



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 10:22 AM UTC

PDB ID : 8Y15 / pdb_00008y15
EMDB ID : EMD-38825
Title : Cryo-EM structure of Light-harvesting complex from Spinacia oleracea
Authors : Seki, S.; Miyata, T.; Tanaka, H.; Namba, K.; Kurisu, G.; Fujii, R.
Deposited on : 2024-01-23
Resolution : 2.17 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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
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) : 2.49

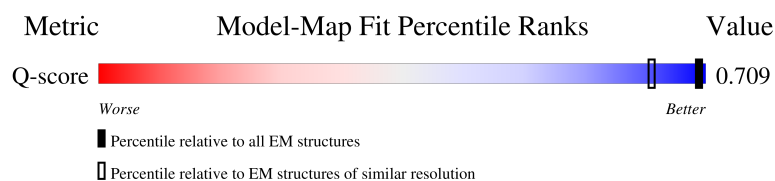
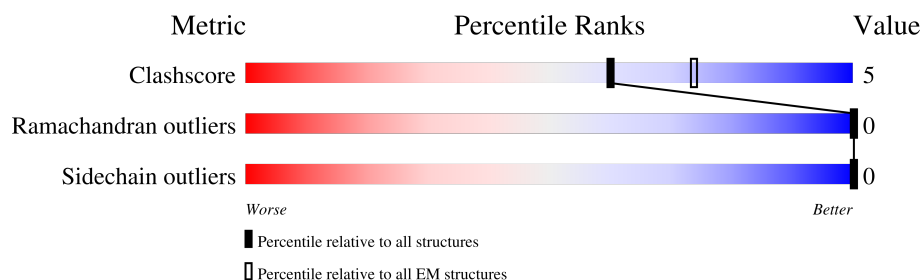
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

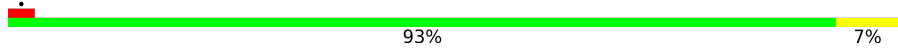
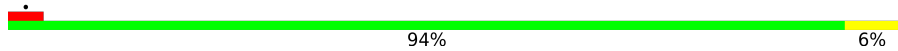
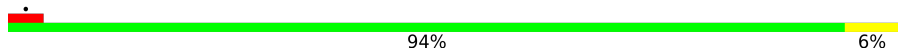
The reported resolution of this entry is 2.17 Å.

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	2651 (1.67 - 2.67)

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	216	
1	B	216	
1	C	216	

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	605	X	-	-	-
2	CHL	A	606	X	-	-	-
2	CHL	A	607	X	-	-	-
2	CHL	A	608	X	-	-	-
2	CHL	A	609	X	-	-	-
2	CHL	B	601	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	C	601	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	-	-	-
3	CLA	A	602	X	-	-	-
3	CLA	A	603	X	-	-	-
3	CLA	A	604	X	-	-	-
3	CLA	A	610	X	-	-	-
3	CLA	A	611	X	-	-	-
3	CLA	A	612	X	-	-	-
3	CLA	A	613	X	-	-	-
3	CLA	A	614	X	-	-	-
3	CLA	B	602	X	-	-	-
3	CLA	B	603	X	-	-	-
3	CLA	B	604	X	-	-	-
3	CLA	B	610	X	-	-	-
3	CLA	B	611	X	-	-	-
3	CLA	B	612	X	-	-	-
3	CLA	B	613	X	-	-	-
3	CLA	B	614	X	-	-	-
3	CLA	C	602	X	-	-	-
3	CLA	C	603	X	-	-	-
3	CLA	C	604	X	-	-	-
3	CLA	C	610	X	-	-	-
3	CLA	C	611	X	-	-	-
3	CLA	C	612	X	-	-	-
3	CLA	C	613	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CLA	C	614	X	-	-	-
7	XAT	A	1004	X	-	-	-
7	XAT	B	1004	X	-	-	-
7	XAT	C	1004	X	-	-	-

2 Entry composition [i](#)

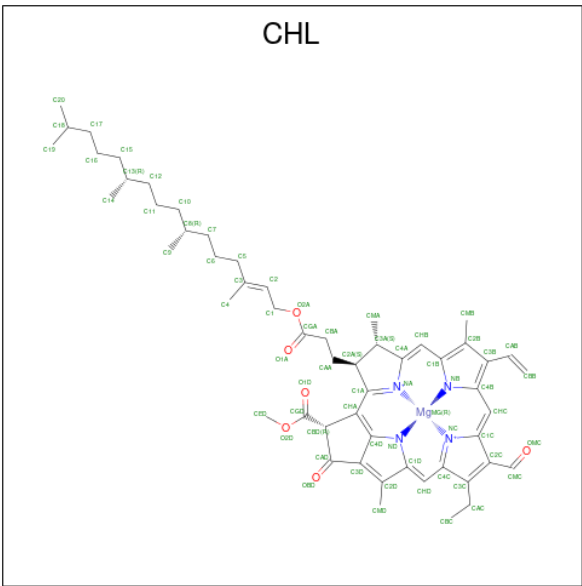
There are 8 unique types of molecules in this entry. The entry contains 8181 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	216	Total	C	N	O	S	0	0
			1650	1072	268	303	7		
1	B	216	Total	C	N	O	S	0	0
			1650	1072	268	303	7		
1	C	216	Total	C	N	O	S	0	0
			1650	1072	268	303	7		

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



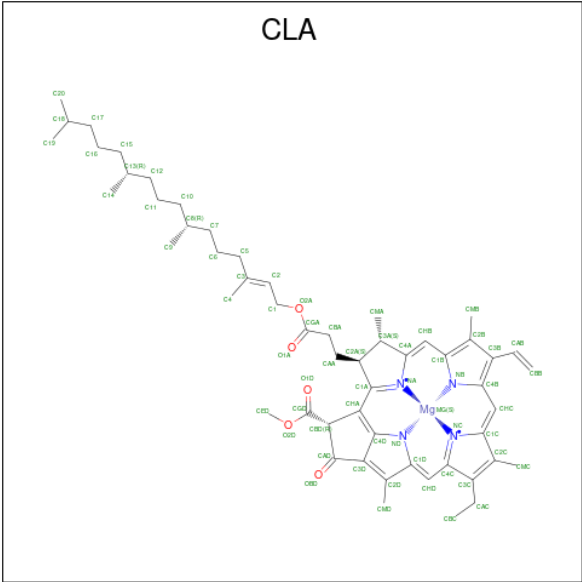
Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
2	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
2	A	1	Total	C	Mg	N	O	0
			51	40	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
2	A	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
2	A	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
2	B	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
2	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
2	B	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
2	B	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
2	B	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
2	B	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
2	C	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
2	C	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
2	C	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
2	C	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
2	C	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
2	C	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 3 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



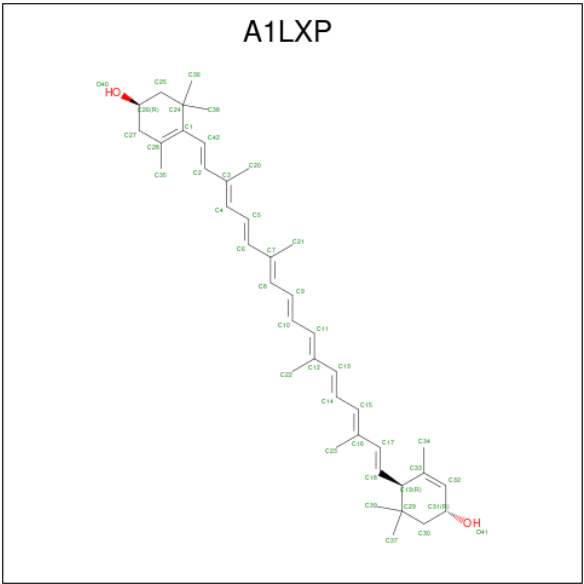
Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
3	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
3	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
3	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
3	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
3	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
3	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
3	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	C	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
3	C	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
3	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	C	1	Total	C	Mg	N	O	0
			42	34	1	4	3	

- Molecule 4 is Lutein (CCD ID: A1LXP) (formula: C₄₀H₅₆O₂) (labeled as "Ligand of Interest" by depositor).



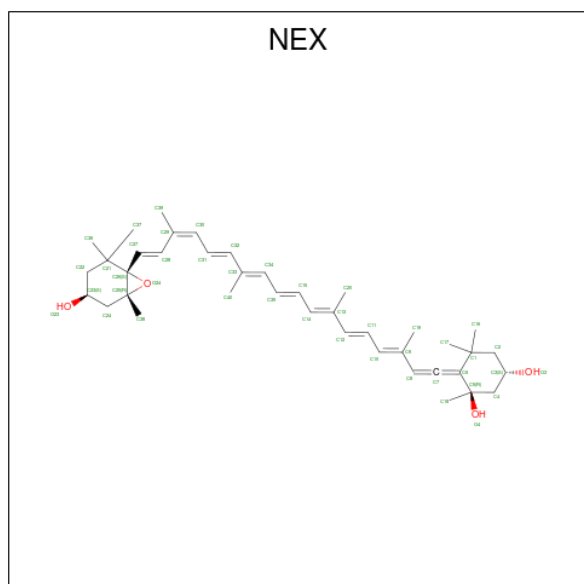
Mol	Chain	Residues	Atoms			AltConf
4	A	1	Total	C	O	0
			42	40	2	

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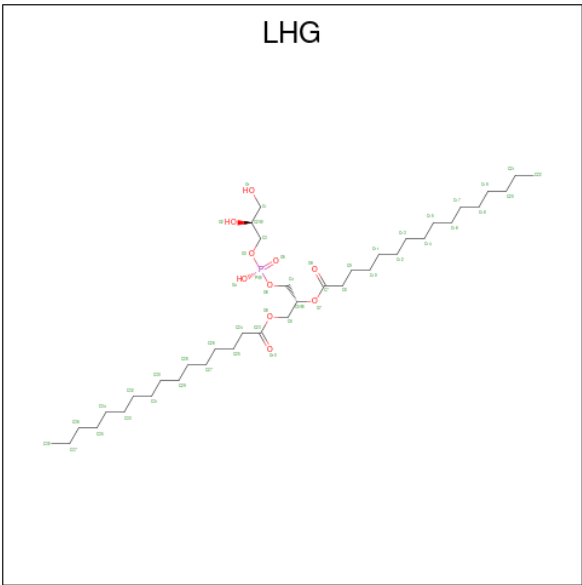
Mol	Chain	Residues	Atoms			AltConf
4	A	1	Total	C	O	0
			42	40	2	
4	B	1	Total	C	O	0
			42	40	2	
4	B	1	Total	C	O	0
			42	40	2	
4	C	1	Total	C	O	0
			42	40	2	
4	C	1	Total	C	O	0
			42	40	2	

- Molecule 5 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-TETRAMETHYLOCTADECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE]-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (CCD ID: NEX) (formula: C₄₀H₅₆O₄) (labeled as "Ligand of Interest" by depositor).



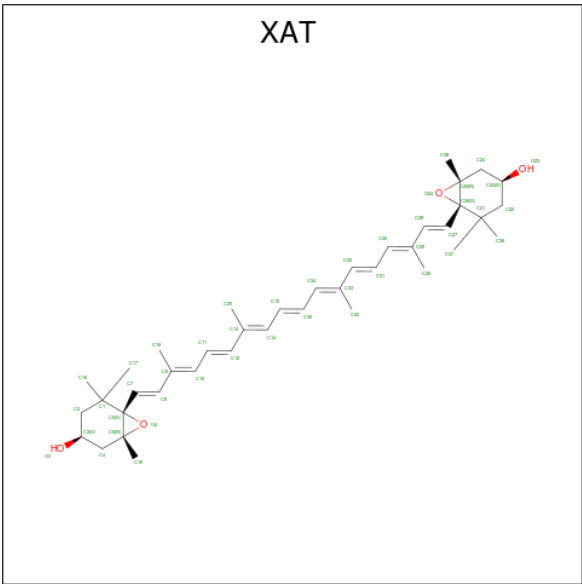
Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total	C	O	0
			44	40	4	
5	B	1	Total	C	O	0
			44	40	4	
5	C	1	Total	C	O	0
			44	40	4	

- Molecule 6 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	O	P	0
			49	38	10	1	
6	B	1	Total	C	O	P	0
			49	38	10	1	
6	C	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 7 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: C₄₀H₅₆O₄) (labeled as "Ligand of Interest" by depositor).



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

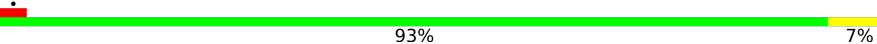
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		AltConf
8	A	45	Total	O	0
			45	45	
8	B	44	Total	O	0
			44	44	
8	C	43	Total	O	0
			43	43	

3 Residue-property plots [i](#)

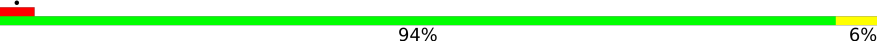
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

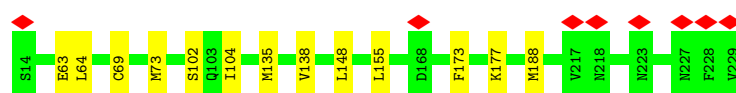
- Molecule 1: Chlorophyll a-b binding protein, chloroplastic

Chain A:  93% 7%

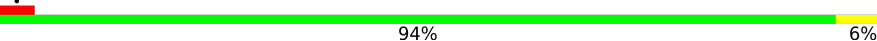


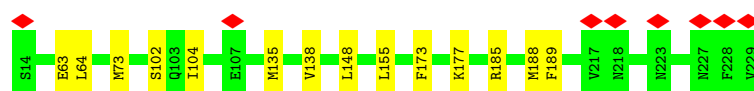
- Molecule 1: Chlorophyll a-b binding protein, chloroplastic

Chain B:  94% 6%



- Molecule 1: Chlorophyll a-b binding protein, chloroplastic

Chain C:  94% 6%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	479808	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	80	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	60000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.880	Depositor
Minimum map value	-1.503	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.069	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	219.904, 219.904, 219.904	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.859, 0.859, 0.859	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, A1LXP, XAT, NEX, CHL, LHG

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	0.12	0/1701	0.28	0/2316
1	B	0.12	0/1701	0.26	0/2316
1	C	0.12	0/1701	0.27	0/2316
All	All	0.12	0/5103	0.27	0/6948

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	1650	0	1582	10	0
1	B	1650	0	1582	9	0
1	C	1650	0	1582	10	0
2	A	335	0	296	7	0
2	B	335	0	296	8	0
2	C	335	0	296	8	0
3	A	477	0	489	11	0
3	B	477	0	489	9	0
3	C	477	0	489	10	0
4	A	84	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	84	0	0	1	0
4	C	84	0	0	1	0
5	A	44	0	53	0	0
5	B	44	0	53	0	0
5	C	44	0	53	0	0
6	A	49	0	74	2	0
6	B	49	0	74	4	0
6	C	49	0	74	6	0
7	A	44	0	56	3	0
7	B	44	0	56	2	0
7	C	44	0	56	1	0
8	A	45	0	0	0	0
8	B	44	0	0	0	0
8	C	43	0	0	0	0
All	All	8181	0	7650	71	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 (71) 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:185:ARG:HA	1:A:188:MET:HE3	1.76	0.67
1:A:148:LEU:HG	2:A:608:CHL:HAB	1.83	0.61
1:B:148:LEU:HG	2:B:608:CHL:HAB	1.83	0.60
7:B:1004:XAT:H12	6:C:1005:LHG:H191	1.83	0.59
7:A:1004:XAT:H363	6:B:1005:LHG:HC41	1.86	0.56
2:A:606:CHL:HBD	2:A:606:CHL:HBA2	1.87	0.56
2:B:606:CHL:HBD	2:B:606:CHL:HBA2	1.87	0.56
1:C:148:LEU:HG	2:C:608:CHL:HAB	1.87	0.56
1:C:185:ARG:HA	1:C:188:MET:HE3	1.88	0.55
2:C:606:CHL:HBA2	2:C:606:CHL:HBD	1.87	0.55
7:A:1004:XAT:H361	6:B:1005:LHG:HC92	1.89	0.55
2:B:601:CHL:HED3	6:B:1005:LHG:H142	1.90	0.54
3:C:610:CLA:H8	3:C:612:CLA:H102	1.90	0.54
6:A:1005:LHG:HC41	7:C:1004:XAT:H363	1.89	0.53
3:B:610:CLA:H8	3:B:612:CLA:H102	1.89	0.53
7:B:1004:XAT:H363	6:C:1005:LHG:HC41	1.90	0.53
1:C:64:LEU:HD13	3:C:603:CLA:HBA1	1.90	0.53
1:A:69:CYS:SG	1:A:188:MET:HE2	2.50	0.51
2:C:601:CHL:H202	6:C:1005:LHG:H221	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:LEU:HD13	3:B:603:CLA:HBA1	1.93	0.50
3:C:603:CLA:HBB1	2:C:609:CHL:H161	1.94	0.50
1:A:64:LEU:HD13	3:A:603:CLA:HBA1	1.93	0.49
1:C:189:PHE:HZ	6:C:1005:LHG:H151	1.79	0.48
3:A:610:CLA:H8	3:A:612:CLA:H102	1.94	0.48
1:A:63:GLU:HA	1:A:155:LEU:HD11	1.96	0.47
1:B:102:SER:HB3	2:B:607:CHL:HED2	1.97	0.47
3:A:603:CLA:HBB1	2:A:609:CHL:H13	1.95	0.47
2:C:601:CHL:HBA1	2:C:601:CHL:H3A	1.69	0.46
1:B:63:GLU:HA	1:B:155:LEU:HD11	1.97	0.46
2:B:601:CHL:HBA1	2:B:601:CHL:H3A	1.68	0.46
6:C:1005:LHG:H301	6:C:1005:LHG:H341	1.97	0.46
3:B:603:CLA:HBB1	2:B:609:CHL:H13	1.98	0.46
3:B:604:CLA:HBD	3:B:604:CLA:HBA1	1.98	0.46
3:A:602:CLA:H41	3:A:602:CLA:H61	1.67	0.45
1:C:135:MET:HA	1:C:138:VAL:HG22	1.97	0.45
1:A:135:MET:HA	1:A:138:VAL:HG22	1.98	0.45
3:C:612:CLA:HMA3	3:C:612:CLA:H101	1.98	0.45
3:A:603:CLA:HAB	4:A:1002:A1LXP:C10	2.47	0.44
3:A:604:CLA:HBA1	3:A:604:CLA:HBD	1.99	0.44
3:B:613:CLA:H51	3:B:613:CLA:C3C	2.47	0.44
1:C:102:SER:HB3	2:C:607:CHL:HED2	1.99	0.44
1:B:135:MET:HA	1:B:138:VAL:HG22	1.99	0.44
7:A:1004:XAT:H10	6:B:1005:LHG:H211	1.99	0.44
1:B:73:MET:SD	3:B:610:CLA:HAB	2.58	0.44
3:A:613:CLA:H51	3:A:613:CLA:C3C	2.47	0.44
3:C:613:CLA:C3C	3:C:613:CLA:H51	2.48	0.43
3:A:603:CLA:C4B	2:A:609:CHL:H111	2.48	0.43
3:C:604:CLA:HBD	3:C:604:CLA:HBA1	2.00	0.43
3:C:610:CLA:H41	3:C:612:CLA:H92	2.00	0.43
1:C:63:GLU:HA	1:C:155:LEU:HD11	1.99	0.43
3:A:603:CLA:HBB1	2:A:609:CHL:H161	2.00	0.43
3:B:603:CLA:HAB	4:B:1002:A1LXP:C10	2.48	0.43
1:B:69:CYS:SG	1:B:188:MET:HE2	2.59	0.43
3:B:603:CLA:C4B	2:B:609:CHL:H111	2.49	0.43
3:C:603:CLA:HAB	4:C:1002:A1LXP:C10	2.49	0.43
3:B:610:CLA:H41	3:B:612:CLA:H92	2.01	0.42
1:A:173:PHE:CZ	1:A:177:LYS:HE3	2.54	0.42
2:C:601:CHL:H162	6:C:1005:LHG:H221	2.01	0.42
3:C:603:CLA:C4B	2:C:609:CHL:H111	2.49	0.42
1:A:102:SER:HB3	2:A:607:CHL:HED2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:610:CLA:H41	3:A:612:CLA:H92	2.02	0.42
1:C:73:MET:SD	3:C:610:CLA:HAB	2.60	0.42
2:A:601:CHL:HMA3	6:A:1005:LHG:H121	2.02	0.41
1:C:173:PHE:CZ	1:C:177:LYS:HE3	2.55	0.41
1:B:173:PHE:CZ	1:B:177:LYS:HE3	2.55	0.41
1:A:203:LYS:HD2	1:A:207:GLU:HG2	2.01	0.41
2:B:601:CHL:H62	2:B:601:CHL:H41	1.81	0.41
1:C:104:ILE:HD12	1:C:104:ILE:HA	1.90	0.41
1:A:24:TYR:HB3	1:A:44:TYR:HB3	2.03	0.41
1:B:104:ILE:HD12	1:B:104:ILE:HA	1.90	0.40
3:A:613:CLA:H2	3:A:613:CLA:H61	1.82	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	214/216 (99%)	211 (99%)	3 (1%)	0	100	100
1	B	214/216 (99%)	212 (99%)	2 (1%)	0	100	100
1	C	214/216 (99%)	212 (99%)	2 (1%)	0	100	100
All	All	642/648 (99%)	635 (99%)	7 (1%)	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	167/167 (100%)	167 (100%)	0	100	100
1	B	167/167 (100%)	167 (100%)	0	100	100
1	C	167/167 (100%)	167 (100%)	0	100	100
All	All	501/501 (100%)	501 (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. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	183	ASN
1	B	183	ASN
1	B	208	ASN
1	C	183	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

57 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	611	6	69,73,73	1.67	8 (11%)	82,113,113	1.15	8 (9%)
3	CLA	C	602	1	69,73,73	1.64	9 (13%)	82,113,113	1.02	9 (10%)
2	CHL	A	608	8	55,69,74	1.44	4 (7%)	52,108,114	1.89	7 (13%)
3	CLA	A	604	8	59,63,73	1.81	8 (13%)	70,101,113	1.21	8 (11%)
6	LHG	C	1005	3	48,48,48	0.23	0	51,54,54	0.27	0
3	CLA	B	613	1	69,73,73	1.63	8 (11%)	82,113,113	1.03	9 (10%)
2	CHL	C	606	8	45,59,74	1.58	4 (8%)	40,96,114	2.21	8 (20%)
3	CLA	A	603	1	59,63,73	1.75	8 (13%)	70,101,113	1.22	9 (12%)
4	A1LXP	C	1001	-	42,43,43	0.47	1 (2%)	51,60,60	0.28	0
2	CHL	B	607	8	40,54,74	1.68	4 (10%)	34,90,114	2.40	6 (17%)
4	A1LXP	B	1002	-	42,43,43	0.45	1 (2%)	51,60,60	0.28	0
3	CLA	C	610	1	69,73,73	1.65	9 (13%)	82,113,113	1.04	9 (10%)
3	CLA	C	614	1	46,50,73	2.01	9 (19%)	53,85,113	1.32	8 (15%)
3	CLA	B	603	1	59,63,73	1.77	8 (13%)	70,101,113	1.22	9 (12%)
2	CHL	C	609	1	60,74,74	1.40	4 (6%)	58,114,114	1.78	7 (12%)
2	CHL	A	606	8	45,59,74	1.61	4 (8%)	40,96,114	2.21	8 (20%)
3	CLA	A	614	1	46,50,73	2.02	9 (19%)	53,85,113	1.31	8 (15%)
5	NEX	A	1003	-	40,46,46	2.34	4 (10%)	50,70,70	0.59	1 (2%)
4	A1LXP	B	1001	-	42,43,43	0.47	1 (2%)	51,60,60	0.27	0
2	CHL	B	601	1	60,74,74	1.38	4 (6%)	58,114,114	1.84	7 (12%)
2	CHL	A	607	8	40,54,74	1.68	4 (10%)	34,90,114	2.42	6 (17%)
3	CLA	C	613	1	69,73,73	1.64	8 (11%)	82,113,113	1.03	9 (10%)
3	CLA	A	611	6	69,73,73	1.66	8 (11%)	82,113,113	1.16	8 (9%)
2	CHL	C	607	8	40,54,74	1.69	4 (10%)	34,90,114	2.41	6 (17%)
3	CLA	B	602	1	69,73,73	1.64	9 (13%)	82,113,113	1.01	9 (10%)
2	CHL	B	605	1	38,53,74	1.73	4 (10%)	31,88,114	2.40	6 (19%)
3	CLA	C	611	6	69,73,73	1.67	8 (11%)	82,113,113	1.16	8 (9%)
6	LHG	A	1005	3	48,48,48	0.23	0	51,54,54	0.28	0
3	CLA	A	602	1	69,73,73	1.64	9 (13%)	82,113,113	1.01	9 (10%)
7	XAT	A	1004	-	41,47,47	0.14	0	54,74,74	2.27	2 (3%)
3	CLA	A	612	1	69,73,73	1.63	8 (11%)	82,113,113	1.11	9 (10%)
4	A1LXP	A	1002	-	42,43,43	0.46	1 (2%)	51,60,60	0.29	0
3	CLA	C	604	8	59,63,73	1.80	8 (13%)	70,101,113	1.22	9 (12%)
3	CLA	C	603	1	59,63,73	1.76	8 (13%)	70,101,113	1.21	9 (12%)
3	CLA	C	612	1	69,73,73	1.63	8 (11%)	82,113,113	1.11	9 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	CHL	B	608	8	55,69,74	1.46	4 (7%)	52,108,114	1.90	6 (11%)
4	A1LXP	A	1001	-	42,43,43	0.46	1 (2%)	51,60,60	0.28	0
2	CHL	A	601	1	60,74,74	1.39	4 (6%)	58,114,114	1.87	6 (10%)
3	CLA	B	612	1	69,73,73	1.63	8 (11%)	82,113,113	1.11	9 (10%)
2	CHL	C	605	1	38,53,74	1.74	4 (10%)	31,88,114	2.40	6 (19%)
5	NEX	C	1003	-	40,46,46	2.33	4 (10%)	50,70,70	0.58	1 (2%)
7	XAT	B	1004	-	41,47,47	0.13	0	54,74,74	2.26	2 (3%)
6	LHG	B	1005	3	48,48,48	0.23	0	51,54,54	0.28	0
2	CHL	C	601	1	60,74,74	1.37	4 (6%)	58,114,114	1.85	6 (10%)
3	CLA	A	610	1	69,73,73	1.65	8 (11%)	82,113,113	1.05	9 (10%)
3	CLA	B	614	1	46,50,73	2.01	9 (19%)	53,85,113	1.31	8 (15%)
2	CHL	A	609	1	60,74,74	1.40	4 (6%)	58,114,114	1.77	7 (12%)
2	CHL	A	605	1	38,53,74	1.74	4 (10%)	31,88,114	2.40	6 (19%)
2	CHL	B	606	8	45,59,74	1.60	4 (8%)	40,96,114	2.21	8 (20%)
3	CLA	B	604	8	59,63,73	1.80	8 (13%)	70,101,113	1.21	9 (12%)
3	CLA	B	610	1	69,73,73	1.65	9 (13%)	82,113,113	1.04	9 (10%)
7	XAT	C	1004	-	41,47,47	0.13	0	54,74,74	2.27	2 (3%)
4	A1LXP	C	1002	-	42,43,43	0.45	1 (2%)	51,60,60	0.28	0
5	NEX	B	1003	-	40,46,46	2.26	3 (7%)	50,70,70	0.59	1 (2%)
2	CHL	B	609	1	60,74,74	1.39	4 (6%)	58,114,114	1.77	7 (12%)
2	CHL	C	608	8	55,69,74	1.45	4 (7%)	52,108,114	1.90	6 (11%)
3	CLA	A	613	1	69,73,73	1.64	8 (11%)	82,113,113	1.03	9 (10%)

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	611	6	2/2/15/20	13/39/115/115	-
3	CLA	C	602	1	2/2/15/20	6/39/115/115	-
2	CHL	A	608	8	4/4/19/26	3/33/131/137	-
3	CLA	A	604	8	2/2/13/20	6/27/103/115	-
6	LHG	C	1005	3	-	10/53/53/53	-
3	CLA	B	613	1	2/2/15/20	6/39/115/115	-
2	CHL	C	606	8	3/3/17/26	6/21/119/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CLA	A	603	1	2/2/13/20	6/27/103/115	-
4	A1LXP	C	1001	-	-	2/29/67/67	0/2/2/2
2	CHL	B	607	8	3/3/16/26	4/15/113/137	-
4	A1LXP	B	1002	-	-	2/29/67/67	0/2/2/2
3	CLA	C	610	1	2/2/15/20	2/39/115/115	-
3	CLA	C	614	1	1/1/10/20	4/12/88/115	-
3	CLA	B	603	1	2/2/13/20	5/27/103/115	-
2	CHL	C	609	1	4/4/20/26	7/39/137/137	-
2	CHL	A	606	8	3/3/17/26	4/21/119/137	-
3	CLA	A	614	1	1/1/10/20	4/12/88/115	-
5	NEX	A	1003	-	-	2/27/83/83	0/3/3/3
4	A1LXP	B	1001	-	-	1/29/67/67	0/2/2/2
2	CHL	B	601	1	4/4/20/26	7/39/137/137	-
2	CHL	A	607	8	3/3/16/26	3/15/113/137	-
3	CLA	C	613	1	2/2/15/20	6/39/115/115	-
3	CLA	A	611	6	2/2/15/20	13/39/115/115	-
2	CHL	C	607	8	3/3/16/26	3/15/113/137	-
3	CLA	B	602	1	2/2/15/20	10/39/115/115	-
2	CHL	B	605	1	3/3/15/26	4/14/112/137	-
3	CLA	C	611	6	2/2/15/20	14/39/115/115	-
6	LHG	A	1005	3	-	7/53/53/53	-
3	CLA	A	602	1	2/2/15/20	7/39/115/115	-
7	XAT	A	1004	-	2/2/12/26	0/31/93/93	0/4/4/4
3	CLA	A	612	1	2/2/15/20	6/39/115/115	-
4	A1LXP	A	1002	-	-	1/29/67/67	0/2/2/2
3	CLA	C	604	8	2/2/13/20	6/27/103/115	-
3	CLA	C	603	1	2/2/13/20	6/27/103/115	-
3	CLA	C	612	1	2/2/15/20	6/39/115/115	-
2	CHL	B	608	8	4/4/19/26	3/33/131/137	-
7	XAT	B	1004	-	2/2/12/26	0/31/93/93	0/4/4/4
2	CHL	A	601	1	4/4/20/26	9/39/137/137	-
3	CLA	B	612	1	2/2/15/20	6/39/115/115	-
2	CHL	C	605	1	3/3/15/26	4/14/112/137	-
4	A1LXP	A	1001	-	-	2/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NEX	C	1003	-	-	2/27/83/83	0/3/3/3
6	LHG	B	1005	3	-	11/53/53/53	-
2	CHL	C	601	1	4/4/20/26	8/39/137/137	-
3	CLA	A	610	1	2/2/15/20	2/39/115/115	-
3	CLA	B	614	1	1/1/10/20	4/12/88/115	-
2	CHL	A	609	1	4/4/20/26	6/39/137/137	-
2	CHL	A	605	1	3/3/15/26	4/14/112/137	-
2	CHL	B	606	8	3/3/17/26	6/21/119/137	-
3	CLA	B	604	8	2/2/13/20	6/27/103/115	-
3	CLA	B	610	1	2/2/15/20	2/39/115/115	-
7	XAT	C	1004	-	2/2/12/26	0/31/93/93	0/4/4/4
4	A1LXP	C	1002	-	-	2/29/67/67	0/2/2/2
5	NEX	B	1003	-	-	2/27/83/83	0/3/3/3
2	CHL	B	609	1	4/4/20/26	5/39/137/137	-
2	CHL	C	608	8	4/4/19/26	6/33/131/137	-
3	CLA	A	613	1	2/2/15/20	6/39/115/115	-

All (289) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1003	NEX	C40-C33	-13.41	1.23	1.50
5	B	1003	NEX	C40-C33	-13.06	1.24	1.50
5	C	1003	NEX	C40-C33	-12.86	1.24	1.50
3	A	614	CLA	C4B-NB	8.14	1.48	1.37
3	B	603	CLA	C4B-NB	8.14	1.48	1.37
3	A	603	CLA	C4B-NB	8.04	1.48	1.37
3	C	614	CLA	C4B-NB	8.03	1.48	1.37
3	B	614	CLA	C4B-NB	8.02	1.48	1.37
3	C	603	CLA	C4B-NB	8.01	1.48	1.37
3	B	602	CLA	C4B-NB	8.00	1.48	1.37
3	C	612	CLA	C4B-NB	7.96	1.48	1.37
3	A	602	CLA	C4B-NB	7.93	1.48	1.37
3	B	612	CLA	C4B-NB	7.92	1.48	1.37
3	A	604	CLA	C4B-NB	7.91	1.48	1.37
3	C	610	CLA	C4B-NB	7.90	1.48	1.37
3	B	610	CLA	C4B-NB	7.88	1.48	1.37
3	A	610	CLA	C4B-NB	7.87	1.48	1.37
3	B	613	CLA	C4B-NB	7.86	1.48	1.37
3	C	602	CLA	C4B-NB	7.86	1.48	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	612	CLA	C4B-NB	7.86	1.48	1.37
3	A	613	CLA	C4B-NB	7.85	1.48	1.37
3	B	604	CLA	C4B-NB	7.83	1.48	1.37
3	C	604	CLA	C4B-NB	7.83	1.48	1.37
3	C	613	CLA	C4B-NB	7.83	1.48	1.37
3	C	611	CLA	C4B-NB	7.78	1.48	1.37
3	B	611	CLA	C4B-NB	7.77	1.48	1.37
2	A	601	CHL	C1B-C2B	7.75	1.48	1.39
3	A	611	CLA	C4B-NB	7.75	1.48	1.37
2	B	606	CHL	C1B-C2B	7.69	1.48	1.39
2	A	606	CHL	C1B-C2B	7.65	1.48	1.39
2	C	606	CHL	C1B-C2B	7.61	1.48	1.39
2	B	601	CHL	C1B-C2B	7.54	1.48	1.39
2	C	605	CHL	C1B-C2B	7.50	1.48	1.39
2	C	607	CHL	C1B-C2B	7.49	1.48	1.39
2	B	605	CHL	C1B-C2B	7.48	1.48	1.39
2	A	605	CHL	C1B-C2B	7.48	1.48	1.39
2	A	609	CHL	C1B-C2B	7.47	1.48	1.39
2	A	607	CHL	C1B-C2B	7.46	1.48	1.39
2	C	609	CHL	C1B-C2B	7.44	1.48	1.39
2	B	607	CHL	C1B-C2B	7.43	1.48	1.39
2	B	608	CHL	C1B-C2B	7.40	1.48	1.39
2	C	608	CHL	C1B-C2B	7.39	1.48	1.39
2	B	609	CHL	C1B-C2B	7.38	1.47	1.39
2	C	601	CHL	C1B-C2B	7.36	1.47	1.39
2	A	608	CHL	C1B-C2B	7.36	1.47	1.39
3	C	611	CLA	MG-NB	-5.09	1.95	2.05
3	A	604	CLA	MG-NB	-5.09	1.95	2.05
3	C	604	CLA	MG-NB	-5.07	1.95	2.05
3	B	611	CLA	MG-NB	-5.04	1.95	2.05
3	C	610	CLA	MG-NB	-5.03	1.95	2.05
3	B	604	CLA	MG-NB	-5.03	1.95	2.05
3	A	604	CLA	MG-ND	-5.02	1.95	2.05
3	C	613	CLA	MG-NB	-5.02	1.95	2.05
3	B	602	CLA	MG-NB	-5.01	1.95	2.05
3	B	610	CLA	MG-NB	-5.01	1.95	2.05
3	A	602	CLA	MG-NB	-5.01	1.95	2.05
3	A	610	CLA	MG-NB	-5.00	1.95	2.05
3	C	602	CLA	MG-NB	-5.00	1.95	2.05
3	B	613	CLA	MG-NB	-4.99	1.95	2.05
3	B	604	CLA	MG-ND	-4.99	1.95	2.05
3	C	604	CLA	MG-ND	-4.98	1.95	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	613	CLA	MG-NB	-4.98	1.95	2.05
3	B	611	CLA	MG-ND	-4.96	1.96	2.05
3	A	611	CLA	MG-NB	-4.95	1.96	2.05
5	C	1003	NEX	C28-C27	4.93	1.43	1.32
3	C	611	CLA	MG-ND	-4.92	1.96	2.05
3	A	611	CLA	MG-ND	-4.91	1.96	2.05
3	C	610	CLA	MG-ND	-4.90	1.96	2.05
3	B	610	CLA	MG-ND	-4.89	1.96	2.05
3	C	602	CLA	MG-ND	-4.87	1.96	2.05
3	A	610	CLA	MG-ND	-4.86	1.96	2.05
3	A	602	CLA	MG-ND	-4.85	1.96	2.05
3	B	602	CLA	MG-ND	-4.85	1.96	2.05
3	A	614	CLA	MG-NB	-4.84	1.96	2.05
3	C	614	CLA	MG-NB	-4.83	1.96	2.05
3	C	613	CLA	MG-ND	-4.82	1.96	2.05
3	B	614	CLA	MG-NB	-4.81	1.96	2.05
3	A	613	CLA	MG-ND	-4.81	1.96	2.05
3	B	613	CLA	MG-ND	-4.79	1.96	2.05
3	B	612	CLA	MG-NB	-4.76	1.96	2.05
3	C	612	CLA	MG-NB	-4.75	1.96	2.05
3	A	612	CLA	MG-NB	-4.74	1.96	2.05
3	A	612	CLA	MG-ND	-4.71	1.96	2.05
3	B	612	CLA	MG-ND	-4.69	1.96	2.05
3	C	612	CLA	MG-ND	-4.68	1.96	2.05
3	B	603	CLA	MG-NB	-4.65	1.96	2.05
3	C	603	CLA	MG-NB	-4.63	1.96	2.05
3	B	614	CLA	MG-ND	-4.59	1.96	2.05
3	A	614	CLA	MG-ND	-4.58	1.96	2.05
3	A	603	CLA	MG-NB	-4.58	1.96	2.05
3	C	614	CLA	MG-ND	-4.57	1.96	2.05
3	B	603	CLA	MG-ND	-4.52	1.96	2.05
3	A	603	CLA	MG-ND	-4.51	1.96	2.05
3	C	603	CLA	MG-ND	-4.51	1.96	2.05
3	A	611	CLA	MG-NA	-4.28	1.96	2.06
3	B	611	CLA	MG-NA	-4.27	1.96	2.06
3	C	611	CLA	MG-NA	-4.22	1.96	2.06
3	C	604	CLA	MG-NA	-4.17	1.96	2.06
3	B	604	CLA	MG-NA	-4.16	1.96	2.06
3	A	604	CLA	MG-NA	-4.12	1.96	2.06
3	C	610	CLA	MG-NA	-4.09	1.96	2.06
3	A	610	CLA	MG-NA	-4.08	1.96	2.06
3	B	610	CLA	MG-NA	-4.03	1.96	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1003	NEX	C28-C27	3.95	1.41	1.32
3	C	603	CLA	C1D-ND	3.95	1.43	1.37
2	B	608	CHL	C3B-C4B	3.92	1.45	1.41
2	B	601	CHL	C3B-C4B	3.92	1.45	1.41
3	C	614	CLA	C1D-ND	3.92	1.43	1.37
2	C	608	CHL	C3B-C4B	3.92	1.45	1.41
2	A	608	CHL	C3B-C4B	3.90	1.45	1.41
3	A	614	CLA	C1D-ND	3.90	1.43	1.37
2	C	609	CHL	C3B-C4B	3.90	1.45	1.41
2	C	605	CHL	C3B-C4B	3.89	1.45	1.41
2	C	601	CHL	C3B-C4B	3.89	1.45	1.41
2	A	605	CHL	C3B-C4B	3.89	1.45	1.41
3	B	614	CLA	C1D-ND	3.88	1.43	1.37
3	A	603	CLA	C1D-ND	3.88	1.43	1.37
3	B	612	CLA	C1D-ND	3.87	1.42	1.37
3	B	603	CLA	C1D-ND	3.87	1.42	1.37
3	C	613	CLA	MG-NA	-3.86	1.97	2.06
2	A	609	CHL	C3B-C4B	3.86	1.45	1.41
3	B	602	CLA	MG-NA	-3.84	1.97	2.06
3	A	612	CLA	C1D-ND	3.84	1.42	1.37
2	B	609	CHL	C3B-C4B	3.82	1.45	1.41
3	C	612	CLA	C1D-ND	3.81	1.42	1.37
2	A	606	CHL	C3B-C4B	3.81	1.45	1.41
3	B	613	CLA	MG-NA	-3.81	1.97	2.06
2	C	606	CHL	C3B-C4B	3.80	1.45	1.41
2	B	605	CHL	C3B-C4B	3.80	1.45	1.41
2	A	601	CHL	C3B-C4B	3.80	1.45	1.41
3	A	613	CLA	MG-NA	-3.79	1.97	2.06
3	C	602	CLA	MG-NA	-3.79	1.97	2.06
2	B	606	CHL	C3B-C4B	3.77	1.45	1.41
3	A	602	CLA	MG-NA	-3.77	1.97	2.06
2	B	607	CHL	C3B-C4B	3.76	1.45	1.41
2	C	607	CHL	C3B-C4B	3.73	1.45	1.41
3	A	613	CLA	C1D-ND	3.71	1.42	1.37
3	A	614	CLA	MG-NA	-3.68	1.97	2.06
2	A	607	CHL	C3B-C4B	3.67	1.45	1.41
3	B	611	CLA	MG-NC	-3.67	1.97	2.06
3	A	604	CLA	C1D-ND	3.67	1.42	1.37
3	B	614	CLA	MG-NA	-3.67	1.97	2.06
3	C	604	CLA	C1D-ND	3.66	1.42	1.37
3	A	611	CLA	C1D-ND	3.65	1.42	1.37
3	B	611	CLA	C1D-ND	3.64	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	614	CLA	MG-NA	-3.63	1.97	2.06
3	B	604	CLA	C1D-ND	3.62	1.42	1.37
3	B	613	CLA	C1D-ND	3.62	1.42	1.37
3	A	611	CLA	MG-NC	-3.62	1.97	2.06
2	B	609	CHL	C1A-CHA	-3.62	1.35	1.40
3	C	613	CLA	C1D-ND	3.62	1.42	1.37
3	C	604	CLA	MG-NC	-3.61	1.97	2.06
3	C	611	CLA	MG-NC	-3.61	1.97	2.06
2	C	609	CHL	C1A-CHA	-3.60	1.35	1.40
3	A	604	CLA	MG-NC	-3.60	1.97	2.06
3	B	604	CLA	MG-NC	-3.59	1.97	2.06
3	C	611	CLA	C1D-ND	3.59	1.42	1.37
3	B	610	CLA	C1D-ND	3.58	1.42	1.37
3	B	612	CLA	MG-NA	-3.57	1.97	2.06
3	A	612	CLA	MG-NA	-3.56	1.97	2.06
2	A	609	CHL	C1A-CHA	-3.54	1.36	1.40
3	A	610	CLA	MG-NC	-3.54	1.97	2.06
3	C	612	CLA	MG-NA	-3.53	1.97	2.06
2	B	605	CHL	C1A-CHA	-3.53	1.36	1.40
3	A	610	CLA	C1D-ND	3.53	1.42	1.37
2	C	605	CHL	C1A-CHA	-3.53	1.36	1.40
5	B	1003	NEX	C28-C27	3.53	1.40	1.32
3	A	602	CLA	C1D-ND	3.52	1.42	1.37
3	C	610	CLA	MG-NC	-3.51	1.97	2.06
3	C	602	CLA	C1D-ND	3.51	1.42	1.37
3	B	610	CLA	MG-NC	-3.50	1.98	2.06
3	B	614	CLA	MG-NC	-3.48	1.98	2.06
3	A	614	CLA	MG-NC	-3.47	1.98	2.06
2	B	608	CHL	C1A-CHA	-3.47	1.36	1.40
3	C	614	CLA	MG-NC	-3.46	1.98	2.06
3	B	602	CLA	C1D-ND	3.45	1.42	1.37
2	C	608	CHL	C1A-CHA	-3.45	1.36	1.40
2	A	601	CHL	C1A-CHA	-3.44	1.36	1.40
2	A	605	CHL	C1A-CHA	-3.44	1.36	1.40
2	C	601	CHL	C1A-CHA	-3.44	1.36	1.40
3	C	603	CLA	MG-NA	-3.44	1.98	2.06
2	B	606	CHL	C1A-CHA	-3.43	1.36	1.40
3	B	603	CLA	MG-NA	-3.42	1.98	2.06
2	A	608	CHL	C1A-CHA	-3.42	1.36	1.40
3	C	610	CLA	C1D-ND	3.41	1.42	1.37
2	B	601	CHL	C1A-CHA	-3.41	1.36	1.40
2	A	606	CHL	C1A-CHA	-3.39	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	603	CLA	MG-NA	-3.37	1.98	2.06
2	B	607	CHL	C1A-CHA	-3.36	1.36	1.40
2	C	607	CHL	C1A-CHA	-3.36	1.36	1.40
3	B	603	CLA	MG-NC	-3.35	1.98	2.06
5	C	1003	NEX	C39-C29	-3.35	1.44	1.50
3	A	603	CLA	MG-NC	-3.34	1.98	2.06
2	C	606	CHL	C1A-CHA	-3.34	1.36	1.40
3	B	613	CLA	MG-NC	-3.32	1.98	2.06
3	C	602	CLA	MG-NC	-3.32	1.98	2.06
2	A	607	CHL	C1A-CHA	-3.31	1.36	1.40
3	A	613	CLA	MG-NC	-3.31	1.98	2.06
3	A	602	CLA	MG-NC	-3.30	1.98	2.06
3	C	613	CLA	MG-NC	-3.29	1.98	2.06
3	B	602	CLA	MG-NC	-3.27	1.98	2.06
3	C	603	CLA	MG-NC	-3.26	1.98	2.06
3	B	612	CLA	MG-NC	-3.23	1.98	2.06
3	C	612	CLA	MG-NC	-3.23	1.98	2.06
3	A	612	CLA	MG-NC	-3.22	1.98	2.06
3	B	614	CLA	C1B-NB	3.21	1.42	1.37
3	A	603	CLA	C1B-NB	3.18	1.42	1.37
3	B	603	CLA	C1B-NB	3.15	1.42	1.37
3	A	611	CLA	C1B-NB	3.14	1.42	1.37
3	C	611	CLA	C1B-NB	3.14	1.42	1.37
3	C	603	CLA	C1B-NB	3.14	1.42	1.37
3	C	614	CLA	C1B-NB	3.14	1.42	1.37
3	B	611	CLA	C1B-NB	3.11	1.41	1.37
3	A	614	CLA	C1B-NB	3.10	1.41	1.37
3	C	610	CLA	C1B-NB	3.10	1.41	1.37
3	A	613	CLA	C1B-NB	3.08	1.41	1.37
3	B	610	CLA	C1B-NB	3.08	1.41	1.37
3	C	613	CLA	C1B-NB	3.06	1.41	1.37
3	C	604	CLA	C1B-NB	3.06	1.41	1.37
3	A	604	CLA	C1B-NB	3.05	1.41	1.37
3	A	610	CLA	C1B-NB	3.05	1.41	1.37
3	C	612	CLA	C1B-NB	3.05	1.41	1.37
3	A	602	CLA	C1B-NB	3.05	1.41	1.37
3	C	602	CLA	C1B-NB	3.05	1.41	1.37
3	B	612	CLA	C1B-NB	3.03	1.41	1.37
3	A	612	CLA	C1B-NB	3.00	1.41	1.37
3	B	604	CLA	C1B-NB	2.99	1.41	1.37
3	B	613	CLA	C1B-NB	2.96	1.41	1.37
3	B	602	CLA	C1B-NB	2.95	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1003	NEX	C39-C29	-2.95	1.44	1.50
5	A	1003	NEX	C39-C29	-2.86	1.45	1.50
4	B	1001	A1LXP	C30-C31	-2.73	1.49	1.52
4	C	1001	A1LXP	C30-C31	-2.72	1.49	1.52
4	A	1001	A1LXP	C30-C31	-2.64	1.49	1.52
4	A	1002	A1LXP	C30-C31	-2.61	1.49	1.52
4	B	1002	A1LXP	C30-C31	-2.54	1.49	1.52
5	A	1003	NEX	C34-C33	-2.53	1.29	1.35
4	C	1002	A1LXP	C30-C31	-2.53	1.49	1.52
5	C	1003	NEX	C34-C33	-2.50	1.30	1.35
2	B	601	CHL	C3B-C2B	-2.38	1.37	1.40
2	C	607	CHL	C3B-C2B	-2.36	1.37	1.40
3	C	610	CLA	C1D-C2D	-2.34	1.40	1.45
2	B	607	CHL	C3B-C2B	-2.33	1.37	1.40
3	A	610	CLA	C1D-C2D	-2.33	1.40	1.45
3	B	610	CLA	C1D-C2D	-2.33	1.40	1.45
3	B	604	CLA	C1D-C2D	-2.33	1.40	1.45
3	C	611	CLA	C1D-C2D	-2.33	1.40	1.45
3	C	612	CLA	C1D-C2D	-2.33	1.40	1.45
3	A	611	CLA	C1D-C2D	-2.33	1.40	1.45
3	B	611	CLA	C1D-C2D	-2.33	1.40	1.45
2	A	607	CHL	C3B-C2B	-2.32	1.37	1.40
3	B	612	CLA	C1D-C2D	-2.32	1.40	1.45
2	C	601	CHL	C3B-C2B	-2.32	1.37	1.40
3	A	612	CLA	C1D-C2D	-2.32	1.40	1.45
3	C	604	CLA	C1D-C2D	-2.31	1.40	1.45
3	C	602	CLA	C1D-C2D	-2.31	1.40	1.45
3	A	613	CLA	C1D-C2D	-2.31	1.40	1.45
3	A	602	CLA	C1D-C2D	-2.31	1.40	1.45
3	C	603	CLA	C1D-C2D	-2.31	1.40	1.45
3	C	614	CLA	C1D-C2D	-2.30	1.40	1.45
3	A	604	CLA	C1D-C2D	-2.30	1.40	1.45
3	B	602	CLA	C1C-C2C	2.30	1.49	1.44
3	B	602	CLA	C1D-C2D	-2.29	1.40	1.45
3	A	614	CLA	C1D-C2D	-2.29	1.40	1.45
3	B	614	CLA	C1D-C2D	-2.28	1.40	1.45
2	B	605	CHL	C3B-C2B	-2.28	1.37	1.40
2	B	608	CHL	C3B-C2B	-2.27	1.37	1.40
3	B	603	CLA	C1D-C2D	-2.27	1.40	1.45
3	C	613	CLA	C1D-C2D	-2.27	1.40	1.45
2	C	605	CHL	C3B-C2B	-2.27	1.37	1.40
2	A	605	CHL	C3B-C2B	-2.26	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	613	CLA	C1D-C2D	-2.26	1.40	1.45
3	A	603	CLA	C1D-C2D	-2.25	1.40	1.45
2	A	608	CHL	C3B-C2B	-2.25	1.37	1.40
2	A	601	CHL	C3B-C2B	-2.25	1.37	1.40
3	C	602	CLA	C1C-C2C	2.24	1.49	1.44
2	C	608	CHL	C3B-C2B	-2.21	1.37	1.40
2	A	609	CHL	C3B-C2B	-2.16	1.37	1.40
2	B	609	CHL	C3B-C2B	-2.15	1.37	1.40
2	C	609	CHL	C3B-C2B	-2.15	1.37	1.40
2	A	606	CHL	C3B-C2B	-2.13	1.37	1.40
3	A	602	CLA	C1C-C2C	2.13	1.48	1.44
3	C	610	CLA	C1C-C2C	2.09	1.48	1.44
2	B	606	CHL	C3B-C2B	-2.08	1.37	1.40
2	C	606	CHL	C3B-C2B	-2.06	1.37	1.40
3	A	614	CLA	C1C-C2C	2.04	1.48	1.44
3	B	614	CLA	C1C-C2C	2.03	1.48	1.44
3	B	610	CLA	C1C-C2C	2.02	1.48	1.44
3	C	614	CLA	C1C-C2C	2.02	1.48	1.44

All (337) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1004	XAT	O24-C25-C24	-14.77	99.65	113.49
7	C	1004	XAT	O24-C25-C24	-14.77	99.65	113.49
7	B	1004	XAT	O24-C25-C24	-14.68	99.73	113.49
2	A	601	CHL	C1B-CHB-C4A	11.30	128.59	121.32
2	C	607	CHL	C1B-CHB-C4A	11.20	128.53	121.32
2	A	607	CHL	C1B-CHB-C4A	11.19	128.52	121.32
2	C	601	CHL	C1B-CHB-C4A	11.18	128.52	121.32
2	B	607	CHL	C1B-CHB-C4A	11.04	128.42	121.32
2	B	601	CHL	C1B-CHB-C4A	11.04	128.42	121.32
2	C	606	CHL	C1B-CHB-C4A	11.02	128.41	121.32
2	B	606	CHL	C1B-CHB-C4A	11.00	128.40	121.32
2	A	606	CHL	C1B-CHB-C4A	10.96	128.37	121.32
2	C	608	CHL	C1B-CHB-C4A	10.80	128.27	121.32
2	B	608	CHL	C1B-CHB-C4A	10.77	128.25	121.32
2	A	608	CHL	C1B-CHB-C4A	10.68	128.19	121.32
2	B	609	CHL	C1B-CHB-C4A	10.56	128.11	121.32
2	C	609	CHL	C1B-CHB-C4A	10.56	128.11	121.32
2	A	605	CHL	C1B-CHB-C4A	10.47	128.06	121.32
2	A	609	CHL	C1B-CHB-C4A	10.44	128.04	121.32
2	C	605	CHL	C1B-CHB-C4A	10.43	128.03	121.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	605	CHL	C1B-CHB-C4A	10.43	128.03	121.32
7	A	1004	XAT	O24-C26-C27	-6.98	96.89	116.88
7	C	1004	XAT	O24-C26-C27	-6.93	97.03	116.88
7	B	1004	XAT	O24-C26-C27	-6.93	97.04	116.88
3	C	611	CLA	C4A-NA-C1A	-6.19	103.86	106.68
3	A	611	CLA	C4A-NA-C1A	-6.18	103.86	106.68
3	B	611	CLA	C4A-NA-C1A	-6.09	103.90	106.68
3	C	604	CLA	C4A-NA-C1A	-5.84	104.02	106.68
3	A	604	CLA	C4A-NA-C1A	-5.76	104.05	106.68
3	B	604	CLA	C4A-NA-C1A	-5.65	104.10	106.68
3	A	603	CLA	C4A-NA-C1A	-5.45	104.19	106.68
3	B	603	CLA	C4A-NA-C1A	-5.44	104.19	106.68
3	C	603	CLA	C4A-NA-C1A	-5.23	104.29	106.68
3	A	612	CLA	C4A-NA-C1A	-5.14	104.33	106.68
3	B	612	CLA	C4A-NA-C1A	-5.10	104.35	106.68
3	B	614	CLA	C4A-NA-C1A	-5.08	104.36	106.68
3	C	612	CLA	C4A-NA-C1A	-5.07	104.36	106.68
3	A	614	CLA	C4A-NA-C1A	-5.04	104.38	106.68
3	C	614	CLA	C4A-NA-C1A	-5.03	104.39	106.68
3	A	610	CLA	C4A-NA-C1A	-4.69	104.54	106.68
3	B	610	CLA	C4A-NA-C1A	-4.56	104.60	106.68
3	C	610	CLA	C4A-NA-C1A	-4.55	104.60	106.68
3	C	602	CLA	C4A-NA-C1A	-4.27	104.73	106.68
3	B	602	CLA	C4A-NA-C1A	-4.25	104.74	106.68
3	A	602	CLA	C4A-NA-C1A	-4.14	104.79	106.68
3	A	613	CLA	C4A-NA-C1A	-4.09	104.81	106.68
3	C	613	CLA	C4A-NA-C1A	-4.02	104.85	106.68
3	B	613	CLA	C4A-NA-C1A	-4.01	104.85	106.68
2	B	607	CHL	C1A-CHA-C4D	3.77	125.27	118.98
2	B	607	CHL	C3D-C4D-CHA	3.73	114.21	108.54
2	A	607	CHL	C1A-CHA-C4D	3.71	125.17	118.98
2	A	601	CHL	C3D-C4D-CHA	3.71	114.18	108.54
2	C	607	CHL	C1A-CHA-C4D	3.71	125.17	118.98
2	B	606	CHL	C3D-C4D-CHA	3.70	114.17	108.54
2	A	607	CHL	C3D-C4D-CHA	3.70	114.16	108.54
2	A	605	CHL	C3D-C4D-CHA	3.70	114.16	108.54
2	A	606	CHL	C3D-C4D-CHA	3.69	114.16	108.54
2	C	605	CHL	C3D-C4D-CHA	3.69	114.16	108.54
2	B	605	CHL	C3D-C4D-CHA	3.69	114.15	108.54
2	C	606	CHL	C3D-C4D-CHA	3.68	114.14	108.54
2	C	607	CHL	C3D-C4D-CHA	3.68	114.14	108.54
2	B	605	CHL	C1A-CHA-C4D	3.68	125.12	118.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	CHL	C3D-C4D-CHA	3.68	114.13	108.54
2	C	601	CHL	C3D-C4D-CHA	3.68	114.13	108.54
2	A	605	CHL	C1A-CHA-C4D	3.67	125.11	118.98
2	C	605	CHL	C1A-CHA-C4D	3.65	125.07	118.98
2	C	608	CHL	C1A-CHA-C4D	3.64	125.06	118.98
2	B	608	CHL	C3D-C4D-CHA	3.64	114.08	108.54
2	C	608	CHL	C3D-C4D-CHA	3.64	114.07	108.54
2	A	606	CHL	C1A-CHA-C4D	3.64	125.06	118.98
2	A	608	CHL	C3D-C4D-CHA	3.64	114.07	108.54
2	C	609	CHL	C3D-C4D-CHA	3.63	114.06	108.54
2	C	606	CHL	C1A-CHA-C4D	3.63	125.03	118.98
2	B	606	CHL	C1A-CHA-C4D	3.63	125.03	118.98
2	B	601	CHL	C1A-CHA-C4D	3.62	125.02	118.98
2	A	609	CHL	C3D-C4D-CHA	3.61	114.02	108.54
2	B	608	CHL	C1A-CHA-C4D	3.60	124.99	118.98
2	A	608	CHL	C1A-CHA-C4D	3.60	124.99	118.98
2	B	609	CHL	C3D-C4D-CHA	3.60	114.01	108.54
2	A	601	CHL	C1A-CHA-C4D	3.58	124.96	118.98
2	C	601	CHL	C1A-CHA-C4D	3.58	124.96	118.98
2	A	609	CHL	C1A-CHA-C4D	3.49	124.81	118.98
2	C	609	CHL	C1A-CHA-C4D	3.47	124.77	118.98
2	B	609	CHL	C1A-CHA-C4D	3.46	124.76	118.98
3	C	603	CLA	C1D-ND-C4D	-3.19	104.07	106.31
3	B	612	CLA	C1D-ND-C4D	-3.13	104.11	106.31
3	C	614	CLA	C1D-ND-C4D	-3.12	104.12	106.31
3	A	612	CLA	C1D-ND-C4D	-3.10	104.14	106.31
3	A	603	CLA	C1D-ND-C4D	-3.09	104.14	106.31
3	B	603	CLA	C1D-ND-C4D	-3.09	104.14	106.31
3	A	614	CLA	C1D-ND-C4D	-3.08	104.15	106.31
3	C	612	CLA	C1D-ND-C4D	-3.08	104.15	106.31
3	B	614	CLA	C1D-ND-C4D	-3.05	104.17	106.31
3	A	613	CLA	C1D-ND-C4D	-2.98	104.22	106.31
2	B	607	CHL	C4D-CHA-CBD	-2.97	105.98	108.97
2	A	607	CHL	C4D-CHA-CBD	-2.93	106.02	108.97
3	B	613	CLA	C1D-ND-C4D	-2.90	104.28	106.31
2	C	607	CHL	C4D-CHA-CBD	-2.90	106.04	108.97
3	C	613	CLA	C1D-ND-C4D	-2.88	104.29	106.31
3	C	602	CLA	C1D-ND-C4D	-2.86	104.31	106.31
2	A	606	CHL	C4D-CHA-CBD	-2.84	106.10	108.97
2	B	606	CHL	C4D-CHA-CBD	-2.83	106.11	108.97
3	A	603	CLA	C1-C2-C3	-2.81	121.59	126.20
3	A	602	CLA	C1D-ND-C4D	-2.81	104.34	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	606	CHL	C4D-CHA-CBD	-2.81	106.14	108.97
3	A	612	CLA	C1-C2-C3	-2.80	121.61	126.20
3	B	603	CLA	C1-C2-C3	-2.79	121.62	126.20
3	B	610	CLA	C1D-ND-C4D	-2.79	104.35	106.31
3	B	602	CLA	C1D-ND-C4D	-2.78	104.36	106.31
3	C	612	CLA	C1-C2-C3	-2.77	121.65	126.20
3	A	610	CLA	CHD-C1D-ND	-2.77	120.90	124.80
3	C	610	CLA	C1D-ND-C4D	-2.77	104.37	106.31
3	A	610	CLA	C1D-ND-C4D	-2.77	104.37	106.31
3	B	612	CLA	C1-C2-C3	-2.74	121.71	126.20
2	C	609	CHL	C4C-CHD-C1D	2.73	125.83	116.07
2	B	609	CHL	C4C-CHD-C1D	2.73	125.83	116.07
3	C	614	CLA	CHD-C1D-ND	-2.73	120.96	124.80
2	A	609	CHL	C4C-CHD-C1D	2.72	125.81	116.07
2	A	601	CHL	C4C-CHD-C1D	2.72	125.78	116.07
2	A	608	CHL	C4C-CHD-C1D	2.71	125.77	116.07
2	C	601	CHL	C4C-CHD-C1D	2.71	125.77	116.07
2	B	608	CHL	C4C-CHD-C1D	2.71	125.76	116.07
2	B	601	CHL	C4C-CHD-C1D	2.71	125.75	116.07
2	C	608	CHL	C4C-CHD-C1D	2.70	125.72	116.07
2	B	606	CHL	C4C-CHD-C1D	2.70	125.72	116.07
2	C	606	CHL	C4C-CHD-C1D	2.69	125.71	116.07
2	A	606	CHL	C4C-CHD-C1D	2.69	125.70	116.07
3	B	610	CLA	CHD-C1D-ND	-2.69	121.02	124.80
3	C	610	CLA	CHD-C1D-ND	-2.69	121.02	124.80
3	C	603	CLA	C1-C2-C3	-2.68	121.80	126.20
2	C	607	CHL	C4C-CHD-C1D	2.68	125.67	116.07
2	B	607	CHL	C4C-CHD-C1D	2.68	125.66	116.07
2	A	607	CHL	C4C-CHD-C1D	2.67	125.64	116.07
3	C	602	CLA	CHD-C1D-ND	-2.67	121.04	124.80
3	A	614	CLA	CHD-C1D-ND	-2.66	121.06	124.80
3	A	611	CLA	CHD-C1D-ND	-2.66	121.06	124.80
3	C	604	CLA	C1D-ND-C4D	-2.66	104.45	106.31
2	B	605	CHL	C4C-CHD-C1D	2.65	125.55	116.07
3	B	614	CLA	CHD-C1D-ND	-2.65	121.07	124.80
3	B	604	CLA	CHD-C1D-ND	-2.64	121.08	124.80
3	B	604	CLA	C1D-ND-C4D	-2.64	104.46	106.31
2	A	605	CHL	C4C-CHD-C1D	2.64	125.53	116.07
3	A	611	CLA	C1D-ND-C4D	-2.64	104.46	106.31
3	A	604	CLA	C1D-ND-C4D	-2.64	104.46	106.31
2	C	605	CHL	C4C-CHD-C1D	2.64	125.51	116.07
3	A	613	CLA	CHD-C1D-ND	-2.64	121.09	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	604	CLA	CHD-C1D-ND	-2.63	121.10	124.80
3	B	603	CLA	CHD-C1D-ND	-2.63	121.10	124.80
3	A	612	CLA	CHC-C1C-C2C	-2.63	119.48	126.95
2	C	608	CHL	C4D-CHA-CBD	-2.63	106.32	108.97
3	C	603	CLA	CHD-C1D-ND	-2.63	121.11	124.80
3	B	602	CLA	CHD-C1D-ND	-2.62	121.11	124.80
3	A	604	CLA	CHD-C1D-ND	-2.62	121.11	124.80
2	A	601	CHL	C4D-CHA-CBD	-2.62	106.33	108.97
3	A	602	CLA	CHD-C1D-ND	-2.61	121.12	124.80
2	A	605	CHL	C4D-CHA-CBD	-2.61	106.33	108.97
2	B	605	CHL	C4D-CHA-CBD	-2.61	106.34	108.97
3	B	613	CLA	CHD-C1D-ND	-2.60	121.14	124.80
3	C	612	CLA	CHC-C1C-C2C	-2.60	119.56	126.95
3	C	611	CLA	C1D-ND-C4D	-2.60	104.49	106.31
3	B	603	CLA	CHC-C1C-C2C	-2.60	119.57	126.95
3	C	613	CLA	CHD-C1D-ND	-2.59	121.15	124.80
3	B	613	CLA	CHC-C1C-C2C	-2.59	119.58	126.95
3	C	613	CLA	CHC-C1C-C2C	-2.59	119.59	126.95
2	B	608	CHL	C4D-CHA-CBD	-2.59	106.36	108.97
3	B	611	CLA	CHD-C1D-ND	-2.59	121.16	124.80
3	A	603	CLA	CHC-C1C-C2C	-2.58	119.60	126.95
3	C	603	CLA	CHC-C1C-C2C	-2.58	119.60	126.95
3	B	611	CLA	C1D-ND-C4D	-2.58	104.50	106.31
3	B	612	CLA	CHC-C1C-C2C	-2.58	119.61	126.95
3	A	613	CLA	CHC-C1C-C2C	-2.58	119.61	126.95
3	A	603	CLA	CHD-C1D-ND	-2.58	121.17	124.80
3	A	612	CLA	CHD-C1D-ND	-2.58	121.17	124.80
2	A	608	CHL	C4D-CHA-CBD	-2.58	106.37	108.97
3	B	612	CLA	CHD-C1D-ND	-2.58	121.18	124.80
2	C	605	CHL	C4D-CHA-CBD	-2.57	106.37	108.97
3	C	611	CLA	CHD-C1D-ND	-2.57	121.19	124.80
3	C	612	CLA	CHD-C1D-ND	-2.54	121.22	124.80
2	C	601	CHL	C4D-CHA-CBD	-2.54	106.41	108.97
2	B	601	CHL	C4D-CHA-CBD	-2.52	106.43	108.97
3	A	611	CLA	CHC-C1C-C2C	-2.51	119.82	126.95
3	C	612	CLA	C2C-C1C-NC	2.50	112.60	109.98
3	A	610	CLA	CHC-C1C-C2C	-2.49	119.88	126.95
3	C	614	CLA	CHC-C1C-C2C	-2.48	119.89	126.95
3	A	614	CLA	CHC-C1C-C2C	-2.48	119.90	126.95
3	C	604	CLA	CHC-C1C-C2C	-2.48	119.90	126.95
3	C	611	CLA	CHC-C1C-C2C	-2.48	119.90	126.95
3	B	604	CLA	CHC-C1C-C2C	-2.48	119.91	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	614	CLA	CHC-C1C-C2C	-2.48	119.91	126.95
3	B	611	CLA	CHC-C1C-C2C	-2.47	119.92	126.95
3	C	602	CLA	C1-C2-C3	-2.47	122.15	126.20
2	C	609	CHL	C4D-CHA-CBD	-2.46	106.48	108.97
3	B	611	CLA	CHA-C1A-NA	-2.46	120.81	126.39
3	A	611	CLA	CHA-C1A-NA	-2.46	120.81	126.39
3	A	604	CLA	CHC-C1C-C2C	-2.46	119.95	126.95
3	C	611	CLA	CHA-C1A-NA	-2.46	120.82	126.39
3	A	612	CLA	C2C-C1C-NC	2.46	112.56	109.98
3	B	610	CLA	CHC-C1C-C2C	-2.46	119.96	126.95
3	B	603	CLA	CHC-C1C-NC	2.45	128.01	124.31
3	C	610	CLA	C1-C2-C3	-2.45	122.18	126.20
3	C	610	CLA	CHC-C1C-C2C	-2.44	120.01	126.95
3	B	612	CLA	C2C-C1C-NC	2.44	112.55	109.98
3	A	602	CLA	CHC-C1C-C2C	-2.44	120.02	126.95
3	A	603	CLA	CHC-C1C-NC	2.43	127.98	124.31
3	C	603	CLA	CHC-C1C-NC	2.43	127.97	124.31
2	A	609	CHL	C4D-CHA-CBD	-2.43	106.52	108.97
3	A	612	CLA	CHC-C1C-NC	2.42	127.95	124.31
3	C	604	CLA	CHC-C1C-NC	2.42	127.95	124.31
3	B	613	CLA	C2C-C1C-NC	2.41	112.52	109.98
3	B	604	CLA	CHA-C1A-NA	-2.41	120.93	126.39
3	C	604	CLA	CHA-C1A-NA	-2.40	120.95	126.39
2	B	609	CHL	C4D-CHA-CBD	-2.40	106.54	108.97
3	C	613	CLA	C2C-C1C-NC	2.40	112.50	109.98
3	A	613	CLA	CHC-C1C-NC	2.40	127.92	124.31
3	A	604	CLA	CHA-C1A-NA	-2.39	120.97	126.39
3	B	604	CLA	CHC-C1C-NC	2.38	127.89	124.31
3	C	613	CLA	CHC-C1C-NC	2.37	127.89	124.31
3	C	602	CLA	CHC-C1C-C2C	-2.37	120.22	126.95
3	A	611	CLA	CHC-C1C-NC	2.37	127.88	124.31
3	B	613	CLA	CHC-C1C-NC	2.37	127.88	124.31
3	B	602	CLA	CHC-C1C-C2C	-2.36	120.24	126.95
2	B	605	CHL	C3C-C4C-NC	-2.35	108.89	114.65
3	A	604	CLA	CHC-C1C-NC	2.34	127.84	124.31
3	B	612	CLA	CHC-C1C-NC	2.34	127.84	124.31
3	A	613	CLA	C2C-C1C-NC	2.34	112.44	109.98
3	C	612	CLA	CHC-C1C-NC	2.34	127.84	124.31
2	C	605	CHL	C3C-C4C-NC	-2.34	108.93	114.65
3	C	614	CLA	CHC-C1C-NC	2.34	127.83	124.31
3	A	614	CLA	CHC-C1C-NC	2.34	127.83	124.31
3	A	610	CLA	C1-C2-C3	-2.34	122.37	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	605	CHL	C3C-C4C-NC	-2.33	108.95	114.65
3	B	611	CLA	CHC-C1C-NC	2.32	127.81	124.31
3	A	610	CLA	CHC-C1C-NC	2.32	127.81	124.31
3	C	610	CLA	CHC-C1C-NC	2.32	127.81	124.31
3	C	611	CLA	CHC-C1C-NC	2.32	127.80	124.31
3	B	614	CLA	CHC-C1C-NC	2.31	127.80	124.31
3	C	603	CLA	C2C-C1C-NC	2.31	112.41	109.98
3	A	603	CLA	C2C-C1C-NC	2.30	112.40	109.98
3	B	603	CLA	C2C-C1C-NC	2.30	112.40	109.98
5	A	1003	NEX	O24-C25-C24	2.28	115.63	113.49
3	B	610	CLA	C1-C2-C3	-2.28	122.47	126.20
3	B	610	CLA	CHC-C1C-NC	2.27	127.74	124.31
3	B	602	CLA	CHA-C1A-NA	-2.25	121.30	126.39
5	B	1003	NEX	O24-C25-C24	2.24	115.59	113.49
3	A	602	CLA	CHA-C1A-NA	-2.24	121.33	126.39
2	A	608	CHL	C3C-C4C-NC	-2.23	109.21	114.65
3	A	612	CLA	CHA-C1A-NA	-2.23	121.35	126.39
3	C	614	CLA	CHA-C1A-NA	-2.23	121.35	126.39
3	A	602	CLA	C2C-C1C-NC	2.23	112.32	109.98
3	B	612	CLA	CHA-C1A-NA	-2.22	121.38	126.39
3	C	612	CLA	CHA-C1A-NA	-2.21	121.38	126.39
3	B	613	CLA	CHA-C1A-NA	-2.21	121.38	126.39
2	B	608	CHL	C3C-C4C-NC	-2.21	109.25	114.65
3	B	613	CLA	C1-C2-C3	-2.21	122.58	126.20
3	A	614	CLA	CHA-C1A-NA	-2.21	121.39	126.39
3	C	602	CLA	CHA-C1A-NA	-2.21	121.39	126.39
2	C	608	CHL	C3C-C4C-NC	-2.20	109.26	114.65
3	B	614	CLA	CHA-C1A-NA	-2.20	121.40	126.39
3	A	610	CLA	C2C-C1C-NC	2.20	112.30	109.98
2	C	609	CHL	C3C-C4C-NC	-2.20	109.28	114.65
5	C	1003	NEX	O24-C25-C24	2.20	115.55	113.49
3	C	610	CLA	CHA-C1A-NA	-2.20	121.42	126.39
2	C	607	CHL	C3C-C4C-NC	-2.19	109.29	114.65
3	C	602	CLA	CHC-C1C-NC	2.19	127.61	124.31
3	A	602	CLA	CHC-C1C-NC	2.19	127.61	124.31
3	B	602	CLA	CHC-C1C-NC	2.19	127.60	124.31
3	B	610	CLA	C2C-C1C-NC	2.19	112.28	109.98
3	A	613	CLA	CHA-C1A-NA	-2.18	121.45	126.39
3	A	611	CLA	C2C-C1C-NC	2.18	112.27	109.98
3	C	613	CLA	CHA-C1A-NA	-2.18	121.46	126.39
3	A	610	CLA	CHA-C1A-NA	-2.17	121.47	126.39
3	C	611	CLA	C2C-C1C-NC	2.17	112.26	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	610	CLA	CHA-C1A-NA	-2.17	121.48	126.39
3	B	604	CLA	C1-C2-C3	-2.17	122.64	126.20
2	B	609	CHL	C3C-C4C-NC	-2.17	109.35	114.65
3	A	604	CLA	C1-C2-C3	-2.17	122.65	126.20
3	C	604	CLA	C1-C2-C3	-2.16	122.65	126.20
3	B	602	CLA	C1-C2-C3	-2.16	122.65	126.20
2	B	607	CHL	C3C-C4C-NC	-2.16	109.37	114.65
3	B	614	CLA	C2C-C1C-NC	2.16	112.25	109.98
2	A	609	CHL	C3C-C4C-NC	-2.15	109.39	114.65
3	A	613	CLA	C1-C2-C3	-2.15	122.67	126.20
2	B	601	CHL	C3C-C4C-NC	-2.14	109.41	114.65
3	B	611	CLA	CHB-C1B-NB	-2.14	120.83	124.05
2	C	606	CHL	C3C-C4C-NC	-2.14	109.41	114.65
3	B	611	CLA	C2C-C1C-NC	2.14	112.23	109.98
3	C	614	CLA	C2C-C1C-NC	2.14	112.23	109.98
2	A	607	CHL	C3C-C4C-NC	-2.14	109.43	114.65
3	A	614	CLA	C2C-C1C-NC	2.14	112.23	109.98
3	A	603	CLA	CHA-C1A-NA	-2.13	121.56	126.39
3	A	613	CLA	CHB-C1B-NB	-2.13	120.85	124.05
3	B	603	CLA	CHA-C1A-NA	-2.13	121.58	126.39
2	B	606	CHL	C3C-C4C-NC	-2.12	109.46	114.65
3	C	603	CLA	CHA-C1A-NA	-2.12	121.59	126.39
3	B	613	CLA	CHB-C1B-NB	-2.12	120.87	124.05
3	C	613	CLA	CHB-C1B-NB	-2.12	120.87	124.05
2	C	601	CHL	C3C-C4C-NC	-2.12	109.47	114.65
2	B	601	CHL	C1-C2-C3	-2.12	122.73	126.20
3	A	611	CLA	CHB-C1B-NB	-2.12	120.88	124.05
3	C	612	CLA	CHB-C1B-NB	-2.12	120.88	124.05
2	A	601	CHL	C3C-C4C-NC	-2.11	109.48	114.65
3	C	610	CLA	CHB-C1B-NB	-2.11	120.88	124.05
3	C	603	CLA	CHB-C1B-NB	-2.11	120.89	124.05
3	B	612	CLA	CHB-C1B-NB	-2.10	120.90	124.05
3	C	613	CLA	C1-C2-C3	-2.10	122.76	126.20
3	B	602	CLA	CHB-C1B-NB	-2.10	120.90	124.05
2	B	606	CHL	C1-C2-C3	-2.09	123.38	126.76
2	A	606	CHL	C3C-C4C-NC	-2.09	109.54	114.65
3	C	611	CLA	CHB-C1B-NB	-2.09	120.91	124.05
3	B	610	CLA	CHB-C1B-NB	-2.09	120.91	124.05
3	A	602	CLA	CHB-C1B-NB	-2.09	120.92	124.05
3	C	602	CLA	CHB-C1B-NB	-2.08	120.92	124.05
3	A	604	CLA	C2C-C1C-NC	2.08	112.17	109.98
3	A	612	CLA	CHB-C1B-NB	-2.08	120.92	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	610	CLA	C2C-C1C-NC	2.08	112.17	109.98
3	A	603	CLA	CHB-C1B-NB	-2.08	120.93	124.05
3	A	602	CLA	C1-C2-C3	-2.08	122.79	126.20
3	B	604	CLA	C2C-C1C-NC	2.08	112.17	109.98
3	A	614	CLA	CHB-C1B-NB	-2.07	120.94	124.05
3	B	603	CLA	CHB-C1B-NB	-2.07	120.94	124.05
2	A	606	CHL	C1-C2-C3	-2.07	123.41	126.76
3	B	614	CLA	CHB-C1B-NB	-2.07	120.94	124.05
2	A	609	CHL	CMB-C2B-C3B	2.07	128.82	124.68
3	C	614	CLA	CHB-C1B-NB	-2.07	120.95	124.05
3	A	610	CLA	CHB-C1B-NB	-2.06	120.95	124.05
3	B	604	CLA	CHB-C1B-NB	-2.05	120.97	124.05
2	B	609	CHL	CMB-C2B-C3B	2.05	128.78	124.68
2	C	606	CHL	C1-C2-C3	-2.05	123.45	126.76
2	C	609	CHL	CMB-C2B-C3B	2.05	128.77	124.68
3	C	604	CLA	C2C-C1C-NC	2.04	112.12	109.98
3	B	602	CLA	C2C-C1C-NC	2.03	112.11	109.98
3	C	602	CLA	C2C-C1C-NC	2.03	112.11	109.98
2	B	606	CHL	CMB-C2B-C3B	2.03	128.73	124.68
2	A	606	CHL	CMB-C2B-C3B	2.02	128.73	124.68
2	C	606	CHL	CMB-C2B-C3B	2.02	128.71	124.68
2	A	608	CHL	CMB-C2B-C3B	2.01	128.71	124.68
3	C	604	CLA	CHB-C1B-NB	-2.01	121.04	124.05

All (114) chirality outliers are listed below:

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

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

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Mol	Chain	Res	Type	Atom
2	C	608	CHL	NA
2	C	608	CHL	C8
2	C	609	CHL	ND
2	C	609	CHL	NC
2	C	609	CHL	NA
2	C	609	CHL	C8
3	A	602	CLA	ND
3	A	602	CLA	C8
3	A	603	CLA	ND
3	A	603	CLA	C8
3	A	604	CLA	ND
3	A	604	CLA	C8
3	A	610	CLA	ND
3	A	610	CLA	C8
3	A	611	CLA	ND
3	A	611	CLA	C8
3	A	612	CLA	ND
3	A	612	CLA	C8
3	A	613	CLA	ND
3	A	613	CLA	C8
3	A	614	CLA	ND
3	B	602	CLA	ND
3	B	602	CLA	C8
3	B	603	CLA	ND
3	B	603	CLA	C8
3	B	604	CLA	ND
3	B	604	CLA	C8
3	B	610	CLA	ND
3	B	610	CLA	C8
3	B	611	CLA	ND
3	B	611	CLA	C8
3	B	612	CLA	ND
3	B	612	CLA	C8
3	B	613	CLA	ND
3	B	613	CLA	C8
3	B	614	CLA	ND
3	C	602	CLA	ND
3	C	602	CLA	C8
3	C	603	CLA	ND
3	C	603	CLA	C8
3	C	604	CLA	ND
3	C	604	CLA	C8

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Mol	Chain	Res	Type	Atom
3	C	610	CLA	ND
3	C	610	CLA	C8
3	C	611	CLA	ND
3	C	611	CLA	C8
3	C	612	CLA	ND
3	C	612	CLA	C8
3	C	613	CLA	ND
3	C	613	CLA	C8
3	C	614	CLA	ND
7	A	1004	XAT	C26
7	A	1004	XAT	C25
7	B	1004	XAT	C26
7	B	1004	XAT	C25
7	C	1004	XAT	C26
7	C	1004	XAT	C25

All (288) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	CHL	C3A-C2A-CAA-CBA
2	A	601	CHL	C1C-C2C-CMC-OMC
2	A	601	CHL	C3C-C2C-CMC-OMC
2	A	605	CHL	C1C-C2C-CMC-OMC
2	A	605	CHL	C3C-C2C-CMC-OMC
2	A	609	CHL	C6-C7-C8-C9
2	B	601	CHL	C3A-C2A-CAA-CBA
2	B	601	CHL	C1C-C2C-CMC-OMC
2	B	601	CHL	C3C-C2C-CMC-OMC
2	B	605	CHL	C1C-C2C-CMC-OMC
2	B	605	CHL	C3C-C2C-CMC-OMC
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	609	CHL	C6-C7-C8-C9
2	C	601	CHL	C3A-C2A-CAA-CBA
2	C	601	CHL	C1C-C2C-CMC-OMC
2	C	601	CHL	C3C-C2C-CMC-OMC
2	C	605	CHL	C1C-C2C-CMC-OMC
2	C	605	CHL	C3C-C2C-CMC-OMC
2	C	606	CHL	C1C-C2C-CMC-OMC
2	C	607	CHL	C1C-C2C-CMC-OMC
2	C	607	CHL	C3C-C2C-CMC-OMC

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Mol	Chain	Res	Type	Atoms
2	C	608	CHL	C1C-C2C-CMC-OMC
2	C	608	CHL	C3C-C2C-CMC-OMC
2	C	609	CHL	C1C-C2C-CMC-OMC
2	C	609	CHL	C3C-C2C-CMC-OMC
2	C	609	CHL	C6-C7-C8-C9
3	A	602	CLA	CHA-CBD-CGD-O1D
3	A	602	CLA	CHA-CBD-CGD-O2D
3	A	603	CLA	C2B-C3B-CAB-CBB
3	A	603	CLA	C4B-C3B-CAB-CBB
3	A	604	CLA	C1A-C2A-CAA-CBA
3	A	611	CLA	C1A-C2A-CAA-CBA
3	A	611	CLA	C2B-C3B-CAB-CBB
3	A	611	CLA	C4B-C3B-CAB-CBB
3	A	612	CLA	C2B-C3B-CAB-CBB
3	A	612	CLA	C4B-C3B-CAB-CBB
3	A	614	CLA	C2B-C3B-CAB-CBB
3	A	614	CLA	C4B-C3B-CAB-CBB
3	B	602	CLA	CHA-CBD-CGD-O1D
3	B	602	CLA	CHA-CBD-CGD-O2D
3	B	603	CLA	C2B-C3B-CAB-CBB
3	B	603	CLA	C4B-C3B-CAB-CBB
3	B	604	CLA	C1A-C2A-CAA-CBA
3	B	611	CLA	C1A-C2A-CAA-CBA
3	B	612	CLA	C2B-C3B-CAB-CBB
3	B	612	CLA	C4B-C3B-CAB-CBB
3	B	614	CLA	C2B-C3B-CAB-CBB
3	B	614	CLA	C4B-C3B-CAB-CBB
3	C	602	CLA	CHA-CBD-CGD-O1D
3	C	602	CLA	CHA-CBD-CGD-O2D
3	C	603	CLA	C4B-C3B-CAB-CBB
3	C	604	CLA	C1A-C2A-CAA-CBA
3	C	611	CLA	C1A-C2A-CAA-CBA
3	C	611	CLA	C4B-C3B-CAB-CBB
3	C	612	CLA	C4B-C3B-CAB-CBB
3	C	614	CLA	C2B-C3B-CAB-CBB
3	C	614	CLA	C4B-C3B-CAB-CBB
6	A	1005	LHG	C3-O3-P-O4
6	A	1005	LHG	C3-O3-P-O6
6	B	1005	LHG	C3-O3-P-O4
6	B	1005	LHG	C3-O3-P-O6
6	B	1005	LHG	C4-O6-P-O3
6	B	1005	LHG	C4-O6-P-O5

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Mol	Chain	Res	Type	Atoms
6	C	1005	LHG	C3-O3-P-O4
6	C	1005	LHG	C3-O3-P-O6
2	A	601	CHL	C11-C10-C8-C9
2	C	601	CHL	C11-C10-C8-C9
2	B	601	CHL	C5-C6-C7-C8
2	A	608	CHL	C2A-CAA-CBA-CGA
2	B	608	CHL	C2A-CAA-CBA-CGA
2	C	608	CHL	C2A-CAA-CBA-CGA
3	A	602	CLA	C4-C3-C5-C6
2	C	608	CHL	C5-C6-C7-C8
3	B	604	CLA	C4B-C3B-CAB-CBB
3	B	611	CLA	C4B-C3B-CAB-CBB
2	A	608	CHL	C5-C6-C7-C8
2	B	608	CHL	C5-C6-C7-C8
3	A	603	CLA	C3A-C2A-CAA-CBA
3	B	603	CLA	C3A-C2A-CAA-CBA
3	C	603	CLA	C3A-C2A-CAA-CBA
3	A	602	CLA	C2-C3-C5-C6
3	C	603	CLA	C2B-C3B-CAB-CBB
3	C	611	CLA	C2B-C3B-CAB-CBB
3	C	612	CLA	C2B-C3B-CAB-CBB
6	B	1005	LHG	C23-C24-C25-C26
2	A	601	CHL	C11-C12-C13-C14
2	C	601	CHL	C11-C12-C13-C14
3	C	611	CLA	C5-C6-C7-C8
3	A	611	CLA	C5-C6-C7-C8
6	A	1005	LHG	C23-C24-C25-C26
3	A	603	CLA	C1A-C2A-CAA-CBA
3	B	603	CLA	C1A-C2A-CAA-CBA
3	C	603	CLA	C1A-C2A-CAA-CBA
2	C	601	CHL	C6-C7-C8-C10
6	C	1005	LHG	C23-C24-C25-C26
3	A	613	CLA	C2-C3-C5-C6
3	C	613	CLA	C2-C3-C5-C6
3	B	611	CLA	C5-C6-C7-C8
2	A	605	CHL	CHA-CBD-CGD-O1D
2	A	605	CHL	CHA-CBD-CGD-O2D
2	B	605	CHL	CHA-CBD-CGD-O1D
2	B	605	CHL	CHA-CBD-CGD-O2D
2	C	605	CHL	CHA-CBD-CGD-O1D
2	C	605	CHL	CHA-CBD-CGD-O2D
2	B	606	CHL	C3C-C2C-CMC-OMC

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Mol	Chain	Res	Type	Atoms
2	C	606	CHL	C3C-C2C-CMC-OMC
3	A	613	CLA	C4-C3-C5-C6
3	B	602	CLA	C4-C3-C5-C6
3	B	613	CLA	C2-C3-C5-C6
2	B	607	CHL	C2A-CAA-CBA-CGA
6	C	1005	LHG	C31-C32-C33-C34
3	B	602	CLA	C11-C10-C8-C9
3	A	604	CLA	C4B-C3B-CAB-CBB
3	A	610	CLA	C4B-C3B-CAB-CBB
3	A	613	CLA	C4B-C3B-CAB-CBB
3	B	610	CLA	C4B-C3B-CAB-CBB
3	B	613	CLA	C4B-C3B-CAB-CBB
3	C	604	CLA	C4B-C3B-CAB-CBB
3	C	613	CLA	C4B-C3B-CAB-CBB
2	A	609	CHL	C6-C7-C8-C10
2	B	609	CHL	C6-C7-C8-C10
2	C	609	CHL	C6-C7-C8-C10
2	C	609	CHL	C8-C10-C11-C12
2	B	609	CHL	C8-C10-C11-C12
2	A	609	CHL	C2-C3-C5-C6
2	A	601	CHL	C1A-C2A-CAA-CBA
2	B	601	CHL	C1A-C2A-CAA-CBA
2	C	601	CHL	C1A-C2A-CAA-CBA
3	B	613	CLA	C4-C3-C5-C6
3	C	613	CLA	C4-C3-C5-C6
4	A	1001	A1LXP	C24-C1-C42-C2
4	C	1001	A1LXP	C24-C1-C42-C2
2	A	609	CHL	C4-C3-C5-C6
2	A	609	CHL	C8-C10-C11-C12
2	C	607	CHL	C2A-CAA-CBA-CGA
3	C	604	CLA	C4-C3-C5-C6
3	A	604	CLA	C4-C3-C5-C6
3	A	612	CLA	C4-C3-C5-C6
3	B	604	CLA	C4-C3-C5-C6
3	B	602	CLA	C2-C3-C5-C6
3	C	602	CLA	C11-C12-C13-C14
2	B	609	CHL	C4-C3-C5-C6
3	C	612	CLA	C4-C3-C5-C6
2	A	606	CHL	C3A-C2A-CAA-CBA
2	B	606	CHL	C3A-C2A-CAA-CBA
3	B	612	CLA	C4-C3-C5-C6
3	A	604	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
3	C	604	CLA	C2-C3-C5-C6
6	B	1005	LHG	C25-C26-C27-C28
3	A	612	CLA	C2-C3-C5-C6
3	C	614	CLA	CAD-CBD-CGD-O2D
2	A	607	CHL	C2A-CAA-CBA-CGA
3	A	603	CLA	CHA-CBD-CGD-O1D
3	A	603	CLA	CHA-CBD-CGD-O2D
3	A	614	CLA	CAD-CBD-CGD-O1D
3	B	614	CLA	CAD-CBD-CGD-O1D
3	C	603	CLA	CHA-CBD-CGD-O1D
3	C	603	CLA	CHA-CBD-CGD-O2D
3	C	614	CLA	CAD-CBD-CGD-O1D
6	A	1005	LHG	C4-O6-P-O3
6	B	1005	LHG	C4-O6-P-O4
6	C	1005	LHG	C4-O6-P-O3
3	A	611	CLA	C13-C15-C16-C17
3	A	613	CLA	C2B-C3B-CAB-CBB
3	B	604	CLA	C2B-C3B-CAB-CBB
3	B	611	CLA	C2B-C3B-CAB-CBB
3	B	613	CLA	C2B-C3B-CAB-CBB
4	B	1001	A1LXP	C24-C1-C42-C2
2	B	609	CHL	C2-C3-C5-C6
3	B	604	CLA	C2-C3-C5-C6
3	C	602	CLA	C11-C12-C13-C15
3	C	611	CLA	C12-C13-C15-C16
3	B	602	CLA	C3-C5-C6-C7
3	A	602	CLA	C3-C5-C6-C7
3	B	611	CLA	C13-C15-C16-C17
3	C	611	CLA	C13-C15-C16-C17
2	C	606	CHL	C2A-CAA-CBA-CGA
3	B	611	CLA	C4-C3-C5-C6
3	C	610	CLA	C4B-C3B-CAB-CBB
2	C	606	CHL	C3A-C2A-CAA-CBA
3	C	612	CLA	C2-C3-C5-C6
5	A	1003	NEX	C39-C29-C30-C31
5	B	1003	NEX	C39-C29-C30-C31
5	C	1003	NEX	C39-C29-C30-C31
3	A	611	CLA	C4-C3-C5-C6
3	B	612	CLA	C2-C3-C5-C6
6	C	1005	LHG	C12-C13-C14-C15
3	A	611	CLA	C11-C10-C8-C9
3	A	613	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
3	B	611	CLA	C11-C10-C8-C9
3	C	613	CLA	C6-C7-C8-C9
6	B	1005	LHG	C16-C17-C18-C19
3	B	611	CLA	C3-C5-C6-C7
2	A	606	CHL	C2A-CAA-CBA-CGA
2	B	606	CHL	C2A-CAA-CBA-CGA
5	A	1003	NEX	C28-C29-C30-C31
5	B	1003	NEX	C28-C29-C30-C31
5	C	1003	NEX	C28-C29-C30-C31
3	A	602	CLA	C2B-C3B-CAB-CBB
3	A	604	CLA	C2B-C3B-CAB-CBB
3	B	602	CLA	C2B-C3B-CAB-CBB
3	C	604	CLA	C2B-C3B-CAB-CBB
3	C	613	CLA	C2B-C3B-CAB-CBB
4	A	1002	A1LXP	C24-C1-C42-C2
4	B	1002	A1LXP	C24-C1-C42-C2
4	C	1002	A1LXP	C24-C1-C42-C2
3	A	611	CLA	C12-C13-C15-C16
3	B	611	CLA	C12-C13-C15-C16
2	B	601	CHL	C4-C3-C5-C6
3	A	611	CLA	C2-C3-C5-C6
3	B	611	CLA	C2-C3-C5-C6
2	C	601	CHL	C2-C1-O2A-CGA
3	B	602	CLA	C14-C13-C15-C16
3	C	611	CLA	C4-C3-C5-C6
6	C	1005	LHG	C25-C26-C27-C28
3	A	611	CLA	C3-C5-C6-C7
3	B	604	CLA	CAA-CBA-CGA-O2A
3	C	611	CLA	C2-C3-C5-C6
3	C	611	CLA	C3-C5-C6-C7
3	B	613	CLA	C6-C7-C8-C9
3	C	611	CLA	C11-C10-C8-C9
3	C	604	CLA	CAA-CBA-CGA-O2A
6	B	1005	LHG	C11-C10-C9-C8
3	A	611	CLA	CAA-CBA-CGA-O2A
3	C	611	CLA	CAA-CBA-CGA-O2A
2	A	601	CHL	C6-C7-C8-C10
2	A	601	CHL	C11-C10-C8-C7
2	C	608	CHL	C6-C7-C8-C10
3	B	602	CLA	C12-C13-C15-C16
3	A	610	CLA	C2B-C3B-CAB-CBB
3	B	610	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
3	C	602	CLA	C2B-C3B-CAB-CBB
3	C	610	CLA	C2B-C3B-CAB-CBB
4	A	1001	A1LXP	C28-C1-C42-C2
4	B	1002	A1LXP	C28-C1-C42-C2
4	C	1001	A1LXP	C28-C1-C42-C2
4	C	1002	A1LXP	C28-C1-C42-C2
3	A	604	CLA	CAA-CBA-CGA-O2A
2	A	607	CHL	CAA-CBA-CGA-O2A
2	C	609	CHL	C2-C3-C5-C6
6	C	1005	LHG	O8-C23-C24-C25
3	B	611	CLA	CAA-CBA-CGA-O2A
3	B	612	CLA	CAA-CBA-CGA-O2A
3	C	612	CLA	CAA-CBA-CGA-O2A
6	A	1005	LHG	O8-C23-C24-C25
6	B	1005	LHG	O8-C23-C24-C25
3	C	611	CLA	C14-C13-C15-C16
2	B	606	CHL	CAA-CBA-CGA-O2A
3	A	602	CLA	C4B-C3B-CAB-CBB
3	B	602	CLA	C4B-C3B-CAB-CBB
3	C	602	CLA	C4B-C3B-CAB-CBB
2	C	606	CHL	CAA-CBA-CGA-O2A
3	A	612	CLA	CAA-CBA-CGA-O2A
2	A	606	CHL	CAA-CBA-CGA-O2A
2	C	609	CHL	C4-C3-C5-C6
2	A	601	CHL	C2-C1-O2A-CGA
2	B	601	CHL	C2-C1-O2A-CGA
2	A	608	CHL	C6-C7-C8-C10
2	A	607	CHL	CAA-CBA-CGA-O1A
3	A	611	CLA	C3A-C2A-CAA-CBA
3	B	611	CLA	C3A-C2A-CAA-CBA
3	C	611	CLA	C3A-C2A-CAA-CBA
6	C	1005	LHG	C15-C16-C17-C18
6	A	1005	LHG	C25-C26-C27-C28
3	C	613	CLA	C2A-CAA-CBA-CGA
3	B	611	CLA	CAA-CBA-CGA-O1A
3	A	611	CLA	CAA-CBA-CGA-O1A
3	C	611	CLA	CAA-CBA-CGA-O1A
2	B	607	CHL	CAA-CBA-CGA-O2A
3	A	612	CLA	CAA-CBA-CGA-O1A
2	A	606	CHL	CAA-CBA-CGA-O1A
3	B	612	CLA	CAA-CBA-CGA-O1A
3	A	613	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
2	B	606	CHL	CAA-CBA-CGA-O1A
3	C	612	CLA	CAA-CBA-CGA-O1A
2	A	609	CHL	C15-C16-C17-C18
2	C	606	CHL	CAA-CBA-CGA-O1A
3	A	614	CLA	CAD-CBD-CGD-O2D
3	B	603	CLA	CAD-CBD-CGD-O2D
3	B	614	CLA	CAD-CBD-CGD-O2D
6	A	1005	LHG	O10-C23-C24-C25
6	B	1005	LHG	O10-C23-C24-C25
6	C	1005	LHG	O10-C23-C24-C25
3	B	613	CLA	C2A-CAA-CBA-CGA
2	C	608	CHL	CAA-CBA-CGA-O2A
2	B	608	CHL	CAA-CBA-CGA-O2A

There are no ring outliers.

40 monomers are involved in 54 short contacts:

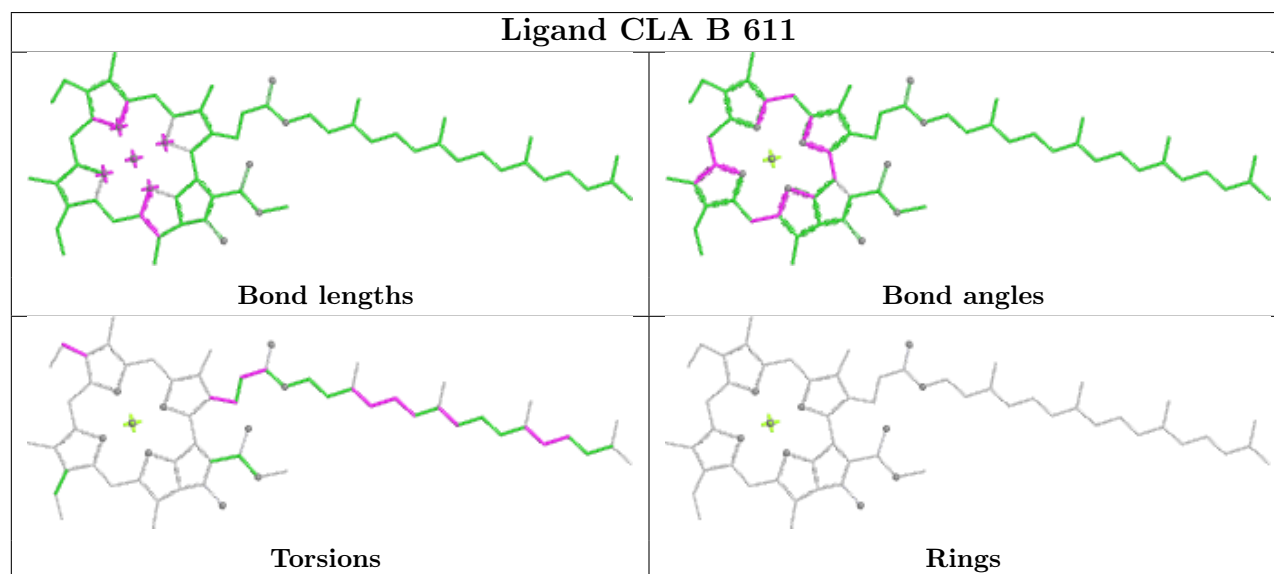
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	608	CHL	1	0
3	A	604	CLA	1	0
6	C	1005	LHG	6	0
3	B	613	CLA	1	0
2	C	606	CHL	1	0
3	A	603	CLA	5	0
2	B	607	CHL	1	0
4	B	1002	A1LXP	1	0
3	C	610	CLA	3	0
3	B	603	CLA	4	0
2	C	609	CHL	2	0
2	A	606	CHL	1	0
2	B	601	CHL	3	0
2	A	607	CHL	1	0
3	C	613	CLA	1	0
2	C	607	CHL	1	0
6	A	1005	LHG	2	0
3	A	602	CLA	1	0
7	A	1004	XAT	3	0
3	A	612	CLA	2	0
4	A	1002	A1LXP	1	0
3	C	604	CLA	1	0
3	C	603	CLA	4	0
3	C	612	CLA	3	0

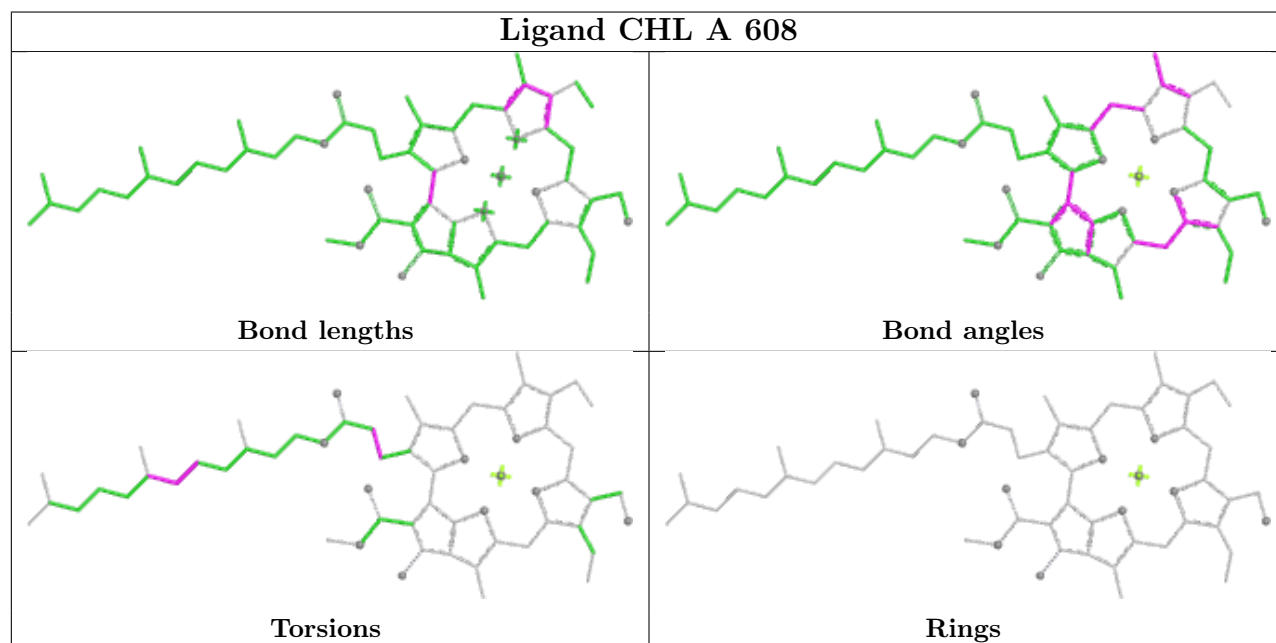
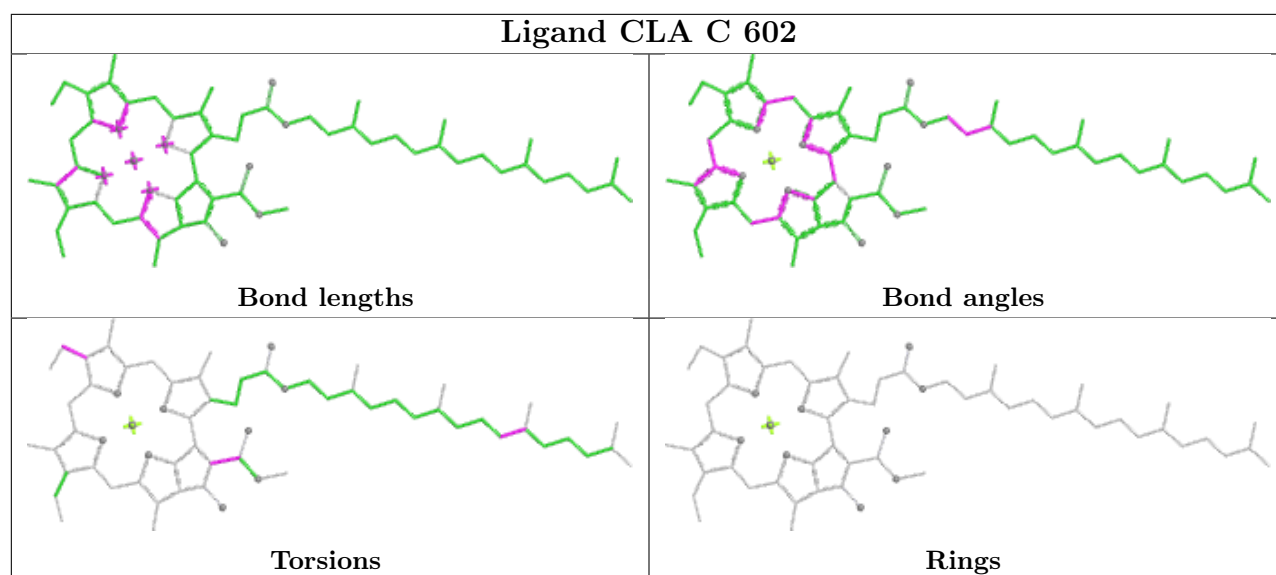
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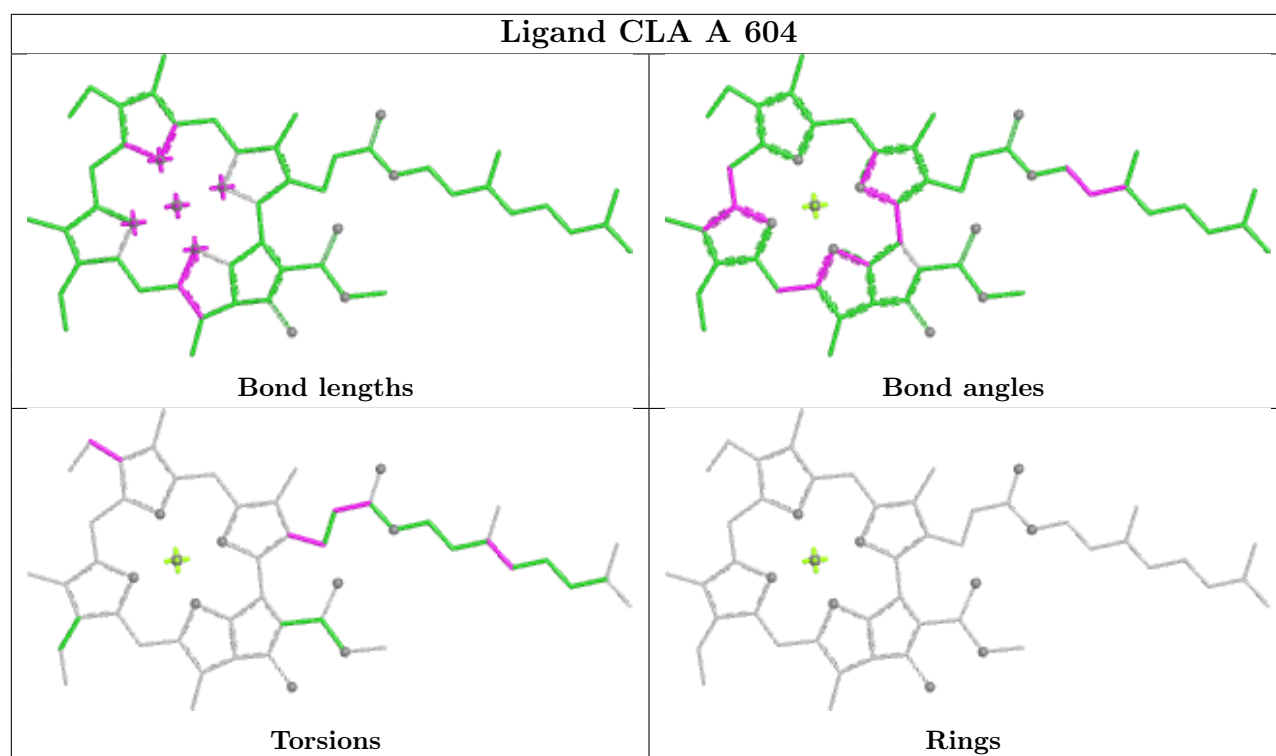
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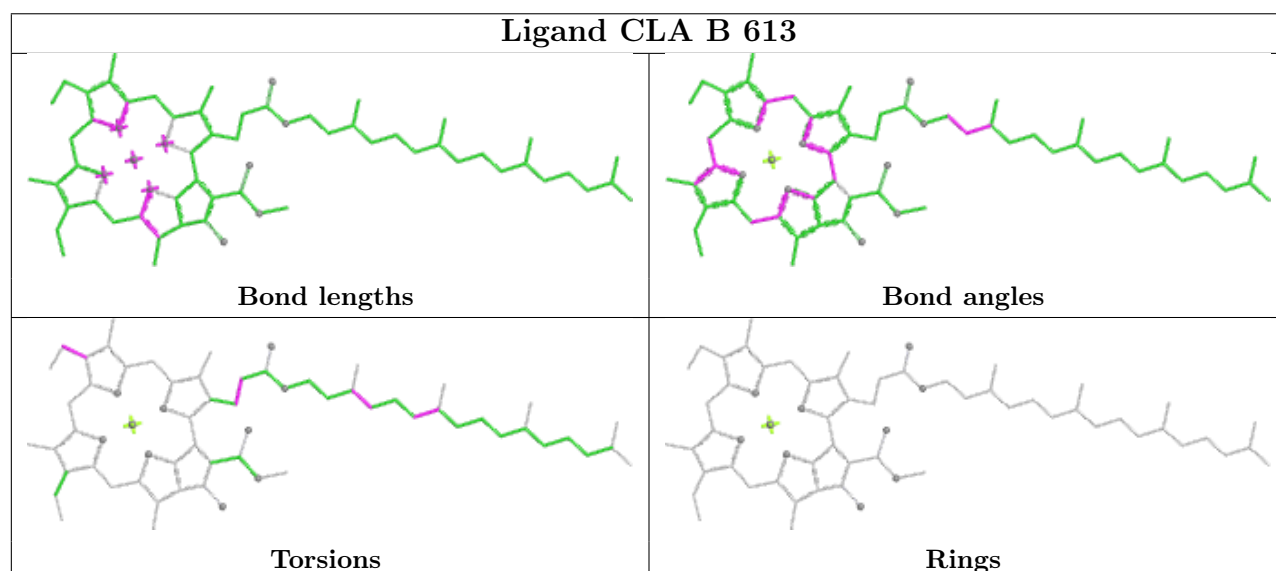
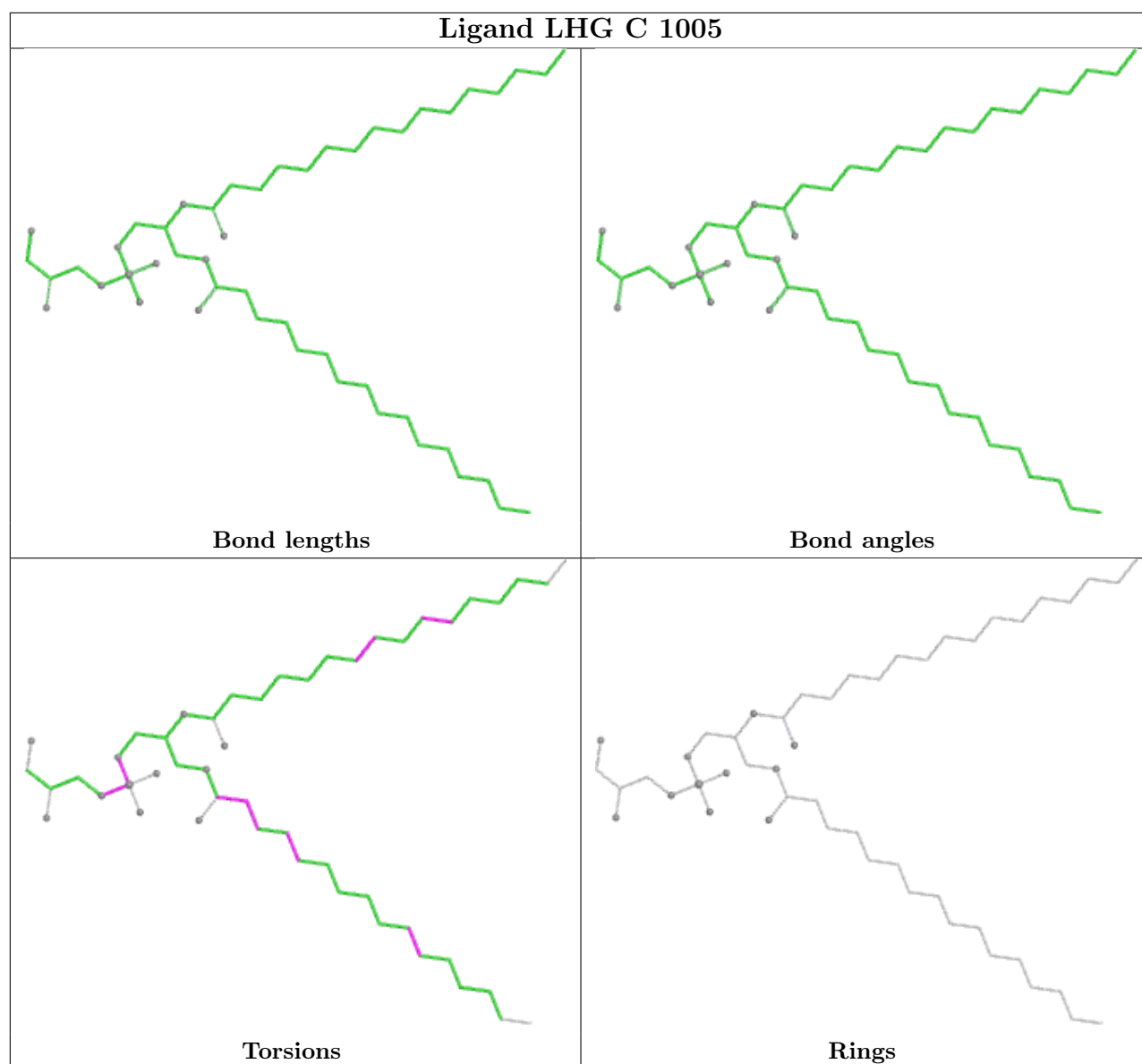
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	608	CHL	1	0
2	A	601	CHL	1	0
3	B	612	CLA	2	0
7	B	1004	XAT	2	0
6	B	1005	LHG	4	0
2	C	601	CHL	3	0
3	A	610	CLA	2	0
2	A	609	CHL	3	0
2	B	606	CHL	1	0
3	B	604	CLA	1	0
3	B	610	CLA	3	0
7	C	1004	XAT	1	0
4	C	1002	A1LXP	1	0
2	B	609	CHL	2	0
2	C	608	CHL	1	0
3	A	613	CLA	2	0

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.

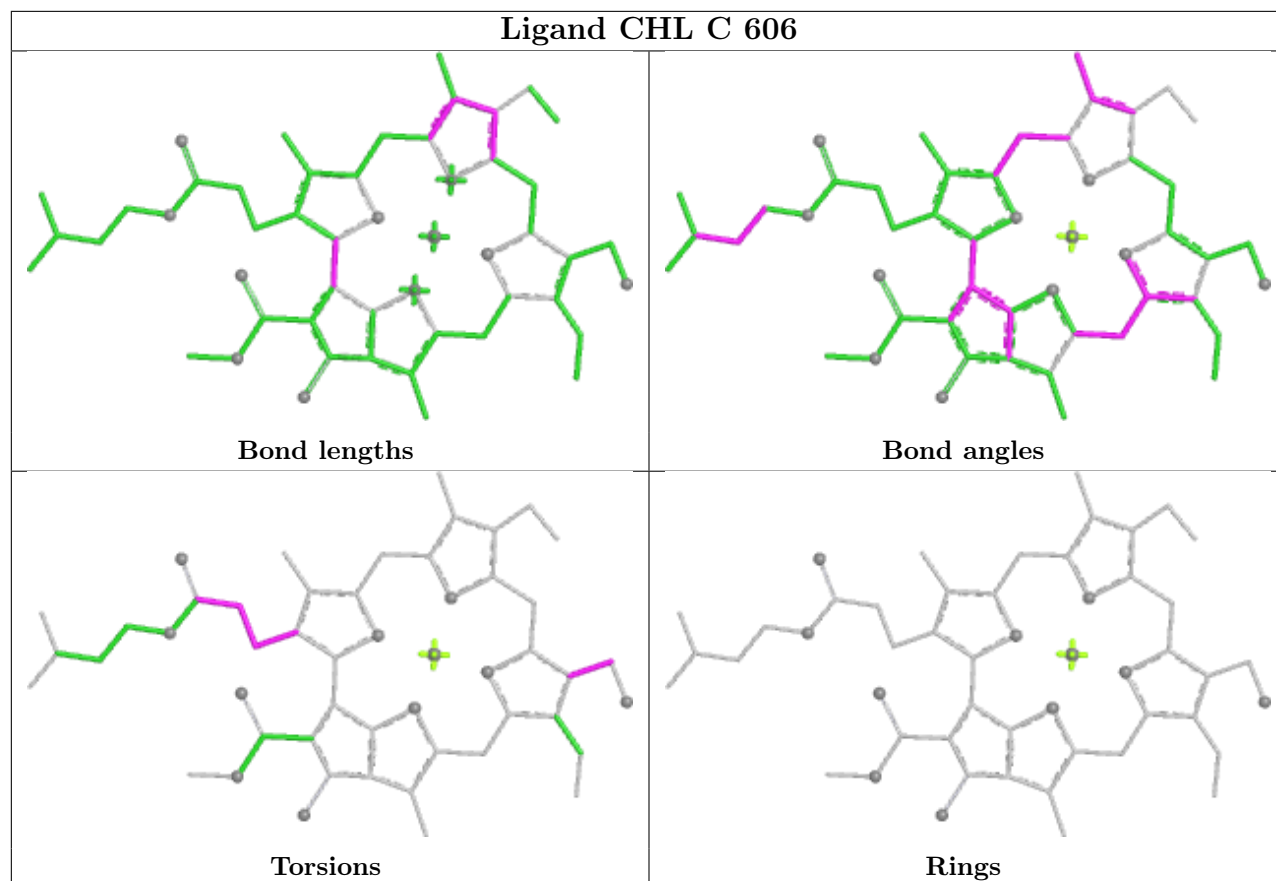




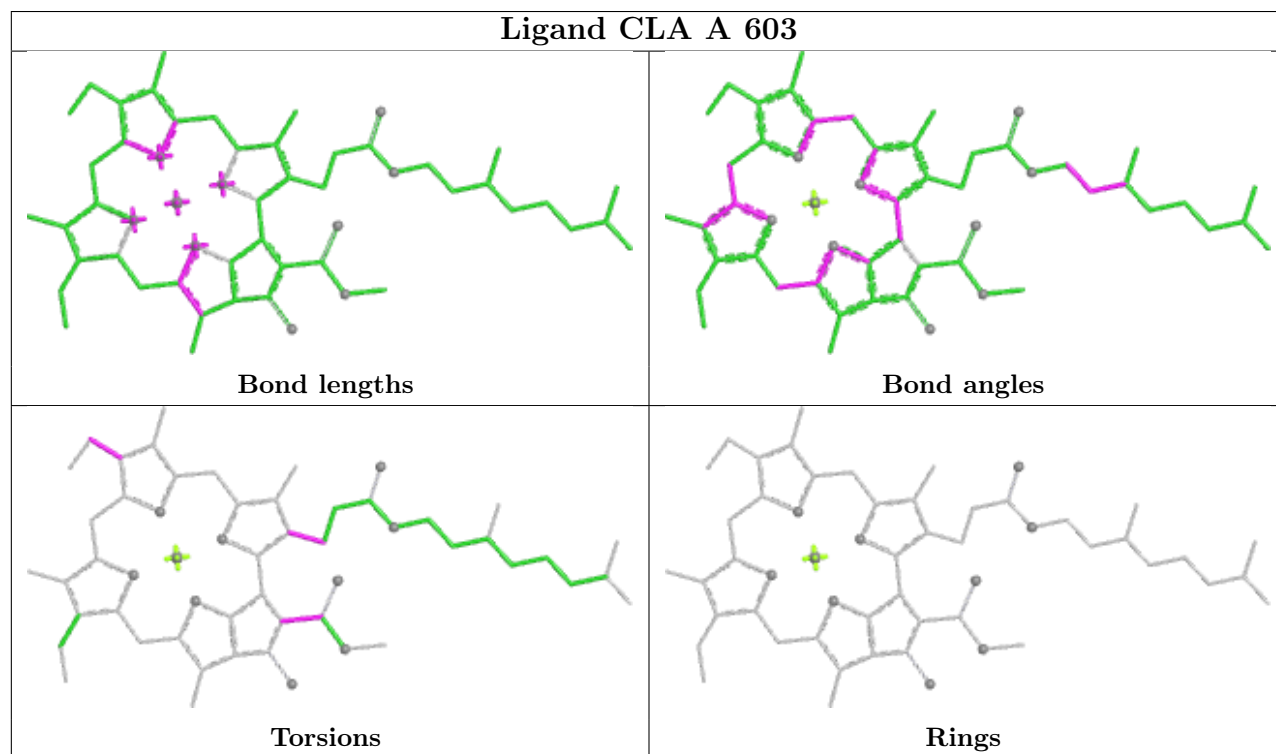




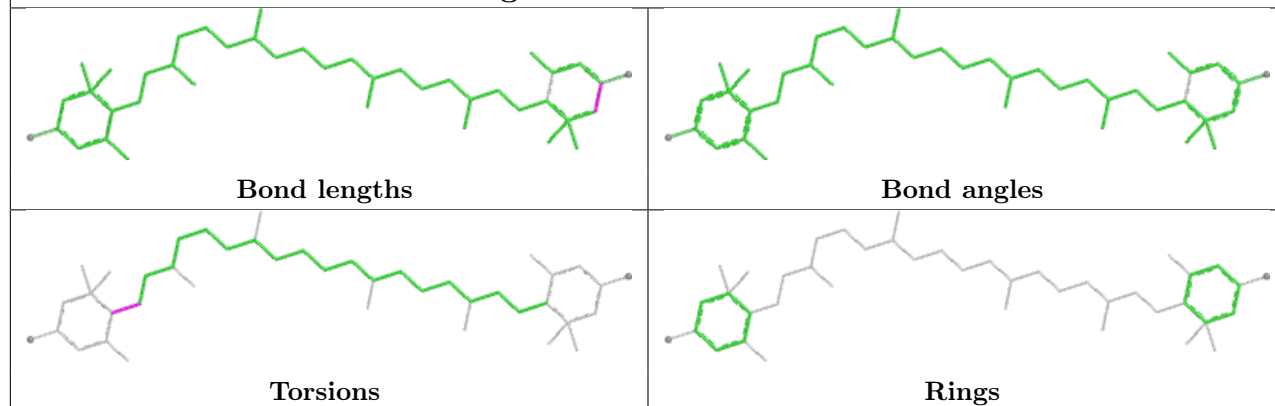
Ligand CHL C 606



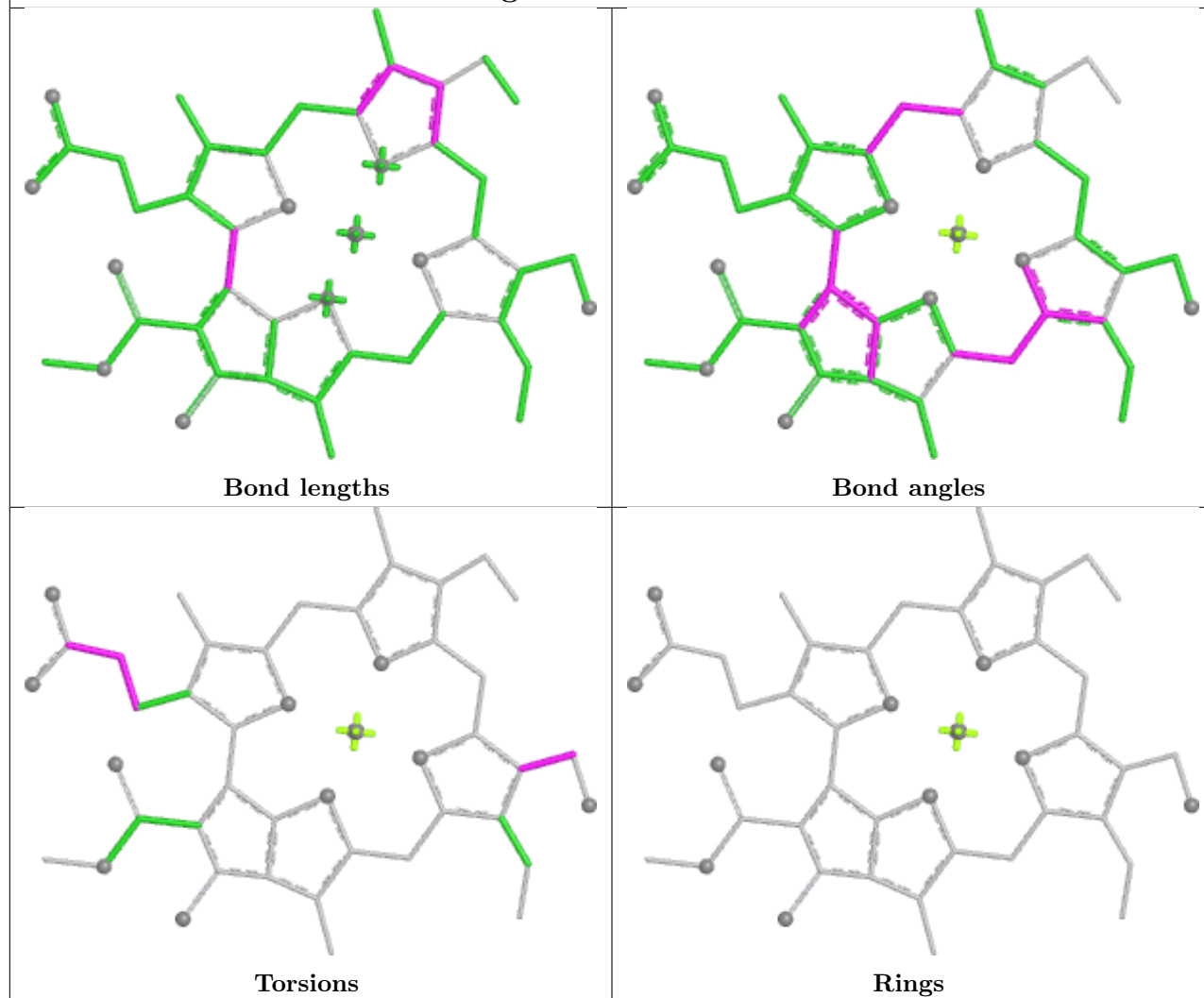
Ligand CLA A 603

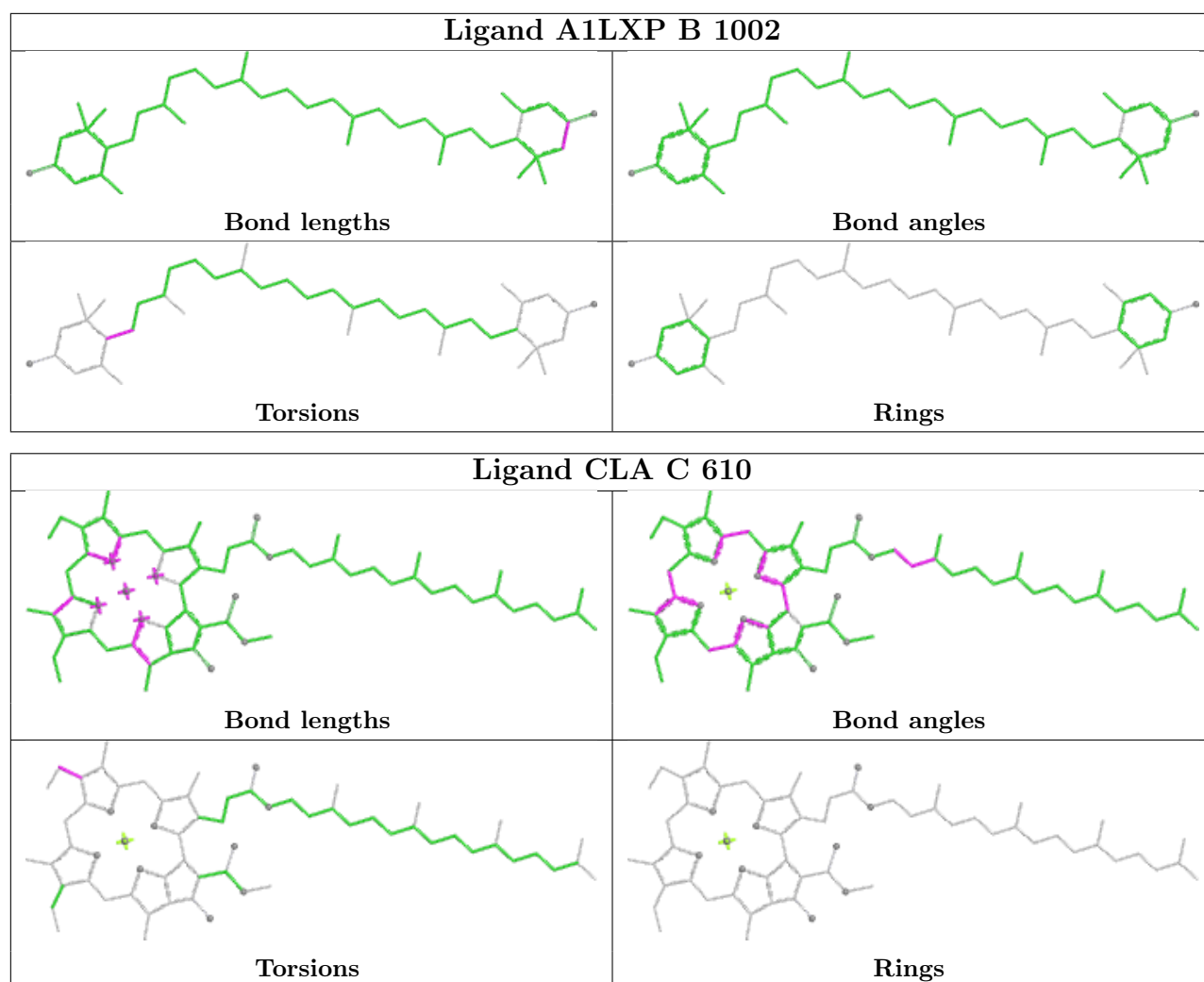


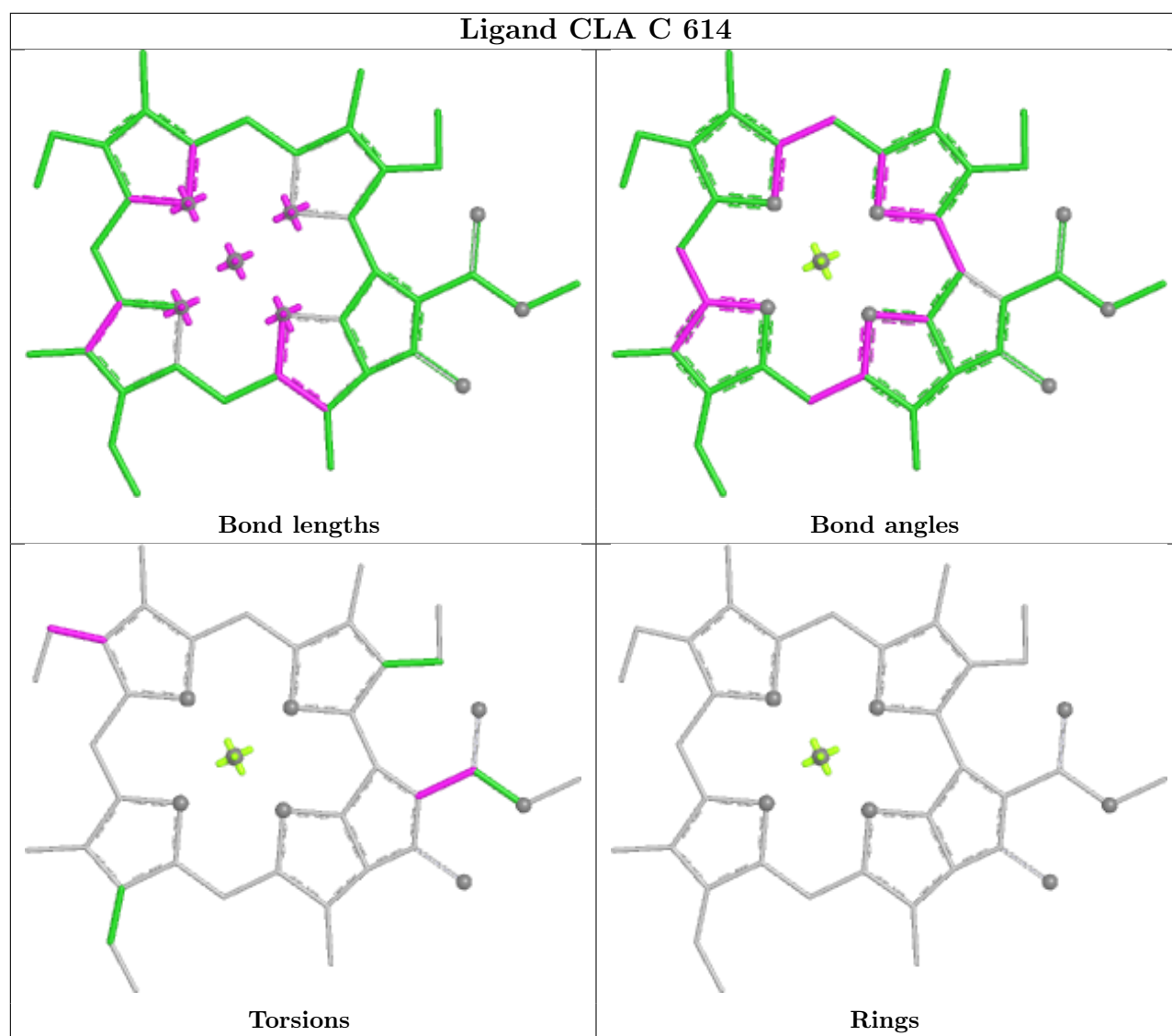
Ligand A1LXP C 1001

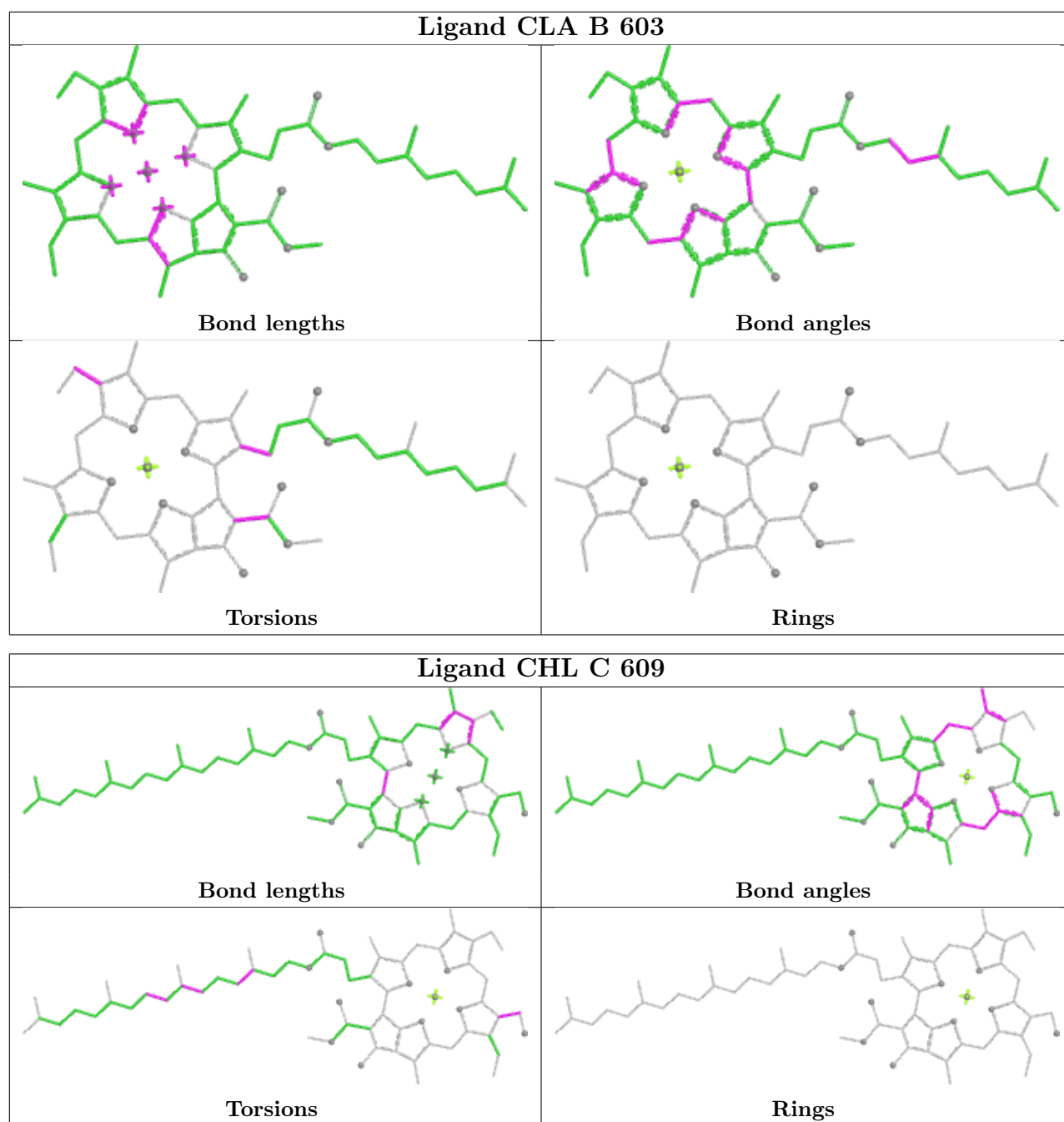


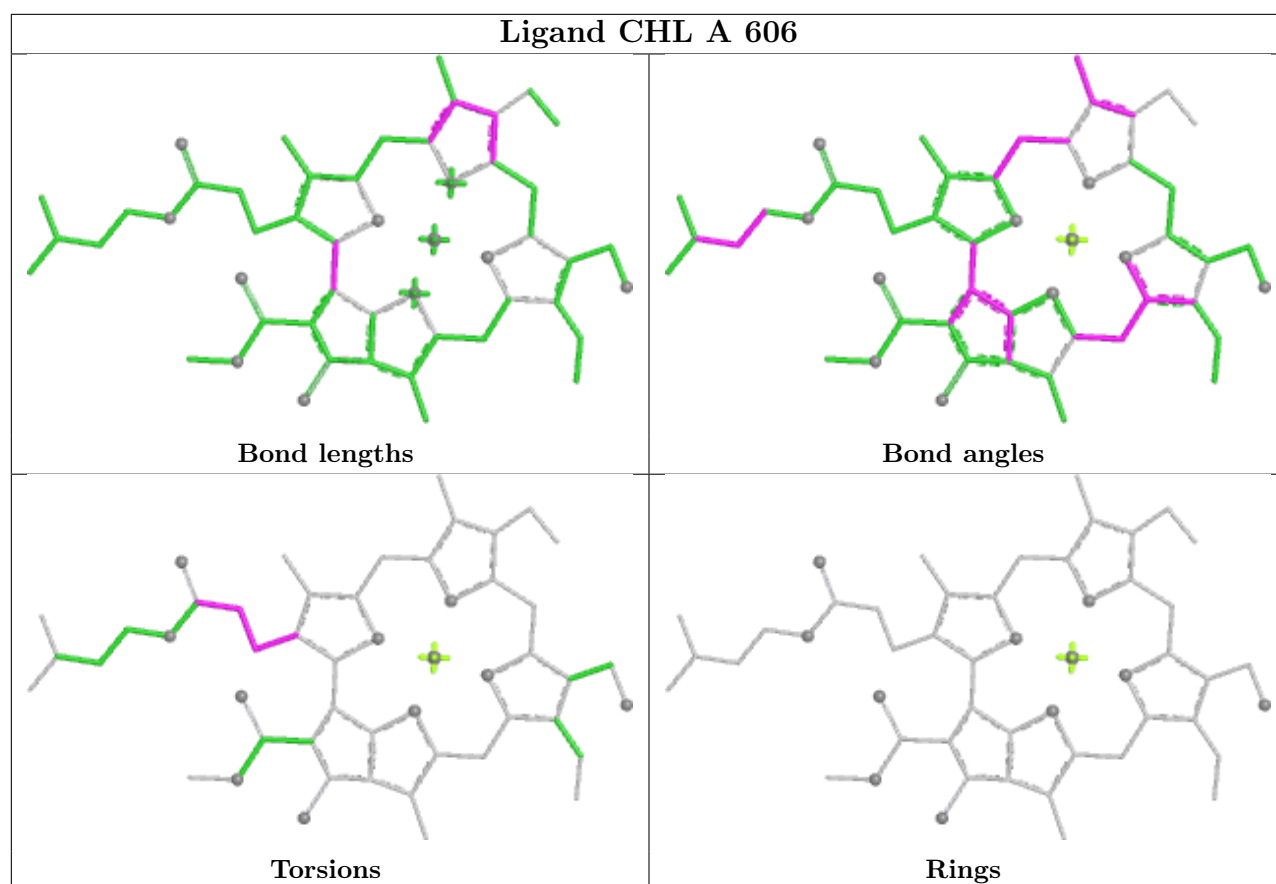
Ligand CHL B 607



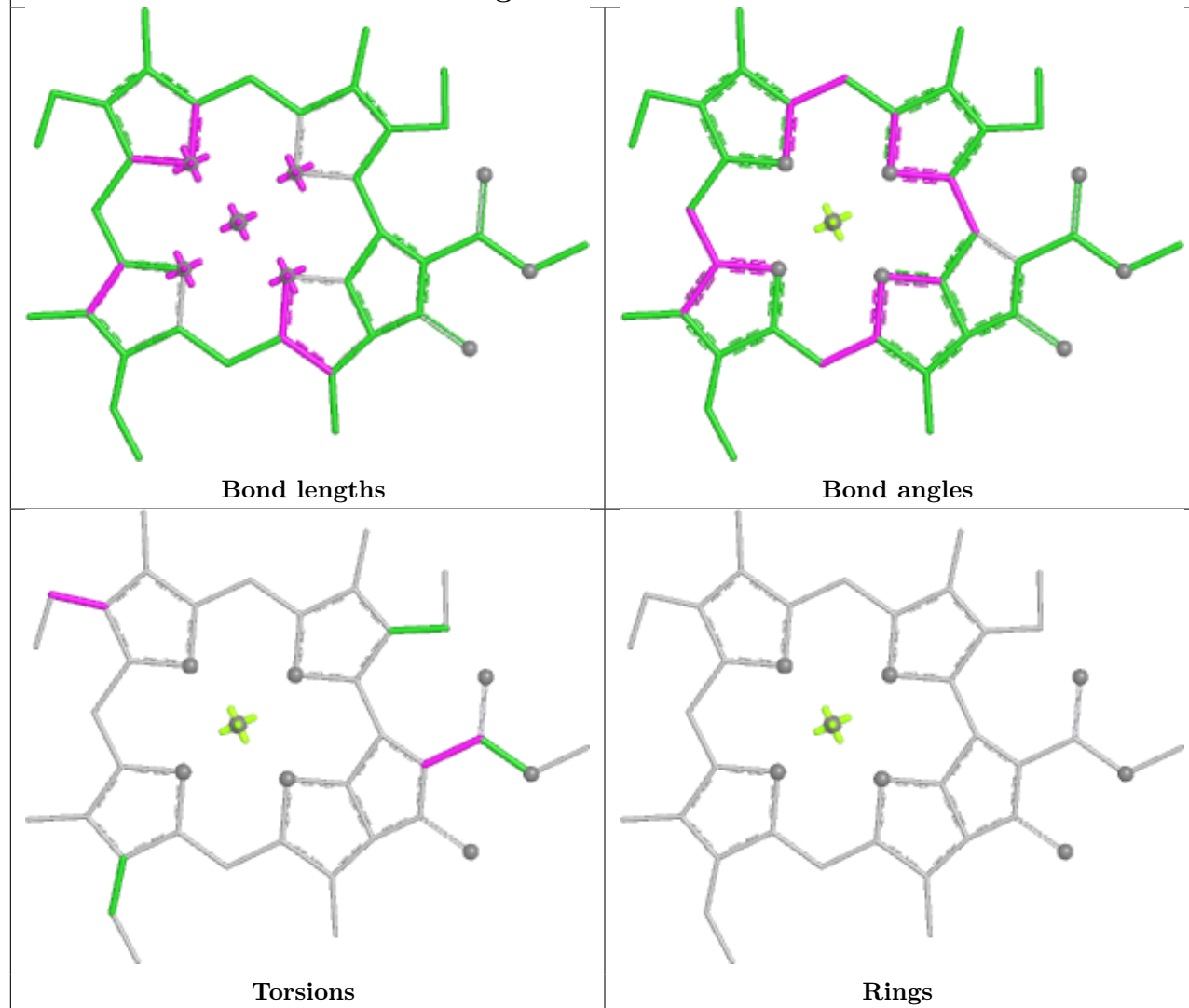




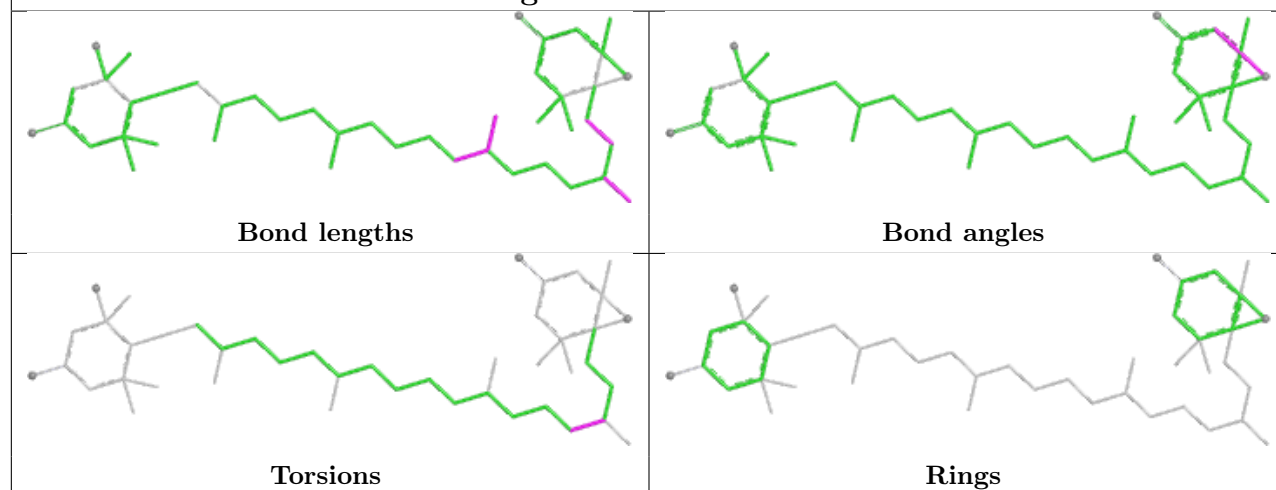


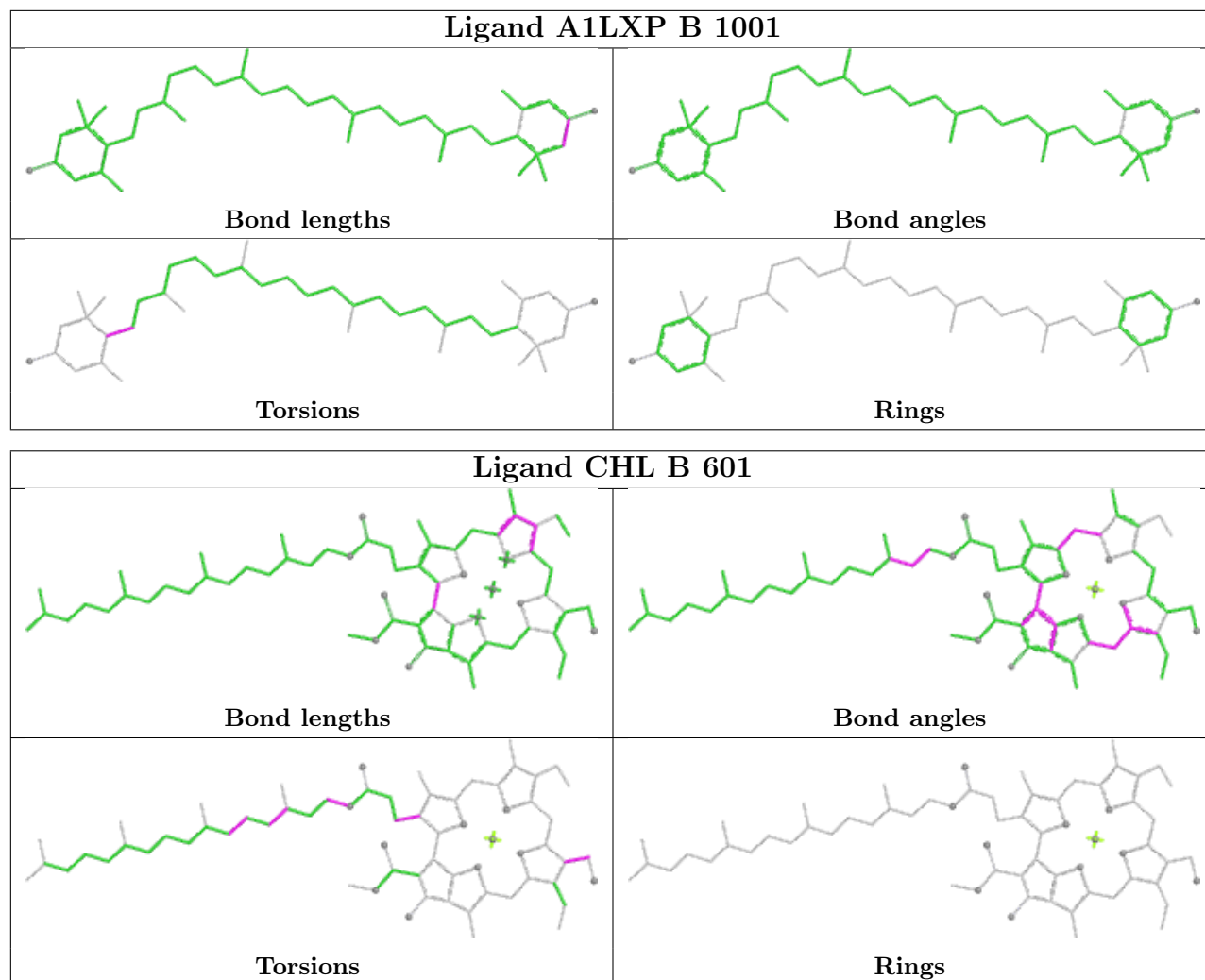


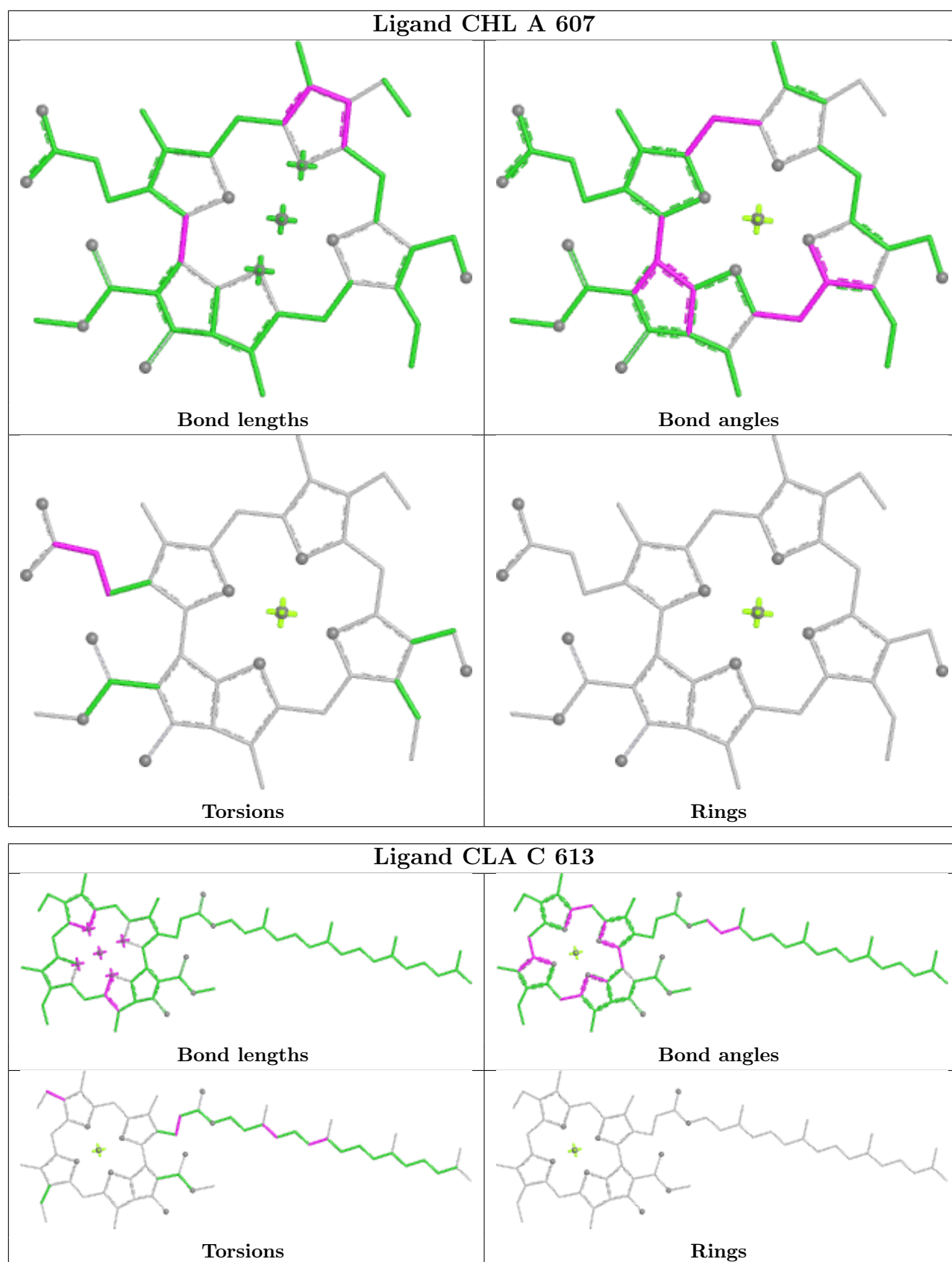
Ligand CLA A 614

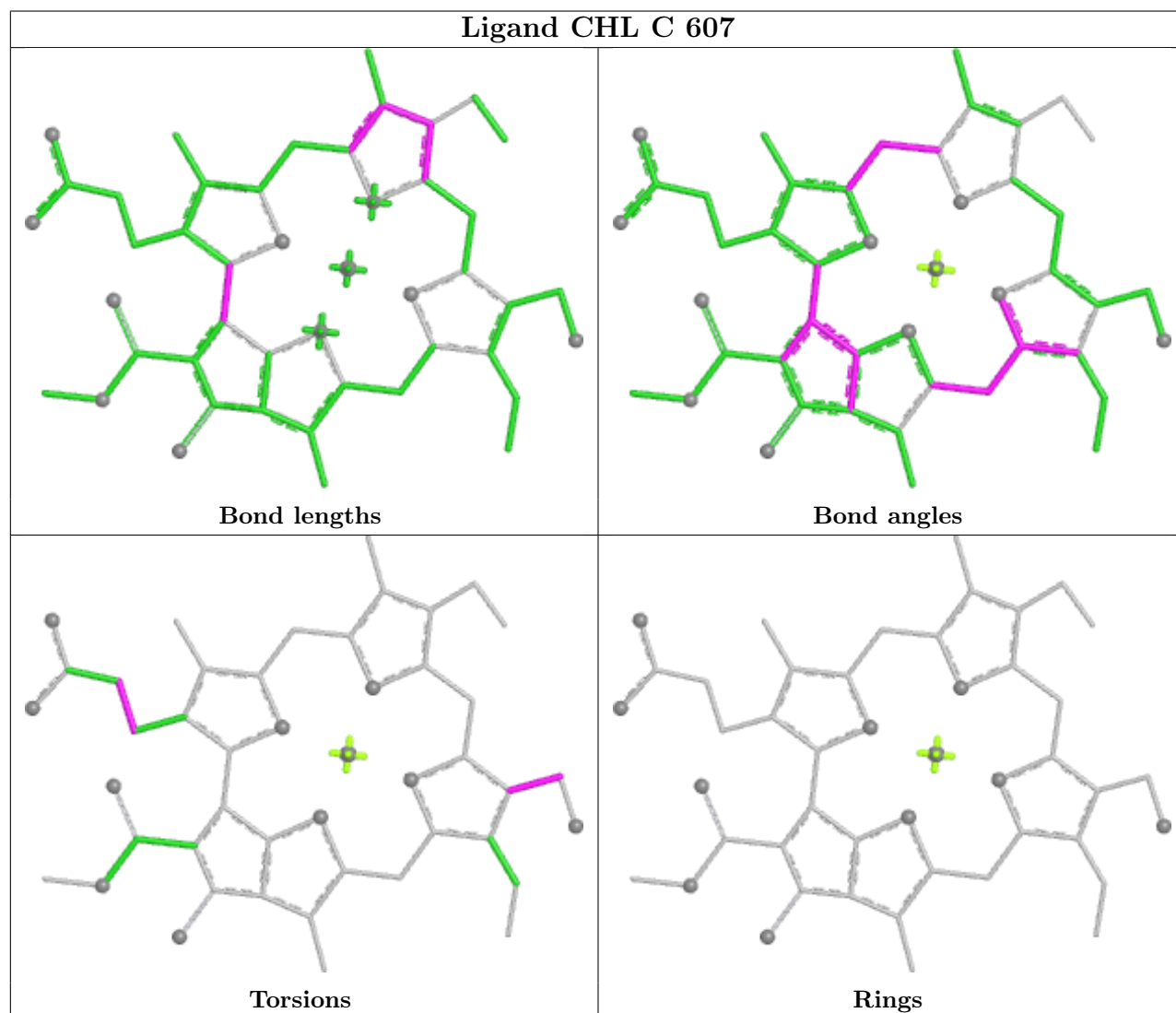
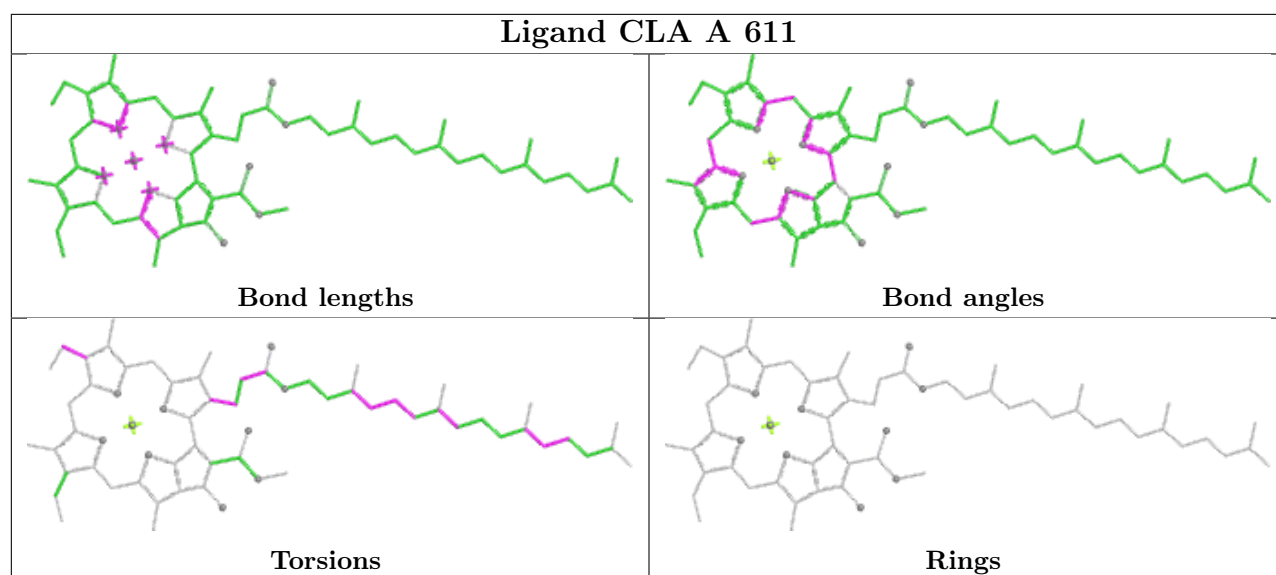


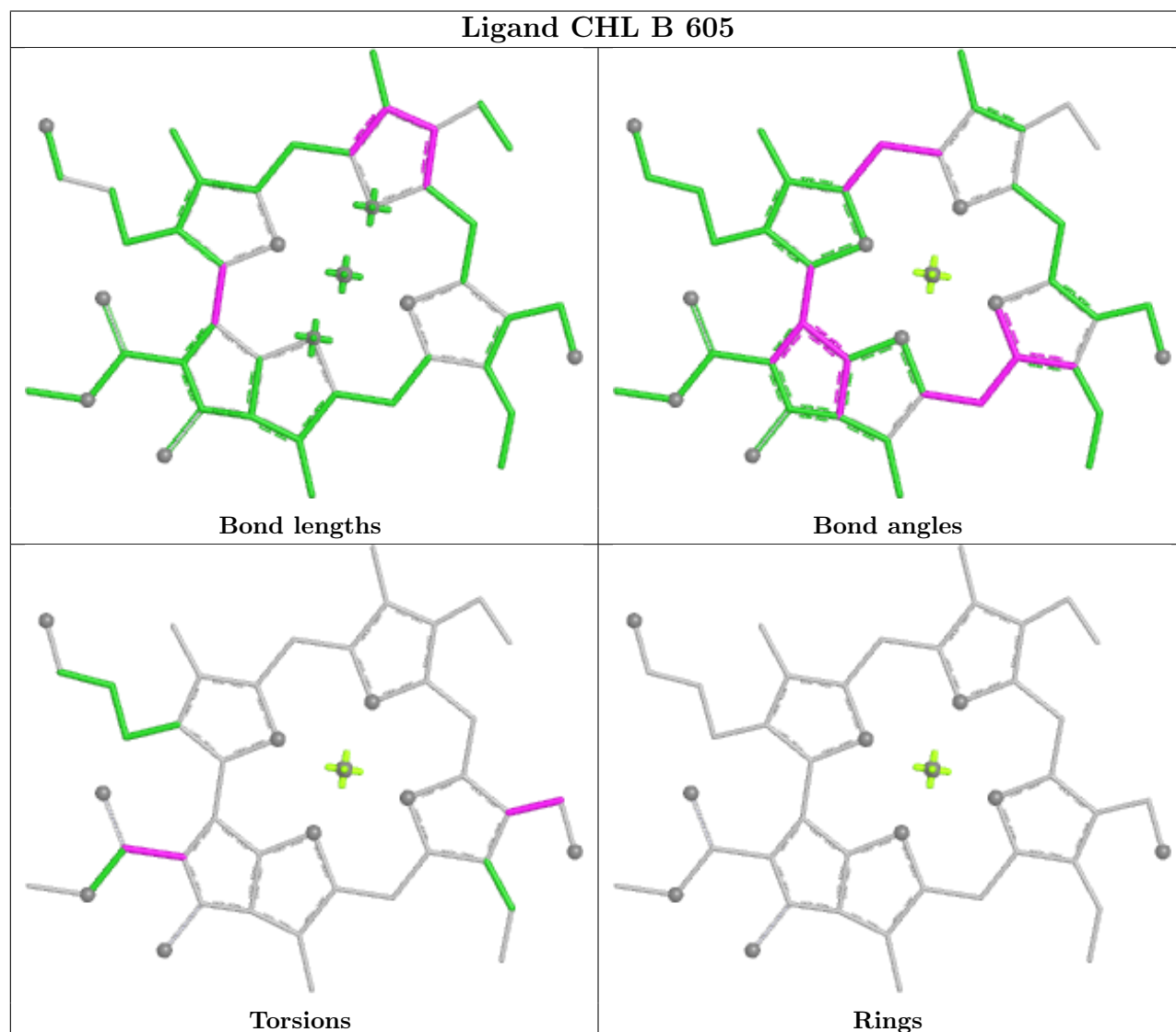
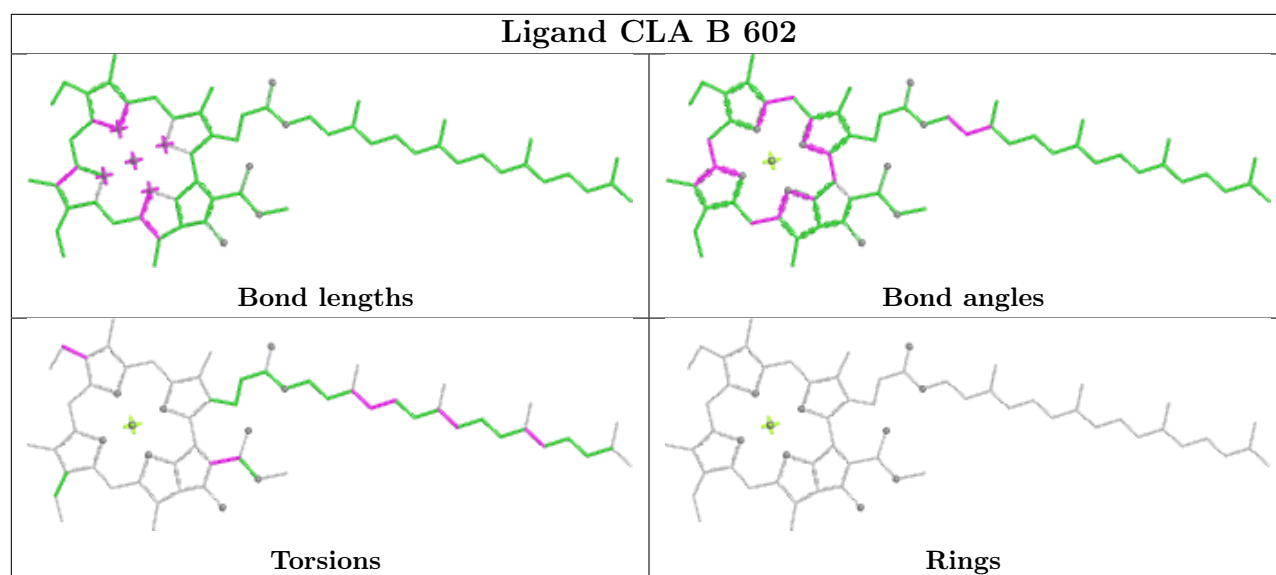
Ligand NEX A 1003

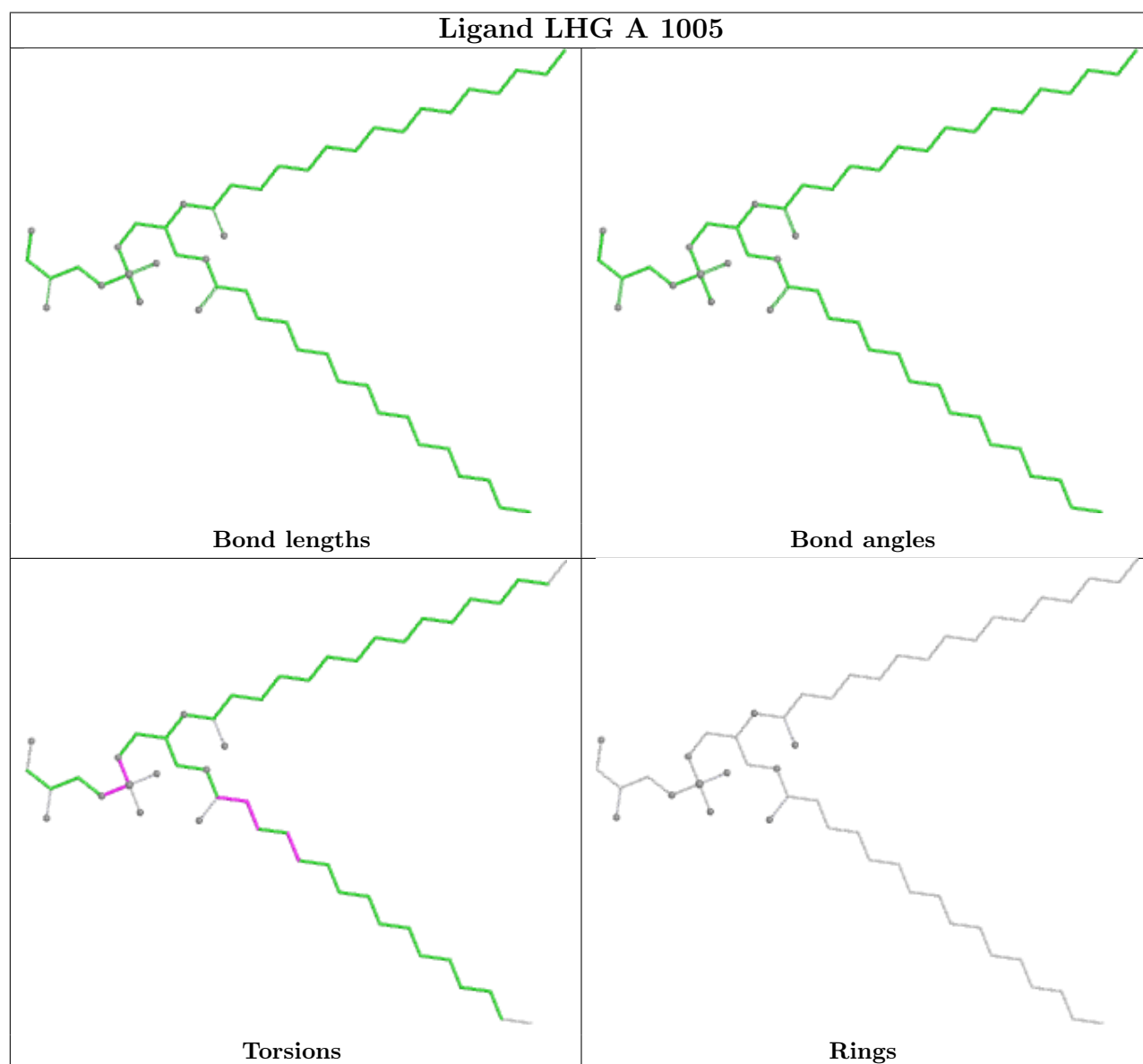
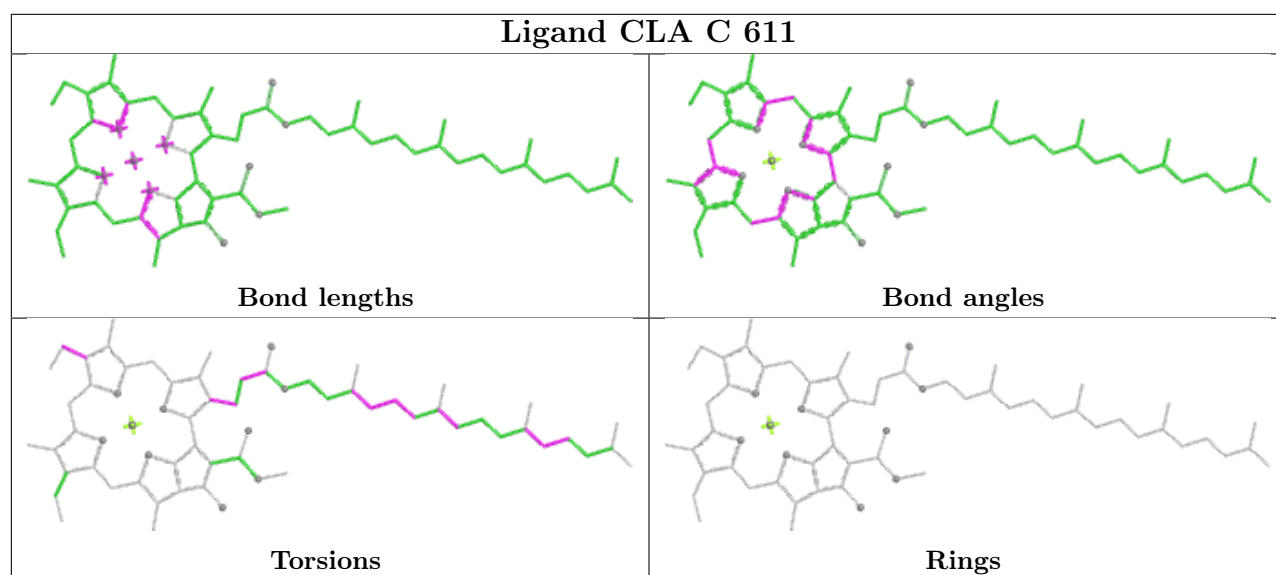


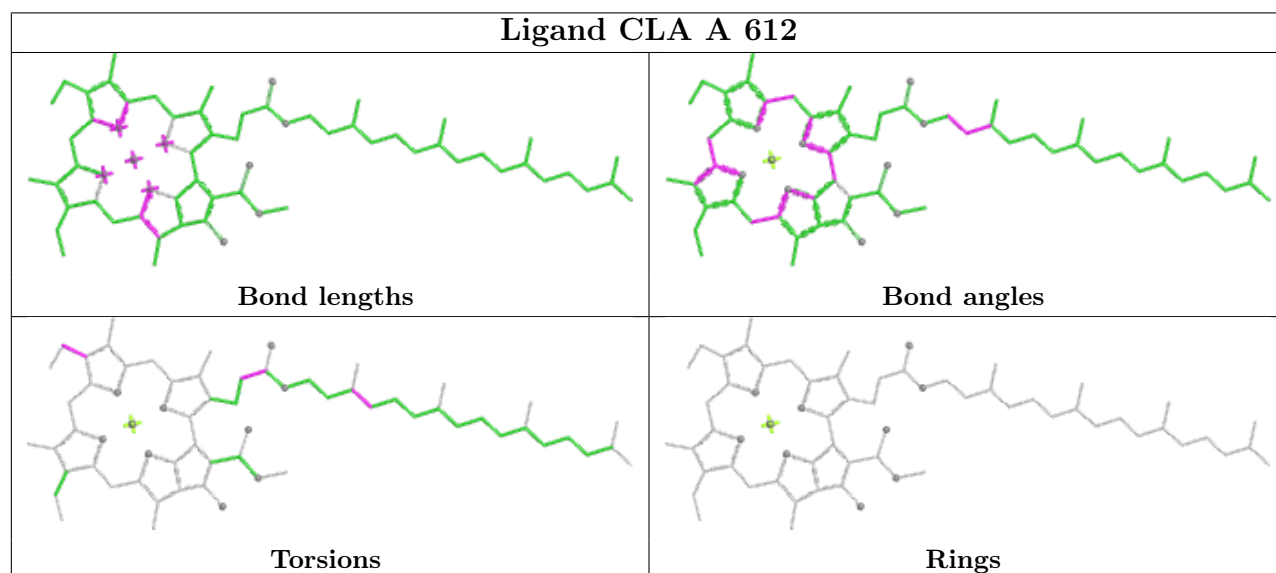
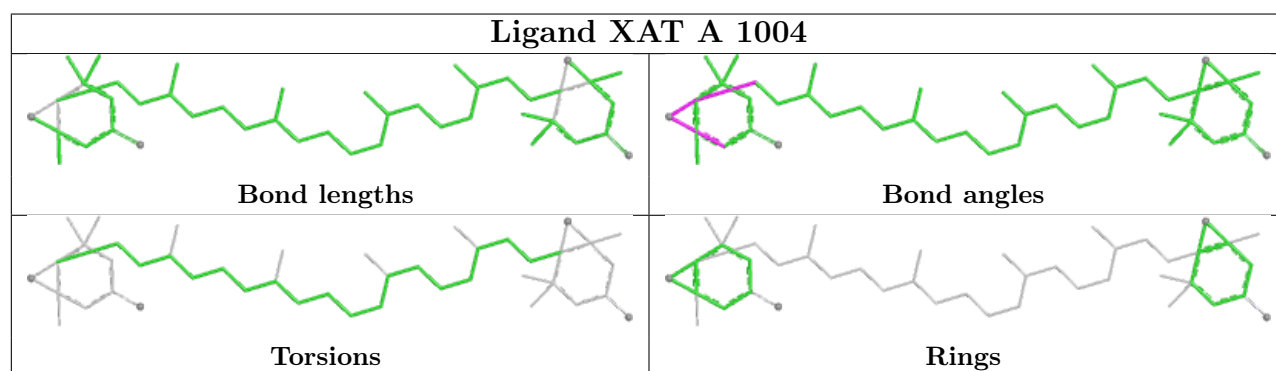
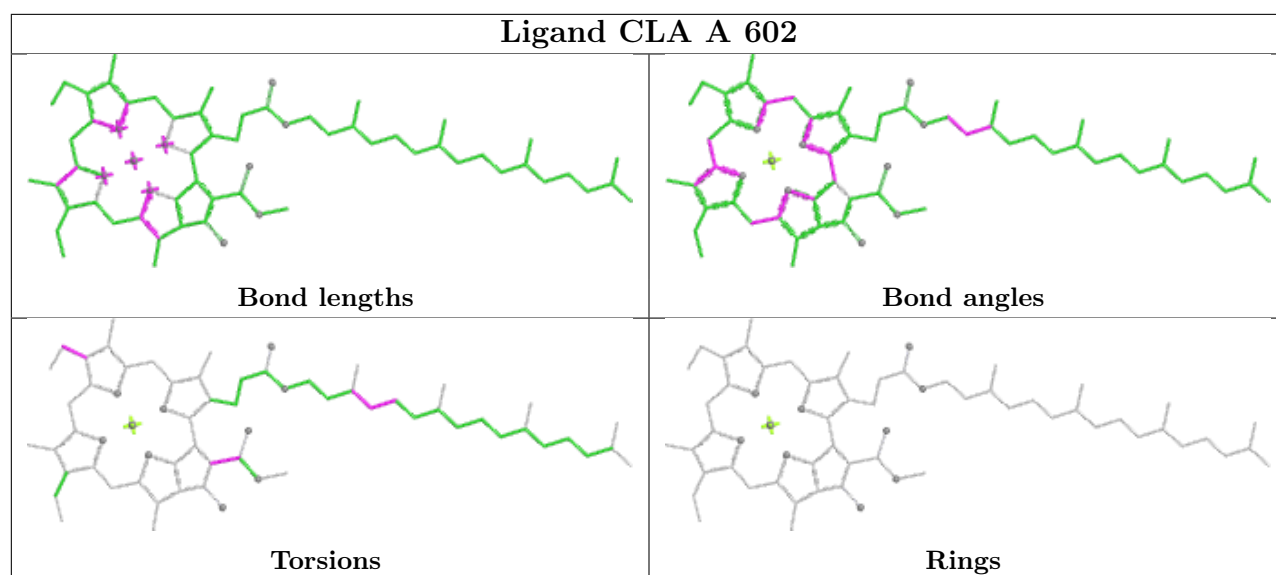




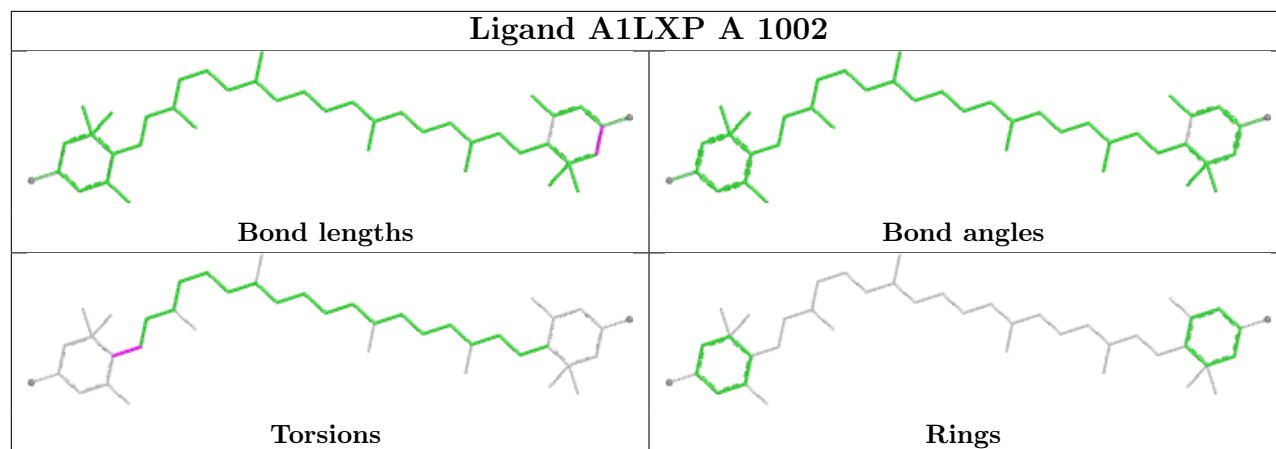




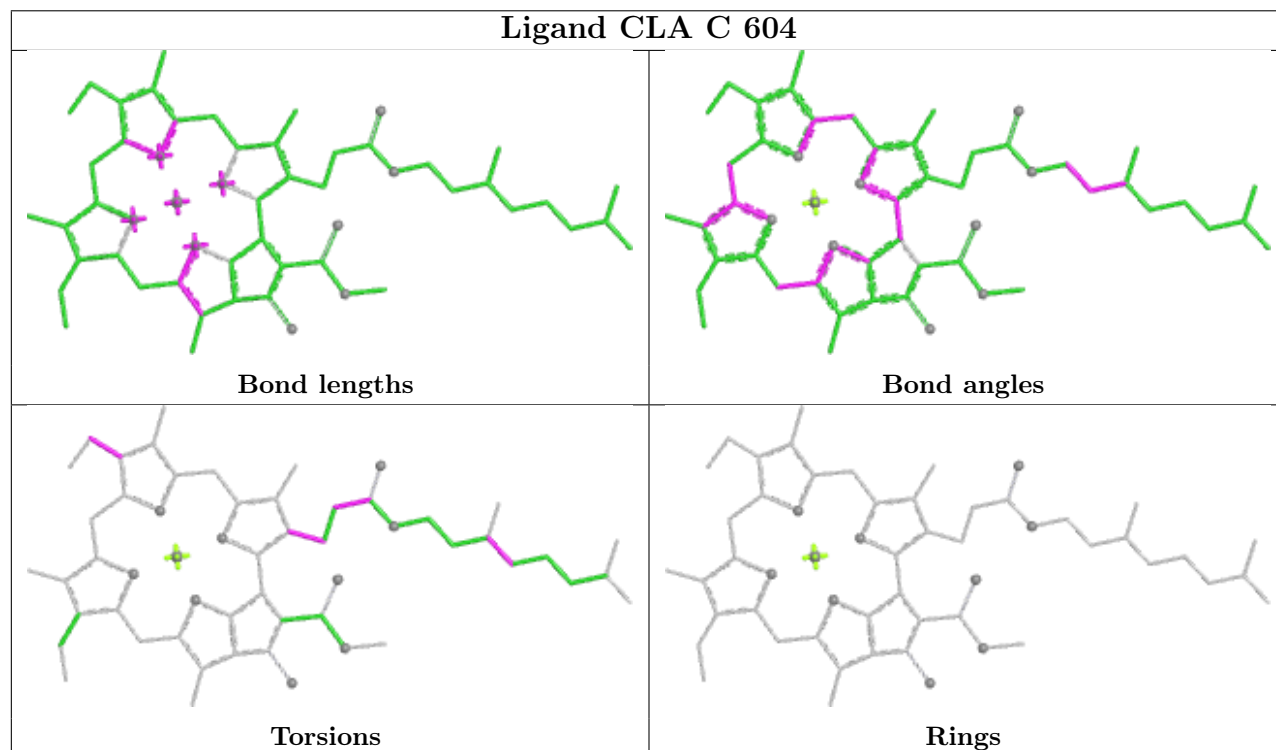


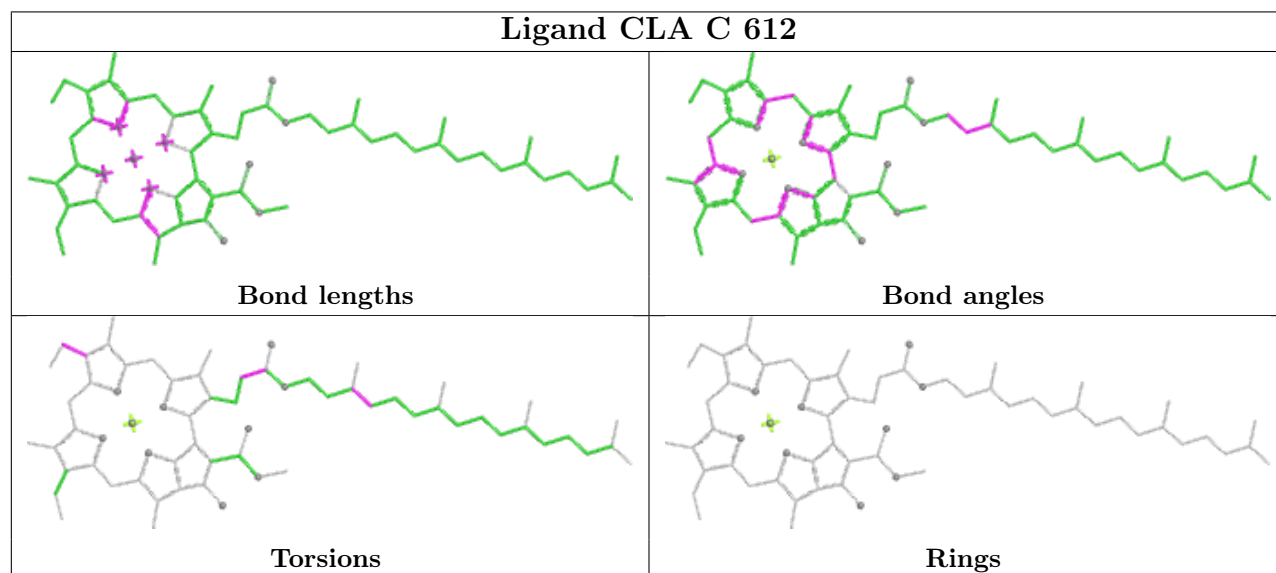
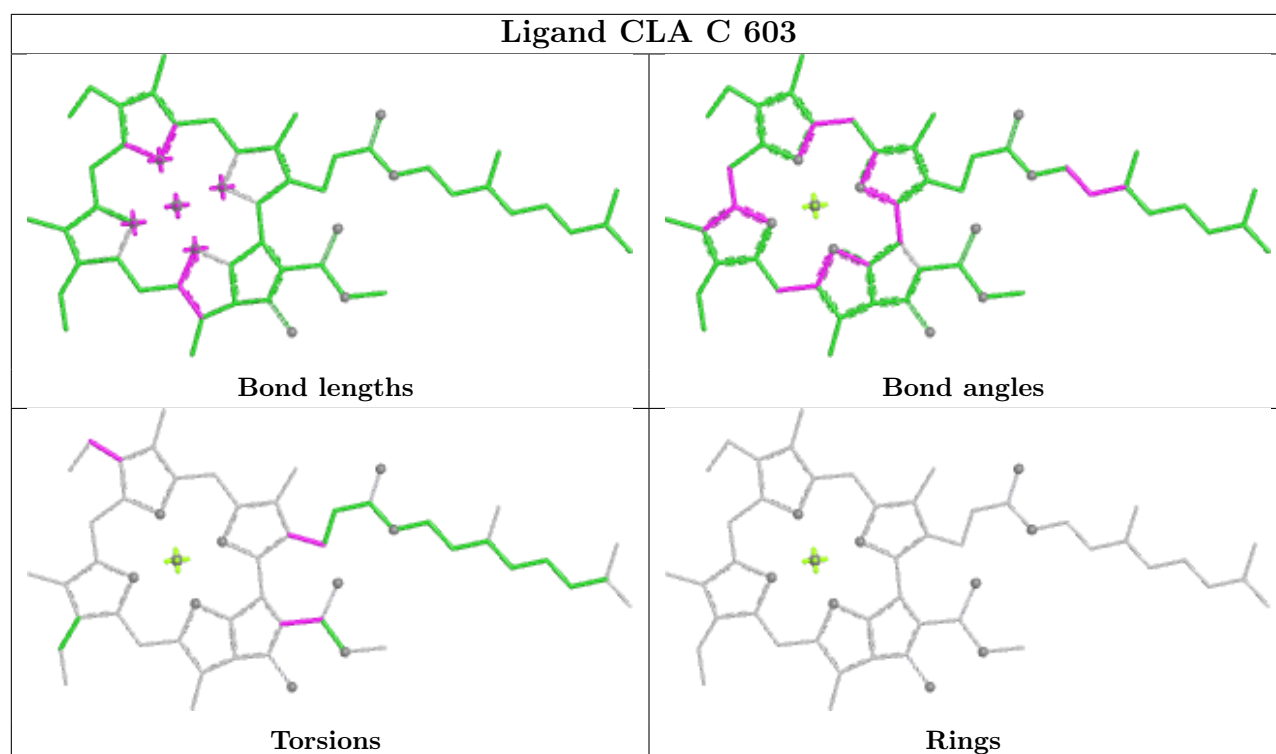


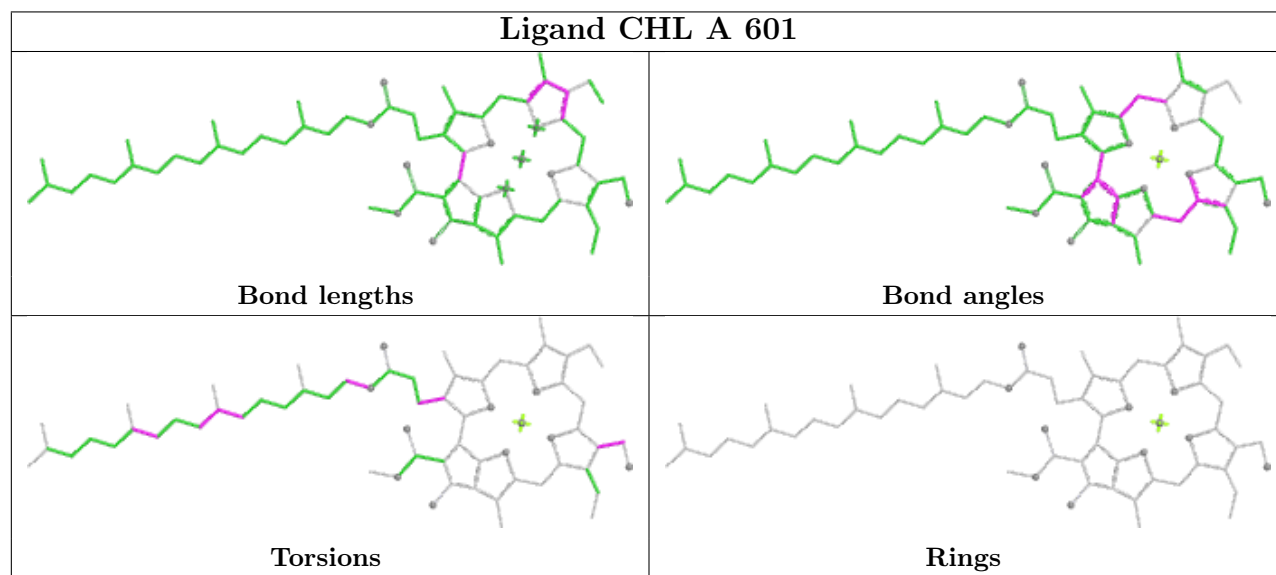
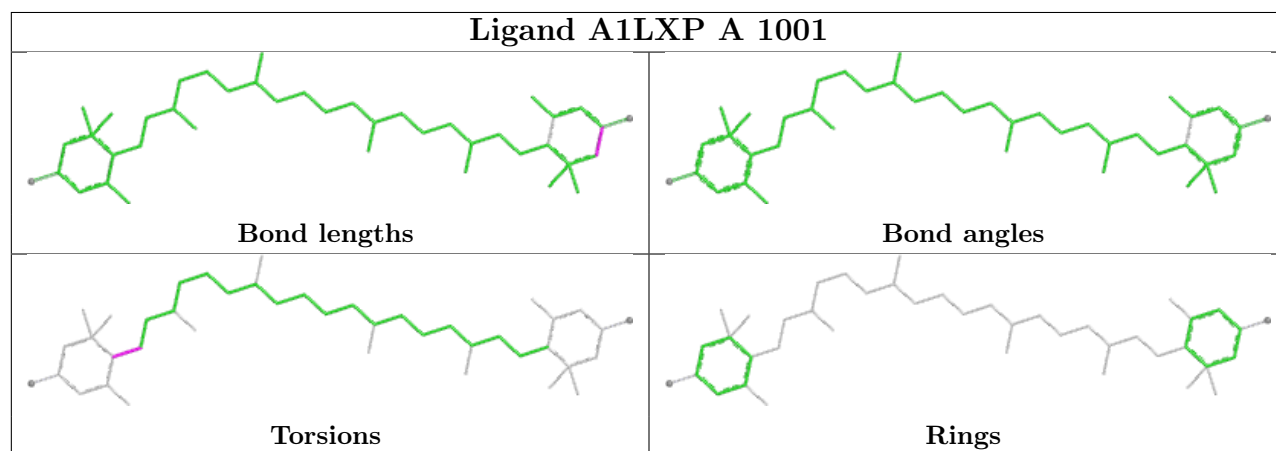
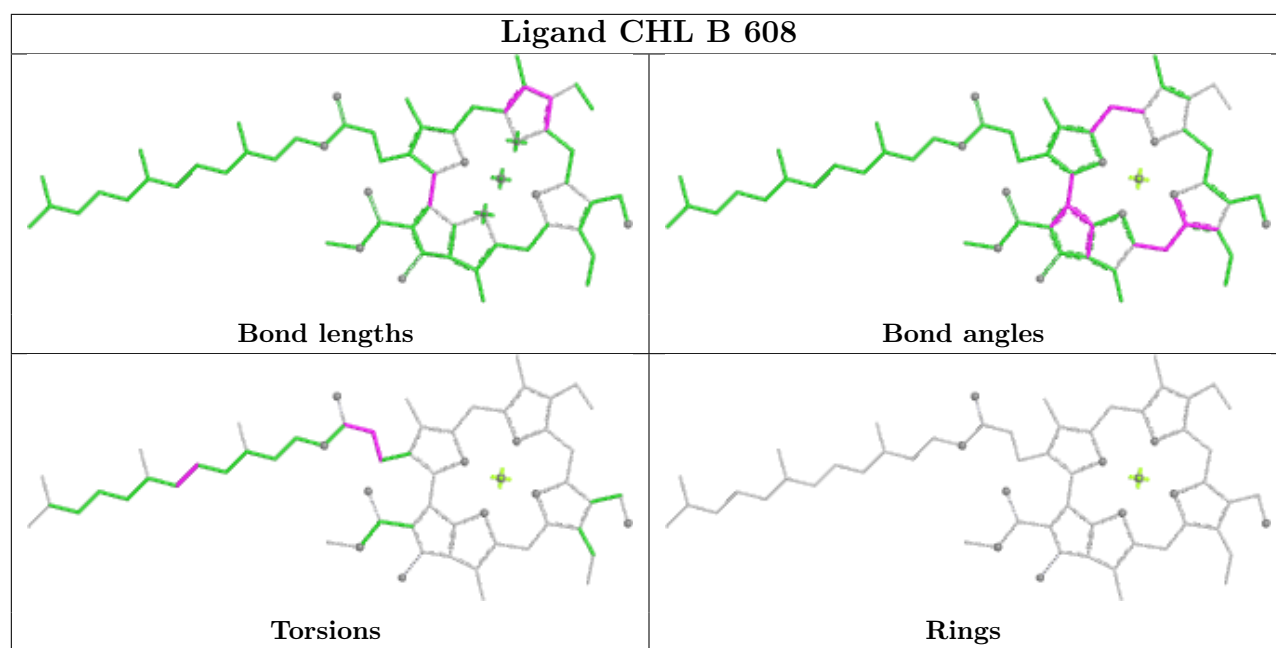
Ligand A1LXP A 1002

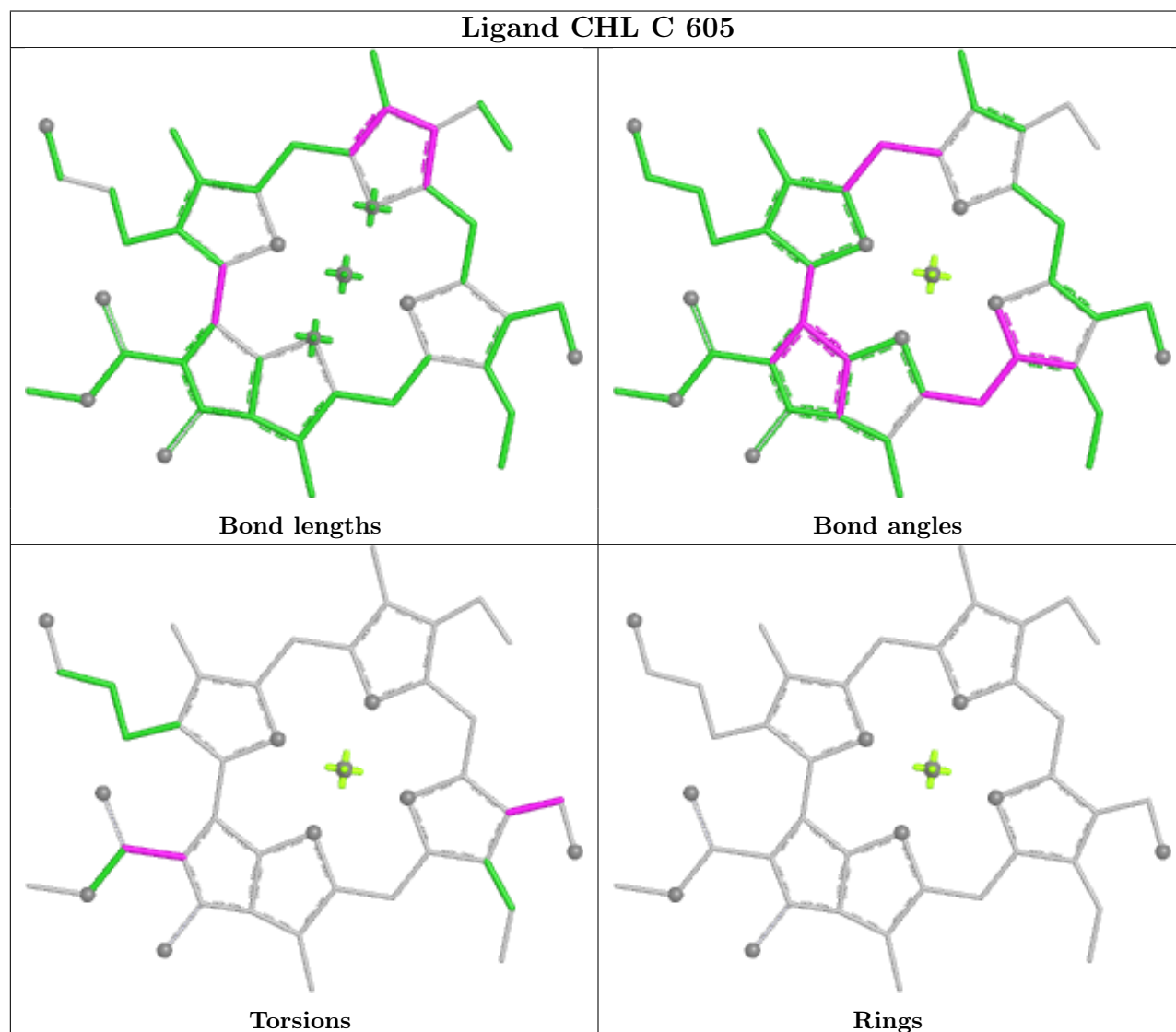
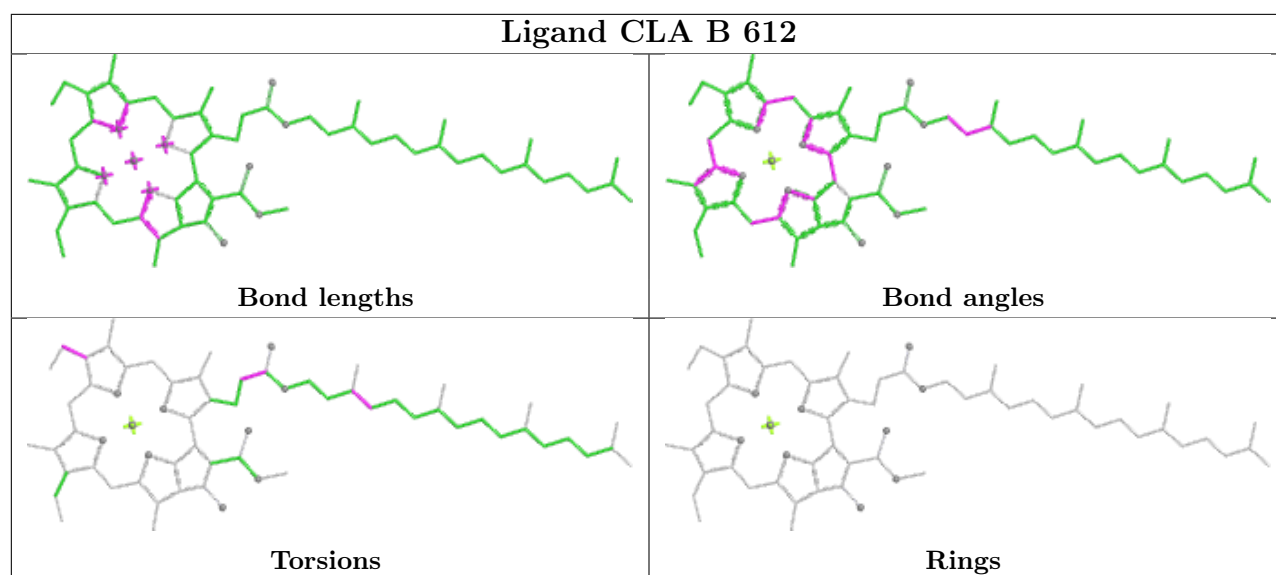


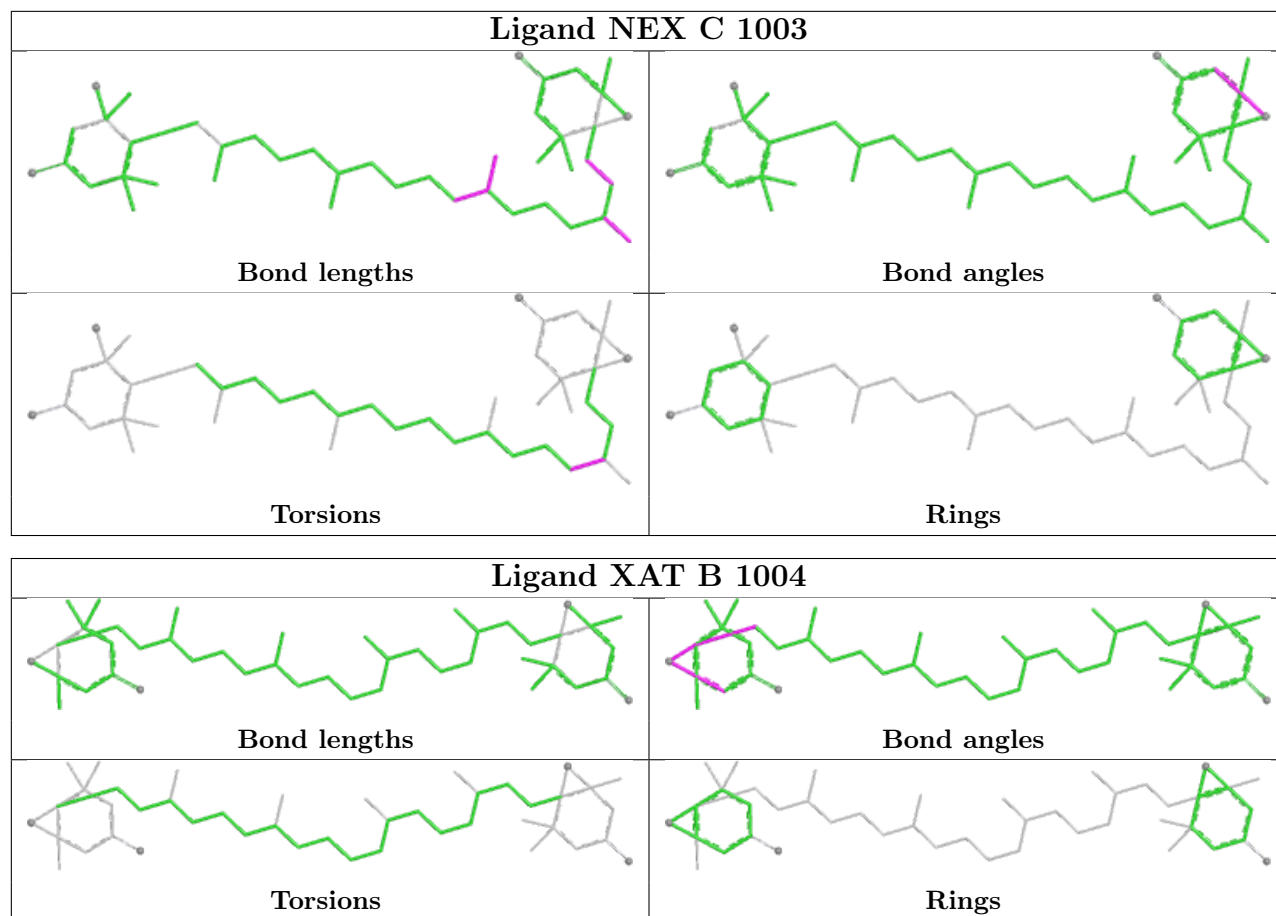
Ligand CLA C 604

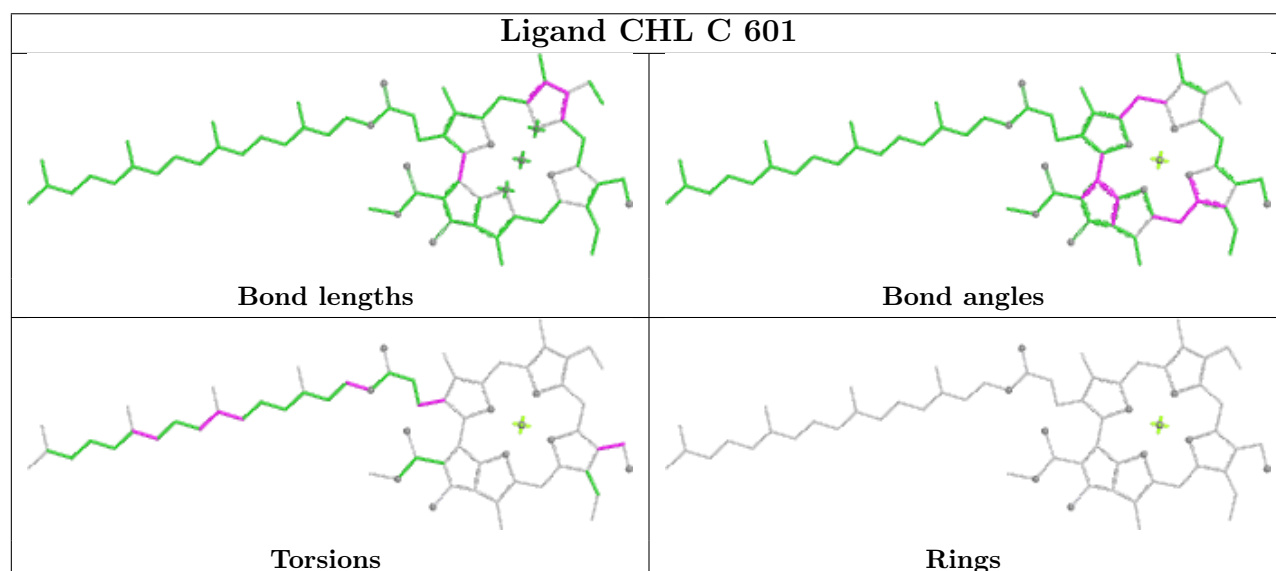
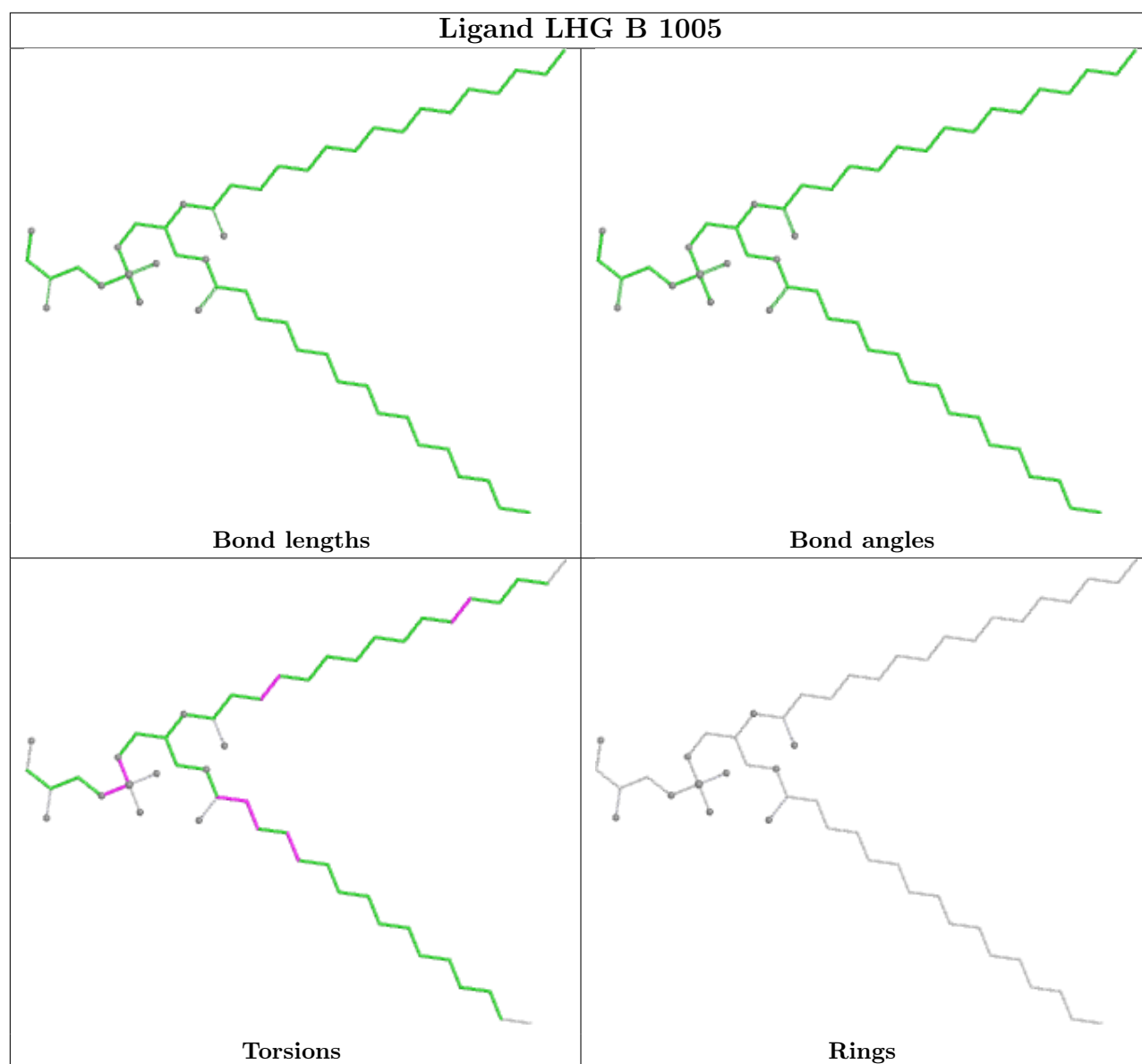


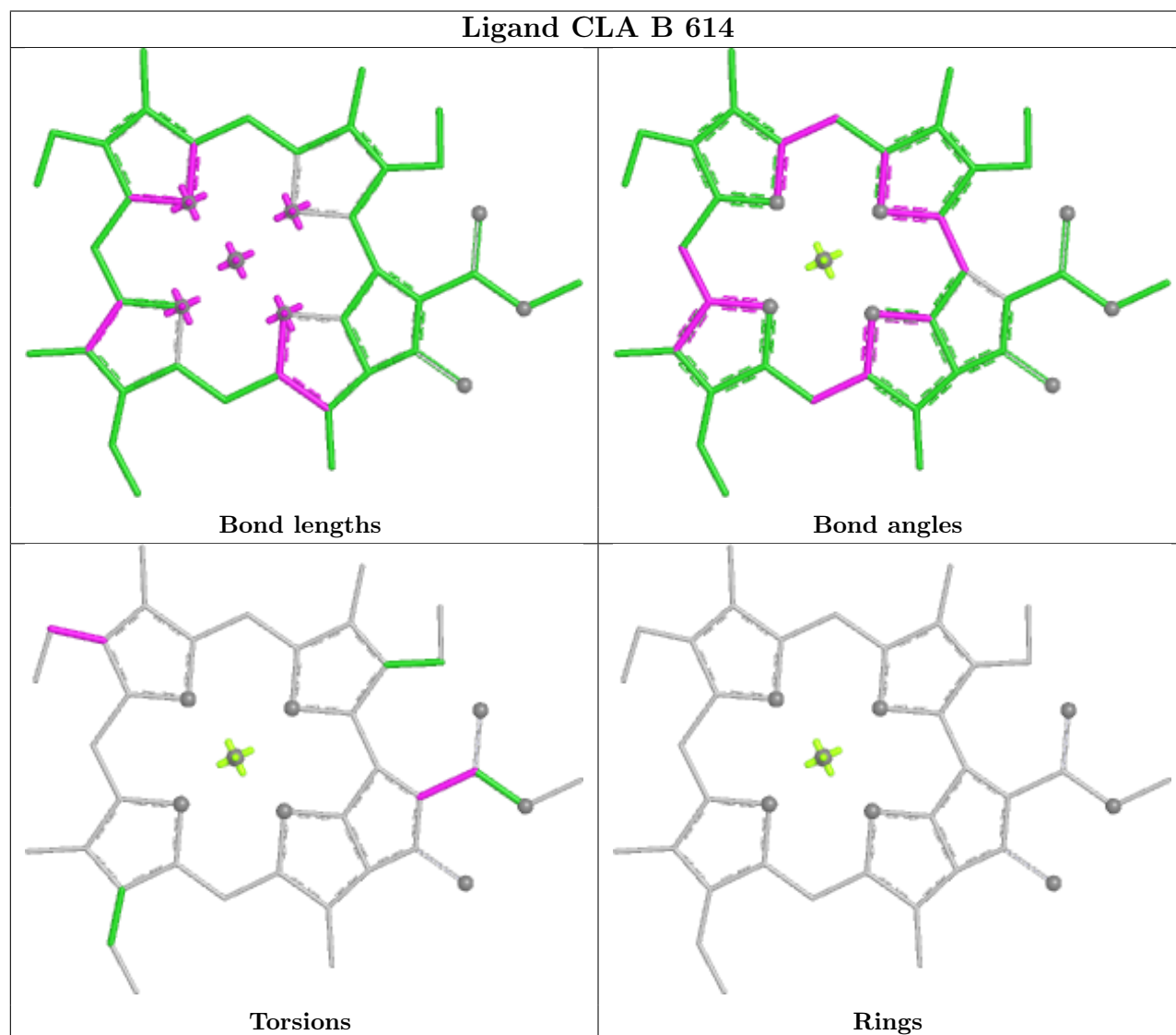
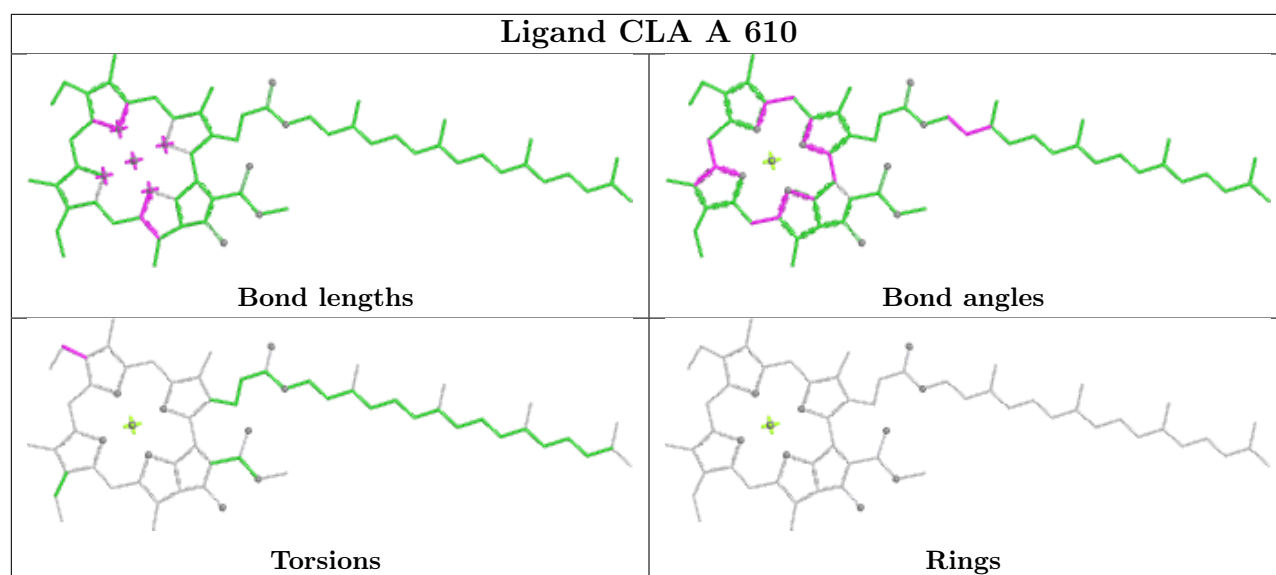


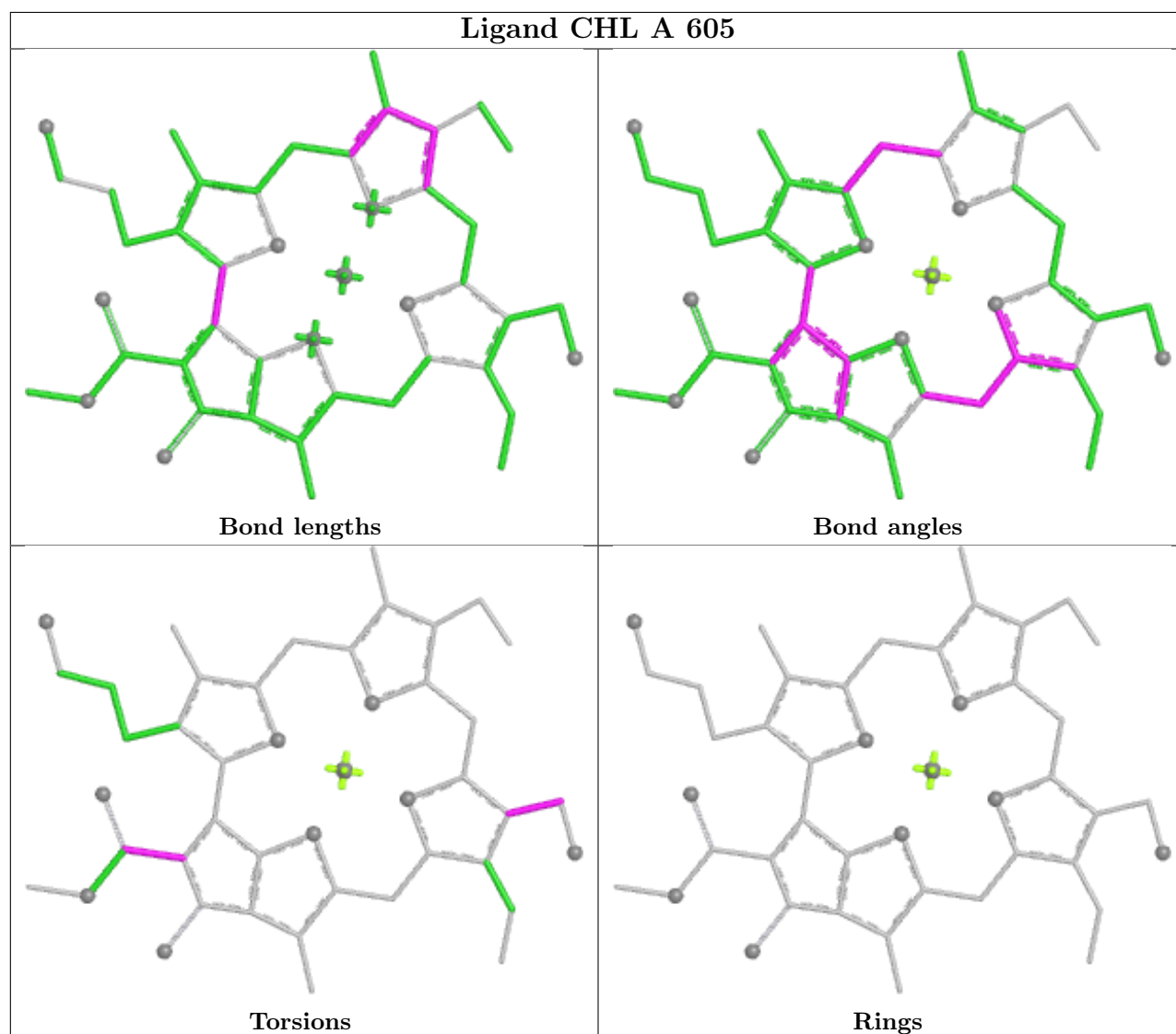
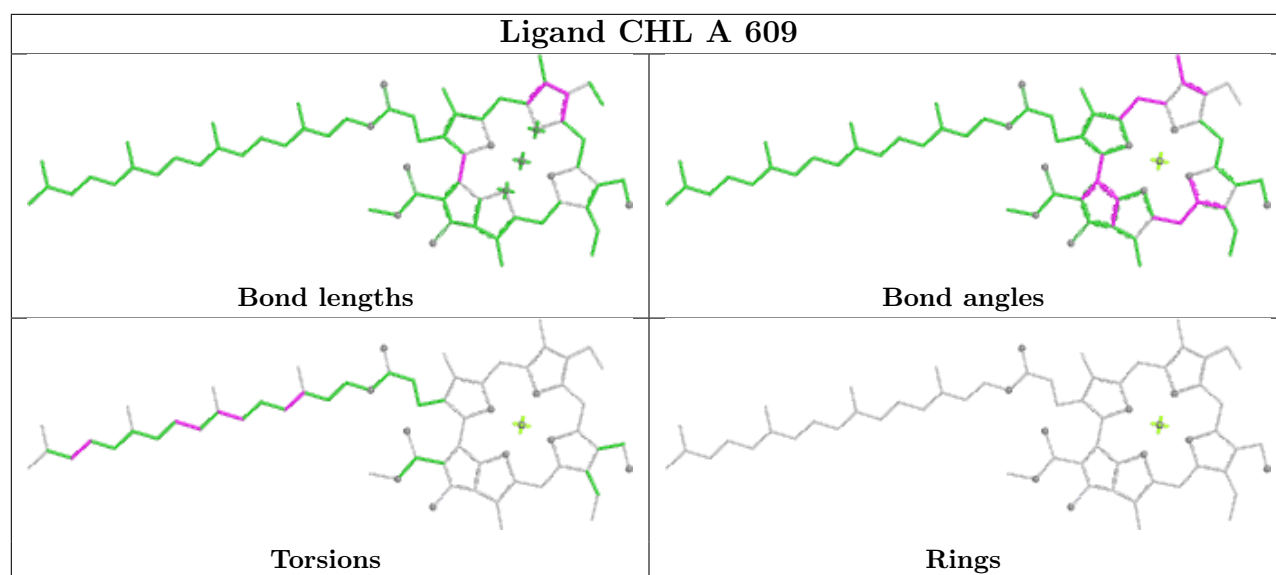


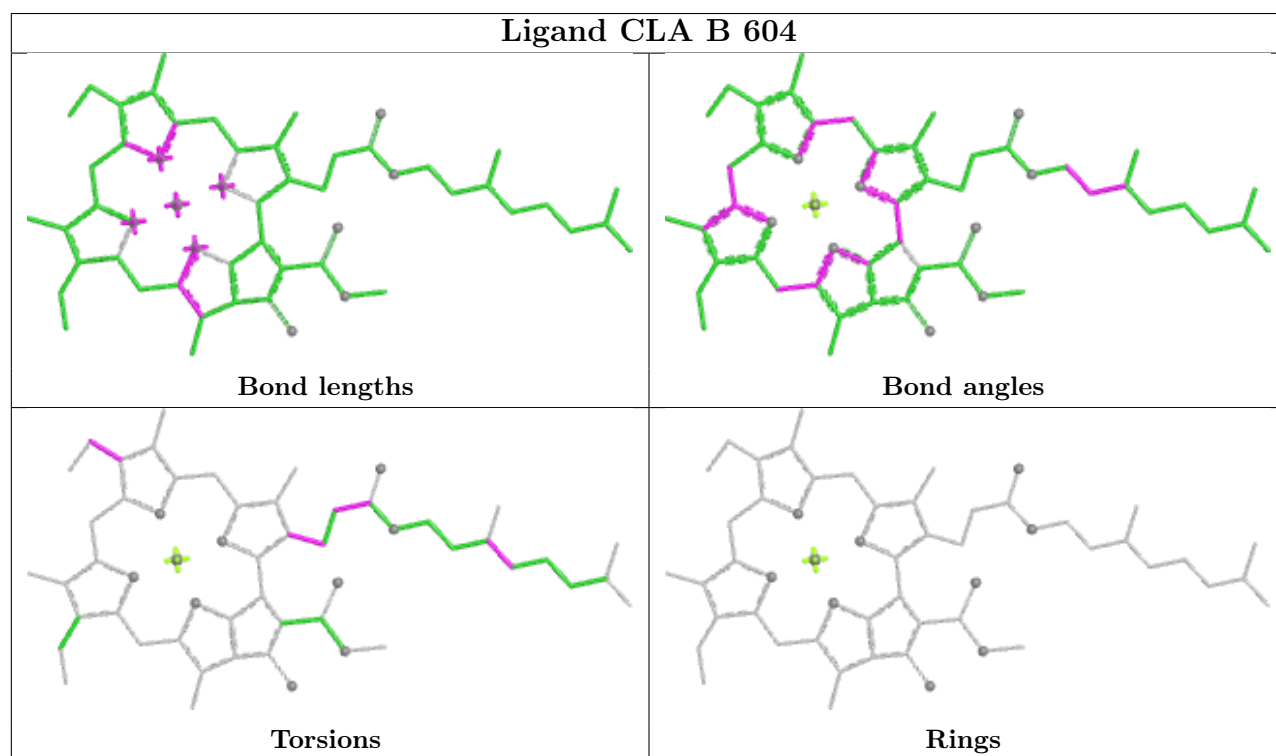
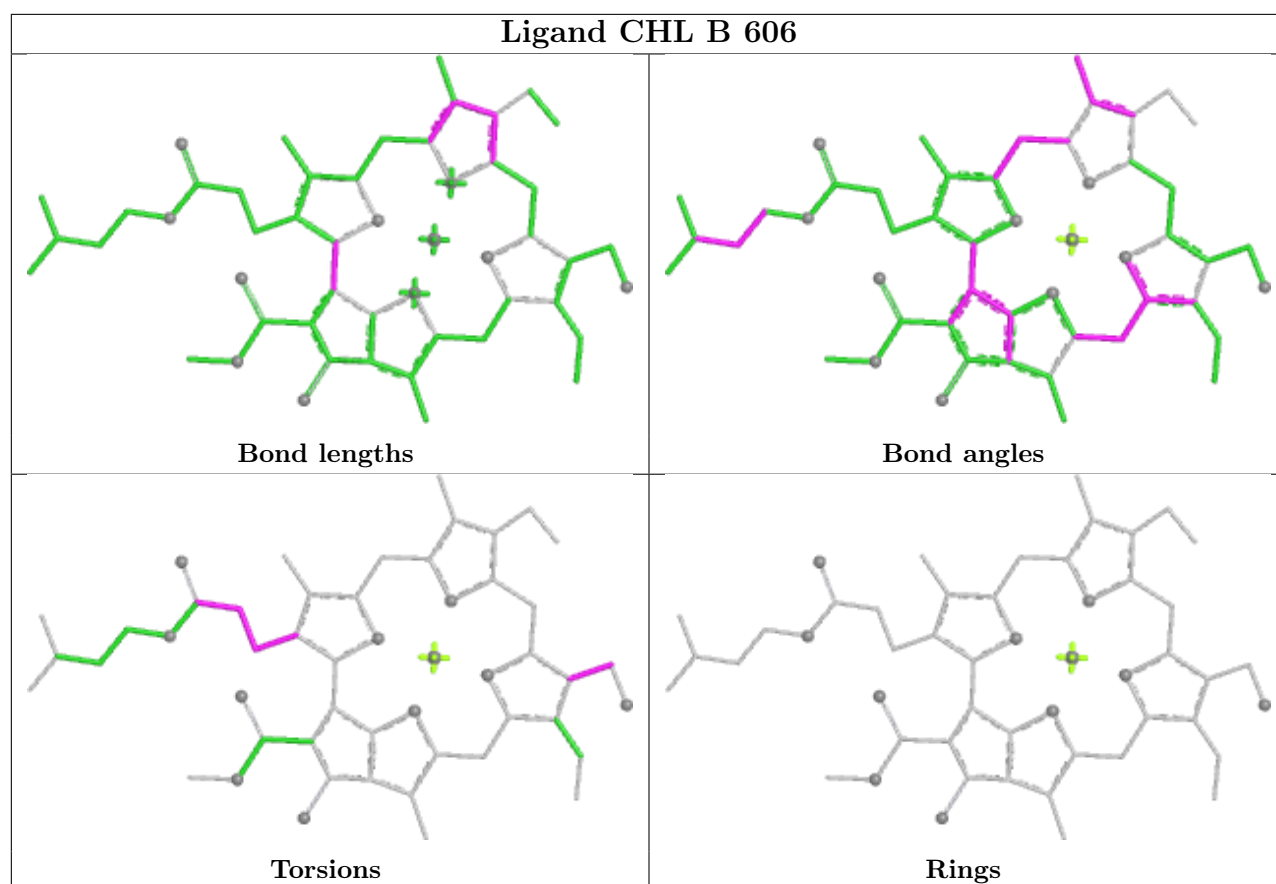


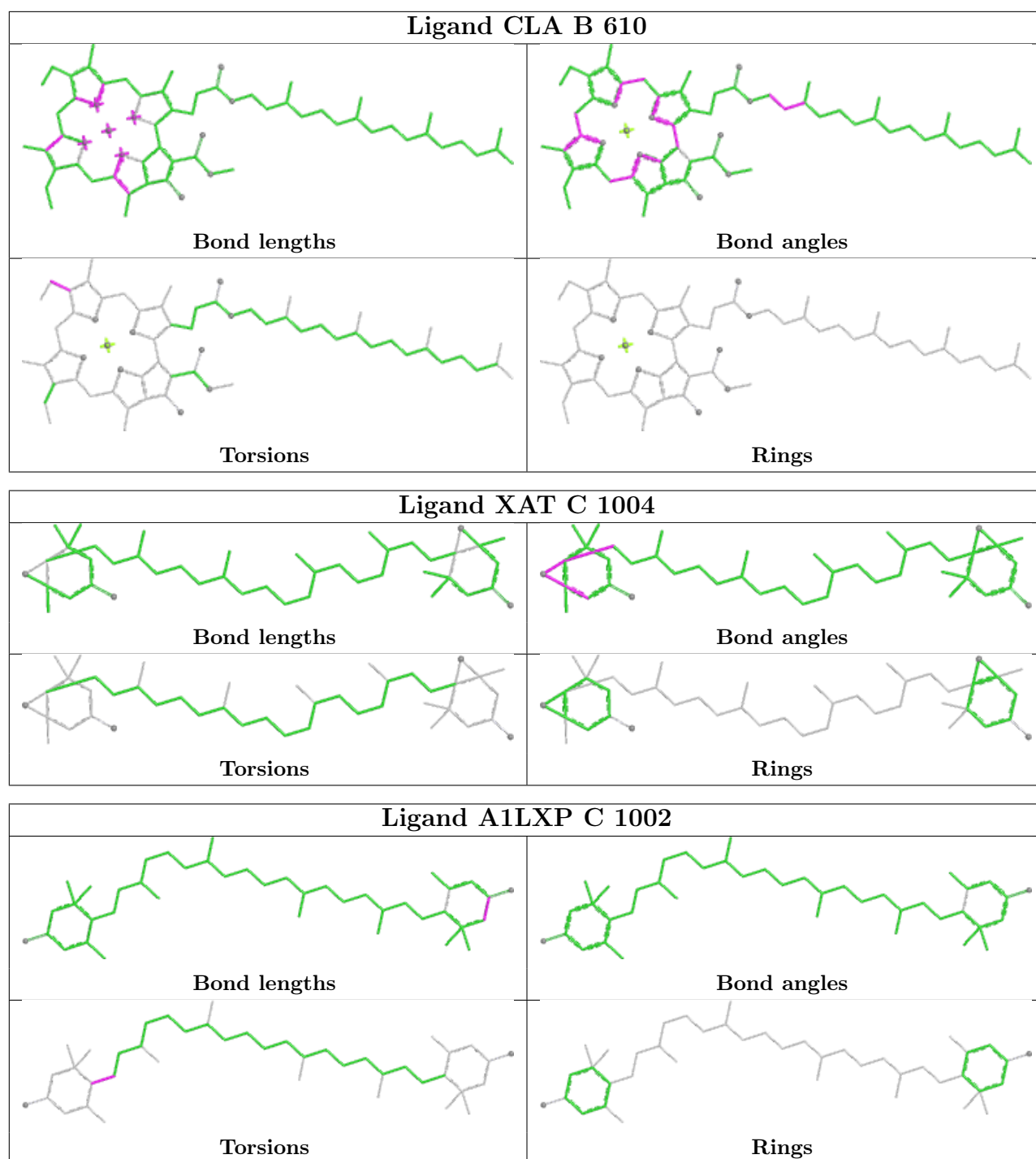


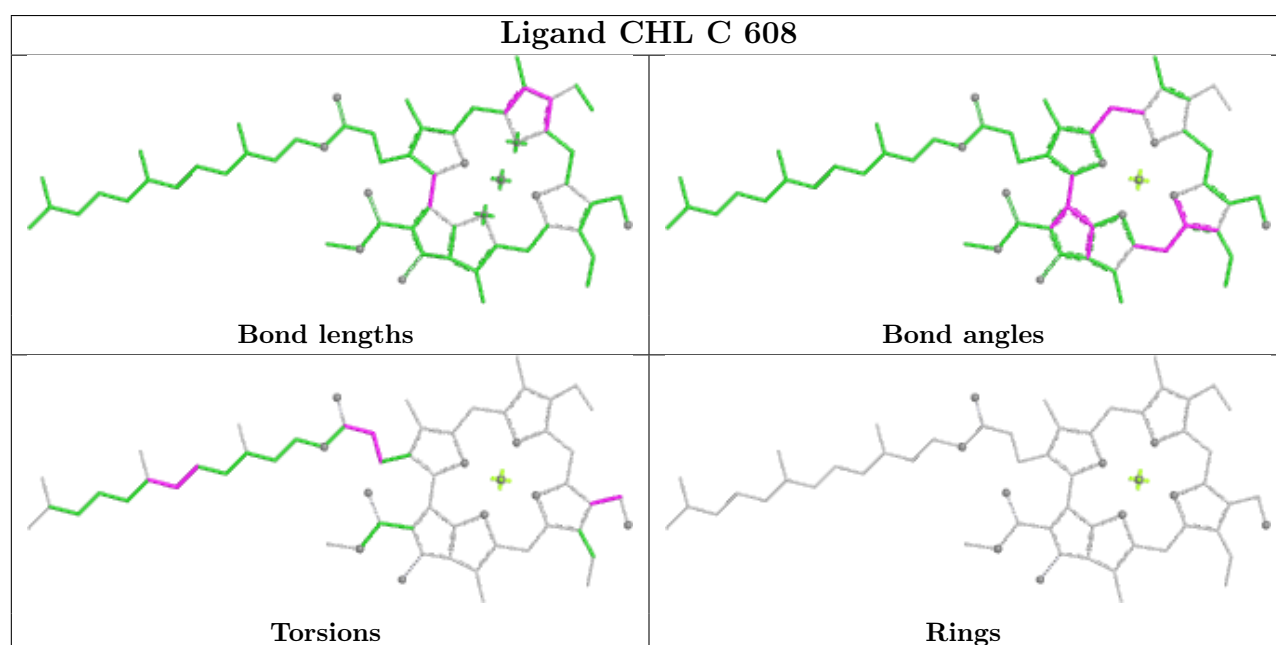
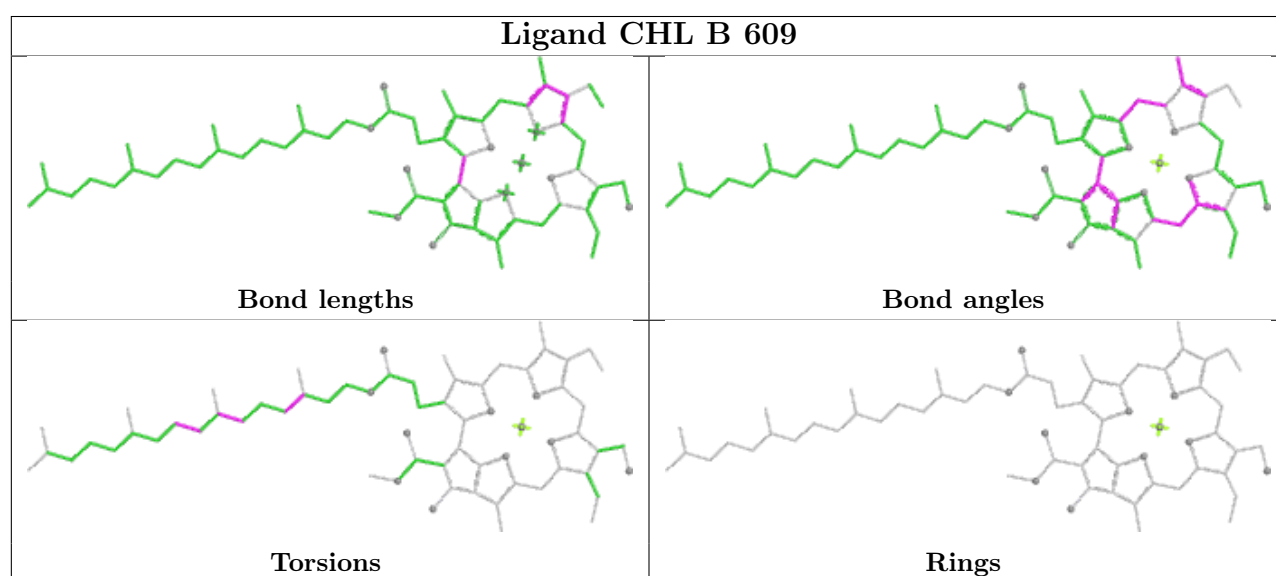
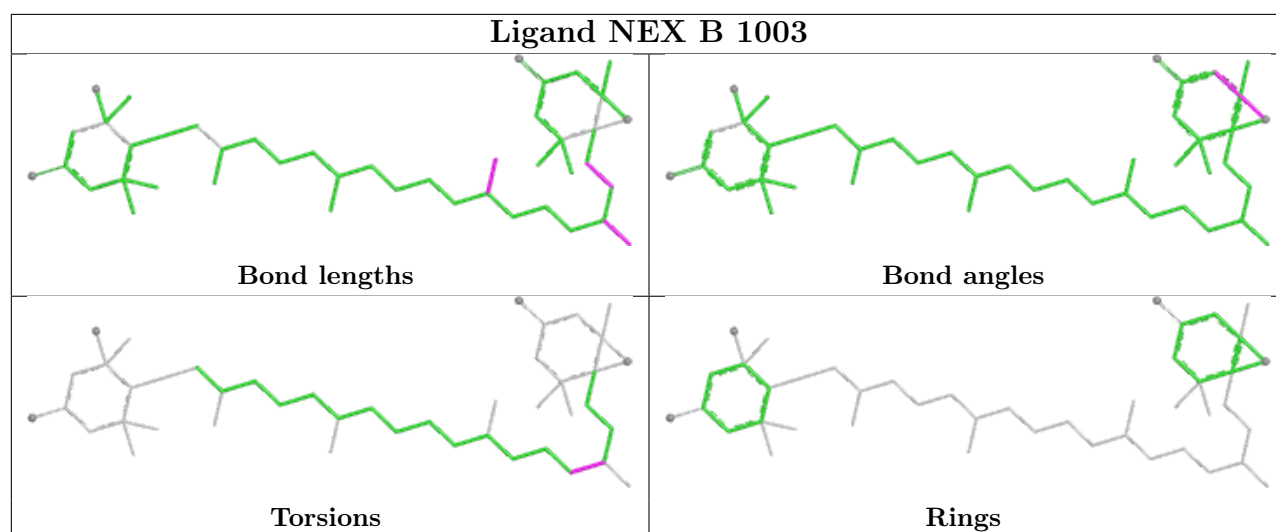


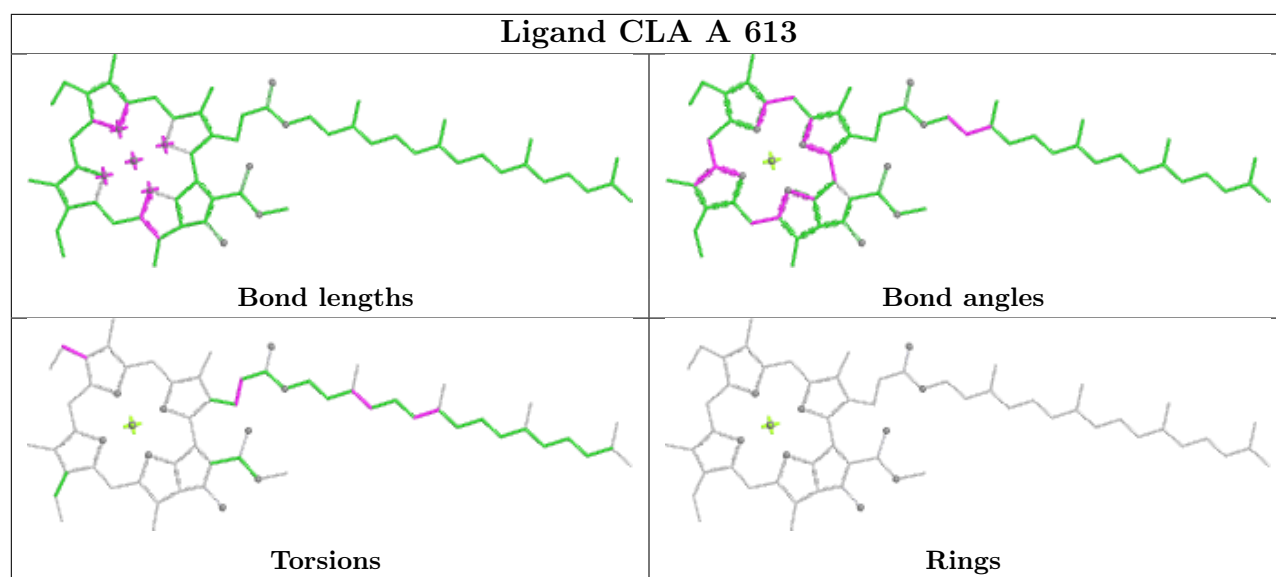












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

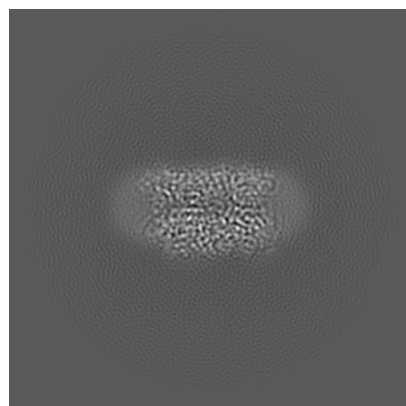
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38825. These allow visual inspection of the internal detail of the map and identification of artifacts.

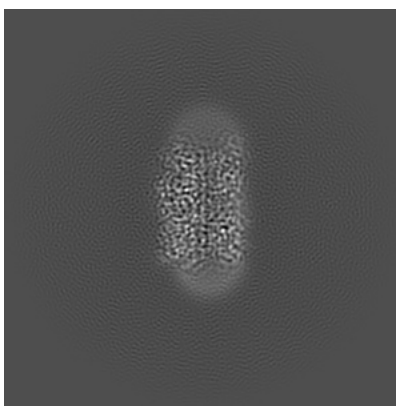
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

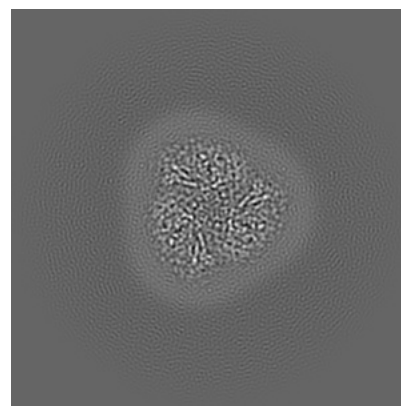
6.1.1 Primary map



X

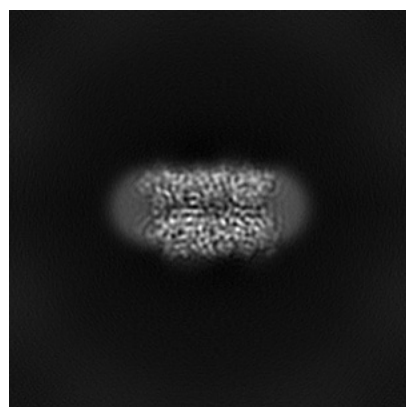


Y

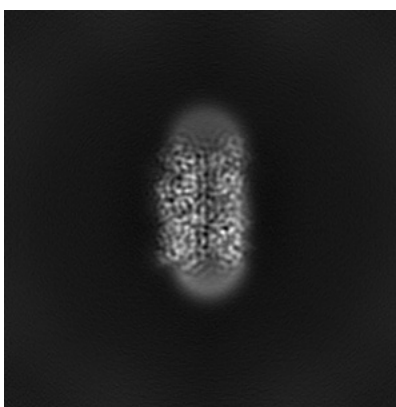


Z

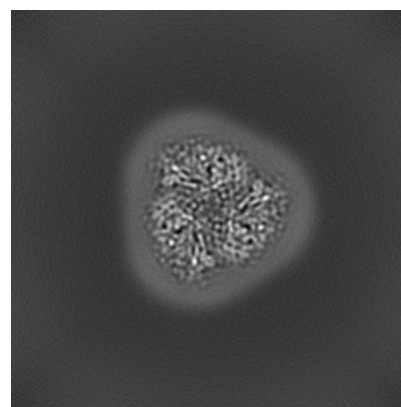
6.1.2 Raw map



X



Y

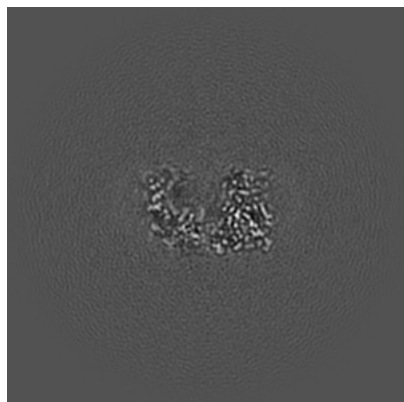


Z

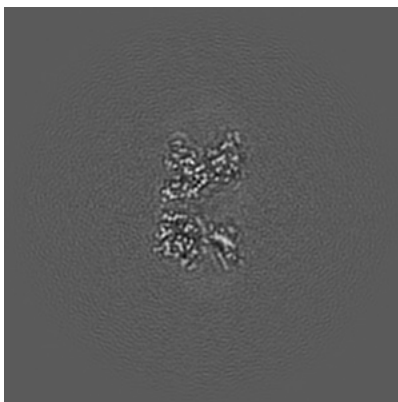
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

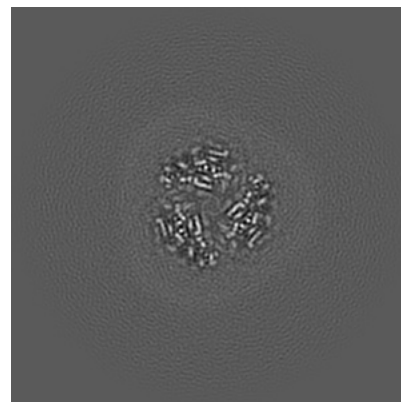
6.2.1 Primary map



X Index: 128

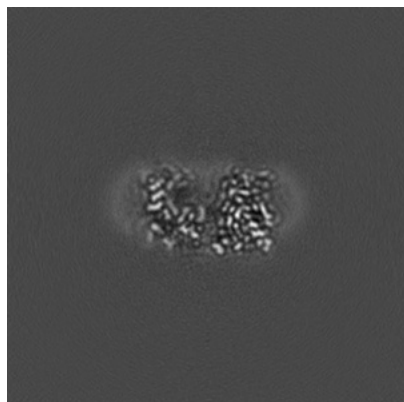


Y Index: 128

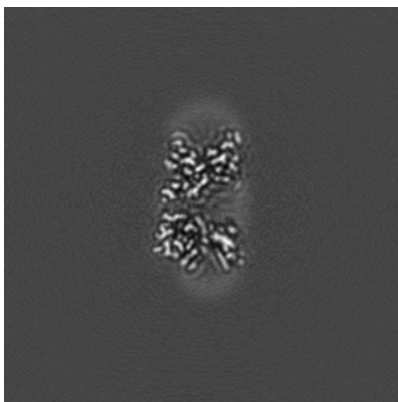


Z Index: 128

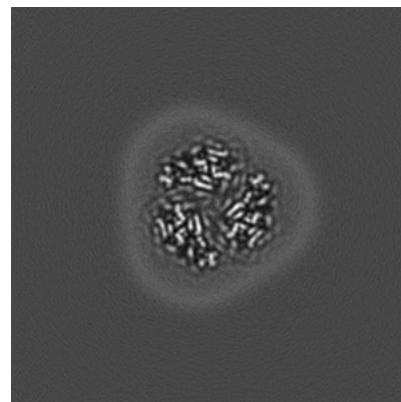
6.2.2 Raw map



X Index: 128



Y Index: 128

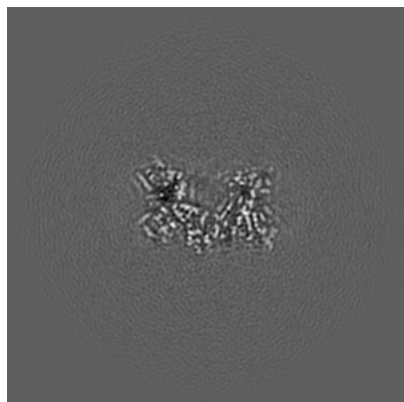


Z Index: 128

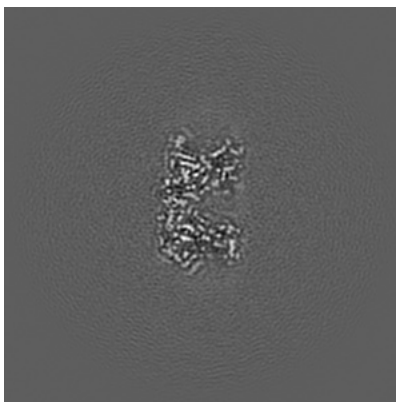
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

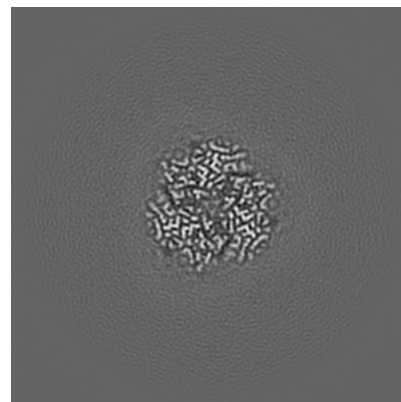
6.3.1 Primary map



X Index: 120

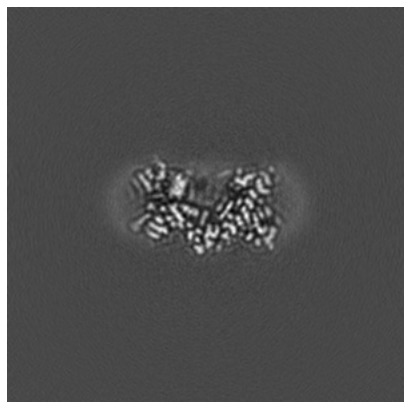


Y Index: 122

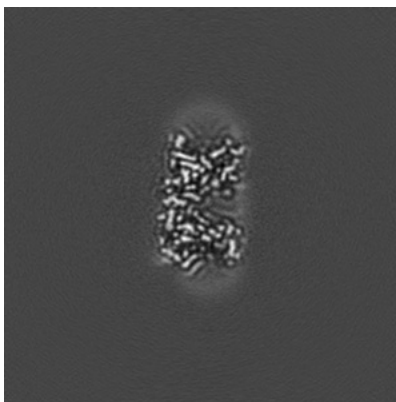


Z Index: 121

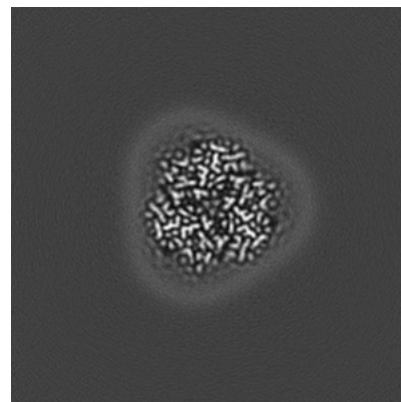
6.3.2 Raw map



X Index: 121



Y Index: 122

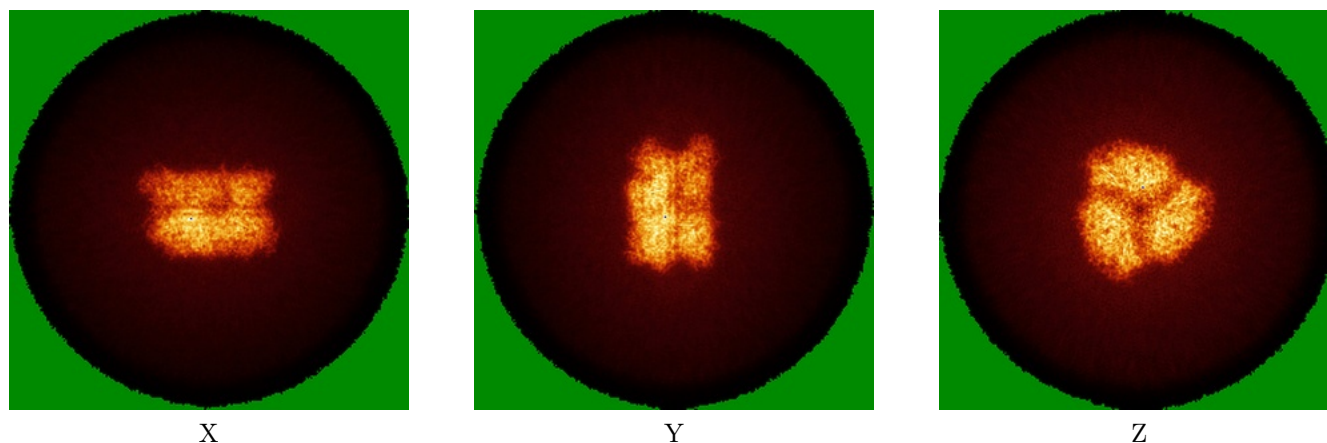


Z Index: 121

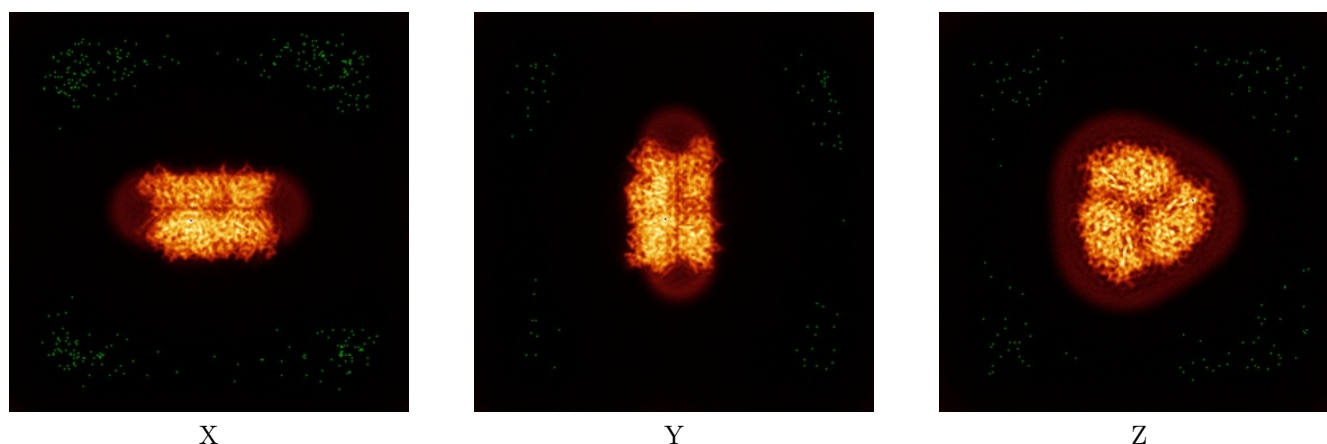
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

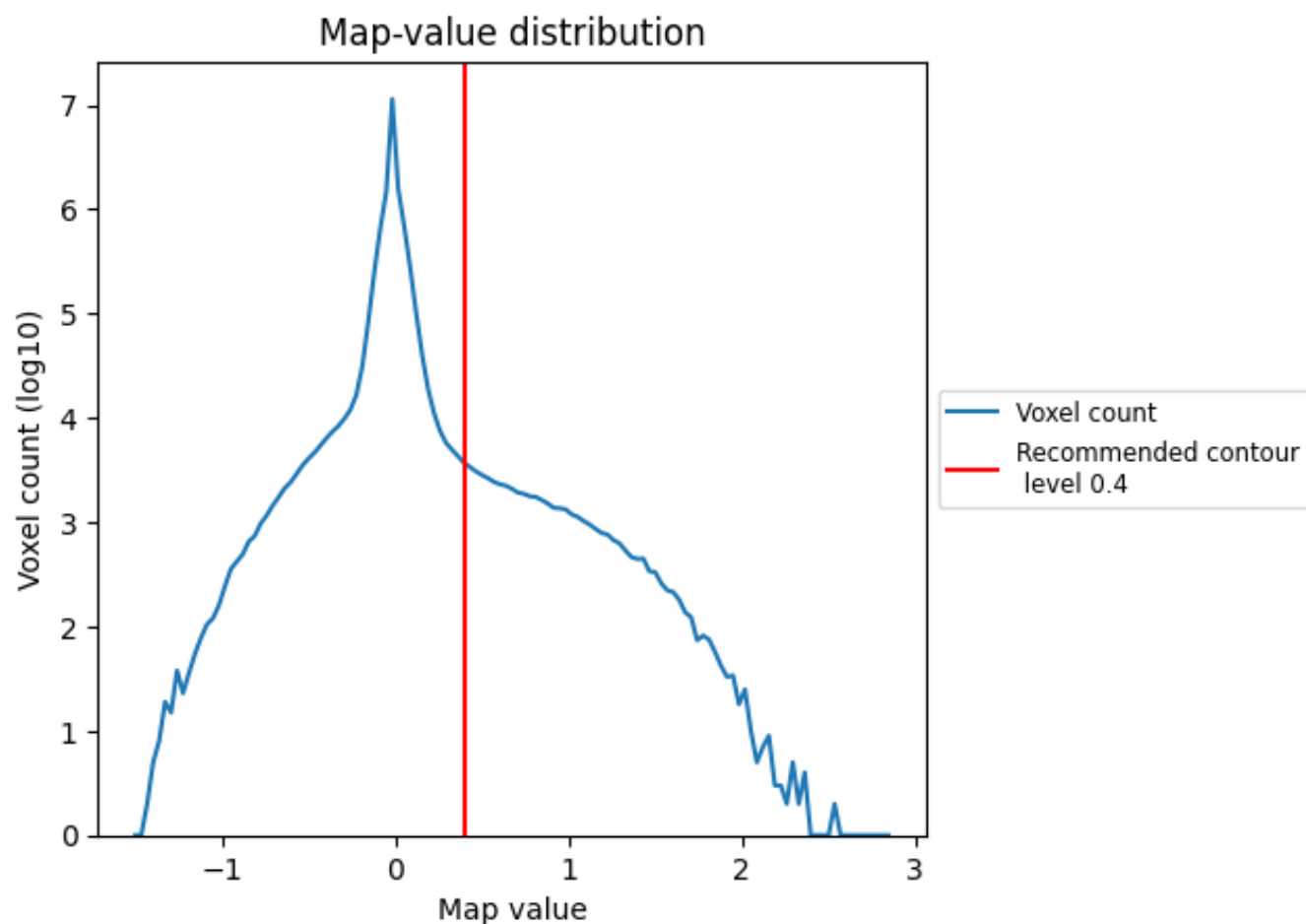
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

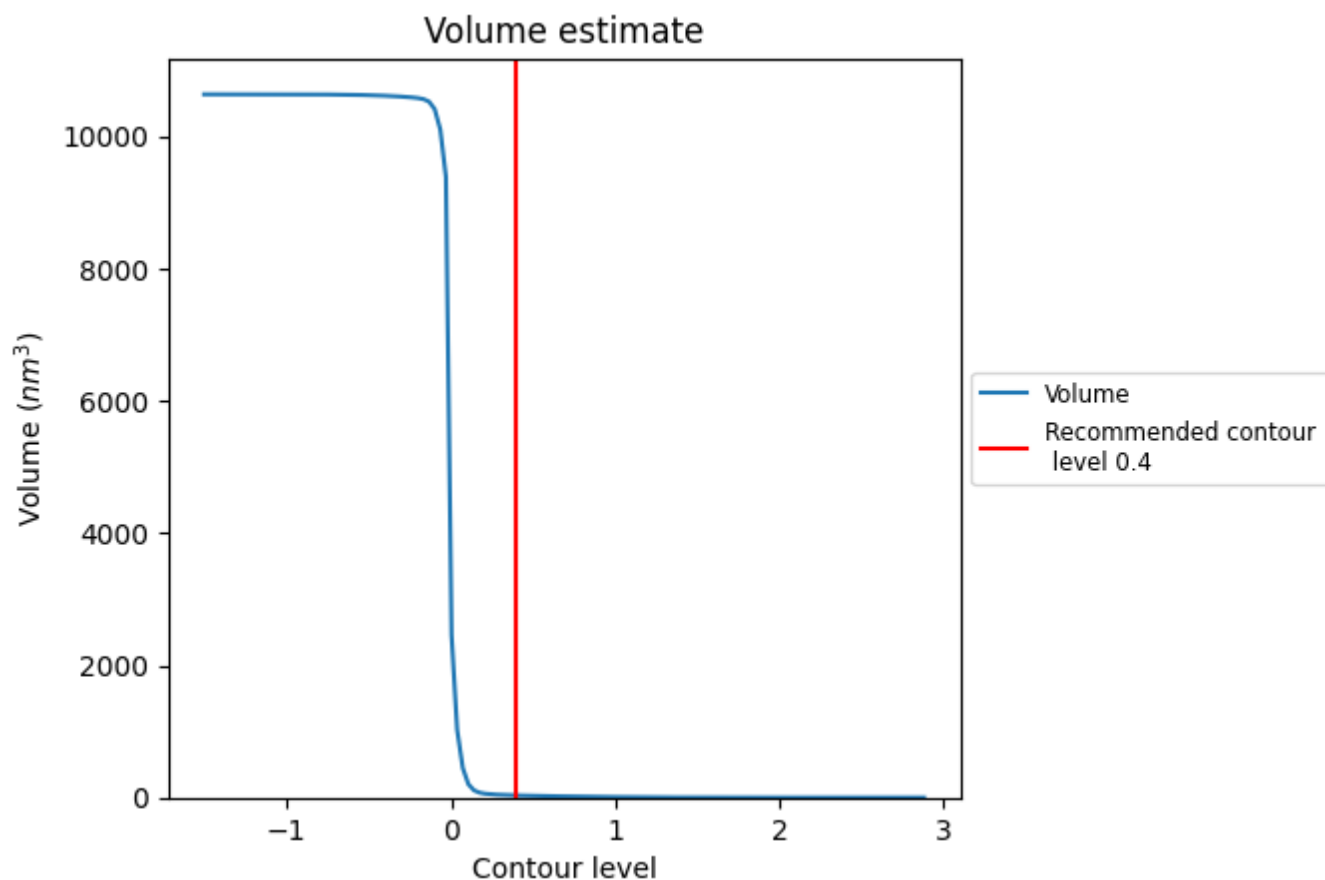
This section contains the results of statistical analysis of the map.

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.

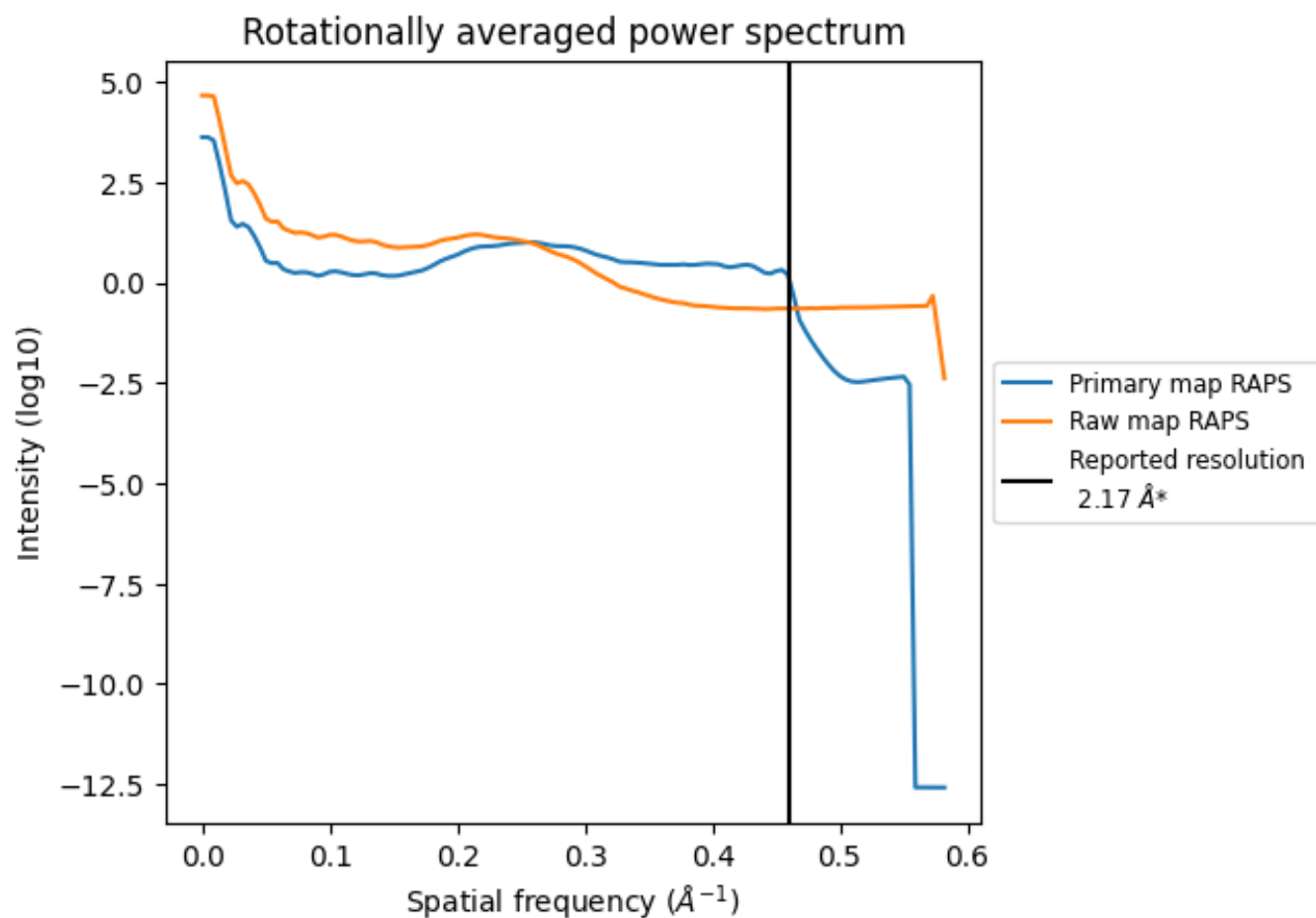
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 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 ⓘ

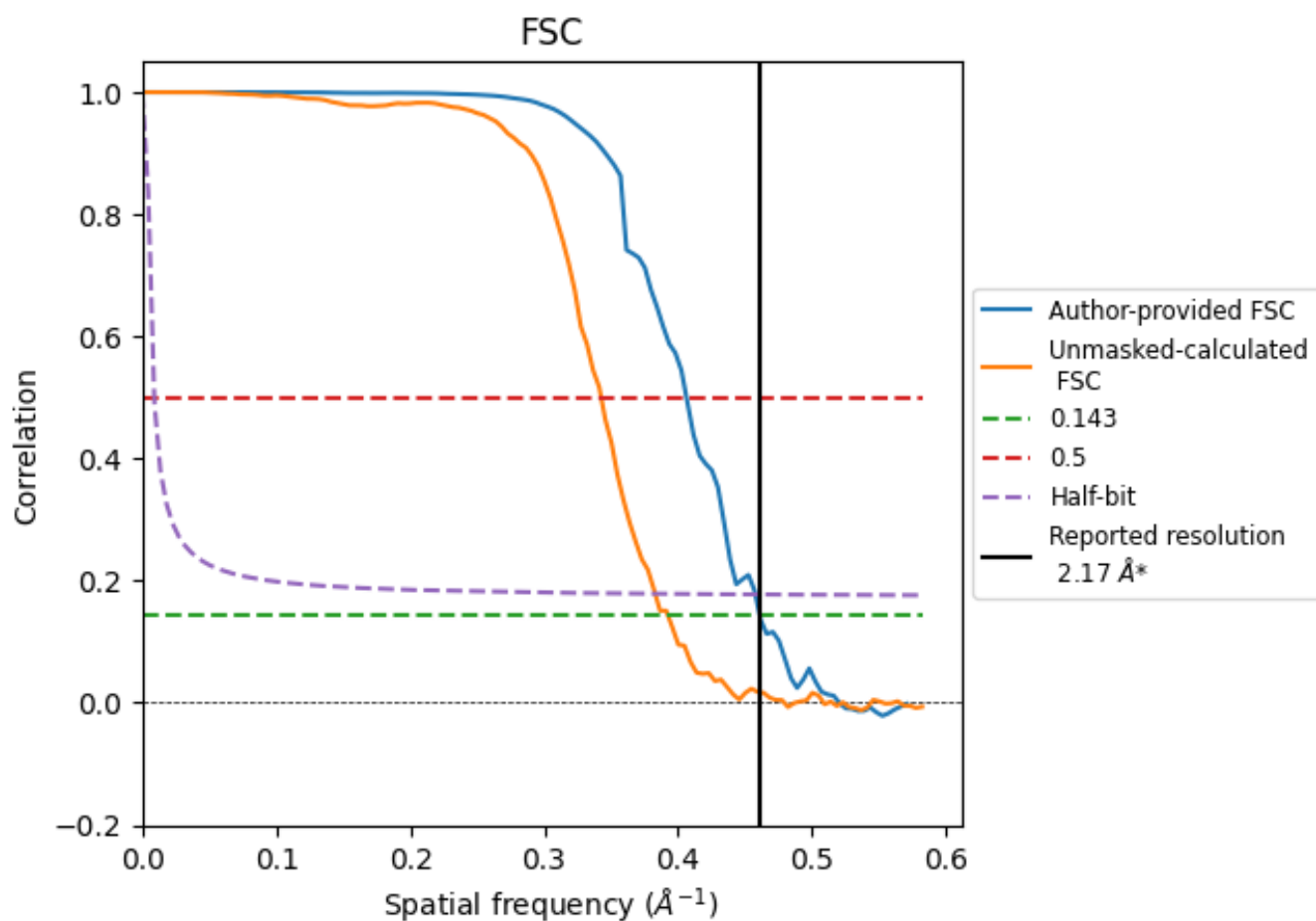


*Reported resolution corresponds to spatial frequency of 0.461 Å⁻¹

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 0.461 Å⁻¹

8.2 Resolution estimates [i](#)

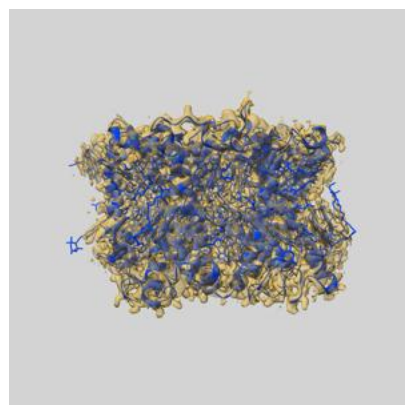
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.17	-	-
Author-provided FSC curve	2.17	2.46	2.19
Unmasked-calculated*	2.55	2.92	2.61

*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 2.55 differs from the reported value 2.17 by more than 10 %

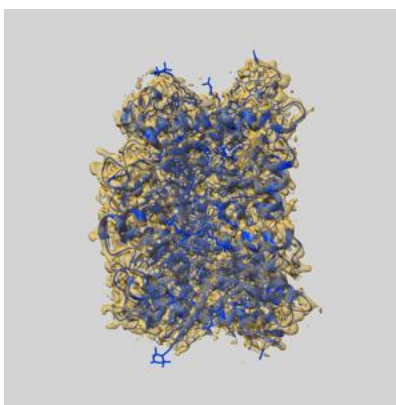
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-38825 and PDB model 8Y15. Per-residue inclusion information can be found in section [3](#) on page [12](#).

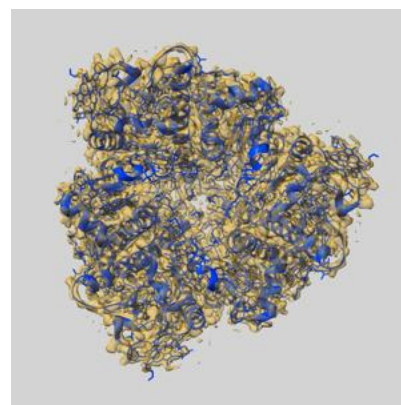
9.1 Map-model overlay [i](#)



X



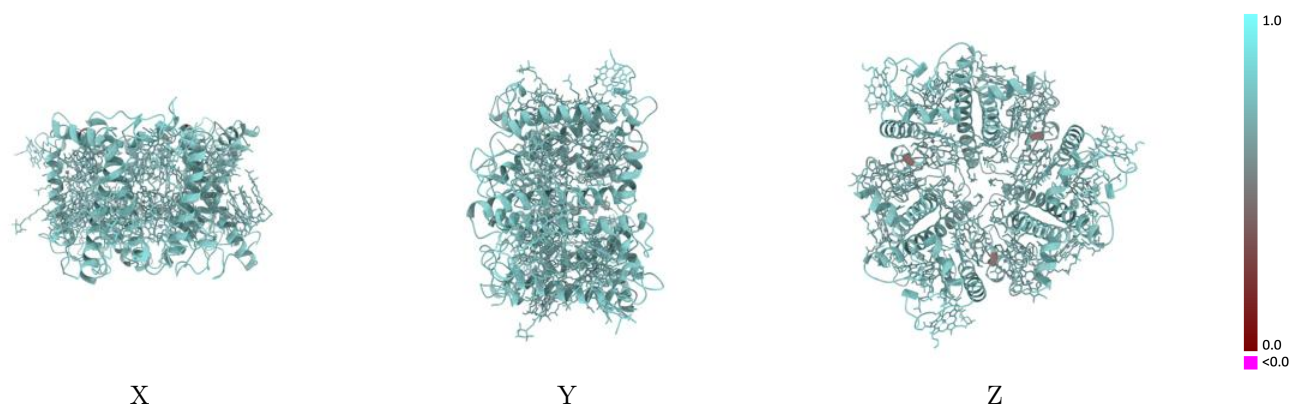
Y



Z

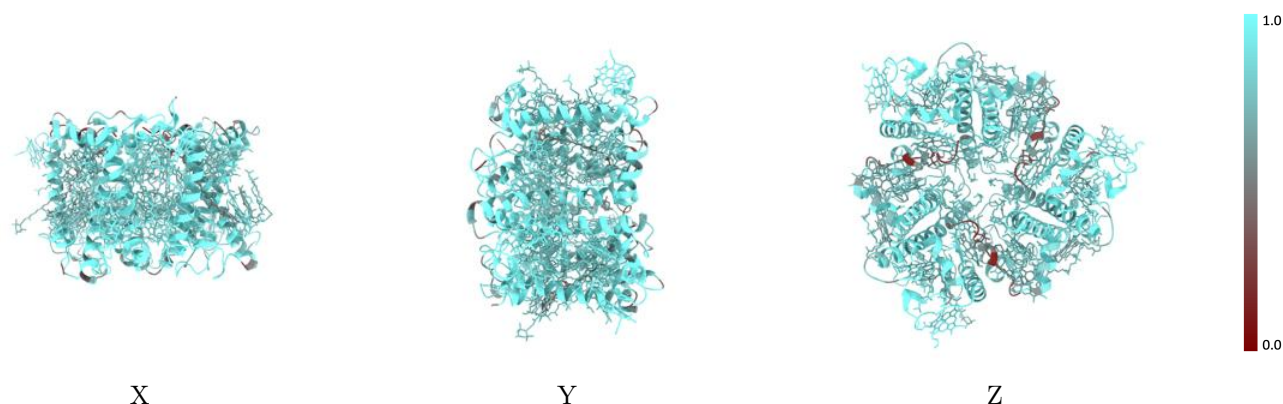
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



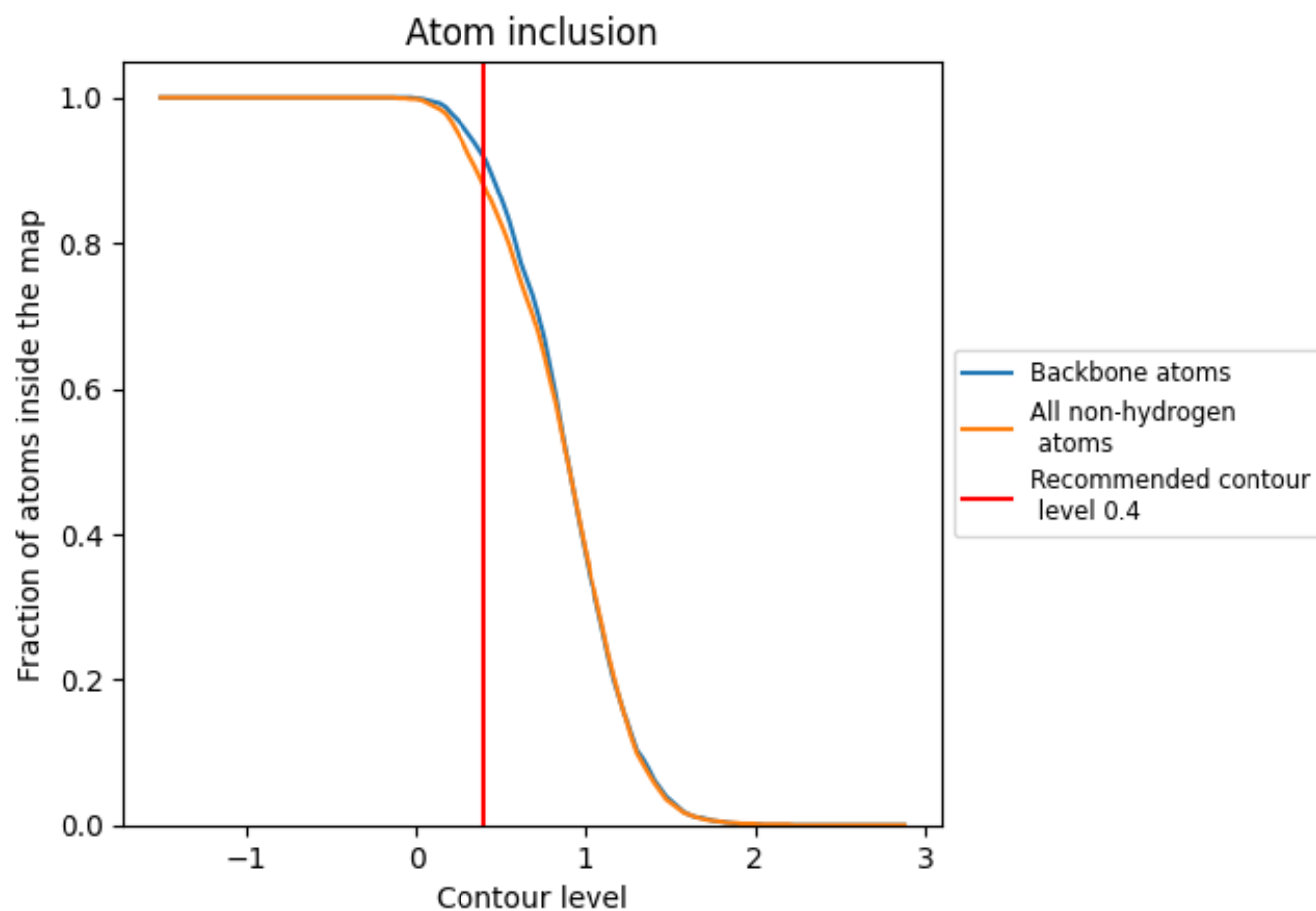
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.4).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 88% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8810	0.7090
A	0.8800	0.7090
B	0.8780	0.7090
C	0.8780	0.7090

