



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 11:00 AM UTC

PDB ID : 8YEE / pdb_00008yee
EMDB ID : EMD-39192
Title : Cryo-EM structure of in vitro reconstituted Light-harvesting complex II trimer
Authors : Seki, S.; Miyata, T.; Tanaka, H.; Namba, K.; Kurisu, G.; Fujii, R.
Deposited on : 2024-02-22
Resolution : 2.37 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:

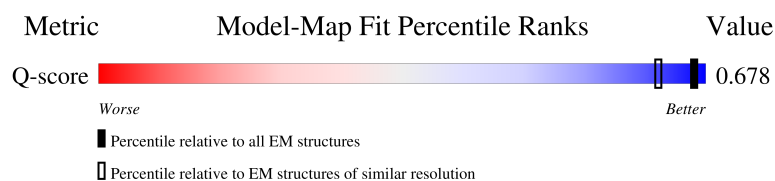
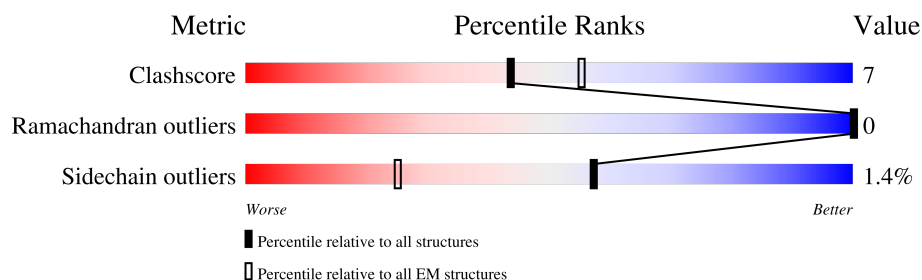
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMD 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 2.37 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	4742 (1.87 - 2.87)

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	225	 80% 12% 7%
1	B	225	 78% 15% 7%
1	C	225	 81% 12% 7%

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	-	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7776 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.

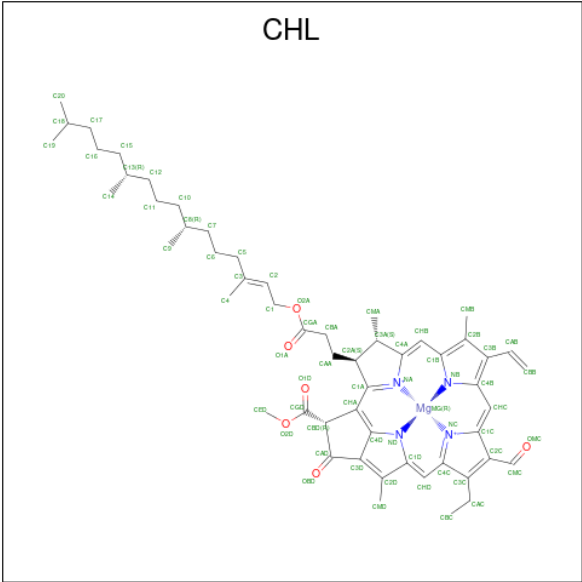
- Molecule 1 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	210	Total	C	N	O	S	0	0
			1601	1038	261	295	7		
1	B	210	Total	C	N	O	S	0	0
			1601	1038	261	295	7		
1	C	210	Total	C	N	O	S	0	0
			1601	1038	261	295	7		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	233	HIS	-	expression tag	UNP P12333
A	234	HIS	-	expression tag	UNP P12333
A	235	HIS	-	expression tag	UNP P12333
A	236	HIS	-	expression tag	UNP P12333
A	237	HIS	-	expression tag	UNP P12333
A	238	HIS	-	expression tag	UNP P12333
B	233	HIS	-	expression tag	UNP P12333
B	234	HIS	-	expression tag	UNP P12333
B	235	HIS	-	expression tag	UNP P12333
B	236	HIS	-	expression tag	UNP P12333
B	237	HIS	-	expression tag	UNP P12333
B	238	HIS	-	expression tag	UNP P12333
C	233	HIS	-	expression tag	UNP P12333
C	234	HIS	-	expression tag	UNP P12333
C	235	HIS	-	expression tag	UNP P12333
C	236	HIS	-	expression tag	UNP P12333
C	237	HIS	-	expression tag	UNP P12333
C	238	HIS	-	expression tag	UNP P12333

- Molecule 2 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



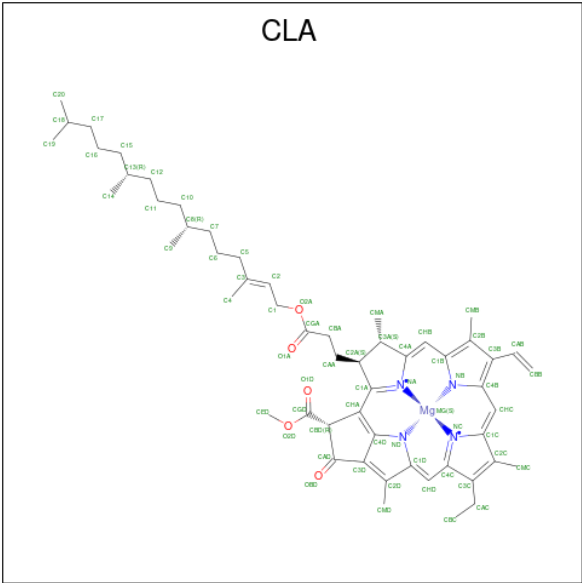
Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
2	A	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
2	A	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
2	A	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
2	A	1	Total	C	Mg	N	O	0
			52	41	1	4	6	
2	A	1	Total	C	Mg	N	O	0
			57	46	1	4	6	
2	B	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
2	B	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
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
			52	41	1	4	6	
2	B	1	Total	C	Mg	N	O	0
			57	46	1	4	6	
2	C	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
2	C	1	Total	C	Mg	N	O	0
			44	35	1	4	4	

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Mol	Chain	Residues	Atoms					AltConf
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
			52	41	1	4	6	
2	C	1	Total	C	Mg	N	O	0
			57	46	1	4	6	

- Molecule 3 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



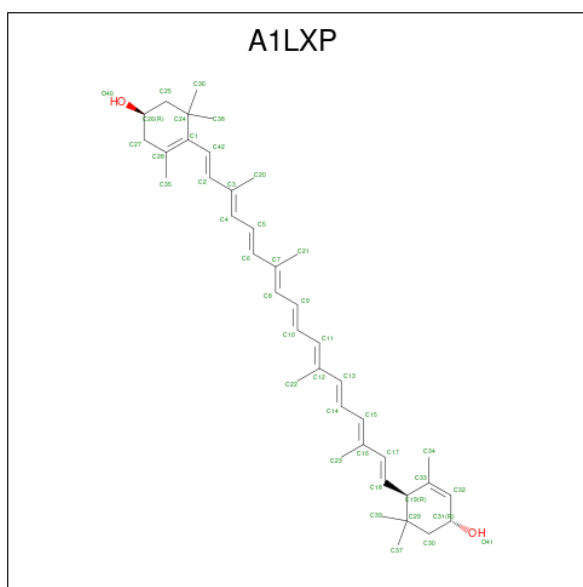
Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
3	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
3	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	A	1	Total	C	Mg	N	O	0
			57	47	1	4	5	

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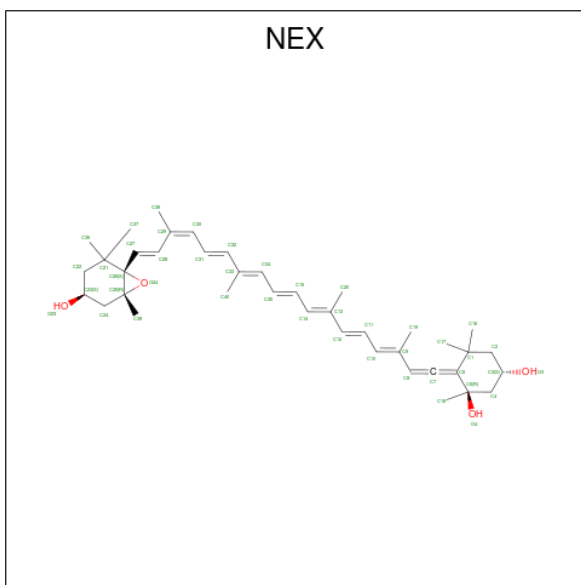
Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
3	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
3	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
3	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	B	1	Total	C	Mg	N	O	0
			57	47	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
			57	47	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).



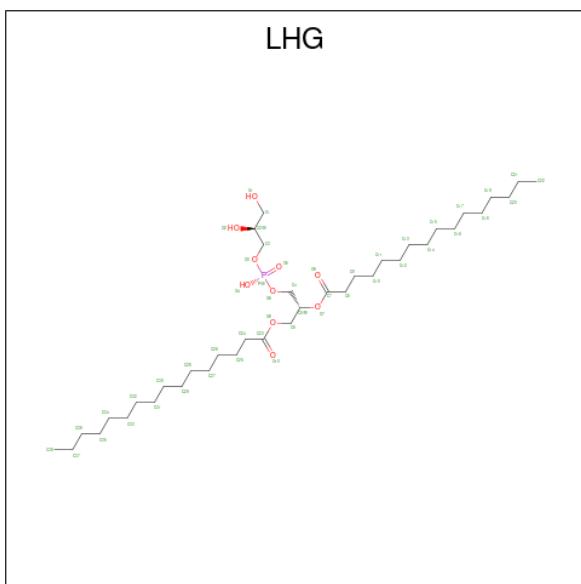
Mol	Chain	Residues	Atoms			AltConf
4	A	1	Total	C	O	0
			42	40	2	
4	A	1	Total	C	O	0
			42	40	2	
4	B	1	Total	C	O	0
			42	40	2	
4	B	1	Total	C	O	0
			42	40	2	
4	C	1	Total	C	O	0
			42	40	2	
4	C	1	Total	C	O	0
			42	40	2	

- 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-TETRAMETHYLOCTA DECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE}-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (CCD ID: NEX) (formula: C₄₀H₅₆O₄).



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

- Molecule 6 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $\text{C}_{38}\text{H}_{75}\text{O}_{10}\text{P}$).



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	

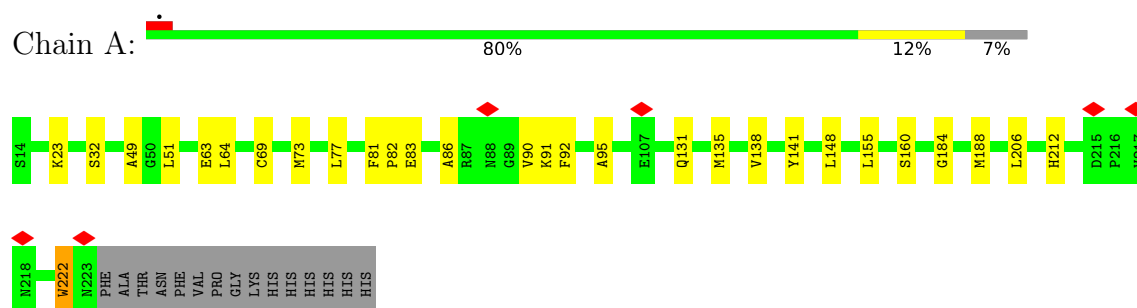
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		AltConf
7	A	43	Total	O	0
			43	43	
7	B	42	Total	O	0
			42	42	
7	C	41	Total	O	0
			41	41	

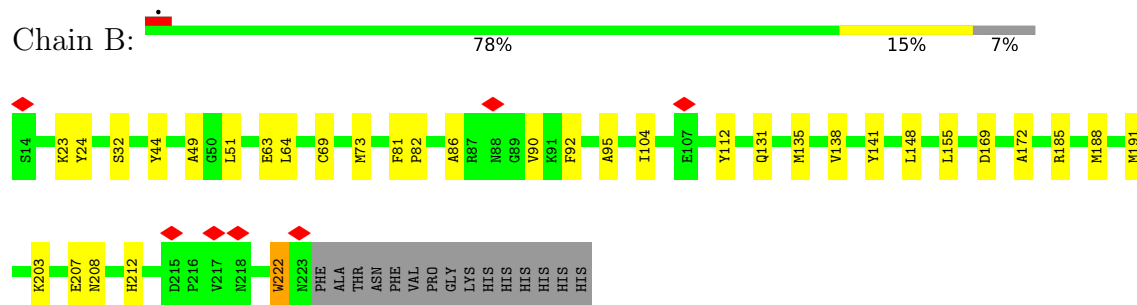
3 Residue-property plots [i](#)

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.

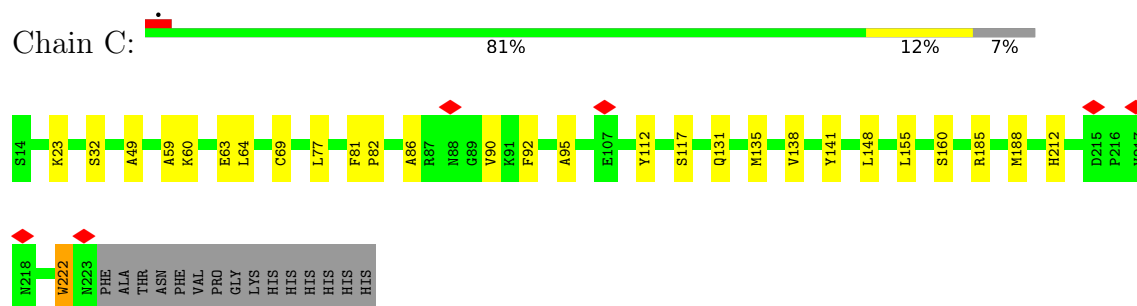
- Molecule 1: Chlorophyll a-b binding protein, chloroplastic



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



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	179318	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	2.652	Depositor
Minimum map value	-1.600	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.066	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	223.488, 223.488, 223.488	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.873, 0.873, 0.873	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, NEX, A1LXP, 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	0.13	0/1650	0.33	0/2246
1	B	0.13	0/1650	0.34	0/2246
1	C	0.13	0/1650	0.33	0/2246
All	All	0.13	0/4950	0.34	0/6738

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	1601	0	1537	21	0
1	B	1601	0	1537	28	0
1	C	1601	0	1537	21	0
2	A	303	0	228	7	0
2	B	303	0	228	7	0
2	C	303	0	228	6	0
3	A	469	0	470	7	0
3	B	469	0	470	9	0
3	C	469	0	470	10	0
4	A	84	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	84	0	0	2	0
4	C	84	0	0	0	0
5	A	44	0	56	2	0
5	B	44	0	56	1	0
5	C	44	0	56	1	0
6	A	49	0	74	4	0
6	B	49	0	74	2	0
6	C	49	0	74	4	0
7	A	43	0	0	0	0
7	B	42	0	0	0	0
7	C	41	0	0	0	0
All	All	7776	0	7095	96	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (96) 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)
3:B:613:CLA:H91	6:B:618:LHG:H321	1.76	0.66
1:A:51:LEU:HD11	3:B:603:CLA:H12	1.77	0.66
3:C:613:CLA:H91	6:C:618:LHG:H321	1.78	0.66
2:B:601:CHL:HED3	6:B:618:LHG:H142	1.81	0.63
2:C:601:CHL:HED3	6:C:618:LHG:H142	1.80	0.63
3:A:613:CLA:H91	6:A:618:LHG:H321	1.80	0.62
2:B:606:CHL:HBD	2:B:606:CHL:HBA2	1.82	0.62
2:A:601:CHL:HED3	6:A:618:LHG:H142	1.81	0.61
2:C:606:CHL:HBA2	2:C:606:CHL:HBD	1.83	0.60
2:A:606:CHL:HBD	2:A:606:CHL:HBA2	1.84	0.59
1:B:185:ARG:HA	1:B:188:MET:HE3	1.83	0.59
1:B:69:CYS:O	1:B:73:MET:HG3	2.02	0.59
1:B:64:LEU:HD13	3:B:603:CLA:HBA1	1.86	0.58
3:B:602:CLA:H93	3:B:603:CLA:HMA1	1.87	0.56
1:A:49:ALA:HA	1:B:64:LEU:HD11	1.88	0.55
1:A:64:LEU:HD11	1:C:49:ALA:HA	1.89	0.55
1:C:59:ALA:O	1:C:63:GLU:HG3	2.07	0.55
1:B:73:MET:HB3	4:B:615:A1LXP:C10	2.37	0.54
1:A:64:LEU:HD13	3:A:603:CLA:HBA1	1.89	0.54
1:C:64:LEU:HD13	3:C:603:CLA:HBA1	1.91	0.53
1:C:148:LEU:HG	2:C:608:CHL:HAB	1.90	0.53
1:B:49:ALA:HA	1:C:64:LEU:HD11	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:GLU:HA	1:B:155:LEU:HD21	1.92	0.51
1:B:135:MET:HA	1:B:138:VAL:HG22	1.91	0.51
1:B:203:LYS:HB2	1:B:208:ASN:HD21	1.76	0.51
1:B:63:GLU:HA	1:B:155:LEU:HD11	1.93	0.51
1:A:135:MET:HA	1:A:138:VAL:HG22	1.92	0.51
1:C:63:GLU:HA	1:C:155:LEU:HD21	1.92	0.51
1:C:222:TRP:HA	1:C:222:TRP:CE3	2.46	0.50
1:A:148:LEU:HG	2:A:608:CHL:HAB	1.92	0.50
1:A:63:GLU:HA	1:A:155:LEU:HD21	1.93	0.50
1:B:222:TRP:HA	1:B:222:TRP:CE3	2.46	0.50
1:C:131:GLN:OE1	2:C:607:CHL:HMC	2.12	0.50
1:C:135:MET:HA	1:C:138:VAL:HG22	1.94	0.50
1:A:63:GLU:HA	1:A:155:LEU:HD11	1.94	0.49
1:A:222:TRP:HA	1:A:222:TRP:CE3	2.46	0.49
1:C:77:LEU:HD21	3:C:612:CLA:H202	1.94	0.49
1:C:63:GLU:HA	1:C:155:LEU:HD11	1.95	0.48
1:A:23:LYS:HE2	1:A:32:SER:HB2	1.95	0.48
1:B:148:LEU:HG	2:B:608:CHL:HAB	1.93	0.48
1:C:23:LYS:HE2	1:C:32:SER:HB2	1.96	0.48
1:A:131:GLN:OE1	2:A:607:CHL:HMC	2.15	0.47
1:B:23:LYS:HE2	1:B:32:SER:HB2	1.96	0.47
1:A:69:CYS:SG	1:A:188:MET:HE2	2.55	0.47
3:A:610:CLA:H62	3:A:612:CLA:H92	1.97	0.46
1:C:69:CYS:SG	1:C:188:MET:HE2	2.56	0.46
1:C:86:ALA:HA	1:C:90:VAL:O	2.16	0.46
3:C:610:CLA:H62	3:C:612:CLA:H92	1.98	0.45
1:B:69:CYS:SG	1:B:188:MET:HE2	2.57	0.45
1:A:81:PHE:HB3	1:A:82:PRO:HD3	1.99	0.45
1:B:51:LEU:HD13	3:B:602:CLA:H42	1.98	0.45
2:C:601:CHL:HBA1	2:C:601:CHL:H3A	1.71	0.45
1:B:81:PHE:HB3	1:B:82:PRO:HD3	1.99	0.45
3:B:610:CLA:H62	3:B:612:CLA:H92	1.98	0.45
1:B:203:LYS:HE2	1:B:207:GLU:OE2	2.17	0.45
1:C:81:PHE:HB3	1:C:82:PRO:HD3	1.98	0.45
3:C:602:CLA:H62	3:C:603:CLA:H3A	1.99	0.45
1:A:184:GLY:O	1:A:188:MET:HG3	2.18	0.44
2:A:601:CHL:H62	2:A:601:CHL:H41	1.79	0.44
1:B:112:TYR:CE1	3:B:604:CLA:H2	2.53	0.44
1:A:69:CYS:O	1:A:73:MET:HG3	2.18	0.44
1:B:51:LEU:HD11	3:C:603:CLA:H12	2.00	0.44
1:A:92:PHE:HB2	1:A:95:ALA:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:ALA:HA	1:B:90:VAL:O	2.18	0.43
1:C:60:LYS:HA	1:C:60:LYS:HD2	1.89	0.43
1:B:212:HIS:CD2	3:B:614:CLA:NC	2.86	0.43
1:C:92:PHE:HB2	1:C:95:ALA:HB2	2.00	0.43
2:A:601:CHL:HMA3	6:A:618:LHG:H121	2.00	0.43
1:B:141:TYR:HE2	5:B:617:NEX:H202	1.84	0.43
1:C:112:TYR:CE1	3:C:604:CLA:H2	2.53	0.43
3:C:602:CLA:H61	3:C:602:CLA:H41	1.64	0.43
1:C:141:TYR:HE2	5:C:617:NEX:H202	1.84	0.42
2:A:601:CHL:HBA1	2:A:601:CHL:H3A	1.69	0.42
1:B:131:GLN:OE1	2:B:607:CHL:HMC	2.18	0.42
1:A:141:TYR:HE2	5:A:617:NEX:H202	1.83	0.42
6:A:618:LHG:H282	6:A:618:LHG:HC82	2.02	0.42
3:C:604:CLA:HBD	3:C:604:CLA:HBA1	2.01	0.42
1:A:86:ALA:HA	1:A:90:VAL:O	2.19	0.42
1:A:83:GLU:HB3	1:A:206:LEU:HD12	2.02	0.42
1:B:92:PHE:HB2	1:B:95:ALA:HB2	2.02	0.42
1:C:212:HIS:CD2	3:C:614:CLA:NC	2.87	0.42
3:A:604:CLA:C1C	5:A:617:NEX:H222	2.50	0.42
1:A:77:LEU:HD21	3:A:612:CLA:H202	2.02	0.42
3:B:604:CLA:HBD	3:B:604:CLA:HBA1	2.01	0.41
2:B:601:CHL:HBA1	2:B:601:CHL:H3A	1.73	0.41
6:C:618:LHG:H282	6:C:618:LHG:HC82	2.03	0.41
1:A:212:HIS:CD2	3:A:614:CLA:NC	2.88	0.41
2:C:601:CHL:HMA3	6:C:618:LHG:H121	2.02	0.41
1:B:104:ILE:HD12	1:B:104:ILE:HA	1.89	0.41
1:C:185:ARG:HA	1:C:188:MET:HE3	2.03	0.41
1:B:24:TYR:HB3	1:B:44:TYR:HB3	2.02	0.41
1:B:169:ASP:HB3	1:B:172:ALA:HB3	2.03	0.41
1:B:191:MET:HE2	4:B:616:A1LXP:C4	2.51	0.40
2:B:601:CHL:H62	2:B:601:CHL:H41	1.82	0.40
3:A:604:CLA:HBD	3:A:604:CLA:HBA1	2.03	0.40
2:B:606:CHL:HMB1	2:B:609:CHL:HMC	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	208/225 (92%)	207 (100%)	1 (0%)	0	100	100
1	B	208/225 (92%)	207 (100%)	1 (0%)	0	100	100
1	C	208/225 (92%)	207 (100%)	1 (0%)	0	100	100
All	All	624/675 (92%)	621 (100%)	3 (0%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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	162/175 (93%)	159 (98%)	3 (2%)	50	69
1	B	162/175 (93%)	161 (99%)	1 (1%)	78	88
1	C	162/175 (93%)	159 (98%)	3 (2%)	50	69
All	All	486/525 (93%)	479 (99%)	7 (1%)	57	77

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	91	LYS
1	A	160	SER
1	A	222	TRP
1	B	222	TRP
1	C	117	SER

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Mol	Chain	Res	Type
1	C	160	SER
1	C	222	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

54 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	$\# Z > 2$
2	CHL	B	609	1	51,65,74	1.51	4 (7%)	47,103,114	1.96	7 (14%)
4	A1LXP	B	616	-	42,43,43	0.48	1 (2%)	51,60,60	0.29	0
3	CLA	B	611	6	69,73,73	1.66	8 (11%)	82,113,113	1.13	9 (10%)
5	NEX	C	617	-	40,46,46	1.34	3 (7%)	50,70,70	0.55	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	CHL	B	608	7	46,60,74	1.57	4 (8%)	40,97,114	2.12	6 (15%)
3	CLA	B	610	1	69,73,73	1.66	9 (13%)	82,113,113	1.05	9 (10%)
6	LHG	C	618	3	48,48,48	0.23	0	51,54,54	0.30	0
2	CHL	B	606	7	45,59,74	1.58	4 (8%)	40,96,114	2.21	7 (17%)
3	CLA	B	612	1	69,73,73	1.63	8 (11%)	82,113,113	1.09	9 (10%)
4	A1LXP	C	615	-	42,43,43	0.42	1 (2%)	51,60,60	0.30	0
3	CLA	A	612	1	69,73,73	1.64	8 (11%)	82,113,113	1.09	9 (10%)
3	CLA	B	614	1	46,50,73	2.02	9 (19%)	53,85,113	1.29	8 (15%)
5	NEX	A	617	-	40,46,46	1.20	3 (7%)	50,70,70	0.55	1 (2%)
5	NEX	B	617	-	40,46,46	1.48	4 (10%)	50,70,70	0.54	1 (2%)
3	CLA	A	613	1	61,65,73	1.75	9 (14%)	72,103,113	1.12	9 (12%)
6	LHG	B	618	3	48,48,48	0.23	0	51,54,54	0.29	0
3	CLA	C	612	1	69,73,73	1.63	8 (11%)	82,113,113	1.09	9 (10%)
2	CHL	B	607	7	40,54,74	1.70	4 (10%)	34,90,114	2.37	7 (20%)
3	CLA	C	610	1	69,73,73	1.66	9 (13%)	82,113,113	1.05	9 (10%)
3	CLA	A	603	1	59,63,73	1.78	9 (15%)	70,101,113	1.20	9 (12%)
2	CHL	C	606	7	45,59,74	1.59	4 (8%)	40,96,114	2.19	7 (17%)
3	CLA	B	603	1	59,63,73	1.77	8 (13%)	70,101,113	1.20	9 (12%)
3	CLA	B	613	1	61,65,73	1.75	9 (14%)	72,103,113	1.12	9 (12%)
3	CLA	A	602	1	69,73,73	1.65	9 (13%)	82,113,113	1.04	9 (10%)
6	LHG	A	618	3	48,48,48	0.23	0	51,54,54	0.29	0
2	CHL	A	601	1	47,61,74	1.56	4 (8%)	41,98,114	2.21	6 (14%)
2	CHL	C	607	7	40,54,74	1.71	4 (10%)	34,90,114	2.38	6 (17%)
3	CLA	A	614	1	46,50,73	2.02	9 (19%)	53,85,113	1.29	8 (15%)
3	CLA	C	614	1	46,50,73	2.02	9 (19%)	53,85,113	1.29	8 (15%)
2	CHL	A	609	1	51,65,74	1.51	4 (7%)	47,103,114	1.95	6 (12%)
3	CLA	A	610	1	69,73,73	1.66	9 (13%)	82,113,113	1.05	9 (10%)
4	A1LXP	A	616	-	42,43,43	0.46	1 (2%)	51,60,60	0.29	0
2	CHL	A	606	7	45,59,74	1.60	4 (8%)	40,96,114	2.20	7 (17%)
2	CHL	B	605	1	38,52,74	1.74	4 (10%)	31,87,114	2.41	6 (19%)
3	CLA	C	613	1	61,65,73	1.75	9 (14%)	72,103,113	1.12	9 (12%)
2	CHL	C	601	1	47,61,74	1.55	4 (8%)	41,98,114	2.18	6 (14%)
3	CLA	B	602	1	69,73,73	1.65	9 (13%)	82,113,113	1.06	9 (10%)
3	CLA	C	603	1	59,63,73	1.77	8 (13%)	70,101,113	1.19	9 (12%)
3	CLA	C	604	7	59,63,73	1.82	8 (13%)	70,101,113	1.26	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	CLA	C	611	6	69,73,73	1.67	8 (11%)	82,113,113	1.13	10 (12%)
2	CHL	C	605	1	38,52,74	1.75	4 (10%)	31,87,114	2.40	6 (19%)
4	A1LXP	C	616	-	42,43,43	0.45	1 (2%)	51,60,60	0.28	0
3	CLA	C	602	1	69,73,73	1.65	9 (13%)	82,113,113	1.04	9 (10%)
2	CHL	A	608	7	46,60,74	1.57	4 (8%)	40,97,114	2.13	6 (15%)
4	A1LXP	A	615	-	42,43,43	0.42	1 (2%)	51,60,60	0.30	0
2	CHL	C	609	1	51,65,74	1.50	4 (7%)	47,103,114	1.96	7 (14%)
2	CHL	A	607	7	40,54,74	1.70	4 (10%)	34,90,114	2.37	6 (17%)
3	CLA	A	611	6	69,73,73	1.66	8 (11%)	82,113,113	1.13	10 (12%)
2	CHL	C	608	7	46,60,74	1.59	4 (8%)	40,97,114	2.13	7 (17%)
3	CLA	B	604	7	59,63,73	1.82	8 (13%)	70,101,113	1.26	7 (10%)
4	A1LXP	B	615	-	42,43,43	0.42	1 (2%)	51,60,60	0.31	0
2	CHL	B	601	1	47,61,74	1.56	4 (8%)	41,98,114	2.19	6 (14%)
3	CLA	A	604	7	59,63,73	1.82	8 (13%)	70,101,113	1.27	7 (10%)
2	CHL	A	605	1	38,52,74	1.76	4 (10%)	31,87,114	2.40	6 (19%)

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
2	CHL	B	609	1	4/4/18/26	6/29/127/137	-
4	A1LXP	B	616	-	-	2/29/67/67	0/2/2/2
3	CLA	B	611	6	2/2/15/20	5/39/115/115	-
5	NEX	C	617	-	-	2/27/83/83	0/3/3/3
2	CHL	B	608	7	3/3/17/26	6/23/121/137	-
3	CLA	B	610	1	2/2/15/20	4/39/115/115	-
6	LHG	C	618	3	-	13/53/53/53	-
2	CHL	B	606	7	3/3/17/26	4/21/119/137	-
3	CLA	B	612	1	2/2/15/20	9/39/115/115	-
4	A1LXP	C	615	-	-	2/29/67/67	0/2/2/2
3	CLA	A	612	1	2/2/15/20	9/39/115/115	-
3	CLA	B	614	1	1/1/10/20	2/12/88/115	-
5	NEX	A	617	-	-	2/27/83/83	0/3/3/3
5	NEX	B	617	-	-	2/27/83/83	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CLA	A	613	1	2/2/13/20	5/30/106/115	-
6	LHG	B	618	3	-	12/53/53/53	-
3	CLA	C	612	1	2/2/15/20	9/39/115/115	-
2	CHL	B	607	7	3/3/16/26	5/15/113/137	-
3	CLA	C	610	1	2/2/15/20	4/39/115/115	-
3	CLA	A	603	1	2/2/13/20	7/27/103/115	-
2	CHL	C	606	7	3/3/17/26	3/21/119/137	-
3	CLA	B	603	1	2/2/13/20	5/27/103/115	-
3	CLA	B	613	1	2/2/13/20	5/30/106/115	-
3	CLA	A	602	1	2/2/15/20	7/39/115/115	-
6	LHG	A	618	3	-	12/53/53/53	-
2	CHL	A	601	1	3/3/17/26	6/24/122/137	-
2	CHL	C	607	7	3/3/16/26	5/15/113/137	-
3	CLA	A	614	1	1/1/10/20	2/12/88/115	-
3	CLA	C	614	1	1/1/10/20	2/12/88/115	-
2	CHL	A	609	1	4/4/18/26	4/29/127/137	-
3	CLA	A	610	1	2/2/15/20	4/39/115/115	-
4	A1LXP	A	616	-	-	2/29/67/67	0/2/2/2
2	CHL	A	606	7	3/3/17/26	2/21/119/137	-
2	CHL	B	605	1	3/3/15/26	2/13/111/137	-
3	CLA	C	613	1	2/2/13/20	5/30/106/115	-
2	CHL	C	601	1	3/3/17/26	7/24/122/137	-
3	CLA	B	602	1	2/2/15/20	6/39/115/115	-
3	CLA	C	603	1	2/2/13/20	5/27/103/115	-
3	CLA	C	604	7	2/2/13/20	4/27/103/115	-
3	CLA	C	611	6	2/2/15/20	5/39/115/115	-
2	CHL	C	605	1	3/3/15/26	2/13/111/137	-
4	A1LXP	C	616	-	-	2/29/67/67	0/2/2/2
3	CLA	C	602	1	2/2/15/20	7/39/115/115	-
2	CHL	A	608	7	3/3/17/26	3/23/121/137	-
4	A1LXP	A	615	-	-	2/29/67/67	0/2/2/2
2	CHL	C	609	1	4/4/18/26	6/29/127/137	-
2	CHL	A	607	7	3/3/16/26	4/15/113/137	-
3	CLA	A	611	6	2/2/15/20	5/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CHL	C	608	7	3/3/17/26	6/23/121/137	-
3	CLA	B	604	7	2/2/13/20	4/27/103/115	-
4	A1LXP	B	615	-	-	2/29/67/67	0/2/2/2
2	CHL	B	601	1	3/3/17/26	6/24/122/137	-
3	CLA	A	604	7	2/2/13/20	4/27/103/115	-
2	CHL	A	605	1	3/3/15/26	2/13/111/137	-

All (293) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	614	CLA	C4B-NB	8.03	1.48	1.37
3	C	614	CLA	C4B-NB	8.02	1.48	1.37
3	B	614	CLA	C4B-NB	7.99	1.48	1.37
3	A	603	CLA	C4B-NB	7.98	1.48	1.37
3	B	612	CLA	C4B-NB	7.95	1.48	1.37
3	A	612	CLA	C4B-NB	7.93	1.48	1.37
3	B	613	CLA	C4B-NB	7.92	1.48	1.37
3	C	603	CLA	C4B-NB	7.92	1.48	1.37
3	C	613	CLA	C4B-NB	7.91	1.48	1.37
3	B	603	CLA	C4B-NB	7.89	1.48	1.37
3	B	602	CLA	C4B-NB	7.88	1.48	1.37
3	A	613	CLA	C4B-NB	7.87	1.48	1.37
3	A	602	CLA	C4B-NB	7.86	1.48	1.37
3	C	612	CLA	C4B-NB	7.86	1.48	1.37
3	C	610	CLA	C4B-NB	7.86	1.48	1.37
3	A	604	CLA	C4B-NB	7.85	1.48	1.37
3	C	611	CLA	C4B-NB	7.83	1.48	1.37
3	B	604	CLA	C4B-NB	7.82	1.48	1.37
3	B	611	CLA	C4B-NB	7.81	1.48	1.37
3	C	602	CLA	C4B-NB	7.80	1.48	1.37
3	C	604	CLA	C4B-NB	7.78	1.48	1.37
3	A	610	CLA	C4B-NB	7.73	1.48	1.37
3	B	610	CLA	C4B-NB	7.72	1.48	1.37
3	A	611	CLA	C4B-NB	7.71	1.48	1.37
2	A	605	CHL	C1B-C2B	7.66	1.48	1.39
2	C	605	CHL	C1B-C2B	7.63	1.48	1.39
2	B	605	CHL	C1B-C2B	7.60	1.48	1.39
2	B	601	CHL	C1B-C2B	7.58	1.48	1.39
2	C	607	CHL	C1B-C2B	7.57	1.48	1.39
2	A	607	CHL	C1B-C2B	7.56	1.48	1.39
2	C	601	CHL	C1B-C2B	7.55	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	CHL	C1B-C2B	7.51	1.48	1.39
2	B	607	CHL	C1B-C2B	7.51	1.48	1.39
2	A	606	CHL	C1B-C2B	7.48	1.48	1.39
2	C	606	CHL	C1B-C2B	7.44	1.48	1.39
2	B	609	CHL	C1B-C2B	7.43	1.48	1.39
2	A	609	CHL	C1B-C2B	7.41	1.48	1.39
2	C	609	CHL	C1B-C2B	7.40	1.48	1.39
2	C	608	CHL	C1B-C2B	7.37	1.47	1.39
2	B	606	CHL	C1B-C2B	7.36	1.47	1.39
2	B	608	CHL	C1B-C2B	7.30	1.47	1.39
2	A	608	CHL	C1B-C2B	7.27	1.47	1.39
5	B	617	NEX	C40-C33	-6.69	1.37	1.50
3	C	604	CLA	MG-NB	-5.26	1.95	2.05
5	C	617	NEX	C40-C33	-5.23	1.40	1.50
3	A	604	CLA	MG-NB	-5.22	1.95	2.05
3	B	604	CLA	MG-NB	-5.19	1.95	2.05
3	B	610	CLA	MG-NB	-5.12	1.95	2.05
3	A	610	CLA	MG-NB	-5.11	1.95	2.05
3	B	611	CLA	MG-NB	-5.08	1.95	2.05
3	C	610	CLA	MG-NB	-5.07	1.95	2.05
3	A	602	CLA	MG-NB	-5.07	1.95	2.05
3	A	611	CLA	MG-NB	-5.05	1.95	2.05
3	B	604	CLA	MG-ND	-5.05	1.95	2.05
3	B	602	CLA	MG-NB	-5.05	1.95	2.05
3	C	604	CLA	MG-ND	-5.05	1.95	2.05
3	C	611	CLA	MG-NB	-5.05	1.95	2.05
3	A	604	CLA	MG-ND	-5.04	1.95	2.05
3	C	602	CLA	MG-NB	-5.03	1.95	2.05
3	A	610	CLA	MG-ND	-5.03	1.95	2.05
3	C	610	CLA	MG-ND	-5.02	1.95	2.05
3	B	610	CLA	MG-ND	-5.00	1.95	2.05
3	B	614	CLA	MG-NB	-4.97	1.95	2.05
3	A	613	CLA	MG-NB	-4.97	1.95	2.05
3	C	614	CLA	MG-NB	-4.96	1.96	2.05
3	B	613	CLA	MG-NB	-4.95	1.96	2.05
3	A	611	CLA	MG-ND	-4.94	1.96	2.05
3	C	613	CLA	MG-NB	-4.94	1.96	2.05
3	A	602	CLA	MG-ND	-4.92	1.96	2.05
3	C	611	CLA	MG-ND	-4.92	1.96	2.05
3	A	614	CLA	MG-NB	-4.92	1.96	2.05
5	C	617	NEX	C34-C33	-4.91	1.24	1.35
3	C	602	CLA	MG-ND	-4.89	1.96	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	611	CLA	MG-ND	-4.87	1.96	2.05
3	B	602	CLA	MG-ND	-4.86	1.96	2.05
5	B	617	NEX	C34-C33	-4.82	1.24	1.35
3	B	603	CLA	MG-NB	-4.79	1.96	2.05
3	C	613	CLA	MG-ND	-4.79	1.96	2.05
3	A	613	CLA	MG-ND	-4.78	1.96	2.05
3	B	613	CLA	MG-ND	-4.77	1.96	2.05
3	A	612	CLA	MG-NB	-4.76	1.96	2.05
3	B	614	CLA	MG-ND	-4.76	1.96	2.05
3	C	603	CLA	MG-NB	-4.75	1.96	2.05
3	C	612	CLA	MG-NB	-4.74	1.96	2.05
3	C	614	CLA	MG-ND	-4.74	1.96	2.05
3	A	614	CLA	MG-ND	-4.72	1.96	2.05
3	A	603	CLA	MG-NB	-4.70	1.96	2.05
5	A	617	NEX	C34-C33	-4.69	1.24	1.35
3	C	612	CLA	MG-ND	-4.68	1.96	2.05
3	B	612	CLA	MG-NB	-4.67	1.96	2.05
3	A	603	CLA	MG-ND	-4.65	1.96	2.05
3	A	612	CLA	MG-ND	-4.65	1.96	2.05
3	C	603	CLA	MG-ND	-4.65	1.96	2.05
3	B	612	CLA	MG-ND	-4.65	1.96	2.05
3	B	603	CLA	MG-ND	-4.64	1.96	2.05
5	A	617	NEX	C40-C33	-4.48	1.41	1.50
3	A	604	CLA	MG-NA	-4.39	1.95	2.06
3	B	604	CLA	MG-NA	-4.35	1.95	2.06
3	C	604	CLA	MG-NA	-4.35	1.95	2.06
3	B	610	CLA	MG-NA	-4.25	1.96	2.06
3	C	611	CLA	MG-NA	-4.25	1.96	2.06
3	B	611	CLA	MG-NA	-4.24	1.96	2.06
3	A	611	CLA	MG-NA	-4.22	1.96	2.06
3	A	610	CLA	MG-NA	-4.20	1.96	2.06
3	C	610	CLA	MG-NA	-4.14	1.96	2.06
3	B	602	CLA	MG-NA	-3.96	1.96	2.06
3	A	602	CLA	MG-NA	-3.95	1.96	2.06
3	C	602	CLA	MG-NA	-3.91	1.97	2.06
3	A	613	CLA	MG-NA	-3.91	1.97	2.06
3	C	613	CLA	MG-NA	-3.90	1.97	2.06
3	B	613	CLA	MG-NA	-3.89	1.97	2.06
2	A	606	CHL	C3B-C4B	3.86	1.45	1.41
2	A	601	CHL	C3B-C4B	3.85	1.45	1.41
3	A	612	CLA	C1D-ND	3.85	1.42	1.37
2	A	605	CHL	C3B-C4B	3.84	1.45	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	606	CHL	C3B-C4B	3.84	1.45	1.41
3	B	604	CLA	MG-NC	-3.84	1.97	2.06
2	B	601	CHL	C3B-C4B	3.84	1.45	1.41
2	B	605	CHL	C3B-C4B	3.83	1.45	1.41
3	A	603	CLA	C1D-ND	3.83	1.42	1.37
3	B	612	CLA	C1D-ND	3.83	1.42	1.37
3	A	604	CLA	MG-NC	-3.83	1.97	2.06
2	C	605	CHL	C3B-C4B	3.83	1.45	1.41
2	B	606	CHL	C3B-C4B	3.82	1.45	1.41
2	C	608	CHL	C3B-C4B	3.81	1.45	1.41
3	A	614	CLA	MG-NA	-3.80	1.97	2.06
3	C	603	CLA	C1D-ND	3.79	1.42	1.37
3	C	604	CLA	MG-NC	-3.79	1.97	2.06
3	B	603	CLA	C1D-ND	3.78	1.42	1.37
3	A	603	CLA	MG-NA	-3.78	1.97	2.06
3	C	612	CLA	C1D-ND	3.78	1.42	1.37
3	B	603	CLA	MG-NA	-3.78	1.97	2.06
2	A	609	CHL	C3B-C4B	3.77	1.45	1.41
2	A	608	CHL	C3B-C4B	3.77	1.45	1.41
2	C	609	CHL	C3B-C4B	3.77	1.45	1.41
3	C	614	CLA	MG-NA	-3.76	1.97	2.06
3	C	603	CLA	MG-NA	-3.76	1.97	2.06
2	C	607	CHL	C3B-C4B	3.75	1.45	1.41
2	B	609	CHL	C3B-C4B	3.75	1.45	1.41
3	B	614	CLA	MG-NA	-3.74	1.97	2.06
2	C	601	CHL	C3B-C4B	3.73	1.45	1.41
2	B	608	CHL	C3B-C4B	3.73	1.45	1.41
2	B	607	CHL	C3B-C4B	3.71	1.45	1.41
3	A	614	CLA	C1D-ND	3.71	1.42	1.37
3	B	614	CLA	C1D-ND	3.70	1.42	1.37
3	A	610	CLA	MG-NC	-3.70	1.97	2.06
3	C	614	CLA	C1D-ND	3.68	1.42	1.37
2	A	607	CHL	C3B-C4B	3.67	1.45	1.41
3	B	612	CLA	MG-NA	-3.67	1.97	2.06
3	C	610	CLA	MG-NC	-3.67	1.97	2.06
3	A	613	CLA	C1D-ND	3.67	1.42	1.37
3	B	610	CLA	MG-NC	-3.66	1.97	2.06
3	C	612	CLA	MG-NA	-3.66	1.97	2.06
3	B	613	CLA	C1D-ND	3.66	1.42	1.37
3	A	612	CLA	MG-NA	-3.65	1.97	2.06
3	A	611	CLA	MG-NC	-3.62	1.97	2.06
3	C	611	CLA	MG-NC	-3.62	1.97	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	611	CLA	MG-NC	-3.59	1.97	2.06
3	C	613	CLA	C1D-ND	3.58	1.42	1.37
2	B	609	CHL	C1A-CHA	-3.58	1.35	1.40
3	B	604	CLA	C1D-ND	3.57	1.42	1.37
3	C	602	CLA	C1D-ND	3.57	1.42	1.37
2	A	609	CHL	C1A-CHA	-3.54	1.36	1.40
3	C	614	CLA	MG-NC	-3.52	1.97	2.06
3	A	603	CLA	MG-NC	-3.52	1.97	2.06
2	C	609	CHL	C1A-CHA	-3.51	1.36	1.40
3	B	602	CLA	C1D-ND	3.51	1.42	1.37
3	A	602	CLA	C1D-ND	3.51	1.42	1.37
3	C	603	CLA	MG-NC	-3.51	1.97	2.06
3	C	604	CLA	C1D-ND	3.50	1.42	1.37
2	B	605	CHL	C1A-CHA	-3.49	1.36	1.40
3	B	614	CLA	MG-NC	-3.49	1.98	2.06
2	A	608	CHL	C1A-CHA	-3.48	1.36	1.40
2	B	607	CHL	C1A-CHA	-3.47	1.36	1.40
2	B	608	CHL	C1A-CHA	-3.47	1.36	1.40
3	B	603	CLA	MG-NC	-3.47	1.98	2.06
2	C	605	CHL	C1A-CHA	-3.46	1.36	1.40
3	C	611	CLA	C1D-ND	3.46	1.42	1.37
3	A	614	CLA	MG-NC	-3.45	1.98	2.06
3	B	602	CLA	MG-NC	-3.45	1.98	2.06
2	A	607	CHL	C1A-CHA	-3.44	1.36	1.40
2	C	608	CHL	C1A-CHA	-3.44	1.36	1.40
3	C	610	CLA	C1D-ND	3.44	1.42	1.37
3	C	602	CLA	MG-NC	-3.44	1.98	2.06
2	A	605	CHL	C1A-CHA	-3.44	1.36	1.40
3	A	611	CLA	C1D-ND	3.44	1.42	1.37
2	A	601	CHL	C1A-CHA	-3.43	1.36	1.40
2	C	607	CHL	C1A-CHA	-3.43	1.36	1.40
3	A	604	CLA	C1D-ND	3.43	1.42	1.37
3	B	610	CLA	C1D-ND	3.43	1.42	1.37
2	C	601	CHL	C1A-CHA	-3.41	1.36	1.40
2	B	601	CHL	C1A-CHA	-3.41	1.36	1.40
3	B	611	CLA	C1D-ND	3.40	1.42	1.37
3	A	610	CLA	C1D-ND	3.40	1.42	1.37
2	B	606	CHL	C1A-CHA	-3.39	1.36	1.40
3	C	613	CLA	MG-NC	-3.39	1.98	2.06
3	B	613	CLA	MG-NC	-3.38	1.98	2.06
3	A	602	CLA	MG-NC	-3.37	1.98	2.06
3	A	613	CLA	MG-NC	-3.36	1.98	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	612	CLA	MG-NC	-3.35	1.98	2.06
2	C	606	CHL	C1A-CHA	-3.34	1.36	1.40
2	A	606	CHL	C1A-CHA	-3.34	1.36	1.40
3	B	612	CLA	MG-NC	-3.33	1.98	2.06
3	C	612	CLA	MG-NC	-3.33	1.98	2.06
5	B	617	NEX	C39-C29	-3.31	1.44	1.50
5	C	617	NEX	C39-C29	-3.25	1.44	1.50
3	C	611	CLA	C1B-NB	3.21	1.42	1.37
3	B	614	CLA	C1B-NB	3.17	1.42	1.37
3	B	611	CLA	C1B-NB	3.16	1.42	1.37
3	C	602	CLA	C1B-NB	3.14	1.42	1.37
3	B	602	CLA	C1B-NB	3.12	1.42	1.37
3	A	611	CLA	C1B-NB	3.12	1.42	1.37
3	A	614	CLA	C1B-NB	3.12	1.42	1.37
3	A	602	CLA	C1B-NB	3.11	1.41	1.37
3	C	614	CLA	C1B-NB	3.07	1.41	1.37
3	B	613	CLA	C1B-NB	3.07	1.41	1.37
3	B	603	CLA	C1B-NB	3.06	1.41	1.37
3	A	612	CLA	C1B-NB	3.06	1.41	1.37
3	A	613	CLA	C1B-NB	3.06	1.41	1.37
5	A	617	NEX	C39-C29	-3.05	1.44	1.50
3	C	613	CLA	C1B-NB	3.04	1.41	1.37
3	B	612	CLA	C1B-NB	3.03	1.41	1.37
3	A	603	CLA	C1B-NB	3.02	1.41	1.37
3	C	612	CLA	C1B-NB	3.01	1.41	1.37
3	C	604	CLA	C1B-NB	2.99	1.41	1.37
3	B	604	CLA	C1B-NB	2.99	1.41	1.37
3	C	603	CLA	C1B-NB	2.99	1.41	1.37
3	B	610	CLA	C1B-NB	2.97	1.41	1.37
3	A	604	CLA	C1B-NB	2.94	1.41	1.37
3	A	610	CLA	C1B-NB	2.94	1.41	1.37
3	C	610	CLA	C1B-NB	2.92	1.41	1.37
4	B	616	A1LXP	C30-C31	-2.66	1.49	1.52
4	A	616	A1LXP	C30-C31	-2.53	1.49	1.52
4	C	616	A1LXP	C30-C31	-2.47	1.49	1.52
2	B	608	CHL	C3B-C2B	-2.36	1.37	1.40
3	C	612	CLA	C1D-C2D	-2.36	1.40	1.45
3	B	612	CLA	C1D-C2D	-2.35	1.40	1.45
3	A	612	CLA	C1D-C2D	-2.34	1.40	1.45
3	B	614	CLA	C1D-C2D	-2.34	1.40	1.45
3	C	602	CLA	C1D-C2D	-2.34	1.40	1.45
3	A	610	CLA	C1D-C2D	-2.33	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	603	CLA	C1D-C2D	-2.32	1.40	1.45
3	C	603	CLA	C1D-C2D	-2.32	1.40	1.45
3	B	613	CLA	C1D-C2D	-2.32	1.40	1.45
3	C	614	CLA	C1D-C2D	-2.32	1.40	1.45
3	A	613	CLA	C1D-C2D	-2.32	1.40	1.45
2	A	607	CHL	C3B-C2B	-2.32	1.37	1.40
2	C	607	CHL	C3B-C2B	-2.31	1.37	1.40
2	C	601	CHL	C3B-C2B	-2.31	1.37	1.40
2	A	605	CHL	C3B-C2B	-2.31	1.37	1.40
3	A	614	CLA	C1D-C2D	-2.31	1.40	1.45
3	C	610	CLA	C1D-C2D	-2.31	1.40	1.45
2	B	601	CHL	C3B-C2B	-2.31	1.37	1.40
3	B	610	CLA	C1D-C2D	-2.30	1.40	1.45
2	B	605	CHL	C3B-C2B	-2.30	1.37	1.40
3	C	613	CLA	C1D-C2D	-2.29	1.40	1.45
3	A	604	CLA	C1D-C2D	-2.29	1.40	1.45
3	B	602	CLA	C1D-C2D	-2.29	1.40	1.45
2	A	601	CHL	C3B-C2B	-2.28	1.37	1.40
3	B	604	CLA	C1D-C2D	-2.28	1.40	1.45
3	B	611	CLA	C1D-C2D	-2.28	1.40	1.45
2	C	605	CHL	C3B-C2B	-2.28	1.37	1.40
3	A	603	CLA	C1D-C2D	-2.27	1.40	1.45
3	A	602	CLA	C1D-C2D	-2.27	1.40	1.45
3	A	611	CLA	C1D-C2D	-2.27	1.40	1.45
3	C	611	CLA	C1D-C2D	-2.26	1.40	1.45
3	C	604	CLA	C1D-C2D	-2.26	1.40	1.45
2	C	608	CHL	C3B-C2B	-2.25	1.37	1.40
2	A	608	CHL	C3B-C2B	-2.25	1.37	1.40
2	A	609	CHL	C3B-C2B	-2.24	1.37	1.40
2	B	607	CHL	C3B-C2B	-2.24	1.37	1.40
2	A	606	CHL	C3B-C2B	-2.22	1.37	1.40
4	B	615	A1LXP	C30-C31	-2.20	1.50	1.52
2	B	606	CHL	C3B-C2B	-2.20	1.37	1.40
4	A	615	A1LXP	C30-C31	-2.19	1.50	1.52
4	C	615	A1LXP	C30-C31	-2.19	1.50	1.52
2	C	606	CHL	C3B-C2B	-2.19	1.37	1.40
2	B	609	CHL	C3B-C2B	-2.18	1.37	1.40
2	C	609	CHL	C3B-C2B	-2.16	1.37	1.40
3	A	602	CLA	C1C-C2C	2.05	1.48	1.44
5	B	617	NEX	C32-C33	-2.05	1.41	1.46
3	A	614	CLA	C1C-C2C	2.04	1.48	1.44
3	C	614	CLA	C1C-C2C	2.03	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	602	CLA	C1C-C2C	2.02	1.48	1.44
3	A	613	CLA	C1C-C2C	2.02	1.48	1.44
3	B	602	CLA	C1C-C2C	2.02	1.48	1.44
3	A	610	CLA	C1C-C2C	2.01	1.48	1.44
3	C	613	CLA	C1C-C2C	2.01	1.48	1.44
3	B	614	CLA	C1C-C2C	2.01	1.48	1.44
3	B	610	CLA	C1C-C2C	2.00	1.48	1.44
3	B	613	CLA	C1C-C2C	2.00	1.48	1.44
3	C	610	CLA	C1C-C2C	2.00	1.48	1.44
3	A	603	CLA	C3D-C4D	-2.00	1.39	1.44

All (327) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	CHL	C1B-CHB-C4A	11.31	128.60	121.32
2	B	601	CHL	C1B-CHB-C4A	11.20	128.53	121.32
2	C	601	CHL	C1B-CHB-C4A	11.09	128.46	121.32
2	C	607	CHL	C1B-CHB-C4A	11.00	128.40	121.32
2	A	607	CHL	C1B-CHB-C4A	10.97	128.38	121.32
2	B	607	CHL	C1B-CHB-C4A	10.93	128.35	121.32
2	B	606	CHL	C1B-CHB-C4A	10.77	128.25	121.32
2	A	606	CHL	C1B-CHB-C4A	10.75	128.24	121.32
2	C	606	CHL	C1B-CHB-C4A	10.68	128.19	121.32
2	B	609	CHL	C1B-CHB-C4A	10.55	128.11	121.32
2	B	605	CHL	C1B-CHB-C4A	10.52	128.09	121.32
2	C	605	CHL	C1B-CHB-C4A	10.48	128.07	121.32
2	C	609	CHL	C1B-CHB-C4A	10.48	128.06	121.32
2	A	605	CHL	C1B-CHB-C4A	10.48	128.06	121.32
2	A	608	CHL	C1B-CHB-C4A	10.47	128.06	121.32
2	A	609	CHL	C1B-CHB-C4A	10.46	128.05	121.32
2	C	608	CHL	C1B-CHB-C4A	10.41	128.02	121.32
2	B	608	CHL	C1B-CHB-C4A	10.30	127.95	121.32
3	A	604	CLA	C4A-NA-C1A	-6.38	103.77	106.68
3	C	604	CLA	C4A-NA-C1A	-6.31	103.80	106.68
3	B	604	CLA	C4A-NA-C1A	-6.28	103.81	106.68
3	C	611	CLA	C4A-NA-C1A	-5.31	104.26	106.68
3	A	611	CLA	C4A-NA-C1A	-5.28	104.27	106.68
3	B	611	CLA	C4A-NA-C1A	-5.28	104.27	106.68
3	A	603	CLA	C4A-NA-C1A	-5.13	104.34	106.68
3	C	603	CLA	C4A-NA-C1A	-5.01	104.39	106.68
3	B	603	CLA	C4A-NA-C1A	-5.00	104.40	106.68
3	C	610	CLA	C4A-NA-C1A	-4.81	104.48	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	610	CLA	C4A-NA-C1A	-4.78	104.50	106.68
3	B	610	CLA	C4A-NA-C1A	-4.76	104.51	106.68
3	B	612	CLA	C4A-NA-C1A	-4.76	104.51	106.68
3	C	612	CLA	C4A-NA-C1A	-4.76	104.51	106.68
3	B	614	CLA	C4A-NA-C1A	-4.72	104.53	106.68
3	C	614	CLA	C4A-NA-C1A	-4.71	104.53	106.68
3	A	612	CLA	C4A-NA-C1A	-4.70	104.54	106.68
3	A	614	CLA	C4A-NA-C1A	-4.62	104.57	106.68
3	C	602	CLA	C4A-NA-C1A	-4.34	104.70	106.68
3	A	602	CLA	C4A-NA-C1A	-4.34	104.70	106.68
3	B	602	CLA	C4A-NA-C1A	-4.24	104.74	106.68
3	C	613	CLA	C4A-NA-C1A	-4.21	104.76	106.68
3	A	613	CLA	C4A-NA-C1A	-4.10	104.81	106.68
3	B	613	CLA	C4A-NA-C1A	-4.06	104.83	106.68
2	B	606	CHL	C3D-C4D-CHA	3.75	114.25	108.54
2	C	606	CHL	C3D-C4D-CHA	3.74	114.23	108.54
2	A	606	CHL	C3D-C4D-CHA	3.72	114.20	108.54
2	B	607	CHL	C3D-C4D-CHA	3.69	114.14	108.54
2	C	607	CHL	C3D-C4D-CHA	3.68	114.14	108.54
2	A	607	CHL	C3D-C4D-CHA	3.67	114.12	108.54
2	B	606	CHL	C1A-CHA-C4D	3.66	125.10	118.98
2	C	601	CHL	C1A-CHA-C4D	3.66	125.09	118.98
2	C	605	CHL	C1A-CHA-C4D	3.66	125.09	118.98
2	B	608	CHL	C3D-C4D-CHA	3.66	114.10	108.54
2	C	608	CHL	C3D-C4D-CHA	3.66	114.10	108.54
2	A	601	CHL	C3D-C4D-CHA	3.65	114.09	108.54
2	B	605	CHL	C3D-C4D-CHA	3.65	114.09	108.54
2	A	601	CHL	C1A-CHA-C4D	3.65	125.07	118.98
2	A	605	CHL	C3D-C4D-CHA	3.65	114.09	108.54
2	C	606	CHL	C1A-CHA-C4D	3.65	125.06	118.98
2	C	601	CHL	C3D-C4D-CHA	3.64	114.08	108.54
2	A	605	CHL	C1A-CHA-C4D	3.64	125.05	118.98
2	C	605	CHL	C3D-C4D-CHA	3.62	114.05	108.54
2	B	601	CHL	C1A-CHA-C4D	3.62	125.02	118.98
2	C	609	CHL	C3D-C4D-CHA	3.62	114.04	108.54
2	B	605	CHL	C1A-CHA-C4D	3.62	125.02	118.98
2	C	608	CHL	C1A-CHA-C4D	3.62	125.02	118.98
2	B	601	CHL	C3D-C4D-CHA	3.61	114.03	108.54
2	A	606	CHL	C1A-CHA-C4D	3.61	125.00	118.98
2	C	607	CHL	C1A-CHA-C4D	3.61	125.00	118.98
2	A	608	CHL	C3D-C4D-CHA	3.61	114.02	108.54
2	B	608	CHL	C1A-CHA-C4D	3.60	124.99	118.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	607	CHL	C1A-CHA-C4D	3.59	124.97	118.98
2	B	609	CHL	C3D-C4D-CHA	3.59	114.00	108.54
2	A	608	CHL	C1A-CHA-C4D	3.57	124.94	118.98
2	A	609	CHL	C3D-C4D-CHA	3.57	113.97	108.54
2	B	607	CHL	C1A-CHA-C4D	3.56	124.93	118.98
2	C	609	CHL	C1A-CHA-C4D	3.55	124.91	118.98
2	B	609	CHL	C1A-CHA-C4D	3.53	124.87	118.98
2	A	609	CHL	C1A-CHA-C4D	3.52	124.86	118.98
3	B	602	CLA	C1-C2-C3	-3.44	120.56	126.20
3	B	612	CLA	C1D-ND-C4D	-3.19	104.07	106.31
3	A	611	CLA	CAA-C2A-C1A	-3.19	101.51	111.97
3	A	603	CLA	C1D-ND-C4D	-3.18	104.08	106.31
3	C	603	CLA	C1D-ND-C4D	-3.18	104.08	106.31
3	C	612	CLA	C1D-ND-C4D	-3.16	104.09	106.31
3	B	603	CLA	C1D-ND-C4D	-3.14	104.11	106.31
3	B	611	CLA	CAA-C2A-C1A	-3.14	101.70	111.97
3	A	612	CLA	C1D-ND-C4D	-3.11	104.13	106.31
3	C	611	CLA	CAA-C2A-C1A	-3.10	101.80	111.97
3	B	613	CLA	C1D-ND-C4D	-3.09	104.14	106.31
3	A	611	CLA	C1D-ND-C4D	-3.08	104.15	106.31
3	B	611	CLA	C1D-ND-C4D	-3.04	104.18	106.31
2	B	606	CHL	C4D-CHA-CBD	-3.02	105.92	108.97
3	B	614	CLA	C1D-ND-C4D	-3.02	104.19	106.31
3	A	613	CLA	C1D-ND-C4D	-3.01	104.20	106.31
3	C	613	CLA	C1D-ND-C4D	-3.01	104.20	106.31
3	C	611	CLA	C1D-ND-C4D	-3.00	104.21	106.31
3	A	614	CLA	C1D-ND-C4D	-2.99	104.22	106.31
2	C	606	CHL	C4D-CHA-CBD	-2.99	105.96	108.97
3	C	602	CLA	C1D-ND-C4D	-2.97	104.23	106.31
3	C	614	CLA	C1D-ND-C4D	-2.95	104.24	106.31
3	B	602	CLA	C1D-ND-C4D	-2.94	104.25	106.31
2	A	606	CHL	C4D-CHA-CBD	-2.94	106.00	108.97
3	A	602	CLA	C1D-ND-C4D	-2.90	104.28	106.31
3	A	613	CLA	C1-C2-C3	-2.85	121.53	126.20
3	C	613	CLA	C1-C2-C3	-2.85	121.53	126.20
3	B	613	CLA	C1-C2-C3	-2.83	121.57	126.20
3	B	603	CLA	C1-C2-C3	-2.82	121.58	126.20
3	A	610	CLA	C1D-ND-C4D	-2.82	104.33	106.31
3	C	610	CLA	C1D-ND-C4D	-2.82	104.33	106.31
3	B	610	CLA	C1D-ND-C4D	-2.81	104.34	106.31
3	A	611	CLA	CHD-C1D-ND	-2.77	120.91	124.80
3	B	612	CLA	C1-C2-C3	-2.76	121.67	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	611	CLA	CHD-C1D-ND	-2.76	120.92	124.80
3	B	611	CLA	CHD-C1D-ND	-2.74	120.95	124.80
3	B	610	CLA	CHD-C1D-ND	-2.74	120.95	124.80
3	A	612	CLA	C1-C2-C3	-2.74	121.71	126.20
3	B	604	CLA	C1D-ND-C4D	-2.73	104.39	106.31
2	C	607	CHL	C4C-CHD-C1D	2.73	125.83	116.07
2	C	608	CHL	C4D-CHA-CBD	-2.73	106.22	108.97
3	B	604	CLA	CHD-C1D-ND	-2.73	120.97	124.80
2	B	607	CHL	C4C-CHD-C1D	2.72	125.82	116.07
2	A	609	CHL	C4C-CHD-C1D	2.72	125.79	116.07
3	A	610	CLA	CHD-C1D-ND	-2.72	120.98	124.80
2	B	609	CHL	C4C-CHD-C1D	2.71	125.78	116.07
3	A	604	CLA	CHD-C1D-ND	-2.71	120.98	124.80
2	C	609	CHL	C4C-CHD-C1D	2.71	125.77	116.07
2	C	601	CHL	C4C-CHD-C1D	2.71	125.76	116.07
3	C	612	CLA	C1-C2-C3	-2.71	121.76	126.20
2	A	607	CHL	C4C-CHD-C1D	2.70	125.74	116.07
2	C	606	CHL	C4C-CHD-C1D	2.70	125.74	116.07
2	A	601	CHL	C4C-CHD-C1D	2.70	125.73	116.07
3	C	602	CLA	CHD-C1D-ND	-2.70	121.01	124.80
2	B	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	A	603	CLA	CHD-C1D-ND	-2.69	121.02	124.80
3	C	603	CLA	CHD-C1D-ND	-2.69	121.02	124.80
3	C	610	CLA	CHD-C1D-ND	-2.69	121.02	124.80
2	B	601	CHL	C4C-CHD-C1D	2.68	125.67	116.07
2	C	608	CHL	C4C-CHD-C1D	2.68	125.65	116.07
2	B	608	CHL	C4C-CHD-C1D	2.67	125.64	116.07
3	B	602	CLA	CHD-C1D-ND	-2.67	121.04	124.80
3	C	604	CLA	CHD-C1D-ND	-2.67	121.05	124.80
2	B	608	CHL	C4D-CHA-CBD	-2.67	106.28	108.97
2	A	608	CHL	C4C-CHD-C1D	2.66	125.60	116.07
3	B	613	CLA	CHD-C1D-ND	-2.66	121.06	124.80
2	B	605	CHL	C4C-CHD-C1D	2.66	125.59	116.07
3	B	603	CLA	CHD-C1D-ND	-2.66	121.06	124.80
3	A	614	CLA	CHD-C1D-ND	-2.65	121.07	124.80
3	A	603	CLA	C1-C2-C3	-2.64	121.87	126.20
3	C	614	CLA	CHD-C1D-ND	-2.64	121.08	124.80
2	C	605	CHL	C4C-CHD-C1D	2.64	125.51	116.07
3	A	602	CLA	CHD-C1D-ND	-2.64	121.09	124.80
3	C	613	CLA	CHD-C1D-ND	-2.64	121.09	124.80
2	A	605	CHL	C4C-CHD-C1D	2.64	125.50	116.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	613	CLA	CHD-C1D-ND	-2.64	121.09	124.80
3	A	604	CLA	C1D-ND-C4D	-2.63	104.47	106.31
3	C	603	CLA	CHC-C1C-C2C	-2.63	119.48	126.95
3	B	614	CLA	CHD-C1D-ND	-2.62	121.11	124.80
3	A	612	CLA	CHC-C1C-C2C	-2.62	119.49	126.95
3	C	604	CLA	C1D-ND-C4D	-2.62	104.47	106.31
3	B	603	CLA	CHC-C1C-C2C	-2.62	119.51	126.95
3	B	612	CLA	CHC-C1C-C2C	-2.62	119.52	126.95
2	A	608	CHL	C4D-CHA-CBD	-2.61	106.33	108.97
3	C	612	CLA	CHD-C1D-ND	-2.60	121.14	124.80
2	B	607	CHL	C4D-CHA-CBD	-2.60	106.35	108.97
3	A	603	CLA	CHC-C1C-C2C	-2.60	119.56	126.95
3	C	612	CLA	CHC-C1C-C2C	-2.60	119.56	126.95
2	C	607	CHL	C4D-CHA-CBD	-2.59	106.35	108.97
2	A	605	CHL	C4D-CHA-CBD	-2.59	106.35	108.97
3	C	603	CLA	C1-C2-C3	-2.59	121.95	126.20
2	C	605	CHL	C4D-CHA-CBD	-2.59	106.36	108.97
2	A	607	CHL	C4D-CHA-CBD	-2.58	106.36	108.97
2	B	605	CHL	C4D-CHA-CBD	-2.58	106.37	108.97
3	B	612	CLA	CHD-C1D-ND	-2.57	121.19	124.80
2	A	601	CHL	C4D-CHA-CBD	-2.56	106.38	108.97
3	A	612	CLA	CHD-C1D-ND	-2.55	121.21	124.80
3	C	613	CLA	CHC-C1C-C2C	-2.54	119.73	126.95
3	B	613	CLA	CHC-C1C-C2C	-2.53	119.76	126.95
2	B	601	CHL	C4D-CHA-CBD	-2.53	106.42	108.97
3	A	602	CLA	C1-C2-C3	-2.52	122.06	126.20
3	A	613	CLA	CHC-C1C-C2C	-2.52	119.78	126.95
3	A	611	CLA	CHC-C1C-C2C	-2.52	119.80	126.95
3	C	602	CLA	C1-C2-C3	-2.51	122.08	126.20
3	A	604	CLA	CHC-C1C-C2C	-2.51	119.82	126.95
3	C	604	CLA	CHC-C1C-C2C	-2.50	119.83	126.95
3	B	614	CLA	CHC-C1C-C2C	-2.50	119.84	126.95
3	B	611	CLA	CHC-C1C-C2C	-2.50	119.85	126.95
3	C	611	CLA	CHC-C1C-C2C	-2.49	119.88	126.95
3	C	614	CLA	CHC-C1C-C2C	-2.49	119.88	126.95
3	A	614	CLA	CHC-C1C-C2C	-2.49	119.88	126.95
3	C	603	CLA	CHC-C1C-NC	2.49	128.06	124.31
2	C	601	CHL	C4D-CHA-CBD	-2.48	106.47	108.97
3	B	604	CLA	CHC-C1C-C2C	-2.47	119.92	126.95
3	A	610	CLA	CHC-C1C-C2C	-2.46	119.95	126.95
3	C	610	CLA	CHC-C1C-C2C	-2.46	119.96	126.95
3	B	612	CLA	C2C-C1C-NC	2.45	112.56	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	603	CLA	CHC-C1C-NC	2.45	128.00	124.31
3	A	603	CLA	CHC-C1C-NC	2.45	128.00	124.31
3	B	602	CLA	CHC-C1C-C2C	-2.44	120.00	126.95
3	B	610	CLA	CHC-C1C-C2C	-2.44	120.00	126.95
3	C	612	CLA	C2C-C1C-NC	2.44	112.54	109.98
3	A	612	CLA	C2C-C1C-NC	2.43	112.54	109.98
3	A	612	CLA	CHC-C1C-NC	2.43	127.97	124.31
3	A	602	CLA	CHC-C1C-C2C	-2.42	120.06	126.95
3	C	604	CLA	CHC-C1C-NC	2.42	127.96	124.31
3	C	602	CLA	CHC-C1C-C2C	-2.42	120.07	126.95
2	A	609	CHL	C4D-CHA-CBD	-2.40	106.55	108.97
3	A	604	CLA	CHC-C1C-NC	2.39	127.91	124.31
3	B	612	CLA	CHC-C1C-NC	2.39	127.91	124.31
3	B	604	CLA	CHC-C1C-NC	2.39	127.91	124.31
2	B	609	CHL	C4D-CHA-CBD	-2.38	106.57	108.97
3	C	612	CLA	CHC-C1C-NC	2.38	127.89	124.31
2	B	606	CHL	C1-C2-C3	-2.37	122.92	126.76
3	C	604	CLA	CHA-C1A-NA	-2.37	121.02	126.39
3	A	604	CLA	CHA-C1A-NA	-2.37	121.03	126.39
3	B	611	CLA	CHC-C1C-NC	2.37	127.88	124.31
5	A	617	NEX	O24-C25-C24	2.37	115.71	113.49
2	A	606	CHL	C1-C2-C3	-2.36	122.94	126.76
2	C	609	CHL	C4D-CHA-CBD	-2.36	106.58	108.97
3	B	604	CLA	CHA-C1A-NA	-2.36	121.05	126.39
3	C	613	CLA	CHC-C1C-NC	2.36	127.86	124.31
3	B	613	CLA	CHC-C1C-NC	2.35	127.86	124.31
2	A	605	CHL	C3C-C4C-NC	-2.35	108.90	114.65
2	B	605	CHL	C3C-C4C-NC	-2.35	108.90	114.65
2	C	605	CHL	C3C-C4C-NC	-2.35	108.91	114.65
3	A	611	CLA	CHC-C1C-NC	2.35	127.84	124.31
2	C	606	CHL	C1-C2-C3	-2.34	122.97	126.76
3	B	603	CLA	C2C-C1C-NC	2.34	112.44	109.98
3	A	613	CLA	CHC-C1C-NC	2.34	127.84	124.31
3	C	611	CLA	CHC-C1C-NC	2.34	127.84	124.31
3	C	610	CLA	CHC-C1C-NC	2.34	127.83	124.31
3	C	603	CLA	C2C-C1C-NC	2.32	112.42	109.98
5	C	617	NEX	O24-C25-C24	2.31	115.66	113.49
3	A	610	CLA	C1-C2-C3	-2.31	122.41	126.20
3	A	603	CLA	C2C-C1C-NC	2.31	112.41	109.98
3	A	614	CLA	CHC-C1C-NC	2.30	127.78	124.31
3	B	614	CLA	C2C-C1C-NC	2.30	112.40	109.98
3	C	614	CLA	CHC-C1C-NC	2.30	127.77	124.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	CLA	CHC-C1C-NC	2.29	127.76	124.31
3	C	613	CLA	C2C-C1C-NC	2.29	112.38	109.98
3	A	610	CLA	CHC-C1C-NC	2.29	127.75	124.31
3	A	613	CLA	C2C-C1C-NC	2.28	112.37	109.98
2	C	609	CHL	C3C-C4C-NC	-2.27	109.09	114.65
3	B	613	CLA	C2C-C1C-NC	2.27	112.37	109.98
2	A	609	CHL	C3C-C4C-NC	-2.27	109.10	114.65
3	B	610	CLA	CHC-C1C-NC	2.27	127.73	124.31
3	B	614	CLA	CHC-C1C-NC	2.27	127.73	124.31
3	B	610	CLA	CHA-C1A-NA	-2.26	121.27	126.39
3	C	610	CLA	CHA-C1A-NA	-2.26	121.27	126.39
3	A	611	CLA	C2C-C1C-NC	2.25	112.35	109.98
2	B	609	CHL	C3C-C4C-NC	-2.25	109.15	114.65
3	A	610	CLA	CHA-C1A-NA	-2.24	121.31	126.39
3	C	610	CLA	C1-C2-C3	-2.24	122.53	126.20
2	A	601	CHL	C3C-C4C-NC	-2.23	109.19	114.65
3	C	614	CLA	C2C-C1C-NC	2.23	112.32	109.98
2	C	601	CHL	C3C-C4C-NC	-2.22	109.22	114.65
5	B	617	NEX	O24-C25-C24	2.22	115.57	113.49
3	A	614	CLA	C2C-C1C-NC	2.22	112.31	109.98
3	A	602	CLA	CHA-C1A-NA	-2.22	121.37	126.39
2	B	601	CHL	C3C-C4C-NC	-2.22	109.23	114.65
3	B	610	CLA	C1-C2-C3	-2.22	122.56	126.20
3	B	614	CLA	CHA-C1A-NA	-2.22	121.37	126.39
3	A	614	CLA	CHA-C1A-NA	-2.22	121.37	126.39
2	B	606	CHL	C3C-C4C-NC	-2.22	109.23	114.65
3	C	602	CLA	CHC-C1C-NC	2.22	127.65	124.31
3	C	614	CLA	CHA-C1A-NA	-2.21	121.38	126.39
2	C	606	CHL	C3C-C4C-NC	-2.21	109.24	114.65
3	A	602	CLA	CHC-C1C-NC	2.21	127.64	124.31
3	C	602	CLA	CHA-C1A-NA	-2.21	121.38	126.39
2	C	608	CHL	C3C-C4C-NC	-2.20	109.26	114.65
2	A	606	CHL	C3C-C4C-NC	-2.20	109.27	114.65
3	A	612	CLA	CHA-C1A-NA	-2.20	121.41	126.39
2	B	608	CHL	C3C-C4C-NC	-2.19	109.30	114.65
2	A	607	CHL	C3C-C4C-NC	-2.19	109.30	114.65
3	B	602	CLA	CHA-C1A-NA	-2.19	121.43	126.39
2	B	607	CHL	C3C-C4C-NC	-2.19	109.31	114.65
3	C	611	CLA	C2C-C1C-NC	2.18	112.28	109.98
2	C	607	CHL	C3C-C4C-NC	-2.18	109.32	114.65
3	C	612	CLA	CHA-C1A-NA	-2.18	121.45	126.39
3	B	611	CLA	C2C-C1C-NC	2.17	112.27	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	612	CLA	CHB-C1B-NB	-2.17	120.79	124.05
3	A	610	CLA	C2C-C1C-NC	2.16	112.25	109.98
2	A	608	CHL	C3C-C4C-NC	-2.16	109.38	114.65
3	B	612	CLA	CHA-C1A-NA	-2.14	121.53	126.39
3	A	604	CLA	C2C-C1C-NC	2.14	112.23	109.98
3	B	610	CLA	C2C-C1C-NC	2.14	112.23	109.98
3	A	602	CLA	C2C-C1C-NC	2.14	112.23	109.98
3	A	612	CLA	CHB-C1B-NB	-2.13	120.85	124.05
3	C	612	CLA	CHB-C1B-NB	-2.13	120.85	124.05
3	A	613	CLA	CHA-C1A-NA	-2.13	121.56	126.39
3	B	611	CLA	C1-C2-C3	-2.13	122.71	126.20
3	B	603	CLA	CHB-C1B-NB	-2.13	120.86	124.05
3	A	613	CLA	CHB-C1B-NB	-2.12	120.86	124.05
3	C	613	CLA	CHA-C1A-NA	-2.12	121.59	126.39
3	C	602	CLA	C2C-C1C-NC	2.12	112.20	109.98
3	C	603	CLA	CHB-C1B-NB	-2.11	120.88	124.05
3	C	613	CLA	CHB-C1B-NB	-2.11	120.88	124.05
3	B	602	CLA	CHB-C1B-NB	-2.11	120.88	124.05
3	B	613	CLA	CHA-C1A-NA	-2.11	121.61	126.39
3	A	602	CLA	CHB-C1B-NB	-2.10	120.89	124.05
3	B	610	CLA	CHB-C1B-NB	-2.10	120.89	124.05
3	C	602	CLA	CHB-C1B-NB	-2.10	120.90	124.05
3	C	610	CLA	C2C-C1C-NC	2.10	112.19	109.98
3	B	613	CLA	CHB-C1B-NB	-2.10	120.90	124.05
3	A	603	CLA	CHB-C1B-NB	-2.10	120.90	124.05
3	B	602	CLA	C2C-C1C-NC	2.10	112.18	109.98
3	B	603	CLA	CHA-C1A-NA	-2.08	121.67	126.39
3	C	603	CLA	CHA-C1A-NA	-2.08	121.67	126.39
3	A	614	CLA	CHB-C1B-NB	-2.08	120.93	124.05
3	C	604	CLA	C2C-C1C-NC	2.08	112.17	109.98
3	C	611	CLA	C1-C2-C3	-2.08	122.80	126.20
3	A	610	CLA	CHB-C1B-NB	-2.08	120.94	124.05
3	A	603	CLA	CHA-C1A-NA	-2.07	121.69	126.39
3	B	614	CLA	CHB-C1B-NB	-2.07	120.94	124.05
3	C	614	CLA	CHB-C1B-NB	-2.07	120.95	124.05
3	C	611	CLA	CHB-C1B-NB	-2.07	120.95	124.05
3	B	604	CLA	C2C-C1C-NC	2.04	112.12	109.98
3	C	610	CLA	CHB-C1B-NB	-2.04	120.99	124.05
3	A	611	CLA	C1-C2-C3	-2.04	122.86	126.20
3	B	611	CLA	CHB-C1B-NB	-2.04	121.00	124.05
3	A	611	CLA	CHB-C1B-NB	-2.02	121.01	124.05
2	C	609	CHL	CMB-C2B-C3B	2.02	128.72	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	607	CHL	CHA-C1A-C2A	-2.01	128.59	133.31
3	A	611	CLA	CHA-C1A-NA	-2.01	121.84	126.39
3	C	611	CLA	CHA-C1A-NA	-2.01	121.84	126.39
2	B	609	CHL	CMB-C2B-C3B	2.01	128.69	124.68
2	C	608	CHL	CMB-C2B-C3B	2.00	128.69	124.68

All (102) chirality outliers are listed below:

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

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

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Mol	Chain	Res	Type	Atom
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
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

All (258) 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	601	CHL	C4-C3-C5-C6
2	A	605	CHL	C1C-C2C-CMC-OMC
2	A	605	CHL	C3C-C2C-CMC-OMC
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	609	CHL	C1C-C2C-CMC-OMC
2	A	609	CHL	C3C-C2C-CMC-OMC

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Mol	Chain	Res	Type	Atoms
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	C1C-C2C-CMC-OMC
2	B	609	CHL	C3C-C2C-CMC-OMC
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
2	C	607	CHL	CHA-CBD-CGD-O1D
2	C	607	CHL	CHA-CBD-CGD-O2D
2	C	609	CHL	C1C-C2C-CMC-OMC
2	C	609	CHL	C3C-C2C-CMC-OMC
3	A	602	CLA	CHA-CBD-CGD-O1D
3	A	602	CLA	CHA-CBD-CGD-O2D
3	A	603	CLA	C1A-C2A-CAA-CBA
3	A	604	CLA	C1A-C2A-CAA-CBA
3	A	611	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	604	CLA	C1A-C2A-CAA-CBA
3	B	611	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	604	CLA	C1A-C2A-CAA-CBA
3	C	611	CLA	C4B-C3B-CAB-CBB
3	C	614	CLA	C2B-C3B-CAB-CBB
3	C	614	CLA	C4B-C3B-CAB-CBB
6	A	618	LHG	C3-O3-P-O5

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Mol	Chain	Res	Type	Atoms
6	A	618	LHG	C4-O6-P-O3
6	A	618	LHG	C4-O6-P-O5
6	B	618	LHG	C3-O3-P-O5
6	B	618	LHG	C4-O6-P-O3
6	B	618	LHG	C4-O6-P-O5
6	C	618	LHG	C3-O3-P-O5
6	C	618	LHG	C3-O3-P-O6
6	C	618	LHG	C4-O6-P-O3
6	C	618	LHG	C4-O6-P-O5
3	B	602	CLA	C3-C5-C6-C7
2	B	601	CHL	C4-C3-C5-C6
2	C	601	CHL	C4-C3-C5-C6
3	A	602	CLA	C4-C3-C5-C6
2	A	601	CHL	C2-C3-C5-C6
2	C	601	CHL	C2-C3-C5-C6
3	A	602	CLA	C2-C3-C5-C6
6	A	618	LHG	O2-C2-C3-O3
6	B	618	LHG	O2-C2-C3-O3
6	C	618	LHG	O2-C2-C3-O3
3	C	602	CLA	C4-C3-C5-C6
2	B	601	CHL	C2-C3-C5-C6
6	A	618	LHG	C1-C2-C3-O3
6	B	618	LHG	C1-C2-C3-O3
3	C	602	CLA	C2-C3-C5-C6
6	C	618	LHG	C1-C2-C3-O3
2	A	608	CHL	C2A-CAA-CBA-CGA
2	B	608	CHL	C2A-CAA-CBA-CGA
3	A	603	CLA	C4B-C3B-CAB-CBB
3	A	612	CLA	C4B-C3B-CAB-CBB
3	B	603	CLA	C4B-C3B-CAB-CBB
3	B	612	CLA	C4B-C3B-CAB-CBB
3	C	603	CLA	C4B-C3B-CAB-CBB
3	C	612	CLA	C4B-C3B-CAB-CBB
2	C	608	CHL	C2A-CAA-CBA-CGA
2	A	609	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	611	CLA	C2B-C3B-CAB-CBB
3	B	611	CLA	C2B-C3B-CAB-CBB
3	C	611	CLA	C2B-C3B-CAB-CBB
3	C	611	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
3	A	611	CLA	C10-C11-C12-C13
3	B	611	CLA	C10-C11-C12-C13
6	A	618	LHG	C23-C24-C25-C26
6	B	618	LHG	C23-C24-C25-C26
2	C	609	CHL	C5-C6-C7-C8
6	C	618	LHG	C23-C24-C25-C26
2	B	609	CHL	C5-C6-C7-C8
3	B	603	CLA	C1A-C2A-CAA-CBA
3	C	603	CLA	C1A-C2A-CAA-CBA
2	A	607	CHL	CHA-CBD-CGD-O2D
2	B	607	CHL	CHA-CBD-CGD-O2D
3	A	612	CLA	C10-C11-C12-C13
3	C	612	CLA	C10-C11-C12-C13
3	B	612	CLA	C10-C11-C12-C13
2	A	606	CHL	C3C-C2C-CMC-OMC
2	B	606	CHL	C3C-C2C-CMC-OMC
2	C	606	CHL	C3C-C2C-CMC-OMC
2	C	608	CHL	C3C-C2C-CMC-OMC
3	A	611	CLA	CAA-CBA-CGA-O2A
3	B	613	CLA	C4-C3-C5-C6
3	B	611	CLA	CAA-CBA-CGA-O2A
3	A	602	CLA	C4B-C3B-CAB-CBB
3	A	610	CLA	C4B-C3B-CAB-CBB
3	B	610	CLA	C4B-C3B-CAB-CBB
3	B	613	CLA	C4B-C3B-CAB-CBB
3	C	602	CLA	C4B-C3B-CAB-CBB
3	C	610	CLA	C4B-C3B-CAB-CBB
3	C	613	CLA	C4B-C3B-CAB-CBB
3	A	613	CLA	C4-C3-C5-C6
3	C	611	CLA	CAA-CBA-CGA-O2A
2	A	601	CHL	C1A-C2A-CAA-CBA
2	B	601	CHL	C1A-C2A-CAA-CBA
2	C	601	CHL	C1A-C2A-CAA-CBA
2	B	609	CHL	C4-C3-C5-C6
2	B	609	CHL	C2-C3-C5-C6
4	A	615	A1LXP	C24-C1-C42-C2
4	B	615	A1LXP	C24-C1-C42-C2
4	C	615	A1LXP	C24-C1-C42-C2
3	B	613	CLA	C2-C3-C5-C6
3	C	613	CLA	C4-C3-C5-C6
3	A	613	CLA	C2-C3-C5-C6
3	C	613	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
2	C	609	CHL	C4-C3-C5-C6
2	A	609	CHL	C6-C7-C8-C9
3	A	610	CLA	C11-C10-C8-C9
3	B	610	CLA	C11-C10-C8-C9
3	B	612	CLA	C4-C3-C5-C6
2	A	607	CHL	CHA-CBD-CGD-O1D
2	A	608	CHL	CHA-CBD-CGD-O2D
2	B	607	CHL	CHA-CBD-CGD-O1D
2	B	608	CHL	CHA-CBD-CGD-O1D
2	B	608	CHL	CHA-CBD-CGD-O2D
2	C	608	CHL	CHA-CBD-CGD-O1D
2	C	608	CHL	CHA-CBD-CGD-O2D
3	A	603	CLA	CHA-CBD-CGD-O1D
3	A	603	CLA	CHA-CBD-CGD-O2D
3	A	612	CLA	CHA-CBD-CGD-O1D
3	A	612	CLA	CHA-CBD-CGD-O2D
3	B	612	CLA	CHA-CBD-CGD-O1D
3	B	612	CLA	CHA-CBD-CGD-O2D
3	C	612	CLA	CHA-CBD-CGD-O1D
3	C	612	CLA	CHA-CBD-CGD-O2D
6	A	618	LHG	C4-O6-P-O4
6	B	618	LHG	C4-O6-P-O4
6	C	618	LHG	C4-O6-P-O4
3	C	602	CLA	C3-C5-C6-C7
3	A	612	CLA	C4-C3-C5-C6
3	C	612	CLA	C4-C3-C5-C6
3	A	603	CLA	C2B-C3B-CAB-CBB
3	A	610	CLA	C2B-C3B-CAB-CBB
3	A	612	CLA	C2B-C3B-CAB-CBB
3	B	603	CLA	C2B-C3B-CAB-CBB
3	B	612	CLA	C2B-C3B-CAB-CBB
3	C	603	CLA	C2B-C3B-CAB-CBB
3	C	610	CLA	C2B-C3B-CAB-CBB
3	C	612	CLA	C2B-C3B-CAB-CBB
2	C	609	CHL	C2-C3-C5-C6
3	C	610	CLA	C11-C10-C8-C9
2	C	608	CHL	C1C-C2C-CMC-OMC
3	B	612	CLA	C2-C3-C5-C6
3	C	612	CLA	C2-C3-C5-C6
3	A	613	CLA	C4B-C3B-CAB-CBB
3	B	602	CLA	C4B-C3B-CAB-CBB
3	C	604	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
3	A	611	CLA	CAA-CBA-CGA-O1A
3	A	612	CLA	C2-C3-C5-C6
5	A	617	NEX	C39-C29-C30-C31
5	B	617	NEX	C39-C29-C30-C31
5	C	617	NEX	C39-C29-C30-C31
6	A	618	LHG	C25-C26-C27-C28
2	B	608	CHL	C4-C3-C5-C6
3	B	611	CLA	CAA-CBA-CGA-O1A
2	B	609	CHL	C6-C7-C8-C9
2	C	609	CHL	C6-C7-C8-C9
5	A	617	NEX	C28-C29-C30-C31
5	B	617	NEX	C28-C29-C30-C31
5	C	617	NEX	C28-C29-C30-C31
6	C	618	LHG	C25-C26-C27-C28
3	A	604	CLA	C2B-C3B-CAB-CBB
3	B	604	CLA	C2B-C3B-CAB-CBB
3	B	610	CLA	C2B-C3B-CAB-CBB
3	C	604	CLA	C2B-C3B-CAB-CBB
4	A	615	A1LXP	C28-C1-C42-C2
4	A	616	A1LXP	C24-C1-C42-C2
4	C	615	A1LXP	C28-C1-C42-C2
4	C	616	A1LXP	C24-C1-C42-C2
6	C	618	LHG	C5-C4-O6-P
6	A	618	LHG	C5-C4-O6-P
3	B	604	CLA	CAA-CBA-CGA-O2A
6	B	618	LHG	C25-C26-C27-C28
3	A	602	CLA	C3-C5-C6-C7
3	A	604	CLA	C4B-C3B-CAB-CBB
3	B	604	CLA	C4B-C3B-CAB-CBB
3	C	611	CLA	CAA-CBA-CGA-O1A
3	A	604	CLA	CAA-CBA-CGA-O2A
3	C	604	CLA	CAA-CBA-CGA-O2A
2	C	601	CHL	CHA-CBD-CGD-O2D
6	B	618	LHG	C5-C4-O6-P
3	A	603	CLA	C4-C3-C5-C6
3	A	602	CLA	C2B-C3B-CAB-CBB
3	A	613	CLA	C2B-C3B-CAB-CBB
3	B	602	CLA	C2B-C3B-CAB-CBB
3	B	613	CLA	C2B-C3B-CAB-CBB
3	C	602	CLA	C2B-C3B-CAB-CBB
3	C	613	CLA	C2B-C3B-CAB-CBB
4	A	616	A1LXP	C28-C1-C42-C2

Continued on next page...

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Mol	Chain	Res	Type	Atoms
4	B	615	A1LXP	C28-C1-C42-C2
4	B	616	A1LXP	C24-C1-C42-C2
4	B	616	A1LXP	C28-C1-C42-C2
4	C	616	A1LXP	C28-C1-C42-C2
3	B	610	CLA	C15-C16-C17-C18
3	C	612	CLA	CAA-CBA-CGA-O2A
3	A	612	CLA	CAA-CBA-CGA-O2A
3	B	612	CLA	CAA-CBA-CGA-O2A
6	A	618	LHG	O8-C23-C24-C25
6	C	618	LHG	O8-C23-C24-C25
6	B	618	LHG	O8-C23-C24-C25
3	A	613	CLA	C2A-CAA-CBA-CGA
2	C	607	CHL	CAA-CBA-CGA-O2A
3	B	613	CLA	C2A-CAA-CBA-CGA
3	C	613	CLA	C2A-CAA-CBA-CGA
3	A	610	CLA	C15-C16-C17-C18
3	B	602	CLA	C5-C6-C7-C8
2	B	606	CHL	C3A-C2A-CAA-CBA
2	C	606	CHL	C3A-C2A-CAA-CBA
2	C	608	CHL	CAA-CBA-CGA-O2A
6	B	618	LHG	C28-C29-C30-C31
3	C	610	CLA	C15-C16-C17-C18
6	C	618	LHG	O10-C23-C24-C25
6	A	618	LHG	O10-C23-C24-C25
2	B	607	CHL	CAA-CBA-CGA-O2A
6	A	618	LHG	C28-C29-C30-C31
3	A	612	CLA	CAA-CBA-CGA-O1A
6	B	618	LHG	O10-C23-C24-C25
2	B	606	CHL	CAA-CBA-CGA-O2A
3	C	612	CLA	CAA-CBA-CGA-O1A
6	C	618	LHG	C28-C29-C30-C31
3	B	603	CLA	CAD-CBD-CGD-O2D
3	C	603	CLA	CAD-CBD-CGD-O2D
2	A	608	CHL	CAA-CBA-CGA-O2A
2	B	608	CHL	CAA-CBA-CGA-O2A
3	B	612	CLA	CAA-CBA-CGA-O1A
2	B	608	CHL	CAA-CBA-CGA-O1A

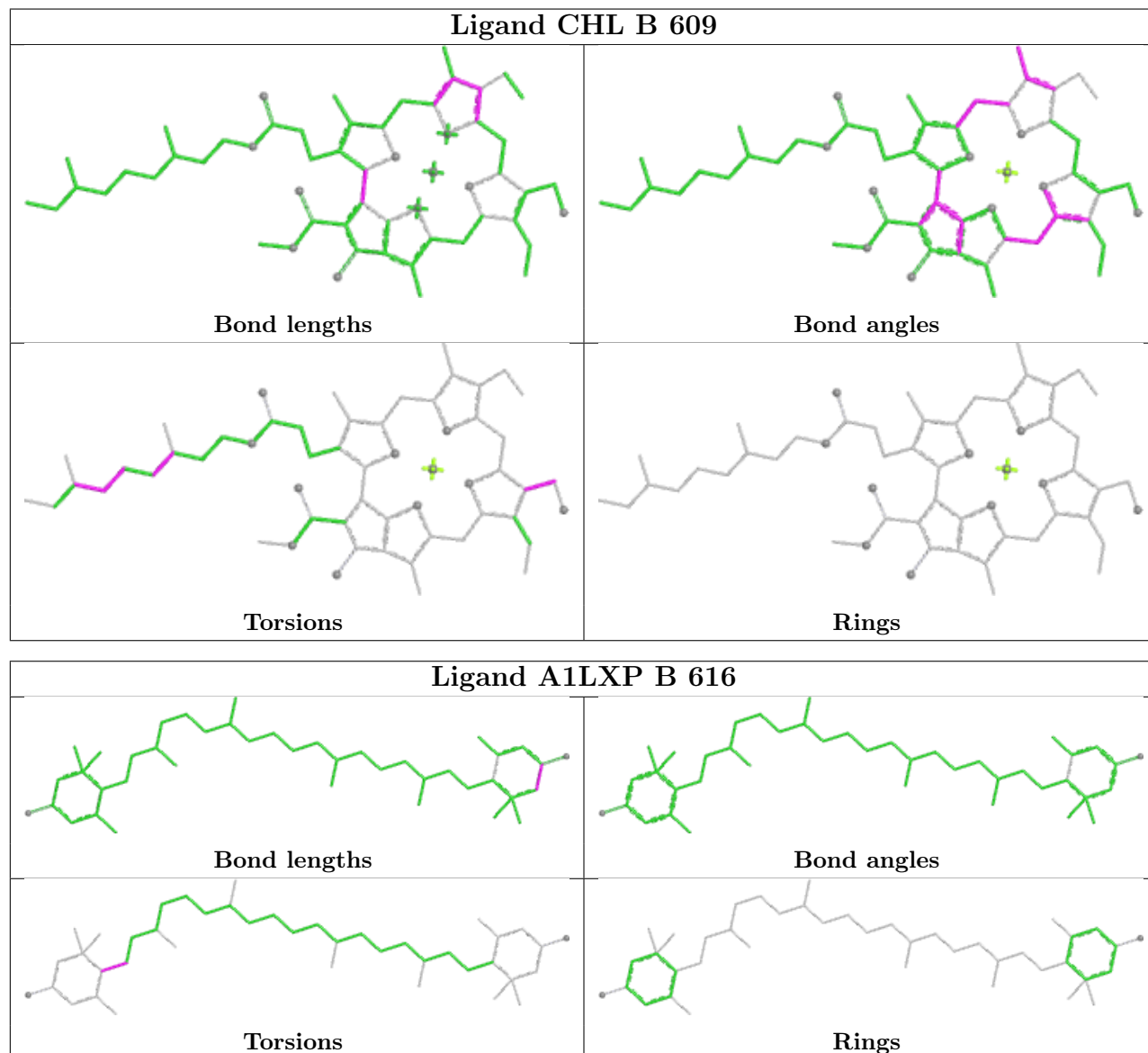
There are no ring outliers.

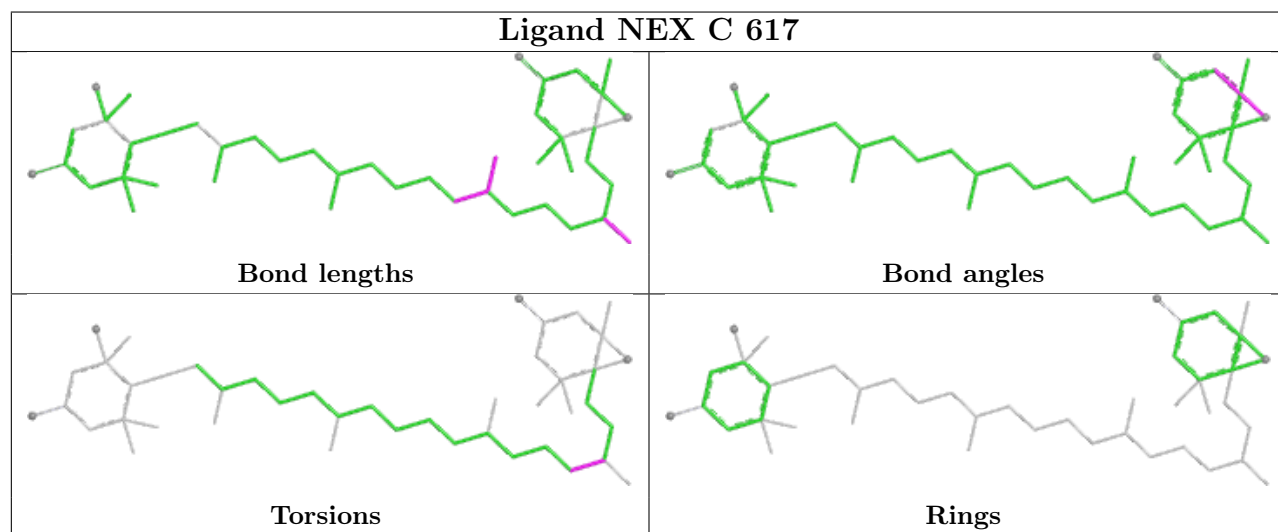
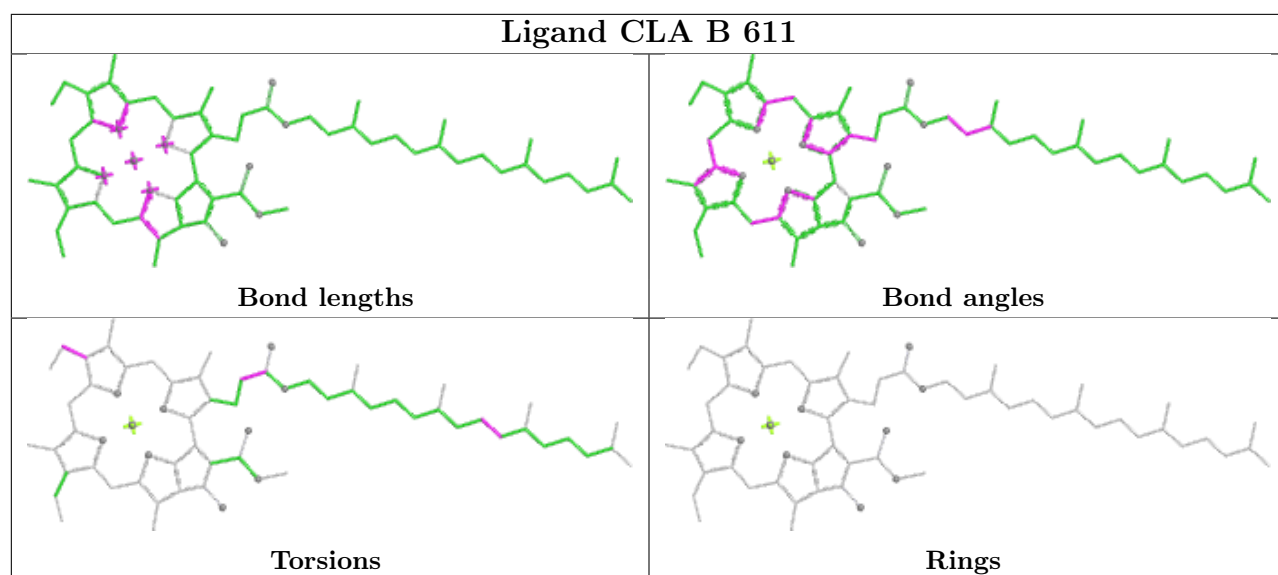
41 monomers are involved in 53 short contacts:

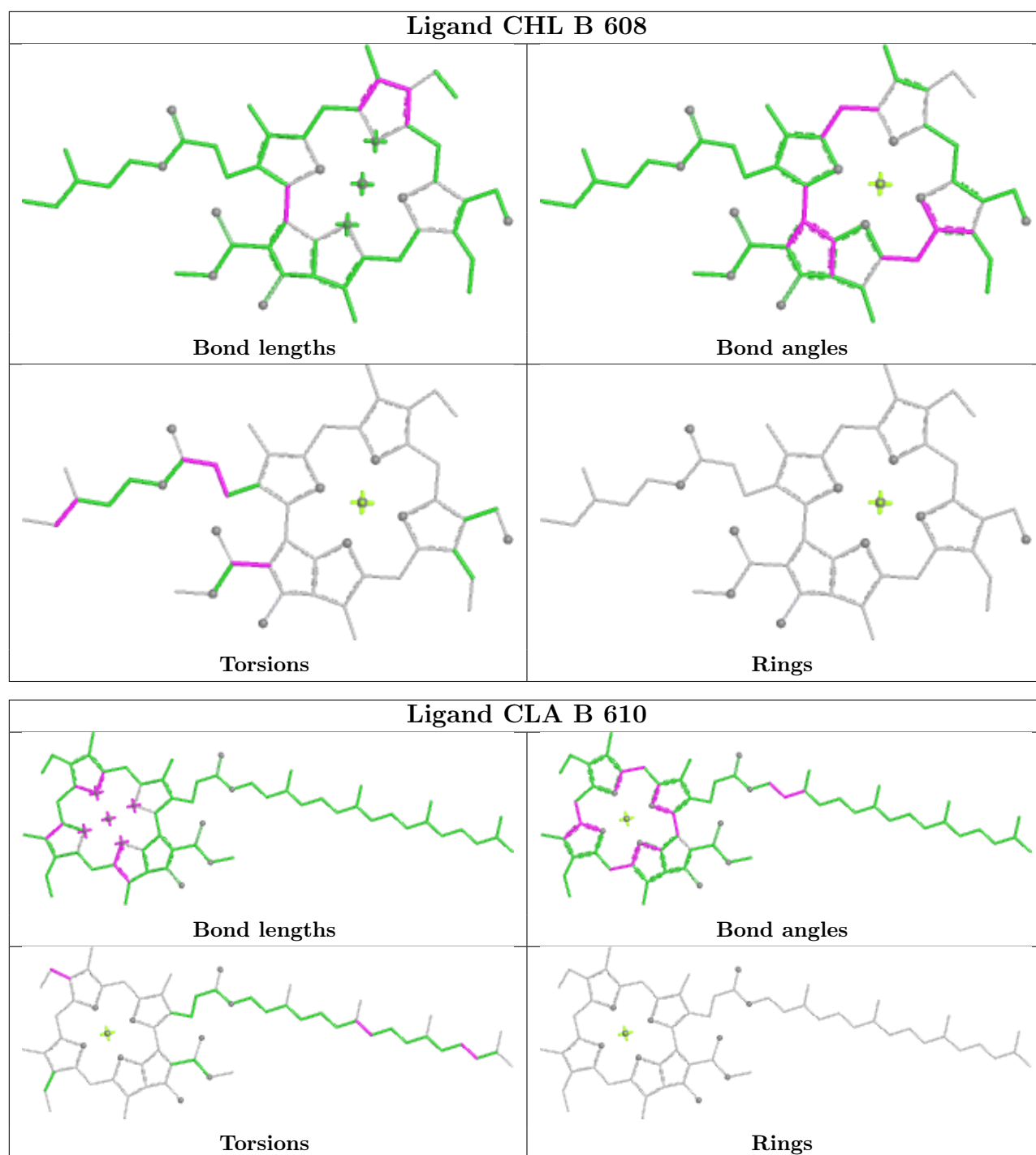
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	609	CHL	1	0
4	B	616	A1LXP	1	0
5	C	617	NEX	1	0
2	B	608	CHL	1	0
3	B	610	CLA	1	0
6	C	618	LHG	4	0
2	B	606	CHL	2	0
3	B	612	CLA	1	0
3	A	612	CLA	2	0
3	B	614	CLA	1	0
5	A	617	NEX	2	0
5	B	617	NEX	1	0
3	A	613	CLA	1	0
6	B	618	LHG	2	0
3	C	612	CLA	2	0
2	B	607	CHL	1	0
3	C	610	CLA	1	0
3	A	603	CLA	1	0
2	C	606	CHL	1	0
3	B	603	CLA	3	0
3	B	613	CLA	1	0
6	A	618	LHG	4	0
2	A	601	CHL	4	0
2	C	607	CHL	1	0
3	A	614	CLA	1	0
3	C	614	CLA	1	0
3	A	610	CLA	1	0
2	A	606	CHL	1	0
3	C	613	CLA	1	0
2	C	601	CHL	3	0
3	B	602	CLA	2	0
3	C	603	CLA	3	0
3	C	604	CLA	2	0
3	C	602	CLA	2	0
2	A	608	CHL	1	0
2	A	607	CHL	1	0
2	C	608	CHL	1	0
3	B	604	CLA	2	0
4	B	615	A1LXP	1	0
2	B	601	CHL	3	0
3	A	604	CLA	2	0

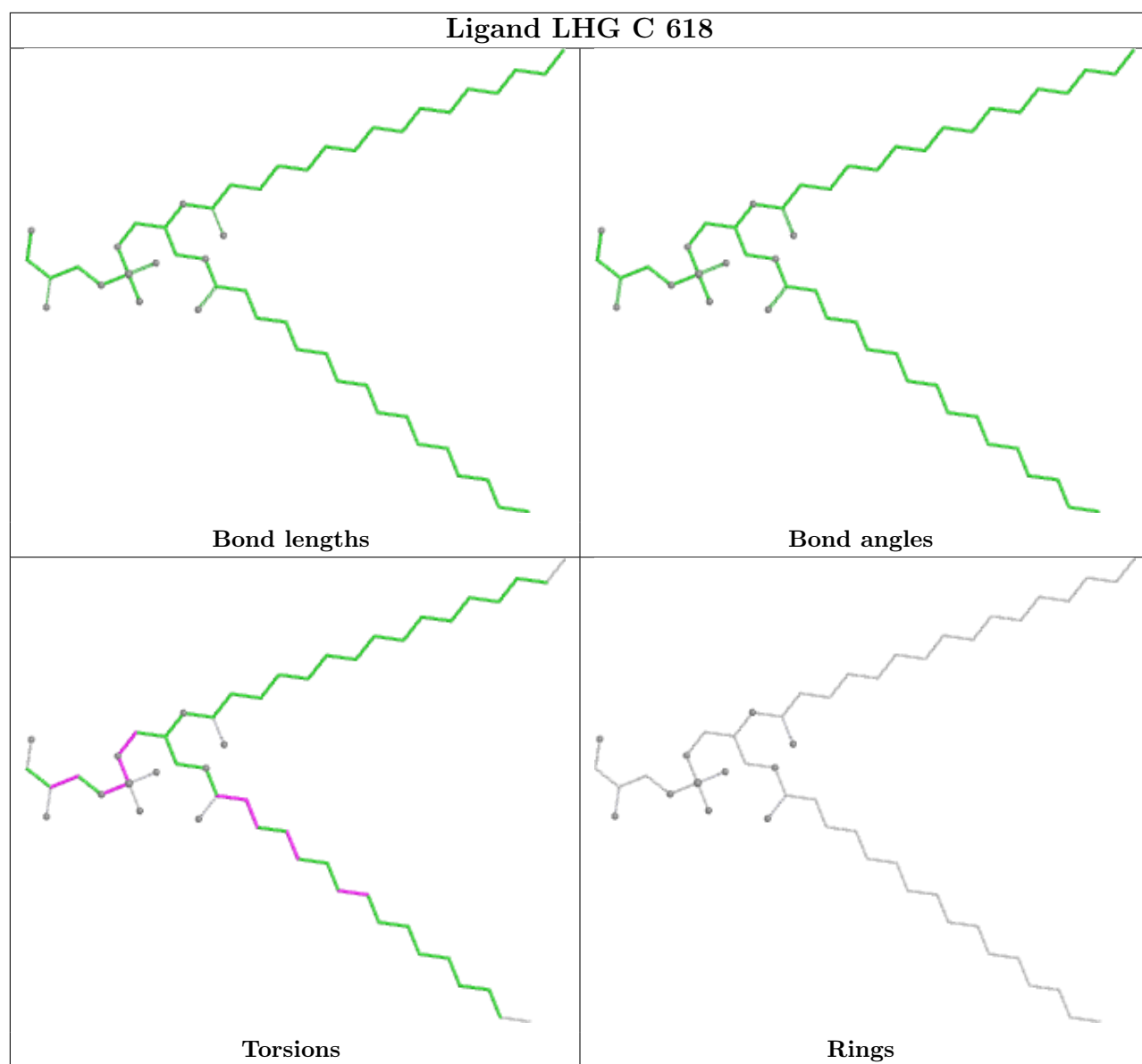
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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.

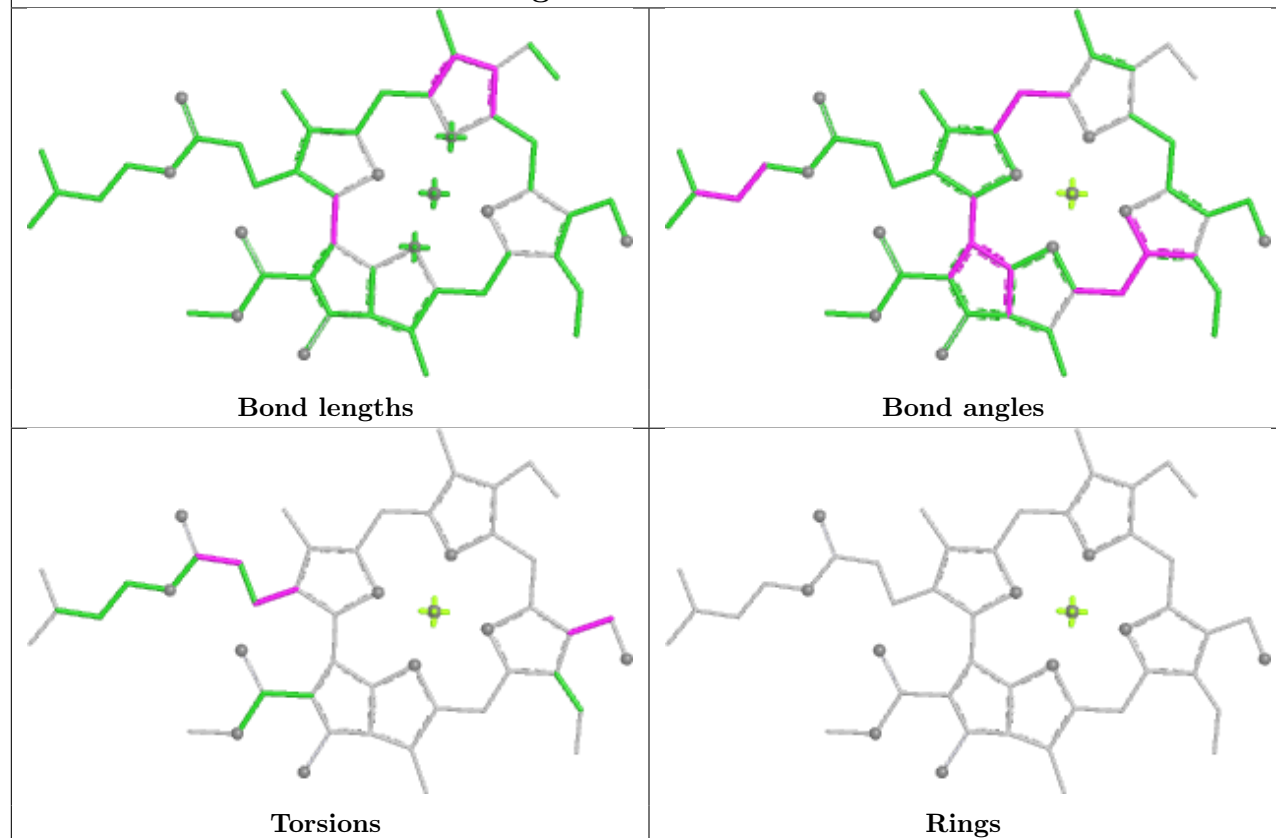




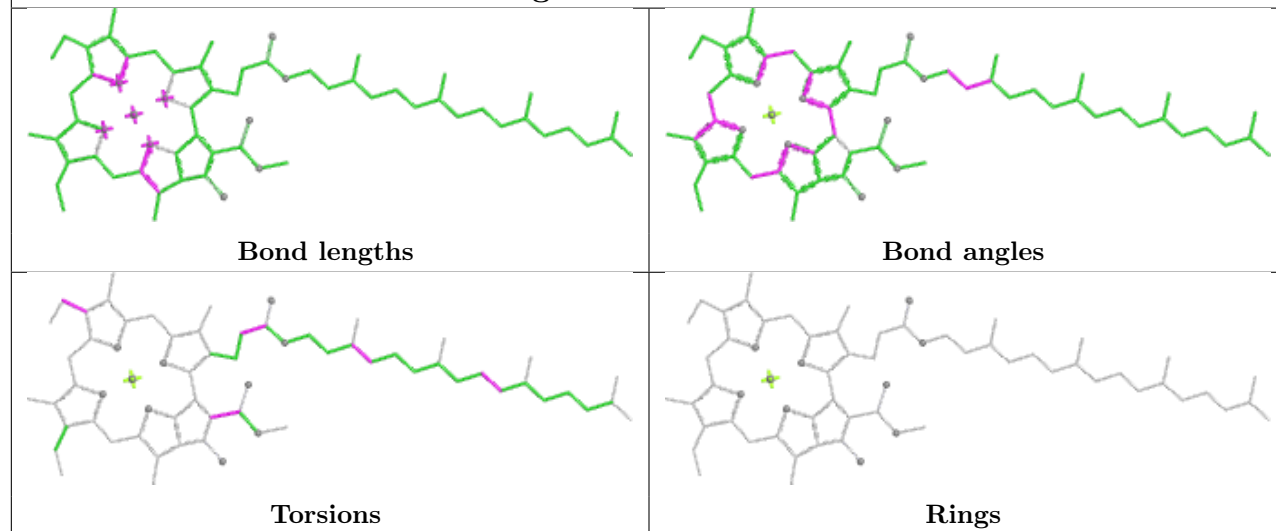


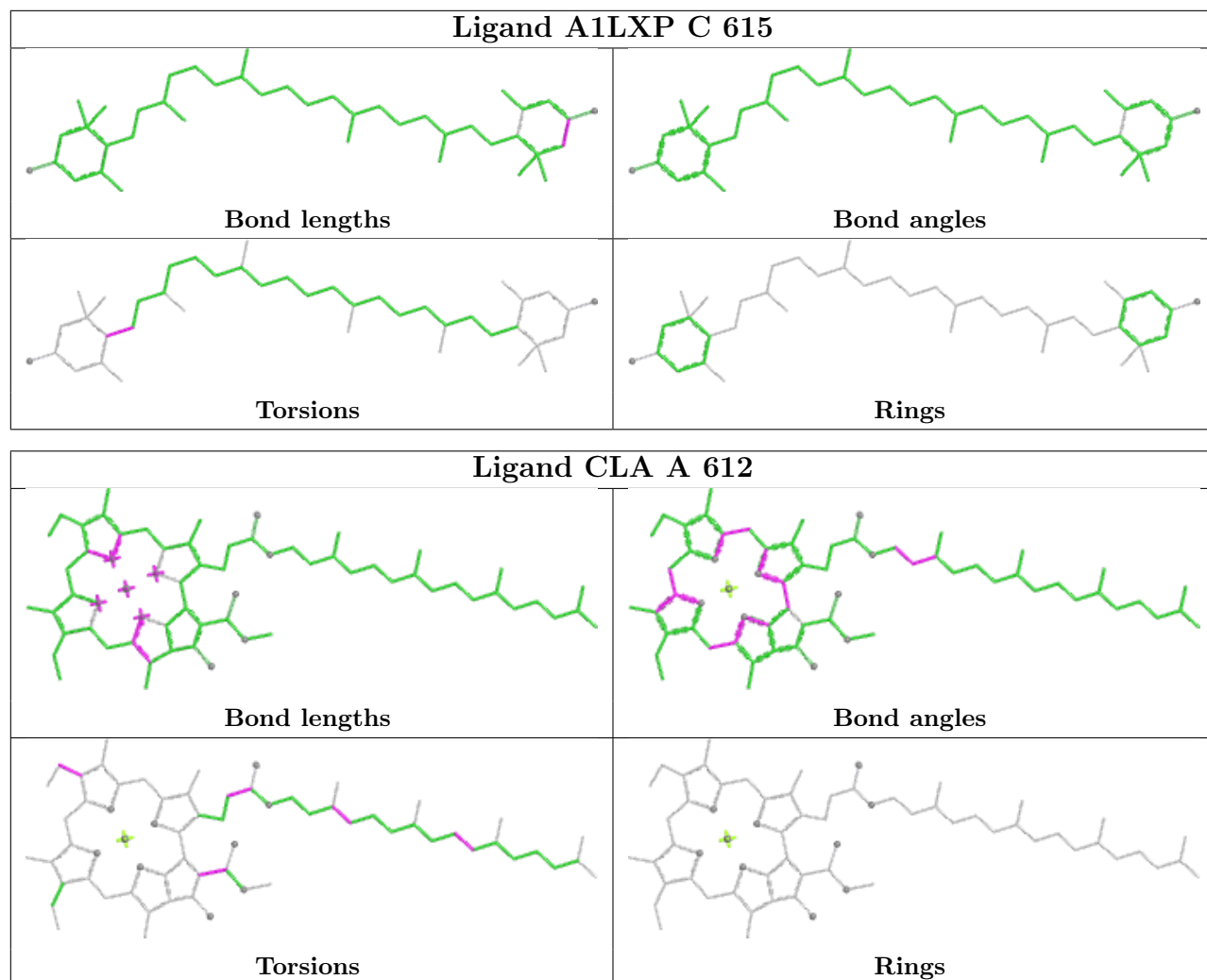


Ligand CHL B 606

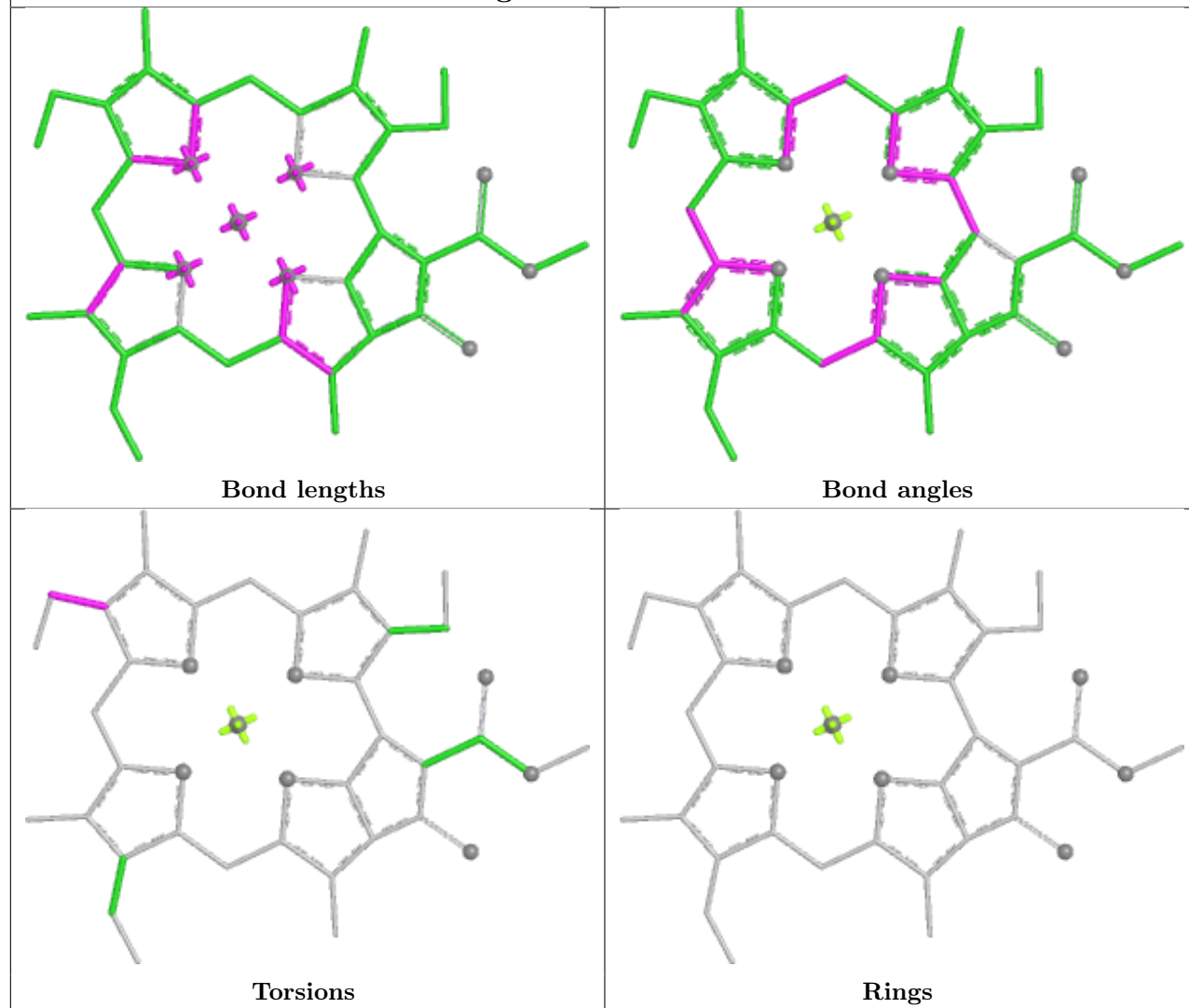


Ligand CLA B 612

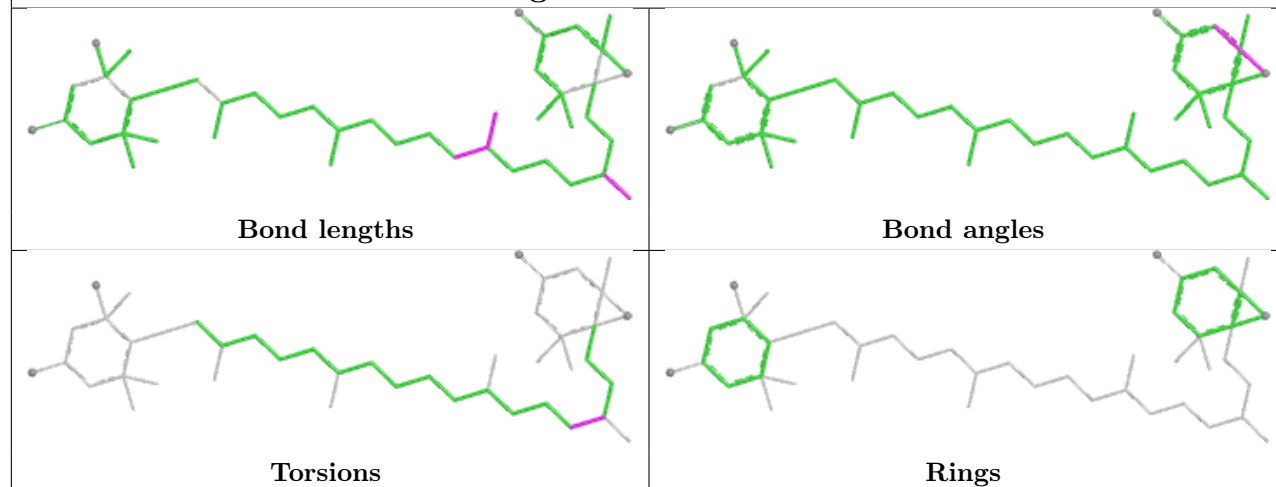


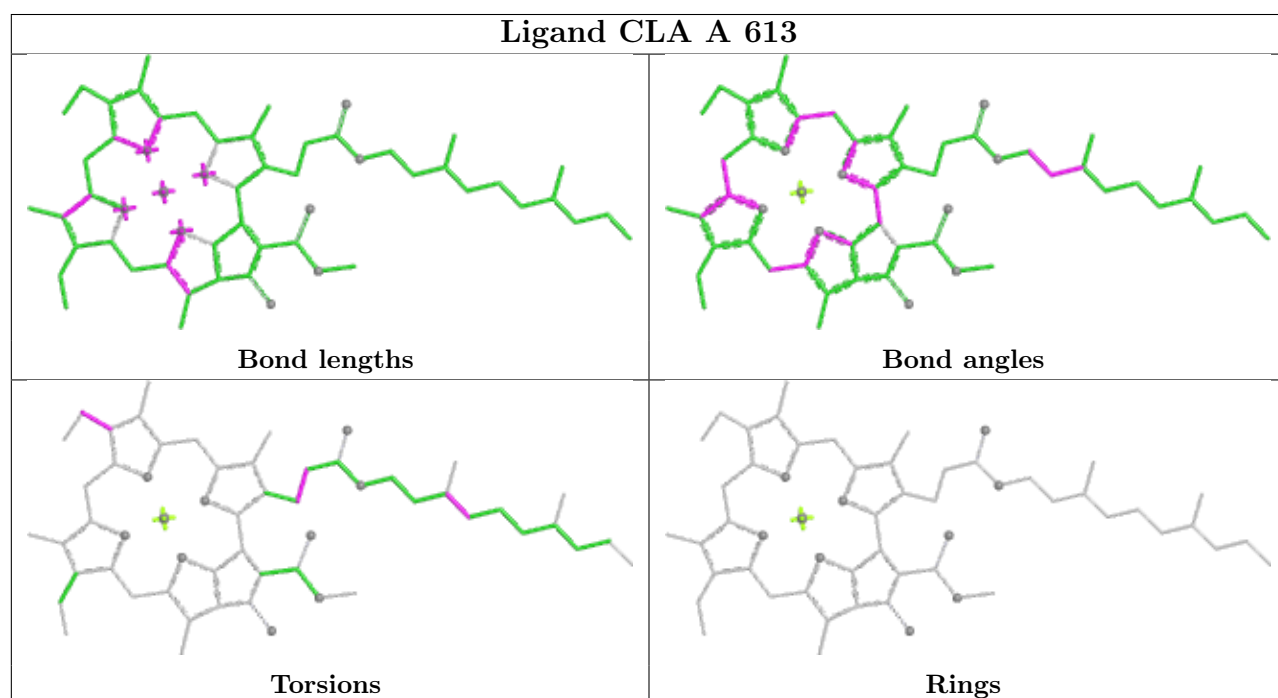
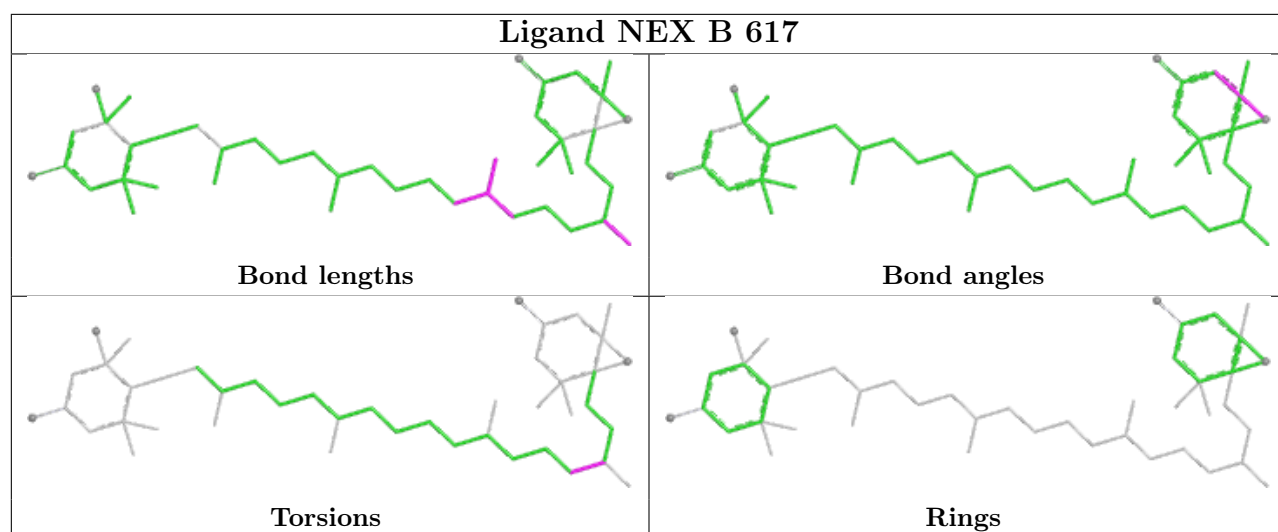


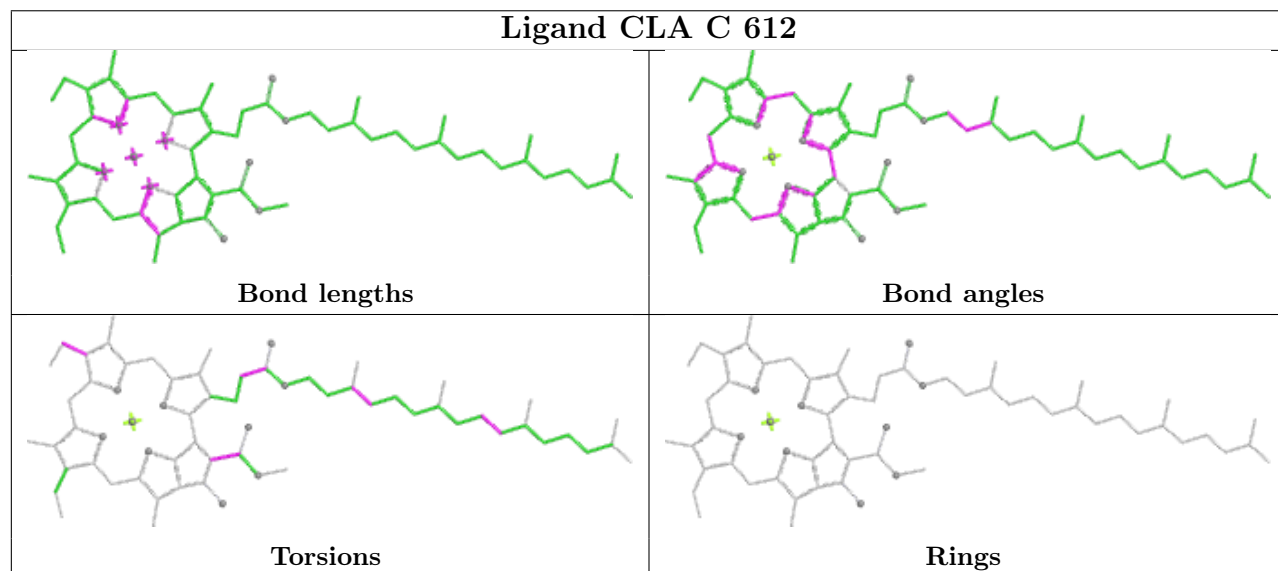
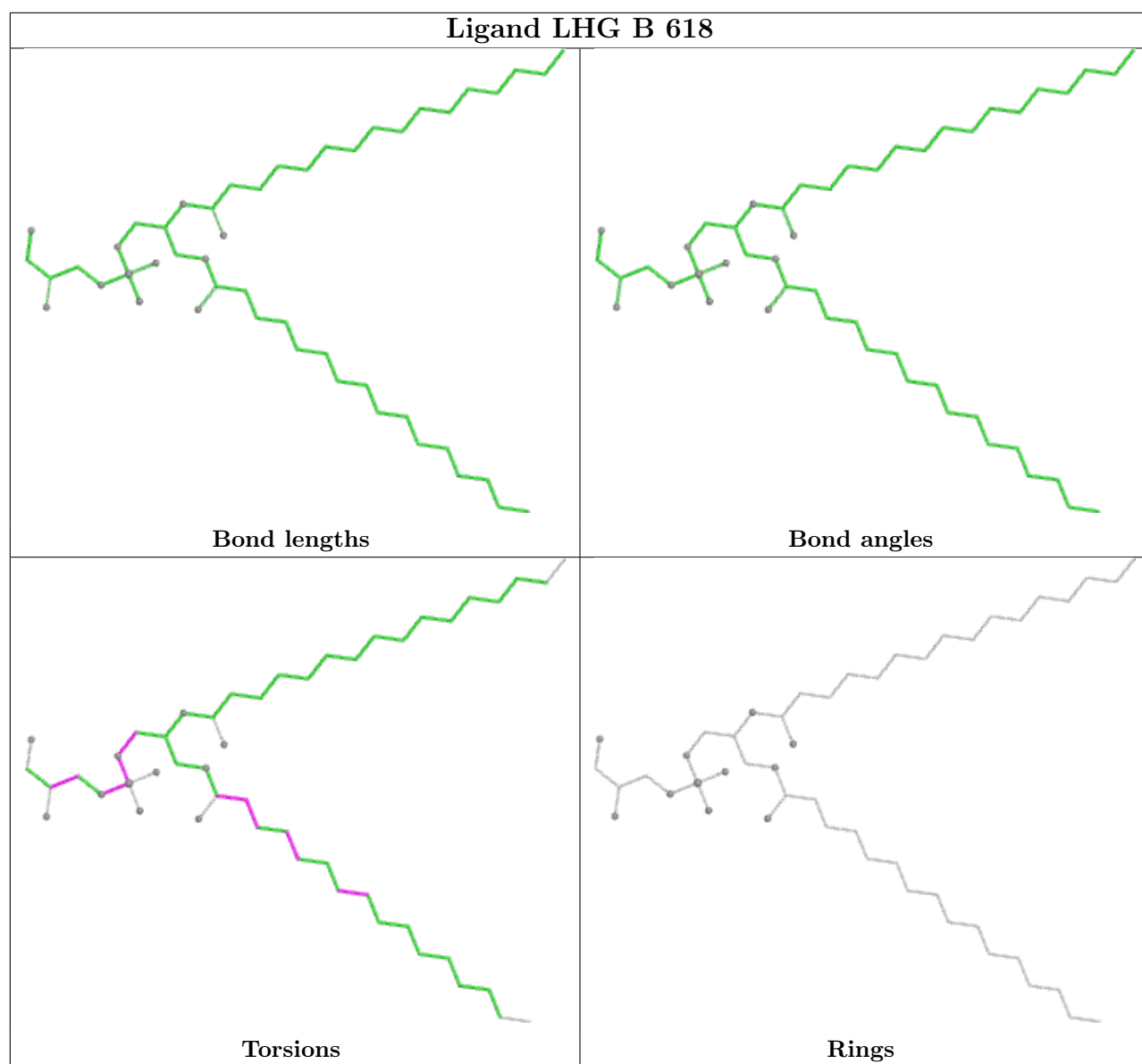
Ligand CLA B 614



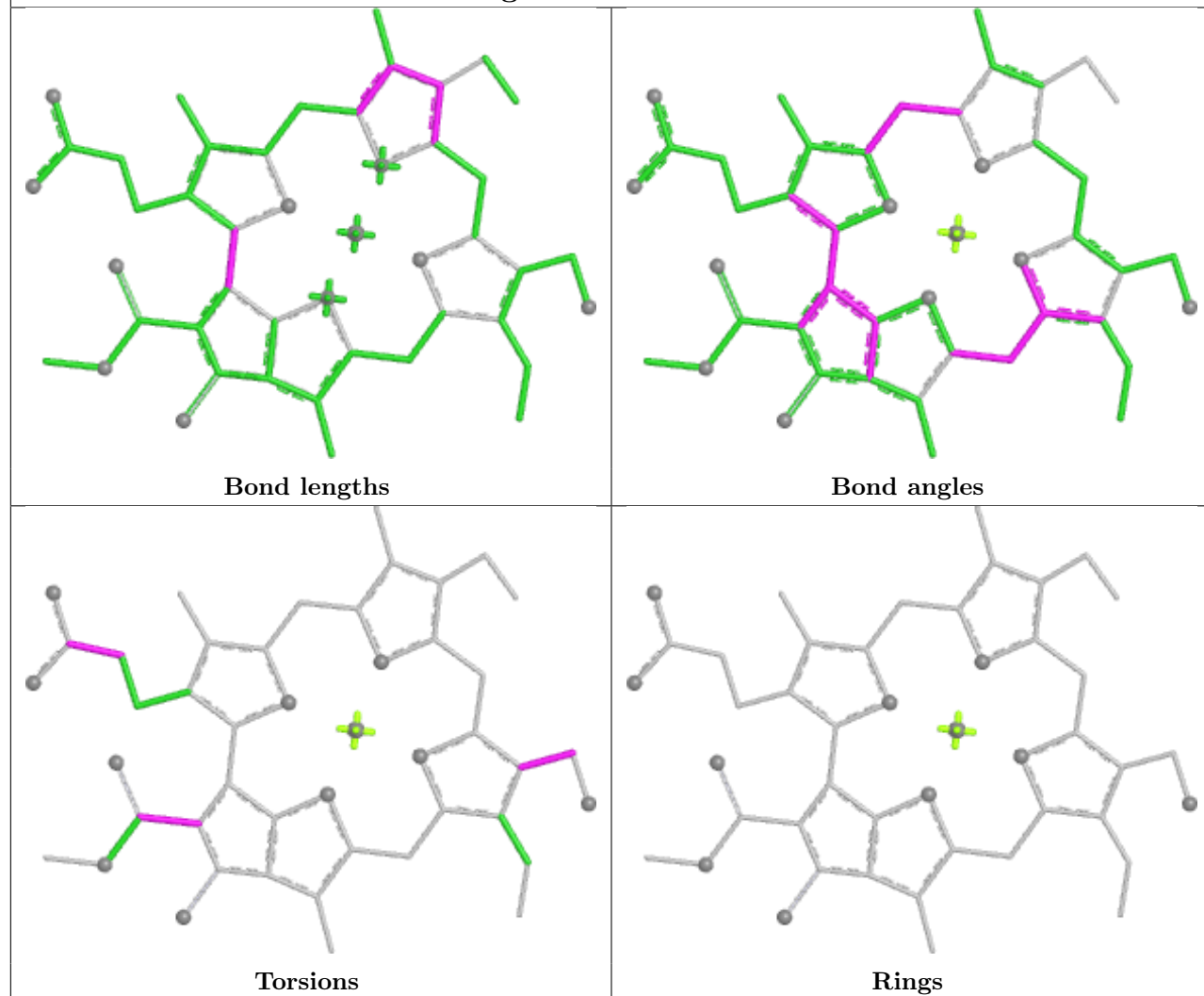
Ligand NEX A 617



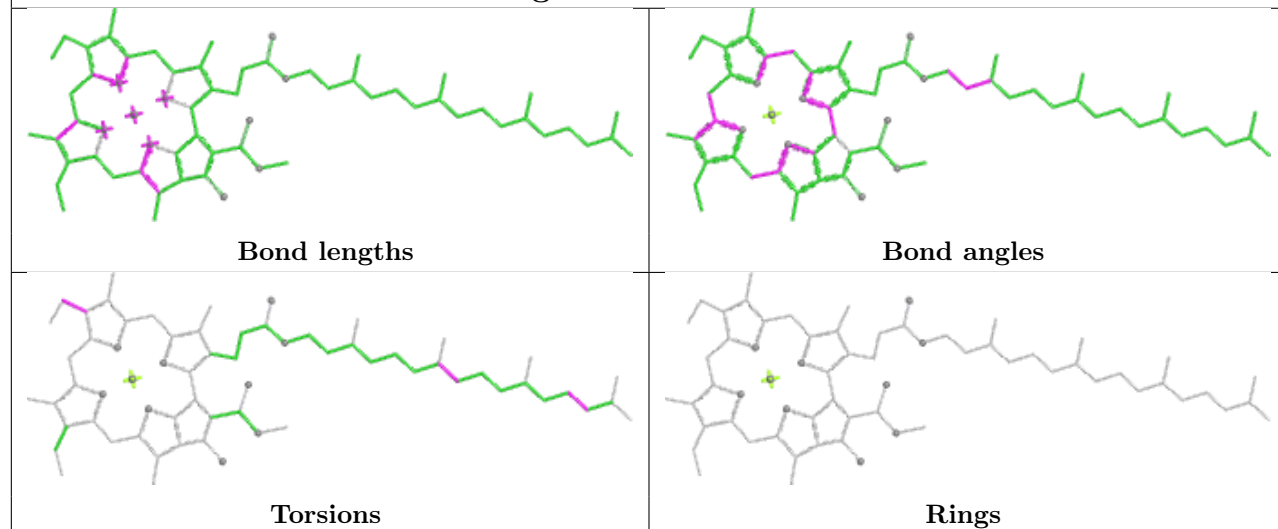




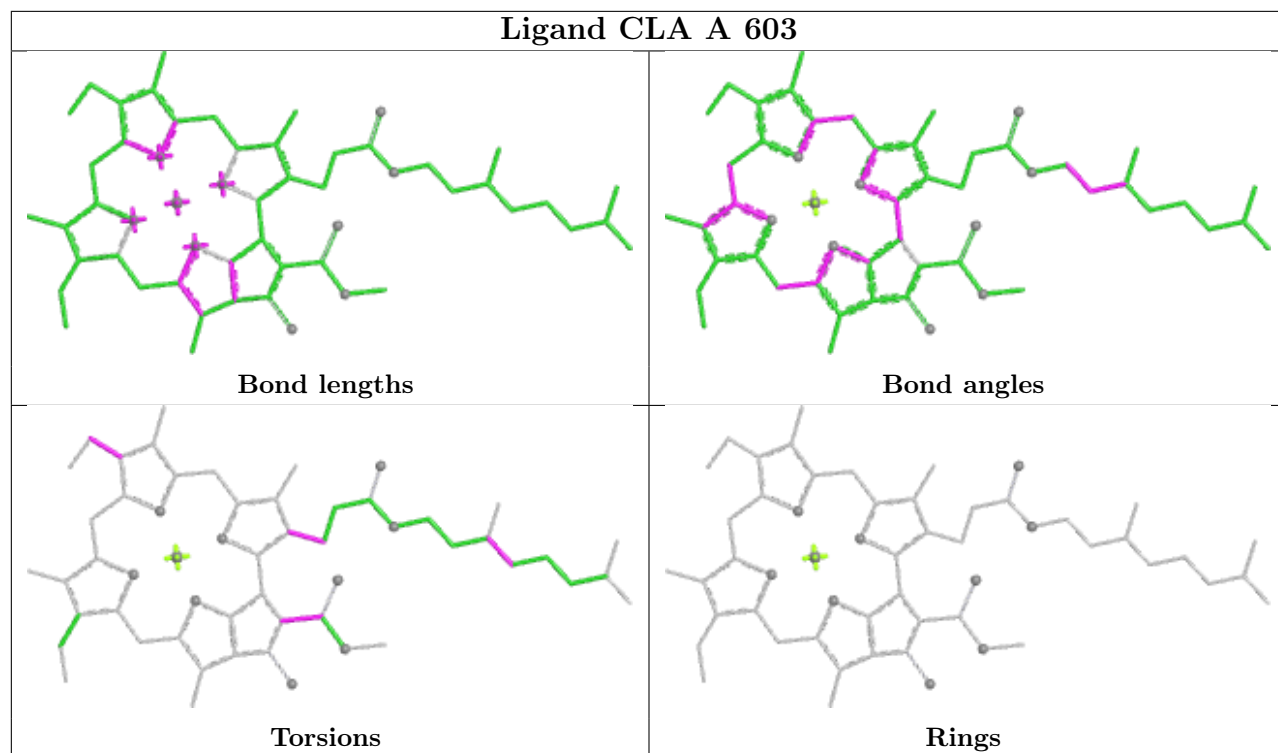
Ligand CHL B 607



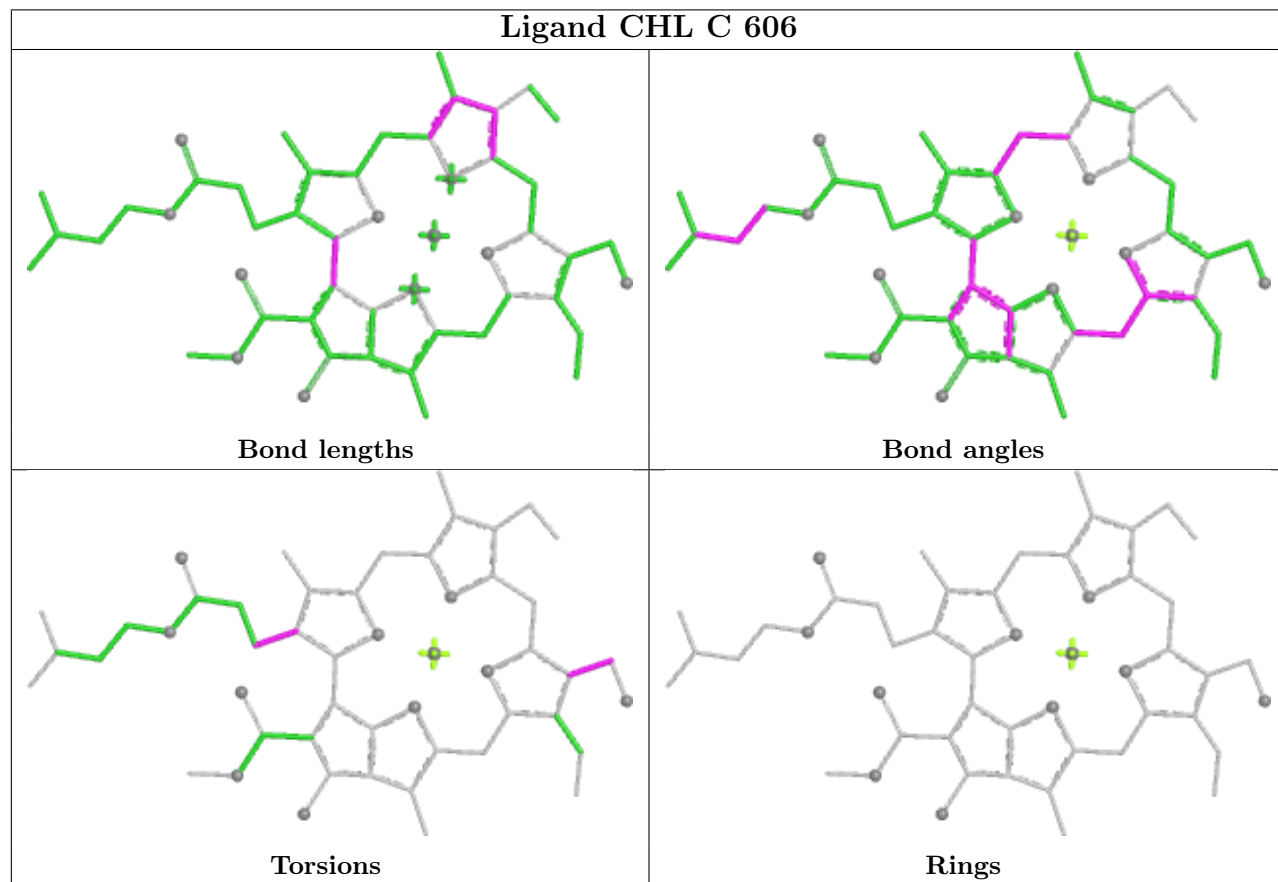
Ligand CLA C 610



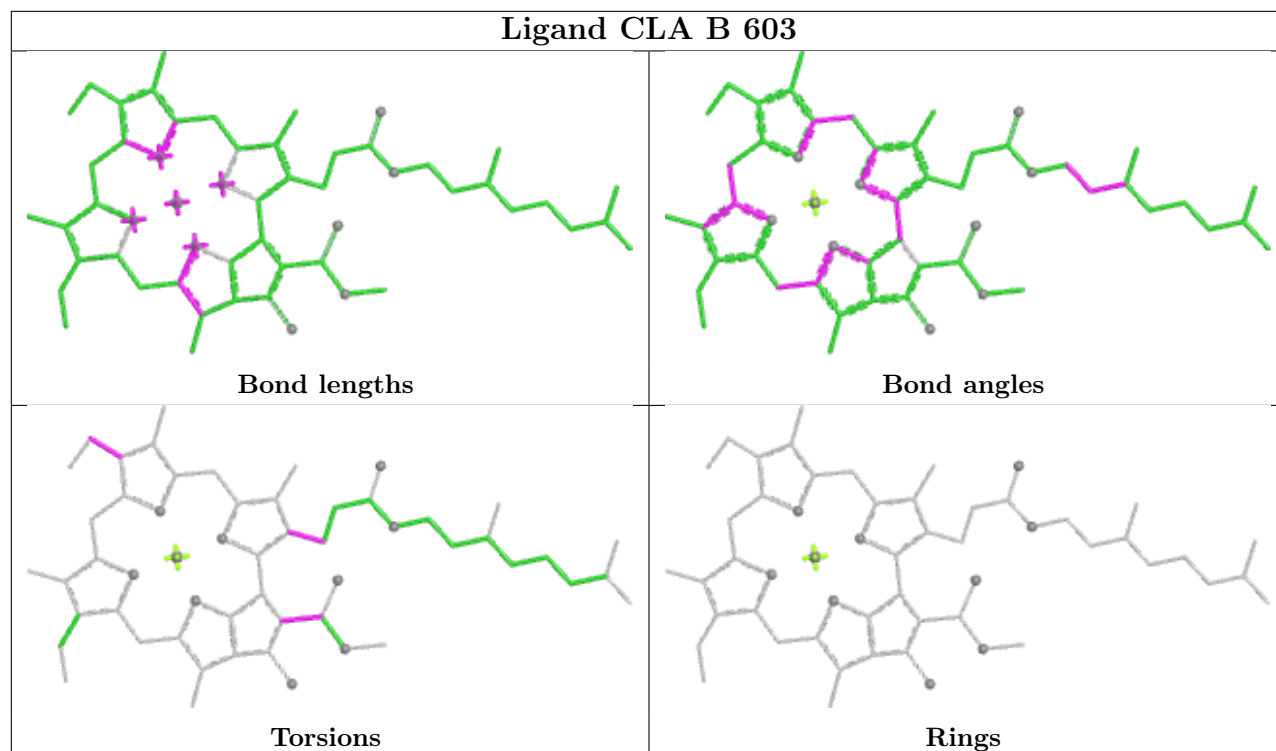
Ligand CLA A 603



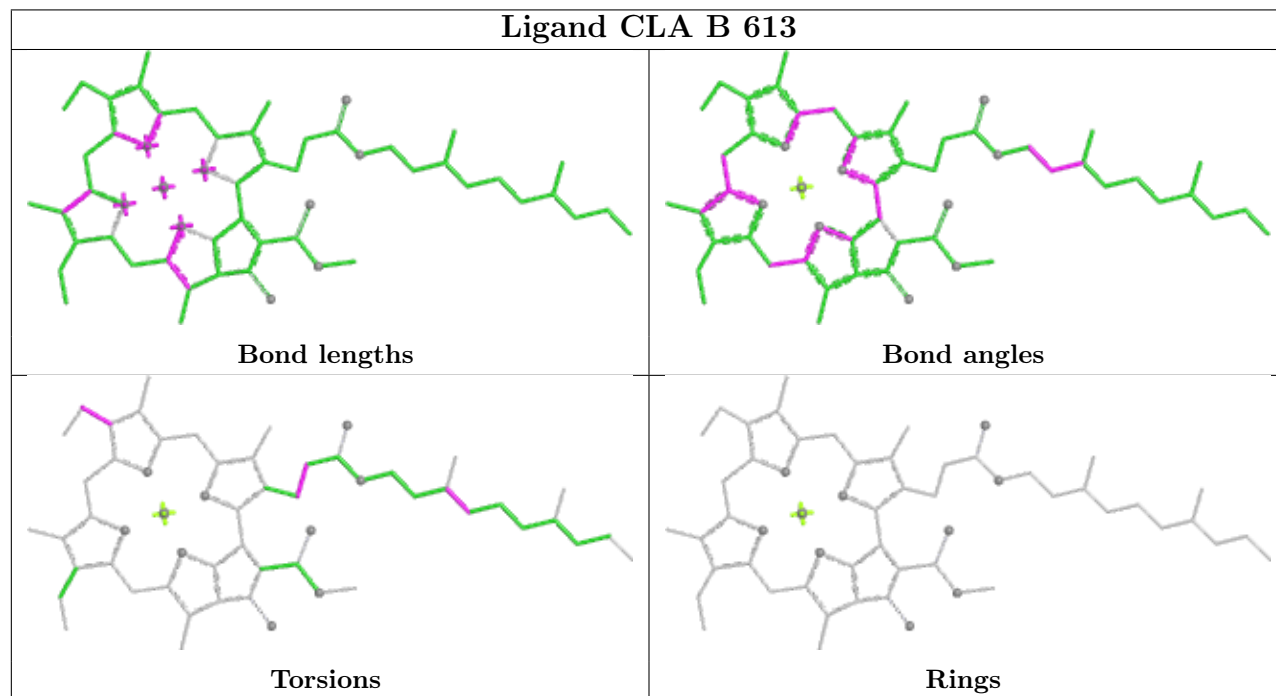
Ligand CHL C 606

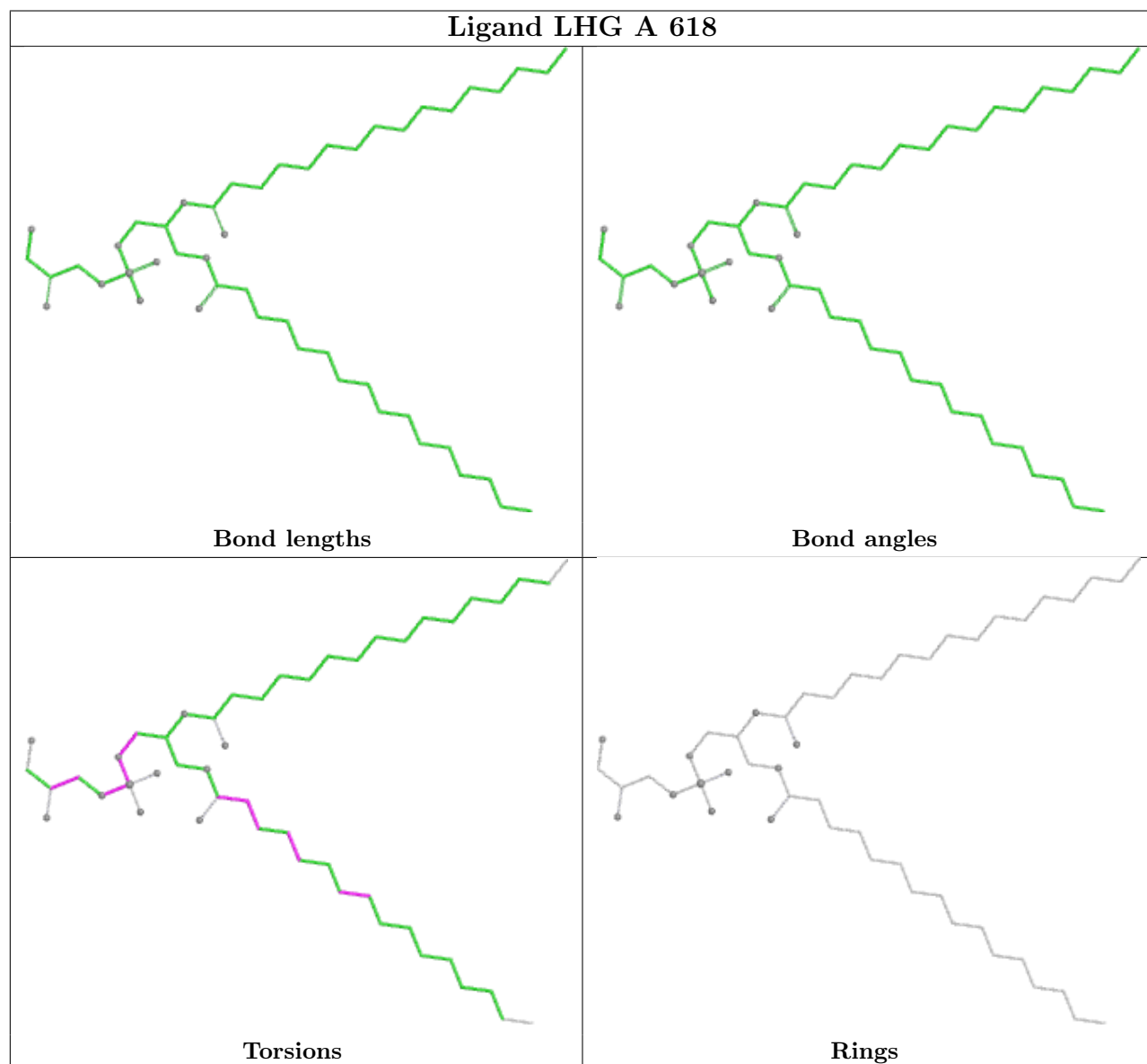
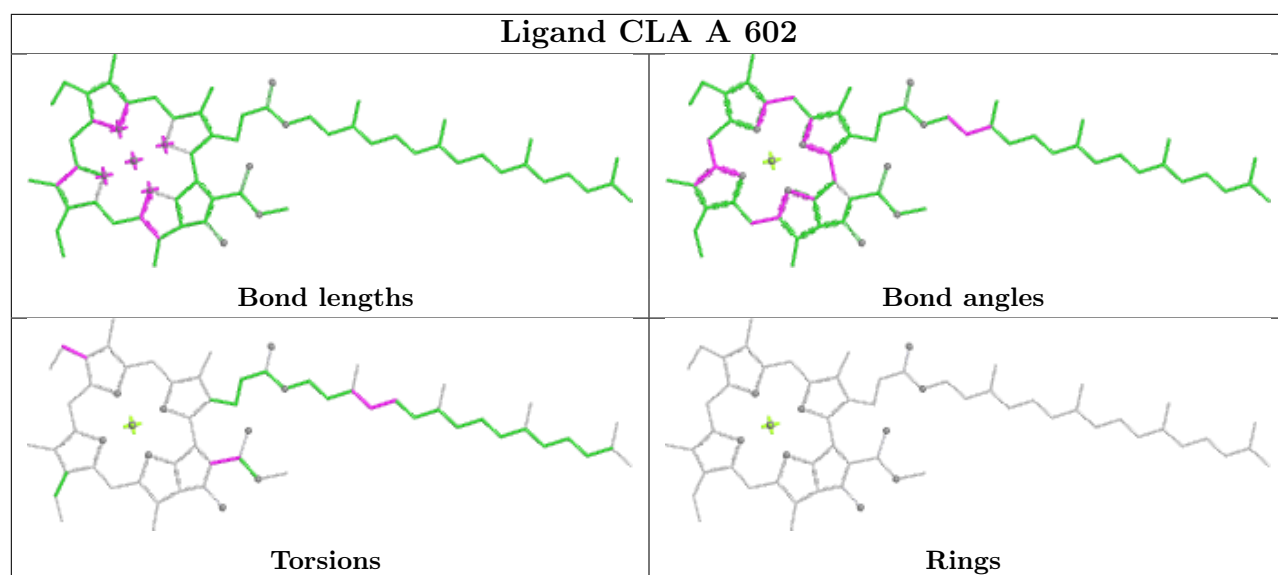


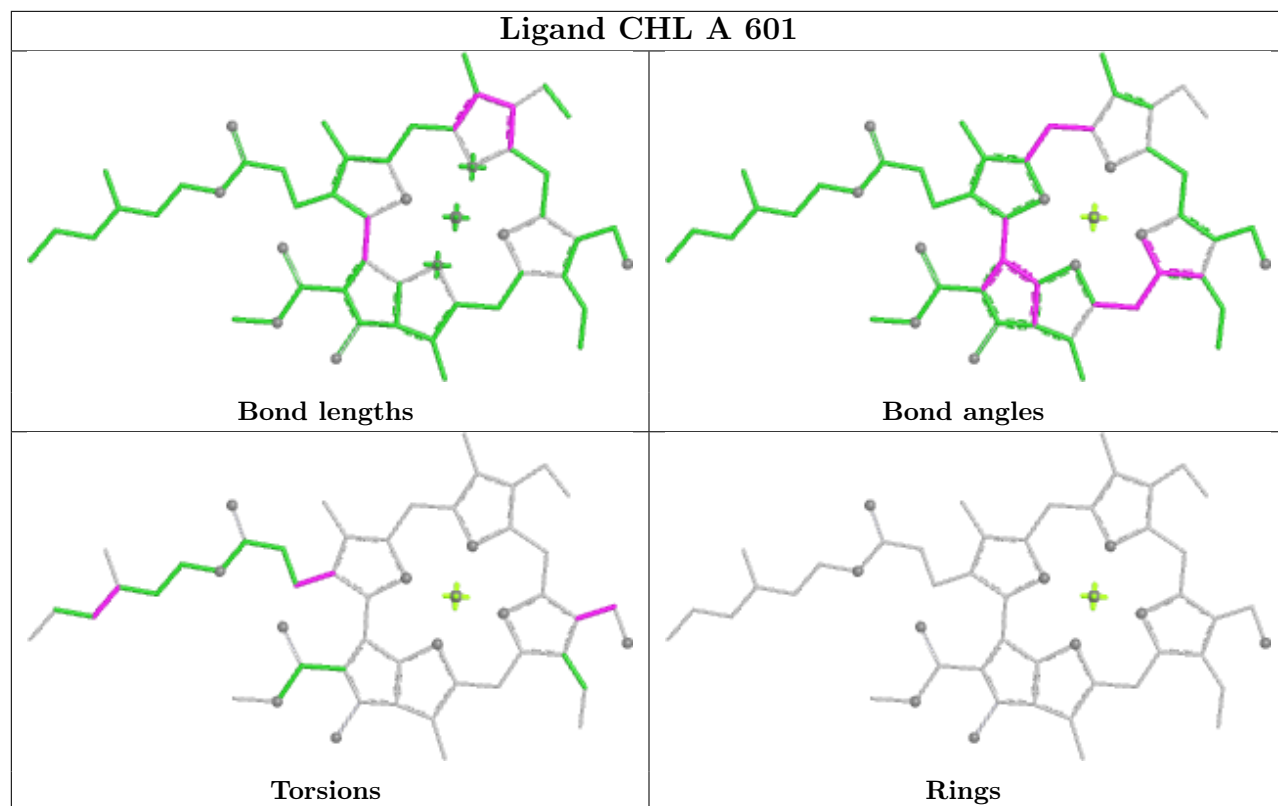
Ligand CLA B 603

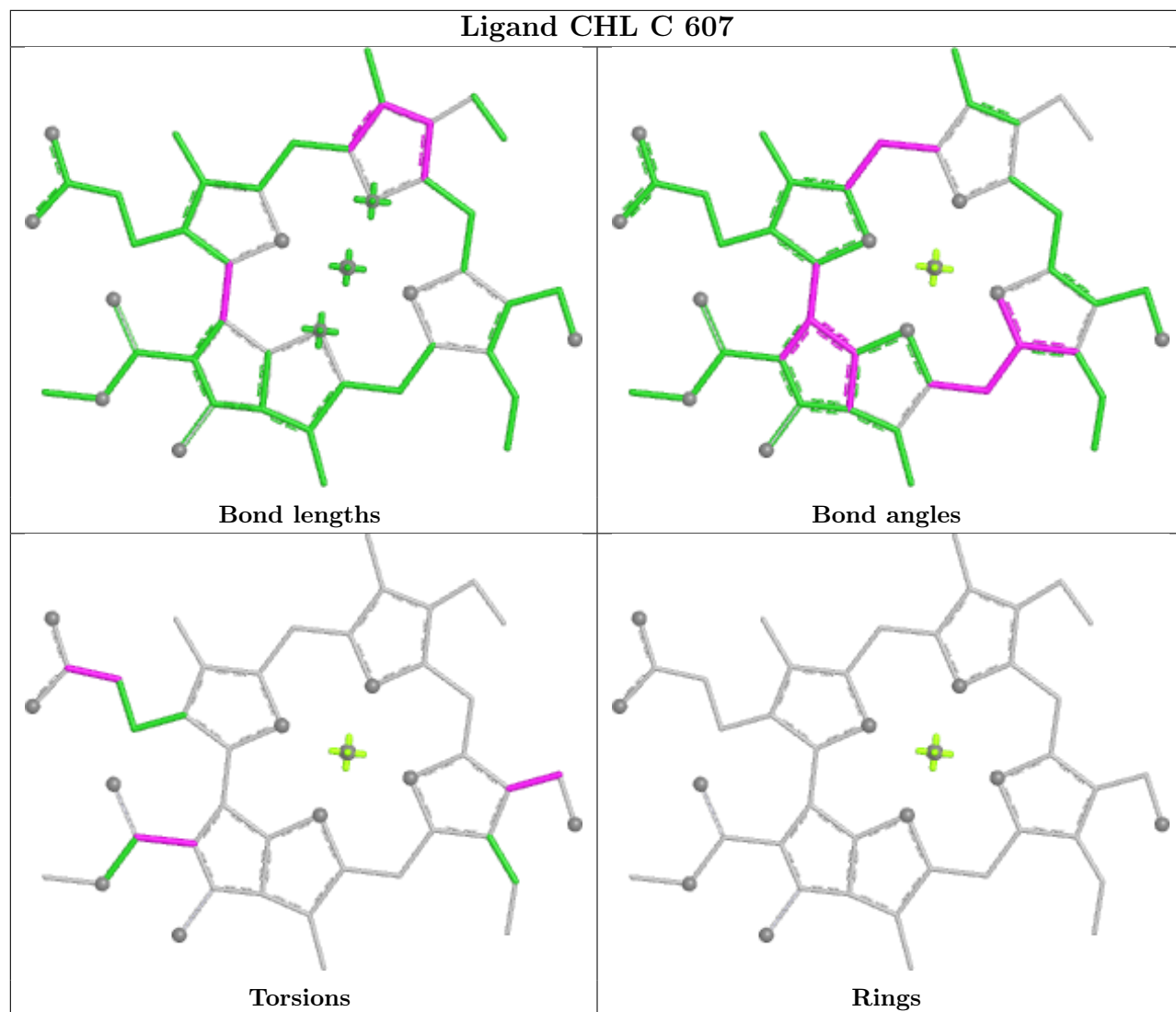


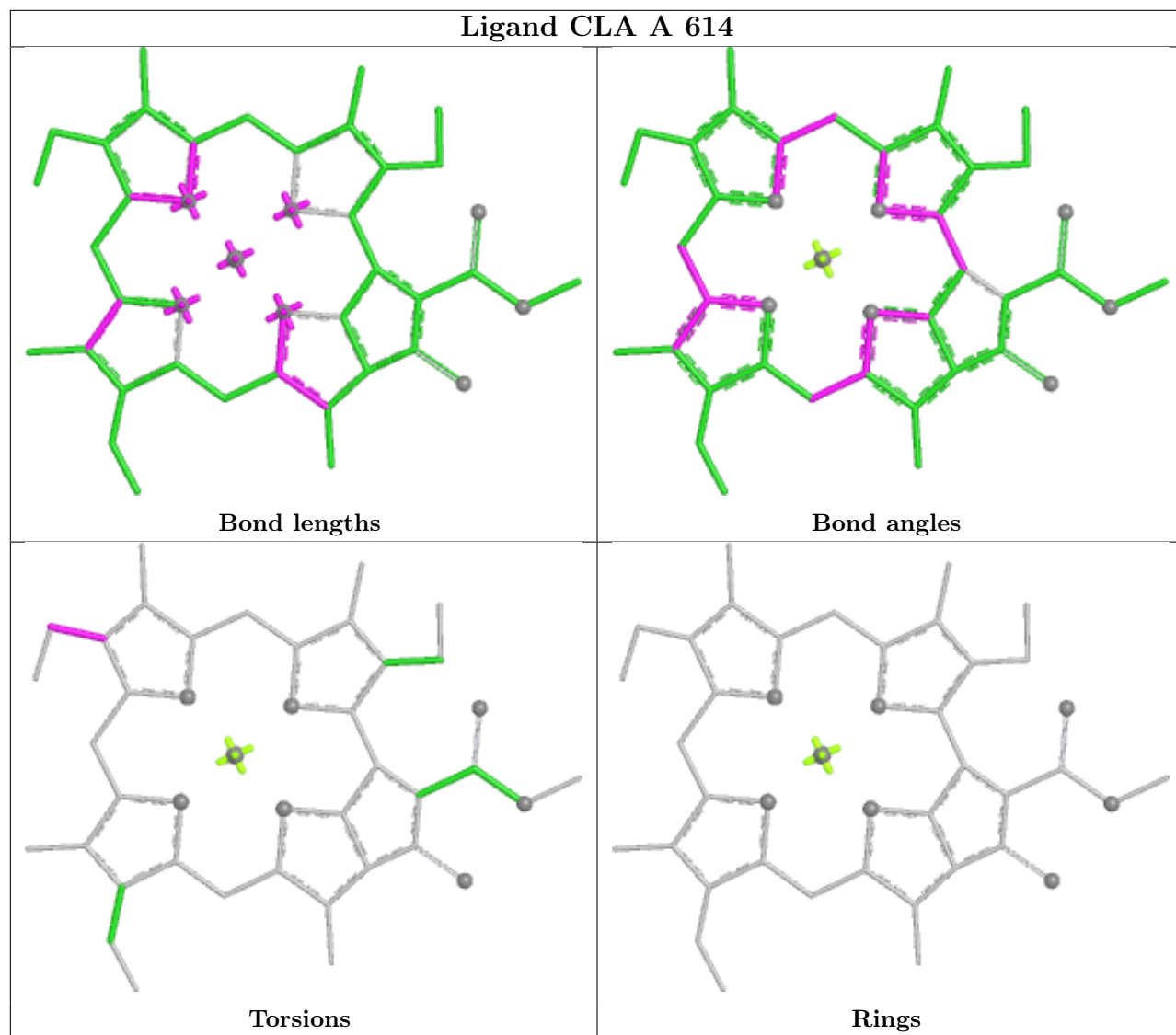
Ligand CLA B 613

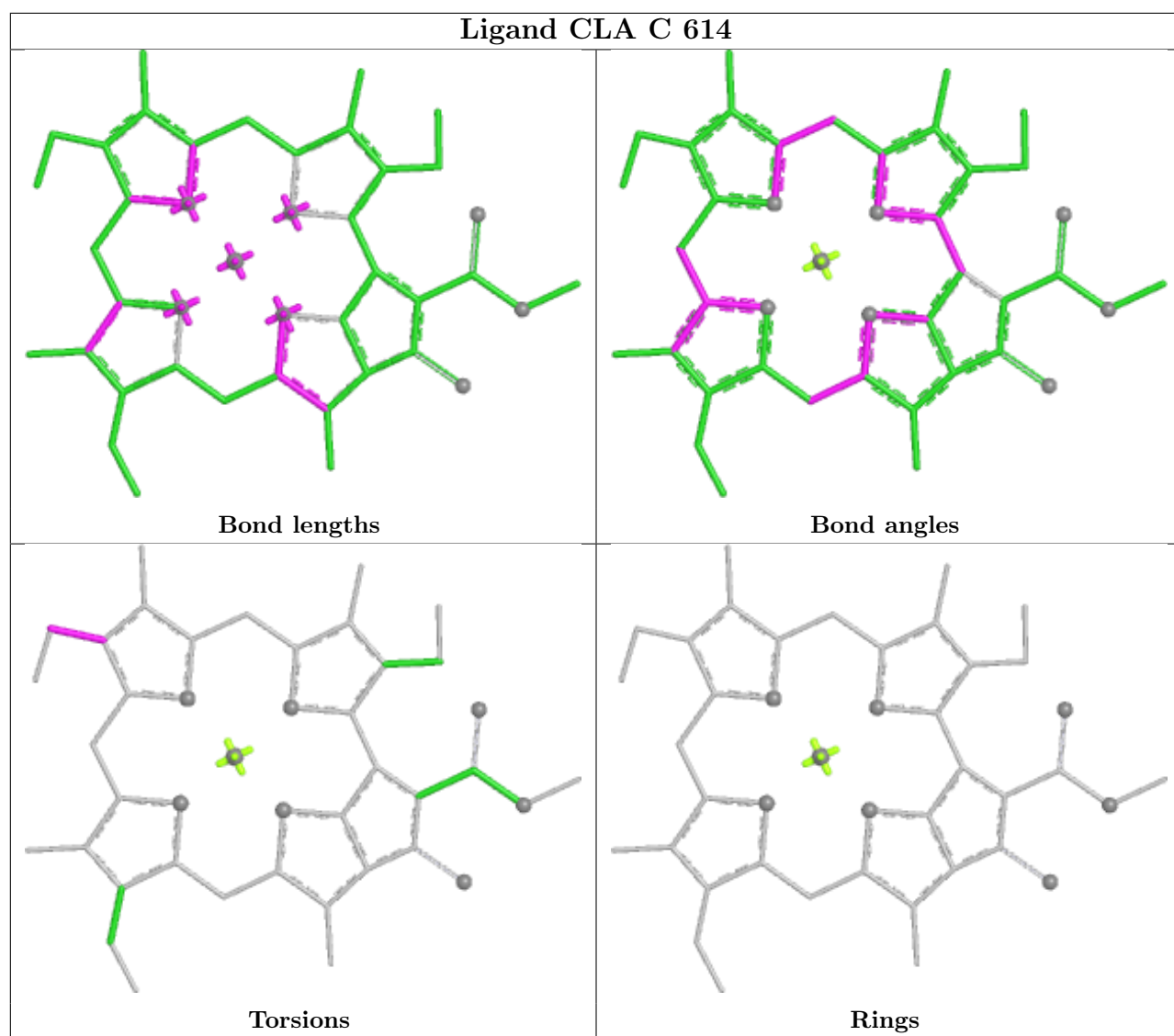


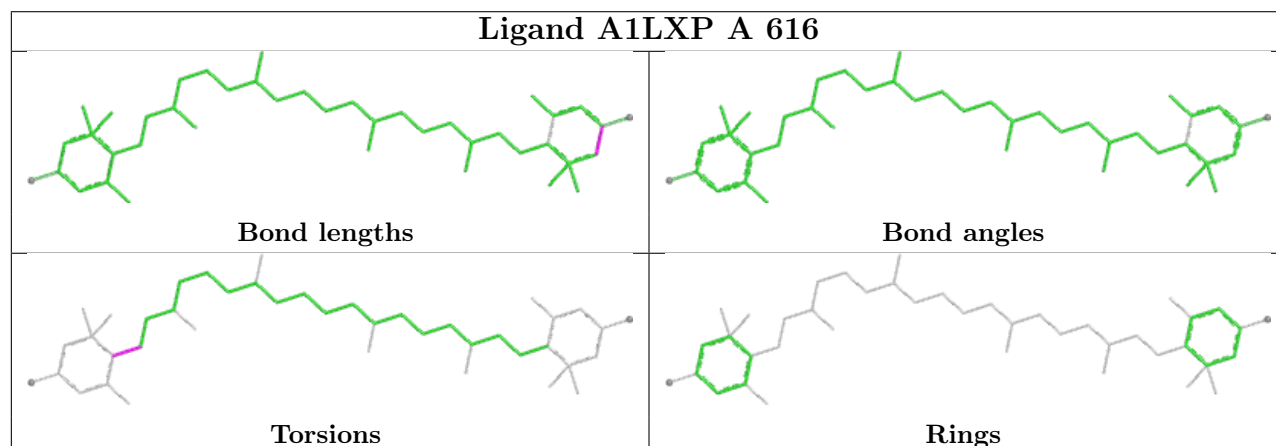
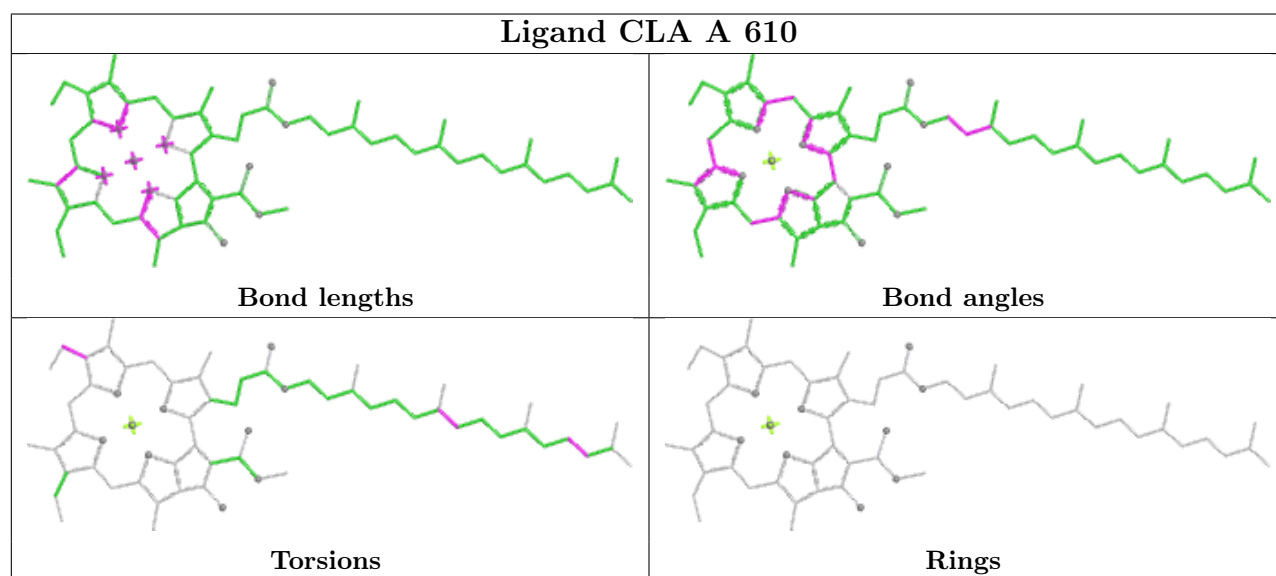
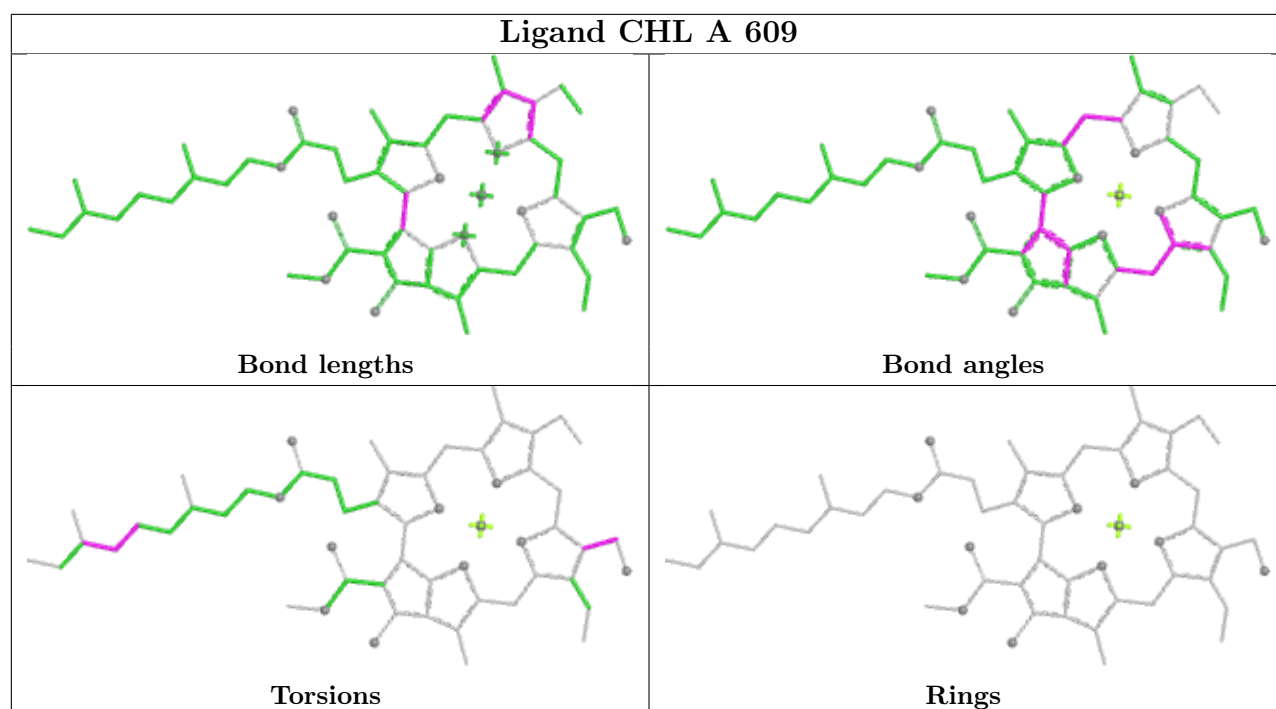


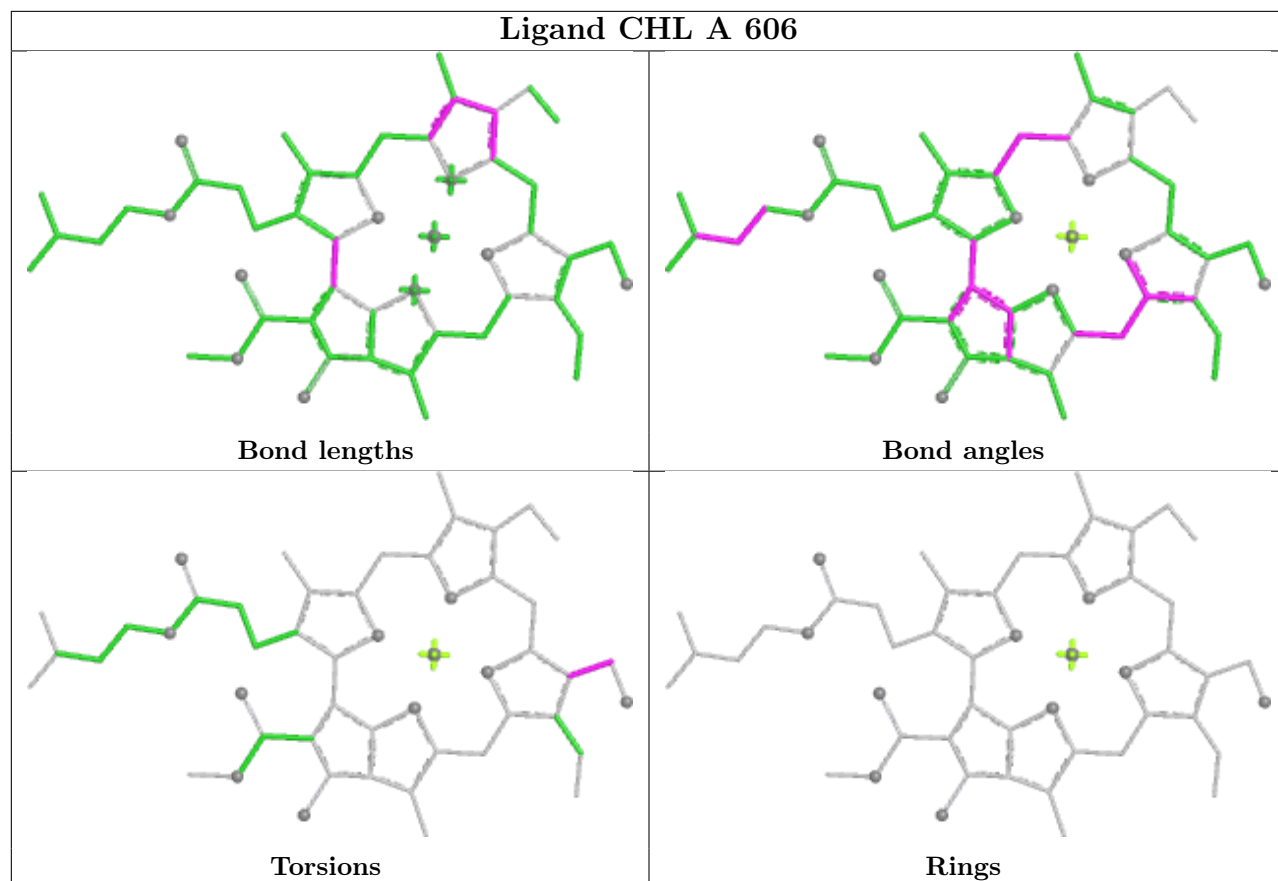




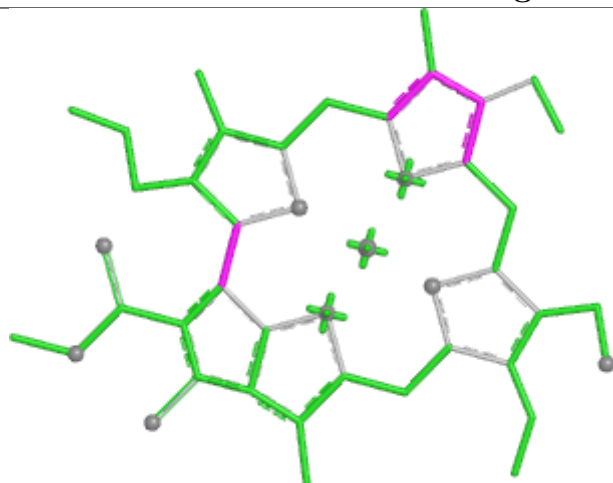




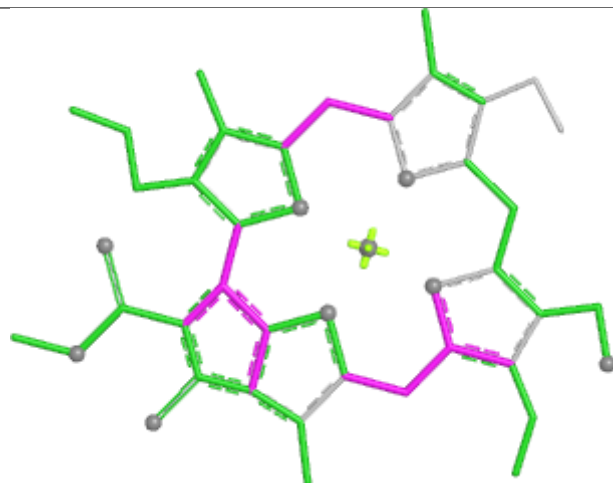




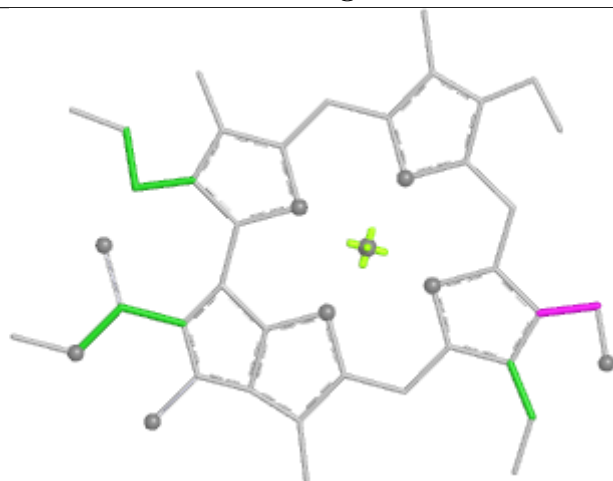
Ligand CHL B 605



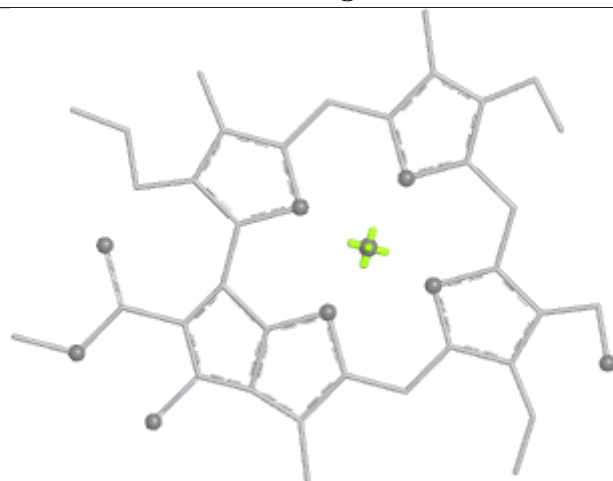
Bond lengths



Bond angles

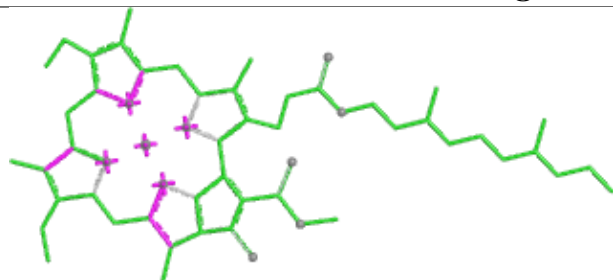


Torsions

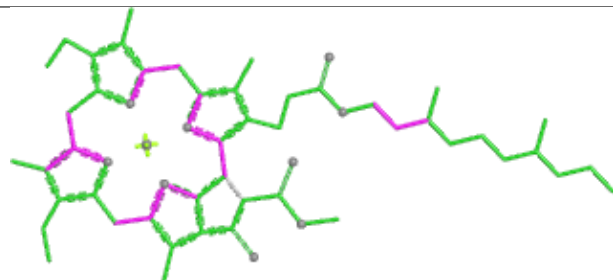


Rings

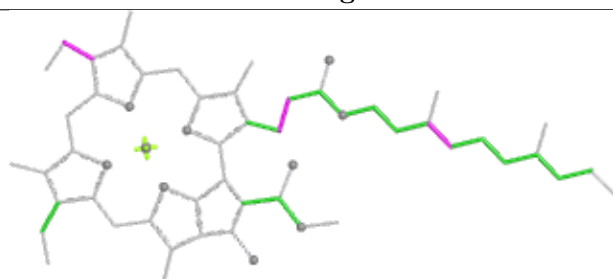
Ligand CLA C 613



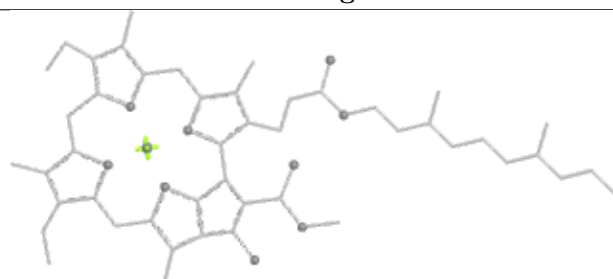
Bond lengths



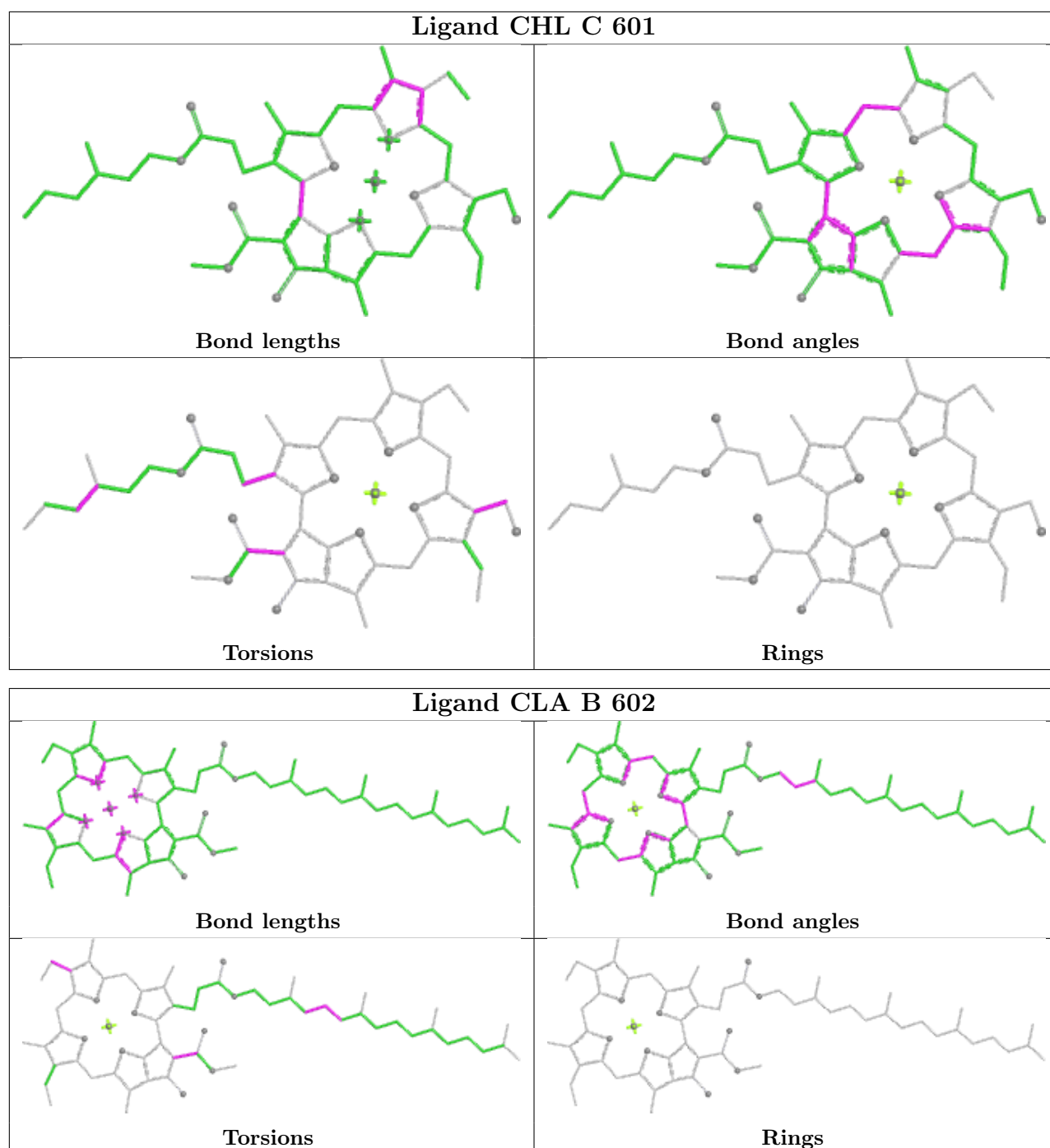
Bond angles

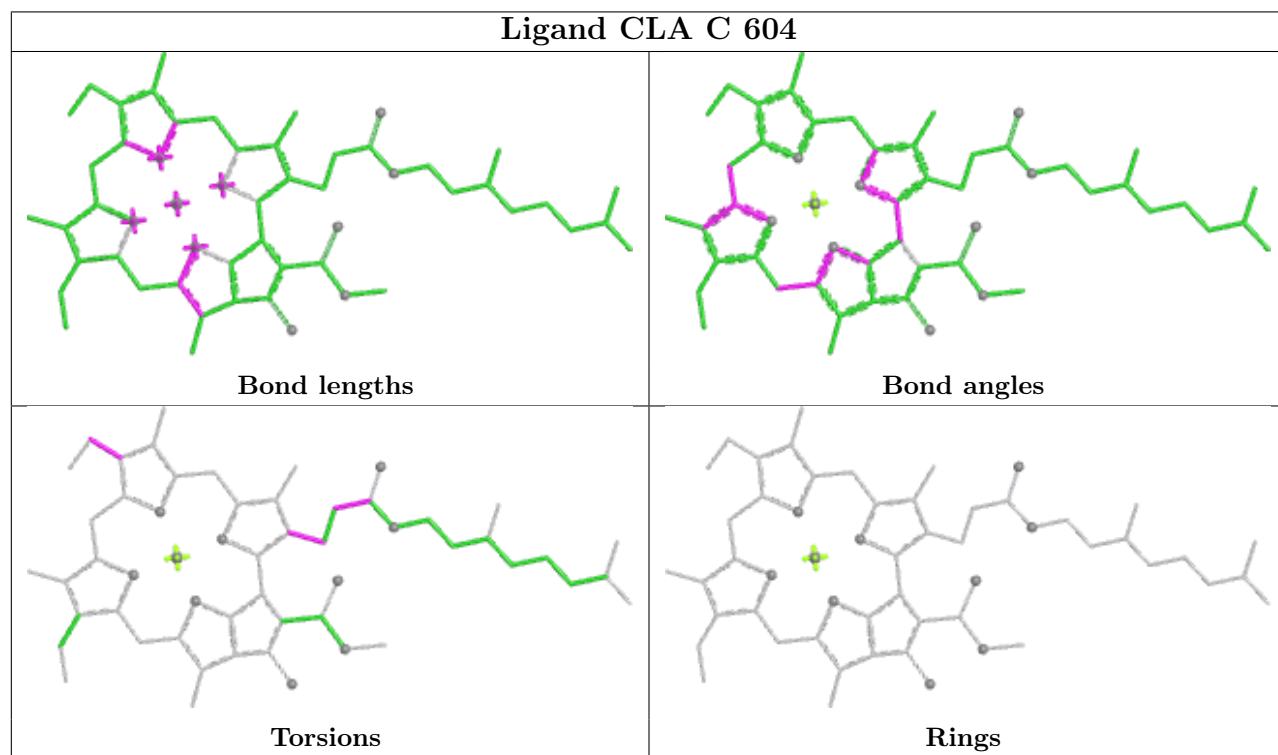
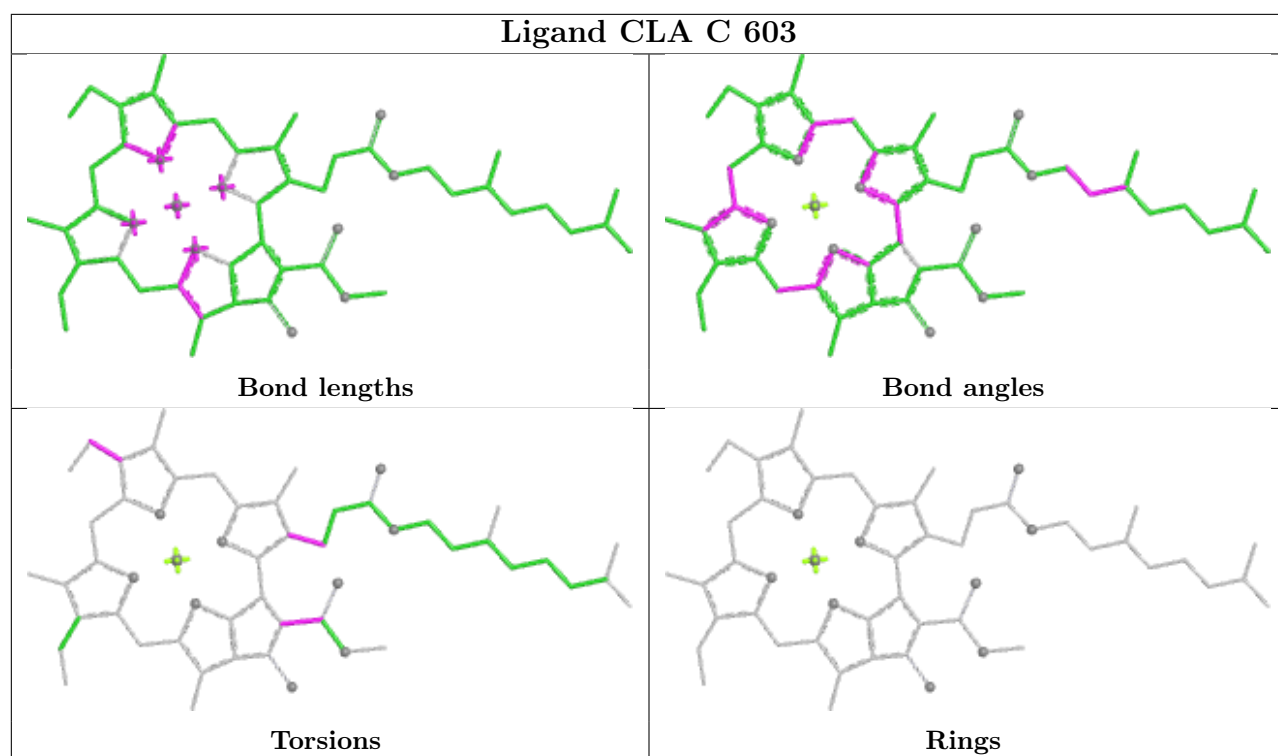


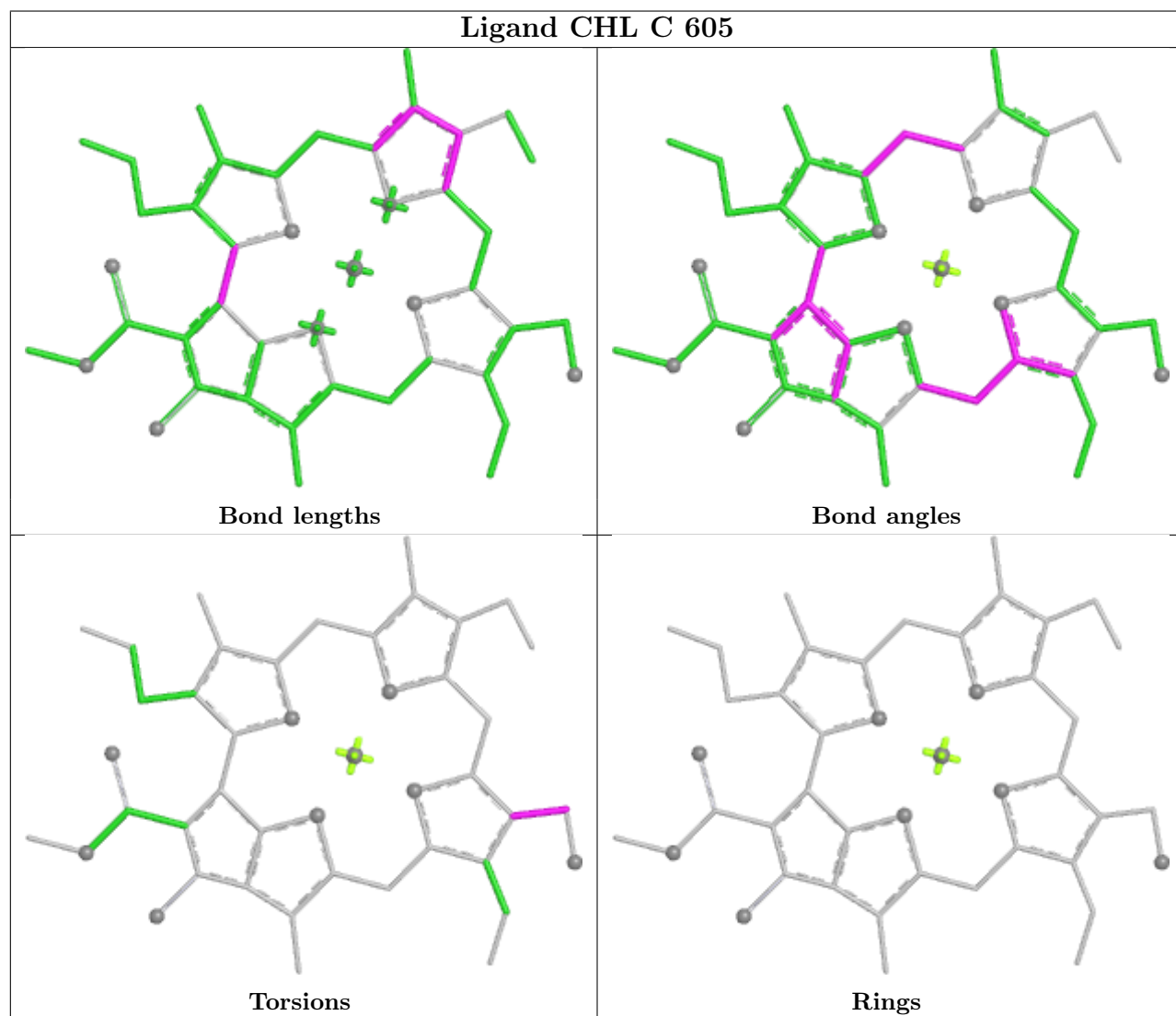
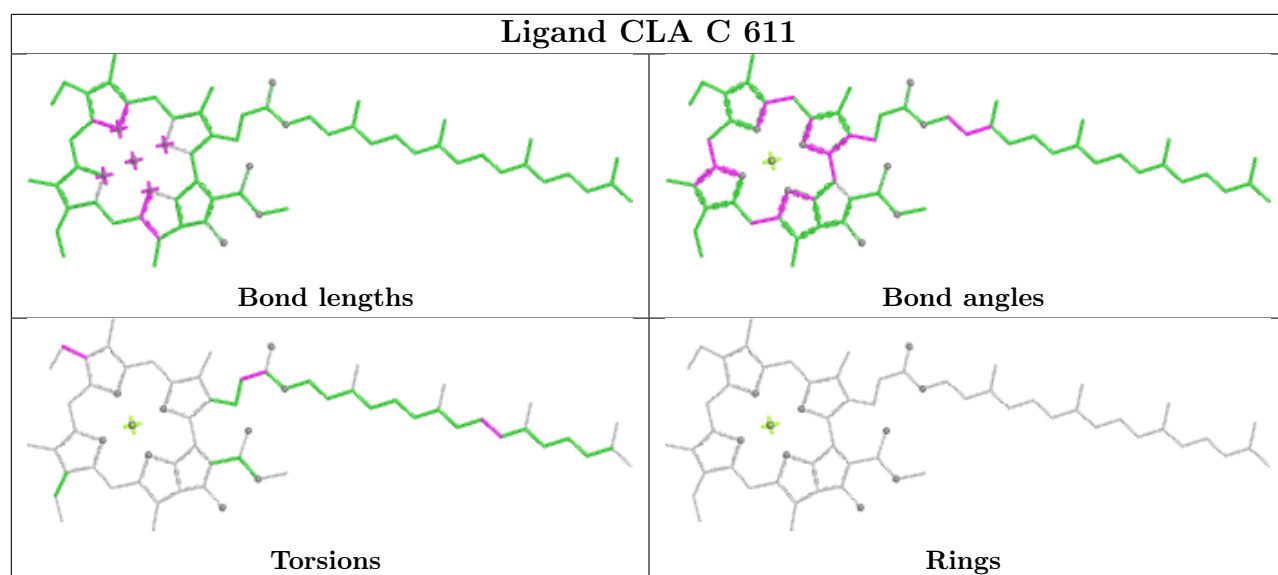
Torsions

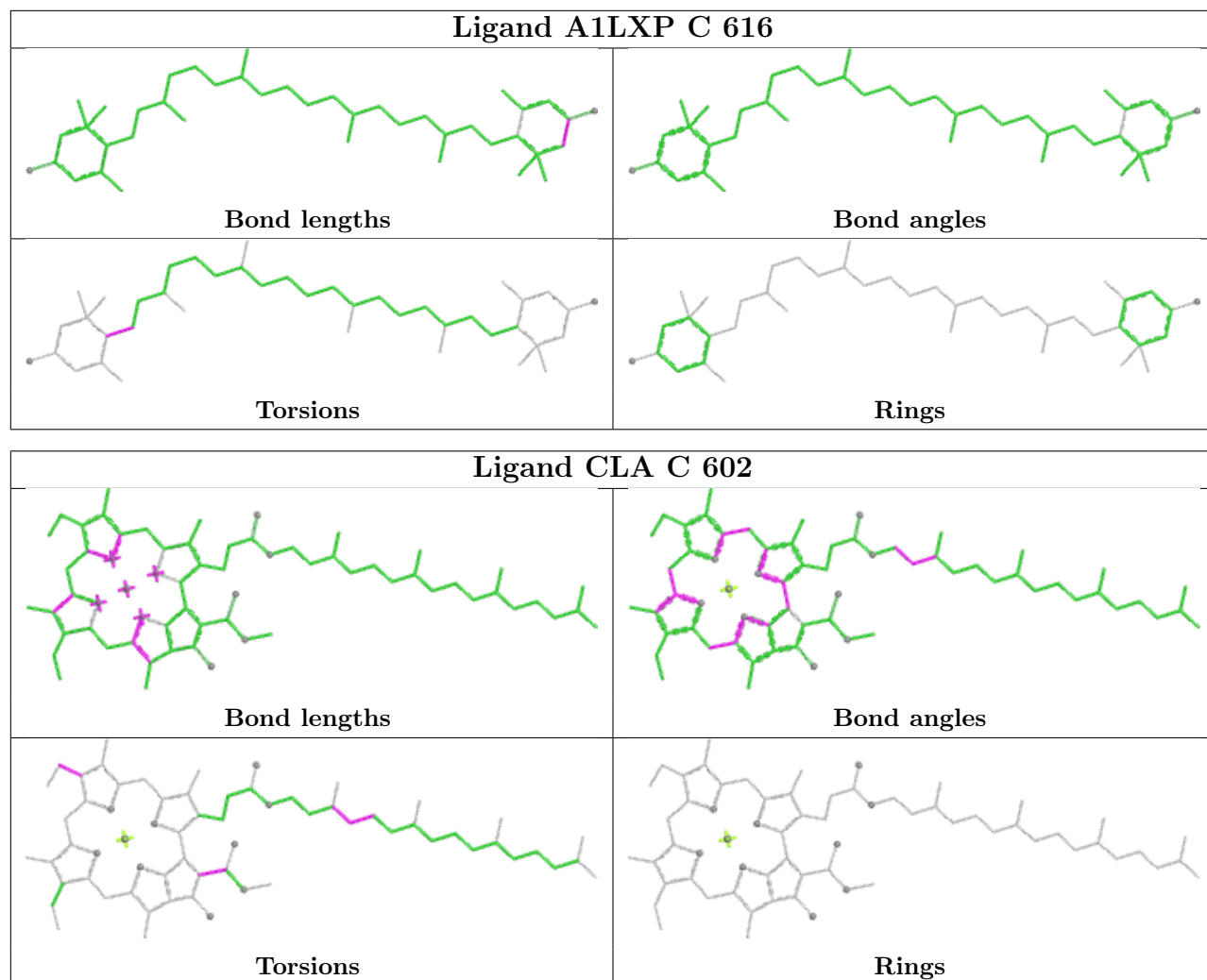


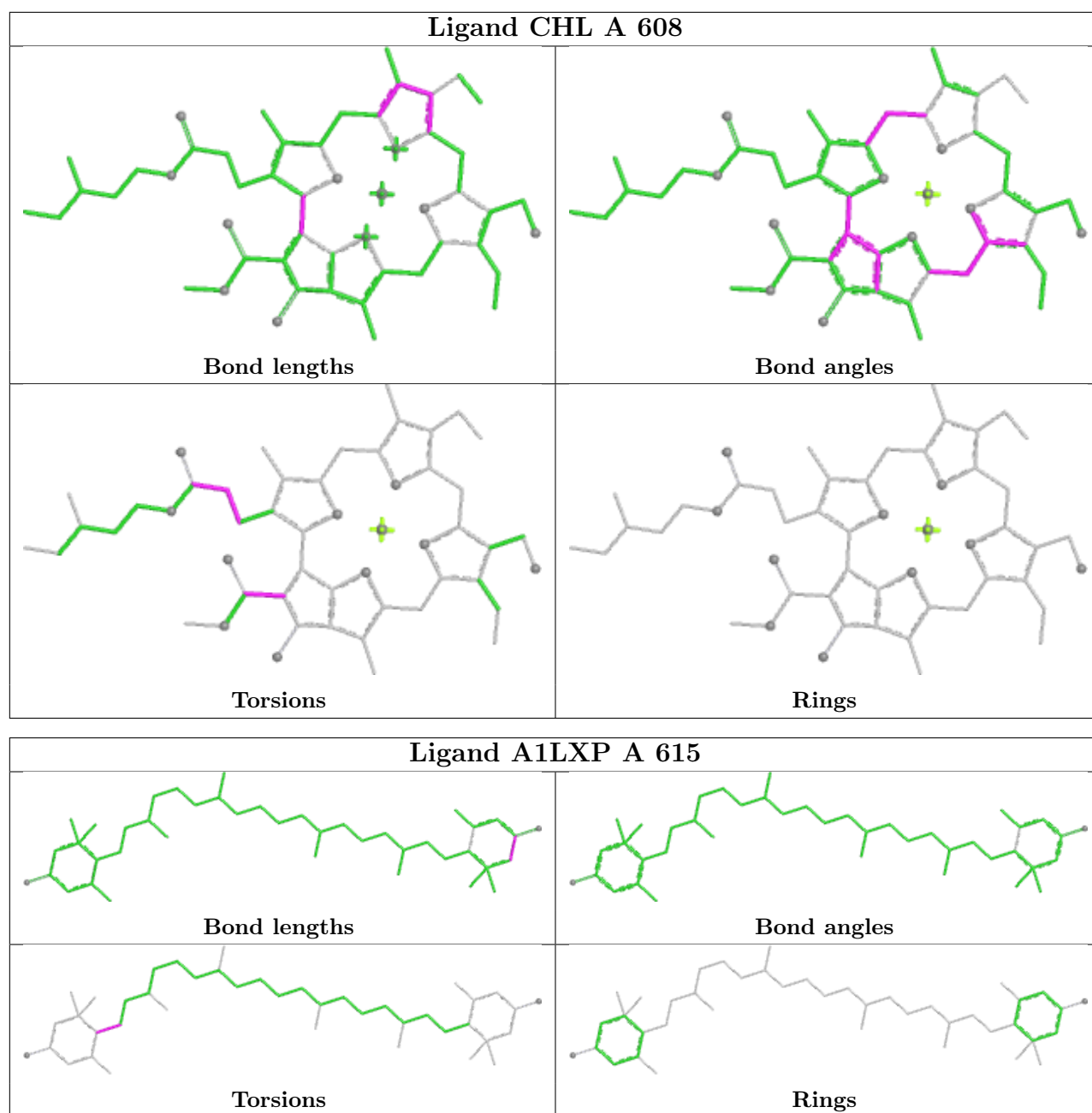
Rings

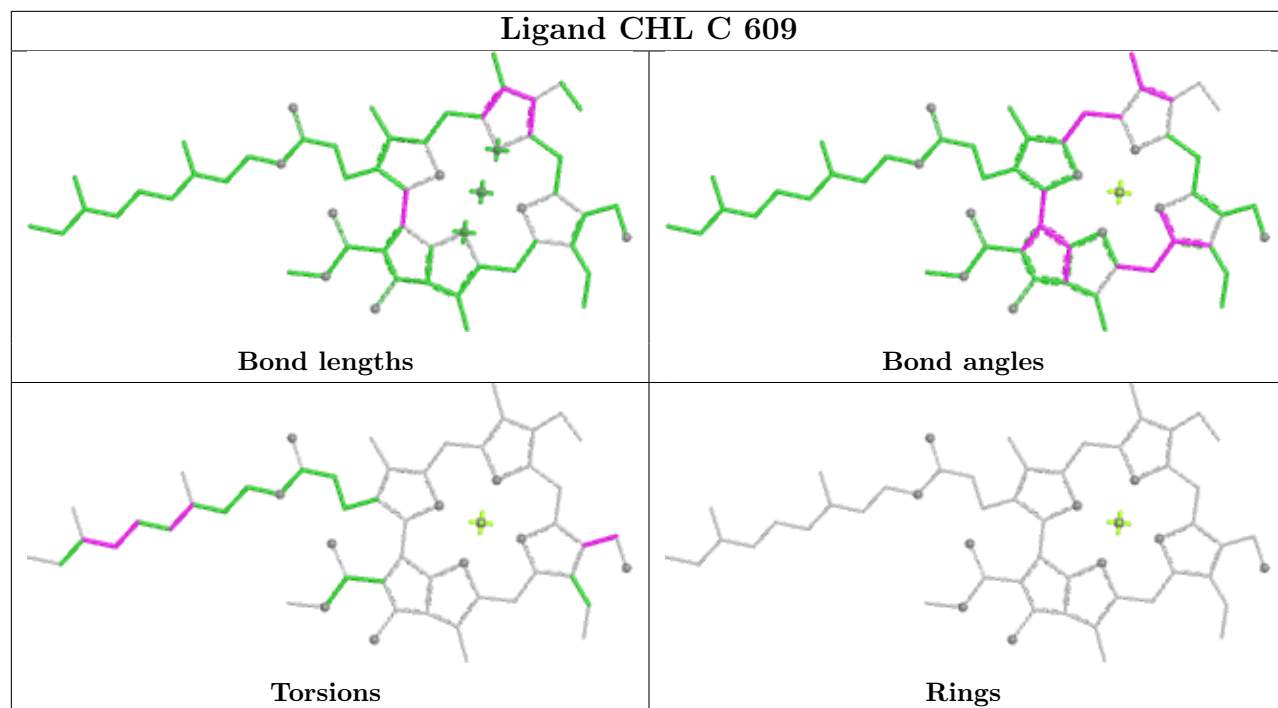




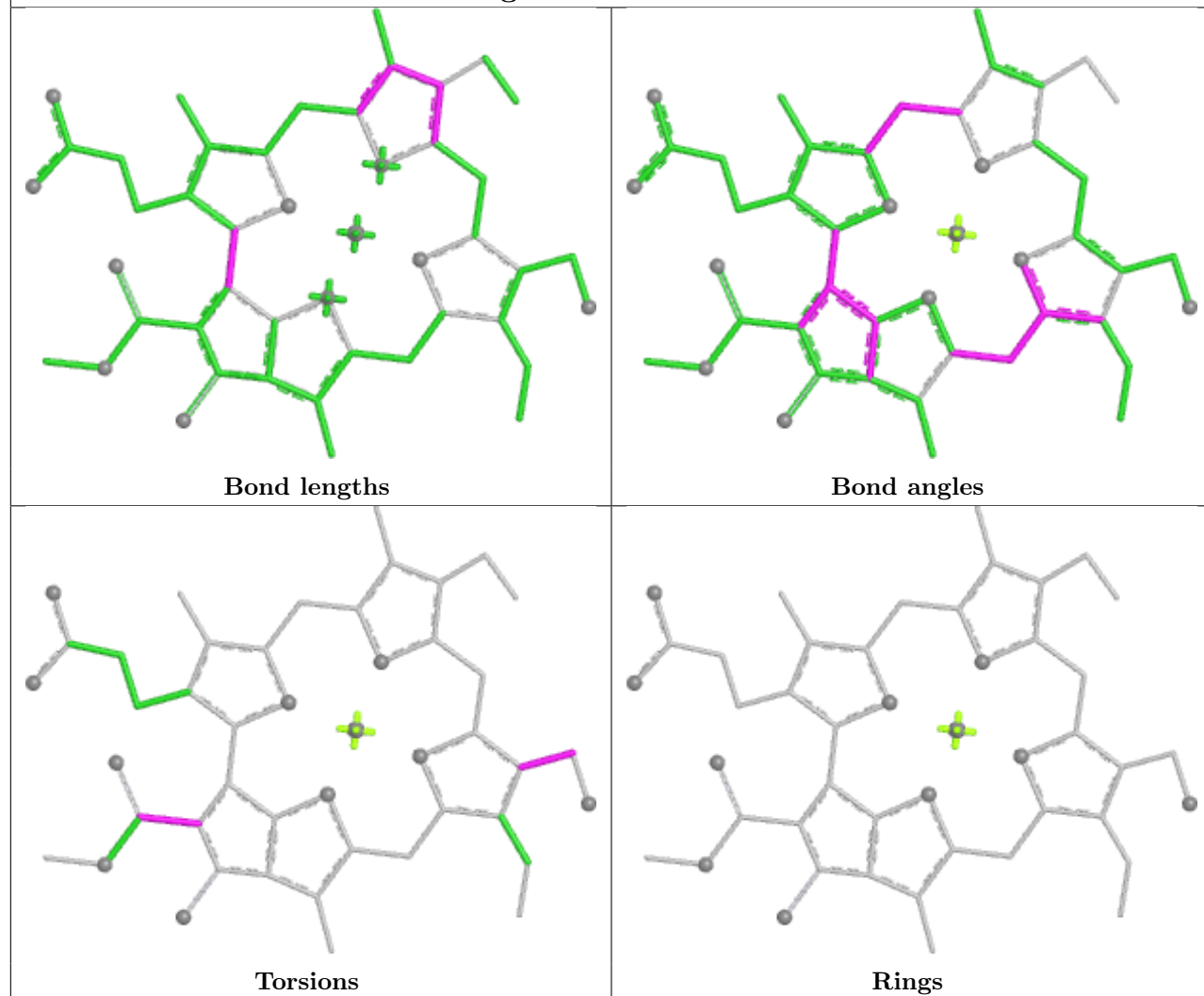




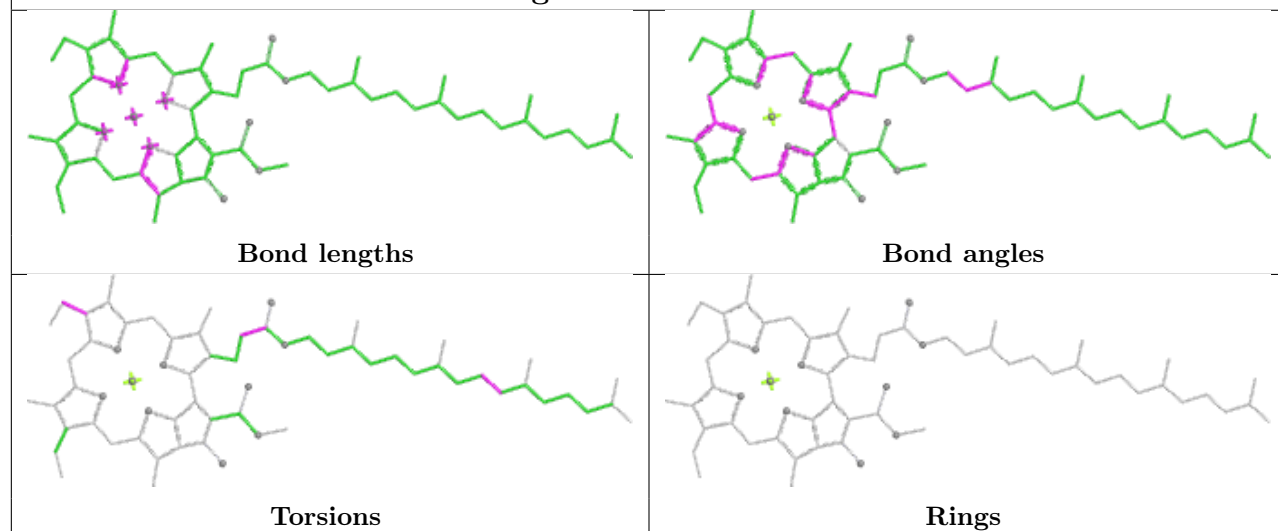


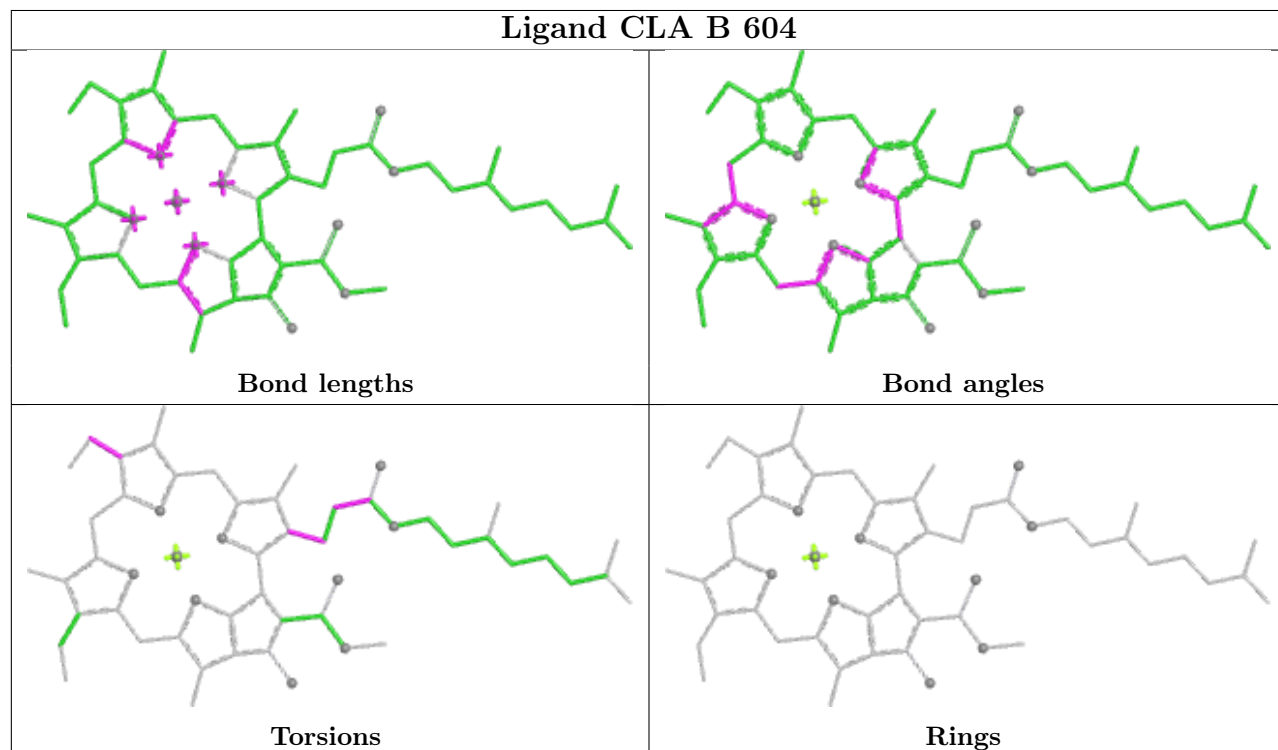
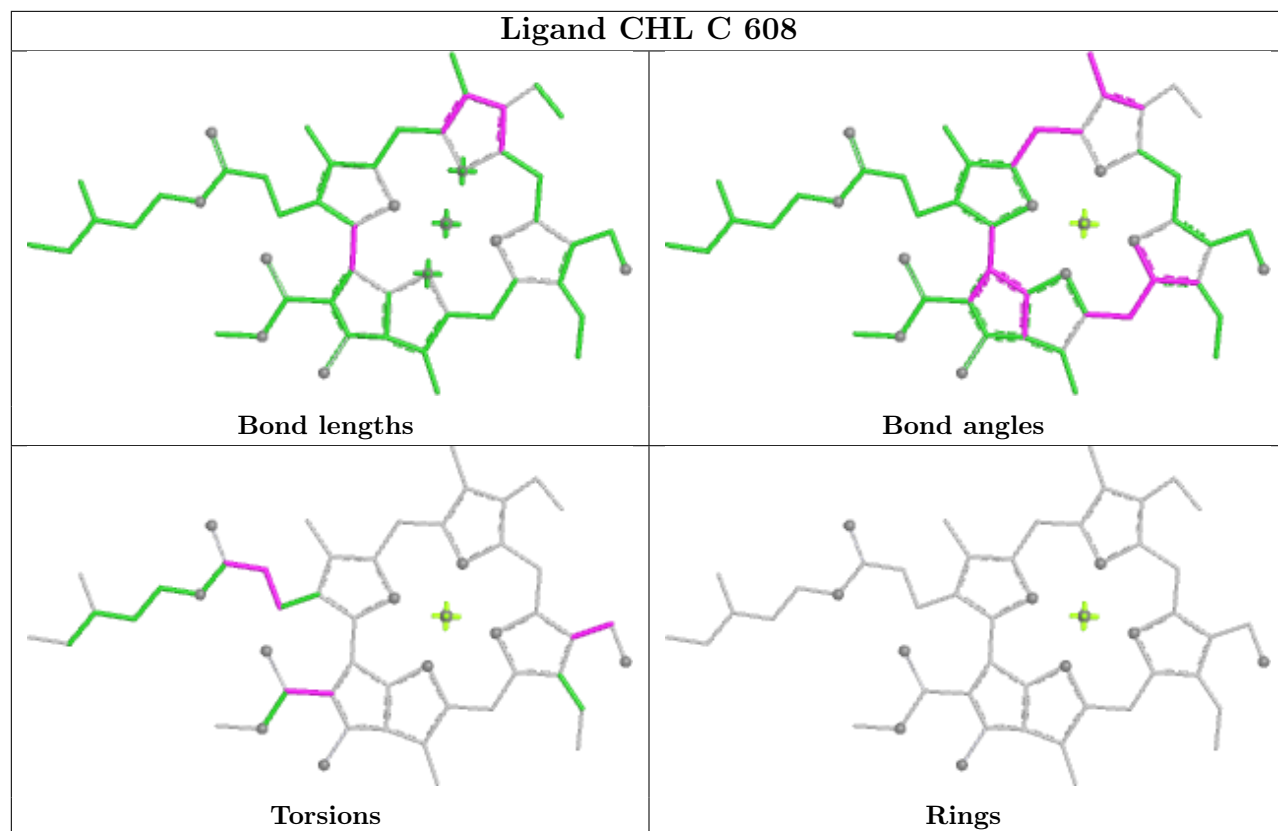


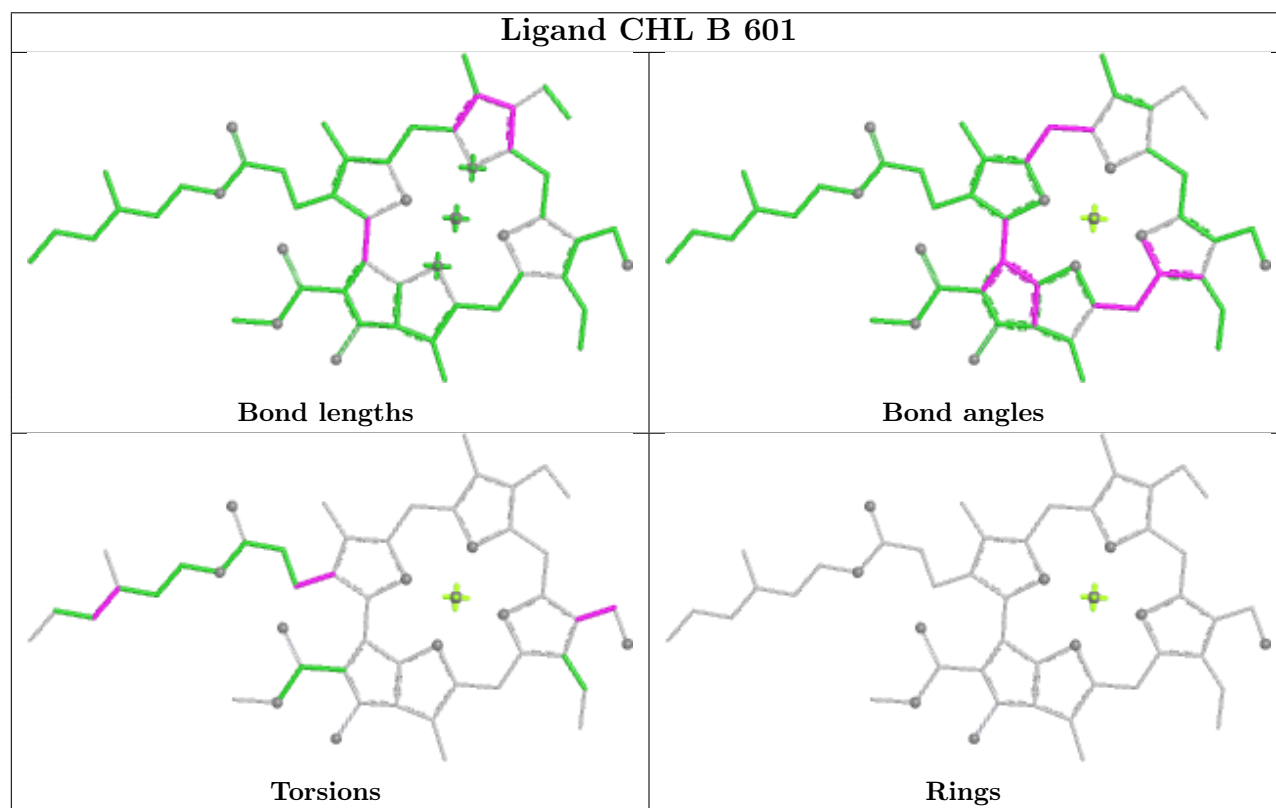
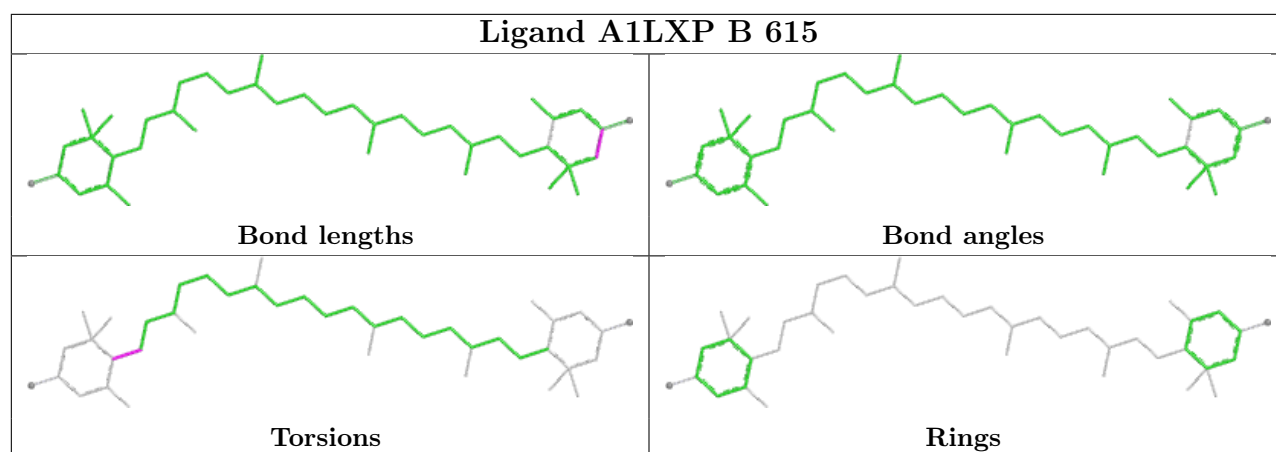
Ligand CHL A 607

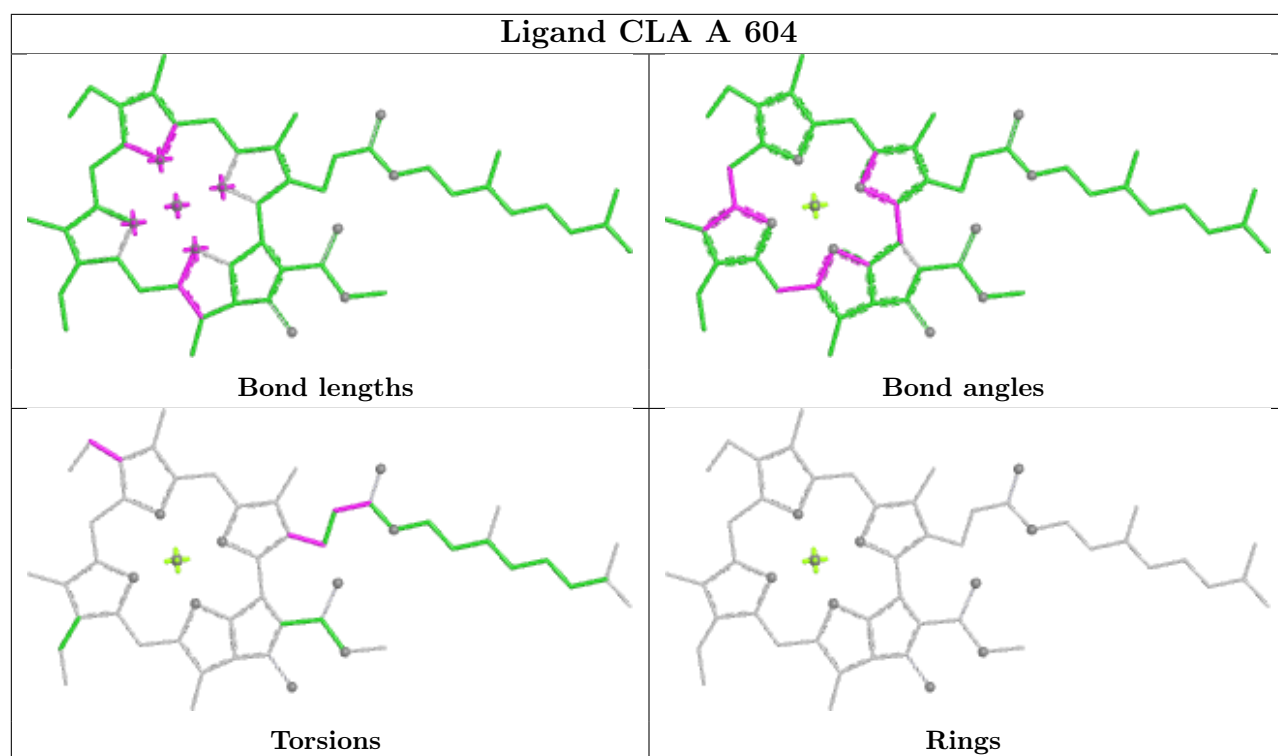


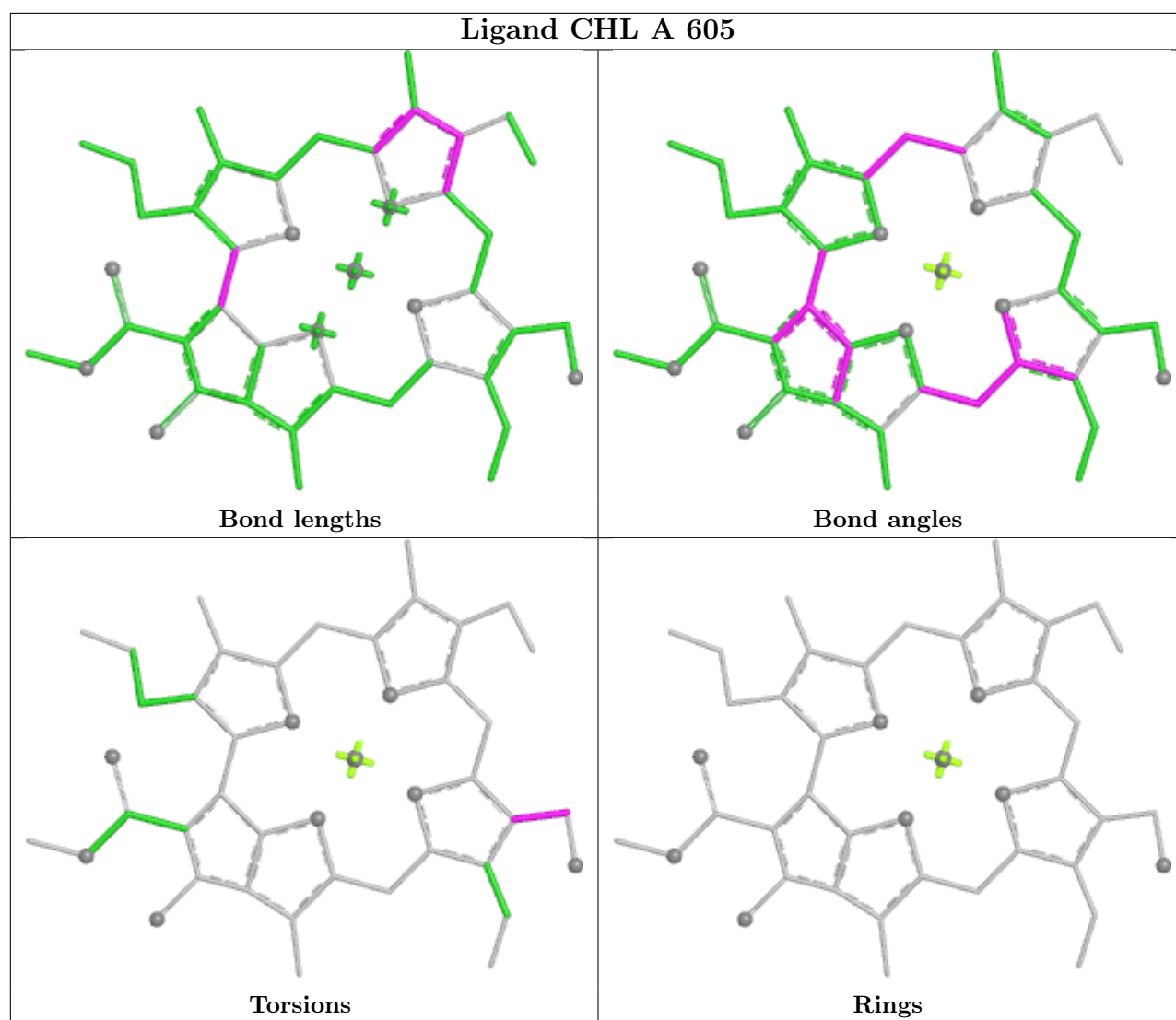
Ligand CLA A 611











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.

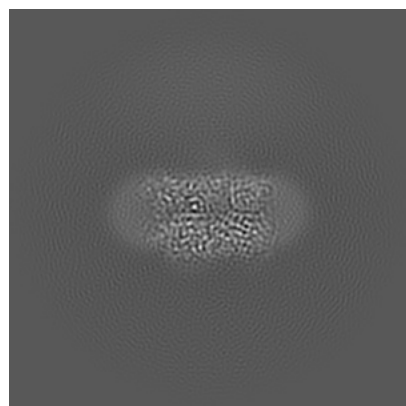
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39192. These allow visual inspection of the internal detail of the map and identification of artifacts.

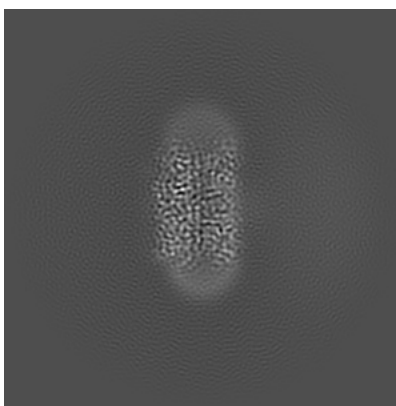
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

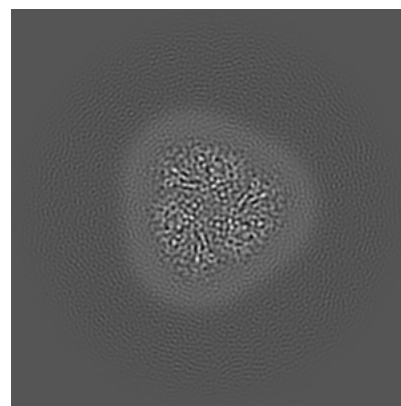
6.1.1 Primary map



X

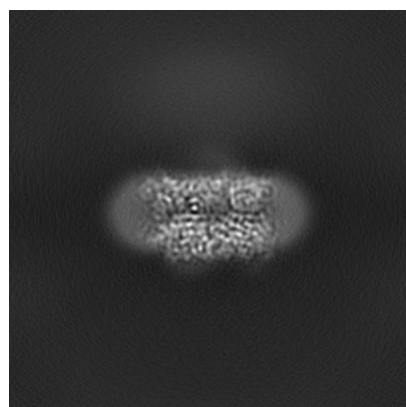


Y

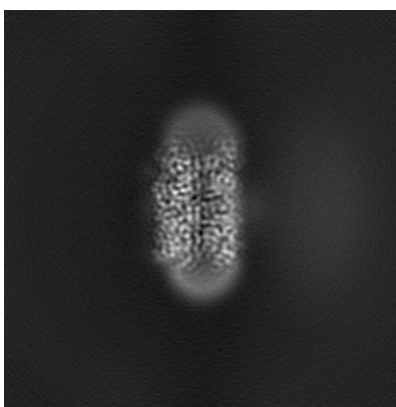


Z

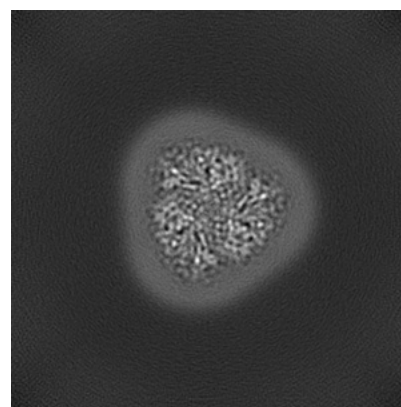
6.1.2 Raw map



X



Y

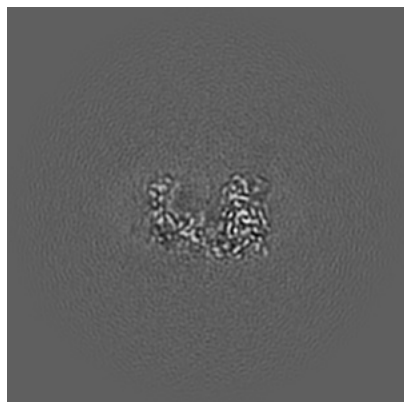


Z

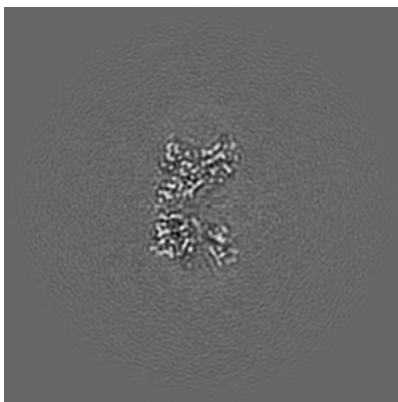
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

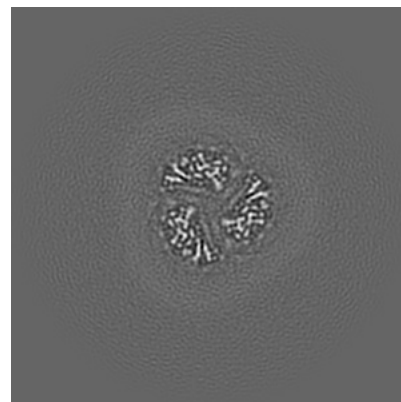
6.2.1 Primary map



X Index: 128

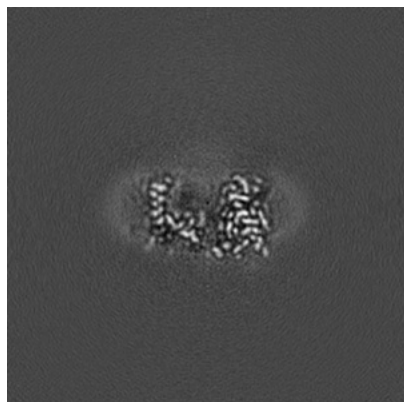


Y Index: 128

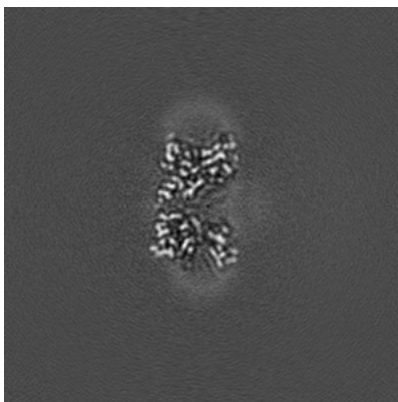


Z Index: 128

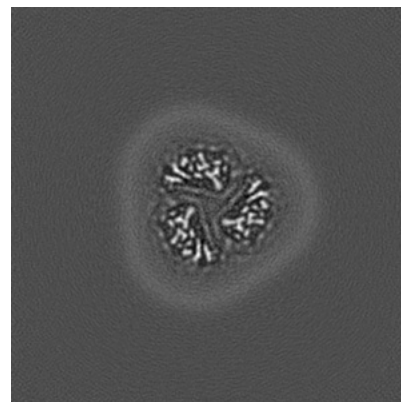
6.2.2 Raw map



X Index: 128



Y Index: 128

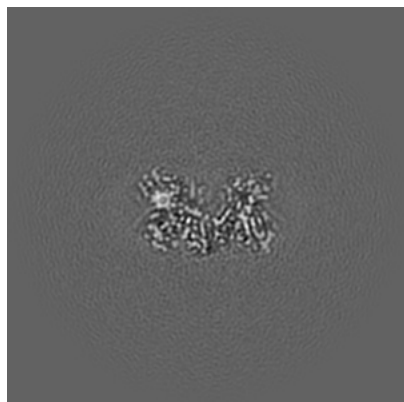


Z Index: 128

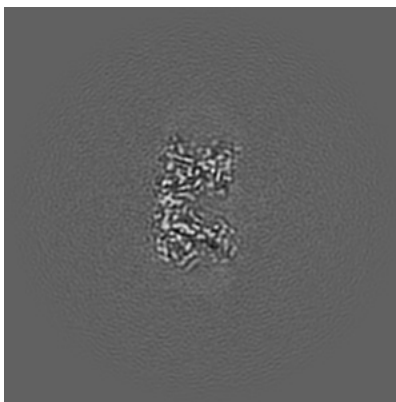
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

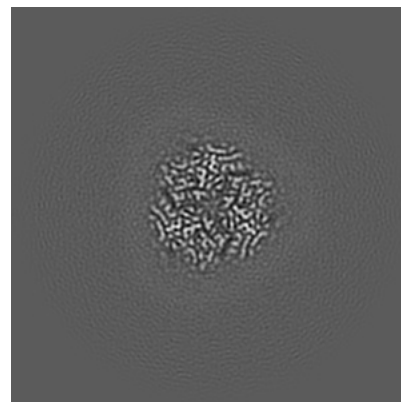
6.3.1 Primary map



X Index: 119

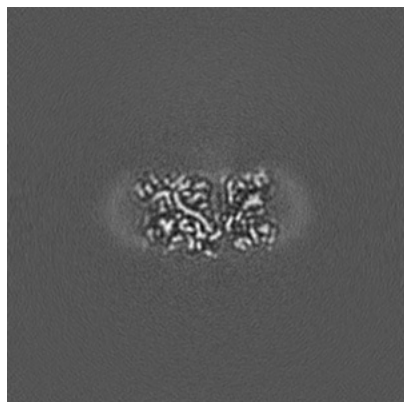


Y Index: 122

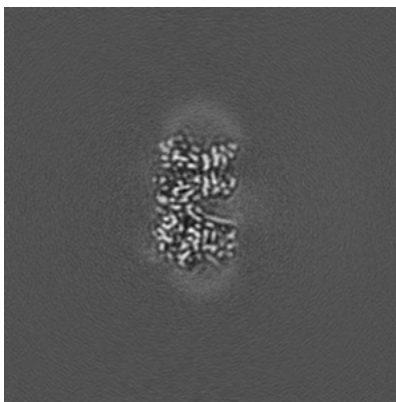


Z Index: 118

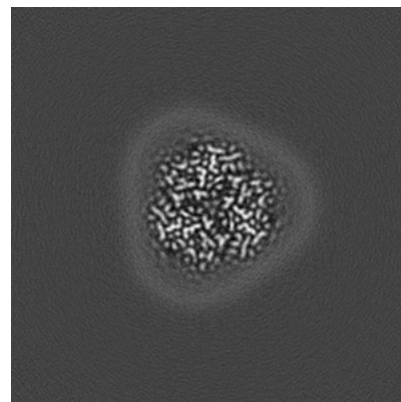
6.3.2 Raw map



X Index: 115



Y Index: 118

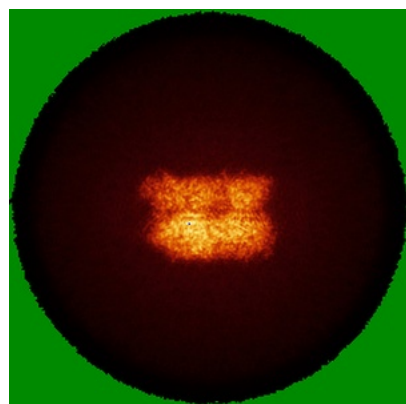


Z Index: 118

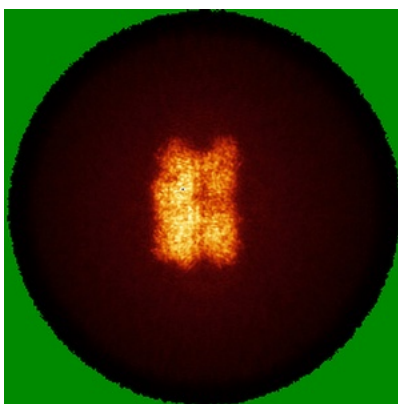
The images above show the largest variance slices of the map in three orthogonal directions.

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

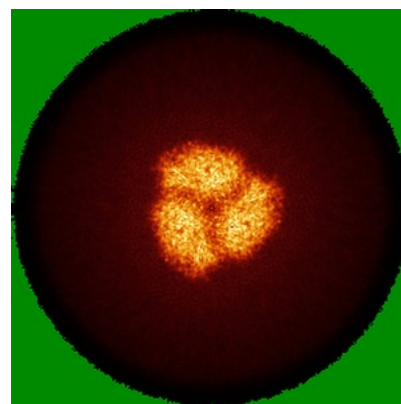
6.4.1 Primary map



X

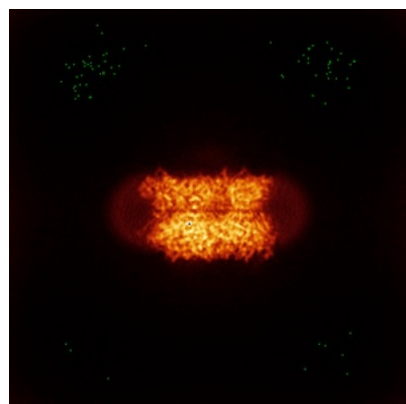


Y

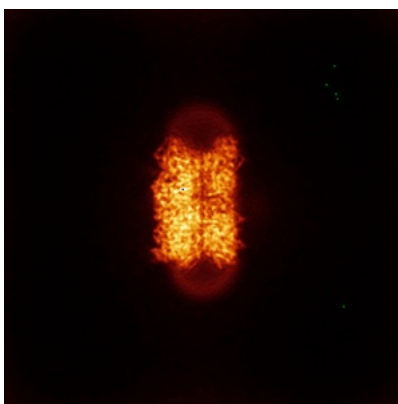


Z

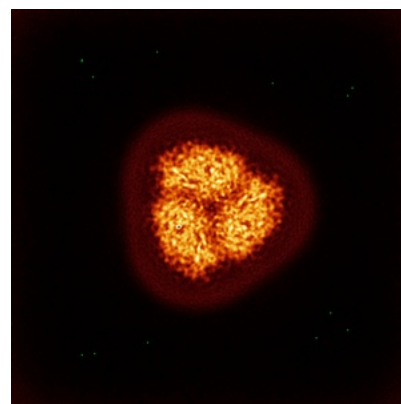
6.4.2 Raw map



X



Y

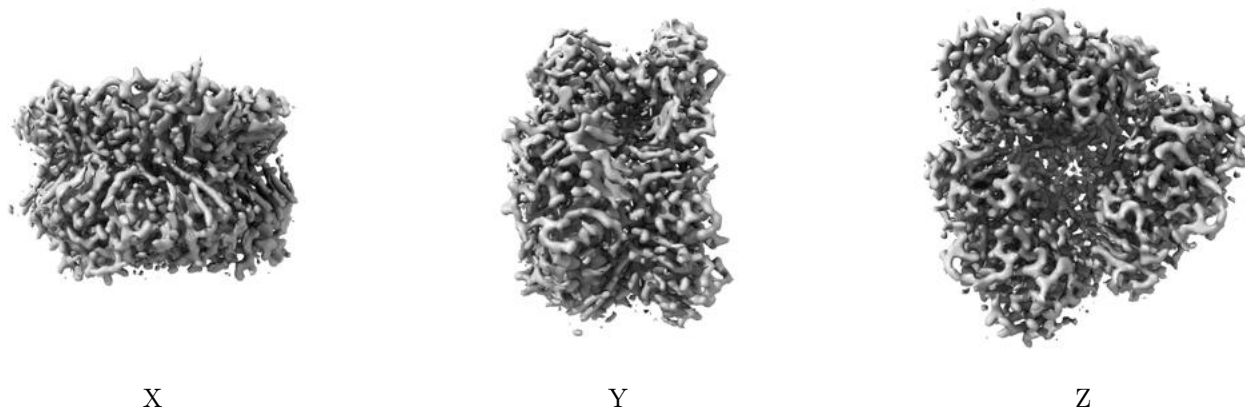


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

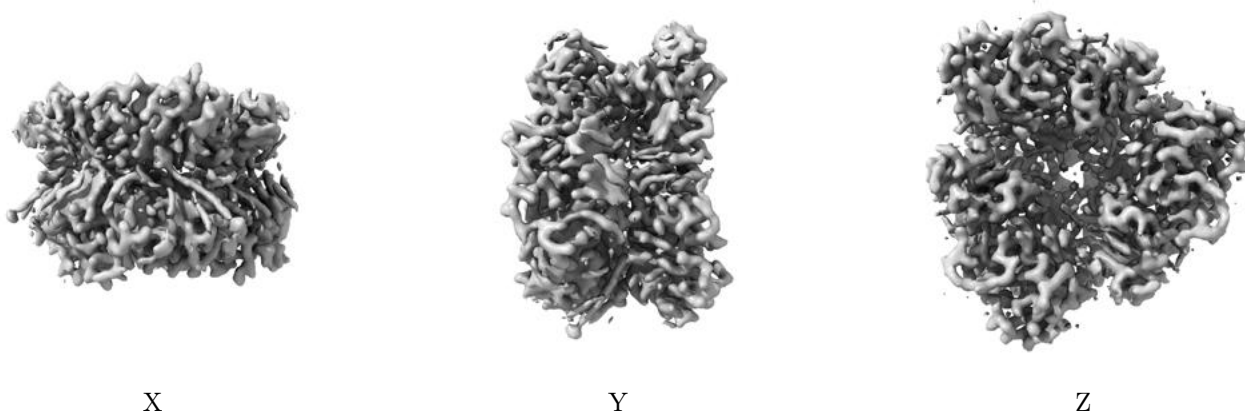
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

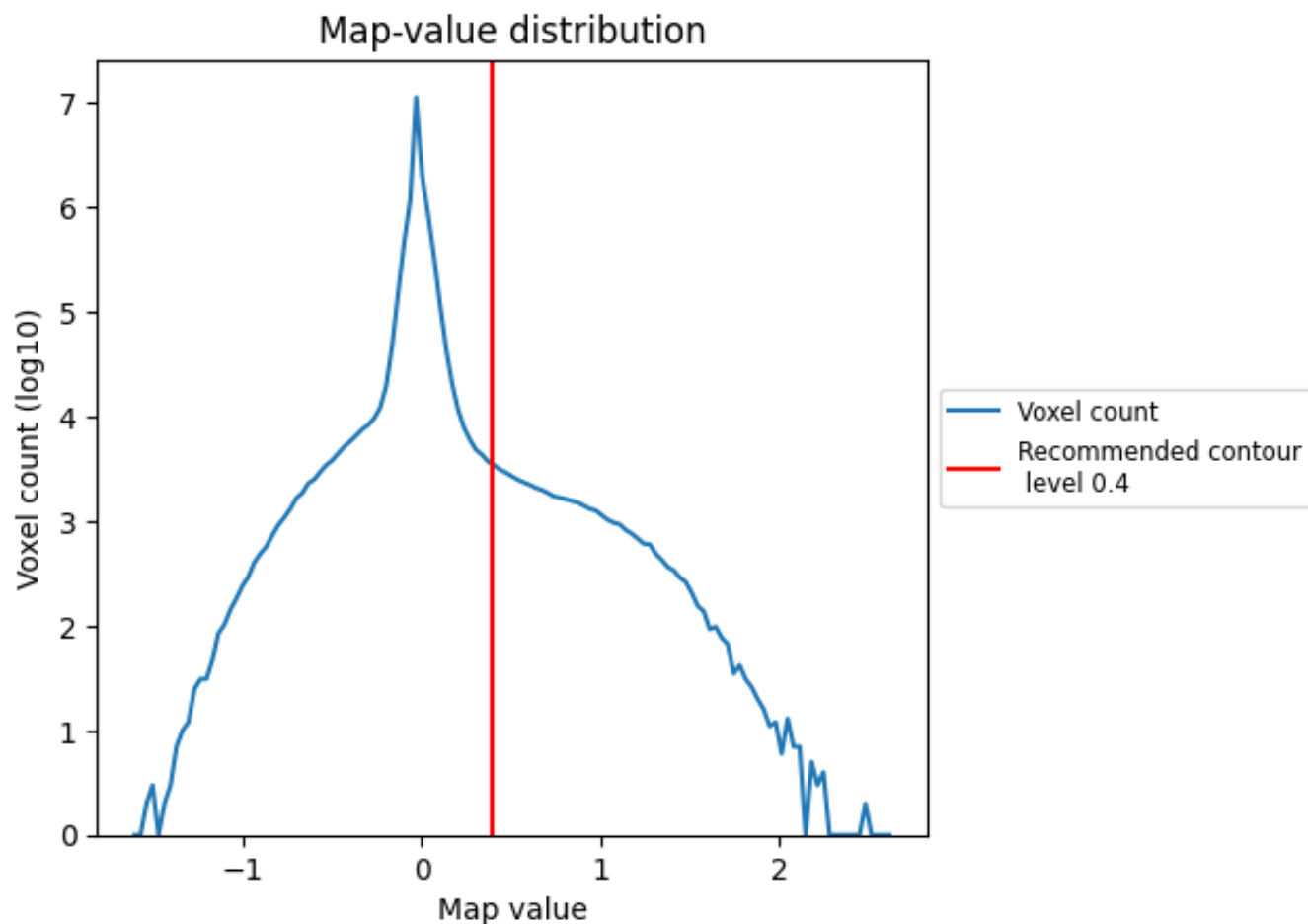
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

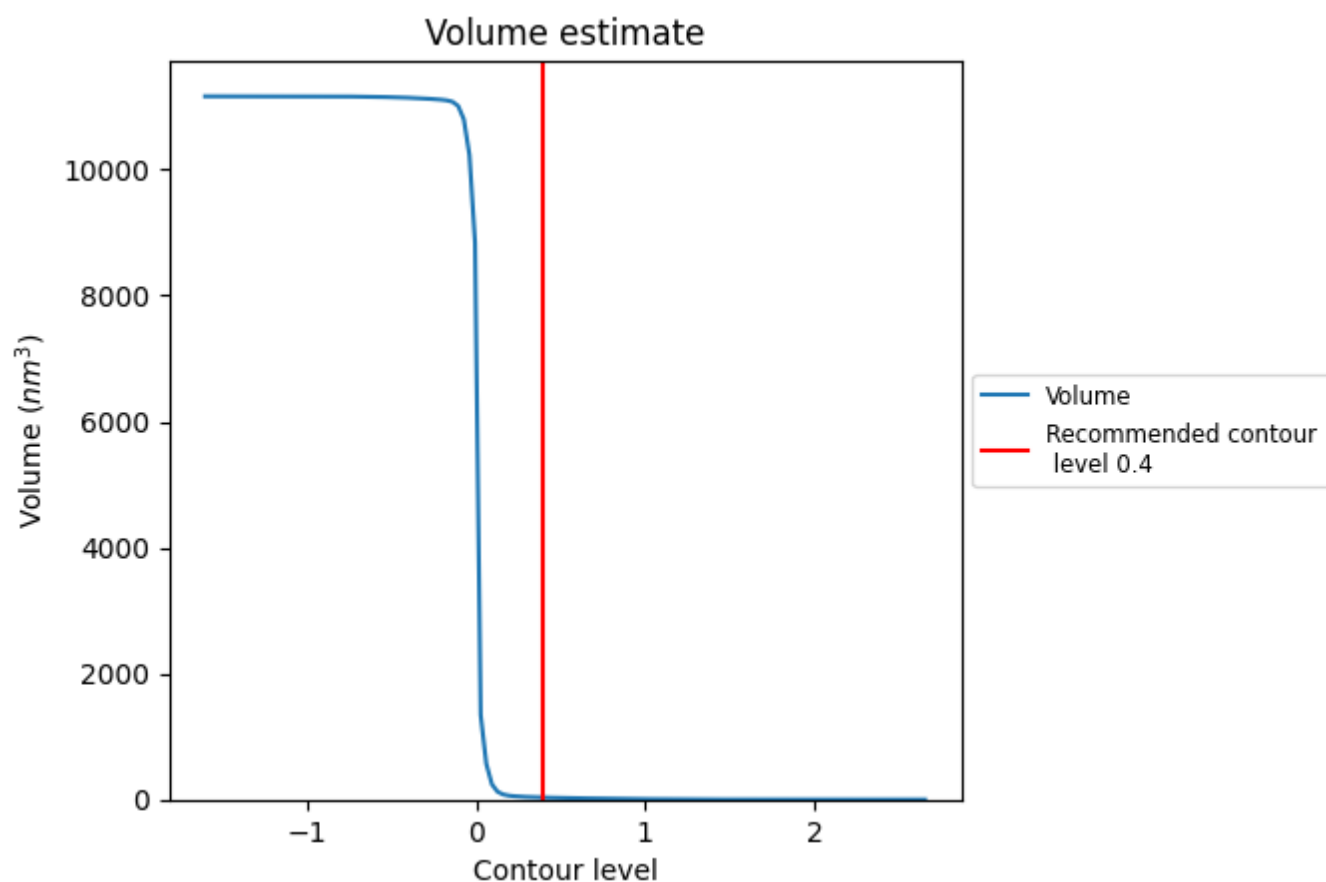
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

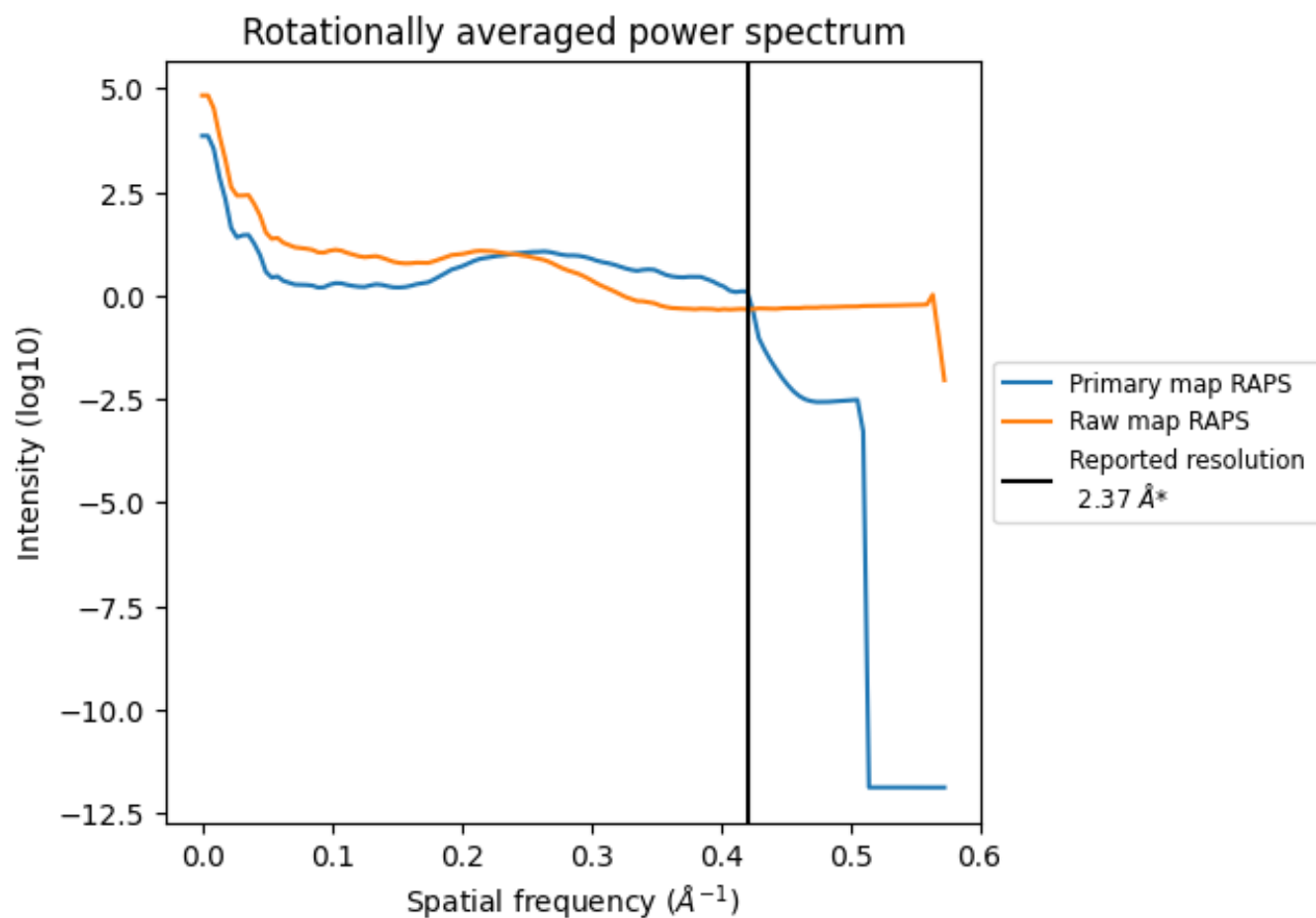
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 33 nm³; this corresponds to an approximate mass of 30 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 ⓘ

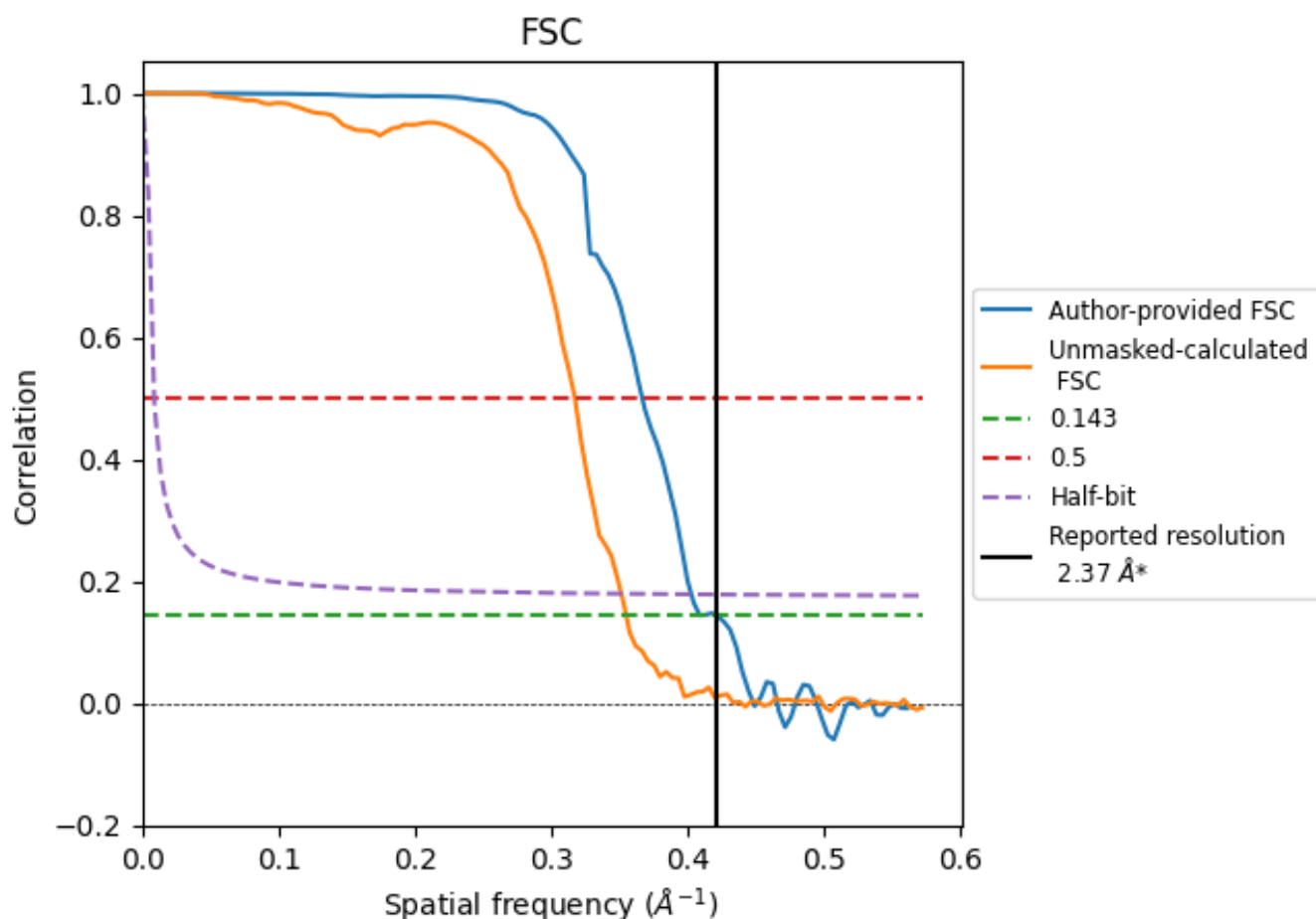


*Reported resolution corresponds to spatial frequency of 0.422 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.422 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

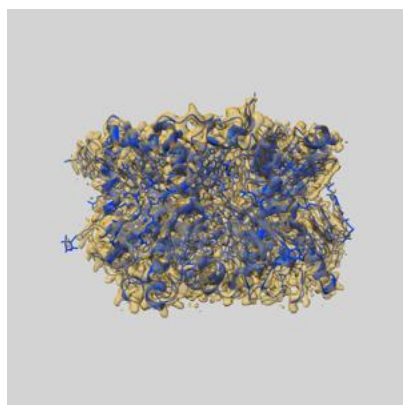
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.37	-	-
Author-provided FSC curve	2.37	2.72	2.48
Unmasked-calculated*	2.81	3.15	2.84

*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 2.81 differs from the reported value 2.37 by more than 10 %

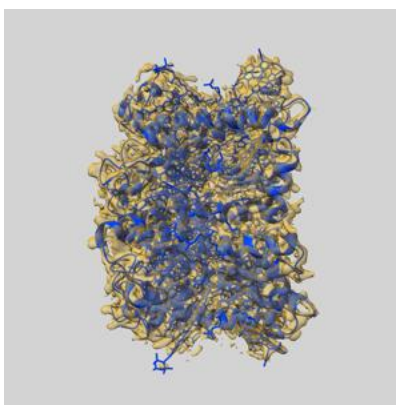
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-39192 and PDB model 8YEE. Per-residue inclusion information can be found in section 3 on page 12.

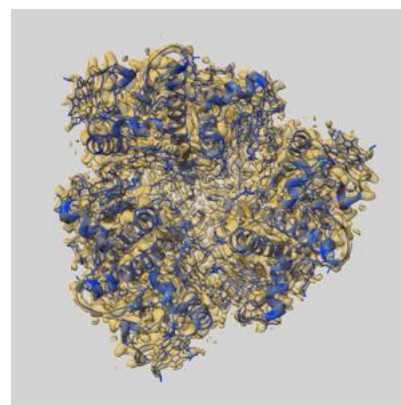
9.1 Map-model overlay [i](#)



X



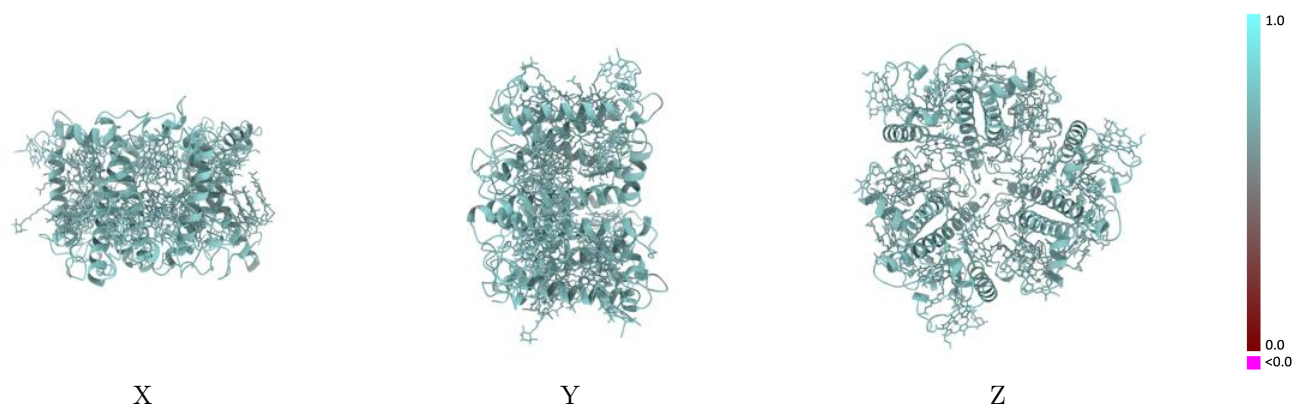
Y



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](#)



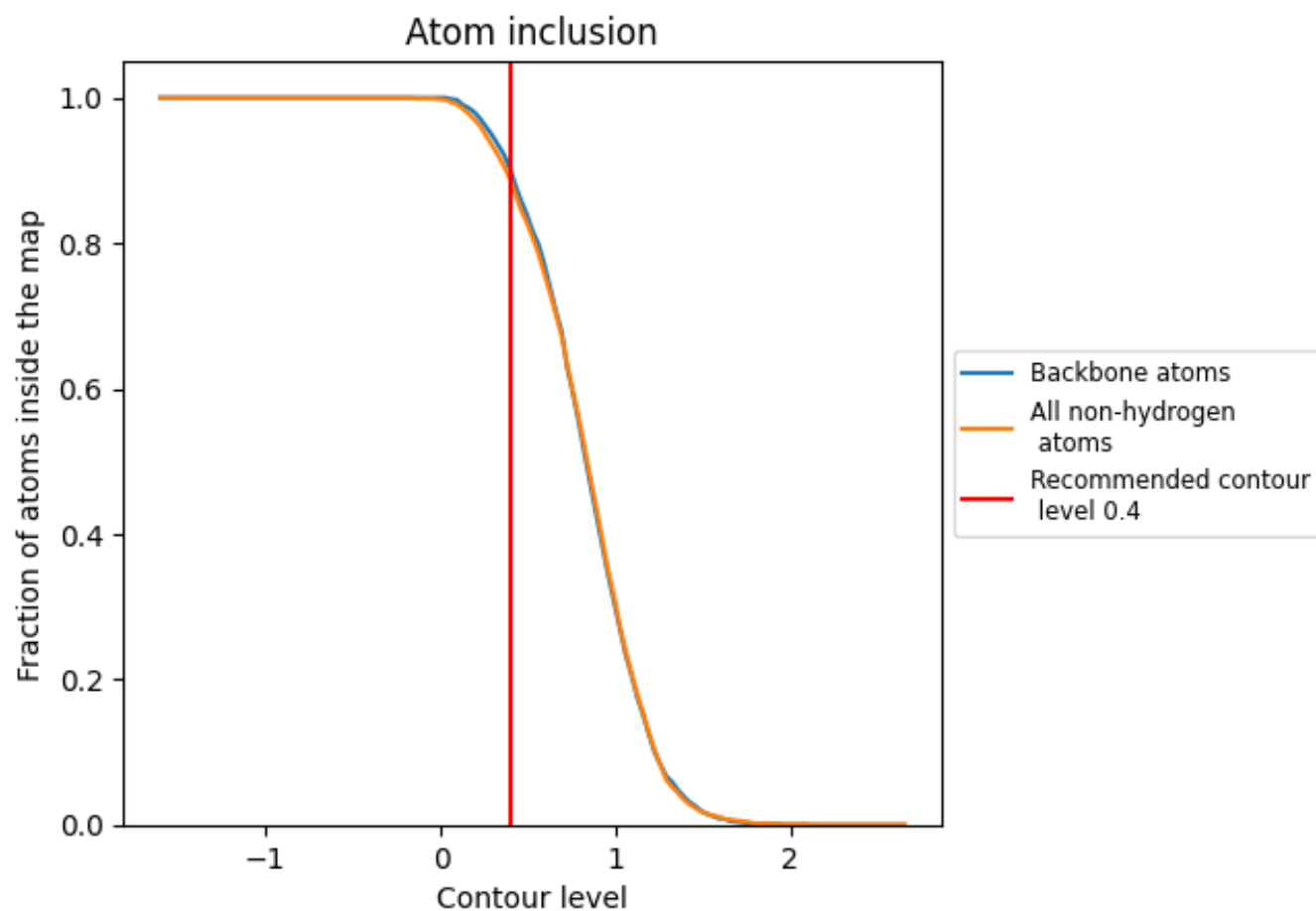
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 90% of all backbone atoms, 89% 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	0.8870	0.6780
A	0.8890	0.6780
B	0.8880	0.6780
C	0.8820	0.6770

