



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 11:05 AM UTC

PDB ID : 9UC6 / pdb_00009uc6
EMDB ID : EMD-64036
Title : Cryo-EM structure of the Lhcp trimer from *Ostreococcus tauri* at 1.94 angstrom resolution
Authors : Seki, S.; Kubota, M.; Ishii, A.; Kim, E.; Tanaka, H.; Miyata, T.; Namba, K.; Kurisu, G.; Minagawa, J.; Fujii, R.
Deposited on : 2025-04-03
Resolution : 1.94 Å (reported)
Based on initial model : 8HG3

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:

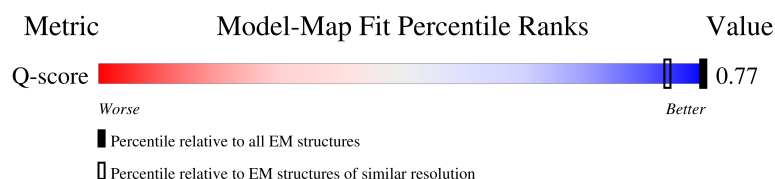
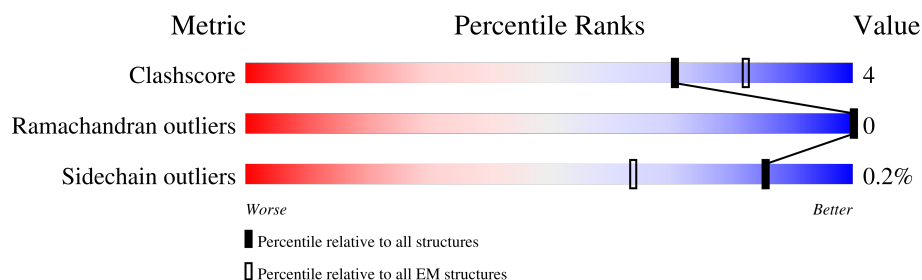
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

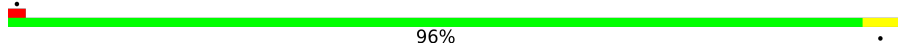
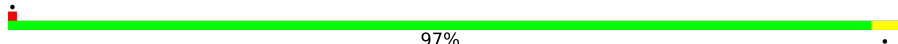
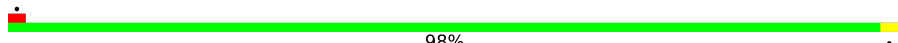
The reported resolution of this entry is 1.94 Å.

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	1283 (1.45 - 2.44)

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	202	 96% .
1	B	202	 97% .
1	C	202	 98% .

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
12	A1LYW	B	323	X	-	-	-
2	CLA	A	301	X	-	-	-
2	CLA	A	303	X	-	-	-
2	CLA	A	307	X	-	-	-
2	CLA	A	309	X	-	-	-
2	CLA	A	310	X	-	-	-
2	CLA	A	311	X	-	-	-
2	CLA	A	312	X	-	-	-
2	CLA	B	302	X	-	-	-
2	CLA	B	304	X	-	-	-
2	CLA	B	308	X	-	-	-
2	CLA	B	310	X	-	-	-
2	CLA	B	311	X	-	-	-
2	CLA	B	312	X	-	-	-
2	CLA	B	313	X	-	-	-
2	CLA	C	302	X	-	-	-
2	CLA	C	304	X	-	-	-
2	CLA	C	308	X	-	-	-
2	CLA	C	310	X	-	-	-
2	CLA	C	311	X	-	-	-
2	CLA	C	312	X	-	-	-
2	CLA	C	313	X	-	-	-
3	CHL	A	302	X	-	-	-
3	CHL	A	304	X	-	-	-
3	CHL	A	305	X	-	-	-
3	CHL	A	306	X	-	-	-
3	CHL	A	313	X	-	-	-
3	CHL	A	314	X	-	-	-
3	CHL	B	303	X	-	-	-
3	CHL	B	305	X	-	-	-
3	CHL	B	306	X	-	-	-
3	CHL	B	307	X	-	-	-
3	CHL	B	314	X	-	-	-
3	CHL	B	315	X	-	-	-
3	CHL	C	303	X	-	-	-
3	CHL	C	305	X	-	-	-
3	CHL	C	306	X	-	-	-
3	CHL	C	307	X	-	-	-
3	CHL	C	314	X	-	-	-
3	CHL	C	315	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	A1L0F	A	308	X	-	-	-
4	A1L0F	B	309	X	-	-	-
4	A1L0F	C	309	X	-	-	-
5	IWJ	A	315	X	-	-	-
5	IWJ	A	318	X	-	-	-
5	IWJ	B	316	X	-	-	-
5	IWJ	B	319	X	-	-	-
5	IWJ	C	316	X	-	-	-
5	IWJ	C	319	X	-	-	-

2 Entry composition [i](#)

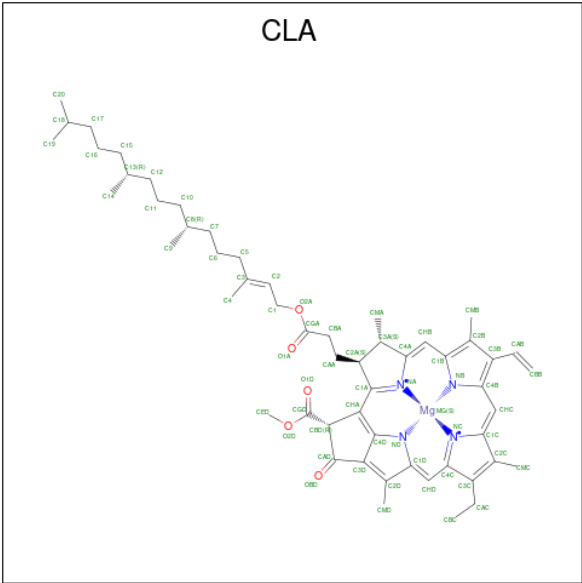
There are 13 unique types of molecules in this entry. The entry contains 8379 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	202	Total	C	N	O	S	0	0
			1512	971	247	288	6		
1	B	202	Total	C	N	O	S	0	0
			1512	971	247	288	6		
1	C	202	Total	C	N	O	S	0	0
			1512	971	247	288	6		

- Molecule 2 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



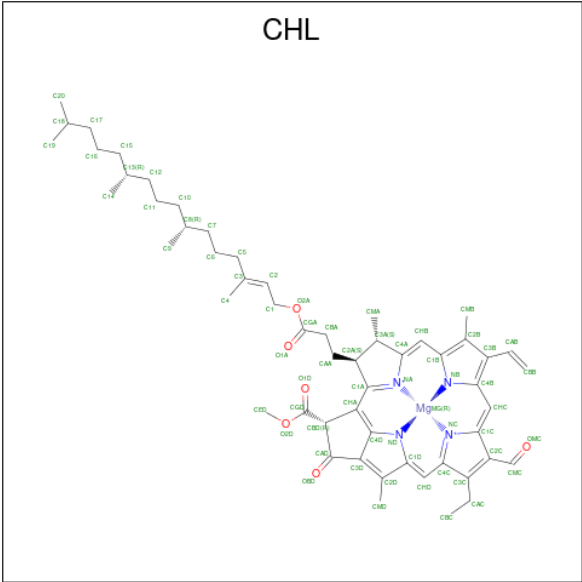
Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
2	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
2	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
2	A	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
2	A	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
2	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
2	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
2	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
2	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
2	B	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
2	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
2	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
2	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
2	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
2	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
2	C	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
2	C	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
2	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 3 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



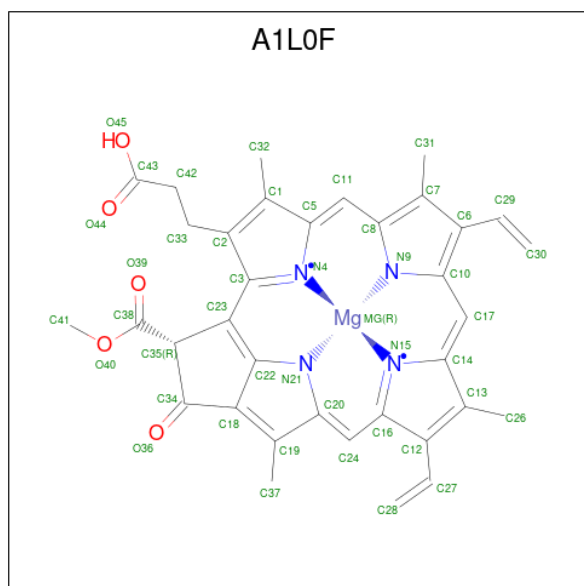
Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total 63	C 52	Mg 1	N 4	O 6	0
3	A	1	Total 66	C 55	Mg 1	N 4	O 6	0
3	A	1	Total 48	C 37	Mg 1	N 4	O 6	0
3	A	1	Total 66	C 55	Mg 1	N 4	O 6	0
3	A	1	Total 53	C 42	Mg 1	N 4	O 6	0
3	A	1	Total 66	C 55	Mg 1	N 4	O 6	0
3	B	1	Total 63	C 52	Mg 1	N 4	O 6	0
3	B	1	Total 66	C 55	Mg 1	N 4	O 6	0
3	B	1	Total 48	C 37	Mg 1	N 4	O 6	0
3	B	1	Total 66	C 55	Mg 1	N 4	O 6	0
3	B	1	Total 53	C 42	Mg 1	N 4	O 6	0
3	B	1	Total 66	C 55	Mg 1	N 4	O 6	0
3	C	1	Total 63	C 52	Mg 1	N 4	O 6	0
3	C	1	Total 66	C 55	Mg 1	N 4	O 6	0

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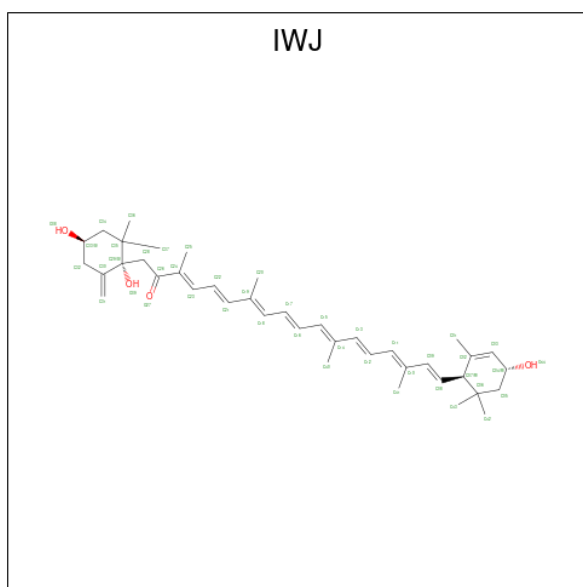
Mol	Chain	Residues	Atoms					AltConf
3	C	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
3	C	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
3	C	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
3	C	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 4 is Mg-2,4-divinyl-phaeoporphyrin a5-monomethyl ester (CCD ID: A1L0F) (formula: $C_{35}H_{30}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



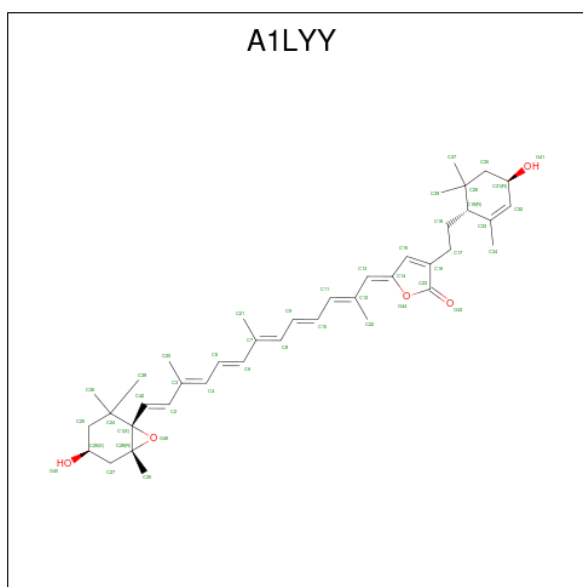
Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
4	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
4	C	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 5 is (3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-1-[(1 {S},4 {S})-2,2-dimethyl-6-methylidene-1,4-bis(oxidanyl)cyclohexyl]-3,7,12,16-tetramethyl-18-[(1 {R},4 {R})-2,6,6-trimethyl-4-oxidanyl-cyclohex-2-en-1-yl]octadeca-3,5,7,9,11,13,15,17-octaen-2-one (CCD ID: IWJ) (formula: $C_{40}H_{56}O_4$) (labeled as "Ligand of Interest" by depositor).



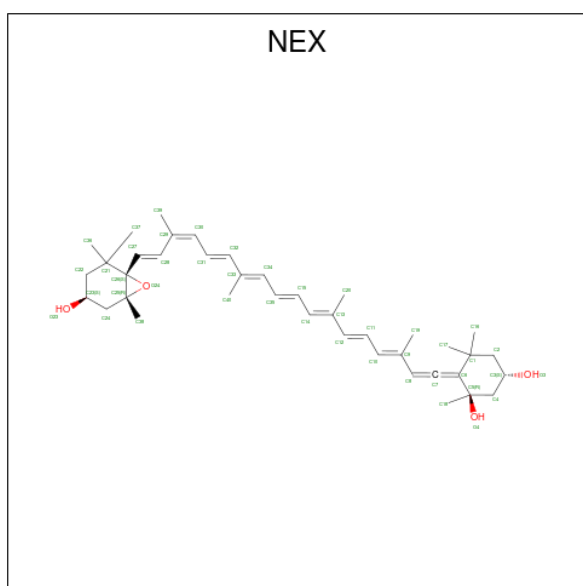
Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total	C	O	0
			44	40	4	
5	A	1	Total	C	O	0
			44	40	4	
5	B	1	Total	C	O	0
			44	40	4	
5	B	1	Total	C	O	0
			44	40	4	
5	C	1	Total	C	O	0
			44	40	4	
5	C	1	Total	C	O	0
			44	40	4	

- Molecule 6 is (5 {Z})-3-[2-[(1 {R},4 {R})-2,6,6-trimethyl-4-oxidanyl-cyclohex-2-en-1-yl]ethyl]-5-[(2 {E},4 {E},6 {E},8 {E},10 {E},12 {E})-2,7,11-trimethyl-13-[(1 {S},4 {S},6 {R})-2,2,6-trimethyl-4-oxidanyl-7-oxabicyclo[4.1.0]heptan-1-yl]trideca-2,4,6,8,10,12-hexaenylidene]furan-2-one (CCD ID: A1LYY) (formula: C₄₀H₅₄O₅) (labeled as "Ligand of Interest" by depositor).



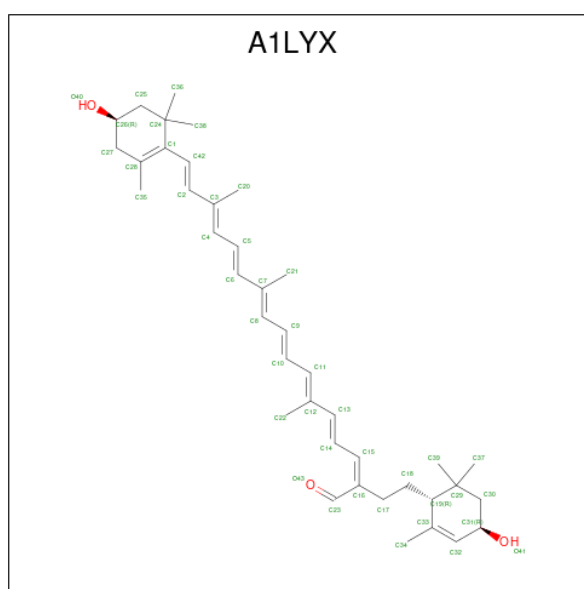
Mol	Chain	Residues	Atoms			AltConf
6	A	1	Total	C	O	0
			45	40	5	
6	B	1	Total	C	O	0
			45	40	5	
6	C	1	Total	C	O	0
			45	40	5	

- Molecule 7 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).



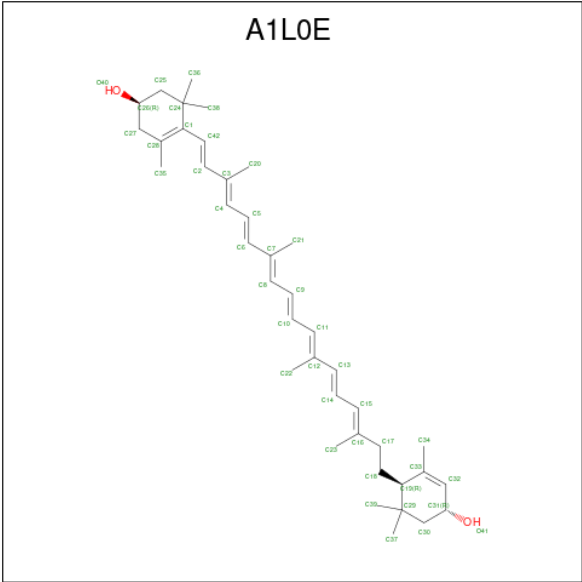
Mol	Chain	Residues	Atoms			AltConf
7	A	1	Total	C	O	0
			44	40	4	
7	B	1	Total	C	O	0
			44	40	4	
7	C	1	Total	C	O	0
			44	40	4	

- Molecule 8 is (2 {Z},4 {E},6 {E},8 {E},10 {E},12 {E},14 {E},16 {E})-6,11,15-trimethyl-17-[(4 {R})-2,6,6-trimethyl-4-oxidanyl-cyclohexen-1-yl]-2-[2-[(1 {R},4 {R})-2,6,6-trimethyl-4-oxidanyl-cyclohex-2-en-1-yl]ethyl]heptadeca-2,4,6,8,10,12,14,16-octaenal (CCD ID: A1LYX) (formula: C₄₀H₅₆O₃) (labeled as "Ligand of Interest" by depositor).



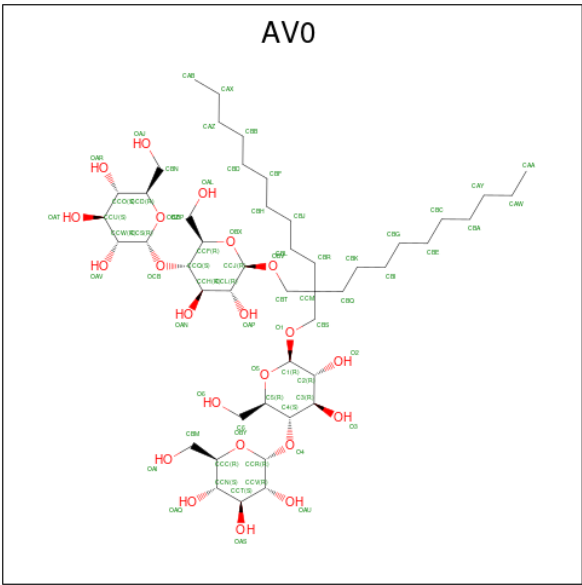
Mol	Chain	Residues	Atoms			AltConf
8	A	1	Total	C	O	0
			43	40	3	
8	B	1	Total	C	O	0
			43	40	3	
8	C	1	Total	C	O	0
			43	40	3	

- Molecule 9 is (1 {R})-3,5,5-trimethyl-4-[(1 {E},3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E})-3,7,12,16-tetramethyl-18-[(1 {R},4 {R})-2,6,6-trimethyl-4-oxidanyl-cyclohex-2-en-1-yl]octadeca-1,3,5,7,9,11,13,15-octaenyl]cyclohex-3-en-1-ol (CCD ID: A1L0E) (formula: C₄₀H₅₈O₂) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 10 is Lauryl Maltose Neopentyl Glycol (CCD ID: AV0) (formula: C₄₇H₈₈O₂₂).



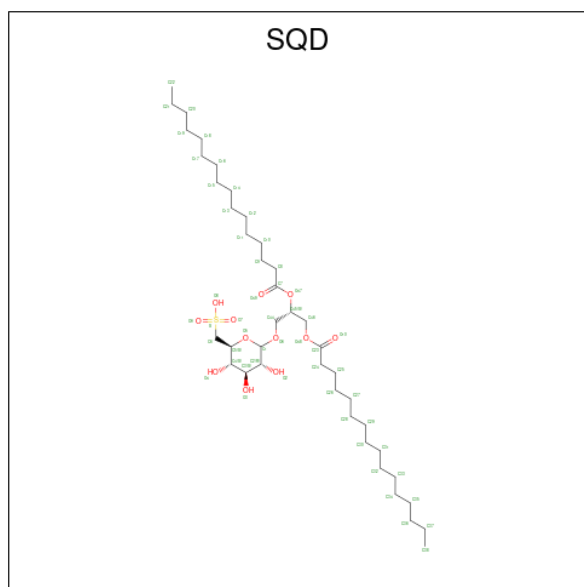
Mol	Chain	Residues	Atoms			AltConf
10	A	1	Total	C	O	0
			25	23	2	

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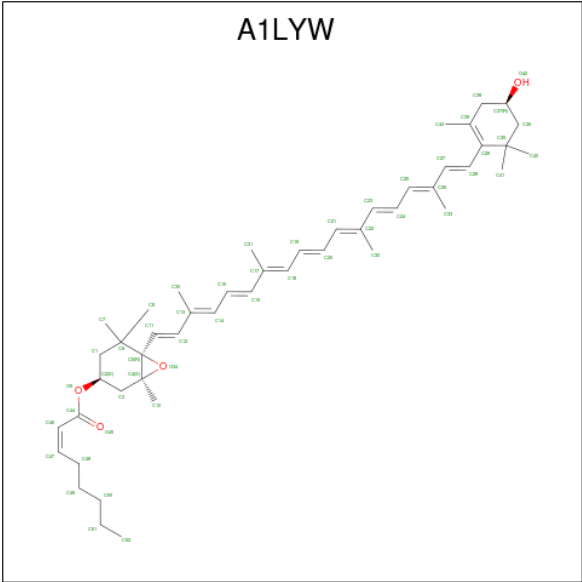
Mol	Chain	Residues	Atoms			AltConf
10	B	1	Total	C	O	0
			25	23	2	
10	C	1	Total	C	O	0
			25	23	2	

- Molecule 11 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
11	A	1	Total	C	O	0
			41	36	5	
11	B	1	Total	C	O	0
			41	36	5	
11	C	1	Total	C	O	0
			41	36	5	

- Molecule 12 is [(1 {S},3 {S},6 {R})-1,5,5-trimethyl-6-[(1 {E},3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-[(4 {R})-2,6,6-trimethyl-4-oxidanyl-cyclohexen-1-yl]octadeca-1,3,5,7,9,11,13,15,17-nonaenyl]-7-oxabicyclo[4.1.0]heptan-3-yl] ({Z})-oct-2-enoate (CCD ID: A1LYW) (formula: C₄₈H₆₈O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
12	A	1	Total	C	O	0
			52	48	4	
12	B	1	Total	C	O	0
			52	48	4	
12	B	1	Total	C	O	0
			52	48	4	

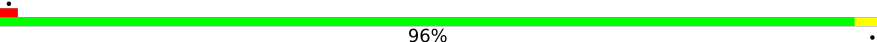
- Molecule 13 is water.

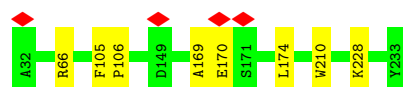
Mol	Chain	Residues	Atoms		AltConf
13	A	62	Total	O	0
			62	62	
13	B	62	Total	O	0
			62	62	
13	C	62	Total	O	0
			62	62	

3 Residue-property plots

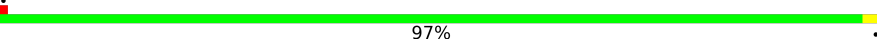
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

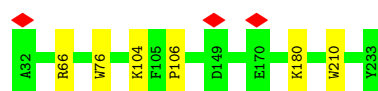
- Molecule 1: Chlorophyll a-b binding protein, chloroplastic

Chain A:  96%

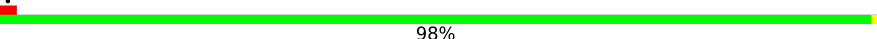


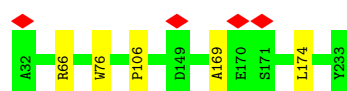
- Molecule 1: Chlorophyll a-b binding protein, chloroplastic

Chain B:  97%



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

Chain C:  98%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	1153594	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	3.771	Depositor
Minimum map value	-1.904	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.084	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: CHL, CLA, A1LYX, A1L0E, A1LYW, A1LYY, AV0, IWJ, NEX, A1L0F, SQD

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	0.18	0/1558	0.36	0/2129
1	B	0.18	0/1558	0.37	0/2129
1	C	0.18	0/1558	0.37	0/2129
All	All	0.18	0/4674	0.37	0/6387

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	1512	0	1434	6	0
1	B	1512	0	1434	7	0
1	C	1512	0	1434	4	0
2	A	432	0	454	11	0
2	B	432	0	454	9	0
2	C	432	0	454	11	0
3	A	362	0	345	5	0
3	B	362	0	345	7	0
3	C	362	0	345	8	0
4	A	45	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	45	0	0	0	0
4	C	45	0	0	0	0
5	A	88	0	0	1	0
5	B	88	0	0	0	0
5	C	88	0	0	0	0
6	A	45	0	0	0	0
6	B	45	0	0	0	0
6	C	45	0	0	0	0
7	A	44	0	56	0	0
7	B	44	0	56	0	0
7	C	44	0	56	0	0
8	A	43	0	0	0	0
8	B	43	0	0	0	0
8	C	43	0	0	0	0
9	A	84	0	0	0	0
9	C	42	0	0	0	0
10	A	25	0	0	0	0
10	B	25	0	0	0	0
10	C	25	0	0	0	0
11	A	41	0	67	2	0
11	B	41	0	67	4	0
11	C	41	0	67	3	0
12	A	52	0	0	0	0
12	B	104	0	0	0	0
13	A	62	0	0	0	0
13	B	62	0	0	0	0
13	C	62	0	0	0	0
All	All	8379	0	7068	54	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 4.

All (54) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:304:CLA:HMA2	3:C:306:CHL:HBC3	1.70	0.72
2:B:304:CLA:HMA2	3:B:306:CHL:HBC3	1.79	0.64
3:C:305:CHL:H203	2:C:308:CLA:H193	1.79	0.63
2:A:303:CLA:HMA2	3:A:305:CHL:HBC3	1.81	0.62
1:A:210:TRP:CE2	11:A:322:SQD:H101	2.40	0.56
3:C:305:CHL:H111	3:C:315:CHL:H13	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:312:CLA:HMA1	11:C:322:SQD:H361	1.88	0.55
3:B:305:CHL:H192	2:B:308:CLA:H162	1.88	0.55
2:A:307:CLA:H71	2:A:309:CLA:H151	1.88	0.55
2:C:311:CLA:H143	11:C:322:SQD:H291	1.89	0.53
3:B:305:CHL:H111	3:B:315:CHL:H13	1.91	0.52
2:B:311:CLA:H152	11:B:322:SQD:H141	1.92	0.51
2:A:311:CLA:HMB1	2:A:311:CLA:HBB1	1.92	0.51
1:B:66:ARG:HG2	2:B:310:CLA:C3C	2.40	0.51
2:A:310:CLA:H143	11:A:322:SQD:H292	1.93	0.50
1:A:66:ARG:HG2	2:A:309:CLA:C3C	2.41	0.50
2:C:313:CLA:HBB1	2:C:313:CLA:HMB1	1.93	0.50
1:B:210:TRP:CE2	11:B:322:SQD:H112	2.47	0.49
1:C:66:ARG:HG2	2:C:310:CLA:C3C	2.43	0.48
3:A:304:CHL:H203	2:A:307:CLA:H193	1.95	0.48
1:C:106:PRO:HG2	3:C:315:CHL:O1D	2.14	0.48
1:A:106:PRO:HG2	3:A:314:CHL:O1D	2.14	0.47
1:C:169:ALA:HB1	1:C:174:LEU:HD13	1.97	0.47
2:A:307:CLA:H192	5:A:318:IWJ:C10	2.46	0.46
1:B:104:LYS:HA	1:B:104:LYS:HD3	1.70	0.46
2:B:308:CLA:H71	2:B:310:CLA:H151	1.98	0.46
2:C:312:CLA:HBB1	2:C:312:CLA:HMB1	1.97	0.46
1:B:106:PRO:HG2	3:B:315:CHL:O1D	2.16	0.45
3:C:305:CHL:H192	2:C:308:CLA:H161	1.98	0.45
3:A:304:CHL:H162	3:A:314:CHL:H71	1.97	0.45
1:B:210:TRP:NE1	11:B:322:SQD:H112	2.33	0.44
2:B:304:CLA:H12	2:B:304:CLA:H51	1.81	0.44
2:A:312:CLA:H61	2:A:312:CLA:H102	1.72	0.44
3:B:306:CHL:C3C	3:B:307:CHL:HBC3	2.48	0.44
3:C:306:CHL:C3C	3:C:307:CHL:HBC3	2.47	0.43
2:A:303:CLA:H12	2:A:303:CLA:H51	1.83	0.43
3:C:303:CHL:H142	3:C:307:CHL:H8	2.00	0.43
1:B:76:TRP:CZ2	11:B:322:SQD:H101	2.53	0.43
1:C:76:TRP:CZ2	11:C:322:SQD:H92	2.53	0.43
2:C:313:CLA:H61	2:C:313:CLA:H102	1.67	0.43
1:A:228:LYS:HE3	1:A:228:LYS:HB2	1.78	0.42
3:A:305:CHL:C3C	3:A:306:CHL:HBC3	2.49	0.42
1:A:169:ALA:HB1	1:A:174:LEU:HD13	2.01	0.41
2:A:312:CLA:H192	2:A:312:CLA:H161	1.95	0.41
2:A:310:CLA:H62	2:A:310:CLA:H2	1.83	0.41
3:B:305:CHL:H162	3:B:315:CHL:H71	2.03	0.41
1:A:105:PHE:HA	1:A:106:PRO:HD3	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:313:CLA:H92	2:B:313:CLA:H111	1.95	0.41
2:C:304:CLA:H51	2:C:304:CLA:H12	1.83	0.41
3:B:307:CHL:H2	3:B:307:CHL:H61	1.85	0.41
2:C:308:CLA:H8	2:C:310:CLA:H162	2.03	0.41
2:B:304:CLA:H101	2:B:304:CLA:H62	1.91	0.40
1:B:180:LYS:HD3	2:B:312:CLA:HBA2	2.03	0.40
3:C:307:CHL:H142	3:C:307:CHL:H112	1.92	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	200/202 (99%)	198 (99%)	2 (1%)	0	100	100
1	B	200/202 (99%)	199 (100%)	1 (0%)	0	100	100
1	C	200/202 (99%)	197 (98%)	3 (2%)	0	100	100
All	All	600/606 (99%)	594 (99%)	6 (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	153/153 (100%)	152 (99%)	1 (1%)	76	74
1	B	153/153 (100%)	153 (100%)	0	100	100
1	C	153/153 (100%)	153 (100%)	0	100	100
All	All	459/459 (100%)	458 (100%)	1 (0%)	85	87

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	170	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	211	GLN

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 ⓘ

69 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	CHL	A	304	1	60,74,74	1.39	4 (6%)	58,114,114	1.85	8 (13%)
6	A1LYY	B	317	-	45,48,48	0.55	1 (2%)	58,73,73	0.99	3 (5%)
3	CHL	C	303	1	57,71,74	1.40	5 (8%)	54,110,114	1.80	8 (14%)
9	A1L0E	C	301	-	43,43,43	0.14	0	54,60,60	0.45	0
5	IWJ	A	318	-	43,45,45	0.46	1 (2%)	47,65,65	1.39	3 (6%)
12	A1LYW	B	301	-	51,54,54	0.37	0	66,77,77	1.28	7 (10%)
5	IWJ	A	315	-	43,45,45	0.57	1 (2%)	47,65,65	1.33	3 (6%)
8	A1LYX	A	319	-	43,44,44	0.46	1 (2%)	52,61,61	2.05	4 (7%)
11	SQD	B	322	-	40,40,54	0.20	0	42,42,65	0.21	0
12	A1LYW	B	323	-	51,54,54	0.39	0	66,77,77	1.27	6 (9%)
2	CLA	A	307	13	69,73,73	1.56	8 (11%)	82,113,113	1.02	9 (10%)
3	CHL	B	305	1	60,74,74	1.37	4 (6%)	58,114,114	1.90	9 (15%)
7	NEX	A	317	-	40,46,46	1.53	5 (12%)	50,70,70	0.72	2 (4%)
2	CLA	A	310	1	65,69,73	1.60	8 (12%)	77,108,113	1.03	9 (11%)
9	A1L0E	A	320	-	43,43,43	0.19	0	54,60,60	0.45	0
2	CLA	B	308	-	69,73,73	1.54	9 (13%)	82,113,113	1.02	9 (10%)
7	NEX	B	318	-	40,46,46	1.93	6 (15%)	50,70,70	0.75	3 (6%)
9	A1L0E	A	324	-	43,43,43	0.20	0	54,60,60	0.44	0
10	AV0	C	321	-	24,24,72	0.14	0	26,26,98	0.69	1 (3%)
11	SQD	C	322	-	40,40,54	0.20	0	42,42,65	0.19	0
3	CHL	B	306	-	42,56,74	1.61	5 (11%)	36,92,114	2.37	8 (22%)
2	CLA	B	302	1	69,73,73	1.57	9 (13%)	82,113,113	0.96	6 (7%)
3	CHL	B	315	1	60,74,74	1.38	4 (6%)	58,114,114	1.81	8 (13%)
4	A1L0F	B	309	1	50,53,53	1.96	11 (22%)	60,89,89	2.45	11 (18%)
3	CHL	B	303	1	57,71,74	1.42	5 (8%)	54,110,114	1.89	9 (16%)
3	CHL	A	314	1	60,74,74	1.37	4 (6%)	58,114,114	1.81	8 (13%)
6	A1LYY	A	316	-	45,48,48	0.51	1 (2%)	58,73,73	0.92	3 (5%)
3	CHL	C	306	-	42,56,74	1.64	5 (11%)	36,92,114	2.41	7 (19%)
5	IWJ	C	316	-	43,45,45	0.56	1 (2%)	47,65,65	1.33	3 (6%)
4	A1L0F	C	309	1	50,53,53	1.99	11 (22%)	60,89,89	2.70	11 (18%)
3	CHL	B	314	1	47,61,74	1.54	4 (8%)	41,98,114	2.05	6 (14%)
2	CLA	C	308	-	69,73,73	1.53	9 (13%)	82,113,113	1.05	9 (10%)
2	CLA	A	301	1	69,73,73	1.59	9 (13%)	82,113,113	0.97	7 (8%)
2	CLA	C	302	1	69,73,73	1.60	10 (14%)	82,113,113	0.96	6 (7%)
2	CLA	C	310	1	69,73,73	1.54	10 (14%)	82,113,113	1.00	9 (10%)
2	CLA	C	312	1	50,54,73	1.82	9 (18%)	59,90,113	1.22	9 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	CHL	C	315	1	60,74,74	1.41	4 (6%)	58,114,114	1.81	8 (13%)
2	CLA	B	311	1	65,69,73	1.60	8 (12%)	77,108,113	1.01	9 (11%)
11	SQD	A	322	-	40,40,54	0.22	0	42,42,65	0.20	0
3	CHL	A	305	13	42,56,74	1.73	5 (11%)	36,92,114	2.38	7 (19%)
2	CLA	B	313	1	69,73,73	1.51	9 (13%)	82,113,113	0.97	8 (9%)
10	AV0	A	321	-	24,24,72	0.14	0	26,26,98	0.70	1 (3%)
2	CLA	C	313	1	69,73,73	1.53	9 (13%)	82,113,113	0.97	8 (9%)
5	IWJ	B	316	-	43,45,45	0.53	1 (2%)	47,65,65	1.32	2 (4%)
3	CHL	B	307	-	60,74,74	1.35	4 (6%)	58,114,114	1.80	8 (13%)
3	CHL	A	306	13	60,74,74	1.35	3 (5%)	58,114,114	1.82	8 (13%)
5	IWJ	B	319	-	43,45,45	0.46	1 (2%)	47,65,65	1.40	3 (6%)
8	A1LYX	B	320	-	43,44,44	0.37	0	52,61,61	2.11	4 (7%)
10	AV0	B	321	-	24,24,72	0.13	0	26,26,98	0.70	1 (3%)
2	CLA	A	303	13	69,73,73	1.54	9 (13%)	82,113,113	0.95	8 (9%)
2	CLA	C	311	1	65,69,73	1.60	9 (13%)	77,108,113	1.03	8 (10%)
2	CLA	A	309	1	69,73,73	1.56	9 (13%)	82,113,113	1.03	7 (8%)
2	CLA	A	312	1	69,73,73	1.53	9 (13%)	82,113,113	0.96	8 (9%)
2	CLA	B	304	-	69,73,73	1.54	9 (13%)	82,113,113	0.97	8 (9%)
6	A1LYY	C	317	-	45,48,48	0.54	1 (2%)	58,73,73	0.89	3 (5%)
8	A1LYX	C	320	-	43,44,44	0.53	1 (2%)	52,61,61	2.01	4 (7%)
3	CHL	A	302	1	57,71,74	1.38	6 (10%)	54,110,114	1.86	8 (14%)
2	CLA	B	310	1	69,73,73	1.57	9 (13%)	82,113,113	0.99	8 (9%)
2	CLA	B	312	1	50,54,73	1.81	8 (16%)	59,90,113	1.23	9 (15%)
4	A1LOF	A	308	1	50,53,53	1.90	10 (20%)	60,89,89	2.57	13 (21%)
12	A1LYW	A	323	-	51,54,54	0.40	0	66,77,77	1.26	6 (9%)
5	IWJ	C	319	-	43,45,45	0.45	1 (2%)	47,65,65	1.37	3 (6%)
2	CLA	A	311	1	50,54,73	1.81	9 (18%)	59,90,113	1.21	8 (13%)
3	CHL	C	307	-	60,74,74	1.34	4 (6%)	58,114,114	1.82	7 (12%)
3	CHL	A	313	1	47,61,74	1.59	5 (10%)	41,98,114	1.95	7 (17%)
3	CHL	C	305	1	60,74,74	1.41	5 (8%)	58,114,114	1.84	9 (15%)
2	CLA	C	304	-	69,73,73	1.55	8 (11%)	82,113,113	0.96	8 (9%)
7	NEX	C	318	-	40,46,46	1.53	7 (17%)	50,70,70	0.75	2 (4%)
3	CHL	C	314	1	47,61,74	1.57	5 (10%)	41,98,114	1.99	6 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CHL	A	304	1	4/4/20/26	8/39/137/137	-
6	A1LYY	B	317	-	-	0/27/90/90	0/4/4/4
3	CHL	C	303	1	4/4/19/26	5/36/134/137	-
9	A1L0E	C	301	-	-	1/29/67/67	0/2/2/2
5	IWJ	A	318	-	1/1/13/26	1/33/76/76	0/2/2/2
12	A1LYW	B	301	-	-	2/41/91/91	0/3/3/3
5	IWJ	A	315	-	1/1/13/26	1/33/76/76	0/2/2/2
12	A1LYW	B	323	-	1/1/13/29	2/41/91/91	0/3/3/3
8	A1LYX	A	319	-	-	2/31/69/69	0/2/2/2
11	SQD	B	322	-	-	6/42/42/69	-
2	CLA	A	307	13	2/2/15/20	3/39/115/115	-
3	CHL	B	305	1	4/4/20/26	7/39/137/137	-
7	NEX	A	317	-	-	2/27/83/83	0/3/3/3
2	CLA	A	310	1	2/2/14/20	6/35/111/115	-
9	A1L0E	A	320	-	-	1/29/67/67	0/2/2/2
2	CLA	B	308	-	2/2/15/20	6/39/115/115	-
7	NEX	B	318	-	-	2/27/83/83	0/3/3/3
9	A1L0E	A	324	-	-	1/29/67/67	0/2/2/2
10	AV0	C	321	-	-	1/28/28/130	-
11	SQD	C	322	-	-	11/42/42/69	-
3	CHL	B	306	-	3/3/16/26	2/18/116/137	-
2	CLA	B	302	1	2/2/15/20	6/39/115/115	-
3	CHL	B	315	1	4/4/20/26	9/39/137/137	-
4	A1L0F	B	309	1	1/1/6/11	1/15/71/71	-
3	CHL	B	303	1	4/4/19/26	6/36/134/137	-
3	CHL	A	314	1	4/4/20/26	9/39/137/137	-
6	A1LYY	A	316	-	-	0/27/90/90	0/4/4/4
3	CHL	C	306	-	3/3/16/26	1/18/116/137	-
5	IWJ	C	316	-	1/1/13/26	1/33/76/76	0/2/2/2
4	A1L0F	C	309	1	1/1/6/11	5/15/71/71	-
3	CHL	B	314	1	3/3/17/26	4/24/122/137	-
2	CLA	C	308	-	2/2/15/20	5/39/115/115	-
2	CLA	A	301	1	2/2/15/20	5/39/115/115	-
2	CLA	C	302	1	2/2/15/20	5/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CLA	C	310	1	2/2/15/20	3/39/115/115	-
2	CLA	C	312	1	1/1/11/20	2/17/93/115	-
3	CHL	C	315	1	4/4/20/26	11/39/137/137	-
2	CLA	B	311	1	2/2/14/20	7/35/111/115	-
11	SQD	A	322	-	-	8/42/42/69	-
3	CHL	A	305	13	3/3/16/26	2/18/116/137	-
2	CLA	B	313	1	2/2/15/20	10/39/115/115	-
10	AV0	A	321	-	-	1/28/28/130	-
2	CLA	C	313	1	2/2/15/20	10/39/115/115	-
5	IWJ	B	316	-	1/1/13/26	1/33/76/76	0/2/2/2
3	CHL	B	307	-	4/4/20/26	12/39/137/137	-
3	CHL	A	306	13	4/4/20/26	8/39/137/137	-
5	IWJ	B	319	-	1/1/13/26	2/33/76/76	0/2/2/2
8	A1LYX	B	320	-	-	3/31/69/69	0/2/2/2
10	AV0	B	321	-	-	1/28/28/130	-
2	CLA	A	303	13	2/2/15/20	0/39/115/115	-
2	CLA	C	311	1	2/2/14/20	7/35/111/115	-
2	CLA	A	309	1	2/2/15/20	4/39/115/115	-
2	CLA	A	312	1	2/2/15/20	10/39/115/115	-
2	CLA	B	304	-	2/2/15/20	1/39/115/115	-
6	A1LYY	C	317	-	-	0/27/90/90	0/4/4/4
8	A1LYX	C	320	-	-	3/31/69/69	0/2/2/2
3	CHL	A	302	1	4/4/19/26	5/36/134/137	-
2	CLA	B	310	1	2/2/15/20	5/39/115/115	-
2	CLA	B	312	1	1/1/11/20	2/17/93/115	-
4	A1LOF	A	308	1	1/1/6/11	1/15/71/71	-
12	A1LYW	A	323	-	-	2/41/91/91	0/3/3/3
5	IWJ	C	319	-	1/1/13/26	1/33/76/76	0/2/2/2
2	CLA	A	311	1	1/1/11/20	4/17/93/115	-
3	CHL	C	307	-	4/4/20/26	11/39/137/137	-
3	CHL	A	313	1	3/3/17/26	4/24/122/137	-
3	CHL	C	305	1	4/4/20/26	7/39/137/137	-
2	CLA	C	304	-	2/2/15/20	2/39/115/115	-
7	NEX	C	318	-	-	2/27/83/83	0/3/3/3
3	CHL	C	314	1	3/3/17/26	4/24/122/137	-

All (328) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	CLA	C4B-NB	8.77	1.49	1.37
2	C	302	CLA	C4B-NB	8.59	1.49	1.37
2	B	302	CLA	C4B-NB	8.31	1.48	1.37
3	A	305	CHL	C1B-C2B	8.21	1.48	1.39
2	A	303	CLA	C4B-NB	7.91	1.48	1.37
2	B	304	CLA	C4B-NB	7.91	1.48	1.37
2	C	304	CLA	C4B-NB	7.88	1.48	1.37
2	A	307	CLA	C4B-NB	7.85	1.48	1.37
2	B	311	CLA	C4B-NB	7.76	1.48	1.37
2	C	310	CLA	C4B-NB	7.72	1.48	1.37
2	A	312	CLA	C4B-NB	7.70	1.48	1.37
2	A	309	CLA	C4B-NB	7.70	1.48	1.37
2	B	310	CLA	C4B-NB	7.67	1.47	1.37
3	C	315	CHL	C1B-C2B	7.66	1.48	1.39
3	A	313	CHL	C1B-C2B	7.65	1.48	1.39
2	C	313	CLA	C4B-NB	7.63	1.47	1.37
3	C	305	CHL	C1B-C2B	7.60	1.48	1.39
2	C	312	CLA	C4B-NB	7.55	1.47	1.37
2	C	308	CLA	C4B-NB	7.55	1.47	1.37
3	A	314	CHL	C1B-C2B	7.54	1.48	1.39
3	B	315	CHL	C1B-C2B	7.53	1.48	1.39
2	A	311	CLA	C4B-NB	7.48	1.47	1.37
2	B	313	CLA	C4B-NB	7.42	1.47	1.37
2	B	308	CLA	C4B-NB	7.41	1.47	1.37
3	C	314	CHL	C1B-C2B	7.41	1.48	1.39
2	B	312	CLA	C4B-NB	7.38	1.47	1.37
2	C	311	CLA	C4B-NB	7.32	1.47	1.37
3	B	307	CHL	C1B-C2B	7.32	1.47	1.39
2	A	310	CLA	C4B-NB	7.27	1.47	1.37
3	A	306	CHL	C1B-C2B	7.24	1.47	1.39
3	C	306	CHL	C1B-C2B	7.22	1.47	1.39
3	A	304	CHL	C1B-C2B	7.21	1.47	1.39
3	C	307	CHL	C1B-C2B	7.20	1.47	1.39
3	B	314	CHL	C1B-C2B	7.17	1.47	1.39
3	B	306	CHL	C1B-C2B	7.04	1.47	1.39
3	B	305	CHL	C1B-C2B	7.01	1.47	1.39
3	C	303	CHL	C1B-C2B	6.87	1.47	1.39
3	B	303	CHL	C1B-C2B	6.84	1.47	1.39
3	A	302	CHL	C1B-C2B	6.82	1.47	1.39
7	B	318	NEX	C30-C29	6.71	1.51	1.35
4	C	309	A1L0F	C24-C16	6.65	1.54	1.39
4	A	308	A1L0F	C24-C16	6.45	1.53	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	318	NEX	C28-C29	6.37	1.59	1.46
4	B	309	A1L0F	C24-C16	6.32	1.53	1.39
4	C	309	A1L0F	MG-N4	5.45	2.19	2.06
4	B	309	A1L0F	MG-N4	5.36	2.19	2.06
4	B	309	A1L0F	MG-N15	5.26	2.18	2.06
2	C	311	CLA	MG-NB	-5.08	1.95	2.05
7	A	317	NEX	C30-C29	5.02	1.47	1.35
2	A	310	CLA	MG-NB	-4.96	1.96	2.05
2	B	310	CLA	MG-NB	-4.95	1.96	2.05
7	A	317	NEX	C28-C29	4.89	1.56	1.46
4	C	309	A1L0F	MG-N15	4.89	2.17	2.06
2	B	310	CLA	MG-ND	-4.87	1.96	2.05
2	A	309	CLA	MG-ND	-4.84	1.96	2.05
2	C	310	CLA	MG-NB	-4.81	1.96	2.05
7	C	318	NEX	C30-C29	4.78	1.46	1.35
2	B	308	CLA	MG-NB	-4.78	1.96	2.05
4	A	308	A1L0F	MG-N4	4.77	2.17	2.06
2	A	309	CLA	MG-NB	-4.74	1.96	2.05
2	C	304	CLA	MG-NB	-4.69	1.96	2.05
7	B	318	NEX	C32-C33	-4.69	1.35	1.46
2	A	307	CLA	MG-NB	-4.69	1.96	2.05
2	C	313	CLA	MG-ND	-4.67	1.96	2.05
2	B	302	CLA	MG-NB	-4.66	1.96	2.05
2	C	313	CLA	MG-NB	-4.65	1.96	2.05
2	C	302	CLA	MG-NB	-4.63	1.96	2.05
2	C	302	CLA	MG-ND	-4.63	1.96	2.05
2	A	312	CLA	MG-ND	-4.62	1.96	2.05
4	B	309	A1L0F	C11-C8	4.60	1.49	1.39
2	A	301	CLA	MG-NB	-4.60	1.96	2.05
2	C	308	CLA	MG-ND	-4.60	1.96	2.05
2	B	313	CLA	MG-ND	-4.57	1.96	2.05
2	A	307	CLA	MG-ND	-4.56	1.96	2.05
2	B	311	CLA	MG-NB	-4.55	1.96	2.05
2	A	303	CLA	MG-NB	-4.54	1.96	2.05
4	A	308	A1L0F	C11-C8	4.52	1.49	1.39
2	B	304	CLA	MG-NB	-4.51	1.96	2.05
2	C	312	CLA	MG-NB	-4.50	1.96	2.05
2	C	310	CLA	MG-ND	-4.49	1.96	2.05
2	A	311	CLA	MG-NB	-4.48	1.96	2.05
2	B	308	CLA	MG-ND	-4.45	1.97	2.05
2	C	308	CLA	MG-NB	-4.44	1.97	2.05
2	B	313	CLA	MG-NB	-4.44	1.97	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	311	CLA	MG-ND	-4.42	1.97	2.05
2	A	310	CLA	MG-ND	-4.42	1.97	2.05
4	C	309	A1L0F	C11-C8	4.42	1.49	1.39
2	B	312	CLA	MG-NB	-4.39	1.97	2.05
7	B	318	NEX	C40-C33	-4.35	1.42	1.50
4	A	308	A1L0F	MG-N15	4.34	2.16	2.06
2	B	302	CLA	MG-ND	-4.32	1.97	2.05
2	A	312	CLA	MG-NB	-4.27	1.97	2.05
3	B	303	CHL	C3B-C4B	4.24	1.45	1.41
2	C	304	CLA	MG-ND	-4.24	1.97	2.05
2	B	312	CLA	MG-ND	-4.23	1.97	2.05
2	B	311	CLA	MG-ND	-4.21	1.97	2.05
7	C	318	NEX	C28-C29	4.21	1.55	1.46
2	B	304	CLA	MG-ND	-4.12	1.97	2.05
2	A	301	CLA	MG-ND	-4.10	1.97	2.05
2	A	303	CLA	MG-ND	-4.10	1.97	2.05
2	A	311	CLA	MG-ND	-4.09	1.97	2.05
3	B	305	CHL	C3B-C4B	4.08	1.45	1.41
3	C	306	CHL	C3B-C4B	4.06	1.45	1.41
3	A	302	CHL	C3B-C4B	4.03	1.45	1.41
2	C	312	CLA	MG-ND	-4.00	1.97	2.05
2	B	312	CLA	C1D-ND	3.96	1.43	1.37
3	A	304	CHL	C3B-C4B	3.95	1.45	1.41
3	C	305	CHL	C3B-C4B	3.93	1.45	1.41
3	A	314	CHL	C3B-C4B	3.92	1.45	1.41
7	C	318	NEX	C39-C29	-3.90	1.43	1.50
3	C	315	CHL	C3B-C4B	3.90	1.45	1.41
3	B	306	CHL	C3B-C4B	3.89	1.45	1.41
3	B	315	CHL	C3B-C4B	3.88	1.45	1.41
7	A	317	NEX	C40-C33	-3.86	1.43	1.50
3	A	305	CHL	C3B-C4B	3.86	1.45	1.41
3	C	303	CHL	C3B-C4B	3.85	1.45	1.41
3	A	306	CHL	C1A-CHA	-3.74	1.35	1.40
3	C	303	CHL	C1A-CHA	-3.74	1.35	1.40
3	B	314	CHL	C3B-C4B	3.70	1.45	1.41
2	B	311	CLA	MG-NA	-3.70	1.97	2.06
2	C	312	CLA	C1D-ND	3.70	1.42	1.37
3	B	307	CHL	C3B-C4B	3.66	1.45	1.41
2	C	304	CLA	C1D-ND	3.63	1.42	1.37
2	A	310	CLA	MG-NA	-3.62	1.97	2.06
3	C	314	CHL	C1A-CHA	-3.62	1.35	1.40
7	A	317	NEX	C28-C27	-3.62	1.24	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	311	CLA	C1D-ND	3.61	1.42	1.37
3	C	307	CHL	C1A-CHA	-3.59	1.35	1.40
3	A	313	CHL	C3B-C4B	3.59	1.44	1.41
3	C	314	CHL	C3B-C4B	3.59	1.44	1.41
3	C	307	CHL	C3B-C4B	3.57	1.44	1.41
3	A	313	CHL	C1A-CHA	-3.56	1.36	1.40
4	B	309	A1L0F	C17-C10	3.56	1.47	1.39
3	B	314	CHL	C1A-CHA	-3.55	1.36	1.40
3	A	306	CHL	C3B-C4B	3.55	1.44	1.41
2	B	308	CLA	C1D-ND	3.54	1.42	1.37
2	A	311	CLA	C1D-ND	3.54	1.42	1.37
3	A	302	CHL	C1A-CHA	-3.53	1.36	1.40
3	A	304	CHL	C1A-CHA	-3.53	1.36	1.40
2	C	311	CLA	MG-NA	-3.52	1.97	2.06
3	B	303	CHL	C1A-CHA	-3.51	1.36	1.40
3	C	305	CHL	C1A-CHA	-3.51	1.36	1.40
2	B	311	CLA	C1D-ND	3.51	1.42	1.37
2	A	311	CLA	MG-NA	-3.50	1.98	2.06
2	B	304	CLA	C1D-ND	3.50	1.42	1.37
3	B	307	CHL	C1A-CHA	-3.50	1.36	1.40
3	C	315	CHL	C1A-CHA	-3.49	1.36	1.40
3	B	305	CHL	C1A-CHA	-3.47	1.36	1.40
2	A	310	CLA	C1D-ND	3.46	1.42	1.37
2	C	312	CLA	MG-NA	-3.44	1.98	2.06
2	B	310	CLA	MG-NA	-3.43	1.98	2.06
3	C	306	CHL	C1A-CHA	-3.41	1.36	1.40
2	A	307	CLA	C1D-ND	3.41	1.42	1.37
3	B	315	CHL	C1A-CHA	-3.39	1.36	1.40
2	A	303	CLA	MG-NA	-3.39	1.98	2.06
3	A	314	CHL	C1A-CHA	-3.39	1.36	1.40
2	A	303	CLA	C1D-ND	3.39	1.42	1.37
2	C	304	CLA	MG-NA	-3.37	1.98	2.06
3	B	306	CHL	C1A-CHA	-3.37	1.36	1.40
2	B	312	CLA	MG-NA	-3.37	1.98	2.06
2	C	310	CLA	MG-NA	-3.36	1.98	2.06
2	B	313	CLA	C1D-ND	3.35	1.42	1.37
3	A	305	CHL	C1A-CHA	-3.34	1.36	1.40
4	C	309	A1L0F	O40-C41	-3.33	1.37	1.45
2	C	308	CLA	C1D-ND	3.32	1.42	1.37
2	C	313	CLA	C1D-ND	3.29	1.42	1.37
4	A	308	A1L0F	C17-C10	3.28	1.46	1.39
2	B	302	CLA	C1D-ND	3.27	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	CLA	C1D-ND	3.27	1.42	1.37
2	A	309	CLA	MG-NA	-3.26	1.98	2.06
4	C	309	A1L0F	C17-C10	3.26	1.46	1.39
6	B	317	A1LYY	C30-C31	-3.24	1.49	1.52
2	C	308	CLA	MG-NA	-3.24	1.98	2.06
2	A	312	CLA	MG-NA	-3.22	1.98	2.06
2	B	308	CLA	MG-NA	-3.21	1.98	2.06
4	A	308	A1L0F	O40-C41	-3.21	1.38	1.45
2	B	302	CLA	MG-NA	-3.20	1.98	2.06
7	B	318	NEX	C39-C29	-3.18	1.44	1.50
7	A	317	NEX	C39-C29	3.18	1.57	1.50
4	B	309	A1L0F	O40-C41	-3.17	1.38	1.45
7	C	318	NEX	C28-C27	-3.16	1.25	1.32
2	B	310	CLA	MG-NC	-3.14	1.98	2.06
6	C	317	A1LYY	C30-C31	-3.14	1.49	1.52
2	B	304	CLA	MG-NA	-3.14	1.98	2.06
2	B	313	CLA	MG-NA	-3.13	1.98	2.06
2	C	302	CLA	MG-NA	-3.10	1.98	2.06
2	C	310	CLA	MG-NC	-3.10	1.98	2.06
5	C	316	IWJ	C05-C04	-3.10	1.49	1.52
2	A	309	CLA	C1B-NB	3.10	1.41	1.37
2	C	313	CLA	MG-NA	-3.09	1.98	2.06
5	A	315	IWJ	C05-C04	-3.09	1.49	1.52
2	A	307	CLA	MG-NA	-3.08	1.99	2.06
2	A	311	CLA	MG-NC	-3.08	1.99	2.06
2	A	311	CLA	C1B-NB	3.08	1.41	1.37
2	B	308	CLA	MG-NC	-3.07	1.99	2.06
2	A	310	CLA	MG-NC	-3.07	1.99	2.06
2	A	301	CLA	MG-NA	-3.07	1.99	2.06
2	A	307	CLA	MG-NC	-3.06	1.99	2.06
2	B	304	CLA	MG-NC	-3.05	1.99	2.06
7	C	318	NEX	C35-C34	-3.05	1.33	1.43
2	B	311	CLA	MG-NC	-3.04	1.99	2.06
2	A	312	CLA	C1D-ND	3.03	1.41	1.37
8	C	320	A1LYX	C30-C31	-3.02	1.49	1.52
2	B	312	CLA	MG-NC	-3.01	1.99	2.06
2	B	310	CLA	C1D-ND	3.00	1.41	1.37
2	C	308	CLA	MG-NC	-3.00	1.99	2.06
6	A	316	A1LYY	C30-C31	-3.00	1.49	1.52
2	A	303	CLA	MG-NC	-2.99	1.99	2.06
2	A	309	CLA	MG-NC	-2.99	1.99	2.06
2	B	312	CLA	C1B-NB	2.99	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	304	CLA	MG-NC	-2.94	1.99	2.06
2	A	312	CLA	MG-NC	-2.92	1.99	2.06
5	B	316	IWJ	C05-C04	-2.91	1.49	1.52
2	C	311	CLA	MG-NC	-2.91	1.99	2.06
2	C	302	CLA	C1D-ND	2.90	1.41	1.37
2	C	312	CLA	MG-NC	-2.88	1.99	2.06
2	A	309	CLA	C1D-ND	2.87	1.41	1.37
2	C	312	CLA	C1B-NB	2.86	1.41	1.37
4	A	308	A1L0F	C35-C34	-2.86	1.43	1.56
4	B	309	A1L0F	C35-C34	-2.85	1.43	1.56
4	C	309	A1L0F	C3-C2	2.83	1.51	1.45
2	B	308	CLA	C1B-NB	2.83	1.41	1.37
4	C	309	A1L0F	C35-C34	-2.81	1.44	1.56
2	C	308	CLA	C1B-NB	2.81	1.41	1.37
2	C	310	CLA	C1D-ND	2.80	1.41	1.37
2	C	302	CLA	MG-NC	-2.79	1.99	2.06
2	B	310	CLA	C1B-NB	2.78	1.41	1.37
2	A	301	CLA	MG-NC	-2.77	1.99	2.06
2	C	310	CLA	C1B-NB	2.73	1.41	1.37
2	A	310	CLA	C1B-NB	2.72	1.41	1.37
2	A	307	CLA	C1B-NB	2.72	1.41	1.37
2	B	302	CLA	MG-NC	-2.71	1.99	2.06
4	A	308	A1L0F	C3-C2	2.70	1.51	1.45
2	B	313	CLA	MG-NC	-2.68	1.99	2.06
4	A	308	A1L0F	C14-N15	2.67	1.42	1.37
2	B	313	CLA	C1B-NB	2.62	1.41	1.37
2	C	304	CLA	C1B-NB	2.60	1.41	1.37
4	C	309	A1L0F	C14-N15	2.59	1.42	1.37
2	C	302	CLA	C1C-C2C	2.58	1.49	1.44
7	B	318	NEX	C28-C27	-2.57	1.27	1.32
2	C	302	CLA	C1B-NB	2.57	1.41	1.37
2	A	303	CLA	C1C-C2C	2.55	1.49	1.44
7	C	318	NEX	C31-C30	-2.54	1.35	1.43
2	A	301	CLA	C1C-C2C	2.54	1.49	1.44
2	B	304	CLA	C1B-NB	2.53	1.41	1.37
2	B	311	CLA	C1B-NB	2.53	1.41	1.37
3	B	303	CHL	C3B-C2B	-2.50	1.37	1.40
3	A	313	CHL	C3B-C2B	-2.48	1.37	1.40
2	C	311	CLA	C1B-NB	2.47	1.41	1.37
8	A	319	A1LYX	C30-C31	-2.47	1.49	1.52
2	A	303	CLA	C1B-NB	2.46	1.41	1.37
3	B	314	CHL	C3B-C2B	-2.45	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	314	CHL	C3B-C2B	-2.45	1.37	1.40
2	A	312	CLA	C1B-NB	2.43	1.41	1.37
7	C	318	NEX	C40-C33	-2.43	1.45	1.50
4	B	309	A1L0F	C14-N15	2.42	1.41	1.37
2	C	313	CLA	MG-NC	-2.42	2.00	2.06
5	B	319	IWJ	C05-C04	-2.41	1.49	1.52
2	C	312	CLA	C1C-C2C	2.41	1.49	1.44
2	A	312	CLA	C1C-C2C	2.40	1.49	1.44
2	A	310	CLA	C1D-C2D	-2.38	1.40	1.45
2	B	302	CLA	C1B-NB	2.37	1.41	1.37
4	B	309	A1L0F	C3-C2	2.37	1.50	1.45
2	A	311	CLA	C1D-C2D	-2.36	1.40	1.45
2	B	304	CLA	C1C-C2C	2.35	1.49	1.44
2	B	311	CLA	C1D-C2D	-2.35	1.40	1.45
2	C	313	CLA	C1D-C2D	-2.35	1.40	1.45
2	B	302	CLA	C1C-C2C	2.35	1.49	1.44
2	C	312	CLA	C1D-C2D	-2.32	1.40	1.45
2	C	310	CLA	C1D-C2D	-2.30	1.40	1.45
2	C	302	CLA	C1D-C2D	-2.30	1.40	1.45
3	B	303	CHL	CHB-C4A	-2.30	1.35	1.38
2	B	312	CLA	C1D-C2D	-2.30	1.40	1.45
2	C	311	CLA	C1D-C2D	-2.30	1.40	1.45
3	A	305	CHL	C3B-C2B	-2.29	1.37	1.40
2	A	301	CLA	C1B-NB	2.29	1.40	1.37
3	B	306	CHL	C3B-C2B	-2.29	1.37	1.40
5	A	318	IWJ	C05-C04	-2.27	1.50	1.52
2	C	304	CLA	C1D-C2D	-2.27	1.40	1.45
2	A	309	CLA	C1D-C2D	-2.27	1.40	1.45
2	B	302	CLA	C1D-C2D	-2.27	1.40	1.45
3	C	303	CHL	C3B-C2B	-2.26	1.37	1.40
5	C	319	IWJ	C05-C04	-2.26	1.50	1.52
2	C	313	CLA	C1C-C2C	2.26	1.49	1.44
2	A	303	CLA	C1D-C2D	-2.26	1.40	1.45
2	B	310	CLA	C1D-C2D	-2.25	1.40	1.45
2	B	313	CLA	C1D-C2D	-2.23	1.40	1.45
3	A	302	CHL	C3B-C2B	-2.23	1.37	1.40
2	B	304	CLA	C1D-C2D	-2.23	1.40	1.45
3	A	304	CHL	C3B-C2B	-2.23	1.37	1.40
2	A	307	CLA	C1D-C2D	-2.22	1.40	1.45
4	C	309	A1L0F	C17-C14	-2.22	1.34	1.38
3	C	306	CHL	CHA-CBD	2.22	1.54	1.51
2	B	308	CLA	C1D-C2D	-2.21	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	312	CLA	C1D-C2D	-2.21	1.41	1.45
3	B	307	CHL	C3B-C2B	-2.21	1.37	1.40
2	B	313	CLA	C1C-C2C	2.20	1.49	1.44
2	C	308	CLA	C1D-C2D	-2.20	1.41	1.45
3	A	305	CHL	CHA-CBD	2.20	1.54	1.51
3	C	315	CHL	C3B-C2B	-2.20	1.37	1.40
2	A	301	CLA	C1D-C2D	-2.20	1.41	1.45
3	B	306	CHL	CHA-CBD	2.19	1.54	1.51
2	C	313	CLA	C1B-NB	2.18	1.40	1.37
3	C	305	CHL	C3B-C2B	-2.14	1.37	1.40
4	A	308	A1L0F	C8-C7	-2.14	1.38	1.43
3	C	307	CHL	C3B-C2B	-2.14	1.37	1.40
2	C	310	CLA	C1C-C2C	2.12	1.48	1.44
3	B	305	CHL	C3B-C2B	-2.11	1.37	1.40
2	C	311	CLA	C1C-C2C	2.10	1.48	1.44
4	B	309	A1L0F	C17-C14	-2.08	1.34	1.38
3	C	306	CHL	C3B-C2B	-2.08	1.37	1.40
4	C	309	A1L0F	C8-C7	-2.08	1.38	1.43
4	B	309	A1L0F	C8-C7	-2.06	1.38	1.43
3	C	303	CHL	CHB-C4A	-2.06	1.36	1.38
3	A	313	CHL	CHC-C4B	-2.06	1.36	1.39
2	B	308	CLA	C3D-C4D	-2.05	1.39	1.44
3	A	302	CHL	CHA-CBD	2.04	1.54	1.51
3	A	302	CHL	CHB-C4A	-2.04	1.36	1.38
3	B	315	CHL	C3B-C2B	-2.03	1.37	1.40
2	C	308	CLA	C3D-C4D	-2.03	1.39	1.44
3	A	314	CHL	C3B-C2B	-2.02	1.37	1.40
2	A	309	CLA	C3D-C4D	-2.01	1.39	1.44
2	C	310	CLA	C3D-C4D	-2.01	1.39	1.44
2	B	310	CLA	C3D-C4D	-2.01	1.39	1.44
3	C	314	CHL	CHC-C4B	-2.01	1.36	1.39
2	C	302	CLA	C3D-C4D	-2.01	1.39	1.44
3	C	305	CHL	C3A-C2A	-2.01	1.53	1.54
2	A	311	CLA	C1C-C2C	2.01	1.48	1.44

All (411) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	309	A1L0F	C5-N4-C3	16.70	114.30	106.68
4	A	308	A1L0F	C5-N4-C3	15.28	113.65	106.68
4	B	309	A1L0F	C5-N4-C3	14.80	113.43	106.68
3	C	306	CHL	C1B-CHB-C4A	11.80	128.91	121.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	305	CHL	C1B-CHB-C4A	11.53	128.74	121.32
3	B	305	CHL	C1B-CHB-C4A	11.35	128.63	121.32
3	B	306	CHL	C1B-CHB-C4A	11.28	128.58	121.32
3	A	304	CHL	C1B-CHB-C4A	11.11	128.47	121.32
3	C	305	CHL	C1B-CHB-C4A	10.98	128.38	121.32
3	B	303	CHL	C1B-CHB-C4A	10.95	128.37	121.32
3	A	314	CHL	C1B-CHB-C4A	10.89	128.33	121.32
3	C	315	CHL	C1B-CHB-C4A	10.86	128.31	121.32
3	B	315	CHL	C1B-CHB-C4A	10.73	128.22	121.32
3	A	302	CHL	C1B-CHB-C4A	10.70	128.21	121.32
3	A	306	CHL	C1B-CHB-C4A	10.63	128.16	121.32
3	B	307	CHL	C1B-CHB-C4A	10.57	128.12	121.32
3	C	307	CHL	C1B-CHB-C4A	10.53	128.09	121.32
3	B	314	CHL	C1B-CHB-C4A	10.38	128.00	121.32
3	C	303	CHL	C1B-CHB-C4A	10.16	127.86	121.32
3	C	314	CHL	C1B-CHB-C4A	10.03	127.78	121.32
8	B	320	A1LYX	O41-C31-C30	9.81	127.45	110.06
8	B	320	A1LYX	C30-C31-C32	9.71	125.61	111.18
8	A	319	A1LYX	C30-C31-C32	9.64	125.50	111.18
3	A	313	CHL	C1B-CHB-C4A	9.58	127.48	121.32
8	C	320	A1LYX	C30-C31-C32	9.48	125.26	111.18
8	A	319	A1LYX	O41-C31-C30	9.35	126.62	110.06
8	C	320	A1LYX	O41-C31-C30	9.06	126.11	110.06
5	B	319	IWJ	C28-C29-C35	-8.14	98.25	111.97
5	A	318	IWJ	C28-C29-C35	-7.93	98.61	111.97
5	C	319	IWJ	C28-C29-C35	-7.92	98.63	111.97
5	C	316	IWJ	C28-C29-C35	-7.65	99.09	111.97
5	A	315	IWJ	C28-C29-C35	-7.64	99.10	111.97
5	B	316	IWJ	C28-C29-C35	-7.54	99.26	111.97
12	B	301	A1LYW	C28-C27-C26	-5.49	118.11	126.23
12	B	323	A1LYW	C28-C27-C26	-5.20	118.55	126.23
12	A	323	A1LYW	C28-C27-C26	-5.15	118.62	126.23
12	B	323	A1LYW	O34-C4-C3	-4.92	108.88	113.49
2	C	312	CLA	C4A-NA-C1A	-4.75	104.51	106.68
2	A	309	CLA	C4A-NA-C1A	-4.75	104.51	106.68
6	B	317	A1LYY	C42-C2-C3	4.73	132.87	125.53
12	A	323	A1LYW	O34-C4-C3	-4.63	109.15	113.49
2	B	312	CLA	C4A-NA-C1A	-4.63	104.57	106.68
4	B	309	A1L0F	C22-C18-C34	-4.62	103.09	108.11
4	A	308	A1L0F	C22-C18-C34	-4.54	103.18	108.11
4	C	309	A1L0F	C22-C18-C34	-4.45	103.27	108.11
6	A	316	A1LYY	C42-C2-C3	4.34	132.26	125.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	301	A1LYW	O34-C4-C3	-4.27	109.49	113.49
2	C	308	CLA	C4A-NA-C1A	-4.23	104.75	106.68
2	A	311	CLA	C4A-NA-C1A	-4.21	104.76	106.68
3	C	307	CHL	C1A-CHA-C4D	4.16	125.92	118.98
2	C	310	CLA	C4A-NA-C1A	-4.11	104.80	106.68
2	B	310	CLA	C4A-NA-C1A	-4.04	104.84	106.68
6	C	317	A1LYY	C42-C2-C3	4.04	131.80	125.53
4	C	309	A1L0F	C2-C3-C23	3.98	131.72	127.50
2	B	304	CLA	C4A-NA-C1A	-3.88	104.91	106.68
3	B	306	CHL	C3D-C4D-CHA	3.88	114.44	108.54
2	A	307	CLA	C4A-NA-C1A	-3.87	104.91	106.68
2	C	311	CLA	C4A-NA-C1A	-3.85	104.92	106.68
3	A	305	CHL	C3D-C4D-CHA	3.84	114.38	108.54
3	B	305	CHL	C1A-CHA-C4D	3.83	125.38	118.98
3	B	307	CHL	C1A-CHA-C4D	3.80	125.32	118.98
2	C	302	CLA	C4A-NA-C1A	-3.80	104.94	106.68
12	B	301	A1LYW	C27-C28-C29	3.80	137.14	127.00
3	B	305	CHL	C3D-C4D-CHA	3.77	114.27	108.54
3	B	307	CHL	C3D-C4D-CHA	3.77	114.27	108.54
3	C	306	CHL	C3D-C4D-CHA	3.76	114.25	108.54
3	B	306	CHL	C1A-CHA-C4D	3.75	125.25	118.98
3	A	304	CHL	C1A-CHA-C4D	3.75	125.24	118.98
3	C	305	CHL	C1A-CHA-C4D	3.74	125.23	118.98
3	A	306	CHL	C1A-CHA-C4D	3.73	125.21	118.98
5	A	318	IWJ	O39-C29-C30	3.73	115.24	108.13
3	A	302	CHL	C3D-C4D-CHA	3.71	114.19	108.54
3	B	303	CHL	C3D-C4D-CHA	3.71	114.17	108.54
3	C	307	CHL	C3D-C4D-CHA	3.70	114.17	108.54
3	A	304	CHL	C3D-C4D-CHA	3.70	114.16	108.54
3	B	314	CHL	C3D-C4D-CHA	3.69	114.15	108.54
3	C	305	CHL	C3D-C4D-CHA	3.66	114.10	108.54
5	B	316	IWJ	O39-C29-C30	3.66	115.10	108.13
2	B	308	CLA	C4A-NA-C1A	-3.65	105.01	106.68
3	C	314	CHL	C3D-C4D-CHA	3.65	114.09	108.54
5	B	319	IWJ	O39-C29-C30	3.64	115.07	108.13
3	B	315	CHL	C3D-C4D-CHA	3.64	114.08	108.54
3	B	303	CHL	C1A-CHA-C4D	3.64	125.05	118.98
3	A	306	CHL	C3D-C4D-CHA	3.63	114.06	108.54
3	C	303	CHL	C3D-C4D-CHA	3.63	114.06	108.54
4	A	308	A1L0F	C2-C3-C23	3.61	131.33	127.50
5	C	319	IWJ	O39-C29-C30	3.61	115.01	108.13
3	A	313	CHL	C3D-C4D-CHA	3.61	114.03	108.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	323	A1LYW	C11-C12-C13	3.61	131.13	125.53
12	B	323	A1LYW	C27-C28-C29	3.60	136.61	127.00
3	A	314	CHL	C3D-C4D-CHA	3.58	113.98	108.54
8	B	320	A1LYX	O41-C31-C32	-3.55	103.14	110.39
3	C	303	CHL	C1A-CHA-C4D	3.55	124.91	118.98
3	C	315	CHL	C3D-C4D-CHA	3.54	113.93	108.54
3	B	315	CHL	C1A-CHA-C4D	3.54	124.89	118.98
3	C	306	CHL	C1A-CHA-C4D	3.48	124.78	118.98
5	C	316	IWJ	O39-C29-C30	3.48	114.75	108.13
2	C	304	CLA	C4A-NA-C1A	-3.48	105.09	106.68
3	A	305	CHL	C1A-CHA-C4D	3.47	124.77	118.98
2	B	302	CLA	C4A-NA-C1A	-3.46	105.10	106.68
3	C	315	CHL	C1A-CHA-C4D	3.46	124.75	118.98
5	A	315	IWJ	O39-C29-C30	3.42	114.65	108.13
2	A	301	CLA	C4A-NA-C1A	-3.37	105.14	106.68
2	A	303	CLA	C4A-NA-C1A	-3.36	105.14	106.68
12	B	323	A1LYW	C11-C12-C13	3.34	130.72	125.53
2	A	310	CLA	C4A-NA-C1A	-3.34	105.16	106.68
3	B	314	CHL	C1A-CHA-C4D	3.33	124.53	118.98
3	A	302	CHL	C1A-CHA-C4D	3.31	124.51	118.98
4	C	309	A1L0F	C27-C12-C13	-3.31	117.68	128.43
3	A	314	CHL	C1A-CHA-C4D	3.30	124.48	118.98
8	A	319	A1LYX	O41-C31-C32	-3.29	103.68	110.39
3	A	313	CHL	C1A-CHA-C4D	3.27	124.44	118.98
12	A	323	A1LYW	C27-C28-C29	3.27	135.72	127.00
12	B	301	A1LYW	C11-C12-C13	3.26	130.59	125.53
8	C	320	A1LYX	O41-C31-C32	-3.22	103.83	110.39
4	A	308	A1L0F	C27-C12-C13	-3.21	118.00	128.43
4	B	309	A1L0F	C41-O40-C38	3.21	123.19	115.92
4	B	309	A1L0F	C27-C12-C13	-3.21	118.01	128.43
4	A	308	A1L0F	C17-C14-N15	3.17	129.09	124.31
2	C	308	CLA	C1-C2-C3	-3.17	121.00	126.20
10	A	321	AV0	CBR-CCM-CBQ	-3.16	104.09	109.96
4	B	309	A1L0F	C2-C3-C23	3.15	130.84	127.50
4	A	308	A1L0F	C33-C2-C1	-3.08	122.09	127.87
10	B	321	AV0	CBR-CCM-CBQ	-3.07	104.26	109.96
4	A	308	A1L0F	C41-O40-C38	3.07	122.87	115.92
3	C	314	CHL	C1A-CHA-C4D	3.06	124.09	118.98
2	A	312	CLA	C4A-NA-C1A	-3.05	105.29	106.68
2	A	310	CLA	C1D-ND-C4D	-3.04	104.18	106.31
2	B	311	CLA	C4A-NA-C1A	-3.04	105.29	106.68
2	C	312	CLA	C1D-ND-C4D	-3.03	104.18	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	313	CLA	C4A-NA-C1A	-3.03	105.30	106.68
10	C	321	AV0	CBR-CCM-CBQ	-2.99	104.41	109.96
4	C	309	A1L0F	C33-C2-C1	-2.97	122.30	127.87
6	B	317	A1LYY	O45-C1-C42	-2.94	108.46	116.88
6	B	317	A1LYY	O45-C28-C1	-2.92	56.61	58.93
2	A	311	CLA	C1D-ND-C4D	-2.90	104.28	106.31
2	B	311	CLA	C1D-ND-C4D	-2.87	104.30	106.31
3	B	306	CHL	C4D-CHA-CBD	-2.85	106.09	108.97
4	C	309	A1L0F	C1-C5-N4	-2.84	106.99	109.98
3	B	305	CHL	C4D-CHA-CBD	-2.84	106.10	108.97
2	A	301	CLA	CHD-C1D-ND	-2.84	120.81	124.80
3	C	307	CHL	C4D-CHA-CBD	-2.83	106.11	108.97
2	A	303	CLA	C1D-ND-C4D	-2.83	104.33	106.31
7	B	318	NEX	O24-C25-C24	2.82	116.14	113.49
4	C	309	A1L0F	C41-O40-C38	2.82	122.31	115.92
2	B	312	CLA	C1D-ND-C4D	-2.82	104.33	106.31
4	C	309	A1L0F	C17-C14-N15	2.82	128.56	124.31
3	A	305	CHL	C4C-CHD-C1D	2.81	126.12	116.07
2	C	313	CLA	C2C-C1C-NC	2.80	112.92	109.98
3	B	305	CHL	C4C-CHD-C1D	2.79	126.05	116.07
3	A	302	CHL	C4C-CHD-C1D	2.78	126.03	116.07
2	B	313	CLA	C4A-NA-C1A	-2.78	105.41	106.68
2	C	311	CLA	CHD-C1D-ND	-2.78	120.90	124.80
2	A	303	CLA	CHD-C1D-ND	-2.77	120.90	124.80
3	C	306	CHL	C4C-CHD-C1D	2.77	125.97	116.07
3	C	305	CHL	C4C-CHD-C1D	2.77	125.97	116.07
2	B	311	CLA	CHD-C1D-ND	-2.77	120.91	124.80
3	C	306	CHL	C4D-CHA-CBD	-2.76	106.18	108.97
2	A	309	CLA	CHD-C1D-ND	-2.75	120.93	124.80
3	A	306	CHL	C4C-CHD-C1D	2.75	125.92	116.07
3	A	314	CHL	C4C-CHD-C1D	2.75	125.91	116.07
2	C	310	CLA	C1-C2-C3	-2.75	121.69	126.20
2	C	310	CLA	CHD-C1D-ND	-2.75	120.93	124.80
3	B	314	CHL	C4D-CHA-CBD	-2.74	106.20	108.97
2	A	310	CLA	CHD-C1D-ND	-2.74	120.95	124.80
2	C	304	CLA	C1D-ND-C4D	-2.74	104.39	106.31
3	A	304	CHL	C4C-CHD-C1D	2.73	125.82	116.07
2	C	311	CLA	C1D-ND-C4D	-2.72	104.40	106.31
3	B	315	CHL	C4C-CHD-C1D	2.72	125.80	116.07
3	B	307	CHL	C4C-CHD-C1D	2.72	125.79	116.07
3	C	315	CHL	C4C-CHD-C1D	2.71	125.78	116.07
12	A	323	A1LYW	C25-C24-C23	-2.71	115.35	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	302	CLA	C1D-ND-C4D	-2.71	104.41	106.31
3	B	314	CHL	C4C-CHD-C1D	2.71	125.76	116.07
2	A	309	CLA	C1-C2-C3	-2.71	121.76	126.20
3	B	303	CHL	C4C-CHD-C1D	2.71	125.75	116.07
2	B	313	CLA	C1D-ND-C4D	-2.70	104.42	106.31
2	B	310	CLA	CHD-C1D-ND	-2.70	121.00	124.80
3	C	307	CHL	C4C-CHD-C1D	2.69	125.70	116.07
2	A	311	CLA	CHD-C1D-ND	-2.69	121.02	124.80
3	B	306	CHL	C4C-CHD-C1D	2.67	125.64	116.07
2	B	304	CLA	CHD-C1D-ND	-2.67	121.04	124.80
2	C	312	CLA	CHD-C1D-ND	-2.67	121.04	124.80
8	B	320	A1LYX	C39-C29-C30	-2.67	104.43	109.41
2	B	308	CLA	CHC-C1C-C2C	-2.67	119.37	126.95
3	A	313	CHL	C4C-CHD-C1D	2.66	125.60	116.07
12	B	301	A1LYW	C25-C24-C23	-2.66	115.50	123.20
3	C	314	CHL	C4C-CHD-C1D	2.66	125.58	116.07
3	C	305	CHL	C4D-CHA-CBD	-2.66	106.29	108.97
3	A	305	CHL	C4D-CHA-CBD	-2.65	106.29	108.97
8	A	319	A1LYX	C39-C29-C30	-2.65	104.47	109.41
2	C	308	CLA	CHD-C1D-ND	-2.65	121.08	124.80
2	B	308	CLA	C1-C2-C3	-2.65	121.86	126.20
4	A	308	A1L0F	C1-C5-N4	-2.64	107.20	109.98
3	C	303	CHL	C4C-CHD-C1D	2.64	125.50	116.07
4	A	308	A1L0F	C11-C5-C1	-2.63	119.46	126.95
2	B	310	CLA	C1D-ND-C4D	-2.63	104.47	106.31
12	B	323	A1LYW	C25-C24-C23	-2.62	115.60	123.20
2	B	302	CLA	CHD-C1D-ND	-2.62	121.11	124.80
8	C	320	A1LYX	C39-C29-C30	-2.62	104.53	109.41
2	C	302	CLA	CHD-C1D-ND	-2.62	121.12	124.80
2	A	311	CLA	CAA-C2A-C1A	-2.61	103.41	111.97
4	B	309	A1L0F	C1-C5-N4	-2.61	107.24	109.98
6	A	316	A1LYY	O45-C1-C42	-2.60	109.42	116.88
2	B	313	CLA	CHD-C1D-ND	-2.60	121.14	124.80
2	A	307	CLA	CHD-C1D-ND	-2.60	121.14	124.80
3	A	302	CHL	C4D-CHA-CBD	-2.60	106.35	108.97
2	B	312	CLA	CHD-C1D-ND	-2.59	121.15	124.80
2	C	304	CLA	CHC-C1C-C2C	-2.59	119.58	126.95
2	B	308	CLA	C2C-C1C-NC	2.59	112.70	109.98
2	A	307	CLA	C1-C2-C3	-2.58	121.96	126.20
2	C	304	CLA	CHD-C1D-ND	-2.58	121.17	124.80
3	A	304	CHL	C4D-CHA-CBD	-2.57	106.37	108.97
6	C	317	A1LYY	O45-C1-C42	-2.57	109.50	116.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	311	CLA	CHC-C1C-C2C	-2.56	119.66	126.95
6	A	316	A1LYY	O45-C28-C1	-2.56	56.90	58.93
2	B	313	CLA	CHC-C1C-C2C	-2.56	119.68	126.95
2	B	304	CLA	C1D-ND-C4D	-2.56	104.52	106.31
2	B	313	CLA	C2C-C1C-NC	2.55	112.67	109.98
4	B	309	A1L0F	C20-N21-C22	2.55	108.10	106.31
2	B	312	CLA	CAA-C2A-C1A	-2.55	103.62	111.97
2	A	301	CLA	C1D-ND-C4D	-2.55	104.52	106.31
7	C	318	NEX	C31-C30-C29	2.55	130.85	127.28
4	C	309	A1L0F	C20-N21-C22	2.55	108.10	106.31
2	B	312	CLA	CHC-C1C-C2C	-2.54	119.74	126.95
2	B	308	CLA	CHD-C1D-ND	-2.53	121.24	124.80
3	B	307	CHL	C4D-CHA-CBD	-2.53	106.42	108.97
7	A	317	NEX	C5-C6-C1	2.53	122.21	119.70
3	B	315	CHL	C4D-CHA-CBD	-2.53	106.42	108.97
3	A	306	CHL	C4D-CHA-CBD	-2.52	106.42	108.97
3	A	313	CHL	C4D-CHA-CBD	-2.52	106.42	108.97
2	A	307	CLA	CHC-C1C-C2C	-2.52	119.79	126.95
2	A	312	CLA	CHD-C1D-ND	-2.51	121.27	124.80
2	C	308	CLA	CHC-C1C-C2C	-2.50	119.83	126.95
3	B	303	CHL	C4D-CHA-CBD	-2.50	106.44	108.97
3	C	315	CHL	C4D-CHA-CBD	-2.49	106.45	108.97
3	C	303	CHL	CHA-C1A-C2A	-2.49	127.47	133.31
2	C	313	CLA	CHA-C1A-NA	-2.48	120.77	126.39
3	B	305	CHL	C1-C2-C3	-2.48	122.13	126.20
2	B	311	CLA	CHC-C1C-C2C	-2.48	119.91	126.95
4	A	308	A1L0F	C24-C20-N21	2.48	128.29	124.80
2	A	310	CLA	CHC-C1C-C2C	-2.47	119.94	126.95
4	B	309	A1L0F	C33-C2-C1	-2.47	123.25	127.87
2	A	311	CLA	C2C-C1C-NC	2.46	112.57	109.98
2	A	312	CLA	CHC-C1C-C2C	-2.46	119.96	126.95
2	A	312	CLA	CHA-C1A-NA	-2.46	120.83	126.39
2	B	313	CLA	CHA-C1A-NA	-2.44	120.87	126.39
2	C	313	CLA	CHC-C1C-C2C	-2.43	120.03	126.95
2	A	309	CLA	C1D-ND-C4D	-2.43	104.61	106.31
2	A	312	CLA	CHB-C1B-NB	-2.43	120.41	124.05
2	C	302	CLA	CHA-C1A-NA	-2.42	120.91	126.39
2	A	301	CLA	CHA-C1A-NA	-2.41	120.93	126.39
2	A	307	CLA	CHA-C1A-NA	-2.41	120.94	126.39
2	C	310	CLA	C1D-ND-C4D	-2.41	104.62	106.31
2	C	304	CLA	C2C-C1C-NC	2.41	112.51	109.98
2	B	312	CLA	C2C-C1C-NC	2.40	112.50	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	314	CHL	C4D-CHA-CBD	-2.40	106.55	108.97
2	B	313	CLA	CHB-C1B-NB	-2.39	120.47	124.05
2	B	311	CLA	CHC-C1C-NC	2.38	127.90	124.31
2	C	304	CLA	CHC-C1C-NC	2.38	127.90	124.31
3	B	315	CHL	CMB-C2B-C3B	2.38	129.44	124.68
2	B	308	CLA	CHC-C1C-NC	2.38	127.90	124.31
2	C	312	CLA	CHC-C1C-C2C	-2.38	120.19	126.95
2	C	302	CLA	C1D-ND-C4D	-2.38	104.64	106.31
2	C	308	CLA	CHA-C1A-NA	-2.37	121.01	126.39
2	A	310	CLA	C2C-C1C-NC	2.37	112.47	109.98
4	A	308	A1L0F	C20-N21-C22	2.36	107.97	106.31
3	A	304	CHL	C1-C2-C3	-2.36	122.32	126.20
2	B	304	CLA	CHC-C1C-C2C	-2.36	120.24	126.95
3	C	314	CHL	C4D-CHA-CBD	-2.36	106.59	108.97
3	C	305	CHL	C1-C2-C3	-2.35	122.34	126.20
3	C	315	CHL	C3C-C4C-NC	-2.34	108.92	114.65
2	A	307	CLA	C1D-ND-C4D	-2.34	104.67	106.31
3	A	306	CHL	CMB-C2B-C3B	2.34	129.36	124.68
4	B	309	A1L0F	C8-C11-C5	2.34	131.74	126.25
2	C	313	CLA	CHD-C1D-ND	-2.34	121.52	124.80
3	A	313	CHL	CHA-C1A-C2A	-2.34	127.82	133.31
2	B	302	CLA	CHA-C1A-NA	-2.33	121.11	126.39
2	B	304	CLA	CHA-C1A-NA	-2.33	121.11	126.39
2	A	307	CLA	CHC-C1C-NC	2.33	127.82	124.31
2	B	310	CLA	CHC-C1C-C2C	-2.33	120.33	126.95
12	B	301	A1LYW	C27-C26-C25	-2.32	115.35	119.01
5	A	318	IWJ	C35-C29-C30	-2.32	106.39	108.78
4	B	309	A1L0F	C37-C19-C20	2.32	128.82	124.73
2	C	308	CLA	CHC-C1C-NC	2.32	127.80	124.31
2	A	312	CLA	C1D-ND-C4D	-2.31	104.69	106.31
2	C	311	CLA	CHC-C1C-C2C	-2.31	120.37	126.95
2	A	303	CLA	CHC-C1C-C2C	-2.31	120.38	126.95
2	C	311	CLA	CHA-C1A-NA	-2.31	121.16	126.39
2	C	313	CLA	CHB-C1B-NB	-2.31	120.59	124.05
3	A	314	CHL	C3C-C4C-NC	-2.31	109.01	114.65
2	A	312	CLA	C2C-C1C-NC	2.30	112.40	109.98
3	C	303	CHL	C4D-CHA-CBD	-2.30	106.65	108.97
2	B	308	CLA	C1D-ND-C4D	-2.29	104.70	106.31
2	A	309	CLA	CHC-C1C-C2C	-2.29	120.45	126.95
2	A	311	CLA	CHC-C1C-NC	2.29	127.76	124.31
2	A	307	CLA	C2C-C1C-NC	2.29	112.38	109.98
5	C	319	IWJ	C35-C29-C30	-2.29	106.43	108.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	314	CHL	CMB-C2B-C3B	2.29	129.25	124.68
2	B	312	CLA	CHC-C1C-NC	2.28	127.75	124.31
3	B	314	CHL	CHA-C1A-C2A	-2.28	127.95	133.31
2	C	312	CLA	CAA-C2A-C1A	-2.28	104.50	111.97
2	C	310	CLA	CHC-C1C-C2C	-2.28	120.47	126.95
4	C	309	A1L0F	C37-C19-C20	2.28	128.74	124.73
2	B	308	CLA	CHA-C1A-NA	-2.28	121.24	126.39
7	B	318	NEX	C5-C6-C1	2.27	121.95	119.70
5	B	319	IWJ	C35-C29-C30	-2.26	106.46	108.78
3	B	315	CHL	C3C-C4C-NC	-2.26	109.12	114.65
2	C	308	CLA	C2C-C1C-NC	2.26	112.35	109.98
2	C	310	CLA	CHA-C1A-NA	-2.26	121.28	126.39
3	B	303	CHL	C1-C2-C3	-2.26	122.50	126.20
2	C	312	CLA	C2C-C1C-NC	2.25	112.35	109.98
3	B	306	CHL	C3C-C4C-NC	-2.25	109.16	114.65
3	A	305	CHL	CHA-C1A-C2A	-2.24	128.05	133.31
2	B	304	CLA	CHC-C1C-NC	2.23	127.67	124.31
12	A	323	A1LYW	C27-C26-C25	-2.23	115.50	119.01
3	A	302	CHL	C1-C2-C3	-2.23	122.54	126.20
5	A	315	IWJ	C35-C29-C30	-2.23	106.49	108.78
2	A	303	CLA	CHA-C1A-NA	-2.23	121.35	126.39
3	B	305	CHL	CMB-C2B-C3B	2.23	129.13	124.68
12	B	323	A1LYW	C27-C26-C25	-2.22	115.51	119.01
2	B	313	CLA	CHC-C1C-NC	2.22	127.66	124.31
2	B	310	CLA	CHA-C1A-NA	-2.22	121.36	126.39
3	A	305	CHL	C3C-C4C-NC	-2.22	109.23	114.65
7	A	317	NEX	O24-C25-C24	2.22	115.57	113.49
3	C	315	CHL	CMB-C2B-C3B	2.22	129.11	124.68
2	A	312	CLA	CHC-C1C-NC	2.21	127.64	124.31
3	A	302	CHL	CHA-C1A-C2A	-2.21	128.12	133.31
3	A	306	CHL	C3C-C4C-NC	-2.21	109.25	114.65
2	B	311	CLA	CHA-C1A-NA	-2.21	121.39	126.39
3	C	314	CHL	CHA-C1A-C2A	-2.21	128.12	133.31
6	C	317	A1LYY	O45-C28-C1	-2.20	57.18	58.93
3	A	304	CHL	C3C-C4C-NC	-2.20	109.27	114.65
2	B	302	CLA	CHC-C1C-C2C	-2.20	120.69	126.95
2	A	311	CLA	CHB-C1B-NB	-2.20	120.75	124.05
4	C	309	A1L0F	C3-C2-C1	2.19	109.52	106.63
3	B	305	CHL	C3C-C4C-NC	-2.19	109.29	114.65
2	A	301	CLA	CHC-C1C-C2C	-2.19	120.71	126.95
3	B	307	CHL	C3C-C4C-NC	-2.19	109.29	114.65
2	C	304	CLA	CHA-C1A-NA	-2.19	121.43	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	308	A1L0F	C3-C2-C1	2.19	109.51	106.63
3	A	306	CHL	CHA-C1A-C2A	-2.19	128.17	133.31
2	A	309	CLA	CHA-C1A-NA	-2.18	121.45	126.39
2	A	310	CLA	C1-C2-C3	-2.18	122.63	126.20
3	C	305	CHL	C3C-C4C-NC	-2.17	109.34	114.65
2	C	313	CLA	C1-C2-C3	-2.17	122.64	126.20
2	A	310	CLA	CHC-C1C-NC	2.17	127.58	124.31
2	A	310	CLA	CHA-C1A-NA	-2.17	121.48	126.39
2	C	302	CLA	CHC-C1C-NC	2.17	127.57	124.31
2	C	302	CLA	CHC-C1C-C2C	-2.17	120.80	126.95
2	A	309	CLA	CHC-C1C-NC	2.16	127.57	124.31
2	B	310	CLA	C1-C2-C3	-2.16	122.66	126.20
3	C	306	CHL	C3C-C4C-NC	-2.16	109.37	114.65
2	A	301	CLA	CHC-C1C-NC	2.16	127.56	124.31
2	C	313	CLA	C1D-ND-C4D	-2.15	104.80	106.31
2	C	312	CLA	CHB-C1B-NB	-2.15	120.82	124.05
4	A	308	A1L0F	C37-C19-C20	2.15	128.51	124.73
3	A	304	CHL	CMB-C2B-C3B	2.15	128.97	124.68
2	B	312	CLA	CHB-C1B-NB	-2.14	120.83	124.05
2	C	308	CLA	C1D-ND-C4D	-2.14	104.81	106.31
3	B	307	CHL	CHA-C1A-C2A	-2.13	128.31	133.31
3	C	303	CHL	C3C-C4C-NC	-2.13	109.45	114.65
3	C	307	CHL	CMB-C2B-C3B	2.13	128.93	124.68
2	B	310	CLA	C2C-C1C-NC	2.12	112.21	109.98
3	C	307	CHL	C3C-C4C-NC	-2.11	109.49	114.65
2	A	303	CLA	CHC-C1C-NC	2.11	127.49	124.31
3	B	303	CHL	CHA-C1A-C2A	-2.11	128.36	133.31
2	A	301	CLA	C3B-C4B-NB	-2.10	108.65	110.53
3	B	306	CHL	CMB-C2B-C3B	2.10	128.88	124.68
2	B	311	CLA	CHB-C1B-NB	-2.10	120.90	124.05
2	C	311	CLA	C2C-C1C-NC	2.10	112.19	109.98
3	A	302	CHL	CMB-C2B-C3B	2.10	128.88	124.68
3	A	314	CHL	CHA-C1A-C2A	-2.10	128.38	133.31
2	B	311	CLA	C2C-C1C-NC	2.10	112.19	109.98
5	C	316	IWJ	C35-C29-C30	-2.10	106.63	108.78
2	B	308	CLA	CHB-C1B-NB	-2.09	120.91	124.05
2	B	310	CLA	CHC-C1C-NC	2.09	127.46	124.31
2	C	311	CLA	C1-C2-C3	-2.09	122.78	126.20
3	B	303	CHL	CMB-C2B-C3B	2.09	128.85	124.68
4	B	309	A1L0F	C3-C2-C1	2.09	109.38	106.63
2	A	303	CLA	CHB-C1B-NB	-2.08	120.92	124.05
2	B	311	CLA	C1-C2-C3	-2.08	122.78	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	302	CLA	CHC-C1C-NC	2.08	127.44	124.31
2	C	311	CLA	CHC-C1C-NC	2.07	127.44	124.31
2	C	312	CLA	CHC-C1C-NC	2.07	127.43	124.31
2	A	310	CLA	CHB-C1B-NB	-2.07	120.94	124.05
3	B	306	CHL	CHA-C1A-C2A	-2.07	128.45	133.31
3	B	307	CHL	CMB-C2B-C3B	2.06	128.81	124.68
3	C	305	CHL	CMB-C2B-C3B	2.06	128.80	124.68
2	A	307	CLA	CHB-C1B-NB	-2.06	120.96	124.05
2	C	310	CLA	CHC-C1C-NC	2.06	127.41	124.31
3	C	303	CHL	CMB-C2B-C3B	2.05	128.79	124.68
3	C	306	CHL	CMB-C2B-C3B	2.05	128.78	124.68
7	C	318	NEX	C5-C6-C1	2.04	121.72	119.70
2	B	312	CLA	CHA-C1A-NA	-2.04	121.78	126.39
2	C	310	CLA	C2C-C1C-NC	2.04	112.12	109.98
3	A	313	CHL	C3C-C4C-NC	-2.03	109.68	114.65
3	C	315	CHL	CHA-C1A-C2A	-2.03	128.54	133.31
2	A	303	CLA	C2C-C1C-NC	2.03	112.11	109.98
7	B	318	NEX	C31-C30-C29	2.03	130.12	127.28
2	C	310	CLA	CHB-C1B-NB	-2.03	121.00	124.05
2	C	304	CLA	CHB-C1B-NB	-2.03	121.01	124.05
2	B	304	CLA	CHB-C1B-NB	-2.03	121.01	124.05
3	C	305	CHL	CHA-C1A-C2A	-2.02	128.55	133.31
3	B	315	CHL	CHA-C1A-C2A	-2.02	128.56	133.31
12	B	301	A1LYW	C24-C25-C26	2.02	130.11	127.28
3	B	305	CHL	CHA-C1A-C2A	-2.01	128.59	133.31
2	C	308	CLA	CHB-C1B-NB	-2.01	121.04	124.05
2	B	304	CLA	C2C-C1C-NC	2.01	112.09	109.98
2	C	312	CLA	CHA-C1A-NA	-2.00	121.85	126.39
3	B	303	CHL	C3C-C4C-NC	-2.00	109.76	114.65

All (115) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	301	CLA	C8
2	A	301	CLA	ND
2	A	303	CLA	C8
2	A	303	CLA	ND
2	A	307	CLA	C8
2	A	307	CLA	ND
2	A	309	CLA	C8
2	A	309	CLA	ND
2	A	310	CLA	C8

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Mol	Chain	Res	Type	Atom
2	A	310	CLA	ND
2	A	311	CLA	ND
2	A	312	CLA	C8
2	A	312	CLA	ND
2	B	302	CLA	C8
2	B	302	CLA	ND
2	B	304	CLA	C8
2	B	304	CLA	ND
2	B	308	CLA	C8
2	B	308	CLA	ND
2	B	310	CLA	C8
2	B	310	CLA	ND
2	B	311	CLA	C8
2	B	311	CLA	ND
2	B	312	CLA	ND
2	B	313	CLA	C8
2	B	313	CLA	ND
2	C	302	CLA	C8
2	C	302	CLA	ND
2	C	304	CLA	C8
2	C	304	CLA	ND
2	C	308	CLA	C8
2	C	308	CLA	ND
2	C	310	CLA	C8
2	C	310	CLA	ND
2	C	311	CLA	C8
2	C	311	CLA	ND
2	C	312	CLA	ND
2	C	313	CLA	C8
2	C	313	CLA	ND
3	A	302	CHL	NA
3	A	302	CHL	C8
3	A	302	CHL	NC
3	A	302	CHL	ND
3	A	304	CHL	NA
3	A	304	CHL	C8
3	A	304	CHL	NC
3	A	304	CHL	ND
3	A	305	CHL	NA
3	A	305	CHL	NC
3	A	305	CHL	ND
3	A	306	CHL	NA

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Mol	Chain	Res	Type	Atom
3	A	306	CHL	C8
3	A	306	CHL	NC
3	A	306	CHL	ND
3	A	313	CHL	NA
3	A	313	CHL	NC
3	A	313	CHL	ND
3	A	314	CHL	NA
3	A	314	CHL	C8
3	A	314	CHL	NC
3	A	314	CHL	ND
3	B	303	CHL	NA
3	B	303	CHL	C8
3	B	303	CHL	NC
3	B	303	CHL	ND
3	B	305	CHL	NA
3	B	305	CHL	C8
3	B	305	CHL	NC
3	B	305	CHL	ND
3	B	306	CHL	NA
3	B	306	CHL	NC
3	B	306	CHL	ND
3	B	307	CHL	NA
3	B	307	CHL	C8
3	B	307	CHL	NC
3	B	307	CHL	ND
3	B	314	CHL	NA
3	B	314	CHL	NC
3	B	314	CHL	ND
3	B	315	CHL	NA
3	B	315	CHL	C8
3	B	315	CHL	NC
3	B	315	CHL	ND
3	C	303	CHL	NA
3	C	303	CHL	C8
3	C	303	CHL	NC
3	C	303	CHL	ND
3	C	305	CHL	NA
3	C	305	CHL	C8
3	C	305	CHL	NC
3	C	305	CHL	ND
3	C	306	CHL	NA
3	C	306	CHL	NC

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Mol	Chain	Res	Type	Atom
3	C	306	CHL	ND
3	C	307	CHL	NA
3	C	307	CHL	C8
3	C	307	CHL	NC
3	C	307	CHL	ND
3	C	314	CHL	NA
3	C	314	CHL	NC
3	C	314	CHL	ND
3	C	315	CHL	NA
3	C	315	CHL	C8
3	C	315	CHL	NC
3	C	315	CHL	ND
4	A	308	A1L0F	N21
4	B	309	A1L0F	N21
4	C	309	A1L0F	N21
5	A	315	IWJ	C29
5	A	318	IWJ	C29
5	B	316	IWJ	C29
5	B	319	IWJ	C29
5	C	316	IWJ	C29
5	C	319	IWJ	C29
12	B	323	A1LYW	C4

All (283) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	310	CLA	C2B-C3B-CAB-CBB
2	A	310	CLA	C4B-C3B-CAB-CBB
2	B	311	CLA	C2B-C3B-CAB-CBB
2	B	311	CLA	C4B-C3B-CAB-CBB
2	B	313	CLA	C6-C7-C8-C10
2	B	313	CLA	C11-C10-C8-C9
2	C	311	CLA	C2B-C3B-CAB-CBB
2	C	311	CLA	C4B-C3B-CAB-CBB
2	C	313	CLA	C11-C10-C8-C9
3	A	302	CHL	C1C-C2C-CMC-OMC
3	A	304	CHL	C1C-C2C-CMC-OMC
3	A	305	CHL	C3C-C2C-CMC-OMC
3	A	314	CHL	C1C-C2C-CMC-OMC
3	A	314	CHL	C3C-C2C-CMC-OMC
3	B	303	CHL	C3C-C2C-CMC-OMC
3	B	305	CHL	C1C-C2C-CMC-OMC

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Mol	Chain	Res	Type	Atoms
3	B	306	CHL	C1C-C2C-CMC-OMC
3	B	314	CHL	C1C-C2C-CMC-OMC
3	B	314	CHL	C3C-C2C-CMC-OMC
3	B	315	CHL	C1C-C2C-CMC-OMC
3	B	315	CHL	C3C-C2C-CMC-OMC
3	C	303	CHL	C1C-C2C-CMC-OMC
3	C	303	CHL	C3C-C2C-CMC-OMC
3	C	305	CHL	C1C-C2C-CMC-OMC
3	C	314	CHL	C1C-C2C-CMC-OMC
3	C	314	CHL	C3C-C2C-CMC-OMC
3	C	315	CHL	C1C-C2C-CMC-OMC
3	C	315	CHL	C3C-C2C-CMC-OMC
4	A	308	A1L0F	C13-C12-C27-C28
4	B	309	A1L0F	C13-C12-C27-C28
4	C	309	A1L0F	C13-C12-C27-C28
8	B	320	A1LYX	C15-C16-C23-O43
2	A	307	CLA	C14-C13-C15-C16
2	A	312	CLA	C11-C10-C8-C9
2	B	302	CLA	C11-C10-C8-C9
3	A	306	CHL	C6-C7-C8-C9
3	B	307	CHL	C6-C7-C8-C9
3	C	307	CHL	C6-C7-C8-C9
12	A	323	A1LYW	C33-C26-C27-C28
12	B	301	A1LYW	C33-C26-C27-C28
12	B	323	A1LYW	C33-C26-C27-C28
12	A	323	A1LYW	C25-C26-C27-C28
12	B	301	A1LYW	C25-C26-C27-C28
12	B	323	A1LYW	C25-C26-C27-C28
3	B	315	CHL	C5-C6-C7-C8
11	C	322	SQD	C23-C24-C25-C26
3	C	307	CHL	C8-C10-C11-C12
3	A	314	CHL	C5-C6-C7-C8
3	B	307	CHL	C8-C10-C11-C12
3	C	315	CHL	C5-C6-C7-C8
3	B	305	CHL	C13-C15-C16-C17
3	C	305	CHL	C5-C6-C7-C8
2	A	312	CLA	C8-C10-C11-C12
2	C	308	CLA	C5-C6-C7-C8
3	A	306	CHL	C5-C6-C7-C8
3	A	304	CHL	C13-C15-C16-C17
2	A	309	CLA	C15-C16-C17-C18
2	C	313	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
2	A	311	CLA	C3A-C2A-CAA-CBA
2	B	312	CLA	C3A-C2A-CAA-CBA
2	C	312	CLA	C3A-C2A-CAA-CBA
3	C	305	CHL	C13-C15-C16-C17
3	B	315	CHL	C3-C5-C6-C7
3	C	303	CHL	C11-C12-C13-C14
11	C	322	SQD	C9-C10-C11-C12
11	C	322	SQD	C24-C25-C26-C27
11	B	322	SQD	C11-C10-C9-C8
3	A	302	CHL	C5-C6-C7-C8
11	B	322	SQD	C31-C32-C33-C34
2	C	311	CLA	C4-C3-C5-C6
2	A	311	CLA	C1A-C2A-CAA-CBA
2	B	312	CLA	C1A-C2A-CAA-CBA
2	C	312	CLA	C1A-C2A-CAA-CBA
2	C	310	CLA	C15-C16-C17-C18
3	C	315	CHL	C3-C5-C6-C7
2	A	301	CLA	C11-C12-C13-C15
2	A	312	CLA	C6-C7-C8-C10
2	C	308	CLA	C11-C10-C8-C7
3	C	305	CHL	C11-C10-C8-C7
2	A	310	CLA	C2-C3-C5-C6
2	B	311	CLA	C2-C3-C5-C6
2	A	301	CLA	C11-C12-C13-C14
2	C	302	CLA	C11-C12-C13-C14
3	A	304	CHL	C11-C10-C8-C9
3	B	305	CHL	C11-C10-C8-C9
3	C	303	CHL	C11-C10-C8-C9
11	A	322	SQD	C44-C45-C46-O48
3	C	307	CHL	C5-C6-C7-C8
11	C	322	SQD	C11-C10-C9-C8
2	B	311	CLA	C4-C3-C5-C6
2	C	311	CLA	C2-C3-C5-C6
2	B	308	CLA	C16-C17-C18-C20
2	A	312	CLA	C15-C16-C17-C18
3	A	306	CHL	C15-C16-C17-C18
3	C	307	CHL	C15-C16-C17-C18
3	A	302	CHL	C3C-C2C-CMC-OMC
3	A	304	CHL	C3C-C2C-CMC-OMC
3	A	313	CHL	C3C-C2C-CMC-OMC
3	B	305	CHL	C3C-C2C-CMC-OMC
3	B	306	CHL	C3C-C2C-CMC-OMC

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Mol	Chain	Res	Type	Atoms
3	B	307	CHL	C3C-C2C-CMC-OMC
3	C	305	CHL	C3C-C2C-CMC-OMC
3	C	306	CHL	C3C-C2C-CMC-OMC
10	B	321	AV0	CAZ-CBB-CBD-CBF
3	B	307	CHL	C2-C3-C5-C6
3	C	307	CHL	C2-C3-C5-C6
10	A	321	AV0	CAZ-CBB-CBD-CBF
3	A	305	CHL	C1C-C2C-CMC-OMC
3	A	313	CHL	C1C-C2C-CMC-OMC
3	B	303	CHL	C1C-C2C-CMC-OMC
3	B	307	CHL	C1C-C2C-CMC-OMC
2	C	313	CLA	C15-C16-C17-C18
11	C	322	SQD	C10-C11-C12-C13
2	A	310	CLA	C4-C3-C5-C6
2	B	313	CLA	C6-C7-C8-C9
2	C	308	CLA	C11-C10-C8-C9
3	C	305	CHL	C11-C10-C8-C9
10	C	321	AV0	CAZ-CBB-CBD-CBF
2	A	307	CLA	C12-C13-C15-C16
2	B	313	CLA	C11-C10-C8-C7
2	C	313	CLA	C11-C10-C8-C7
3	A	304	CHL	C11-C10-C8-C7
3	B	305	CHL	C11-C10-C8-C7
3	A	313	CHL	C4-C3-C5-C6
3	C	315	CHL	C13-C15-C16-C17
11	C	322	SQD	C44-C45-C46-O48
3	C	307	CHL	C4-C3-C5-C6
11	C	322	SQD	C28-C29-C30-C31
3	A	313	CHL	C2-C3-C5-C6
2	B	310	CLA	C8-C10-C11-C12
2	B	313	CLA	C15-C16-C17-C18
3	A	304	CHL	C10-C11-C12-C13
2	B	310	CLA	C15-C16-C17-C18
3	B	305	CHL	C10-C11-C12-C13
3	B	307	CHL	C4-C3-C5-C6
3	B	314	CHL	C4-C3-C5-C6
3	C	305	CHL	C10-C11-C12-C13
11	A	322	SQD	C7-C8-C9-C10
2	B	302	CLA	C3-C5-C6-C7
2	C	313	CLA	C14-C13-C15-C16
11	B	322	SQD	C11-C12-C13-C14
8	C	320	A1LYX	C15-C16-C23-O43

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Mol	Chain	Res	Type	Atoms
2	A	309	CLA	C10-C11-C12-C13
2	A	312	CLA	C11-C10-C8-C7
2	C	302	CLA	C11-C12-C13-C15
11	A	322	SQD	C13-C14-C15-C16
3	C	314	CHL	C4-C3-C5-C6
11	C	322	SQD	C45-C44-O6-C1
2	B	308	CLA	C16-C17-C18-C19
3	B	314	CHL	C2-C3-C5-C6
3	B	307	CHL	C15-C16-C17-C18
11	C	322	SQD	O47-C45-C46-O48
2	B	308	CLA	C14-C13-C15-C16
2	B	313	CLA	C14-C13-C15-C16
3	C	315	CHL	C11-C12-C13-C14
3	A	306	CHL	C8-C10-C11-C12
2	C	304	CLA	C5-C6-C7-C8
5	B	319	IWJ	C22-C23-C24-C26
5	C	316	IWJ	C22-C23-C24-C26
3	B	315	CHL	C13-C15-C16-C17
11	A	322	SQD	C23-C24-C25-C26
3	A	306	CHL	C4C-C3C-CAC-CBC
3	B	307	CHL	C4C-C3C-CAC-CBC
3	C	307	CHL	C4C-C3C-CAC-CBC
5	B	319	IWJ	C26-C28-C29-C30
3	A	306	CHL	C6-C7-C8-C10
3	C	315	CHL	C6-C7-C8-C10
11	B	322	SQD	C45-C44-O6-C1
2	A	309	CLA	C8-C10-C11-C12
11	A	322	SQD	O47-C45-C46-O48
3	C	314	CHL	C2-C3-C5-C6
3	B	307	CHL	C5-C6-C7-C8
8	A	319	A1LYX	C17-C18-C19-C29
8	B	320	A1LYX	C17-C18-C19-C29
8	C	320	A1LYX	C17-C18-C19-C29
9	A	320	A1L0E	C17-C18-C19-C29
9	A	324	A1L0E	C17-C18-C19-C29
9	C	301	A1L0E	C17-C18-C19-C29
2	A	301	CLA	C3-C5-C6-C7
2	C	302	CLA	C3-C5-C6-C7
2	B	310	CLA	C10-C11-C12-C13
11	C	322	SQD	C11-C12-C13-C14
2	A	301	CLA	C11-C10-C8-C9
2	A	312	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
2	B	302	CLA	C11-C12-C13-C14
5	A	315	IWJ	C22-C23-C24-C26
5	A	318	IWJ	C22-C23-C24-C26
5	C	319	IWJ	C22-C23-C24-C26
4	C	309	A1L0F	C35-C38-O40-C41
3	A	314	CHL	C3-C5-C6-C7
2	C	311	CLA	C6-C7-C8-C9
2	A	310	CLA	C6-C7-C8-C10
2	A	312	CLA	C12-C13-C15-C16
2	B	313	CLA	C12-C13-C15-C16
2	B	308	CLA	C15-C16-C17-C18
7	A	317	NEX	C39-C29-C30-C31
7	B	318	NEX	C39-C29-C30-C31
7	C	318	NEX	C39-C29-C30-C31
2	C	310	CLA	C10-C11-C12-C13
2	A	310	CLA	C6-C7-C8-C9
2	B	308	CLA	C6-C7-C8-C9
2	C	302	CLA	C11-C10-C8-C9
3	B	303	CHL	C11-C12-C13-C14
3	A	302	CHL	C1A-C2A-CAA-CBA
3	B	303	CHL	C1A-C2A-CAA-CBA
7	A	317	NEX	C28-C29-C30-C31
7	B	318	NEX	C28-C29-C30-C31
7	C	318	NEX	C28-C29-C30-C31
11	C	322	SQD	C17-C18-C19-C20
2	C	308	CLA	C4-C3-C5-C6
2	A	307	CLA	C11-C10-C8-C7
2	B	302	CLA	C11-C12-C13-C15
2	B	310	CLA	C6-C7-C8-C10
2	C	311	CLA	C6-C7-C8-C10
2	C	313	CLA	C12-C13-C15-C16
3	B	315	CHL	C6-C7-C8-C10
3	C	307	CHL	C6-C7-C8-C10
2	C	302	CLA	C10-C11-C12-C13
2	C	310	CLA	C8-C10-C11-C12
2	B	308	CLA	C3-C5-C6-C7
5	B	316	IWJ	C22-C23-C24-C26
2	B	310	CLA	C13-C15-C16-C17
2	B	311	CLA	C6-C7-C8-C9
8	B	320	A1LYX	C14-C15-C16-C23
8	C	320	A1LYX	C14-C15-C16-C23
2	A	312	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
4	C	309	A1L0F	O39-C38-O40-C41
2	A	312	CLA	C16-C17-C18-C19
3	A	314	CHL	CHA-CBD-CGD-O1D
3	A	314	CHL	CHA-CBD-CGD-O2D
3	B	315	CHL	CHA-CBD-CGD-O1D
3	B	315	CHL	CHA-CBD-CGD-O2D
3	C	307	CHL	CHA-CBD-CGD-O2D
3	C	315	CHL	CHA-CBD-CGD-O1D
3	C	315	CHL	CHA-CBD-CGD-O2D
2	C	313	CLA	C8-C10-C11-C12
3	B	307	CHL	C10-C11-C12-C13
2	C	313	CLA	C6-C7-C8-C9
3	A	314	CHL	CAA-CBA-CGA-O2A
11	A	322	SQD	C45-C44-O6-C1
11	B	322	SQD	C15-C16-C17-C18
3	B	303	CHL	C5-C6-C7-C8
4	C	309	A1L0F	C16-C12-C27-C28
11	A	322	SQD	O48-C23-C24-C25
2	B	302	CLA	C14-C13-C15-C16
3	A	314	CHL	C11-C12-C13-C14
3	C	315	CHL	C6-C7-C8-C9
2	C	313	CLA	C16-C17-C18-C20
3	C	307	CHL	C10-C11-C12-C13
3	C	307	CHL	C2A-CAA-CBA-CGA
2	B	302	CLA	C11-C10-C8-C7
2	B	311	CLA	C6-C7-C8-C10
3	B	307	CHL	C6-C7-C8-C10
3	C	303	CHL	C11-C12-C13-C15
2	B	304	CLA	C2B-C3B-CAB-CBB
8	A	319	A1LYX	C14-C15-C16-C23
2	B	313	CLA	C16-C17-C18-C20
2	C	313	CLA	C16-C17-C18-C19
11	B	322	SQD	C26-C27-C28-C29
3	A	304	CHL	CAA-CBA-CGA-O2A
2	A	309	CLA	C13-C15-C16-C17
2	C	304	CLA	C4-C3-C5-C6
2	B	313	CLA	C16-C17-C18-C19
2	B	311	CLA	C2-C1-O2A-CGA
3	A	306	CHL	C2-C1-O2A-CGA
3	A	314	CHL	C6-C7-C8-C10
2	A	301	CLA	C10-C11-C12-C13
2	B	313	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
2	A	312	CLA	C6-C7-C8-C9
3	B	315	CHL	C6-C7-C8-C9
11	A	322	SQD	O10-C23-C24-C25
3	C	315	CHL	CAA-CBA-CGA-O2A
2	C	308	CLA	C13-C15-C16-C17
4	C	309	A1L0F	C33-C42-C43-O45
3	A	306	CHL	C2-C3-C5-C6
3	A	304	CHL	CAA-CBA-CGA-O1A
2	A	311	CLA	CAD-CBD-CGD-O2D
3	A	302	CHL	CAD-CBD-CGD-O2D
3	B	303	CHL	CAD-CBD-CGD-O2D
2	C	311	CLA	C2-C1-O2A-CGA
3	B	307	CHL	C2-C1-O2A-CGA
3	B	305	CHL	CAA-CBA-CGA-O2A
2	A	311	CLA	CAA-CBA-CGA-O2A

There are no ring outliers.

35 monomers are involved in 49 short contacts:

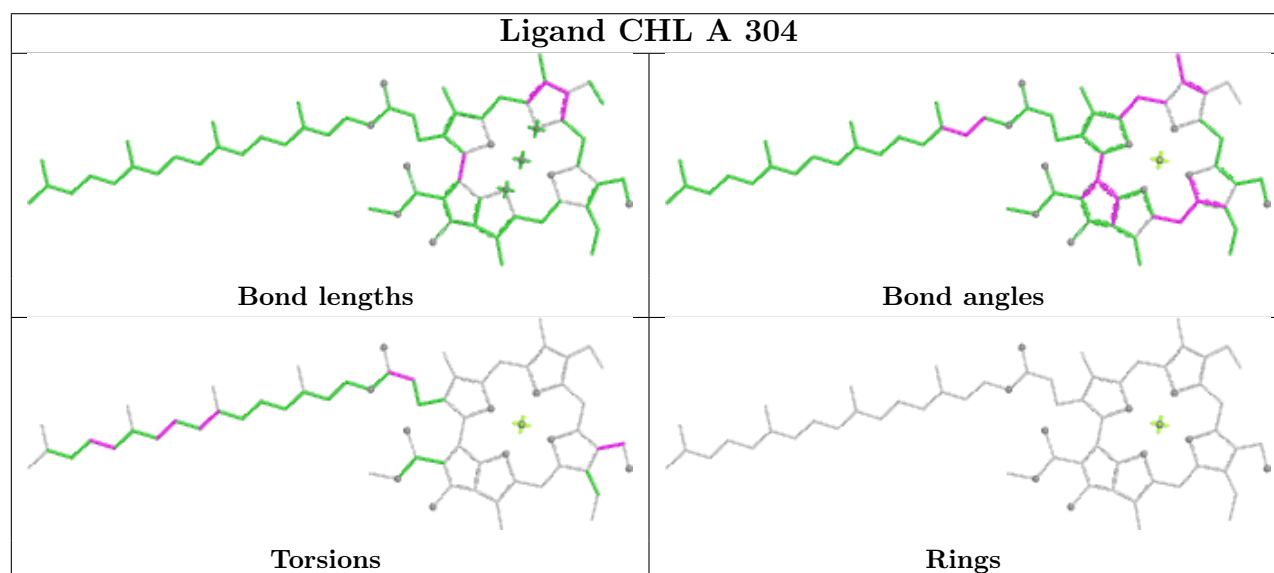
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	304	CHL	2	0
3	C	303	CHL	1	0
5	A	318	IWJ	1	0
11	B	322	SQD	4	0
2	A	307	CLA	3	0
3	B	305	CHL	3	0
2	A	310	CLA	2	0
2	B	308	CLA	2	0
11	C	322	SQD	3	0
3	B	306	CHL	2	0
3	B	315	CHL	3	0
3	A	314	CHL	2	0
3	C	306	CHL	2	0
2	C	308	CLA	3	0
2	C	310	CLA	2	0
2	C	312	CLA	2	0
3	C	315	CHL	2	0
2	B	311	CLA	1	0
11	A	322	SQD	2	0
3	A	305	CHL	2	0
2	B	313	CLA	1	0
2	C	313	CLA	2	0

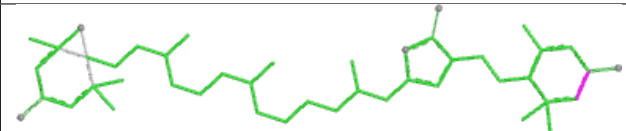
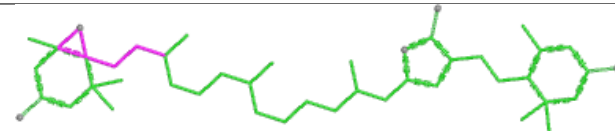
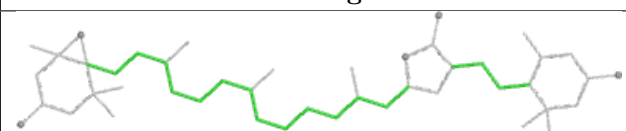
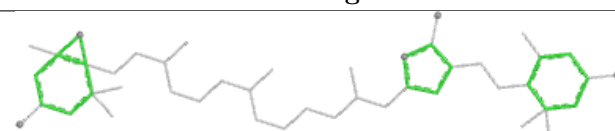
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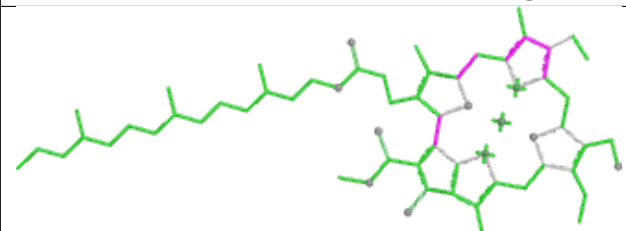
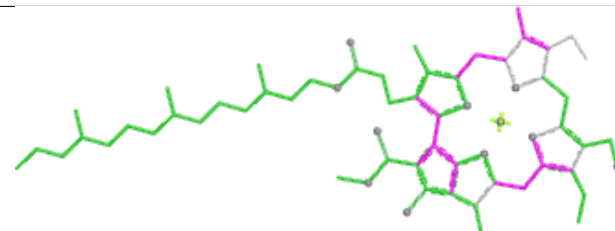
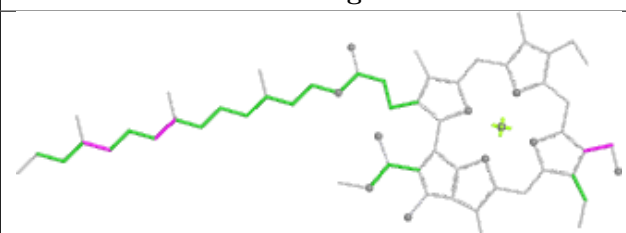
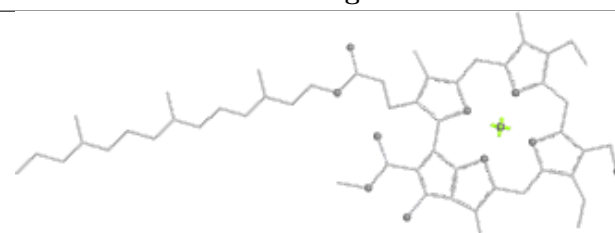
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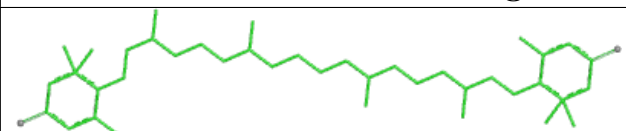
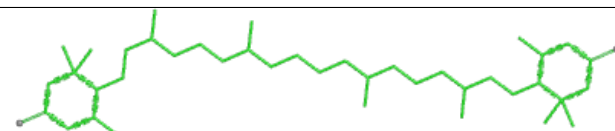
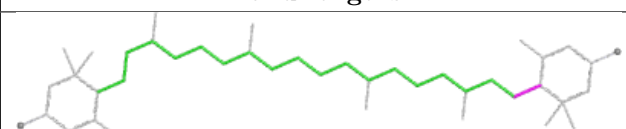
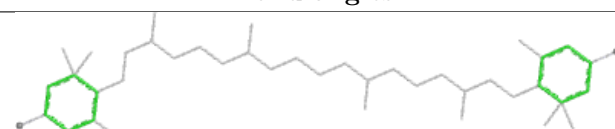
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	307	CHL	2	0
3	A	306	CHL	1	0
2	A	303	CLA	2	0
2	C	311	CLA	1	0
2	A	309	CLA	2	0
2	A	312	CLA	2	0
2	B	304	CLA	3	0
2	B	310	CLA	2	0
2	B	312	CLA	1	0
2	A	311	CLA	1	0
3	C	307	CHL	3	0
3	C	305	CHL	3	0
2	C	304	CLA	2	0

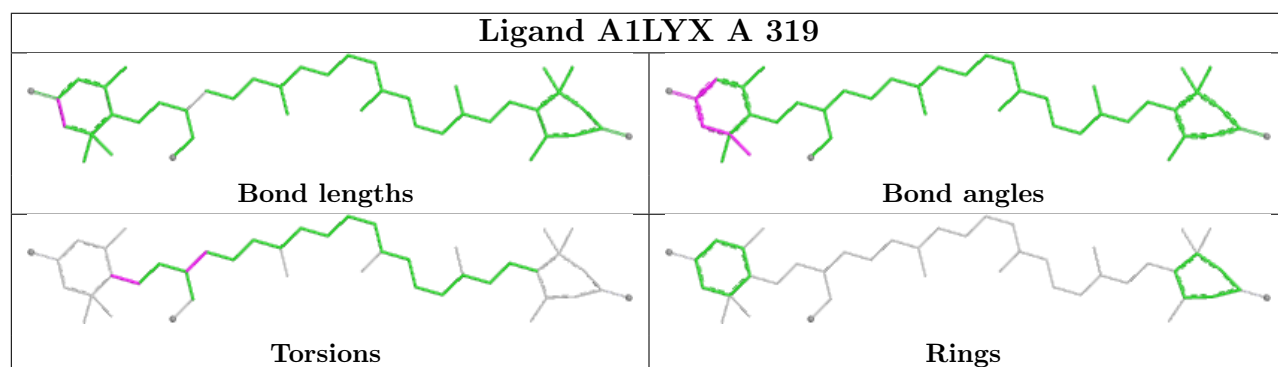
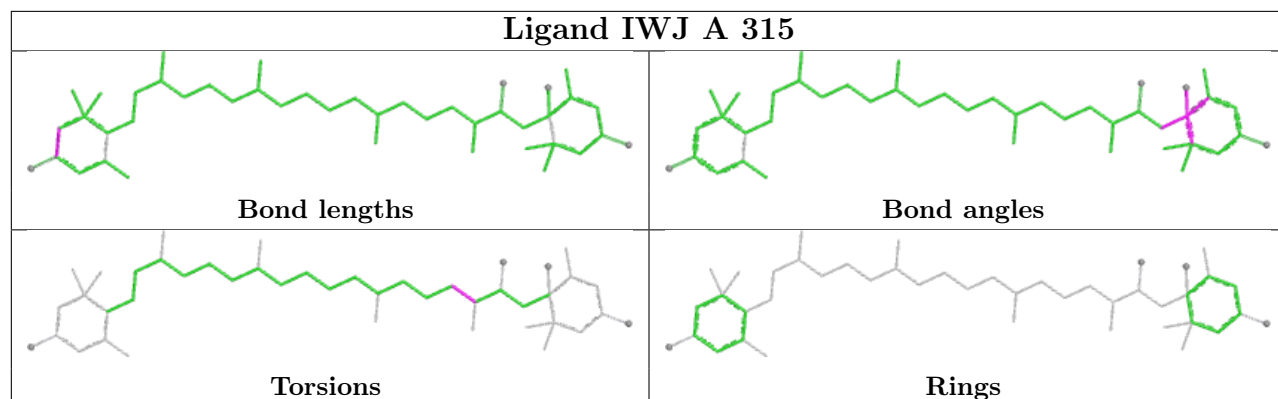
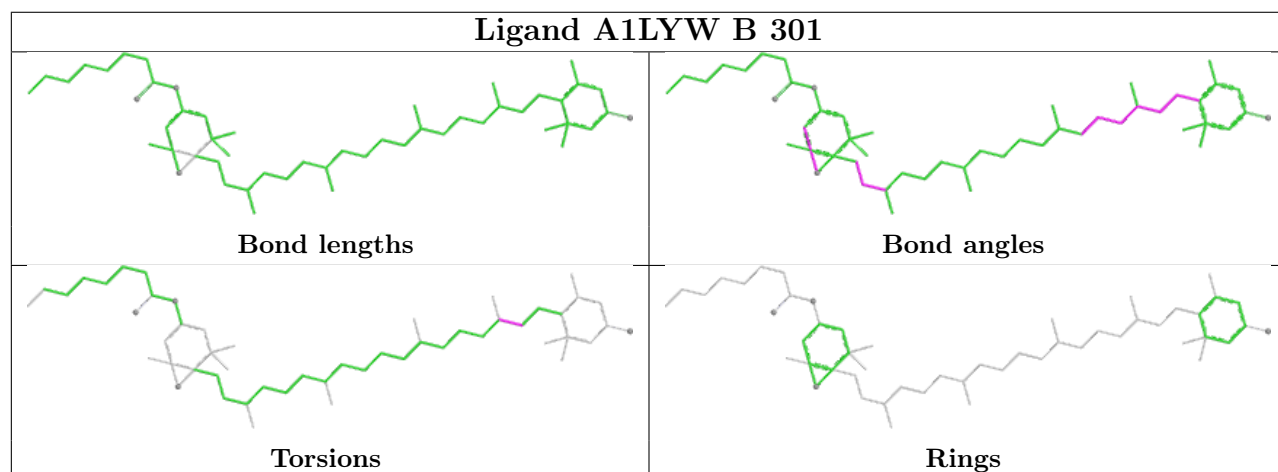
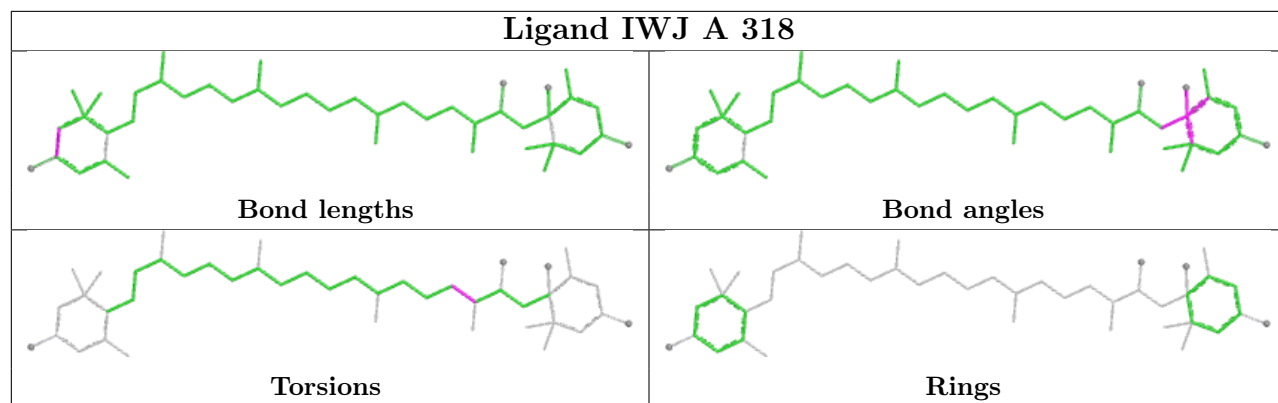
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

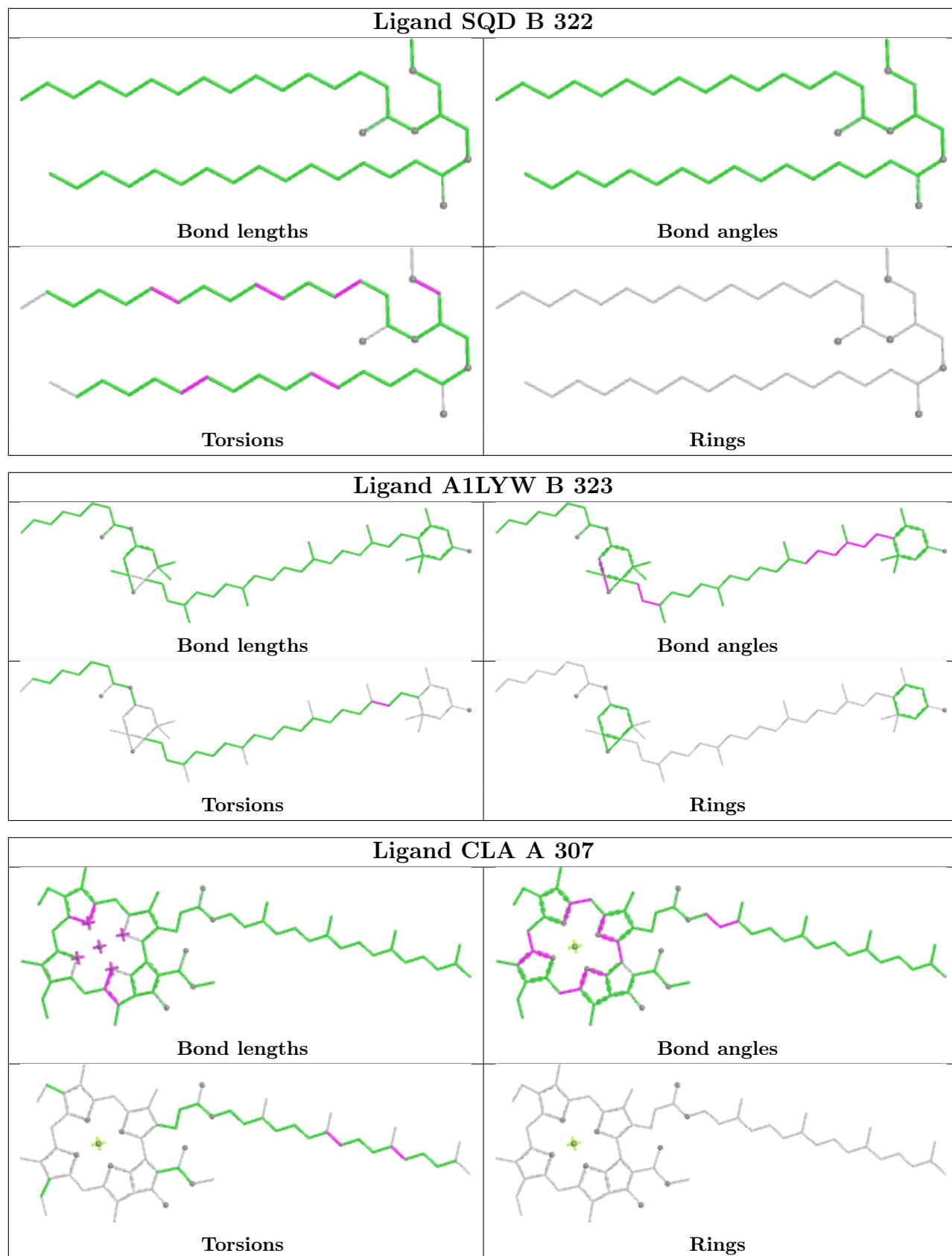


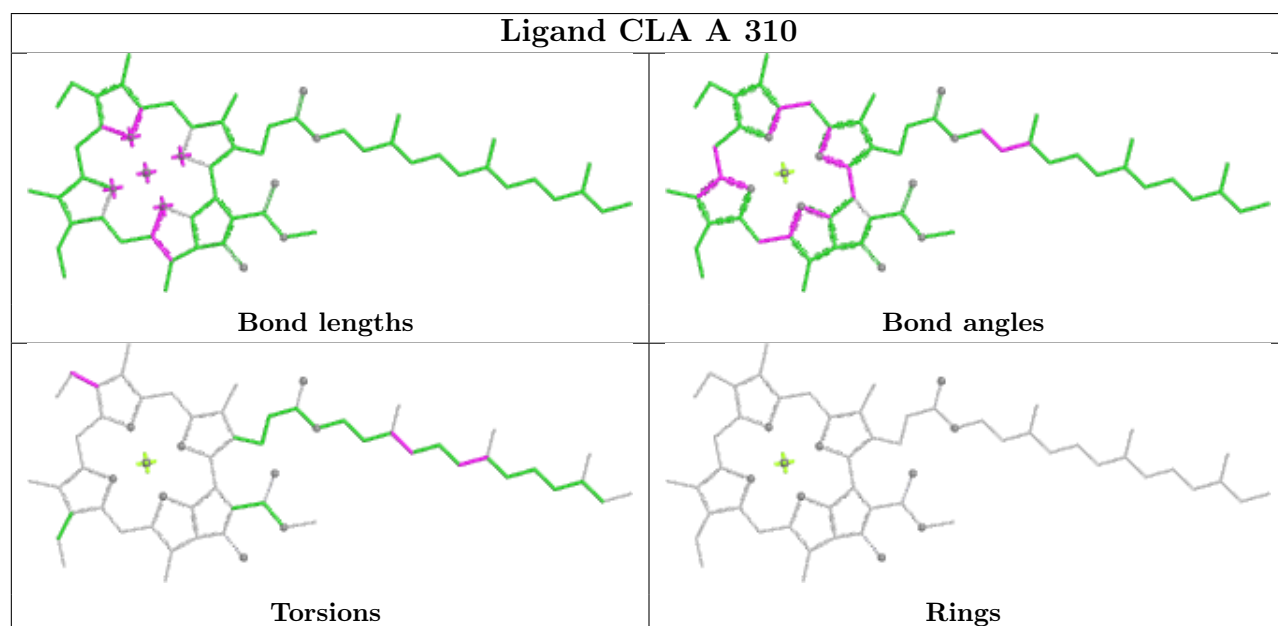
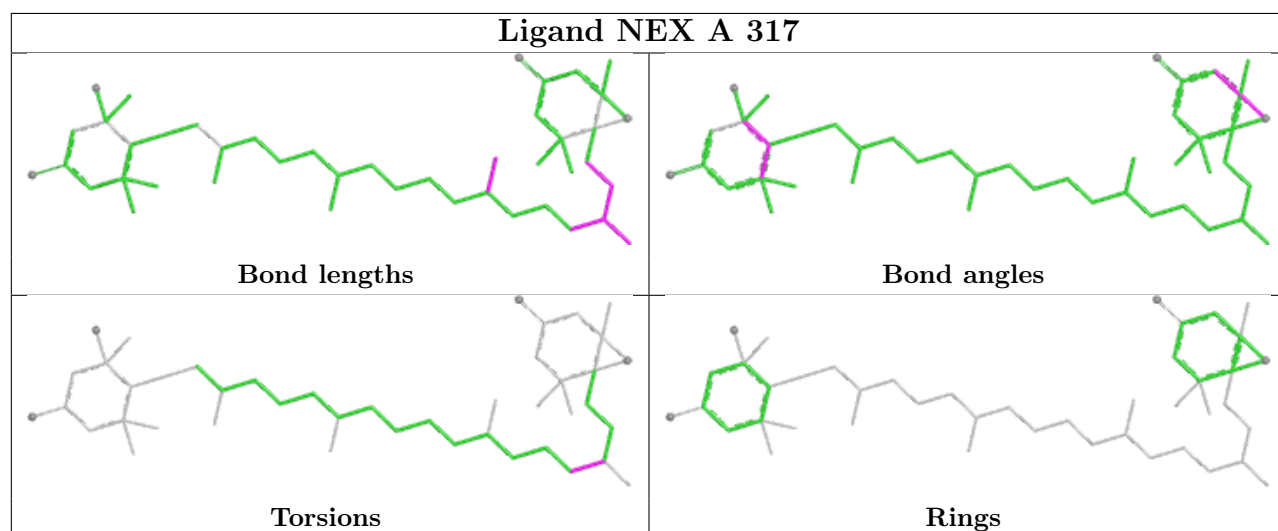
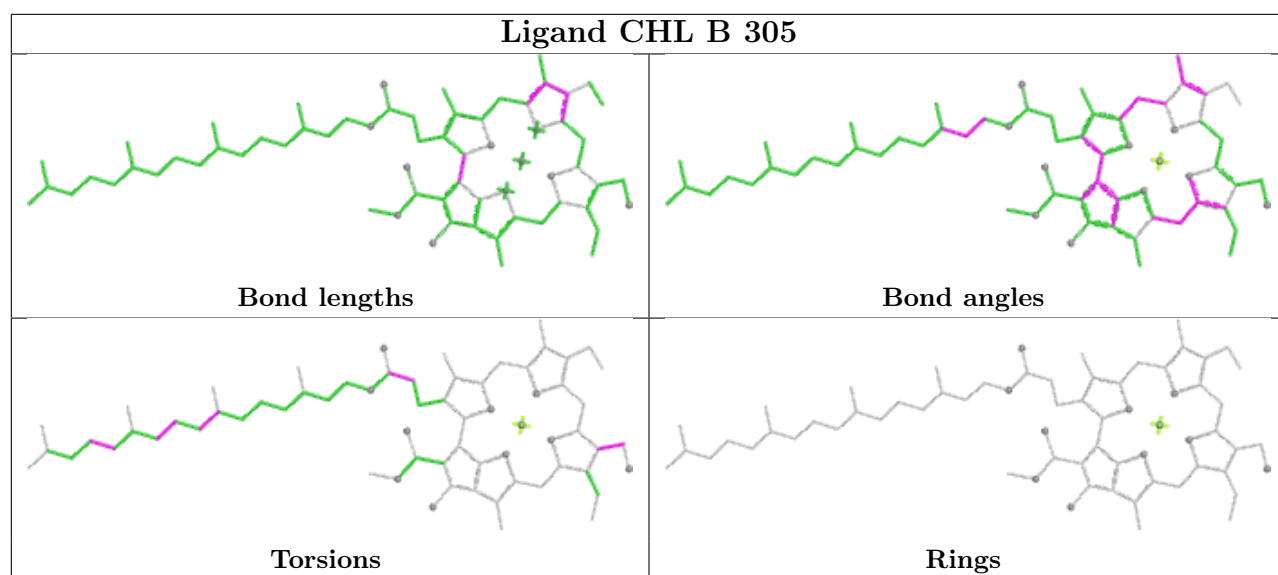
Ligand A1LYY B 317	
	
Bond lengths	Bond angles
	
Torsions	Rings

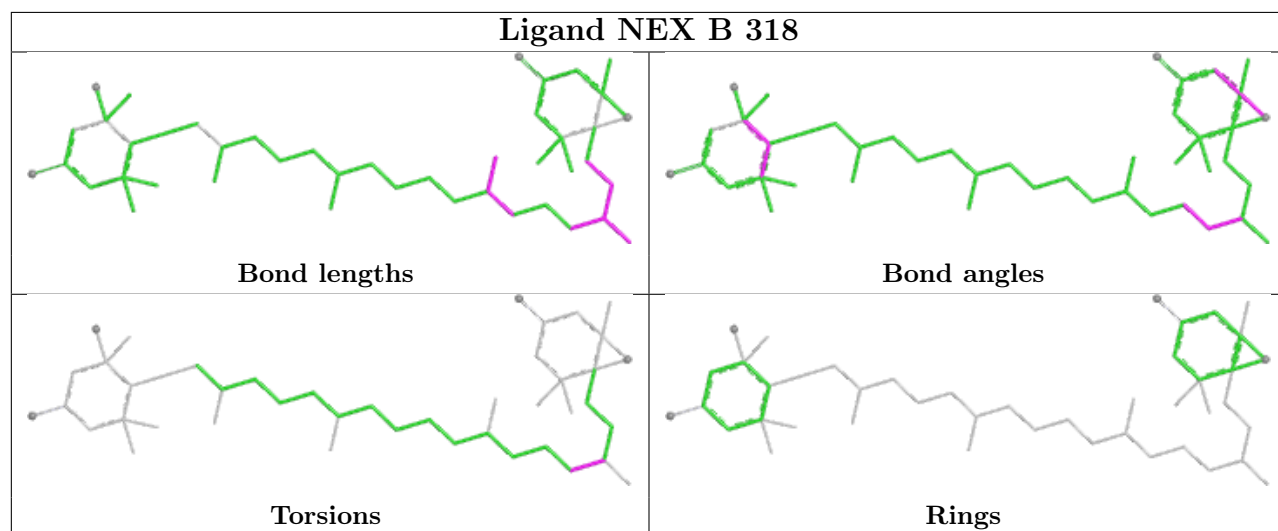
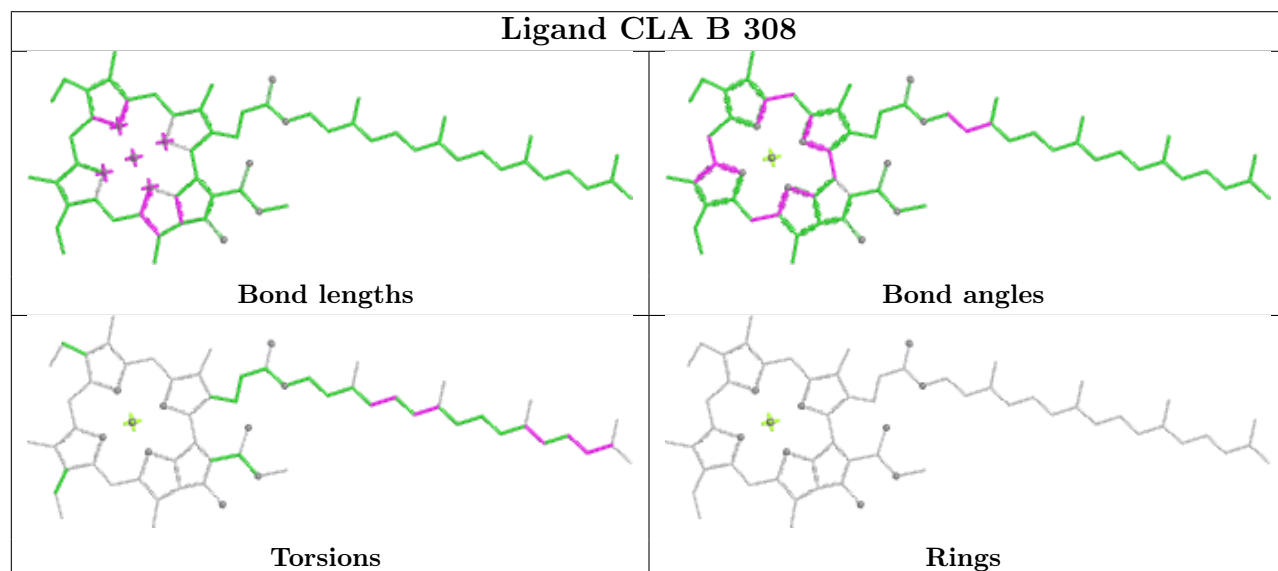
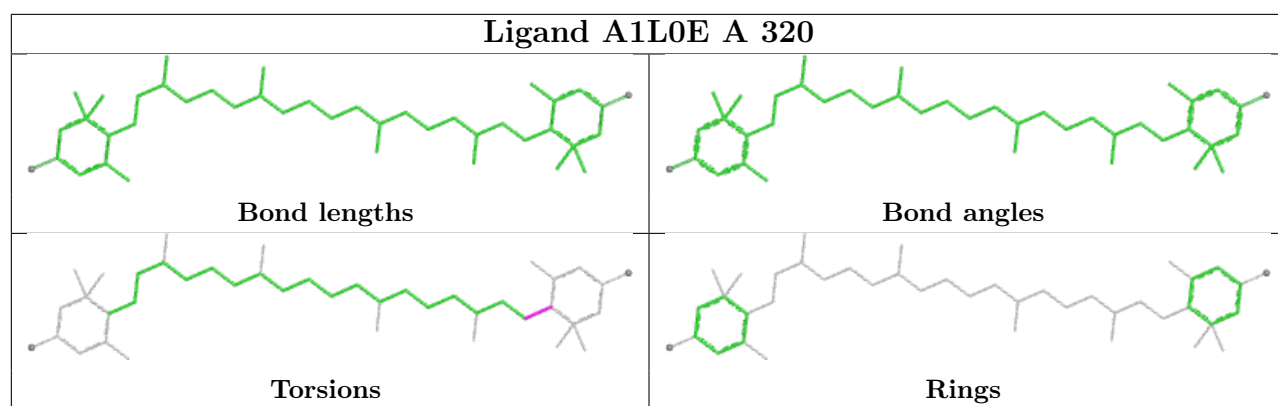
Ligand CHL C 303	
	
Bond lengths	Bond angles
	
Torsions	Rings

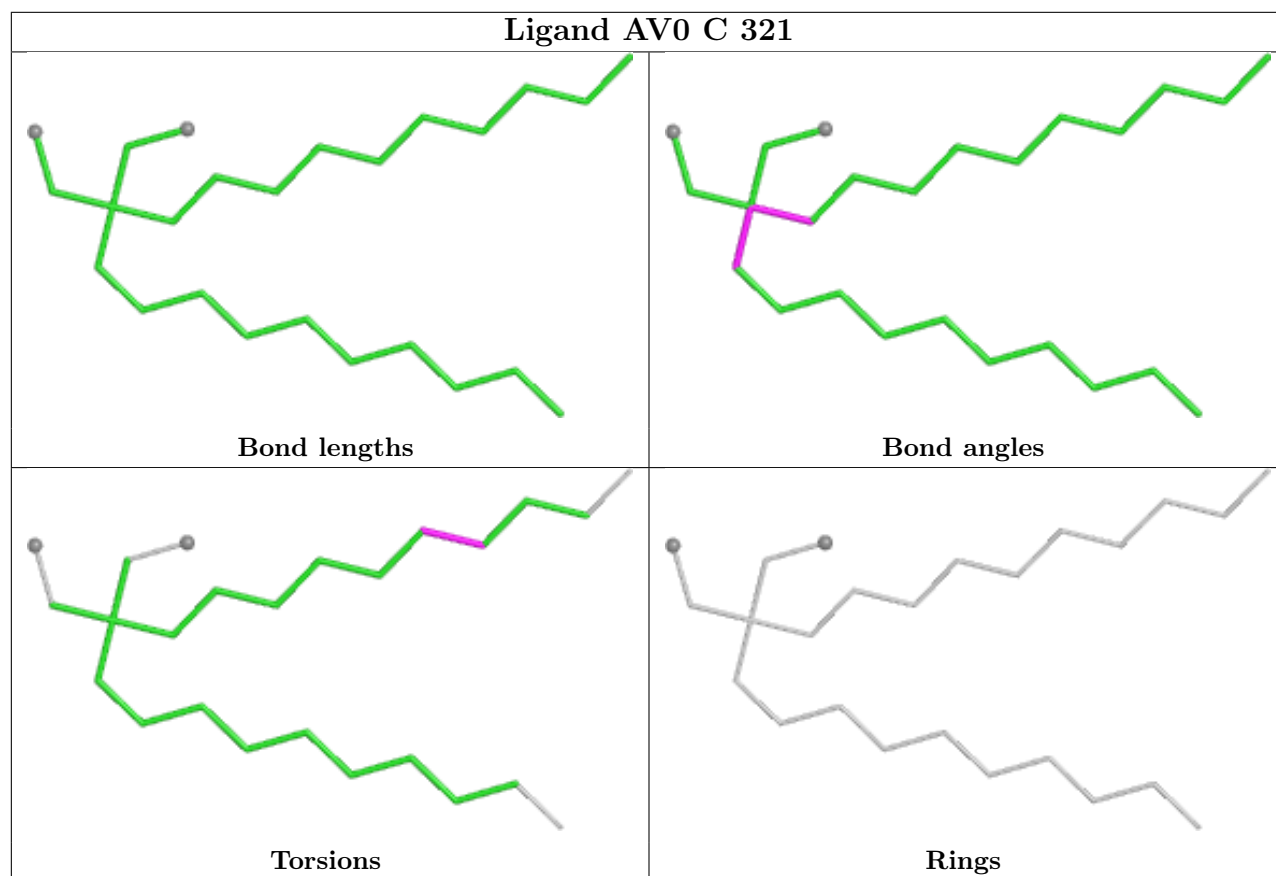
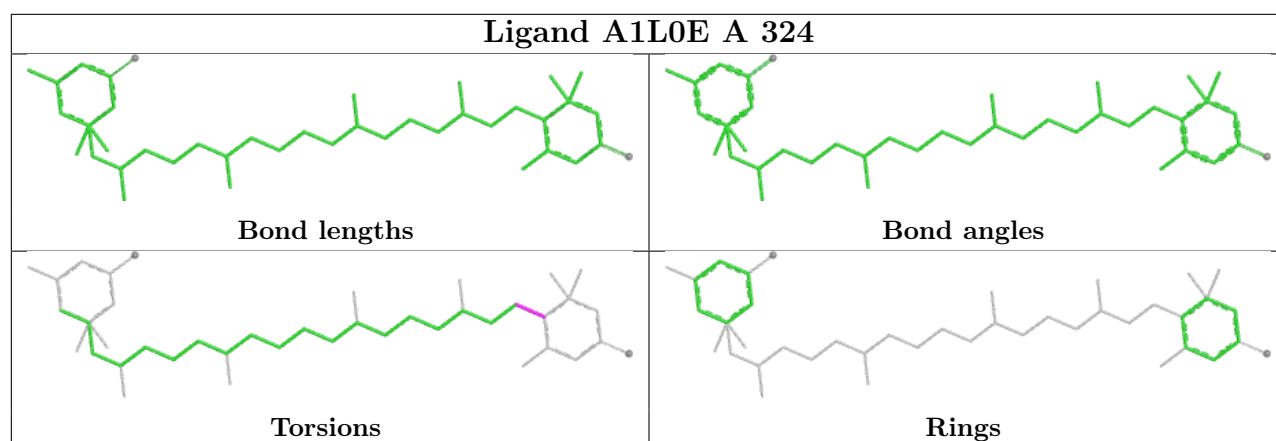
Ligand A1L0E C 301	
	
Bond lengths	Bond angles
	
Torsions	Rings

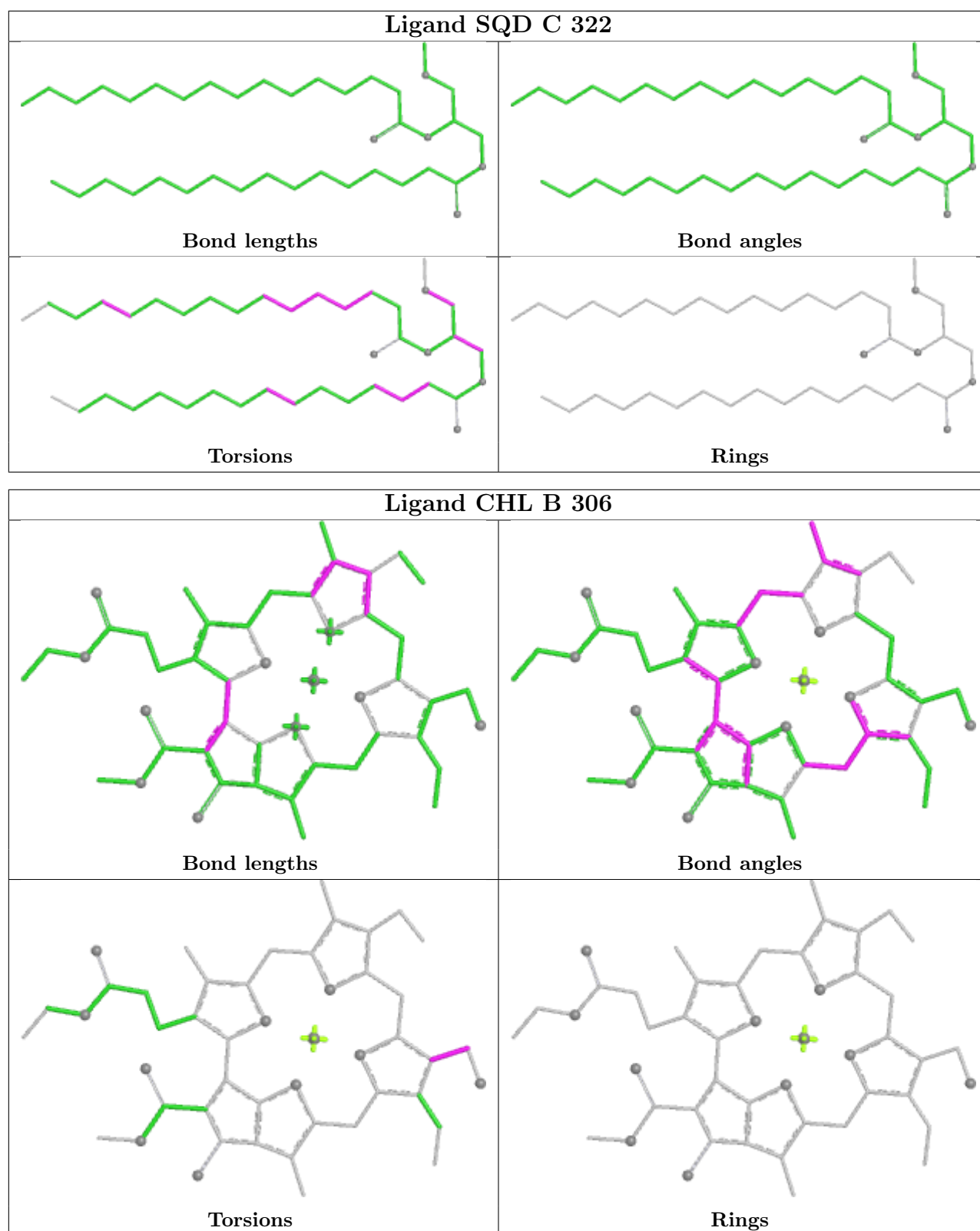


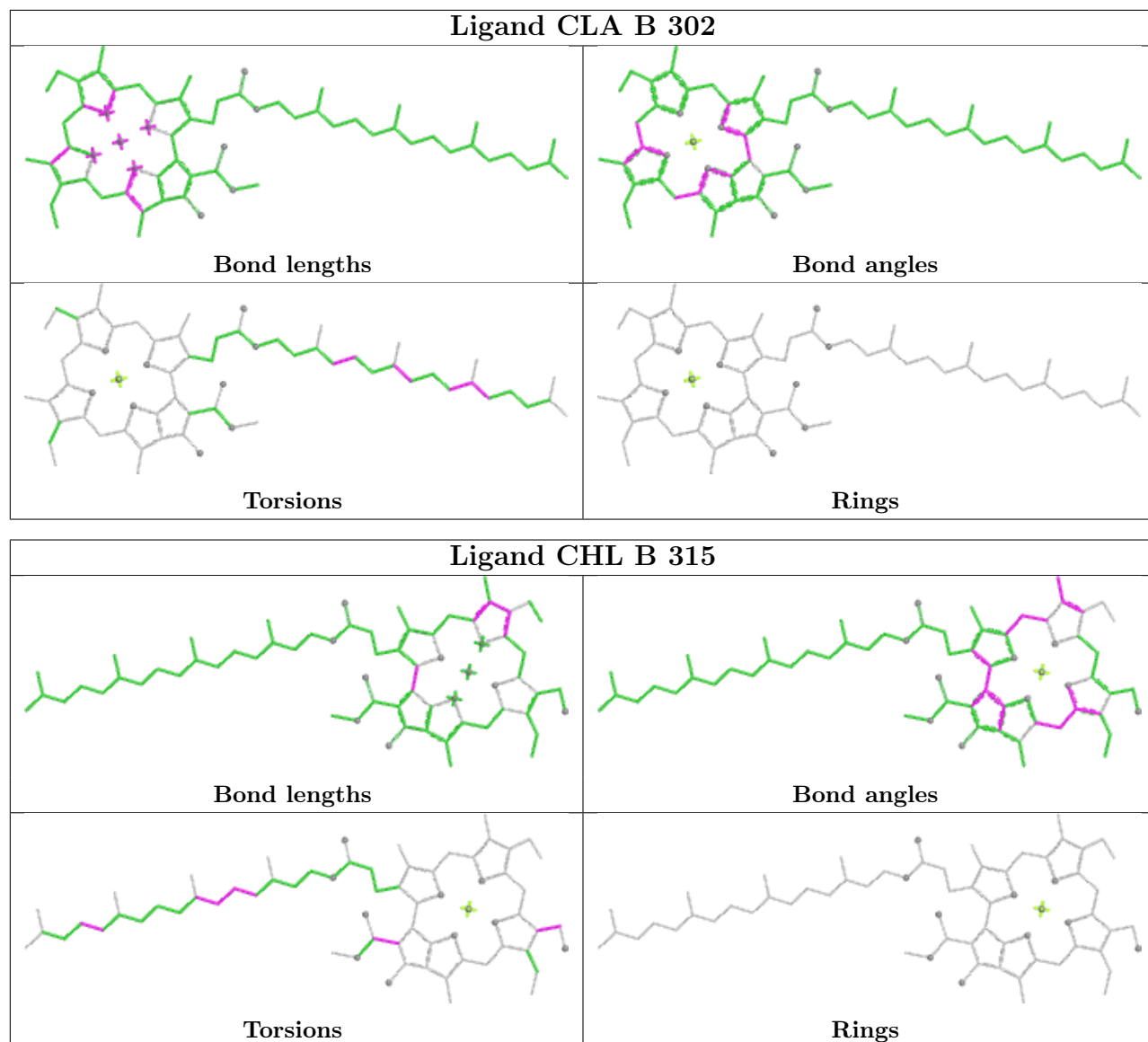




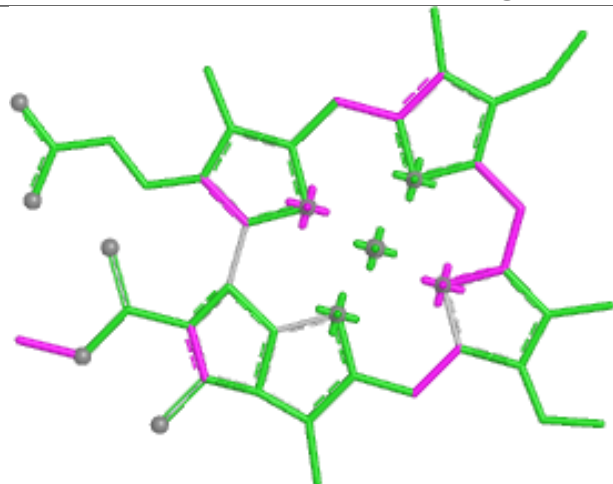




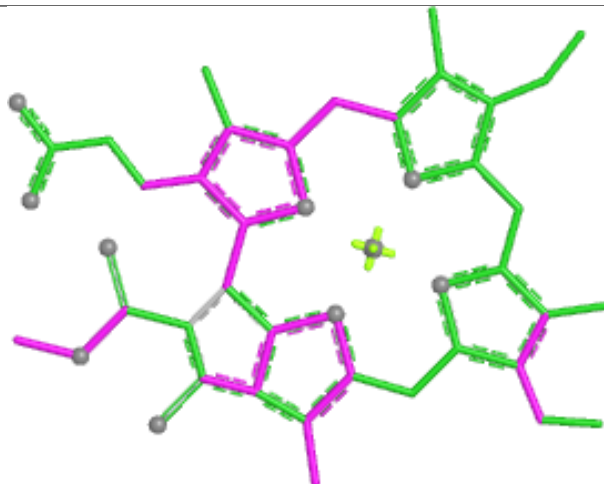




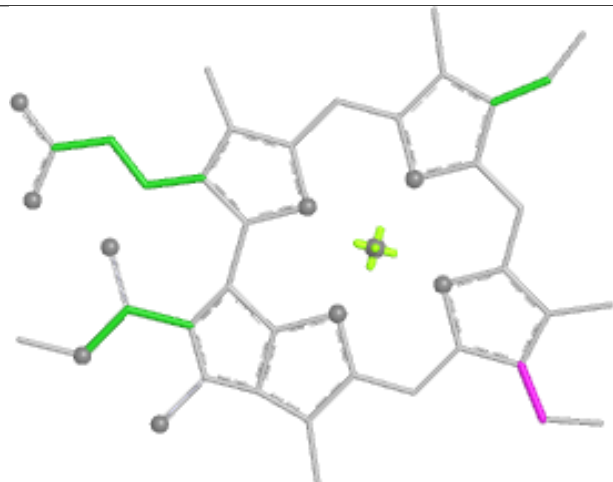
Ligand A1L0F B 309



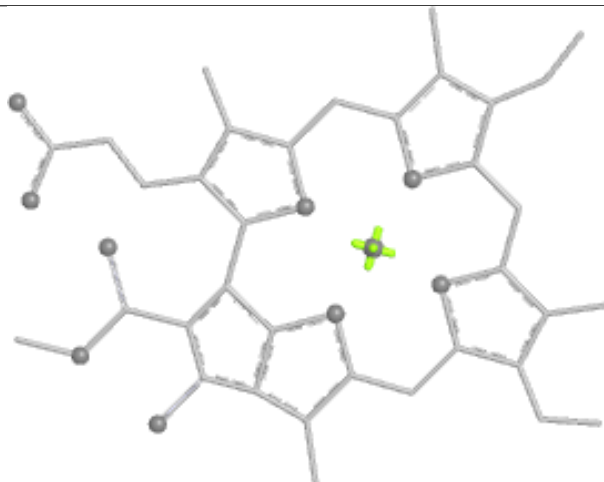
Bond lengths



Bond angles

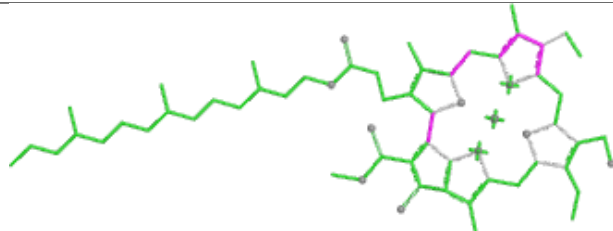


Torsions

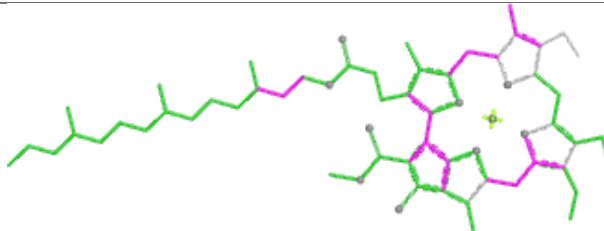


Rings

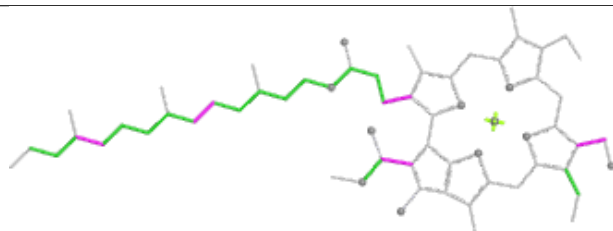
Ligand CHL B 303



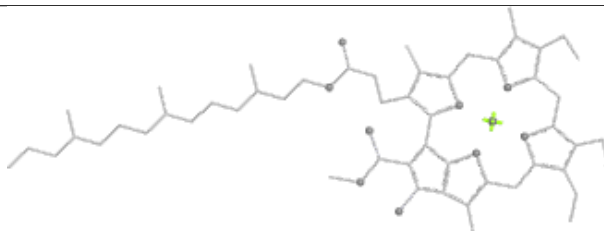
Bond lengths



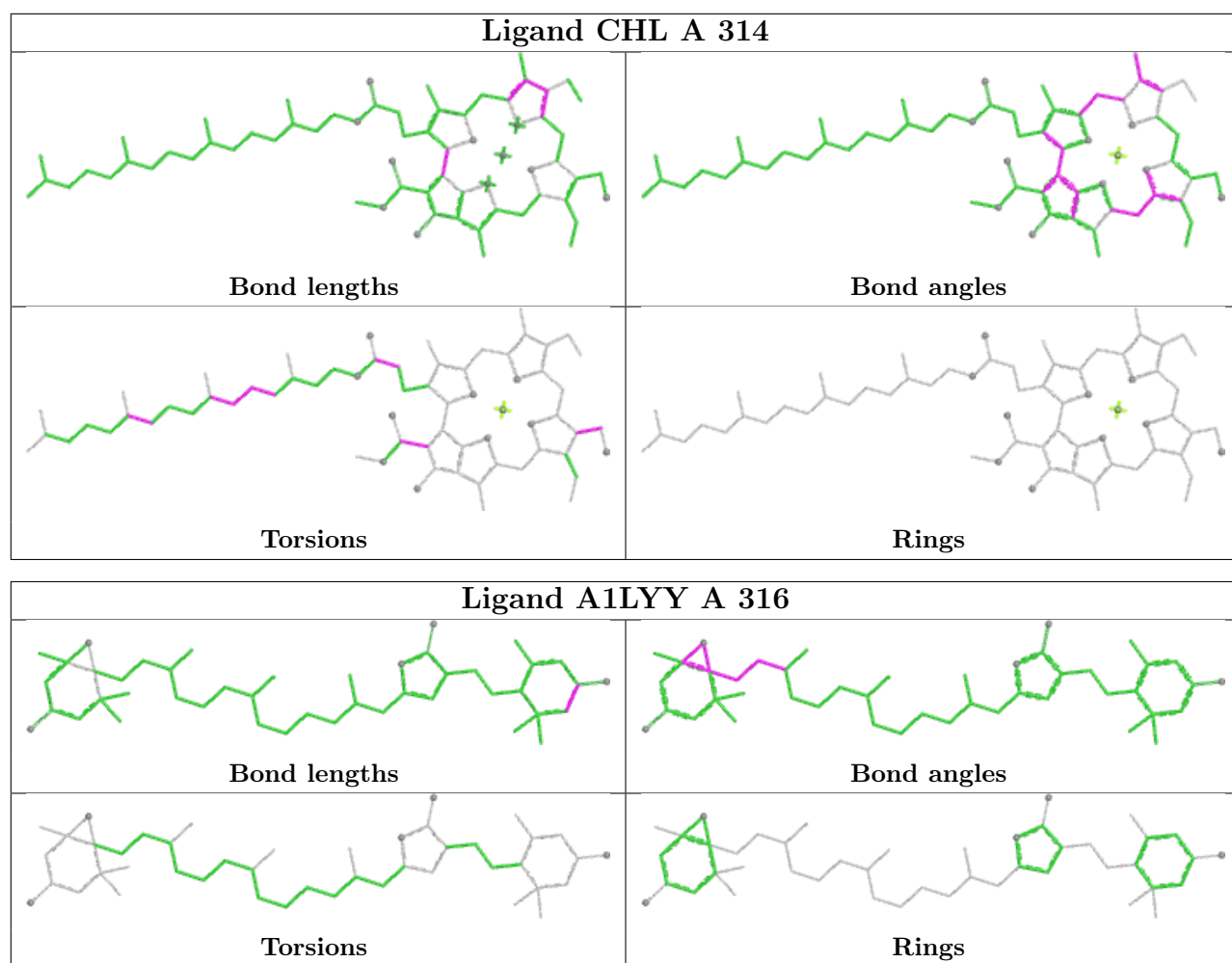
Bond angles

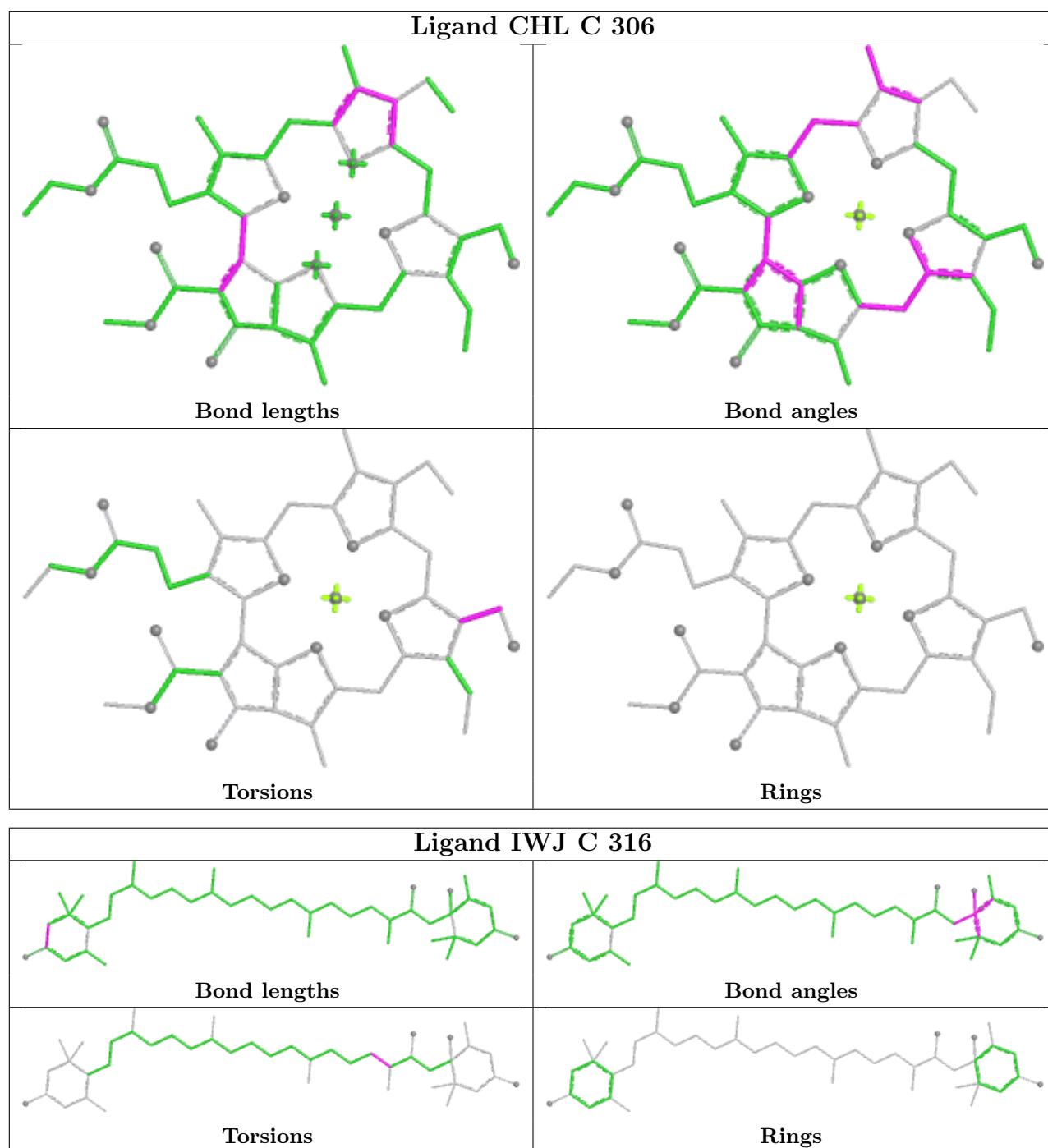


Torsions

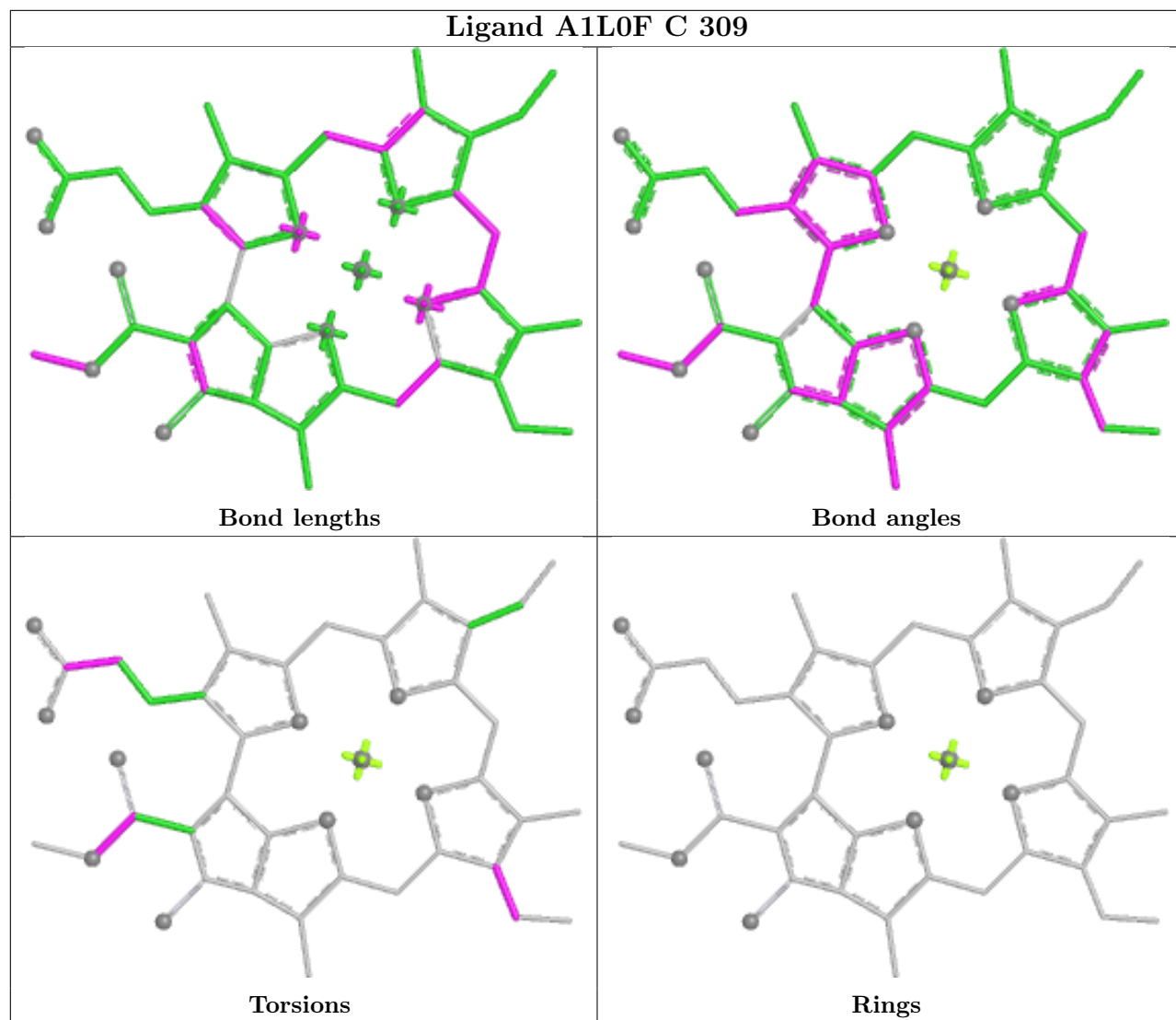


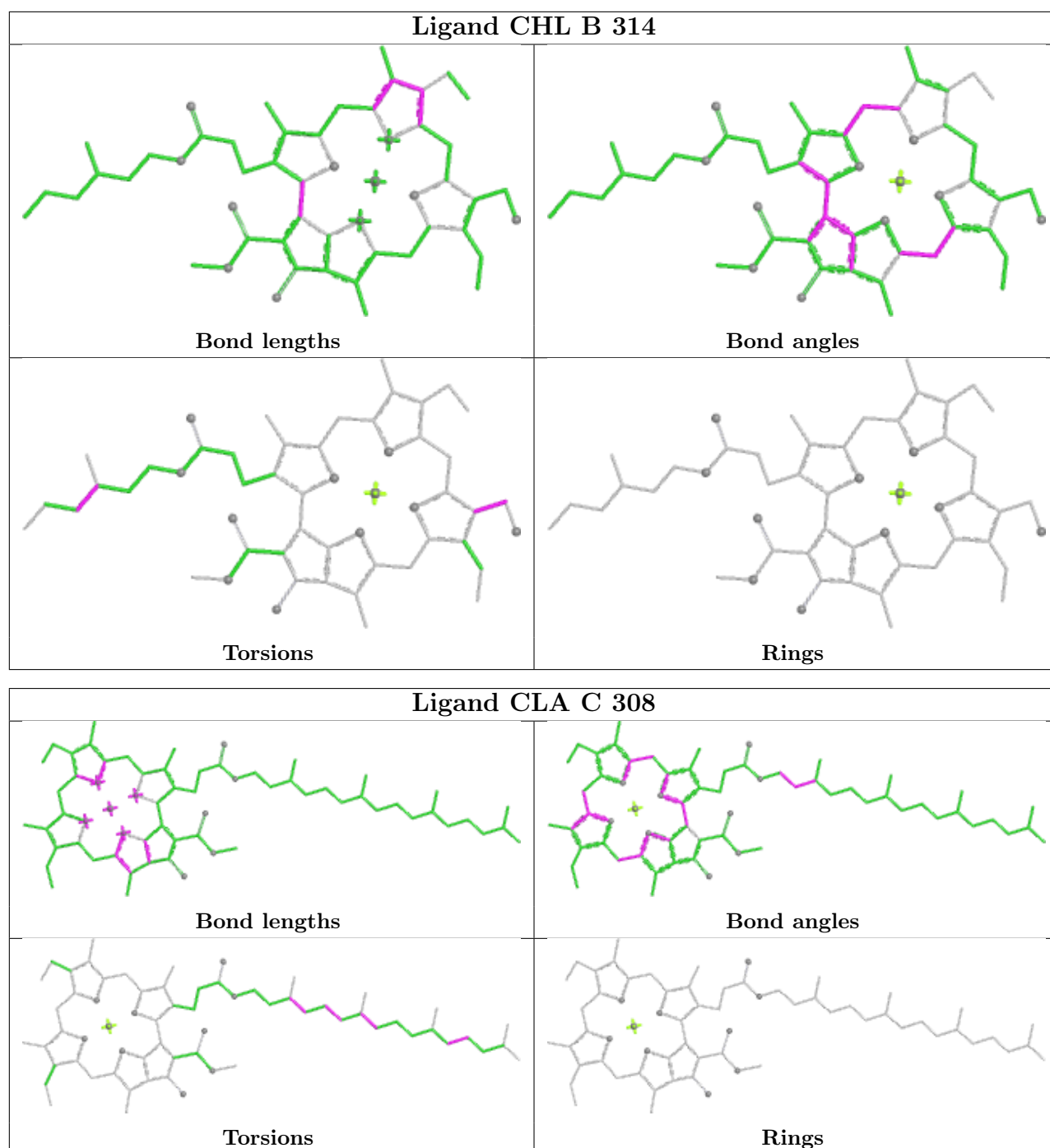
Rings

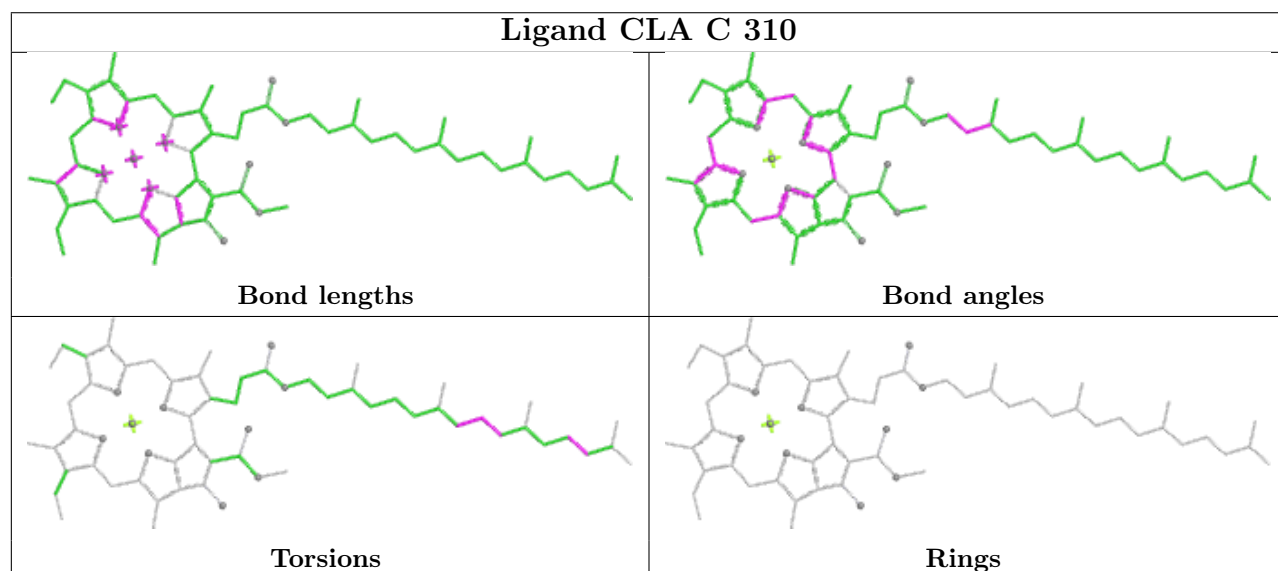
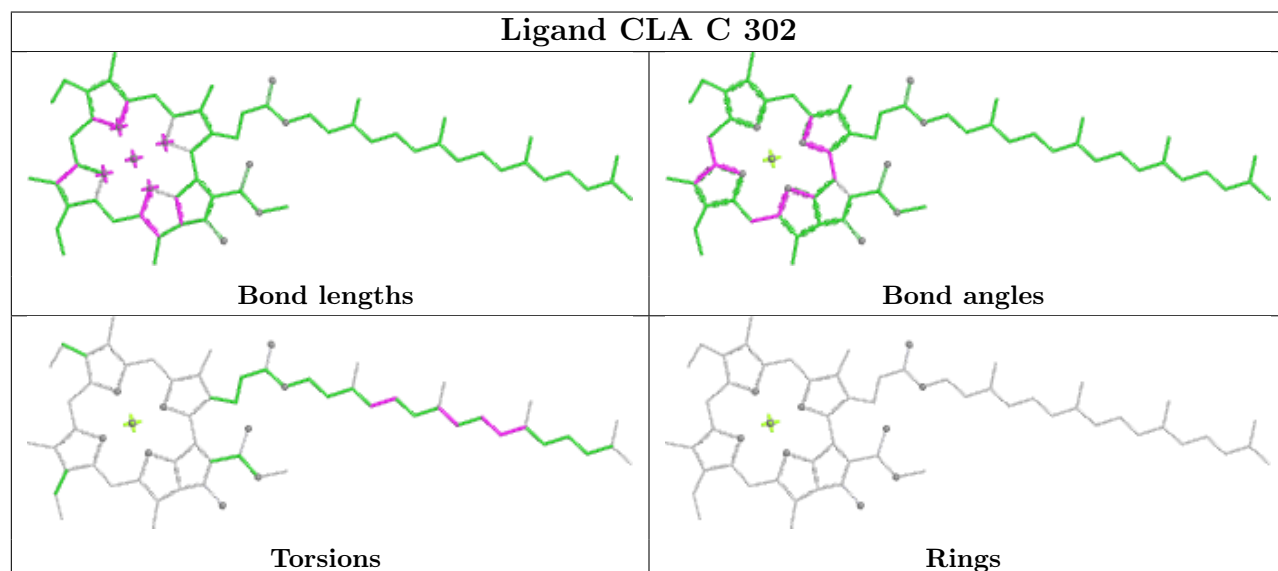
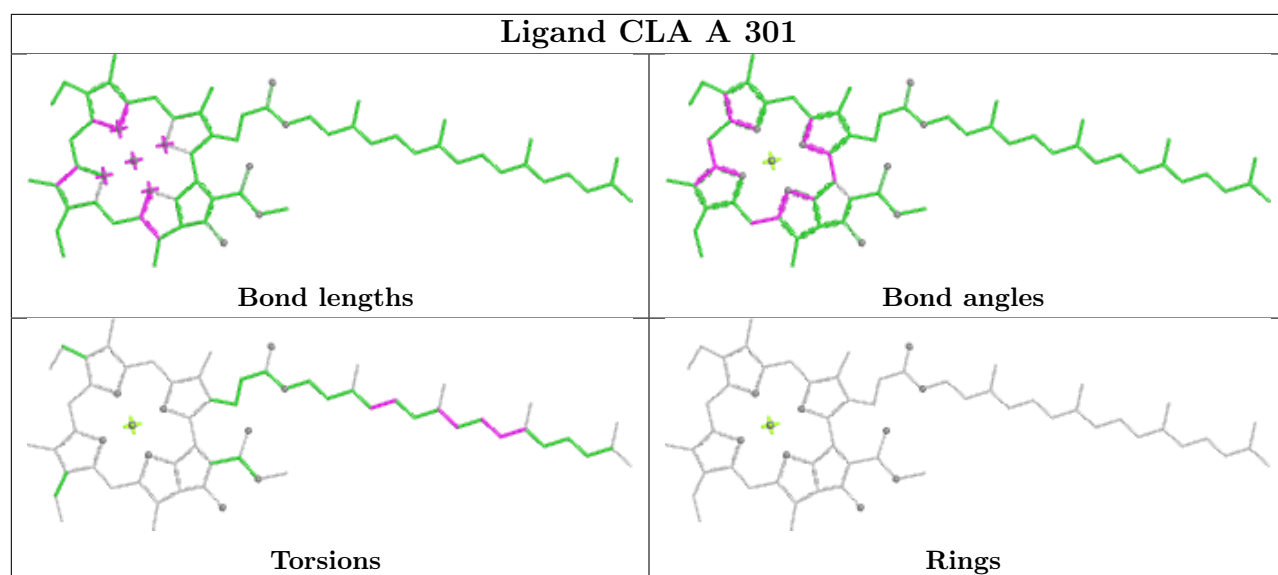




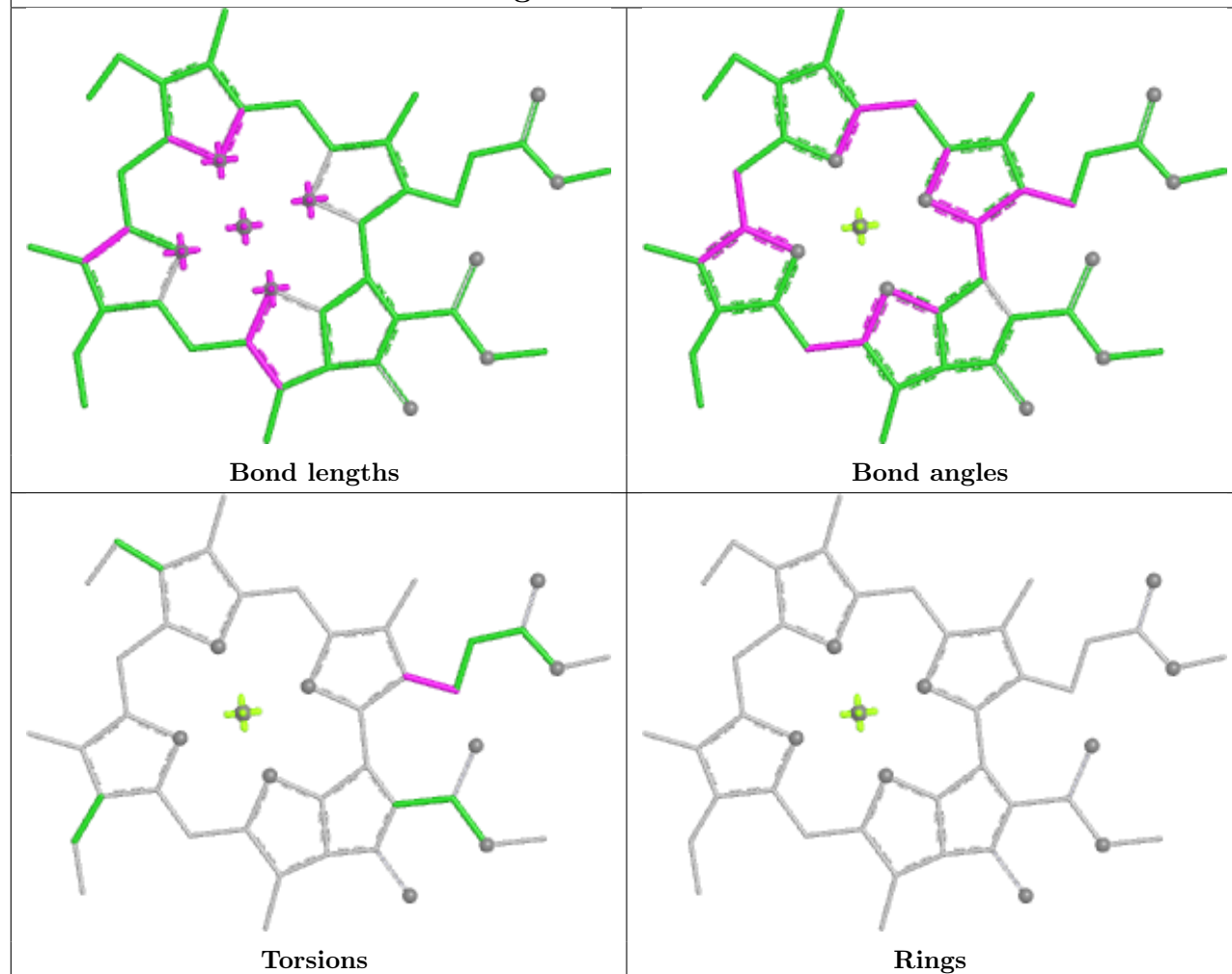
Ligand A1L0F C 309



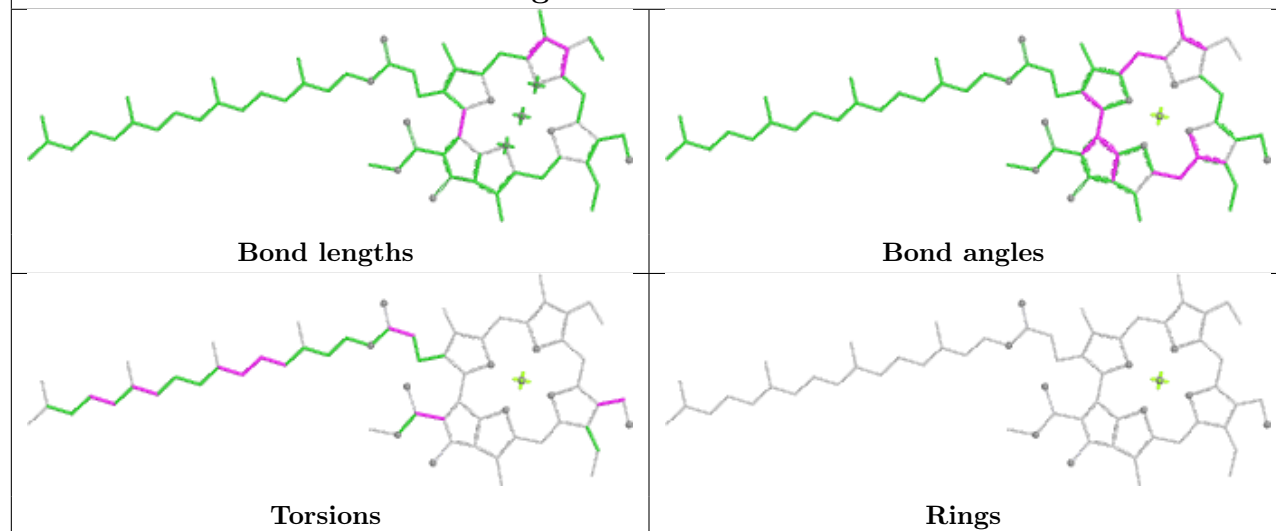


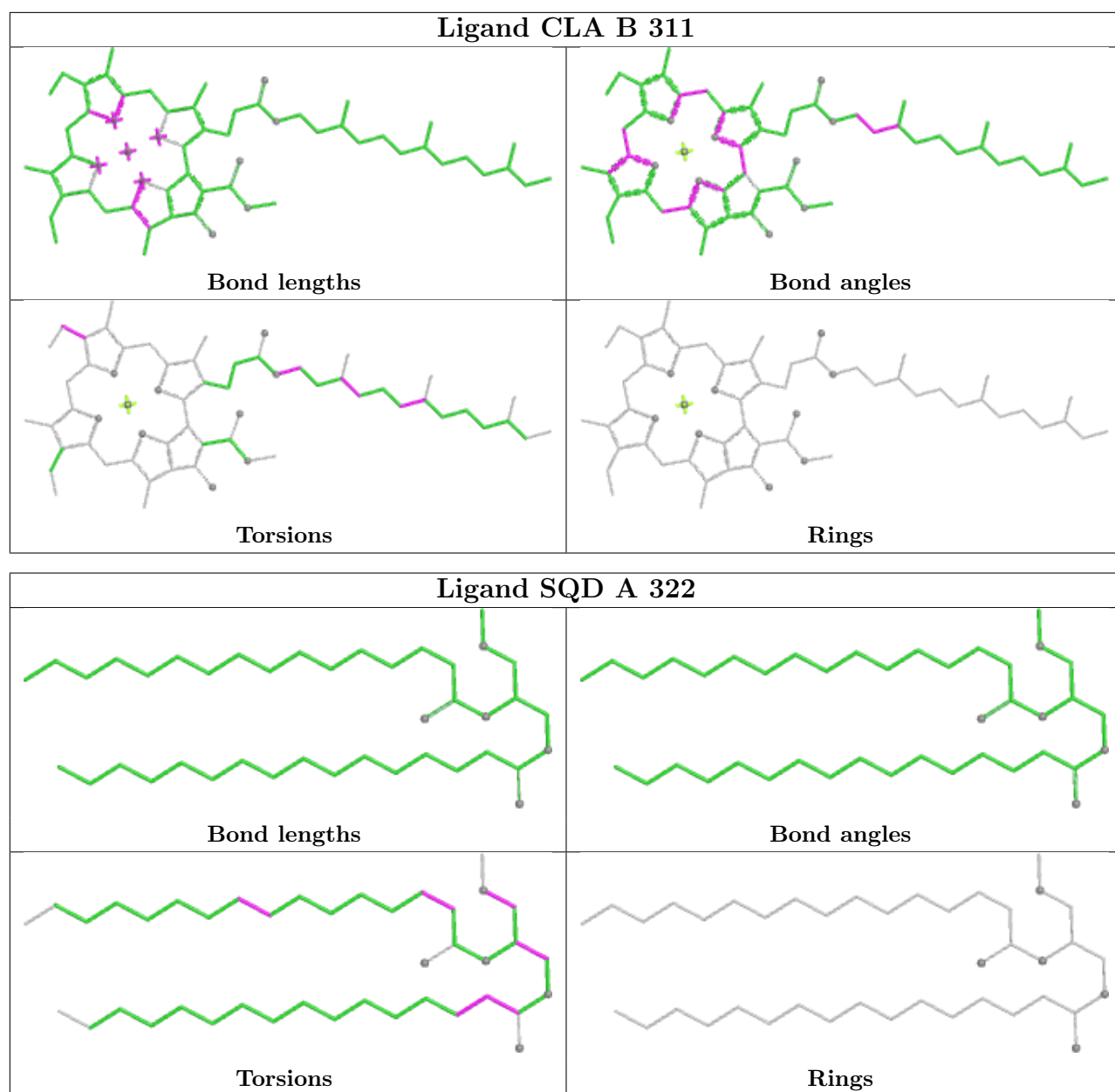


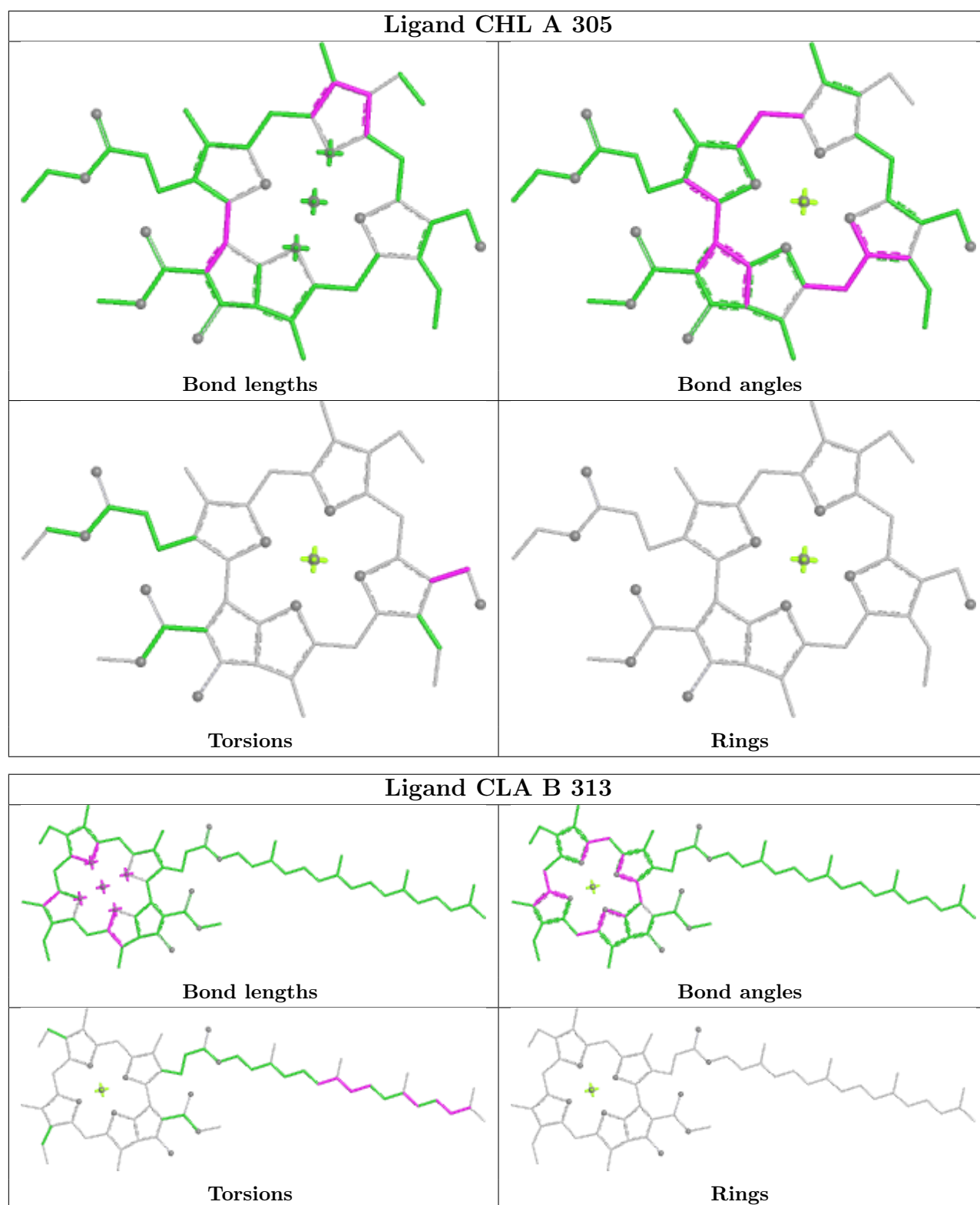
Ligand CLA C 312

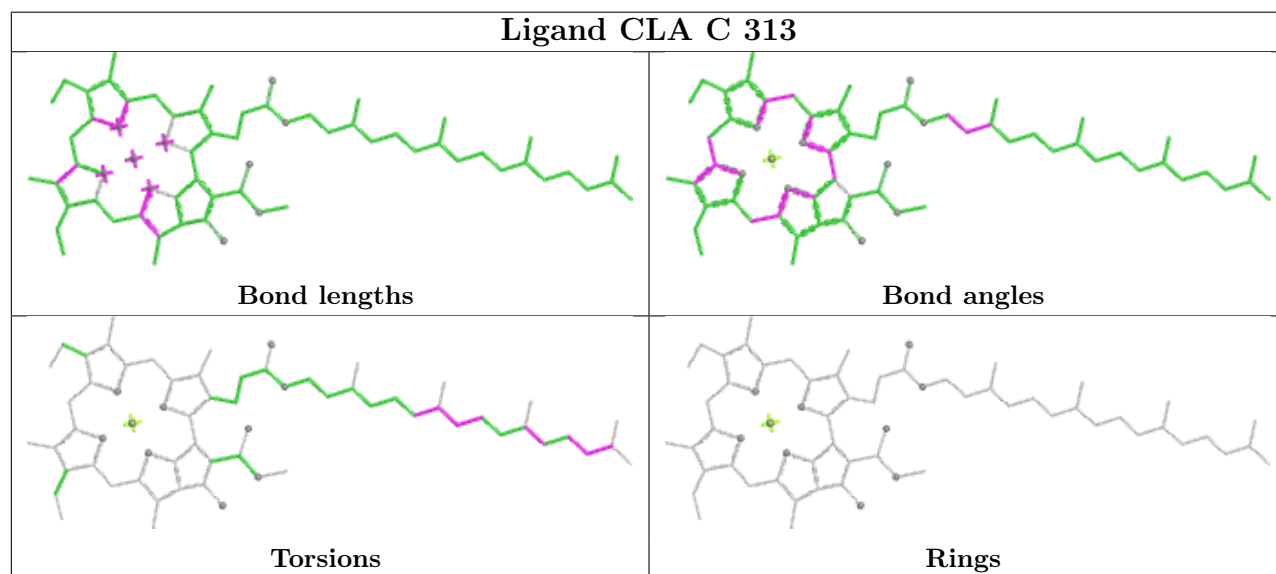
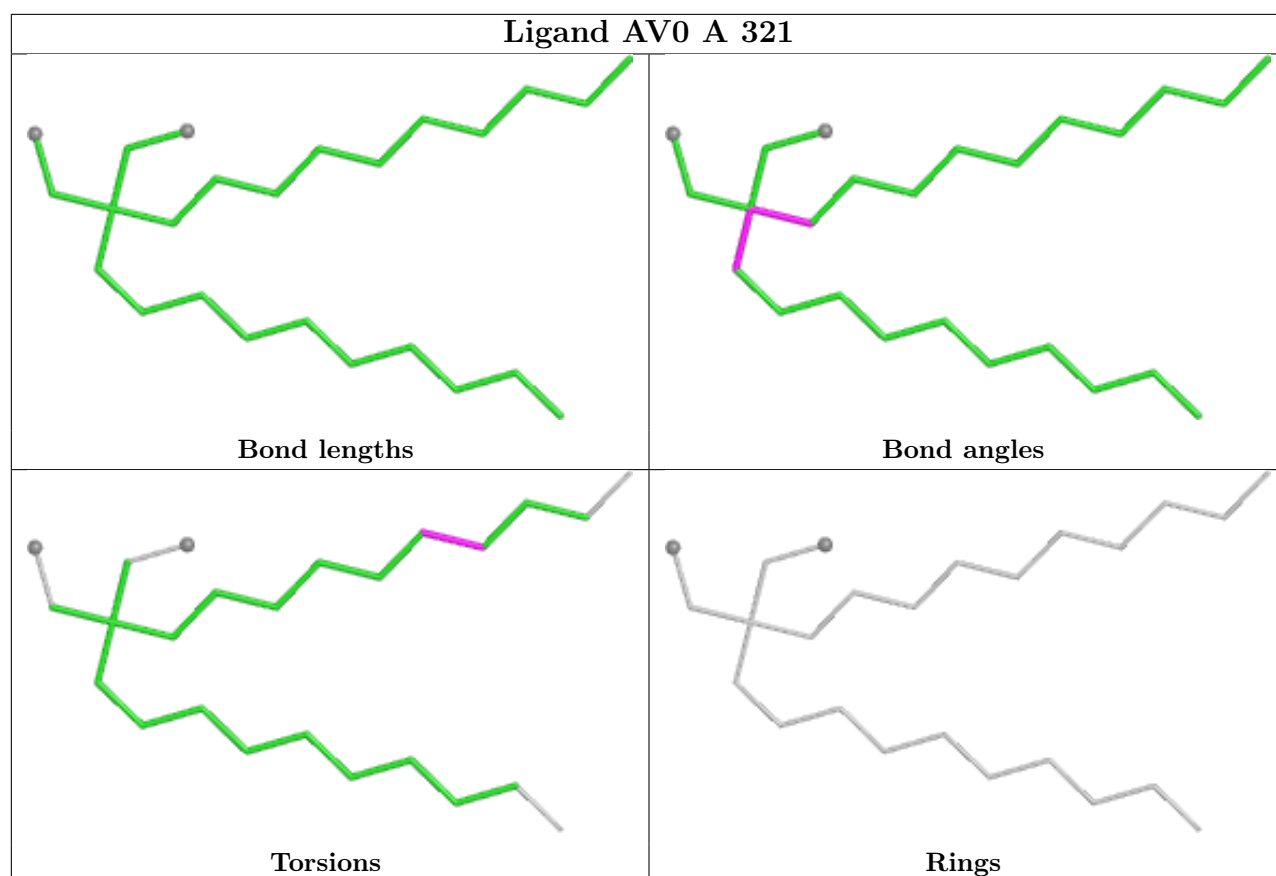


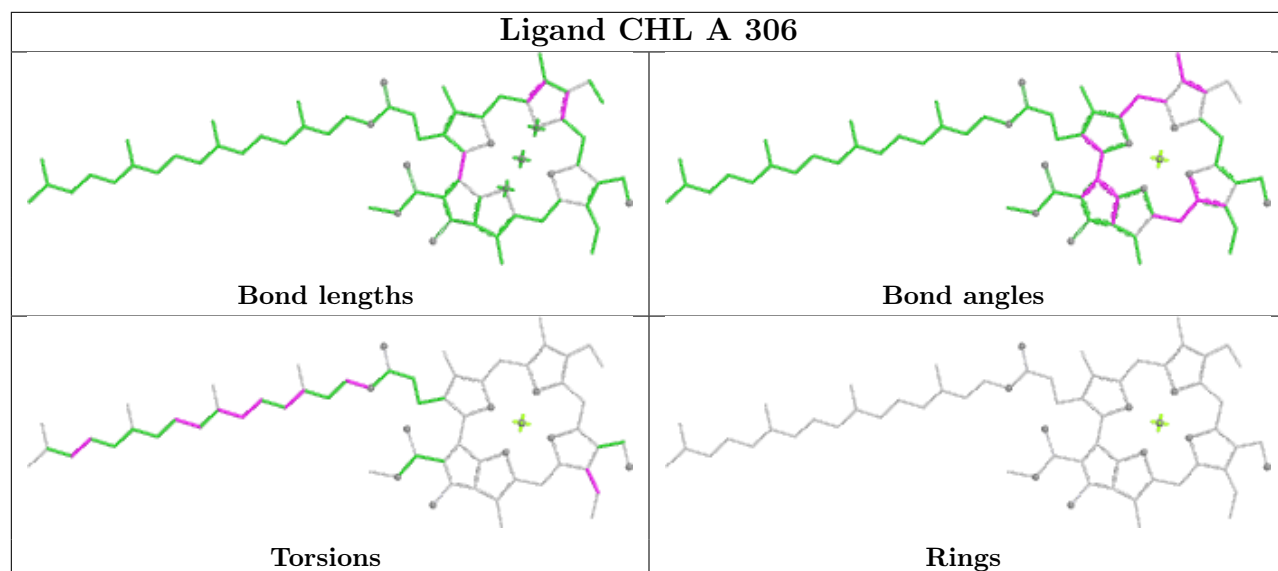
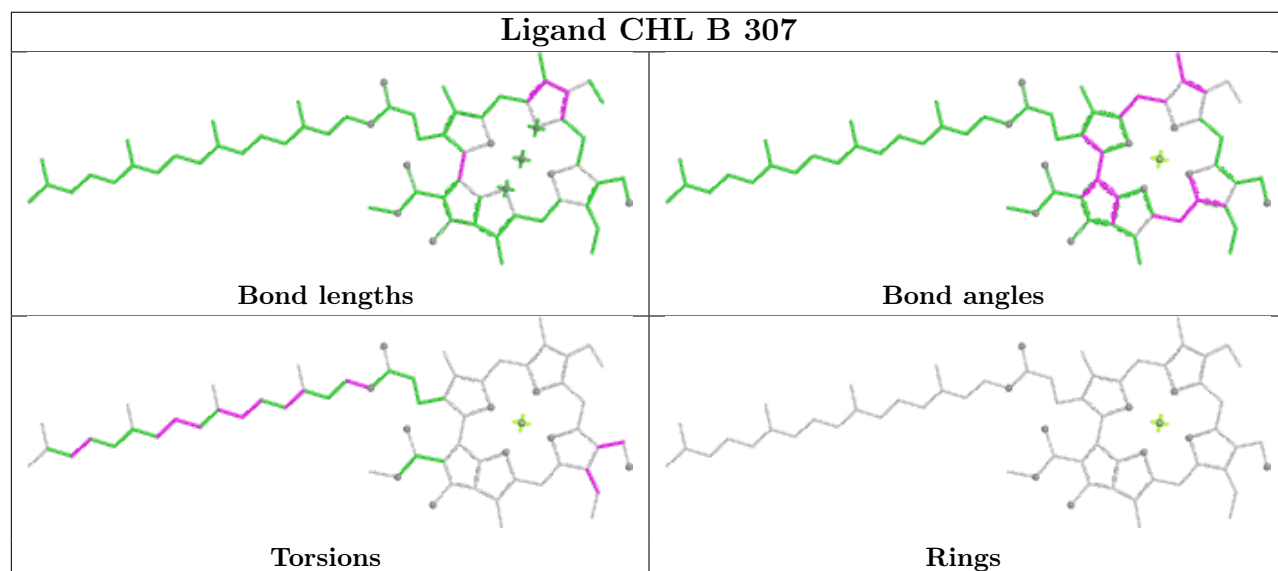
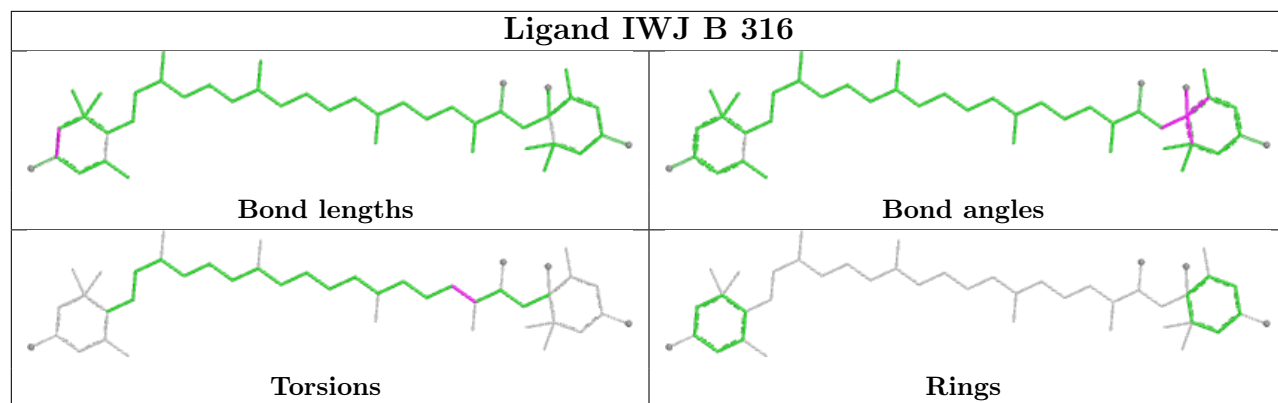
Ligand CHL C 315

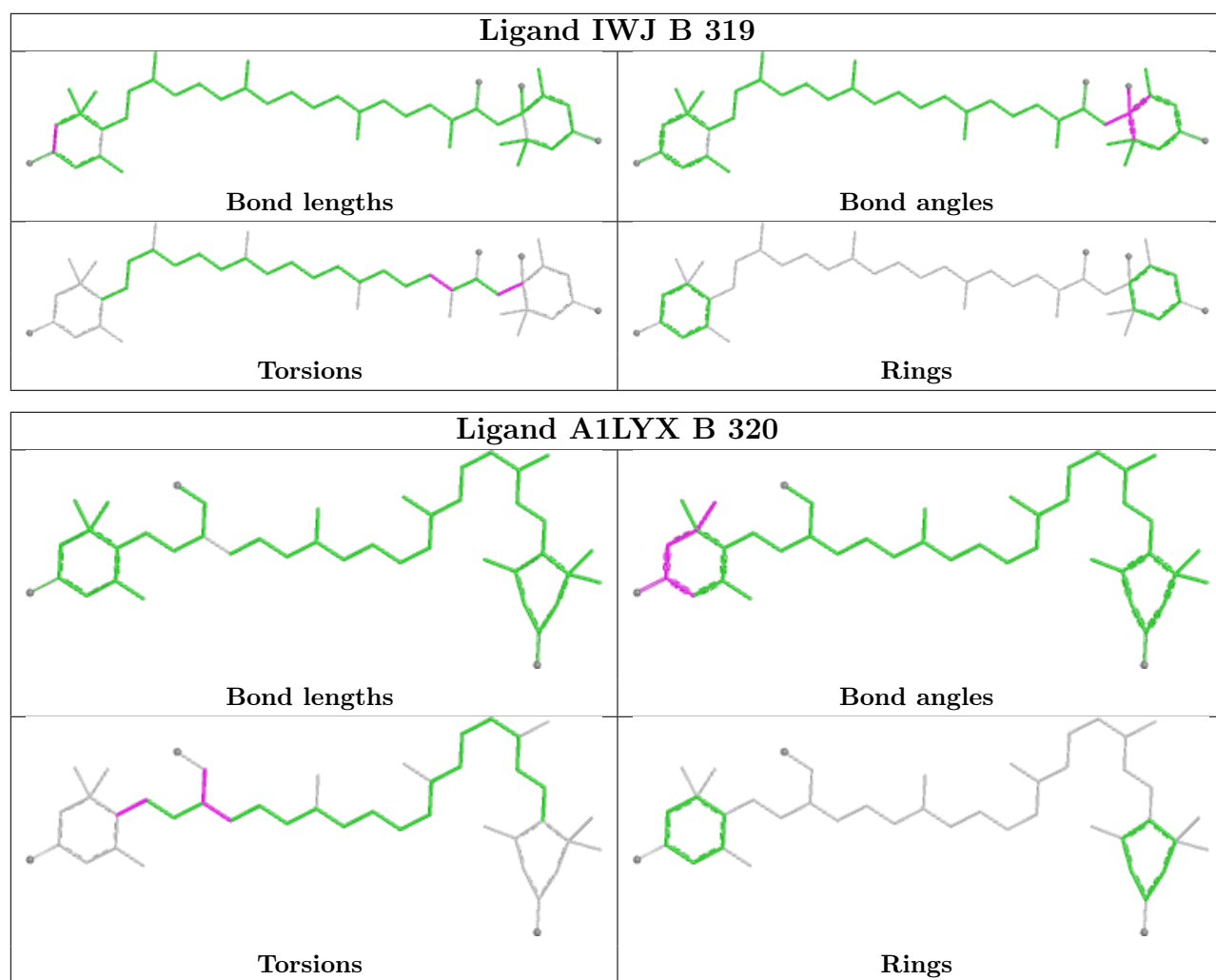


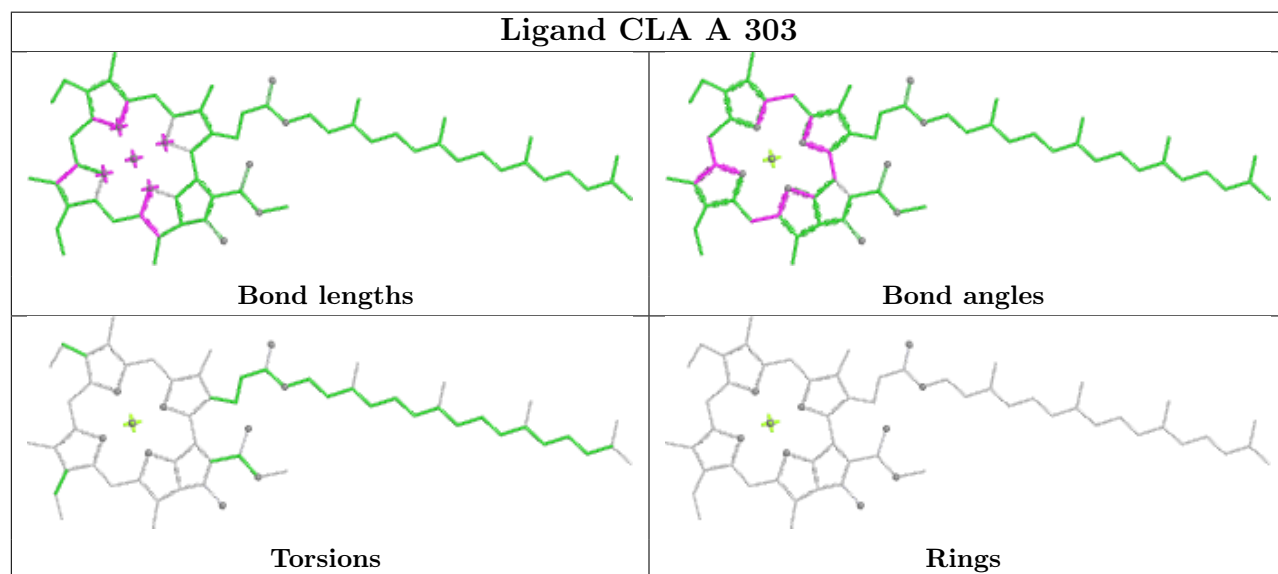
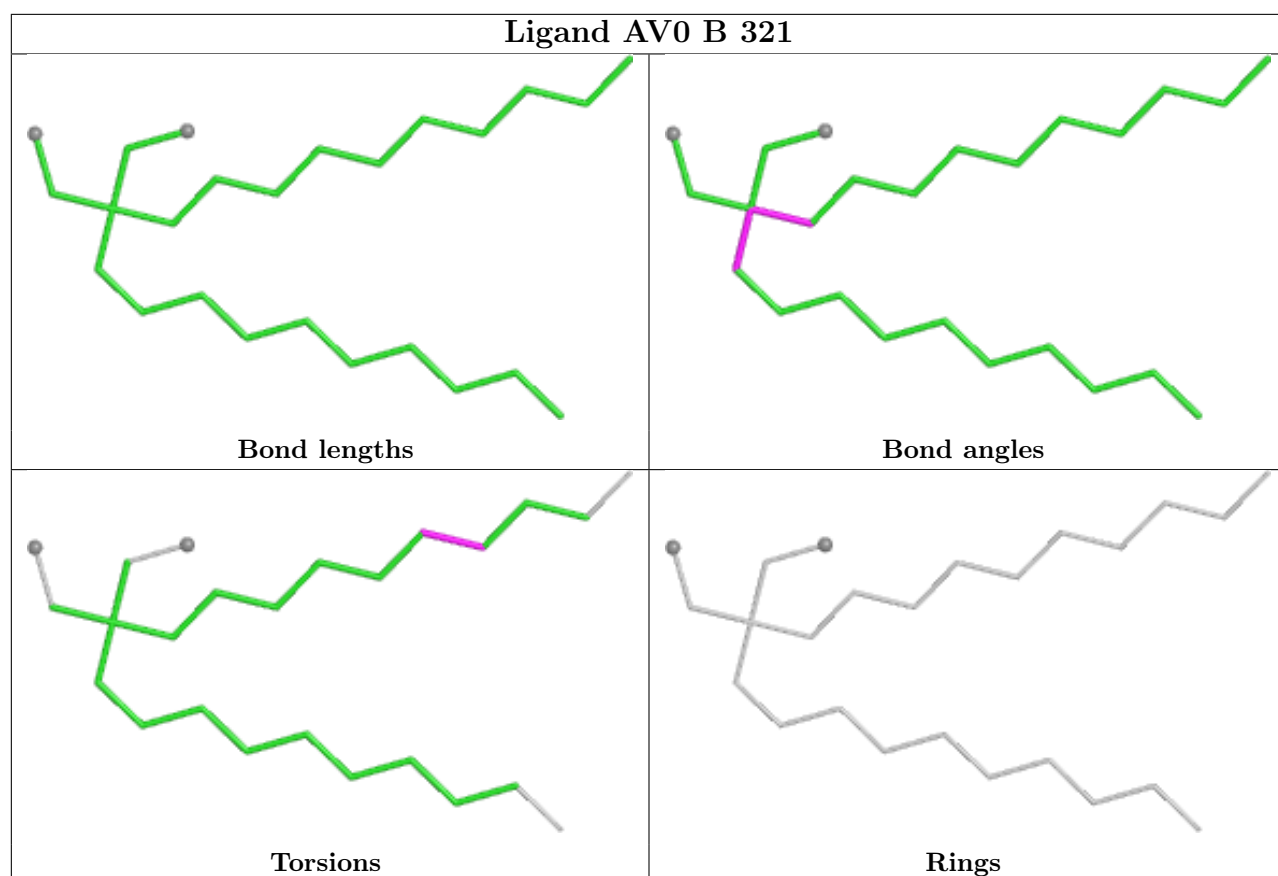


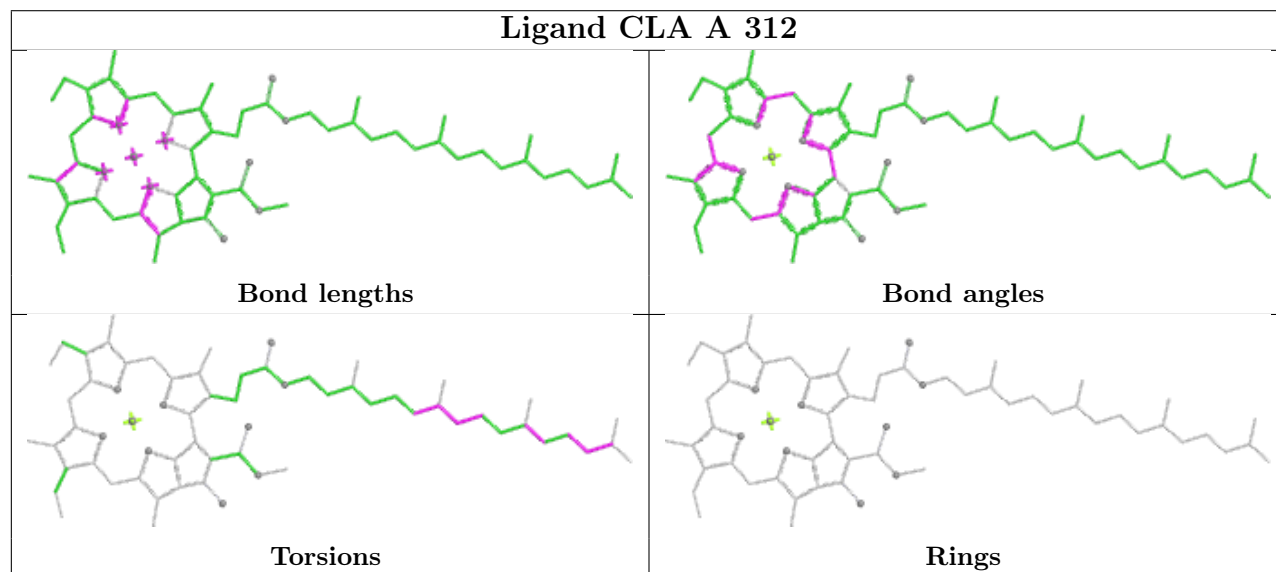
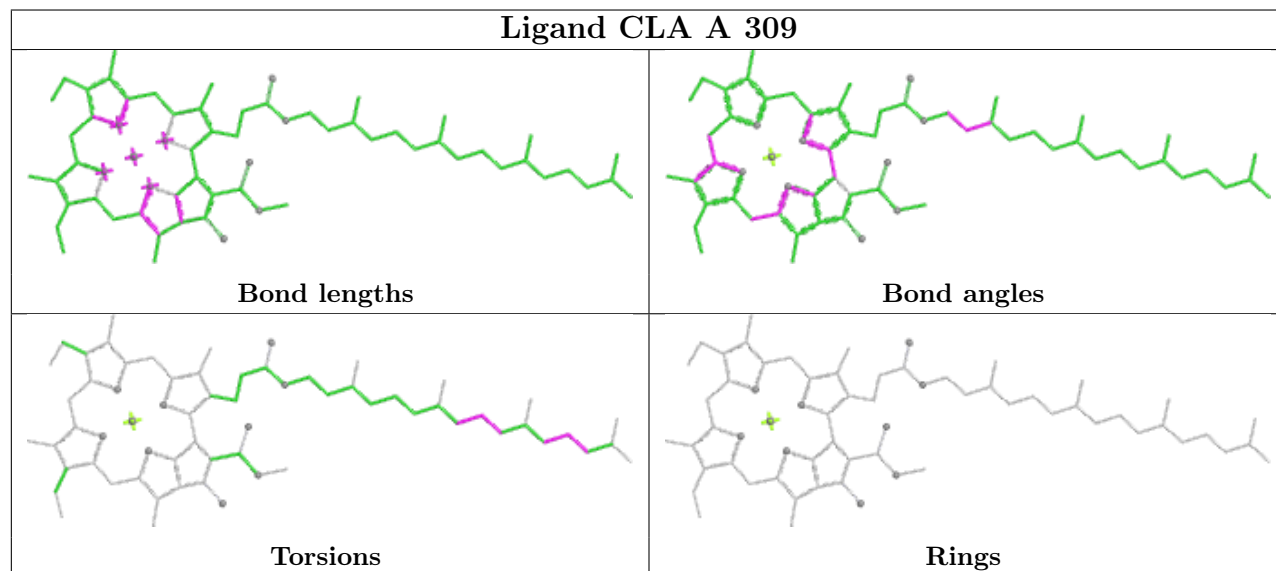
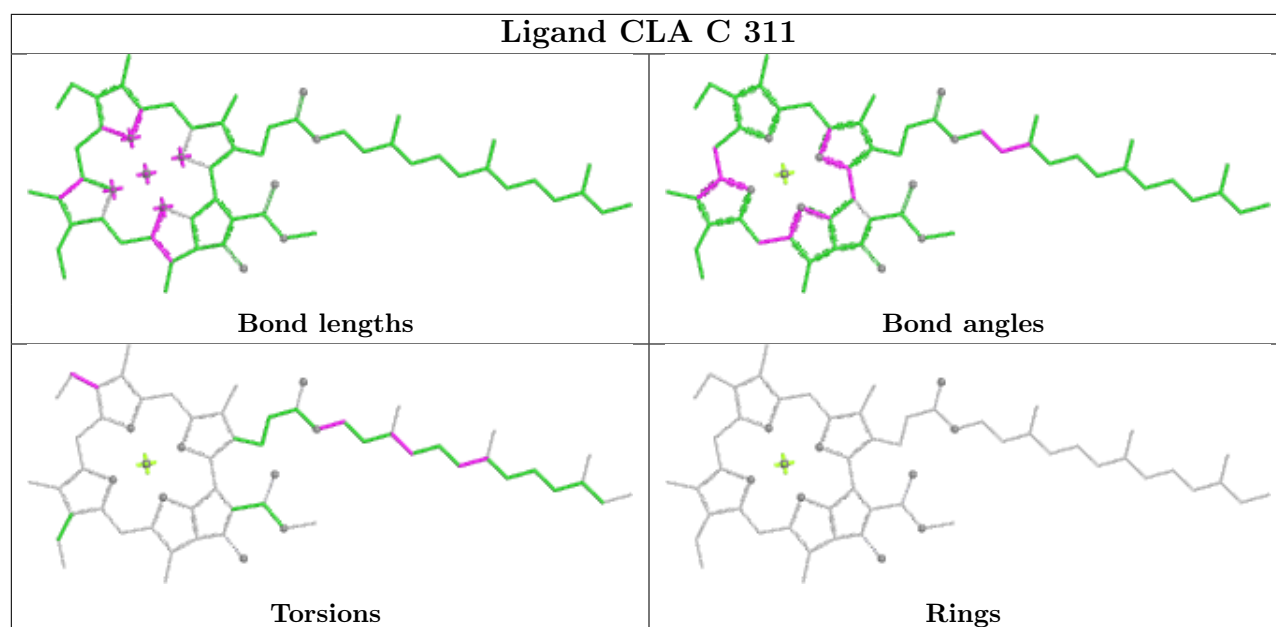


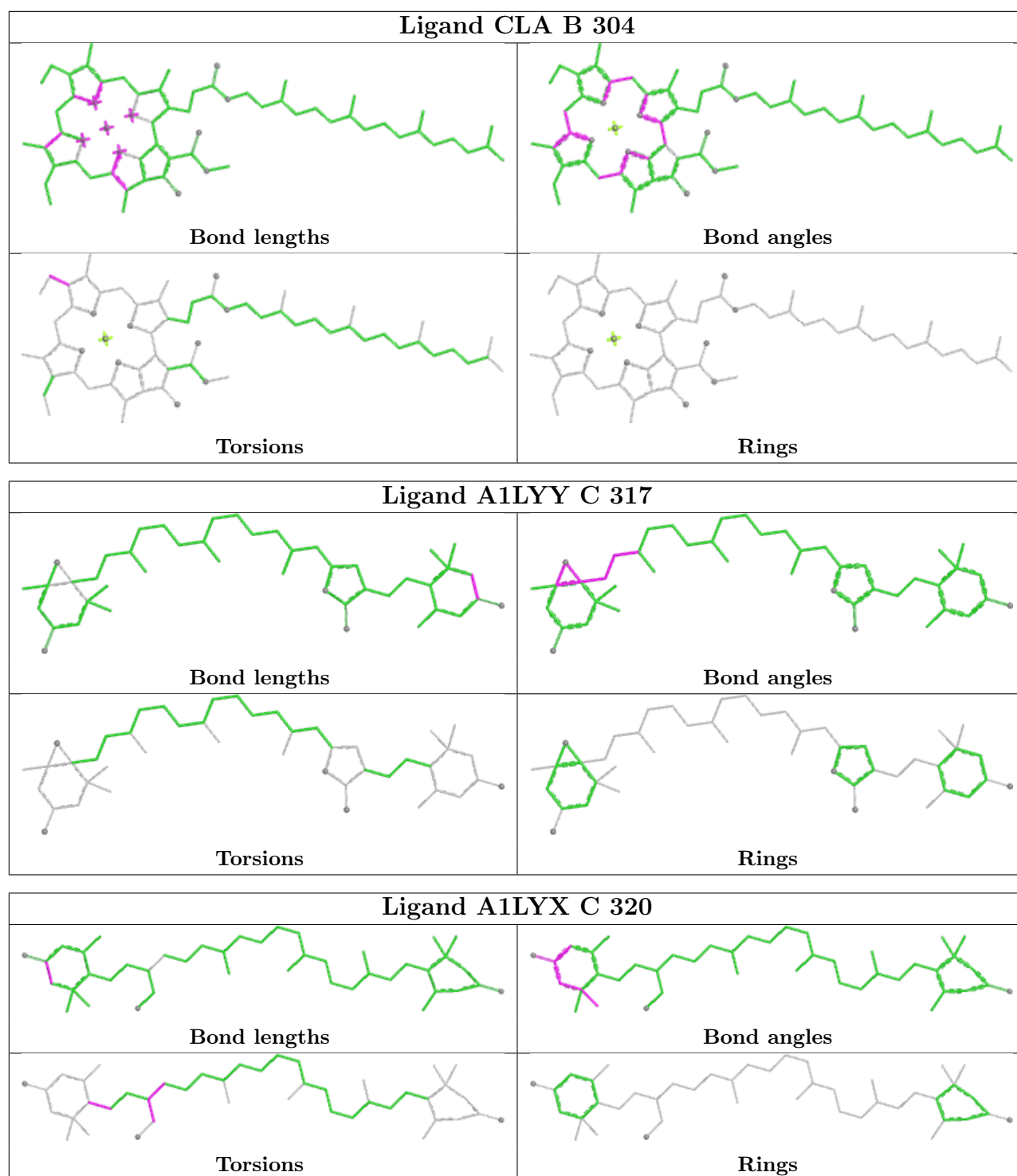


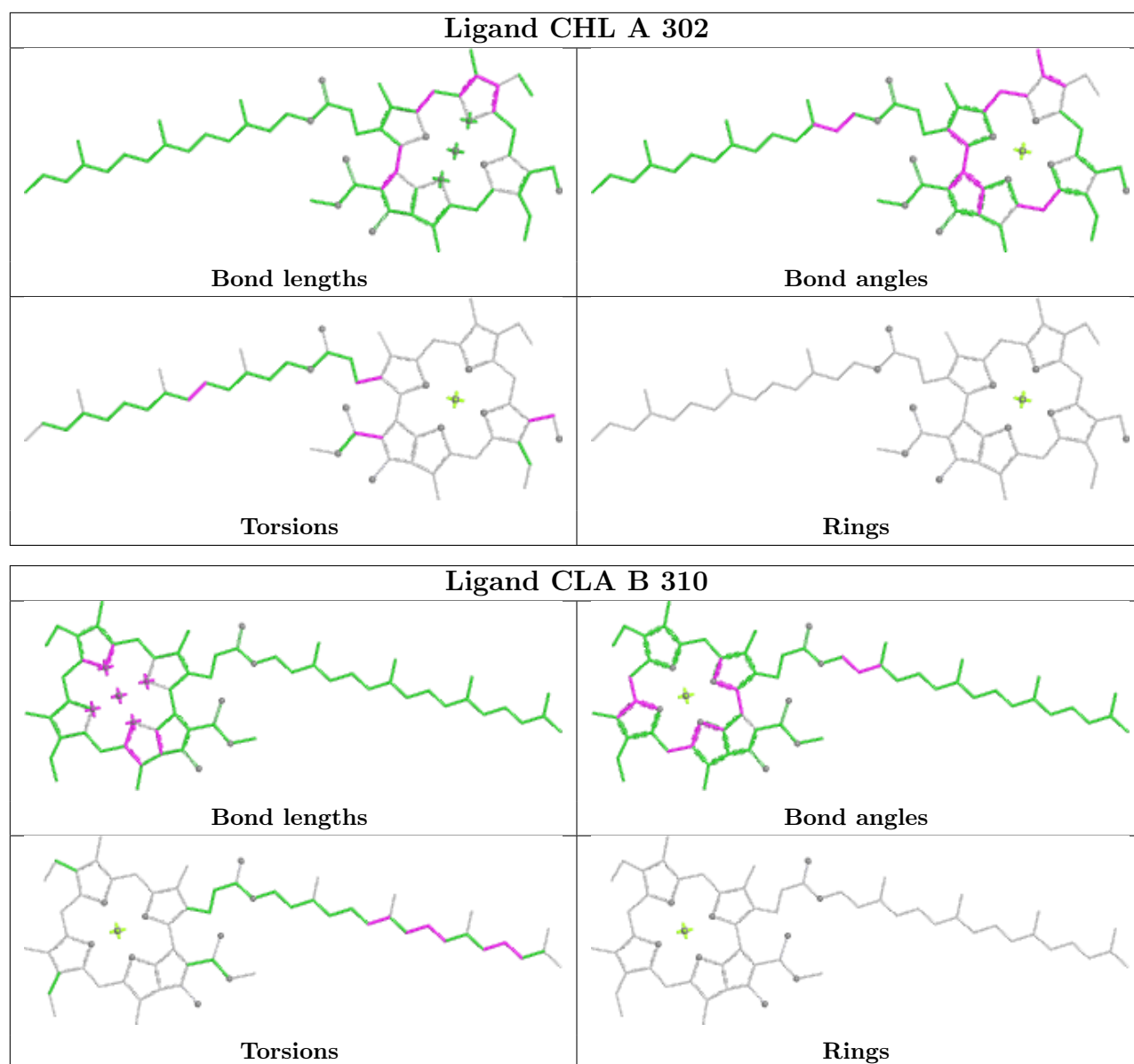


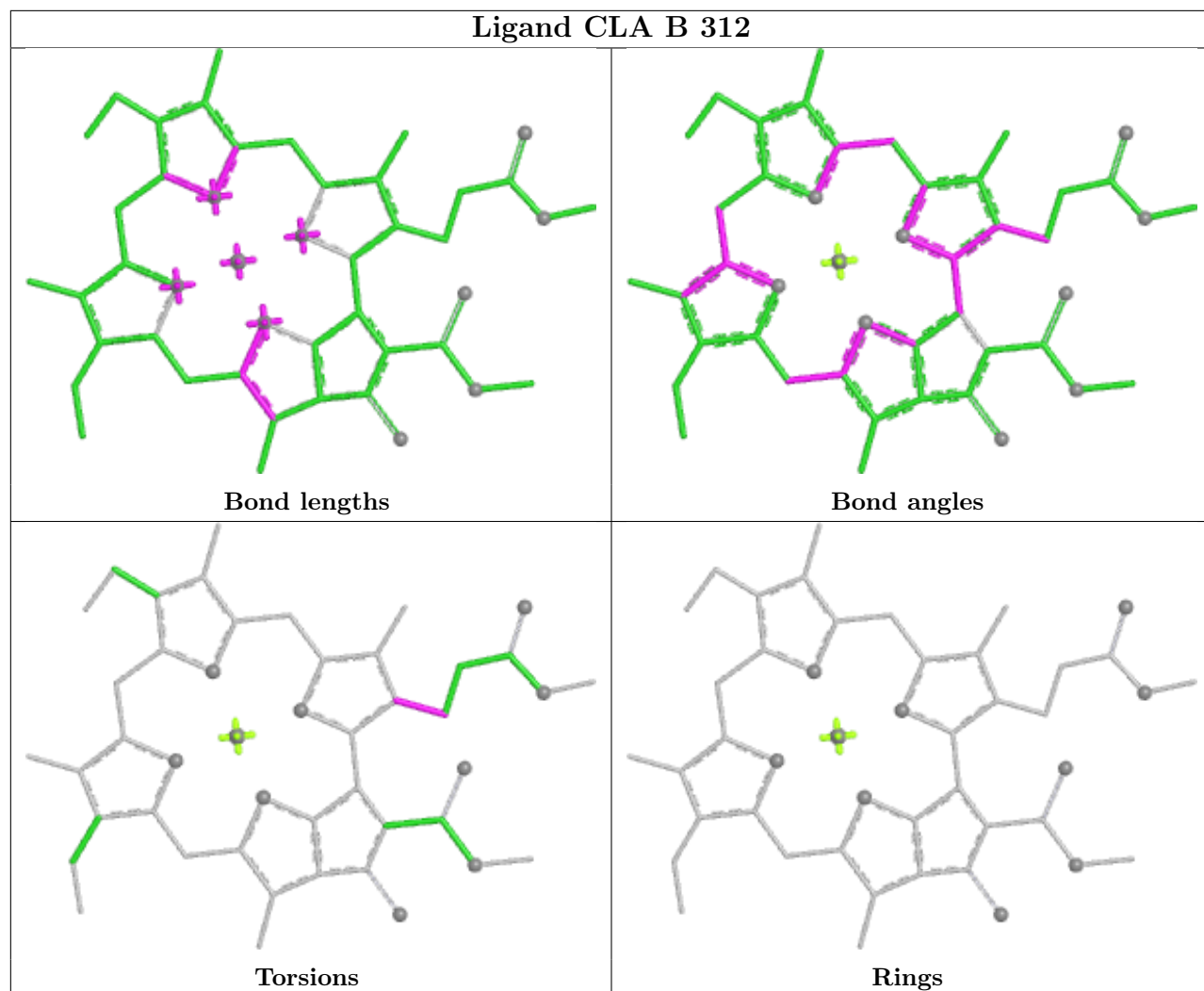




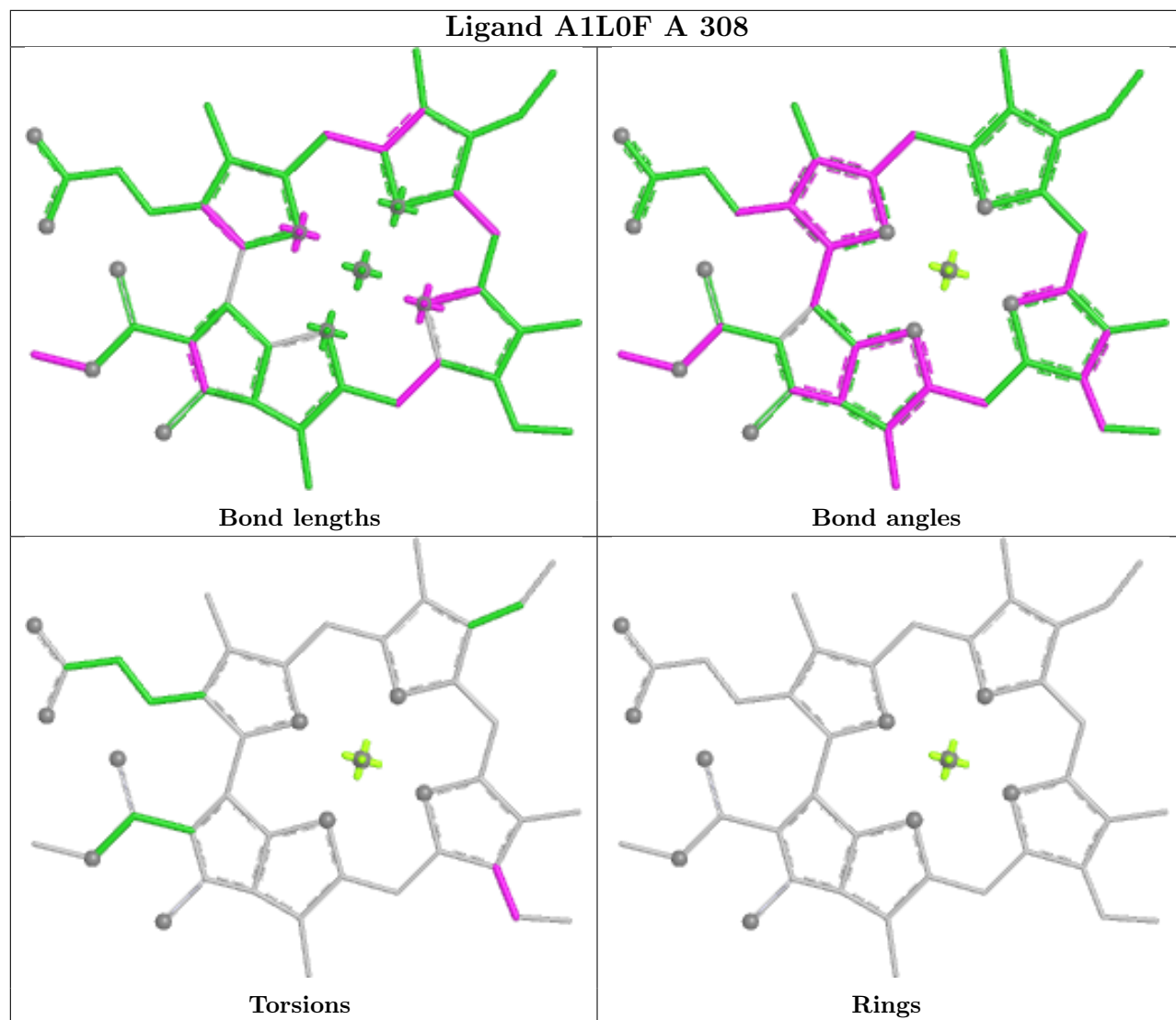


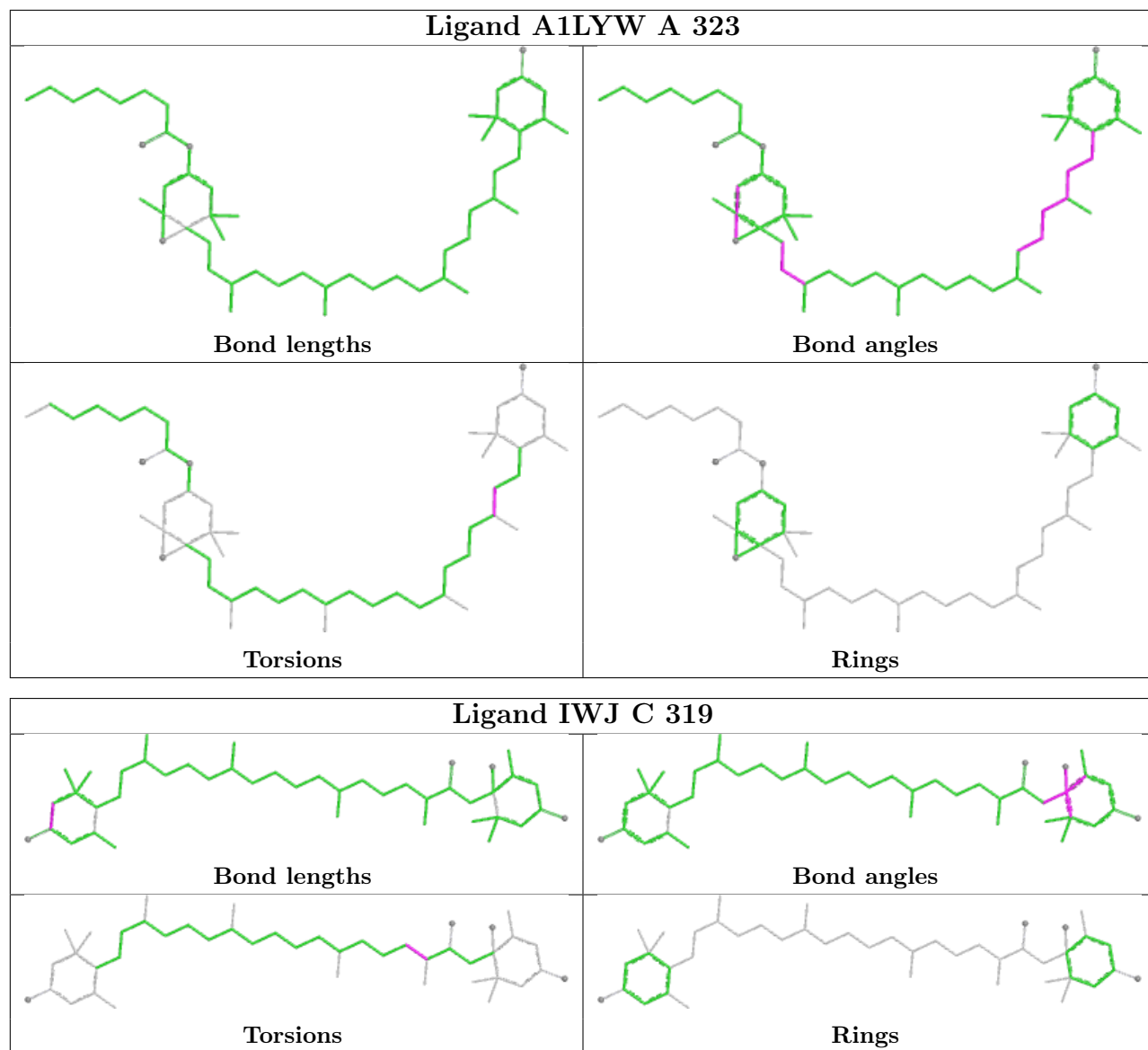




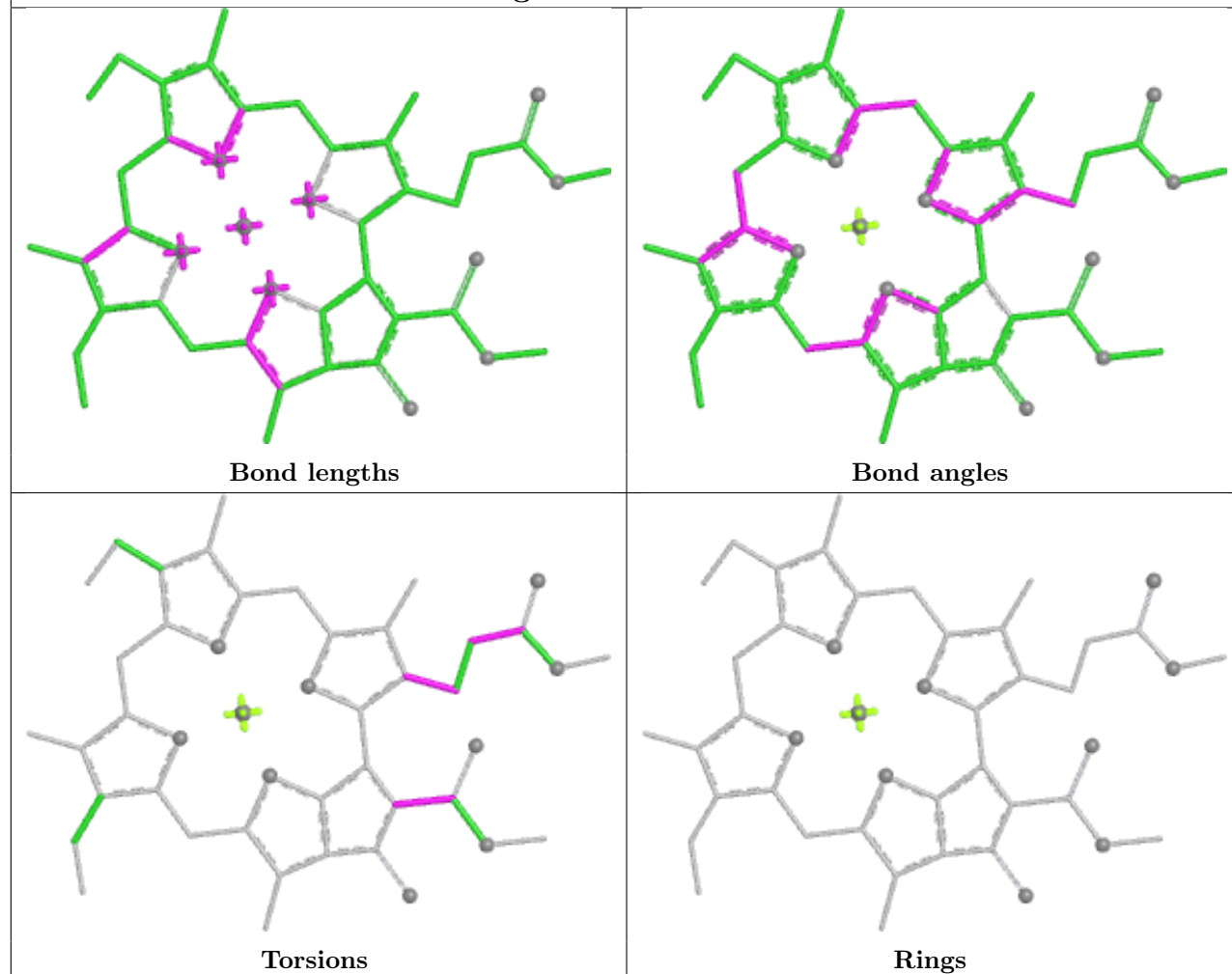


Ligand A1L0F A 308

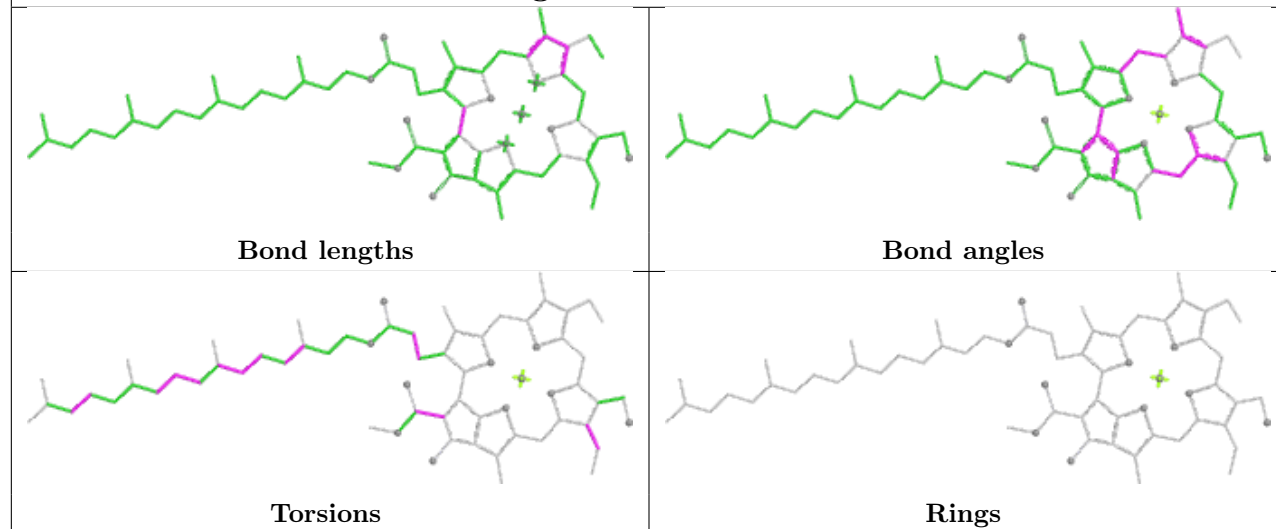


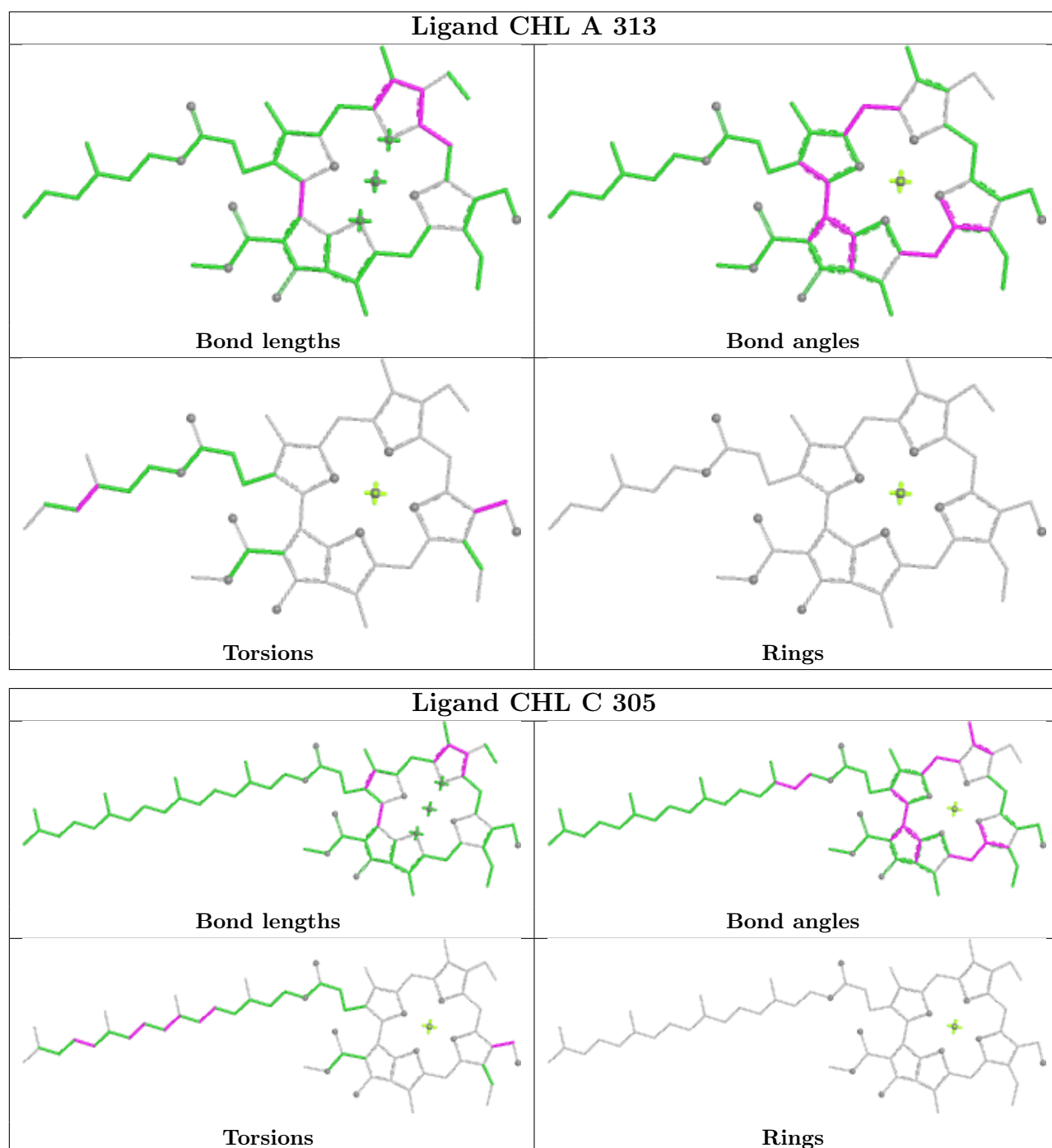


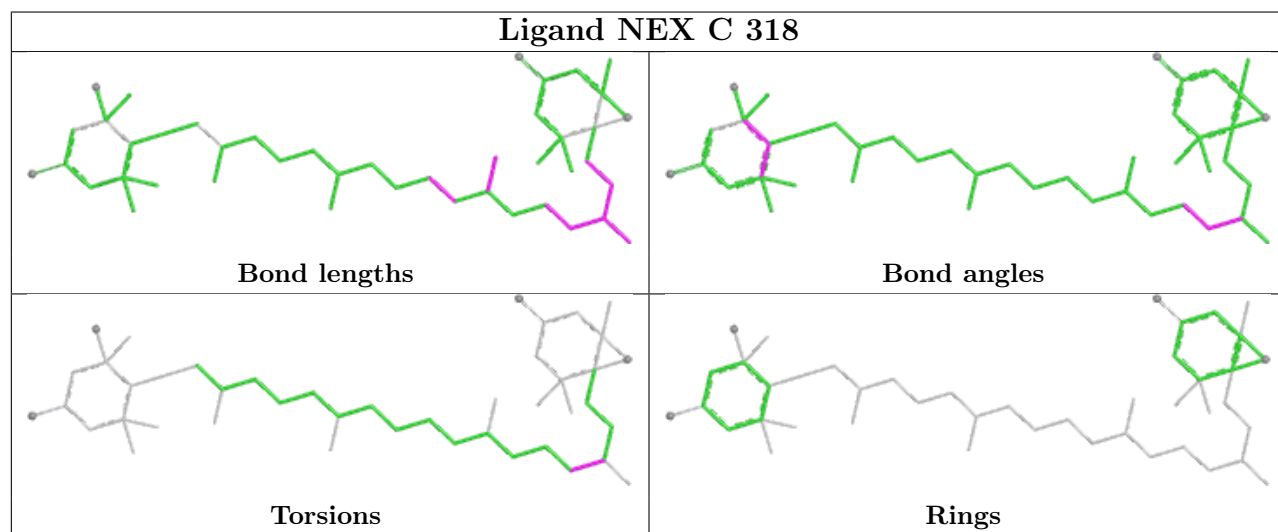
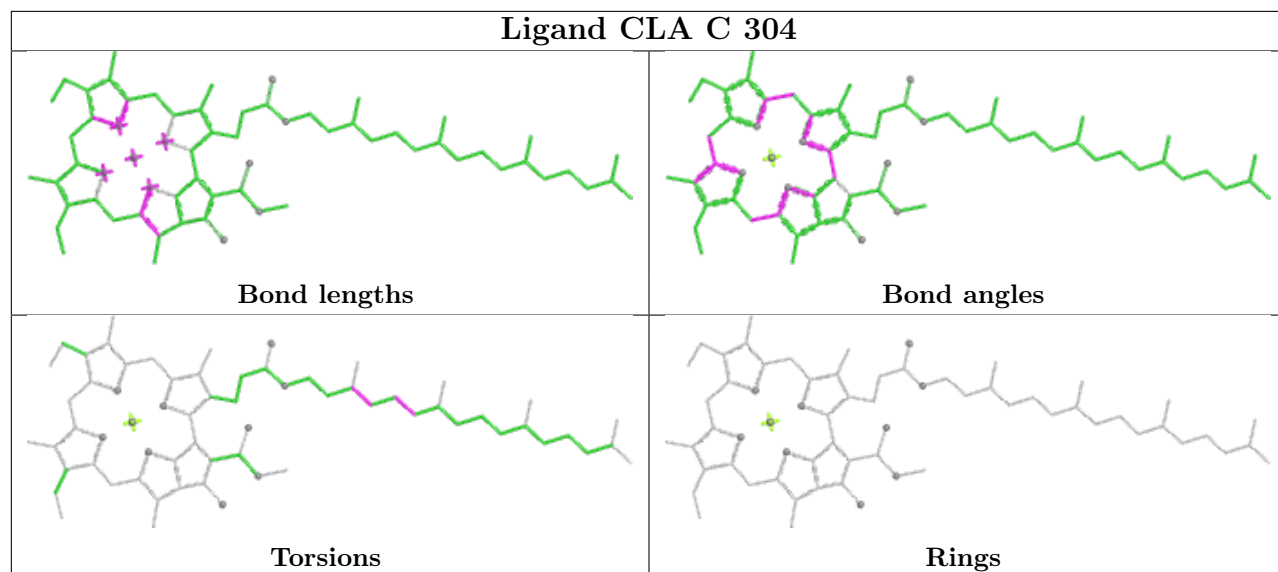
Ligand CLA A 311

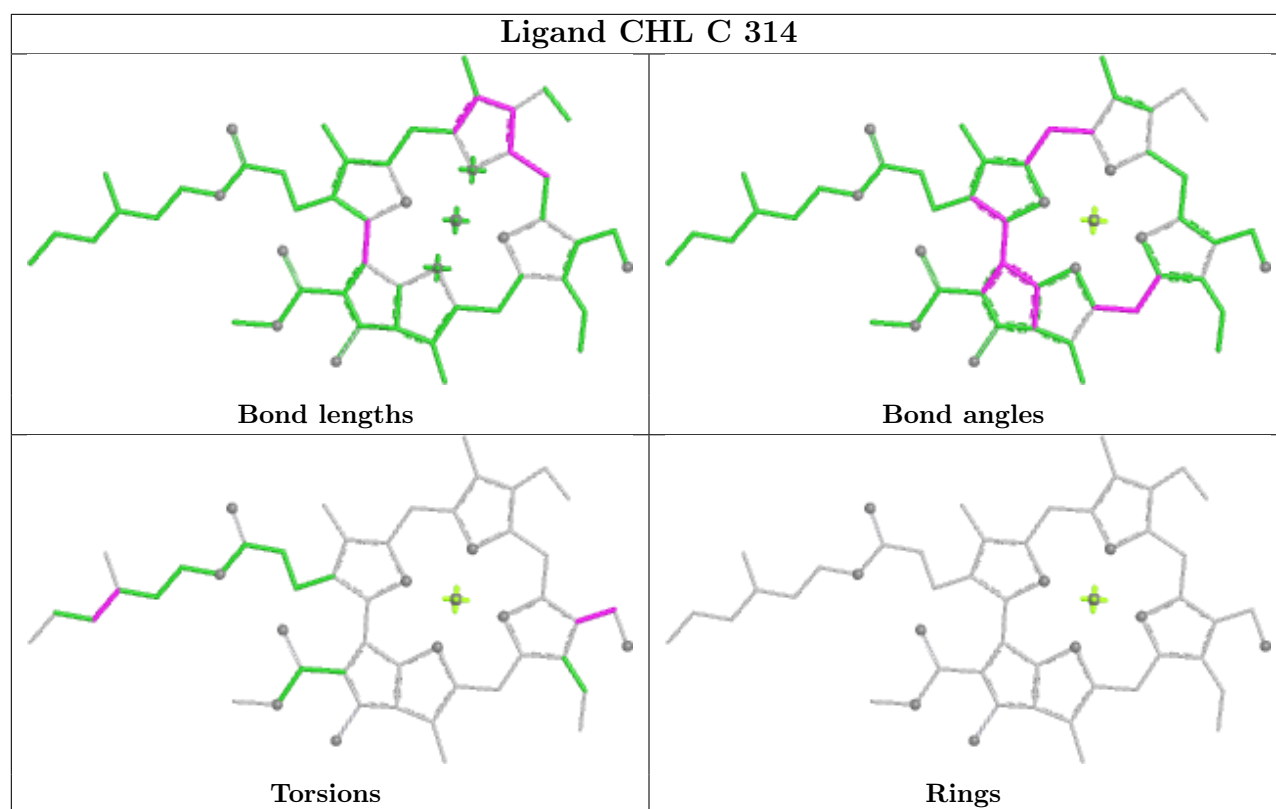


Ligand CHL C 307









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.

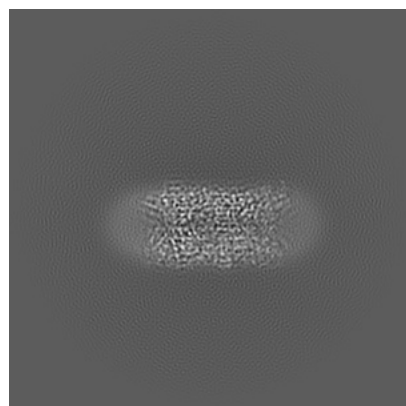
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-64036. These allow visual inspection of the internal detail of the map and identification of artifacts.

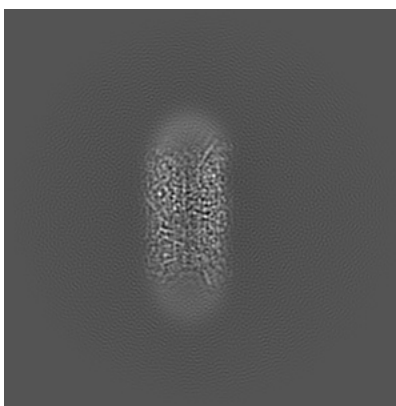
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

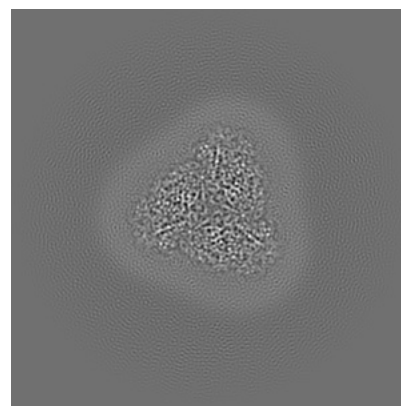
6.1.1 Primary map



X

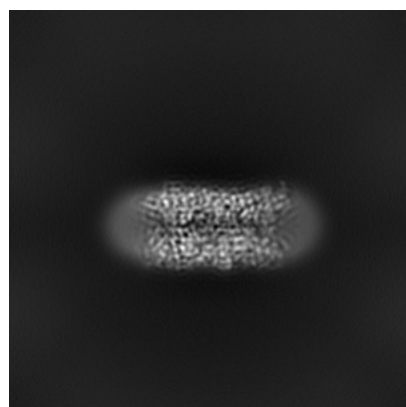


Y

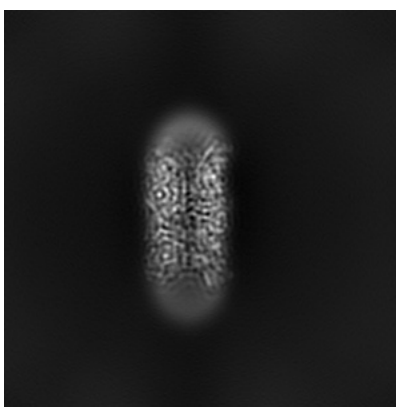


Z

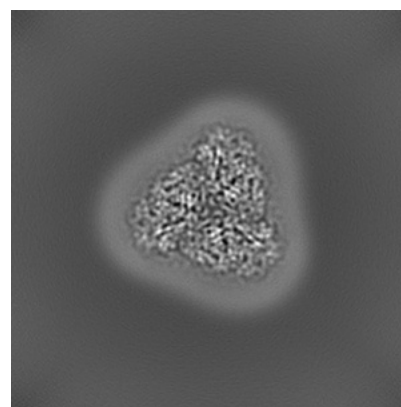
6.1.2 Raw map



X



Y

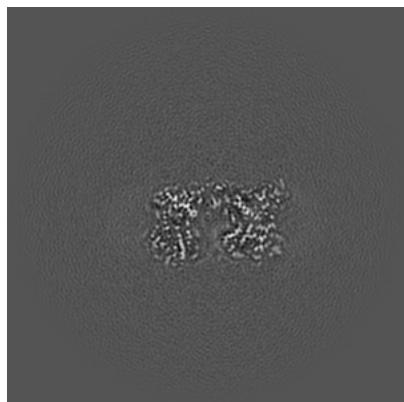


Z

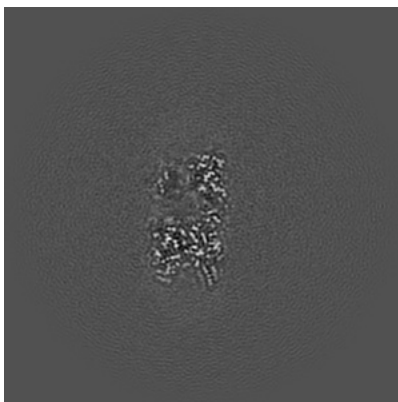
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

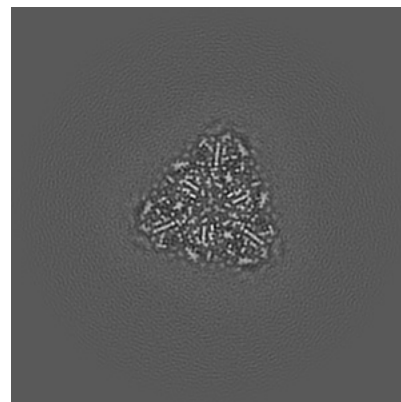
6.2.1 Primary map



X Index: 128

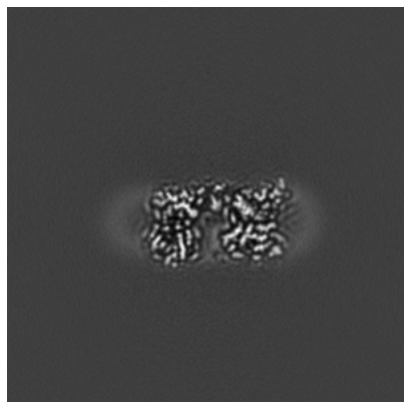


Y Index: 128

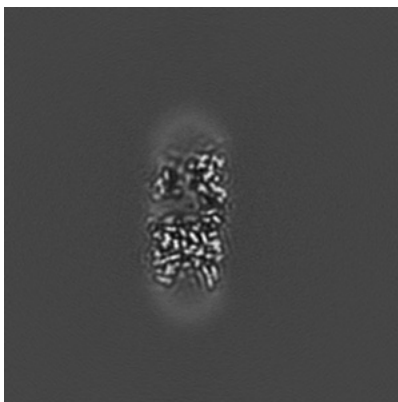


Z Index: 128

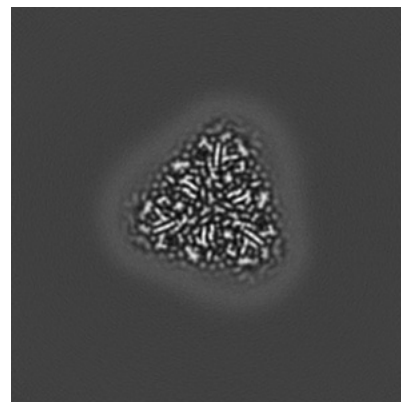
6.2.2 Raw map



X Index: 128



Y Index: 128

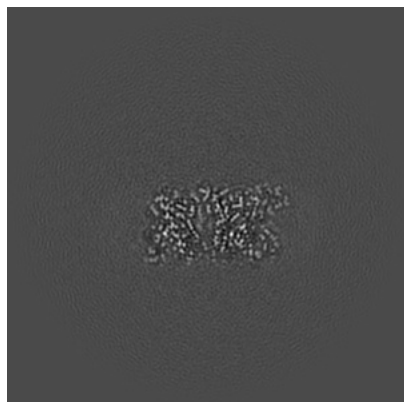


Z Index: 128

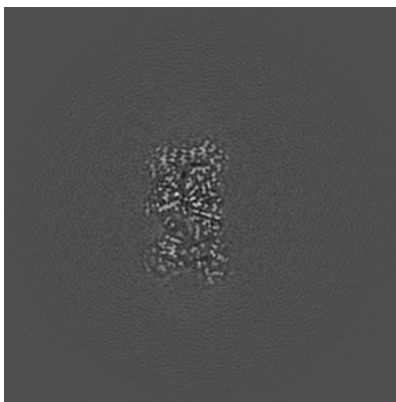
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

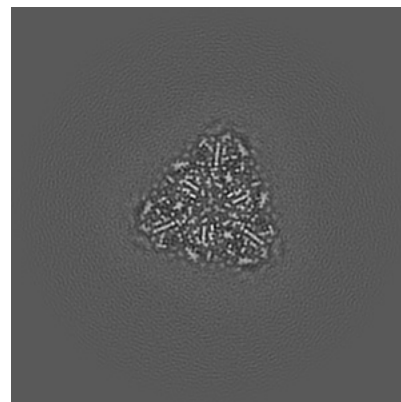
6.3.1 Primary map



X Index: 139

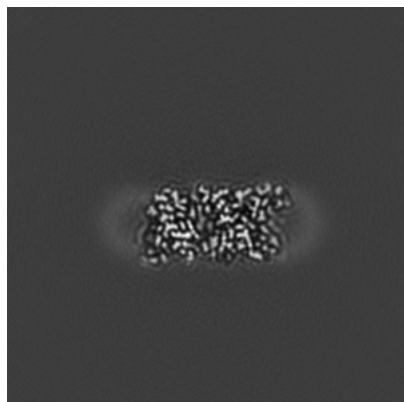


Y Index: 111

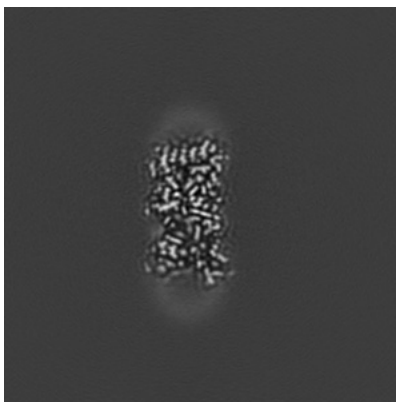


Z Index: 128

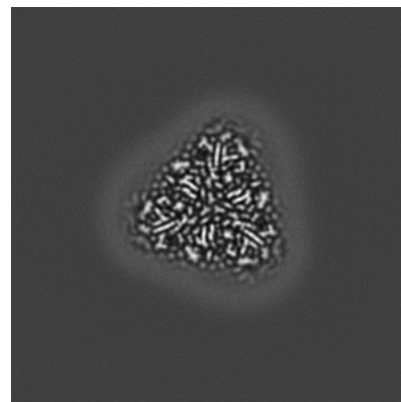
6.3.2 Raw map



X Index: 140



Y Index: 111

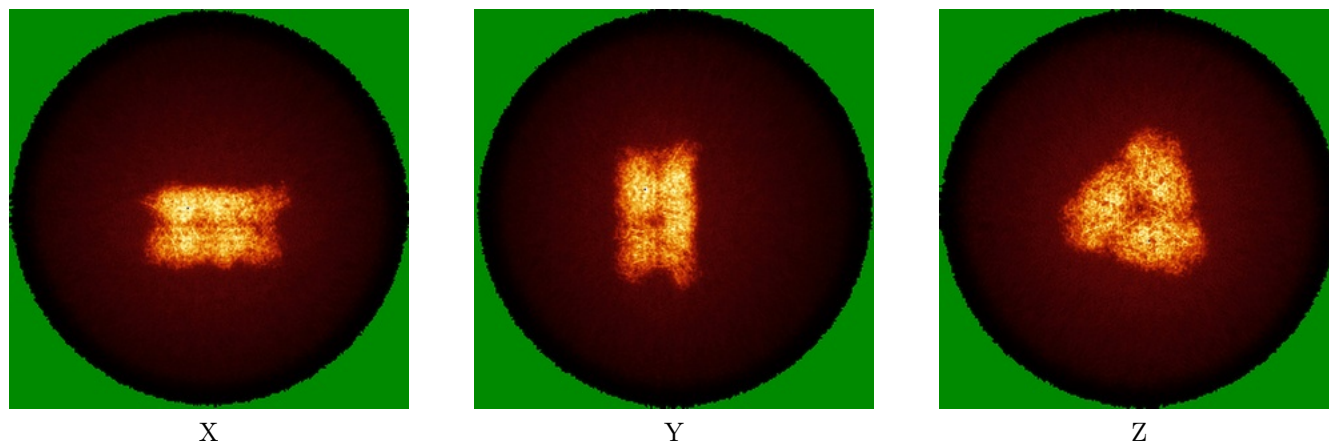


Z Index: 128

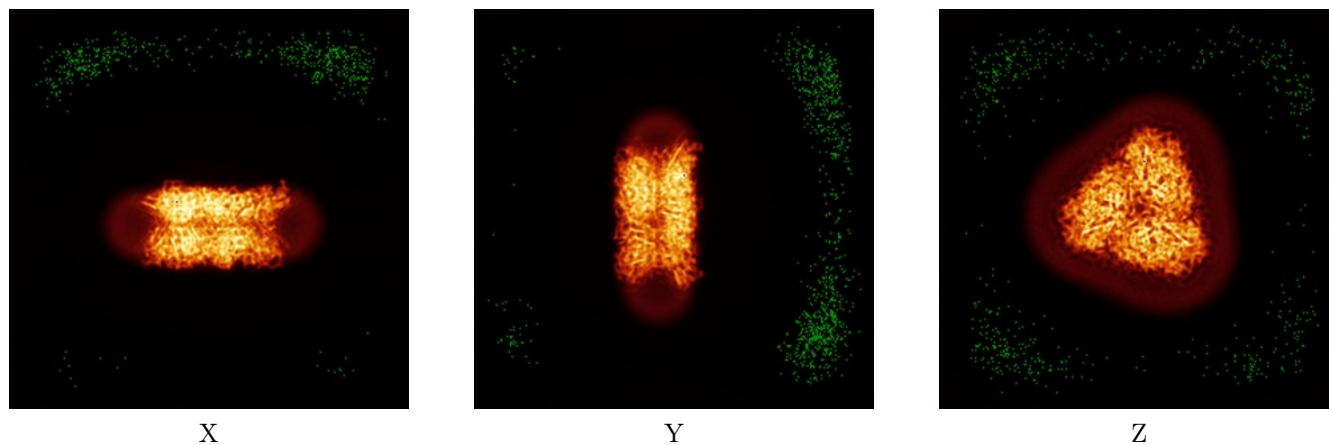
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



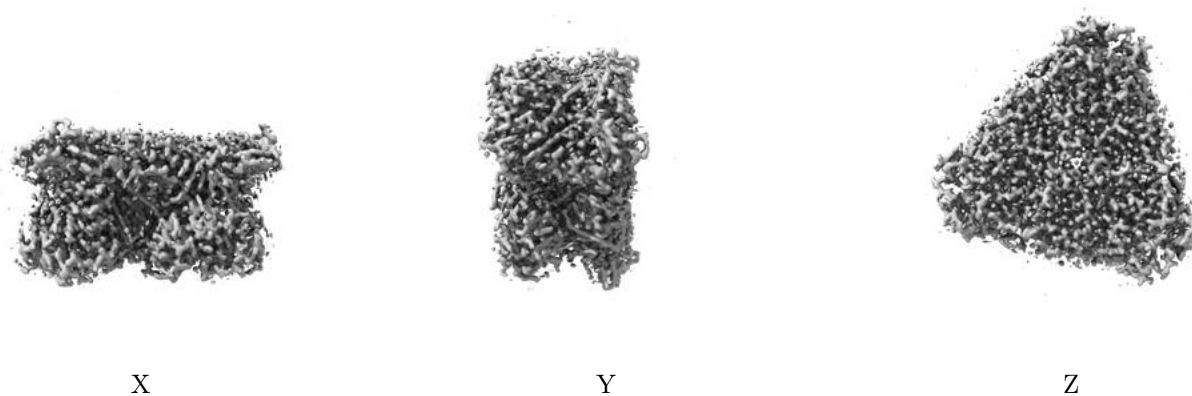
6.4.2 Raw map



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](#)

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.

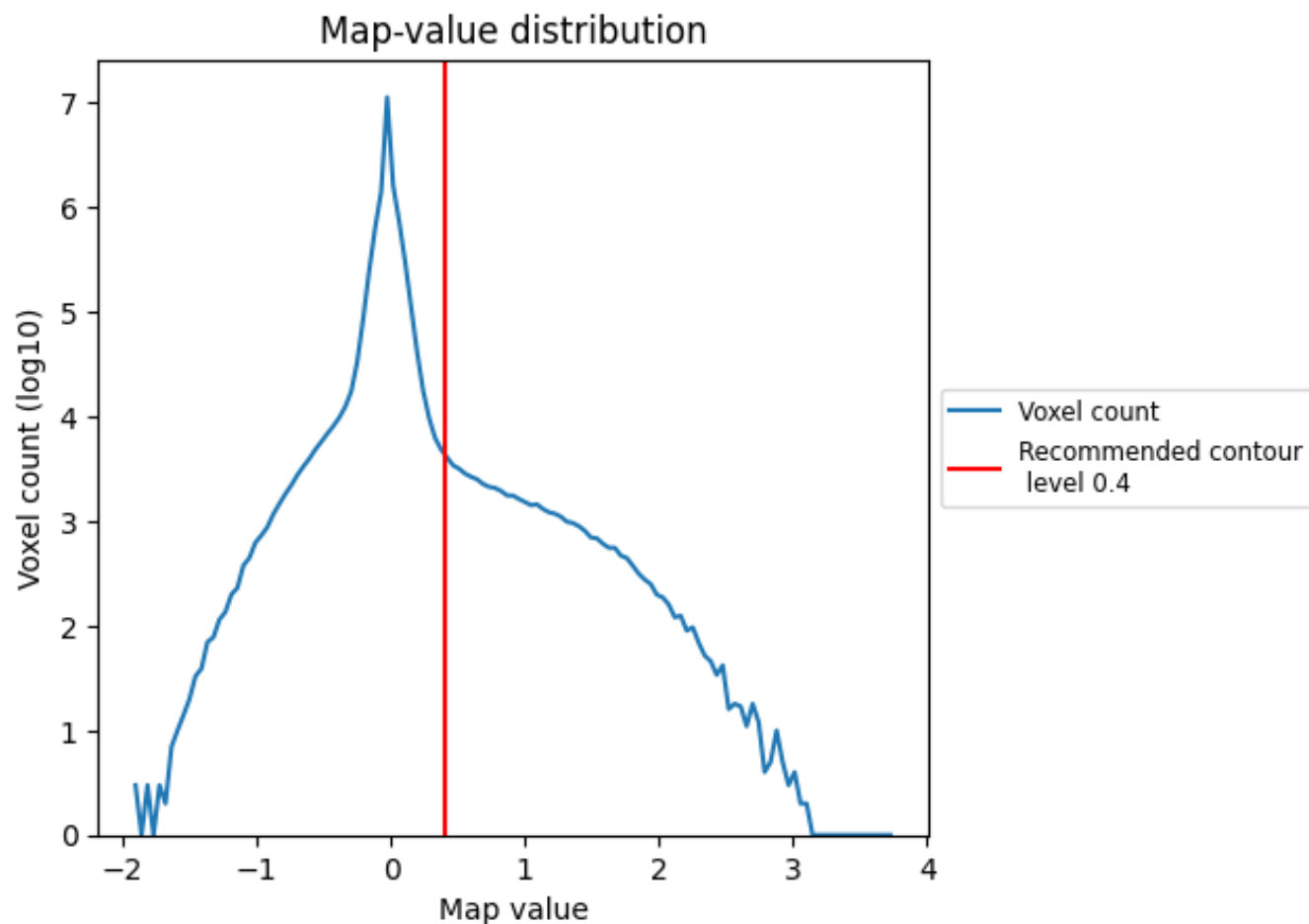
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

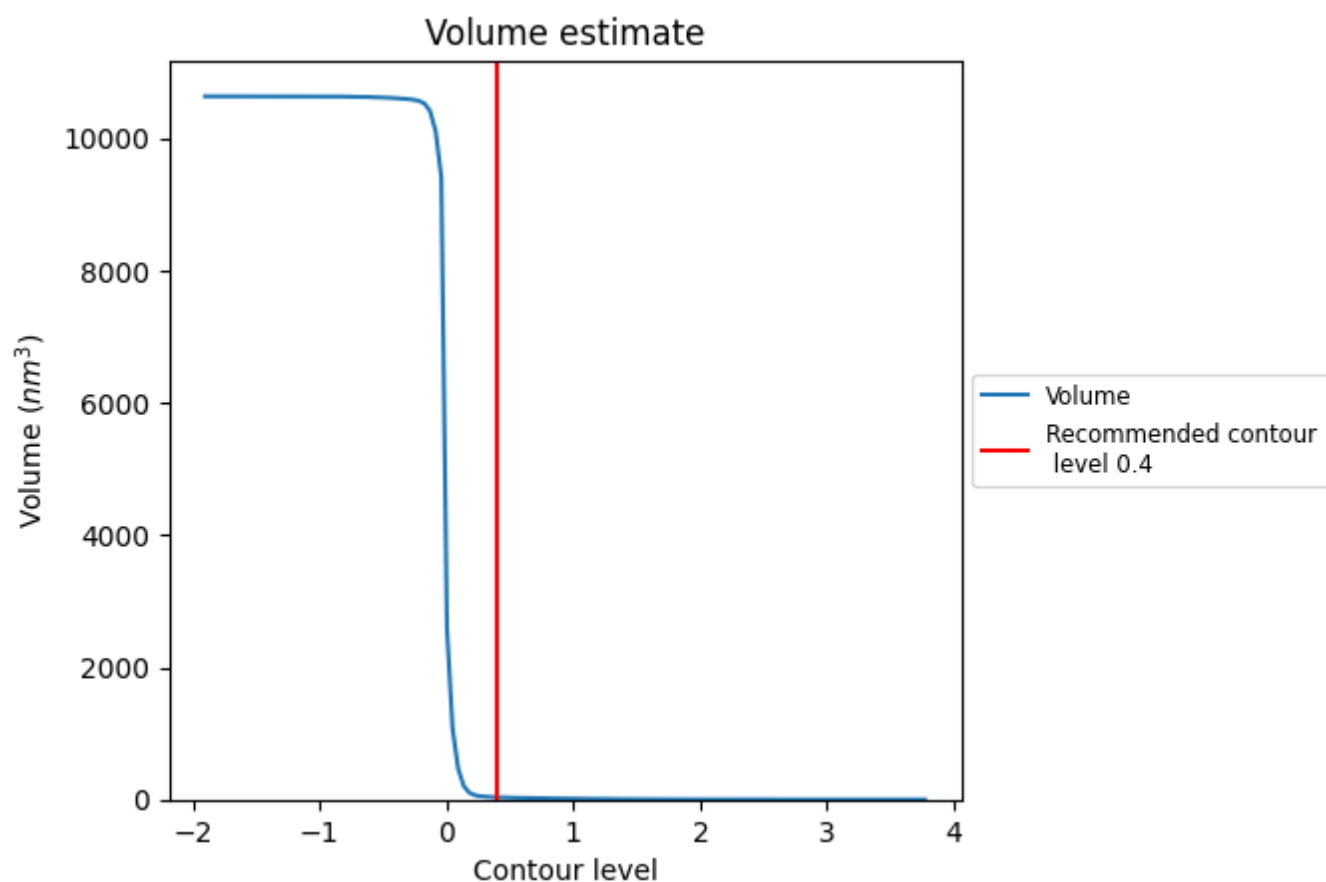
This section contains the results of statistical analysis of the map.

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.

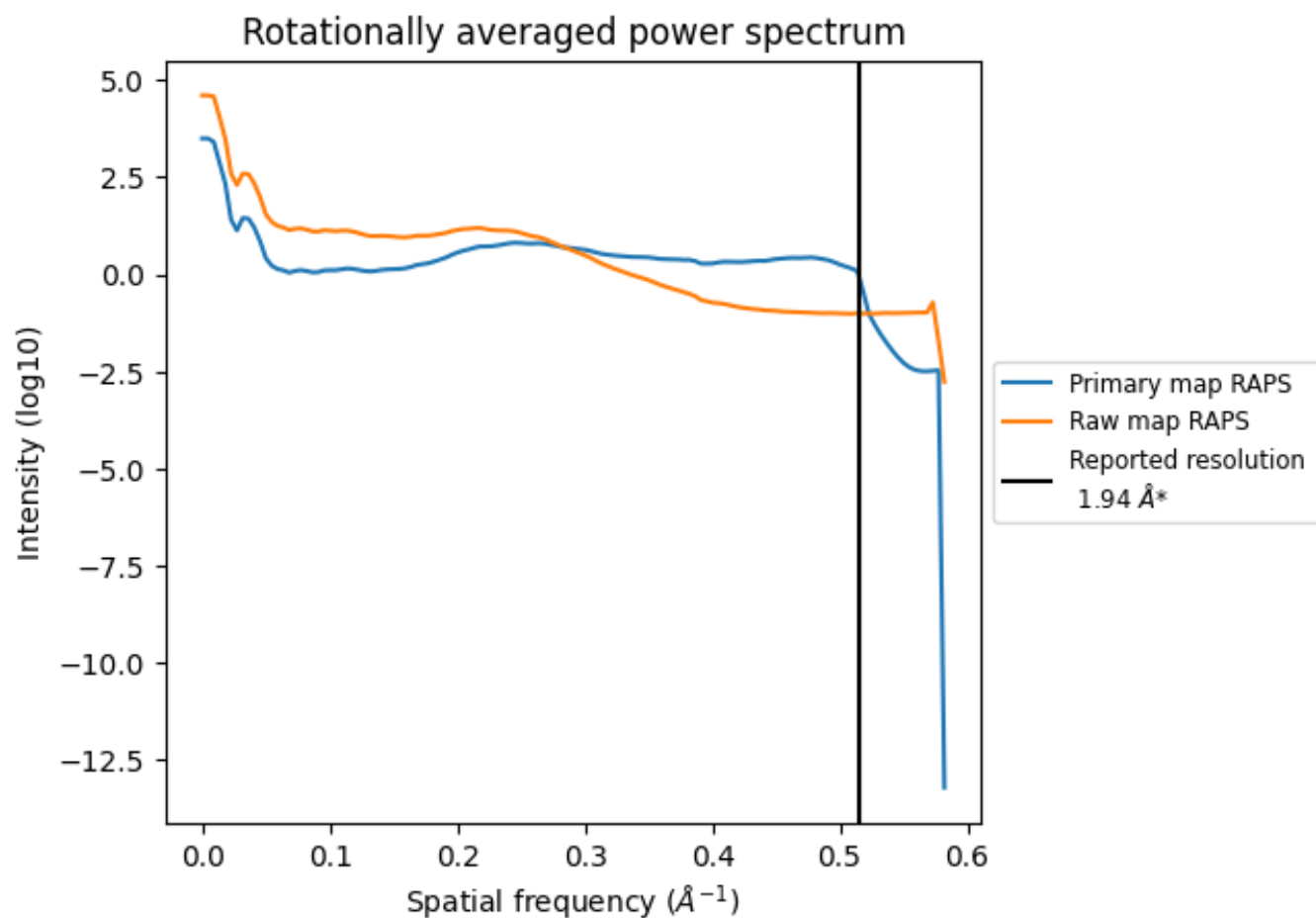
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 34 nm^3 ; this corresponds to an approximate mass of 31 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 ⓘ

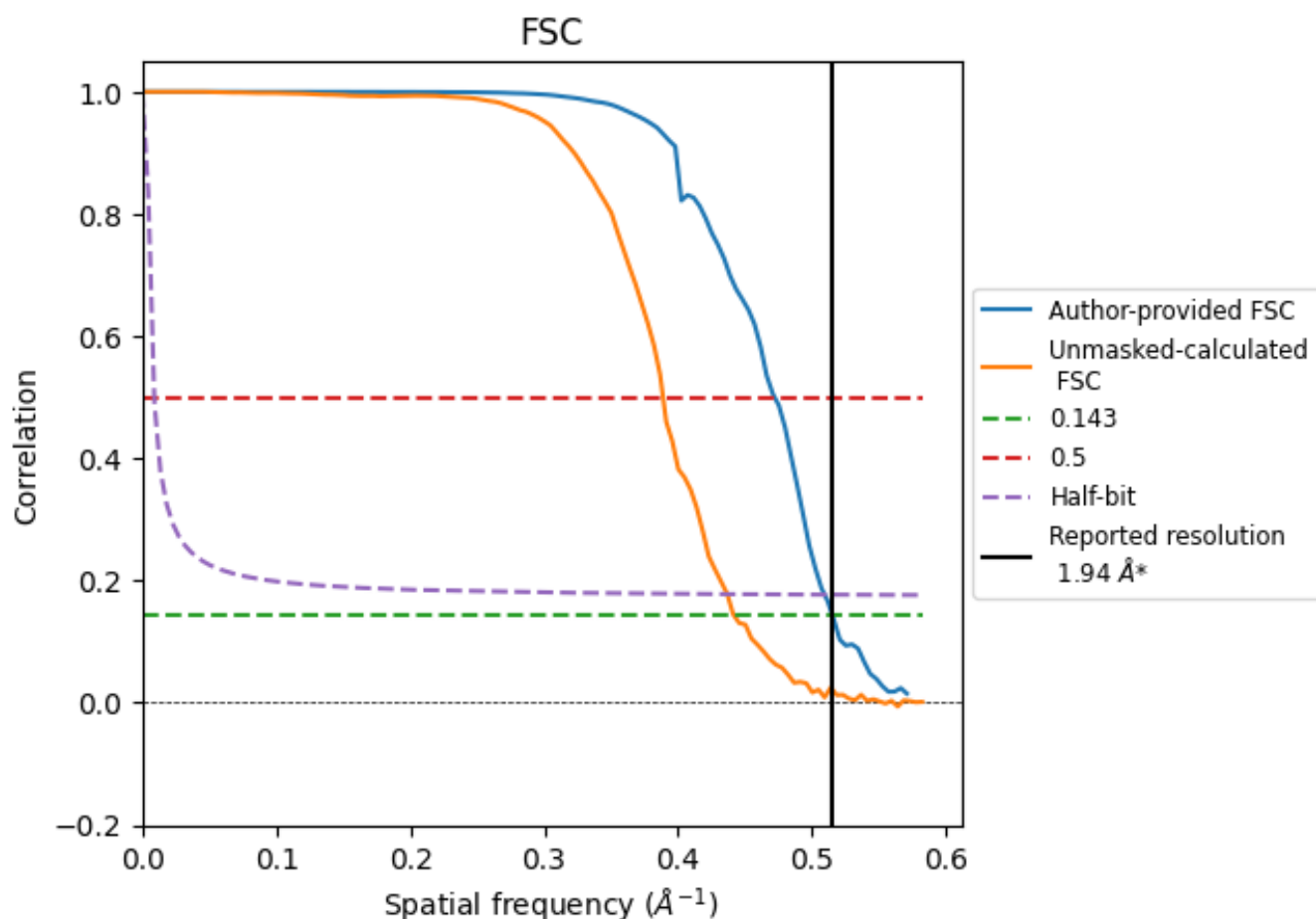


*Reported resolution corresponds to spatial frequency of 0.515 Å⁻¹

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 0.515 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	1.94	-	-
Author-provided FSC curve	1.94	2.12	1.96
Unmasked-calculated*	2.26	2.57	2.29

*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 2.26 differs from the reported value 1.94 by more than 10 %

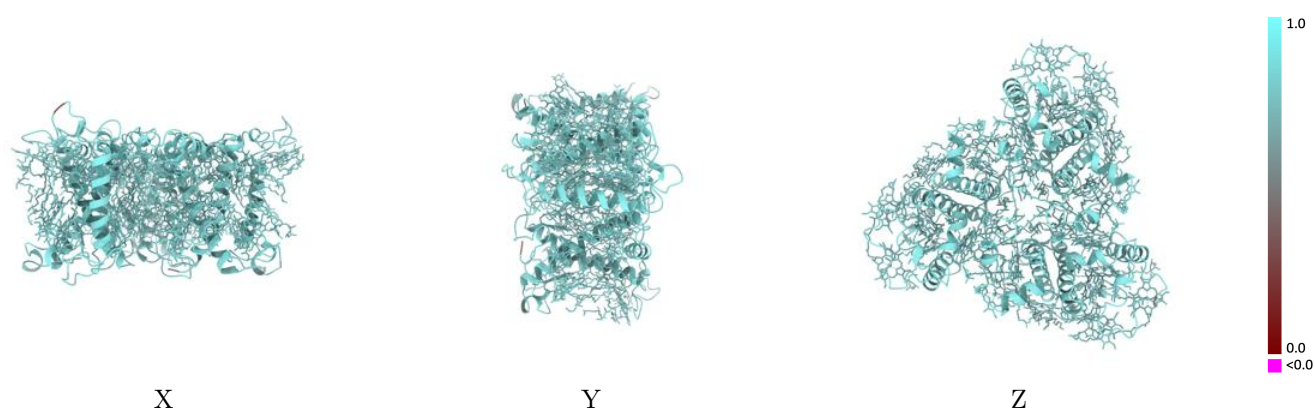
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-64036 and PDB model 9UC6. Per-residue inclusion information can be found in section 3 on page 15.

9.1 Map-model overlay [i](#)

This section was not generated.

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

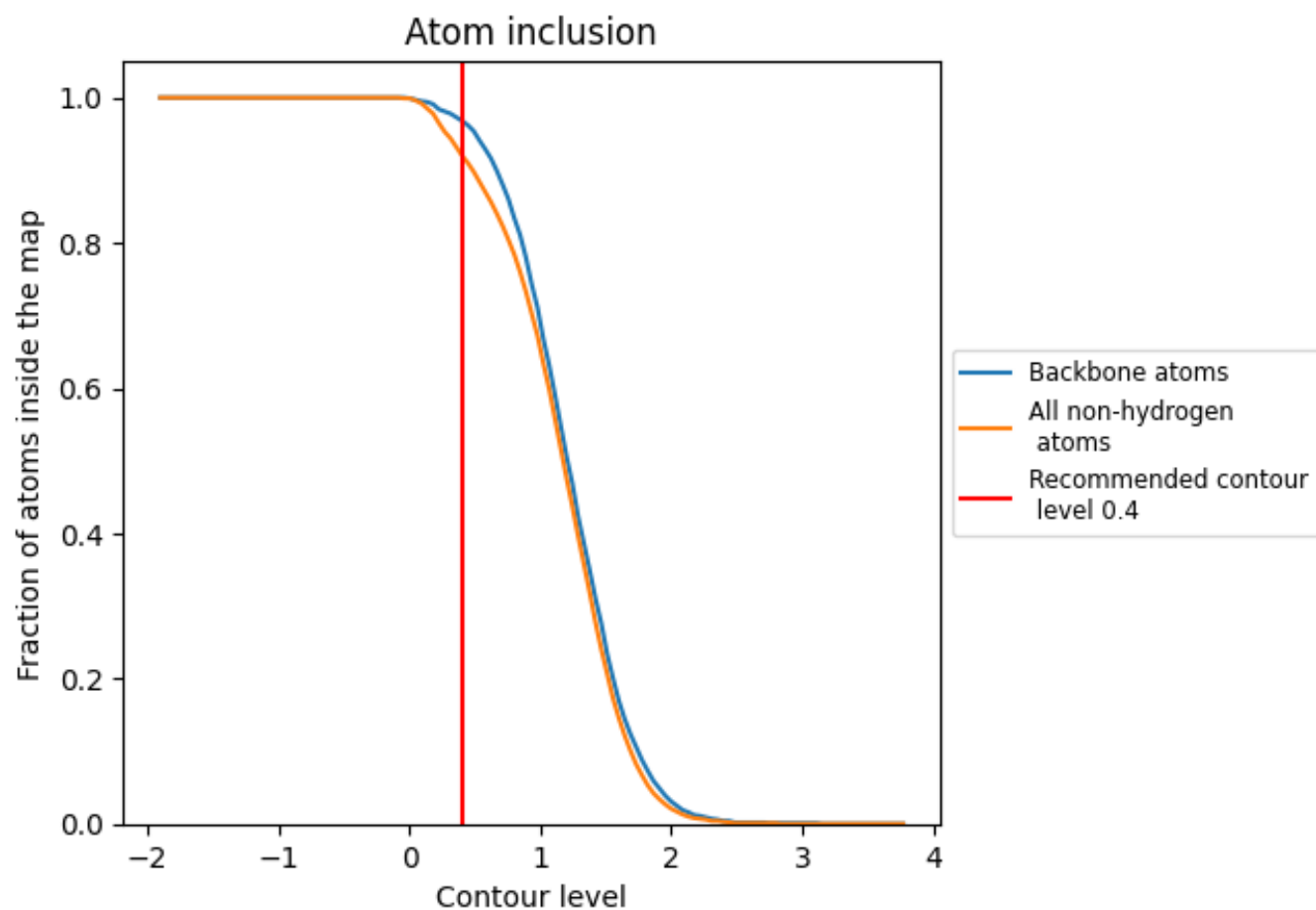


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 92% 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	0.9210	0.7700
A	0.9200	0.7710
B	0.9140	0.7690
C	0.9170	0.7700

