



Full wwPDB EM Validation Report ⓘ

Aug 6, 2026 – 07:33 PM JST

PDB ID : 8IX0 / pdb_00008ix0
EMDB ID : EMD-35785
Title : Cryo-EM structure of unprotonated LHCII nanodisc at high pH value
Authors : Ruan, M.X.; Ding, W.
Deposited on : 2023-03-31
Resolution : 2.64 Å(reported)

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.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
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) : 2.50

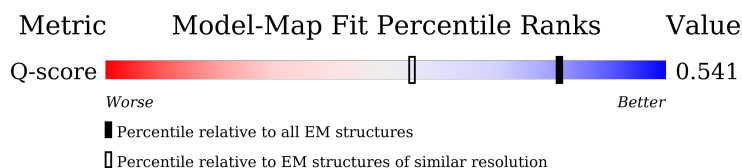
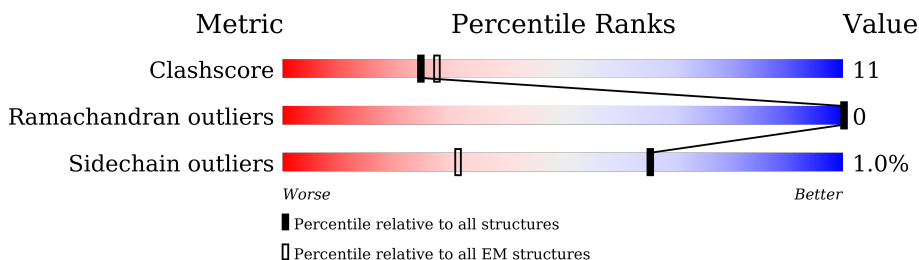
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.64 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	8968 (2.14 - 3.14)

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	G	218	 84% 16%
1	N	218	 89% 10% •
1	Y	218	 89% 11%

2 Entry composition [i](#)

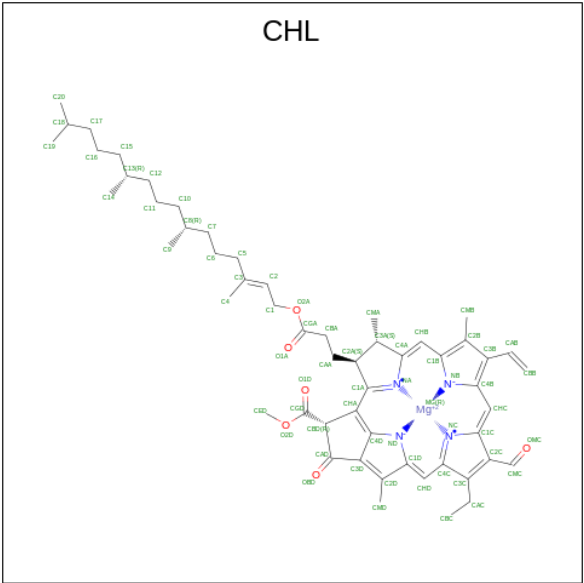
There are 7 unique types of molecules in this entry. The entry contains 8238 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	N	218	Total	C	N	O	S	0	0
			1661	1079	270	305	7		
1	G	218	Total	C	N	O	S	0	0
			1661	1079	270	305	7		
1	Y	218	Total	C	N	O	S	0	0
			1661	1079	270	305	7		

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



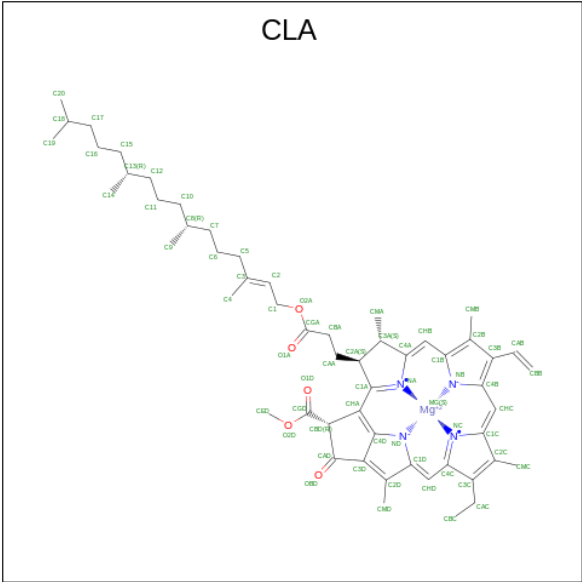
Mol	Chain	Residues	Atoms					AltConf
2	N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
2	N	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
2	N	1	Total	C	Mg	N	O	0
			51	40	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
2	N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
2	N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
2	N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
2	G	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
2	G	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
2	G	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
2	G	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
2	G	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
2	G	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
2	G	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
2	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
2	Y	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
2	Y	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
2	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
2	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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



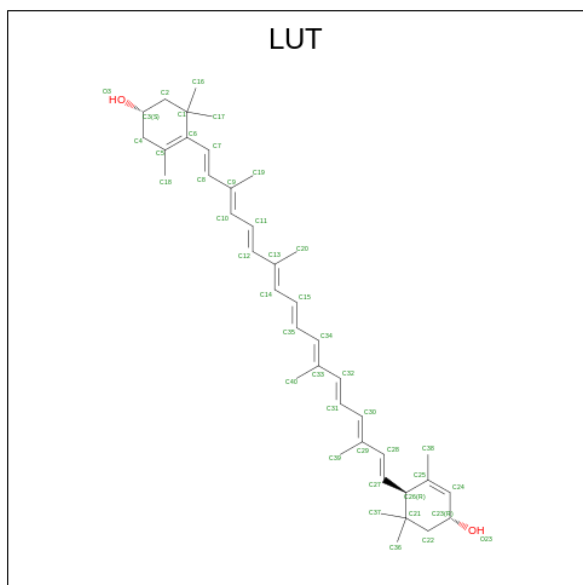
Mol	Chain	Residues	Atoms					AltConf
3	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	N	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
3	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	N	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
3	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	G	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
3	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
3	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	G	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
3	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	Y	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
3	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	Y	1	Total	C	Mg	N	O	0
			49	39	1	4	5	

- Molecule 4 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: C₄₀H₅₆O₂).



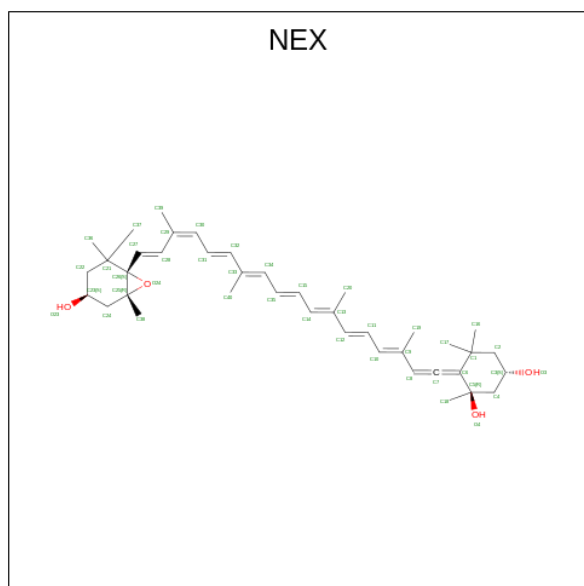
Mol	Chain	Residues	Atoms			AltConf
4	N	1	Total	C	O	0
			42	40	2	

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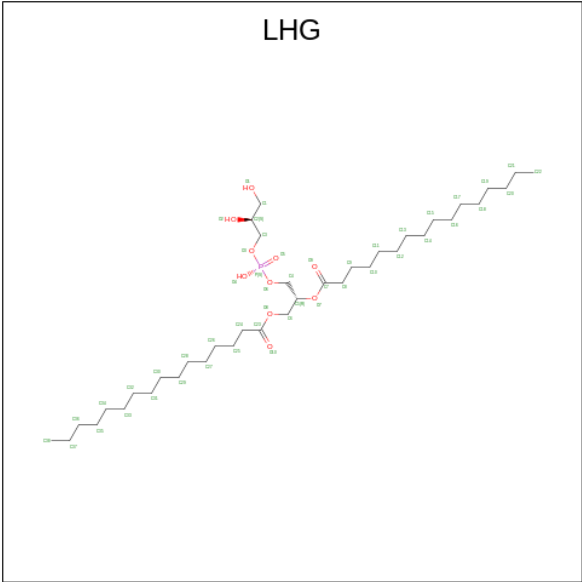
Mol	Chain	Residues	Atoms			AltConf
4	N	1	Total	C	O	0
			42	40	2	
4	G	1	Total	C	O	0
			42	40	2	
4	G	1	Total	C	O	0
			42	40	2	
4	Y	1	Total	C	O	0
			42	40	2	
4	Y	1	Total	C	O	0
			42	40	2	

- Molecule 5 is (1R,3R)-6-[(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTADECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE]-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (CCD ID: NEX) (formula: C₄₀H₅₆O₄) (labeled as "Ligand of Interest" by depositor).



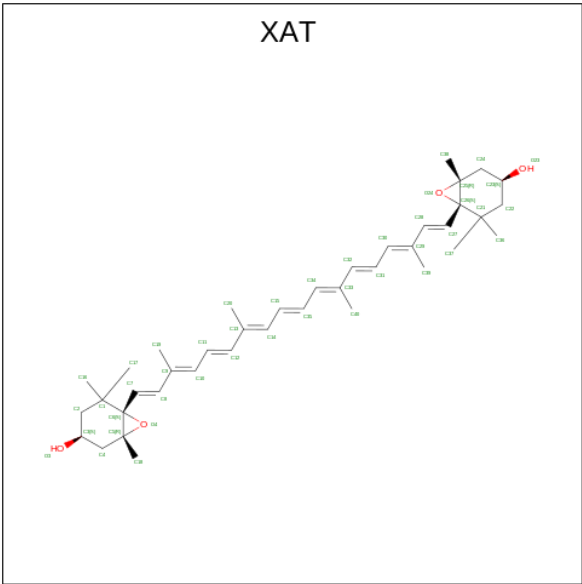
Mol	Chain	Residues	Atoms			AltConf
5	N	1	Total	C	O	0
			44	40	4	
5	G	1	Total	C	O	0
			44	40	4	
5	Y	1	Total	C	O	0
			44	40	4	

- Molecule 6 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



Mol	Chain	Residues	Atoms				AltConf
6	N	1	Total	C	O	P	0
			49	38	10	1	
6	G	1	Total	C	O	P	0
			49	38	10	1	
6	Y	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 7 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA, BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: C₄₀H₅₆O₄).



Mol	Chain	Residues	Atoms			AltConf
7	N	1	Total 44	C 40	O 4	0
7	G	1	Total 44	C 40	O 4	0
7	Y	1	Total 44	C 40	O 4	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.

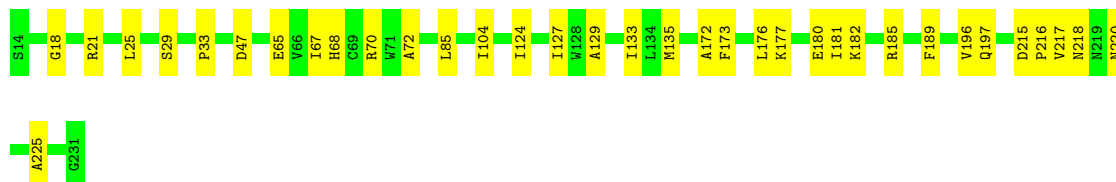
- Molecule 1: Chlorophyll a-b binding protein, chloroplastic

Chain N: 



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

Chain G: 



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

Chain Y: 



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	817473	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	22500	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.490	Depositor
Minimum map value	-0.118	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	208.0, 208.0, 208.0	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	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: LHG, CHL, CLA, XAT, NEX, LUT

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	G	0.26	0/1713	0.53	0/2333
1	N	0.27	0/1713	0.50	0/2333
1	Y	0.22	0/1713	0.46	0/2333
All	All	0.25	0/5139	0.50	0/6999

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	G	1661	0	1592	25	0
1	N	1661	0	1591	20	0
1	Y	1661	0	1592	22	0
2	G	429	0	420	14	0
2	N	363	0	350	13	0
2	Y	297	0	280	8	0
3	G	501	0	534	19	0
3	N	501	0	534	18	0
3	Y	501	0	534	25	0
4	G	84	0	112	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	N	84	0	112	9	0
4	Y	84	0	112	13	0
5	G	44	0	56	3	0
5	N	44	0	56	4	0
5	Y	44	0	56	4	0
6	G	49	0	74	2	0
6	N	49	0	74	1	0
6	Y	49	0	74	0	0
7	G	44	0	56	5	0
7	N	44	0	56	4	0
7	Y	44	0	56	6	0
All	All	8238	0	8321	175	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 11.

All (175) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:610:CLA:H52	4:G:615:LUT:H28	1.68	0.74
1:G:196:VAL:HG11	3:G:613:CLA:HAC2	1.70	0.73
3:N:610:CLA:H52	4:N:615:LUT:H28	1.73	0.70
3:Y:312:CLA:HMC1	4:Y:315:LUT:H203	1.74	0.68
1:N:208:ASN:ND2	3:N:613:CLA:O1D	2.30	0.64
1:G:182:LYS:HZ3	6:G:618:LHG:HC42	1.64	0.63
3:Y:310:CLA:H52	4:Y:315:LUT:H28	1.81	0.62
3:N:610:CLA:H72	4:N:615:LUT:H30	1.81	0.62
1:G:173:PHE:O	1:G:177:LYS:HG3	2.00	0.61
1:G:65:GLU:OE2	1:G:185:ARG:NH1	2.34	0.61
1:G:197:GLN:NE2	3:G:613:CLA:NA	2.49	0.61
1:G:217:VAL:O	1:G:220:ASN:ND2	2.34	0.60
3:G:610:CLA:H61	4:G:615:LUT:C37	2.32	0.59
3:G:610:CLA:H61	4:G:615:LUT:H371	1.84	0.59
1:N:193:GLY:O	1:N:197:GLN:HG2	2.04	0.58
1:N:196:VAL:HG11	3:N:613:CLA:HAC2	1.85	0.58
1:Y:172:ALA:O	1:Y:176:LEU:HG	2.03	0.57
1:Y:21:ARG:NH2	1:Y:43:ASP:OD2	2.38	0.57
1:Y:176:LEU:HD13	3:Y:310:CLA:H3A	1.86	0.57
2:G:619:CHL:HHD	2:Y:307:CHL:HBC2	1.86	0.56
1:N:25:LEU:HB3	1:N:29:SER:HA	1.86	0.56
2:G:605:CHL:HBB1	2:G:605:CHL:HHC	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:610:CLA:H71	3:G:612:CLA:H91	1.88	0.56
1:Y:103:GLN:OE1	1:Y:103:GLN:N	2.34	0.55
3:G:610:CLA:H62	3:G:612:CLA:H92	1.87	0.55
1:G:70:ARG:NH2	1:G:180:GLU:OE1	2.30	0.54
1:N:197:GLN:HE22	3:N:613:CLA:C1D	2.21	0.54
1:G:67:ILE:HD12	1:G:68:HIS:N	2.22	0.54
1:N:135:MET:HE1	2:N:609:CHL:C2C	2.38	0.53
1:G:18:GLY:O	1:G:21:ARG:NH1	2.38	0.53
1:G:182:LYS:HE3	3:G:611:CLA:C3D	2.39	0.53
1:N:23:LYS:HE3	1:N:32:SER:HB3	1.91	0.53
5:N:617:NEX:H183	5:N:617:NEX:H192	1.91	0.52
2:G:606:CHL:HMC	2:G:607:CHL:C4C	2.39	0.52
3:Y:312:CLA:H122	3:Y:312:CLA:HMB2	1.91	0.52
3:Y:312:CLA:CMC	4:Y:315:LUT:H203	2.40	0.52
1:N:225:ALA:HB1	7:N:619:XAT:H42	1.91	0.52
3:G:610:CLA:H72	4:G:615:LUT:C30	2.40	0.52
2:N:601:CHL:H102	6:N:618:LHG:H191	1.91	0.51
3:G:610:CLA:H8	4:G:615:LUT:H371	1.92	0.51
3:Y:304:CLA:HED2	3:Y:304:CLA:H2A	1.93	0.50
3:N:610:CLA:H51	3:N:610:CLA:HBB1	1.93	0.50
1:Y:225:ALA:HA	7:Y:301:XAT:H22	1.92	0.50
1:N:194:PHE:HE1	4:N:615:LUT:H41	1.76	0.49
2:N:606:CHL:HBC2	2:N:607:CHL:HHD	1.93	0.49
5:G:617:NEX:H183	5:G:617:NEX:H192	1.93	0.49
2:N:607:CHL:H18	2:N:609:CHL:H52	1.95	0.49
1:G:33:PRO:HG2	1:G:47:ASP:HB3	1.94	0.49
2:G:607:CHL:H3A	2:G:607:CHL:H12	1.95	0.48
1:N:131:GLN:HA	2:N:606:CHL:HMA3	1.95	0.48
1:Y:25:LEU:HB2	1:Y:29:SER:HA	1.95	0.48
1:Y:76:ALA:O	1:Y:80:VAL:HG12	2.12	0.48
3:Y:303:CLA:H52	4:Y:316:LUT:H28	1.94	0.48
3:Y:312:CLA:HMB2	3:Y:312:CLA:C12	2.44	0.48
1:N:25:LEU:HA	1:N:25:LEU:HD12	1.75	0.47
2:G:601:CHL:H161	2:G:619:CHL:H142	1.96	0.47
3:Y:310:CLA:H93	3:Y:312:CLA:H91	1.96	0.47
1:G:72:ALA:HB2	4:G:616:LUT:H202	1.95	0.47
1:G:225:ALA:HB1	7:G:620:XAT:H42	1.95	0.47
7:Y:301:XAT:H11	7:Y:301:XAT:H191	1.77	0.47
3:Y:310:CLA:CBB	4:Y:315:LUT:H32	2.44	0.47
3:N:610:CLA:H41	3:N:610:CLA:H61	1.63	0.47
4:N:615:LUT:H11	4:N:615:LUT:H191	1.76	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:172:ALA:O	1:G:176:LEU:HD12	2.14	0.47
4:G:616:LUT:H201	4:G:616:LUT:H15	1.79	0.47
3:Y:313:CLA:HMB2	4:Y:315:LUT:H183	1.96	0.47
3:G:613:CLA:H61	3:G:613:CLA:H2	1.62	0.47
1:G:104:ILE:HG12	1:G:124:ILE:CG2	2.45	0.46
3:Y:304:CLA:HMD2	2:Y:309:CHL:C3D	2.45	0.46
7:Y:301:XAT:H35	7:Y:301:XAT:H401	1.78	0.46
5:Y:317:NEX:H15	5:Y:317:NEX:H201	1.71	0.46
1:N:102:SER:O	1:N:102:SER:OG	2.30	0.46
3:Y:310:CLA:H121	3:Y:312:CLA:H172	1.98	0.46
4:N:615:LUT:H35	4:N:615:LUT:H401	1.79	0.46
1:G:218:ASN:OD1	1:G:218:ASN:N	2.48	0.46
1:N:76:ALA:HA	1:N:191:MET:HE1	1.98	0.45
4:N:616:LUT:H11	4:N:616:LUT:H191	1.83	0.45
1:G:182:LYS:NZ	6:G:618:LHG:HC42	2.30	0.45
4:G:615:LUT:H11	4:G:615:LUT:H191	1.81	0.45
7:Y:301:XAT:H31	7:Y:301:XAT:H391	1.80	0.45
2:N:601:CHL:H11	2:G:609:CHL:HBA1	1.98	0.45
3:N:613:CLA:H2	3:N:613:CLA:H61	1.70	0.45
2:G:606:CHL:HBC2	2:G:607:CHL:HHD	1.99	0.45
7:G:620:XAT:H35	7:G:620:XAT:H401	1.80	0.45
1:N:59:ALA:O	1:N:63:GLU:HG3	2.17	0.45
2:G:608:CHL:H162	2:G:608:CHL:H121	1.74	0.45
5:G:617:NEX:H35	5:G:617:NEX:H401	1.76	0.45
1:Y:112:TYR:HB3	1:Y:118:LEU:HD12	1.98	0.45
7:Y:301:XAT:H15	7:Y:301:XAT:H201	1.72	0.45
3:Y:304:CLA:HBC2	2:Y:309:CHL:HMD2	1.99	0.45
1:N:60:LYS:NZ	1:Y:48:THR:O	2.47	0.45
2:N:601:CHL:H3A	2:N:601:CHL:HBA1	1.76	0.45
3:N:602:CLA:H141	3:N:602:CLA:H161	1.84	0.45
1:Y:103:GLN:O	1:Y:106:SER:OG	2.28	0.45
7:N:619:XAT:H31	7:N:619:XAT:H391	1.80	0.44
1:G:85:LEU:HD23	1:G:85:LEU:HA	1.82	0.44
5:N:617:NEX:H35	5:N:617:NEX:H401	1.77	0.44
1:G:124:ILE:HA	1:G:127:ILE:HG13	2.00	0.44
3:Y:310:CLA:H71	3:Y:312:CLA:H8	1.98	0.44
3:G:603:CLA:H143	3:G:603:CLA:H111	1.81	0.44
5:Y:317:NEX:H183	5:Y:317:NEX:H192	2.00	0.44
4:Y:315:LUT:H191	4:Y:315:LUT:H11	1.74	0.44
3:N:612:CLA:H72	3:N:612:CLA:H112	1.92	0.44
3:N:611:CLA:HBA1	3:N:611:CLA:H3A	1.79	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:N:619:XAT:H35	7:N:619:XAT:H401	1.79	0.43
3:Y:304:CLA:H143	3:Y:304:CLA:H112	1.73	0.43
3:G:610:CLA:H62	3:G:612:CLA:C9	2.48	0.43
1:Y:225:ALA:HB1	7:Y:301:XAT:H42	2.00	0.43
1:N:212:HIS:HE1	3:N:614:CLA:NB	2.11	0.43
3:N:611:CLA:H171	3:N:611:CLA:H13	1.88	0.43
2:G:608:CHL:H142	2:G:608:CHL:H112	1.81	0.43
4:Y:316:LUT:H15	4:Y:316:LUT:H201	1.78	0.43
4:Y:316:LUT:H31	4:Y:316:LUT:H391	1.81	0.43
3:Y:313:CLA:H111	3:Y:313:CLA:H152	1.92	0.43
4:G:615:LUT:H35	4:G:615:LUT:H401	1.80	0.43
2:Y:308:CHL:H3A	2:Y:308:CHL:HBA2	1.84	0.43
4:Y:315:LUT:H31	4:Y:315:LUT:H391	1.76	0.43
5:Y:317:NEX:H35	5:Y:317:NEX:H401	1.76	0.43
5:G:617:NEX:H11	5:G:617:NEX:H191	1.77	0.43
1:Y:21:ARG:O	1:Y:23:LYS:NZ	2.44	0.43
1:Y:142:ARG:HG2	2:Y:308:CHL:CHD	2.49	0.43
3:N:614:CLA:HBA1	3:N:614:CLA:H3A	1.76	0.42
1:Y:85:LEU:HD12	1:Y:85:LEU:HA	1.83	0.42
2:N:608:CHL:H121	2:N:608:CHL:H162	1.88	0.42
4:Y:315:LUT:H35	4:Y:315:LUT:H401	1.76	0.42
2:N:608:CHL:HBA2	2:N:608:CHL:H3A	1.72	0.42
1:G:177:LYS:O	1:G:181:ILE:HG22	2.19	0.42
3:G:614:CLA:H2A	3:G:614:CLA:O1D	2.19	0.42
3:Y:311:CLA:HBA1	3:Y:311:CLA:H3A	1.73	0.42
3:G:602:CLA:H52	4:G:616:LUT:H28	2.01	0.42
1:N:197:GLN:HE22	3:N:613:CLA:CHD	2.31	0.42
4:N:616:LUT:H401	4:N:616:LUT:H35	1.78	0.42
3:G:602:CLA:H161	3:G:602:CLA:H141	1.78	0.42
2:N:601:CHL:H202	2:G:607:CHL:H142	2.01	0.42
1:Y:199:ILE:HD12	1:Y:199:ILE:HA	1.88	0.42
1:G:197:GLN:NE2	3:G:613:CLA:C4A	2.83	0.42
2:G:607:CHL:H143	2:G:607:CHL:H111	1.91	0.42
1:Y:176:LEU:CD1	3:Y:310:CLA:H3A	2.49	0.42
1:Y:20:ASP:N	1:Y:20:ASP:OD1	2.53	0.41
2:N:601:CHL:H91	2:N:601:CHL:H112	1.61	0.41
3:Y:310:CLA:HBB2	4:Y:315:LUT:H32	2.01	0.41
1:G:129:ALA:O	1:G:133:ILE:HG22	2.20	0.41
7:G:620:XAT:H31	7:G:620:XAT:H391	1.78	0.41
1:Y:18:GLY:O	1:Y:21:ARG:NH1	2.38	0.41
4:Y:315:LUT:H201	4:Y:315:LUT:H15	1.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:115:ASN:HB3	1:N:118:LEU:HG	2.02	0.41
2:N:601:CHL:H202	2:N:601:CHL:H161	1.60	0.41
2:Y:308:CHL:H61	2:Y:308:CHL:H2	1.61	0.41
3:Y:310:CLA:H141	3:Y:310:CLA:H161	1.51	0.41
3:Y:311:CLA:H93	3:Y:311:CLA:H62	1.81	0.41
1:G:135:MET:HE1	2:G:606:CHL:HMB3	2.03	0.41
1:G:215:ASP:HA	1:G:216:PRO:HD3	1.91	0.41
2:G:601:CHL:H203	7:G:620:XAT:H171	2.02	0.41
1:Y:100:ALA:HA	1:Y:103:GLN:HE22	1.86	0.41
3:Y:304:CLA:H61	3:Y:304:CLA:H2	1.75	0.41
4:N:616:LUT:H391	4:N:616:LUT:H31	1.79	0.41
5:N:617:NEX:H15	5:N:617:NEX:H201	1.70	0.41
3:N:611:CLA:H93	3:N:611:CLA:H62	1.73	0.41
3:Y:310:CLA:H51	3:Y:312:CLA:HMA1	2.02	0.41
2:G:619:CHL:H42	1:Y:199:ILE:HD13	2.03	0.41
3:N:604:CLA:H71	3:N:604:CLA:H112	1.83	0.40
3:G:610:CLA:HBB2	4:G:615:LUT:H32	2.02	0.40
7:G:620:XAT:H11	7:G:620:XAT:H191	1.75	0.40
5:Y:317:NEX:H373	5:Y:317:NEX:H23	1.89	0.40
5:N:617:NEX:H11	5:N:617:NEX:H191	1.73	0.40
1:Y:96:VAL:HB	1:Y:99:LYS:HB3	2.03	0.40
1:N:24:TYR:CE2	2:N:601:CHL:HAA1	2.56	0.40
1:N:203:LYS:HE2	1:N:203:LYS:HB3	1.92	0.40
1:G:25:LEU:HB3	1:G:29:SER:HA	2.03	0.40
3:G:602:CLA:H101	4:G:616:LUT:H371	2.02	0.40
1:Y:142:ARG:HG2	2:Y:308:CHL:C1D	2.51	0.40
2:Y:308:CHL:H162	2:Y:308:CHL:H121	1.90	0.40
3:Y:314:CLA:HBA1	3:Y:314:CLA:H3A	1.79	0.40
3:N:610:CLA:H72	4:N:615:LUT:C30	2.48	0.40
7:N:619:XAT:H3	7:N:619:XAT:H173	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	216/218 (99%)	207 (96%)	9 (4%)	0	100	100
1	N	216/218 (99%)	209 (97%)	7 (3%)	0	100	100
1	Y	216/218 (99%)	209 (97%)	7 (3%)	0	100	100
All	All	648/654 (99%)	625 (96%)	23 (4%)	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	G	168/168 (100%)	167 (99%)	1 (1%)	78	87
1	N	168/168 (100%)	166 (99%)	2 (1%)	63	78
1	Y	168/168 (100%)	166 (99%)	2 (1%)	63	78
All	All	504/504 (100%)	499 (99%)	5 (1%)	65	80

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	23	LYS
1	N	194	PHE
1	G	189	PHE
1	Y	92	PHE
1	Y	176	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	N	103	GLN
1	N	115	ASN

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Mol	Chain	Res	Type
1	G	197	GLN
1	G	208	ASN
1	G	220	ASN
1	Y	68	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

57 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	CLA	G	610	1	69,73,73	1.25	9 (13%)	83,113,113	1.25	6 (7%)
2	CHL	N	607	-	70,74,74	1.21	8 (11%)	80,114,114	1.22	6 (7%)
7	XAT	Y	301	-	39,47,47	0.92	0	54,74,74	2.80	17 (31%)
3	CLA	Y	311	6	69,73,73	1.25	5 (7%)	83,113,113	1.13	5 (6%)
2	CHL	N	606	1	55,59,74	1.36	6 (10%)	62,96,114	1.30	7 (11%)
3	CLA	Y	305	-	66,70,73	1.27	7 (10%)	79,109,113	1.18	5 (6%)
3	CLA	Y	314	1	53,57,73	1.40	7 (13%)	62,93,113	1.33	8 (12%)
4	LUT	N	615	-	42,43,43	0.76	0	51,60,60	1.74	11 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	CLA	G	611	6	69,73,73	1.25	8 (11%)	83,113,113	1.17	7 (8%)
3	CLA	Y	303	1	69,73,73	1.25	6 (8%)	83,113,113	1.14	4 (4%)
2	CHL	G	608	-	70,74,74	1.20	6 (8%)	80,114,114	1.17	8 (10%)
2	CHL	Y	302	1	70,74,74	1.22	5 (7%)	80,114,114	1.10	7 (8%)
3	CLA	G	603	-	69,73,73	1.25	7 (10%)	83,113,113	1.18	4 (4%)
7	XAT	N	619	-	39,47,47	0.93	0	54,74,74	2.82	17 (31%)
4	LUT	Y	315	-	42,43,43	0.79	0	51,60,60	1.98	15 (29%)
3	CLA	G	614	1	53,57,73	1.40	5 (9%)	62,93,113	1.26	7 (11%)
3	CLA	N	610	1	69,73,73	1.22	8 (11%)	83,113,113	1.16	5 (6%)
2	CHL	Y	306	1	52,56,74	1.38	6 (11%)	58,92,114	1.23	9 (15%)
3	CLA	G	613	1	69,73,73	1.26	6 (8%)	83,113,113	1.16	5 (6%)
2	CHL	G	606	-	55,59,74	1.34	6 (10%)	62,96,114	1.27	7 (11%)
2	CHL	G	605	-	52,56,74	1.41	5 (9%)	58,92,114	1.33	6 (10%)
4	LUT	Y	316	-	42,43,43	0.76	0	51,60,60	1.78	12 (23%)
3	CLA	Y	312	1	69,73,73	1.26	9 (13%)	83,113,113	1.24	9 (10%)
3	CLA	N	612	1	69,73,73	1.25	7 (10%)	83,113,113	1.19	6 (7%)
6	LHG	N	618	3	48,48,48	0.94	2 (4%)	51,54,54	1.08	4 (7%)
3	CLA	G	604	-	66,70,73	1.28	8 (12%)	79,109,113	1.23	5 (6%)
3	CLA	Y	304	1	69,73,73	1.27	6 (8%)	83,113,113	1.30	11 (13%)
4	LUT	N	616	-	42,43,43	0.76	0	51,60,60	1.90	11 (21%)
2	CHL	N	608	-	70,74,74	1.21	8 (11%)	80,114,114	1.16	7 (8%)
4	LUT	G	616	-	42,43,43	0.75	0	51,60,60	1.81	11 (21%)
7	XAT	G	620	-	39,47,47	0.93	0	54,74,74	2.78	18 (33%)
2	CHL	G	601	1	70,74,74	1.22	7 (10%)	80,114,114	1.09	6 (7%)
2	CHL	Y	307	-	55,59,74	1.35	7 (12%)	62,96,114	1.30	7 (11%)
2	CHL	G	607	-	70,74,74	1.22	7 (10%)	80,114,114	1.22	7 (8%)
3	CLA	N	613	1	69,73,73	1.27	6 (8%)	83,113,113	1.17	5 (6%)
4	LUT	G	615	-	42,43,43	0.72	0	51,60,60	1.73	12 (23%)
5	NEX	G	617	-	38,46,46	0.98	1 (2%)	50,70,70	2.40	15 (30%)
6	LHG	G	618	3	48,48,48	0.95	2 (4%)	51,54,54	1.08	4 (7%)
3	CLA	N	614	1	53,57,73	1.41	6 (11%)	62,93,113	1.19	5 (8%)
2	CHL	Y	308	-	70,74,74	1.22	7 (10%)	80,114,114	1.12	8 (10%)
3	CLA	N	611	6	69,73,73	1.25	6 (8%)	83,113,113	1.16	6 (7%)
3	CLA	G	612	1	69,73,73	1.26	8 (11%)	83,113,113	1.22	9 (10%)
3	CLA	G	602	1	69,73,73	1.26	6 (8%)	83,113,113	1.16	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	CLA	N	604	-	66,70,73	1.27	6 (9%)	79,109,113	1.18	5 (6%)
2	CHL	N	605	-	52,56,74	1.38	5 (9%)	58,92,114	1.29	7 (12%)
5	NEX	Y	317	-	38,46,46	0.93	1 (2%)	50,70,70	2.41	16 (32%)
6	LHG	Y	318	3	48,48,48	0.94	2 (4%)	51,54,54	1.01	2 (3%)
2	CHL	G	619	-	70,74,74	1.22	6 (8%)	80,114,114	1.25	6 (7%)
2	CHL	N	609	1	70,74,74	1.23	9 (12%)	80,114,114	1.42	8 (10%)
2	CHL	Y	309	1	70,74,74	1.23	8 (11%)	80,114,114	1.29	7 (8%)
3	CLA	Y	310	1	69,73,73	1.20	8 (11%)	83,113,113	1.23	8 (9%)
2	CHL	G	609	1	70,74,74	1.21	8 (11%)	80,114,114	1.31	9 (11%)
3	CLA	N	603	1	69,73,73	1.26	7 (10%)	83,113,113	1.19	8 (9%)
3	CLA	Y	313	1	69,73,73	1.25	7 (10%)	83,113,113	1.19	5 (6%)
3	CLA	N	602	1	69,73,73	1.26	7 (10%)	83,113,113	1.14	5 (6%)
5	NEX	N	617	-	38,46,46	0.95	1 (2%)	50,70,70	2.38	14 (28%)
2	CHL	N	601	1	70,74,74	1.21	9 (12%)	80,114,114	1.16	8 (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	G	610	1	-	10/39/115/115	-
2	CHL	N	607	-	-	16/41/117/117	-
7	XAT	Y	301	-	-	0/31/93/93	0/4/4/4
3	CLA	Y	311	6	-	20/39/115/115	-
2	CHL	N	606	1	-	8/23/99/117	-
3	CLA	Y	305	-	-	8/36/112/115	-
3	CLA	Y	314	1	-	12/20/96/115	-
4	LUT	N	615	-	-	4/29/67/67	0/2/2/2
3	CLA	G	611	6	-	16/39/115/115	-
3	CLA	Y	303	1	-	12/39/115/115	-
2	CHL	G	608	-	-	10/41/117/117	-
2	CHL	Y	302	1	-	17/41/117/117	-
3	CLA	G	603	-	-	16/39/115/115	-
7	XAT	N	619	-	-	0/31/93/93	0/4/4/4
4	LUT	Y	315	-	-	4/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CLA	G	614	1	-	11/20/96/115	-
3	CLA	N	610	1	-	20/39/115/115	-
2	CHL	Y	306	1	-	11/20/96/117	-
3	CLA	G	613	1	-	14/39/115/115	-
2	CHL	G	606	-	-	8/23/99/117	-
2	CHL	G	605	-	-	4/20/96/117	-
4	LUT	Y	316	-	-	4/29/67/67	0/2/2/2
3	CLA	Y	312	1	-	21/39/115/115	-
3	CLA	N	612	1	-	18/39/115/115	-
6	LHG	N	618	3	-	13/53/53/53	-
3	CLA	G	604	-	-	12/36/112/115	-
3	CLA	Y	304	1	-	18/39/115/115	-
4	LUT	N	616	-	-	1/29/67/67	0/2/2/2
2	CHL	N	608	-	-	14/41/117/117	-
4	LUT	G	616	-	-	6/29/67/67	0/2/2/2
7	XAT	G	620	-	-	0/31/93/93	0/4/4/4
2	CHL	G	601	1	-	16/41/117/117	-
2	CHL	Y	307	-	-	6/23/99/117	-
2	CHL	G	607	-	-	14/41/117/117	-
3	CLA	N	613	1	-	14/39/115/115	-
4	LUT	G	615	-	-	3/29/67/67	0/2/2/2
5	NEX	G	617	-	-	5/27/83/83	0/3/3/3
6	LHG	G	618	3	-	15/53/53/53	-
3	CLA	N	614	1	-	16/20/96/115	-
2	CHL	Y	308	-	-	16/41/117/117	-
3	CLA	N	611	6	-	22/39/115/115	-
3	CLA	G	612	1	-	19/39/115/115	-
3	CLA	G	602	1	-	14/39/115/115	-
3	CLA	N	604	-	-	7/36/112/115	-
2	CHL	N	605	-	-	6/20/96/117	-
5	NEX	Y	317	-	-	3/27/83/83	0/3/3/3
6	LHG	Y	318	3	-	13/53/53/53	-
2	CHL	G	619	-	-	19/41/117/117	-
2	CHL	N	609	1	-	12/41/117/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CHL	Y	309	1	-	11/41/117/117	-
3	CLA	Y	310	1	-	16/39/115/115	-
2	CHL	G	609	1	-	17/41/117/117	-
3	CLA	N	603	1	-	11/39/115/115	-
3	CLA	Y	313	1	-	12/39/115/115	-
3	CLA	N	602	1	-	10/39/115/115	-
5	NEX	N	617	-	-	3/27/83/83	0/3/3/3
2	CHL	N	601	1	-	22/41/117/117	-

All (297) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	Y	318	LHG	O8-C23	4.28	1.45	1.33
6	G	618	LHG	O8-C23	4.26	1.45	1.33
6	N	618	LHG	O8-C23	4.25	1.45	1.33
6	G	618	LHG	O7-C7	4.16	1.46	1.34
6	N	618	LHG	O7-C7	4.14	1.46	1.34
6	Y	318	LHG	O7-C7	4.14	1.46	1.34
3	Y	304	CLA	C1D-ND	4.07	1.42	1.37
3	N	603	CLA	C1D-ND	4.01	1.42	1.37
3	N	613	CLA	C1D-ND	3.97	1.42	1.37
2	G	601	CHL	C1D-ND	3.91	1.42	1.37
2	Y	308	CHL	C1D-ND	3.89	1.42	1.37
2	G	606	CHL	C1D-ND	3.89	1.42	1.37
3	G	611	CLA	C1D-ND	3.86	1.42	1.37
2	G	605	CHL	C1D-ND	3.85	1.42	1.37
3	N	602	CLA	C1D-ND	3.84	1.42	1.37
2	N	606	CHL	C1D-ND	3.84	1.42	1.37
3	G	602	CLA	C1D-ND	3.84	1.42	1.37
3	G	613	CLA	C1D-ND	3.83	1.42	1.37
3	G	614	CLA	C1D-ND	3.82	1.42	1.37
2	Y	302	CHL	C1D-ND	3.82	1.42	1.37
3	Y	303	CLA	C1D-ND	3.82	1.42	1.37
2	N	605	CHL	C1D-ND	3.81	1.42	1.37
3	Y	311	CLA	C1D-ND	3.80	1.42	1.37
2	G	608	CHL	C1D-ND	3.80	1.42	1.37
3	N	611	CLA	C1D-ND	3.79	1.42	1.37
3	Y	313	CLA	C1D-ND	3.79	1.42	1.37
3	G	604	CLA	C1D-ND	3.79	1.42	1.37
2	Y	306	CHL	C1D-ND	3.79	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Y	307	CHL	C1D-ND	3.78	1.42	1.37
2	G	619	CHL	C1D-ND	3.78	1.42	1.37
3	N	614	CLA	C1D-ND	3.76	1.42	1.37
3	G	612	CLA	C1D-ND	3.76	1.42	1.37
2	G	607	CHL	C1D-ND	3.75	1.42	1.37
3	Y	305	CLA	C1D-ND	3.75	1.42	1.37
3	N	604	CLA	C1D-ND	3.74	1.42	1.37
2	N	608	CHL	C1D-ND	3.71	1.42	1.37
2	G	609	CHL	C1D-ND	3.71	1.42	1.37
2	G	605	CHL	C4B-NB	3.70	1.42	1.37
3	N	612	CLA	C1D-ND	3.70	1.42	1.37
3	G	603	CLA	C1D-ND	3.69	1.42	1.37
3	Y	314	CLA	C1D-ND	3.68	1.42	1.37
2	N	607	CHL	C1D-ND	3.64	1.42	1.37
3	G	612	CLA	C4B-NB	3.64	1.42	1.37
3	N	614	CLA	C4B-NB	3.63	1.42	1.37
3	N	602	CLA	C4B-NB	3.62	1.42	1.37
2	G	601	CHL	C4B-NB	3.62	1.42	1.37
3	Y	303	CLA	C4B-NB	3.61	1.42	1.37
2	Y	309	CHL	C1D-ND	3.61	1.42	1.37
3	G	613	CLA	C4B-NB	3.60	1.42	1.37
2	Y	302	CHL	C4B-NB	3.53	1.42	1.37
3	N	610	CLA	C4B-NB	3.51	1.42	1.37
3	G	602	CLA	C4B-NB	3.51	1.42	1.37
2	Y	306	CHL	C4B-NB	3.51	1.42	1.37
3	N	603	CLA	C4B-NB	3.50	1.42	1.37
3	N	613	CLA	C4B-NB	3.47	1.42	1.37
3	Y	313	CLA	C4B-NB	3.47	1.42	1.37
3	Y	311	CLA	C4B-NB	3.46	1.42	1.37
3	N	611	CLA	C4B-NB	3.45	1.42	1.37
2	N	606	CHL	C4B-NB	3.44	1.42	1.37
3	G	604	CLA	C4B-NB	3.44	1.42	1.37
3	G	603	CLA	C4B-NB	3.42	1.42	1.37
2	N	609	CHL	C1D-ND	3.42	1.42	1.37
3	G	611	CLA	C4B-NB	3.42	1.42	1.37
3	N	612	CLA	C4B-NB	3.41	1.42	1.37
3	G	614	CLA	C4B-NB	3.40	1.42	1.37
2	G	607	CHL	C4B-NB	3.39	1.42	1.37
3	Y	304	CLA	C4B-NB	3.39	1.42	1.37
3	G	610	CLA	C4B-NB	3.38	1.41	1.37
2	N	605	CHL	C4B-NB	3.37	1.41	1.37
2	Y	308	CHL	C4B-NB	3.37	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	604	CLA	C4B-NB	3.36	1.41	1.37
3	Y	310	CLA	C1D-ND	3.36	1.41	1.37
3	N	610	CLA	C1D-ND	3.36	1.41	1.37
3	Y	312	CLA	C4D-ND	-3.34	1.33	1.37
3	Y	305	CLA	C4B-NB	3.34	1.41	1.37
3	Y	312	CLA	C1D-ND	3.33	1.41	1.37
3	Y	314	CLA	C4B-NB	3.33	1.41	1.37
3	Y	310	CLA	C4B-NB	3.32	1.41	1.37
2	G	606	CHL	C4B-NB	3.32	1.41	1.37
2	N	607	CHL	C4B-NB	3.31	1.41	1.37
2	G	619	CHL	C4B-NB	3.31	1.41	1.37
2	Y	309	CHL	C4B-NB	3.31	1.41	1.37
2	Y	307	CHL	C4B-NB	3.31	1.41	1.37
2	N	608	CHL	C4B-NB	3.31	1.41	1.37
3	G	610	CLA	C4D-ND	-3.31	1.33	1.37
2	G	605	CHL	C3B-C4B	3.27	1.50	1.42
3	N	610	CLA	C4D-ND	-3.26	1.33	1.37
3	N	612	CLA	C4D-ND	-3.25	1.33	1.37
2	N	601	CHL	C1D-ND	3.25	1.41	1.37
2	Y	309	CHL	C4D-ND	-3.24	1.33	1.37
2	G	608	CHL	C4B-NB	3.22	1.41	1.37
2	N	601	CHL	C4D-ND	-3.21	1.33	1.37
2	N	609	CHL	C4D-ND	-3.19	1.33	1.37
3	G	610	CLA	C1D-ND	3.18	1.41	1.37
2	N	609	CHL	C4B-NB	3.17	1.41	1.37
5	G	617	NEX	C7-C8	-3.15	1.26	1.32
3	Y	312	CLA	C4B-NB	3.14	1.41	1.37
3	G	612	CLA	C3B-C4B	3.12	1.50	1.42
3	N	613	CLA	C4D-ND	-3.11	1.33	1.37
3	Y	310	CLA	C4D-ND	-3.09	1.33	1.37
2	N	601	CHL	C4B-NB	3.07	1.41	1.37
3	Y	313	CLA	C4D-ND	-3.07	1.33	1.37
3	Y	303	CLA	C4D-ND	-3.06	1.33	1.37
3	Y	311	CLA	C4D-ND	-3.05	1.33	1.37
2	G	609	CHL	C4D-ND	-3.05	1.33	1.37
5	N	617	NEX	C7-C8	-3.02	1.26	1.32
2	G	609	CHL	C4B-NB	3.02	1.41	1.37
3	N	604	CLA	C4D-ND	-3.01	1.33	1.37
3	Y	304	CLA	C4D-ND	-3.00	1.33	1.37
3	Y	312	CLA	C3B-C4B	3.00	1.49	1.42
3	G	602	CLA	C4D-ND	-2.98	1.33	1.37
3	Y	314	CLA	C4D-ND	-2.98	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Y	304	CLA	C3B-C4B	2.98	1.49	1.42
2	N	607	CHL	C4D-ND	-2.98	1.33	1.37
3	G	611	CLA	C4D-ND	-2.98	1.33	1.37
3	N	611	CLA	C4D-ND	-2.98	1.33	1.37
2	G	619	CHL	C4D-ND	-2.97	1.33	1.37
3	Y	305	CLA	C4D-ND	-2.97	1.33	1.37
5	Y	317	NEX	C7-C8	-2.96	1.27	1.32
2	G	601	CHL	C3B-C4B	2.95	1.49	1.42
2	G	607	CHL	C4D-ND	-2.94	1.33	1.37
3	N	602	CLA	C4D-ND	-2.93	1.33	1.37
3	G	612	CLA	C4D-ND	-2.93	1.33	1.37
3	N	614	CLA	C4D-ND	-2.93	1.33	1.37
2	N	609	CHL	C3B-C4B	2.92	1.49	1.42
3	G	603	CLA	C3B-C4B	2.92	1.49	1.42
3	G	613	CLA	C4D-ND	-2.91	1.33	1.37
3	G	614	CLA	C4D-ND	-2.91	1.33	1.37
2	Y	309	CHL	C3B-C4B	2.91	1.49	1.42
2	Y	308	CHL	C3B-C4B	2.90	1.49	1.42
2	G	607	CHL	C3B-C4B	2.89	1.49	1.42
2	N	608	CHL	C3B-C4B	2.88	1.49	1.42
3	N	603	CLA	C3B-C4B	2.88	1.49	1.42
3	Y	311	CLA	C3B-C4B	2.88	1.49	1.42
3	G	603	CLA	C4D-ND	-2.88	1.33	1.37
2	Y	302	CHL	C3B-C4B	2.87	1.49	1.42
2	N	606	CHL	C4D-ND	-2.85	1.33	1.37
3	N	603	CLA	C4D-ND	-2.85	1.33	1.37
3	N	602	CLA	C3B-C4B	2.84	1.49	1.42
2	N	607	CHL	C3B-C4B	2.84	1.49	1.42
3	G	604	CLA	C4D-ND	-2.83	1.33	1.37
2	G	619	CHL	C3B-C4B	2.83	1.49	1.42
3	G	602	CLA	C3B-C4B	2.83	1.49	1.42
2	G	606	CHL	C1B-C2B	2.82	1.49	1.43
3	G	611	CLA	C3B-C4B	2.82	1.49	1.42
3	Y	314	CLA	C3B-C4B	2.81	1.49	1.42
3	N	611	CLA	C3B-C4B	2.81	1.49	1.42
3	N	604	CLA	C3B-C4B	2.81	1.49	1.42
2	Y	306	CHL	C3B-C4B	2.81	1.49	1.42
2	N	608	CHL	C4D-ND	-2.81	1.33	1.37
2	N	606	CHL	C3B-C4B	2.81	1.49	1.42
2	G	609	CHL	C3B-C4B	2.81	1.49	1.42
3	G	614	CLA	C3B-C4B	2.80	1.49	1.42
3	Y	303	CLA	C3B-C4B	2.80	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	605	CHL	C4D-ND	-2.80	1.33	1.37
2	G	601	CHL	C4D-ND	-2.80	1.33	1.37
2	G	608	CHL	C3B-C4B	2.80	1.49	1.42
2	Y	302	CHL	C4D-ND	-2.79	1.33	1.37
3	N	612	CLA	C3B-C4B	2.79	1.49	1.42
3	Y	305	CLA	C3B-C4B	2.78	1.49	1.42
2	Y	308	CHL	C4D-ND	-2.77	1.33	1.37
3	N	614	CLA	C3B-C4B	2.77	1.49	1.42
3	N	613	CLA	C3B-C4B	2.76	1.49	1.42
3	Y	313	CLA	C3B-C4B	2.76	1.49	1.42
2	Y	307	CHL	C3B-C4B	2.76	1.49	1.42
3	G	604	CLA	C3B-C4B	2.76	1.49	1.42
3	G	613	CLA	C3B-C4B	2.76	1.49	1.42
2	G	605	CHL	C4D-ND	-2.75	1.33	1.37
2	N	605	CHL	C3B-C4B	2.72	1.49	1.42
2	Y	307	CHL	C4D-ND	-2.68	1.34	1.37
2	G	608	CHL	C1B-C2B	2.68	1.49	1.43
2	N	601	CHL	C3B-C4B	2.67	1.49	1.42
2	G	606	CHL	C4D-ND	-2.66	1.34	1.37
2	Y	307	CHL	C1B-C2B	2.66	1.49	1.43
3	Y	305	CLA	C1B-C2B	2.66	1.49	1.43
3	G	604	CLA	C1B-C2B	2.65	1.49	1.43
2	G	606	CHL	C3B-C4B	2.65	1.49	1.42
3	G	610	CLA	CMB-C2B	-2.64	1.45	1.50
3	N	604	CLA	C1B-C2B	2.64	1.49	1.43
3	Y	311	CLA	C1B-C2B	2.64	1.49	1.43
2	G	619	CHL	C1B-C2B	2.64	1.49	1.43
2	Y	306	CHL	C4D-ND	-2.63	1.34	1.37
3	N	611	CLA	C1B-C2B	2.63	1.49	1.43
3	G	611	CLA	C1B-C2B	2.62	1.49	1.43
3	N	602	CLA	C1B-C2B	2.62	1.49	1.43
3	Y	303	CLA	C1B-C2B	2.61	1.49	1.43
2	Y	309	CHL	C1B-C2B	2.61	1.49	1.43
3	G	602	CLA	C1B-C2B	2.61	1.49	1.43
2	N	606	CHL	C1B-C2B	2.60	1.49	1.43
2	N	607	CHL	C1B-C2B	2.60	1.49	1.43
3	N	614	CLA	C1B-C2B	2.60	1.49	1.43
2	Y	308	CHL	C1B-C2B	2.60	1.49	1.43
3	N	610	CLA	C3B-C4B	2.59	1.48	1.42
2	Y	302	CHL	C1B-C2B	2.59	1.49	1.43
3	G	614	CLA	C1B-C2B	2.59	1.49	1.43
3	Y	313	CLA	C1B-C2B	2.58	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	613	CLA	C1B-C2B	2.58	1.49	1.43
2	Y	306	CHL	C1B-C2B	2.58	1.49	1.43
3	G	603	CLA	C1B-C2B	2.58	1.49	1.43
2	G	607	CHL	C1B-C2B	2.57	1.49	1.43
3	N	603	CLA	C1B-C2B	2.57	1.49	1.43
2	G	608	CHL	C4D-ND	-2.56	1.34	1.37
3	G	613	CLA	C1B-C2B	2.56	1.49	1.43
2	N	605	CHL	C1B-C2B	2.55	1.49	1.43
2	G	601	CHL	C1B-C2B	2.54	1.49	1.43
2	N	609	CHL	C1B-C2B	2.54	1.49	1.43
3	Y	314	CLA	C1B-C2B	2.53	1.49	1.43
3	N	612	CLA	C1B-C2B	2.48	1.49	1.43
3	N	610	CLA	C1B-C2B	2.46	1.49	1.43
2	G	605	CHL	C1B-C2B	2.46	1.49	1.43
3	Y	310	CLA	C3B-C4B	2.45	1.48	1.42
3	Y	304	CLA	C1B-C2B	2.43	1.49	1.43
2	G	609	CHL	CMB-C2B	-2.41	1.45	1.50
2	N	608	CHL	C1B-C2B	2.41	1.48	1.43
3	G	610	CLA	C3B-C4B	2.40	1.48	1.42
2	N	601	CHL	C1B-C2B	2.39	1.48	1.43
2	G	609	CHL	C1B-C2B	2.38	1.48	1.43
3	Y	312	CLA	CMD-C2D	-2.37	1.45	1.50
2	N	609	CHL	CHC-C1C	2.36	1.43	1.38
3	Y	312	CLA	CMB-C2B	-2.36	1.45	1.50
3	Y	312	CLA	MG-NB	-2.34	2.01	2.05
3	G	610	CLA	CMD-C2D	-2.33	1.45	1.50
2	N	601	CHL	CMD-C2D	-2.28	1.46	1.50
3	G	610	CLA	C1B-C2B	2.27	1.48	1.43
3	G	612	CLA	CMB-C2B	-2.22	1.46	1.50
3	Y	310	CLA	C1B-C2B	2.22	1.48	1.43
3	N	612	CLA	CMD-C2D	-2.20	1.46	1.50
2	G	609	CHL	CHC-C1C	2.19	1.43	1.38
2	N	609	CHL	MG-NB	-2.19	2.01	2.05
3	N	610	CLA	CMB-C2B	-2.16	1.46	1.50
2	N	608	CHL	CHC-C1C	2.15	1.42	1.38
2	Y	309	CHL	CHC-C1C	2.14	1.42	1.38
3	N	612	CLA	CMB-C2B	-2.12	1.46	1.50
3	N	610	CLA	CMD-C2D	-2.12	1.46	1.50
2	G	608	CHL	CHC-C1C	2.11	1.42	1.38
3	G	612	CLA	CMD-C2D	-2.10	1.46	1.50
2	Y	307	CHL	CHC-C1C	2.10	1.42	1.38
3	G	612	CLA	C1B-C2B	2.10	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	610	CLA	CMC-C2C	-2.10	1.46	1.50
2	G	607	CHL	CHC-C1C	2.10	1.42	1.38
3	Y	304	CLA	CMD-C2D	-2.09	1.46	1.50
2	N	601	CHL	CMB-C2B	-2.09	1.46	1.50
2	N	607	CHL	CHC-C1C	2.08	1.42	1.38
3	G	603	CLA	CHC-C1C	2.08	1.42	1.38
3	N	614	CLA	CMD-C2D	-2.08	1.46	1.50
3	Y	310	CLA	CMB-C2B	-2.08	1.46	1.50
3	G	610	CLA	MG-ND	-2.07	2.01	2.05
2	Y	308	CHL	CHC-C1C	2.07	1.42	1.38
2	N	601	CHL	MG-NB	-2.07	2.01	2.05
3	G	610	CLA	MG-NB	-2.07	2.01	2.05
2	N	609	CHL	CMD-C2D	-2.06	1.46	1.50
3	Y	312	CLA	C1B-C2B	2.06	1.48	1.43
3	Y	314	CLA	CHC-C1C	2.06	1.42	1.38
3	N	613	CLA	CMD-C2D	-2.05	1.46	1.50
2	N	606	CHL	CMD-C2D	-2.05	1.46	1.50
3	Y	310	CLA	CMD-C2D	-2.05	1.46	1.50
3	N	604	CLA	CHC-C1C	2.05	1.42	1.38
3	G	603	CLA	CMD-C2D	-2.04	1.46	1.50
3	G	604	CLA	CMB-C2B	-2.04	1.46	1.50
3	G	613	CLA	CMB-C2B	-2.04	1.46	1.50
2	G	609	CHL	CMD-C2D	-2.04	1.46	1.50
3	G	604	CLA	CMD-C2D	-2.04	1.46	1.50
2	G	619	CHL	CHC-C1C	2.04	1.42	1.38
3	Y	303	CLA	CMB-C2B	-2.04	1.46	1.50
3	Y	313	CLA	CHC-C1C	2.04	1.42	1.38
3	Y	313	CLA	CMD-C2D	-2.04	1.46	1.50
2	Y	308	CHL	CMB-C2B	-2.03	1.46	1.50
3	G	612	CLA	CMC-C2C	-2.03	1.46	1.50
2	Y	309	CHL	CMD-C2D	-2.03	1.46	1.50
2	G	601	CHL	CMB-C2B	-2.03	1.46	1.50
3	Y	305	CLA	CMD-C2D	-2.03	1.46	1.50
3	Y	312	CLA	CMC-C2C	-2.03	1.46	1.50
3	Y	314	CLA	CMD-C2D	-2.03	1.46	1.50
3	N	603	CLA	CMD-C2D	-2.03	1.46	1.50
3	G	611	CLA	CHC-C1C	2.03	1.42	1.38
2	N	608	CHL	CMD-C2D	-2.02	1.46	1.50
3	G	604	CLA	CHC-C1C	2.02	1.42	1.38
2	Y	309	CHL	CMB-C2B	-2.02	1.46	1.50
3	N	602	CLA	CMD-C2D	-2.02	1.46	1.50
3	Y	310	CLA	CMC-C2C	-2.02	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	609	CHL	CMB-C2B	-2.02	1.46	1.50
2	N	608	CHL	CMB-C2B	-2.02	1.46	1.50
3	N	603	CLA	CMB-C2B	-2.01	1.46	1.50
3	G	611	CLA	CMD-C2D	-2.01	1.46	1.50
3	G	611	CLA	CMB-C2B	-2.01	1.46	1.50
2	N	607	CHL	CMD-C2D	-2.01	1.46	1.50
2	Y	306	CHL	CMB-C2B	-2.01	1.46	1.50
2	G	601	CHL	CMD-C2D	-2.01	1.46	1.50
2	Y	307	CHL	CMD-C2D	-2.01	1.46	1.50
3	G	602	CLA	CMB-C2B	-2.01	1.46	1.50
3	N	602	CLA	CMB-C2B	-2.01	1.46	1.50
2	N	601	CHL	CHC-C1C	2.01	1.42	1.38
3	N	611	CLA	CMD-C2D	-2.01	1.46	1.50
2	N	607	CHL	CMB-C2B	-2.00	1.46	1.50
2	G	606	CHL	CMB-C2B	-2.00	1.46	1.50
3	Y	305	CLA	CHC-C1C	2.00	1.42	1.38
2	G	607	CHL	CMD-C2D	-2.00	1.46	1.50

All (457) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	N	619	XAT	O4-C5-C4	8.85	120.03	113.38
7	G	620	XAT	O4-C5-C4	8.78	119.98	113.38
7	Y	301	XAT	O4-C5-C4	8.38	119.68	113.38
7	N	619	XAT	O24-C25-C24	8.06	119.44	113.38
5	Y	317	NEX	O24-C25-C24	7.86	119.29	113.38
7	Y	301	XAT	O24-C25-C24	7.84	119.27	113.38
5	N	617	NEX	O24-C25-C24	7.75	119.20	113.38
5	G	617	NEX	O24-C25-C24	7.43	118.97	113.38
7	G	620	XAT	O24-C25-C24	7.39	118.93	113.38
5	Y	317	NEX	C38-C25-C26	-6.43	111.49	122.26
5	N	617	NEX	C38-C25-C26	-6.42	111.50	122.26
5	G	617	NEX	C38-C25-C26	-6.38	111.56	122.26
7	G	620	XAT	C38-C25-C26	-6.33	111.65	122.26
2	N	609	CHL	C4A-NA-C1A	6.29	109.54	106.71
7	Y	301	XAT	C38-C25-C26	-6.27	111.75	122.26
7	N	619	XAT	C38-C25-C26	-6.23	111.82	122.26
7	G	620	XAT	C18-C5-C6	-6.16	111.93	122.26
7	Y	301	XAT	C18-C5-C6	-6.10	112.03	122.26
7	N	619	XAT	C18-C5-C6	-6.07	112.08	122.26
3	G	603	CLA	C4A-NA-C1A	5.74	109.29	106.71
3	G	604	CLA	C4A-NA-C1A	5.68	109.26	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Y	309	CHL	C4A-NA-C1A	5.56	109.20	106.71
3	Y	313	CLA	C4A-NA-C1A	5.21	109.05	106.71
5	G	617	NEX	C15-C14-C13	-5.19	119.91	127.31
3	G	602	CLA	C4A-NA-C1A	5.16	109.03	106.71
3	Y	305	CLA	C4A-NA-C1A	5.15	109.02	106.71
3	G	611	CLA	C4A-NA-C1A	5.14	109.02	106.71
3	Y	314	CLA	C4A-NA-C1A	5.09	109.00	106.71
2	G	619	CHL	C4A-NA-C1A	5.08	108.99	106.71
7	Y	301	XAT	C15-C14-C13	-5.03	120.14	127.31
5	N	617	NEX	C15-C14-C13	-5.02	120.14	127.31
5	Y	317	NEX	C15-C14-C13	-5.02	120.14	127.31
3	N	610	CLA	C4A-NA-C1A	5.02	108.96	106.71
3	G	610	CLA	C4A-NA-C1A	4.96	108.94	106.71
7	N	619	XAT	C11-C10-C9	-4.93	120.27	127.31
3	N	611	CLA	C4A-NA-C1A	4.91	108.91	106.71
3	N	604	CLA	C4A-NA-C1A	4.87	108.90	106.71
3	N	602	CLA	C4A-NA-C1A	4.81	108.87	106.71
3	Y	311	CLA	C4A-NA-C1A	4.77	108.85	106.71
3	N	613	CLA	C4A-NA-C1A	4.73	108.83	106.71
4	Y	315	LUT	C11-C10-C9	-4.72	120.57	127.31
4	N	616	LUT	C7-C8-C9	-4.70	119.13	126.23
4	Y	316	LUT	C35-C34-C33	-4.69	120.62	127.31
4	N	615	LUT	C11-C10-C9	-4.67	120.64	127.31
2	N	609	CHL	CHD-C1D-ND	-4.65	120.18	124.45
7	N	619	XAT	C15-C14-C13	-4.65	120.67	127.31
3	G	613	CLA	C4A-NA-C1A	4.65	108.80	106.71
7	G	620	XAT	C15-C14-C13	-4.60	120.74	127.31
3	Y	303	CLA	C4A-NA-C1A	4.58	108.77	106.71
4	N	616	LUT	C11-C10-C9	-4.58	120.77	127.31
4	Y	315	LUT	C7-C8-C9	-4.56	119.35	126.23
7	G	620	XAT	C11-C10-C9	-4.52	120.86	127.31
4	G	616	LUT	C35-C34-C33	-4.51	120.87	127.31
7	G	620	XAT	O24-C25-C38	4.49	120.43	115.06
5	G	617	NEX	O24-C25-C38	4.45	120.39	115.06
5	Y	317	NEX	O24-C25-C38	4.43	120.37	115.06
7	Y	301	XAT	C11-C10-C9	-4.41	121.02	127.31
5	N	617	NEX	O24-C25-C38	4.40	120.33	115.06
2	G	609	CHL	C4A-NA-C1A	4.38	108.68	106.71
5	G	617	NEX	C11-C10-C9	-4.37	121.07	127.31
4	Y	315	LUT	C35-C34-C33	-4.37	121.08	127.31
4	N	615	LUT	C7-C8-C9	-4.36	119.65	126.23
5	N	617	NEX	C11-C10-C9	-4.35	121.11	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	Y	315	LUT	C31-C30-C29	-4.34	121.12	127.31
2	Y	307	CHL	C4A-NA-C1A	4.34	108.66	106.71
5	G	617	NEX	C35-C34-C33	-4.30	121.17	127.31
5	Y	317	NEX	C35-C34-C33	-4.27	121.22	127.31
2	G	607	CHL	C4A-NA-C1A	4.24	108.61	106.71
2	N	607	CHL	C4A-NA-C1A	4.22	108.60	106.71
4	N	615	LUT	C35-C34-C33	-4.20	121.32	127.31
4	N	616	LUT	C31-C30-C29	-4.20	121.32	127.31
7	Y	301	XAT	C35-C34-C33	-4.18	121.34	127.31
2	G	605	CHL	C4A-NA-C1A	4.18	108.59	106.71
5	Y	317	NEX	C11-C10-C9	-4.18	121.34	127.31
7	Y	301	XAT	O4-C5-C18	4.17	120.05	115.06
7	Y	301	XAT	O24-C25-C38	4.16	120.04	115.06
7	N	619	XAT	O24-C25-C38	4.15	120.03	115.06
4	G	616	LUT	C31-C30-C29	-4.15	121.39	127.31
4	G	615	LUT	C35-C34-C33	-4.13	121.41	127.31
2	N	606	CHL	C4A-NA-C1A	4.13	108.56	106.71
4	Y	316	LUT	C15-C14-C13	-4.12	121.43	127.31
4	Y	315	LUT	C15-C14-C13	-4.11	121.44	127.31
4	N	616	LUT	C35-C34-C33	-4.10	121.45	127.31
5	G	617	NEX	C31-C30-C29	-4.07	121.51	127.31
7	G	620	XAT	C31-C30-C29	-4.07	121.51	127.31
5	N	617	NEX	C35-C34-C33	-4.03	121.55	127.31
3	G	614	CLA	C4A-NA-C1A	4.03	108.52	106.71
7	N	619	XAT	C31-C30-C29	-4.02	121.58	127.31
4	N	616	LUT	C15-C14-C13	-4.01	121.58	127.31
4	G	616	LUT	C15-C14-C13	-4.01	121.59	127.31
7	N	619	XAT	C35-C34-C33	-4.00	121.60	127.31
7	G	620	XAT	O4-C5-C18	3.98	119.83	115.06
4	G	615	LUT	C11-C10-C9	-3.98	121.62	127.31
3	N	614	CLA	C4A-NA-C1A	3.94	108.48	106.71
7	Y	301	XAT	C31-C30-C29	-3.94	121.69	127.31
4	G	616	LUT	C7-C8-C9	-3.93	120.29	126.23
3	Y	310	CLA	C4A-NA-C1A	3.93	108.47	106.71
6	G	618	LHG	O7-C7-C8	3.91	119.92	111.50
2	G	606	CHL	C4A-NA-C1A	3.89	108.46	106.71
7	N	619	XAT	O4-C5-C18	3.89	119.71	115.06
6	N	618	LHG	O7-C7-C8	3.86	119.83	111.50
4	Y	316	LUT	C31-C30-C29	-3.86	121.80	127.31
5	Y	317	NEX	C31-C30-C29	-3.81	121.87	127.31
3	Y	312	CLA	CHB-C1B-NB	3.80	128.28	124.26
4	Y	316	LUT	C11-C10-C9	-3.78	121.91	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	612	CLA	CHB-C1B-NB	3.78	128.26	124.26
4	G	615	LUT	C15-C14-C13	-3.76	121.95	127.31
6	Y	318	LHG	O7-C7-C8	3.75	119.58	111.50
4	G	615	LUT	C31-C30-C29	-3.74	121.98	127.31
2	Y	309	CHL	CHD-C1D-ND	-3.72	121.03	124.45
7	G	620	XAT	C35-C34-C33	-3.68	122.05	127.31
7	N	619	XAT	C7-C8-C9	-3.68	119.82	125.53
4	Y	315	LUT	C18-C5-C6	-3.67	120.40	124.53
3	Y	304	CLA	C4A-NA-C1A	3.62	108.33	106.71
7	G	620	XAT	C7-C8-C9	-3.61	119.92	125.53
4	G	616	LUT	C11-C10-C9	-3.61	122.17	127.31
4	N	615	LUT	C31-C30-C29	-3.60	122.17	127.31
3	N	603	CLA	C4A-NA-C1A	3.57	108.31	106.71
5	Y	317	NEX	C27-C28-C29	-3.55	120.02	125.53
2	N	605	CHL	C4A-NA-C1A	3.55	108.30	106.71
5	N	617	NEX	C27-C28-C29	-3.48	120.13	125.53
4	N	615	LUT	C15-C14-C13	-3.46	122.37	127.31
3	N	612	CLA	C4A-NA-C1A	3.44	108.25	106.71
7	Y	301	XAT	C26-C27-C28	-3.41	118.79	125.99
4	G	615	LUT	C7-C8-C9	-3.40	121.10	126.23
5	N	617	NEX	C31-C30-C29	-3.40	122.46	127.31
3	G	610	CLA	C1-C2-C3	-3.37	120.21	126.04
2	N	609	CHL	C3B-C4B-NB	-3.33	107.43	110.52
2	G	609	CHL	C3B-C4B-NB	-3.33	107.43	110.52
3	Y	310	CLA	O2D-CGD-O1D	-3.29	117.41	123.84
4	Y	316	LUT	C18-C5-C6	-3.27	120.86	124.53
7	Y	301	XAT	C7-C8-C9	-3.26	120.47	125.53
4	Y	316	LUT	C7-C8-C9	-3.26	121.32	126.23
5	G	617	NEX	C27-C28-C29	-3.20	120.56	125.53
5	G	617	NEX	C26-C27-C28	-3.19	119.24	125.99
7	N	619	XAT	C26-C27-C28	-3.18	119.27	125.99
2	Y	308	CHL	C4A-NA-C1A	3.18	108.14	106.71
2	N	608	CHL	CHD-C1D-ND	-3.17	121.54	124.45
2	G	608	CHL	O2D-CGD-O1D	-3.15	117.67	123.84
4	N	615	LUT	C18-C5-C6	-3.15	120.99	124.53
2	N	607	CHL	CHD-C1D-ND	-3.14	121.57	124.45
3	Y	310	CLA	CHB-C4A-NA	3.12	128.83	124.51
3	G	614	CLA	O2D-CGD-O1D	-3.12	117.74	123.84
7	G	620	XAT	C26-C27-C28	-3.11	119.41	125.99
3	G	612	CLA	O2D-CGD-O1D	-3.11	117.77	123.84
4	G	615	LUT	C18-C5-C6	-3.09	121.06	124.53
3	Y	304	CLA	CHB-C1B-NB	3.07	127.51	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	608	CHL	C4A-NA-C1A	3.07	108.09	106.71
2	Y	307	CHL	O2D-CGD-O1D	-3.07	117.83	123.84
3	N	612	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
3	Y	304	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
3	Y	314	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
7	Y	301	XAT	C6-C7-C8	-3.02	119.62	125.99
3	N	614	CLA	O2D-CGD-O1D	-3.00	117.98	123.84
2	G	619	CHL	O2D-CGD-O1D	-2.99	118.00	123.84
2	N	608	CHL	O2D-CGD-O1D	-2.98	118.01	123.84
3	G	611	CLA	O2D-CGD-O1D	-2.98	118.02	123.84
2	G	609	CHL	CHD-C1D-ND	-2.97	121.73	124.45
2	G	619	CHL	CHD-C1D-ND	-2.96	121.73	124.45
2	G	605	CHL	OMC-CMC-C2C	-2.96	118.99	125.69
4	Y	315	LUT	C2-C3-C4	2.95	114.34	110.30
3	G	612	CLA	C1-C2-C3	-2.94	120.96	126.04
3	G	604	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
3	Y	312	CLA	O2D-CGD-O1D	-2.93	118.10	123.84
2	N	601	CHL	C4A-NA-C1A	2.90	108.01	106.71
3	G	613	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
4	N	616	LUT	C21-C26-C27	-2.90	109.03	112.70
2	Y	309	CHL	O2D-CGD-O1D	-2.90	118.17	123.84
2	N	606	CHL	O2D-CGD-O1D	-2.89	118.18	123.84
5	N	617	NEX	C26-C27-C28	-2.88	119.90	125.99
6	N	618	LHG	O8-C23-C24	2.87	120.93	111.91
2	G	606	CHL	O2D-CGD-O1D	-2.87	118.22	123.84
2	N	601	CHL	OMC-CMC-C2C	-2.87	119.20	125.69
4	Y	316	LUT	C21-C26-C27	-2.87	109.08	112.70
6	Y	318	LHG	O8-C23-C24	2.87	120.90	111.91
3	N	603	CLA	O2D-CGD-O1D	-2.87	118.24	123.84
3	Y	313	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
3	Y	303	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
2	G	607	CHL	CHD-C1D-ND	-2.84	121.84	124.45
2	N	607	CHL	O2D-CGD-O1D	-2.83	118.30	123.84
4	N	616	LUT	C18-C5-C6	-2.83	121.35	124.53
3	N	603	CLA	CHB-C4A-NA	2.83	128.43	124.51
3	N	602	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
4	G	615	LUT	C31-C32-C33	-2.80	118.56	126.42
2	G	607	CHL	O2D-CGD-O1D	-2.79	118.38	123.84
5	G	617	NEX	C24-C23-C22	-2.79	105.39	110.77
5	Y	317	NEX	C26-C27-C28	-2.79	120.10	125.99
2	N	605	CHL	O2D-CGD-O1D	-2.79	118.39	123.84
2	G	605	CHL	O2D-CGD-O1D	-2.79	118.39	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Y	309	CHL	C3B-C4B-NB	-2.79	107.93	110.52
3	G	603	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
3	N	611	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
5	N	617	NEX	C24-C23-C22	-2.77	105.43	110.77
2	N	601	CHL	C3B-C4B-NB	-2.76	107.96	110.52
4	G	616	LUT	C2-C3-C4	-2.75	106.53	110.30
3	Y	311	CLA	O2D-CGD-O1D	-2.75	118.45	123.84
2	G	609	CHL	O2D-CGD-O1D	-2.75	118.46	123.84
2	Y	306	CHL	O2D-CGD-O1D	-2.75	118.46	123.84
2	N	609	CHL	C1D-CHD-C4C	-2.73	120.16	126.06
6	G	618	LHG	O8-C23-C24	2.73	120.48	111.91
2	G	606	CHL	OMC-CMC-C2C	-2.73	119.52	125.69
3	Y	305	CLA	O2D-CGD-O1D	-2.73	118.51	123.84
3	N	604	CLA	O2D-CGD-O1D	-2.73	118.51	123.84
3	N	613	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
3	N	610	CLA	CHB-C4A-NA	2.70	128.24	124.51
7	G	620	XAT	C24-C23-C22	-2.69	105.57	110.77
3	G	602	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
3	Y	304	CLA	CHC-C4B-NB	2.68	127.10	124.26
3	Y	304	CLA	C2A-C1A-CHA	2.68	128.55	123.86
4	Y	315	LUT	C21-C26-C27	-2.68	109.31	112.70
3	G	610	CLA	CHB-C4A-NA	2.68	128.22	124.51
3	Y	304	CLA	CHB-C4A-NA	2.68	128.21	124.51
3	Y	310	CLA	C1-C2-C3	-2.67	121.42	126.04
2	Y	302	CHL	CHD-C1D-ND	-2.67	122.00	124.45
2	Y	308	CHL	O2D-CGD-O1D	-2.67	118.61	123.84
7	N	619	XAT	C27-C28-C29	-2.66	121.41	125.53
2	N	609	CHL	CHD-C1D-C2D	2.64	131.03	125.48
3	Y	313	CLA	CHB-C4A-NA	2.64	128.17	124.51
2	Y	302	CHL	O2D-CGD-O1D	-2.64	118.67	123.84
4	G	616	LUT	C21-C26-C27	-2.64	109.36	112.70
2	N	606	CHL	C1-C2-C3	-2.64	122.48	126.75
2	Y	302	CHL	OMC-CMC-C2C	-2.64	119.73	125.69
3	Y	312	CLA	C4A-NA-C1A	2.64	107.89	106.71
2	N	605	CHL	CHD-C1D-ND	-2.63	122.03	124.45
3	G	610	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
2	N	609	CHL	O2D-CGD-O1D	-2.63	118.70	123.84
2	N	607	CHL	OMC-CMC-C2C	-2.62	119.75	125.69
6	G	618	LHG	C5-O7-C7	-2.62	111.35	117.79
2	N	606	CHL	CHB-C4A-NA	2.61	128.12	124.51
2	G	601	CHL	O2D-CGD-O1D	-2.60	118.75	123.84
6	G	618	LHG	C6-C5-C4	-2.60	105.63	111.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	610	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
3	Y	314	CLA	CHB-C4A-NA	2.58	128.08	124.51
5	N	617	NEX	C39-C29-C30	-2.57	119.32	122.92
2	G	607	CHL	OMC-CMC-C2C	-2.57	119.88	125.69
3	G	614	CLA	CHB-C4A-NA	2.57	128.06	124.51
2	G	601	CHL	CHD-C1D-ND	-2.56	122.10	124.45
2	Y	306	CHL	C4A-NA-C1A	2.56	107.86	106.71
2	Y	306	CHL	CHD-C1D-ND	-2.56	122.10	124.45
4	Y	315	LUT	C18-C5-C4	2.56	119.09	114.36
7	Y	301	XAT	C24-C23-C22	-2.55	105.85	110.77
2	N	601	CHL	O2D-CGD-O1D	-2.55	118.86	123.84
3	Y	305	CLA	CHB-C4A-NA	2.54	128.03	124.51
4	G	616	LUT	C18-C5-C6	-2.54	121.67	124.53
7	G	620	XAT	C27-C28-C29	-2.53	121.60	125.53
2	G	609	CHL	OMC-CMC-C2C	-2.53	119.96	125.69
3	Y	312	CLA	CMB-C2B-C1B	-2.53	121.52	125.37
2	G	601	CHL	OMC-CMC-C2C	-2.52	119.98	125.69
3	N	612	CLA	CHB-C4A-NA	2.52	128.00	124.51
2	N	609	CHL	C1-C2-C3	-2.52	121.68	126.04
3	N	602	CLA	CHB-C4A-NA	2.52	128.00	124.51
2	G	619	CHL	OMC-CMC-C2C	-2.52	120.00	125.69
2	G	606	CHL	C2A-C1A-CHA	2.51	128.25	123.86
2	Y	302	CHL	C4A-NA-C1A	2.51	107.83	106.71
2	Y	307	CHL	C1-C2-C3	-2.50	122.70	126.75
2	G	606	CHL	C1-C2-C3	-2.50	122.70	126.75
2	Y	309	CHL	OMC-CMC-C2C	-2.50	120.04	125.69
3	G	604	CLA	CHB-C4A-NA	2.50	127.96	124.51
3	Y	303	CLA	CHB-C4A-NA	2.48	127.95	124.51
3	N	604	CLA	CHB-C4A-NA	2.48	127.94	124.51
5	Y	317	NEX	C24-C23-C22	-2.48	105.99	110.77
3	N	613	CLA	CHB-C4A-NA	2.48	127.94	124.51
5	Y	317	NEX	C39-C29-C30	-2.47	119.47	122.92
4	N	616	LUT	C18-C5-C4	2.47	118.92	114.36
4	G	616	LUT	C3-C4-C5	-2.46	106.95	111.85
7	Y	301	XAT	C27-C28-C29	-2.46	121.71	125.53
4	N	616	LUT	C38-C25-C24	-2.46	118.30	123.56
5	N	617	NEX	C19-C9-C10	-2.46	119.48	122.92
2	G	605	CHL	CHB-C4A-NA	2.46	127.91	124.51
3	N	611	CLA	CHD-C1D-ND	-2.46	122.20	124.45
6	N	618	LHG	C5-O7-C7	-2.45	111.75	117.79
4	Y	316	LUT	C31-C32-C33	-2.45	119.55	126.42
3	G	611	CLA	CHD-C1D-ND	-2.44	122.21	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	608	CHL	CHB-C4A-NA	2.44	127.88	124.51
6	N	618	LHG	C6-C5-C4	-2.43	106.04	111.79
3	G	612	CLA	CHB-C1B-C2B	-2.43	120.38	127.24
7	N	619	XAT	C24-C23-C22	-2.43	106.09	110.77
7	N	619	XAT	C6-C7-C8	-2.43	120.86	125.99
3	G	602	CLA	CHB-C4A-NA	2.42	127.86	124.51
3	N	612	CLA	CHB-C1B-NB	2.41	126.81	124.26
3	Y	314	CLA	CMB-C2B-C1B	-2.41	121.70	125.37
2	G	607	CHL	C3B-C4B-NB	-2.41	108.28	110.52
4	N	616	LUT	C3-C4-C5	-2.41	107.06	111.85
2	N	608	CHL	C4A-NA-C1A	2.41	107.79	106.71
2	G	609	CHL	C1-C2-C3	-2.40	121.89	126.04
3	Y	312	CLA	CHB-C4A-NA	2.40	127.83	124.51
3	Y	311	CLA	CHB-C4A-NA	2.39	127.81	124.51
3	N	614	CLA	CHB-C4A-NA	2.38	127.81	124.51
3	Y	311	CLA	CHD-C1D-ND	-2.37	122.27	124.45
3	Y	305	CLA	CHD-C1D-ND	-2.37	122.27	124.45
2	Y	308	CHL	O2A-CGA-O1A	-2.37	117.62	123.59
2	N	607	CHL	C3B-C4B-NB	-2.36	108.32	110.52
2	N	605	CHL	CHB-C4A-NA	2.36	127.78	124.51
4	G	616	LUT	C38-C25-C24	-2.36	118.50	123.56
5	G	617	NEX	C39-C29-C30	-2.36	119.62	122.92
2	Y	308	CHL	CHD-C1D-ND	-2.36	122.29	124.45
2	G	605	CHL	CHD-C1D-ND	-2.36	122.29	124.45
2	G	608	CHL	CHD-C1D-ND	-2.36	122.29	124.45
4	N	615	LUT	C35-C15-C14	-2.35	118.65	123.47
7	G	620	XAT	C6-C7-C8	-2.35	121.02	125.99
4	Y	315	LUT	C1-C2-C3	2.35	118.95	113.64
3	G	603	CLA	CHB-C4A-NA	2.35	127.76	124.51
5	N	617	NEX	C11-C12-C13	-2.35	119.81	126.42
2	Y	302	CHL	CHB-C4A-NA	2.34	127.75	124.51
3	G	602	CLA	CHD-C1D-ND	-2.33	122.31	124.45
4	G	616	LUT	C16-C1-C6	-2.33	106.52	110.30
2	G	619	CHL	C3B-C4B-NB	-2.33	108.35	110.52
3	Y	304	CLA	C2C-C1C-NC	2.32	112.15	109.97
3	G	613	CLA	CHB-C4A-NA	2.32	127.72	124.51
3	G	611	CLA	CHB-C4A-NA	2.32	127.72	124.51
3	G	614	CLA	CMB-C2B-C1B	-2.31	121.85	125.37
2	G	609	CHL	CHB-C1B-NB	2.31	126.70	124.26
5	G	617	NEX	C19-C9-C10	-2.31	119.69	122.92
2	G	601	CHL	CHB-C4A-NA	2.30	127.70	124.51
3	G	610	CLA	CHB-C1B-NB	2.30	126.69	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	601	CHL	C4A-NA-C1A	2.30	107.74	106.71
4	G	615	LUT	C40-C33-C34	-2.30	119.70	122.92
3	Y	312	CLA	CHB-C1B-C2B	-2.30	120.75	127.24
3	N	611	CLA	CHB-C4A-NA	2.30	127.69	124.51
3	G	612	CLA	C4A-NA-C1A	2.30	107.74	106.71
3	Y	312	CLA	C3B-C4B-NB	-2.29	108.39	110.52
5	N	617	NEX	C20-C13-C14	-2.28	119.72	122.92
3	G	610	CLA	CHC-C4B-NB	2.28	126.67	124.26
3	N	612	CLA	CHC-C4B-NB	2.27	126.66	124.26
2	N	608	CHL	C3B-C4B-NB	-2.27	108.41	110.52
2	G	609	CHL	CHB-C4A-NA	2.27	127.65	124.51
2	Y	306	CHL	OMC-CMC-C2C	-2.27	120.56	125.69
7	N	619	XAT	C11-C12-C13	-2.26	120.05	126.42
4	Y	316	LUT	C38-C25-C24	-2.25	118.74	123.56
3	N	604	CLA	C1-C2-C3	-2.25	122.16	126.04
7	Y	301	XAT	C11-C12-C13	-2.24	120.12	126.42
3	G	612	CLA	CMB-C2B-C1B	-2.24	121.96	125.37
3	Y	304	CLA	CHB-C1B-C2B	-2.23	120.93	127.24
2	Y	307	CHL	CHB-C4A-NA	2.23	127.59	124.51
2	Y	308	CHL	O1D-CGD-CBD	2.22	129.03	124.48
2	N	601	CHL	C1-C2-C3	-2.22	122.20	126.04
2	G	605	CHL	CHB-C1B-NB	2.22	126.61	124.26
2	G	601	CHL	CHB-C1B-NB	2.22	126.61	124.26
2	Y	307	CHL	C2A-C1A-CHA	2.22	127.74	123.86
3	N	610	CLA	C1-C2-C3	-2.21	122.21	126.04
2	G	608	CHL	CMB-C2B-C1B	-2.21	122.00	125.37
3	Y	313	CLA	CHD-C1D-ND	-2.21	122.42	124.45
3	Y	304	CLA	C1-C2-C3	-2.21	122.22	126.04
3	Y	312	CLA	O2A-CGA-O1A	-2.20	118.03	123.59
4	G	615	LUT	C20-C13-C14	-2.20	119.84	122.92
5	G	617	NEX	C11-C12-C13	-2.20	120.24	126.42
3	N	604	CLA	CHD-C1D-ND	-2.20	122.44	124.45
5	Y	317	NEX	C11-C12-C13	-2.20	120.25	126.42
3	G	604	CLA	CHD-C1D-ND	-2.19	122.44	124.45
4	Y	315	LUT	C35-C15-C14	-2.19	118.99	123.47
4	Y	316	LUT	C18-C5-C4	2.19	118.41	114.36
7	G	620	XAT	C11-C12-C13	-2.18	120.28	126.42
3	Y	314	CLA	CHD-C1D-ND	-2.18	122.45	124.45
4	N	615	LUT	C38-C25-C24	-2.18	118.89	123.56
2	Y	308	CHL	CHB-C1B-NB	2.18	126.56	124.26
3	Y	312	CLA	C1-C2-C3	-2.18	122.27	126.04
4	G	615	LUT	C38-C25-C24	-2.18	118.90	123.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	615	LUT	C18-C5-C4	2.18	118.39	114.36
3	G	614	CLA	CHD-C1D-ND	-2.17	122.46	124.45
4	Y	315	LUT	C31-C32-C33	-2.16	120.34	126.42
2	G	607	CHL	CHB-C4A-NA	2.16	127.50	124.51
3	N	603	CLA	CHB-C1B-NB	2.16	126.55	124.26
2	Y	308	CHL	CHB-C4A-NA	2.15	127.49	124.51
4	G	615	LUT	C32-C33-C34	2.15	122.24	118.94
2	Y	307	CHL	O2A-CGA-O1A	-2.15	118.17	123.59
3	G	611	CLA	O2D-CGD-CBD	2.15	115.09	111.27
3	G	604	CLA	O2A-CGA-O1A	-2.14	118.18	123.59
2	N	601	CHL	CHB-C1B-NB	2.14	126.53	124.26
2	N	607	CHL	CHB-C4A-NA	2.14	127.47	124.51
2	G	608	CHL	CHB-C1B-NB	2.14	126.52	124.26
3	N	614	CLA	CHD-C1D-ND	-2.14	122.49	124.45
3	G	611	CLA	C3B-C4B-NB	-2.13	108.53	110.52
2	G	607	CHL	CHB-C1B-NB	2.13	126.52	124.26
4	Y	315	LUT	C38-C25-C24	-2.13	119.01	123.56
3	G	603	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
4	N	615	LUT	C21-C26-C27	-2.12	110.02	112.70
2	G	606	CHL	O2A-CGA-O1A	-2.12	118.24	123.59
2	N	608	CHL	OMC-CMC-C2C	-2.12	120.90	125.69
3	Y	313	CLA	CHB-C1B-NB	2.12	126.50	124.26
7	Y	301	XAT	C15-C35-C34	-2.12	119.14	123.47
3	G	612	CLA	CHD-C1D-ND	-2.12	122.51	124.45
3	Y	314	CLA	CMB-C2B-C3B	2.12	131.71	126.59
2	G	619	CHL	CHB-C4A-NA	2.12	127.44	124.51
3	N	603	CLA	CHC-C4B-NB	2.11	126.49	124.26
2	Y	306	CHL	CHB-C4A-NA	2.11	127.43	124.51
3	N	602	CLA	CHD-C1D-ND	-2.11	122.52	124.45
3	G	612	CLA	CHB-C4A-NA	2.11	127.43	124.51
5	Y	317	NEX	C19-C9-C10	-2.11	119.97	122.92
3	N	613	CLA	CHD-C1D-ND	-2.11	122.52	124.45
2	Y	306	CHL	CHB-C1B-NB	2.11	126.49	124.26
2	N	608	CHL	C1-C2-C3	-2.10	122.41	126.04
2	G	608	CHL	C1-C2-C3	-2.10	122.42	126.04
3	Y	310	CLA	O2D-CGD-CBD	2.10	114.99	111.27
3	N	614	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
3	Y	314	CLA	CHB-C1B-NB	2.09	126.47	124.26
3	G	613	CLA	CHD-C1D-ND	-2.09	122.53	124.45
2	N	606	CHL	O2A-CGA-O1A	-2.08	118.34	123.59
2	N	601	CHL	CHD-C1D-ND	-2.08	122.54	124.45
5	G	617	NEX	C15-C35-C34	-2.08	119.21	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	609	CHL	C11-C12-C13	-2.08	109.19	115.92
3	N	610	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
3	G	614	CLA	CMB-C2B-C3B	2.08	131.62	126.59
4	N	615	LUT	C16-C1-C6	-2.08	106.93	110.30
7	G	620	XAT	C20-C13-C14	-2.08	120.02	122.92
2	Y	309	CHL	CHD-C1D-C2D	2.08	129.83	125.48
3	N	603	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
4	N	616	LUT	C22-C23-C24	-2.07	109.39	111.74
4	Y	316	LUT	C8-C7-C6	-2.07	121.40	127.20
3	Y	310	CLA	CHB-C1B-NB	2.07	126.44	124.26
3	Y	304	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
3	N	612	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
2	N	601	CHL	CHB-C4A-NA	2.06	127.37	124.51
3	Y	310	CLA	CHD-C1D-ND	-2.06	122.56	124.45
3	N	603	CLA	CAA-C2A-C3A	-2.06	107.13	112.78
3	Y	304	CLA	CAA-C2A-C3A	-2.06	107.13	112.78
5	Y	317	NEX	C20-C13-C14	-2.06	120.03	122.92
2	N	606	CHL	CHD-C1D-ND	-2.06	122.56	124.45
3	G	602	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
7	N	619	XAT	C19-C9-C10	-2.06	120.04	122.92
5	Y	317	NEX	C17-C1-C6	-2.06	108.63	110.47
2	Y	306	CHL	O2A-CGA-O1A	-2.06	118.40	123.59
3	N	611	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
2	N	605	CHL	OMC-CMC-C2C	-2.06	121.04	125.69
3	Y	305	CLA	C1-C2-C3	-2.05	122.49	126.04
2	Y	308	CHL	C3B-C4B-NB	-2.05	108.61	110.52
2	Y	302	CHL	CHB-C1B-NB	2.05	126.43	124.26
2	N	609	CHL	O2A-CGA-O1A	-2.05	118.41	123.59
3	G	614	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
3	N	603	CLA	C2A-C1A-CHA	2.05	127.45	123.86
2	Y	307	CHL	CMB-C2B-C1B	-2.05	122.25	125.37
3	N	602	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
3	Y	314	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
4	Y	316	LUT	C3-C4-C5	-2.05	107.78	111.85
3	Y	311	CLA	O2A-CGA-O1A	-2.05	118.43	123.59
3	Y	310	CLA	C3B-C4B-NB	-2.05	108.62	110.52
3	G	613	CLA	O2A-CGA-O1A	-2.04	118.43	123.59
2	Y	302	CHL	O2A-CGA-O1A	-2.04	118.43	123.59
3	G	611	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
5	Y	317	NEX	C15-C35-C34	-2.04	119.30	123.47
2	Y	306	CHL	C3B-C4B-NB	-2.04	108.63	110.52
2	G	606	CHL	CHB-C4A-NA	2.03	127.33	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	Y	315	LUT	C19-C9-C10	-2.03	120.08	122.92
7	G	620	XAT	C19-C9-C10	-2.03	120.08	122.92
4	N	615	LUT	C11-C12-C13	-2.03	120.71	126.42
3	N	611	CLA	CMB-C2B-C1B	-2.03	122.28	125.37
2	Y	306	CHL	C2A-C1A-CHA	2.03	127.40	123.86
2	N	605	CHL	O2A-CGA-O1A	-2.02	118.48	123.59
2	N	608	CHL	O2A-CGA-O1A	-2.02	118.48	123.59
2	Y	309	CHL	O2A-CGA-O1A	-2.02	118.49	123.59
2	G	608	CHL	O2A-CGA-O1A	-2.02	118.49	123.59
3	G	612	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
2	N	606	CHL	CHB-C1B-NB	2.02	126.39	124.26
3	Y	303	CLA	CHB-C1B-NB	2.01	126.39	124.26
5	G	617	NEX	C5-C4-C3	-2.01	109.36	111.75
4	Y	315	LUT	C11-C12-C13	-2.01	120.77	126.42
2	N	605	CHL	CHB-C1B-NB	2.01	126.39	124.26
3	N	613	CLA	O2A-CGA-O1A	-2.01	118.52	123.59

There are no chirality outliers.

All (650) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	N	601	CHL	C2B-C3B-CAB-CBB
2	N	601	CHL	C4B-C3B-CAB-CBB
2	N	601	CHL	C1C-C2C-CMC-OMC
2	N	601	CHL	C3C-C2C-CMC-OMC
2	N	605	CHL	C2B-C3B-CAB-CBB
2	N	605	CHL	C4B-C3B-CAB-CBB
2	N	605	CHL	C1C-C2C-CMC-OMC
2	N	605	CHL	C3C-C2C-CMC-OMC
2	N	606	CHL	C1C-C2C-CMC-OMC
2	N	607	CHL	C1C-C2C-CMC-OMC
2	N	607	CHL	C3C-C2C-CMC-OMC
2	N	607	CHL	CBD-CGD-O2D-CED
2	N	608	CHL	C1A-C2A-CAA-CBA
2	N	608	CHL	C3A-C2A-CAA-CBA
2	N	608	CHL	C1C-C2C-CMC-OMC
2	N	608	CHL	C3C-C2C-CMC-OMC
2	N	608	CHL	CBD-CGD-O2D-CED
2	N	609	CHL	C1A-C2A-CAA-CBA
2	N	609	CHL	C1C-C2C-CMC-OMC
2	N	609	CHL	C3C-C2C-CMC-OMC
2	G	601	CHL	C1C-C2C-CMC-OMC

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Mol	Chain	Res	Type	Atoms
2	G	601	CHL	C3C-C2C-CMC-OMC
2	G	601	CHL	CHA-CBD-CGD-O1D
2	G	605	CHL	C1C-C2C-CMC-OMC
2	G	605	CHL	C3C-C2C-CMC-OMC
2	G	606	CHL	C1C-C2C-CMC-OMC
2	G	606	CHL	C3C-C2C-CMC-OMC
2	G	607	CHL	C1C-C2C-CMC-OMC
2	G	607	CHL	C3C-C2C-CMC-OMC
2	G	608	CHL	C1A-C2A-CAA-CBA
2	G	608	CHL	C3A-C2A-CAA-CBA
2	G	608	CHL	C1C-C2C-CMC-OMC
2	G	608	CHL	C3C-C2C-CMC-OMC
2	G	608	CHL	CBD-CGD-O2D-CED
2	G	609	CHL	C1A-C2A-CAA-CBA
2	G	609	CHL	C2B-C3B-CAB-CBB
2	G	609	CHL	C4B-C3B-CAB-CBB
2	G	609	CHL	C1C-C2C-CMC-OMC
2	G	609	CHL	C3C-C2C-CMC-OMC
2	G	619	CHL	C2A-CAA-CBA-CGA
2	G	619	CHL	C1C-C2C-CMC-OMC
2	G	619	CHL	C3C-C2C-CMC-OMC
2	G	619	CHL	CBD-CGD-O2D-CED
2	Y	302	CHL	C1C-C2C-CMC-OMC
2	Y	302	CHL	C3C-C2C-CMC-OMC
2	Y	306	CHL	C2B-C3B-CAB-CBB
2	Y	306	CHL	C4B-C3B-CAB-CBB
2	Y	306	CHL	C1C-C2C-CMC-OMC
2	Y	306	CHL	C3C-C2C-CMC-OMC
2	Y	307	CHL	C1A-C2A-CAA-CBA
2	Y	307	CHL	C3A-C2A-CAA-CBA
2	Y	308	CHL	C1A-C2A-CAA-CBA
2	Y	308	CHL	CHA-CBD-CGD-O1D
2	Y	308	CHL	CHA-CBD-CGD-O2D
2	Y	308	CHL	CBD-CGD-O2D-CED
2	Y	309	CHL	C4B-C3B-CAB-CBB
2	Y	309	CHL	C1C-C2C-CMC-OMC
2	Y	309	CHL	C3C-C2C-CMC-OMC
3	N	603	CLA	C2B-C3B-CAB-CBB
3	N	603	CLA	C4B-C3B-CAB-CBB
3	N	610	CLA	C2B-C3B-CAB-CBB
3	N	610	CLA	C4B-C3B-CAB-CBB
3	N	611	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
3	N	611	CLA	CHA-CBD-CGD-O1D
3	N	611	CLA	CHA-CBD-CGD-O2D
3	N	612	CLA	C2B-C3B-CAB-CBB
3	N	612	CLA	C4B-C3B-CAB-CBB
3	N	614	CLA	C1A-C2A-CAA-CBA
3	N	614	CLA	C3A-C2A-CAA-CBA
3	N	614	CLA	CHA-CBD-CGD-O1D
3	N	614	CLA	CHA-CBD-CGD-O2D
3	N	614	CLA	CAD-CBD-CGD-O1D
3	N	614	CLA	CAD-CBD-CGD-O2D
3	N	614	CLA	CBD-CGD-O2D-CED
3	G	603	CLA	CBD-CGD-O2D-CED
3	G	604	CLA	C2A-CAA-CBA-CGA
3	G	604	CLA	CHA-CBD-CGD-O1D
3	G	604	CLA	CHA-CBD-CGD-O2D
3	G	610	CLA	C2B-C3B-CAB-CBB
3	G	610	CLA	C4B-C3B-CAB-CBB
3	G	611	CLA	C1A-C2A-CAA-CBA
3	G	611	CLA	C2B-C3B-CAB-CBB
3	G	611	CLA	C4B-C3B-CAB-CBB
3	G	611	CLA	C6-C7-C8-C9
3	G	613	CLA	CHA-CBD-CGD-O1D
3	G	613	CLA	CHA-CBD-CGD-O2D
3	G	613	CLA	CBD-CGD-O2D-CED
3	G	614	CLA	CAD-CBD-CGD-O1D
3	G	614	CLA	CAD-CBD-CGD-O2D
3	G	614	CLA	CBD-CGD-O2D-CED
3	Y	303	CLA	CHA-CBD-CGD-O1D
3	Y	303	CLA	CHA-CBD-CGD-O2D
3	Y	311	CLA	C1A-C2A-CAA-CBA
3	Y	311	CLA	C3A-C2A-CAA-CBA
3	Y	311	CLA	CHA-CBD-CGD-O1D
3	Y	311	CLA	CHA-CBD-CGD-O2D
3	Y	314	CLA	C1A-C2A-CAA-CBA
3	Y	314	CLA	CHA-CBD-CGD-O1D
3	Y	314	CLA	CHA-CBD-CGD-O2D
3	Y	314	CLA	CAD-CBD-CGD-O1D
3	Y	314	CLA	CAD-CBD-CGD-O2D
3	Y	314	CLA	CBD-CGD-O2D-CED
4	G	615	LUT	C1-C6-C7-C8
4	G	616	LUT	C1-C6-C7-C8
4	G	616	LUT	C7-C8-C9-C19

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Mol	Chain	Res	Type	Atoms
4	G	616	LUT	C31-C32-C33-C34
4	G	616	LUT	C31-C32-C33-C40
4	Y	315	LUT	C1-C6-C7-C8
4	Y	316	LUT	C31-C32-C33-C34
4	Y	316	LUT	C31-C32-C33-C40
5	G	617	NEX	C7-C8-C9-C10
5	G	617	NEX	C7-C8-C9-C19
6	N	618	LHG	C4-O6-P-O4
6	G	618	LHG	C3-O3-P-O5
6	G	618	LHG	C4-O6-P-O4
6	Y	318	LHG	C4-O6-P-O5
2	N	608	CHL	O1D-CGD-O2D-CED
2	Y	308	CHL	O1D-CGD-O2D-CED
2	N	601	CHL	CBD-CGD-O2D-CED
2	G	609	CHL	CBD-CGD-O2D-CED
2	Y	307	CHL	CBD-CGD-O2D-CED
3	N	613	CLA	CBD-CGD-O2D-CED
3	G	610	CLA	CBD-CGD-O2D-CED
3	Y	303	CLA	CBD-CGD-O2D-CED
3	Y	304	CLA	CBD-CGD-O2D-CED
3	Y	310	CLA	CBD-CGD-O2D-CED
3	Y	311	CLA	CBD-CGD-O2D-CED
2	G	606	CHL	O1A-CGA-O2A-C1
3	G	610	CLA	O1D-CGD-O2D-CED
3	Y	303	CLA	O1D-CGD-O2D-CED
3	Y	310	CLA	O1D-CGD-O2D-CED
2	G	608	CHL	O1D-CGD-O2D-CED
2	G	619	CHL	O1D-CGD-O2D-CED
3	N	614	CLA	O1D-CGD-O2D-CED
3	G	603	CLA	O1D-CGD-O2D-CED
3	G	614	CLA	O1D-CGD-O2D-CED
3	Y	314	CLA	O1D-CGD-O2D-CED
3	N	612	CLA	CBD-CGD-O2D-CED
3	Y	313	CLA	CBD-CGD-O2D-CED
2	N	606	CHL	O1A-CGA-O2A-C1
2	N	607	CHL	O1A-CGA-O2A-C1
2	Y	306	CHL	O1A-CGA-O2A-C1
2	Y	307	CHL	O1A-CGA-O2A-C1
3	G	613	CLA	O1D-CGD-O2D-CED
3	G	612	CLA	CBD-CGD-O2D-CED
2	N	607	CHL	O1D-CGD-O2D-CED
3	N	613	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
3	Y	304	CLA	O1D-CGD-O2D-CED
3	G	603	CLA	C3-C5-C6-C7
3	G	612	CLA	C3-C5-C6-C7
3	Y	305	CLA	C3-C5-C6-C7
2	N	606	CHL	CBA-CGA-O2A-C1
2	G	606	CHL	CBA-CGA-O2A-C1
2	Y	306	CHL	CBA-CGA-O2A-C1
2	Y	307	CHL	CBA-CGA-O2A-C1
2	Y	309	CHL	CBD-CGD-O2D-CED
2	G	619	CHL	O1A-CGA-O2A-C1
3	G	604	CLA	CBD-CGD-O2D-CED
2	G	607	CHL	C2A-CAA-CBA-CGA
2	N	607	CHL	CBA-CGA-O2A-C1
3	Y	314	CLA	CBA-CGA-O2A-C1
2	G	609	CHL	O1D-CGD-O2D-CED
3	N	610	CLA	CBD-CGD-O2D-CED
2	N	601	CHL	C3-C5-C6-C7
2	Y	308	CHL	C3-C5-C6-C7
2	G	619	CHL	CBA-CGA-O2A-C1
2	G	607	CHL	O1A-CGA-O2A-C1
2	N	601	CHL	O1D-CGD-O2D-CED
2	Y	307	CHL	O1D-CGD-O2D-CED
2	G	601	CHL	CBA-CGA-O2A-C1
2	G	607	CHL	CBA-CGA-O2A-C1
3	Y	311	CLA	O1D-CGD-O2D-CED
3	N	610	CLA	C4-C3-C5-C6
3	N	610	CLA	C2-C3-C5-C6
2	N	607	CHL	C2A-CAA-CBA-CGA
2	G	601	CHL	O1A-CGA-O2A-C1
3	Y	314	CLA	O1A-CGA-O2A-C1
3	N	604	CLA	C3-C5-C6-C7
3	N	612	CLA	O1D-CGD-O2D-CED
2	N	608	CHL	CBA-CGA-O2A-C1
3	N	614	CLA	CBA-CGA-O2A-C1
3	G	604	CLA	CBA-CGA-O2A-C1
3	G	614	CLA	CBA-CGA-O2A-C1
2	G	607	CHL	CBD-CGD-O2D-CED
3	N	602	CLA	C10-C11-C12-C13
3	N	614	CLA	O1A-CGA-O2A-C1
2	N	601	CHL	C11-C10-C8-C9
2	G	609	CHL	C11-C10-C8-C9
3	N	611	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
3	N	612	CLA	C14-C13-C15-C16
3	G	612	CLA	C14-C13-C15-C16
3	Y	311	CLA	C6-C7-C8-C9
3	Y	312	CLA	C6-C7-C8-C9
3	Y	312	CLA	C14-C13-C15-C16
3	Y	313	CLA	O1D-CGD-O2D-CED
4	N	615	LUT	C11-C12-C13-C20
4	Y	315	LUT	C11-C12-C13-C20
2	N	608	CHL	O1A-CGA-O2A-C1
3	N	610	CLA	C13-C15-C16-C17
3	G	603	CLA	C5-C6-C7-C8
3	Y	303	CLA	C10-C11-C12-C13
3	G	610	CLA	C13-C15-C16-C17
3	G	611	CLA	C5-C6-C7-C8
3	Y	310	CLA	C5-C6-C7-C8
3	G	614	CLA	O1A-CGA-O2A-C1
2	N	601	CHL	C15-C16-C17-C18
2	Y	308	CHL	C5-C6-C7-C8
3	N	611	CLA	C5-C6-C7-C8
3	N	611	CLA	C10-C11-C12-C13
3	N	612	CLA	C15-C16-C17-C18
3	Y	310	CLA	C13-C15-C16-C17
3	N	610	CLA	C5-C6-C7-C8
3	G	612	CLA	C5-C6-C7-C8
3	G	612	CLA	C15-C16-C17-C18
3	Y	312	CLA	C15-C16-C17-C18
3	G	612	CLA	O1D-CGD-O2D-CED
3	N	611	CLA	C12-C13-C15-C16
3	G	610	CLA	C11-C12-C13-C15
3	G	611	CLA	C11-C10-C8-C7
3	Y	310	CLA	C11-C12-C13-C15
3	G	604	CLA	O1A-CGA-O2A-C1
2	N	606	CHL	CBD-CGD-O2D-CED
2	G	606	CHL	CBD-CGD-O2D-CED
3	Y	312	CLA	C8-C10-C11-C12
2	G	619	CHL	C5-C6-C7-C8
3	Y	304	CLA	C10-C11-C12-C13
2	Y	302	CHL	CBA-CGA-O2A-C1
6	N	618	LHG	C4-O6-P-O3
6	G	618	LHG	C4-O6-P-O3
6	Y	318	LHG	C4-O6-P-O3
3	G	612	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
2	Y	309	CHL	O1D-CGD-O2D-CED
2	N	608	CHL	C5-C6-C7-C8
3	G	611	CLA	C4-C3-C5-C6
3	G	602	CLA	C15-C16-C17-C18
6	N	618	LHG	C24-C23-O8-C6
2	Y	306	CHL	CBD-CGD-O2D-CED
6	G	618	LHG	C8-C7-O7-C5
3	G	613	CLA	C3-C5-C6-C7
3	Y	312	CLA	C16-C17-C18-C20
3	G	604	CLA	O1D-CGD-O2D-CED
6	G	618	LHG	O9-C7-O7-C5
3	N	611	CLA	C4-C3-C5-C6
3	G	611	CLA	C2-C3-C5-C6
3	G	611	CLA	C14-C13-C15-C16
3	Y	311	CLA	C14-C13-C15-C16
4	G	616	LUT	C7-C8-C9-C10
6	N	618	LHG	C14-C15-C16-C17
2	N	609	CHL	C4B-C3B-CAB-CBB
3	N	602	CLA	C4B-C3B-CAB-CBB
3	G	602	CLA	C4B-C3B-CAB-CBB
3	G	613	CLA	C4B-C3B-CAB-CBB
3	Y	303	CLA	C4B-C3B-CAB-CBB
3	Y	310	CLA	C4B-C3B-CAB-CBB
3	Y	311	CLA	C4B-C3B-CAB-CBB
6	N	618	LHG	C24-C25-C26-C27
6	Y	318	LHG	C14-C15-C16-C17
3	N	612	CLA	C8-C10-C11-C12
3	G	612	CLA	O1A-CGA-O2A-C1
6	N	618	LHG	O10-C23-O8-C6
2	N	606	CHL	C3A-C2A-CAA-CBA
2	G	606	CHL	C3A-C2A-CAA-CBA
2	G	609	CHL	C3A-C2A-CAA-CBA
2	Y	306	CHL	C3A-C2A-CAA-CBA
2	Y	308	CHL	C3A-C2A-CAA-CBA
3	N	603	CLA	C3A-C2A-CAA-CBA
3	N	611	CLA	C3A-C2A-CAA-CBA
3	Y	304	CLA	C3A-C2A-CAA-CBA
2	N	601	CHL	C13-C15-C16-C17
3	N	610	CLA	O1D-CGD-O2D-CED
2	Y	302	CHL	O1A-CGA-O2A-C1
6	N	618	LHG	C8-C7-O7-C5
6	Y	318	LHG	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
6	G	618	LHG	C7-C8-C9-C10
2	N	609	CHL	C2B-C3B-CAB-CBB
2	Y	309	CHL	C2B-C3B-CAB-CBB
3	N	602	CLA	C2B-C3B-CAB-CBB
3	G	602	CLA	C2B-C3B-CAB-CBB
3	G	613	CLA	C2B-C3B-CAB-CBB
3	Y	303	CLA	C2B-C3B-CAB-CBB
3	Y	310	CLA	C2B-C3B-CAB-CBB
3	N	610	CLA	C10-C11-C12-C13
6	N	618	LHG	O9-C7-O7-C5
3	Y	305	CLA	C2-C1-O2A-CGA
3	G	610	CLA	C5-C6-C7-C8
4	G	615	LUT	C5-C6-C7-C8
4	G	616	LUT	C5-C6-C7-C8
4	Y	315	LUT	C5-C6-C7-C8
4	Y	316	LUT	C1-C6-C7-C8
4	Y	316	LUT	C5-C6-C7-C8
3	Y	312	CLA	CBA-CGA-O2A-C1
6	G	618	LHG	C24-C23-O8-C6
2	N	608	CHL	C13-C15-C16-C17
3	G	602	CLA	C8-C10-C11-C12
3	Y	310	CLA	C8-C10-C11-C12
2	G	601	CHL	C6-C7-C8-C10
2	G	619	CHL	C11-C10-C8-C7
3	N	603	CLA	C6-C7-C8-C10
3	N	611	CLA	C2-C3-C5-C6
3	N	611	CLA	C6-C7-C8-C10
3	N	613	CLA	C6-C7-C8-C10
3	N	613	CLA	C11-C12-C13-C15
3	G	603	CLA	C11-C10-C8-C7
3	G	613	CLA	C12-C13-C15-C16
3	Y	311	CLA	C6-C7-C8-C10
3	Y	311	CLA	C11-C10-C8-C7
3	Y	312	CLA	O1A-CGA-O2A-C1
3	G	611	CLA	C13-C15-C16-C17
3	N	610	CLA	CBA-CGA-O2A-C1
3	N	612	CLA	CBA-CGA-O2A-C1
6	N	618	LHG	C15-C16-C17-C18
2	Y	306	CHL	C2A-CAA-CBA-CGA
3	Y	311	CLA	C5-C6-C7-C8
2	Y	302	CHL	C2C-C3C-CAC-CBC
2	N	601	CHL	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
3	Y	304	CLA	C8-C10-C11-C12
2	N	601	CHL	C16-C17-C18-C19
2	G	601	CHL	C6-C7-C8-C9
2	G	619	CHL	C11-C10-C8-C9
3	N	603	CLA	C6-C7-C8-C9
3	N	613	CLA	C6-C7-C8-C9
3	N	613	CLA	C11-C12-C13-C14
3	G	603	CLA	C11-C10-C8-C9
3	G	611	CLA	C11-C10-C8-C9
3	G	613	CLA	C14-C13-C15-C16
3	Y	312	CLA	C11-C12-C13-C14
3	N	613	CLA	C3-C5-C6-C7
6	Y	318	LHG	C16-C17-C18-C19
3	N	612	CLA	O1A-CGA-O2A-C1
6	G	618	LHG	O10-C23-O8-C6
2	N	606	CHL	C1A-C2A-CAA-CBA
2	G	605	CHL	C1A-C2A-CAA-CBA
2	G	606	CHL	C1A-C2A-CAA-CBA
2	Y	306	CHL	C1A-C2A-CAA-CBA
2	Y	309	CHL	C1A-C2A-CAA-CBA
3	N	603	CLA	C1A-C2A-CAA-CBA
3	N	604	CLA	C1A-C2A-CAA-CBA
3	G	610	CLA	C1A-C2A-CAA-CBA
3	Y	304	CLA	C1A-C2A-CAA-CBA
3	Y	305	CLA	C1A-C2A-CAA-CBA
3	Y	310	CLA	C1A-C2A-CAA-CBA
6	Y	318	LHG	C15-C16-C17-C18
2	G	608	CHL	C5-C6-C7-C8
2	N	601	CHL	C4-C3-C5-C6
3	N	610	CLA	O1A-CGA-O2A-C1
2	G	608	CHL	C2A-CAA-CBA-CGA
3	Y	313	CLA	C2A-CAA-CBA-CGA
2	G	601	CHL	C15-C16-C17-C18
2	N	609	CHL	C4-C3-C5-C6
3	G	603	CLA	C15-C16-C17-C18
2	G	607	CHL	O1D-CGD-O2D-CED
3	N	613	CLA	C2A-CAA-CBA-CGA
3	N	604	CLA	C2-C1-O2A-CGA
3	N	604	CLA	CBA-CGA-O2A-C1
3	Y	305	CLA	CBA-CGA-O2A-C1
2	N	606	CHL	O1D-CGD-O2D-CED
2	G	606	CHL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
3	Y	311	CLA	C4-C3-C5-C6
3	Y	312	CLA	C4-C3-C5-C6
2	N	607	CHL	C12-C13-C15-C16
2	G	607	CHL	C11-C10-C8-C7
3	N	612	CLA	C11-C12-C13-C15
3	N	613	CLA	C12-C13-C15-C16
3	G	604	CLA	C6-C7-C8-C10
3	G	611	CLA	C6-C7-C8-C10
3	G	612	CLA	C11-C10-C8-C7
3	Y	312	CLA	C2-C3-C5-C6
3	Y	312	CLA	C11-C12-C13-C15
3	Y	313	CLA	C11-C10-C8-C7
2	N	607	CHL	C14-C13-C15-C16
2	G	601	CHL	C14-C13-C15-C16
2	G	607	CHL	C11-C10-C8-C9
2	G	607	CHL	C14-C13-C15-C16
2	G	619	CHL	C14-C13-C15-C16
3	N	602	CLA	C6-C7-C8-C9
3	N	610	CLA	C14-C13-C15-C16
3	N	611	CLA	C11-C10-C8-C9
3	N	611	CLA	C14-C13-C15-C16
3	N	612	CLA	C11-C12-C13-C14
3	N	613	CLA	C14-C13-C15-C16
3	G	602	CLA	C6-C7-C8-C9
3	G	604	CLA	C6-C7-C8-C9
3	G	612	CLA	C11-C10-C8-C9
3	G	612	CLA	C11-C12-C13-C14
3	Y	310	CLA	C11-C12-C13-C14
3	Y	311	CLA	C11-C10-C8-C9
3	Y	313	CLA	C11-C10-C8-C9
3	Y	313	CLA	C3-C5-C6-C7
3	Y	313	CLA	CBA-CGA-O2A-C1
3	G	612	CLA	C8-C10-C11-C12
3	Y	313	CLA	C13-C15-C16-C17
2	N	607	CHL	C4B-C3B-CAB-CBB
2	G	601	CHL	C4B-C3B-CAB-CBB
2	G	619	CHL	C4B-C3B-CAB-CBB
2	Y	302	CHL	C4B-C3B-CAB-CBB
2	Y	308	CHL	C4B-C3B-CAB-CBB
3	G	603	CLA	C4B-C3B-CAB-CBB
3	Y	304	CLA	C4B-C3B-CAB-CBB
3	Y	312	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
3	G	602	CLA	C10-C11-C12-C13
2	Y	306	CHL	O1D-CGD-O2D-CED
3	N	612	CLA	C4-C3-C5-C6
3	N	612	CLA	C2-C3-C5-C6
3	Y	311	CLA	C2-C3-C5-C6
3	G	612	CLA	C10-C11-C12-C13
3	N	613	CLA	CBA-CGA-O2A-C1
2	G	605	CHL	C3A-C2A-CAA-CBA
3	G	611	CLA	C3A-C2A-CAA-CBA
3	Y	314	CLA	C3A-C2A-CAA-CBA
3	Y	310	CLA	C16-C17-C18-C20
6	Y	318	LHG	C4-C5-C6-O8
3	Y	305	CLA	O1A-CGA-O2A-C1
3	G	612	CLA	C4-C3-C5-C6
3	Y	310	CLA	C16-C17-C18-C19
2	N	606	CHL	C3C-C2C-CMC-OMC
3	N	604	CLA	O1A-CGA-O2A-C1
2	N	607	CHL	C2B-C3B-CAB-CBB
2	G	601	CHL	C2B-C3B-CAB-CBB
3	Y	311	CLA	C2B-C3B-CAB-CBB
3	Y	312	CLA	C2B-C3B-CAB-CBB
6	Y	318	LHG	O7-C5-C6-O8
3	N	610	CLA	C16-C17-C18-C20
2	Y	302	CHL	C4C-C3C-CAC-CBC
3	G	612	CLA	C2-C3-C5-C6
2	N	607	CHL	C11-C10-C8-C9
2	N	609	CHL	C14-C13-C15-C16
2	Y	302	CHL	C14-C13-C15-C16
3	N	610	CLA	C11-C10-C8-C9
3	N	612	CLA	C6-C7-C8-C9
3	G	610	CLA	C11-C12-C13-C14
3	Y	303	CLA	C6-C7-C8-C9
3	Y	310	CLA	C14-C13-C15-C16
3	Y	303	CLA	C8-C10-C11-C12
3	G	610	CLA	C2A-CAA-CBA-CGA
2	N	601	CHL	C16-C17-C18-C20
3	G	614	CLA	O2A-C1-C2-C3
2	N	607	CHL	C15-C16-C17-C18
2	N	605	CHL	CAA-CBA-CGA-O2A
4	N	615	LUT	C11-C12-C13-C14
4	Y	315	LUT	C11-C12-C13-C14
2	G	609	CHL	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
3	N	610	CLA	C8-C10-C11-C12
2	G	619	CHL	C15-C16-C17-C18
2	N	607	CHL	C11-C10-C8-C7
2	N	609	CHL	C12-C13-C15-C16
2	G	601	CHL	C12-C13-C15-C16
2	G	607	CHL	C12-C13-C15-C16
2	G	619	CHL	C12-C13-C15-C16
2	Y	302	CHL	C12-C13-C15-C16
2	Y	309	CHL	C12-C13-C15-C16
3	N	602	CLA	C6-C7-C8-C10
3	N	610	CLA	C11-C10-C8-C7
3	N	610	CLA	C12-C13-C15-C16
3	N	611	CLA	C11-C10-C8-C7
3	G	602	CLA	C6-C7-C8-C10
3	G	611	CLA	C12-C13-C15-C16
3	G	612	CLA	C11-C12-C13-C15
3	Y	303	CLA	C6-C7-C8-C10
3	Y	311	CLA	C12-C13-C15-C16
3	Y	312	CLA	C12-C13-C15-C16
3	Y	313	CLA	C12-C13-C15-C16
3	Y	310	CLA	C2A-CAA-CBA-CGA
3	N	610	CLA	C16-C17-C18-C19
2	G	607	CHL	CAD-CBD-CGD-O2D
2	G	609	CHL	CAD-CBD-CGD-O2D
3	Y	312	CLA	CAD-CBD-CGD-O2D
3	N	603	CLA	CBA-CGA-O2A-C1
3	Y	313	CLA	O1A-CGA-O2A-C1
2	G	601	CHL	CHA-CBD-CGD-O2D
3	N	613	CLA	O1A-CGA-O2A-C1
2	N	609	CHL	C2-C3-C5-C6
2	N	601	CHL	C6-C7-C8-C9
2	Y	309	CHL	C14-C13-C15-C16
3	G	602	CLA	C11-C12-C13-C14
3	Y	304	CLA	C6-C7-C8-C9
3	Y	313	CLA	C14-C13-C15-C16
3	Y	312	CLA	C10-C11-C12-C13
2	Y	309	CHL	C8-C10-C11-C12
2	N	601	CHL	C2-C3-C5-C6
3	Y	312	CLA	C4B-C3B-CAB-CBB
6	Y	318	LHG	C4-O6-P-O4
3	N	614	CLA	O2A-C1-C2-C3
3	Y	314	CLA	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
3	N	603	CLA	O1A-CGA-O2A-C1
3	Y	303	CLA	CAD-CBD-CGD-O1D
3	G	602	CLA	C16-C17-C18-C20
2	G	609	CHL	C11-C10-C8-C7
3	N	612	CLA	C12-C13-C15-C16
3	G	602	CLA	C11-C12-C13-C15
3	G	603	CLA	C12-C13-C15-C16
3	G	612	CLA	C12-C13-C15-C16
3	G	613	CLA	C11-C10-C8-C7
3	Y	304	CLA	C6-C7-C8-C10
3	G	613	CLA	C2A-CAA-CBA-CGA
3	N	613	CLA	C13-C15-C16-C17
3	Y	304	CLA	CBA-CGA-O2A-C1
2	G	609	CHL	C6-C7-C8-C9
2	Y	308	CHL	C6-C7-C8-C9
3	G	603	CLA	C14-C13-C15-C16
2	G	619	CHL	C2B-C3B-CAB-CBB
2	Y	302	CHL	C2B-C3B-CAB-CBB
2	Y	308	CHL	C2B-C3B-CAB-CBB
3	N	614	CLA	C2B-C3B-CAB-CBB
3	G	603	CLA	C2B-C3B-CAB-CBB
3	Y	304	CLA	C2B-C3B-CAB-CBB
3	Y	310	CLA	C4-C3-C5-C6
3	N	614	CLA	C1-C2-C3-C4
3	G	614	CLA	C1-C2-C3-C4
3	Y	314	CLA	C1-C2-C3-C4
2	N	608	CHL	C2A-CAA-CBA-CGA
3	N	610	CLA	C2A-CAA-CBA-CGA
6	Y	318	LHG	C13-C14-C15-C16
3	Y	304	CLA	O1A-CGA-O2A-C1
3	N	610	CLA	C2-C1-O2A-CGA
3	G	604	CLA	C2-C1-O2A-CGA
3	Y	304	CLA	C2-C1-O2A-CGA
4	N	615	LUT	C5-C6-C7-C8
6	N	618	LHG	C3-O3-P-O6
6	G	618	LHG	C3-O3-P-O6
6	Y	318	LHG	C3-O3-P-O6
3	Y	312	CLA	C11-C10-C8-C7
2	G	608	CHL	C16-C17-C18-C20
3	G	602	CLA	C16-C17-C18-C19
2	G	607	CHL	C4B-C3B-CAB-CBB
3	N	614	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
3	G	602	CLA	C2A-CAA-CBA-CGA
2	Y	308	CHL	CBA-CGA-O2A-C1
3	Y	304	CLA	C5-C6-C7-C8
3	N	611	CLA	CBD-CGD-O2D-CED
2	N	608	CHL	C11-C10-C8-C9
2	G	609	CHL	C11-C12-C13-C14
6	Y	318	LHG	C27-C28-C29-C30
5	N	617	NEX	C39-C29-C30-C31
5	G	617	NEX	C39-C29-C30-C31
5	Y	317	NEX	C39-C29-C30-C31
2	G	608	CHL	C16-C17-C18-C19
2	N	607	CHL	C1A-C2A-CAA-CBA
3	N	602	CLA	C11-C12-C13-C15
3	N	602	CLA	C2A-CAA-CBA-CGA
3	N	602	CLA	C13-C15-C16-C17
2	Y	308	CHL	O1A-CGA-O2A-C1
5	N	617	NEX	C28-C29-C30-C31
5	G	617	NEX	C28-C29-C30-C31
5	Y	317	NEX	C28-C29-C30-C31
2	Y	302	CHL	C6-C7-C8-C9
3	Y	304	CLA	C11-C12-C13-C14
3	G	603	CLA	C16-C17-C18-C20
4	N	615	LUT	C1-C6-C7-C8
4	N	616	LUT	C1-C6-C7-C8
3	G	602	CLA	C13-C15-C16-C17
2	Y	309	CHL	C4-C3-C5-C6
3	N	611	CLA	C8-C10-C11-C12
6	G	618	LHG	C27-C28-C29-C30
3	N	611	CLA	C13-C15-C16-C17
3	Y	304	CLA	C3-C5-C6-C7
3	N	613	CLA	C4B-C3B-CAB-CBB
3	Y	313	CLA	C4B-C3B-CAB-CBB
3	N	611	CLA	O1D-CGD-O2D-CED
2	N	601	CHL	C6-C7-C8-C10
2	G	609	CHL	C2-C3-C5-C6
3	N	604	CLA	C11-C10-C8-C7
3	N	611	CLA	CAA-CBA-CGA-O2A
2	G	609	CHL	C2A-CAA-CBA-CGA
6	G	618	LHG	C23-C24-C25-C26
2	G	619	CHL	C4-C3-C5-C6
2	Y	308	CHL	C11-C12-C13-C14
3	G	613	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
2	N	601	CHL	C3A-C2A-CAA-CBA
2	N	607	CHL	C3A-C2A-CAA-CBA
2	N	608	CHL	CAD-CBD-CGD-O2D
2	G	619	CHL	CAD-CBD-CGD-O2D
2	Y	308	CHL	C2A-CAA-CBA-CGA
3	G	603	CLA	C2-C1-O2A-CGA
3	G	604	CLA	C4-C3-C5-C6
6	G	618	LHG	O8-C23-C24-C25
5	N	617	NEX	O24-C26-C27-C28
5	G	617	NEX	O24-C26-C27-C28
5	Y	317	NEX	O24-C26-C27-C28
3	G	613	CLA	CBA-CGA-O2A-C1
3	G	603	CLA	CAA-CBA-CGA-O2A
2	N	609	CHL	C2C-C3C-CAC-CBC
3	N	603	CLA	C15-C16-C17-C18
3	N	614	CLA	CAA-CBA-CGA-O2A
2	Y	302	CHL	CHA-CBD-CGD-O1D
2	Y	302	CHL	CHA-CBD-CGD-O2D
3	N	603	CLA	CHA-CBD-CGD-O2D
3	N	604	CLA	CHA-CBD-CGD-O1D
3	G	602	CLA	CHA-CBD-CGD-O1D
3	G	614	CLA	CHA-CBD-CGD-O1D
3	G	614	CLA	CHA-CBD-CGD-O2D
3	Y	304	CLA	CHA-CBD-CGD-O1D
3	Y	304	CLA	CHA-CBD-CGD-O2D
3	Y	305	CLA	CHA-CBD-CGD-O1D
3	Y	305	CLA	CHA-CBD-CGD-O2D
2	G	619	CHL	C2-C3-C5-C6
3	G	611	CLA	CAA-CBA-CGA-O2A
6	N	618	LHG	C33-C34-C35-C36
3	Y	312	CLA	CAA-CBA-CGA-O2A
3	Y	311	CLA	CAA-CBA-CGA-O2A
6	N	618	LHG	O8-C23-C24-C25
2	N	601	CHL	C12-C13-C15-C16
3	G	603	CLA	C16-C17-C18-C19
3	G	612	CLA	CAA-CBA-CGA-O2A
3	N	602	CLA	C11-C12-C13-C14
3	G	604	CLA	C2B-C3B-CAB-CBB
3	G	613	CLA	O1A-CGA-O2A-C1
3	Y	311	CLA	C13-C15-C16-C17
3	Y	303	CLA	C2A-CAA-CBA-CGA
2	N	609	CHL	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
3	Y	310	CLA	C2-C3-C5-C6
3	N	611	CLA	CBA-CGA-O2A-C1
3	N	602	CLA	C8-C10-C11-C12
2	N	601	CHL	C1A-C2A-CAA-CBA
2	G	607	CHL	C1A-C2A-CAA-CBA
2	G	619	CHL	C1A-C2A-CAA-CBA
3	N	611	CLA	O1A-CGA-O2A-C1
3	Y	305	CLA	O1D-CGD-O2D-CED
2	N	608	CHL	C2-C1-O2A-CGA
6	G	618	LHG	C9-C10-C11-C12
3	N	611	CLA	CAA-CBA-CGA-O1A
3	G	614	CLA	C2A-CAA-CBA-CGA
2	G	601	CHL	C16-C17-C18-C20
2	N	605	CHL	CAA-CBA-CGA-O1A
6	G	618	LHG	O10-C23-C24-C25
3	N	614	CLA	CAA-CBA-CGA-O1A
3	G	612	CLA	CAA-CBA-CGA-O1A
3	N	612	CLA	C10-C11-C12-C13
6	Y	318	LHG	C3-O3-P-O5
3	G	611	CLA	CAA-CBA-CGA-O1A
6	N	618	LHG	O10-C23-C24-C25
2	G	601	CHL	C13-C15-C16-C17
3	G	603	CLA	CAA-CBA-CGA-O1A
2	G	609	CHL	C4-C3-C5-C6
6	G	618	LHG	C29-C30-C31-C32
2	N	601	CHL	CAD-CBD-CGD-O1D
2	Y	302	CHL	CAD-CBD-CGD-O1D
2	N	601	CHL	C14-C13-C15-C16
3	N	612	CLA	CAA-CBA-CGA-O2A
2	G	601	CHL	CAA-CBA-CGA-O2A
3	Y	312	CLA	CAA-CBA-CGA-O1A
2	N	609	CHL	C3A-C2A-CAA-CBA
2	Y	302	CHL	C6-C7-C8-C10
2	Y	308	CHL	C6-C7-C8-C10
3	Y	312	CLA	C6-C7-C8-C10
2	Y	302	CHL	CAA-CBA-CGA-O2A
4	G	615	LUT	C11-C12-C13-C14
3	N	603	CLA	CAA-CBA-CGA-O2A
3	N	612	CLA	CAA-CBA-CGA-O1A
3	Y	311	CLA	CAA-CBA-CGA-O1A
2	Y	302	CHL	CAA-CBA-CGA-O1A

There are no ring outliers.

50 monomers are involved in 135 short contacts:

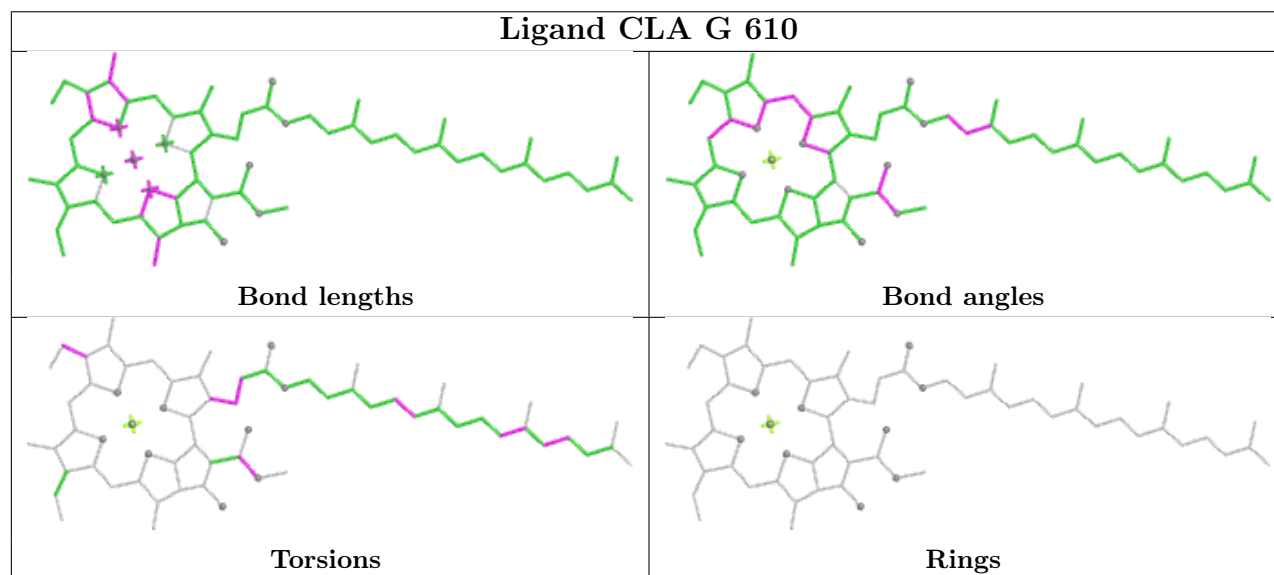
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	610	CLA	9	0
2	N	607	CHL	2	0
7	Y	301	XAT	6	0
3	Y	311	CLA	2	0
2	N	606	CHL	2	0
3	Y	314	CLA	1	0
4	N	615	LUT	6	0
3	G	611	CLA	1	0
3	Y	303	CLA	1	0
2	G	608	CHL	2	0
3	G	603	CLA	1	0
7	N	619	XAT	4	0
4	Y	315	LUT	10	0
3	G	614	CLA	1	0
3	N	610	CLA	5	0
3	G	613	CLA	4	0
2	G	606	CHL	3	0
2	G	605	CHL	1	0
4	Y	316	LUT	3	0
3	Y	312	CLA	8	0
3	N	612	CLA	1	0
6	N	618	LHG	1	0
3	Y	304	CLA	5	0
4	N	616	LUT	3	0
2	N	608	CHL	2	0
4	G	616	LUT	4	0
7	G	620	XAT	5	0
2	G	601	CHL	2	0
2	Y	307	CHL	1	0
2	G	607	CHL	5	0
3	N	613	CLA	5	0
4	G	615	LUT	8	0
5	G	617	NEX	3	0
6	G	618	LHG	2	0
3	N	614	CLA	2	0
2	Y	308	CHL	5	0
3	N	611	CLA	3	0
3	G	612	CLA	3	0
3	G	602	CLA	3	0
3	N	604	CLA	1	0
5	Y	317	NEX	4	0
2	G	619	CHL	3	0

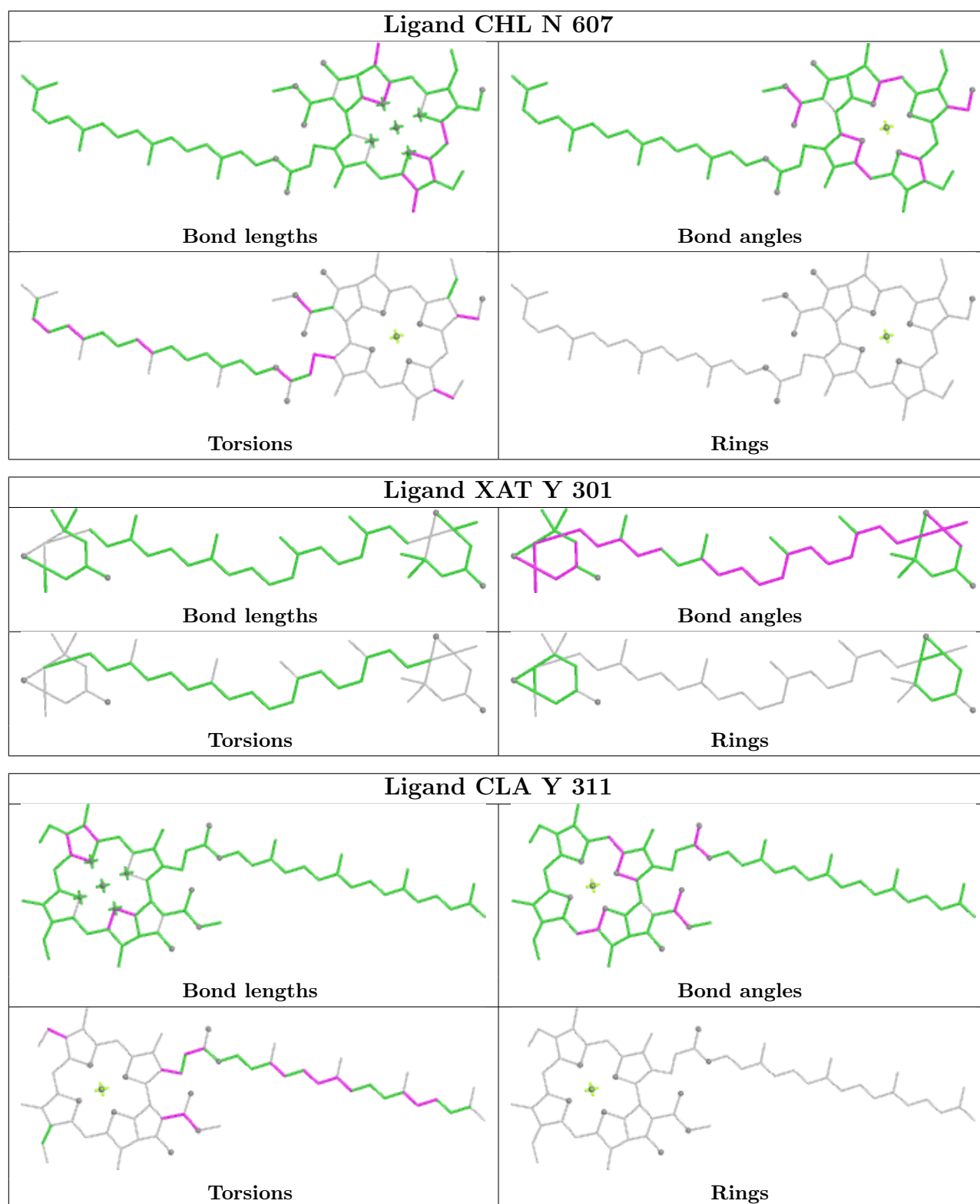
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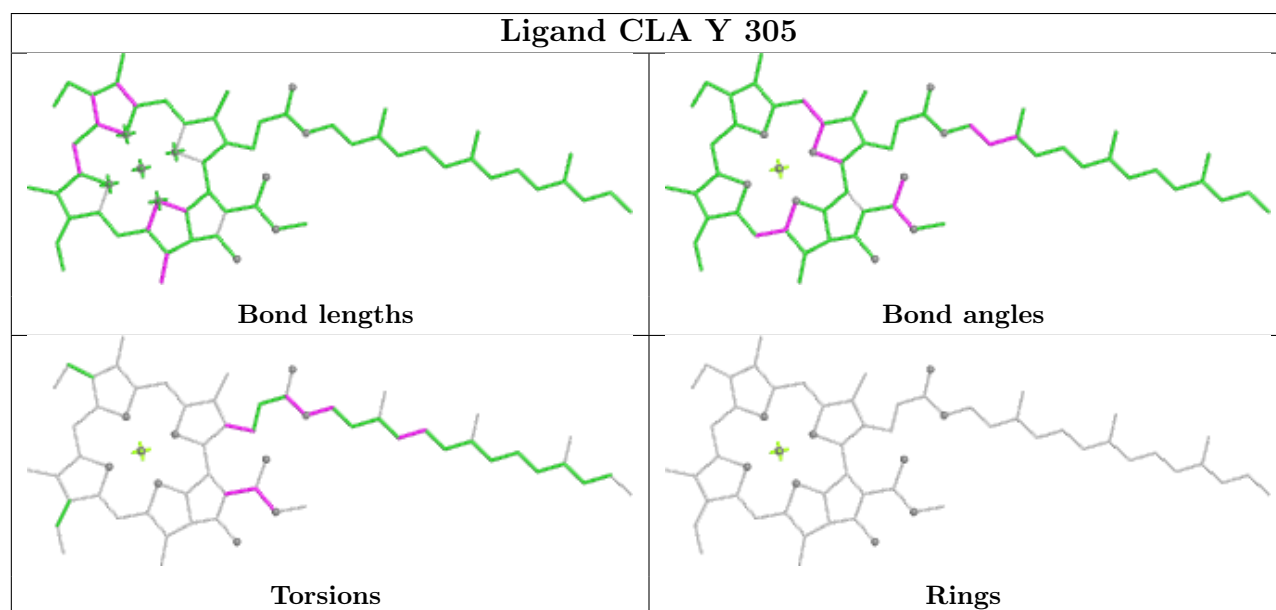
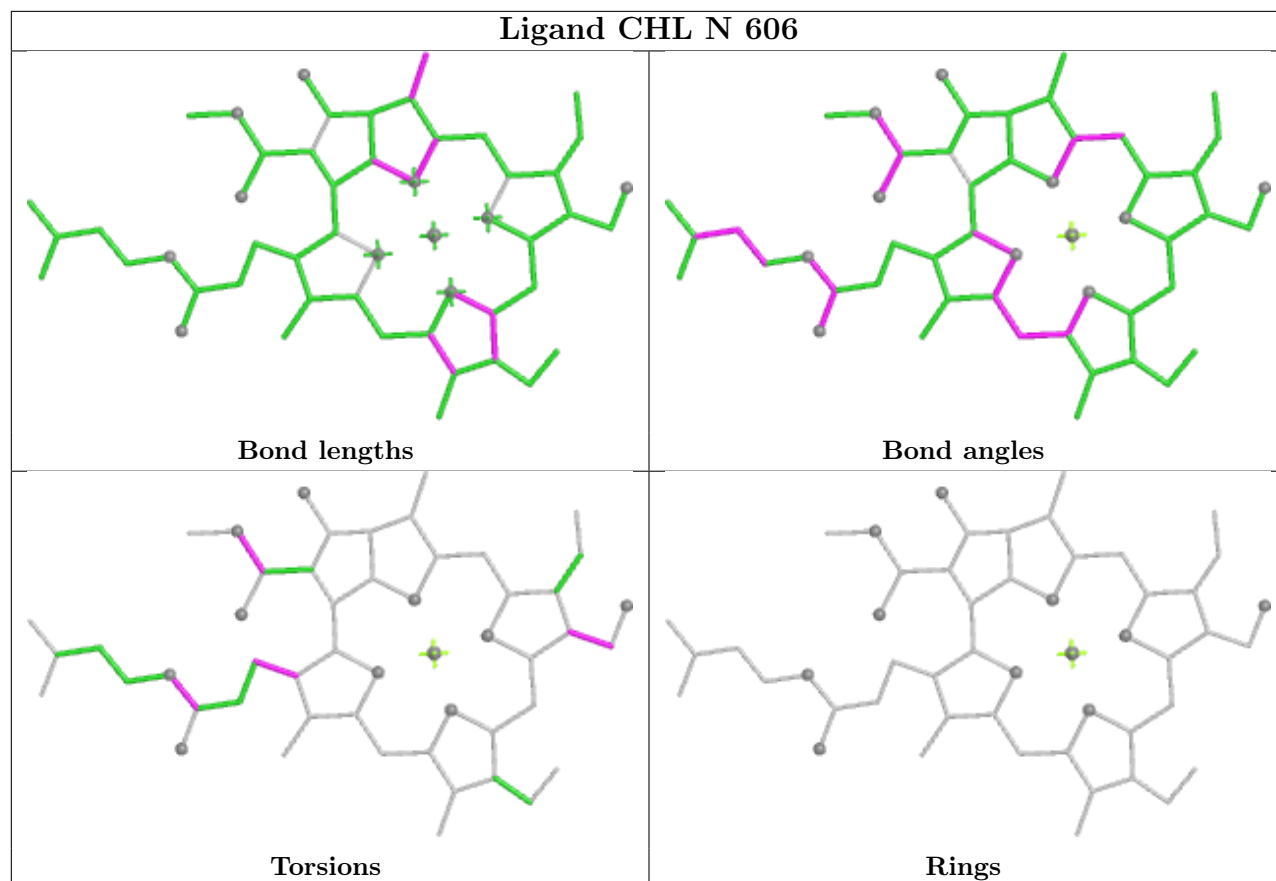
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	N	609	CHL	2	0
2	Y	309	CHL	2	0
3	Y	310	CLA	10	0
2	G	609	CHL	1	0
3	Y	313	CLA	2	0
3	N	602	CLA	1	0
5	N	617	NEX	4	0
2	N	601	CHL	7	0

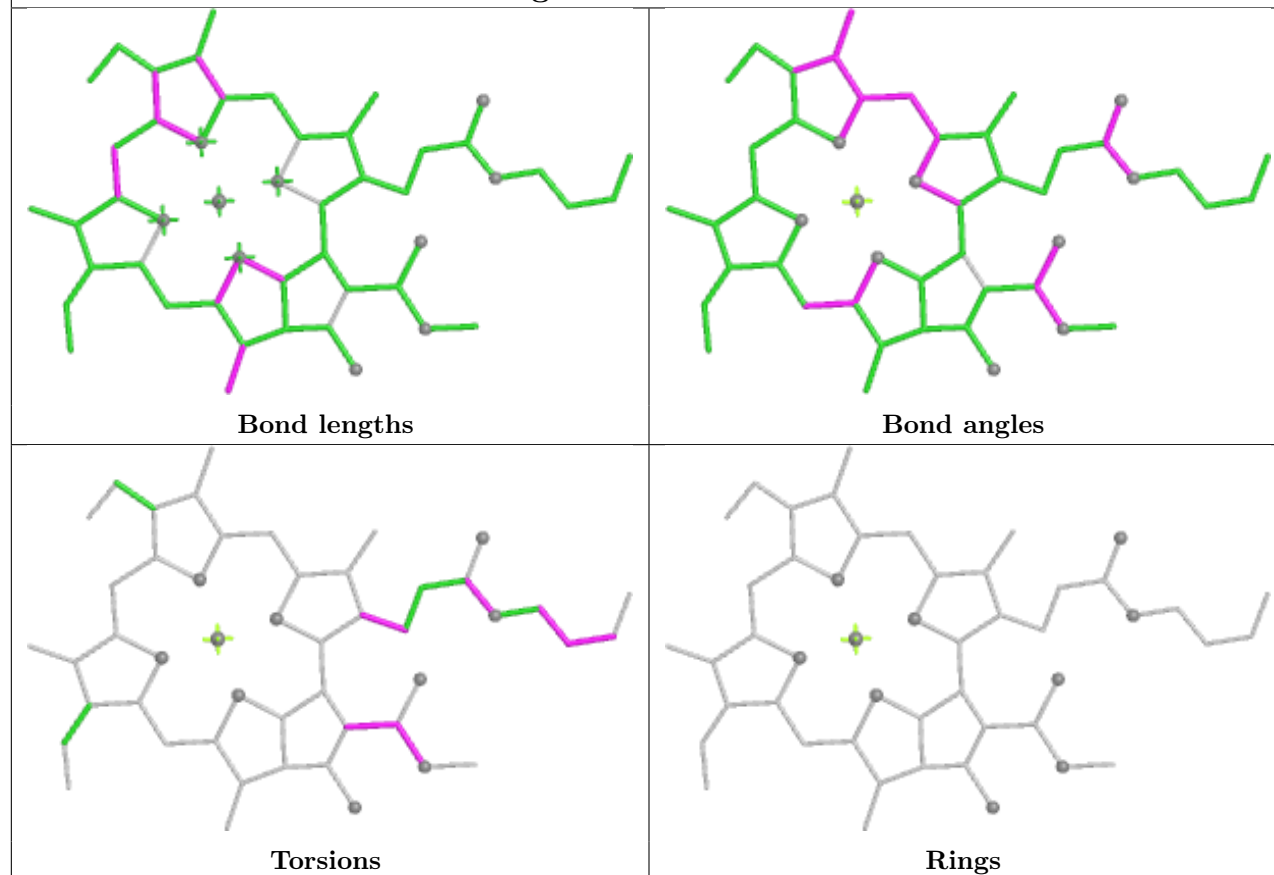
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



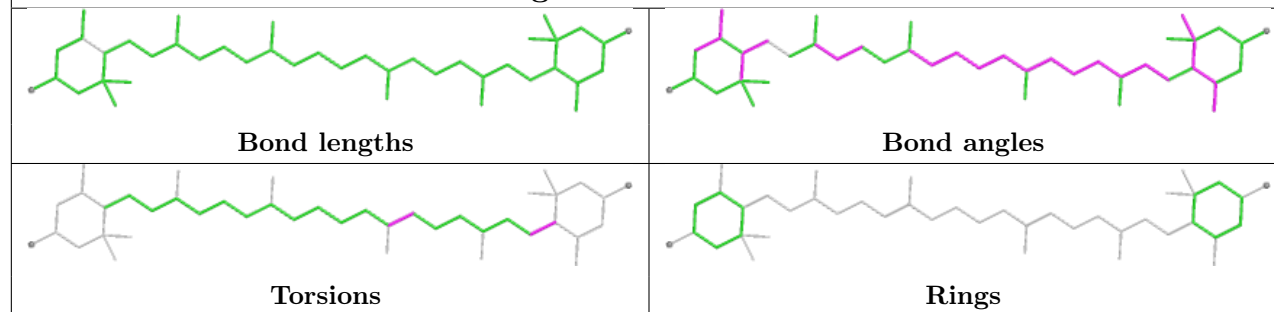


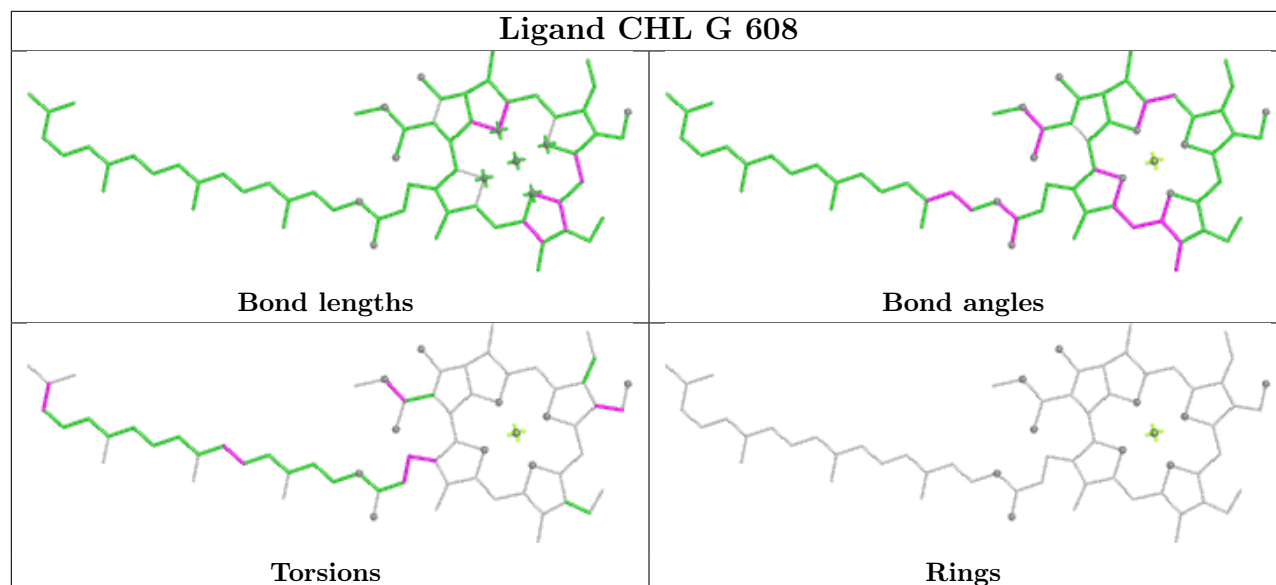
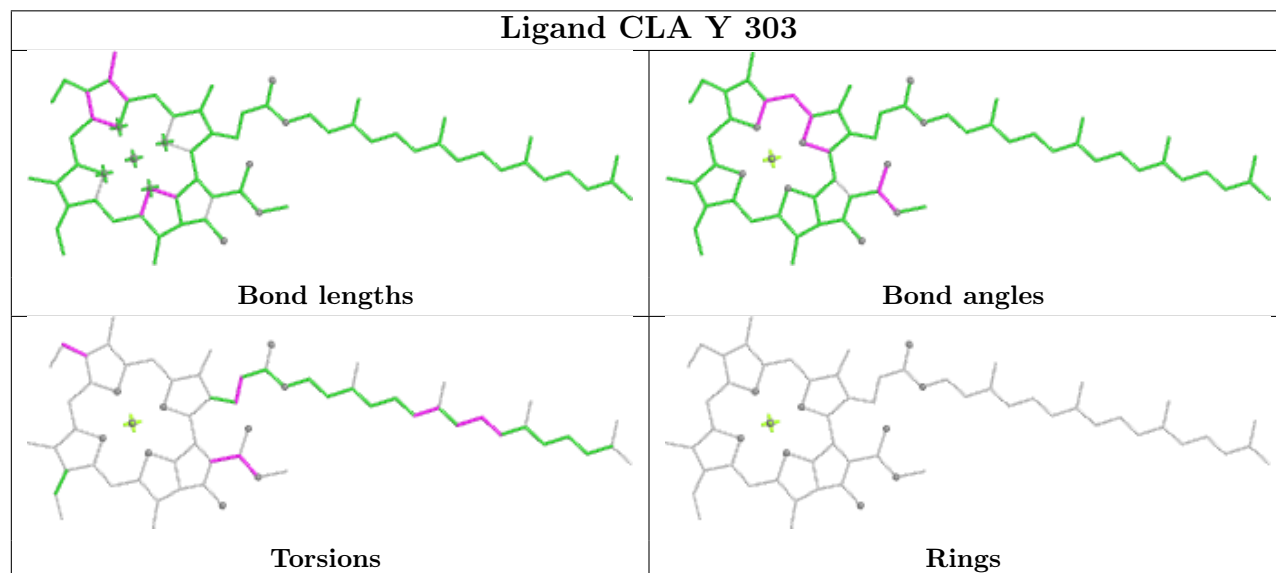
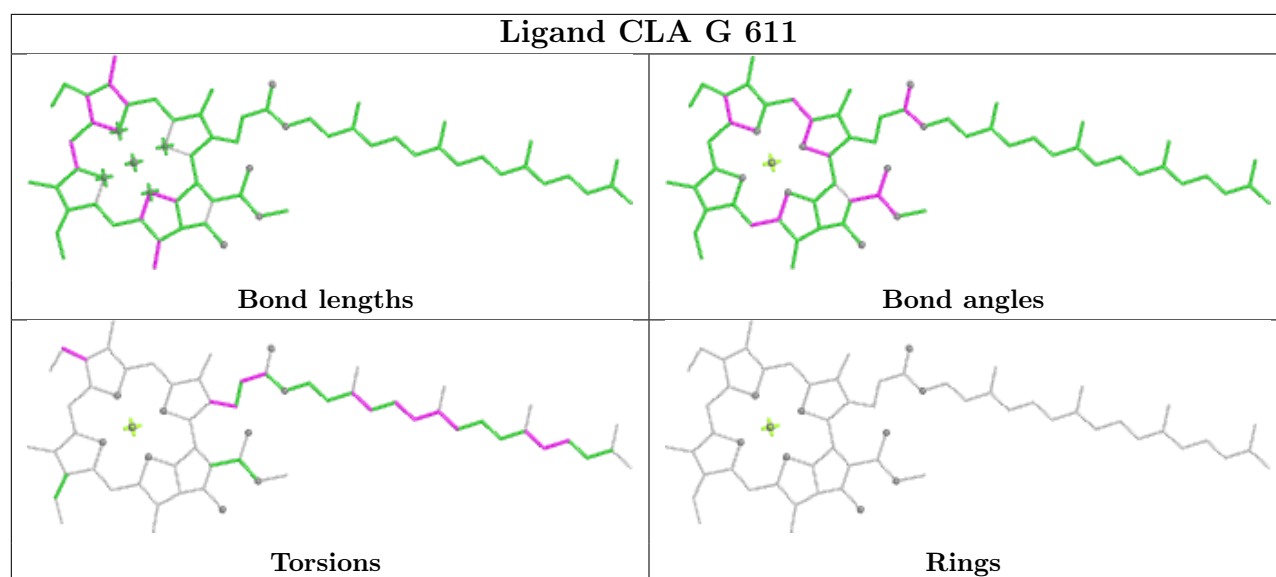


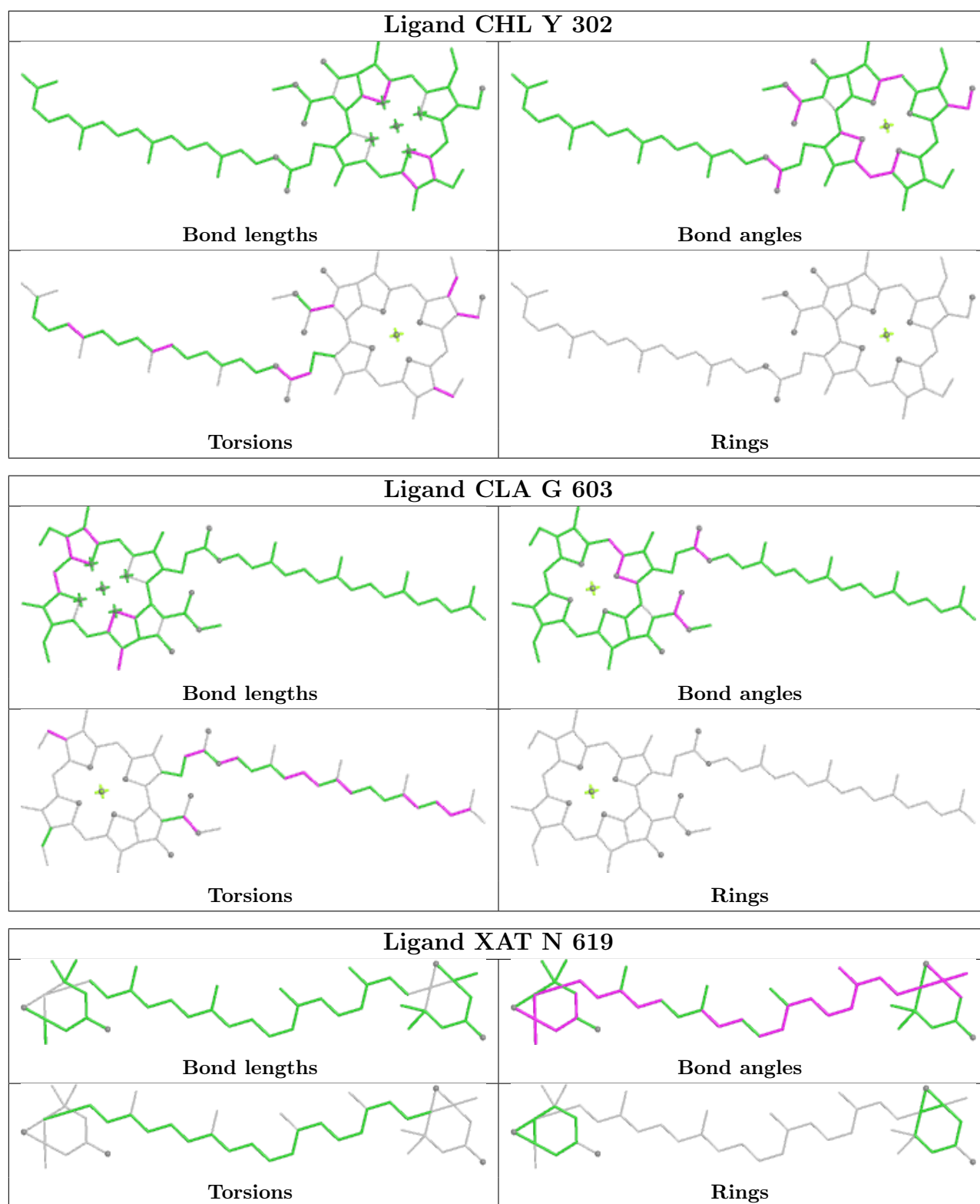
Ligand CLA Y 314

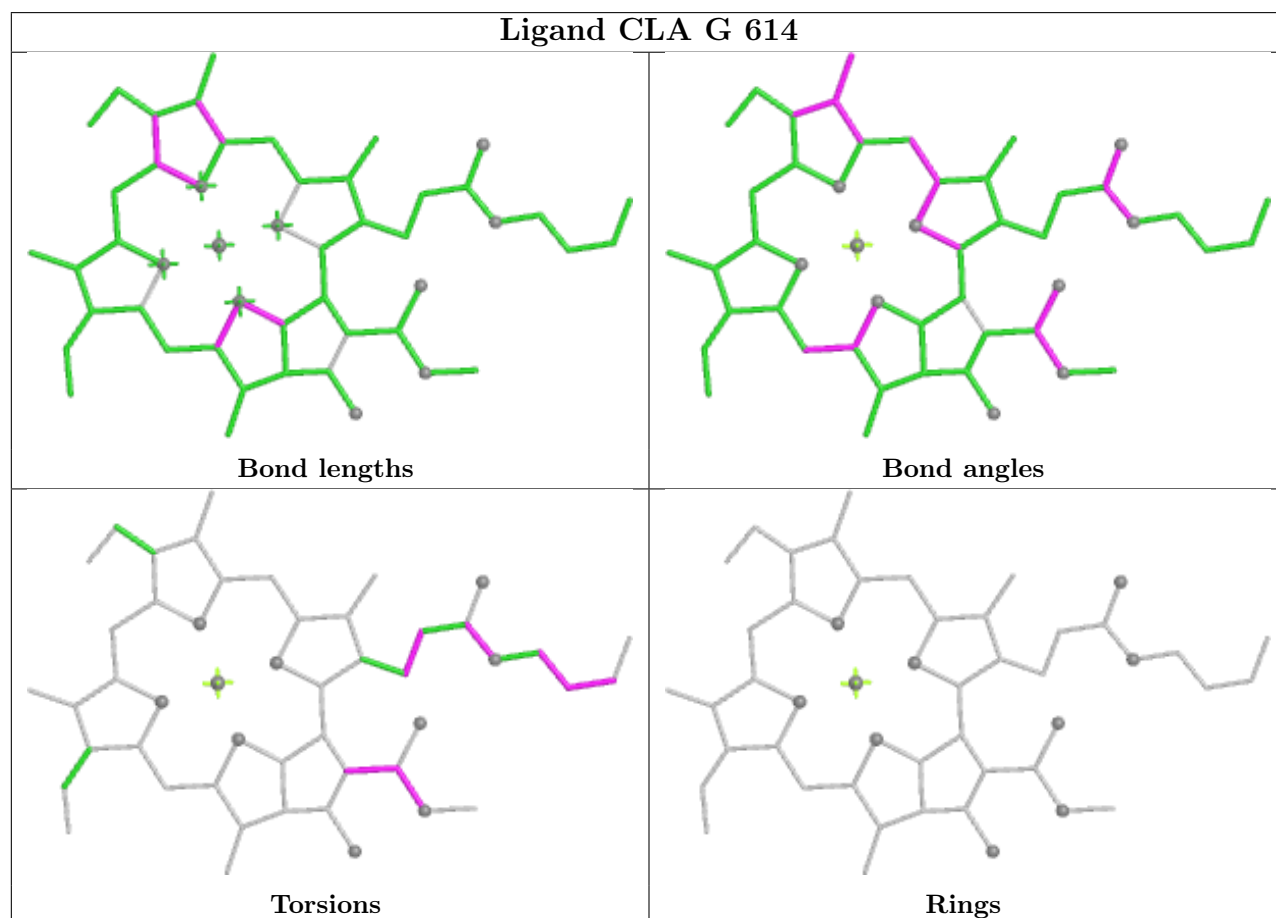
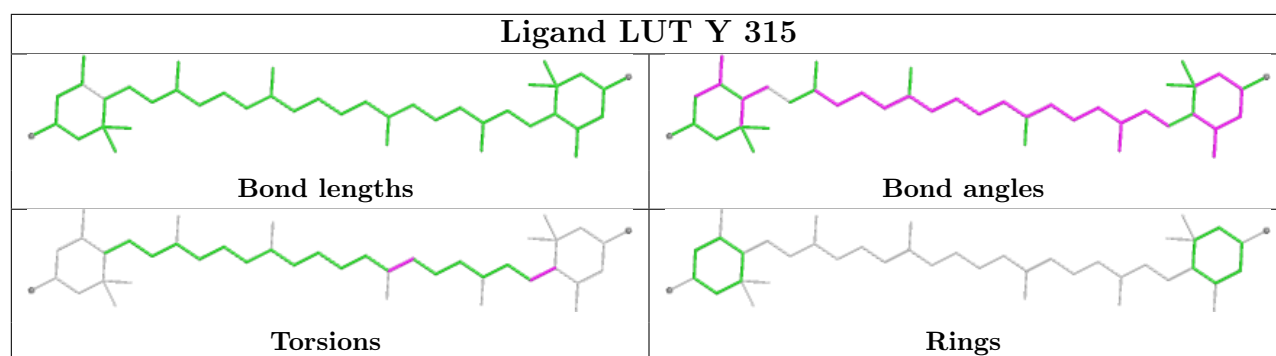


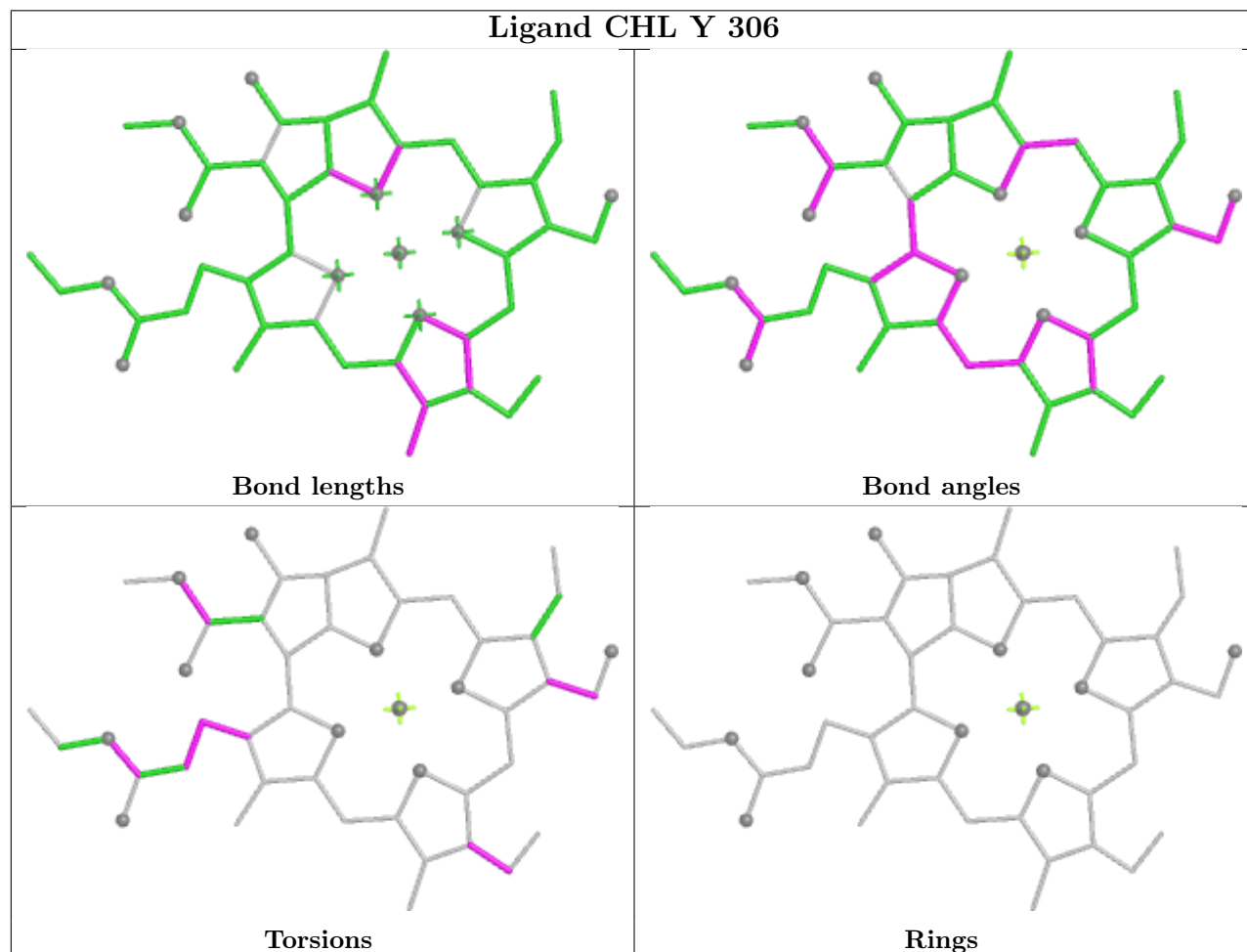
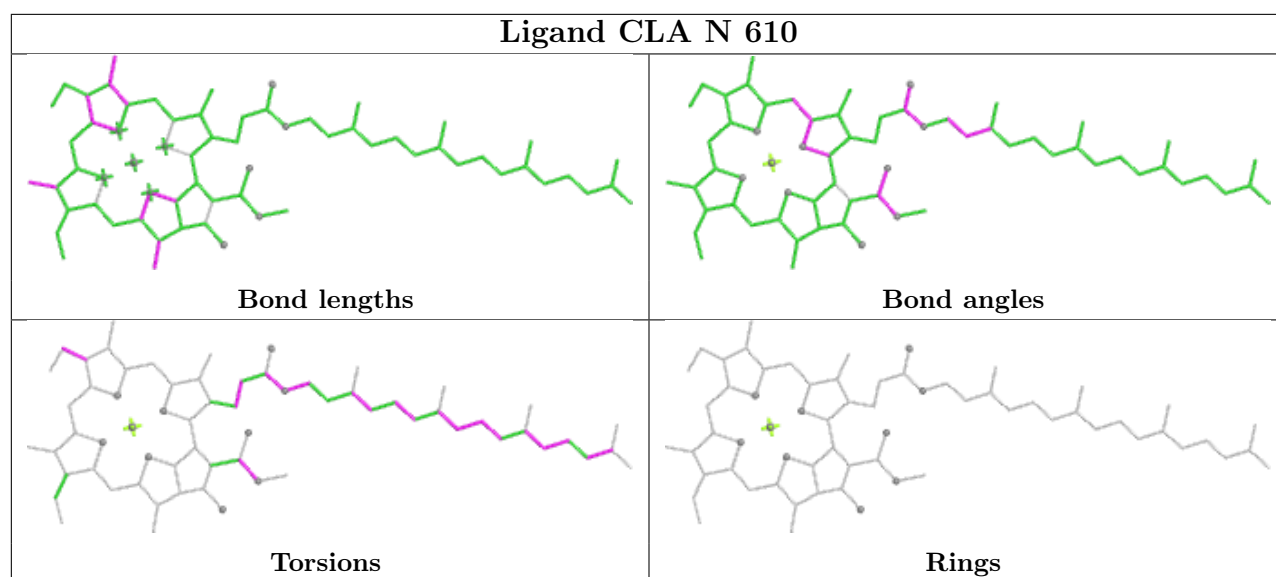
Ligand LUT N 615

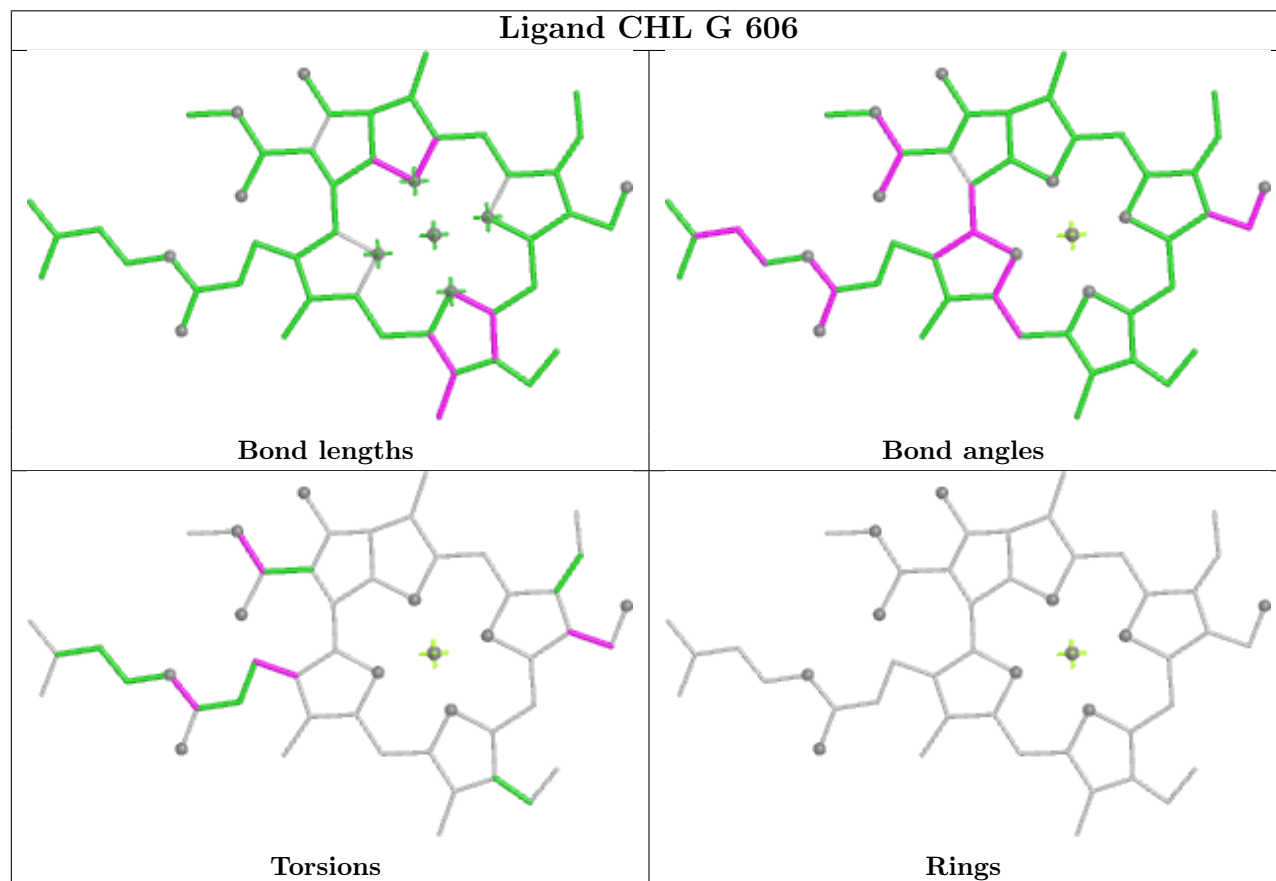
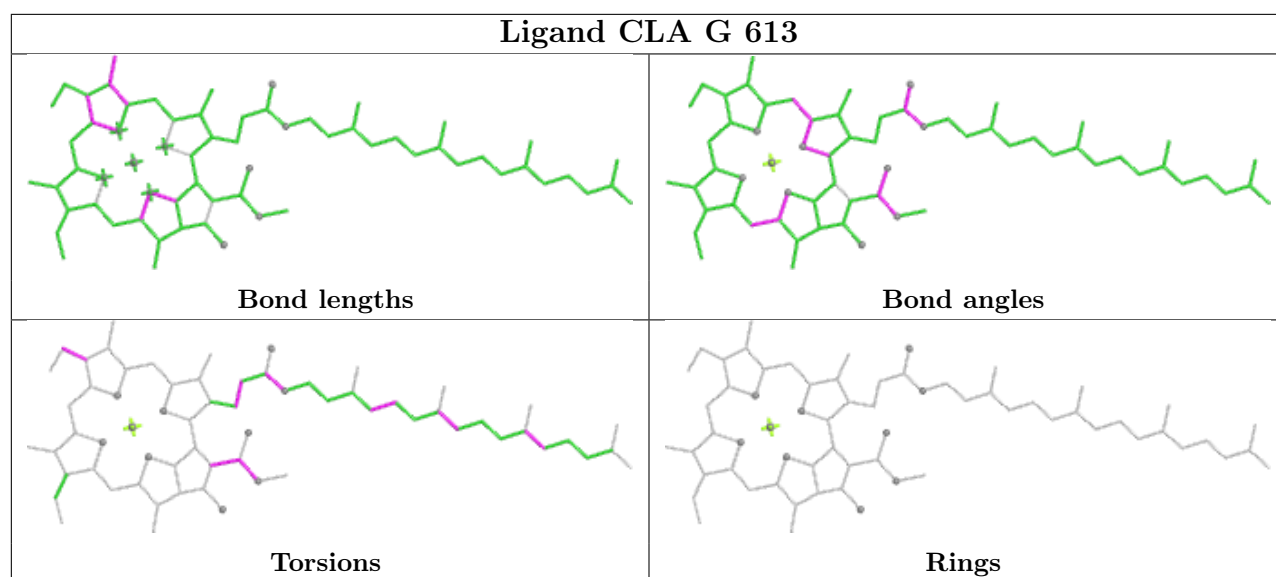


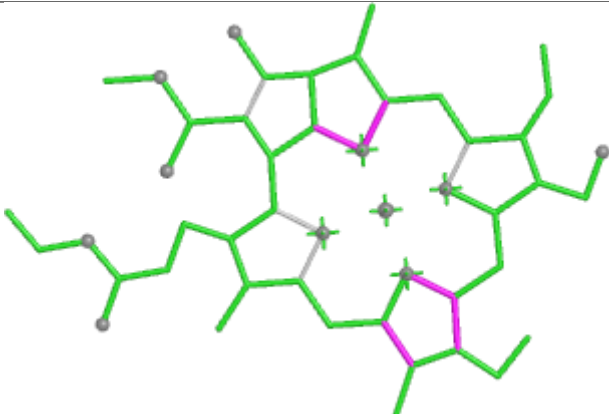
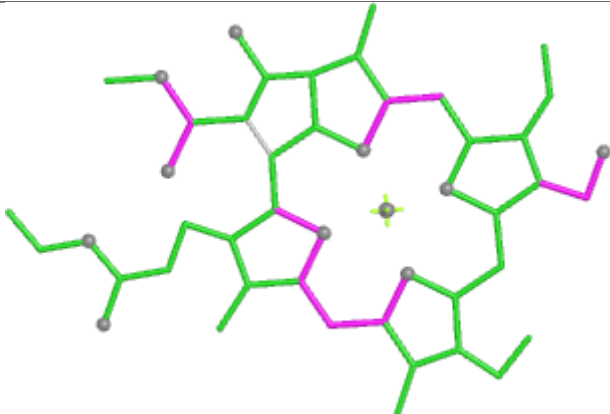
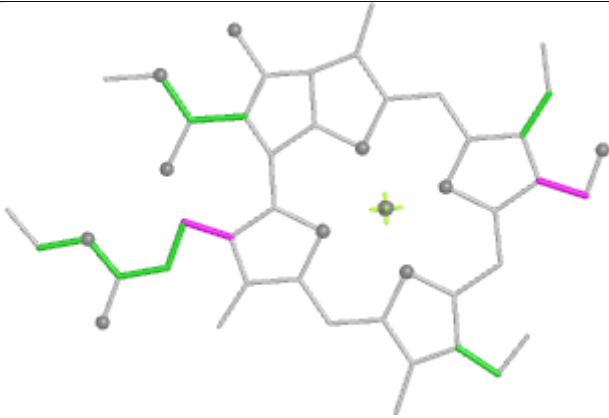
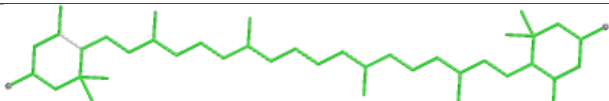
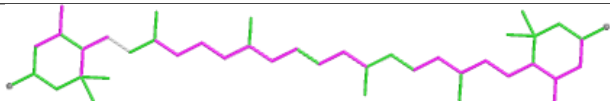


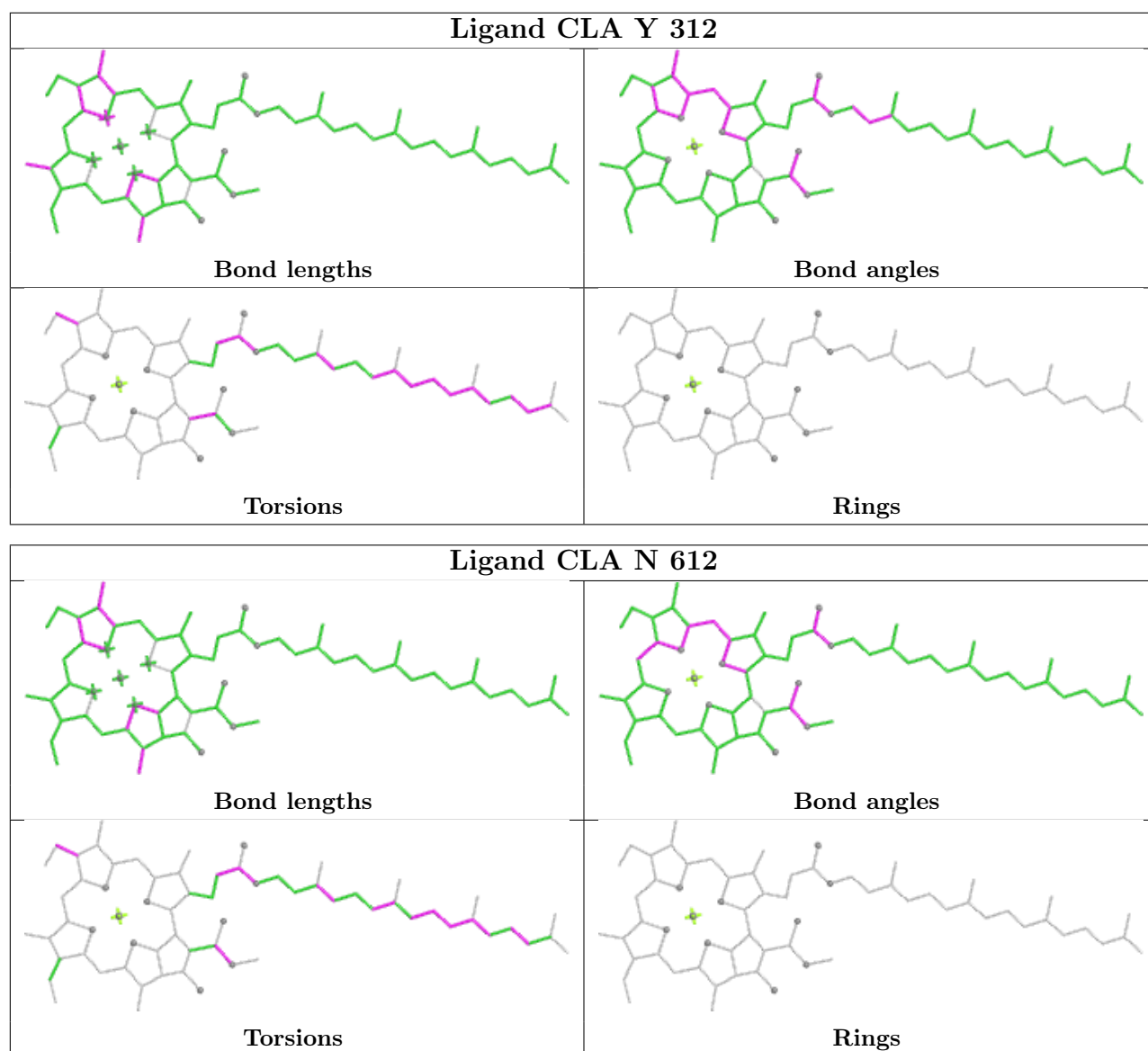


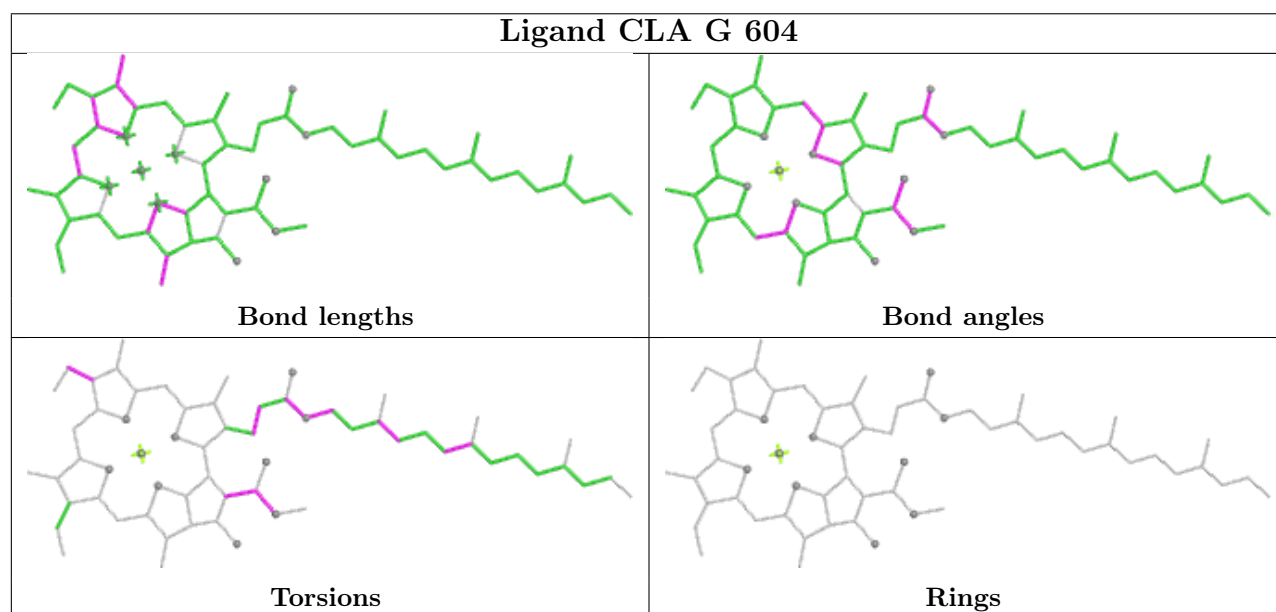
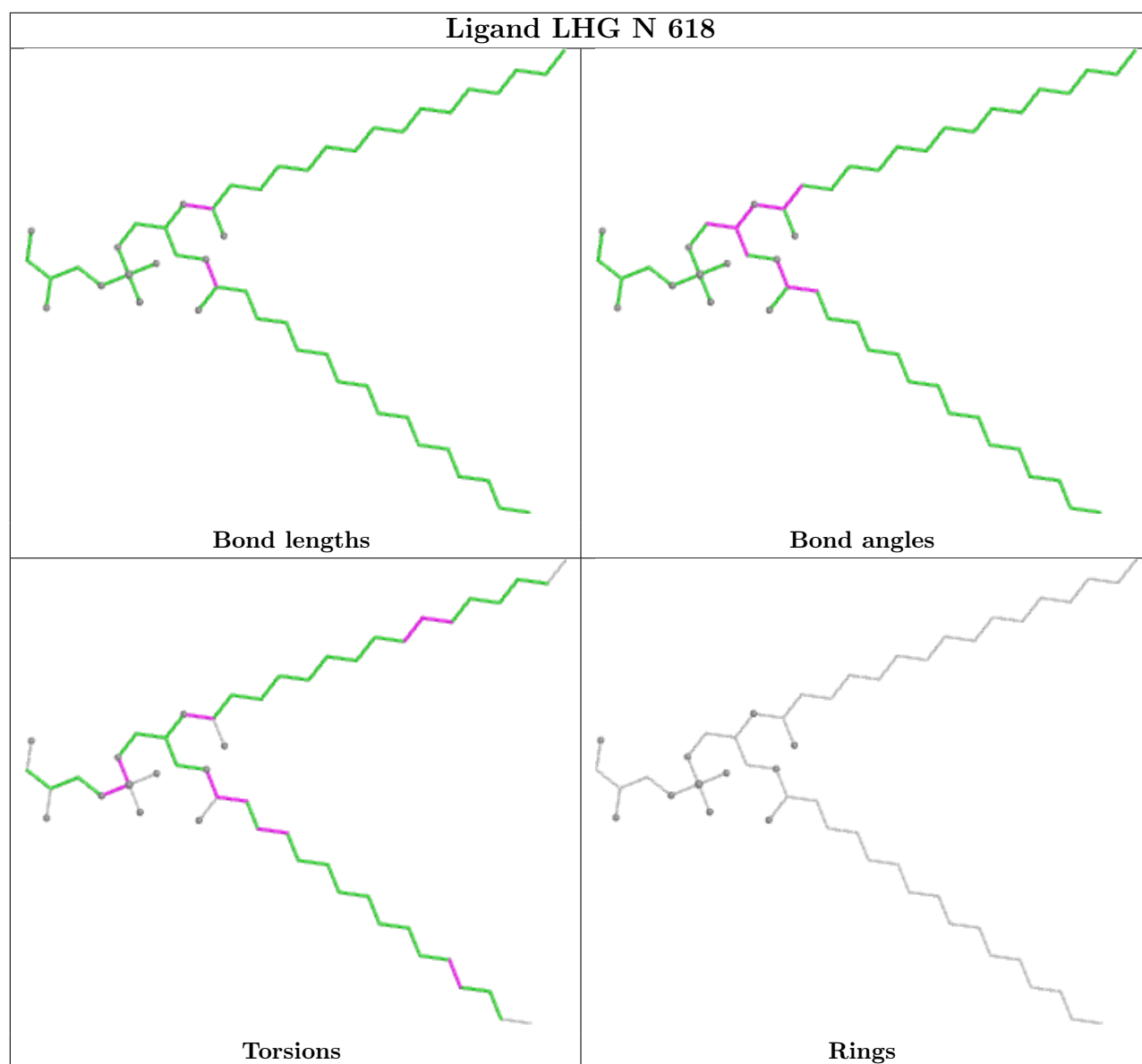


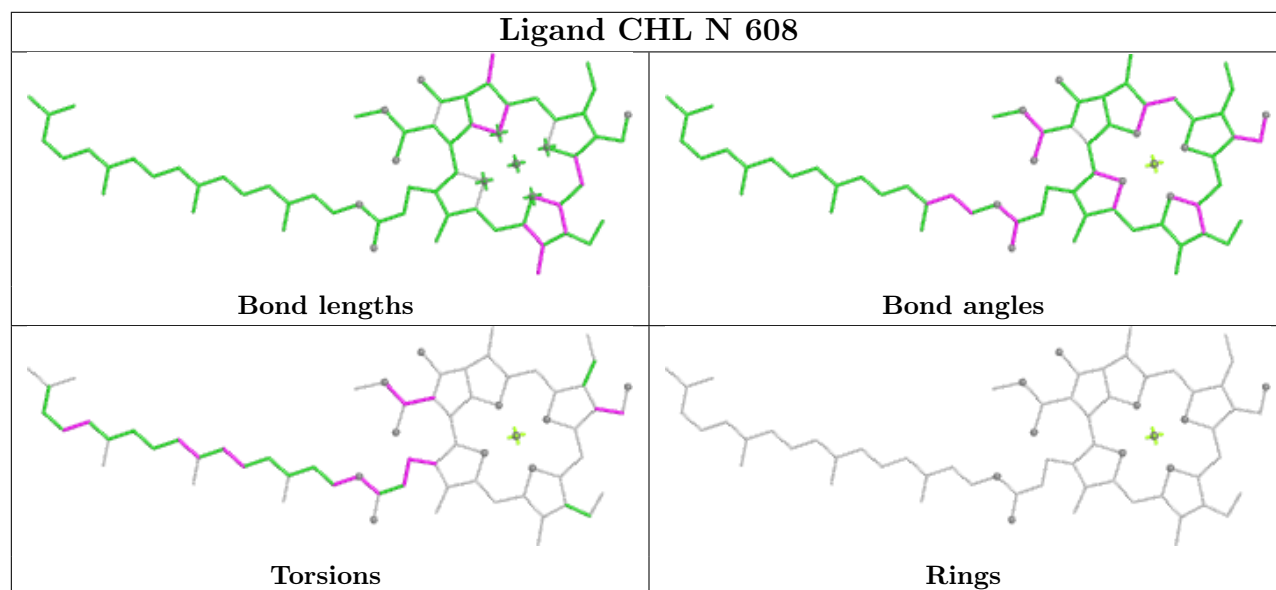
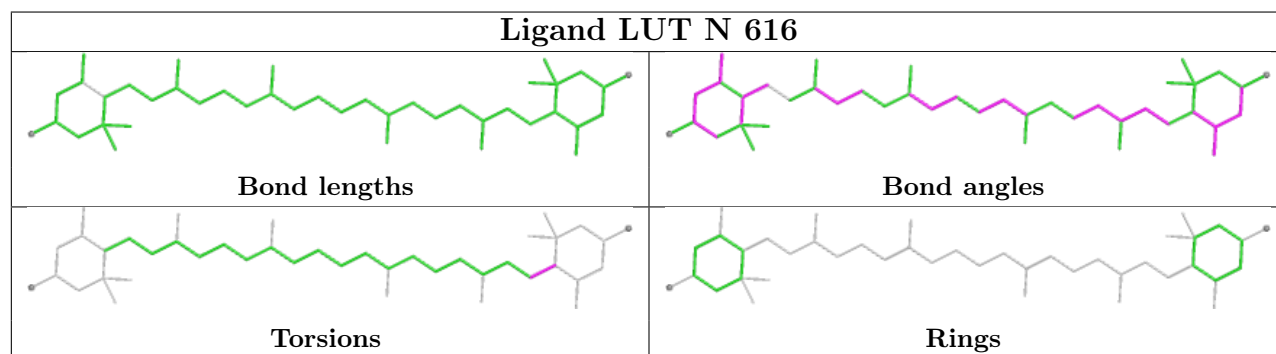
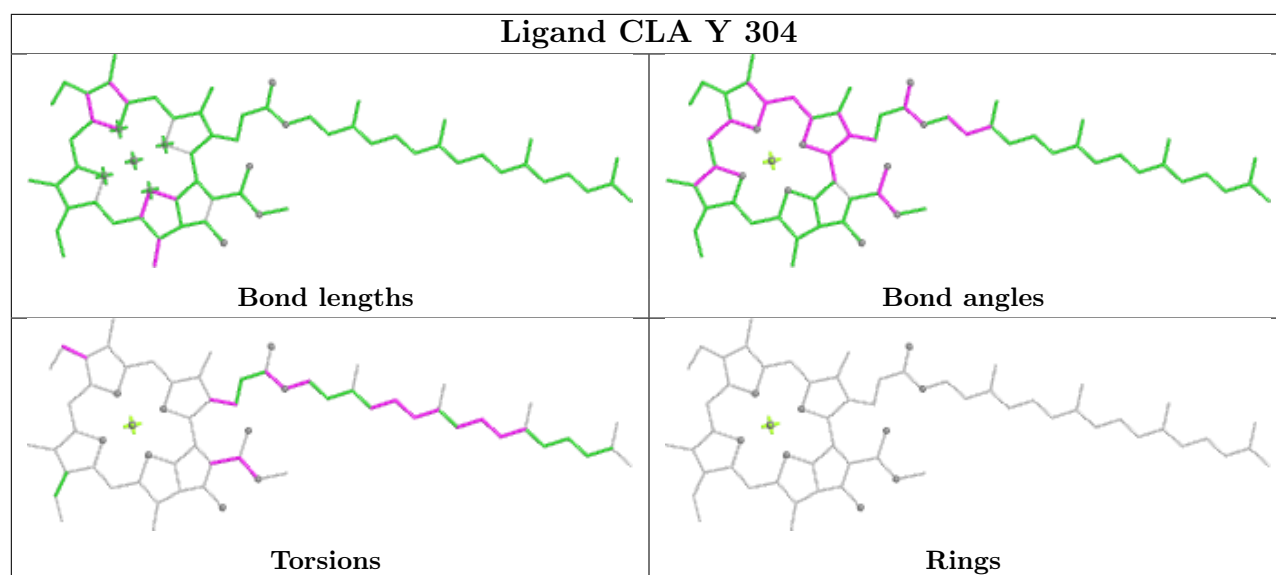


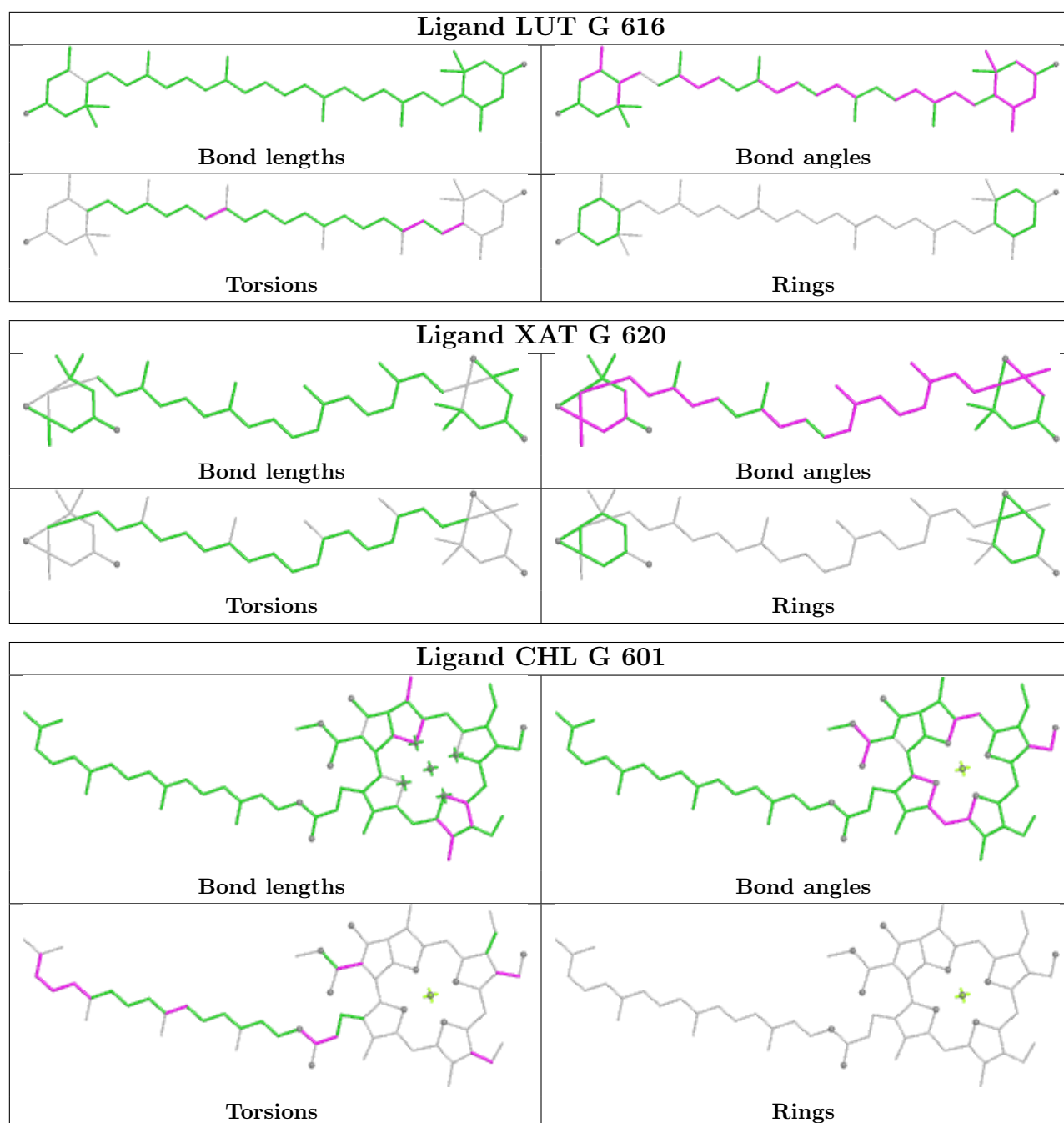


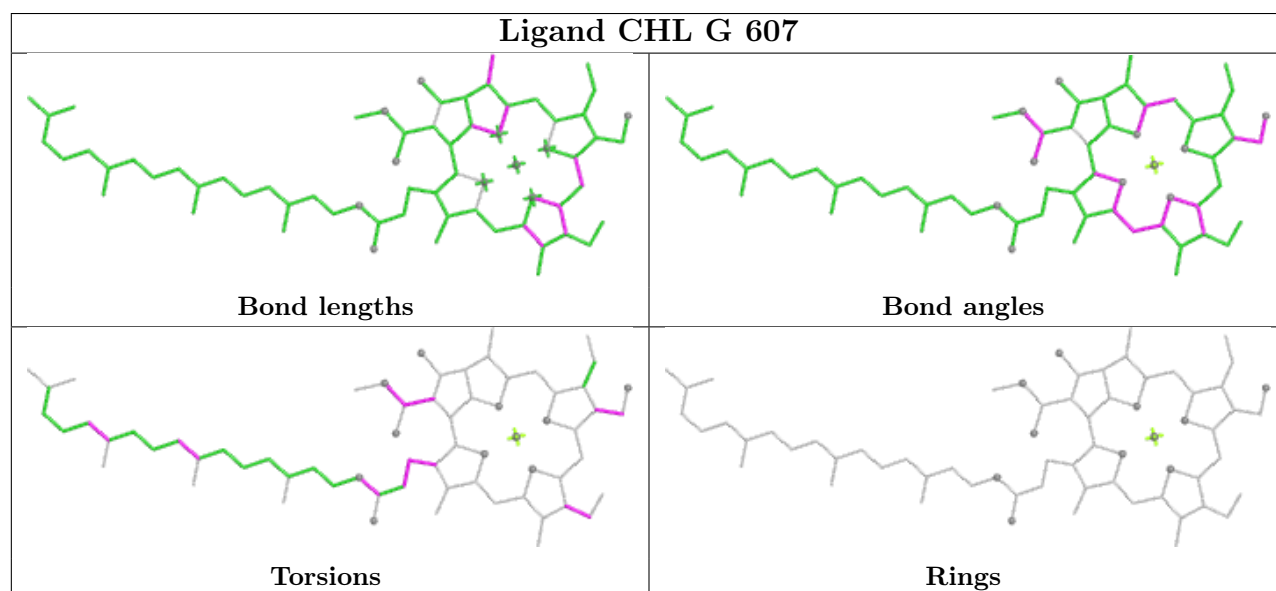
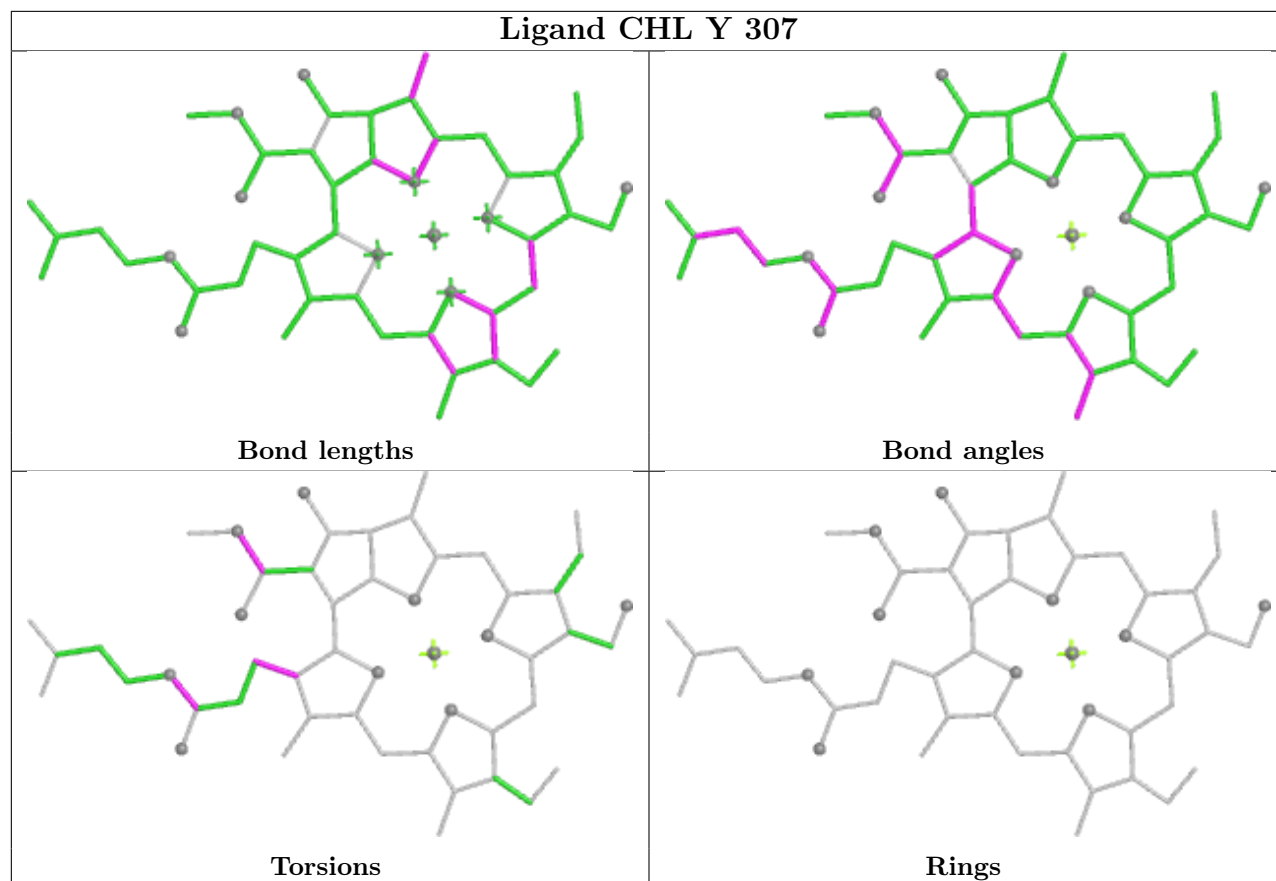
Ligand CHL G 605	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand LUT Y 316	
	
Bond lengths	Bond angles
	
Torsions	Rings

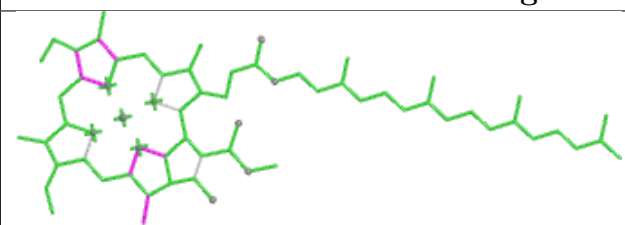
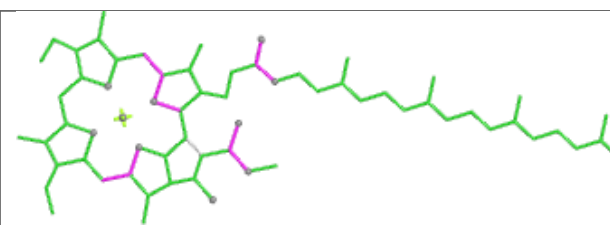
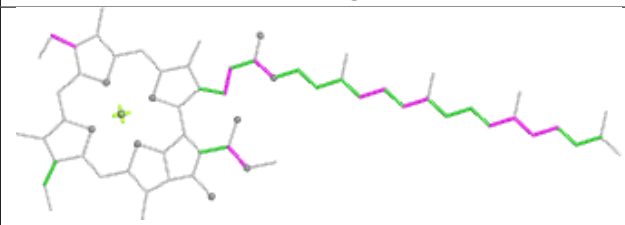
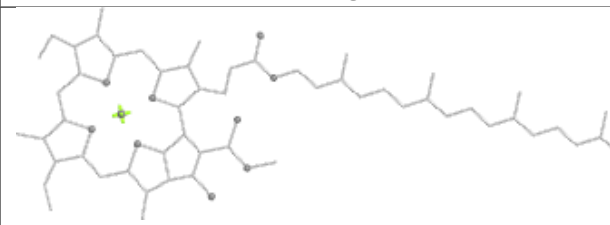


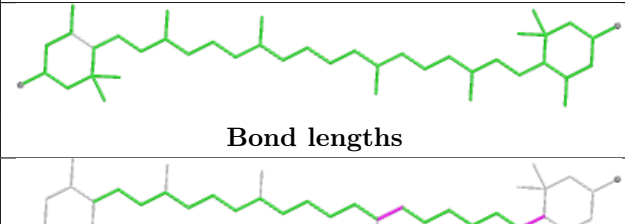
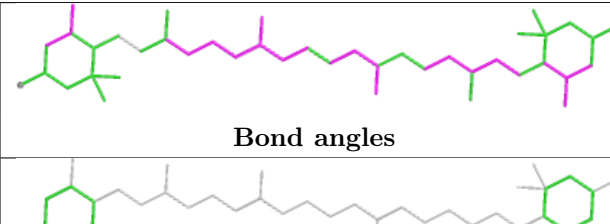
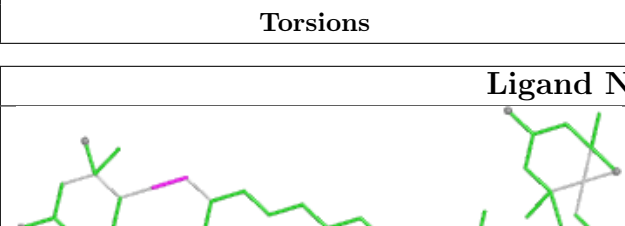
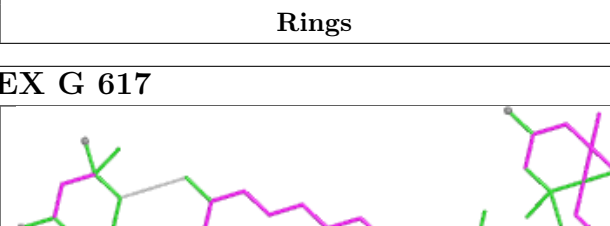


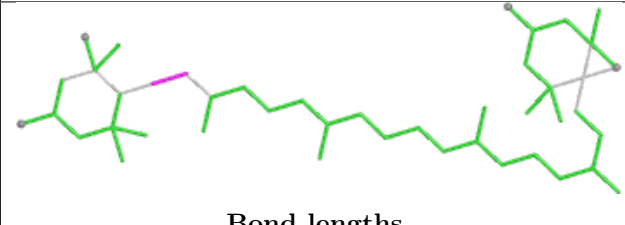
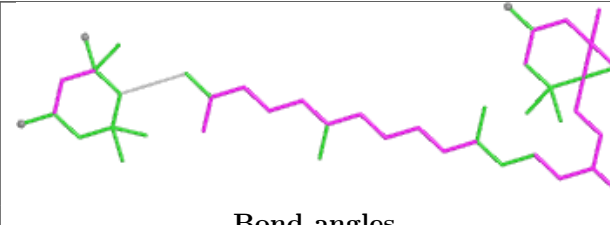
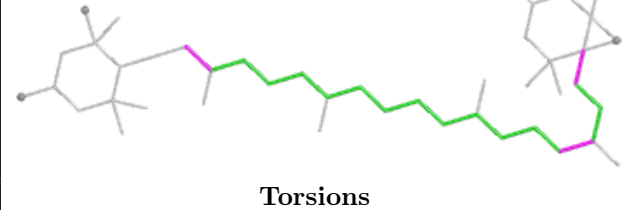
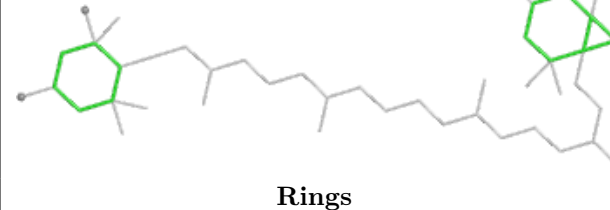


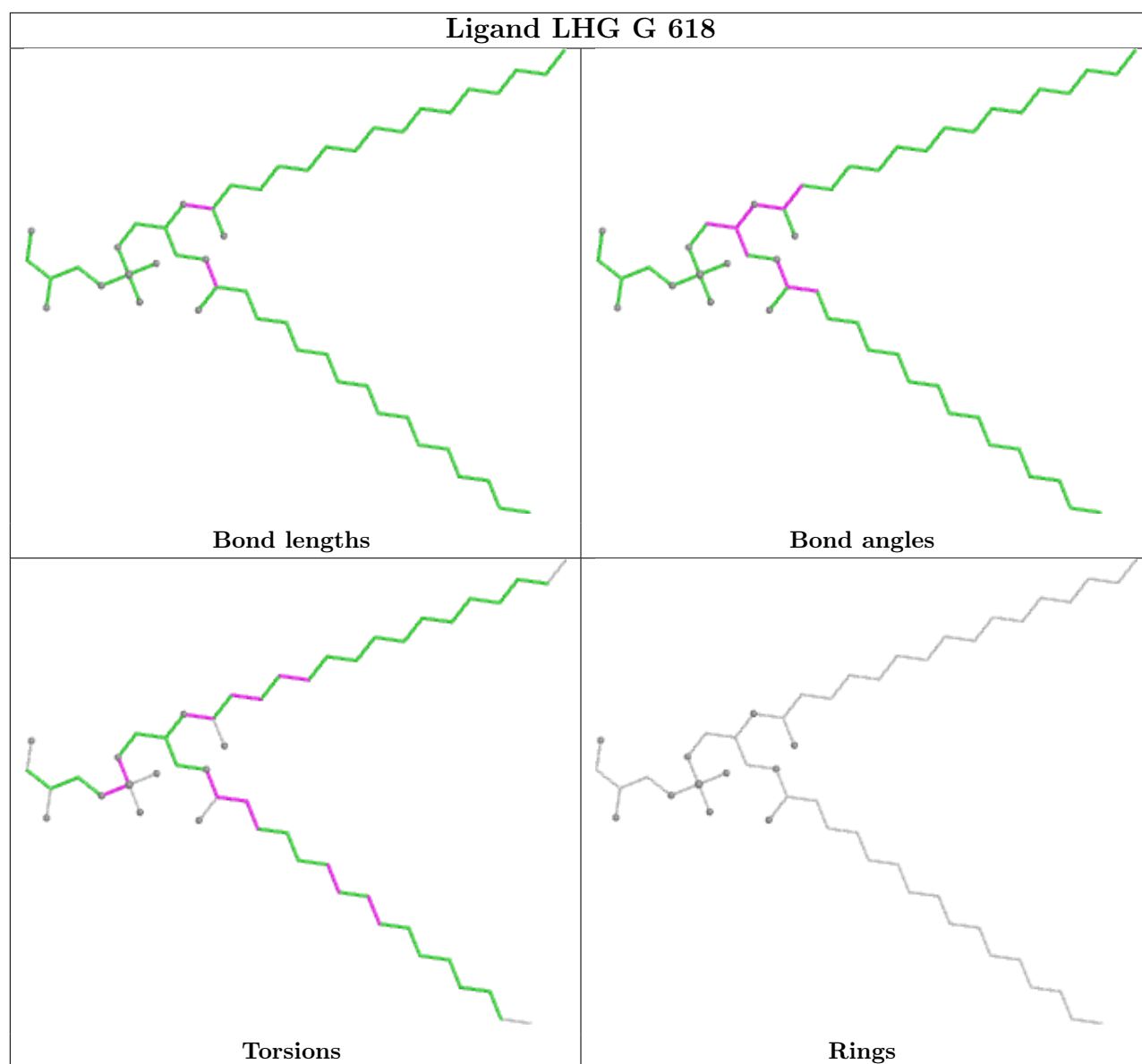




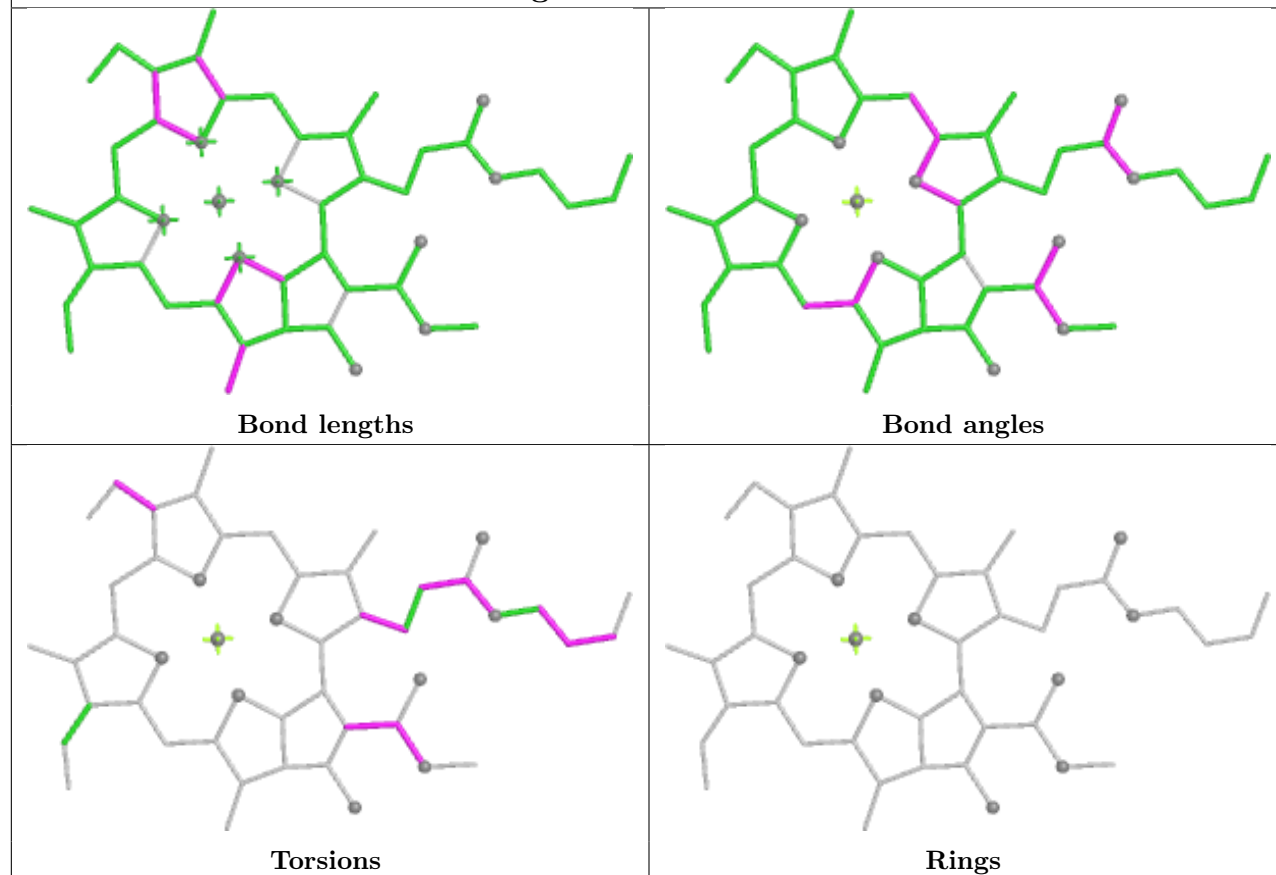
Ligand CLA N 613	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LUT G 615	
	
Bond lengths	Bond angles
	
Torsions	Rings

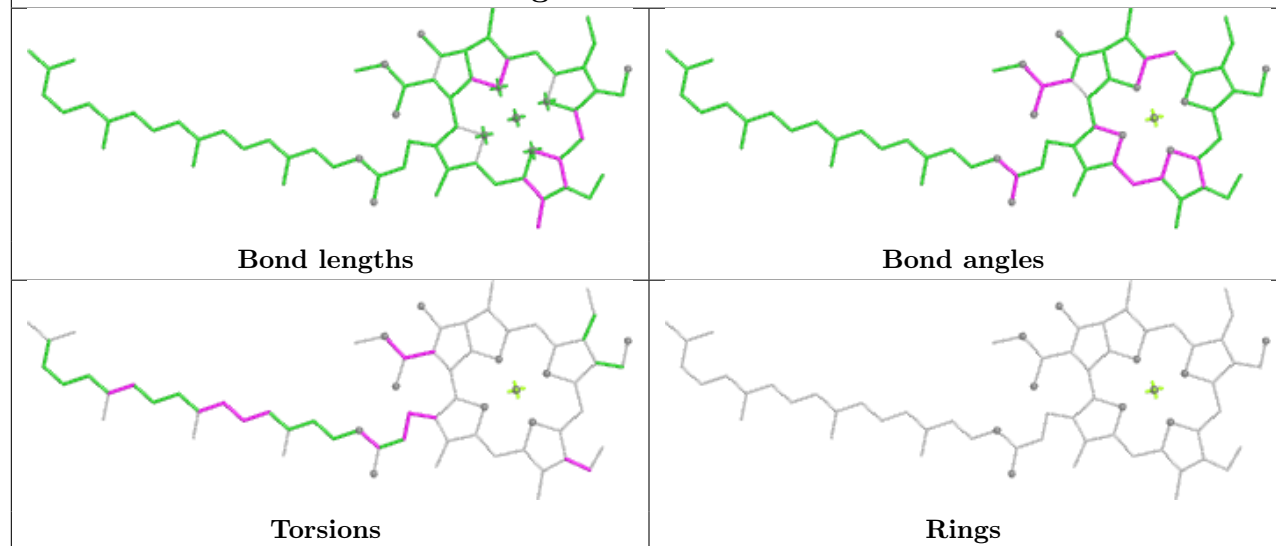
Ligand NEX G 617	
	
Bond lengths	Bond angles
	
Torsions	Rings

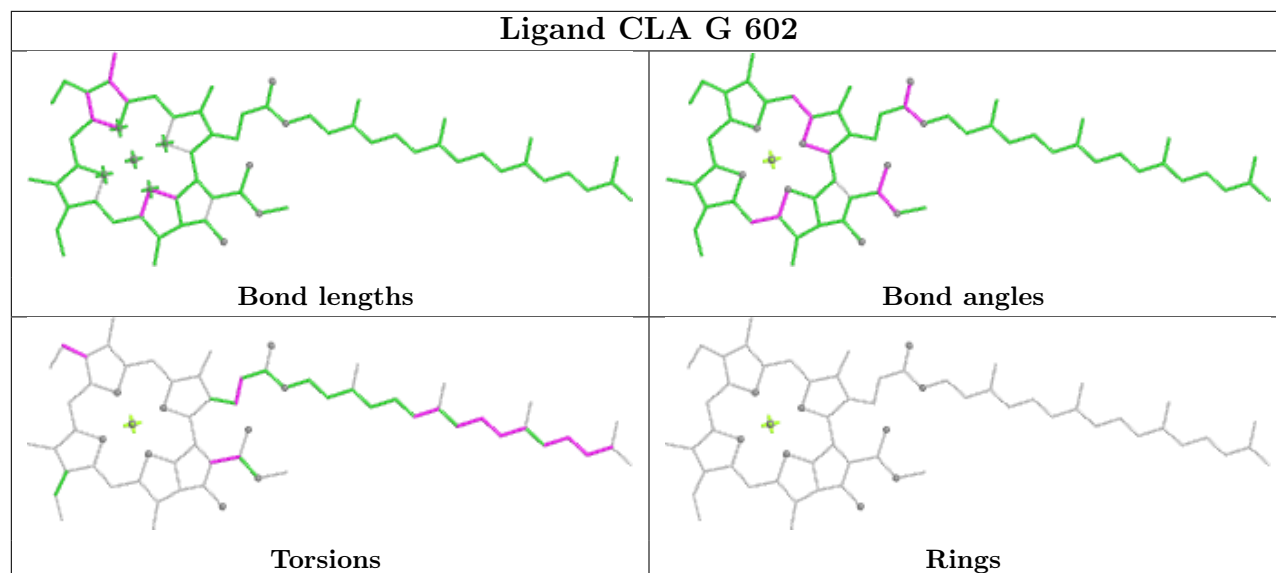
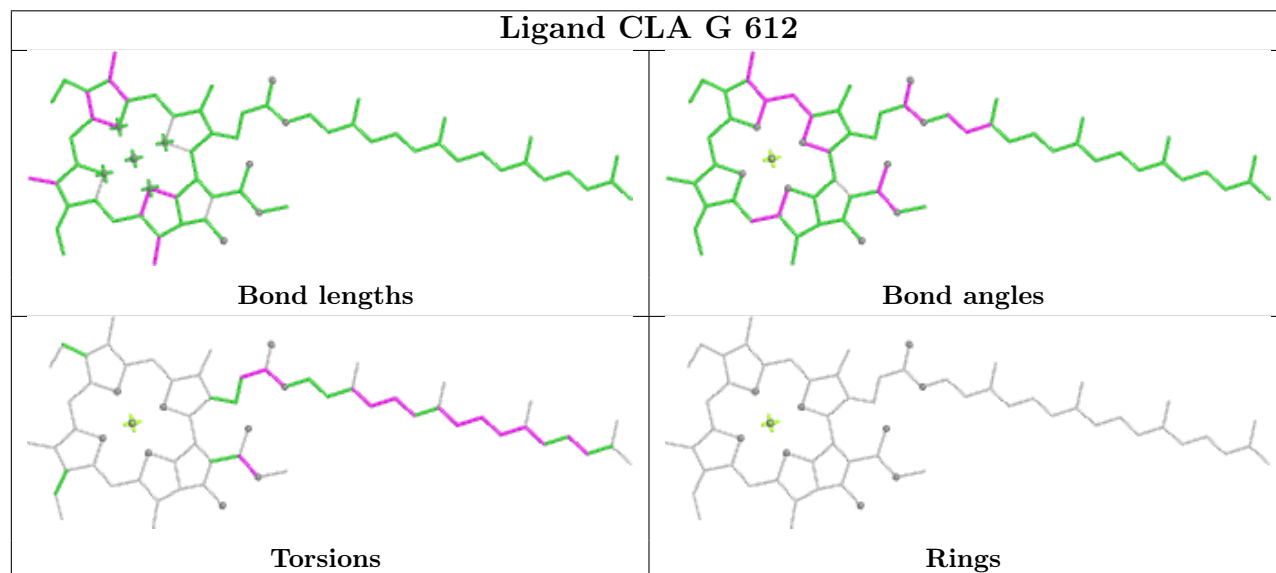
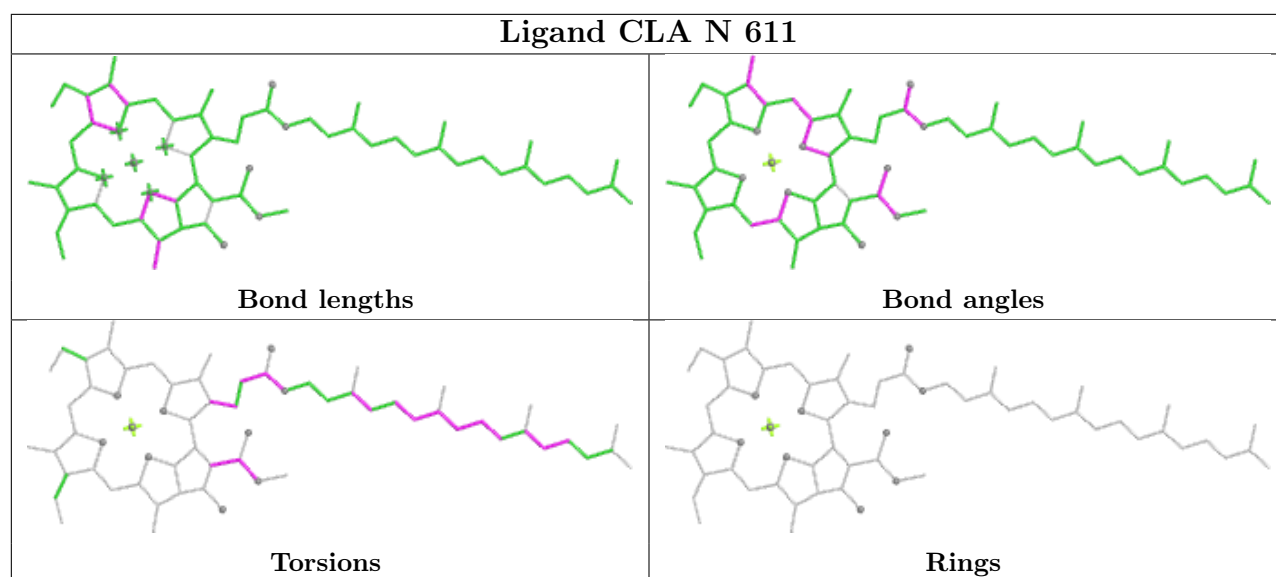


Ligand CLA N 614

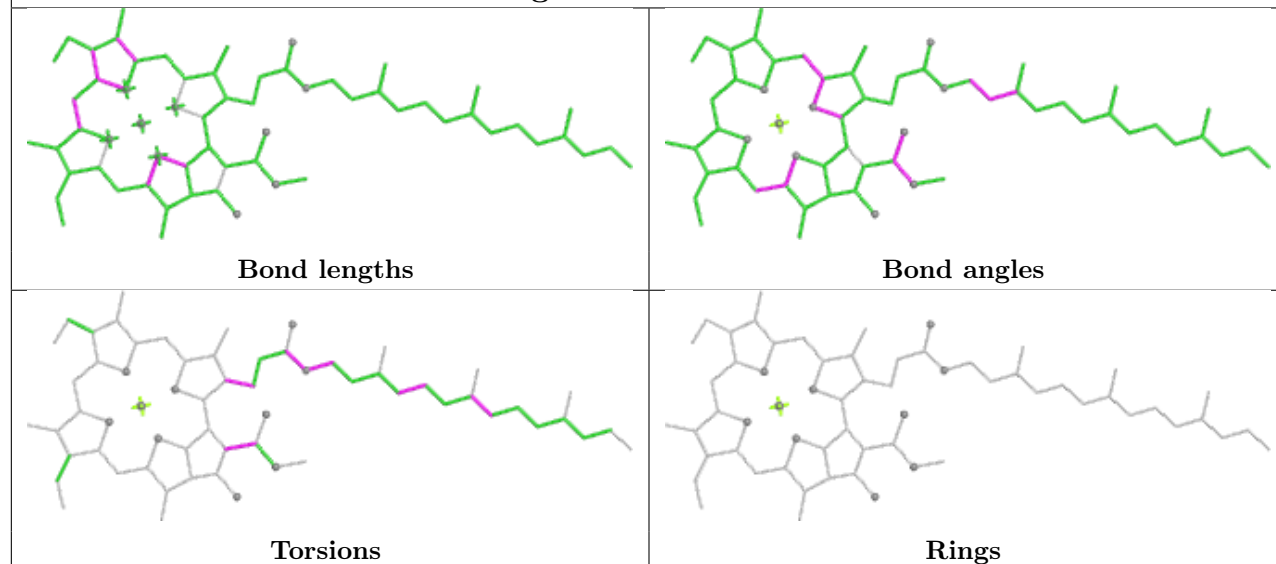


Ligand CHL Y 308

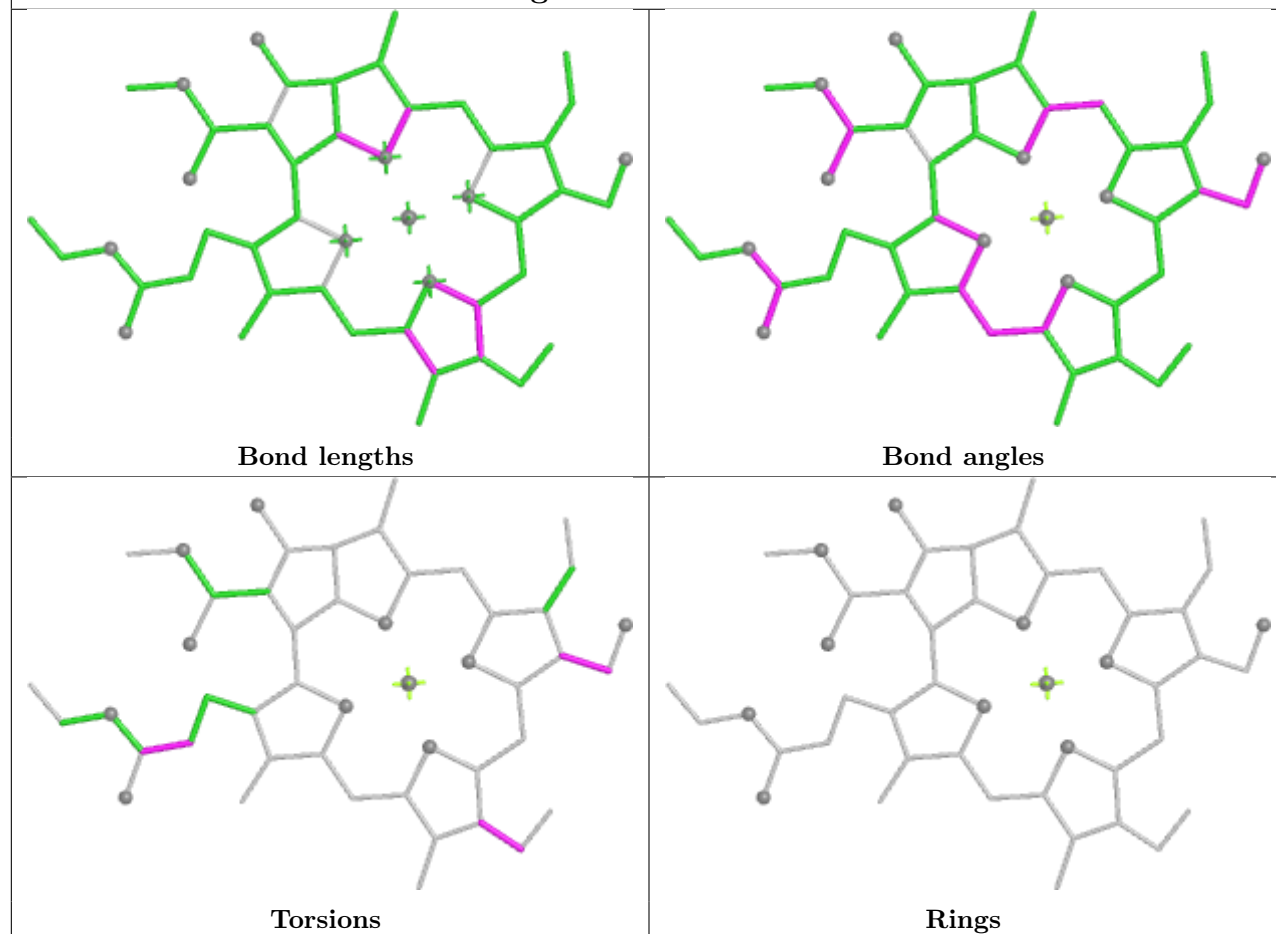


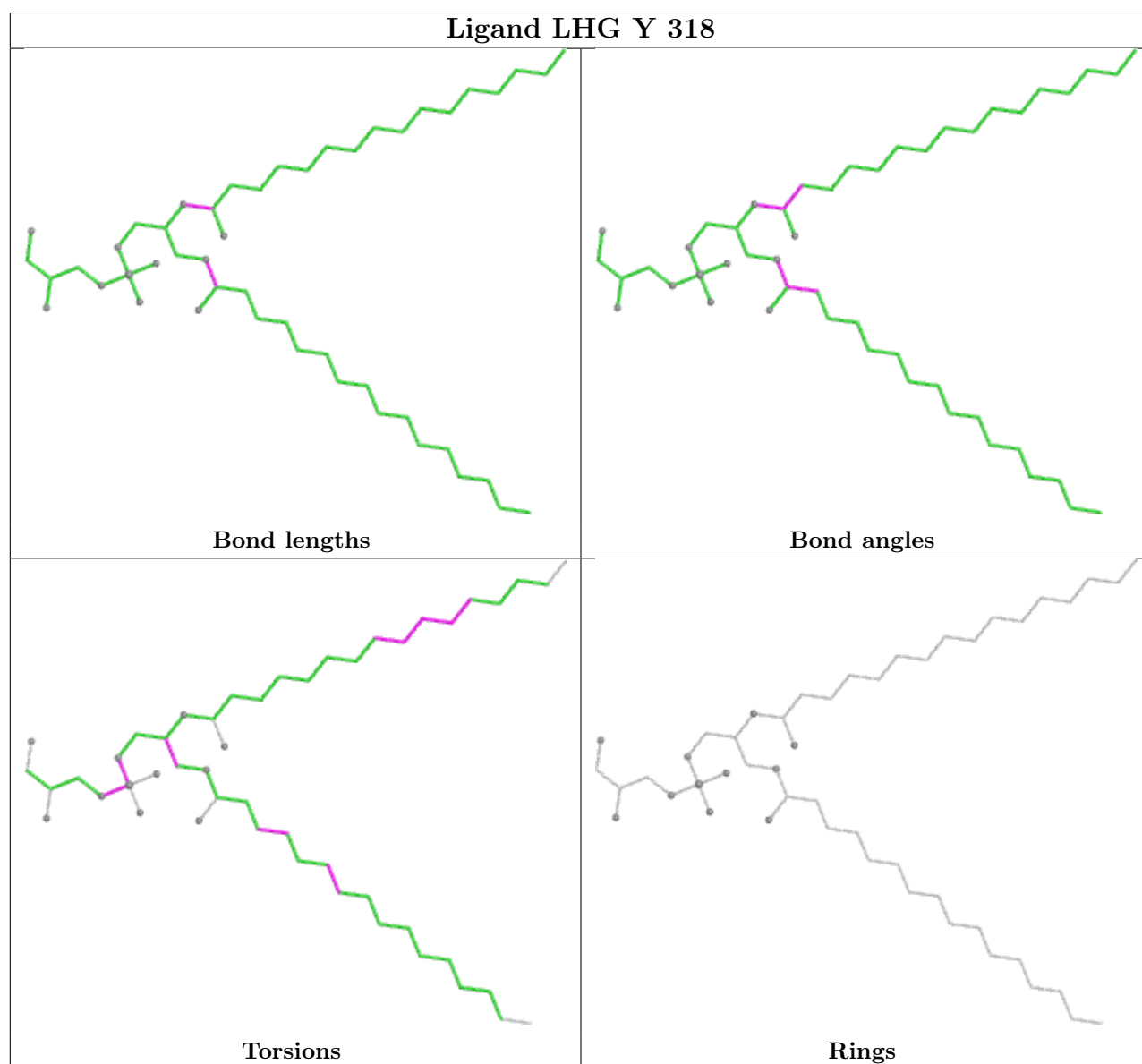
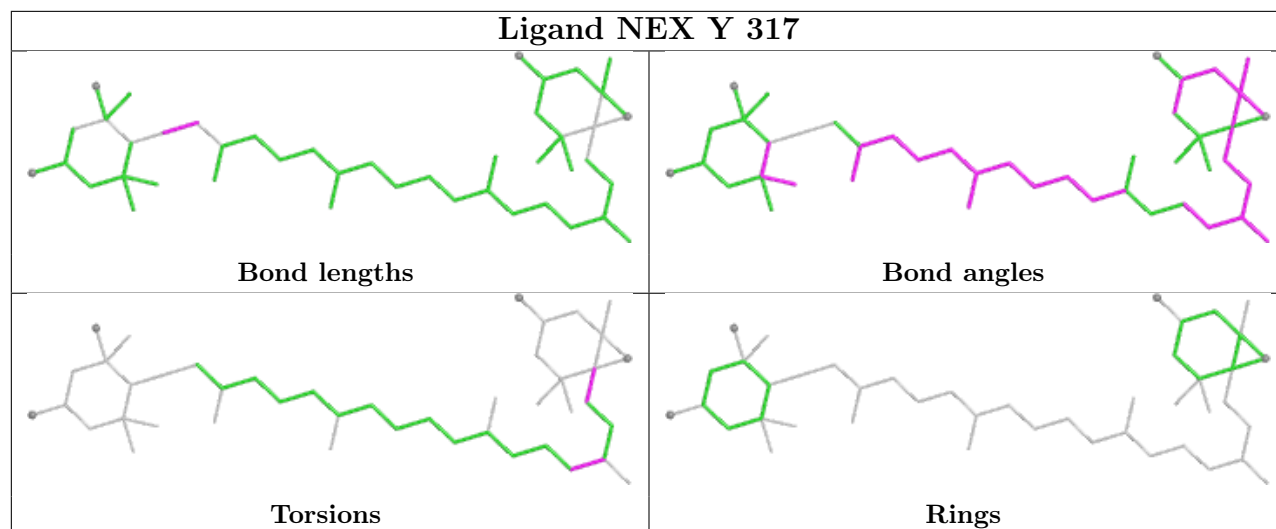


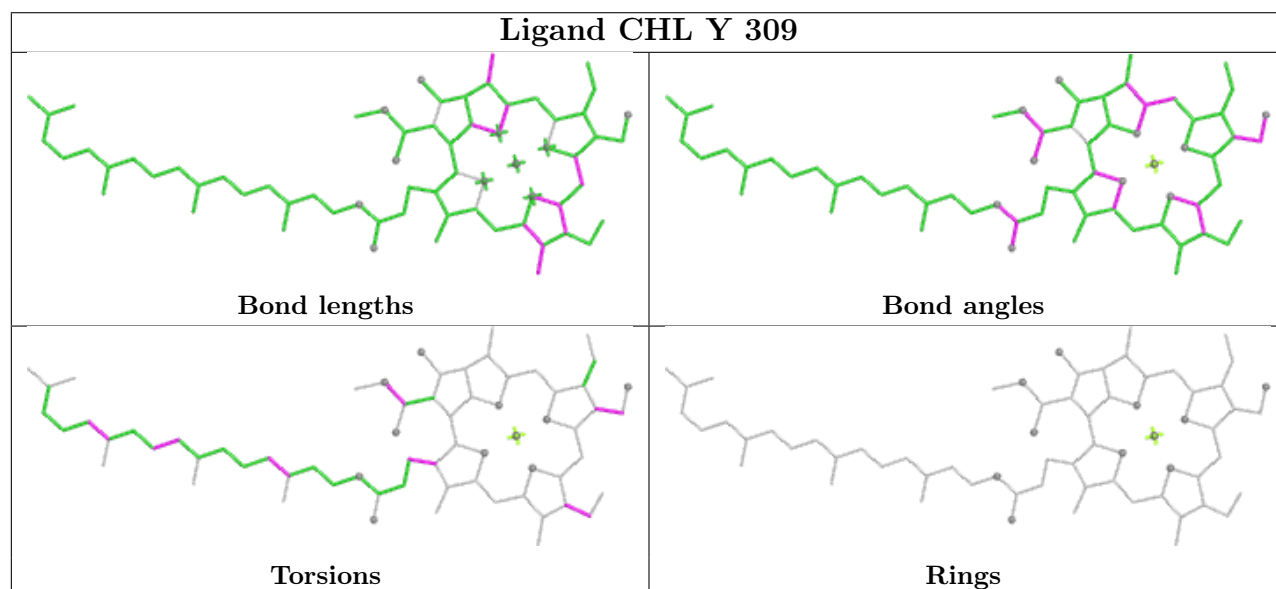
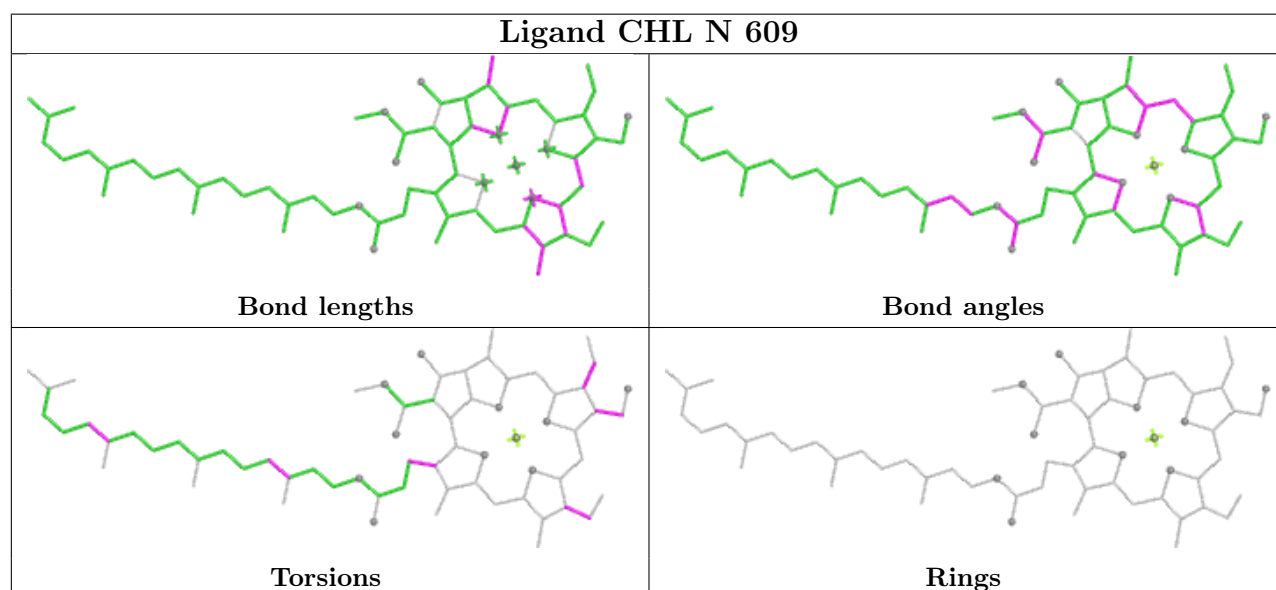
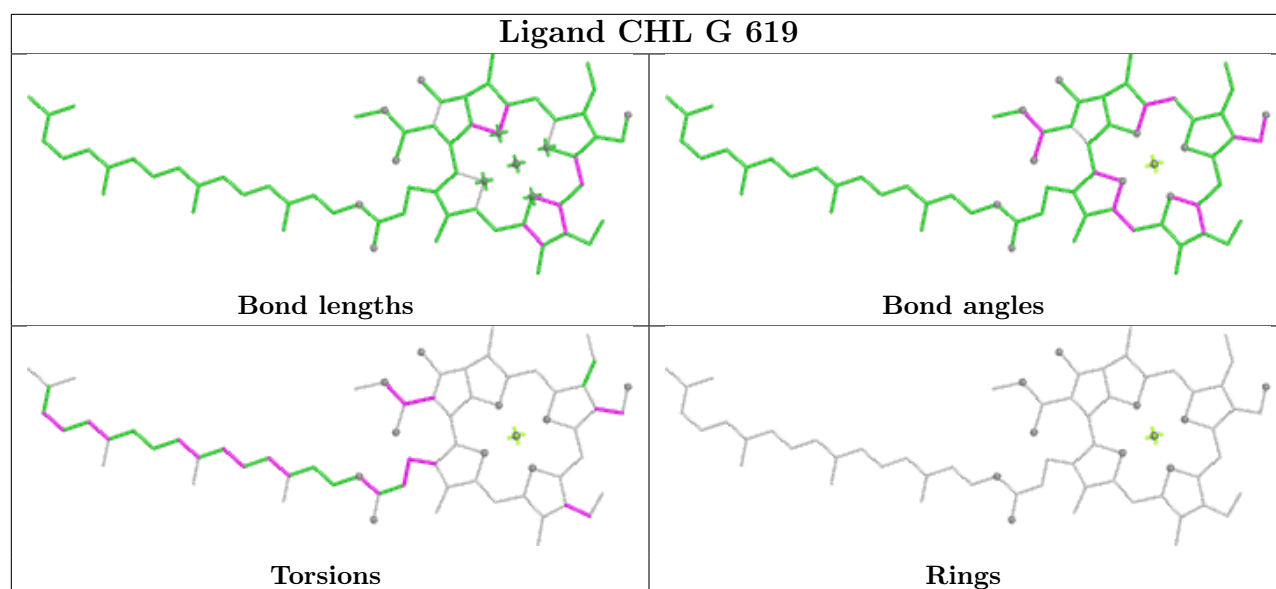
Ligand CLA N 604

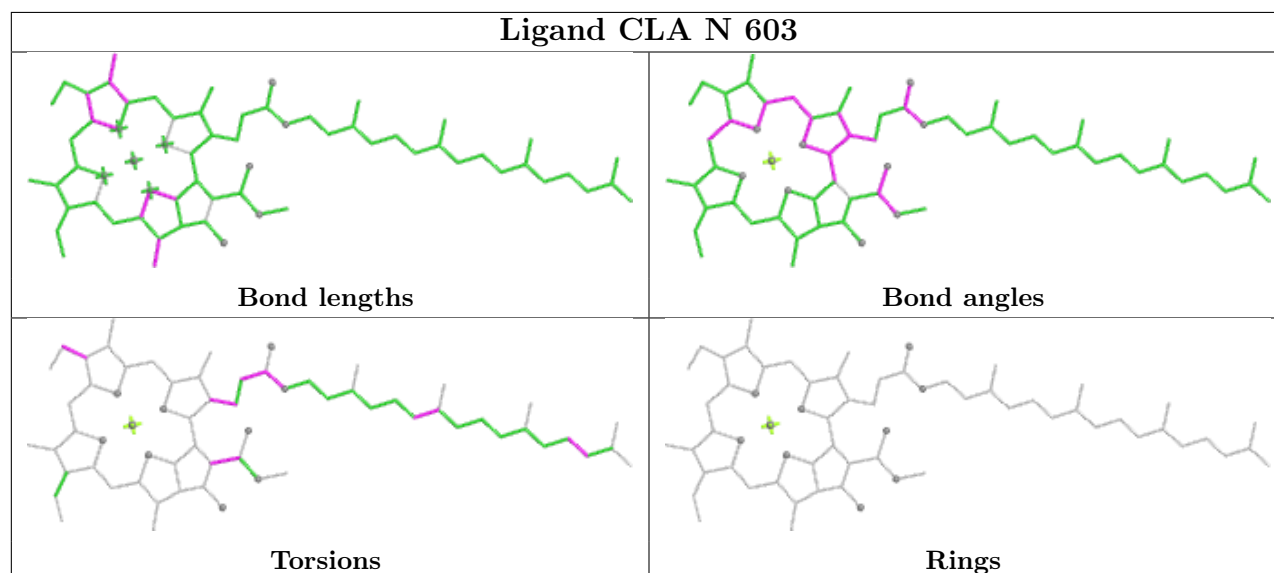
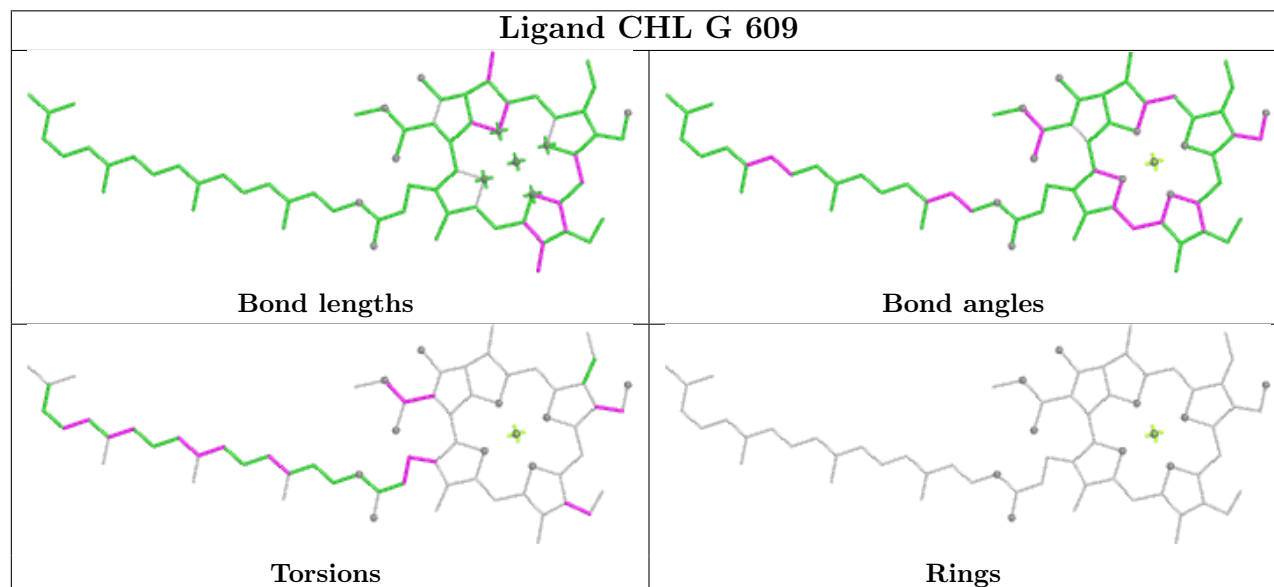
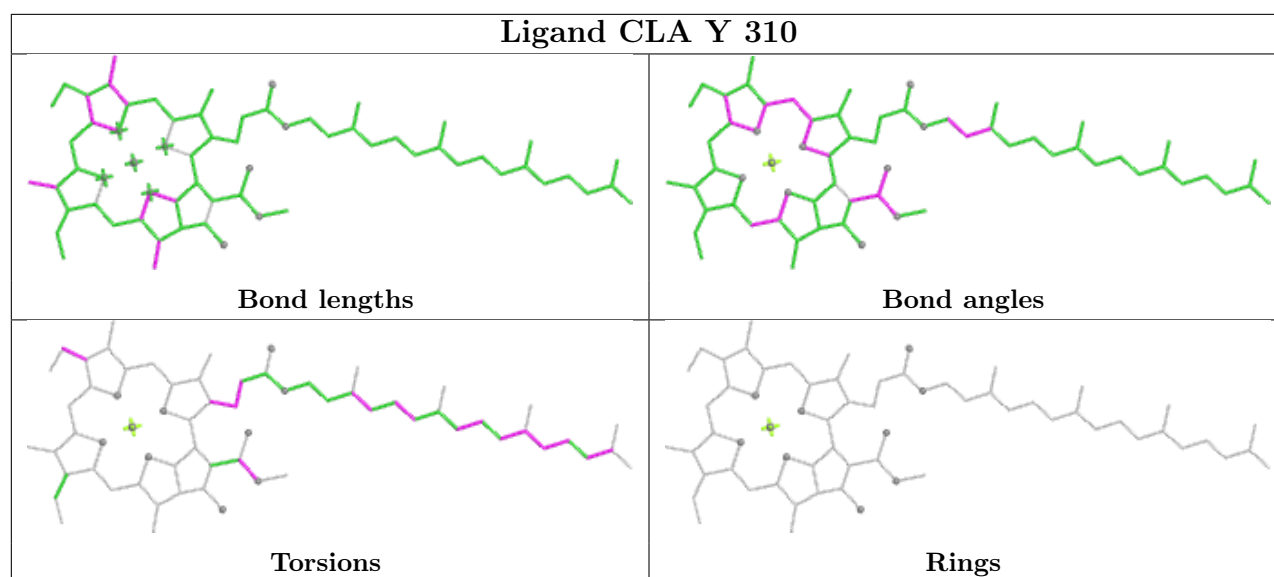


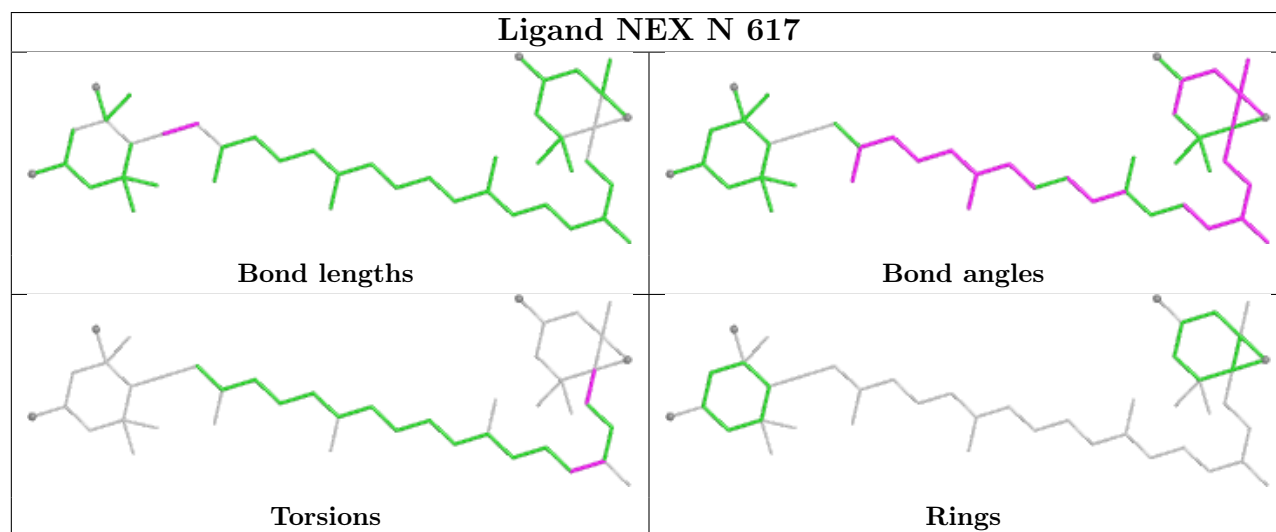
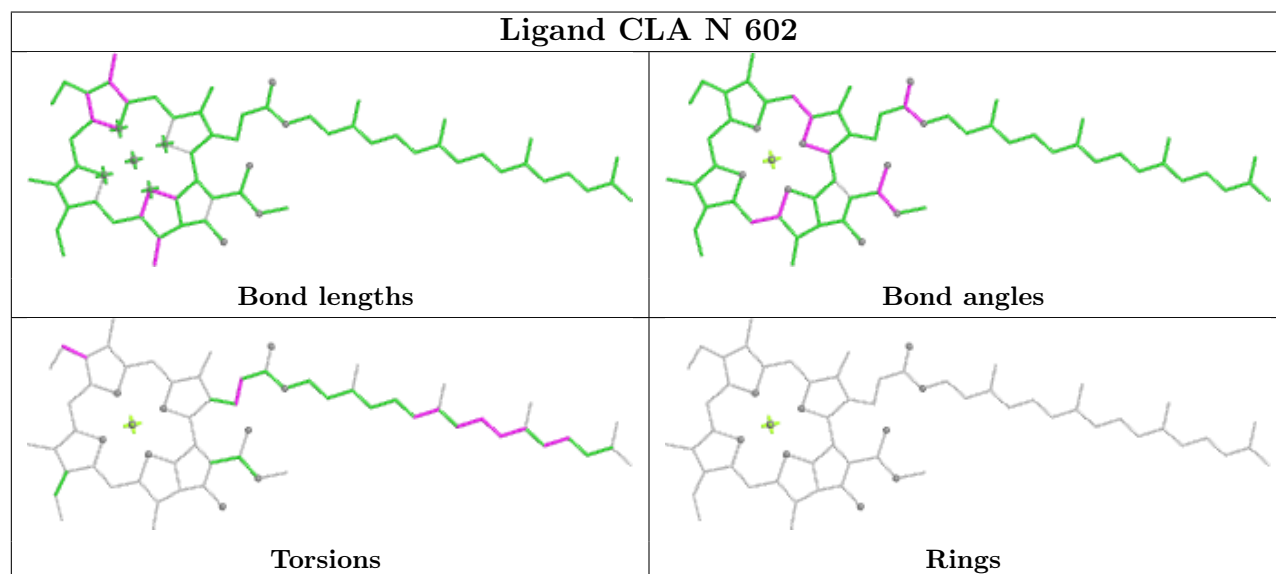
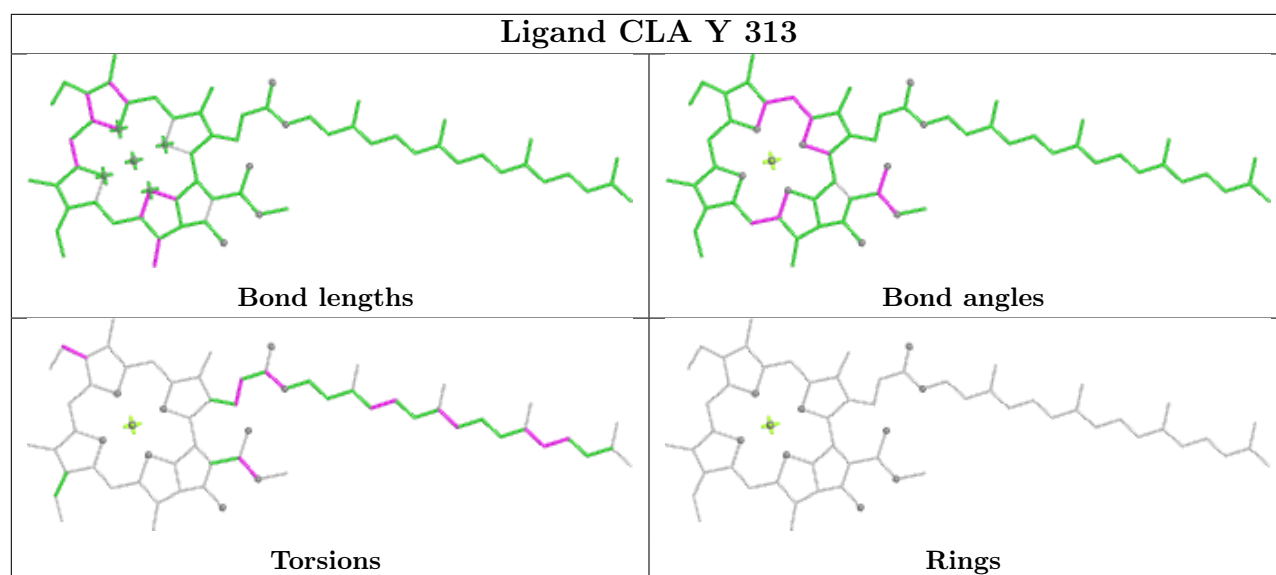
Ligand CHL N 605

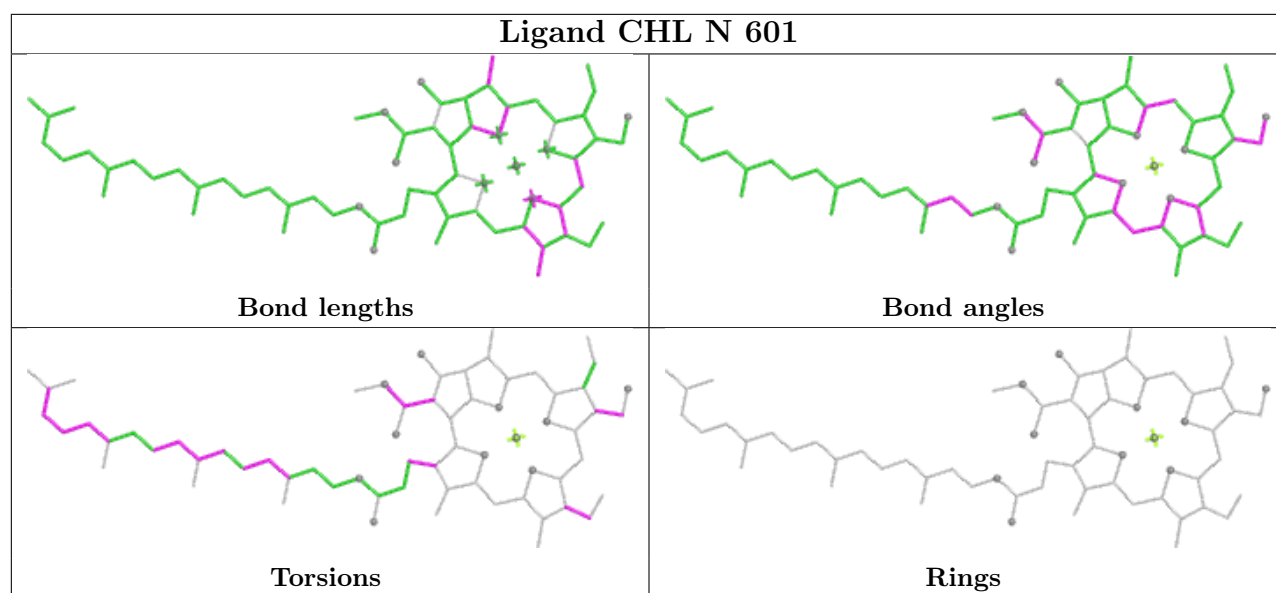












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

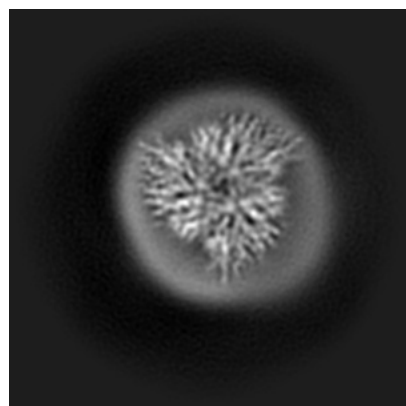
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35785. These allow visual inspection of the internal detail of the map and identification of artifacts.

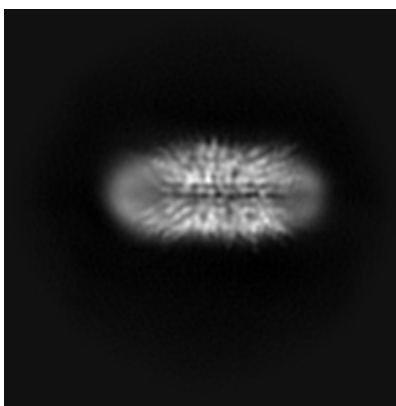
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

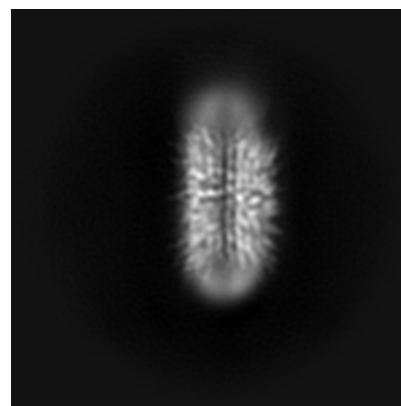
6.1.1 Primary map



X

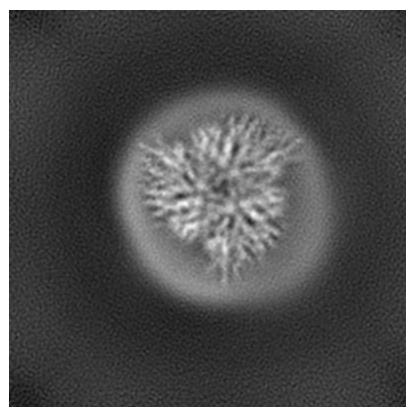


Y

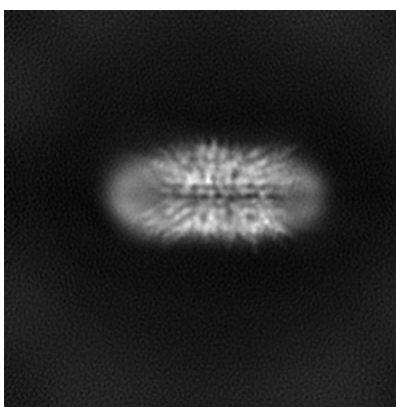


Z

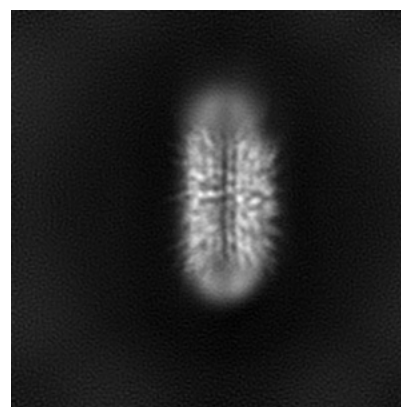
6.1.2 Raw map



X



Y

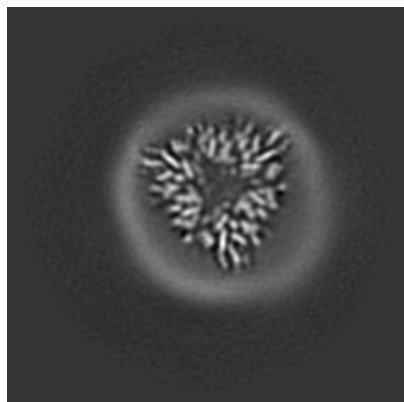


Z

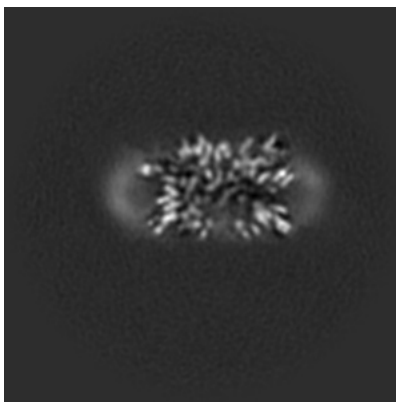
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

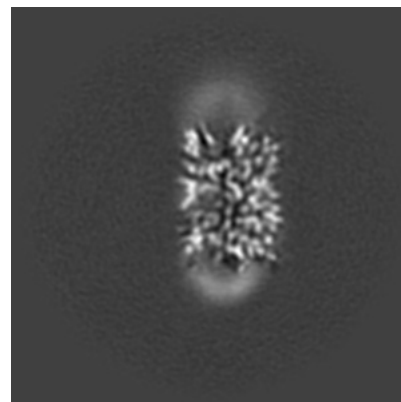
6.2.1 Primary map



X Index: 100

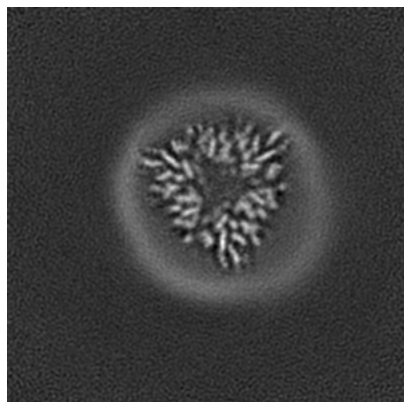


Y Index: 100

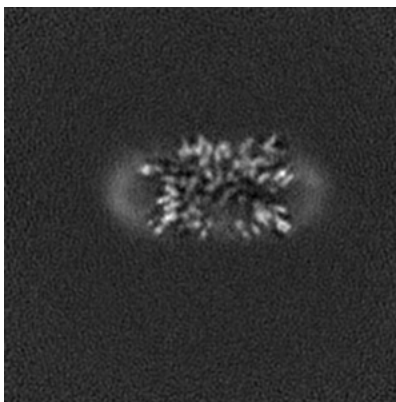


Z Index: 100

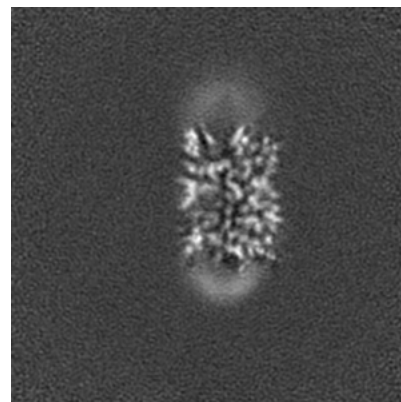
6.2.2 Raw map



X Index: 100



Y Index: 100

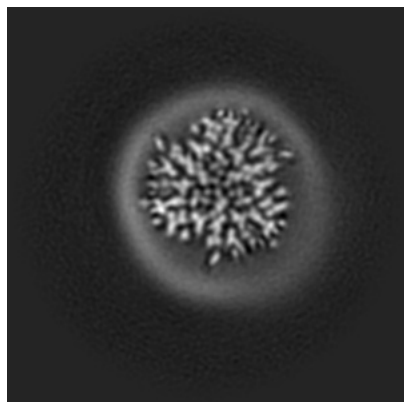


Z Index: 100

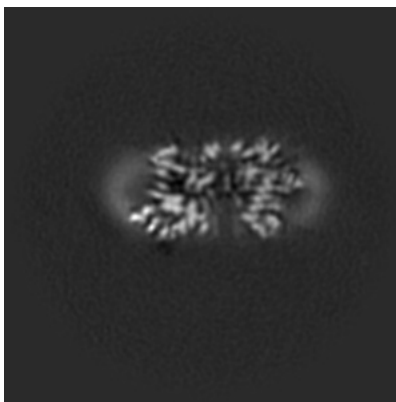
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

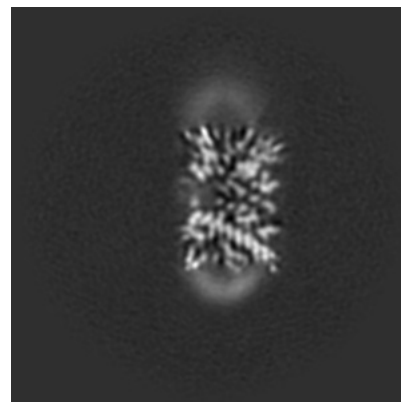
6.3.1 Primary map



X Index: 114

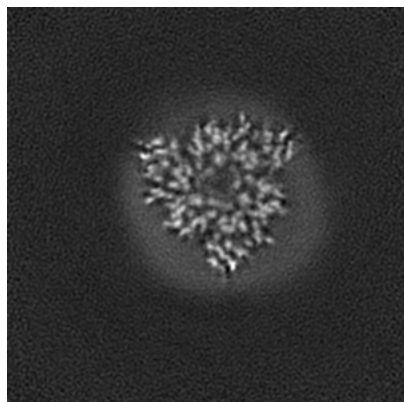


Y Index: 108

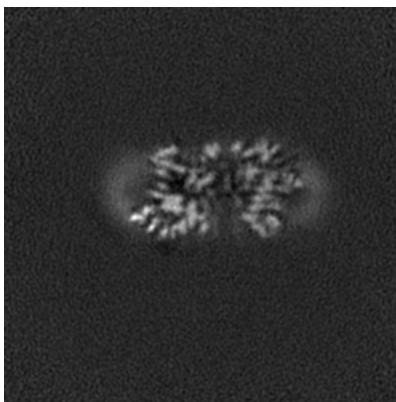


Z Index: 103

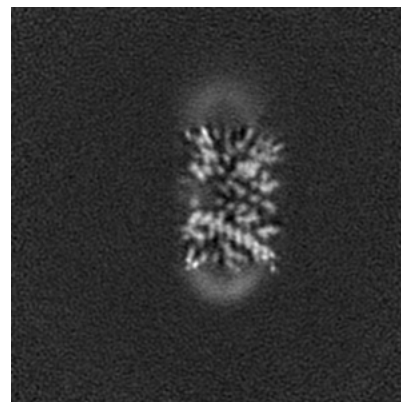
6.3.2 Raw map



X Index: 92



Y Index: 108

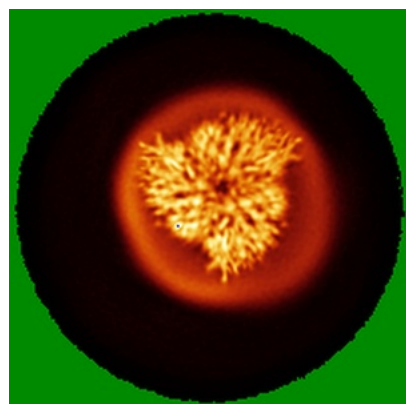


Z Index: 103

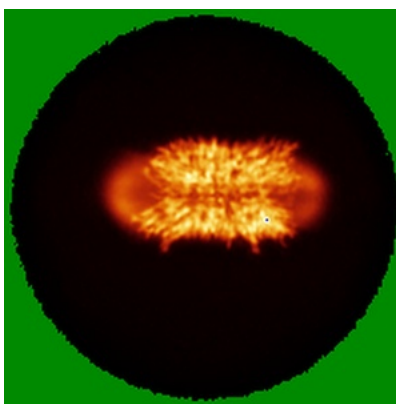
The images above show the largest variance slices of the map in three orthogonal directions.

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

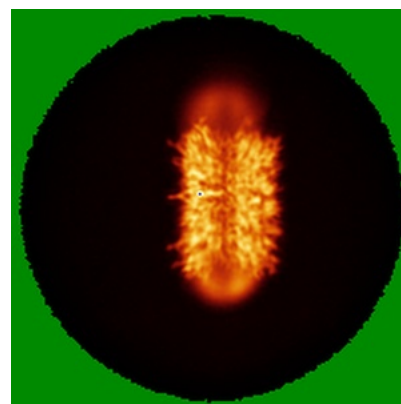
6.4.1 Primary map



X

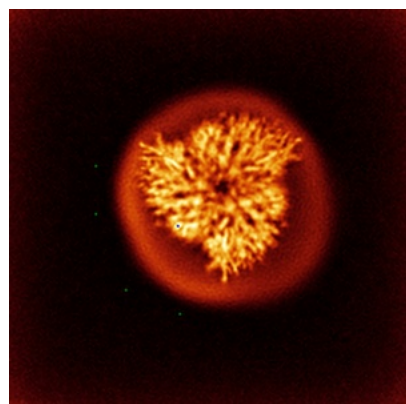


Y

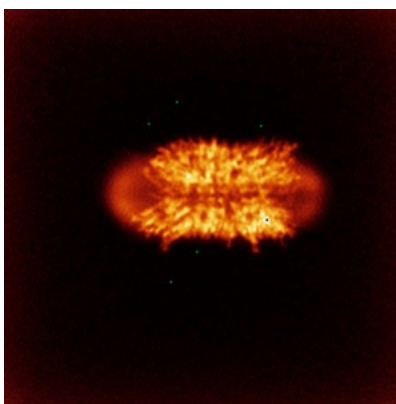


Z

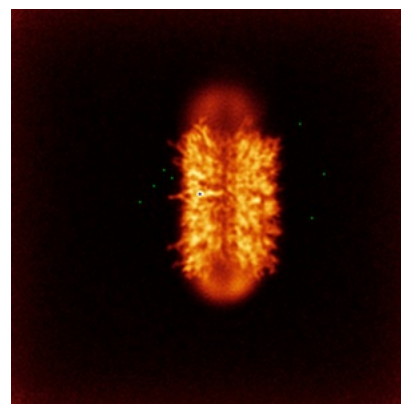
6.4.2 Raw map



X



Y

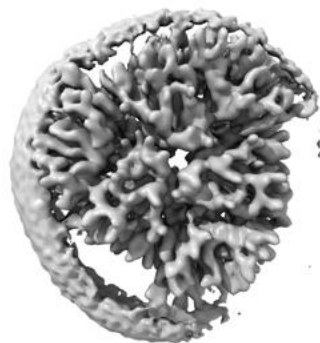


Z

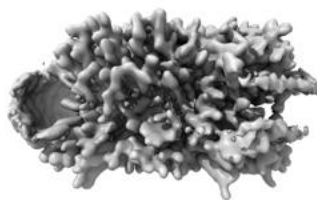
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

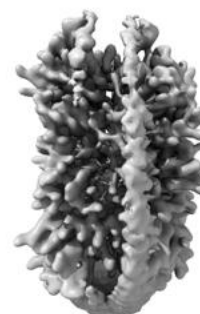
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

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

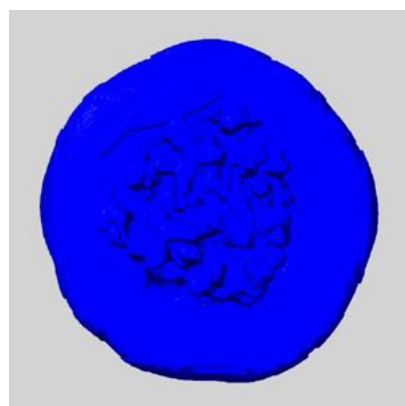
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

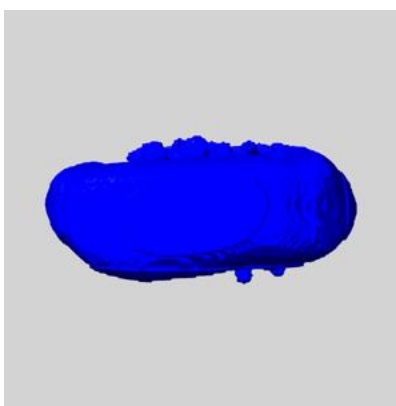
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

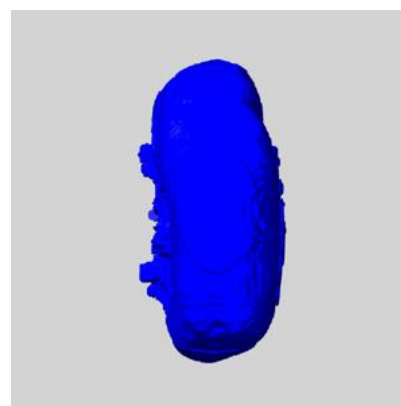
6.6.1 emd_35785_msk_1.map [i](#)



X



Y

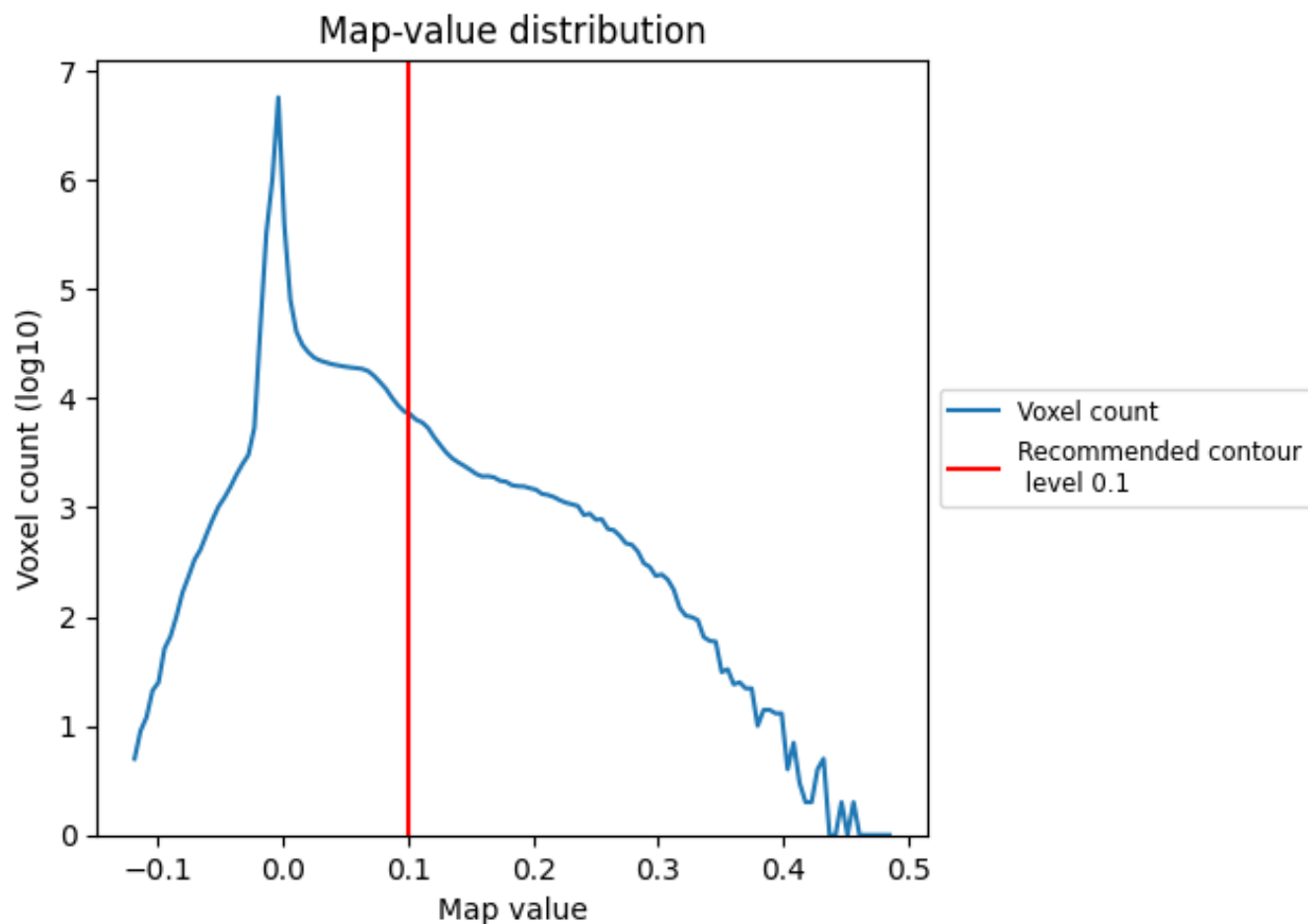


Z

7 Map analysis [i](#)

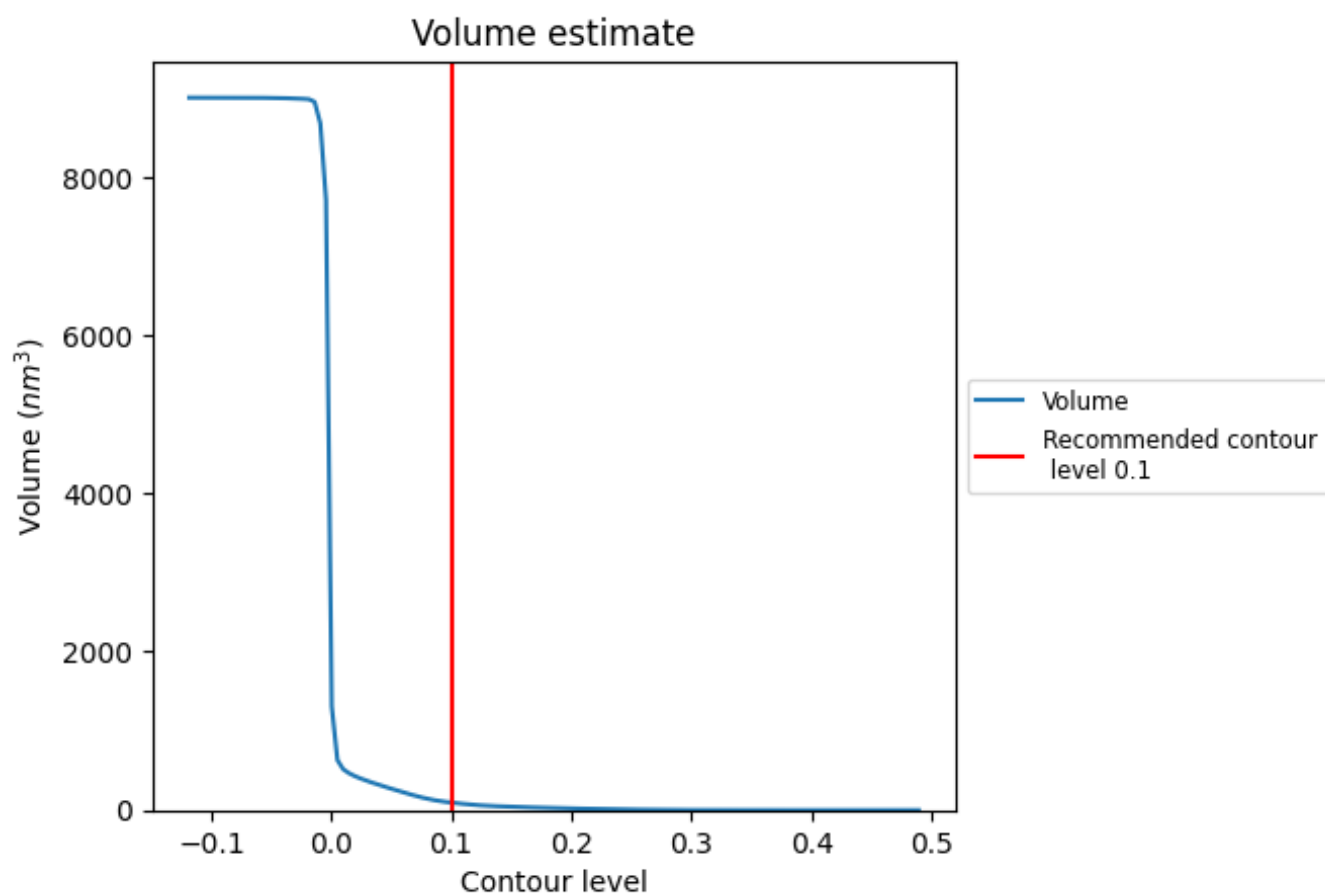
This section contains the results of statistical analysis of the map.

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.

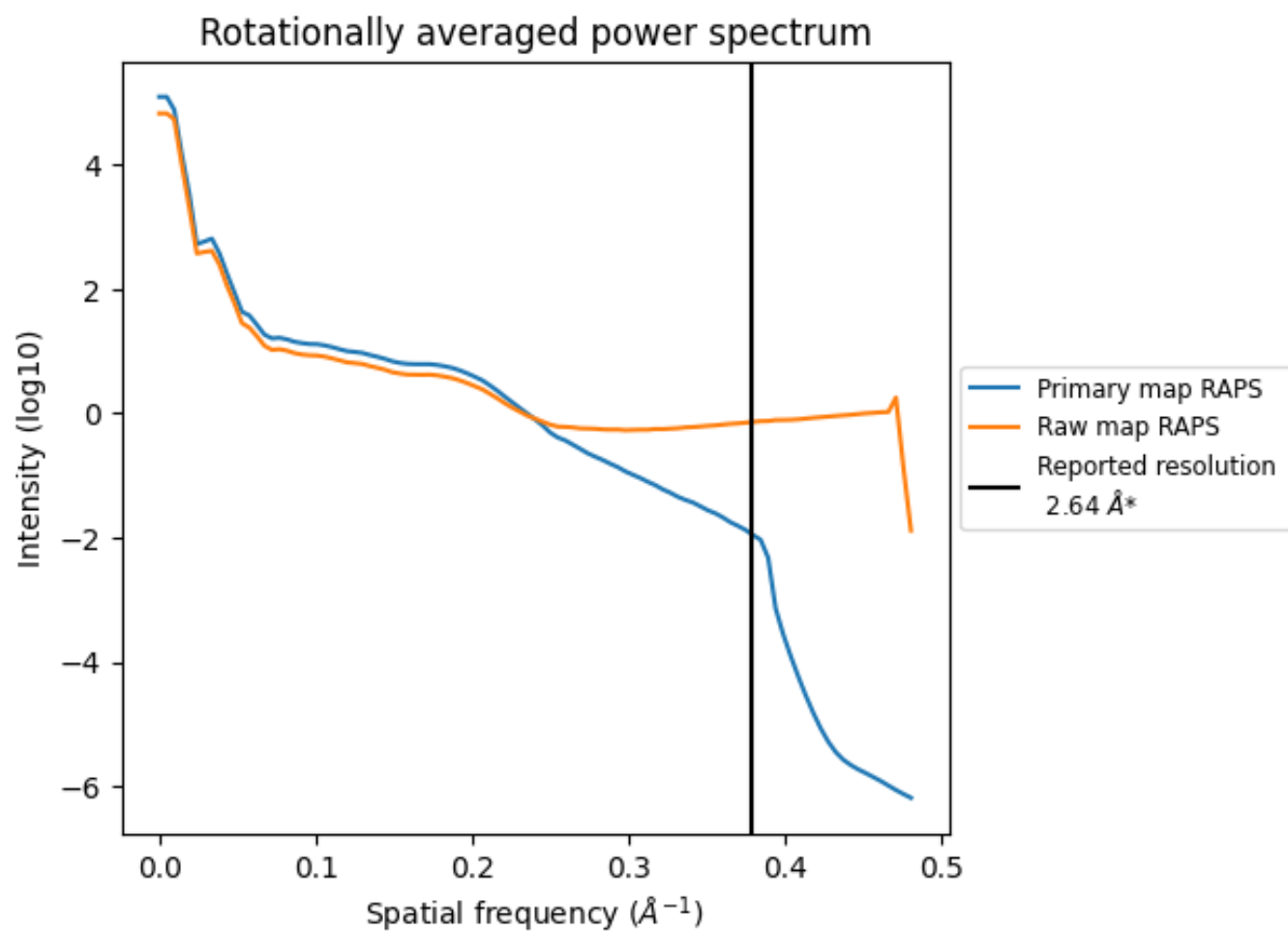
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 95 nm³; this corresponds to an approximate mass of 86 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 ⓘ

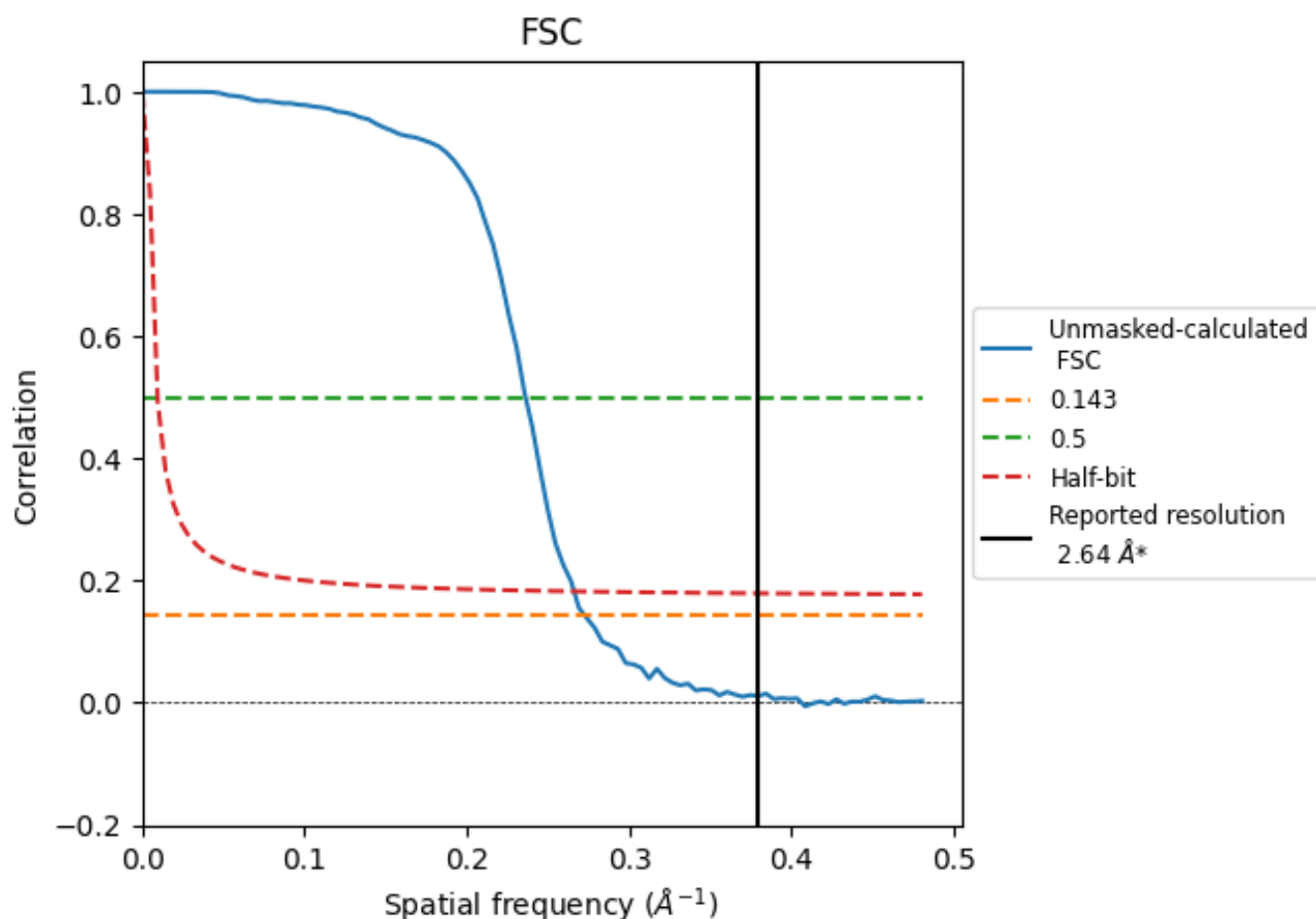


*Reported resolution corresponds to spatial frequency of $0.379 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.379 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

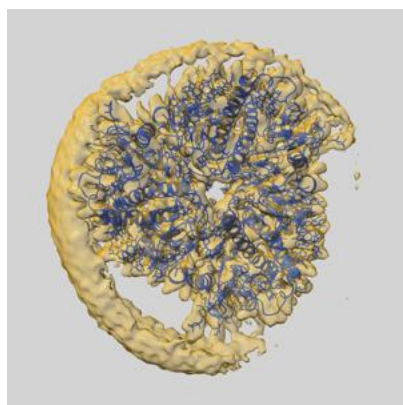
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.64	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.67	4.23	3.76

*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 3.67 differs from the reported value 2.64 by more than 10 %

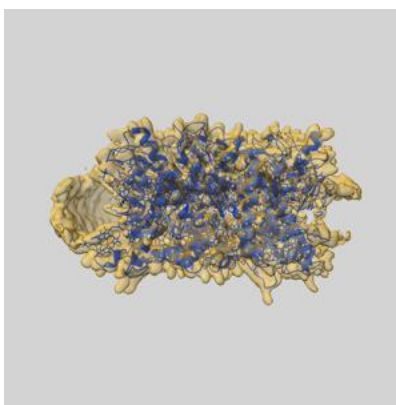
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-35785 and PDB model 8IX0. Per-residue inclusion information can be found in section 3 on page 10.

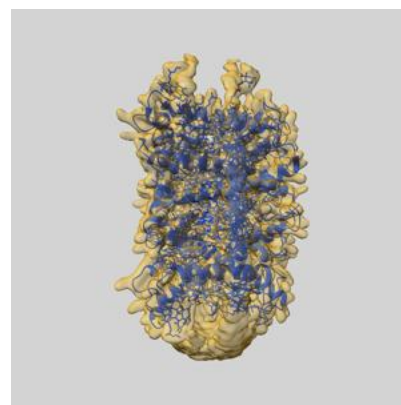
9.1 Map-model overlay [i](#)



X



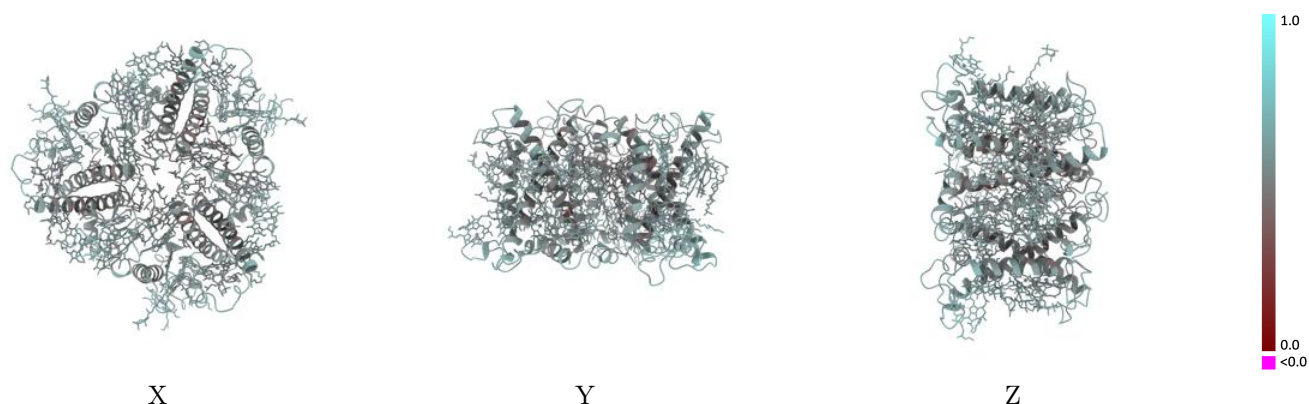
Y



Z

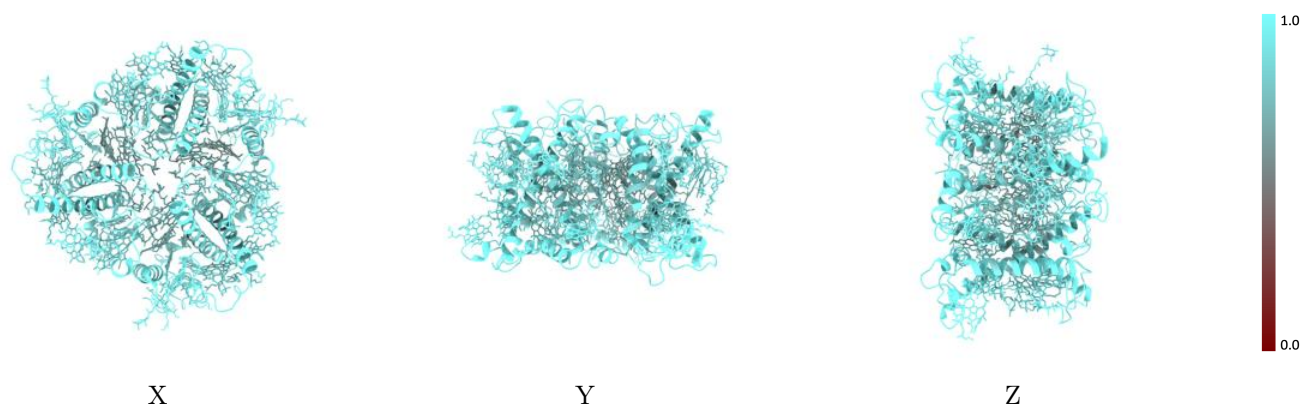
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



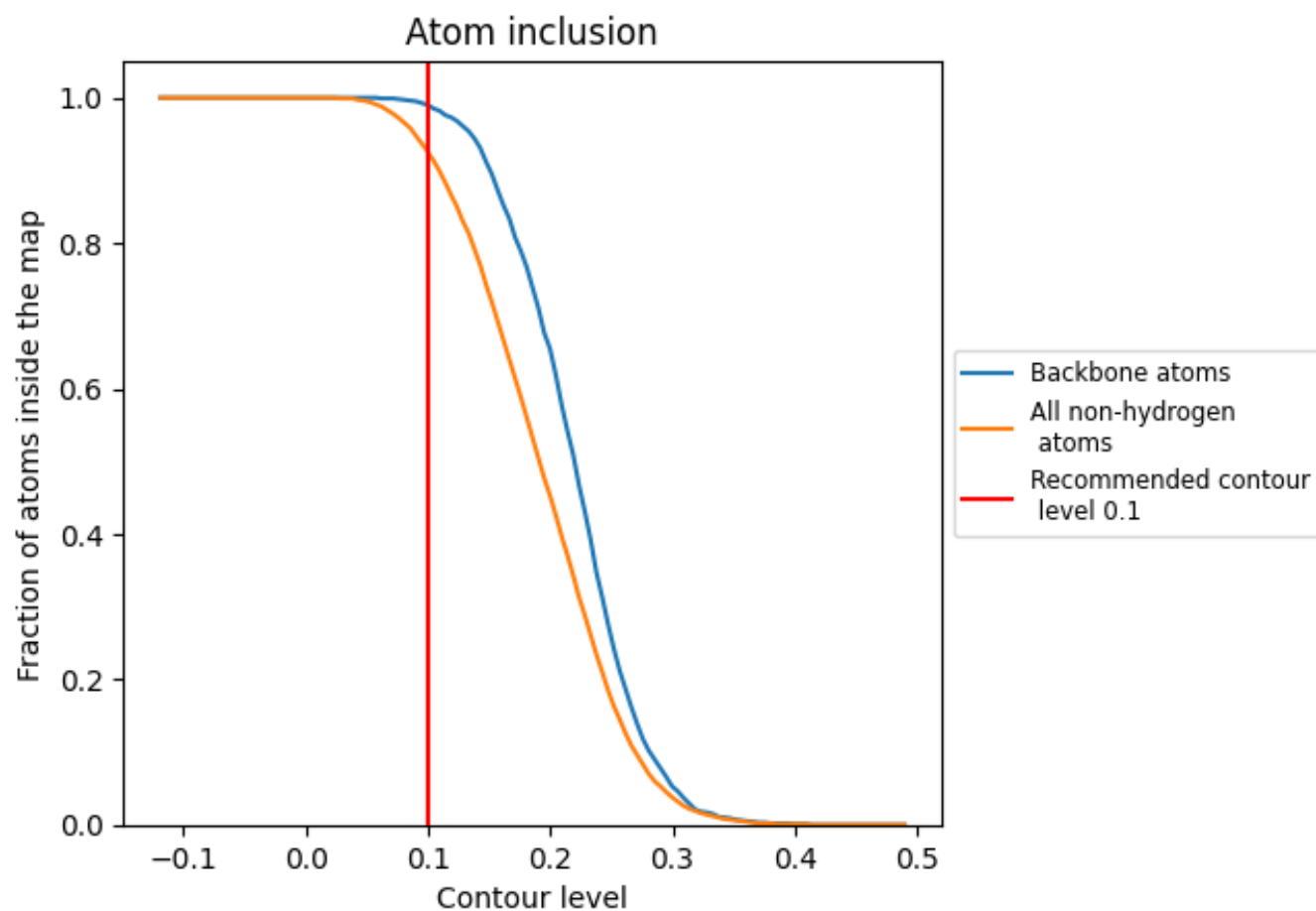
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 93% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9260	0.5410
G	0.9140	0.5440
N	0.9270	0.5380
Y	0.9360	0.5410

