Full wwPDB EM Validation Report ⓘ

May 30, 2024 – 11:33 AM JST

PDB ID	:	8XKL
EMDB ID	:	EMD-38419
Title	:	Structure of ACPII-CCPII from cryptophyte algae
Authors	:	Li, X.Y.; Mao, Z.Y.; Shen, J.R.; Han, G.Y.
Deposited on	:	2023-12-23
Resolution	:	2.84 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:

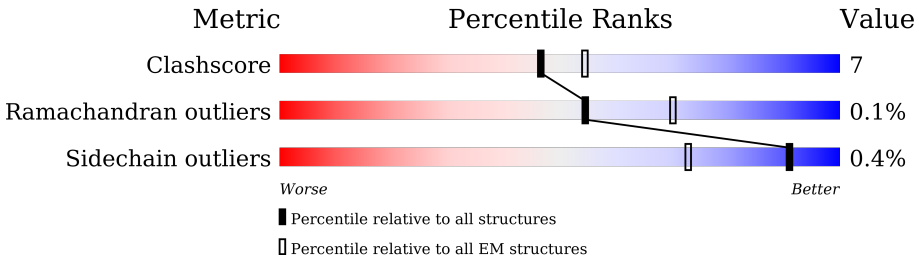
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.84 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	0	226	5% 66% 10% 24%
2	7	235	6% 70% 12% 17%
3	8	217	66% 13% 20%
4	9	222	73% 8% 20%
5	G	64	55% 100%
6	P	220	71% 7% 21%
7	p	218	6% 85% 14%
8	s	285	42% 71% 29%

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
9	CLA	0	601	X	-	-	-
9	CLA	0	602	X	-	-	-
9	CLA	0	603	X	-	-	-
9	CLA	0	604	X	-	-	-
9	CLA	0	605	X	-	-	-
9	CLA	0	606	X	-	-	-
9	CLA	0	607	X	-	-	-
9	CLA	0	608	X	-	-	-
9	CLA	0	609	X	-	-	-
9	CLA	0	611	X	-	-	-
9	CLA	0	612	X	-	-	-
9	CLA	0	613	X	-	-	-
9	CLA	7	601	X	-	-	-
9	CLA	7	602	X	-	-	-
9	CLA	7	603	X	-	-	-
9	CLA	7	604	X	-	-	-
9	CLA	7	605	X	-	-	-
9	CLA	7	606	X	-	-	-
9	CLA	7	607	X	-	-	-
9	CLA	7	608	X	-	-	-
9	CLA	7	609	X	-	-	-
9	CLA	7	611	X	-	-	-
9	CLA	7	612	X	-	-	-
9	CLA	7	613	X	-	-	-
9	CLA	8	601	X	-	-	-
9	CLA	8	602	X	-	-	-
9	CLA	8	603	X	-	-	-
9	CLA	8	604	X	-	-	-
9	CLA	8	605	X	-	-	-
9	CLA	8	606	X	-	-	-
9	CLA	8	607	X	-	-	-
9	CLA	8	608	X	-	-	-
9	CLA	8	609	X	-	-	-
9	CLA	8	611	X	-	-	-
9	CLA	8	612	X	-	-	-
9	CLA	9	601	X	-	-	-
9	CLA	9	602	X	-	-	-
9	CLA	9	603	X	-	-	-
9	CLA	9	604	X	-	-	-
9	CLA	9	605	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
9	CLA	9	606	X	-	-	-
9	CLA	9	607	X	-	-	-
9	CLA	9	608	X	-	-	-
9	CLA	9	609	X	-	-	-
9	CLA	9	610	X	-	-	-
9	CLA	9	611	X	-	-	-
9	CLA	G	101	X	-	-	-
9	CLA	P	601	X	-	-	-
9	CLA	P	602	X	-	-	-
9	CLA	P	603	X	-	-	-
9	CLA	P	604	X	-	-	-
9	CLA	P	606	X	-	-	-
9	CLA	P	607	X	-	-	-
9	CLA	P	608	X	-	-	-
9	CLA	P	610	X	-	-	-
9	CLA	P	611	X	-	-	-
9	CLA	p	303	X	-	-	-
9	CLA	p	304	X	-	-	-
9	CLA	p	305	X	-	-	-
9	CLA	p	306	X	-	-	-
9	CLA	p	307	X	-	-	-
9	CLA	p	308	X	-	-	-
9	CLA	p	309	X	-	-	-
9	CLA	p	310	X	-	-	-
9	CLA	p	311	X	-	-	-
9	CLA	p	313	X	-	-	-
9	CLA	p	314	X	-	-	-
9	CLA	s	303	X	-	-	-

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 15357 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 ACPII-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	172	Total	C	N	O	S	0	0
			1308	845	225	229	9		

- Molecule 2 is a protein called ACPII-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	7	194	Total	C	N	O	S	0	0
			1472	946	256	262	8		

- Molecule 3 is a protein called ACPII-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	8	173	Total	C	N	O	S	0	0
			1362	899	222	238	3		

- Molecule 4 is a protein called ACPII-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	9	178	Total	C	N	O	S	0	0
			1371	885	230	247	9		

- Molecule 5 is a protein called Photosystem II reaction center protein G.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	G	64	Total	C	N	O	0	0
			320	192	64	64		

- Molecule 6 is a protein called ACPII-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	P	173	Total	C	N	O	S	0	0
			1344	878	221	237	8		

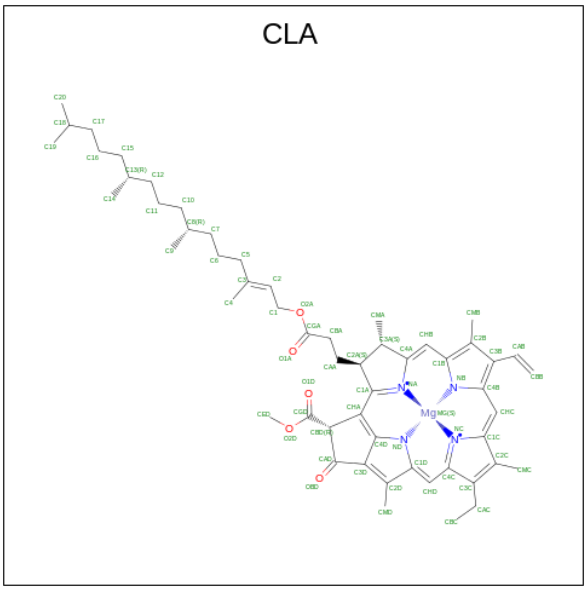
- Molecule 7 is a protein called ACPII-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	p	187	Total	C	N	O	S	0	0
			1471	956	243	267	5		

- Molecule 8 is a protein called CCPII-S.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	s	203	Total	C	N	O	S	0	0
			1563	1005	255	299	4		

- Molecule 9 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
9	0	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
9	0	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
9	0	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
9	0	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
9	0	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
9	0	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
9	0	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	0	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
9	0	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
9	0	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	0	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	0	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	7	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
9	7	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
9	7	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
9	7	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
9	7	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
9	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	7	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
9	7	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
9	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	8	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
9	8	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
9	8	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
9	8	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
9	8	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
9	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	8	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
9	8	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
9	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	9	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
9	9	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
9	9	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
9	9	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
9	9	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
9	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	9	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
9	9	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
9	9	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
9	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	P	1	Total	C	Mg	N	O	0
			42	34	1	4	3	

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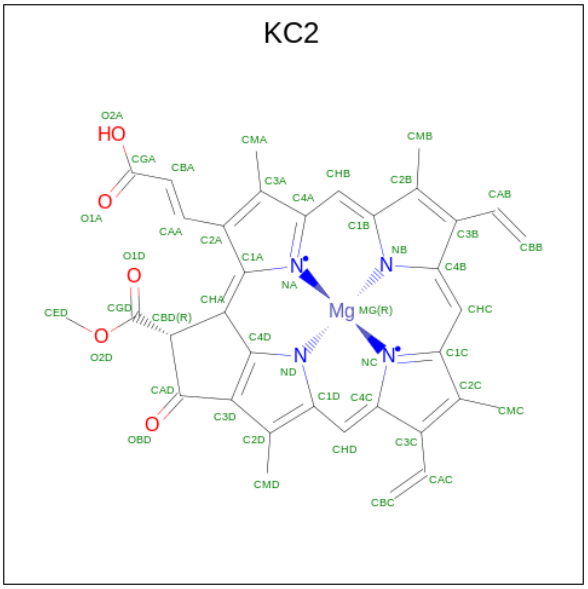
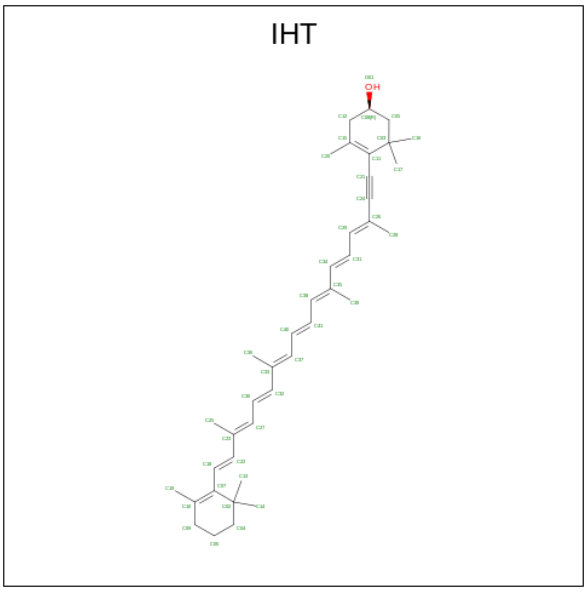
Mol	Chain	Residues	Atoms					AltConf
9	P	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
9	P	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
9	P	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
9	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	P	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
9	P	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
9	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	p	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
9	p	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
9	p	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
9	p	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
9	p	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
9	p	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	p	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	p	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
9	p	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
9	p	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	p	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	s	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	s	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 10 is Chlorophyll c2 (three-letter code: KC2) (formula: $C_{35}H_{28}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



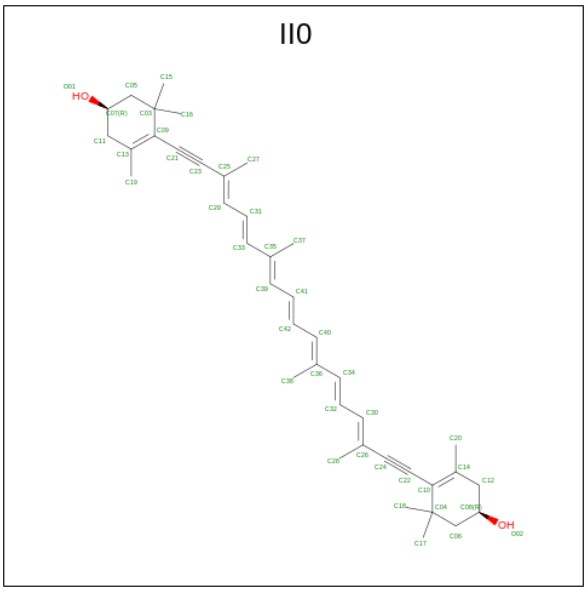
Mol	Chain	Residues	Atoms					AltConf
10	0	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
10	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
10	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
10	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
10	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
10	p	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 11 is (1 {R})-3,5,5-trimethyl-4-[(3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-(2,6,6-trimethylcyclohexen-1-yl)octadeca-3,5,7,9,11,13,15,17-octaen-1-ynyl]cyclohex-3-en-1-ol (three-letter code: IHT) (formula: $C_{40}H_{54}O$).



Mol	Chain	Residues	Atoms			AltConf
11	0	1	Total	C	O	0
			41	40	1	
11	0	1	Total	C	O	0
			41	40	1	
11	7	1	Total	C	O	0
			41	40	1	
11	8	1	Total	C	O	0
			41	40	1	
11	p	1	Total	C	O	0
			41	40	1	

- Molecule 12 is (1 {R})-3,5,5-trimethyl-4-[(3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E})-3,7,12,16-tetramethyl-18-[(4 {R})-2,6,6-trimethyl-4-oxidanyl-cyclohexen-1-yl]octadeca-3,5,7,9,11,13,15-heptaen-1,17-diynyl]cyclohex-3-en-1-ol (three-letter code: II0) (formula: $C_{40}H_{52}O_2$).



Mol	Chain	Residues	Atoms			AltConf
12	0	1	Total	C	O	0
			42	40	2	
12	0	1	Total	C	O	0
			42	40	2	
12	0	1	Total	C	O	0
			42	40	2	
12	7	1	Total	C	O	0
			42	40	2	
12	7	1	Total	C	O	0
			42	40	2	
12	7	1	Total	C	O	0
			42	40	2	
12	7	1	Total	C	O	0
			42	40	2	
12	8	1	Total	C	O	0
			42	40	2	
12	8	1	Total	C	O	0
			42	40	2	
12	8	1	Total	C	O	0
			42	40	2	
12	8	1	Total	C	O	0
			42	40	2	
12	9	1	Total	C	O	0
			42	40	2	
12	9	1	Total	C	O	0
			42	40	2	
12	9	1	Total	C	O	0
			42	40	2	

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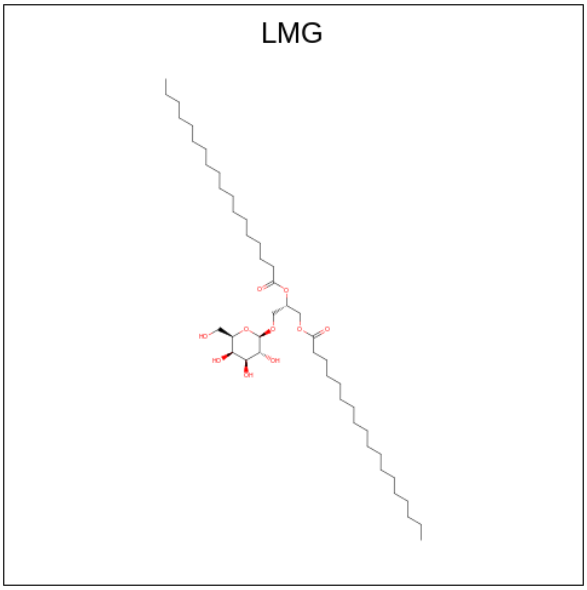
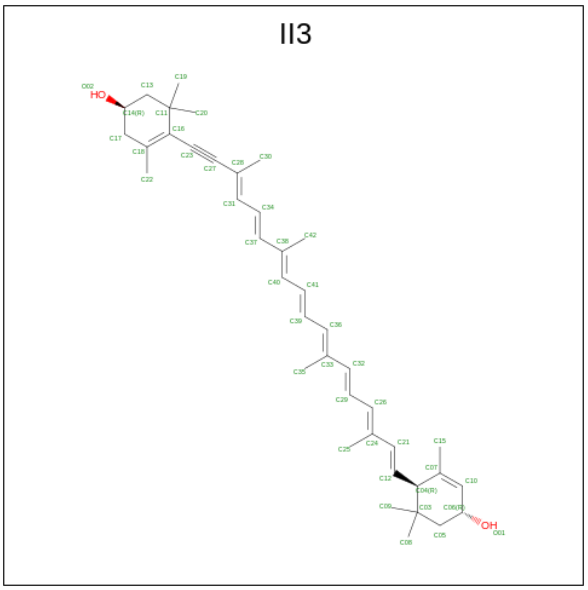
Mol	Chain	Residues	Atoms	AltConf
12	P	1	Total C O 42 40 2	0
12	P	1	Total C O 42 40 2	0
12	p	1	Total C O 42 40 2	0
12	p	1	Total C O 42 40 2	0
12	p	1	Total C O 42 40 2	0
12	p	1	Total C O 42 40 2	0
12	p	1	Total C O 42 40 2	0

- Molecule 13 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



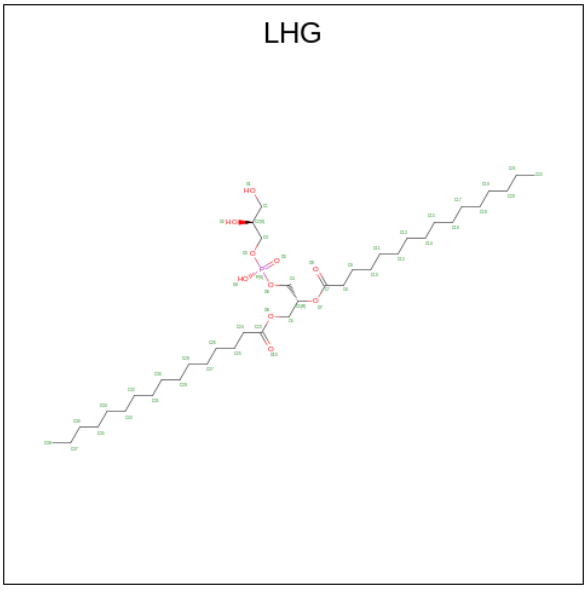
Mol	Chain	Residues	Atoms	AltConf
13	0	1	Total C O 36 26 10	0
13	8	1	Total C O 36 26 10	0
13	G	1	Total C O 28 18 10	0
13	G	1	Total C O 28 18 10	0

- Molecule 14 is (1 {R})-3,5,5-trimethyl-4-[(3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-[(1 {R},4 {R})-2,6,6-trimethyl-4-oxidanyl-cyclohex-2-en-1-yl]octadeca-3,5,7,9,11,13,15,17-octaen-1-ynyl]cyclohex-3-en-1-ol (three-letter code: II3) (formula: $C_{40}H_{54}O_2$).



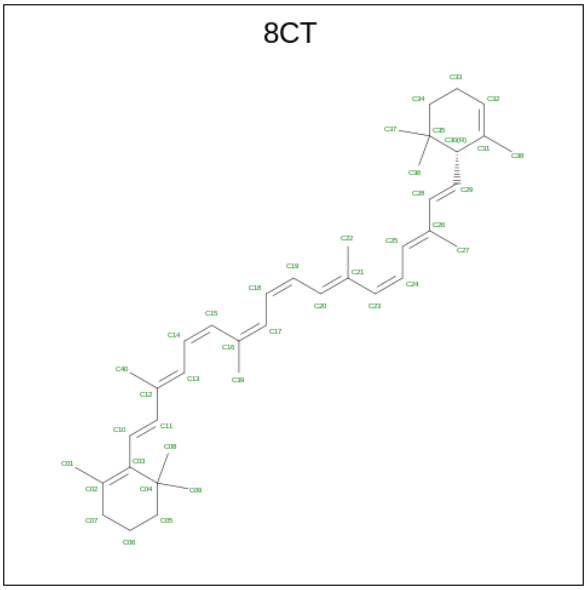
Mol	Chain	Residues	Atoms			AltConf
14	7	1	Total	C	O	0
			42	40	2	
14	P	1	Total	C	O	0
			42	40	2	

- Molecule 15 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).



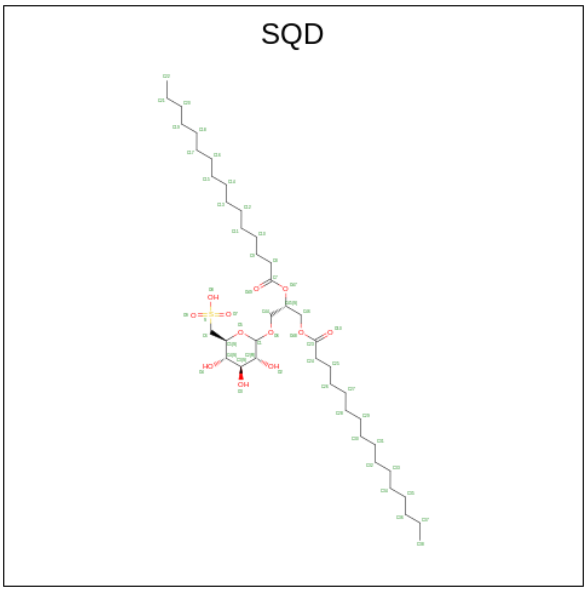
Mol	Chain	Residues	Atoms				AltConf
15	8	1	Total	C	O	P	0
			22	12	9	1	
15	s	1	Total	C	O	P	0
			37	26	10	1	

- Molecule 16 is (6'R,11cis,11'cis,13cis,15cis)-4',5'-didehydro-5',6'-dihydro-beta,beta-carotene (three-letter code: 8CT) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		AltConf
16	9	1	Total	C	0
			40	40	
16	P	1	Total	C	0
			40	40	

- Molecule 17 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$) (labeled as "Ligand of Interest" by depositor).



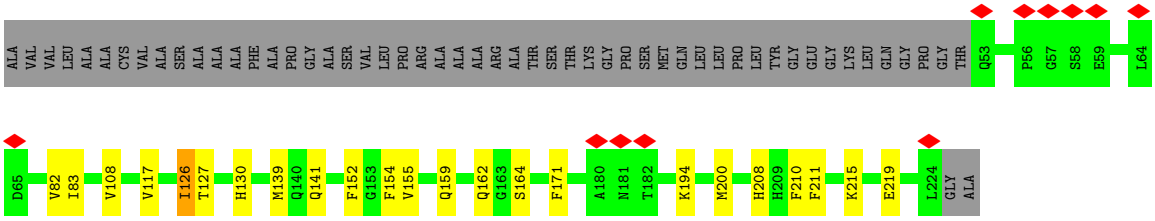
Mol	Chain	Residues	Atoms				AltConf
17	p	1	Total	C	O	S	0
			35	22	12	1	

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.

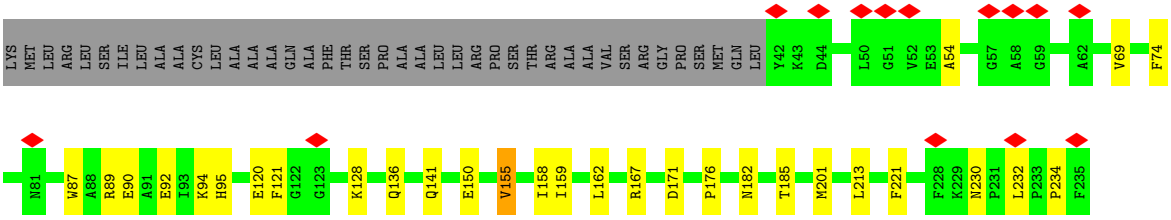
• Molecule 1: ACPII-4

Chain 0:



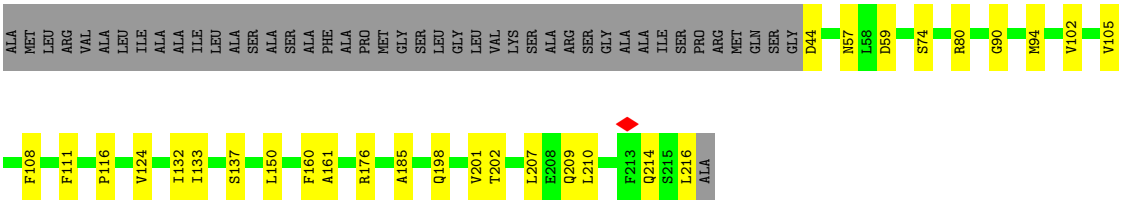
• Molecule 2: ACPII-1

Chain 7:



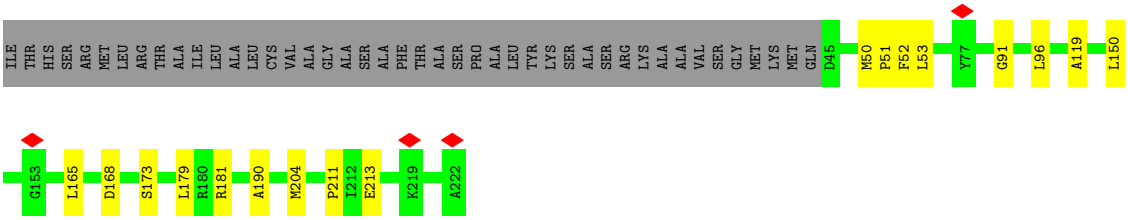
• Molecule 3: ACPII-2

Chain 8:

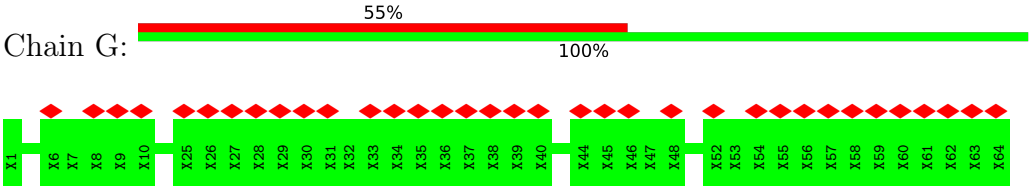


• Molecule 4: ACPII-3

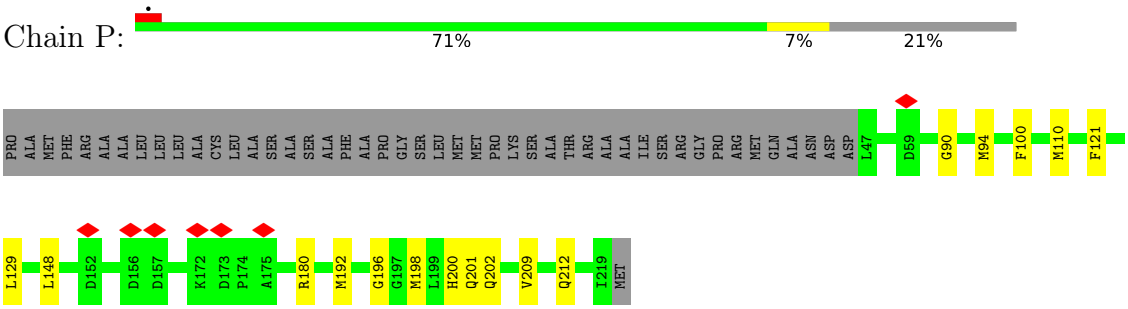
Chain 9:



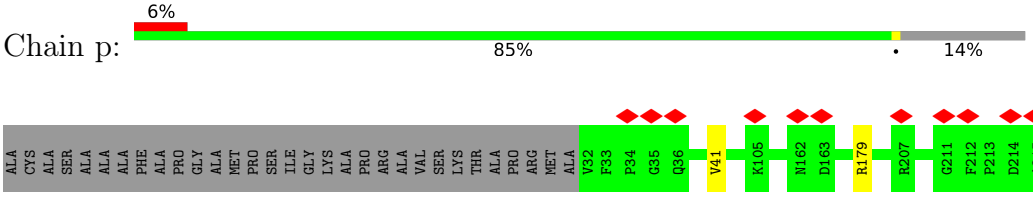
• Molecule 5: Photosystem II reaction center protein G



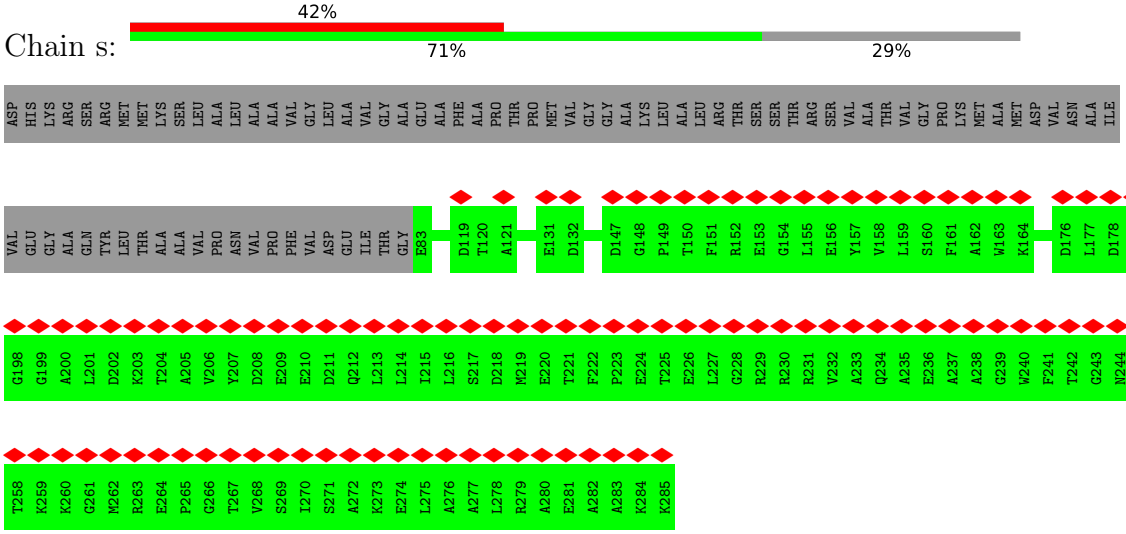
• Molecule 6: ACPII-6



• Molecule 7: ACPII-5



• Molecule 8: CCPII-S



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	610800	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.131	Depositor
Minimum map value	-0.417	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.266	Depositor
Map size (Å)	532.48, 532.48, 532.48	wwPDB
Map dimensions	512, 512, 512	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: II3, II0, LHG, SQD, 8CT, KC2, CLA, LMG, IHT

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	0	0.29	0/1339	0.46	0/1814
2	7	0.30	0/1507	0.47	0/2043
3	8	0.33	0/1399	0.44	0/1893
4	9	0.29	0/1404	0.44	0/1895
6	P	0.31	0/1380	0.46	0/1870
7	p	0.32	0/1510	0.46	0/2046
8	s	0.28	0/1603	0.48	0/2180
All	All	0.30	0/10142	0.46	0/13741

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	0	1308	0	1323	16	0
2	7	1472	0	1473	22	0
3	8	1362	0	1348	22	0
4	9	1371	0	1370	12	0
5	G	320	0	70	0	0
6	P	1344	0	1329	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	p	1471	0	1445	0	0
8	s	1563	0	1540	0	0
9	0	582	0	469	16	0
9	7	582	0	469	22	0
9	8	547	0	456	17	0
9	9	548	0	456	11	0
9	G	45	0	33	2	0
9	P	442	0	364	9	0
9	p	547	0	456	0	0
9	s	110	0	105	0	0
10	0	45	0	0	0	0
10	7	45	0	0	0	0
10	8	45	0	0	0	0
10	P	90	0	0	0	0
10	p	45	0	0	0	0
11	0	82	0	0	0	0
11	7	41	0	0	0	0
11	8	41	0	0	0	0
11	p	41	0	0	0	0
12	0	126	0	0	1	0
12	7	168	0	0	1	0
12	8	168	0	0	3	0
12	9	126	0	0	0	0
12	P	84	0	0	0	0
12	p	210	0	0	0	0
13	0	36	0	42	0	0
13	8	36	0	42	2	0
13	G	56	0	52	0	0
14	7	42	0	0	0	0
14	P	42	0	0	0	0
15	8	22	0	20	0	0
15	s	37	0	44	0	0
16	9	40	0	0	0	0
16	P	40	0	0	0	0
17	p	35	0	34	0	0
All	All	15357	0	12940	127	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 7.

All (127) 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)
6:P:192:MET:HE1	9:P:602:CLA:HAB	1.69	0.75
3:8:90:GLY:HA3	3:8:185:ALA:HB1	1.69	0.74
4:9:91:GLY:HA3	4:9:190:ALA:HB1	1.70	0.72
2:7:155:VAL:HG22	9:7:607:CLA:HMA1	1.72	0.72
2:7:90:GLU:HG2	2:7:158:ILE:HD11	1.75	0.69
9:0:608:CLA:HBB1	9:0:608:CLA:H51	1.78	0.66
2:7:232:LEU:O	2:7:234:PRO:HD3	1.95	0.65
9:7:602:CLA:H2A	9:7:602:CLA:HED3	1.78	0.65
2:7:94:LYS:NZ	2:7:150:GLU:OE2	2.24	0.65
9:9:606:CLA:HHC	9:9:606:CLA:HBB1	1.81	0.62
9:7:603:CLA:HMA2	9:7:603:CLA:H11	1.80	0.62
2:7:150:GLU:HG2	9:7:607:CLA:NB	2.15	0.62
3:8:160:PHE:HA	4:9:52:PHE:HB3	1.81	0.61
4:9:211:PRO:O	4:9:213:GLU:N	2.32	0.61
1:0:130:HIS:ND1	1:0:139:MET:SD	2.73	0.60
6:P:201:GLN:HB3	6:P:212:GLN:HE22	1.66	0.60
2:7:89:ARG:NH1	2:7:92:GLU:OE1	2.35	0.60
9:0:603:CLA:HBC1	9:0:607:CLA:HBC2	1.82	0.60
2:7:69:VAL:O	2:7:89:ARG:NH2	2.35	0.60
9:7:603:CLA:HMB1	9:7:603:CLA:HBB1	1.85	0.59
1:0:154:PHE:HB2	9:0:607:CLA:HMA1	1.85	0.59
2:7:182:ASN:HD22	2:7:185:THR:H	1.51	0.59
3:8:201:VAL:HG23	3:8:202:THR:HG23	1.85	0.58
9:7:606:CLA:HMB1	9:7:606:CLA:HBB1	1.86	0.57
2:7:141:GLN:HG2	9:7:605:CLA:ND	2.20	0.56
3:8:80:ARG:HB3	3:8:150:LEU:HD11	1.88	0.56
6:P:196:GLY:O	6:P:200:HIS:ND1	2.30	0.56
6:P:180:ARG:HE	9:P:607:CLA:H43	1.68	0.56
9:7:612:CLA:HED2	9:7:612:CLA:H2A	1.87	0.56
1:0:117:VAL:HG23	9:0:613:CLA:HBC3	1.88	0.55
3:8:108:PHE:HB2	3:8:111:PHE:HD2	1.74	0.53
2:7:167:ARG:NH1	2:7:171:ASP:O	2.39	0.53
6:P:90:GLY:O	6:P:94:MET:HB2	2.08	0.53
9:7:605:CLA:HBA1	9:8:611:CLA:HBD	1.91	0.53
9:7:603:CLA:HMC1	9:7:606:CLA:HBB2	1.92	0.52
9:P:610:CLA:HBC1	9:P:611:CLA:HMB3	1.92	0.52
6:P:148:LEU:HD13	9:P:606:CLA:HMB3	1.92	0.52
4:9:173:SER:HB2	4:9:179:LEU:HD13	1.92	0.52
4:9:150:LEU:HD22	9:9:606:CLA:HMA1	1.92	0.51
3:8:132:ILE:HD12	9:8:606:CLA:HBC1	1.93	0.50
4:9:165:LEU:HB2	9:9:607:CLA:HMD1	1.93	0.50
2:7:221:PHE:HE2	9:7:611:CLA:HMA3	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:7:608:CLA:H2A	9:7:608:CLA:HED3	1.94	0.49
9:G:101:CLA:HHD	9:P:606:CLA:O1A	2.13	0.49
9:P:611:CLA:HED2	9:P:611:CLA:H2A	1.94	0.49
9:8:603:CLA:HAC1	9:8:606:CLA:HAB	1.94	0.49
3:8:102:VAL:HA	3:8:105:VAL:HG12	1.96	0.48
3:8:116:PRO:O	12:8:614:II0:O01	2.30	0.48
9:0:608:CLA:H2A	9:0:608:CLA:HED3	1.96	0.48
3:8:133:ILE:HD11	13:8:617:LMG:HC8	1.96	0.48
1:0:159:GLN:HB3	1:0:164:SER:HB3	1.95	0.48
9:8:605:CLA:HBA2	9:9:610:CLA:HBD	1.96	0.48
1:0:152:PHE:HA	1:0:155:VAL:HG22	1.96	0.47
1:0:171:PHE:HB2	9:0:608:CLA:HMD1	1.96	0.47
9:9:605:CLA:H3A	9:9:605:CLA:HBA2	1.43	0.47
9:0:603:CLA:HMD1	9:0:607:CLA:HBA2	1.96	0.47
3:8:44:ASP:N	3:8:44:ASP:OD1	2.48	0.47
9:0:612:CLA:H2A	9:0:612:CLA:O2D	2.15	0.46
1:0:126:ILE:HD13	1:0:210:PHE:CD1	2.50	0.46
6:P:100:PHE:HD2	6:P:198:MET:HG3	1.80	0.46
9:9:607:CLA:H142	9:9:607:CLA:H111	1.70	0.46
3:8:102:VAL:HG12	9:8:604:CLA:HMD3	1.97	0.46
2:7:128:LYS:HD3	2:7:234:PRO:HG2	1.98	0.46
1:0:82:VAL:HG23	1:0:83:ILE:HG12	1.98	0.46
2:7:120:GLU:HG2	2:7:136:GLN:HG3	1.98	0.46
9:0:601:CLA:H2A	9:0:601:CLA:HED3	1.98	0.46
9:8:605:CLA:HAB	12:8:619:II0:C42	2.46	0.46
2:7:155:VAL:O	2:7:159:ILE:HG13	2.16	0.46
9:8:602:CLA:HBA2	9:8:602:CLA:H3A	1.28	0.46
9:7:602:CLA:H93	9:7:602:CLA:H61	1.76	0.45
4:9:168:ASP:N	4:9:168:ASP:OD1	2.48	0.45
9:9:602:CLA:H3A	9:9:602:CLA:HBA2	1.30	0.45
2:7:121:PHE:HD2	9:7:604:CLA:HED1	1.81	0.45
9:7:602:CLA:H62	9:7:602:CLA:H41	1.71	0.45
3:8:176:ARG:HG2	9:8:609:CLA:HED1	1.98	0.45
9:8:606:CLA:HBB1	9:8:606:CLA:HHC	1.99	0.45
3:8:137:SER:CB	9:8:607:CLA:HAB	2.47	0.44
3:8:137:SER:HB3	9:8:607:CLA:HAB	1.99	0.44
3:8:161:ALA:HB3	4:9:51:PRO:HB2	1.99	0.44
3:8:198:GLN:HB3	3:8:209:GLN:HE22	1.83	0.44
9:7:606:CLA:H3A	9:7:606:CLA:HBA2	1.40	0.44
9:8:602:CLA:H72	9:8:603:CLA:HMA1	1.99	0.44
4:9:96:LEU:O	9:9:604:CLA:HMC3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:7:95:HIS:HB3	2:7:201:MET:SD	2.57	0.44
4:9:119:ALA:H	4:9:204:MET:HE3	1.82	0.44
6:P:148:LEU:HD22	9:P:606:CLA:HMA1	1.99	0.44
1:0:159:GLN:HA	1:0:162:GLN:HG2	1.99	0.44
6:P:121:PHE:CZ	6:P:129:LEU:HD11	2.53	0.44
9:7:611:CLA:HAA1	9:7:613:CLA:C1C	2.48	0.44
9:P:602:CLA:H3A	9:P:602:CLA:HBA2	1.32	0.43
2:7:54:ALA:HB3	2:7:74:PHE:HB2	2.00	0.43
1:0:108:VAL:HG12	9:0:604:CLA:HMD3	2.00	0.43
2:7:176:PRO:O	12:7:614:II0:O01	2.37	0.43
9:9:607:CLA:CGA	9:9:607:CLA:H3A	2.49	0.43
1:0:215:LYS:HB3	1:0:219:GLU:HG3	2.01	0.43
9:7:605:CLA:HBA1	9:7:605:CLA:H3A	1.88	0.42
9:0:608:CLA:H91	9:0:608:CLA:H112	1.90	0.42
1:0:127:THR:HG21	1:0:211:PHE:HE1	1.84	0.42
6:P:110:MET:SD	6:P:110:MET:N	2.93	0.42
3:8:207:LEU:HD23	3:8:210:LEU:HD12	2.00	0.42
6:P:202:GLN:HE21	6:P:209:VAL:HG13	1.83	0.42
1:0:194:LYS:NZ	12:0:616:II0:O02	2.52	0.42
3:8:57:ASN:ND2	3:8:74:SER:O	2.47	0.42
9:P:604:CLA:H3A	9:P:604:CLA:HBA2	1.81	0.42
2:7:213:LEU:HG	9:7:612:CLA:HED3	2.02	0.42
9:7:602:CLA:HBA2	9:7:602:CLA:H3A	1.35	0.42
9:G:101:CLA:HBA2	9:G:101:CLA:H3A	1.72	0.41
3:8:59:ASP:N	3:8:59:ASP:OD1	2.53	0.41
3:8:94:MET:CE	9:8:608:CLA:HAB	2.50	0.41
1:0:200:MET:SD	9:0:602:CLA:HAB	2.61	0.41
9:8:608:CLA:H2A	9:8:608:CLA:HED3	2.02	0.41
4:9:50:MET:HB2	4:9:53:LEU:HB2	2.01	0.41
2:7:87:TRP:HE3	2:7:162:LEU:HD11	1.85	0.41
9:7:611:CLA:HBD	9:7:611:CLA:HAA2	2.02	0.41
9:0:602:CLA:HBA2	9:0:602:CLA:H3A	1.43	0.41
2:7:230:ASN:OD1	2:7:230:ASN:N	2.53	0.41
4:9:204:MET:HB3	4:9:204:MET:HE2	1.84	0.41
1:0:141:GLN:HE21	9:0:605:CLA:HMA3	1.86	0.41
3:8:214:GLN:HE22	3:8:216:LEU:HB2	1.85	0.41
9:8:603:CLA:HMD2	9:8:607:CLA:C1D	2.50	0.41
2:7:221:PHE:CE2	9:7:611:CLA:HMA3	2.56	0.41
3:8:124:VAL:O	13:8:617:LMG:O3	2.34	0.41
1:0:208:HIS:HE1	9:0:612:CLA:NA	2.19	0.40
9:0:607:CLA:HMB2	9:9:609:CLA:H122	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:9:607:CLA:HED3	9:9:607:CLA:HBD	1.86	0.40
9:8:608:CLA:HMC2	12:8:613:II0:C31	2.51	0.40
9:8:606:CLA:HHC	9:8:606:CLA:CBB	2.52	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	0	170/226 (75%)	167 (98%)	2 (1%)	1 (1%)	25 46
2	7	192/235 (82%)	183 (95%)	9 (5%)	0	100 100
3	8	171/217 (79%)	170 (99%)	1 (1%)	0	100 100
4	9	176/222 (79%)	172 (98%)	4 (2%)	0	100 100
6	P	171/220 (78%)	171 (100%)	0	0	100 100
7	p	185/218 (85%)	183 (99%)	2 (1%)	0	100 100
8	s	201/285 (70%)	180 (90%)	21 (10%)	0	100 100
All	All	1266/1623 (78%)	1226 (97%)	39 (3%)	1 (0%)	54 75

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	0	126	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	0	136/169 (80%)	136 (100%)	0	100 100
2	7	149/179 (83%)	148 (99%)	1 (1%)	84 91
3	8	139/167 (83%)	139 (100%)	0	100 100
4	9	143/175 (82%)	142 (99%)	1 (1%)	84 91
6	P	141/174 (81%)	141 (100%)	0	100 100
7	p	157/175 (90%)	155 (99%)	2 (1%)	69 84
8	s	159/219 (73%)	159 (100%)	0	100 100
All	All	1024/1258 (81%)	1020 (100%)	4 (0%)	91 95

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	7	155	VAL
4	9	181	ARG
7	p	41	VAL
7	p	179	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	208	HIS
2	7	182	ASN
3	8	209	GLN
4	9	104	GLN
6	P	144	ASN
6	P	201	GLN
6	P	212	GLN
7	p	202	GLN

5.3.3 RNA

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)

112 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	$\#\|Z\| > 2$
12	II0	p	317	-	39,43,43	2.74	4 (10%)	50,60,60	1.70	9 (18%)
12	II0	p	301	-	39,43,43	2.71	4 (10%)	50,60,60	1.79	11 (22%)
9	CLA	P	610	-	45,53,73	1.72	8 (17%)	52,89,113	1.64	8 (15%)
9	CLA	P	607	6	60,68,73	1.52	8 (13%)	70,107,113	1.42	6 (8%)
9	CLA	9	601	4	42,50,73	1.78	7 (16%)	48,85,113	1.63	6 (12%)
9	CLA	9	604	4	55,63,73	1.61	8 (14%)	64,101,113	1.46	9 (14%)
12	II0	7	616	-	39,43,43	2.76	4 (10%)	50,60,60	1.76	11 (22%)
9	CLA	P	611	-	45,53,73	1.77	8 (17%)	52,89,113	1.59	7 (13%)
9	CLA	7	612	-	45,53,73	1.78	7 (15%)	52,89,113	1.55	6 (11%)
9	CLA	0	606	-	45,53,73	1.76	6 (13%)	52,89,113	1.54	7 (13%)
11	IHT	p	318	-	40,42,42	1.99	2 (5%)	53,58,58	1.81	11 (20%)
9	CLA	0	609	-	41,49,73	1.81	6 (14%)	47,84,113	1.61	8 (17%)
17	SQD	p	319	-	34,35,54	1.73	7 (20%)	43,46,65	1.60	7 (16%)
15	LHG	8	618	9	21,21,48	0.78	0	23,26,54	1.26	2 (8%)
9	CLA	9	603	-	50,58,73	1.63	7 (14%)	58,95,113	1.59	8 (13%)
10	KC2	7	610	-	48,53,53	1.89	10 (20%)	54,89,89	2.13	13 (24%)
9	CLA	0	608	-	60,68,73	1.52	7 (11%)	70,107,113	1.44	8 (11%)
13	LMG	8	617	-	36,36,55	0.89	1 (2%)	44,44,63	1.30	6 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	CLA	p	308	-	45,53,73	1.76	8 (17%)	52,89,113	1.57	7 (13%)
9	CLA	7	603	-	50,58,73	1.61	7 (14%)	58,95,113	1.59	7 (12%)
9	CLA	9	607	4	60,68,73	1.52	8 (13%)	70,107,113	1.43	6 (8%)
9	CLA	7	602	2	59,67,73	1.51	8 (13%)	68,105,113	1.42	8 (11%)
9	CLA	0	612	-	45,53,73	1.78	5 (11%)	52,89,113	1.58	8 (15%)
12	II0	8	614	-	39,43,43	2.72	4 (10%)	50,60,60	1.69	8 (16%)
9	CLA	P	601	6	42,50,73	1.76	7 (16%)	48,85,113	1.56	6 (12%)
10	KC2	0	610	1	48,53,53	1.89	10 (20%)	54,89,89	2.17	15 (27%)
12	II0	8	615	-	39,43,43	2.72	5 (12%)	50,60,60	1.84	10 (20%)
16	8CT	9	615	-	40,41,41	4.64	23 (57%)	50,56,56	2.87	20 (40%)
10	KC2	8	610	-	48,53,53	1.91	11 (22%)	54,89,89	2.19	14 (25%)
9	CLA	9	608	-	41,49,73	1.78	6 (14%)	47,84,113	1.66	8 (17%)
9	CLA	9	602	4	59,67,73	1.51	7 (11%)	68,105,113	1.48	8 (11%)
9	CLA	8	606	-	45,53,73	1.76	8 (17%)	52,89,113	1.59	7 (13%)
9	CLA	0	611	-	45,53,73	1.77	6 (13%)	52,89,113	1.55	6 (11%)
9	CLA	8	611	3	45,53,73	1.70	8 (17%)	52,89,113	1.63	7 (13%)
11	IHT	0	617	-	40,42,42	1.99	3 (7%)	53,58,58	2.04	15 (28%)
14	II3	P	613	-	40,43,43	2.00	2 (5%)	47,60,60	1.59	10 (21%)
9	CLA	7	601	-	42,50,73	1.81	6 (14%)	48,85,113	1.56	6 (12%)
9	CLA	p	304	7	59,67,73	1.55	9 (15%)	68,105,113	1.39	10 (14%)
9	CLA	7	608	2	60,68,73	1.51	9 (15%)	70,107,113	1.43	8 (11%)
12	II0	P	614	-	39,43,43	2.74	4 (10%)	50,60,60	1.71	11 (22%)
16	8CT	P	615	-	40,41,41	4.66	23 (57%)	50,56,56	2.68	19 (38%)
11	IHT	7	618	-	40,42,42	2.01	2 (5%)	53,58,58	1.95	13 (24%)
9	CLA	p	313	-	45,53,73	1.72	7 (15%)	52,89,113	1.62	7 (13%)
12	II0	7	619	-	39,43,43	2.69	4 (10%)	50,60,60	1.67	11 (22%)
9	CLA	9	611	-	45,53,73	1.74	7 (15%)	52,89,113	1.57	7 (13%)
9	CLA	0	613	1	45,53,73	1.79	7 (15%)	52,89,113	1.54	7 (13%)
9	CLA	p	310	7	60,68,73	1.52	8 (13%)	70,107,113	1.44	7 (10%)
9	CLA	G	101	-	45,53,73	1.78	7 (15%)	52,89,113	1.57	7 (13%)
9	CLA	7	605	-	50,58,73	1.68	9 (18%)	58,95,113	1.51	8 (13%)
12	II0	7	614	-	39,43,43	2.73	4 (10%)	50,60,60	1.75	10 (20%)
12	II0	0	619	-	39,43,43	2.68	4 (10%)	50,60,60	1.69	13 (26%)
12	II0	8	619	-	39,43,43	2.74	4 (10%)	50,60,60	1.73	8 (16%)
9	CLA	0	601	1	42,50,73	1.81	6 (14%)	48,85,113	1.58	6 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	CLA	7	607	-	45,53,73	1.74	9 (20%)	52,89,113	1.53	7 (13%)
9	CLA	8	601	3	42,50,73	1.76	8 (19%)	48,85,113	1.62	6 (12%)
9	CLA	p	306	-	55,63,73	1.56	7 (12%)	64,101,113	1.49	7 (10%)
13	LMG	0	618	-	36,36,55	0.89	1 (2%)	44,44,63	1.29	6 (13%)
9	CLA	s	303	8	65,73,73	1.51	6 (9%)	76,113,113	1.37	7 (9%)
12	II0	9	614	-	39,43,43	2.71	4 (10%)	50,60,60	1.69	11 (22%)
12	II0	9	612	-	39,43,43	2.73	4 (10%)	50,60,60	1.70	10 (20%)
9	CLA	9	609	-	60,68,73	1.51	7 (11%)	70,107,113	1.43	7 (10%)
9	CLA	P	603	-	50,58,73	1.66	7 (14%)	58,95,113	1.60	8 (13%)
10	KC2	p	312	-	48,53,53	1.90	10 (20%)	54,89,89	2.14	15 (27%)
12	II0	9	613	-	39,43,43	2.73	4 (10%)	50,60,60	1.74	9 (18%)
9	CLA	p	314	-	45,53,73	1.76	7 (15%)	52,89,113	1.56	6 (11%)
13	LMG	G	103	-	28,28,55	1.00	0	36,36,63	1.33	5 (13%)
9	CLA	8	612	-	45,53,73	1.75	8 (17%)	52,89,113	1.55	7 (13%)
9	CLA	9	610	4	45,53,73	1.72	7 (15%)	52,89,113	1.62	7 (13%)
9	CLA	0	605	1	50,58,73	1.68	7 (14%)	58,95,113	1.50	7 (12%)
9	CLA	p	309	7	45,53,73	1.74	7 (15%)	52,89,113	1.63	7 (13%)
11	IHT	8	616	-	40,42,42	2.04	3 (7%)	53,58,58	2.03	15 (28%)
12	II0	0	615	-	39,43,43	2.70	4 (10%)	50,60,60	1.75	12 (24%)
9	CLA	7	613	-	45,53,73	1.78	6 (13%)	52,89,113	1.56	7 (13%)
9	CLA	9	606	-	45,53,73	1.79	8 (17%)	52,89,113	1.49	6 (11%)
9	CLA	0	604	-	55,63,73	1.62	9 (16%)	64,101,113	1.45	9 (14%)
11	IHT	0	614	-	40,42,42	1.98	2 (5%)	53,58,58	1.79	13 (24%)
9	CLA	0	607	1	45,53,73	1.77	6 (13%)	52,89,113	1.52	8 (15%)
9	CLA	8	604	-	55,63,73	1.56	7 (12%)	64,101,113	1.50	7 (10%)
12	II0	8	613	-	39,43,43	2.75	4 (10%)	50,60,60	1.77	10 (20%)
12	II0	p	315	-	39,43,43	2.69	4 (10%)	50,60,60	1.75	12 (24%)
9	CLA	P	604	-	55,63,73	1.60	9 (16%)	64,101,113	1.51	7 (10%)
9	CLA	8	609	15	41,49,73	1.81	7 (17%)	47,84,113	1.65	7 (14%)
10	KC2	P	609	6	48,53,53	1.89	10 (20%)	54,89,89	2.16	14 (25%)
15	LHG	s	301	-	36,36,48	0.72	1 (2%)	39,42,54	1.24	4 (10%)
12	II0	p	316	-	39,43,43	2.71	4 (10%)	50,60,60	1.60	10 (20%)
10	KC2	P	605	-	48,53,53	1.91	10 (20%)	54,89,89	2.05	12 (22%)
9	CLA	p	307	-	60,68,73	1.52	7 (11%)	70,107,113	1.40	8 (11%)
9	CLA	7	604	2	55,63,73	1.57	7 (12%)	64,101,113	1.53	8 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	II3	7	615	-	40,43,43	1.99	2 (5%)	47,60,60	1.63	9 (19%)
9	CLA	8	603	-	50,58,73	1.64	8 (16%)	58,95,113	1.53	8 (13%)
9	CLA	p	303	7	42,50,73	1.77	7 (16%)	48,85,113	1.59	6 (12%)
9	CLA	p	311	-	41,49,73	1.81	6 (14%)	47,84,113	1.61	8 (17%)
12	II0	0	616	-	39,43,43	2.77	4 (10%)	50,60,60	1.75	12 (24%)
9	CLA	0	602	1	59,67,73	1.54	8 (13%)	68,105,113	1.41	9 (13%)
9	CLA	8	602	3	59,67,73	1.51	8 (13%)	68,105,113	1.47	9 (13%)
12	II0	p	302	-	39,43,43	2.72	4 (10%)	50,60,60	1.76	11 (22%)
9	CLA	0	603	-	50,58,73	1.65	7 (14%)	58,95,113	1.55	8 (13%)
13	LMG	G	102	-	28,28,55	0.94	0	36,36,63	1.30	5 (13%)
9	CLA	8	605	3	60,68,73	1.53	8 (13%)	70,107,113	1.41	8 (11%)
9	CLA	8	607	3	45,53,73	1.72	8 (17%)	52,89,113	1.57	7 (13%)
9	CLA	p	305	-	50,58,73	1.67	7 (14%)	58,95,113	1.56	8 (13%)
9	CLA	s	302	-	45,53,73	1.77	6 (13%)	52,89,113	1.62	6 (11%)
12	II0	P	612	-	39,43,43	2.70	4 (10%)	50,60,60	1.77	10 (20%)
9	CLA	9	605	-	46,54,73	1.74	7 (15%)	53,90,113	1.52	6 (11%)
12	II0	7	617	-	39,43,43	2.75	4 (10%)	50,60,60	1.72	10 (20%)
9	CLA	7	606	-	45,53,73	1.71	6 (13%)	52,89,113	1.65	6 (11%)
9	CLA	P	608	-	41,49,73	1.80	7 (17%)	47,84,113	1.61	7 (14%)
9	CLA	P	602	6	59,67,73	1.54	9 (15%)	68,105,113	1.42	9 (13%)
9	CLA	8	608	3	60,68,73	1.51	8 (13%)	70,107,113	1.43	8 (11%)
9	CLA	7	611	-	45,53,73	1.73	6 (13%)	52,89,113	1.59	6 (11%)
9	CLA	P	606	6	45,53,73	1.77	6 (13%)	52,89,113	1.53	9 (17%)
9	CLA	7	609	-	41,49,73	1.82	6 (14%)	47,84,113	1.63	7 (14%)

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
12	II0	p	317	-	-	5/21/67/67	0/2/2/2
12	II0	p	301	-	-	2/21/67/67	0/2/2/2
9	CLA	P	610	-	1/1/11/20	6/13/91/115	-
9	CLA	P	607	6	1/1/14/20	5/31/109/115	-
9	CLA	9	601	4	1/1/10/20	3/10/88/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	CLA	9	604	4	1/1/13/20	6/25/103/115	-
12	II0	7	616	-	-	5/21/67/67	0/2/2/2
9	CLA	P	611	-	1/1/11/20	5/13/91/115	-
9	CLA	7	612	-	1/1/11/20	5/13/91/115	-
9	CLA	0	606	-	1/1/11/20	5/13/91/115	-
11	IHT	p	318	-	-	0/25/65/65	0/2/2/2
9	CLA	0	609	-	1/1/10/20	2/8/86/115	-
17	SQD	p	319	-	-	19/30/50/69	0/1/1/1
15	LHG	8	618	9	-	11/24/24/53	-
9	CLA	9	603	-	1/1/12/20	6/19/97/115	-
10	KC2	7	610	-	-	11/15/71/71	-
9	CLA	0	608	-	1/1/14/20	9/31/109/115	-
13	LMG	8	617	-	-	10/31/51/70	0/1/1/1
9	CLA	p	308	-	1/1/11/20	4/13/91/115	-
9	CLA	7	603	-	1/1/12/20	8/19/97/115	-
9	CLA	9	607	4	1/1/14/20	6/31/109/115	-
9	CLA	7	602	2	1/1/13/20	12/30/108/115	-
9	CLA	0	612	-	1/1/11/20	5/13/91/115	-
12	II0	8	614	-	-	0/21/67/67	0/2/2/2
9	CLA	P	601	6	1/1/10/20	0/10/88/115	-
10	KC2	0	610	1	-	11/15/71/71	-
12	II0	8	615	-	-	3/21/67/67	0/2/2/2
16	8CT	9	615	-	-	9/29/63/63	0/2/2/2
10	KC2	8	610	-	-	9/15/71/71	-
9	CLA	9	608	-	1/1/10/20	1/8/86/115	-
9	CLA	9	602	4	1/1/13/20	11/30/108/115	-
9	CLA	8	606	-	1/1/11/20	2/13/91/115	-
9	CLA	0	611	-	1/1/11/20	7/13/91/115	-
9	CLA	8	611	3	1/1/11/20	6/13/91/115	-
11	IHT	0	617	-	-	5/25/65/65	0/2/2/2
14	II3	P	613	-	-	1/25/67/67	0/2/2/2
9	CLA	7	601	-	1/1/10/20	3/10/88/115	-
9	CLA	p	304	7	1/1/13/20	12/30/108/115	-
9	CLA	7	608	2	1/1/14/20	8/31/109/115	-
12	II0	P	614	-	-	3/21/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	8CT	P	615	-	-	4/29/63/63	0/2/2/2
11	IHT	7	618	-	-	2/25/65/65	0/2/2/2
9	CLA	p	313	-	1/1/11/20	8/13/91/115	-
12	II0	7	619	-	-	2/21/67/67	0/2/2/2
9	CLA	9	611	-	1/1/11/20	4/13/91/115	-
9	CLA	0	613	1	1/1/11/20	6/13/91/115	-
9	CLA	p	310	7	1/1/14/20	9/31/109/115	-
9	CLA	G	101	-	1/1/11/20	7/13/91/115	-
9	CLA	7	605	-	1/1/12/20	6/19/97/115	-
12	II0	7	614	-	-	0/21/67/67	0/2/2/2
12	II0	0	619	-	-	2/21/67/67	0/2/2/2
12	II0	8	619	-	-	1/21/67/67	0/2/2/2
9	CLA	0	601	1	1/1/10/20	5/10/88/115	-
9	CLA	7	607	-	1/1/11/20	7/13/91/115	-
9	CLA	8	601	3	1/1/10/20	4/10/88/115	-
9	CLA	p	306	-	1/1/13/20	9/25/103/115	-
13	LMG	0	618	-	-	10/31/51/70	0/1/1/1
9	CLA	s	303	8	1/1/15/20	15/37/115/115	-
12	II0	9	614	-	-	4/21/67/67	0/2/2/2
12	II0	9	612	-	-	2/21/67/67	0/2/2/2
9	CLA	9	609	-	1/1/14/20	7/31/109/115	-
9	CLA	P	603	-	1/1/12/20	3/19/97/115	-
10	KC2	p	312	-	-	10/15/71/71	-
12	II0	9	613	-	-	1/21/67/67	0/2/2/2
9	CLA	p	314	-	1/1/11/20	5/13/91/115	-
13	LMG	G	103	-	-	7/23/43/70	0/1/1/1
9	CLA	8	612	-	1/1/11/20	6/13/91/115	-
9	CLA	9	610	4	1/1/11/20	7/13/91/115	-
9	CLA	0	605	1	1/1/12/20	7/19/97/115	-
9	CLA	p	309	7	1/1/11/20	4/13/91/115	-
11	IHT	8	616	-	-	1/25/65/65	0/2/2/2
12	II0	0	615	-	-	0/21/67/67	0/2/2/2
9	CLA	7	613	-	1/1/11/20	7/13/91/115	-
9	CLA	9	606	-	1/1/11/20	1/13/91/115	-
9	CLA	0	604	-	1/1/13/20	7/25/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	IHT	0	614	-	-	5/25/65/65	0/2/2/2
9	CLA	0	607	1	1/1/11/20	0/13/91/115	-
9	CLA	8	604	-	1/1/13/20	3/25/103/115	-
12	II0	8	613	-	-	0/21/67/67	0/2/2/2
12	II0	p	315	-	-	1/21/67/67	0/2/2/2
9	CLA	P	604	-	1/1/13/20	4/25/103/115	-
9	CLA	8	609	15	1/1/10/20	2/8/86/115	-
10	KC2	P	609	6	-	12/15/71/71	-
15	LHG	s	301	-	-	20/41/41/53	-
12	II0	p	316	-	-	4/21/67/67	0/2/2/2
10	KC2	P	605	-	-	10/15/71/71	-
9	CLA	p	307	-	1/1/14/20	13/31/109/115	-
9	CLA	7	604	2	1/1/13/20	5/25/103/115	-
14	II3	7	615	-	-	1/25/67/67	0/2/2/2
9	CLA	8	603	-	1/1/12/20	7/19/97/115	-
9	CLA	p	303	7	1/1/10/20	6/10/88/115	-
9	CLA	p	311	-	1/1/10/20	3/8/86/115	-
12	II0	0	616	-	-	4/21/67/67	0/2/2/2
9	CLA	0	602	1	1/1/13/20	11/30/108/115	-
9	CLA	8	602	3	1/1/13/20	11/30/108/115	-
12	II0	p	302	-	-	1/21/67/67	0/2/2/2
9	CLA	0	603	-	1/1/12/20	5/19/97/115	-
13	LMG	G	102	-	-	9/23/43/70	0/1/1/1
9	CLA	8	605	3	1/1/14/20	11/31/109/115	-
9	CLA	8	607	3	1/1/11/20	3/13/91/115	-
9	CLA	p	305	-	1/1/12/20	10/19/97/115	-
9	CLA	s	302	-	-	5/13/91/115	-
12	II0	P	612	-	-	0/21/67/67	0/2/2/2
9	CLA	9	605	-	1/1/11/20	5/15/93/115	-
12	II0	7	617	-	-	4/21/67/67	0/2/2/2
9	CLA	7	606	-	1/1/11/20	9/13/91/115	-
9	CLA	P	608	-	1/1/10/20	0/8/86/115	-
9	CLA	P	602	6	1/1/13/20	14/30/108/115	-
9	CLA	8	608	3	1/1/14/20	8/31/109/115	-
9	CLA	7	611	-	1/1/11/20	6/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	CLA	P	606	6	1/1/11/20	4/13/91/115	-
9	CLA	7	609	-	1/1/10/20	1/8/86/115	-

All (717) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	9	615	8CT	C02-C03	13.96	1.58	1.34
16	P	615	8CT	C02-C03	13.88	1.58	1.34
16	P	615	8CT	C32-C31	13.81	1.59	1.32
16	9	615	8CT	C32-C31	13.63	1.59	1.32
12	0	616	II0	C24-C26	-8.78	1.25	1.42
12	7	617	II0	C23-C25	-8.75	1.25	1.42
12	7	616	II0	C23-C25	-8.73	1.25	1.42
12	9	612	II0	C23-C25	-8.72	1.25	1.42
12	P	614	II0	C23-C25	-8.71	1.25	1.42
12	8	613	II0	C24-C26	-8.70	1.25	1.42
12	8	614	II0	C24-C26	-8.70	1.25	1.42
12	7	614	II0	C23-C25	-8.69	1.25	1.42
12	7	616	II0	C24-C26	-8.68	1.25	1.42
12	9	613	II0	C24-C26	-8.68	1.25	1.42
12	p	317	II0	C23-C25	-8.68	1.25	1.42
12	9	612	II0	C24-C26	-8.65	1.25	1.42
12	8	619	II0	C24-C26	-8.65	1.25	1.42
12	8	613	II0	C23-C25	-8.65	1.25	1.42
12	p	301	II0	C24-C26	-8.65	1.25	1.42
11	8	616	IHT	C24-C26	-8.63	1.25	1.42
11	p	318	IHT	C24-C26	-8.62	1.26	1.42
11	7	618	IHT	C24-C26	-8.62	1.26	1.42
12	p	316	II0	C24-C26	-8.62	1.26	1.42
14	7	615	II3	C27-C28	-8.61	1.26	1.42
12	9	614	II0	C23-C25	-8.60	1.26	1.42
14	P	613	II3	C27-C28	-8.59	1.26	1.42
12	0	616	II0	C23-C25	-8.59	1.26	1.42
12	9	614	II0	C24-C26	-8.58	1.26	1.42
12	8	619	II0	C23-C25	-8.58	1.26	1.42
11	0	617	IHT	C24-C26	-8.57	1.26	1.42
11	0	614	IHT	C24-C26	-8.56	1.26	1.42
12	9	613	II0	C23-C25	-8.56	1.26	1.42
12	0	615	II0	C24-C26	-8.56	1.26	1.42
12	7	617	II0	C24-C26	-8.55	1.26	1.42
12	8	615	II0	C24-C26	-8.54	1.26	1.42
12	P	614	II0	C24-C26	-8.53	1.26	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	7	614	II0	C24-C26	-8.51	1.26	1.42
12	7	619	II0	C24-C26	-8.51	1.26	1.42
12	p	315	II0	C23-C25	-8.50	1.26	1.42
12	P	612	II0	C24-C26	-8.50	1.26	1.42
12	8	615	II0	C23-C25	-8.50	1.26	1.42
12	p	301	II0	C23-C25	-8.49	1.26	1.42
12	p	302	II0	C24-C26	-8.49	1.26	1.42
12	P	612	II0	C23-C25	-8.48	1.26	1.42
12	p	317	II0	C24-C26	-8.48	1.26	1.42
12	p	302	II0	C23-C25	-8.44	1.26	1.42
12	p	315	II0	C24-C26	-8.42	1.26	1.42
12	7	619	II0	C23-C25	-8.41	1.26	1.42
12	0	619	II0	C24-C26	-8.41	1.26	1.42
12	p	316	II0	C23-C25	-8.41	1.26	1.42
12	0	615	II0	C23-C25	-8.40	1.26	1.42
12	0	619	II0	C23-C25	-8.40	1.26	1.42
16	P	615	8CT	C34-C35	-8.40	1.36	1.54
12	8	614	II0	C23-C25	-8.37	1.26	1.42
16	9	615	8CT	C34-C35	-8.27	1.37	1.54
12	0	616	II0	C22-C10	-8.05	1.25	1.42
11	7	618	IHT	C21-C11	-7.99	1.25	1.42
12	8	619	II0	C22-C10	-7.96	1.25	1.42
12	P	614	II0	C21-C09	-7.94	1.25	1.42
12	9	613	II0	C22-C10	-7.94	1.25	1.42
12	7	616	II0	C22-C10	-7.94	1.25	1.42
12	p	302	II0	C22-C10	-7.93	1.25	1.42
12	7	617	II0	C21-C09	-7.92	1.25	1.42
12	7	614	II0	C21-C09	-7.90	1.25	1.42
12	7	617	II0	C22-C10	-7.90	1.25	1.42
12	p	317	II0	C21-C09	-7.89	1.25	1.42
12	7	616	II0	C21-C09	-7.89	1.25	1.42
11	8	616	IHT	C21-C11	-7.88	1.25	1.42
12	8	614	II0	C22-C10	-7.88	1.25	1.42
11	0	614	IHT	C21-C11	-7.87	1.25	1.42
12	p	301	II0	C22-C10	-7.87	1.25	1.42
11	p	318	IHT	C21-C11	-7.86	1.25	1.42
12	8	613	II0	C22-C10	-7.84	1.26	1.42
12	8	613	II0	C21-C09	-7.84	1.26	1.42
12	9	614	II0	C21-C09	-7.84	1.26	1.42
12	8	619	II0	C21-C09	-7.84	1.26	1.42
12	p	316	II0	C22-C10	-7.84	1.26	1.42
12	p	301	II0	C21-C09	-7.83	1.26	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	9	612	II0	C21-C09	-7.83	1.26	1.42
12	p	317	II0	C22-C10	-7.82	1.26	1.42
12	0	619	II0	C22-C10	-7.81	1.26	1.42
12	P	612	II0	C21-C09	-7.81	1.26	1.42
14	7	615	II3	C23-C16	-7.81	1.26	1.42
12	7	614	II0	C22-C10	-7.81	1.26	1.42
12	9	612	II0	C22-C10	-7.80	1.26	1.42
14	P	613	II3	C23-C16	-7.80	1.26	1.42
12	0	616	II0	C21-C09	-7.79	1.26	1.42
12	0	615	II0	C22-C10	-7.79	1.26	1.42
11	0	617	IHT	C21-C11	-7.78	1.26	1.42
12	8	615	II0	C22-C10	-7.78	1.26	1.42
12	9	614	II0	C22-C10	-7.77	1.26	1.42
12	P	614	II0	C22-C10	-7.77	1.26	1.42
12	7	619	II0	C22-C10	-7.77	1.26	1.42
12	9	613	II0	C21-C09	-7.77	1.26	1.42
12	P	612	II0	C22-C10	-7.75	1.26	1.42
12	0	615	II0	C21-C09	-7.74	1.26	1.42
12	p	315	II0	C21-C09	-7.74	1.26	1.42
12	8	615	II0	C21-C09	-7.72	1.26	1.42
12	p	315	II0	C22-C10	-7.71	1.26	1.42
12	7	619	II0	C21-C09	-7.67	1.26	1.42
12	8	614	II0	C21-C09	-7.64	1.26	1.42
12	p	316	II0	C21-C09	-7.64	1.26	1.42
12	p	302	II0	C21-C09	-7.59	1.26	1.42
12	0	619	II0	C21-C09	-7.59	1.26	1.42
9	s	303	CLA	C4B-NB	7.57	1.42	1.35
9	9	606	CLA	C4B-NB	7.44	1.41	1.35
9	0	612	CLA	C4B-NB	7.44	1.41	1.35
9	G	101	CLA	C4B-NB	7.39	1.41	1.35
9	0	613	CLA	C4B-NB	7.38	1.41	1.35
9	7	601	CLA	C4B-NB	7.36	1.41	1.35
9	0	604	CLA	C4B-NB	7.32	1.41	1.35
9	7	612	CLA	C4B-NB	7.31	1.41	1.35
9	0	607	CLA	C4B-NB	7.30	1.41	1.35
9	0	601	CLA	C4B-NB	7.29	1.41	1.35
9	9	604	CLA	C4B-NB	7.28	1.41	1.35
9	7	613	CLA	C4B-NB	7.27	1.41	1.35
9	0	605	CLA	C4B-NB	7.25	1.41	1.35
9	7	609	CLA	C4B-NB	7.24	1.41	1.35
9	9	605	CLA	C4B-NB	7.24	1.41	1.35
9	P	611	CLA	C4B-NB	7.23	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	P	606	CLA	C4B-NB	7.21	1.41	1.35
9	0	611	CLA	C4B-NB	7.21	1.41	1.35
9	0	609	CLA	C4B-NB	7.20	1.41	1.35
9	p	314	CLA	C4B-NB	7.20	1.41	1.35
9	8	605	CLA	C4B-NB	7.19	1.41	1.35
9	8	606	CLA	C4B-NB	7.19	1.41	1.35
9	0	606	CLA	C4B-NB	7.15	1.41	1.35
9	P	604	CLA	C4B-NB	7.13	1.41	1.35
9	p	311	CLA	C4B-NB	7.10	1.41	1.35
9	7	605	CLA	C4B-NB	7.09	1.41	1.35
9	P	603	CLA	C4B-NB	7.06	1.41	1.35
9	9	601	CLA	C4B-NB	7.05	1.41	1.35
9	0	603	CLA	C4B-NB	7.05	1.41	1.35
9	8	612	CLA	C4B-NB	7.05	1.41	1.35
9	p	305	CLA	C4B-NB	7.05	1.41	1.35
9	0	602	CLA	C4B-NB	7.04	1.41	1.35
9	8	609	CLA	C4B-NB	7.04	1.41	1.35
9	9	611	CLA	C4B-NB	7.01	1.41	1.35
9	P	608	CLA	C4B-NB	7.01	1.41	1.35
9	p	303	CLA	C4B-NB	6.99	1.41	1.35
9	s	302	CLA	C4B-NB	6.98	1.41	1.35
9	p	308	CLA	C4B-NB	6.98	1.41	1.35
9	P	602	CLA	C4B-NB	6.98	1.41	1.35
9	p	304	CLA	C4B-NB	6.98	1.41	1.35
9	0	608	CLA	C4B-NB	6.96	1.41	1.35
9	p	307	CLA	C4B-NB	6.95	1.41	1.35
10	7	610	KC2	C4D-CHA	-6.95	1.36	1.45
10	8	610	KC2	C4D-CHA	-6.95	1.36	1.45
9	P	607	CLA	C4B-NB	6.94	1.41	1.35
10	0	610	KC2	C4D-CHA	-6.92	1.36	1.45
9	p	310	CLA	C4B-NB	6.92	1.41	1.35
9	P	601	CLA	C4B-NB	6.91	1.41	1.35
10	p	312	KC2	C4D-CHA	-6.90	1.36	1.45
9	8	601	CLA	C4B-NB	6.89	1.41	1.35
9	9	608	CLA	C4B-NB	6.89	1.41	1.35
9	9	609	CLA	C4B-NB	6.89	1.41	1.35
9	9	607	CLA	C4B-NB	6.88	1.41	1.35
9	p	309	CLA	C4B-NB	6.87	1.41	1.35
9	7	608	CLA	C4B-NB	6.86	1.41	1.35
9	8	604	CLA	C4B-NB	6.86	1.41	1.35
9	7	611	CLA	C4B-NB	6.84	1.41	1.35
9	7	607	CLA	C4B-NB	6.84	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	p	313	CLA	C4B-NB	6.83	1.41	1.35
9	9	603	CLA	C4B-NB	6.83	1.41	1.35
9	8	608	CLA	C4B-NB	6.83	1.41	1.35
10	P	605	KC2	C4D-CHA	-6.82	1.36	1.45
9	9	610	CLA	C4B-NB	6.81	1.41	1.35
9	8	603	CLA	C4B-NB	6.80	1.41	1.35
10	P	609	KC2	C4D-CHA	-6.80	1.36	1.45
9	7	604	CLA	C4B-NB	6.79	1.41	1.35
9	P	610	CLA	C4B-NB	6.78	1.41	1.35
9	7	602	CLA	C4B-NB	6.75	1.41	1.35
9	7	606	CLA	C4B-NB	6.72	1.41	1.35
9	p	306	CLA	C4B-NB	6.71	1.41	1.35
9	8	607	CLA	C4B-NB	6.67	1.41	1.35
9	9	602	CLA	C4B-NB	6.65	1.41	1.35
9	7	603	CLA	C4B-NB	6.63	1.41	1.35
9	8	611	CLA	C4B-NB	6.53	1.41	1.35
9	8	602	CLA	C4B-NB	6.47	1.41	1.35
16	P	615	8CT	C05-C06	-6.41	1.36	1.52
16	9	615	8CT	C05-C06	-6.37	1.36	1.52
16	P	615	8CT	C15-C16	6.29	1.59	1.45
16	9	615	8CT	C15-C16	6.22	1.59	1.45
16	P	615	8CT	C28-C26	6.22	1.59	1.45
16	9	615	8CT	C28-C26	6.09	1.59	1.45
16	9	615	8CT	C04-C03	-5.83	1.45	1.53
16	P	615	8CT	C04-C03	-5.73	1.45	1.53
16	P	615	8CT	C23-C21	5.72	1.58	1.45
16	9	615	8CT	C23-C21	5.62	1.58	1.45
10	P	605	KC2	CHD-C4C	5.51	1.49	1.35
10	7	610	KC2	CHD-C4C	5.42	1.48	1.35
10	0	610	KC2	CHD-C4C	5.42	1.48	1.35
10	P	609	KC2	CHD-C4C	5.42	1.48	1.35
10	p	312	KC2	CHD-C4C	5.36	1.48	1.35
10	8	610	KC2	CHD-C4C	5.34	1.48	1.35
16	9	615	8CT	C34-C33	5.14	1.64	1.52
16	P	615	8CT	C34-C33	5.14	1.64	1.52
16	P	615	8CT	C05-C04	4.97	1.65	1.54
16	9	615	8CT	C05-C04	4.95	1.65	1.54
16	9	615	8CT	C06-C07	4.69	1.67	1.52
16	P	615	8CT	C06-C07	4.57	1.66	1.52
17	p	319	SQD	O48-C23	4.56	1.46	1.33
16	P	615	8CT	C19-C20	4.41	1.57	1.43
10	8	610	KC2	MG-NB	-4.40	1.97	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	P	605	KC2	MG-NB	-4.39	1.97	2.05
16	9	615	8CT	C19-C20	4.31	1.56	1.43
10	0	610	KC2	MG-NB	-4.27	1.97	2.05
10	p	312	KC2	MG-NB	-4.21	1.97	2.05
10	P	609	KC2	MG-NB	-4.20	1.97	2.05
10	7	610	KC2	MG-NB	-4.11	1.97	2.05
10	0	610	KC2	CHC-C1C	4.08	1.48	1.39
10	p	312	KC2	CHC-C1C	4.08	1.48	1.39
10	P	609	KC2	CHC-C1C	4.08	1.48	1.39
10	P	605	KC2	CHC-C1C	4.05	1.48	1.39
16	P	615	8CT	C24-C25	4.05	1.56	1.43
16	9	615	8CT	C24-C25	4.04	1.56	1.43
10	P	605	KC2	CHC-C4B	4.02	1.46	1.38
10	0	610	KC2	CHC-C4B	4.01	1.46	1.38
10	p	312	KC2	CHC-C4B	3.97	1.46	1.38
10	7	610	KC2	CHC-C1C	3.97	1.48	1.39
10	P	609	KC2	CHC-C4B	3.96	1.46	1.38
10	8	610	KC2	CHC-C1C	3.90	1.48	1.39
9	P	606	CLA	C1D-ND	3.84	1.42	1.37
9	7	613	CLA	C1D-ND	3.82	1.42	1.37
9	s	302	CLA	C1D-ND	3.80	1.42	1.37
16	P	615	8CT	C14-C13	3.78	1.55	1.43
10	7	610	KC2	CHC-C4B	3.77	1.45	1.38
10	8	610	KC2	CHC-C4B	3.76	1.45	1.38
9	s	303	CLA	C1D-ND	3.76	1.42	1.37
9	0	611	CLA	C1D-ND	3.75	1.42	1.37
9	0	612	CLA	C1D-ND	3.75	1.42	1.37
9	0	601	CLA	C1D-ND	3.74	1.42	1.37
16	9	615	8CT	C14-C13	3.73	1.55	1.43
9	7	601	CLA	C1D-ND	3.71	1.42	1.37
9	0	609	CLA	C1D-ND	3.71	1.42	1.37
9	0	606	CLA	C1D-ND	3.68	1.42	1.37
9	9	605	CLA	C1D-ND	3.68	1.42	1.37
9	7	609	CLA	C1D-ND	3.67	1.42	1.37
9	P	607	CLA	C1D-ND	3.66	1.42	1.37
9	p	314	CLA	C1D-ND	3.65	1.42	1.37
9	7	604	CLA	C1D-ND	3.65	1.42	1.37
16	P	615	8CT	C11-C12	3.65	1.53	1.45
9	9	609	CLA	C1D-ND	3.64	1.42	1.37
9	7	612	CLA	C1D-ND	3.64	1.42	1.37
9	0	608	CLA	C1D-ND	3.64	1.42	1.37
9	0	604	CLA	C1D-ND	3.63	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	9	607	CLA	C1D-ND	3.63	1.42	1.37
9	9	604	CLA	C1D-ND	3.61	1.42	1.37
16	9	615	8CT	C11-C12	3.60	1.53	1.45
9	p	308	CLA	C1D-ND	3.60	1.42	1.37
9	p	309	CLA	C1D-ND	3.59	1.42	1.37
9	8	604	CLA	C1D-ND	3.59	1.42	1.37
9	P	611	CLA	C1D-ND	3.58	1.42	1.37
9	9	601	CLA	C1D-ND	3.58	1.42	1.37
9	0	613	CLA	C1D-ND	3.57	1.42	1.37
9	0	605	CLA	C1D-ND	3.57	1.42	1.37
9	p	304	CLA	C1D-ND	3.56	1.42	1.37
9	7	605	CLA	C1D-ND	3.56	1.42	1.37
9	P	603	CLA	C1D-ND	3.56	1.42	1.37
9	p	305	CLA	C1D-ND	3.55	1.42	1.37
9	9	611	CLA	C1D-ND	3.54	1.42	1.37
9	p	307	CLA	C1D-ND	3.53	1.42	1.37
9	8	609	CLA	C1D-ND	3.52	1.42	1.37
9	G	101	CLA	C1D-ND	3.52	1.42	1.37
9	p	306	CLA	C1D-ND	3.52	1.42	1.37
9	0	607	CLA	C1D-ND	3.52	1.42	1.37
9	8	607	CLA	C1D-ND	3.52	1.42	1.37
9	9	606	CLA	C1D-ND	3.52	1.42	1.37
9	P	602	CLA	C1D-ND	3.51	1.42	1.37
9	p	311	CLA	C1D-ND	3.51	1.42	1.37
9	7	611	CLA	C1D-ND	3.51	1.42	1.37
9	0	603	CLA	C1D-ND	3.50	1.42	1.37
9	p	310	CLA	C1D-ND	3.50	1.42	1.37
9	8	602	CLA	C4D-ND	-3.50	1.32	1.37
9	P	608	CLA	C1D-ND	3.50	1.42	1.37
9	8	603	CLA	C1D-ND	3.50	1.42	1.37
16	P	615	8CT	C28-C29	3.49	1.40	1.32
9	0	602	CLA	C1D-ND	3.47	1.42	1.37
9	8	611	CLA	C1D-ND	3.46	1.42	1.37
9	7	603	CLA	C1D-ND	3.46	1.42	1.37
9	9	603	CLA	C1D-ND	3.45	1.42	1.37
9	p	303	CLA	C1D-ND	3.44	1.42	1.37
9	9	602	CLA	C1D-ND	3.44	1.42	1.37
9	9	602	CLA	C4D-ND	-3.44	1.33	1.37
9	8	606	CLA	C1D-ND	3.44	1.42	1.37
9	9	610	CLA	C1D-ND	3.44	1.42	1.37
9	8	608	CLA	C1D-ND	3.43	1.42	1.37
9	8	612	CLA	C1D-ND	3.43	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	7	608	CLA	C1D-ND	3.43	1.42	1.37
9	8	605	CLA	C1D-ND	3.42	1.42	1.37
9	9	608	CLA	C1D-ND	3.42	1.42	1.37
9	7	607	CLA	C1D-ND	3.42	1.42	1.37
9	s	302	CLA	C4D-ND	-3.41	1.33	1.37
9	8	601	CLA	C1D-ND	3.41	1.42	1.37
9	7	606	CLA	C1D-ND	3.40	1.42	1.37
9	P	604	CLA	C1D-ND	3.39	1.42	1.37
16	9	615	8CT	C28-C29	3.39	1.40	1.32
9	P	601	CLA	C1D-ND	3.39	1.42	1.37
9	p	313	CLA	C1D-ND	3.36	1.41	1.37
9	7	602	CLA	C1D-ND	3.34	1.41	1.37
17	p	319	SQD	O47-C7	3.33	1.43	1.34
9	8	608	CLA	C4D-ND	-3.33	1.33	1.37
17	p	319	SQD	O5-C1	3.33	1.50	1.41
9	P	610	CLA	C1D-ND	3.33	1.41	1.37
9	7	607	CLA	C4D-ND	-3.30	1.33	1.37
9	7	603	CLA	C4D-ND	-3.30	1.33	1.37
9	p	305	CLA	C4D-ND	-3.30	1.33	1.37
9	7	602	CLA	C4D-ND	-3.30	1.33	1.37
9	P	602	CLA	C4D-ND	-3.29	1.33	1.37
17	p	319	SQD	O47-C45	-3.29	1.38	1.46
9	8	603	CLA	C4D-ND	-3.29	1.33	1.37
9	8	602	CLA	C1D-ND	3.27	1.41	1.37
9	9	607	CLA	C4D-ND	-3.27	1.33	1.37
9	8	611	CLA	C4D-ND	-3.25	1.33	1.37
16	9	615	8CT	C35-C30	3.25	1.65	1.56
9	7	606	CLA	C4D-ND	-3.24	1.33	1.37
9	7	608	CLA	C4D-ND	-3.24	1.33	1.37
16	9	615	8CT	C01-C02	3.24	1.56	1.50
9	p	304	CLA	CHC-C1C	3.23	1.43	1.35
9	P	604	CLA	C4D-ND	-3.23	1.33	1.37
9	9	608	CLA	C4D-ND	-3.23	1.33	1.37
9	8	609	CLA	C4D-ND	-3.22	1.33	1.37
9	9	603	CLA	C4D-ND	-3.22	1.33	1.37
9	p	309	CLA	C4D-ND	-3.22	1.33	1.37
9	p	311	CLA	C4D-ND	-3.22	1.33	1.37
9	p	304	CLA	C4D-ND	-3.21	1.33	1.37
9	P	601	CLA	C4D-ND	-3.21	1.33	1.37
9	7	604	CLA	C4D-ND	-3.20	1.33	1.37
9	9	604	CLA	CHC-C1C	3.20	1.43	1.35
9	8	604	CLA	C4D-ND	-3.19	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	p	306	CLA	C4D-ND	-3.19	1.33	1.37
9	p	303	CLA	C4D-ND	-3.18	1.33	1.37
9	P	602	CLA	CHC-C1C	3.18	1.43	1.35
9	P	610	CLA	C4D-ND	-3.18	1.33	1.37
9	9	606	CLA	CHC-C1C	3.18	1.43	1.35
9	p	310	CLA	C4D-ND	-3.18	1.33	1.37
9	7	605	CLA	C4D-ND	-3.17	1.33	1.37
9	0	603	CLA	C4D-ND	-3.17	1.33	1.37
9	9	604	CLA	C4D-ND	-3.16	1.33	1.37
9	8	606	CLA	C4D-ND	-3.16	1.33	1.37
9	8	601	CLA	C4D-ND	-3.15	1.33	1.37
9	7	611	CLA	C4D-ND	-3.15	1.33	1.37
16	9	615	8CT	C30-C29	3.15	1.54	1.50
9	P	608	CLA	C4D-ND	-3.15	1.33	1.37
16	P	615	8CT	C35-C30	3.14	1.65	1.56
9	8	607	CLA	C4D-ND	-3.14	1.33	1.37
9	9	609	CLA	C4D-ND	-3.14	1.33	1.37
9	P	603	CLA	C4D-ND	-3.13	1.33	1.37
9	0	613	CLA	CHC-C1C	3.13	1.43	1.35
16	P	615	8CT	C01-C02	3.13	1.56	1.50
9	7	612	CLA	C4D-ND	-3.13	1.33	1.37
9	s	303	CLA	CHC-C1C	3.13	1.43	1.35
9	0	604	CLA	CHC-C1C	3.13	1.43	1.35
9	8	605	CLA	C4D-ND	-3.12	1.33	1.37
9	9	610	CLA	C4D-ND	-3.12	1.33	1.37
9	p	313	CLA	C4D-ND	-3.12	1.33	1.37
9	0	602	CLA	C4D-ND	-3.12	1.33	1.37
9	0	608	CLA	C4D-ND	-3.12	1.33	1.37
9	p	309	CLA	CHC-C1C	3.11	1.42	1.35
9	p	308	CLA	C4D-ND	-3.11	1.33	1.37
9	9	606	CLA	C4D-ND	-3.11	1.33	1.37
9	P	603	CLA	CHC-C1C	3.11	1.42	1.35
9	0	602	CLA	CHC-C1C	3.10	1.42	1.35
9	7	609	CLA	CHC-C1C	3.10	1.42	1.35
9	P	606	CLA	CHC-C1C	3.10	1.42	1.35
9	8	612	CLA	C4D-ND	-3.10	1.33	1.37
9	9	611	CLA	C4D-ND	-3.10	1.33	1.37
9	p	307	CLA	C4D-ND	-3.10	1.33	1.37
9	7	612	CLA	CHC-C1C	3.09	1.42	1.35
9	7	609	CLA	C4D-ND	-3.09	1.33	1.37
9	s	302	CLA	CHC-C1C	3.08	1.42	1.35
9	8	607	CLA	CHC-C1C	3.08	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	0	601	CLA	CHC-C1C	3.08	1.42	1.35
9	9	605	CLA	CHC-C1C	3.08	1.42	1.35
16	P	615	8CT	C30-C29	3.08	1.54	1.50
9	0	612	CLA	CHC-C1C	3.08	1.42	1.35
9	0	607	CLA	CHC-C1C	3.07	1.42	1.35
9	0	611	CLA	CHC-C1C	3.07	1.42	1.35
9	p	310	CLA	CHC-C1C	3.07	1.42	1.35
9	G	101	CLA	C4D-ND	-3.07	1.33	1.37
9	8	609	CLA	CHC-C1C	3.07	1.42	1.35
9	0	604	CLA	C4D-ND	-3.06	1.33	1.37
9	p	311	CLA	CHC-C1C	3.06	1.42	1.35
9	0	609	CLA	CHC-C1C	3.06	1.42	1.35
9	s	303	CLA	C4D-ND	-3.06	1.33	1.37
9	7	601	CLA	CHC-C1C	3.06	1.42	1.35
9	p	314	CLA	C4D-ND	-3.05	1.33	1.37
9	p	314	CLA	CHC-C1C	3.05	1.42	1.35
9	P	608	CLA	CHC-C1C	3.05	1.42	1.35
9	9	609	CLA	CHC-C1C	3.05	1.42	1.35
9	p	305	CLA	CHC-C1C	3.04	1.42	1.35
9	P	607	CLA	CHC-C1C	3.04	1.42	1.35
9	0	607	CLA	C4D-ND	-3.04	1.33	1.37
9	7	607	CLA	CHC-C1C	3.04	1.42	1.35
9	0	606	CLA	C4D-ND	-3.04	1.33	1.37
9	7	613	CLA	CHC-C1C	3.04	1.42	1.35
9	0	608	CLA	CHC-C1C	3.03	1.42	1.35
9	7	601	CLA	C4D-ND	-3.03	1.33	1.37
9	9	601	CLA	CHC-C1C	3.03	1.42	1.35
9	P	611	CLA	CHC-C1C	3.03	1.42	1.35
9	9	607	CLA	CHC-C1C	3.03	1.42	1.35
9	0	603	CLA	CHC-C1C	3.03	1.42	1.35
9	G	101	CLA	CHC-C1C	3.02	1.42	1.35
9	P	611	CLA	C4D-ND	-3.02	1.33	1.37
9	9	601	CLA	C4D-ND	-3.02	1.33	1.37
9	8	612	CLA	CHC-C1C	3.02	1.42	1.35
9	9	611	CLA	CHC-C1C	3.02	1.42	1.35
9	7	608	CLA	CHC-C1C	3.02	1.42	1.35
9	0	609	CLA	C4D-ND	-3.02	1.33	1.37
9	9	608	CLA	CHC-C1C	3.02	1.42	1.35
9	9	602	CLA	CHC-C1C	3.02	1.42	1.35
9	7	604	CLA	CHC-C1C	3.02	1.42	1.35
9	0	606	CLA	CHC-C1C	3.01	1.42	1.35
9	0	613	CLA	C4D-ND	-3.01	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	P	615	8CT	C18-C17	3.01	1.52	1.43
9	0	611	CLA	C4D-ND	-3.00	1.33	1.37
9	7	613	CLA	C4D-ND	-2.99	1.33	1.37
9	7	611	CLA	CHC-C1C	2.99	1.42	1.35
9	P	604	CLA	CHC-C1C	2.99	1.42	1.35
9	0	605	CLA	CHC-C1C	2.99	1.42	1.35
9	p	313	CLA	CHC-C1C	2.99	1.42	1.35
9	P	601	CLA	CHC-C1C	2.99	1.42	1.35
9	8	603	CLA	CHC-C1C	2.99	1.42	1.35
16	9	615	8CT	C18-C17	2.99	1.52	1.43
9	P	607	CLA	C4D-ND	-2.98	1.33	1.37
9	9	603	CLA	CHC-C1C	2.98	1.42	1.35
9	7	602	CLA	CHC-C1C	2.98	1.42	1.35
9	p	303	CLA	CHC-C1C	2.98	1.42	1.35
9	8	604	CLA	CHC-C1C	2.97	1.42	1.35
9	p	307	CLA	CHC-C1C	2.97	1.42	1.35
9	8	608	CLA	CHC-C1C	2.97	1.42	1.35
9	9	610	CLA	CHC-C1C	2.96	1.42	1.35
9	P	610	CLA	CHC-C1C	2.96	1.42	1.35
9	p	308	CLA	CHC-C1C	2.96	1.42	1.35
9	9	605	CLA	C4D-ND	-2.96	1.33	1.37
9	7	605	CLA	CHC-C1C	2.96	1.42	1.35
9	0	605	CLA	C4D-ND	-2.95	1.33	1.37
9	P	606	CLA	C4D-ND	-2.95	1.33	1.37
9	7	603	CLA	CHC-C1C	2.95	1.42	1.35
9	8	605	CLA	CHC-C1C	2.95	1.42	1.35
9	8	601	CLA	CHC-C1C	2.94	1.42	1.35
9	0	612	CLA	C4D-ND	-2.92	1.33	1.37
9	8	602	CLA	CHC-C1C	2.92	1.42	1.35
9	8	611	CLA	CHC-C1C	2.92	1.42	1.35
9	0	601	CLA	C4D-ND	-2.92	1.33	1.37
9	7	606	CLA	CHC-C1C	2.91	1.42	1.35
16	P	615	8CT	C07-C02	-2.89	1.45	1.51
16	P	615	8CT	C10-C03	2.89	1.55	1.45
9	p	306	CLA	CHC-C1C	2.89	1.42	1.35
10	8	610	KC2	C4B-NB	-2.89	1.34	1.37
16	9	615	8CT	C10-C03	2.87	1.55	1.45
10	7	610	KC2	CBA-CGA	-2.85	1.41	1.48
9	8	606	CLA	CHC-C1C	2.84	1.42	1.35
10	P	605	KC2	CBA-CGA	-2.82	1.42	1.48
10	P	605	KC2	C4B-NB	-2.80	1.34	1.37
9	8	605	CLA	CMB-C2B	-2.78	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	p	312	KC2	CBA-CGA	-2.78	1.42	1.48
10	P	609	KC2	CBA-CGA	-2.78	1.42	1.48
10	0	610	KC2	CBA-CGA	-2.77	1.42	1.48
10	8	610	KC2	CBA-CGA	-2.77	1.42	1.48
9	p	307	CLA	CMB-C2B	-2.77	1.45	1.51
9	7	605	CLA	CMB-C2B	-2.76	1.45	1.51
16	9	615	8CT	C07-C02	-2.74	1.45	1.51
9	p	308	CLA	CMB-C2B	-2.73	1.46	1.51
9	0	605	CLA	CMB-C2B	-2.71	1.46	1.51
10	7	610	KC2	C4B-NB	-2.70	1.34	1.37
9	8	608	CLA	CMB-C2B	-2.70	1.46	1.51
9	8	602	CLA	CMB-C2B	-2.64	1.46	1.51
9	8	606	CLA	CMB-C2B	-2.64	1.46	1.51
9	P	607	CLA	CMB-C2B	-2.63	1.46	1.51
9	0	608	CLA	CMB-C2B	-2.62	1.46	1.51
10	P	609	KC2	C4B-NB	-2.62	1.34	1.37
9	9	606	CLA	CMB-C2B	-2.62	1.46	1.51
10	p	312	KC2	C4B-NB	-2.61	1.34	1.37
9	7	607	CLA	CMB-C2B	-2.61	1.46	1.51
9	8	612	CLA	CMB-C2B	-2.60	1.46	1.51
9	p	310	CLA	CMB-C2B	-2.60	1.46	1.51
9	7	608	CLA	CMB-C2B	-2.60	1.46	1.51
9	P	604	CLA	CMB-C2B	-2.59	1.46	1.51
9	9	609	CLA	CMB-C2B	-2.59	1.46	1.51
9	9	607	CLA	CMB-C2B	-2.59	1.46	1.51
9	9	603	CLA	CMB-C2B	-2.58	1.46	1.51
12	8	615	II0	C13-C09	-2.58	1.32	1.34
9	7	612	CLA	CMB-C2B	-2.58	1.46	1.51
9	p	304	CLA	CMB-C2B	-2.57	1.46	1.51
9	0	604	CLA	CMB-C2B	-2.57	1.46	1.51
11	8	616	IHT	C02-C07	-2.56	1.50	1.53
9	p	313	CLA	CMB-C2B	-2.56	1.46	1.51
9	8	601	CLA	CMB-C2B	-2.56	1.46	1.51
9	P	610	CLA	CMB-C2B	-2.56	1.46	1.51
10	0	610	KC2	C4B-NB	-2.56	1.34	1.37
9	s	302	CLA	CMB-C2B	-2.56	1.46	1.51
9	8	607	CLA	CMB-C2B	-2.56	1.46	1.51
9	9	604	CLA	CMB-C2B	-2.55	1.46	1.51
9	P	608	CLA	CMB-C2B	-2.55	1.46	1.51
9	7	611	CLA	CMB-C2B	-2.55	1.46	1.51
9	p	306	CLA	CMB-C2B	-2.55	1.46	1.51
9	p	303	CLA	CMB-C2B	-2.55	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	0	613	CLA	CMB-C2B	-2.54	1.46	1.51
9	8	611	CLA	CMB-C2B	-2.54	1.46	1.51
9	8	609	CLA	CMB-C2B	-2.54	1.46	1.51
9	0	607	CLA	CMB-C2B	-2.54	1.46	1.51
9	p	309	CLA	CMB-C2B	-2.54	1.46	1.51
9	8	604	CLA	CMB-C2B	-2.54	1.46	1.51
9	9	611	CLA	CMB-C2B	-2.53	1.46	1.51
9	P	603	CLA	CMB-C2B	-2.53	1.46	1.51
9	8	603	CLA	CMB-C2B	-2.53	1.46	1.51
9	P	602	CLA	CMB-C2B	-2.53	1.46	1.51
9	9	602	CLA	CMB-C2B	-2.53	1.46	1.51
9	7	602	CLA	CMB-C2B	-2.53	1.46	1.51
9	0	612	CLA	CMB-C2B	-2.52	1.46	1.51
9	7	606	CLA	CMB-C2B	-2.52	1.46	1.51
9	P	611	CLA	CMB-C2B	-2.51	1.46	1.51
9	p	305	CLA	CMB-C2B	-2.51	1.46	1.51
9	9	608	CLA	CMB-C2B	-2.51	1.46	1.51
9	0	601	CLA	CMB-C2B	-2.51	1.46	1.51
9	7	604	CLA	CMB-C2B	-2.50	1.46	1.51
9	9	605	CLA	CMB-C2B	-2.50	1.46	1.51
9	9	610	CLA	CMB-C2B	-2.50	1.46	1.51
9	P	601	CLA	CMB-C2B	-2.50	1.46	1.51
9	7	603	CLA	CMB-C2B	-2.49	1.46	1.51
9	0	602	CLA	CMB-C2B	-2.49	1.46	1.51
9	7	613	CLA	CMB-C2B	-2.49	1.46	1.51
9	0	603	CLA	CMB-C2B	-2.48	1.46	1.51
9	s	303	CLA	CMB-C2B	-2.48	1.46	1.51
9	9	601	CLA	CMB-C2B	-2.47	1.46	1.51
9	p	311	CLA	CMB-C2B	-2.47	1.46	1.51
9	0	606	CLA	CMB-C2B	-2.47	1.46	1.51
9	0	609	CLA	CMB-C2B	-2.47	1.46	1.51
9	p	314	CLA	CMB-C2B	-2.47	1.46	1.51
9	0	611	CLA	CMB-C2B	-2.45	1.46	1.51
9	7	609	CLA	CMB-C2B	-2.45	1.46	1.51
9	G	101	CLA	CMB-C2B	-2.44	1.46	1.51
9	7	601	CLA	CMB-C2B	-2.42	1.46	1.51
11	0	617	IHT	C02-C07	-2.40	1.50	1.53
16	9	615	8CT	C33-C32	-2.39	1.43	1.50
10	8	610	KC2	C4A-C3A	-2.38	1.40	1.44
9	P	606	CLA	CMB-C2B	-2.36	1.46	1.51
9	p	305	CLA	CMD-C2D	-2.35	1.45	1.50
10	8	610	KC2	C1C-C2C	-2.35	1.40	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	p	312	KC2	C4A-C3A	-2.35	1.40	1.44
16	P	615	8CT	C33-C32	-2.32	1.44	1.50
9	P	610	CLA	CMD-C2D	-2.30	1.45	1.50
13	8	617	LMG	O7-C8	-2.27	1.40	1.46
10	7	610	KC2	C4A-C3A	-2.27	1.40	1.44
13	0	618	LMG	O7-C8	-2.26	1.40	1.46
9	7	607	CLA	CMD-C2D	-2.26	1.46	1.50
9	8	611	CLA	CMD-C2D	-2.26	1.46	1.50
9	P	603	CLA	CMD-C2D	-2.24	1.46	1.50
15	s	301	LHG	O7-C5	-2.23	1.41	1.46
10	7	610	KC2	C1C-C2C	-2.23	1.40	1.44
9	8	601	CLA	CMD-C2D	-2.23	1.46	1.50
10	P	605	KC2	C1D-CHD	2.22	1.47	1.41
9	8	609	CLA	CMD-C2D	-2.21	1.46	1.50
9	p	306	CLA	CMD-C2D	-2.21	1.46	1.50
9	9	606	CLA	CMD-C2D	-2.21	1.46	1.50
9	7	605	CLA	C3B-C2B	-2.20	1.37	1.40
9	8	602	CLA	CMD-C2D	-2.20	1.46	1.50
9	p	304	CLA	CMD-C2D	-2.20	1.46	1.50
9	p	307	CLA	CMD-C2D	-2.20	1.46	1.50
10	p	312	KC2	C1C-C2C	-2.19	1.40	1.44
9	7	606	CLA	CMD-C2D	-2.19	1.46	1.50
9	7	609	CLA	CMD-C2D	-2.19	1.46	1.50
9	P	608	CLA	CMD-C2D	-2.19	1.46	1.50
10	P	605	KC2	C4A-C3A	-2.18	1.40	1.44
9	8	602	CLA	C3B-CAB	-2.18	1.43	1.47
9	7	604	CLA	CMD-C2D	-2.18	1.46	1.50
9	7	608	CLA	C3B-C2B	-2.18	1.37	1.40
9	P	604	CLA	CMD-C2D	-2.17	1.46	1.50
9	P	604	CLA	C3B-CAB	-2.17	1.43	1.47
9	0	602	CLA	CMD-C2D	-2.17	1.46	1.50
9	8	602	CLA	CMC-C2C	-2.17	1.46	1.50
9	G	101	CLA	CMD-C2D	-2.17	1.46	1.50
10	P	609	KC2	C4A-C3A	-2.17	1.40	1.44
17	p	319	SQD	C24-C23	2.17	1.59	1.51
9	7	603	CLA	CMD-C2D	-2.17	1.46	1.50
9	8	608	CLA	CMC-C2C	-2.16	1.46	1.50
9	9	601	CLA	CMD-C2D	-2.16	1.46	1.50
9	9	608	CLA	CMD-C2D	-2.16	1.46	1.50
9	8	606	CLA	CMD-C2D	-2.16	1.46	1.50
9	0	603	CLA	CMD-C2D	-2.16	1.46	1.50
9	0	604	CLA	C3B-C2B	-2.15	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	P	606	CLA	CMD-C2D	-2.15	1.46	1.50
9	p	310	CLA	CMD-C2D	-2.15	1.46	1.50
9	8	607	CLA	CMD-C2D	-2.15	1.46	1.50
9	8	606	CLA	C3B-C2B	-2.15	1.37	1.40
10	0	610	KC2	C1D-CHD	2.15	1.47	1.41
9	8	603	CLA	CMD-C2D	-2.14	1.46	1.50
9	p	304	CLA	C3B-C2B	-2.14	1.37	1.40
9	p	309	CLA	CMC-C2C	-2.14	1.46	1.50
9	P	601	CLA	CMD-C2D	-2.14	1.46	1.50
10	P	605	KC2	C1C-C2C	-2.14	1.40	1.44
9	8	612	CLA	CMD-C2D	-2.14	1.46	1.50
9	P	604	CLA	CMC-C2C	-2.14	1.46	1.50
9	9	603	CLA	CMD-C2D	-2.14	1.46	1.50
9	p	308	CLA	C3B-C2B	-2.13	1.37	1.40
9	7	604	CLA	CMC-C2C	-2.13	1.46	1.50
9	p	303	CLA	CMD-C2D	-2.13	1.46	1.50
9	p	308	CLA	CMD-C2D	-2.13	1.46	1.50
9	7	607	CLA	C3B-C2B	-2.13	1.37	1.40
9	8	605	CLA	C3B-C2B	-2.13	1.37	1.40
9	7	608	CLA	CMD-C2D	-2.13	1.46	1.50
9	9	610	CLA	CMD-C2D	-2.13	1.46	1.50
9	p	309	CLA	CMD-C2D	-2.13	1.46	1.50
9	8	612	CLA	CMC-C2C	-2.12	1.46	1.50
9	P	611	CLA	CMD-C2D	-2.12	1.46	1.50
9	0	604	CLA	CMD-C2D	-2.12	1.46	1.50
9	0	609	CLA	CMD-C2D	-2.12	1.46	1.50
9	p	310	CLA	CMC-C2C	-2.12	1.46	1.50
10	P	609	KC2	C1C-C2C	-2.12	1.40	1.44
9	P	607	CLA	CMD-C2D	-2.12	1.46	1.50
9	p	313	CLA	CMD-C2D	-2.12	1.46	1.50
9	8	601	CLA	CMC-C2C	-2.12	1.46	1.50
9	8	608	CLA	CMD-C2D	-2.12	1.46	1.50
9	P	602	CLA	CMC-C2C	-2.12	1.46	1.50
9	p	311	CLA	CMD-C2D	-2.12	1.46	1.50
9	P	602	CLA	CMD-C2D	-2.11	1.46	1.50
17	p	319	SQD	O9-S	2.11	1.51	1.45
9	7	611	CLA	CMD-C2D	-2.11	1.46	1.50
9	9	609	CLA	CMD-C2D	-2.11	1.46	1.50
9	8	604	CLA	CMD-C2D	-2.11	1.46	1.50
9	9	606	CLA	C3B-C2B	-2.11	1.37	1.40
9	P	601	CLA	C3B-C2B	-2.11	1.37	1.40
9	7	602	CLA	CMC-C2C	-2.11	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	0	607	CLA	CMD-C2D	-2.11	1.46	1.50
9	p	306	CLA	CMC-C2C	-2.11	1.46	1.50
9	9	602	CLA	CMC-C2C	-2.10	1.46	1.50
9	9	602	CLA	CMD-C2D	-2.10	1.46	1.50
9	0	606	CLA	CMD-C2D	-2.10	1.46	1.50
9	9	604	CLA	CMD-C2D	-2.10	1.46	1.50
9	0	605	CLA	CMD-C2D	-2.10	1.46	1.50
9	8	605	CLA	CMC-C2C	-2.10	1.46	1.50
9	7	608	CLA	CMC-C2C	-2.10	1.46	1.50
9	8	605	CLA	CMD-C2D	-2.10	1.46	1.50
9	7	602	CLA	CMD-C2D	-2.09	1.46	1.50
10	P	609	KC2	C1D-CHD	2.09	1.46	1.41
10	7	610	KC2	C1D-CHD	2.09	1.46	1.41
9	7	612	CLA	CMD-C2D	-2.09	1.46	1.50
9	9	607	CLA	CMD-C2D	-2.09	1.46	1.50
9	s	303	CLA	CMD-C2D	-2.09	1.46	1.50
9	8	603	CLA	C3B-CAB	-2.09	1.43	1.47
9	p	314	CLA	CMD-C2D	-2.08	1.46	1.50
10	8	610	KC2	C1B-NB	-2.08	1.35	1.37
9	0	613	CLA	CMD-C2D	-2.08	1.46	1.50
9	8	603	CLA	CMC-C2C	-2.08	1.46	1.50
9	9	611	CLA	CMD-C2D	-2.08	1.46	1.50
9	P	611	CLA	CMC-C2C	-2.08	1.46	1.50
9	7	605	CLA	CMD-C2D	-2.08	1.46	1.50
9	0	608	CLA	CMD-C2D	-2.08	1.46	1.50
9	0	611	CLA	CMD-C2D	-2.08	1.46	1.50
9	7	607	CLA	CMC-C2C	-2.08	1.46	1.50
9	8	604	CLA	CMC-C2C	-2.08	1.46	1.50
9	p	313	CLA	CMC-C2C	-2.08	1.46	1.50
9	7	602	CLA	C3B-CAB	-2.08	1.43	1.47
9	p	305	CLA	CMC-C2C	-2.07	1.46	1.50
9	p	304	CLA	CMC-C2C	-2.07	1.46	1.50
9	8	611	CLA	CMC-C2C	-2.07	1.46	1.50
9	9	604	CLA	CMC-C2C	-2.06	1.46	1.50
9	P	607	CLA	C3B-C2B	-2.06	1.37	1.40
9	9	607	CLA	CMC-C2C	-2.06	1.46	1.50
10	0	610	KC2	C4A-C3A	-2.06	1.40	1.44
9	0	605	CLA	C3B-C2B	-2.06	1.37	1.40
9	P	604	CLA	C3B-C2B	-2.06	1.37	1.40
10	0	610	KC2	C1C-C2C	-2.06	1.40	1.44
9	8	607	CLA	CMC-C2C	-2.06	1.46	1.50
9	9	605	CLA	CMD-C2D	-2.05	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	P	608	CLA	CMC-C2C	-2.05	1.46	1.50
9	7	613	CLA	CMD-C2D	-2.05	1.46	1.50
9	9	610	CLA	CMC-C2C	-2.05	1.46	1.50
9	0	604	CLA	CMC-C2C	-2.04	1.46	1.50
9	0	602	CLA	C3B-CAB	-2.04	1.43	1.47
9	7	605	CLA	C3B-CAB	-2.04	1.43	1.47
9	7	605	CLA	CMC-C2C	-2.04	1.46	1.50
9	8	609	CLA	CMC-C2C	-2.04	1.46	1.50
9	9	603	CLA	CMC-C2C	-2.04	1.46	1.50
9	9	606	CLA	CMC-C2C	-2.04	1.46	1.50
9	p	303	CLA	CMC-C2C	-2.04	1.46	1.50
9	P	602	CLA	C3B-CAB	-2.04	1.43	1.47
9	8	612	CLA	C3B-C2B	-2.04	1.37	1.40
9	P	603	CLA	CMC-C2C	-2.04	1.46	1.50
9	p	304	CLA	C3B-CAB	-2.04	1.43	1.47
17	p	319	SQD	O7-S	2.04	1.51	1.45
9	0	601	CLA	CMD-C2D	-2.04	1.46	1.50
10	p	312	KC2	C1D-CHD	2.04	1.46	1.41
9	0	603	CLA	CMC-C2C	-2.03	1.46	1.50
9	0	604	CLA	C3B-CAB	-2.03	1.43	1.47
9	G	101	CLA	CMC-C2C	-2.03	1.46	1.50
9	9	611	CLA	CMC-C2C	-2.03	1.46	1.50
9	p	307	CLA	CMC-C2C	-2.03	1.46	1.50
9	P	610	CLA	CMC-C2C	-2.03	1.46	1.50
9	8	606	CLA	CMC-C2C	-2.03	1.46	1.50
9	P	607	CLA	CMC-C2C	-2.03	1.46	1.50
9	p	308	CLA	CMC-C2C	-2.03	1.46	1.50
9	0	602	CLA	CMC-C2C	-2.02	1.46	1.50
9	7	612	CLA	CMC-C2C	-2.02	1.46	1.50
9	7	601	CLA	CMD-C2D	-2.02	1.46	1.50
9	s	302	CLA	CMD-C2D	-2.02	1.46	1.50
9	7	607	CLA	C3B-CAB	-2.02	1.43	1.47
9	9	601	CLA	CMC-C2C	-2.02	1.46	1.50
9	9	605	CLA	CMC-C2C	-2.02	1.46	1.50
10	8	610	KC2	C1D-CHD	2.02	1.46	1.41
9	7	603	CLA	CMC-C2C	-2.01	1.46	1.50
9	8	601	CLA	C3B-C2B	-2.01	1.37	1.40
9	P	611	CLA	C3B-CAB	-2.01	1.43	1.47
9	8	611	CLA	MG-ND	-2.01	2.01	2.05
9	P	610	CLA	MG-ND	-2.01	2.01	2.05
9	0	608	CLA	C3B-C2B	-2.01	1.37	1.40
9	8	608	CLA	C3B-C2B	-2.01	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	8	607	CLA	C3B-C2B	-2.01	1.37	1.40
9	P	602	CLA	C3B-C2B	-2.01	1.37	1.40
9	0	613	CLA	CMC-C2C	-2.01	1.46	1.50
9	9	604	CLA	C3B-C2B	-2.00	1.37	1.40
9	p	310	CLA	C3B-C2B	-2.00	1.37	1.40
9	9	609	CLA	CMC-C2C	-2.00	1.46	1.50
9	7	608	CLA	C3B-CAB	-2.00	1.43	1.47
9	9	607	CLA	C3B-CAB	-2.00	1.43	1.47
9	p	314	CLA	CMC-C2C	-2.00	1.46	1.50

All (964) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	9	615	8CT	C33-C32-C31	-8.64	116.57	124.85
16	P	615	8CT	C33-C32-C31	-8.01	117.17	124.85
10	0	610	KC2	CHB-C1B-NB	7.41	131.26	124.45
10	8	610	KC2	CHC-C4B-NB	7.14	131.02	124.45
10	8	610	KC2	CHB-C1B-NB	7.13	131.01	124.45
10	p	312	KC2	CHB-C1B-NB	7.07	130.95	124.45
9	7	604	CLA	C4A-NA-C1A	6.98	109.85	106.71
10	7	610	KC2	CHB-C1B-NB	6.95	130.84	124.45
9	8	611	CLA	C4A-NA-C1A	6.95	109.83	106.71
10	P	609	KC2	CHB-C1B-NB	6.94	130.84	124.45
10	P	605	KC2	CHB-C1B-NB	6.92	130.82	124.45
9	7	606	CLA	C4A-NA-C1A	6.86	109.79	106.71
16	9	615	8CT	C18-C17-C16	-6.85	117.54	127.31
9	p	306	CLA	C4A-NA-C1A	6.84	109.78	106.71
9	9	603	CLA	C4A-NA-C1A	6.84	109.78	106.71
9	9	609	CLA	C4A-NA-C1A	6.83	109.78	106.71
9	7	608	CLA	C4A-NA-C1A	6.82	109.77	106.71
9	0	608	CLA	C4A-NA-C1A	6.81	109.77	106.71
9	p	310	CLA	C4A-NA-C1A	6.80	109.76	106.71
9	7	611	CLA	C4A-NA-C1A	6.78	109.75	106.71
9	9	601	CLA	C4A-NA-C1A	6.77	109.75	106.71
9	9	607	CLA	C4A-NA-C1A	6.76	109.74	106.71
10	0	610	KC2	CHC-C4B-NB	6.74	130.65	124.45
16	9	615	8CT	C04-C03-C02	-6.73	113.13	122.61
9	P	607	CLA	C4A-NA-C1A	6.72	109.73	106.71
9	8	606	CLA	C4A-NA-C1A	6.72	109.73	106.71
10	P	609	KC2	CHC-C4B-NB	6.71	130.62	124.45
9	9	610	CLA	C4A-NA-C1A	6.70	109.72	106.71
9	P	604	CLA	C4A-NA-C1A	6.69	109.71	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	8	605	CLA	C4A-NA-C1A	6.67	109.70	106.71
9	0	605	CLA	C4A-NA-C1A	6.62	109.68	106.71
9	0	612	CLA	C4A-NA-C1A	6.62	109.68	106.71
9	p	307	CLA	C4A-NA-C1A	6.60	109.67	106.71
9	7	603	CLA	C4A-NA-C1A	6.59	109.67	106.71
9	8	601	CLA	C4A-NA-C1A	6.58	109.66	106.71
9	P	610	CLA	C4A-NA-C1A	6.56	109.66	106.71
9	p	309	CLA	C4A-NA-C1A	6.56	109.65	106.71
9	P	603	CLA	C4A-NA-C1A	6.56	109.65	106.71
9	s	303	CLA	C4A-NA-C1A	6.56	109.65	106.71
9	0	603	CLA	C4A-NA-C1A	6.53	109.64	106.71
9	7	613	CLA	C4A-NA-C1A	6.53	109.64	106.71
9	p	314	CLA	C4A-NA-C1A	6.52	109.64	106.71
9	G	101	CLA	C4A-NA-C1A	6.52	109.64	106.71
9	8	609	CLA	C4A-NA-C1A	6.50	109.63	106.71
9	8	608	CLA	C4A-NA-C1A	6.49	109.62	106.71
16	P	615	8CT	C14-C13-C12	-6.49	118.05	127.31
10	7	610	KC2	CHC-C4B-NB	6.48	130.41	124.45
9	9	611	CLA	C4A-NA-C1A	6.47	109.62	106.71
9	8	604	CLA	C4A-NA-C1A	6.45	109.61	106.71
9	9	604	CLA	C4A-NA-C1A	6.43	109.60	106.71
9	9	605	CLA	C4A-NA-C1A	6.41	109.59	106.71
9	0	601	CLA	C4A-NA-C1A	6.40	109.58	106.71
9	p	303	CLA	C4A-NA-C1A	6.39	109.58	106.71
9	0	611	CLA	C4A-NA-C1A	6.38	109.57	106.71
9	0	602	CLA	C4A-NA-C1A	6.37	109.57	106.71
9	7	609	CLA	C4A-NA-C1A	6.37	109.57	106.71
10	P	605	KC2	CHC-C4B-NB	6.37	130.30	124.45
9	7	612	CLA	C4A-NA-C1A	6.36	109.57	106.71
9	9	602	CLA	C4A-NA-C1A	6.36	109.56	106.71
9	p	313	CLA	C4A-NA-C1A	6.35	109.56	106.71
9	7	607	CLA	C4A-NA-C1A	6.33	109.55	106.71
9	9	608	CLA	C4A-NA-C1A	6.32	109.55	106.71
9	7	601	CLA	C4A-NA-C1A	6.30	109.54	106.71
9	p	308	CLA	C4A-NA-C1A	6.29	109.54	106.71
9	P	608	CLA	C4A-NA-C1A	6.29	109.53	106.71
9	8	602	CLA	C4A-NA-C1A	6.27	109.53	106.71
9	P	601	CLA	C4A-NA-C1A	6.27	109.53	106.71
10	p	312	KC2	CHC-C4B-NB	6.25	130.20	124.45
9	8	612	CLA	C4A-NA-C1A	6.23	109.51	106.71
9	7	605	CLA	C4A-NA-C1A	6.22	109.50	106.71
9	7	602	CLA	C4A-NA-C1A	6.18	109.49	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	0	609	CLA	C4A-NA-C1A	6.15	109.47	106.71
9	0	607	CLA	C4A-NA-C1A	6.11	109.45	106.71
9	P	611	CLA	C4A-NA-C1A	6.10	109.45	106.71
9	0	606	CLA	C4A-NA-C1A	6.09	109.44	106.71
9	8	607	CLA	C4A-NA-C1A	6.08	109.44	106.71
9	p	305	CLA	C4A-NA-C1A	6.05	109.43	106.71
9	0	613	CLA	C4A-NA-C1A	6.00	109.40	106.71
9	8	603	CLA	C4A-NA-C1A	5.98	109.40	106.71
9	0	604	CLA	C4A-NA-C1A	5.97	109.39	106.71
9	p	311	CLA	C4A-NA-C1A	5.93	109.37	106.71
9	P	606	CLA	C4A-NA-C1A	5.91	109.36	106.71
9	P	602	CLA	C4A-NA-C1A	5.86	109.34	106.71
9	p	304	CLA	C4A-NA-C1A	5.86	109.34	106.71
9	9	606	CLA	C4A-NA-C1A	5.74	109.29	106.71
11	0	617	IHT	C40-C37-C33	-5.66	119.23	127.31
9	s	302	CLA	C4A-NA-C1A	5.63	109.23	106.71
16	P	615	8CT	C18-C17-C16	-5.57	119.36	127.31
16	9	615	8CT	C14-C13-C12	-5.34	119.68	127.31
11	0	617	IHT	C41-C38-C35	-5.30	119.75	127.31
10	p	312	KC2	O2D-CGD-CBD	5.28	120.65	111.27
16	9	615	8CT	C07-C02-C03	-5.24	115.12	122.73
11	8	616	IHT	C18-C22-C23	-5.23	118.33	126.23
12	9	613	II0	C42-C40-C36	-5.20	119.89	127.31
12	0	615	II0	C42-C40-C36	-5.18	119.92	127.31
11	7	618	IHT	C41-C38-C35	-5.10	120.03	127.31
11	p	318	IHT	C41-C38-C35	-5.10	120.04	127.31
12	p	317	II0	C42-C40-C36	-5.06	120.09	127.31
16	9	615	8CT	C01-C02-C03	-5.04	118.87	124.53
12	8	615	II0	C03-C09-C13	-5.00	115.57	122.63
16	9	615	8CT	C24-C25-C26	-4.97	120.21	127.31
12	P	612	II0	C41-C39-C35	-4.96	120.23	127.31
10	P	605	KC2	O2D-CGD-CBD	4.95	120.07	111.27
16	P	615	8CT	C24-C25-C26	-4.92	120.29	127.31
12	p	315	II0	C41-C39-C35	-4.91	120.31	127.31
11	8	616	IHT	C30-C27-C23	-4.87	120.37	127.31
12	8	614	II0	C42-C40-C36	-4.86	120.38	127.31
10	7	610	KC2	O2D-CGD-CBD	4.82	119.84	111.27
11	8	616	IHT	C41-C38-C35	-4.81	120.45	127.31
10	P	609	KC2	O2D-CGD-CBD	4.73	119.67	111.27
12	7	616	II0	C42-C40-C36	-4.72	120.57	127.31
12	7	614	II0	C41-C39-C35	-4.72	120.58	127.31
10	0	610	KC2	O2D-CGD-CBD	4.70	119.62	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	7	618	IHT	C30-C27-C23	-4.68	120.64	127.31
11	0	614	IHT	C41-C38-C35	-4.66	120.66	127.31
16	P	615	8CT	C04-C03-C02	-4.66	116.05	122.61
12	p	301	II0	C41-C39-C35	-4.63	120.71	127.31
12	8	613	II0	C41-C39-C35	-4.61	120.73	127.31
16	P	615	8CT	C10-C11-C12	-4.60	119.28	126.23
12	0	616	II0	C41-C39-C35	-4.59	120.76	127.31
11	0	614	IHT	C19-C10-C07	-4.57	119.39	124.53
11	0	617	IHT	C18-C22-C23	-4.53	119.39	126.23
16	P	615	8CT	C01-C02-C03	-4.53	119.44	124.53
16	P	615	8CT	C07-C02-C03	-4.53	116.16	122.73
12	9	612	II0	C41-C39-C35	-4.52	120.86	127.31
11	7	618	IHT	C18-C22-C23	-4.48	119.46	126.23
12	7	617	II0	C42-C40-C36	-4.48	120.92	127.31
12	8	619	II0	C42-C40-C36	-4.47	120.93	127.31
11	0	617	IHT	C19-C10-C07	-4.47	119.51	124.53
12	8	615	II0	C42-C40-C36	-4.44	120.97	127.31
12	7	616	II0	C41-C39-C35	-4.44	120.98	127.31
12	p	302	II0	C42-C40-C36	-4.42	121.00	127.31
12	p	301	II0	C42-C40-C36	-4.41	121.02	127.31
11	8	616	IHT	C19-C10-C07	-4.32	119.68	124.53
15	s	301	LHG	O4-P-O5	4.16	132.83	112.24
9	p	309	CLA	CMB-C2B-C1B	-4.16	122.07	128.46
15	8	618	LHG	O4-P-O5	4.16	132.81	112.24
10	P	605	KC2	C4B-CHC-C1C	-4.14	117.12	126.06
12	8	619	II0	C41-C39-C35	-4.14	121.40	127.31
14	7	615	II3	C39-C36-C33	-4.10	121.46	127.31
10	8	610	KC2	C4B-CHC-C1C	-4.10	117.22	126.06
12	8	613	II0	C42-C40-C36	-4.09	121.48	127.31
9	s	302	CLA	CMB-C2B-C1B	-4.07	122.20	128.46
17	p	319	SQD	O47-C7-C8	4.07	120.27	111.50
9	7	603	CLA	CMB-C2B-C1B	-4.06	122.22	128.46
10	P	609	KC2	C4B-CHC-C1C	-4.04	117.33	126.06
9	8	604	CLA	CMB-C2B-C1B	-4.04	122.25	128.46
9	7	606	CLA	CMB-C2B-C1B	-4.03	122.27	128.46
12	0	619	II0	C42-C40-C36	-4.02	121.57	127.31
12	p	302	II0	C20-C14-C10	-4.00	118.92	124.35
12	9	614	II0	C42-C40-C36	-3.98	121.64	127.31
11	8	616	IHT	C40-C37-C33	-3.97	121.64	127.31
10	0	610	KC2	C4B-CHC-C1C	-3.97	117.50	126.06
11	p	318	IHT	C18-C22-C23	-3.95	120.27	126.23
10	8	610	KC2	O1D-CGD-CBD	-3.92	116.46	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	7	610	KC2	C4B-CHC-C1C	-3.91	117.61	126.06
12	P	614	II0	C42-C40-C36	-3.91	121.73	127.31
14	P	613	II3	C39-C36-C33	-3.90	121.75	127.31
12	7	616	II0	C20-C14-C10	-3.88	119.07	124.35
12	0	616	II0	C42-C40-C36	-3.88	121.78	127.31
9	9	603	CLA	CMB-C2B-C1B	-3.86	122.53	128.46
9	9	602	CLA	CMB-C2B-C1B	-3.85	122.55	128.46
10	p	312	KC2	C4B-CHC-C1C	-3.85	117.76	126.06
12	7	617	II0	C41-C39-C35	-3.82	121.86	127.31
12	8	619	II0	C20-C14-C10	-3.81	119.17	124.35
16	P	615	8CT	C19-C20-C21	-3.80	121.88	127.31
12	p	302	II0	C41-C39-C35	-3.79	121.90	127.31
12	8	615	II0	C19-C13-C11	3.79	121.38	114.36
10	P	609	KC2	C3D-CAD-CBD	-3.77	102.64	107.61
9	8	611	CLA	CMB-C2B-C1B	-3.76	122.69	128.46
12	p	315	II0	C19-C13-C09	-3.76	119.25	124.35
12	p	301	II0	C19-C13-C09	-3.74	119.26	124.35
9	P	603	CLA	CMB-C2B-C1B	-3.74	122.72	128.46
12	p	316	II0	C42-C40-C36	-3.73	121.98	127.31
9	9	607	CLA	CMB-C2B-C1B	-3.73	122.74	128.46
14	P	613	II3	C22-C18-C16	-3.73	119.29	124.35
12	p	302	II0	C03-C09-C13	-3.72	117.39	122.63
11	p	318	IHT	C19-C10-C07	-3.70	120.37	124.53
16	9	615	8CT	C19-C20-C21	-3.70	122.03	127.31
12	8	613	II0	C19-C13-C09	-3.70	119.33	124.35
10	8	610	KC2	CHC-C4B-C3B	-3.69	118.94	125.26
9	8	608	CLA	CMB-C2B-C1B	-3.69	122.79	128.46
12	8	613	II0	C20-C14-C10	-3.69	119.34	124.35
11	0	614	IHT	C20-C15-C11	-3.69	119.34	124.35
17	p	319	SQD	O7-S-C6	3.68	111.31	106.94
9	0	603	CLA	CMB-C2B-C1B	-3.67	122.82	128.46
9	8	602	CLA	CMB-C2B-C1B	-3.67	122.83	128.46
11	7	618	IHT	C40-C37-C33	-3.67	122.08	127.31
12	8	615	II0	C20-C14-C10	-3.66	119.37	124.35
12	P	614	II0	C19-C13-C09	-3.66	119.38	124.35
9	p	313	CLA	CMB-C2B-C1B	-3.65	122.86	128.46
9	8	603	CLA	CMB-C2B-C1B	-3.64	122.87	128.46
17	p	319	SQD	O9-S-O7	-3.64	101.36	113.95
9	P	610	CLA	CMB-C2B-C1B	-3.64	122.87	128.46
9	7	611	CLA	CMB-C2B-C1B	-3.63	122.89	128.46
12	7	619	II0	C42-C40-C36	-3.63	122.13	127.31
9	7	602	CLA	CMB-C2B-C1B	-3.61	122.91	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	9	606	CLA	CMB-C2B-C1B	-3.59	122.94	128.46
12	0	615	II0	C19-C13-C09	-3.59	119.47	124.35
12	7	619	II0	C20-C14-C10	-3.59	119.47	124.35
9	8	607	CLA	CMB-C2B-C1B	-3.58	122.96	128.46
9	9	608	CLA	CMB-C2B-C1B	-3.58	122.96	128.46
12	9	614	II0	C41-C39-C35	-3.58	122.21	127.31
12	9	612	II0	C20-C14-C10	-3.57	119.50	124.35
9	p	309	CLA	CMB-C2B-C3B	3.56	131.34	124.68
9	P	604	CLA	CMB-C2B-C1B	-3.55	123.00	128.46
12	0	616	II0	C20-C14-C10	-3.55	119.52	124.35
9	P	611	CLA	CMB-C2B-C1B	-3.55	123.01	128.46
9	p	303	CLA	CMB-C2B-C1B	-3.55	123.01	128.46
9	7	604	CLA	CMB-C2B-C1B	-3.55	123.01	128.46
12	P	612	II0	C20-C14-C10	-3.54	119.53	124.35
16	9	615	8CT	C11-C10-C03	-3.54	117.26	127.20
14	7	615	II3	C41-C40-C38	-3.52	122.28	127.31
9	G	101	CLA	CMB-C2B-C1B	-3.51	123.08	128.46
10	P	609	KC2	CHC-C4B-C3B	-3.50	119.27	125.26
12	8	615	II0	C41-C39-C35	-3.50	122.31	127.31
10	7	610	KC2	CHC-C4B-C3B	-3.49	119.28	125.26
12	0	619	II0	C03-C09-C13	-3.49	117.70	122.63
11	0	617	IHT	C20-C15-C11	-3.49	119.61	124.35
9	8	612	CLA	CMB-C2B-C1B	-3.49	123.10	128.46
12	P	612	II0	C19-C13-C09	-3.49	119.61	124.35
9	p	314	CLA	CMB-C2B-C1B	-3.49	123.11	128.46
9	p	310	CLA	CMB-C2B-C1B	-3.48	123.11	128.46
11	0	617	IHT	C30-C27-C23	-3.48	122.35	127.31
12	7	619	II0	C41-C39-C35	-3.48	122.35	127.31
9	0	611	CLA	CMB-C2B-C1B	-3.47	123.13	128.46
9	9	610	CLA	CMB-C2B-C1B	-3.47	123.14	128.46
12	9	612	II0	C42-C40-C36	-3.47	122.36	127.31
9	9	604	CLA	CMB-C2B-C1B	-3.46	123.14	128.46
12	9	613	II0	C19-C13-C09	-3.46	119.64	124.35
9	7	613	CLA	CMB-C2B-C1B	-3.46	123.14	128.46
12	7	614	II0	C19-C13-C09	-3.45	119.66	124.35
9	7	607	CLA	CMB-C2B-C1B	-3.45	123.16	128.46
9	7	603	CLA	CMB-C2B-C3B	3.45	131.13	124.68
16	P	615	8CT	C01-C02-C07	3.45	120.24	113.62
12	P	614	II0	C41-C39-C35	-3.44	122.39	127.31
9	0	606	CLA	CMB-C2B-C1B	-3.44	123.18	128.46
9	0	609	CLA	CMB-C2B-C1B	-3.44	123.18	128.46
9	9	601	CLA	CMB-C2B-C1B	-3.44	123.18	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	8	616	IHT	C20-C15-C11	-3.44	119.68	124.35
14	7	615	II3	C22-C18-C16	-3.43	119.68	124.35
11	7	618	IHT	C19-C10-C07	-3.42	120.69	124.53
9	P	607	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
9	8	604	CLA	CMB-C2B-C3B	3.42	131.07	124.68
9	8	606	CLA	CMB-C2B-C1B	-3.41	123.22	128.46
9	p	308	CLA	CMB-C2B-C1B	-3.41	123.22	128.46
10	0	610	KC2	CHC-C4B-C3B	-3.41	119.43	125.26
12	p	315	II0	C42-C40-C36	-3.41	122.45	127.31
9	p	311	CLA	CMB-C2B-C1B	-3.40	123.23	128.46
9	0	607	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
9	7	601	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
10	8	610	KC2	C3D-CAD-CBD	-3.40	103.13	107.61
9	7	606	CLA	CMB-C2B-C3B	3.40	131.03	124.68
12	9	614	II0	C19-C13-C09	-3.39	119.74	124.35
11	p	318	IHT	C20-C15-C11	-3.39	119.74	124.35
9	9	609	CLA	CMB-C2B-C1B	-3.39	123.25	128.46
9	s	303	CLA	CMB-C2B-C1B	-3.39	123.26	128.46
17	p	319	SQD	O48-C23-C24	3.39	120.26	111.38
10	0	610	KC2	CHB-C1B-C2B	-3.38	118.38	125.48
9	7	608	CLA	CMB-C2B-C1B	-3.38	123.26	128.46
9	p	306	CLA	CMB-C2B-C1B	-3.38	123.27	128.46
9	9	605	CLA	CMB-C2B-C1B	-3.38	123.27	128.46
10	0	610	KC2	C1A-NA-C4A	-3.38	105.19	106.71
9	0	613	CLA	CMB-C2B-C1B	-3.38	123.28	128.46
9	P	602	CLA	CMB-C2B-C1B	-3.38	123.28	128.46
12	7	614	II0	C42-C40-C36	-3.37	122.50	127.31
11	0	614	IHT	C40-C37-C33	-3.37	122.50	127.31
9	7	609	CLA	CMB-C2B-C1B	-3.37	123.29	128.46
9	8	601	CLA	CMB-C2B-C1B	-3.37	123.29	128.46
9	0	608	CLA	CMB-C2B-C1B	-3.37	123.29	128.46
9	8	609	CLA	CMB-C2B-C1B	-3.37	123.29	128.46
9	P	608	CLA	CMB-C2B-C1B	-3.36	123.29	128.46
9	P	606	CLA	CMB-C2B-C1B	-3.36	123.30	128.46
11	7	618	IHT	C06-C09-C10	-3.35	108.09	114.08
9	P	610	CLA	O2D-CGD-O1D	-3.35	117.28	123.84
12	9	613	II0	C06-C08-C12	-3.35	105.72	110.30
9	7	612	CLA	CMB-C2B-C1B	-3.35	123.32	128.46
12	9	612	II0	C19-C13-C09	-3.35	119.80	124.35
12	p	315	II0	C20-C14-C10	-3.35	119.80	124.35
9	9	611	CLA	CMB-C2B-C1B	-3.34	123.32	128.46
10	p	312	KC2	CHB-C1B-C2B	-3.34	118.47	125.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	0	602	CLA	CMB-C2B-C1B	-3.34	123.33	128.46
12	8	614	II0	C20-C14-C10	-3.34	119.81	124.35
12	p	316	II0	C19-C13-C09	-3.34	119.82	124.35
9	0	601	CLA	CMB-C2B-C1B	-3.34	123.34	128.46
12	P	614	II0	C20-C14-C12	3.33	120.53	114.36
9	0	604	CLA	CMB-C2B-C1B	-3.33	123.34	128.46
12	P	612	II0	C42-C40-C36	-3.33	122.56	127.31
9	8	605	CLA	CMB-C2B-C1B	-3.32	123.36	128.46
12	7	614	II0	C20-C14-C10	-3.32	119.83	124.35
12	7	619	II0	C19-C13-C09	-3.32	119.84	124.35
9	7	605	CLA	CMB-C2B-C1B	-3.32	123.36	128.46
9	9	602	CLA	CMB-C2B-C3B	3.31	130.86	124.68
12	8	619	II0	C19-C13-C09	-3.30	119.86	124.35
9	0	612	CLA	CMB-C2B-C1B	-3.30	123.39	128.46
16	9	615	8CT	C35-C30-C31	3.30	117.32	111.42
9	p	305	CLA	CMB-C2B-C1B	-3.29	123.41	128.46
9	s	302	CLA	CMB-C2B-C3B	3.28	130.82	124.68
9	p	304	CLA	CMB-C2B-C1B	-3.28	123.43	128.46
9	8	603	CLA	O2D-CGD-O1D	-3.27	117.44	123.84
10	7	610	KC2	CHB-C1B-C2B	-3.27	118.61	125.48
12	0	619	II0	C20-C14-C10	-3.27	119.90	124.35
9	9	609	CLA	O2D-CGD-O1D	-3.27	117.44	123.84
11	p	318	IHT	C40-C37-C33	-3.27	122.65	127.31
17	p	319	SQD	O9-S-C6	3.26	110.82	106.94
9	P	601	CLA	CMB-C2B-C1B	-3.26	123.46	128.46
9	p	307	CLA	CMB-C2B-C1B	-3.26	123.46	128.46
12	0	616	II0	C19-C13-C11	3.24	120.36	114.36
9	p	305	CLA	O2D-CGD-O1D	-3.24	117.50	123.84
12	p	317	II0	C41-C39-C35	-3.24	122.69	127.31
10	8	610	KC2	CHB-C1B-C2B	-3.23	118.70	125.48
9	p	308	CLA	O2D-CGD-O1D	-3.23	117.52	123.84
9	7	604	CLA	O2D-CGD-O1D	-3.23	117.52	123.84
12	p	317	II0	C19-C13-C09	-3.23	119.96	124.35
11	7	618	IHT	C20-C15-C11	-3.22	119.97	124.35
9	0	604	CLA	O2D-CGD-O1D	-3.22	117.54	123.84
9	9	603	CLA	CMB-C2B-C3B	3.22	130.70	124.68
9	8	611	CLA	CMB-C2B-C3B	3.21	130.69	124.68
9	8	602	CLA	O2D-CGD-O1D	-3.21	117.57	123.84
9	p	313	CLA	O2D-CGD-O1D	-3.21	117.57	123.84
10	p	312	KC2	CHC-C4B-C3B	-3.20	119.78	125.26
12	p	315	II0	C05-C07-C11	-3.20	105.92	110.30
9	P	603	CLA	O2D-CGD-O1D	-3.20	117.59	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	7	617	II0	C19-C13-C11	3.19	120.26	114.36
9	0	612	CLA	O2D-CGD-O1D	-3.18	117.62	123.84
9	P	611	CLA	O2D-CGD-O1D	-3.18	117.62	123.84
9	0	605	CLA	CMB-C2B-C1B	-3.18	123.58	128.46
12	7	616	II0	C19-C13-C09	-3.18	120.03	124.35
11	0	614	IHT	C18-C22-C23	-3.18	121.44	126.23
12	8	615	II0	C07-C11-C13	-3.17	105.55	111.85
12	0	619	II0	C19-C13-C11	3.16	120.22	114.36
9	0	608	CLA	O2D-CGD-O1D	-3.15	117.67	123.84
12	9	613	II0	C20-C14-C10	-3.15	120.06	124.35
10	P	609	KC2	CHB-C1B-C2B	-3.15	118.87	125.48
12	p	301	II0	C06-C08-C12	-3.15	105.99	110.30
12	7	617	II0	C20-C14-C10	-3.14	120.08	124.35
10	8	610	KC2	O2D-CGD-CBD	3.13	116.83	111.27
12	0	616	II0	C41-C42-C40	-3.13	117.07	123.47
12	9	614	II0	C20-C14-C10	-3.13	120.10	124.35
9	8	602	CLA	CMB-C2B-C3B	3.12	130.52	124.68
9	P	603	CLA	CMB-C2B-C3B	3.12	130.52	124.68
12	8	614	II0	C19-C13-C09	-3.12	120.11	124.35
9	p	305	CLA	C1-C2-C3	-3.12	121.70	126.75
12	0	615	II0	C20-C14-C10	-3.12	120.11	124.35
9	8	607	CLA	O2D-CGD-O1D	-3.12	117.75	123.84
9	7	602	CLA	CMB-C2B-C3B	3.12	130.51	124.68
10	P	605	KC2	CHC-C4B-C3B	-3.11	119.94	125.26
9	8	603	CLA	CMB-C2B-C3B	3.10	130.49	124.68
9	7	611	CLA	CMB-C2B-C3B	3.10	130.48	124.68
9	9	602	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
9	P	604	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
12	p	316	II0	C41-C39-C35	-3.09	122.89	127.31
9	8	604	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
9	p	313	CLA	CMB-C2B-C3B	3.09	130.45	124.68
12	8	614	II0	C06-C08-C12	-3.08	106.09	110.30
12	8	614	II0	C41-C39-C35	-3.08	122.92	127.31
9	P	604	CLA	CMB-C2B-C3B	3.07	130.42	124.68
12	9	614	II0	C05-C07-C11	-3.07	106.11	110.30
9	0	603	CLA	CMB-C2B-C3B	3.06	130.40	124.68
9	8	609	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
10	0	610	KC2	C3D-CAD-CBD	-3.06	103.58	107.61
14	7	615	II3	C29-C26-C24	-3.05	122.95	127.31
9	7	604	CLA	CMB-C2B-C3B	3.05	130.39	124.68
9	9	607	CLA	CMB-C2B-C3B	3.05	130.38	124.68
12	P	612	II0	C05-C07-C11	-3.04	106.14	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	P	612	II0	C06-C08-C12	-3.04	106.14	110.30
9	P	610	CLA	CMB-C2B-C3B	3.03	130.36	124.68
9	9	604	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
9	7	605	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
9	p	310	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
10	P	605	KC2	CHB-C1B-C2B	-3.03	119.13	125.48
12	7	614	II0	C06-C08-C12	-3.02	106.16	110.30
9	7	612	CLA	O2D-CGD-O1D	-3.02	117.92	123.84
9	P	611	CLA	CMB-C2B-C3B	3.02	130.33	124.68
9	P	601	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
16	9	615	8CT	C10-C11-C12	-3.02	121.68	126.23
12	0	615	II0	C41-C39-C35	-3.02	123.01	127.31
12	7	617	II0	C19-C13-C09	-3.01	120.25	124.35
9	8	608	CLA	CMB-C2B-C3B	3.01	130.31	124.68
12	8	614	II0	C05-C07-C11	-3.01	106.19	110.30
12	7	619	II0	C05-C07-C11	-3.00	106.20	110.30
9	9	610	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
9	8	605	CLA	O2D-CGD-O1D	-3.00	117.98	123.84
9	P	606	CLA	CMB-C2B-C3B	2.99	130.28	124.68
9	8	607	CLA	CMB-C2B-C3B	2.99	130.28	124.68
12	p	317	II0	C20-C14-C10	-2.99	120.28	124.35
9	p	303	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
9	0	601	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
9	7	608	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
9	P	602	CLA	O2D-CGD-O1D	-2.98	118.02	123.84
9	8	608	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
11	p	318	IHT	C30-C27-C23	-2.97	123.07	127.31
12	9	613	II0	C42-C41-C39	-2.97	117.39	123.47
9	0	603	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
9	8	601	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
16	9	615	8CT	C18-C19-C20	-2.96	117.41	123.47
9	p	314	CLA	CMB-C2B-C3B	2.96	130.21	124.68
13	G	103	LMG	O6-C1-O1	-2.95	102.99	109.97
9	p	306	CLA	CMB-C2B-C3B	2.95	130.20	124.68
12	7	617	II0	C06-C08-C12	-2.95	106.27	110.30
9	0	611	CLA	CMB-C2B-C3B	2.95	130.19	124.68
12	8	613	II0	C05-C07-C11	-2.95	106.27	110.30
11	7	618	IHT	C20-C15-C12	2.94	119.80	114.36
9	8	606	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
9	P	602	CLA	CMB-C2B-C3B	2.94	130.18	124.68
12	p	315	II0	C06-C08-C12	-2.94	106.28	110.30
9	p	306	CLA	O2D-CGD-O1D	-2.93	118.11	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	P	606	CLA	C1B-CHB-C4A	-2.93	124.31	130.12
9	9	608	CLA	CMB-C2B-C3B	2.93	130.16	124.68
16	9	615	8CT	C01-C02-C07	2.93	119.24	113.62
9	9	610	CLA	CMB-C2B-C3B	2.93	130.15	124.68
12	0	616	II0	C19-C13-C09	-2.92	120.38	124.35
9	8	611	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
9	9	611	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
9	7	603	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
10	8	610	KC2	O2D-CGD-O1D	-2.92	118.13	123.84
9	8	612	CLA	CMB-C2B-C3B	2.92	130.13	124.68
11	0	617	IHT	C19-C10-C09	2.92	119.22	113.62
9	7	613	CLA	CMB-C2B-C3B	2.91	130.13	124.68
12	0	619	II0	C19-C13-C09	-2.91	120.40	124.35
9	0	606	CLA	CMB-C2B-C3B	2.91	130.12	124.68
9	9	608	CLA	CAA-C2A-C3A	-2.90	109.32	116.10
9	0	602	CLA	CMB-C2B-C3B	2.90	130.11	124.68
12	p	301	II0	C20-C14-C10	-2.90	120.41	124.35
9	p	304	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
9	G	101	CLA	CMB-C2B-C3B	2.90	130.10	124.68
12	0	619	II0	C41-C39-C35	-2.90	123.17	127.31
9	P	608	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
12	p	316	II0	C20-C14-C10	-2.90	120.41	124.35
9	p	303	CLA	CMB-C2B-C3B	2.89	130.09	124.68
10	p	312	KC2	C1A-NA-C4A	-2.89	105.41	106.71
9	p	310	CLA	CMB-C2B-C3B	2.89	130.08	124.68
9	0	613	CLA	O2D-CGD-O1D	-2.89	118.20	123.84
9	7	607	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
9	7	602	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
9	s	303	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
11	8	616	IHT	C19-C10-C09	2.88	119.15	113.62
9	s	302	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
9	9	603	CLA	O2D-CGD-O1D	-2.88	118.22	123.84
9	p	314	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
9	P	607	CLA	CMB-C2B-C3B	2.87	130.05	124.68
12	p	317	II0	C20-C14-C12	2.87	119.67	114.36
12	7	616	II0	C19-C13-C11	2.86	119.66	114.36
9	8	612	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
12	p	302	II0	C19-C13-C09	-2.86	120.46	124.35
9	9	601	CLA	CMB-C2B-C3B	2.86	130.03	124.68
12	P	614	II0	C20-C14-C10	-2.86	120.47	124.35
12	p	302	II0	C19-C13-C11	2.86	119.65	114.36
9	7	607	CLA	CMB-C2B-C3B	2.86	130.02	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	9	601	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
13	8	617	LMG	O6-C1-O1	-2.85	103.22	109.97
12	9	612	II0	C05-C07-C11	-2.85	106.41	110.30
17	p	319	SQD	O8-S-C6	2.85	110.28	105.74
9	7	601	CLA	CMB-C2B-C3B	2.85	130.00	124.68
9	9	611	CLA	CMB-C2B-C3B	2.85	130.00	124.68
9	9	605	CLA	O2D-CGD-O1D	-2.85	118.28	123.84
9	p	311	CLA	CMB-C2B-C3B	2.84	129.99	124.68
9	P	608	CLA	CMB-C2B-C3B	2.84	129.99	124.68
9	9	604	CLA	CMB-C2B-C3B	2.84	129.99	124.68
9	0	608	CLA	CMB-C2B-C3B	2.83	129.97	124.68
9	0	602	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
9	8	601	CLA	CMB-C2B-C3B	2.83	129.97	124.68
12	0	616	II0	C20-C14-C12	2.82	119.58	114.36
12	7	619	II0	C06-C08-C12	-2.82	106.44	110.30
11	8	616	IHT	C05-C08-C12	-2.82	106.44	110.30
9	9	605	CLA	CMB-C2B-C3B	2.82	129.95	124.68
9	p	305	CLA	CMB-C2B-C3B	2.82	129.95	124.68
9	0	606	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
9	0	609	CLA	CMB-C2B-C3B	2.82	129.95	124.68
10	8	610	KC2	C1A-NA-C4A	-2.81	105.44	106.71
9	8	609	CLA	CMB-C2B-C3B	2.81	129.94	124.68
10	P	609	KC2	C1A-NA-C4A	-2.80	105.44	106.71
16	9	615	8CT	C35-C30-C29	-2.80	109.16	112.70
9	0	611	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
9	0	609	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
9	P	607	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
9	G	101	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
12	8	615	II0	C32-C34-C36	-2.80	118.56	126.42
10	p	312	KC2	C3D-CAD-CBD	-2.79	103.93	107.61
11	p	318	IHT	C20-C15-C12	2.79	119.53	114.36
12	p	316	II0	C05-C07-C11	-2.79	106.48	110.30
9	7	612	CLA	CMB-C2B-C3B	2.79	129.90	124.68
14	P	613	II3	C39-C41-C40	-2.79	117.76	123.47
9	0	605	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
9	0	604	CLA	CMB-C2B-C3B	2.79	129.89	124.68
9	0	613	CLA	CMB-C2B-C3B	2.78	129.89	124.68
9	0	607	CLA	CMB-C2B-C3B	2.78	129.88	124.68
9	9	609	CLA	CMB-C2B-C3B	2.78	129.88	124.68
12	p	317	II0	C32-C34-C36	-2.77	118.62	126.42
9	7	606	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
9	p	304	CLA	CMB-C2B-C3B	2.77	129.86	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	7	609	CLA	CMB-C2B-C3B	2.77	129.86	124.68
16	P	615	8CT	C40-C12-C13	-2.77	119.05	122.92
9	s	303	CLA	CMB-C2B-C3B	2.77	129.85	124.68
12	8	613	II0	C06-C08-C12	-2.77	106.52	110.30
12	9	612	II0	C06-C08-C12	-2.77	106.52	110.30
14	7	615	II3	C05-C06-C10	-2.76	108.60	111.74
11	0	614	IHT	C30-C27-C23	-2.76	123.37	127.31
16	P	615	8CT	C35-C30-C31	2.75	116.35	111.42
9	p	311	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
9	0	601	CLA	CMB-C2B-C3B	2.75	129.81	124.68
9	7	609	CLA	O2D-CGD-O1D	-2.74	118.47	123.84
13	0	618	LMG	O6-C1-O1	-2.74	103.48	109.97
9	9	606	CLA	CMB-C2B-C3B	2.74	129.80	124.68
12	0	619	II0	C06-C08-C12	-2.74	106.56	110.30
9	9	606	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
10	p	312	KC2	CHD-C4C-NC	2.73	128.34	124.20
13	G	103	LMG	O1-C1-C2	-2.72	104.05	108.30
9	0	612	CLA	CMB-C2B-C3B	2.71	129.76	124.68
9	P	601	CLA	CMB-C2B-C3B	2.71	129.76	124.68
9	7	601	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
11	p	318	IHT	C31-C34-C35	-2.71	118.80	126.42
10	7	610	KC2	C1A-NA-C4A	-2.71	105.49	106.71
9	7	613	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
9	0	607	CLA	O2D-CGD-O1D	-2.71	118.55	123.84
9	7	611	CLA	O2D-CGD-O1D	-2.70	118.55	123.84
10	p	312	KC2	CBD-CHA-C1A	2.70	133.91	128.88
11	7	618	IHT	C19-C10-C09	2.69	118.79	113.62
12	p	301	II0	C05-C07-C11	-2.69	106.62	110.30
9	9	608	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
9	P	603	CLA	C1-C2-C3	-2.69	122.41	126.75
9	s	302	CLA	C1B-CHB-C4A	-2.69	124.80	130.12
12	p	302	II0	C32-C30-C26	-2.68	118.79	126.58
16	P	615	8CT	C18-C19-C20	-2.68	117.98	123.47
9	7	608	CLA	CMB-C2B-C3B	2.68	129.69	124.68
9	0	607	CLA	C1B-CHB-C4A	-2.68	124.81	130.12
10	P	605	KC2	CBD-CHA-C1A	2.67	133.86	128.88
10	7	610	KC2	O1D-CGD-CBD	-2.67	119.02	124.48
9	7	609	CLA	CAA-C2A-C3A	-2.67	109.87	116.10
9	9	602	CLA	C1-C2-C3	-2.67	121.43	126.04
12	P	614	II0	C04-C10-C14	-2.66	118.87	122.63
12	9	614	II0	C06-C08-C12	-2.66	106.66	110.30
11	0	614	IHT	C05-C08-C12	-2.66	106.66	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	p	308	CLA	CMB-C2B-C3B	2.66	129.65	124.68
9	7	605	CLA	CMB-C2B-C3B	2.66	129.65	124.68
9	9	607	CLA	O2D-CGD-O1D	-2.65	118.65	123.84
9	8	606	CLA	CMB-C2B-C3B	2.65	129.64	124.68
12	7	614	II0	C05-C07-C11	-2.65	106.68	110.30
15	8	618	LHG	O8-C23-C24	2.65	120.22	111.91
12	7	619	II0	C20-C14-C12	2.64	119.25	114.36
15	s	301	LHG	O8-C23-C24	2.64	120.20	111.91
9	8	608	CLA	CHB-C4A-NA	2.64	128.16	124.51
9	9	606	CLA	C1B-CHB-C4A	-2.64	124.89	130.12
10	7	610	KC2	CBD-CHA-C1A	2.64	133.80	128.88
9	9	603	CLA	CHB-C4A-NA	2.63	128.16	124.51
9	P	607	CLA	CHB-C4A-NA	2.63	128.16	124.51
10	8	610	KC2	CBD-CHA-C1A	2.63	133.79	128.88
9	0	602	CLA	CHB-C4A-NA	2.63	128.15	124.51
10	P	609	KC2	O1D-CGD-CBD	-2.63	119.11	124.48
12	P	614	II0	C05-C07-C11	-2.63	106.71	110.30
9	0	608	CLA	CHB-C4A-NA	2.62	128.14	124.51
14	P	613	II3	C05-C06-C10	-2.61	108.77	111.74
9	p	311	CLA	CAA-C2A-C3A	-2.61	110.00	116.10
9	P	604	CLA	CHB-C4A-NA	2.61	128.12	124.51
10	P	605	KC2	C3D-CAD-CBD	-2.61	104.17	107.61
10	0	610	KC2	CHD-C4C-NC	2.60	128.15	124.20
12	0	616	II0	C31-C29-C25	-2.60	119.03	126.58
9	8	611	CLA	CHB-C4A-NA	2.60	128.10	124.51
12	8	614	II0	C42-C41-C39	-2.59	118.17	123.47
13	G	102	LMG	O6-C1-O1	-2.59	103.84	109.97
9	0	612	CLA	CHB-C4A-NA	2.59	128.09	124.51
16	9	615	8CT	C39-C16-C17	-2.59	119.30	122.92
12	8	619	II0	C19-C13-C11	2.59	119.15	114.36
12	p	317	II0	C19-C13-C11	2.58	119.14	114.36
16	9	615	8CT	C13-C14-C15	-2.58	115.15	123.22
15	s	301	LHG	C11-C10-C9	-2.58	101.31	114.42
9	p	309	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
9	7	606	CLA	CHB-C4A-NA	2.58	128.08	124.51
12	0	615	II0	C05-C07-C11	-2.58	106.78	110.30
12	0	615	II0	C06-C08-C12	-2.58	106.78	110.30
9	9	610	CLA	CHB-C4A-NA	2.58	128.07	124.51
9	p	309	CLA	CHB-C4A-NA	2.57	128.07	124.51
9	7	604	CLA	CHB-C4A-NA	2.57	128.07	124.51
12	0	616	II0	C31-C33-C35	-2.57	119.20	126.42
9	9	607	CLA	CHB-C4A-NA	2.57	128.06	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	9	613	II0	C05-C07-C11	-2.57	106.79	110.30
9	7	611	CLA	CHB-C4A-NA	2.56	128.06	124.51
9	p	307	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
9	p	307	CLA	CMB-C2B-C3B	2.56	129.47	124.68
10	7	610	KC2	C3D-CAD-CBD	-2.56	104.24	107.61
12	P	614	II0	C31-C29-C25	-2.56	119.16	126.58
9	9	605	CLA	C1B-CHB-C4A	-2.55	125.06	130.12
9	0	605	CLA	CMB-C2B-C3B	2.55	129.45	124.68
9	7	607	CLA	C1B-CHB-C4A	-2.55	125.07	130.12
9	8	605	CLA	CMB-C2B-C3B	2.55	129.45	124.68
11	0	617	IHT	C05-C08-C12	-2.54	106.82	110.30
16	P	615	8CT	C11-C10-C03	-2.54	120.06	127.20
11	0	617	IHT	C20-C15-C12	2.54	119.06	114.36
9	P	610	CLA	CHB-C4A-NA	2.54	128.02	124.51
9	p	310	CLA	CHB-C4A-NA	2.53	128.02	124.51
16	P	615	8CT	C14-C15-C16	-2.53	119.30	126.42
9	7	612	CLA	C1B-CHB-C4A	-2.53	125.10	130.12
9	9	601	CLA	CHB-C4A-NA	2.53	128.01	124.51
9	8	612	CLA	C1B-CHB-C4A	-2.53	125.10	130.12
9	9	609	CLA	CHB-C4A-NA	2.53	128.01	124.51
9	0	604	CLA	C1B-CHB-C4A	-2.53	125.11	130.12
12	0	615	II0	C20-C14-C12	2.53	119.04	114.36
12	7	614	II0	C19-C13-C11	2.53	119.03	114.36
9	p	306	CLA	CHB-C4A-NA	2.53	128.00	124.51
9	0	609	CLA	CAA-C2A-C3A	-2.52	110.21	116.10
12	7	614	II0	C08-C12-C14	-2.52	106.83	111.85
9	s	303	CLA	CHB-C4A-NA	2.52	128.00	124.51
10	P	609	KC2	CHD-C4C-NC	2.52	128.03	124.20
11	p	318	IHT	C31-C29-C26	-2.52	119.27	126.58
9	P	603	CLA	CHB-C4A-NA	2.52	127.99	124.51
9	9	604	CLA	CHB-C4A-NA	2.52	127.99	124.51
12	p	316	II0	C20-C14-C12	2.51	119.01	114.36
12	P	612	II0	C31-C33-C35	-2.51	119.36	126.42
9	p	304	CLA	C1B-CHB-C4A	-2.51	125.14	130.12
10	P	609	KC2	O2D-CGD-O1D	-2.51	118.93	123.84
9	8	601	CLA	CHB-C4A-NA	2.51	127.98	124.51
9	7	603	CLA	CHB-C4A-NA	2.51	127.98	124.51
9	7	608	CLA	CHB-C4A-NA	2.51	127.98	124.51
9	8	605	CLA	CHB-C4A-NA	2.51	127.98	124.51
12	7	614	II0	C20-C14-C12	2.51	119.00	114.36
12	8	619	II0	C20-C14-C12	2.50	119.00	114.36
9	P	602	CLA	C1B-CHB-C4A	-2.50	125.16	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	P	606	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
14	P	613	II3	C25-C24-C21	2.50	122.01	118.08
9	9	608	CLA	C1B-CHB-C4A	-2.49	125.18	130.12
9	7	609	CLA	CHB-C4A-NA	2.49	127.96	124.51
9	7	605	CLA	C1B-CHB-C4A	-2.49	125.18	130.12
9	9	611	CLA	CHB-C4A-NA	2.49	127.96	124.51
9	p	304	CLA	CHB-C4A-NA	2.49	127.96	124.51
12	p	317	II0	C42-C41-C39	-2.49	118.38	123.47
9	p	313	CLA	CHB-C4A-NA	2.49	127.95	124.51
12	0	616	II0	C06-C08-C12	2.49	113.71	110.30
12	p	302	II0	C20-C14-C12	2.48	118.95	114.36
12	9	614	II0	C08-C12-C14	-2.48	106.92	111.85
9	7	613	CLA	CHB-C4A-NA	2.48	127.94	124.51
9	p	314	CLA	CHB-C4A-NA	2.48	127.94	124.51
9	9	608	CLA	CHB-C4A-NA	2.48	127.94	124.51
9	7	603	CLA	C1-C2-C3	-2.47	122.75	126.75
9	9	602	CLA	CHB-C4A-NA	2.47	127.93	124.51
9	8	602	CLA	CHB-C4A-NA	2.47	127.93	124.51
9	8	606	CLA	CHB-C4A-NA	2.47	127.93	124.51
9	8	602	CLA	C1B-CHB-C4A	-2.47	125.23	130.12
12	8	619	II0	C05-C07-C11	-2.47	106.93	110.30
9	8	609	CLA	CAA-C2A-C3A	-2.47	110.34	116.10
10	p	312	KC2	C1A-C2A-C3A	-2.46	105.16	107.11
9	8	607	CLA	C1B-CHB-C4A	-2.46	125.24	130.12
12	8	615	II0	C06-C08-C12	-2.46	106.94	110.30
9	P	604	CLA	C1B-CHB-C4A	-2.46	125.25	130.12
9	0	605	CLA	C1B-CHB-C4A	-2.46	125.25	130.12
9	8	604	CLA	CHB-C4A-NA	2.46	127.91	124.51
9	0	601	CLA	CHB-C4A-NA	2.46	127.91	124.51
9	8	602	CLA	C1-C2-C3	-2.45	121.80	126.04
9	0	613	CLA	CHB-C4A-NA	2.45	127.90	124.51
9	0	606	CLA	C1B-CHB-C4A	-2.45	125.27	130.12
10	P	605	KC2	O1D-CGD-CBD	-2.45	119.47	124.48
9	8	612	CLA	CHB-C4A-NA	2.45	127.90	124.51
9	G	101	CLA	CHB-C4A-NA	2.45	127.89	124.51
12	0	616	II0	C03-C09-C13	-2.44	119.19	122.63
9	9	605	CLA	CHB-C4A-NA	2.44	127.89	124.51
9	8	604	CLA	C1B-CHB-C4A	-2.43	125.30	130.12
9	p	314	CLA	C1B-CHB-C4A	-2.43	125.30	130.12
9	0	608	CLA	C1B-CHB-C4A	-2.43	125.31	130.12
14	7	615	II3	C13-C14-C17	2.43	113.63	110.30
13	8	617	LMG	O3-C3-C2	-2.43	104.74	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	9	604	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
9	G	101	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
9	8	607	CLA	CHB-C4A-NA	2.42	127.86	124.51
12	9	614	II0	C31-C29-C25	-2.42	119.55	126.58
9	7	612	CLA	CHB-C4A-NA	2.42	127.86	124.51
9	8	608	CLA	C1B-CHB-C4A	-2.42	125.33	130.12
9	0	603	CLA	CHB-C4A-NA	2.41	127.85	124.51
13	G	102	LMG	O1-C7-C8	-2.41	105.07	110.90
11	0	617	IHT	C31-C34-C35	-2.41	119.64	126.42
9	7	602	CLA	CHB-C4A-NA	2.41	127.85	124.51
9	9	602	CLA	C1B-CHB-C4A	-2.41	125.34	130.12
11	0	614	IHT	C20-C15-C12	2.41	118.82	114.36
9	P	611	CLA	CHB-C4A-NA	2.41	127.84	124.51
9	8	606	CLA	C1B-CHB-C4A	-2.41	125.35	130.12
9	8	605	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
14	P	613	II3	C26-C29-C32	-2.40	115.72	123.22
13	G	103	LMG	O3-C3-C2	-2.40	104.80	110.35
9	7	601	CLA	CHB-C4A-NA	2.40	127.83	124.51
10	P	605	KC2	CHD-C4C-NC	2.40	127.84	124.20
9	8	603	CLA	CHB-C4A-NA	2.40	127.83	124.51
9	8	609	CLA	CHB-C4A-NA	2.40	127.83	124.51
13	0	618	LMG	O3-C3-C2	-2.40	104.81	110.35
9	p	306	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
13	G	103	LMG	O1-C7-C8	-2.39	105.13	110.90
11	8	616	IHT	C31-C29-C26	-2.39	119.64	126.58
12	p	316	II0	C08-C12-C14	-2.39	107.10	111.85
12	0	615	II0	C42-C41-C39	-2.38	118.59	123.47
10	P	605	KC2	C1B-CHB-C4A	-2.38	120.91	126.06
13	0	618	LMG	O1-C7-C8	-2.38	105.15	110.90
9	0	611	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
10	p	312	KC2	O1D-CGD-CBD	-2.38	119.61	124.48
12	p	317	II0	C38-C36-C40	-2.38	119.59	122.92
9	0	605	CLA	CHB-C4A-NA	2.38	127.80	124.51
12	9	614	II0	C31-C33-C35	-2.38	119.73	126.42
9	0	604	CLA	CHB-C4A-NA	2.38	127.80	124.51
13	G	103	LMG	O2-C2-C1	-2.38	104.27	110.05
11	0	617	IHT	C31-C29-C26	-2.38	119.67	126.58
16	9	615	8CT	C10-C03-C02	-2.38	115.70	121.46
10	7	610	KC2	O2D-CGD-O1D	-2.38	119.19	123.84
9	0	611	CLA	CHB-C4A-NA	2.37	127.79	124.51
9	7	607	CLA	CHB-C4A-NA	2.37	127.79	124.51
9	0	602	CLA	C1B-CHB-C4A	-2.37	125.42	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	P	615	8CT	C27-C26-C25	-2.37	119.60	122.92
12	p	301	II0	C31-C29-C25	-2.37	119.70	126.58
9	7	603	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
9	0	612	CLA	O2D-CGD-CBD	2.37	115.48	111.27
10	7	610	KC2	C1B-CHB-C4A	-2.37	120.95	126.06
9	p	305	CLA	CHB-C4A-NA	2.37	127.78	124.51
9	7	601	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
9	p	309	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
11	8	616	IHT	C31-C34-C35	-2.36	119.78	126.42
9	P	602	CLA	CHB-C4A-NA	2.36	127.78	124.51
12	P	614	II0	C31-C33-C35	-2.36	119.78	126.42
12	7	617	II0	C03-C09-C13	-2.36	119.30	122.63
9	9	611	CLA	C1B-CHB-C4A	-2.36	125.45	130.12
9	9	603	CLA	C1-C2-C3	-2.35	122.94	126.75
11	8	616	IHT	C41-C40-C37	-2.35	118.65	123.47
12	P	612	II0	C37-C35-C39	-2.35	119.62	122.92
13	8	617	LMG	O2-C2-C1	-2.35	104.33	110.05
10	7	610	KC2	CHD-C4C-NC	2.35	127.77	124.20
12	0	615	II0	C08-C12-C14	-2.35	107.17	111.85
13	G	102	LMG	O3-C3-C2	-2.35	104.92	110.35
9	9	610	CLA	C1B-CHB-C4A	-2.35	125.47	130.12
14	P	613	II3	C31-C34-C37	-2.34	115.91	123.22
12	0	619	II0	C20-C14-C12	2.34	118.69	114.36
9	7	613	CLA	C1B-CHB-C4A	-2.34	125.49	130.12
9	p	313	CLA	C1B-CHB-C4A	-2.34	125.49	130.12
9	p	305	CLA	C1B-CHB-C4A	-2.34	125.49	130.12
12	7	616	II0	C31-C29-C25	-2.33	119.80	126.58
9	p	308	CLA	CHB-C4A-NA	2.33	127.74	124.51
9	7	604	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
9	9	607	CLA	C1B-CHB-C4A	-2.33	125.51	130.12
13	0	618	LMG	O2-C2-C1	-2.33	104.39	110.05
9	P	607	CLA	C1B-CHB-C4A	-2.33	125.51	130.12
12	0	619	II0	C18-C04-C10	-2.33	106.77	110.47
9	P	610	CLA	C1B-CHB-C4A	-2.32	125.51	130.12
12	P	612	II0	C31-C29-C25	-2.32	119.83	126.58
9	P	611	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
9	0	609	CLA	CHB-C4A-NA	2.32	127.72	124.51
9	9	609	CLA	C1B-CHB-C4A	-2.32	125.53	130.12
9	P	601	CLA	CHB-C4A-NA	2.31	127.70	124.51
9	8	611	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
9	p	310	CLA	C1B-CHB-C4A	-2.31	125.55	130.12
13	G	102	LMG	O1-C1-C2	-2.31	104.70	108.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	0	601	CLA	C1B-CHB-C4A	-2.31	125.55	130.12
9	p	303	CLA	CHB-C4A-NA	2.30	127.70	124.51
12	7	619	II0	C31-C29-C25	-2.30	119.89	126.58
9	0	613	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
14	7	615	II3	C22-C18-C17	2.30	118.62	114.36
9	7	602	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
9	0	606	CLA	CHB-C4A-NA	2.30	127.69	124.51
12	p	301	II0	C20-C14-C12	2.30	118.61	114.36
16	9	615	8CT	C30-C31-C32	-2.29	118.65	121.47
9	0	607	CLA	CHB-C4A-NA	2.29	127.68	124.51
9	9	603	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
9	7	604	CLA	O2D-CGD-CBD	2.29	115.34	111.27
9	p	311	CLA	CHB-C4A-NA	2.29	127.68	124.51
9	8	609	CLA	C1B-CHB-C4A	-2.29	125.59	130.12
9	s	303	CLA	C1B-CHB-C4A	-2.29	125.59	130.12
10	0	610	KC2	O1D-CGD-CBD	-2.28	119.81	124.48
11	p	318	IHT	C19-C10-C09	2.28	118.00	113.62
12	0	619	II0	C08-C12-C14	-2.28	107.31	111.85
16	9	615	8CT	C27-C26-C25	-2.28	119.73	122.92
9	P	602	CLA	C1-C2-C3	-2.28	122.10	126.04
9	P	603	CLA	O2A-CGA-O1A	-2.28	117.85	123.59
10	8	610	KC2	C1B-CHB-C4A	-2.28	121.15	126.06
13	8	617	LMG	O1-C7-C8	-2.28	105.41	110.90
14	7	615	II3	C39-C41-C40	-2.28	118.81	123.47
9	0	603	CLA	C1-C2-C3	-2.27	123.08	126.75
9	P	608	CLA	CAA-C2A-C3A	-2.27	110.80	116.10
9	P	608	CLA	CHB-C4A-NA	2.27	127.65	124.51
9	7	605	CLA	CHD-C1D-ND	-2.27	122.37	124.45
10	8	610	KC2	CHD-C4C-NC	2.27	127.65	124.20
14	P	613	II3	C22-C18-C17	2.27	118.55	114.36
9	0	609	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
12	p	315	II0	C19-C13-C11	2.26	118.55	114.36
9	7	609	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
9	P	608	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
9	P	603	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
12	7	616	II0	C31-C33-C35	-2.26	120.07	126.42
9	0	612	CLA	C1B-CHB-C4A	-2.26	125.65	130.12
13	8	617	LMG	O7-C10-O9	-2.25	118.25	123.70
9	p	307	CLA	CHB-C4A-NA	2.25	127.62	124.51
12	9	614	II0	C20-C14-C12	2.25	118.52	114.36
12	P	614	II0	C08-C12-C14	-2.25	107.38	111.85
11	0	617	IHT	C22-C18-C07	-2.24	120.90	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	0	614	IHT	C31-C29-C26	-2.24	120.07	126.58
9	p	307	CLA	C1B-CHB-C4A	-2.24	125.69	130.12
9	7	604	CLA	O2A-CGA-O1A	-2.24	117.95	123.59
15	s	301	LHG	C27-C26-C25	-2.24	103.08	114.42
12	7	617	II0	C31-C33-C35	-2.24	120.14	126.42
12	p	302	II0	C38-C36-C40	-2.23	119.79	122.92
12	9	613	II0	C41-C39-C35	-2.23	124.12	127.31
9	7	606	CLA	C1B-CHB-C4A	-2.23	125.70	130.12
13	8	617	LMG	O1-C1-C2	-2.23	104.83	108.30
10	0	610	KC2	O2D-CGD-O1D	-2.22	119.49	123.84
12	P	612	II0	C19-C13-C11	2.22	118.47	114.36
9	7	605	CLA	CHB-C4A-NA	2.22	127.59	124.51
11	0	614	IHT	C19-C10-C09	2.22	117.89	113.62
9	7	611	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
9	8	603	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
9	0	607	CLA	O2A-CGA-O1A	-2.22	117.77	123.30
9	p	308	CLA	C1B-CHB-C4A	-2.22	125.73	130.12
12	7	616	II0	C20-C14-C12	2.21	118.45	114.36
12	7	617	II0	C42-C41-C39	-2.21	118.95	123.47
12	p	315	II0	C41-C42-C40	-2.21	118.96	123.47
9	9	610	CLA	O2A-CGA-O1A	-2.20	117.81	123.30
12	9	614	II0	C19-C13-C11	2.20	118.44	114.36
10	P	609	KC2	C1A-C2A-C3A	-2.20	105.37	107.11
12	9	612	II0	C32-C30-C26	-2.20	120.19	126.58
10	0	610	KC2	C1B-CHB-C4A	-2.20	121.31	126.06
9	P	606	CLA	CAA-CBA-CGA	-2.20	106.67	112.51
9	9	606	CLA	CHB-C4A-NA	2.20	127.55	124.51
14	P	613	II3	C30-C28-C27	2.20	121.19	116.84
9	0	604	CLA	O2D-CGD-CBD	2.20	115.17	111.27
9	s	303	CLA	O2A-CGA-O1A	-2.19	118.05	123.59
12	8	615	II0	C19-C13-C09	-2.19	121.37	124.35
9	9	609	CLA	O2D-CGD-CBD	2.19	115.17	111.27
10	0	610	KC2	CBD-CHA-C1A	2.19	132.97	128.88
12	p	316	II0	C32-C30-C26	-2.19	120.22	126.58
10	p	312	KC2	C1B-CHB-C4A	-2.19	121.33	126.06
12	9	613	II0	C19-C13-C11	2.19	118.41	114.36
9	9	602	CLA	O2A-CGA-O1A	-2.19	118.07	123.59
10	p	312	KC2	O2D-CGD-O1D	-2.19	119.56	123.84
12	p	301	II0	C31-C33-C35	-2.19	120.27	126.42
16	P	615	8CT	C04-C03-C10	2.19	121.96	115.78
10	0	610	KC2	C1A-C2A-C3A	-2.19	105.38	107.11
11	0	617	IHT	C41-C40-C37	-2.18	119.00	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	9	601	CLA	C1B-CHB-C4A	-2.18	125.80	130.12
11	0	617	IHT	C39-C35-C38	-2.18	119.87	122.92
9	p	311	CLA	C1B-CHB-C4A	-2.18	125.80	130.12
11	0	617	IHT	C36-C33-C37	-2.18	119.87	122.92
17	p	319	SQD	C4-C3-C2	2.17	114.62	110.82
9	8	601	CLA	C1B-CHB-C4A	-2.17	125.82	130.12
12	8	613	II0	C19-C13-C11	2.17	118.38	114.36
9	7	608	CLA	C1B-CHB-C4A	-2.17	125.82	130.12
9	8	608	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
12	p	301	II0	C19-C13-C11	2.17	118.37	114.36
9	0	604	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
9	p	303	CLA	C1B-CHB-C4A	-2.17	125.83	130.12
9	8	605	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
9	p	304	CLA	CHD-C1D-ND	-2.16	122.47	124.45
9	0	608	CLA	CHD-C1D-ND	-2.15	122.47	124.45
10	p	312	KC2	CHB-C4A-C3A	-2.15	121.62	124.98
12	9	612	II0	C41-C42-C40	-2.15	119.08	123.47
13	0	618	LMG	O1-C1-C2	-2.15	104.95	108.30
12	0	615	II0	C38-C36-C40	-2.14	119.92	122.92
12	p	301	II0	C08-C12-C14	-2.14	107.59	111.85
9	8	602	CLA	O2D-CGD-CBD	2.14	115.07	111.27
12	p	302	II0	C31-C29-C25	-2.14	120.37	126.58
9	p	313	CLA	O2A-CGA-O1A	-2.14	117.97	123.30
9	8	603	CLA	O2A-CGA-O1A	-2.14	118.20	123.59
9	8	604	CLA	O2A-CGA-O1A	-2.14	118.20	123.59
12	p	315	II0	C37-C35-C39	-2.13	119.93	122.92
16	P	615	8CT	C39-C16-C17	-2.13	119.94	122.92
9	8	611	CLA	O2A-CGA-O1A	-2.13	117.99	123.30
9	s	302	CLA	CHB-C4A-NA	2.13	127.46	124.51
9	9	604	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
9	P	601	CLA	C1B-CHB-C4A	-2.13	125.91	130.12
12	p	316	II0	C29-C31-C33	-2.13	116.58	123.22
9	8	608	CLA	CHD-C1D-ND	-2.12	122.50	124.45
12	p	315	II0	C20-C14-C12	2.12	118.29	114.36
9	9	608	CLA	CMA-C3A-C2A	-2.12	111.14	116.10
12	0	616	II0	C32-C30-C26	-2.12	120.42	126.58
9	P	602	CLA	CHD-C1D-ND	-2.12	122.50	124.45
9	0	608	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
12	9	612	II0	C20-C14-C12	2.12	118.28	114.36
12	P	614	II0	C19-C13-C11	2.12	118.28	114.36
11	8	616	IHT	C22-C18-C07	-2.12	121.25	127.20
9	p	306	CLA	O2A-CGA-O1A	-2.12	118.25	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	9	612	II0	C19-C13-C11	2.12	118.28	114.36
11	8	616	IHT	C25-C23-C27	-2.12	119.96	122.92
9	7	602	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
11	7	618	IHT	C25-C23-C27	-2.11	119.96	122.92
12	8	613	II0	C41-C42-C40	-2.11	119.14	123.47
11	0	614	IHT	C31-C34-C35	-2.11	120.48	126.42
9	7	602	CLA	CHD-C1D-ND	-2.11	122.51	124.45
12	7	616	II0	C41-C42-C40	-2.11	119.15	123.47
9	P	604	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
12	8	613	II0	C20-C14-C12	2.11	118.26	114.36
10	8	610	KC2	CHB-C4A-C3A	-2.11	121.68	124.98
9	7	608	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
9	p	305	CLA	CHD-C1D-ND	-2.11	122.52	124.45
9	8	602	CLA	CHD-C1D-ND	-2.11	122.52	124.45
12	7	616	II0	C42-C41-C39	-2.11	119.16	123.47
9	0	603	CLA	C1B-CHB-C4A	-2.10	125.95	130.12
9	p	311	CLA	CMA-C3A-C2A	-2.10	111.19	116.10
12	7	619	II0	C19-C13-C11	2.10	118.25	114.36
9	p	310	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
12	9	613	II0	C20-C14-C12	2.10	118.25	114.36
9	P	606	CLA	CHD-C1D-ND	-2.10	122.53	124.45
14	7	615	II3	C25-C24-C21	2.09	121.38	118.08
12	7	616	II0	C32-C30-C26	-2.09	120.50	126.58
11	0	614	IHT	C22-C18-C07	-2.09	121.32	127.20
11	7	618	IHT	C39-C35-C38	-2.09	119.99	122.92
12	8	619	II0	C32-C30-C26	-2.09	120.52	126.58
9	0	609	CLA	CMA-C3A-C2A	-2.09	111.22	116.10
9	0	602	CLA	C1-C2-C3	-2.09	122.43	126.04
12	7	619	II0	C37-C35-C39	-2.09	120.00	122.92
9	p	307	CLA	CHD-C1D-ND	-2.09	122.54	124.45
11	p	318	IHT	C41-C40-C37	-2.09	119.20	123.47
13	0	618	LMG	C1-O6-C5	-2.09	109.59	113.69
14	P	613	II3	C42-C38-C37	2.09	121.36	118.08
13	G	102	LMG	O2-C2-C1	-2.08	104.98	110.05
11	7	618	IHT	C41-C40-C37	-2.08	119.20	123.47
9	8	603	CLA	CHD-C1D-ND	-2.08	122.54	124.45
9	p	307	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
10	P	605	KC2	O2D-CGD-O1D	-2.08	119.77	123.84
12	0	615	II0	C32-C30-C26	-2.08	120.55	126.58
9	p	304	CLA	C1-C2-C3	-2.08	122.45	126.04
10	P	609	KC2	C1B-CHB-C4A	-2.08	121.58	126.06
12	0	619	II0	C32-C30-C26	-2.07	120.56	126.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	7	618	IHT	C05-C08-C12	2.07	113.14	110.30
9	0	602	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
16	9	615	8CT	C40-C12-C13	-2.07	120.03	122.92
11	8	616	IHT	C20-C15-C12	2.07	118.18	114.36
9	0	607	CLA	CHD-C1D-ND	-2.06	122.56	124.45
9	p	304	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
10	P	609	KC2	C2A-C3A-C4A	2.06	108.02	106.49
9	P	606	CLA	CHB-C4A-NA	2.06	127.36	124.51
9	0	604	CLA	C1-C2-C3	-2.05	122.49	126.04
9	9	603	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
9	8	612	CLA	O2A-CGA-O1A	-2.05	118.18	123.30
12	7	617	II0	C20-C14-C12	2.05	118.16	114.36
12	p	315	II0	C32-C34-C36	-2.05	120.66	126.42
9	P	610	CLA	O2A-CGA-O1A	-2.05	118.19	123.30
9	0	612	CLA	O2A-CGA-O1A	-2.05	118.19	123.30
12	8	615	II0	C18-C04-C10	-2.05	107.21	110.47
12	0	619	II0	C06-C04-C10	2.04	113.75	109.62
9	P	610	CLA	O2D-CGD-CBD	2.04	114.89	111.27
9	P	602	CLA	O2D-CGD-CBD	2.04	114.89	111.27
9	7	605	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
12	8	613	II0	C37-C35-C39	-2.04	120.07	122.92
9	9	604	CLA	CHD-C1D-ND	-2.04	122.58	124.45
9	0	606	CLA	O2A-CGA-O1A	-2.03	118.23	123.30
9	0	603	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
9	7	607	CLA	O2A-CGA-O1A	-2.03	118.23	123.30
9	7	608	CLA	CHD-C1D-ND	-2.03	122.59	124.45
9	P	606	CLA	C2D-C1D-ND	-2.03	108.61	110.10
9	G	101	CLA	O2A-CGA-O1A	-2.03	118.24	123.30
9	8	605	CLA	CHD-C1D-ND	-2.03	122.59	124.45
12	0	615	II0	C32-C34-C36	-2.02	120.73	126.42
12	7	614	II0	C07-C11-C13	-2.02	107.83	111.85
9	7	613	CLA	O2A-CGA-O1A	-2.02	118.26	123.30
9	8	606	CLA	O2A-CGA-O1A	-2.02	118.27	123.30
12	p	302	II0	C31-C33-C35	-2.02	120.75	126.42
12	7	619	II0	C04-C06-C08	-2.02	109.09	113.64
12	8	614	II0	C19-C13-C11	2.02	118.09	114.36
11	0	614	IHT	C39-C35-C38	-2.01	120.10	122.92
11	8	616	IHT	C06-C09-C10	-2.01	110.48	114.08
9	p	308	CLA	O2A-CGA-O1A	-2.01	118.28	123.30
12	0	619	II0	C30-C32-C34	-2.01	116.94	123.22
9	p	309	CLA	O2A-CGA-O1A	-2.01	118.28	123.30
9	p	304	CLA	O2D-CGD-CBD	2.01	114.84	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	P	611	CLA	CHD-C1D-ND	-2.01	122.61	124.45
9	9	604	CLA	O2D-CGD-CBD	2.01	114.84	111.27
12	p	315	II0	C31-C33-C35	-2.01	120.77	126.42
10	0	610	KC2	O2A-CGA-O1A	-2.01	118.50	122.67
9	8	607	CLA	O2A-CGA-O1A	-2.01	118.30	123.30
16	P	615	8CT	C35-C30-C29	-2.00	110.17	112.70
9	0	613	CLA	O2A-CGA-O1A	-2.00	118.31	123.30
9	0	602	CLA	CHD-C1D-ND	-2.00	122.61	124.45
12	p	316	II0	C06-C08-C12	-2.00	107.56	110.30
9	0	605	CLA	CHD-C1D-ND	-2.00	122.62	124.45
9	9	611	CLA	O2A-CGA-O1A	-2.00	118.31	123.30

All (68) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
9	0	601	CLA	ND
9	0	602	CLA	ND
9	0	603	CLA	ND
9	0	604	CLA	ND
9	0	605	CLA	ND
9	0	606	CLA	ND
9	0	607	CLA	ND
9	0	608	CLA	ND
9	0	609	CLA	ND
9	0	611	CLA	ND
9	0	612	CLA	ND
9	0	613	CLA	ND
9	7	601	CLA	ND
9	7	602	CLA	ND
9	7	603	CLA	ND
9	7	604	CLA	ND
9	7	605	CLA	ND
9	7	606	CLA	ND
9	7	607	CLA	ND
9	7	608	CLA	ND
9	7	609	CLA	ND
9	7	611	CLA	ND
9	7	612	CLA	ND
9	7	613	CLA	ND
9	8	601	CLA	ND
9	8	602	CLA	ND
9	8	603	CLA	ND

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Mol	Chain	Res	Type	Atom
9	8	604	CLA	ND
9	8	605	CLA	ND
9	8	606	CLA	ND
9	8	607	CLA	ND
9	8	608	CLA	ND
9	8	609	CLA	ND
9	8	611	CLA	ND
9	8	612	CLA	ND
9	9	601	CLA	ND
9	9	602	CLA	ND
9	9	603	CLA	ND
9	9	604	CLA	ND
9	9	605	CLA	ND
9	9	606	CLA	ND
9	9	607	CLA	ND
9	9	608	CLA	ND
9	9	609	CLA	ND
9	9	610	CLA	ND
9	9	611	CLA	ND
9	G	101	CLA	ND
9	P	601	CLA	ND
9	P	602	CLA	ND
9	P	603	CLA	ND
9	P	604	CLA	ND
9	P	606	CLA	ND
9	P	607	CLA	ND
9	P	608	CLA	ND
9	P	610	CLA	ND
9	P	611	CLA	ND
9	p	303	CLA	ND
9	p	304	CLA	ND
9	p	305	CLA	ND
9	p	306	CLA	ND
9	p	307	CLA	ND
9	p	308	CLA	ND
9	p	309	CLA	ND
9	p	310	CLA	ND
9	p	311	CLA	ND
9	p	313	CLA	ND
9	p	314	CLA	ND
9	s	303	CLA	ND

All (638) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	0	602	CLA	C1A-C2A-CAA-CBA
9	0	602	CLA	C3A-C2A-CAA-CBA
9	0	602	CLA	CHA-CBD-CGD-O1D
9	0	602	CLA	CHA-CBD-CGD-O2D
9	0	603	CLA	C1A-C2A-CAA-CBA
9	0	605	CLA	CBD-CGD-O2D-CED
9	0	611	CLA	CHA-CBD-CGD-O1D
9	0	611	CLA	CHA-CBD-CGD-O2D
9	0	612	CLA	CBD-CGD-O2D-CED
9	7	602	CLA	C1A-C2A-CAA-CBA
9	7	602	CLA	C3A-C2A-CAA-CBA
9	7	602	CLA	CBD-CGD-O2D-CED
9	7	603	CLA	C1A-C2A-CAA-CBA
9	7	603	CLA	C3A-C2A-CAA-CBA
9	7	605	CLA	C1A-C2A-CAA-CBA
9	7	605	CLA	C3A-C2A-CAA-CBA
9	7	605	CLA	CBD-CGD-O2D-CED
9	7	606	CLA	C1A-C2A-CAA-CBA
9	7	606	CLA	C3A-C2A-CAA-CBA
9	7	607	CLA	C1A-C2A-CAA-CBA
9	7	607	CLA	C3A-C2A-CAA-CBA
9	7	611	CLA	CBD-CGD-O2D-CED
9	7	611	CLA	O1D-CGD-O2D-CED
9	7	612	CLA	CBD-CGD-O2D-CED
9	7	613	CLA	CBD-CGD-O2D-CED
9	8	602	CLA	C1A-C2A-CAA-CBA
9	8	602	CLA	C3A-C2A-CAA-CBA
9	8	602	CLA	CHA-CBD-CGD-O1D
9	8	602	CLA	CHA-CBD-CGD-O2D
9	8	603	CLA	C1A-C2A-CAA-CBA
9	8	603	CLA	C3A-C2A-CAA-CBA
9	8	603	CLA	CHA-CBD-CGD-O1D
9	8	603	CLA	CHA-CBD-CGD-O2D
9	8	611	CLA	C1A-C2A-CAA-CBA
9	8	611	CLA	C3A-C2A-CAA-CBA
9	8	611	CLA	CBD-CGD-O2D-CED
9	8	612	CLA	CBD-CGD-O2D-CED
9	9	601	CLA	CBD-CGD-O2D-CED
9	9	602	CLA	C1A-C2A-CAA-CBA
9	9	602	CLA	C3A-C2A-CAA-CBA
9	9	604	CLA	CHA-CBD-CGD-O1D
9	9	604	CLA	CHA-CBD-CGD-O2D
9	9	605	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
9	9	607	CLA	CBD-CGD-O2D-CED
9	9	610	CLA	CHA-CBD-CGD-O1D
9	9	610	CLA	CHA-CBD-CGD-O2D
9	G	101	CLA	C1A-C2A-CAA-CBA
9	G	101	CLA	CHA-CBD-CGD-O1D
9	G	101	CLA	CHA-CBD-CGD-O2D
9	P	602	CLA	C1A-C2A-CAA-CBA
9	P	602	CLA	C3A-C2A-CAA-CBA
9	P	610	CLA	CHA-CBD-CGD-O1D
9	P	610	CLA	CHA-CBD-CGD-O2D
9	p	304	CLA	C1A-C2A-CAA-CBA
9	p	304	CLA	C3A-C2A-CAA-CBA
9	p	306	CLA	CHA-CBD-CGD-O1D
9	p	306	CLA	CHA-CBD-CGD-O2D
9	p	307	CLA	C1A-C2A-CAA-CBA
9	p	307	CLA	C3A-C2A-CAA-CBA
9	p	307	CLA	CHA-CBD-CGD-O1D
9	p	307	CLA	CHA-CBD-CGD-O2D
9	p	307	CLA	CBD-CGD-O2D-CED
9	p	309	CLA	C1A-C2A-CAA-CBA
9	p	313	CLA	C1A-C2A-CAA-CBA
9	p	313	CLA	C3A-C2A-CAA-CBA
9	p	313	CLA	CHA-CBD-CGD-O1D
9	p	313	CLA	CHA-CBD-CGD-O2D
9	s	302	CLA	C1A-C2A-CAA-CBA
9	s	302	CLA	C3A-C2A-CAA-CBA
9	s	302	CLA	CBD-CGD-O2D-CED
10	0	610	KC2	C1A-C2A-CAA-CBA
10	0	610	KC2	C2B-C3B-CAB-CBB
10	0	610	KC2	C4B-C3B-CAB-CBB
10	0	610	KC2	C2C-C3C-CAC-CBC
10	0	610	KC2	C4C-C3C-CAC-CBC
10	0	610	KC2	C2A-CAA-CBA-CGA
10	0	610	KC2	CAA-CBA-CGA-O2A
10	7	610	KC2	C1A-C2A-CAA-CBA
10	7	610	KC2	C2B-C3B-CAB-CBB
10	7	610	KC2	C4B-C3B-CAB-CBB
10	7	610	KC2	CAA-CBA-CGA-O2A
10	7	610	KC2	CBD-CGD-O2D-CED
10	8	610	KC2	C1A-C2A-CAA-CBA
10	8	610	KC2	C3A-C2A-CAA-CBA
10	8	610	KC2	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
10	P	605	KC2	C1A-C2A-CAA-CBA
10	P	605	KC2	C2B-C3B-CAB-CBB
10	P	605	KC2	C4B-C3B-CAB-CBB
10	P	605	KC2	C2C-C3C-CAC-CBC
10	P	605	KC2	C4C-C3C-CAC-CBC
10	P	605	KC2	CBD-CGD-O2D-CED
10	P	609	KC2	C1A-C2A-CAA-CBA
10	P	609	KC2	C2B-C3B-CAB-CBB
10	P	609	KC2	C4B-C3B-CAB-CBB
10	P	609	KC2	C2C-C3C-CAC-CBC
10	P	609	KC2	C4C-C3C-CAC-CBC
10	P	609	KC2	CAA-CBA-CGA-O2A
10	p	312	KC2	C2B-C3B-CAB-CBB
10	p	312	KC2	C4B-C3B-CAB-CBB
10	p	312	KC2	C2C-C3C-CAC-CBC
10	p	312	KC2	C4C-C3C-CAC-CBC
11	0	614	IHT	C30-C32-C33-C36
11	0	614	IHT	C30-C32-C33-C37
11	0	617	IHT	C30-C32-C33-C36
11	0	617	IHT	C30-C32-C33-C37
11	0	617	IHT	C33-C37-C40-C41
12	0	619	II0	C26-C30-C32-C34
12	7	616	II0	C09-C21-C23-C25
12	7	617	II0	C31-C33-C35-C37
12	7	617	II0	C31-C33-C35-C39
12	9	614	II0	C31-C33-C35-C37
12	9	614	II0	C31-C33-C35-C39
12	P	614	II0	C31-C33-C35-C37
12	P	614	II0	C31-C33-C35-C39
12	p	301	II0	C31-C33-C35-C37
12	p	301	II0	C31-C33-C35-C39
12	p	316	II0	C09-C21-C23-C25
12	p	317	II0	C32-C34-C36-C38
12	p	317	II0	C32-C34-C36-C40
13	G	102	LMG	C11-C10-O7-C8
14	P	613	II3	C16-C23-C27-C28
15	8	618	LHG	O1-C1-C2-C3
15	8	618	LHG	O2-C2-C3-O3
15	s	301	LHG	C3-O3-P-O4
15	s	301	LHG	C4-O6-P-O5
15	s	301	LHG	O9-C7-O7-C5
15	s	301	LHG	C8-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
16	9	615	8CT	C12-C13-C14-C15
16	9	615	8CT	C22-C21-C23-C24
16	P	615	8CT	C04-C03-C10-C11
17	p	319	SQD	O5-C1-O6-C44
17	p	319	SQD	C8-C7-O47-C45
17	p	319	SQD	C5-C6-S-O7
17	p	319	SQD	C5-C6-S-O8
17	p	319	SQD	C5-C6-S-O9
9	0	611	CLA	O1D-CGD-O2D-CED
9	7	601	CLA	O1D-CGD-O2D-CED
9	7	613	CLA	O1D-CGD-O2D-CED
9	9	601	CLA	O1D-CGD-O2D-CED
9	9	607	CLA	O1D-CGD-O2D-CED
10	P	605	KC2	O1D-CGD-O2D-CED
9	0	605	CLA	O1D-CGD-O2D-CED
9	s	302	CLA	O1D-CGD-O2D-CED
10	7	610	KC2	O1D-CGD-O2D-CED
9	0	611	CLA	CBD-CGD-O2D-CED
9	0	613	CLA	CBD-CGD-O2D-CED
9	7	601	CLA	CBD-CGD-O2D-CED
9	8	609	CLA	CBD-CGD-O2D-CED
9	p	311	CLA	CBD-CGD-O2D-CED
9	p	313	CLA	CBD-CGD-O2D-CED
10	8	610	KC2	CBD-CGD-O2D-CED
9	p	307	CLA	O1D-CGD-O2D-CED
9	7	612	CLA	O1D-CGD-O2D-CED
9	8	612	CLA	O1D-CGD-O2D-CED
9	0	601	CLA	CBD-CGD-O2D-CED
9	0	608	CLA	CBD-CGD-O2D-CED
9	7	604	CLA	CBD-CGD-O2D-CED
9	7	606	CLA	CBD-CGD-O2D-CED
9	7	608	CLA	CBD-CGD-O2D-CED
9	8	601	CLA	CBD-CGD-O2D-CED
9	9	603	CLA	CBD-CGD-O2D-CED
9	P	606	CLA	CBD-CGD-O2D-CED
9	P	610	CLA	CBD-CGD-O2D-CED
9	P	611	CLA	CBD-CGD-O2D-CED
17	p	319	SQD	O10-C23-O48-C46
9	7	602	CLA	O1D-CGD-O2D-CED
9	7	605	CLA	O1D-CGD-O2D-CED
9	0	612	CLA	O1D-CGD-O2D-CED
9	8	611	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
13	G	102	LMG	O9-C10-O7-C8
17	p	319	SQD	O49-C7-O47-C45
9	0	602	CLA	C3-C5-C6-C7
9	9	609	CLA	C3-C5-C6-C7
9	8	608	CLA	CBD-CGD-O2D-CED
10	7	610	KC2	CAA-CBA-CGA-O1A
9	p	303	CLA	CBD-CGD-O2D-CED
9	p	310	CLA	CBD-CGD-O2D-CED
9	p	314	CLA	CBD-CGD-O2D-CED
9	s	303	CLA	C2A-CAA-CBA-CGA
9	s	303	CLA	C3-C5-C6-C7
17	p	319	SQD	C24-C23-O48-C46
9	p	313	CLA	O1D-CGD-O2D-CED
9	0	613	CLA	O1D-CGD-O2D-CED
10	0	610	KC2	CAA-CBA-CGA-O1A
10	P	609	KC2	CAA-CBA-CGA-O1A
9	7	607	CLA	CBD-CGD-O2D-CED
9	P	602	CLA	CBD-CGD-O2D-CED
9	0	604	CLA	C3-C5-C6-C7
9	8	602	CLA	CBD-CGD-O2D-CED
9	8	607	CLA	CBD-CGD-O2D-CED
9	9	610	CLA	CBD-CGD-O2D-CED
10	P	609	KC2	CBD-CGD-O2D-CED
9	8	609	CLA	O1D-CGD-O2D-CED
9	p	311	CLA	O1D-CGD-O2D-CED
10	8	610	KC2	CAA-CBA-CGA-O2A
9	0	613	CLA	C2A-CAA-CBA-CGA
15	s	301	LHG	C28-C29-C30-C31
13	G	102	LMG	O6-C1-O1-C7
9	p	305	CLA	CBA-CGA-O2A-C1
9	0	601	CLA	O1D-CGD-O2D-CED
10	8	610	KC2	CAA-CBA-CGA-O1A
9	7	608	CLA	O1D-CGD-O2D-CED
9	P	606	CLA	O1D-CGD-O2D-CED
9	P	610	CLA	O1D-CGD-O2D-CED
15	8	618	LHG	C1-C2-C3-O3
9	8	603	CLA	O1A-CGA-O2A-C1
9	p	305	CLA	O1A-CGA-O2A-C1
9	8	601	CLA	O1D-CGD-O2D-CED
9	0	605	CLA	CBA-CGA-O2A-C1
9	7	603	CLA	CBA-CGA-O2A-C1
9	8	603	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
9	s	303	CLA	CBA-CGA-O2A-C1
9	7	604	CLA	O1D-CGD-O2D-CED
11	0	617	IHT	C23-C27-C30-C32
17	p	319	SQD	C2-C1-O6-C44
9	0	608	CLA	O1D-CGD-O2D-CED
9	P	611	CLA	O1D-CGD-O2D-CED
9	0	611	CLA	C2A-CAA-CBA-CGA
12	7	616	II0	C31-C33-C35-C37
16	9	615	8CT	C14-C15-C16-C39
9	P	607	CLA	C8-C10-C11-C12
9	P	607	CLA	C10-C11-C12-C13
9	p	310	CLA	C8-C10-C11-C12
13	0	618	LMG	C10-C11-C12-C13
15	8	618	LHG	C23-C24-C25-C26
9	8	608	CLA	C8-C10-C11-C12
9	7	606	CLA	O1D-CGD-O2D-CED
10	8	610	KC2	O1D-CGD-O2D-CED
9	9	607	CLA	C10-C11-C12-C13
9	P	602	CLA	C6-C7-C8-C10
9	0	605	CLA	O1A-CGA-O2A-C1
9	s	303	CLA	O1A-CGA-O2A-C1
11	0	614	IHT	C23-C27-C30-C32
9	9	603	CLA	O1D-CGD-O2D-CED
9	7	603	CLA	O1A-CGA-O2A-C1
9	0	604	CLA	CBD-CGD-O2D-CED
13	0	618	LMG	O6-C1-O1-C7
9	p	306	CLA	C5-C6-C7-C8
9	0	602	CLA	C5-C6-C7-C8
9	7	608	CLA	C8-C10-C11-C12
9	s	303	CLA	C13-C15-C16-C17
15	s	301	LHG	C3-O3-P-O6
9	8	608	CLA	O1D-CGD-O2D-CED
9	p	304	CLA	CBD-CGD-O2D-CED
15	s	301	LHG	C23-C24-C25-C26
9	p	314	CLA	O1D-CGD-O2D-CED
9	0	602	CLA	C4-C3-C5-C6
9	P	611	CLA	C2A-CAA-CBA-CGA
9	p	307	CLA	CBA-CGA-O2A-C1
12	0	616	II0	C35-C39-C41-C42
12	0	616	II0	C36-C40-C42-C41
12	p	316	II0	C36-C40-C42-C41
12	p	317	II0	C26-C30-C32-C34

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Mol	Chain	Res	Type	Atoms
10	P	609	KC2	C2A-CAA-CBA-CGA
10	p	312	KC2	C2A-CAA-CBA-CGA
17	p	319	SQD	C44-C45-O47-C7
9	p	303	CLA	O1D-CGD-O2D-CED
9	p	310	CLA	O1D-CGD-O2D-CED
15	8	618	LHG	C24-C25-C26-C27
13	0	618	LMG	C28-C29-C30-C31
13	0	618	LMG	C2-C1-O1-C7
13	G	102	LMG	O7-C8-C9-O8
9	7	608	CLA	C11-C12-C13-C14
9	p	310	CLA	C11-C12-C13-C14
15	s	301	LHG	C24-C25-C26-C27
10	P	605	KC2	CAA-CBA-CGA-O1A
10	p	312	KC2	CAA-CBA-CGA-O2A
16	9	615	8CT	C14-C15-C16-C17
16	9	615	8CT	C20-C21-C23-C24
13	8	617	LMG	C14-C15-C16-C17
9	0	608	CLA	C11-C12-C13-C14
9	0	608	CLA	C11-C12-C13-C15
9	8	608	CLA	C10-C11-C12-C13
17	p	319	SQD	C11-C10-C9-C8
17	p	319	SQD	C7-C8-C9-C10
9	7	608	CLA	C10-C11-C12-C13
15	s	301	LHG	C27-C28-C29-C30
9	0	603	CLA	CBA-CGA-O2A-C1
15	s	301	LHG	C11-C10-C9-C8
9	0	603	CLA	C3A-C2A-CAA-CBA
9	9	603	CLA	C3A-C2A-CAA-CBA
9	P	603	CLA	C3A-C2A-CAA-CBA
9	p	305	CLA	C3A-C2A-CAA-CBA
9	p	307	CLA	C8-C10-C11-C12
15	s	301	LHG	C30-C31-C32-C33
17	p	319	SQD	C11-C12-C13-C14
9	p	310	CLA	C11-C12-C13-C15
9	p	305	CLA	CBD-CGD-O2D-CED
9	7	605	CLA	CBA-CGA-O2A-C1
10	p	312	KC2	CAA-CBA-CGA-O1A
15	8	618	LHG	O1-C1-C2-O2
9	p	307	CLA	O1A-CGA-O2A-C1
11	0	614	IHT	C02-C07-C18-C22
11	0	614	IHT	C10-C07-C18-C22
11	7	618	IHT	C02-C07-C18-C22

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Mol	Chain	Res	Type	Atoms
11	7	618	IHT	C10-C07-C18-C22
16	9	615	8CT	C04-C03-C10-C11
9	7	607	CLA	O1D-CGD-O2D-CED
9	8	602	CLA	CBA-CGA-O2A-C1
9	P	602	CLA	CBA-CGA-O2A-C1
9	p	304	CLA	CBA-CGA-O2A-C1
9	9	604	CLA	C5-C6-C7-C8
9	7	602	CLA	C4-C3-C5-C6
9	9	602	CLA	C4-C3-C5-C6
9	0	603	CLA	O1A-CGA-O2A-C1
9	7	605	CLA	O1A-CGA-O2A-C1
9	P	602	CLA	O1A-CGA-O2A-C1
9	7	602	CLA	C5-C6-C7-C8
9	7	608	CLA	C11-C12-C13-C15
9	p	314	CLA	C2A-CAA-CBA-CGA
9	P	602	CLA	O1D-CGD-O2D-CED
15	s	301	LHG	C25-C26-C27-C28
9	8	607	CLA	O1D-CGD-O2D-CED
13	8	617	LMG	C30-C31-C32-C33
10	7	610	KC2	C2C-C3C-CAC-CBC
9	8	608	CLA	C11-C12-C13-C15
9	9	607	CLA	C11-C12-C13-C15
9	0	608	CLA	C8-C10-C11-C12
9	9	610	CLA	O1D-CGD-O2D-CED
10	7	610	KC2	C4C-C3C-CAC-CBC
10	8	610	KC2	C4B-C3B-CAB-CBB
9	0	606	CLA	CBD-CGD-O2D-CED
9	8	602	CLA	O1A-CGA-O2A-C1
9	p	304	CLA	O1A-CGA-O2A-C1
17	p	319	SQD	O47-C45-C46-O48
13	0	618	LMG	O6-C5-C6-O5
9	8	602	CLA	O1D-CGD-O2D-CED
9	0	602	CLA	C2-C3-C5-C6
12	0	616	II0	C10-C22-C24-C26
12	8	615	II0	C09-C21-C23-C25
12	9	613	II0	C10-C22-C24-C26
12	9	614	II0	C09-C21-C23-C25
12	P	614	II0	C10-C22-C24-C26
12	p	316	II0	C10-C22-C24-C26
12	p	317	II0	C09-C21-C23-C25
9	P	602	CLA	C6-C7-C8-C9
9	s	303	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
9	p	306	CLA	C2A-CAA-CBA-CGA
9	0	612	CLA	C1A-C2A-CAA-CBA
9	7	612	CLA	C1A-C2A-CAA-CBA
9	8	612	CLA	C1A-C2A-CAA-CBA
9	9	603	CLA	C1A-C2A-CAA-CBA
9	9	605	CLA	C1A-C2A-CAA-CBA
9	9	610	CLA	C1A-C2A-CAA-CBA
9	9	611	CLA	C1A-C2A-CAA-CBA
9	P	603	CLA	C1A-C2A-CAA-CBA
9	p	305	CLA	C1A-C2A-CAA-CBA
9	p	314	CLA	C1A-C2A-CAA-CBA
9	8	608	CLA	C11-C12-C13-C14
15	8	618	LHG	C4-O6-P-O3
9	7	602	CLA	CBA-CGA-O2A-C1
9	7	602	CLA	C2-C3-C5-C6
13	G	103	LMG	O1-C7-C8-C9
15	s	301	LHG	C4-C5-C6-O8
9	0	602	CLA	C11-C12-C13-C14
9	0	602	CLA	CBA-CGA-O2A-C1
13	8	617	LMG	O6-C5-C6-O5
15	s	301	LHG	C32-C33-C34-C35
13	G	103	LMG	O6-C5-C6-O5
10	8	610	KC2	C2A-CAA-CBA-CGA
9	p	310	CLA	C10-C11-C12-C13
9	p	313	CLA	C2A-CAA-CBA-CGA
9	0	604	CLA	O1D-CGD-O2D-CED
9	7	604	CLA	C5-C6-C7-C8
13	G	102	LMG	O1-C7-C8-O7
9	P	602	CLA	C11-C12-C13-C14
9	0	602	CLA	O1A-CGA-O2A-C1
9	7	602	CLA	O1A-CGA-O2A-C1
9	p	304	CLA	C11-C10-C8-C7
9	p	307	CLA	C11-C10-C8-C7
9	s	303	CLA	C6-C7-C8-C10
9	p	306	CLA	C3-C5-C6-C7
9	8	605	CLA	C6-C7-C8-C9
9	9	609	CLA	C6-C7-C8-C9
9	P	602	CLA	C11-C10-C8-C9
9	p	307	CLA	C11-C10-C8-C9
9	s	303	CLA	C11-C12-C13-C14
9	8	604	CLA	C2A-CAA-CBA-CGA
9	9	604	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
16	9	615	8CT	C10-C11-C12-C40
13	0	618	LMG	C32-C33-C34-C35
13	G	103	LMG	C28-C29-C30-C31
9	9	602	CLA	CBA-CGA-O2A-C1
13	8	617	LMG	C29-C28-O8-C9
9	9	603	CLA	CBA-CGA-O2A-C1
9	9	610	CLA	C3A-C2A-CAA-CBA
9	G	101	CLA	C3A-C2A-CAA-CBA
9	p	309	CLA	C3A-C2A-CAA-CBA
13	0	618	LMG	O1-C7-C8-C9
13	8	617	LMG	O1-C7-C8-C9
13	8	617	LMG	C7-C8-C9-O8
13	G	102	LMG	O1-C7-C8-C9
13	G	102	LMG	C7-C8-C9-O8
17	p	319	SQD	C44-C45-C46-O48
9	7	602	CLA	C11-C12-C13-C14
9	0	604	CLA	C5-C6-C7-C8
13	G	103	LMG	C29-C30-C31-C32
13	G	103	LMG	C29-C28-O8-C9
15	s	301	LHG	C31-C32-C33-C34
13	8	617	LMG	O1-C7-C8-O7
13	G	103	LMG	O1-C7-C8-O7
15	s	301	LHG	O7-C5-C6-O8
9	9	607	CLA	C11-C12-C13-C14
13	8	617	LMG	C32-C33-C34-C35
9	7	603	CLA	C2-C1-O2A-CGA
9	8	605	CLA	C2-C1-O2A-CGA
9	p	304	CLA	O1D-CGD-O2D-CED
15	s	301	LHG	C26-C27-C28-C29
9	0	601	CLA	C1A-C2A-CAA-CBA
9	8	601	CLA	C1A-C2A-CAA-CBA
9	9	601	CLA	C1A-C2A-CAA-CBA
9	p	303	CLA	C1A-C2A-CAA-CBA
12	7	616	II0	C31-C33-C35-C39
9	p	305	CLA	O1D-CGD-O2D-CED
9	0	606	CLA	O1D-CGD-O2D-CED
9	8	605	CLA	C6-C7-C8-C10
9	8	605	CLA	C11-C10-C8-C7
9	9	609	CLA	C6-C7-C8-C10
9	P	602	CLA	C11-C10-C8-C7
9	s	303	CLA	C11-C12-C13-C15
9	0	608	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
12	8	619	II0	C26-C30-C32-C34
9	0	603	CLA	CAD-CBD-CGD-O2D
9	0	606	CLA	CAD-CBD-CGD-O2D
9	7	603	CLA	CAD-CBD-CGD-O2D
9	7	607	CLA	CAD-CBD-CGD-O2D
9	P	603	CLA	CAD-CBD-CGD-O2D
9	p	311	CLA	CAD-CBD-CGD-O2D
9	0	604	CLA	C2A-CAA-CBA-CGA
10	0	610	KC2	CBD-CGD-O2D-CED
9	0	605	CLA	CHA-CBD-CGD-O1D
9	0	605	CLA	CHA-CBD-CGD-O2D
9	7	613	CLA	CHA-CBD-CGD-O1D
9	8	608	CLA	CHA-CBD-CGD-O1D
9	8	611	CLA	CHA-CBD-CGD-O1D
9	8	611	CLA	CHA-CBD-CGD-O2D
9	p	304	CLA	CHA-CBD-CGD-O1D
9	p	304	CLA	CHA-CBD-CGD-O2D
9	p	305	CLA	CHA-CBD-CGD-O1D
10	7	610	KC2	CHA-CBD-CGD-O2D
10	P	609	KC2	CHA-CBD-CGD-O1D
10	p	312	KC2	CHA-CBD-CGD-O2D
9	9	602	CLA	O1A-CGA-O2A-C1
9	9	603	CLA	O1A-CGA-O2A-C1
11	8	616	IHT	C11-C21-C24-C26
12	0	616	II0	C09-C21-C23-C25
12	7	616	II0	C10-C22-C24-C26
12	7	617	II0	C09-C21-C23-C25
12	7	617	II0	C10-C22-C24-C26
12	7	619	II0	C09-C21-C23-C25
12	7	619	II0	C10-C22-C24-C26
12	8	615	II0	C10-C22-C24-C26
12	9	612	II0	C09-C21-C23-C25
12	9	612	II0	C10-C22-C24-C26
12	9	614	II0	C10-C22-C24-C26
12	p	302	II0	C09-C21-C23-C25
12	p	315	II0	C10-C22-C24-C26
14	7	615	II3	C16-C23-C27-C28
9	8	605	CLA	C11-C10-C8-C9
9	8	605	CLA	C8-C10-C11-C12
9	7	604	CLA	C2A-CAA-CBA-CGA
13	G	102	LMG	O10-C28-O8-C9
16	P	615	8CT	C10-C11-C12-C40

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Mol	Chain	Res	Type	Atoms
16	9	615	8CT	C10-C11-C12-C13
16	P	615	8CT	C10-C11-C12-C13
11	0	617	IHT	C35-C38-C41-C40
15	8	618	LHG	C3-O3-P-O6
9	9	602	CLA	C2-C3-C5-C6
15	8	618	LHG	C3-O3-P-O4
15	8	618	LHG	C4-O6-P-O5
9	9	605	CLA	C2A-CAA-CBA-CGA
9	0	604	CLA	C6-C7-C8-C10
9	8	603	CLA	CAD-CBD-CGD-O1D
9	p	305	CLA	CAD-CBD-CGD-O1D
15	8	618	LHG	O6-C4-C5-C6
9	8	602	CLA	C11-C10-C8-C7
9	9	609	CLA	C11-C10-C8-C7
9	7	603	CLA	CBD-CGD-O2D-CED
9	P	604	CLA	C2A-CAA-CBA-CGA
9	9	605	CLA	CAA-CBA-CGA-O2A
13	0	618	LMG	O1-C7-C8-O7
13	8	617	LMG	O7-C8-C9-O8
9	s	303	CLA	C10-C11-C12-C13
9	8	602	CLA	C2A-CAA-CBA-CGA
9	P	602	CLA	C2A-CAA-CBA-CGA
9	p	305	CLA	C2-C1-O2A-CGA
15	s	301	LHG	C4-O6-P-O3
9	8	602	CLA	C11-C10-C8-C9
9	9	609	CLA	C11-C10-C8-C9
9	p	304	CLA	C11-C10-C8-C9
9	7	606	CLA	C4C-C3C-CAC-CBC
9	7	606	CLA	C2C-C3C-CAC-CBC
13	G	102	LMG	C29-C28-O8-C9
9	P	604	CLA	C5-C6-C7-C8
9	G	101	CLA	C2A-CAA-CBA-CGA
9	p	306	CLA	C3A-C2A-CAA-CBA
9	0	611	CLA	CAA-CBA-CGA-O1A
9	7	603	CLA	O1D-CGD-O2D-CED
9	8	605	CLA	CAA-CBA-CGA-O2A
12	p	317	II0	C10-C22-C24-C26
9	s	303	CLA	C12-C13-C15-C16
9	7	613	CLA	CAA-CBA-CGA-O1A
17	p	319	SQD	O48-C23-C24-C25
9	0	605	CLA	CAA-CBA-CGA-O2A
9	P	610	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
9	P	610	CLA	CAA-CBA-CGA-O2A
9	9	607	CLA	C2A-CAA-CBA-CGA
10	0	610	KC2	C3A-C2A-CAA-CBA
10	7	610	KC2	C3A-C2A-CAA-CBA
10	P	605	KC2	C3A-C2A-CAA-CBA
10	P	609	KC2	C3A-C2A-CAA-CBA
10	p	312	KC2	C3A-C2A-CAA-CBA
9	P	604	CLA	C6-C7-C8-C10
9	0	611	CLA	CAA-CBA-CGA-O2A
9	9	611	CLA	O1D-CGD-O2D-CED
9	0	608	CLA	C10-C11-C12-C13
9	7	602	CLA	C3-C5-C6-C7
13	0	618	LMG	C29-C30-C31-C32
9	7	613	CLA	CAA-CBA-CGA-O2A
9	9	602	CLA	C2A-CAA-CBA-CGA
9	9	611	CLA	CBD-CGD-O2D-CED
9	p	313	CLA	C2C-C3C-CAC-CBC
9	P	611	CLA	CAA-CBA-CGA-O1A
12	7	616	II0	C26-C30-C32-C34
12	p	316	II0	C25-C29-C31-C33
17	p	319	SQD	C45-C44-O6-C1
9	7	611	CLA	CAA-CBA-CGA-O2A
9	P	607	CLA	C11-C12-C13-C15
17	p	319	SQD	C9-C10-C11-C12
9	7	607	CLA	CAA-CBA-CGA-O2A
9	9	610	CLA	C2A-CAA-CBA-CGA
17	p	319	SQD	C12-C13-C14-C15
9	8	612	CLA	CAA-CBA-CGA-O2A
9	8	605	CLA	C11-C12-C13-C15
9	7	611	CLA	CAA-CBA-CGA-O1A
9	0	612	CLA	CAA-CBA-CGA-O2A
9	7	607	CLA	CAA-CBA-CGA-O1A
9	7	612	CLA	CAA-CBA-CGA-O2A
9	0	606	CLA	CAA-CBA-CGA-O2A
9	0	613	CLA	CAD-CBD-CGD-O2D
9	7	609	CLA	CAD-CBD-CGD-O2D
9	8	601	CLA	CAD-CBD-CGD-O2D
9	8	607	CLA	CAD-CBD-CGD-O2D
9	8	612	CLA	CAD-CBD-CGD-O2D
9	9	606	CLA	CAD-CBD-CGD-O2D
9	9	608	CLA	CAD-CBD-CGD-O2D
9	P	606	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
9	s	302	CLA	CAD-CBD-CGD-O2D
10	P	605	KC2	CAD-CBD-CGD-O2D
9	7	602	CLA	C2A-CAA-CBA-CGA
9	0	613	CLA	CAA-CBA-CGA-O2A
9	p	309	CLA	CAA-CBA-CGA-O2A
9	p	306	CLA	CAA-CBA-CGA-O2A
9	9	602	CLA	C11-C12-C13-C14
12	8	615	II0	C32-C34-C36-C40
9	0	613	CLA	CAA-CBA-CGA-O1A
9	9	609	CLA	O2A-C1-C2-C3
9	0	612	CLA	CAA-CBA-CGA-O1A
9	0	601	CLA	CHA-CBD-CGD-O1D
9	0	601	CLA	CHA-CBD-CGD-O2D
9	0	608	CLA	CHA-CBD-CGD-O1D
9	0	608	CLA	CHA-CBD-CGD-O2D
9	0	609	CLA	CHA-CBD-CGD-O1D
9	0	609	CLA	CHA-CBD-CGD-O2D
9	7	606	CLA	CHA-CBD-CGD-O1D
9	7	608	CLA	CHA-CBD-CGD-O1D
9	7	608	CLA	CHA-CBD-CGD-O2D
9	7	611	CLA	CHA-CBD-CGD-O1D
9	7	611	CLA	CHA-CBD-CGD-O2D
9	7	613	CLA	CHA-CBD-CGD-O2D
9	8	605	CLA	CHA-CBD-CGD-O1D
9	8	605	CLA	CHA-CBD-CGD-O2D
9	8	608	CLA	CHA-CBD-CGD-O2D
9	9	602	CLA	CHA-CBD-CGD-O1D
9	9	602	CLA	CHA-CBD-CGD-O2D
9	9	605	CLA	CHA-CBD-CGD-O1D
9	9	611	CLA	CHA-CBD-CGD-O1D
9	P	602	CLA	CHA-CBD-CGD-O1D
9	P	602	CLA	CHA-CBD-CGD-O2D
9	P	607	CLA	CHA-CBD-CGD-O1D
9	P	607	CLA	CHA-CBD-CGD-O2D
9	p	303	CLA	CHA-CBD-CGD-O1D
9	p	303	CLA	CHA-CBD-CGD-O2D
9	p	305	CLA	CHA-CBD-CGD-O2D
9	p	308	CLA	CHA-CBD-CGD-O2D
9	p	310	CLA	CHA-CBD-CGD-O1D
9	p	310	CLA	CHA-CBD-CGD-O2D
9	p	314	CLA	CHA-CBD-CGD-O1D
9	s	303	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
9	s	303	CLA	CHA-CBD-CGD-O2D
10	0	610	KC2	CHA-CBD-CGD-O1D
10	P	609	KC2	CHA-CBD-CGD-O2D
10	p	312	KC2	CHA-CBD-CGD-O1D
9	7	606	CLA	CAA-CBA-CGA-O2A
9	0	606	CLA	CAA-CBA-CGA-O1A
9	7	612	CLA	CAA-CBA-CGA-O1A
9	8	612	CLA	CAA-CBA-CGA-O1A
9	p	309	CLA	CAA-CBA-CGA-O1A
9	s	303	CLA	CAA-CBA-CGA-O2A
13	0	618	LMG	C15-C16-C17-C18
9	p	308	CLA	O1D-CGD-O2D-CED
9	p	304	CLA	C11-C12-C13-C14
9	P	611	CLA	CAA-CBA-CGA-O2A
9	P	606	CLA	C1A-C2A-CAA-CBA
9	p	306	CLA	C1A-C2A-CAA-CBA
9	p	307	CLA	CAA-CBA-CGA-O2A
9	p	310	CLA	C2A-CAA-CBA-CGA
15	s	301	LHG	O10-C23-C24-C25
9	8	606	CLA	CAA-CBA-CGA-O2A
13	8	617	LMG	O9-C10-C11-C12
9	P	604	CLA	CAA-CBA-CGA-O2A
9	p	308	CLA	CAA-CBA-CGA-O2A
9	p	304	CLA	C2A-CAA-CBA-CGA
9	p	306	CLA	CAA-CBA-CGA-O1A
9	7	606	CLA	CAA-CBA-CGA-O1A
9	G	101	CLA	CAA-CBA-CGA-O2A
15	s	301	LHG	C29-C30-C31-C32
9	7	613	CLA	CAD-CBD-CGD-O1D
9	8	605	CLA	CAD-CBD-CGD-O1D
9	p	303	CLA	CAD-CBD-CGD-O1D
9	s	303	CLA	CAA-CBA-CGA-O1A
9	8	604	CLA	CAA-CBA-CGA-O2A
9	9	604	CLA	CAA-CBA-CGA-O2A
13	G	103	LMG	O8-C28-C29-C30
9	p	308	CLA	CAA-CBA-CGA-O1A
9	7	601	CLA	C3A-C2A-CAA-CBA
9	9	602	CLA	C11-C10-C8-C7
16	9	615	8CT	C28-C29-C30-C31
16	P	615	8CT	C28-C29-C30-C31
9	8	606	CLA	CAA-CBA-CGA-O1A
12	0	619	II0	C32-C34-C36-C40

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Mol	Chain	Res	Type	Atoms
9	7	604	CLA	CAA-CBA-CGA-O2A
9	9	604	CLA	CAA-CBA-CGA-O1A
9	0	604	CLA	CAA-CBA-CGA-O2A
9	9	609	CLA	CAA-CBA-CGA-O2A
9	p	307	CLA	CAA-CBA-CGA-O1A
9	G	101	CLA	CAA-CBA-CGA-O1A
9	8	604	CLA	CAA-CBA-CGA-O1A

There are no ring outliers.

48 monomers are involved in 78 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	P	610	CLA	1	0
9	P	607	CLA	1	0
9	9	604	CLA	1	0
9	P	611	CLA	2	0
9	7	612	CLA	2	0
9	0	608	CLA	4	0
13	8	617	LMG	2	0
9	7	603	CLA	3	0
9	9	607	CLA	4	0
9	7	602	CLA	4	0
9	0	612	CLA	2	0
12	8	614	II0	1	0
9	9	602	CLA	1	0
9	8	606	CLA	4	0
9	8	611	CLA	1	0
9	7	608	CLA	1	0
9	0	613	CLA	1	0
9	G	101	CLA	2	0
9	7	605	CLA	3	0
12	7	614	II0	1	0
12	8	619	II0	1	0
9	0	601	CLA	1	0
9	7	607	CLA	2	0
9	9	609	CLA	1	0
9	9	610	CLA	1	0
9	0	605	CLA	1	0
9	7	613	CLA	1	0
9	9	606	CLA	2	0
9	0	604	CLA	1	0
9	0	607	CLA	4	0

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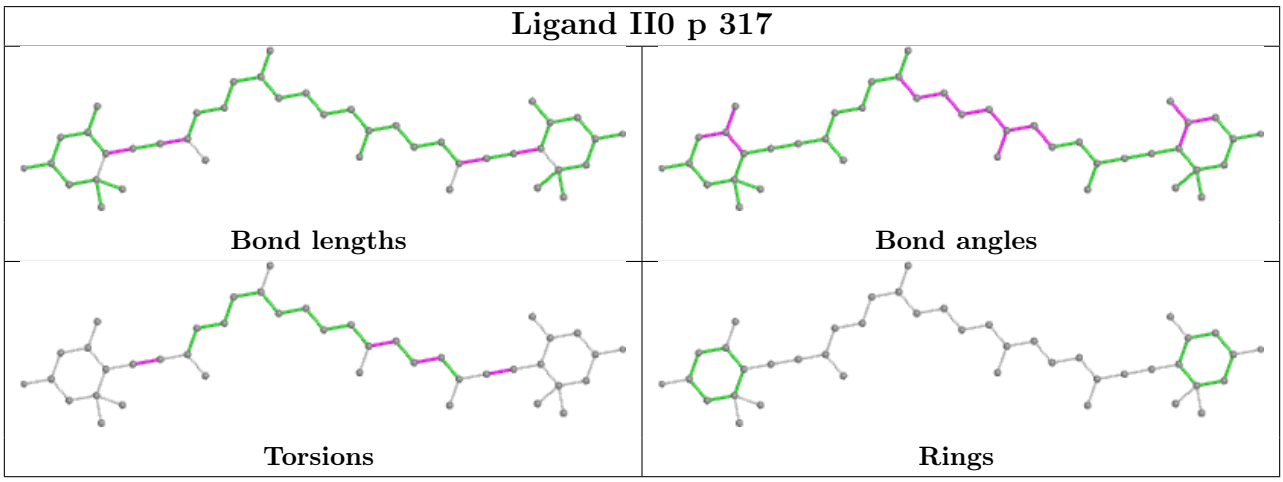
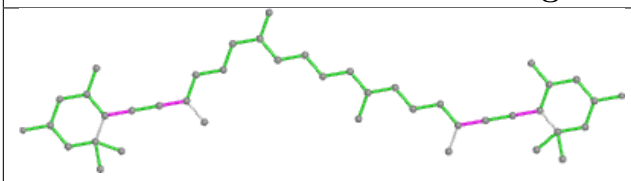
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	8	604	CLA	1	0
12	8	613	II0	1	0
9	P	604	CLA	1	0
9	8	609	CLA	1	0
9	7	604	CLA	1	0
9	8	603	CLA	3	0
12	0	616	II0	1	0
9	0	602	CLA	2	0
9	8	602	CLA	2	0
9	0	603	CLA	2	0
9	8	605	CLA	2	0
9	8	607	CLA	3	0
9	9	605	CLA	1	0
9	7	606	CLA	3	0
9	P	602	CLA	2	0
9	8	608	CLA	3	0
9	7	611	CLA	4	0
9	P	606	CLA	3	0

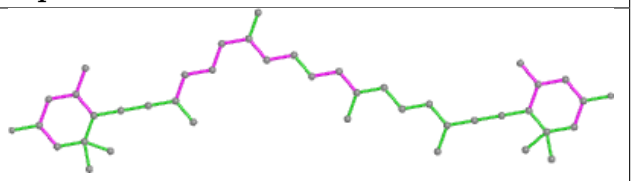
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



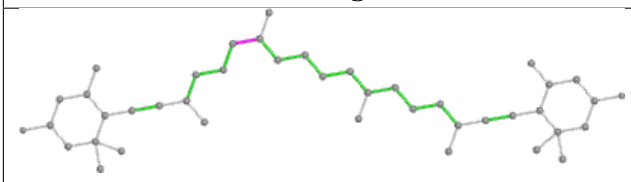
Ligand II0 p 301



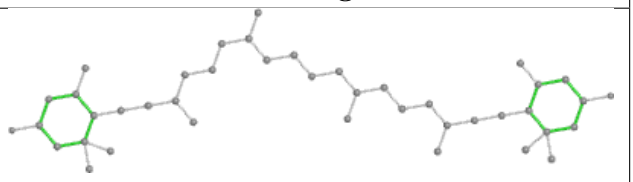
Bond lengths



Bond angles

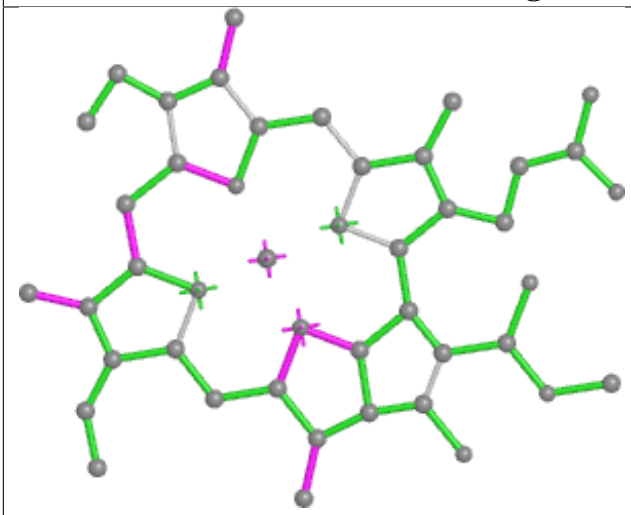


Torsions

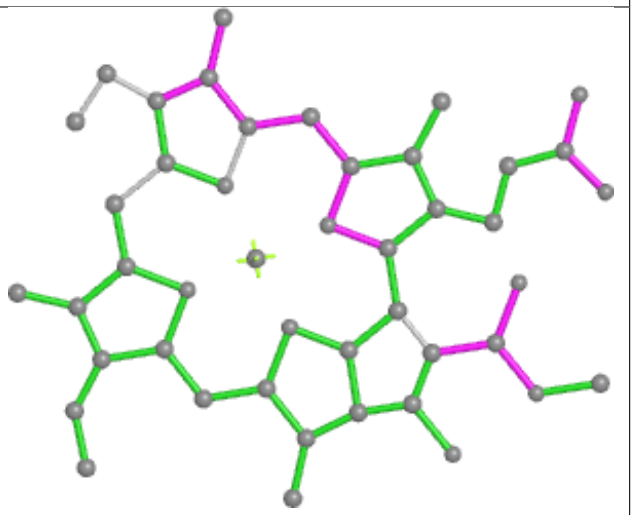


Rings

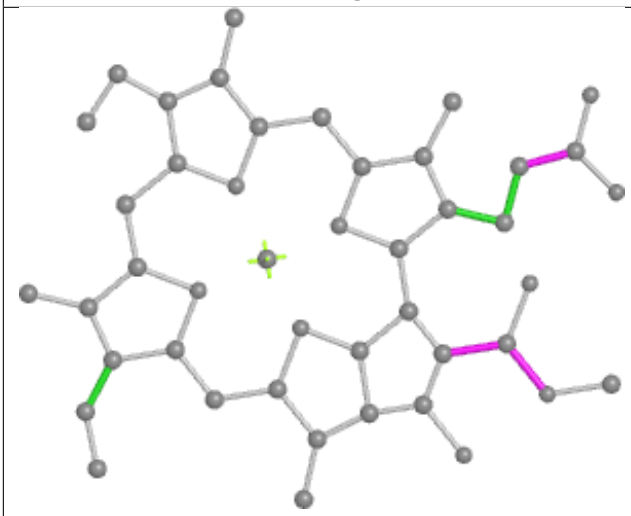
Ligand CLA P 610



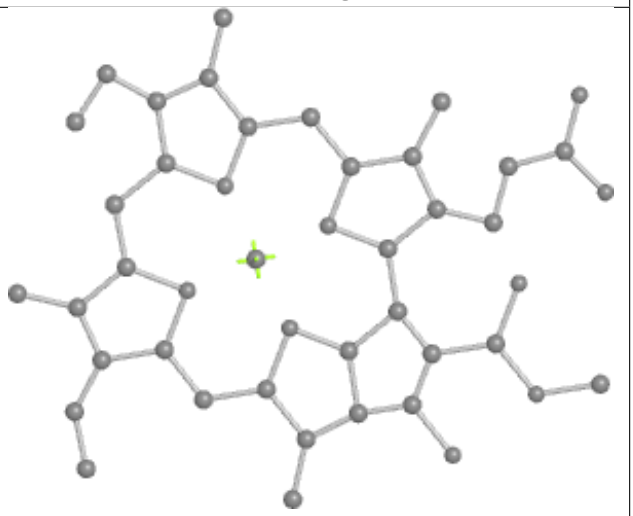
Bond lengths



Bond angles

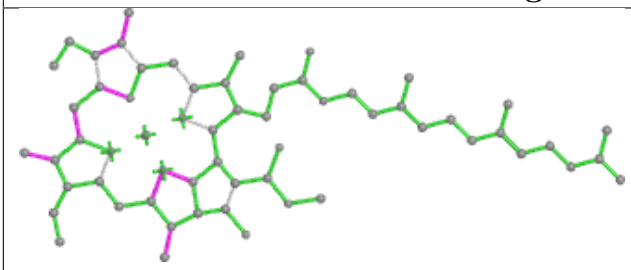


Torsions

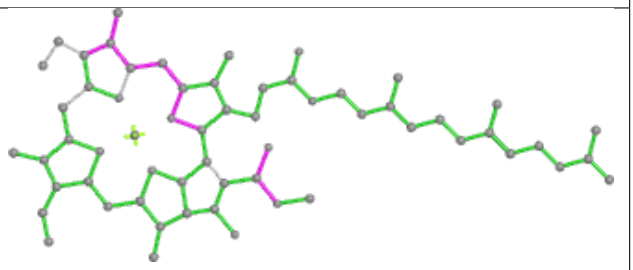


Rings

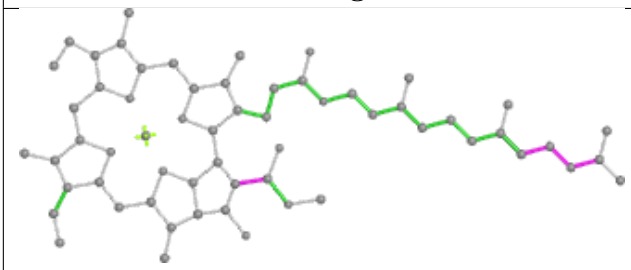
Ligand CLA P 607



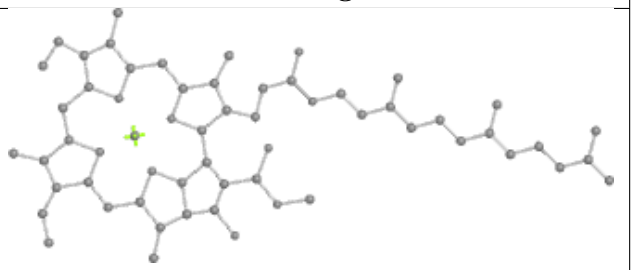
Bond lengths



Bond angles

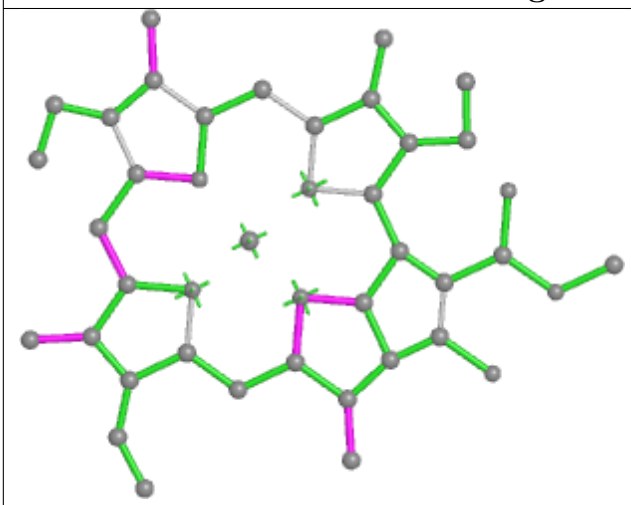


Torsions

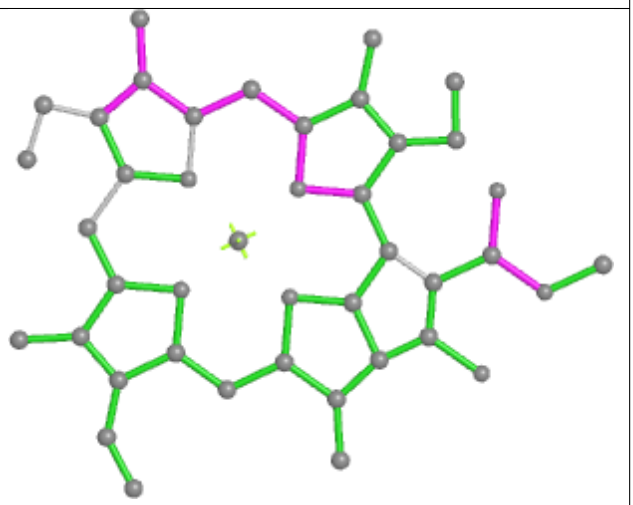


Rings

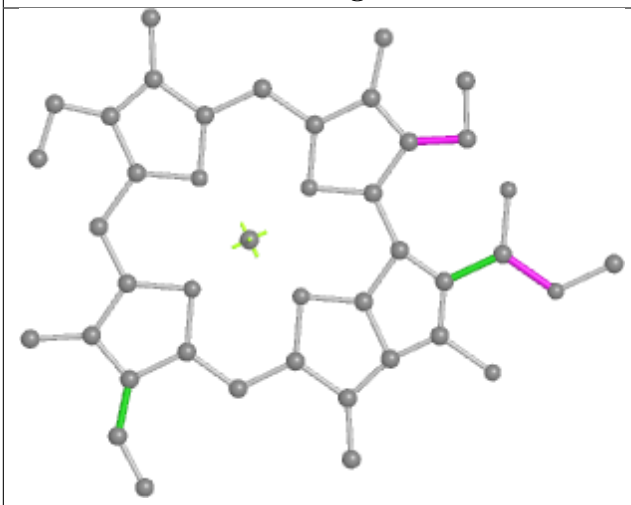
Ligand CLA 9 601



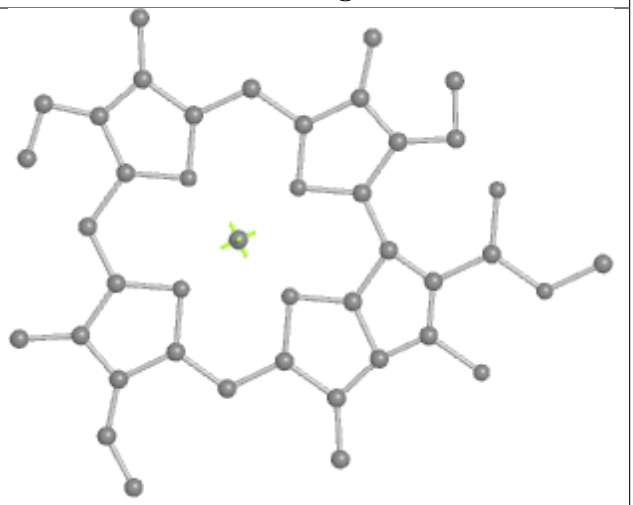
Bond lengths



Bond angles

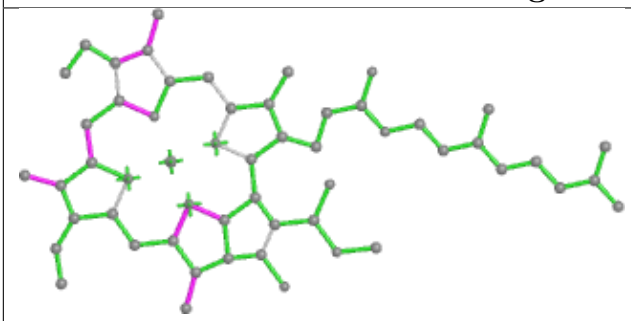


Torsions

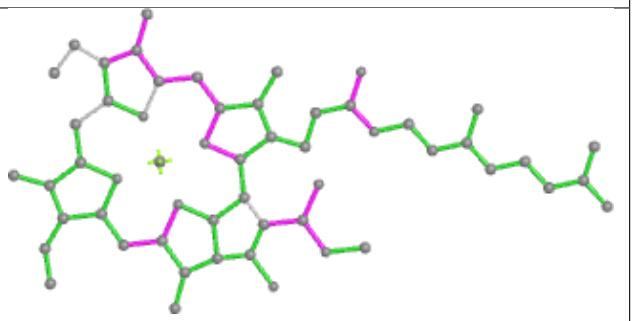


Rings

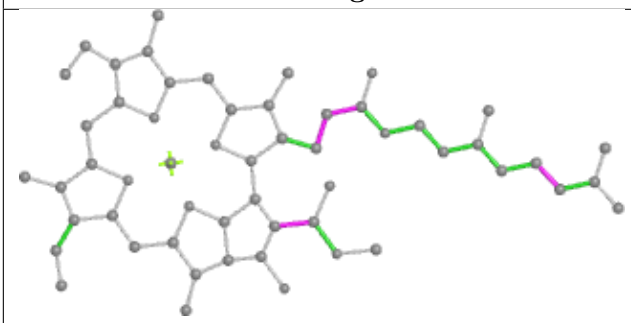
Ligand CLA 9 604



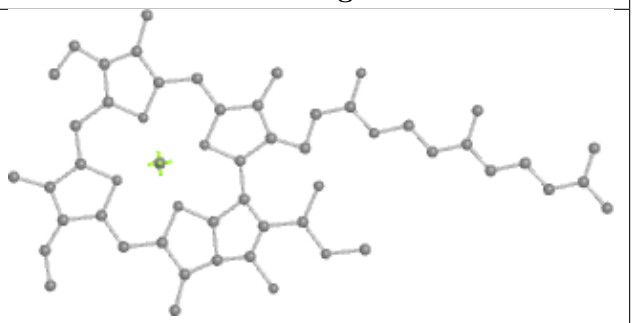
Bond lengths



Bond angles

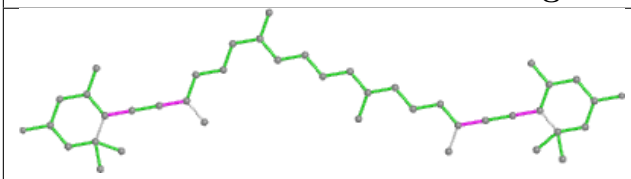


Torsions

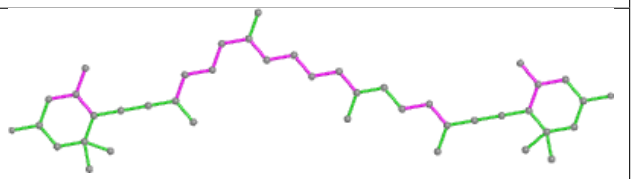


Rings

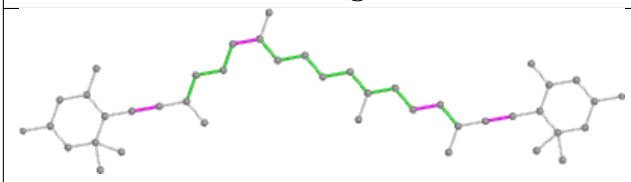
Ligand II0 7 616



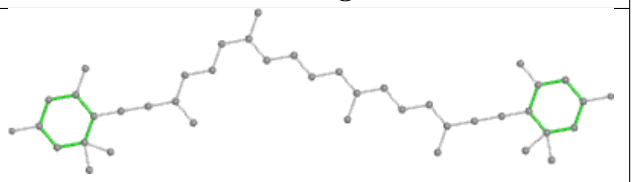
Bond lengths



Bond angles

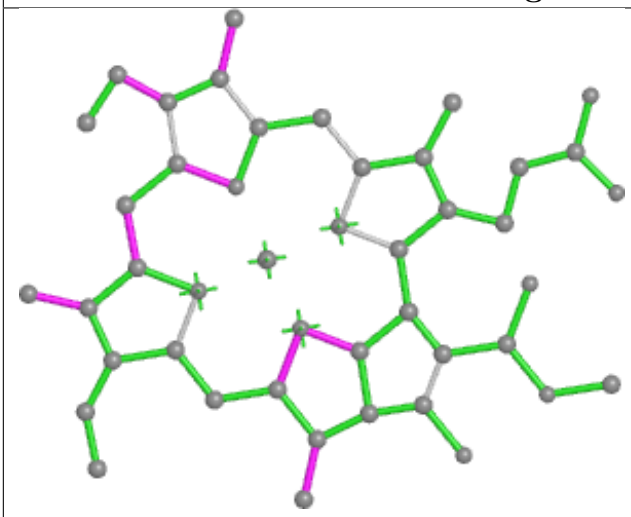


Torsions

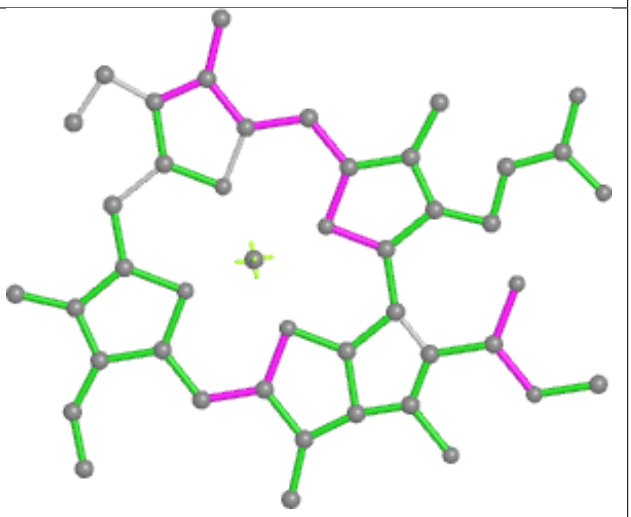


Rings

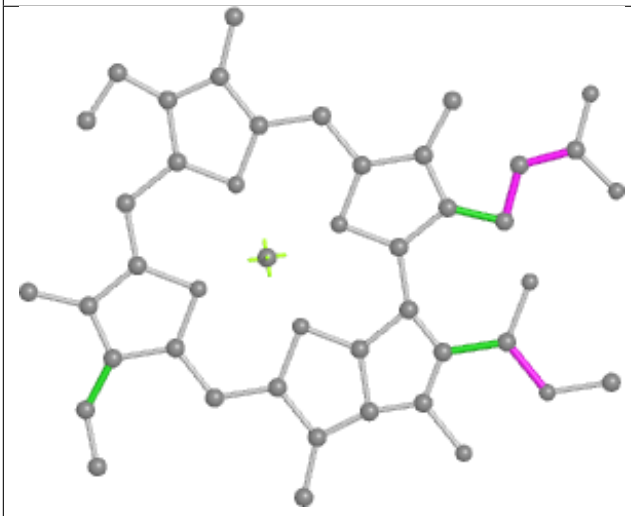
Ligand CLA P 611



Bond lengths



Bond angles



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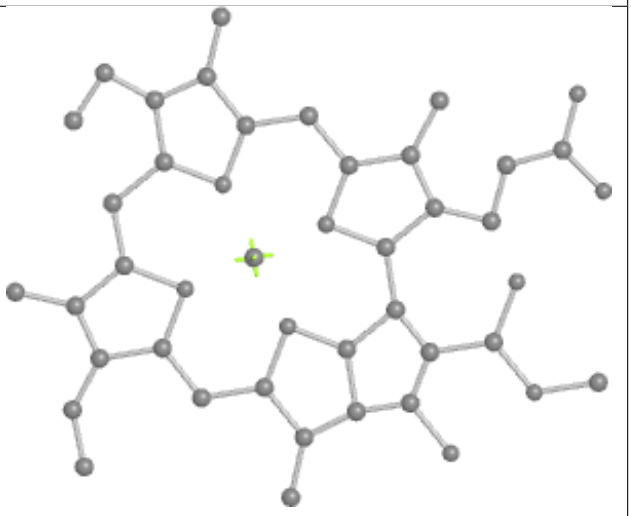
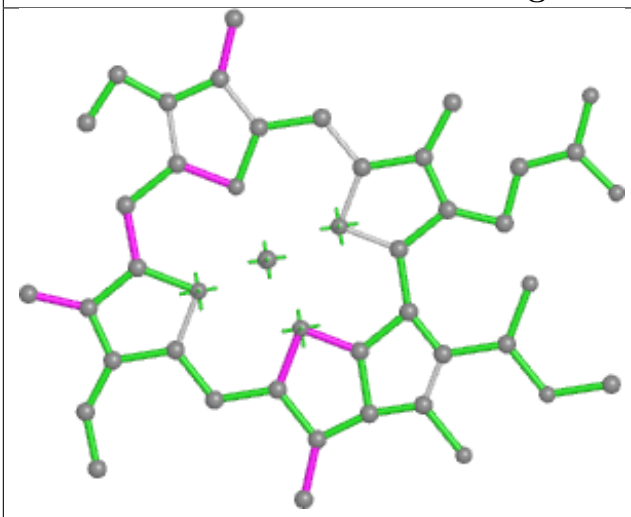


Rings

Ligand CLA 7 612



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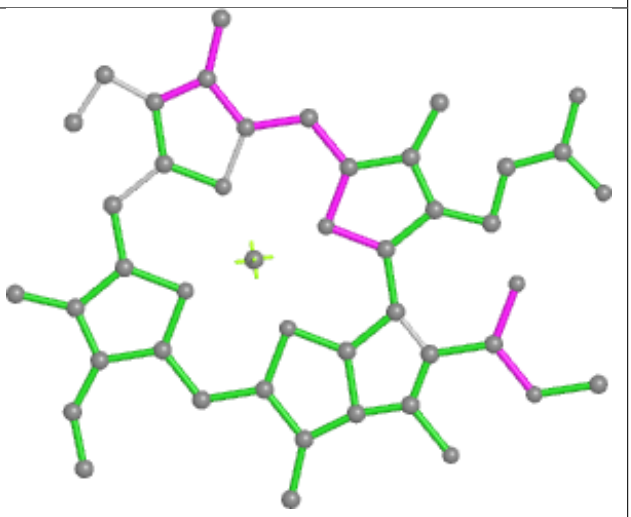
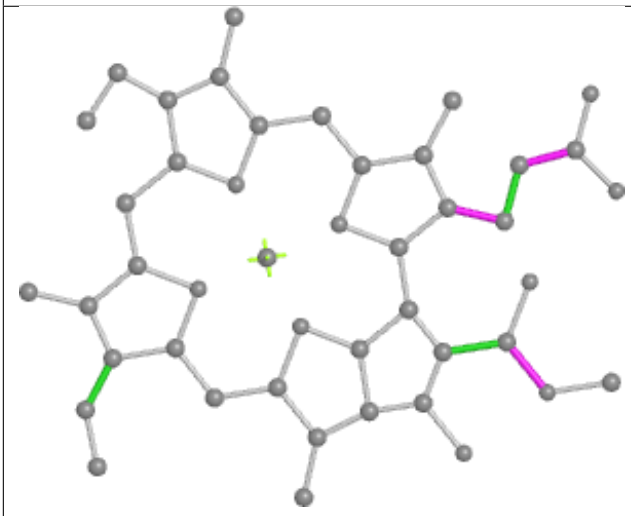


Bond angles



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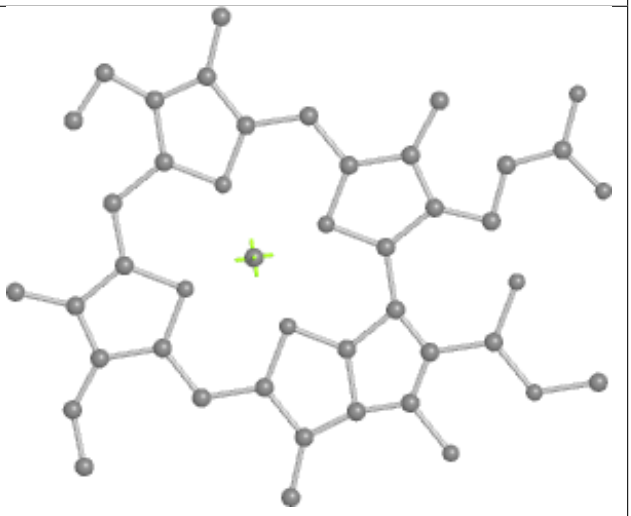
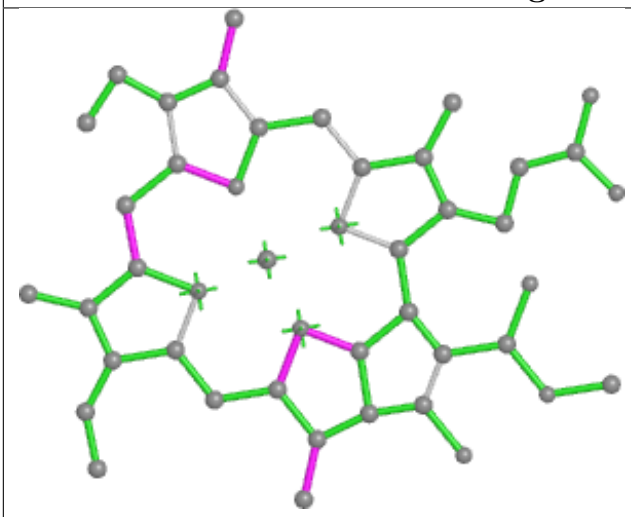


Rings

Ligand CLA 0 606



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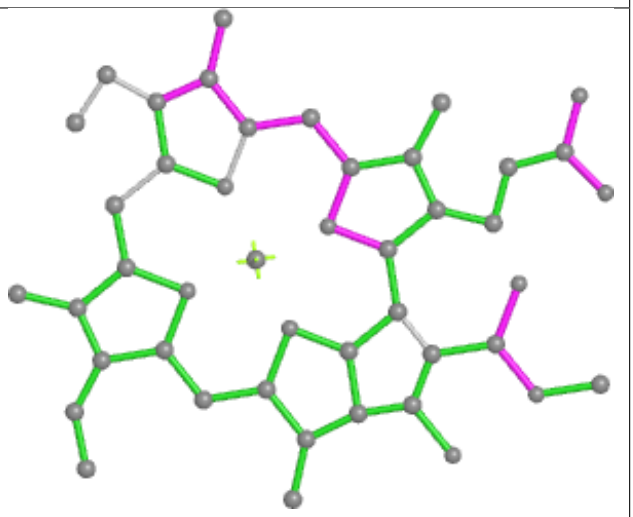
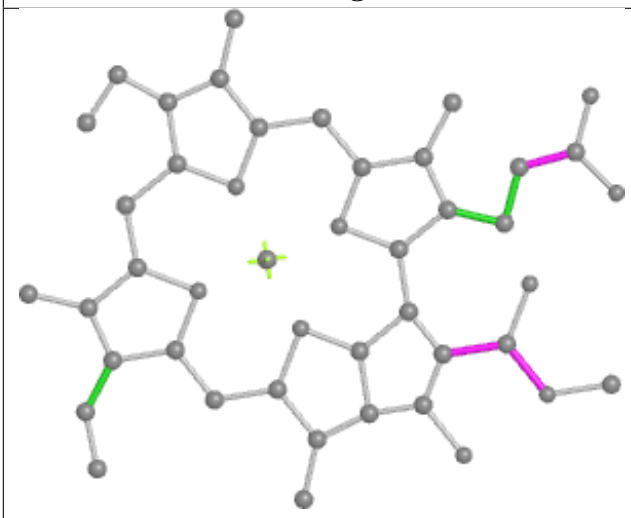


Bond angles



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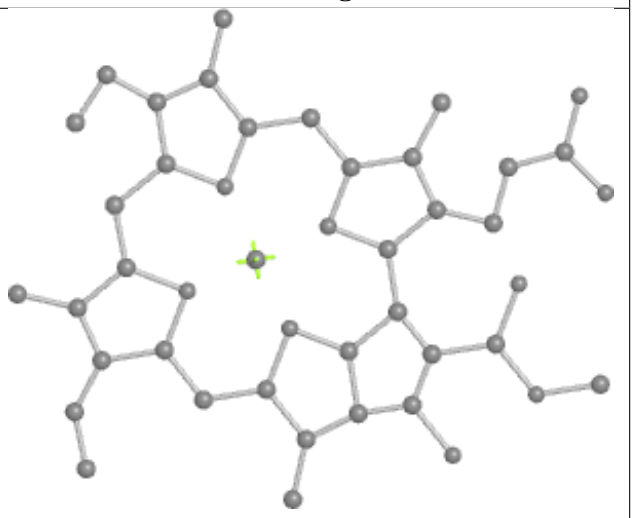
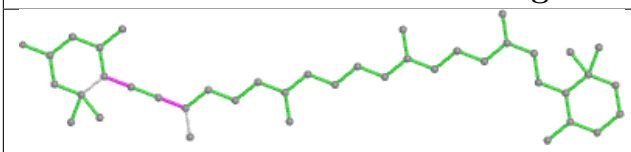


Rings

Ligand IHT p 318



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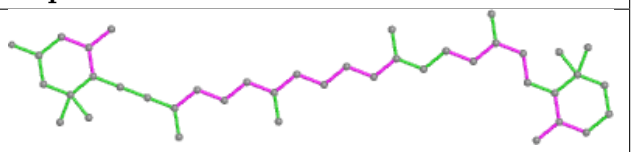
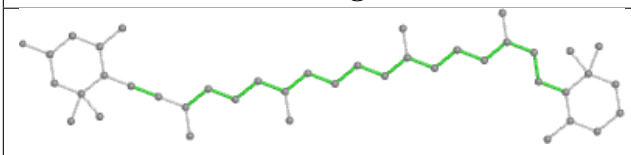


Bond angles



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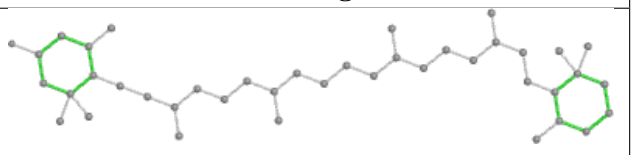
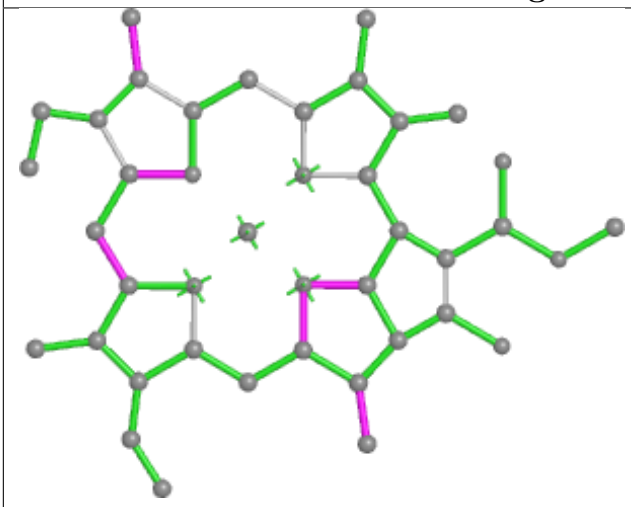


Rings

Ligand CLA 0 609



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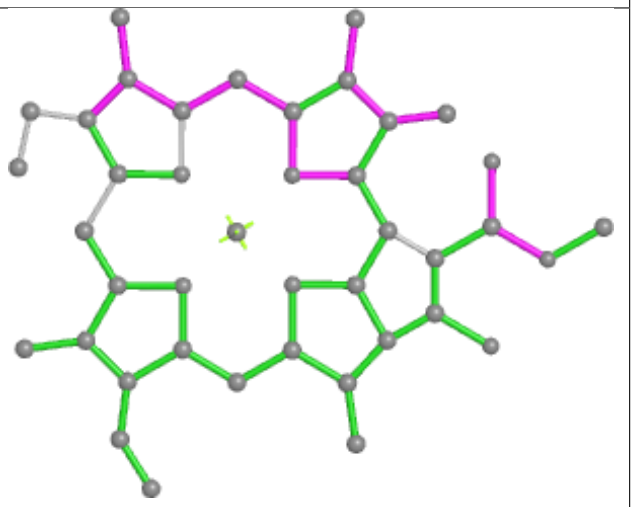
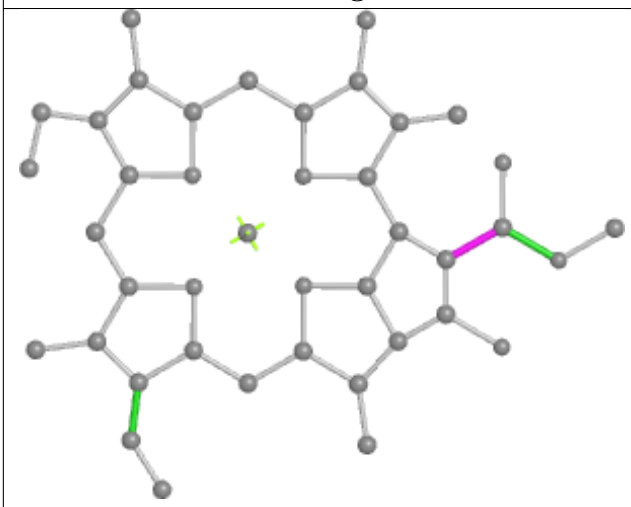


Bond angles



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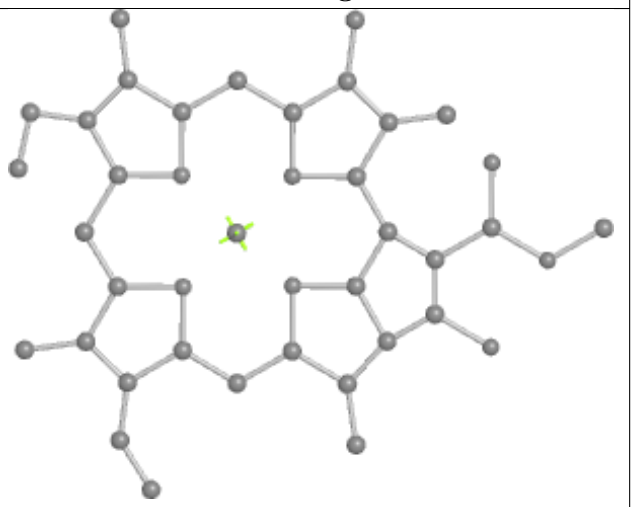
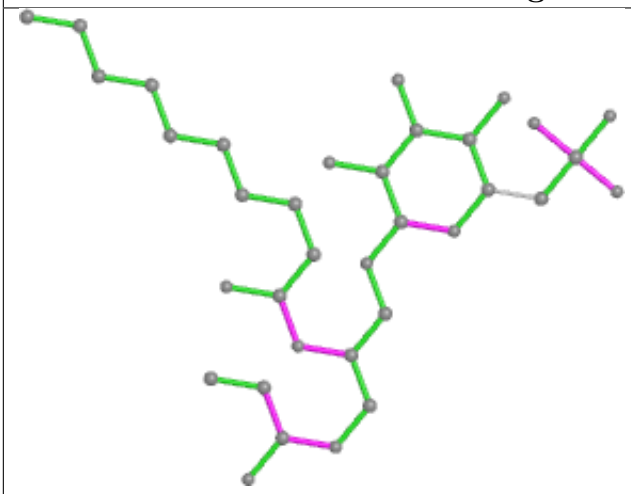
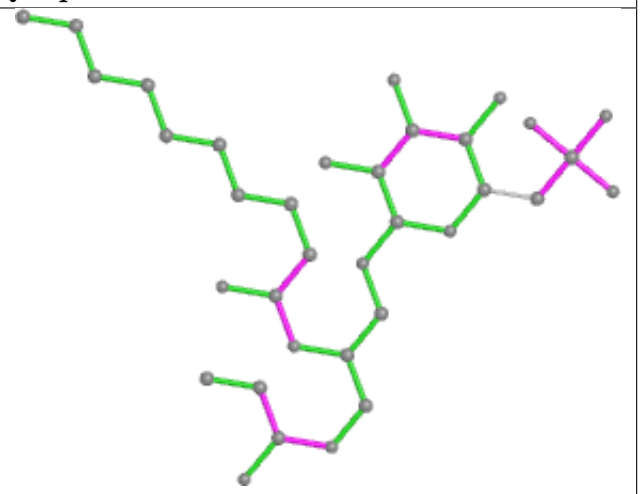


Rings

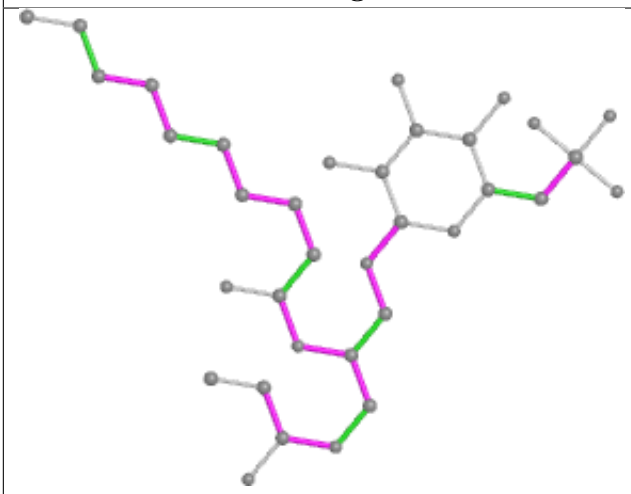
Ligand SQD p 319



Bond lengths



Bond angles



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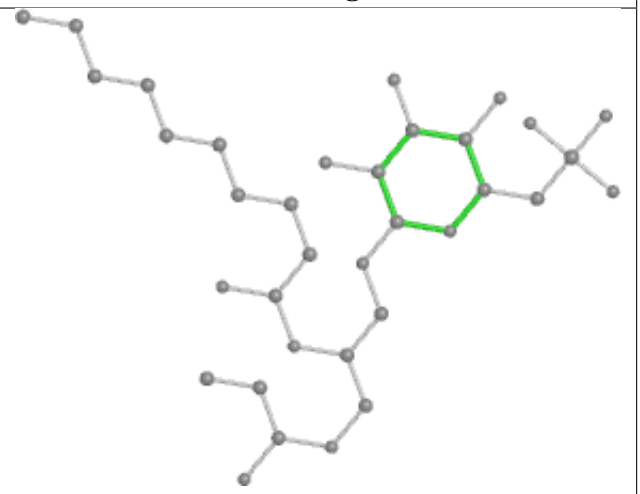
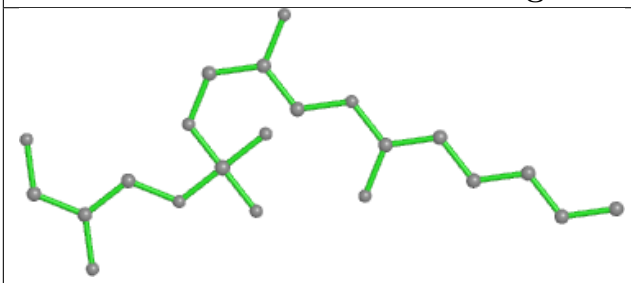


Rings

Ligand LHG 8 618



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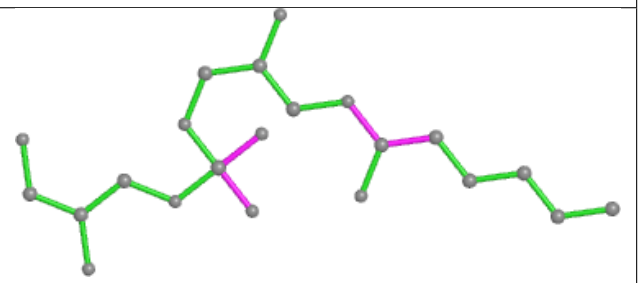
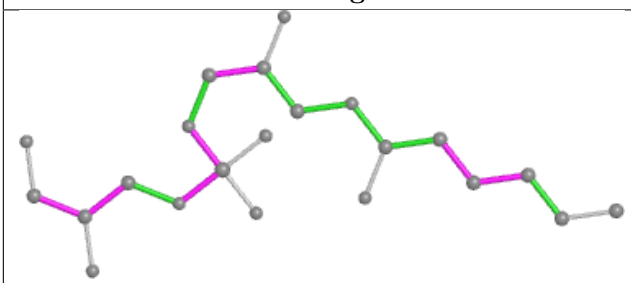
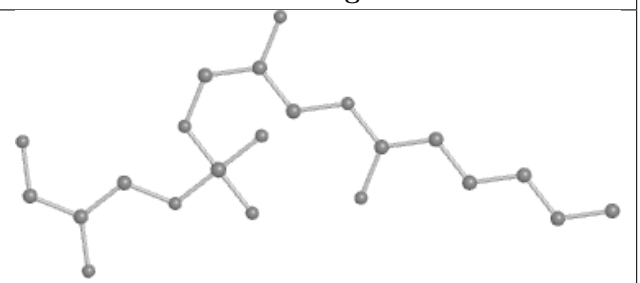


Bond angles

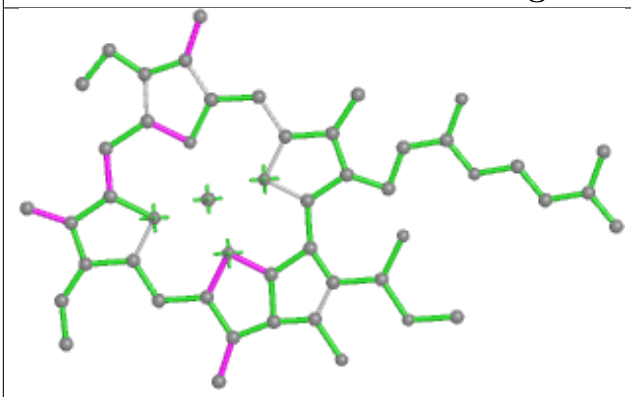


Torsions



Rings

Ligand CLA 9 603



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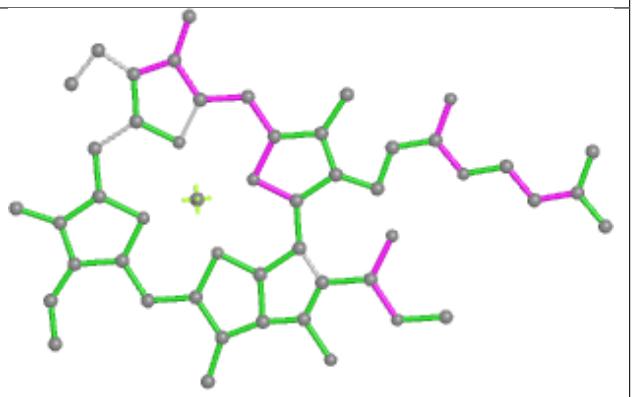
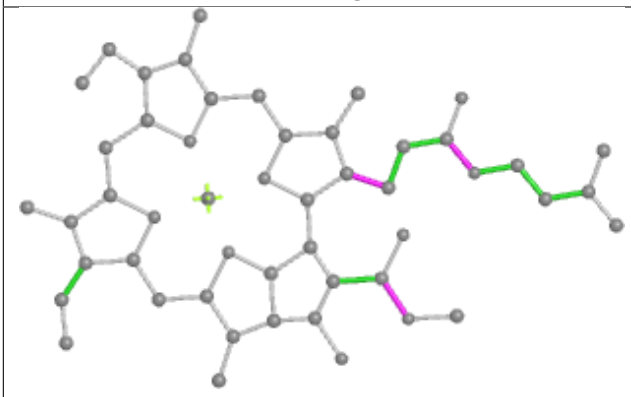
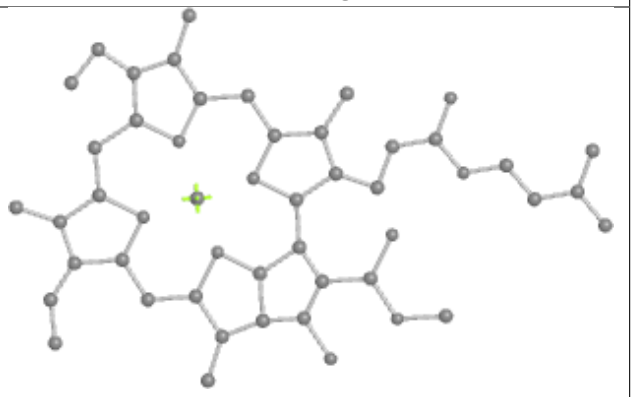


Bond angles

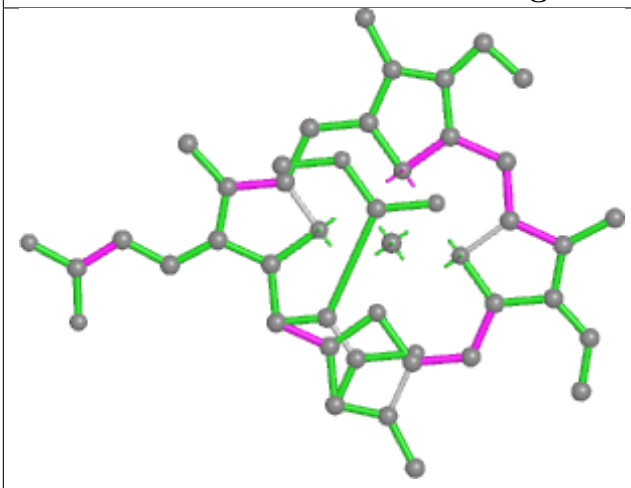


Torsions



Rings

Ligand KC2 7 610



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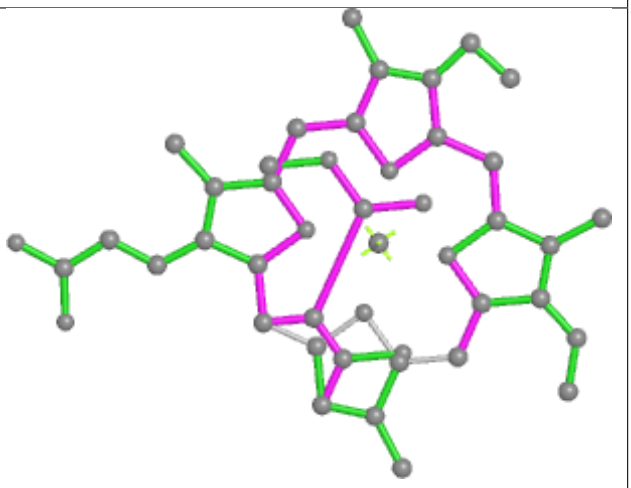
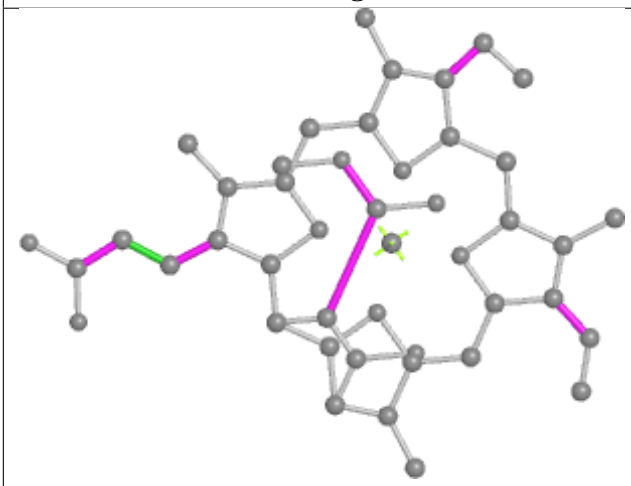
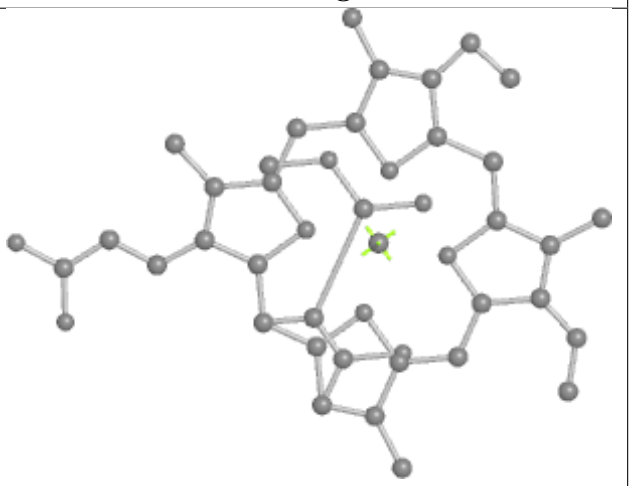


Bond angles

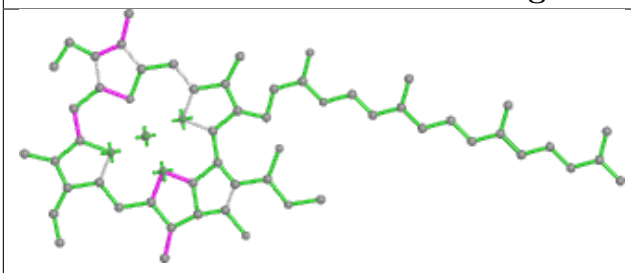


Torsions

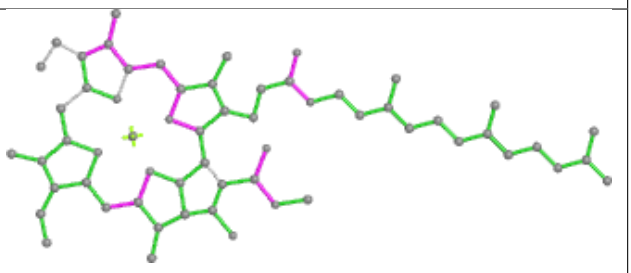


Rings

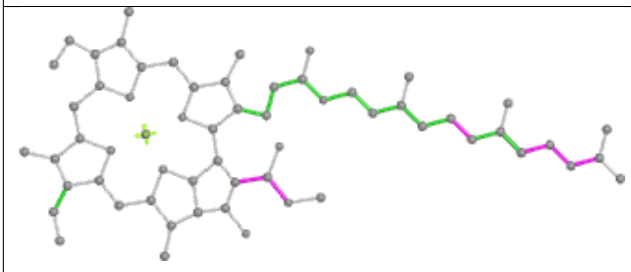
Ligand CLA 0 608



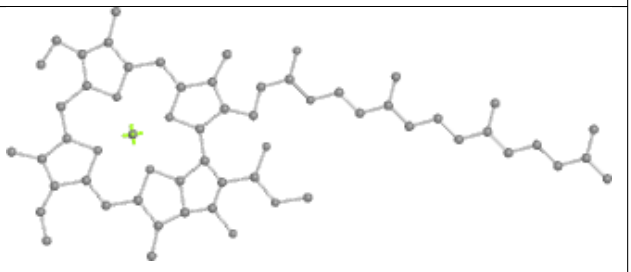
Bond lengths



Bond angles

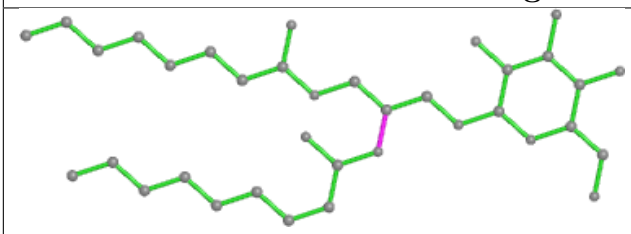


Torsions

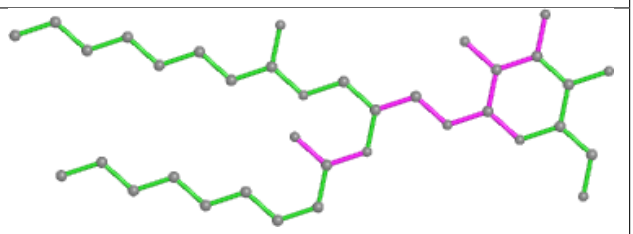


Rings

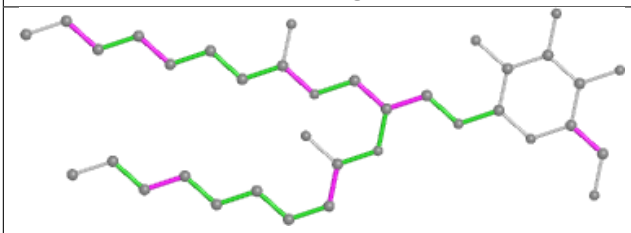
Ligand LMG 8 617



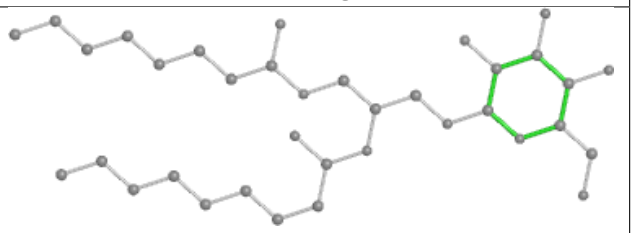
Bond lengths



Bond angles

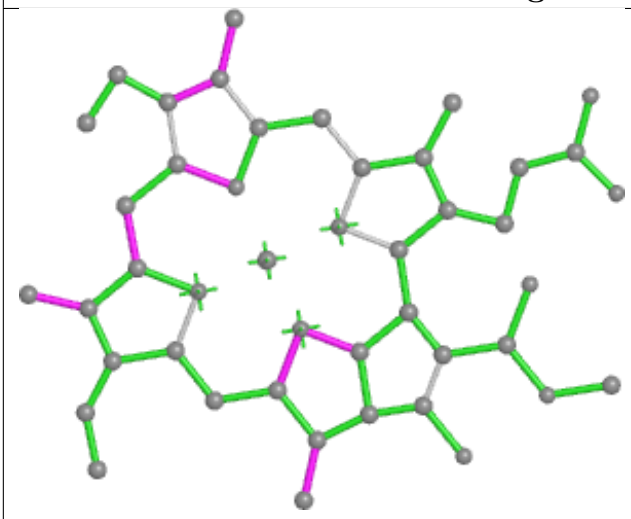


Torsions

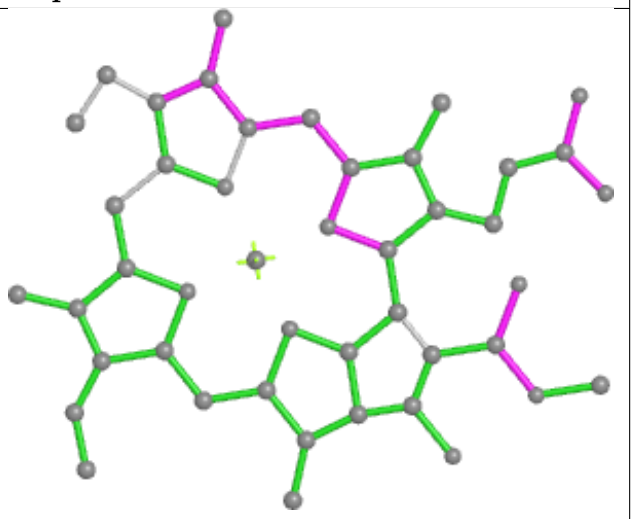


Rings

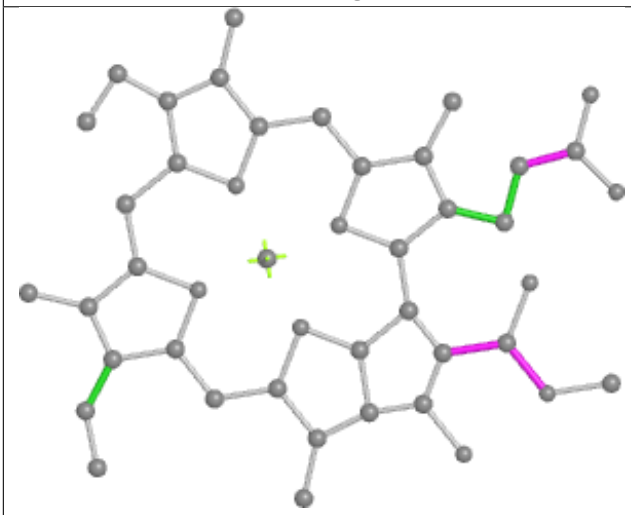
Ligand CLA p 308



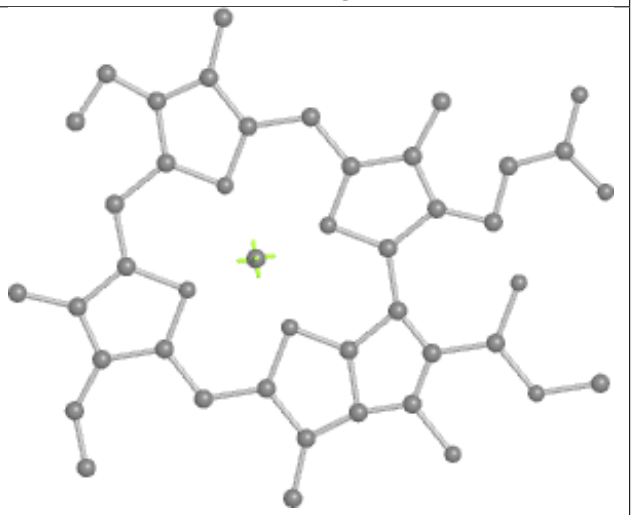
Bond lengths



Bond angles

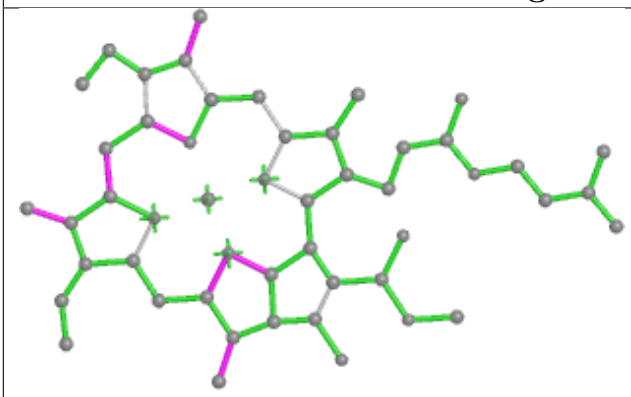


Torsions

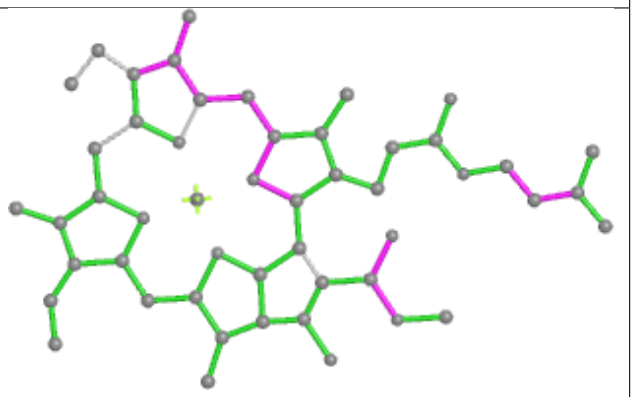


Rings

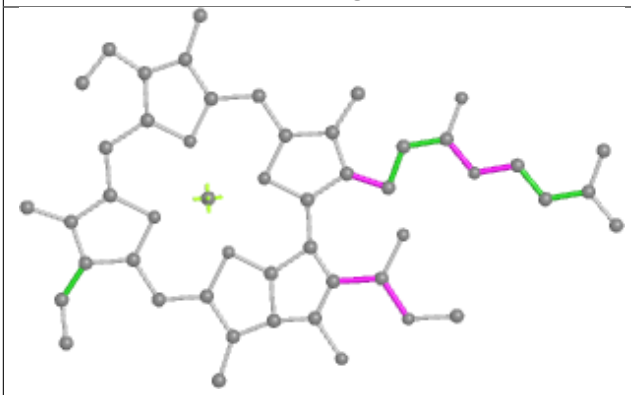
Ligand CLA 7 603



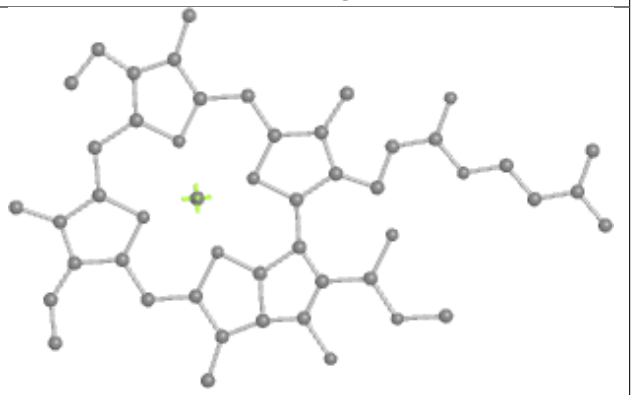
Bond lengths



Bond angles

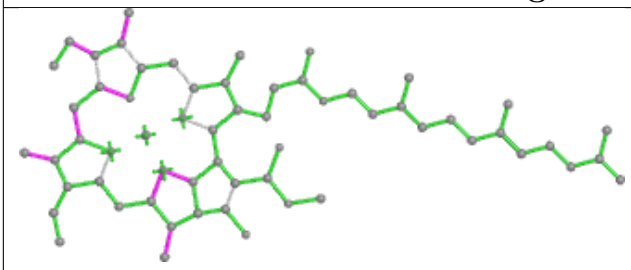


Torsions

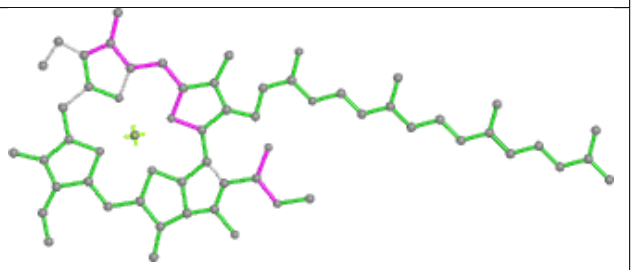


Rings

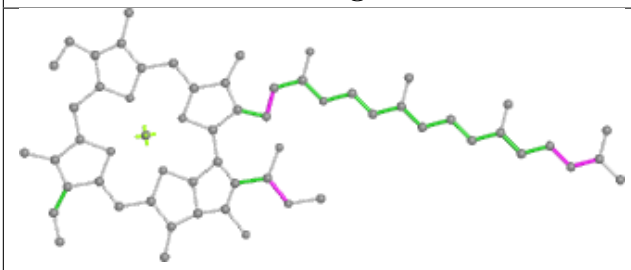
Ligand CLA 9 607



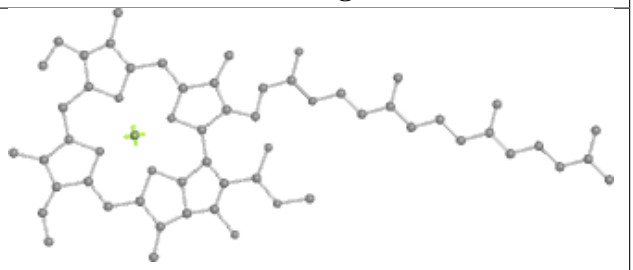
Bond lengths



Bond angles

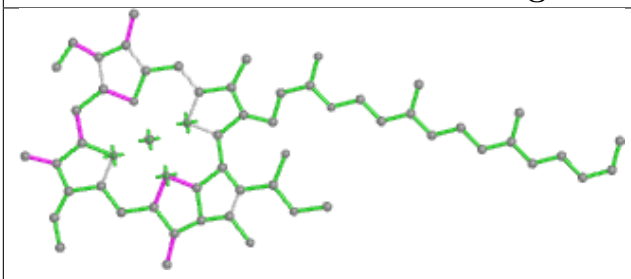


Torsions

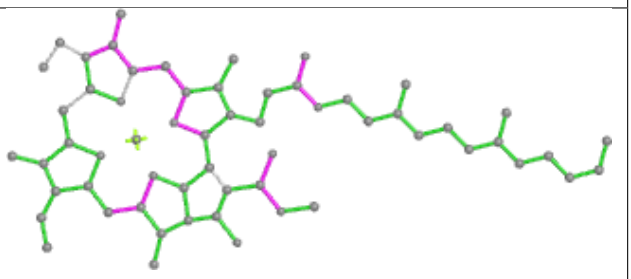


Rings

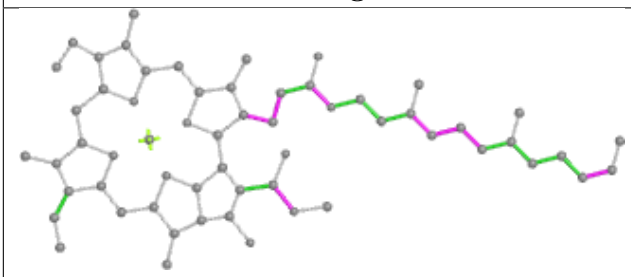
Ligand CLA 7 602



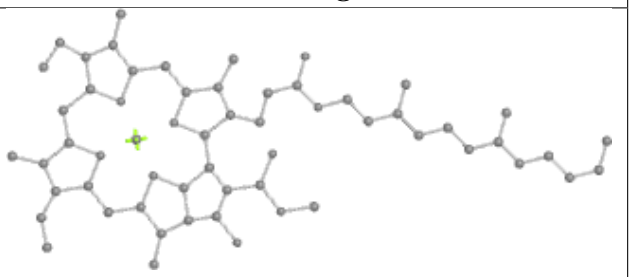
Bond lengths



Bond angles

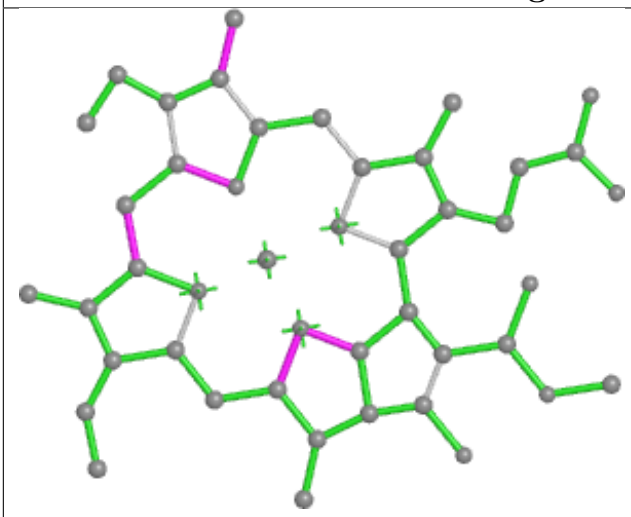


Torsions

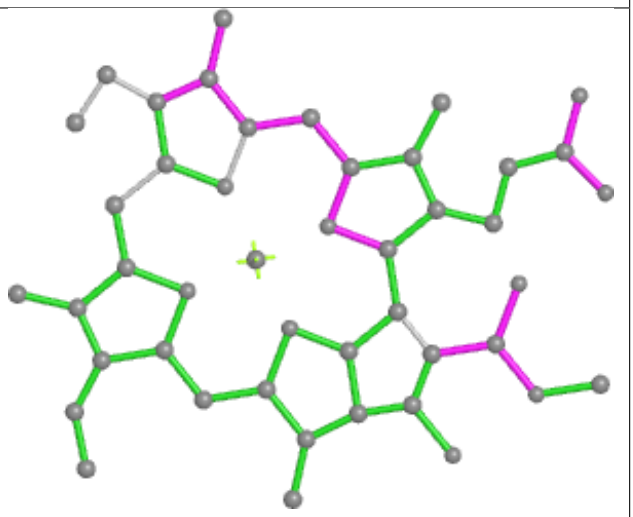


Rings

Ligand CLA 0 612



Bond lengths



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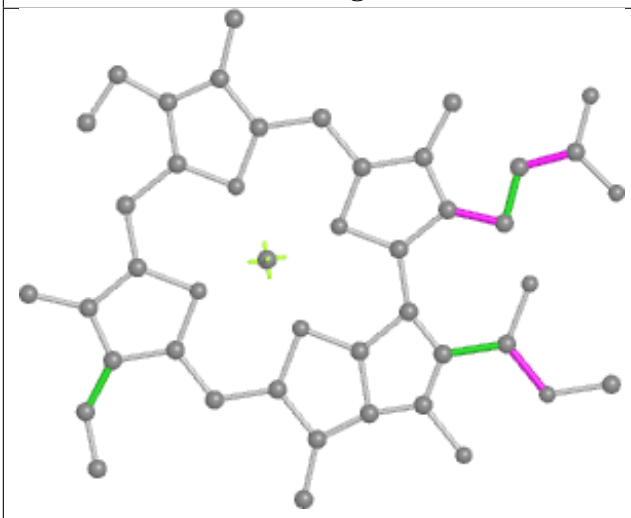
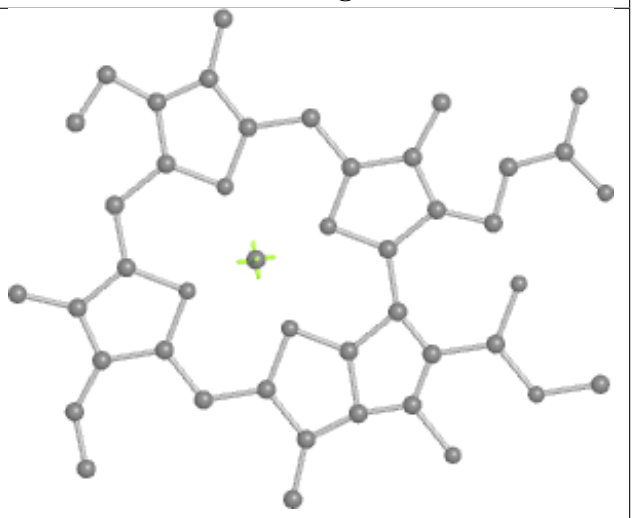
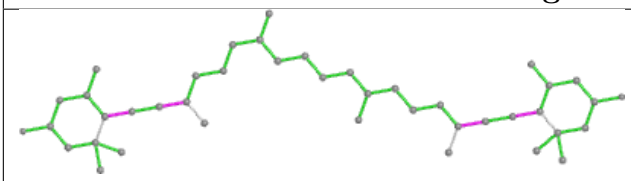


Torsions



Rings

Ligand II0 8 614



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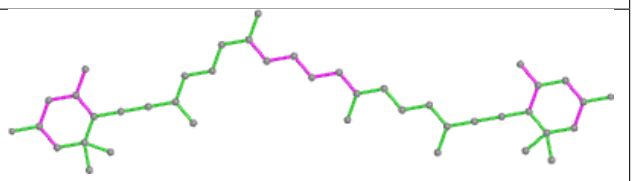
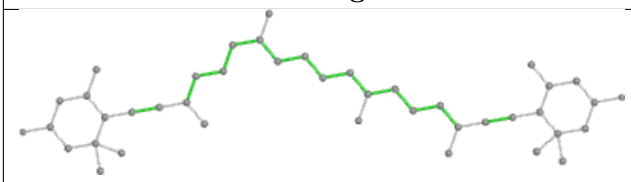


Bond angles



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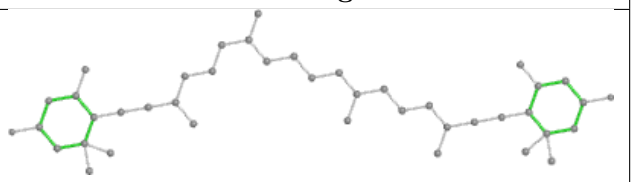
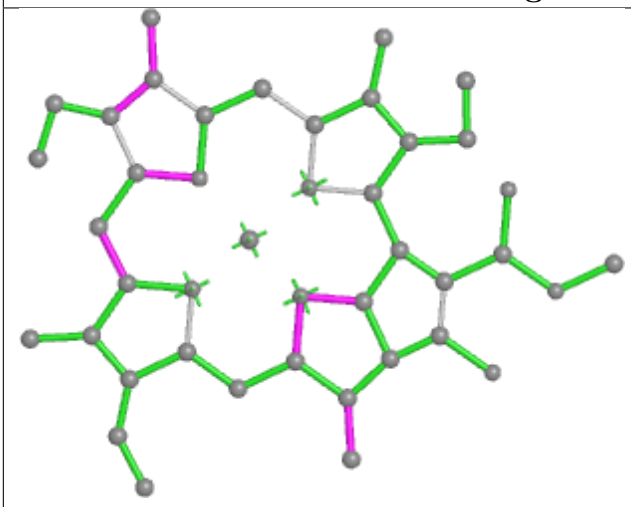


Rings

Ligand CLA P 601



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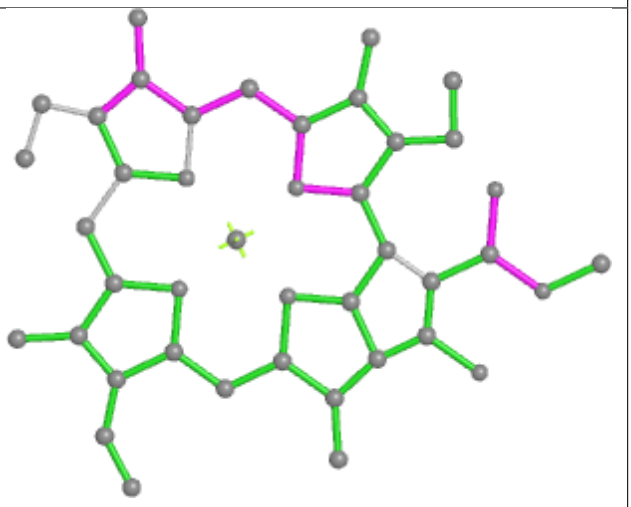
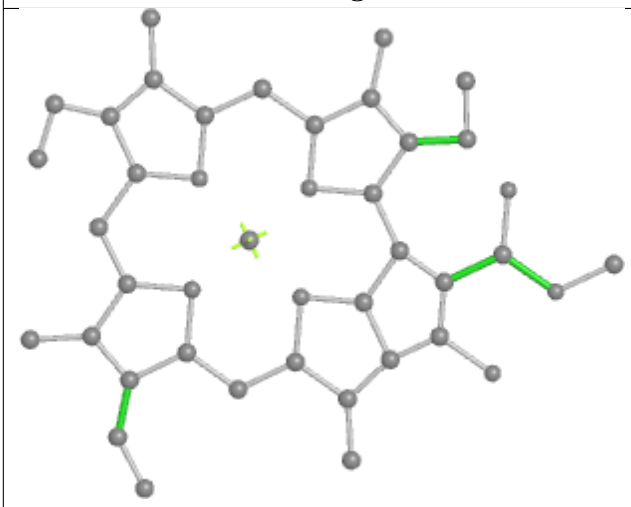


Bond angles



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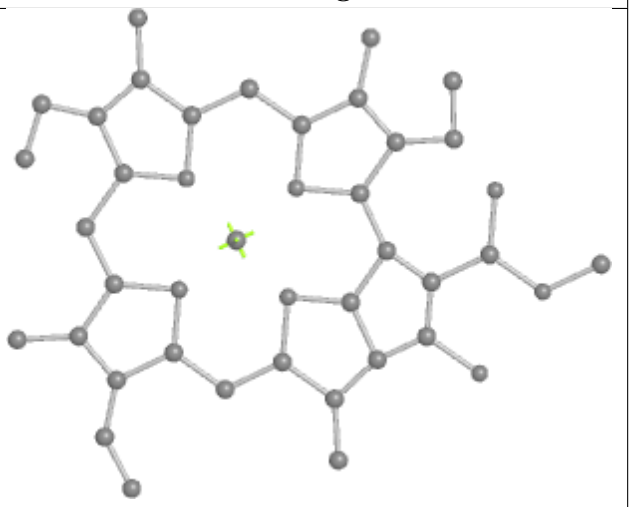
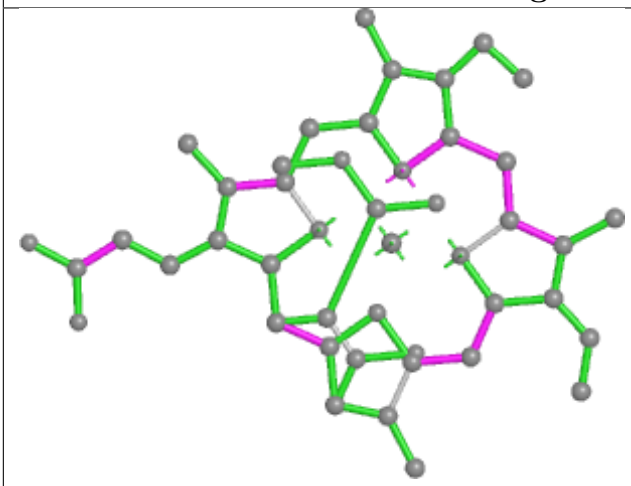


Rings

Ligand KC2 0 610



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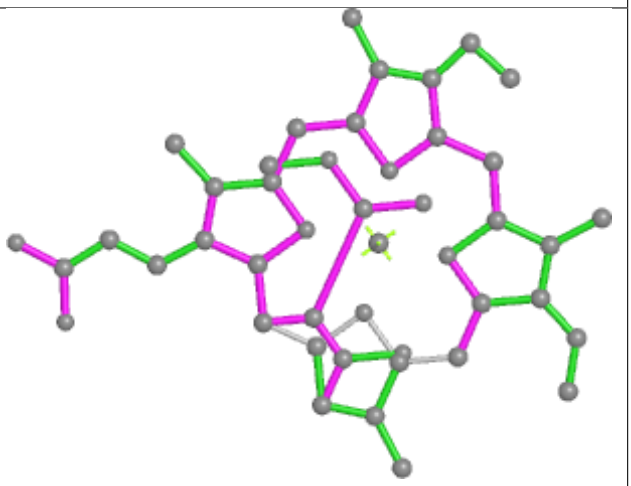
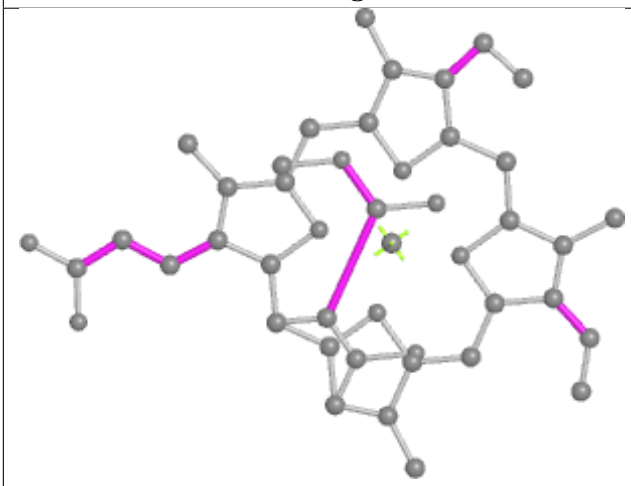
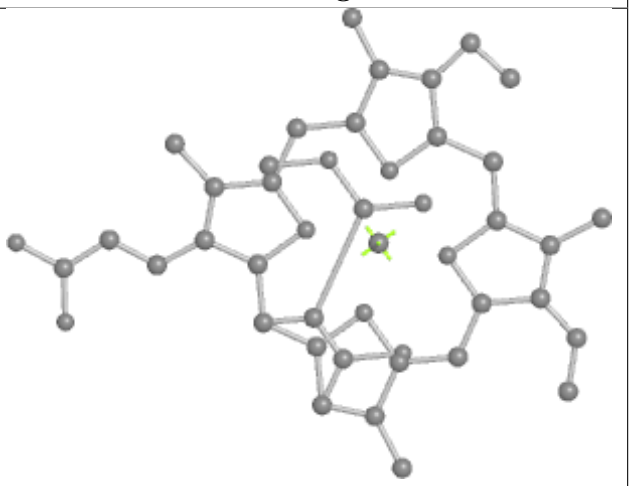


Bond angles

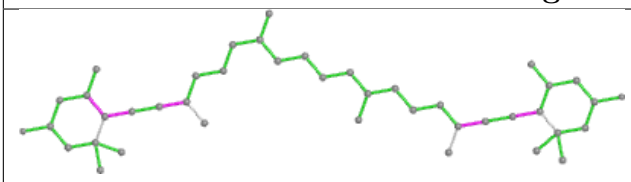


Torsions



Rings

Ligand II0 8 615



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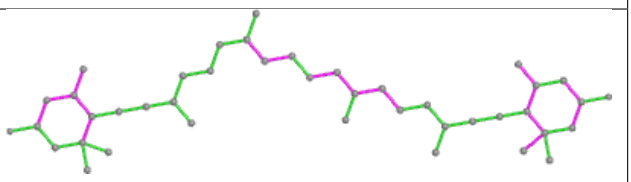
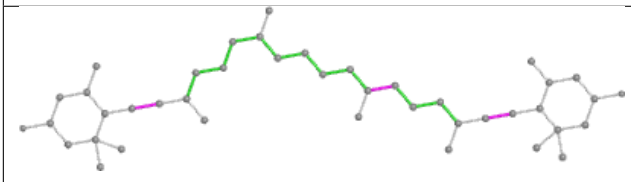
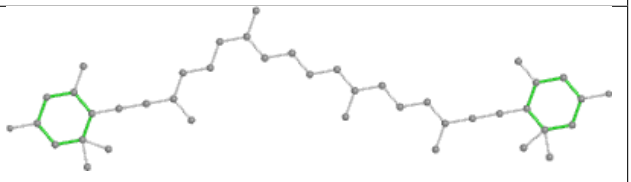


Bond angles

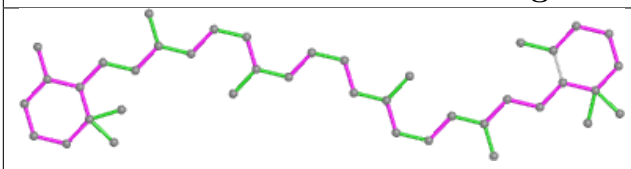


Torsions



Rings

Ligand 8CT 9 615



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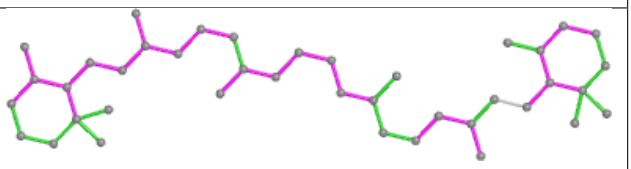

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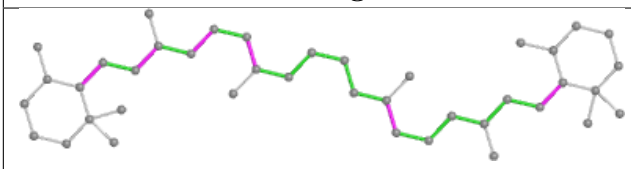
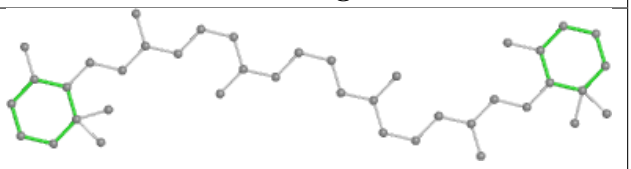
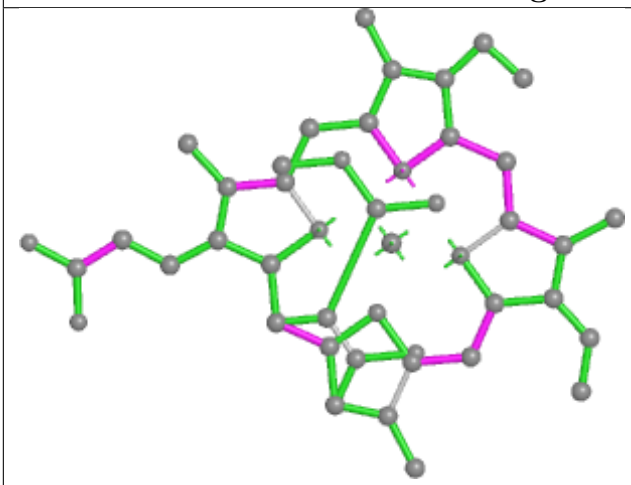


Torsions



Rings

Ligand KC2 8 610



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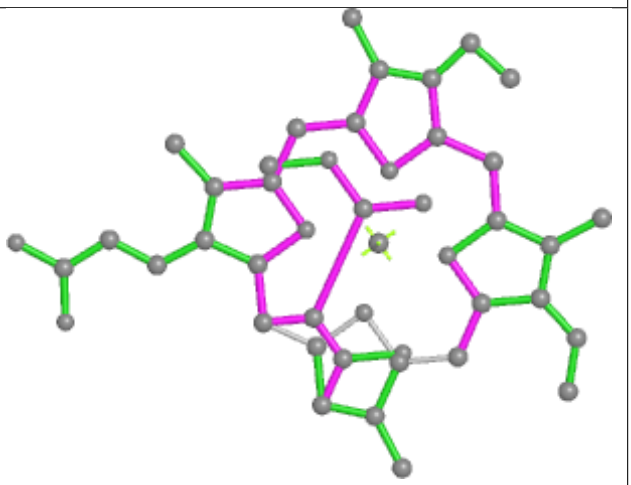
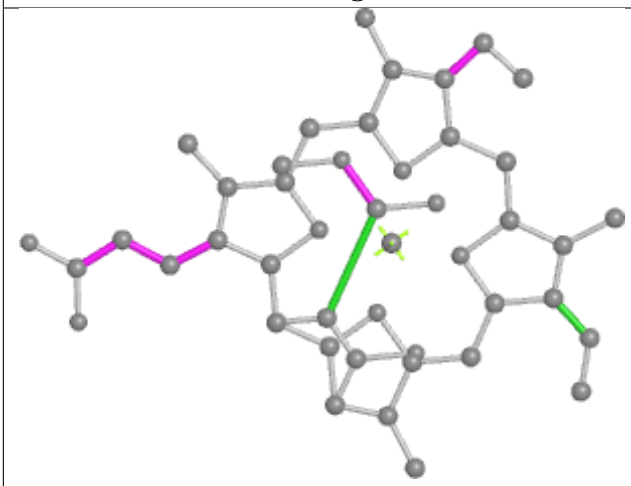


Bond angles



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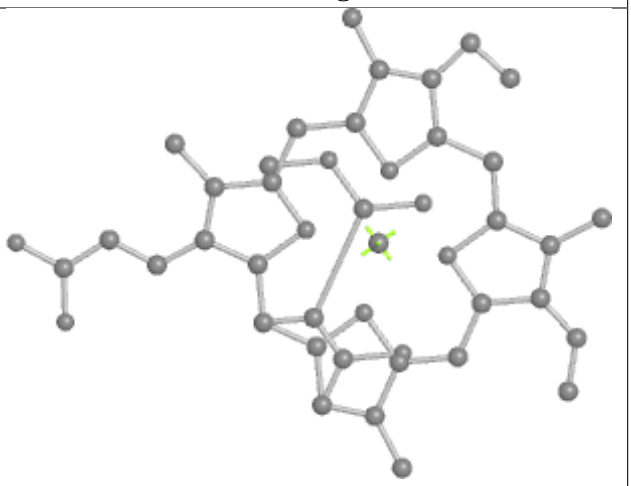
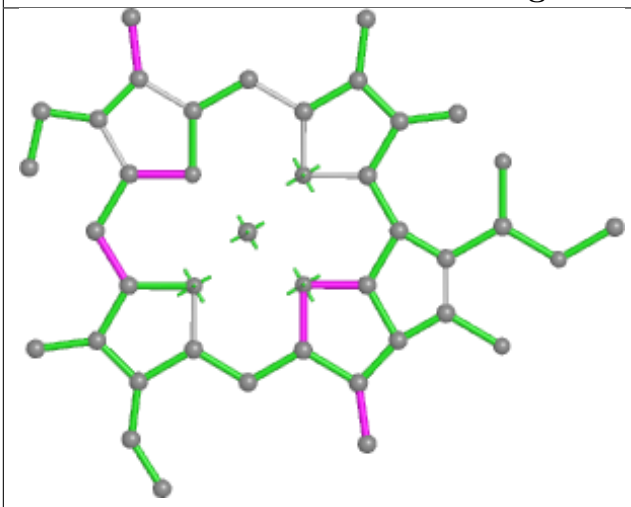
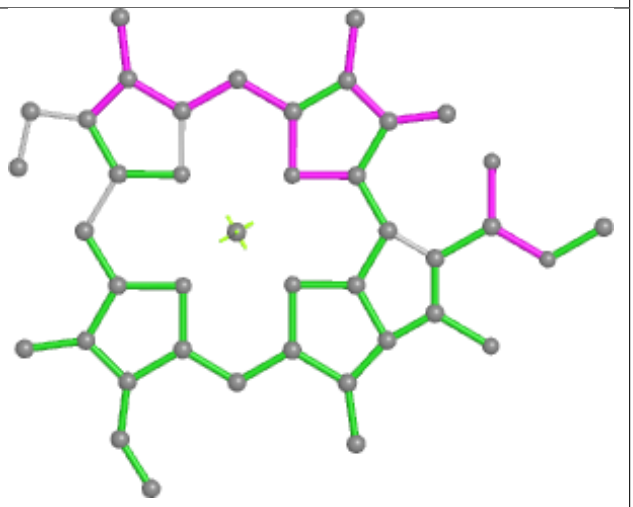


Rings

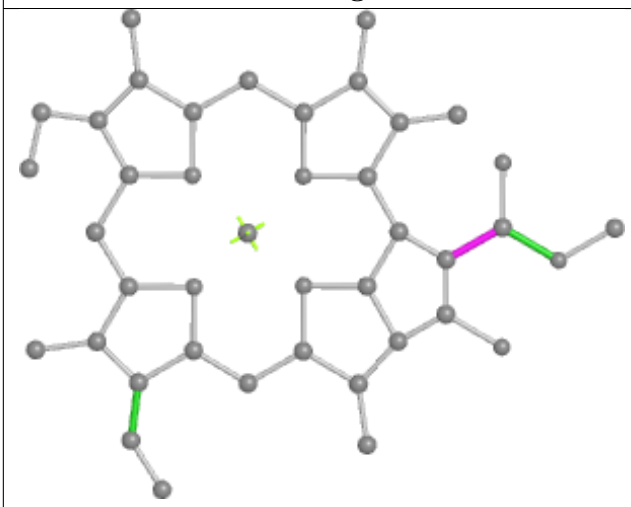
Ligand CLA 9 608



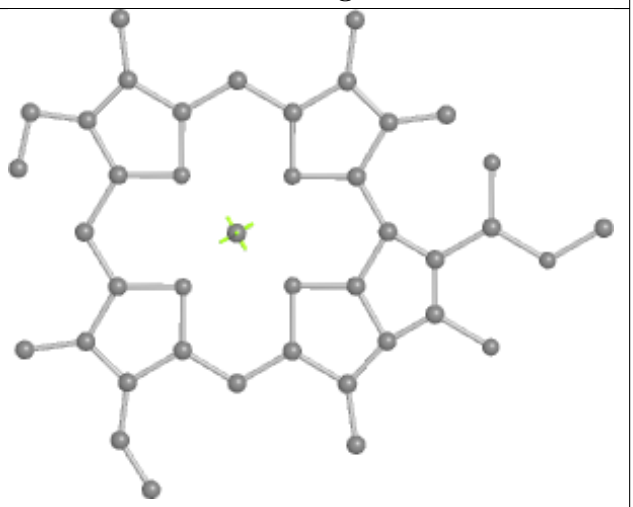
Bond lengths



Bond angles

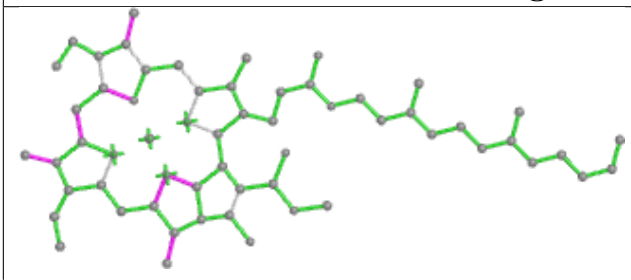


Torsions



Rings

Ligand CLA 9 602



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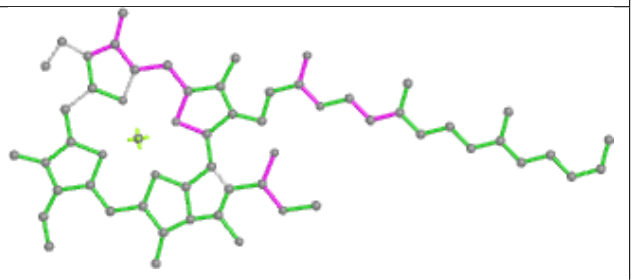
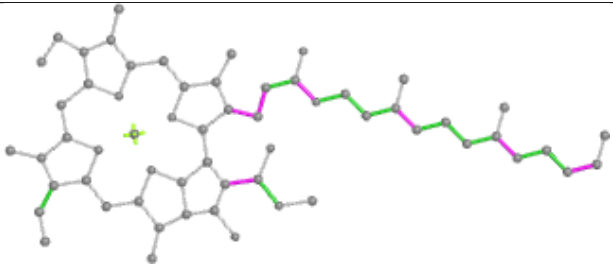
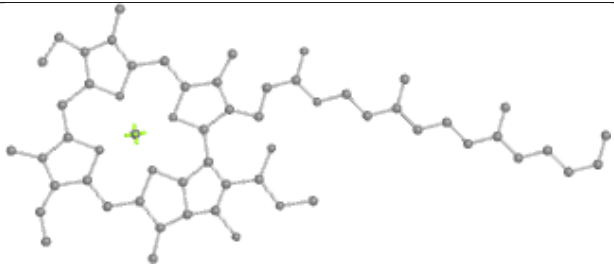


Bond angles

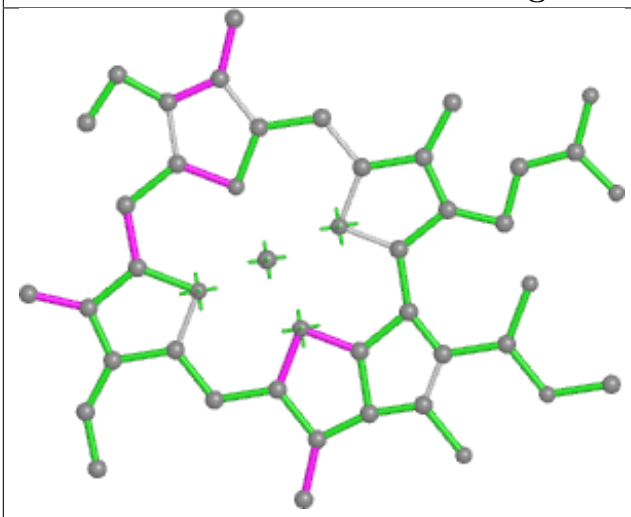


Torsions



Rings

Ligand CLA 8 606



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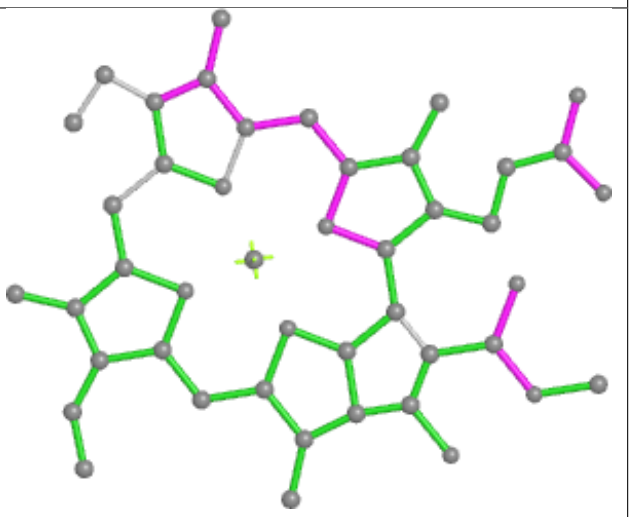

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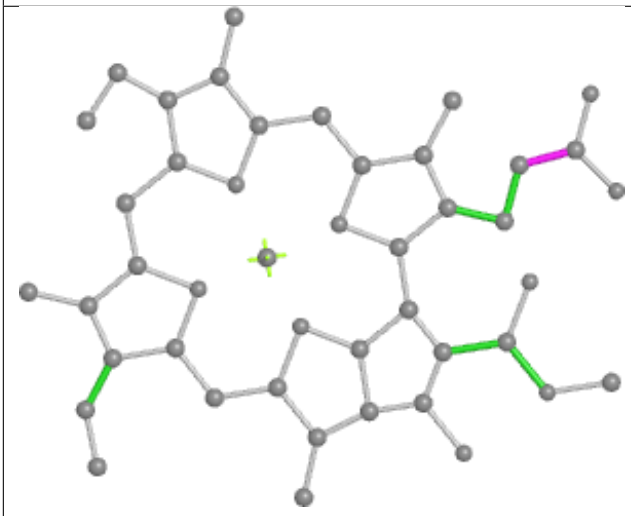
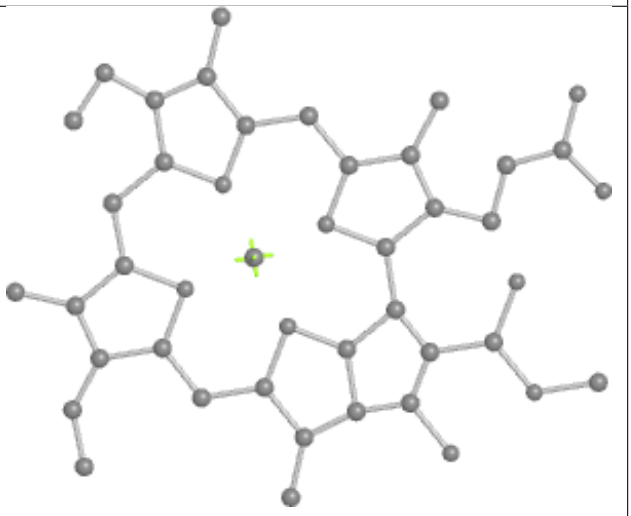
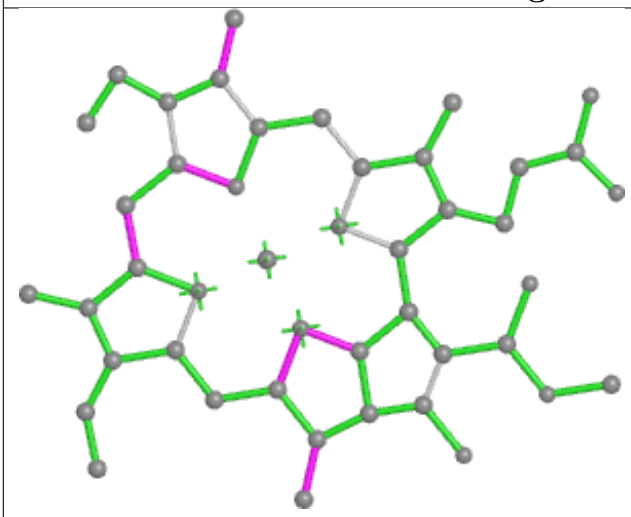


Torsions

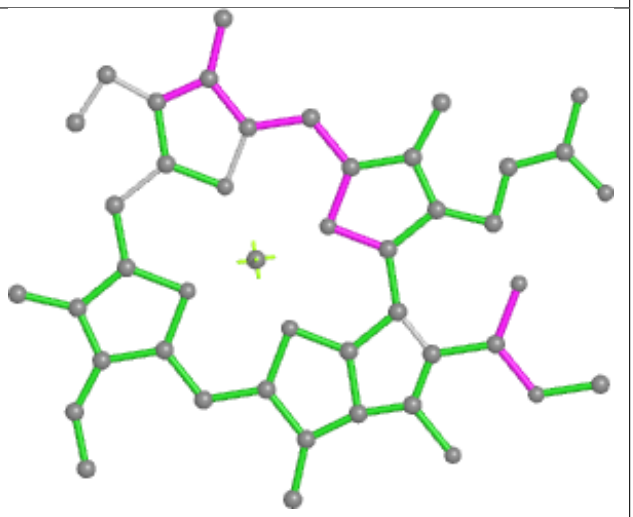


Rings

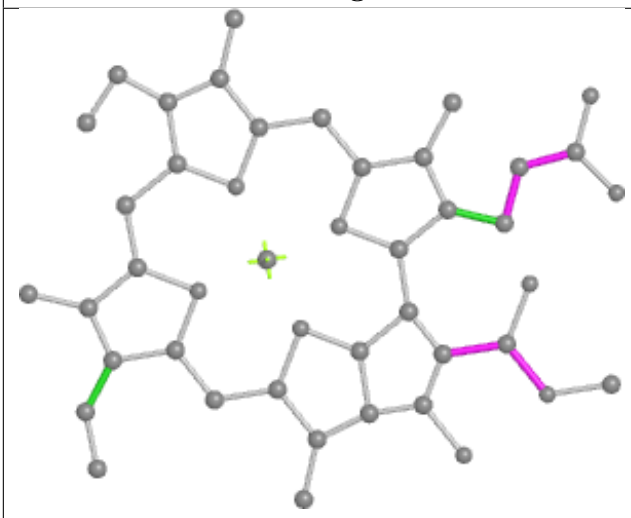
Ligand CLA 0 611



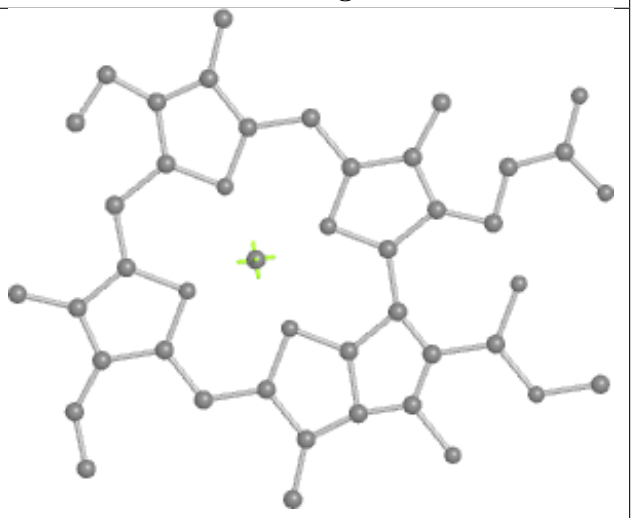
Bond lengths



Bond angles

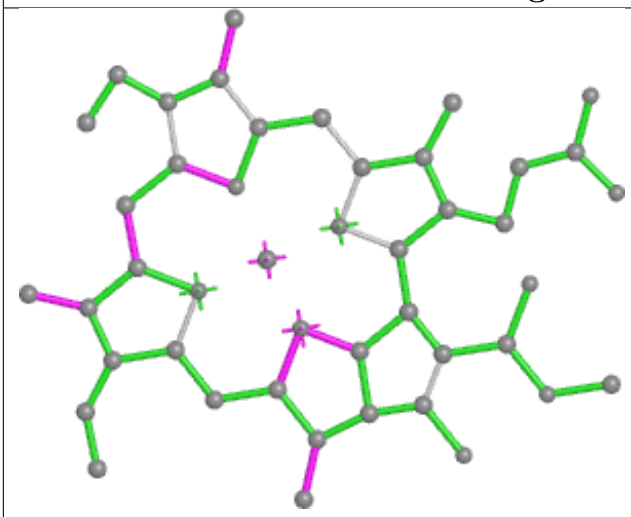


Torsions



Rings

Ligand CLA 8 611



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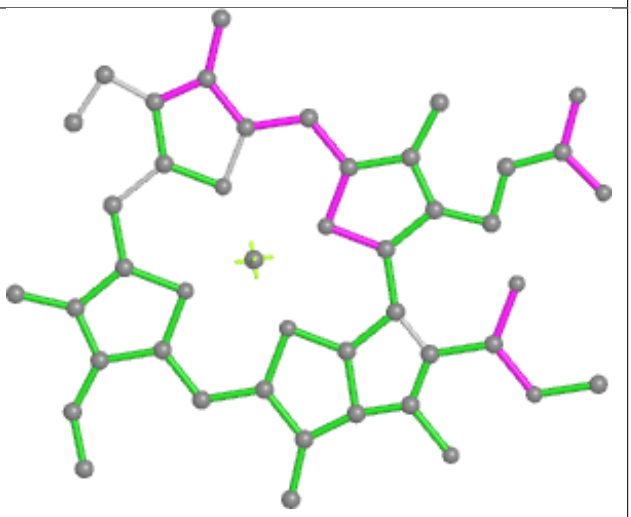

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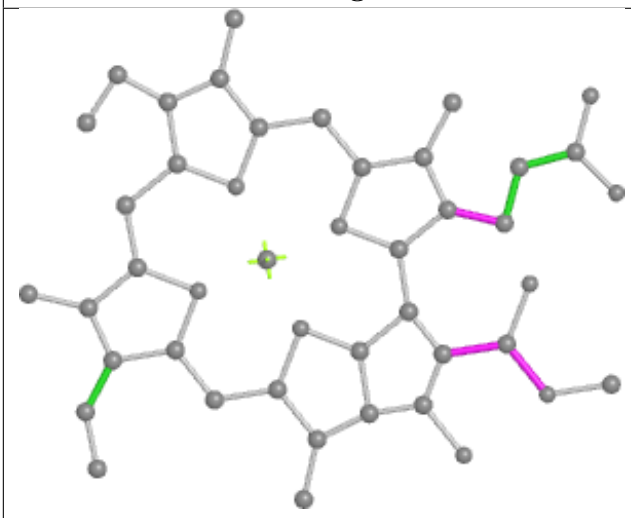
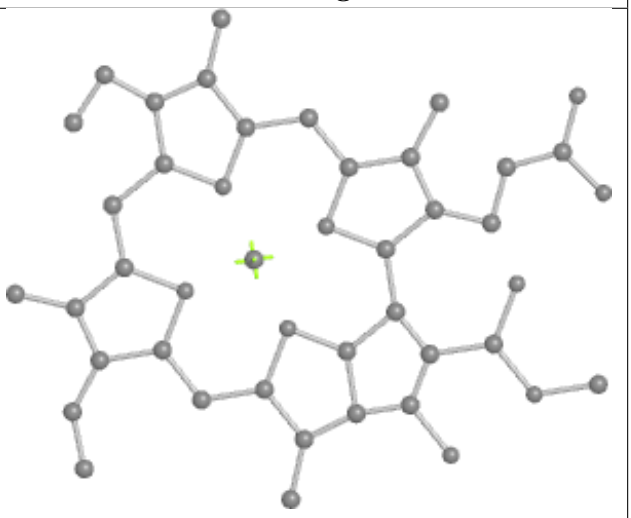
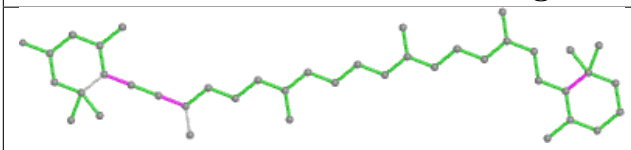


Torsions

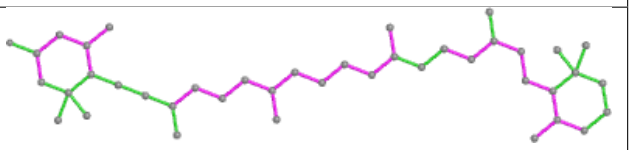


Rings

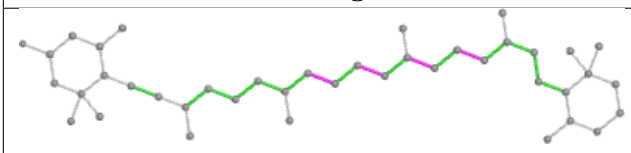
Ligand IHT 0 617



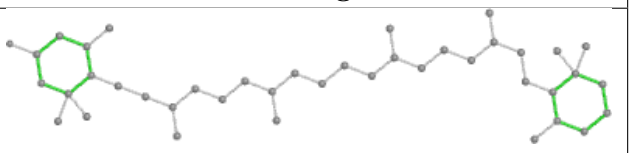
Bond lengths



Bond angles

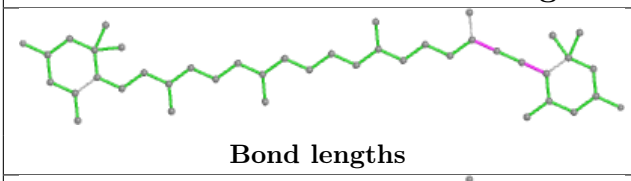


Torsions

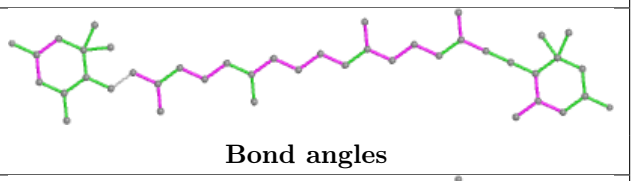


Rings

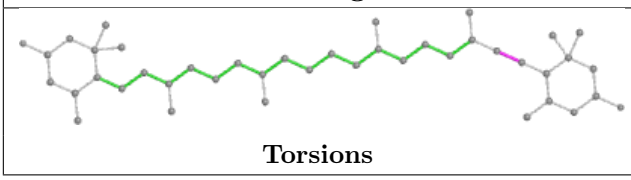
Ligand II3 P 613



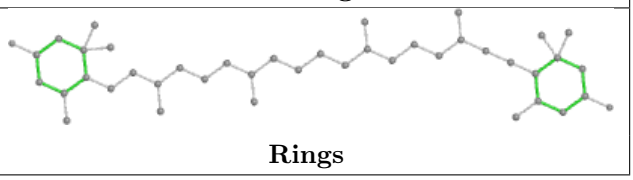
Bond lengths



Bond angles

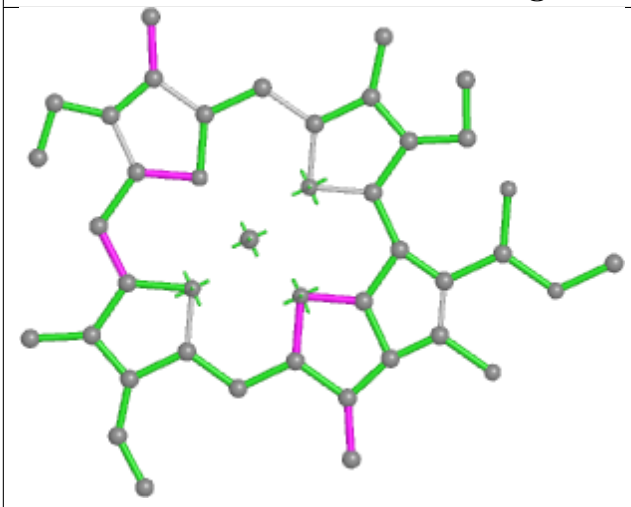


Torsions

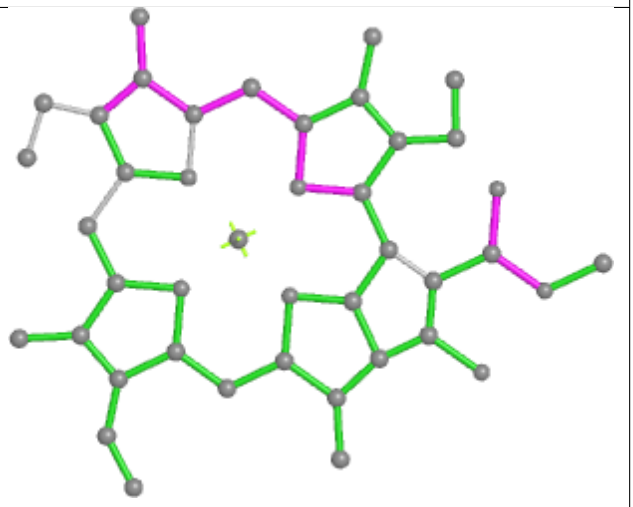


Rings

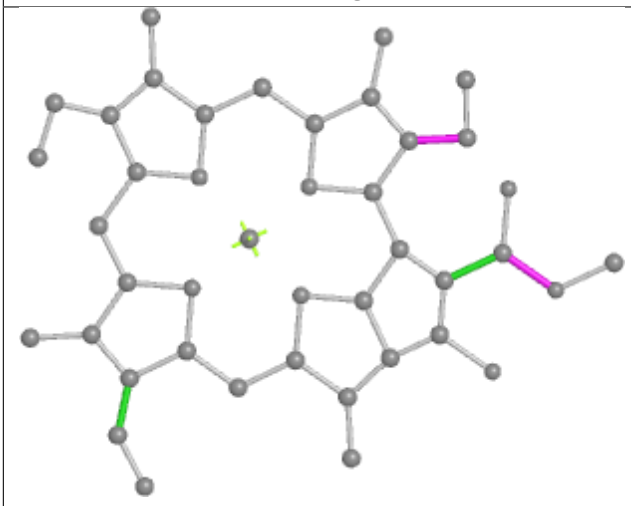
Ligand CLA 7 601



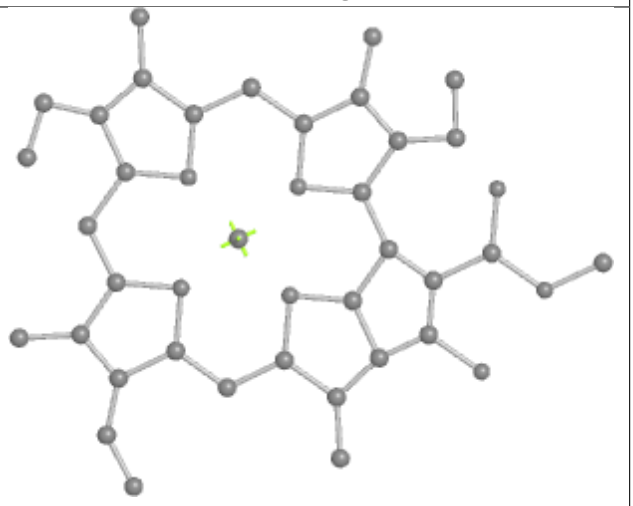
Bond lengths



Bond angles

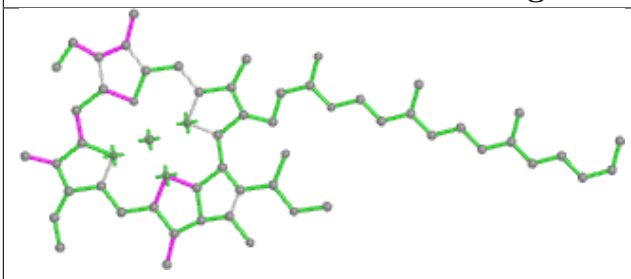


Torsions

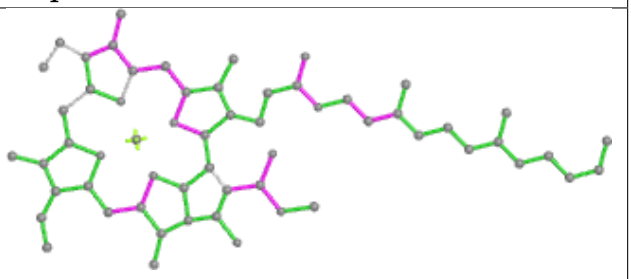


Rings

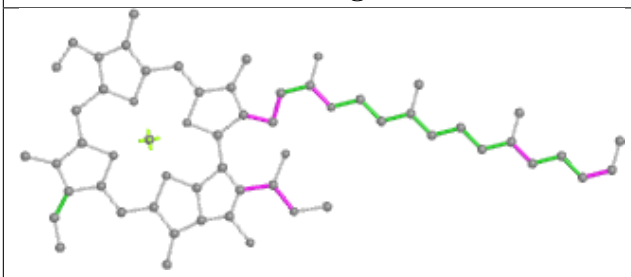
Ligand CLA p 304



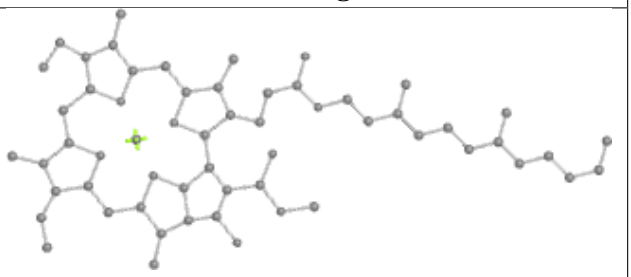
Bond lengths



Bond angles

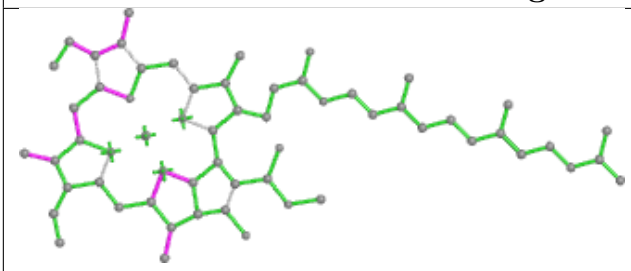


Torsions

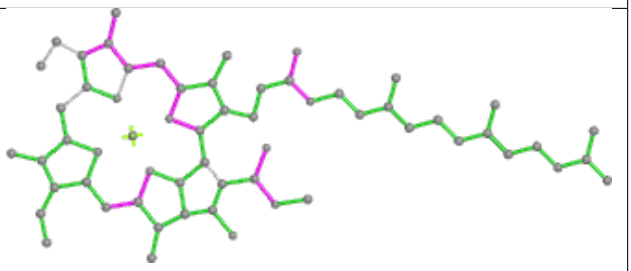


Rings

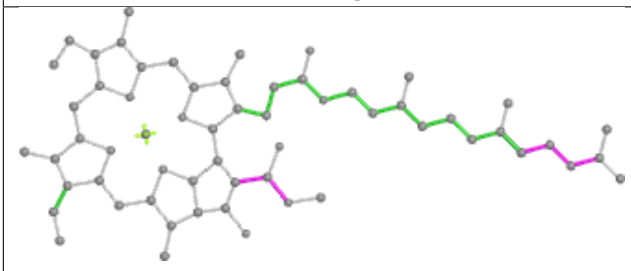
Ligand CLA 7 608



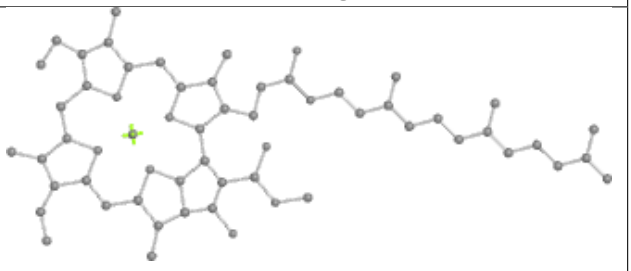
Bond lengths



Bond angles

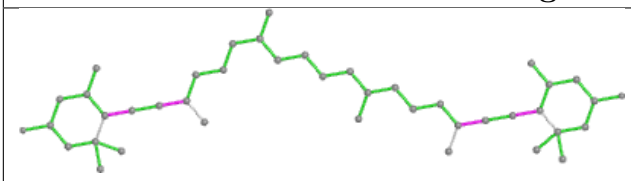


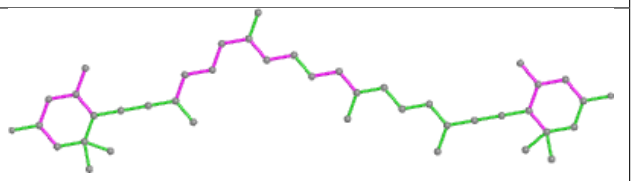
Torsions

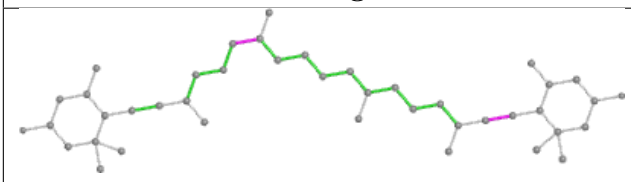


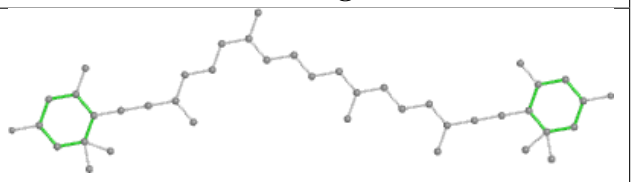
Rings

Ligand II0 P 614

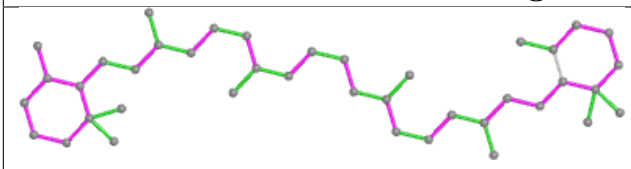

Bond lengths

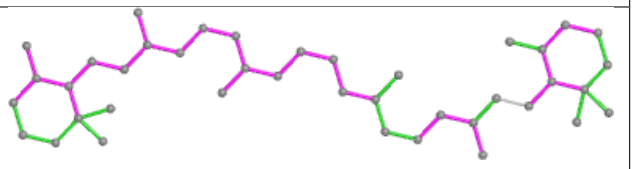

Bond angles

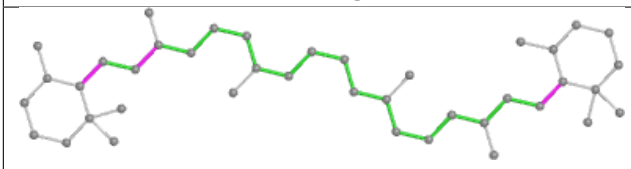

Torsions

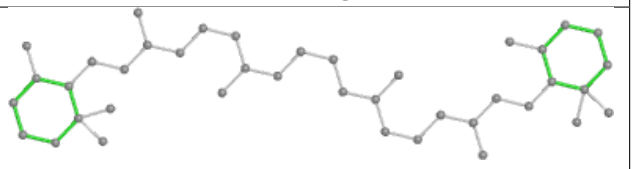

Rings

Ligand 8CT P 615

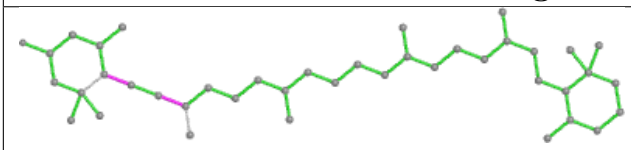

Bond lengths

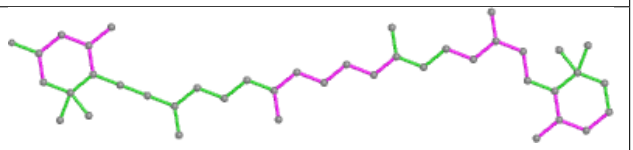

Bond angles

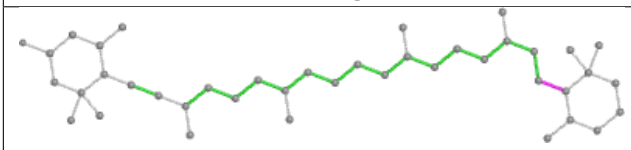

Torsions

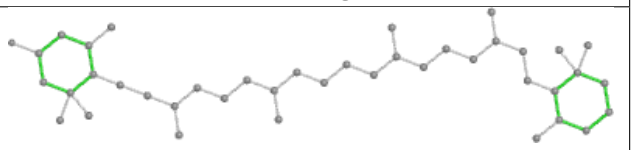

Rings

Ligand IHT 7 618

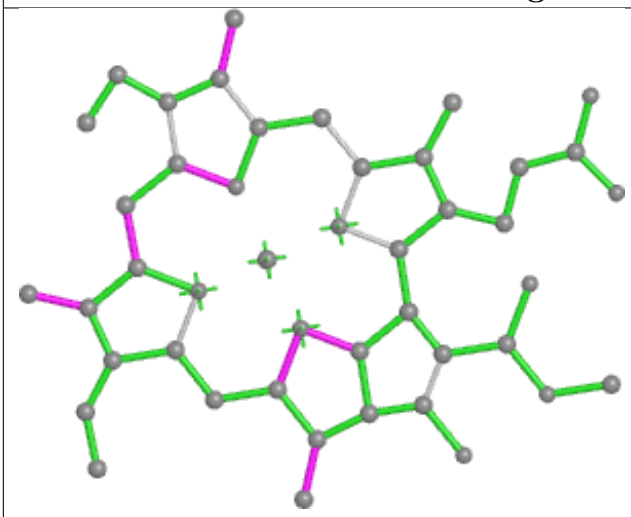

Bond lengths


Bond angles

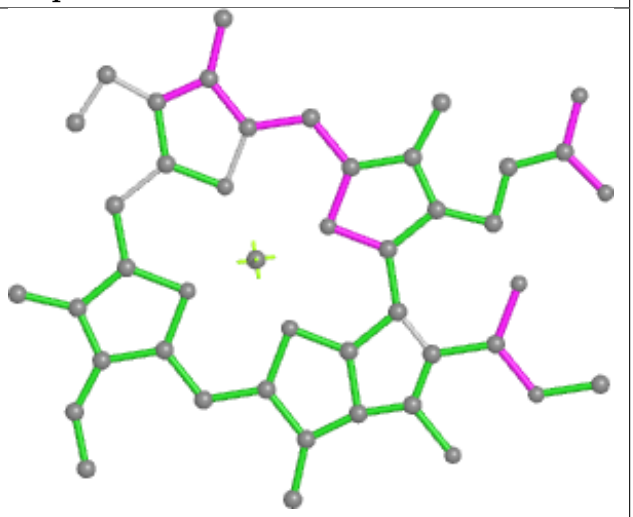

Torsions


Rings

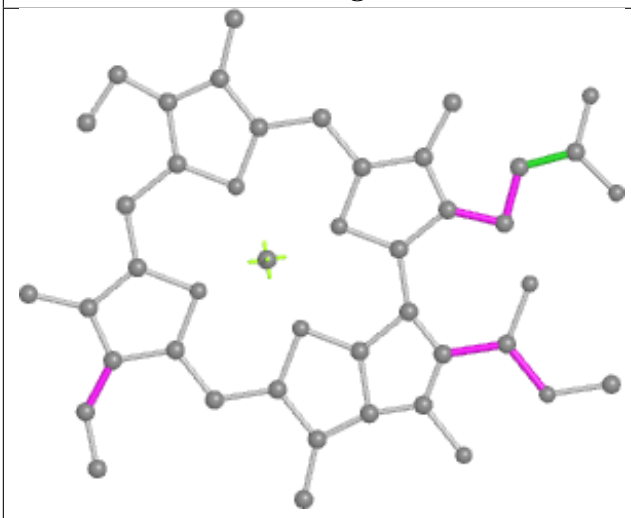
Ligand CLA p 313



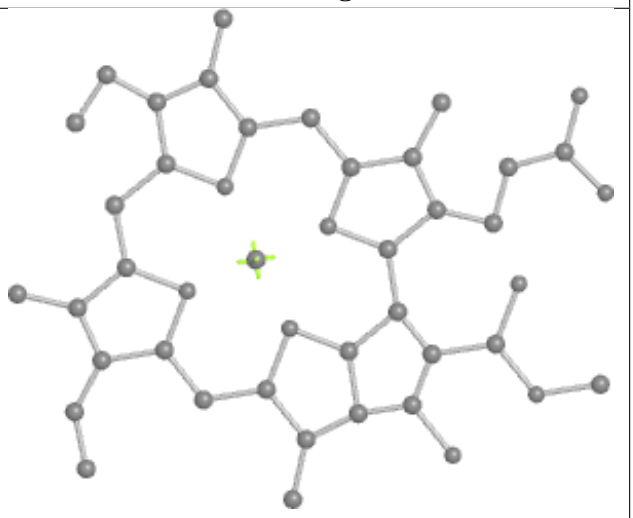
Bond lengths



Bond angles

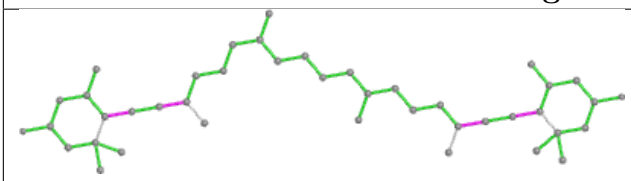


Torsions

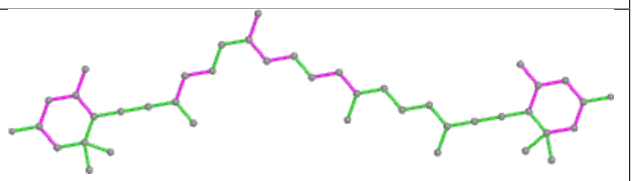


Rings

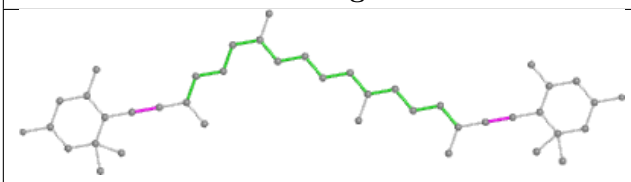
Ligand II0 7 619



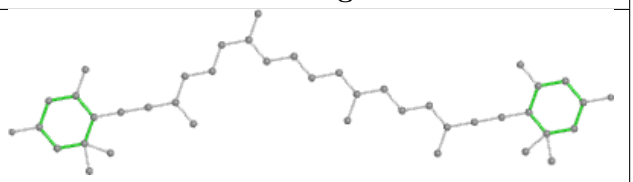
Bond lengths



Bond angles

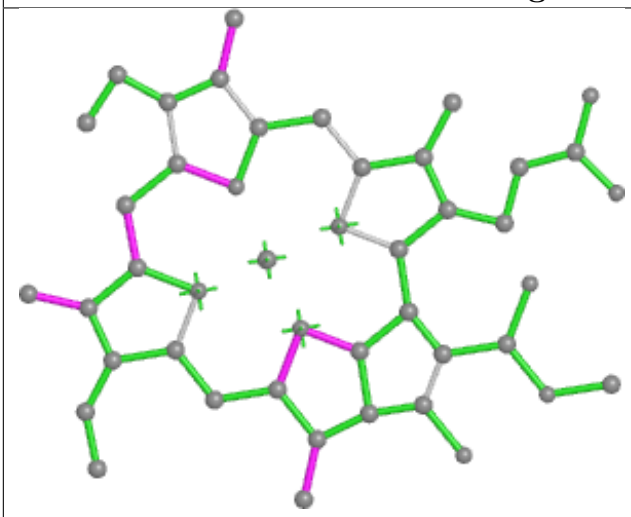


Torsions

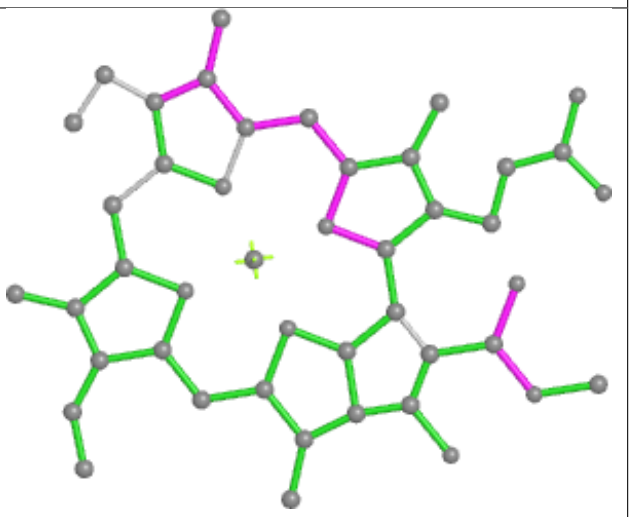


Rings

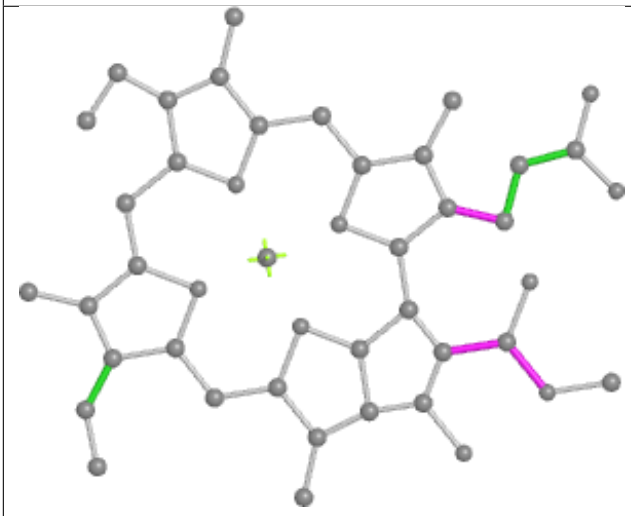
Ligand CLA 9 611



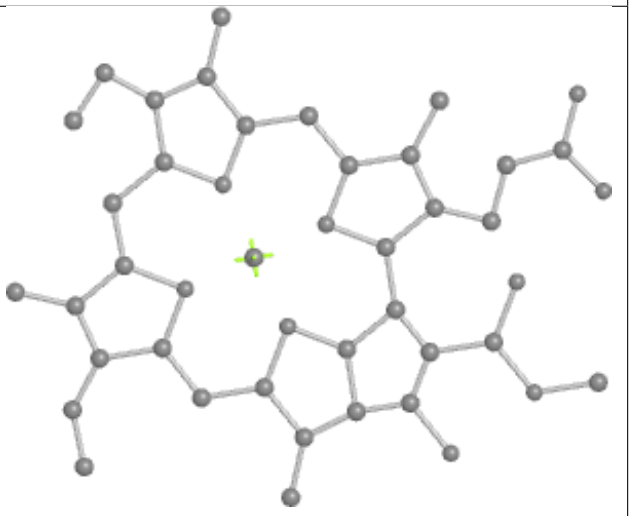
Bond lengths



Bond angles

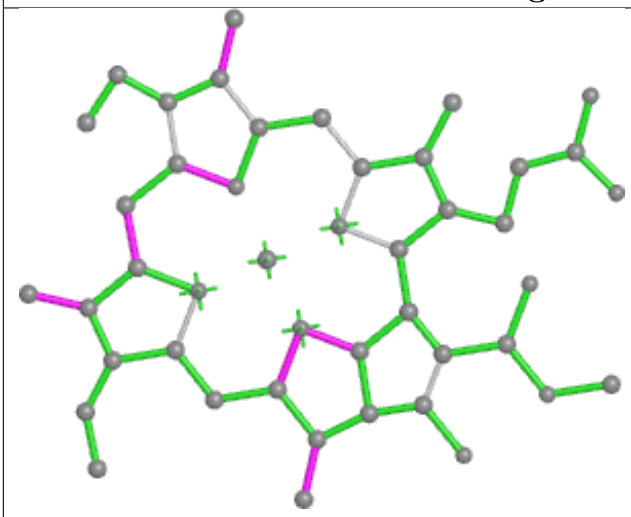


Torsions

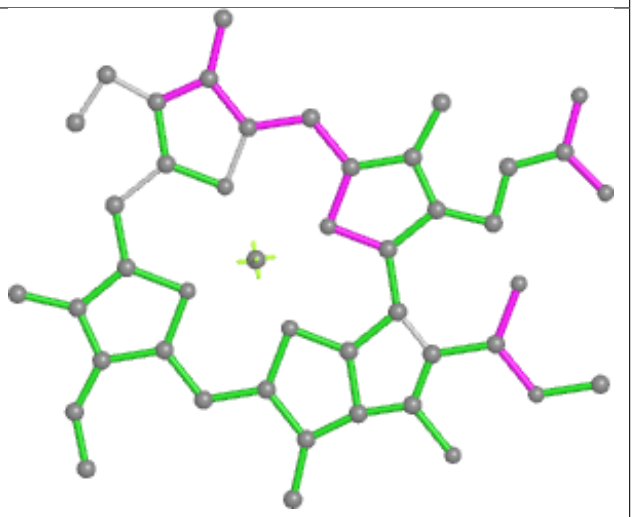


Rings

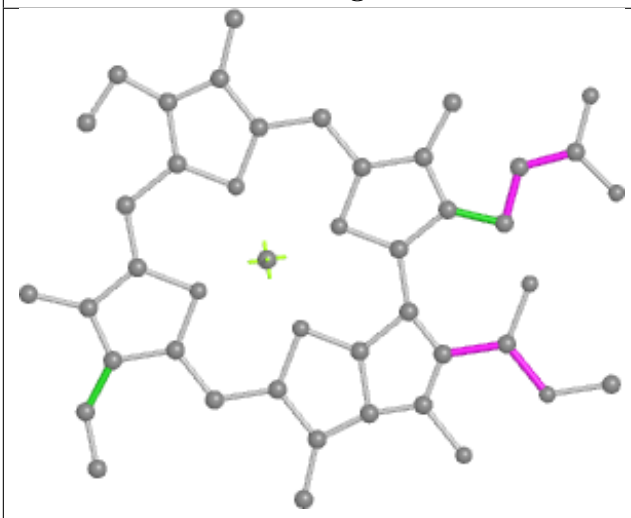
Ligand CLA 0 613



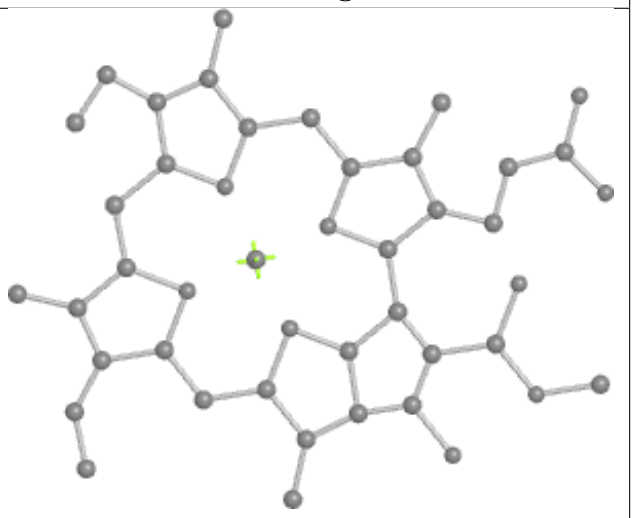
Bond lengths



Bond angles

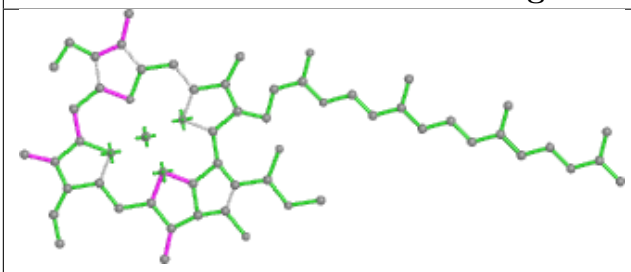


Torsions



Rings

Ligand CLA p 310



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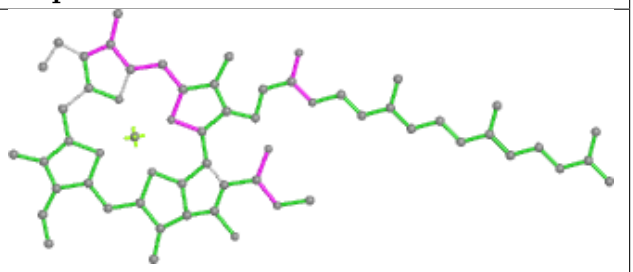
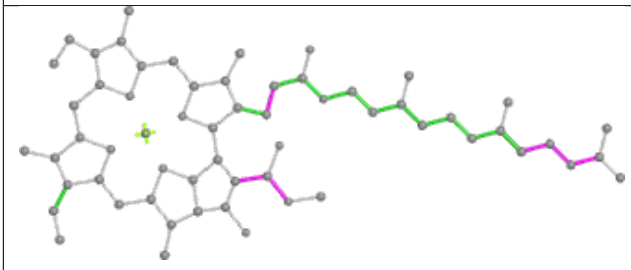


Bond angles



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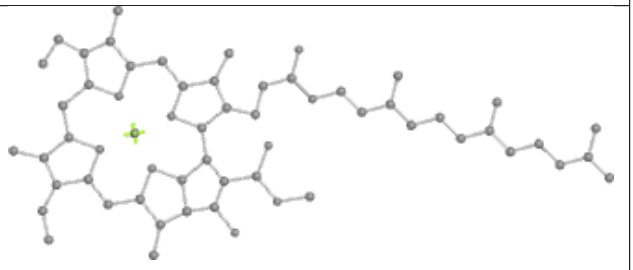
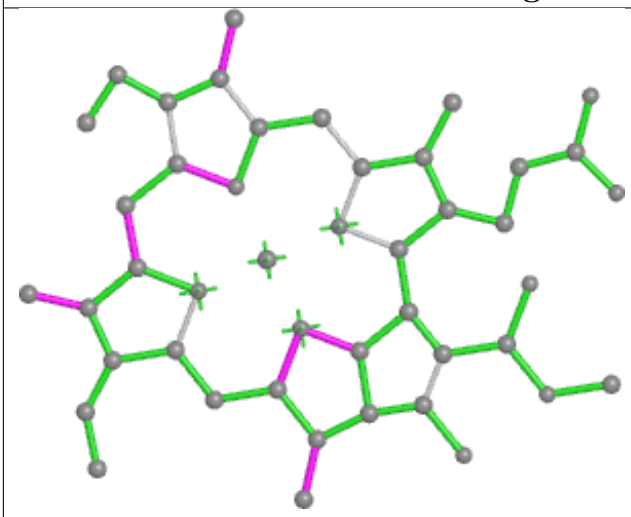
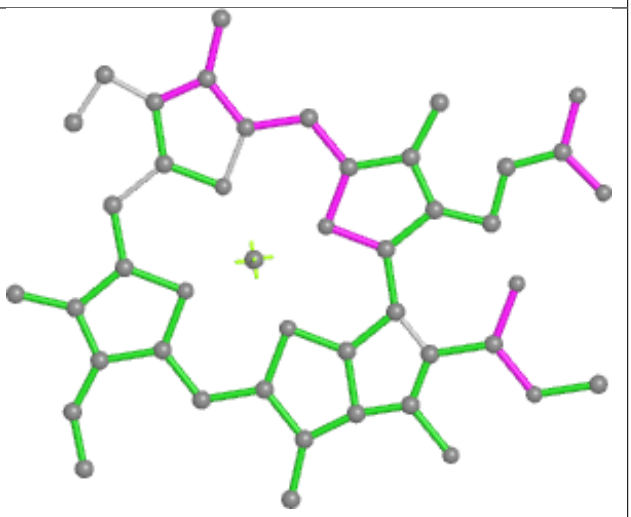


Rings

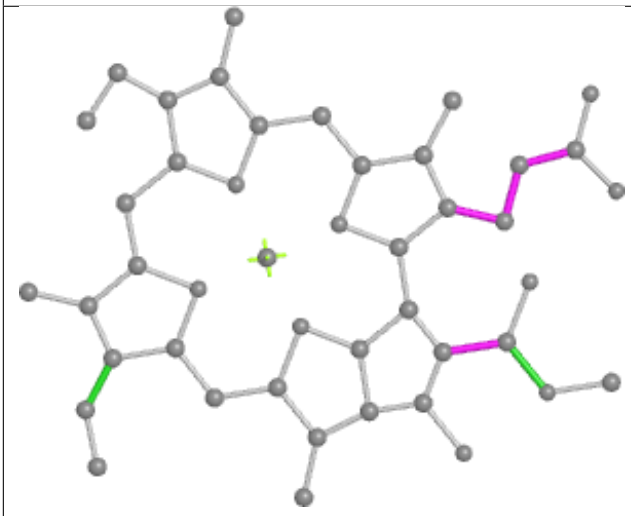
Ligand CLA G 101



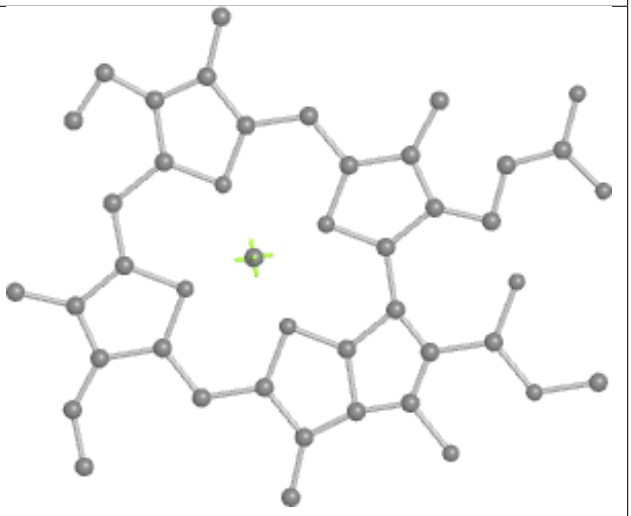
Bond lengths



Bond angles

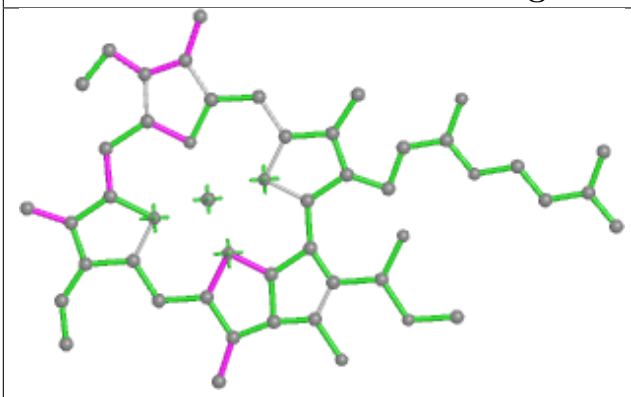


Torsions

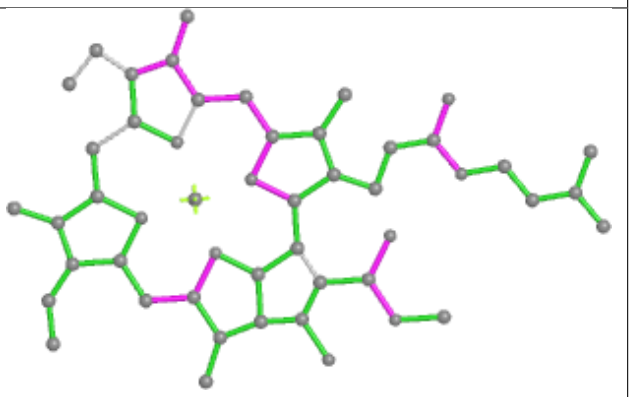


Rings

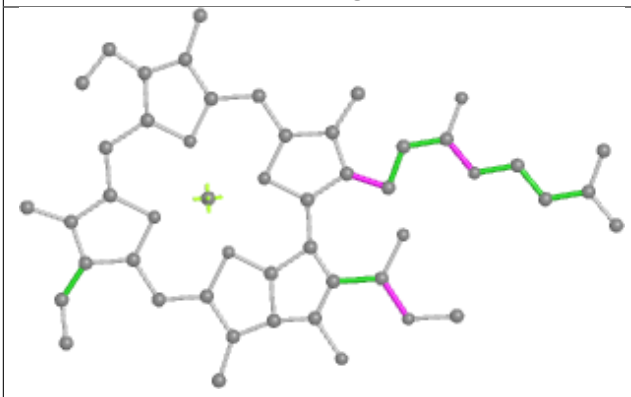
Ligand CLA 7 605



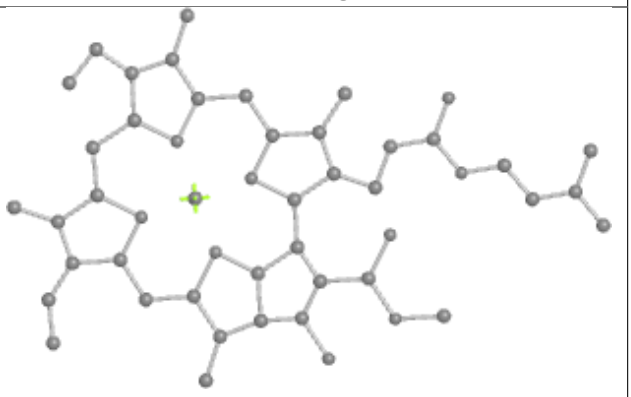
Bond lengths



Bond angles

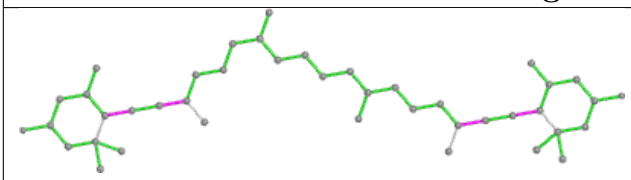


Torsions



Rings

Ligand II0 7 614



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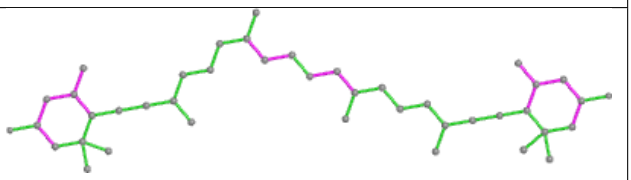
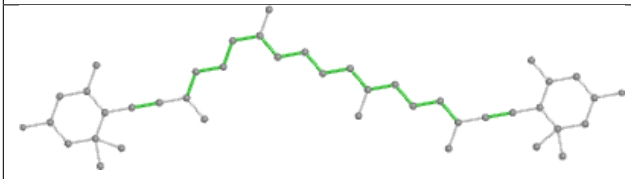
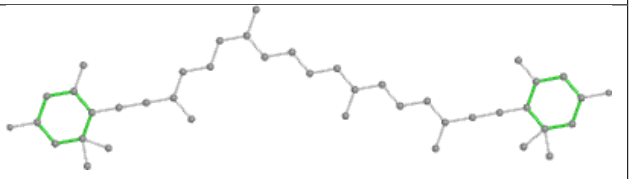


Bond angles

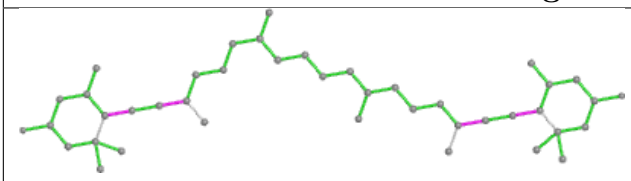


Torsions

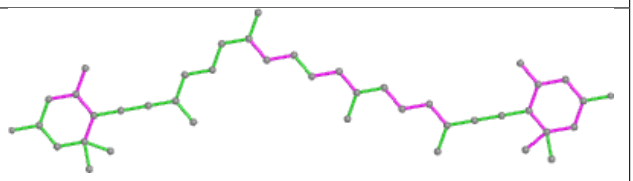


Rings

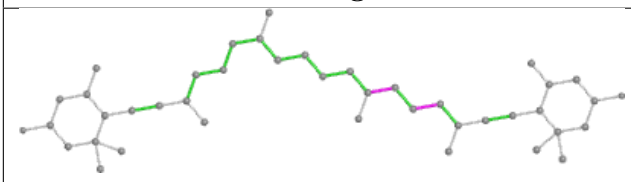
Ligand II0 0 619



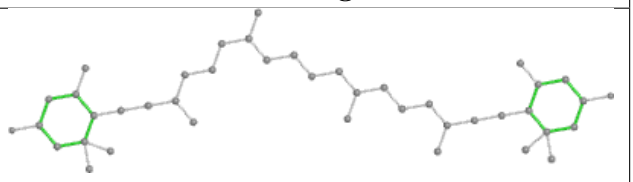
Bond lengths



Bond angles

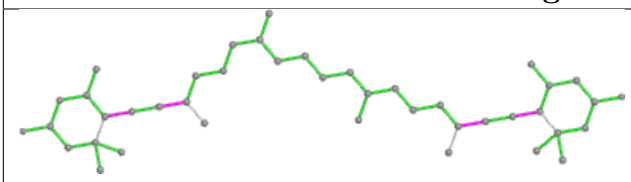


Torsions



Rings

Ligand II0 8 619



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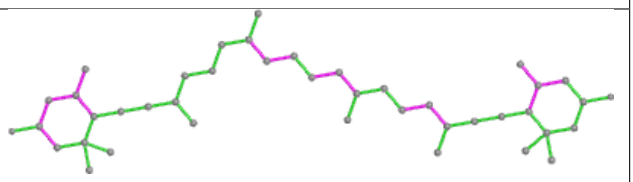
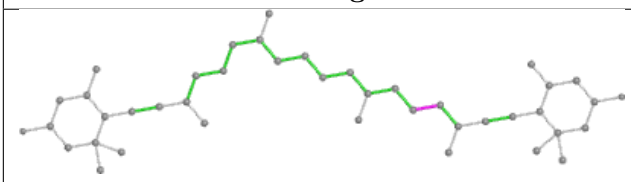
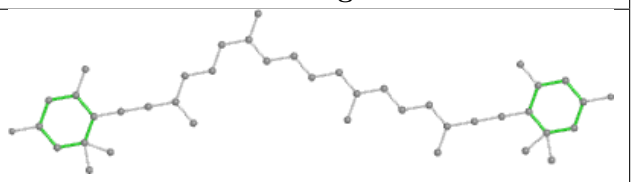


Bond angles

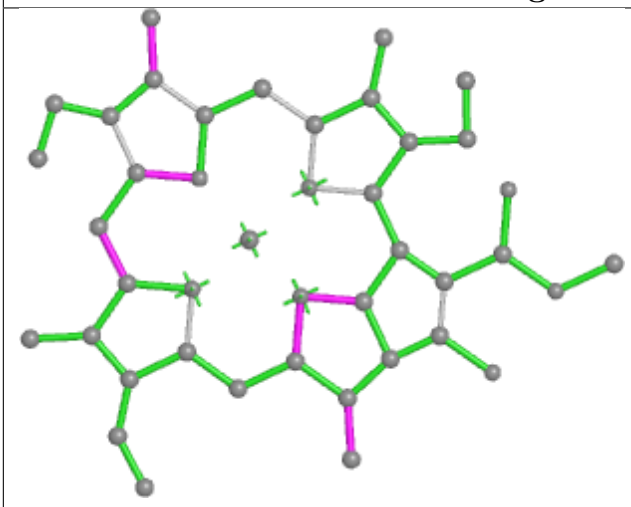


Torsions



Rings

Ligand CLA 0 601



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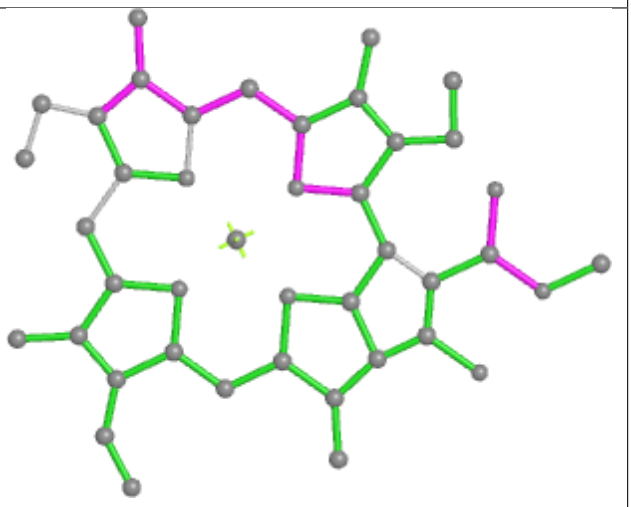
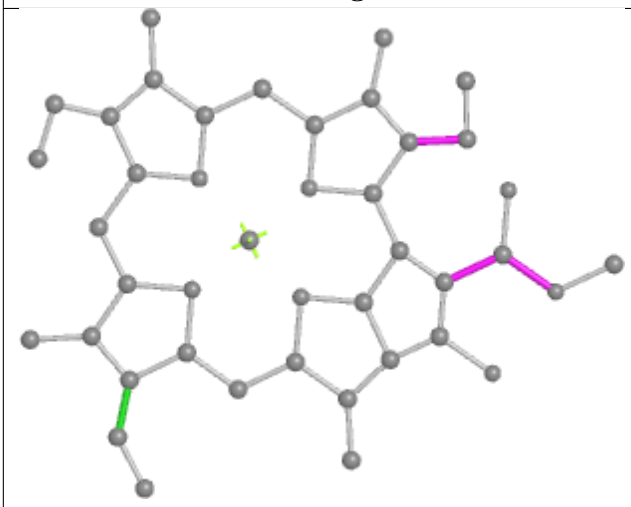


Bond angles



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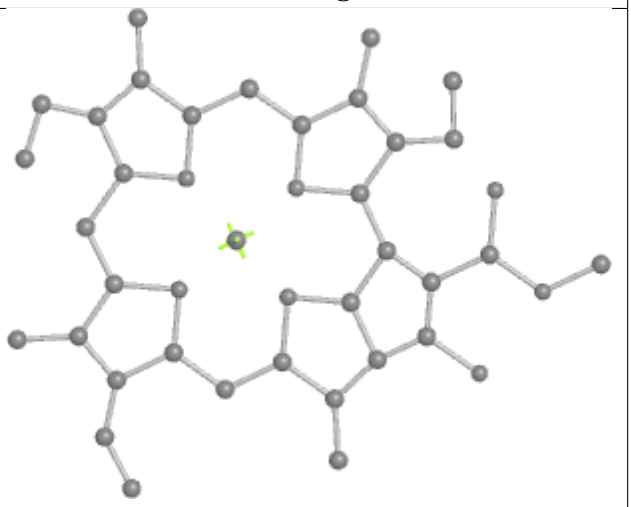
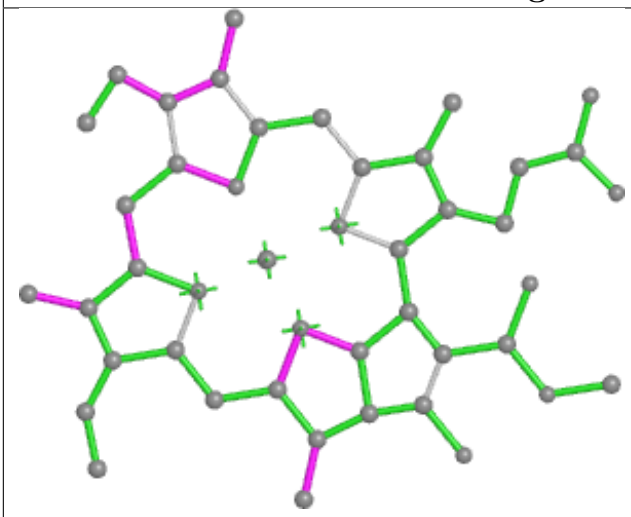


Rings

Ligand CLA 7 607



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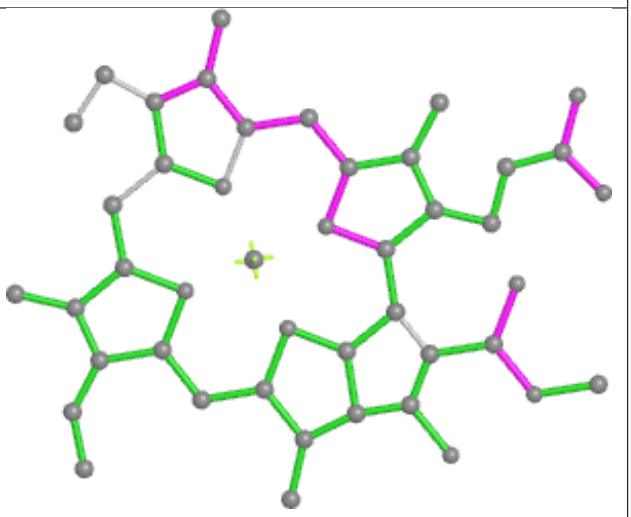

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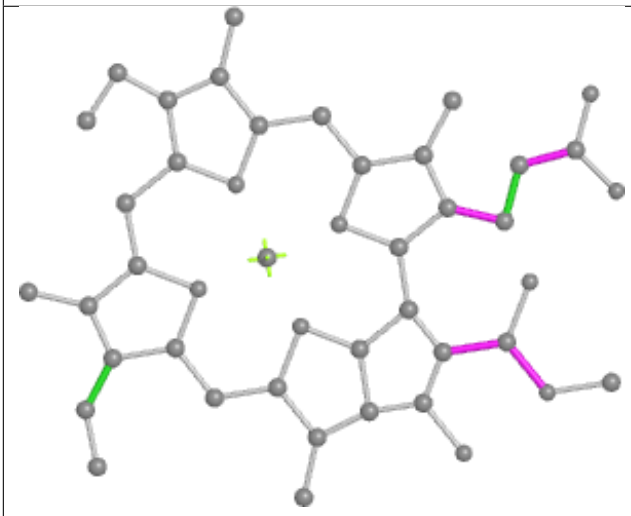
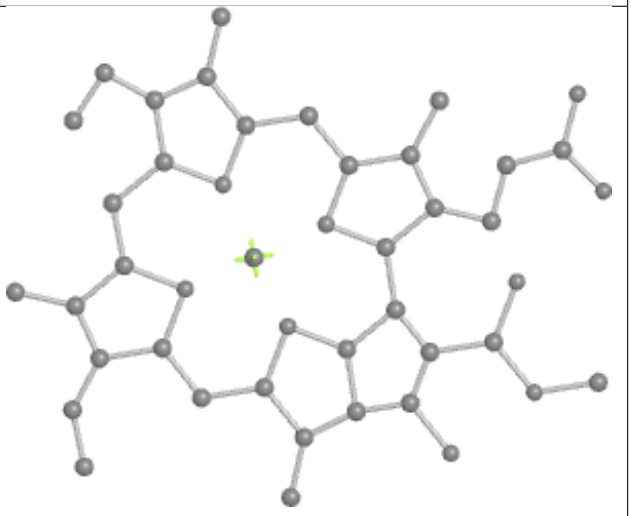
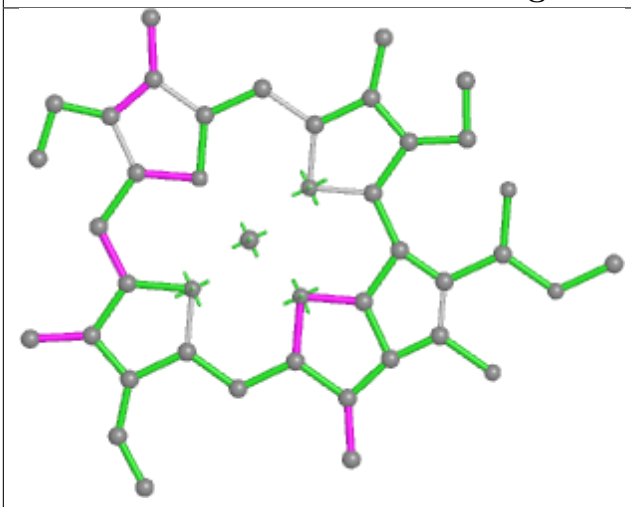


Torsions



Rings

Ligand CLA 8 601



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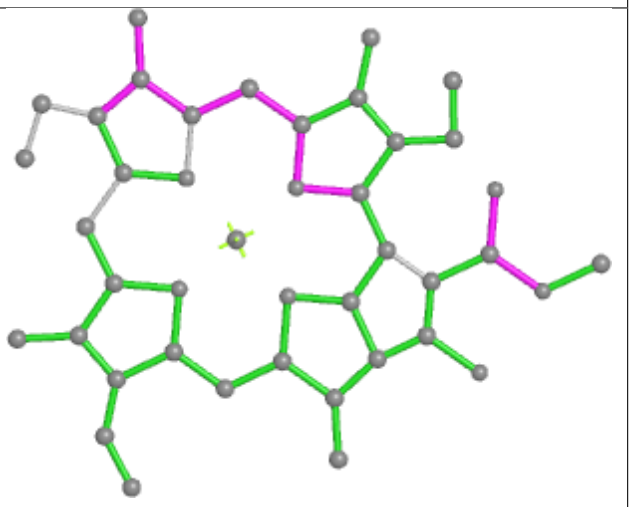
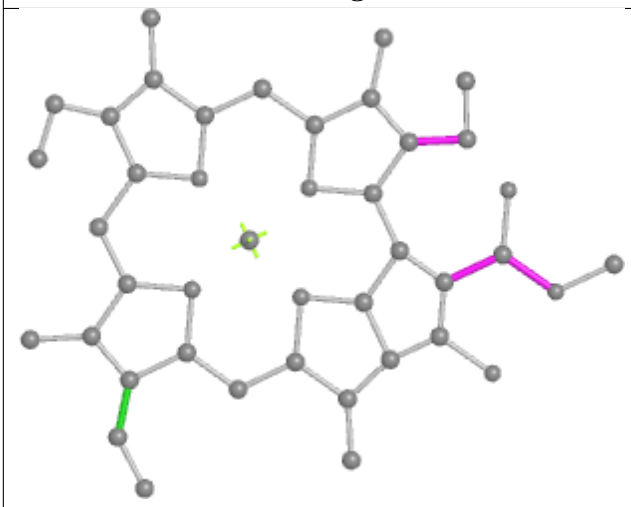
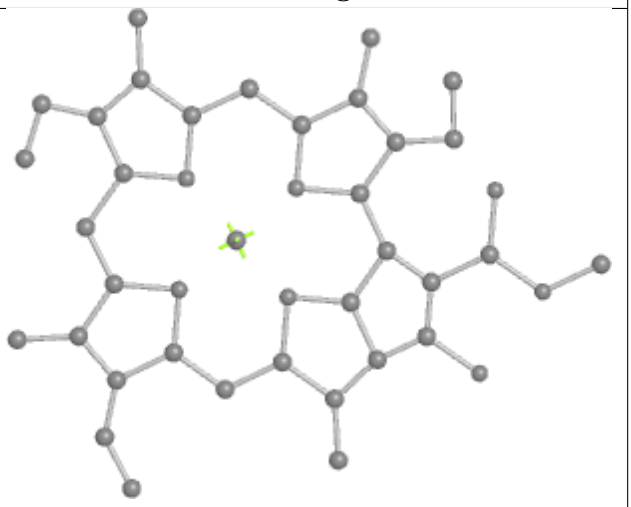


Bond angles

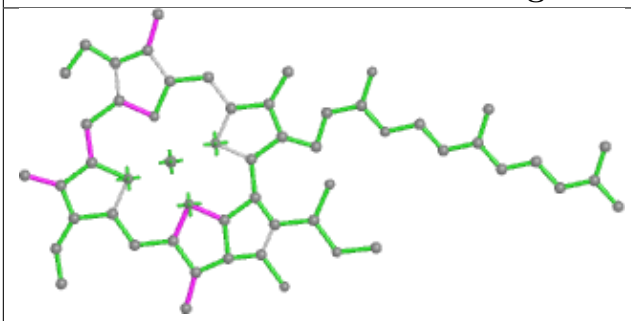


Torsions



Rings

Ligand CLA p 306



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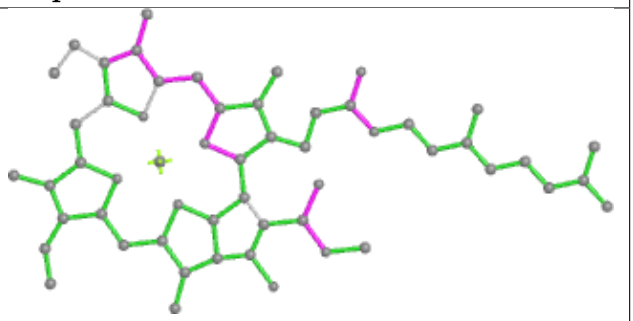
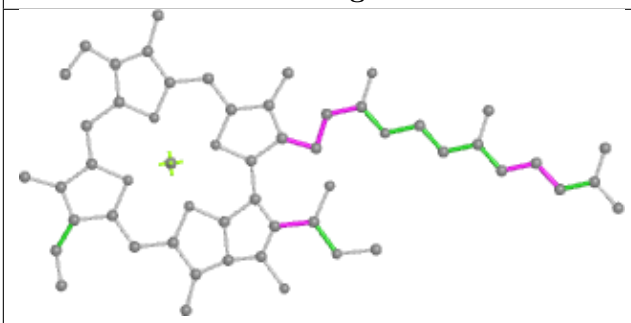


Bond angles



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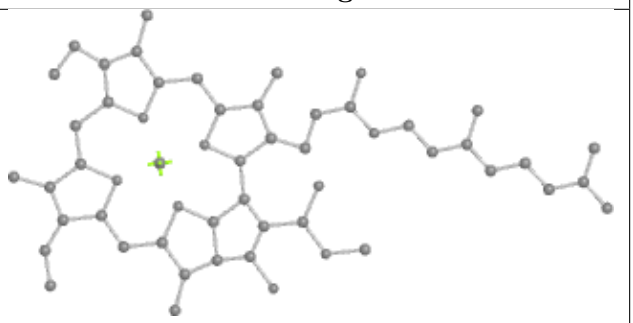
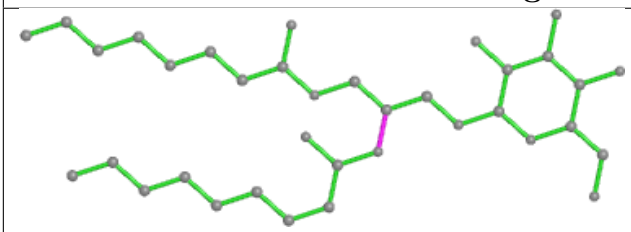


Rings

Ligand LMG 0 618



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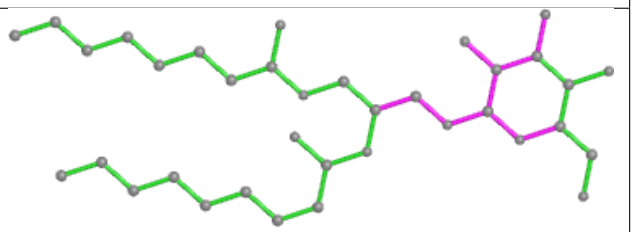

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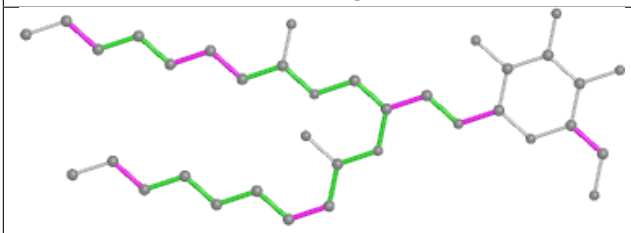
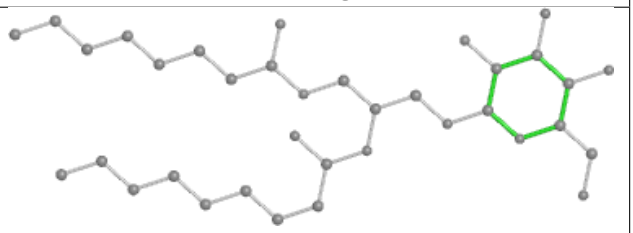
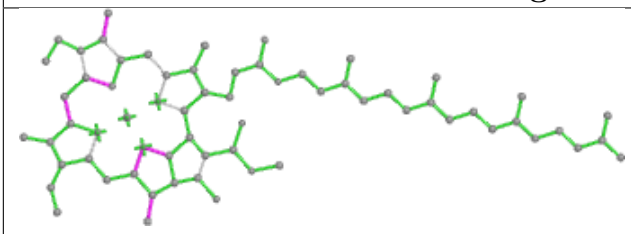


Torsions



Rings

Ligand CLA s 303



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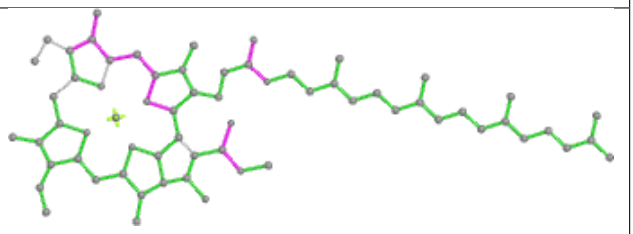
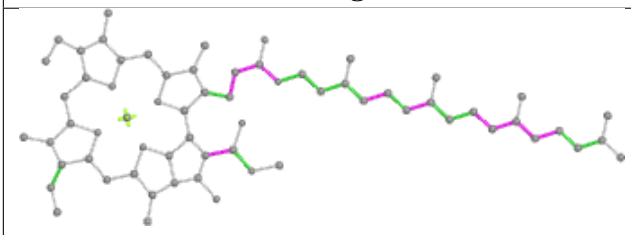


Bond angles



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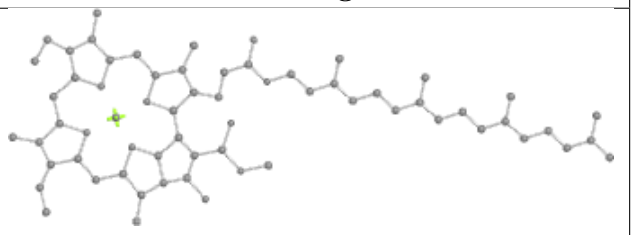
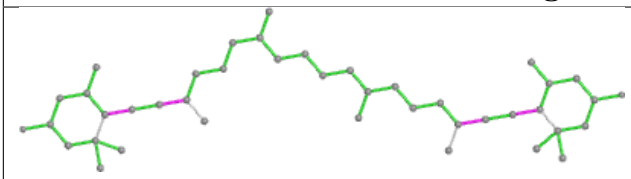


Rings

Ligand II0 9 614



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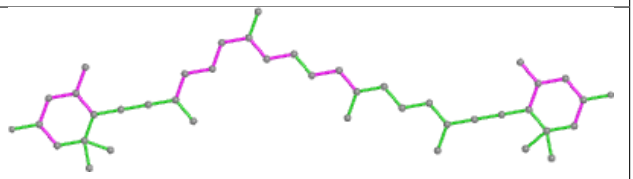
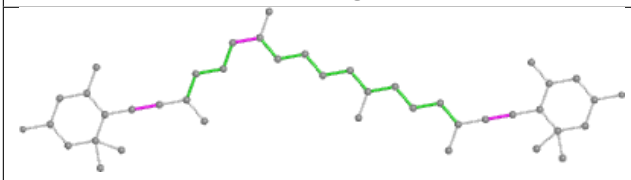
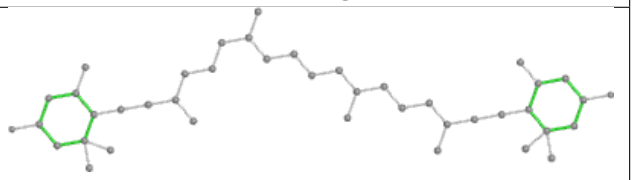


Bond angles

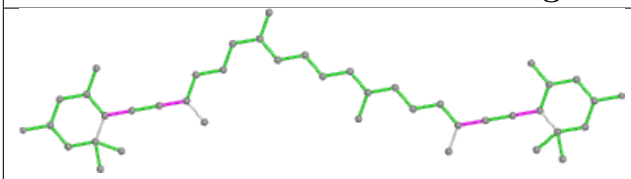


Torsions

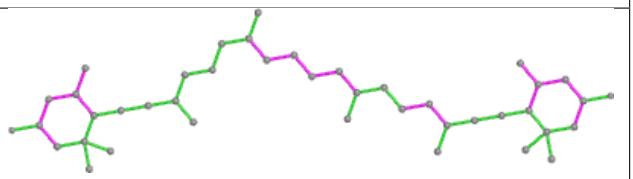


Rings

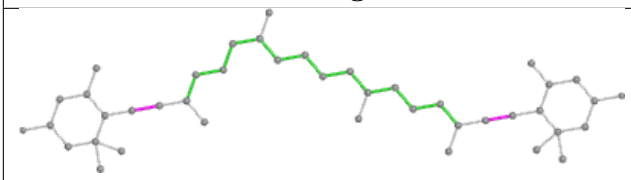
Ligand II0 9 612



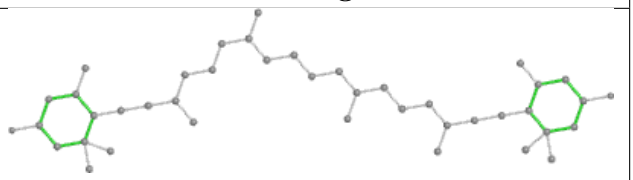
Bond lengths



Bond angles

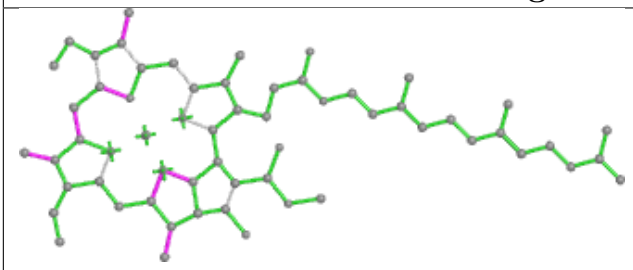


Torsions

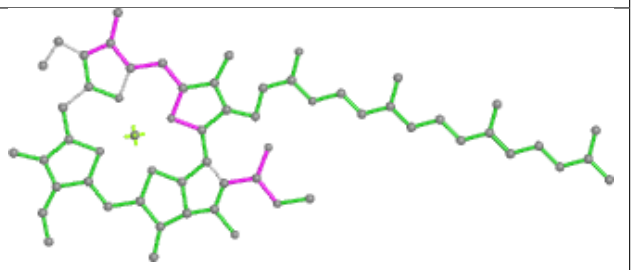


Rings

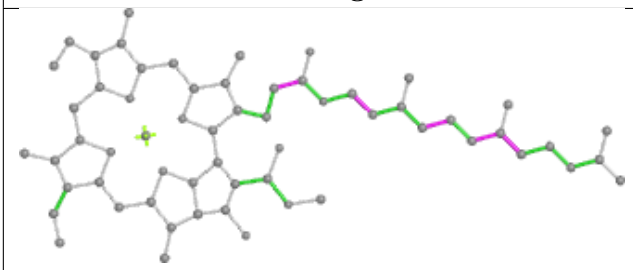
Ligand CLA 9 609



Bond lengths



Bond angles



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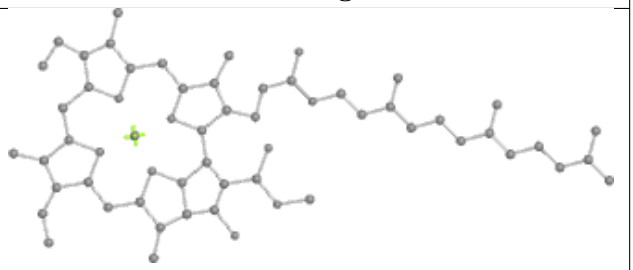
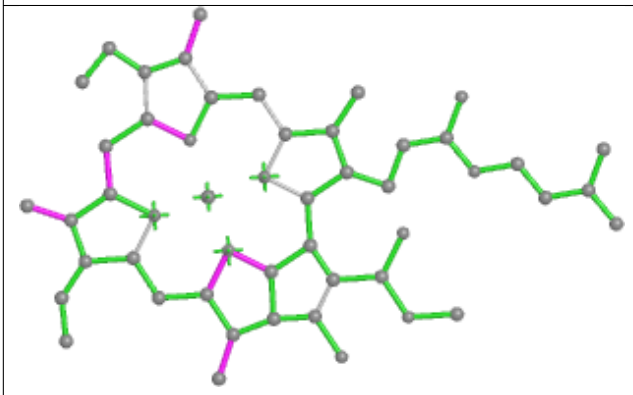


Rings

Ligand CLA P 603



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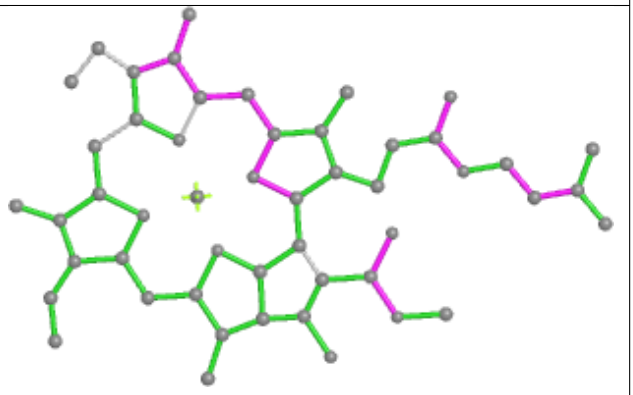
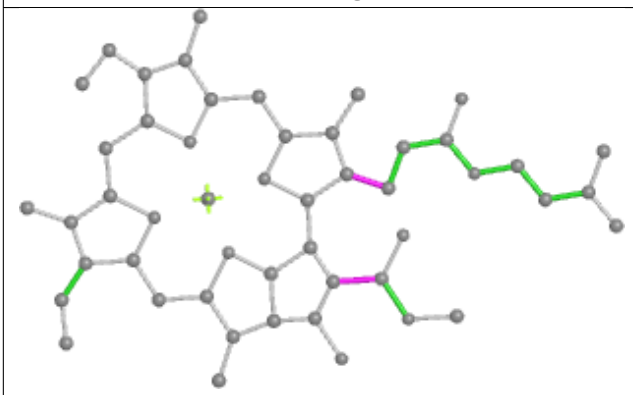
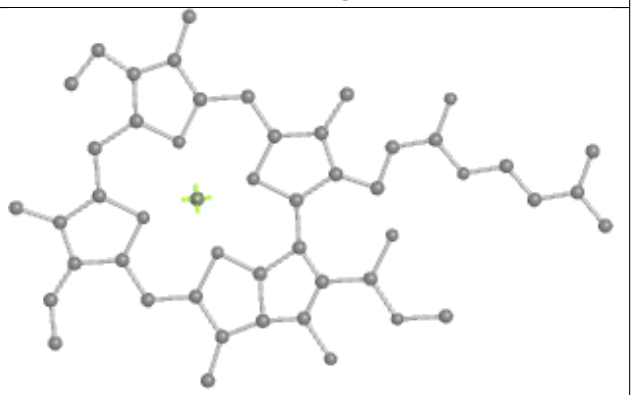


Bond angles

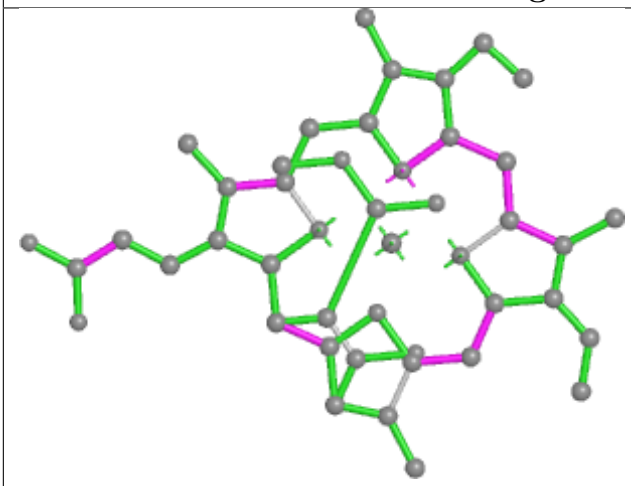


Torsions

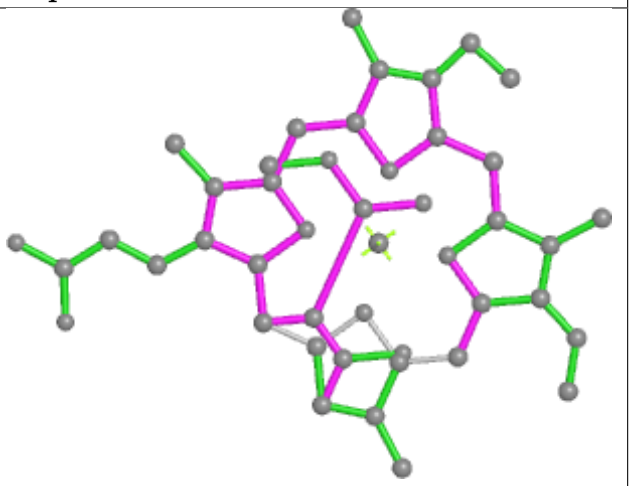


Rings

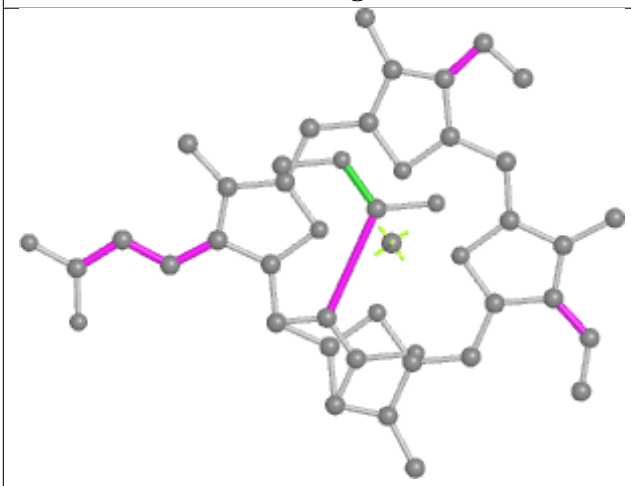
Ligand KC2 p 312



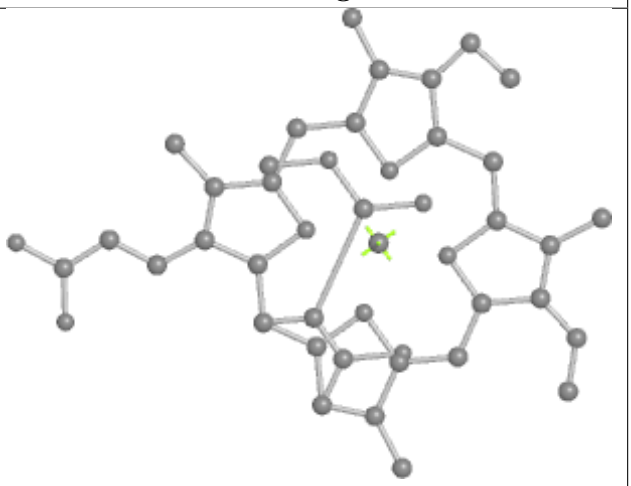
Bond lengths



Bond angles

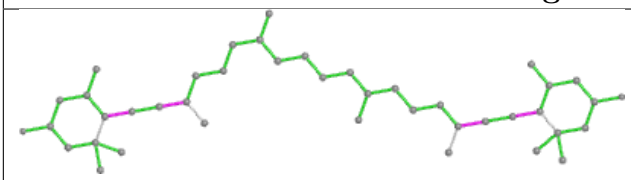


Torsions

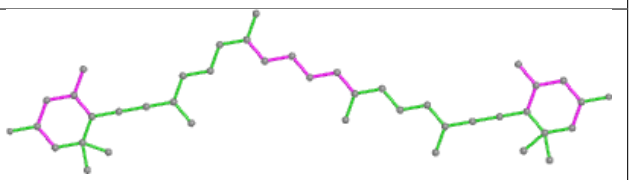


Rings

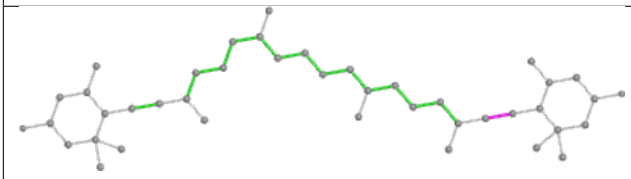
Ligand II0 9 613



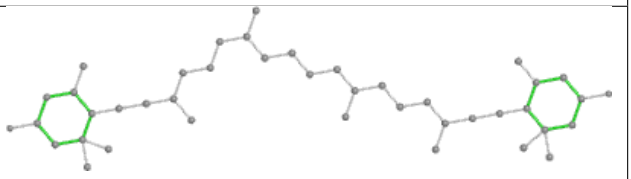
Bond lengths



Bond angles

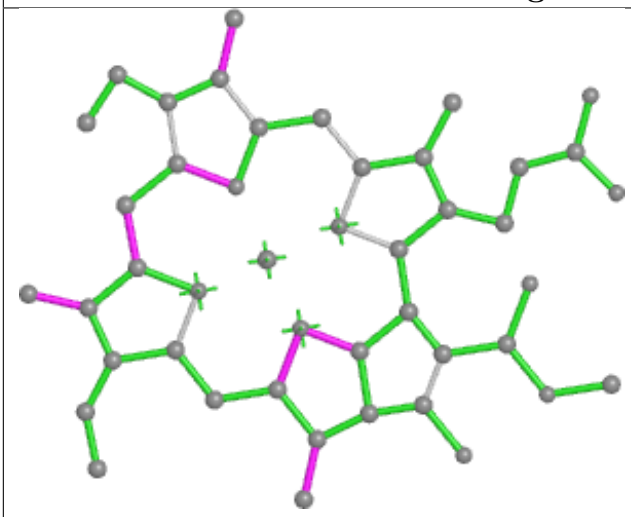


Torsions

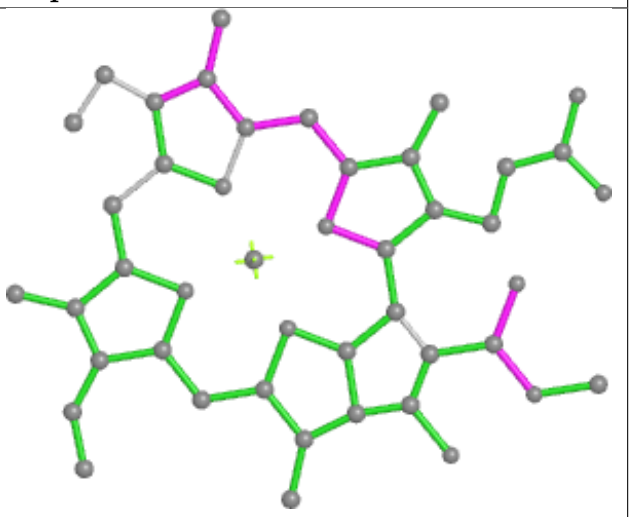


Rings

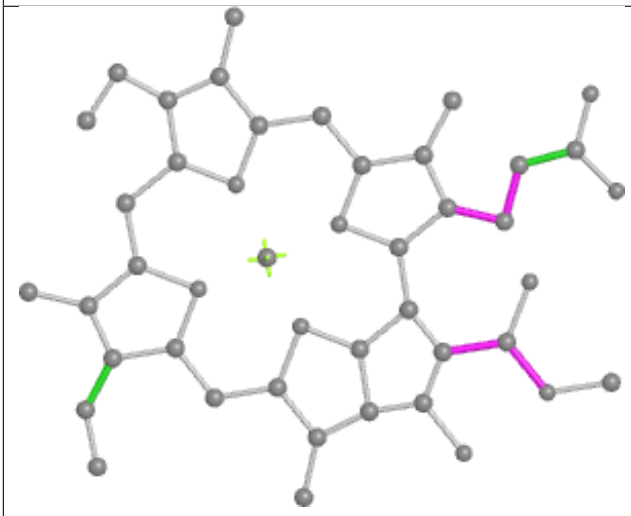
Ligand CLA p 314



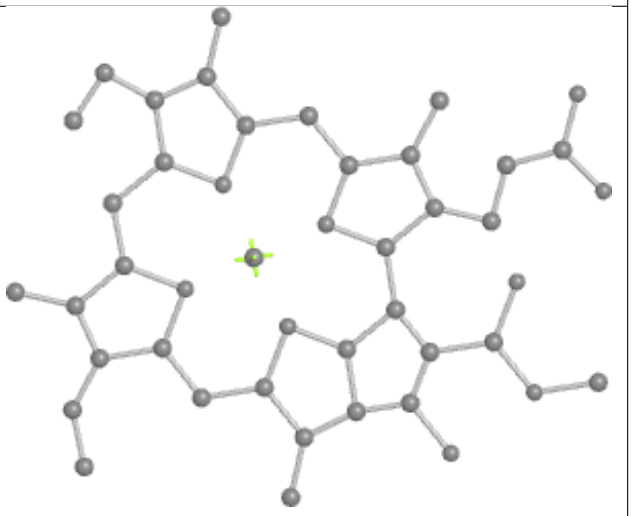
Bond lengths



Bond angles

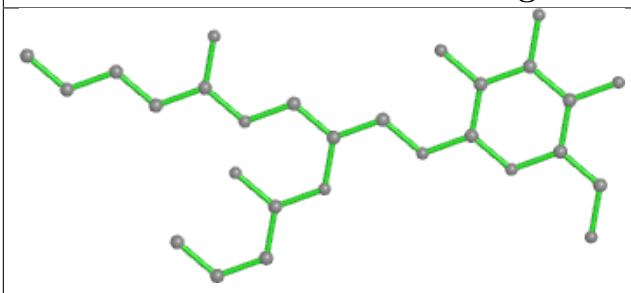


Torsions

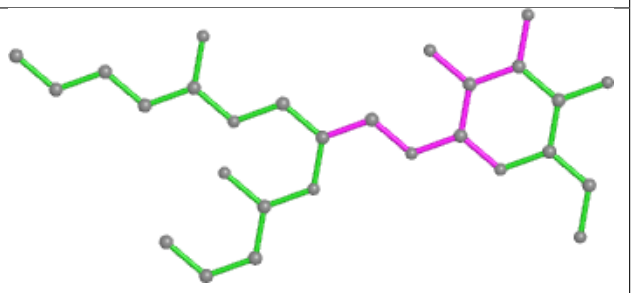


Rings

Ligand LMG G 103



Bond lengths



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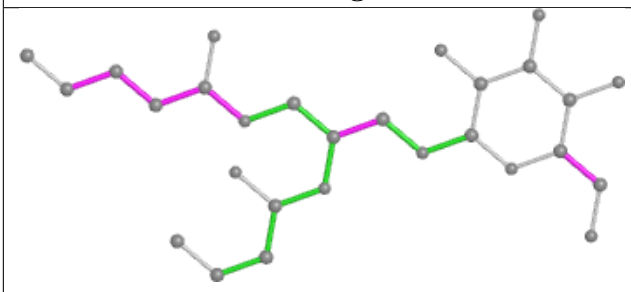

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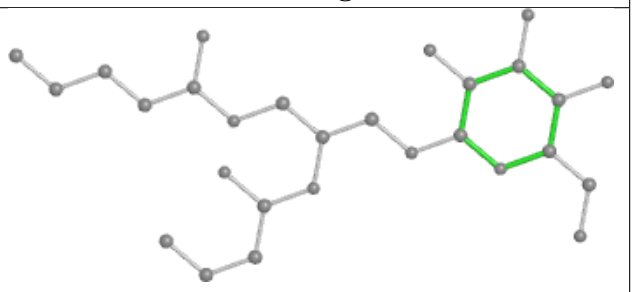
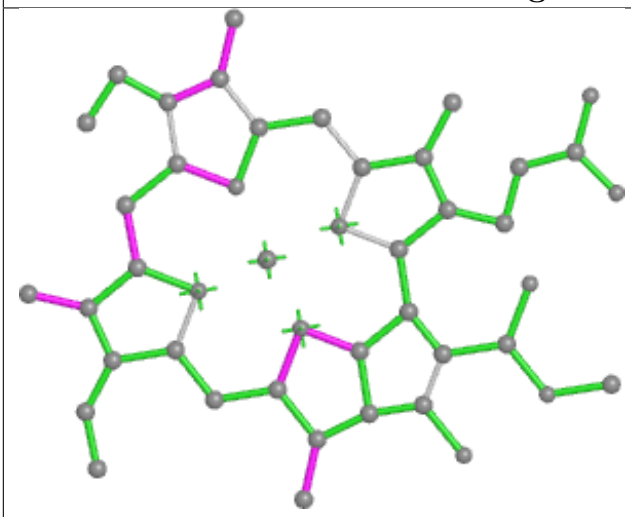


Rings

Ligand CLA 8 612



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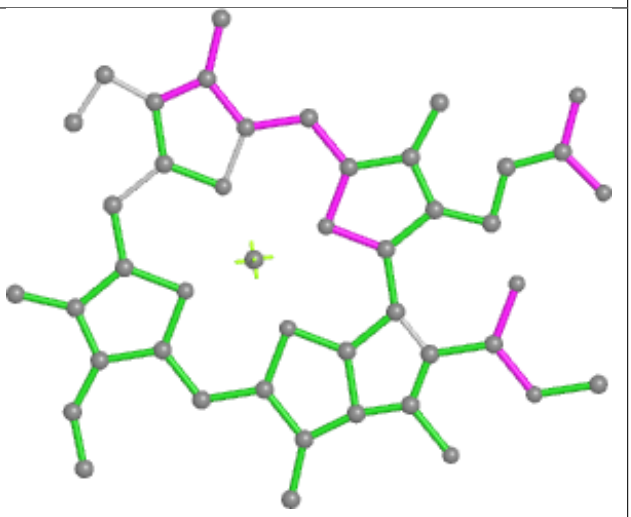

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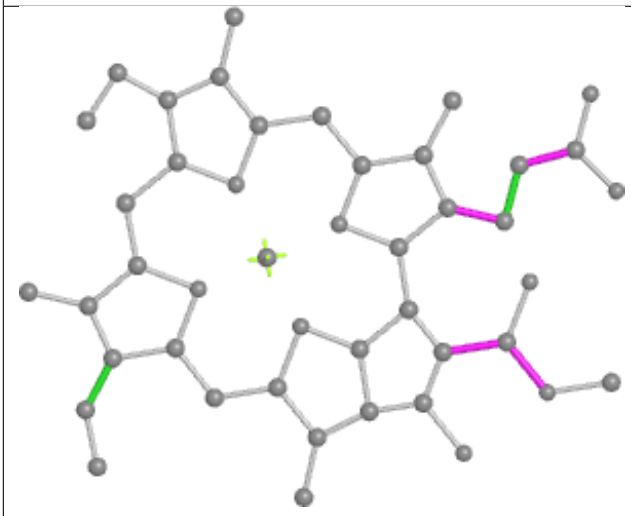

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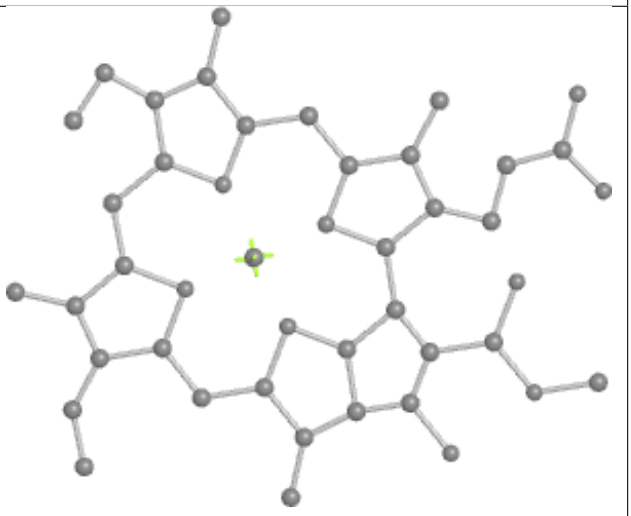
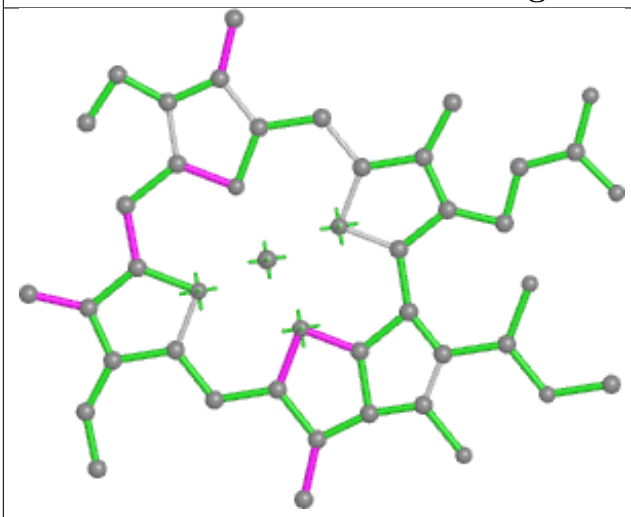


Rings

Ligand CLA 9 610



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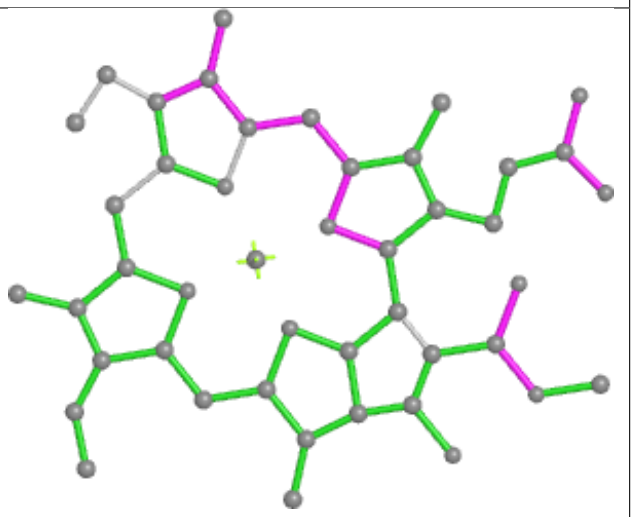

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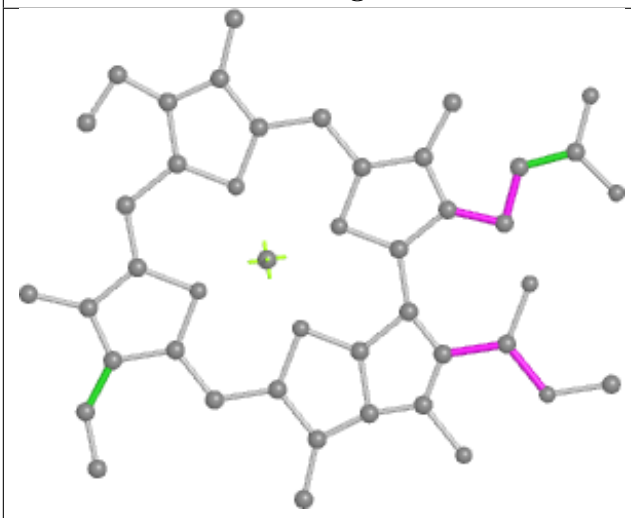

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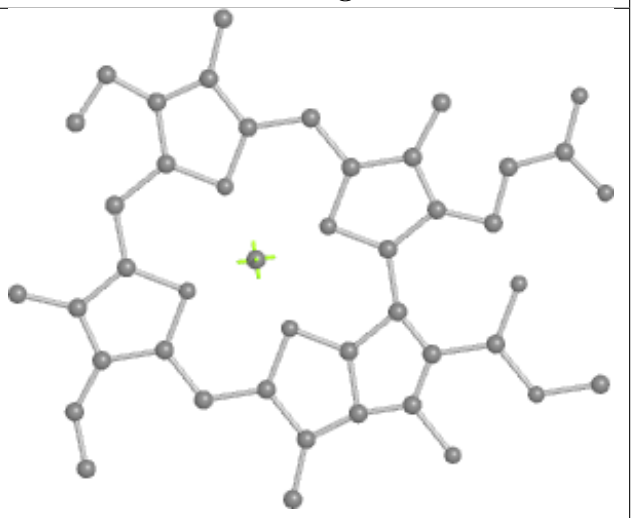
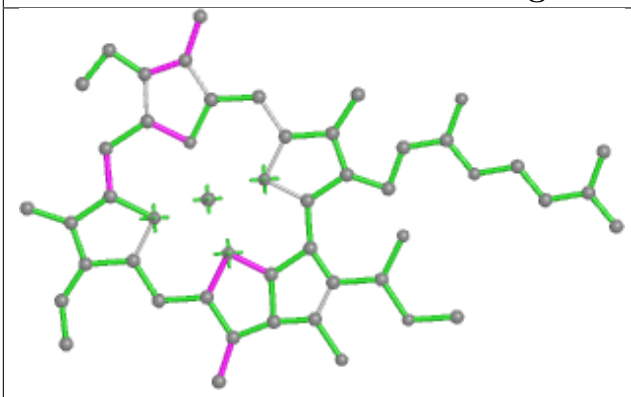


Rings

Ligand CLA 0 605



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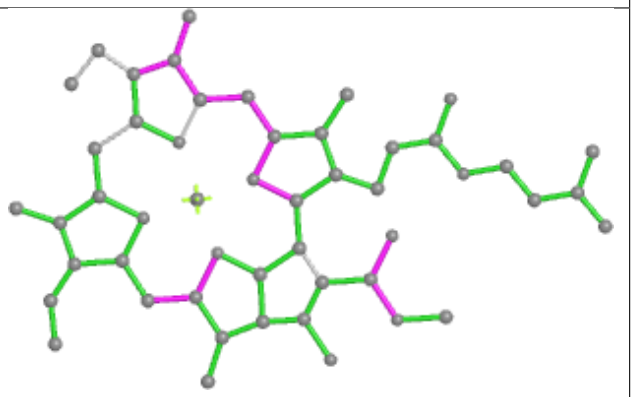
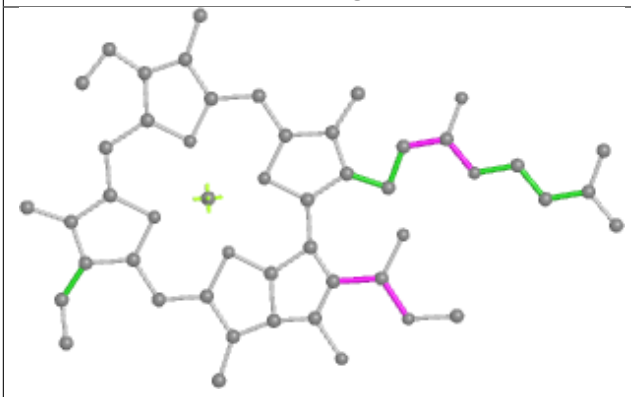


Bond angles



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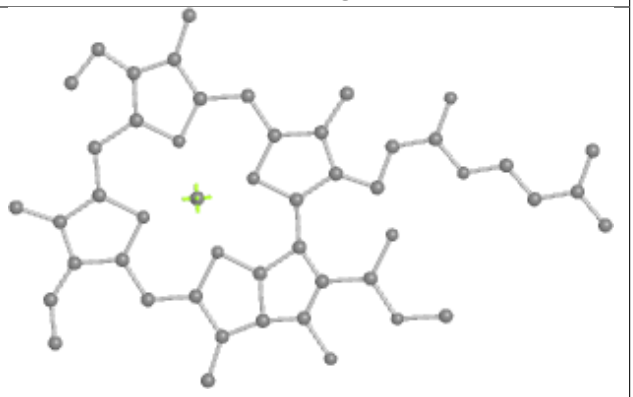
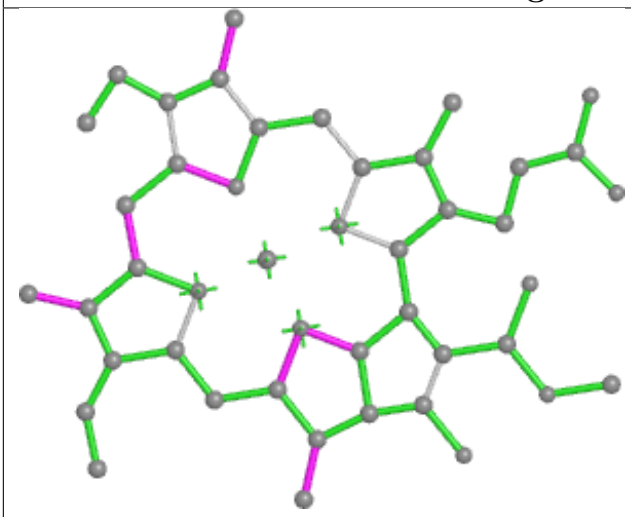


Rings

Ligand CLA p 309



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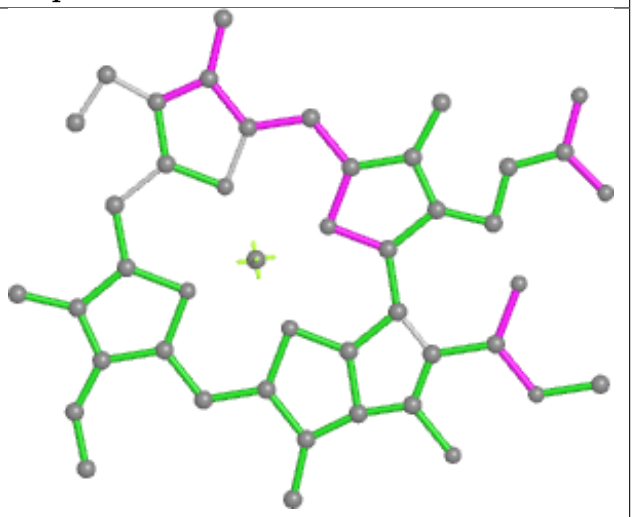
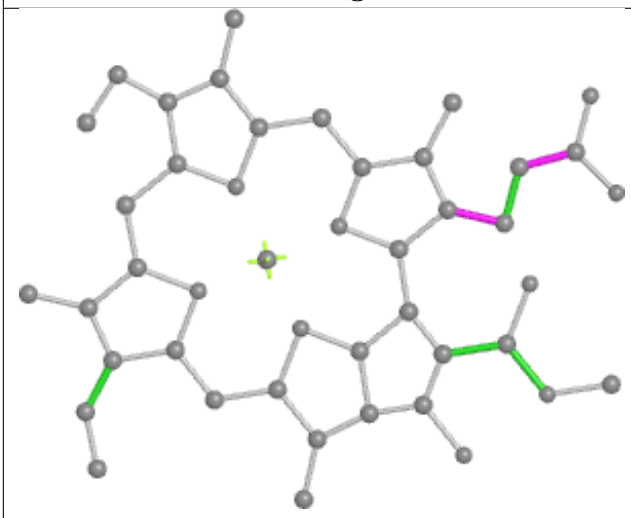


Bond angles



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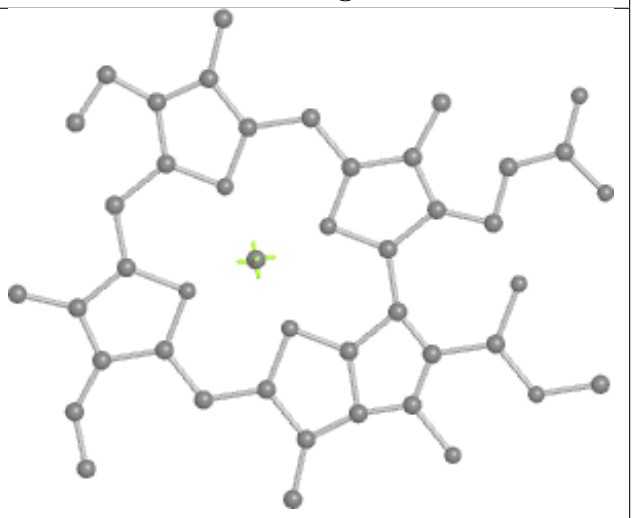
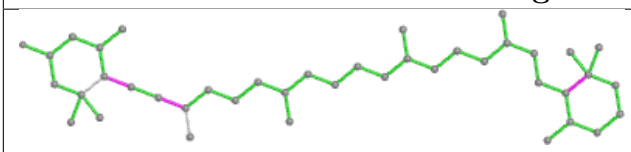


Rings

Ligand IHT 8 616



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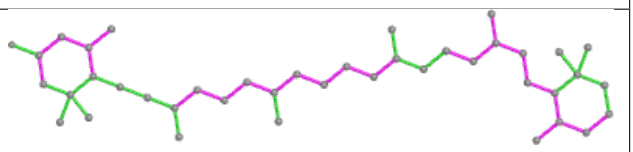

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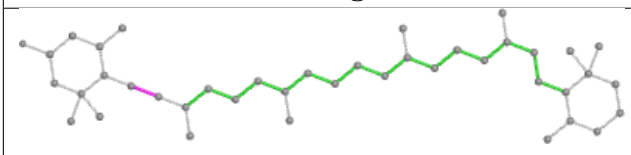

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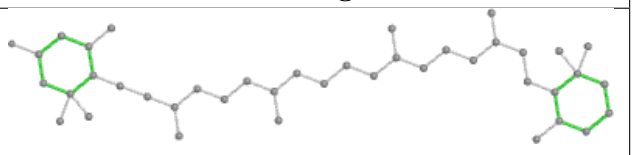
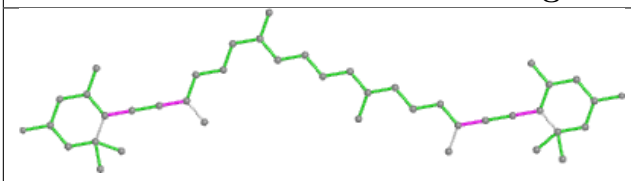


Rings

Ligand II0 0 615



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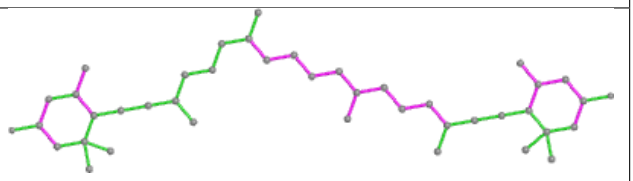
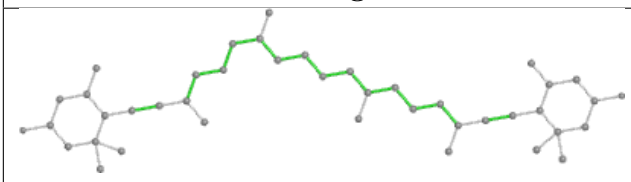


Bond angles



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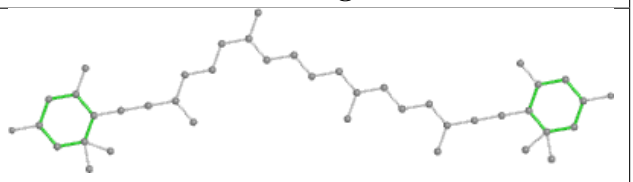
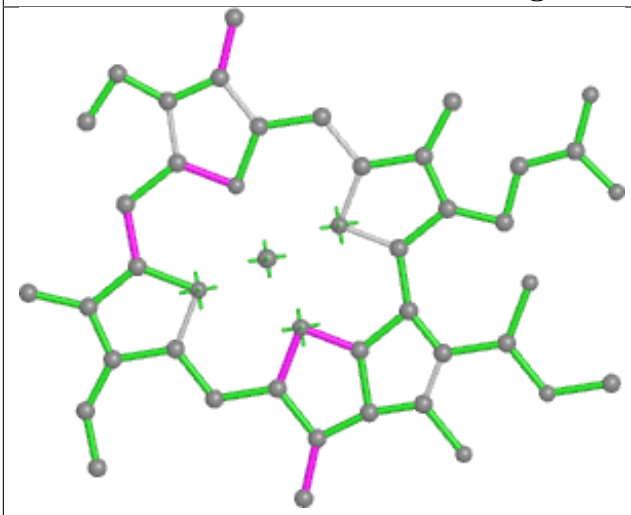


Rings

Ligand CLA 7 613



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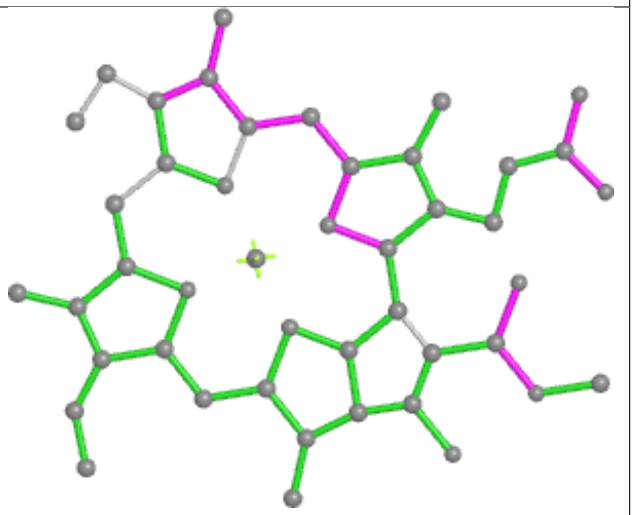
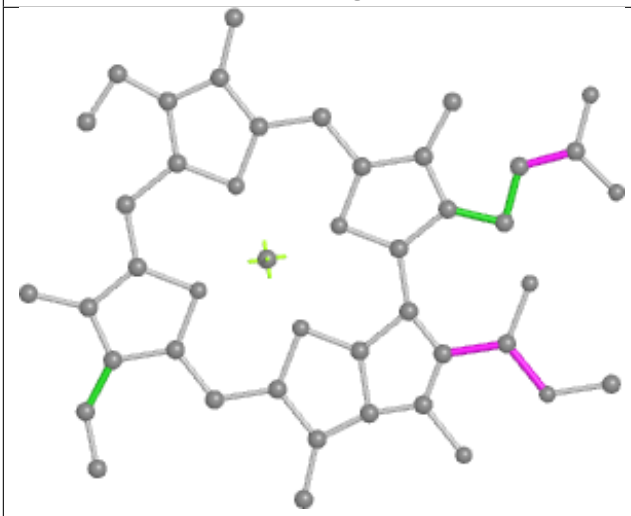
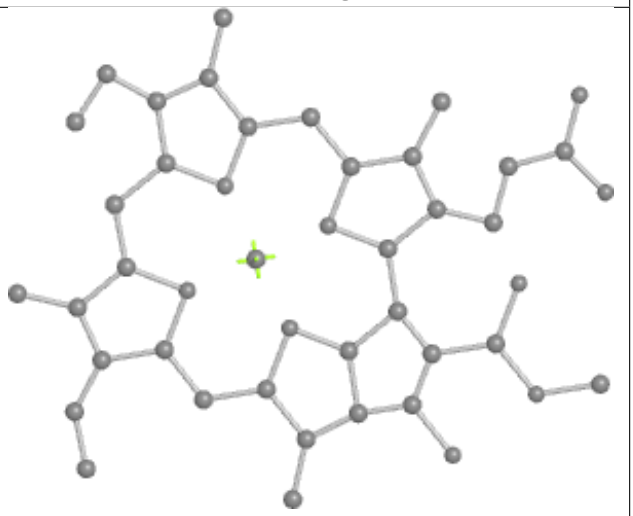


Bond angles

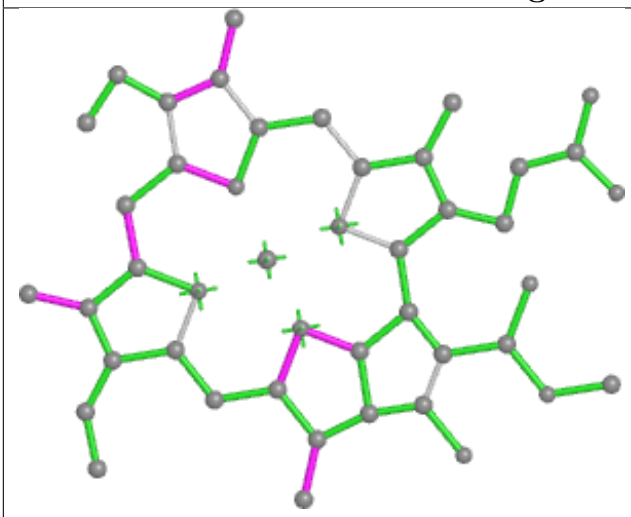


Torsions



Rings

Ligand CLA 9 606



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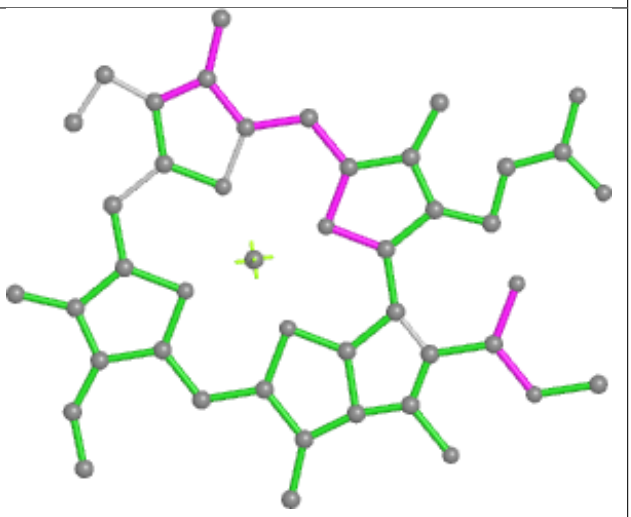

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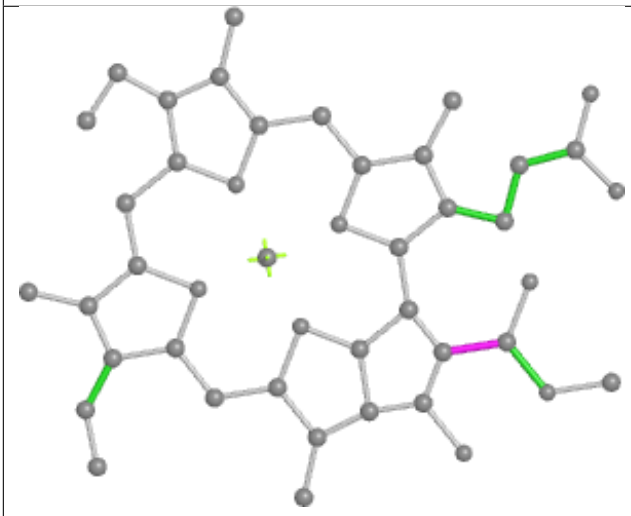

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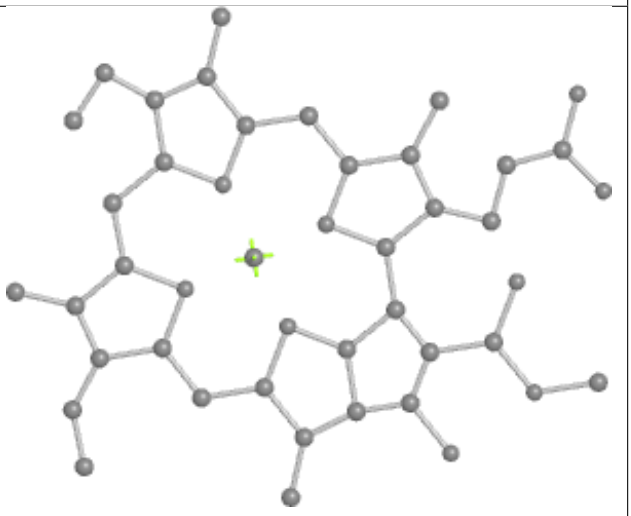
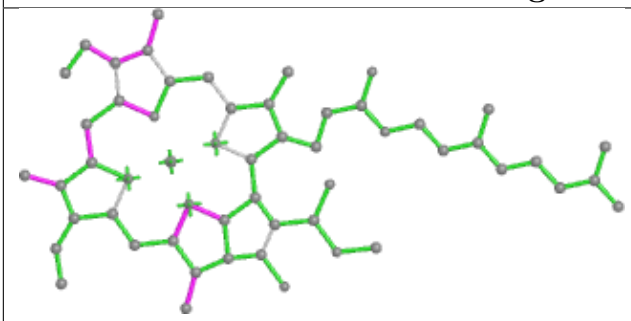


Rings

Ligand CLA 0 604



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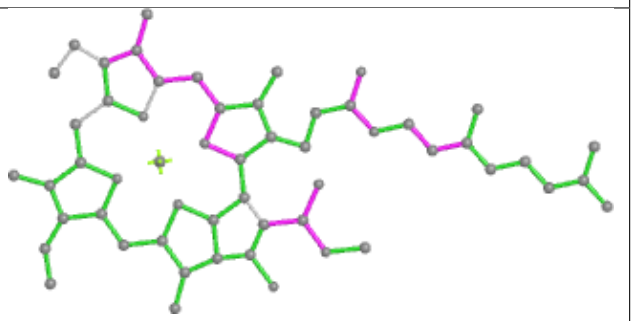
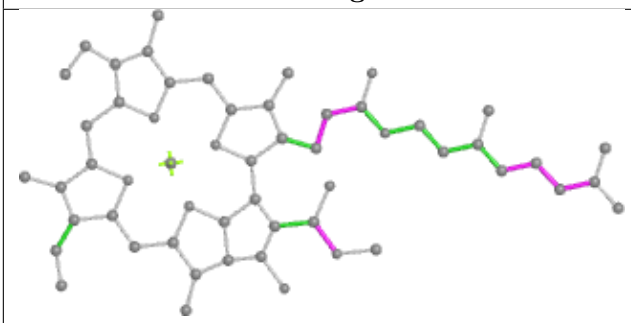


Bond angles



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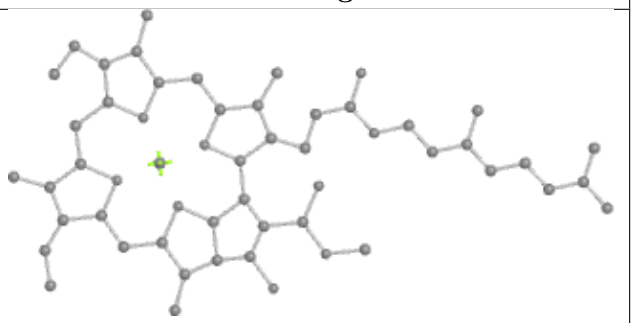
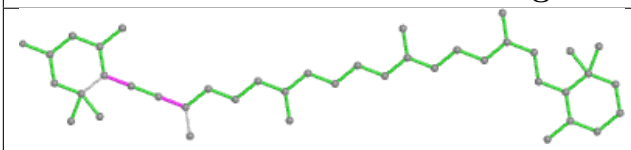


Rings

Ligand IHT 0 614



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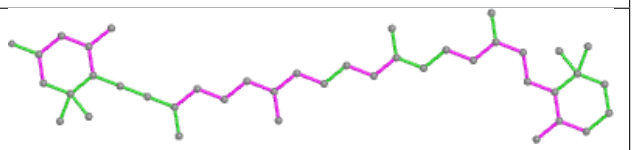
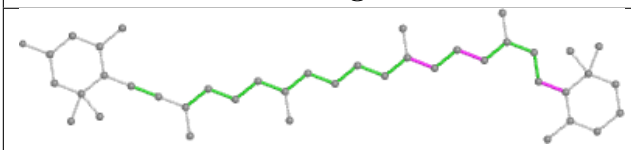
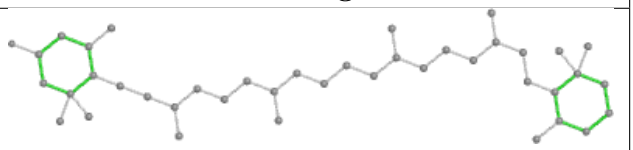


Bond angles

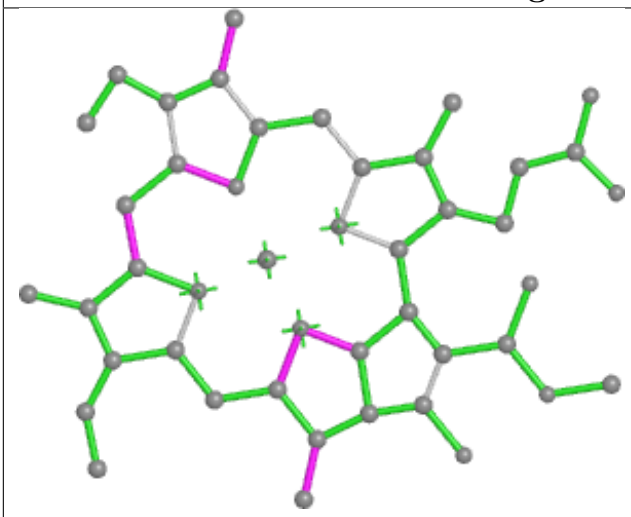


Torsions



Rings

Ligand CLA 0 607



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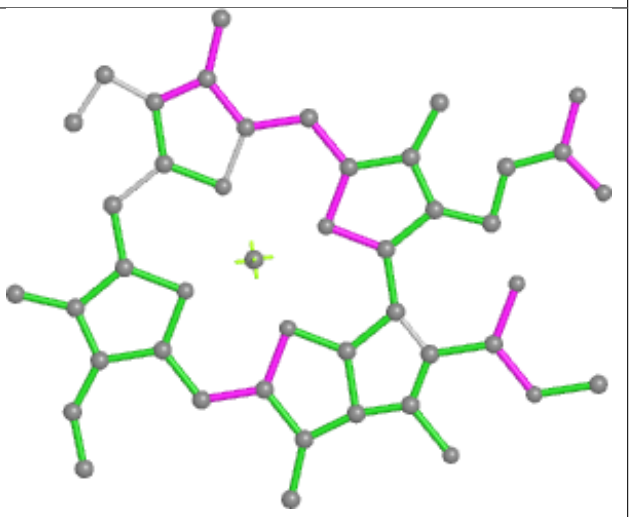
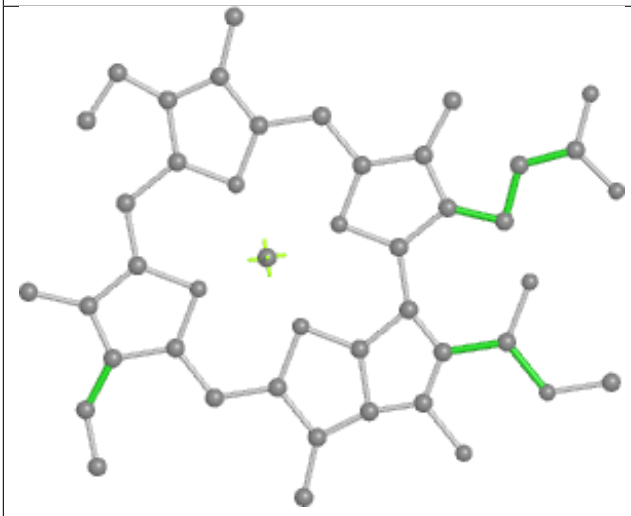
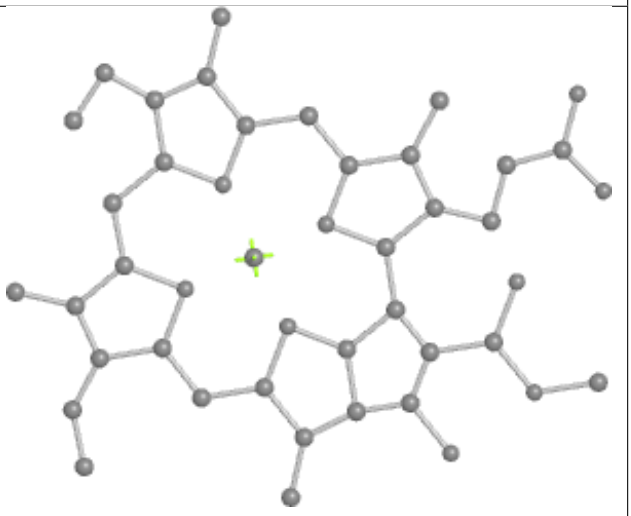


Bond angles

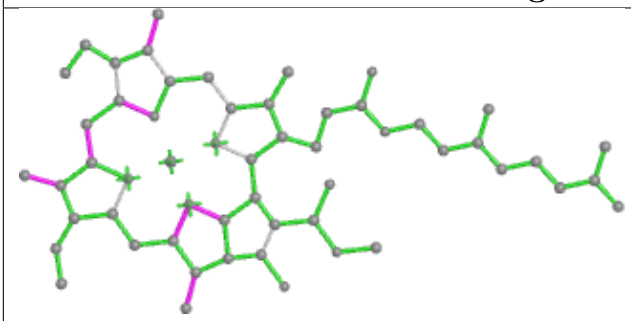


Torsions

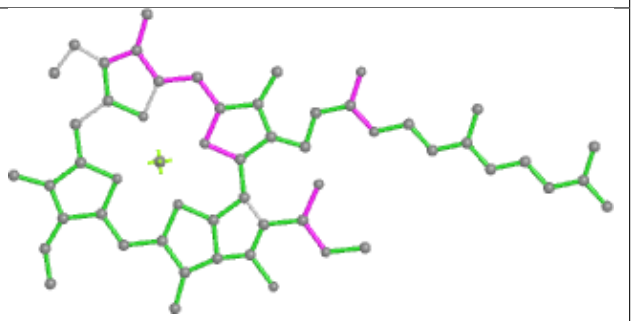


Rings

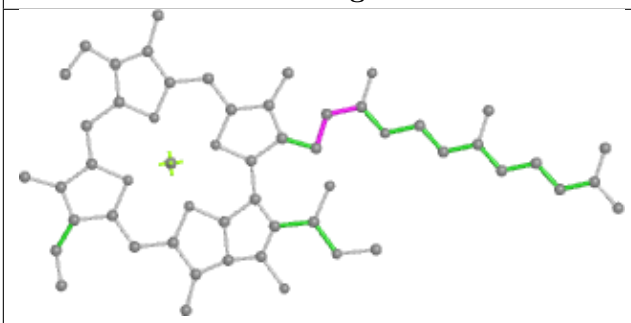
Ligand CLA 8 604



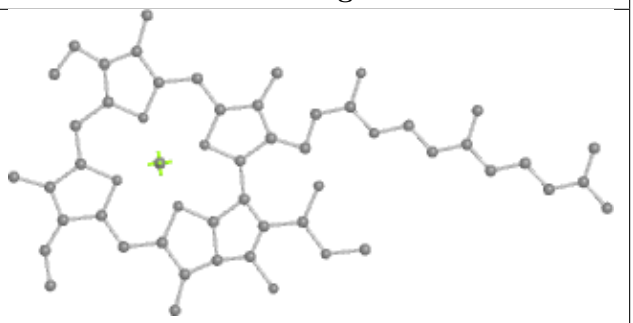
Bond lengths



Bond angles

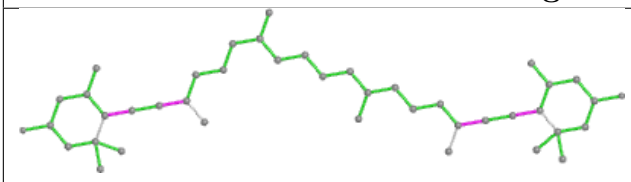


Torsions

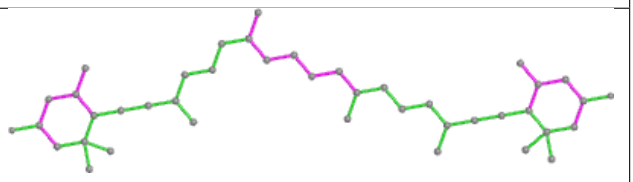


Rings

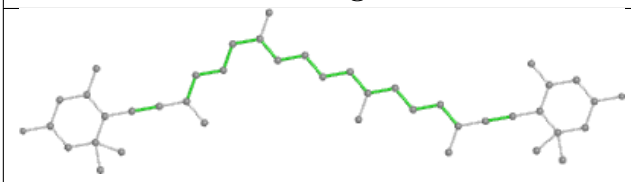
Ligand II0 8 613



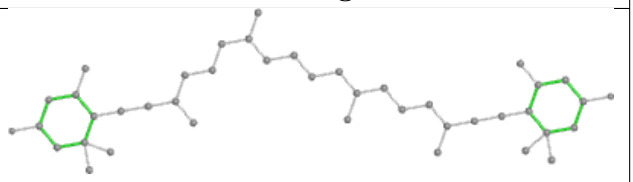
Bond lengths



Bond angles

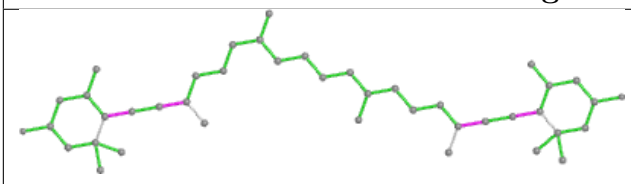


Torsions

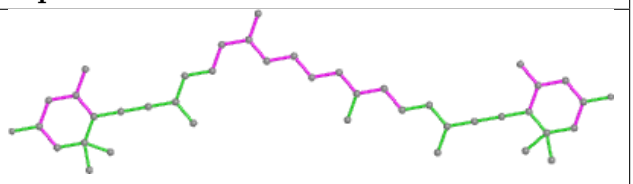


Rings

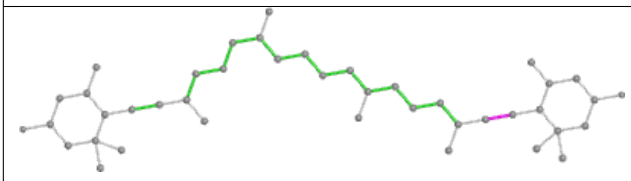
Ligand II0 p 315



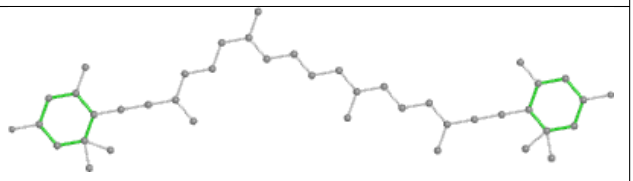
Bond lengths



Bond angles

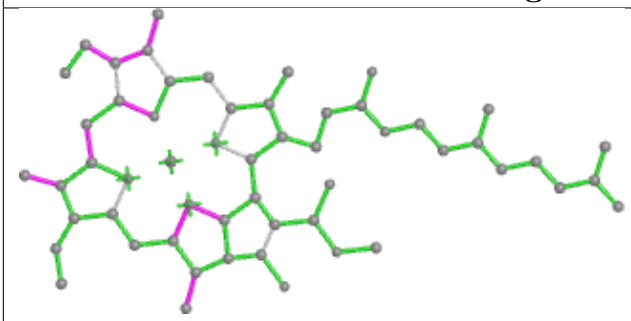


Torsions



Rings

Ligand CLA P 604



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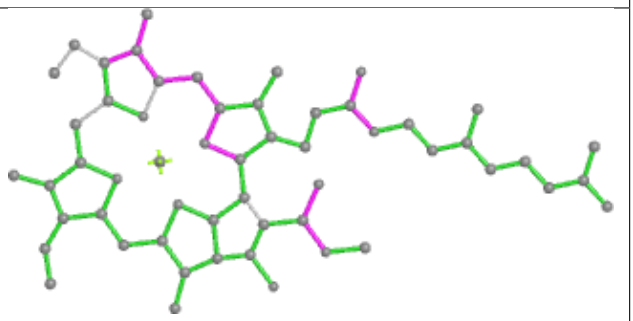
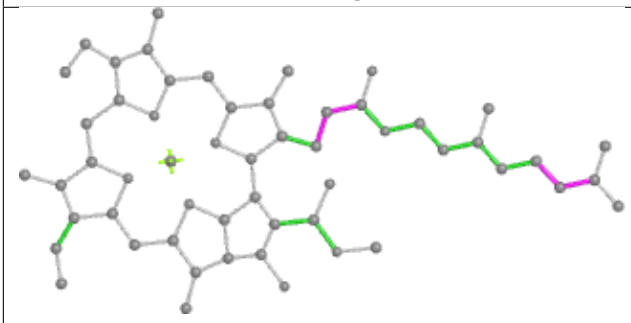
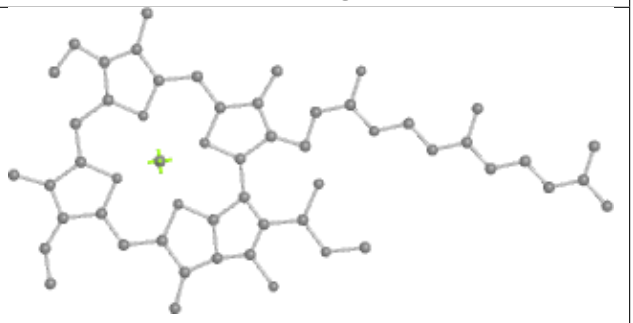


Bond angles

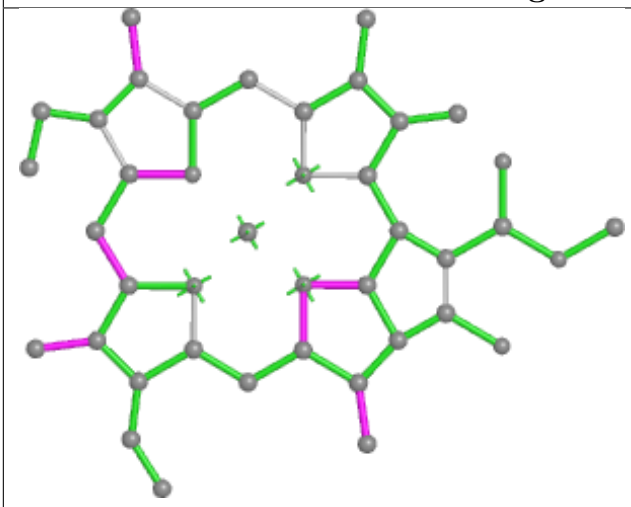


Torsions



Rings

Ligand CLA 8 609



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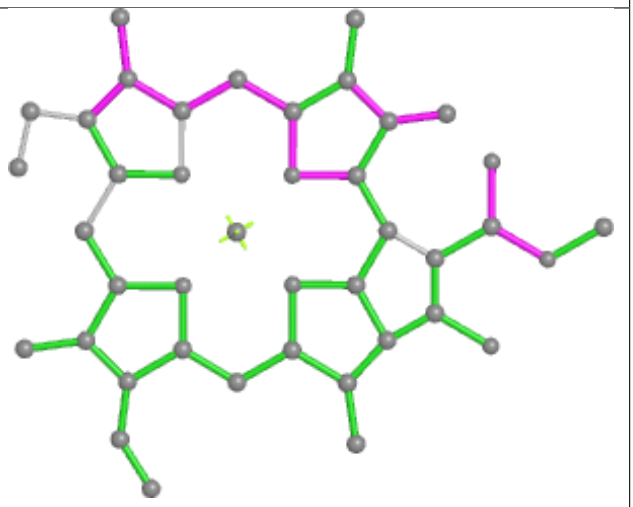
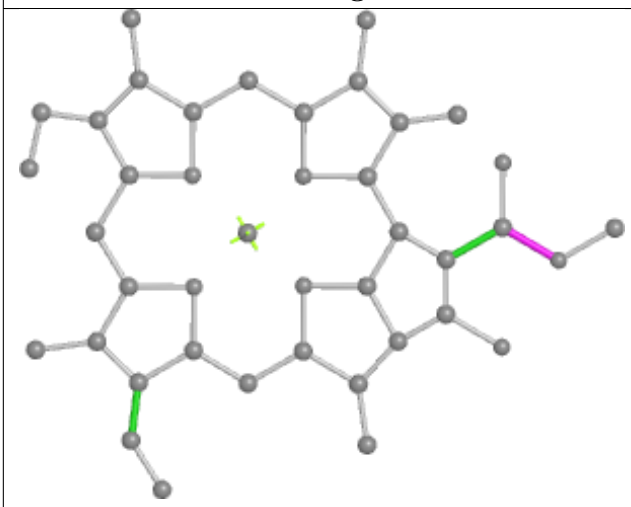


Bond angles



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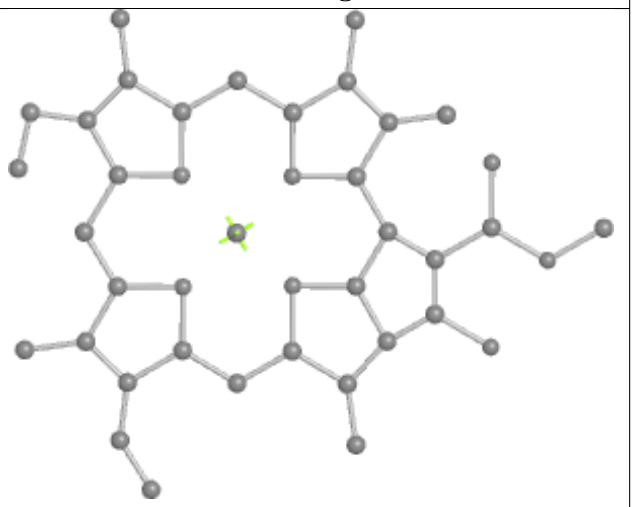
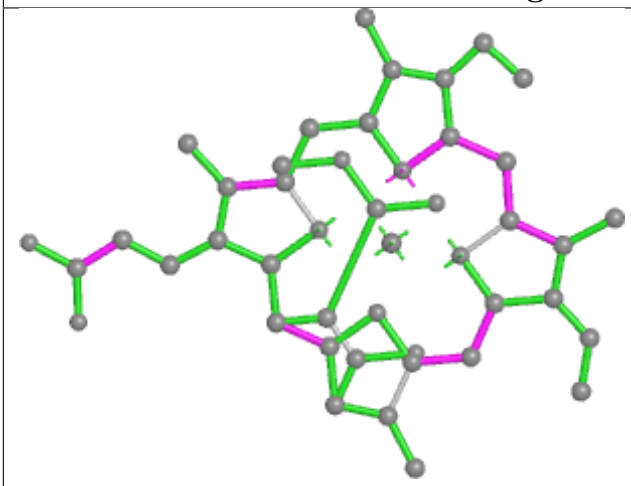


Rings

Ligand KC2 P 609



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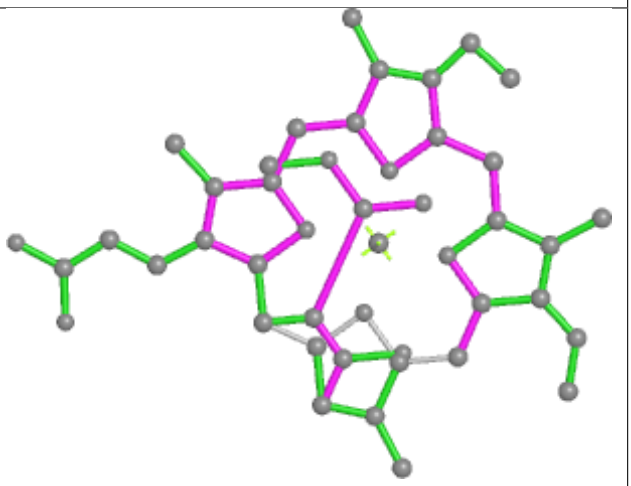
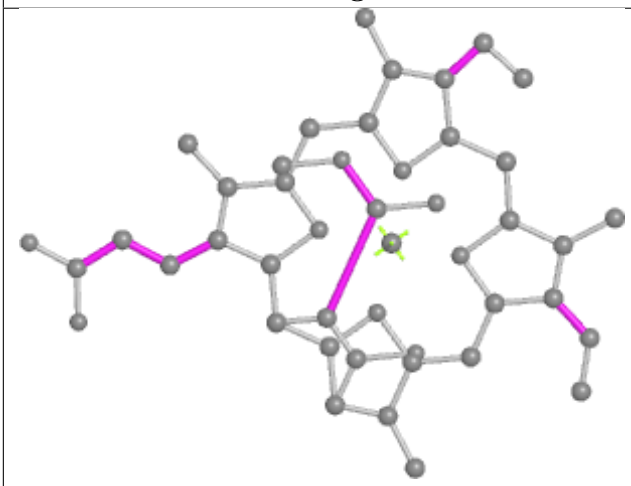
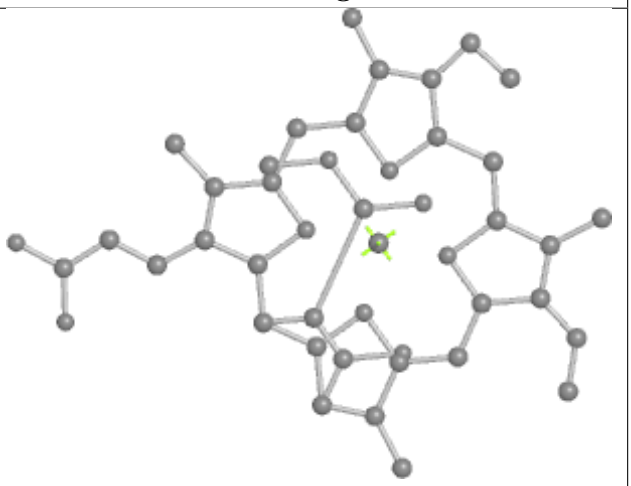


Bond angles

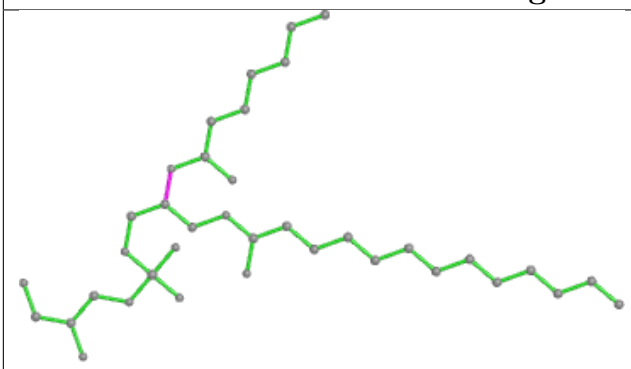


Torsions



Rings

Ligand LHG s 301



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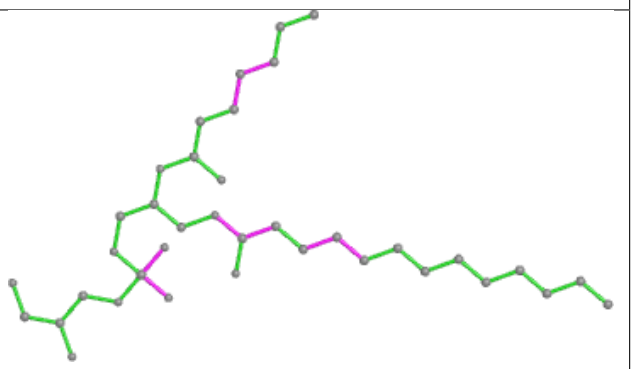
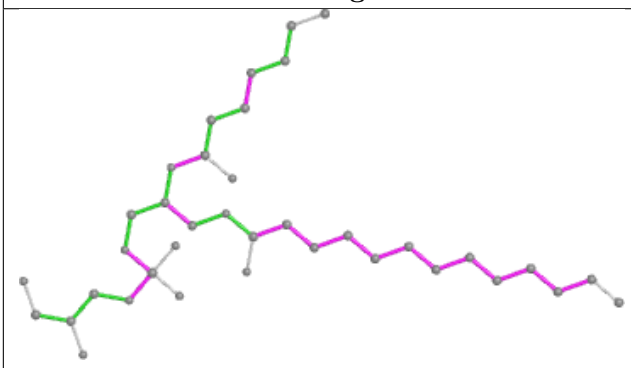


Bond angles



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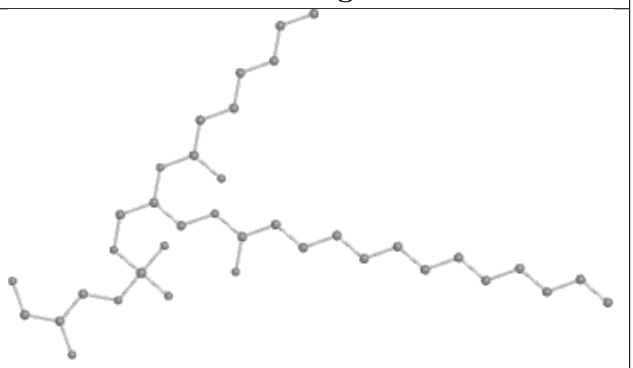
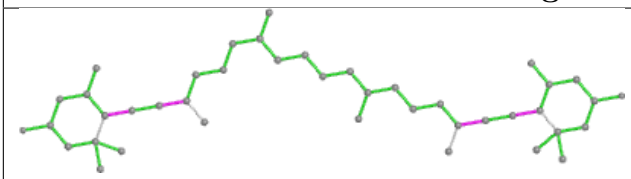
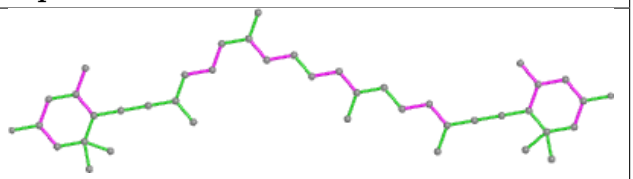


Rings

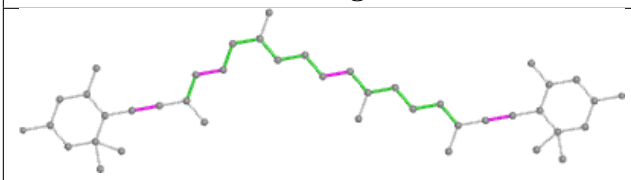
Ligand II0 p 316



Bond lengths



Bond angles



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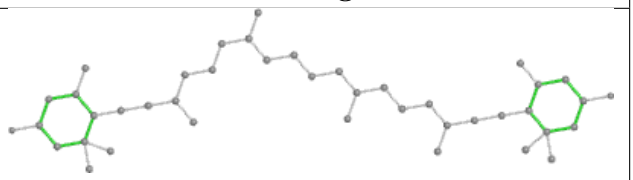
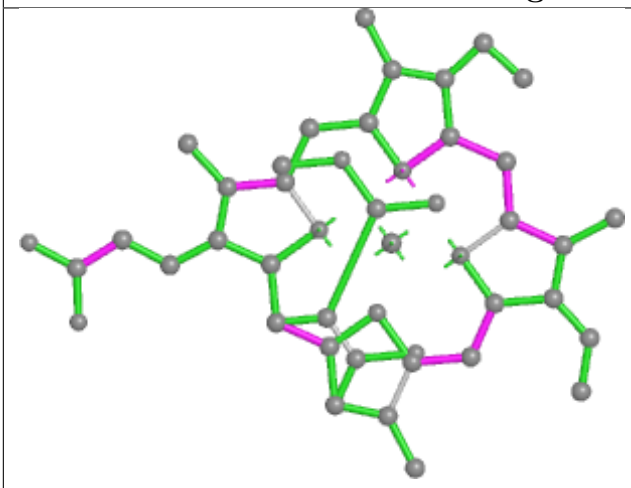
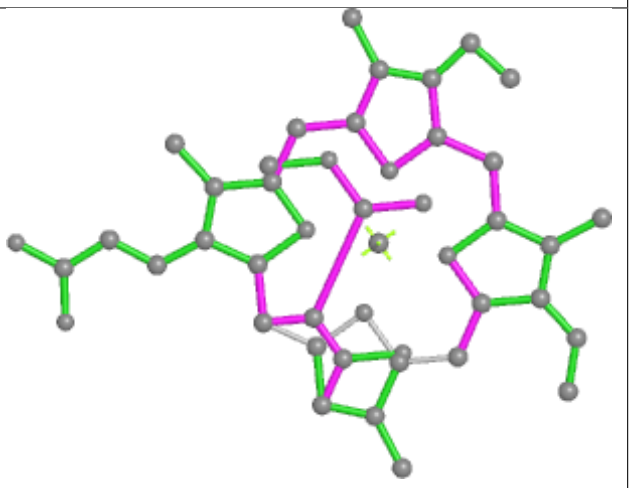


Rings

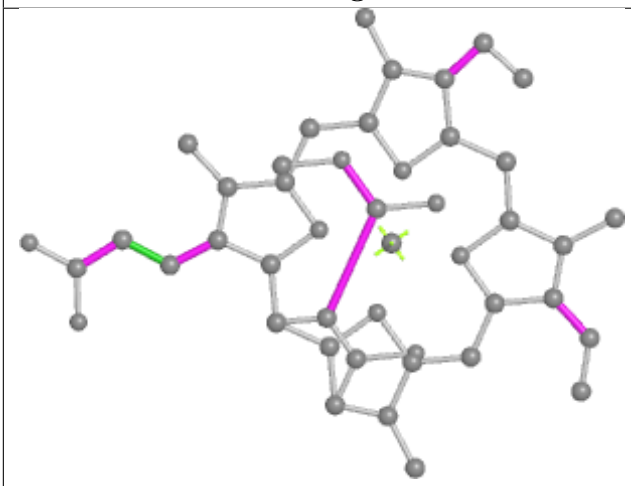
Ligand KC2 P 605



Bond lengths



Bond angles



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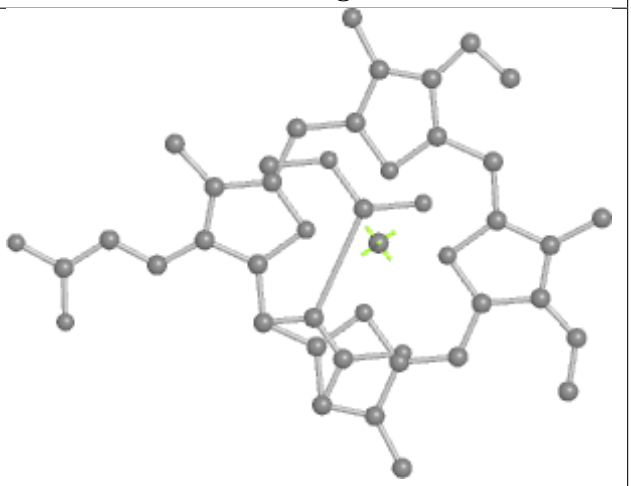
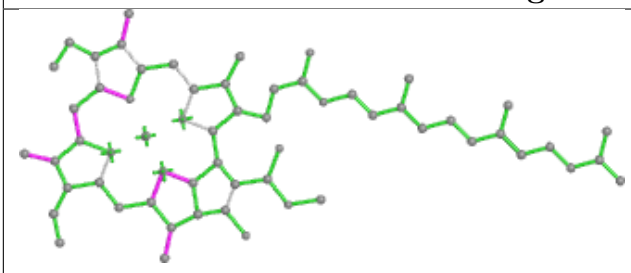
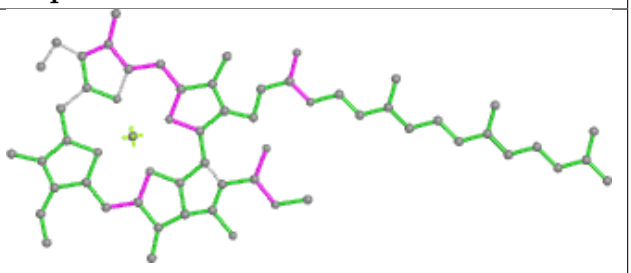


Rings

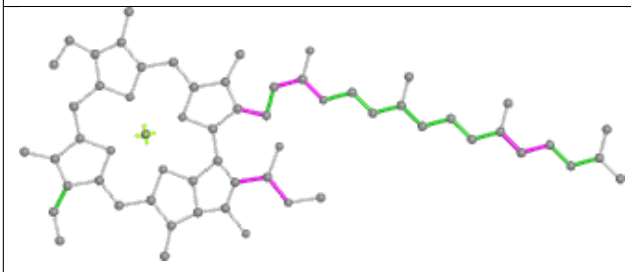
Ligand CLA p 307



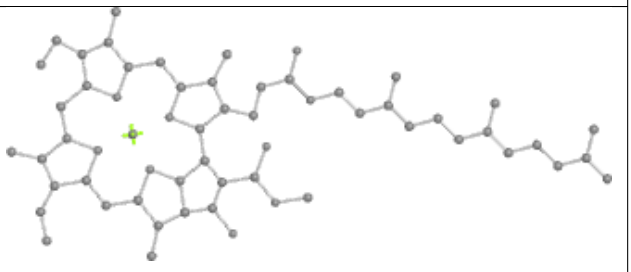
Bond lengths



Bond angles

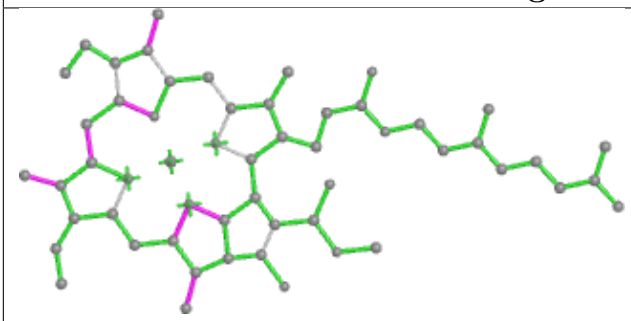


Torsions

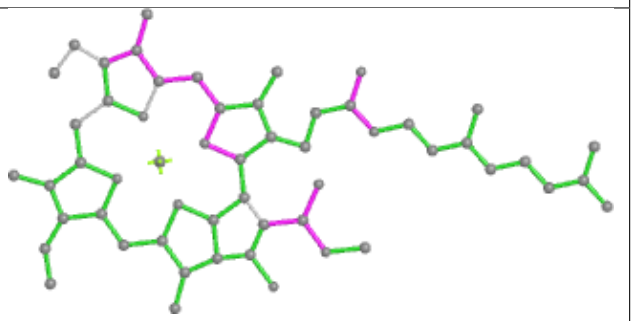


Rings

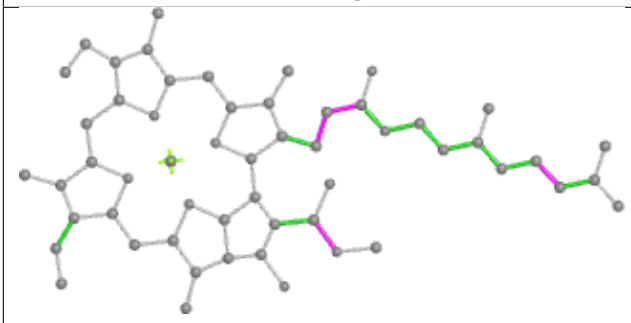
Ligand CLA 7 604



Bond lengths



Bond angles



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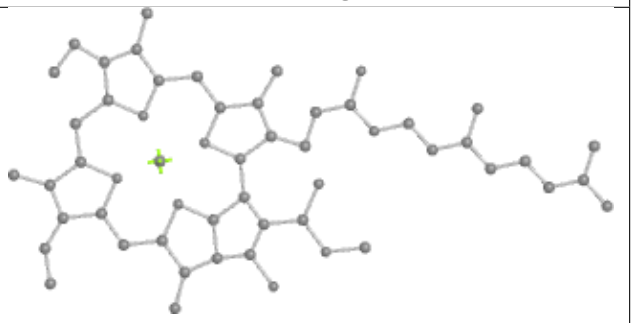
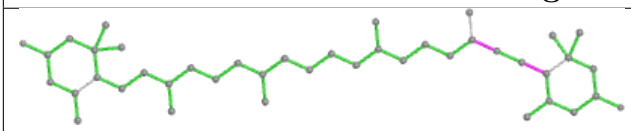
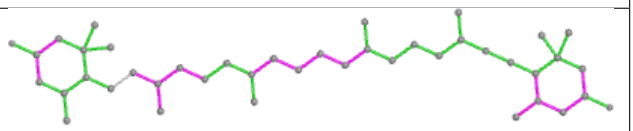


Rings

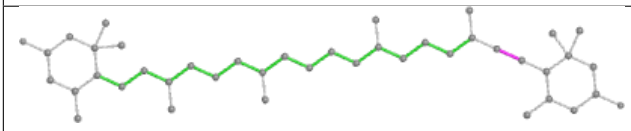
Ligand II3 7 615



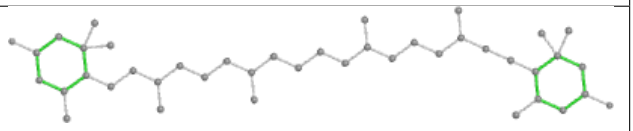
Bond lengths



Bond angles

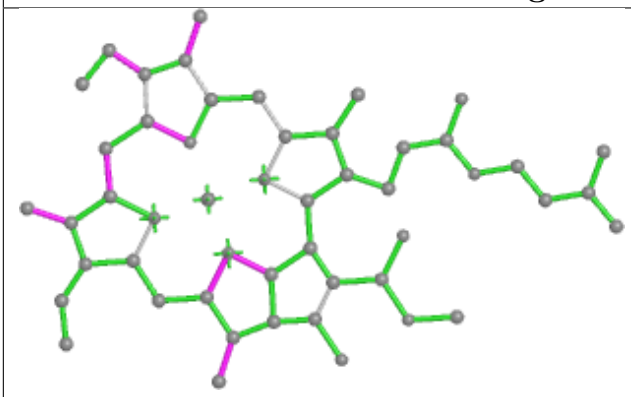


Torsions

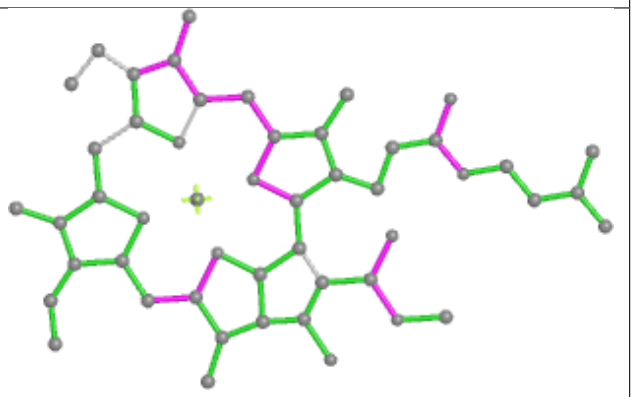


Rings

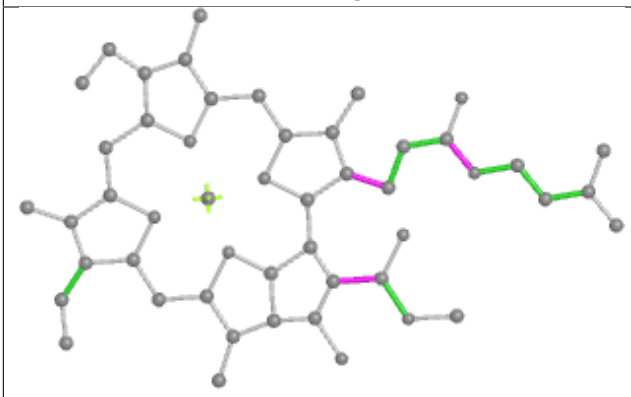
Ligand CLA 8 603



Bond lengths



Bond angles



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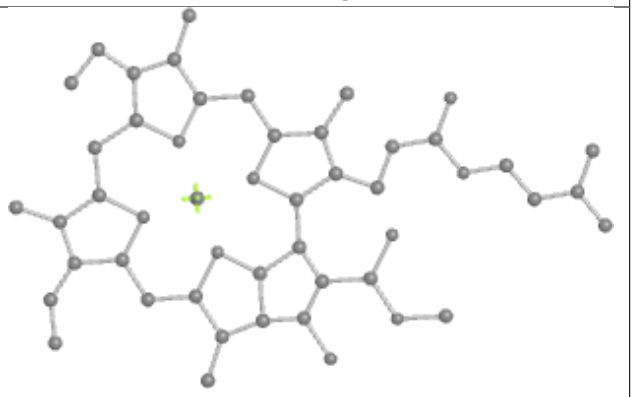
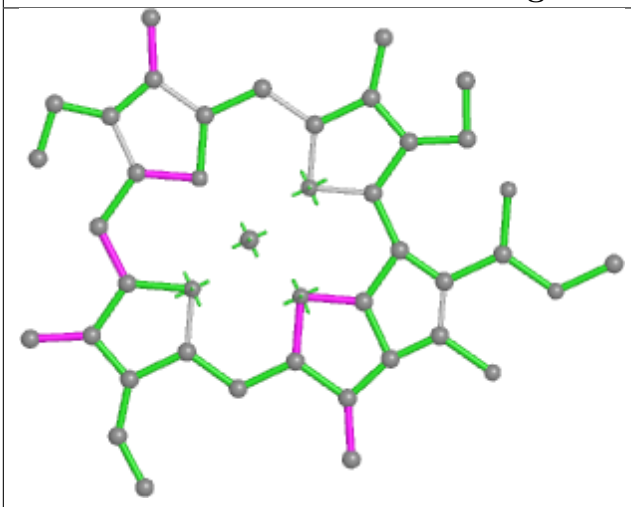
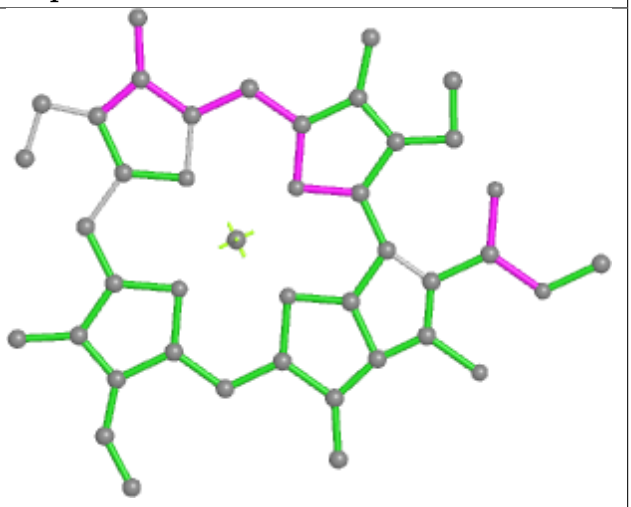


Rings

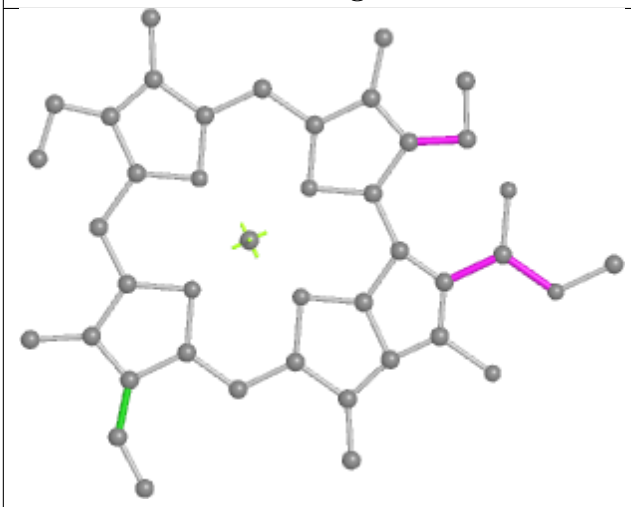
Ligand CLA p 303



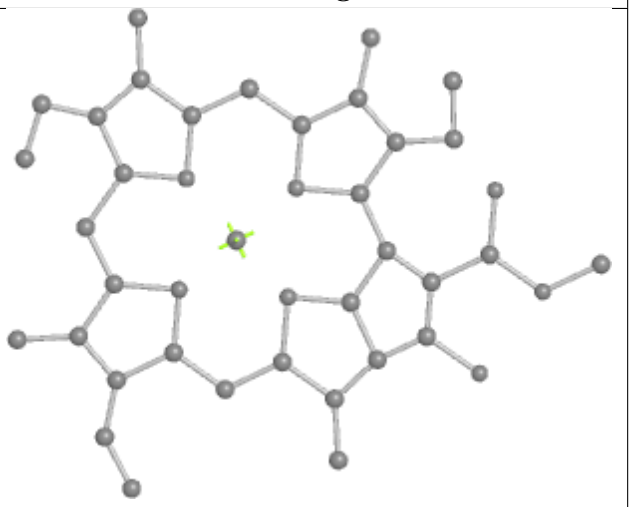
Bond lengths



Bond angles

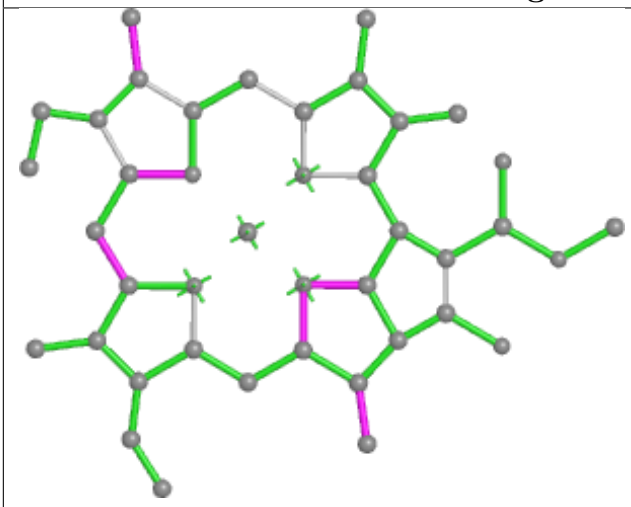


Torsions

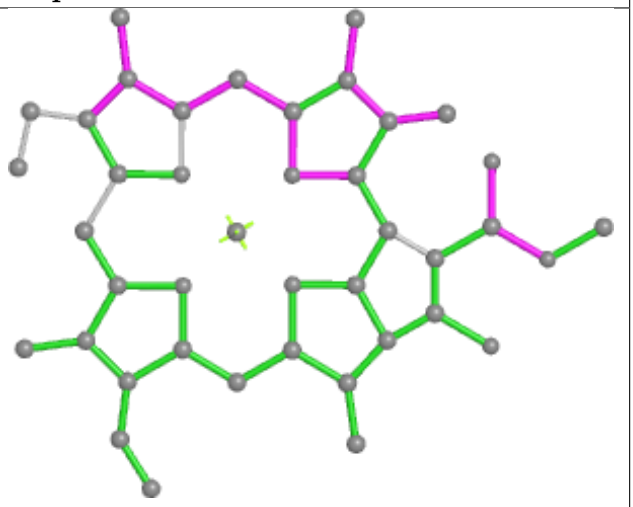


Rings

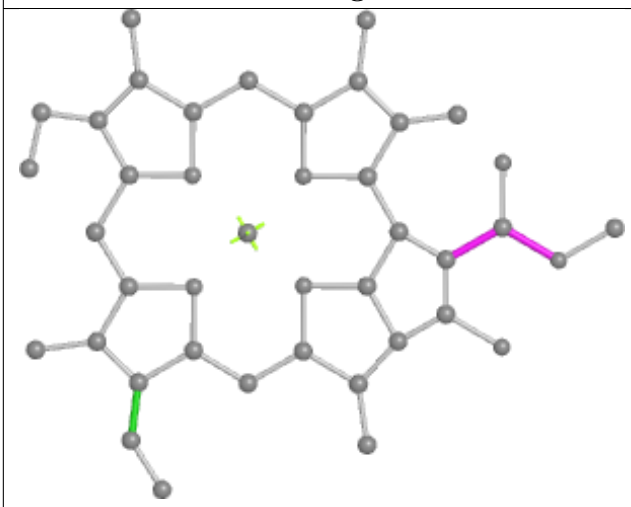
Ligand CLA p 311



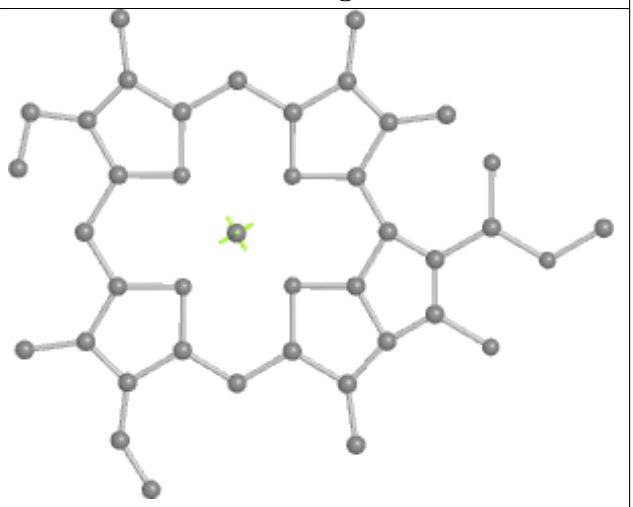
Bond lengths



Bond angles

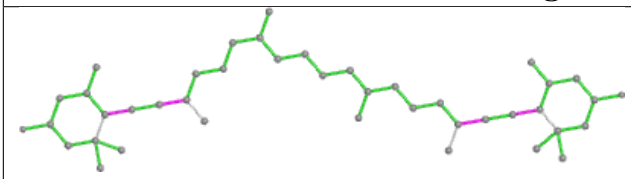


Torsions

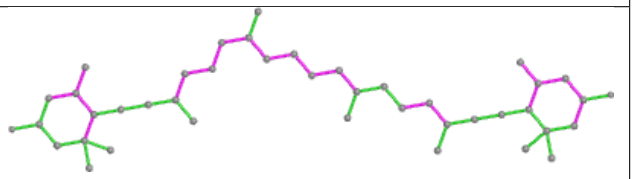


Rings

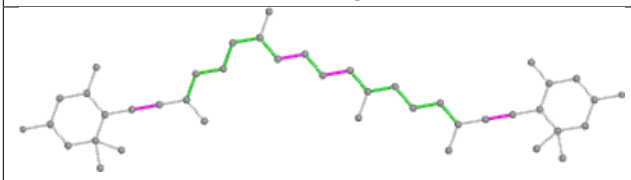
Ligand II0 0 616



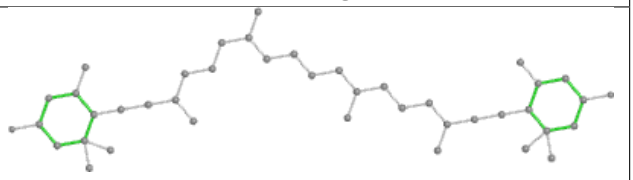
Bond lengths



Bond angles

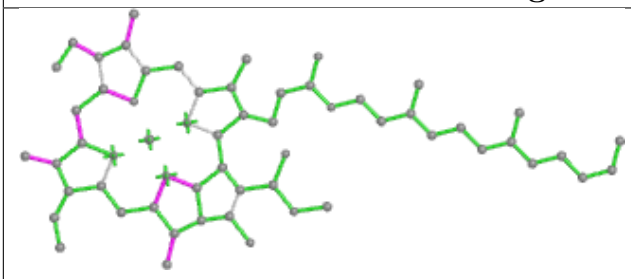


Torsions

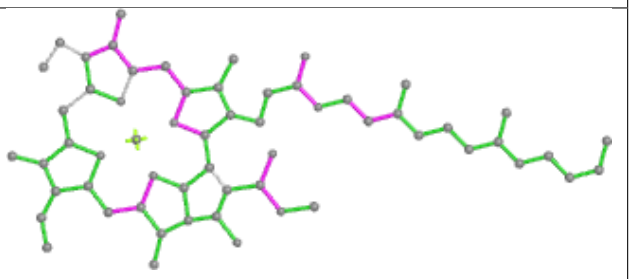


Rings

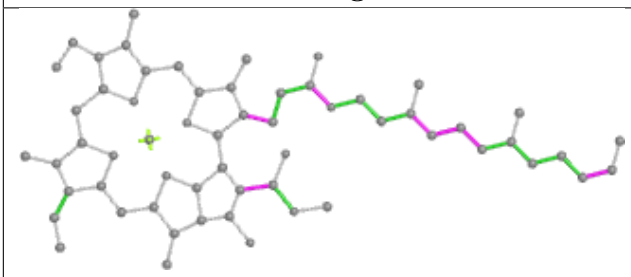
Ligand CLA 0 602



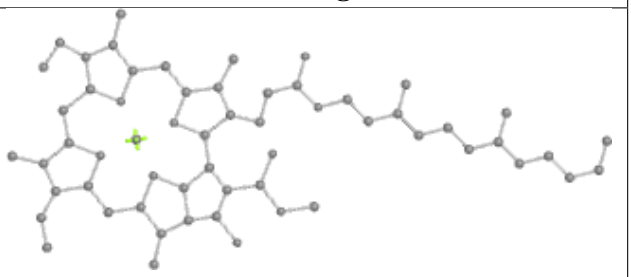
Bond lengths



Bond angles

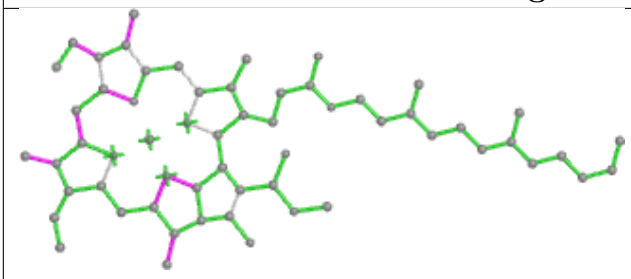


Torsions



Rings

Ligand CLA 8 602



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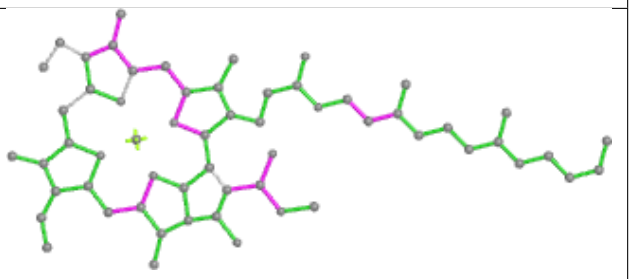
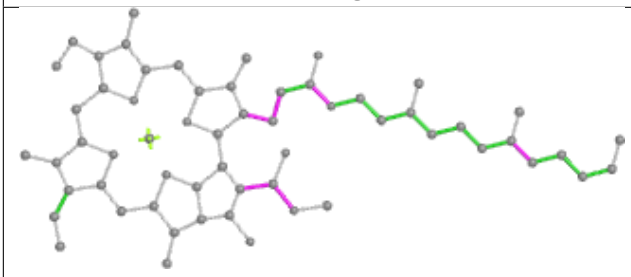


Bond angles



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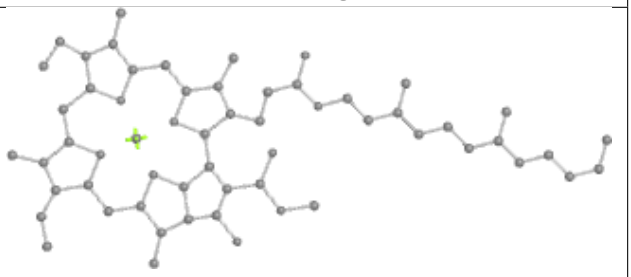
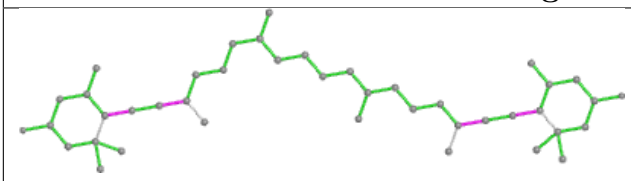


Rings

Ligand II0 p 302



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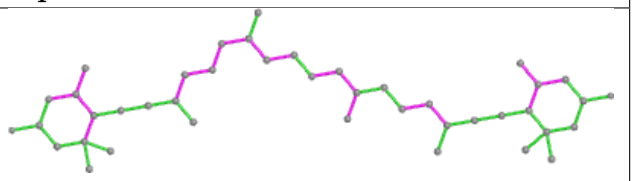
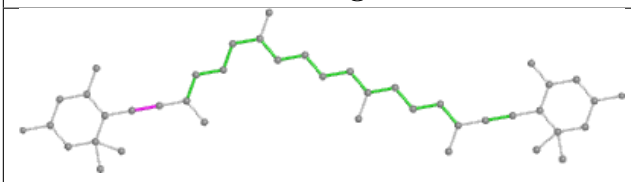


Bond angles



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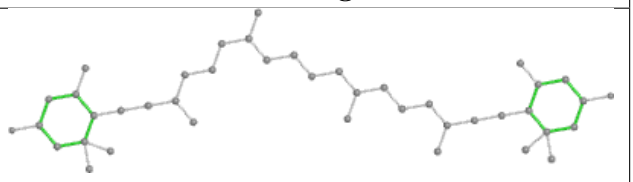
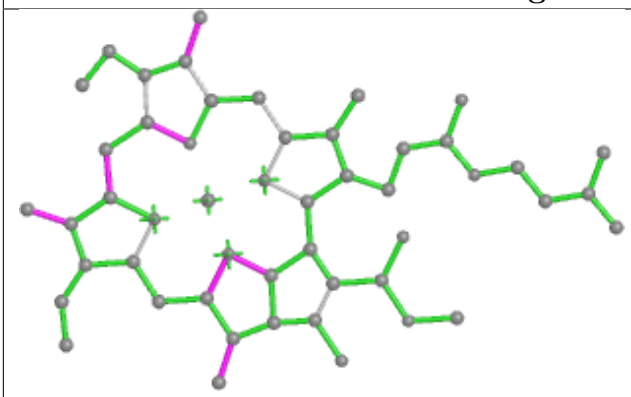


Rings

Ligand CLA 0 603



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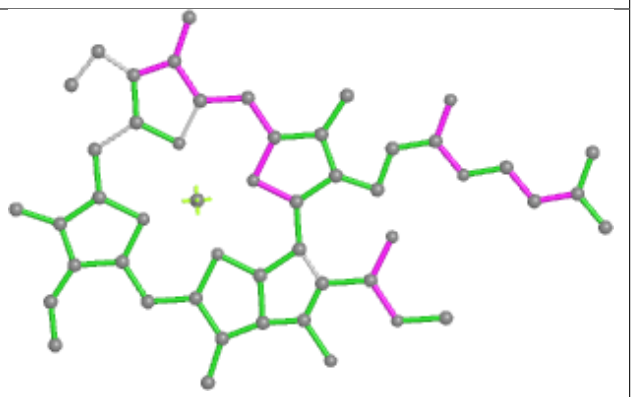
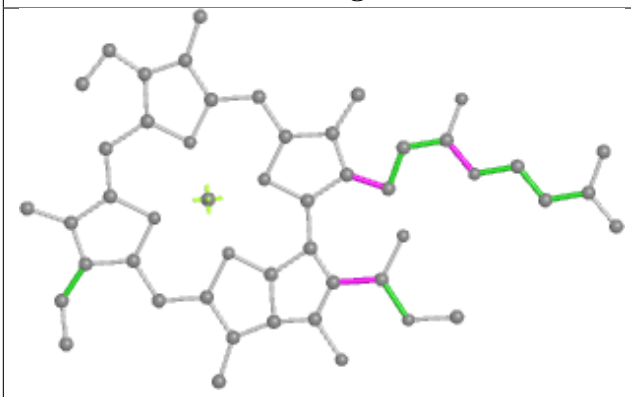


Bond angles



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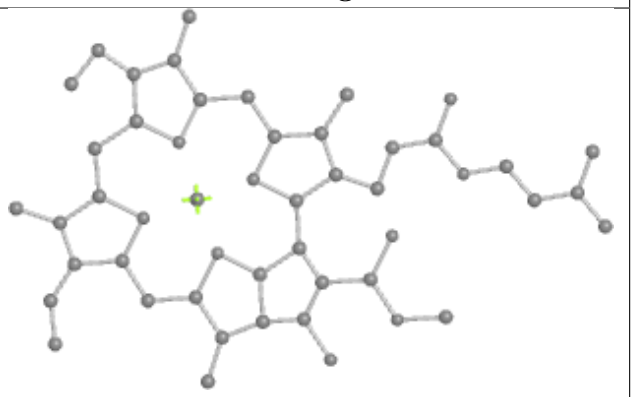
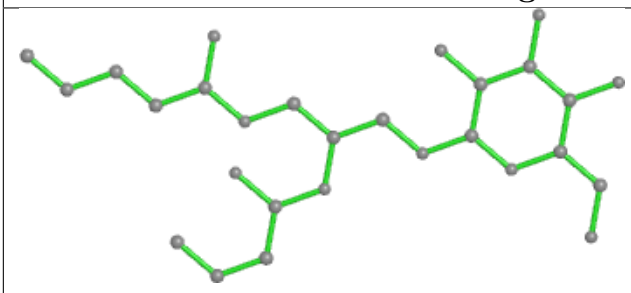


Rings

Ligand LMG G 102



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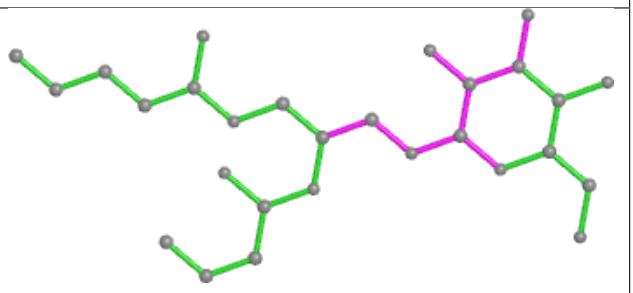
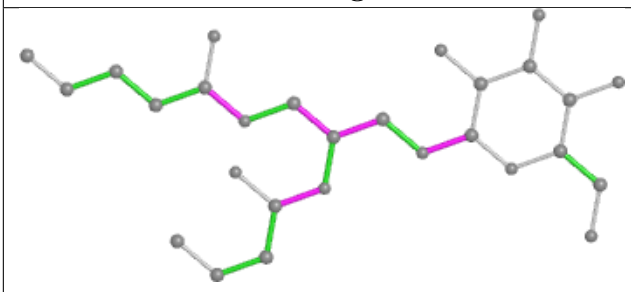


Bond angles



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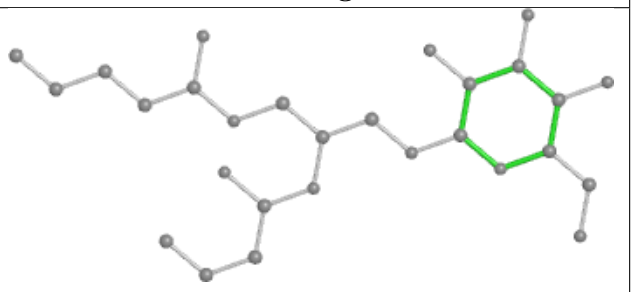
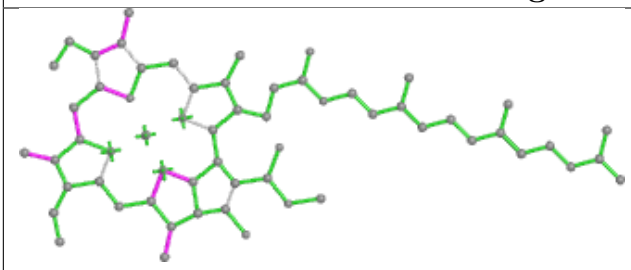


Rings

Ligand CLA 8 605



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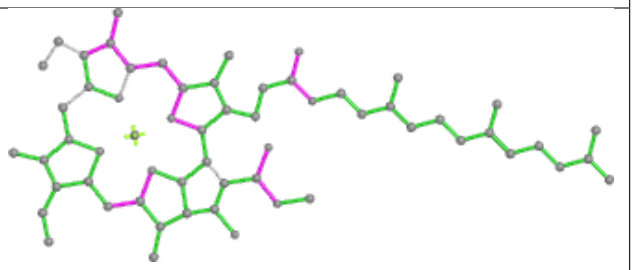
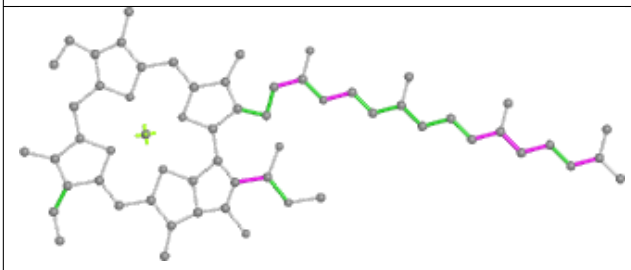


Bond angles



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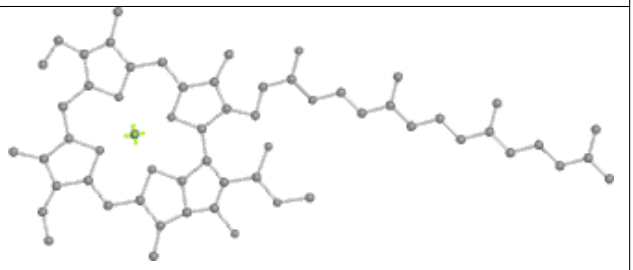
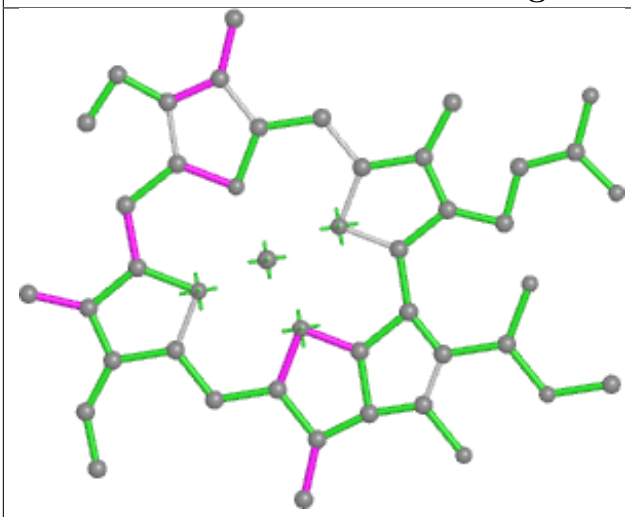


Rings

Ligand CLA 8 607



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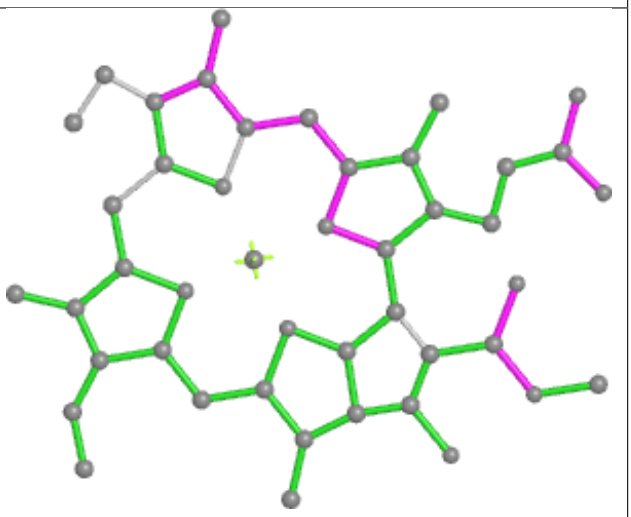

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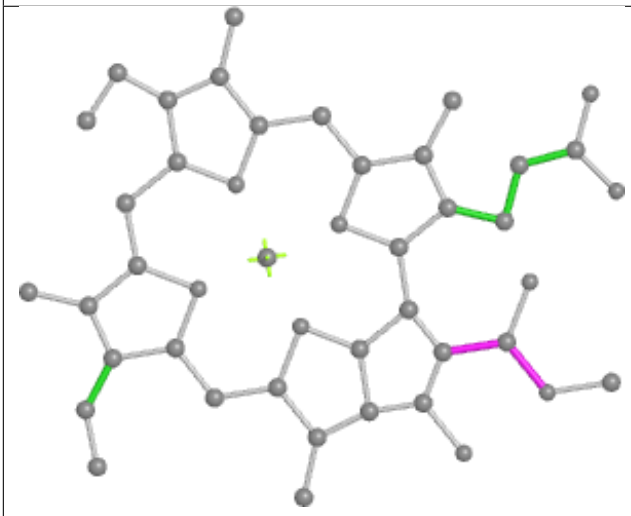

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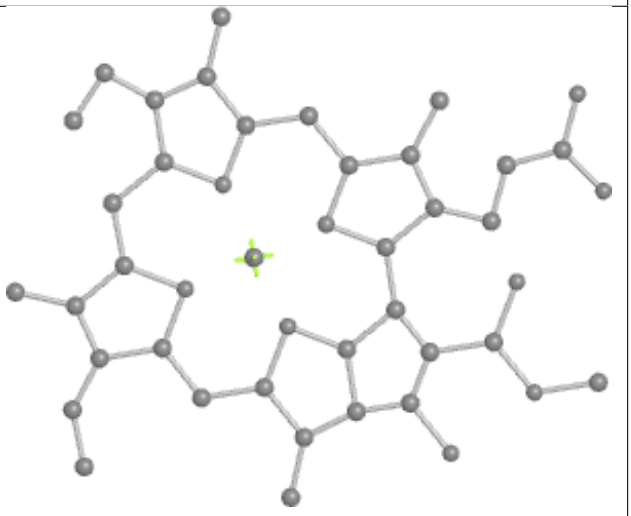
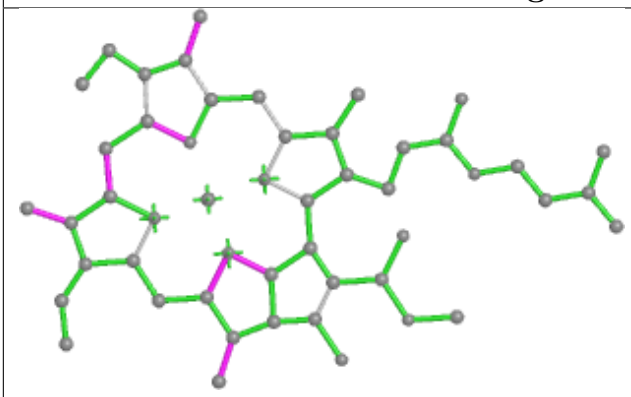


Rings

Ligand CLA p 305



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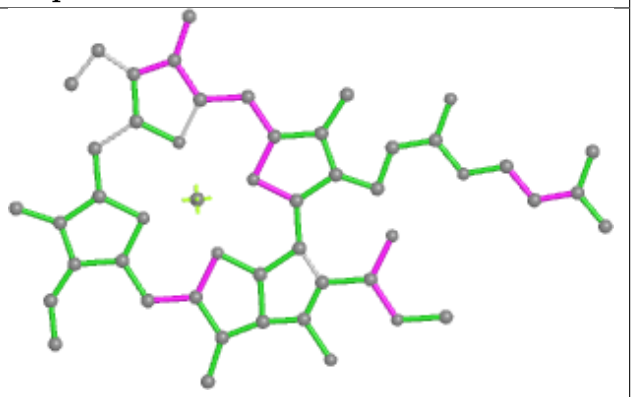

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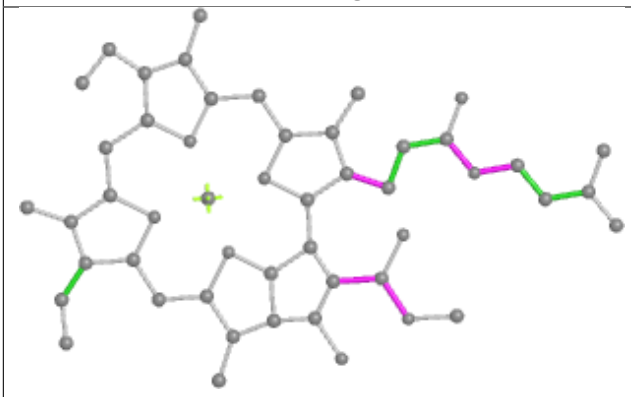

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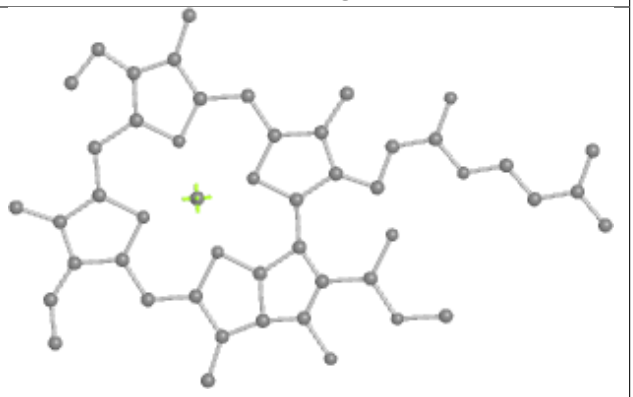
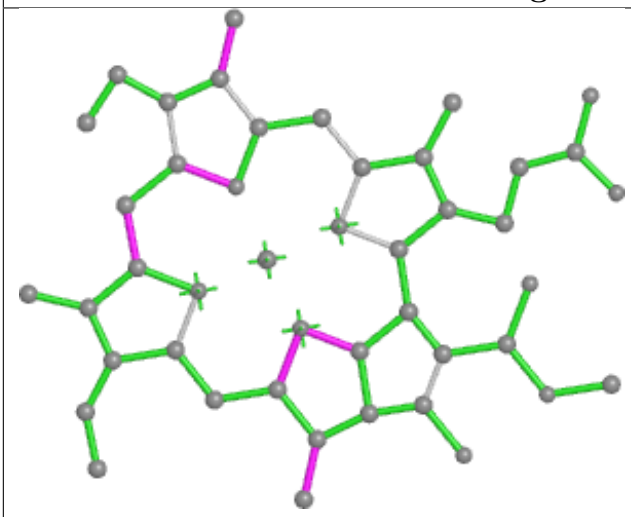


Rings

Ligand CLA s 302



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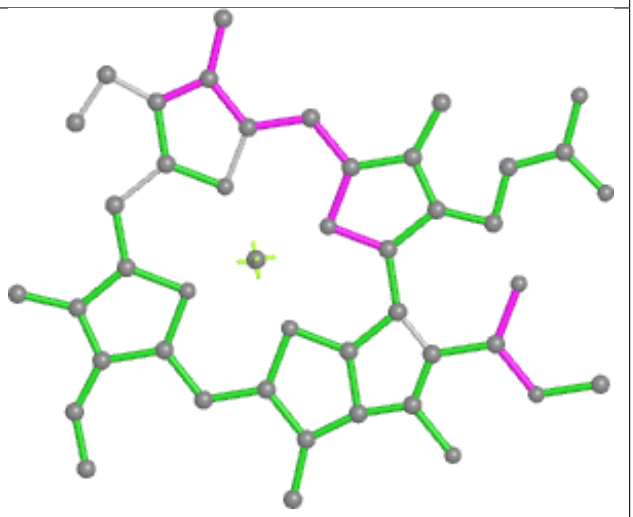
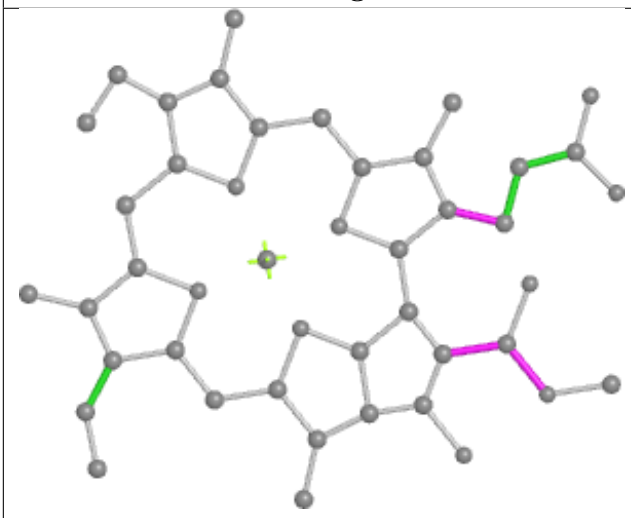


Bond angles



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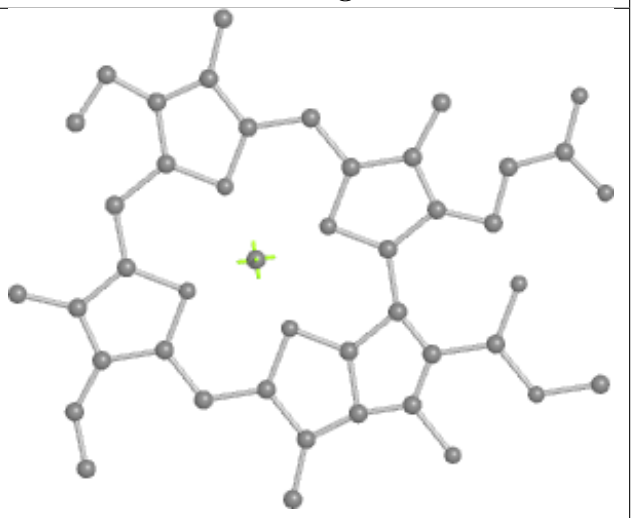
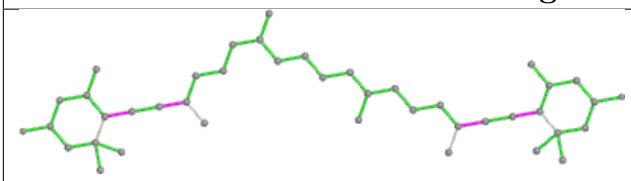


Rings

Ligand II0 P 612



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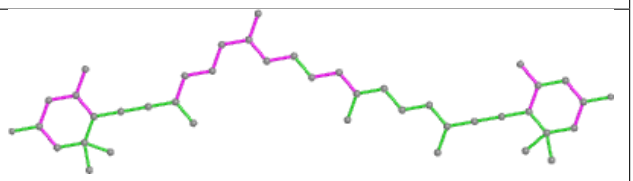
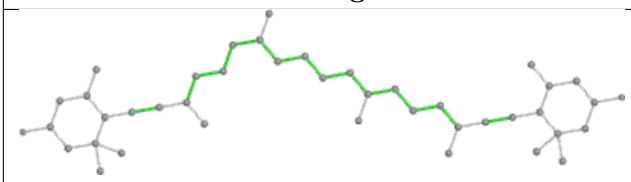
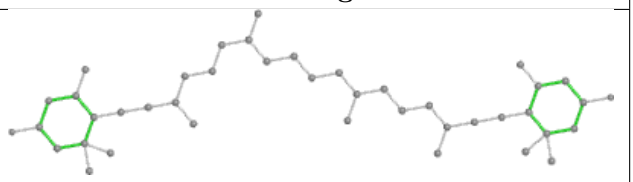


Bond angles

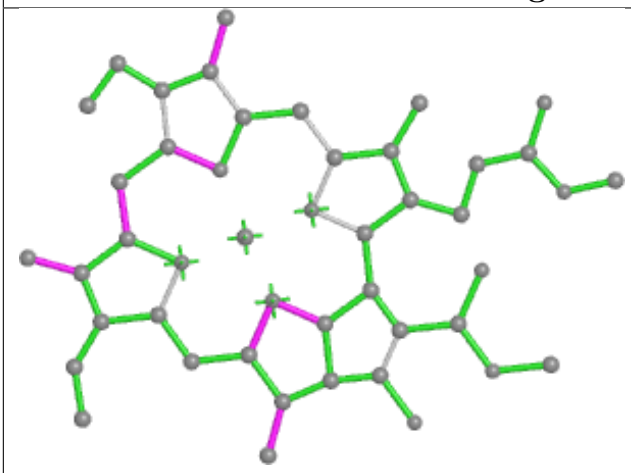


Torsions



Rings

Ligand CLA 9 605



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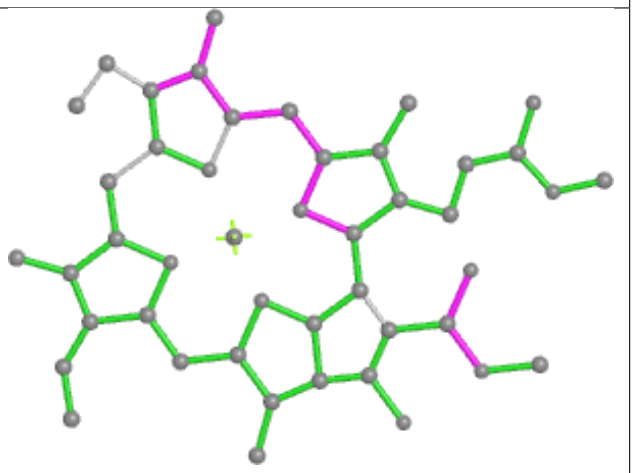
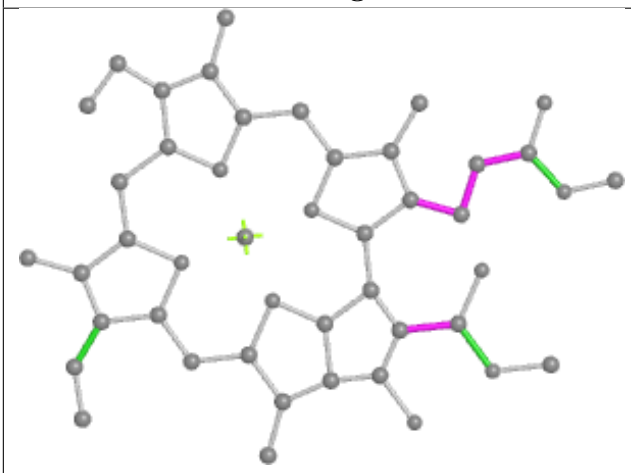
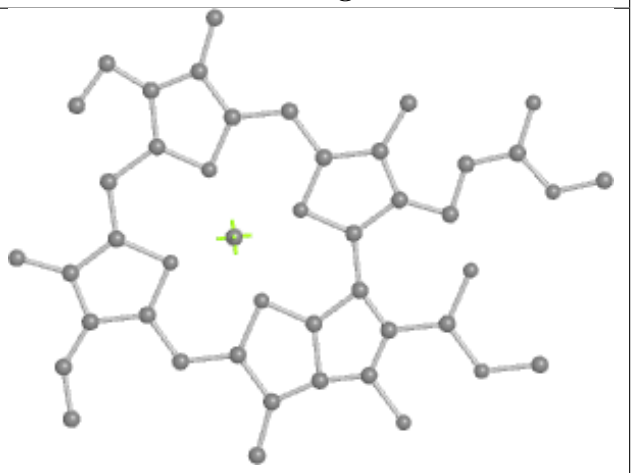


Bond angles

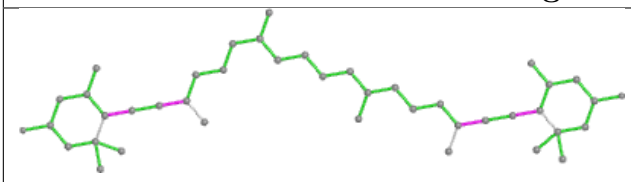


Torsions



Rings

Ligand II0 7 617



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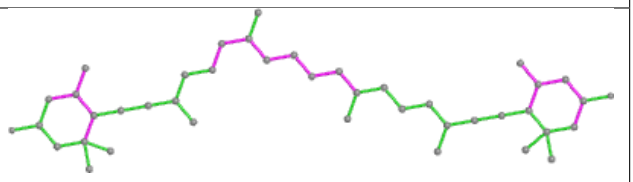
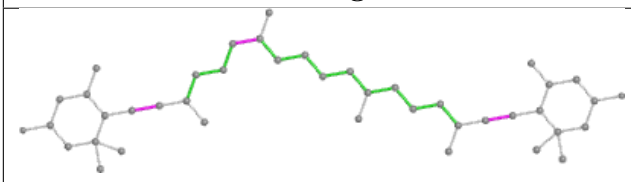


Bond angles



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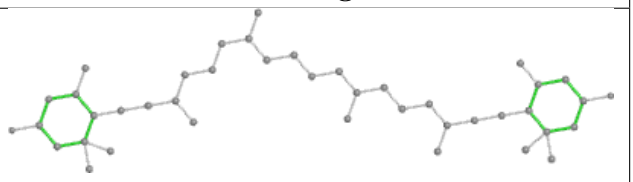
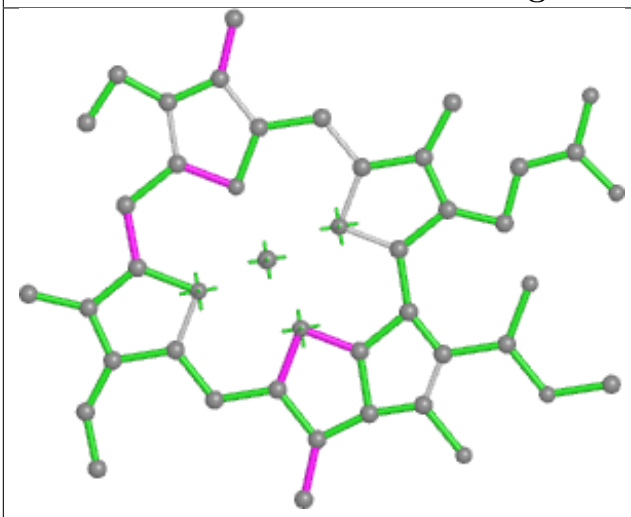


Rings

Ligand CLA 7 606



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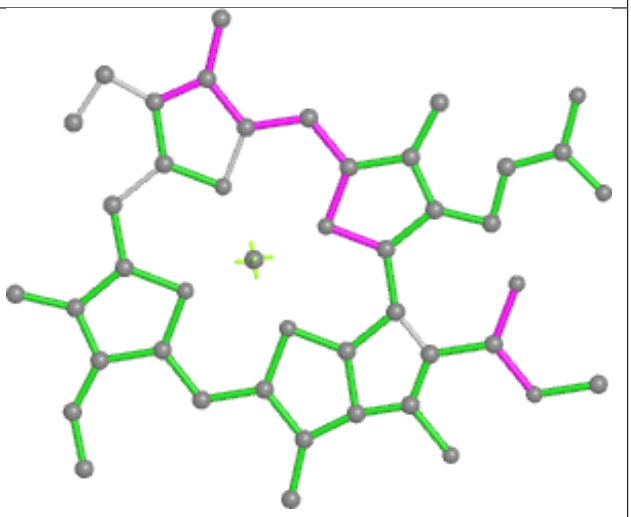
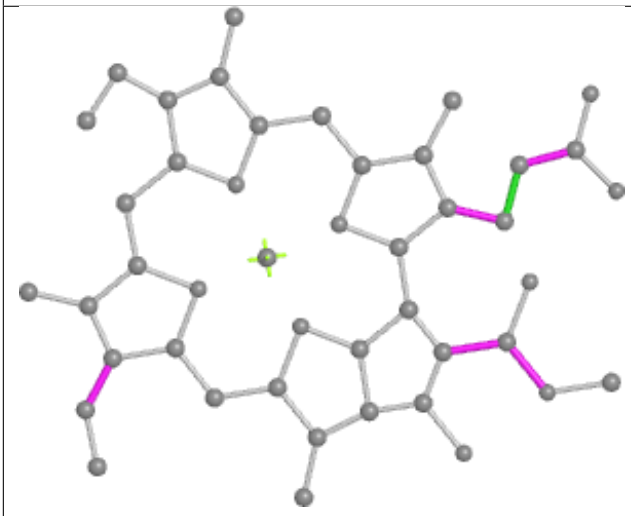


Bond angles



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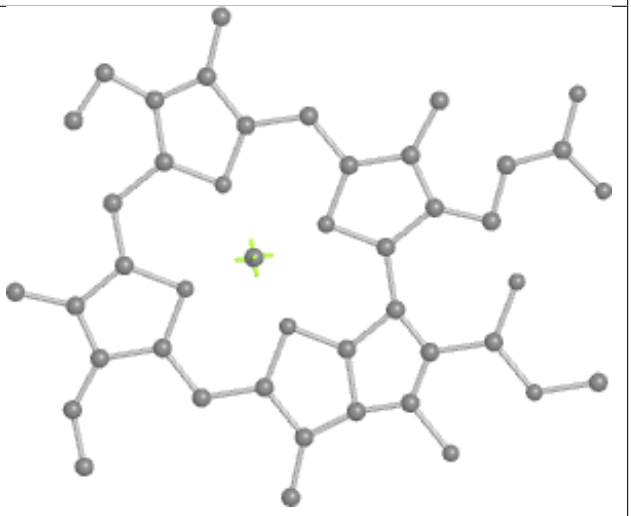
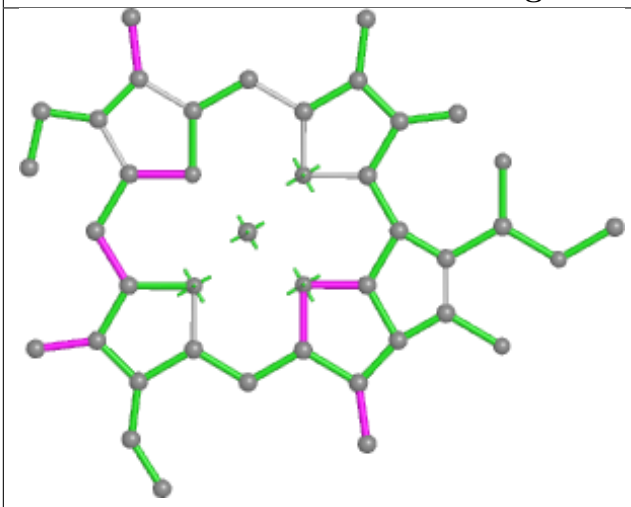
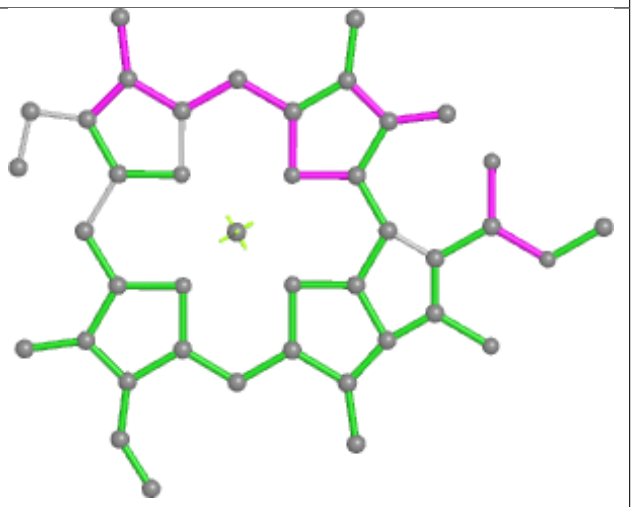


Rings

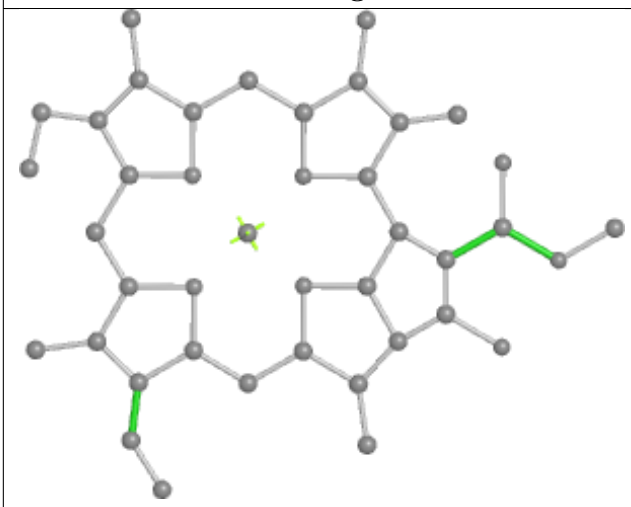
Ligand CLA P 608



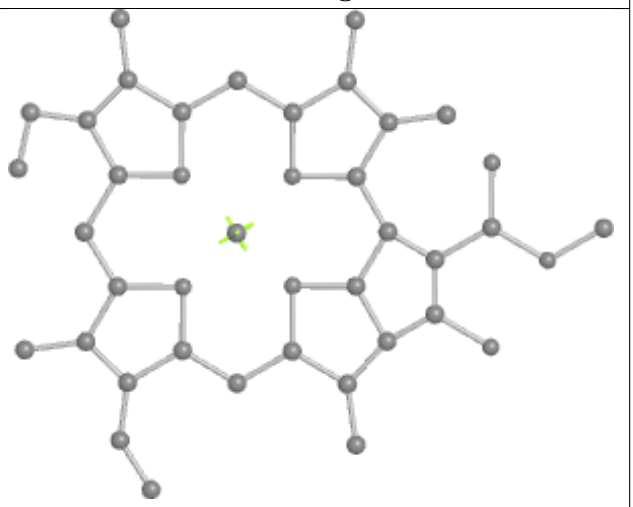
Bond lengths



Bond angles

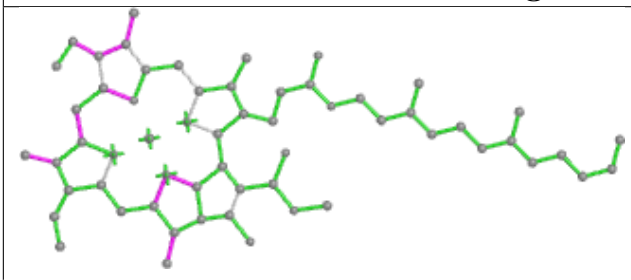


Torsions

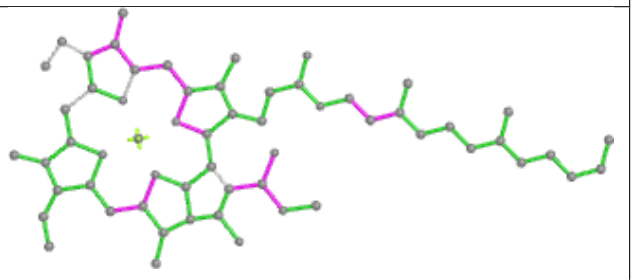


Rings

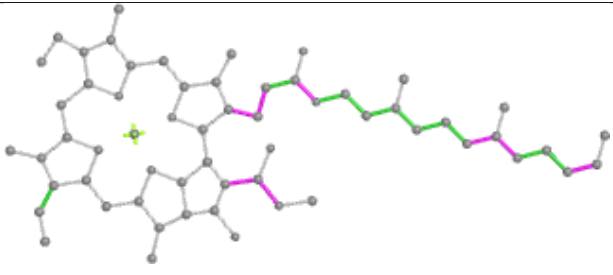
Ligand CLA P 602



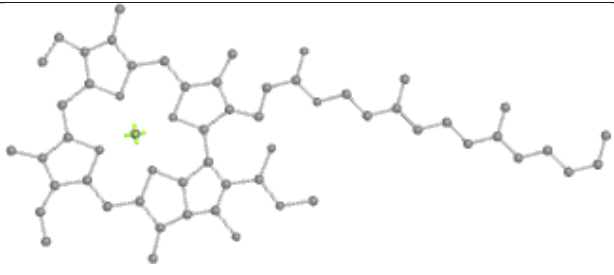
Bond lengths



Bond angles

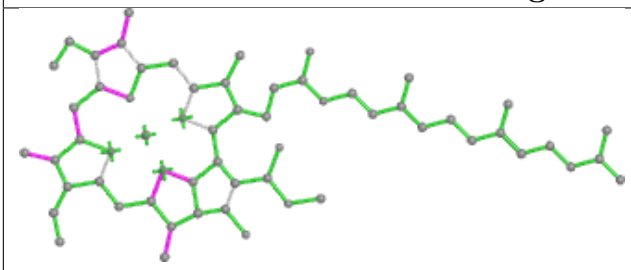


Torsions

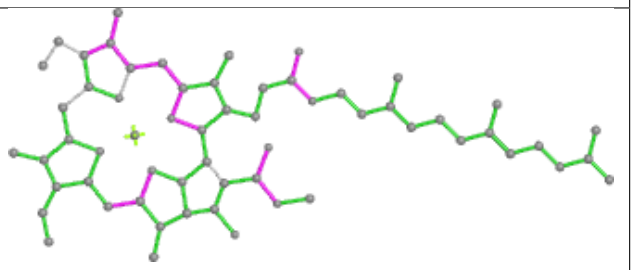


Rings

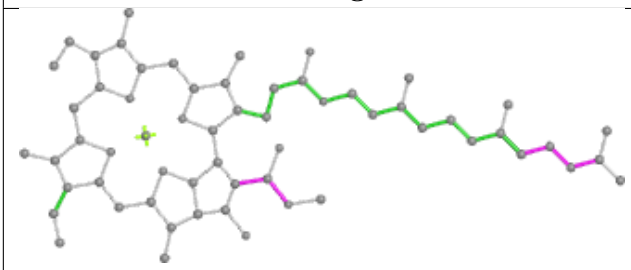
Ligand CLA 8 608



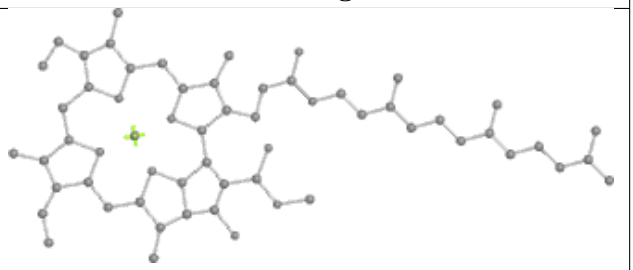
Bond lengths



Bond angles

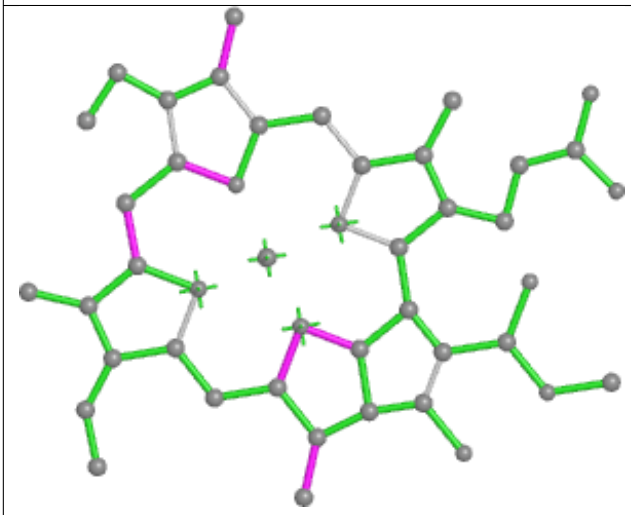


Torsions

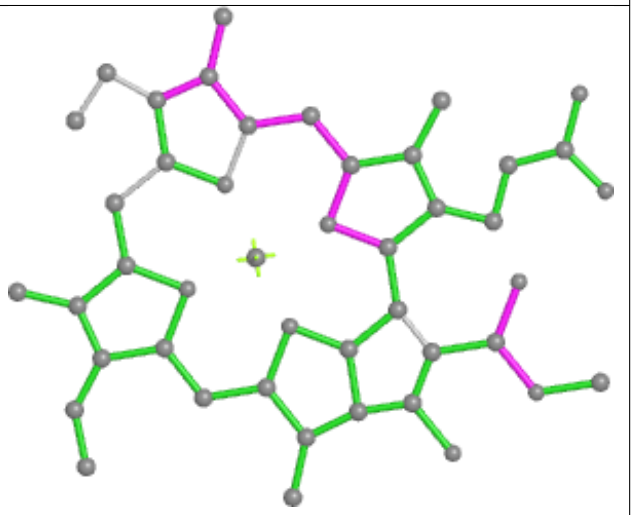


Rings

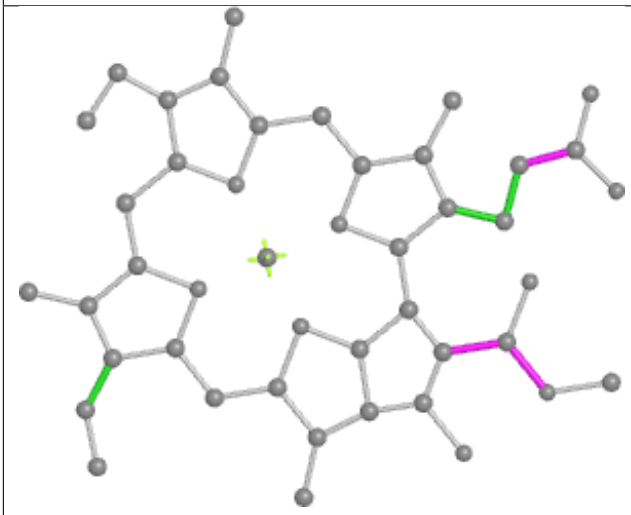
Ligand CLA 7 611



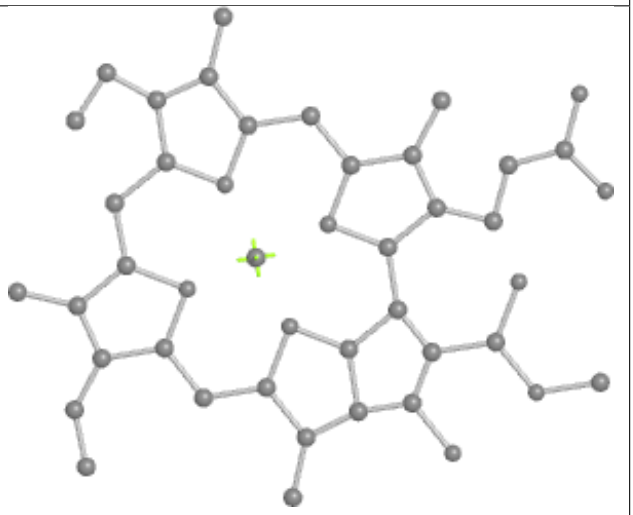
Bond lengths



Bond angles

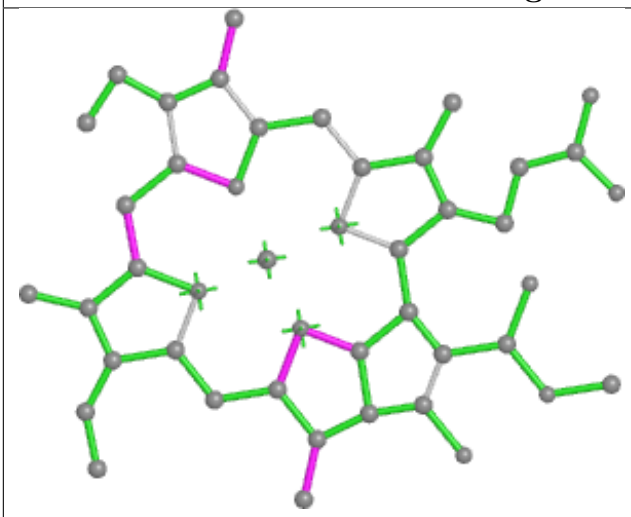


Torsions

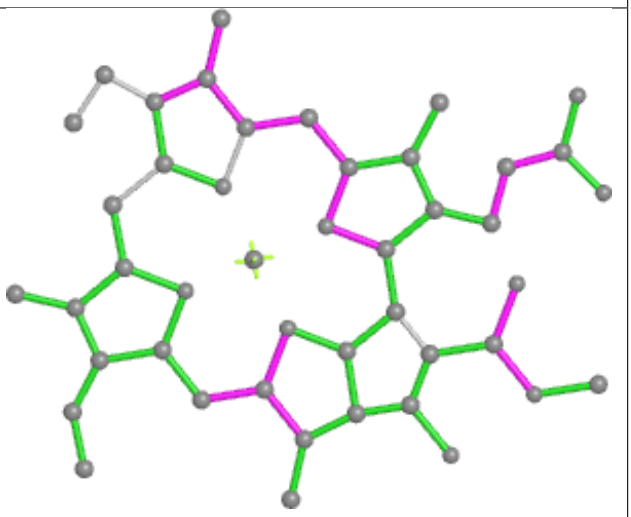


Rings

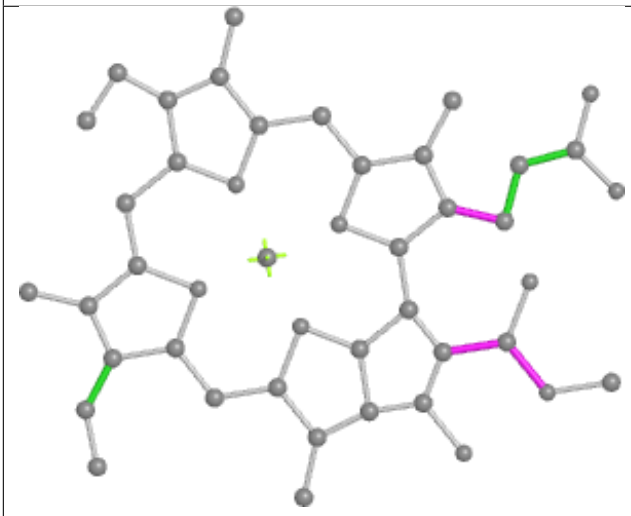
Ligand CLA P 606



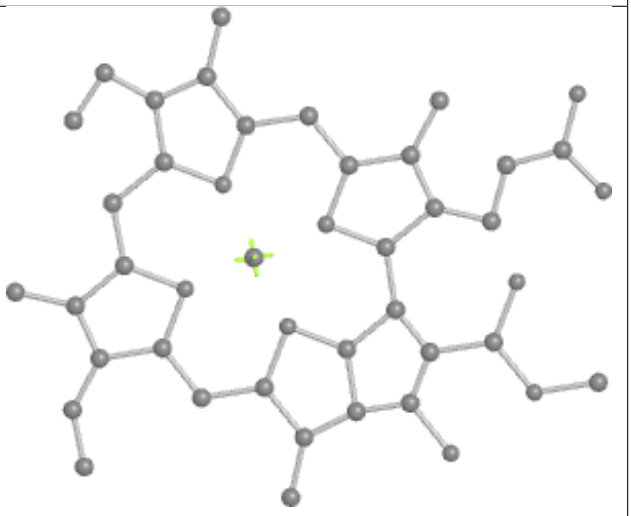
Bond lengths



Bond angles

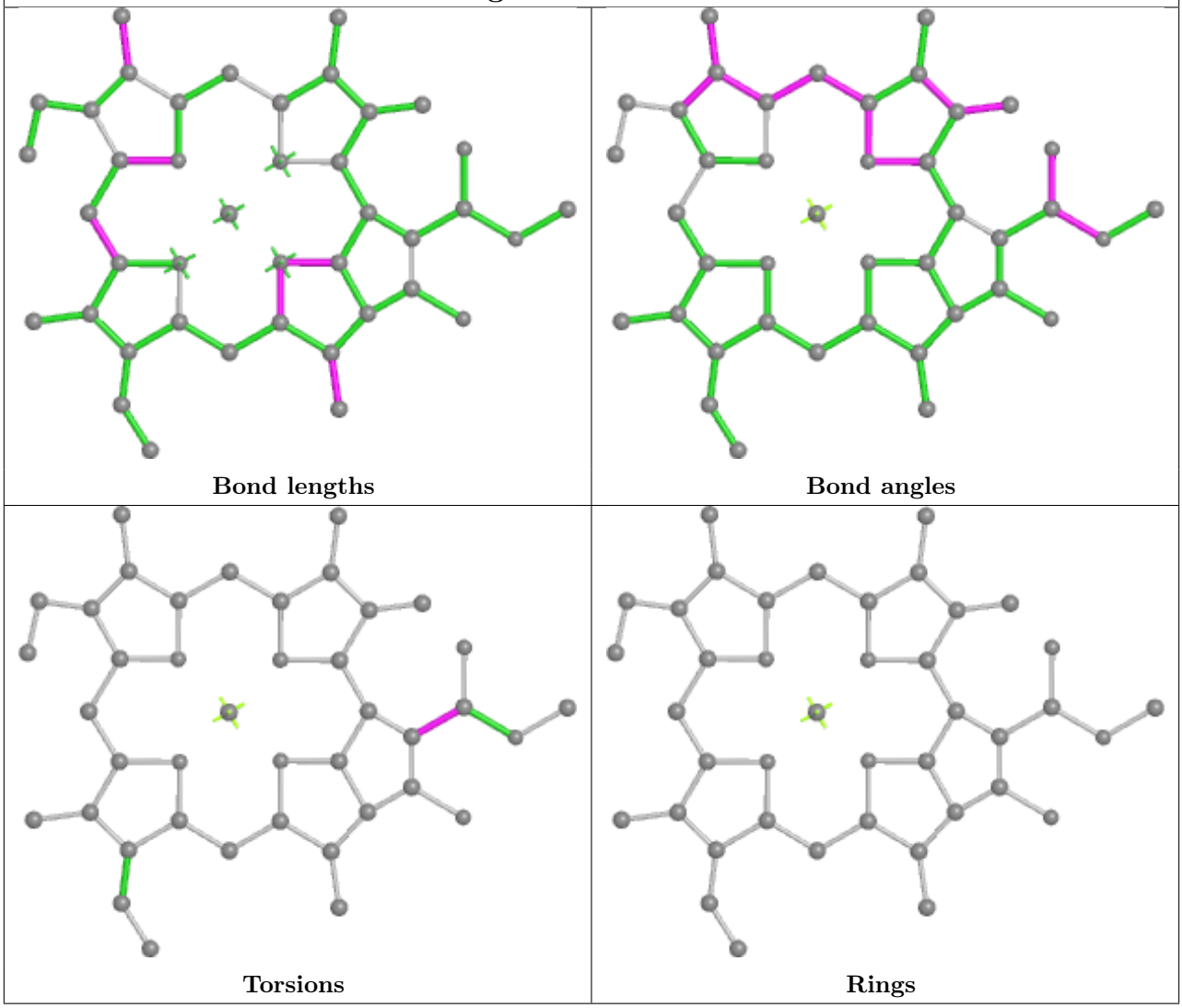


Torsions



Rings

Ligand CLA 7 609



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

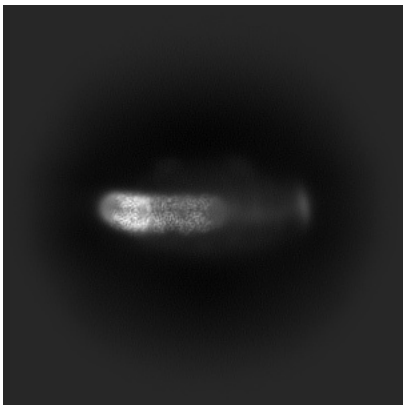
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-38419. These allow visual inspection of the internal detail of the map and identification of artifacts.

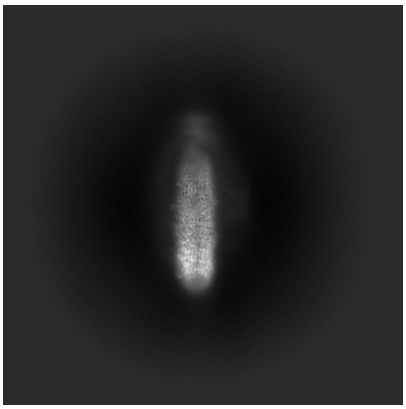
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

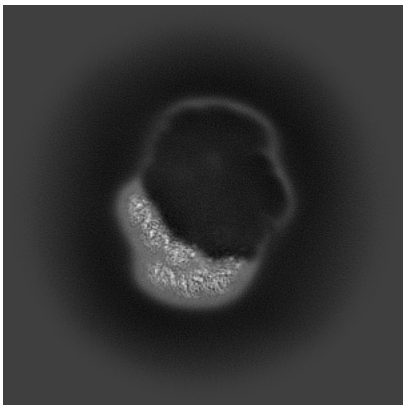
6.1.1 Primary map



X

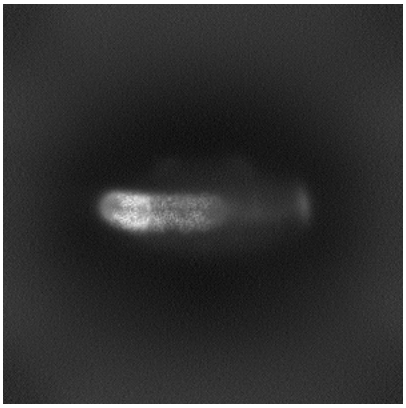


Y

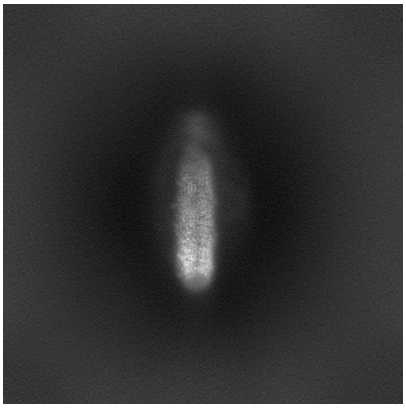


Z

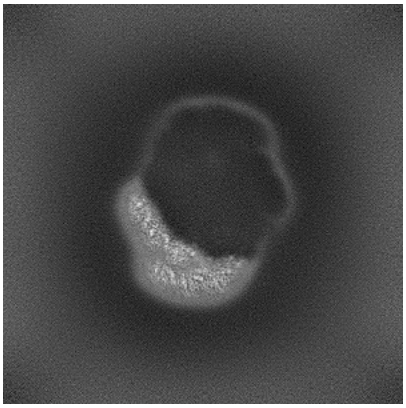
6.1.2 Raw map



X



Y

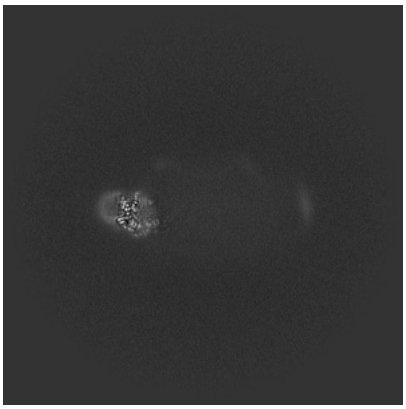


Z

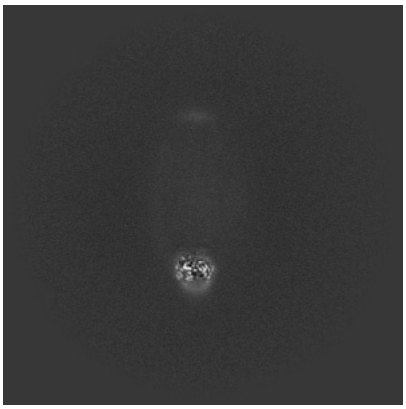
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

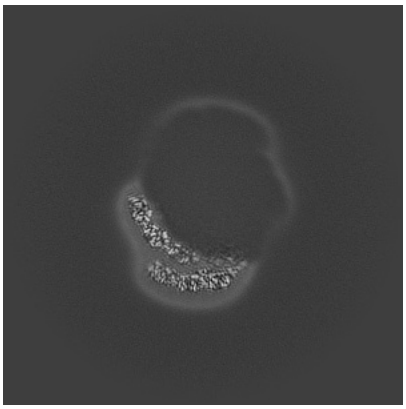
6.2.1 Primary map



X Index: 256

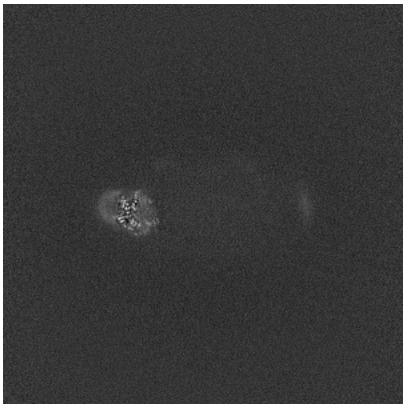


Y Index: 256

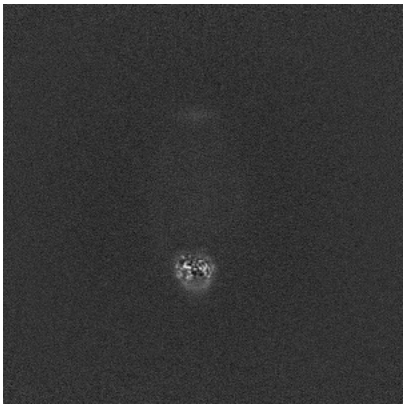


Z Index: 256

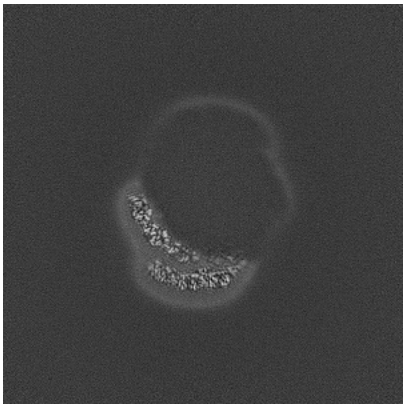
6.2.2 Raw map



X Index: 256



Y Index: 256

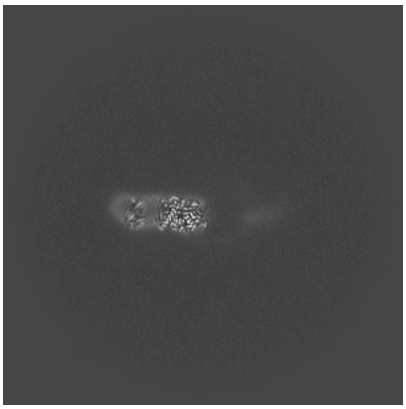


Z Index: 256

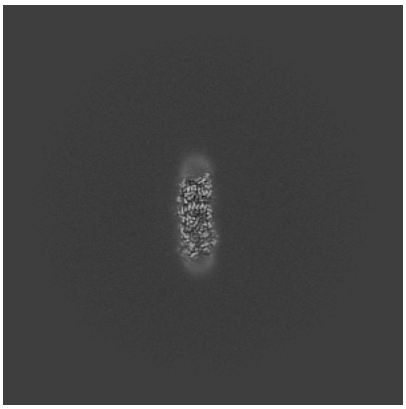
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

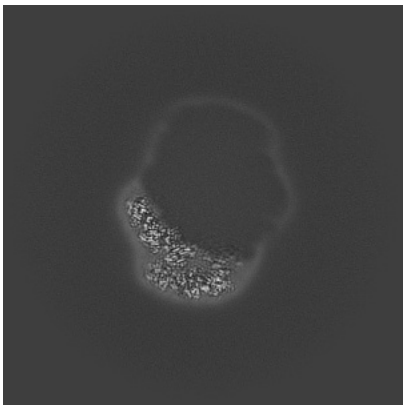
6.3.1 Primary map



X Index: 188

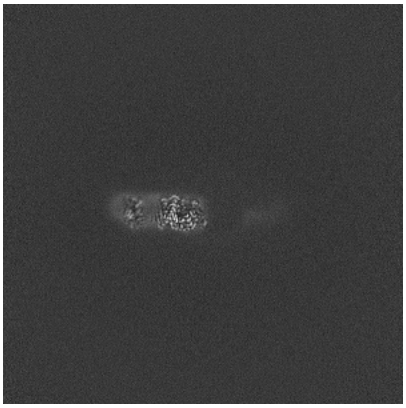


Y Index: 159

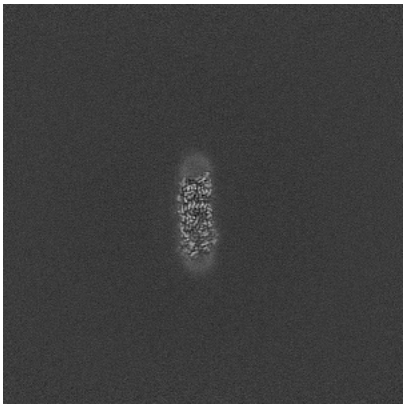


Z Index: 237

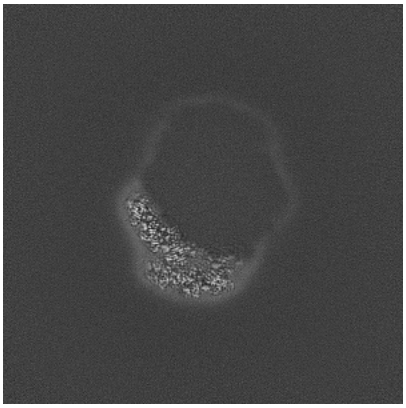
6.3.2 Raw map



X Index: 189



Y Index: 159

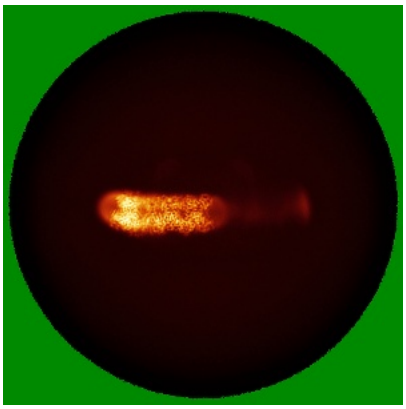


Z Index: 236

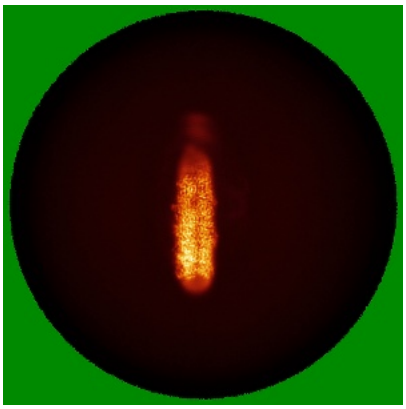
The images above show the largest variance slices of the map in three orthogonal directions.

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

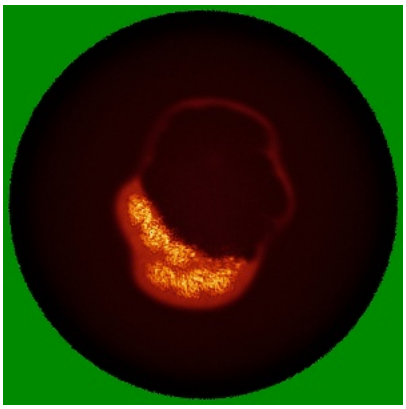
6.4.1 Primary map



X

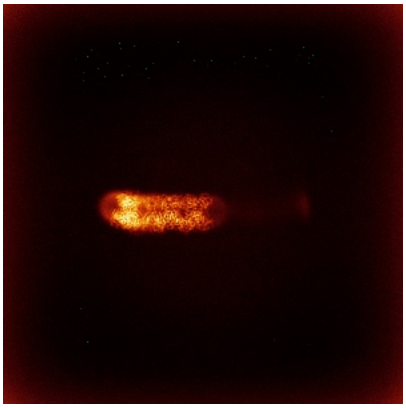


Y

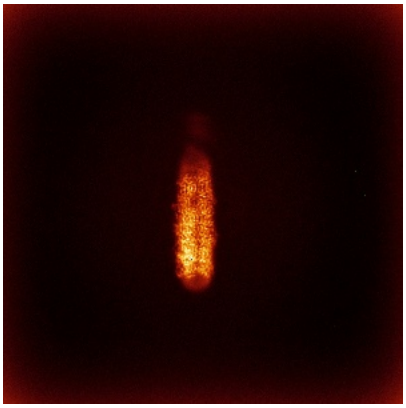


Z

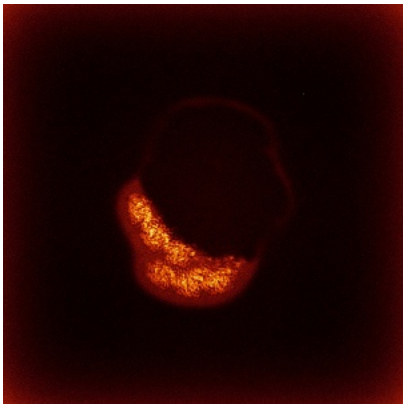
6.4.2 Raw map



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 0.266. 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.

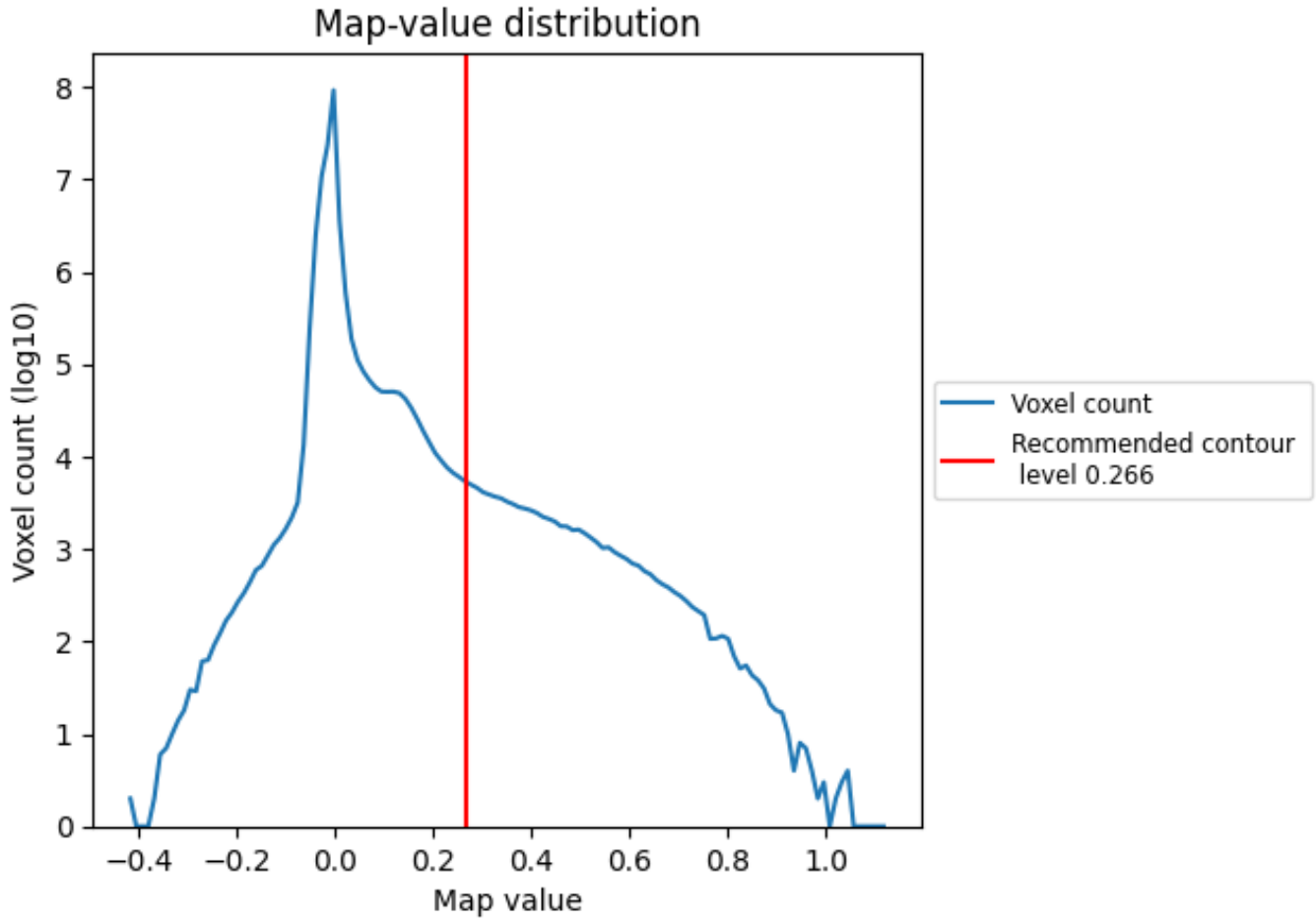
6.6 Mask visualisation (i)

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

7 Map analysis

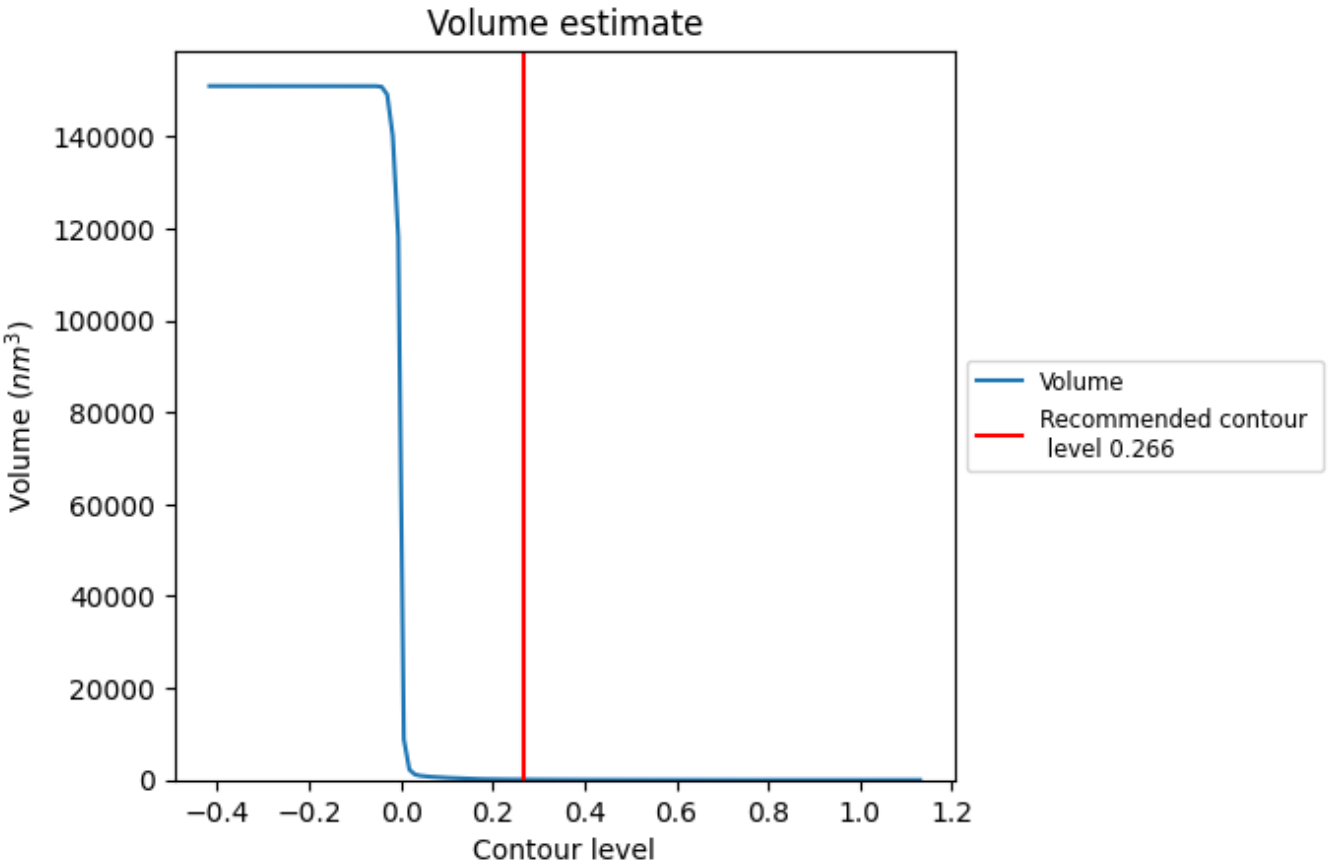
This section contains the results of statistical analysis of the map.

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.

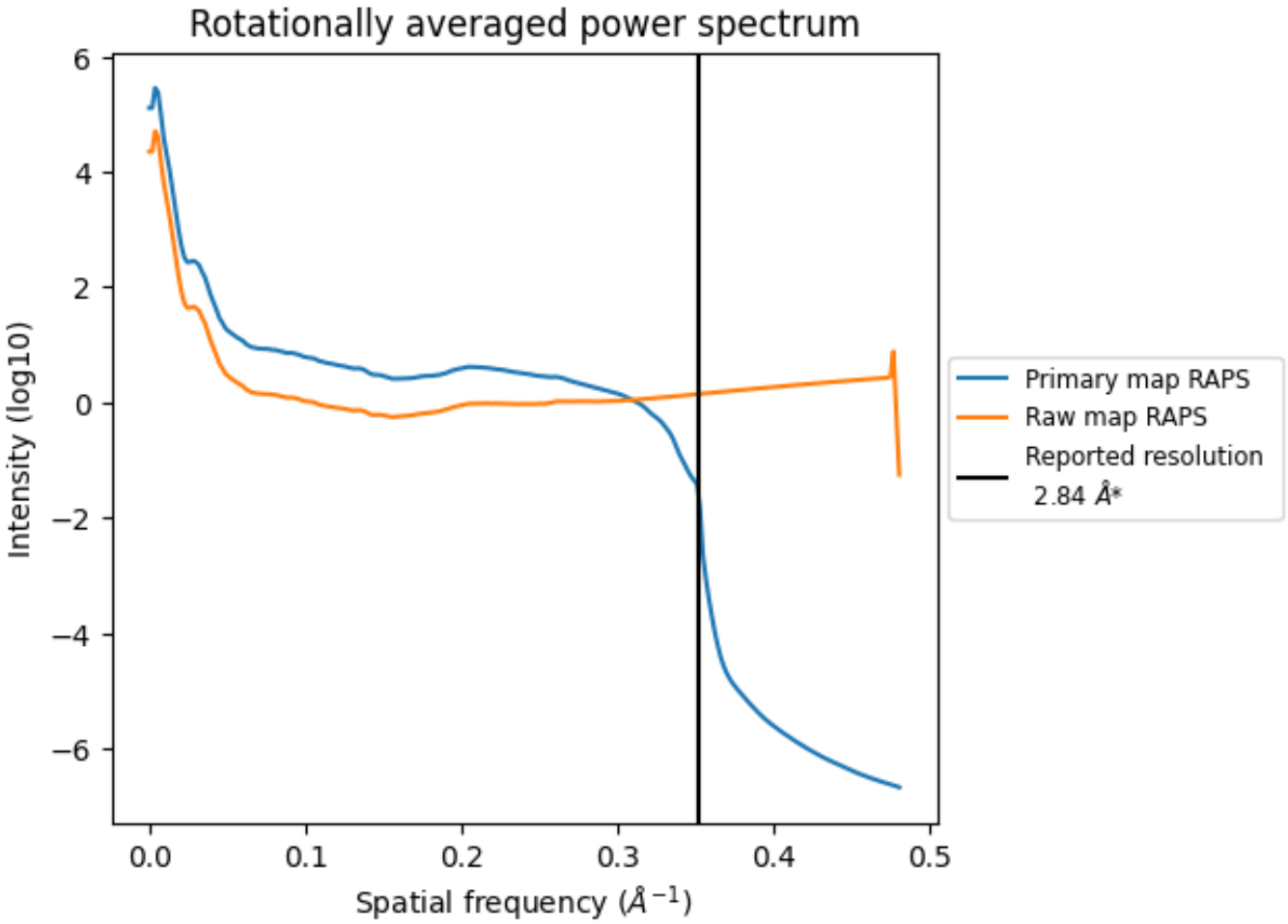
7.2 Volume estimate



The volume at the recommended contour level is 84 nm^3; this corresponds to an approximate mass of 76 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)

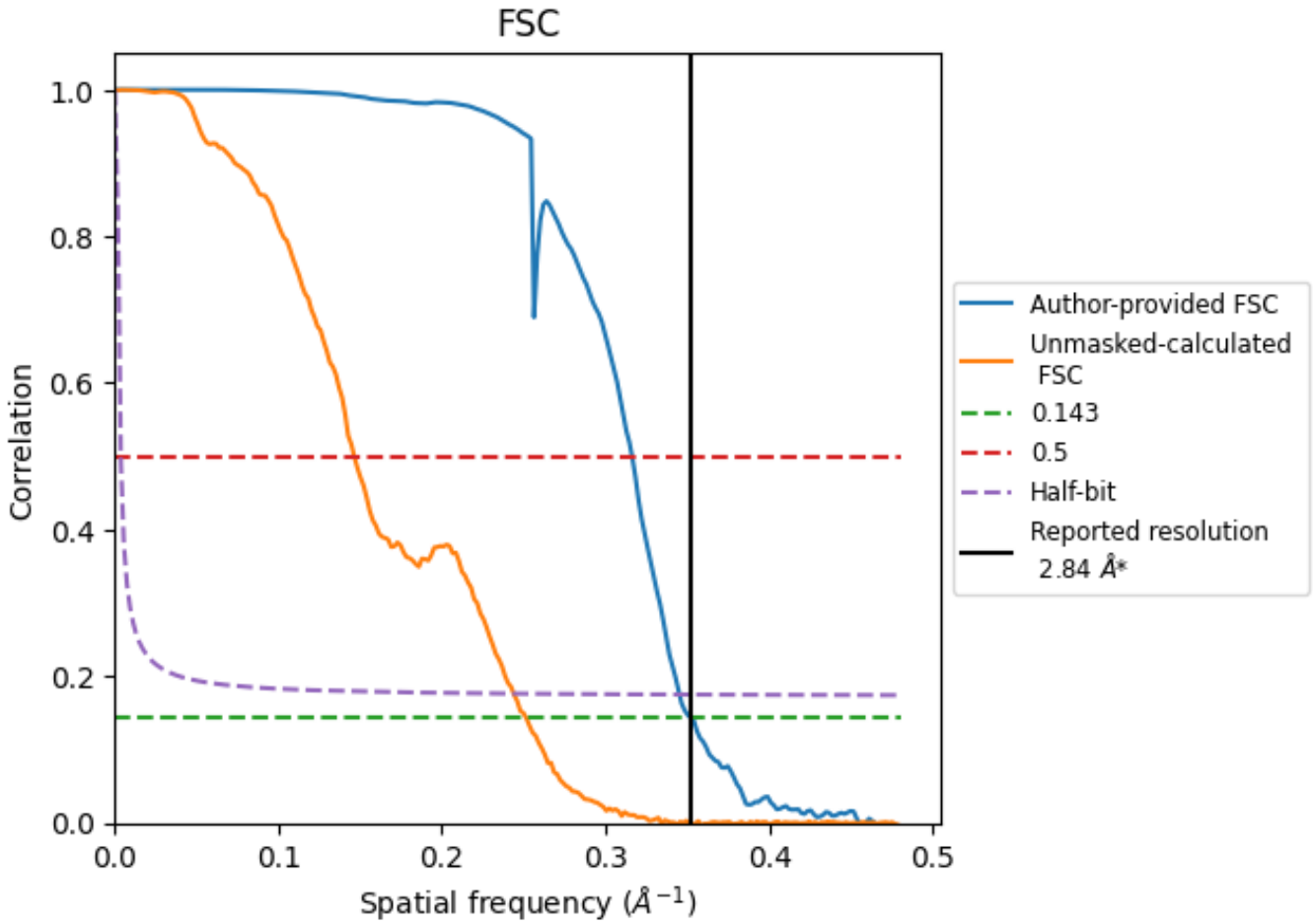


*Reported resolution corresponds to spatial frequency of 0.352 Å^{-1}

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 0.352 $Å^{-1}$

8.2 Resolution estimates (i)

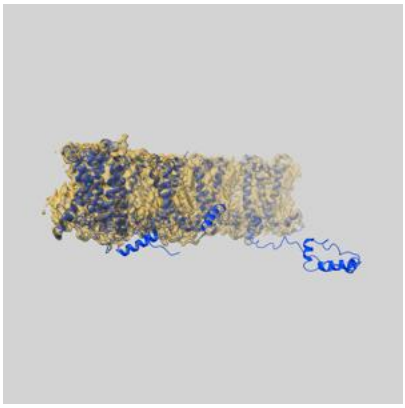
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.84	-	-
Author-provided FSC curve	2.84	3.16	2.90
Unmasked-calculated*	3.98	6.83	4.10

*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 3.98 differs from the reported value 2.84 by more than 10 %

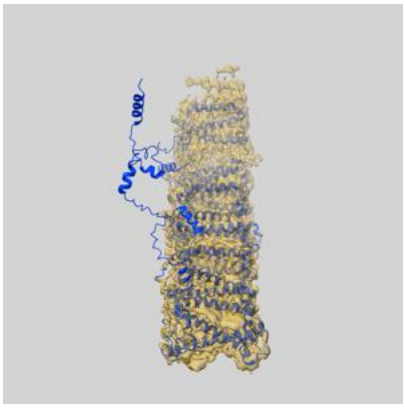
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-38419 and PDB model 8XKL. Per-residue inclusion information can be found in section 3 on page 17.

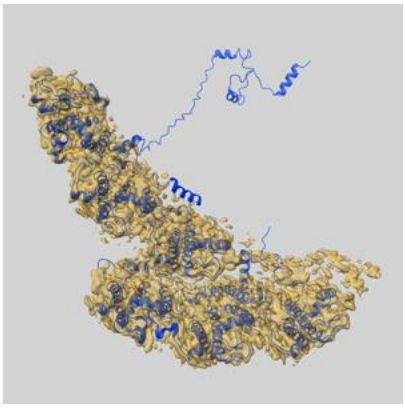
9.1 Map-model overlay



X



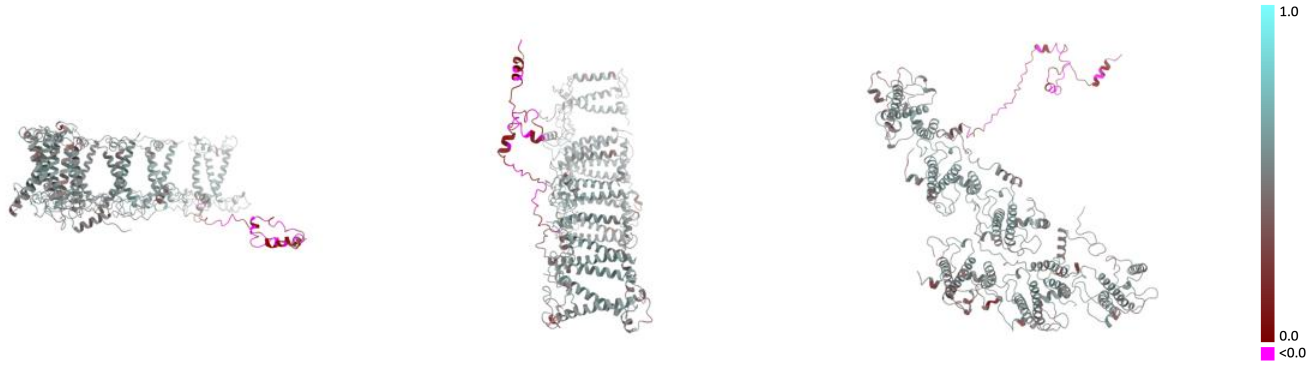
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.266 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.

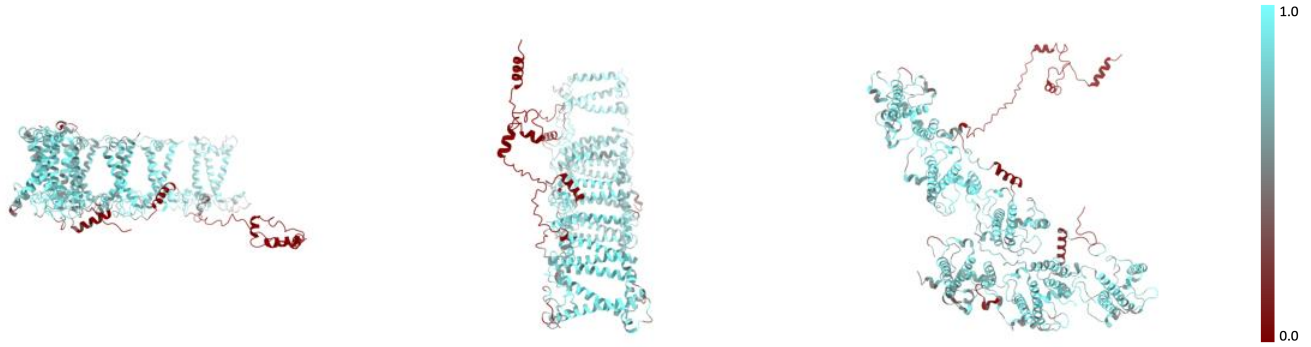
9.2 Q-score mapped to coordinate model (i)



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.

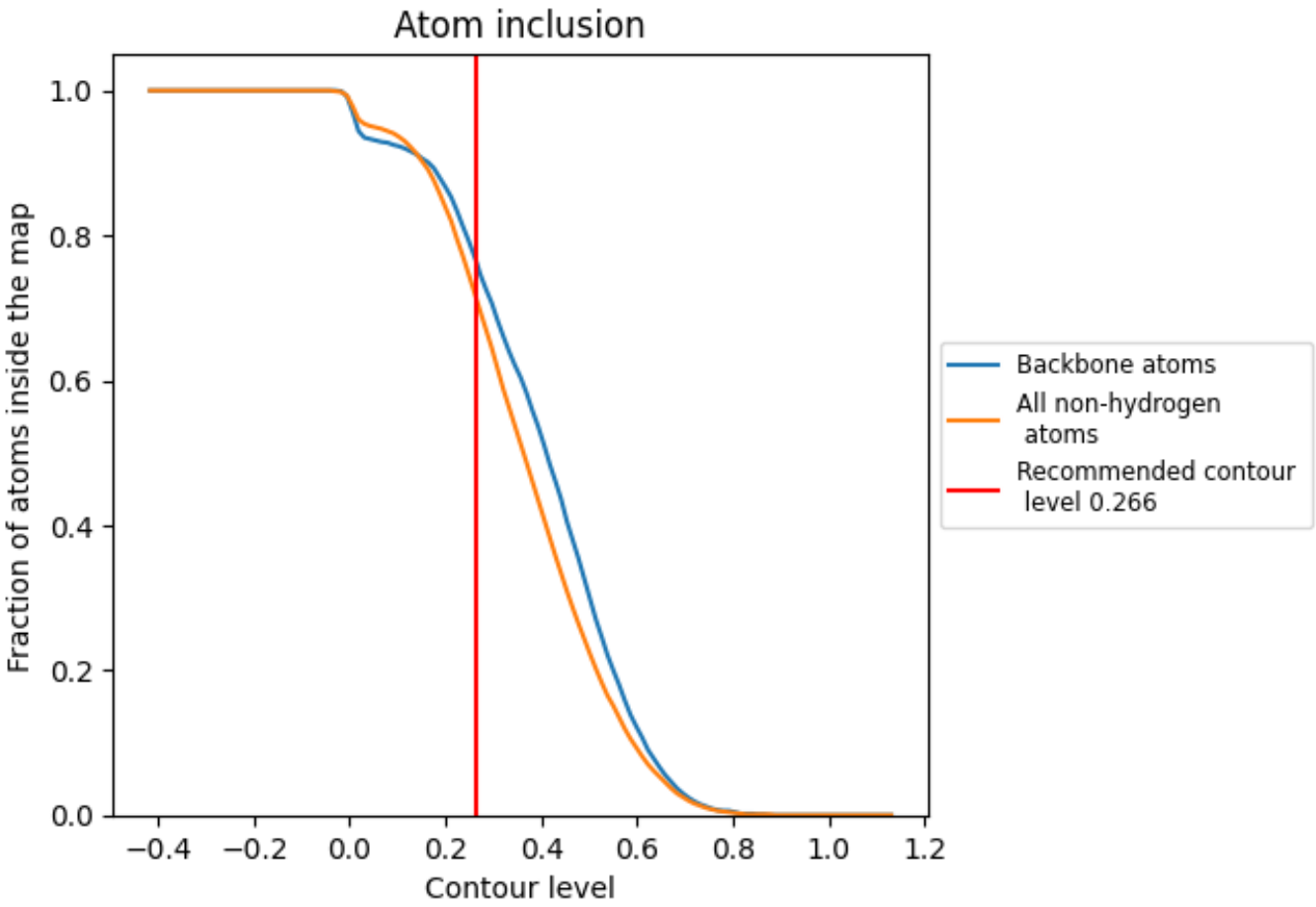
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.266).

9.4 Atom inclusion (i)



At the recommended contour level, 76% of all backbone atoms, 71% 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 (0.266) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7090	0.4900
0	0.7050	0.4920
7	0.7430	0.5020
8	0.8400	0.5470
9	0.7770	0.5340
G	0.4410	0.4780
P	0.7690	0.4930
p	0.7700	0.5160
s	0.3310	0.3040