



Full wwPDB EM Validation Report ⓘ

Aug 6, 2026 – 11:01 PM JST

PDB ID : 8W4O / pdb_00008w4o
EMDB ID : EMD-37267
Title : Structure of PSII-FCPII-G/H complex in the PSII-FCPII supercomplex from *Cyclotella meneghiniana*
Authors : Shen, L.L.; Li, Z.H.; Shen, J.R.; Wang, W.D.
Deposited on : 2023-08-24
Resolution : 3.23 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.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

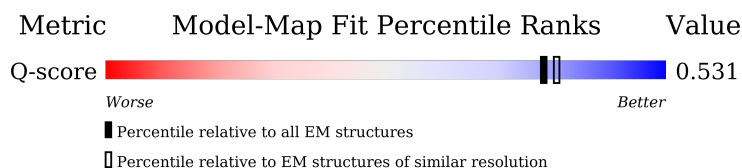
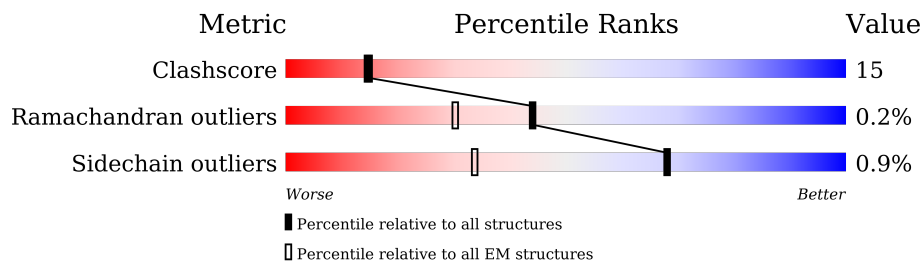
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.23 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14612 (2.73 - 3.73)

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 $\leq 5\%$. 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	5	169	13% 75% 25%
2	7	164	21% 70% 30%
3	6	164	12% 71% 27% .

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 6046 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 FCPII-G, Fucoxanthin chlorophyll a/c binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	5	169	Total	C	N	O	S	0	0
			1280	827	211	239	3		

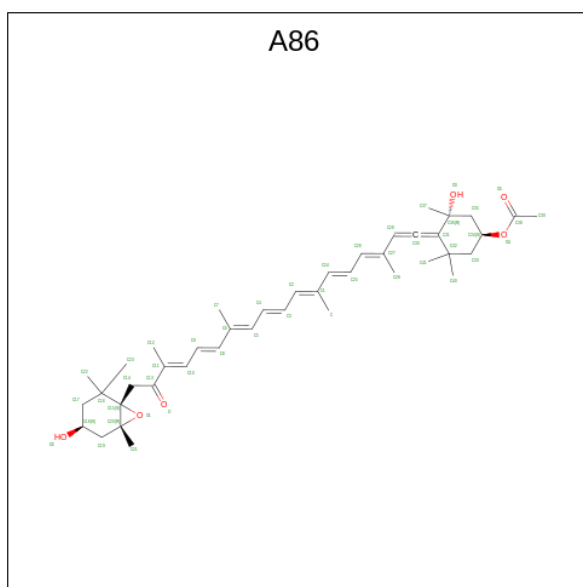
- Molecule 2 is a protein called FCPII-H2, Fucoxanthin chlorophyll a/c binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	7	164	Total	C	N	O	S	0	0
			1222	808	198	212	4		

- Molecule 3 is a protein called FCPII-H1, Fucoxanthin chlorophyll a/c binding protein.

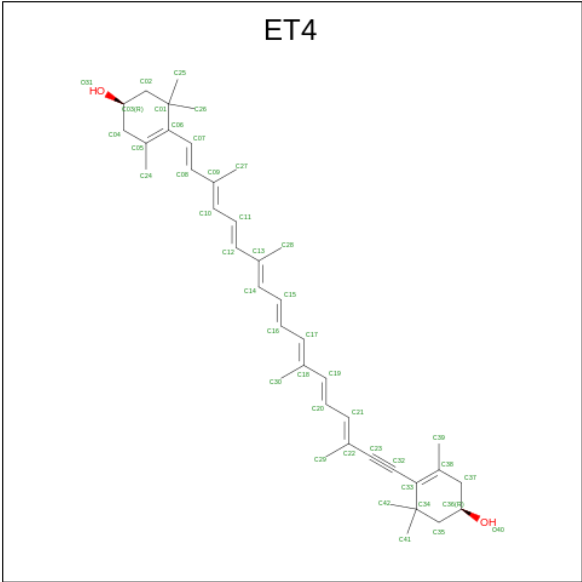
Mol	Chain	Residues	Atoms					AltConf	Trace
3	6	164	Total	C	N	O	S	0	0
			1209	796	210	201	2		

- Molecule 4 is (3S,3'S,5R,5'R,6S,6'R,8'R)-3,5'-dihydroxy-8-oxo-6',7'-didehydro-5,5',6,6',7,8-hexahydro-5,6-epoxy-beta,beta-caroten-3'-yl acetate (CCD ID: A86) (formula: C₄₂H₅₈O₆) (labeled as "Ligand of Interest" by depositor).



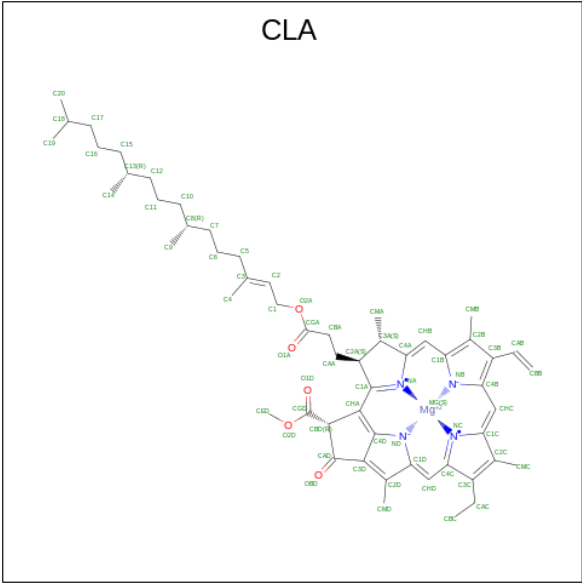
Mol	Chain	Residues	Atoms			AltConf
4	5	1	Total	C	O	0
			48	42	6	
4	5	1	Total	C	O	0
			48	42	6	
4	5	1	Total	C	O	0
			48	42	6	
4	7	1	Total	C	O	0
			48	42	6	
4	7	1	Total	C	O	0
			48	42	6	
4	6	1	Total	C	O	0
			48	42	6	

- Molecule 5 is (1 {R})-3,5,5-trimethyl-4-[(1 {E},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-1,3,5,7,9,11,13,15-octaen-17-ynyl]cyclohex-3-en-1-ol (CCD ID: ET4) (formula: C₄₀H₅₄O₂).



Mol	Chain	Residues	Atoms			AltConf
5	5	1	Total	C	O	0
			42	40	2	

- Molecule 6 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
6	5	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
6	5	1	Total	C	Mg	N	O	0
			61	51	1	4	5	

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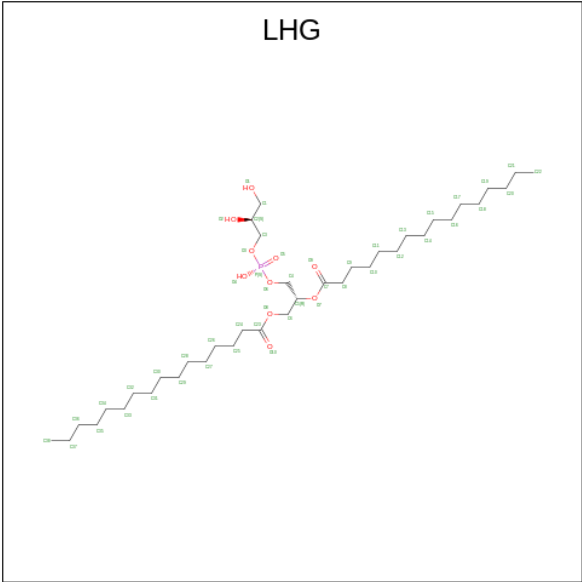
Mol	Chain	Residues	Atoms					AltConf
6	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
6	5	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
6	5	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
6	5	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
6	5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
6	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
6	5	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
6	5	1	Total	C	Mg	N	O	0
			38	32	1	4	1	
6	5	1	Total	C	Mg	N	O	0
			38	32	1	4	1	
6	7	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
6	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
6	7	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
6	7	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
6	7	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
6	7	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
6	7	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
6	7	1	Total	C	Mg	N	O	0
			36	30	1	4	1	
6	7	1	Total	C	Mg	N	O	0
			38	32	1	4	1	
6	7	1	Total	C	Mg	N	O	0
			38	32	1	4	1	
6	7	1	Total	C	Mg	N	O	0
			38	32	1	4	1	
6	7	1	Total	C	Mg	N	O	0
			41	33	1	4	3	

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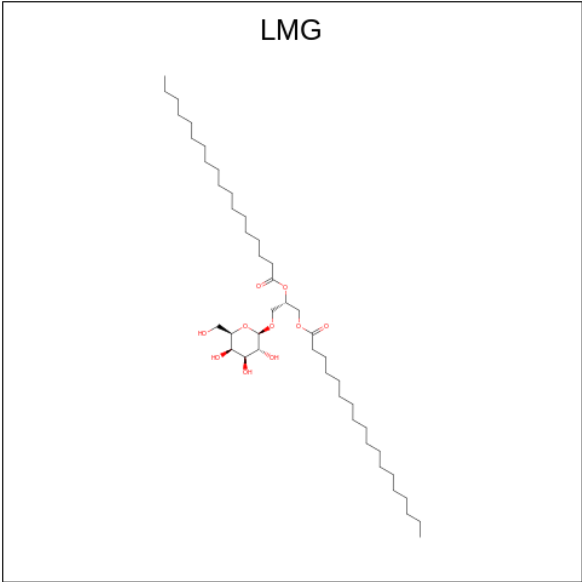
Mol	Chain	Residues	Atoms					AltConf
6	6	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
6	6	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
6	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
6	6	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
6	6	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
6	6	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
6	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
6	6	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
6	6	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
6	6	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
6	6	1	Total	C	Mg	N	O	0
			38	32	1	4	1	
6	6	1	Total	C	Mg	N	O	0
			38	32	1	4	1	
6	6	1	Total	C	Mg	N	O	0
			38	32	1	4	1	

- Molecule 7 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P) (labeled as "Ligand of Interest" by depositor).



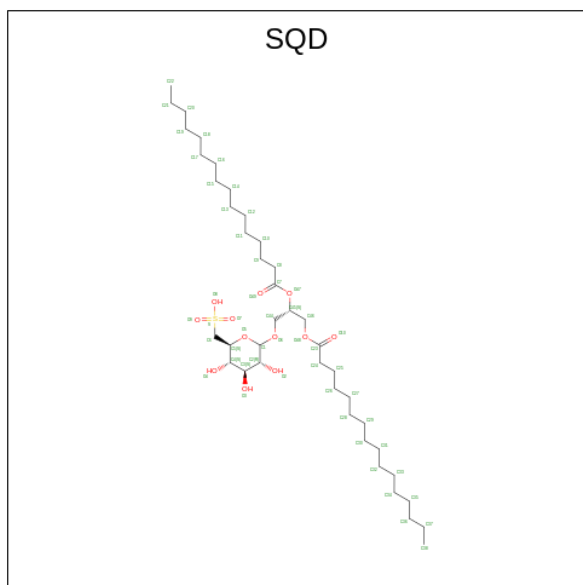
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
7	5	1	42	31	10	1	0
7	5	1	34	23	10	1	0
7	5	1	28	19	8	1	0

- Molecule 8 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀) (labeled as "Ligand of Interest" by depositor).



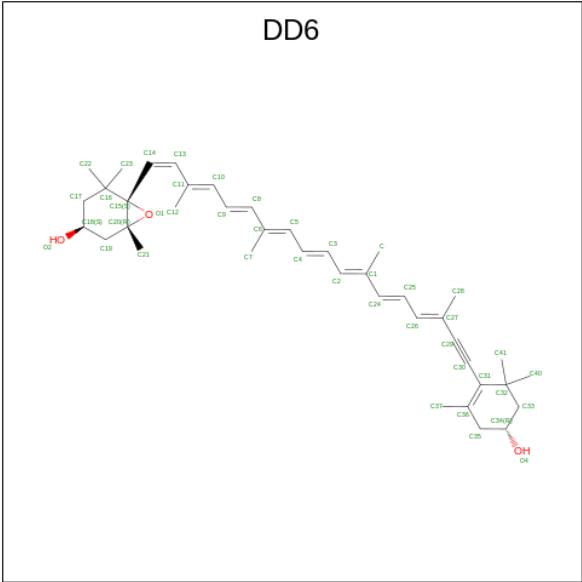
Mol	Chain	Residues	Atoms			AltConf
8	5	1	Total	C	O	0
			48	38	10	

- Molecule 9 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
9	5	1	Total	C	O	S	0
			48	35	12	1	

- Molecule 10 is (3S,3'R,5R,6S,7cis)-7',8'-didehydro-5,6-dihydro-5,6-epoxy-beta,beta-carotene -3,3'-diol (CCD ID: DD6) (formula: $C_{40}H_{54}O_3$).

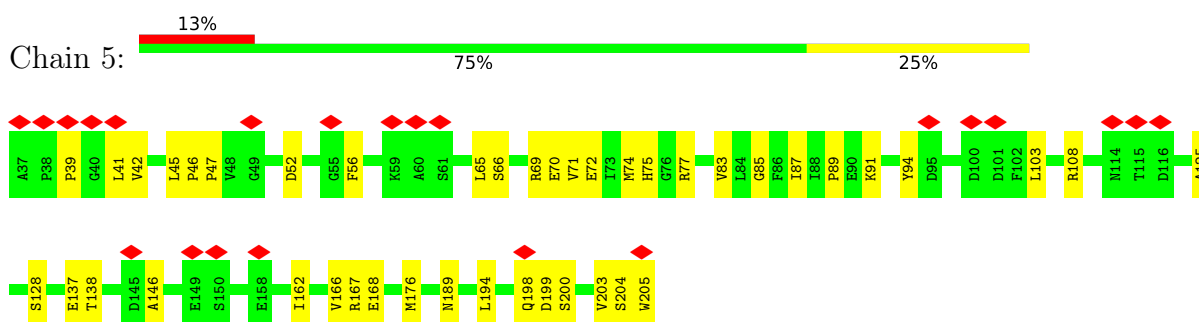


Mol	Chain	Residues	Atoms			AltConf
10	7	1	Total	C	O	0
			43	40	3	
10	7	1	Total	C	O	0
			43	40	3	
10	6	1	Total	C	O	0
			43	40	3	
10	6	1	Total	C	O	0
			43	40	3	

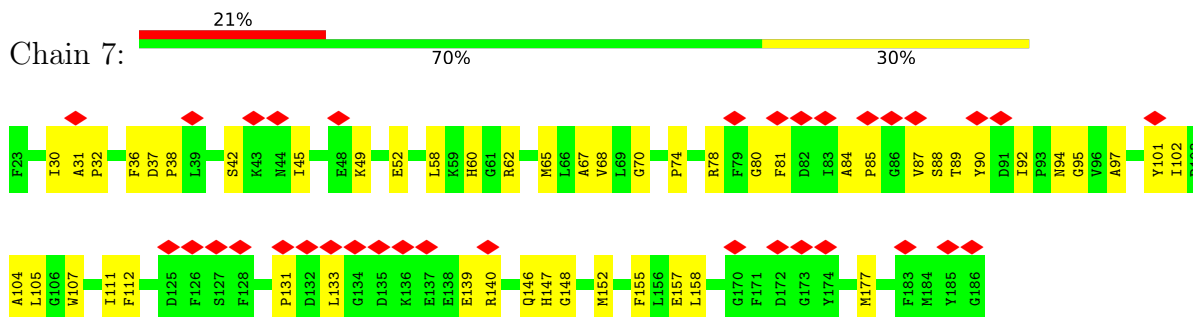
3 Residue-property plots

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.

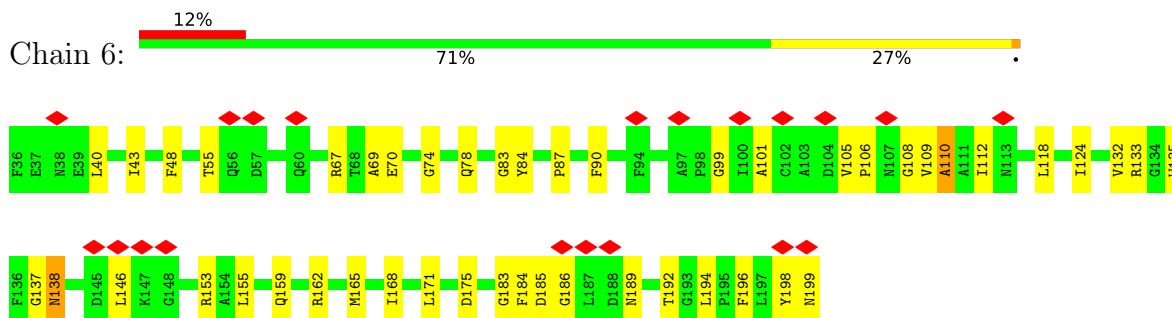
- Molecule 1: FCPHII-G, Fucoxanthin chlorophyll a/c binding protein



- Molecule 2: FCPHII-H2, Fucoxanthin chlorophyll a/c binding protein



- Molecule 3: FCPHII-H1, Fucoxanthin chlorophyll a/c binding protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	314409	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.873	Depositor
Minimum map value	-0.442	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.313	Depositor
Map size (Å)	542.72, 542.72, 542.72	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CLA, DD6, LHG, ET4, A86, SQD, LMG

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	5	0.27	0/1312	0.49	0/1792
2	7	0.24	0/1258	0.44	0/1714
3	6	0.31	0/1242	0.47	0/1697
All	All	0.27	0/3812	0.47	0/5203

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	5	1280	0	1242	39	0
2	7	1222	0	1142	64	0
3	6	1209	0	1150	40	0
4	5	144	0	0	1	0
4	6	48	0	0	1	0
4	7	96	0	0	0	0
5	5	42	0	0	0	0
6	5	528	0	439	16	0
6	6	580	0	441	15	0
6	7	525	0	395	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	5	104	0	121	2	0
8	5	48	0	69	1	0
9	5	48	0	63	5	0
10	6	86	0	0	3	0
10	7	86	0	0	26	0
All	All	6046	0	5062	168	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 15.

All (168) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:7:65:MET:HG2	10:7:304:DD6:C3	1.71	1.19
2:7:37:ASP:HA	10:7:303:DD6:O2	1.54	1.06
2:7:155:PHE:CE2	10:7:303:DD6:C24	2.39	1.05
2:7:68:VAL:HG11	10:7:304:DD6:C26	1.89	1.01
10:7:304:DD6:C8	6:7:310:CLA:HHC	1.92	1.00
2:7:36:PHE:CD2	10:7:303:DD6:C22	2.45	1.00
10:7:304:DD6:C8	6:7:310:CLA:CHC	2.56	0.83
2:7:38:PRO:HD2	10:7:303:DD6:C18	2.09	0.82
3:6:189:ASN:HB3	3:6:199:ASN:C	2.09	0.77
1:5:71:VAL:HG13	1:5:75:HIS:CE1	2.20	0.76
2:7:155:PHE:CD2	10:7:303:DD6:C24	2.69	0.76
2:7:38:PRO:HD2	10:7:303:DD6:C19	2.19	0.73
1:5:41:LEU:HD12	1:5:69:ARG:HE	1.55	0.71
1:5:167:ARG:HD3	6:5:311:CLA:HBA1	1.72	0.70
7:5:315:LHG:H241	7:5:318:LHG:HC81	1.73	0.69
2:7:107:TRP:O	2:7:111:ILE:HG13	1.93	0.69
2:7:37:ASP:CA	10:7:303:DD6:O2	2.38	0.68
3:6:165:MET:HE1	6:6:206:CLA:HHC	1.76	0.66
2:7:133:LEU:HD21	6:7:310:CLA:HAA2	1.78	0.65
2:7:36:PHE:CE2	10:7:303:DD6:C22	2.81	0.64
1:5:41:LEU:HB3	1:5:69:ARG:HH21	1.62	0.63
2:7:84:ALA:HB3	2:7:87:VAL:HG12	1.80	0.63
2:7:155:PHE:CZ	10:7:303:DD6:C24	2.82	0.62
3:6:194:LEU:HB3	3:6:196:PHE:CZ	2.35	0.62
6:5:313:CLA:HBB2	9:5:319:SQD:H251	1.82	0.62
2:7:155:PHE:CZ	10:7:303:DD6:C26	2.83	0.62
2:7:65:MET:SD	6:7:310:CLA:HMC3	2.39	0.61
1:5:138:THR:HG23	6:5:308:CLA:HAC2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:194:LEU:HD11	1:5:205:TRP:HZ3	1.66	0.61
3:6:70:GLU:OE2	3:6:162:ARG:NE	2.27	0.60
10:7:303:DD6:C9	6:7:306:CLA:HMC1	2.31	0.60
2:7:155:PHE:CE1	10:7:303:DD6:C26	2.85	0.60
3:6:74:GLY:O	3:6:78:GLN:HG3	2.01	0.60
2:7:36:PHE:HD2	10:7:303:DD6:C22	2.08	0.59
2:7:38:PRO:CD	10:7:303:DD6:C18	2.81	0.58
2:7:84:ALA:HB1	2:7:85:PRO:HD2	1.85	0.58
2:7:38:PRO:HD2	10:7:303:DD6:O2	2.04	0.57
3:6:165:MET:HE1	6:6:206:CLA:CHC	2.34	0.57
1:5:42:VAL:HG23	1:5:162:ILE:HG23	1.86	0.57
3:6:132:VAL:HG13	3:6:133:ARG:H	1.68	0.57
3:6:159:GLN:OE1	3:6:162:ARG:NH1	2.38	0.56
2:7:38:PRO:CD	10:7:303:DD6:O2	2.53	0.56
1:5:47:PRO:HG3	6:5:304:CLA:NB	2.21	0.56
3:6:40:LEU:O	3:6:67:ARG:NH2	2.39	0.56
1:5:66:SER:O	1:5:70:GLU:HG2	2.05	0.55
2:7:133:LEU:HD12	2:7:140:ARG:HG3	1.89	0.55
1:5:71:VAL:HG13	1:5:75:HIS:HE1	1.71	0.55
1:5:74:MET:HE1	6:5:308:CLA:OBD	2.07	0.55
1:5:39:PRO:HG2	1:5:41:LEU:HD23	1.89	0.54
2:7:30:ILE:HG22	2:7:31:ALA:H	1.72	0.54
2:7:81:PHE:O	2:7:89:THR:HG22	2.07	0.54
3:6:84:TYR:HD2	3:6:171:LEU:HD13	1.72	0.53
2:7:30:ILE:HG22	2:7:32:PRO:HD2	1.90	0.53
2:7:60:HIS:CB	2:7:152:MET:HE2	2.38	0.53
3:6:83:GLY:O	3:6:87:PRO:HD2	2.09	0.53
1:5:47:PRO:HG3	6:5:304:CLA:C4B	2.38	0.53
2:7:68:VAL:CG1	10:7:304:DD6:C26	2.76	0.52
3:6:165:MET:O	3:6:168:ILE:HG22	2.09	0.52
2:7:32:PRO:HG3	6:7:305:CLA:C4B	2.39	0.52
3:6:99:GLY:O	3:6:101:ALA:N	2.40	0.52
3:6:133:ARG:HH21	6:6:201:CLA:HED1	1.76	0.51
1:5:146:ALA:HA	6:5:308:CLA:HBC2	1.93	0.51
1:5:204:SER:O	3:6:186:GLY:HA3	2.11	0.51
7:5:315:LHG:H131	7:5:315:LHG:H261	1.92	0.51
3:6:108:GLY:HA3	3:6:175:ASP:OD2	2.11	0.51
1:5:42:VAL:HG22	1:5:166:VAL:HG23	1.93	0.50
3:6:132:VAL:HG13	3:6:133:ARG:N	2.26	0.50
10:7:303:DD6:C37	6:7:307:CLA:C2B	2.89	0.50
1:5:137:GLU:HG3	6:5:308:CLA:HMC2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:7:30:ILE:HG22	2:7:31:ALA:N	2.27	0.49
1:5:74:MET:HE2	1:5:77:ARG:HD2	1.94	0.49
1:5:103:LEU:HD22	1:5:108:ARG:O	2.13	0.48
1:5:45:LEU:HB3	1:5:47:PRO:HD2	1.95	0.48
2:7:104:ALA:HB3	3:6:112:ILE:O	2.13	0.48
6:7:309:CLA:H12	6:6:201:CLA:HMD2	1.94	0.48
6:5:308:CLA:O1A	6:5:308:CLA:H2A	2.12	0.48
2:7:102:ILE:HB	2:7:107:TRP:NE1	2.28	0.48
2:7:65:MET:HE2	2:7:147:HIS:HB3	1.96	0.48
2:7:74:PRO:HB2	2:7:94:ASN:ND2	2.29	0.48
1:5:194:LEU:HD11	1:5:205:TRP:CZ3	2.48	0.48
2:7:80:GLY:HA2	2:7:90:TYR:CE2	2.49	0.48
1:5:85:GLY:O	1:5:89:PRO:HD2	2.13	0.48
3:6:43:ILE:HD12	3:6:155:LEU:HD21	1.96	0.48
10:6:204:DD6:C10	6:6:211:CLA:H52	2.43	0.48
2:7:78:ARG:HB3	2:7:89:THR:O	2.12	0.48
3:6:78:GLN:HB3	10:6:204:DD6:C3	2.43	0.48
6:5:304:CLA:HBC2	6:5:311:CLA:HBC1	1.96	0.47
3:6:171:LEU:HD23	3:6:171:LEU:HA	1.77	0.47
9:5:319:SQD:H45	9:5:319:SQD:H1	1.72	0.47
2:7:92:ILE:HG13	6:7:307:CLA:HED3	1.96	0.47
2:7:102:ILE:HD11	6:7:307:CLA:HAA2	1.96	0.47
6:7:309:CLA:HBB1	6:7:309:CLA:HMB3	1.95	0.46
4:6:202:A86:C21	6:6:214:CLA:H3A	2.45	0.46
2:7:80:GLY:H	2:7:89:THR:HG23	1.80	0.46
3:6:48:PHE:CZ	3:6:55:THR:HG21	2.50	0.46
2:7:45:ILE:HG22	2:7:49:LYS:HB2	1.97	0.46
10:7:303:DD6:C8	6:7:306:CLA:HMC1	2.45	0.46
6:6:210:CLA:CHA	6:6:210:CLA:HBA1	2.45	0.46
1:5:69:ARG:NH1	1:5:72:GLU:OE1	2.49	0.46
9:5:319:SQD:H252	9:5:319:SQD:H82	1.98	0.45
3:6:105:VAL:HG12	3:6:106:PRO:O	2.16	0.45
3:6:109:VAL:N	3:6:175:ASP:OD2	2.44	0.45
3:6:135:TRP:C	3:6:137:GLY:H	2.25	0.45
2:7:65:MET:HE3	2:7:148:GLY:CA	2.47	0.45
3:6:48:PHE:HZ	3:6:55:THR:HG21	1.82	0.45
1:5:46:PRO:O	1:5:47:PRO:C	2.60	0.45
1:5:199:ASP:O	1:5:200:SER:OG	2.24	0.45
2:7:65:MET:HE3	2:7:148:GLY:HA2	1.97	0.45
2:7:105:LEU:HD13	3:6:112:ILE:HG21	1.99	0.45
3:6:165:MET:CE	6:6:206:CLA:HHC	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:45:LEU:HD21	1:5:166:VAL:HG11	1.99	0.44
2:7:37:ASP:OD2	2:7:42:SER:OG	2.28	0.44
2:7:131:PRO:HD2	6:7:310:CLA:HED3	1.98	0.44
1:5:52:ASP:OD1	6:5:305:CLA:HBA2	2.17	0.44
3:6:87:PRO:HA	3:6:90:PHE:O	2.16	0.44
3:6:196:PHE:C	3:6:198:TYR:H	2.25	0.44
6:7:309:CLA:H62	6:7:309:CLA:H41	1.71	0.44
2:7:112:PHE:HA	6:7:309:CLA:HBB2	1.99	0.44
6:5:305:CLA:CGA	6:5:305:CLA:H3A	2.48	0.44
3:6:138:ASN:O	3:6:138:ASN:ND2	2.51	0.44
6:5:308:CLA:H51	6:5:308:CLA:H12	1.79	0.44
2:7:37:ASP:OD2	6:7:306:CLA:HBA2	2.18	0.43
6:6:211:CLA:H92	6:6:211:CLA:H61	1.69	0.43
8:5:316:LMG:O5	8:5:316:LMG:O4	2.35	0.43
2:7:157:GLU:HB2	6:7:312:CLA:C4B	2.49	0.43
3:6:110:ALA:C	3:6:112:ILE:H	2.25	0.43
1:5:91:LYS:HE2	9:5:319:SQD:H442	2.00	0.43
3:6:124:ILE:O	6:6:210:CLA:HAB	2.18	0.43
2:7:49:LYS:O	2:7:52:GLU:N	2.51	0.43
2:7:158:LEU:HG	10:7:304:DD6:C37	2.49	0.43
6:7:309:CLA:CGA	3:6:132:VAL:HG11	2.48	0.43
2:7:60:HIS:HB3	2:7:152:MET:HE2	1.99	0.43
1:5:94:TYR:CD2	1:5:194:LEU:HD23	2.53	0.43
6:5:307:CLA:H3A	6:5:307:CLA:HBA2	1.47	0.43
3:6:109:VAL:C	3:6:110:ALA:O	2.62	0.43
2:7:88:SER:C	2:7:90:TYR:H	2.28	0.42
2:7:92:ILE:HG22	2:7:101:TYR:CD2	2.54	0.42
10:6:203:DD6:C9	6:6:206:CLA:HMC1	2.49	0.42
2:7:60:HIS:HB2	2:7:152:MET:HE2	2.01	0.42
2:7:147:HIS:CD2	6:7:310:CLA:HBB2	2.55	0.42
1:5:65:LEU:HD12	1:5:65:LEU:HA	1.79	0.42
2:7:95:GLY:O	2:7:97:ALA:N	2.46	0.42
3:6:118:LEU:HB3	6:6:209:CLA:O1D	2.20	0.42
3:6:69:ALA:HB2	6:6:210:CLA:HED3	2.02	0.41
1:5:56:PHE:CD2	6:5:305:CLA:H42	2.55	0.41
1:5:83:VAL:HG11	4:5:303:A86:C8	2.50	0.41
2:7:36:PHE:HB3	6:7:306:CLA:C3D	2.50	0.41
1:5:71:VAL:O	1:5:75:HIS:ND1	2.31	0.41
2:7:84:ALA:HB1	2:7:85:PRO:CD	2.49	0.41
1:5:168:GLU:HB2	6:5:310:CLA:C1B	2.50	0.41
2:7:65:MET:CG	10:7:304:DD6:C3	2.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:6:146:LEU:HD13	3:6:153:ARG:HG3	2.02	0.41
6:6:210:CLA:H41	6:6:210:CLA:H62	1.70	0.41
3:6:183:GLY:C	3:6:185:ASP:H	2.28	0.41
2:7:30:ILE:HD12	2:7:146:GLN:CD	2.45	0.41
6:6:210:CLA:HED2	6:6:210:CLA:HBD	1.86	0.41
1:5:83:VAL:O	1:5:87:ILE:HG12	2.20	0.41
1:5:189:ASN:O	1:5:189:ASN:OD1	2.38	0.41
2:7:148:GLY:O	2:7:152:MET:HG3	2.21	0.41
2:7:177:MET:HE2	2:7:177:MET:HB2	1.93	0.41
2:7:58:LEU:O	2:7:62:ARG:HG3	2.21	0.40
2:7:67:ALA:O	2:7:70:GLY:N	2.52	0.40
1:5:125:ALA:O	1:5:128:SER:OG	2.30	0.40
10:7:304:DD6:C5	6:7:310:CLA:HAB	2.52	0.40
1:5:198:GLN:HA	1:5:203:VAL:HG22	2.04	0.40
9:5:319:SQD:O4	3:6:184:PHE:O	2.30	0.40
6:7:309:CLA:H111	6:7:309:CLA:H71	1.69	0.40
1:5:75:HIS:HB2	1:5:176:MET:HE2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	5	167/169 (99%)	144 (86%)	23 (14%)	0	100	100
2	7	162/164 (99%)	143 (88%)	19 (12%)	0	100	100
3	6	162/164 (99%)	135 (83%)	26 (16%)	1 (1%)	21	53
All	All	491/497 (99%)	422 (86%)	68 (14%)	1 (0%)	44	72

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	6	110	ALA

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	5	129/136 (95%)	129 (100%)	0	100	100
2	7	110/131 (84%)	109 (99%)	1 (1%)	70	79
3	6	107/129 (83%)	105 (98%)	2 (2%)	50	70
All	All	346/396 (87%)	343 (99%)	3 (1%)	68	79

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	7	139	GLU
3	6	138	ASN
3	6	192	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	5	171	GLN
1	5	185	GLN
1	5	189	ASN
1	5	196	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

52 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
6	CLA	7	311	2	47,51,73	1.48	8 (17%)	56,86,113	1.41	6 (10%)
10	DD6	7	303	-	39,45,45	1.99	3 (7%)	52,67,67	2.20	17 (32%)
10	DD6	7	304	-	39,45,45	2.05	3 (7%)	52,67,67	2.51	17 (32%)
6	CLA	5	306	-	49,53,73	1.47	8 (16%)	59,89,113	1.44	5 (8%)
4	A86	5	303	-	44,50,50	1.27	4 (9%)	51,76,76	2.43	20 (39%)
6	CLA	7	307	-	51,55,73	1.44	9 (17%)	61,91,113	1.46	7 (11%)
6	CLA	6	210	3	69,73,73	1.23	8 (11%)	83,113,113	1.34	7 (8%)
6	CLA	5	308	-	65,69,73	1.30	9 (13%)	78,108,113	1.34	7 (8%)
6	CLA	6	216	3	41,46,73	1.55	7 (17%)	51,80,113	1.50	5 (9%)
6	CLA	6	215	3	41,46,73	1.54	8 (19%)	51,80,113	1.54	6 (11%)
5	ET4	5	302	-	41,43,43	1.73	11 (26%)	54,60,60	2.22	17 (31%)
6	CLA	7	306	2	49,53,73	1.47	8 (16%)	59,89,113	1.46	5 (8%)
6	CLA	7	305	-	45,49,73	1.52	9 (20%)	54,84,113	1.53	7 (12%)
6	CLA	6	213	3	43,48,73	1.54	8 (18%)	51,83,113	1.48	5 (9%)
7	LHG	5	318	-	27,27,48	0.87	2 (7%)	31,32,54	1.72	4 (12%)
6	CLA	7	315	2	41,46,73	1.56	7 (17%)	51,80,113	1.53	5 (9%)
6	CLA	6	211	3	59,63,73	1.36	9 (15%)	71,101,113	1.34	7 (9%)
6	CLA	6	209	3	48,52,73	1.56	10 (20%)	61,88,113	1.50	8 (13%)
10	DD6	6	203	-	39,45,45	1.99	3 (7%)	52,67,67	2.20	17 (32%)
6	CLA	7	308	2	48,52,73	1.56	9 (18%)	61,88,113	1.49	6 (9%)
6	CLA	5	307	-	65,69,73	1.29	8 (12%)	78,108,113	1.34	5 (6%)
6	CLA	6	208	-	51,55,73	1.44	7 (13%)	61,91,113	1.43	6 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	A86	5	301	-	44,50,50	1.29	3 (6%)	51,76,76	2.93	19 (37%)
7	LHG	5	317	-	33,33,48	0.73	0	36,39,54	1.35	4 (11%)
6	CLA	5	312	-	46,50,73	1.50	9 (19%)	55,85,113	1.46	4 (7%)
6	CLA	7	313	2	41,46,73	1.57	8 (19%)	51,80,113	1.52	6 (11%)
9	SQD	5	319	-	47,48,54	1.03	5 (10%)	56,59,65	1.45	8 (14%)
6	CLA	5	311	-	49,53,73	1.47	8 (16%)	59,89,113	1.49	4 (6%)
6	CLA	7	314	2	41,46,73	1.56	9 (21%)	51,80,113	1.55	8 (15%)
6	CLA	6	214	3	41,46,73	1.55	8 (19%)	51,80,113	1.56	6 (11%)
4	A86	5	320	-	44,50,50	1.29	3 (6%)	51,76,76	2.94	18 (35%)
4	A86	6	202	-	44,50,50	1.32	4 (9%)	51,76,76	2.90	16 (31%)
6	CLA	6	201	2	48,52,73	1.56	10 (20%)	61,88,113	1.53	8 (13%)
8	LMG	5	316	-	48,48,55	0.77	0	56,56,63	1.29	6 (10%)
6	CLA	7	312	2	40,44,73	1.70	9 (22%)	49,77,113	1.62	8 (16%)
4	A86	7	301	-	44,50,50	1.30	3 (6%)	51,76,76	2.97	19 (37%)
6	CLA	5	309	1	45,49,73	1.51	9 (20%)	54,84,113	1.53	7 (12%)
6	CLA	5	310	1	59,63,73	1.34	8 (13%)	71,101,113	1.36	7 (9%)
6	CLA	5	313	1	41,46,73	1.55	8 (19%)	51,80,113	1.56	7 (13%)
4	A86	7	302	-	44,50,50	1.52	6 (13%)	51,76,76	3.25	18 (35%)
6	CLA	6	206	3	49,53,73	1.46	8 (16%)	59,89,113	1.51	6 (10%)
6	CLA	6	212	3	45,49,73	1.51	8 (17%)	54,84,113	1.51	6 (11%)
6	CLA	7	309	2	63,67,73	1.30	9 (14%)	75,105,113	1.34	8 (10%)
6	CLA	7	310	2	59,63,73	1.35	9 (15%)	71,101,113	1.38	8 (11%)
10	DD6	6	204	-	39,45,45	2.22	4 (10%)	52,67,67	2.34	17 (32%)
6	CLA	5	304	-	45,49,73	1.51	9 (20%)	54,84,113	1.53	6 (11%)
6	CLA	6	207	3	48,52,73	1.56	9 (18%)	61,88,113	1.48	8 (13%)
6	CLA	6	205	-	45,49,73	1.52	8 (17%)	54,84,113	1.50	7 (12%)
7	LHG	5	315	-	41,41,48	0.65	1 (2%)	44,47,54	1.14	3 (6%)
6	CLA	5	314	1	41,46,73	1.56	8 (19%)	51,80,113	1.53	5 (9%)
6	CLA	5	305	1	65,69,73	1.31	10 (15%)	78,108,113	1.35	8 (10%)
6	CLA	7	316	-	45,49,73	1.52	7 (15%)	54,84,113	1.51	7 (12%)

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
6	CLA	7	311	2	-	7/13/89/115	-
10	DD6	7	303	-	-	2/26/80/80	0/3/3/3
10	DD6	7	304	-	-	10/26/80/80	0/3/3/3
6	CLA	5	306	-	-	4/15/91/115	-
4	A86	5	303	-	-	5/34/90/90	0/3/3/3
6	CLA	7	307	-	-	5/18/94/115	-
6	CLA	6	210	3	-	16/39/115/115	-
6	CLA	5	308	-	-	14/35/111/115	-
6	CLA	6	216	3	-	2/4/80/115	-
6	CLA	6	215	3	-	0/4/80/115	-
5	ET4	5	302	-	-	9/25/67/67	0/2/2/2
6	CLA	7	306	2	-	3/15/91/115	-
6	CLA	7	305	-	-	6/10/86/115	-
6	CLA	6	213	3	-	6/8/84/115	-
7	LHG	5	318	-	-	17/29/29/53	-
6	CLA	7	315	2	-	2/4/80/115	-
6	CLA	6	211	3	-	5/27/103/115	-
6	CLA	6	209	3	-	6/13/89/115	-
10	DD6	6	203	-	-	2/26/80/80	0/3/3/3
6	CLA	7	308	2	-	7/13/89/115	-
6	CLA	5	307	-	-	21/35/111/115	-
6	CLA	6	208	-	-	7/18/94/115	-
4	A86	5	301	-	-	10/34/90/90	0/3/3/3
7	LHG	5	317	-	-	26/38/38/53	-
6	CLA	5	312	-	-	9/12/88/115	-
6	CLA	7	313	2	-	2/4/80/115	-
9	SQD	5	319	-	-	18/43/63/69	0/1/1/1
6	CLA	5	311	-	-	9/15/91/115	-
6	CLA	7	314	2	-	0/4/80/115	-
6	CLA	6	214	3	-	0/4/80/115	-
4	A86	5	320	-	-	8/34/90/90	0/3/3/3
4	A86	6	202	-	-	7/34/90/90	0/3/3/3
6	CLA	6	201	2	-	4/13/89/115	-
8	LMG	5	316	-	-	25/43/63/70	0/1/1/1
6	CLA	7	312	2	-	0/2/78/115	-
4	A86	7	301	-	-	8/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	CLA	5	309	1	-	4/10/86/115	-
6	CLA	5	310	1	-	5/27/103/115	-
6	CLA	5	313	1	-	2/4/80/115	-
4	A86	7	302	-	-	8/34/90/90	0/3/3/3
6	CLA	6	206	3	-	8/15/91/115	-
6	CLA	6	212	3	-	4/10/86/115	-
6	CLA	7	309	2	-	10/32/108/115	-
6	CLA	7	310	2	-	10/27/103/115	-
10	DD6	6	204	-	-	5/26/80/80	0/3/3/3
6	CLA	5	304	-	-	4/10/86/115	-
6	CLA	6	207	3	-	6/13/89/115	-
6	CLA	6	205	-	-	4/10/86/115	-
7	LHG	5	315	-	-	10/46/46/53	-
6	CLA	5	314	1	-	0/4/80/115	-
6	CLA	5	305	1	-	17/35/111/115	-
6	CLA	7	316	-	-	2/10/86/115	-

All (358) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	6	204	DD6	C29-C27	-9.29	1.24	1.42
10	7	304	DD6	C29-C27	-8.70	1.25	1.42
10	6	204	DD6	C30-C31	-8.46	1.24	1.42
10	6	203	DD6	C29-C27	-8.37	1.26	1.42
10	7	303	DD6	C29-C27	-8.36	1.26	1.42
10	7	304	DD6	C30-C31	-8.00	1.25	1.42
10	6	203	DD6	C30-C31	-7.64	1.26	1.42
10	7	303	DD6	C30-C31	-7.64	1.26	1.42
4	5	301	A86	O4-C38	5.13	1.46	1.35
4	6	202	A86	O4-C38	5.13	1.46	1.35
4	7	302	A86	O4-C38	5.00	1.46	1.35
4	7	301	A86	O4-C38	4.93	1.46	1.35
4	5	320	A86	O4-C38	4.89	1.46	1.35
4	5	303	A86	O4-C38	4.49	1.45	1.35
5	5	302	ET4	C08-C07	4.38	1.46	1.33
4	7	302	A86	C30-C29	-4.18	1.25	1.32
5	5	302	ET4	C19-C18	3.97	1.54	1.45
6	7	312	CLA	C3C-C4C	3.86	1.46	1.40
6	7	308	CLA	C1D-ND	3.85	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	6	205	CLA	C1D-ND	3.84	1.42	1.37
6	7	305	CLA	C1D-ND	3.81	1.42	1.37
4	7	302	A86	C32-C31	-3.80	1.48	1.54
6	6	209	CLA	C1D-ND	3.80	1.42	1.37
6	7	316	CLA	C1D-ND	3.80	1.42	1.37
4	7	302	A86	O1-C20	-3.79	1.40	1.46
6	5	314	CLA	C1D-ND	3.78	1.42	1.37
6	6	208	CLA	C1D-ND	3.78	1.42	1.37
6	7	313	CLA	C1D-ND	3.77	1.42	1.37
6	6	213	CLA	C1D-ND	3.77	1.42	1.37
5	5	302	ET4	C08-C09	3.76	1.54	1.45
6	6	212	CLA	C1D-ND	3.76	1.42	1.37
6	6	211	CLA	C1D-ND	3.75	1.42	1.37
6	6	214	CLA	C1D-ND	3.75	1.42	1.37
6	5	307	CLA	C1D-ND	3.75	1.42	1.37
6	5	309	CLA	C1D-ND	3.74	1.42	1.37
4	5	303	A86	C30-C29	-3.73	1.25	1.32
6	7	315	CLA	C1D-ND	3.73	1.42	1.37
6	6	207	CLA	C1D-ND	3.71	1.42	1.37
6	7	310	CLA	C1D-ND	3.70	1.42	1.37
6	5	304	CLA	C1D-ND	3.69	1.42	1.37
6	5	312	CLA	C1D-ND	3.68	1.42	1.37
6	7	314	CLA	C1D-ND	3.68	1.42	1.37
6	5	308	CLA	C1D-ND	3.67	1.42	1.37
6	7	312	CLA	C1D-ND	3.67	1.42	1.37
6	7	311	CLA	C1D-ND	3.66	1.42	1.37
6	6	215	CLA	C1D-ND	3.66	1.42	1.37
6	5	306	CLA	C1D-ND	3.66	1.42	1.37
6	7	307	CLA	C1D-ND	3.65	1.42	1.37
6	6	216	CLA	C1D-ND	3.65	1.42	1.37
4	7	301	A86	C30-C29	-3.64	1.25	1.32
4	6	202	A86	C30-C29	-3.64	1.25	1.32
6	5	310	CLA	C1D-ND	3.63	1.42	1.37
6	5	313	CLA	C1D-ND	3.63	1.42	1.37
6	6	201	CLA	C1D-ND	3.62	1.42	1.37
6	5	305	CLA	C1D-ND	3.61	1.42	1.37
6	6	210	CLA	C1D-ND	3.58	1.42	1.37
6	6	206	CLA	C1D-ND	3.58	1.42	1.37
4	7	301	A86	O1-C20	-3.56	1.41	1.46
6	7	309	CLA	C1D-ND	3.54	1.42	1.37
6	5	311	CLA	C1D-ND	3.52	1.42	1.37
6	7	306	CLA	C1D-ND	3.51	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	5	302	ET4	C12-C13	3.50	1.53	1.45
4	5	301	A86	C30-C29	-3.47	1.26	1.32
4	5	320	A86	O1-C20	-3.46	1.41	1.46
4	5	320	A86	C30-C29	-3.46	1.26	1.32
6	5	304	CLA	C4B-NB	3.36	1.41	1.37
6	7	305	CLA	C4B-NB	3.36	1.41	1.37
6	7	308	CLA	C4B-NB	3.29	1.41	1.37
6	6	213	CLA	C4B-NB	3.28	1.41	1.37
6	7	313	CLA	C4B-NB	3.27	1.41	1.37
6	5	305	CLA	C4D-ND	-3.26	1.33	1.37
4	5	301	A86	O1-C20	-3.26	1.41	1.46
6	7	316	CLA	C4B-NB	3.26	1.41	1.37
6	7	306	CLA	C4B-NB	3.25	1.41	1.37
6	7	314	CLA	C4B-NB	3.22	1.41	1.37
6	6	205	CLA	C4B-NB	3.22	1.41	1.37
6	5	313	CLA	C4B-NB	3.20	1.41	1.37
6	5	314	CLA	C4B-NB	3.20	1.41	1.37
6	6	216	CLA	C4B-NB	3.20	1.41	1.37
6	6	201	CLA	C4B-NB	3.20	1.41	1.37
6	6	214	CLA	C4B-NB	3.20	1.41	1.37
6	6	207	CLA	C4B-NB	3.19	1.41	1.37
6	6	208	CLA	C4B-NB	3.18	1.41	1.37
6	5	307	CLA	C4B-NB	3.18	1.41	1.37
6	7	315	CLA	C4B-NB	3.18	1.41	1.37
6	7	312	CLA	C4B-NB	3.17	1.41	1.37
6	7	311	CLA	C4B-NB	3.17	1.41	1.37
6	6	211	CLA	C4B-NB	3.17	1.41	1.37
6	6	207	CLA	C4D-ND	-3.16	1.33	1.37
6	7	307	CLA	C4D-ND	-3.15	1.33	1.37
6	7	309	CLA	C4D-ND	-3.15	1.33	1.37
6	5	306	CLA	C4B-NB	3.15	1.41	1.37
6	6	209	CLA	C4B-NB	3.15	1.41	1.37
6	5	308	CLA	C4B-NB	3.14	1.41	1.37
6	5	305	CLA	C4B-NB	3.14	1.41	1.37
6	6	206	CLA	C4D-ND	-3.14	1.33	1.37
6	6	201	CLA	C4D-ND	-3.13	1.33	1.37
6	5	310	CLA	C4B-NB	3.13	1.41	1.37
6	5	309	CLA	C4B-NB	3.13	1.41	1.37
6	6	212	CLA	C4B-NB	3.12	1.41	1.37
6	5	312	CLA	C4B-NB	3.12	1.41	1.37
6	6	210	CLA	C4B-NB	3.12	1.41	1.37
4	6	202	A86	O1-C20	-3.12	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	6	208	CLA	C4D-ND	-3.11	1.33	1.37
6	5	311	CLA	C4B-NB	3.11	1.41	1.37
6	7	310	CLA	C4D-ND	-3.10	1.33	1.37
6	6	215	CLA	C4B-NB	3.10	1.41	1.37
6	7	307	CLA	C4B-NB	3.10	1.41	1.37
9	5	319	SQD	O48-C23	3.10	1.42	1.33
6	6	201	CLA	CAB-C3B	-3.09	1.44	1.50
6	6	209	CLA	CAB-C3B	-3.09	1.44	1.50
6	6	211	CLA	C4D-ND	-3.09	1.33	1.37
6	6	207	CLA	CAB-C3B	-3.06	1.44	1.50
6	5	308	CLA	C4D-ND	-3.06	1.33	1.37
6	7	310	CLA	C4B-NB	3.06	1.41	1.37
6	7	308	CLA	CAB-C3B	-3.05	1.44	1.50
6	7	314	CLA	C4D-ND	-3.05	1.33	1.37
6	6	205	CLA	C4D-ND	-3.04	1.33	1.37
6	5	306	CLA	C4D-ND	-3.04	1.33	1.37
6	7	306	CLA	C4D-ND	-3.04	1.33	1.37
6	7	315	CLA	C4D-ND	-3.03	1.33	1.37
6	5	309	CLA	C4D-ND	-3.03	1.33	1.37
6	7	309	CLA	C4B-NB	3.03	1.41	1.37
6	6	214	CLA	C4D-ND	-3.02	1.33	1.37
6	5	312	CLA	C4D-ND	-3.00	1.33	1.37
6	7	311	CLA	C4D-ND	-3.00	1.33	1.37
6	6	212	CLA	C4D-ND	-3.00	1.33	1.37
6	6	216	CLA	C4D-ND	-2.99	1.33	1.37
6	6	206	CLA	C3B-C4B	2.99	1.49	1.42
6	7	308	CLA	C4D-ND	-2.98	1.33	1.37
6	5	304	CLA	C4D-ND	-2.98	1.33	1.37
6	6	215	CLA	C4D-ND	-2.97	1.33	1.37
6	6	209	CLA	C4D-ND	-2.97	1.33	1.37
6	5	311	CLA	C4D-ND	-2.96	1.33	1.37
6	5	307	CLA	C4D-ND	-2.96	1.33	1.37
6	5	310	CLA	C4D-ND	-2.95	1.33	1.37
6	5	314	CLA	C4D-ND	-2.95	1.33	1.37
6	7	312	CLA	C3B-C4B	2.94	1.49	1.42
6	7	310	CLA	C3B-C4B	2.93	1.49	1.42
6	6	213	CLA	C4D-ND	-2.93	1.33	1.37
6	7	312	CLA	C4D-ND	-2.93	1.33	1.37
6	6	206	CLA	C4B-NB	2.93	1.41	1.37
6	7	305	CLA	C4D-ND	-2.92	1.33	1.37
6	7	313	CLA	C4D-ND	-2.92	1.33	1.37
6	6	210	CLA	C4D-ND	-2.92	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	7	316	CLA	C4D-ND	-2.90	1.33	1.37
6	7	316	CLA	C3B-C4B	2.90	1.49	1.42
6	7	305	CLA	C3B-C4B	2.89	1.49	1.42
6	7	311	CLA	C3B-C4B	2.87	1.49	1.42
6	7	313	CLA	C3B-C4B	2.87	1.49	1.42
6	6	211	CLA	C3B-C4B	2.87	1.49	1.42
6	5	313	CLA	C4D-ND	-2.86	1.33	1.37
6	5	304	CLA	C3B-C4B	2.85	1.49	1.42
6	6	208	CLA	C3B-C4B	2.85	1.49	1.42
6	5	306	CLA	C3B-C4B	2.85	1.49	1.42
6	7	306	CLA	C3B-C4B	2.85	1.49	1.42
6	6	212	CLA	C3B-C4B	2.84	1.49	1.42
6	5	307	CLA	C3B-C4B	2.83	1.49	1.42
6	5	308	CLA	C3B-C4B	2.82	1.49	1.42
6	5	309	CLA	C3B-C4B	2.82	1.49	1.42
6	6	216	CLA	C3B-C4B	2.81	1.49	1.42
6	7	309	CLA	C3B-C4B	2.80	1.49	1.42
6	6	214	CLA	C3B-C4B	2.80	1.49	1.42
6	6	205	CLA	C3B-C4B	2.79	1.49	1.42
6	5	313	CLA	C3B-C4B	2.79	1.49	1.42
6	5	305	CLA	C3B-C4B	2.79	1.49	1.42
6	6	215	CLA	C3B-C4B	2.78	1.49	1.42
6	5	314	CLA	C3B-C4B	2.78	1.49	1.42
6	7	314	CLA	C3B-C4B	2.78	1.49	1.42
6	5	310	CLA	C3B-C4B	2.77	1.49	1.42
6	6	213	CLA	C3B-C4B	2.77	1.49	1.42
9	5	319	SQD	O47-C7	2.76	1.42	1.34
6	7	315	CLA	C3B-C4B	2.76	1.49	1.42
6	5	311	CLA	C3B-C4B	2.74	1.49	1.42
6	7	307	CLA	C3B-C4B	2.74	1.49	1.42
6	5	312	CLA	C3B-C4B	2.72	1.49	1.42
6	6	210	CLA	C1B-C2B	2.72	1.49	1.43
6	6	210	CLA	C3B-C4B	2.71	1.49	1.42
6	6	214	CLA	C1B-C2B	2.69	1.49	1.43
6	6	209	CLA	C4B-C3B	2.64	1.49	1.43
6	5	307	CLA	C1B-C2B	2.64	1.49	1.43
6	5	311	CLA	C1B-C2B	2.63	1.49	1.43
6	6	212	CLA	C1B-C2B	2.63	1.49	1.43
6	6	216	CLA	C1B-C2B	2.63	1.49	1.43
6	5	314	CLA	C1B-C2B	2.63	1.49	1.43
6	6	215	CLA	C1B-C2B	2.63	1.49	1.43
6	7	315	CLA	C1B-C2B	2.62	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	6	206	CLA	C1B-C2B	2.61	1.49	1.43
6	6	205	CLA	C1B-C2B	2.61	1.49	1.43
6	6	207	CLA	C4B-C3B	2.61	1.49	1.43
5	5	302	ET4	C23-C22	2.61	1.47	1.42
6	6	209	CLA	C1B-C2B	2.60	1.49	1.43
5	5	302	ET4	C20-C21	2.60	1.51	1.43
6	5	313	CLA	C1B-C2B	2.60	1.49	1.43
6	7	308	CLA	C1B-C2B	2.59	1.49	1.43
6	7	306	CLA	C1B-C2B	2.59	1.49	1.43
6	6	201	CLA	C4B-C3B	2.59	1.49	1.43
6	6	211	CLA	C1B-C2B	2.59	1.49	1.43
6	5	310	CLA	C1B-C2B	2.58	1.49	1.43
6	5	312	CLA	C1B-C2B	2.58	1.49	1.43
6	5	304	CLA	C1B-C2B	2.57	1.49	1.43
6	6	207	CLA	C1B-C2B	2.57	1.49	1.43
6	7	313	CLA	C1B-C2B	2.56	1.49	1.43
6	7	310	CLA	C1B-C2B	2.56	1.49	1.43
6	7	314	CLA	C1B-C2B	2.56	1.49	1.43
6	7	311	CLA	C1B-C2B	2.56	1.49	1.43
6	6	208	CLA	C1B-C2B	2.56	1.49	1.43
6	7	316	CLA	C1B-C2B	2.55	1.49	1.43
6	7	312	CLA	C1B-C2B	2.55	1.49	1.43
6	6	201	CLA	C1B-C2B	2.54	1.49	1.43
6	7	305	CLA	C1B-C2B	2.54	1.49	1.43
6	6	213	CLA	C1B-C2B	2.54	1.49	1.43
6	7	307	CLA	C1B-C2B	2.54	1.49	1.43
6	5	308	CLA	C1B-C2B	2.53	1.49	1.43
6	7	308	CLA	C4B-C3B	2.52	1.49	1.43
4	5	303	A86	O1-C20	-2.51	1.42	1.46
6	5	306	CLA	C1B-C2B	2.50	1.49	1.43
6	5	309	CLA	C1B-C2B	2.49	1.49	1.43
6	7	309	CLA	C1B-C2B	2.46	1.49	1.43
6	7	306	CLA	CHC-C1C	2.35	1.43	1.38
10	7	303	DD6	O1-C20	-2.34	1.42	1.46
6	7	309	CLA	MG-NB	-2.33	2.01	2.05
10	6	203	DD6	O1-C20	-2.31	1.42	1.46
6	7	310	CLA	CHC-C1C	2.30	1.43	1.38
6	5	305	CLA	MG-NB	-2.30	2.01	2.05
6	6	206	CLA	CHC-C1C	2.30	1.43	1.38
6	5	305	CLA	C1B-C2B	2.30	1.48	1.43
6	5	305	CLA	CMC-C2C	-2.30	1.45	1.50
6	7	306	CLA	MG-NB	-2.30	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	5	308	CLA	MG-NB	-2.29	2.01	2.05
6	6	201	CLA	MG-NB	-2.28	2.01	2.05
6	7	314	CLA	MG-NB	-2.27	2.01	2.05
6	5	305	CLA	CMB-C2B	-2.27	1.46	1.50
6	5	309	CLA	CHC-C1C	2.27	1.43	1.38
5	5	302	ET4	C16-C17	2.26	1.50	1.43
6	5	306	CLA	MG-NB	-2.26	2.01	2.05
6	7	307	CLA	CHC-C1C	2.26	1.43	1.38
6	6	216	CLA	CHC-C1C	2.25	1.43	1.38
6	6	212	CLA	MG-NB	-2.25	2.01	2.05
6	7	313	CLA	CHC-C1C	2.25	1.43	1.38
6	6	207	CLA	CHC-C1C	2.24	1.43	1.38
6	7	312	CLA	CHC-C1C	2.24	1.43	1.38
6	6	211	CLA	CHC-C1C	2.24	1.43	1.38
6	7	311	CLA	MG-NB	-2.24	2.01	2.05
6	6	207	CLA	MG-NB	-2.23	2.01	2.05
6	5	312	CLA	MG-NB	-2.22	2.01	2.05
9	5	319	SQD	O2-C2	-2.22	1.37	1.43
6	5	314	CLA	CHC-C1C	2.21	1.43	1.38
5	5	302	ET4	C15-C14	2.21	1.50	1.43
6	7	307	CLA	MG-NB	-2.20	2.01	2.05
6	7	315	CLA	CHC-C1C	2.20	1.43	1.38
6	6	208	CLA	CHC-C1C	2.20	1.43	1.38
6	5	307	CLA	CHC-C1C	2.19	1.43	1.38
6	7	316	CLA	CHC-C1C	2.19	1.43	1.38
6	5	306	CLA	CHC-C1C	2.19	1.43	1.38
6	6	201	CLA	CHC-C1C	2.19	1.43	1.38
6	5	310	CLA	MG-NB	-2.19	2.01	2.05
6	7	308	CLA	MG-NB	-2.19	2.01	2.05
7	5	318	LHG	P-O6	2.19	1.67	1.60
6	7	315	CLA	MG-NB	-2.19	2.01	2.05
4	6	202	A86	C13-C11	-2.19	1.45	1.49
6	6	209	CLA	CHC-C1C	2.19	1.43	1.38
6	7	311	CLA	CHC-C1C	2.18	1.43	1.38
6	6	212	CLA	CHC-C1C	2.18	1.43	1.38
4	7	302	A86	C13-C11	-2.18	1.45	1.49
6	5	313	CLA	MG-NB	-2.18	2.01	2.05
6	6	213	CLA	MG-NB	-2.18	2.01	2.05
5	5	302	ET4	C11-C10	2.17	1.50	1.43
6	5	313	CLA	CHC-C1C	2.17	1.42	1.38
9	5	319	SQD	O4-C4	-2.17	1.37	1.43
6	5	314	CLA	MG-NB	-2.17	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	7	309	CLA	CHC-C1C	2.16	1.42	1.38
6	6	205	CLA	CHC-C1C	2.16	1.42	1.38
6	5	307	CLA	MG-NB	-2.16	2.01	2.05
6	6	205	CLA	MG-NB	-2.16	2.01	2.05
6	5	312	CLA	CHC-C1C	2.16	1.42	1.38
10	6	204	DD6	O1-C20	-2.16	1.43	1.46
6	5	309	CLA	MG-NB	-2.15	2.01	2.05
4	5	303	A86	C32-C31	-2.15	1.50	1.54
6	6	208	CLA	MG-NB	-2.15	2.01	2.05
6	6	206	CLA	MG-NB	-2.15	2.01	2.05
6	5	310	CLA	CHC-C1C	2.15	1.42	1.38
6	6	211	CLA	MG-NB	-2.14	2.01	2.05
9	5	319	SQD	O3-C3	-2.14	1.37	1.43
5	5	302	ET4	C01-C06	2.14	1.56	1.53
6	5	310	CLA	CMD-C2D	-2.14	1.46	1.50
6	7	310	CLA	MG-NB	-2.13	2.01	2.05
6	7	314	CLA	CMD-C2D	-2.13	1.46	1.50
6	7	305	CLA	CHC-C1C	2.13	1.42	1.38
6	6	214	CLA	MG-NB	-2.13	2.01	2.05
6	5	311	CLA	CHC-C1C	2.13	1.42	1.38
6	7	313	CLA	MG-NB	-2.13	2.01	2.05
6	5	308	CLA	CHC-C1C	2.13	1.42	1.38
6	5	308	CLA	CMD-C2D	-2.13	1.46	1.50
6	6	213	CLA	CHC-C1C	2.12	1.42	1.38
6	7	312	CLA	MG-NB	-2.12	2.01	2.05
5	5	302	ET4	C38-C33	2.12	1.37	1.34
6	6	215	CLA	MG-NB	-2.12	2.01	2.05
6	7	309	CLA	CMB-C2B	-2.12	1.46	1.50
6	5	304	CLA	CHC-C1C	2.12	1.42	1.38
6	7	309	CLA	CMD-C2D	-2.12	1.46	1.50
6	6	210	CLA	CHC-C1C	2.11	1.42	1.38
6	6	215	CLA	CHC-C1C	2.11	1.42	1.38
6	5	311	CLA	MG-NB	-2.11	2.01	2.05
6	6	209	CLA	MG-NB	-2.11	2.01	2.05
6	6	214	CLA	CHC-C1C	2.10	1.42	1.38
6	7	305	CLA	MG-NB	-2.10	2.01	2.05
6	7	314	CLA	CHC-C1C	2.10	1.42	1.38
6	7	310	CLA	CMC-C2C	-2.10	1.46	1.50
6	7	314	CLA	CMB-C2B	-2.10	1.46	1.50
7	5	318	LHG	O7-C5	-2.09	1.41	1.46
6	5	305	CLA	CHC-C1C	2.09	1.42	1.38
6	7	316	CLA	MG-NB	-2.09	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	6	210	CLA	MG-NB	-2.08	2.01	2.05
4	7	302	A86	C26-C27	-2.08	1.33	1.35
6	5	304	CLA	MG-NB	-2.07	2.01	2.05
6	6	201	CLA	CMB-C2B	-2.07	1.46	1.50
6	7	308	CLA	CHC-C1C	2.07	1.42	1.38
6	6	210	CLA	CMD-C2D	-2.06	1.46	1.50
6	7	307	CLA	CMB-C2B	-2.06	1.46	1.50
6	5	306	CLA	CMD-C2D	-2.06	1.46	1.50
6	6	216	CLA	CMD-C2D	-2.06	1.46	1.50
6	7	306	CLA	CMC-C2C	-2.05	1.46	1.50
6	6	201	CLA	CMD-C2D	-2.05	1.46	1.50
6	7	305	CLA	CMD-C2D	-2.05	1.46	1.50
6	5	307	CLA	CMD-C2D	-2.05	1.46	1.50
6	6	214	CLA	CMD-C2D	-2.05	1.46	1.50
6	7	311	CLA	CMD-C2D	-2.05	1.46	1.50
6	6	207	CLA	CMD-C2D	-2.04	1.46	1.50
6	6	209	CLA	CMD-C2D	-2.04	1.46	1.50
6	5	309	CLA	CMB-C2B	-2.04	1.46	1.50
6	7	305	CLA	CMB-C2B	-2.04	1.46	1.50
6	6	211	CLA	CMD-C2D	-2.04	1.46	1.50
6	5	304	CLA	CMD-C2D	-2.04	1.46	1.50
6	6	212	CLA	CMD-C2D	-2.04	1.46	1.50
7	5	315	LHG	P-O6	2.04	1.67	1.59
6	5	309	CLA	CMD-C2D	-2.03	1.46	1.50
6	7	310	CLA	CMD-C2D	-2.03	1.46	1.50
10	6	204	DD6	C36-C31	-2.03	1.32	1.34
6	6	215	CLA	CMB-C2B	-2.02	1.46	1.50
6	5	312	CLA	CMD-C2D	-2.02	1.46	1.50
6	5	313	CLA	CMD-C2D	-2.02	1.46	1.50
6	5	308	CLA	CMB-C2B	-2.02	1.46	1.50
6	5	311	CLA	CMD-C2D	-2.02	1.46	1.50
6	6	209	CLA	CMB-C2B	-2.02	1.46	1.50
6	6	211	CLA	CMC-C2C	-2.02	1.46	1.50
6	7	313	CLA	CMD-C2D	-2.02	1.46	1.50
6	5	305	CLA	CMD-C2D	-2.01	1.46	1.50
6	5	314	CLA	CMD-C2D	-2.01	1.46	1.50
6	6	206	CLA	CMD-C2D	-2.01	1.46	1.50
6	6	213	CLA	CMD-C2D	-2.01	1.46	1.50
6	7	308	CLA	CMD-C2D	-2.01	1.46	1.50
10	7	304	DD6	O1-C20	-2.01	1.43	1.46
6	7	312	CLA	CMD-C2D	-2.01	1.46	1.50
6	6	205	CLA	CMD-C2D	-2.01	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	7	307	CLA	CMD-C2D	-2.01	1.46	1.50
6	5	312	CLA	CMB-C2B	-2.00	1.46	1.50
6	5	304	CLA	CMB-C2B	-2.00	1.46	1.50

All (451) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	7	302	A86	O1-C15-C14	-13.42	86.28	113.21
4	7	301	A86	O1-C15-C14	-12.11	88.91	113.21
4	5	320	A86	O1-C15-C14	-12.00	89.12	113.21
4	6	202	A86	O1-C15-C14	-11.25	90.63	113.21
4	5	301	A86	O1-C15-C14	8.62	130.51	113.21
10	7	304	DD6	C4-C5-C6	-8.04	115.84	127.31
4	5	301	A86	C25-C26-C27	-7.80	116.17	127.31
4	5	320	A86	C17-C16-C15	7.80	117.12	109.16
4	7	301	A86	C17-C16-C15	7.79	117.11	109.16
4	6	202	A86	C17-C16-C15	7.71	117.03	109.16
10	7	304	DD6	C14-C13-C11	-7.56	113.80	125.53
4	7	302	A86	C3-C2-C1	-7.36	116.81	127.31
6	6	206	CLA	C4A-NA-C1A	7.03	109.87	106.71
4	5	303	A86	O1-C20-C19	-7.00	108.12	113.38
6	6	210	CLA	C4A-NA-C1A	6.99	109.85	106.71
6	5	307	CLA	C4A-NA-C1A	6.93	109.82	106.71
10	7	303	DD6	C9-C10-C11	-6.88	117.49	127.31
10	6	203	DD6	C9-C10-C11	-6.87	117.50	127.31
10	7	304	DD6	C9-C10-C11	-6.78	117.64	127.31
6	5	311	CLA	C4A-NA-C1A	6.75	109.74	106.71
6	6	214	CLA	C4A-NA-C1A	6.75	109.74	106.71
6	7	306	CLA	C4A-NA-C1A	6.69	109.72	106.71
6	7	310	CLA	C4A-NA-C1A	6.68	109.71	106.71
10	6	204	DD6	C14-C13-C11	-6.67	115.18	125.53
4	7	302	A86	O1-C20-C21	-6.58	107.17	115.06
6	7	315	CLA	C4A-NA-C1A	6.54	109.65	106.71
6	5	305	CLA	C4A-NA-C1A	6.53	109.64	106.71
6	5	304	CLA	C4A-NA-C1A	6.52	109.64	106.71
6	5	313	CLA	C4A-NA-C1A	6.51	109.64	106.71
6	6	205	CLA	C4A-NA-C1A	6.46	109.61	106.71
6	6	212	CLA	C4A-NA-C1A	6.43	109.60	106.71
6	6	208	CLA	C4A-NA-C1A	6.42	109.59	106.71
6	6	215	CLA	C4A-NA-C1A	6.42	109.59	106.71
6	7	305	CLA	C4A-NA-C1A	6.41	109.59	106.71
6	5	309	CLA	C4A-NA-C1A	6.39	109.58	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	6	213	CLA	C4A-NA-C1A	6.39	109.58	106.71
4	7	302	A86	O4-C38-C39	6.39	122.84	111.09
6	7	313	CLA	C4A-NA-C1A	6.38	109.57	106.71
6	6	211	CLA	C4A-NA-C1A	6.37	109.57	106.71
10	6	204	DD6	C3-C2-C1	-6.37	118.22	127.31
6	5	314	CLA	C4A-NA-C1A	6.36	109.56	106.71
6	7	307	CLA	C4A-NA-C1A	6.36	109.56	106.71
6	5	310	CLA	C4A-NA-C1A	6.35	109.56	106.71
6	5	312	CLA	C4A-NA-C1A	6.35	109.56	106.71
6	5	306	CLA	C4A-NA-C1A	6.34	109.56	106.71
6	7	309	CLA	C4A-NA-C1A	6.34	109.56	106.71
6	7	316	CLA	C4A-NA-C1A	6.33	109.55	106.71
6	6	209	CLA	C4A-NA-C1A	6.33	109.55	106.71
4	6	202	A86	C3-C2-C1	-6.32	118.29	127.31
4	5	301	A86	O1-C20-C19	6.32	118.13	113.38
6	7	314	CLA	C4A-NA-C1A	6.29	109.53	106.71
6	6	216	CLA	C4A-NA-C1A	6.22	109.50	106.71
6	7	312	CLA	C4A-NA-C1A	6.17	109.48	106.71
6	7	308	CLA	C4A-NA-C1A	6.13	109.46	106.71
6	5	308	CLA	C4A-NA-C1A	6.13	109.46	106.71
4	5	301	A86	O4-C38-C39	6.11	122.34	111.09
10	6	204	DD6	C9-C10-C11	-6.05	118.68	127.31
6	6	201	CLA	C4A-NA-C1A	5.97	109.39	106.71
4	7	302	A86	C35-C34-C33	-5.94	99.51	109.88
6	7	311	CLA	C4A-NA-C1A	5.87	109.34	106.71
4	5	320	A86	C35-C34-C33	-5.83	99.71	109.88
4	7	302	A86	C17-C16-C15	5.80	115.08	109.16
4	7	301	A86	C35-C34-C33	-5.76	99.82	109.88
7	5	318	LHG	O4-P-O5	5.70	133.01	110.68
6	6	207	CLA	C4A-NA-C1A	5.56	109.21	106.71
4	6	202	A86	C25-C26-C27	-5.51	119.45	127.31
4	5	303	A86	C3-C2-C1	-5.43	119.56	127.31
5	5	302	ET4	C29-C22-C23	5.39	127.51	116.84
10	7	303	DD6	C4-C5-C6	-5.38	119.63	127.31
10	6	203	DD6	C4-C5-C6	-5.38	119.64	127.31
4	5	301	A86	C17-C16-C15	5.32	114.59	109.16
4	5	303	A86	O1-C20-C21	-5.24	108.78	115.06
4	5	301	A86	C35-C34-C33	-5.24	100.74	109.88
10	6	204	DD6	C4-C5-C6	-5.14	119.97	127.31
4	7	301	A86	C3-C2-C1	-5.13	119.99	127.31
4	6	202	A86	C4-C5-C6	-4.96	120.23	127.31
5	5	302	ET4	C24-C05-C06	-4.92	119.01	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	7	301	A86	C4-C5-C6	-4.89	120.34	127.31
10	6	203	DD6	C3-C2-C1	-4.84	120.40	127.31
10	7	303	DD6	C3-C2-C1	-4.83	120.42	127.31
5	5	302	ET4	C30-C18-C17	-4.76	116.25	122.92
10	7	304	DD6	O1-C20-C19	4.70	116.92	113.38
4	5	320	A86	C3-C2-C1	-4.69	120.61	127.31
5	5	302	ET4	C27-C09-C10	-4.68	116.37	122.92
4	5	320	A86	C4-C5-C6	-4.65	120.68	127.31
4	5	301	A86	C4-C5-C6	-4.54	120.84	127.31
7	5	318	LHG	O3-P-O6	-4.51	94.72	106.73
5	5	302	ET4	C19-C18-C17	4.51	125.86	118.94
4	5	303	A86	C36-C31-C32	4.50	124.16	119.70
4	7	302	A86	C4-C5-C6	-4.41	121.01	127.31
4	5	301	A86	C20-C19-C18	4.40	121.46	112.75
4	5	303	A86	C4-C5-C6	-4.34	121.11	127.31
7	5	317	LHG	O4-P-O5	4.19	132.94	112.24
4	5	303	A86	O4-C38-C39	4.18	118.78	111.09
10	6	204	DD6	C21-C20-C19	4.17	118.97	114.28
5	5	302	ET4	C16-C15-C14	4.16	132.00	123.47
7	5	315	LHG	O4-P-O5	4.11	132.58	112.24
10	7	303	DD6	C21-C20-C19	4.08	118.87	114.28
10	6	203	DD6	C21-C20-C19	4.06	118.85	114.28
4	5	301	A86	C12-C11-C13	4.05	122.82	116.02
4	5	320	A86	O4-C34-C33	4.00	117.55	107.59
4	7	301	A86	O1-C20-C21	-4.00	110.27	115.06
4	5	320	A86	O1-C20-C21	-3.99	110.28	115.06
4	5	301	A86	C3-C2-C1	-3.97	121.65	127.31
10	7	304	DD6	C21-C20-C15	-3.94	115.65	122.26
4	6	202	A86	C9-C10-C11	-3.94	115.03	126.61
4	5	320	A86	O4-C38-C39	3.86	118.18	111.09
4	7	301	A86	C41-C32-C31	-3.85	107.03	110.47
4	6	202	A86	C40-C32-C31	-3.80	107.07	110.47
4	7	301	A86	O4-C34-C33	3.78	117.00	107.59
4	6	202	A86	C35-C34-C33	-3.76	103.32	109.88
9	5	319	SQD	O9-S-C6	3.75	111.39	106.94
9	5	319	SQD	O9-S-O7	-3.68	101.23	113.95
4	7	301	A86	O4-C38-C39	3.68	117.85	111.09
4	5	320	A86	C41-C32-C31	-3.65	107.20	110.47
6	6	207	CLA	C3B-C4B-NB	-3.63	107.80	110.23
10	7	304	DD6	C37-C36-C31	-3.62	119.43	124.35
5	5	302	ET4	O40-C36-C35	3.61	116.99	109.80
4	6	202	A86	C3-C4-C5	-3.57	116.15	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	6	201	CLA	C3B-C4B-NB	-3.57	107.84	110.23
10	7	304	DD6	C21-C20-C19	3.55	118.27	114.28
6	6	201	CLA	O2D-CGD-O1D	-3.54	116.91	123.84
9	5	319	SQD	O7-S-C6	3.52	111.12	106.94
10	6	203	DD6	C37-C36-C31	-3.50	119.59	124.35
6	7	307	CLA	O2D-CGD-O1D	-3.50	117.00	123.84
4	7	302	A86	C3-C4-C5	-3.49	116.32	123.47
10	7	303	DD6	C37-C36-C31	-3.49	119.61	124.35
7	5	317	LHG	O8-C23-C24	3.49	120.53	111.38
6	6	209	CLA	C3B-C4B-NB	-3.48	107.90	110.23
6	5	305	CLA	CMB-C2B-C1B	-3.45	120.12	125.37
4	5	303	A86	C34-O4-C38	-3.44	111.48	117.90
10	6	203	DD6	C15-C14-C13	-3.42	118.76	125.99
10	7	303	DD6	C15-C14-C13	-3.42	118.77	125.99
9	5	319	SQD	O47-C7-C8	3.41	118.86	111.50
4	7	302	A86	O1-C15-C20	-3.39	56.08	59.40
4	5	301	A86	C28-C27-C26	-3.37	118.20	122.92
4	5	303	A86	C17-C16-C15	3.35	112.58	109.16
6	7	308	CLA	C3B-C4B-NB	-3.33	108.00	110.23
4	6	202	A86	O4-C38-C39	3.32	117.21	111.09
5	5	302	ET4	C35-C34-C33	3.32	116.35	109.62
4	7	302	A86	C25-C26-C27	-3.31	122.58	127.31
4	5	301	A86	O1-C15-C20	-3.29	56.18	59.40
6	5	304	CLA	O2D-CGD-O1D	-3.29	117.40	123.84
6	6	210	CLA	O2D-CGD-O1D	-3.26	117.47	123.84
4	7	301	A86	O1-C15-C20	-3.26	56.22	59.40
4	5	320	A86	O1-C15-C20	-3.25	56.22	59.40
6	7	305	CLA	CAA-C2A-C3A	-3.20	108.63	116.10
10	6	203	DD6	C12-C11-C10	-3.19	118.45	122.92
10	6	204	DD6	C4-C3-C2	-3.19	116.95	123.47
10	7	303	DD6	C12-C11-C10	-3.16	118.49	122.92
4	6	202	A86	C9-C8-C6	-3.09	117.74	126.42
6	7	305	CLA	O2D-CGD-O1D	-3.08	117.81	123.84
6	7	306	CLA	C3B-C4B-NB	-3.08	107.66	110.52
4	5	301	A86	O4-C38-O5	-3.08	116.85	122.96
6	5	312	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
5	5	302	ET4	C01-C06-C07	3.05	124.41	115.78
10	6	204	DD6	C28-C27-C29	3.05	122.87	116.84
6	7	316	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
4	7	302	A86	O4-C38-O5	-3.03	116.94	122.96
6	7	313	CLA	C3B-C4B-NB	-3.02	107.72	110.52
10	7	303	DD6	C13-C11-C10	3.01	123.56	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	5	302	ET4	C42-C34-C33	-3.01	105.69	110.47
10	6	203	DD6	C13-C11-C10	3.00	123.55	118.94
10	6	204	DD6	C37-C36-C31	-2.99	120.28	124.35
4	7	302	A86	C41-C32-C31	-2.99	107.80	110.47
10	6	204	DD6	C21-C20-C15	-2.97	117.28	122.26
4	5	303	A86	C40-C32-C31	-2.97	107.81	110.47
10	7	303	DD6	C-C1-C2	-2.97	118.77	122.92
4	5	303	A86	O1-C15-C14	-2.96	107.27	113.21
10	7	304	DD6	C37-C36-C35	2.95	119.81	114.36
6	7	308	CLA	O2D-CGD-O1D	-2.94	118.08	123.84
10	6	203	DD6	C-C1-C2	-2.94	118.80	122.92
6	5	306	CLA	C3B-C4B-NB	-2.94	107.79	110.52
6	5	314	CLA	CBD-CHA-C1A	2.94	132.13	127.43
6	6	215	CLA	CBD-CHA-C1A	2.93	132.12	127.43
6	6	206	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
6	5	313	CLA	CBD-CHA-C1A	2.90	132.07	127.43
6	7	307	CLA	C3B-C4B-NB	-2.89	107.83	110.52
6	7	313	CLA	CBD-CHA-C1A	2.89	132.06	127.43
6	5	307	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
6	5	309	CLA	C3B-C4B-NB	-2.89	107.84	110.52
6	6	208	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
9	5	319	SQD	O8-S-C6	2.88	110.33	105.74
6	6	216	CLA	CBD-CHA-C1A	2.88	132.04	127.43
6	5	310	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
6	7	310	CLA	C3B-C4B-NB	-2.88	107.84	110.52
6	7	309	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
6	5	309	CLA	CAA-C2A-C3A	-2.87	109.41	116.10
6	5	304	CLA	CAA-C2A-C3A	-2.87	109.41	116.10
4	7	302	A86	C9-C10-C11	-2.86	118.19	126.61
6	5	313	CLA	C3B-C4B-NB	-2.86	107.86	110.52
4	5	303	A86	C-C1-C2	-2.85	118.93	122.92
6	5	311	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
6	6	209	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
6	6	211	CLA	C3B-C4B-NB	-2.83	107.89	110.52
6	6	212	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
10	6	203	DD6	C33-C34-C35	-2.82	106.44	110.30
6	7	311	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
10	6	204	DD6	C25-C24-C1	-2.81	118.51	126.42
10	7	303	DD6	C7-C6-C5	-2.81	118.98	122.92
4	7	302	A86	C33-C32-C31	2.81	111.94	109.21
6	7	312	CLA	CBD-CHA-C1A	2.80	131.92	127.43
6	6	206	CLA	CHB-C4A-NA	2.80	128.38	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	6	204	DD6	O1-C20-C21	-2.80	111.70	115.06
6	7	315	CLA	C3B-C4B-NB	-2.80	107.92	110.52
9	5	319	SQD	O6-C1-C2	2.79	112.66	108.30
6	5	309	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
10	7	303	DD6	C33-C34-C35	-2.78	106.50	110.30
6	7	305	CLA	C3B-C4B-NB	-2.78	107.94	110.52
6	5	306	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
6	7	315	CLA	CBD-CHA-C1A	2.78	131.88	127.43
10	6	203	DD6	C7-C6-C5	-2.78	119.03	122.92
6	5	304	CLA	C3B-C4B-NB	-2.77	107.94	110.52
5	5	302	ET4	C07-C06-C05	-2.77	114.74	121.46
6	7	306	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
6	7	310	CLA	O2D-CGD-O1D	-2.76	118.43	123.84
6	5	307	CLA	C3B-C4B-NB	-2.76	107.95	110.52
6	7	313	CLA	CAA-C2A-C3A	-2.76	109.66	116.10
6	6	206	CLA	C3B-C4B-NB	-2.76	107.95	110.52
6	6	211	CLA	O2D-CGD-O1D	-2.74	118.47	123.84
6	6	208	CLA	C3B-C4B-NB	-2.74	107.97	110.52
6	6	215	CLA	CAA-C2A-C3A	-2.74	109.70	116.10
6	6	205	CLA	C3B-C4B-NB	-2.74	107.97	110.52
7	5	318	LHG	O8-C23-C24	2.74	120.49	111.91
4	5	303	A86	C19-C18-C17	-2.73	105.50	110.77
6	6	216	CLA	C3B-C4B-NB	-2.73	107.98	110.52
6	6	205	CLA	O2D-CGD-O1D	-2.72	118.51	123.84
6	5	308	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
6	6	207	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
6	6	214	CLA	CBD-CHA-C1A	2.72	131.78	127.43
6	7	311	CLA	C3B-C4B-NB	-2.71	108.00	110.52
6	5	313	CLA	CAA-C2A-C3A	-2.71	109.77	116.10
4	5	320	A86	C23-C16-C17	-2.71	104.28	108.98
6	6	210	CLA	CHB-C4A-NA	2.71	128.25	124.51
6	5	314	CLA	CAA-C2A-C3A	-2.70	109.79	116.10
6	5	314	CLA	C3B-C4B-NB	-2.70	108.01	110.52
4	6	202	A86	O1-C15-C20	-2.70	56.76	59.40
6	7	312	CLA	C3B-C4B-NB	-2.69	108.02	110.52
4	7	301	A86	C23-C16-C17	-2.69	104.31	108.98
6	7	314	CLA	CAA-C2A-C3A	-2.69	109.83	116.10
4	5	301	A86	C25-C24-C1	-2.67	118.92	126.42
10	7	304	DD6	C19-C18-C17	2.67	115.92	110.77
5	5	302	ET4	C08-C09-C10	2.66	123.03	118.94
5	5	302	ET4	C28-C13-C14	-2.66	119.20	122.92
6	7	315	CLA	CAA-C2A-C3A	-2.66	109.89	116.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	7	314	CLA	CBD-CHA-C1A	2.66	131.69	127.43
5	5	302	ET4	C35-C36-C37	-2.65	106.68	110.30
4	5	303	A86	C33-C32-C31	2.65	111.78	109.21
6	6	213	CLA	O2D-CGD-O1D	-2.64	118.08	124.09
6	6	216	CLA	CAA-C2A-C3A	-2.64	109.94	116.10
6	6	205	CLA	CAA-C2A-C3A	-2.64	109.95	116.10
4	5	301	A86	O-C13-C11	-2.63	115.33	121.15
6	6	212	CLA	CAA-C2A-C3A	-2.63	109.95	116.10
6	6	215	CLA	C3B-C4B-NB	-2.63	108.08	110.52
6	6	213	CLA	C3B-C4B-NB	-2.62	108.09	110.52
4	7	301	A86	C20-C19-C18	2.62	117.93	112.75
6	5	311	CLA	CHB-C4A-NA	2.61	128.12	124.51
6	7	309	CLA	C3B-C4B-NB	-2.61	108.09	110.52
4	5	303	A86	C41-C32-C31	-2.61	108.14	110.47
6	5	309	CLA	CHB-C4A-NA	2.61	128.12	124.51
6	6	214	CLA	CHB-C4A-NA	2.60	128.11	124.51
7	5	315	LHG	O8-C23-C24	2.60	120.06	111.91
6	5	312	CLA	C3B-C4B-NB	-2.60	108.11	110.52
6	5	305	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
4	5	320	A86	C20-C19-C18	2.58	117.85	112.75
6	7	308	CLA	CAB-C3B-C2B	2.58	130.27	123.59
6	6	214	CLA	CAA-C2A-C3A	-2.57	110.09	116.10
4	7	302	A86	C-C1-C2	-2.57	119.32	122.92
6	6	211	CLA	CHB-C4A-NA	2.56	128.06	124.51
6	5	310	CLA	C3B-C4B-NB	-2.56	108.14	110.52
6	6	210	CLA	C3B-C4B-NB	-2.56	108.14	110.52
6	5	313	CLA	CHB-C4A-NA	2.56	128.05	124.51
6	7	312	CLA	CAA-C2A-C3A	-2.56	110.12	116.10
6	6	212	CLA	C3B-C4B-NB	-2.53	108.17	110.52
10	6	204	DD6	C9-C8-C6	-2.53	119.31	126.42
8	5	316	LMG	O6-C1-O1	-2.53	103.99	109.97
4	7	302	A86	C25-C24-C1	-2.52	119.33	126.42
10	6	204	DD6	C32-C33-C34	-2.52	107.95	113.64
6	5	307	CLA	CHB-C4A-NA	2.52	128.00	124.51
10	7	303	DD6	C21-C20-C15	-2.52	118.04	122.26
10	6	203	DD6	C21-C20-C15	-2.52	118.04	122.26
6	7	316	CLA	CAA-C2A-C3A	-2.51	110.23	116.10
6	7	305	CLA	CHB-C4A-NA	2.51	127.99	124.51
10	6	204	DD6	C26-C25-C24	-2.51	115.38	123.22
6	6	201	CLA	CMB-C2B-C3B	2.50	130.08	123.59
6	6	208	CLA	CHB-C4A-NA	2.50	127.97	124.51
6	6	216	CLA	CHB-C4A-NA	2.50	127.97	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	7	301	A86	O4-C34-C35	2.50	113.81	107.59
6	5	305	CLA	CMB-C2B-C3B	2.49	132.62	126.59
6	6	212	CLA	CHB-C4A-NA	2.49	127.95	124.51
6	6	207	CLA	CMB-C2B-C3B	2.49	130.03	123.59
6	6	215	CLA	CHB-C4A-NA	2.48	127.95	124.51
6	7	314	CLA	C3B-C4B-NB	-2.48	108.21	110.52
6	5	312	CLA	CHB-C4A-NA	2.48	127.94	124.51
6	6	201	CLA	CAB-C3B-C2B	2.48	130.00	123.59
6	7	313	CLA	CHB-C4A-NA	2.47	127.93	124.51
6	6	214	CLA	C3B-C4B-NB	-2.47	108.22	110.52
6	5	308	CLA	C3B-C4B-NB	-2.46	108.23	110.52
4	7	301	A86	C9-C10-C11	-2.46	119.37	126.61
6	7	312	CLA	CHB-C4A-NA	2.46	127.92	124.51
6	6	209	CLA	CAB-C3B-C2B	2.46	129.96	123.59
6	6	205	CLA	CHB-C4A-NA	2.45	127.89	124.51
6	6	210	CLA	CAA-C2A-C3A	-2.44	106.08	112.78
6	7	310	CLA	CHB-C4A-NA	2.44	127.89	124.51
6	5	311	CLA	C3B-C4B-NB	-2.44	108.25	110.52
6	5	314	CLA	CHB-C4A-NA	2.44	127.89	124.51
6	7	316	CLA	C3B-C4B-NB	-2.44	108.25	110.52
6	7	314	CLA	CHB-C4A-NA	2.44	127.89	124.51
6	6	207	CLA	CAB-C3B-C2B	2.44	129.91	123.59
6	5	305	CLA	CHB-C1B-NB	2.44	126.84	124.26
4	5	320	A86	C9-C10-C11	-2.44	119.45	126.61
6	6	201	CLA	O2D-CGD-CBD	2.43	115.59	111.27
6	6	210	CLA	O2D-CGD-CBD	2.43	115.59	111.27
6	7	309	CLA	CMB-C2B-C1B	-2.43	121.67	125.37
6	5	304	CLA	CHB-C4A-NA	2.43	127.87	124.51
6	5	310	CLA	CHB-C4A-NA	2.43	127.87	124.51
6	6	213	CLA	CAA-C2A-C3A	-2.43	110.44	116.10
10	6	204	DD6	C37-C36-C35	2.43	118.85	114.36
6	7	315	CLA	CHB-C4A-NA	2.42	127.86	124.51
6	7	312	CLA	CHC-C1C-C2C	-2.42	124.01	129.77
6	7	308	CLA	CMB-C2B-C3B	2.42	129.86	123.59
6	5	306	CLA	CHB-C4A-NA	2.41	127.85	124.51
6	6	207	CLA	CHB-C1B-NB	2.41	126.81	124.26
4	5	301	A86	C36-C31-C32	-2.41	117.30	119.70
6	7	307	CLA	CHB-C4A-NA	2.41	127.84	124.51
6	6	209	CLA	CHB-C4A-NA	2.41	127.84	124.51
5	5	302	ET4	C02-C03-C04	-2.41	107.01	110.30
6	6	209	CLA	CMB-C2B-C3B	2.40	129.82	123.59
10	7	304	DD6	C7-C6-C5	-2.40	119.56	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	7	302	A86	C20-C19-C18	2.40	117.49	112.75
6	7	306	CLA	CHB-C4A-NA	2.39	127.82	124.51
7	5	317	LHG	C11-C10-C9	-2.39	102.30	114.42
10	6	203	DD6	O1-C20-C21	-2.38	112.20	115.06
10	7	303	DD6	O1-C20-C21	-2.37	112.22	115.06
6	6	213	CLA	CHB-C4A-NA	2.36	127.78	124.51
9	5	319	SQD	O48-C23-C24	2.36	119.33	111.91
6	7	316	CLA	CHB-C4A-NA	2.36	127.78	124.51
6	5	305	CLA	C3B-C4B-NB	-2.35	108.33	110.52
6	7	309	CLA	CHB-C1B-NB	2.35	126.74	124.26
4	5	320	A86	C9-C8-C6	-2.35	119.83	126.42
6	6	201	CLA	CHB-C4A-NA	2.34	127.75	124.51
6	7	316	CLA	CHD-C1D-ND	-2.34	122.30	124.45
8	5	316	LMG	C38-C37-C36	-2.33	102.58	114.42
6	7	308	CLA	CHB-C4A-NA	2.33	127.73	124.51
6	5	308	CLA	O2A-CGA-O1A	-2.32	117.73	123.59
6	7	311	CLA	CHB-C4A-NA	2.32	127.72	124.51
10	7	304	DD6	C-C1-C24	2.32	121.73	118.08
6	7	309	CLA	CHB-C4A-NA	2.31	127.71	124.51
8	5	316	LMG	C40-C39-C38	-2.30	102.73	114.42
6	6	214	CLA	CMA-C3A-C2A	-2.30	110.73	116.10
6	7	307	CLA	CHD-C1D-ND	-2.29	122.35	124.45
6	5	308	CLA	CHB-C4A-NA	2.28	127.67	124.51
6	6	207	CLA	CHB-C4A-NA	2.28	127.67	124.51
4	7	301	A86	C9-C8-C6	-2.28	120.03	126.42
10	6	204	DD6	C12-C11-C10	-2.27	119.75	122.92
4	5	320	A86	O4-C34-C35	2.27	113.24	107.59
10	7	304	DD6	C12-C11-C10	-2.26	119.75	122.92
6	7	311	CLA	CMB-C2B-C1B	-2.26	121.92	125.37
10	6	203	DD6	C9-C8-C6	-2.26	120.08	126.42
4	6	202	A86	C25-C24-C1	-2.25	120.09	126.42
10	7	304	DD6	C26-C25-C24	-2.25	116.20	123.22
10	7	303	DD6	C9-C8-C6	-2.24	120.12	126.42
10	7	304	DD6	C8-C6-C5	2.24	122.38	118.94
10	7	303	DD6	C37-C36-C35	2.24	118.50	114.36
10	7	304	DD6	C3-C4-C5	-2.24	118.89	123.47
6	6	208	CLA	CHB-C1B-NB	2.24	126.62	124.26
10	7	303	DD6	C24-C1-C2	2.24	122.37	118.94
10	6	203	DD6	C37-C36-C35	2.23	118.49	114.36
10	6	203	DD6	C24-C1-C2	2.23	122.36	118.94
6	6	201	CLA	CHB-C1B-NB	2.23	126.62	124.26
4	6	202	A86	C26-C25-C24	-2.23	116.27	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	5	308	CLA	C1-C2-C3	-2.22	122.20	126.04
6	5	307	CLA	C1-C2-C3	-2.22	122.21	126.04
4	5	303	A86	C9-C8-C6	-2.21	120.20	126.42
4	5	301	A86	C-C1-C2	-2.21	119.83	122.92
6	7	305	CLA	O2D-CGD-CBD	2.21	115.19	111.27
6	7	314	CLA	CMB-C2B-C1B	-2.20	122.02	125.37
6	6	208	CLA	O2A-CGA-O1A	-2.20	118.04	123.59
6	7	310	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
6	5	310	CLA	O2A-CGA-O1A	-2.19	118.07	123.59
4	5	303	A86	C25-C26-C27	-2.19	124.19	127.31
6	7	307	CLA	CHB-C1B-NB	2.19	126.57	124.26
6	6	206	CLA	CMC-C2C-C1C	2.18	128.36	125.04
6	5	309	CLA	CHB-C1B-NB	2.18	126.56	124.26
6	7	311	CLA	CHB-C1B-NB	2.17	126.56	124.26
6	6	211	CLA	C1-C2-C3	-2.17	122.29	126.04
4	7	301	A86	C26-C25-C24	-2.17	116.45	123.22
10	7	303	DD6	C8-C6-C5	2.16	122.26	118.94
6	6	212	CLA	CMB-C2B-C1B	-2.16	122.08	125.37
6	6	211	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
6	7	312	CLA	C1C-NC-C4C	2.15	107.67	106.71
8	5	316	LMG	O3-C3-C2	-2.15	105.38	110.35
6	7	314	CLA	CHB-C1B-NB	2.15	126.53	124.26
4	5	301	A86	O-C13-C14	-2.14	117.30	121.66
9	5	319	SQD	O5-C5-C4	2.14	113.59	109.69
6	7	312	CLA	CMB-C2B-C1B	-2.14	122.11	125.37
10	6	203	DD6	C8-C6-C5	2.14	122.22	118.94
7	5	318	LHG	C27-C26-C25	-2.13	103.62	114.42
6	5	309	CLA	CMA-C3A-C2A	-2.13	111.14	116.10
6	5	305	CLA	CHB-C4A-NA	2.12	127.45	124.51
8	5	316	LMG	C42-C41-C40	-2.12	103.66	114.42
6	6	210	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
7	5	317	LHG	C18-C17-C16	-2.12	103.66	114.42
6	6	209	CLA	CHB-C1B-NB	2.12	126.50	124.26
6	7	310	CLA	CHD-C1D-ND	-2.11	122.51	124.45
6	5	304	CLA	CHB-C1B-NB	2.11	126.50	124.26
5	5	302	ET4	C39-C38-C33	2.11	127.22	124.35
4	7	301	A86	C12-C11-C13	2.11	119.57	116.02
4	7	301	A86	C3-C4-C5	-2.11	119.15	123.47
10	7	304	DD6	C28-C27-C29	2.11	121.01	116.84
4	5	320	A86	C12-C11-C13	2.10	119.55	116.02
6	7	310	CLA	CHB-C1B-NB	2.10	126.48	124.26
6	7	314	CLA	CHD-C1D-ND	-2.10	122.53	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	7	305	CLA	CHB-C1B-NB	2.10	126.48	124.26
4	5	301	A86	C41-C32-C31	-2.09	108.60	110.47
4	6	202	A86	C12-C11-C13	2.09	119.53	116.02
6	5	308	CLA	CHB-C1B-NB	2.08	126.46	124.26
4	5	303	A86	C9-C10-C11	-2.08	120.48	126.61
6	5	313	CLA	CHB-C1B-NB	2.08	126.46	124.26
6	5	306	CLA	CHB-C1B-NB	2.08	126.46	124.26
6	7	306	CLA	CHB-C1B-NB	2.07	126.45	124.26
6	6	215	CLA	CHB-C1B-NB	2.07	126.45	124.26
4	5	303	A86	C4-C3-C2	-2.07	119.24	123.47
10	7	304	DD6	C13-C11-C10	2.07	122.11	118.94
4	5	303	A86	C12-C11-C13	2.06	119.49	116.02
6	6	209	CLA	CHD-C1D-ND	-2.06	122.56	124.45
6	7	316	CLA	CMB-C2B-C1B	-2.06	122.24	125.37
5	5	302	ET4	C36-C37-C38	2.05	115.94	111.85
10	6	204	DD6	C24-C1-C2	2.05	122.09	118.94
6	7	313	CLA	CHB-C1B-NB	2.05	126.43	124.26
6	5	313	CLA	CHD-C1D-ND	-2.05	122.57	124.45
4	7	302	A86	C23-C16-C17	-2.05	105.43	108.98
6	6	211	CLA	CHD-C1D-ND	-2.05	122.57	124.45
8	5	316	LMG	O2-C2-C1	-2.05	105.08	110.05
6	7	307	CLA	O2A-CGA-O1A	-2.04	118.43	123.59
6	7	310	CLA	C1-C2-C3	-2.04	122.51	126.04
4	6	202	A86	C7-C6-C8	2.04	121.29	118.08
4	5	320	A86	C25-C26-C27	-2.04	124.40	127.31
4	5	320	A86	C26-C25-C24	-2.04	116.86	123.22
6	6	207	CLA	CHD-C1D-ND	-2.03	122.59	124.45
6	5	305	CLA	CHD-C1D-ND	-2.03	122.59	124.45
6	5	310	CLA	CHB-C1B-NB	2.02	126.39	124.26
4	7	301	A86	C25-C26-C27	-2.02	124.43	127.31
7	5	315	LHG	C11-C10-C9	-2.02	104.19	114.42
6	5	310	CLA	C1-C2-C3	-2.02	122.56	126.04
4	5	303	A86	C35-C34-C33	-2.02	106.36	109.88
6	7	309	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
6	6	205	CLA	CHD-C1D-ND	-2.01	122.61	124.45
6	7	309	CLA	CMB-C2B-C3B	2.01	131.45	126.59
6	6	205	CLA	CHB-C1B-NB	2.01	126.38	124.26
6	6	206	CLA	O2A-CGA-O1A	-2.00	118.31	123.30

There are no chirality outliers.

All (381) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	5	301	A86	C10-C11-C13-O
4	5	301	A86	C10-C11-C13-C14
4	5	301	A86	C12-C11-C13-O
4	5	301	A86	C13-C14-C15-C16
4	5	301	A86	C13-C14-C15-O1
4	5	303	A86	C5-C6-C8-C9
4	5	303	A86	C7-C6-C8-C9
4	5	320	A86	C10-C11-C13-O
4	5	320	A86	C12-C11-C13-O
4	5	320	A86	C12-C11-C13-C14
4	7	301	A86	C10-C11-C13-O
4	7	301	A86	C12-C11-C13-O
4	7	301	A86	C12-C11-C13-C14
5	5	302	ET4	C17-C18-C19-C20
5	5	302	ET4	C30-C18-C19-C20
5	5	302	ET4	C01-C06-C07-C08
5	5	302	ET4	C05-C06-C07-C08
5	5	302	ET4	C07-C08-C09-C10
5	5	302	ET4	C07-C08-C09-C27
6	5	307	CLA	C1A-C2A-CAA-CBA
6	5	307	CLA	CBD-CGD-O2D-CED
6	5	307	CLA	C2-C3-C5-C6
6	5	307	CLA	C4-C3-C5-C6
6	5	307	CLA	C6-C7-C8-C9
6	5	309	CLA	CBD-CGD-O2D-CED
6	5	312	CLA	CAD-CBD-CGD-O1D
6	5	312	CLA	CAD-CBD-CGD-O2D
6	7	309	CLA	CBD-CGD-O2D-CED
6	7	310	CLA	CBD-CGD-O2D-CED
6	7	311	CLA	CHA-CBD-CGD-O1D
6	7	311	CLA	CHA-CBD-CGD-O2D
6	7	311	CLA	CAD-CBD-CGD-O1D
6	6	205	CLA	CHA-CBD-CGD-O1D
6	6	205	CLA	CHA-CBD-CGD-O2D
6	6	206	CLA	CHA-CBD-CGD-O1D
6	6	206	CLA	CHA-CBD-CGD-O2D
6	6	208	CLA	CHA-CBD-CGD-O1D
6	6	208	CLA	CHA-CBD-CGD-O2D
6	6	209	CLA	C1A-C2A-CAA-CBA
6	6	210	CLA	C1A-C2A-CAA-CBA
6	6	210	CLA	CBD-CGD-O2D-CED
6	6	211	CLA	CBD-CGD-O2D-CED
6	6	212	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
6	6	212	CLA	CHA-CBD-CGD-O2D
6	6	212	CLA	CBD-CGD-O2D-CED
6	6	216	CLA	C2B-C3B-CAB-CBB
6	6	216	CLA	C4B-C3B-CAB-CBB
7	5	315	LHG	C3-O3-P-O5
7	5	315	LHG	C3-O3-P-O6
7	5	317	LHG	C4-O6-P-O3
7	5	317	LHG	C4-O6-P-O4
7	5	317	LHG	C4-O6-P-O5
7	5	317	LHG	O6-C4-C5-O7
7	5	318	LHG	C4-O6-P-O3
7	5	318	LHG	C4-O6-P-O4
7	5	318	LHG	C4-O6-P-O5
7	5	318	LHG	O7-C5-C6-O8
8	5	316	LMG	O6-C1-O1-C7
8	5	316	LMG	O7-C8-C9-O8
9	5	319	SQD	C45-C44-O6-C1
9	5	319	SQD	C5-C6-S-O7
10	7	304	DD6	C-C1-C24-C25
10	7	304	DD6	C2-C1-C24-C25
10	7	304	DD6	C13-C14-C15-C16
10	7	304	DD6	C13-C14-C15-C20
10	6	204	DD6	C12-C11-C13-C14
10	6	204	DD6	C1-C2-C3-C4
4	5	320	A86	C39-C38-O4-C34
4	7	301	A86	C39-C38-O4-C34
4	6	202	A86	C39-C38-O4-C34
6	7	310	CLA	O1D-CGD-O2D-CED
6	6	211	CLA	O1D-CGD-O2D-CED
6	5	312	CLA	CBD-CGD-O2D-CED
6	7	308	CLA	CBD-CGD-O2D-CED
6	7	311	CLA	CBD-CGD-O2D-CED
6	6	207	CLA	CBD-CGD-O2D-CED
6	6	208	CLA	CBD-CGD-O2D-CED
8	5	316	LMG	O10-C28-O8-C9
6	5	309	CLA	O1D-CGD-O2D-CED
6	5	312	CLA	O1D-CGD-O2D-CED
6	6	212	CLA	O1D-CGD-O2D-CED
6	7	309	CLA	O1D-CGD-O2D-CED
6	6	210	CLA	O1D-CGD-O2D-CED
8	5	316	LMG	C29-C28-O8-C9
6	6	201	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
6	5	305	CLA	O1A-CGA-O2A-C1
6	5	308	CLA	O1A-CGA-O2A-C1
6	7	309	CLA	O1A-CGA-O2A-C1
4	5	320	A86	O5-C38-O4-C34
4	7	301	A86	O5-C38-O4-C34
4	6	202	A86	O5-C38-O4-C34
6	5	307	CLA	O1D-CGD-O2D-CED
7	5	315	LHG	O9-C7-O7-C5
6	5	308	CLA	C3-C5-C6-C7
6	5	310	CLA	C3-C5-C6-C7
7	5	317	LHG	C8-C7-O7-C5
6	6	207	CLA	O1D-CGD-O2D-CED
6	7	307	CLA	CBD-CGD-O2D-CED
6	5	304	CLA	CBD-CGD-O2D-CED
6	5	308	CLA	CBD-CGD-O2D-CED
6	5	305	CLA	CBA-CGA-O2A-C1
6	5	308	CLA	CBA-CGA-O2A-C1
6	7	309	CLA	CBA-CGA-O2A-C1
6	7	308	CLA	O1D-CGD-O2D-CED
7	5	317	LHG	O9-C7-O7-C5
6	6	208	CLA	O1D-CGD-O2D-CED
10	7	304	DD6	C24-C25-C26-C27
10	6	204	DD6	C3-C4-C5-C6
4	5	303	A86	C39-C38-O4-C34
6	7	311	CLA	O1D-CGD-O2D-CED
6	5	307	CLA	C3-C5-C6-C7
7	5	315	LHG	C24-C23-O8-C6
4	5	301	A86	C39-C38-O4-C34
4	5	303	A86	O5-C38-O4-C34
4	7	302	A86	C39-C38-O4-C34
7	5	315	LHG	C8-C7-O7-C5
4	5	301	A86	O5-C38-O4-C34
4	7	302	A86	O5-C38-O4-C34
7	5	315	LHG	O10-C23-O8-C6
6	6	210	CLA	CBA-CGA-O2A-C1
6	6	210	CLA	O1A-CGA-O2A-C1
6	6	201	CLA	O1D-CGD-O2D-CED
7	5	318	LHG	C24-C23-O8-C6
8	5	316	LMG	C28-C29-C30-C31
8	5	316	LMG	C2-C1-O1-C7
6	5	308	CLA	C11-C10-C8-C9
6	7	309	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
6	6	210	CLA	C11-C12-C13-C14
10	7	303	DD6	C12-C11-C13-C14
10	6	203	DD6	C12-C11-C13-C14
10	7	303	DD6	C10-C11-C13-C14
10	6	203	DD6	C10-C11-C13-C14
10	6	204	DD6	C10-C11-C13-C14
6	6	209	CLA	CBD-CGD-O2D-CED
6	5	307	CLA	C8-C10-C11-C12
6	7	310	CLA	C5-C6-C7-C8
9	5	319	SQD	C7-C8-C9-C10
9	5	319	SQD	C31-C32-C33-C34
6	7	309	CLA	C11-C10-C8-C7
10	7	304	DD6	C1-C2-C3-C4
10	6	204	DD6	C11-C10-C9-C8
6	5	308	CLA	C5-C6-C7-C8
9	5	319	SQD	C27-C28-C29-C30
6	6	211	CLA	C5-C6-C7-C8
6	5	305	CLA	C5-C6-C7-C8
7	5	318	LHG	C8-C7-O7-C5
7	5	317	LHG	C3-O3-P-O6
9	5	319	SQD	C35-C36-C37-C38
6	7	310	CLA	CBA-CGA-O2A-C1
10	7	304	DD6	C11-C10-C9-C8
10	7	304	DD6	C3-C4-C5-C6
7	5	317	LHG	C7-C8-C9-C10
7	5	317	LHG	C16-C17-C18-C19
6	5	304	CLA	O1D-CGD-O2D-CED
6	5	308	CLA	O1D-CGD-O2D-CED
6	7	307	CLA	O1D-CGD-O2D-CED
7	5	317	LHG	C9-C10-C11-C12
8	5	316	LMG	C31-C32-C33-C34
6	6	210	CLA	C14-C13-C15-C16
7	5	318	LHG	C23-C24-C25-C26
10	7	304	DD6	C7-C6-C8-C9
7	5	317	LHG	O1-C1-C2-C3
10	7	304	DD6	C5-C6-C8-C9
8	5	316	LMG	C29-C30-C31-C32
8	5	316	LMG	C33-C34-C35-C36
9	5	319	SQD	C10-C11-C12-C13
6	5	309	CLA	C4B-C3B-CAB-CBB
6	7	313	CLA	C4B-C3B-CAB-CBB
6	6	213	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
8	5	316	LMG	C30-C31-C32-C33
9	5	319	SQD	C11-C12-C13-C14
9	5	319	SQD	C23-C24-C25-C26
7	5	317	LHG	C15-C16-C17-C18
6	5	307	CLA	C3A-C2A-CAA-CBA
6	5	311	CLA	C3A-C2A-CAA-CBA
6	7	308	CLA	C3A-C2A-CAA-CBA
6	6	209	CLA	C3A-C2A-CAA-CBA
6	6	210	CLA	C3A-C2A-CAA-CBA
6	7	310	CLA	C6-C7-C8-C10
6	6	206	CLA	CBD-CGD-O2D-CED
6	7	310	CLA	O1A-CGA-O2A-C1
6	5	309	CLA	C2B-C3B-CAB-CBB
6	7	313	CLA	C2B-C3B-CAB-CBB
6	6	213	CLA	C2B-C3B-CAB-CBB
7	5	317	LHG	C10-C11-C12-C13
6	5	305	CLA	C4-C3-C5-C6
6	5	305	CLA	C2-C3-C5-C6
6	6	210	CLA	C11-C12-C13-C15
6	6	210	CLA	C12-C13-C15-C16
6	5	311	CLA	CBD-CGD-O2D-CED
6	5	310	CLA	C2A-CAA-CBA-CGA
6	7	311	CLA	C2A-CAA-CBA-CGA
6	5	305	CLA	CBD-CGD-O2D-CED
6	5	307	CLA	C10-C11-C12-C13
6	7	310	CLA	C6-C7-C8-C9
6	5	307	CLA	C2A-CAA-CBA-CGA
6	5	311	CLA	C1A-C2A-CAA-CBA
6	7	306	CLA	C1A-C2A-CAA-CBA
6	7	308	CLA	C1A-C2A-CAA-CBA
6	7	309	CLA	C1A-C2A-CAA-CBA
7	5	318	LHG	O9-C7-O7-C5
7	5	318	LHG	C28-C29-C30-C31
5	5	302	ET4	C09-C10-C11-C12
6	6	210	CLA	C8-C10-C11-C12
4	6	202	A86	C35-C34-O4-C38
8	5	316	LMG	C34-C35-C36-C37
6	6	210	CLA	C3-C5-C6-C7
7	5	318	LHG	C5-C4-O6-P
7	5	317	LHG	O6-C4-C5-C6
7	5	318	LHG	O6-C4-C5-C6
8	5	316	LMG	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
6	6	210	CLA	C4-C3-C5-C6
8	5	316	LMG	C7-C8-C9-O8
8	5	316	LMG	C41-C42-C43-C44
8	5	316	LMG	O6-C5-C6-O5
4	7	301	A86	C35-C34-O4-C38
7	5	318	LHG	O10-C23-O8-C6
6	6	209	CLA	O1D-CGD-O2D-CED
7	5	318	LHG	O6-C4-C5-O7
8	5	316	LMG	C16-C17-C18-C19
8	5	316	LMG	O1-C7-C8-O7
4	5	301	A86	C35-C34-O4-C38
4	5	320	A86	C35-C34-O4-C38
6	5	307	CLA	C11-C10-C8-C7
6	5	307	CLA	C11-C12-C13-C15
6	5	307	CLA	C11-C10-C8-C9
6	7	309	CLA	C11-C10-C8-C9
7	5	318	LHG	C26-C27-C28-C29
6	5	307	CLA	C4B-C3B-CAB-CBB
6	7	315	CLA	C4B-C3B-CAB-CBB
6	6	205	CLA	C4B-C3B-CAB-CBB
8	5	316	LMG	C32-C33-C34-C35
8	5	316	LMG	O1-C7-C8-C9
9	5	319	SQD	C12-C13-C14-C15
6	5	310	CLA	C4-C3-C5-C6
6	5	307	CLA	C2B-C3B-CAB-CBB
6	7	315	CLA	C2B-C3B-CAB-CBB
7	5	317	LHG	O7-C5-C6-O8
4	5	320	A86	C10-C11-C13-C14
4	7	301	A86	C10-C11-C13-C14
4	7	302	A86	C10-C11-C13-C14
6	6	210	CLA	C2-C1-O2A-CGA
6	5	305	CLA	C6-C7-C8-C9
6	5	308	CLA	C11-C12-C13-C14
7	5	317	LHG	C2-C3-O3-P
8	5	316	LMG	C42-C43-C44-C45
6	5	305	CLA	O1D-CGD-O2D-CED
6	5	311	CLA	O1D-CGD-O2D-CED
6	6	206	CLA	O1D-CGD-O2D-CED
4	5	303	A86	C11-C10-C9-C8
9	5	319	SQD	C25-C26-C27-C28
4	5	301	A86	C28-C27-C29-C30
6	7	311	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
6	7	309	CLA	C4-C3-C5-C6
6	7	310	CLA	C4-C3-C5-C6
6	5	311	CLA	C2C-C3C-CAC-CBC
4	7	302	A86	C12-C11-C13-O
4	6	202	A86	C12-C11-C13-O
7	5	317	LHG	C4-C5-C6-O8
7	5	318	LHG	C4-C5-C6-O8
6	5	305	CLA	CHA-CBD-CGD-O1D
6	5	311	CLA	CHA-CBD-CGD-O1D
6	7	305	CLA	CHA-CBD-CGD-O1D
7	5	315	LHG	O7-C5-C6-O8
9	5	319	SQD	O47-C45-C46-O48
4	7	302	A86	C10-C11-C13-O
4	6	202	A86	C10-C11-C13-O
9	5	319	SQD	O49-C7-O47-C45
7	5	317	LHG	O10-C23-O8-C6
5	5	302	ET4	C11-C12-C13-C28
6	7	310	CLA	C1A-C2A-CAA-CBA
6	5	307	CLA	CBA-CGA-O2A-C1
6	5	304	CLA	C4B-C3B-CAB-CBB
6	7	305	CLA	C4B-C3B-CAB-CBB
7	5	317	LHG	C3-O3-P-O5
7	5	318	LHG	C29-C30-C31-C32
4	5	301	A86	C26-C27-C29-C30
6	6	208	CLA	CAD-CBD-CGD-O1D
6	5	305	CLA	C11-C10-C8-C7
6	5	308	CLA	C6-C7-C8-C10
6	5	305	CLA	C2A-CAA-CBA-CGA
6	6	213	CLA	CAD-CBD-CGD-O1D
7	5	315	LHG	C4-C5-C6-O8
6	5	305	CLA	O2A-C1-C2-C3
6	7	305	CLA	O1D-CGD-O2D-CED
4	6	202	A86	C33-C34-O4-C38
7	5	317	LHG	C24-C23-O8-C6
4	5	320	A86	C13-C14-C15-C20
4	7	301	A86	C13-C14-C15-C20
4	7	302	A86	C13-C14-C15-C20
6	5	307	CLA	C11-C12-C13-C14
6	5	307	CLA	O1A-CGA-O2A-C1
7	5	317	LHG	O1-C1-C2-O2
6	6	211	CLA	C6-C7-C8-C9
6	6	205	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
4	7	302	A86	C35-C34-O4-C38
6	6	210	CLA	C2-C3-C5-C6
7	5	317	LHG	C12-C13-C14-C15
6	6	210	CLA	C15-C16-C17-C18
4	7	302	A86	C12-C11-C13-C14
7	5	318	LHG	C7-C8-C9-C10
6	5	308	CLA	C11-C12-C13-C15
6	7	310	CLA	C2-C3-C5-C6
6	5	308	CLA	C6-C7-C8-C9
6	5	306	CLA	CAA-CBA-CGA-O1A
5	5	302	ET4	C11-C12-C13-C14
6	7	316	CLA	CBD-CGD-O2D-CED
6	5	313	CLA	C4B-C3B-CAB-CBB
6	7	305	CLA	CBD-CGD-O2D-CED
6	6	206	CLA	CAA-CBA-CGA-O2A
6	7	316	CLA	O1D-CGD-O2D-CED
6	7	306	CLA	CAA-CBA-CGA-O1A
7	5	317	LHG	O10-C23-C24-C25
8	5	316	LMG	C17-C18-C19-C20
9	5	319	SQD	C33-C34-C35-C36
7	5	315	LHG	C12-C13-C14-C15
6	7	306	CLA	CAA-CBA-CGA-O2A
6	5	312	CLA	C2C-C3C-CAC-CBC
6	5	310	CLA	C1A-C2A-CAA-CBA
6	6	206	CLA	C1A-C2A-CAA-CBA
6	6	211	CLA	C1A-C2A-CAA-CBA
6	5	306	CLA	CAA-CBA-CGA-O2A
7	5	317	LHG	O8-C23-C24-C25
6	5	304	CLA	C2B-C3B-CAB-CBB
6	5	313	CLA	C2B-C3B-CAB-CBB
6	7	305	CLA	C2B-C3B-CAB-CBB
6	5	311	CLA	CAA-CBA-CGA-O2A
6	6	201	CLA	CAA-CBA-CGA-O2A
4	6	202	A86	C10-C11-C13-C14
6	6	206	CLA	CAA-CBA-CGA-O1A
6	6	207	CLA	CAA-CBA-CGA-O2A
6	5	311	CLA	CAA-CBA-CGA-O1A
6	5	312	CLA	C4C-C3C-CAC-CBC
7	5	317	LHG	C11-C10-C9-C8
9	5	319	SQD	C32-C33-C34-C35
6	6	207	CLA	CAA-CBA-CGA-O1A
6	5	312	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
6	5	305	CLA	C6-C7-C8-C10
6	5	310	CLA	C2-C3-C5-C6
8	5	316	LMG	O7-C10-C11-C12
6	6	201	CLA	CAA-CBA-CGA-O1A
6	7	308	CLA	CAA-CBA-CGA-O1A
6	7	309	CLA	C2-C3-C5-C6
6	5	305	CLA	C11-C10-C8-C9
6	6	208	CLA	C3A-C2A-CAA-CBA
6	5	306	CLA	CAD-CBD-CGD-O2D
6	6	207	CLA	CAD-CBD-CGD-O2D
6	5	306	CLA	C2A-CAA-CBA-CGA
7	5	317	LHG	O7-C7-C8-C9
6	6	209	CLA	CAA-CBA-CGA-O1A
6	6	208	CLA	C2A-CAA-CBA-CGA
6	5	305	CLA	CHA-CBD-CGD-O2D
6	5	308	CLA	CHA-CBD-CGD-O1D
6	5	308	CLA	CHA-CBD-CGD-O2D
6	5	311	CLA	CHA-CBD-CGD-O2D
6	5	312	CLA	CHA-CBD-CGD-O1D
6	5	312	CLA	CHA-CBD-CGD-O2D
6	7	305	CLA	CHA-CBD-CGD-O2D
6	7	308	CLA	CAA-CBA-CGA-O2A
6	6	209	CLA	CAA-CBA-CGA-O2A
6	5	307	CLA	C6-C7-C8-C10
9	5	319	SQD	C5-C6-S-O8
7	5	315	LHG	C27-C28-C29-C30
6	6	213	CLA	CHA-CBD-CGD-O2D
9	5	319	SQD	C34-C35-C36-C37
6	7	307	CLA	C2A-CAA-CBA-CGA
6	6	206	CLA	C2A-CAA-CBA-CGA
6	5	305	CLA	C10-C11-C12-C13
8	5	316	LMG	C12-C13-C14-C15
8	5	316	LMG	O9-C10-C11-C12
6	5	307	CLA	CAD-CBD-CGD-O1D
6	5	308	CLA	CAD-CBD-CGD-O1D
6	7	307	CLA	CAD-CBD-CGD-O1D
6	7	308	CLA	CAD-CBD-CGD-O1D
6	6	207	CLA	C2C-C3C-CAC-CBC
8	5	316	LMG	C11-C12-C13-C14
9	5	319	SQD	C26-C27-C28-C29
6	6	213	CLA	CHA-CBD-CGD-O1D
6	6	213	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
6	5	305	CLA	CAA-CBA-CGA-O2A
6	7	307	CLA	CAA-CBA-CGA-O2A

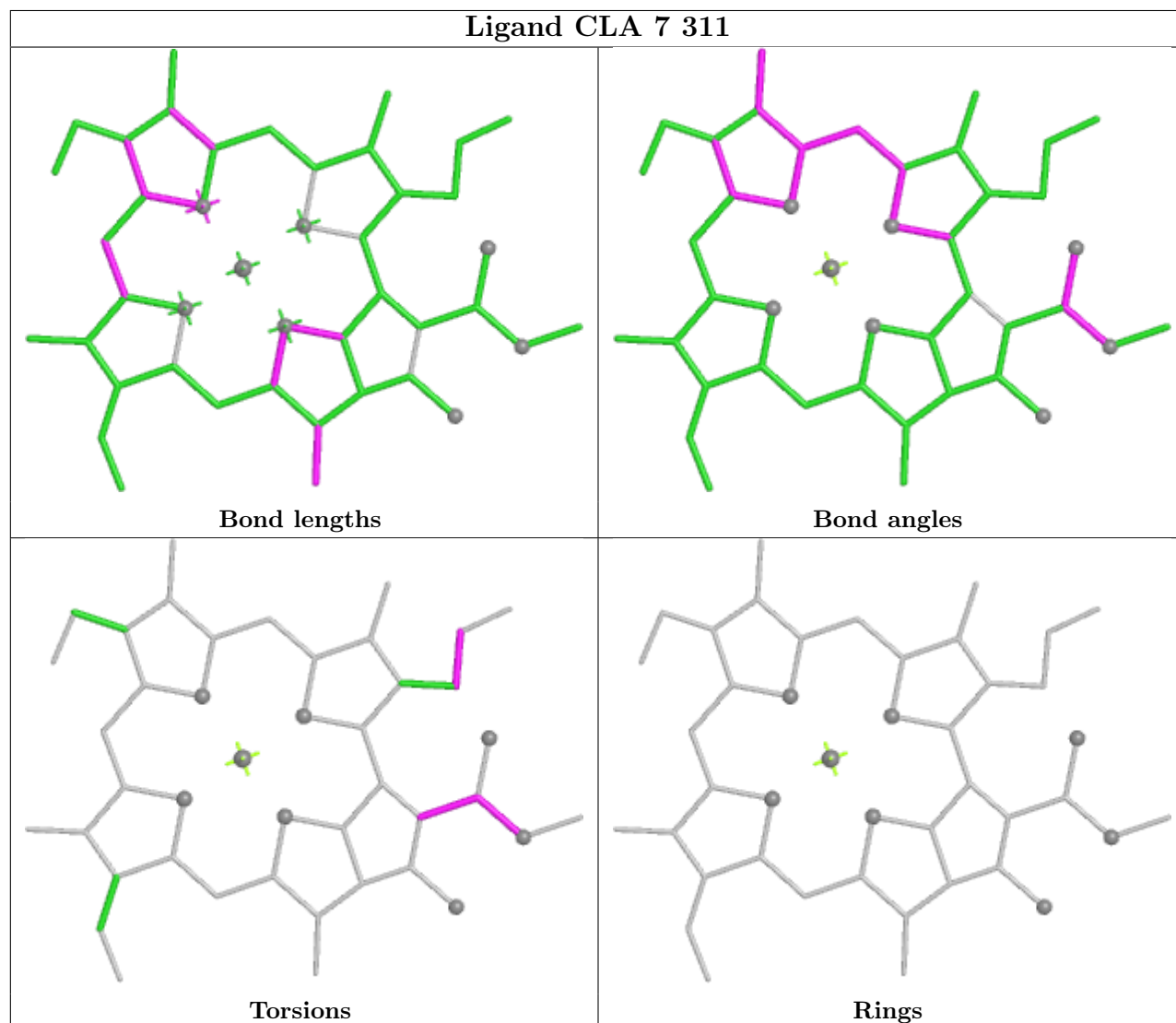
There are no ring outliers.

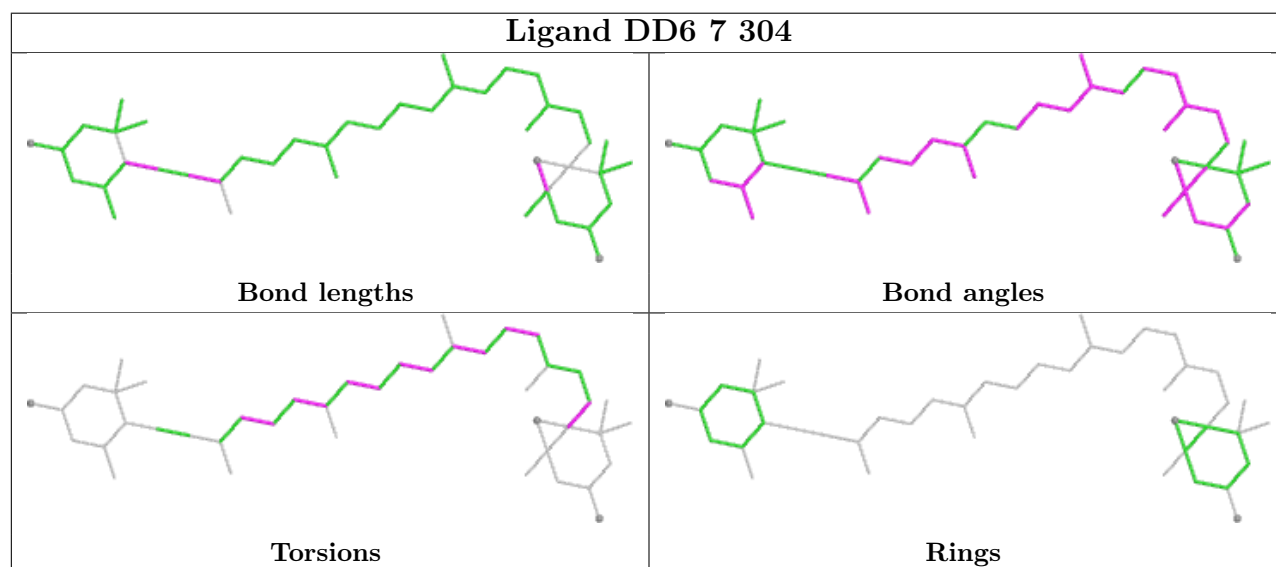
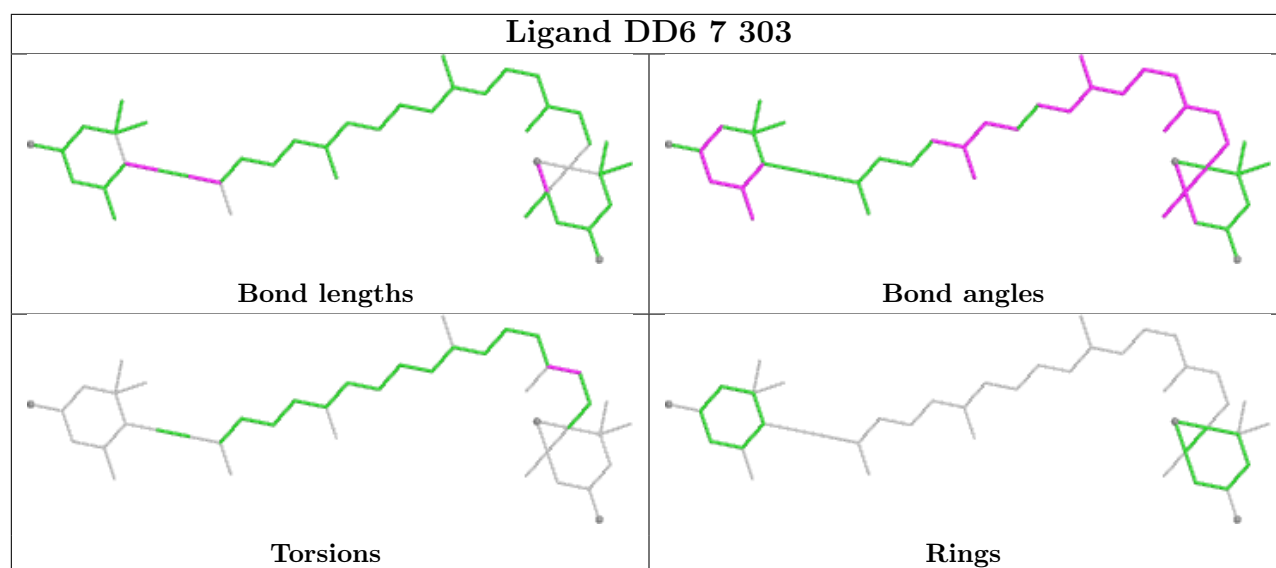
29 monomers are involved in 81 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	7	303	DD6	18	0
10	7	304	DD6	8	0
4	5	303	A86	1	0
6	7	307	CLA	3	0
6	6	210	CLA	5	0
6	5	308	CLA	6	0
6	7	306	CLA	4	0
6	7	305	CLA	1	0
7	5	318	LHG	1	0
6	6	211	CLA	2	0
6	6	209	CLA	1	0
10	6	203	DD6	1	0
6	5	307	CLA	1	0
9	5	319	SQD	5	0
6	5	311	CLA	2	0
6	6	214	CLA	1	0
4	6	202	A86	1	0
6	6	201	CLA	2	0
8	5	316	LMG	1	0
6	7	312	CLA	1	0
6	5	310	CLA	1	0
6	5	313	CLA	1	0
6	6	206	CLA	4	0
6	7	309	CLA	6	0
6	7	310	CLA	7	0
10	6	204	DD6	2	0
6	5	304	CLA	3	0
7	5	315	LHG	2	0
6	5	305	CLA	3	0

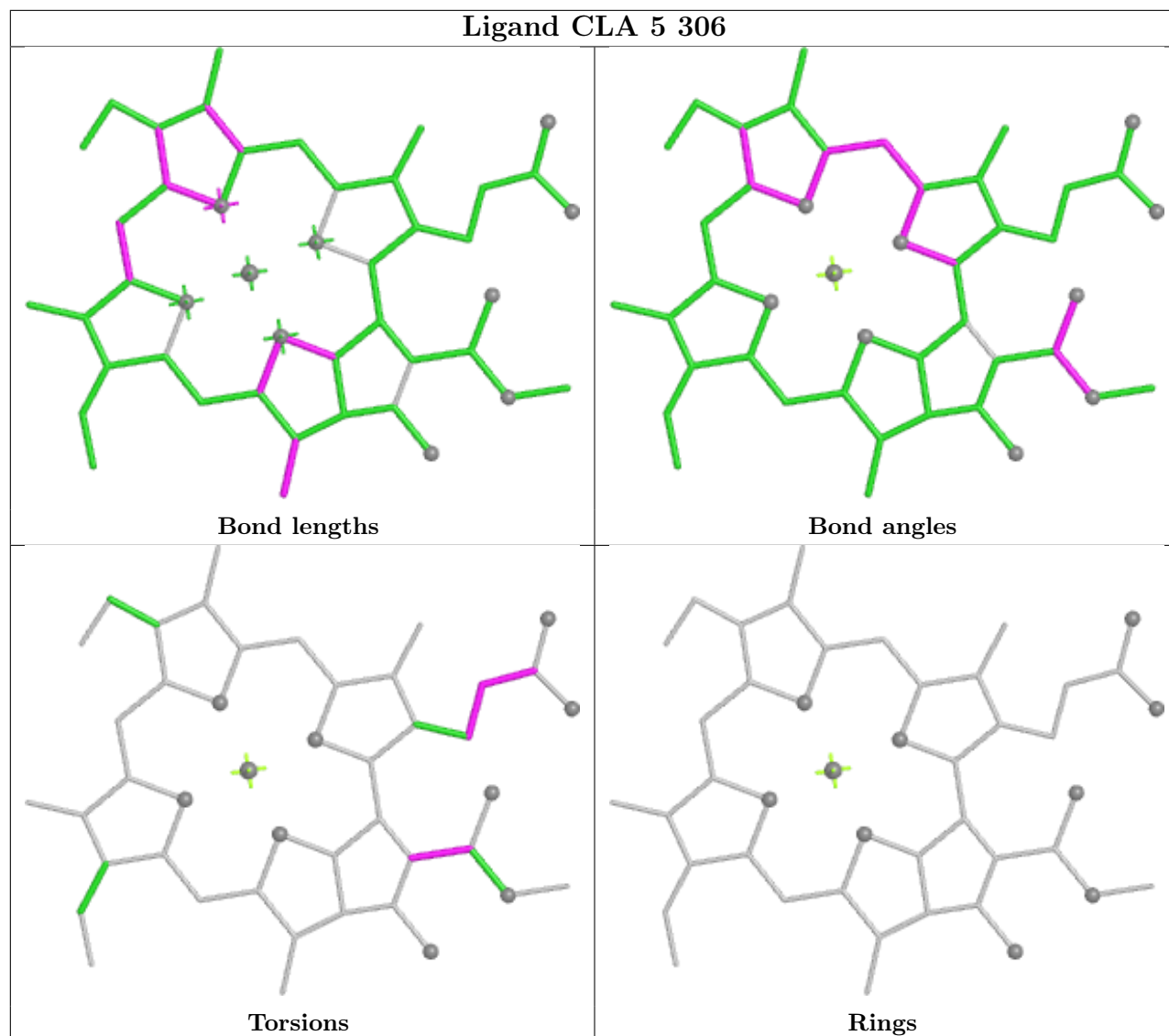
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

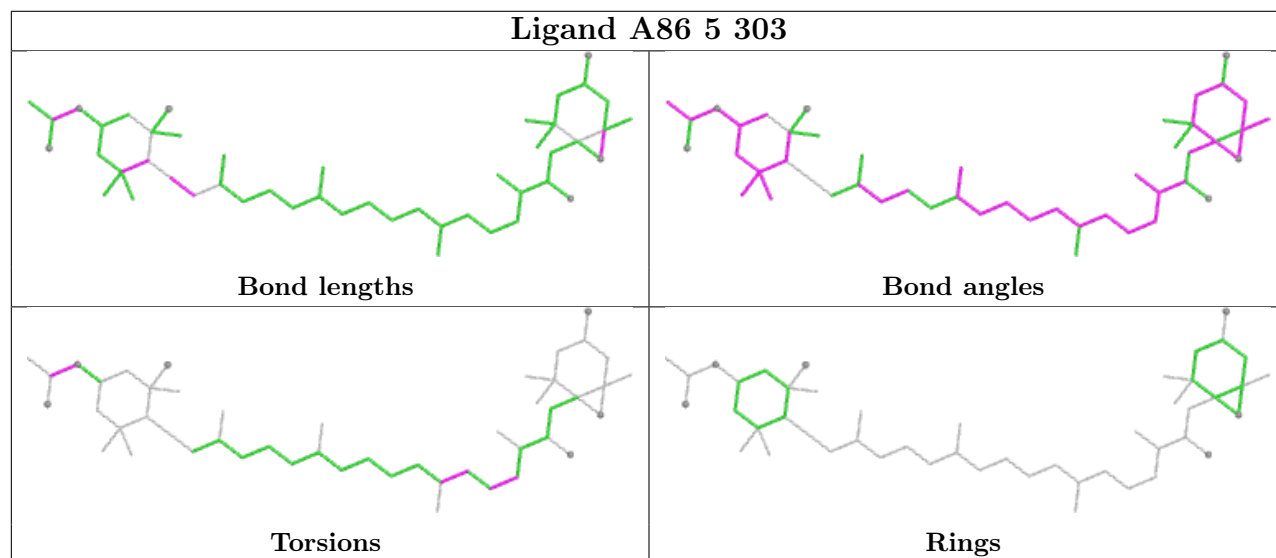




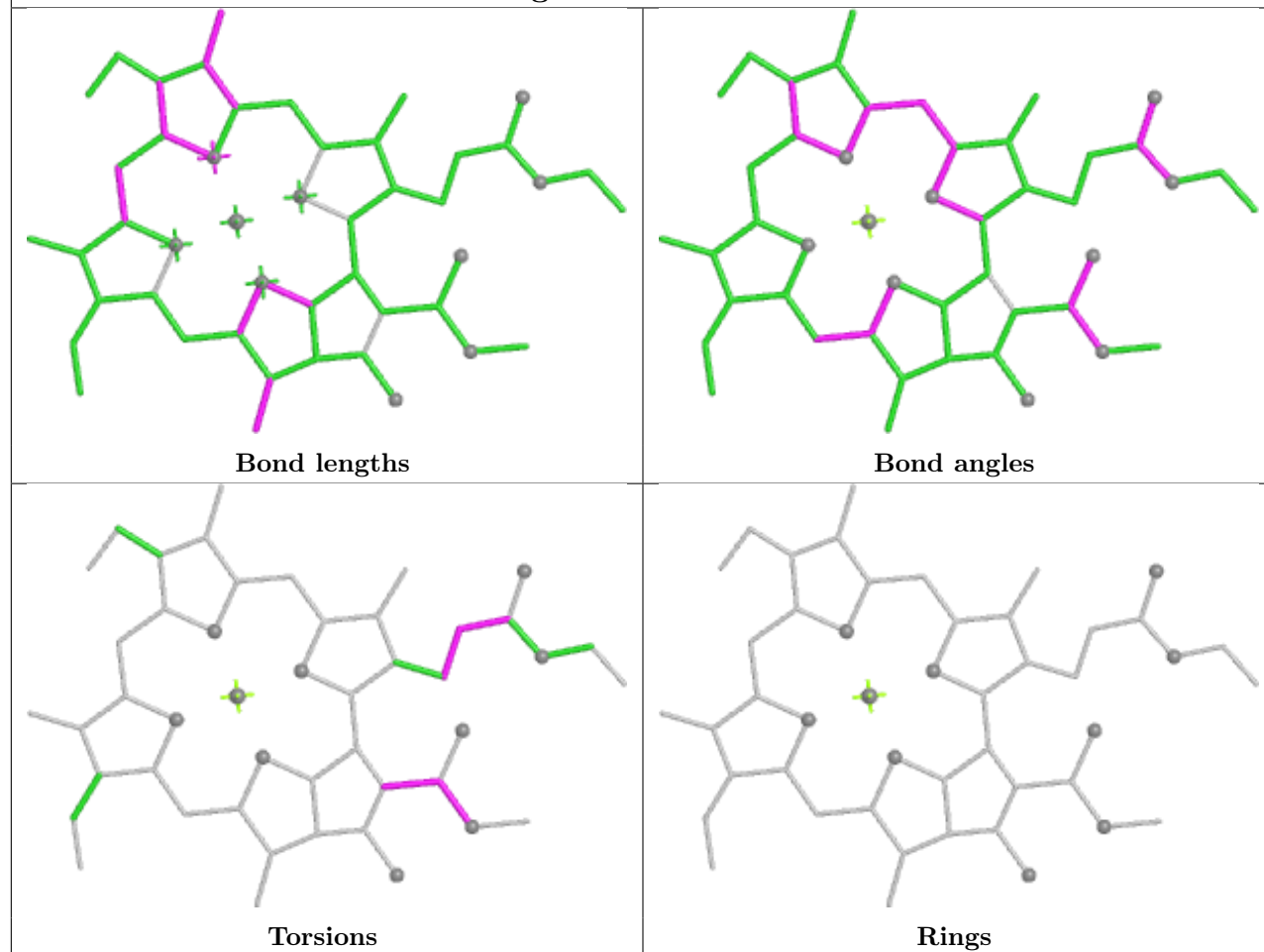
Ligand CLA 5 306



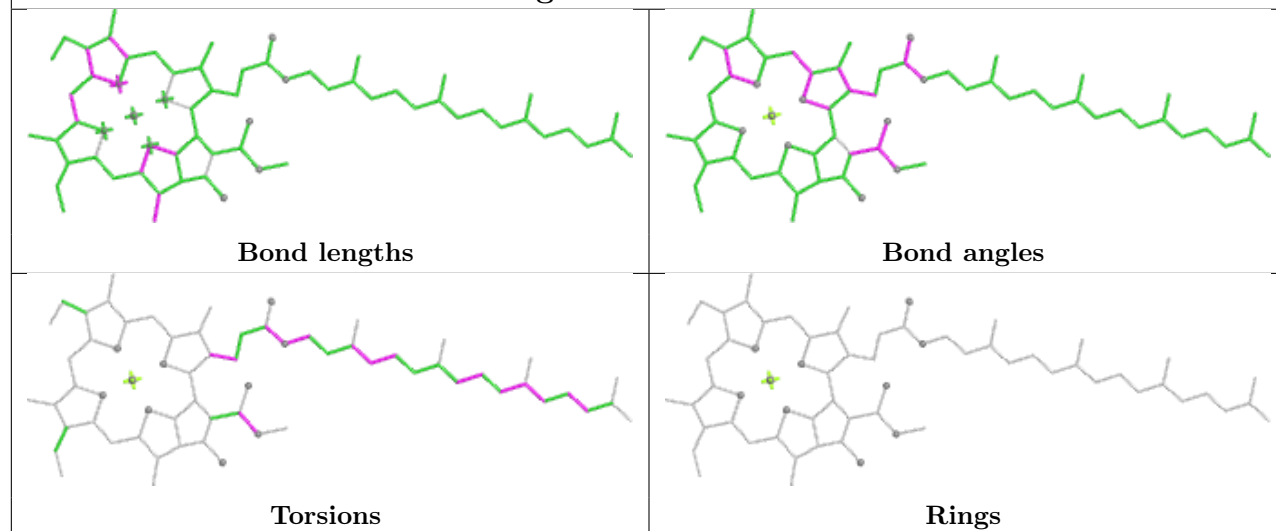
Ligand A86 5 303

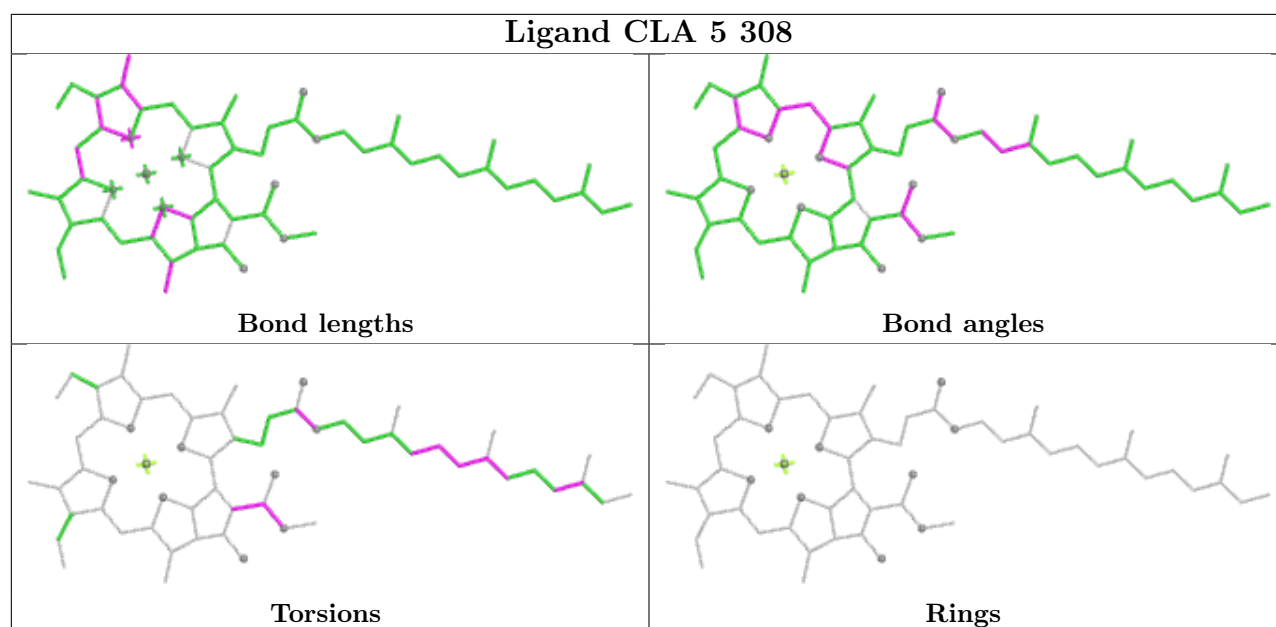


Ligand CLA 7 307

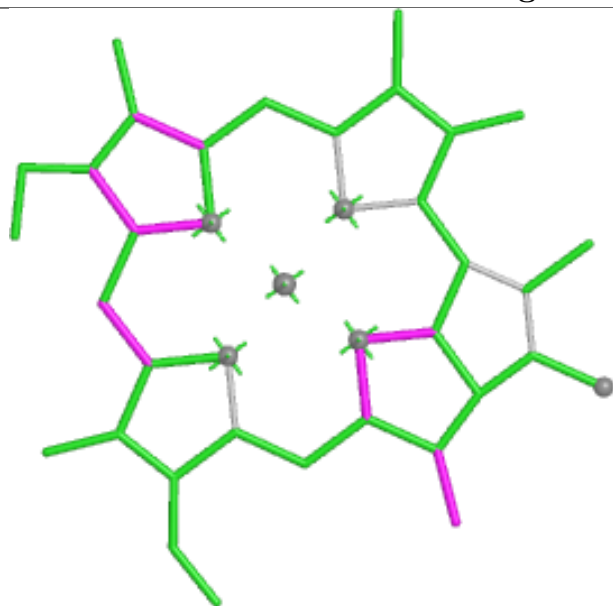


Ligand CLA 6 210





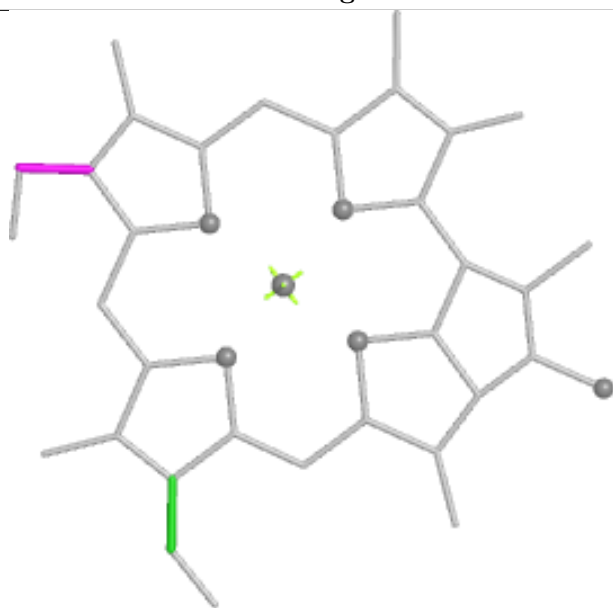
Ligand CLA 6 216



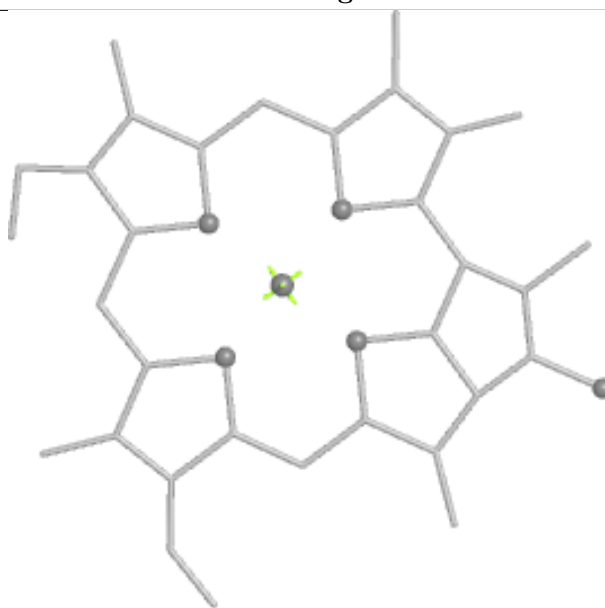
Bond lengths



Bond angles

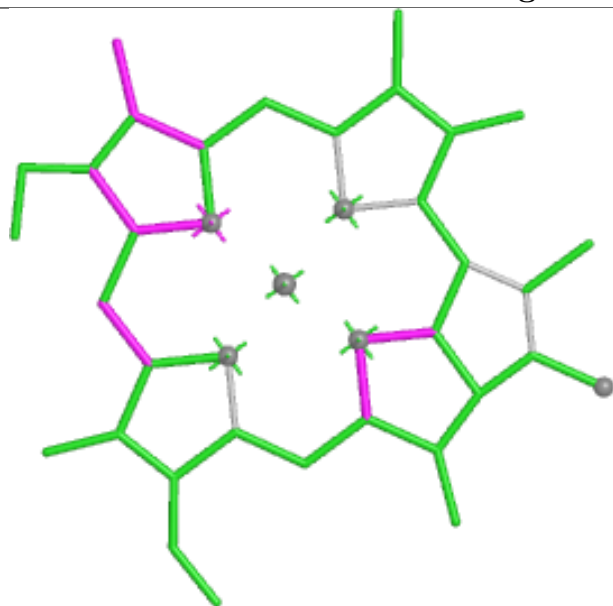


Torsions

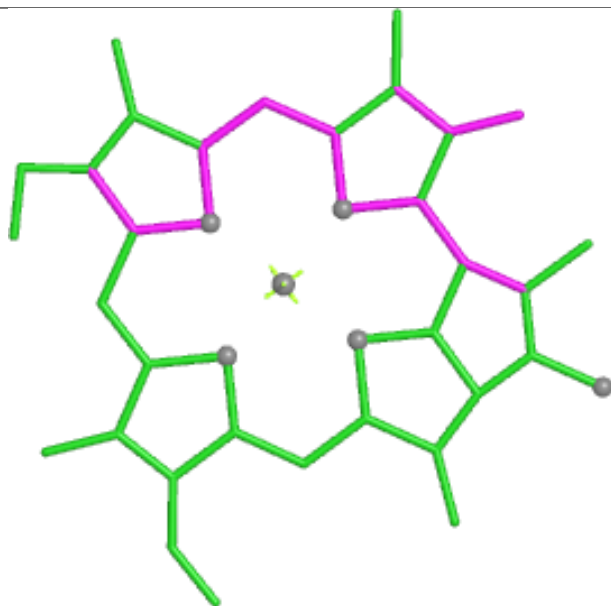


Rings

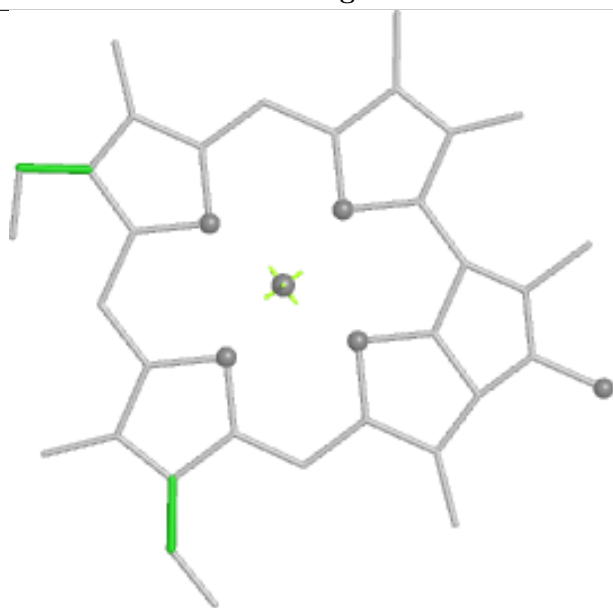
Ligand CLA 6 215



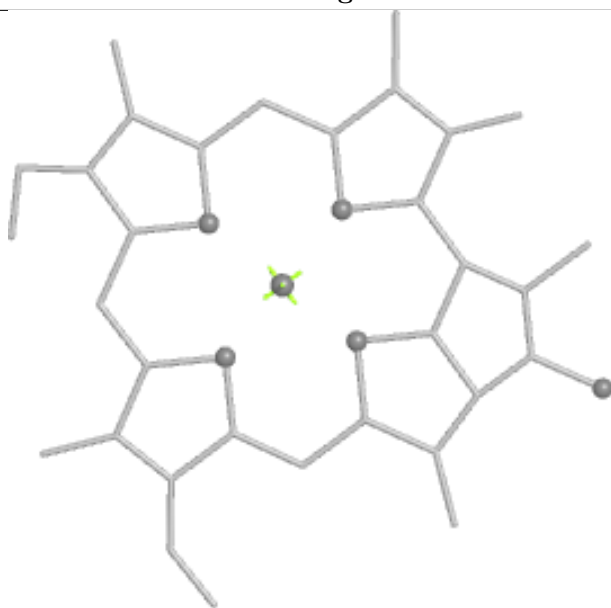
Bond lengths



Bond angles

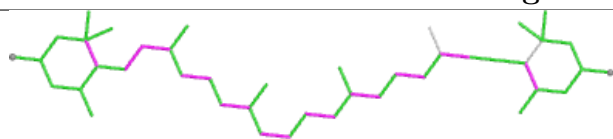


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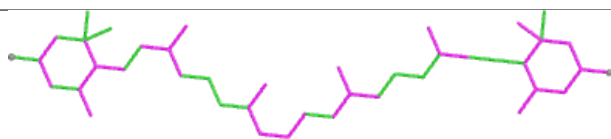


Rings

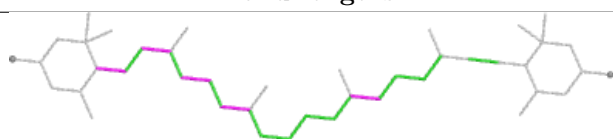
Ligand ET4 5 302



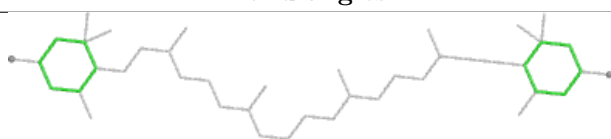
Bond lengths



Bond angles

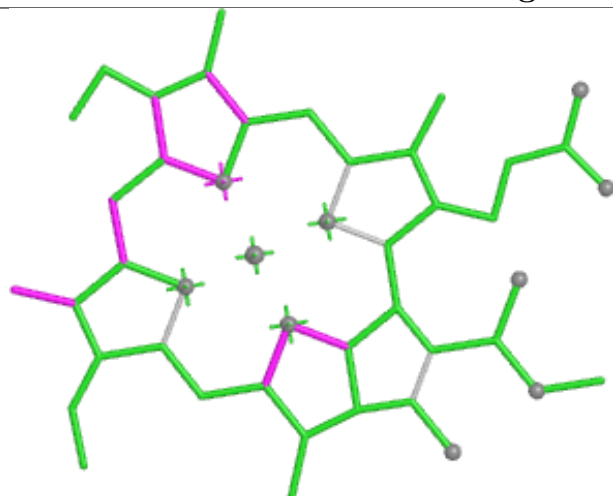


Torsions

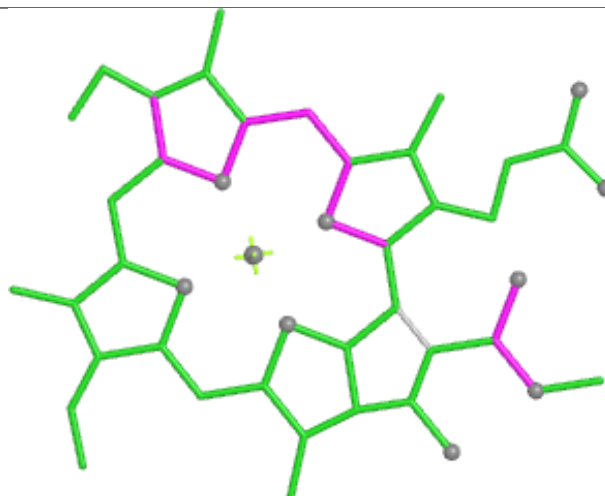


Rings

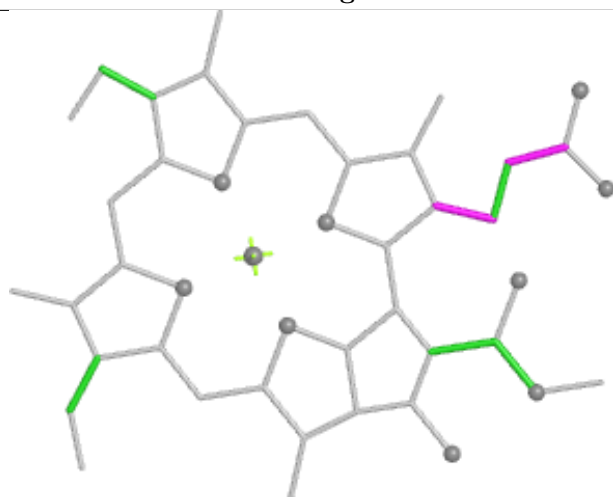
Ligand CLA 7 306



Bond lengths



Bond angles

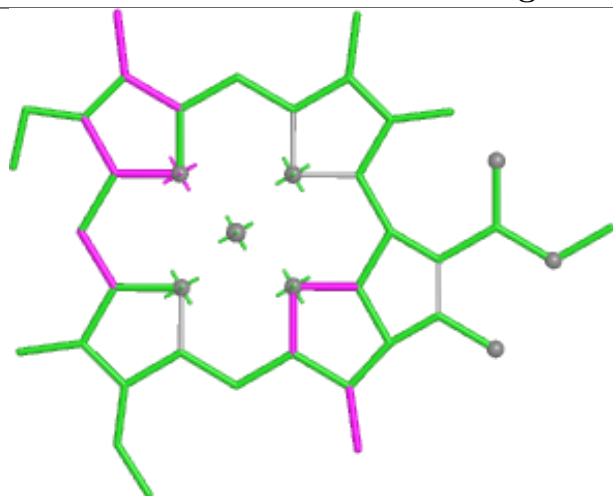


Torsions

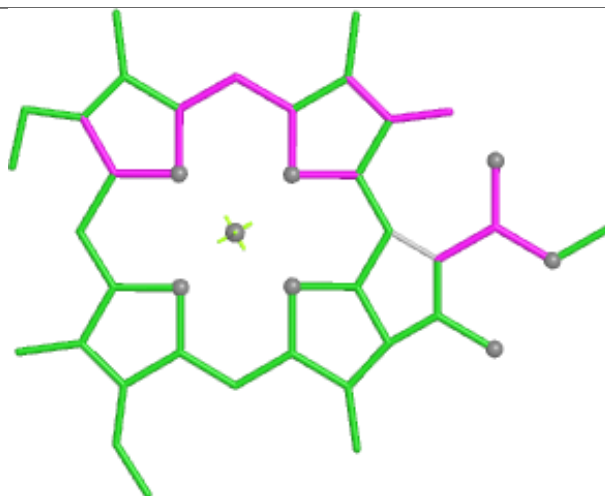


Rings

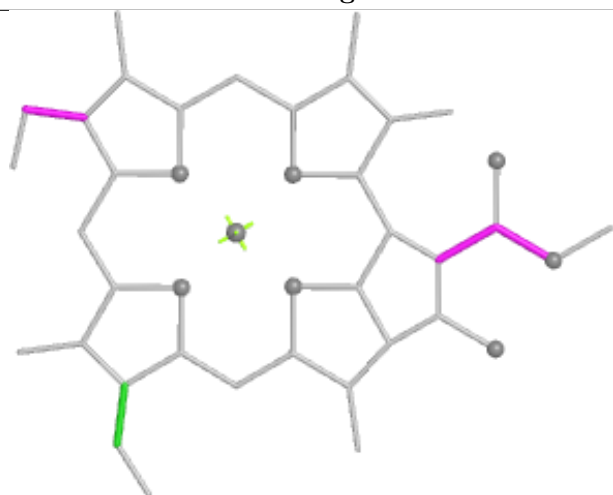
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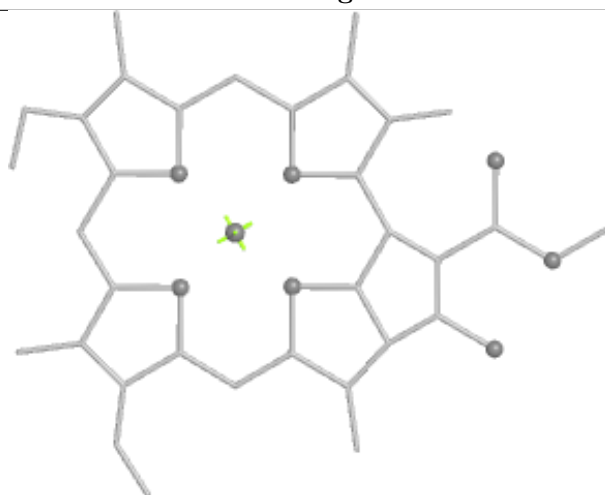
Bond lengths



Bond angles

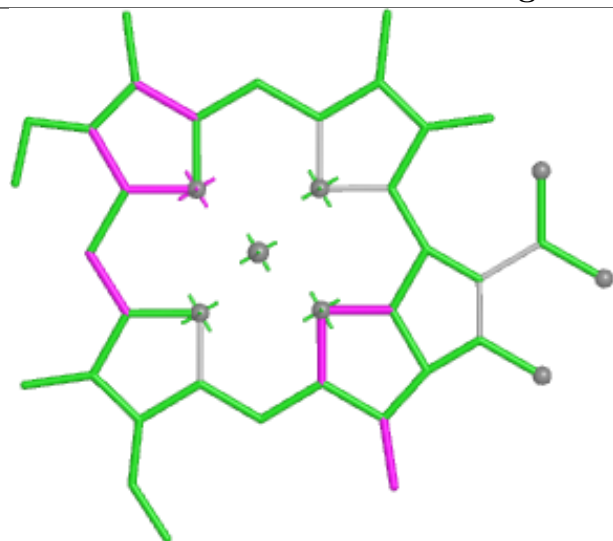


Torsions

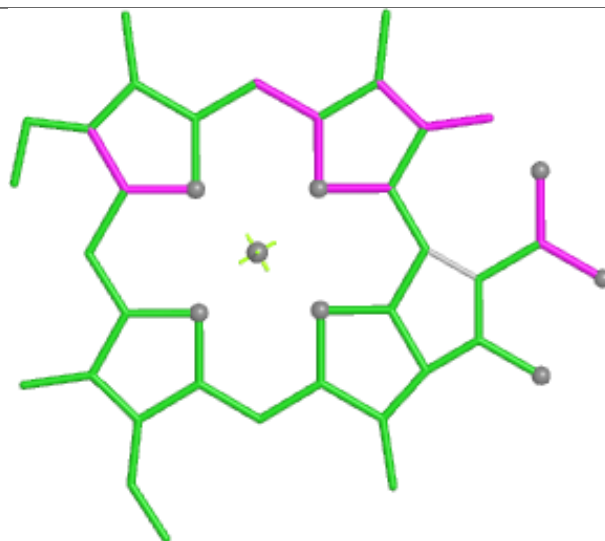


Rings

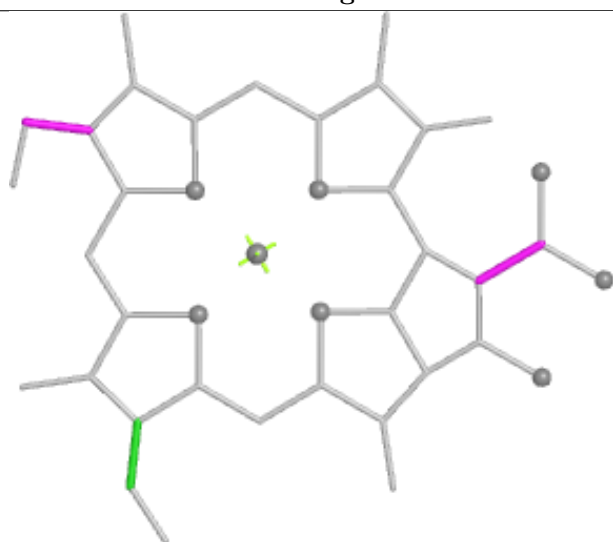
Ligand CLA 6 213



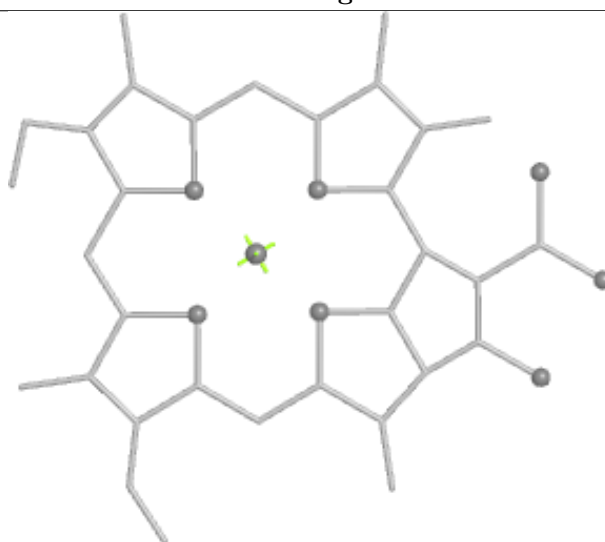
Bond lengths



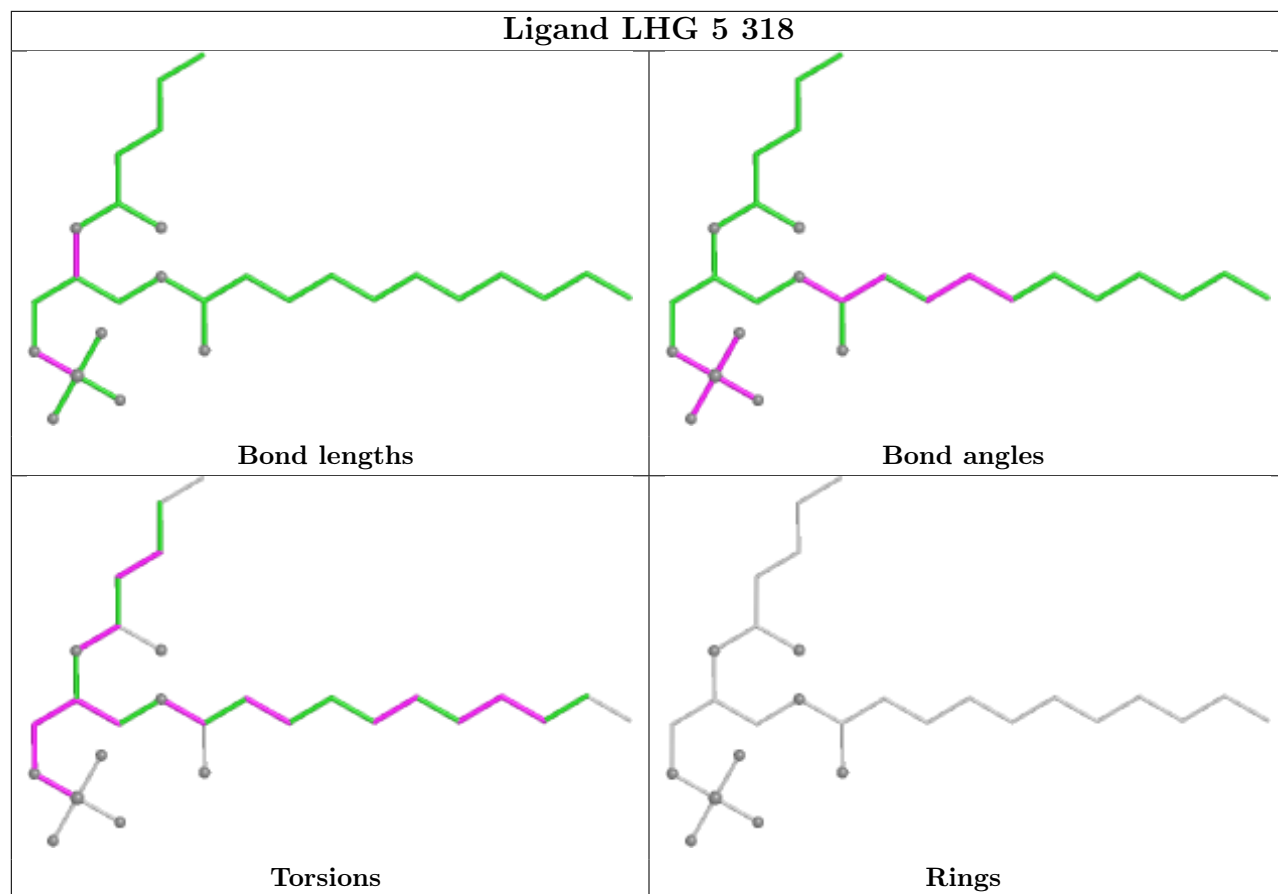
Bond angles



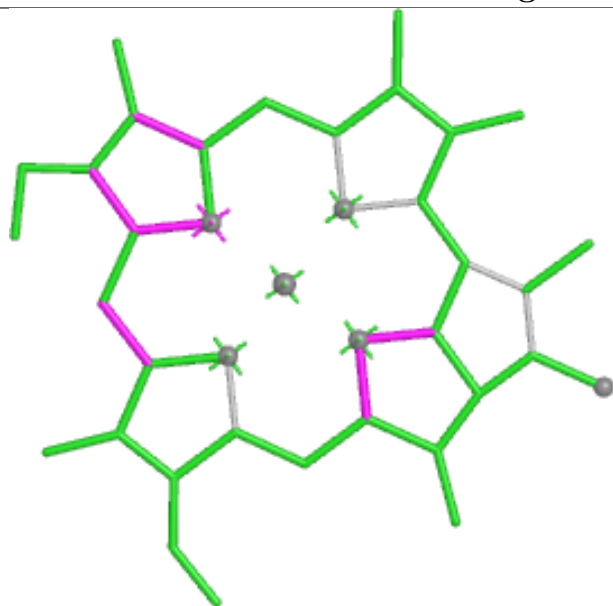
Torsions



Rings



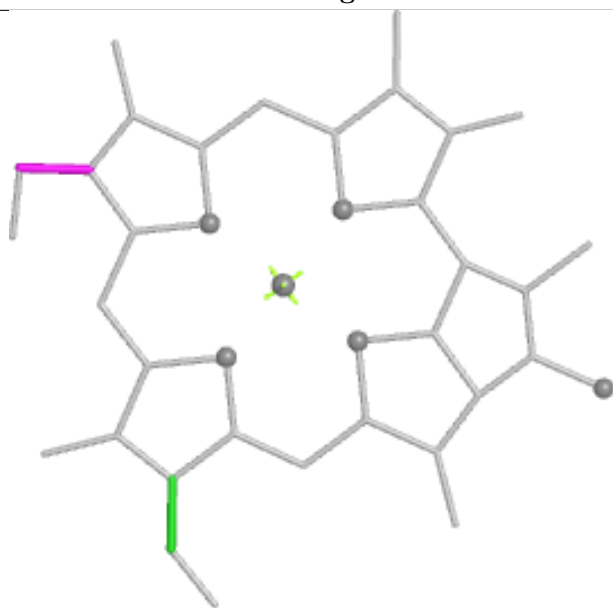
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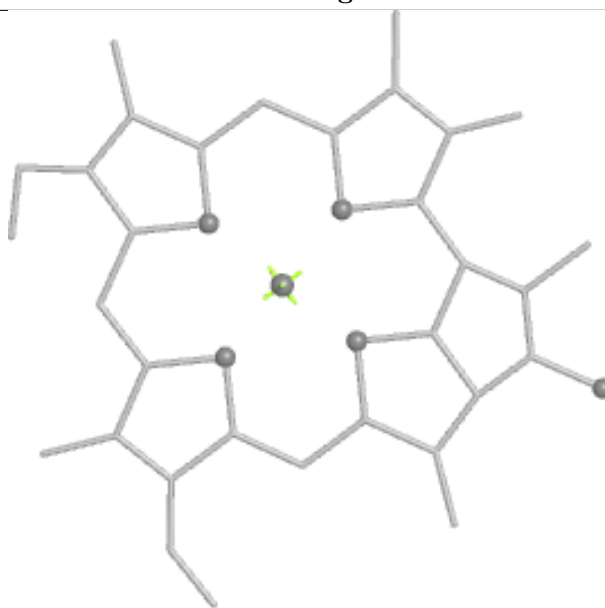
Bond lengths



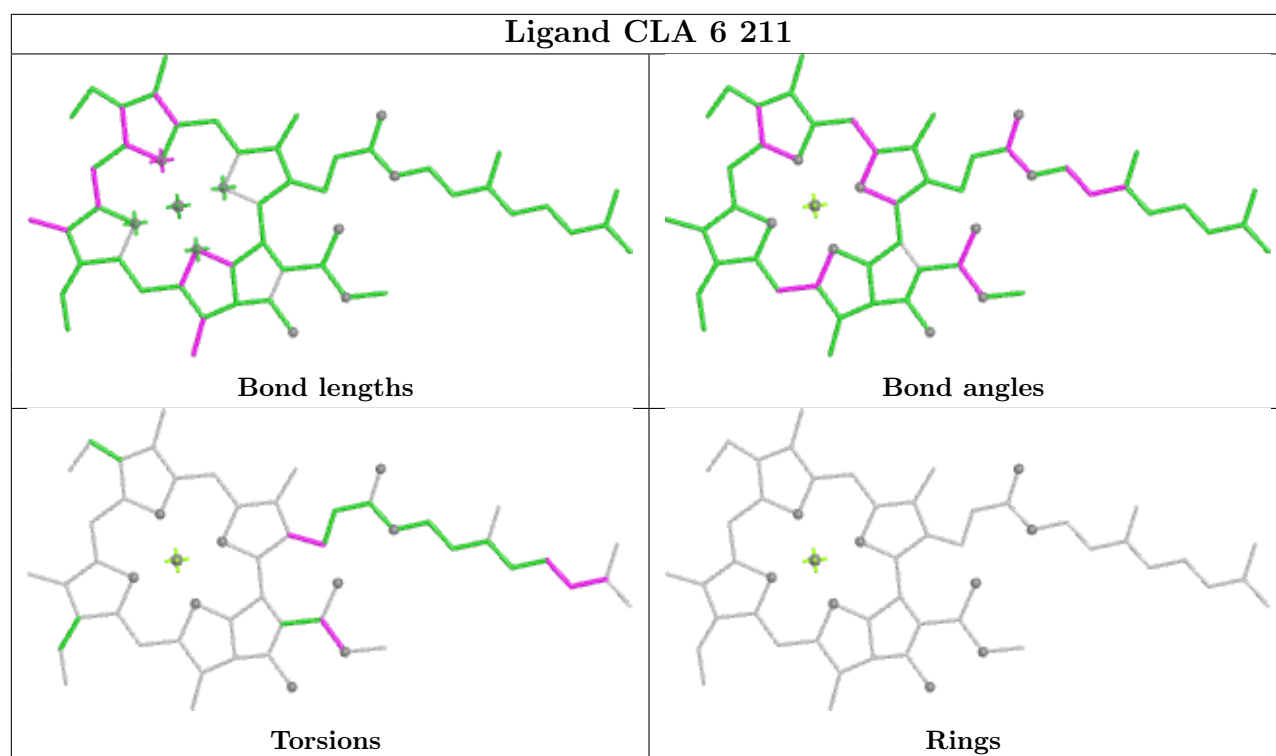
Bond angles



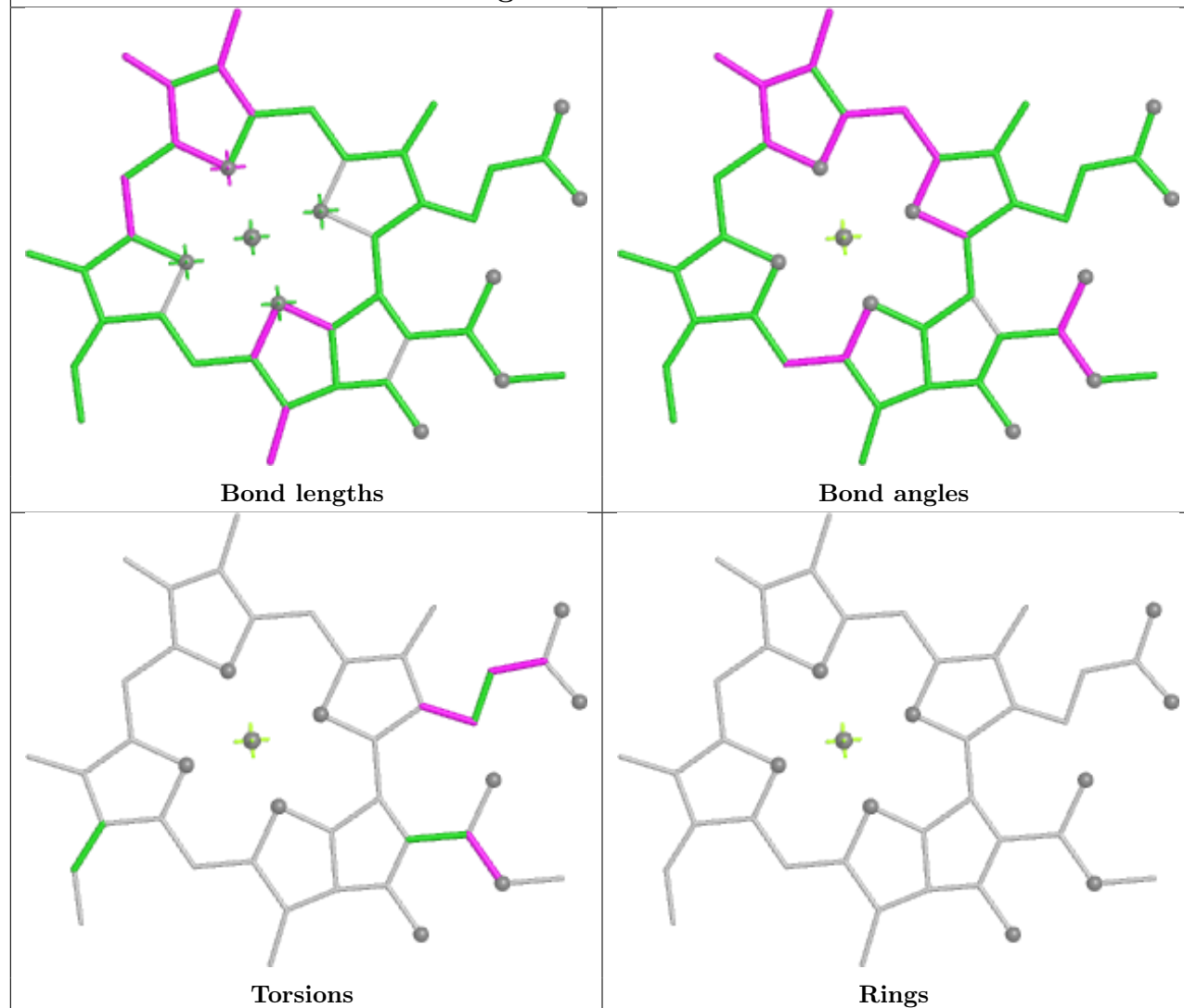
Torsions



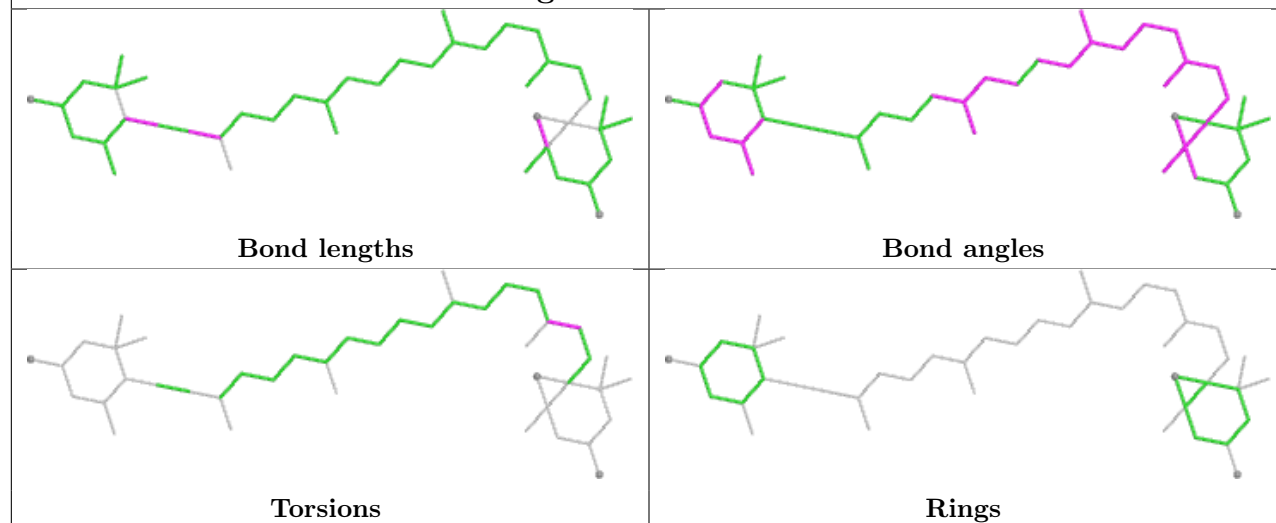
Rings



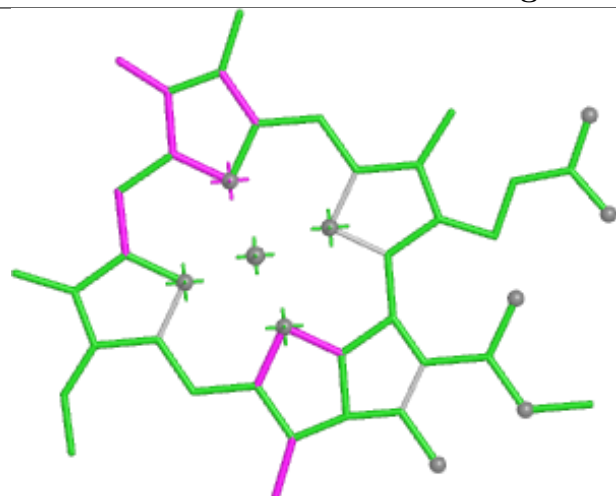
Ligand CLA 6 209



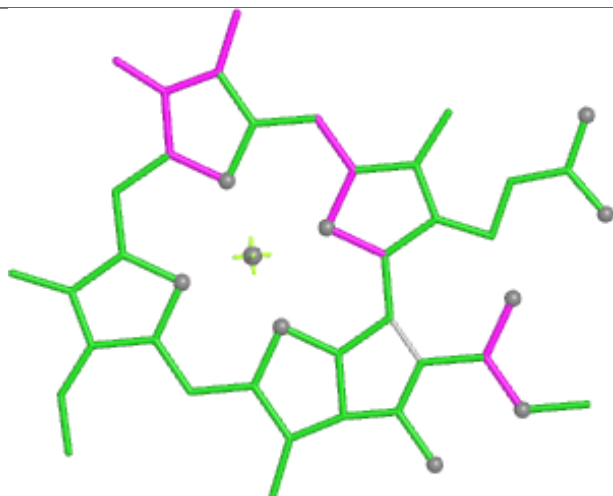
Ligand DD6 6 203



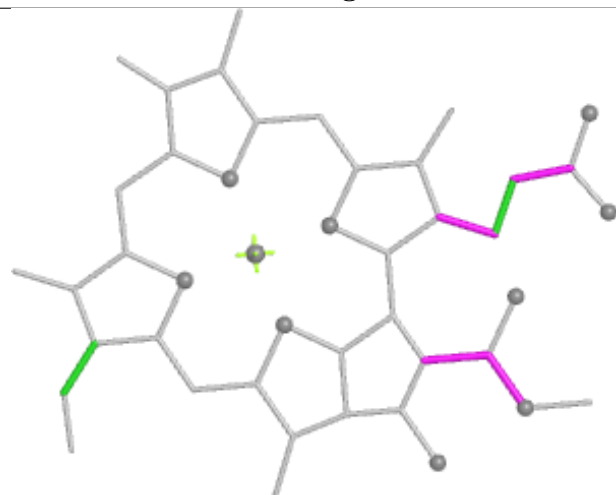
Ligand CLA 7 308



Bond lengths



Bond angles

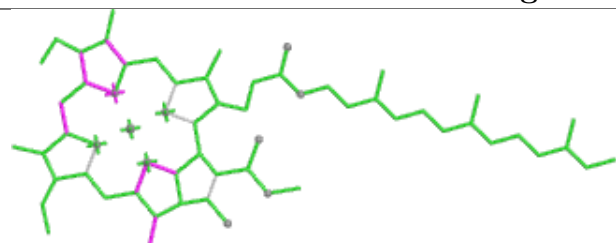


Torsions

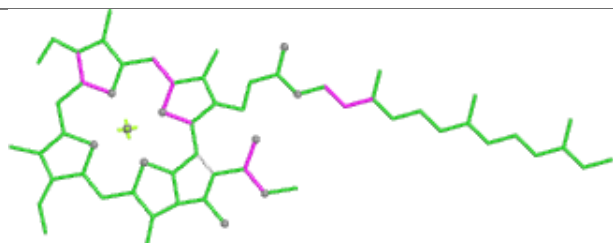


Rings

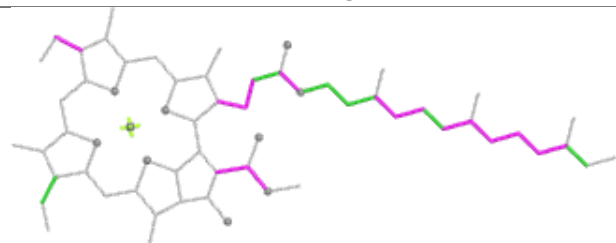
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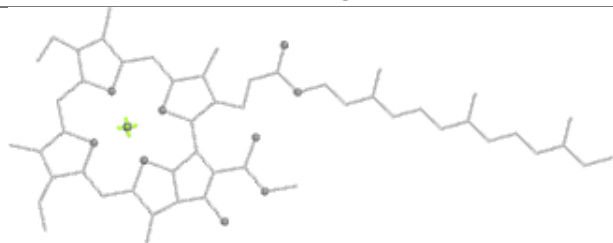
Bond lengths



Bond angles

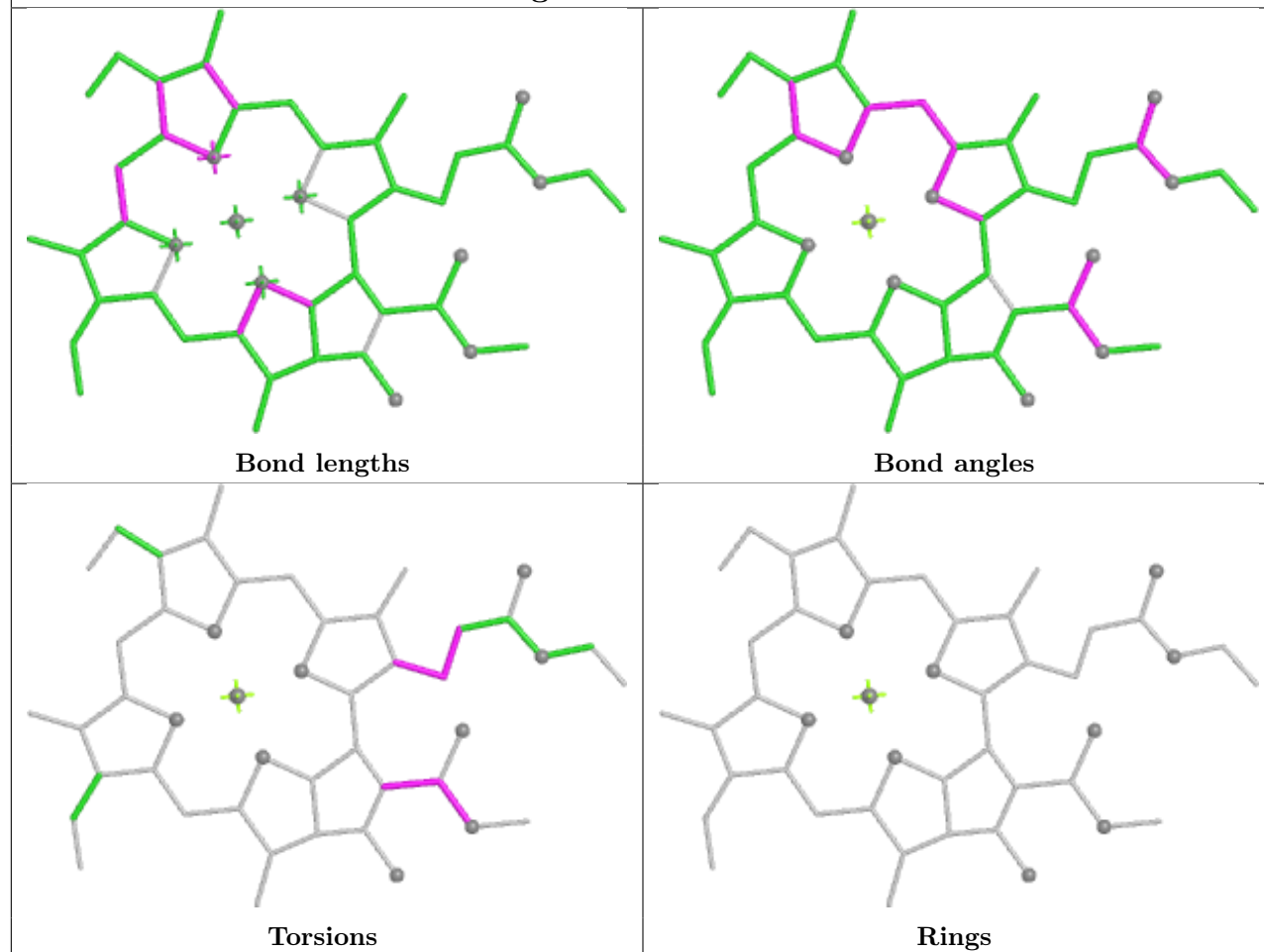


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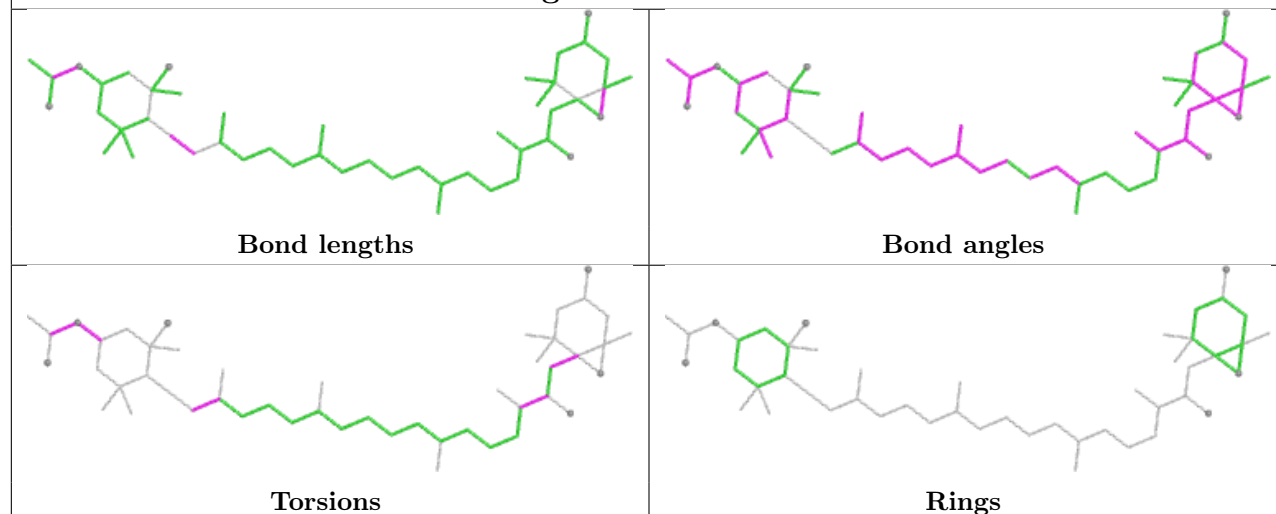


Rings

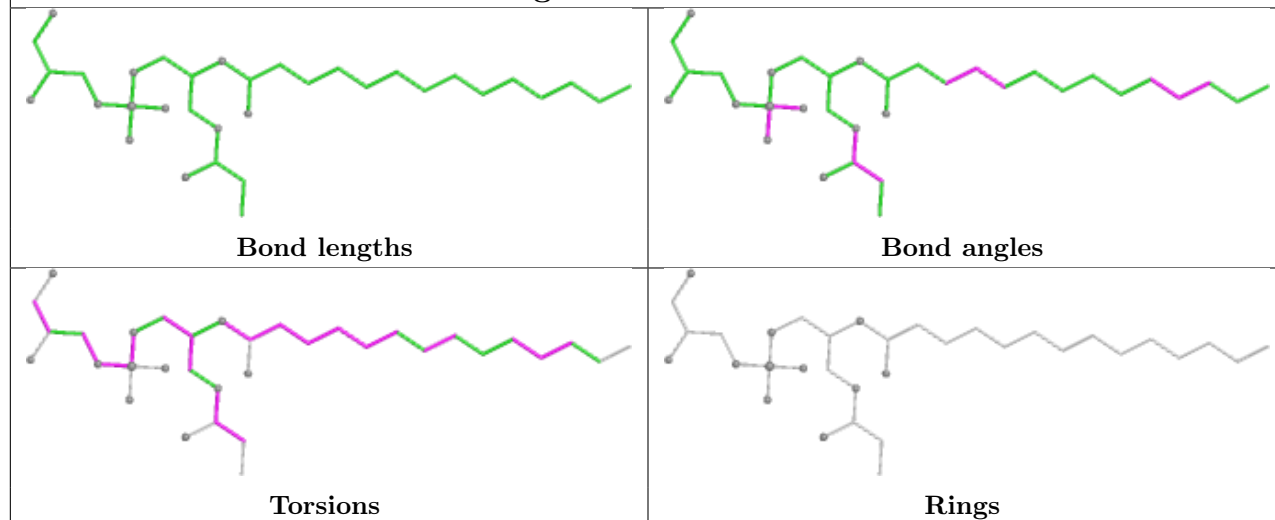
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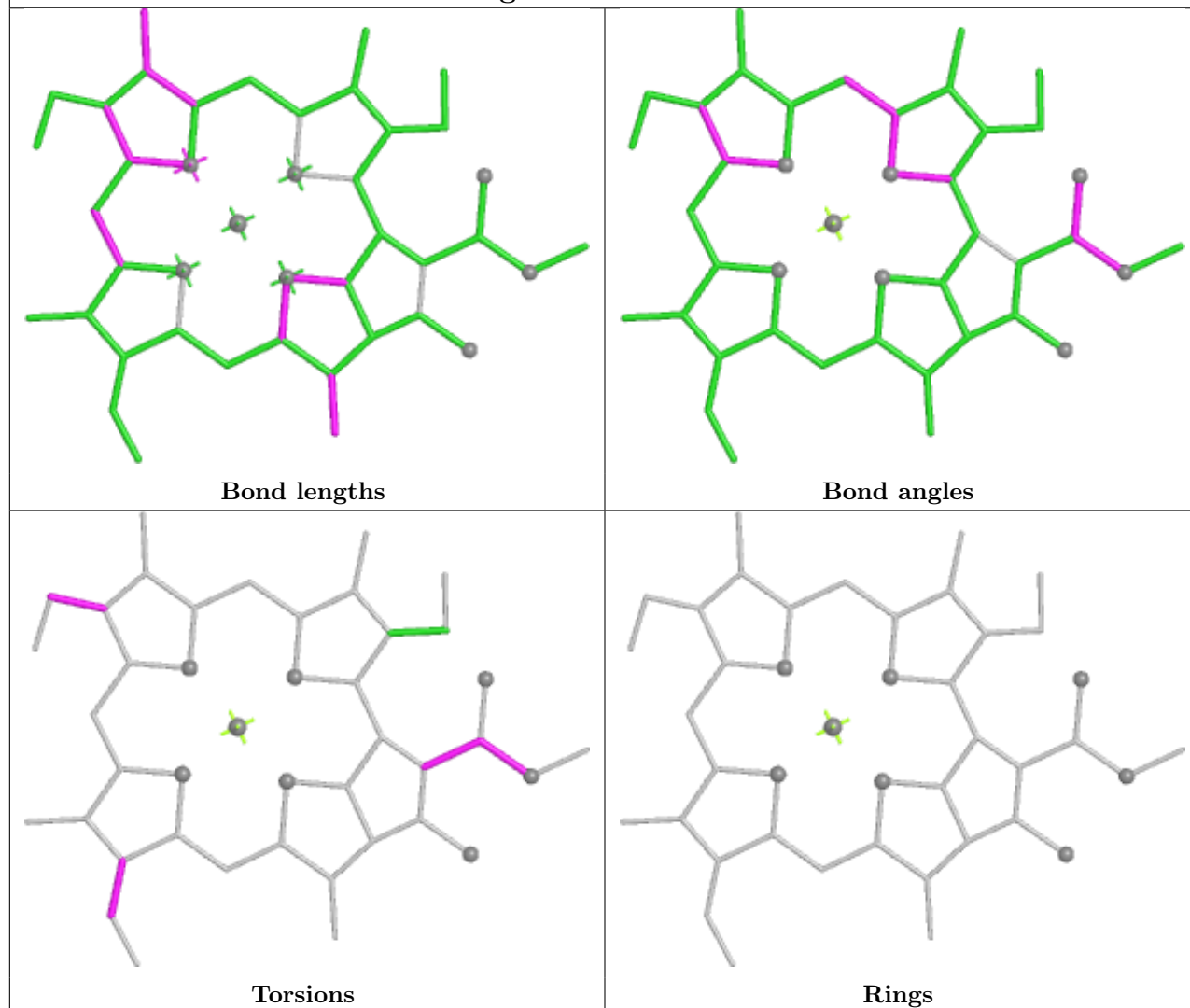
Ligand A86 5 301



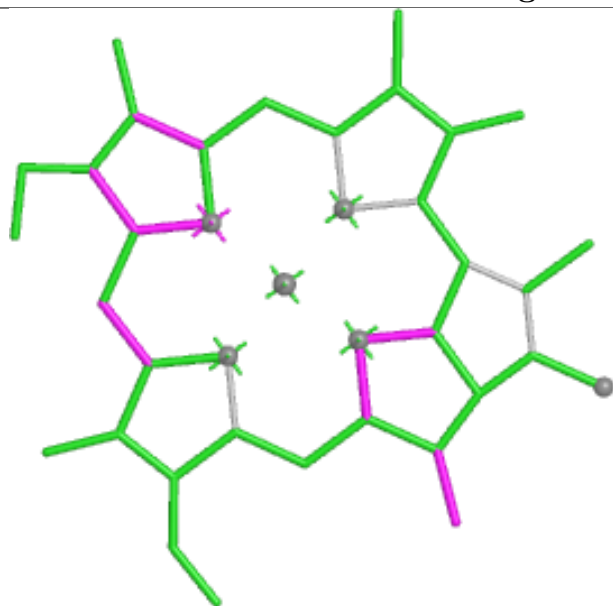
Ligand LHG 5 317



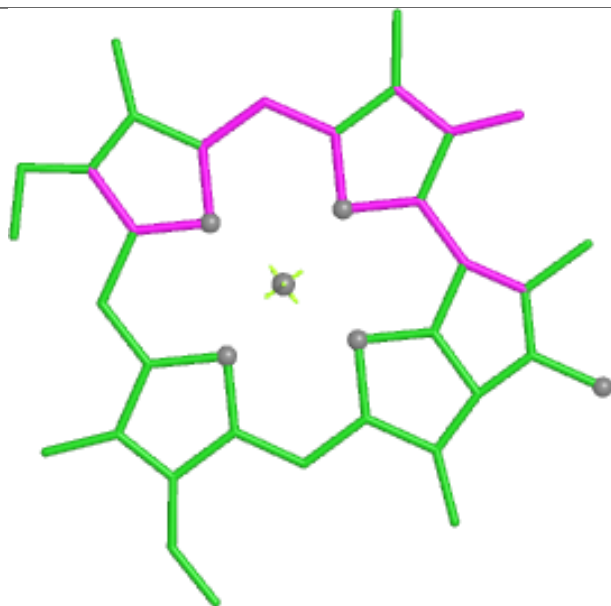
Ligand CLA 5 312



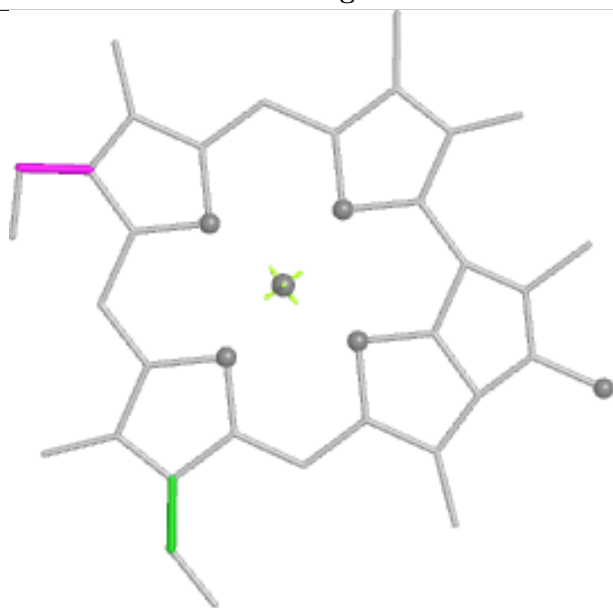
Ligand CLA 7 313



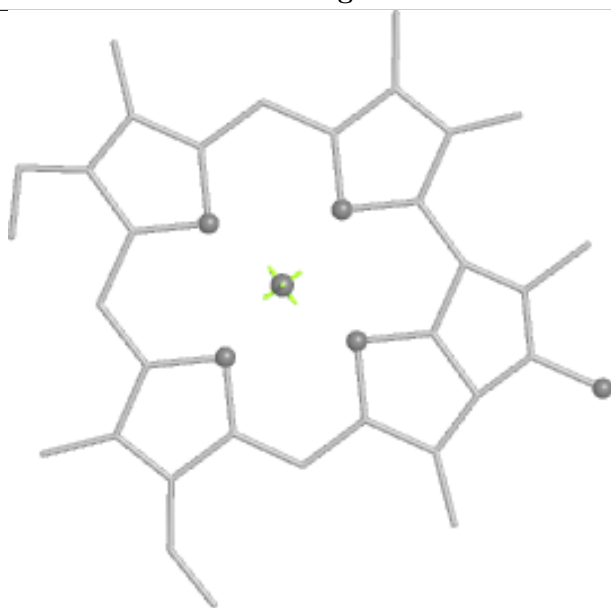
Bond lengths



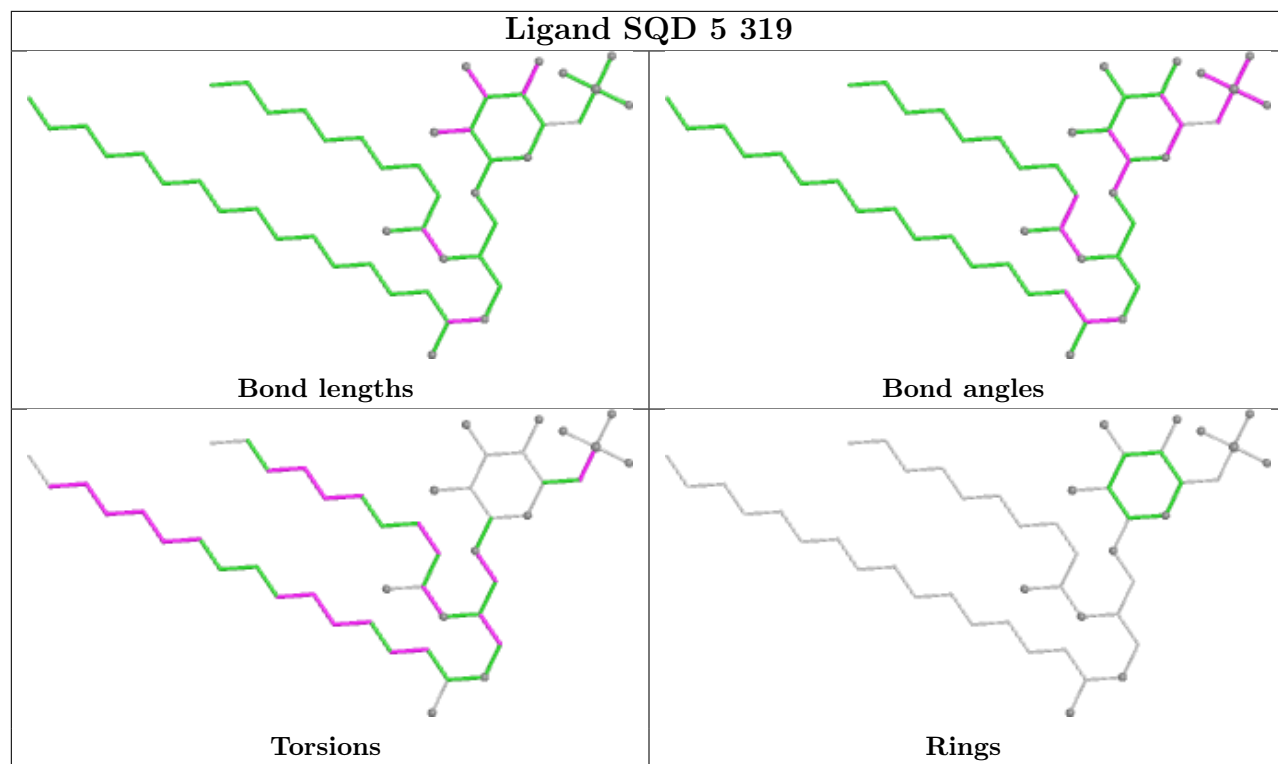
Bond angles



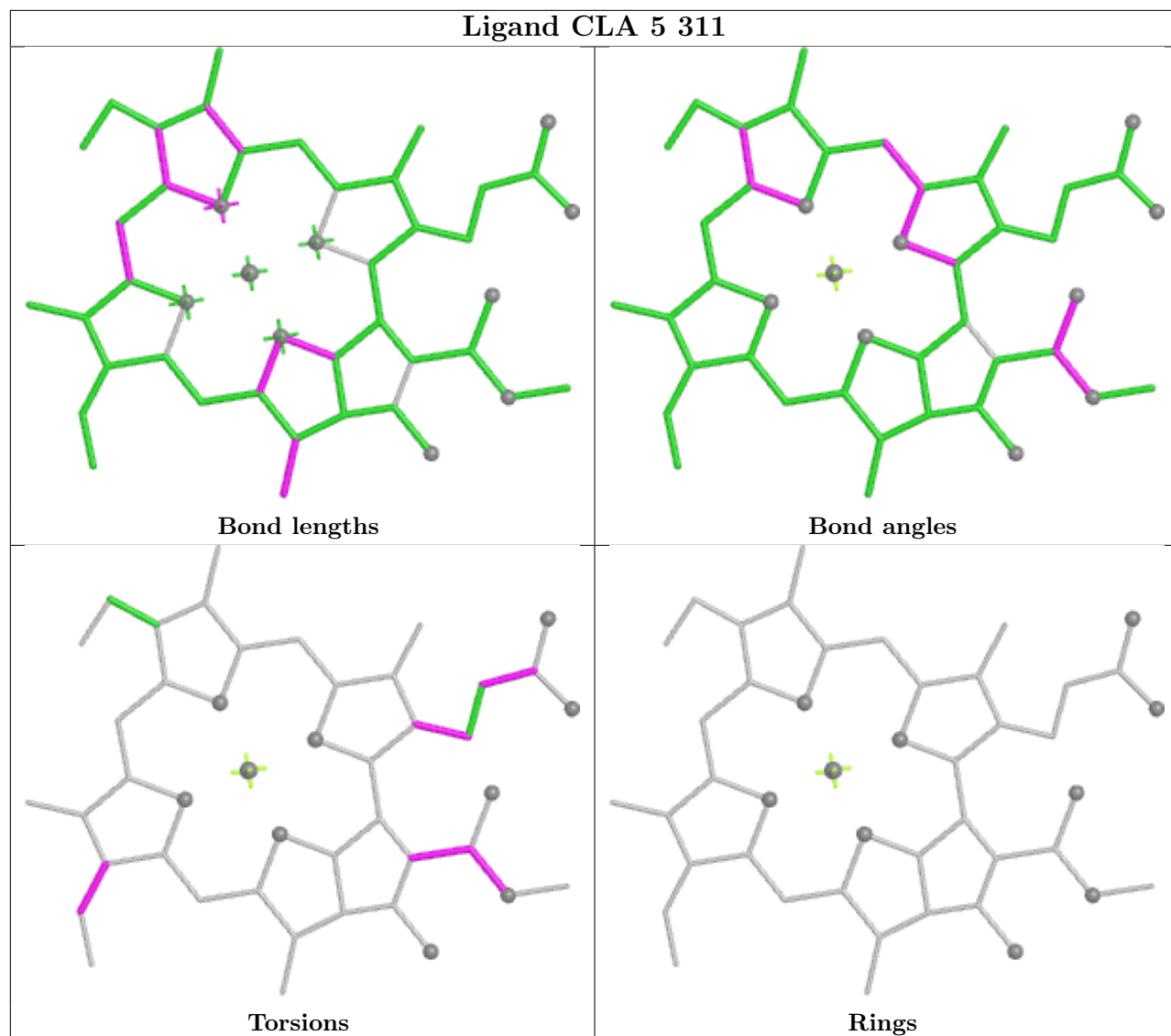
Torsions



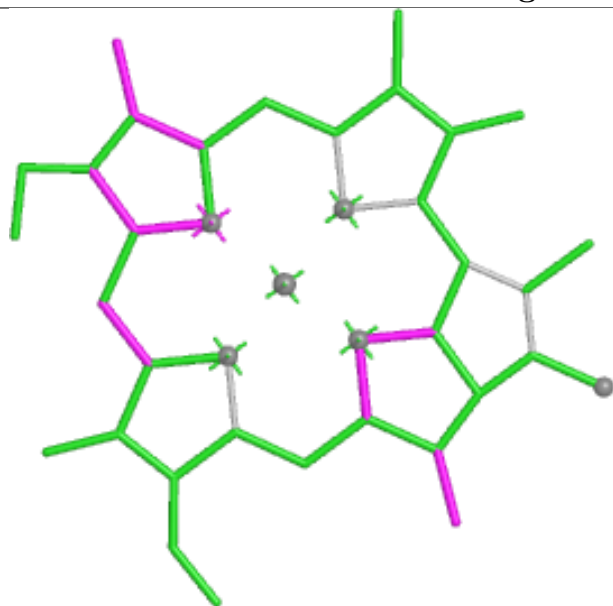
Rings



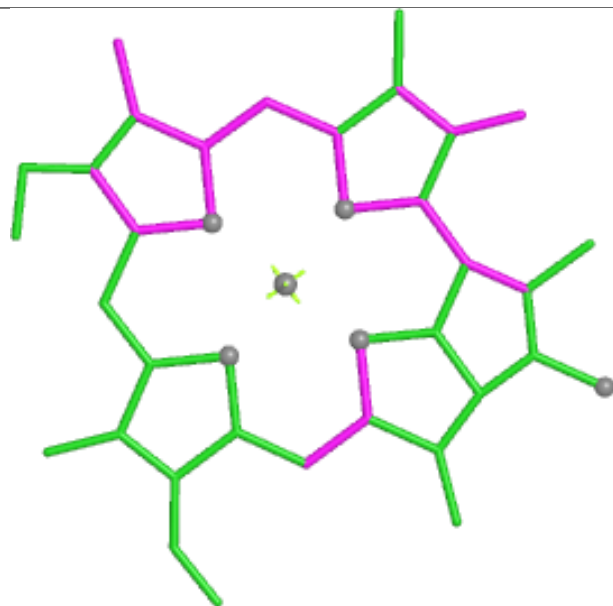
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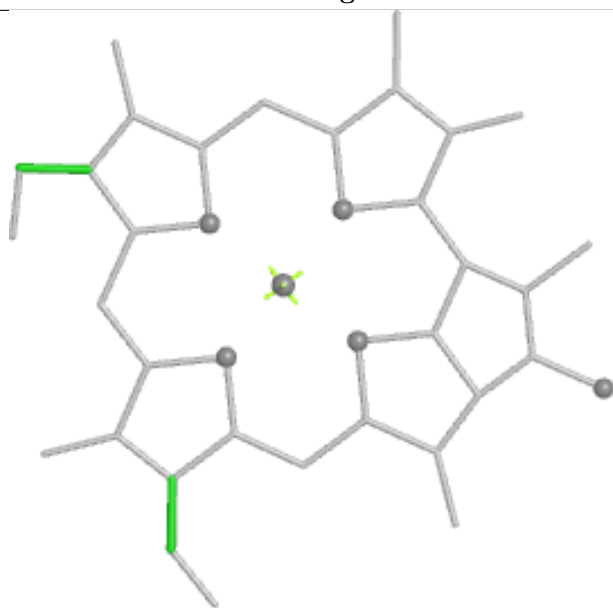
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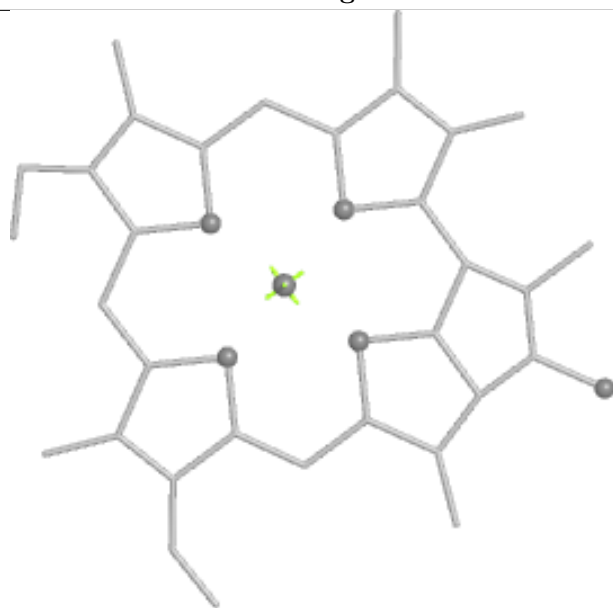
Bond lengths



Bond angles

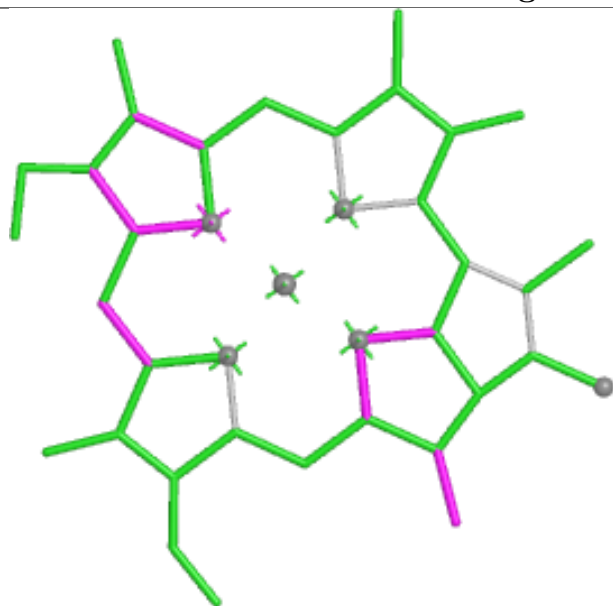


Torsions

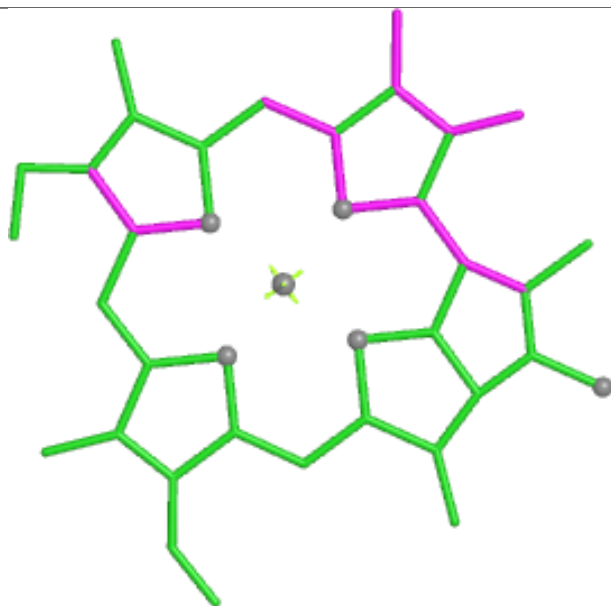


Rings

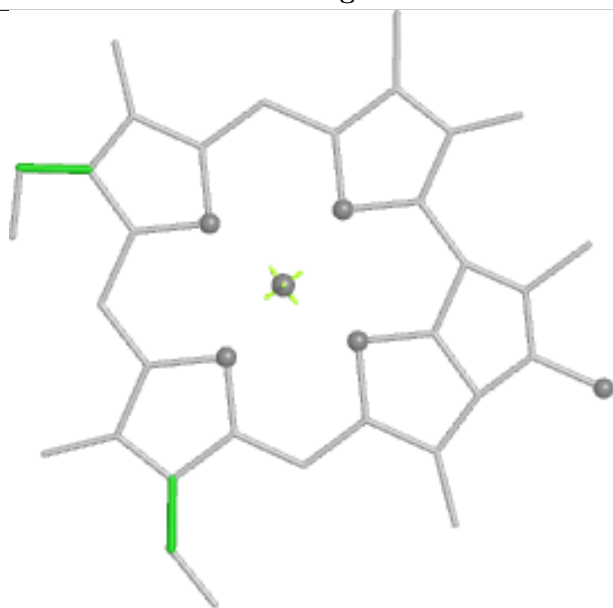
Ligand CLA 6 214



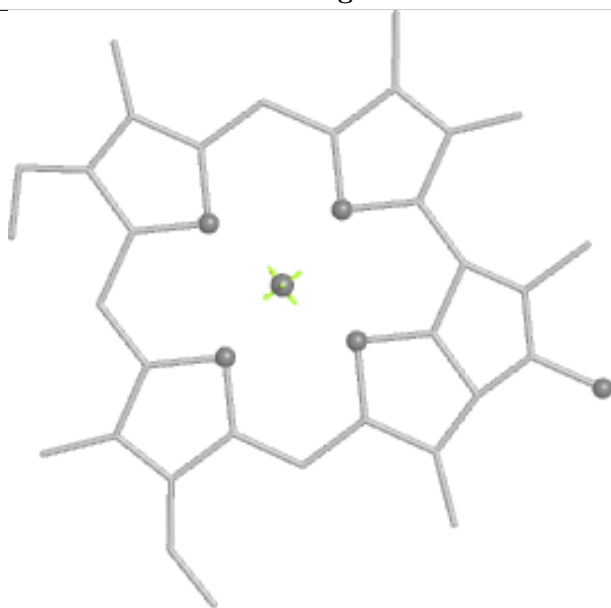
Bond lengths



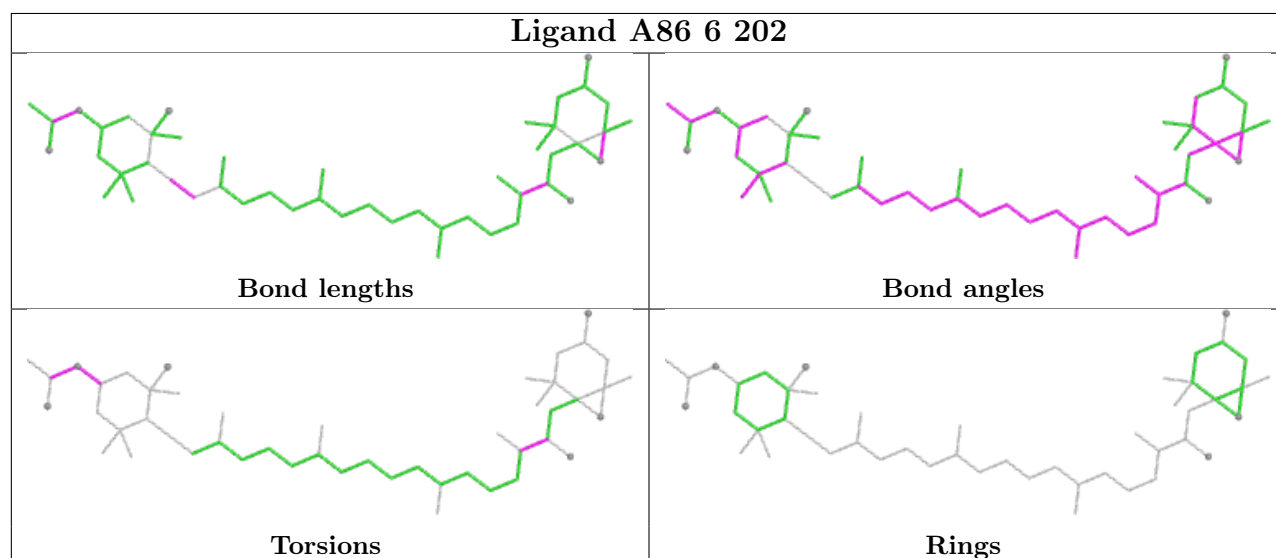
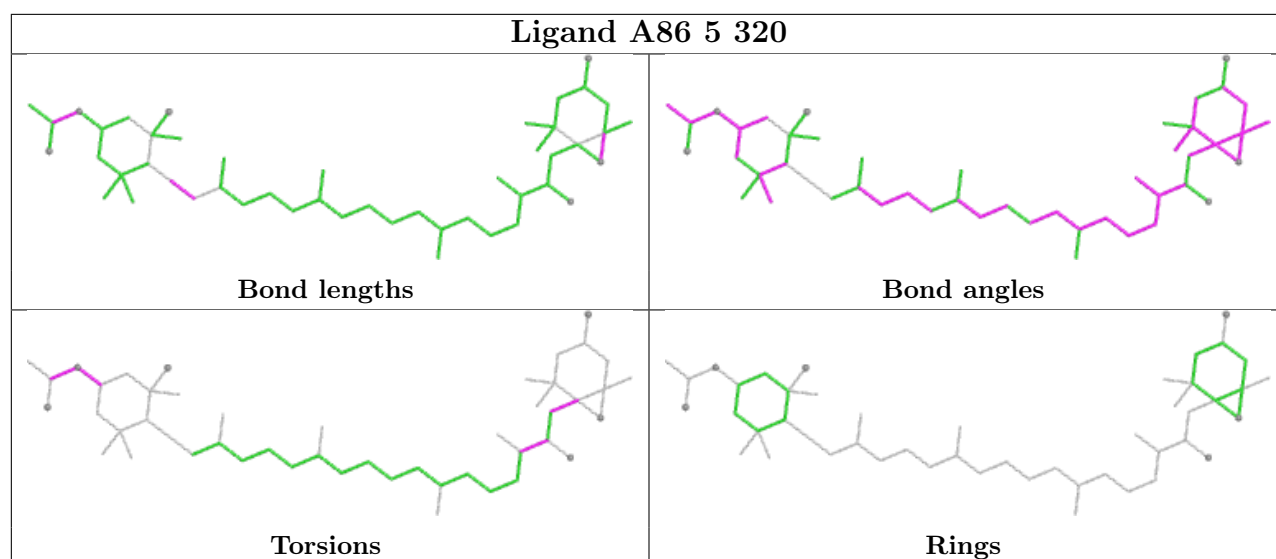
Bond angles



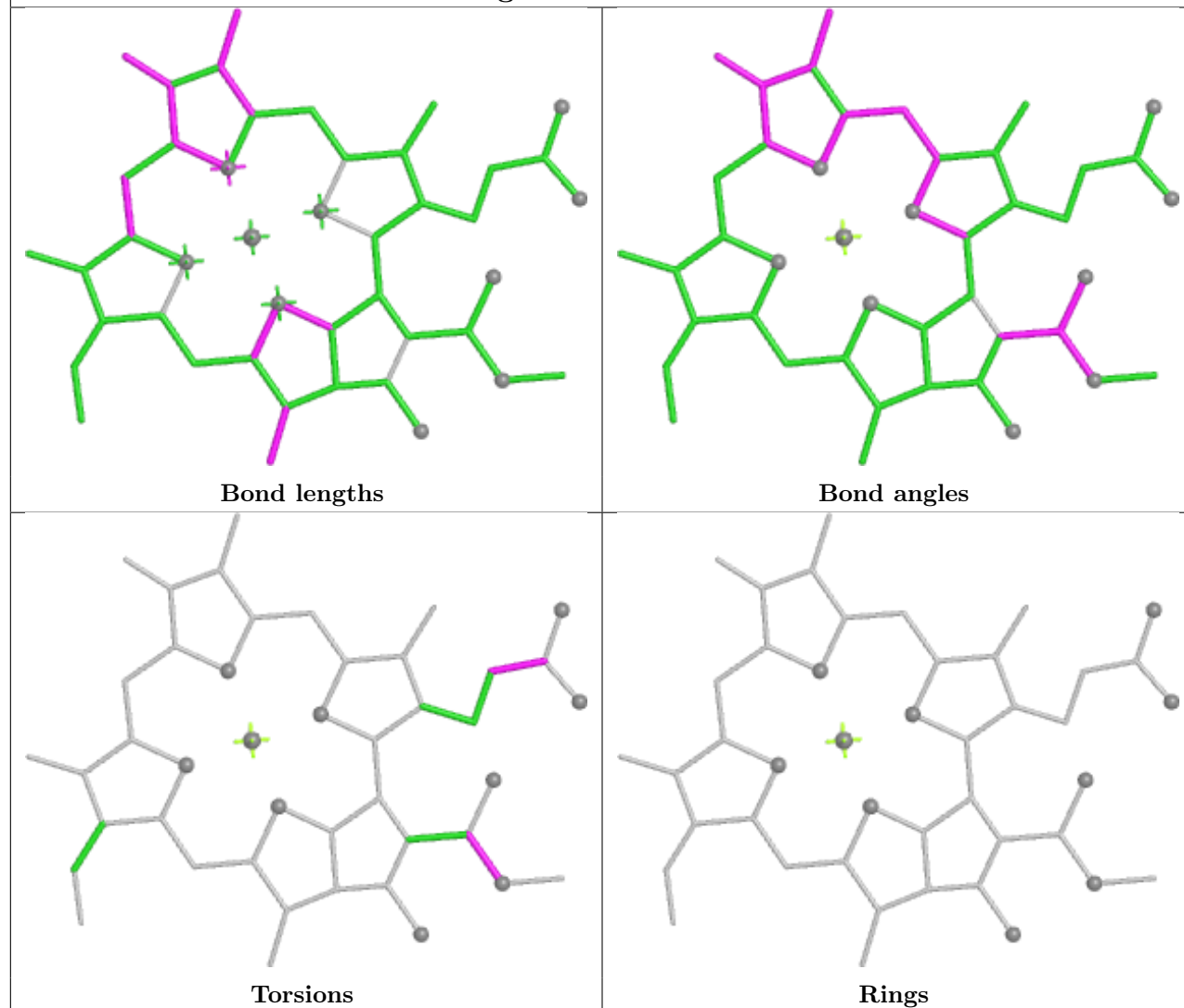
Torsions



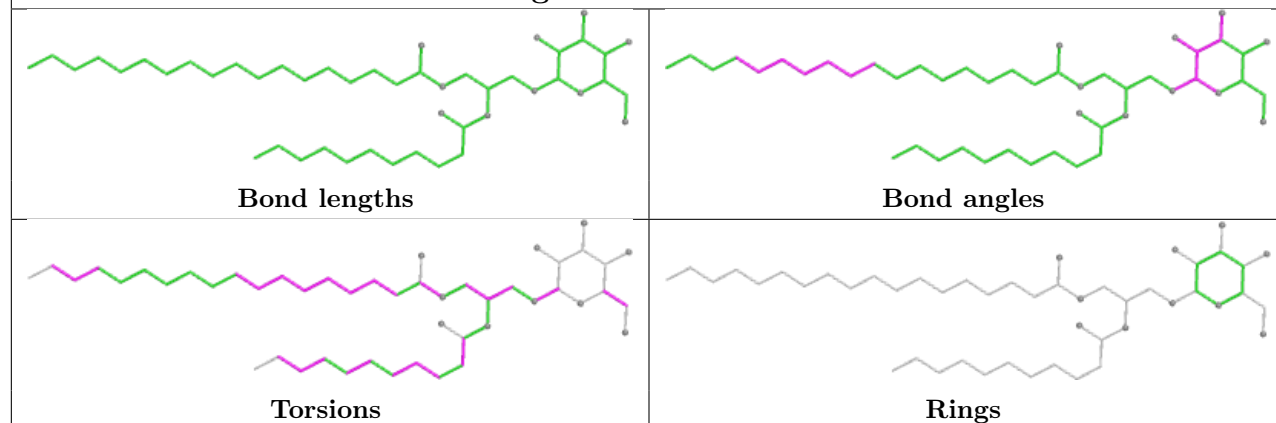
Rings



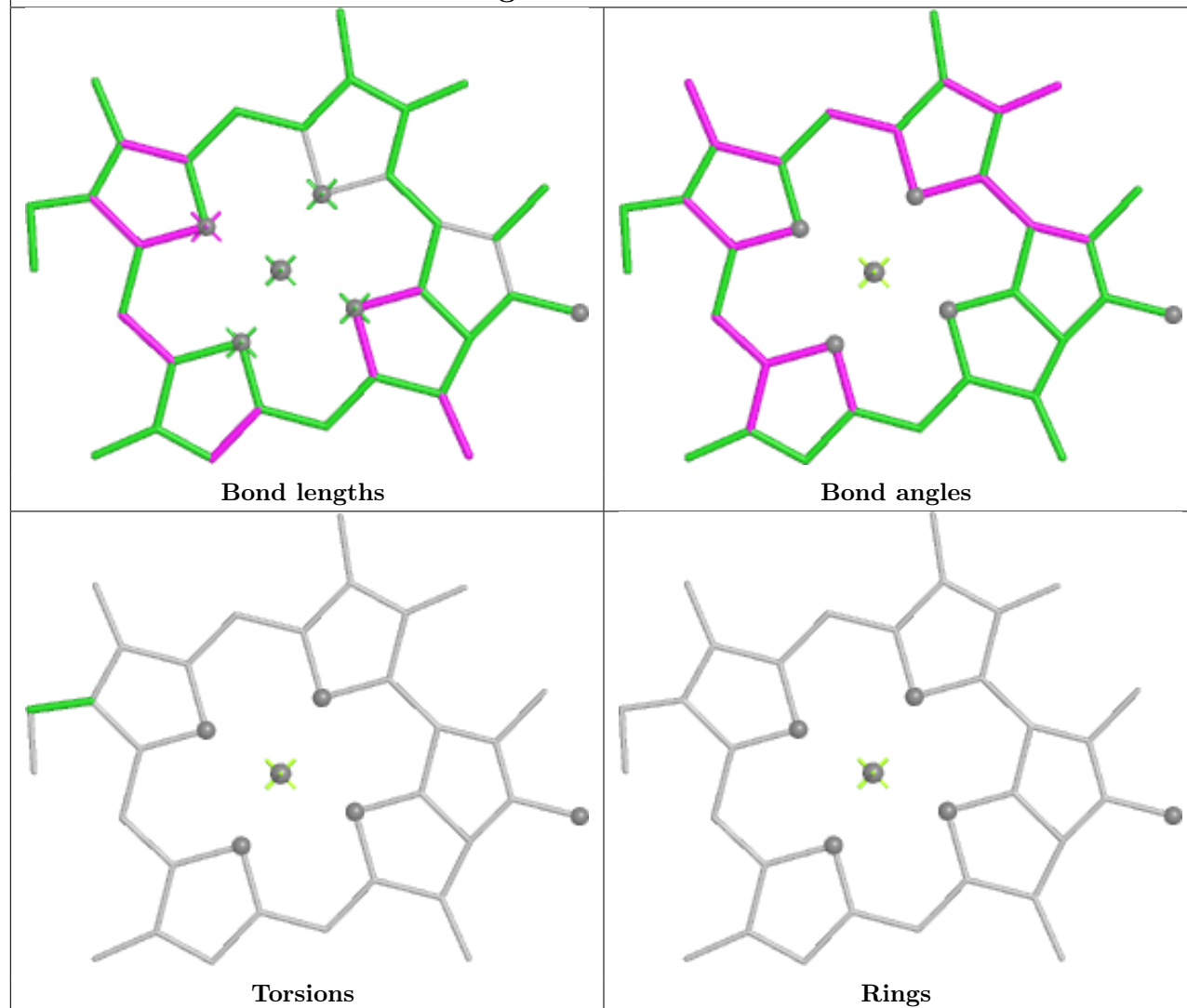
Ligand CLA 6 201



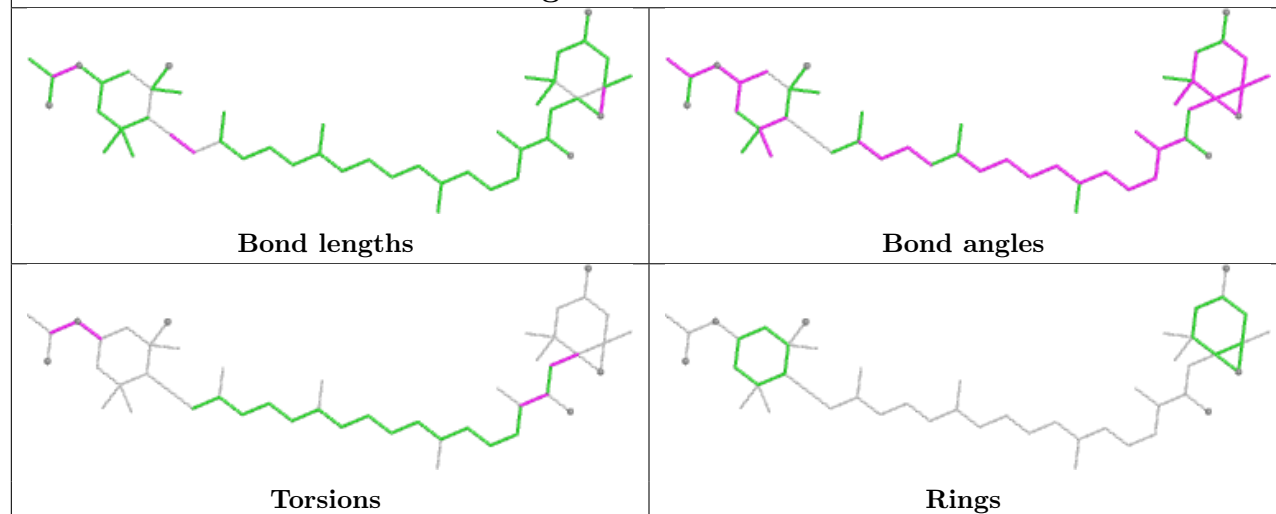
Ligand LMG 5 316



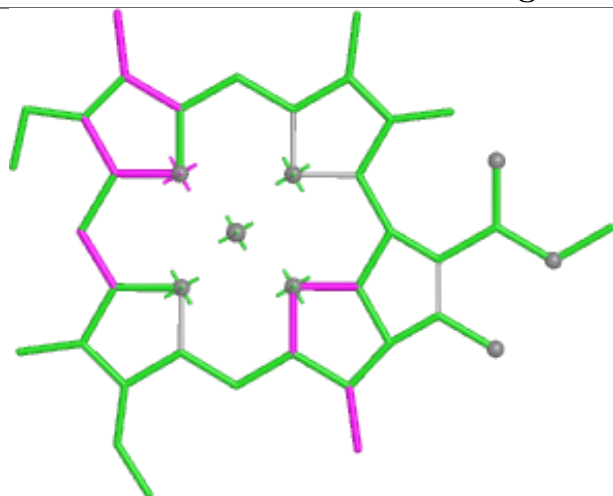
Ligand CLA 7 312



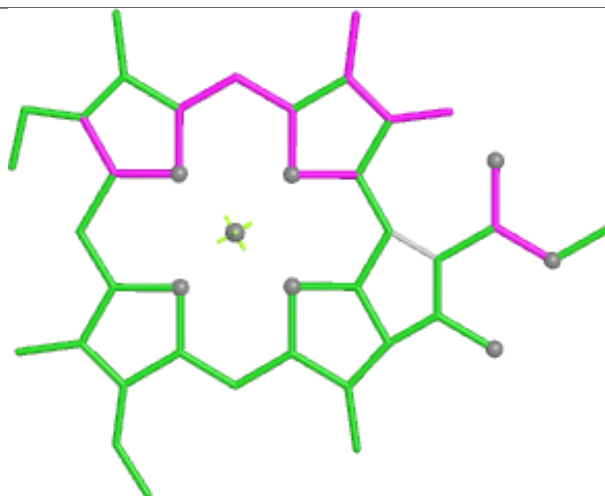
Ligand A86 7 301



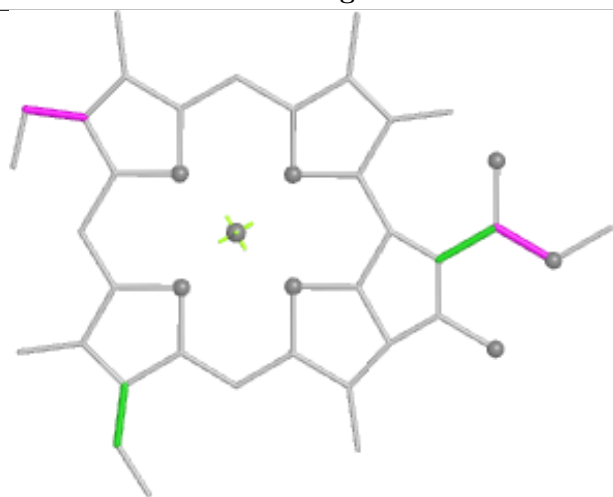
Ligand CLA 5 309



Bond lengths



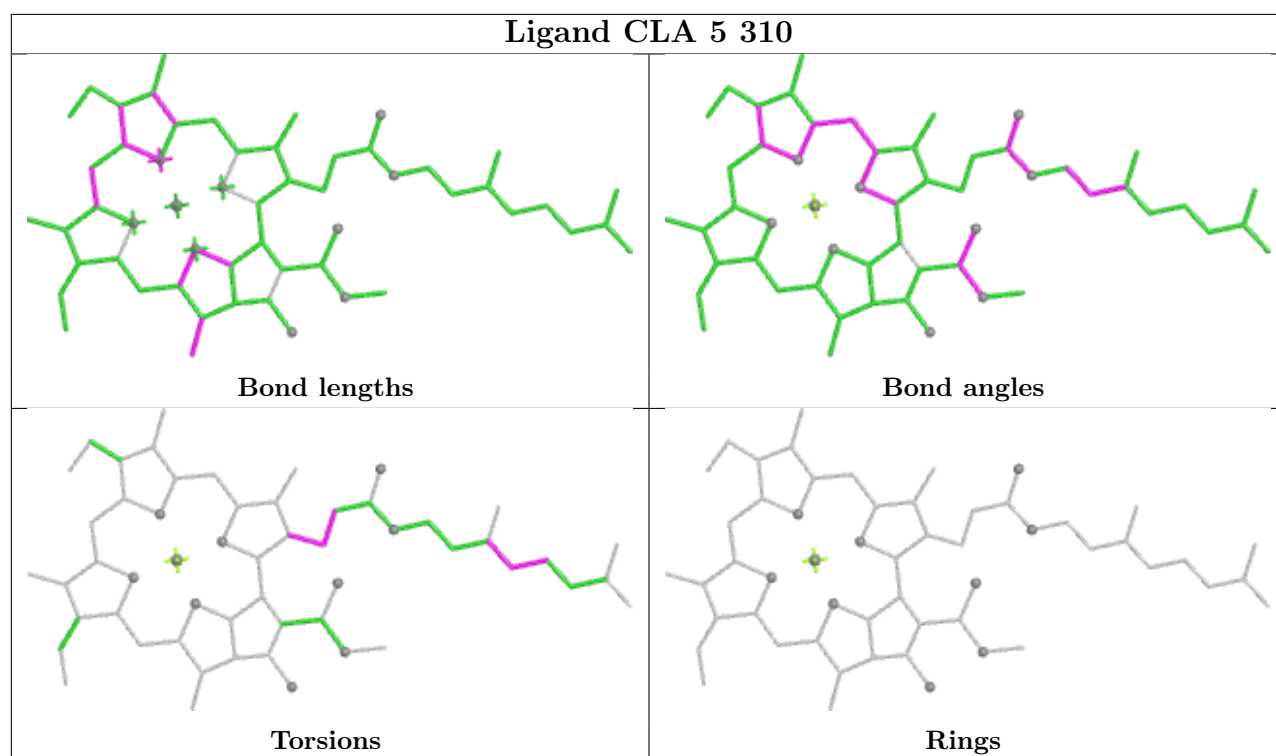
Bond angles



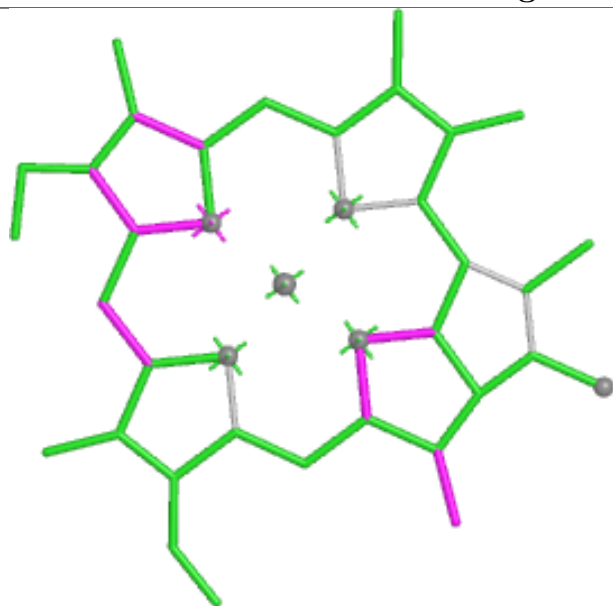
Torsions



Rings



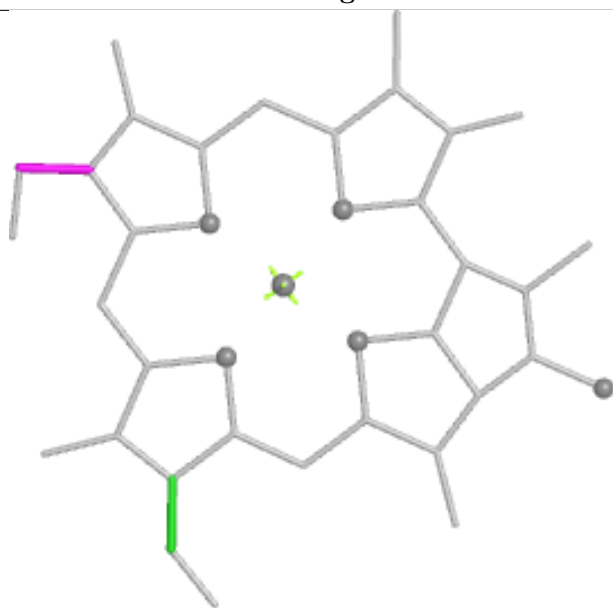
Ligand CLA 5 313



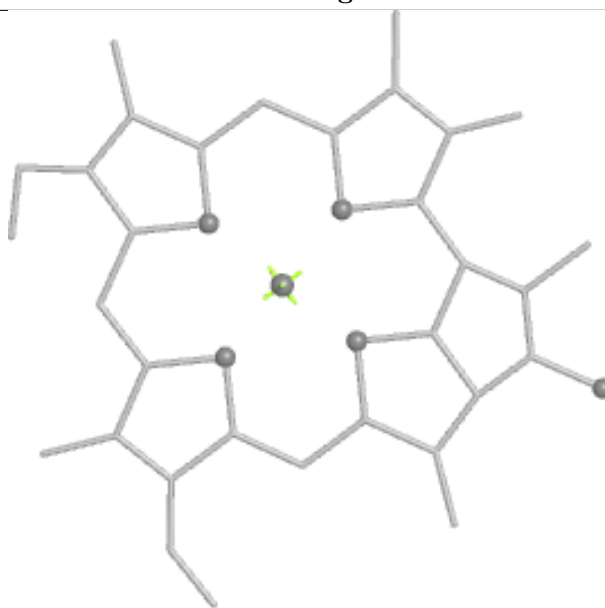
Bond lengths



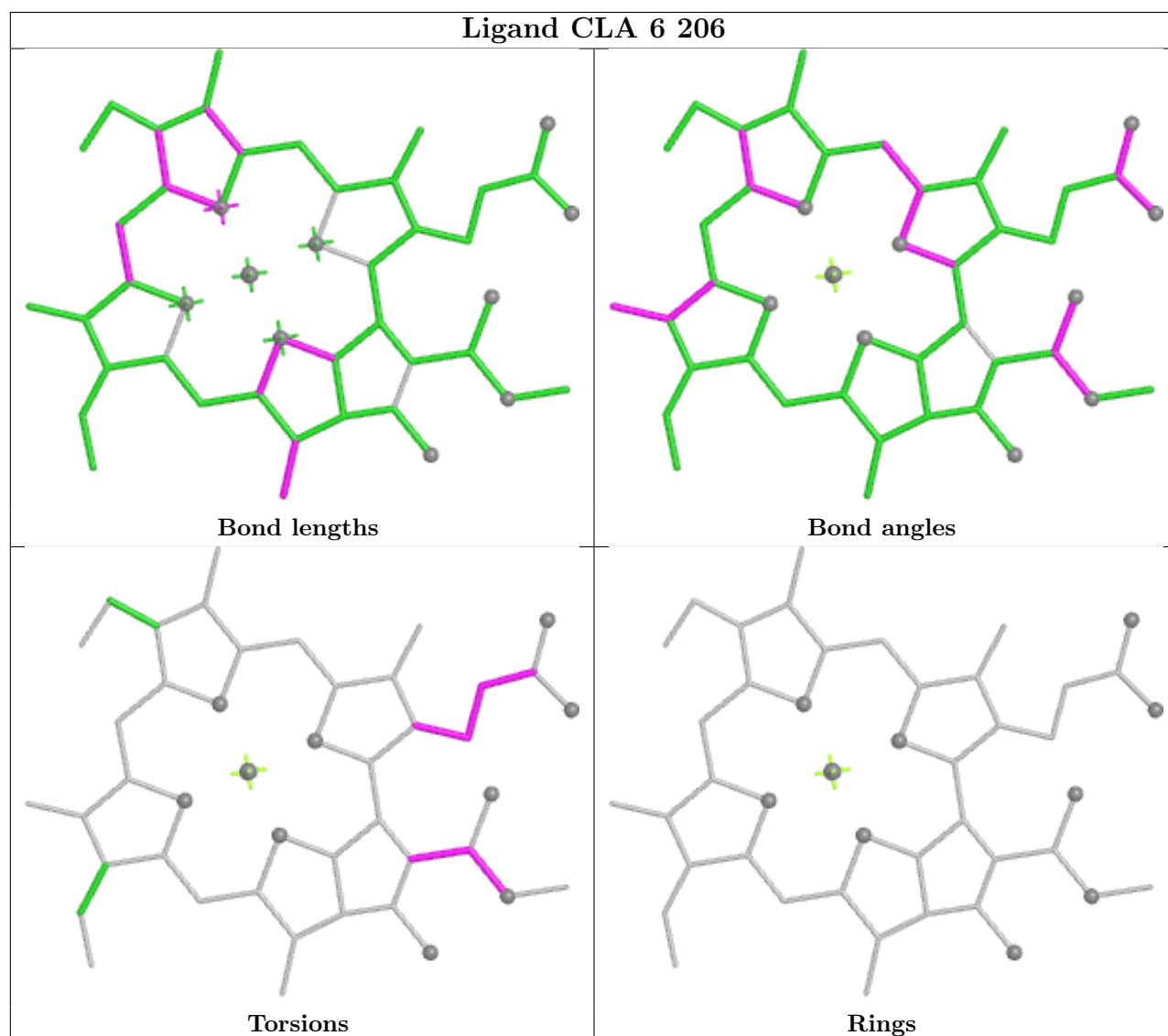
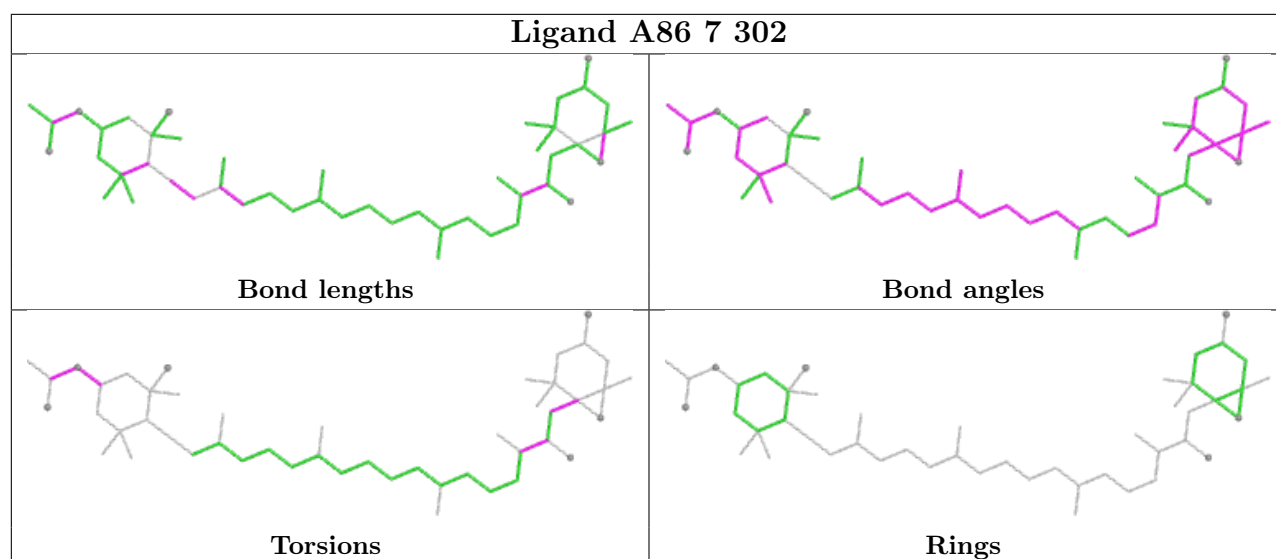
Bond angles



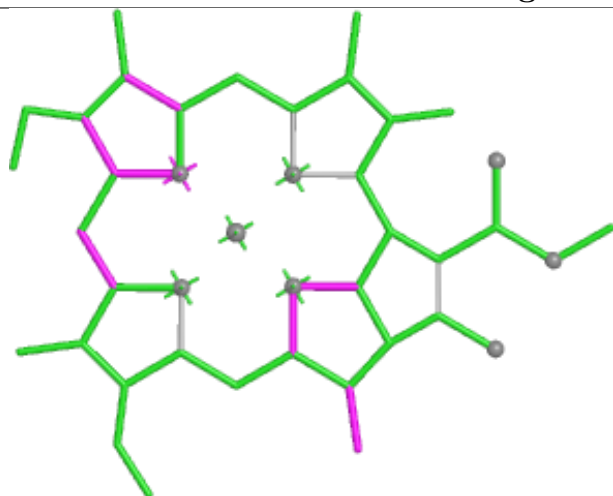
Torsions



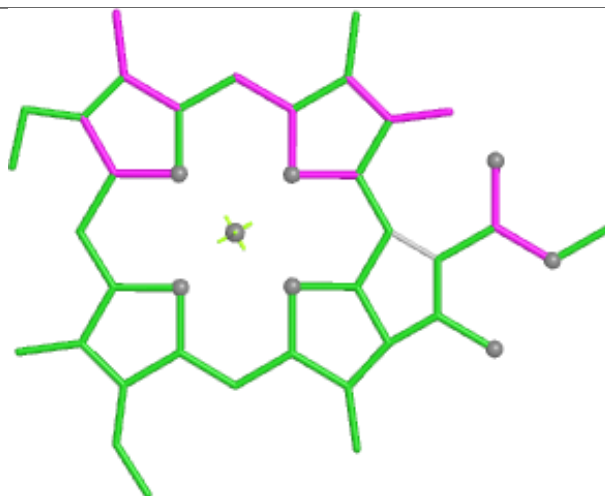
Rings



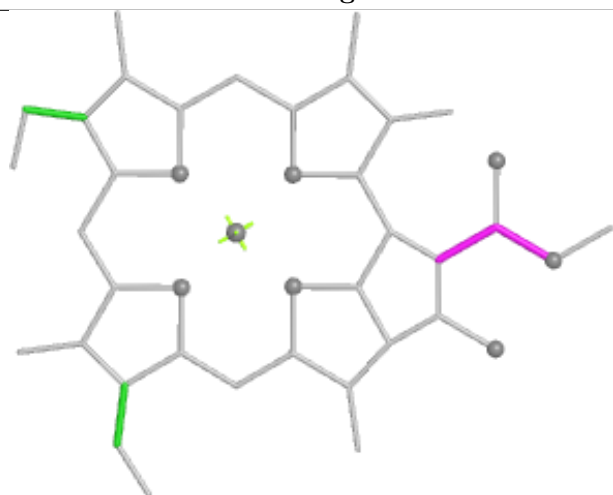
Ligand CLA 6 212



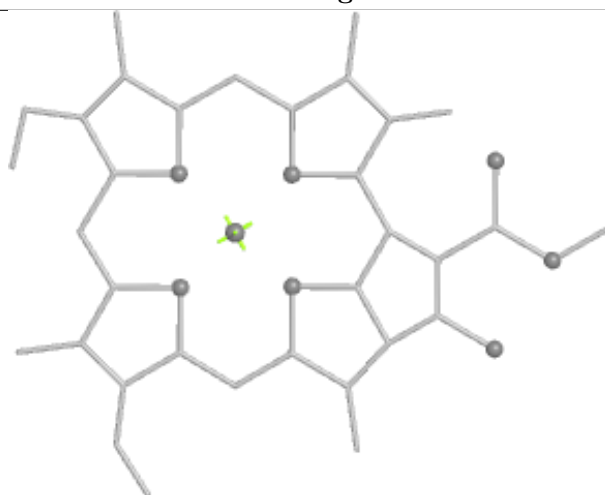
Bond lengths



Bond angles

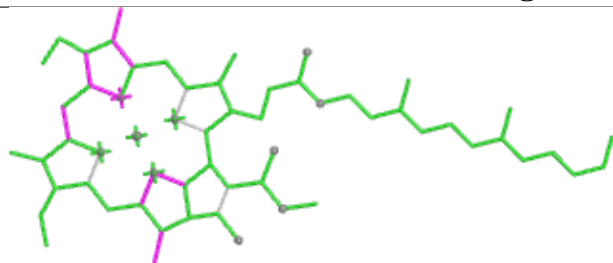


Torsions

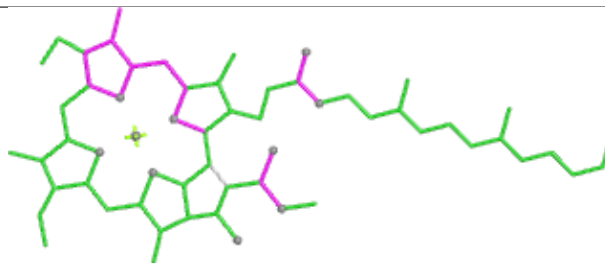


Rings

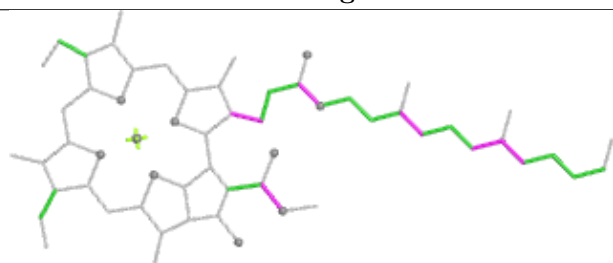
Ligand CLA 7 309



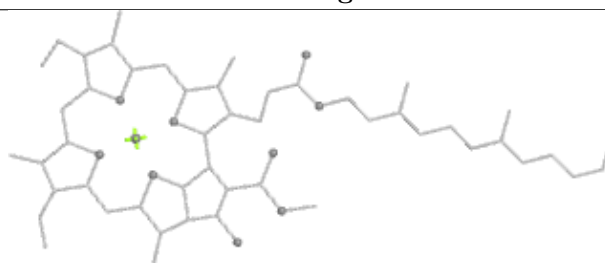
Bond lengths



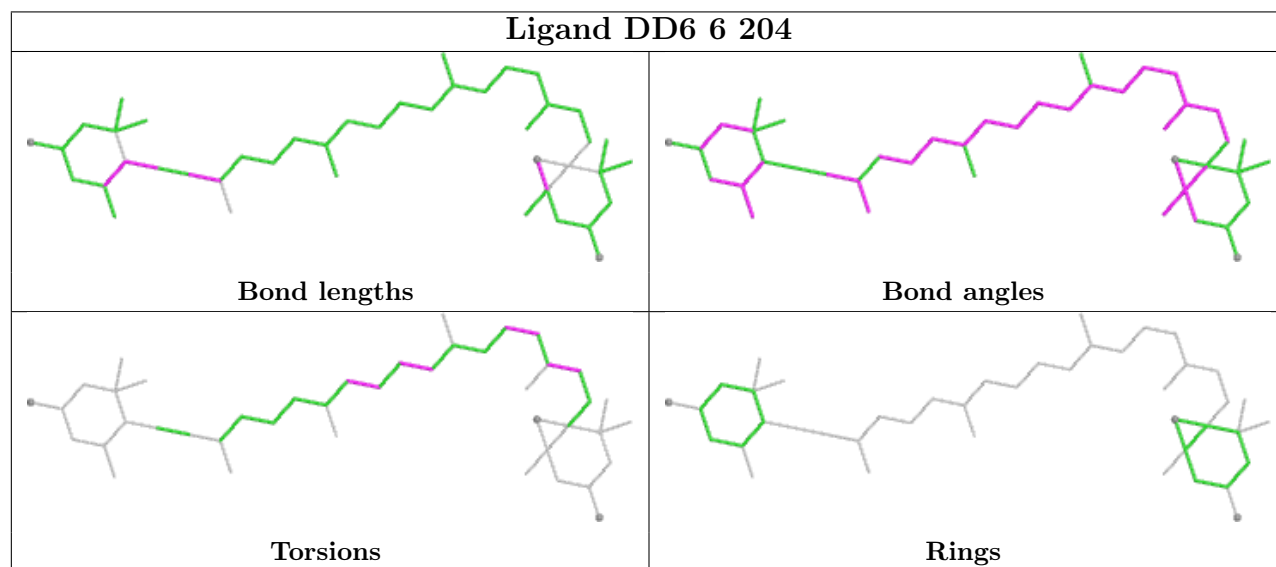
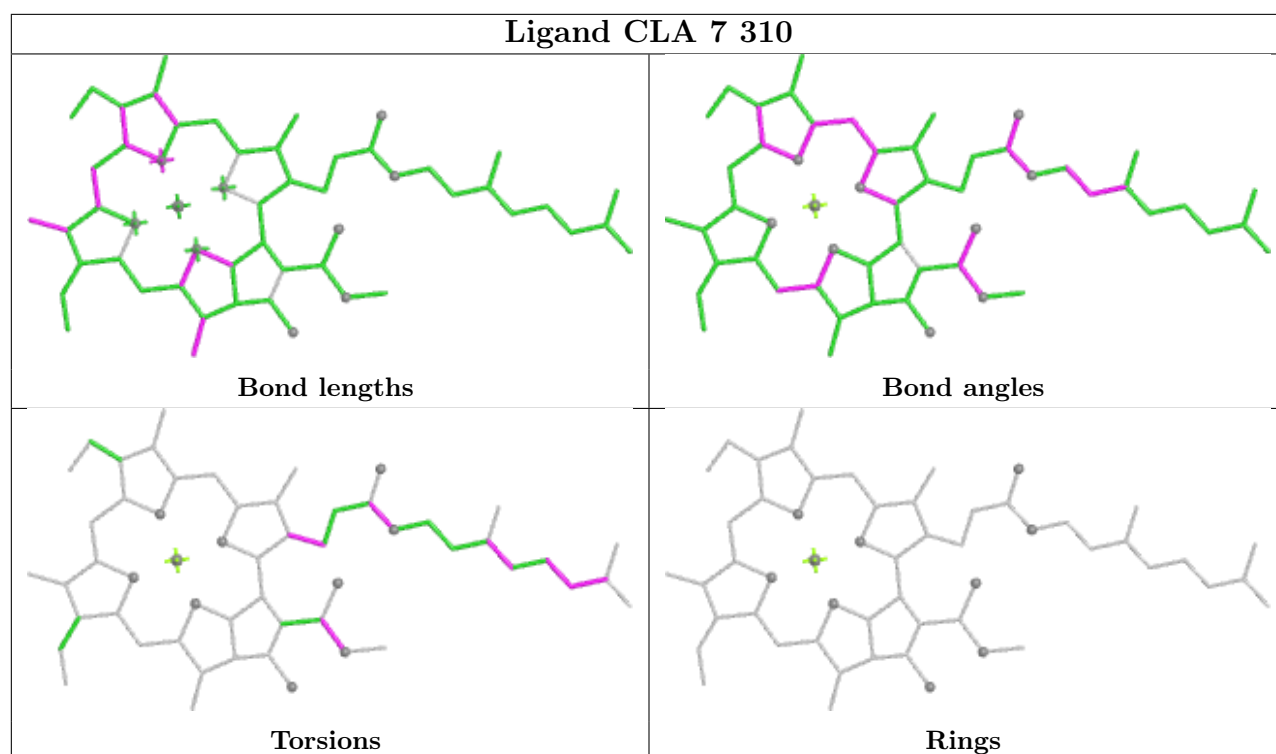
Bond angles



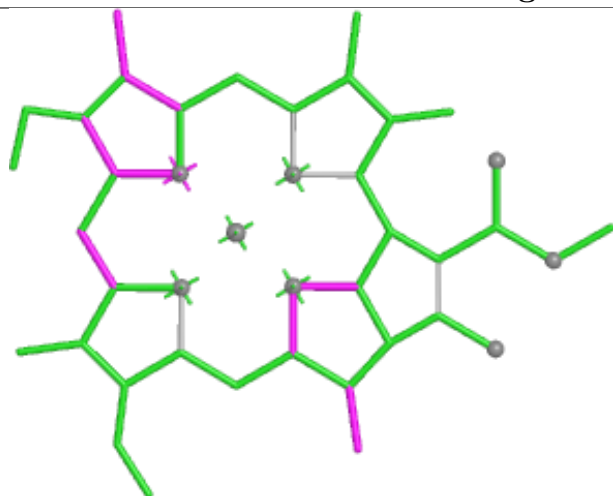
Torsions



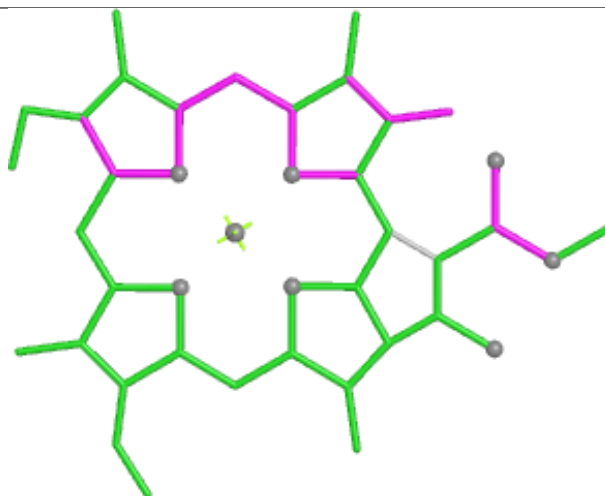
Rings



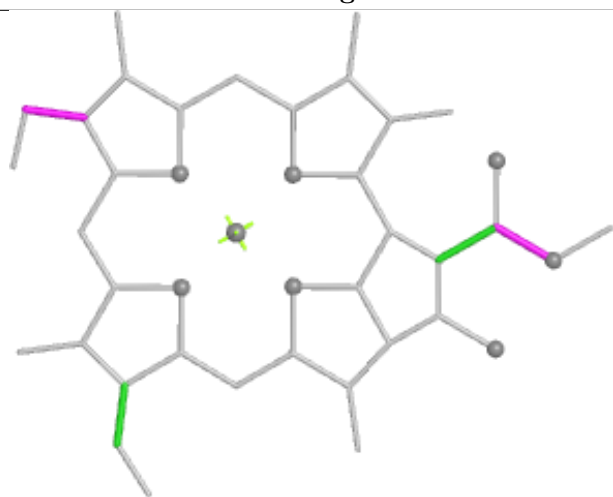
Ligand CLA 5 304



Bond lengths



Bond angles

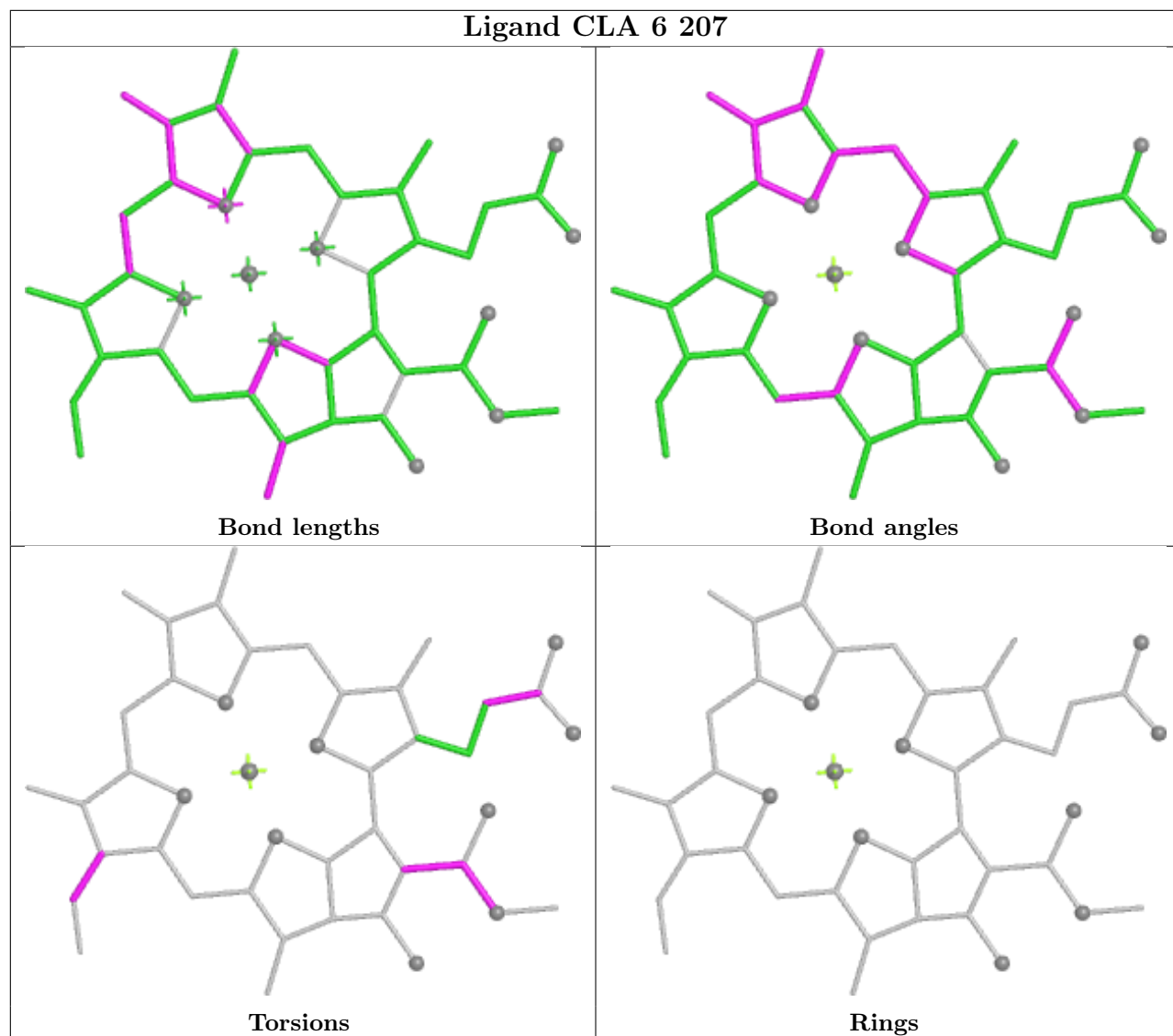


Torsions

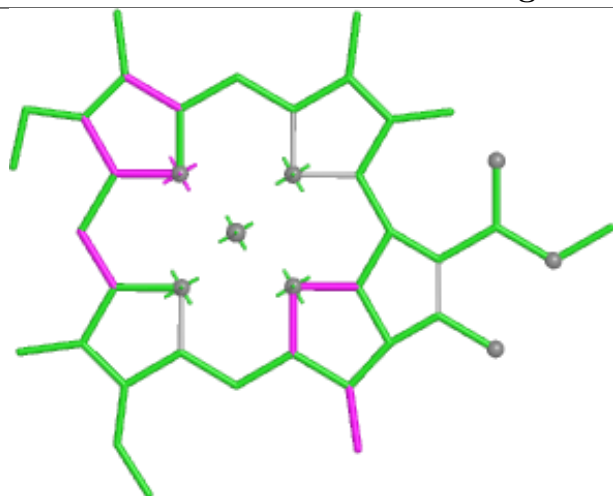


Rings

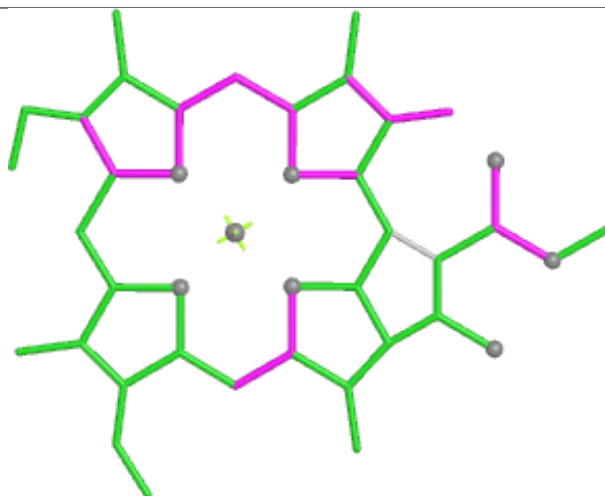
Ligand CLA 6 207



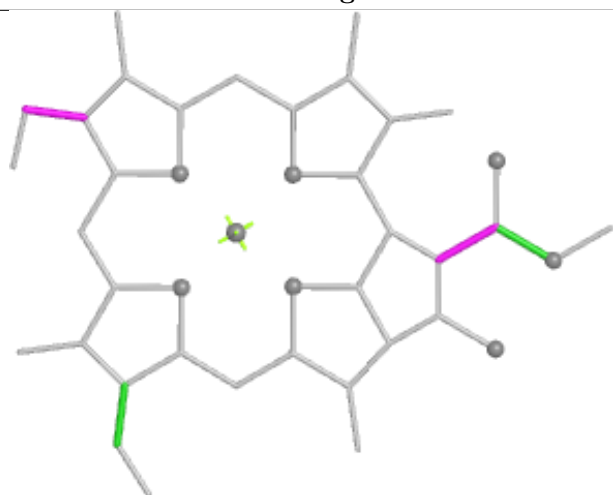
Ligand CLA 6 205



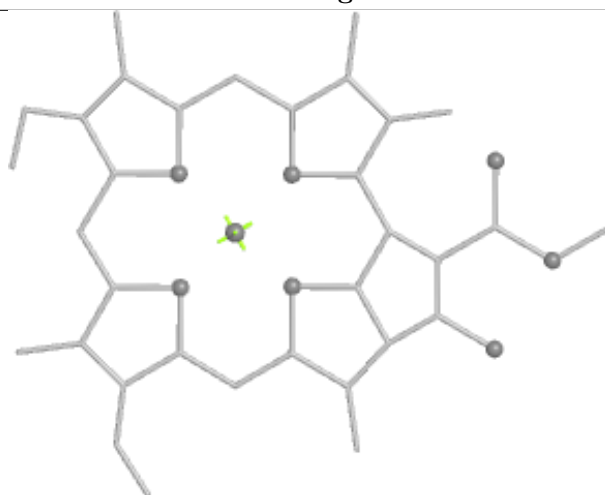
Bond lengths



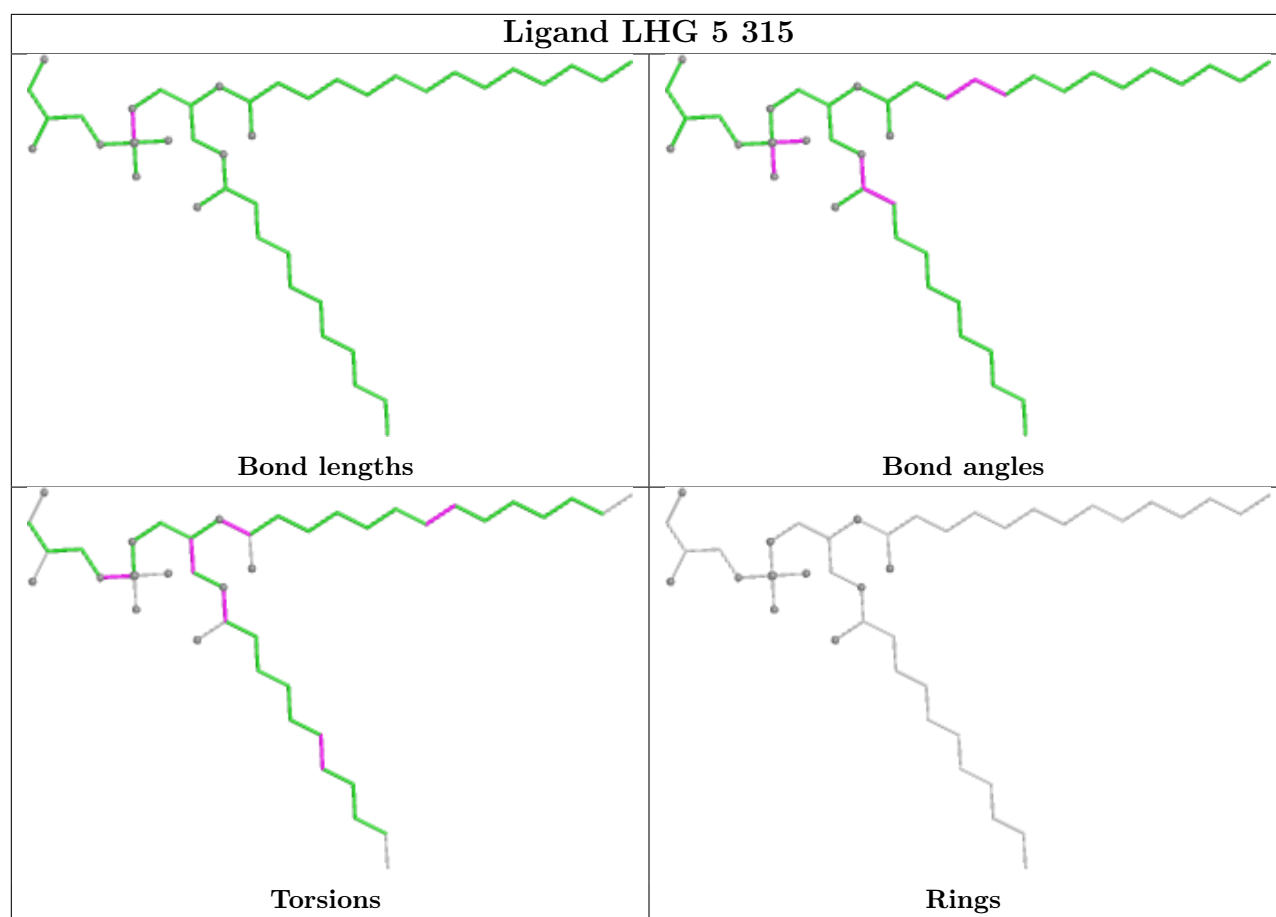
Bond angles



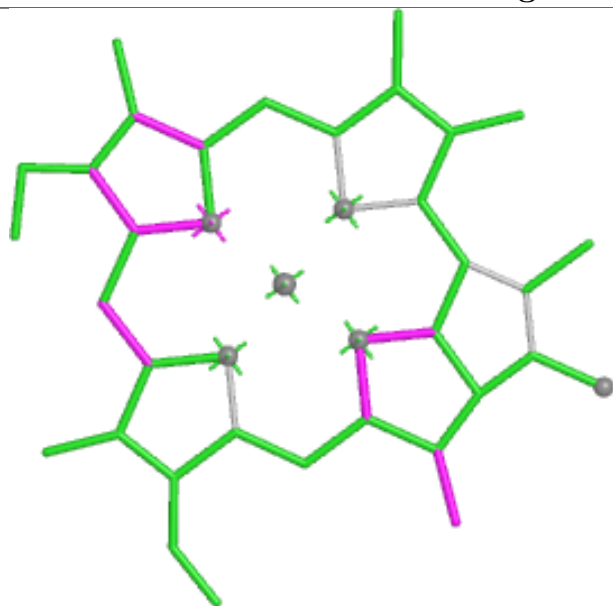
Torsions



Rings



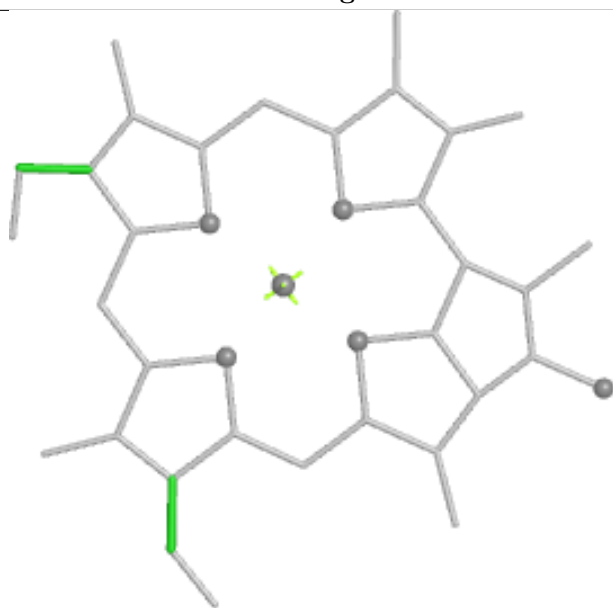
Ligand CLA 5 314



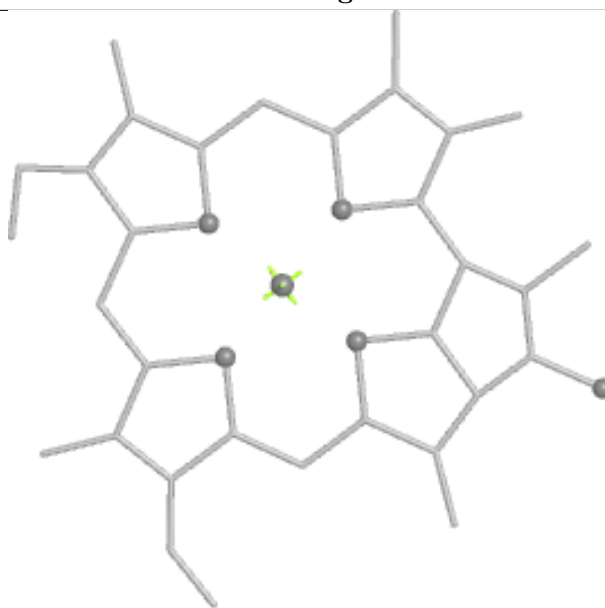
Bond lengths



Bond angles

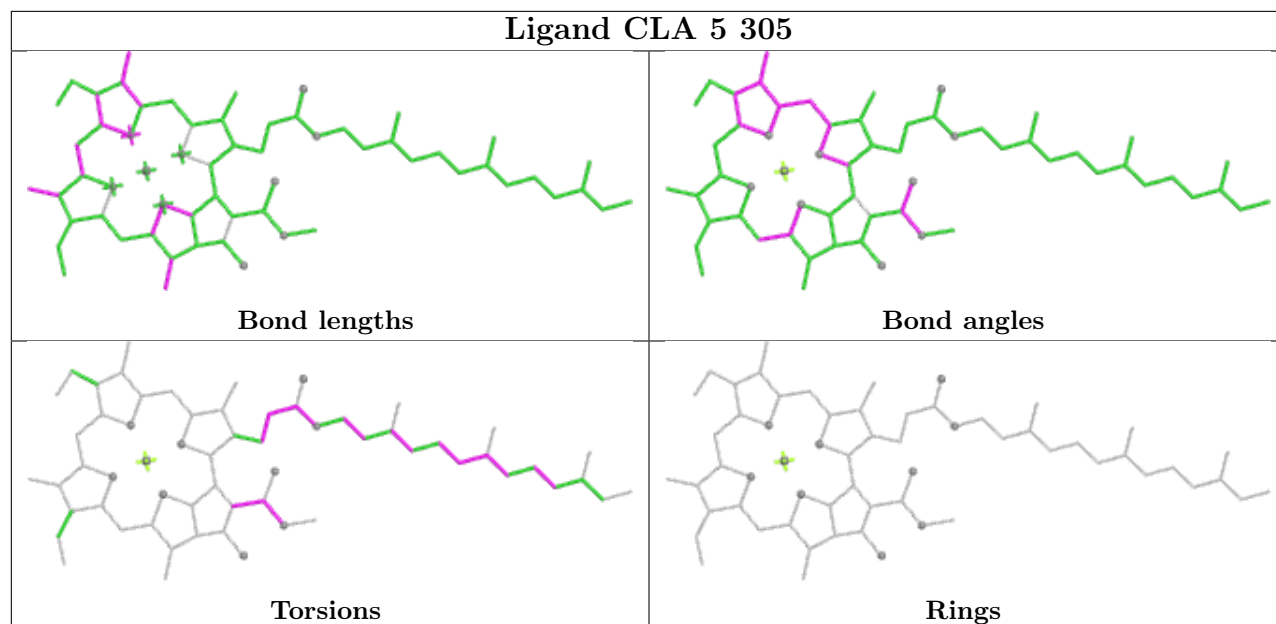


Torsions

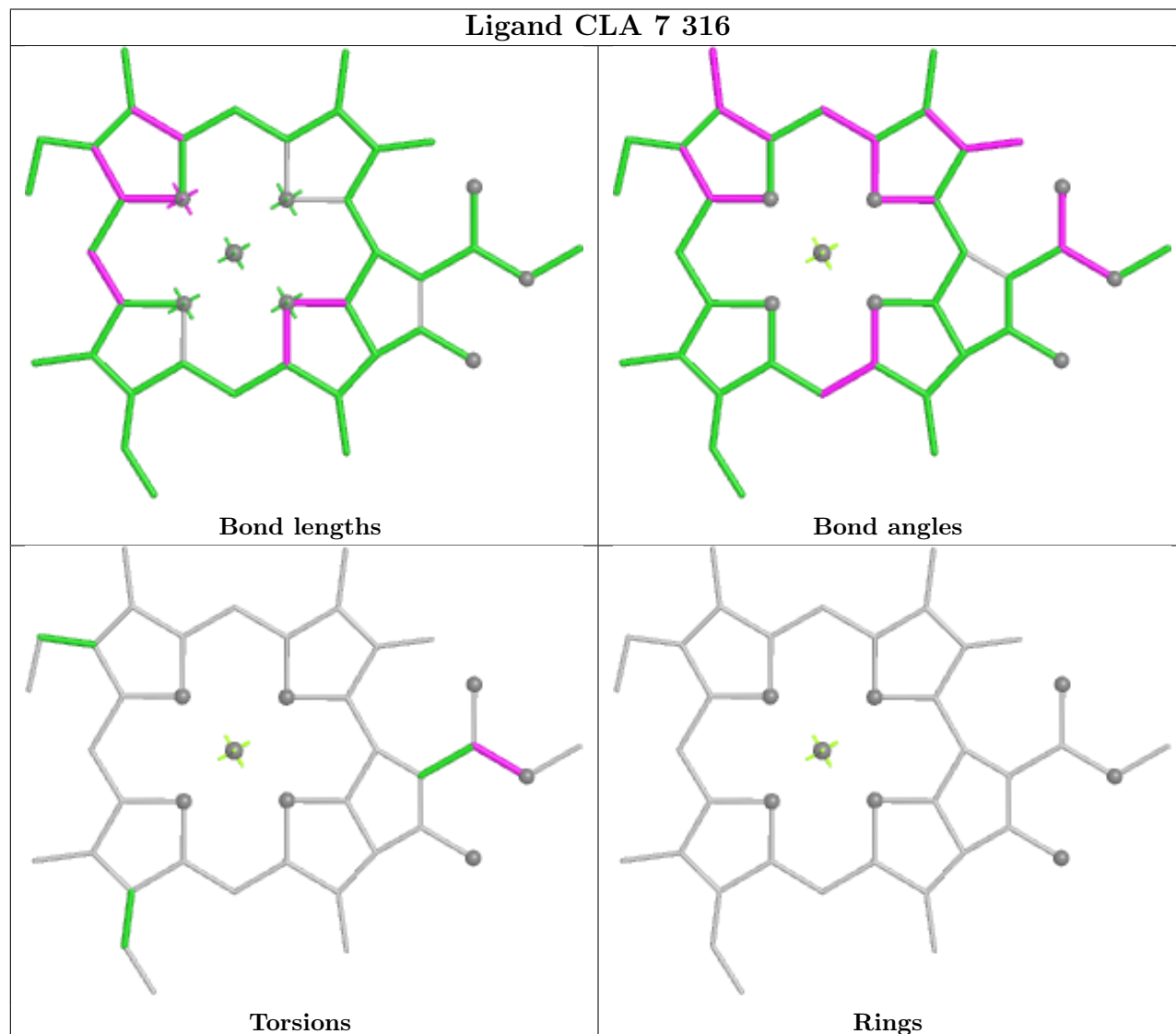


Rings

Ligand CLA 5 305



Ligand CLA 7 316



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

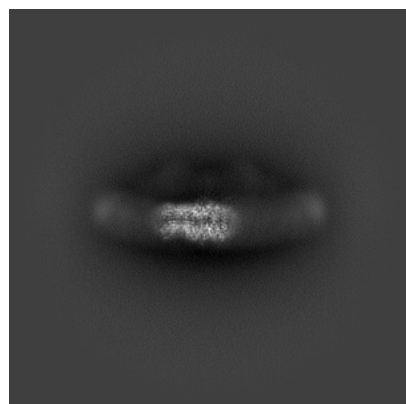
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37267. These allow visual inspection of the internal detail of the map and identification of artifacts.

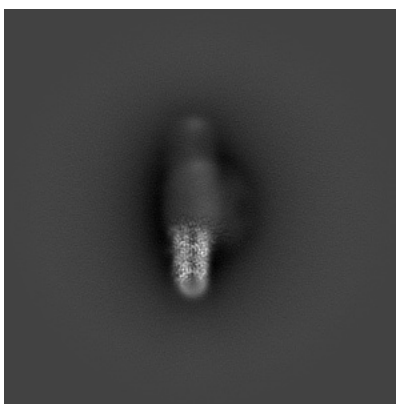
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

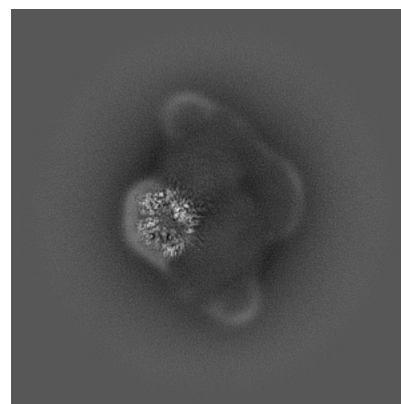
6.1.1 Primary map



X

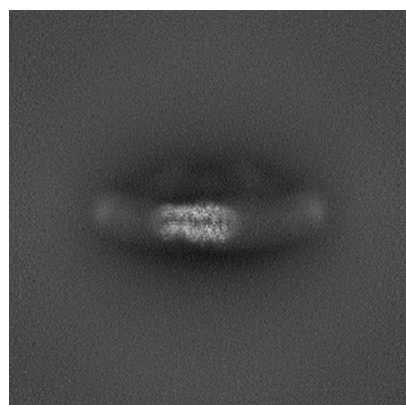


Y

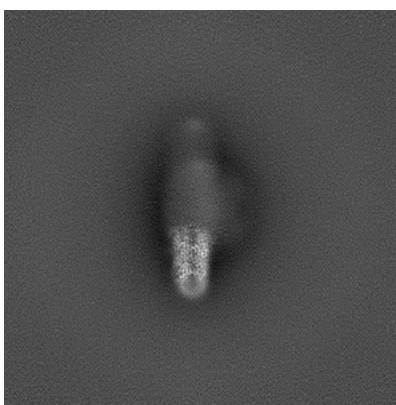


Z

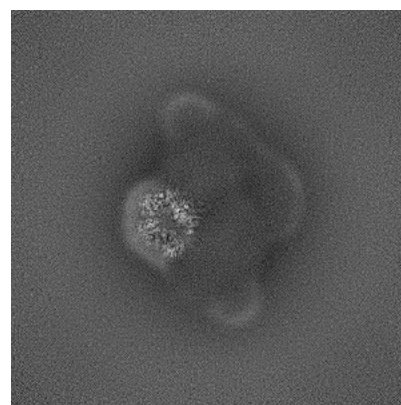
6.1.2 Raw map



X



Y

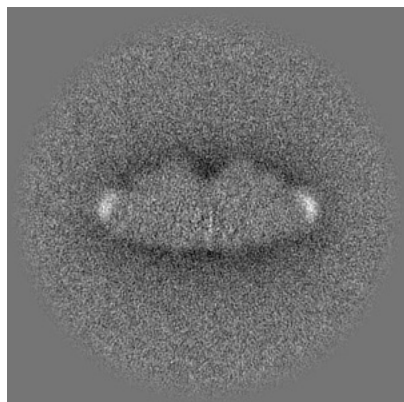


Z

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

6.2 Central slices [i](#)

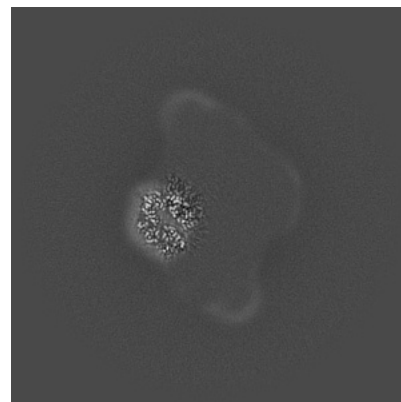
6.2.1 Primary map



X Index: 256

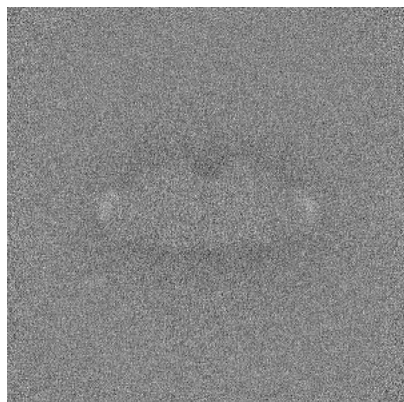


Y Index: 256



Z Index: 256

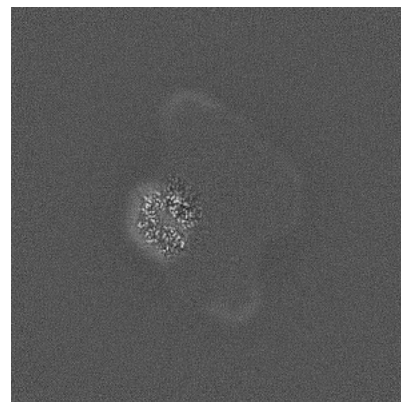
6.2.2 Raw map



X Index: 256



Y Index: 256



Z Index: 256

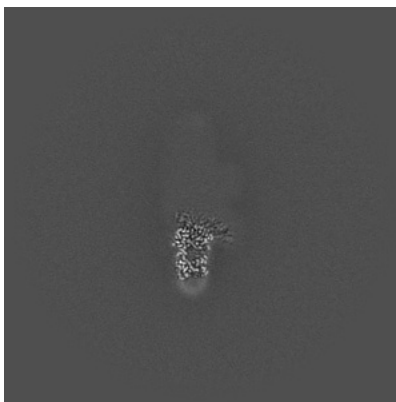
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

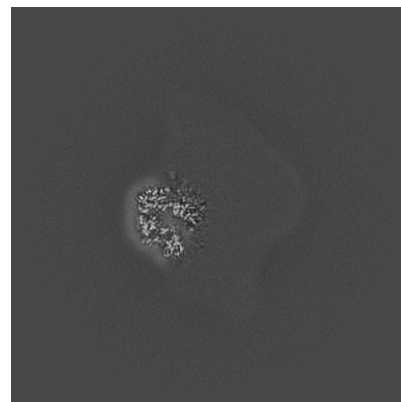
6.3.1 Primary map



X Index: 210

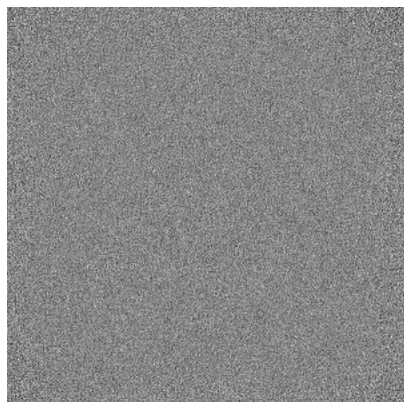


Y Index: 257

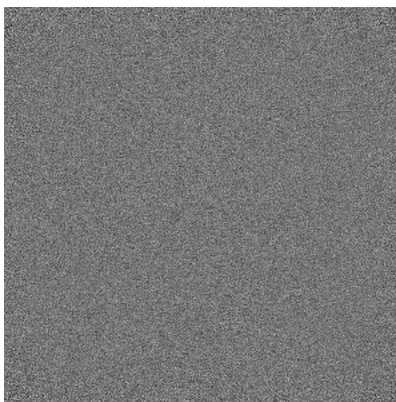


Z Index: 230

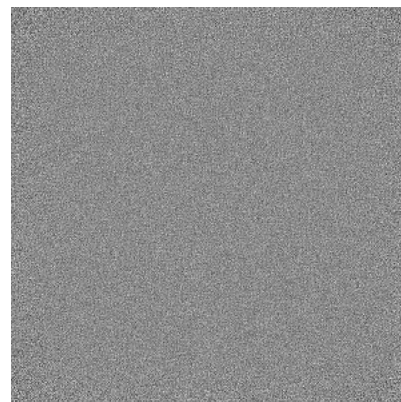
6.3.2 Raw map



X Index: 0



Y Index: 0

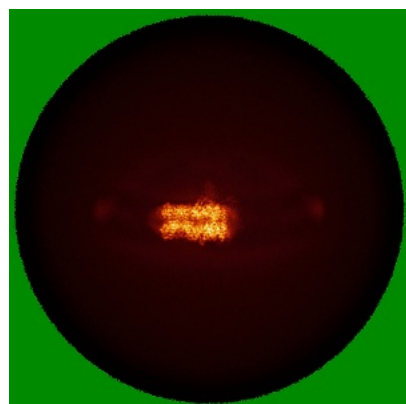


Z Index: 511

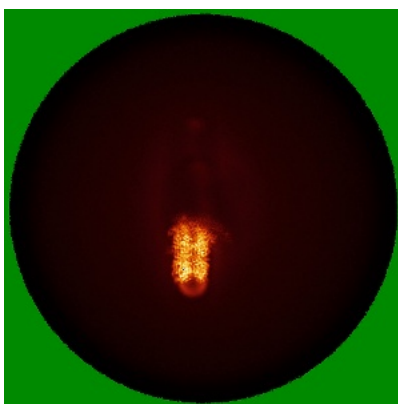
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

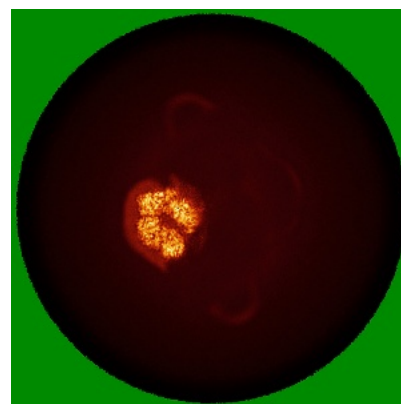
6.4.1 Primary map



X

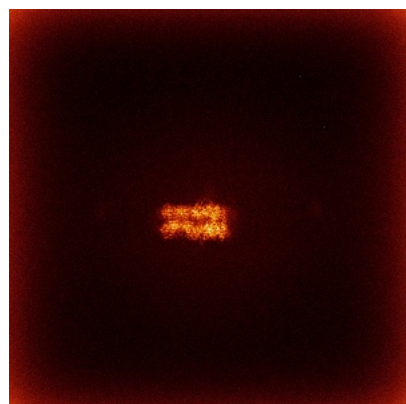


Y

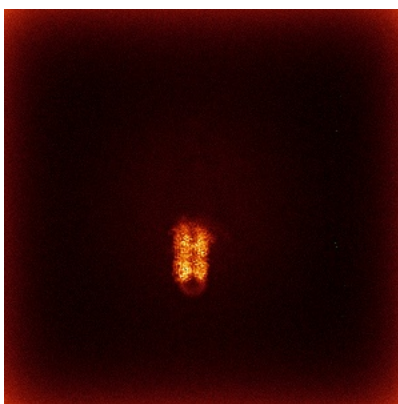


Z

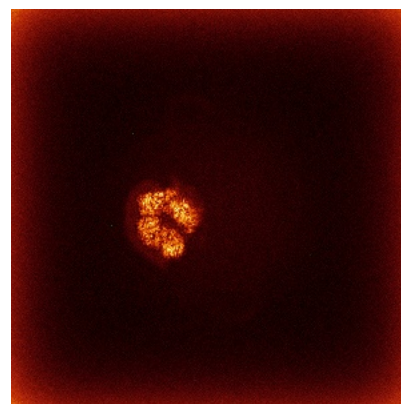
6.4.2 Raw map



X



Y

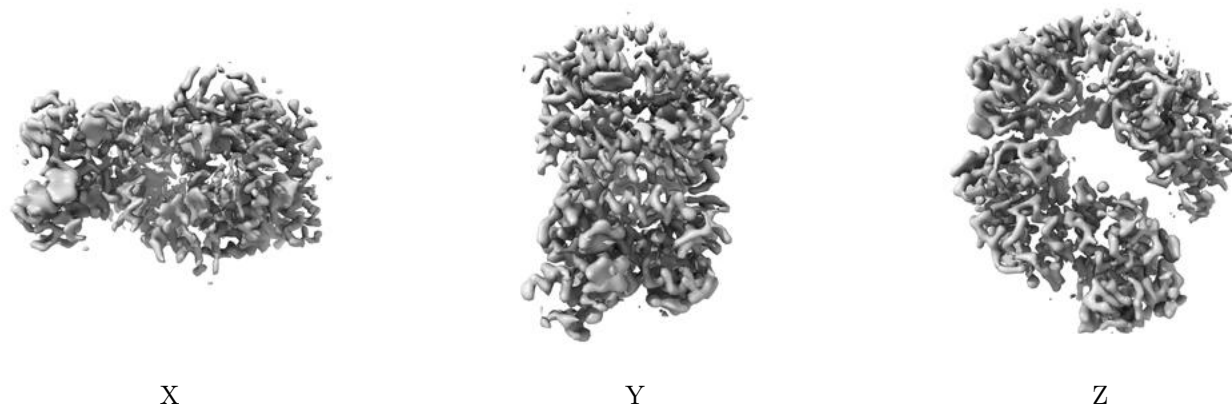


Z

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.

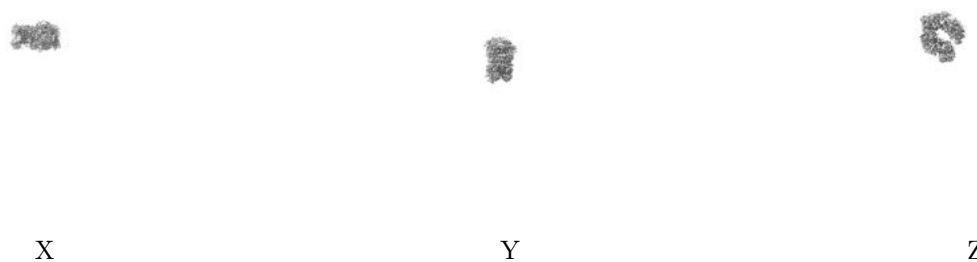
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.313. 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



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.

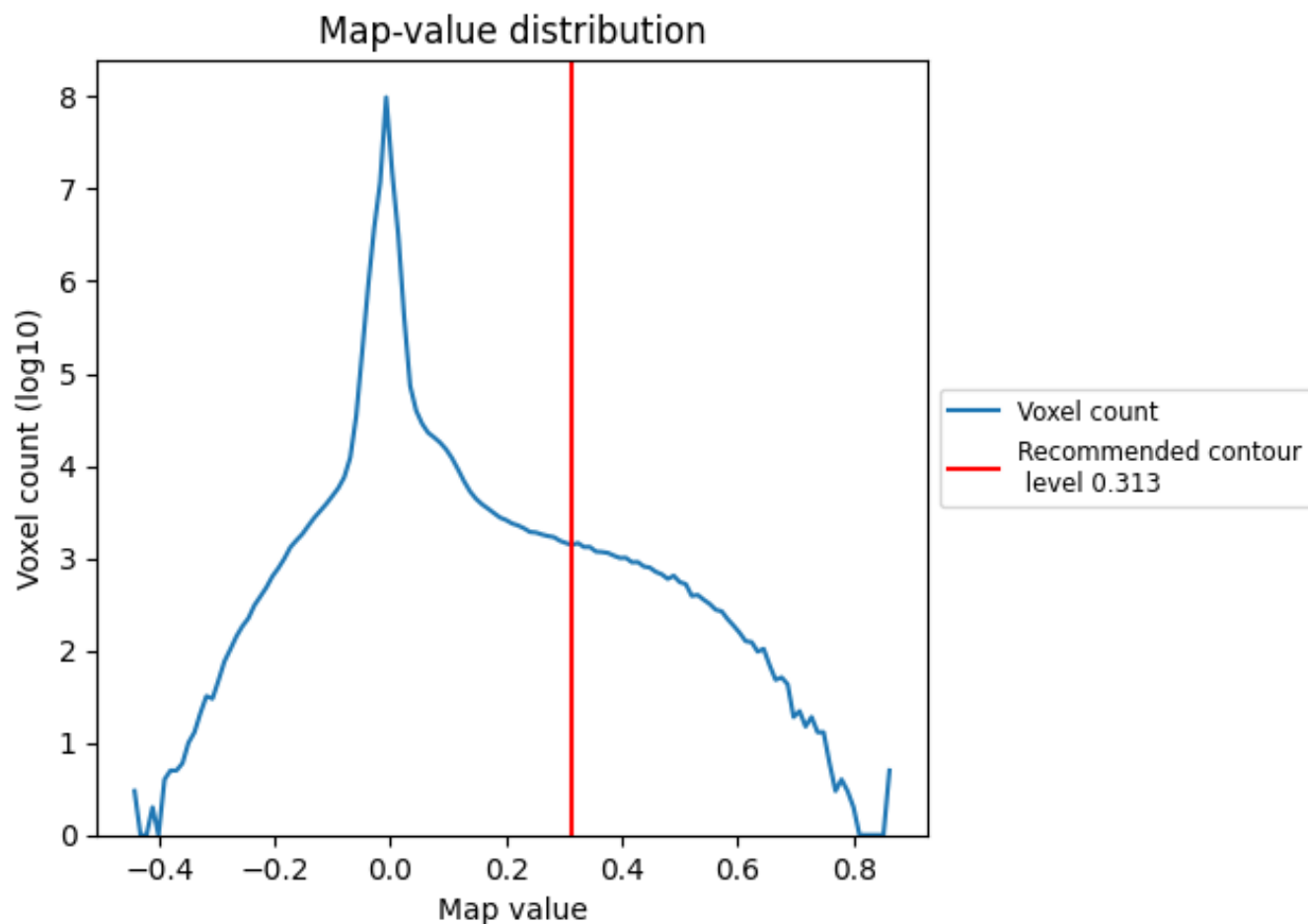
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

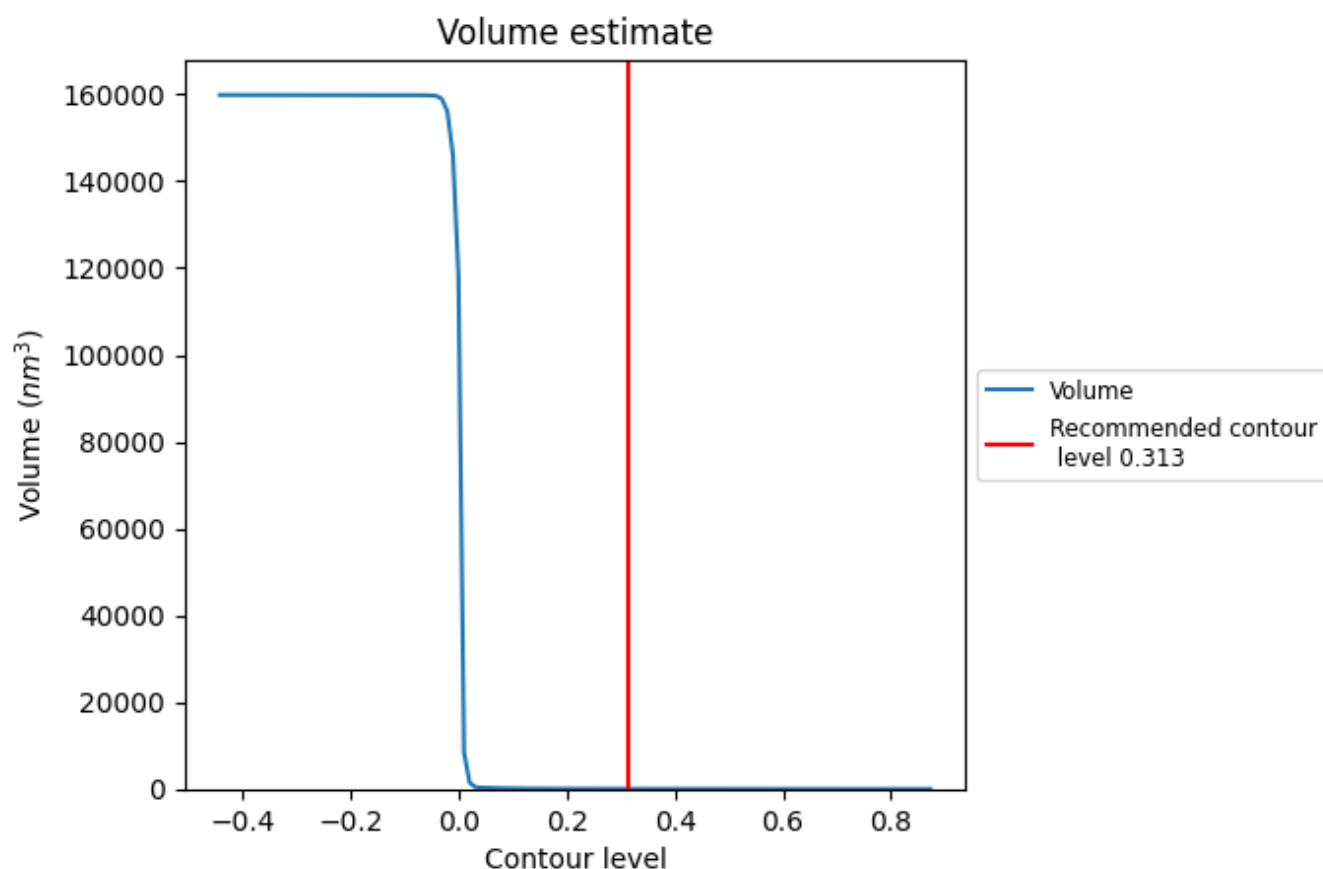
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

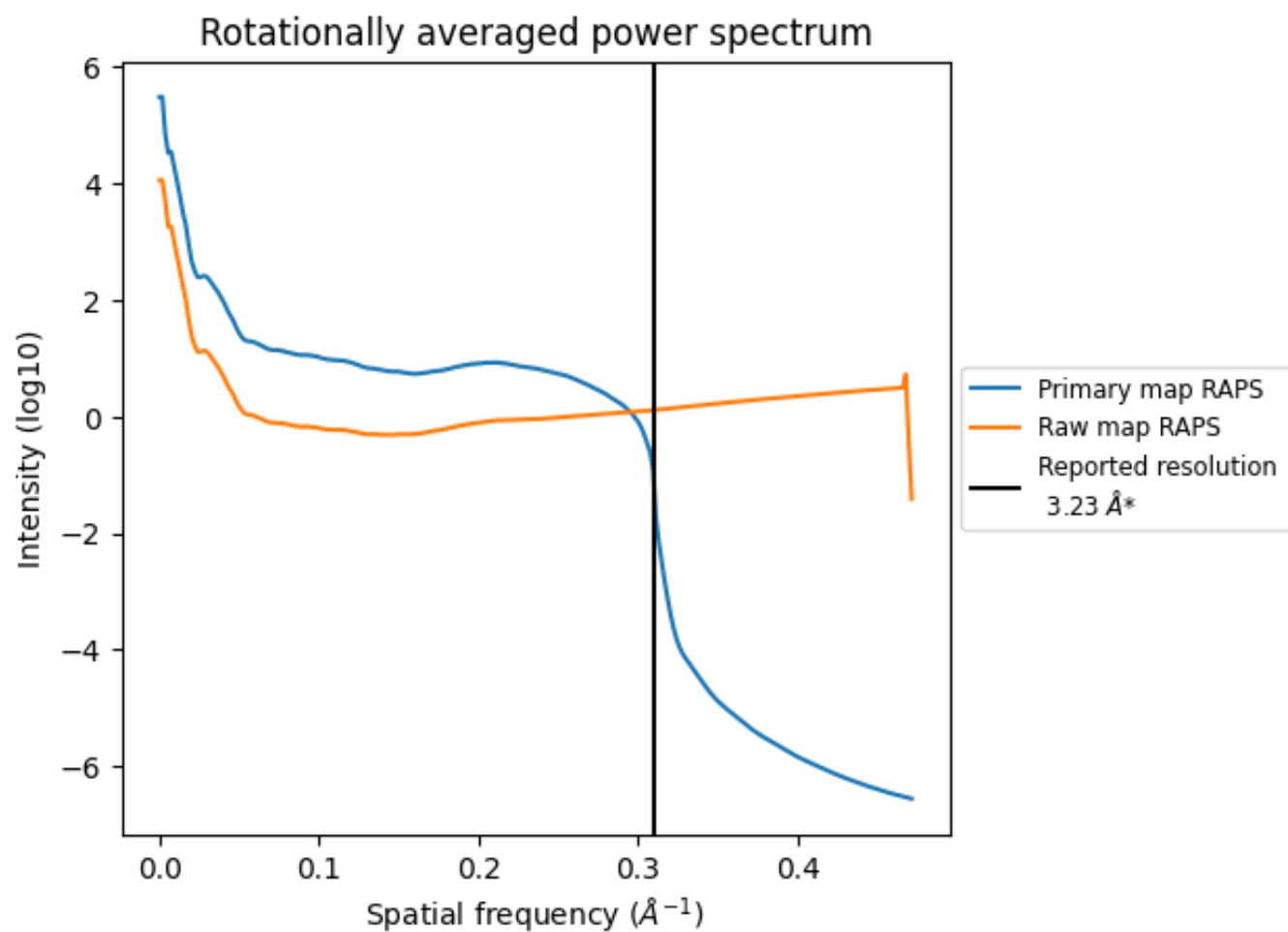
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 27 nm³; this corresponds to an approximate mass of 24 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 ⓘ

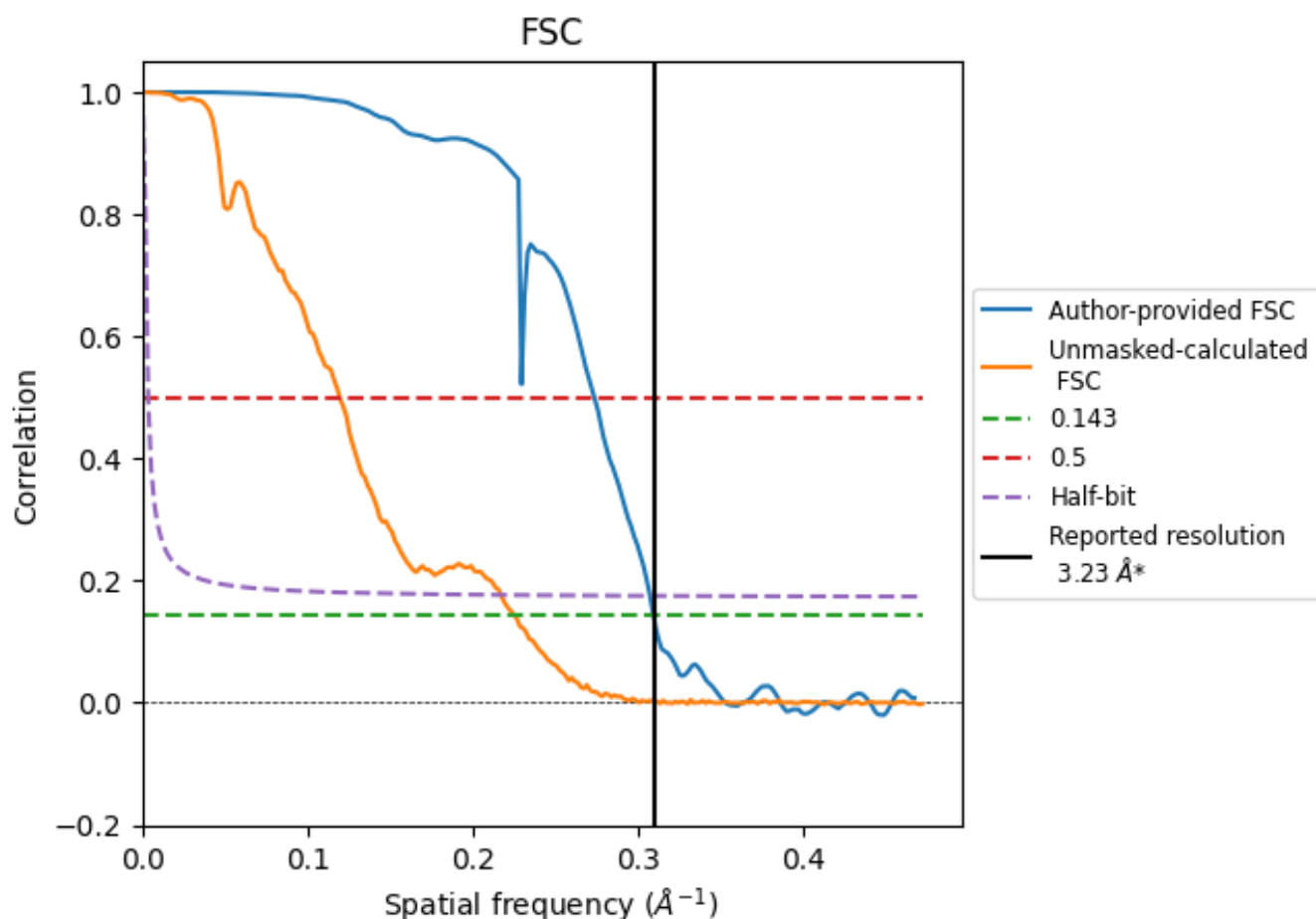


*Reported resolution corresponds to spatial frequency of 0.310 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.310 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

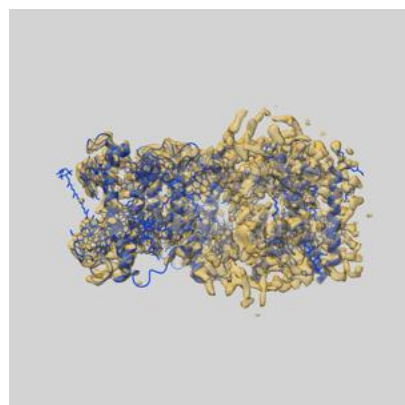
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.23	-	-
Author-provided FSC curve	3.23	3.66	3.26
Unmasked-calculated*	4.44	8.37	4.61

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.44 differs from the reported value 3.23 by more than 10 %

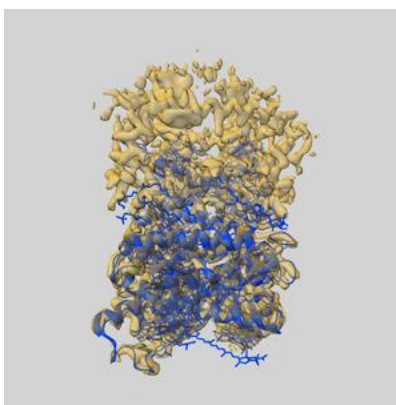
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-37267 and PDB model 8W4O. Per-residue inclusion information can be found in section [3](#) on page [11](#).

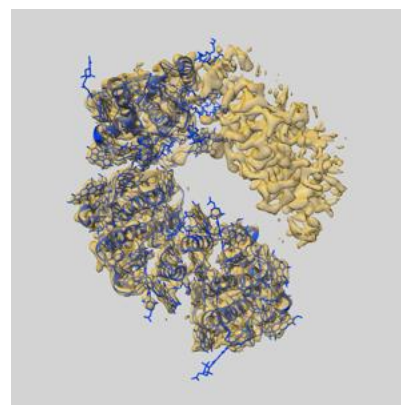
9.1 Map-model overlay [i](#)



X



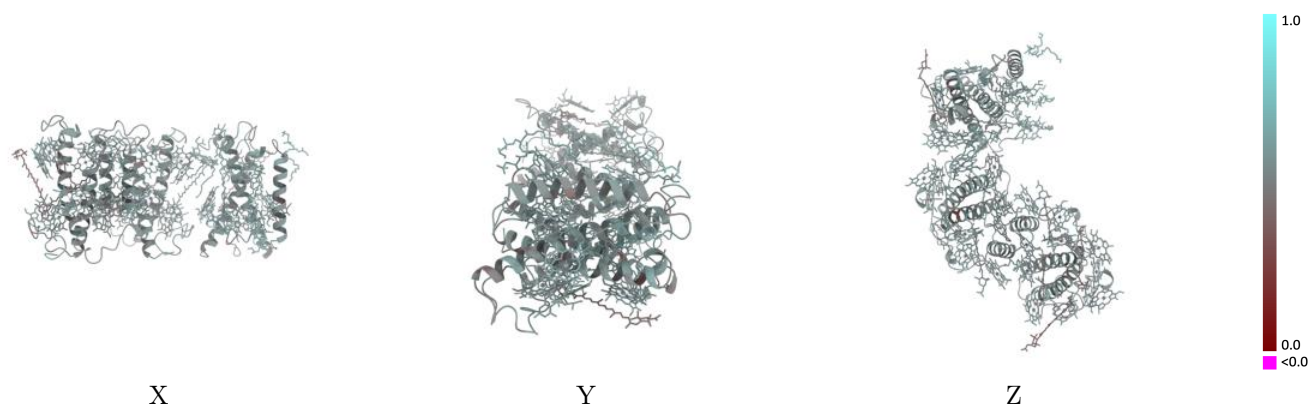
Y



Z

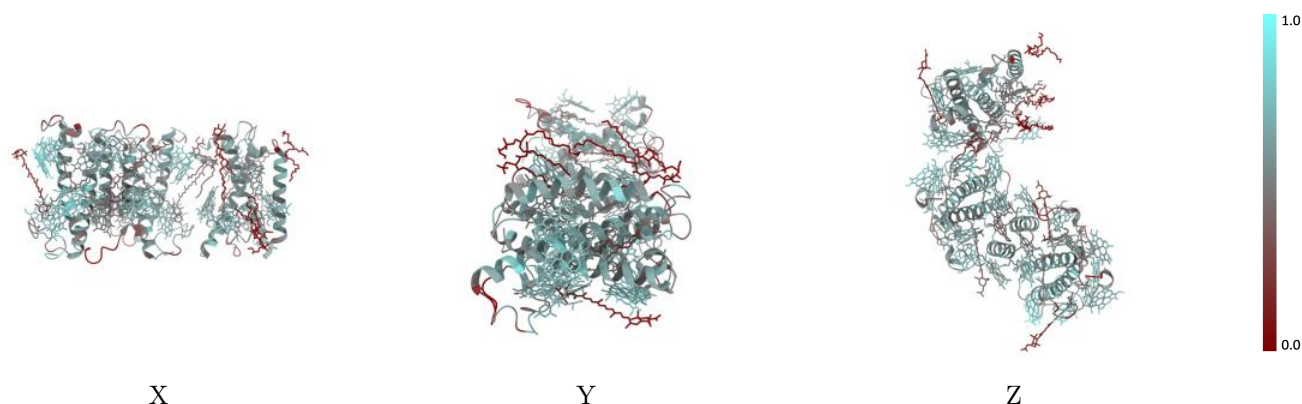
The images above show the 3D surface view of the map at the recommended contour level 0.313 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



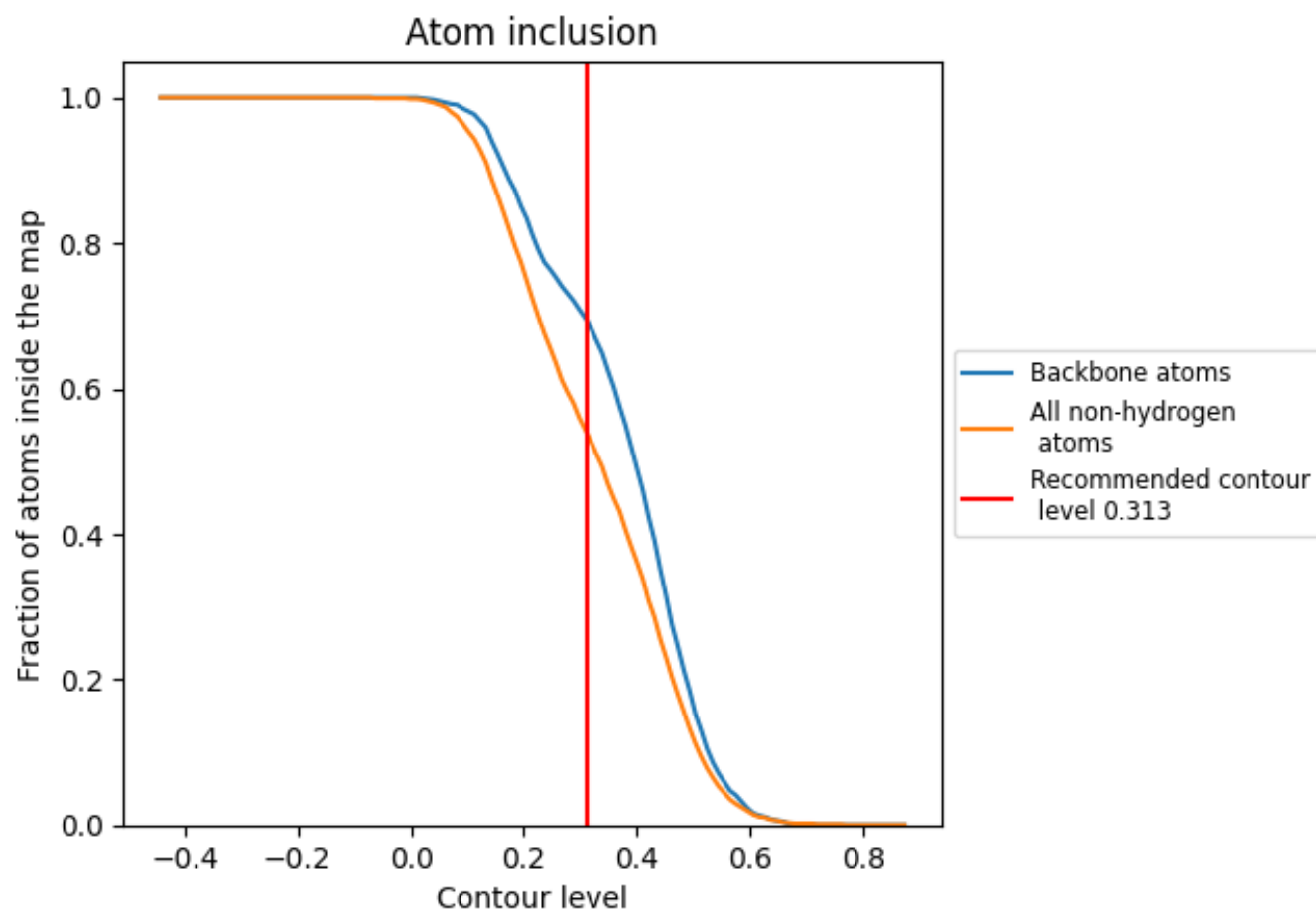
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



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 (0.313).

9.4 Atom inclusion [i](#)



At the recommended contour level, 69% of all backbone atoms, 54% 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 (0.313) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5360	0.5310
5	0.5040	0.5380
6	0.5690	0.5340
7	0.5380	0.5200

