



Full wwPDB EM Validation Report ⓘ

Nov 14, 2022 – 07:13 PM JST

PDB ID : 7WLM
EMDB ID : EMD-32588
Title : The Cryo-EM structure of siphonaxanthin chlorophyll a/b type light-harvesting complex II
Authors : Seki, S.; Nakaniwa, T.; Castro-Hartmann, P.; Sader, K.; Kawamoto, A.; Tanaka, H.; Qian, P.; Kurisu, G.; Fujii, R.
Deposited on : 2022-01-13
Resolution : 2.80 Å (reported)
Based on initial model : 1RWT

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.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

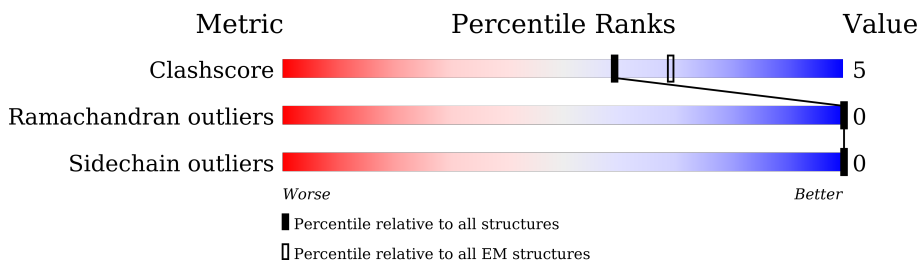
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	A	223	 82% 8% 10%
1	B	223	 81% 9% 10%
1	C	223	 82% 8% 10%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CHL	A	601	X	-	-	-
2	CHL	A	602	X	-	-	-
2	CHL	A	605	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CHL	A	606	X	-	-	-
2	CHL	A	607	X	-	-	-
2	CHL	A	608	X	-	-	-
2	CHL	A	609	X	-	-	-
2	CHL	A	610	X	-	-	-
2	CHL	B	601	X	-	-	-
2	CHL	B	602	X	-	-	-
2	CHL	B	605	X	-	-	-
2	CHL	B	606	X	-	-	-
2	CHL	B	607	X	-	-	-
2	CHL	B	608	X	-	-	-
2	CHL	B	609	X	-	-	-
2	CHL	B	610	X	-	-	-
2	CHL	C	601	X	-	-	-
2	CHL	C	602	X	-	-	-
2	CHL	C	605	X	-	-	-
2	CHL	C	606	X	-	-	-
2	CHL	C	607	X	-	-	-
2	CHL	C	608	X	-	-	-
2	CHL	C	609	X	-	-	-
2	CHL	C	610	X	-	-	-
3	CLA	A	603	X	-	-	-
3	CLA	A	604	X	-	-	-
3	CLA	A	611	X	-	-	-
3	CLA	A	612	X	-	-	-
3	CLA	A	613	X	-	-	-
3	CLA	B	603	X	-	-	-
3	CLA	B	604	X	-	-	-
3	CLA	B	611	X	-	-	-
3	CLA	B	612	X	-	-	-
3	CLA	B	613	X	-	-	-
3	CLA	C	603	X	-	-	-
3	CLA	C	604	X	-	-	-
3	CLA	C	611	X	-	-	-
3	CLA	C	612	X	-	-	-
3	CLA	C	613	X	-	-	-

2 Entry composition [i](#)

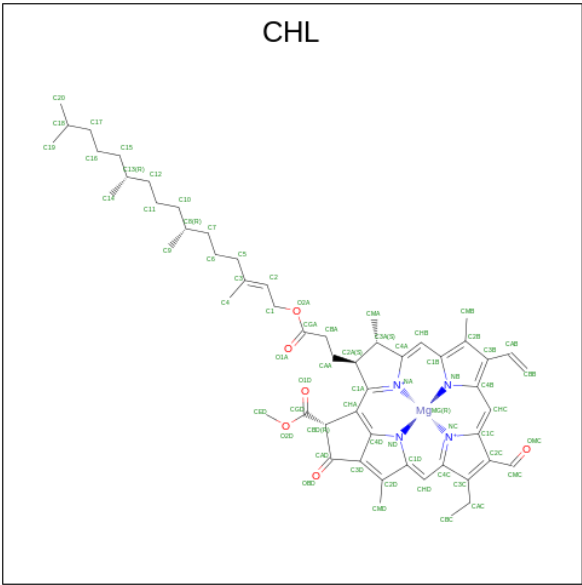
There are 8 unique types of molecules in this entry. The entry contains 7308 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 siphonaxanthin chlorophyll a/b binding light-harvesting complex II.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	201	Total	C	N	O	S	0	0
			1539	1001	242	290	6		
1	B	201	Total	C	N	O	S	0	0
			1539	1001	242	290	6		
1	C	201	Total	C	N	O	S	0	0
			1539	1001	242	290	6		

- Molecule 2 is CHLOROPHYLL B (three-letter code: CHL) (formula: C₅₅H₇₀MgN₄O₆) (labeled as "Ligand of Interest" by depositor).



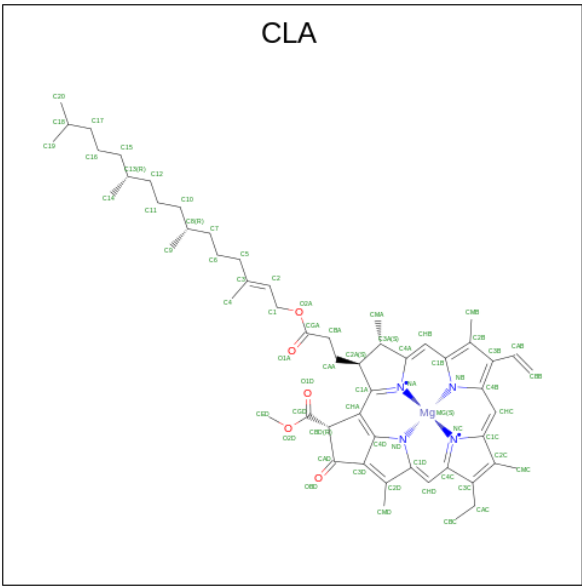
Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	Mg	N	O	0
			441	353	8	32	48	
2	A	1	Total	C	Mg	N	O	0
			441	353	8	32	48	
2	A	1	Total	C	Mg	N	O	0
			441	353	8	32	48	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total 441	C 353	Mg 8	N 32	O 48	0
2	A	1	Total 441	C 353	Mg 8	N 32	O 48	0
2	A	1	Total 441	C 353	Mg 8	N 32	O 48	0
2	A	1	Total 441	C 353	Mg 8	N 32	O 48	0
2	A	1	Total 441	C 353	Mg 8	N 32	O 48	0
2	B	1	Total 441	C 353	Mg 8	N 32	O 48	0
2	B	1	Total 441	C 353	Mg 8	N 32	O 48	0
2	B	1	Total 441	C 353	Mg 8	N 32	O 48	0
2	B	1	Total 441	C 353	Mg 8	N 32	O 48	0
2	B	1	Total 441	C 353	Mg 8	N 32	O 48	0
2	B	1	Total 441	C 353	Mg 8	N 32	O 48	0
2	B	1	Total 441	C 353	Mg 8	N 32	O 48	0
2	B	1	Total 441	C 353	Mg 8	N 32	O 48	0
2	B	1	Total 441	C 353	Mg 8	N 32	O 48	0
2	C	1	Total 441	C 353	Mg 8	N 32	O 48	0
2	C	1	Total 441	C 353	Mg 8	N 32	O 48	0
2	C	1	Total 441	C 353	Mg 8	N 32	O 48	0
2	C	1	Total 441	C 353	Mg 8	N 32	O 48	0
2	C	1	Total 441	C 353	Mg 8	N 32	O 48	0
2	C	1	Total 441	C 353	Mg 8	N 32	O 48	0
2	C	1	Total 441	C 353	Mg 8	N 32	O 48	0
2	C	1	Total 441	C 353	Mg 8	N 32	O 48	0

- Molecule 3 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



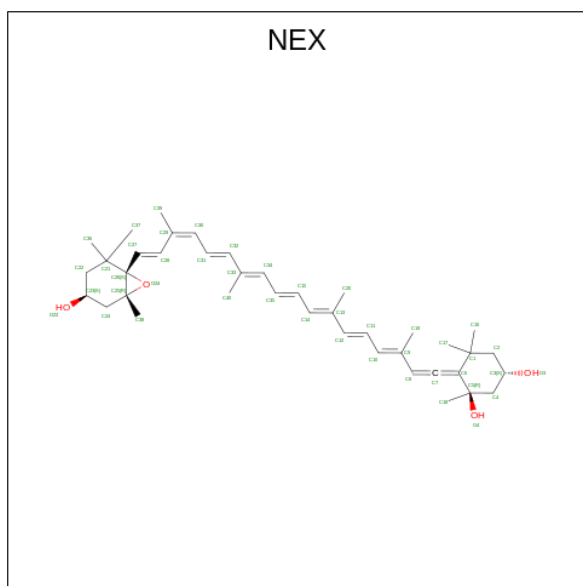
Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	Mg	N	O	0
			253	203	5	20	25	
3	A	1	Total	C	Mg	N	O	0
			253	203	5	20	25	
3	A	1	Total	C	Mg	N	O	0
			253	203	5	20	25	
3	A	1	Total	C	Mg	N	O	0
			253	203	5	20	25	
3	A	1	Total	C	Mg	N	O	0
			253	203	5	20	25	
3	B	1	Total	C	Mg	N	O	0
			253	203	5	20	25	
3	B	1	Total	C	Mg	N	O	0
			253	203	5	20	25	
3	B	1	Total	C	Mg	N	O	0
			253	203	5	20	25	
3	B	1	Total	C	Mg	N	O	0
			253	203	5	20	25	
3	B	1	Total	C	Mg	N	O	0
			253	203	5	20	25	
3	C	1	Total	C	Mg	N	O	0
			253	203	5	20	25	
3	C	1	Total	C	Mg	N	O	0
			253	203	5	20	25	
3	C	1	Total	C	Mg	N	O	0
			253	203	5	20	25	

Continued on next page...

Continued from previous page...

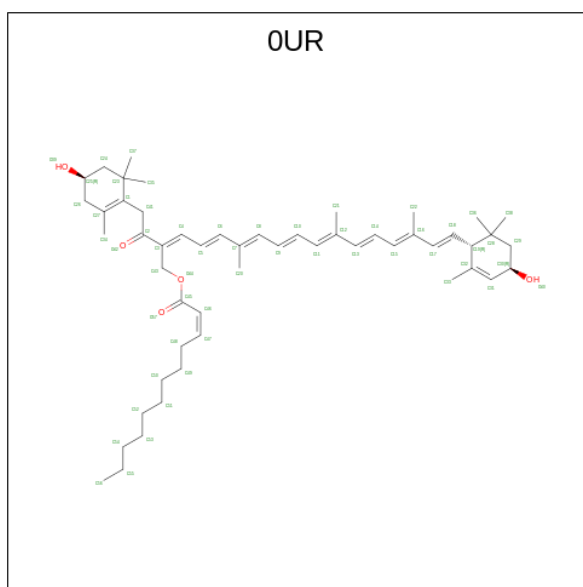
Mol	Chain	Residues	Atoms					AltConf
3	C	1	Total	C	Mg	N	O	0
			253	203	5	20	25	
3	C	1	Total	C	Mg	N	O	0
			253	203	5	20	25	

- Molecule 4 is (1R,3R)-6-[(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTA DECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE]-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (three-letter code: NEX) (formula: $C_{40}H_{56}O_4$).



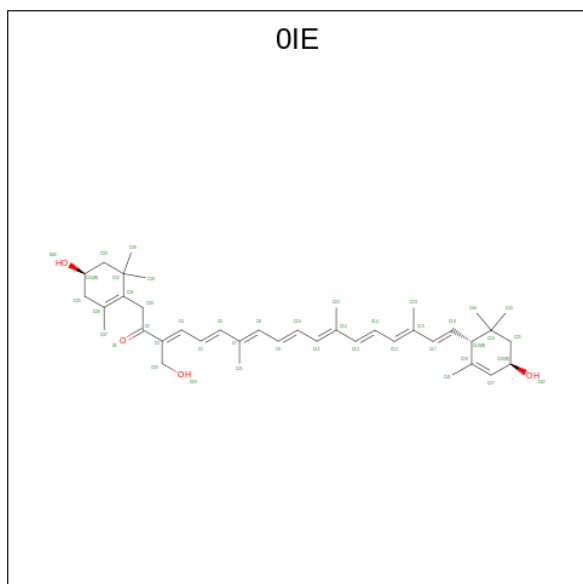
Mol	Chain	Residues	Atoms			AltConf
4	A	1	Total	C	O	0
			44	40	4	
4	B	1	Total	C	O	0
			44	40	4	
4	C	1	Total	C	O	0
			44	40	4	

- Molecule 5 is Siphonein (three-letter code: 0UR) (formula: $C_{52}H_{76}O_5$) (labeled as "Ligand of Interest" by depositor).



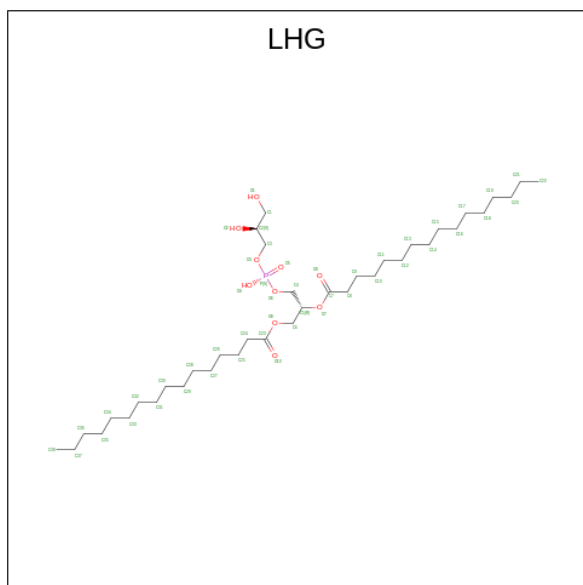
Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total	C	O	0
			57	52	5	
5	B	1	Total	C	O	0
			57	52	5	
5	C	1	Total	C	O	0
			57	52	5	

- Molecule 6 is Siphonaxanthin (three-letter code: 0IE) (formula: $C_{40}H_{56}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
6	A	1	Total	C	O	0
			44	40	4	
6	B	1	Total	C	O	0
			44	40	4	
6	C	1	Total	C	O	0
			44	40	4	

- Molecule 7 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				AltConf
7	A	1	Total	C	O	P	0
			40	29	10	1	
7	B	1	Total	C	O	P	0
			40	29	10	1	
7	C	1	Total	C	O	P	0
			40	29	10	1	

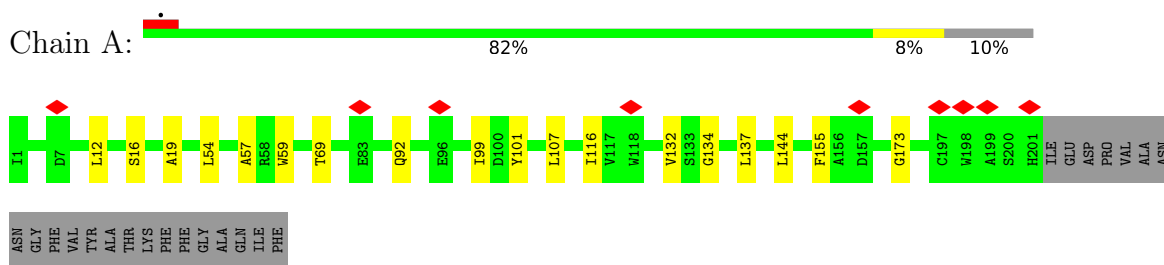
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		AltConf
8	A	18	Total	O	0
			18	18	
8	B	18	Total	O	0
			18	18	
8	C	18	Total	O	0
			18	18	

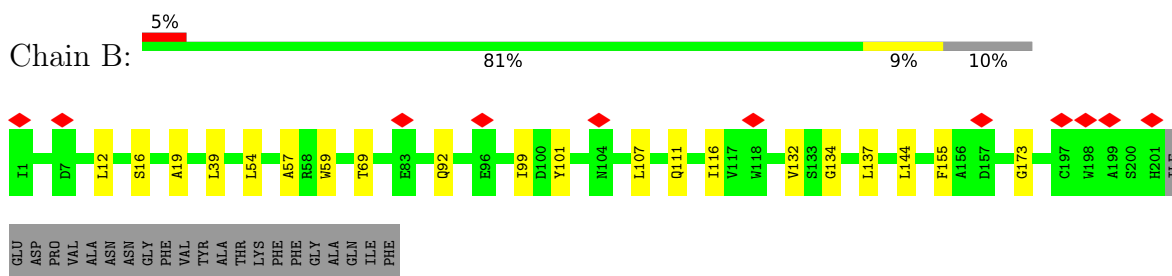
3 Residue-property plots [i](#)

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

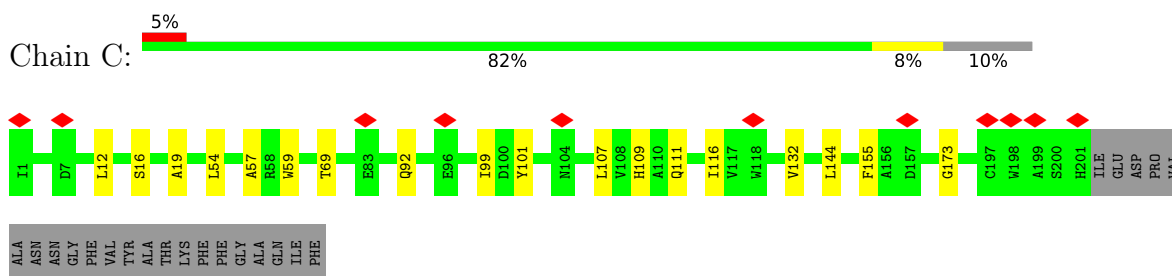
- Molecule 1: siphonaxanthin chlorophyll a/b binding light-harvesting complex II



- Molecule 1: siphonaxanthin chlorophyll a/b binding light-harvesting complex II



- Molecule 1: siphonaxanthin chlorophyll a/b binding light-harvesting complex II



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	250633	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 ($e^-/\text{\AA}^2$)	50.75	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	120000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.375	Depositor
Minimum map value	-0.195	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.0528	Depositor
Map size (\AA)	217.136, 217.136, 217.136	wwPDB
Map dimensions	328, 328, 328	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.662, 0.662, 0.662	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, OUR, NEX, OIE, LHG, CHL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.27	0/1588	0.43	0/2161
1	B	0.26	0/1588	0.44	0/2161
1	C	0.27	0/1588	0.43	0/2161
All	All	0.27	0/4764	0.43	0/6483

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	A	1539	0	1456	15	0
1	B	1539	0	1456	16	0
1	C	1539	0	1456	13	0
2	A	441	0	380	12	0
2	B	441	0	380	14	0
2	C	441	0	380	8	0
3	A	253	0	209	3	0
3	B	253	0	209	2	0
3	C	253	0	209	2	0
4	A	44	0	56	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	44	0	56	1	0
4	C	44	0	56	2	0
5	A	57	0	0	0	0
5	B	57	0	0	0	0
5	C	57	0	0	0	0
6	A	44	0	0	0	0
6	B	44	0	0	0	0
6	C	44	0	0	0	0
7	A	40	0	50	1	0
7	B	40	0	50	1	0
7	C	40	0	50	1	0
8	A	18	0	0	0	0
8	B	18	0	0	0	0
8	C	18	0	0	0	0
All	All	7308	0	6453	66	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 5.

All (66) 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)
1:A:137:LEU:HD13	2:A:608:CHL:HAB	1.63	0.78
1:B:137:LEU:HD13	2:B:608:CHL:HAB	1.78	0.64
1:A:155:PHE:HB2	2:A:610:CHL:HBA1	1.78	0.64
1:B:155:PHE:HB2	2:B:610:CHL:HBA1	1.80	0.63
1:C:155:PHE:HB2	2:C:610:CHL:HBA1	1.80	0.63
1:A:57:ALA:HB1	1:A:173:GLY:HA3	1.85	0.58
1:C:57:ALA:HB1	1:C:173:GLY:HA3	1.86	0.58
1:C:92:GLN:HB2	1:C:99:ILE:HG12	1.86	0.57
1:B:57:ALA:HB1	1:B:173:GLY:HA3	1.86	0.57
1:A:12:LEU:HB2	1:A:16:SER:HB3	1.87	0.57
2:C:610:CHL:HMB1	2:C:610:CHL:HBB1	1.86	0.57
1:A:92:GLN:HB2	1:A:99:ILE:HG12	1.87	0.56
1:B:12:LEU:HB2	1:B:16:SER:HB3	1.87	0.56
1:C:12:LEU:HB2	1:C:16:SER:HB3	1.88	0.56
1:B:92:GLN:HB2	1:B:99:ILE:HG12	1.88	0.54
1:B:54:LEU:HD23	1:B:144:LEU:HB3	1.90	0.53
1:C:54:LEU:HD23	1:C:144:LEU:HB3	1.90	0.53
1:B:116:ILE:HG12	2:B:605:CHL:HAC1	1.92	0.52
1:A:116:ILE:HG12	2:A:605:CHL:HAC1	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:LEU:HD23	1:A:144:LEU:HB3	1.91	0.52
2:B:610:CHL:HBB1	2:B:610:CHL:HMB1	1.92	0.52
1:B:132:VAL:HG11	1:C:19:ALA:HB2	1.92	0.51
1:C:116:ILE:HG12	2:C:605:CHL:HAC1	1.92	0.51
2:C:606:CHL:HBA2	2:C:606:CHL:HBD	1.92	0.51
1:B:111:GLN:HB2	2:B:605:CHL:HBB1	1.93	0.51
2:A:606:CHL:HBD	2:A:606:CHL:HBA2	1.92	0.50
1:A:19:ALA:HB2	1:C:132:VAL:HG11	1.94	0.49
2:B:606:CHL:HBD	2:B:606:CHL:HBA2	1.92	0.49
1:A:132:VAL:HG11	1:B:19:ALA:HB2	1.93	0.49
2:C:605:CHL:HBA1	2:C:605:CHL:H3A	1.71	0.48
2:A:610:CHL:HBB1	2:A:610:CHL:HMB1	1.96	0.47
1:C:109:HIS:CD2	1:C:111:GLN:HE22	2.32	0.47
1:B:134:GLY:O	2:B:608:CHL:HMC	2.15	0.47
3:A:603:CLA:H12	1:B:39:LEU:HD21	1.97	0.46
2:B:601:CHL:HMD3	7:B:617:LHG:HC61	1.97	0.46
2:A:602:CHL:H18	2:A:602:CHL:H152	1.78	0.46
2:B:610:CHL:H62	2:B:610:CHL:H41	1.64	0.46
1:A:59:TRP:CD1	2:A:609:CHL:HMD3	2.51	0.45
1:C:59:TRP:CD1	2:C:609:CHL:HMD3	2.51	0.45
2:B:605:CHL:HBA1	2:B:605:CHL:H3A	1.72	0.45
2:A:605:CHL:HBA1	2:A:605:CHL:H3A	1.72	0.45
2:B:602:CHL:H18	2:B:602:CHL:H152	1.77	0.44
2:C:601:CHL:HMD3	7:C:617:LHG:HC61	1.98	0.44
1:A:137:LEU:CD1	2:A:608:CHL:HAB	2.40	0.44
4:C:614:NEX:H401	4:C:614:NEX:H35	1.76	0.43
1:A:134:GLY:O	2:A:608:CHL:HMC	2.18	0.43
1:C:69:THR:HG21	3:C:604:CLA:HAC2	2.01	0.43
2:A:601:CHL:HMD3	7:A:617:LHG:HC61	2.00	0.43
4:A:614:NEX:H35	4:A:614:NEX:H401	1.76	0.43
3:C:611:CLA:H62	3:C:611:CLA:H41	1.73	0.42
3:B:603:CLA:H72	2:C:602:CHL:H91	2.00	0.42
2:A:606:CHL:HMB3	2:A:609:CHL:HMC	2.01	0.42
1:A:101:TYR:O	1:A:107:LEU:HD12	2.20	0.41
4:B:614:NEX:H401	4:B:614:NEX:H35	1.76	0.41
1:C:101:TYR:O	1:C:107:LEU:HD12	2.20	0.41
1:A:69:THR:HG21	3:A:604:CLA:HAC2	2.03	0.41
3:A:611:CLA:H41	3:A:611:CLA:H62	1.72	0.41
1:C:12:LEU:HD23	1:C:12:LEU:HA	1.93	0.41
4:A:614:NEX:H31	4:A:614:NEX:H28	1.83	0.41
1:B:59:TRP:CD1	2:B:609:CHL:HMD3	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:THR:HG21	3:B:604:CLA:HAC2	2.03	0.41
1:B:101:TYR:O	1:B:107:LEU:HD12	2.21	0.41
1:B:137:LEU:CD1	2:B:608:CHL:HAB	2.46	0.40
1:A:12:LEU:HD23	1:A:12:LEU:HA	1.92	0.40
2:B:606:CHL:HMB3	2:B:609:CHL:HMC	2.03	0.40
4:C:614:NEX:H31	4:C:614:NEX:H28	1.84	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	199/223 (89%)	196 (98%)	3 (2%)	0	100	100
1	B	199/223 (89%)	196 (98%)	3 (2%)	0	100	100
1	C	199/223 (89%)	195 (98%)	4 (2%)	0	100	100
All	All	597/669 (89%)	587 (98%)	10 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	153/170 (90%)	153 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	153/170 (90%)	153 (100%)	0	100	100
1	C	153/170 (90%)	153 (100%)	0	100	100
All	All	459/510 (90%)	459 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

51 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
3	CLA	B	604	8	50,58,73	2.66	7 (14%)	58,95,113	1.44	10 (17%)
5	OUR	C	615	-	55,58,58	0.68	2 (3%)	63,77,77	1.61	12 (19%)
3	CLA	C	613	1	45,53,73	2.85	7 (15%)	52,89,113	1.54	10 (19%)
3	CLA	B	612	1	45,53,73	2.80	7 (15%)	52,89,113	1.37	8 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	CHL	A	602	1	66,74,74	1.47	5 (7%)	73,114,114	1.88	11 (15%)
4	NEX	A	614	-	38,46,46	3.00	8 (21%)	50,70,70	0.64	1 (2%)
3	CLA	A	611	7	57,65,73	2.52	7 (12%)	66,103,113	1.34	9 (13%)
2	CHL	C	607	8	46,54,74	1.83	4 (8%)	49,90,114	2.25	14 (28%)
2	CHL	C	609	1	56,64,74	1.67	4 (7%)	61,102,114	1.91	11 (18%)
3	CLA	B	611	7	57,65,73	2.53	9 (15%)	66,103,113	1.35	9 (13%)
4	NEX	B	614	-	38,46,46	3.01	8 (21%)	50,70,70	0.64	1 (2%)
7	LHG	C	617	3	39,39,48	0.26	0	42,45,54	0.31	0
6	OIE	A	616	-	42,45,45	0.25	0	49,63,63	1.16	3 (6%)
7	LHG	A	617	3	39,39,48	0.26	0	42,45,54	0.31	0
2	CHL	B	610	1	66,74,74	1.49	5 (7%)	73,114,114	1.81	11 (15%)
2	CHL	C	602	1	66,74,74	1.48	6 (9%)	73,114,114	1.89	12 (16%)
2	CHL	A	607	8	46,54,74	1.83	4 (8%)	49,90,114	2.25	14 (28%)
2	CHL	A	605	1	46,54,74	1.91	5 (10%)	49,90,114	2.06	10 (20%)
2	CHL	A	606	8	46,54,74	1.78	5 (10%)	49,90,114	2.15	11 (22%)
3	CLA	C	612	1	45,53,73	2.79	7 (15%)	52,89,113	1.36	8 (15%)
6	OIE	B	616	-	42,45,45	0.25	0	49,63,63	1.20	3 (6%)
3	CLA	B	603	-	56,64,73	2.48	8 (14%)	65,102,113	1.31	8 (12%)
2	CHL	C	601	1	52,60,74	1.69	4 (7%)	56,97,114	2.11	11 (19%)
3	CLA	A	612	1	45,53,73	2.79	7 (15%)	52,89,113	1.36	8 (15%)
4	NEX	C	614	-	38,46,46	3.02	8 (21%)	50,70,70	0.62	1 (2%)
3	CLA	C	611	7	57,65,73	2.52	8 (14%)	66,103,113	1.34	9 (13%)
2	CHL	C	608	8	63,71,74	1.53	4 (6%)	69,110,114	1.76	9 (13%)
2	CHL	A	601	1	52,60,74	1.69	4 (7%)	56,97,114	2.12	11 (19%)
2	CHL	B	605	1	46,54,74	1.92	5 (10%)	49,90,114	2.07	10 (20%)
2	CHL	B	602	1	66,74,74	1.47	5 (7%)	73,114,114	1.88	11 (15%)
2	CHL	C	606	8	46,54,74	1.79	5 (10%)	49,90,114	2.17	11 (22%)
2	CHL	C	610	1	66,74,74	1.48	5 (7%)	73,114,114	1.80	12 (16%)
2	CHL	B	608	8	63,71,74	1.54	4 (6%)	69,110,114	1.79	10 (14%)
2	CHL	A	609	1	56,64,74	1.65	4 (7%)	61,102,114	1.89	11 (18%)
3	CLA	A	613	1	45,53,73	2.85	7 (15%)	52,89,113	1.53	10 (19%)
3	CLA	C	603	-	56,64,73	2.47	8 (14%)	65,102,113	1.29	7 (10%)
2	CHL	A	610	1	66,74,74	1.49	5 (7%)	73,114,114	1.82	12 (16%)
3	CLA	B	613	1	45,53,73	2.85	7 (15%)	52,89,113	1.53	10 (19%)
2	CHL	B	601	1	52,60,74	1.68	4 (7%)	56,97,114	2.12	11 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	CHL	C	605	1	46,54,74	1.89	5 (10%)	49,90,114	2.07	10 (20%)
7	LHG	B	617	3	39,39,48	0.26	0	42,45,54	0.31	0
2	CHL	B	606	8	46,54,74	1.80	5 (10%)	49,90,114	2.15	11 (22%)
2	CHL	B	607	8	46,54,74	1.84	4 (8%)	49,90,114	2.24	14 (28%)
3	CLA	A	604	8	50,58,73	2.67	8 (16%)	58,95,113	1.45	10 (17%)
3	CLA	A	603	-	56,64,73	2.47	8 (14%)	65,102,113	1.29	7 (10%)
3	CLA	C	604	8	50,58,73	2.67	7 (14%)	58,95,113	1.43	10 (17%)
5	OUR	A	615	-	55,58,58	0.67	2 (3%)	63,77,77	1.61	12 (19%)
5	OUR	B	615	-	55,58,58	0.67	2 (3%)	63,77,77	1.59	12 (19%)
2	CHL	A	608	8	63,71,74	1.56	5 (7%)	69,110,114	1.76	10 (14%)
2	CHL	B	609	1	56,64,74	1.65	4 (7%)	61,102,114	1.89	11 (18%)
6	OIE	C	616	-	42,45,45	0.25	0	49,63,63	1.12	3 (6%)

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
3	CLA	B	604	8	1/1/12/20	2/19/97/115	-
5	OUR	C	615	-	-	7/47/86/86	0/2/2/2
3	CLA	C	613	1	1/1/11/20	4/13/91/115	-
3	CLA	B	612	1	1/1/11/20	3/13/91/115	-
2	CHL	A	602	1	4/4/20/26	7/39/137/137	-
4	NEX	A	614	-	-	2/27/83/83	0/3/3/3
3	CLA	A	611	7	2/2/13/20	5/28/106/115	-
2	CHL	C	607	8	3/3/16/26	2/15/113/137	-
2	CHL	C	609	1	4/4/18/26	6/27/125/137	-
3	CLA	B	611	7	2/2/13/20	4/28/106/115	-
4	NEX	B	614	-	-	2/27/83/83	0/3/3/3
7	LHG	C	617	3	-	7/44/44/53	-
6	OIE	A	616	-	-	3/33/72/72	0/2/2/2
7	LHG	A	617	3	-	7/44/44/53	-
2	CHL	B	610	1	4/4/20/26	7/39/137/137	-
2	CHL	C	602	1	4/4/20/26	7/39/137/137	-
2	CHL	A	607	8	3/3/16/26	3/15/113/137	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CHL	A	605	1	3/3/16/26	5/15/113/137	-
2	CHL	A	606	8	3/3/16/26	6/15/113/137	-
3	CLA	C	612	1	1/1/11/20	3/13/91/115	-
6	OIE	B	616	-	-	3/33/72/72	0/2/2/2
3	CLA	B	603	-	2/2/13/20	1/27/105/115	-
2	CHL	C	601	1	3/3/17/26	7/23/121/137	-
3	CLA	A	612	1	1/1/11/20	3/13/91/115	-
4	NEX	C	614	-	-	2/27/83/83	0/3/3/3
3	CLA	C	611	7	2/2/13/20	4/28/106/115	-
2	CHL	C	608	8	4/4/19/26	4/36/134/137	-
2	CHL	A	601	1	3/3/17/26	6/23/121/137	-
2	CHL	B	605	1	3/3/16/26	5/15/113/137	-
2	CHL	B	602	1	4/4/20/26	7/39/137/137	-
2	CHL	C	606	8	3/3/16/26	6/15/113/137	-
2	CHL	C	610	1	4/4/20/26	7/39/137/137	-
2	CHL	B	608	8	4/4/19/26	6/36/134/137	-
2	CHL	A	609	1	4/4/18/26	6/27/125/137	-
3	CLA	A	613	1	1/1/11/20	4/13/91/115	-
3	CLA	C	603	-	2/2/13/20	1/27/105/115	-
2	CHL	A	610	1	4/4/20/26	7/39/137/137	-
3	CLA	B	613	1	1/1/11/20	4/13/91/115	-
2	CHL	B	601	1	3/3/17/26	6/23/121/137	-
2	CHL	C	605	1	3/3/16/26	5/15/113/137	-
7	LHG	B	617	3	-	7/44/44/53	-
2	CHL	B	606	8	3/3/16/26	6/15/113/137	-
2	CHL	B	607	8	3/3/16/26	2/15/113/137	-
3	CLA	A	604	8	1/1/12/20	2/19/97/115	-
3	CLA	A	603	-	2/2/13/20	2/27/105/115	-
3	CLA	C	604	8	1/1/12/20	2/19/97/115	-
5	OUR	A	615	-	-	7/47/86/86	0/2/2/2
5	OUR	B	615	-	-	7/47/86/86	0/2/2/2
2	CHL	A	608	8	4/4/19/26	6/36/134/137	-
2	CHL	B	609	1	4/4/18/26	5/27/125/137	-
6	OIE	C	616	-	-	3/33/72/72	0/2/2/2

All (252) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	612	CLA	C4B-NB	14.51	1.48	1.35
3	C	612	CLA	C4B-NB	14.49	1.48	1.35
3	A	612	CLA	C4B-NB	14.44	1.48	1.35
3	A	611	CLA	C4B-NB	14.42	1.48	1.35
3	B	613	CLA	C4B-NB	14.41	1.48	1.35
3	B	611	CLA	C4B-NB	14.39	1.48	1.35
3	A	613	CLA	C4B-NB	14.39	1.48	1.35
3	C	611	CLA	C4B-NB	14.38	1.48	1.35
3	C	613	CLA	C4B-NB	14.34	1.48	1.35
3	C	604	CLA	C4B-NB	14.34	1.48	1.35
3	A	604	CLA	C4B-NB	14.31	1.48	1.35
3	C	603	CLA	C4B-NB	14.31	1.48	1.35
3	B	603	CLA	C4B-NB	14.30	1.48	1.35
3	A	603	CLA	C4B-NB	14.21	1.47	1.35
3	B	604	CLA	C4B-NB	14.18	1.47	1.35
2	B	605	CHL	C4B-NB	11.51	1.45	1.35
2	A	605	CHL	C4B-NB	11.37	1.45	1.35
2	C	605	CHL	C4B-NB	11.28	1.45	1.35
4	B	614	NEX	C34-C33	-11.05	1.21	1.35
4	C	614	NEX	C34-C33	-10.90	1.21	1.35
2	C	609	CHL	C4B-NB	10.88	1.44	1.35
2	B	607	CHL	C4B-NB	10.87	1.44	1.35
2	C	607	CHL	C4B-NB	10.84	1.44	1.35
2	A	607	CHL	C4B-NB	10.82	1.44	1.35
2	B	609	CHL	C4B-NB	10.78	1.44	1.35
2	A	609	CHL	C4B-NB	10.77	1.44	1.35
2	A	608	CHL	C4B-NB	10.62	1.44	1.35
4	A	614	NEX	C34-C33	-10.61	1.21	1.35
2	A	601	CHL	C4B-NB	10.57	1.44	1.35
2	B	606	CHL	C4B-NB	10.54	1.44	1.35
2	B	608	CHL	C4B-NB	10.52	1.44	1.35
2	B	601	CHL	C4B-NB	10.52	1.44	1.35
2	C	601	CHL	C4B-NB	10.51	1.44	1.35
2	B	610	CHL	C4B-NB	10.49	1.44	1.35
2	C	606	CHL	C4B-NB	10.47	1.44	1.35
2	A	610	CHL	C4B-NB	10.47	1.44	1.35
2	C	608	CHL	C4B-NB	10.44	1.44	1.35
2	A	606	CHL	C4B-NB	10.43	1.44	1.35
2	C	610	CHL	C4B-NB	10.40	1.44	1.35
2	C	602	CHL	C4B-NB	10.37	1.44	1.35
2	A	602	CHL	C4B-NB	10.32	1.44	1.35
2	B	602	CHL	C4B-NB	10.29	1.44	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	614	NEX	C30-C29	-9.20	1.23	1.35
4	C	614	NEX	C30-C29	-8.58	1.24	1.35
4	B	614	NEX	C30-C29	-8.13	1.25	1.35
3	C	613	CLA	C1B-NB	7.76	1.42	1.35
3	B	613	CLA	C1B-NB	7.73	1.42	1.35
3	B	611	CLA	C1B-NB	7.73	1.42	1.35
3	A	613	CLA	C1B-NB	7.72	1.42	1.35
3	C	611	CLA	C1B-NB	7.64	1.42	1.35
3	A	611	CLA	C1B-NB	7.62	1.42	1.35
3	A	604	CLA	C1B-NB	7.33	1.41	1.35
3	B	604	CLA	C1B-NB	7.32	1.41	1.35
3	C	604	CLA	C1B-NB	7.32	1.41	1.35
3	A	612	CLA	C1B-NB	7.23	1.41	1.35
3	B	612	CLA	C1B-NB	7.19	1.41	1.35
3	C	612	CLA	C1B-NB	7.16	1.41	1.35
3	B	603	CLA	C1B-NB	6.96	1.41	1.35
3	A	603	CLA	C1B-NB	6.94	1.41	1.35
3	C	603	CLA	C1B-NB	6.89	1.41	1.35
4	B	614	NEX	C39-C29	-6.19	1.38	1.50
4	C	614	NEX	C39-C29	-6.17	1.38	1.50
4	B	614	NEX	C31-C30	-6.08	1.24	1.43
4	C	614	NEX	C31-C30	-6.00	1.24	1.43
4	A	614	NEX	C39-C29	-5.76	1.39	1.50
4	A	614	NEX	C31-C30	-5.60	1.26	1.43
4	B	614	NEX	C32-C33	-5.27	1.34	1.45
3	A	613	CLA	MG-ND	-5.11	1.95	2.05
3	C	613	CLA	MG-ND	-5.09	1.95	2.05
4	A	614	NEX	C32-C33	-5.08	1.35	1.45
3	A	604	CLA	MG-ND	-5.06	1.95	2.05
3	B	604	CLA	MG-ND	-5.06	1.95	2.05
3	B	613	CLA	MG-ND	-5.06	1.95	2.05
3	C	604	CLA	MG-ND	-5.03	1.95	2.05
3	B	611	CLA	MG-ND	-4.93	1.96	2.05
3	C	611	CLA	MG-ND	-4.92	1.96	2.05
4	C	614	NEX	C32-C33	-4.89	1.35	1.45
3	A	611	CLA	MG-ND	-4.89	1.96	2.05
4	A	614	NEX	C35-C34	-4.86	1.28	1.43
3	B	603	CLA	MG-ND	-4.70	1.96	2.05
3	A	603	CLA	MG-ND	-4.68	1.96	2.05
4	B	614	NEX	C35-C34	-4.66	1.29	1.43
3	C	603	CLA	MG-ND	-4.65	1.96	2.05
3	C	612	CLA	MG-ND	-4.63	1.96	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	612	CLA	MG-ND	-4.63	1.96	2.05
3	B	612	CLA	MG-ND	-4.63	1.96	2.05
4	C	614	NEX	C35-C34	-4.59	1.29	1.43
4	A	614	NEX	C40-C33	-4.59	1.41	1.50
3	C	613	CLA	MG-NA	-4.48	1.95	2.06
3	A	613	CLA	MG-NA	-4.42	1.95	2.06
3	B	604	CLA	MG-NA	-4.42	1.95	2.06
3	B	613	CLA	MG-NA	-4.42	1.95	2.06
3	B	611	CLA	MG-NA	-4.41	1.95	2.06
3	A	611	CLA	MG-NA	-4.40	1.95	2.06
3	A	604	CLA	MG-NA	-4.40	1.95	2.06
4	C	614	NEX	C40-C33	-4.39	1.41	1.50
3	C	611	CLA	MG-NA	-4.39	1.95	2.06
3	C	604	CLA	MG-NA	-4.37	1.95	2.06
4	B	614	NEX	C40-C33	-4.11	1.42	1.50
3	C	612	CLA	C1D-ND	4.07	1.42	1.37
3	A	612	CLA	C1D-ND	4.07	1.42	1.37
3	B	612	CLA	C1D-ND	4.03	1.42	1.37
3	A	603	CLA	C1D-ND	3.93	1.42	1.37
3	B	603	CLA	C1D-ND	3.92	1.42	1.37
3	B	603	CLA	MG-NA	-3.91	1.97	2.06
3	C	603	CLA	C1D-ND	3.89	1.42	1.37
3	C	603	CLA	MG-NA	-3.89	1.97	2.06
3	A	603	CLA	MG-NA	-3.88	1.97	2.06
3	A	604	CLA	C1D-ND	3.83	1.42	1.37
3	C	604	CLA	C1D-ND	3.81	1.42	1.37
3	B	604	CLA	MG-NC	-3.81	1.97	2.06
3	B	604	CLA	C1D-ND	3.80	1.42	1.37
3	C	604	CLA	MG-NC	-3.80	1.97	2.06
3	A	613	CLA	C1D-ND	3.79	1.42	1.37
3	A	613	CLA	MG-NC	-3.79	1.97	2.06
3	A	604	CLA	MG-NC	-3.78	1.97	2.06
3	B	613	CLA	MG-NC	-3.78	1.97	2.06
3	B	611	CLA	MG-NC	-3.77	1.97	2.06
3	C	613	CLA	C1D-ND	3.76	1.42	1.37
3	B	613	CLA	C1D-ND	3.75	1.42	1.37
3	C	611	CLA	MG-NC	-3.75	1.97	2.06
3	C	613	CLA	MG-NC	-3.74	1.97	2.06
3	B	612	CLA	MG-NA	-3.74	1.97	2.06
3	A	611	CLA	MG-NC	-3.74	1.97	2.06
3	A	612	CLA	MG-NA	-3.72	1.97	2.06
3	C	612	CLA	MG-NA	-3.72	1.97	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	611	CLA	C1D-ND	3.67	1.42	1.37
3	C	611	CLA	C1D-ND	3.64	1.42	1.37
3	A	611	CLA	C1D-ND	3.60	1.42	1.37
3	A	603	CLA	MG-NC	-3.57	1.97	2.06
3	B	603	CLA	MG-NC	-3.54	1.97	2.06
3	C	603	CLA	MG-NC	-3.52	1.97	2.06
3	C	612	CLA	MG-NC	-3.47	1.98	2.06
3	A	612	CLA	MG-NC	-3.44	1.98	2.06
3	B	612	CLA	MG-NC	-3.42	1.98	2.06
4	C	614	NEX	C31-C32	-3.14	1.26	1.34
4	B	614	NEX	C31-C32	-2.91	1.27	1.34
2	A	608	CHL	C3B-C2B	-2.59	1.36	1.40
4	A	614	NEX	C31-C32	-2.55	1.28	1.34
2	B	608	CHL	C3B-C2B	-2.51	1.36	1.40
3	C	612	CLA	C1D-C2D	-2.49	1.40	1.45
3	B	612	CLA	C1D-C2D	-2.45	1.40	1.45
3	A	612	CLA	C1D-C2D	-2.42	1.40	1.45
2	C	608	CHL	C3B-C2B	-2.42	1.37	1.40
5	C	615	0UR	C17-C18	-2.41	1.26	1.32
5	B	615	0UR	C19-C18	-2.35	1.46	1.50
5	C	615	0UR	C19-C18	-2.35	1.46	1.50
3	A	604	CLA	C1D-C2D	-2.35	1.40	1.45
5	A	615	0UR	C19-C18	-2.35	1.46	1.50
3	B	604	CLA	C1D-C2D	-2.35	1.40	1.45
5	A	615	0UR	C17-C18	-2.34	1.26	1.32
2	B	609	CHL	C3B-C2B	-2.33	1.37	1.40
3	C	613	CLA	C1D-C2D	-2.33	1.40	1.45
3	C	604	CLA	C1D-C2D	-2.33	1.40	1.45
2	C	601	CHL	C3B-C2B	-2.31	1.37	1.40
2	C	609	CHL	C3B-C2B	-2.31	1.37	1.40
2	A	601	CHL	C3B-C2B	-2.31	1.37	1.40
5	B	615	0UR	C17-C18	-2.30	1.26	1.32
3	B	613	CLA	C1D-C2D	-2.29	1.40	1.45
2	B	605	CHL	C3B-C2B	-2.29	1.37	1.40
2	A	610	CHL	C1D-C2D	-2.29	1.40	1.45
3	C	603	CLA	C1D-C2D	-2.29	1.40	1.45
2	B	610	CHL	C1D-C2D	-2.28	1.40	1.45
2	C	601	CHL	C1D-C2D	-2.28	1.40	1.45
3	C	611	CLA	C1D-C2D	-2.27	1.40	1.45
2	B	601	CHL	C3B-C2B	-2.27	1.37	1.40
3	A	603	CLA	C1D-C2D	-2.27	1.40	1.45
3	B	611	CLA	C1D-C2D	-2.27	1.40	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	607	CHL	C1D-C2D	-2.26	1.40	1.45
3	B	603	CLA	C1D-C2D	-2.26	1.40	1.45
2	A	609	CHL	C3B-C2B	-2.26	1.37	1.40
2	C	610	CHL	C1D-C2D	-2.26	1.40	1.45
2	B	601	CHL	C1D-C2D	-2.26	1.40	1.45
3	A	611	CLA	C1D-C2D	-2.25	1.40	1.45
2	C	605	CHL	C3B-C2B	-2.25	1.37	1.40
2	A	602	CHL	C1D-C2D	-2.25	1.40	1.45
3	A	613	CLA	C1D-C2D	-2.25	1.40	1.45
2	C	607	CHL	C1D-C2D	-2.25	1.40	1.45
2	A	601	CHL	C1D-C2D	-2.23	1.40	1.45
2	A	605	CHL	C3B-C2B	-2.23	1.37	1.40
2	C	608	CHL	C1D-C2D	-2.22	1.40	1.45
2	B	608	CHL	C1D-C2D	-2.22	1.40	1.45
2	A	606	CHL	C1D-C2D	-2.22	1.40	1.45
2	C	602	CHL	C1D-C2D	-2.22	1.40	1.45
2	A	607	CHL	C1D-C2D	-2.21	1.41	1.45
2	C	606	CHL	C1D-C2D	-2.20	1.41	1.45
2	B	602	CHL	C1D-C2D	-2.20	1.41	1.45
2	A	606	CHL	C3B-C2B	-2.20	1.37	1.40
2	A	607	CHL	C3B-C2B	-2.20	1.37	1.40
2	C	607	CHL	C3B-C2B	-2.20	1.37	1.40
2	B	606	CHL	C1D-C2D	-2.19	1.41	1.45
2	C	609	CHL	C1D-C2D	-2.19	1.41	1.45
2	B	605	CHL	C1D-C2D	-2.19	1.41	1.45
2	A	608	CHL	C1D-C2D	-2.19	1.41	1.45
2	B	609	CHL	C1D-C2D	-2.19	1.41	1.45
2	B	607	CHL	C3B-C2B	-2.19	1.37	1.40
2	C	606	CHL	C3B-C2B	-2.18	1.37	1.40
2	C	602	CHL	C3D-C4D	-2.17	1.39	1.44
2	A	609	CHL	C1D-C2D	-2.17	1.41	1.45
2	A	605	CHL	C1D-C2D	-2.16	1.41	1.45
2	C	605	CHL	C1D-C2D	-2.16	1.41	1.45
2	B	606	CHL	C3B-C2B	-2.16	1.37	1.40
2	A	610	CHL	C1C-NC	-2.15	1.34	1.37
2	A	609	CHL	C3D-C4D	-2.14	1.39	1.44
2	B	609	CHL	C3D-C4D	-2.13	1.39	1.44
2	B	602	CHL	C3D-C4D	-2.12	1.39	1.44
2	C	601	CHL	C3D-C4D	-2.12	1.39	1.44
2	A	602	CHL	C3D-C4D	-2.12	1.39	1.44
2	C	608	CHL	C3D-C4D	-2.11	1.39	1.44
2	B	601	CHL	C3D-C4D	-2.11	1.39	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	CHL	C3D-C4D	-2.10	1.39	1.44
2	C	609	CHL	C3D-C4D	-2.10	1.39	1.44
2	C	606	CHL	C3D-C4D	-2.10	1.39	1.44
2	C	610	CHL	C1C-NC	-2.09	1.34	1.37
2	B	607	CHL	C3D-C4D	-2.08	1.39	1.44
2	B	608	CHL	C3D-C4D	-2.08	1.39	1.44
2	A	610	CHL	CHC-C1C	2.08	1.40	1.35
2	B	606	CHL	C3D-C4D	-2.08	1.39	1.44
2	A	606	CHL	CHC-C1C	2.07	1.40	1.35
2	C	606	CHL	CHC-C1C	2.06	1.40	1.35
2	A	607	CHL	C3D-C4D	-2.06	1.39	1.44
2	A	606	CHL	C3D-C4D	-2.06	1.39	1.44
2	A	608	CHL	C3D-C4D	-2.06	1.39	1.44
2	C	610	CHL	C3D-C4D	-2.06	1.39	1.44
2	A	610	CHL	C3D-C4D	-2.06	1.39	1.44
2	C	605	CHL	C3D-C4D	-2.06	1.39	1.44
2	C	610	CHL	CHC-C1C	2.05	1.40	1.35
2	C	607	CHL	C3D-C4D	-2.05	1.39	1.44
2	B	610	CHL	C3D-C4D	-2.05	1.39	1.44
2	B	602	CHL	C1C-NC	-2.05	1.34	1.37
2	C	602	CHL	C1C-NC	-2.04	1.34	1.37
2	B	606	CHL	CHC-C1C	2.04	1.40	1.35
3	C	603	CLA	C3D-C4D	-2.04	1.39	1.44
2	B	610	CHL	CHC-C1C	2.04	1.40	1.35
2	A	605	CHL	CHC-C1C	2.04	1.40	1.35
2	B	602	CHL	CHC-C1C	2.04	1.40	1.35
2	B	610	CHL	C1C-NC	-2.04	1.34	1.37
3	A	603	CLA	C3D-C4D	-2.03	1.39	1.44
2	A	608	CHL	CHC-C1C	2.03	1.40	1.35
3	B	611	CLA	C3D-C4D	-2.03	1.39	1.44
2	A	605	CHL	C3D-C4D	-2.03	1.39	1.44
2	A	602	CHL	CHC-C1C	2.02	1.40	1.35
2	C	602	CHL	CHC-C1C	2.02	1.40	1.35
3	B	603	CLA	C3D-C4D	-2.02	1.39	1.44
2	B	605	CHL	CHC-C1C	2.02	1.40	1.35
3	C	611	CLA	C3D-C4D	-2.02	1.39	1.44
3	B	611	CLA	C1C-C2C	2.01	1.48	1.44
2	C	605	CHL	CHC-C1C	2.01	1.40	1.35
2	A	602	CHL	C1C-NC	-2.01	1.34	1.37
2	C	602	CHL	C3B-C2B	-2.00	1.37	1.40
2	B	605	CHL	C3D-C4D	-2.00	1.39	1.44
3	A	604	CLA	C3D-C4D	-2.00	1.39	1.44

All (450) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	602	CHL	C4A-NA-C1A	11.88	112.05	106.71
2	B	602	CHL	C4A-NA-C1A	11.85	112.03	106.71
2	A	602	CHL	C4A-NA-C1A	11.84	112.03	106.71
2	A	601	CHL	C4A-NA-C1A	11.77	112.00	106.71
2	B	601	CHL	C4A-NA-C1A	11.77	112.00	106.71
2	C	601	CHL	C4A-NA-C1A	11.64	111.94	106.71
2	A	607	CHL	C4A-NA-C1A	11.60	111.92	106.71
2	C	607	CHL	C4A-NA-C1A	11.50	111.88	106.71
2	B	607	CHL	C4A-NA-C1A	11.46	111.86	106.71
2	C	606	CHL	C4A-NA-C1A	10.86	111.59	106.71
2	A	606	CHL	C4A-NA-C1A	10.74	111.53	106.71
2	B	606	CHL	C4A-NA-C1A	10.72	111.53	106.71
2	A	610	CHL	C4A-NA-C1A	10.65	111.50	106.71
2	B	608	CHL	C4A-NA-C1A	10.61	111.48	106.71
2	B	610	CHL	C4A-NA-C1A	10.57	111.46	106.71
2	C	609	CHL	C4A-NA-C1A	10.51	111.43	106.71
2	C	608	CHL	C4A-NA-C1A	10.49	111.42	106.71
2	C	610	CHL	C4A-NA-C1A	10.42	111.39	106.71
2	A	609	CHL	C4A-NA-C1A	10.41	111.39	106.71
2	B	609	CHL	C4A-NA-C1A	10.41	111.38	106.71
2	A	608	CHL	C4A-NA-C1A	10.34	111.35	106.71
2	C	605	CHL	C4A-NA-C1A	10.14	111.27	106.71
2	B	605	CHL	C4A-NA-C1A	10.06	111.23	106.71
2	A	605	CHL	C4A-NA-C1A	10.04	111.22	106.71
6	B	616	OIE	O1-C2-C3	-7.01	107.86	120.66
6	A	616	OIE	O1-C2-C3	-6.70	108.41	120.66
3	C	613	CLA	C4A-NA-C1A	-6.57	103.75	106.71
3	B	613	CLA	C4A-NA-C1A	-6.52	103.77	106.71
3	A	613	CLA	C4A-NA-C1A	-6.49	103.79	106.71
6	C	616	OIE	O1-C2-C3	-6.43	108.90	120.66
3	B	611	CLA	C4A-NA-C1A	-6.18	103.93	106.71
3	A	611	CLA	C4A-NA-C1A	-6.14	103.95	106.71
3	C	611	CLA	C4A-NA-C1A	-6.12	103.96	106.71
3	A	604	CLA	C4A-NA-C1A	-5.84	104.08	106.71
3	B	604	CLA	C4A-NA-C1A	-5.75	104.12	106.71
3	C	604	CLA	C4A-NA-C1A	-5.66	104.16	106.71
3	B	603	CLA	C4A-NA-C1A	-5.52	104.22	106.71
5	A	615	OUR	C4-C3-C2	-5.44	115.41	120.08
3	A	603	CLA	C4A-NA-C1A	-5.41	104.28	106.71
5	B	615	OUR	C4-C3-C2	-5.34	115.50	120.08
5	B	615	OUR	C28-C19-C18	-5.32	105.98	112.70
5	C	615	OUR	C4-C3-C2	-5.31	115.52	120.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	603	CLA	C4A-NA-C1A	-5.30	104.33	106.71
5	C	615	0UR	C28-C19-C18	-5.15	106.19	112.70
5	A	615	0UR	C28-C19-C18	-5.10	106.26	112.70
3	C	612	CLA	C4A-NA-C1A	-4.80	104.55	106.71
3	B	612	CLA	C4A-NA-C1A	-4.79	104.55	106.71
3	A	612	CLA	C4A-NA-C1A	-4.76	104.57	106.71
2	C	610	CHL	CHD-C1D-ND	-4.62	120.21	124.45
2	A	610	CHL	CHD-C1D-ND	-4.60	120.23	124.45
2	A	602	CHL	CHD-C1D-ND	-4.50	120.32	124.45
2	B	610	CHL	CHD-C1D-ND	-4.50	120.32	124.45
5	A	615	0UR	O40-C30-C29	-4.50	99.37	110.74
2	C	602	CHL	CHD-C1D-ND	-4.47	120.35	124.45
5	C	615	0UR	O40-C30-C29	-4.46	99.45	110.74
2	C	609	CHL	CHD-C1D-ND	-4.43	120.38	124.45
2	B	602	CHL	CHD-C1D-ND	-4.43	120.39	124.45
2	A	609	CHL	CHD-C1D-ND	-4.40	120.41	124.45
2	C	606	CHL	CHD-C1D-ND	-4.39	120.42	124.45
2	B	605	CHL	CHD-C1D-ND	-4.38	120.43	124.45
2	C	607	CHL	CHD-C1D-ND	-4.38	120.43	124.45
2	A	606	CHL	CHD-C1D-ND	-4.36	120.45	124.45
2	B	609	CHL	CHD-C1D-ND	-4.36	120.45	124.45
2	C	610	CHL	CMB-C2B-C1B	-4.36	121.77	128.46
2	A	605	CHL	CHD-C1D-ND	-4.35	120.46	124.45
2	B	606	CHL	CHD-C1D-ND	-4.35	120.46	124.45
2	C	605	CHL	CHD-C1D-ND	-4.33	120.48	124.45
2	B	608	CHL	CHD-C1D-ND	-4.30	120.50	124.45
2	B	607	CHL	CHD-C1D-ND	-4.28	120.52	124.45
2	C	601	CHL	CHD-C1D-ND	-4.27	120.53	124.45
2	A	608	CHL	CHD-C1D-ND	-4.27	120.53	124.45
2	B	610	CHL	CMB-C2B-C1B	-4.27	121.90	128.46
2	C	608	CHL	CHD-C1D-ND	-4.26	120.54	124.45
2	A	601	CHL	CHD-C1D-ND	-4.25	120.55	124.45
2	B	601	CHL	CHD-C1D-ND	-4.24	120.56	124.45
2	A	607	CHL	CHD-C1D-ND	-4.23	120.57	124.45
2	A	610	CHL	CMB-C2B-C1B	-4.19	122.03	128.46
5	B	615	0UR	O40-C30-C29	-3.99	100.65	110.74
3	B	611	CLA	CHD-C1D-ND	-3.85	120.92	124.45
3	C	611	CLA	CHD-C1D-ND	-3.83	120.94	124.45
3	A	611	CLA	CHD-C1D-ND	-3.82	120.95	124.45
3	C	603	CLA	CHD-C1D-ND	-3.82	120.95	124.45
3	B	613	CLA	CHD-C1D-ND	-3.81	120.95	124.45
3	B	603	CLA	CHD-C1D-ND	-3.80	120.96	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	613	CLA	CHD-C1D-ND	-3.78	120.98	124.45
3	A	603	CLA	CHD-C1D-ND	-3.76	121.00	124.45
3	A	604	CLA	CHD-C1D-ND	-3.76	121.00	124.45
3	C	604	CLA	CHD-C1D-ND	-3.74	121.01	124.45
3	B	604	CLA	CHD-C1D-ND	-3.73	121.02	124.45
2	A	610	CHL	CHC-C1C-NC	3.73	129.86	124.20
3	A	613	CLA	CHD-C1D-ND	-3.72	121.03	124.45
2	C	607	CHL	CHC-C1C-NC	3.70	129.82	124.20
2	C	610	CHL	CHC-C1C-NC	3.69	129.80	124.20
2	B	607	CHL	CHC-C1C-NC	3.68	129.79	124.20
2	B	610	CHL	CHC-C1C-NC	3.67	129.77	124.20
2	C	602	CHL	CHC-C1C-NC	3.65	129.74	124.20
2	A	607	CHL	CHC-C1C-NC	3.65	129.74	124.20
2	C	609	CHL	CHC-C1C-NC	3.64	129.72	124.20
2	B	608	CHL	CHC-C1C-NC	3.63	129.72	124.20
2	A	601	CHL	CHC-C1C-NC	3.63	129.71	124.20
2	A	602	CHL	CHC-C1C-NC	3.63	129.70	124.20
2	C	606	CHL	CHC-C1C-NC	3.62	129.69	124.20
2	A	609	CHL	CHC-C1C-NC	3.60	129.67	124.20
2	C	601	CHL	CHC-C1C-NC	3.60	129.67	124.20
2	A	608	CHL	CHC-C1C-NC	3.60	129.67	124.20
2	B	606	CHL	CHC-C1C-NC	3.60	129.67	124.20
2	B	602	CHL	CHC-C1C-NC	3.59	129.66	124.20
2	B	601	CHL	CHC-C1C-NC	3.59	129.65	124.20
2	C	605	CHL	CHC-C1C-NC	3.59	129.65	124.20
2	B	609	CHL	CHC-C1C-NC	3.58	129.64	124.20
2	A	605	CHL	CHC-C1C-NC	3.58	129.64	124.20
2	A	606	CHL	CHC-C1C-NC	3.58	129.63	124.20
3	B	612	CLA	CHD-C1D-ND	-3.56	121.18	124.45
2	C	602	CHL	CMB-C2B-C1B	-3.55	123.00	128.46
2	C	610	CHL	C2A-C1A-CHA	3.55	130.07	123.86
2	B	605	CHL	CHC-C1C-NC	3.55	129.59	124.20
3	C	612	CLA	CHD-C1D-ND	-3.55	121.19	124.45
2	B	610	CHL	C2A-C1A-CHA	3.54	130.05	123.86
2	B	602	CHL	CMB-C2B-C1B	-3.54	123.02	128.46
2	A	610	CHL	C2A-C1A-CHA	3.53	130.03	123.86
2	C	608	CHL	CHC-C1C-NC	3.53	129.56	124.20
2	A	602	CHL	CMB-C2B-C1B	-3.48	123.11	128.46
3	A	612	CLA	CHD-C1D-ND	-3.48	121.26	124.45
2	C	606	CHL	CMB-C2B-C1B	-3.46	123.15	128.46
2	A	607	CHL	CMB-C2B-C1B	-3.44	123.17	128.46
5	C	615	OUR	C17-C16-C15	-3.43	113.68	118.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	605	CHL	CMB-C2B-C1B	-3.43	123.20	128.46
2	C	607	CHL	CMB-C2B-C1B	-3.42	123.21	128.46
2	B	606	CHL	CMB-C2B-C1B	-3.41	123.22	128.46
2	B	607	CHL	CMB-C2B-C1B	-3.41	123.22	128.46
2	A	605	CHL	CMB-C2B-C1B	-3.40	123.23	128.46
2	C	609	CHL	CMB-C2B-C1B	-3.40	123.24	128.46
2	A	609	CHL	CMB-C2B-C1B	-3.40	123.24	128.46
2	B	609	CHL	CMB-C2B-C1B	-3.39	123.25	128.46
2	C	605	CHL	CMB-C2B-C1B	-3.38	123.27	128.46
2	A	606	CHL	CMB-C2B-C1B	-3.37	123.28	128.46
2	C	601	CHL	CHB-C4A-NA	3.35	129.14	124.51
2	B	601	CHL	CHB-C4A-NA	3.34	129.13	124.51
2	A	601	CHL	CHB-C4A-NA	3.32	129.11	124.51
4	A	614	NEX	O24-C25-C24	3.32	115.88	113.38
2	C	602	CHL	C4D-CHA-C1A	3.29	125.25	121.25
4	B	614	NEX	O24-C25-C24	3.27	115.84	113.38
5	A	615	OUR	C17-C16-C15	-3.25	113.96	118.94
2	B	601	CHL	C4D-CHA-C1A	3.25	125.20	121.25
2	C	601	CHL	CMB-C2B-C1B	-3.25	123.48	128.46
3	B	612	CLA	C1D-ND-C4D	-3.24	104.03	106.33
2	B	601	CHL	CMB-C2B-C1B	-3.23	123.50	128.46
3	C	612	CLA	C1D-ND-C4D	-3.21	104.05	106.33
2	A	601	CHL	CMB-C2B-C1B	-3.21	123.53	128.46
2	B	602	CHL	C4D-CHA-C1A	3.21	125.16	121.25
3	A	612	CLA	C1D-ND-C4D	-3.20	104.06	106.33
5	A	615	OUR	O42-C2-C3	-3.20	114.81	120.66
2	C	607	CHL	CHB-C4A-NA	3.20	128.94	124.51
2	C	601	CHL	C4D-CHA-C1A	3.20	125.14	121.25
5	B	615	OUR	O42-C2-C3	-3.19	114.83	120.66
2	A	601	CHL	C4D-CHA-C1A	3.19	125.13	121.25
2	B	608	CHL	CMB-C2B-C1B	-3.18	123.57	128.46
2	B	607	CHL	CHB-C4A-NA	3.18	128.91	124.51
2	A	607	CHL	CHB-C4A-NA	3.18	128.91	124.51
2	A	605	CHL	C4D-CHA-C1A	3.17	125.11	121.25
5	C	615	OUR	C38-C28-C19	3.17	114.34	109.55
2	A	608	CHL	CMB-C2B-C1B	-3.17	123.60	128.46
5	B	615	OUR	C17-C16-C15	-3.17	114.08	118.94
2	A	606	CHL	C4D-CHA-C1A	3.17	125.10	121.25
2	B	608	CHL	C4D-CHA-C1A	3.16	125.10	121.25
2	A	602	CHL	C4D-CHA-C1A	3.16	125.10	121.25
2	C	607	CHL	C4D-CHA-C1A	3.16	125.10	121.25
2	B	607	CHL	C4D-CHA-C1A	3.16	125.09	121.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	605	CHL	C4D-CHA-C1A	3.15	125.09	121.25
2	C	608	CHL	CMB-C2B-C1B	-3.15	123.62	128.46
2	A	606	CHL	C2A-C1A-CHA	3.15	129.37	123.86
2	B	606	CHL	C2A-C1A-CHA	3.15	129.37	123.86
2	C	606	CHL	C2A-C1A-CHA	3.15	129.37	123.86
4	C	614	NEX	O24-C25-C24	3.14	115.74	113.38
2	B	605	CHL	C4D-CHA-C1A	3.14	125.07	121.25
2	A	607	CHL	C4D-CHA-C1A	3.13	125.05	121.25
2	B	606	CHL	C4D-CHA-C1A	3.12	125.04	121.25
2	C	606	CHL	C4D-CHA-C1A	3.12	125.04	121.25
3	C	603	CLA	C1D-ND-C4D	-3.09	104.14	106.33
3	B	603	CLA	C1D-ND-C4D	-3.09	104.14	106.33
2	C	608	CHL	C4D-CHA-C1A	3.08	125.00	121.25
2	C	609	CHL	C4D-CHA-C1A	3.08	125.00	121.25
3	A	603	CLA	C1D-ND-C4D	-3.08	104.15	106.33
5	A	615	0UR	C38-C28-C19	3.08	114.21	109.55
2	A	608	CHL	C4D-CHA-C1A	3.07	124.98	121.25
2	A	609	CHL	C4D-CHA-C1A	3.07	124.98	121.25
5	C	615	0UR	O42-C2-C3	-3.06	115.07	120.66
2	C	609	CHL	CHB-C4A-NA	3.05	128.73	124.51
2	B	609	CHL	CHB-C4A-NA	3.04	128.72	124.51
2	A	609	CHL	CHB-C4A-NA	3.04	128.71	124.51
2	B	608	CHL	C2A-C1A-CHA	3.03	129.16	123.86
3	B	611	CLA	C1D-ND-C4D	-3.03	104.19	106.33
2	B	609	CHL	C4D-CHA-C1A	3.00	124.90	121.25
2	A	608	CHL	C2A-C1A-CHA	3.00	129.10	123.86
2	A	610	CHL	C4D-CHA-C1A	3.00	124.89	121.25
2	A	602	CHL	CHB-C4A-NA	2.99	128.65	124.51
5	B	615	0UR	C29-C30-C31	2.99	115.15	111.74
2	C	606	CHL	CHB-C4A-NA	2.99	128.65	124.51
2	C	608	CHL	C2A-C1A-CHA	2.98	129.08	123.86
3	C	611	CLA	C1D-ND-C4D	-2.98	104.22	106.33
2	B	606	CHL	CHB-C4A-NA	2.98	128.63	124.51
2	B	602	CHL	CHB-C4A-NA	2.97	128.62	124.51
6	B	616	0IE	C5-C4-C3	-2.96	123.45	127.00
2	C	602	CHL	CHB-C4A-NA	2.95	128.59	124.51
5	C	615	0UR	C36-C28-C29	-2.95	103.85	109.44
2	C	610	CHL	C4D-CHA-C1A	2.94	124.83	121.25
2	A	609	CHL	C2A-C1A-CHA	2.94	129.00	123.86
2	C	609	CHL	C2A-C1A-CHA	2.94	129.00	123.86
2	A	606	CHL	CHB-C4A-NA	2.94	128.57	124.51
3	A	611	CLA	C1D-ND-C4D	-2.94	104.25	106.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	615	0UR	C38-C28-C19	2.93	113.98	109.55
2	B	608	CHL	CHB-C4A-NA	2.92	128.55	124.51
5	B	615	0UR	C36-C28-C29	-2.91	103.93	109.44
3	C	611	CLA	CAA-C2A-C1A	-2.90	102.46	111.97
2	B	610	CHL	C4D-CHA-C1A	2.90	124.78	121.25
2	B	609	CHL	C2A-C1A-CHA	2.90	128.93	123.86
2	C	608	CHL	CHB-C4A-NA	2.90	128.52	124.51
3	A	611	CLA	CAA-C2A-C1A	-2.89	102.51	111.97
3	B	611	CLA	CAA-C2A-C1A	-2.88	102.53	111.97
6	A	616	0IE	C5-C4-C3	-2.88	123.55	127.00
2	C	602	CHL	C2A-C1A-CHA	2.87	128.88	123.86
2	B	601	CHL	C2A-C1A-CHA	2.87	128.88	123.86
2	A	608	CHL	CHB-C4A-NA	2.87	128.48	124.51
2	A	607	CHL	C2A-C1A-CHA	2.87	128.87	123.86
5	A	615	0UR	C36-C28-C29	-2.87	104.00	109.44
2	C	607	CHL	C2A-C1A-CHA	2.87	128.87	123.86
3	A	612	CLA	C2C-C1C-NC	2.87	112.66	109.97
2	A	601	CHL	C2A-C1A-CHA	2.86	128.86	123.86
6	C	616	0IE	C5-C4-C3	-2.86	123.57	127.00
3	B	603	CLA	C1-C2-C3	-2.85	121.11	126.04
2	B	607	CHL	C2A-C1A-CHA	2.83	128.81	123.86
2	C	601	CHL	C2A-C1A-CHA	2.83	128.81	123.86
2	B	605	CHL	C2A-C1A-CHA	2.83	128.81	123.86
2	A	605	CHL	C2A-C1A-CHA	2.82	128.79	123.86
2	A	610	CHL	CHB-C4A-NA	2.82	128.41	124.51
2	B	610	CHL	CHB-C4A-NA	2.81	128.40	124.51
3	B	604	CLA	C1-C2-C3	-2.81	122.21	126.75
2	C	605	CHL	C2A-C1A-CHA	2.81	128.76	123.86
3	A	604	CLA	C1-C2-C3	-2.80	122.22	126.75
3	C	612	CLA	C2C-C1C-NC	2.80	112.59	109.97
2	C	605	CHL	CHB-C4A-NA	2.79	128.38	124.51
2	B	602	CHL	C2A-C1A-CHA	2.79	128.74	123.86
3	C	604	CLA	C1-C2-C3	-2.78	122.25	126.75
3	C	613	CLA	C1D-ND-C4D	-2.78	104.36	106.33
2	B	605	CHL	CHB-C4A-NA	2.78	128.36	124.51
3	B	612	CLA	C2C-C1C-NC	2.78	112.58	109.97
2	A	605	CHL	CHB-C4A-NA	2.77	128.34	124.51
3	A	613	CLA	C1D-ND-C4D	-2.76	104.37	106.33
2	C	610	CHL	CHB-C4A-NA	2.76	128.33	124.51
3	B	604	CLA	C1D-ND-C4D	-2.76	104.38	106.33
2	A	602	CHL	C2A-C1A-CHA	2.75	128.67	123.86
3	A	604	CLA	C1D-ND-C4D	-2.75	104.38	106.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	613	CLA	C1D-ND-C4D	-2.75	104.38	106.33
3	C	604	CLA	C1D-ND-C4D	-2.73	104.40	106.33
5	B	615	0UR	C36-C28-C19	2.72	113.66	109.55
5	C	615	0UR	C36-C28-C19	2.71	113.66	109.55
2	C	610	CHL	CMB-C2B-C3B	2.68	129.70	124.68
3	C	603	CLA	C1-C2-C3	-2.67	121.42	126.04
3	B	612	CLA	CHC-C1C-C2C	-2.64	119.42	126.72
3	A	612	CLA	CHC-C1C-C2C	-2.63	119.44	126.72
2	B	610	CHL	CMB-C2B-C3B	2.62	129.58	124.68
5	A	615	0UR	C36-C28-C19	2.62	113.51	109.55
3	C	612	CLA	CHC-C1C-C2C	-2.61	119.49	126.72
2	A	610	CHL	CMB-C2B-C3B	2.57	129.49	124.68
6	B	616	0IE	O1-C2-C30	2.57	124.30	120.58
5	A	615	0UR	C29-C30-C31	2.56	114.66	111.74
3	A	604	CLA	CHC-C1C-C2C	-2.55	119.68	126.72
3	C	604	CLA	CHC-C1C-C2C	-2.54	119.69	126.72
3	B	604	CLA	CHC-C1C-C2C	-2.53	119.72	126.72
3	A	603	CLA	CHC-C1C-C2C	-2.53	119.73	126.72
3	C	603	CLA	CHC-C1C-C2C	-2.52	119.76	126.72
3	C	604	CLA	C2C-C1C-NC	2.52	112.33	109.97
3	B	603	CLA	CHC-C1C-C2C	-2.52	119.76	126.72
6	A	616	0IE	O1-C2-C30	2.51	124.21	120.58
3	A	604	CLA	C2C-C1C-NC	2.50	112.32	109.97
3	B	604	CLA	C2C-C1C-NC	2.50	112.32	109.97
3	B	612	CLA	CHC-C1C-NC	2.50	128.00	124.20
3	A	604	CLA	CHC-C1C-NC	2.48	127.97	124.20
3	C	604	CLA	CHC-C1C-NC	2.47	127.95	124.20
3	A	613	CLA	CHC-C1C-C2C	-2.47	119.90	126.72
3	C	603	CLA	CHC-C1C-NC	2.46	127.94	124.20
3	B	603	CLA	CHC-C1C-NC	2.46	127.94	124.20
3	A	603	CLA	CHC-C1C-NC	2.46	127.93	124.20
3	C	613	CLA	CHC-C1C-C2C	-2.45	119.94	126.72
3	B	604	CLA	CHC-C1C-NC	2.45	127.92	124.20
3	A	613	CLA	CHC-C1C-NC	2.45	127.92	124.20
3	C	612	CLA	CHC-C1C-NC	2.44	127.91	124.20
3	B	613	CLA	CHC-C1C-C2C	-2.44	119.97	126.72
3	A	612	CLA	CHC-C1C-NC	2.43	127.90	124.20
3	B	611	CLA	CHC-C1C-C2C	-2.43	120.00	126.72
3	B	613	CLA	CHC-C1C-NC	2.43	127.89	124.20
3	C	611	CLA	CHC-C1C-C2C	-2.43	120.01	126.72
3	A	611	CLA	CHC-C1C-C2C	-2.43	120.01	126.72
3	A	603	CLA	C2C-C1C-NC	2.42	112.24	109.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	603	CLA	C1-C2-C3	-2.42	121.86	126.04
2	B	610	CHL	C1-C2-C3	-2.41	121.87	126.04
5	C	615	0UR	C29-C30-C31	2.41	114.48	111.74
3	C	613	CLA	CHC-C1C-NC	2.41	127.85	124.20
5	A	615	0UR	C36-C28-C38	-2.40	104.36	107.89
3	B	611	CLA	CHC-C1C-NC	2.40	127.84	124.20
3	B	603	CLA	C2C-C1C-NC	2.39	112.21	109.97
5	B	615	0UR	C36-C28-C38	-2.39	104.38	107.89
2	A	610	CHL	C1-C2-C3	-2.39	121.92	126.04
3	C	603	CLA	C2C-C1C-NC	2.38	112.20	109.97
2	B	605	CHL	C3B-C4B-NB	-2.38	106.14	109.21
3	C	611	CLA	CHC-C1C-NC	2.37	127.80	124.20
3	A	611	CLA	C2C-C1C-NC	2.37	112.19	109.97
3	C	613	CLA	C2C-C1C-NC	2.37	112.19	109.97
3	A	611	CLA	CHC-C1C-NC	2.36	127.78	124.20
3	C	611	CLA	C2C-C1C-NC	2.35	112.17	109.97
5	C	615	0UR	C36-C28-C38	-2.34	104.44	107.89
3	B	604	CLA	CHA-C1A-NA	-2.33	121.06	126.40
3	A	613	CLA	C2C-C1C-NC	2.33	112.15	109.97
2	A	605	CHL	C3B-C4B-NB	-2.33	106.20	109.21
3	A	604	CLA	CHA-C1A-NA	-2.32	121.09	126.40
5	A	615	0UR	O42-C2-C41	2.31	123.92	120.58
3	B	611	CLA	C2C-C1C-NC	2.31	112.14	109.97
2	B	606	CHL	C3B-C4B-NB	-2.30	106.23	109.21
2	C	606	CHL	C3B-C4B-NB	-2.30	106.23	109.21
3	C	613	CLA	CHA-C1A-NA	-2.30	121.13	126.40
5	B	615	0UR	O42-C2-C41	2.30	123.91	120.58
3	B	613	CLA	CHA-C1A-NA	-2.29	121.15	126.40
2	C	610	CHL	C1-C2-C3	-2.29	122.08	126.04
3	B	613	CLA	C2C-C1C-NC	2.29	112.12	109.97
3	A	613	CLA	CHA-C1A-NA	-2.29	121.15	126.40
3	B	604	CLA	C1B-CHB-C4A	-2.29	125.59	130.12
3	C	604	CLA	CHA-C1A-NA	-2.28	121.17	126.40
2	A	606	CHL	C3B-C4B-NB	-2.28	106.27	109.21
2	C	605	CHL	C3B-C4B-NB	-2.28	106.27	109.21
3	C	604	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
3	A	604	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
2	C	602	CHL	C1-C2-C3	-2.25	122.16	126.04
6	C	616	0IE	O1-C2-C30	2.23	123.81	120.58
2	B	602	CHL	CMB-C2B-C3B	2.23	128.84	124.68
2	C	602	CHL	CMB-C2B-C3B	2.22	128.83	124.68
3	C	613	CLA	C1B-CHB-C4A	-2.20	125.77	130.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	613	CLA	C1B-CHB-C4A	-2.19	125.77	130.12
2	A	602	CHL	CMB-C2B-C3B	2.18	128.76	124.68
3	B	613	CLA	C1B-CHB-C4A	-2.18	125.80	130.12
2	A	607	CHL	C3A-C2A-C1A	2.18	104.60	101.34
5	C	615	OUR	O42-C2-C41	2.17	123.72	120.58
3	A	611	CLA	C1B-CHB-C4A	-2.17	125.82	130.12
2	C	602	CHL	C3B-C4B-NB	-2.17	106.41	109.21
2	B	610	CHL	C3B-C4B-NB	-2.16	106.42	109.21
2	C	606	CHL	CMB-C2B-C3B	2.16	128.72	124.68
2	C	607	CHL	C3A-C2A-C1A	2.16	104.57	101.34
2	C	609	CHL	C3B-C4B-NB	-2.15	106.42	109.21
2	A	608	CHL	C3B-C4B-NB	-2.15	106.43	109.21
2	A	602	CHL	C1-C2-C3	-2.15	122.33	126.04
2	C	602	CHL	CHD-C1D-C2D	2.15	129.98	125.48
2	A	602	CHL	C3B-C4B-NB	-2.14	106.44	109.21
2	A	609	CHL	C3B-C4B-NB	-2.14	106.44	109.21
3	C	611	CLA	C1B-CHB-C4A	-2.14	125.88	130.12
2	B	607	CHL	C3A-C2A-C1A	2.14	104.54	101.34
3	B	611	CLA	C1B-CHB-C4A	-2.14	125.88	130.12
3	A	612	CLA	CHA-C1A-NA	-2.14	121.50	126.40
2	B	609	CHL	C3B-C4B-NB	-2.14	106.45	109.21
2	B	602	CHL	C3B-C4B-NB	-2.13	106.46	109.21
2	B	606	CHL	CMB-C2B-C3B	2.13	128.66	124.68
2	A	602	CHL	CHD-C1D-C2D	2.13	129.94	125.48
2	B	607	CHL	CAA-C2A-C1A	2.13	118.95	111.97
3	B	612	CLA	CHA-C1A-NA	-2.13	121.53	126.40
2	C	610	CHL	C3B-C4B-NB	-2.12	106.47	109.21
2	C	607	CHL	CAA-C2A-C1A	2.12	118.93	111.97
2	B	606	CHL	CHA-C1A-NA	-2.12	121.54	126.40
3	C	612	CLA	CHA-C1A-NA	-2.12	121.54	126.40
2	B	608	CHL	C3B-C4B-NB	-2.12	106.47	109.21
2	A	607	CHL	CAA-C2A-C1A	2.12	118.92	111.97
2	A	606	CHL	CHA-C1A-NA	-2.12	121.55	126.40
2	B	602	CHL	C1-C2-C3	-2.12	122.38	126.04
2	C	607	CHL	CMB-C2B-C3B	2.12	128.64	124.68
2	A	609	CHL	CMB-C2B-C3B	2.12	128.64	124.68
2	A	610	CHL	C3B-C4B-NB	-2.11	106.48	109.21
2	B	601	CHL	CHA-C1A-NA	-2.11	121.56	126.40
2	A	601	CHL	CHA-C1A-NA	-2.11	121.56	126.40
2	B	602	CHL	CHD-C1D-C2D	2.11	129.91	125.48
2	C	601	CHL	CHA-C1A-NA	-2.11	121.57	126.40
2	A	607	CHL	CMB-C2B-C3B	2.11	128.62	124.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	607	CHL	CMB-C2B-C3B	2.11	128.62	124.68
2	A	609	CHL	CHD-C1D-C2D	2.11	129.90	125.48
3	C	604	CLA	CMB-C2B-C1B	-2.10	125.23	128.46
2	C	609	CHL	CHD-C1D-C2D	2.10	129.89	125.48
2	C	606	CHL	CHA-C1A-NA	-2.10	121.58	126.40
3	A	613	CLA	CAA-C2A-C1A	-2.09	105.11	111.97
2	A	606	CHL	CHD-C1D-C2D	2.09	129.87	125.48
3	C	613	CLA	CAA-C2A-C1A	-2.09	105.13	111.97
2	C	607	CHL	CHA-C1A-NA	-2.09	121.61	126.40
2	C	606	CHL	CHD-C1D-C2D	2.09	129.86	125.48
2	B	609	CHL	CMB-C2B-C3B	2.09	128.58	124.68
2	B	607	CHL	CHA-C1A-NA	-2.09	121.62	126.40
2	A	607	CHL	C3B-C4B-NB	-2.08	106.52	109.21
2	B	608	CHL	CHA-C1A-NA	-2.08	121.63	126.40
2	C	609	CHL	CMB-C2B-C3B	2.08	128.57	124.68
2	B	609	CHL	CHD-C1D-C2D	2.08	129.84	125.48
2	A	605	CHL	CHA-C1A-NA	-2.08	121.63	126.40
2	B	607	CHL	C3B-C4B-NB	-2.08	106.52	109.21
2	A	605	CHL	CHD-C1D-C2D	2.08	129.84	125.48
2	B	606	CHL	CHD-C1D-C2D	2.08	129.84	125.48
2	A	606	CHL	CMB-C2B-C3B	2.08	128.57	124.68
2	C	607	CHL	C3B-C4B-NB	-2.08	106.53	109.21
2	B	605	CHL	CHD-C1D-C2D	2.08	129.84	125.48
2	C	605	CHL	CHD-C1D-C2D	2.08	129.83	125.48
3	B	613	CLA	CAA-C2A-C1A	-2.07	105.18	111.97
3	A	604	CLA	CMB-C2B-C1B	-2.07	125.28	128.46
2	C	607	CHL	CHD-C1D-C2D	2.07	129.82	125.48
2	A	607	CHL	CHA-C1A-NA	-2.07	121.66	126.40
3	B	604	CLA	CMB-C2B-C1B	-2.07	125.29	128.46
2	C	605	CHL	CHA-C1A-NA	-2.06	121.67	126.40
5	C	615	OUR	C24-C25-C26	-2.06	107.48	110.30
2	C	609	CHL	CHA-C1A-NA	-2.06	121.67	126.40
2	C	610	CHL	CHD-C1D-C2D	2.06	129.80	125.48
2	A	609	CHL	CHA-C1A-NA	-2.06	121.68	126.40
3	A	611	CLA	CMB-C2B-C1B	-2.06	125.30	128.46
3	C	611	CLA	CMB-C2B-C1B	-2.06	125.30	128.46
2	C	601	CHL	C3B-C4B-NB	-2.06	106.55	109.21
2	B	608	CHL	CHD-C1D-C2D	2.06	129.79	125.48
2	B	605	CHL	CHA-C1A-NA	-2.05	121.69	126.40
2	C	610	CHL	CHA-C1A-NA	-2.05	121.69	126.40
2	A	608	CHL	CHD-C1D-C2D	2.05	129.78	125.48
3	B	612	CLA	CMB-C2B-C1B	-2.05	125.32	128.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	610	CHL	CHA-C1A-NA	-2.05	121.71	126.40
2	B	610	CHL	CHA-C1A-NA	-2.05	121.71	126.40
2	B	609	CHL	CHA-C1A-NA	-2.05	121.71	126.40
2	A	608	CHL	CHA-C1A-NA	-2.04	121.72	126.40
3	B	611	CLA	CMB-C2B-C1B	-2.04	125.33	128.46
3	A	612	CLA	CMB-C2B-C1B	-2.04	125.33	128.46
5	A	615	0UR	C24-C25-C26	-2.04	107.51	110.30
2	C	608	CHL	CHA-C1A-NA	-2.04	121.73	126.40
2	A	610	CHL	CHD-C1D-C2D	2.04	129.75	125.48
3	A	613	CLA	CMB-C2B-C1B	-2.04	125.34	128.46
2	B	607	CHL	CHD-C1D-C2D	2.03	129.75	125.48
2	B	607	CHL	CHC-C1C-C2C	-2.03	118.75	126.11
2	C	608	CHL	CHD-C1D-C2D	2.03	129.73	125.48
2	A	607	CHL	CHD-C1D-C2D	2.03	129.73	125.48
2	A	601	CHL	C3B-C4B-NB	-2.03	106.59	109.21
3	B	613	CLA	CMB-C2B-C1B	-2.02	125.35	128.46
3	C	613	CLA	CMB-C2B-C1B	-2.02	125.35	128.46
2	C	607	CHL	CHC-C1C-C2C	-2.02	118.78	126.11
2	B	601	CHL	CMB-C2B-C3B	2.02	128.46	124.68
2	C	602	CHL	CHA-C1A-NA	-2.02	121.78	126.40
2	A	601	CHL	CHD-C1D-C2D	2.02	129.71	125.48
2	A	607	CHL	CHC-C1C-C2C	-2.01	118.81	126.11
3	C	612	CLA	CMB-C2B-C1B	-2.01	125.37	128.46
3	B	603	CLA	CMB-C2B-C1B	-2.01	125.37	128.46
2	C	601	CHL	CHD-C1D-C2D	2.00	129.69	125.48
5	B	615	0UR	C24-C25-C26	-2.00	107.56	110.30
2	B	601	CHL	CHD-C1D-C2D	2.00	129.68	125.48
2	A	601	CHL	CHC-C1C-C2C	-2.00	118.85	126.11
2	C	601	CHL	CMB-C2B-C3B	2.00	128.42	124.68
2	B	601	CHL	C3B-C4B-NB	-2.00	106.62	109.21

All (105) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	601	CHL	NA
2	A	601	CHL	ND
2	A	601	CHL	NC
2	A	602	CHL	NA
2	A	602	CHL	C8
2	A	602	CHL	ND
2	A	602	CHL	NC
2	A	605	CHL	NA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
2	A	605	CHL	ND
2	A	605	CHL	NC
2	A	606	CHL	NA
2	A	606	CHL	ND
2	A	606	CHL	NC
2	A	607	CHL	NA
2	A	607	CHL	ND
2	A	607	CHL	NC
2	A	608	CHL	NA
2	A	608	CHL	C8
2	A	608	CHL	ND
2	A	608	CHL	NC
2	A	609	CHL	NA
2	A	609	CHL	C8
2	A	609	CHL	ND
2	A	609	CHL	NC
2	A	610	CHL	NA
2	A	610	CHL	C8
2	A	610	CHL	ND
2	A	610	CHL	NC
2	B	601	CHL	NA
2	B	601	CHL	ND
2	B	601	CHL	NC
2	B	602	CHL	NA
2	B	602	CHL	C8
2	B	602	CHL	ND
2	B	602	CHL	NC
2	B	605	CHL	NA
2	B	605	CHL	ND
2	B	605	CHL	NC
2	B	606	CHL	NA
2	B	606	CHL	ND
2	B	606	CHL	NC
2	B	607	CHL	NA
2	B	607	CHL	ND
2	B	607	CHL	NC
2	B	608	CHL	NA
2	B	608	CHL	C8
2	B	608	CHL	ND
2	B	608	CHL	NC
2	B	609	CHL	NA
2	B	609	CHL	C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
2	B	609	CHL	ND
2	B	609	CHL	NC
2	B	610	CHL	NA
2	B	610	CHL	C8
2	B	610	CHL	ND
2	B	610	CHL	NC
2	C	601	CHL	NA
2	C	601	CHL	ND
2	C	601	CHL	NC
2	C	602	CHL	NA
2	C	602	CHL	C8
2	C	602	CHL	ND
2	C	602	CHL	NC
2	C	605	CHL	NA
2	C	605	CHL	ND
2	C	605	CHL	NC
2	C	606	CHL	NA
2	C	606	CHL	ND
2	C	606	CHL	NC
2	C	607	CHL	NA
2	C	607	CHL	ND
2	C	607	CHL	NC
2	C	608	CHL	NA
2	C	608	CHL	C8
2	C	608	CHL	ND
2	C	608	CHL	NC
2	C	609	CHL	NA
2	C	609	CHL	C8
2	C	609	CHL	ND
2	C	609	CHL	NC
2	C	610	CHL	NA
2	C	610	CHL	C8
2	C	610	CHL	ND
2	C	610	CHL	NC
3	A	603	CLA	ND
3	A	603	CLA	C8
3	A	604	CLA	ND
3	A	611	CLA	ND
3	A	611	CLA	C8
3	A	612	CLA	ND
3	A	613	CLA	ND
3	B	603	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
3	B	603	CLA	C8
3	B	604	CLA	ND
3	B	611	CLA	ND
3	B	611	CLA	C8
3	B	612	CLA	ND
3	B	613	CLA	ND
3	C	603	CLA	ND
3	C	603	CLA	C8
3	C	604	CLA	ND
3	C	611	CLA	ND
3	C	611	CLA	C8
3	C	612	CLA	ND
3	C	613	CLA	ND

All (235) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	CHL	C1C-C2C-CMC-OMC
2	A	601	CHL	C3C-C2C-CMC-OMC
2	A	601	CHL	C2-C3-C5-C6
2	A	602	CHL	C1C-C2C-CMC-OMC
2	A	605	CHL	C3A-C2A-CAA-CBA
2	A	605	CHL	C1C-C2C-CMC-OMC
2	A	605	CHL	C3C-C2C-CMC-OMC
2	A	606	CHL	C1A-C2A-CAA-CBA
2	A	606	CHL	C1C-C2C-CMC-OMC
2	A	607	CHL	C1C-C2C-CMC-OMC
2	A	607	CHL	C3C-C2C-CMC-OMC
2	A	608	CHL	C3C-C2C-CMC-OMC
2	A	609	CHL	C1C-C2C-CMC-OMC
2	A	609	CHL	C3C-C2C-CMC-OMC
2	A	610	CHL	C1A-C2A-CAA-CBA
2	A	610	CHL	C3A-C2A-CAA-CBA
2	A	610	CHL	C1C-C2C-CMC-OMC
2	A	610	CHL	C3C-C2C-CMC-OMC
2	A	610	CHL	C2-C3-C5-C6
2	A	610	CHL	C4-C3-C5-C6
2	B	601	CHL	C1C-C2C-CMC-OMC
2	B	601	CHL	C3C-C2C-CMC-OMC
2	B	601	CHL	C2-C3-C5-C6
2	B	602	CHL	C1C-C2C-CMC-OMC
2	B	602	CHL	C3C-C2C-CMC-OMC

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	605	CHL	C3A-C2A-CAA-CBA
2	B	605	CHL	C1C-C2C-CMC-OMC
2	B	605	CHL	C3C-C2C-CMC-OMC
2	B	606	CHL	C1A-C2A-CAA-CBA
2	B	606	CHL	C1C-C2C-CMC-OMC
2	B	607	CHL	C1C-C2C-CMC-OMC
2	B	607	CHL	C3C-C2C-CMC-OMC
2	B	608	CHL	C3C-C2C-CMC-OMC
2	B	609	CHL	C1C-C2C-CMC-OMC
2	B	609	CHL	C3C-C2C-CMC-OMC
2	B	610	CHL	C1A-C2A-CAA-CBA
2	B	610	CHL	C3A-C2A-CAA-CBA
2	B	610	CHL	C1C-C2C-CMC-OMC
2	B	610	CHL	C3C-C2C-CMC-OMC
2	B	610	CHL	C2-C3-C5-C6
2	B	610	CHL	C4-C3-C5-C6
2	C	601	CHL	C1C-C2C-CMC-OMC
2	C	601	CHL	C3C-C2C-CMC-OMC
2	C	601	CHL	C2-C3-C5-C6
2	C	602	CHL	C1C-C2C-CMC-OMC
2	C	602	CHL	C3C-C2C-CMC-OMC
2	C	605	CHL	C3A-C2A-CAA-CBA
2	C	605	CHL	C1C-C2C-CMC-OMC
2	C	605	CHL	C3C-C2C-CMC-OMC
2	C	606	CHL	C1A-C2A-CAA-CBA
2	C	606	CHL	C1C-C2C-CMC-OMC
2	C	607	CHL	C1C-C2C-CMC-OMC
2	C	607	CHL	C3C-C2C-CMC-OMC
2	C	609	CHL	C1C-C2C-CMC-OMC
2	C	609	CHL	C3C-C2C-CMC-OMC
2	C	610	CHL	C1A-C2A-CAA-CBA
2	C	610	CHL	C3A-C2A-CAA-CBA
2	C	610	CHL	C1C-C2C-CMC-OMC
2	C	610	CHL	C3C-C2C-CMC-OMC
3	A	604	CLA	C1A-C2A-CAA-CBA
3	A	611	CLA	C2-C3-C5-C6
3	A	611	CLA	C4-C3-C5-C6
3	B	611	CLA	C2-C3-C5-C6
3	B	611	CLA	C4-C3-C5-C6
3	C	611	CLA	C2-C3-C5-C6
3	C	611	CLA	C4-C3-C5-C6
7	A	617	LHG	C1-C2-C3-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	B	617	LHG	C1-C2-C3-O3
7	C	617	LHG	C1-C2-C3-O3
2	C	610	CHL	C4-C3-C5-C6
2	A	608	CHL	C2A-CAA-CBA-CGA
2	B	608	CHL	C2A-CAA-CBA-CGA
2	C	608	CHL	C2A-CAA-CBA-CGA
5	A	615	0UR	O44-C45-C46-C47
5	B	615	0UR	O44-C45-C46-C47
5	C	615	0UR	O44-C45-C46-C47
2	C	610	CHL	C2-C3-C5-C6
5	B	615	0UR	O57-C45-C46-C47
5	C	615	0UR	O57-C45-C46-C47
2	A	608	CHL	C13-C15-C16-C17
2	B	608	CHL	C13-C15-C16-C17
2	C	608	CHL	C13-C15-C16-C17
5	A	615	0UR	O57-C45-C46-C47
7	A	617	LHG	O2-C2-C3-O3
7	B	617	LHG	O2-C2-C3-O3
7	C	617	LHG	O2-C2-C3-O3
3	A	603	CLA	C3-C5-C6-C7
2	A	602	CHL	C13-C15-C16-C17
2	B	602	CHL	C13-C15-C16-C17
2	B	602	CHL	C15-C16-C17-C18
2	C	602	CHL	C13-C15-C16-C17
2	C	602	CHL	C15-C16-C17-C18
3	B	604	CLA	C1A-C2A-CAA-CBA
3	C	604	CLA	C1A-C2A-CAA-CBA
2	A	602	CHL	C15-C16-C17-C18
2	A	608	CHL	C5-C6-C7-C8
2	A	609	CHL	C4-C3-C5-C6
2	C	608	CHL	C5-C6-C7-C8
3	A	611	CLA	CAA-CBA-CGA-O2A
2	C	609	CHL	C4-C3-C5-C6
2	A	606	CHL	C3A-C2A-CAA-CBA
2	B	606	CHL	C3A-C2A-CAA-CBA
2	C	606	CHL	C3A-C2A-CAA-CBA
5	A	615	0UR	C49-C50-C51-C52
2	B	608	CHL	C5-C6-C7-C8
2	A	609	CHL	C2-C3-C5-C6
5	C	615	0UR	C49-C50-C51-C52
2	A	602	CHL	C3C-C2C-CMC-OMC
2	A	606	CHL	C3C-C2C-CMC-OMC

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	606	CHL	C3C-C2C-CMC-OMC
2	C	606	CHL	C3C-C2C-CMC-OMC
3	C	611	CLA	CAA-CBA-CGA-O2A
5	B	615	0UR	C49-C50-C51-C52
2	A	610	CHL	C2-C1-O2A-CGA
2	B	609	CHL	C2-C1-O2A-CGA
2	C	609	CHL	C2-C3-C5-C6
7	C	617	LHG	C11-C12-C13-C14
7	B	617	LHG	C11-C12-C13-C14
2	A	601	CHL	C4-C3-C5-C6
2	B	601	CHL	C4-C3-C5-C6
2	C	601	CHL	C4-C3-C5-C6
7	A	617	LHG	C11-C12-C13-C14
6	A	616	0IE	C13-C14-C15-C16
6	B	616	0IE	C13-C14-C15-C16
6	C	616	0IE	C13-C14-C15-C16
5	A	615	0UR	O42-C2-C3-C4
5	B	615	0UR	O42-C2-C3-C4
5	C	615	0UR	O42-C2-C3-C4
6	A	616	0IE	O1-C2-C3-C4
6	B	616	0IE	O1-C2-C3-C4
6	C	616	0IE	O1-C2-C3-C4
3	B	611	CLA	CAA-CBA-CGA-O2A
3	A	603	CLA	CAD-CBD-CGD-O2D
3	A	604	CLA	CAD-CBD-CGD-O2D
3	B	604	CLA	CAD-CBD-CGD-O2D
3	C	603	CLA	CAD-CBD-CGD-O2D
3	C	604	CLA	CAD-CBD-CGD-O2D
5	B	615	0UR	C48-C49-C50-C51
2	B	609	CHL	C4-C3-C5-C6
2	A	605	CHL	C1A-C2A-CAA-CBA
2	B	605	CHL	C1A-C2A-CAA-CBA
2	C	605	CHL	C1A-C2A-CAA-CBA
5	C	615	0UR	C48-C49-C50-C51
5	A	615	0UR	C48-C49-C50-C51
6	A	616	0IE	O1-C2-C3-C20
6	B	616	0IE	O1-C2-C3-C20
6	C	616	0IE	O1-C2-C3-C20
2	A	608	CHL	C1C-C2C-CMC-OMC
2	B	608	CHL	C1C-C2C-CMC-OMC
2	B	609	CHL	C2-C3-C5-C6
2	A	609	CHL	C2-C1-O2A-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	610	CHL	C2-C1-O2A-CGA
2	C	609	CHL	C2-C1-O2A-CGA
2	C	610	CHL	C2-C1-O2A-CGA
7	A	617	LHG	C3-O3-P-O6
7	B	617	LHG	C3-O3-P-O6
7	C	617	LHG	C3-O3-P-O6
4	A	614	NEX	C39-C29-C30-C31
4	B	614	NEX	C39-C29-C30-C31
4	C	614	NEX	C39-C29-C30-C31
3	A	613	CLA	C1A-C2A-CAA-CBA
3	B	613	CLA	C1A-C2A-CAA-CBA
3	C	613	CLA	C1A-C2A-CAA-CBA
7	A	617	LHG	C29-C30-C31-C32
4	A	614	NEX	C28-C29-C30-C31
4	B	614	NEX	C28-C29-C30-C31
4	C	614	NEX	C28-C29-C30-C31
3	A	612	CLA	CAA-CBA-CGA-O2A
3	B	612	CLA	CAA-CBA-CGA-O2A
2	A	606	CHL	CAA-CBA-CGA-O2A
2	B	606	CHL	CAA-CBA-CGA-O2A
3	B	612	CLA	CAA-CBA-CGA-O1A
7	B	617	LHG	C29-C30-C31-C32
2	C	606	CHL	CAA-CBA-CGA-O2A
3	C	612	CLA	CAA-CBA-CGA-O2A
7	C	617	LHG	O8-C23-C24-C25
3	A	611	CLA	CAA-CBA-CGA-O1A
3	B	613	CLA	CAA-CBA-CGA-O2A
7	A	617	LHG	O8-C23-C24-C25
3	C	613	CLA	CAA-CBA-CGA-O2A
7	C	617	LHG	C29-C30-C31-C32
5	A	615	OUR	C46-C47-C48-C49
5	B	615	OUR	C46-C47-C48-C49
3	A	612	CLA	CAD-CBD-CGD-O2D
3	B	603	CLA	CAD-CBD-CGD-O2D
3	B	612	CLA	CAD-CBD-CGD-O2D
3	C	612	CLA	CAD-CBD-CGD-O2D
7	B	617	LHG	O8-C23-C24-C25
5	C	615	OUR	C46-C47-C48-C49
2	A	608	CHL	C10-C11-C12-C13
3	C	612	CLA	CAA-CBA-CGA-O1A
3	B	613	CLA	CAA-CBA-CGA-O1A
2	B	608	CHL	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	C	608	CHL	C10-C11-C12-C13
3	A	612	CLA	CAA-CBA-CGA-O1A
3	A	613	CLA	CAA-CBA-CGA-O2A
3	C	611	CLA	CAA-CBA-CGA-O1A
2	A	601	CHL	CHA-CBD-CGD-O1D
2	A	601	CHL	CHA-CBD-CGD-O2D
2	A	602	CHL	CHA-CBD-CGD-O1D
2	A	602	CHL	CHA-CBD-CGD-O2D
2	B	601	CHL	CHA-CBD-CGD-O1D
2	B	601	CHL	CHA-CBD-CGD-O2D
2	B	602	CHL	CHA-CBD-CGD-O1D
2	B	602	CHL	CHA-CBD-CGD-O2D
2	C	601	CHL	CHA-CBD-CGD-O1D
2	C	601	CHL	CHA-CBD-CGD-O2D
2	C	602	CHL	CHA-CBD-CGD-O1D
2	C	602	CHL	CHA-CBD-CGD-O2D
2	B	606	CHL	CAA-CBA-CGA-O1A
3	A	613	CLA	CAA-CBA-CGA-O1A
3	C	613	CLA	CAA-CBA-CGA-O1A
2	A	606	CHL	CAA-CBA-CGA-O1A
2	C	606	CHL	CAA-CBA-CGA-O1A
2	A	607	CHL	C1A-C2A-CAA-CBA
3	A	611	CLA	C2-C1-O2A-CGA
2	A	609	CHL	C6-C7-C8-C9
7	B	617	LHG	O10-C23-C24-C25
7	A	617	LHG	O10-C23-C24-C25
7	C	617	LHG	O10-C23-C24-C25
2	C	609	CHL	C6-C7-C8-C9
2	C	602	CHL	CAA-CBA-CGA-O2A
2	C	601	CHL	CAD-CBD-CGD-O1D
2	B	602	CHL	CAA-CBA-CGA-O2A
2	A	605	CHL	CAA-CBA-CGA-O2A
2	B	605	CHL	CAA-CBA-CGA-O2A
3	A	613	CLA	C3A-C2A-CAA-CBA
3	B	613	CLA	C3A-C2A-CAA-CBA
3	C	613	CLA	C3A-C2A-CAA-CBA
5	A	615	OUR	O42-C2-C3-C43
5	B	615	OUR	O42-C2-C3-C43
5	C	615	OUR	O42-C2-C3-C43
2	C	605	CHL	CAA-CBA-CGA-O2A
2	A	602	CHL	CAA-CBA-CGA-O2A
3	B	611	CLA	CAA-CBA-CGA-O1A

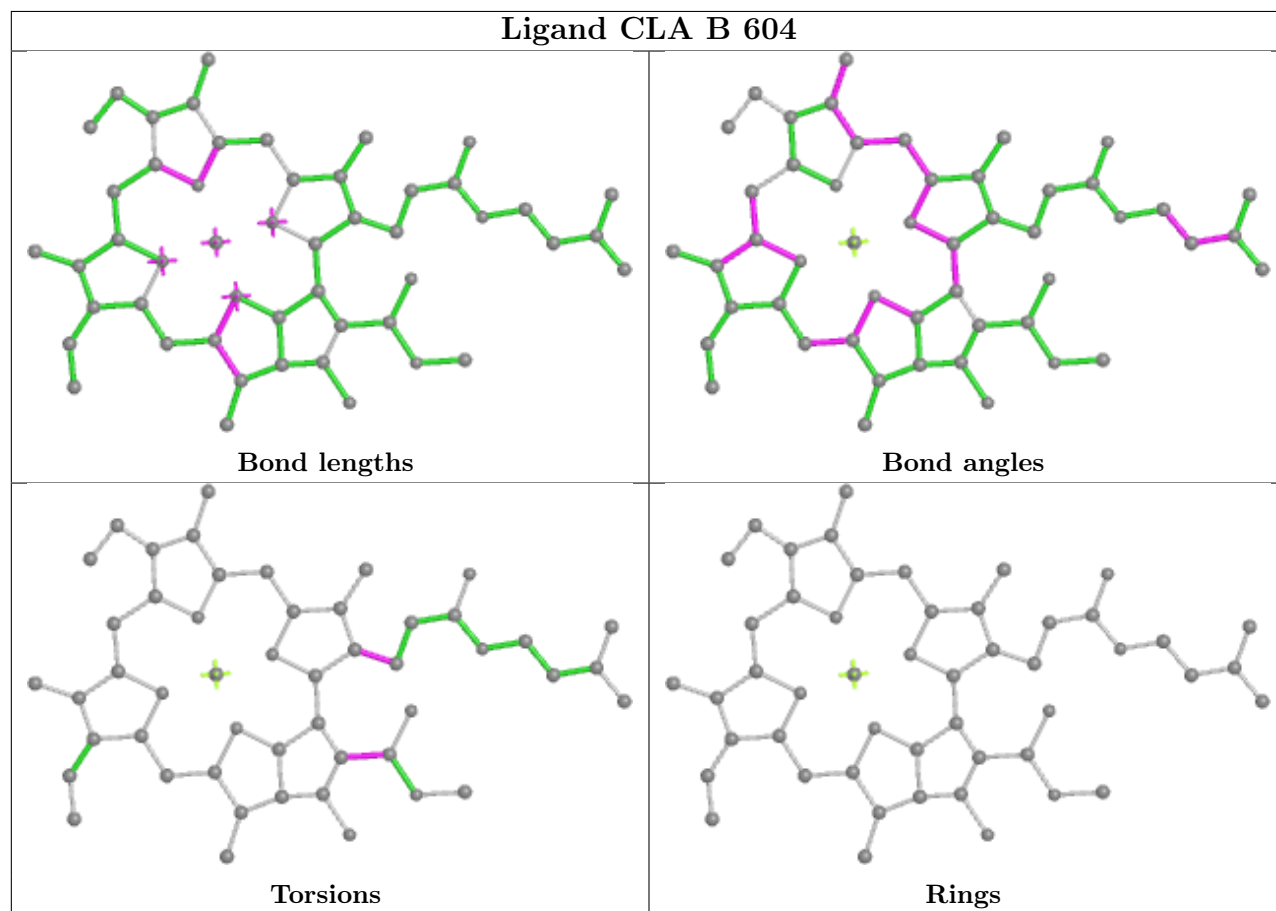
There are no ring outliers.

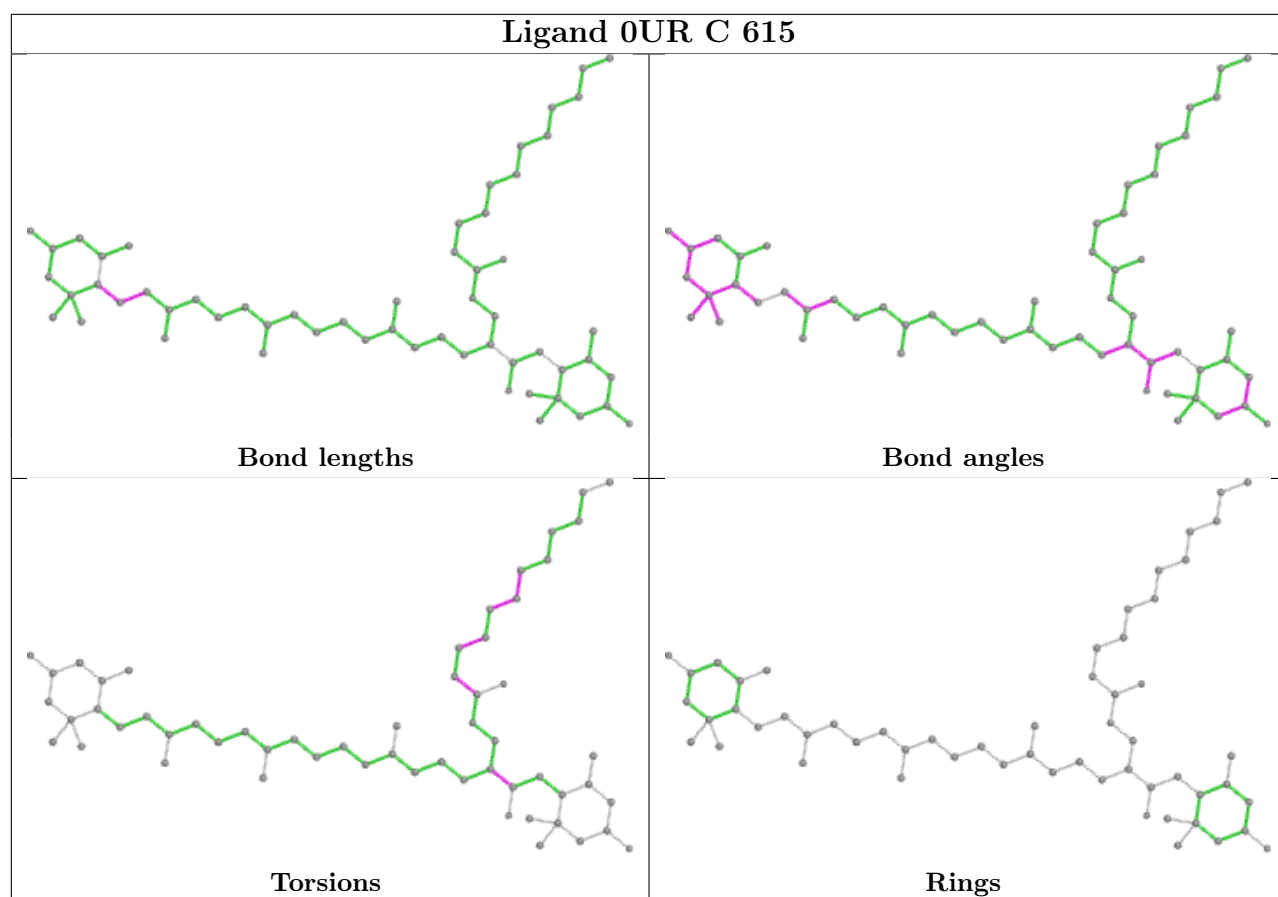
33 monomers are involved in 45 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	604	CLA	1	0
2	A	602	CHL	1	0
4	A	614	NEX	2	0
3	A	611	CLA	1	0
2	C	609	CHL	1	0
4	B	614	NEX	1	0
7	C	617	LHG	1	0
7	A	617	LHG	1	0
2	B	610	CHL	3	0
2	C	602	CHL	1	0
2	A	605	CHL	2	0
2	A	606	CHL	2	0
3	B	603	CLA	1	0
2	C	601	CHL	1	0
4	C	614	NEX	2	0
3	C	611	CLA	1	0
2	A	601	CHL	1	0
2	B	605	CHL	3	0
2	B	602	CHL	1	0
2	C	606	CHL	1	0
2	C	610	CHL	2	0
2	B	608	CHL	3	0
2	A	609	CHL	2	0
2	A	610	CHL	2	0
2	B	601	CHL	1	0
2	C	605	CHL	2	0
7	B	617	LHG	1	0
2	B	606	CHL	2	0
3	A	604	CLA	1	0
3	A	603	CLA	1	0
3	C	604	CLA	1	0
2	A	608	CHL	3	0
2	B	609	CHL	2	0

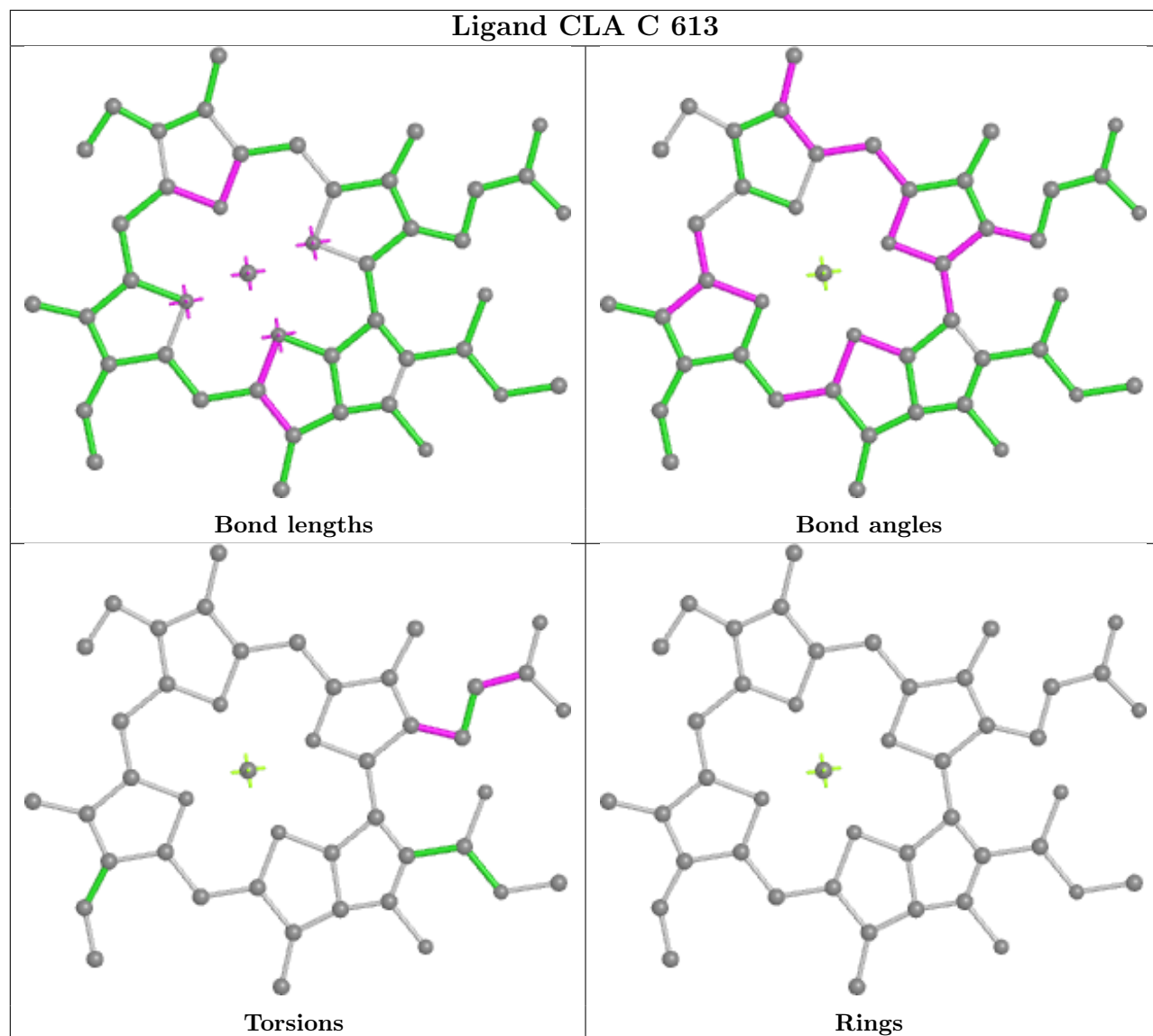
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

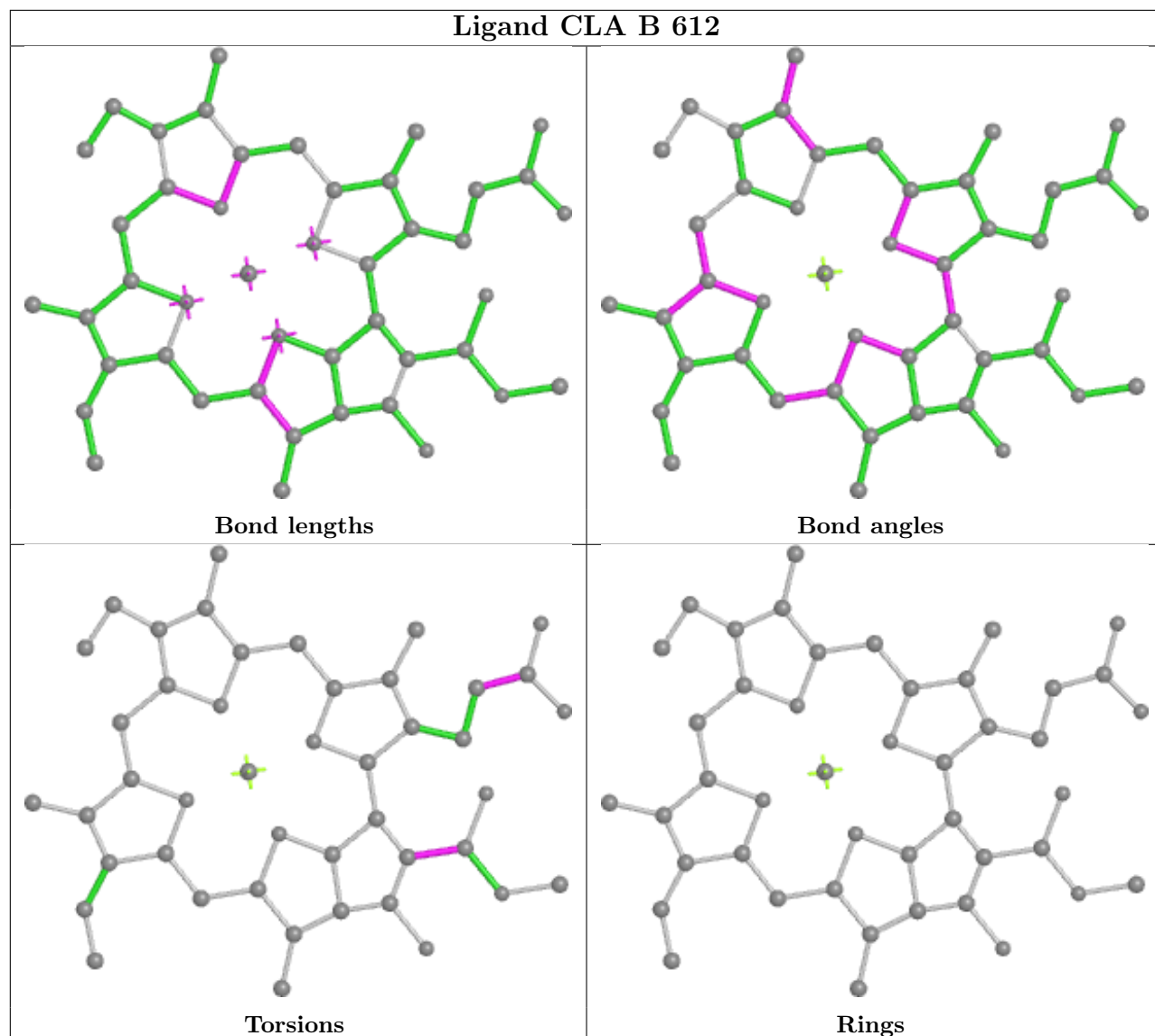




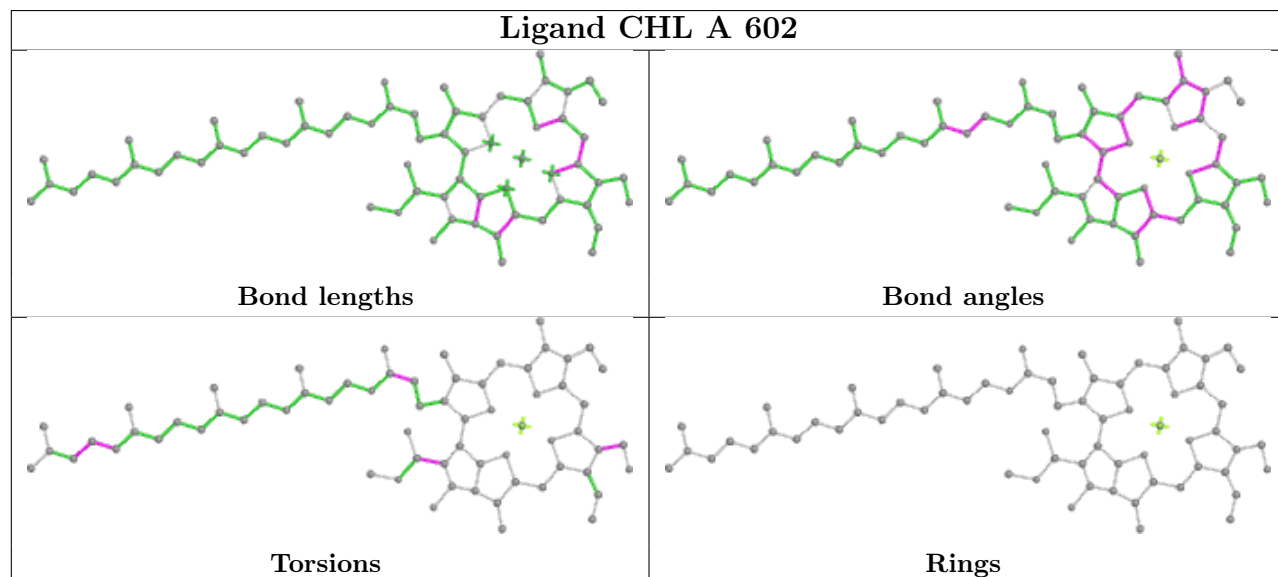
Ligand CLA C 613

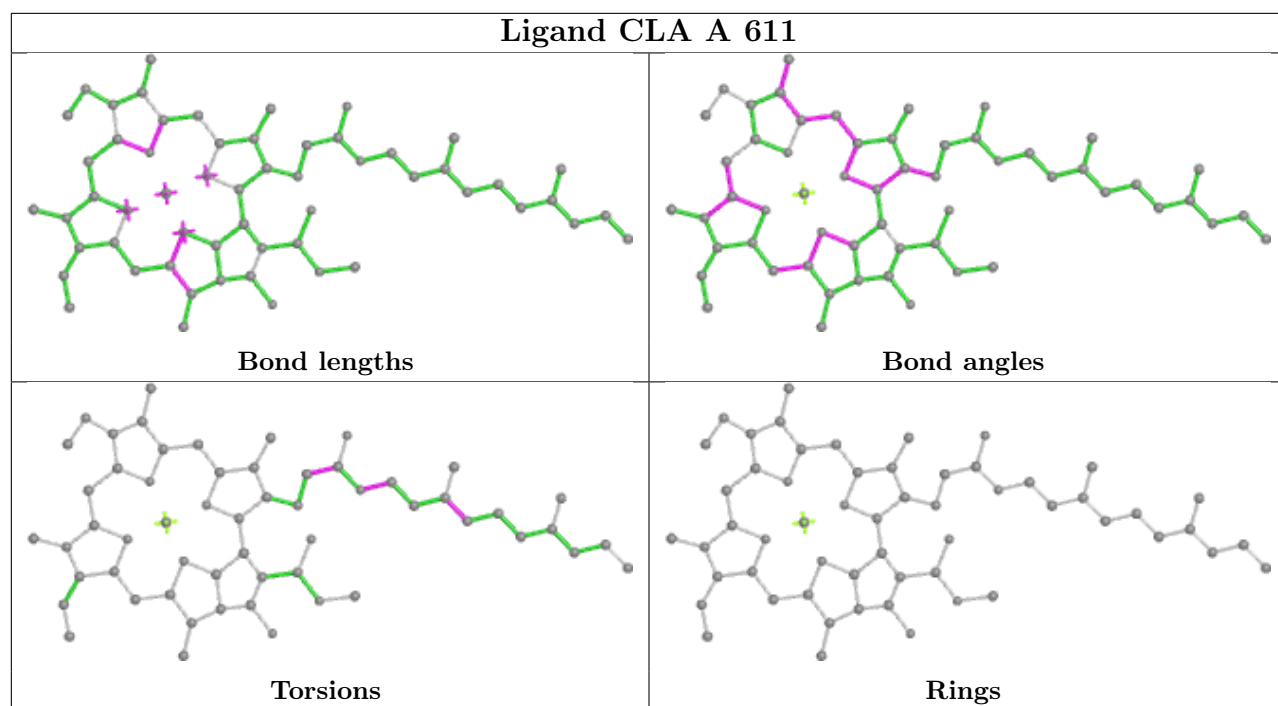
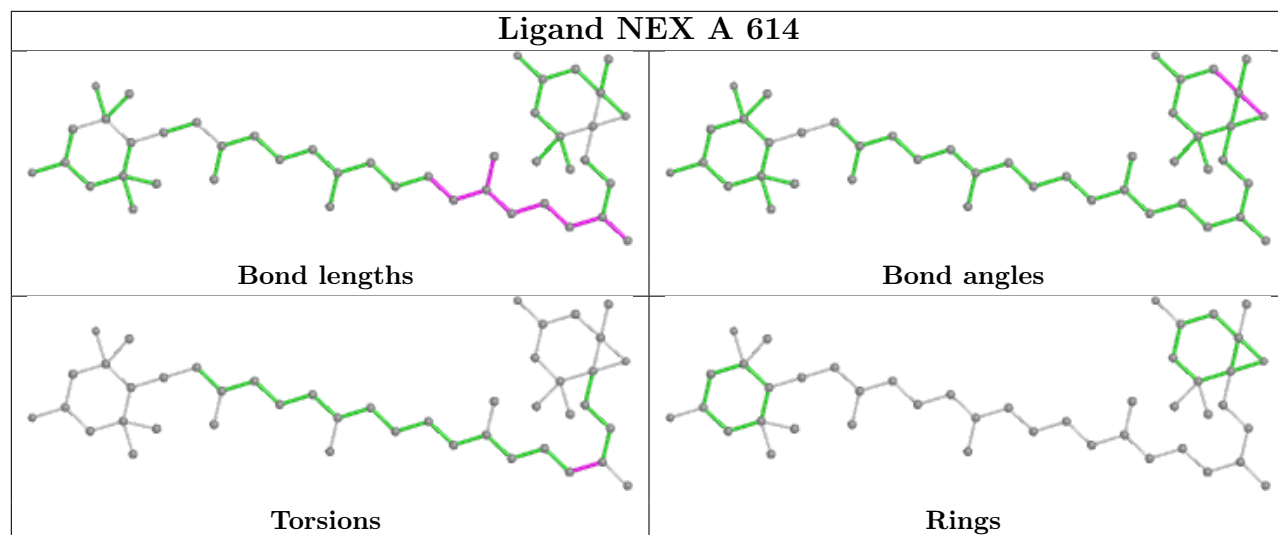


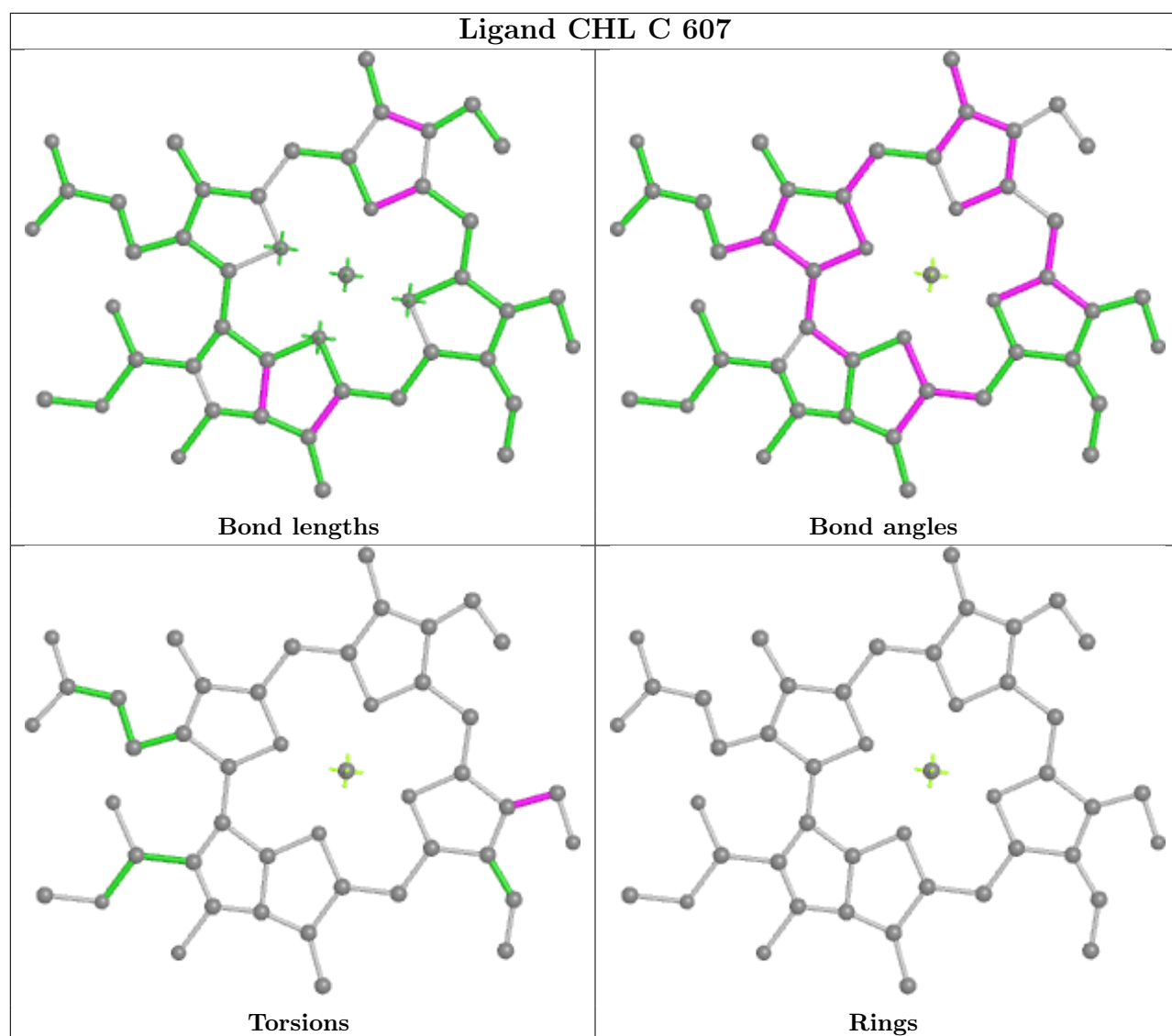
Ligand CLA B 612

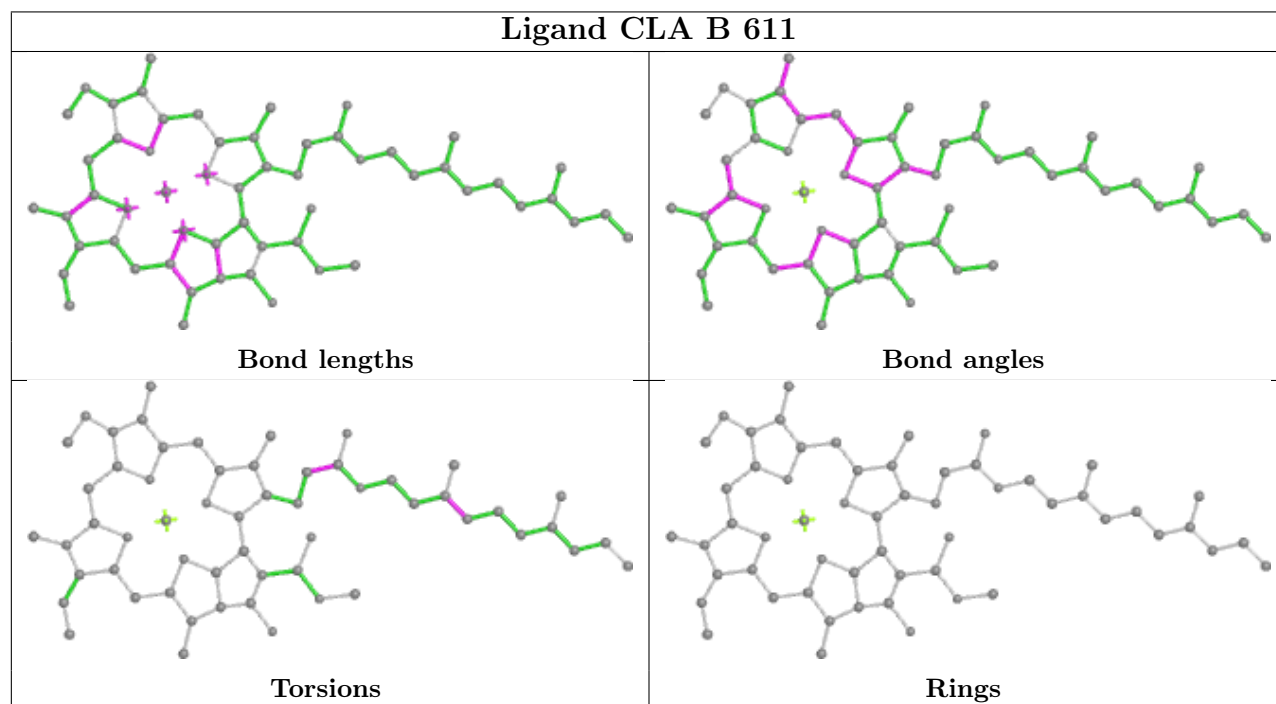
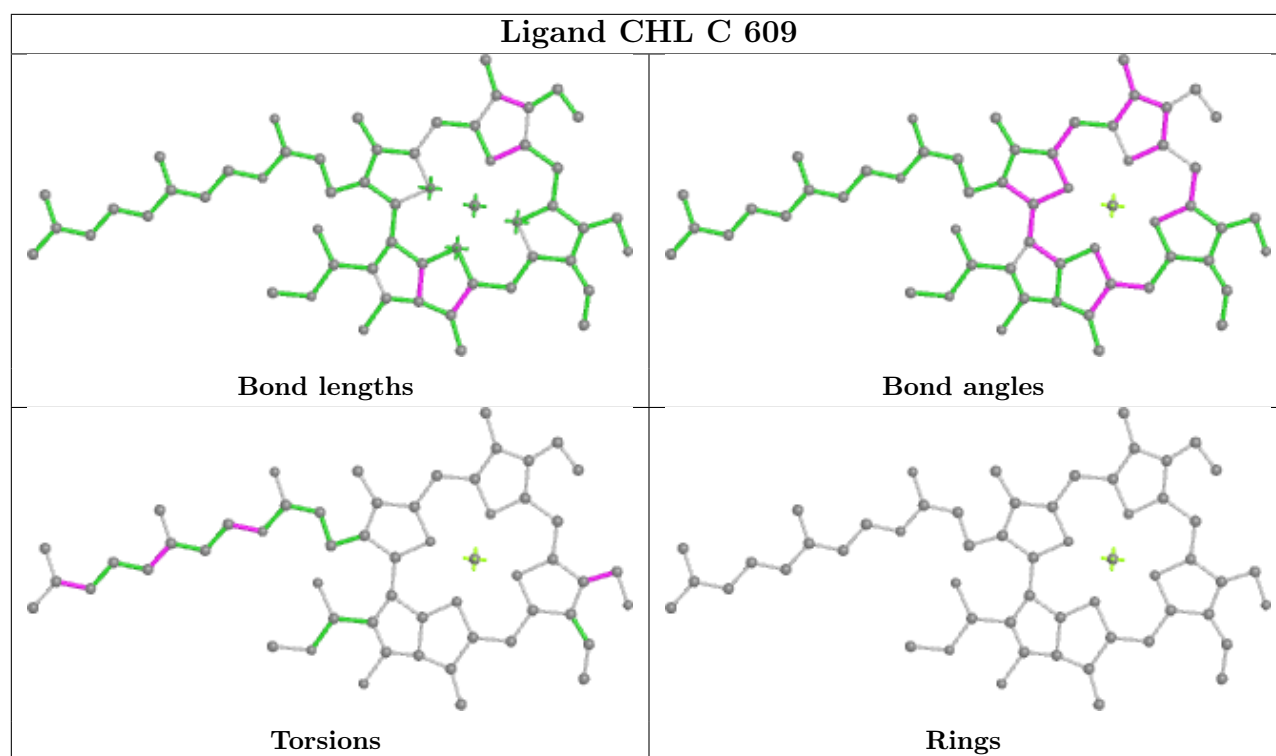


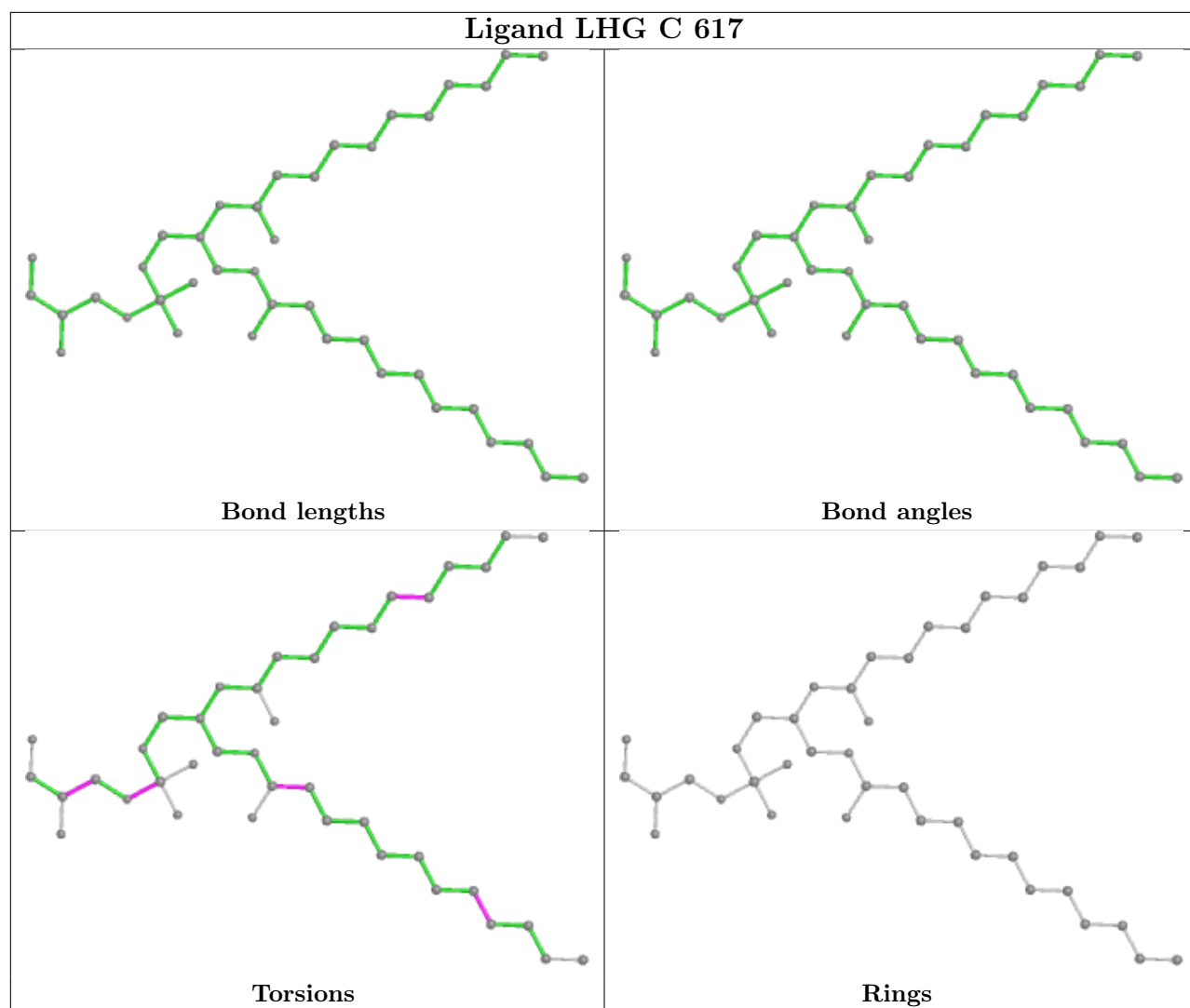
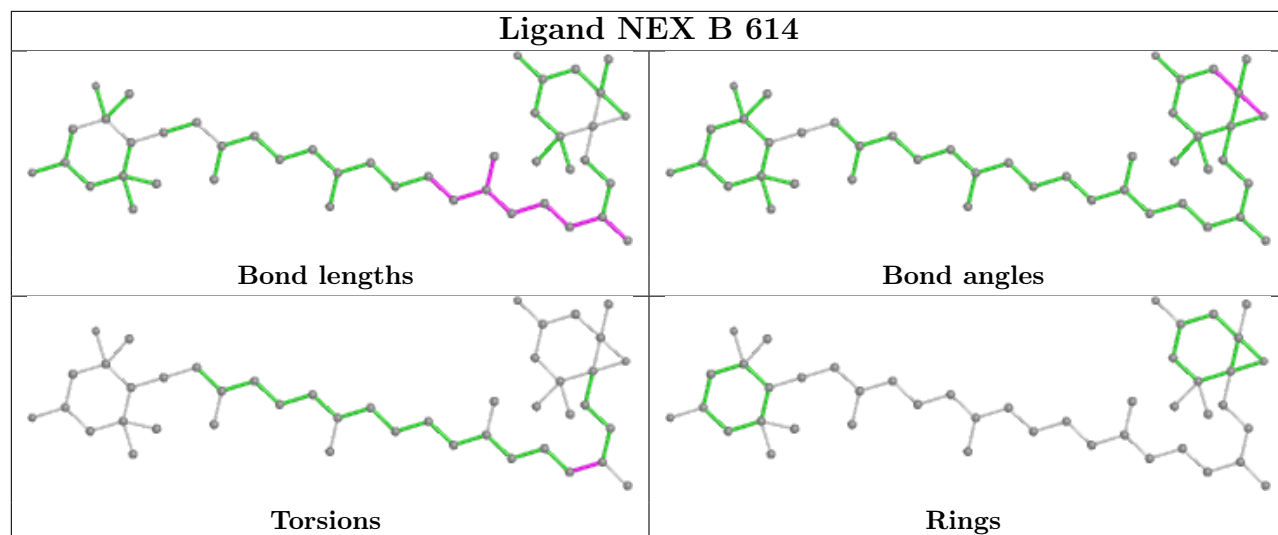
Ligand CHL A 602

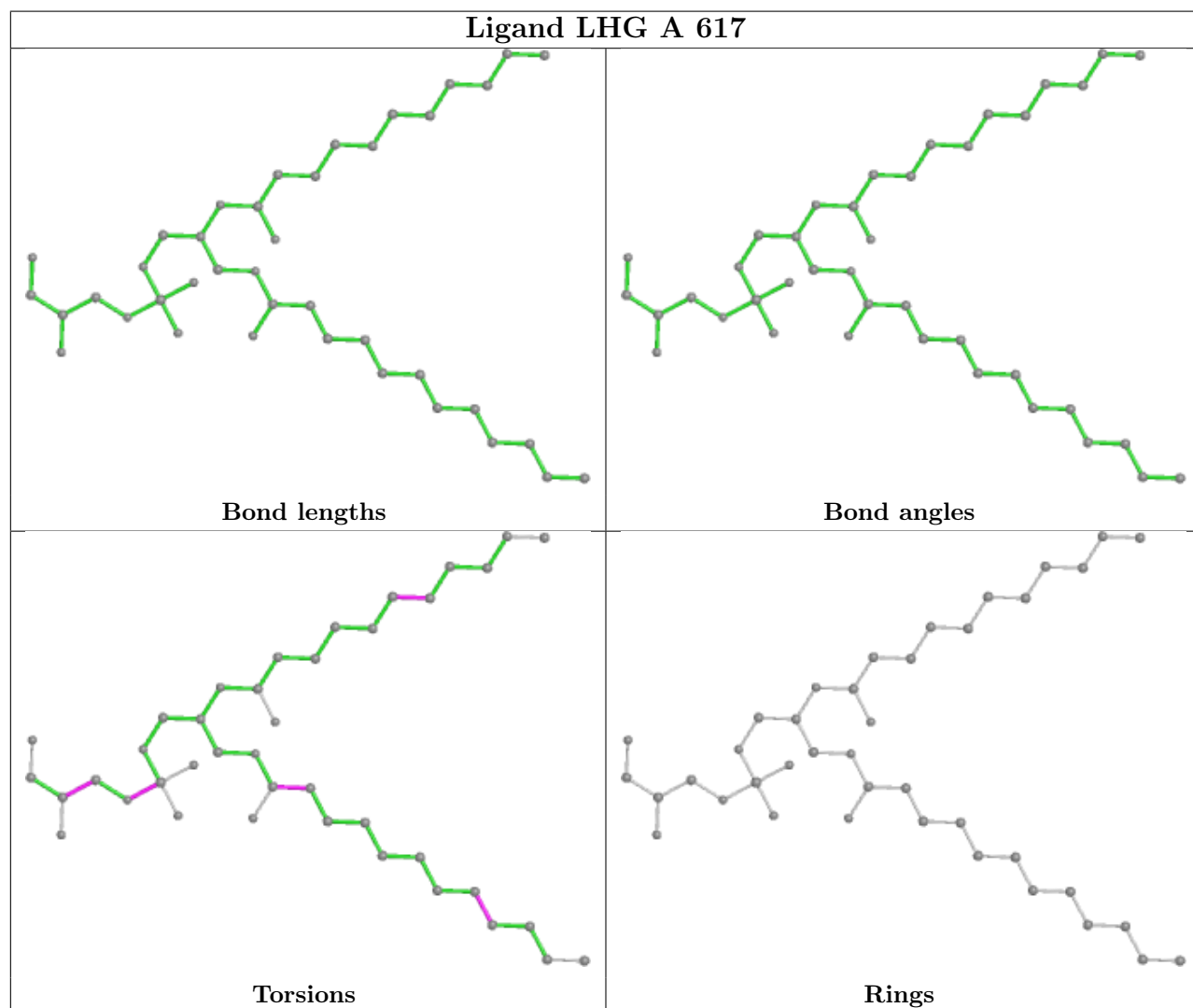
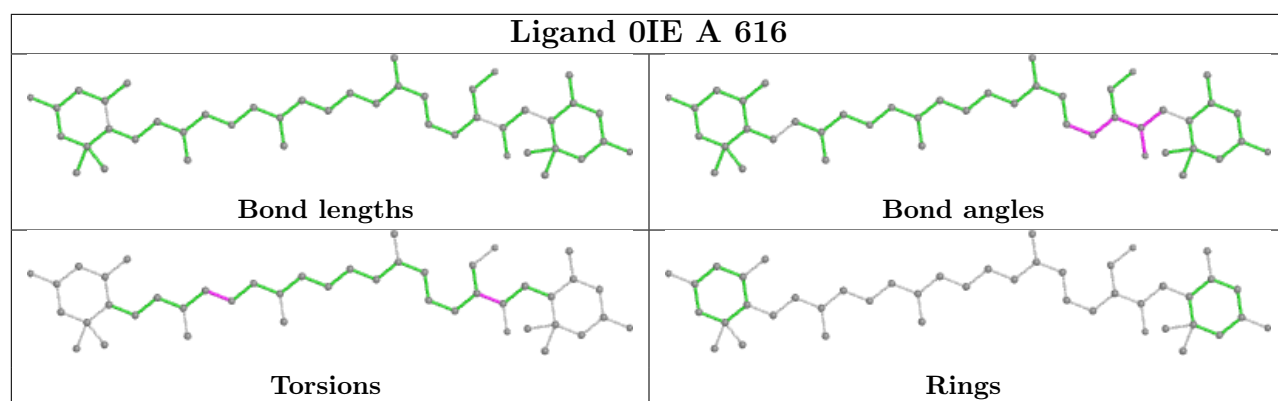


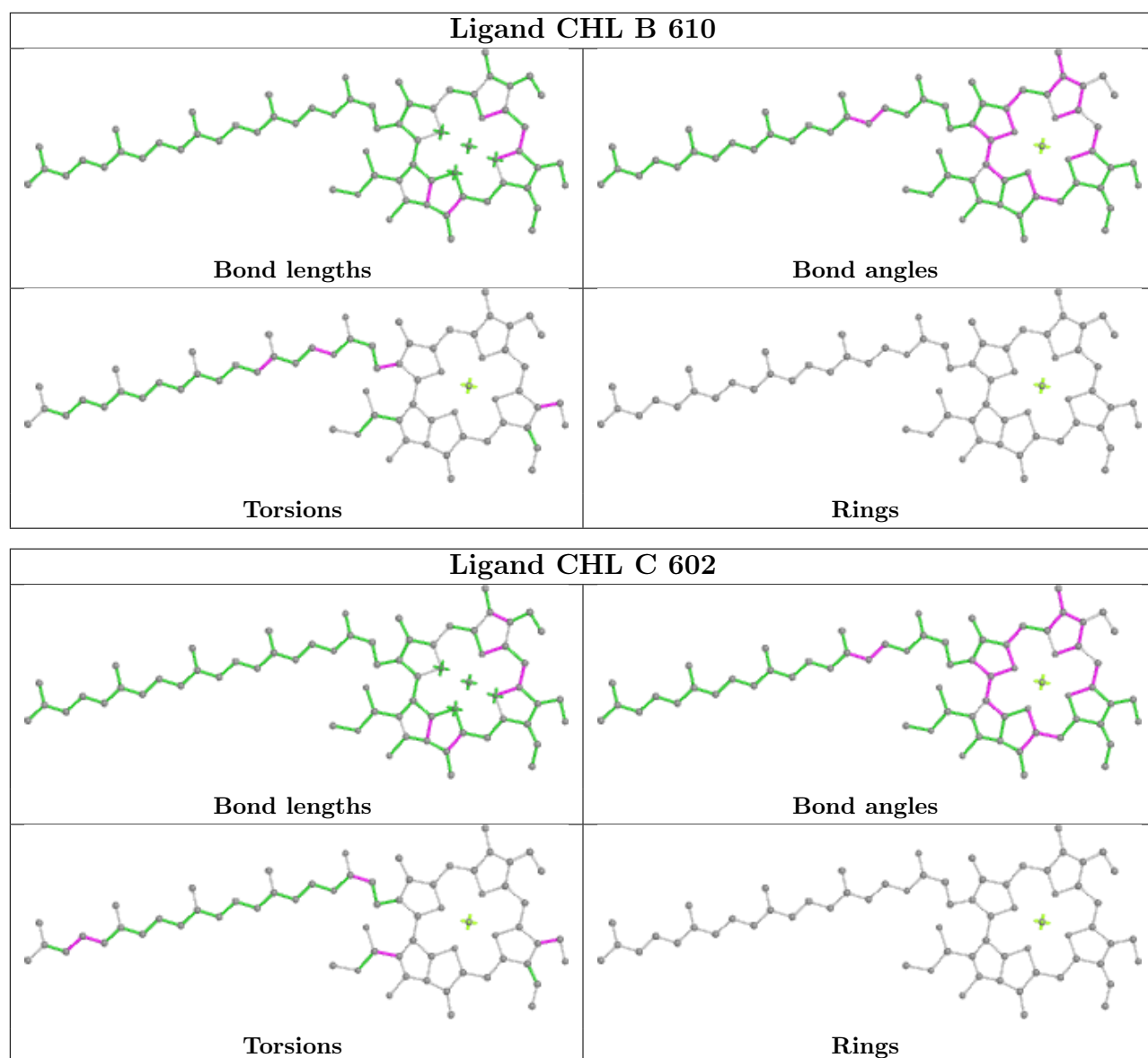


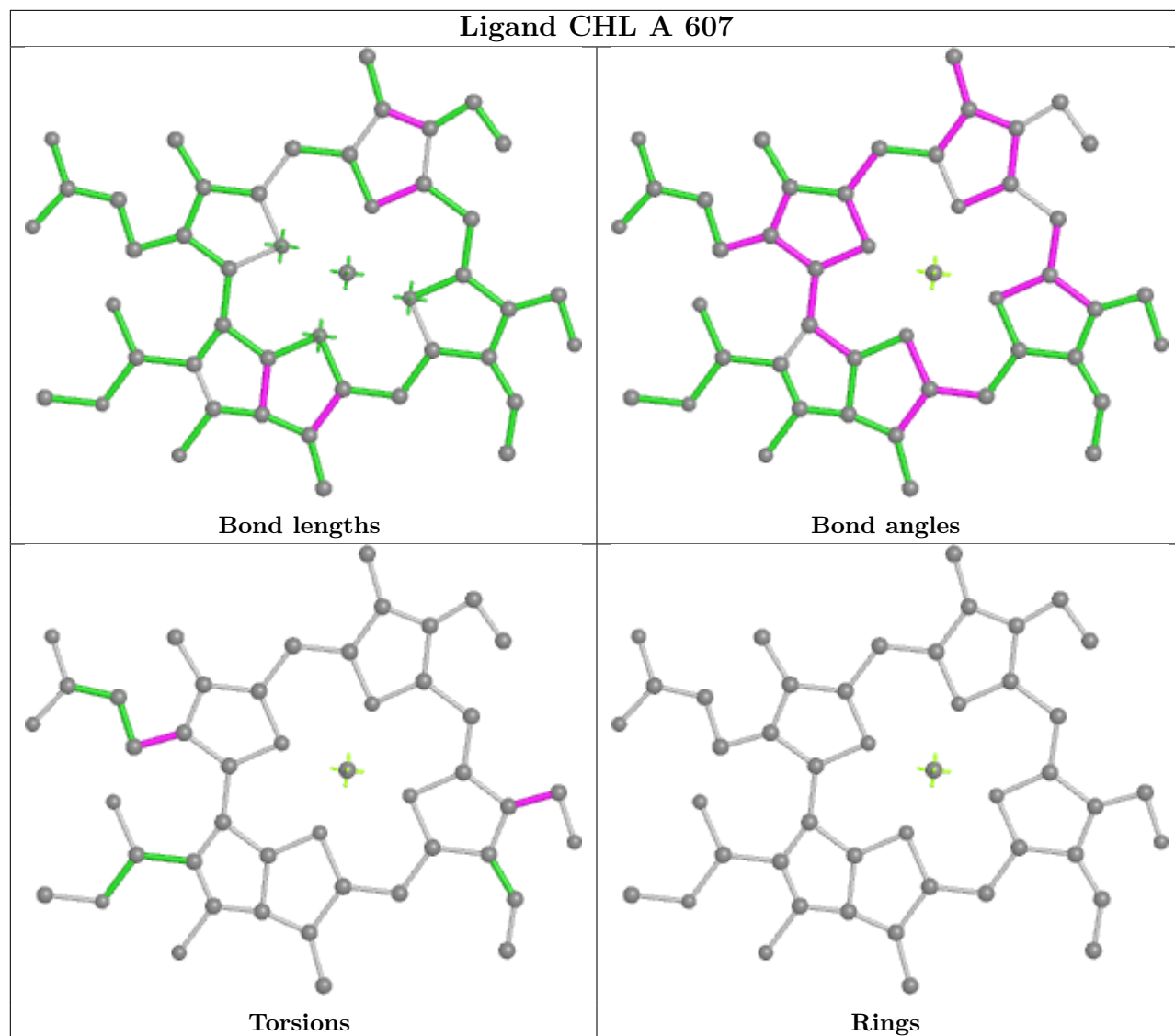


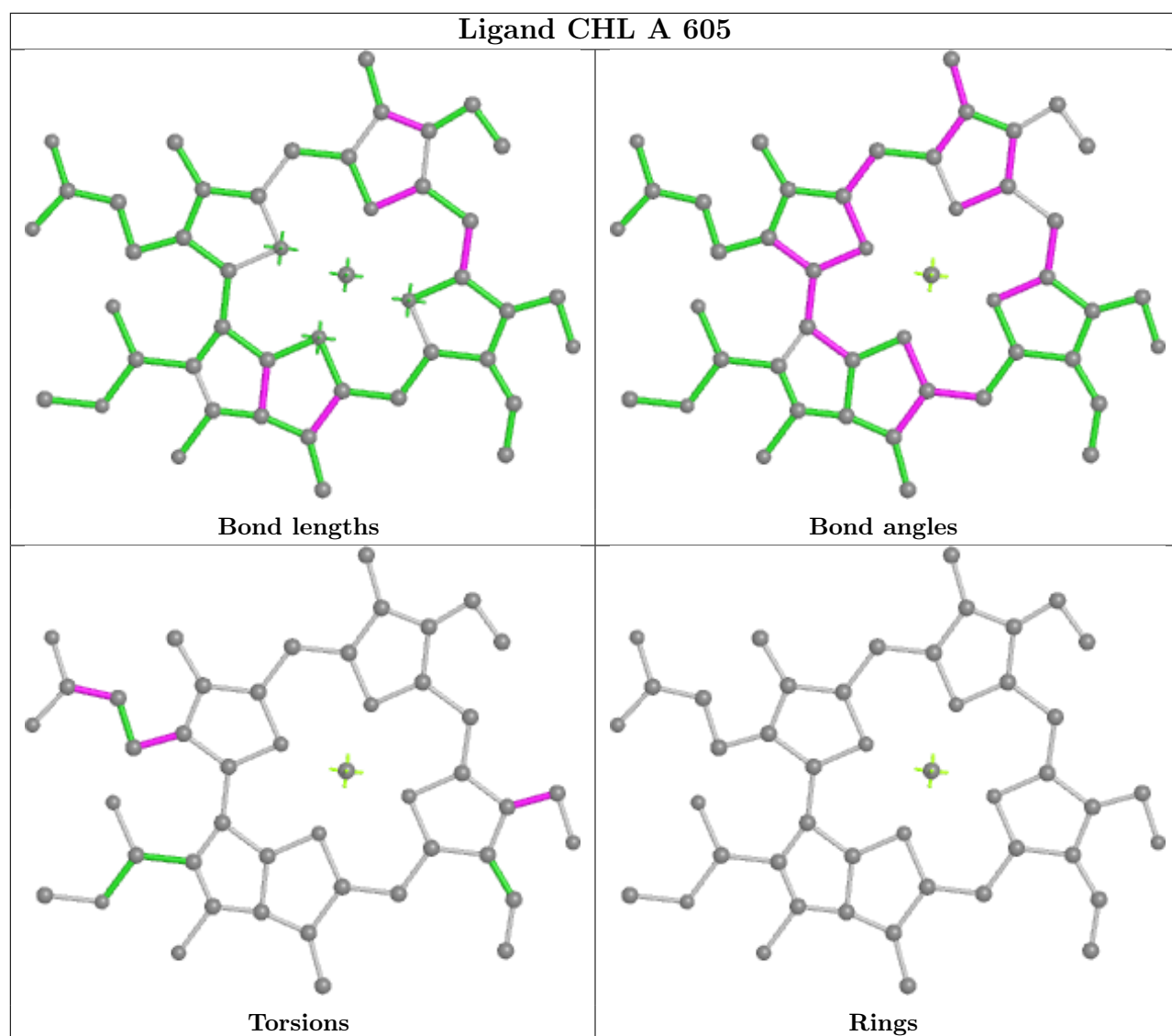


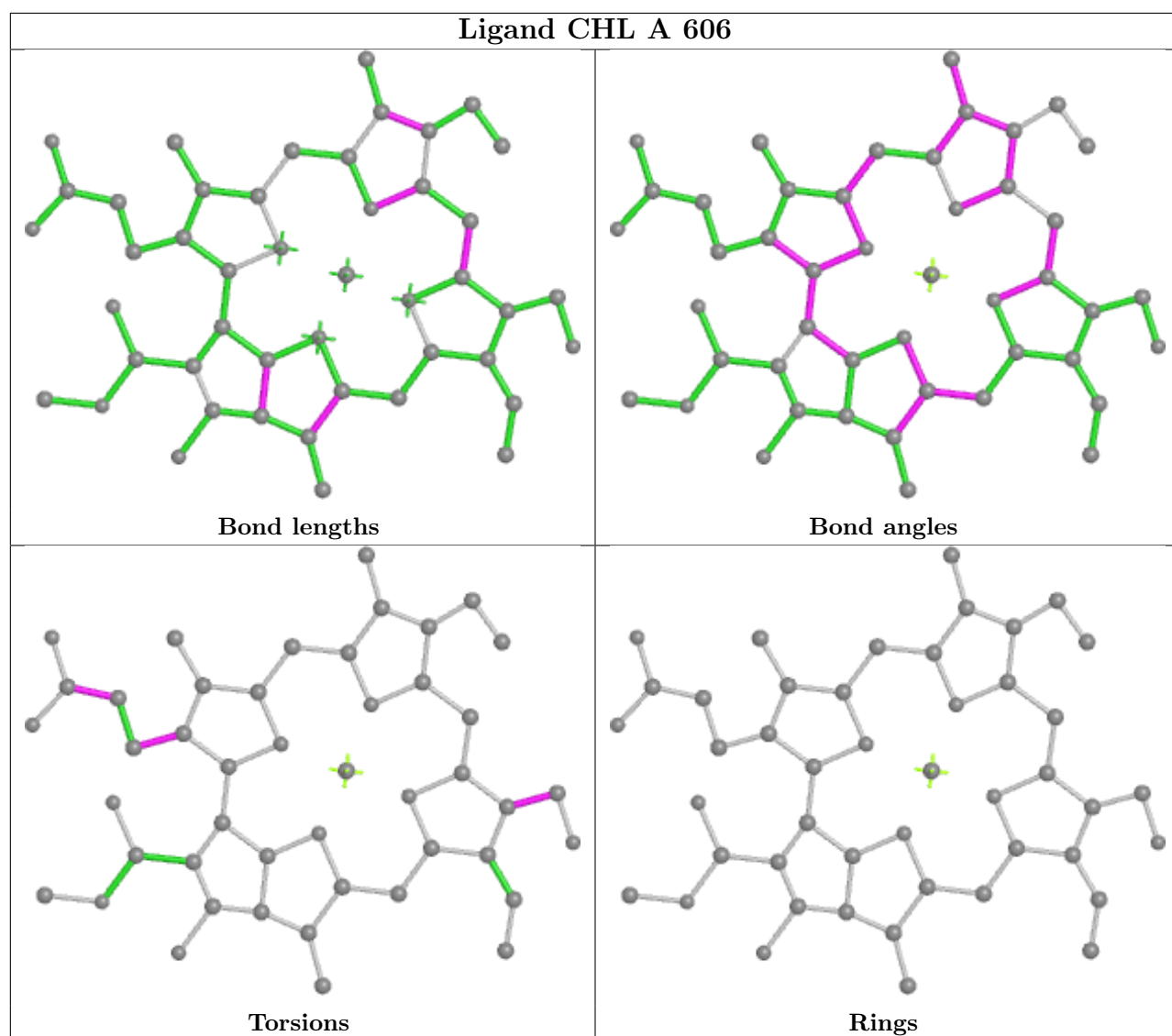




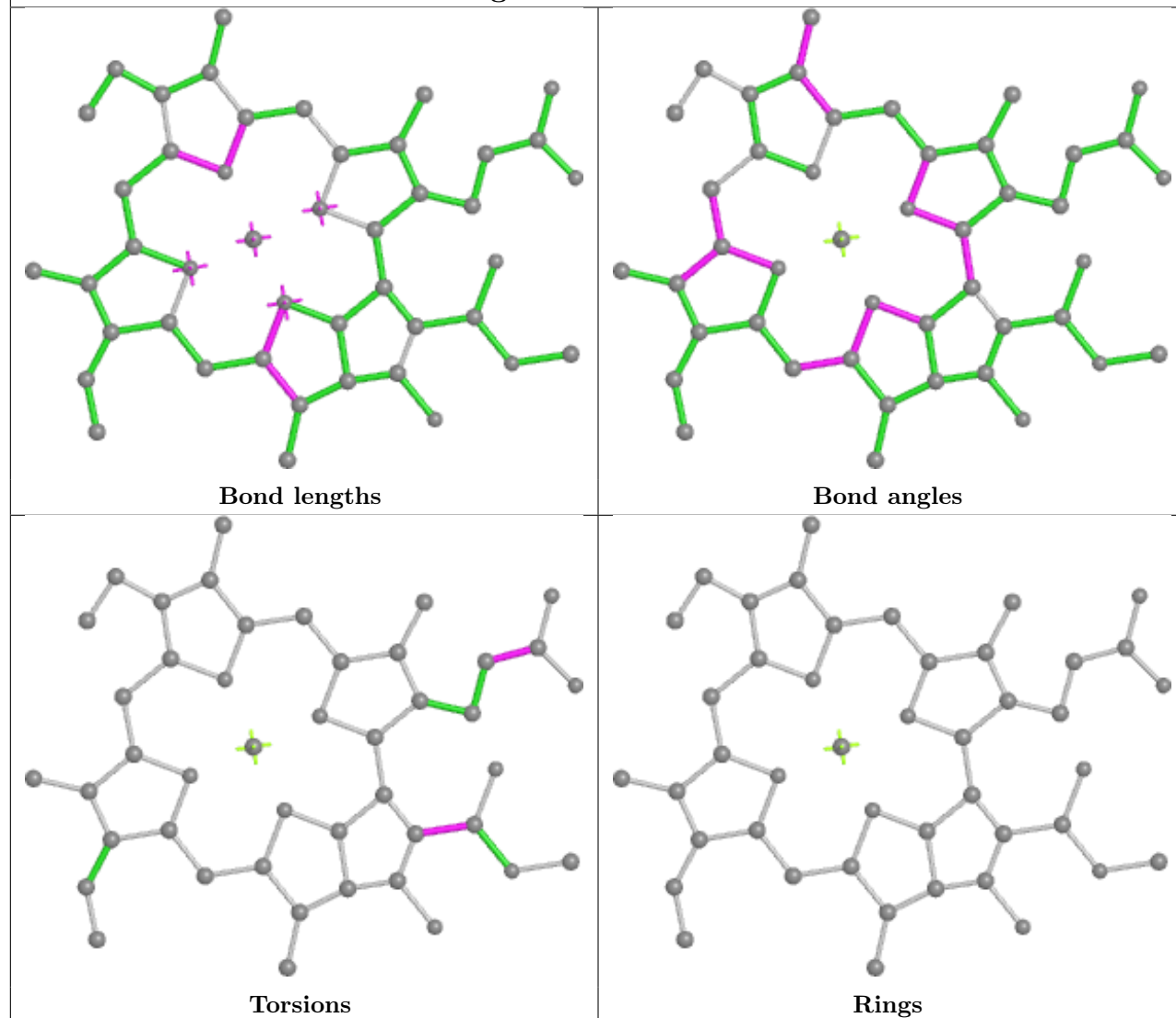




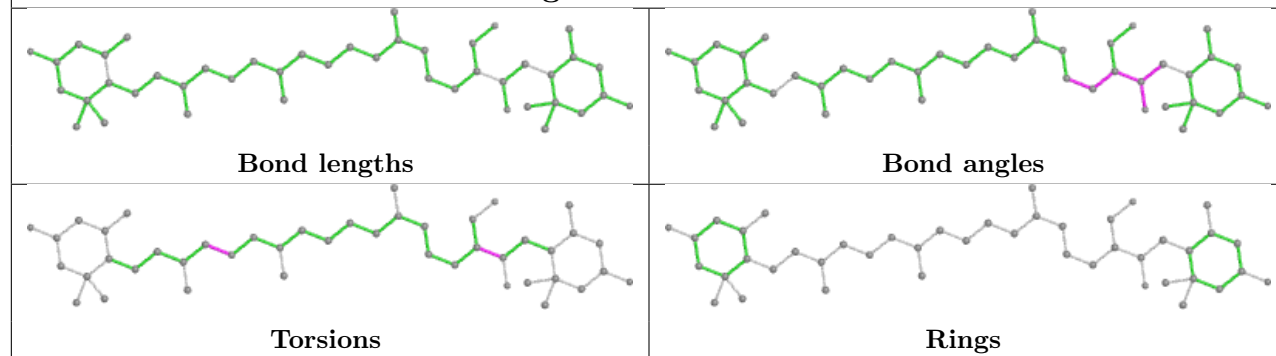


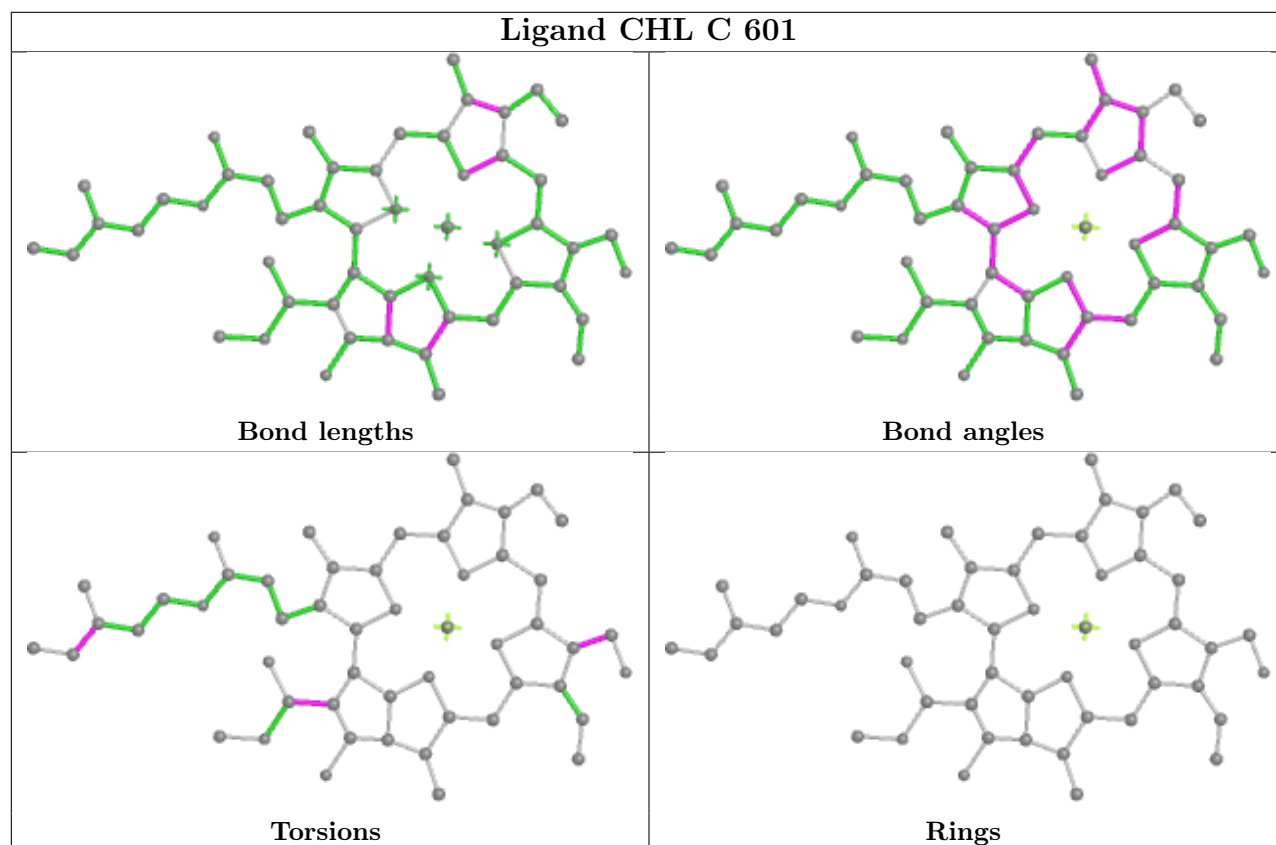
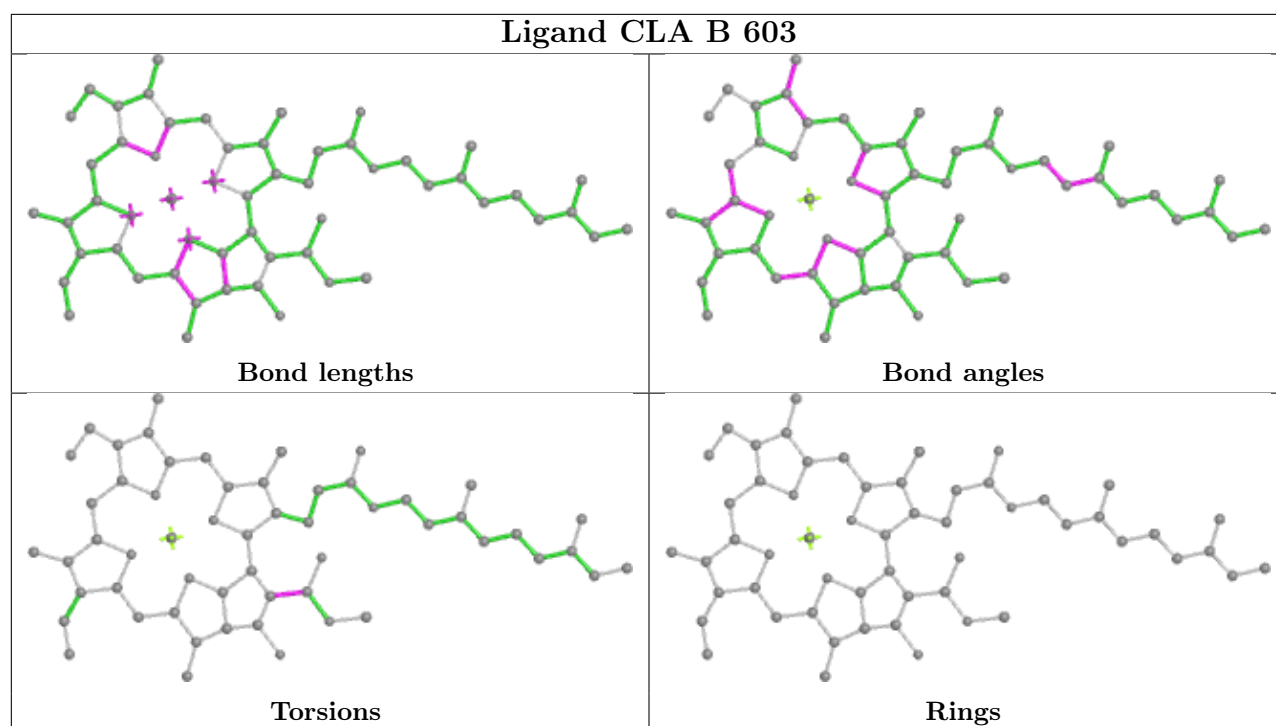


Ligand CLA C 612

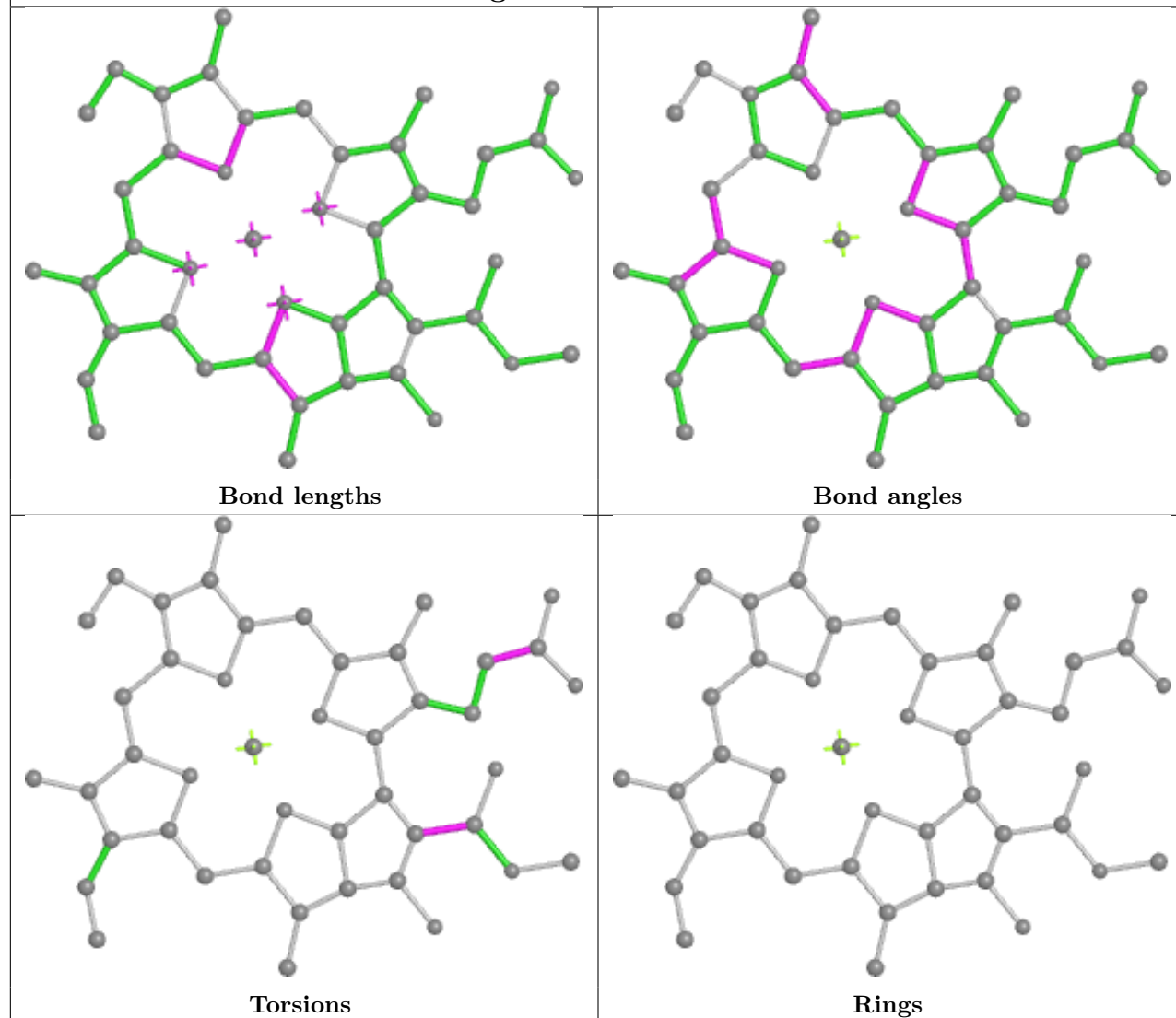


Ligand OIE B 616

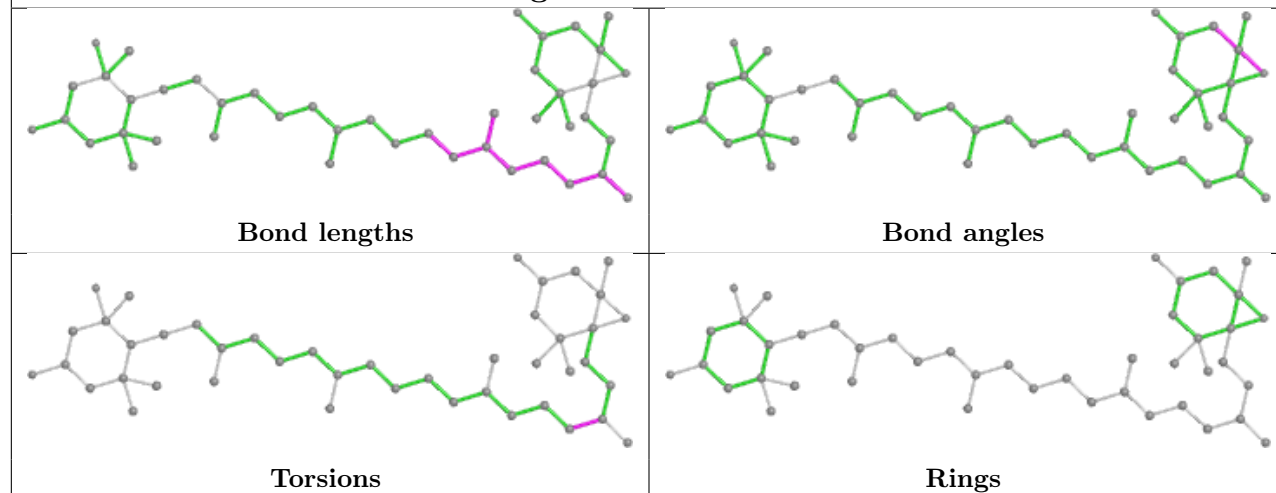


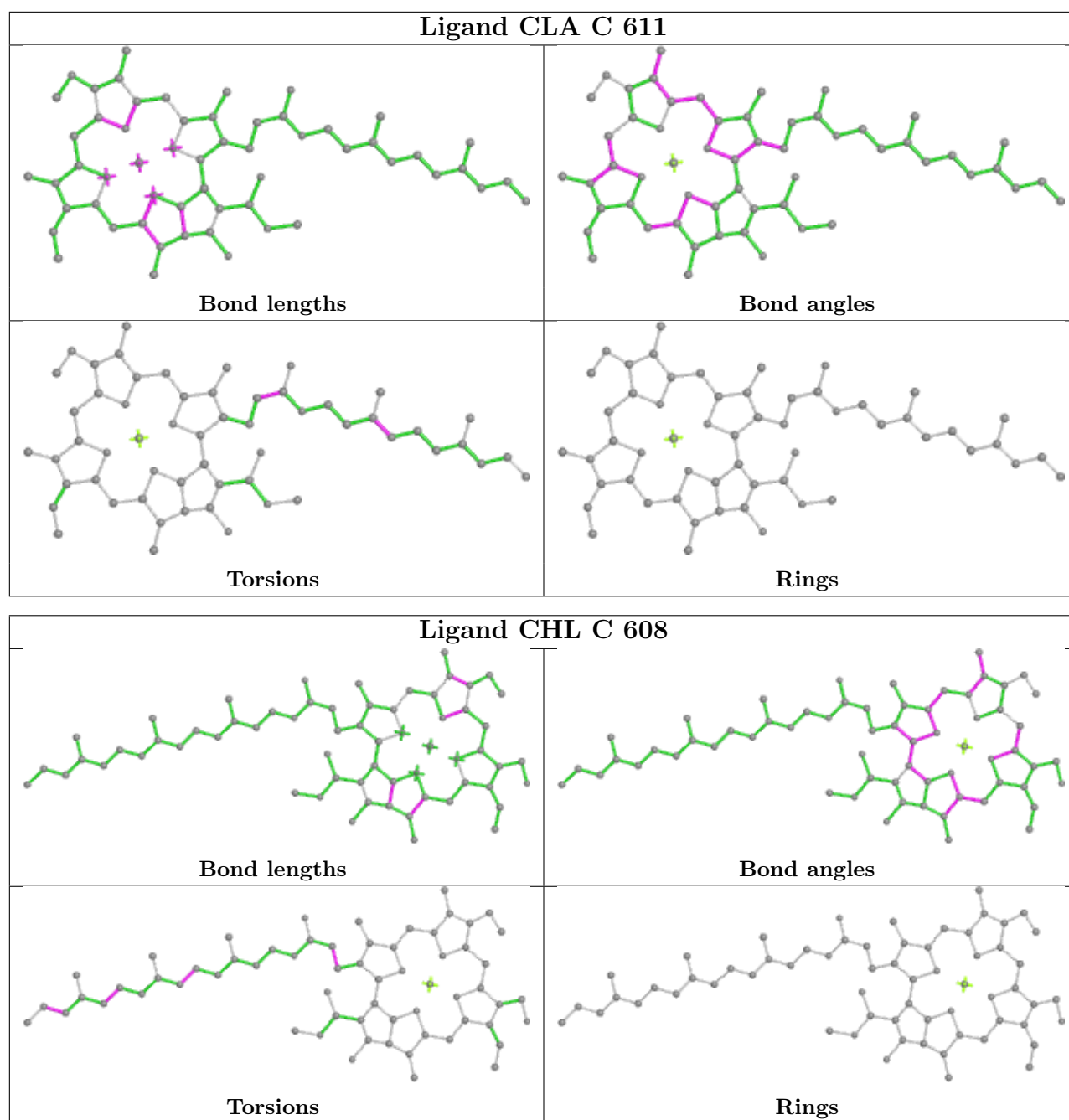


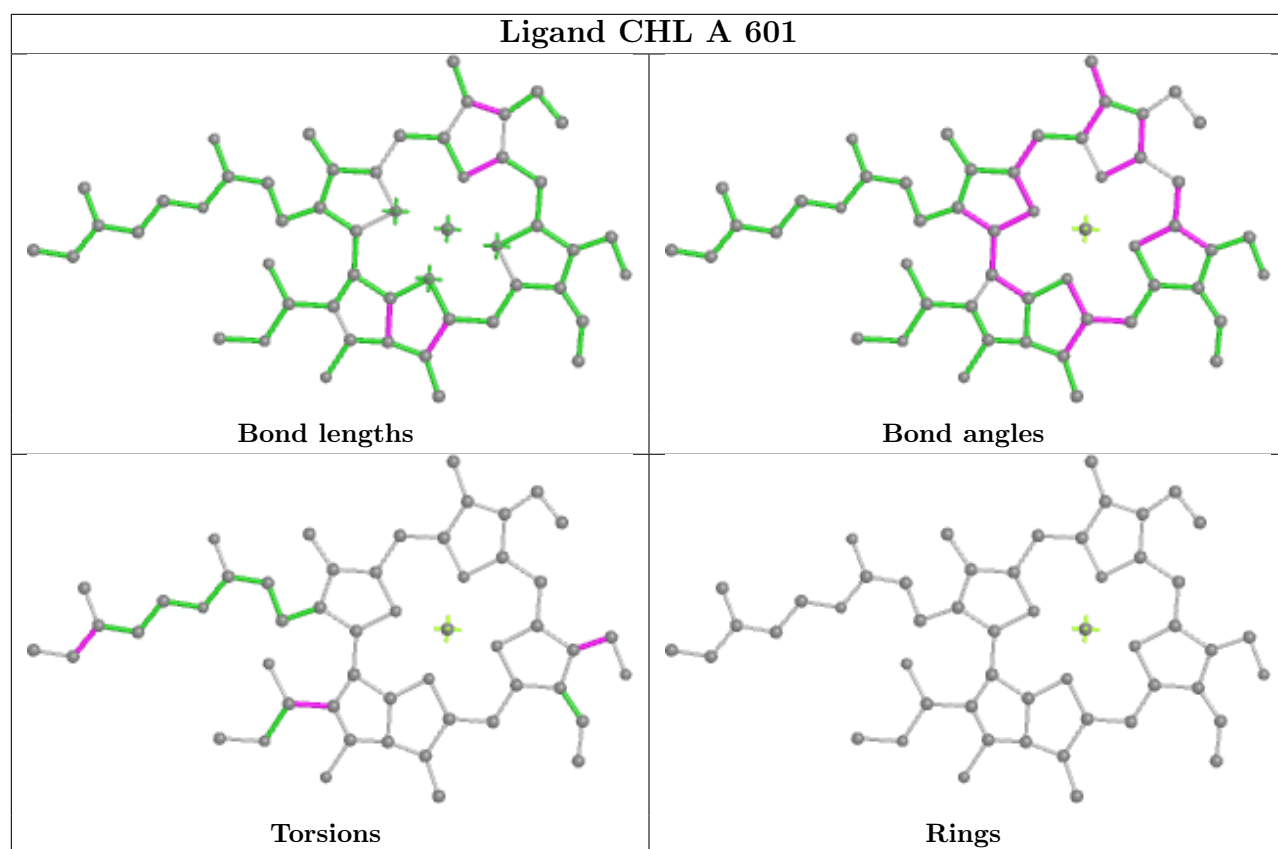
Ligand CLA A 612



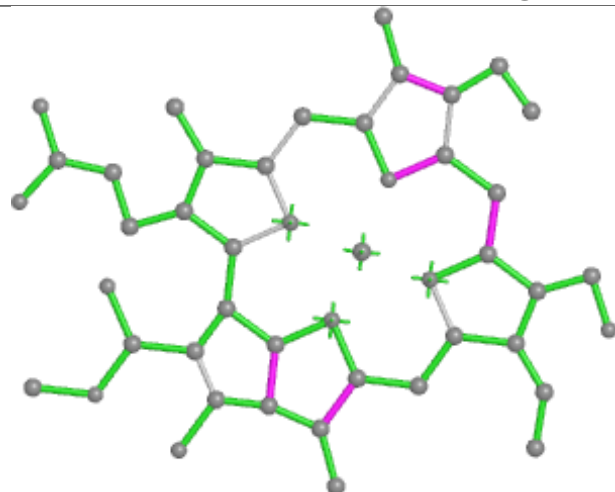
Ligand NEX C 614



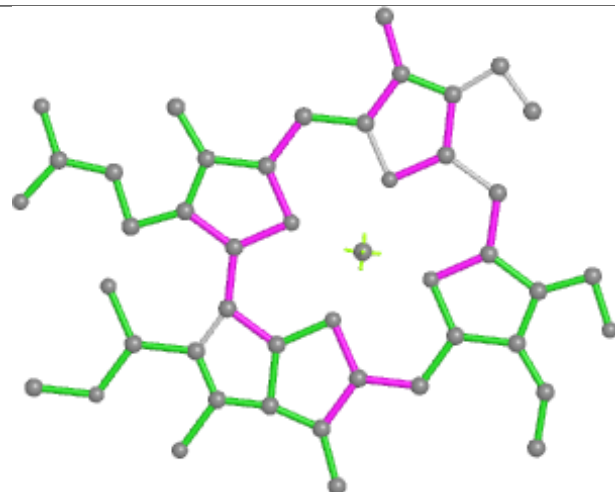




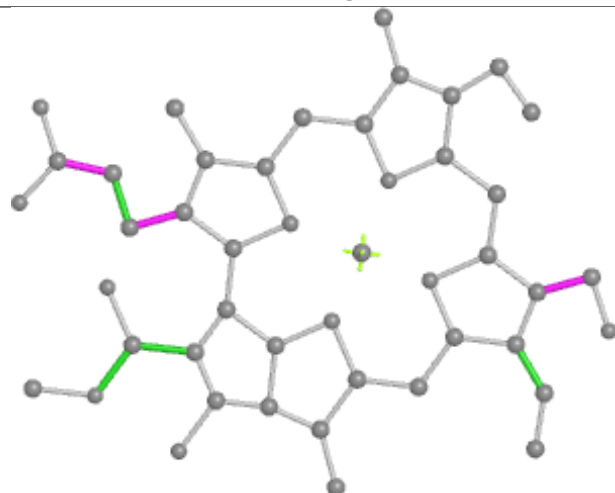
Ligand CHL B 605



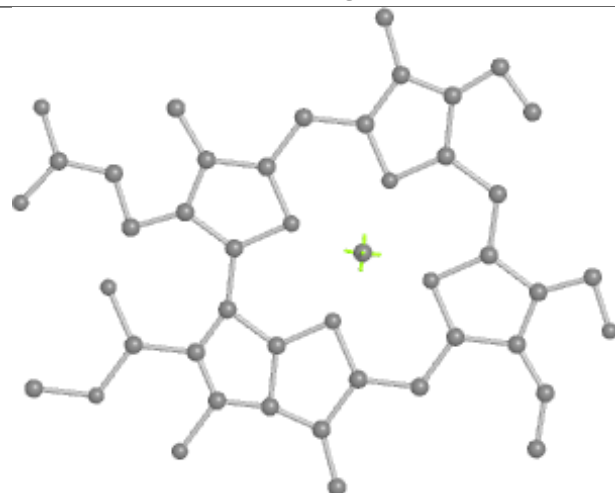
Bond lengths



Bond angles

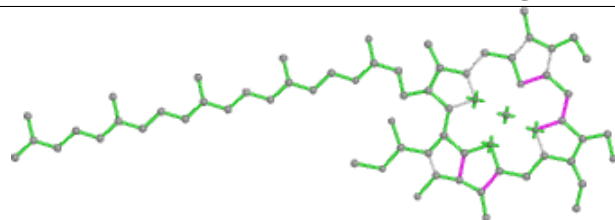


Torsions

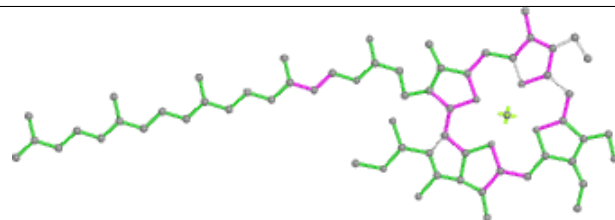


Rings

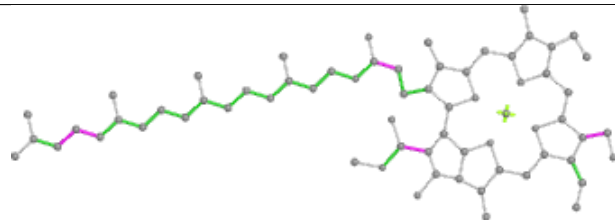
Ligand CHL B 602



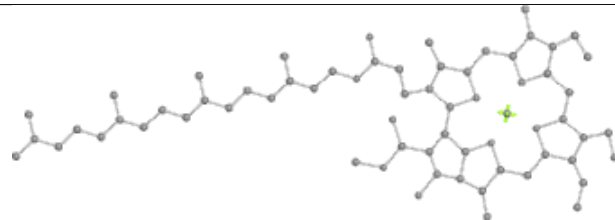
Bond lengths



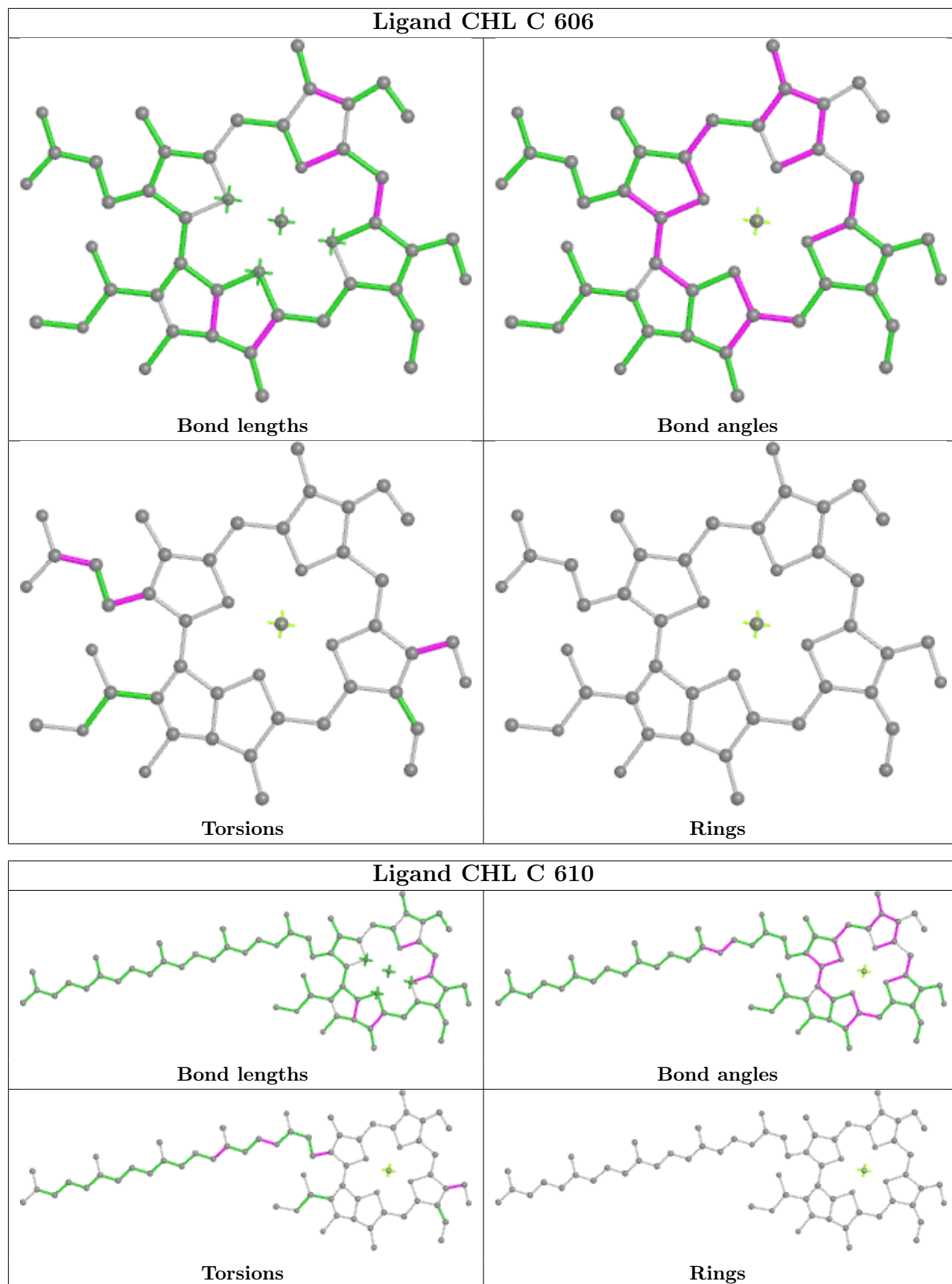
Bond angles

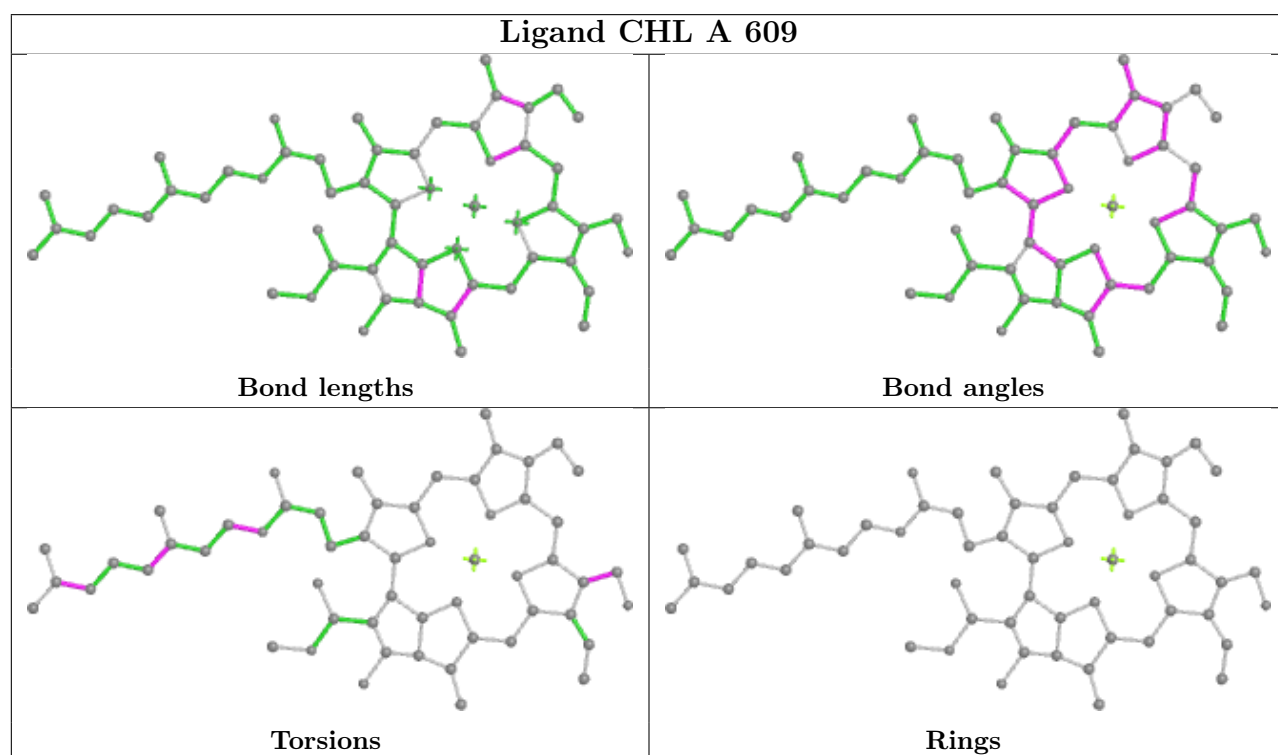
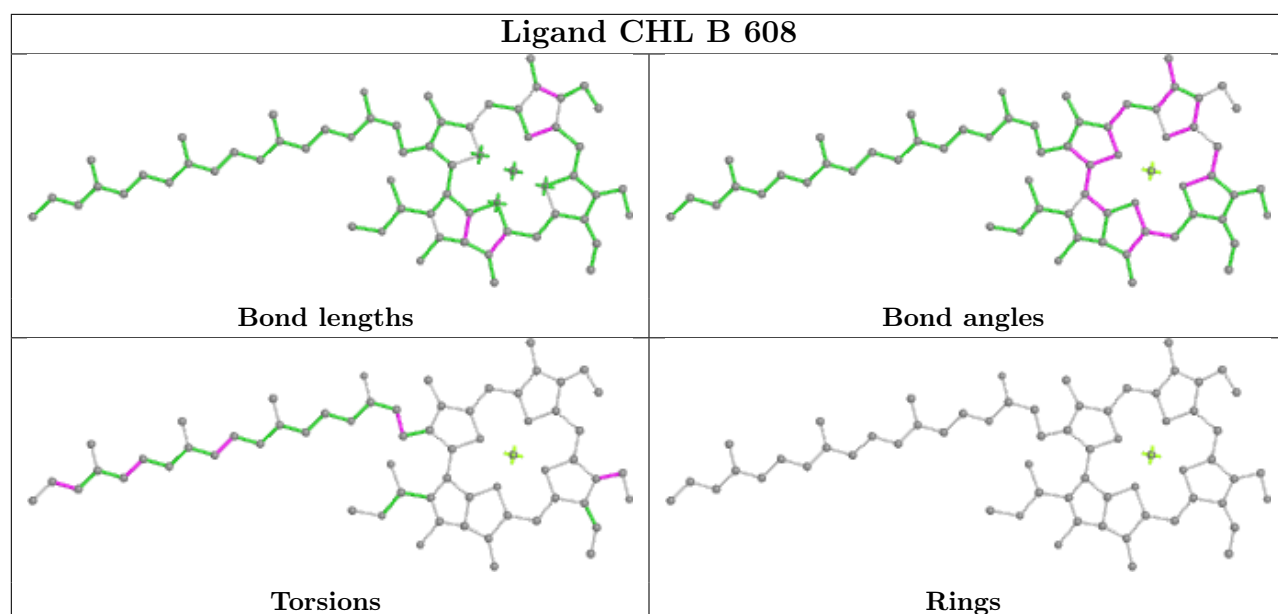


Torsions

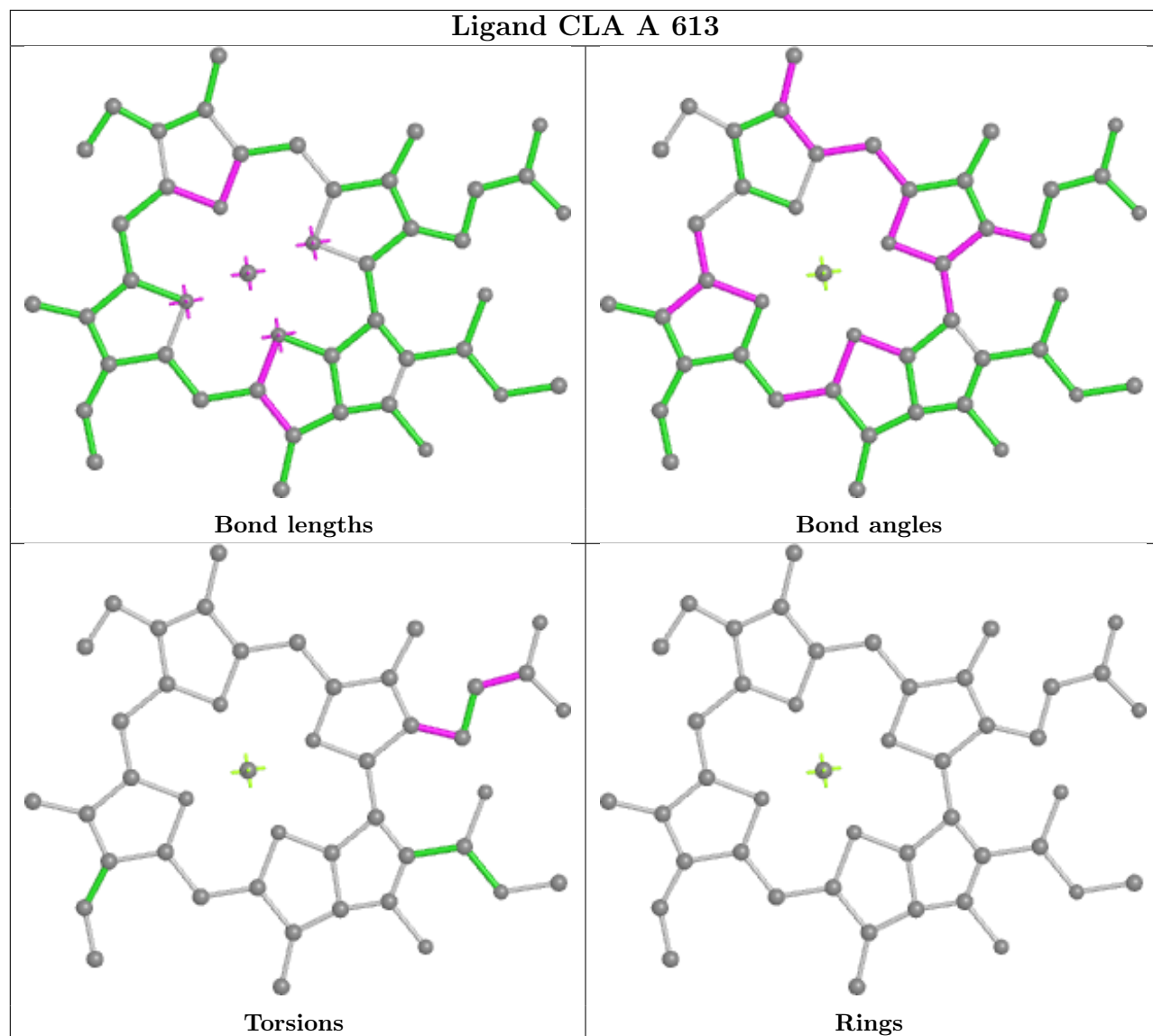


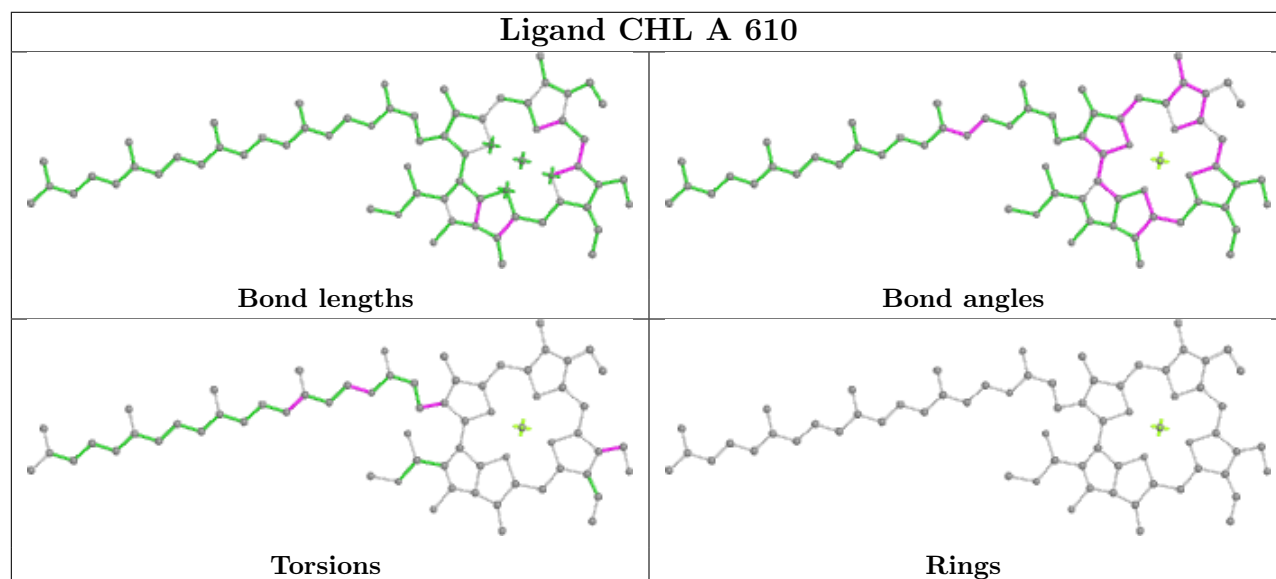
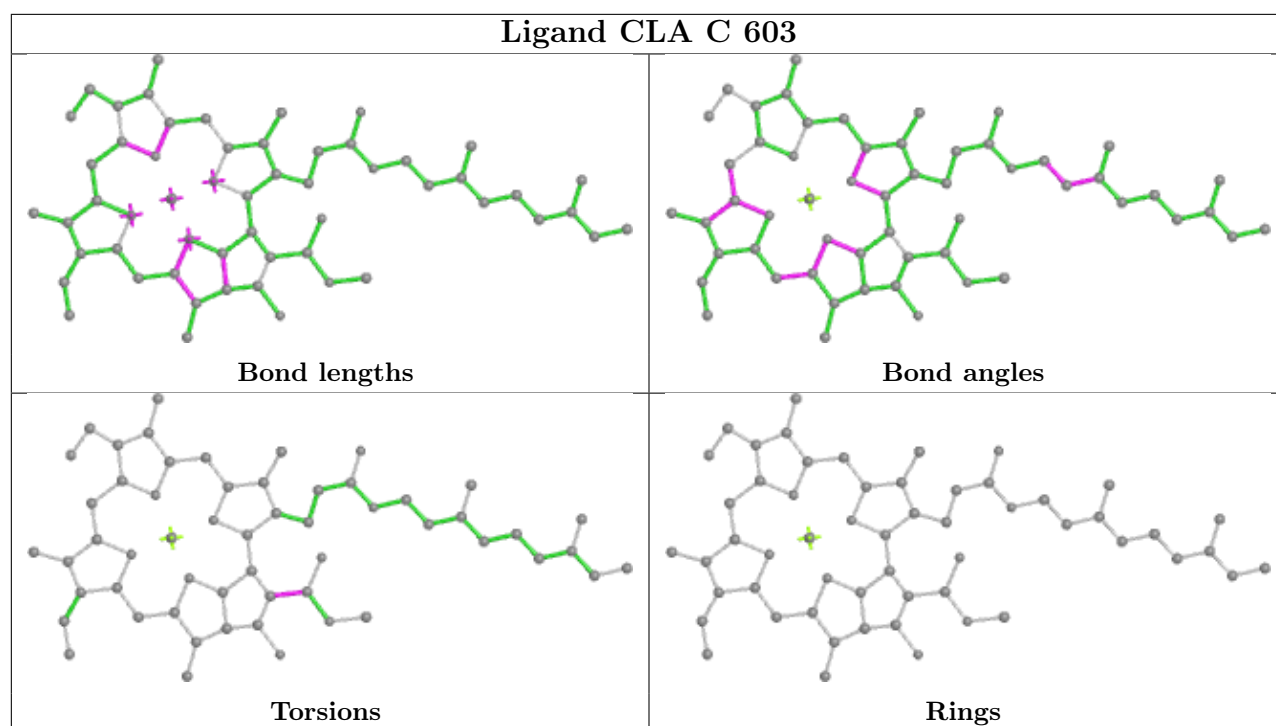
Rings



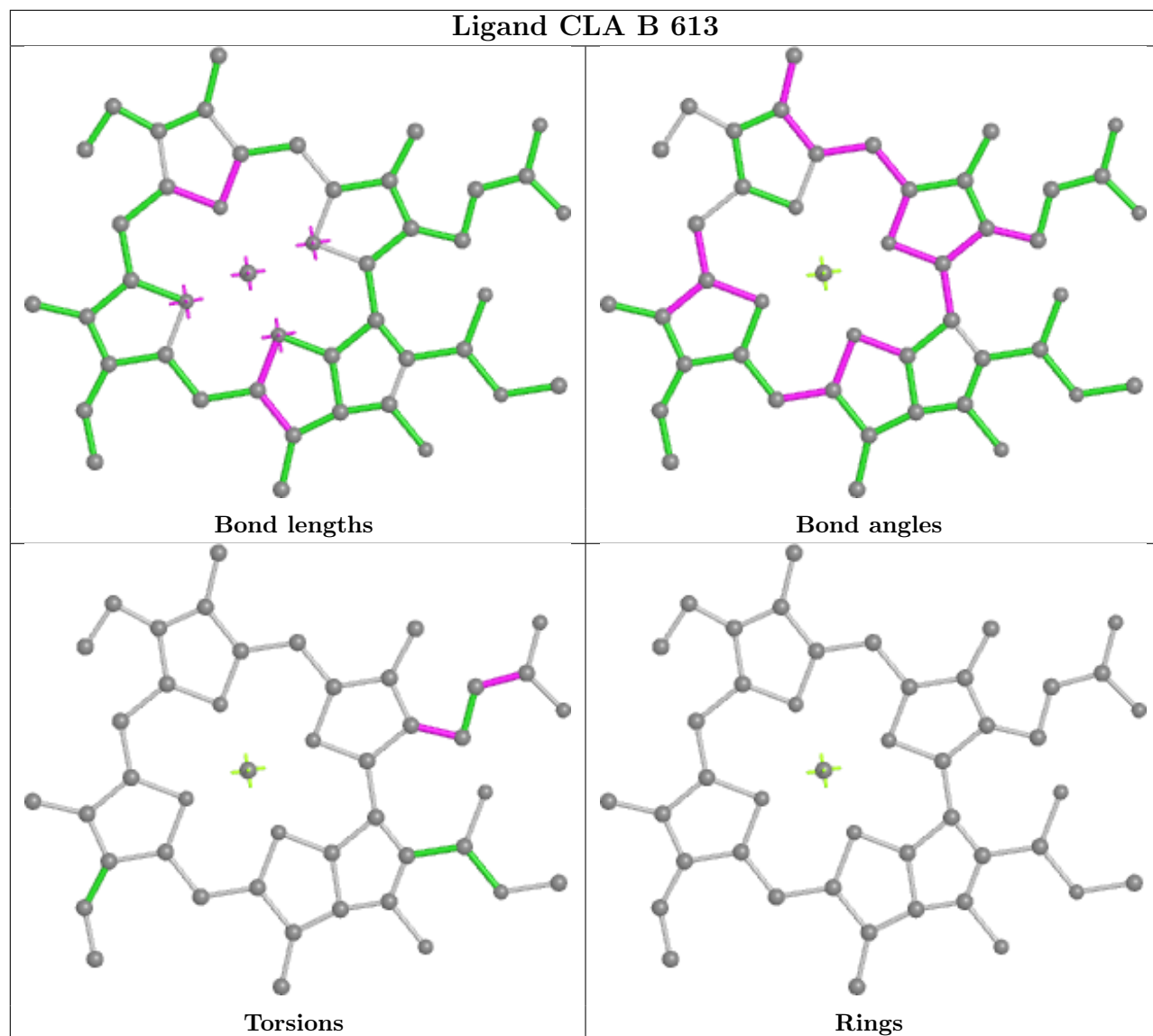


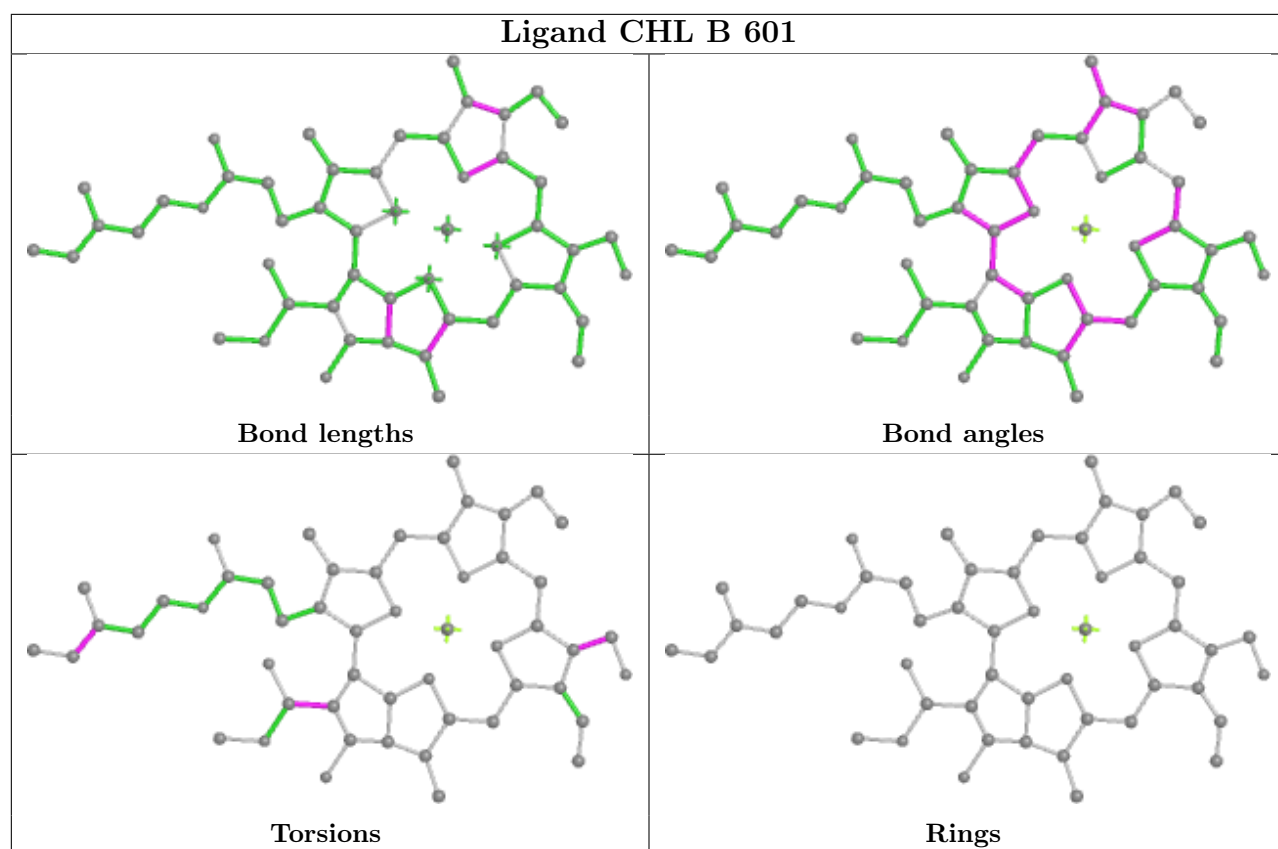
Ligand CLA A 613

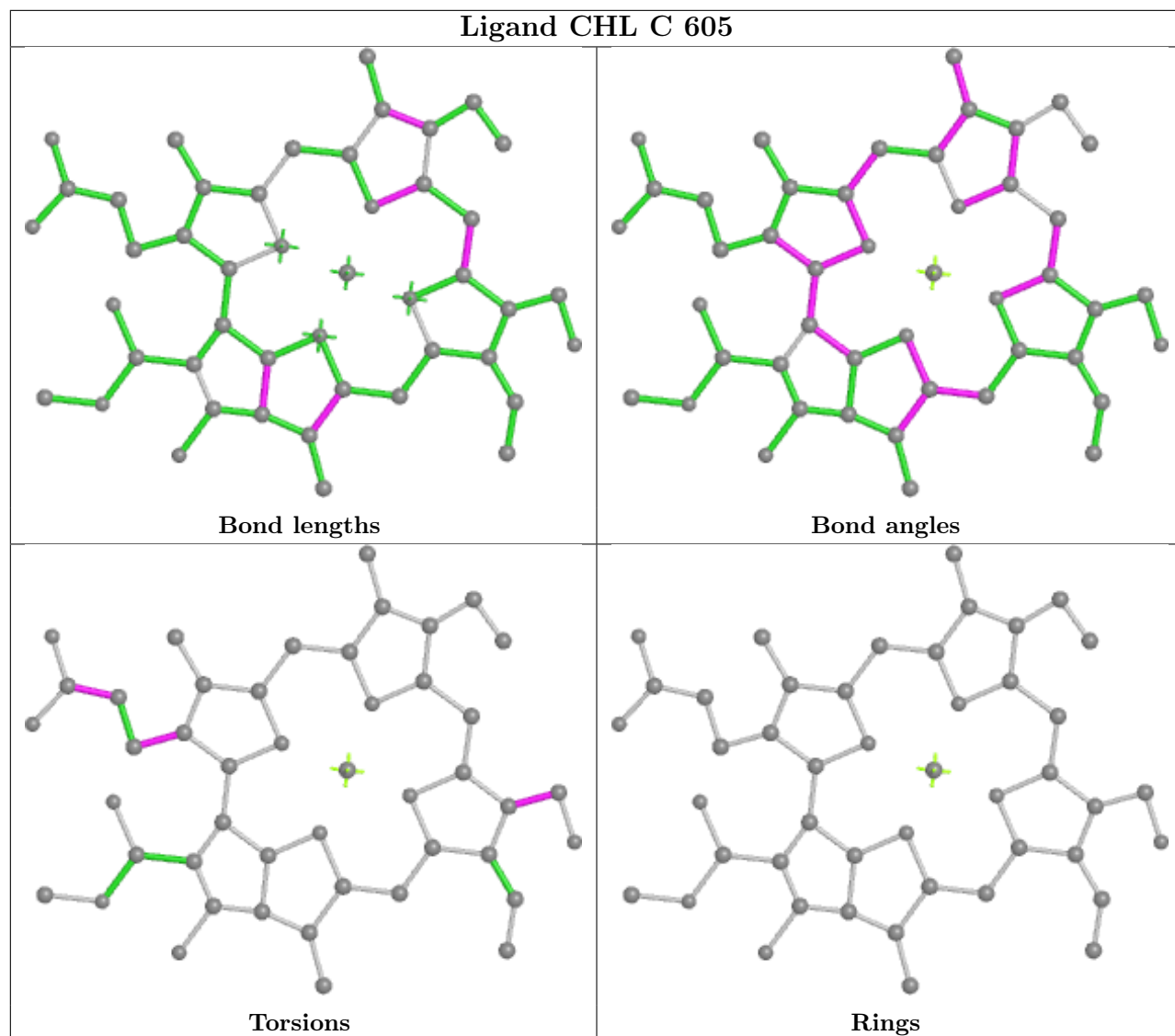


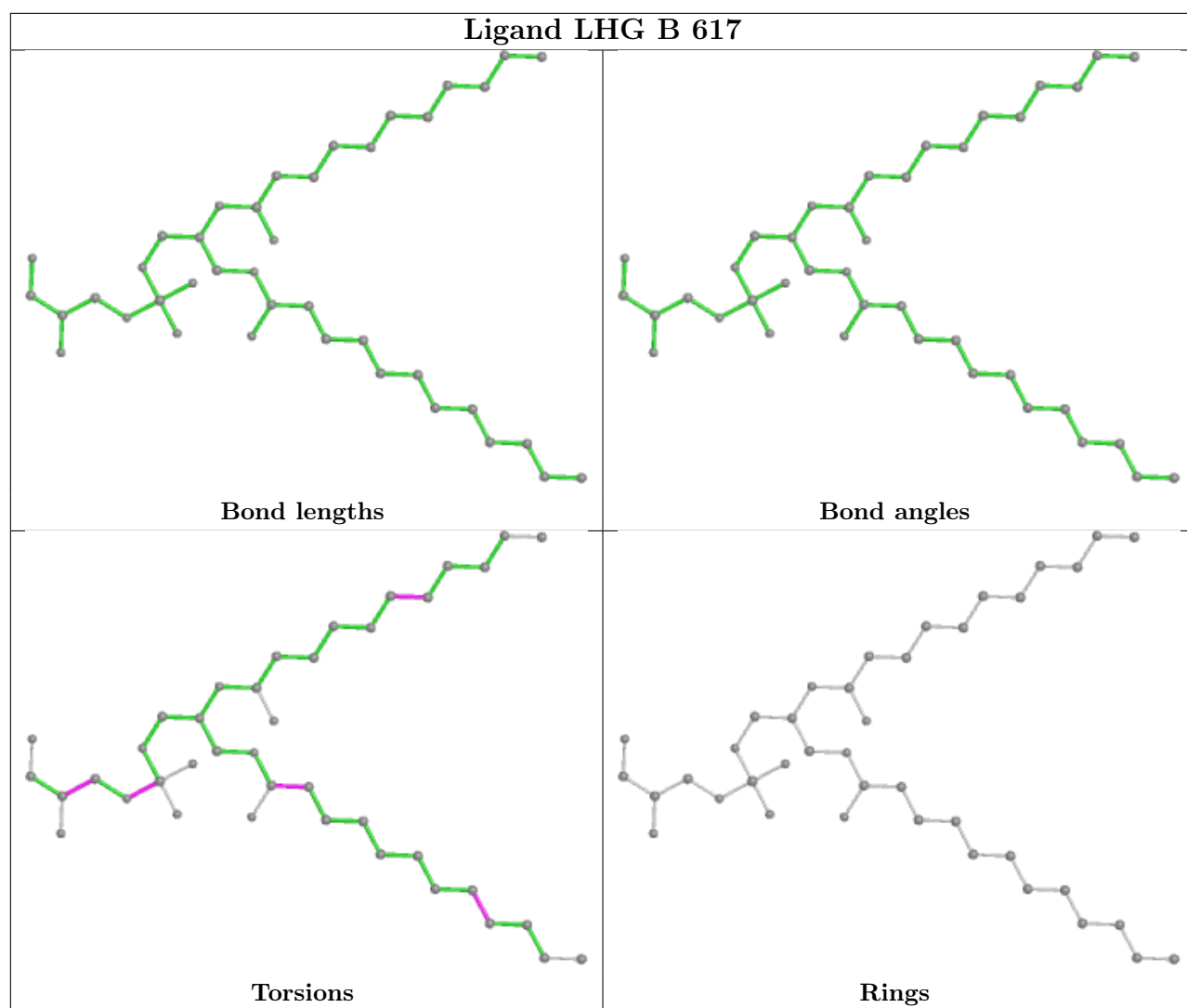


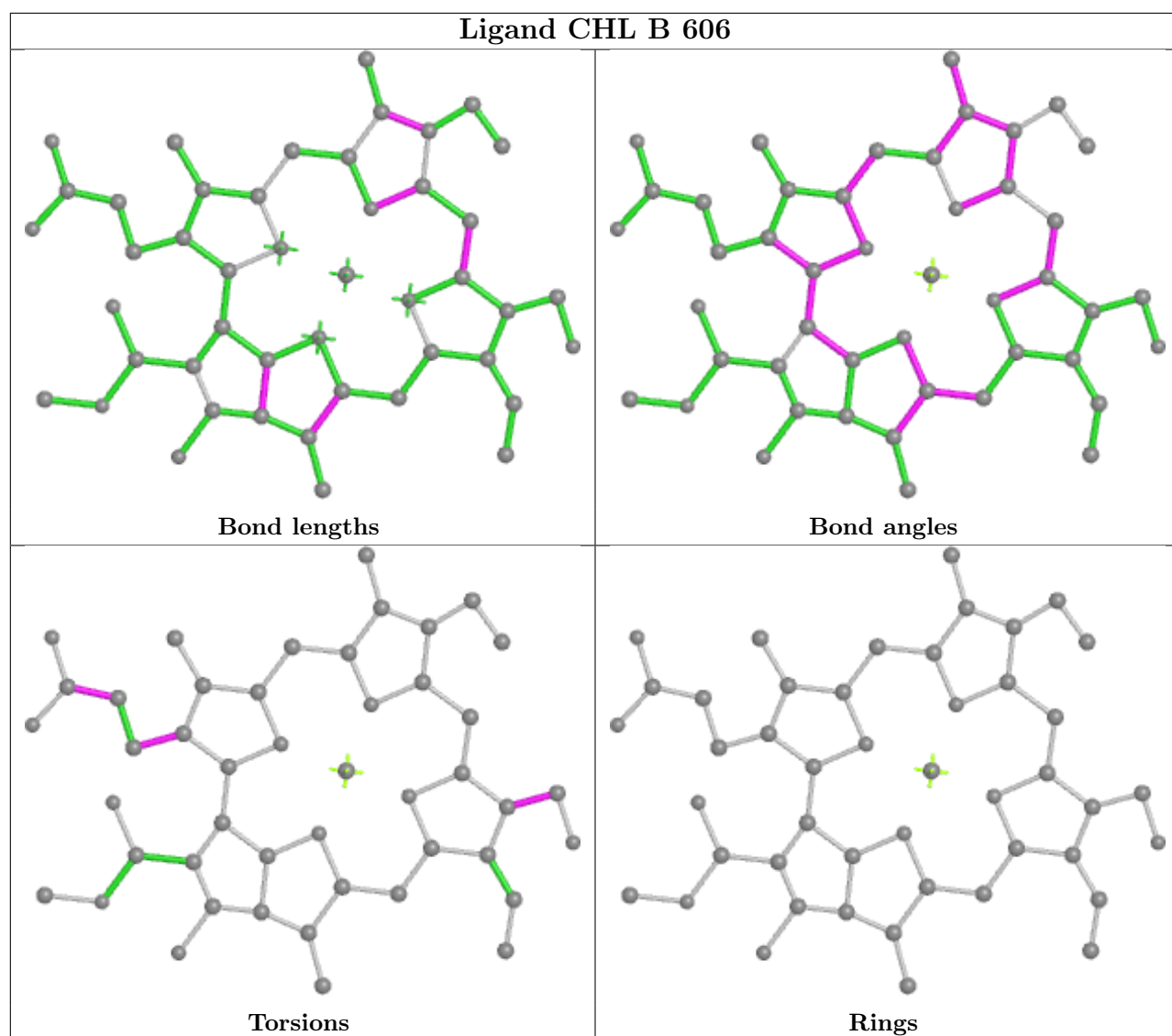
Ligand CLA B 613

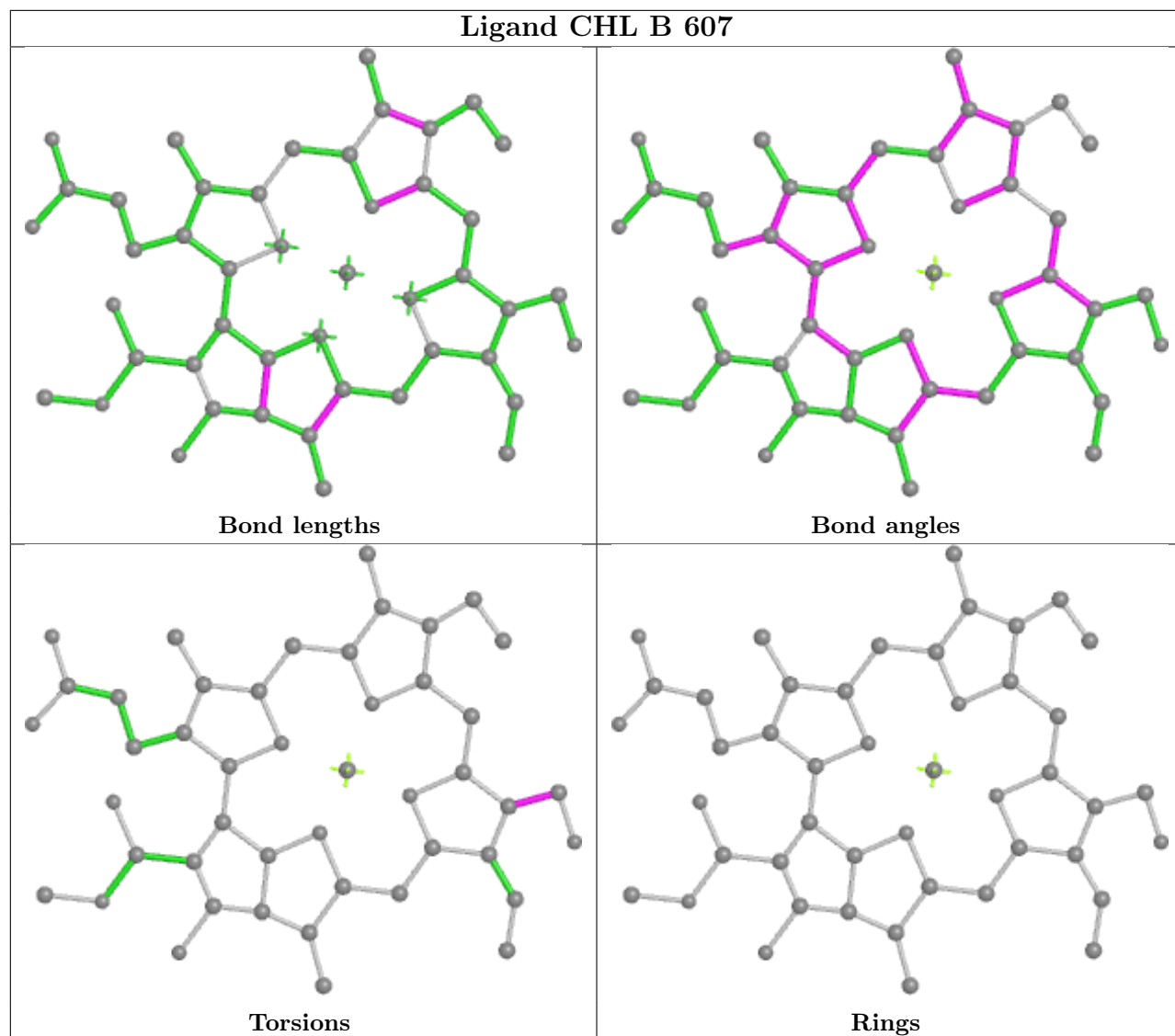




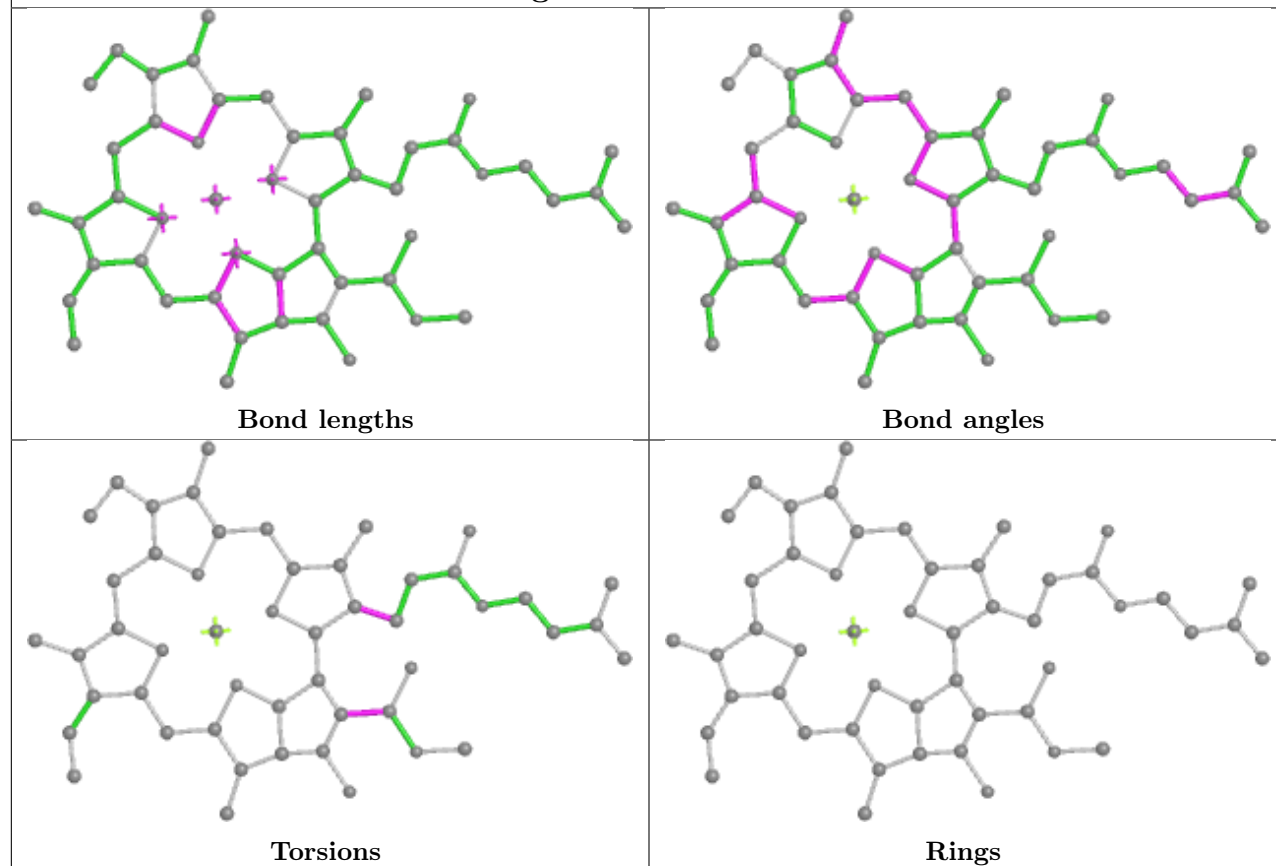




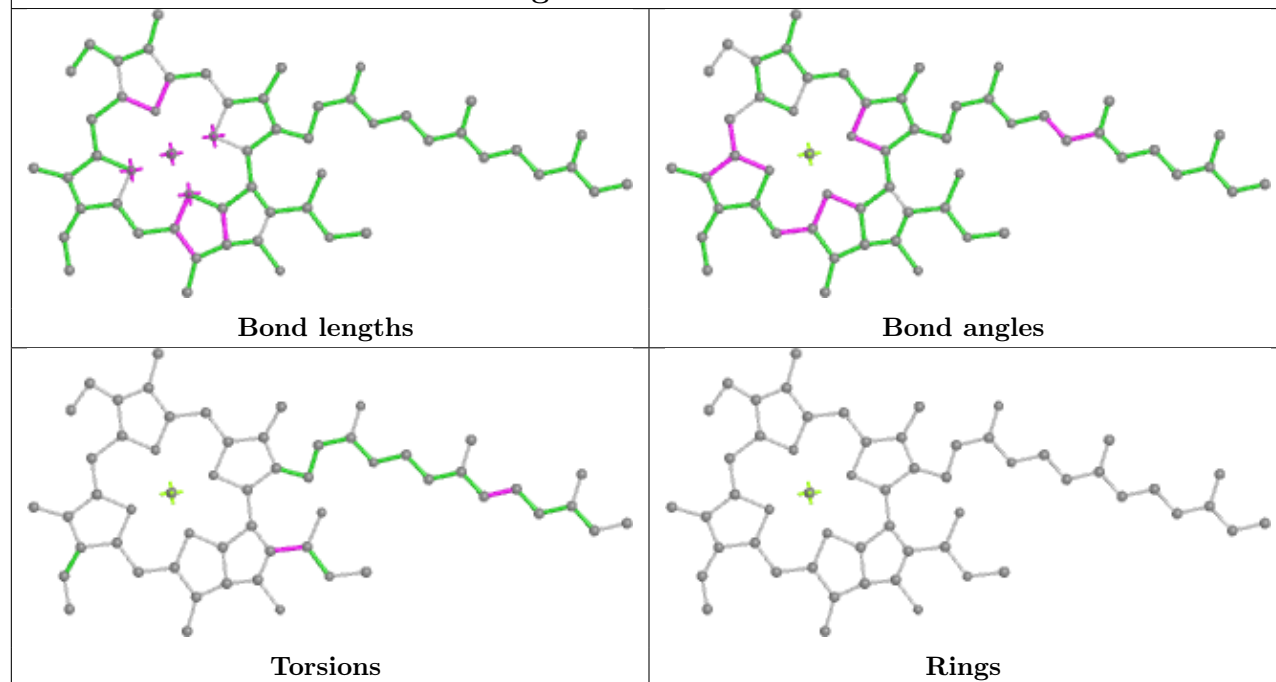


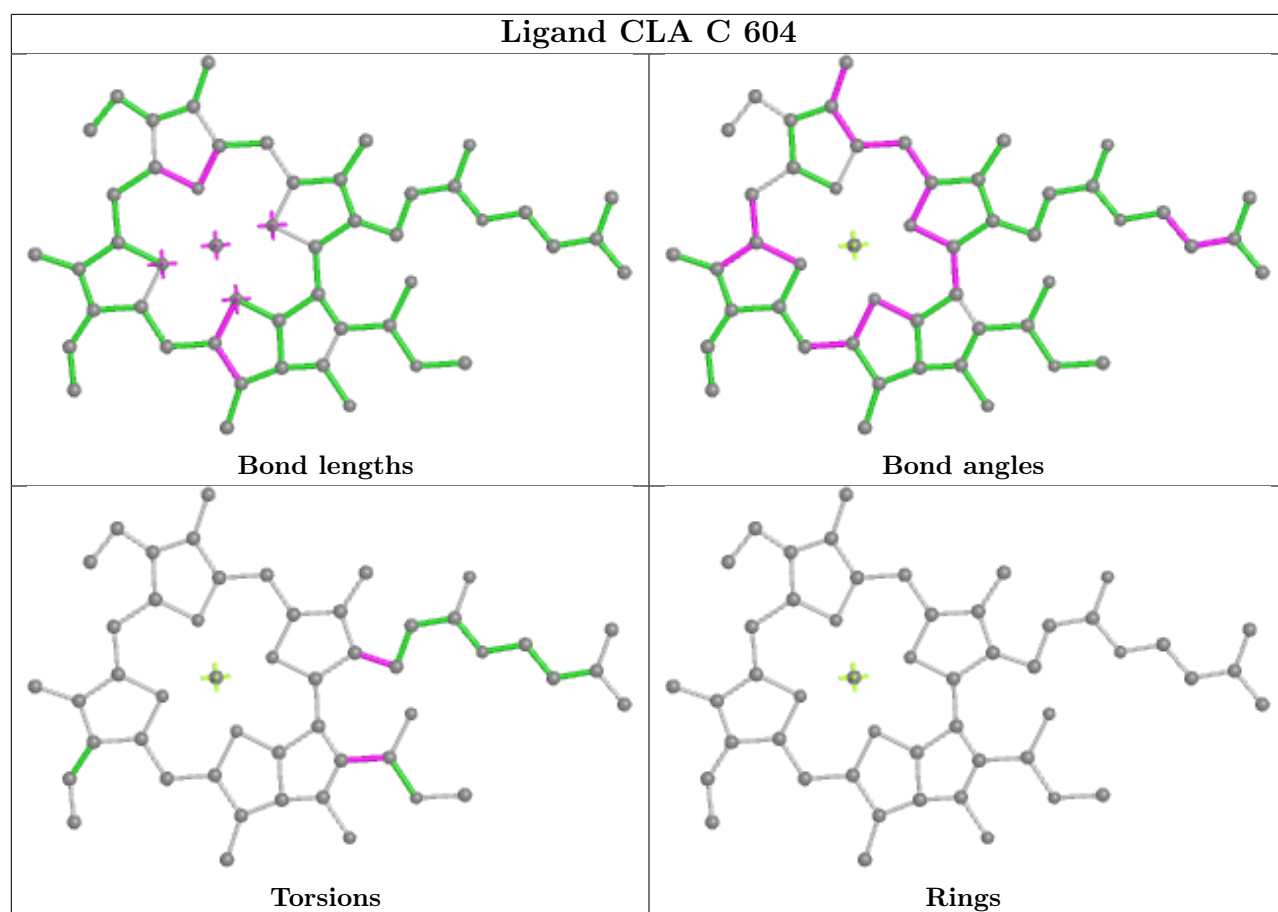


Ligand CLA A 604

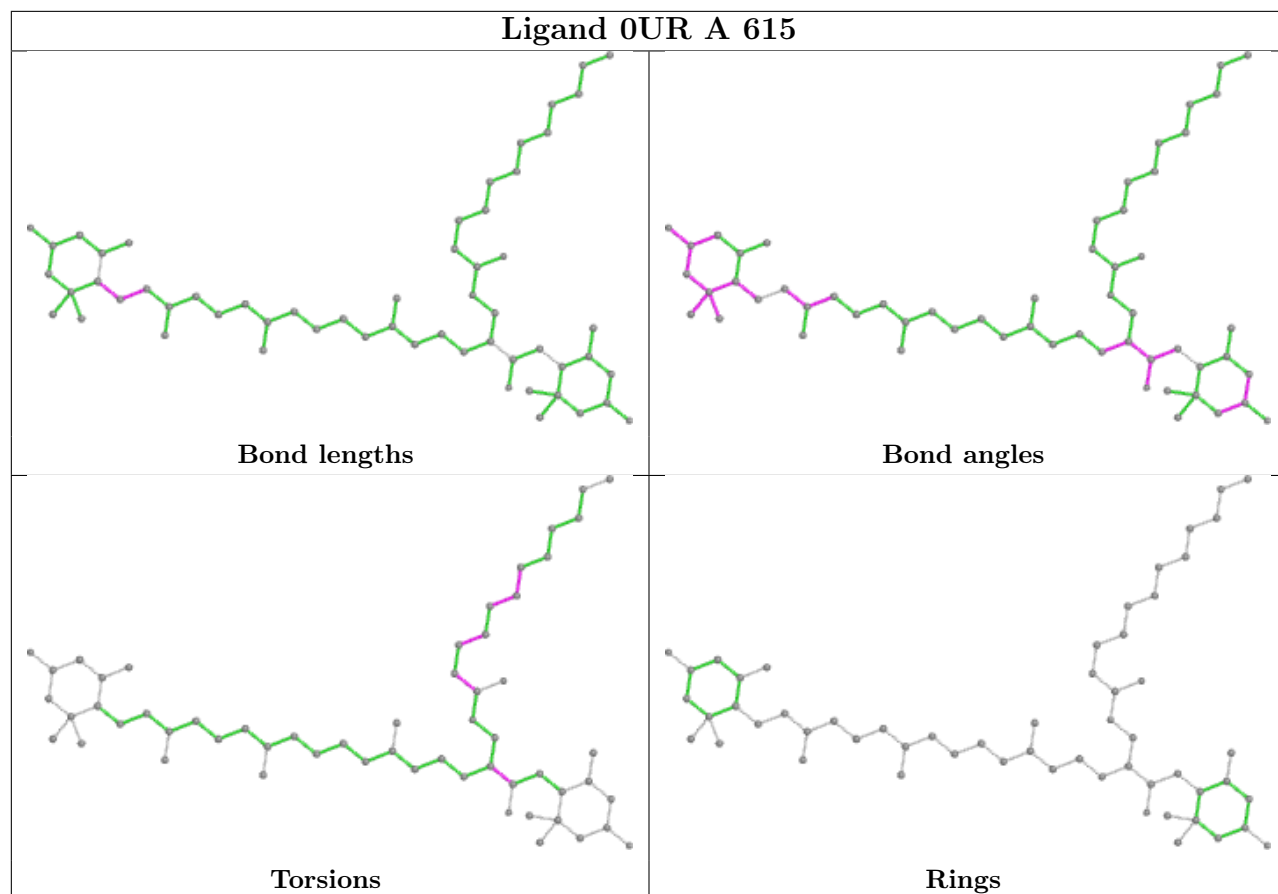


Ligand CLA A 603

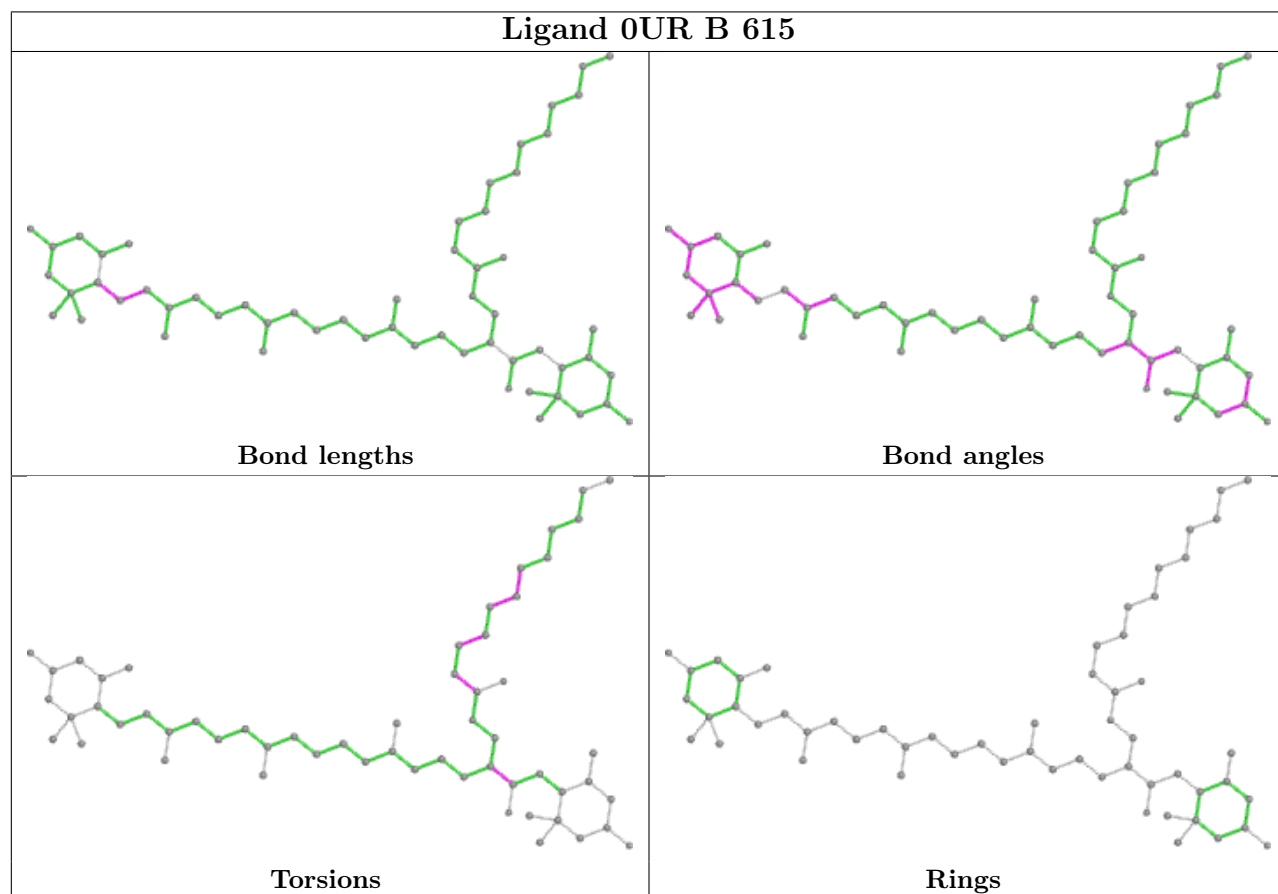


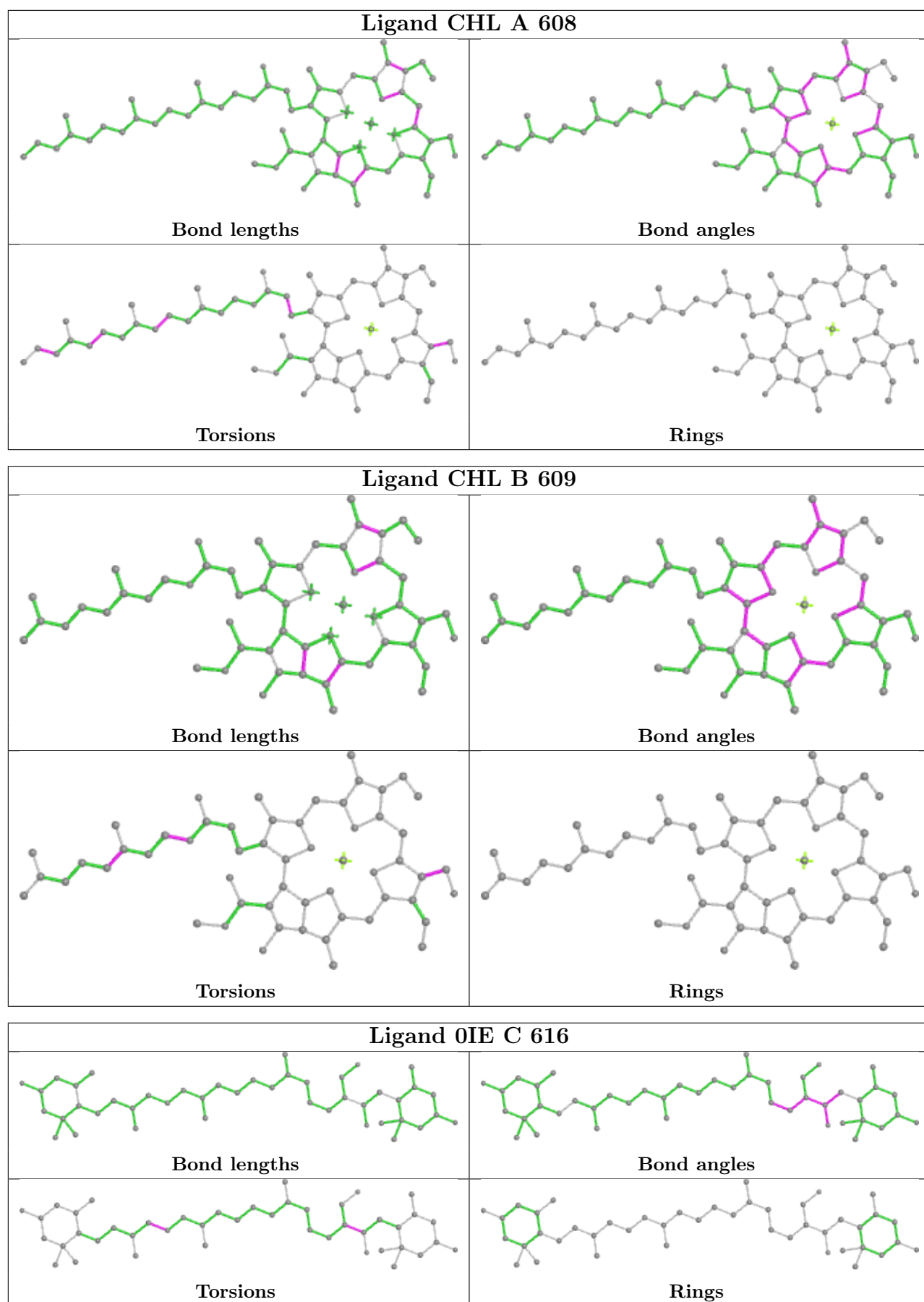


Ligand 0UR A 615



Ligand 0UR B 615





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

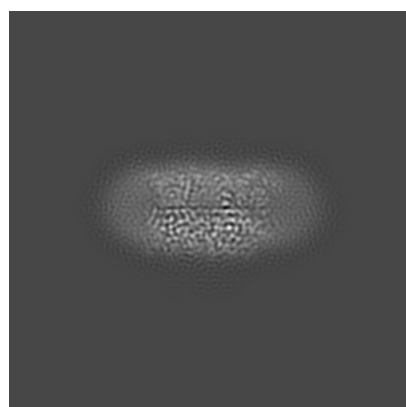
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32588. These allow visual inspection of the internal detail of the map and identification of artifacts.

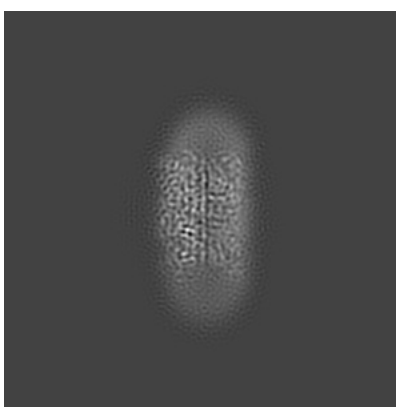
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

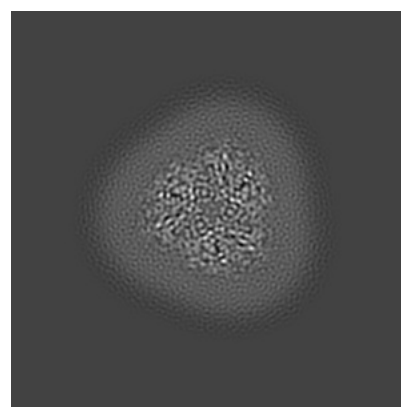
6.1.1 Primary map



X



Y

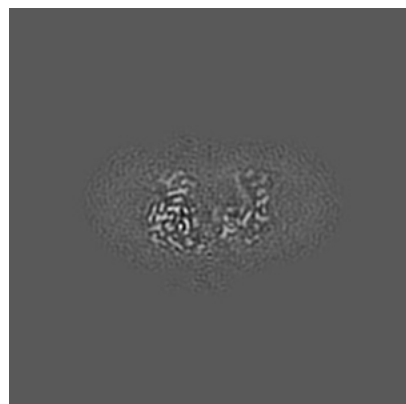


Z

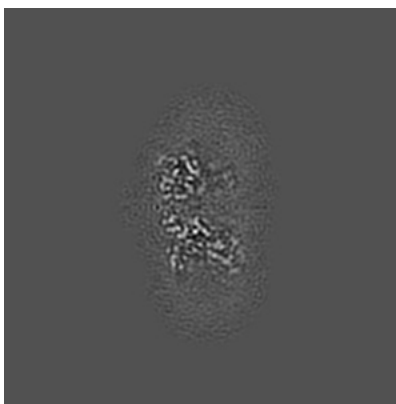
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

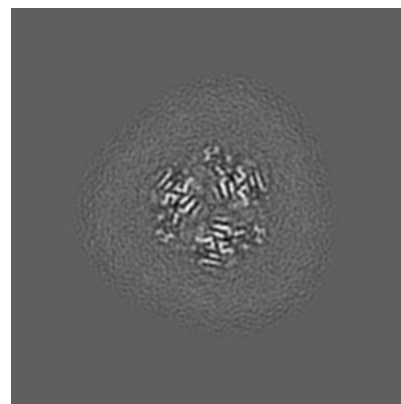
6.2.1 Primary map



X Index: 164



Y Index: 164

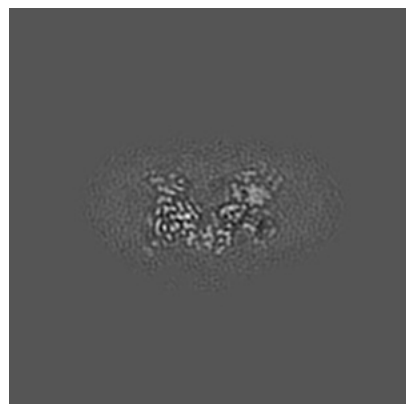


Z Index: 164

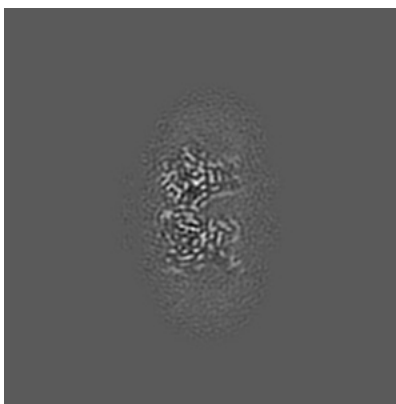
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

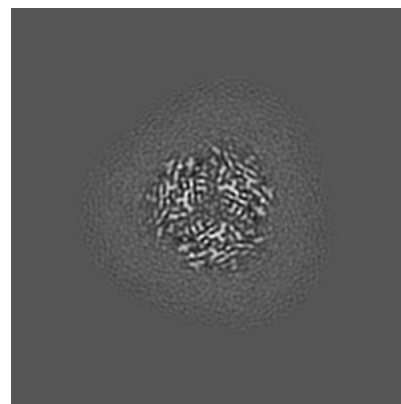
6.3.1 Primary map



X Index: 173



Y Index: 178



Z Index: 149

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0528. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

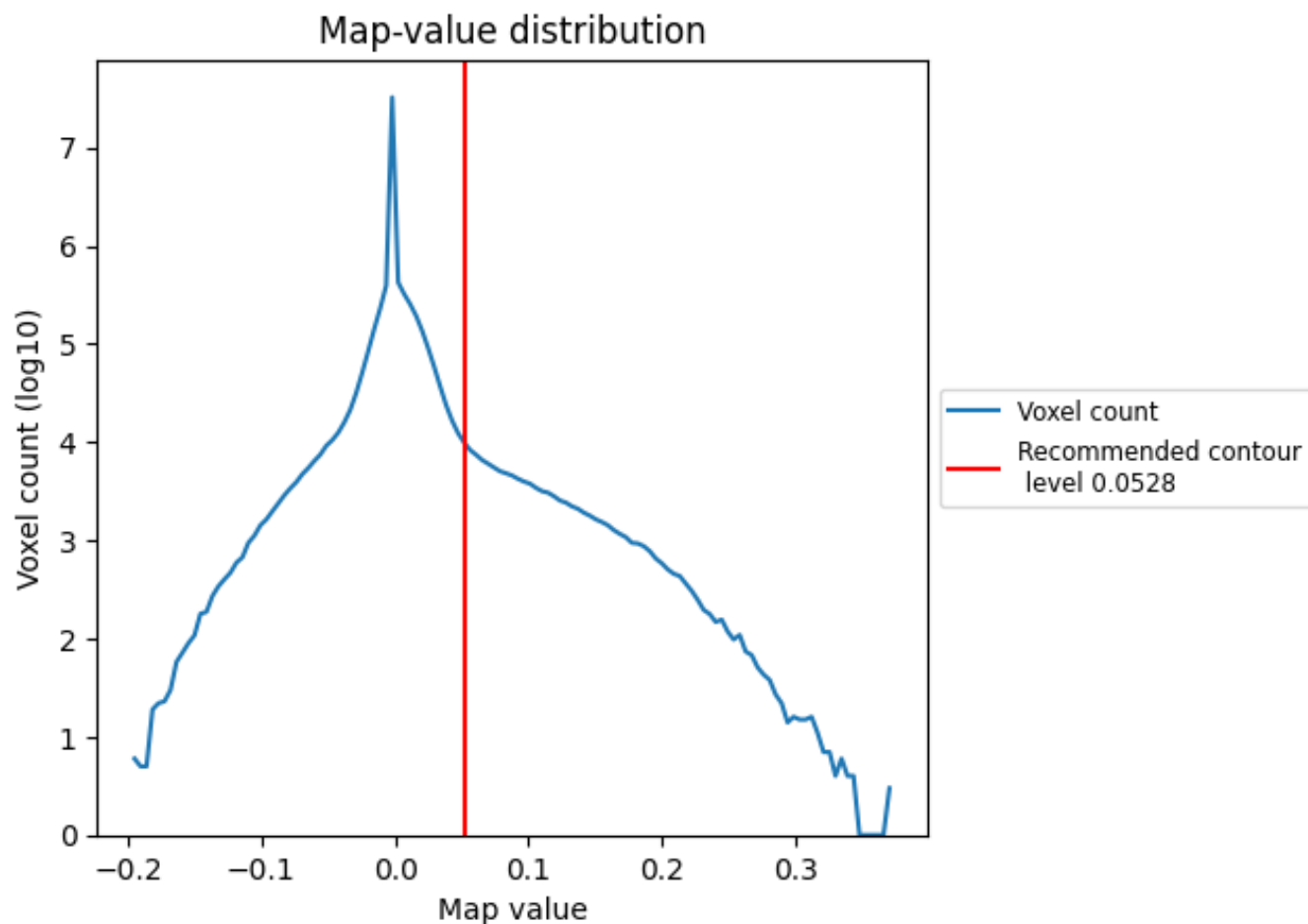
6.5 Mask visualisation

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

7 Map analysis [i](#)

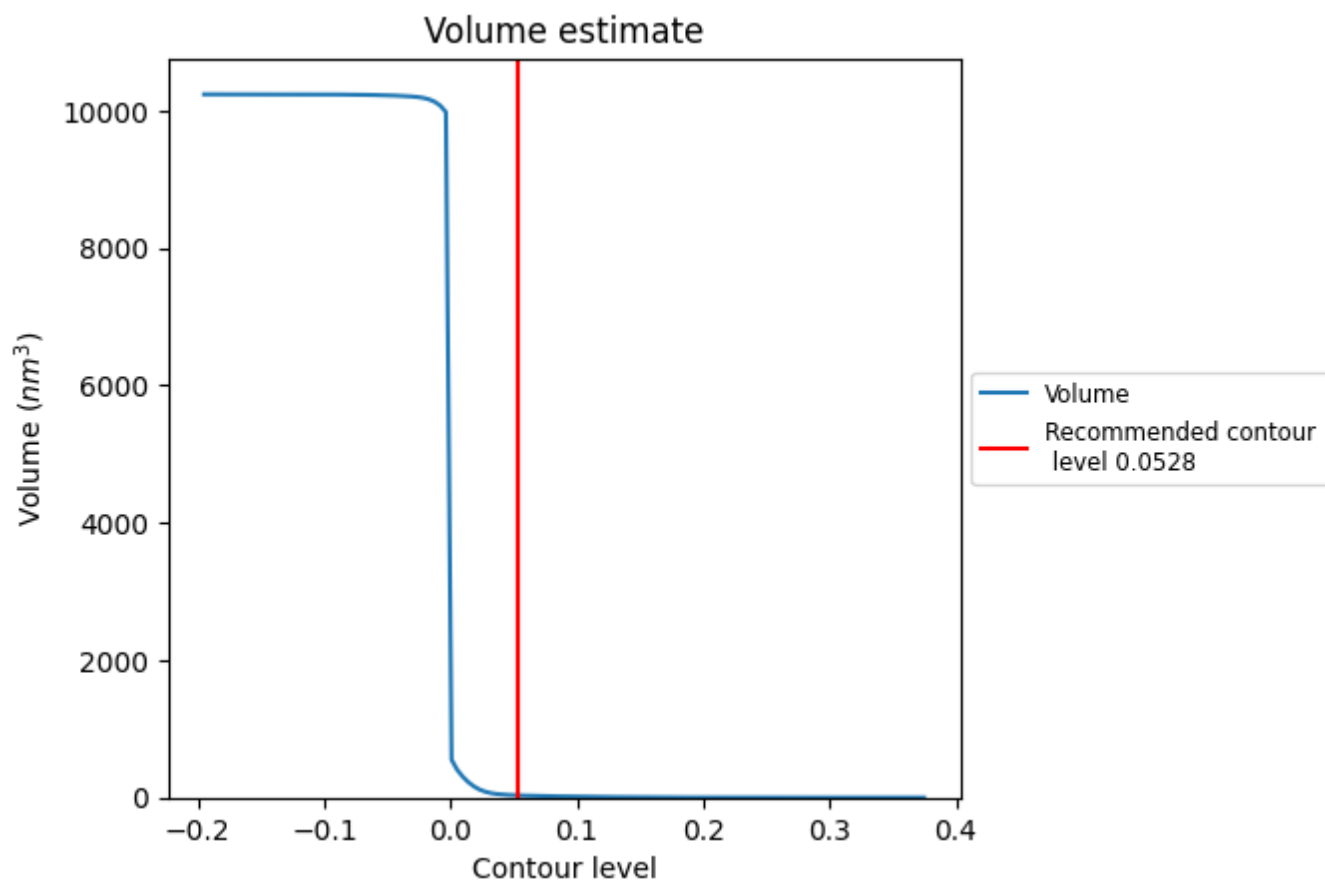
This section contains the results of statistical analysis of the map.

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.

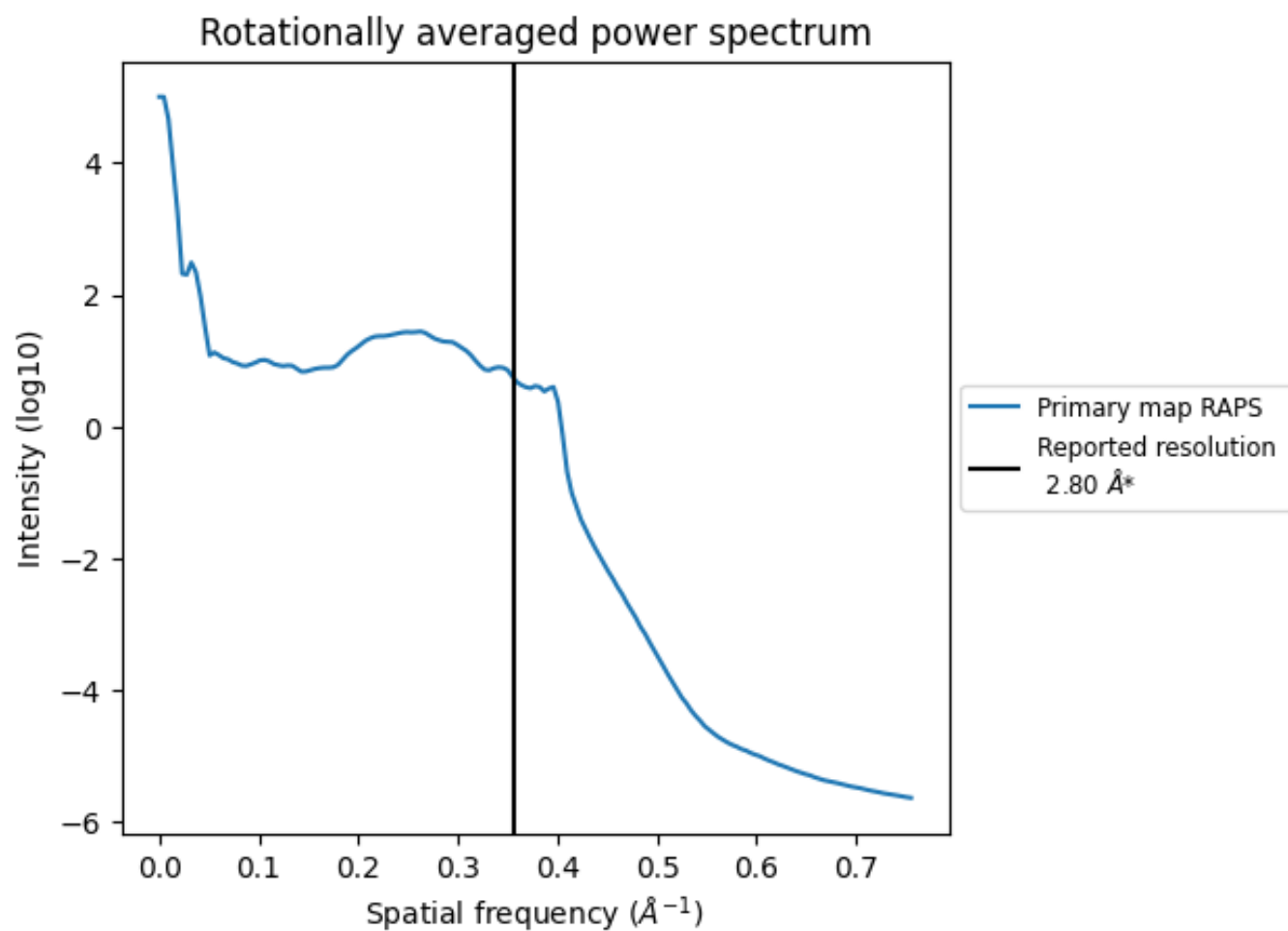
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 32 nm³; this corresponds to an approximate mass of 29 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [i](#)

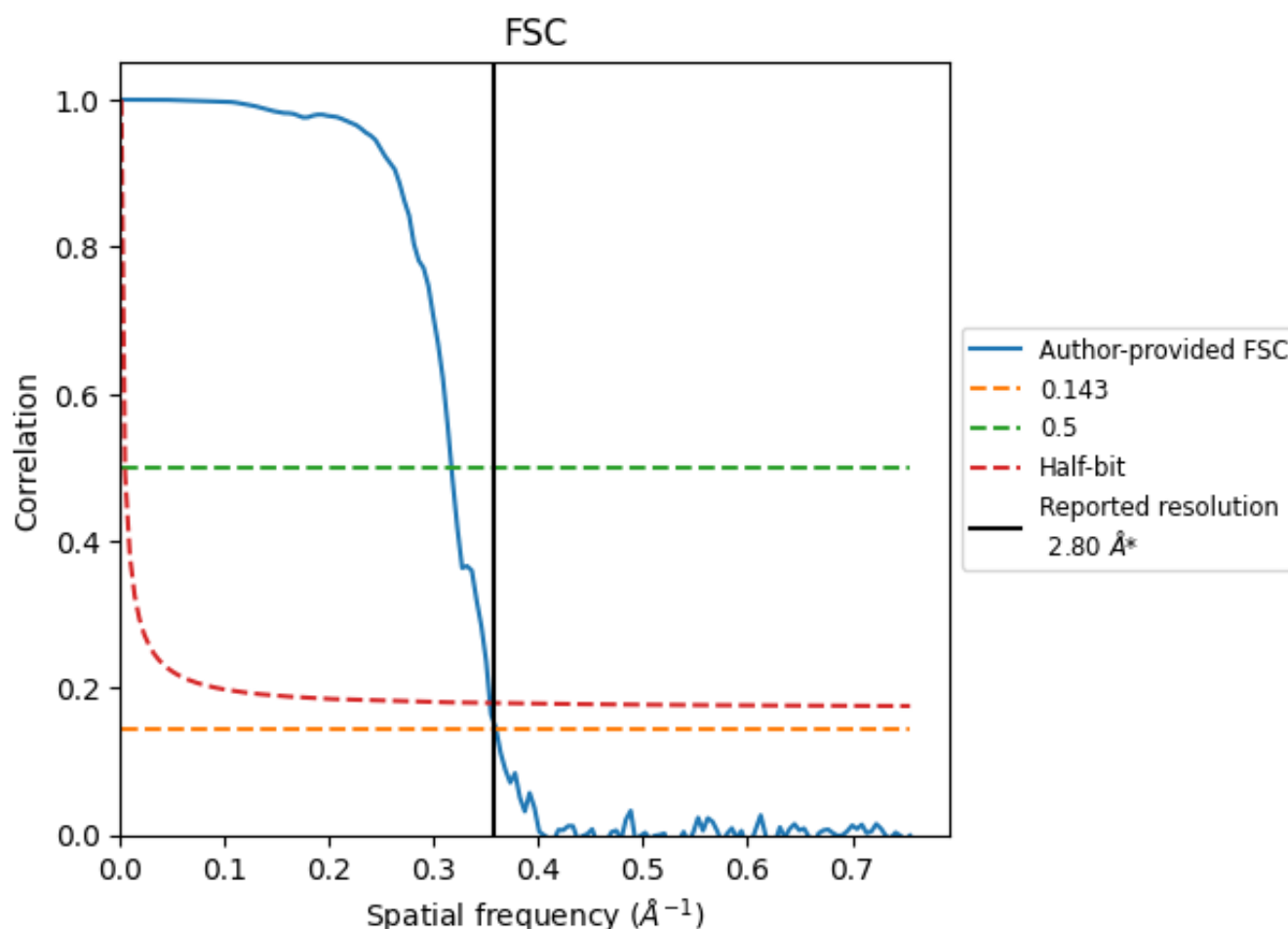


*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

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 0.357 \AA^{-1}

8.2 Resolution estimates [i](#)

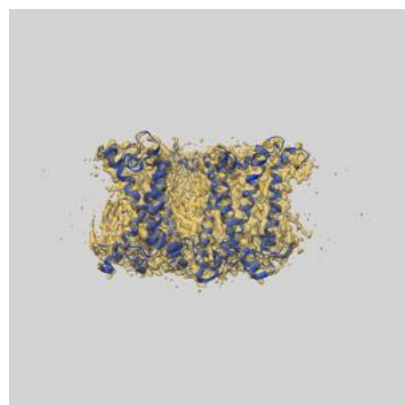
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.78	3.16	2.83
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

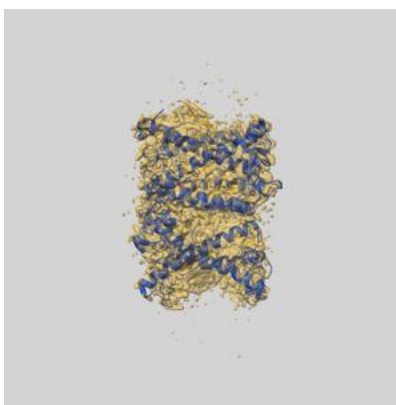
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-32588 and PDB model 7WLM. Per-residue inclusion information can be found in [section 3](#) on [page 10](#).

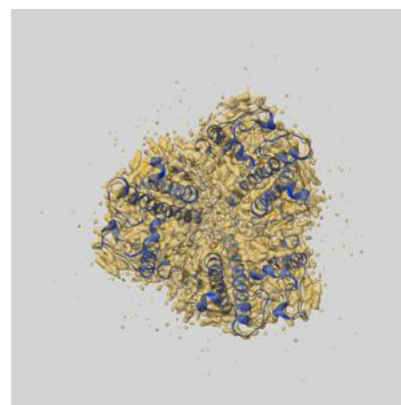
9.1 Map-model overlay [i](#)



X



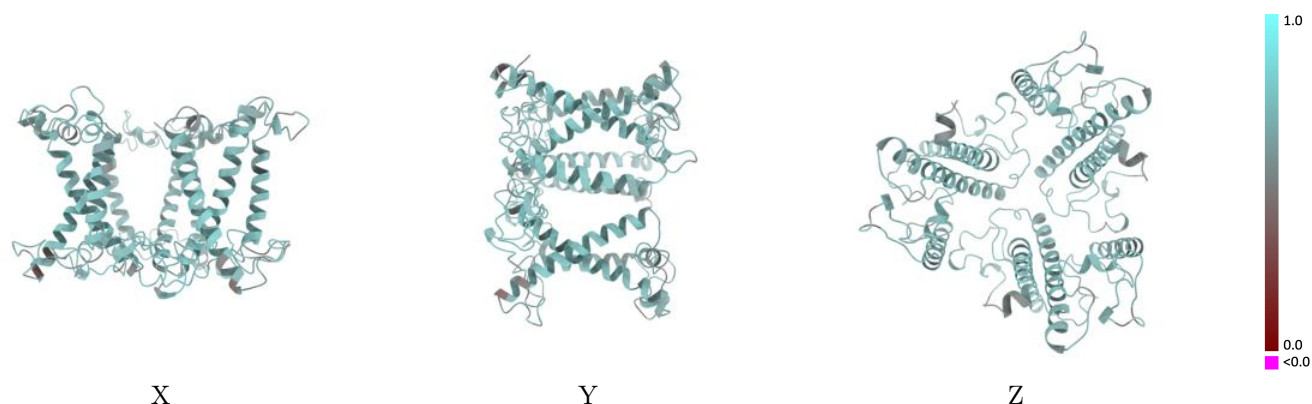
Y



Z

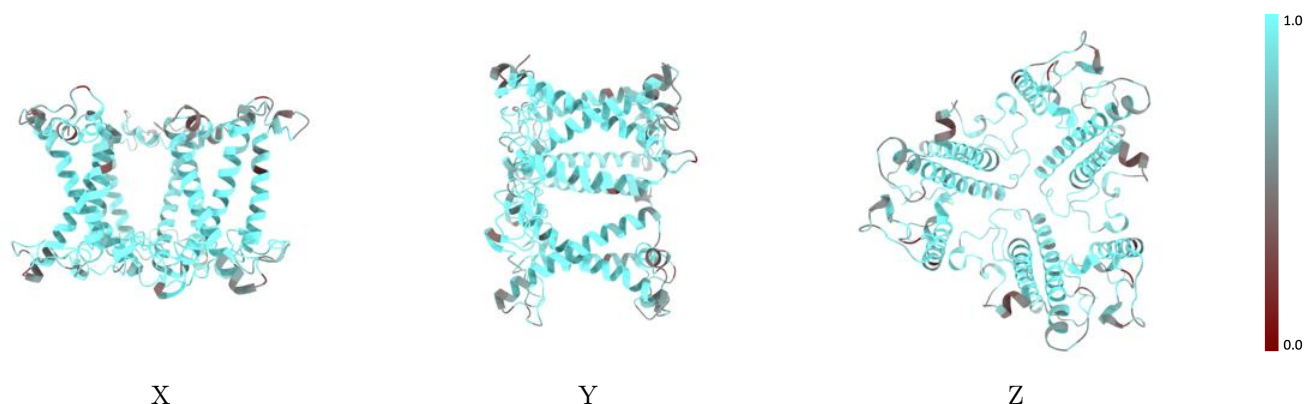
The images above show the 3D surface view of the map at the recommended contour level 0.0528 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



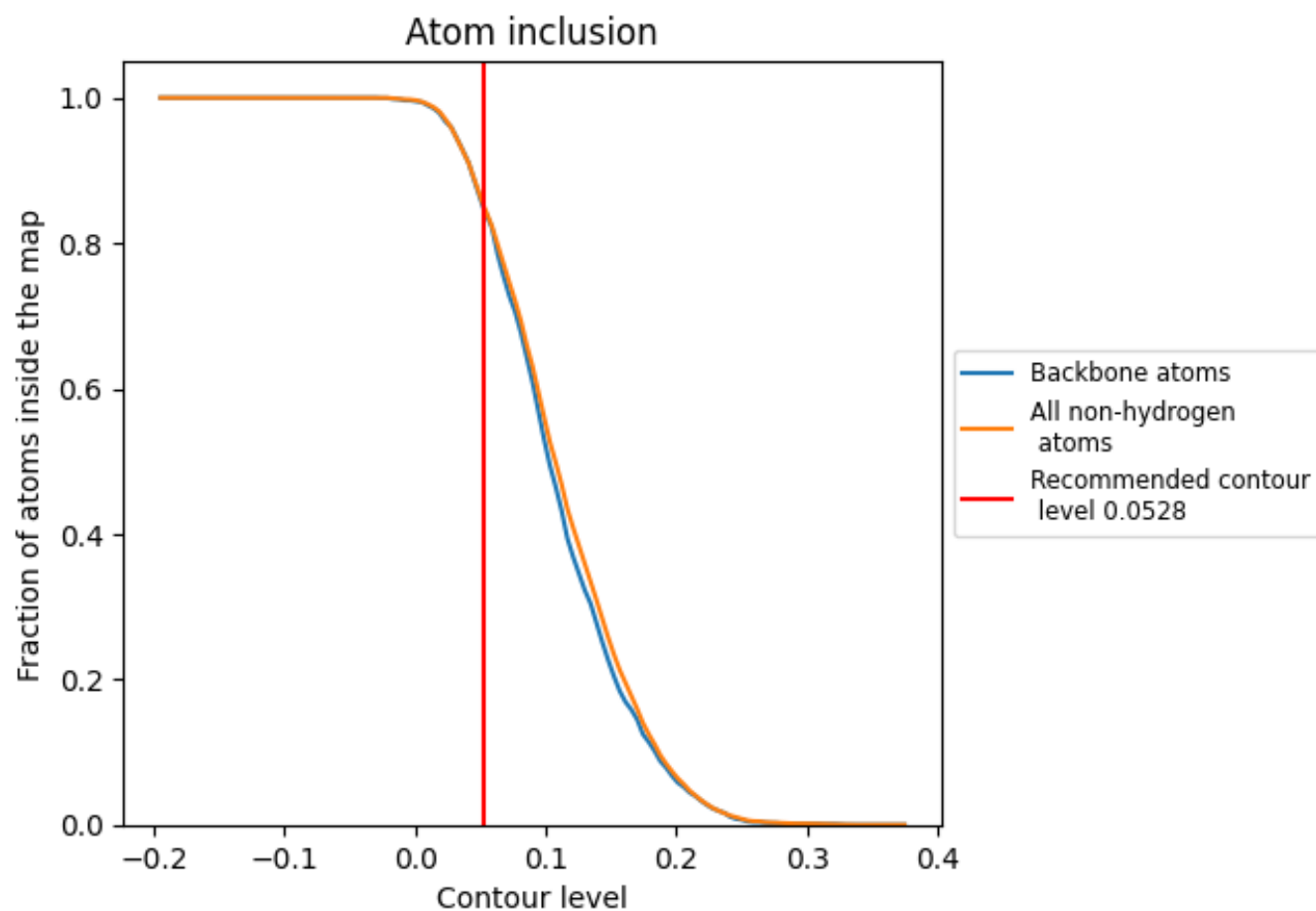
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0528).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 85% 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 (0.0528) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8494	<div></div> 0.6490
A	<div></div> 0.8506	<div></div> 0.6490
B	<div></div> 0.8480	<div></div> 0.6490
C	<div></div> 0.8471	<div></div> 0.6500

