



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 04:51 AM UTC

PDB ID : 9MCC / pdb_00009mcc
EMDB ID : EMD-63799
Title : Cryo-EM structure of violaxanthin-chlorophyll-a-binding protein with red shifted Chl a (rVCP) from Trachydiscus minutus at 2.4 angstrom
Authors : Seki, S.; Litvin, R.; Bina, D.; Tanaka, H.; Miyata, T.; Namba, K.; Kurisu, G.; Polivka, T.; Fujii, R.
Deposited on : 2025-03-17
Resolution : 2.42 Å(reported)
Based on initial model : 1RWT

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

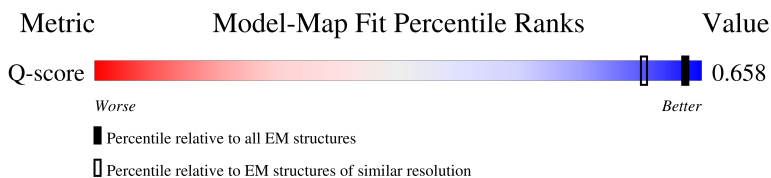
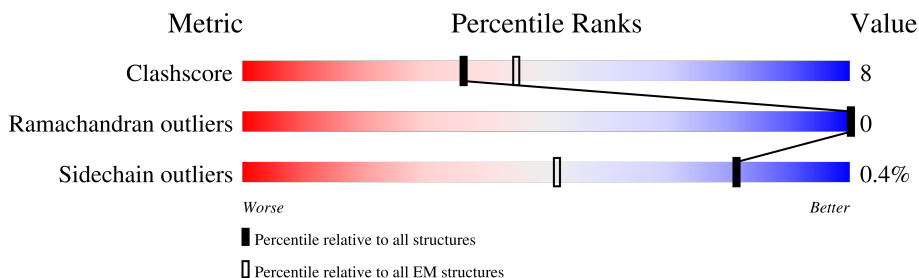
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.42 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	5729 (1.92 - 2.92)

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	229	 65% 10% 25%
1	C	229	 64% 11% 25%
2	B	221	 65% 16% 19%

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Mol	Chain	Length	Quality of chain
2	D	221	

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
3	CLA	A	201	X	-	-	-
3	CLA	A	202	X	-	-	-
3	CLA	A	203	X	-	-	-
3	CLA	A	204	X	-	-	-
3	CLA	A	205	X	-	-	-
3	CLA	A	206	X	-	-	-
3	CLA	A	207	X	-	-	-
3	CLA	A	208	X	-	-	-
3	CLA	A	209	X	-	-	-
3	CLA	A	210	X	-	-	-
3	CLA	A	211	X	-	-	-
3	CLA	A	212	X	-	-	-
3	CLA	B	301	X	-	-	-
3	CLA	B	302	X	-	-	-
3	CLA	B	303	X	-	-	-
3	CLA	B	304	X	-	-	-
3	CLA	B	305	X	-	-	-
3	CLA	B	306	X	-	-	-
3	CLA	B	307	X	-	-	-
3	CLA	B	308	X	-	-	-
3	CLA	B	309	X	-	-	-
3	CLA	B	310	X	-	-	-
3	CLA	B	311	X	-	-	-
3	CLA	C	201	X	-	-	-
3	CLA	C	202	X	-	-	-
3	CLA	C	203	X	-	-	-
3	CLA	C	204	X	-	-	-
3	CLA	C	205	X	-	-	-
3	CLA	C	206	X	-	-	-
3	CLA	C	207	X	-	-	-
3	CLA	C	208	X	-	-	-
3	CLA	C	209	X	-	-	-
3	CLA	C	210	X	-	-	-
3	CLA	C	211	X	-	-	-
3	CLA	C	212	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CLA	D	301	X	-	-	-
3	CLA	D	302	X	-	-	-
3	CLA	D	303	X	-	-	-
3	CLA	D	304	X	-	-	-
3	CLA	D	305	X	-	-	-
3	CLA	D	306	X	-	-	-
3	CLA	D	307	X	-	-	-
3	CLA	D	308	X	-	-	-
3	CLA	D	309	X	-	-	-
3	CLA	D	310	X	-	-	-
3	CLA	D	311	X	-	-	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 8978 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.

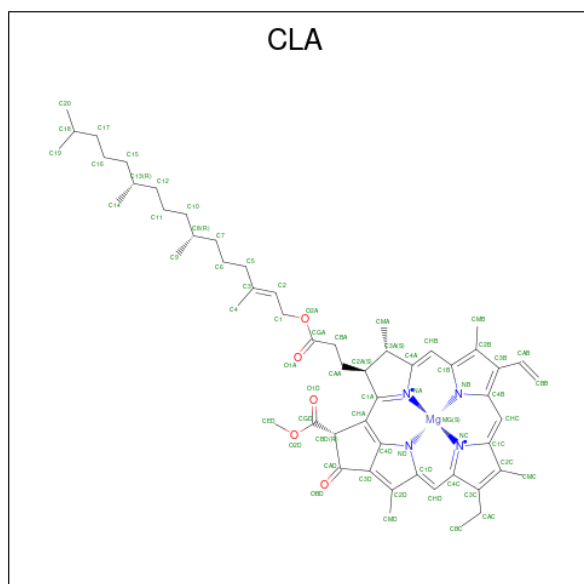
- Molecule 1 is a protein called Light-harvesting complex.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	172	Total	C	N	O	S	0	0
			1311	859	209	240	3		
1	C	172	Total	C	N	O	S	0	0
			1311	859	209	240	3		

- Molecule 2 is a protein called light-harvesting complex.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	178	Total	C	N	O	S	0	0
			1392	913	229	247	3		
2	D	178	Total	C	N	O	S	0	0
			1392	913	229	247	3		

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



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
3	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	A	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
3	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
3	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
3	A	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
3	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
3	A	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
3	A	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
3	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
3	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	B	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
3	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	B	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
3	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	B	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
3	B	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
3	B	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
3	B	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
3	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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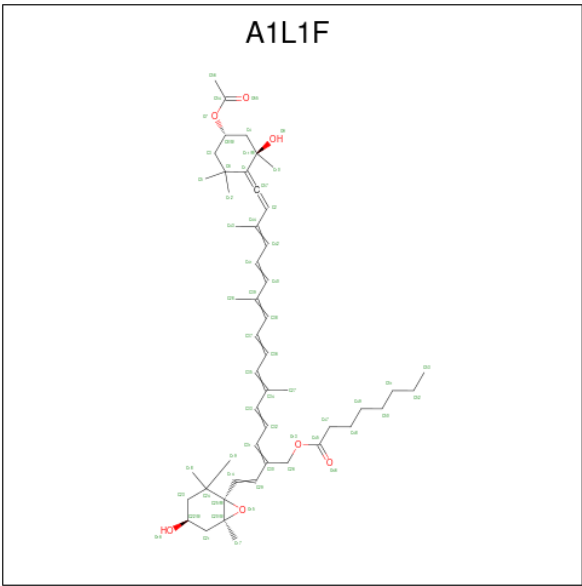
Mol	Chain	Residues	Atoms					AltConf
3	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
3	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	C	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
3	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	C	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
3	C	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
3	C	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
3	C	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
3	C	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
3	C	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
3	C	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
3	C	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
3	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	D	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
3	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	D	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
3	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	D	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
3	D	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
3	D	1	Total	C	Mg	N	O	0
			52	42	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
3	D	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
3	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	D	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

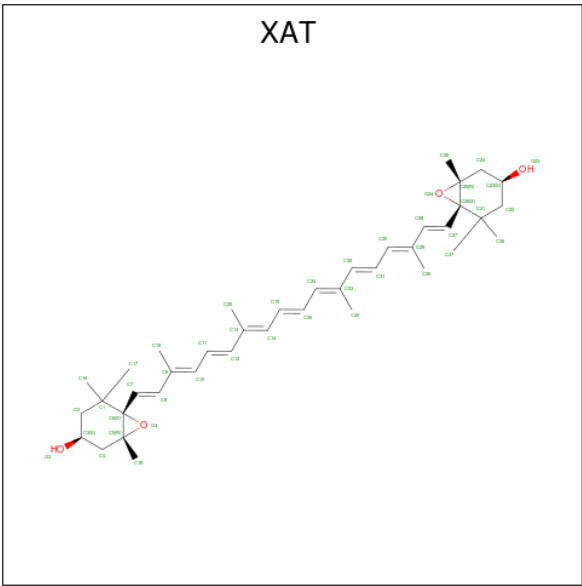
- Molecule 4 is [(2 {Z},4 {E},6 {E},8 {E},10 {E},12 {E},14 {E})-17-[(4 {S},6 {R})-4-acetyloxy-2,2,6-trimethyl-6-oxidanyl-cyclohexylidene]-6,11,15-trimethyl-2-[({E})-2-[(1 {S},4 {S},6 {R})-2,2,6-trimethyl-4-oxidanyl-7-oxabicyclo[4.1.0]heptan-1-yl]ethenyl]heptadeca-2,4,6,8,10,12,14,16-octaenyl] octanoate (CCD ID: A1L1F) (formula: C₅₀H₇₂O₇).



Mol	Chain	Residues	Atoms			AltConf
4	A	1	Total	C	O	0
			57	50	7	
4	A	1	Total	C	O	0
			57	50	7	
4	B	1	Total	C	O	0
			57	50	7	
4	C	1	Total	C	O	0
			57	50	7	
4	C	1	Total	C	O	0
			57	50	7	
4	D	1	Total	C	O	0
			57	50	7	

- Molecule 5 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA,

BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: C₄₀H₅₆O₄).



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	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	
5	D	1	Total	C	O	0
			44	40	4	
5	D	1	Total	C	O	0
			44	40	4	
5	D	1	Total	C	O	0
			44	40	4	

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		AltConf
6	A	19	Total	O	0
			19	19	

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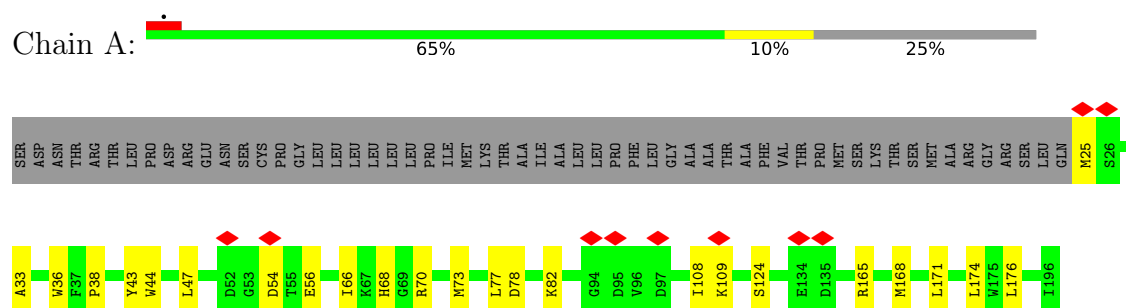
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Mol	Chain	Residues	Atoms		AltConf
6	B	15	Total 15	O 15	0
6	C	19	Total 19	O 19	0
6	D	15	Total 15	O 15	0

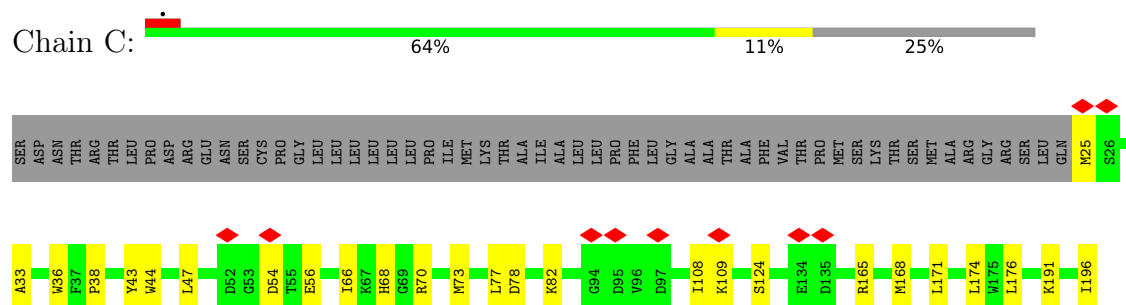
3 Residue-property plots

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.

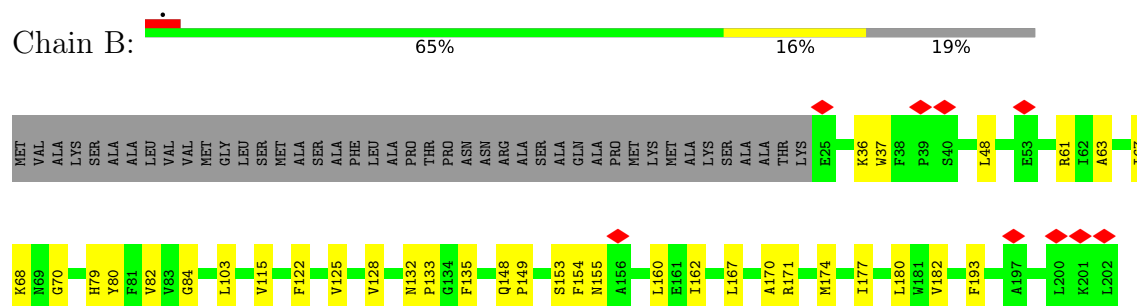
- Molecule 1: Light-harvesting complex



- Molecule 1: Light-harvesting complex

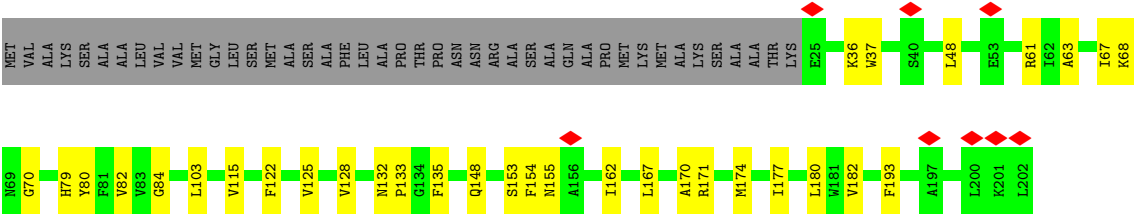


- Molecule 2: light-harvesting complex



- Molecule 2: light-harvesting complex





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	290174	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	80	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	60000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.538	Depositor
Minimum map value	-1.574	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.067	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	223.488, 223.488, 223.488	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.873, 0.873, 0.873	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: A1L1F, CLA, XAT

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.13	0/1353	0.31	0/1848
1	C	0.13	0/1353	0.31	0/1848
2	B	0.13	0/1440	0.28	0/1968
2	D	0.13	0/1440	0.28	0/1968
All	All	0.13	0/5586	0.29	0/7632

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	1311	0	1290	24	0
1	C	1311	0	1290	25	0
2	B	1392	0	1353	29	0
2	D	1392	0	1353	27	0
3	A	711	0	699	15	0
3	B	650	0	641	20	0
3	C	711	0	699	15	0
3	D	650	0	641	19	0
4	A	114	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	57	0	0	0	0
4	C	114	0	0	2	0
4	D	57	0	0	0	0
5	A	88	0	112	5	0
5	B	132	0	168	7	0
5	C	88	0	112	5	0
5	D	132	0	168	6	0
6	A	19	0	0	1	0
6	B	15	0	0	0	0
6	C	19	0	0	1	0
6	D	15	0	0	0	0
All	All	8978	0	8526	135	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 8.

All (135) 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:D:70:GLY:HA3	2:D:170:ALA:HB1	1.67	0.76
2:B:70:GLY:HA3	2:B:170:ALA:HB1	1.67	0.75
3:C:201:CLA:H51	3:C:202:CLA:HBA1	1.81	0.63
3:A:201:CLA:H51	3:A:202:CLA:HBA1	1.81	0.62
2:B:132:ASN:HB3	2:B:133:PRO:HD3	1.82	0.62
2:D:132:ASN:HB3	2:D:133:PRO:HD3	1.82	0.61
1:A:82:LYS:NZ	6:A:302:HOH:O	2.35	0.59
2:B:170:ALA:O	2:B:174:MET:HG3	2.03	0.58
1:C:82:LYS:NZ	6:C:302:HOH:O	2.35	0.58
2:D:170:ALA:O	2:D:174:MET:HG3	2.03	0.58
3:D:303:CLA:O1A	5:D:314:XAT:H35	2.04	0.58
3:B:303:CLA:O1A	5:B:314:XAT:H35	2.04	0.58
2:B:48:LEU:HD12	5:B:313:XAT:H221	1.85	0.57
2:B:115:VAL:HG13	3:B:310:CLA:H201	1.87	0.57
2:D:48:LEU:HD12	5:D:313:XAT:H221	1.85	0.57
2:D:115:VAL:HG13	3:D:310:CLA:H201	1.87	0.57
2:D:61:ARG:HH22	3:D:304:CLA:HBA1	1.70	0.55
1:A:66:ILE:O	1:A:70:ARG:HG3	2.07	0.55
2:B:61:ARG:HH22	3:B:304:CLA:HBA1	1.70	0.55
1:C:66:ILE:O	1:C:70:ARG:HG3	2.07	0.54
1:A:171:LEU:HD22	5:A:214:XAT:H30	1.92	0.52
2:B:79:HIS:HB2	3:B:303:CLA:C1C	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:68:HIS:HD2	5:C:214:XAT:H15	1.75	0.52
1:A:68:HIS:HD2	5:A:214:XAT:H35	1.75	0.52
1:C:171:LEU:HD22	5:C:214:XAT:H10	1.92	0.51
2:D:79:HIS:HB2	3:D:303:CLA:C1C	2.40	0.51
1:A:70:ARG:HA	1:A:73:MET:HE3	1.93	0.50
2:D:82:VAL:HG21	3:D:303:CLA:HAC2	1.93	0.50
1:C:124:SER:HB3	3:C:204:CLA:HAB	1.95	0.49
1:A:124:SER:HB3	3:A:204:CLA:HAB	1.94	0.49
1:C:38:PRO:HG2	2:D:135:PHE:HB2	1.94	0.49
1:C:70:ARG:HA	1:C:73:MET:HE3	1.93	0.49
1:A:78:ASP:HB2	3:A:203:CLA:C1C	2.43	0.49
1:A:165:ARG:HA	1:A:168:MET:HE3	1.95	0.49
2:B:82:VAL:HG21	3:B:303:CLA:HAC2	1.93	0.48
1:A:38:PRO:HG2	2:B:135:PHE:HB2	1.94	0.48
1:C:165:ARG:HA	1:C:168:MET:HE3	1.95	0.48
1:C:78:ASP:HB2	3:C:203:CLA:C1C	2.43	0.48
3:A:209:CLA:H111	3:A:209:CLA:H72	1.66	0.47
3:C:205:CLA:H143	3:C:210:CLA:H141	1.97	0.47
3:C:209:CLA:C4B	2:D:128:VAL:HG22	2.45	0.47
1:A:25:MET:SD	1:A:43:TYR:OH	2.70	0.47
2:B:68:LYS:HD2	3:B:304:CLA:C3D	2.45	0.47
3:A:209:CLA:C4B	2:B:128:VAL:HG22	2.45	0.47
3:A:205:CLA:H143	3:A:210:CLA:H141	1.97	0.46
2:B:177:ILE:HA	2:B:180:LEU:HD12	1.97	0.46
3:B:301:CLA:H62	5:B:313:XAT:H28	1.97	0.46
1:C:171:LEU:HA	1:C:174:LEU:HD12	1.97	0.46
3:C:209:CLA:H52	2:D:125:VAL:HG22	1.97	0.46
2:B:80:TYR:HA	2:B:103:LEU:HD11	1.97	0.46
2:D:177:ILE:HA	2:D:180:LEU:HD12	1.97	0.46
2:B:155:ASN:O	3:B:305:CLA:HBA1	2.16	0.46
2:D:68:LYS:HD2	3:D:304:CLA:C3D	2.45	0.46
1:C:25:MET:SD	1:C:43:TYR:OH	2.70	0.46
1:C:70:ARG:HD2	3:C:205:CLA:C4C	2.46	0.46
1:A:171:LEU:HA	1:A:174:LEU:HD12	1.97	0.45
1:A:108:ILE:HG22	1:A:109:LYS:HE2	1.97	0.45
1:A:109:LYS:HA	1:A:109:LYS:HD3	1.74	0.45
1:C:168:MET:HG2	5:C:214:XAT:C15	2.46	0.45
2:D:80:TYR:HA	2:D:103:LEU:HD11	1.97	0.45
2:D:155:ASN:O	3:D:305:CLA:HBA1	2.16	0.45
3:D:301:CLA:H62	5:D:313:XAT:H28	1.97	0.45
1:A:70:ARG:HD2	3:A:205:CLA:C4C	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:210:CLA:H93	3:D:307:CLA:H71	1.99	0.45
3:A:209:CLA:H52	2:B:125:VAL:HG22	1.97	0.45
1:C:108:ILE:HG22	1:C:109:LYS:HE2	1.98	0.45
1:A:36:TRP:HE1	1:A:44:TRP:CD1	2.35	0.45
3:A:210:CLA:H3A	3:A:210:CLA:HBA2	1.44	0.45
1:A:168:MET:HG2	5:A:214:XAT:C35	2.46	0.45
3:B:306:CLA:HAC1	5:B:315:XAT:H27	1.99	0.45
2:B:182:VAL:HB	3:B:308:CLA:HBC3	1.98	0.45
2:D:148:GLN:HG2	2:D:154:PHE:CG	2.52	0.45
2:D:182:VAL:HB	3:D:308:CLA:HBC3	1.98	0.44
1:C:109:LYS:HD3	1:C:109:LYS:HA	1.74	0.44
3:A:204:CLA:H71	3:A:204:CLA:H111	1.83	0.44
3:B:305:CLA:HHD	3:B:310:CLA:HMC3	1.98	0.44
1:C:36:TRP:HE1	1:C:44:TRP:CD1	2.35	0.44
2:D:171:ARG:HA	2:D:174:MET:HE3	2.00	0.44
3:D:305:CLA:HHD	3:D:310:CLA:HMC3	1.98	0.44
3:B:306:CLA:H51	3:B:307:CLA:C3D	2.48	0.44
3:D:306:CLA:HAC1	5:D:315:XAT:H27	1.99	0.44
3:B:302:CLA:OBD	3:B:304:CLA:HAA2	2.18	0.44
2:B:84:GLY:HA3	2:B:193:PHE:CE2	2.53	0.44
3:C:210:CLA:H3A	3:C:210:CLA:HBA2	1.44	0.44
3:D:302:CLA:OBD	3:D:304:CLA:HAA2	2.18	0.43
1:A:73:MET:HG2	4:A:213:A1L1F:C37	2.48	0.43
3:D:306:CLA:H51	3:D:307:CLA:C3D	2.48	0.43
1:A:47:LEU:HD22	5:A:214:XAT:H172	2.00	0.43
2:B:171:ARG:HA	2:B:174:MET:HE3	2.00	0.43
3:B:307:CLA:H71	3:C:210:CLA:H93	1.99	0.43
2:B:148:GLN:HG2	2:B:154:PHE:CG	2.52	0.43
1:C:73:MET:HG2	4:C:213:A1L1F:C37	2.48	0.43
1:C:191:LYS:HG2	1:C:196:ILE:HG13	2.01	0.43
2:D:63:ALA:O	2:D:67:ILE:HG13	2.19	0.43
3:A:212:CLA:H112	3:A:212:CLA:H151	1.89	0.42
2:B:79:HIS:HB2	3:B:303:CLA:CHC	2.49	0.42
2:B:162:ILE:HD12	2:B:162:ILE:HA	1.91	0.42
1:C:47:LEU:HD22	5:C:214:XAT:H372	2.00	0.42
3:C:204:CLA:H71	3:C:204:CLA:H111	1.83	0.42
3:C:209:CLA:H72	3:C:209:CLA:H111	1.66	0.42
2:D:79:HIS:HB2	3:D:303:CLA:CHC	2.49	0.42
2:D:84:GLY:HA3	2:D:193:PHE:CE2	2.53	0.42
2:D:122:PHE:CG	3:D:310:CLA:H143	2.54	0.42
2:B:122:PHE:CG	3:B:310:CLA:H143	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:HIS:HB3	1:A:168:MET:SD	2.59	0.42
1:C:68:HIS:HB3	1:C:168:MET:SD	2.59	0.42
3:D:310:CLA:H61	3:D:310:CLA:H41	1.78	0.42
2:D:67:ILE:HG12	2:D:167:LEU:HD21	2.02	0.42
2:B:67:ILE:HG12	2:B:167:LEU:HD21	2.02	0.42
1:A:54:ASP:C	1:A:56:GLU:H	2.28	0.41
2:B:63:ALA:O	2:B:67:ILE:HG13	2.19	0.41
1:C:176:LEU:HD23	1:C:176:LEU:HA	1.83	0.41
3:C:212:CLA:H62	3:C:212:CLA:H41	1.79	0.41
2:D:36:LYS:O	3:D:309:CLA:HMA3	2.21	0.41
2:B:48:LEU:HD12	5:B:313:XAT:H362	2.02	0.41
3:B:301:CLA:HBA1	5:B:313:XAT:H382	2.03	0.41
1:C:33:ALA:HB2	3:C:201:CLA:HED2	2.02	0.41
1:A:171:LEU:CD2	5:A:214:XAT:H30	2.50	0.41
2:D:48:LEU:HD12	5:D:313:XAT:H362	2.03	0.41
1:C:171:LEU:CD2	5:C:214:XAT:H10	2.50	0.41
1:A:33:ALA:HB2	3:A:201:CLA:HED2	2.02	0.41
2:D:162:ILE:HD12	2:D:162:ILE:HA	1.92	0.41
1:C:77:LEU:HB3	3:C:203:CLA:HMC2	2.02	0.41
2:D:37:TRP:CH2	5:D:315:XAT:H362	2.56	0.41
1:A:77:LEU:HB3	3:A:203:CLA:HMC2	2.02	0.41
2:B:160:LEU:HD23	2:B:160:LEU:HA	1.93	0.41
3:B:307:CLA:HBB1	3:B:307:CLA:HMB3	2.03	0.41
3:A:211:CLA:H43	4:A:215:A1L1F:C41	2.51	0.41
2:B:37:TRP:CH2	5:B:315:XAT:H362	2.56	0.41
1:C:54:ASP:C	1:C:56:GLU:H	2.28	0.40
1:A:176:LEU:HA	1:A:176:LEU:HD23	1.83	0.40
2:B:36:LYS:O	3:B:309:CLA:HMA3	2.21	0.40
3:C:211:CLA:H43	4:C:215:A1L1F:C41	2.51	0.40
3:D:307:CLA:HMB3	3:D:307:CLA:HBB1	2.03	0.40
2:B:149:PRO:HB2	3:B:310:CLA:HED1	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	170/229 (74%)	169 (99%)	1 (1%)	0	100	100
1	C	170/229 (74%)	169 (99%)	1 (1%)	0	100	100
2	B	176/221 (80%)	171 (97%)	5 (3%)	0	100	100
2	D	176/221 (80%)	171 (97%)	5 (3%)	0	100	100
All	All	692/900 (77%)	680 (98%)	12 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	134/182 (74%)	134 (100%)	0	100	100
1	C	134/182 (74%)	134 (100%)	0	100	100
2	B	144/174 (83%)	143 (99%)	1 (1%)	76	87
2	D	144/174 (83%)	143 (99%)	1 (1%)	76	87
All	All	556/712 (78%)	554 (100%)	2 (0%)	81	92

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	153	SER
2	D	153	SER

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

Mol	Chain	Res	Type
2	B	132	ASN
2	D	155	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

62 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	CLA	D	307	2	60,64,73	1.76	8 (13%)	71,102,113	1.15	9 (12%)
3	CLA	B	301	2	69,73,73	1.66	9 (13%)	82,113,113	1.09	8 (9%)
4	A1L1F	D	312	-	52,59,59	0.40	1 (1%)	63,85,85	0.80	3 (4%)
3	CLA	D	305	2	69,73,73	1.67	10 (14%)	82,113,113	1.07	7 (8%)
3	CLA	A	203	1	69,73,73	1.66	9 (13%)	82,113,113	1.08	9 (10%)
5	XAT	B	315	-	41,47,47	0.13	0	54,74,74	0.48	0
3	CLA	C	208	6	55,59,73	1.81	8 (14%)	64,96,113	1.18	9 (14%)
3	CLA	B	308	6	56,60,73	1.85	9 (16%)	65,97,113	1.21	8 (12%)
3	CLA	B	303	2	69,73,73	1.64	8 (11%)	82,113,113	1.07	9 (10%)
3	CLA	D	310	2	69,73,73	1.68	10 (14%)	82,113,113	1.16	9 (10%)
3	CLA	C	209	1	65,69,73	1.75	9 (13%)	77,108,113	1.22	8 (10%)
4	A1L1F	A	213	-	52,59,59	0.43	1 (1%)	63,85,85	0.56	1 (1%)
5	XAT	A	216	-	41,47,47	0.15	0	54,74,74	0.50	0
3	CLA	D	308	6	56,60,73	1.85	9 (16%)	65,97,113	1.21	8 (12%)
3	CLA	C	205	1	64,68,73	1.71	8 (12%)	76,107,113	1.08	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	A1L1F	C	213	-	52,59,59	0.43	1 (1%)	63,85,85	0.56	1 (1%)
5	XAT	C	216	-	41,47,47	0.15	0	54,74,74	0.50	0
5	XAT	B	314	-	41,47,47	0.16	0	54,74,74	0.77	3 (5%)
3	CLA	A	207	1	56,60,73	1.80	8 (14%)	65,97,113	1.21	9 (13%)
3	CLA	A	204	1	65,69,73	1.74	8 (12%)	77,108,113	1.31	9 (11%)
3	CLA	A	211	1	59,63,73	1.84	9 (15%)	70,101,113	1.29	8 (11%)
3	CLA	B	309	2	61,65,73	1.82	9 (14%)	72,103,113	1.29	9 (12%)
3	CLA	A	202	1	64,68,73	1.71	9 (14%)	76,107,113	1.14	9 (11%)
3	CLA	A	206	6	59,63,73	1.78	8 (13%)	70,101,113	1.16	9 (12%)
5	XAT	C	214	-	41,47,47	0.17	0	54,74,74	0.87	1 (1%)
3	CLA	B	306	6	61,65,73	1.80	9 (14%)	72,103,113	1.31	8 (11%)
3	CLA	A	205	1	64,68,73	1.71	8 (12%)	76,107,113	1.09	9 (11%)
3	CLA	C	210	1	65,69,73	1.69	8 (12%)	77,108,113	1.05	9 (11%)
3	CLA	A	201	1	69,73,73	1.64	8 (11%)	82,113,113	1.02	9 (10%)
3	CLA	C	207	1	56,60,73	1.80	8 (14%)	65,97,113	1.22	9 (13%)
3	CLA	D	311	2	54,58,73	1.87	10 (18%)	64,95,113	1.18	9 (14%)
4	A1L1F	A	215	-	52,59,59	0.41	1 (1%)	63,85,85	0.43	0
5	XAT	D	313	-	41,47,47	0.17	0	54,74,74	0.92	2 (3%)
3	CLA	C	212	6	69,73,73	1.64	8 (11%)	82,113,113	1.03	9 (10%)
4	A1L1F	C	215	-	52,59,59	0.41	1 (1%)	63,85,85	0.44	0
5	XAT	B	313	-	41,47,47	0.17	0	54,74,74	0.93	2 (3%)
5	XAT	D	314	-	41,47,47	0.16	0	54,74,74	0.77	3 (5%)
3	CLA	B	305	2	69,73,73	1.67	10 (14%)	82,113,113	1.07	7 (8%)
3	CLA	A	209	1	65,69,73	1.75	9 (13%)	77,108,113	1.22	8 (10%)
3	CLA	D	302	2	65,69,73	1.69	9 (13%)	77,108,113	1.15	9 (11%)
3	CLA	D	309	2	61,65,73	1.82	9 (14%)	72,103,113	1.31	9 (12%)
5	XAT	A	214	-	41,47,47	0.17	0	54,74,74	0.87	2 (3%)
3	CLA	C	204	1	65,69,73	1.74	8 (12%)	77,108,113	1.31	9 (11%)
3	CLA	B	310	2	69,73,73	1.67	9 (13%)	82,113,113	1.15	9 (10%)
3	CLA	B	311	2	54,58,73	1.87	9 (16%)	64,95,113	1.17	9 (14%)
3	CLA	B	304	2	61,65,73	1.77	9 (14%)	72,103,113	1.25	9 (12%)
3	CLA	C	211	1	59,63,73	1.84	9 (15%)	70,101,113	1.29	8 (11%)
3	CLA	D	306	6	61,65,73	1.80	9 (14%)	72,103,113	1.31	8 (11%)
5	XAT	D	315	-	41,47,47	0.13	0	54,74,74	0.48	0
3	CLA	B	307	2	60,64,73	1.76	8 (13%)	71,102,113	1.15	9 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	A1L1F	B	312	-	52,59,59	0.40	1 (1%)	63,85,85	0.81	3 (4%)
3	CLA	B	302	2	65,69,73	1.70	9 (13%)	77,108,113	1.16	9 (11%)
3	CLA	D	301	2	69,73,73	1.66	8 (11%)	82,113,113	1.08	8 (9%)
3	CLA	C	206	6	59,63,73	1.78	8 (13%)	70,101,113	1.16	9 (12%)
3	CLA	A	212	6	69,73,73	1.64	8 (11%)	82,113,113	1.03	9 (10%)
3	CLA	C	202	1	64,68,73	1.71	9 (14%)	76,107,113	1.14	9 (11%)
3	CLA	D	303	2	69,73,73	1.65	8 (11%)	82,113,113	1.07	9 (10%)
3	CLA	C	203	1	69,73,73	1.66	9 (13%)	82,113,113	1.07	9 (10%)
3	CLA	A	208	6	55,59,73	1.81	8 (14%)	64,96,113	1.18	9 (14%)
3	CLA	A	210	1	65,69,73	1.69	8 (12%)	77,108,113	1.05	9 (11%)
3	CLA	D	304	2	61,65,73	1.77	9 (14%)	72,103,113	1.25	9 (12%)
3	CLA	C	201	1	69,73,73	1.65	8 (11%)	82,113,113	1.03	9 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CLA	D	307	2	2/2/13/20	2/29/105/115	-
3	CLA	B	301	2	2/2/15/20	5/39/115/115	-
4	A1L1F	D	312	-	-	5/43/99/99	0/3/3/3
3	CLA	D	305	2	2/2/15/20	5/39/115/115	-
3	CLA	A	203	1	2/2/15/20	9/39/115/115	-
5	XAT	B	315	-	-	1/31/93/93	0/4/4/4
3	CLA	C	208	6	1/1/12/20	5/23/99/115	-
3	CLA	B	308	6	1/1/12/20	3/24/100/115	-
3	CLA	B	303	2	2/2/15/20	6/39/115/115	-
3	CLA	D	310	2	2/2/15/20	11/39/115/115	-
3	CLA	C	209	1	2/2/14/20	6/35/111/115	-
4	A1L1F	A	213	-	-	4/43/99/99	0/3/3/3
5	XAT	A	216	-	-	1/31/93/93	0/4/4/4
3	CLA	D	308	6	1/1/12/20	3/24/100/115	-
3	CLA	C	205	1	2/2/14/20	4/33/109/115	-
4	A1L1F	C	213	-	-	4/43/99/99	0/3/3/3
5	XAT	C	216	-	-	1/31/93/93	0/4/4/4
5	XAT	B	314	-	-	0/31/93/93	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CLA	A	207	1	1/1/12/20	4/24/100/115	-
3	CLA	A	204	1	2/2/14/20	13/35/111/115	-
3	CLA	A	211	1	2/2/13/20	7/27/103/115	-
3	CLA	B	309	2	2/2/13/20	4/30/106/115	-
3	CLA	A	202	1	2/2/14/20	10/33/109/115	-
3	CLA	A	206	6	2/2/13/20	4/27/103/115	-
5	XAT	C	214	-	-	0/31/93/93	0/4/4/4
3	CLA	B	306	6	2/2/13/20	5/30/106/115	-
3	CLA	A	205	1	2/2/14/20	4/33/109/115	-
3	CLA	C	210	1	2/2/14/20	9/35/111/115	-
3	CLA	A	201	1	2/2/15/20	6/39/115/115	-
3	CLA	C	207	1	1/1/12/20	4/24/100/115	-
3	CLA	D	311	2	1/1/12/20	2/21/97/115	-
4	A1L1F	A	215	-	-	2/43/99/99	0/3/3/3
5	XAT	D	313	-	-	0/31/93/93	0/4/4/4
3	CLA	C	212	6	2/2/15/20	7/39/115/115	-
4	A1L1F	C	215	-	-	2/43/99/99	0/3/3/3
5	XAT	B	313	-	-	0/31/93/93	0/4/4/4
5	XAT	D	314	-	-	0/31/93/93	0/4/4/4
3	CLA	B	305	2	2/2/15/20	5/39/115/115	-
3	CLA	A	209	1	2/2/14/20	6/35/111/115	-
3	CLA	D	302	2	2/2/14/20	5/35/111/115	-
3	CLA	D	309	2	2/2/13/20	4/30/106/115	-
5	XAT	A	214	-	-	0/31/93/93	0/4/4/4
3	CLA	C	204	1	2/2/14/20	13/35/111/115	-
3	CLA	B	310	2	2/2/15/20	11/39/115/115	-
3	CLA	B	311	2	1/1/12/20	2/21/97/115	-
3	CLA	B	304	2	2/2/13/20	6/30/106/115	-
3	CLA	C	211	1	2/2/13/20	7/27/103/115	-
3	CLA	D	306	6	2/2/13/20	5/30/106/115	-
5	XAT	D	315	-	-	1/31/93/93	0/4/4/4
3	CLA	B	307	2	2/2/13/20	2/29/105/115	-
4	A1L1F	B	312	-	-	5/43/99/99	0/3/3/3
3	CLA	B	302	2	2/2/14/20	5/35/111/115	-
3	CLA	D	301	2	2/2/15/20	5/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CLA	C	206	6	2/2/13/20	4/27/103/115	-
3	CLA	A	212	6	2/2/15/20	7/39/115/115	-
3	CLA	C	202	1	2/2/14/20	10/33/109/115	-
3	CLA	D	303	2	2/2/15/20	6/39/115/115	-
3	CLA	C	203	1	2/2/15/20	9/39/115/115	-
3	CLA	A	208	6	1/1/12/20	5/23/99/115	-
3	CLA	A	210	1	2/2/14/20	9/35/111/115	-
3	CLA	D	304	2	2/2/13/20	6/30/106/115	-
3	CLA	C	201	1	2/2/15/20	6/39/115/115	-

All (403) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	303	CLA	C4B-NB	8.07	1.48	1.37
3	C	207	CLA	C4B-NB	8.01	1.48	1.37
3	B	308	CLA	C4B-NB	7.99	1.48	1.37
3	D	308	CLA	C4B-NB	7.99	1.48	1.37
3	A	207	CLA	C4B-NB	7.98	1.48	1.37
3	B	303	CLA	C4B-NB	7.97	1.48	1.37
3	D	302	CLA	C4B-NB	7.97	1.48	1.37
3	C	203	CLA	C4B-NB	7.97	1.48	1.37
3	B	302	CLA	C4B-NB	7.95	1.48	1.37
3	A	206	CLA	C4B-NB	7.91	1.48	1.37
3	A	203	CLA	C4B-NB	7.91	1.48	1.37
3	C	206	CLA	C4B-NB	7.88	1.48	1.37
3	C	201	CLA	C4B-NB	7.87	1.48	1.37
3	A	209	CLA	C4B-NB	7.87	1.48	1.37
3	C	209	CLA	C4B-NB	7.87	1.48	1.37
3	A	201	CLA	C4B-NB	7.86	1.48	1.37
3	A	212	CLA	C4B-NB	7.84	1.48	1.37
3	C	212	CLA	C4B-NB	7.84	1.48	1.37
3	A	202	CLA	C4B-NB	7.84	1.48	1.37
3	C	202	CLA	C4B-NB	7.84	1.48	1.37
3	B	309	CLA	C4B-NB	7.84	1.48	1.37
3	D	309	CLA	C4B-NB	7.84	1.48	1.37
3	B	307	CLA	C4B-NB	7.82	1.48	1.37
3	D	307	CLA	C4B-NB	7.82	1.48	1.37
3	B	311	CLA	C4B-NB	7.82	1.48	1.37
3	D	311	CLA	C4B-NB	7.82	1.48	1.37
3	A	211	CLA	C4B-NB	7.78	1.48	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	211	CLA	C4B-NB	7.78	1.48	1.37
3	A	210	CLA	C4B-NB	7.75	1.48	1.37
3	C	210	CLA	C4B-NB	7.75	1.48	1.37
3	B	310	CLA	C4B-NB	7.75	1.48	1.37
3	D	310	CLA	C4B-NB	7.73	1.48	1.37
3	B	306	CLA	C4B-NB	7.72	1.48	1.37
3	D	306	CLA	C4B-NB	7.72	1.48	1.37
3	C	208	CLA	C4B-NB	7.72	1.48	1.37
3	B	301	CLA	C4B-NB	7.72	1.48	1.37
3	D	301	CLA	C4B-NB	7.71	1.48	1.37
3	A	208	CLA	C4B-NB	7.70	1.48	1.37
3	A	205	CLA	C4B-NB	7.70	1.48	1.37
3	C	205	CLA	C4B-NB	7.70	1.48	1.37
3	A	204	CLA	C4B-NB	7.66	1.47	1.37
3	C	204	CLA	C4B-NB	7.66	1.47	1.37
3	B	305	CLA	C4B-NB	7.59	1.47	1.37
3	D	305	CLA	C4B-NB	7.59	1.47	1.37
3	B	304	CLA	C4B-NB	7.54	1.47	1.37
3	D	304	CLA	C4B-NB	7.54	1.47	1.37
3	C	211	CLA	MG-NB	-5.38	1.95	2.05
3	A	211	CLA	MG-NB	-5.36	1.95	2.05
3	A	204	CLA	MG-NB	-5.36	1.95	2.05
3	C	204	CLA	MG-NB	-5.36	1.95	2.05
3	B	309	CLA	MG-NB	-5.36	1.95	2.05
3	A	209	CLA	MG-NB	-5.35	1.95	2.05
3	C	209	CLA	MG-NB	-5.35	1.95	2.05
3	D	309	CLA	MG-NB	-5.34	1.95	2.05
3	D	301	CLA	MG-NB	-5.28	1.95	2.05
3	B	301	CLA	MG-NB	-5.28	1.95	2.05
3	B	305	CLA	MG-NB	-5.28	1.95	2.05
3	D	305	CLA	MG-NB	-5.28	1.95	2.05
3	B	301	CLA	MG-ND	-5.26	1.95	2.05
3	D	301	CLA	MG-ND	-5.22	1.95	2.05
3	D	311	CLA	MG-NB	-5.21	1.95	2.05
3	A	209	CLA	MG-ND	-5.21	1.95	2.05
3	C	209	CLA	MG-ND	-5.21	1.95	2.05
3	B	306	CLA	MG-NB	-5.20	1.95	2.05
3	D	306	CLA	MG-NB	-5.20	1.95	2.05
3	D	310	CLA	MG-NB	-5.19	1.95	2.05
3	B	304	CLA	MG-NB	-5.18	1.95	2.05
3	B	305	CLA	MG-ND	-5.18	1.95	2.05
3	D	304	CLA	MG-NB	-5.18	1.95	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	305	CLA	MG-ND	-5.18	1.95	2.05
3	B	311	CLA	MG-NB	-5.16	1.95	2.05
3	A	204	CLA	MG-ND	-5.13	1.95	2.05
3	C	204	CLA	MG-ND	-5.13	1.95	2.05
3	B	310	CLA	MG-NB	-5.13	1.95	2.05
3	B	309	CLA	MG-ND	-5.12	1.95	2.05
3	D	309	CLA	MG-ND	-5.12	1.95	2.05
3	A	205	CLA	MG-ND	-5.09	1.95	2.05
3	C	205	CLA	MG-ND	-5.09	1.95	2.05
3	C	203	CLA	MG-NB	-5.08	1.95	2.05
3	A	205	CLA	MG-NB	-5.07	1.95	2.05
3	C	205	CLA	MG-NB	-5.07	1.95	2.05
3	A	203	CLA	MG-NB	-5.07	1.95	2.05
3	A	211	CLA	MG-ND	-5.07	1.95	2.05
3	B	310	CLA	MG-ND	-5.05	1.95	2.05
3	C	201	CLA	MG-NB	-5.05	1.95	2.05
3	C	211	CLA	MG-ND	-5.05	1.95	2.05
3	D	310	CLA	MG-ND	-5.03	1.95	2.05
3	A	201	CLA	MG-NB	-5.02	1.95	2.05
3	A	203	CLA	MG-ND	-4.99	1.95	2.05
3	D	303	CLA	MG-NB	-4.99	1.95	2.05
3	C	210	CLA	MG-NB	-4.99	1.95	2.05
3	B	303	CLA	MG-NB	-4.98	1.95	2.05
3	D	311	CLA	MG-ND	-4.98	1.95	2.05
3	B	306	CLA	MG-ND	-4.98	1.95	2.05
3	D	306	CLA	MG-ND	-4.98	1.95	2.05
3	B	302	CLA	MG-NB	-4.98	1.95	2.05
3	C	203	CLA	MG-ND	-4.98	1.95	2.05
3	D	302	CLA	MG-NB	-4.97	1.95	2.05
3	B	311	CLA	MG-ND	-4.97	1.95	2.05
3	C	212	CLA	MG-NB	-4.96	1.96	2.05
3	B	308	CLA	MG-NB	-4.96	1.96	2.05
3	D	308	CLA	MG-NB	-4.96	1.96	2.05
3	A	210	CLA	MG-NB	-4.96	1.96	2.05
3	B	304	CLA	MG-ND	-4.95	1.96	2.05
3	D	304	CLA	MG-ND	-4.95	1.96	2.05
3	C	208	CLA	MG-NB	-4.94	1.96	2.05
3	A	208	CLA	MG-NB	-4.94	1.96	2.05
3	A	202	CLA	MG-NB	-4.93	1.96	2.05
3	C	202	CLA	MG-NB	-4.93	1.96	2.05
3	A	212	CLA	MG-NB	-4.92	1.96	2.05
3	A	212	CLA	MG-ND	-4.91	1.96	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	206	CLA	MG-NB	-4.90	1.96	2.05
3	A	201	CLA	MG-ND	-4.90	1.96	2.05
3	C	201	CLA	MG-ND	-4.90	1.96	2.05
3	A	206	CLA	MG-NB	-4.90	1.96	2.05
3	C	212	CLA	MG-ND	-4.88	1.96	2.05
3	B	308	CLA	MG-ND	-4.84	1.96	2.05
3	D	308	CLA	MG-ND	-4.84	1.96	2.05
3	B	307	CLA	MG-NB	-4.83	1.96	2.05
3	D	307	CLA	MG-NB	-4.82	1.96	2.05
3	B	307	CLA	MG-ND	-4.81	1.96	2.05
3	D	307	CLA	MG-ND	-4.80	1.96	2.05
3	A	206	CLA	MG-ND	-4.80	1.96	2.05
3	A	210	CLA	MG-ND	-4.80	1.96	2.05
3	C	206	CLA	MG-ND	-4.80	1.96	2.05
3	C	210	CLA	MG-ND	-4.80	1.96	2.05
3	A	202	CLA	MG-ND	-4.79	1.96	2.05
3	C	202	CLA	MG-ND	-4.79	1.96	2.05
3	A	208	CLA	MG-ND	-4.76	1.96	2.05
3	C	208	CLA	MG-ND	-4.74	1.96	2.05
3	A	204	CLA	MG-NA	-4.70	1.95	2.06
3	C	204	CLA	MG-NA	-4.70	1.95	2.06
3	B	302	CLA	MG-ND	-4.70	1.96	2.05
3	D	303	CLA	MG-ND	-4.70	1.96	2.05
3	A	207	CLA	MG-NB	-4.68	1.96	2.05
3	C	207	CLA	MG-NB	-4.68	1.96	2.05
3	D	302	CLA	MG-ND	-4.68	1.96	2.05
3	B	303	CLA	MG-ND	-4.67	1.96	2.05
3	D	309	CLA	MG-NA	-4.65	1.95	2.06
3	B	309	CLA	MG-NA	-4.61	1.95	2.06
3	B	306	CLA	MG-NA	-4.56	1.95	2.06
3	D	306	CLA	MG-NA	-4.56	1.95	2.06
3	A	211	CLA	MG-NA	-4.52	1.95	2.06
3	C	207	CLA	MG-ND	-4.52	1.96	2.05
3	A	207	CLA	MG-ND	-4.51	1.96	2.05
3	B	304	CLA	MG-NA	-4.50	1.95	2.06
3	D	304	CLA	MG-NA	-4.50	1.95	2.06
3	C	211	CLA	MG-NA	-4.49	1.95	2.06
3	A	209	CLA	MG-NA	-4.34	1.96	2.06
3	C	209	CLA	MG-NA	-4.34	1.96	2.06
3	D	310	CLA	MG-NA	-4.24	1.96	2.06
3	B	305	CLA	MG-NA	-4.23	1.96	2.06
3	D	305	CLA	MG-NA	-4.23	1.96	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	310	CLA	MG-NA	-4.22	1.96	2.06
3	B	308	CLA	MG-NA	-4.17	1.96	2.06
3	D	308	CLA	MG-NA	-4.17	1.96	2.06
3	A	203	CLA	MG-NA	-4.07	1.96	2.06
3	C	203	CLA	MG-NA	-4.02	1.96	2.06
3	D	303	CLA	MG-NA	-4.00	1.96	2.06
3	B	303	CLA	MG-NA	-3.97	1.96	2.06
3	A	204	CLA	MG-NC	-3.96	1.96	2.06
3	C	204	CLA	MG-NC	-3.96	1.96	2.06
3	B	311	CLA	MG-NA	-3.95	1.96	2.06
3	D	311	CLA	MG-NA	-3.95	1.96	2.06
3	A	206	CLA	MG-NA	-3.94	1.96	2.06
3	C	206	CLA	MG-NA	-3.94	1.96	2.06
3	B	309	CLA	MG-NC	-3.94	1.96	2.06
3	D	309	CLA	MG-NC	-3.94	1.96	2.06
3	A	205	CLA	MG-NA	-3.93	1.96	2.06
3	C	205	CLA	MG-NA	-3.93	1.96	2.06
3	C	201	CLA	MG-NA	-3.91	1.97	2.06
3	B	301	CLA	MG-NA	-3.91	1.97	2.06
3	D	301	CLA	MG-NA	-3.91	1.97	2.06
3	A	201	CLA	MG-NA	-3.91	1.97	2.06
3	A	202	CLA	MG-NA	-3.90	1.97	2.06
3	C	202	CLA	MG-NA	-3.90	1.97	2.06
3	C	211	CLA	MG-NC	-3.89	1.97	2.06
3	A	211	CLA	MG-NC	-3.86	1.97	2.06
3	B	307	CLA	MG-NA	-3.85	1.97	2.06
3	A	208	CLA	MG-NA	-3.84	1.97	2.06
3	C	208	CLA	MG-NA	-3.84	1.97	2.06
3	D	307	CLA	MG-NA	-3.83	1.97	2.06
3	B	306	CLA	MG-NC	-3.81	1.97	2.06
3	D	306	CLA	MG-NC	-3.81	1.97	2.06
3	B	302	CLA	MG-NA	-3.80	1.97	2.06
3	A	210	CLA	MG-NA	-3.79	1.97	2.06
3	C	210	CLA	MG-NA	-3.79	1.97	2.06
3	B	304	CLA	MG-NC	-3.79	1.97	2.06
3	D	304	CLA	MG-NC	-3.79	1.97	2.06
3	A	210	CLA	C1D-ND	3.79	1.42	1.37
3	C	210	CLA	C1D-ND	3.79	1.42	1.37
3	A	209	CLA	MG-NC	-3.78	1.97	2.06
3	C	209	CLA	MG-NC	-3.78	1.97	2.06
3	A	212	CLA	C1D-ND	3.78	1.42	1.37
3	D	302	CLA	MG-NA	-3.75	1.97	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	207	CLA	MG-NA	-3.74	1.97	2.06
3	C	207	CLA	MG-NA	-3.74	1.97	2.06
3	C	212	CLA	C1D-ND	3.74	1.42	1.37
3	C	212	CLA	MG-NA	-3.72	1.97	2.06
3	A	212	CLA	MG-NA	-3.71	1.97	2.06
3	B	305	CLA	MG-NC	-3.66	1.97	2.06
3	D	305	CLA	MG-NC	-3.66	1.97	2.06
3	B	307	CLA	C1D-ND	3.66	1.42	1.37
3	D	307	CLA	C1D-ND	3.66	1.42	1.37
3	B	308	CLA	MG-NC	-3.65	1.97	2.06
3	D	308	CLA	MG-NC	-3.65	1.97	2.06
3	A	202	CLA	C1D-ND	3.65	1.42	1.37
3	C	202	CLA	C1D-ND	3.65	1.42	1.37
3	B	302	CLA	C1D-ND	3.61	1.42	1.37
3	A	207	CLA	C1D-ND	3.59	1.42	1.37
3	A	206	CLA	C1D-ND	3.59	1.42	1.37
3	C	206	CLA	C1D-ND	3.59	1.42	1.37
3	D	302	CLA	C1D-ND	3.58	1.42	1.37
3	C	207	CLA	C1D-ND	3.57	1.42	1.37
3	C	203	CLA	MG-NC	-3.55	1.97	2.06
3	D	310	CLA	C1D-ND	3.54	1.42	1.37
3	B	310	CLA	C1D-ND	3.54	1.42	1.37
3	C	203	CLA	C1D-ND	3.53	1.42	1.37
3	B	308	CLA	C1D-ND	3.53	1.42	1.37
3	D	308	CLA	C1D-ND	3.53	1.42	1.37
3	A	211	CLA	C1D-ND	3.53	1.42	1.37
3	C	211	CLA	C1D-ND	3.53	1.42	1.37
3	D	302	CLA	MG-NC	-3.53	1.97	2.06
3	A	203	CLA	C1D-ND	3.53	1.42	1.37
3	B	302	CLA	MG-NC	-3.52	1.97	2.06
3	A	208	CLA	C1D-ND	3.51	1.42	1.37
3	C	208	CLA	C1D-ND	3.51	1.42	1.37
3	A	203	CLA	MG-NC	-3.51	1.97	2.06
3	D	310	CLA	MG-NC	-3.50	1.97	2.06
3	B	311	CLA	MG-NC	-3.50	1.98	2.06
3	A	205	CLA	C1D-ND	3.49	1.42	1.37
3	C	205	CLA	C1D-ND	3.49	1.42	1.37
3	B	303	CLA	C1D-ND	3.49	1.42	1.37
3	D	303	CLA	C1D-ND	3.49	1.42	1.37
3	A	201	CLA	MG-NC	-3.49	1.98	2.06
3	C	201	CLA	MG-NC	-3.49	1.98	2.06
3	B	304	CLA	C1D-ND	3.49	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	304	CLA	C1D-ND	3.49	1.42	1.37
3	B	310	CLA	MG-NC	-3.49	1.98	2.06
3	D	311	CLA	MG-NC	-3.48	1.98	2.06
3	A	202	CLA	MG-NC	-3.48	1.98	2.06
3	C	202	CLA	MG-NC	-3.48	1.98	2.06
3	A	206	CLA	MG-NC	-3.47	1.98	2.06
3	C	206	CLA	MG-NC	-3.47	1.98	2.06
3	A	205	CLA	MG-NC	-3.46	1.98	2.06
3	C	205	CLA	MG-NC	-3.46	1.98	2.06
3	D	311	CLA	C1D-ND	3.46	1.42	1.37
3	B	301	CLA	C1D-ND	3.43	1.42	1.37
3	D	301	CLA	C1D-ND	3.43	1.42	1.37
3	B	301	CLA	MG-NC	-3.41	1.98	2.06
3	C	201	CLA	C1D-ND	3.41	1.42	1.37
3	D	301	CLA	MG-NC	-3.40	1.98	2.06
3	A	210	CLA	MG-NC	-3.39	1.98	2.06
3	C	210	CLA	MG-NC	-3.39	1.98	2.06
3	B	311	CLA	C1D-ND	3.38	1.42	1.37
3	A	201	CLA	C1D-ND	3.37	1.42	1.37
3	B	303	CLA	MG-NC	-3.37	1.98	2.06
3	A	207	CLA	MG-NC	-3.36	1.98	2.06
3	C	207	CLA	MG-NC	-3.36	1.98	2.06
3	A	212	CLA	MG-NC	-3.36	1.98	2.06
3	D	303	CLA	MG-NC	-3.35	1.98	2.06
3	B	306	CLA	C1D-ND	3.34	1.42	1.37
3	D	306	CLA	C1D-ND	3.34	1.42	1.37
3	A	209	CLA	C1D-ND	3.34	1.42	1.37
3	C	209	CLA	C1D-ND	3.34	1.42	1.37
3	D	307	CLA	MG-NC	-3.34	1.98	2.06
3	C	212	CLA	MG-NC	-3.34	1.98	2.06
3	B	307	CLA	MG-NC	-3.33	1.98	2.06
3	B	309	CLA	C1D-ND	3.32	1.42	1.37
3	D	309	CLA	C1D-ND	3.32	1.42	1.37
3	A	204	CLA	C1D-ND	3.29	1.42	1.37
3	A	208	CLA	MG-NC	-3.28	1.98	2.06
3	C	208	CLA	MG-NC	-3.28	1.98	2.06
3	C	204	CLA	C1D-ND	3.26	1.42	1.37
3	D	310	CLA	C1B-NB	3.24	1.42	1.37
3	B	305	CLA	C1D-ND	3.24	1.42	1.37
3	D	305	CLA	C1D-ND	3.21	1.42	1.37
3	B	306	CLA	C1B-NB	3.18	1.42	1.37
3	D	306	CLA	C1B-NB	3.18	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	310	CLA	C1B-NB	3.17	1.42	1.37
3	B	309	CLA	C1B-NB	3.14	1.42	1.37
3	A	211	CLA	C1B-NB	3.12	1.42	1.37
3	C	211	CLA	C1B-NB	3.12	1.42	1.37
3	A	204	CLA	C1B-NB	3.05	1.41	1.37
3	C	204	CLA	C1B-NB	3.05	1.41	1.37
3	B	303	CLA	C1B-NB	3.05	1.41	1.37
3	D	309	CLA	C1B-NB	3.04	1.41	1.37
3	D	303	CLA	C1B-NB	3.03	1.41	1.37
3	A	212	CLA	C1B-NB	3.02	1.41	1.37
3	C	212	CLA	C1B-NB	3.02	1.41	1.37
3	B	308	CLA	C1B-NB	3.01	1.41	1.37
3	D	308	CLA	C1B-NB	3.01	1.41	1.37
3	C	206	CLA	C1B-NB	3.01	1.41	1.37
3	A	202	CLA	C1B-NB	2.99	1.41	1.37
3	C	202	CLA	C1B-NB	2.99	1.41	1.37
3	A	206	CLA	C1B-NB	2.97	1.41	1.37
3	A	209	CLA	C1B-NB	2.97	1.41	1.37
3	C	209	CLA	C1B-NB	2.97	1.41	1.37
3	A	210	CLA	C1B-NB	2.97	1.41	1.37
3	C	210	CLA	C1B-NB	2.96	1.41	1.37
3	D	311	CLA	C1B-NB	2.95	1.41	1.37
3	B	304	CLA	C1B-NB	2.93	1.41	1.37
3	D	304	CLA	C1B-NB	2.93	1.41	1.37
3	B	311	CLA	C1B-NB	2.91	1.41	1.37
3	B	302	CLA	C1B-NB	2.90	1.41	1.37
3	D	302	CLA	C1B-NB	2.89	1.41	1.37
3	C	208	CLA	C1B-NB	2.88	1.41	1.37
3	B	307	CLA	C1B-NB	2.87	1.41	1.37
3	D	307	CLA	C1B-NB	2.87	1.41	1.37
3	A	207	CLA	C1B-NB	2.87	1.41	1.37
3	C	207	CLA	C1B-NB	2.87	1.41	1.37
3	A	208	CLA	C1B-NB	2.86	1.41	1.37
3	A	205	CLA	C1B-NB	2.85	1.41	1.37
3	C	205	CLA	C1B-NB	2.85	1.41	1.37
4	A	213	A1L1F	C6-C1	-2.84	1.49	1.54
4	C	213	A1L1F	C6-C1	-2.84	1.49	1.54
3	C	201	CLA	C1B-NB	2.84	1.41	1.37
3	A	203	CLA	C1B-NB	2.80	1.41	1.37
3	A	201	CLA	C1B-NB	2.79	1.41	1.37
3	C	203	CLA	C1B-NB	2.79	1.41	1.37
4	A	215	A1L1F	C6-C1	-2.77	1.49	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	215	A1L1F	C6-C1	-2.77	1.49	1.54
3	B	301	CLA	C1B-NB	2.73	1.41	1.37
3	B	305	CLA	C1B-NB	2.73	1.41	1.37
3	D	305	CLA	C1B-NB	2.73	1.41	1.37
3	D	301	CLA	C1B-NB	2.69	1.41	1.37
4	B	312	A1L1F	C6-C1	-2.61	1.50	1.54
4	D	312	A1L1F	C6-C1	-2.61	1.50	1.54
3	A	209	CLA	C1D-C2D	-2.41	1.40	1.45
3	C	209	CLA	C1D-C2D	-2.41	1.40	1.45
3	C	201	CLA	C1D-C2D	-2.39	1.40	1.45
3	B	302	CLA	C1D-C2D	-2.38	1.40	1.45
3	C	212	CLA	C1D-C2D	-2.38	1.40	1.45
3	A	201	CLA	C1D-C2D	-2.37	1.40	1.45
3	A	210	CLA	C1D-C2D	-2.37	1.40	1.45
3	A	212	CLA	C1D-C2D	-2.37	1.40	1.45
3	C	210	CLA	C1D-C2D	-2.37	1.40	1.45
3	B	307	CLA	C1D-C2D	-2.37	1.40	1.45
3	D	307	CLA	C1D-C2D	-2.37	1.40	1.45
3	D	311	CLA	C1D-C2D	-2.36	1.40	1.45
3	B	310	CLA	C1D-C2D	-2.36	1.40	1.45
3	D	310	CLA	C1D-C2D	-2.36	1.40	1.45
3	B	311	CLA	C1D-C2D	-2.35	1.40	1.45
3	D	301	CLA	C1D-C2D	-2.34	1.40	1.45
3	B	309	CLA	C1D-C2D	-2.34	1.40	1.45
3	D	309	CLA	C1D-C2D	-2.34	1.40	1.45
3	B	306	CLA	C1D-C2D	-2.33	1.40	1.45
3	D	302	CLA	C1D-C2D	-2.33	1.40	1.45
3	D	306	CLA	C1D-C2D	-2.33	1.40	1.45
3	A	203	CLA	C1D-C2D	-2.33	1.40	1.45
3	C	203	CLA	C1D-C2D	-2.33	1.40	1.45
3	C	205	CLA	C1D-C2D	-2.32	1.40	1.45
3	C	208	CLA	C1D-C2D	-2.32	1.40	1.45
3	A	202	CLA	C1D-C2D	-2.31	1.40	1.45
3	A	207	CLA	C1D-C2D	-2.31	1.40	1.45
3	C	207	CLA	C1D-C2D	-2.31	1.40	1.45
3	B	301	CLA	C1D-C2D	-2.31	1.40	1.45
3	A	205	CLA	C1D-C2D	-2.30	1.40	1.45
3	B	304	CLA	C1D-C2D	-2.30	1.40	1.45
3	D	304	CLA	C1D-C2D	-2.30	1.40	1.45
3	A	204	CLA	C1D-C2D	-2.29	1.40	1.45
3	A	206	CLA	C1D-C2D	-2.29	1.40	1.45
3	C	206	CLA	C1D-C2D	-2.29	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	204	CLA	C1D-C2D	-2.29	1.40	1.45
3	B	308	CLA	C1D-C2D	-2.29	1.40	1.45
3	D	308	CLA	C1D-C2D	-2.29	1.40	1.45
3	B	303	CLA	C1D-C2D	-2.28	1.40	1.45
3	C	202	CLA	C1D-C2D	-2.28	1.40	1.45
3	D	303	CLA	C1D-C2D	-2.28	1.40	1.45
3	D	305	CLA	C1D-C2D	-2.25	1.40	1.45
3	A	208	CLA	C1D-C2D	-2.25	1.40	1.45
3	A	211	CLA	C1D-C2D	-2.24	1.40	1.45
3	C	211	CLA	C1D-C2D	-2.24	1.40	1.45
3	B	305	CLA	C1D-C2D	-2.21	1.41	1.45
3	A	209	CLA	C1C-C2C	2.19	1.49	1.44
3	C	209	CLA	C1C-C2C	2.19	1.49	1.44
3	B	309	CLA	C1C-C2C	2.10	1.48	1.44
3	D	309	CLA	C1C-C2C	2.10	1.48	1.44
3	B	305	CLA	C3D-C4D	-2.06	1.39	1.44
3	D	305	CLA	C3D-C4D	-2.06	1.39	1.44
3	B	310	CLA	C1C-C2C	2.06	1.48	1.44
3	D	310	CLA	C1C-C2C	2.06	1.48	1.44
3	A	202	CLA	C3D-C4D	-2.06	1.39	1.44
3	B	308	CLA	C1C-C2C	2.06	1.48	1.44
3	A	211	CLA	C1C-C2C	2.05	1.48	1.44
3	C	211	CLA	C1C-C2C	2.05	1.48	1.44
3	C	202	CLA	C3D-C4D	-2.04	1.39	1.44
3	B	306	CLA	C1C-C2C	2.03	1.48	1.44
3	D	306	CLA	C1C-C2C	2.03	1.48	1.44
3	D	308	CLA	C1C-C2C	2.03	1.48	1.44
3	B	304	CLA	C3D-C4D	-2.03	1.39	1.44
3	D	311	CLA	C1C-C2C	2.02	1.48	1.44
3	A	203	CLA	C1C-C2C	2.02	1.48	1.44
3	C	203	CLA	C1C-C2C	2.02	1.48	1.44
3	D	304	CLA	C3D-C4D	-2.02	1.39	1.44
3	B	305	CLA	C3A-C2A	-2.01	1.49	1.54
3	D	305	CLA	C3A-C2A	-2.01	1.49	1.54
3	B	302	CLA	C3D-C4D	-2.01	1.39	1.44
3	D	302	CLA	C3D-C4D	-2.01	1.39	1.44
3	B	301	CLA	C3D-C4D	-2.01	1.39	1.44
3	D	311	CLA	C3D-C4D	-2.00	1.39	1.44
3	B	311	CLA	C3D-C4D	-2.00	1.39	1.44
3	D	310	CLA	C3D-C4D	-2.00	1.39	1.44

All (421) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	204	CLA	C4A-NA-C1A	-7.16	103.41	106.68
3	A	204	CLA	C4A-NA-C1A	-7.13	103.43	106.68
3	B	306	CLA	C4A-NA-C1A	-6.95	103.51	106.68
3	D	306	CLA	C4A-NA-C1A	-6.95	103.51	106.68
3	D	309	CLA	C4A-NA-C1A	-6.72	103.61	106.68
3	B	309	CLA	C4A-NA-C1A	-6.53	103.70	106.68
3	A	209	CLA	C4A-NA-C1A	-6.35	103.78	106.68
3	C	209	CLA	C4A-NA-C1A	-6.35	103.78	106.68
3	A	211	CLA	C4A-NA-C1A	-6.33	103.79	106.68
3	C	211	CLA	C4A-NA-C1A	-6.29	103.81	106.68
3	D	310	CLA	C4A-NA-C1A	-6.20	103.85	106.68
3	B	304	CLA	C4A-NA-C1A	-6.09	103.90	106.68
3	D	304	CLA	C4A-NA-C1A	-6.09	103.90	106.68
3	B	310	CLA	C4A-NA-C1A	-6.09	103.90	106.68
3	B	302	CLA	C4A-NA-C1A	-5.51	104.16	106.68
3	D	302	CLA	C4A-NA-C1A	-5.39	104.22	106.68
3	B	308	CLA	C4A-NA-C1A	-5.08	104.36	106.68
3	D	308	CLA	C4A-NA-C1A	-5.08	104.36	106.68
3	C	202	CLA	C4A-NA-C1A	-5.05	104.38	106.68
3	A	202	CLA	C4A-NA-C1A	-5.00	104.40	106.68
3	B	305	CLA	C4A-NA-C1A	-4.96	104.42	106.68
3	D	305	CLA	C4A-NA-C1A	-4.96	104.42	106.68
3	B	301	CLA	C4A-NA-C1A	-4.92	104.44	106.68
3	D	301	CLA	C4A-NA-C1A	-4.83	104.48	106.68
3	A	207	CLA	C4A-NA-C1A	-4.78	104.50	106.68
3	C	207	CLA	C4A-NA-C1A	-4.78	104.50	106.68
3	A	206	CLA	C4A-NA-C1A	-4.78	104.50	106.68
3	C	206	CLA	C4A-NA-C1A	-4.78	104.50	106.68
3	B	307	CLA	C4A-NA-C1A	-4.69	104.54	106.68
3	D	307	CLA	C4A-NA-C1A	-4.69	104.54	106.68
3	B	311	CLA	C4A-NA-C1A	-4.57	104.59	106.68
3	A	203	CLA	C4A-NA-C1A	-4.55	104.60	106.68
3	D	311	CLA	C4A-NA-C1A	-4.54	104.61	106.68
5	B	313	XAT	C7-C8-C9	4.51	132.53	125.53
5	D	313	XAT	C7-C8-C9	4.50	132.51	125.53
3	C	203	CLA	C4A-NA-C1A	-4.40	104.67	106.68
3	B	303	CLA	C4A-NA-C1A	-4.33	104.70	106.68
3	D	303	CLA	C4A-NA-C1A	-4.33	104.70	106.68
3	A	205	CLA	C4A-NA-C1A	-4.29	104.72	106.68
3	C	205	CLA	C4A-NA-C1A	-4.24	104.74	106.68
3	C	201	CLA	C4A-NA-C1A	-4.20	104.76	106.68
3	A	201	CLA	C4A-NA-C1A	-4.15	104.79	106.68
3	A	208	CLA	C4A-NA-C1A	-4.05	104.83	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	312	A1L1F	O15-C20-C21	-4.00	109.74	113.49
4	D	312	A1L1F	O15-C20-C21	-4.00	109.74	113.49
5	C	214	XAT	C7-C8-C9	3.95	131.66	125.53
3	C	208	CLA	C4A-NA-C1A	-3.95	104.88	106.68
3	A	210	CLA	C4A-NA-C1A	-3.95	104.88	106.68
3	C	210	CLA	C4A-NA-C1A	-3.95	104.88	106.68
5	A	214	XAT	C27-C28-C29	3.94	131.65	125.53
3	A	212	CLA	C4A-NA-C1A	-3.80	104.95	106.68
3	C	212	CLA	C4A-NA-C1A	-3.75	104.97	106.68
3	A	203	CLA	C1-C2-C3	-3.49	120.47	126.20
3	C	203	CLA	C1-C2-C3	-3.48	120.49	126.20
3	B	303	CLA	C1-C2-C3	-3.29	120.80	126.20
3	D	303	CLA	C1-C2-C3	-3.29	120.80	126.20
3	C	207	CLA	C1D-ND-C4D	-3.25	104.03	106.31
3	C	202	CLA	C1D-ND-C4D	-3.24	104.04	106.31
3	A	202	CLA	C1D-ND-C4D	-3.23	104.04	106.31
3	A	207	CLA	C1D-ND-C4D	-3.23	104.05	106.31
3	C	211	CLA	C1-C2-C3	-3.15	121.03	126.20
3	C	206	CLA	C1D-ND-C4D	-3.14	104.11	106.31
3	A	209	CLA	C1-C2-C3	-3.12	121.08	126.20
3	C	209	CLA	C1-C2-C3	-3.12	121.08	126.20
3	A	211	CLA	C1-C2-C3	-3.11	121.09	126.20
3	B	302	CLA	C1D-ND-C4D	-3.11	104.13	106.31
3	A	206	CLA	C1D-ND-C4D	-3.10	104.14	106.31
3	B	303	CLA	C1D-ND-C4D	-3.08	104.15	106.31
3	D	303	CLA	C1D-ND-C4D	-3.08	104.15	106.31
3	D	302	CLA	C1D-ND-C4D	-3.05	104.17	106.31
5	B	314	XAT	C27-C28-C29	3.04	130.25	125.53
5	D	314	XAT	C27-C28-C29	3.04	130.25	125.53
3	B	307	CLA	C1D-ND-C4D	-3.04	104.18	106.31
3	D	307	CLA	C1D-ND-C4D	-3.04	104.18	106.31
3	B	308	CLA	C1D-ND-C4D	-2.99	104.21	106.31
3	D	308	CLA	C1D-ND-C4D	-2.99	104.21	106.31
3	C	201	CLA	C1D-ND-C4D	-2.98	104.22	106.31
3	A	201	CLA	C1D-ND-C4D	-2.97	104.23	106.31
3	A	203	CLA	C1D-ND-C4D	-2.97	104.23	106.31
3	B	301	CLA	C1D-ND-C4D	-2.93	104.26	106.31
3	A	208	CLA	C1D-ND-C4D	-2.93	104.26	106.31
3	C	212	CLA	C1D-ND-C4D	-2.91	104.27	106.31
3	C	203	CLA	C1D-ND-C4D	-2.91	104.27	106.31
3	B	304	CLA	CAA-C2A-C1A	-2.90	102.48	111.97
3	D	304	CLA	CAA-C2A-C1A	-2.90	102.48	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	208	CLA	C1D-ND-C4D	-2.87	104.30	106.31
3	A	212	CLA	C1D-ND-C4D	-2.87	104.30	106.31
3	B	301	CLA	C1-C2-C3	-2.86	121.52	126.20
3	D	311	CLA	C1D-ND-C4D	-2.85	104.31	106.31
3	D	301	CLA	C1D-ND-C4D	-2.85	104.31	106.31
3	D	301	CLA	C1-C2-C3	-2.83	121.55	126.20
3	B	304	CLA	C1D-ND-C4D	-2.81	104.34	106.31
3	D	304	CLA	C1D-ND-C4D	-2.81	104.34	106.31
3	D	305	CLA	CHD-C1D-ND	-2.80	120.87	124.80
4	B	312	A1L1F	O15-C25-C14	-2.79	108.87	116.88
4	D	312	A1L1F	O15-C25-C14	-2.79	108.87	116.88
3	B	303	CLA	CHD-C1D-ND	-2.79	120.87	124.80
3	D	303	CLA	CHD-C1D-ND	-2.78	120.89	124.80
3	A	205	CLA	C1D-ND-C4D	-2.78	104.36	106.31
3	C	205	CLA	C1D-ND-C4D	-2.78	104.36	106.31
3	B	305	CLA	CHD-C1D-ND	-2.77	120.91	124.80
3	B	311	CLA	C1D-ND-C4D	-2.75	104.38	106.31
3	A	206	CLA	CHD-C1D-ND	-2.73	120.96	124.80
3	C	206	CLA	CHD-C1D-ND	-2.73	120.96	124.80
3	B	304	CLA	CHD-C1D-ND	-2.73	120.96	124.80
3	D	304	CLA	CHD-C1D-ND	-2.73	120.96	124.80
3	A	210	CLA	C1D-ND-C4D	-2.73	104.40	106.31
3	A	204	CLA	CHD-C1D-ND	-2.71	120.99	124.80
3	A	211	CLA	CHD-C1D-ND	-2.71	120.99	124.80
3	C	211	CLA	CHD-C1D-ND	-2.71	120.99	124.80
3	A	205	CLA	CHD-C1D-ND	-2.71	120.99	124.80
3	B	307	CLA	CHD-C1D-ND	-2.70	121.00	124.80
3	D	307	CLA	CHD-C1D-ND	-2.70	121.00	124.80
3	B	308	CLA	CHD-C1D-ND	-2.70	121.00	124.80
3	C	204	CLA	CHD-C1D-ND	-2.70	121.00	124.80
3	D	308	CLA	CHD-C1D-ND	-2.70	121.00	124.80
3	C	202	CLA	CHD-C1D-ND	-2.70	121.01	124.80
3	C	207	CLA	CHD-C1D-ND	-2.70	121.01	124.80
3	A	202	CLA	CHD-C1D-ND	-2.69	121.01	124.80
3	A	210	CLA	C1-C2-C3	-2.69	121.79	126.20
3	C	210	CLA	C1-C2-C3	-2.69	121.79	126.20
3	C	205	CLA	CHD-C1D-ND	-2.69	121.02	124.80
3	A	207	CLA	CHD-C1D-ND	-2.68	121.02	124.80
3	B	309	CLA	CHD-C1D-ND	-2.68	121.03	124.80
3	D	309	CLA	CHD-C1D-ND	-2.68	121.03	124.80
3	A	203	CLA	CHD-C1D-ND	-2.68	121.03	124.80
3	B	306	CLA	C1D-ND-C4D	-2.68	104.44	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	306	CLA	C1D-ND-C4D	-2.68	104.44	106.31
3	B	306	CLA	CHD-C1D-ND	-2.67	121.04	124.80
3	D	306	CLA	CHD-C1D-ND	-2.67	121.04	124.80
3	C	210	CLA	C1D-ND-C4D	-2.67	104.44	106.31
3	C	203	CLA	CHD-C1D-ND	-2.66	121.06	124.80
3	B	302	CLA	CHD-C1D-ND	-2.65	121.07	124.80
3	D	305	CLA	C1D-ND-C4D	-2.65	104.45	106.31
3	C	212	CLA	CHD-C1D-ND	-2.63	121.11	124.80
3	B	307	CLA	CHC-C1C-C2C	-2.62	119.49	126.95
3	D	307	CLA	CHC-C1C-C2C	-2.62	119.49	126.95
3	B	309	CLA	C1D-ND-C4D	-2.62	104.48	106.31
3	D	309	CLA	C1D-ND-C4D	-2.62	104.48	106.31
3	C	208	CLA	CHD-C1D-ND	-2.61	121.13	124.80
3	C	212	CLA	CHC-C1C-C2C	-2.61	119.53	126.95
3	A	208	CLA	CHD-C1D-ND	-2.60	121.14	124.80
3	B	305	CLA	C1D-ND-C4D	-2.60	104.49	106.31
3	A	212	CLA	CHC-C1C-C2C	-2.60	119.57	126.95
3	C	208	CLA	CHC-C1C-C2C	-2.60	119.57	126.95
3	D	310	CLA	C1D-ND-C4D	-2.60	104.49	106.31
3	A	208	CLA	CHC-C1C-C2C	-2.59	119.58	126.95
3	A	212	CLA	CHD-C1D-ND	-2.59	121.16	124.80
3	D	302	CLA	CHD-C1D-ND	-2.59	121.16	124.80
3	C	201	CLA	CHD-C1D-ND	-2.59	121.16	124.80
3	C	207	CLA	CHC-C1C-C2C	-2.58	119.61	126.95
3	A	207	CLA	CHC-C1C-C2C	-2.58	119.62	126.95
3	B	310	CLA	C1D-ND-C4D	-2.57	104.51	106.31
3	A	205	CLA	C1-C2-C3	-2.57	121.99	126.20
3	C	205	CLA	C1-C2-C3	-2.57	121.99	126.20
3	A	211	CLA	C1D-ND-C4D	-2.57	104.51	106.31
3	C	211	CLA	C1D-ND-C4D	-2.57	104.51	106.31
3	A	201	CLA	CHD-C1D-ND	-2.57	121.19	124.80
3	D	311	CLA	CHD-C1D-ND	-2.56	121.20	124.80
3	A	206	CLA	CHC-C1C-C2C	-2.56	119.69	126.95
3	A	202	CLA	CHC-C1C-C2C	-2.55	119.69	126.95
3	C	202	CLA	CHC-C1C-C2C	-2.55	119.69	126.95
3	C	206	CLA	CHC-C1C-C2C	-2.54	119.72	126.95
3	B	311	CLA	CHD-C1D-ND	-2.54	121.23	124.80
3	B	301	CLA	CHD-C1D-ND	-2.54	121.23	124.80
3	D	301	CLA	CHD-C1D-ND	-2.54	121.23	124.80
3	D	302	CLA	CHC-C1C-C2C	-2.54	119.73	126.95
3	C	210	CLA	CHC-C1C-C2C	-2.53	119.77	126.95
3	B	310	CLA	CHD-C1D-ND	-2.52	121.25	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	210	CLA	CHC-C1C-C2C	-2.52	119.78	126.95
3	D	310	CLA	CHD-C1D-ND	-2.52	121.26	124.80
3	B	302	CLA	CHC-C1C-C2C	-2.52	119.80	126.95
3	B	305	CLA	CHC-C1C-C2C	-2.52	119.80	126.95
3	B	304	CLA	CHC-C1C-C2C	-2.51	119.81	126.95
3	D	304	CLA	CHC-C1C-C2C	-2.51	119.81	126.95
3	A	206	CLA	C1-C2-C3	-2.51	122.08	126.20
3	C	206	CLA	C1-C2-C3	-2.51	122.08	126.20
3	D	305	CLA	CHC-C1C-C2C	-2.50	119.84	126.95
3	C	202	CLA	C1-C2-C3	-2.49	122.12	126.20
3	B	302	CLA	C1-C2-C3	-2.48	122.13	126.20
3	A	205	CLA	CHC-C1C-C2C	-2.48	119.89	126.95
3	C	205	CLA	CHC-C1C-C2C	-2.48	119.89	126.95
3	D	302	CLA	C1-C2-C3	-2.48	122.13	126.20
3	A	202	CLA	C1-C2-C3	-2.48	122.14	126.20
3	A	209	CLA	C1D-ND-C4D	-2.48	104.57	106.31
3	C	209	CLA	C1D-ND-C4D	-2.48	104.57	106.31
3	D	311	CLA	CHC-C1C-C2C	-2.48	119.91	126.95
3	A	209	CLA	CHD-C1D-ND	-2.47	121.32	124.80
3	C	209	CLA	CHD-C1D-ND	-2.47	121.32	124.80
3	B	307	CLA	CHC-C1C-NC	2.47	128.03	124.31
3	D	307	CLA	CHC-C1C-NC	2.47	128.03	124.31
3	B	308	CLA	CHC-C1C-C2C	-2.47	119.94	126.95
3	B	311	CLA	CHC-C1C-C2C	-2.46	119.95	126.95
3	B	310	CLA	C1-C2-C3	-2.46	122.16	126.20
3	D	310	CLA	C1-C2-C3	-2.46	122.16	126.20
3	A	204	CLA	CHA-C1A-NA	-2.45	120.84	126.39
3	C	204	CLA	CHA-C1A-NA	-2.45	120.84	126.39
3	A	212	CLA	C2C-C1C-NC	2.45	112.55	109.98
3	C	207	CLA	CHC-C1C-NC	2.44	127.99	124.31
3	B	301	CLA	CHC-C1C-C2C	-2.44	120.01	126.95
3	D	301	CLA	CHC-C1C-C2C	-2.44	120.01	126.95
3	D	308	CLA	CHC-C1C-C2C	-2.44	120.01	126.95
3	B	303	CLA	CHC-C1C-C2C	-2.43	120.03	126.95
3	C	203	CLA	CHC-C1C-C2C	-2.43	120.03	126.95
3	D	303	CLA	CHC-C1C-C2C	-2.43	120.03	126.95
3	A	207	CLA	CHC-C1C-NC	2.43	127.98	124.31
3	A	203	CLA	CHC-C1C-C2C	-2.43	120.05	126.95
3	C	211	CLA	CHA-C1A-NA	-2.42	120.90	126.39
3	C	212	CLA	C2C-C1C-NC	2.42	112.53	109.98
3	B	311	CLA	C1-C2-C3	-2.42	122.84	126.76
3	D	311	CLA	C1-C2-C3	-2.42	122.84	126.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	306	CLA	CHA-C1A-NA	-2.42	120.91	126.39
3	A	201	CLA	CHC-C1C-C2C	-2.42	120.07	126.95
3	B	305	CLA	CHA-C1A-NA	-2.42	120.91	126.39
3	D	305	CLA	CHA-C1A-NA	-2.42	120.91	126.39
3	A	204	CLA	CHC-C1C-NC	2.42	127.95	124.31
3	C	204	CLA	CHC-C1C-NC	2.42	127.95	124.31
3	B	310	CLA	CHC-C1C-C2C	-2.41	120.09	126.95
3	D	310	CLA	CHC-C1C-C2C	-2.41	120.09	126.95
3	B	304	CLA	CHC-C1C-NC	2.41	127.95	124.31
3	D	304	CLA	CHC-C1C-NC	2.41	127.95	124.31
3	A	204	CLA	CHC-C1C-C2C	-2.41	120.09	126.95
3	C	204	CLA	CHC-C1C-C2C	-2.41	120.09	126.95
3	C	201	CLA	CHC-C1C-C2C	-2.41	120.10	126.95
3	C	208	CLA	C2C-C1C-NC	2.41	112.51	109.98
3	A	209	CLA	CHA-C1A-NA	-2.41	120.94	126.39
3	C	209	CLA	CHA-C1A-NA	-2.41	120.94	126.39
3	D	306	CLA	CHA-C1A-NA	-2.41	120.94	126.39
3	A	202	CLA	CHC-C1C-NC	2.41	127.94	124.31
3	C	202	CLA	CHC-C1C-NC	2.41	127.94	124.31
3	A	211	CLA	CHA-C1A-NA	-2.40	120.95	126.39
3	B	308	CLA	CHC-C1C-NC	2.40	127.93	124.31
3	A	208	CLA	C2C-C1C-NC	2.40	112.50	109.98
3	D	309	CLA	C1-C2-C3	-2.40	122.27	126.20
3	A	206	CLA	CHC-C1C-NC	2.40	127.92	124.31
3	C	212	CLA	CHC-C1C-NC	2.40	127.92	124.31
3	B	306	CLA	CHC-C1C-C2C	-2.38	120.17	126.95
3	D	306	CLA	CHC-C1C-C2C	-2.38	120.17	126.95
3	D	310	CLA	CHA-C1A-NA	-2.38	120.99	126.39
3	C	208	CLA	CHC-C1C-NC	2.38	127.90	124.31
3	A	208	CLA	CHC-C1C-NC	2.38	127.90	124.31
3	A	210	CLA	CHD-C1D-ND	-2.38	121.46	124.80
3	C	210	CLA	CHD-C1D-ND	-2.38	121.46	124.80
3	B	301	CLA	CHA-C1A-NA	-2.37	121.01	126.39
3	D	301	CLA	CHA-C1A-NA	-2.37	121.03	126.39
3	B	305	CLA	CHC-C1C-NC	2.37	127.88	124.31
3	D	308	CLA	CHC-C1C-NC	2.37	127.88	124.31
3	A	205	CLA	CHC-C1C-NC	2.37	127.88	124.31
3	C	205	CLA	CHC-C1C-NC	2.37	127.88	124.31
3	D	302	CLA	CHC-C1C-NC	2.36	127.87	124.31
3	B	310	CLA	CHA-C1A-NA	-2.36	121.05	126.39
3	B	309	CLA	C1-C2-C3	-2.36	122.33	126.20
3	A	212	CLA	CHC-C1C-NC	2.36	127.86	124.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	206	CLA	CHC-C1C-NC	2.35	127.86	124.31
3	C	201	CLA	CHA-C1A-NA	-2.35	121.07	126.39
3	C	212	CLA	CHA-C1A-NA	-2.35	121.08	126.39
3	A	212	CLA	CHA-C1A-NA	-2.35	121.08	126.39
3	D	305	CLA	CHC-C1C-NC	2.34	127.84	124.31
3	A	201	CLA	CHA-C1A-NA	-2.34	121.09	126.39
3	B	302	CLA	CHC-C1C-NC	2.34	127.83	124.31
3	A	210	CLA	CHA-C1A-NA	-2.34	121.10	126.39
3	C	210	CLA	CHA-C1A-NA	-2.34	121.10	126.39
3	B	307	CLA	C1-C2-C3	-2.33	122.38	126.20
3	D	307	CLA	C1-C2-C3	-2.33	122.38	126.20
3	A	210	CLA	CHC-C1C-NC	2.33	127.82	124.31
3	C	210	CLA	CHC-C1C-NC	2.33	127.82	124.31
3	A	208	CLA	CHA-C1A-NA	-2.33	121.12	126.39
3	C	208	CLA	CHA-C1A-NA	-2.33	121.12	126.39
3	D	309	CLA	CHA-C1A-NA	-2.32	121.13	126.39
3	B	309	CLA	CHC-C1C-C2C	-2.32	120.35	126.95
3	D	309	CLA	CHC-C1C-C2C	-2.32	120.35	126.95
3	C	206	CLA	C2C-C1C-NC	2.32	112.42	109.98
3	A	204	CLA	C1D-ND-C4D	-2.31	104.69	106.31
3	A	205	CLA	CHA-C1A-NA	-2.31	121.16	126.39
3	A	211	CLA	CHC-C1C-C2C	-2.31	120.39	126.95
3	C	211	CLA	CHC-C1C-C2C	-2.31	120.39	126.95
3	B	309	CLA	CHC-C1C-NC	2.30	127.78	124.31
3	D	309	CLA	CHC-C1C-NC	2.30	127.78	124.31
3	A	207	CLA	C2C-C1C-NC	2.30	112.40	109.98
3	C	207	CLA	C2C-C1C-NC	2.30	112.40	109.98
3	D	302	CLA	C2C-C1C-NC	2.30	112.40	109.98
3	A	206	CLA	C2C-C1C-NC	2.29	112.39	109.98
3	B	309	CLA	CHA-C1A-NA	-2.29	121.20	126.39
3	C	204	CLA	C1D-ND-C4D	-2.29	104.71	106.31
3	C	205	CLA	CHA-C1A-NA	-2.29	121.21	126.39
3	B	303	CLA	CHC-C1C-NC	2.28	127.75	124.31
3	D	303	CLA	CHC-C1C-NC	2.28	127.75	124.31
3	C	203	CLA	CHC-C1C-NC	2.28	127.75	124.31
3	A	211	CLA	CHC-C1C-NC	2.28	127.75	124.31
3	C	211	CLA	CHC-C1C-NC	2.28	127.75	124.31
3	A	204	CLA	C3A-C2A-C1A	-2.28	97.92	101.34
3	C	204	CLA	C3A-C2A-C1A	-2.28	97.92	101.34
3	C	210	CLA	C2C-C1C-NC	2.28	112.38	109.98
3	D	311	CLA	CHC-C1C-NC	2.28	127.74	124.31
4	B	312	A1L1F	O15-C20-C25	-2.27	57.13	58.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	312	A1L1F	O15-C20-C25	-2.27	57.13	58.93
3	A	202	CLA	C2C-C1C-NC	2.27	112.36	109.98
3	B	311	CLA	C2C-C1C-NC	2.27	112.36	109.98
3	C	202	CLA	C2C-C1C-NC	2.27	112.36	109.98
3	B	302	CLA	C2C-C1C-NC	2.27	112.36	109.98
3	A	203	CLA	CHC-C1C-NC	2.27	127.72	124.31
3	A	210	CLA	C2C-C1C-NC	2.27	112.36	109.98
3	C	204	CLA	C2A-C3A-C4A	-2.26	98.22	101.87
3	A	201	CLA	CHC-C1C-NC	2.26	127.71	124.31
3	C	201	CLA	CHC-C1C-NC	2.26	127.71	124.31
3	A	208	CLA	C1-C2-C3	-2.26	122.50	126.20
3	B	307	CLA	C2C-C1C-NC	2.25	112.35	109.98
3	D	307	CLA	C2C-C1C-NC	2.25	112.35	109.98
5	B	313	XAT	O4-C5-C4	-2.25	111.38	113.49
5	D	313	XAT	O4-C5-C4	-2.25	111.38	113.49
3	A	204	CLA	C2A-C3A-C4A	-2.25	98.23	101.87
3	C	208	CLA	C1-C2-C3	-2.25	122.51	126.20
3	A	209	CLA	CHC-C1C-C2C	-2.25	120.56	126.95
3	C	209	CLA	CHC-C1C-C2C	-2.25	120.56	126.95
3	B	310	CLA	CHC-C1C-NC	2.24	127.68	124.31
3	D	310	CLA	CHC-C1C-NC	2.24	127.68	124.31
3	C	207	CLA	C1-C2-C3	-2.23	122.54	126.20
3	B	306	CLA	CHC-C1C-NC	2.23	127.67	124.31
3	D	306	CLA	CHC-C1C-NC	2.23	127.67	124.31
3	A	207	CLA	C1-C2-C3	-2.23	122.55	126.20
3	D	311	CLA	C2C-C1C-NC	2.23	112.32	109.98
3	B	311	CLA	CHC-C1C-NC	2.23	127.67	124.31
3	B	308	CLA	C1-C2-C3	-2.22	122.56	126.20
3	D	308	CLA	C1-C2-C3	-2.22	122.56	126.20
3	B	301	CLA	CHC-C1C-NC	2.21	127.64	124.31
3	D	301	CLA	CHC-C1C-NC	2.21	127.64	124.31
3	A	203	CLA	CHA-C1A-NA	-2.21	121.39	126.39
3	B	301	CLA	C2C-C1C-NC	2.21	112.30	109.98
3	D	301	CLA	C2C-C1C-NC	2.21	112.30	109.98
3	C	210	CLA	CHB-C1B-NB	-2.21	120.74	124.05
3	B	311	CLA	CHA-C1A-NA	-2.20	121.40	126.39
3	D	311	CLA	CHA-C1A-NA	-2.20	121.40	126.39
3	A	208	CLA	CHB-C1B-NB	-2.20	120.75	124.05
3	C	203	CLA	CHA-C1A-NA	-2.19	121.42	126.39
3	B	307	CLA	CHB-C1B-NB	-2.19	120.76	124.05
3	D	307	CLA	CHB-C1B-NB	-2.19	120.76	124.05
3	C	208	CLA	CHB-C1B-NB	-2.19	120.77	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	305	CLA	C2C-C1C-NC	2.19	112.28	109.98
3	D	305	CLA	C2C-C1C-NC	2.19	112.28	109.98
3	A	210	CLA	CHB-C1B-NB	-2.18	120.77	124.05
3	A	207	CLA	CHB-C1B-NB	-2.18	120.78	124.05
3	C	207	CLA	CHB-C1B-NB	-2.18	120.78	124.05
3	B	302	CLA	CHA-C1A-NA	-2.18	121.46	126.39
3	D	302	CLA	CHA-C1A-NA	-2.17	121.48	126.39
3	B	308	CLA	CHA-C1A-NA	-2.17	121.48	126.39
3	D	308	CLA	CHA-C1A-NA	-2.17	121.48	126.39
3	C	201	CLA	CHB-C1B-NB	-2.16	120.81	124.05
3	B	304	CLA	C2C-C1C-NC	2.16	112.25	109.98
3	D	304	CLA	C2C-C1C-NC	2.16	112.25	109.98
3	B	307	CLA	CHA-C1A-NA	-2.15	121.52	126.39
3	D	307	CLA	CHA-C1A-NA	-2.15	121.52	126.39
3	A	201	CLA	CHB-C1B-NB	-2.15	120.82	124.05
3	B	302	CLA	CHB-C1B-NB	-2.14	120.83	124.05
3	D	302	CLA	CHB-C1B-NB	-2.14	120.83	124.05
3	B	310	CLA	C2C-C1C-NC	2.14	112.23	109.98
3	D	310	CLA	C2C-C1C-NC	2.14	112.23	109.98
3	A	206	CLA	CHA-C1A-NA	-2.14	121.55	126.39
3	C	206	CLA	CHA-C1A-NA	-2.14	121.55	126.39
3	A	209	CLA	CHC-C1C-NC	2.13	127.53	124.31
3	C	209	CLA	CHC-C1C-NC	2.13	127.53	124.31
3	C	212	CLA	CHB-C1B-NB	-2.13	120.85	124.05
3	C	201	CLA	C1-C2-C3	-2.13	122.71	126.20
3	B	303	CLA	C2C-C1C-NC	2.12	112.21	109.98
3	D	303	CLA	C2C-C1C-NC	2.12	112.21	109.98
5	D	314	XAT	C7-C8-C9	2.12	128.82	125.53
5	B	314	XAT	O24-C25-C24	-2.12	111.50	113.49
5	D	314	XAT	O24-C25-C24	-2.12	111.50	113.49
3	A	201	CLA	C1-C2-C3	-2.12	122.73	126.20
5	B	314	XAT	C7-C8-C9	2.11	128.81	125.53
3	A	212	CLA	CHB-C1B-NB	-2.11	120.89	124.05
3	D	310	CLA	CHB-C1B-NB	-2.10	120.90	124.05
3	B	310	CLA	CHB-C1B-NB	-2.10	120.90	124.05
3	A	203	CLA	CHB-C1B-NB	-2.09	120.91	124.05
3	A	204	CLA	CHB-C1B-NB	-2.09	120.91	124.05
3	C	204	CLA	CHB-C1B-NB	-2.09	120.91	124.05
3	B	303	CLA	CHA-C1A-NA	-2.09	121.66	126.39
3	D	303	CLA	CHA-C1A-NA	-2.09	121.66	126.39
3	A	211	CLA	CHB-C1B-NB	-2.09	120.92	124.05
3	B	308	CLA	CHB-C1B-NB	-2.09	120.92	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	211	CLA	CHB-C1B-NB	-2.09	120.92	124.05
3	D	308	CLA	CHB-C1B-NB	-2.09	120.92	124.05
3	D	309	CLA	CHB-C1B-NB	-2.09	120.92	124.05
3	A	205	CLA	C2C-C1C-NC	2.09	112.17	109.98
3	C	205	CLA	C2C-C1C-NC	2.09	112.17	109.98
3	A	202	CLA	CHA-C1A-NA	-2.08	121.67	126.39
3	B	309	CLA	CHB-C1B-NB	-2.08	120.93	124.05
3	B	309	CLA	C2A-C3A-C4A	-2.08	98.52	101.87
3	C	202	CLA	CHA-C1A-NA	-2.08	121.69	126.39
3	B	304	CLA	C1-C2-C3	-2.08	122.80	126.20
3	D	304	CLA	C1-C2-C3	-2.08	122.80	126.20
3	C	203	CLA	CHB-C1B-NB	-2.07	120.94	124.05
3	C	212	CLA	C1-C2-C3	-2.07	122.80	126.20
3	B	306	CLA	C2C-C1C-NC	2.07	112.16	109.98
3	D	306	CLA	C2C-C1C-NC	2.07	112.16	109.98
3	A	209	CLA	CHB-C1B-NB	-2.07	120.95	124.05
3	C	209	CLA	CHB-C1B-NB	-2.07	120.95	124.05
3	D	303	CLA	CHB-C1B-NB	-2.07	120.95	124.05
3	A	203	CLA	C2C-C1C-NC	2.06	112.15	109.98
3	C	203	CLA	C2C-C1C-NC	2.06	112.15	109.98
3	D	309	CLA	C2A-C3A-C4A	-2.06	98.54	101.87
5	A	214	XAT	O4-C5-C4	-2.06	111.56	113.49
3	A	206	CLA	CHB-C1B-NB	-2.05	120.97	124.05
3	B	304	CLA	CHB-C1B-NB	-2.05	120.97	124.05
3	D	304	CLA	CHB-C1B-NB	-2.05	120.97	124.05
3	D	311	CLA	CHB-C1B-NB	-2.05	120.98	124.05
3	A	201	CLA	C2C-C1C-NC	2.05	112.13	109.98
3	B	306	CLA	CHB-C1B-NB	-2.05	120.98	124.05
3	D	306	CLA	CHB-C1B-NB	-2.05	120.98	124.05
3	C	206	CLA	CHB-C1B-NB	-2.05	120.98	124.05
3	A	205	CLA	CHB-C1B-NB	-2.04	120.99	124.05
3	C	205	CLA	CHB-C1B-NB	-2.04	120.99	124.05
4	A	213	A1L1F	O15-C20-C21	-2.03	111.58	113.49
3	A	202	CLA	CHB-C1B-NB	-2.03	121.00	124.05
3	C	202	CLA	CHB-C1B-NB	-2.03	121.00	124.05
3	A	207	CLA	CHA-C1A-NA	-2.03	121.79	126.39
3	B	303	CLA	CHB-C1B-NB	-2.03	121.00	124.05
3	C	207	CLA	CHA-C1A-NA	-2.03	121.80	126.39
3	A	212	CLA	C1-C2-C3	-2.03	122.88	126.20
3	C	201	CLA	C2C-C1C-NC	2.02	112.11	109.98
4	C	213	A1L1F	O15-C20-C21	-2.02	111.60	113.49
3	B	311	CLA	CHB-C1B-NB	-2.00	121.05	124.05

All (84) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	201	CLA	ND
3	A	201	CLA	C8
3	A	202	CLA	ND
3	A	202	CLA	C8
3	A	203	CLA	ND
3	A	203	CLA	C8
3	A	204	CLA	ND
3	A	204	CLA	C8
3	A	205	CLA	ND
3	A	205	CLA	C8
3	A	206	CLA	ND
3	A	206	CLA	C8
3	A	207	CLA	ND
3	A	208	CLA	ND
3	A	209	CLA	ND
3	A	209	CLA	C8
3	A	210	CLA	ND
3	A	210	CLA	C8
3	A	211	CLA	ND
3	A	211	CLA	C8
3	A	212	CLA	ND
3	A	212	CLA	C8
3	B	301	CLA	ND
3	B	301	CLA	C8
3	B	302	CLA	ND
3	B	302	CLA	C8
3	B	303	CLA	ND
3	B	303	CLA	C8
3	B	304	CLA	ND
3	B	304	CLA	C8
3	B	305	CLA	ND
3	B	305	CLA	C8
3	B	306	CLA	ND
3	B	306	CLA	C8
3	B	307	CLA	ND
3	B	307	CLA	C8
3	B	308	CLA	ND
3	B	309	CLA	ND
3	B	309	CLA	C8
3	B	310	CLA	ND
3	B	310	CLA	C8
3	B	311	CLA	ND

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Mol	Chain	Res	Type	Atom
3	C	201	CLA	ND
3	C	201	CLA	C8
3	C	202	CLA	ND
3	C	202	CLA	C8
3	C	203	CLA	ND
3	C	203	CLA	C8
3	C	204	CLA	ND
3	C	204	CLA	C8
3	C	205	CLA	ND
3	C	205	CLA	C8
3	C	206	CLA	ND
3	C	206	CLA	C8
3	C	207	CLA	ND
3	C	208	CLA	ND
3	C	209	CLA	ND
3	C	209	CLA	C8
3	C	210	CLA	ND
3	C	210	CLA	C8
3	C	211	CLA	ND
3	C	211	CLA	C8
3	C	212	CLA	ND
3	C	212	CLA	C8
3	D	301	CLA	ND
3	D	301	CLA	C8
3	D	302	CLA	ND
3	D	302	CLA	C8
3	D	303	CLA	ND
3	D	303	CLA	C8
3	D	304	CLA	ND
3	D	304	CLA	C8
3	D	305	CLA	ND
3	D	305	CLA	C8
3	D	306	CLA	ND
3	D	306	CLA	C8
3	D	307	CLA	ND
3	D	307	CLA	C8
3	D	308	CLA	ND
3	D	309	CLA	ND
3	D	309	CLA	C8
3	D	310	CLA	ND
3	D	310	CLA	C8
3	D	311	CLA	ND

All (302) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	204	CLA	C1A-C2A-CAA-CBA
3	A	205	CLA	CHA-CBD-CGD-O1D
3	A	205	CLA	CHA-CBD-CGD-O2D
3	A	207	CLA	CHA-CBD-CGD-O1D
3	A	207	CLA	CHA-CBD-CGD-O2D
3	A	208	CLA	C1A-C2A-CAA-CBA
3	A	210	CLA	C1A-C2A-CAA-CBA
3	A	210	CLA	C3A-C2A-CAA-CBA
3	A	210	CLA	C2B-C3B-CAB-CBB
3	A	210	CLA	C4B-C3B-CAB-CBB
3	A	211	CLA	C2B-C3B-CAB-CBB
3	A	211	CLA	C4B-C3B-CAB-CBB
3	B	305	CLA	CHA-CBD-CGD-O1D
3	B	305	CLA	CHA-CBD-CGD-O2D
3	B	306	CLA	C1A-C2A-CAA-CBA
3	B	307	CLA	CHA-CBD-CGD-O2D
3	B	308	CLA	C2B-C3B-CAB-CBB
3	B	308	CLA	C4B-C3B-CAB-CBB
3	B	309	CLA	C2B-C3B-CAB-CBB
3	B	309	CLA	C4B-C3B-CAB-CBB
3	C	204	CLA	C1A-C2A-CAA-CBA
3	C	205	CLA	CHA-CBD-CGD-O1D
3	C	205	CLA	CHA-CBD-CGD-O2D
3	C	207	CLA	CHA-CBD-CGD-O1D
3	C	207	CLA	CHA-CBD-CGD-O2D
3	C	208	CLA	C1A-C2A-CAA-CBA
3	C	210	CLA	C1A-C2A-CAA-CBA
3	C	210	CLA	C3A-C2A-CAA-CBA
3	C	210	CLA	C2B-C3B-CAB-CBB
3	C	210	CLA	C4B-C3B-CAB-CBB
3	C	211	CLA	C2B-C3B-CAB-CBB
3	C	211	CLA	C4B-C3B-CAB-CBB
3	D	305	CLA	CHA-CBD-CGD-O1D
3	D	305	CLA	CHA-CBD-CGD-O2D
3	D	306	CLA	C1A-C2A-CAA-CBA
3	D	307	CLA	CHA-CBD-CGD-O2D
3	D	308	CLA	C2B-C3B-CAB-CBB
3	D	308	CLA	C4B-C3B-CAB-CBB
3	D	309	CLA	C2B-C3B-CAB-CBB
3	D	309	CLA	C4B-C3B-CAB-CBB
4	A	213	A1L1F	C14-C29-C30-C31
4	B	312	A1L1F	C29-C14-C25-C20

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Mol	Chain	Res	Type	Atoms
4	C	213	A1L1F	C14-C29-C30-C31
4	D	312	A1L1F	C29-C14-C25-C20
5	A	216	XAT	O24-C26-C27-C28
5	C	216	XAT	O24-C26-C27-C28
3	B	310	CLA	C4-C3-C5-C6
3	D	310	CLA	C4-C3-C5-C6
3	B	310	CLA	C2-C3-C5-C6
3	D	310	CLA	C2-C3-C5-C6
3	A	206	CLA	C4-C3-C5-C6
3	C	206	CLA	C4-C3-C5-C6
3	A	206	CLA	C2-C3-C5-C6
3	C	206	CLA	C2-C3-C5-C6
3	A	205	CLA	C6-C7-C8-C9
3	C	205	CLA	C6-C7-C8-C9
3	B	306	CLA	C3-C5-C6-C7
3	D	306	CLA	C3-C5-C6-C7
3	A	210	CLA	C2A-CAA-CBA-CGA
3	B	305	CLA	C2A-CAA-CBA-CGA
3	C	210	CLA	C2A-CAA-CBA-CGA
3	D	305	CLA	C2A-CAA-CBA-CGA
3	A	201	CLA	C5-C6-C7-C8
3	C	201	CLA	C5-C6-C7-C8
3	A	204	CLA	C8-C10-C11-C12
3	C	204	CLA	C8-C10-C11-C12
3	A	210	CLA	C8-C10-C11-C12
3	C	210	CLA	C8-C10-C11-C12
3	A	211	CLA	C3-C5-C6-C7
3	C	211	CLA	C3-C5-C6-C7
3	A	202	CLA	C4B-C3B-CAB-CBB
3	A	204	CLA	C4B-C3B-CAB-CBB
3	B	306	CLA	C4B-C3B-CAB-CBB
3	B	310	CLA	C4B-C3B-CAB-CBB
3	B	311	CLA	C4B-C3B-CAB-CBB
3	C	202	CLA	C4B-C3B-CAB-CBB
3	C	204	CLA	C4B-C3B-CAB-CBB
3	D	306	CLA	C4B-C3B-CAB-CBB
3	D	310	CLA	C4B-C3B-CAB-CBB
3	D	311	CLA	C4B-C3B-CAB-CBB
3	A	210	CLA	C5-C6-C7-C8
3	C	210	CLA	C5-C6-C7-C8
3	B	310	CLA	C2B-C3B-CAB-CBB
3	B	311	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
3	D	310	CLA	C2B-C3B-CAB-CBB
3	D	311	CLA	C2B-C3B-CAB-CBB
3	A	203	CLA	C6-C7-C8-C9
3	A	209	CLA	C6-C7-C8-C9
3	C	203	CLA	C6-C7-C8-C9
3	C	209	CLA	C6-C7-C8-C9
3	D	310	CLA	C13-C15-C16-C17
3	B	310	CLA	C13-C15-C16-C17
3	A	209	CLA	C1A-C2A-CAA-CBA
3	B	308	CLA	C1A-C2A-CAA-CBA
3	B	310	CLA	C1A-C2A-CAA-CBA
3	C	209	CLA	C1A-C2A-CAA-CBA
3	D	308	CLA	C1A-C2A-CAA-CBA
3	D	310	CLA	C1A-C2A-CAA-CBA
3	A	202	CLA	C4-C3-C5-C6
3	C	202	CLA	C4-C3-C5-C6
3	A	202	CLA	C2-C3-C5-C6
3	C	202	CLA	C2-C3-C5-C6
3	A	208	CLA	C2A-CAA-CBA-CGA
3	C	208	CLA	C2A-CAA-CBA-CGA
3	A	207	CLA	C2-C3-C5-C6
3	C	207	CLA	C2-C3-C5-C6
3	A	204	CLA	C4-C3-C5-C6
3	A	209	CLA	C4-C3-C5-C6
3	C	204	CLA	C4-C3-C5-C6
3	C	209	CLA	C4-C3-C5-C6
3	A	203	CLA	C4B-C3B-CAB-CBB
3	A	208	CLA	C4B-C3B-CAB-CBB
3	A	212	CLA	C4B-C3B-CAB-CBB
3	B	304	CLA	C4B-C3B-CAB-CBB
3	C	203	CLA	C4B-C3B-CAB-CBB
3	C	208	CLA	C4B-C3B-CAB-CBB
3	C	212	CLA	C4B-C3B-CAB-CBB
3	D	303	CLA	C4B-C3B-CAB-CBB
3	D	304	CLA	C4B-C3B-CAB-CBB
3	A	201	CLA	C11-C12-C13-C15
3	A	204	CLA	C11-C12-C13-C15
3	B	310	CLA	C6-C7-C8-C10
3	C	201	CLA	C11-C12-C13-C15
3	C	204	CLA	C11-C12-C13-C15
3	D	310	CLA	C6-C7-C8-C10
3	A	207	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
3	B	303	CLA	C3A-C2A-CAA-CBA
3	C	207	CLA	C4-C3-C5-C6
3	D	303	CLA	C3A-C2A-CAA-CBA
3	A	204	CLA	C2-C3-C5-C6
3	C	204	CLA	C2-C3-C5-C6
3	A	209	CLA	C2-C3-C5-C6
3	C	209	CLA	C2-C3-C5-C6
4	B	312	A1L1F	C14-C29-C30-C31
4	D	312	A1L1F	C14-C29-C30-C31
3	A	202	CLA	C3-C5-C6-C7
3	C	202	CLA	C3-C5-C6-C7
3	A	212	CLA	C5-C6-C7-C8
3	C	212	CLA	C5-C6-C7-C8
3	A	201	CLA	C11-C12-C13-C14
3	B	305	CLA	C6-C7-C8-C9
3	C	201	CLA	C11-C12-C13-C14
3	D	305	CLA	C6-C7-C8-C9
4	A	215	A1L1F	O13-C26-C30-C29
4	C	215	A1L1F	O13-C26-C30-C29
3	A	210	CLA	C4-C3-C5-C6
3	C	210	CLA	C4-C3-C5-C6
3	B	303	CLA	C4B-C3B-CAB-CBB
3	B	309	CLA	C1A-C2A-CAA-CBA
3	D	309	CLA	C1A-C2A-CAA-CBA
4	A	215	A1L1F	O13-C26-C30-C31
4	C	215	A1L1F	O13-C26-C30-C31
3	A	202	CLA	C6-C7-C8-C10
3	C	202	CLA	C6-C7-C8-C10
3	B	310	CLA	C6-C7-C8-C9
3	D	310	CLA	C6-C7-C8-C9
3	A	203	CLA	CAD-CBD-CGD-O2D
3	C	203	CLA	CAD-CBD-CGD-O2D
3	A	203	CLA	CAD-CBD-CGD-O1D
3	B	302	CLA	CHA-CBD-CGD-O2D
3	B	307	CLA	CHA-CBD-CGD-O1D
3	C	203	CLA	CAD-CBD-CGD-O1D
3	D	302	CLA	CHA-CBD-CGD-O2D
3	D	307	CLA	CHA-CBD-CGD-O1D
3	A	202	CLA	C2B-C3B-CAB-CBB
3	A	204	CLA	C2B-C3B-CAB-CBB
3	A	212	CLA	C2B-C3B-CAB-CBB
3	B	306	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
3	C	202	CLA	C2B-C3B-CAB-CBB
3	C	204	CLA	C2B-C3B-CAB-CBB
3	C	212	CLA	C2B-C3B-CAB-CBB
3	D	306	CLA	C2B-C3B-CAB-CBB
3	B	304	CLA	C11-C10-C8-C9
3	D	304	CLA	C11-C10-C8-C9
3	B	310	CLA	C15-C16-C17-C18
3	D	310	CLA	C15-C16-C17-C18
3	B	304	CLA	CAA-CBA-CGA-O2A
3	B	305	CLA	CAA-CBA-CGA-O2A
3	D	304	CLA	CAA-CBA-CGA-O2A
3	D	305	CLA	CAA-CBA-CGA-O2A
3	B	303	CLA	CAA-CBA-CGA-O2A
3	D	303	CLA	CAA-CBA-CGA-O2A
3	B	301	CLA	C4-C3-C5-C6
3	D	301	CLA	C4-C3-C5-C6
3	A	204	CLA	C11-C12-C13-C14
3	C	204	CLA	C11-C12-C13-C14
3	A	204	CLA	C11-C10-C8-C7
3	B	304	CLA	C11-C10-C8-C7
3	C	204	CLA	C11-C10-C8-C7
3	D	304	CLA	C11-C10-C8-C7
3	A	210	CLA	C2-C3-C5-C6
3	C	210	CLA	C2-C3-C5-C6
4	B	312	A1L1F	C14-C29-C30-C26
4	D	312	A1L1F	C14-C29-C30-C26
3	A	212	CLA	C4-C3-C5-C6
3	C	212	CLA	C4-C3-C5-C6
3	B	301	CLA	C14-C13-C15-C16
3	D	301	CLA	C14-C13-C15-C16
3	C	202	CLA	C5-C6-C7-C8
3	B	301	CLA	C2-C3-C5-C6
3	D	301	CLA	C2-C3-C5-C6
3	A	202	CLA	C5-C6-C7-C8
3	B	303	CLA	C1A-C2A-CAA-CBA
3	D	303	CLA	C1A-C2A-CAA-CBA
3	A	201	CLA	C2B-C3B-CAB-CBB
3	B	301	CLA	C2B-C3B-CAB-CBB
3	B	304	CLA	C2B-C3B-CAB-CBB
3	C	201	CLA	C2B-C3B-CAB-CBB
3	D	301	CLA	C2B-C3B-CAB-CBB
3	D	304	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
3	A	203	CLA	C4-C3-C5-C6
3	C	201	CLA	C4-C3-C5-C6
3	C	203	CLA	C4-C3-C5-C6
3	A	211	CLA	C2A-CAA-CBA-CGA
3	C	211	CLA	C2A-CAA-CBA-CGA
3	A	201	CLA	C4-C3-C5-C6
3	A	203	CLA	C2-C3-C5-C6
3	C	203	CLA	C2-C3-C5-C6
3	B	306	CLA	C4-C3-C5-C6
3	D	306	CLA	C4-C3-C5-C6
3	B	301	CLA	C4B-C3B-CAB-CBB
3	D	301	CLA	C4B-C3B-CAB-CBB
3	B	303	CLA	C11-C12-C13-C14
3	D	303	CLA	C11-C12-C13-C14
3	A	204	CLA	C3A-C2A-CAA-CBA
3	B	304	CLA	C3A-C2A-CAA-CBA
3	C	204	CLA	C3A-C2A-CAA-CBA
3	D	304	CLA	C3A-C2A-CAA-CBA
4	A	213	A1L1F	C29-C14-C25-O15
4	B	312	A1L1F	C29-C14-C25-O15
4	C	213	A1L1F	C29-C14-C25-O15
4	D	312	A1L1F	C29-C14-C25-O15
3	A	202	CLA	C6-C7-C8-C9
3	C	202	CLA	C6-C7-C8-C9
3	A	203	CLA	C6-C7-C8-C10
3	A	205	CLA	C6-C7-C8-C10
3	A	209	CLA	C11-C10-C8-C7
3	A	212	CLA	C6-C7-C8-C10
3	C	203	CLA	C6-C7-C8-C10
3	C	205	CLA	C6-C7-C8-C10
3	C	209	CLA	C11-C10-C8-C7
3	C	212	CLA	C6-C7-C8-C10
3	A	203	CLA	C2B-C3B-CAB-CBB
3	A	206	CLA	C2B-C3B-CAB-CBB
3	A	208	CLA	C2B-C3B-CAB-CBB
3	B	302	CLA	C2B-C3B-CAB-CBB
3	B	303	CLA	C2B-C3B-CAB-CBB
3	C	203	CLA	C2B-C3B-CAB-CBB
3	C	206	CLA	C2B-C3B-CAB-CBB
3	C	208	CLA	C2B-C3B-CAB-CBB
3	D	302	CLA	C2B-C3B-CAB-CBB
3	D	303	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
3	A	202	CLA	CAA-CBA-CGA-O2A
3	C	202	CLA	CAA-CBA-CGA-O2A
4	C	213	A1L1F	O13-C45-C47-C48
4	A	213	A1L1F	O13-C45-C47-C48
3	A	212	CLA	C2-C3-C5-C6
3	C	212	CLA	C2-C3-C5-C6
3	B	310	CLA	C11-C12-C13-C14
3	D	310	CLA	C11-C12-C13-C14
3	A	201	CLA	C4B-C3B-CAB-CBB
3	A	206	CLA	C4B-C3B-CAB-CBB
3	A	211	CLA	C1A-C2A-CAA-CBA
3	B	302	CLA	C4B-C3B-CAB-CBB
3	C	201	CLA	C4B-C3B-CAB-CBB
3	C	206	CLA	C4B-C3B-CAB-CBB
3	C	211	CLA	C1A-C2A-CAA-CBA
3	D	302	CLA	C4B-C3B-CAB-CBB
3	A	204	CLA	CAA-CBA-CGA-O2A
3	B	302	CLA	CAA-CBA-CGA-O2A
3	D	302	CLA	CAA-CBA-CGA-O2A
5	B	315	XAT	C11-C12-C13-C14
5	D	315	XAT	C11-C12-C13-C14
3	C	204	CLA	CAA-CBA-CGA-O2A
3	A	204	CLA	C10-C11-C12-C13
3	C	204	CLA	C10-C11-C12-C13
3	A	212	CLA	C2A-CAA-CBA-CGA
3	C	212	CLA	C2A-CAA-CBA-CGA
3	A	208	CLA	C3A-C2A-CAA-CBA
3	A	209	CLA	C3A-C2A-CAA-CBA
3	A	211	CLA	C3A-C2A-CAA-CBA
3	B	309	CLA	C3A-C2A-CAA-CBA
3	B	310	CLA	C3A-C2A-CAA-CBA
3	C	208	CLA	C3A-C2A-CAA-CBA
3	C	209	CLA	C3A-C2A-CAA-CBA
3	C	211	CLA	C3A-C2A-CAA-CBA
3	D	309	CLA	C3A-C2A-CAA-CBA
3	D	310	CLA	C3A-C2A-CAA-CBA
3	A	202	CLA	CAA-CBA-CGA-O1A
3	C	202	CLA	CAA-CBA-CGA-O1A
3	B	302	CLA	CAA-CBA-CGA-O1A
3	D	302	CLA	CAA-CBA-CGA-O1A
4	C	213	A1L1F	O46-C45-C47-C48
4	A	213	A1L1F	O46-C45-C47-C48

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Mol	Chain	Res	Type	Atoms
3	A	203	CLA	C2A-CAA-CBA-CGA
3	C	203	CLA	C2A-CAA-CBA-CGA
3	A	204	CLA	CAA-CBA-CGA-O1A
3	C	204	CLA	CAA-CBA-CGA-O1A
3	A	211	CLA	CAA-CBA-CGA-O2A
3	C	211	CLA	CAA-CBA-CGA-O2A
4	B	312	A1L1F	O13-C45-C47-C48
4	D	312	A1L1F	O13-C45-C47-C48

There are no ring outliers.

50 monomers are involved in 85 short contacts:

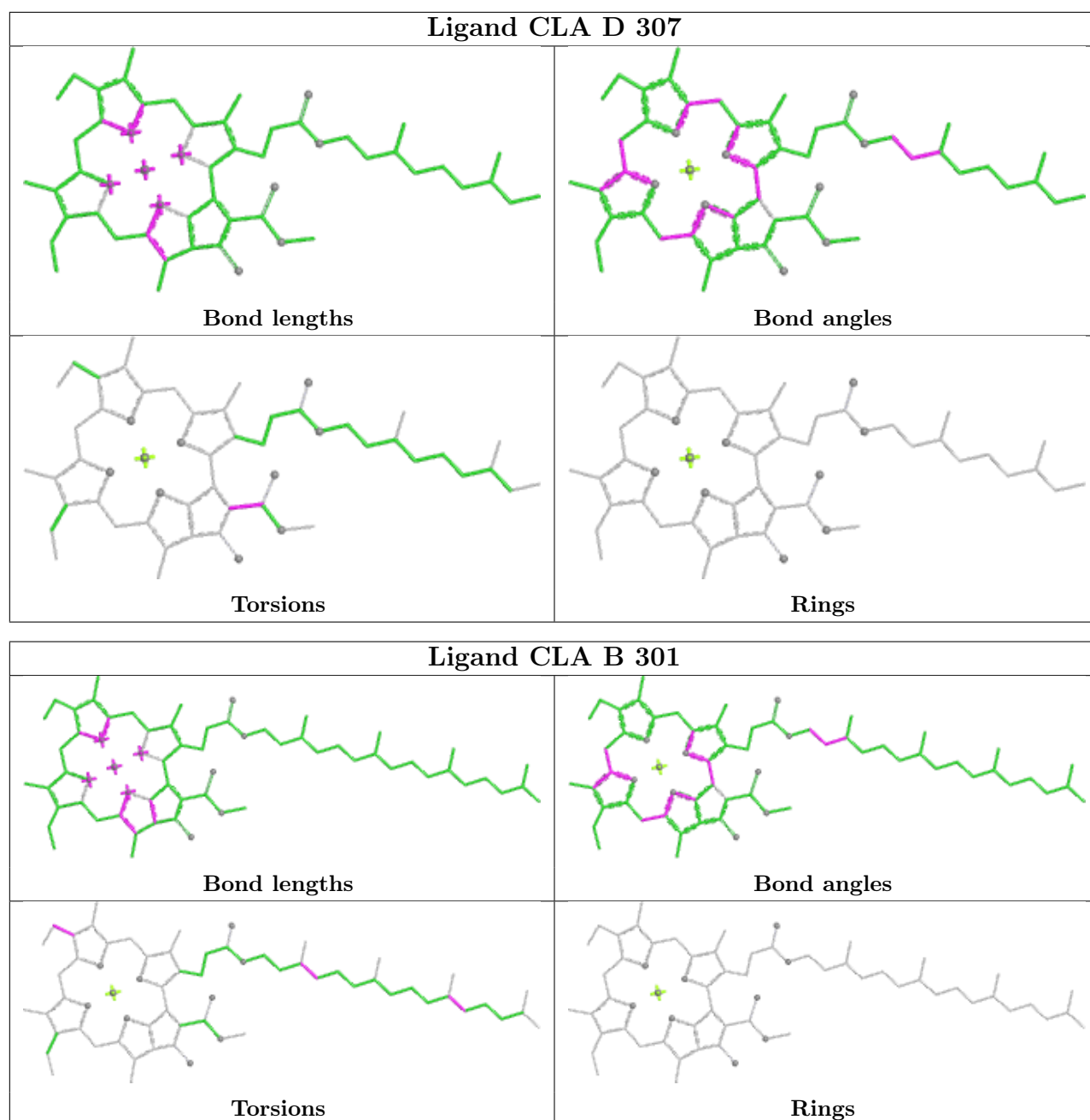
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	307	CLA	3	0
3	B	301	CLA	2	0
3	D	305	CLA	2	0
3	A	203	CLA	2	0
5	B	315	XAT	2	0
3	B	308	CLA	1	0
3	B	303	CLA	4	0
3	D	310	CLA	4	0
3	C	209	CLA	3	0
4	A	213	A1L1F	1	0
3	D	308	CLA	1	0
3	C	205	CLA	2	0
4	C	213	A1L1F	1	0
5	B	314	XAT	1	0
3	A	204	CLA	2	0
3	A	211	CLA	1	0
3	B	309	CLA	1	0
3	A	202	CLA	1	0
5	C	214	XAT	5	0
3	B	306	CLA	2	0
3	A	205	CLA	2	0
3	C	210	CLA	3	0
3	A	201	CLA	2	0
4	A	215	A1L1F	1	0
5	D	313	XAT	3	0
3	C	212	CLA	1	0
4	C	215	A1L1F	1	0
5	B	313	XAT	4	0
5	D	314	XAT	1	0

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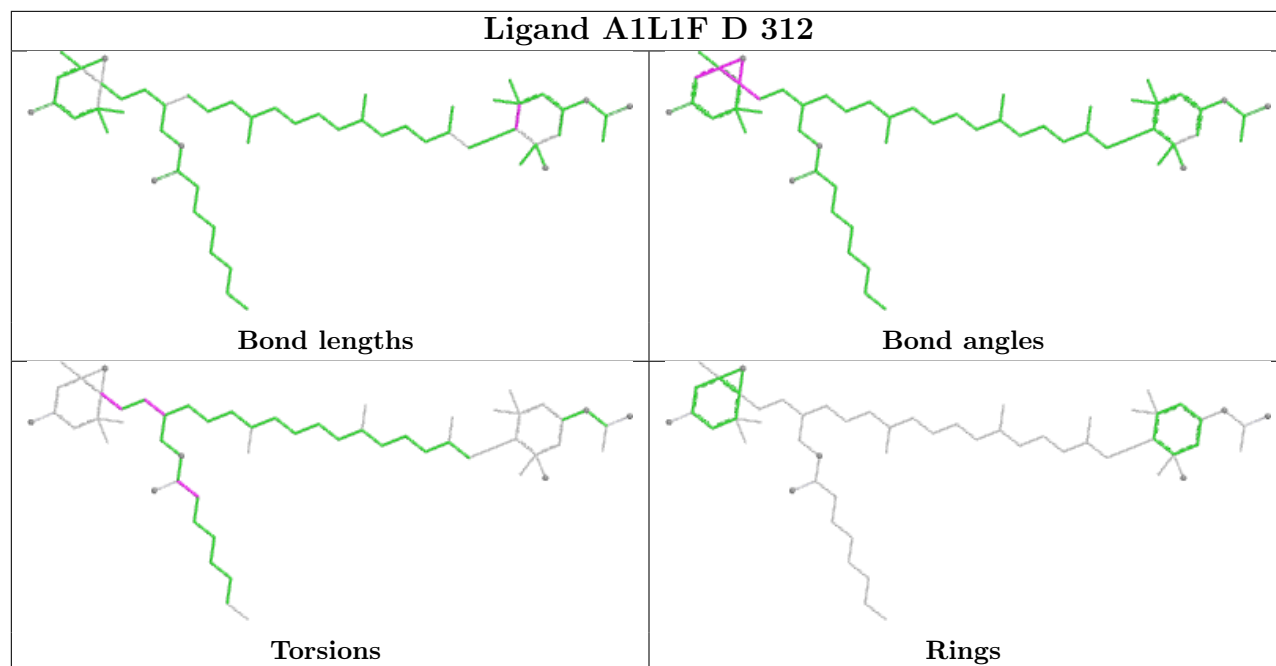
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	305	CLA	2	0
3	A	209	CLA	3	0
3	D	302	CLA	1	0
3	D	309	CLA	1	0
5	A	214	XAT	5	0
3	C	204	CLA	2	0
3	B	310	CLA	4	0
3	B	304	CLA	3	0
3	C	211	CLA	1	0
3	D	306	CLA	2	0
5	D	315	XAT	2	0
3	B	307	CLA	3	0
3	B	302	CLA	1	0
3	D	301	CLA	1	0
3	A	212	CLA	1	0
3	C	202	CLA	1	0
3	D	303	CLA	4	0
3	C	203	CLA	2	0
3	A	210	CLA	3	0
3	D	304	CLA	3	0
3	C	201	CLA	2	0

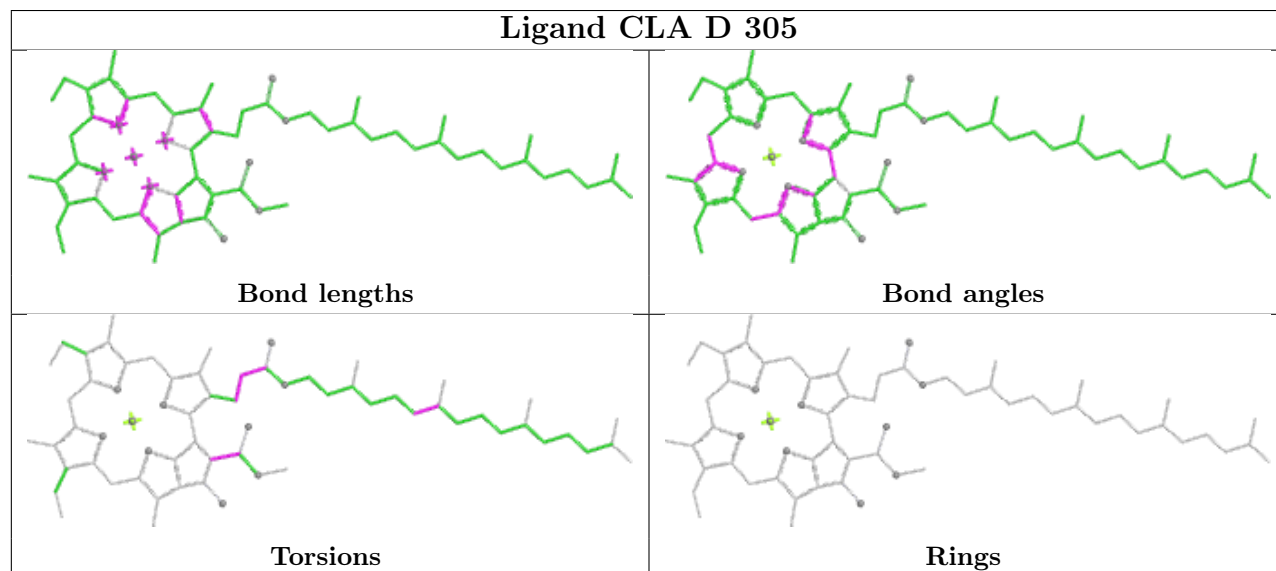
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

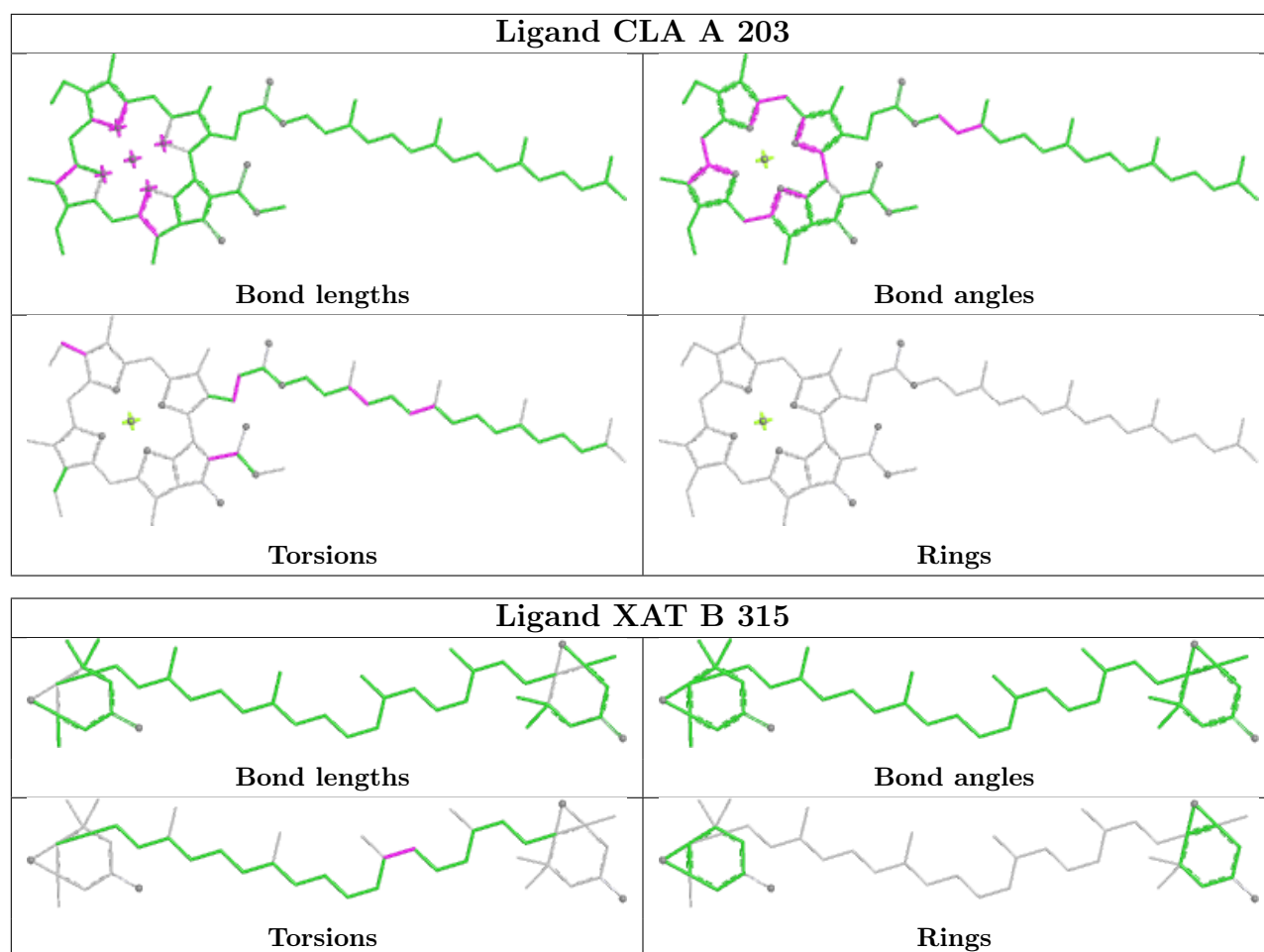


Ligand A1L1F D 312

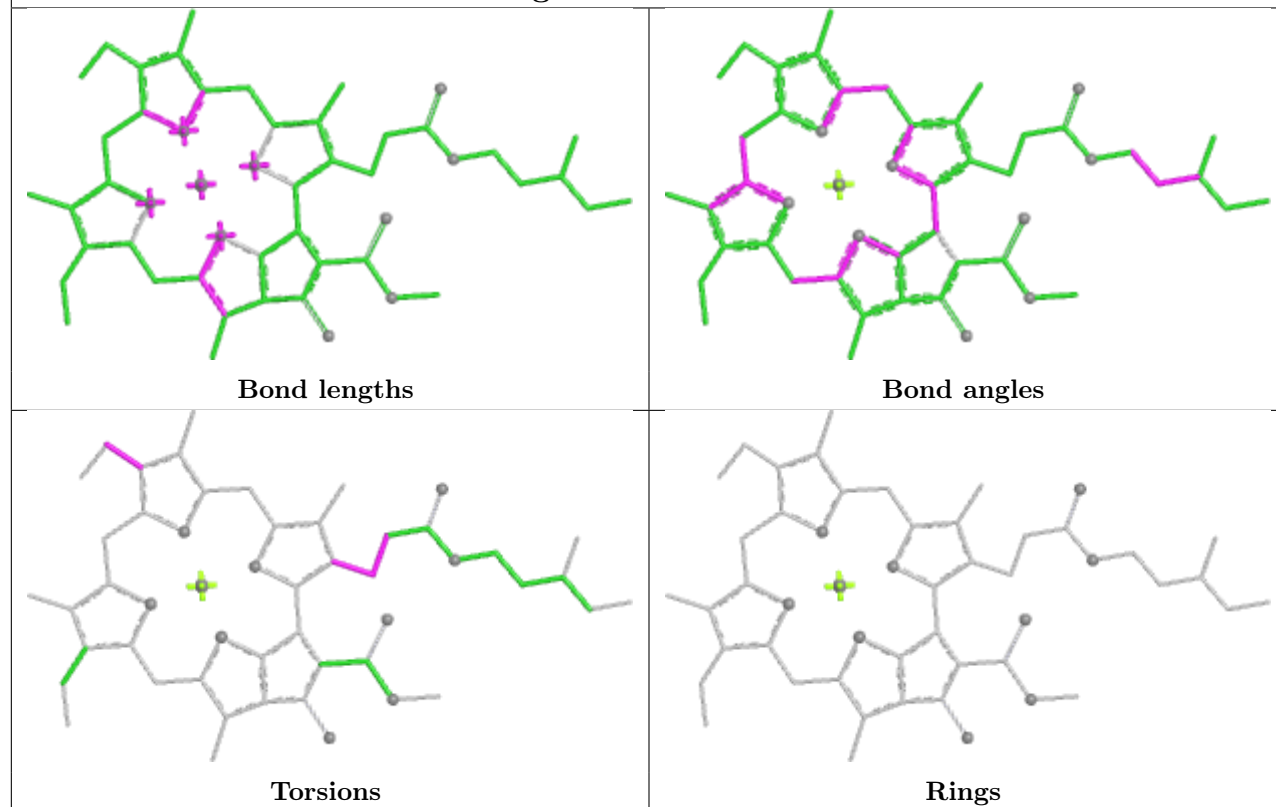


Ligand CLA D 305

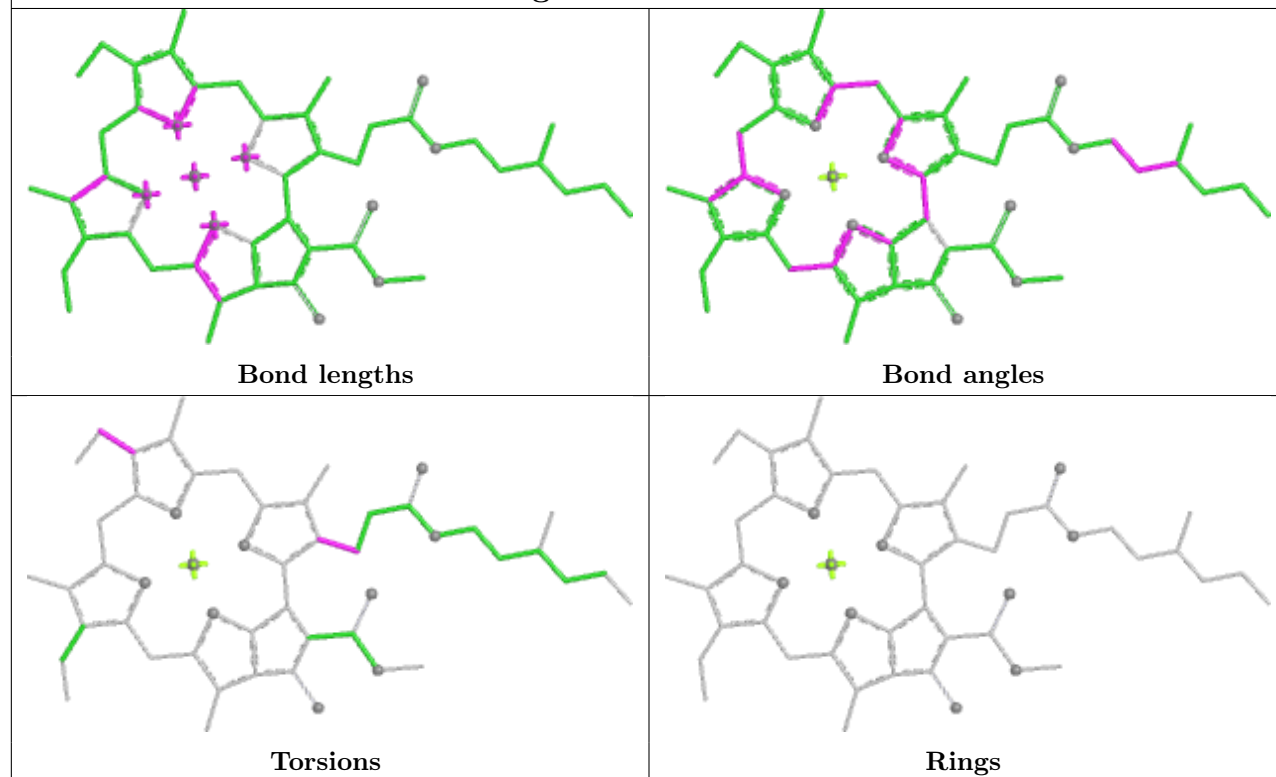


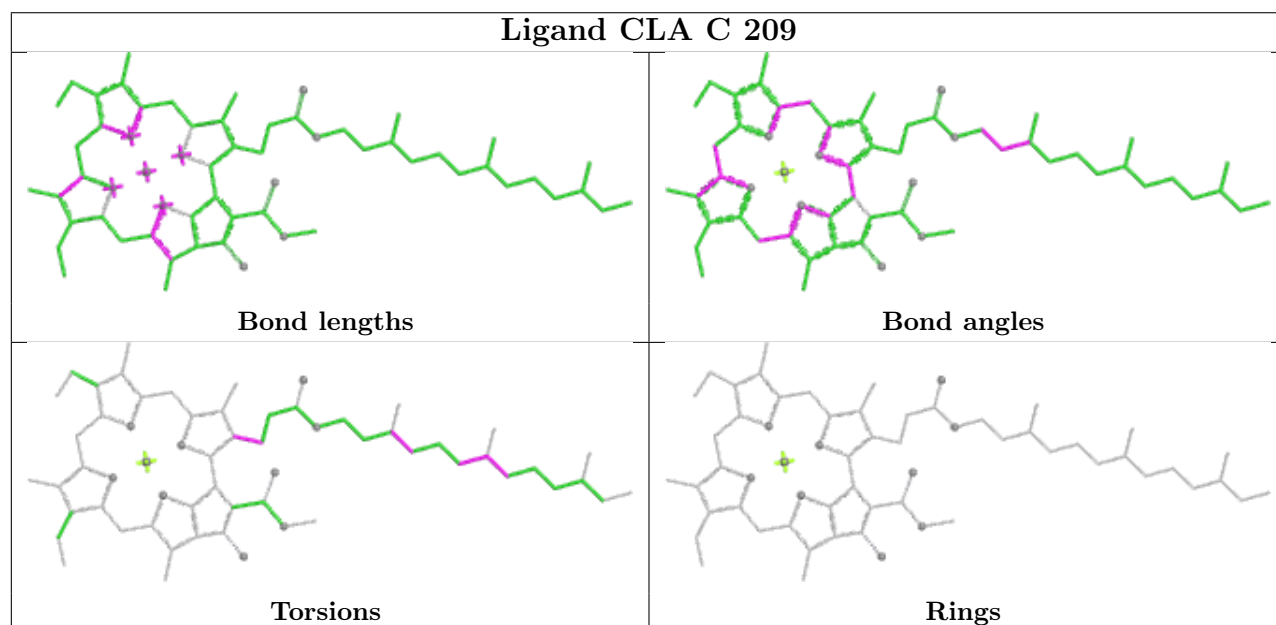
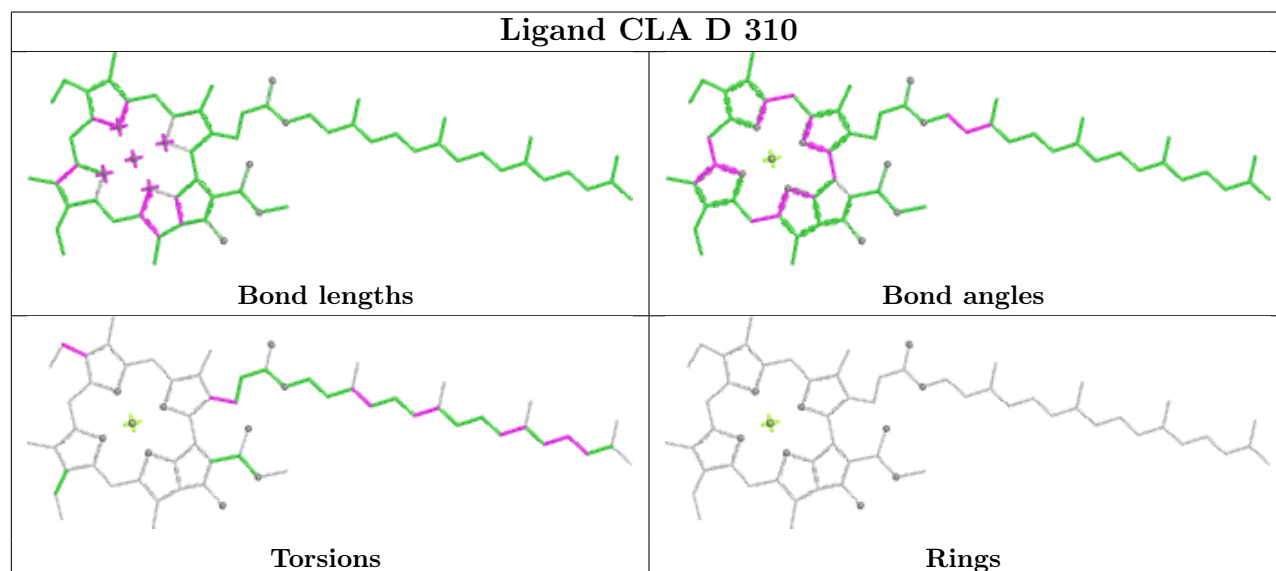
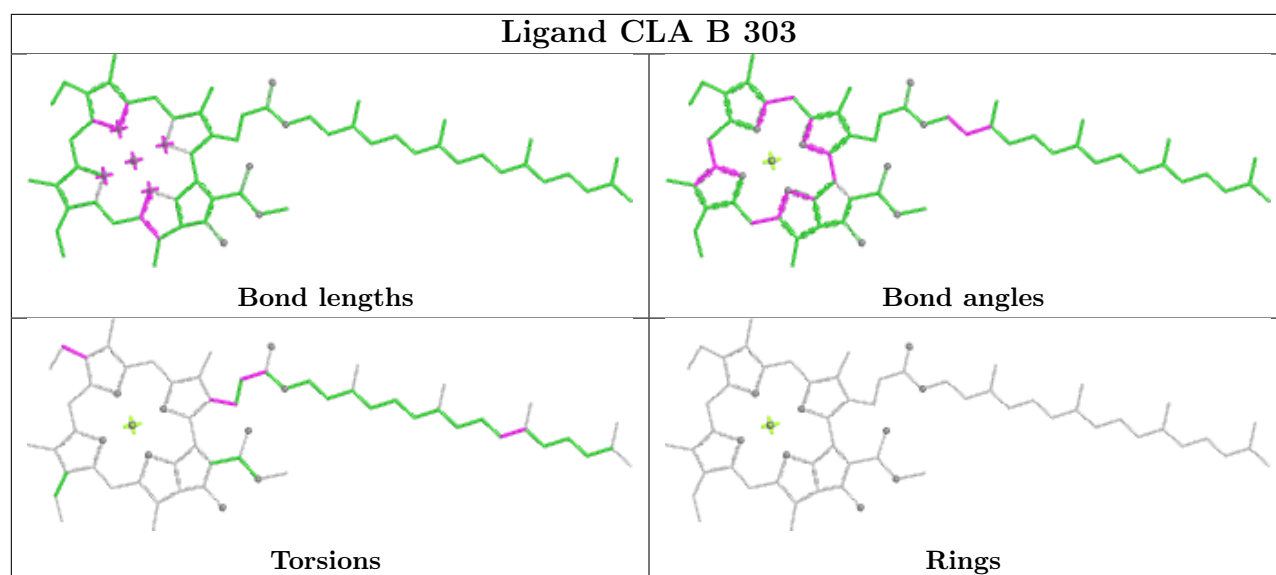


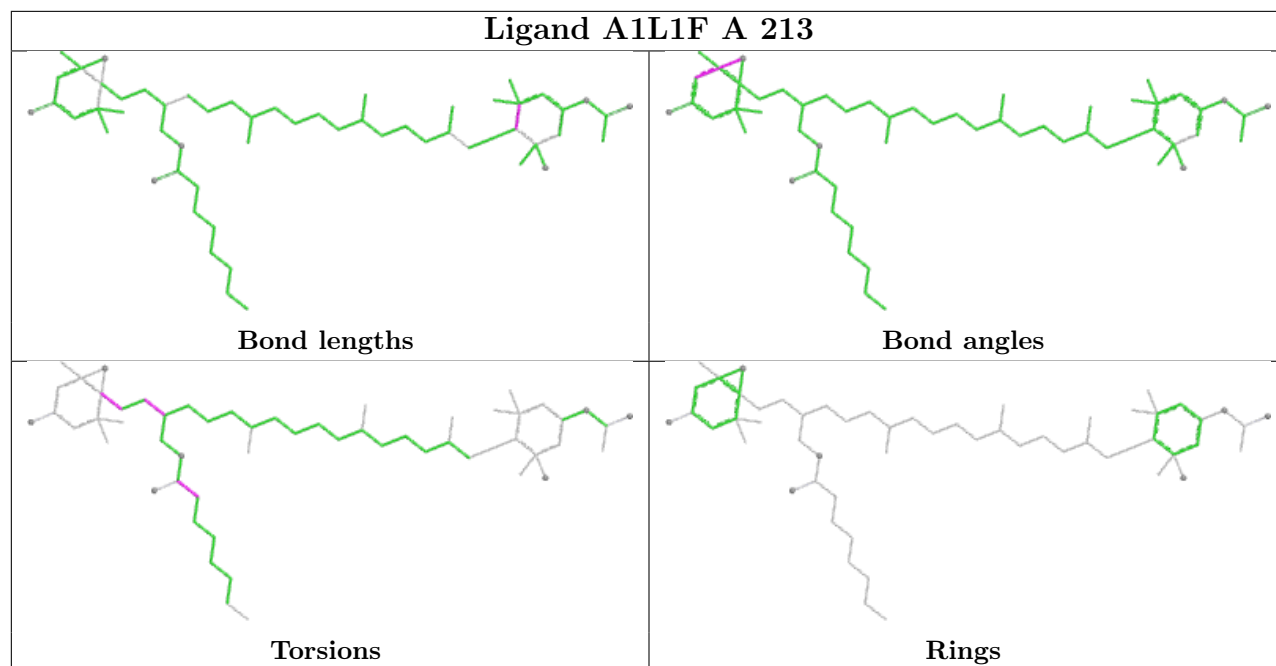
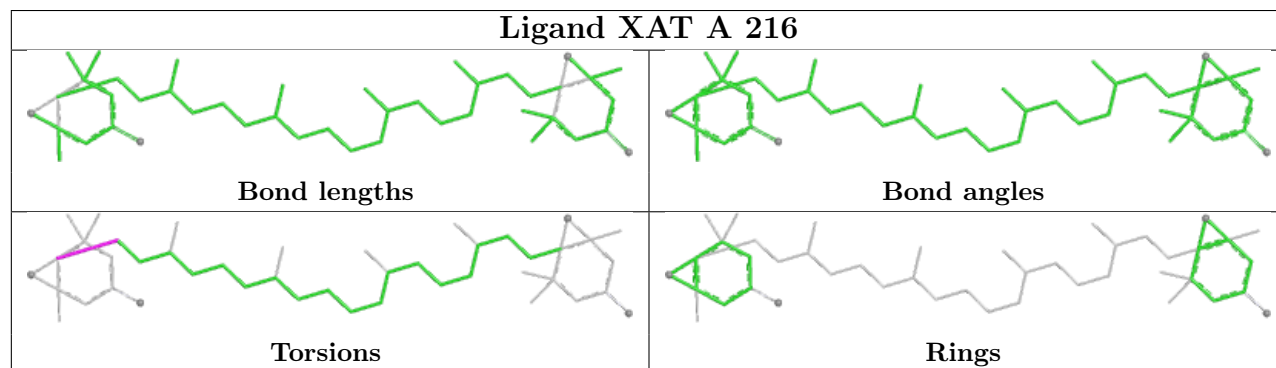
Ligand CLA C 208

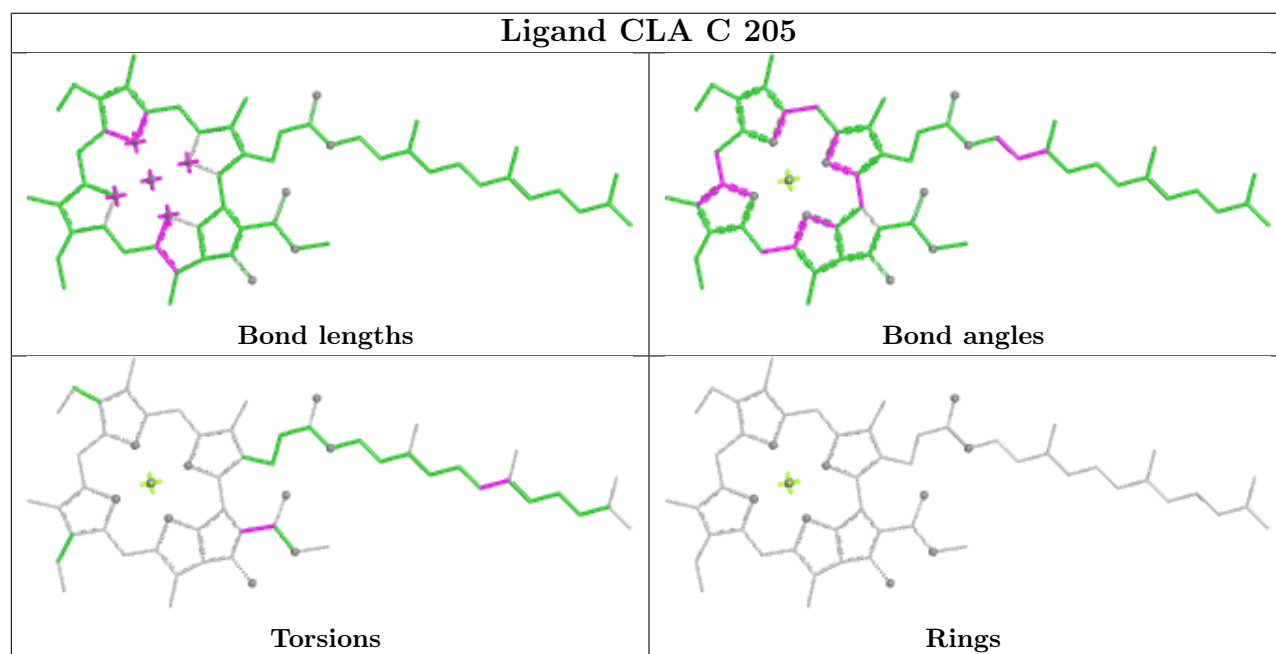
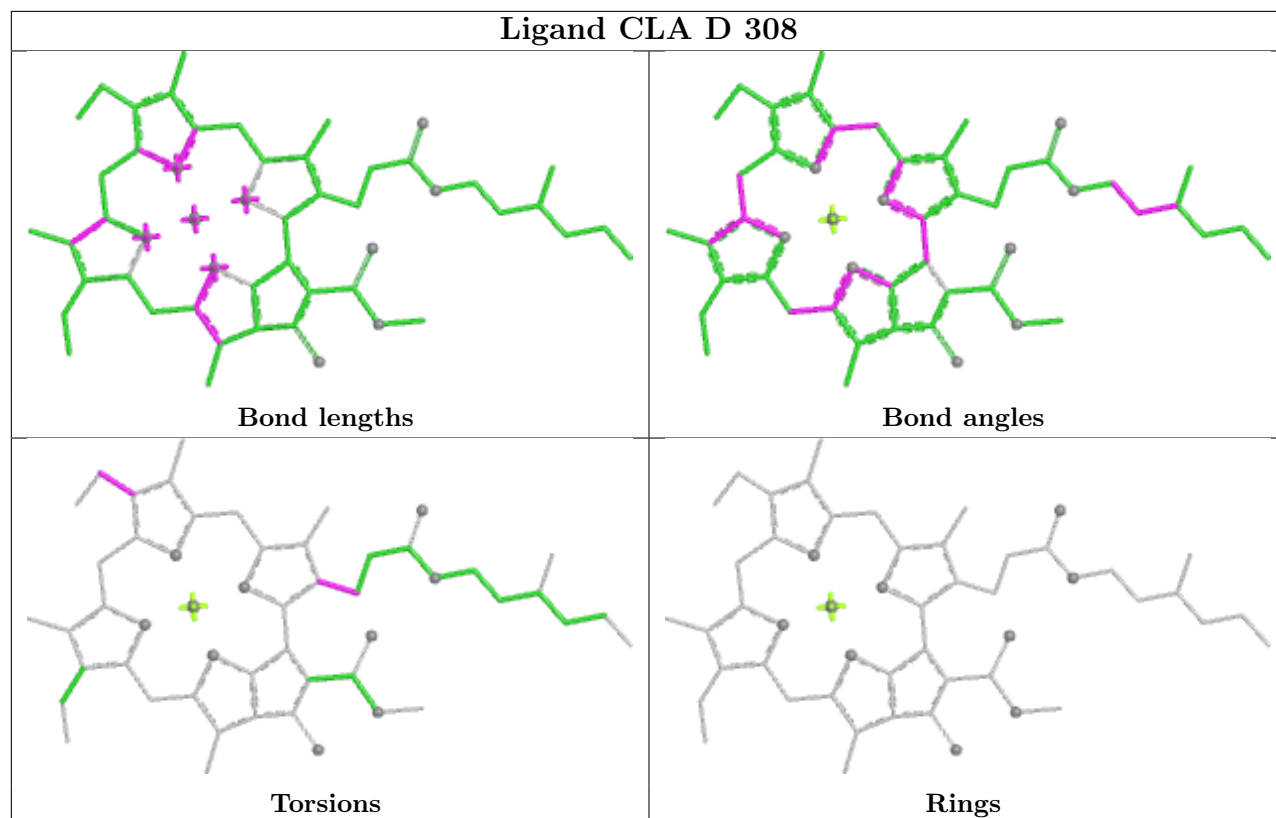


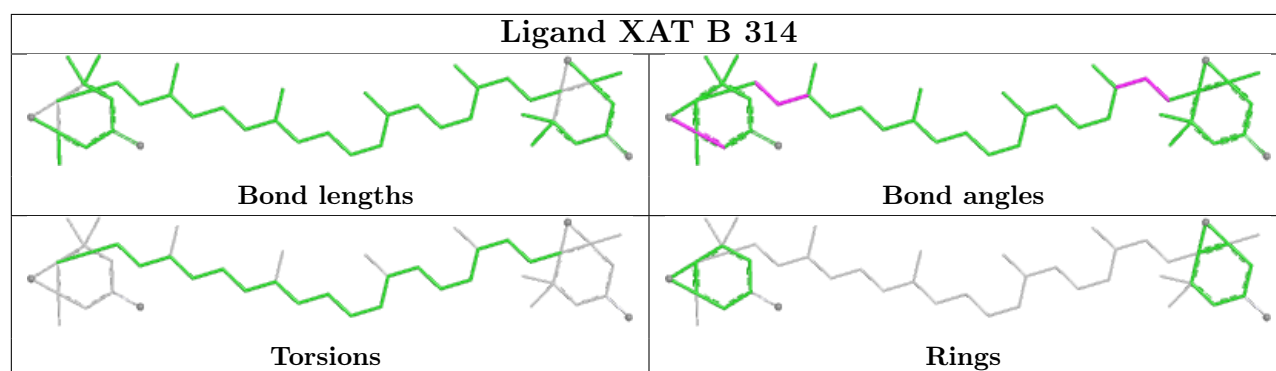
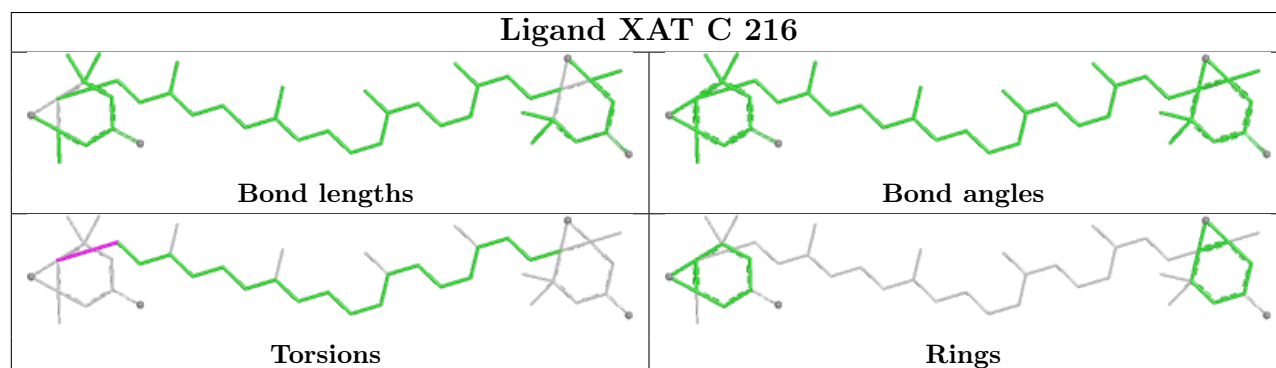
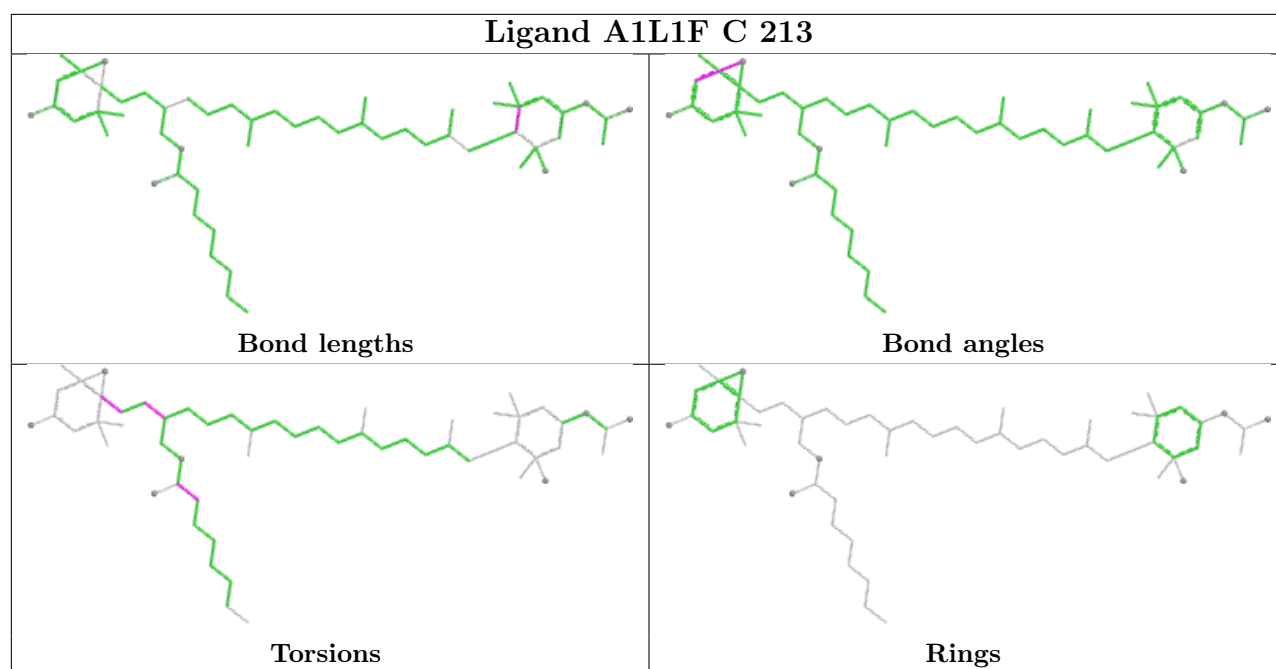
Ligand CLA B 308

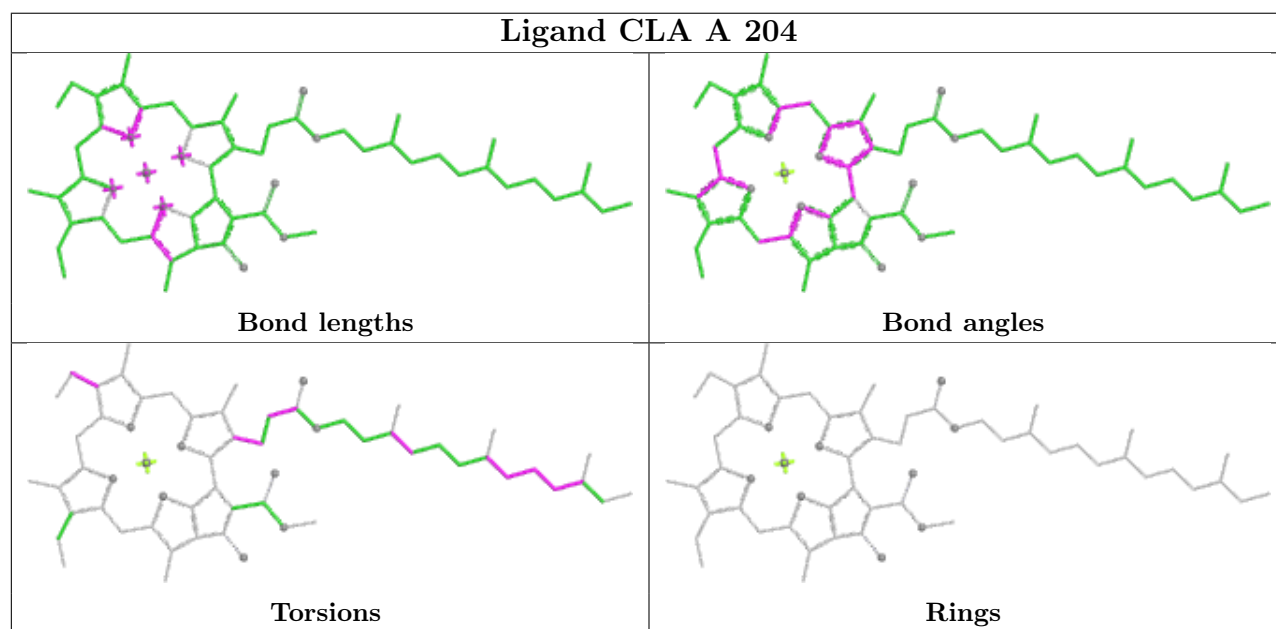
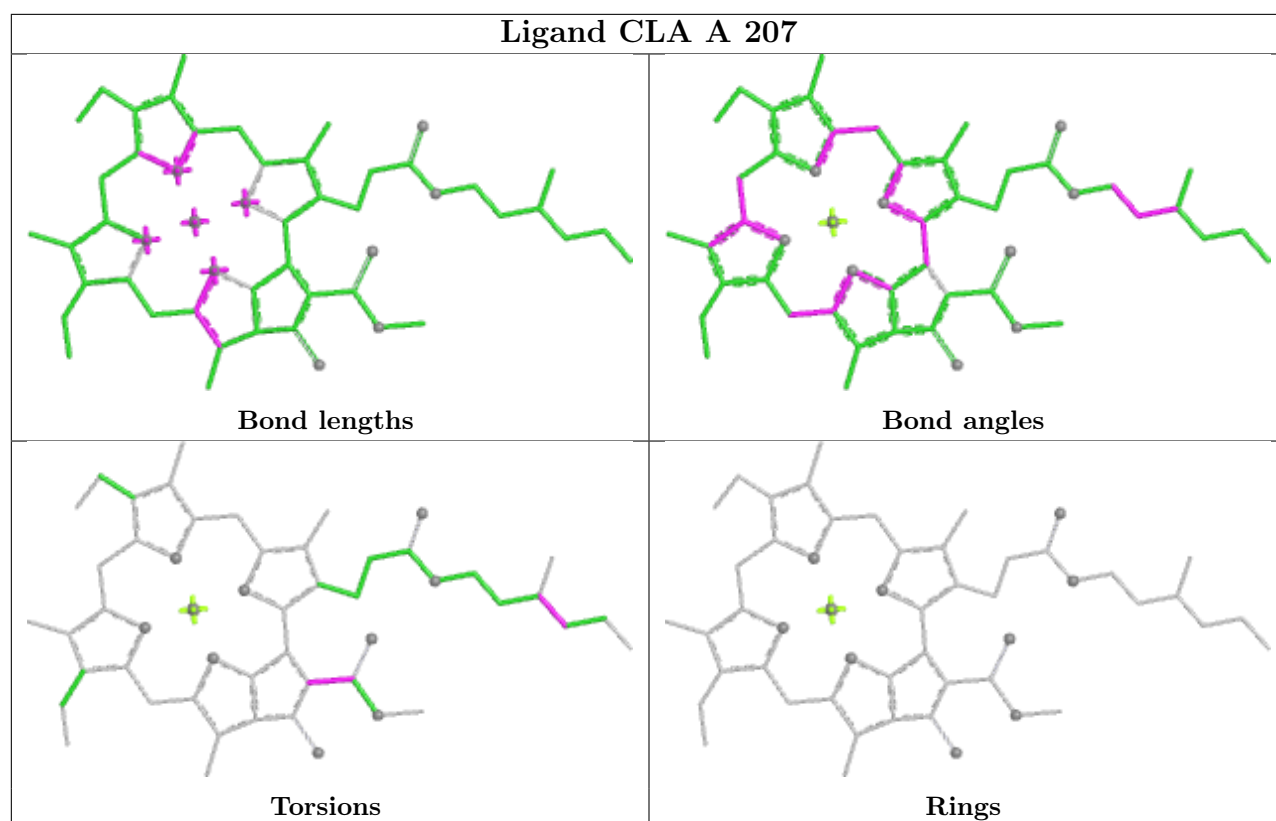




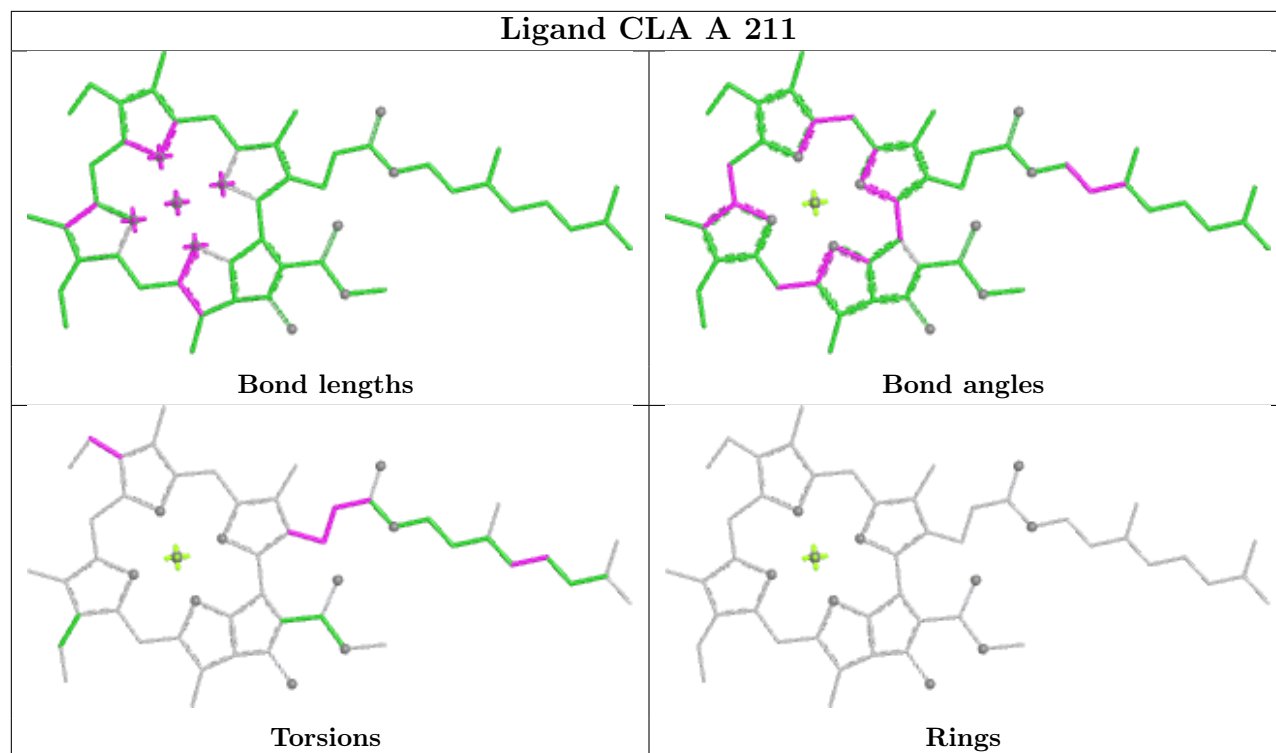
Ligand A1L1F A 213**Ligand XAT A 216**



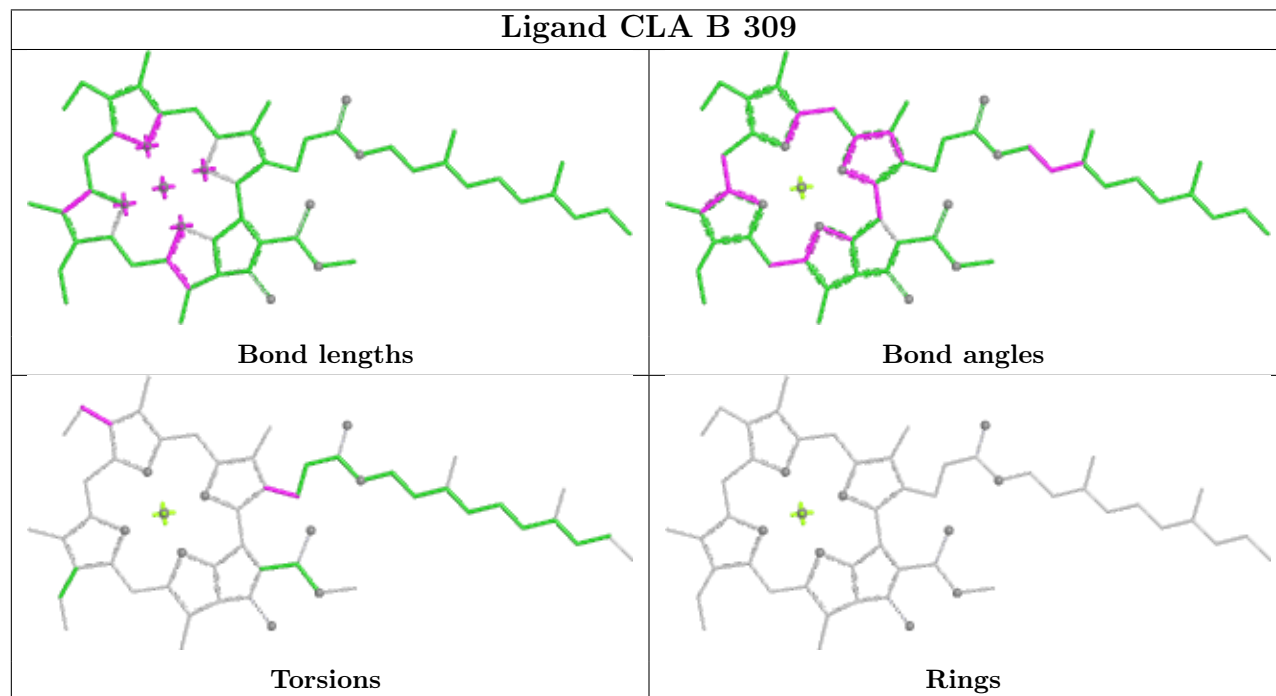


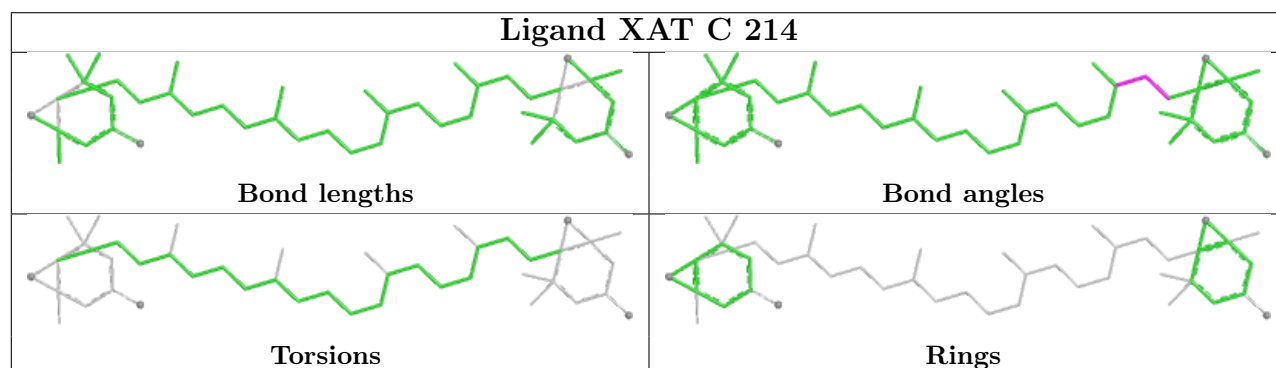
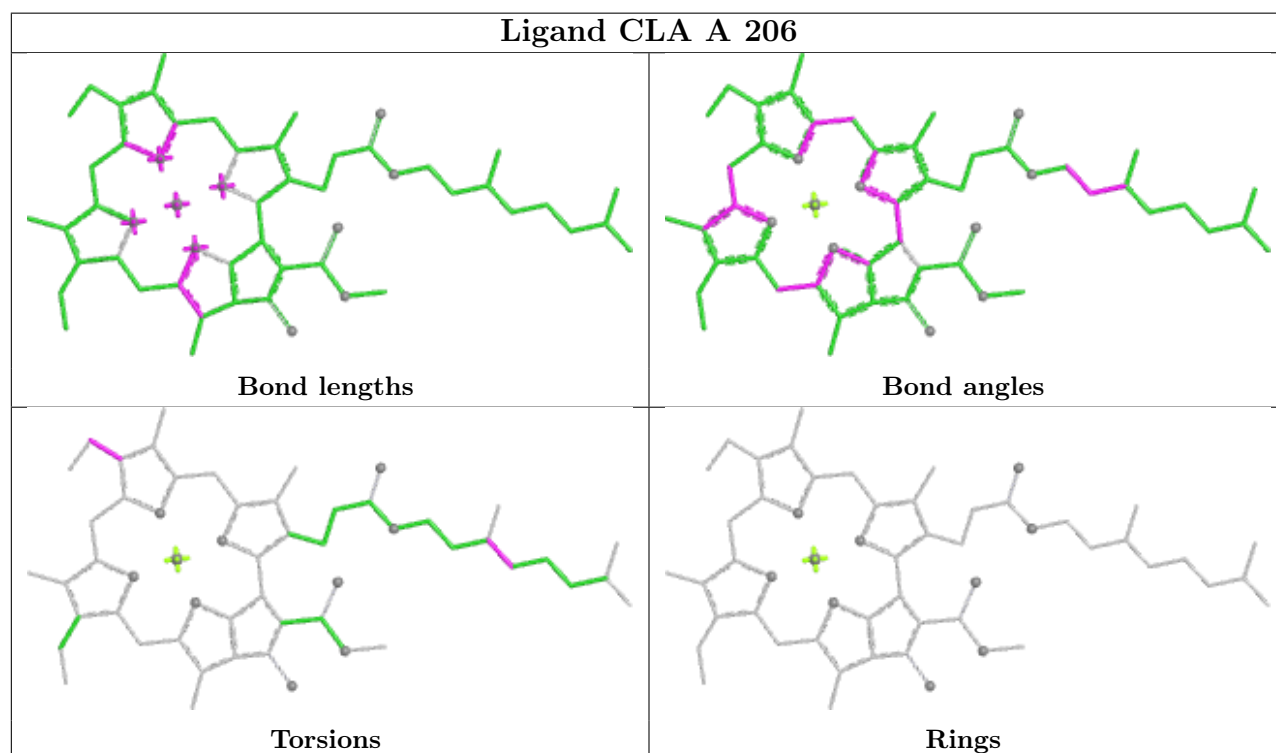
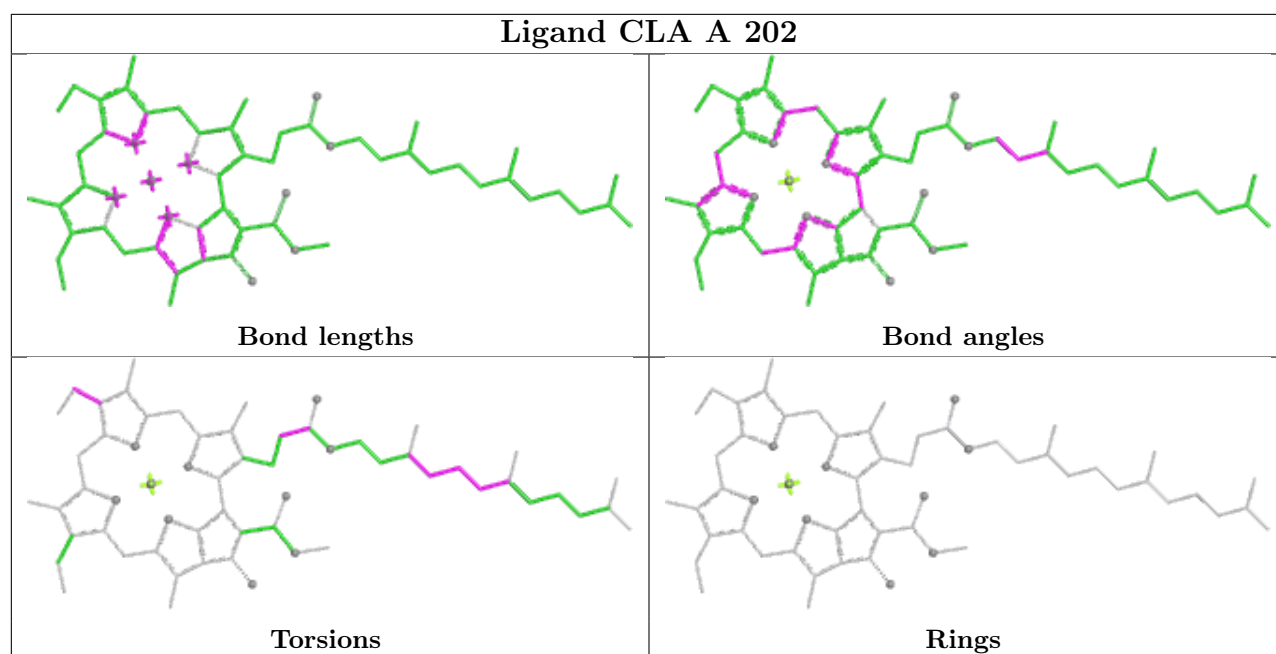


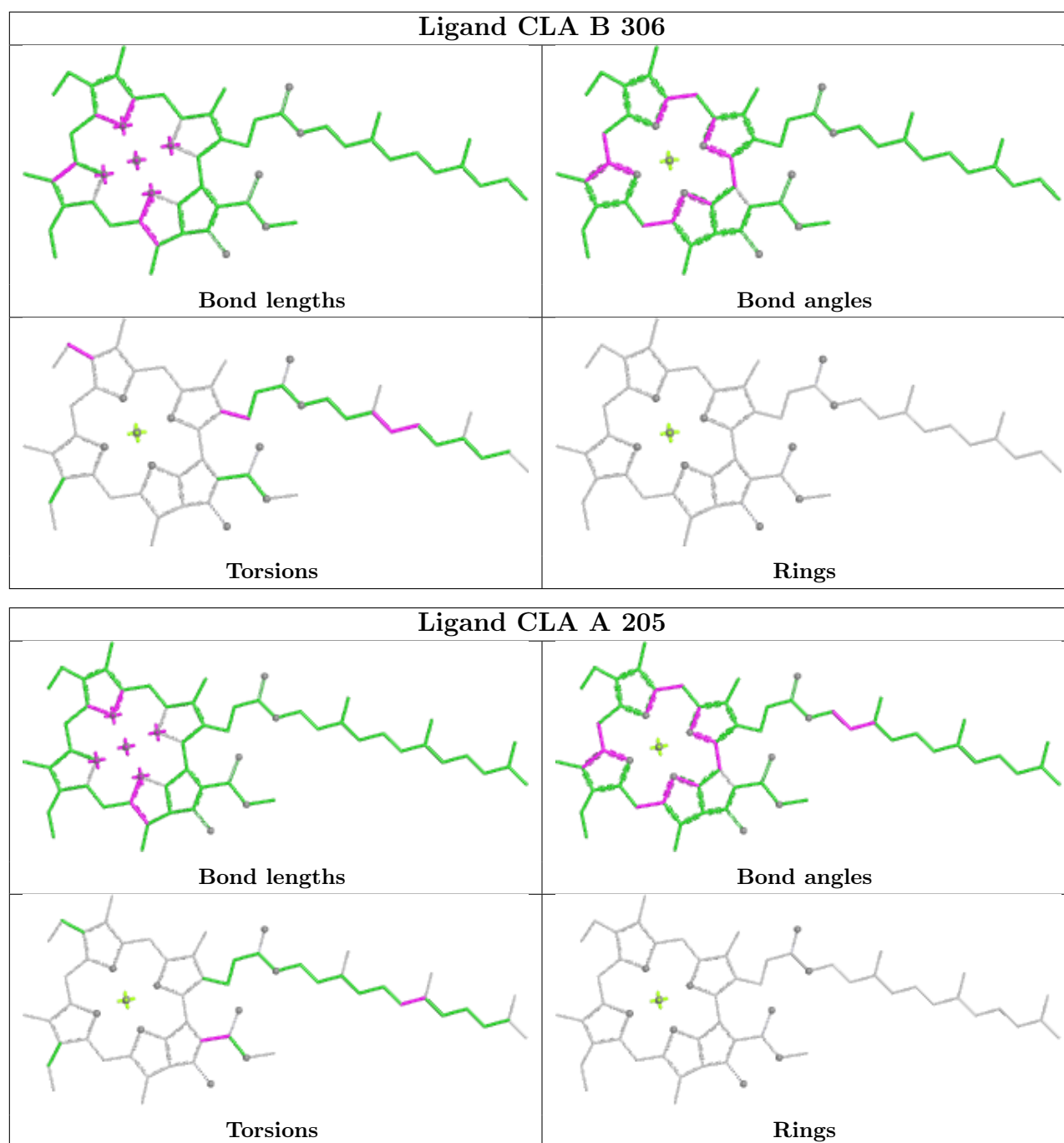
Ligand CLA A 211

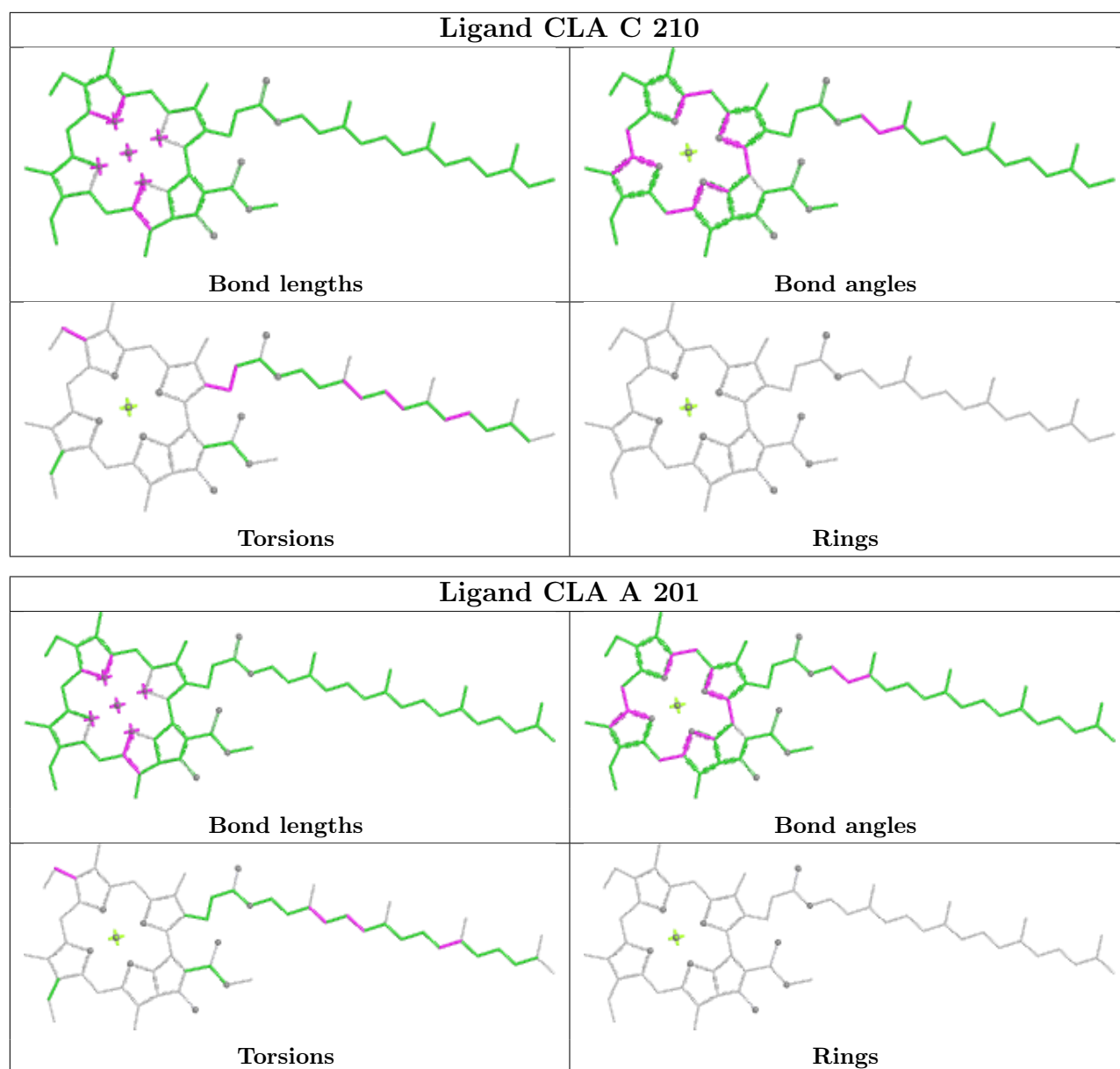


Ligand CLA B 309

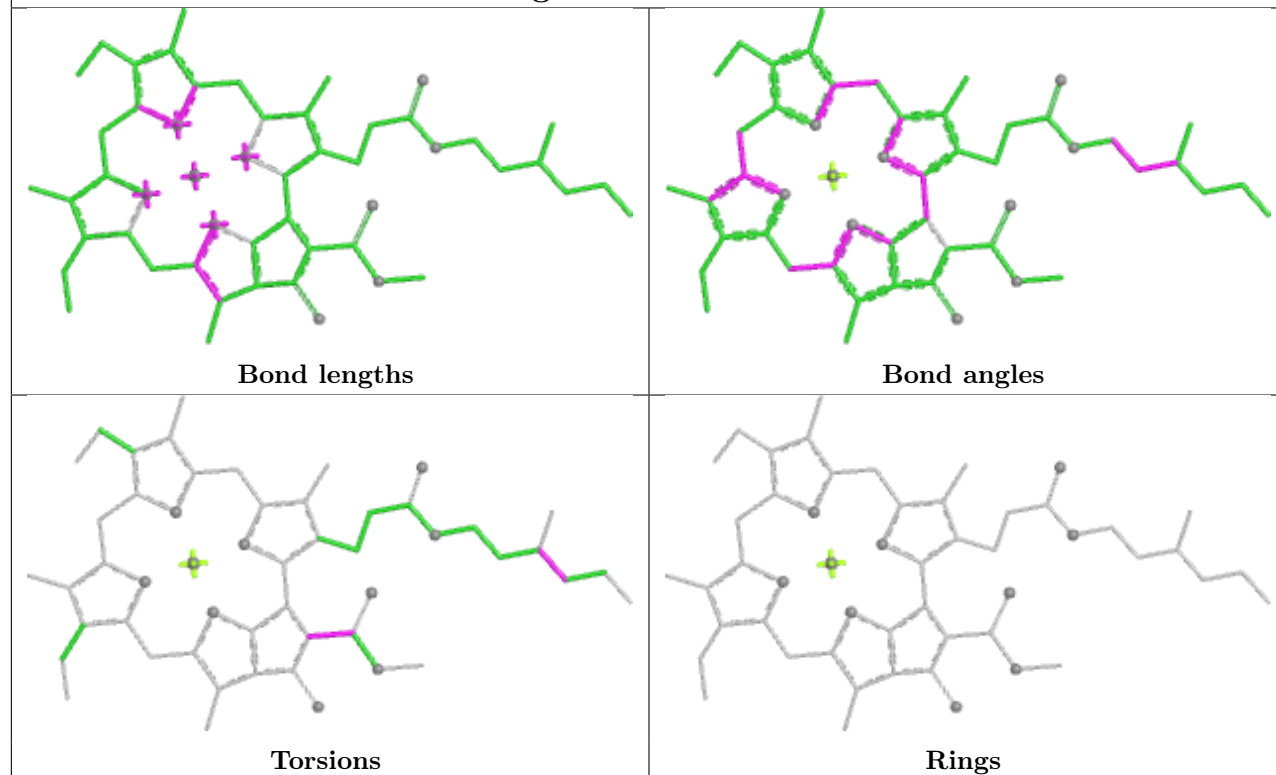




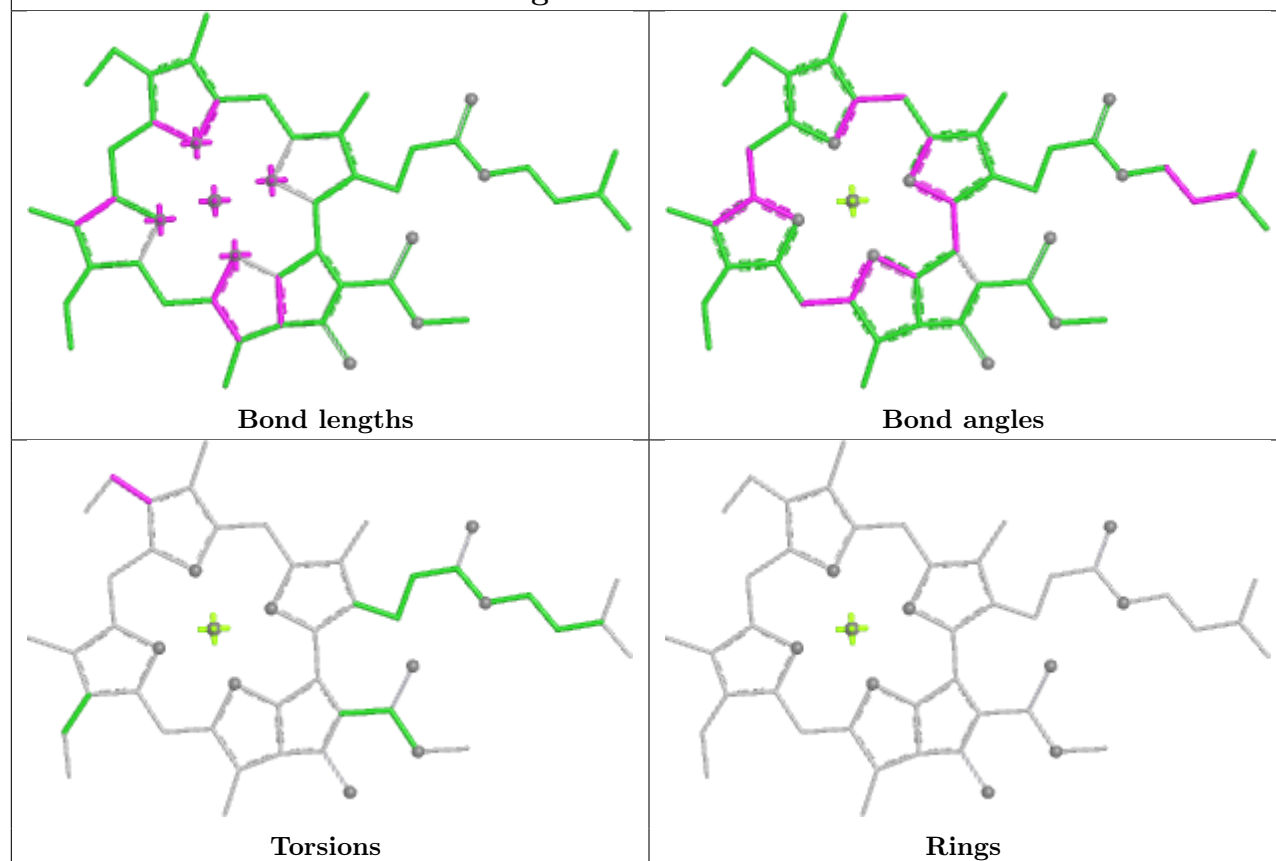




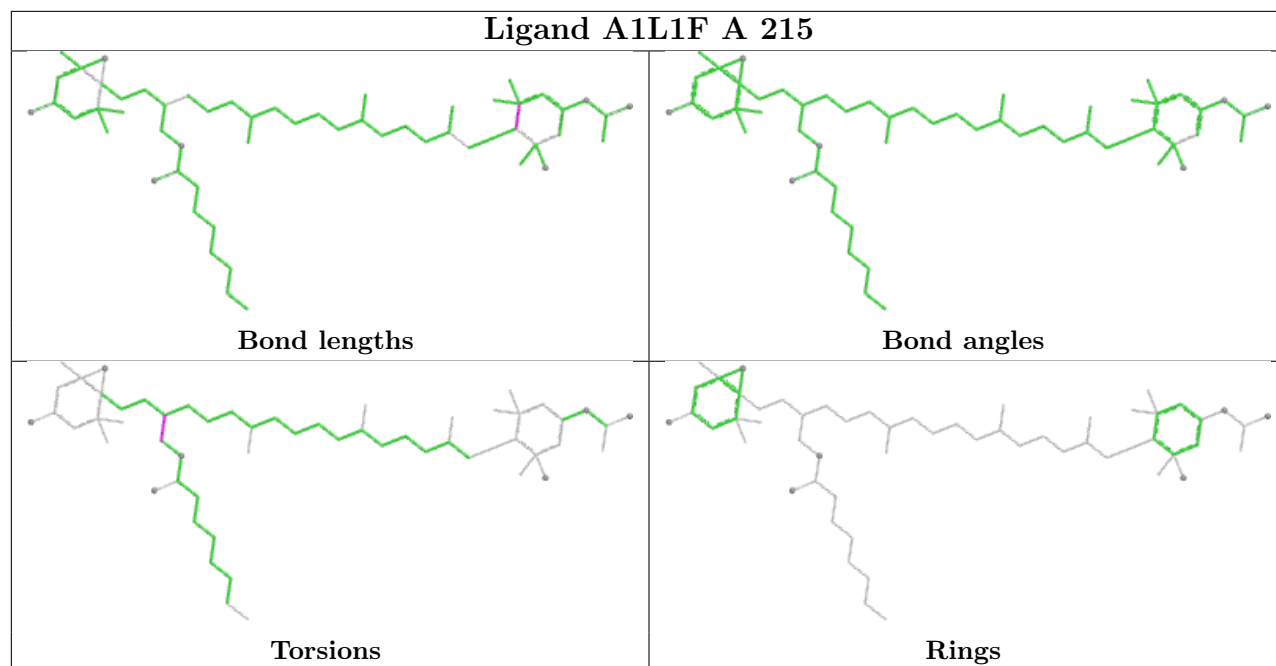
Ligand CLA C 207



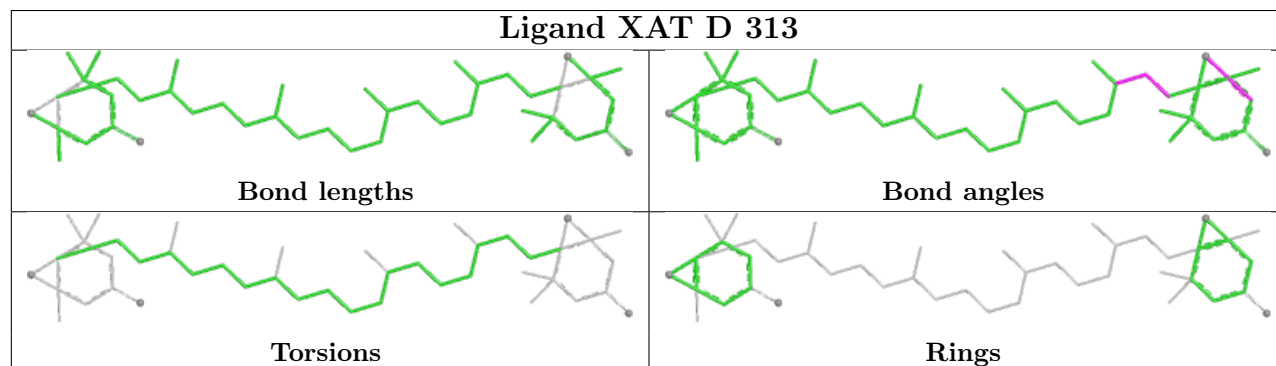
Ligand CLA D 311



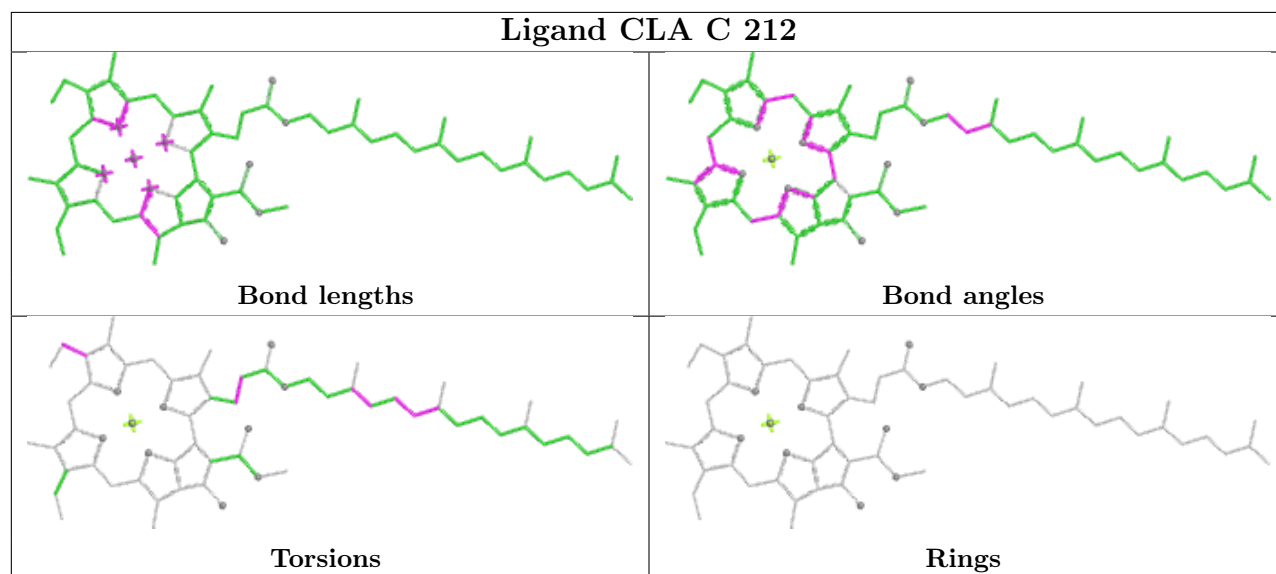
Ligand A1L1F A 215

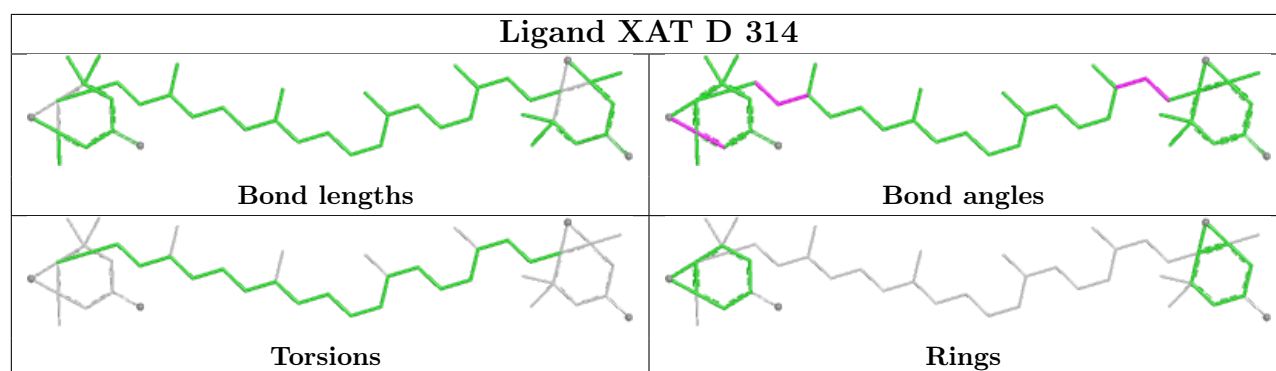
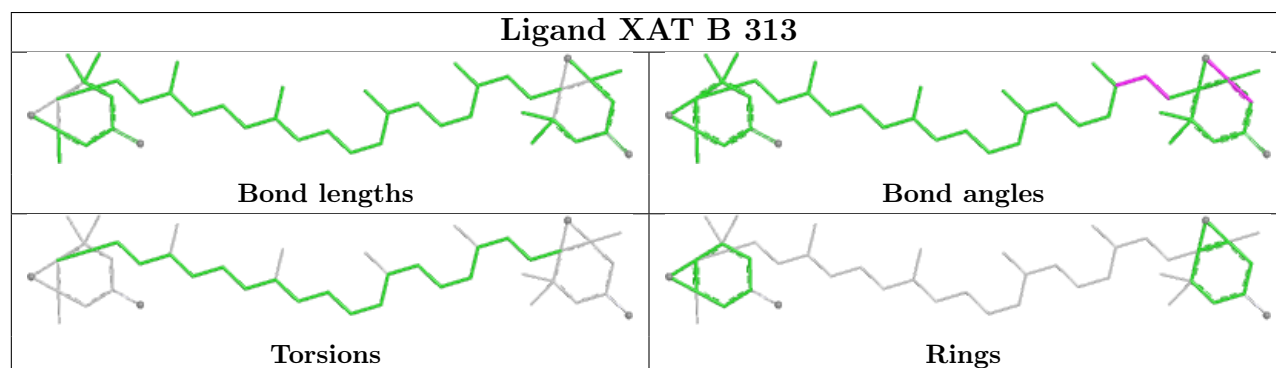
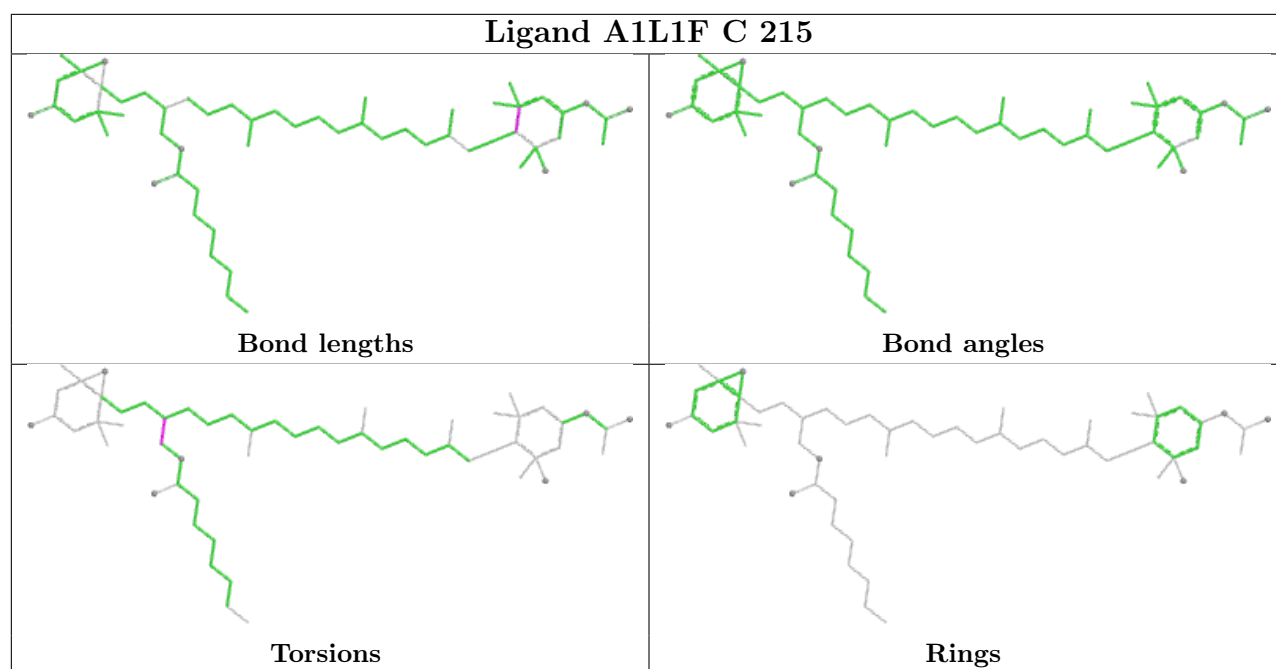


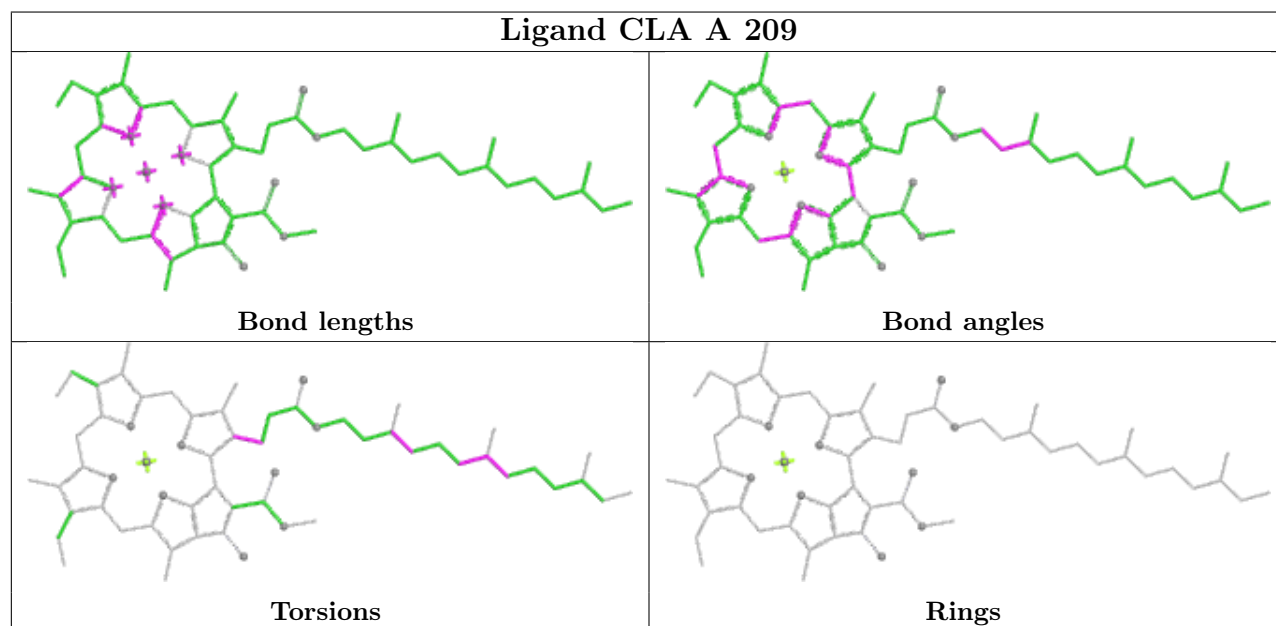
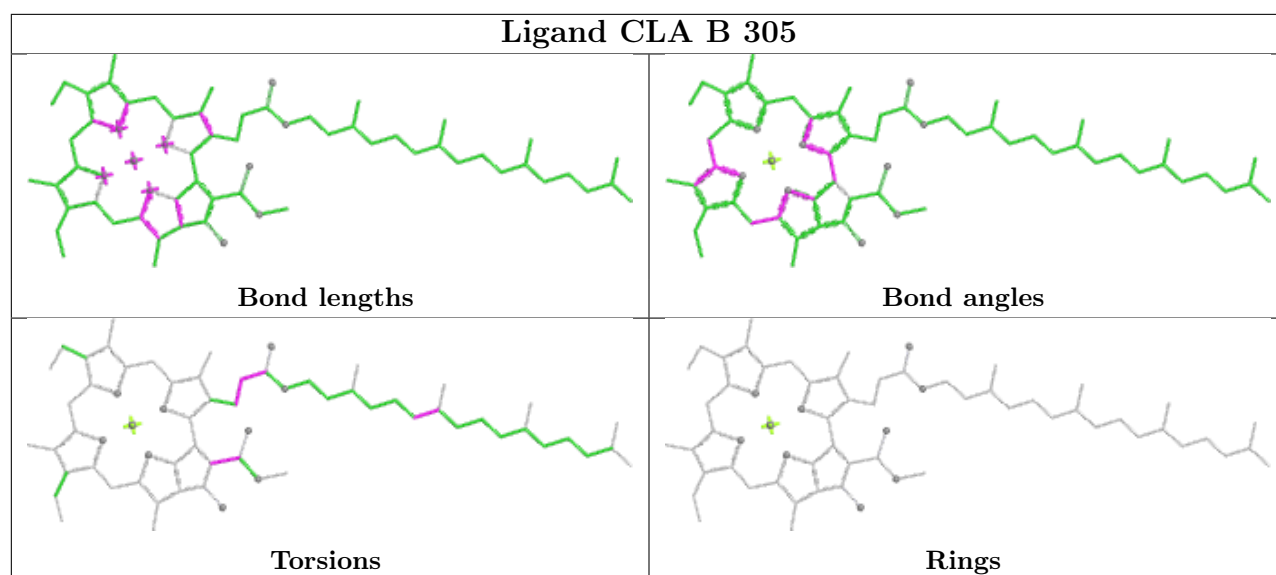
Ligand XAT D 313

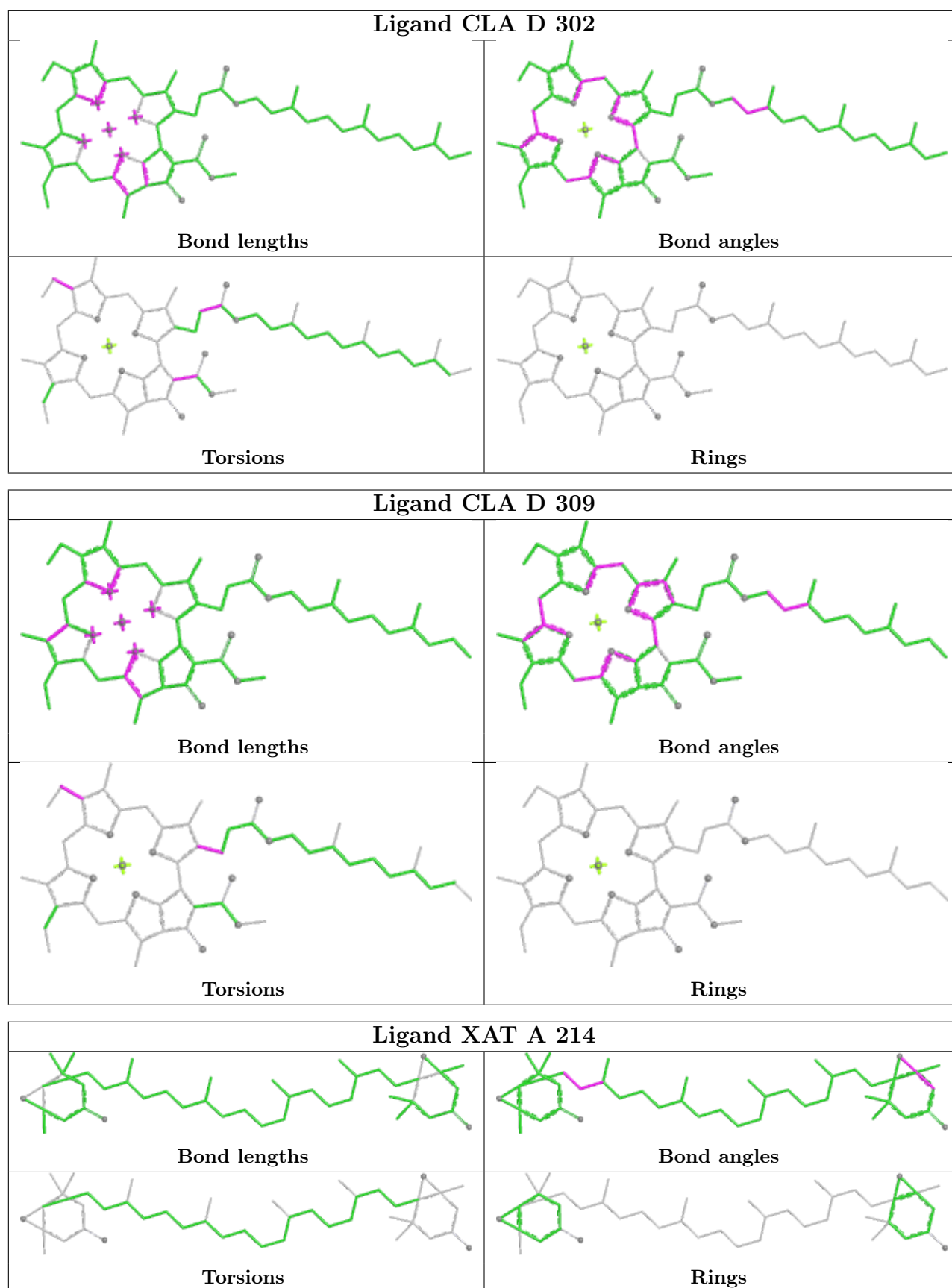


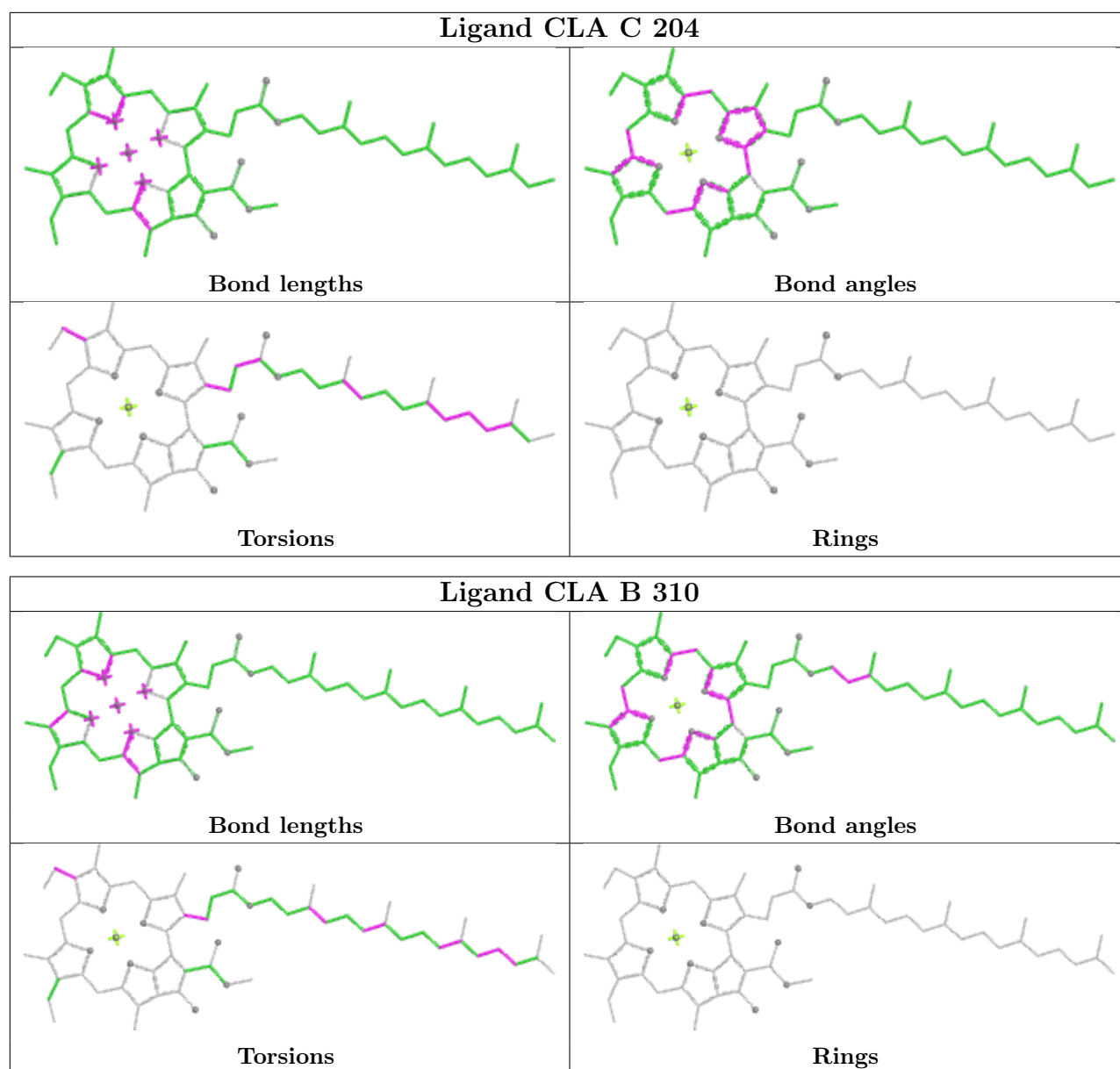
Ligand CLA C 212



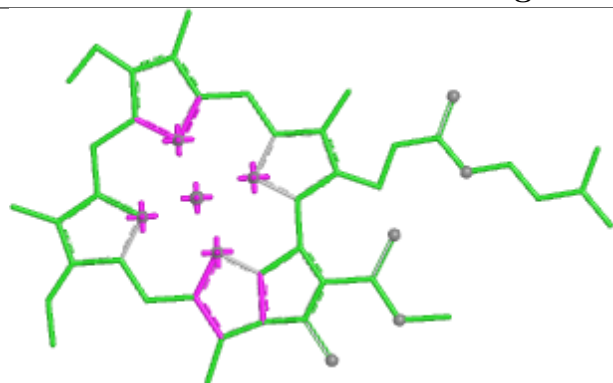




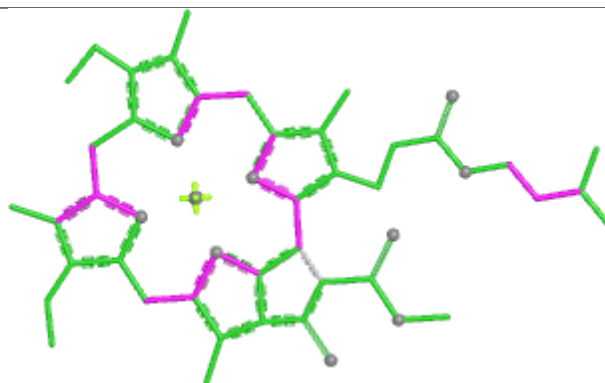




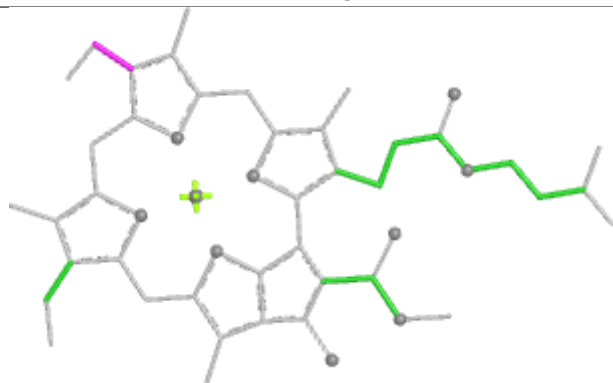
Ligand CLA B 311



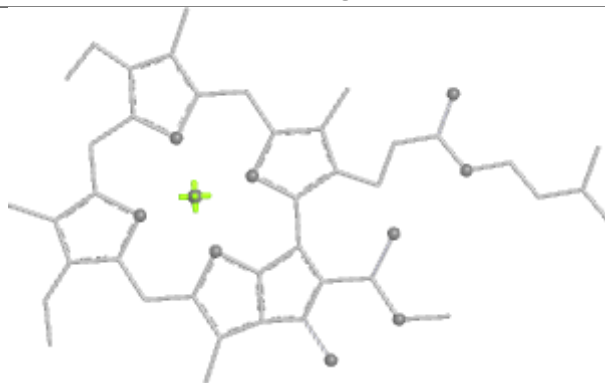
Bond lengths



Bond angles

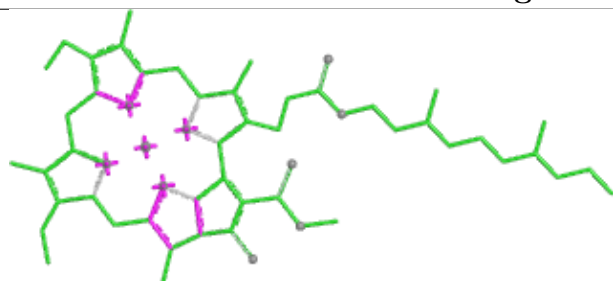


Torsions

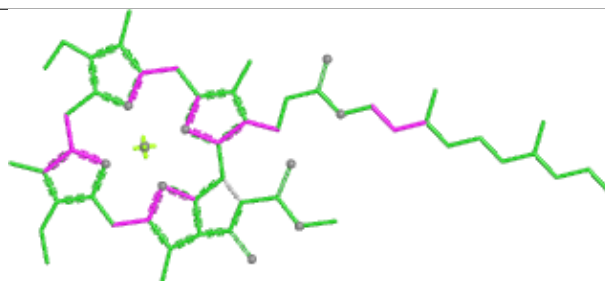


Rings

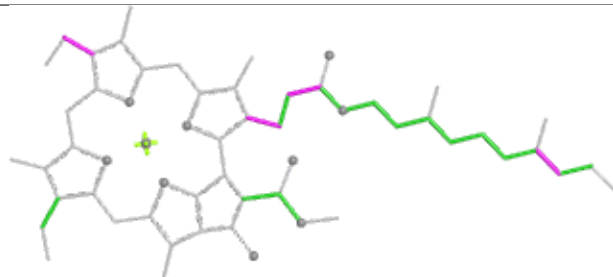
Ligand CLA B 304



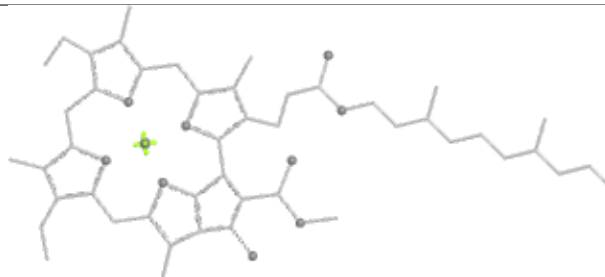
Bond lengths



Bond angles

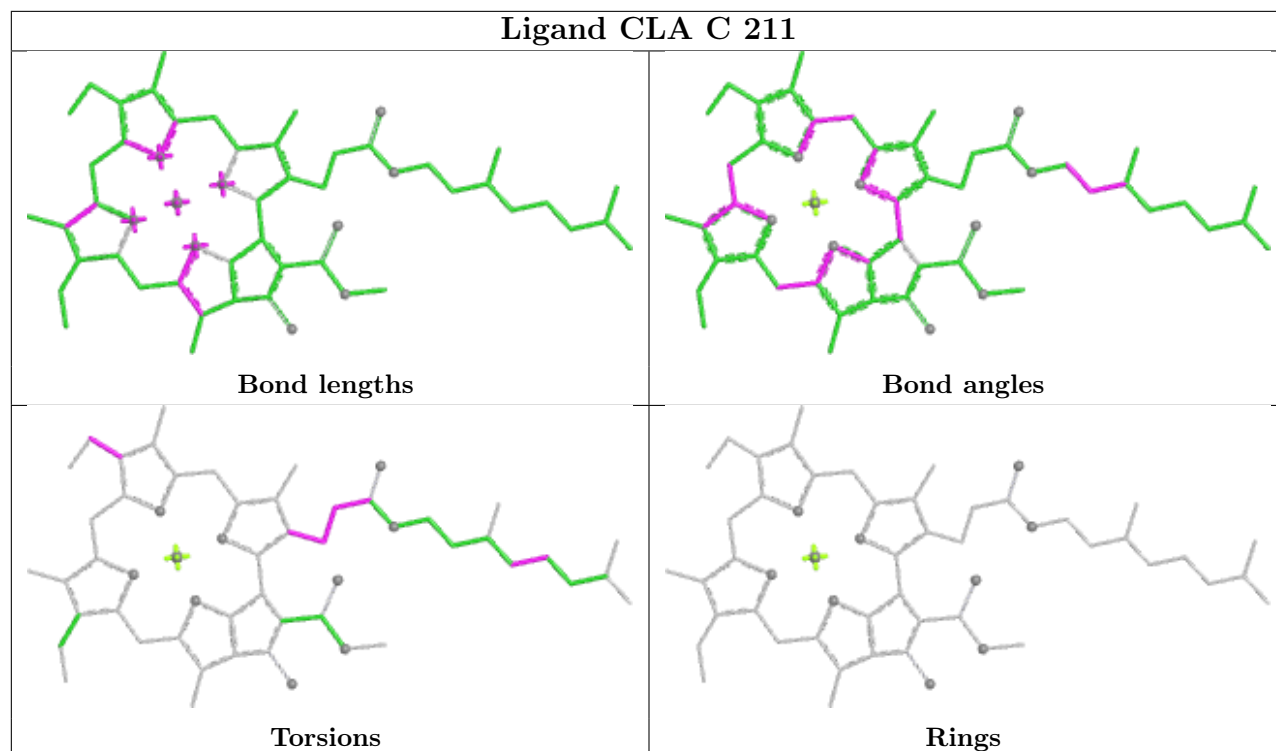


Torsions

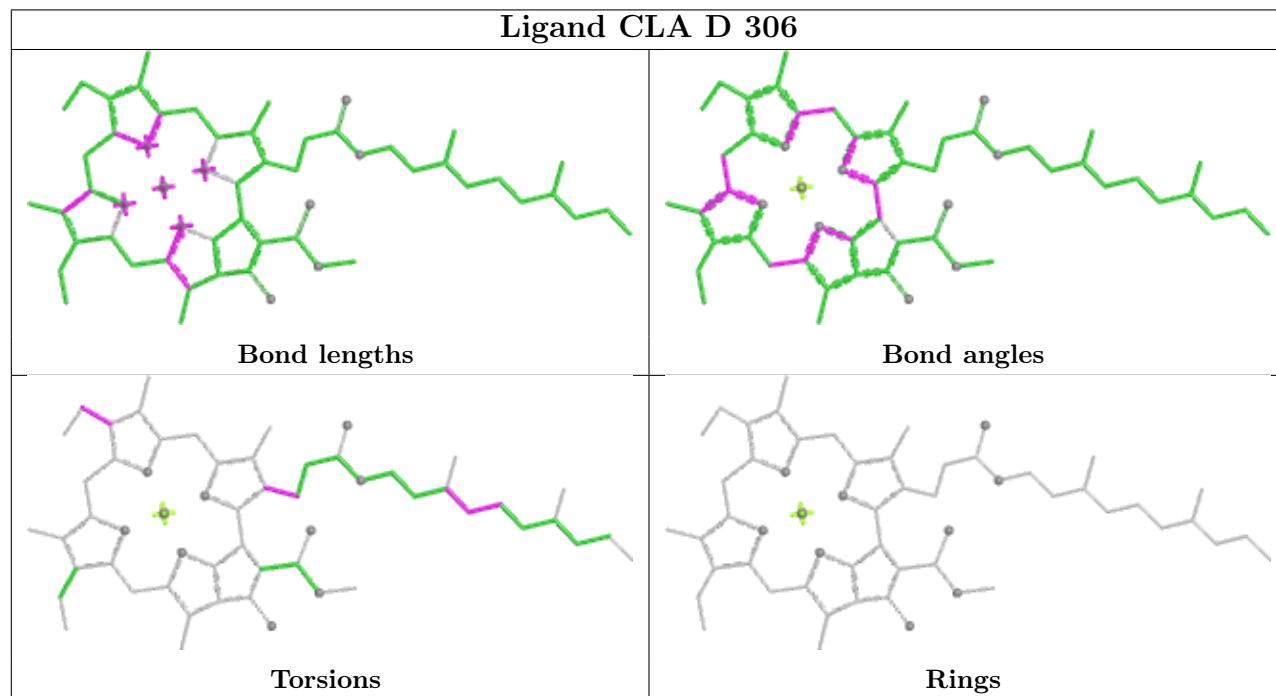


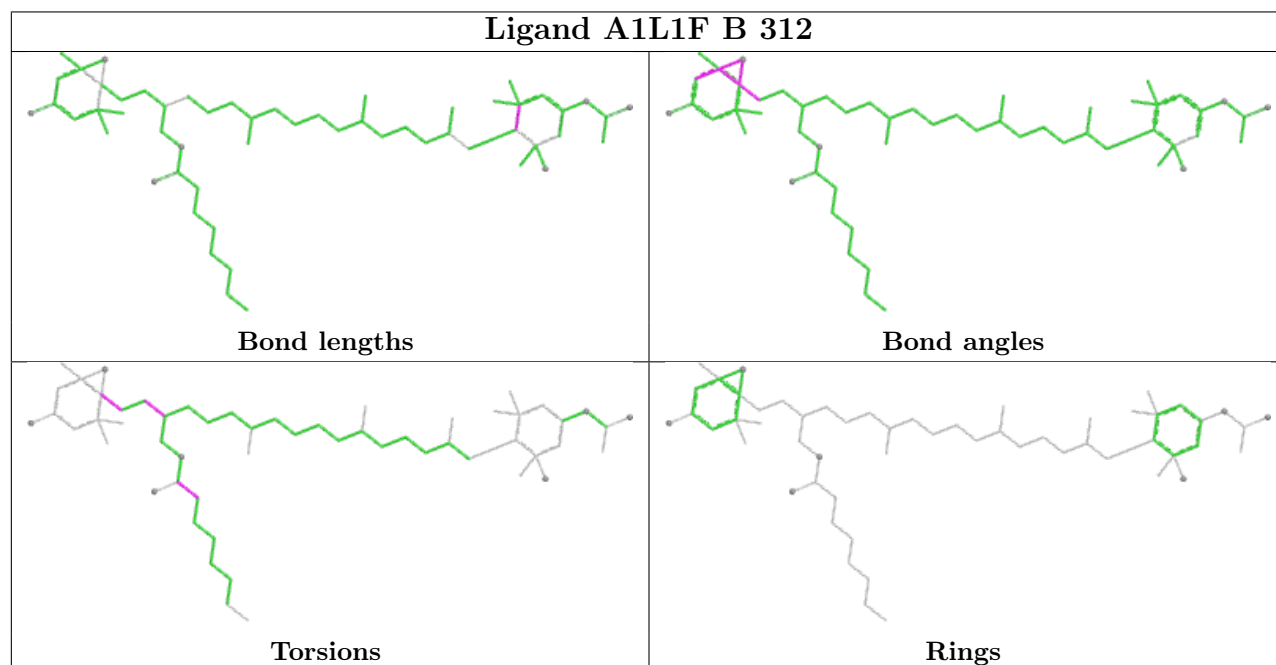
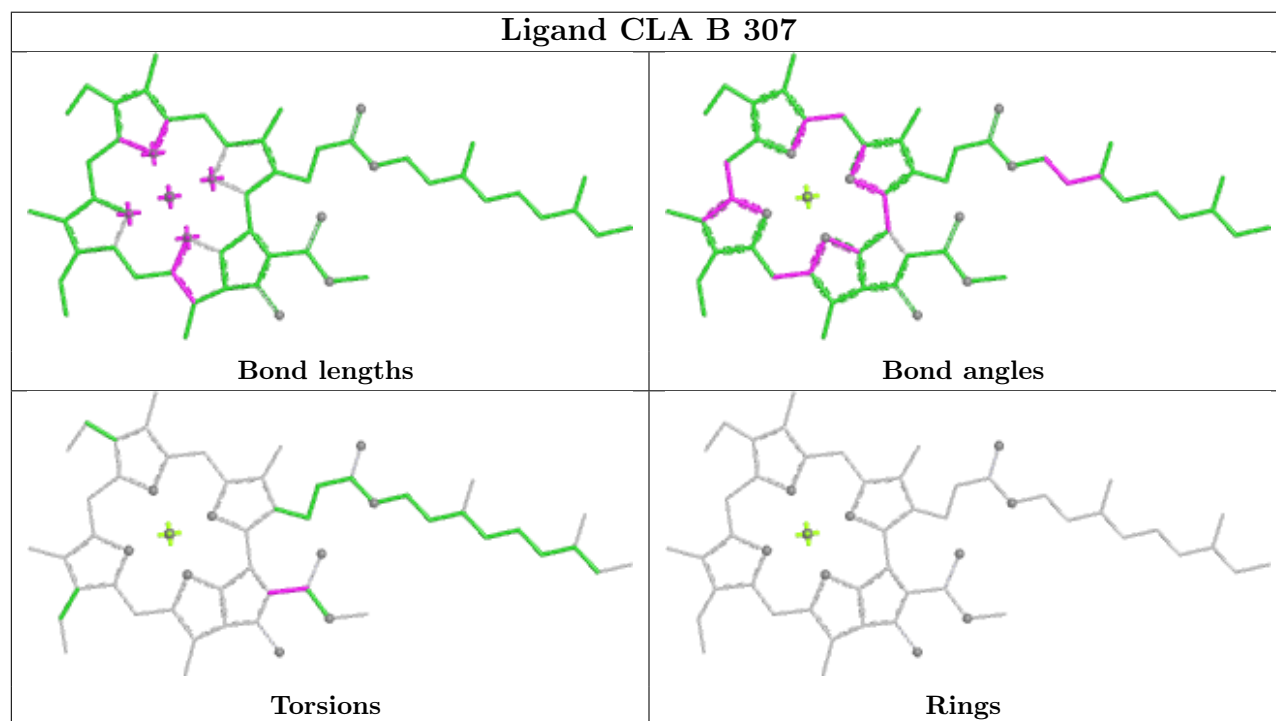
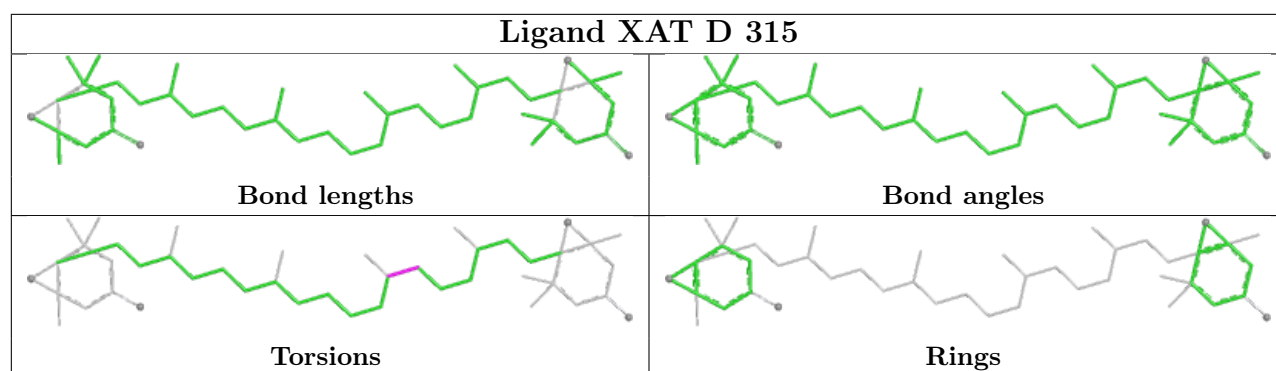
Rings

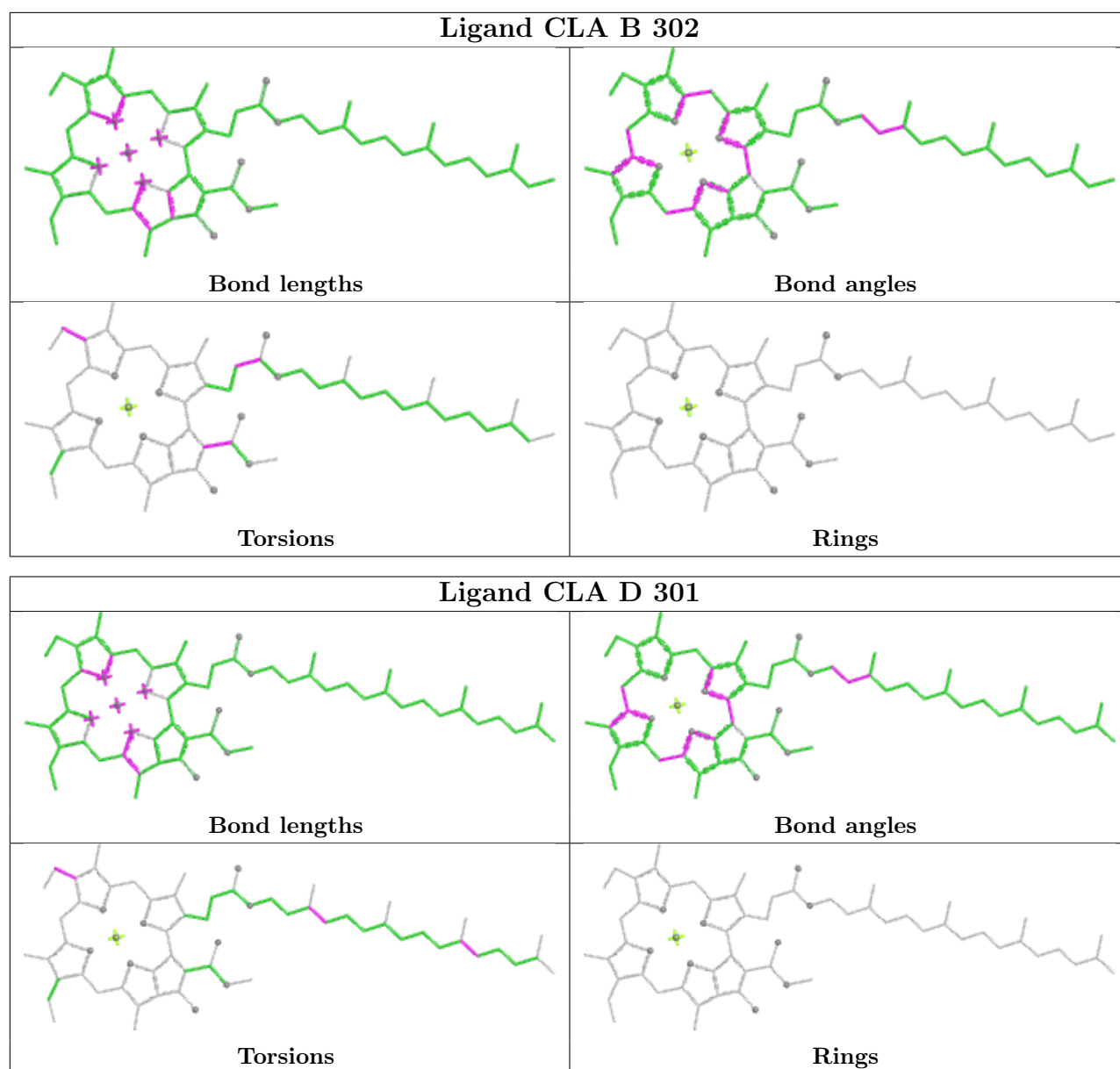
Ligand CLA C 211

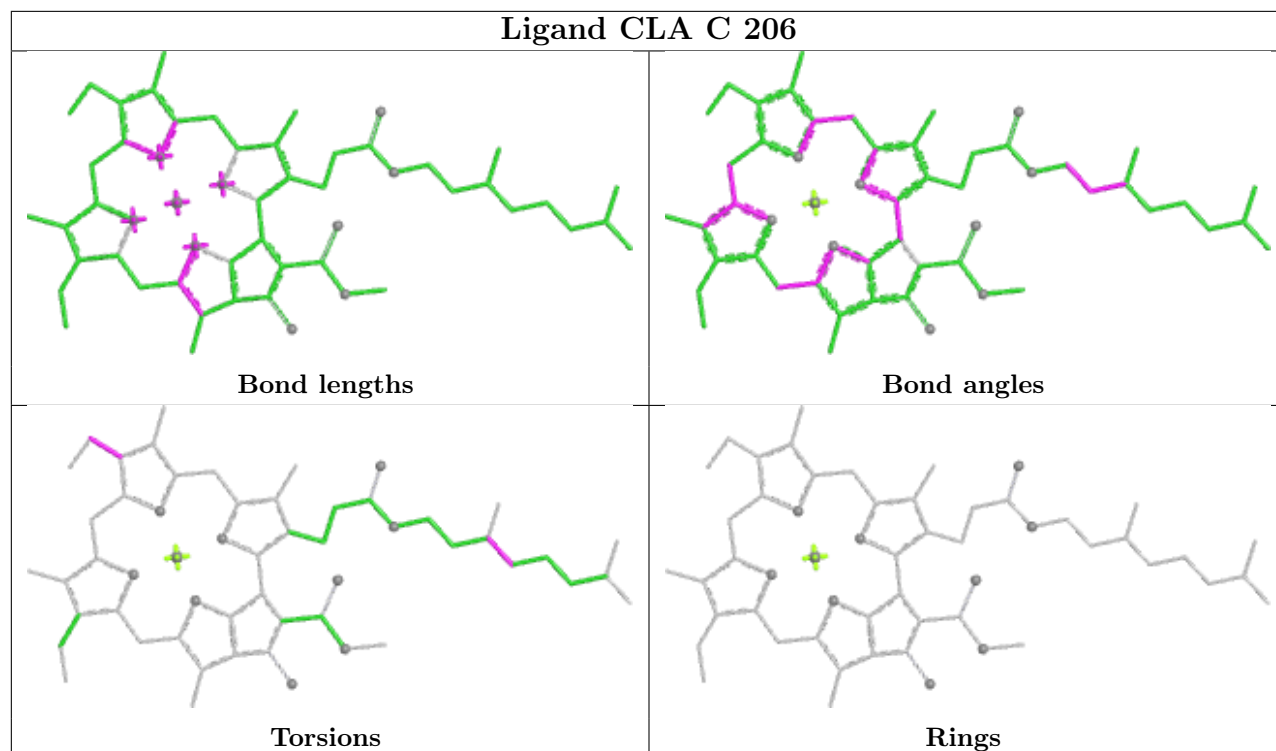
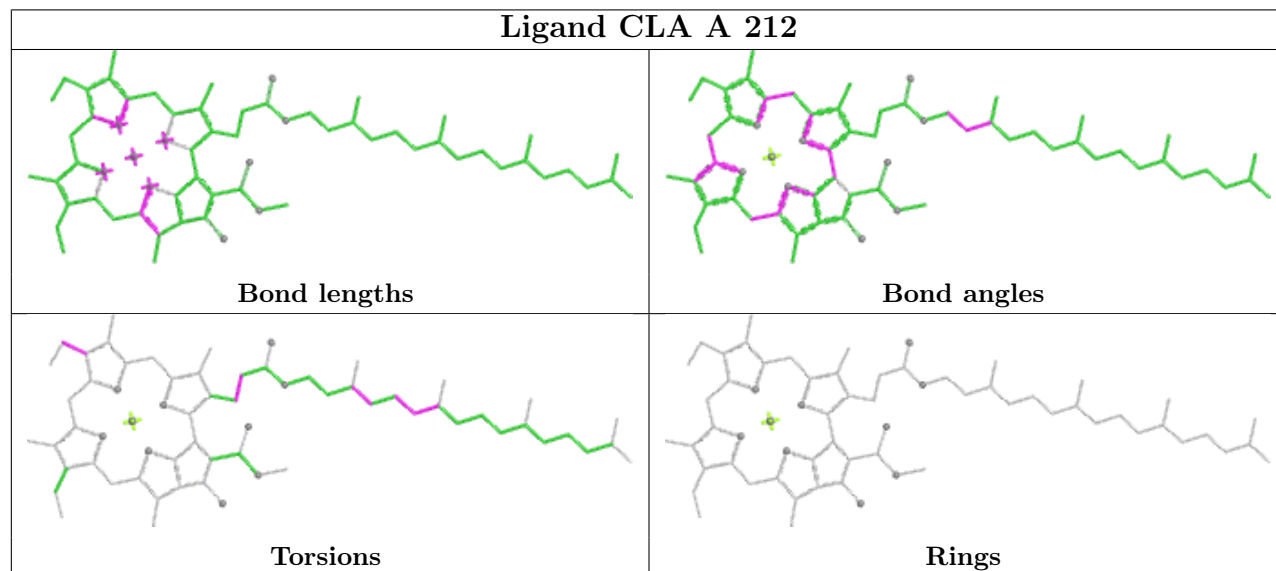


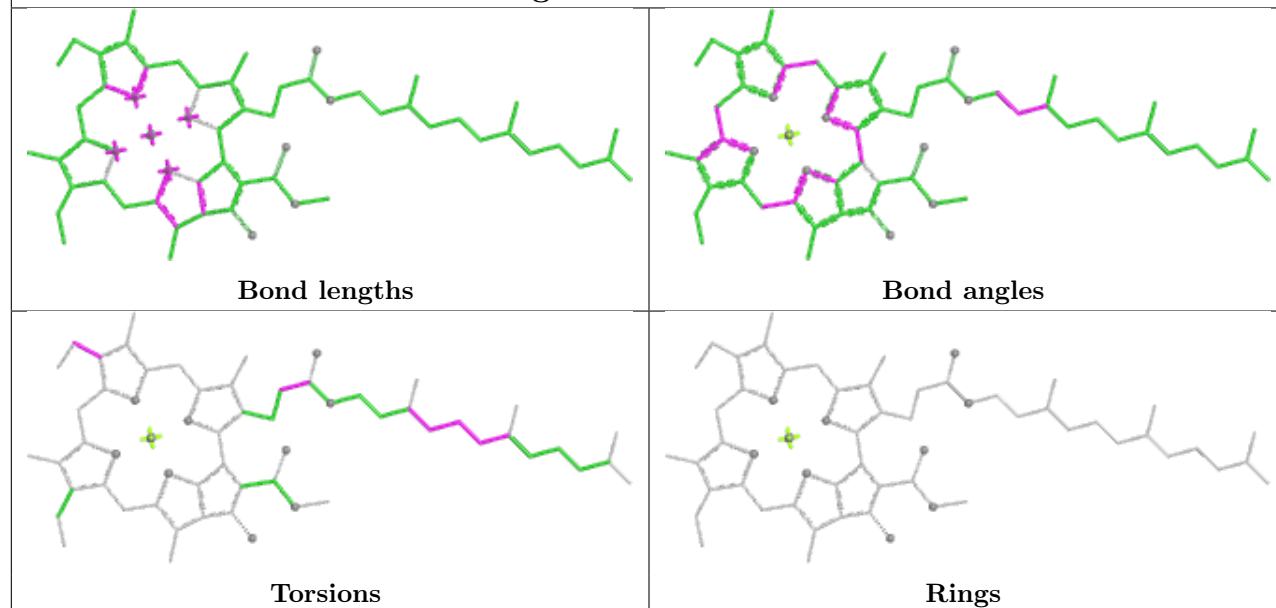
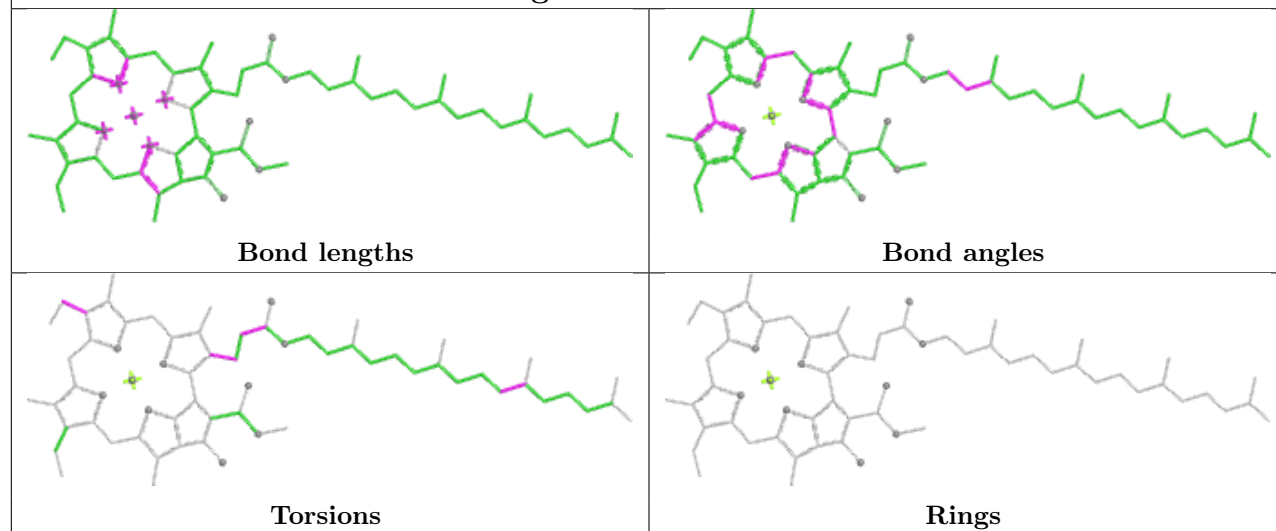
Ligand CLA D 306

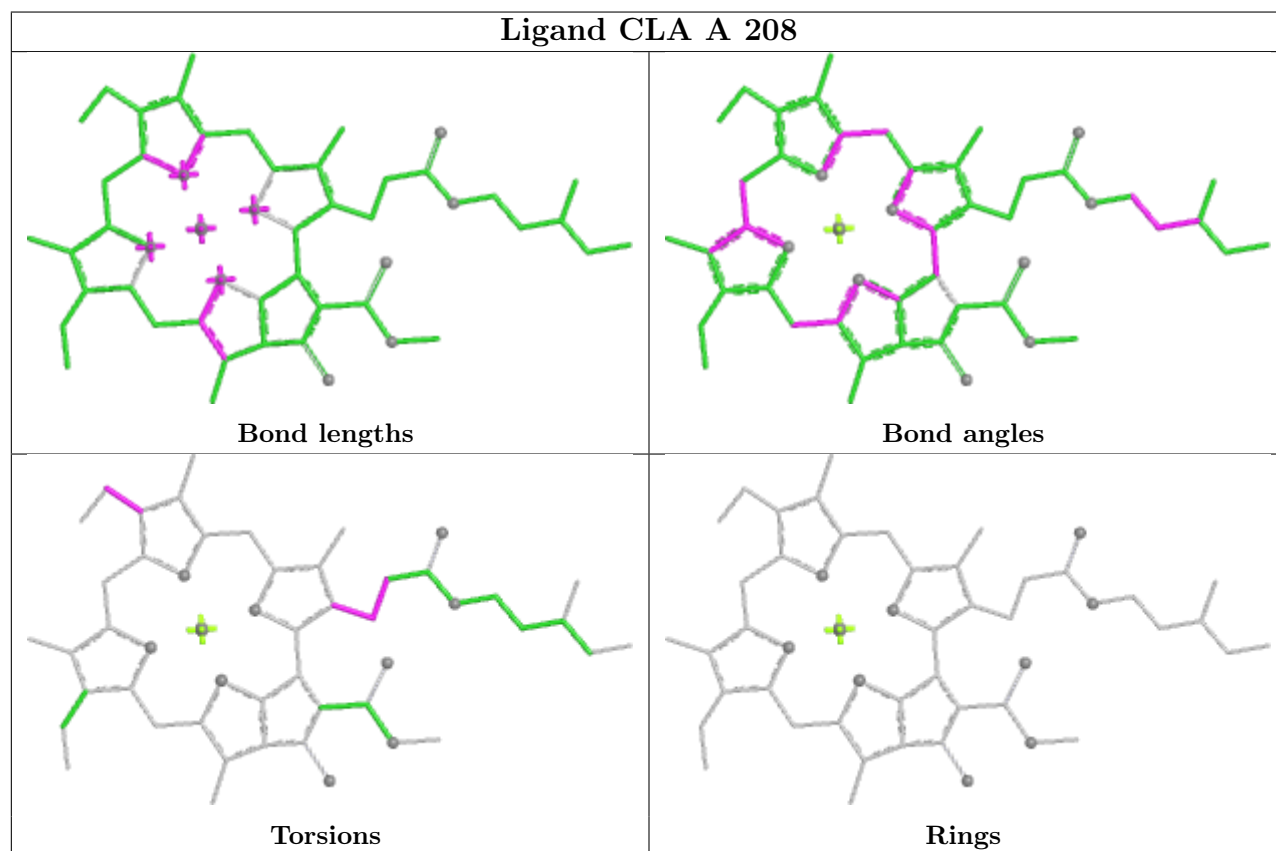
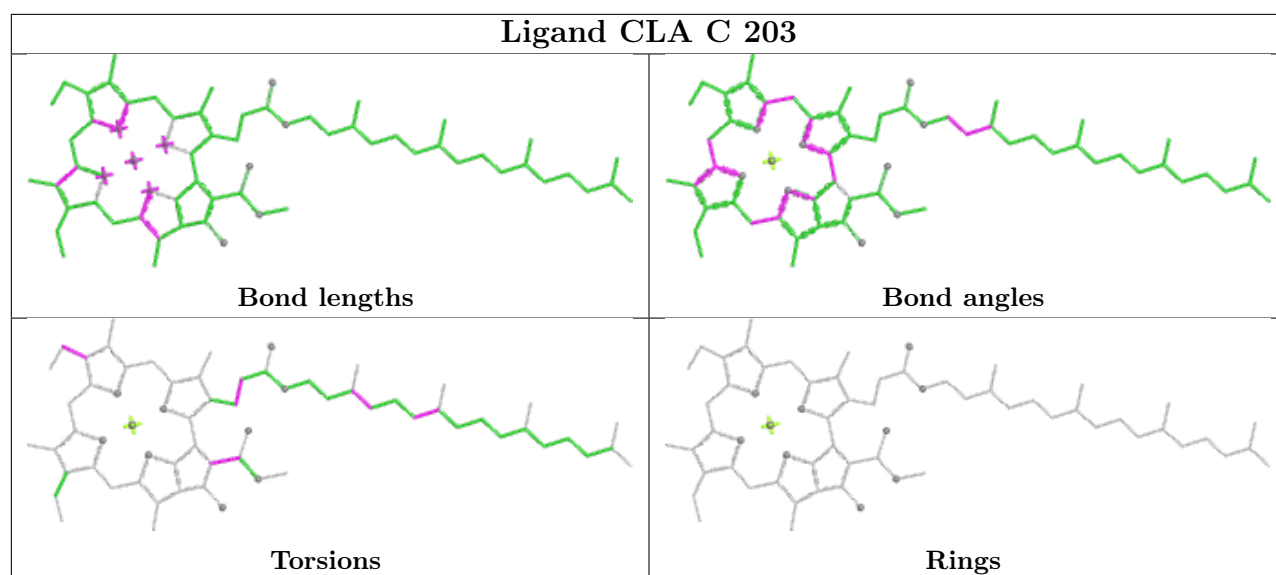


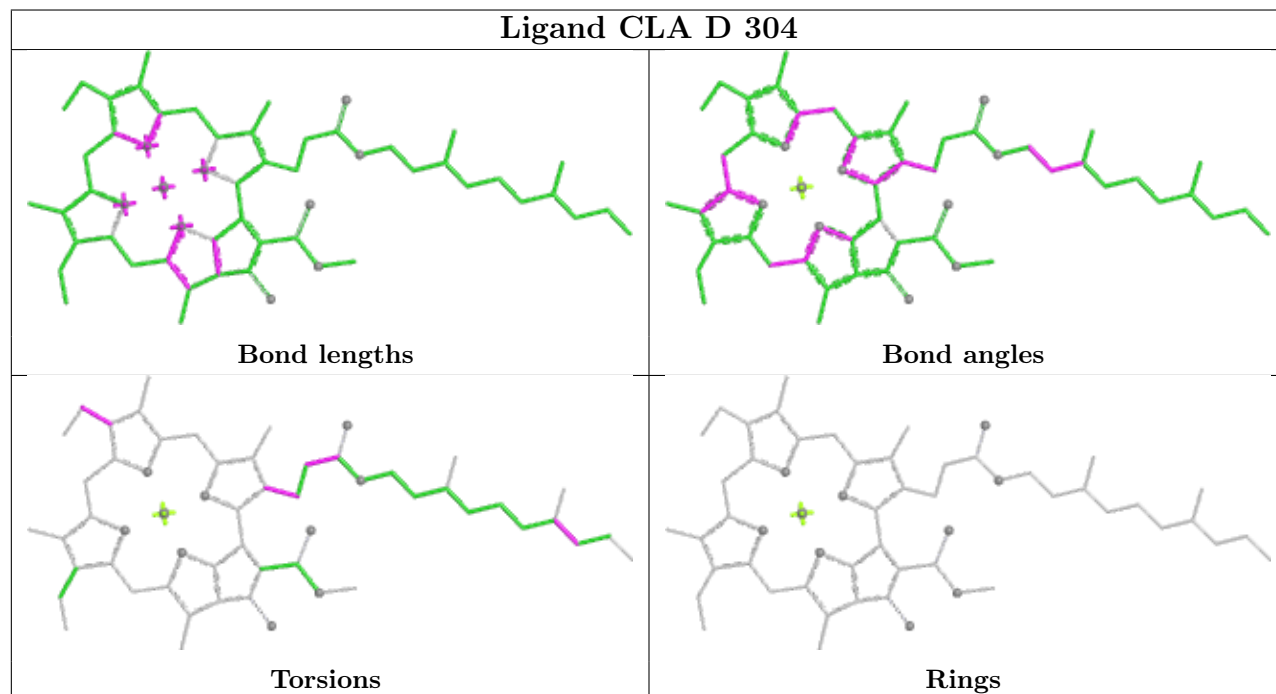
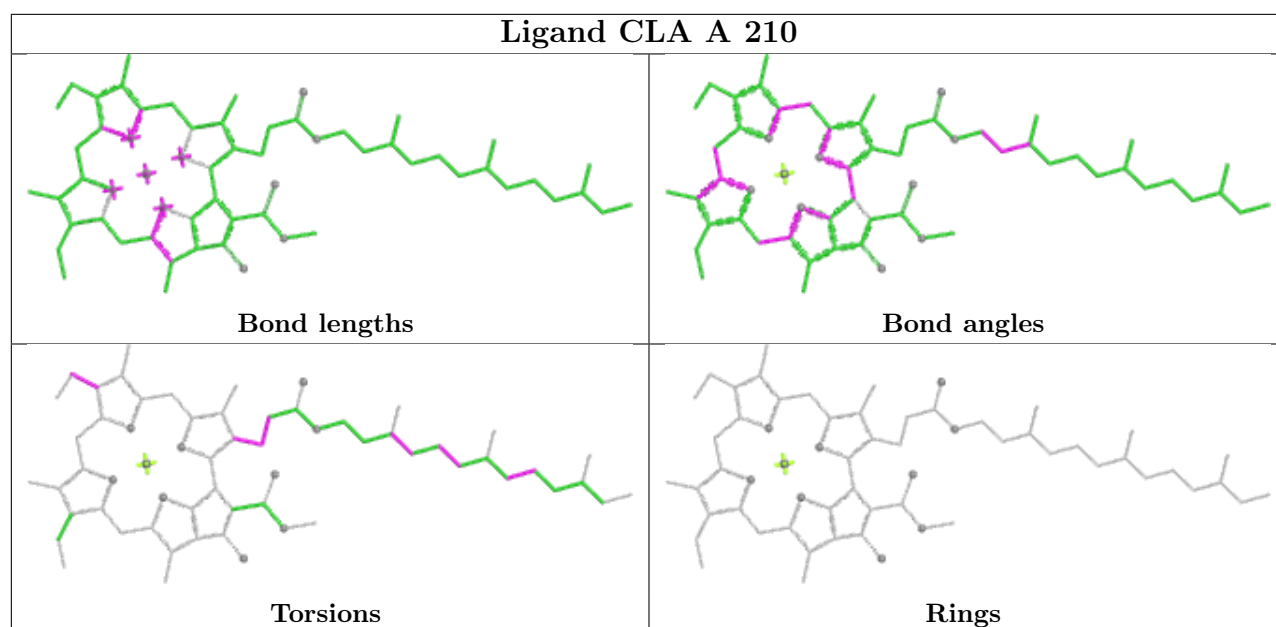


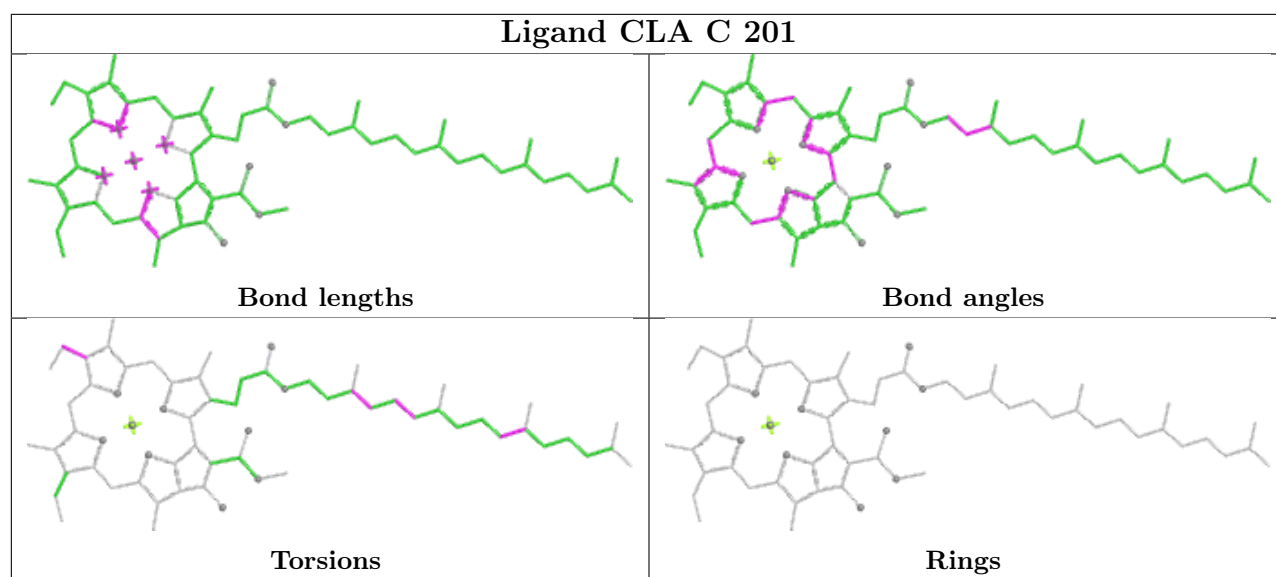


Ligand CLA C 206**Ligand CLA A 212**

Ligand CLA C 202**Ligand CLA D 303**







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.

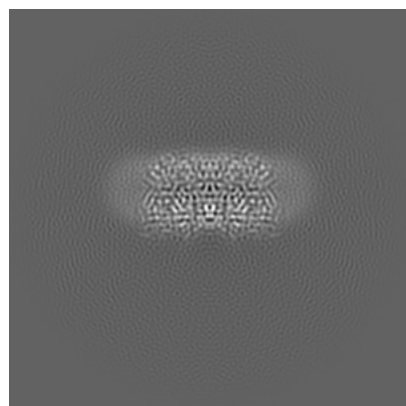
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-63799. These allow visual inspection of the internal detail of the map and identification of artifacts.

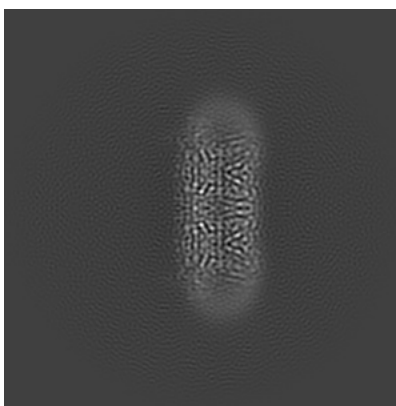
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

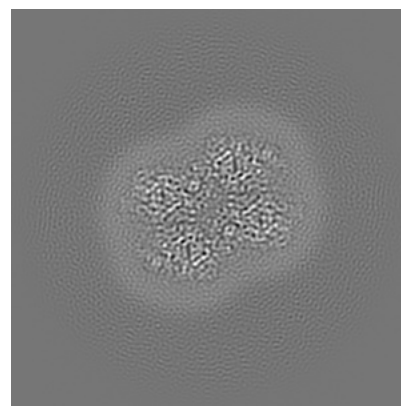
6.1.1 Primary map



X

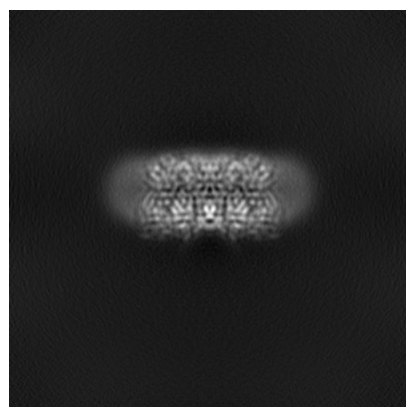


Y

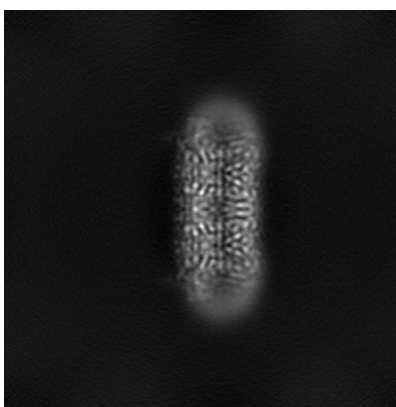


Z

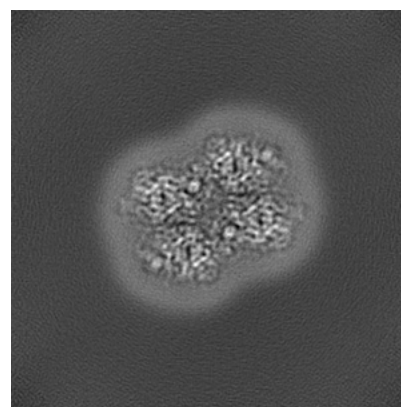
6.1.2 Raw map



X



Y

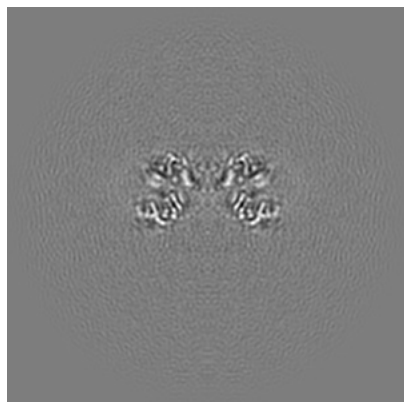


Z

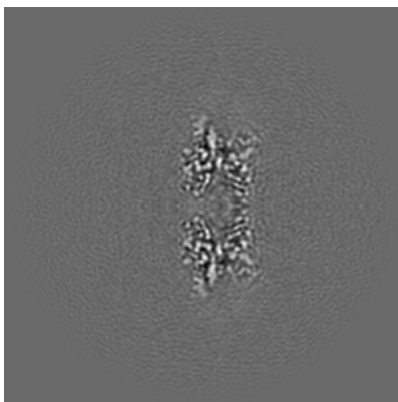
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

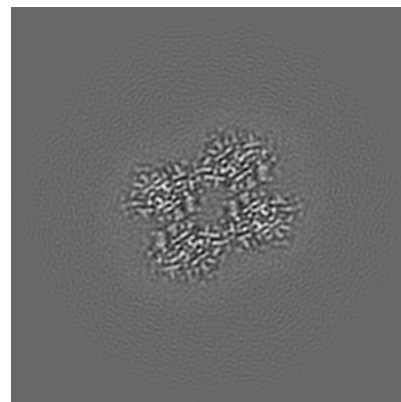
6.2.1 Primary map



X Index: 128

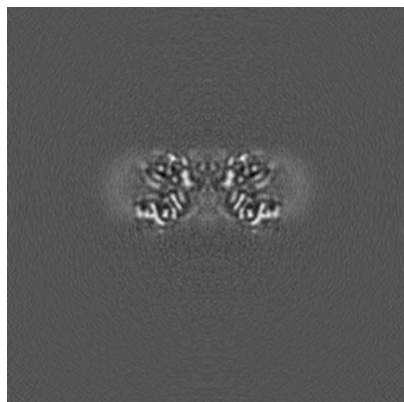


Y Index: 128

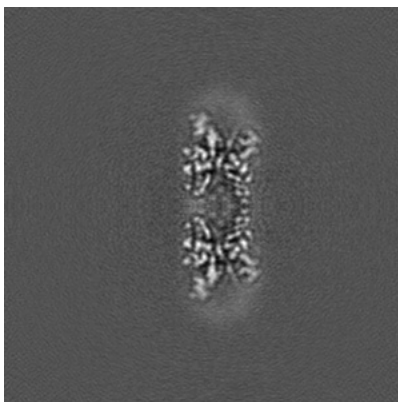


Z Index: 128

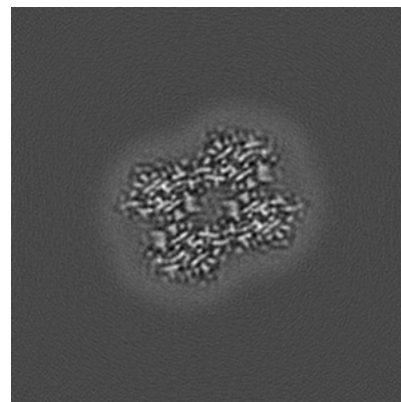
6.2.2 Raw map



X Index: 128



Y Index: 128

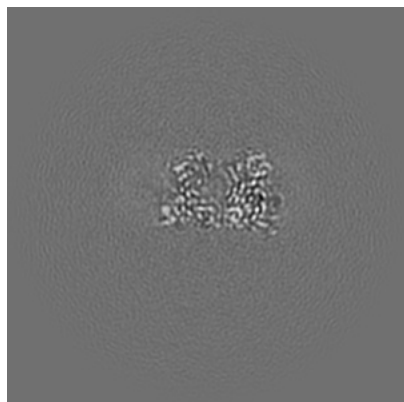


Z Index: 128

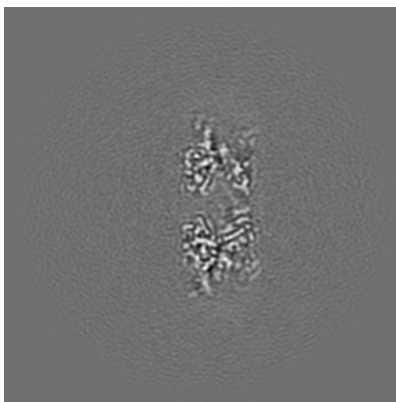
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

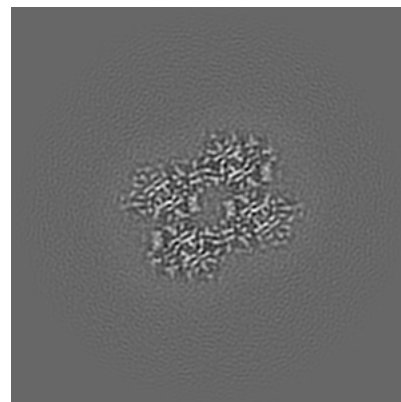
6.3.1 Primary map



X Index: 139

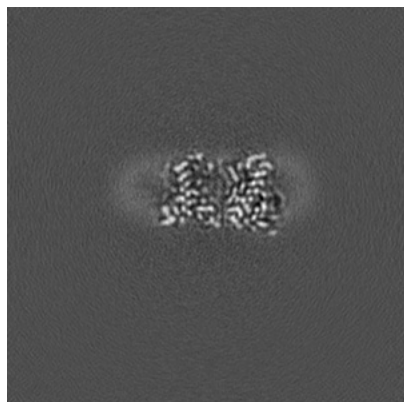


Y Index: 130

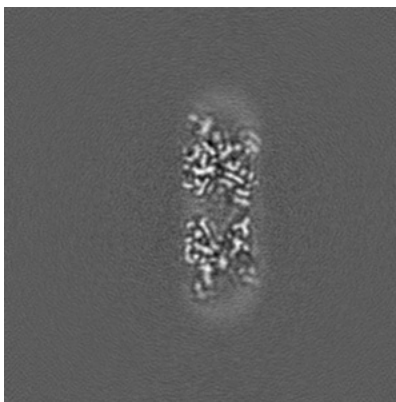


Z Index: 127

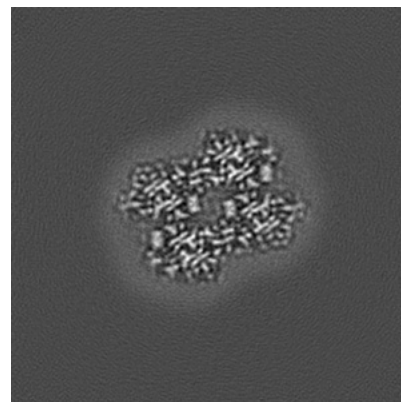
6.3.2 Raw map



X Index: 139



Y Index: 126

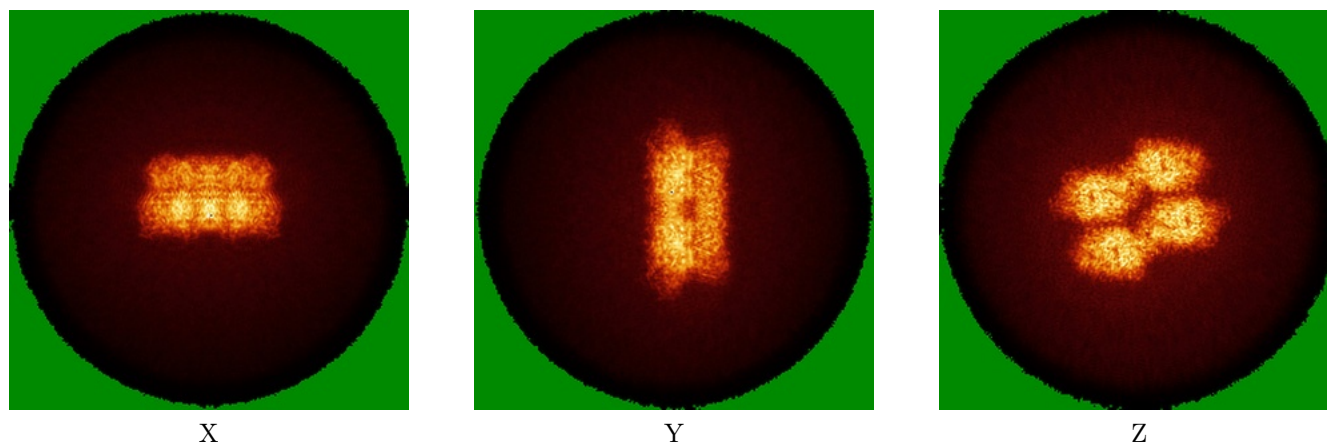


Z Index: 127

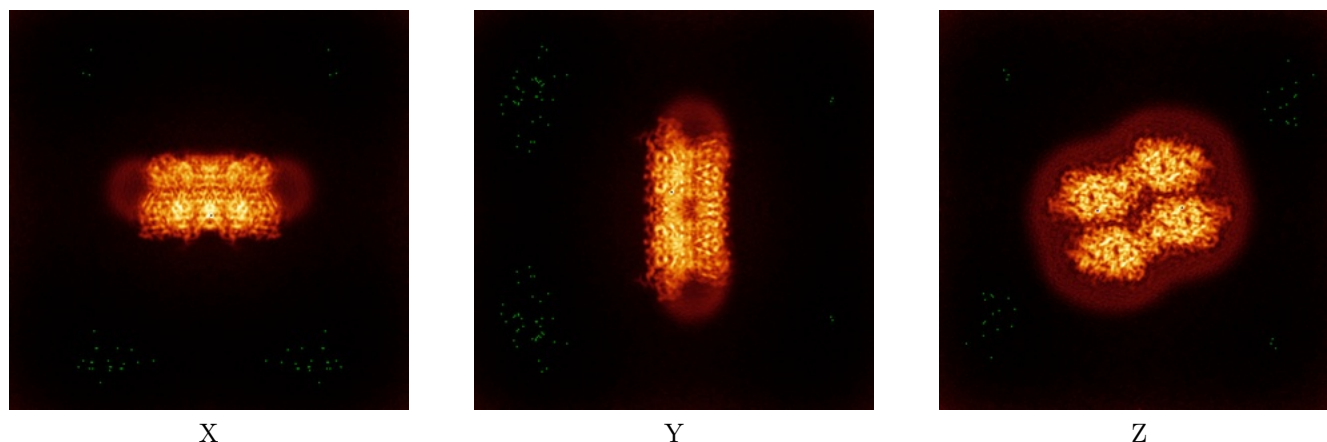
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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

6.5 Orthogonal surface views [i](#)

This section was not generated.

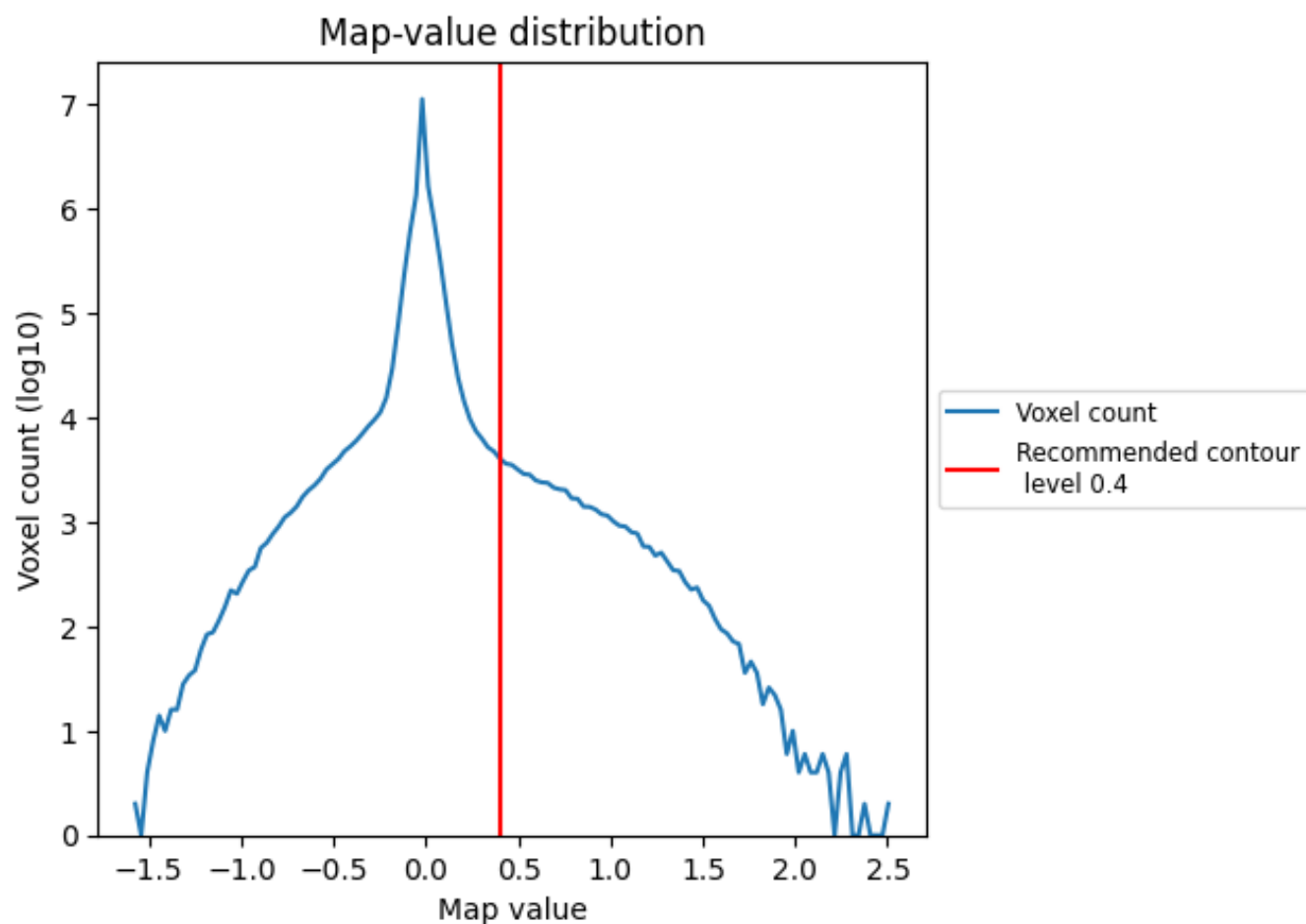
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

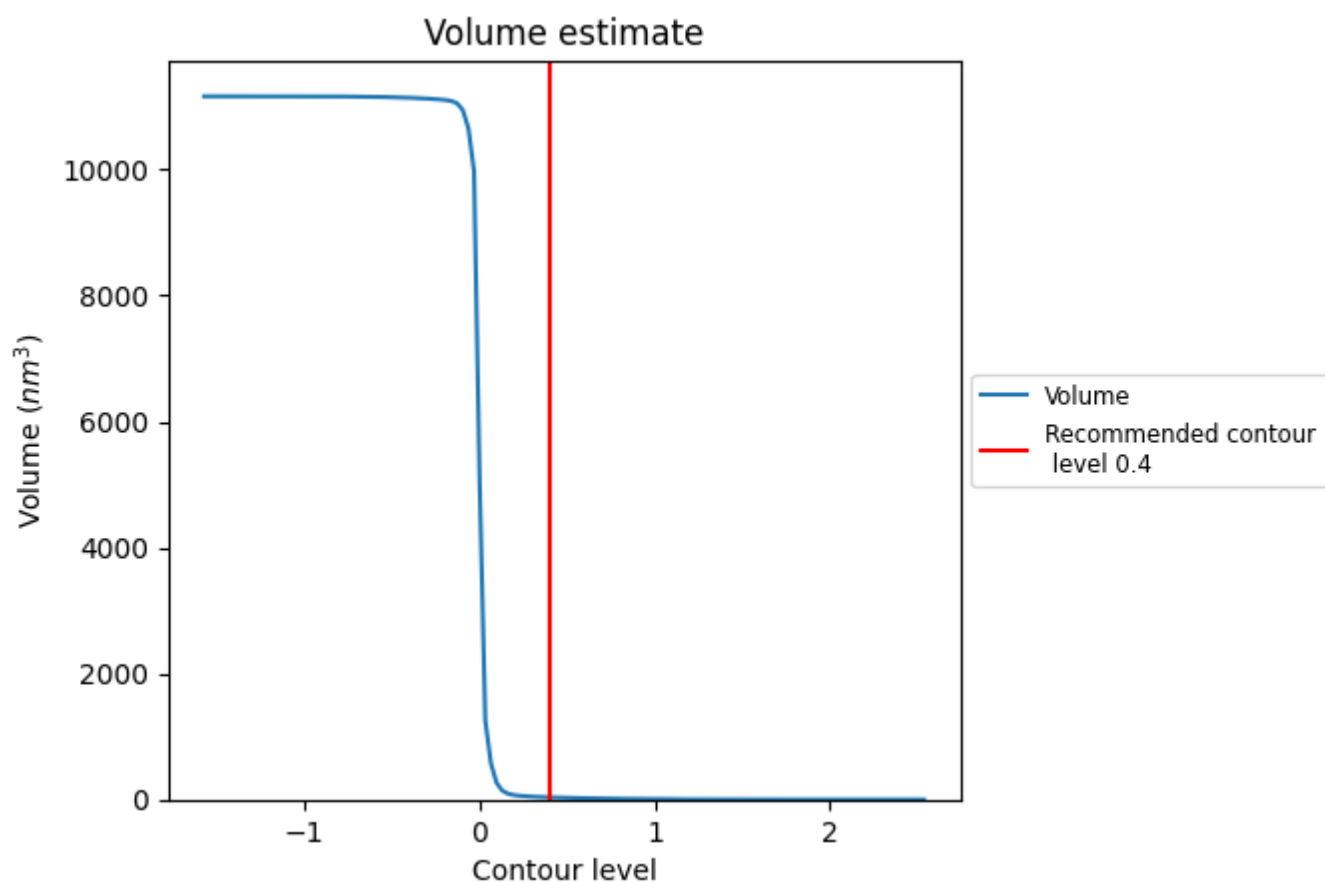
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

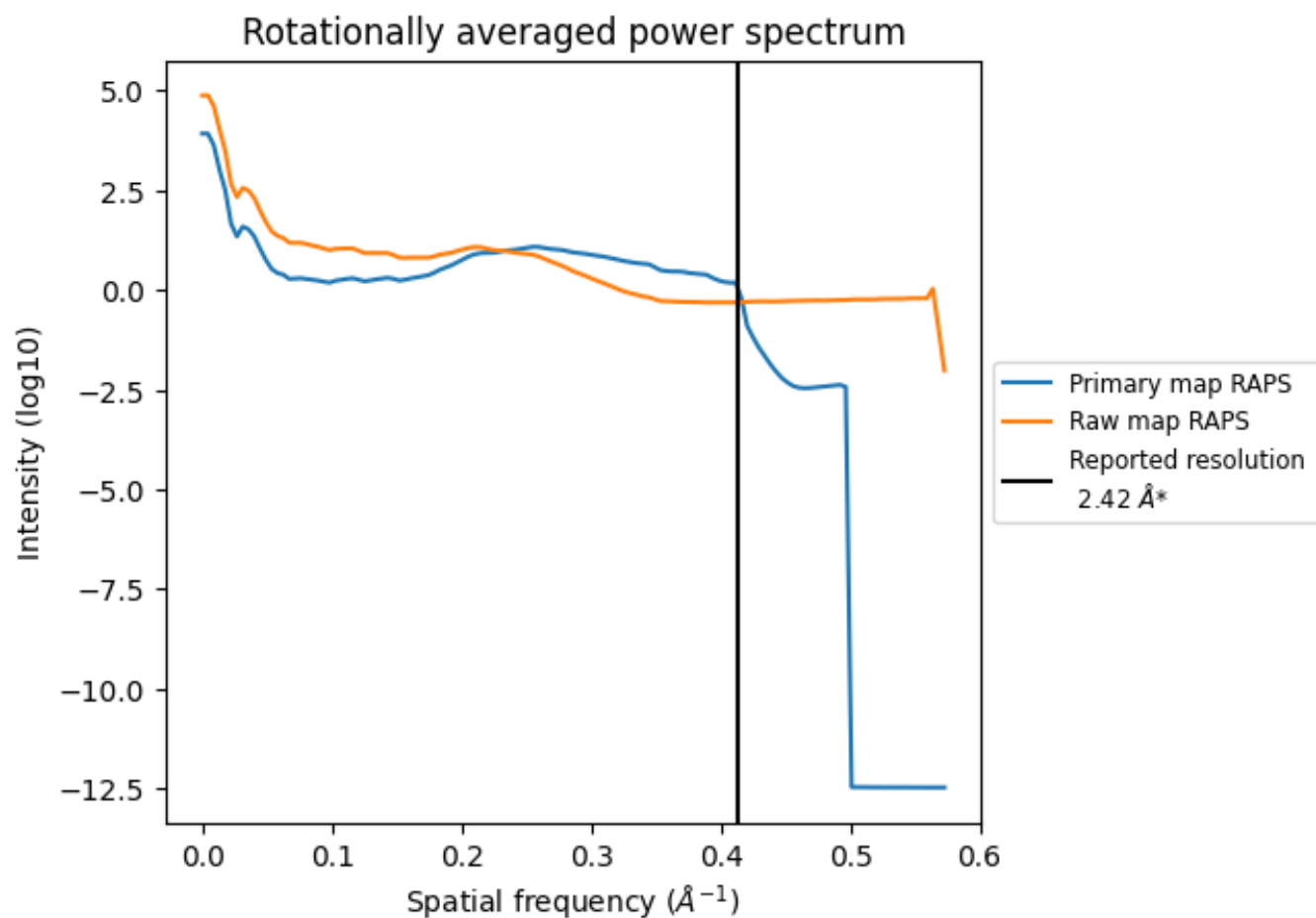
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 35 nm³; this corresponds to an approximate mass of 32 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 ⓘ

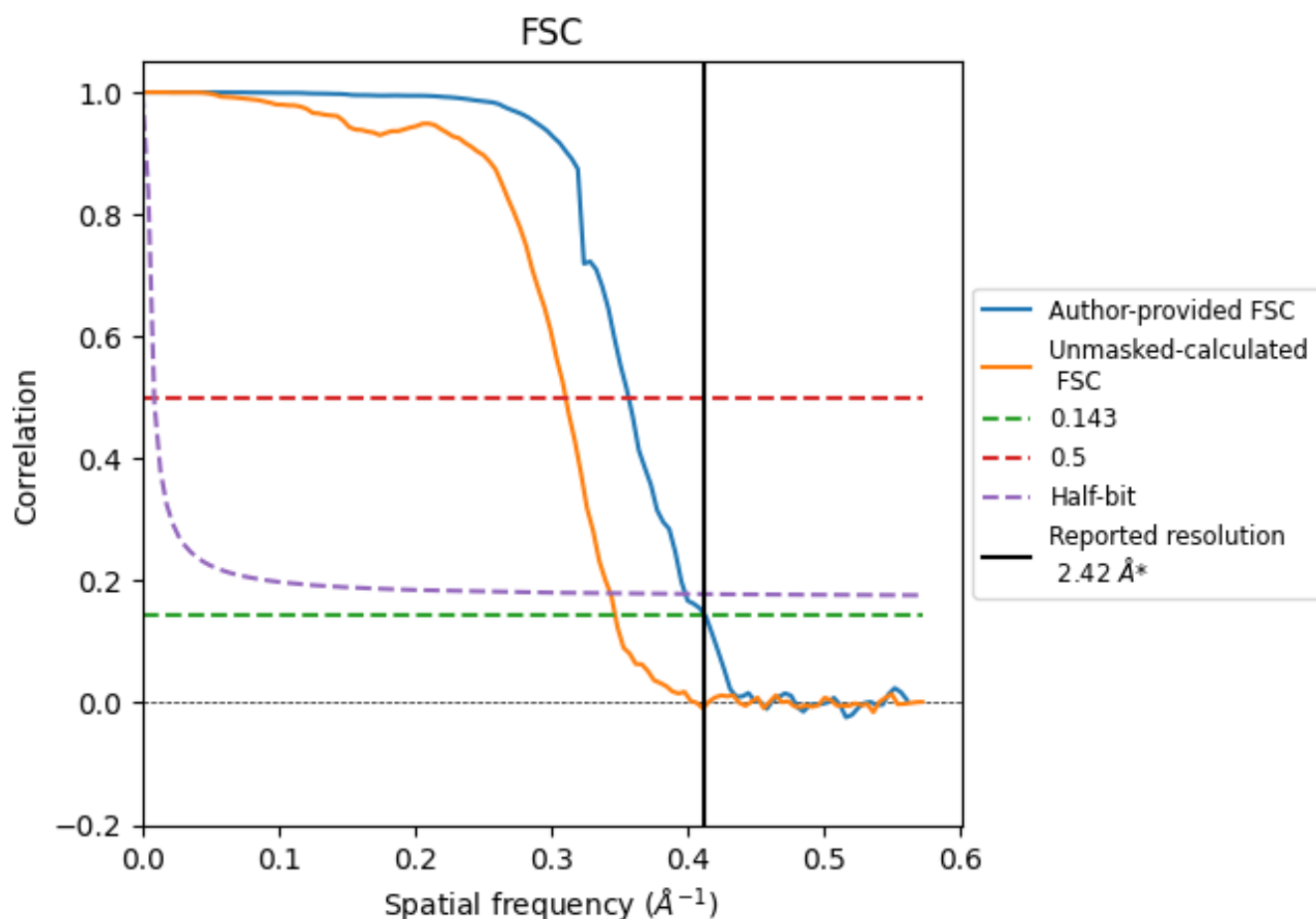


*Reported resolution corresponds to spatial frequency of 0.413 Å⁻¹

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 0.413 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

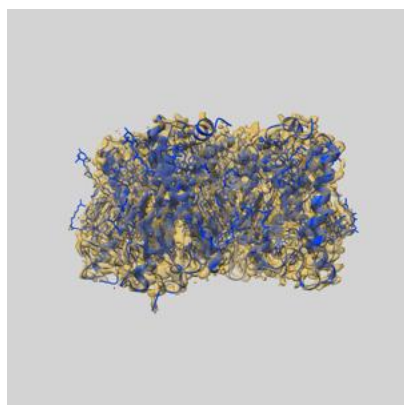
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.42	-	-
Author-provided FSC curve	2.42	2.80	2.51
Unmasked-calculated*	2.88	3.22	2.91

*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 2.88 differs from the reported value 2.42 by more than 10 %

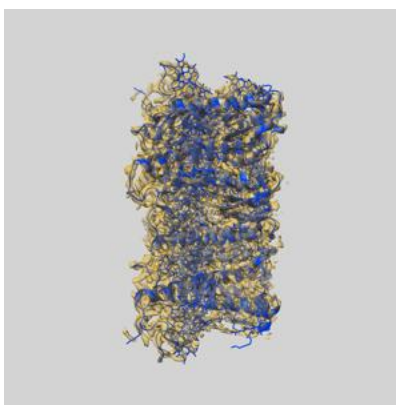
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-63799 and PDB model 9MCC. Per-residue inclusion information can be found in [section 3](#) on [page 11](#).

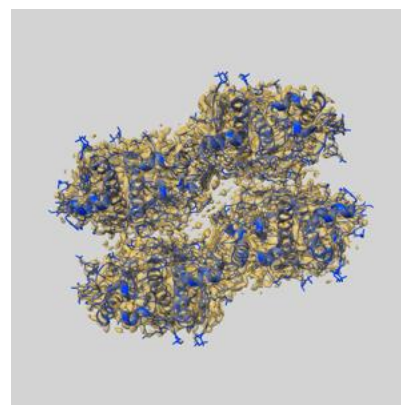
9.1 Map-model overlay [i](#)



X



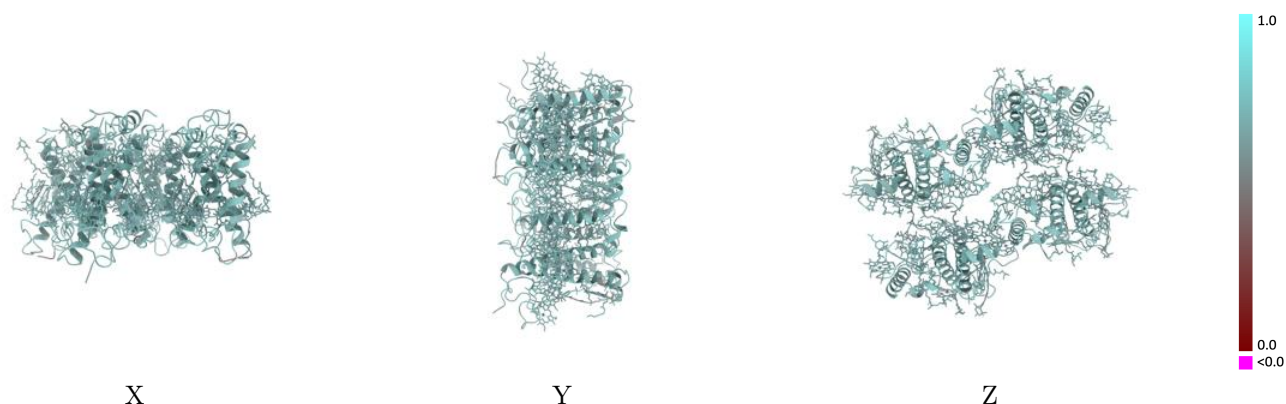
Y



Z

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

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

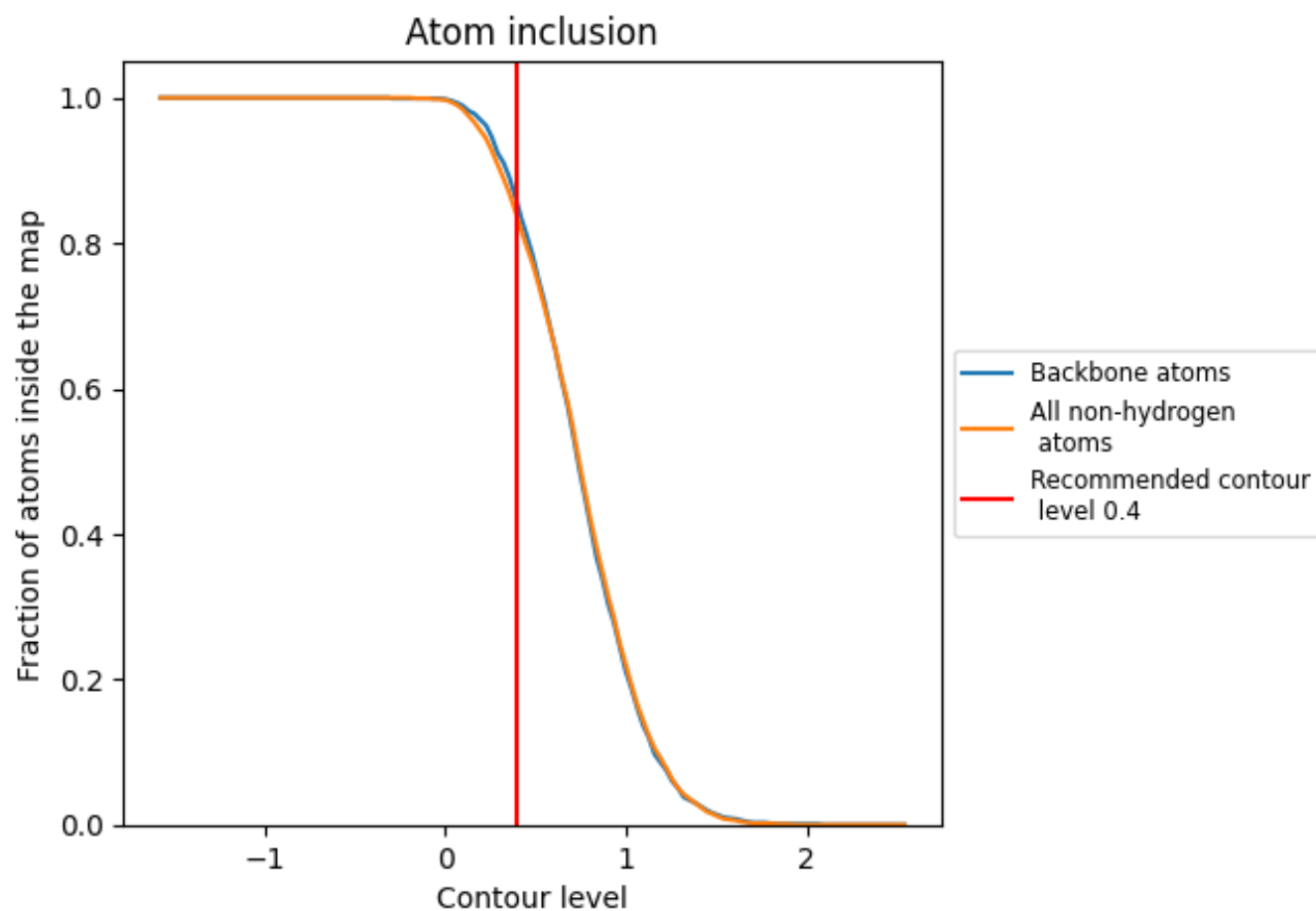


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 83% 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	0.8340	0.6580
A	0.8310	0.6580
B	0.8320	0.6580
C	0.8310	0.6580
D	0.8340	0.6580

