



Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 09:08 PM UTC

PDB ID : 8IWZ / pdb_00008iwz
EMDB ID : EMD-35784
Title : Cryo-EM structure of unprotonated LHCII in detergent solution at low pH value
Authors : Ruan, M.X.; Ding, W.
Deposited on : 2023-03-31
Resolution : 2.52 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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

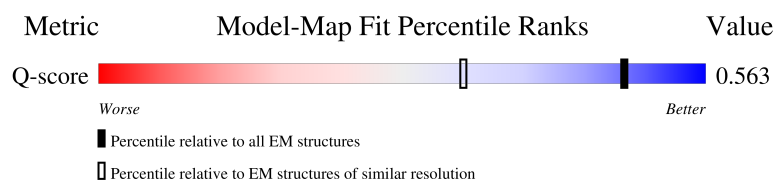
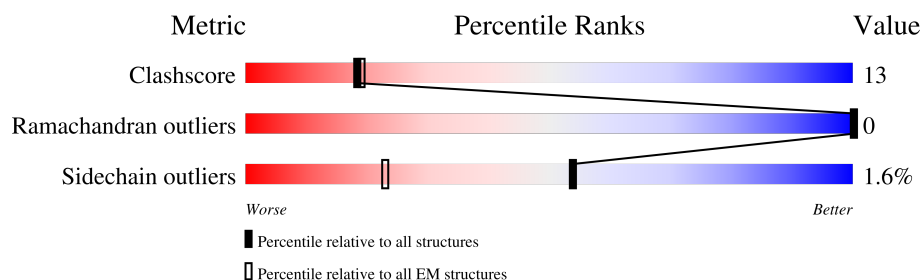
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.52 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	7226 (2.02 - 3.02)

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	
1	N	218	
1	Y	218	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CHL	G	601	X	-	-	-
2	CHL	G	605	X	-	-	-
2	CHL	G	606	X	-	-	-
2	CHL	G	607	X	-	-	-
2	CHL	G	608	X	-	-	-
2	CHL	G	609	X	-	-	-
2	CHL	N	601	X	-	-	-
2	CHL	N	605	X	-	-	-
2	CHL	N	606	X	-	-	-
2	CHL	N	607	X	-	-	-
2	CHL	N	608	X	-	-	-
2	CHL	N	609	X	-	-	-
2	CHL	Y	302	X	-	-	-
2	CHL	Y	306	X	-	-	-
2	CHL	Y	307	X	-	-	-
2	CHL	Y	308	X	-	-	-
2	CHL	Y	309	X	-	-	-
2	CHL	Y	310	X	-	-	-
3	CLA	G	602	X	-	-	-
3	CLA	G	603	X	-	-	-
3	CLA	G	610	X	-	-	-
3	CLA	G	612	X	-	-	-
3	CLA	G	614	X	-	-	-
3	CLA	N	602	X	-	-	-
3	CLA	N	603	X	-	-	-
3	CLA	N	604	X	-	-	-
3	CLA	N	610	X	-	-	-
3	CLA	N	611	X	-	-	-
3	CLA	N	612	X	-	-	-
3	CLA	N	613	X	-	-	-
3	CLA	N	614	X	-	-	-
3	CLA	Y	303	X	-	-	-
3	CLA	Y	304	X	-	-	-
3	CLA	Y	305	X	-	-	-
3	CLA	Y	311	X	-	-	-
3	CLA	Y	313	X	-	-	-
3	CLA	Y	314	X	-	-	-
3	CLA	Y	315	X	-	-	-

2 Entry composition [i](#)

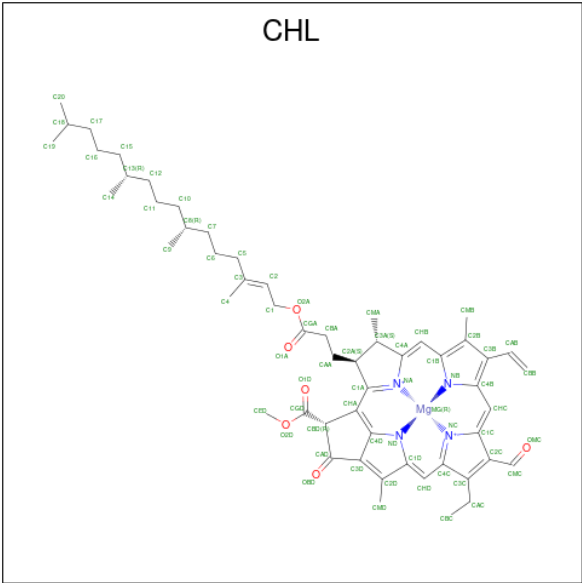
There are 7 unique types of molecules in this entry. The entry contains 8238 atoms, of which 0 are hydrogens and 0 are deuteriums.

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).



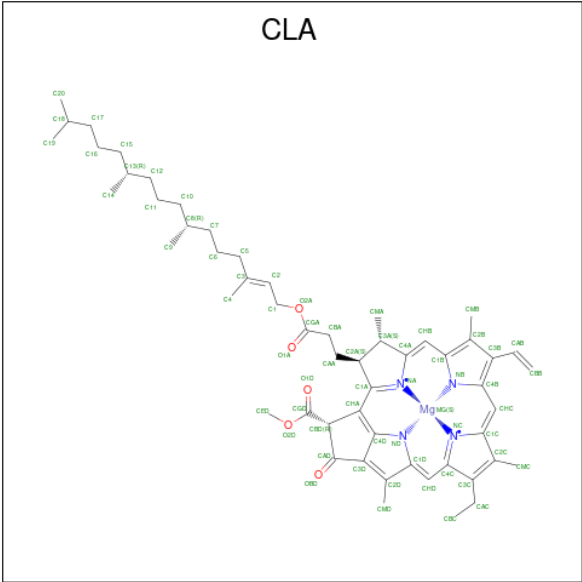
Mol	Chain	Residues	Atoms					AltConf
2	N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
2	N	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
2	N	1	Total	C	Mg	N	O	0
			51	40	1	4	6	

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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	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	
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).



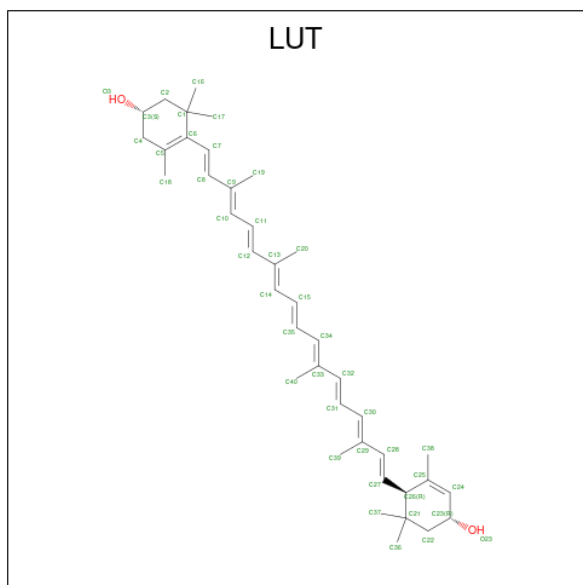
Mol	Chain	Residues	Atoms					AltConf
3	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	N	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
3	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	N	1	Total	C	Mg	N	O	0
			65	55	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).



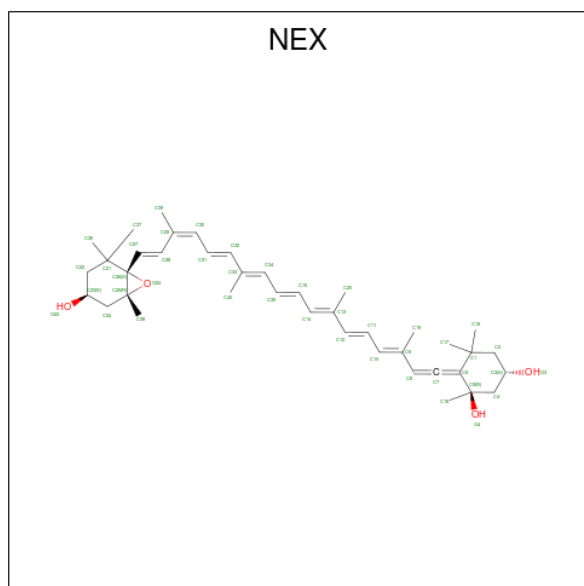
Mol	Chain	Residues	Atoms			AltConf
4	N	1	Total	C	O	0
			42	40	2	

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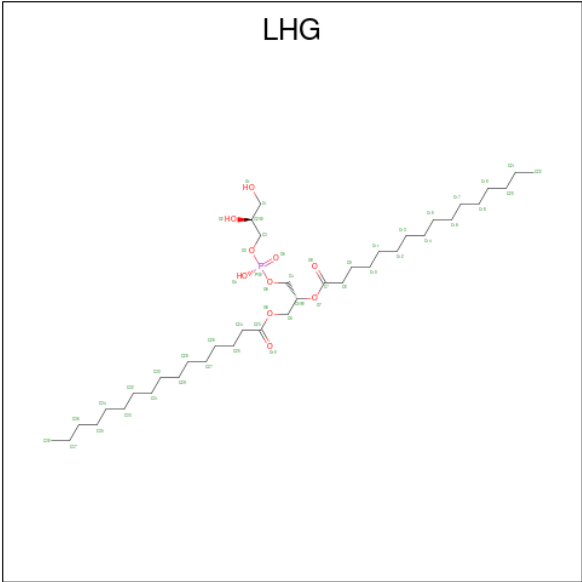
Mol	Chain	Residues	Atoms			AltConf
4	N	1	Total	C	O	0
			42	40	2	
4	G	1	Total	C	O	0
			42	40	2	
4	G	1	Total	C	O	0
			42	40	2	
4	Y	1	Total	C	O	0
			42	40	2	
4	Y	1	Total	C	O	0
			42	40	2	

- 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: $C_{40}H_{56}O_4$) (labeled as "Ligand of Interest" by depositor).



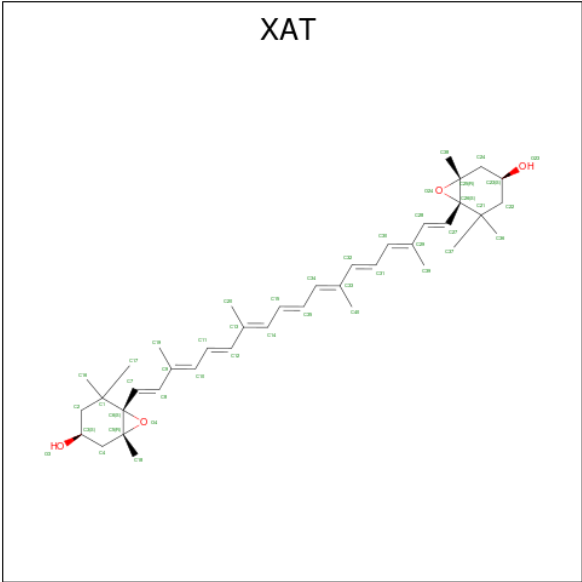
Mol	Chain	Residues	Atoms			AltConf
5	N	1	Total	C	O	0
			44	40	4	
5	G	1	Total	C	O	0
			44	40	4	
5	Y	1	Total	C	O	0
			44	40	4	

- Molecule 6 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



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 [i](#)

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

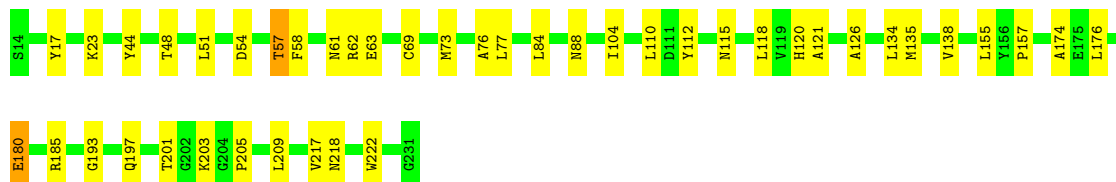
- Molecule 1: Chlorophyll a-b binding protein, chloroplastic

Chain N:  86% 14%



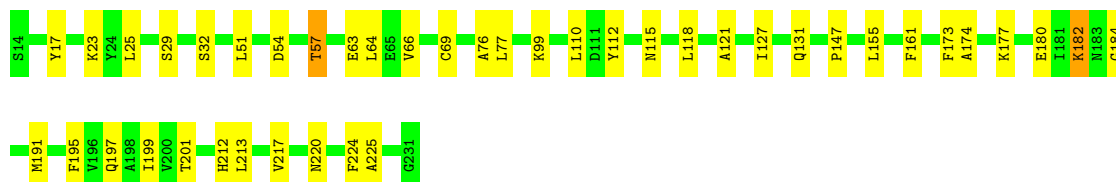
- Molecule 1: Chlorophyll a-b binding protein, chloroplastic

Chain G:  80% 19% .



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

Chain Y:  81% 18% .



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	879190	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	0.506	Depositor
Minimum map value	-0.199	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	273.92, 273.92, 273.92	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	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: XAT, NEX, CLA, LUT, CHL, LHG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	G	0.37	0/1713	0.64	1/2333 (0.0%)
1	N	0.39	0/1713	0.63	0/2333
1	Y	0.32	0/1713	0.60	0/2333
All	All	0.36	0/5139	0.62	1/6999 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	180	GLU	CB-CA-C	-5.69	102.19	110.96

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	1590	43	0
1	N	1661	0	1591	29	0
1	Y	1661	0	1592	36	0
2	G	363	0	350	26	0
2	N	363	0	350	21	0
2	Y	363	0	350	20	0
3	G	501	0	534	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	N	501	0	534	18	0
3	Y	501	0	534	23	0
4	G	84	0	112	11	0
4	N	84	0	112	5	0
4	Y	84	0	112	9	0
5	G	44	0	56	4	0
5	N	44	0	56	3	0
5	Y	44	0	56	2	0
6	G	49	0	74	6	0
6	N	49	0	74	7	0
6	Y	49	0	74	5	0
7	G	44	0	56	6	0
7	N	44	0	56	5	0
7	Y	44	0	56	7	0
All	All	8238	0	8319	216	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 13.

All (216) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:54:ASP:HB3	1:G:57:THR:CG2	1.66	1.23
1:Y:54:ASP:HB3	1:Y:57:THR:CG2	1.75	1.14
1:Y:54:ASP:HB3	1:Y:57:THR:HG22	1.30	1.12
1:G:54:ASP:HB3	1:G:57:THR:HG22	1.30	1.05
1:G:54:ASP:CB	1:G:57:THR:CG2	2.45	0.93
1:Y:54:ASP:O	1:Y:57:THR:HG23	1.73	0.88
1:G:54:ASP:O	1:G:57:THR:HG23	1.74	0.86
3:N:602:CLA:HAB	4:N:616:LUT:H32	1.62	0.82
1:N:46:TRP:HZ3	3:N:602:CLA:HBC2	1.46	0.80
1:Y:54:ASP:CB	1:Y:57:THR:CG2	2.63	0.75
2:G:601:CHL:HAC1	6:G:618:LHG:HC12	1.67	0.74
2:G:601:CHL:H8	7:G:619:XAT:H14	1.69	0.74
3:N:611:CLA:H152	3:N:612:CLA:HBB1	1.71	0.73
1:G:73:MET:HE2	4:G:615:LUT:H34	1.72	0.71
1:N:46:TRP:CZ3	3:N:602:CLA:HBC2	2.25	0.71
1:N:48:THR:HG21	2:G:609:CHL:HAA1	1.73	0.71
1:G:54:ASP:HB3	1:G:57:THR:HG23	1.71	0.70
1:N:191:MET:HG2	4:N:616:LUT:H12	1.75	0.68
3:N:603:CLA:HBB1	2:N:609:CHL:H13	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:601:CHL:HMC	7:N:619:XAT:H242	1.78	0.65
1:Y:110:LEU:HB3	1:Y:121:ALA:HB3	1.78	0.65
1:Y:191:MET:HG2	4:Y:317:LUT:H12	1.78	0.65
3:Y:311:CLA:H52	3:Y:311:CLA:HBB1	1.80	0.64
3:N:613:CLA:H93	6:N:618:LHG:H131	1.79	0.63
3:Y:305:CLA:HBA1	5:Y:318:NEX:H241	1.81	0.63
1:Y:182:LYS:HE3	6:Y:319:LHG:HC42	1.80	0.63
7:Y:301:XAT:H242	2:Y:302:CHL:HMC	1.80	0.62
1:G:135:MET:HE1	2:G:609:CHL:C2C	2.30	0.62
2:G:601:CHL:CHC	7:G:619:XAT:H383	2.31	0.61
1:G:185:ARG:HG2	6:G:618:LHG:H252	1.81	0.61
1:N:131:GLN:HG3	2:N:606:CHL:HMA3	1.81	0.61
6:G:618:LHG:H281	6:G:618:LHG:HC91	1.82	0.61
3:G:610:CLA:HBB1	4:G:615:LUT:H30	1.81	0.61
1:Y:213:LEU:HD23	3:Y:315:CLA:HBB1	1.81	0.60
2:N:609:CHL:HHC	2:Y:302:CHL:H52	1.83	0.60
1:N:173:PHE:CZ	1:N:177:LYS:HD3	2.37	0.60
2:G:601:CHL:HHD	6:G:618:LHG:HC41	1.84	0.59
1:N:63:GLU:HA	1:N:155:LEU:HD11	1.83	0.59
3:G:602:CLA:H52	4:G:616:LUT:H28	1.85	0.59
3:Y:303:CLA:HAB	4:Y:317:LUT:H32	1.85	0.58
1:Y:69:CYS:HB3	1:Y:184:GLY:HA3	1.86	0.58
2:N:601:CHL:H52	2:G:609:CHL:HHC	1.85	0.58
1:G:110:LEU:HB3	1:G:121:ALA:HB3	1.86	0.58
1:G:135:MET:HA	1:G:138:VAL:HG22	1.85	0.57
1:G:84:LEU:O	1:G:88:ASN:ND2	2.33	0.57
3:Y:314:CLA:H71	6:Y:319:LHG:H151	1.86	0.57
1:N:70:ARG:NH1	2:N:608:CHL:OBD	2.38	0.56
1:N:173:PHE:CE2	1:N:177:LYS:HD3	2.40	0.56
1:Y:201:THR:HG22	1:Y:224:PHE:HE2	1.70	0.56
6:Y:319:LHG:H281	6:Y:319:LHG:HC91	1.86	0.56
2:G:607:CHL:H18	2:G:609:CHL:H52	1.87	0.56
1:Y:197:GLN:O	1:Y:201:THR:OG1	2.21	0.55
1:Y:51:LEU:HD13	3:Y:303:CLA:H42	1.88	0.55
1:N:177:LYS:HA	1:N:180:GLU:HG2	1.89	0.55
1:Y:115:ASN:HB3	1:Y:118:LEU:HB2	1.88	0.55
1:G:54:ASP:CB	1:G:57:THR:HG21	2.33	0.54
1:G:73:MET:HE2	4:G:615:LUT:C34	2.38	0.54
1:G:201:THR:HG22	1:G:203:LYS:HG3	1.89	0.54
2:G:608:CHL:HHC	2:G:608:CHL:HBB1	1.90	0.54
2:N:609:CHL:HMC	2:Y:302:CHL:H72	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:69:CYS:O	1:G:73:MET:HG3	2.08	0.53
1:N:115:ASN:HD22	1:N:118:LEU:HD13	1.71	0.53
3:N:610:CLA:CBB	4:N:615:LUT:H32	2.39	0.53
1:N:42:GLY:HA3	1:N:181:ILE:HG21	1.91	0.53
1:N:174:ALA:HA	1:N:177:LYS:HE2	1.91	0.53
1:N:112:TYR:HD2	1:N:118:LEU:HD23	1.75	0.52
3:N:613:CLA:H141	3:N:614:CLA:H2	1.91	0.52
1:G:54:ASP:C	1:G:57:THR:HG23	2.33	0.52
1:Y:217:VAL:O	1:Y:220:ASN:ND2	2.43	0.52
3:Y:311:CLA:H61	4:Y:316:LUT:H371	1.91	0.52
3:G:610:CLA:H61	4:G:615:LUT:H371	1.91	0.51
1:G:126:ALA:HB3	2:G:605:CHL:HMC	1.93	0.51
1:N:63:GLU:HG2	2:N:609:CHL:HED2	1.92	0.51
3:G:610:CLA:H51	3:G:612:CLA:HMA1	1.93	0.50
1:G:209:LEU:HD11	3:G:614:CLA:HMC1	1.94	0.50
1:Y:112:TYR:HB3	1:Y:118:LEU:HB3	1.94	0.50
6:N:618:LHG:HC91	6:N:618:LHG:H282	1.92	0.50
2:N:601:CHL:HMA3	6:N:618:LHG:H121	1.94	0.50
1:Y:173:PHE:O	1:Y:177:LYS:HG3	2.11	0.49
3:G:610:CLA:CBB	4:G:615:LUT:H32	2.42	0.49
3:G:611:CLA:HBB1	7:G:619:XAT:H221	1.95	0.49
1:G:120:HIS:ND1	1:G:121:ALA:N	2.60	0.49
3:G:612:CLA:H2A	3:G:612:CLA:H12	1.95	0.49
3:Y:303:CLA:HAB	4:Y:317:LUT:H30	1.95	0.48
2:N:601:CHL:H202	6:N:618:LHG:H221	1.94	0.48
1:G:77:LEU:HD21	3:G:612:CLA:H18	1.94	0.48
3:N:611:CLA:HBD	3:N:612:CLA:OBD	2.13	0.48
1:G:61:ASN:HB3	3:G:602:CLA:HHB	1.94	0.48
1:N:115:ASN:HB3	1:N:118:LEU:HB2	1.96	0.48
1:Y:195:PHE:O	1:Y:199:ILE:HG13	2.14	0.48
3:Y:312:CLA:H152	3:Y:313:CLA:HBB1	1.96	0.48
1:G:193:GLY:O	1:G:197:GLN:HG3	2.13	0.48
2:G:608:CHL:H162	2:G:608:CHL:H121	1.62	0.48
1:Y:99:LYS:HA	2:Y:308:CHL:HED3	1.95	0.48
2:N:609:CHL:CHC	2:Y:302:CHL:H2	2.44	0.47
2:G:601:CHL:H202	2:G:601:CHL:H161	1.65	0.47
1:Y:63:GLU:HA	1:Y:155:LEU:HD11	1.95	0.47
1:N:51:LEU:HB2	3:N:602:CLA:O1A	2.14	0.47
1:G:135:MET:HE1	2:G:609:CHL:C1C	2.45	0.47
1:N:79:CYS:HG	1:N:97:TRP:CG	2.32	0.47
3:Y:303:CLA:H52	4:Y:317:LUT:H28	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Y:319:LHG:HC62	6:Y:319:LHG:H262	1.97	0.47
1:Y:161:PHE:HD1	2:Y:309:CHL:H61	1.78	0.47
2:N:609:CHL:H93	2:N:609:CHL:H112	1.81	0.47
2:G:608:CHL:H171	2:G:608:CHL:HAA2	1.97	0.46
1:N:185:ARG:HG2	6:N:618:LHG:H252	1.98	0.46
1:G:76:ALA:HB1	4:G:615:LUT:H12	1.98	0.46
2:N:609:CHL:H202	2:N:609:CHL:H161	1.66	0.46
1:G:44:TYR:CE2	2:G:601:CHL:HMD1	2.50	0.46
2:N:601:CHL:H2	2:G:609:CHL:CHC	2.46	0.46
1:G:205:PRO:HB2	4:G:615:LUT:H173	1.98	0.46
4:G:616:LUT:H15	4:G:616:LUT:H201	1.81	0.46
1:G:63:GLU:HA	1:G:155:LEU:HD11	1.98	0.46
1:Y:76:ALA:HB1	4:Y:316:LUT:H12	1.98	0.46
1:G:48:THR:HG21	2:Y:310:CHL:H2A	1.97	0.45
1:G:115:ASN:HB3	1:G:118:LEU:HB2	1.98	0.45
2:Y:302:CHL:H202	2:Y:302:CHL:H161	1.82	0.45
1:Y:225:ALA:O	7:Y:301:XAT:O3	2.32	0.45
1:Y:64:LEU:HD11	3:Y:304:CLA:HAA2	1.99	0.45
1:G:54:ASP:CB	1:G:57:THR:HG23	2.39	0.45
3:Y:311:CLA:H51	3:Y:313:CLA:HMA1	1.97	0.45
6:N:618:LHG:H202	7:N:619:XAT:H10	1.99	0.45
2:G:601:CHL:H62	6:G:618:LHG:H171	1.99	0.45
2:N:608:CHL:H152	5:N:617:NEX:H402	1.99	0.45
2:N:609:CHL:H62	2:N:609:CHL:H2	1.69	0.45
7:N:619:XAT:H15	7:N:619:XAT:H201	1.69	0.45
3:N:602:CLA:H92	3:N:603:CLA:HMA1	1.99	0.44
3:G:613:CLA:H61	3:G:613:CLA:H2	1.68	0.44
1:N:51:LEU:HB2	3:N:602:CLA:H11	1.99	0.44
1:G:51:LEU:HD13	3:G:602:CLA:H42	2.00	0.44
3:N:603:CLA:H72	3:N:603:CLA:H112	1.79	0.44
1:G:44:TYR:CD2	2:G:601:CHL:HMD1	2.53	0.44
1:G:176:LEU:O	1:G:180:GLU:HG2	2.18	0.44
2:N:609:CHL:HMB2	2:Y:302:CHL:H3A	2.00	0.44
1:Y:25:LEU:HB2	1:Y:29:SER:HA	2.00	0.44
1:Y:213:LEU:CD2	3:Y:315:CLA:CBB	2.96	0.44
2:N:601:CHL:HBA1	2:N:601:CHL:H3A	1.63	0.43
3:N:611:CLA:H112	3:N:611:CLA:H91	1.65	0.43
5:N:617:NEX:H11	5:N:617:NEX:H191	1.82	0.43
2:G:601:CHL:HHC	7:G:619:XAT:H383	2.00	0.43
5:G:617:NEX:H11	5:G:617:NEX:H191	1.81	0.43
6:G:618:LHG:H212	3:Y:304:CLA:H201	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:304:CLA:H2	3:Y:304:CLA:H61	1.76	0.43
1:G:58:PHE:O	1:G:62:ARG:HG3	2.18	0.43
7:Y:301:XAT:H35	7:Y:301:XAT:H401	1.81	0.43
1:N:174:ALA:O	1:N:178:VAL:HG23	2.18	0.43
1:N:217:VAL:O	1:N:220:ASN:ND2	2.51	0.43
2:G:601:CHL:H2	2:Y:310:CHL:C3B	2.48	0.43
3:G:611:CLA:H143	3:G:611:CLA:H111	1.81	0.43
4:G:615:LUT:H11	4:G:615:LUT:H191	1.91	0.43
2:Y:308:CHL:HBB2	2:Y:310:CHL:HBC1	2.01	0.43
4:N:616:LUT:H201	4:N:616:LUT:H15	1.82	0.43
5:N:617:NEX:H35	5:N:617:NEX:H401	1.81	0.43
2:G:607:CHL:H143	2:G:607:CHL:H111	1.81	0.43
1:Y:66:VAL:HG21	1:Y:155:LEU:HD13	2.01	0.43
1:Y:147:PRO:HB3	5:Y:318:NEX:H183	2.01	0.43
1:N:56:GLU:O	1:N:60:LYS:HG2	2.19	0.43
1:Y:17:TYR:CE2	1:Y:174:ALA:HB1	2.54	0.43
1:Y:213:LEU:HD23	3:Y:315:CLA:CBB	2.47	0.43
1:G:180:GLU:OE1	3:G:610:CLA:C2B	2.67	0.43
2:Y:309:CHL:H171	2:Y:309:CHL:HAA2	2.00	0.43
3:Y:312:CLA:H143	3:Y:312:CLA:H111	1.84	0.43
4:Y:317:LUT:H15	4:Y:317:LUT:H201	1.86	0.43
6:N:618:LHG:H282	6:N:618:LHG:H312	1.78	0.42
5:G:617:NEX:H15	5:G:617:NEX:H201	1.78	0.42
1:N:157:PRO:HB3	2:N:608:CHL:HBC2	2.01	0.42
7:Y:301:XAT:H201	7:Y:301:XAT:H15	1.75	0.42
4:N:615:LUT:H15	4:N:615:LUT:H201	1.90	0.42
7:N:619:XAT:H35	7:N:619:XAT:H401	1.78	0.42
3:G:602:CLA:CBB	4:G:616:LUT:H32	2.50	0.42
1:N:17:TYR:CE2	1:N:174:ALA:HB1	2.55	0.42
2:Y:308:CHL:H93	2:Y:308:CHL:H61	1.79	0.42
1:N:46:TRP:HE3	3:N:602:CLA:HMD1	1.85	0.42
2:G:608:CHL:H152	5:G:617:NEX:H402	2.00	0.42
3:Y:314:CLA:H151	3:Y:315:CLA:HBA2	2.02	0.42
7:N:619:XAT:H11	7:N:619:XAT:H191	1.92	0.42
1:G:134:LEU:HD21	2:G:606:CHL:H42	2.01	0.42
7:Y:301:XAT:H11	7:Y:301:XAT:H191	1.91	0.42
1:N:85:LEU:HD23	1:N:85:LEU:HA	1.93	0.41
3:Y:304:CLA:H102	2:Y:310:CHL:H143	2.01	0.41
3:Y:311:CLA:CBB	4:Y:316:LUT:H32	2.50	0.41
1:N:112:TYR:HB3	1:N:118:LEU:HB3	2.01	0.41
2:N:608:CHL:HHB	2:N:608:CHL:H13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Y:316:LUT:H31	4:Y:316:LUT:H391	1.93	0.41
1:N:64:LEU:HD11	3:N:603:CLA:HAA2	2.03	0.41
1:Y:77:LEU:HD21	3:Y:313:CLA:H202	2.02	0.41
2:Y:308:CHL:H12	2:Y:308:CHL:HMA2	2.01	0.41
3:G:602:CLA:H93	3:G:602:CLA:H111	1.84	0.41
3:G:602:CLA:H161	3:G:602:CLA:H141	1.85	0.41
1:G:112:TYR:HB3	1:G:118:LEU:HB3	2.02	0.41
1:G:217:VAL:HG23	1:G:218:ASN:OD1	2.21	0.41
2:G:601:CHL:H141	2:G:601:CHL:H162	1.77	0.41
7:G:619:XAT:H35	7:G:619:XAT:H401	1.87	0.41
1:Y:54:ASP:HB3	1:Y:57:THR:HG21	1.83	0.41
1:Y:182:LYS:NZ	3:Y:312:CLA:O1D	2.43	0.41
3:G:613:CLA:H8	3:G:614:CLA:HMD3	2.03	0.41
7:Y:301:XAT:H14	2:Y:302:CHL:H8	2.03	0.41
2:Y:308:CHL:H18	2:Y:310:CHL:H52	2.03	0.41
2:Y:308:CHL:H111	2:Y:308:CHL:H143	1.82	0.41
1:G:180:GLU:OE1	3:G:610:CLA:C1B	2.69	0.41
1:G:157:PRO:HB3	2:G:608:CHL:HBC2	2.03	0.40
1:G:222:TRP:CZ2	3:G:614:CLA:HED2	2.55	0.40
2:G:607:CHL:H93	2:G:607:CHL:H61	1.82	0.40
1:Y:23:LYS:HE2	1:Y:32:SER:HB3	2.04	0.40
7:Y:301:XAT:H12	2:Y:302:CHL:H111	2.03	0.40
3:N:613:CLA:H61	3:N:613:CLA:H2	1.58	0.40
5:G:617:NEX:H35	5:G:617:NEX:H401	1.85	0.40
2:N:607:CHL:H143	2:N:607:CHL:H111	1.80	0.40
3:N:611:CLA:H62	3:N:611:CLA:H101	1.47	0.40
1:G:104:ILE:HD12	1:G:104:ILE:HA	1.87	0.40
1:Y:127:ILE:O	1:Y:131:GLN:HG2	2.22	0.40
2:Y:302:CHL:H202	6:Y:319:LHG:H221	2.03	0.40
1:G:17:TYR:CE2	1:G:174:ALA:HB1	2.57	0.40
7:G:619:XAT:H31	7:G:619:XAT:H391	1.82	0.40
1:Y:17:TYR:HE2	1:Y:174:ALA:HB1	1.86	0.40
1:Y:212:HIS:ND1	3:Y:314:CLA:HAA2	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	216/218 (99%)	210 (97%)	6 (3%)	0	100	100
1	N	216/218 (99%)	206 (95%)	10 (5%)	0	100	100
1	Y	216/218 (99%)	208 (96%)	8 (4%)	0	100	100
All	All	648/654 (99%)	624 (96%)	24 (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%)	166 (99%)	2 (1%)	63	82
1	N	168/168 (100%)	165 (98%)	3 (2%)	51	75
1	Y	168/168 (100%)	165 (98%)	3 (2%)	51	75
All	All	504/504 (100%)	496 (98%)	8 (2%)	54	78

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	131	GLN
1	N	135	MET
1	N	182	LYS
1	G	23	LYS
1	G	57	THR

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Mol	Chain	Res	Type
1	Y	57	THR
1	Y	180	GLU
1	Y	182	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	N	61	ASN
1	N	115	ASN
1	G	61	ASN
1	Y	122	GLN

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	$\# Z > 2$
4	LUT	Y	317	-	42,43,43	0.76	0	51,60,60	1.58	11 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	CHL	Y	306	1	42,56,74	2.70	9 (21%)	36,92,114	1.66	13 (36%)
2	CHL	G	607	-	60,74,74	2.21	9 (15%)	58,114,114	1.51	11 (18%)
2	CHL	N	607	-	60,74,74	2.25	9 (15%)	58,114,114	1.53	11 (18%)
3	CLA	N	614	-	53,57,73	1.34	5 (9%)	61,93,113	1.14	5 (8%)
3	CLA	G	614	-	53,57,73	1.33	6 (11%)	61,93,113	1.18	6 (9%)
2	CHL	Y	307	1	45,59,74	2.60	8 (17%)	40,96,114	2.02	15 (37%)
3	CLA	Y	312	6	69,73,73	1.18	9 (13%)	82,113,113	1.27	4 (4%)
4	LUT	Y	316	-	42,43,43	0.79	0	51,60,60	1.54	11 (21%)
5	NEX	Y	318	-	40,46,46	1.21	6 (15%)	50,70,70	1.49	10 (20%)
3	CLA	Y	311	1	69,73,73	1.20	6 (8%)	82,113,113	1.20	8 (9%)
3	CLA	N	602	1	69,73,73	1.16	5 (7%)	82,113,113	1.17	6 (7%)
7	XAT	Y	301	-	41,47,47	0.91	2 (4%)	54,74,74	2.50	19 (35%)
2	CHL	N	609	1	60,74,74	2.22	11 (18%)	58,114,114	1.52	12 (20%)
3	CLA	N	611	6	69,73,73	1.12	8 (11%)	82,113,113	1.20	6 (7%)
2	CHL	Y	302	1	60,74,74	2.25	10 (16%)	58,114,114	1.54	13 (22%)
3	CLA	G	603	-	69,73,73	1.21	7 (10%)	82,113,113	1.20	4 (4%)
3	CLA	Y	314	1	69,73,73	1.16	7 (10%)	82,113,113	1.15	5 (6%)
7	XAT	N	619	-	41,47,47	0.91	2 (4%)	54,74,74	2.55	21 (38%)
3	CLA	N	603	-	69,73,73	1.20	7 (10%)	82,113,113	1.19	4 (4%)
4	LUT	N	616	-	42,43,43	0.76	0	51,60,60	1.60	12 (23%)
4	LUT	G	615	-	42,43,43	0.75	0	51,60,60	1.63	14 (27%)
7	XAT	G	619	-	41,47,47	0.90	2 (4%)	54,74,74	2.49	20 (37%)
2	CHL	N	605	1	42,56,74	2.68	9 (21%)	36,92,114	1.76	13 (36%)
2	CHL	N	601	1	60,74,74	2.27	9 (15%)	58,114,114	1.59	12 (20%)
2	CHL	N	606	-	45,59,74	2.52	11 (24%)	40,96,114	1.97	14 (35%)
5	NEX	G	617	-	40,46,46	1.09	3 (7%)	50,70,70	2.25	15 (30%)
3	CLA	G	612	-	69,73,73	1.15	7 (10%)	82,113,113	1.21	7 (8%)
3	CLA	N	613	1	69,73,73	1.16	5 (7%)	82,113,113	1.22	6 (7%)
3	CLA	Y	315	-	53,57,73	1.35	7 (13%)	61,93,113	1.15	5 (8%)
3	CLA	Y	305	-	66,70,73	1.17	8 (12%)	78,109,113	1.30	8 (10%)
3	CLA	N	612	-	69,73,73	1.20	8 (11%)	82,113,113	1.20	7 (8%)
2	CHL	G	605	1	42,56,74	2.71	9 (21%)	36,92,114	1.62	11 (30%)
3	CLA	Y	303	1	69,73,73	1.17	6 (8%)	82,113,113	1.12	4 (4%)
3	CLA	N	604	-	66,70,73	1.19	7 (10%)	78,109,113	1.22	6 (7%)
3	CLA	Y	313	-	69,73,73	1.18	6 (8%)	82,113,113	1.25	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	CHL	G	609	1	60,74,74	2.27	10 (16%)	58,114,114	1.74	14 (24%)
5	NEX	N	617	-	40,46,46	1.09	3 (7%)	50,70,70	2.28	16 (32%)
2	CHL	Y	310	1	60,74,74	2.31	10 (16%)	58,114,114	1.47	11 (18%)
6	LHG	N	618	3	48,48,48	0.92	2 (4%)	51,54,54	0.95	2 (3%)
2	CHL	Y	308	-	60,74,74	2.24	9 (15%)	58,114,114	1.54	12 (20%)
3	CLA	G	602	-	69,73,73	1.19	8 (11%)	82,113,113	1.16	6 (7%)
3	CLA	G	611	6	69,73,73	1.16	6 (8%)	82,113,113	1.23	8 (9%)
2	CHL	Y	309	-	60,74,74	2.29	9 (15%)	58,114,114	1.42	13 (22%)
2	CHL	G	608	-	60,74,74	2.30	10 (16%)	58,114,114	1.46	10 (17%)
3	CLA	G	604	-	66,70,73	1.19	7 (10%)	78,109,113	1.23	6 (7%)
3	CLA	N	610	1	69,73,73	1.19	7 (10%)	82,113,113	1.16	6 (7%)
2	CHL	N	608	-	60,74,74	2.29	8 (13%)	58,114,114	1.41	12 (20%)
2	CHL	G	601	-	60,74,74	2.26	11 (18%)	58,114,114	1.55	11 (18%)
3	CLA	G	610	-	69,73,73	1.17	8 (11%)	82,113,113	1.20	10 (12%)
6	LHG	G	618	3	48,48,48	0.92	2 (4%)	51,54,54	1.09	3 (5%)
4	LUT	G	616	-	42,43,43	0.72	0	51,60,60	1.51	9 (17%)
4	LUT	N	615	-	42,43,43	0.71	0	51,60,60	1.63	10 (19%)
2	CHL	G	606	-	45,59,74	2.59	10 (22%)	40,96,114	2.00	13 (32%)
3	CLA	G	613	1	69,73,73	1.15	6 (8%)	82,113,113	1.24	4 (4%)
6	LHG	Y	319	3	48,48,48	0.93	2 (4%)	51,54,54	1.07	4 (7%)
3	CLA	Y	304	-	69,73,73	1.18	7 (10%)	82,113,113	1.32	5 (6%)

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
4	LUT	Y	317	-	-	3/29/67/67	0/2/2/2
2	CHL	Y	306	1	3/3/16/26	7/18/116/137	-
2	CHL	G	607	-	3/3/20/26	15/39/137/137	-
2	CHL	N	607	-	3/3/20/26	16/39/137/137	-
3	CLA	N	614	-	1/1/11/20	10/20/96/115	-
3	CLA	G	614	-	1/1/11/20	9/20/96/115	-
2	CHL	Y	307	1	3/3/17/26	6/21/119/137	-
3	CLA	Y	312	6	-	11/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	LUT	Y	316	-	-	4/29/67/67	0/2/2/2
5	NEX	Y	318	-	-	13/27/83/83	0/3/3/3
3	CLA	Y	311	1	1/1/15/20	5/39/115/115	-
3	CLA	N	602	1	1/1/15/20	8/39/115/115	-
7	XAT	Y	301	-	-	6/31/93/93	0/4/4/4
2	CHL	N	609	1	3/3/20/26	17/39/137/137	-
3	CLA	N	611	6	1/1/15/20	15/39/115/115	-
2	CHL	Y	302	1	3/3/20/26	8/39/137/137	-
3	CLA	G	603	-	1/1/15/20	16/39/115/115	-
3	CLA	Y	314	1	1/1/15/20	8/39/115/115	-
7	XAT	N	619	-	-	7/31/93/93	0/4/4/4
3	CLA	N	603	-	1/1/15/20	16/39/115/115	-
4	LUT	N	616	-	-	1/29/67/67	0/2/2/2
4	LUT	G	615	-	-	4/29/67/67	0/2/2/2
7	XAT	G	619	-	-	7/31/93/93	0/4/4/4
2	CHL	N	605	1	3/3/16/26	6/18/116/137	-
2	CHL	N	601	1	3/3/20/26	7/39/137/137	-
2	CHL	N	606	-	3/3/17/26	6/21/119/137	-
5	NEX	G	617	-	-	6/27/83/83	0/3/3/3
3	CLA	G	612	-	1/1/15/20	13/39/115/115	-
3	CLA	N	613	1	1/1/15/20	12/39/115/115	-
3	CLA	Y	315	-	1/1/11/20	9/20/96/115	-
3	CLA	Y	305	-	1/1/14/20	10/36/112/115	-
3	CLA	N	612	-	1/1/15/20	16/39/115/115	-
2	CHL	G	605	1	3/3/16/26	7/18/116/137	-
3	CLA	Y	303	1	1/1/15/20	9/39/115/115	-
3	CLA	N	604	-	1/1/14/20	10/36/112/115	-
3	CLA	Y	313	-	1/1/15/20	18/39/115/115	-
2	CHL	G	609	1	3/3/20/26	17/39/137/137	-
5	NEX	N	617	-	-	6/27/83/83	0/3/3/3
2	CHL	Y	310	1	3/3/20/26	12/39/137/137	-
6	LHG	N	618	3	-	25/53/53/53	-
2	CHL	Y	308	-	3/3/20/26	15/39/137/137	-
3	CLA	G	602	-	1/1/15/20	14/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CLA	G	611	6	-	13/39/115/115	-
2	CHL	Y	309	-	3/3/20/26	14/39/137/137	-
2	CHL	G	608	-	3/3/20/26	11/39/137/137	-
3	CLA	G	604	-	-	16/36/112/115	-
3	CLA	N	610	1	1/1/15/20	5/39/115/115	-
2	CHL	N	608	-	3/3/20/26	12/39/137/137	-
2	CHL	G	601	-	3/3/20/26	11/39/137/137	-
3	CLA	G	610	-	1/1/15/20	4/39/115/115	-
6	LHG	G	618	3	-	28/53/53/53	-
4	LUT	G	616	-	-	3/29/67/67	0/2/2/2
4	LUT	N	615	-	-	5/29/67/67	0/2/2/2
2	CHL	G	606	-	3/3/17/26	4/21/119/137	-
3	CLA	G	613	1	-	11/39/115/115	-
6	LHG	Y	319	3	-	29/53/53/53	-
3	CLA	Y	304	-	1/1/15/20	17/39/115/115	-

All (358) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Y	310	CHL	C3B-C4B	10.00	1.51	1.41
2	N	608	CHL	C3B-C4B	9.66	1.50	1.41
2	Y	309	CHL	C3B-C4B	9.61	1.50	1.41
2	G	609	CHL	C3B-C4B	9.35	1.50	1.41
2	G	608	CHL	C3B-C4B	9.32	1.50	1.41
2	Y	306	CHL	C1B-C2B	8.97	1.49	1.39
2	N	601	CHL	C3B-C4B	8.94	1.50	1.41
2	Y	307	CHL	C1B-C2B	8.87	1.49	1.39
2	G	605	CHL	C1B-C2B	8.86	1.49	1.39
2	G	608	CHL	C1B-C2B	8.74	1.49	1.39
2	G	607	CHL	C1B-C2B	8.66	1.49	1.39
2	G	605	CHL	C3B-C4B	8.66	1.49	1.41
2	N	606	CHL	C1B-C2B	8.65	1.49	1.39
2	N	605	CHL	C3B-C4B	8.64	1.49	1.41
2	N	605	CHL	C1B-C2B	8.64	1.49	1.39
2	Y	302	CHL	C3B-C4B	8.64	1.49	1.41
2	G	606	CHL	C1B-C2B	8.61	1.49	1.39
2	N	607	CHL	C3B-C4B	8.57	1.49	1.41
2	Y	308	CHL	C3B-C4B	8.56	1.49	1.41
2	Y	306	CHL	C3B-C4B	8.55	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Y	302	CHL	C1B-C2B	8.54	1.49	1.39
2	Y	307	CHL	C3B-C4B	8.54	1.49	1.41
2	N	607	CHL	C1B-C2B	8.45	1.49	1.39
2	G	606	CHL	C3B-C4B	8.43	1.49	1.41
2	N	601	CHL	C1B-C2B	8.42	1.49	1.39
2	Y	309	CHL	C1B-C2B	8.41	1.49	1.39
2	G	601	CHL	C1B-C2B	8.40	1.49	1.39
2	N	608	CHL	C1B-C2B	8.40	1.49	1.39
2	N	609	CHL	C3B-C4B	8.35	1.49	1.41
2	Y	308	CHL	C1B-C2B	8.24	1.48	1.39
2	G	601	CHL	C3B-C4B	8.11	1.49	1.41
2	G	609	CHL	C1D-C2D	8.06	1.48	1.39
2	Y	310	CHL	C1D-C2D	8.05	1.48	1.39
2	G	607	CHL	C3B-C4B	8.03	1.49	1.41
2	N	601	CHL	C1D-C2D	7.98	1.48	1.39
2	Y	302	CHL	C1D-C2D	7.98	1.48	1.39
2	Y	310	CHL	C1B-C2B	7.90	1.48	1.39
2	G	608	CHL	C1D-C2D	7.89	1.48	1.39
2	N	609	CHL	C1B-C2B	7.82	1.48	1.39
2	G	605	CHL	C1D-C2D	7.74	1.48	1.39
2	Y	308	CHL	C1D-C2D	7.70	1.48	1.39
2	G	607	CHL	C1D-C2D	7.69	1.48	1.39
2	N	608	CHL	C1D-C2D	7.68	1.48	1.39
2	Y	309	CHL	C1D-C2D	7.67	1.48	1.39
2	N	609	CHL	C1D-C2D	7.64	1.48	1.39
2	Y	306	CHL	C1D-C2D	7.62	1.48	1.39
2	N	607	CHL	C1D-C2D	7.61	1.48	1.39
2	N	605	CHL	C1D-C2D	7.61	1.48	1.39
2	G	601	CHL	C1D-C2D	7.54	1.48	1.39
2	G	606	CHL	C1D-C2D	7.46	1.48	1.39
2	N	606	CHL	C3B-C4B	7.44	1.48	1.41
2	G	609	CHL	C1B-C2B	7.31	1.47	1.39
2	Y	307	CHL	C1D-C2D	7.30	1.47	1.39
2	N	606	CHL	C1D-C2D	7.21	1.47	1.39
2	Y	307	CHL	C3D-C4D	4.71	1.48	1.41
2	G	606	CHL	C3D-C4D	4.54	1.48	1.41
2	N	607	CHL	C3D-C4D	4.54	1.48	1.41
2	G	606	CHL	C2C-C3C	4.52	1.40	1.36
2	N	605	CHL	C3D-C4D	4.46	1.48	1.41
2	Y	309	CHL	C3D-C4D	4.46	1.48	1.41
2	Y	306	CHL	C3D-C4D	4.45	1.48	1.41
2	N	609	CHL	C2C-C3C	4.43	1.40	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	608	CHL	C3D-C4D	4.43	1.48	1.41
2	G	607	CHL	C3D-C4D	4.39	1.48	1.41
2	G	605	CHL	C3D-C4D	4.39	1.48	1.41
2	N	606	CHL	C3D-C4D	4.39	1.48	1.41
6	Y	319	LHG	O8-C23	4.38	1.46	1.33
2	Y	308	CHL	C3D-C4D	4.37	1.48	1.41
2	Y	310	CHL	C3D-C4D	4.36	1.48	1.41
2	G	609	CHL	C2C-C3C	4.25	1.40	1.36
2	N	601	CHL	C3D-C4D	4.20	1.47	1.41
2	G	608	CHL	C3D-C4D	4.19	1.47	1.41
6	G	618	LHG	O8-C23	4.17	1.45	1.33
2	G	609	CHL	C3D-C4D	4.14	1.47	1.41
6	N	618	LHG	O8-C23	4.13	1.45	1.33
2	Y	302	CHL	C3D-C4D	4.11	1.47	1.41
2	Y	307	CHL	C2C-C3C	4.09	1.40	1.36
2	N	609	CHL	C3D-C4D	4.08	1.47	1.41
6	N	618	LHG	O7-C7	4.04	1.45	1.34
6	G	618	LHG	O7-C7	4.04	1.45	1.34
2	Y	308	CHL	C2C-C3C	3.98	1.40	1.36
2	N	607	CHL	C2C-C3C	3.88	1.40	1.36
6	Y	319	LHG	O7-C7	3.88	1.45	1.34
2	G	601	CHL	C3D-C4D	3.75	1.47	1.41
3	Y	315	CLA	C1D-ND	3.72	1.42	1.37
2	G	605	CHL	C2C-C3C	3.71	1.40	1.36
2	N	606	CHL	C2C-C3C	3.71	1.40	1.36
3	N	603	CLA	C1D-ND	3.69	1.42	1.37
3	N	612	CLA	C1D-ND	3.69	1.42	1.37
3	N	610	CLA	C1D-ND	3.66	1.42	1.37
3	N	602	CLA	C1D-ND	3.65	1.42	1.37
3	G	603	CLA	C1D-ND	3.63	1.42	1.37
2	G	601	CHL	C2C-C3C	3.63	1.39	1.36
3	Y	303	CLA	C1D-ND	3.63	1.42	1.37
3	G	602	CLA	C4B-NB	3.61	1.42	1.37
3	N	614	CLA	C1D-ND	3.58	1.42	1.37
2	G	607	CHL	C2C-C3C	3.58	1.39	1.36
3	G	614	CLA	C1D-ND	3.58	1.42	1.37
3	G	603	CLA	C4B-NB	3.53	1.42	1.37
3	Y	304	CLA	C1D-ND	3.52	1.42	1.37
3	Y	311	CLA	C1D-ND	3.49	1.42	1.37
3	N	604	CLA	C1D-ND	3.48	1.42	1.37
3	Y	313	CLA	C1D-ND	3.46	1.42	1.37
3	N	613	CLA	C1D-ND	3.46	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	604	CLA	C1D-ND	3.46	1.42	1.37
3	Y	312	CLA	C4B-NB	3.45	1.42	1.37
2	Y	306	CHL	C2C-C3C	3.43	1.39	1.36
3	Y	313	CLA	C4B-NB	3.41	1.42	1.37
3	G	602	CLA	C1D-ND	3.40	1.42	1.37
3	N	612	CLA	C4B-NB	3.39	1.42	1.37
3	N	614	CLA	C4B-NB	3.38	1.42	1.37
2	G	601	CHL	CAC-C3C	-3.37	1.45	1.51
3	Y	314	CLA	C1D-ND	3.36	1.42	1.37
2	G	601	CHL	C1A-CHA	-3.35	1.36	1.40
3	Y	314	CLA	C4B-NB	3.34	1.42	1.37
2	N	601	CHL	C2C-C3C	3.34	1.39	1.36
2	Y	302	CHL	C2C-C3C	3.33	1.39	1.36
5	G	617	NEX	C7-C6	-3.33	1.26	1.30
3	G	614	CLA	C4B-NB	3.33	1.42	1.37
3	Y	303	CLA	C4B-NB	3.31	1.42	1.37
3	N	603	CLA	C4B-NB	3.30	1.42	1.37
2	N	605	CHL	C2C-C3C	3.30	1.39	1.36
3	G	612	CLA	C1D-ND	3.29	1.42	1.37
3	G	611	CLA	C4B-NB	3.28	1.42	1.37
5	N	617	NEX	C7-C6	-3.27	1.26	1.30
3	Y	315	CLA	C4B-NB	3.26	1.42	1.37
2	G	601	CHL	CMD-C2D	-3.26	1.45	1.51
3	G	613	CLA	C1D-ND	3.25	1.42	1.37
2	N	608	CHL	C2C-C3C	3.24	1.39	1.36
3	N	610	CLA	C4B-NB	3.22	1.42	1.37
3	G	610	CLA	C4B-NB	3.22	1.42	1.37
3	G	604	CLA	C4B-NB	3.21	1.42	1.37
3	N	604	CLA	C4B-NB	3.20	1.42	1.37
2	Y	309	CHL	C2C-C3C	3.20	1.39	1.36
3	Y	305	CLA	C4B-NB	3.20	1.42	1.37
3	G	610	CLA	C1D-ND	3.18	1.42	1.37
3	Y	304	CLA	C4B-NB	3.17	1.42	1.37
3	Y	311	CLA	C1B-C2B	3.09	1.50	1.43
3	G	613	CLA	C4B-NB	3.07	1.41	1.37
3	N	611	CLA	C1D-ND	3.04	1.41	1.37
3	N	613	CLA	C4B-NB	3.04	1.41	1.37
3	Y	305	CLA	C1D-ND	3.02	1.41	1.37
3	N	602	CLA	C4B-NB	3.02	1.41	1.37
2	G	609	CHL	CMB-C2B	-2.98	1.45	1.51
2	N	606	CHL	CMB-C2B	-2.98	1.45	1.51
5	N	617	NEX	C7-C8	-2.98	1.27	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Y	312	CLA	C1D-ND	2.97	1.41	1.37
3	G	611	CLA	C1D-ND	2.96	1.41	1.37
2	G	608	CHL	C2C-C3C	2.92	1.39	1.36
3	G	612	CLA	C4B-NB	2.91	1.41	1.37
2	G	608	CHL	CMD-C2D	-2.90	1.45	1.51
5	G	617	NEX	C7-C8	-2.89	1.27	1.31
2	Y	306	CHL	CAC-C3C	-2.87	1.46	1.51
2	N	601	CHL	C1A-CHA	-2.84	1.36	1.40
2	Y	310	CHL	C2C-C3C	2.84	1.39	1.36
3	Y	304	CLA	C1B-C2B	2.84	1.49	1.43
3	N	614	CLA	C1B-C2B	2.80	1.49	1.43
2	Y	302	CHL	CMD-C2D	-2.80	1.46	1.51
3	Y	314	CLA	C1B-C2B	2.78	1.49	1.43
2	N	609	CHL	CMB-C2B	-2.78	1.46	1.51
7	Y	301	XAT	O4-C5	-2.77	1.42	1.46
2	Y	308	CHL	CMD-C2D	-2.77	1.46	1.51
3	N	613	CLA	C1B-C2B	2.76	1.49	1.43
3	G	613	CLA	C1B-C2B	2.76	1.49	1.43
3	N	603	CLA	C1B-C2B	2.76	1.49	1.43
3	Y	312	CLA	CMD-C2D	-2.74	1.45	1.50
2	N	601	CHL	CMD-C2D	-2.73	1.46	1.51
3	Y	315	CLA	C1B-C2B	2.73	1.49	1.43
3	G	610	CLA	CMB-C2B	-2.73	1.45	1.50
2	G	608	CHL	CMB-C2B	-2.72	1.46	1.51
2	N	605	CHL	CAC-C3C	-2.72	1.46	1.51
3	Y	312	CLA	C1B-C2B	2.72	1.49	1.43
2	G	605	CHL	CMD-C2D	-2.72	1.46	1.51
5	N	617	NEX	O24-C25	-2.71	1.42	1.46
2	Y	310	CHL	CMB-C2B	-2.69	1.46	1.51
2	N	605	CHL	CMD-C2D	-2.69	1.46	1.51
3	Y	303	CLA	C1B-C2B	2.67	1.49	1.43
3	N	611	CLA	C4B-NB	2.65	1.41	1.37
2	Y	302	CHL	C1A-CHA	-2.65	1.37	1.40
3	N	602	CLA	C1B-C2B	2.64	1.49	1.43
3	N	612	CLA	C1B-C2B	2.64	1.49	1.43
3	Y	313	CLA	C3B-C4B	2.63	1.50	1.42
3	Y	313	CLA	C1B-C2B	2.62	1.49	1.43
2	N	608	CHL	CMB-C2B	-2.60	1.46	1.51
2	N	609	CHL	CMD-C2D	-2.60	1.46	1.51
2	N	608	CHL	CMD-C2D	-2.60	1.46	1.51
7	N	619	XAT	O24-C25	-2.60	1.42	1.46
2	G	609	CHL	CMD-C2D	-2.60	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	604	CLA	C1B-C2B	2.59	1.49	1.43
2	G	607	CHL	CMB-C2B	-2.59	1.46	1.51
2	Y	302	CHL	CMB-C2B	-2.59	1.46	1.51
2	N	606	CHL	CMD-C2D	-2.59	1.46	1.51
3	G	603	CLA	C1B-C2B	2.59	1.49	1.43
2	G	601	CHL	CMB-C2B	-2.58	1.46	1.51
2	N	605	CHL	CMB-C2B	-2.58	1.46	1.51
3	G	611	CLA	C1B-C2B	2.58	1.49	1.43
5	G	617	NEX	O24-C25	-2.58	1.42	1.46
3	N	604	CLA	C1B-C2B	2.57	1.49	1.43
2	Y	307	CHL	CMD-C2D	-2.57	1.46	1.51
2	G	606	CHL	CMB-C2B	-2.56	1.46	1.51
2	Y	308	CHL	CMB-C2B	-2.56	1.46	1.51
2	N	601	CHL	CMB-C2B	-2.56	1.46	1.51
2	Y	309	CHL	CMD-C2D	-2.56	1.46	1.51
2	Y	307	CHL	CMB-C2B	-2.56	1.46	1.51
2	Y	306	CHL	CMD-C2D	-2.55	1.46	1.51
5	Y	318	NEX	C32-C33	-2.55	1.40	1.46
2	Y	306	CHL	CMB-C2B	-2.55	1.46	1.51
3	N	612	CLA	C3B-C4B	2.54	1.50	1.42
3	G	602	CLA	CMB-C2B	-2.54	1.45	1.50
2	Y	309	CHL	CAC-C3C	-2.54	1.47	1.51
7	G	619	XAT	O24-C25	-2.54	1.42	1.46
2	N	607	CHL	CMD-C2D	-2.53	1.46	1.51
3	N	610	CLA	CMB-C2B	-2.53	1.45	1.50
2	N	607	CHL	CMB-C2B	-2.52	1.46	1.51
3	N	610	CLA	C1B-C2B	2.52	1.49	1.43
2	N	609	CHL	C1A-CHA	-2.52	1.37	1.40
3	N	611	CLA	C1B-C2B	2.52	1.49	1.43
2	G	606	CHL	CMD-C2D	-2.51	1.46	1.51
7	N	619	XAT	O4-C5	-2.51	1.43	1.46
3	G	612	CLA	C1B-C2B	2.51	1.49	1.43
2	G	605	CHL	CAC-C3C	-2.51	1.47	1.51
2	Y	302	CHL	CAC-C3C	-2.50	1.47	1.51
5	Y	318	NEX	C12-C13	-2.50	1.40	1.46
2	G	607	CHL	CMD-C2D	-2.50	1.46	1.51
2	N	606	CHL	CBD-CGD	-2.50	1.49	1.52
3	G	603	CLA	C3B-C4B	2.50	1.50	1.42
2	Y	310	CHL	CMD-C2D	-2.50	1.46	1.51
2	G	609	CHL	MG-NB	-2.49	2.00	2.05
3	Y	305	CLA	C1B-C2B	2.49	1.49	1.43
2	G	607	CHL	CAC-C3C	-2.48	1.47	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Y	309	CHL	CMB-C2B	-2.48	1.46	1.51
3	Y	311	CLA	MG-NB	-2.48	2.00	2.05
2	G	605	CHL	CMB-C2B	-2.48	1.46	1.51
3	G	614	CLA	C1B-C2B	2.47	1.48	1.43
3	G	614	CLA	C3B-C4B	2.47	1.49	1.42
2	G	609	CHL	C1A-CHA	-2.47	1.37	1.40
2	Y	310	CHL	CHC-C1C	2.46	1.44	1.39
5	Y	318	NEX	C28-C29	-2.46	1.40	1.46
3	G	611	CLA	C3B-C4B	2.44	1.49	1.42
2	N	608	CHL	CAC-C3C	-2.44	1.47	1.51
3	G	602	CLA	C3B-C4B	2.44	1.49	1.42
2	N	605	CHL	CHC-C4B	-2.44	1.35	1.39
3	N	614	CLA	C3B-C4B	2.43	1.49	1.42
7	Y	301	XAT	O24-C25	-2.43	1.43	1.46
3	Y	312	CLA	C3B-C4B	2.43	1.49	1.42
2	G	608	CHL	CAC-C3C	-2.42	1.47	1.51
3	Y	315	CLA	CMD-C2D	-2.41	1.45	1.50
3	Y	311	CLA	C4B-NB	2.41	1.41	1.37
3	Y	304	CLA	CMD-C2D	-2.40	1.45	1.50
2	N	607	CHL	CAC-C3C	-2.40	1.47	1.51
2	Y	308	CHL	CBD-CGD	-2.39	1.49	1.52
2	N	606	CHL	CHC-C4B	-2.39	1.35	1.39
2	N	607	CHL	CBD-CGD	-2.39	1.49	1.52
3	Y	305	CLA	C3B-C4B	2.37	1.49	1.42
2	N	606	CHL	CAC-C3C	-2.36	1.47	1.51
2	G	601	CHL	CBD-CGD	-2.36	1.49	1.52
2	N	601	CHL	CAC-C3C	-2.35	1.47	1.51
7	G	619	XAT	O4-C5	-2.35	1.43	1.46
3	Y	314	CLA	C3B-C4B	2.34	1.49	1.42
3	G	602	CLA	CHC-C1C	2.34	1.43	1.38
3	N	602	CLA	C3B-C4B	2.34	1.49	1.42
3	Y	304	CLA	C3B-C4B	2.33	1.49	1.42
3	Y	303	CLA	C3B-C4B	2.33	1.49	1.42
3	N	603	CLA	C3B-C4B	2.32	1.49	1.42
2	Y	308	CHL	CAC-C3C	-2.31	1.47	1.51
3	Y	305	CLA	CMB-C2B	-2.31	1.46	1.50
3	N	602	CLA	CHC-C1C	2.31	1.43	1.38
2	Y	310	CHL	CAC-C3C	-2.30	1.47	1.51
3	G	610	CLA	C3B-C4B	2.30	1.49	1.42
3	G	611	CLA	CMD-C2D	-2.30	1.46	1.50
2	N	609	CHL	MG-NB	-2.29	2.01	2.05
3	G	604	CLA	CMB-C2B	-2.28	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	603	CLA	CMB-C2B	-2.27	1.46	1.50
3	G	610	CLA	CMD-C2D	-2.27	1.46	1.50
3	G	614	CLA	CMD-C2D	-2.27	1.46	1.50
2	N	609	CHL	CAC-C3C	-2.26	1.47	1.51
3	G	614	CLA	CHC-C1C	2.26	1.43	1.38
2	G	608	CHL	CHC-C4B	-2.26	1.36	1.39
3	N	613	CLA	C3B-C4B	2.26	1.49	1.42
3	Y	315	CLA	C3B-C4B	2.25	1.49	1.42
3	N	604	CLA	C3B-C4B	2.24	1.49	1.42
3	N	604	CLA	CMB-C2B	-2.24	1.46	1.50
3	N	614	CLA	CMD-C2D	-2.24	1.46	1.50
2	N	606	CHL	MG-NB	-2.22	2.01	2.05
3	N	611	CLA	CMC-C2C	-2.21	1.46	1.50
3	G	604	CLA	C3B-C4B	2.21	1.49	1.42
3	Y	305	CLA	CHC-C1C	2.20	1.42	1.38
3	G	612	CLA	C3B-C4B	2.20	1.49	1.42
3	N	611	CLA	CMD-C2D	-2.19	1.46	1.50
3	Y	303	CLA	CMD-C2D	-2.19	1.46	1.50
2	G	605	CHL	CHC-C4B	-2.18	1.36	1.39
2	Y	309	CHL	CHC-C4B	-2.17	1.36	1.39
3	G	612	CLA	CMD-C2D	-2.17	1.46	1.50
3	G	611	CLA	CMB-C2B	-2.17	1.46	1.50
3	Y	305	CLA	CMD-C2D	-2.17	1.46	1.50
3	Y	315	CLA	CHC-C1C	2.17	1.42	1.38
2	G	607	CHL	CHC-C4B	-2.16	1.36	1.39
3	G	613	CLA	C3B-C4B	2.16	1.49	1.42
3	N	611	CLA	MG-NB	-2.16	2.01	2.05
3	Y	311	CLA	MG-ND	-2.15	2.01	2.05
2	Y	310	CHL	MG-NB	-2.14	2.01	2.05
3	N	604	CLA	CMD-C2D	-2.13	1.46	1.50
2	Y	306	CHL	CHC-C4B	-2.13	1.36	1.39
3	Y	313	CLA	C3D-C4D	2.13	1.49	1.44
3	Y	314	CLA	CMD-C2D	-2.13	1.46	1.50
3	G	602	CLA	C1B-C2B	2.13	1.48	1.43
3	G	603	CLA	CMD-C2D	-2.13	1.46	1.50
3	N	604	CLA	CHC-C1C	2.13	1.42	1.38
3	G	612	CLA	CMB-C2B	-2.12	1.46	1.50
5	Y	318	NEX	C14-C13	2.12	1.40	1.35
3	N	603	CLA	CMD-C2D	-2.12	1.46	1.50
2	G	606	CHL	C1A-C2A	2.12	1.55	1.51
3	N	612	CLA	CMC-C2C	-2.11	1.46	1.50
3	Y	311	CLA	CMD-C2D	-2.11	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	609	CHL	CAC-C3C	-2.11	1.48	1.51
3	N	611	CLA	C3B-C4B	2.11	1.48	1.42
2	Y	307	CHL	CAC-C3C	-2.10	1.48	1.51
3	N	612	CLA	C3D-C4D	2.10	1.48	1.44
3	N	610	CLA	CMD-C2D	-2.09	1.46	1.50
3	G	602	CLA	CMC-C2C	-2.09	1.46	1.50
3	Y	304	CLA	CMB-C2B	-2.09	1.46	1.50
3	G	603	CLA	CMC-C2C	-2.09	1.46	1.50
3	G	610	CLA	CHC-C1C	2.08	1.42	1.38
2	Y	302	CHL	CHC-C4B	-2.08	1.36	1.39
3	G	603	CLA	CMB-C2B	-2.08	1.46	1.50
3	G	613	CLA	CMB-C2B	-2.08	1.46	1.50
2	N	609	CHL	MG-ND	-2.08	2.01	2.05
3	Y	303	CLA	CHC-C1C	2.07	1.42	1.38
3	Y	312	CLA	CMB-C2B	-2.07	1.46	1.50
3	N	612	CLA	CMB-C2B	-2.07	1.46	1.50
3	Y	312	CLA	CMC-C2C	-2.07	1.46	1.50
3	N	611	CLA	CMB-C2B	-2.06	1.46	1.50
3	G	604	CLA	CMD-C2D	-2.06	1.46	1.50
5	Y	318	NEX	C30-C29	2.06	1.40	1.35
3	G	610	CLA	CMC-C2C	-2.06	1.46	1.50
5	Y	318	NEX	C34-C33	2.06	1.40	1.35
2	G	606	CHL	CAC-C3C	-2.06	1.48	1.51
3	N	603	CLA	CMC-C2C	-2.05	1.46	1.50
3	N	612	CLA	CMD-C2D	-2.05	1.46	1.50
3	N	610	CLA	C3B-C4B	2.05	1.48	1.42
3	N	610	CLA	CMC-C2C	-2.05	1.46	1.50
3	Y	312	CLA	C3D-C4D	2.05	1.48	1.44
3	G	612	CLA	CMC-C2C	-2.04	1.46	1.50
3	G	613	CLA	CMD-C2D	-2.04	1.46	1.50
3	Y	314	CLA	CMB-C2B	-2.04	1.46	1.50
3	Y	312	CLA	MG-NB	-2.04	2.01	2.05
3	G	604	CLA	CHC-C1C	2.03	1.42	1.38
3	Y	314	CLA	CHC-C1C	2.03	1.42	1.38
3	Y	313	CLA	CMB-C2B	-2.03	1.46	1.50
2	G	601	CHL	MG-NB	-2.02	2.01	2.05
3	G	602	CLA	CMD-C2D	-2.02	1.46	1.50
3	Y	315	CLA	CMB-C2B	-2.02	1.46	1.50
3	N	613	CLA	CMD-C2D	-2.02	1.46	1.50
2	G	608	CHL	C3B-C2B	-2.01	1.37	1.40
3	G	610	CLA	MG-NB	-2.01	2.01	2.05
3	Y	305	CLA	CMC-C2C	-2.00	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	606	CHL	CHC-C4B	-2.00	1.36	1.39
3	Y	304	CLA	CMC-C2C	-2.00	1.46	1.50

All (542) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	N	617	NEX	O24-C25-C24	7.16	120.20	113.49
5	G	617	NEX	O24-C25-C24	7.00	120.05	113.49
2	Y	307	CHL	C1B-CHB-C4A	6.72	125.65	121.32
3	Y	312	CLA	C4A-NA-C1A	6.55	109.67	106.68
7	G	619	XAT	O4-C5-C4	6.51	119.59	113.49
7	Y	301	XAT	O4-C5-C4	6.18	119.28	113.49
2	G	609	CHL	C1B-CHB-C4A	-6.14	117.37	121.32
7	G	619	XAT	O24-C25-C24	6.08	119.19	113.49
7	N	619	XAT	O4-C5-C4	6.08	119.19	113.49
3	G	613	CLA	C4A-NA-C1A	6.04	109.43	106.68
7	N	619	XAT	O24-C25-C24	5.82	118.95	113.49
7	Y	301	XAT	O24-C25-C24	5.71	118.84	113.49
2	N	601	CHL	C1B-CHB-C4A	5.67	124.97	121.32
7	N	619	XAT	C15-C14-C13	-5.51	119.55	127.28
3	Y	314	CLA	C4A-NA-C1A	5.38	109.13	106.68
3	N	613	CLA	C4A-NA-C1A	5.35	109.12	106.68
3	G	604	CLA	C4A-NA-C1A	5.33	109.11	106.68
2	N	606	CHL	C1B-CHB-C4A	5.31	124.74	121.32
2	G	606	CHL	C1B-CHB-C4A	5.26	124.71	121.32
3	Y	304	CLA	C4A-NA-C1A	5.25	109.07	106.68
5	N	617	NEX	C27-C28-C29	-5.18	117.49	125.53
2	G	608	CHL	C1B-CHB-C4A	5.10	124.61	121.32
3	N	604	CLA	C4A-NA-C1A	5.01	108.97	106.68
7	Y	301	XAT	O24-C25-C38	4.94	120.57	115.05
2	Y	302	CHL	C1B-CHB-C4A	4.85	124.44	121.32
3	Y	313	CLA	C4A-NA-C1A	4.83	108.88	106.68
3	N	612	CLA	C4A-NA-C1A	4.81	108.87	106.68
7	N	619	XAT	C18-C5-C6	-4.78	114.44	122.30
7	G	619	XAT	C18-C5-C6	-4.72	114.53	122.30
7	N	619	XAT	O24-C25-C38	4.72	120.32	115.05
7	Y	301	XAT	C15-C14-C13	-4.71	120.67	127.28
3	G	612	CLA	C4A-NA-C1A	4.67	108.81	106.68
7	G	619	XAT	C11-C10-C9	-4.65	120.76	127.28
3	Y	305	CLA	C4A-NA-C1A	4.57	108.76	106.68
2	G	606	CHL	O2D-CGD-CBD	4.57	115.96	110.95
7	Y	301	XAT	C38-C25-C26	-4.55	114.81	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	619	XAT	O4-C5-C18	4.55	120.13	115.05
7	N	619	XAT	C38-C25-C26	-4.54	114.82	122.30
5	N	617	NEX	C15-C14-C13	-4.54	120.91	127.28
3	N	611	CLA	C4A-NA-C1A	4.50	108.73	106.68
7	G	619	XAT	C38-C25-C26	-4.50	114.89	122.30
7	G	619	XAT	O24-C25-C38	4.45	120.02	115.05
7	Y	301	XAT	C18-C5-C6	-4.45	114.98	122.30
3	N	602	CLA	C4A-NA-C1A	4.44	108.70	106.68
5	G	617	NEX	C15-C14-C13	-4.41	121.09	127.28
7	N	619	XAT	C35-C34-C33	-4.41	121.09	127.28
3	Y	303	CLA	C4A-NA-C1A	4.36	108.67	106.68
5	G	617	NEX	C38-C25-C26	-4.34	115.17	122.30
7	N	619	XAT	O4-C5-C18	4.33	119.89	115.05
7	N	619	XAT	C11-C10-C9	-4.31	121.24	127.28
2	G	606	CHL	C4D-CHA-CBD	-4.31	104.63	108.97
5	N	617	NEX	C38-C25-C26	-4.30	115.22	122.30
7	Y	301	XAT	C11-C10-C9	-4.29	121.26	127.28
3	G	611	CLA	C4A-NA-C1A	4.23	108.61	106.68
7	Y	301	XAT	O4-C5-C18	4.22	119.76	115.05
4	N	615	LUT	C35-C34-C33	-4.18	121.41	127.28
5	G	617	NEX	C11-C10-C9	-4.09	121.54	127.28
3	N	603	CLA	C4A-NA-C1A	4.05	108.53	106.68
5	G	617	NEX	C27-C28-C29	-4.03	119.27	125.53
7	Y	301	XAT	C31-C30-C29	-4.03	121.62	127.28
5	G	617	NEX	C17-C1-C6	-4.02	106.88	110.47
5	N	617	NEX	O24-C25-C38	3.98	119.50	115.05
2	G	601	CHL	O2D-CGD-CBD	3.96	115.30	110.95
2	G	601	CHL	C1B-CHB-C4A	3.95	123.86	121.32
2	G	609	CHL	CMB-C2B-C3B	3.95	132.57	124.68
2	N	607	CHL	O2D-CGD-CBD	3.94	115.28	110.95
2	Y	308	CHL	C4D-CHA-CBD	-3.94	105.00	108.97
2	N	607	CHL	C4D-CHA-CBD	-3.92	105.01	108.97
5	N	617	NEX	C35-C34-C33	-3.90	121.80	127.28
7	Y	301	XAT	C35-C34-C33	-3.90	121.81	127.28
7	G	619	XAT	C31-C30-C29	-3.90	121.81	127.28
5	G	617	NEX	O24-C25-C38	3.89	119.40	115.05
2	N	606	CHL	C4D-CHA-CBD	-3.89	105.05	108.97
2	Y	307	CHL	C4D-CHA-CBD	-3.88	105.06	108.97
5	N	617	NEX	C11-C10-C9	-3.82	121.93	127.28
5	Y	318	NEX	C15-C35-C34	3.74	131.16	123.52
4	G	616	LUT	C15-C14-C13	-3.73	122.05	127.28
7	N	619	XAT	C31-C30-C29	-3.72	122.07	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	607	CHL	C4D-CHA-CBD	-3.67	105.27	108.97
4	Y	317	LUT	C7-C8-C9	-3.65	120.84	126.23
3	G	603	CLA	C4A-NA-C1A	3.65	108.34	106.68
4	G	615	LUT	C21-C26-C27	-3.63	108.65	112.83
7	G	619	XAT	C15-C14-C13	-3.60	122.22	127.28
6	Y	319	LHG	O8-C23-C24	3.60	122.80	111.83
6	G	618	LHG	O8-C23-C24	3.58	122.76	111.83
5	Y	318	NEX	C39-C29-C30	-3.56	117.05	122.82
4	N	616	LUT	C35-C34-C33	-3.55	122.29	127.28
4	G	616	LUT	C35-C34-C33	-3.53	122.33	127.28
4	N	616	LUT	C15-C14-C13	-3.50	122.36	127.28
2	G	607	CHL	O2D-CGD-CBD	3.50	114.79	110.95
3	Y	305	CLA	CMB-C2B-C1B	-3.48	120.12	125.42
2	Y	309	CHL	C1B-CHB-C4A	3.46	123.55	121.32
2	N	606	CHL	O2D-CGD-CBD	3.46	114.75	110.95
4	N	615	LUT	C11-C10-C9	-3.44	122.45	127.28
3	Y	304	CLA	CAA-C2A-C3A	-3.43	103.72	113.00
2	N	608	CHL	C4D-CHA-CBD	-3.43	105.51	108.97
5	G	617	NEX	C31-C30-C29	-3.42	122.48	127.28
2	Y	310	CHL	C4D-CHA-CBD	-3.42	105.52	108.97
7	G	619	XAT	C26-C27-C28	-3.42	118.77	125.99
2	Y	309	CHL	C4D-CHA-CBD	-3.42	105.52	108.97
4	N	615	LUT	C35-C15-C14	-3.39	116.59	123.52
4	Y	316	LUT	C7-C8-C9	-3.37	121.25	126.23
3	N	603	CLA	CAA-C2A-C3A	-3.32	104.02	113.00
2	N	605	CHL	C4D-CHA-CBD	-3.32	105.62	108.97
2	G	609	CHL	C1C-CHC-C4B	3.31	127.90	116.07
2	G	608	CHL	C1C-CHC-C4B	3.29	127.86	116.07
3	G	614	CLA	C4A-NA-C1A	3.29	108.18	106.68
3	G	610	CLA	O2D-CGD-O1D	-3.28	117.47	123.85
2	G	609	CHL	C4D-ND-C1D	3.28	107.71	105.22
7	N	619	XAT	C26-C27-C28	-3.28	119.07	125.99
3	Y	305	CLA	O2D-CGD-O1D	-3.27	117.48	123.85
3	G	611	CLA	CMD-C2D-C1D	-3.27	118.97	124.73
4	N	616	LUT	C26-C27-C28	-3.25	119.52	124.58
4	G	615	LUT	C35-C34-C33	-3.25	122.72	127.28
3	N	612	CLA	O2D-CGD-O1D	-3.25	117.52	123.85
6	G	618	LHG	O7-C7-C8	3.25	118.51	111.48
5	N	617	NEX	C8-C7-C6	-3.25	173.83	177.66
4	G	616	LUT	C27-C28-C29	-3.24	119.36	126.32
2	N	609	CHL	CMB-C2B-C3B	3.23	131.15	124.68
4	N	615	LUT	C30-C31-C32	-3.23	113.84	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	602	CLA	C3B-C4B-NB	-3.23	107.65	110.53
3	N	611	CLA	O2D-CGD-O1D	-3.22	117.57	123.85
3	Y	311	CLA	CMA-C3A-C4A	3.22	120.43	111.77
5	Y	318	NEX	C35-C15-C14	3.22	130.11	123.52
5	G	617	NEX	C35-C34-C33	-3.22	122.77	127.28
3	G	611	CLA	O2D-CGD-O1D	-3.22	117.59	123.85
3	N	610	CLA	O2D-CGD-O1D	-3.21	117.60	123.85
3	G	610	CLA	C3B-C4B-NB	-3.20	107.67	110.53
7	N	619	XAT	C11-C12-C13	-3.19	117.61	126.36
2	Y	302	CHL	CHA-C1A-C2A	-3.19	125.81	133.31
2	N	605	CHL	O2D-CGD-O1D	-3.18	117.65	123.85
3	N	602	CLA	O2D-CGD-O1D	-3.18	117.67	123.85
3	G	602	CLA	C4A-NA-C1A	3.17	108.13	106.68
7	G	619	XAT	C35-C34-C33	-3.17	122.84	127.28
3	N	614	CLA	C4A-NA-C1A	3.16	108.12	106.68
4	Y	317	LUT	C15-C14-C13	-3.16	122.85	127.28
3	G	602	CLA	O2D-CGD-O1D	-3.15	117.72	123.85
7	Y	301	XAT	C7-C8-C9	-3.14	120.66	125.53
4	G	615	LUT	C7-C8-C9	-3.14	121.59	126.23
2	Y	308	CHL	O2D-CGD-CBD	3.13	114.39	110.95
7	G	619	XAT	C17-C1-C2	-3.13	103.47	108.97
2	G	601	CHL	CHA-C1A-C2A	-3.13	125.96	133.31
3	N	604	CLA	C1-C2-C3	-3.13	121.08	126.20
2	Y	310	CHL	C3D-C4D-CHA	3.11	113.27	108.54
4	Y	317	LUT	C27-C28-C29	-3.11	119.63	126.32
2	G	609	CHL	C3D-C4D-CHA	3.11	113.27	108.54
7	Y	301	XAT	C27-C28-C29	-3.11	120.71	125.53
4	N	615	LUT	C21-C26-C27	-3.10	109.26	112.83
3	G	604	CLA	O2D-CGD-O1D	-3.09	117.83	123.85
2	G	609	CHL	C4D-CHA-CBD	-3.09	105.85	108.97
6	N	618	LHG	O7-C7-C8	3.08	118.14	111.48
2	Y	309	CHL	C1C-CHC-C4B	3.07	127.06	116.07
4	N	616	LUT	C21-C26-C27	-3.07	109.30	112.83
2	G	607	CHL	O2D-CGD-O1D	-3.07	117.88	123.85
2	Y	306	CHL	O2D-CGD-O1D	-3.07	117.88	123.85
2	G	606	CHL	O2D-CGD-O1D	-3.06	117.89	123.85
2	Y	310	CHL	C4D-ND-C1D	3.05	107.53	105.22
3	Y	311	CLA	O2D-CGD-O1D	-3.05	117.91	123.85
2	N	601	CHL	CHA-C1A-C2A	-3.05	126.15	133.31
2	G	607	CHL	C3D-C4D-CHA	3.04	113.16	108.54
2	N	609	CHL	C3D-C4D-CHA	3.04	113.15	108.54
3	G	614	CLA	O2D-CGD-O1D	-3.03	117.94	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	605	CHL	C1B-CHB-C4A	3.03	123.27	121.32
3	N	613	CLA	O2D-CGD-O1D	-3.03	117.95	123.85
2	Y	306	CHL	O2D-CGD-CBD	3.03	114.28	110.95
5	Y	318	NEX	C32-C33-C34	3.03	123.77	119.01
3	G	612	CLA	C1-C2-C3	-3.03	121.24	126.20
4	N	615	LUT	C7-C8-C9	-3.02	121.77	126.23
2	G	606	CHL	CMB-C2B-C3B	3.02	130.72	124.68
7	G	619	XAT	C15-C35-C34	-3.01	117.36	123.52
7	G	619	XAT	C7-C8-C9	-3.00	120.88	125.53
2	Y	306	CHL	C4D-CHA-CBD	-3.00	105.94	108.97
2	Y	310	CHL	C1C-CHC-C4B	3.00	126.79	116.07
2	G	605	CHL	O2D-CGD-CBD	3.00	114.24	110.95
2	G	607	CHL	OMC-CMC-C2C	-2.99	119.92	125.12
7	Y	301	XAT	C26-C27-C28	-2.99	119.66	125.99
7	Y	301	XAT	C11-C12-C13	-2.99	118.17	126.36
6	Y	319	LHG	O7-C7-C8	2.99	117.94	111.48
4	N	616	LUT	C31-C30-C29	-2.98	123.10	127.28
4	N	615	LUT	C15-C14-C13	-2.97	123.12	127.28
2	N	607	CHL	C3D-C4D-CHA	2.96	113.05	108.54
3	Y	305	CLA	C4-C3-C5	2.96	120.37	115.23
2	G	608	CHL	O2D-CGD-O1D	-2.96	118.08	123.85
2	G	606	CHL	C3D-C4D-CHA	2.95	113.03	108.54
3	G	611	CLA	CMD-C2D-C3D	2.95	134.45	127.69
2	G	605	CHL	C4D-CHA-CBD	-2.95	106.00	108.97
2	G	601	CHL	C3C-C4C-NC	-2.95	107.45	114.65
3	N	614	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
2	Y	310	CHL	OMC-CMC-C2C	-2.94	120.01	125.12
2	G	608	CHL	CHA-C1A-C2A	-2.94	126.40	133.31
5	G	617	NEX	C24-C23-C22	-2.94	105.30	110.79
2	G	601	CHL	O2D-CGD-O1D	-2.93	118.15	123.85
3	N	611	CLA	O2D-CGD-CBD	2.93	116.34	111.23
2	N	606	CHL	C1-C2-C3	-2.92	122.03	126.76
3	Y	314	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
7	N	619	XAT	C18-C5-C4	2.92	117.52	114.24
2	Y	308	CHL	C3D-C4D-CHA	2.91	112.97	108.54
2	G	601	CHL	CMB-C2B-C3B	2.90	130.49	124.68
2	G	605	CHL	O2D-CGD-O1D	-2.90	118.20	123.85
2	Y	308	CHL	CMB-C2B-C3B	2.90	130.48	124.68
2	N	608	CHL	C1C-CHC-C4B	2.90	126.44	116.07
2	Y	302	CHL	O2D-CGD-O1D	-2.89	118.22	123.85
2	N	607	CHL	CMB-C2B-C3B	2.89	130.46	124.68
5	N	617	NEX	C24-C23-C22	-2.89	105.38	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Y	307	CHL	C1C-CHC-C4B	2.89	126.41	116.07
2	G	608	CHL	O2D-CGD-CBD	2.89	114.12	110.95
5	Y	318	NEX	C12-C13-C14	2.89	123.55	119.01
5	Y	318	NEX	C40-C33-C34	-2.88	118.14	122.82
2	N	609	CHL	C1C-CHC-C4B	2.88	126.38	116.07
2	N	606	CHL	C3D-C4D-CHA	2.88	112.92	108.54
4	Y	317	LUT	C21-C26-C27	-2.88	109.51	112.83
4	Y	317	LUT	C11-C10-C9	-2.87	123.25	127.28
2	Y	308	CHL	C1C-CHC-C4B	2.86	126.32	116.07
3	N	610	CLA	C4A-NA-C1A	2.86	107.98	106.68
2	N	601	CHL	O2D-CGD-CBD	2.86	114.09	110.95
2	N	609	CHL	C4D-ND-C1D	2.85	107.39	105.22
7	N	619	XAT	C17-C1-C2	-2.85	103.96	108.97
3	G	603	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
2	G	608	CHL	C4D-CHA-CBD	-2.85	106.09	108.97
3	Y	304	CLA	CHB-C4A-NA	2.84	128.50	124.40
2	Y	308	CHL	C4D-ND-C1D	2.84	107.38	105.22
2	N	607	CHL	C1C-CHC-C4B	2.84	126.24	116.07
2	N	605	CHL	O2D-CGD-CBD	2.84	114.06	110.95
7	G	619	XAT	C11-C12-C13	-2.83	118.59	126.36
3	G	613	CLA	O2D-CGD-O1D	-2.83	118.33	123.85
3	N	613	CLA	CMB-C2B-C1B	-2.82	121.12	125.42
2	N	606	CHL	O2D-CGD-O1D	-2.82	118.36	123.85
5	N	617	NEX	C31-C32-C33	-2.81	118.66	126.36
5	N	617	NEX	C31-C30-C29	-2.81	123.34	127.28
3	Y	303	CLA	O2D-CGD-O1D	-2.81	118.39	123.85
4	G	616	LUT	C7-C8-C9	-2.80	122.09	126.23
4	G	616	LUT	C21-C26-C27	-2.80	109.61	112.83
3	Y	313	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
2	N	601	CHL	O2D-CGD-O1D	-2.80	118.41	123.85
2	Y	307	CHL	C3D-C4D-CHA	2.79	112.78	108.54
3	Y	304	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
2	G	601	CHL	C1C-CHC-C4B	2.78	126.03	116.07
4	Y	316	LUT	C18-C5-C6	-2.78	121.45	124.48
3	Y	315	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
5	Y	318	NEX	C28-C29-C30	2.78	123.38	119.01
5	Y	318	NEX	C20-C13-C14	-2.78	118.31	122.82
4	G	615	LUT	C11-C10-C9	-2.78	123.38	127.28
2	N	609	CHL	C4D-CHA-CBD	-2.78	106.17	108.97
3	G	610	CLA	C4A-NA-C1A	2.77	107.94	106.68
2	G	607	CHL	CMB-C2B-C3B	2.77	130.22	124.68
2	G	607	CHL	C1C-CHC-C4B	2.77	125.97	116.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	Y	301	XAT	C17-C1-C2	-2.77	104.10	108.97
7	Y	301	XAT	C24-C23-C22	-2.77	105.61	110.79
2	N	605	CHL	C1C-CHC-C4B	2.76	125.96	116.07
2	G	601	CHL	OMC-CMC-C2C	-2.76	120.32	125.12
2	Y	309	CHL	O2D-CGD-O1D	-2.76	118.47	123.85
3	G	603	CLA	CHB-C4A-NA	2.76	128.38	124.40
3	N	604	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
3	N	603	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
2	N	601	CHL	CMB-C2B-C3B	2.74	130.16	124.68
2	G	606	CHL	C1C-CHC-C4B	2.73	125.85	116.07
7	Y	301	XAT	C15-C35-C34	-2.73	117.94	123.52
5	N	617	NEX	C15-C35-C34	-2.72	117.95	123.52
5	G	617	NEX	C26-C27-C28	-2.72	120.24	125.99
2	Y	302	CHL	C1-C2-C3	-2.72	121.74	126.20
7	Y	301	XAT	C18-C5-C4	2.72	117.29	114.24
3	Y	305	CLA	C1-C2-C3	-2.72	121.75	126.20
7	G	619	XAT	C27-C28-C29	-2.71	121.33	125.53
2	Y	306	CHL	C1C-CHC-C4B	2.71	125.76	116.07
2	N	609	CHL	OMC-CMC-C2C	-2.71	120.42	125.12
3	N	610	CLA	O2A-CGA-O1A	-2.70	116.86	123.63
2	Y	302	CHL	CMB-C2B-C3B	2.70	130.08	124.68
2	Y	302	CHL	C1C-CHC-C4B	2.70	125.73	116.07
2	G	605	CHL	C1C-CHC-C4B	2.70	125.73	116.07
2	Y	308	CHL	OMC-CMC-C2C	-2.70	120.44	125.12
2	Y	308	CHL	O2D-CGD-O1D	-2.69	118.61	123.85
2	Y	310	CHL	C3C-C4C-NC	-2.69	108.07	114.65
2	N	608	CHL	C3D-C4D-CHA	2.69	112.63	108.54
3	G	604	CLA	CMB-C2B-C1B	-2.69	121.32	125.42
2	Y	309	CHL	C3D-C4D-CHA	2.69	112.63	108.54
4	G	615	LUT	C27-C28-C29	-2.69	120.54	126.32
2	N	608	CHL	O2D-CGD-O1D	-2.69	118.62	123.85
2	Y	307	CHL	CMD-C2D-C3D	2.69	130.05	124.68
3	N	603	CLA	CHB-C4A-NA	2.68	128.27	124.40
2	Y	302	CHL	OMC-CMC-C2C	-2.68	120.47	125.12
3	Y	313	CLA	C1-C2-C3	-2.68	121.81	126.20
3	G	611	CLA	O2D-CGD-CBD	2.67	115.91	111.23
7	N	619	XAT	C27-C28-C29	-2.67	121.39	125.53
4	G	615	LUT	C30-C31-C32	-2.66	115.48	123.20
2	N	609	CHL	C1-C2-C3	-2.66	121.84	126.20
2	N	601	CHL	C1C-CHC-C4B	2.66	125.58	116.07
2	Y	310	CHL	O2D-CGD-O1D	-2.65	118.69	123.85
3	N	604	CLA	CMB-C2B-C1B	-2.65	121.39	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	N	617	NEX	C17-C1-C6	-2.64	108.11	110.47
4	G	615	LUT	C15-C14-C13	-2.64	123.57	127.28
2	Y	310	CHL	O1D-CGD-CBD	2.64	128.73	124.72
2	N	607	CHL	O2D-CGD-O1D	-2.63	118.73	123.85
2	G	609	CHL	C3C-C4C-NC	-2.62	108.24	114.65
2	N	605	CHL	CMB-C2B-C3B	2.62	129.92	124.68
2	N	605	CHL	C3C-C4C-NC	-2.61	108.26	114.65
3	G	612	CLA	CHB-C4A-NA	2.61	128.17	124.40
2	Y	302	CHL	O2D-CGD-CBD	2.61	113.82	110.95
2	Y	306	CHL	C3C-C4C-NC	-2.61	108.27	114.65
5	G	617	NEX	C15-C35-C34	-2.61	118.18	123.52
4	G	615	LUT	C18-C5-C6	-2.61	121.64	124.48
3	G	610	CLA	CHB-C1B-NB	2.60	127.96	124.05
3	G	603	CLA	CAA-C2A-C3A	-2.60	105.98	113.00
3	Y	313	CLA	CAA-C2A-C3A	-2.59	105.99	113.00
3	G	614	CLA	C3B-C4B-NB	-2.59	108.21	110.53
2	N	609	CHL	CMD-C2D-C3D	2.59	129.86	124.68
2	N	609	CHL	C3C-C4C-NC	-2.59	108.32	114.65
2	N	606	CHL	CMD-C2D-C3D	2.59	129.86	124.68
2	Y	306	CHL	C3D-C4D-CHA	2.59	112.47	108.54
2	N	606	CHL	C1C-CHC-C4B	2.59	125.32	116.07
2	G	605	CHL	C3C-C4C-NC	-2.59	108.33	114.65
3	N	611	CLA	CMB-C2B-C1B	-2.58	121.48	125.42
5	Y	318	NEX	C19-C9-C10	-2.58	118.63	122.82
3	G	612	CLA	O2D-CGD-O1D	-2.57	118.84	123.85
4	Y	316	LUT	C21-C26-C27	-2.57	109.87	112.83
2	N	605	CHL	C3D-C4D-CHA	2.57	112.44	108.54
3	G	613	CLA	CHB-C4A-NA	2.57	128.10	124.40
3	Y	305	CLA	CMB-C2B-C3B	2.56	132.57	126.55
2	Y	307	CHL	O2D-CGD-O1D	-2.56	118.87	123.85
4	Y	316	LUT	C11-C10-C9	-2.56	123.69	127.28
7	N	619	XAT	C15-C35-C34	-2.55	118.30	123.52
2	G	607	CHL	C4D-ND-C1D	2.55	107.15	105.22
2	Y	310	CHL	CMB-C2B-C3B	2.55	129.78	124.68
4	Y	316	LUT	C37-C21-C22	-2.54	104.67	109.41
7	N	619	XAT	C6-C7-C8	-2.54	120.62	125.99
2	G	601	CHL	O2A-CGA-O1A	-2.53	117.30	123.63
3	G	602	CLA	CMB-C2B-C1B	-2.53	121.57	125.42
4	Y	317	LUT	C38-C25-C24	-2.53	117.38	123.36
2	N	608	CHL	OMC-CMC-C2C	-2.52	120.74	125.12
3	Y	305	CLA	O2D-CGD-CBD	2.52	115.63	111.23
2	G	609	CHL	OMC-CMC-C2C	-2.52	120.75	125.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	609	CHL	CHA-C1A-C2A	-2.51	127.41	133.31
2	N	608	CHL	O2D-CGD-CBD	2.51	113.70	110.95
2	G	607	CHL	CHA-C1A-C2A	-2.51	127.41	133.31
2	N	608	CHL	C3C-C4C-NC	-2.50	108.54	114.65
3	N	602	CLA	C3B-C4B-NB	-2.50	108.30	110.53
2	N	606	CHL	CMB-C2B-C3B	2.50	129.68	124.68
2	Y	307	CHL	CMB-C2B-C3B	2.50	129.68	124.68
2	N	608	CHL	CMB-C2B-C3B	2.50	129.67	124.68
2	G	609	CHL	CHA-C1A-C2A	-2.50	127.45	133.31
2	Y	308	CHL	C3C-C4C-NC	-2.49	108.55	114.65
3	Y	315	CLA	C4A-NA-C1A	2.49	107.81	106.68
3	N	613	CLA	CMB-C2B-C3B	2.48	132.39	126.55
2	Y	306	CHL	CMB-C2B-C3B	2.48	129.63	124.68
2	G	601	CHL	C4C-CHD-C1D	2.48	124.93	116.07
5	N	617	NEX	C39-C29-C30	-2.47	118.81	122.82
5	N	617	NEX	C28-C29-C30	2.47	122.90	119.01
2	G	608	CHL	C3C-C4C-NC	-2.47	108.62	114.65
3	N	602	CLA	O2D-CGD-CBD	2.46	115.53	111.23
2	N	609	CHL	O2D-CGD-O1D	-2.46	119.06	123.85
4	Y	316	LUT	C15-C14-C13	-2.46	123.83	127.28
4	Y	317	LUT	C35-C34-C33	-2.46	123.83	127.28
3	N	602	CLA	CHB-C4A-NA	2.46	127.94	124.40
3	G	611	CLA	C3B-C4B-NB	-2.45	108.34	110.53
3	Y	315	CLA	C3B-C4B-NB	-2.45	108.34	110.53
2	G	607	CHL	CMD-C2D-C3D	2.45	129.59	124.68
4	G	615	LUT	C10-C11-C12	-2.45	116.10	123.20
4	N	616	LUT	C7-C8-C9	-2.45	122.61	126.23
2	G	609	CHL	O2D-CGD-O1D	-2.45	119.08	123.85
4	N	616	LUT	C30-C31-C32	-2.44	116.14	123.20
2	Y	307	CHL	O2D-CGD-CBD	2.43	113.62	110.95
4	N	616	LUT	C18-C5-C6	-2.43	121.83	124.48
2	N	608	CHL	C4C-CHD-C1D	2.43	124.76	116.07
2	G	607	CHL	C3C-C4C-NC	-2.43	108.72	114.65
4	Y	317	LUT	C31-C30-C29	-2.42	123.88	127.28
4	G	616	LUT	C38-C25-C24	-2.42	117.62	123.36
2	Y	309	CHL	C3C-C4C-NC	-2.42	108.74	114.65
4	N	616	LUT	C16-C1-C6	-2.42	106.45	110.24
2	G	605	CHL	CHA-C1A-C2A	-2.42	127.63	133.31
2	N	607	CHL	OMC-CMC-C2C	-2.41	120.93	125.12
6	N	618	LHG	O8-C23-C24	2.41	119.19	111.83
3	G	602	CLA	CHB-C1B-NB	2.41	127.67	124.05
3	N	604	CLA	CHB-C4A-NA	2.40	127.87	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Y	308	CHL	CAA-C2A-C3A	-2.40	106.50	113.00
2	Y	307	CHL	C1-C2-C3	-2.40	122.88	126.76
6	Y	319	LHG	O8-C23-O10	-2.40	117.62	123.63
3	G	610	CLA	O2D-CGD-CBD	2.40	115.43	111.23
7	G	619	XAT	C18-C5-C4	2.40	116.94	114.24
3	G	604	CLA	CHB-C4A-NA	2.39	127.85	124.40
3	N	613	CLA	CHB-C4A-NA	2.39	127.85	124.40
5	G	617	NEX	C8-C7-C6	-2.39	174.84	177.66
2	G	606	CHL	C4C-CHD-C1D	2.39	124.61	116.07
3	Y	311	CLA	CHC-C4B-NB	2.39	127.63	124.05
2	G	605	CHL	CMB-C2B-C3B	2.39	129.45	124.68
6	G	618	LHG	O8-C23-O10	-2.39	117.66	123.63
2	G	605	CHL	C3D-C4D-CHA	2.38	112.16	108.54
3	Y	305	CLA	CHB-C4A-NA	2.38	127.84	124.40
2	N	607	CHL	C3C-C4C-NC	-2.38	108.83	114.65
3	N	610	CLA	CHB-C1B-NB	2.38	127.62	124.05
2	N	601	CHL	C3C-C4C-NC	-2.38	108.84	114.65
3	Y	313	CLA	CMD-C2D-C3D	2.37	133.13	127.69
3	Y	315	CLA	O2A-CGA-O1A	-2.37	117.71	123.63
2	Y	306	CHL	CHA-C1A-C2A	-2.36	127.77	133.31
2	Y	302	CHL	C3C-C4C-NC	-2.36	108.89	114.65
3	Y	303	CLA	CHB-C4A-NA	2.35	127.80	124.40
3	G	614	CLA	CAA-CBA-CGA	-2.35	106.53	113.21
3	G	610	CLA	O2A-CGA-O1A	-2.35	117.75	123.63
2	Y	309	CHL	C4C-CHD-C1D	2.35	124.48	116.07
2	Y	309	CHL	CMB-C2B-C3B	2.35	129.38	124.68
4	G	616	LUT	C16-C1-C6	-2.35	106.56	110.24
2	N	605	CHL	O1D-CGD-CBD	2.35	128.28	124.72
2	N	607	CHL	CMD-C2D-C3D	2.35	129.37	124.68
2	N	607	CHL	CHA-C1A-C2A	-2.35	127.80	133.31
5	Y	318	NEX	C27-C28-C29	-2.34	121.89	125.53
2	Y	302	CHL	C4D-CHA-CBD	-2.34	106.61	108.97
4	G	616	LUT	C31-C30-C29	-2.33	124.00	127.28
2	Y	306	CHL	C4C-CHD-C1D	2.33	124.42	116.07
2	G	606	CHL	CMD-C2D-C3D	2.33	129.34	124.68
2	Y	307	CHL	C4C-CHD-C1D	2.33	124.40	116.07
2	G	605	CHL	C4C-CHD-C1D	2.33	124.39	116.07
3	N	614	CLA	O2A-CGA-O1A	-2.32	117.83	123.63
3	N	612	CLA	CHB-C4A-NA	2.32	127.74	124.40
2	N	605	CHL	CHA-C1A-C2A	-2.32	127.87	133.31
7	N	619	XAT	C7-C8-C9	-2.31	121.94	125.53
4	N	616	LUT	C10-C11-C12	-2.31	116.51	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	606	CHL	CHA-C1A-C2A	-2.31	127.89	133.31
3	Y	311	CLA	C3B-C4B-NB	-2.30	108.47	110.53
2	Y	309	CHL	O2D-CGD-CBD	2.30	113.47	110.95
2	N	606	CHL	C4C-CHD-C1D	2.30	124.29	116.07
4	Y	316	LUT	C10-C11-C12	-2.30	116.55	123.20
3	Y	311	CLA	O2D-CGD-CBD	2.30	115.24	111.23
2	G	609	CHL	O2A-CGA-O1A	-2.29	117.89	123.63
2	Y	310	CHL	CHA-C1A-C2A	-2.29	127.92	133.31
3	Y	304	CLA	C1-C2-C3	-2.29	122.44	126.20
3	N	614	CLA	C3B-C4B-NB	-2.28	108.49	110.53
3	N	610	CLA	C1D-ND-C4D	-2.28	104.71	106.31
3	Y	312	CLA	CMD-C2D-C3D	2.28	132.91	127.69
2	Y	302	CHL	C3D-C4D-CHA	2.27	111.99	108.54
4	Y	317	LUT	C10-C11-C12	-2.27	116.63	123.20
3	G	614	CLA	CHB-C4A-NA	2.27	127.67	124.40
3	Y	312	CLA	CMD-C2D-C1D	-2.26	120.74	124.73
3	N	611	CLA	CMB-C2B-C3B	2.26	131.87	126.55
3	N	611	CLA	CHB-C4A-NA	2.26	127.66	124.40
4	G	615	LUT	C38-C25-C24	-2.26	118.01	123.36
2	Y	306	CHL	CMD-C2D-C3D	2.26	129.19	124.68
3	Y	313	CLA	CHB-C4A-NA	2.25	127.65	124.40
2	G	608	CHL	C4C-CHD-C1D	2.25	124.12	116.07
2	N	601	CHL	C4C-CHD-C1D	2.25	124.11	116.07
3	N	614	CLA	CHB-C4A-NA	2.25	127.64	124.40
3	Y	314	CLA	CHB-C4A-NA	2.25	127.64	124.40
4	N	615	LUT	C26-C27-C28	-2.24	121.09	124.58
2	G	601	CHL	C4D-CHA-CBD	-2.24	106.71	108.97
2	Y	310	CHL	CMD-C2D-C3D	2.23	129.15	124.68
4	N	616	LUT	C38-C25-C24	-2.23	118.08	123.36
2	N	609	CHL	O1D-CGD-CBD	2.23	128.10	124.72
2	Y	307	CHL	CHA-C1A-C2A	-2.22	128.09	133.31
5	G	617	NEX	C39-C29-C30	-2.22	119.22	122.82
2	G	605	CHL	C1B-CHB-C4A	2.22	122.75	121.32
2	N	605	CHL	C4C-CHD-C1D	2.22	124.01	116.07
2	Y	302	CHL	C4C-CHD-C1D	2.22	124.00	116.07
4	Y	317	LUT	C18-C5-C6	-2.22	122.07	124.48
3	G	613	CLA	CMB-C2B-C1B	-2.21	122.05	125.42
3	G	610	CLA	CMB-C2B-C1B	-2.21	122.05	125.42
2	G	608	CHL	C3D-C4D-CHA	2.21	111.89	108.54
2	Y	309	CHL	CHA-C1A-C2A	-2.21	128.12	133.31
3	G	610	CLA	CHB-C4A-NA	2.20	127.58	124.40
2	G	606	CHL	C1C-C2C-CMC	-2.20	122.83	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Y	309	CHL	CMD-C2D-C3D	2.20	129.08	124.68
3	N	612	CLA	C1-C2-C3	-2.20	122.60	126.20
2	Y	309	CHL	O1D-CGD-CBD	2.20	128.05	124.72
2	N	601	CHL	C3D-C4D-CHA	2.19	111.87	108.54
2	N	607	CHL	C4D-ND-C1D	2.19	106.88	105.22
2	G	605	CHL	O2A-CGA-O1A	-2.19	118.16	123.63
7	N	619	XAT	C38-C25-C24	2.18	116.69	114.24
2	N	606	CHL	C3C-C4C-NC	-2.18	109.32	114.65
3	Y	311	CLA	CMA-C3A-C2A	-2.18	105.55	113.98
2	G	609	CHL	CMD-C2D-C3D	2.18	129.04	124.68
3	G	611	CLA	CHB-C1B-NB	2.18	127.32	124.05
3	Y	303	CLA	CMB-C2B-C1B	-2.18	122.11	125.42
5	N	617	NEX	C11-C12-C13	-2.17	120.41	126.36
4	G	616	LUT	C30-C31-C32	-2.17	116.91	123.20
3	N	612	CLA	O2D-CGD-CBD	2.17	115.02	111.23
2	N	608	CHL	CHA-C1A-C2A	-2.16	128.22	133.31
2	Y	306	CHL	C1B-CHB-C4A	2.16	122.72	121.32
2	Y	308	CHL	C1-C2-C3	-2.16	122.66	126.20
2	Y	307	CHL	CBA-CAA-C2A	-2.15	107.43	113.78
2	G	609	CHL	C1C-C2C-CMC	-2.15	122.92	126.80
2	Y	307	CHL	O2A-CGA-O1A	-2.15	118.24	123.63
3	G	611	CLA	CHB-C4A-NA	2.15	127.51	124.40
2	N	605	CHL	CAA-C2A-C3A	-2.15	107.19	113.00
3	N	604	CLA	CMB-C2B-C3B	2.15	131.60	126.55
2	N	601	CHL	C7-C6-C5	-2.15	107.54	113.26
2	Y	307	CHL	C1C-C2C-CMC	-2.14	122.94	126.80
3	G	604	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
3	Y	312	CLA	C1D-ND-C4D	-2.14	104.81	106.31
3	Y	311	CLA	C2A-C3A-C4A	-2.14	98.41	101.87
2	G	609	CHL	O1D-CGD-CBD	2.14	127.97	124.72
4	N	615	LUT	C38-C25-C24	-2.13	118.31	123.36
2	G	606	CHL	C4D-ND-C1D	2.13	106.84	105.22
2	Y	302	CHL	O1D-CGD-CBD	2.13	127.95	124.72
4	G	615	LUT	C8-C7-C6	-2.13	121.31	127.00
4	Y	316	LUT	C1-C2-C3	2.12	118.25	113.59
2	N	608	CHL	CMD-C2D-C3D	2.12	128.92	124.68
4	N	616	LUT	C27-C28-C29	-2.12	121.77	126.32
2	Y	308	CHL	CHA-C1A-C2A	-2.11	128.34	133.31
3	G	604	CLA	CMB-C2B-C3B	2.11	131.52	126.55
7	G	619	XAT	C24-C23-C22	-2.11	106.84	110.79
3	Y	315	CLA	CHB-C4A-NA	2.11	127.45	124.40
4	Y	317	LUT	C1-C2-C3	2.11	118.22	113.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Y	314	CLA	CMB-C2B-C1B	-2.11	122.20	125.42
2	Y	306	CHL	O2A-CGA-O1A	-2.11	118.35	123.63
3	G	602	CLA	CHB-C4A-NA	2.11	127.44	124.40
4	G	615	LUT	C35-C15-C14	-2.11	119.21	123.52
4	Y	316	LUT	C35-C34-C33	-2.11	124.33	127.28
4	G	615	LUT	C1-C2-C3	2.11	118.21	113.59
7	G	619	XAT	C40-C33-C32	2.11	121.30	118.09
2	G	606	CHL	C3C-C4C-NC	-2.11	109.50	114.65
4	Y	316	LUT	C30-C31-C32	-2.10	117.12	123.20
2	N	601	CHL	C6-C5-C3	2.10	118.58	113.47
2	N	606	CHL	C1C-C2C-CMC	-2.09	123.04	126.80
3	Y	314	CLA	CHD-C1D-ND	-2.09	121.87	124.80
3	N	612	CLA	CAA-C2A-C3A	-2.08	107.37	113.00
3	N	613	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
3	N	602	CLA	CMB-C2B-C1B	-2.08	122.25	125.42
3	G	614	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
7	G	619	XAT	C38-C25-C24	2.07	116.56	114.24
3	Y	313	CLA	C2A-C1A-CHA	2.07	127.45	123.87
2	G	606	CHL	C1-C2-C3	-2.06	123.42	126.76
3	G	612	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
4	Y	316	LUT	C38-C25-C24	-2.06	118.48	123.36
2	N	605	CHL	CMD-C2D-C3D	2.06	128.80	124.68
2	Y	306	CHL	O1D-CGD-CBD	2.06	127.84	124.72
3	Y	311	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
2	Y	307	CHL	C3C-C4C-NC	-2.05	109.63	114.65
3	N	610	CLA	C3B-C4B-NB	-2.05	108.70	110.53
7	N	619	XAT	C24-C23-C22	-2.05	106.96	110.79
3	G	612	CLA	C3B-C4B-NB	-2.05	108.70	110.53
2	N	606	CHL	O2A-CGA-O1A	-2.05	118.51	123.63
7	N	619	XAT	O4-C5-C6	-2.04	57.31	58.93
3	G	612	CLA	CMB-C2B-C1B	-2.04	122.31	125.42
4	N	615	LUT	C27-C28-C29	-2.04	121.94	126.32
6	Y	319	LHG	O4-P-O5	2.04	121.92	112.44
4	G	615	LUT	C26-C27-C28	-2.03	121.42	124.58
3	G	610	CLA	CHB-C1B-C2B	-2.03	121.53	127.43
3	G	610	CLA	CAC-C3C-C4C	2.03	127.43	124.79
2	G	608	CHL	O1D-CGD-CBD	2.02	127.79	124.72
3	N	612	CLA	C2A-C1A-CHA	2.02	127.37	123.87
2	N	601	CHL	C4D-CHA-CBD	-2.02	106.94	108.97
7	Y	301	XAT	C31-C32-C33	-2.01	120.84	126.36
2	Y	309	CHL	OMC-CMC-C2C	-2.01	121.62	125.12
5	G	617	NEX	C40-C33-C32	2.01	121.16	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Y	313	CLA	CMD-C2D-C1D	-2.01	121.19	124.73
2	N	608	CHL	C4D-ND-C1D	2.01	106.74	105.22

All (74) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	N	601	CHL	NA
2	N	601	CHL	ND
2	N	601	CHL	NC
2	N	605	CHL	NA
2	N	605	CHL	ND
2	N	605	CHL	NC
2	N	606	CHL	NA
2	N	606	CHL	ND
2	N	606	CHL	NC
2	N	607	CHL	NA
2	N	607	CHL	ND
2	N	607	CHL	NC
2	N	608	CHL	NA
2	N	608	CHL	ND
2	N	608	CHL	NC
2	N	609	CHL	NA
2	N	609	CHL	ND
2	N	609	CHL	NC
2	G	601	CHL	NA
2	G	601	CHL	ND
2	G	601	CHL	NC
2	G	605	CHL	NA
2	G	605	CHL	ND
2	G	605	CHL	NC
2	G	606	CHL	NA
2	G	606	CHL	ND
2	G	606	CHL	NC
2	G	607	CHL	NA
2	G	607	CHL	ND
2	G	607	CHL	NC
2	G	608	CHL	NA
2	G	608	CHL	ND
2	G	608	CHL	NC
2	G	609	CHL	NA
2	G	609	CHL	ND
2	G	609	CHL	NC

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Mol	Chain	Res	Type	Atom
2	Y	302	CHL	NA
2	Y	302	CHL	ND
2	Y	302	CHL	NC
2	Y	306	CHL	NA
2	Y	306	CHL	ND
2	Y	306	CHL	NC
2	Y	307	CHL	NA
2	Y	307	CHL	ND
2	Y	307	CHL	NC
2	Y	308	CHL	NA
2	Y	308	CHL	ND
2	Y	308	CHL	NC
2	Y	309	CHL	NA
2	Y	309	CHL	ND
2	Y	309	CHL	NC
2	Y	310	CHL	NA
2	Y	310	CHL	ND
2	Y	310	CHL	NC
3	N	602	CLA	ND
3	N	603	CLA	ND
3	N	604	CLA	ND
3	N	610	CLA	ND
3	N	611	CLA	ND
3	N	612	CLA	ND
3	N	613	CLA	ND
3	N	614	CLA	ND
3	G	602	CLA	ND
3	G	603	CLA	ND
3	G	610	CLA	ND
3	G	612	CLA	ND
3	G	614	CLA	ND
3	Y	303	CLA	ND
3	Y	304	CLA	ND
3	Y	305	CLA	ND
3	Y	311	CLA	ND
3	Y	313	CLA	ND
3	Y	314	CLA	ND
3	Y	315	CLA	ND

All (613) torsion outliers are listed below:

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Mol	Chain	Res	Type	Atoms
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Mol	Chain	Res	Type	Atoms
2	N	601	CHL	C1C-C2C-CMC-OMC
2	N	601	CHL	C3C-C2C-CMC-OMC
2	N	606	CHL	C1A-C2A-CAA-CBA
2	N	606	CHL	C3A-C2A-CAA-CBA
2	N	606	CHL	CBA-CGA-O2A-C1
2	N	606	CHL	O1A-CGA-O2A-C1
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	C1C-C2C-CMC-OMC
2	N	608	CHL	C3C-C2C-CMC-OMC
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	N	609	CHL	C4C-C3C-CAC-CBC
2	N	609	CHL	C11-C10-C8-C9
2	G	601	CHL	C1C-C2C-CMC-OMC
2	G	601	CHL	C3C-C2C-CMC-OMC
2	G	605	CHL	C1A-C2A-CAA-CBA
2	G	606	CHL	C1A-C2A-CAA-CBA
2	G	606	CHL	O1A-CGA-O2A-C1
2	G	607	CHL	C1C-C2C-CMC-OMC
2	G	607	CHL	C3C-C2C-CMC-OMC
2	G	608	CHL	C1C-C2C-CMC-OMC
2	G	608	CHL	C3C-C2C-CMC-OMC
2	G	609	CHL	C1A-C2A-CAA-CBA
2	G	609	CHL	C1C-C2C-CMC-OMC
2	G	609	CHL	C3C-C2C-CMC-OMC
2	G	609	CHL	C4C-C3C-CAC-CBC
2	Y	302	CHL	C1C-C2C-CMC-OMC
2	Y	302	CHL	C3C-C2C-CMC-OMC
2	Y	306	CHL	C1C-C2C-CMC-OMC
2	Y	307	CHL	C1A-C2A-CAA-CBA
2	Y	307	CHL	C3C-C2C-CMC-OMC
2	Y	308	CHL	C1C-C2C-CMC-OMC
2	Y	308	CHL	C3C-C2C-CMC-OMC
2	Y	309	CHL	C1C-C2C-CMC-OMC
2	Y	309	CHL	C3C-C2C-CMC-OMC
2	Y	310	CHL	C1C-C2C-CMC-OMC
2	Y	310	CHL	C3C-C2C-CMC-OMC

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Mol	Chain	Res	Type	Atoms
2	Y	310	CHL	CBD-CGD-O2D-CED
3	N	602	CLA	CHA-CBD-CGD-O1D
3	N	602	CLA	CHA-CBD-CGD-O2D
3	N	604	CLA	CBD-CGD-O2D-CED
3	N	610	CLA	C2B-C3B-CAB-CBB
3	N	610	CLA	C4B-C3B-CAB-CBB
3	N	613	CLA	CBD-CGD-O2D-CED
3	N	614	CLA	CBD-CGD-O2D-CED
3	G	602	CLA	C2B-C3B-CAB-CBB
3	G	602	CLA	C4B-C3B-CAB-CBB
3	G	602	CLA	CHA-CBD-CGD-O2D
3	G	604	CLA	C1A-C2A-CAA-CBA
3	G	604	CLA	C3A-C2A-CAA-CBA
3	G	604	CLA	CHA-CBD-CGD-O1D
3	G	604	CLA	CHA-CBD-CGD-O2D
3	G	613	CLA	CBD-CGD-O2D-CED
3	G	614	CLA	CBD-CGD-O2D-CED
3	Y	304	CLA	CBD-CGD-O2D-CED
3	Y	305	CLA	C1A-C2A-CAA-CBA
3	Y	305	CLA	CHA-CBD-CGD-O1D
3	Y	305	CLA	CHA-CBD-CGD-O2D
3	Y	314	CLA	CBD-CGD-O2D-CED
3	Y	315	CLA	C2B-C3B-CAB-CBB
3	Y	315	CLA	C4B-C3B-CAB-CBB
4	G	615	LUT	C27-C28-C29-C30
5	N	617	NEX	O24-C26-C27-C28
5	G	617	NEX	O24-C26-C27-C28
5	Y	318	NEX	C9-C10-C11-C12
5	Y	318	NEX	C28-C29-C30-C31
5	Y	318	NEX	C39-C29-C30-C31
6	G	618	LHG	C3-O3-P-O5
6	G	618	LHG	C4-O6-P-O3
6	G	618	LHG	C4-O6-P-O4
6	Y	319	LHG	O1-C1-C2-C3
6	Y	319	LHG	C3-O3-P-O5
6	Y	319	LHG	C4-O6-P-O3
6	Y	319	LHG	C4-O6-P-O4
6	Y	319	LHG	O10-C23-O8-C6
6	Y	319	LHG	C24-C23-O8-C6
7	N	619	XAT	O4-C6-C7-C8
7	N	619	XAT	C7-C8-C9-C10
7	N	619	XAT	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
7	G	619	XAT	O4-C6-C7-C8
7	G	619	XAT	C7-C8-C9-C10
7	G	619	XAT	C7-C8-C9-C19
7	G	619	XAT	O24-C26-C27-C28
7	G	619	XAT	C31-C32-C33-C34
7	Y	301	XAT	O4-C6-C7-C8
7	Y	301	XAT	C7-C8-C9-C10
7	Y	301	XAT	C7-C8-C9-C19
3	Y	305	CLA	O1D-CGD-O2D-CED
2	G	608	CHL	O1D-CGD-O2D-CED
2	G	608	CHL	CBD-CGD-O2D-CED
2	G	609	CHL	CBD-CGD-O2D-CED
2	Y	306	CHL	CBD-CGD-O2D-CED
3	N	610	CLA	CBD-CGD-O2D-CED
3	Y	303	CLA	CBD-CGD-O2D-CED
3	Y	305	CLA	CBD-CGD-O2D-CED
3	Y	315	CLA	CBD-CGD-O2D-CED
2	Y	307	CHL	O1A-CGA-O2A-C1
6	G	618	LHG	O10-C23-O8-C6
2	Y	307	CHL	CBA-CGA-O2A-C1
2	N	607	CHL	O1A-CGA-O2A-C1
2	G	607	CHL	O1A-CGA-O2A-C1
2	Y	308	CHL	O1A-CGA-O2A-C1
3	Y	315	CLA	O1A-CGA-O2A-C1
6	N	618	LHG	O10-C23-O8-C6
2	N	607	CHL	O1D-CGD-O2D-CED
3	G	613	CLA	O1D-CGD-O2D-CED
3	G	614	CLA	O1D-CGD-O2D-CED
3	Y	303	CLA	O1D-CGD-O2D-CED
2	Y	310	CHL	O1D-CGD-O2D-CED
3	N	614	CLA	O1D-CGD-O2D-CED
3	Y	314	CLA	O1D-CGD-O2D-CED
2	G	601	CHL	C3-C5-C6-C7
2	G	606	CHL	CBA-CGA-O2A-C1
3	Y	315	CLA	CBA-CGA-O2A-C1
6	N	618	LHG	C24-C23-O8-C6
6	G	618	LHG	C24-C23-O8-C6
2	N	605	CHL	CBD-CGD-O2D-CED
2	N	608	CHL	CBD-CGD-O2D-CED
3	Y	313	CLA	CBD-CGD-O2D-CED
3	N	604	CLA	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
2	Y	306	CHL	O1D-CGD-O2D-CED
2	G	607	CHL	C2A-CAA-CBA-CGA
2	G	607	CHL	C3-C5-C6-C7
3	G	604	CLA	C3-C5-C6-C7
3	Y	312	CLA	C3-C5-C6-C7
3	Y	313	CLA	C3-C5-C6-C7
2	N	607	CHL	CBA-CGA-O2A-C1
2	G	607	CHL	CBA-CGA-O2A-C1
2	Y	308	CHL	CBA-CGA-O2A-C1
3	G	612	CLA	CBA-CGA-O2A-C1
4	G	616	LUT	C29-C30-C31-C32
2	G	609	CHL	O1D-CGD-O2D-CED
3	N	611	CLA	C3-C5-C6-C7
3	G	604	CLA	CBD-CGD-O2D-CED
3	Y	315	CLA	O1D-CGD-O2D-CED
3	N	614	CLA	CBA-CGA-O2A-C1
3	G	612	CLA	O1A-CGA-O2A-C1
3	G	603	CLA	CBD-CGD-O2D-CED
3	N	604	CLA	C3-C5-C6-C7
3	N	614	CLA	O1A-CGA-O2A-C1
2	N	607	CHL	C2A-CAA-CBA-CGA
3	N	610	CLA	O1D-CGD-O2D-CED
3	G	614	CLA	CBA-CGA-O2A-C1
2	N	609	CHL	CBD-CGD-O2D-CED
2	G	607	CHL	CBD-CGD-O2D-CED
3	Y	311	CLA	CBD-CGD-O2D-CED
3	G	614	CLA	O1A-CGA-O2A-C1
3	Y	313	CLA	O1D-CGD-O2D-CED
2	Y	308	CHL	C3-C5-C6-C7
2	Y	309	CHL	C11-C12-C13-C14
2	Y	310	CHL	C6-C7-C8-C9
2	N	609	CHL	C2C-C3C-CAC-CBC
6	Y	319	LHG	O2-C2-C3-O3
4	N	615	LUT	C27-C28-C29-C39
4	G	615	LUT	C27-C28-C29-C39
7	N	619	XAT	C7-C8-C9-C19
7	N	619	XAT	C31-C32-C33-C40
7	G	619	XAT	C31-C32-C33-C40
2	N	608	CHL	O1D-CGD-O2D-CED
2	G	605	CHL	CBA-CGA-O2A-C1
3	G	611	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
6	N	618	LHG	C28-C29-C30-C31
2	Y	302	CHL	C15-C16-C17-C18
3	Y	314	CLA	C13-C15-C16-C17
2	N	608	CHL	C12-C13-C15-C16
3	N	611	CLA	C6-C7-C8-C10
3	G	612	CLA	C12-C13-C15-C16
3	G	613	CLA	C3-C5-C6-C7
2	G	601	CHL	C15-C16-C17-C18
3	G	612	CLA	C15-C16-C17-C18
2	Y	308	CHL	C2A-CAA-CBA-CGA
5	Y	318	NEX	C30-C31-C32-C33
2	G	607	CHL	C5-C6-C7-C8
3	N	611	CLA	C10-C11-C12-C13
3	G	602	CLA	C10-C11-C12-C13
3	N	612	CLA	C3-C5-C6-C7
2	N	605	CHL	O1D-CGD-O2D-CED
3	N	603	CLA	C13-C15-C16-C17
3	G	603	CLA	C5-C6-C7-C8
3	Y	305	CLA	CBA-CGA-O2A-C1
6	Y	319	LHG	C23-C24-C25-C26
3	G	612	CLA	C13-C15-C16-C17
2	N	609	CHL	C15-C16-C17-C18
2	Y	308	CHL	C5-C6-C7-C8
3	G	612	CLA	C8-C10-C11-C12
3	G	611	CLA	C3-C5-C6-C7
3	G	611	CLA	O1A-CGA-O2A-C1
6	Y	319	LHG	C1-C2-C3-O3
3	N	612	CLA	CBA-CGA-O2A-C1
3	Y	313	CLA	CBA-CGA-O2A-C1
3	Y	312	CLA	C8-C10-C11-C12
3	N	611	CLA	C5-C6-C7-C8
3	G	603	CLA	C15-C16-C17-C18
3	G	603	CLA	O1D-CGD-O2D-CED
2	G	605	CHL	O1A-CGA-O2A-C1
3	G	604	CLA	O1D-CGD-O2D-CED
3	Y	312	CLA	C10-C11-C12-C13
3	G	603	CLA	C10-C11-C12-C13
6	N	618	LHG	C23-C24-C25-C26
3	G	612	CLA	C5-C6-C7-C8
4	Y	316	LUT	C27-C28-C29-C39
5	G	617	NEX	C11-C12-C13-C20
7	Y	301	XAT	C11-C12-C13-C20

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Mol	Chain	Res	Type	Atoms
3	G	604	CLA	C13-C15-C16-C17
3	Y	305	CLA	O1A-CGA-O2A-C1
2	N	608	CHL	C2A-CAA-CBA-CGA
2	Y	309	CHL	C2A-CAA-CBA-CGA
3	Y	304	CLA	C2A-CAA-CBA-CGA
2	N	601	CHL	C15-C16-C17-C18
3	N	613	CLA	C3-C5-C6-C7
3	Y	305	CLA	C2-C1-O2A-CGA
3	N	611	CLA	C16-C17-C18-C19
3	Y	313	CLA	O1A-CGA-O2A-C1
3	N	611	CLA	C8-C10-C11-C12
2	G	607	CHL	O1D-CGD-O2D-CED
6	Y	319	LHG	C26-C27-C28-C29
5	Y	318	NEX	C14-C15-C35-C34
6	N	618	LHG	C25-C26-C27-C28
6	Y	319	LHG	C32-C33-C34-C35
6	G	618	LHG	C23-C24-C25-C26
6	Y	319	LHG	O1-C1-C2-O2
3	Y	311	CLA	C4B-C3B-CAB-CBB
3	N	611	CLA	C16-C17-C18-C20
3	G	612	CLA	C16-C17-C18-C20
2	N	605	CHL	CBA-CGA-O2A-C1
3	N	612	CLA	O1A-CGA-O2A-C1
3	Y	314	CLA	C3-C5-C6-C7
2	N	605	CHL	C3A-C2A-CAA-CBA
2	G	601	CHL	C3A-C2A-CAA-CBA
2	G	605	CHL	C3A-C2A-CAA-CBA
2	G	606	CHL	C3A-C2A-CAA-CBA
2	Y	306	CHL	C3A-C2A-CAA-CBA
2	Y	307	CHL	C3A-C2A-CAA-CBA
3	N	603	CLA	C3A-C2A-CAA-CBA
3	Y	304	CLA	C3A-C2A-CAA-CBA
3	Y	304	CLA	C10-C11-C12-C13
3	Y	311	CLA	O1D-CGD-O2D-CED
5	Y	318	NEX	C33-C34-C35-C15
3	G	612	CLA	C16-C17-C18-C19
6	Y	319	LHG	C15-C16-C17-C18
6	N	618	LHG	C15-C16-C17-C18
6	G	618	LHG	C9-C10-C11-C12
2	N	609	CHL	O1D-CGD-O2D-CED
3	N	603	CLA	C2B-C3B-CAB-CBB
3	N	612	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
3	G	603	CLA	C2B-C3B-CAB-CBB
3	G	610	CLA	C2B-C3B-CAB-CBB
4	G	615	LUT	C1-C6-C7-C8
2	N	609	CHL	C3-C5-C6-C7
6	N	618	LHG	C32-C33-C34-C35
3	G	613	CLA	C13-C15-C16-C17
6	G	618	LHG	C32-C33-C34-C35
6	G	618	LHG	C14-C15-C16-C17
5	G	617	NEX	C29-C30-C31-C32
6	N	618	LHG	C8-C7-O7-C5
6	G	618	LHG	C8-C7-O7-C5
3	N	604	CLA	C13-C15-C16-C17
6	N	618	LHG	O9-C7-O7-C5
6	G	618	LHG	O9-C7-O7-C5
6	Y	319	LHG	C29-C30-C31-C32
2	G	601	CHL	C10-C11-C12-C13
5	N	617	NEX	C11-C12-C13-C20
6	G	618	LHG	C29-C30-C31-C32
3	G	612	CLA	C10-C11-C12-C13
2	N	605	CHL	O1A-CGA-O2A-C1
3	G	603	CLA	C3-C5-C6-C7
3	N	611	CLA	C13-C15-C16-C17
2	N	609	CHL	C8-C10-C11-C12
3	Y	305	CLA	C3-C5-C6-C7
6	N	618	LHG	C14-C15-C16-C17
2	Y	302	CHL	CBD-CGD-O2D-CED
3	N	612	CLA	CBD-CGD-O2D-CED
6	Y	319	LHG	C28-C29-C30-C31
2	N	601	CHL	C13-C15-C16-C17
3	N	611	CLA	C15-C16-C17-C18
3	Y	313	CLA	C10-C11-C12-C13
3	N	603	CLA	C1A-C2A-CAA-CBA
3	N	604	CLA	C1A-C2A-CAA-CBA
3	N	611	CLA	C1A-C2A-CAA-CBA
3	G	611	CLA	C1A-C2A-CAA-CBA
3	Y	304	CLA	C1A-C2A-CAA-CBA
3	Y	315	CLA	C1A-C2A-CAA-CBA
3	N	612	CLA	C8-C10-C11-C12
3	N	612	CLA	C10-C11-C12-C13
2	N	607	CHL	C12-C13-C15-C16
2	N	608	CHL	C11-C10-C8-C7
2	N	609	CHL	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
2	G	607	CHL	C12-C13-C15-C16
3	N	603	CLA	C6-C7-C8-C10
3	N	613	CLA	C6-C7-C8-C10
3	G	611	CLA	C11-C10-C8-C7
3	G	613	CLA	C12-C13-C15-C16
3	Y	304	CLA	C6-C7-C8-C10
2	N	607	CHL	C15-C16-C17-C18
2	G	608	CHL	C5-C6-C7-C8
3	Y	303	CLA	C15-C16-C17-C18
3	Y	303	CLA	C2A-CAA-CBA-CGA
2	N	607	CHL	C14-C13-C15-C16
2	Y	308	CHL	C11-C10-C8-C9
3	N	611	CLA	C6-C7-C8-C9
3	G	611	CLA	C11-C10-C8-C9
5	N	617	NEX	C29-C30-C31-C32
6	G	618	LHG	C25-C26-C27-C28
3	N	604	CLA	CBA-CGA-O2A-C1
3	G	611	CLA	C8-C10-C11-C12
6	G	618	LHG	C28-C29-C30-C31
2	Y	308	CHL	CHA-CBD-CGD-O1D
3	G	602	CLA	C15-C16-C17-C18
6	G	618	LHG	C10-C11-C12-C13
2	N	606	CHL	C3C-C2C-CMC-OMC
2	Y	306	CHL	C3C-C2C-CMC-OMC
6	Y	319	LHG	C30-C31-C32-C33
2	G	609	CHL	CBA-CGA-O2A-C1
6	G	618	LHG	C33-C34-C35-C36
6	G	618	LHG	C27-C28-C29-C30
2	G	605	CHL	C2A-CAA-CBA-CGA
3	Y	304	CLA	CBA-CGA-O2A-C1
2	Y	307	CHL	C1C-C2C-CMC-OMC
6	N	618	LHG	C24-C25-C26-C27
3	G	604	CLA	CBA-CGA-O2A-C1
6	Y	319	LHG	C27-C28-C29-C30
6	G	618	LHG	O1-C1-C2-O2
2	N	608	CHL	C11-C10-C8-C9
2	N	608	CHL	C14-C13-C15-C16
2	N	609	CHL	C6-C7-C8-C9
2	G	607	CHL	C14-C13-C15-C16
2	G	609	CHL	C14-C13-C15-C16
3	N	603	CLA	C6-C7-C8-C9
3	N	613	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
3	G	612	CLA	C14-C13-C15-C16
3	G	613	CLA	C14-C13-C15-C16
3	Y	304	CLA	C6-C7-C8-C9
3	Y	304	CLA	C8-C10-C11-C12
3	N	603	CLA	C4B-C3B-CAB-CBB
3	N	612	CLA	C4B-C3B-CAB-CBB
3	G	603	CLA	C4B-C3B-CAB-CBB
3	G	610	CLA	C4B-C3B-CAB-CBB
3	G	614	CLA	C4B-C3B-CAB-CBB
6	G	618	LHG	O6-C4-C5-C6
2	N	609	CHL	C11-C10-C8-C7
2	G	607	CHL	C11-C10-C8-C7
2	G	609	CHL	C12-C13-C15-C16
2	Y	308	CHL	C11-C10-C8-C7
3	G	604	CLA	C12-C13-C15-C16
3	Y	313	CLA	C4-C3-C5-C6
4	Y	317	LUT	C29-C30-C31-C32
3	N	604	CLA	O1A-CGA-O2A-C1
3	Y	313	CLA	C8-C10-C11-C12
6	Y	319	LHG	C14-C15-C16-C17
2	N	605	CHL	C1A-C2A-CAA-CBA
2	G	609	CHL	C4-C3-C5-C6
6	G	618	LHG	C15-C16-C17-C18
6	G	618	LHG	C26-C27-C28-C29
4	Y	316	LUT	C1-C6-C7-C8
3	N	602	CLA	C10-C11-C12-C13
3	Y	313	CLA	C2-C3-C5-C6
2	G	607	CHL	C11-C10-C8-C9
2	G	608	CHL	C6-C7-C8-C9
2	Y	308	CHL	C14-C13-C15-C16
3	G	604	CLA	C14-C13-C15-C16
6	N	618	LHG	C27-C28-C29-C30
6	Y	319	LHG	C34-C35-C36-C37
3	N	614	CLA	O2A-C1-C2-C3
3	G	614	CLA	O2A-C1-C2-C3
3	G	604	CLA	O1A-CGA-O2A-C1
2	N	607	CHL	C10-C11-C12-C13
6	N	618	LHG	O1-C1-C2-O2
3	G	612	CLA	C4-C3-C5-C6
4	N	616	LUT	C29-C30-C31-C32
5	Y	318	NEX	C13-C14-C15-C35
2	G	609	CHL	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
3	G	611	CLA	C13-C15-C16-C17
5	Y	318	NEX	C11-C10-C9-C19
3	Y	312	CLA	C5-C6-C7-C8
6	Y	319	LHG	O6-C4-C5-C6
2	N	609	CHL	C16-C17-C18-C20
2	N	607	CHL	C11-C10-C8-C7
2	G	608	CHL	C12-C13-C15-C16
3	N	603	CLA	C11-C12-C13-C15
3	N	604	CLA	C11-C12-C13-C15
3	Y	303	CLA	C11-C12-C13-C15
2	Y	309	CHL	C3-C5-C6-C7
4	N	615	LUT	C27-C28-C29-C30
5	N	617	NEX	C11-C12-C13-C14
5	G	617	NEX	C11-C12-C13-C14
7	Y	301	XAT	C11-C12-C13-C14
3	Y	304	CLA	O1A-CGA-O2A-C1
2	G	608	CHL	C2A-CAA-CBA-CGA
3	N	613	CLA	C16-C17-C18-C20
6	Y	319	LHG	O6-C4-C5-O7
6	G	618	LHG	C4-C5-C6-O8
3	G	612	CLA	C2-C3-C5-C6
6	N	618	LHG	O7-C5-C6-O8
6	G	618	LHG	O7-C5-C6-O8
6	Y	319	LHG	O7-C5-C6-O8
2	G	608	CHL	C11-C12-C13-C14
2	Y	310	CHL	C11-C12-C13-C14
3	N	604	CLA	C11-C12-C13-C14
3	G	603	CLA	C11-C10-C8-C9
3	Y	303	CLA	C11-C12-C13-C14
6	N	618	LHG	C29-C30-C31-C32
6	N	618	LHG	C30-C31-C32-C33
3	G	603	CLA	C13-C15-C16-C17
6	Y	319	LHG	C33-C34-C35-C36
7	N	619	XAT	C9-C10-C11-C12
3	G	602	CLA	C2A-CAA-CBA-CGA
2	G	609	CHL	O1A-CGA-O2A-C1
3	N	612	CLA	O1D-CGD-O2D-CED
3	N	614	CLA	C4B-C3B-CAB-CBB
3	G	602	CLA	C1A-C2A-CAA-CBA
3	G	611	CLA	C4B-C3B-CAB-CBB
3	Y	304	CLA	C4B-C3B-CAB-CBB
3	Y	312	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
4	Y	316	LUT	C27-C28-C29-C30
2	G	609	CHL	C2C-C3C-CAC-CBC
3	G	604	CLA	C2A-CAA-CBA-CGA
2	N	601	CHL	C11-C10-C8-C7
2	Y	308	CHL	C12-C13-C15-C16
2	Y	309	CHL	C6-C7-C8-C10
2	Y	309	CHL	C11-C12-C13-C15
3	N	603	CLA	C12-C13-C15-C16
3	N	612	CLA	C11-C12-C13-C15
3	N	613	CLA	C12-C13-C15-C16
3	G	602	CLA	C11-C12-C13-C15
3	G	603	CLA	C11-C10-C8-C7
3	Y	312	CLA	C11-C10-C8-C7
3	Y	314	CLA	C12-C13-C15-C16
6	G	618	LHG	C30-C31-C32-C33
2	Y	310	CHL	C16-C17-C18-C20
6	Y	319	LHG	C25-C26-C27-C28
6	G	618	LHG	O6-C4-C5-O7
3	N	611	CLA	CBD-CGD-O2D-CED
2	N	601	CHL	C11-C10-C8-C9
2	N	607	CHL	C11-C10-C8-C9
3	N	603	CLA	C11-C12-C13-C14
3	G	603	CLA	C14-C13-C15-C16
3	N	614	CLA	C1-C2-C3-C4
3	G	614	CLA	C1-C2-C3-C4
3	Y	315	CLA	C1-C2-C3-C4
5	Y	318	NEX	C7-C8-C9-C10
3	Y	313	CLA	C5-C6-C7-C8
6	N	618	LHG	C4-C5-C6-O8
6	Y	319	LHG	C4-C5-C6-O8
3	G	603	CLA	C8-C10-C11-C12
3	N	614	CLA	CAD-CBD-CGD-O2D
6	N	618	LHG	C13-C14-C15-C16
2	N	607	CHL	CHA-CBD-CGD-O1D
2	N	607	CHL	CHA-CBD-CGD-O2D
2	G	605	CHL	CHA-CBD-CGD-O1D
2	G	605	CHL	CHA-CBD-CGD-O2D
2	Y	308	CHL	CHA-CBD-CGD-O2D
3	N	614	CLA	CAD-CBD-CGD-O1D
3	G	602	CLA	CHA-CBD-CGD-O1D
6	N	618	LHG	C3-O3-P-O5
7	Y	301	XAT	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
3	N	614	CLA	C2B-C3B-CAB-CBB
3	G	614	CLA	C2B-C3B-CAB-CBB
3	Y	304	CLA	C2B-C3B-CAB-CBB
3	Y	311	CLA	C2B-C3B-CAB-CBB
3	Y	312	CLA	C2B-C3B-CAB-CBB
4	G	615	LUT	C5-C6-C7-C8
5	Y	318	NEX	C11-C12-C13-C20
3	Y	312	CLA	O1D-CGD-O2D-CED
6	G	618	LHG	C4-C5-O7-C7
6	N	618	LHG	O6-C4-C5-C6
2	Y	310	CHL	C11-C10-C8-C9
3	N	602	CLA	C6-C7-C8-C9
3	N	603	CLA	C14-C13-C15-C16
3	Y	313	CLA	C11-C12-C13-C14
3	N	602	CLA	C6-C7-C8-C10
3	N	602	CLA	C11-C12-C13-C15
3	G	603	CLA	C12-C13-C15-C16
3	Y	313	CLA	C11-C12-C13-C15
6	N	618	LHG	O6-C4-C5-O7
2	Y	302	CHL	C13-C15-C16-C17
3	Y	313	CLA	C16-C17-C18-C20
3	Y	304	CLA	C5-C6-C7-C8
2	Y	302	CHL	O1D-CGD-O2D-CED
6	Y	319	LHG	C7-C8-C9-C10
3	G	602	CLA	C8-C10-C11-C12
7	G	619	XAT	C9-C10-C11-C12
3	N	612	CLA	C4-C3-C5-C6
3	N	612	CLA	C11-C12-C13-C14
3	N	603	CLA	CBA-CGA-O2A-C1
3	N	610	CLA	C5-C6-C7-C8
3	N	613	CLA	C16-C17-C18-C19
3	G	604	CLA	C4-C3-C5-C6
3	N	603	CLA	O1A-CGA-O2A-C1
2	N	601	CHL	C3A-C2A-CAA-CBA
2	Y	302	CHL	C3A-C2A-CAA-CBA
2	Y	309	CHL	C4-C3-C5-C6
5	N	617	NEX	C39-C29-C30-C31
5	G	617	NEX	C39-C29-C30-C31
2	G	607	CHL	C15-C16-C17-C18
2	G	609	CHL	C2-C1-O2A-CGA
2	N	609	CHL	C16-C17-C18-C19
2	G	601	CHL	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
2	G	607	CHL	C6-C7-C8-C9
2	Y	309	CHL	C14-C13-C15-C16
3	N	611	CLA	C11-C10-C8-C9
3	N	612	CLA	C11-C10-C8-C9
3	N	613	CLA	C11-C12-C13-C14
3	G	602	CLA	C6-C7-C8-C9
3	G	611	CLA	C14-C13-C15-C16
6	N	618	LHG	C4-C5-O7-C7
6	G	618	LHG	C6-C5-O7-C7
2	G	601	CHL	C1A-C2A-CAA-CBA
2	G	608	CHL	C1A-C2A-CAA-CBA
2	Y	306	CHL	C1A-C2A-CAA-CBA
2	Y	310	CHL	C1A-C2A-CAA-CBA
4	N	615	LUT	C29-C30-C31-C32
3	N	612	CLA	C2-C3-C5-C6
3	N	602	CLA	C2A-CAA-CBA-CGA
3	Y	314	CLA	C2A-CAA-CBA-CGA
3	G	610	CLA	C1A-C2A-CAA-CBA
3	G	614	CLA	C1A-C2A-CAA-CBA
5	N	617	NEX	C28-C29-C30-C31
5	G	617	NEX	C28-C29-C30-C31
4	N	615	LUT	C1-C6-C7-C8
4	G	616	LUT	C1-C6-C7-C8
4	Y	316	LUT	C5-C6-C7-C8
4	Y	317	LUT	C1-C6-C7-C8
2	G	609	CHL	C16-C17-C18-C19
3	Y	315	CLA	O2A-C1-C2-C3
2	Y	310	CHL	C6-C7-C8-C10
3	N	612	CLA	C11-C10-C8-C7
3	G	602	CLA	C6-C7-C8-C10
3	Y	304	CLA	C12-C13-C15-C16
2	N	608	CHL	C16-C17-C18-C20
2	Y	309	CHL	C2-C3-C5-C6
3	G	604	CLA	C2-C3-C5-C6
3	N	603	CLA	C10-C11-C12-C13
5	Y	318	NEX	C11-C12-C13-C14
2	Y	308	CHL	C6-C7-C8-C9
2	Y	310	CHL	C14-C13-C15-C16
3	N	612	CLA	C5-C6-C7-C8
2	G	608	CHL	C16-C17-C18-C19
3	G	613	CLA	C15-C16-C17-C18
3	Y	313	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
3	G	613	CLA	C2A-CAA-CBA-CGA
3	G	602	CLA	C13-C15-C16-C17
2	G	609	CHL	CHA-CBD-CGD-O1D
2	G	609	CHL	CHA-CBD-CGD-O2D
3	Y	312	CLA	C4-C3-C5-C6
2	Y	309	CHL	C6-C7-C8-C9
3	G	602	CLA	C11-C12-C13-C14
3	Y	312	CLA	C11-C10-C8-C9
3	Y	312	CLA	C14-C13-C15-C16
3	Y	313	CLA	C11-C10-C8-C9
3	Y	314	CLA	C14-C13-C15-C16
3	N	604	CLA	C2-C1-O2A-CGA
2	N	609	CHL	C3A-C2A-CAA-CBA
3	N	611	CLA	C4-C3-C5-C6
3	Y	305	CLA	C3A-C2A-CAA-CBA
3	Y	314	CLA	C15-C16-C17-C18
6	N	618	LHG	C34-C35-C36-C37
2	N	607	CHL	C5-C6-C7-C8
7	N	619	XAT	O24-C26-C27-C28
6	Y	319	LHG	C13-C14-C15-C16
3	G	613	CLA	CBA-CGA-O2A-C1
5	Y	318	NEX	C7-C8-C9-C19
3	N	602	CLA	C11-C12-C13-C14
3	G	603	CLA	C16-C17-C18-C20
2	Y	309	CHL	C16-C17-C18-C19
2	Y	310	CHL	C12-C13-C15-C16
3	N	613	CLA	C11-C12-C13-C15
3	G	611	CLA	C12-C13-C15-C16
4	N	615	LUT	C5-C6-C7-C8
4	G	616	LUT	C5-C6-C7-C8
4	Y	317	LUT	C5-C6-C7-C8
3	N	611	CLA	O1D-CGD-O2D-CED
3	G	603	CLA	C16-C17-C18-C19
6	N	618	LHG	C9-C10-C11-C12
6	Y	319	LHG	O8-C23-C24-C25
2	N	608	CHL	CAA-CBA-CGA-O2A
2	Y	309	CHL	CAA-CBA-CGA-O2A
3	Y	303	CLA	C13-C15-C16-C17
2	G	601	CHL	CAA-CBA-CGA-O2A
3	Y	303	CLA	C1A-C2A-CAA-CBA
3	Y	311	CLA	C1A-C2A-CAA-CBA
3	Y	313	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
3	Y	304	CLA	CAA-CBA-CGA-O2A
2	Y	302	CHL	C2-C1-O2A-CGA
3	G	604	CLA	C2-C1-O2A-CGA
3	G	610	CLA	C11-C10-C8-C7
3	G	613	CLA	C11-C12-C13-C15
3	Y	313	CLA	C11-C10-C8-C7
2	G	601	CHL	C16-C17-C18-C20
6	N	618	LHG	C6-C5-O7-C7
3	G	613	CLA	C8-C10-C11-C12
5	Y	318	NEX	C11-C10-C9-C8
6	Y	319	LHG	O10-C23-C24-C25
3	N	613	CLA	C14-C13-C15-C16
2	N	608	CHL	CAA-CBA-CGA-O1A
2	Y	308	CHL	C15-C16-C17-C18
6	G	618	LHG	O8-C23-C24-C25
3	N	603	CLA	C2A-CAA-CBA-CGA
2	Y	309	CHL	CAA-CBA-CGA-O1A
3	N	613	CLA	C13-C15-C16-C17
3	Y	303	CLA	C8-C10-C11-C12
3	Y	313	CLA	CAD-CBD-CGD-O2D
2	Y	306	CHL	O1A-CGA-O2A-C1
2	G	601	CHL	C2-C1-O2A-CGA
3	G	611	CLA	C2-C1-O2A-CGA
3	Y	304	CLA	CAA-CBA-CGA-O1A
3	G	611	CLA	C10-C11-C12-C13
3	N	603	CLA	CAA-CBA-CGA-O2A

There are no ring outliers.

51 monomers are involved in 156 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	Y	317	LUT	5	0
2	G	607	CHL	3	0
2	N	607	CHL	1	0
3	N	614	CLA	1	0
3	G	614	CLA	3	0
3	Y	312	CLA	3	0
4	Y	316	LUT	4	0
5	Y	318	NEX	2	0
3	Y	311	CLA	4	0
3	N	602	CLA	7	0
7	Y	301	XAT	7	0

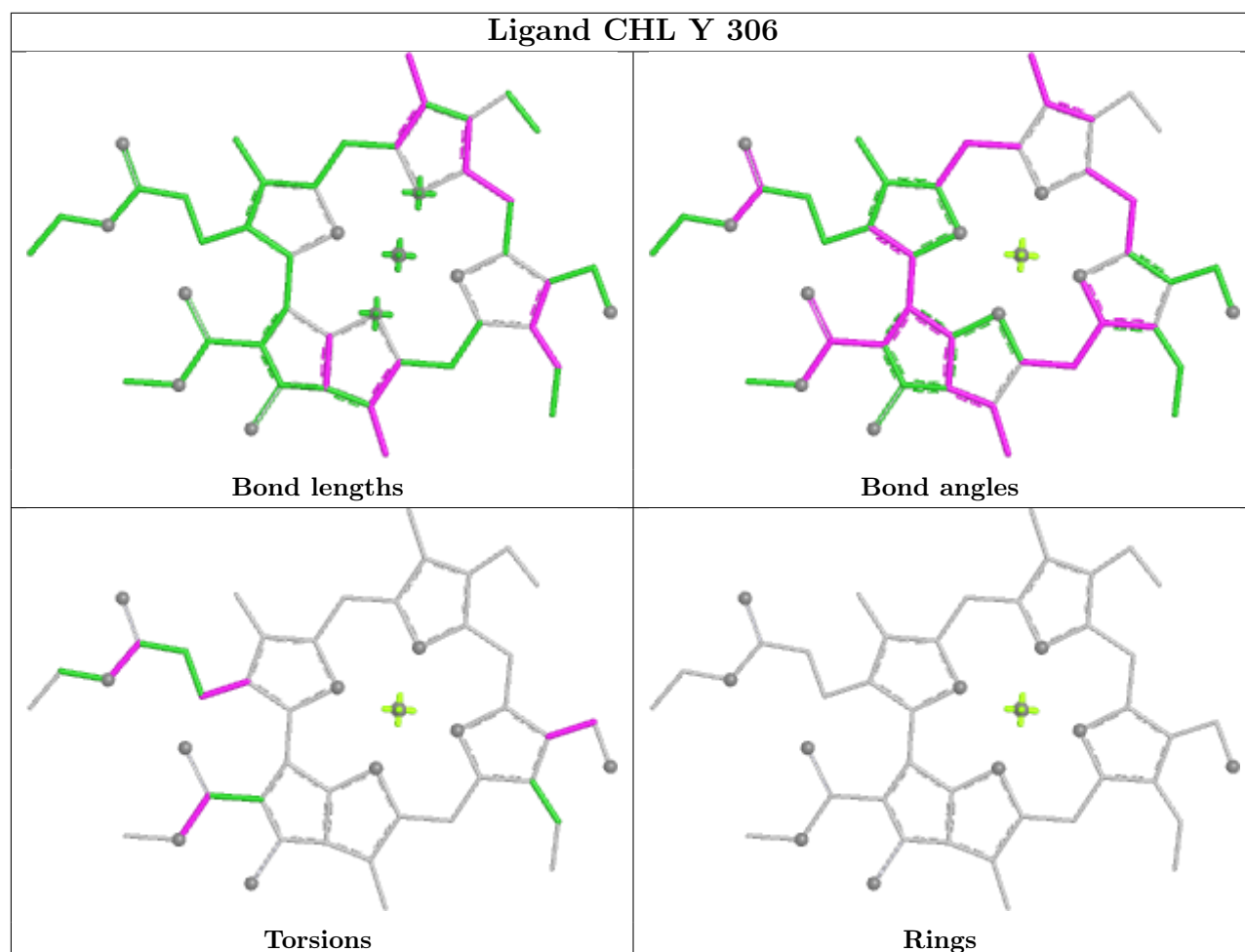
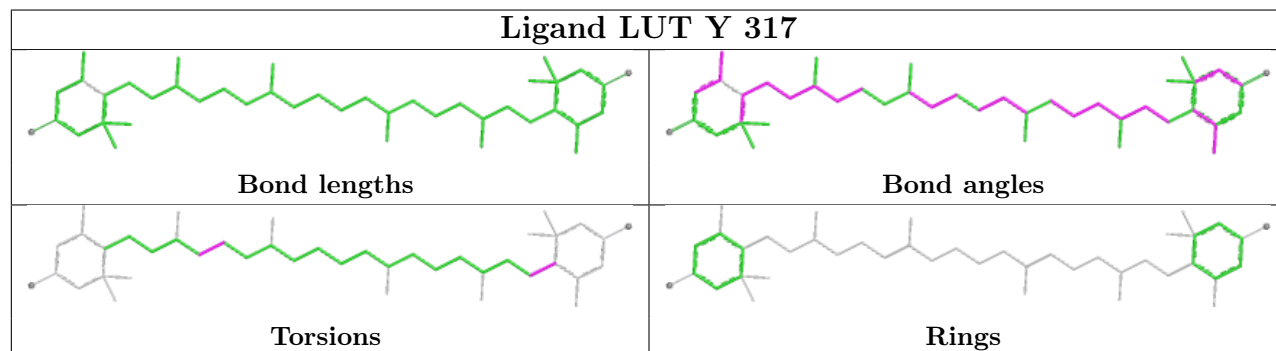
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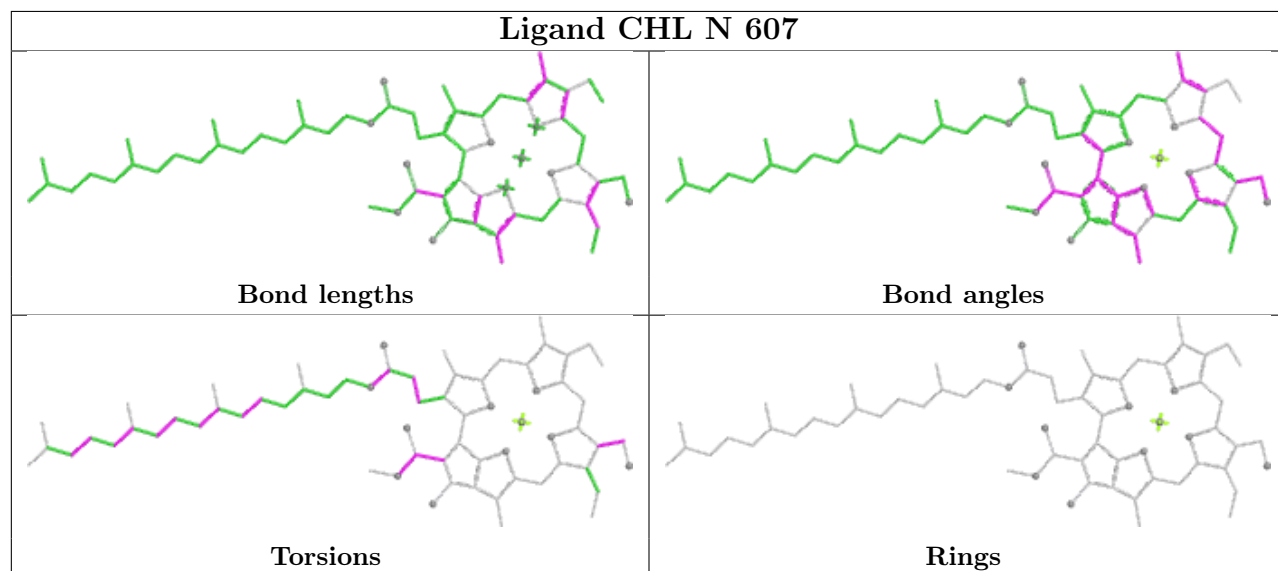
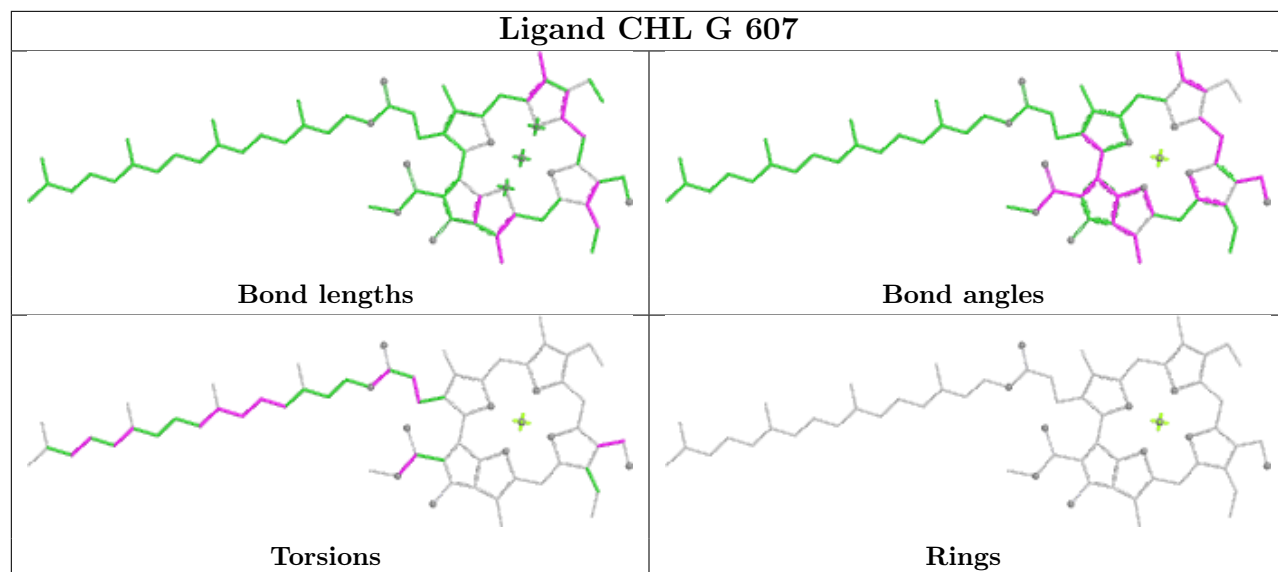
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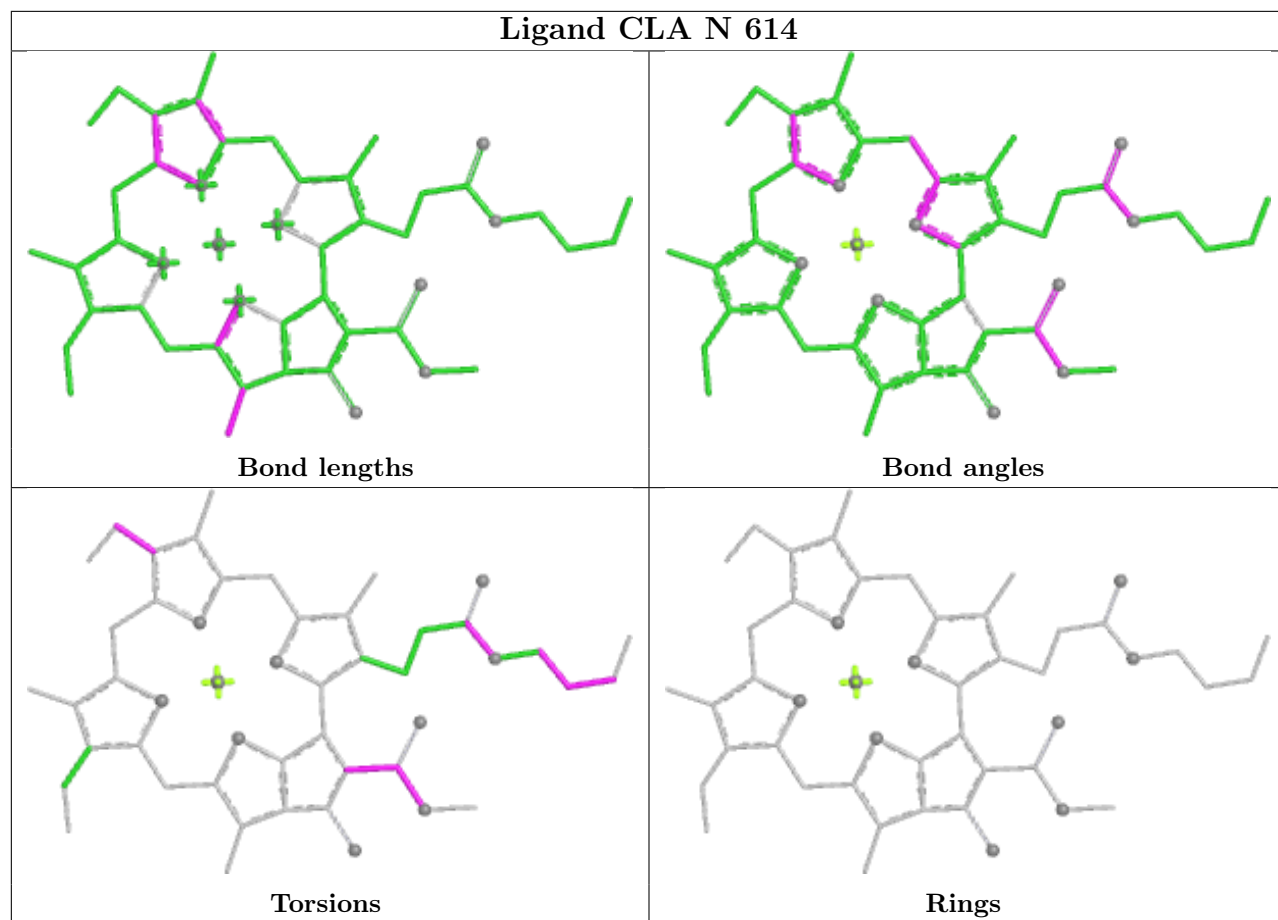
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	N	609	CHL	9	0
3	N	611	CLA	4	0
2	Y	302	CHL	9	0
3	Y	314	CLA	3	0
7	N	619	XAT	5	0
3	N	603	CLA	4	0
4	N	616	LUT	3	0
4	G	615	LUT	8	0
7	G	619	XAT	6	0
2	N	601	CHL	6	0
2	N	606	CHL	1	0
5	G	617	NEX	4	0
3	G	612	CLA	3	0
3	N	613	CLA	3	0
3	Y	315	CLA	4	0
3	Y	305	CLA	1	0
3	N	612	CLA	2	0
2	G	605	CHL	1	0
3	Y	303	CLA	4	0
3	Y	313	CLA	3	0
2	G	609	CHL	6	0
5	N	617	NEX	3	0
2	Y	310	CHL	5	0
6	N	618	LHG	7	0
2	Y	308	CHL	6	0
3	G	602	CLA	6	0
3	G	611	CLA	2	0
2	Y	309	CHL	2	0
2	G	608	CHL	5	0
3	N	610	CLA	1	0
2	N	608	CHL	4	0
2	G	601	CHL	11	0
3	G	610	CLA	6	0
6	G	618	LHG	6	0
4	G	616	LUT	3	0
4	N	615	LUT	2	0
2	G	606	CHL	1	0
3	G	613	CLA	2	0
6	Y	319	LHG	5	0
3	Y	304	CLA	4	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

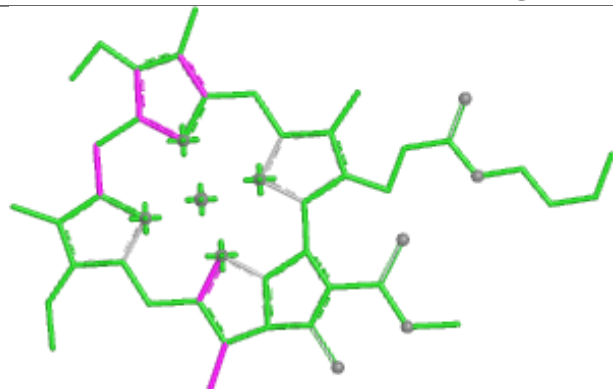
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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.



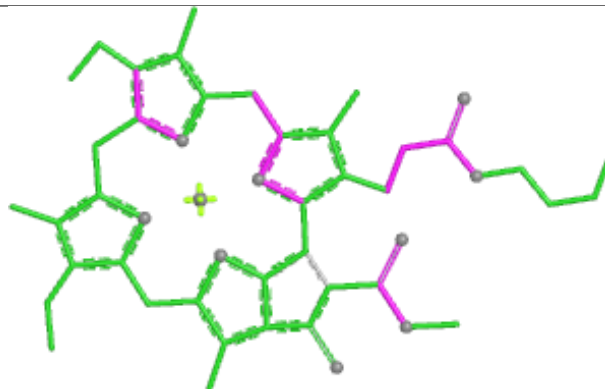




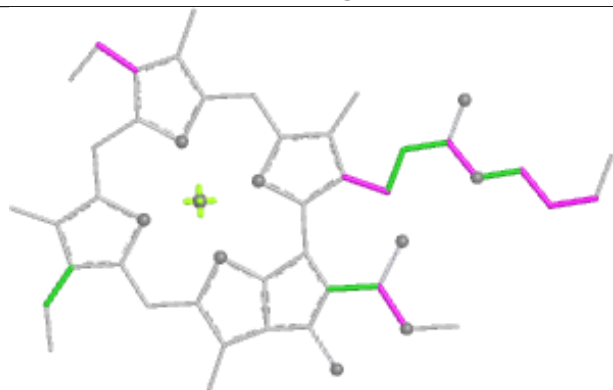
Ligand CLA G 614



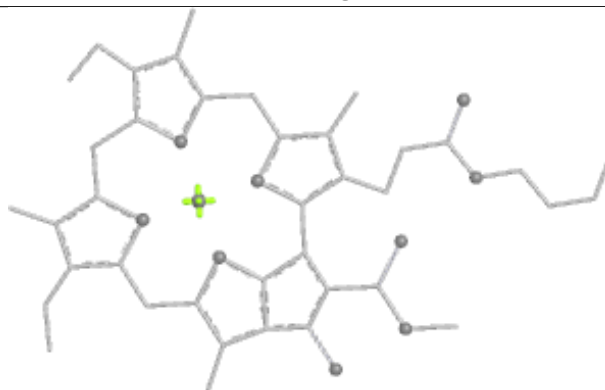
Bond lengths



Bond angles

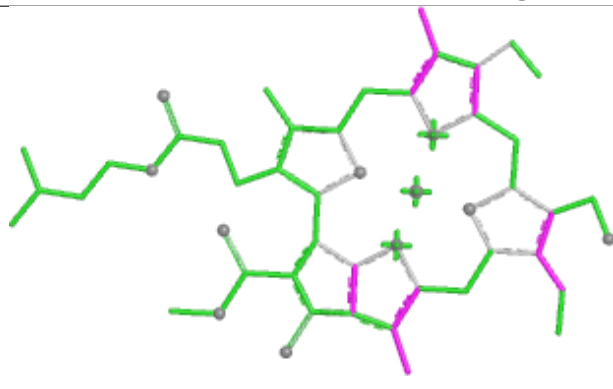


Torsions

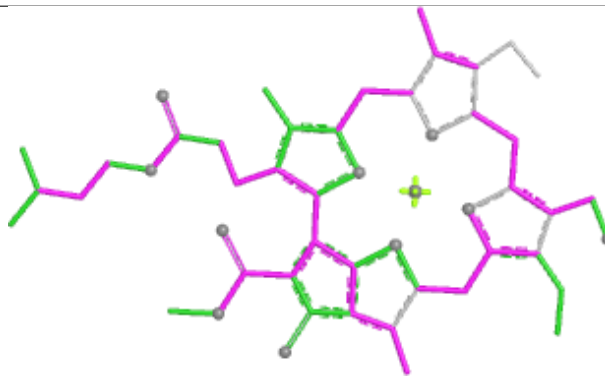


Rings

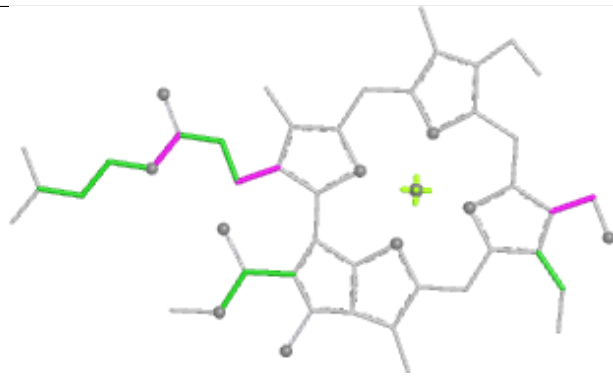
Ligand CHL Y 307



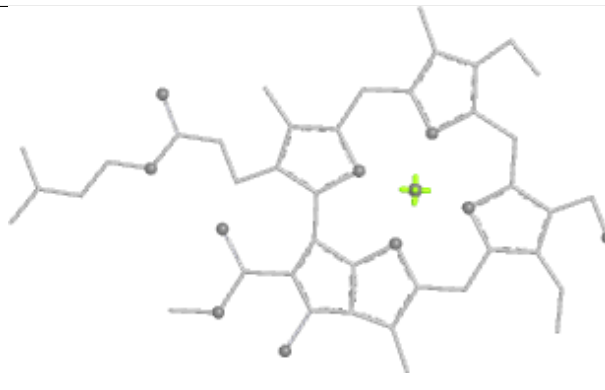
Bond lengths



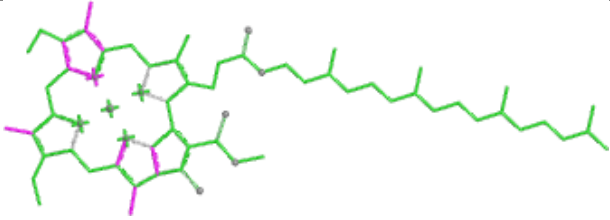
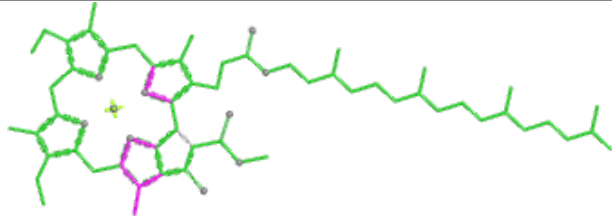
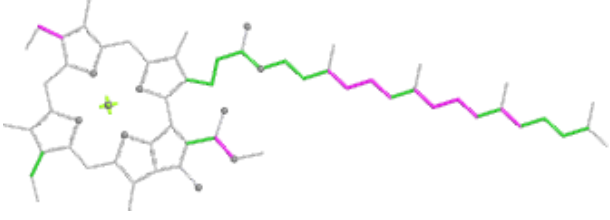
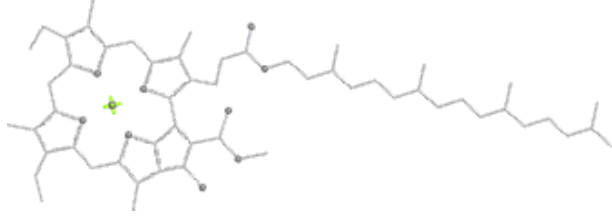
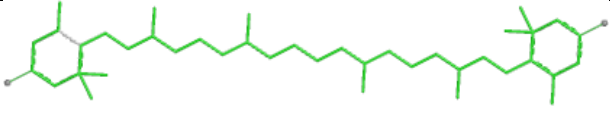
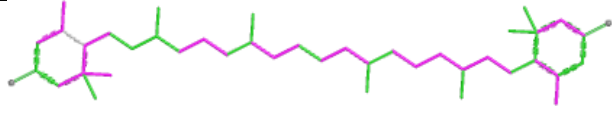
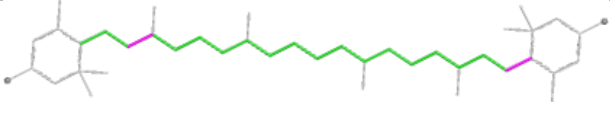
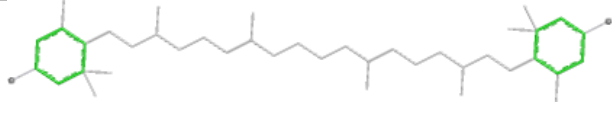
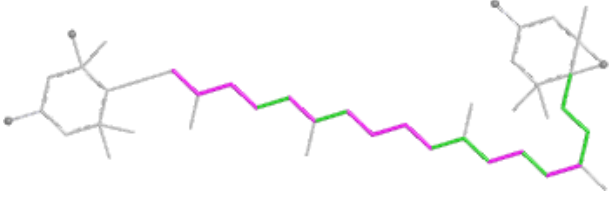
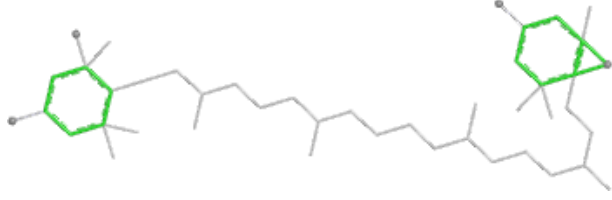
Bond angles

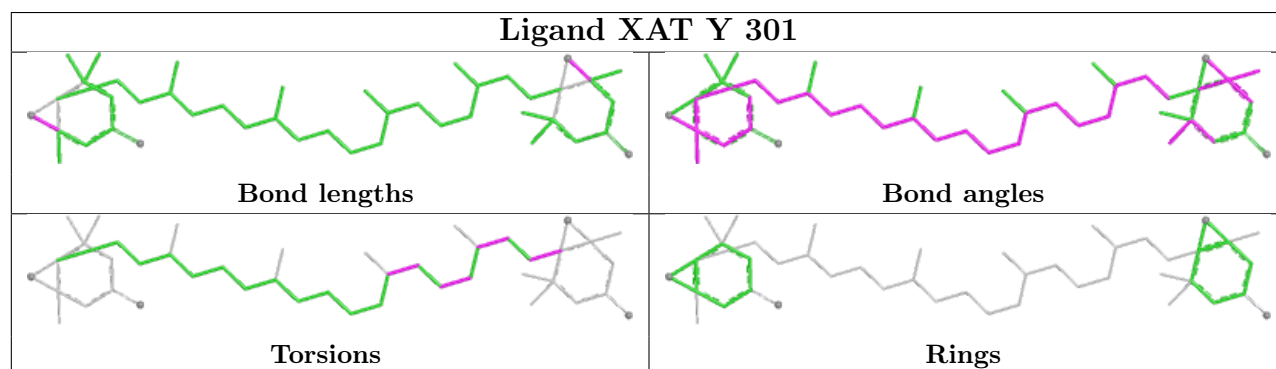
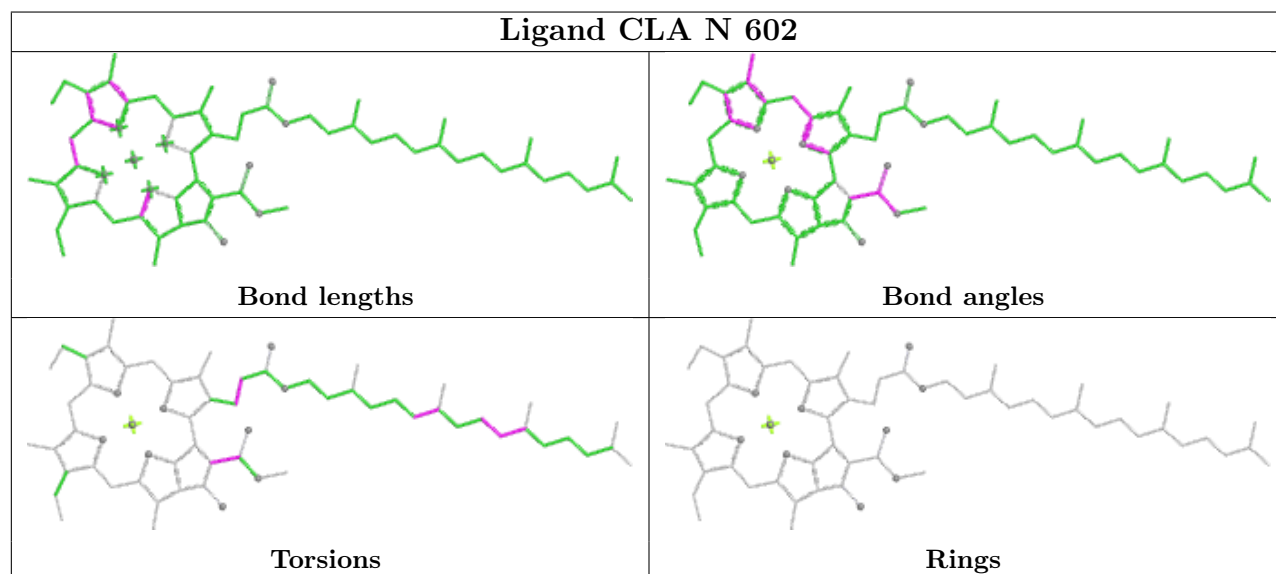
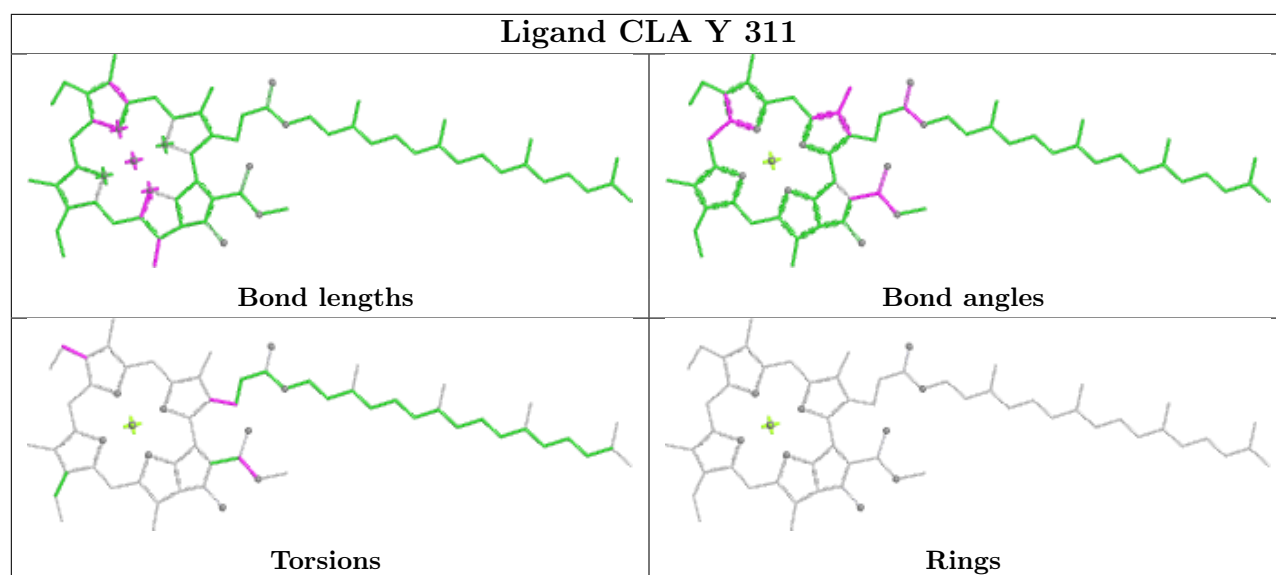


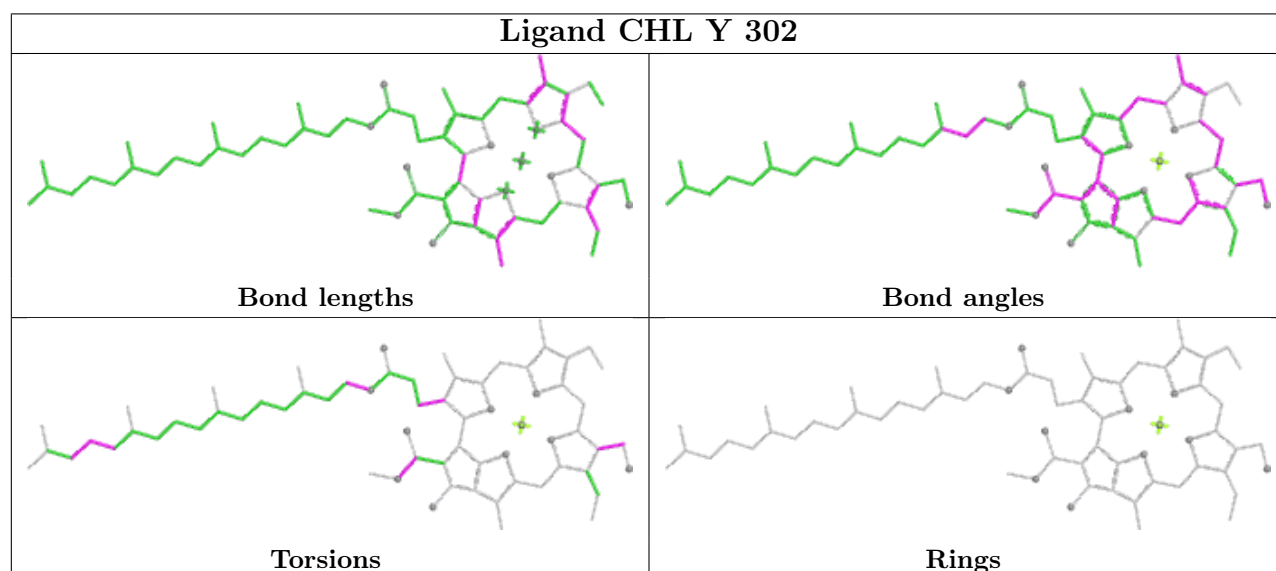
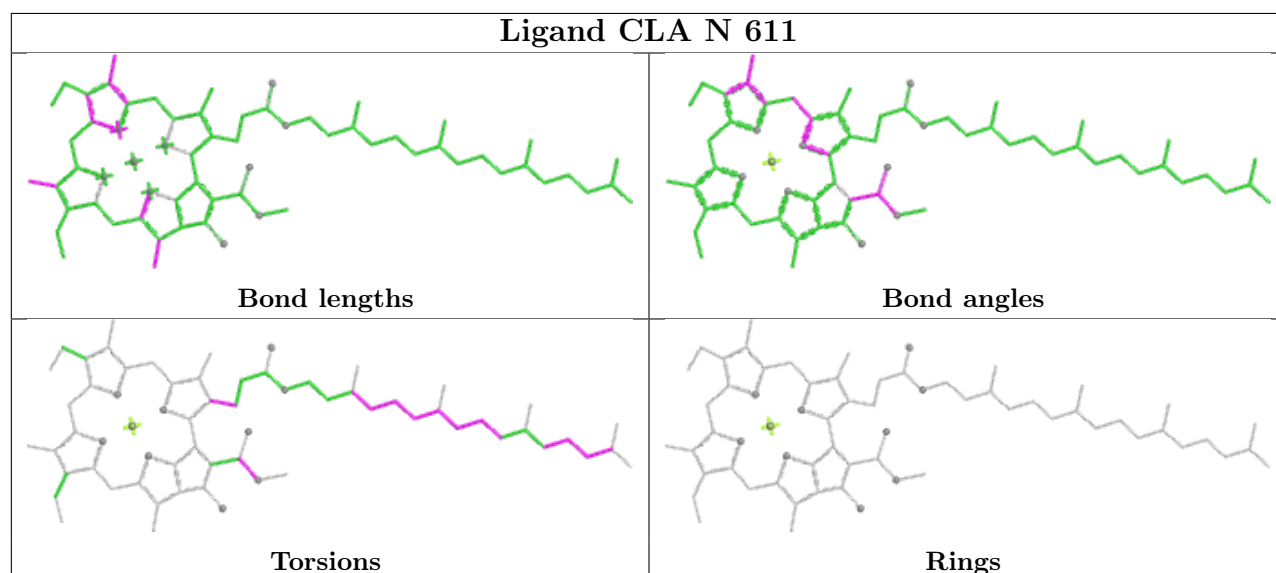
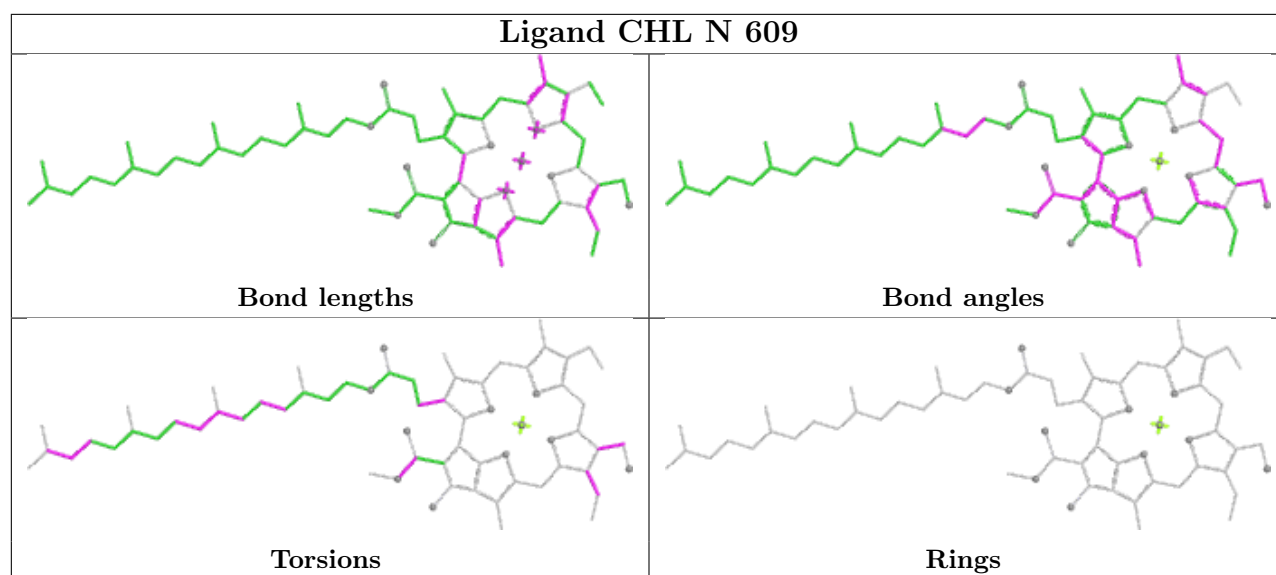
Torsions

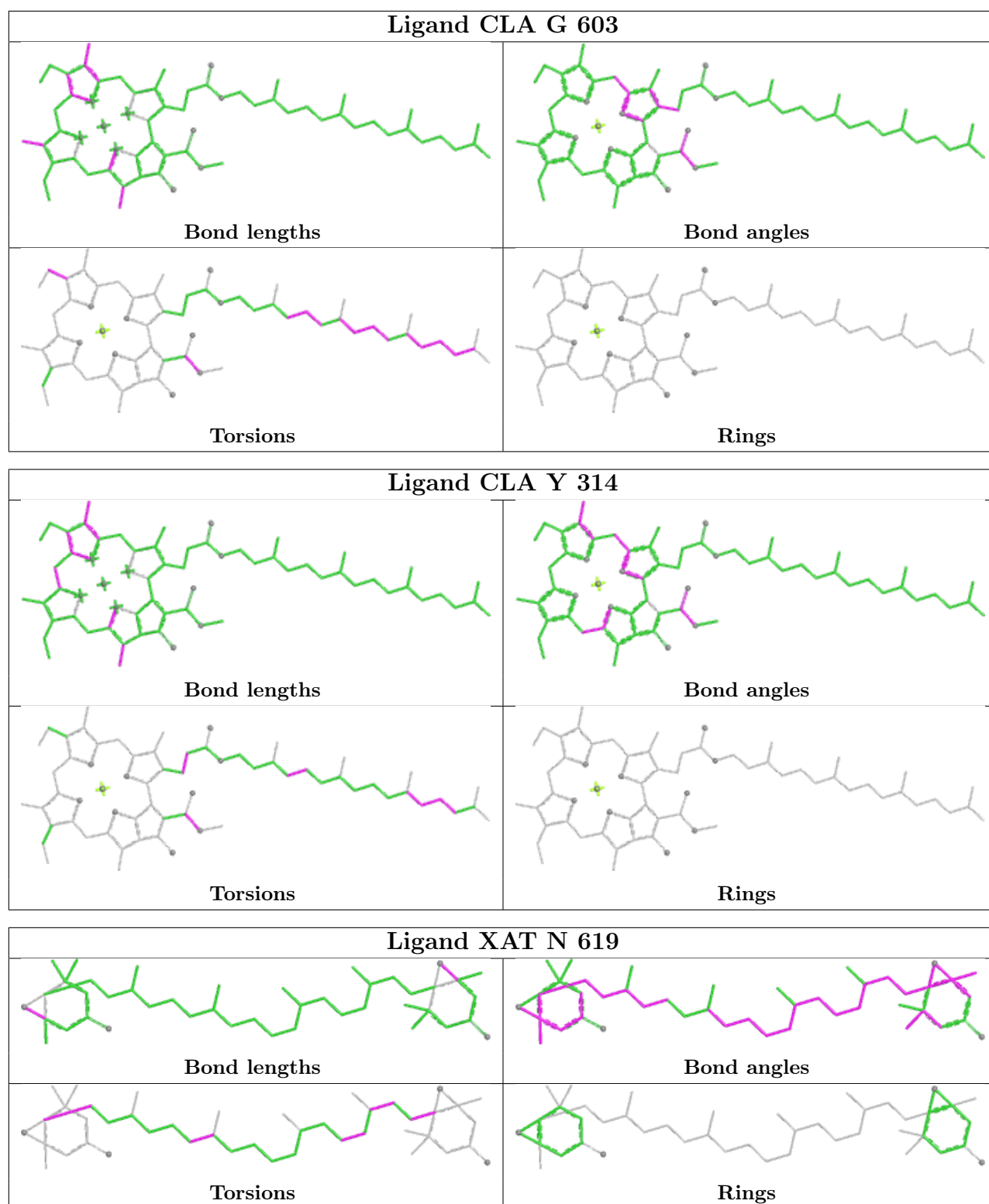


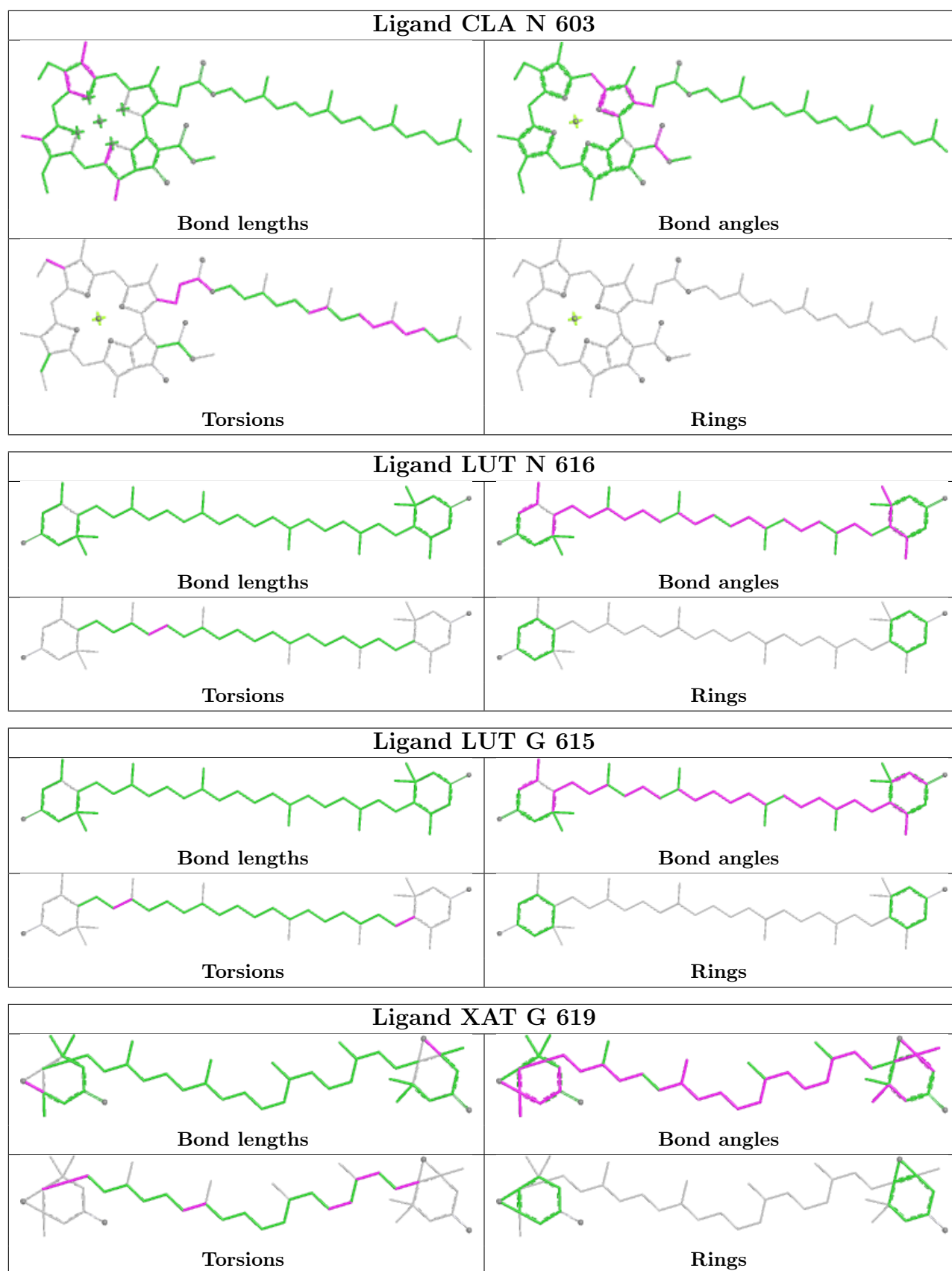
Rings

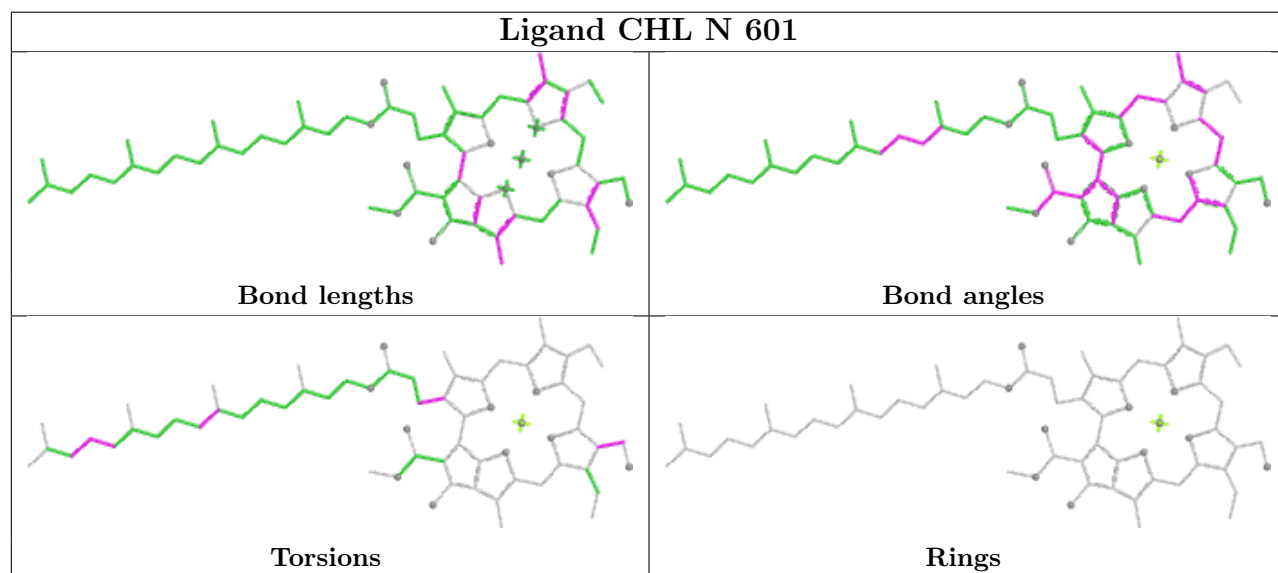
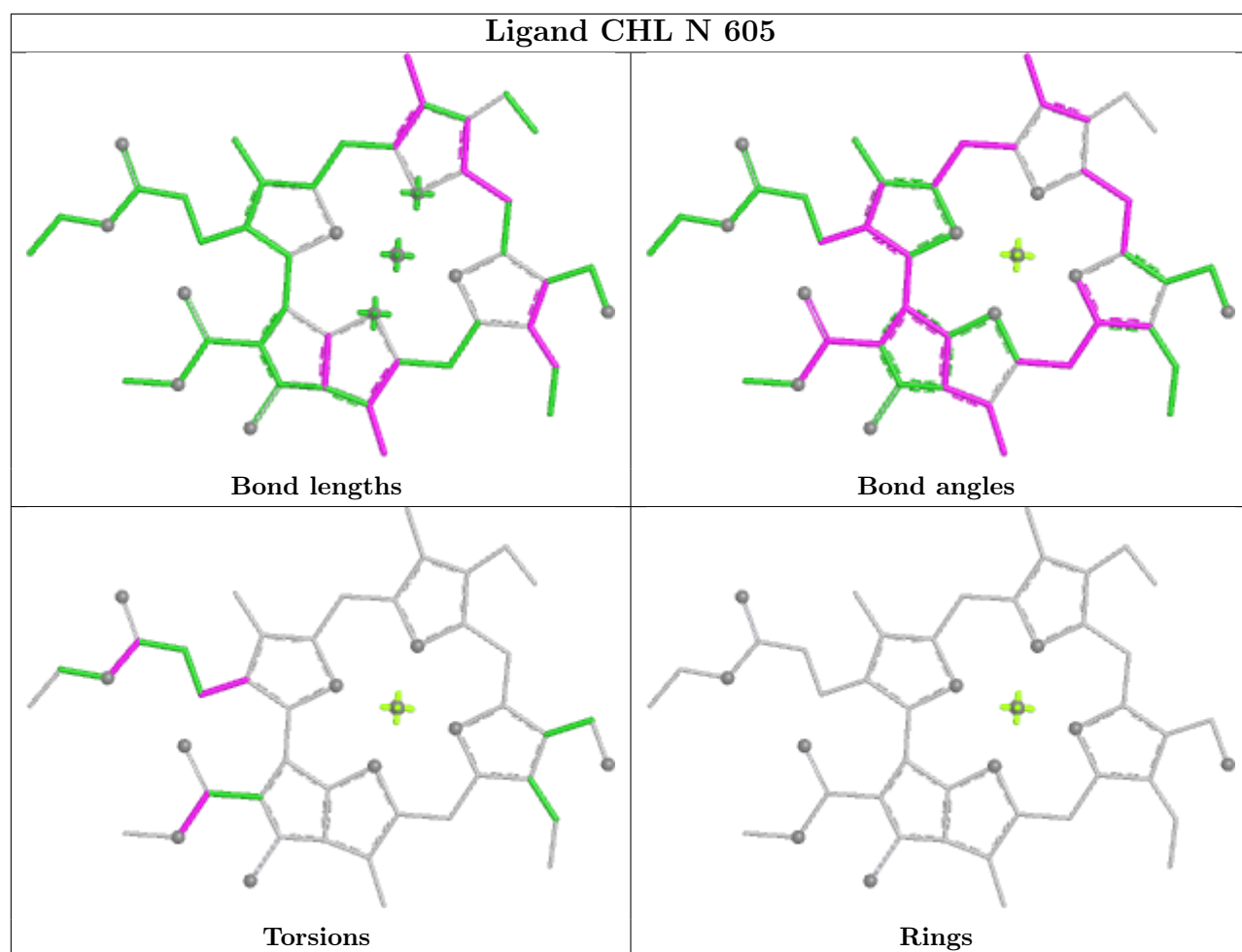
Ligand CLA Y 312	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LUT Y 316	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand NEX Y 318	
 Bond lengths	 Bond angles
 Torsions	 Rings

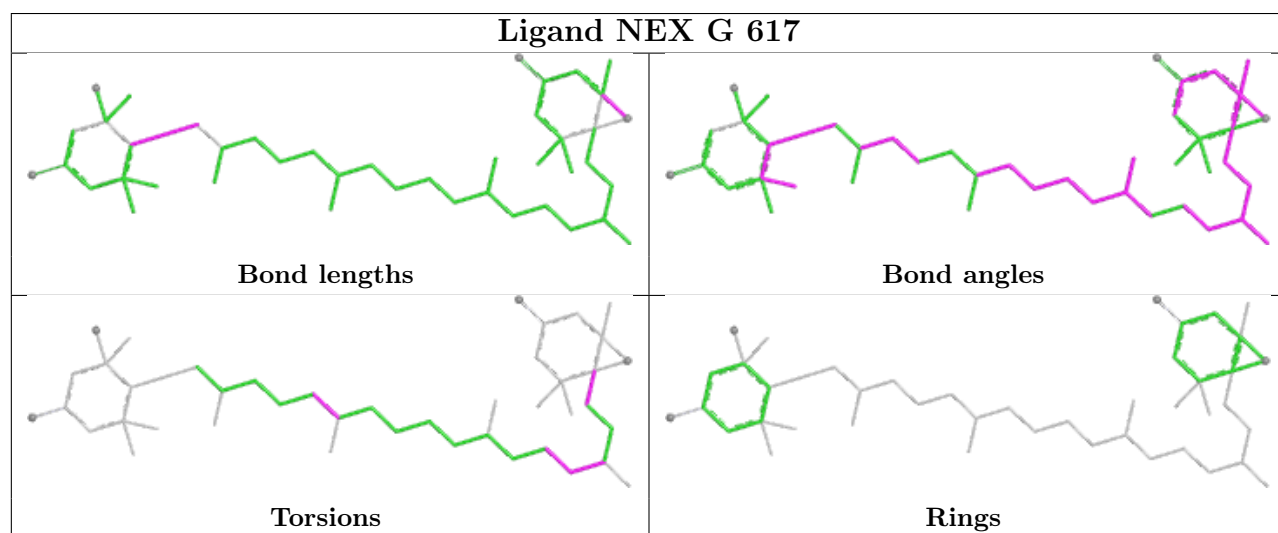
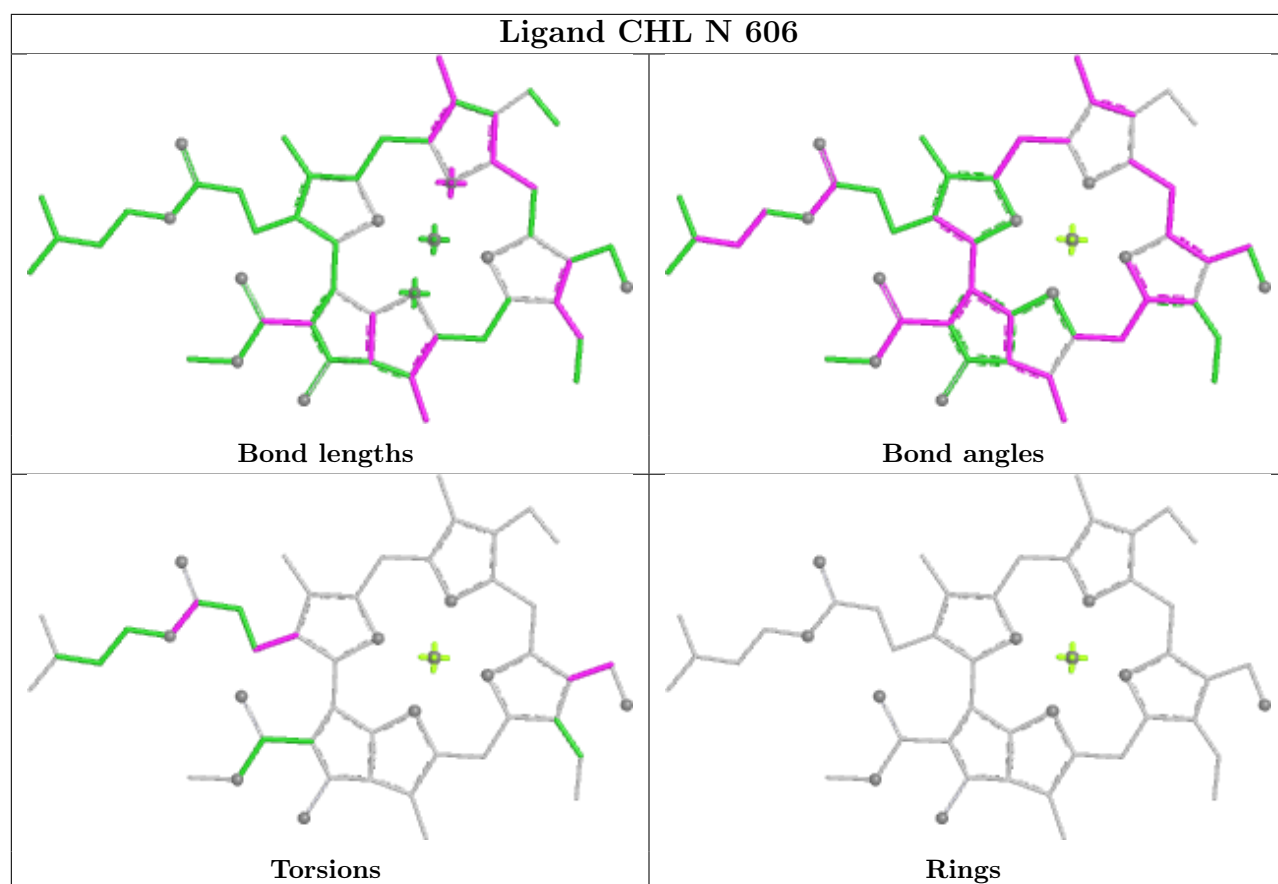


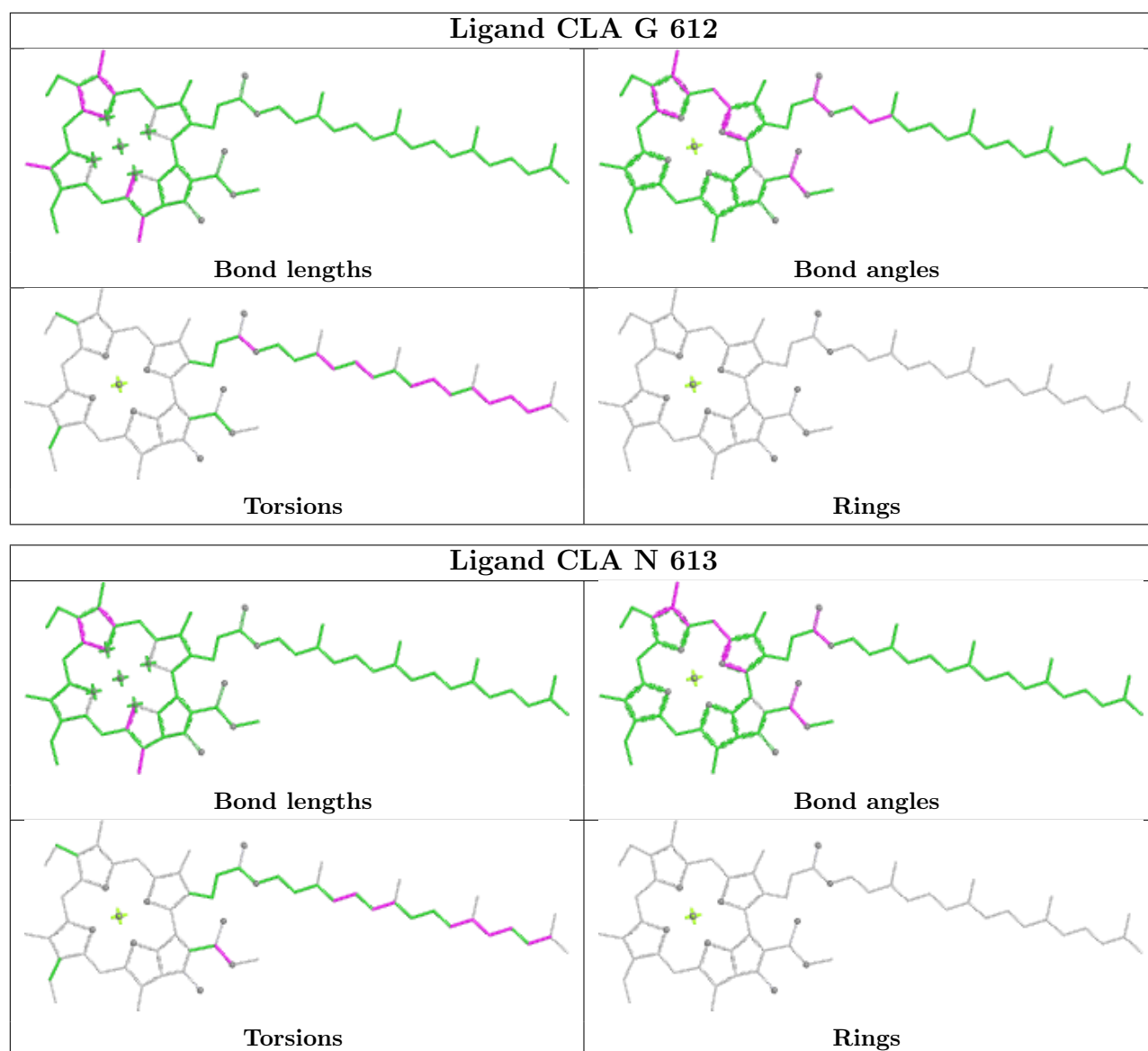




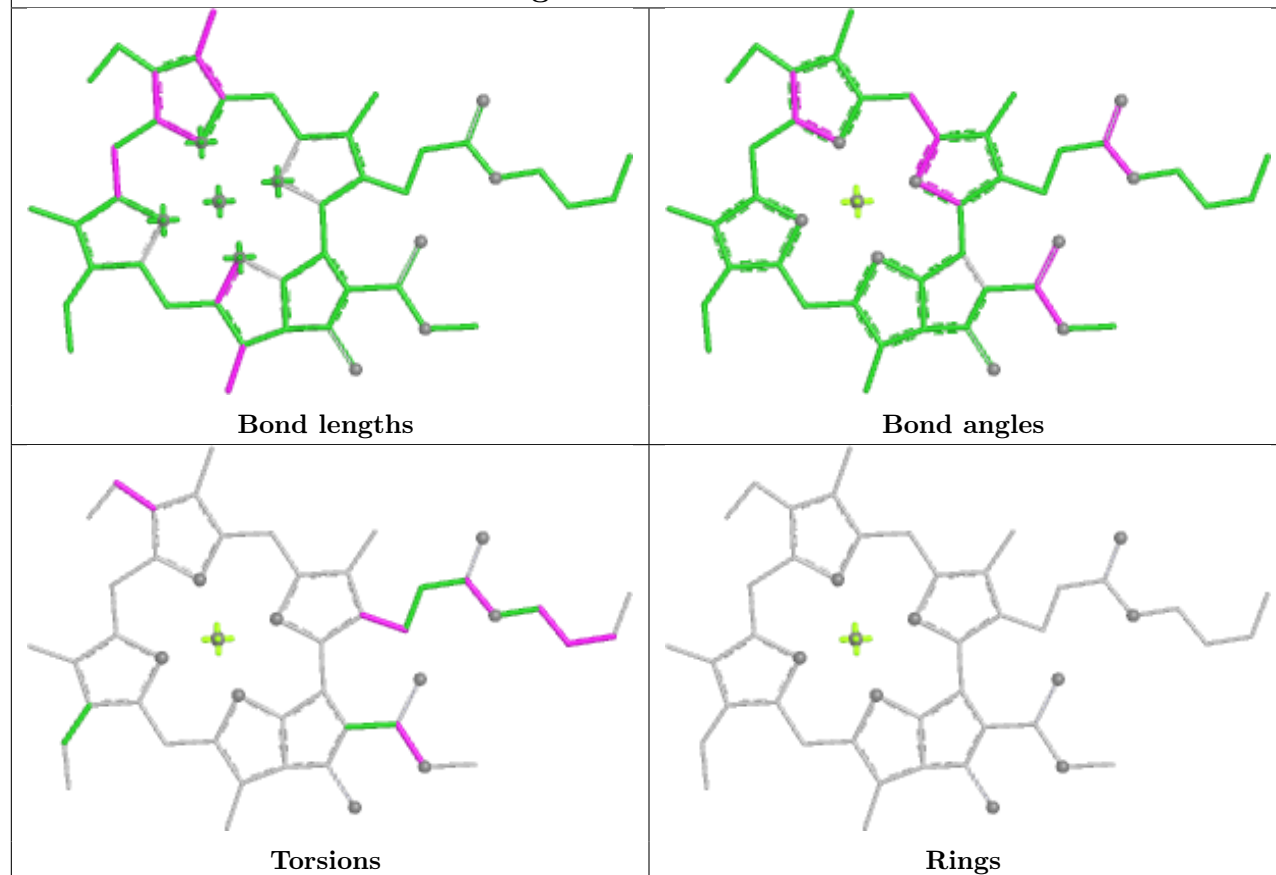




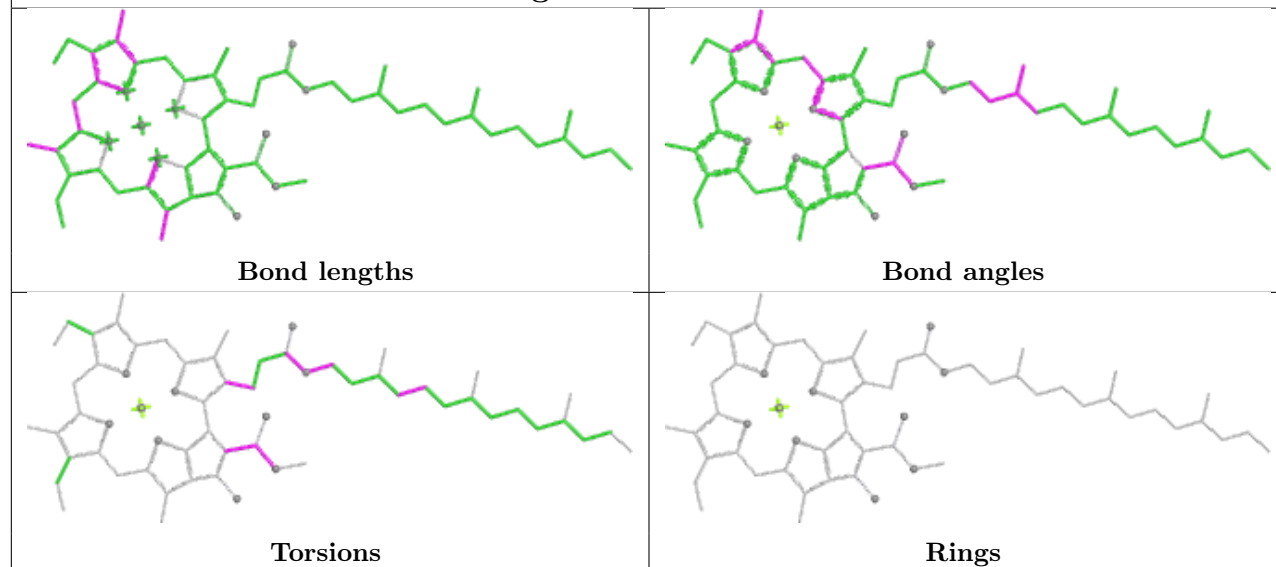


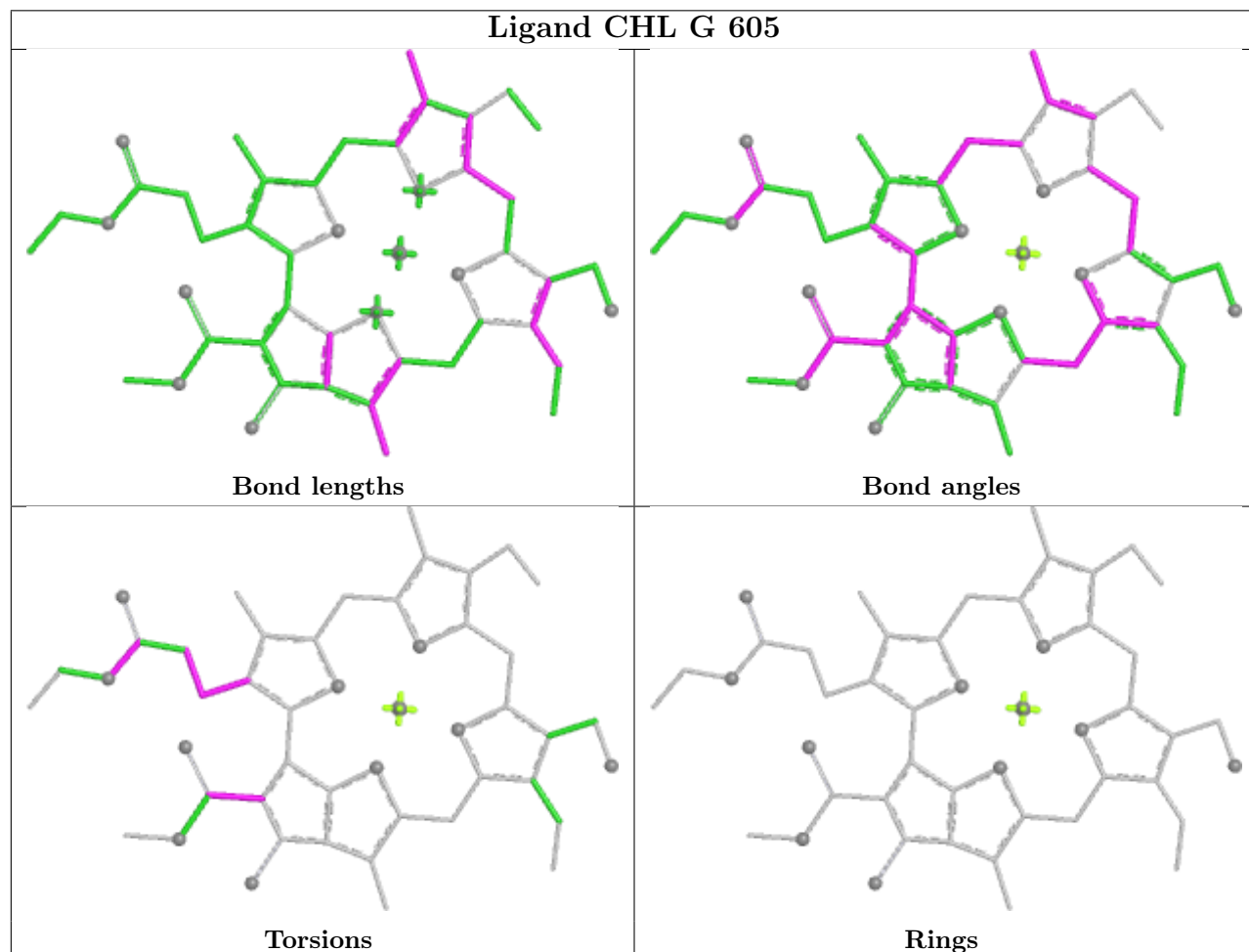
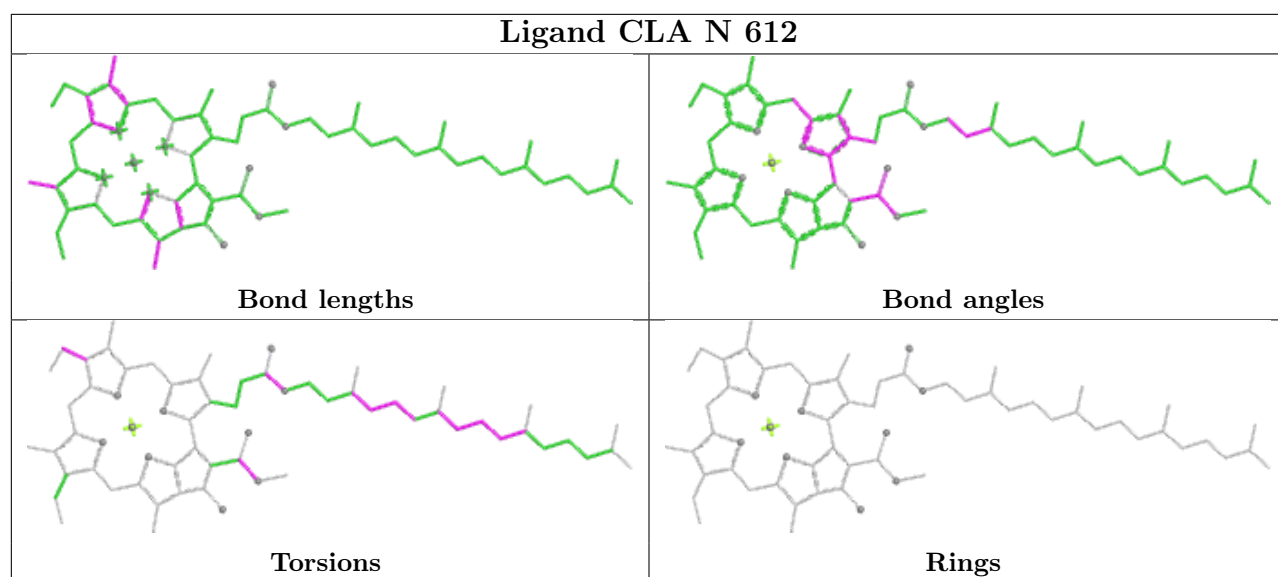


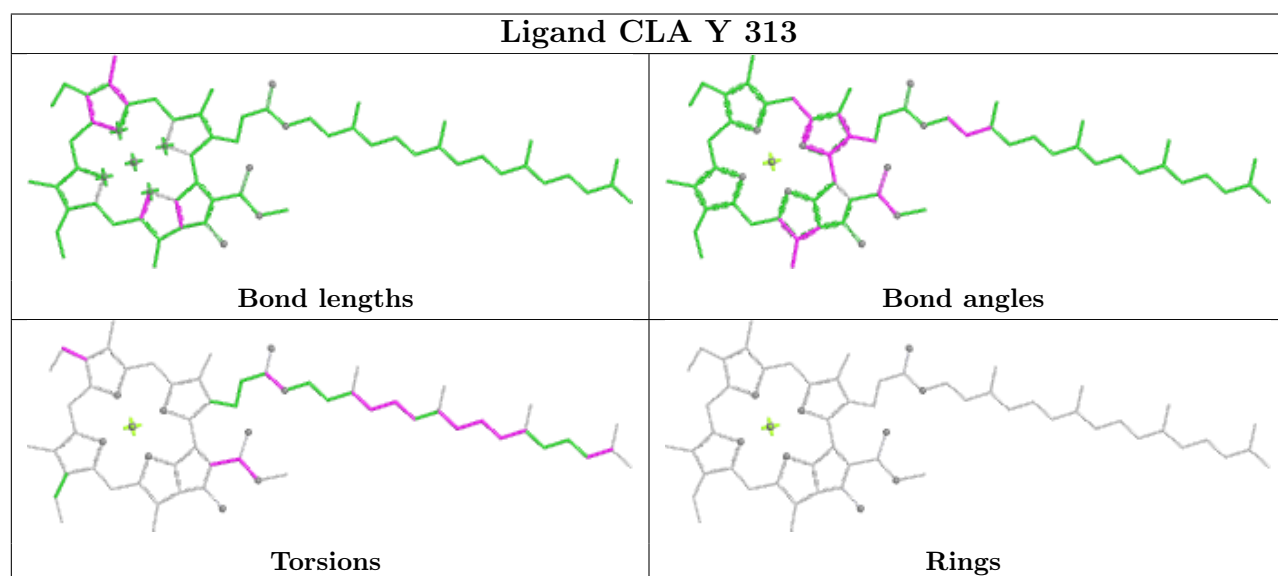
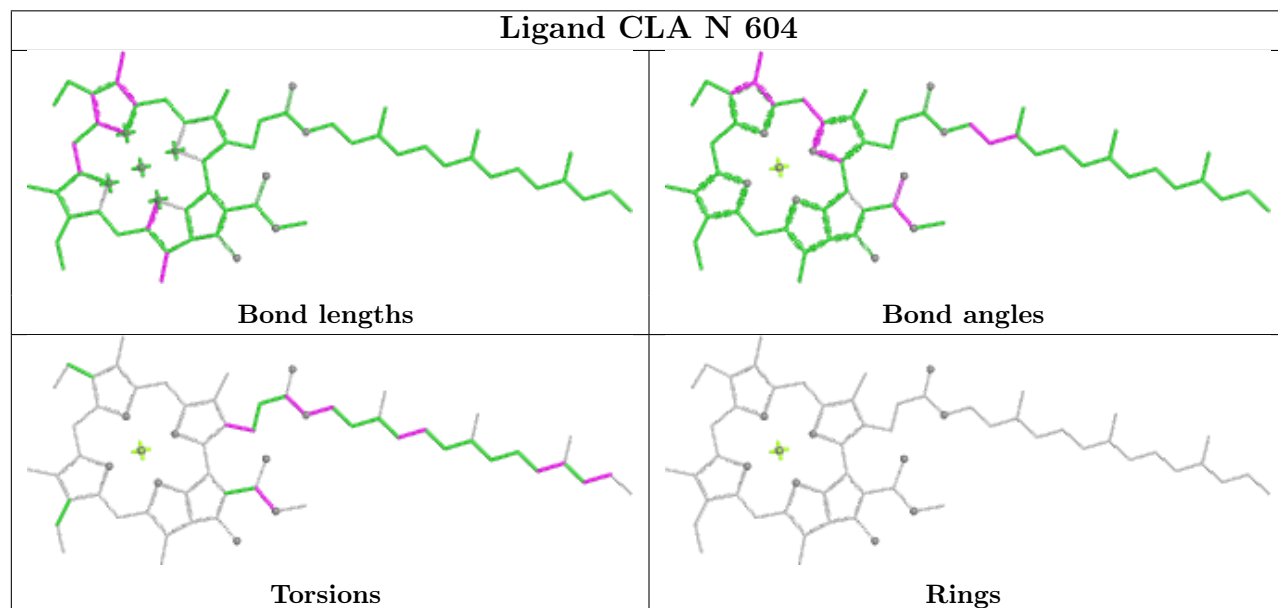
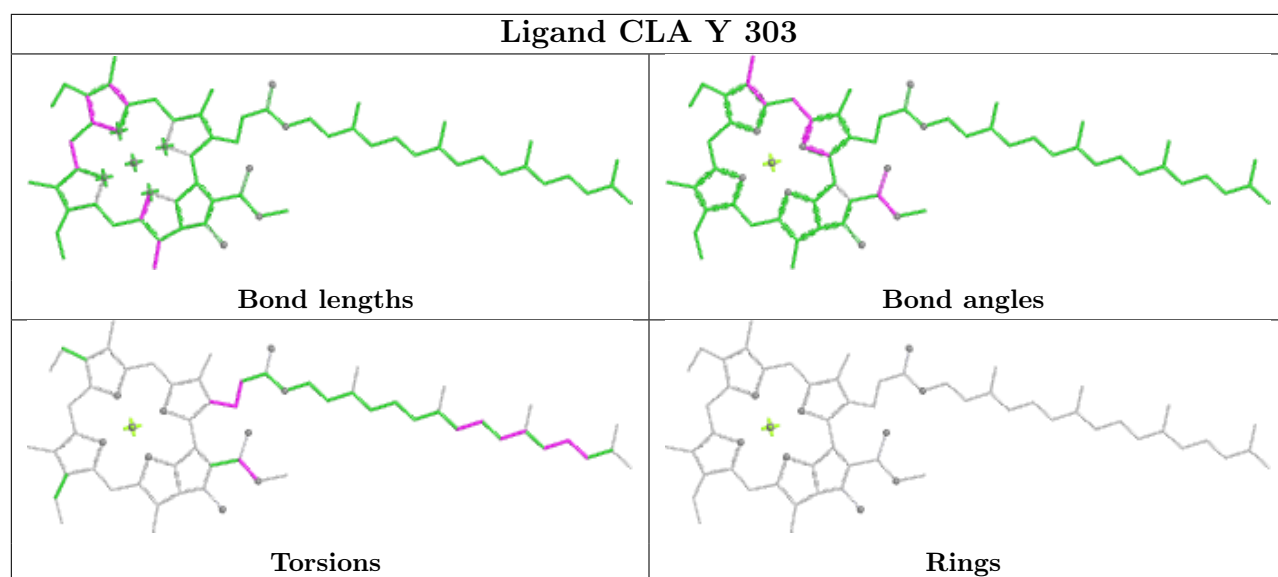
Ligand CLA Y 315

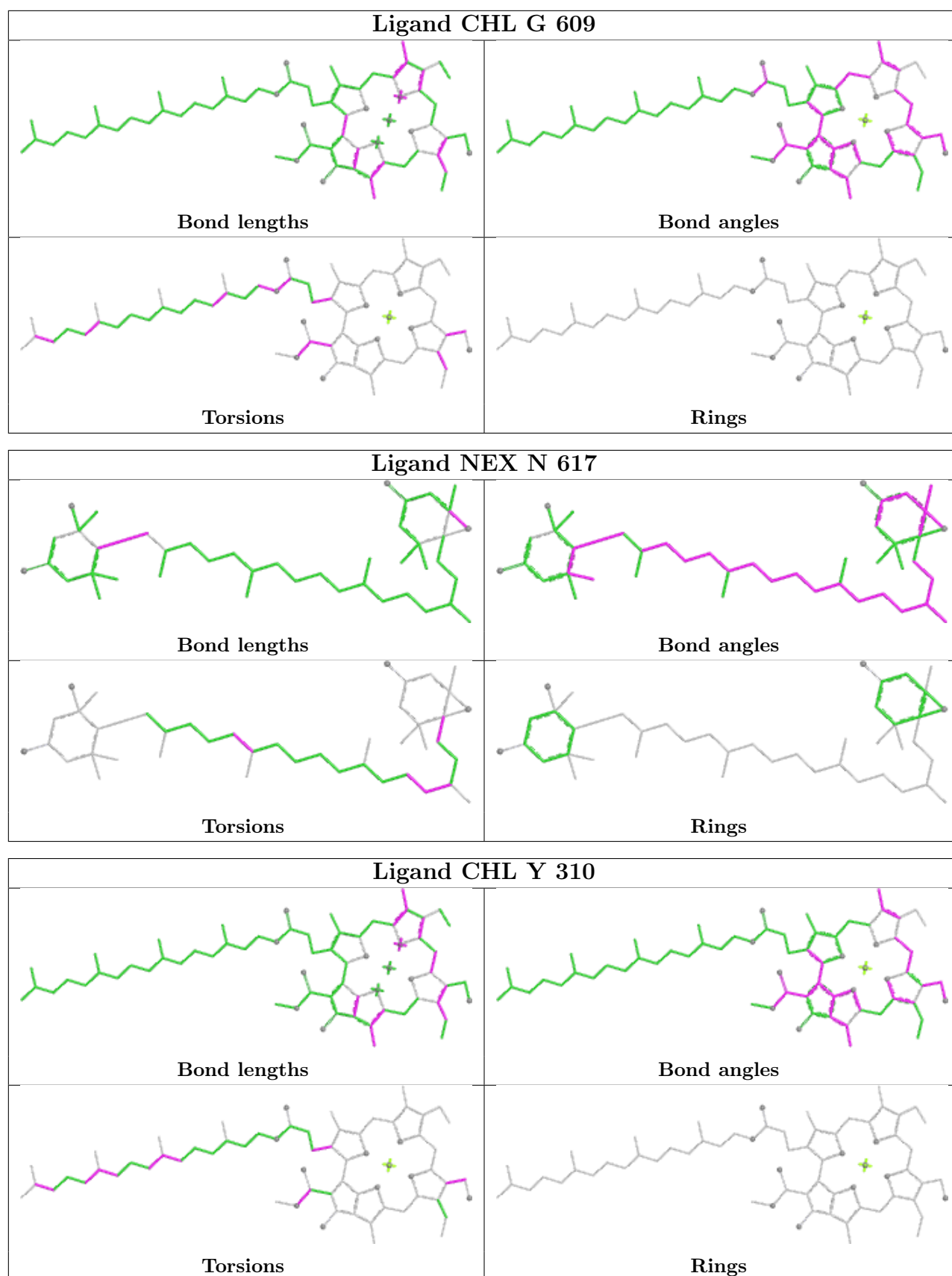


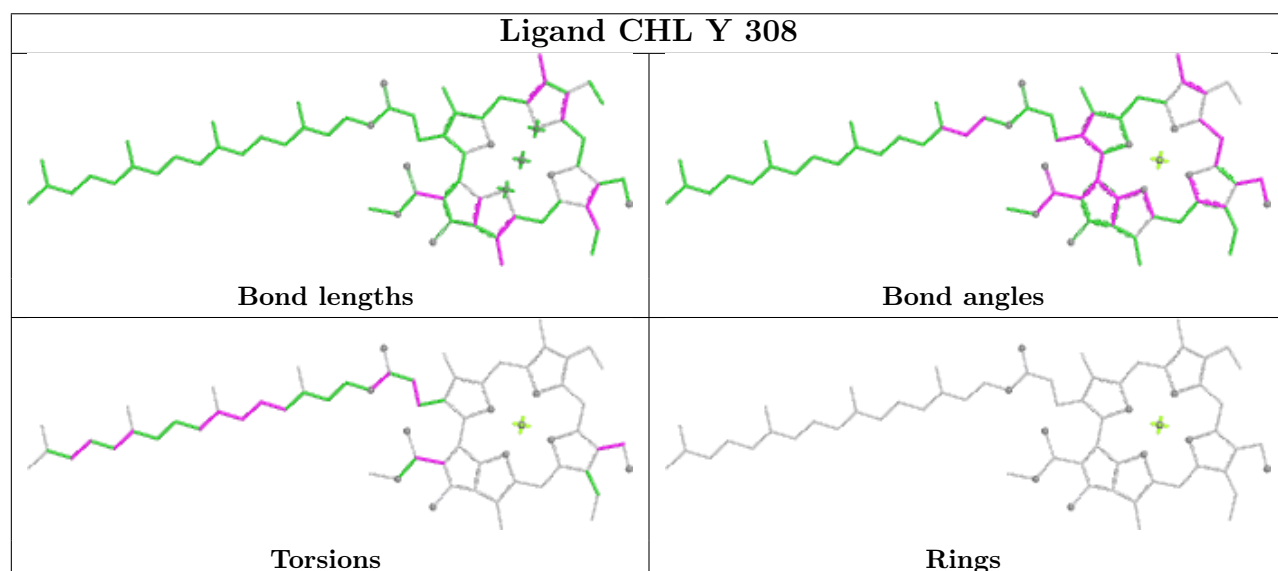
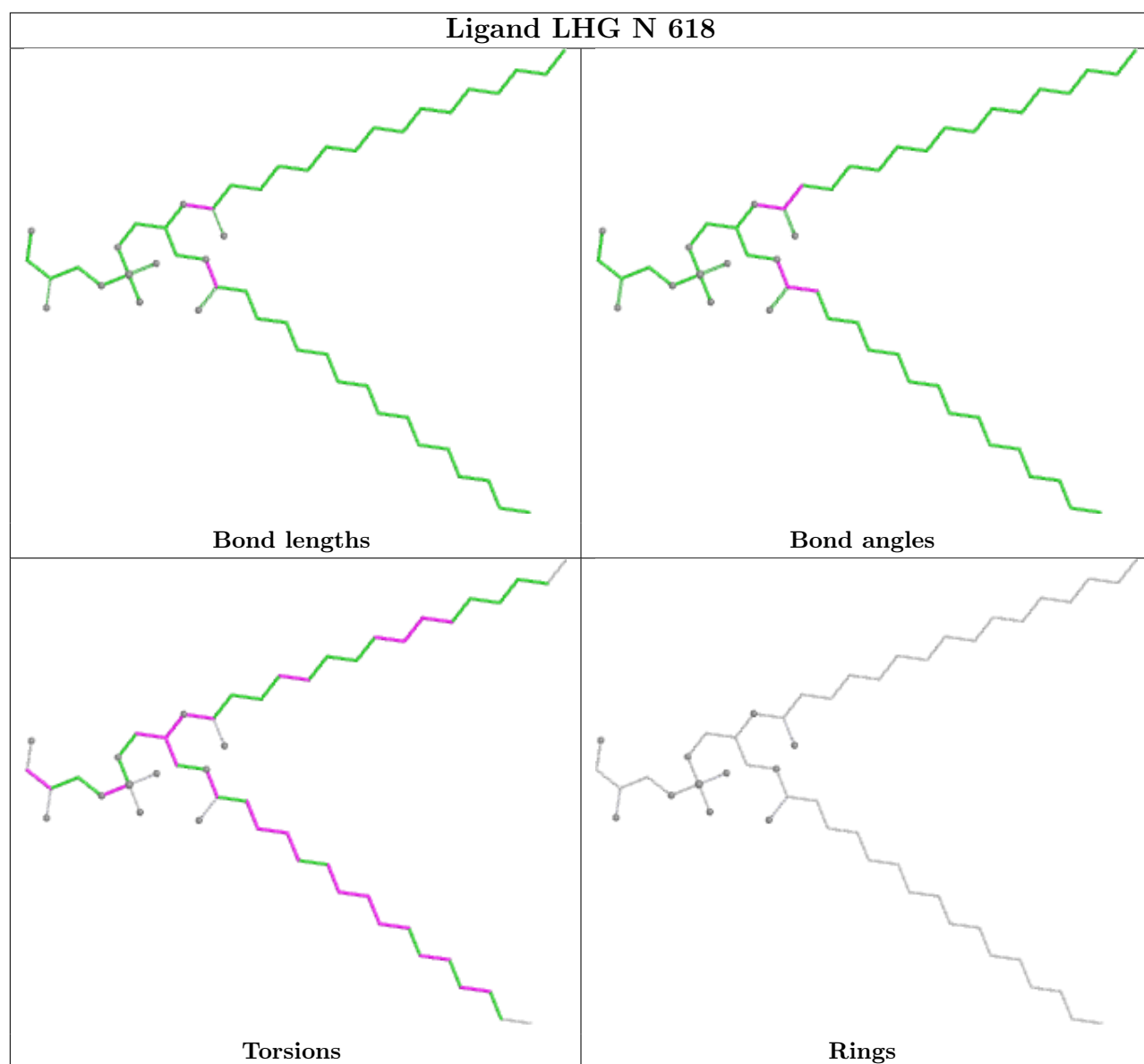
Ligand CLA Y 305

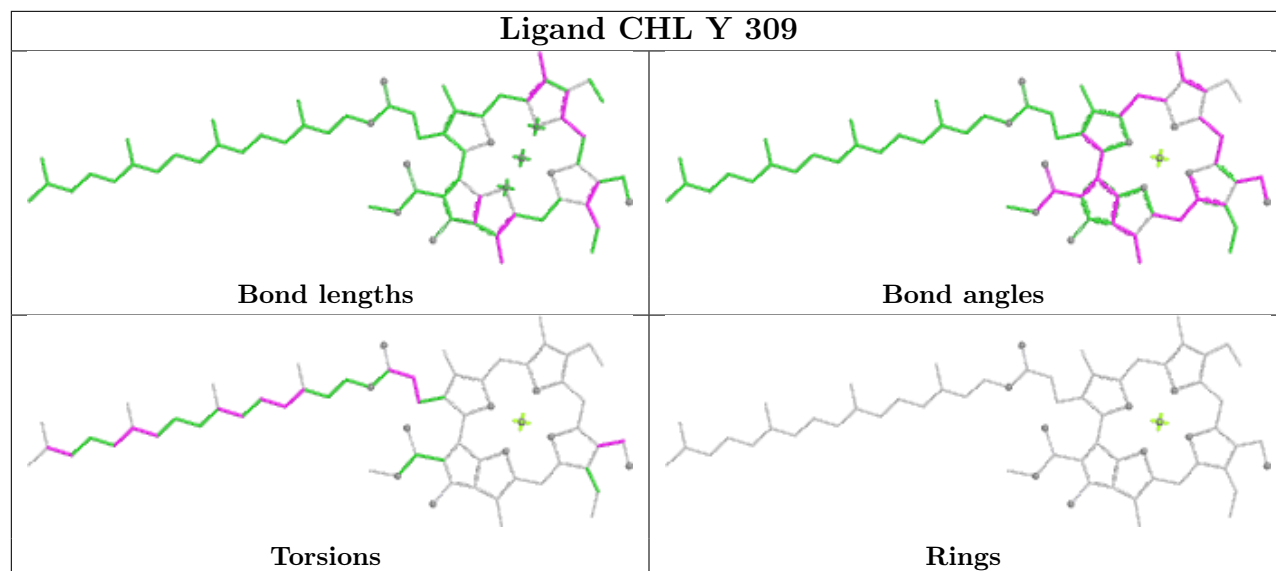
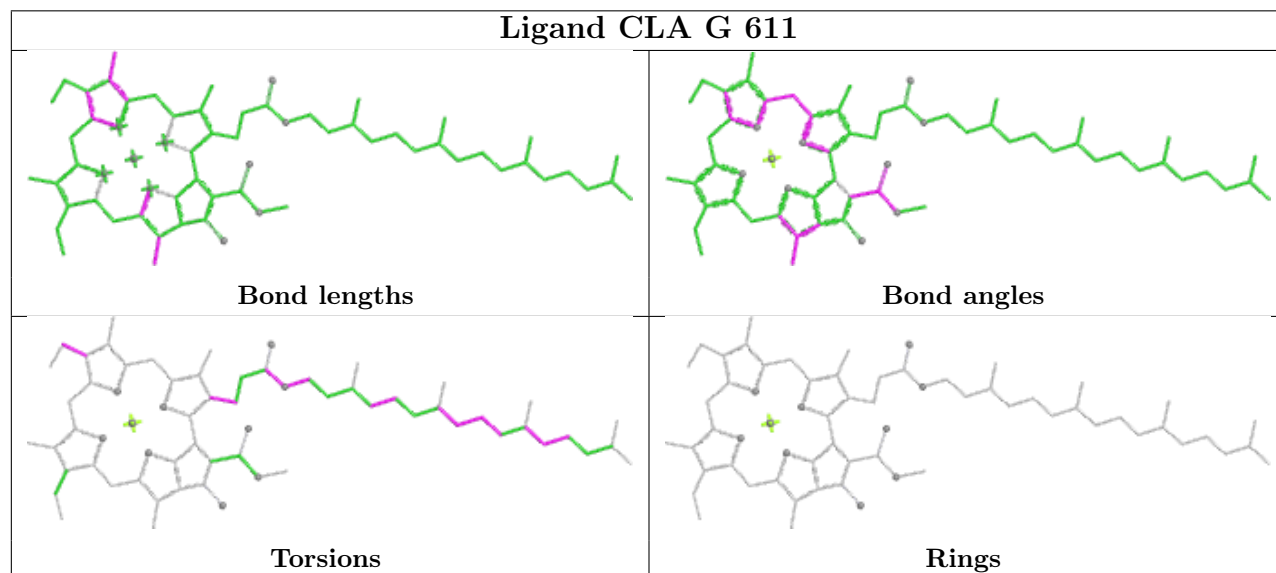
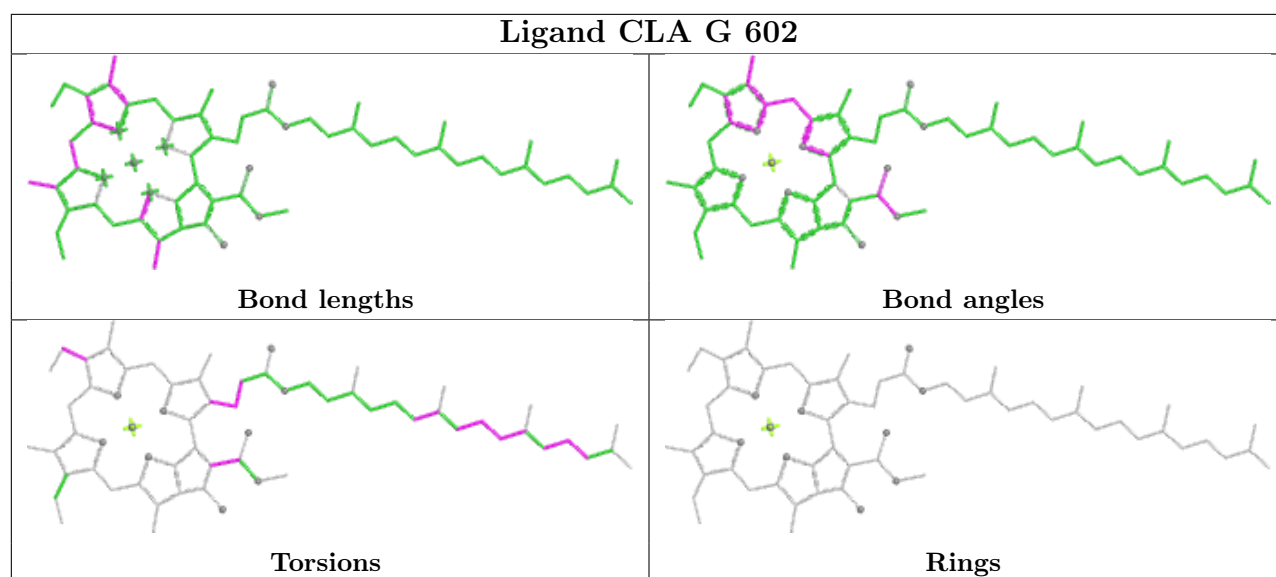


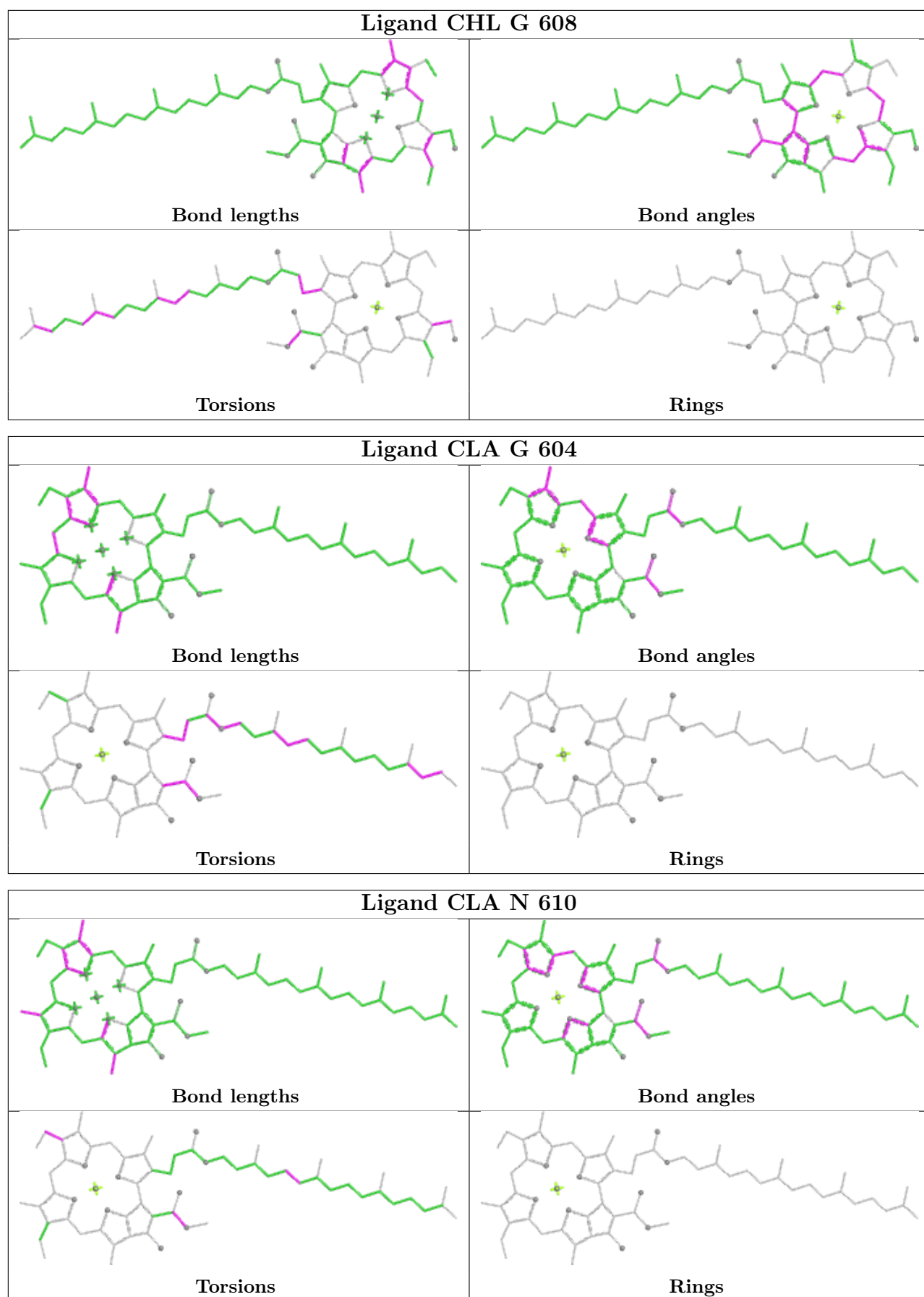


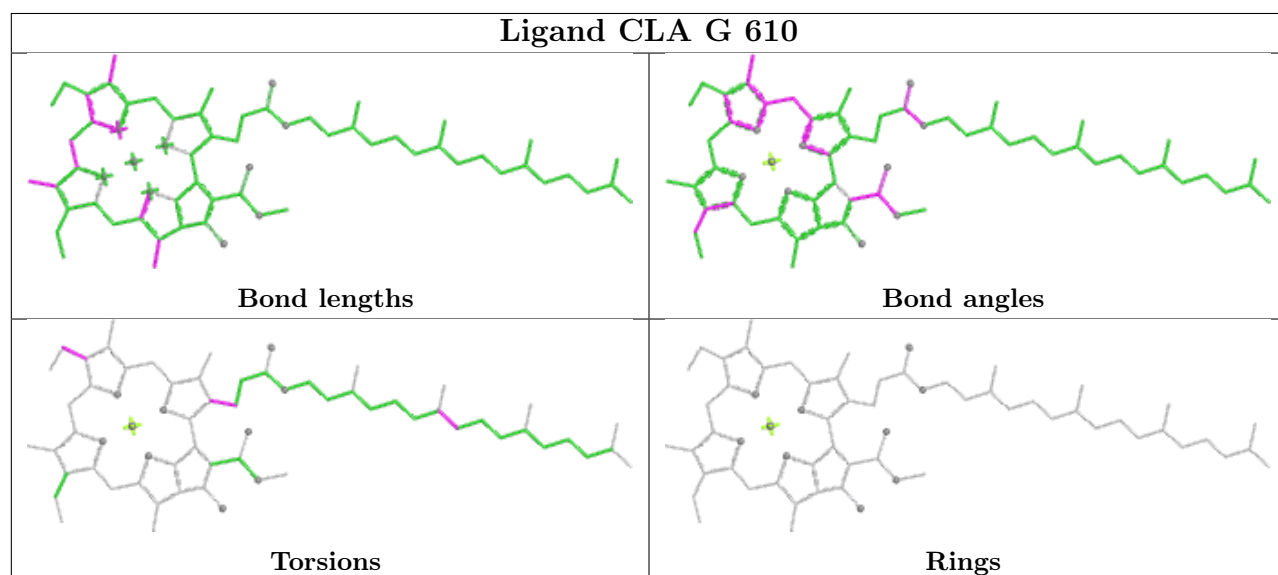
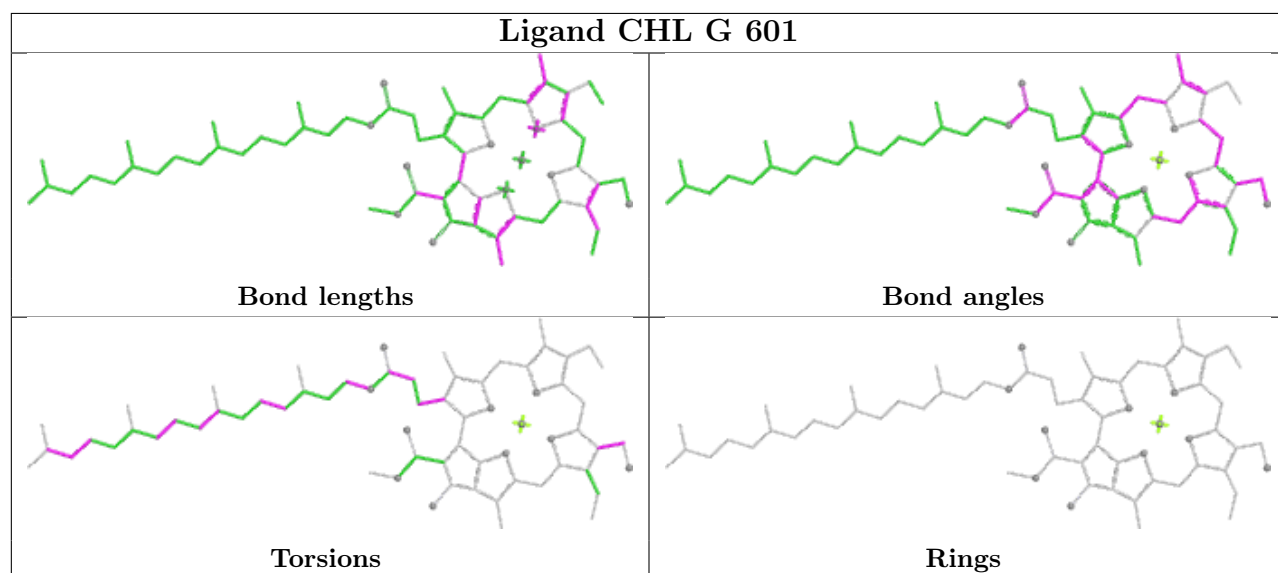
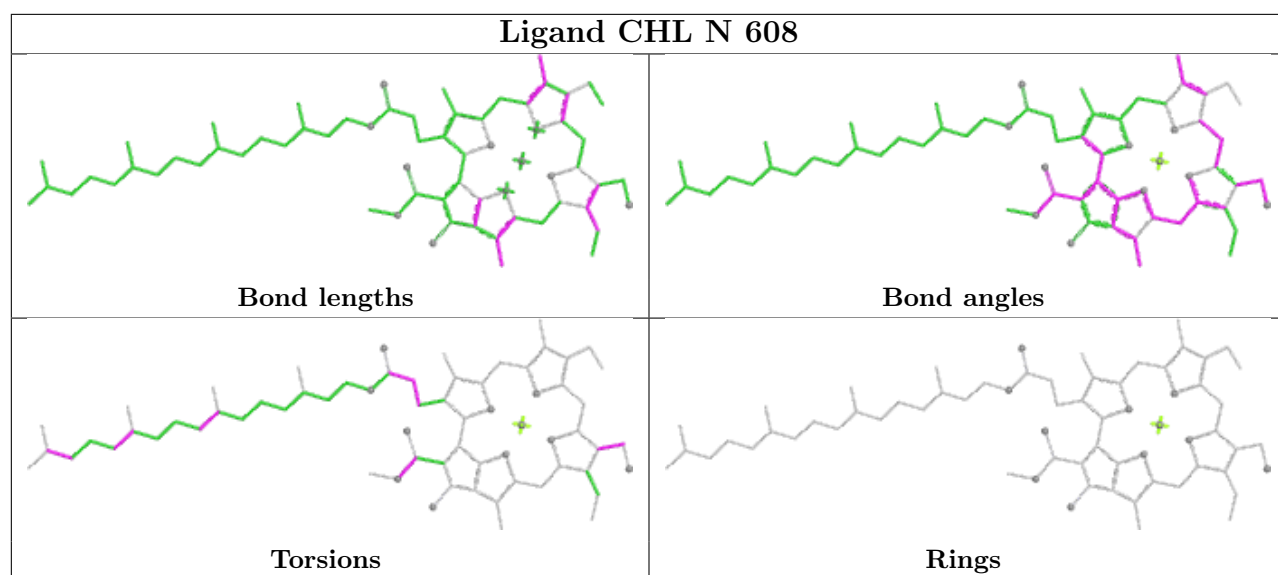


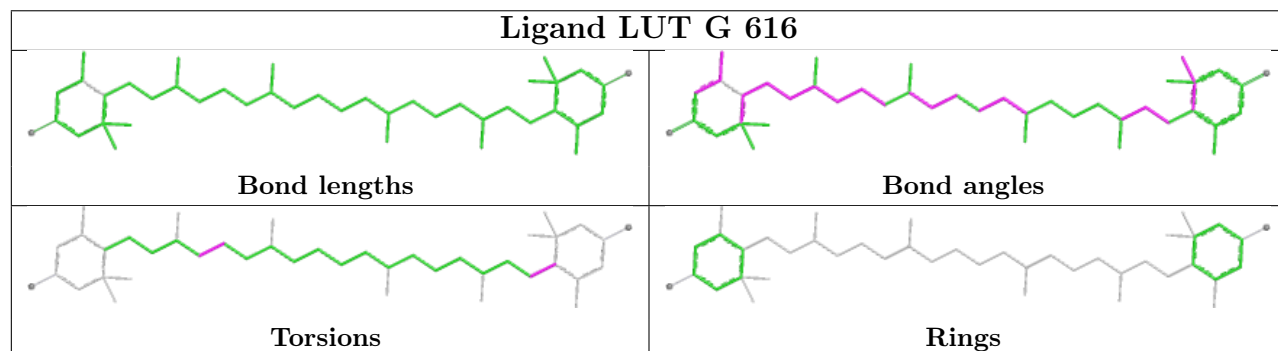
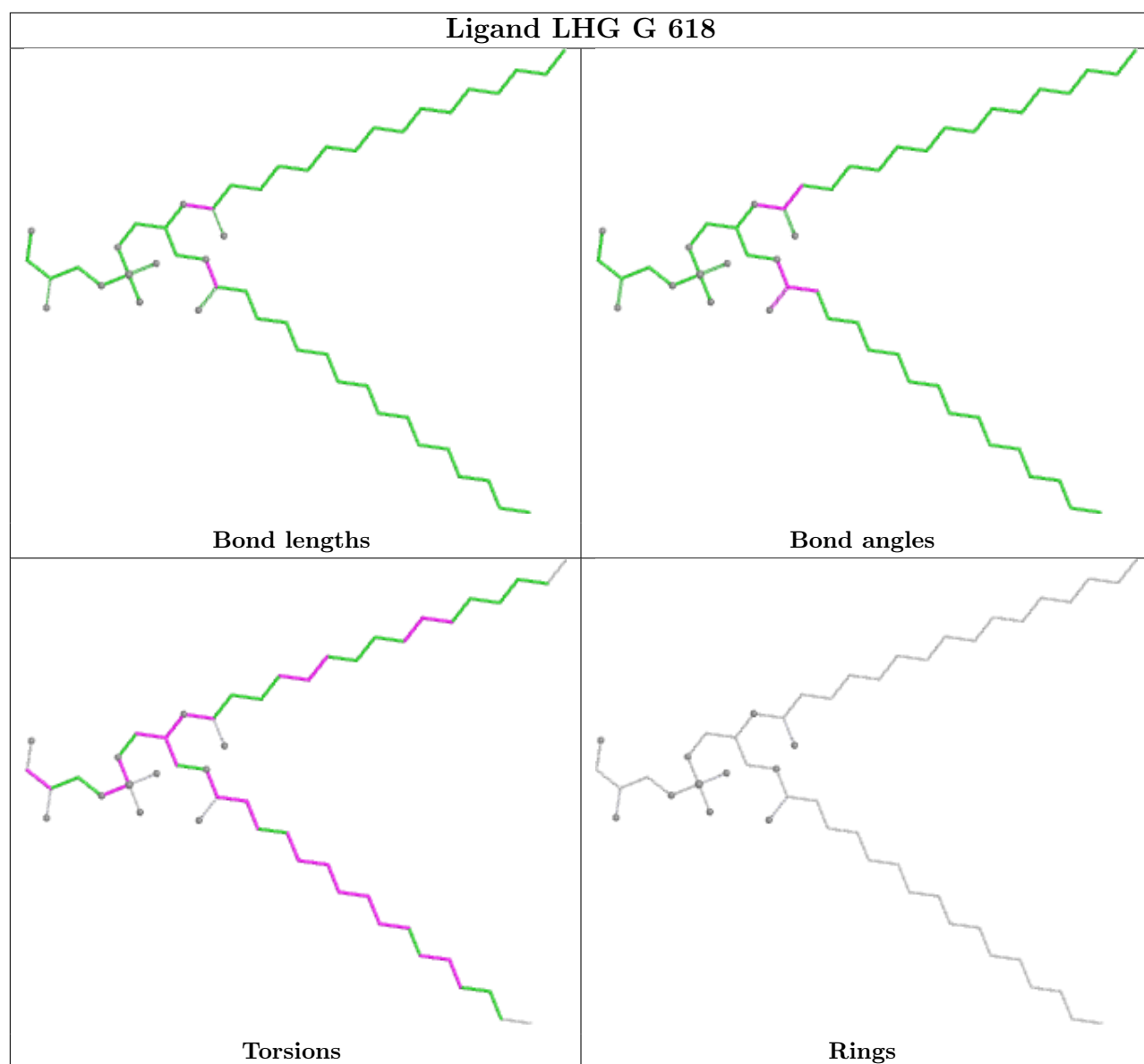


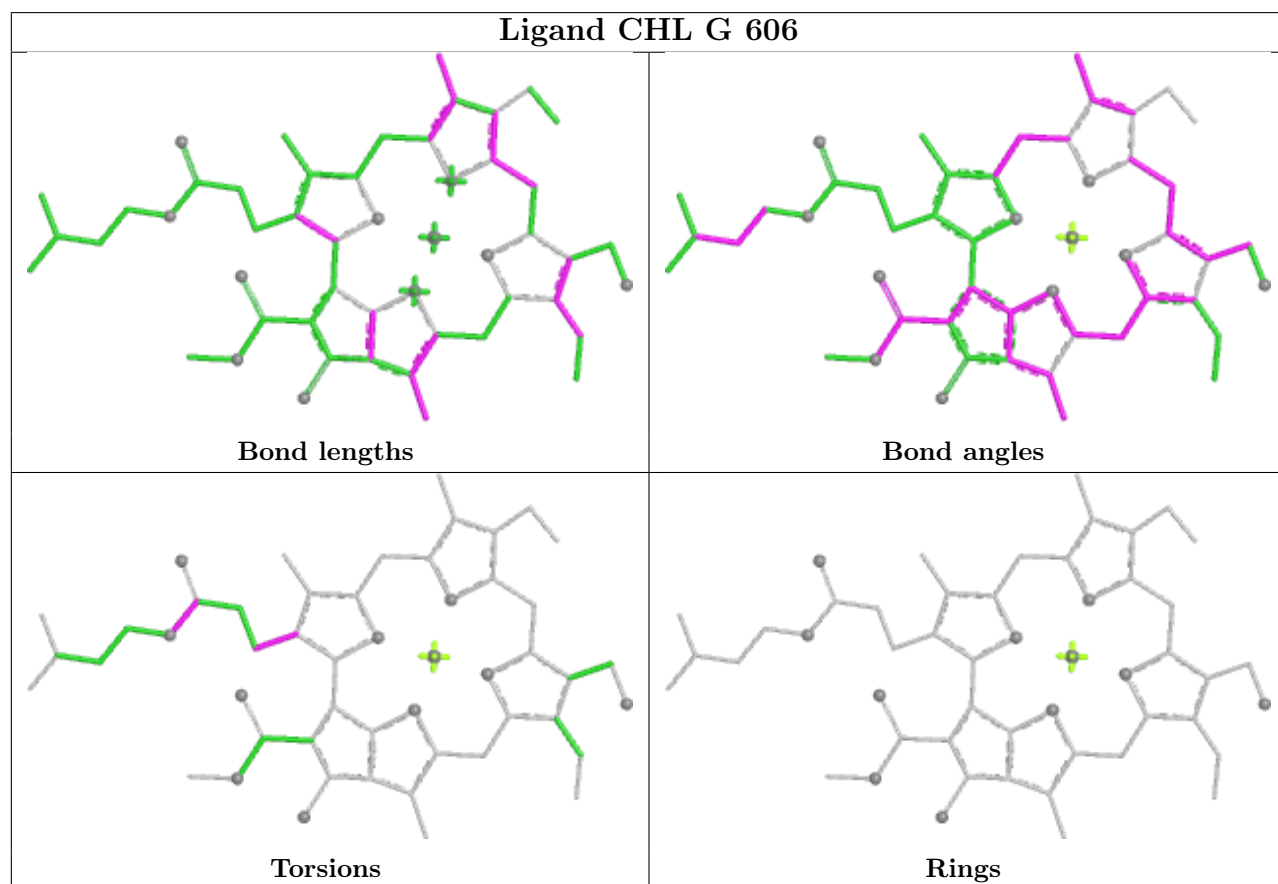
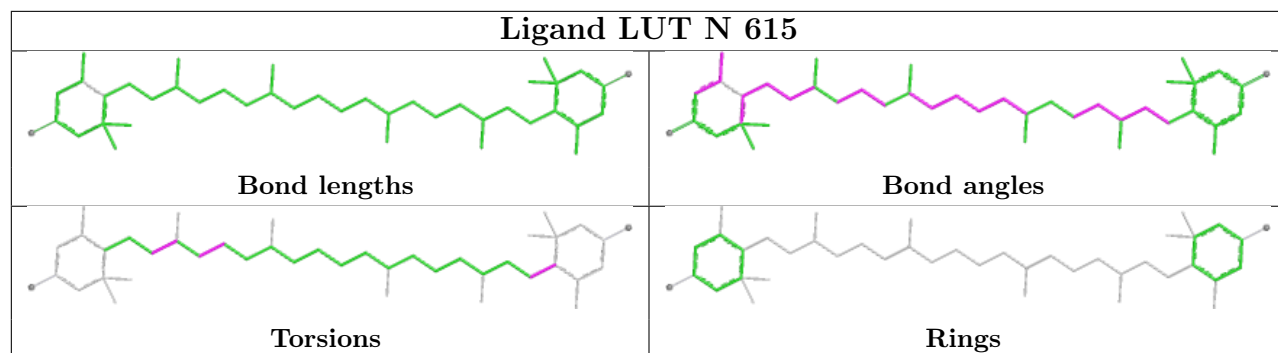


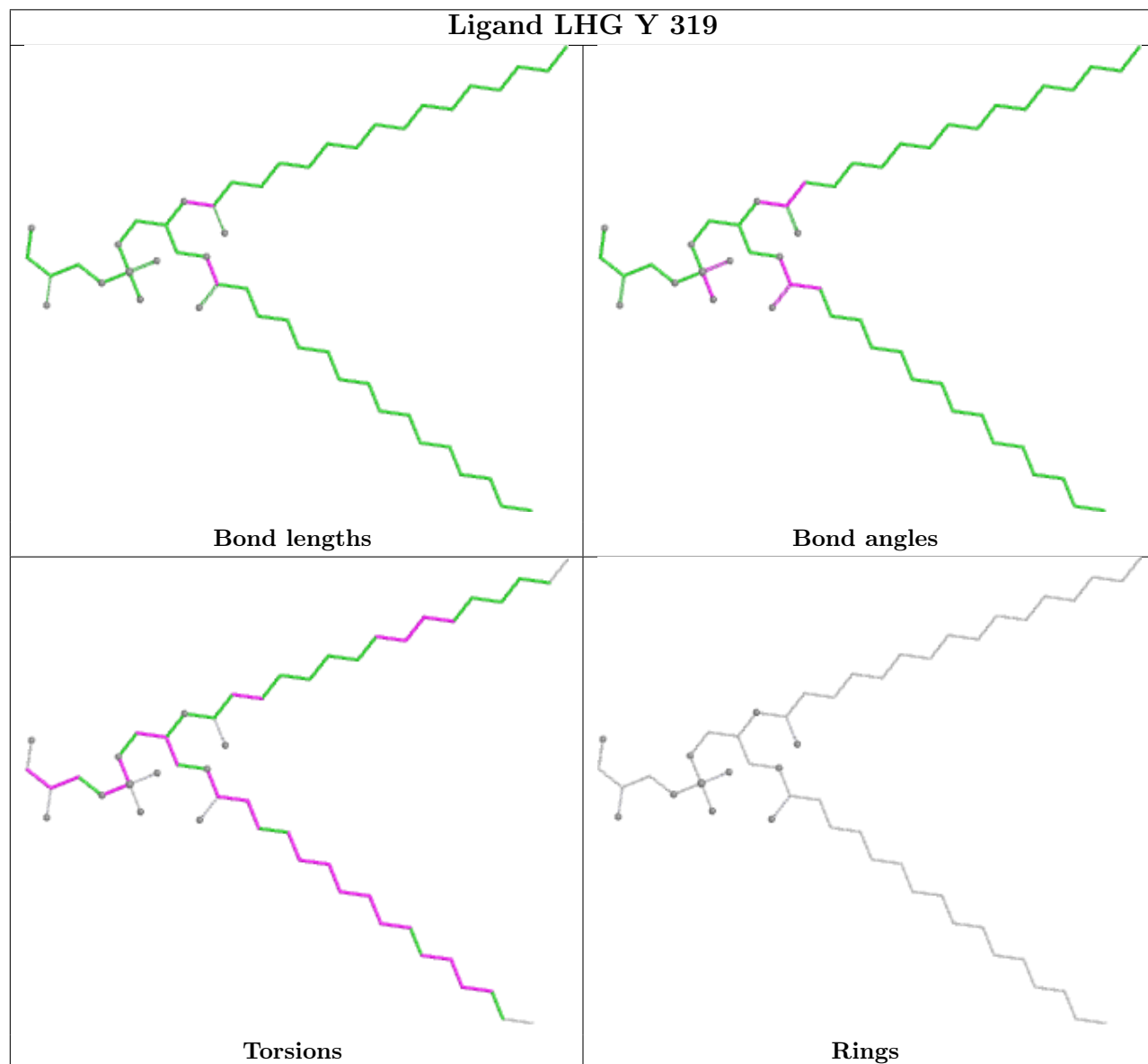
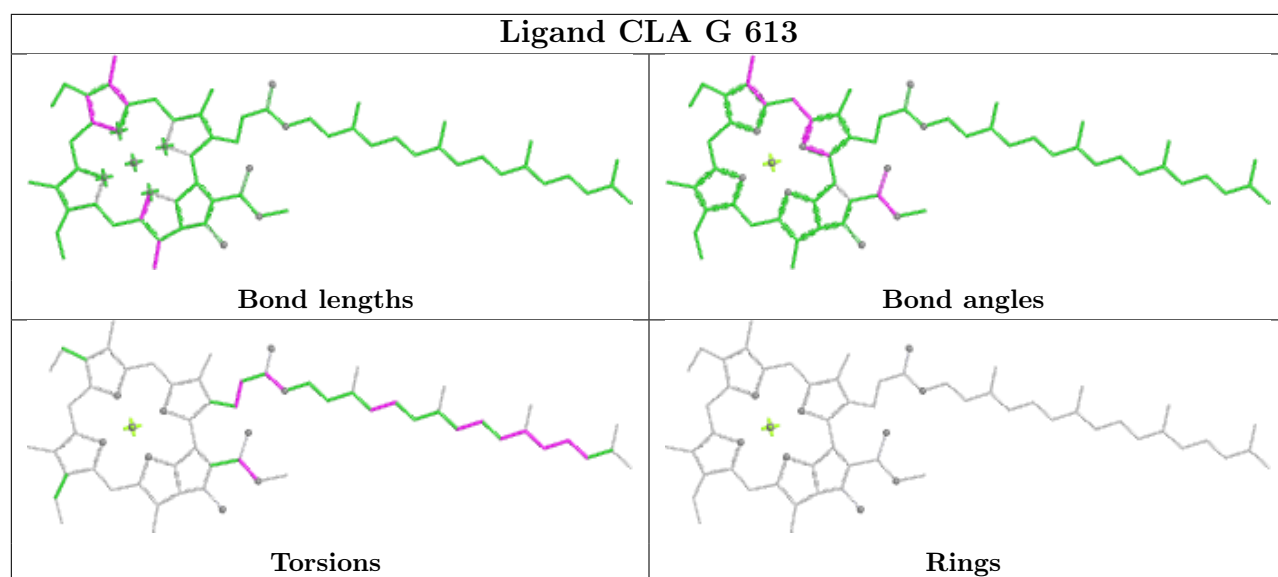


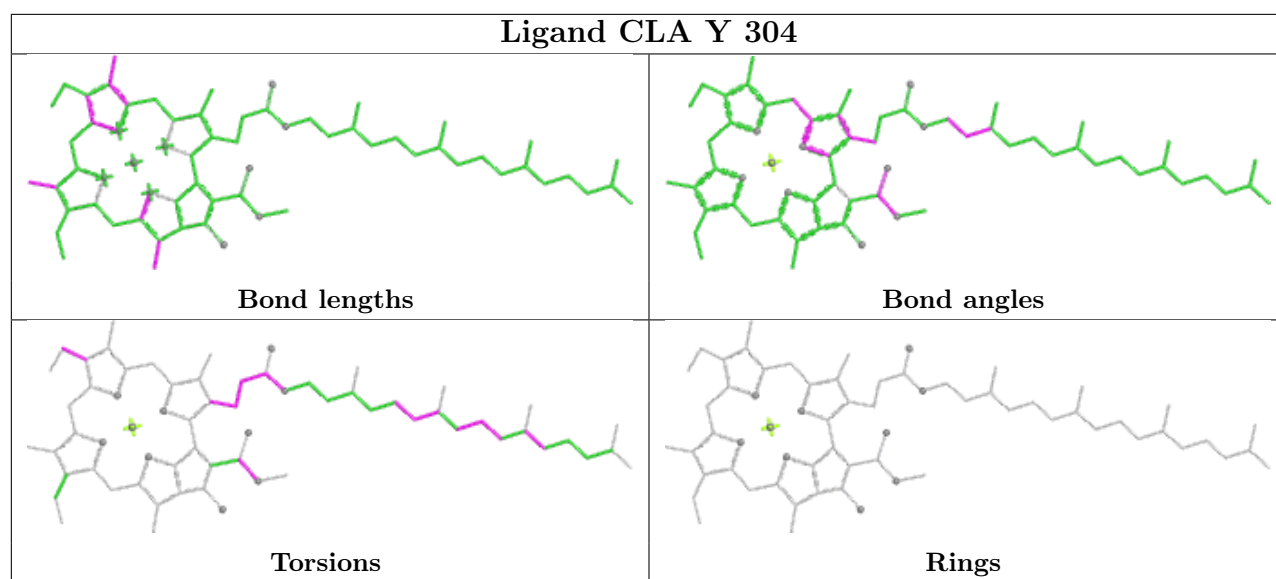












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

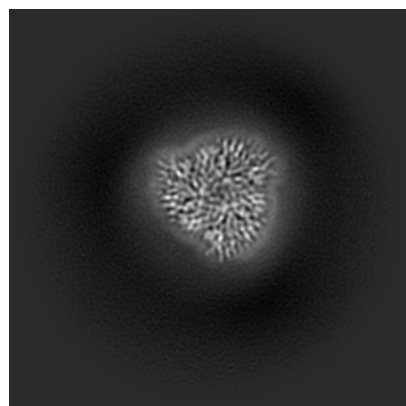
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35784. These allow visual inspection of the internal detail of the map and identification of artifacts.

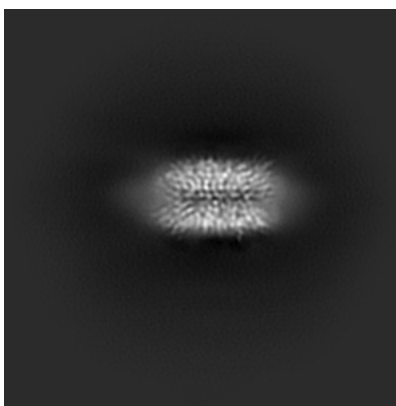
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

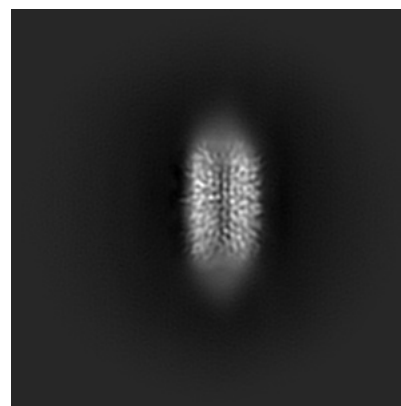
6.1.1 Primary map



X

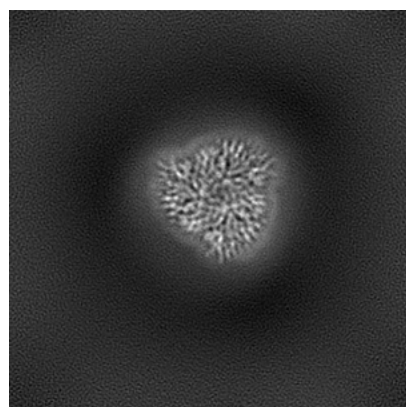


Y

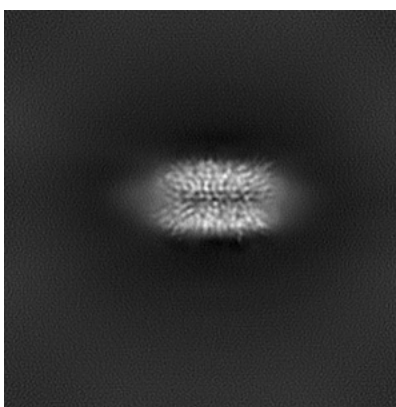


Z

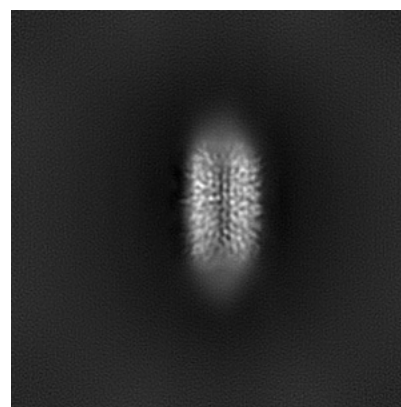
6.1.2 Raw map



X



Y

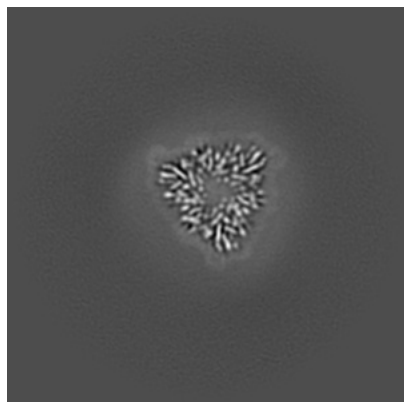


Z

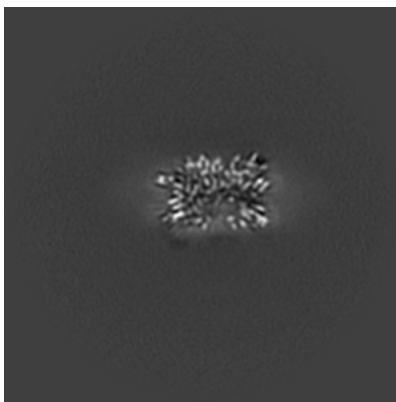
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

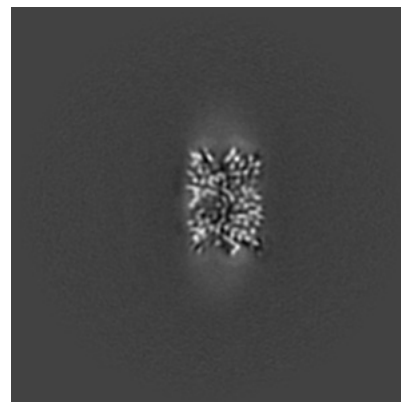
6.2.1 Primary map



X Index: 128

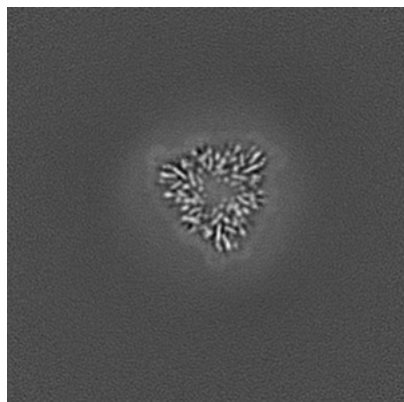


Y Index: 128

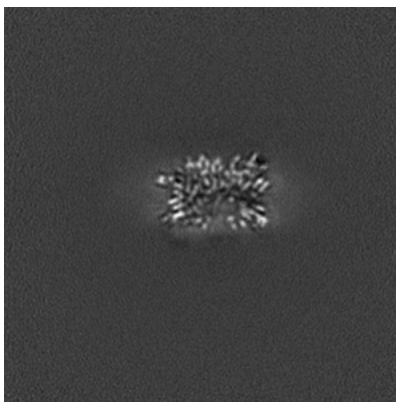


Z Index: 128

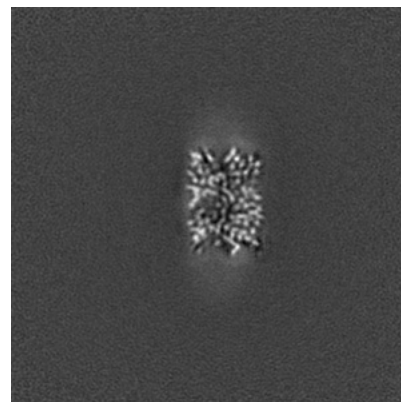
6.2.2 Raw map



X Index: 128



Y Index: 128

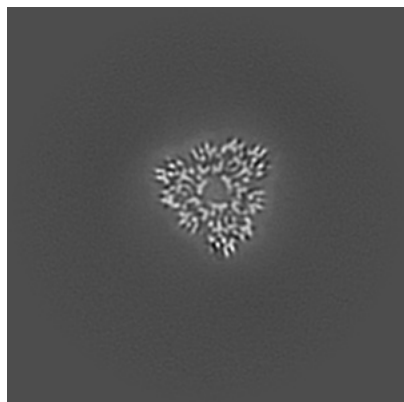


Z Index: 128

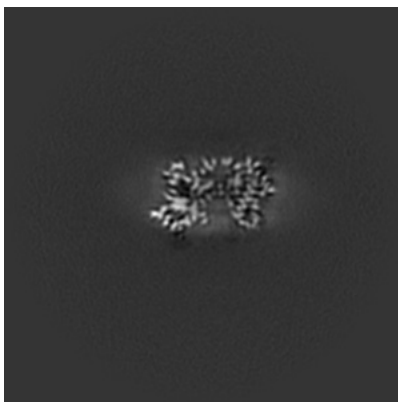
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

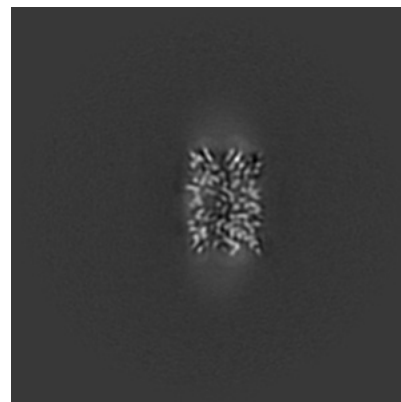
6.3.1 Primary map



X Index: 118

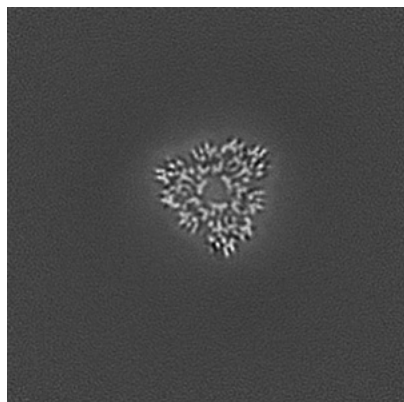


Y Index: 135

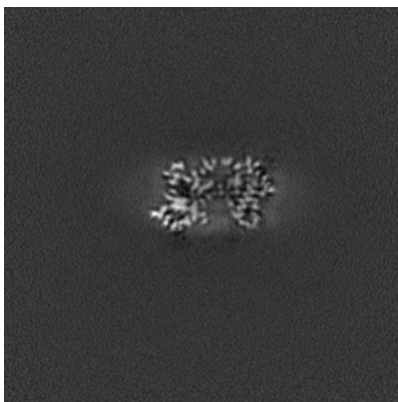


Z Index: 129

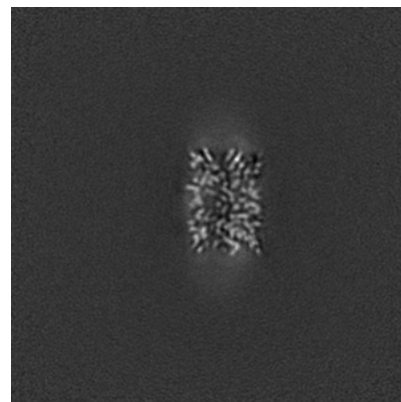
6.3.2 Raw map



X Index: 118



Y Index: 135

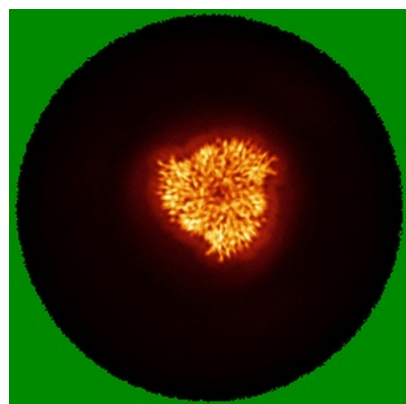


Z Index: 129

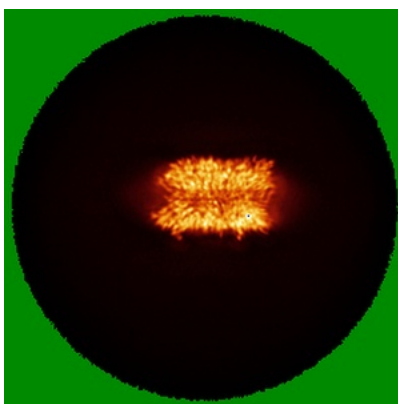
The images above show the largest variance slices of the map in three orthogonal directions.

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

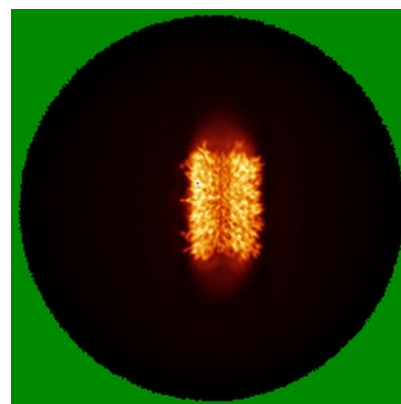
6.4.1 Primary map



X

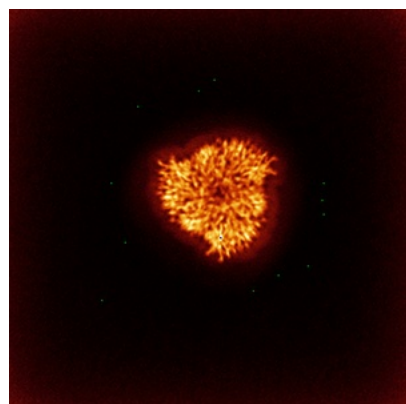


Y

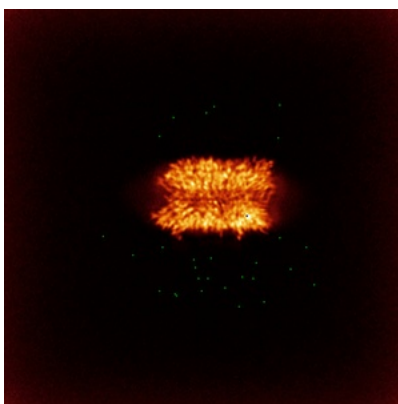


Z

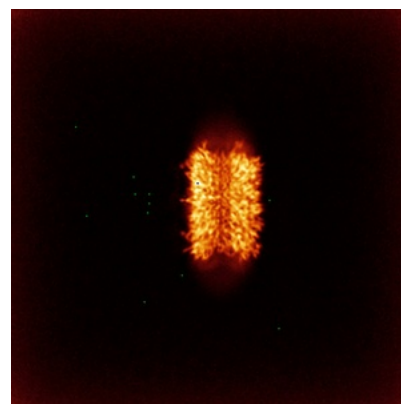
6.4.2 Raw map



X



Y

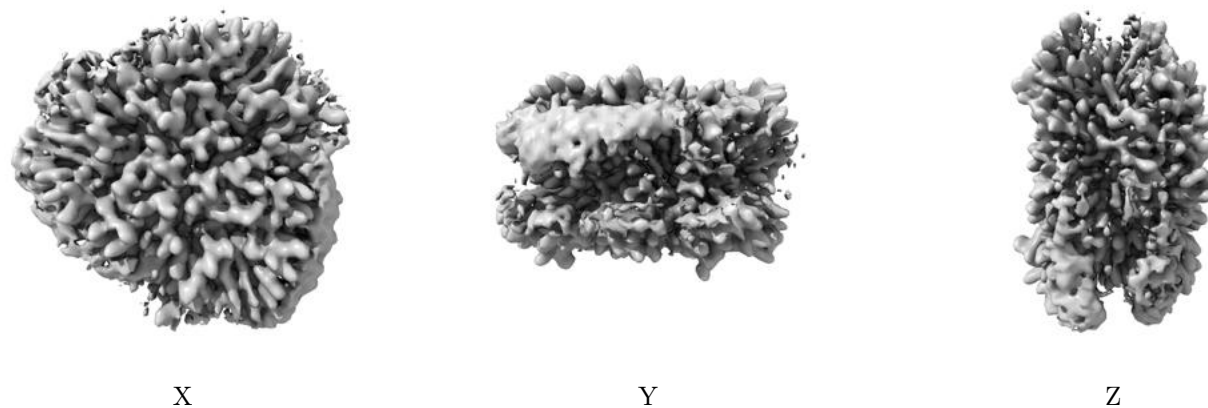


Z

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

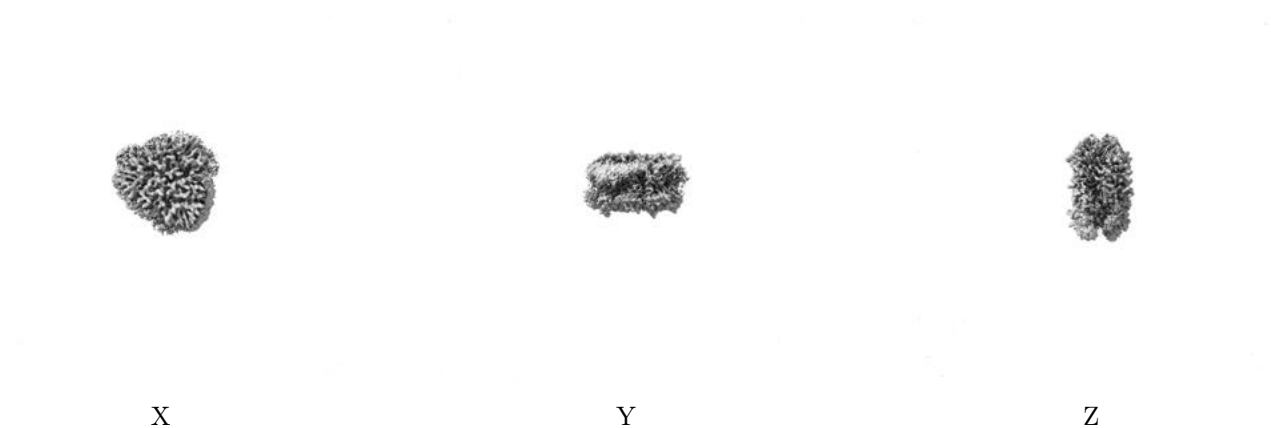
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

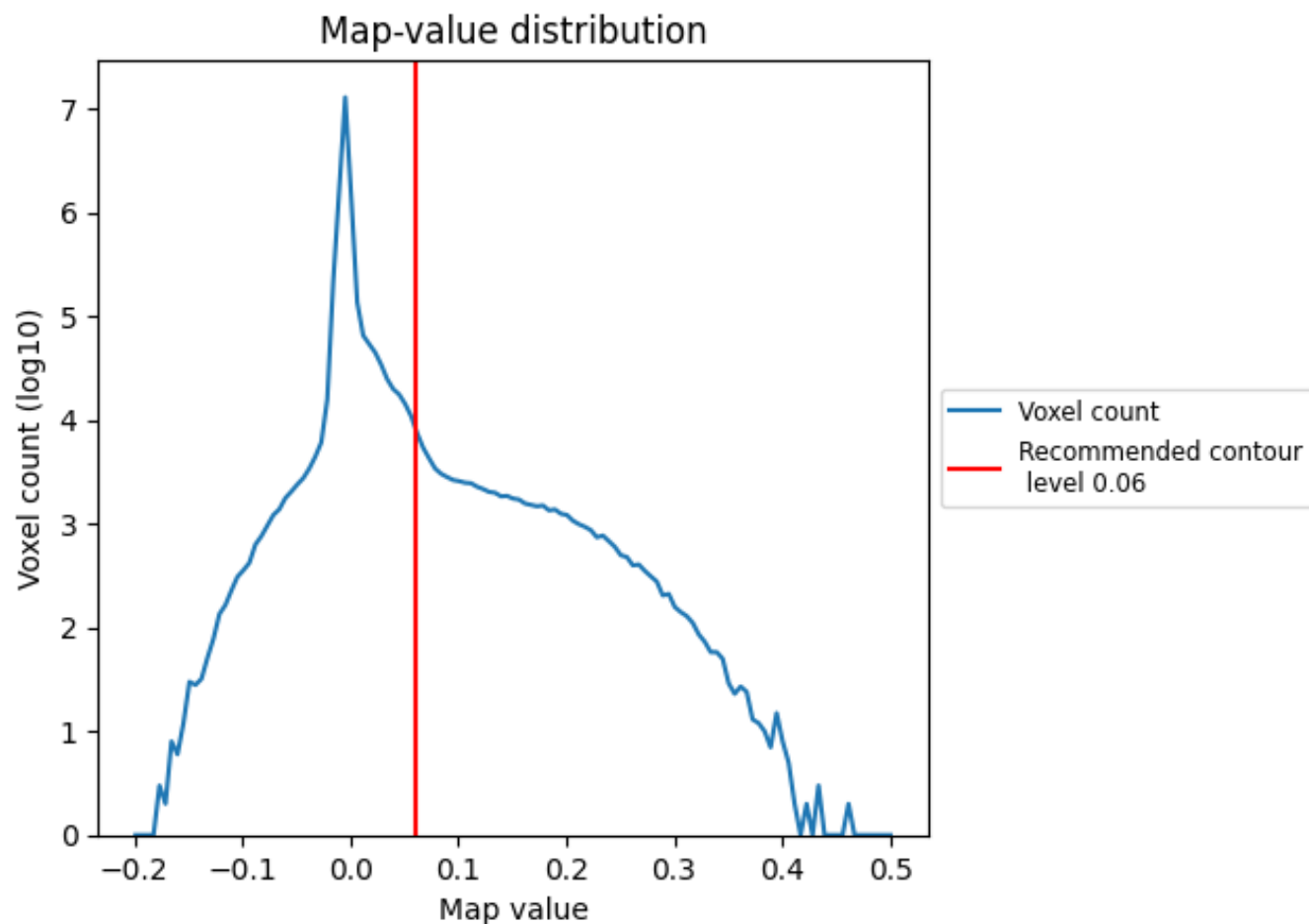
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

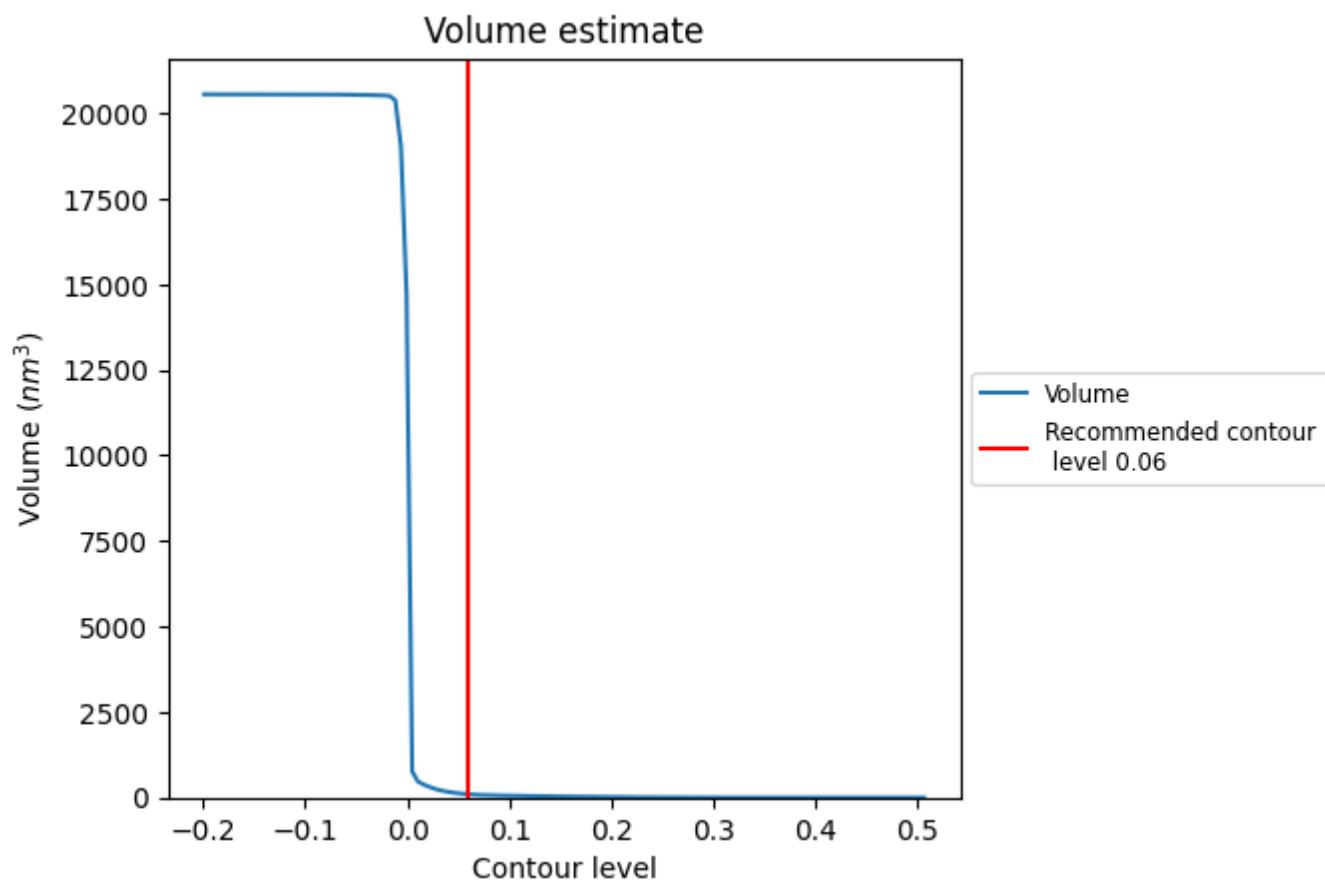
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

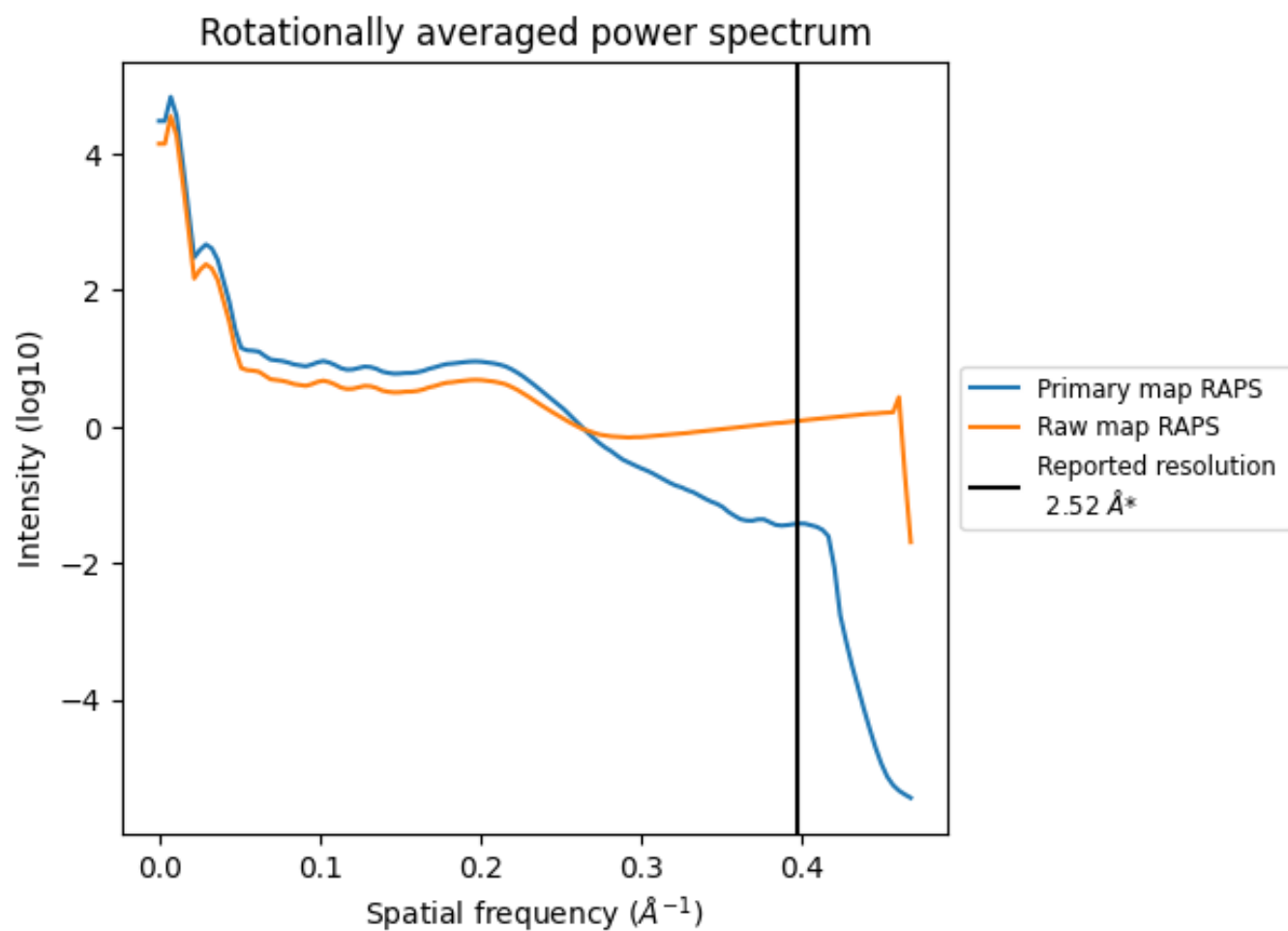
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 95 nm^3 ; 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 ⓘ

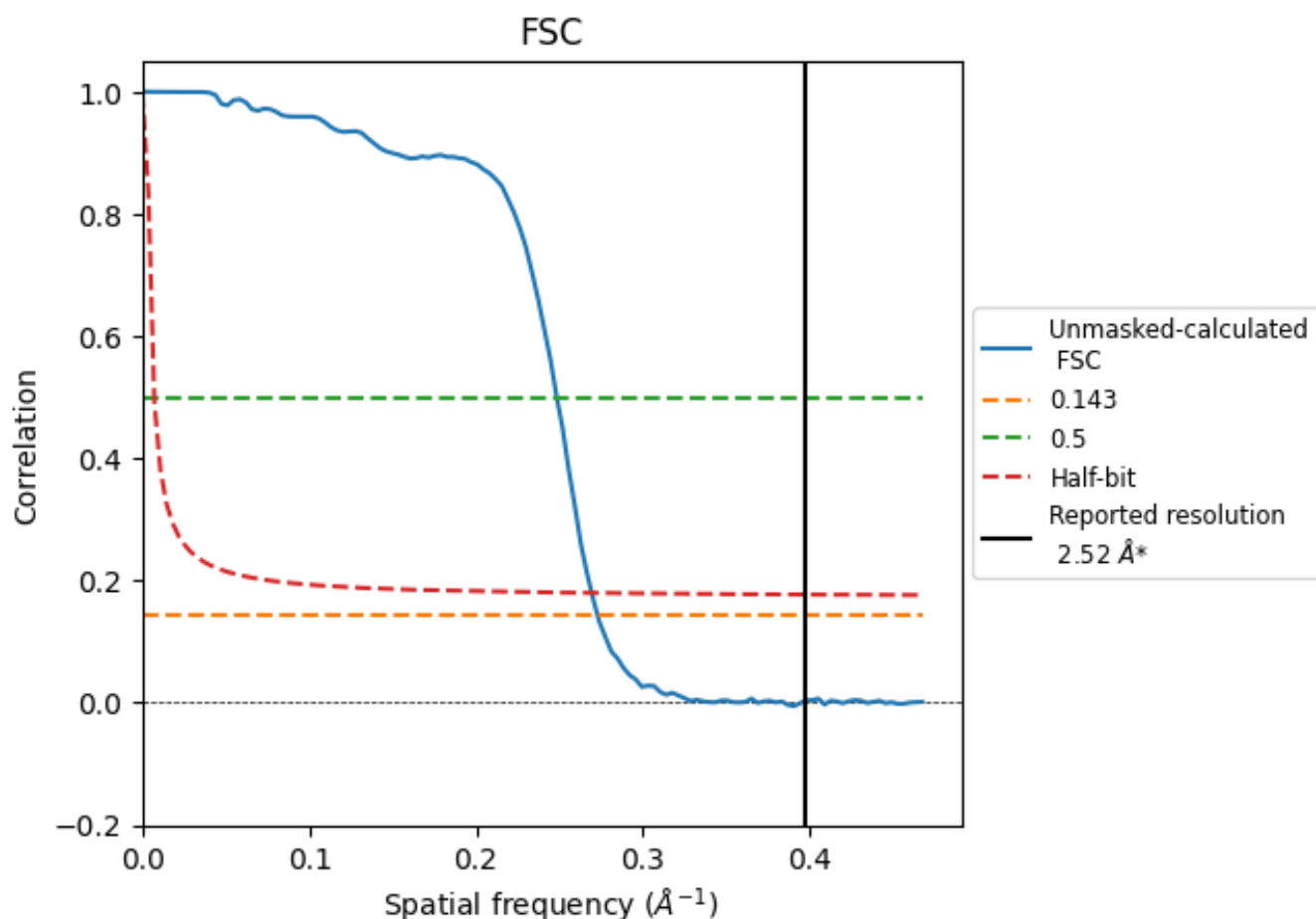


*Reported resolution corresponds to spatial frequency of $0.397 \text{ \AA}^{-1}$

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 $0.397 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

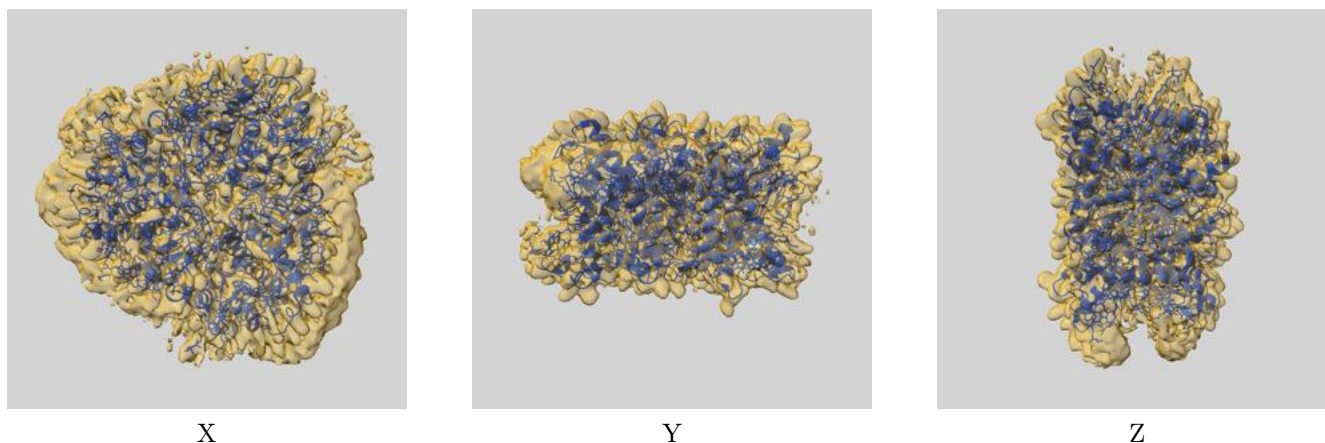
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.52	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.67	4.03	3.71

*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 2.52 by more than 10 %

9 Map-model fit [i](#)

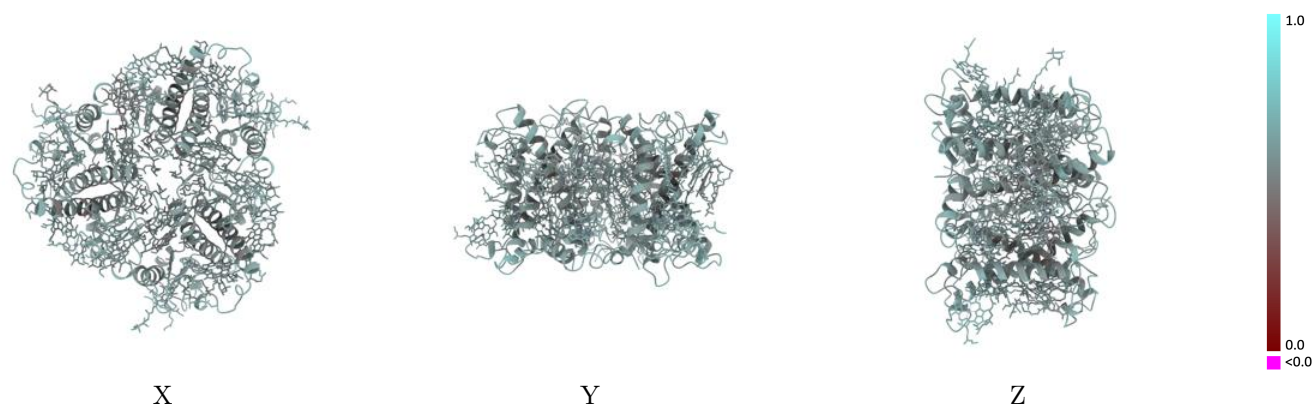
This section contains information regarding the fit between EMDB map EMD-35784 and PDB model 8IWZ. Per-residue inclusion information can be found in section [3](#) on page [11](#).

9.1 Map-model overlay [i](#)



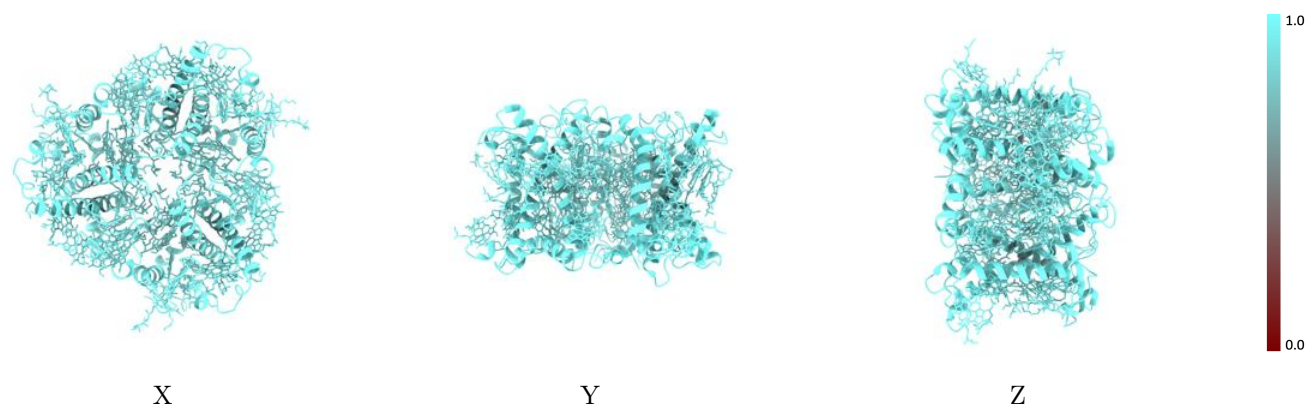
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



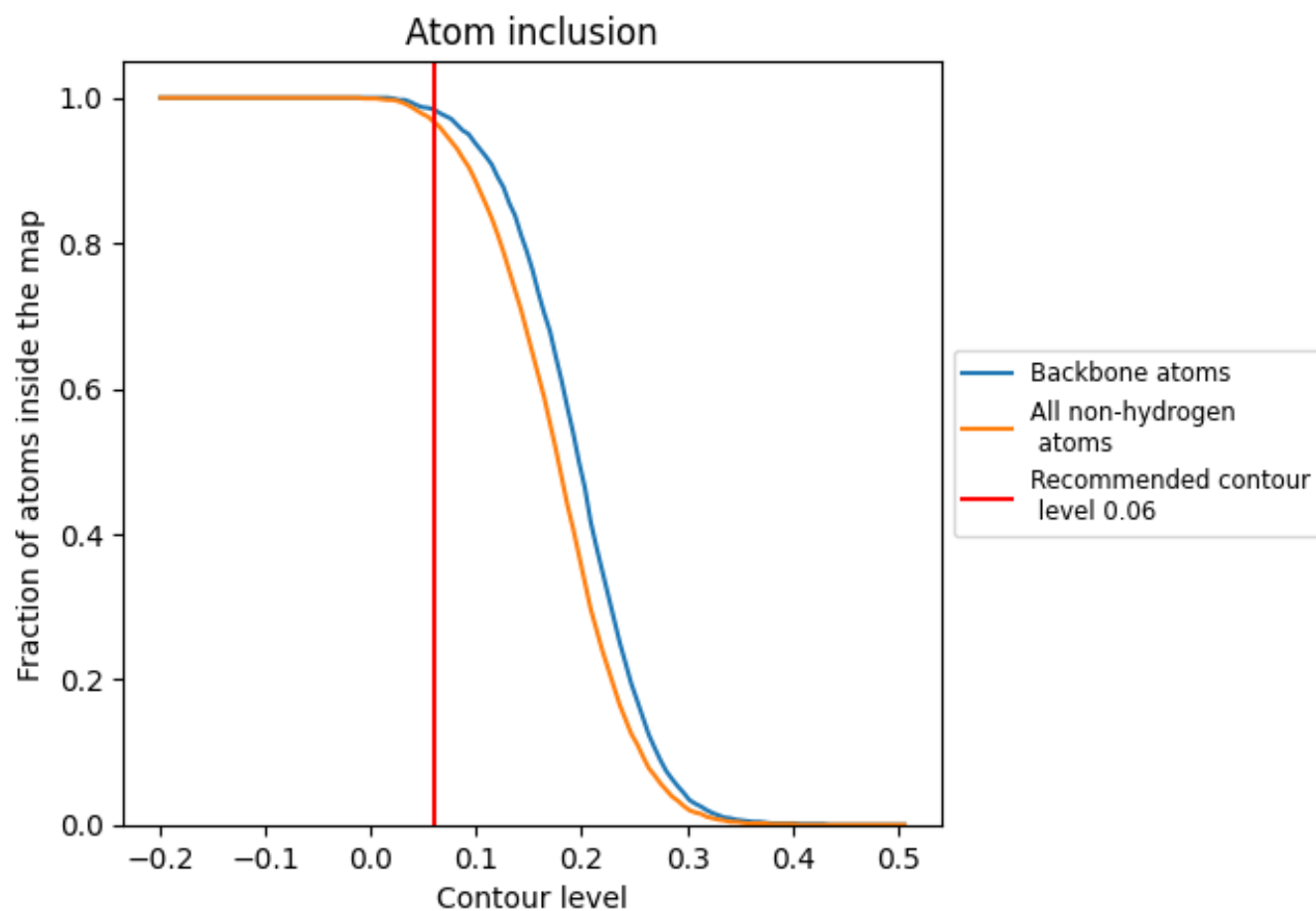
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.06).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 97% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9670	0.5630
G	0.9630	0.5630
N	0.9710	0.5610
Y	0.9660	0.5650

