



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 03:46 AM UTC

PDB ID : 8IWY / pdb_00008iwy
EMDB ID : EMD-35783
Title : Cryo-EM structure of protonated LHCII in detergent solution at low pH value
Authors : Ruan, M.X.; Ding, W.
Deposited on : 2023-03-31
Resolution : 2.68 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

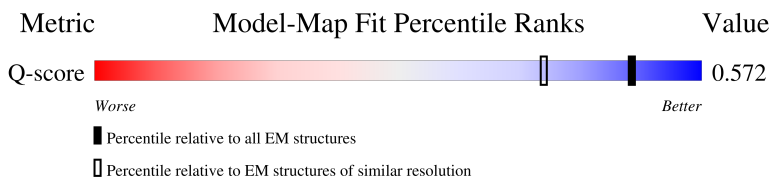
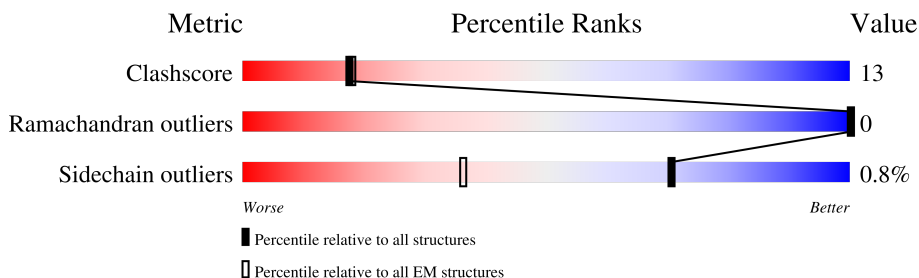
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.68 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	9255 (2.18 - 3.18)

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	81% 18%
1	N	218	81% 19%
1	Y	218	82% 17% .

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	601	X	-	-	-
2	CHL	Y	605	X	-	-	-
2	CHL	Y	606	X	-	-	-
2	CHL	Y	607	X	-	-	-
2	CHL	Y	608	X	-	-	-
2	CHL	Y	609	X	-	-	-
3	CLA	G	602	X	-	-	-
3	CLA	G	603	X	-	-	-
3	CLA	G	604	X	-	-	-
3	CLA	G	610	X	-	-	-
3	CLA	G	612	X	-	-	-
3	CLA	G	613	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	602	X	-	-	-
3	CLA	Y	603	X	-	-	-
3	CLA	Y	604	X	-	-	-
3	CLA	Y	610	X	-	-	-
3	CLA	Y	611	X	-	-	-
3	CLA	Y	612	X	-	-	-
3	CLA	Y	614	X	-	-	-

2 Entry composition [i](#)

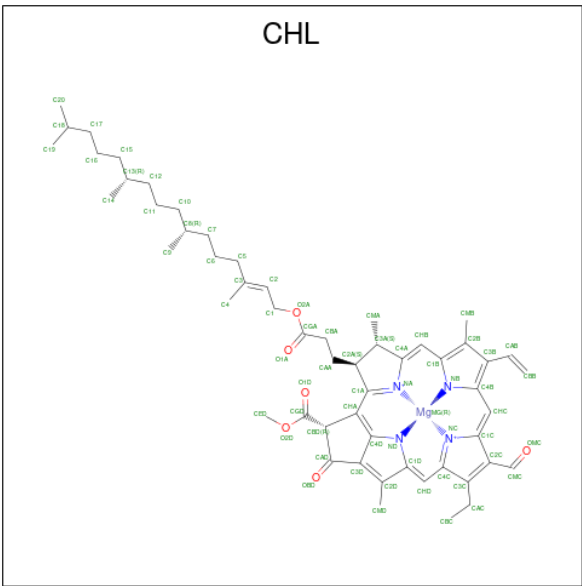
There are 7 unique types of molecules in this entry. The entry contains 8238 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	G	218	Total	C	N	O	S	0	0
			1661	1079	270	305	7		
1	N	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		

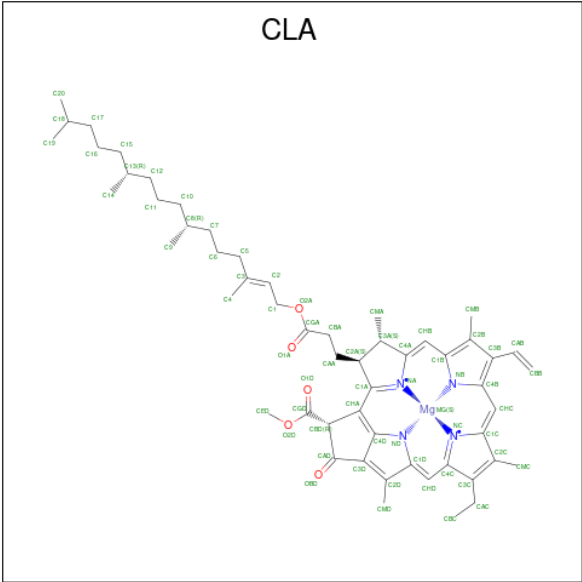
- Molecule 2 is CHLOROPHYLL B (CCD ID: CHL) (formula: C₅₅H₇₀MgN₄O₆) (labeled as "Ligand of Interest" by depositor).



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Mol	Chain	Residues	Atoms					AltConf
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	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	
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	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).



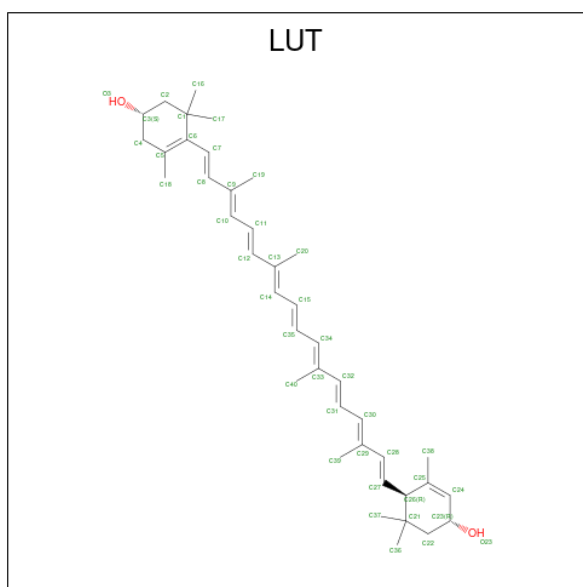
Mol	Chain	Residues	Atoms					AltConf
3	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	G	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
3	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	G	1	Total	C	Mg	N	O	0
			65	55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

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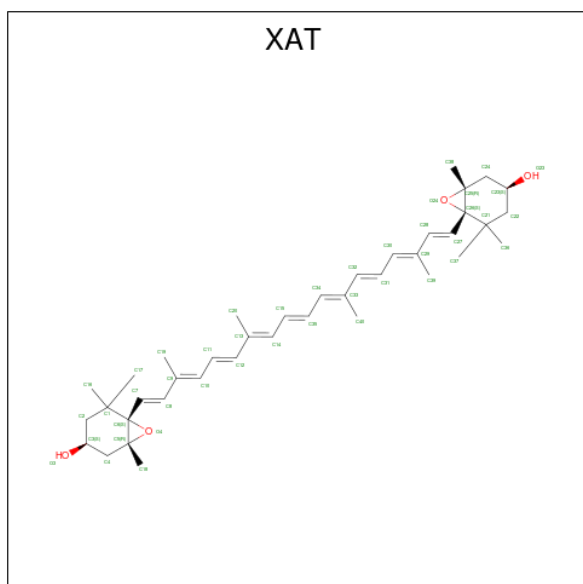
Mol	Chain	Residues	Atoms					AltConf
3	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	N	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
3	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	Y	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
3	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	Y	1	Total	C	Mg	N	O	0
			65	55	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
			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: $C_{40}H_{56}O_2$) (labeled as "Ligand of Interest" by depositor).



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

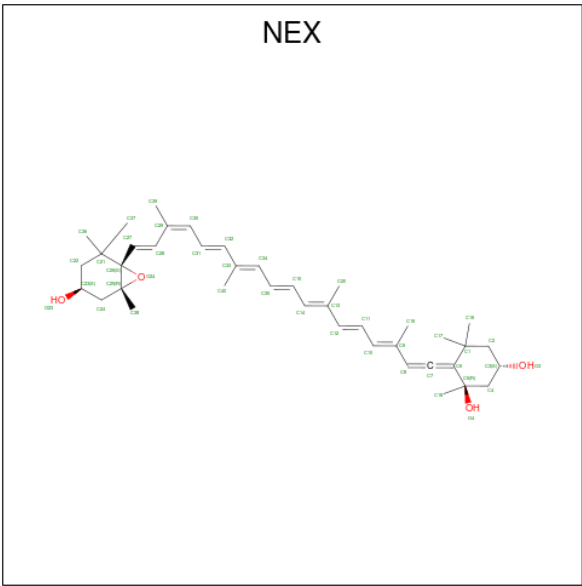
- Molecule 5 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA, BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: C₄₀H₅₆O₄).



Mol	Chain	Residues	Atoms			AltConf
5	G	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	

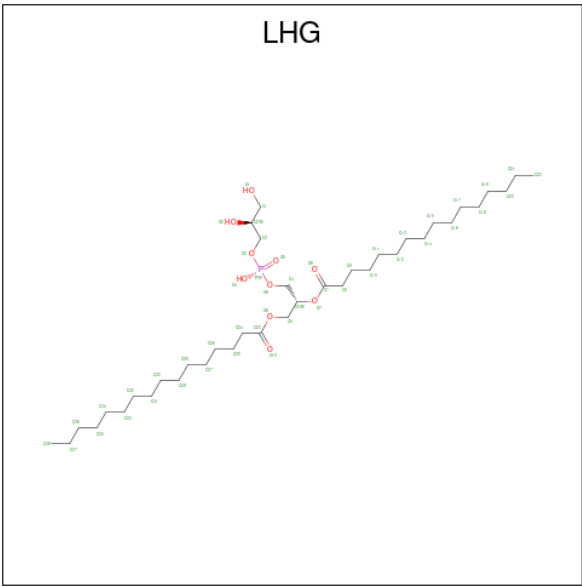
- Molecule 6 is (1R,3R)-6-{(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTADECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE}-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (CCD ID: NEX) (formula: C₄₀H₅₆O₄) (labeled as "Ligand of Interest" by

depositor).



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

- Molecule 7 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).

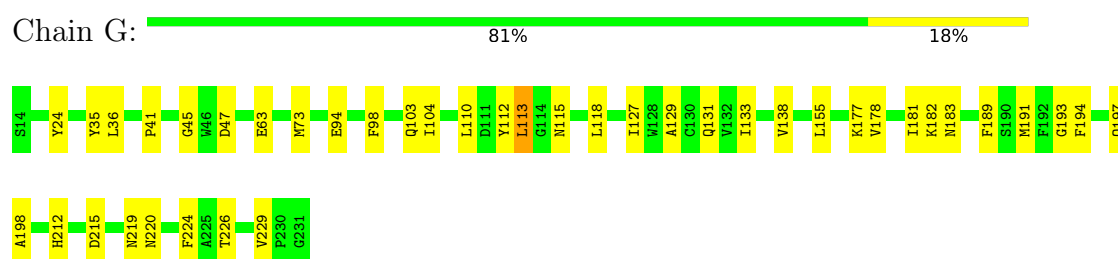


Mol	Chain	Residues	Atoms				AltConf
7	G	1	Total 49	C 38	O 10	P 1	0
7	N	1	Total 49	C 38	O 10	P 1	0
7	Y	1	Total 49	C 38	O 10	P 1	0

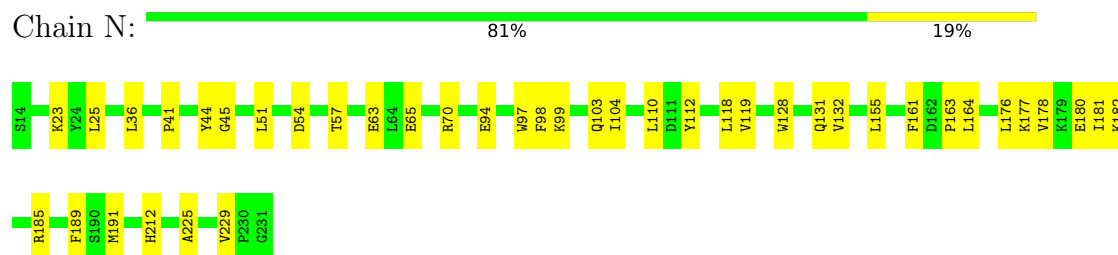
3 Residue-property plots [i](#)

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.

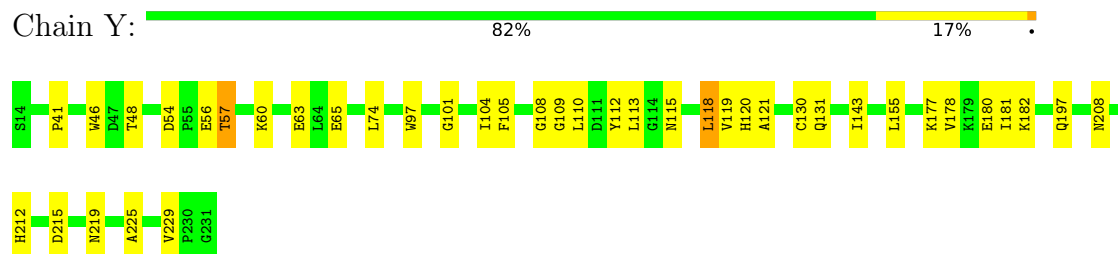
- Molecule 1: Chlorophyll a-b binding protein, chloroplastic



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



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	648142	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	0.494	Depositor
Minimum map value	-0.190	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.04	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: LHG, CHL, LUT, CLA, XAT, NEX

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	0.28	0/1713	0.61	0/2333
1	N	0.29	0/1713	0.59	0/2333
1	Y	0.29	0/1713	0.57	0/2333
All	All	0.29	0/5139	0.59	0/6999

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	1661	0	1591	38	0
1	N	1661	0	1591	32	0
1	Y	1661	0	1591	42	0
2	G	363	0	350	21	0
2	N	363	0	350	29	0
2	Y	363	0	350	26	0
3	G	501	0	534	23	0
3	N	501	0	534	21	0
3	Y	501	0	534	23	0
4	G	84	0	112	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	N	84	0	112	6	0
4	Y	84	0	112	5	0
5	G	88	0	112	13	0
5	Y	44	0	56	5	0
6	G	44	0	56	6	0
6	N	44	0	56	2	0
6	Y	44	0	56	3	0
7	G	49	0	74	6	0
7	N	49	0	74	4	0
7	Y	49	0	74	1	0
All	All	8238	0	8319	223	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 (223) 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:Y:54:ASP:HB2	1:Y:57:THR:CG2	1.56	1.35
1:Y:54:ASP:HB2	1:Y:57:THR:HG23	1.39	1.05
1:Y:54:ASP:HB2	1:Y:57:THR:HG21	1.34	1.04
1:Y:54:ASP:CB	1:Y:57:THR:CG2	2.41	0.97
1:N:191:MET:HG2	4:N:616:LUT:H12	1.52	0.91
1:Y:54:ASP:CB	1:Y:57:THR:HG23	2.03	0.88
1:N:132:VAL:HG23	2:N:609:CHL:HBB2	1.62	0.81
1:Y:41:PRO:HG2	1:Y:177:LYS:HD2	1.70	0.73
1:N:54:ASP:HB2	1:N:57:THR:HG22	1.71	0.71
1:N:41:PRO:HG2	1:N:177:LYS:HD2	1.73	0.69
1:Y:197:GLN:HE22	4:Y:615:LUT:H42	1.57	0.69
1:G:191:MET:HG2	4:G:616:LUT:H12	1.74	0.69
1:Y:115:ASN:HB3	1:Y:118:LEU:HB2	1.75	0.69
5:G:620:XAT:H363	7:N:618:LHG:HC41	1.76	0.68
1:G:63:GLU:HA	1:G:155:LEU:HD11	1.74	0.68
3:G:610:CLA:H52	4:G:615:LUT:H28	1.76	0.67
2:G:609:CHL:HMB3	2:N:601:CHL:HBB	1.77	0.66
1:N:63:GLU:HA	1:N:155:LEU:HD11	1.76	0.66
2:G:601:CHL:H111	5:G:617:XAT:H12	1.78	0.66
1:G:104:ILE:HB	1:G:110:LEU:HB2	1.79	0.65
1:G:194:PHE:CZ	4:G:615:LUT:H8	2.31	0.65
3:N:602:CLA:H52	4:N:616:LUT:H28	1.79	0.65
2:G:601:CHL:HBA2	2:Y:609:CHL:HBA1	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:610:CLA:HBB1	3:G:612:CLA:H3A	1.80	0.64
2:G:608:CHL:H192	2:G:608:CHL:HAA2	1.79	0.64
3:G:613:CLA:C2B	4:G:615:LUT:H183	2.28	0.64
3:Y:613:CLA:H2A	3:Y:613:CLA:HED3	1.79	0.62
1:Y:112:TYR:HD1	3:Y:604:CLA:HBA2	1.64	0.61
3:G:613:CLA:C3B	4:G:615:LUT:H183	2.30	0.61
2:N:607:CHL:H172	2:N:609:CHL:H51	1.82	0.61
1:Y:104:ILE:HB	1:Y:110:LEU:HB2	1.83	0.61
3:G:603:CLA:H151	3:N:602:CLA:H122	1.83	0.60
1:N:104:ILE:HB	1:N:110:LEU:HD13	1.85	0.59
2:Y:608:CHL:H3A	2:Y:608:CHL:H112	1.83	0.59
1:Y:63:GLU:HA	1:Y:155:LEU:HD11	1.85	0.59
3:N:610:CLA:HBB1	3:N:610:CLA:H52	1.86	0.58
1:G:194:PHE:HE1	4:G:615:LUT:C5	2.18	0.57
3:N:613:CLA:H141	3:N:614:CLA:H2	1.85	0.57
2:G:601:CHL:HBA2	2:Y:609:CHL:H3A	1.87	0.57
1:N:180:GLU:OE1	3:N:610:CLA:NB	2.38	0.57
1:Y:208:ASN:HB3	3:Y:613:CLA:HED2	1.86	0.57
4:G:615:LUT:C8	4:G:615:LUT:H181	2.33	0.56
1:G:212:HIS:HD1	3:G:613:CLA:HAA2	1.71	0.56
1:Y:115:ASN:HD22	1:Y:118:LEU:HD23	1.71	0.56
1:Y:104:ILE:HG21	2:Y:606:CHL:HBC1	1.88	0.56
3:N:611:CLA:H2A	3:N:611:CLA:HED3	1.88	0.56
3:Y:603:CLA:HHC	3:Y:603:CLA:HBB1	1.88	0.56
5:G:620:XAT:H373	3:N:611:CLA:HBB1	1.87	0.55
1:G:127:ILE:O	1:G:131:GLN:HB2	2.06	0.55
2:N:609:CHL:HHC	2:N:609:CHL:HBB1	1.87	0.55
2:Y:601:CHL:HMA1	5:Y:617:XAT:H403	1.88	0.55
2:N:609:CHL:H42	3:Y:602:CLA:H143	1.88	0.55
1:G:215:ASP:O	1:G:219:ASN:ND2	2.40	0.55
3:Y:603:CLA:H191	2:Y:609:CHL:H41	1.88	0.54
1:G:110:LEU:HD21	3:G:604:CLA:HAA2	1.89	0.54
7:Y:619:LHG:HC91	7:Y:619:LHG:H282	1.89	0.54
2:N:607:CHL:H151	2:N:609:CHL:H71	1.90	0.53
2:Y:606:CHL:HBC2	2:Y:607:CHL:HHD	1.89	0.53
1:G:41:PRO:HG2	1:G:177:LYS:HD2	1.90	0.53
3:G:613:CLA:H2A	3:G:613:CLA:HED3	1.91	0.53
2:N:607:CHL:H71	2:N:607:CHL:HMB1	1.90	0.53
1:N:94:GLU:HB2	1:N:103:GLN:HB2	1.90	0.52
3:G:602:CLA:H92	3:G:603:CLA:HMA1	1.90	0.52
1:N:110:LEU:HD23	2:N:606:CHL:HMD1	1.89	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:118:LEU:HD11	3:G:604:CLA:H8	1.91	0.52
1:G:189:PHE:HE1	3:G:602:CLA:H191	1.74	0.52
5:G:620:XAT:H173	2:N:601:CHL:H193	1.92	0.52
2:N:601:CHL:H71	7:N:618:LHG:H191	1.91	0.52
1:Y:178:VAL:O	1:Y:182:LYS:HG2	2.10	0.52
1:G:194:PHE:HZ	4:G:615:LUT:H8	1.75	0.52
1:Y:112:TYR:CD1	3:Y:604:CLA:HBA2	2.44	0.52
1:G:112:TYR:HB3	1:G:118:LEU:HD23	1.92	0.51
2:N:607:CHL:H122	2:Y:601:CHL:H18	1.92	0.51
1:N:212:HIS:HD1	3:N:613:CLA:HAA2	1.76	0.51
2:N:606:CHL:HAB	2:N:607:CHL:HHC	1.92	0.51
3:Y:602:CLA:H52	4:Y:616:LUT:H28	1.93	0.51
1:G:127:ILE:HG22	2:G:607:CHL:HBC1	1.93	0.51
1:G:24:TYR:HA	2:G:601:CHL:C1D	2.40	0.50
1:Y:197:GLN:HE22	4:Y:615:LUT:C4	2.22	0.50
5:G:620:XAT:H242	2:N:601:CHL:HMC	1.92	0.50
3:Y:611:CLA:H2	3:Y:612:CLA:HMD2	1.93	0.50
1:G:226:THR:HG21	1:Y:105:PHE:CE2	2.47	0.50
1:Y:180:GLU:HA	3:Y:610:CLA:HBB1	1.94	0.49
3:G:602:CLA:H151	3:Y:603:CLA:H192	1.94	0.49
1:N:178:VAL:HG22	1:N:182:LYS:NZ	2.27	0.49
2:G:606:CHL:HBB2	2:G:607:CHL:CAB	2.42	0.49
1:N:131:GLN:HG2	2:N:606:CHL:HMA3	1.94	0.49
1:Y:143:ILE:HD12	2:Y:609:CHL:HMA3	1.94	0.49
1:G:193:GLY:O	1:G:197:GLN:HG2	2.11	0.49
2:G:601:CHL:H2	2:Y:609:CHL:C4B	2.42	0.49
1:N:128:TRP:HH2	3:Y:613:CLA:H122	1.78	0.49
1:Y:105:PHE:HE2	2:Y:607:CHL:HMD3	1.77	0.49
3:Y:603:CLA:H18	2:Y:609:CHL:H71	1.94	0.49
1:G:112:TYR:HH	6:G:618:NEX:H1	1.54	0.48
1:G:36:LEU:HD12	1:G:45:GLY:HA2	1.95	0.48
1:Y:180:GLU:HB3	3:Y:610:CLA:C2B	2.43	0.48
3:Y:610:CLA:H93	3:Y:612:CLA:H102	1.95	0.48
3:G:613:CLA:H52	5:G:617:XAT:H203	1.96	0.48
2:N:607:CHL:C4D	5:Y:617:XAT:H41	2.44	0.48
2:G:607:CHL:H191	2:G:609:CHL:H52	1.95	0.48
1:Y:74:LEU:HD21	2:Y:608:CHL:H171	1.96	0.48
1:Y:112:TYR:CE2	3:Y:604:CLA:H101	2.49	0.48
1:G:115:ASN:HD22	1:G:118:LEU:HD22	1.79	0.48
2:G:607:CHL:H143	2:G:609:CHL:H101	1.96	0.48
6:G:618:NEX:H35	6:G:618:NEX:H401	1.66	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:607:CHL:H143	2:N:609:CHL:H101	1.96	0.48
1:Y:101:GLY:O	1:Y:105:PHE:HD2	1.96	0.47
1:N:112:TYR:HB3	1:N:118:LEU:HD23	1.95	0.47
1:Y:110:LEU:HD22	2:Y:606:CHL:HAC1	1.96	0.47
3:G:602:CLA:H61	3:G:602:CLA:H41	1.67	0.47
2:N:605:CHL:HAA2	2:N:605:CHL:HED3	1.97	0.47
2:Y:608:CHL:H192	2:Y:608:CHL:H161	1.81	0.47
2:G:601:CHL:H52	2:Y:609:CHL:HHC	1.97	0.47
1:N:98:PHE:HE1	1:N:99:LYS:HE2	1.79	0.47
2:N:609:CHL:HED1	1:Y:48:THR:HB	1.95	0.47
1:N:36:LEU:HD12	1:N:45:GLY:HA2	1.95	0.47
1:G:104:ILE:HG21	2:G:606:CHL:HBC1	1.96	0.46
3:G:611:CLA:H172	3:G:612:CLA:HBB2	1.97	0.46
1:Y:46:TRP:HZ3	3:Y:602:CLA:HBC2	1.80	0.46
1:Y:109:GLY:HA3	1:Y:121:ALA:O	2.15	0.46
4:Y:616:LUT:H15	4:Y:616:LUT:H201	1.81	0.46
1:Y:118:LEU:HD11	3:Y:604:CLA:H8	1.98	0.46
5:G:617:XAT:H361	7:G:619:LHG:HC81	1.98	0.46
2:N:607:CHL:HBD	1:Y:229:VAL:HG11	1.98	0.46
1:Y:212:HIS:HD1	3:Y:613:CLA:HAA2	1.80	0.46
1:G:138:VAL:CG2	6:G:618:NEX:H15	2.46	0.45
1:N:176:LEU:HB3	3:N:610:CLA:HBB	1.98	0.45
5:Y:617:XAT:H11	5:Y:617:XAT:H191	1.75	0.45
3:G:602:CLA:H92	3:G:602:CLA:H62	1.79	0.45
6:N:617:NEX:H15	6:N:617:NEX:H201	1.70	0.45
1:G:220:ASN:HA	1:G:224:PHE:HD2	1.81	0.45
5:Y:617:XAT:H35	5:Y:617:XAT:H401	1.86	0.45
1:G:24:TYR:HA	2:G:601:CHL:CHD	2.47	0.45
2:G:601:CHL:H13	5:G:617:XAT:H10	1.98	0.45
3:N:603:CLA:HBB1	2:N:609:CHL:H122	1.99	0.45
1:Y:112:TYR:HE2	3:Y:604:CLA:H101	1.81	0.45
1:G:194:PHE:CE1	4:G:615:LUT:H8	2.52	0.45
1:N:119:VAL:HG12	2:N:605:CHL:ND	2.32	0.45
6:Y:618:NEX:H35	6:Y:618:NEX:H401	1.68	0.45
1:G:229:VAL:HG11	2:Y:607:CHL:HBD	1.97	0.45
3:G:604:CLA:H102	3:G:604:CLA:H61	1.85	0.45
2:N:608:CHL:H193	2:N:608:CHL:H43	1.98	0.45
2:N:609:CHL:HMB1	2:Y:601:CHL:HBA1	1.97	0.45
2:Y:608:CHL:H111	2:Y:608:CHL:H71	1.48	0.45
6:Y:618:NEX:H192	6:Y:618:NEX:H183	1.99	0.45
1:Y:97:TRP:H	1:Y:97:TRP:CD1	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:161:PHE:O	1:N:163:PRO:HD3	2.18	0.44
1:G:178:VAL:HA	1:G:181:ILE:HG22	1.99	0.44
7:G:619:LHG:H352	7:G:619:LHG:H322	1.58	0.44
1:G:183:ASN:OD1	4:G:615:LUT:H201	2.17	0.44
1:N:23:LYS:HA	1:N:44:TYR:HD1	1.82	0.44
3:N:602:CLA:H61	3:N:602:CLA:H41	1.67	0.44
3:N:603:CLA:H91	3:N:603:CLA:H112	1.82	0.44
3:G:613:CLA:HBC1	7:G:619:LHG:H201	1.98	0.44
1:N:189:PHE:HD2	7:N:618:LHG:H291	1.83	0.44
2:G:609:CHL:HHC	2:G:609:CHL:HBB1	2.00	0.44
1:N:25:LEU:O	2:N:601:CHL:HBB1	2.18	0.44
1:G:113:LEU:HD21	3:G:604:CLA:H121	2.00	0.43
2:G:601:CHL:C3C	5:G:617:XAT:H362	2.48	0.43
3:N:603:CLA:HMD2	2:N:609:CHL:H2	2.00	0.43
2:N:608:CHL:H3A	2:N:608:CHL:HBA2	1.69	0.43
2:Y:607:CHL:HBA1	2:Y:607:CHL:H3A	1.52	0.43
1:Y:65:GLU:HG3	1:Y:181:ILE:HD11	2.00	0.43
1:Y:113:LEU:HB3	1:Y:118:LEU:HG	1.99	0.43
3:Y:603:CLA:H101	3:Y:603:CLA:H13	1.78	0.43
6:Y:618:NEX:H15	6:Y:618:NEX:H201	1.74	0.43
4:G:615:LUT:H35	4:G:615:LUT:H401	1.82	0.43
4:N:615:LUT:H11	4:N:615:LUT:H191	1.85	0.43
1:Y:215:ASP:O	1:Y:219:ASN:ND2	2.50	0.43
1:N:65:GLU:OE2	1:N:185:ARG:NH1	2.39	0.43
3:N:611:CLA:H152	3:N:611:CLA:H111	1.71	0.43
1:N:70:ARG:HE	3:N:610:CLA:C4C	2.31	0.43
1:Y:225:ALA:O	1:Y:229:VAL:HG23	2.18	0.43
3:Y:612:CLA:H101	3:Y:612:CLA:H61	1.64	0.43
5:G:620:XAT:H31	5:G:620:XAT:H391	1.73	0.43
5:G:620:XAT:H35	5:G:620:XAT:H401	1.82	0.43
2:Y:601:CHL:C4A	5:Y:617:XAT:H391	2.48	0.43
1:G:129:ALA:O	1:G:133:ILE:HG22	2.19	0.42
2:G:601:CHL:H93	2:G:601:CHL:H61	1.86	0.42
5:G:617:XAT:H201	5:G:617:XAT:H15	1.60	0.42
6:G:618:NEX:H15	6:G:618:NEX:H201	1.68	0.42
1:G:94:GLU:HB2	1:G:103:GLN:HB2	2.01	0.42
4:G:616:LUT:H35	4:G:616:LUT:H401	1.83	0.42
1:N:225:ALA:O	1:N:229:VAL:HG23	2.20	0.42
2:Y:607:CHL:H143	2:Y:607:CHL:H111	1.80	0.42
1:G:35:TYR:OH	1:G:47:ASP:OD2	2.35	0.42
7:G:619:LHG:HC62	7:G:619:LHG:H242	1.74	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:51:LEU:HD12	3:N:602:CLA:H11	2.02	0.42
2:N:601:CHL:HBA1	2:N:601:CHL:H3A	1.82	0.42
1:Y:108:GLY:HA2	1:Y:120:HIS:HE1	1.84	0.42
6:G:618:NEX:H11	6:G:618:NEX:H191	1.60	0.42
2:G:606:CHL:HBB2	2:G:607:CHL:HAB	2.01	0.42
3:N:602:CLA:H93	3:N:602:CLA:H62	1.79	0.42
5:G:620:XAT:H15	3:N:613:CLA:H72	2.02	0.42
2:N:601:CHL:H61	2:N:601:CHL:H92	1.84	0.42
2:G:606:CHL:H2A	2:G:606:CHL:HED3	2.02	0.42
4:N:616:LUT:H35	4:N:616:LUT:H401	1.89	0.42
6:N:617:NEX:H401	6:N:617:NEX:H35	1.77	0.42
1:G:98:PHE:HE2	1:G:198:ALA:HB1	1.85	0.41
3:G:602:CLA:H93	3:G:602:CLA:H111	1.76	0.41
7:G:619:LHG:H332	7:G:619:LHG:H301	1.98	0.41
1:N:110:LEU:HD21	3:N:604:CLA:HAA2	2.03	0.41
1:N:178:VAL:O	1:N:181:ILE:HG22	2.20	0.41
4:N:615:LUT:H31	4:N:615:LUT:H391	1.94	0.41
2:Y:608:CHL:H161	2:Y:608:CHL:H122	1.39	0.41
3:G:612:CLA:H141	3:G:612:CLA:H162	1.90	0.41
1:N:97:TRP:CD1	1:N:97:TRP:H	2.36	0.41
1:G:182:LYS:NZ	7:G:619:LHG:O5	2.53	0.41
1:N:164:LEU:HD12	4:N:615:LUT:H222	2.03	0.41
3:G:610:CLA:H62	3:G:610:CLA:H41	1.90	0.41
2:Y:608:CHL:H101	2:Y:608:CHL:HMB3	2.03	0.41
1:N:180:GLU:HB3	3:N:610:CLA:C2B	2.51	0.41
1:G:138:VAL:HG22	6:G:618:NEX:H201	2.03	0.41
1:N:189:PHE:CD2	7:N:618:LHG:H291	2.56	0.41
1:G:73:MET:HB2	4:G:615:LUT:C35	2.51	0.40
1:G:110:LEU:CD2	2:G:606:CHL:HHD	2.51	0.40
1:Y:56:GLU:OE2	1:Y:60:LYS:NZ	2.53	0.40
3:G:603:CLA:H52	3:N:602:CLA:H8	2.04	0.40
3:Y:602:CLA:HAB	4:Y:616:LUT:H32	2.03	0.40
1:Y:74:LEU:HD21	2:Y:608:CHL:H18	2.03	0.40
2:Y:608:CHL:H62	2:Y:608:CHL:H41	1.84	0.40
2:N:601:CHL:H141	2:N:601:CHL:H162	1.89	0.40
1:Y:130:CYS:SG	1:Y:131:GLN:N	2.95	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%)	204 (94%)	12 (6%)	0	100	100
1	N	216/218 (99%)	206 (95%)	10 (5%)	0	100	100
1	Y	216/218 (99%)	207 (96%)	9 (4%)	0	100	100
All	All	648/654 (99%)	617 (95%)	31 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	168/168 (100%)	167 (99%)	1 (1%)	78	90
1	N	168/168 (100%)	168 (100%)	0	100	100
1	Y	168/168 (100%)	165 (98%)	3 (2%)	51	76
All	All	504/504 (100%)	500 (99%)	4 (1%)	70	87

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	113	LEU
1	Y	57	THR
1	Y	118	LEU
1	Y	119	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	115	ASN
1	G	120	HIS
1	G	183	ASN
1	N	61	ASN
1	N	208	ASN
1	Y	120	HIS
1	Y	122	GLN
1	Y	131	GLN
1	Y	197	GLN
1	Y	208	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

57 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	CLA	G	611	7	69,73,73	1.17	7 (10%)	82,113,113	1.16	7 (8%)
3	CLA	N	611	7	69,73,73	1.18	8 (11%)	82,113,113	1.15	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	CLA	G	604	-	66,70,73	1.20	7 (10%)	78,109,113	1.22	6 (7%)
6	NEX	Y	618	-	40,46,46	1.15	3 (7%)	50,70,70	2.72	14 (28%)
5	XAT	G	617	-	41,47,47	0.98	0	54,74,74	2.65	13 (24%)
6	NEX	G	618	-	40,46,46	1.29	3 (7%)	50,70,70	3.00	20 (40%)
2	CHL	G	606	-	45,59,74	2.55	10 (22%)	40,96,114	1.68	11 (27%)
7	LHG	N	618	3	48,48,48	0.89	2 (4%)	51,54,54	1.05	2 (3%)
4	LUT	Y	616	-	42,43,43	0.83	1 (2%)	51,60,60	1.80	14 (27%)
3	CLA	N	610	1	69,73,73	1.15	7 (10%)	82,113,113	1.13	7 (8%)
3	CLA	Y	612	-	69,73,73	1.18	7 (10%)	82,113,113	1.14	6 (7%)
2	CHL	G	607	-	60,74,74	2.24	10 (16%)	58,114,114	1.43	8 (13%)
3	CLA	N	603	-	69,73,73	1.16	7 (10%)	82,113,113	1.19	4 (4%)
2	CHL	Y	605	-	42,56,74	2.73	9 (21%)	36,92,114	1.80	12 (33%)
3	CLA	G	613	-	69,73,73	1.16	7 (10%)	82,113,113	1.22	6 (7%)
3	CLA	N	613	-	69,73,73	1.17	7 (10%)	82,113,113	1.22	5 (6%)
3	CLA	Y	613	1	69,73,73	1.14	7 (10%)	82,113,113	1.23	5 (6%)
3	CLA	G	603	-	69,73,73	1.19	6 (8%)	82,113,113	1.16	6 (7%)
6	NEX	N	617	-	40,46,46	1.18	3 (7%)	50,70,70	2.61	13 (26%)
2	CHL	N	601	-	60,74,74	2.29	10 (16%)	58,114,114	1.45	15 (25%)
3	CLA	Y	611	7	69,73,73	1.16	8 (11%)	82,113,113	1.05	4 (4%)
7	LHG	G	619	3	48,48,48	0.91	2 (4%)	51,54,54	1.00	3 (5%)
2	CHL	N	606	-	45,59,74	2.56	9 (20%)	40,96,114	1.81	11 (27%)
3	CLA	G	614	-	53,57,73	1.34	8 (15%)	61,93,113	1.31	6 (9%)
3	CLA	N	602	1	69,73,73	1.16	6 (8%)	82,113,113	1.17	6 (7%)
2	CHL	Y	606	1	45,59,74	2.56	9 (20%)	40,96,114	1.74	12 (30%)
2	CHL	Y	608	-	60,74,74	2.41	12 (20%)	58,114,114	1.72	12 (20%)
3	CLA	N	604	-	66,70,73	1.21	6 (9%)	78,109,113	1.21	5 (6%)
3	CLA	Y	604	-	66,70,73	1.18	6 (9%)	78,109,113	1.21	5 (6%)
2	CHL	G	609	-	60,74,74	2.34	10 (16%)	58,114,114	1.33	9 (15%)
3	CLA	G	602	1	69,73,73	1.16	8 (11%)	82,113,113	1.15	6 (7%)
4	LUT	Y	615	-	42,43,43	1.10	3 (7%)	51,60,60	2.68	21 (41%)
2	CHL	Y	607	-	60,74,74	2.13	11 (18%)	58,114,114	1.72	13 (22%)
2	CHL	G	605	-	42,56,74	2.78	10 (23%)	36,92,114	1.55	13 (36%)
2	CHL	G	608	-	60,74,74	2.29	8 (13%)	58,114,114	1.45	11 (18%)
2	CHL	N	608	-	60,74,74	2.24	11 (18%)	58,114,114	1.37	9 (15%)
5	XAT	Y	617	-	41,47,47	0.99	0	54,74,74	2.60	22 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	CHL	N	609	-	60,74,74	2.33	10 (16%)	58,114,114	1.51	12 (20%)
3	CLA	G	612	-	69,73,73	1.17	8 (11%)	82,113,113	1.41	11 (13%)
4	LUT	N	615	-	42,43,43	0.74	0	51,60,60	1.83	12 (23%)
4	LUT	G	615	-	42,43,43	1.81	3 (7%)	51,60,60	2.17	14 (27%)
3	CLA	N	614	-	53,57,73	1.34	5 (9%)	61,93,113	1.23	7 (11%)
7	LHG	Y	619	3	48,48,48	0.91	2 (4%)	51,54,54	1.10	3 (5%)
5	XAT	G	620	-	41,47,47	0.93	2 (4%)	54,74,74	2.60	21 (38%)
3	CLA	Y	610	-	69,73,73	1.18	7 (10%)	82,113,113	1.12	8 (9%)
4	LUT	G	616	-	42,43,43	0.78	1 (2%)	51,60,60	1.79	14 (27%)
3	CLA	Y	614	-	53,57,73	1.32	7 (13%)	61,93,113	1.19	7 (11%)
2	CHL	Y	601	-	60,74,74	2.24	10 (16%)	58,114,114	1.61	15 (25%)
2	CHL	N	607	-	60,74,74	2.20	11 (18%)	58,114,114	1.69	13 (22%)
3	CLA	N	612	-	69,73,73	1.19	6 (8%)	82,113,113	1.13	4 (4%)
4	LUT	N	616	-	42,43,43	0.79	0	51,60,60	1.48	13 (25%)
3	CLA	Y	603	-	69,73,73	1.22	6 (8%)	82,113,113	1.19	9 (10%)
2	CHL	Y	609	1	60,74,74	2.30	10 (16%)	58,114,114	1.80	13 (22%)
3	CLA	Y	602	-	69,73,73	1.16	6 (8%)	82,113,113	1.19	5 (6%)
3	CLA	G	610	-	69,73,73	1.13	6 (8%)	82,113,113	1.17	8 (9%)
2	CHL	N	605	-	42,56,74	2.82	10 (23%)	36,92,114	1.90	12 (33%)
2	CHL	G	601	-	60,74,74	2.30	10 (16%)	58,114,114	1.53	9 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CLA	N	611	7	1/1/15/20	14/39/115/115	-
3	CLA	G	611	7	-	16/39/115/115	-
3	CLA	G	604	-	1/1/14/20	9/36/112/115	-
6	NEX	Y	618	-	-	5/27/83/83	0/3/3/3
5	XAT	G	617	-	-	2/31/93/93	0/4/4/4
6	NEX	G	618	-	-	3/27/83/83	0/3/3/3
2	CHL	G	606	-	3/3/17/26	11/21/119/137	-
7	LHG	N	618	3	-	23/53/53/53	-
4	LUT	Y	616	-	-	5/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CLA	N	610	1	1/1/15/20	12/39/115/115	-
3	CLA	Y	612	-	1/1/15/20	13/39/115/115	-
2	CHL	G	607	-	3/3/20/26	13/39/137/137	-
3	CLA	N	603	-	1/1/15/20	13/39/115/115	-
2	CHL	Y	605	-	3/3/16/26	8/18/116/137	-
3	CLA	G	613	-	1/1/15/20	12/39/115/115	-
3	CLA	N	613	-	1/1/15/20	16/39/115/115	-
3	CLA	Y	613	1	-	9/39/115/115	-
3	CLA	G	603	-	1/1/15/20	12/39/115/115	-
6	NEX	N	617	-	-	5/27/83/83	0/3/3/3
2	CHL	N	601	-	3/3/20/26	15/39/137/137	-
3	CLA	Y	611	7	1/1/15/20	16/39/115/115	-
7	LHG	G	619	3	-	24/53/53/53	-
2	CHL	N	606	-	3/3/17/26	7/21/119/137	-
3	CLA	G	614	-	1/1/11/20	10/20/96/115	-
3	CLA	N	602	1	1/1/15/20	16/39/115/115	-
2	CHL	Y	606	1	3/3/17/26	9/21/119/137	-
2	CHL	Y	608	-	3/3/20/26	23/39/137/137	-
3	CLA	N	604	-	1/1/14/20	14/36/112/115	-
3	CLA	Y	604	-	1/1/14/20	18/36/112/115	-
2	CHL	G	609	-	3/3/20/26	11/39/137/137	-
3	CLA	G	602	1	1/1/15/20	11/39/115/115	-
4	LUT	Y	615	-	-	6/29/67/67	0/2/2/2
2	CHL	Y	607	-	3/3/20/26	17/39/137/137	-
2	CHL	G	605	-	3/3/16/26	5/18/116/137	-
2	CHL	G	608	-	3/3/20/26	15/39/137/137	-
2	CHL	N	608	-	3/3/20/26	16/39/137/137	-
5	XAT	Y	617	-	-	1/31/93/93	0/4/4/4
2	CHL	N	609	-	3/3/20/26	11/39/137/137	-
3	CLA	G	612	-	1/1/15/20	12/39/115/115	-
4	LUT	N	615	-	-	1/29/67/67	0/2/2/2
4	LUT	G	615	-	-	9/29/67/67	0/2/2/2
3	CLA	N	614	-	1/1/11/20	11/20/96/115	-
7	LHG	Y	619	3	-	27/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	XAT	G	620	-	-	7/31/93/93	0/4/4/4
3	CLA	Y	610	-	1/1/15/20	8/39/115/115	-
4	LUT	G	616	-	-	2/29/67/67	0/2/2/2
3	CLA	Y	614	-	1/1/11/20	12/20/96/115	-
2	CHL	Y	601	-	3/3/20/26	7/39/137/137	-
2	CHL	N	607	-	3/3/20/26	19/39/137/137	-
3	CLA	N	612	-	1/1/15/20	14/39/115/115	-
4	LUT	N	616	-	-	1/29/67/67	0/2/2/2
3	CLA	Y	603	-	1/1/15/20	20/39/115/115	-
2	CHL	Y	609	1	3/3/20/26	14/39/137/137	-
3	CLA	Y	602	-	1/1/15/20	9/39/115/115	-
3	CLA	G	610	-	1/1/15/20	10/39/115/115	-
2	CHL	N	605	-	3/3/16/26	7/18/116/137	-
2	CHL	G	601	-	3/3/20/26	16/39/137/137	-

All (368) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Y	609	CHL	C3B-C4B	10.25	1.51	1.41
2	N	605	CHL	C3B-C4B	9.70	1.50	1.41
2	N	609	CHL	C3B-C4B	9.67	1.50	1.41
2	Y	605	CHL	C3B-C4B	9.59	1.50	1.41
2	G	601	CHL	C3B-C4B	9.43	1.50	1.41
2	G	605	CHL	C3B-C4B	9.42	1.50	1.41
2	G	608	CHL	C3B-C4B	9.42	1.50	1.41
4	G	615	LUT	C19-C9	9.27	1.69	1.50
2	G	609	CHL	C3B-C4B	9.22	1.50	1.41
2	Y	608	CHL	C1B-C2B	8.97	1.49	1.39
2	Y	608	CHL	C3B-C4B	8.92	1.50	1.41
2	N	601	CHL	C1B-C2B	8.70	1.49	1.39
2	Y	608	CHL	C1D-C2D	8.66	1.49	1.39
2	G	605	CHL	C1B-C2B	8.64	1.49	1.39
2	Y	606	CHL	C3B-C4B	8.62	1.49	1.41
2	N	606	CHL	C1B-C2B	8.62	1.49	1.39
2	N	601	CHL	C3B-C4B	8.57	1.49	1.41
2	Y	601	CHL	C1B-C2B	8.55	1.49	1.39
2	Y	601	CHL	C3B-C4B	8.55	1.49	1.41
2	G	608	CHL	C1B-C2B	8.52	1.49	1.39
2	G	606	CHL	C3B-C4B	8.51	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	607	CHL	C3B-C4B	8.49	1.49	1.41
2	N	605	CHL	C1B-C2B	8.46	1.49	1.39
2	G	609	CHL	C1B-C2B	8.45	1.49	1.39
2	N	609	CHL	C1B-C2B	8.45	1.49	1.39
2	N	607	CHL	C1B-C2B	8.42	1.49	1.39
2	Y	605	CHL	C1B-C2B	8.39	1.49	1.39
2	Y	606	CHL	C1B-C2B	8.35	1.49	1.39
2	Y	607	CHL	C3B-C4B	8.34	1.49	1.41
2	N	608	CHL	C3B-C4B	8.30	1.49	1.41
2	N	608	CHL	C1B-C2B	8.28	1.49	1.39
2	G	607	CHL	C1D-C2D	8.24	1.48	1.39
2	G	601	CHL	C1B-C2B	8.23	1.48	1.39
2	Y	609	CHL	C1B-C2B	8.23	1.48	1.39
2	N	607	CHL	C3B-C4B	8.17	1.49	1.41
2	Y	607	CHL	C1B-C2B	8.15	1.48	1.39
2	G	606	CHL	C1B-C2B	8.13	1.48	1.39
2	N	606	CHL	C3B-C4B	8.09	1.49	1.41
2	G	609	CHL	C1D-C2D	8.09	1.48	1.39
2	N	609	CHL	C1D-C2D	8.03	1.48	1.39
2	G	605	CHL	C1D-C2D	8.01	1.48	1.39
2	N	601	CHL	C1D-C2D	8.01	1.48	1.39
2	N	608	CHL	C1D-C2D	7.99	1.48	1.39
2	G	607	CHL	C1B-C2B	7.90	1.48	1.39
2	G	601	CHL	C1D-C2D	7.88	1.48	1.39
2	N	606	CHL	C1D-C2D	7.88	1.48	1.39
2	G	606	CHL	C1D-C2D	7.85	1.48	1.39
2	G	608	CHL	C1D-C2D	7.79	1.48	1.39
2	Y	601	CHL	C1D-C2D	7.72	1.48	1.39
2	Y	606	CHL	C1D-C2D	7.66	1.48	1.39
2	N	605	CHL	C1D-C2D	7.66	1.48	1.39
2	Y	605	CHL	C1D-C2D	7.52	1.48	1.39
2	N	607	CHL	C1D-C2D	7.45	1.48	1.39
2	Y	609	CHL	C1D-C2D	6.84	1.47	1.39
2	Y	607	CHL	C1D-C2D	5.61	1.45	1.39
2	N	605	CHL	C2C-C3C	5.16	1.41	1.36
2	Y	608	CHL	C2C-C3C	4.90	1.41	1.36
4	G	615	LUT	C10-C9	-4.74	1.24	1.35
2	Y	607	CHL	C3D-C4D	4.63	1.48	1.41
2	Y	606	CHL	C3D-C4D	4.53	1.48	1.41
2	N	605	CHL	C3D-C4D	4.50	1.48	1.41
2	N	607	CHL	C3D-C4D	4.49	1.48	1.41
2	Y	605	CHL	C3D-C4D	4.48	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	606	CHL	C3D-C4D	4.45	1.48	1.41
2	G	606	CHL	C3D-C4D	4.44	1.48	1.41
2	Y	609	CHL	C3D-C4D	4.37	1.48	1.41
2	G	601	CHL	C3D-C4D	4.36	1.48	1.41
2	Y	601	CHL	C3D-C4D	4.36	1.48	1.41
2	N	601	CHL	C3D-C4D	4.35	1.48	1.41
2	N	609	CHL	C3D-C4D	4.34	1.48	1.41
2	G	608	CHL	C3D-C4D	4.32	1.48	1.41
2	N	608	CHL	C3D-C4D	4.26	1.48	1.41
2	N	601	CHL	C2C-C3C	4.23	1.40	1.36
2	G	605	CHL	C3D-C4D	4.20	1.47	1.41
7	G	619	LHG	O8-C23	4.15	1.45	1.33
6	G	618	NEX	C7-C6	-4.10	1.25	1.30
7	Y	619	LHG	O8-C23	4.08	1.45	1.33
7	N	618	LHG	O8-C23	4.05	1.45	1.33
2	G	605	CHL	C2C-C3C	4.00	1.40	1.36
2	G	607	CHL	C3D-C4D	3.99	1.47	1.41
2	Y	608	CHL	C3D-C4D	3.99	1.47	1.41
6	N	617	NEX	C7-C6	-3.95	1.26	1.30
2	G	609	CHL	C2C-C3C	3.93	1.40	1.36
3	Y	603	CLA	C1D-ND	3.91	1.43	1.37
4	Y	615	LUT	C19-C9	3.88	1.58	1.50
7	G	619	LHG	O7-C7	3.85	1.45	1.34
7	Y	619	LHG	O7-C7	3.85	1.45	1.34
7	N	618	LHG	O7-C7	3.84	1.45	1.34
2	N	609	CHL	C2C-C3C	3.80	1.40	1.36
6	Y	618	NEX	C7-C6	-3.76	1.26	1.30
6	N	617	NEX	C7-C8	-3.71	1.25	1.31
3	N	612	CLA	C1D-ND	3.71	1.42	1.37
2	N	607	CHL	C2C-C3C	3.69	1.39	1.36
2	G	608	CHL	C2C-C3C	3.68	1.39	1.36
2	G	609	CHL	C3D-C4D	3.68	1.47	1.41
3	Y	604	CLA	C1D-ND	3.67	1.42	1.37
3	N	604	CLA	C1D-ND	3.66	1.42	1.37
3	G	614	CLA	C1D-ND	3.66	1.42	1.37
3	G	603	CLA	C1D-ND	3.66	1.42	1.37
3	Y	603	CLA	C4B-NB	3.66	1.42	1.37
3	N	614	CLA	C1D-ND	3.65	1.42	1.37
2	Y	605	CHL	C2C-C3C	3.64	1.39	1.36
2	Y	607	CHL	C2C-C3C	3.63	1.39	1.36
3	N	611	CLA	C1D-ND	3.62	1.42	1.37
3	Y	612	CLA	C1D-ND	3.62	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Y	602	CLA	C1D-ND	3.62	1.42	1.37
3	G	611	CLA	C1D-ND	3.57	1.42	1.37
3	N	602	CLA	C1D-ND	3.57	1.42	1.37
2	N	608	CHL	C2C-C3C	3.56	1.39	1.36
3	N	613	CLA	C1D-ND	3.54	1.42	1.37
2	G	607	CHL	C1A-CHA	-3.52	1.36	1.40
3	G	604	CLA	C1D-ND	3.51	1.42	1.37
3	Y	611	CLA	C1D-ND	3.51	1.42	1.37
3	N	603	CLA	C1D-ND	3.51	1.42	1.37
3	Y	610	CLA	C1D-ND	3.49	1.42	1.37
2	Y	609	CHL	C2C-C3C	3.49	1.39	1.36
6	G	618	NEX	C7-C8	-3.48	1.26	1.31
3	G	613	CLA	C1D-ND	3.48	1.42	1.37
2	G	601	CHL	C1A-CHA	-3.47	1.36	1.40
3	Y	613	CLA	C1D-ND	3.47	1.42	1.37
3	Y	614	CLA	C1D-ND	3.45	1.42	1.37
3	G	610	CLA	C1D-ND	3.43	1.42	1.37
3	N	610	CLA	C1D-ND	3.42	1.42	1.37
3	G	614	CLA	C4B-NB	3.38	1.42	1.37
3	N	614	CLA	C4B-NB	3.38	1.42	1.37
3	G	602	CLA	C1D-ND	3.37	1.42	1.37
3	G	611	CLA	C4B-NB	3.36	1.42	1.37
3	G	612	CLA	C1D-ND	3.36	1.42	1.37
3	N	611	CLA	C4B-NB	3.35	1.42	1.37
2	N	606	CHL	C2C-C3C	3.33	1.39	1.36
6	Y	618	NEX	C7-C8	-3.33	1.26	1.31
3	N	612	CLA	C4B-NB	3.32	1.42	1.37
3	Y	614	CLA	C4B-NB	3.30	1.42	1.37
2	Y	601	CHL	C2C-C3C	3.30	1.39	1.36
3	G	612	CLA	C4B-NB	3.29	1.42	1.37
2	Y	607	CHL	CMD-C2D	-3.29	1.45	1.51
2	G	607	CHL	C2C-C3C	3.25	1.39	1.36
2	G	601	CHL	C2C-C3C	3.23	1.39	1.36
3	G	603	CLA	C4B-NB	3.23	1.42	1.37
3	G	604	CLA	C4B-NB	3.21	1.42	1.37
3	Y	611	CLA	C4B-NB	3.19	1.42	1.37
2	Y	601	CHL	C1A-CHA	-3.19	1.36	1.40
2	G	606	CHL	C2C-C3C	3.16	1.39	1.36
3	Y	612	CLA	C4B-NB	3.15	1.42	1.37
3	Y	610	CLA	C4B-NB	3.14	1.42	1.37
3	N	604	CLA	C4B-NB	3.12	1.42	1.37
3	G	602	CLA	C4B-NB	3.10	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Y	606	CHL	C2C-C3C	3.09	1.39	1.36
3	N	603	CLA	C4B-NB	3.08	1.41	1.37
3	G	613	CLA	C4B-NB	3.01	1.41	1.37
2	G	609	CHL	CMB-C2B	-2.97	1.45	1.51
4	Y	615	LUT	C10-C9	-2.96	1.29	1.35
3	Y	604	CLA	C4B-NB	2.95	1.41	1.37
3	N	613	CLA	C4B-NB	2.94	1.41	1.37
3	Y	602	CLA	C4B-NB	2.94	1.41	1.37
2	N	608	CHL	C1A-CHA	-2.94	1.36	1.40
3	N	602	CLA	C4B-NB	2.94	1.41	1.37
3	N	610	CLA	C4B-NB	2.93	1.41	1.37
2	G	609	CHL	C1A-CHA	-2.90	1.36	1.40
3	N	613	CLA	C1B-C2B	2.89	1.49	1.43
2	Y	609	CHL	CMD-C2D	-2.89	1.45	1.51
3	Y	612	CLA	C1B-C2B	2.85	1.49	1.43
6	G	618	NEX	O24-C25	-2.83	1.42	1.46
2	Y	606	CHL	CAC-C3C	-2.83	1.46	1.51
3	Y	613	CLA	C4B-NB	2.82	1.41	1.37
2	G	607	CHL	CMD-C2D	-2.80	1.46	1.51
3	Y	613	CLA	C1B-C2B	2.78	1.49	1.43
3	Y	604	CLA	C1B-C2B	2.77	1.49	1.43
3	N	603	CLA	C1B-C2B	2.76	1.49	1.43
2	Y	609	CHL	CAC-C3C	-2.73	1.46	1.51
2	G	601	CHL	CMD-C2D	-2.72	1.46	1.51
2	N	608	CHL	CMB-C2B	-2.71	1.46	1.51
2	N	606	CHL	CMD-C2D	-2.70	1.46	1.51
3	Y	603	CLA	C3B-C4B	2.70	1.50	1.42
3	N	602	CLA	C1B-C2B	2.70	1.49	1.43
3	G	613	CLA	C1B-C2B	2.70	1.49	1.43
2	Y	608	CHL	CMD-C2D	-2.70	1.46	1.51
3	N	604	CLA	C1B-C2B	2.69	1.49	1.43
2	G	606	CHL	CAC-C3C	-2.69	1.47	1.51
3	N	611	CLA	C1B-C2B	2.69	1.49	1.43
2	G	609	CHL	CMD-C2D	-2.68	1.46	1.51
3	Y	602	CLA	C1B-C2B	2.67	1.49	1.43
3	N	614	CLA	C1B-C2B	2.66	1.49	1.43
2	Y	608	CHL	CMB-C2B	-2.66	1.46	1.51
3	N	610	CLA	C1B-C2B	2.65	1.49	1.43
2	G	608	CHL	CMD-C2D	-2.63	1.46	1.51
2	G	607	CHL	CAC-C3C	-2.63	1.47	1.51
5	G	620	XAT	O24-C25	-2.63	1.42	1.46
2	G	605	CHL	C1A-CHA	-2.62	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	607	CHL	CMB-C2B	-2.62	1.46	1.51
2	N	601	CHL	CMD-C2D	-2.61	1.46	1.51
3	N	612	CLA	C1B-C2B	2.60	1.49	1.43
2	G	605	CHL	CAC-C3C	-2.60	1.47	1.51
4	G	615	LUT	C8-C9	2.60	1.51	1.46
5	G	620	XAT	O4-C5	-2.60	1.42	1.46
2	N	609	CHL	CMD-C2D	-2.59	1.46	1.51
3	G	604	CLA	C1B-C2B	2.59	1.49	1.43
2	Y	605	CHL	CMB-C2B	-2.59	1.46	1.51
3	Y	611	CLA	C1B-C2B	2.59	1.49	1.43
2	N	608	CHL	CMD-C2D	-2.58	1.46	1.51
3	Y	614	CLA	C1B-C2B	2.58	1.49	1.43
3	G	614	CLA	C1B-C2B	2.58	1.49	1.43
2	G	606	CHL	CMD-C2D	-2.57	1.46	1.51
2	N	601	CHL	CMB-C2B	-2.57	1.46	1.51
2	N	607	CHL	CMB-C2B	-2.57	1.46	1.51
3	Y	610	CLA	CMD-C2D	-2.57	1.45	1.50
2	Y	608	CHL	MG-NB	-2.56	2.00	2.05
2	N	609	CHL	CMB-C2B	-2.56	1.46	1.51
2	Y	606	CHL	CMD-C2D	-2.56	1.46	1.51
2	G	605	CHL	CMB-C2B	-2.56	1.46	1.51
3	G	602	CLA	C1B-C2B	2.55	1.49	1.43
2	Y	605	CHL	CMD-C2D	-2.55	1.46	1.51
2	G	608	CHL	CMB-C2B	-2.54	1.46	1.51
2	N	605	CHL	CMB-C2B	-2.54	1.46	1.51
2	Y	609	CHL	CMB-C2B	-2.54	1.46	1.51
2	G	609	CHL	CAC-C3C	-2.54	1.47	1.51
3	G	610	CLA	C4B-NB	2.54	1.41	1.37
3	G	610	CLA	C1B-C2B	2.53	1.49	1.43
3	G	603	CLA	C1B-C2B	2.53	1.49	1.43
3	G	611	CLA	C1B-C2B	2.52	1.49	1.43
3	N	612	CLA	C3B-C4B	2.52	1.50	1.42
2	Y	601	CHL	CMD-C2D	-2.52	1.46	1.51
3	G	614	CLA	C3B-C4B	2.50	1.50	1.42
2	N	605	CHL	CMD-C2D	-2.49	1.46	1.51
2	N	606	CHL	CAC-C3C	-2.49	1.47	1.51
2	G	606	CHL	C1A-CHA	-2.49	1.37	1.40
2	G	605	CHL	CMD-C2D	-2.49	1.46	1.51
2	N	607	CHL	CMD-C2D	-2.48	1.46	1.51
2	G	601	CHL	CMB-C2B	-2.47	1.46	1.51
3	Y	603	CLA	C1B-C2B	2.46	1.48	1.43
2	N	601	CHL	C1A-CHA	-2.46	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	608	CHL	CAC-C3C	-2.45	1.47	1.51
3	G	603	CLA	CMD-C2D	-2.44	1.45	1.50
3	G	611	CLA	C3B-C4B	2.44	1.49	1.42
2	N	601	CHL	CAC-C3C	-2.42	1.47	1.51
2	Y	605	CHL	CAC-C3C	-2.42	1.47	1.51
3	Y	614	CLA	C3B-C4B	2.40	1.49	1.42
2	Y	601	CHL	CMB-C2B	-2.40	1.46	1.51
2	N	608	CHL	CAC-C3C	-2.40	1.47	1.51
3	N	611	CLA	C3B-C4B	2.39	1.49	1.42
3	Y	610	CLA	C3B-C4B	2.39	1.49	1.42
3	G	603	CLA	C3B-C4B	2.39	1.49	1.42
2	N	606	CHL	CMB-C2B	-2.39	1.46	1.51
4	Y	616	LUT	C1-C6	-2.38	1.50	1.53
2	N	609	CHL	CAC-C3C	-2.37	1.47	1.51
2	Y	608	CHL	CAC-C3C	-2.37	1.47	1.51
2	Y	607	CHL	CMB-C2B	-2.37	1.46	1.51
3	Y	610	CLA	C1B-C2B	2.36	1.48	1.43
3	G	612	CLA	C3B-C4B	2.36	1.49	1.42
3	G	612	CLA	C1B-C2B	2.36	1.48	1.43
3	Y	611	CLA	C3B-C4B	2.35	1.49	1.42
2	N	607	CHL	CAC-C3C	-2.35	1.47	1.51
2	N	605	CHL	C1A-C2A	2.35	1.55	1.51
3	N	613	CLA	CMD-C2D	-2.34	1.46	1.50
3	G	612	CLA	CHC-C4B	-2.34	1.34	1.39
3	Y	603	CLA	CMD-C2D	-2.34	1.46	1.50
2	G	606	CHL	CMB-C2B	-2.34	1.47	1.51
2	G	601	CHL	C3B-C2B	-2.33	1.37	1.40
2	G	607	CHL	CHC-C4B	-2.33	1.35	1.39
3	Y	610	CLA	CMC-C2C	-2.31	1.46	1.50
3	N	602	CLA	C3B-C4B	2.31	1.49	1.42
3	Y	604	CLA	C3B-C4B	2.30	1.49	1.42
2	N	607	CHL	CHC-C4B	-2.29	1.35	1.39
3	N	604	CLA	CMB-C2B	-2.29	1.46	1.50
2	Y	606	CHL	CMB-C2B	-2.29	1.47	1.51
4	Y	615	LUT	C8-C9	2.29	1.50	1.46
3	G	602	CLA	C3B-C4B	2.29	1.49	1.42
2	Y	601	CHL	CHC-C1C	2.29	1.43	1.39
3	Y	602	CLA	C3B-C4B	2.28	1.49	1.42
2	Y	608	CHL	MG-ND	-2.28	2.01	2.05
3	G	604	CLA	C3B-C4B	2.28	1.49	1.42
2	Y	609	CHL	CHC-C1C	2.27	1.43	1.39
3	G	610	CLA	CMD-C2D	-2.27	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	606	CHL	CHC-C4B	-2.27	1.36	1.39
2	Y	608	CHL	CHC-C1C	2.26	1.43	1.39
2	Y	607	CHL	CAC-C3C	-2.24	1.47	1.51
3	N	613	CLA	C3B-C4B	2.23	1.49	1.42
2	G	609	CHL	MG-NB	-2.23	2.01	2.05
3	N	603	CLA	C3B-C4B	2.23	1.49	1.42
3	N	602	CLA	CHC-C1C	2.22	1.42	1.38
3	G	604	CLA	CMB-C2B	-2.22	1.46	1.50
3	N	614	CLA	CMD-C2D	-2.22	1.46	1.50
3	N	604	CLA	CMD-C2D	-2.22	1.46	1.50
3	G	612	CLA	CMB-C2B	-2.22	1.46	1.50
2	Y	601	CHL	CAC-C3C	-2.22	1.47	1.51
3	N	603	CLA	CMD-C2D	-2.22	1.46	1.50
4	G	616	LUT	C30-C29	2.22	1.40	1.35
2	G	601	CHL	CAC-C3C	-2.22	1.47	1.51
3	N	614	CLA	C3B-C4B	2.21	1.49	1.42
2	N	607	CHL	CMA-C3A	-2.21	1.49	1.53
2	Y	607	CHL	CHC-C4B	-2.21	1.36	1.39
2	Y	607	CHL	MG-NB	-2.18	2.01	2.05
3	G	613	CLA	C3B-C4B	2.18	1.49	1.42
3	Y	612	CLA	C3B-C4B	2.18	1.49	1.42
3	Y	612	CLA	MG-NA	2.17	2.11	2.06
3	G	604	CLA	CMD-C2D	-2.17	1.46	1.50
3	G	614	CLA	CMD-C2D	-2.16	1.46	1.50
3	Y	610	CLA	CHC-C1C	2.16	1.42	1.38
3	Y	602	CLA	CMD-C2D	-2.16	1.46	1.50
3	N	610	CLA	C3B-C4B	2.15	1.49	1.42
3	N	613	CLA	CMC-C2C	-2.15	1.46	1.50
2	Y	605	CHL	CHC-C1C	2.15	1.43	1.39
3	G	613	CLA	CMC-C2C	-2.14	1.46	1.50
3	Y	612	CLA	CMD-C2D	-2.13	1.46	1.50
3	Y	604	CLA	CMD-C2D	-2.13	1.46	1.50
3	N	604	CLA	C3B-C4B	2.13	1.48	1.42
3	N	602	CLA	CMD-C2D	-2.12	1.46	1.50
3	N	603	CLA	CMB-C2B	-2.12	1.46	1.50
3	N	610	CLA	CMD-C2D	-2.12	1.46	1.50
3	Y	602	CLA	CHC-C1C	2.12	1.42	1.38
3	G	611	CLA	CMD-C2D	-2.12	1.46	1.50
3	Y	613	CLA	CMC-C2C	-2.12	1.46	1.50
3	Y	612	CLA	CMC-C2C	-2.11	1.46	1.50
3	N	610	CLA	CMB-C2B	-2.11	1.46	1.50
3	Y	611	CLA	CMC-C2C	-2.10	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Y	603	CLA	CMB-C2B	-2.10	1.46	1.50
3	G	602	CLA	CMD-C2D	-2.10	1.46	1.50
3	N	612	CLA	CMD-C2D	-2.10	1.46	1.50
2	N	605	CHL	CHC-C1C	2.10	1.43	1.39
3	N	611	CLA	CMC-C2C	-2.09	1.46	1.50
3	G	612	CLA	CMC-C2C	-2.09	1.46	1.50
3	Y	614	CLA	CMB-C2B	-2.09	1.46	1.50
2	N	607	CHL	C1A-C2A	2.09	1.55	1.51
3	G	602	CLA	CHC-C1C	2.09	1.42	1.38
2	N	601	CHL	CHC-C1C	2.09	1.43	1.39
6	N	617	NEX	O24-C25	-2.08	1.43	1.46
2	N	608	CHL	CHC-C4B	-2.08	1.36	1.39
3	Y	611	CLA	CMB-C2B	-2.08	1.46	1.50
3	G	611	CLA	CMB-C2B	-2.07	1.46	1.50
3	G	612	CLA	CMD-C2D	-2.07	1.46	1.50
3	N	611	CLA	CHC-C1C	2.06	1.42	1.38
3	Y	611	CLA	CMD-C2D	-2.06	1.46	1.50
3	G	614	CLA	CMC-C2C	-2.06	1.46	1.50
3	N	611	CLA	CMD-C2D	-2.05	1.46	1.50
3	Y	613	CLA	CMB-C2B	-2.05	1.46	1.50
6	Y	618	NEX	O24-C25	-2.05	1.43	1.46
3	Y	611	CLA	CHC-C1C	2.05	1.42	1.38
2	Y	609	CHL	MG-NB	-2.04	2.01	2.05
3	N	613	CLA	CHC-C1C	2.04	1.42	1.38
3	G	610	CLA	CMC-C2C	-2.04	1.46	1.50
3	N	611	CLA	CMB-C2B	-2.03	1.46	1.50
3	Y	614	CLA	CMD-C2D	-2.03	1.46	1.50
3	N	610	CLA	CHC-C1C	2.03	1.42	1.38
3	G	602	CLA	CMC-C2C	-2.03	1.46	1.50
3	Y	604	CLA	CHC-C1C	2.03	1.42	1.38
2	G	606	CHL	CBD-CGD	-2.03	1.50	1.52
2	N	605	CHL	CBD-CGD	-2.02	1.50	1.52
3	N	612	CLA	CMB-C2B	-2.02	1.46	1.50
3	G	611	CLA	CMC-C2C	-2.02	1.46	1.50
3	G	610	CLA	MG-NB	-2.02	2.01	2.05
3	G	604	CLA	CHC-C1C	2.02	1.42	1.38
3	G	614	CLA	CHC-C1C	2.02	1.42	1.38
3	G	614	CLA	CMB-C2B	-2.02	1.46	1.50
2	Y	606	CHL	CHC-C4B	-2.02	1.36	1.39
3	G	613	CLA	CMB-C2B	-2.02	1.46	1.50
2	Y	607	CHL	MG-ND	-2.02	2.01	2.05
2	N	609	CHL	CHC-C4B	-2.01	1.36	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	613	CLA	CHC-C1C	2.01	1.42	1.38
2	N	608	CHL	C3B-C2B	-2.01	1.37	1.40
3	G	603	CLA	CMB-C2B	-2.01	1.46	1.50
3	N	603	CLA	CMC-C2C	-2.01	1.46	1.50
3	Y	613	CLA	CMD-C2D	-2.01	1.46	1.50
2	N	609	CHL	CBD-CGD	-2.01	1.50	1.52
3	Y	614	CLA	CHC-C1C	2.00	1.42	1.38
3	Y	613	CLA	C3B-C4B	2.00	1.48	1.42
2	G	605	CHL	CHC-C1C	2.00	1.43	1.39
3	G	602	CLA	CMB-C2B	-2.00	1.46	1.50
2	Y	608	CHL	C3B-C2B	-2.00	1.37	1.40

All (558) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	618	NEX	C38-C25-C26	-9.21	107.14	122.30
6	Y	618	NEX	C38-C25-C26	-8.68	108.02	122.30
6	N	617	NEX	C38-C25-C26	-8.64	108.08	122.30
5	G	617	XAT	O4-C5-C18	8.04	124.03	115.05
5	Y	617	XAT	O4-C5-C18	7.94	123.92	115.05
5	G	617	XAT	O24-C25-C38	7.59	123.53	115.05
6	G	618	NEX	O24-C25-C38	7.56	123.50	115.05
6	Y	618	NEX	O24-C25-C24	7.38	120.41	113.49
5	Y	617	XAT	O24-C25-C38	7.30	123.21	115.05
6	N	617	NEX	O24-C25-C24	7.25	120.28	113.49
5	G	620	XAT	O24-C25-C24	6.94	120.00	113.49
2	Y	609	CHL	C1B-CHB-C4A	-6.52	117.13	121.32
4	Y	615	LUT	C7-C8-C9	-6.44	116.71	126.23
5	G	617	XAT	C38-C25-C26	-6.39	111.79	122.30
4	Y	615	LUT	C26-C27-C28	-6.31	114.76	124.58
6	Y	618	NEX	O24-C25-C38	6.31	122.10	115.05
5	G	617	XAT	C18-C5-C6	-6.31	111.92	122.30
5	Y	617	XAT	C18-C5-C6	-6.29	111.95	122.30
5	Y	617	XAT	C38-C25-C26	-6.27	111.99	122.30
6	G	618	NEX	C35-C34-C33	-6.21	118.56	127.28
6	N	617	NEX	O24-C25-C38	6.21	121.99	115.05
4	G	615	LUT	C19-C9-C8	-6.15	108.69	118.09
5	G	620	XAT	O4-C5-C4	6.06	119.17	113.49
3	N	613	CLA	C4A-NA-C1A	6.01	109.42	106.68
6	G	618	NEX	C11-C10-C9	-5.98	118.89	127.28
5	G	617	XAT	C15-C14-C13	-5.75	119.22	127.28
6	G	618	NEX	C15-C14-C13	-5.75	119.22	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	Y	615	LUT	C35-C34-C33	-5.66	119.34	127.28
6	G	618	NEX	O24-C25-C24	5.65	118.79	113.49
3	N	604	CLA	C4A-NA-C1A	5.50	109.19	106.68
6	Y	618	NEX	C15-C14-C13	-5.48	119.59	127.28
4	Y	615	LUT	C11-C10-C9	-5.46	119.62	127.28
6	Y	618	NEX	C35-C34-C33	-5.45	119.64	127.28
3	G	613	CLA	C4A-NA-C1A	5.44	109.16	106.68
4	G	615	LUT	C19-C9-C10	-5.41	114.05	122.82
6	N	617	NEX	C15-C14-C13	-5.38	119.73	127.28
5	G	617	XAT	C7-C8-C9	-5.36	117.21	125.53
3	N	611	CLA	C4A-NA-C1A	5.34	109.12	106.68
3	G	604	CLA	C4A-NA-C1A	5.31	109.10	106.68
4	N	615	LUT	C26-C27-C28	-5.30	116.33	124.58
2	G	601	CHL	O2D-CGD-CBD	5.19	116.65	110.95
6	N	617	NEX	C27-C28-C29	-5.10	117.62	125.53
5	G	620	XAT	C31-C30-C29	-5.04	120.21	127.28
3	Y	602	CLA	C4A-NA-C1A	5.00	108.96	106.68
6	Y	618	NEX	C11-C10-C9	-4.95	120.34	127.28
5	G	620	XAT	C38-C25-C26	-4.90	114.24	122.30
3	Y	604	CLA	C4A-NA-C1A	4.85	108.89	106.68
3	Y	613	CLA	C4A-NA-C1A	4.82	108.88	106.68
2	N	605	CHL	C4D-CHA-CBD	-4.81	104.12	108.97
2	Y	607	CHL	O2D-CGD-CBD	4.79	116.21	110.95
2	Y	609	CHL	O2D-CGD-CBD	4.79	116.21	110.95
6	N	617	NEX	C35-C34-C33	-4.76	120.61	127.28
6	Y	618	NEX	C27-C28-C29	-4.70	118.23	125.53
5	G	620	XAT	C18-C5-C6	-4.69	114.58	122.30
2	Y	607	CHL	CMD-C2D-C3D	4.68	134.03	124.68
5	G	617	XAT	C35-C34-C33	-4.67	120.72	127.28
4	Y	615	LUT	C30-C31-C32	-4.67	109.66	123.20
5	G	620	XAT	C15-C14-C13	-4.65	120.76	127.28
3	G	611	CLA	C4A-NA-C1A	4.65	108.80	106.68
2	N	607	CHL	O2D-CGD-O1D	-4.65	114.80	123.85
4	Y	615	LUT	C35-C15-C14	-4.64	114.02	123.52
4	Y	615	LUT	C21-C26-C27	-4.63	107.50	112.83
2	N	607	CHL	O2D-CGD-CBD	4.63	116.03	110.95
5	Y	617	XAT	C31-C30-C29	4.62	133.76	127.28
3	N	602	CLA	C4A-NA-C1A	4.60	108.78	106.68
5	G	620	XAT	C11-C10-C9	-4.57	120.87	127.28
2	Y	608	CHL	C4D-ND-C1D	4.56	108.68	105.22
3	G	612	CLA	C1D-ND-C4D	-4.53	103.14	106.31
3	N	603	CLA	C4A-NA-C1A	4.51	108.74	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	615	LUT	C26-C27-C28	-4.43	117.68	124.58
4	Y	616	LUT	C7-C8-C9	-4.41	119.71	126.23
2	G	608	CHL	C1B-CHB-C4A	4.41	124.16	121.32
4	G	615	LUT	C21-C26-C27	-4.36	107.82	112.83
3	G	614	CLA	C4A-NA-C1A	4.35	108.67	106.68
3	G	602	CLA	C4A-NA-C1A	4.31	108.65	106.68
2	N	606	CHL	C4D-CHA-CBD	-4.30	104.63	108.97
6	G	618	NEX	C27-C28-C29	-4.30	118.86	125.53
4	N	615	LUT	C15-C14-C13	-4.22	121.36	127.28
2	Y	605	CHL	C4D-CHA-CBD	-4.22	104.72	108.97
3	N	610	CLA	C4A-NA-C1A	4.21	108.60	106.68
2	Y	601	CHL	O2D-CGD-CBD	4.19	115.55	110.95
2	N	606	CHL	C1B-CHB-C4A	4.17	124.01	121.32
2	G	607	CHL	CMB-C2B-C3B	4.16	132.99	124.68
5	Y	617	XAT	C11-C10-C9	-4.15	121.45	127.28
5	G	620	XAT	C35-C34-C33	-4.10	121.53	127.28
3	Y	611	CLA	C4A-NA-C1A	4.06	108.53	106.68
4	G	615	LUT	C35-C34-C33	-4.05	121.60	127.28
4	G	616	LUT	C39-C29-C30	-4.05	116.26	122.82
2	G	606	CHL	CMB-C2B-C3B	4.05	132.77	124.68
5	G	620	XAT	O4-C5-C18	4.01	119.53	115.05
2	Y	606	CHL	CMB-C2B-C3B	4.00	132.68	124.68
4	G	615	LUT	C18-C5-C6	-3.97	120.15	124.48
4	Y	616	LUT	C21-C26-C27	-3.97	108.26	112.83
4	Y	616	LUT	C15-C14-C13	-3.93	121.76	127.28
2	Y	607	CHL	CMB-C2B-C3B	3.92	132.52	124.68
2	N	601	CHL	O2D-CGD-CBD	3.90	115.23	110.95
2	G	601	CHL	O2D-CGD-O1D	-3.88	116.30	123.85
3	N	612	CLA	C4A-NA-C1A	3.84	108.43	106.68
5	G	620	XAT	O24-C25-C38	3.84	119.34	115.05
2	N	606	CHL	CMB-C2B-C3B	3.81	132.29	124.68
2	N	607	CHL	CMB-C2B-C3B	3.79	132.25	124.68
4	G	616	LUT	C35-C34-C33	-3.77	121.98	127.28
2	G	601	CHL	CHA-C1A-C2A	-3.71	124.59	133.31
2	Y	601	CHL	CMB-C2B-C3B	3.71	132.09	124.68
4	Y	615	LUT	C39-C29-C28	3.68	123.72	118.09
6	N	617	NEX	C11-C10-C9	-3.68	122.11	127.28
4	N	615	LUT	C21-C26-C27	-3.67	108.60	112.83
3	G	610	CLA	C4A-NA-C1A	3.66	108.35	106.68
2	Y	608	CHL	C4D-CHA-CBD	-3.65	105.28	108.97
2	Y	609	CHL	O2D-CGD-O1D	-3.65	116.74	123.85
4	Y	615	LUT	C19-C9-C10	-3.65	116.90	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Y	617	XAT	C28-C29-C30	-3.62	113.31	119.01
2	Y	607	CHL	C4D-CHA-CBD	-3.62	105.32	108.97
4	N	615	LUT	C35-C34-C33	-3.61	122.21	127.28
2	N	608	CHL	O2D-CGD-CBD	3.60	114.90	110.95
5	Y	617	XAT	C15-C14-C13	-3.60	122.23	127.28
4	G	616	LUT	C39-C29-C28	3.57	123.54	118.09
2	Y	608	CHL	O2D-CGD-CBD	3.56	114.86	110.95
2	Y	608	CHL	C1B-CHB-C4A	-3.56	119.04	121.32
5	G	620	XAT	C7-C8-C9	-3.55	120.03	125.53
6	G	618	NEX	C2-C1-C6	3.53	112.64	109.21
2	N	605	CHL	O2D-CGD-CBD	3.51	114.81	110.95
4	Y	615	LUT	C18-C5-C6	-3.49	120.67	124.48
2	Y	601	CHL	C7-C6-C5	-3.49	103.96	113.26
2	N	609	CHL	C4D-CHA-CBD	-3.49	105.45	108.97
2	Y	606	CHL	C4D-CHA-CBD	-3.47	105.47	108.97
2	N	609	CHL	C1C-CHC-C4B	3.46	128.46	116.07
4	Y	615	LUT	C10-C11-C12	-3.44	113.24	123.20
2	N	607	CHL	C1B-CHB-C4A	3.42	123.52	121.32
4	N	615	LUT	C11-C10-C9	-3.41	122.50	127.28
5	G	617	XAT	C12-C13-C14	3.41	124.37	119.01
2	G	607	CHL	O2D-CGD-CBD	3.41	114.69	110.95
6	G	618	NEX	C5-C6-C1	3.39	123.06	119.70
4	Y	615	LUT	C12-C13-C14	-3.36	113.73	119.01
2	Y	607	CHL	O2D-CGD-O1D	-3.36	117.32	123.85
2	N	607	CHL	C4D-CHA-CBD	-3.35	105.59	108.97
3	G	612	CLA	C2C-C1C-NC	3.35	113.50	109.98
2	G	607	CHL	O2D-CGD-O1D	-3.34	117.35	123.85
3	N	613	CLA	O2D-CGD-O1D	-3.34	117.36	123.85
2	Y	609	CHL	C4D-CHA-CBD	-3.33	105.61	108.97
2	Y	605	CHL	C3D-C4D-CHA	3.32	113.59	108.54
4	N	616	LUT	C7-C8-C9	-3.31	121.34	126.23
4	Y	615	LUT	C19-C9-C8	-3.31	113.03	118.09
3	G	612	CLA	O2D-CGD-O1D	-3.29	117.44	123.85
6	G	618	NEX	C39-C29-C30	-3.29	117.48	122.82
2	Y	609	CHL	CMD-C2D-C3D	3.29	131.26	124.68
4	G	616	LUT	C27-C28-C29	-3.28	119.26	126.32
2	Y	608	CHL	C1-C2-C3	-3.28	120.83	126.20
4	Y	615	LUT	C8-C7-C6	-3.27	118.26	127.00
2	N	609	CHL	C4D-ND-C1D	3.27	107.70	105.22
2	G	606	CHL	C1B-CHB-C4A	3.26	123.42	121.32
7	Y	619	LHG	O7-C7-C8	3.25	118.51	111.48
2	G	606	CHL	CHA-C1A-C2A	-3.24	125.69	133.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	615	LUT	C7-C8-C9	-3.23	121.45	126.23
5	G	620	XAT	C27-C28-C29	-3.23	120.52	125.53
4	N	615	LUT	C7-C8-C9	-3.23	121.45	126.23
7	N	618	LHG	O7-C7-C8	3.23	118.47	111.48
2	Y	608	CHL	C3C-C4C-NC	-3.22	106.78	114.65
2	Y	601	CHL	CHA-C1A-C2A	-3.21	125.77	133.31
2	N	605	CHL	C3D-C4D-CHA	3.17	113.36	108.54
4	G	616	LUT	C26-C27-C28	-3.17	119.64	124.58
5	G	620	XAT	C11-C12-C13	-3.17	117.68	126.36
6	G	618	NEX	C16-C1-C6	-3.16	107.64	110.47
5	G	620	XAT	C18-C5-C4	3.16	117.79	114.24
5	G	617	XAT	C20-C13-C14	-3.14	117.73	122.82
3	N	603	CLA	O2D-CGD-O1D	-3.13	117.75	123.85
3	G	603	CLA	O2D-CGD-O1D	-3.13	117.75	123.85
4	G	615	LUT	C30-C31-C32	-3.12	114.16	123.20
2	Y	607	CHL	C3D-C4D-CHA	3.11	113.27	108.54
4	N	616	LUT	C26-C27-C28	-3.10	119.76	124.58
4	N	615	LUT	C31-C30-C29	-3.09	122.95	127.28
4	Y	616	LUT	C11-C10-C9	-3.07	122.97	127.28
6	G	618	NEX	C28-C29-C30	3.06	123.83	119.01
2	Y	609	CHL	C1C-CHC-C4B	3.05	126.97	116.07
4	Y	616	LUT	C16-C1-C6	-3.03	105.48	110.24
2	Y	606	CHL	CHA-C1A-C2A	-3.03	126.19	133.31
6	G	618	NEX	C24-C23-C22	-3.02	105.14	110.79
2	N	601	CHL	O2D-CGD-O1D	-3.02	117.98	123.85
2	G	609	CHL	O2D-CGD-CBD	3.00	114.25	110.95
5	G	617	XAT	O4-C5-C6	-2.99	56.56	58.93
7	G	619	LHG	O7-C7-C8	2.99	117.94	111.48
2	G	608	CHL	C4D-CHA-CBD	-2.99	105.96	108.97
2	Y	608	CHL	O2D-CGD-O1D	-2.98	118.04	123.85
2	Y	607	CHL	C1C-CHC-C4B	2.98	126.72	116.07
3	N	604	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
4	Y	616	LUT	C27-C28-C29	-2.96	119.96	126.32
4	G	616	LUT	C15-C14-C13	-2.96	123.13	127.28
3	N	612	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
3	Y	603	CLA	O2D-CGD-O1D	-2.95	118.10	123.85
2	N	605	CHL	C4D-ND-C1D	2.95	107.46	105.22
2	Y	601	CHL	O2D-CGD-O1D	-2.95	118.11	123.85
2	Y	605	CHL	C1C-CHC-C4B	2.95	126.61	116.07
2	G	609	CHL	O2D-CGD-O1D	-2.95	118.11	123.85
2	Y	607	CHL	C1-C2-C3	-2.94	121.38	126.20
4	G	615	LUT	C8-C7-C6	-2.94	119.14	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	618	NEX	C11-C12-C13	-2.94	118.31	126.36
2	Y	609	CHL	C3D-C4D-CHA	2.94	113.00	108.54
2	N	608	CHL	CMB-C2B-C3B	2.94	130.55	124.68
4	G	615	LUT	C15-C14-C13	-2.93	123.17	127.28
3	N	614	CLA	C4A-NA-C1A	2.93	108.02	106.68
2	G	609	CHL	C4D-ND-C1D	2.93	107.44	105.22
2	N	607	CHL	O1D-CGD-CBD	2.93	129.16	124.72
3	G	614	CLA	CAA-CBA-CGA	-2.93	104.89	113.21
3	G	612	CLA	C1-C2-C3	-2.93	121.40	126.20
2	G	608	CHL	CHA-C1A-C2A	-2.93	126.44	133.31
3	Y	614	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
3	Y	612	CLA	CAA-C2A-C3A	-2.92	105.10	113.00
4	G	616	LUT	C10-C11-C12	-2.92	114.73	123.20
2	G	609	CHL	C3C-C4C-NC	-2.92	107.52	114.65
2	Y	601	CHL	C1C-CHC-C4B	2.91	126.50	116.07
3	Y	612	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
2	G	608	CHL	C1C-CHC-C4B	2.91	126.49	116.07
4	Y	615	LUT	C20-C13-C12	2.90	122.52	118.09
3	G	611	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
3	N	611	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
2	Y	606	CHL	C1C-CHC-C4B	2.90	126.45	116.07
2	N	609	CHL	C3D-C4D-CHA	2.90	112.94	108.54
2	N	609	CHL	O2D-CGD-CBD	2.90	114.13	110.95
4	Y	615	LUT	C28-C29-C30	-2.90	114.45	119.01
2	N	608	CHL	O2D-CGD-O1D	-2.90	118.21	123.85
2	N	608	CHL	C1C-CHC-C4B	2.89	126.42	116.07
6	G	618	NEX	C19-C9-C10	-2.89	118.13	122.82
4	Y	616	LUT	C31-C30-C29	-2.89	123.23	127.28
3	G	602	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
2	Y	606	CHL	O2A-CGA-O1A	-2.87	116.44	123.63
2	G	606	CHL	C4D-CHA-CBD	-2.87	106.07	108.97
3	G	604	CLA	CMB-C2B-C1B	-2.86	121.07	125.42
3	Y	610	CLA	O2D-CGD-O1D	-2.86	118.29	123.85
2	Y	608	CHL	C1C-CHC-C4B	2.85	126.28	116.07
4	N	616	LUT	C35-C34-C33	-2.85	123.28	127.28
2	Y	606	CHL	O2D-CGD-O1D	-2.85	118.31	123.85
2	Y	605	CHL	O2D-CGD-O1D	-2.83	118.33	123.85
6	Y	618	NEX	C24-C23-C22	-2.83	105.49	110.79
2	Y	608	CHL	C3D-C4D-CHA	2.83	112.84	108.54
2	Y	609	CHL	OMC-CMC-C2C	-2.83	120.21	125.12
3	Y	613	CLA	O2D-CGD-O1D	-2.83	118.35	123.85
3	G	614	CLA	O2D-CGD-O1D	-2.82	118.35	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	620	XAT	C26-C27-C28	-2.81	120.06	125.99
2	N	605	CHL	C1C-C2C-CMC	-2.80	121.75	126.80
2	N	601	CHL	CMB-C2B-C3B	2.80	130.28	124.68
2	G	605	CHL	C3C-C4C-NC	-2.80	107.81	114.65
4	Y	616	LUT	C10-C11-C12	-2.79	115.10	123.20
3	G	612	CLA	O2D-CGD-CBD	2.79	116.11	111.23
2	Y	605	CHL	C4D-ND-C1D	2.79	107.33	105.22
3	G	612	CLA	CAA-C2A-C3A	-2.79	105.47	113.00
3	Y	610	CLA	C3B-C4B-NB	-2.79	108.04	110.53
2	N	605	CHL	O2D-CGD-O1D	-2.78	118.44	123.85
3	N	614	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
2	G	607	CHL	CHA-C1A-C2A	-2.77	126.81	133.31
6	G	618	NEX	C15-C35-C34	-2.76	117.87	123.52
2	N	608	CHL	CHA-C1A-C2A	-2.76	126.82	133.31
3	G	611	CLA	O2D-CGD-CBD	2.76	116.06	111.23
2	G	608	CHL	O2D-CGD-CBD	2.75	113.96	110.95
2	G	606	CHL	C1C-CHC-C4B	2.74	125.88	116.07
3	Y	602	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
2	G	608	CHL	O2D-CGD-O1D	-2.72	118.55	123.85
3	Y	604	CLA	CMB-C2B-C1B	-2.72	121.27	125.42
2	G	605	CHL	C1B-CHB-C4A	2.72	123.07	121.32
4	G	615	LUT	C31-C30-C29	-2.71	123.48	127.28
2	Y	608	CHL	C7-C6-C5	-2.70	106.06	113.26
2	N	605	CHL	C4C-CHD-C1D	2.70	125.73	116.07
4	Y	616	LUT	C26-C27-C28	-2.70	120.38	124.58
2	N	609	CHL	O2D-CGD-O1D	-2.69	118.60	123.85
3	N	602	CLA	O2D-CGD-O1D	-2.69	118.62	123.85
2	N	607	CHL	C3D-C4D-CHA	2.68	112.62	108.54
2	N	606	CHL	C1C-CHC-C4B	2.68	125.66	116.07
2	Y	606	CHL	C3D-C4D-CHA	2.67	112.60	108.54
2	N	606	CHL	C3D-C4D-CHA	2.67	112.60	108.54
3	N	610	CLA	O2D-CGD-O1D	-2.67	118.66	123.85
5	G	620	XAT	C6-C7-C8	-2.67	120.36	125.99
6	G	618	NEX	C40-C33-C34	-2.66	118.50	122.82
5	G	620	XAT	C31-C32-C33	-2.66	119.07	126.36
2	G	605	CHL	C3D-C4D-CHA	2.66	112.58	108.54
2	Y	609	CHL	CHA-C1A-C2A	-2.66	127.07	133.31
5	Y	617	XAT	C6-C7-C8	-2.65	120.38	125.99
2	N	601	CHL	C3C-C4C-NC	-2.65	108.17	114.65
6	N	617	NEX	C24-C23-C22	-2.65	105.84	110.79
4	N	616	LUT	C11-C10-C9	-2.64	123.57	127.28
3	G	603	CLA	CAC-C3C-C4C	2.64	128.23	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	609	CHL	CHA-C1A-C2A	-2.64	127.11	133.31
3	N	610	CLA	C1-C2-C3	-2.64	121.87	126.20
6	N	617	NEX	C39-C29-C30	-2.64	118.55	122.82
4	G	615	LUT	C35-C15-C14	-2.63	118.13	123.52
6	N	617	NEX	C28-C29-C30	2.63	123.14	119.01
5	G	617	XAT	C40-C33-C34	-2.62	118.56	122.82
3	N	610	CLA	C3B-C4B-NB	-2.62	108.19	110.53
3	Y	614	CLA	C4A-NA-C1A	2.61	107.87	106.68
2	G	609	CHL	C3D-C4D-CHA	2.61	112.51	108.54
2	Y	605	CHL	O2D-CGD-CBD	2.61	113.81	110.95
5	Y	617	XAT	C7-C8-C9	-2.60	121.49	125.53
2	G	607	CHL	C3C-C4C-NC	-2.60	108.31	114.65
6	N	617	NEX	C11-C12-C13	-2.60	119.25	126.36
2	N	601	CHL	C1C-CHC-C4B	2.59	125.35	116.07
3	G	613	CLA	O2D-CGD-O1D	-2.59	118.80	123.85
2	G	606	CHL	C3D-C4D-CHA	2.59	112.48	108.54
3	N	614	CLA	O2A-CGA-O1A	-2.59	117.16	123.63
3	Y	604	CLA	O2D-CGD-O1D	-2.59	118.81	123.85
4	N	616	LUT	C21-C26-C27	-2.58	109.86	112.83
2	Y	605	CHL	CMB-C2B-C3B	2.58	129.84	124.68
6	Y	618	NEX	C11-C12-C13	-2.58	119.28	126.36
6	Y	618	NEX	C31-C30-C29	-2.58	123.66	127.28
5	G	617	XAT	O24-C25-C26	-2.58	56.88	58.93
2	Y	606	CHL	O2D-CGD-CBD	2.58	113.78	110.95
3	Y	603	CLA	CHB-C4A-NA	2.58	128.12	124.40
2	N	601	CHL	OMC-CMC-C2C	-2.58	120.65	125.12
2	G	601	CHL	O2A-CGA-O1A	-2.57	117.20	123.63
3	G	610	CLA	C1-C2-C3	-2.57	121.99	126.20
4	Y	615	LUT	C18-C5-C4	2.56	119.13	114.42
3	G	610	CLA	CMB-C2B-C3B	2.56	132.58	126.55
3	G	610	CLA	O2D-CGD-O1D	-2.56	118.87	123.85
7	Y	619	LHG	C5-O7-C7	-2.55	111.68	117.80
2	G	605	CHL	O2D-CGD-O1D	-2.55	118.88	123.85
2	N	606	CHL	O2D-CGD-O1D	-2.55	118.88	123.85
4	Y	615	LUT	C40-C33-C32	2.55	121.99	118.09
4	G	616	LUT	C11-C10-C9	-2.55	123.70	127.28
3	Y	602	CLA	CHB-C4A-NA	2.55	128.08	124.40
2	N	601	CHL	C4C-CHD-C1D	2.55	125.19	116.07
3	N	602	CLA	CMB-C2B-C1B	-2.55	121.54	125.42
2	Y	608	CHL	C11-C12-C13	-2.55	107.50	115.97
2	N	601	CHL	CMA-C3A-C4A	-2.54	109.13	114.61
2	Y	607	CHL	O2A-CGA-O1A	-2.54	117.27	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	604	CLA	C1-C2-C3	-2.54	122.04	126.20
3	G	604	CLA	O2D-CGD-O1D	-2.54	118.91	123.85
2	G	601	CHL	CMB-C2B-C3B	2.54	129.75	124.68
6	Y	618	NEX	C39-C29-C30	-2.54	118.71	122.82
2	G	605	CHL	C4C-CHD-C1D	2.53	125.14	116.07
2	G	601	CHL	C1C-CHC-C4B	2.53	125.12	116.07
2	Y	605	CHL	CMD-C2D-C3D	2.53	129.74	124.68
2	G	606	CHL	O2D-CGD-O1D	-2.52	118.94	123.85
2	G	607	CHL	C1C-CHC-C4B	2.52	125.10	116.07
2	N	606	CHL	C3C-C4C-NC	-2.52	108.48	114.65
3	Y	604	CLA	CHB-C4A-NA	2.52	128.03	124.40
2	N	605	CHL	C3C-C4C-NC	-2.52	108.50	114.65
3	Y	611	CLA	O2D-CGD-O1D	-2.52	118.95	123.85
2	G	608	CHL	C4C-CHD-C1D	2.50	125.03	116.07
2	N	607	CHL	CMA-C3A-C4A	-2.50	109.22	114.61
2	N	608	CHL	C3D-C4D-CHA	2.50	112.34	108.54
3	N	612	CLA	CHB-C4A-NA	2.50	128.01	124.40
2	G	609	CHL	C4C-CHD-C1D	2.50	125.02	116.07
2	N	606	CHL	O2D-CGD-CBD	2.50	113.69	110.95
4	N	616	LUT	C10-C11-C12	-2.49	115.97	123.20
3	Y	602	CLA	CMB-C2B-C1B	-2.49	121.62	125.42
2	G	606	CHL	O2D-CGD-CBD	2.49	113.68	110.95
2	Y	608	CHL	C4C-CHD-C1D	2.49	124.97	116.07
3	N	613	CLA	CHB-C4A-NA	2.49	127.99	124.40
2	Y	606	CHL	C1B-CHB-C4A	2.48	122.92	121.32
3	G	614	CLA	O2A-CGA-O1A	-2.48	117.42	123.63
2	N	607	CHL	C4D-ND-C1D	2.48	107.10	105.22
3	G	610	CLA	CMB-C2B-C1B	-2.48	121.64	125.42
2	G	608	CHL	C3D-C4D-CHA	2.47	112.30	108.54
3	G	612	CLA	CHB-C4A-NA	2.47	127.97	124.40
2	N	606	CHL	C4C-CHD-C1D	2.47	124.90	116.07
2	Y	607	CHL	CHA-C1A-C2A	-2.47	127.51	133.31
4	N	616	LUT	C38-C25-C24	-2.47	117.53	123.36
2	N	607	CHL	CMD-C2D-C3D	2.46	129.60	124.68
4	G	616	LUT	C21-C26-C27	-2.46	110.00	112.83
3	Y	612	CLA	CHC-C4B-NB	2.45	127.73	124.05
7	G	619	LHG	C5-O7-C7	-2.45	111.93	117.80
4	Y	615	LUT	C31-C30-C29	-2.45	123.84	127.28
5	G	620	XAT	C17-C1-C2	-2.45	104.67	108.97
2	G	608	CHL	OMC-CMC-C2C	-2.45	120.87	125.12
3	Y	604	CLA	CMB-C2B-C3B	2.45	132.31	126.55
2	N	607	CHL	C4C-CHD-C1D	2.45	124.83	116.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Y	607	CHL	C4D-ND-C1D	2.45	107.08	105.22
3	Y	612	CLA	C1-C2-C3	-2.44	122.20	126.20
2	G	605	CHL	C4D-CHA-CBD	-2.44	106.51	108.97
5	G	620	XAT	C15-C35-C34	-2.44	118.53	123.52
3	G	610	CLA	CHB-C4A-NA	2.43	127.91	124.40
3	N	603	CLA	CHB-C4A-NA	2.43	127.91	124.40
5	G	617	XAT	C26-C27-C28	-2.43	120.86	125.99
3	G	602	CLA	C3B-C4B-NB	-2.43	108.36	110.53
3	N	603	CLA	O2A-CGA-O1A	-2.43	117.56	123.63
2	Y	601	CHL	O2A-CGA-O1A	-2.43	117.56	123.63
3	G	612	CLA	CHB-C1B-NB	2.42	127.69	124.05
3	G	614	CLA	C3B-C4B-NB	-2.42	108.37	110.53
6	G	618	NEX	O24-C25-C26	-2.41	57.02	58.93
3	G	603	CLA	CHB-C4A-NA	2.41	127.88	124.40
3	N	612	CLA	CAA-C2A-C3A	-2.41	106.48	113.00
3	G	613	CLA	CHB-C4A-NA	2.41	127.88	124.40
3	N	611	CLA	CHB-C4A-NA	2.41	127.87	124.40
5	Y	617	XAT	O24-C25-C26	-2.40	57.02	58.93
2	Y	601	CHL	C6-C5-C3	2.40	119.32	113.47
3	G	612	CLA	CHC-C1C-C2C	-2.40	120.12	126.95
5	Y	617	XAT	C16-C1-C2	-2.40	104.75	108.97
5	Y	617	XAT	C39-C29-C30	2.40	126.70	122.82
2	Y	609	CHL	C3C-C4C-NC	-2.40	108.79	114.65
3	Y	613	CLA	CHB-C4A-NA	2.39	127.85	124.40
2	N	601	CHL	C3D-C4D-CHA	2.39	112.17	108.54
4	N	616	LUT	C18-C5-C6	-2.39	121.88	124.48
7	Y	619	LHG	O8-C23-C24	2.39	119.12	111.83
2	N	605	CHL	CMB-C2B-C3B	2.39	129.45	124.68
5	Y	617	XAT	C8-C9-C10	2.39	122.76	119.01
2	N	601	CHL	C4D-CHA-CBD	-2.39	106.56	108.97
2	N	607	CHL	C3C-C4C-NC	-2.38	108.82	114.65
3	G	610	CLA	CAC-C3C-C4C	2.38	127.89	124.79
3	Y	611	CLA	CHB-C4A-NA	2.38	127.84	124.40
4	N	616	LUT	C15-C14-C13	-2.38	123.94	127.28
3	G	611	CLA	C3B-C4B-NB	-2.38	108.41	110.53
2	Y	609	CHL	CMB-C2B-C3B	2.37	129.43	124.68
2	N	607	CHL	C1C-CHC-C4B	2.37	124.55	116.07
3	N	602	CLA	CHB-C4A-NA	2.37	127.82	124.40
3	N	604	CLA	CMB-C2B-C1B	-2.36	121.82	125.42
2	N	608	CHL	CMD-C2D-C3D	2.36	129.40	124.68
3	G	603	CLA	C1-C2-C3	-2.36	122.33	126.20
3	Y	611	CLA	C3B-C4B-NB	-2.36	108.43	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	608	CHL	C3C-C4C-NC	-2.35	108.90	114.65
3	G	613	CLA	C1-C2-C3	-2.35	122.34	126.20
6	N	617	NEX	O24-C25-C26	-2.35	57.07	58.93
2	G	608	CHL	CMB-C2B-C3B	2.35	129.38	124.68
3	N	604	CLA	CHB-C4A-NA	2.34	127.78	124.40
5	G	620	XAT	C24-C23-C22	-2.34	106.41	110.79
2	G	609	CHL	C1C-CHC-C4B	2.34	124.44	116.07
3	Y	610	CLA	CAC-C3C-C4C	2.34	127.83	124.79
6	G	618	NEX	C38-C25-C24	2.34	116.87	114.24
3	Y	603	CLA	CAC-C3C-C4C	2.33	127.82	124.79
2	G	605	CHL	C1C-CHC-C4B	2.33	124.41	116.07
2	N	608	CHL	C3C-C4C-NC	-2.33	108.96	114.65
4	G	616	LUT	C7-C8-C9	-2.33	122.79	126.23
2	N	605	CHL	CMD-C2D-C3D	2.32	129.32	124.68
2	Y	605	CHL	C3C-C4C-NC	-2.32	108.98	114.65
2	Y	606	CHL	C3C-C4C-NC	-2.32	108.99	114.65
4	G	615	LUT	C10-C11-C12	-2.32	116.49	123.20
4	G	616	LUT	C20-C13-C12	2.32	121.63	118.09
2	N	609	CHL	C3C-C4C-NC	-2.32	108.99	114.65
2	N	608	CHL	C4D-CHA-CBD	-2.31	106.63	108.97
2	G	609	CHL	CMB-C2B-C3B	2.31	129.30	124.68
3	Y	614	CLA	O2A-CGA-O1A	-2.31	117.84	123.63
2	N	609	CHL	C1-O2A-CGA	2.31	122.25	116.65
3	Y	603	CLA	CAA-C2A-C3A	-2.31	106.76	113.00
2	Y	601	CHL	C1B-CHB-C4A	2.31	122.81	121.32
3	G	604	CLA	CMB-C2B-C3B	2.31	131.98	126.55
3	N	611	CLA	C1-C2-C3	-2.30	122.42	126.20
4	Y	616	LUT	C18-C5-C6	-2.30	121.97	124.48
2	N	609	CHL	CMB-C2B-C3B	2.30	129.28	124.68
4	N	615	LUT	C36-C21-C26	2.30	113.03	109.55
4	G	615	LUT	C39-C29-C28	2.30	121.60	118.09
3	Y	603	CLA	C2A-C1A-CHA	2.30	127.85	123.87
2	G	605	CHL	CMB-C2B-C3B	2.30	129.27	124.68
2	Y	601	CHL	CMD-C2D-C3D	2.29	129.26	124.68
3	N	610	CLA	CHB-C4A-NA	2.28	127.69	124.40
4	Y	616	LUT	C18-C5-C4	2.28	118.61	114.42
2	Y	605	CHL	CHA-C1A-C2A	-2.27	127.97	133.31
6	Y	618	NEX	O24-C25-C26	-2.27	57.13	58.93
5	Y	617	XAT	C32-C33-C34	2.27	122.57	119.01
4	Y	616	LUT	C35-C34-C33	-2.26	124.10	127.28
2	N	609	CHL	OMC-CMC-C2C	-2.26	121.20	125.12
3	N	610	CLA	O2A-CGA-O1A	-2.26	117.97	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Y	610	CLA	CHB-C1B-NB	2.26	127.44	124.05
3	N	614	CLA	CHB-C4A-NA	2.26	127.66	124.40
3	G	604	CLA	CHB-C4A-NA	2.26	127.66	124.40
3	N	602	CLA	CMB-C2B-C3B	2.26	131.85	126.55
2	G	606	CHL	C3C-C4C-NC	-2.25	109.14	114.65
3	Y	602	CLA	CMB-C2B-C3B	2.25	131.85	126.55
2	N	601	CHL	CMD-C2D-C3D	2.25	129.17	124.68
3	G	602	CLA	CHB-C4A-NA	2.24	127.63	124.40
4	G	616	LUT	C31-C30-C29	-2.23	124.14	127.28
3	Y	603	CLA	CHC-C1C-C2C	-2.23	120.60	126.95
2	N	601	CHL	CHA-C1A-C2A	-2.23	128.06	133.31
4	N	616	LUT	C31-C30-C29	-2.22	124.16	127.28
3	Y	610	CLA	CHB-C4A-NA	2.22	127.60	124.40
5	Y	617	XAT	C18-C5-C4	2.22	116.73	114.24
5	Y	617	XAT	C12-C13-C14	2.22	122.50	119.01
4	G	616	LUT	C30-C31-C32	-2.22	116.77	123.20
2	G	609	CHL	C4D-CHA-CBD	-2.22	106.73	108.97
2	Y	607	CHL	C1-O2A-CGA	2.22	122.01	116.65
2	N	605	CHL	C1C-CHC-C4B	2.21	123.97	116.07
2	Y	609	CHL	C4D-ND-C1D	2.21	106.89	105.22
2	G	605	CHL	CMD-C2D-C3D	2.21	129.10	124.68
2	Y	601	CHL	OMC-CMC-C2C	-2.20	121.30	125.12
2	G	605	CHL	O2D-CGD-CBD	2.19	113.35	110.95
3	G	614	CLA	CHB-C4A-NA	2.18	127.55	124.40
5	Y	617	XAT	C35-C34-C33	-2.18	124.22	127.28
4	G	616	LUT	C15-C35-C34	-2.18	119.06	123.52
3	Y	613	CLA	O2A-CGA-O1A	-2.18	118.18	123.63
5	Y	617	XAT	C4-C3-C2	-2.18	106.72	110.79
3	G	612	CLA	CHB-C1B-C2B	-2.17	121.11	127.43
2	Y	609	CHL	C1-C2-C3	-2.17	122.64	126.20
2	Y	601	CHL	C3C-C4C-NC	-2.17	109.35	114.65
3	G	612	CLA	CHD-C4C-C3C	-2.16	121.62	124.77
2	G	606	CHL	CMD-C2D-C3D	2.16	129.00	124.68
4	N	616	LUT	C30-C31-C32	-2.16	116.94	123.20
4	Y	616	LUT	C35-C15-C14	-2.16	119.10	123.52
2	G	605	CHL	O2A-CGA-O1A	-2.16	118.23	123.63
4	N	615	LUT	C16-C1-C6	-2.16	106.86	110.24
4	N	615	LUT	C35-C15-C14	-2.16	119.11	123.52
3	Y	614	CLA	CHB-C4A-NA	2.15	127.51	124.40
3	N	604	CLA	O2A-CGA-O1A	-2.15	118.24	123.63
6	N	617	NEX	C38-C25-C24	2.15	116.66	114.24
3	G	611	CLA	CHB-C4A-NA	2.15	127.50	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	606	CHL	C4C-CHD-C1D	2.15	123.76	116.07
3	Y	614	CLA	C3B-C4B-NB	-2.15	108.61	110.53
3	N	610	CLA	CHC-C4B-NB	2.15	127.27	124.05
6	Y	618	NEX	C28-C29-C30	2.14	122.38	119.01
2	N	606	CHL	O2A-CGA-O1A	-2.14	118.28	123.63
2	G	601	CHL	C3C-C4C-NC	-2.14	109.42	114.65
2	N	606	CHL	C4D-ND-C1D	2.14	106.84	105.22
3	N	611	CLA	C3B-C4B-NB	-2.14	108.62	110.53
4	N	615	LUT	C30-C31-C32	-2.14	117.01	123.20
2	G	607	CHL	O1D-CGD-CBD	2.14	127.96	124.72
2	Y	606	CHL	CBC-CAC-C3C	-2.14	109.82	112.87
3	N	613	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
2	Y	601	CHL	C1-C2-C3	-2.13	122.71	126.20
4	Y	615	LUT	C15-C35-C34	-2.12	119.17	123.52
3	G	611	CLA	C1-C2-C3	-2.12	122.72	126.20
4	Y	615	LUT	C32-C33-C34	-2.12	115.68	119.01
3	Y	614	CLA	CAA-CBA-CGA	-2.12	107.19	113.21
6	Y	618	NEX	C26-C27-C28	-2.11	121.53	125.99
2	Y	601	CHL	C4C-CHD-C1D	2.11	123.62	116.07
2	Y	605	CHL	OMC-CMC-C2C	-2.11	121.46	125.12
2	Y	601	CHL	C3D-C4D-CHA	2.11	111.75	108.54
3	G	602	CLA	CMB-C2B-C1B	-2.11	122.21	125.42
3	G	610	CLA	O2A-CGA-O1A	-2.11	118.36	123.63
3	Y	603	CLA	CHA-C1A-NA	-2.11	121.62	126.39
2	N	601	CHL	O2A-CGA-O1A	-2.11	118.36	123.63
2	N	601	CHL	C1B-CHB-C4A	2.10	122.68	121.32
2	Y	607	CHL	OBD-CAD-CBD	-2.10	122.74	125.82
2	Y	606	CHL	O1D-CGD-CBD	2.10	127.91	124.72
3	G	613	CLA	C3B-C4B-NB	-2.10	108.65	110.53
2	G	607	CHL	C4C-CHD-C1D	2.10	123.58	116.07
4	N	616	LUT	C20-C13-C12	2.10	121.29	118.09
3	G	603	CLA	O2D-CGD-CBD	2.09	114.89	111.23
2	G	601	CHL	C11-C10-C8	-2.09	109.01	115.97
3	N	614	CLA	CHB-C1B-NB	2.09	127.19	124.05
4	N	616	LUT	C27-C28-C29	-2.09	121.83	126.32
3	Y	614	CLA	O2D-CGD-CBD	2.09	114.88	111.23
5	G	620	XAT	C36-C21-C22	-2.09	105.30	108.97
3	Y	603	CLA	C2C-C1C-NC	2.09	112.17	109.98
5	Y	617	XAT	C20-C13-C14	-2.09	119.44	122.82
2	N	605	CHL	O2A-CGA-O1A	-2.09	118.41	123.63
2	G	601	CHL	C4-C3-C5	2.08	118.84	115.23
5	Y	617	XAT	C38-C25-C24	2.08	116.58	114.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Y	613	CLA	C1-C2-C3	-2.08	122.80	126.20
3	Y	612	CLA	O2D-CGD-CBD	2.07	114.86	111.23
6	G	618	NEX	C30-C31-C32	-2.07	117.20	123.20
2	Y	605	CHL	O1D-CGD-CBD	2.07	127.86	124.72
4	N	615	LUT	C39-C29-C28	2.06	121.24	118.09
3	G	611	CLA	CHB-C1B-NB	2.05	127.13	124.05
3	G	613	CLA	O2A-CGA-O1A	-2.05	118.49	123.63
3	G	602	CLA	C11-C10-C8	-2.05	109.15	115.97
3	Y	603	CLA	C4A-NA-C1A	2.05	107.61	106.68
3	Y	610	CLA	CHB-C1B-C2B	-2.05	121.49	127.43
3	N	602	CLA	C4-C3-C5	2.04	118.77	115.23
2	N	609	CHL	OBD-CAD-CBD	-2.04	122.83	125.82
3	G	603	CLA	C3B-C4B-NB	-2.04	108.71	110.53
3	Y	610	CLA	CHD-C1D-C2D	2.04	129.72	125.49
3	N	611	CLA	O2A-CGA-O1A	-2.03	118.54	123.63
7	G	619	LHG	O8-C23-C24	2.03	118.03	111.83
3	Y	612	CLA	CHB-C4A-NA	2.03	127.33	124.40
2	G	605	CHL	C4D-ND-C1D	2.03	106.76	105.22
3	N	613	CLA	C3B-C4B-NB	-2.03	108.72	110.53
3	N	614	CLA	CAA-CBA-CGA	-2.02	107.46	113.21
4	Y	616	LUT	C30-C31-C32	-2.02	117.34	123.20
3	Y	610	CLA	CMB-C2B-C3B	2.02	131.30	126.55
2	N	601	CHL	C4D-ND-C1D	2.02	106.75	105.22
3	N	614	CLA	CHC-C4B-NB	2.02	127.07	124.05
5	Y	617	XAT	C40-C33-C34	-2.02	119.55	122.82
2	G	605	CHL	O1D-CGD-CBD	2.01	127.77	124.72
7	N	618	LHG	O8-C6-C5	-2.01	102.60	108.40

All (76) chirality outliers are listed below:

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

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

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Mol	Chain	Res	Type	Atom
2	Y	609	CHL	NA
3	G	602	CLA	ND
3	G	603	CLA	ND
3	G	604	CLA	ND
3	G	610	CLA	ND
3	G	612	CLA	ND
3	G	613	CLA	ND
3	G	614	CLA	ND
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	Y	602	CLA	ND
3	Y	603	CLA	ND
3	Y	604	CLA	ND
3	Y	610	CLA	ND
3	Y	611	CLA	ND
3	Y	612	CLA	ND
3	Y	614	CLA	ND

All (652) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	601	CHL	C1C-C2C-CMC-OMC
2	G	601	CHL	C3C-C2C-CMC-OMC
2	G	605	CHL	O1A-CGA-O2A-C1
2	G	606	CHL	C1C-C2C-CMC-OMC
2	G	606	CHL	C3C-C2C-CMC-OMC
2	G	606	CHL	CHA-CBD-CGD-O1D
2	G	606	CHL	CBD-CGD-O2D-CED
2	G	607	CHL	C1C-C2C-CMC-OMC
2	G	607	CHL	C3C-C2C-CMC-OMC
2	G	607	CHL	CBD-CGD-O2D-CED
2	G	608	CHL	C1C-C2C-CMC-OMC
2	G	608	CHL	C3C-C2C-CMC-OMC
2	N	601	CHL	C1C-C2C-CMC-OMC
2	N	605	CHL	C3A-C2A-CAA-CBA
2	N	605	CHL	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
2	N	606	CHL	C1A-C2A-CAA-CBA
2	N	606	CHL	C1C-C2C-CMC-OMC
2	N	606	CHL	C3C-C2C-CMC-OMC
2	N	607	CHL	C1C-C2C-CMC-OMC
2	N	607	CHL	C3C-C2C-CMC-OMC
2	N	607	CHL	CAD-CBD-CGD-O1D
2	N	607	CHL	CAD-CBD-CGD-O2D
2	N	607	CHL	C11-C10-C8-C9
2	N	608	CHL	C1A-C2A-CAA-CBA
2	N	608	CHL	C3A-C2A-CAA-CBA
2	N	608	CHL	C1C-C2C-CMC-OMC
2	N	608	CHL	C3C-C2C-CMC-OMC
2	N	608	CHL	CBD-CGD-O2D-CED
2	N	609	CHL	C1C-C2C-CMC-OMC
2	N	609	CHL	C3C-C2C-CMC-OMC
2	N	609	CHL	C4C-C3C-CAC-CBC
2	N	609	CHL	C6-C7-C8-C9
2	Y	601	CHL	C1C-C2C-CMC-OMC
2	Y	601	CHL	C3C-C2C-CMC-OMC
2	Y	605	CHL	C1A-C2A-CAA-CBA
2	Y	605	CHL	C1C-C2C-CMC-OMC
2	Y	605	CHL	C3C-C2C-CMC-OMC
2	Y	606	CHL	C1A-C2A-CAA-CBA
2	Y	607	CHL	C1A-C2A-CAA-CBA
2	Y	607	CHL	C3A-C2A-CAA-CBA
2	Y	608	CHL	CBD-CGD-O2D-CED
2	Y	609	CHL	C1C-C2C-CMC-OMC
2	Y	609	CHL	C3C-C2C-CMC-OMC
3	G	604	CLA	CHA-CBD-CGD-O1D
3	G	604	CLA	CHA-CBD-CGD-O2D
3	G	611	CLA	C1A-C2A-CAA-CBA
3	G	611	CLA	CBD-CGD-O2D-CED
3	G	614	CLA	C3A-C2A-CAA-CBA
3	G	614	CLA	CBD-CGD-O2D-CED
3	N	604	CLA	CBD-CGD-O2D-CED
3	N	610	CLA	CBD-CGD-O2D-CED
3	N	612	CLA	CHA-CBD-CGD-O2D
3	N	613	CLA	CAD-CBD-CGD-O1D
3	N	613	CLA	CAD-CBD-CGD-O2D
3	N	614	CLA	C2B-C3B-CAB-CBB
3	N	614	CLA	C4B-C3B-CAB-CBB
3	N	614	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
3	N	614	CLA	CAD-CBD-CGD-O2D
3	N	614	CLA	CBD-CGD-O2D-CED
3	Y	602	CLA	CBD-CGD-O2D-CED
3	Y	603	CLA	CHA-CBD-CGD-O1D
3	Y	603	CLA	CHA-CBD-CGD-O2D
3	Y	610	CLA	CBD-CGD-O2D-CED
3	Y	614	CLA	CHA-CBD-CGD-O1D
3	Y	614	CLA	CHA-CBD-CGD-O2D
3	Y	614	CLA	CBD-CGD-O2D-CED
4	G	615	LUT	C11-C10-C9-C19
4	G	615	LUT	C31-C32-C33-C34
4	G	615	LUT	C31-C32-C33-C40
4	Y	615	LUT	C7-C8-C9-C19
5	G	620	XAT	O4-C6-C7-C8
5	G	620	XAT	O24-C26-C27-C28
5	G	620	XAT	C31-C32-C33-C34
6	G	618	NEX	O24-C26-C27-C28
6	N	617	NEX	O24-C26-C27-C28
6	Y	618	NEX	C7-C8-C9-C19
6	Y	618	NEX	O24-C26-C27-C28
7	G	619	LHG	O1-C1-C2-C3
7	G	619	LHG	C3-O3-P-O5
7	G	619	LHG	C4-O6-P-O3
7	G	619	LHG	C4-O6-P-O4
7	G	619	LHG	C4-O6-P-O5
7	G	619	LHG	C24-C23-O8-C6
7	N	618	LHG	O1-C1-C2-C3
7	N	618	LHG	C4-O6-P-O3
7	N	618	LHG	C4-O6-P-O5
7	Y	619	LHG	O1-C1-C2-C3
7	Y	619	LHG	C4-O6-P-O5
7	Y	619	LHG	C24-C23-O8-C6
2	G	607	CHL	O1D-CGD-O2D-CED
2	G	608	CHL	O1D-CGD-O2D-CED
2	G	609	CHL	O1D-CGD-O2D-CED
2	N	608	CHL	O1D-CGD-O2D-CED
3	Y	613	CLA	O1D-CGD-O2D-CED
3	G	611	CLA	O1D-CGD-O2D-CED
3	N	613	CLA	O1D-CGD-O2D-CED
3	Y	614	CLA	O1D-CGD-O2D-CED
2	G	608	CHL	CBD-CGD-O2D-CED
2	G	609	CHL	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
2	Y	606	CHL	CBD-CGD-O2D-CED
3	G	602	CLA	CBD-CGD-O2D-CED
3	G	610	CLA	CBD-CGD-O2D-CED
3	N	603	CLA	CBD-CGD-O2D-CED
3	N	611	CLA	CBD-CGD-O2D-CED
3	N	613	CLA	CBD-CGD-O2D-CED
3	Y	612	CLA	CBD-CGD-O2D-CED
3	Y	613	CLA	CBD-CGD-O2D-CED
2	Y	607	CHL	O1A-CGA-O2A-C1
3	G	614	CLA	O1A-CGA-O2A-C1
7	G	619	LHG	O10-C23-O8-C6
7	Y	619	LHG	O10-C23-O8-C6
2	G	605	CHL	CBA-CGA-O2A-C1
2	Y	607	CHL	CBA-CGA-O2A-C1
2	N	606	CHL	O1A-CGA-O2A-C1
2	Y	606	CHL	O1A-CGA-O2A-C1
3	G	612	CLA	O1A-CGA-O2A-C1
7	N	618	LHG	O10-C23-O8-C6
3	Y	602	CLA	O1D-CGD-O2D-CED
3	Y	610	CLA	O1D-CGD-O2D-CED
2	G	606	CHL	O1D-CGD-O2D-CED
2	N	605	CHL	O1D-CGD-O2D-CED
2	Y	608	CHL	O1D-CGD-O2D-CED
3	G	614	CLA	O1D-CGD-O2D-CED
3	N	610	CLA	O1D-CGD-O2D-CED
3	N	614	CLA	O1D-CGD-O2D-CED
2	G	601	CHL	C3-C5-C6-C7
2	Y	607	CHL	C3-C5-C6-C7
3	G	604	CLA	C3-C5-C6-C7
2	Y	606	CHL	CBA-CGA-O2A-C1
3	G	612	CLA	CBA-CGA-O2A-C1
3	G	614	CLA	CBA-CGA-O2A-C1
3	Y	603	CLA	CBA-CGA-O2A-C1
7	N	618	LHG	C24-C23-O8-C6
2	G	605	CHL	CBD-CGD-O2D-CED
3	G	613	CLA	CBD-CGD-O2D-CED
3	N	604	CLA	O1D-CGD-O2D-CED
3	Y	612	CLA	O1D-CGD-O2D-CED
3	G	602	CLA	C4-C3-C5-C6
3	N	602	CLA	C4-C3-C5-C6
3	Y	604	CLA	C4-C3-C5-C6
3	G	602	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
3	N	602	CLA	C2-C3-C5-C6
3	N	611	CLA	O1D-CGD-O2D-CED
3	G	602	CLA	C3-C5-C6-C7
2	G	606	CHL	CBA-CGA-O2A-C1
2	N	606	CHL	CBA-CGA-O2A-C1
3	N	614	CLA	CBA-CGA-O2A-C1
2	G	601	CHL	O1A-CGA-O2A-C1
2	G	606	CHL	O1A-CGA-O2A-C1
3	N	614	CLA	O1A-CGA-O2A-C1
3	Y	603	CLA	O1A-CGA-O2A-C1
3	Y	612	CLA	O1A-CGA-O2A-C1
2	Y	606	CHL	O1D-CGD-O2D-CED
3	G	611	CLA	C3-C5-C6-C7
3	N	613	CLA	C3-C5-C6-C7
3	Y	612	CLA	C3-C5-C6-C7
3	Y	611	CLA	CBD-CGD-O2D-CED
2	G	601	CHL	CBA-CGA-O2A-C1
3	Y	612	CLA	CBA-CGA-O2A-C1
3	N	602	CLA	CBD-CGD-O2D-CED
3	Y	604	CLA	C2-C3-C5-C6
2	G	601	CHL	CBD-CGD-O2D-CED
3	G	602	CLA	O1D-CGD-O2D-CED
3	N	603	CLA	O1D-CGD-O2D-CED
3	G	610	CLA	O1D-CGD-O2D-CED
2	G	607	CHL	CBA-CGA-O2A-C1
3	N	604	CLA	CBA-CGA-O2A-C1
3	Y	603	CLA	CBD-CGD-O2D-CED
3	G	612	CLA	CBD-CGD-O2D-CED
3	N	612	CLA	C3-C5-C6-C7
2	N	608	CHL	O1A-CGA-O2A-C1
2	N	608	CHL	CBA-CGA-O2A-C1
3	G	611	CLA	CBA-CGA-O2A-C1
3	Y	614	CLA	CBA-CGA-O2A-C1
7	G	619	LHG	C32-C33-C34-C35
2	Y	608	CHL	C2-C3-C5-C6
3	G	613	CLA	C3-C5-C6-C7
2	G	601	CHL	C11-C12-C13-C14
2	G	608	CHL	C11-C12-C13-C14
2	G	609	CHL	C11-C10-C8-C9
2	G	609	CHL	C11-C12-C13-C14
2	Y	608	CHL	C6-C7-C8-C9
2	Y	609	CHL	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
2	Y	609	CHL	C11-C10-C8-C9
3	G	603	CLA	C14-C13-C15-C16
3	G	610	CLA	C11-C12-C13-C14
3	N	611	CLA	C6-C7-C8-C9
3	Y	611	CLA	C6-C7-C8-C9
3	Y	612	CLA	C11-C10-C8-C9
3	G	613	CLA	O1D-CGD-O2D-CED
2	G	605	CHL	O1D-CGD-O2D-CED
4	G	615	LUT	C7-C8-C9-C19
4	G	615	LUT	C11-C12-C13-C20
5	G	617	XAT	C7-C8-C9-C19
5	G	620	XAT	C31-C32-C33-C40
3	G	611	CLA	O1A-CGA-O2A-C1
3	N	611	CLA	CBA-CGA-O2A-C1
3	N	613	CLA	CBA-CGA-O2A-C1
7	N	618	LHG	O1-C1-C2-O2
2	N	601	CHL	C11-C12-C13-C15
2	Y	608	CHL	C11-C10-C8-C7
2	Y	608	CHL	C12-C13-C15-C16
4	Y	615	LUT	C33-C34-C35-C15
2	N	608	CHL	C10-C11-C12-C13
2	N	608	CHL	C2A-CAA-CBA-CGA
3	N	604	CLA	C2A-CAA-CBA-CGA
2	G	601	CHL	C5-C6-C7-C8
3	Y	611	CLA	C8-C10-C11-C12
3	N	604	CLA	O1A-CGA-O2A-C1
3	N	602	CLA	C5-C6-C7-C8
3	N	604	CLA	C5-C6-C7-C8
2	G	607	CHL	O1A-CGA-O2A-C1
7	G	619	LHG	C23-C24-C25-C26
3	Y	611	CLA	O1D-CGD-O2D-CED
2	Y	608	CHL	C8-C10-C11-C12
2	Y	608	CHL	C15-C16-C17-C18
3	G	602	CLA	C5-C6-C7-C8
3	G	604	CLA	C10-C11-C12-C13
3	G	612	CLA	C5-C6-C7-C8
2	N	605	CHL	CBA-CGA-O2A-C1
2	N	609	CHL	CBD-CGD-O2D-CED
3	N	611	CLA	O1A-CGA-O2A-C1
3	Y	614	CLA	O1A-CGA-O2A-C1
2	N	608	CHL	C8-C10-C11-C12
2	Y	608	CHL	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
3	N	613	CLA	C13-C15-C16-C17
3	N	602	CLA	O1D-CGD-O2D-CED
3	G	602	CLA	C13-C15-C16-C17
3	Y	611	CLA	C10-C11-C12-C13
3	N	611	CLA	C10-C11-C12-C13
3	N	611	CLA	C8-C10-C11-C12
3	N	602	CLA	C6-C7-C8-C9
3	N	610	CLA	C15-C16-C17-C18
4	Y	615	LUT	C11-C10-C9-C19
4	G	616	LUT	C27-C28-C29-C39
6	N	617	NEX	C11-C12-C13-C20
5	G	617	XAT	C7-C8-C9-C10
3	N	613	CLA	O1A-CGA-O2A-C1
2	N	605	CHL	C2A-CAA-CBA-CGA
2	Y	605	CHL	C2A-CAA-CBA-CGA
2	Y	608	CHL	C2A-CAA-CBA-CGA
2	Y	609	CHL	CBD-CGD-O2D-CED
4	Y	616	LUT	C29-C30-C31-C32
7	Y	619	LHG	C28-C29-C30-C31
3	N	612	CLA	CBA-CGA-O2A-C1
2	Y	606	CHL	C2-C1-O2A-CGA
2	Y	607	CHL	C2-C1-O2A-CGA
2	Y	608	CHL	C2-C1-O2A-CGA
2	G	608	CHL	C16-C17-C18-C19
2	Y	608	CHL	C16-C17-C18-C20
7	G	619	LHG	C33-C34-C35-C36
7	N	618	LHG	C27-C28-C29-C30
7	Y	619	LHG	C9-C10-C11-C12
3	Y	603	CLA	O1D-CGD-O2D-CED
3	G	603	CLA	C4B-C3B-CAB-CBB
3	N	610	CLA	C4B-C3B-CAB-CBB
3	N	611	CLA	C4B-C3B-CAB-CBB
3	Y	611	CLA	C4B-C3B-CAB-CBB
3	Y	604	CLA	C11-C10-C8-C7
7	N	618	LHG	C32-C33-C34-C35
7	G	619	LHG	C7-C8-C9-C10
7	Y	619	LHG	C23-C24-C25-C26
2	N	605	CHL	O1A-CGA-O2A-C1
2	N	606	CHL	C3A-C2A-CAA-CBA
2	Y	605	CHL	C3A-C2A-CAA-CBA
2	Y	606	CHL	C3A-C2A-CAA-CBA
3	Y	611	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
3	Y	604	CLA	CBA-CGA-O2A-C1
7	Y	619	LHG	C10-C11-C12-C13
3	N	612	CLA	O1A-CGA-O2A-C1
3	G	603	CLA	C2B-C3B-CAB-CBB
3	N	603	CLA	C2B-C3B-CAB-CBB
3	Y	611	CLA	C2B-C3B-CAB-CBB
7	N	618	LHG	C13-C14-C15-C16
2	Y	608	CHL	C4-C3-C5-C6
3	N	612	CLA	C4-C3-C5-C6
3	N	610	CLA	C10-C11-C12-C13
2	G	608	CHL	C16-C17-C18-C20
7	Y	619	LHG	C32-C33-C34-C35
2	Y	607	CHL	C11-C10-C8-C9
7	N	618	LHG	C24-C25-C26-C27
3	G	603	CLA	C8-C10-C11-C12
3	N	602	CLA	C8-C10-C11-C12
7	N	618	LHG	C23-C24-C25-C26
3	N	610	CLA	C8-C10-C11-C12
5	Y	617	XAT	C29-C30-C31-C32
7	Y	619	LHG	C8-C7-O7-C5
2	N	601	CHL	C5-C6-C7-C8
4	G	615	LUT	C11-C12-C13-C14
2	Y	609	CHL	C16-C17-C18-C20
2	G	601	CHL	O1D-CGD-O2D-CED
3	G	602	CLA	C8-C10-C11-C12
7	G	619	LHG	O6-C4-C5-O7
7	Y	619	LHG	C25-C26-C27-C28
7	N	618	LHG	O7-C5-C6-O8
7	N	618	LHG	C14-C15-C16-C17
3	N	610	CLA	C13-C15-C16-C17
3	N	612	CLA	C15-C16-C17-C18
3	G	613	CLA	C13-C15-C16-C17
2	N	601	CHL	C2-C3-C5-C6
3	N	613	CLA	C2A-CAA-CBA-CGA
2	Y	609	CHL	CBA-CGA-O2A-C1
3	G	612	CLA	O1D-CGD-O2D-CED
2	Y	607	CHL	C10-C11-C12-C13
7	G	619	LHG	O1-C1-C2-O2
7	Y	619	LHG	O1-C1-C2-O2
3	G	614	CLA	C1A-C2A-CAA-CBA
3	N	610	CLA	C1A-C2A-CAA-CBA
3	N	614	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
3	Y	604	CLA	C1A-C2A-CAA-CBA
3	Y	611	CLA	C1A-C2A-CAA-CBA
3	Y	614	CLA	C1A-C2A-CAA-CBA
7	Y	619	LHG	O9-C7-O7-C5
2	G	601	CHL	C11-C10-C8-C7
2	N	607	CHL	C12-C13-C15-C16
2	Y	601	CHL	C12-C13-C15-C16
3	G	603	CLA	C11-C12-C13-C15
3	G	612	CLA	C6-C7-C8-C10
3	N	611	CLA	C12-C13-C15-C16
3	Y	603	CLA	C11-C10-C8-C7
3	Y	603	CLA	C12-C13-C15-C16
3	Y	604	CLA	C6-C7-C8-C10
3	Y	610	CLA	C11-C10-C8-C7
2	N	601	CHL	C4-C3-C5-C6
3	N	612	CLA	C2-C3-C5-C6
2	N	607	CHL	C11-C12-C13-C14
2	Y	608	CHL	C11-C10-C8-C9
2	Y	608	CHL	C11-C12-C13-C14
3	G	604	CLA	C11-C12-C13-C14
3	G	611	CLA	C6-C7-C8-C9
3	G	612	CLA	C6-C7-C8-C9
3	N	604	CLA	C11-C12-C13-C14
3	Y	602	CLA	C6-C7-C8-C9
3	Y	603	CLA	C11-C10-C8-C9
3	Y	611	CLA	C14-C13-C15-C16
2	Y	608	CHL	CBA-CGA-O2A-C1
7	G	619	LHG	C14-C15-C16-C17
2	Y	609	CHL	C16-C17-C18-C19
2	Y	608	CHL	O1A-CGA-O2A-C1
2	G	606	CHL	CHA-CBD-CGD-O2D
2	N	607	CHL	CHA-CBD-CGD-O1D
3	Y	604	CLA	C5-C6-C7-C8
2	N	607	CHL	C8-C10-C11-C12
2	N	609	CHL	O1D-CGD-O2D-CED
2	G	608	CHL	C15-C16-C17-C18
7	G	619	LHG	C27-C28-C29-C30
2	N	601	CHL	C3C-C2C-CMC-OMC
4	N	616	LUT	C29-C30-C31-C32
7	Y	619	LHG	C27-C28-C29-C30
7	Y	619	LHG	C15-C16-C17-C18
7	Y	619	LHG	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
3	G	611	CLA	C2A-CAA-CBA-CGA
3	N	604	CLA	C3-C5-C6-C7
3	Y	603	CLA	C13-C15-C16-C17
7	N	618	LHG	C33-C34-C35-C36
3	N	604	CLA	C4-C3-C5-C6
3	Y	611	CLA	CBA-CGA-O2A-C1
2	G	601	CHL	C11-C10-C8-C9
2	G	608	CHL	C6-C7-C8-C9
2	N	607	CHL	C14-C13-C15-C16
2	Y	601	CHL	C14-C13-C15-C16
2	Y	607	CHL	C14-C13-C15-C16
2	Y	608	CHL	C14-C13-C15-C16
3	G	602	CLA	C6-C7-C8-C9
3	G	603	CLA	C11-C12-C13-C14
3	N	611	CLA	C14-C13-C15-C16
3	Y	603	CLA	C11-C12-C13-C14
3	Y	604	CLA	C6-C7-C8-C9
3	Y	610	CLA	C6-C7-C8-C9
3	Y	610	CLA	C11-C10-C8-C9
3	Y	602	CLA	C10-C11-C12-C13
2	Y	609	CHL	O1A-CGA-O2A-C1
3	N	603	CLA	C4B-C3B-CAB-CBB
3	Y	610	CLA	C4B-C3B-CAB-CBB
3	Y	614	CLA	C4B-C3B-CAB-CBB
2	Y	607	CHL	C8-C10-C11-C12
2	Y	608	CHL	C16-C17-C18-C19
3	Y	613	CLA	C2A-CAA-CBA-CGA
7	N	618	LHG	C30-C31-C32-C33
7	Y	619	LHG	O6-C4-C5-C6
2	G	607	CHL	C6-C7-C8-C10
2	G	609	CHL	C11-C12-C13-C15
2	Y	607	CHL	C12-C13-C15-C16
2	Y	608	CHL	C11-C12-C13-C15
3	G	603	CLA	C6-C7-C8-C10
3	G	604	CLA	C11-C12-C13-C15
3	G	611	CLA	C11-C12-C13-C15
3	N	604	CLA	C11-C12-C13-C15
3	N	610	CLA	C11-C10-C8-C7
3	N	611	CLA	C6-C7-C8-C10
3	N	613	CLA	C12-C13-C15-C16
3	Y	602	CLA	C6-C7-C8-C10
3	Y	611	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
2	Y	609	CHL	O1D-CGD-O2D-CED
2	G	609	CHL	C3A-C2A-CAA-CBA
2	N	607	CHL	C3A-C2A-CAA-CBA
2	Y	608	CHL	C3A-C2A-CAA-CBA
3	G	613	CLA	C4-C3-C5-C6
3	G	610	CLA	C13-C15-C16-C17
3	G	613	CLA	C2-C3-C5-C6
3	Y	604	CLA	O1A-CGA-O2A-C1
5	G	620	XAT	C27-C28-C29-C39
7	N	618	LHG	C15-C16-C17-C18
2	N	605	CHL	C1A-C2A-CAA-CBA
7	Y	619	LHG	O6-C4-C5-O7
3	N	611	CLA	C2B-C3B-CAB-CBB
4	Y	615	LUT	C1-C6-C7-C8
4	Y	616	LUT	C1-C6-C7-C8
3	N	612	CLA	C5-C6-C7-C8
4	Y	615	LUT	C9-C10-C11-C12
3	N	603	CLA	C4-C3-C5-C6
7	G	619	LHG	C29-C30-C31-C32
2	G	607	CHL	C6-C7-C8-C9
2	N	609	CHL	C11-C10-C8-C9
3	G	611	CLA	C11-C12-C13-C14
3	N	610	CLA	C11-C10-C8-C9
7	G	619	LHG	C11-C10-C9-C8
3	N	614	CLA	O2A-C1-C2-C3
3	N	603	CLA	CAA-CBA-CGA-O2A
4	G	615	LUT	C29-C30-C31-C32
3	N	604	CLA	C2-C3-C5-C6
7	N	618	LHG	C10-C11-C12-C13
2	G	607	CHL	C11-C12-C13-C15
2	G	609	CHL	C12-C13-C15-C16
2	N	607	CHL	C11-C10-C8-C7
2	N	609	CHL	C6-C7-C8-C10
2	Y	608	CHL	C6-C7-C8-C10
3	G	610	CLA	C11-C12-C13-C15
3	Y	613	CLA	C12-C13-C15-C16
3	G	604	CLA	C5-C6-C7-C8
6	N	617	NEX	C11-C12-C13-C14
3	Y	611	CLA	O1A-CGA-O2A-C1
2	N	601	CHL	O2A-C1-C2-C3
2	N	609	CHL	O1A-CGA-O2A-C1
7	Y	619	LHG	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
2	N	607	CHL	CAA-CBA-CGA-O2A
2	Y	607	CHL	C2A-CAA-CBA-CGA
3	Y	613	CLA	C14-C13-C15-C16
7	G	619	LHG	C25-C26-C27-C28
7	Y	619	LHG	C33-C34-C35-C36
3	G	612	CLA	C3-C5-C6-C7
3	Y	604	CLA	C2-C1-O2A-CGA
4	N	615	LUT	C33-C34-C35-C15
3	G	603	CLA	C13-C15-C16-C17
3	N	603	CLA	C2-C3-C5-C6
7	Y	619	LHG	C1-C2-C3-O3
3	Y	602	CLA	C16-C17-C18-C20
3	Y	604	CLA	C3-C5-C6-C7
2	N	608	CHL	C3-C5-C6-C7
3	G	610	CLA	C1A-C2A-CAA-CBA
3	G	611	CLA	C4B-C3B-CAB-CBB
3	G	614	CLA	C4B-C3B-CAB-CBB
3	N	612	CLA	C4B-C3B-CAB-CBB
4	Y	616	LUT	C7-C8-C9-C10
2	N	607	CHL	C2A-CAA-CBA-CGA
7	G	619	LHG	O6-C4-C5-C6
3	Y	604	CLA	CBD-CGD-O2D-CED
2	G	608	CHL	C11-C12-C13-C15
3	N	603	CLA	C11-C12-C13-C15
3	N	613	CLA	C6-C7-C8-C10
7	Y	619	LHG	C11-C12-C13-C14
3	G	602	CLA	C16-C17-C18-C20
3	Y	602	CLA	C16-C17-C18-C19
2	N	609	CHL	CBA-CGA-O2A-C1
2	G	609	CHL	C14-C13-C15-C16
3	G	603	CLA	C6-C7-C8-C9
3	G	610	CLA	C11-C10-C8-C9
3	N	613	CLA	C6-C7-C8-C9
2	Y	607	CHL	C5-C6-C7-C8
3	G	614	CLA	C1-C2-C3-C4
3	N	614	CLA	C1-C2-C3-C4
3	Y	614	CLA	C1-C2-C3-C4
6	Y	618	NEX	C7-C8-C9-C10
2	Y	601	CHL	C16-C17-C18-C20
7	N	618	LHG	C4-C5-C6-O8
3	N	602	CLA	C3-C5-C6-C7
2	G	608	CHL	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
2	N	607	CHL	CHA-CBD-CGD-O2D
2	N	608	CHL	CHA-CBD-CGD-O1D
2	N	608	CHL	CHA-CBD-CGD-O2D
2	Y	605	CHL	CHA-CBD-CGD-O2D
3	G	612	CLA	CHA-CBD-CGD-O1D
3	G	612	CLA	CHA-CBD-CGD-O2D
3	N	604	CLA	CHA-CBD-CGD-O1D
3	N	604	CLA	CHA-CBD-CGD-O2D
3	N	612	CLA	CHA-CBD-CGD-O1D
3	Y	612	CLA	CHA-CBD-CGD-O1D
3	Y	612	CLA	CHA-CBD-CGD-O2D
4	G	615	LUT	C9-C10-C11-C12
7	N	618	LHG	C4-O6-P-O4
7	Y	619	LHG	C3-O3-P-O5
7	Y	619	LHG	C4-O6-P-O3
2	N	601	CHL	C16-C17-C18-C20
3	N	610	CLA	C2B-C3B-CAB-CBB
3	Y	614	CLA	C2B-C3B-CAB-CBB
4	Y	616	LUT	C7-C8-C9-C19
2	N	607	CHL	C16-C17-C18-C20
3	G	612	CLA	C10-C11-C12-C13
3	Y	612	CLA	C10-C11-C12-C13
2	G	607	CHL	C11-C12-C13-C14
3	N	603	CLA	C11-C10-C8-C9
3	N	613	CLA	C14-C13-C15-C16
3	G	610	CLA	C11-C10-C8-C7
2	Y	607	CHL	CBD-CGD-O2D-CED
2	G	601	CHL	C16-C17-C18-C20
2	G	607	CHL	C16-C17-C18-C20
5	G	620	XAT	C13-C14-C15-C35
3	Y	612	CLA	C16-C17-C18-C20
7	Y	619	LHG	C30-C31-C32-C33
3	N	612	CLA	C2A-CAA-CBA-CGA
3	Y	602	CLA	C2A-CAA-CBA-CGA
7	G	619	LHG	C15-C16-C17-C18
3	N	602	CLA	C11-C12-C13-C14
3	G	613	CLA	C4B-C3B-CAB-CBB
3	Y	613	CLA	C4B-C3B-CAB-CBB
7	N	618	LHG	C26-C27-C28-C29
2	G	601	CHL	C16-C17-C18-C19
2	Y	609	CHL	C2A-CAA-CBA-CGA
2	G	601	CHL	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
2	G	607	CHL	C11-C10-C8-C7
3	Y	614	CLA	C3A-C2A-CAA-CBA
6	G	618	NEX	C39-C29-C30-C31
6	N	617	NEX	C39-C29-C30-C31
6	Y	618	NEX	C39-C29-C30-C31
2	N	609	CHL	C2C-C3C-CAC-CBC
3	G	611	CLA	C4-C3-C5-C6
3	Y	611	CLA	C13-C15-C16-C17
2	G	601	CHL	C14-C13-C15-C16
2	G	608	CHL	C11-C10-C8-C9
2	G	608	CHL	C14-C13-C15-C16
2	G	609	CHL	C6-C7-C8-C9
2	N	601	CHL	C11-C10-C8-C9
2	N	601	CHL	C11-C12-C13-C14
2	Y	609	CHL	C14-C13-C15-C16
3	N	602	CLA	C14-C13-C15-C16
3	Y	613	CLA	C6-C7-C8-C9
3	N	612	CLA	C16-C17-C18-C20
3	G	604	CLA	O1D-CGD-O2D-CED
2	G	608	CHL	C1A-C2A-CAA-CBA
2	N	607	CHL	C1A-C2A-CAA-CBA
3	G	611	CLA	C5-C6-C7-C8
3	G	613	CLA	C2A-CAA-CBA-CGA
3	N	610	CLA	C2A-CAA-CBA-CGA
6	G	618	NEX	C28-C29-C30-C31
6	N	617	NEX	C28-C29-C30-C31
6	Y	618	NEX	C28-C29-C30-C31
3	G	611	CLA	C2B-C3B-CAB-CBB
3	G	613	CLA	C2B-C3B-CAB-CBB
3	G	614	CLA	C2B-C3B-CAB-CBB
3	N	612	CLA	C2B-C3B-CAB-CBB
4	Y	616	LUT	C5-C6-C7-C8
3	Y	604	CLA	O1D-CGD-O2D-CED
3	Y	612	CLA	C16-C17-C18-C19
3	G	614	CLA	O2A-C1-C2-C3
3	G	613	CLA	C11-C12-C13-C15
3	N	602	CLA	C11-C12-C13-C15
3	Y	603	CLA	C11-C12-C13-C15
3	Y	604	CLA	C11-C12-C13-C15
3	Y	612	CLA	C11-C10-C8-C7
7	N	618	LHG	C31-C32-C33-C34
2	N	608	CHL	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
2	N	601	CHL	O1A-CGA-O2A-C1
3	G	602	CLA	C2A-CAA-CBA-CGA
3	G	604	CLA	CBD-CGD-O2D-CED
3	N	604	CLA	C10-C11-C12-C13
3	G	603	CLA	CAA-CBA-CGA-O2A
3	N	602	CLA	C16-C17-C18-C19
7	G	619	LHG	C1-C2-C3-O3
2	G	609	CHL	CHA-CBD-CGD-O2D
2	N	601	CHL	CHA-CBD-CGD-O1D
2	N	601	CHL	CHA-CBD-CGD-O2D
3	N	602	CLA	C16-C17-C18-C20
2	Y	609	CHL	C6-C7-C8-C10
3	Y	613	CLA	C6-C7-C8-C10
2	Y	601	CHL	C6-C7-C8-C9
3	Y	603	CLA	C6-C7-C8-C9
3	Y	604	CLA	C11-C10-C8-C9
2	G	607	CHL	C16-C17-C18-C19
2	G	605	CHL	C3A-C2A-CAA-CBA
2	G	606	CHL	C3A-C2A-CAA-CBA
3	G	611	CLA	C3A-C2A-CAA-CBA
3	N	603	CLA	C3A-C2A-CAA-CBA
2	G	606	CHL	O2A-C1-C2-C3
2	Y	606	CHL	O2A-C1-C2-C3
2	Y	608	CHL	C3C-C2C-CMC-OMC
7	G	619	LHG	O2-C2-C3-O3
7	Y	619	LHG	C7-C8-C9-C10
3	G	610	CLA	CBA-CGA-O2A-C1
3	G	613	CLA	C15-C16-C17-C18
4	G	616	LUT	C29-C30-C31-C32
3	Y	603	CLA	C14-C13-C15-C16
3	Y	613	CLA	C13-C15-C16-C17
3	N	613	CLA	C16-C17-C18-C20
2	G	601	CHL	C11-C12-C13-C15
2	Y	601	CHL	C6-C7-C8-C10
2	Y	607	CHL	C11-C10-C8-C7
3	N	611	CLA	C11-C12-C13-C15
3	Y	603	CLA	C6-C7-C8-C10
3	N	603	CLA	CAA-CBA-CGA-O1A
3	Y	604	CLA	C2B-C3B-CAB-CBB
3	Y	610	CLA	C2B-C3B-CAB-CBB
4	Y	615	LUT	C5-C6-C7-C8
3	Y	603	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
7	Y	619	LHG	C24-C25-C26-C27
2	N	601	CHL	CBA-CGA-O2A-C1
3	G	613	CLA	CBA-CGA-O2A-C1
3	N	612	CLA	C16-C17-C18-C19
3	Y	603	CLA	CAA-CBA-CGA-O2A
3	N	613	CLA	C2-C3-C5-C6
2	N	601	CHL	C2A-CAA-CBA-CGA
3	Y	610	CLA	C2A-CAA-CBA-CGA
3	Y	612	CLA	C2A-CAA-CBA-CGA
3	G	603	CLA	C5-C6-C7-C8
2	Y	607	CHL	CAA-CBA-CGA-O2A
3	N	613	CLA	C4-C3-C5-C6
3	G	611	CLA	C2-C3-C5-C6
7	G	619	LHG	C13-C14-C15-C16
7	G	619	LHG	C30-C31-C32-C33
2	N	607	CHL	CAA-CBA-CGA-O1A
3	Y	614	CLA	O2A-C1-C2-C3
3	N	603	CLA	C1A-C2A-CAA-CBA
3	Y	603	CLA	C1A-C2A-CAA-CBA
4	G	615	LUT	C6-C7-C8-C9
2	Y	605	CHL	CAA-CBA-CGA-O2A
5	G	620	XAT	C27-C28-C29-C30
3	G	612	CLA	C2A-CAA-CBA-CGA
7	N	618	LHG	C28-C29-C30-C31
2	G	608	CHL	C6-C7-C8-C10
2	Y	609	CHL	C11-C10-C8-C7
3	G	603	CLA	C12-C13-C15-C16
3	N	602	CLA	C6-C7-C8-C10
3	N	611	CLA	C11-C10-C8-C7
3	Y	602	CLA	C11-C12-C13-C15
3	Y	611	CLA	C6-C7-C8-C10
2	G	609	CHL	C16-C17-C18-C20
2	N	606	CHL	O2A-C1-C2-C3
7	N	618	LHG	C5-C4-O6-P
3	Y	603	CLA	C3A-C2A-CAA-CBA
2	N	607	CHL	C5-C6-C7-C8
3	Y	611	CLA	C16-C17-C18-C20
3	N	603	CLA	C11-C12-C13-C14
3	Y	604	CLA	C11-C12-C13-C14
2	Y	607	CHL	CAA-CBA-CGA-O1A
2	Y	605	CHL	CAA-CBA-CGA-O1A
3	G	610	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
3	N	602	CLA	C2A-CAA-CBA-CGA
2	Y	606	CHL	CAA-CBA-CGA-O2A
3	N	602	CLA	CAD-CBD-CGD-O2D
3	Y	604	CLA	CAD-CBD-CGD-O2D
3	Y	603	CLA	CAA-CBA-CGA-O1A
2	G	606	CHL	C1A-C2A-CAA-CBA
2	N	608	CHL	C16-C17-C18-C20

There are no ring outliers.

52 monomers are involved in 171 short contacts:

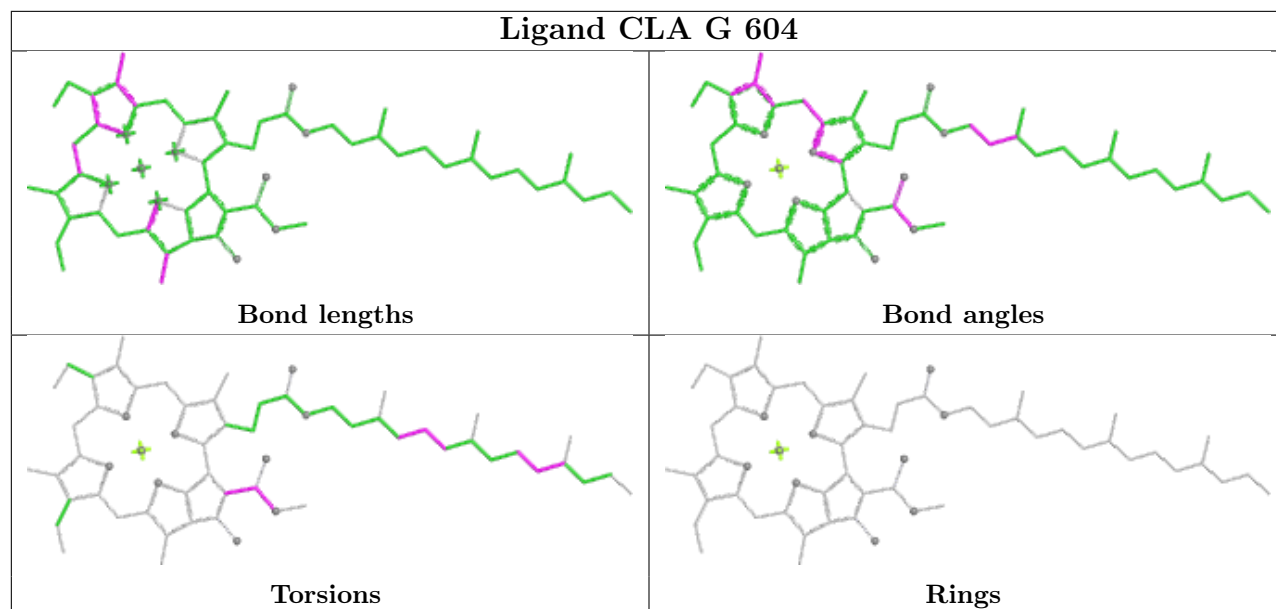
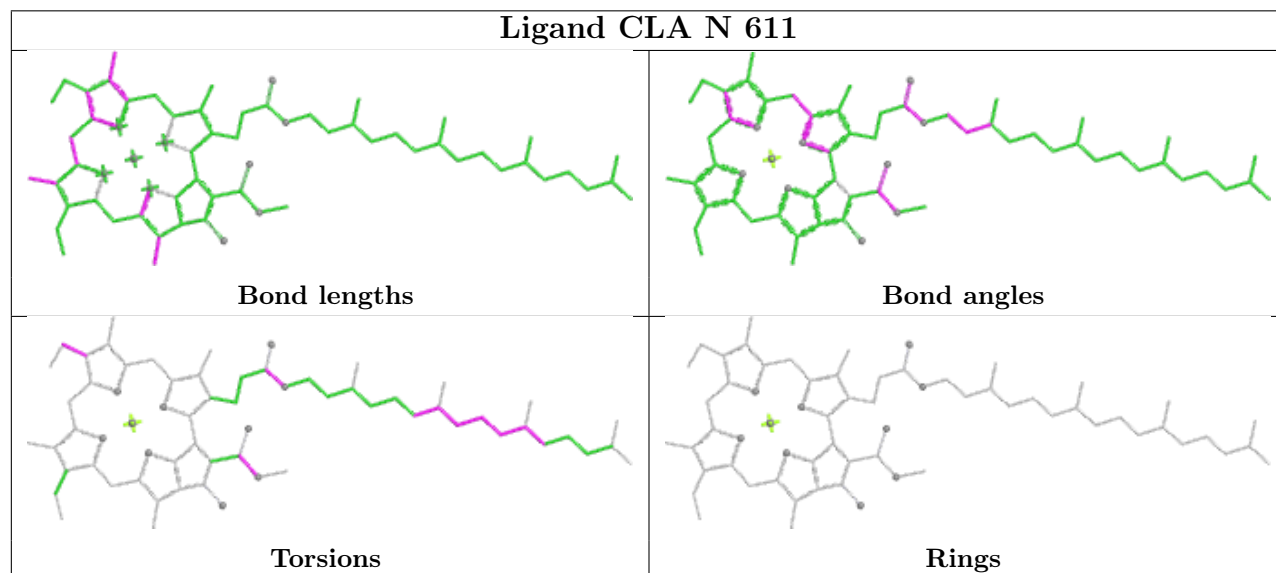
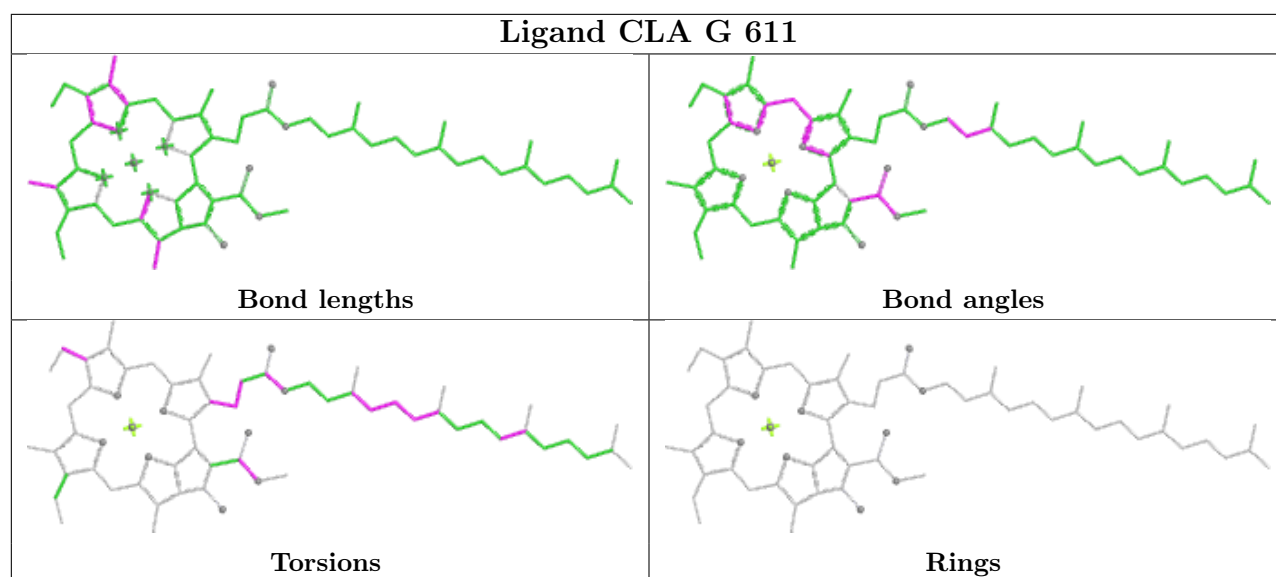
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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3	N	611	CLA	3	0
3	G	604	CLA	4	0
6	Y	618	NEX	3	0
5	G	617	XAT	6	0
6	G	618	NEX	6	0
2	G	606	CHL	5	0
7	N	618	LHG	4	0
4	Y	616	LUT	3	0
3	N	610	CLA	5	0
3	Y	612	CLA	3	0
2	G	607	CHL	5	0
3	N	603	CLA	3	0
3	G	613	CLA	6	0
3	N	613	CLA	3	0
3	Y	613	CLA	4	0
3	G	603	CLA	3	0
6	N	617	NEX	2	0
2	N	601	CHL	8	0
3	Y	611	CLA	1	0
7	G	619	LHG	6	0
2	N	606	CHL	3	0
3	N	602	CLA	6	0
2	Y	606	CHL	3	0
2	Y	608	CHL	8	0
3	N	604	CLA	1	0
3	Y	604	CLA	5	0
2	G	609	CHL	4	0
3	G	602	CLA	6	0
4	Y	615	LUT	2	0

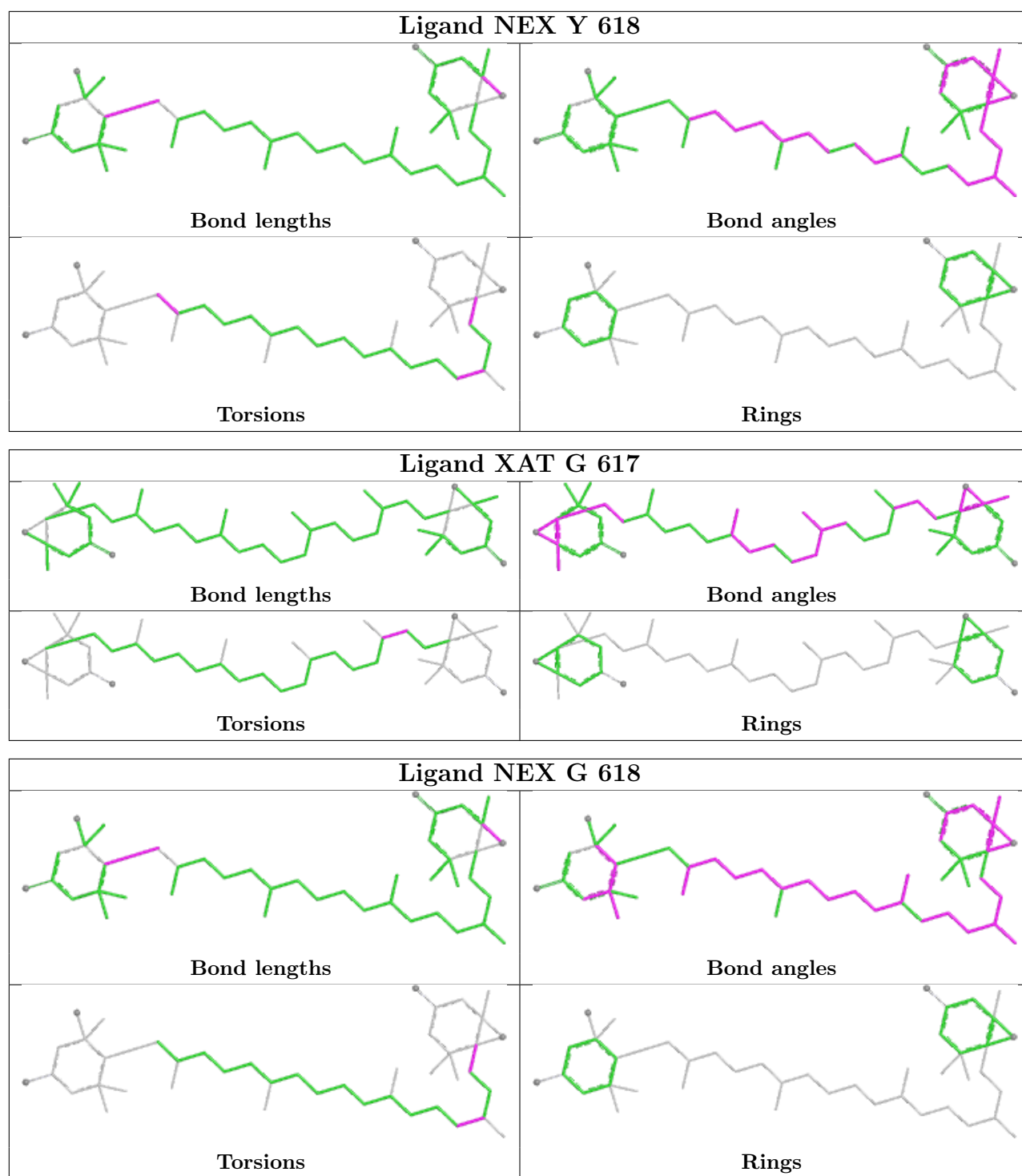
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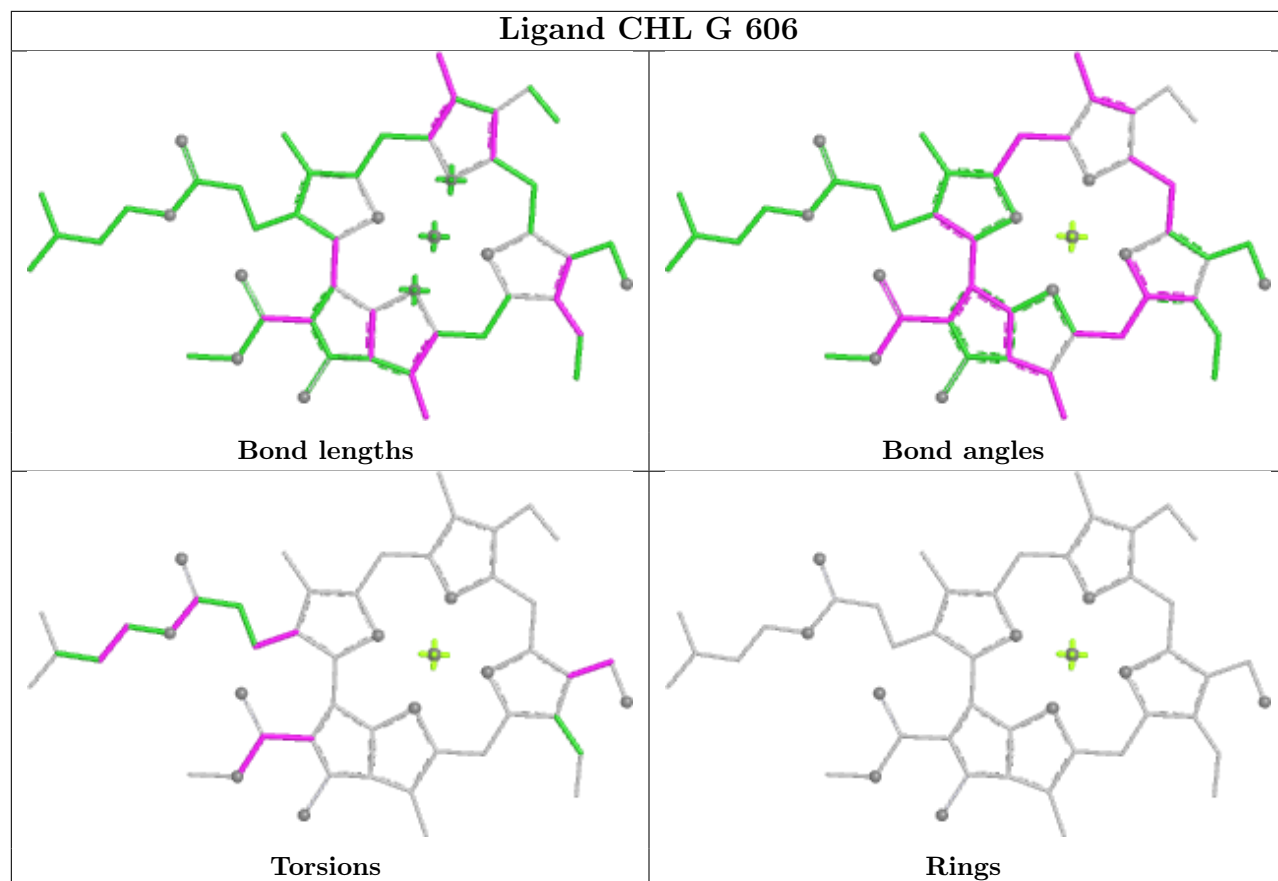
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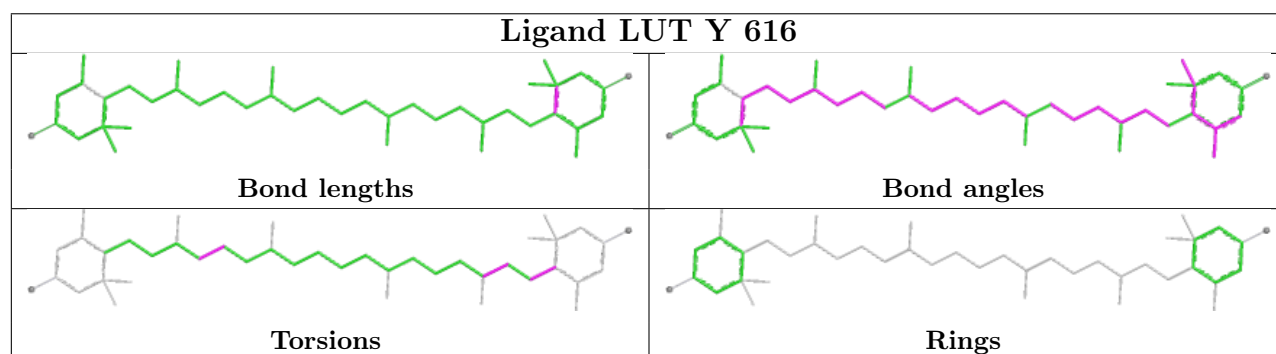
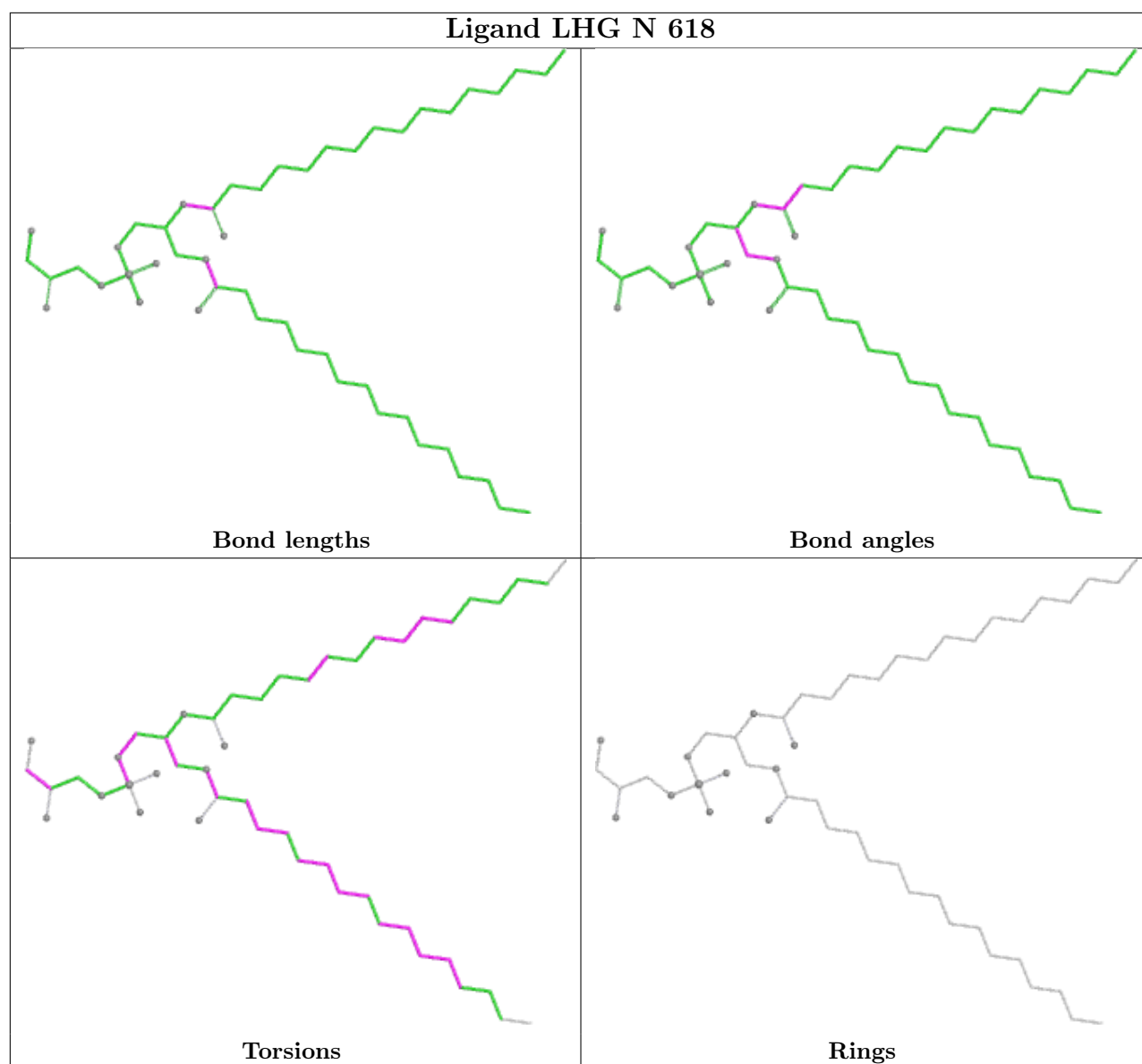
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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2	G	608	CHL	1	0
2	N	608	CHL	2	0
5	Y	617	XAT	5	0
2	N	609	CHL	10	0
3	G	612	CLA	3	0
4	N	615	LUT	3	0
4	G	615	LUT	11	0
3	N	614	CLA	1	0
7	Y	619	LHG	1	0
5	G	620	XAT	7	0
3	Y	610	CLA	3	0
4	G	616	LUT	2	0
2	Y	601	CHL	4	0
2	N	607	CHL	8	0
4	N	616	LUT	3	0
3	Y	603	CLA	5	0
2	Y	609	CHL	7	0
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2	G	601	CHL	10	0

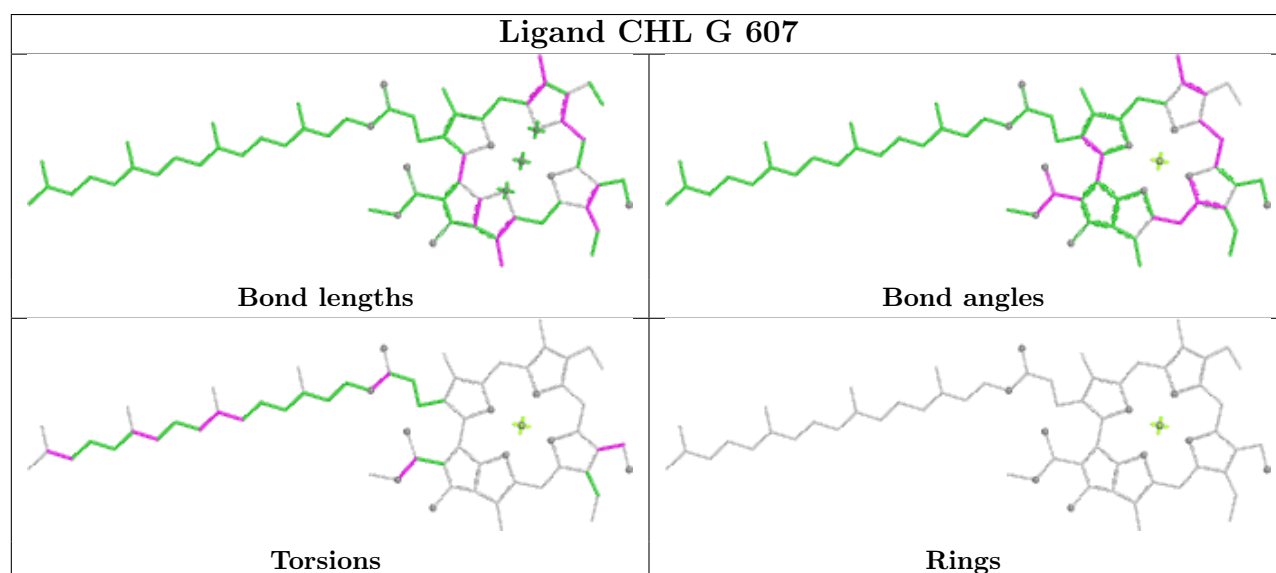
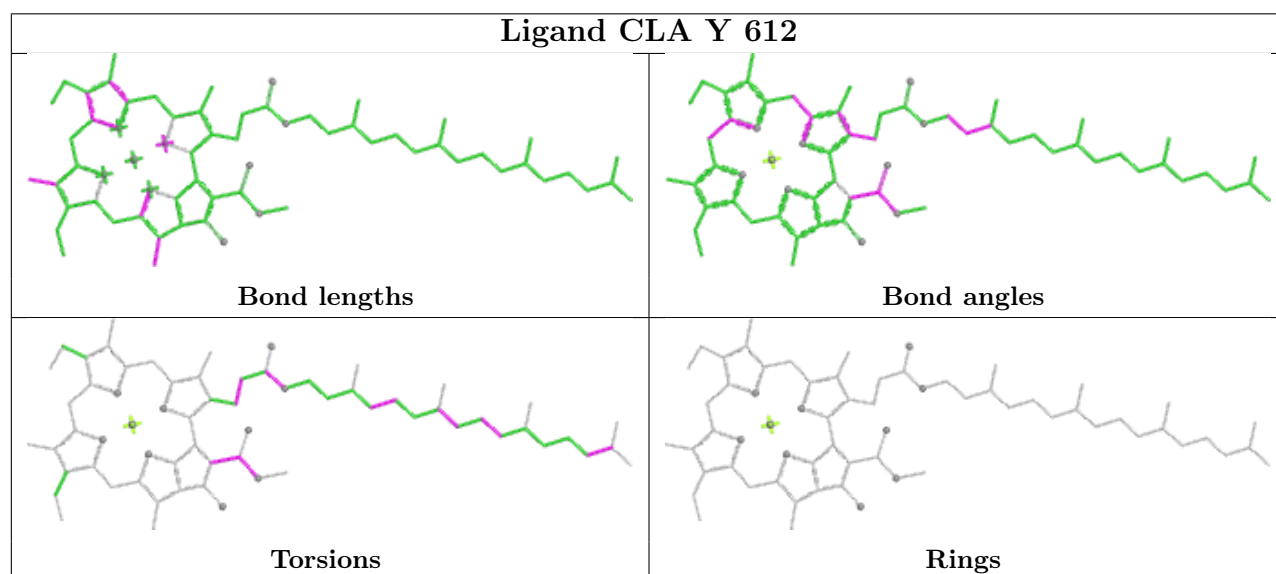
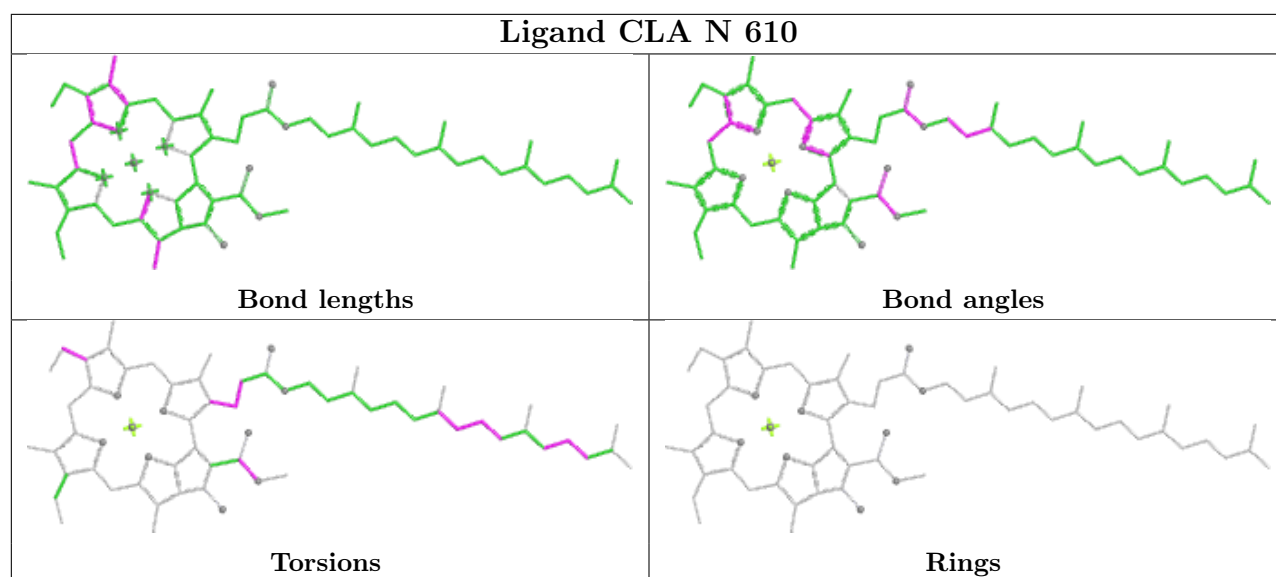
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

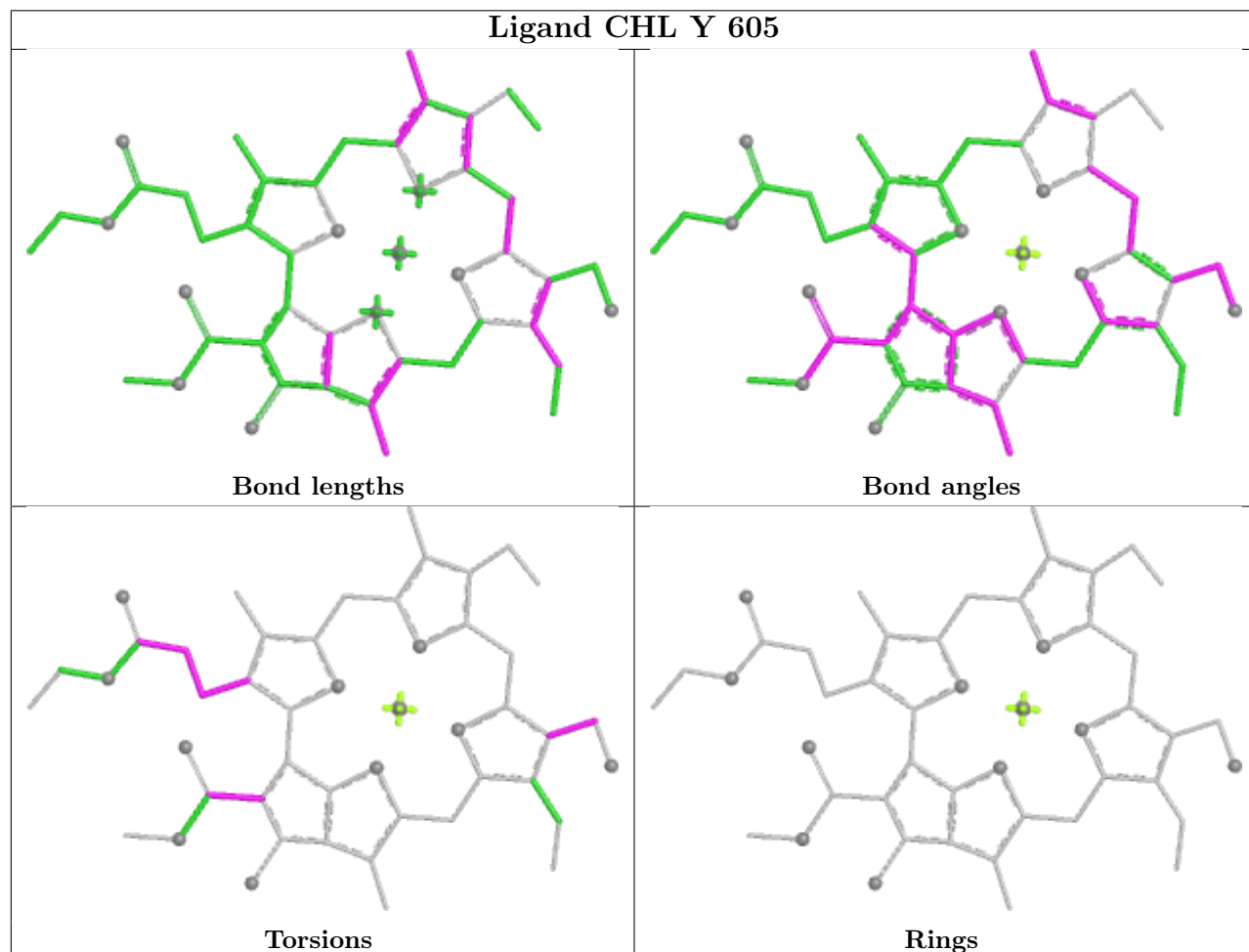
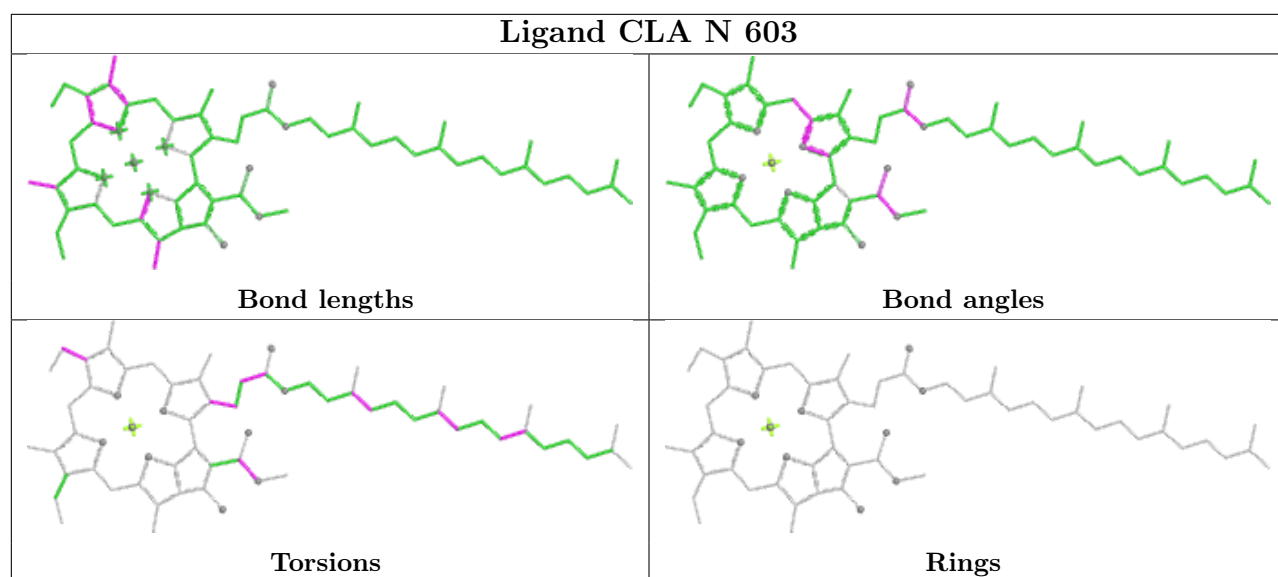


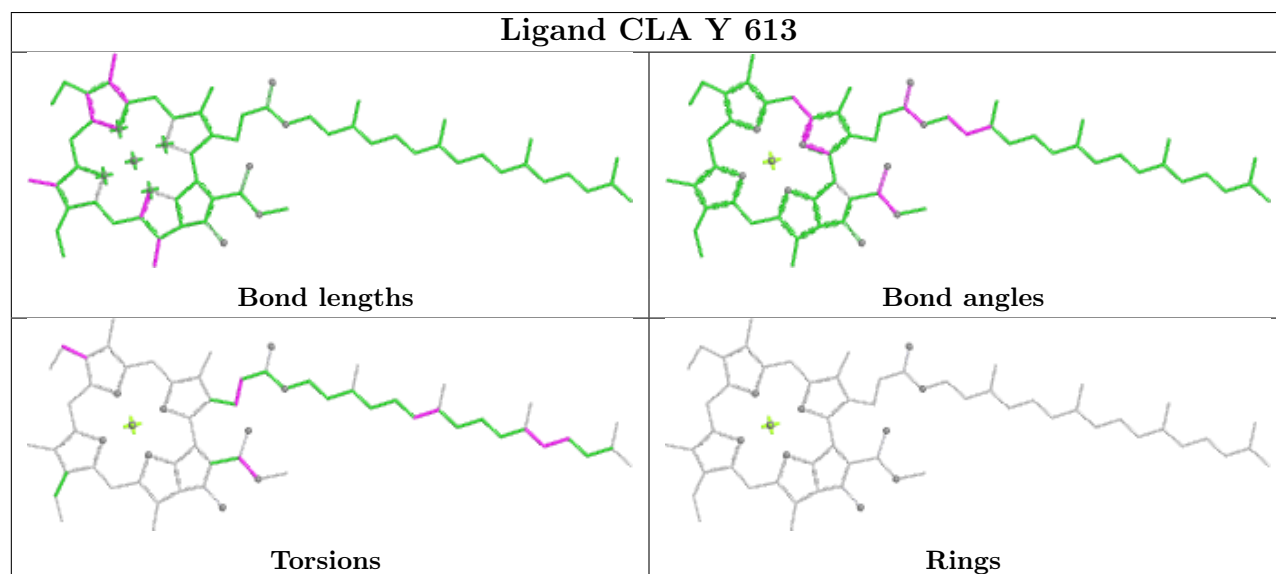
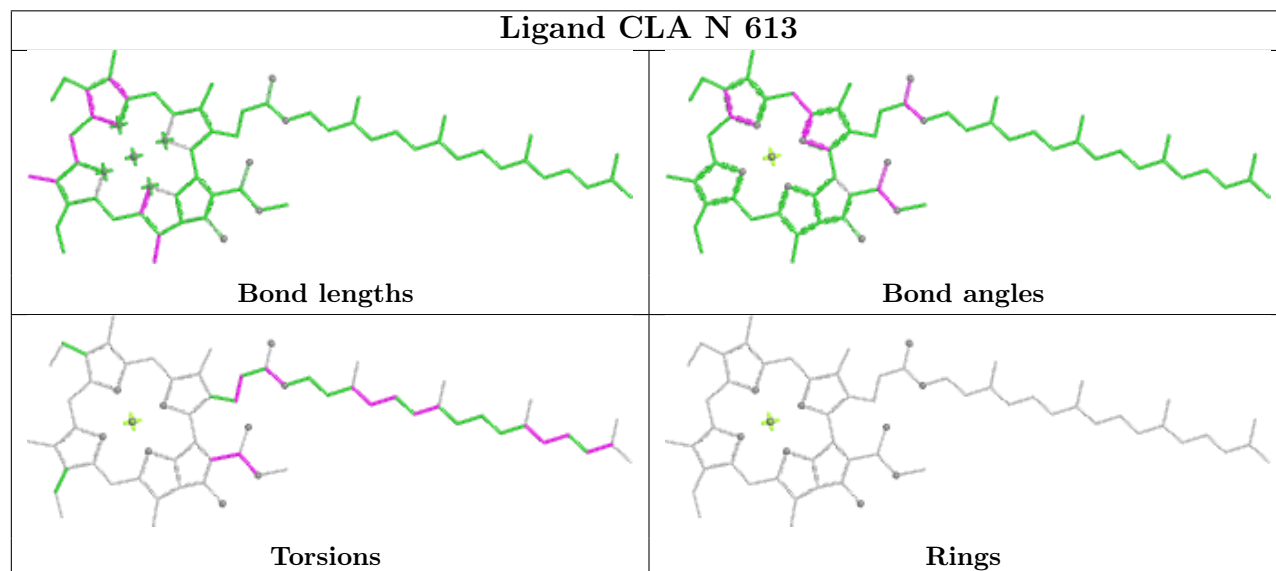
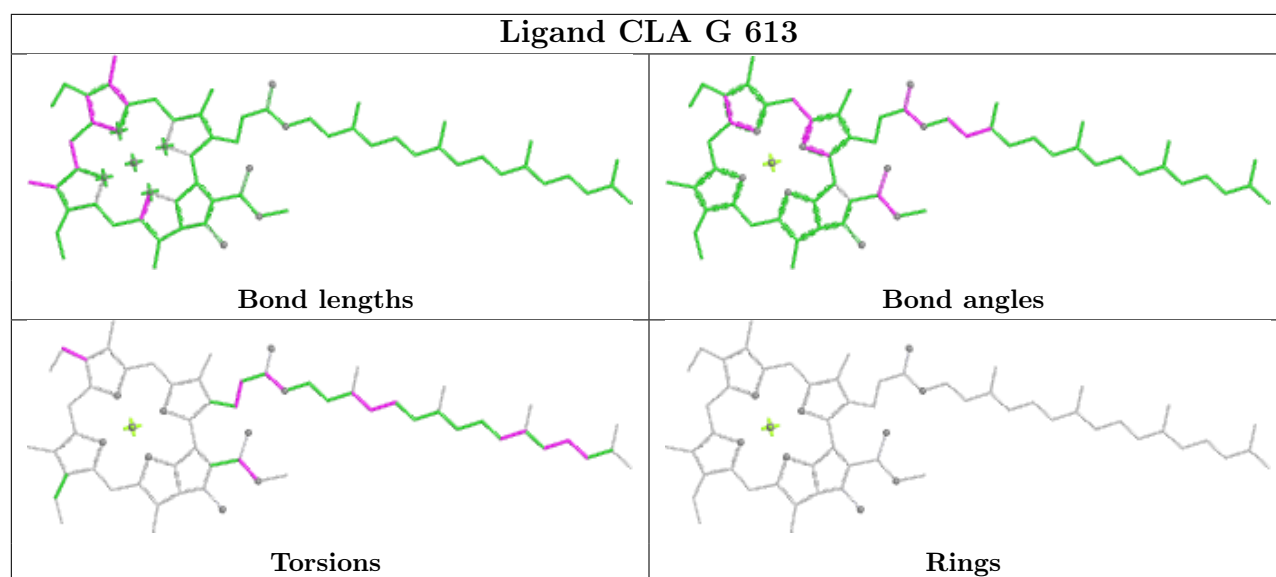


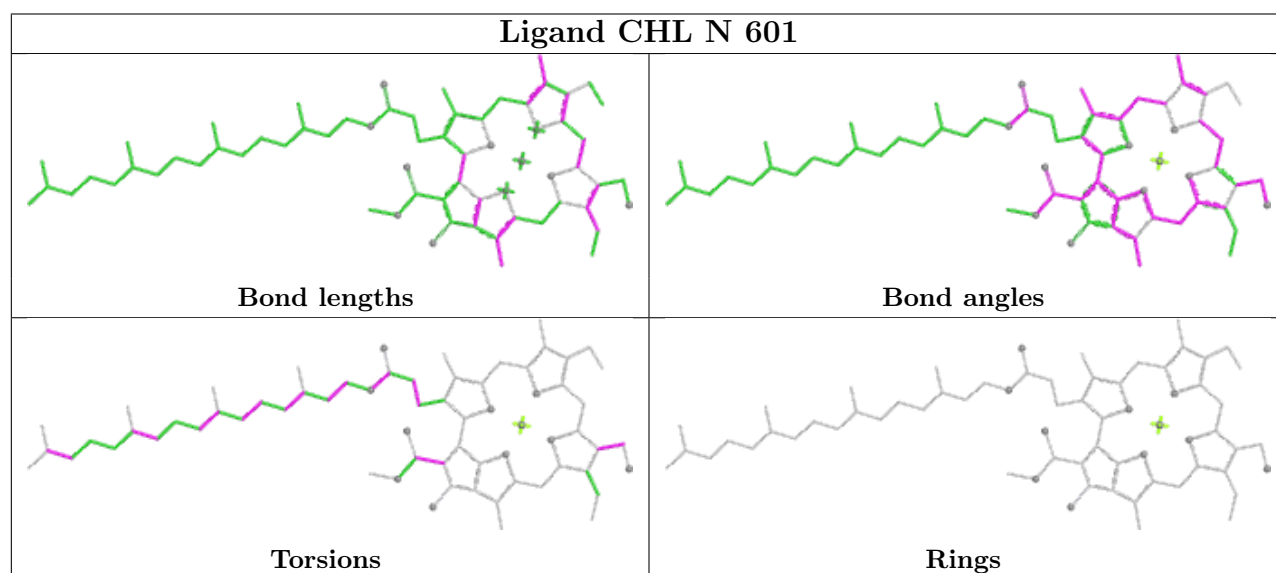
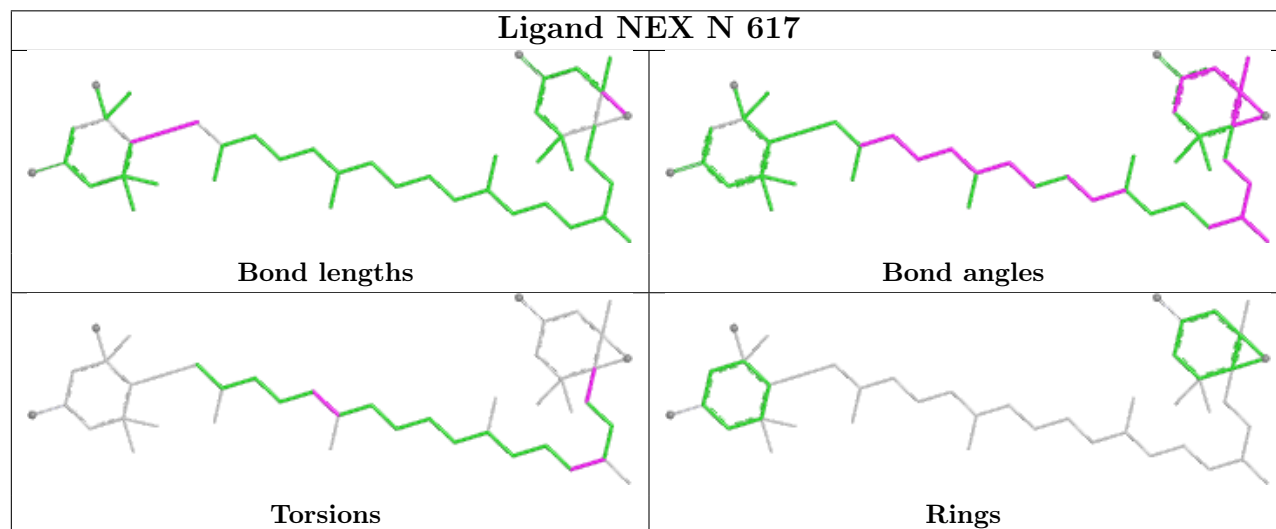
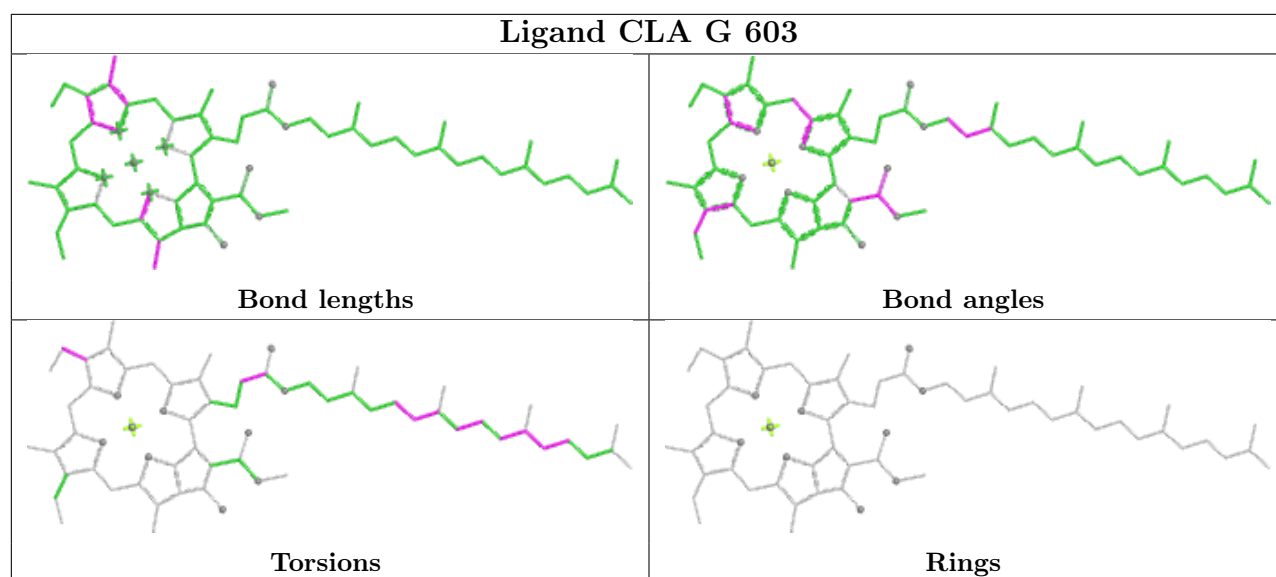


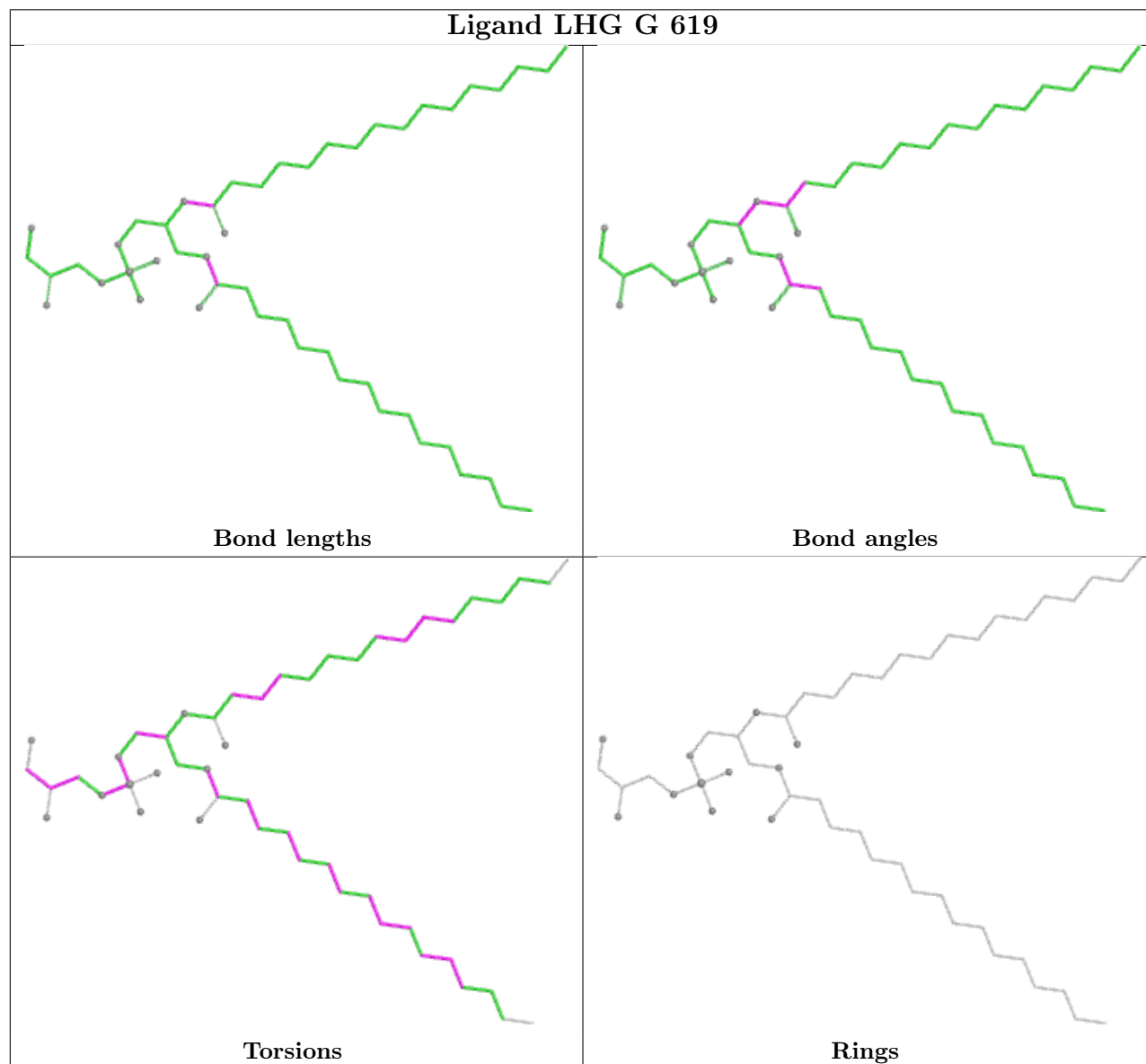
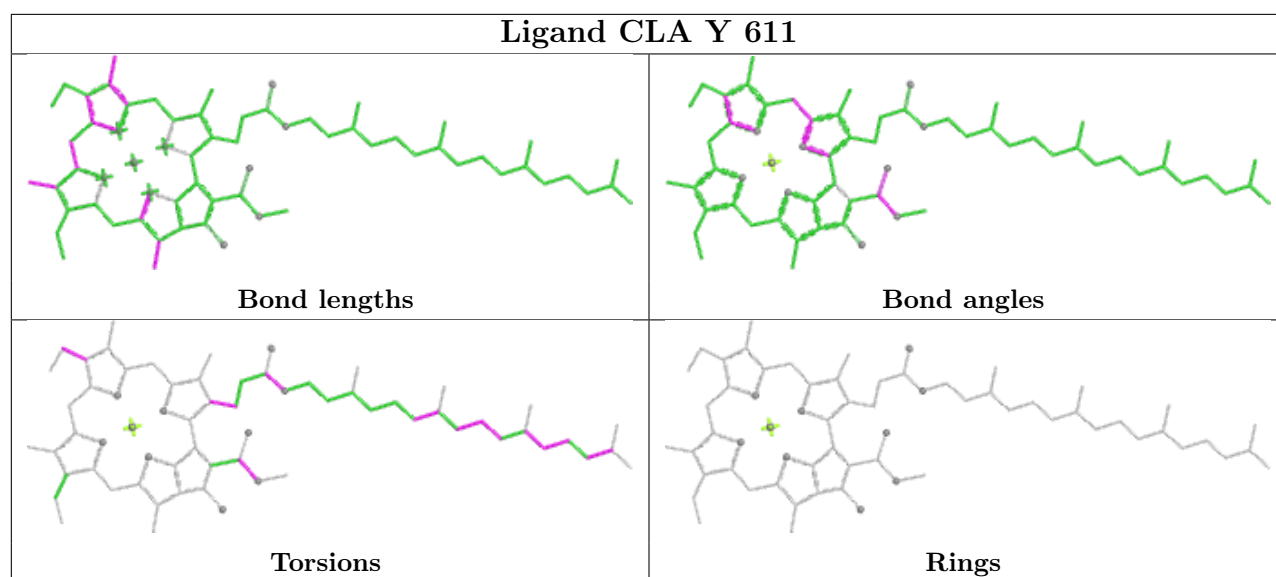




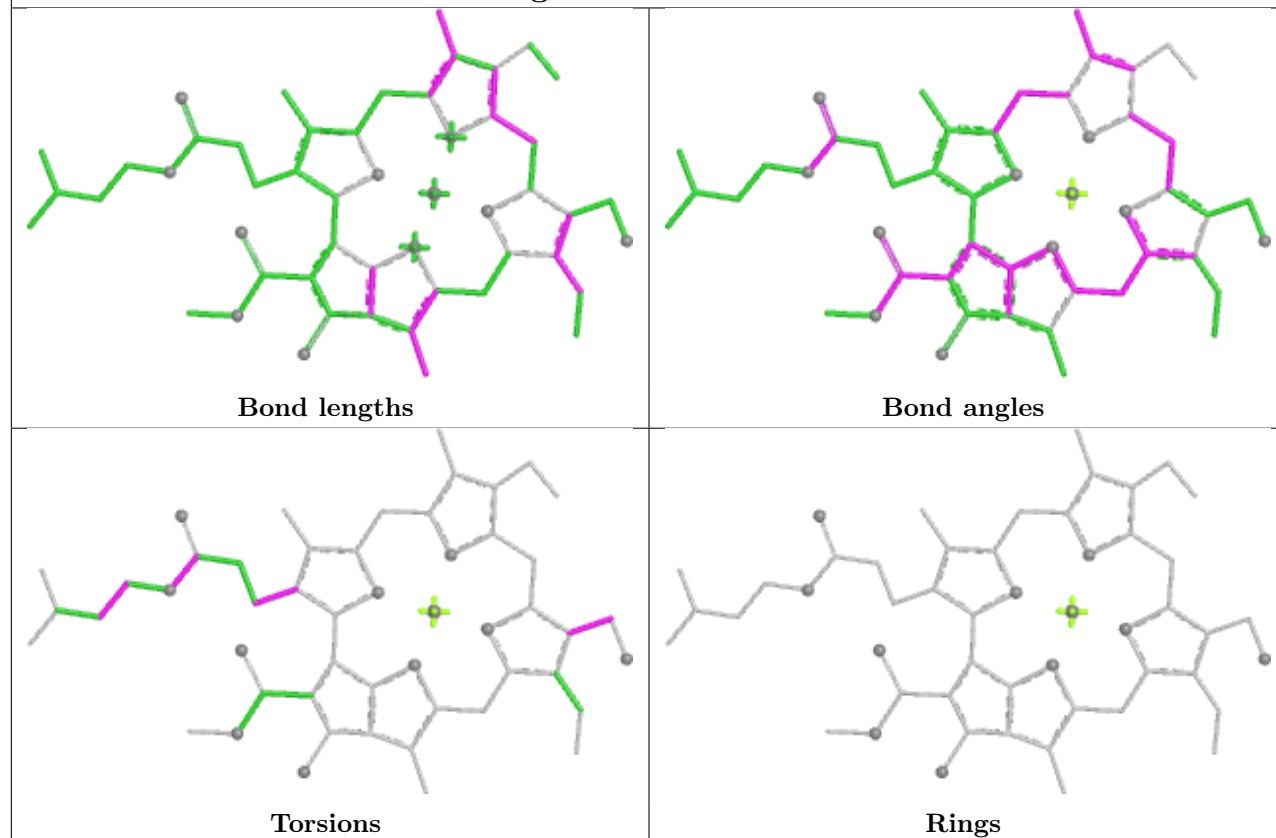




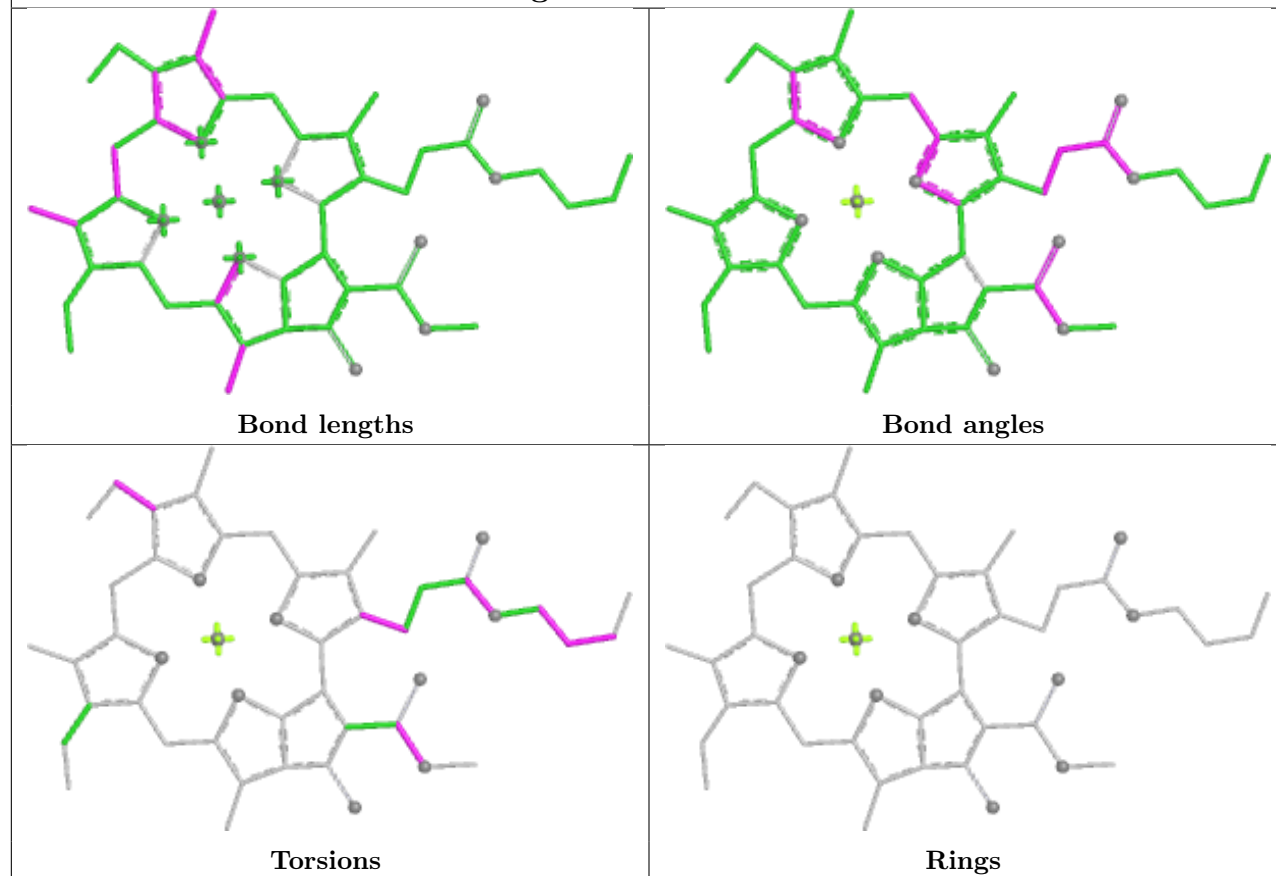


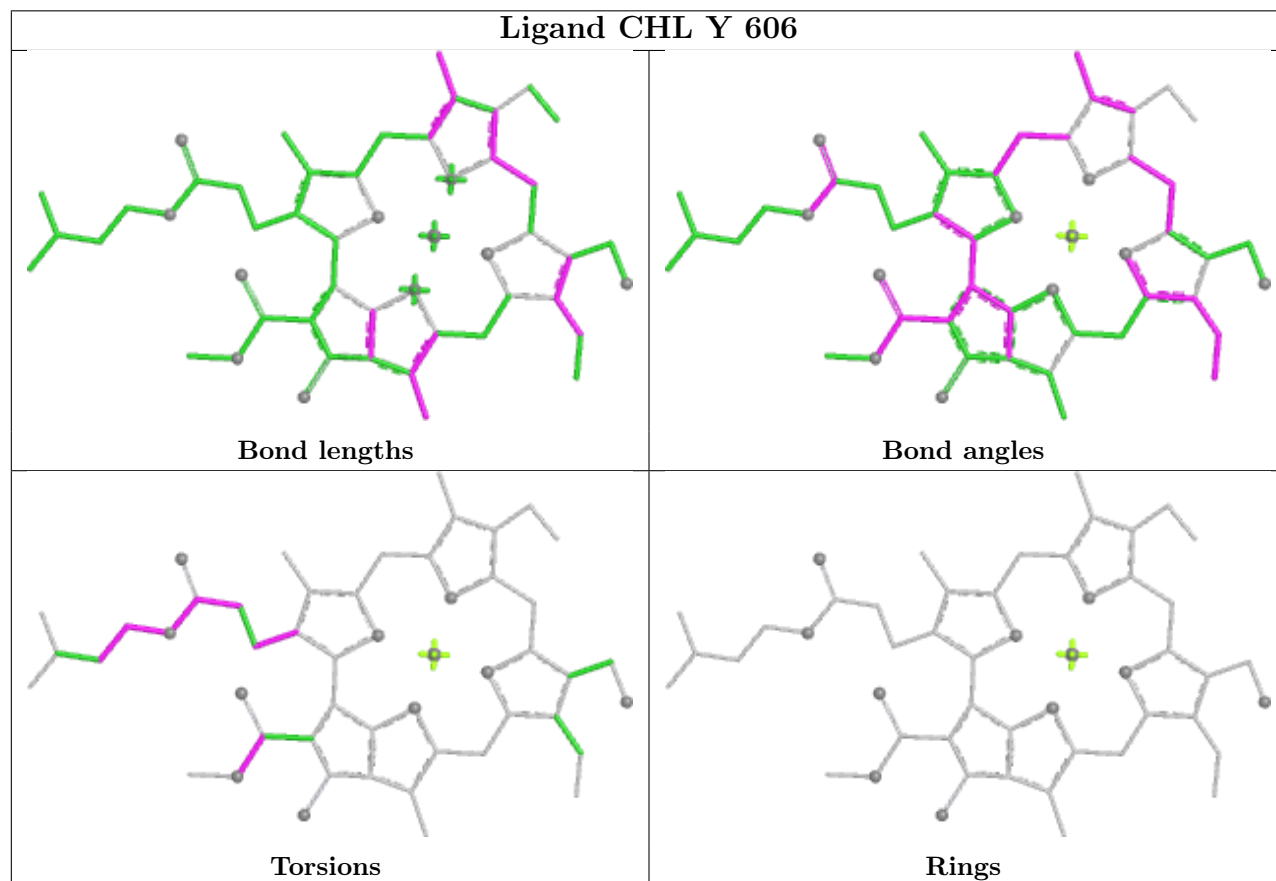
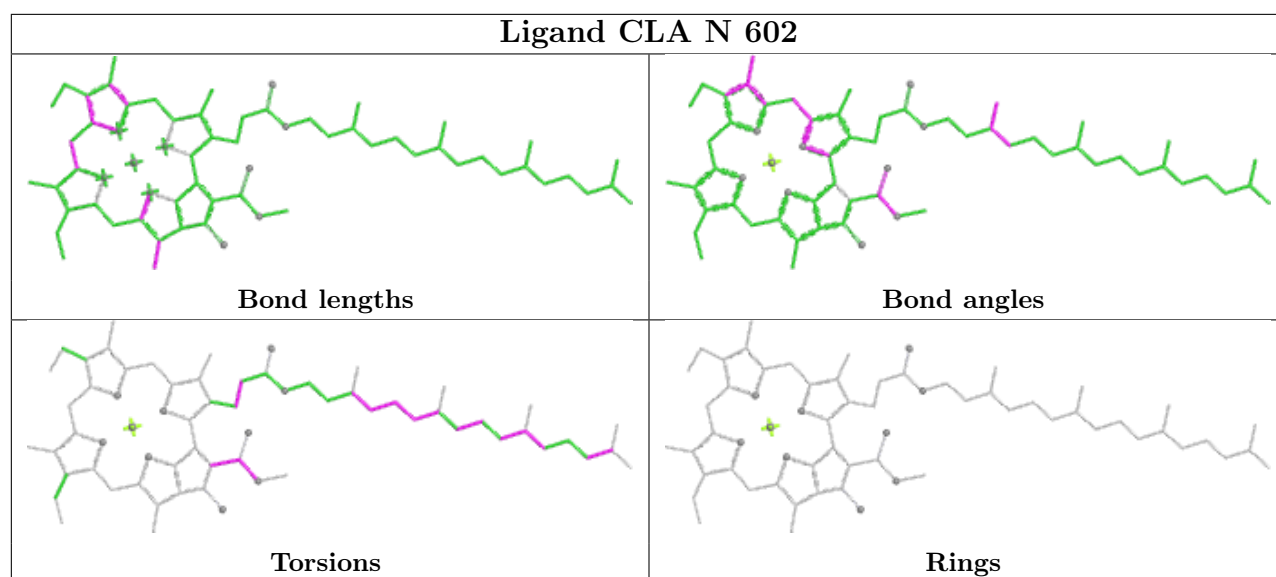


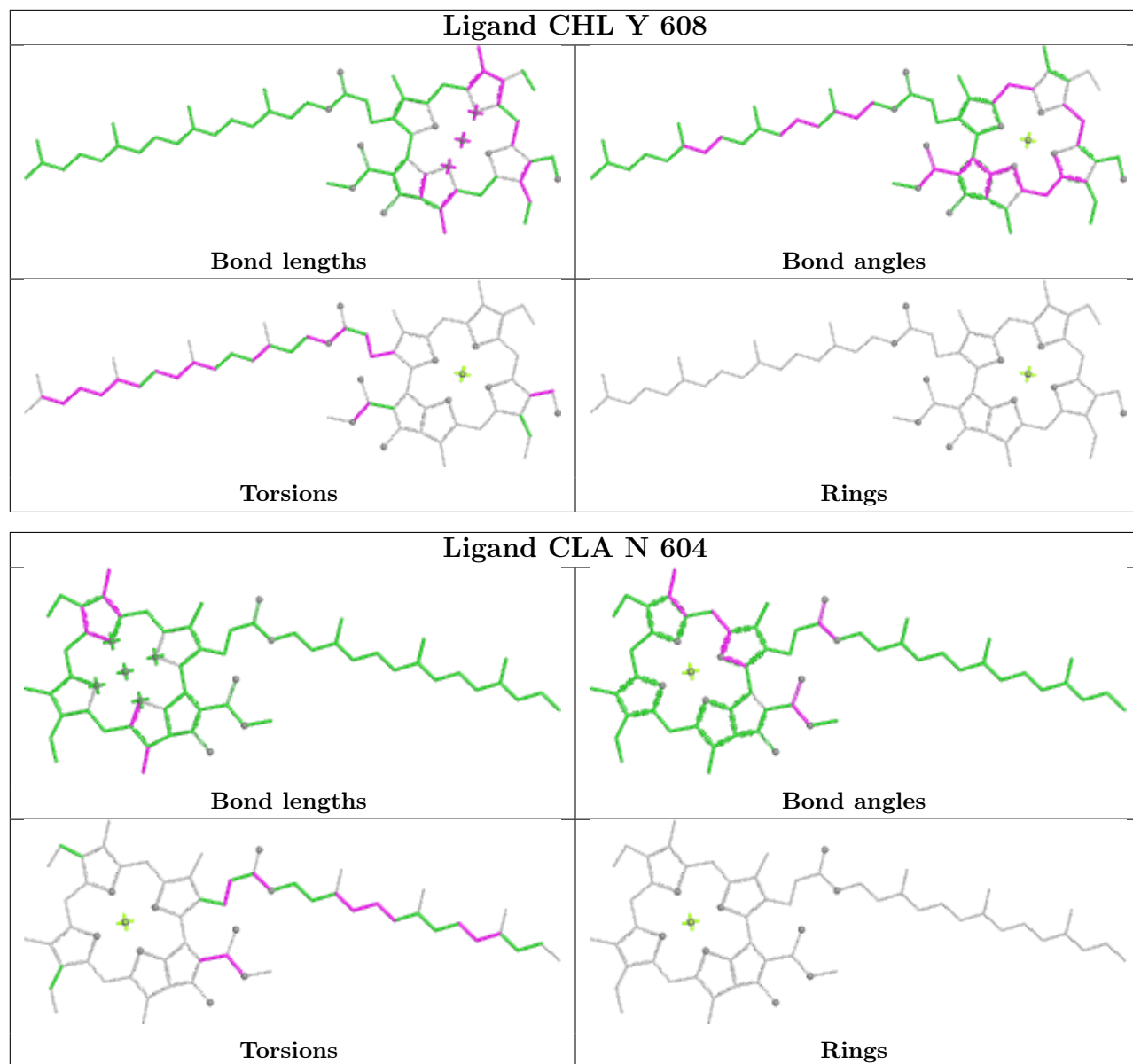
Ligand CHL N 606

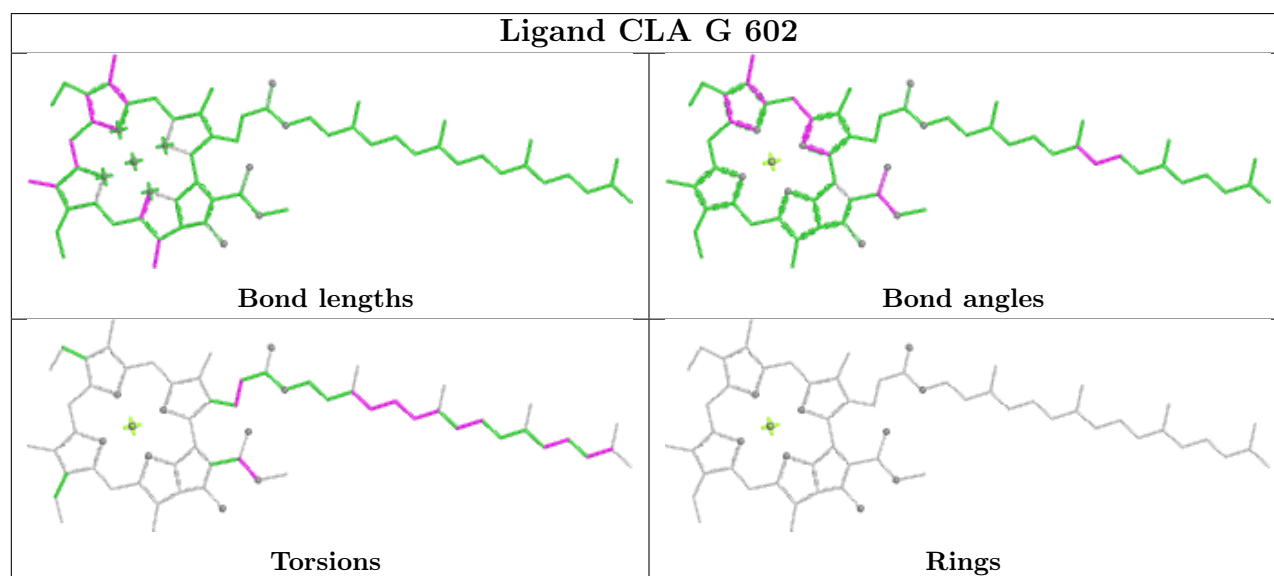
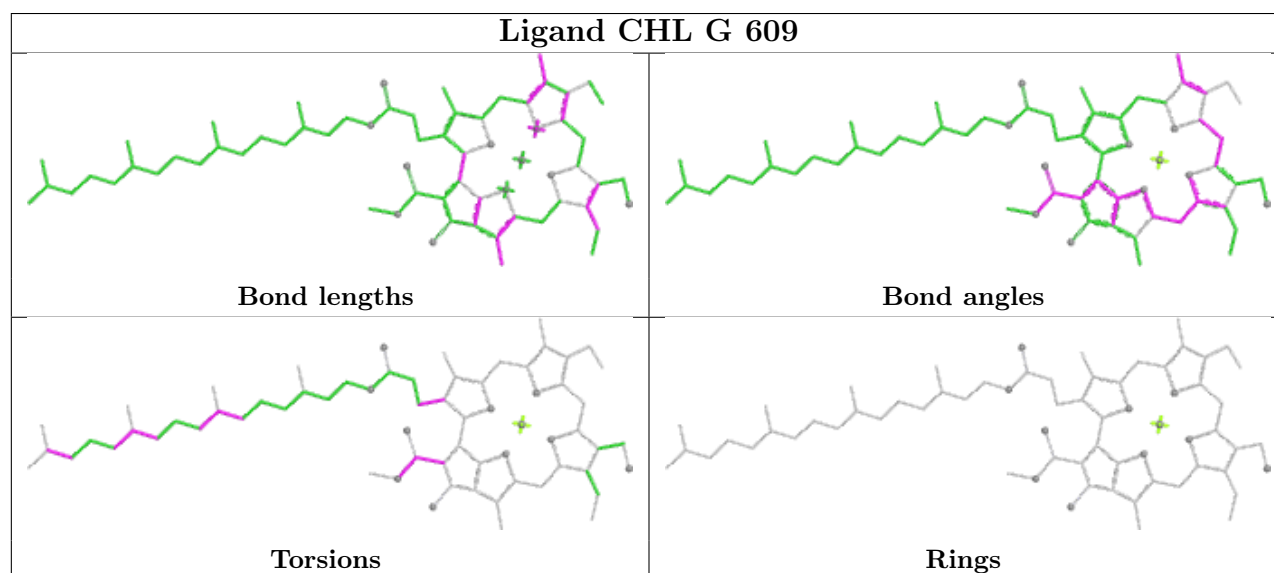
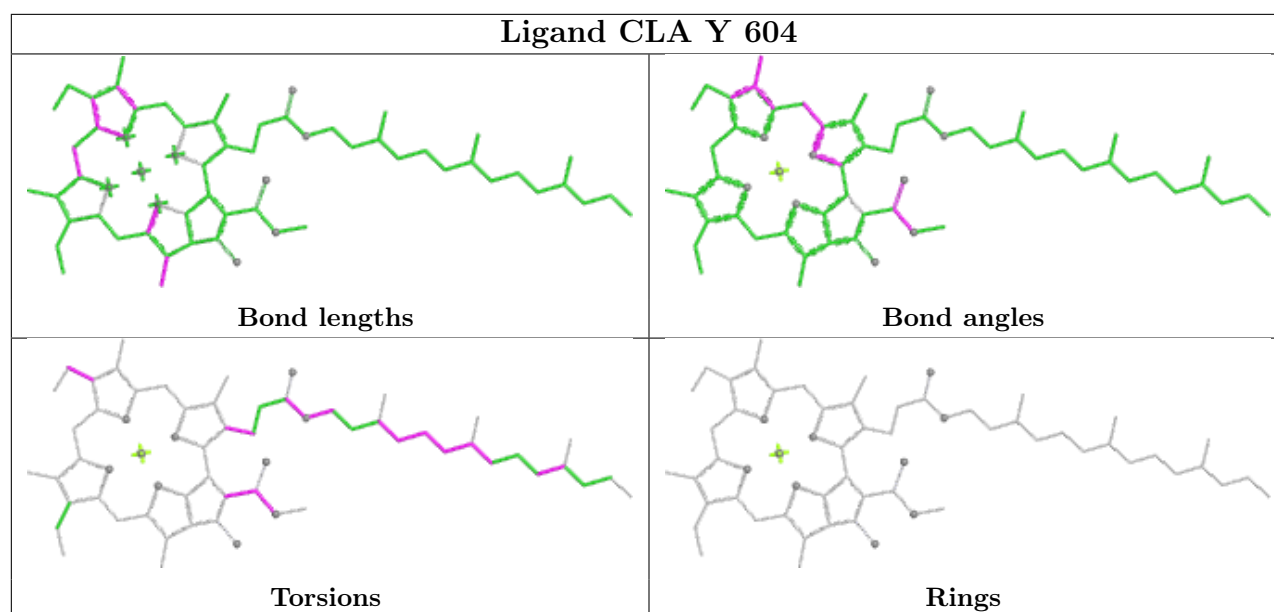


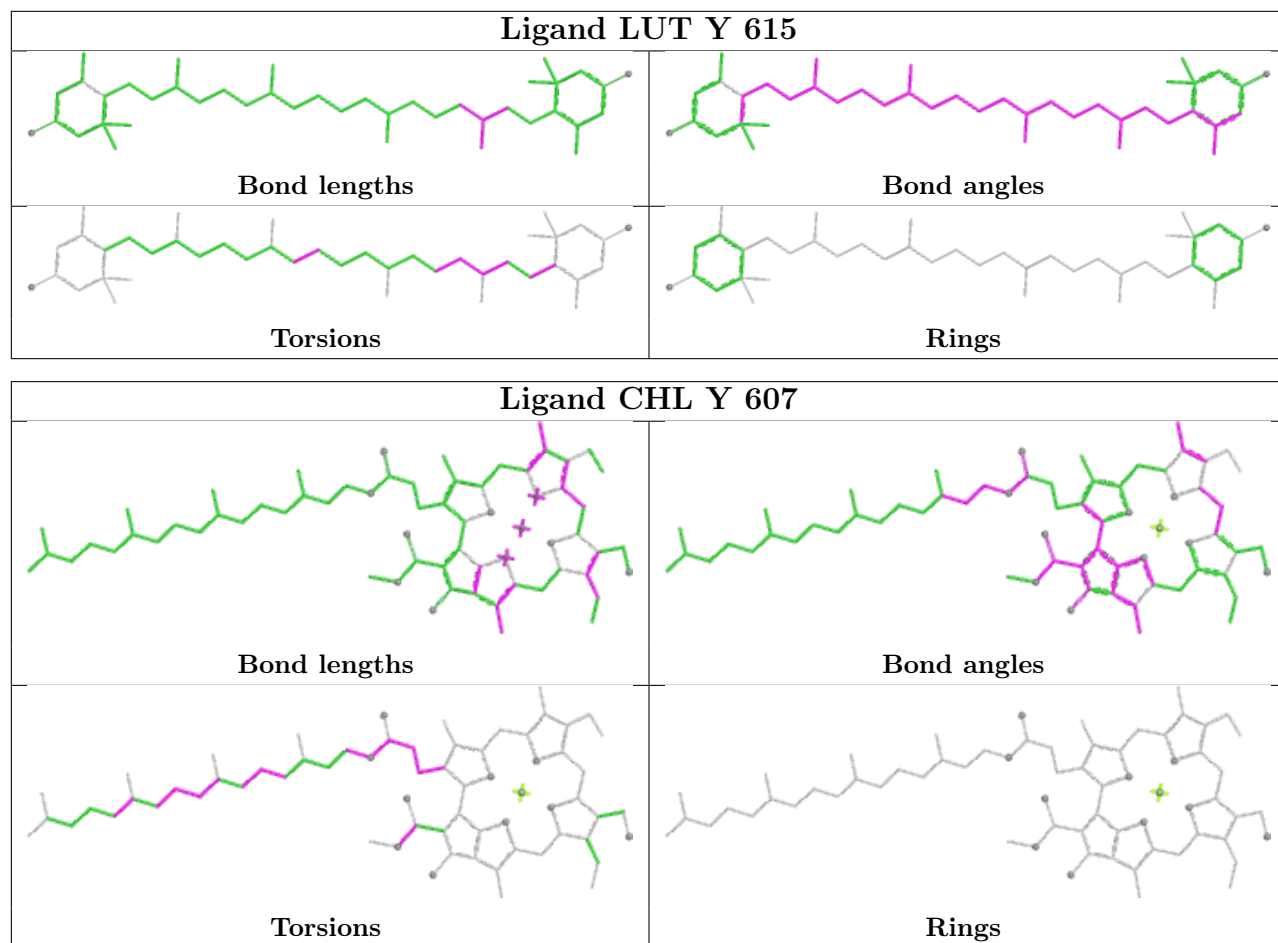
Ligand CLA G 614

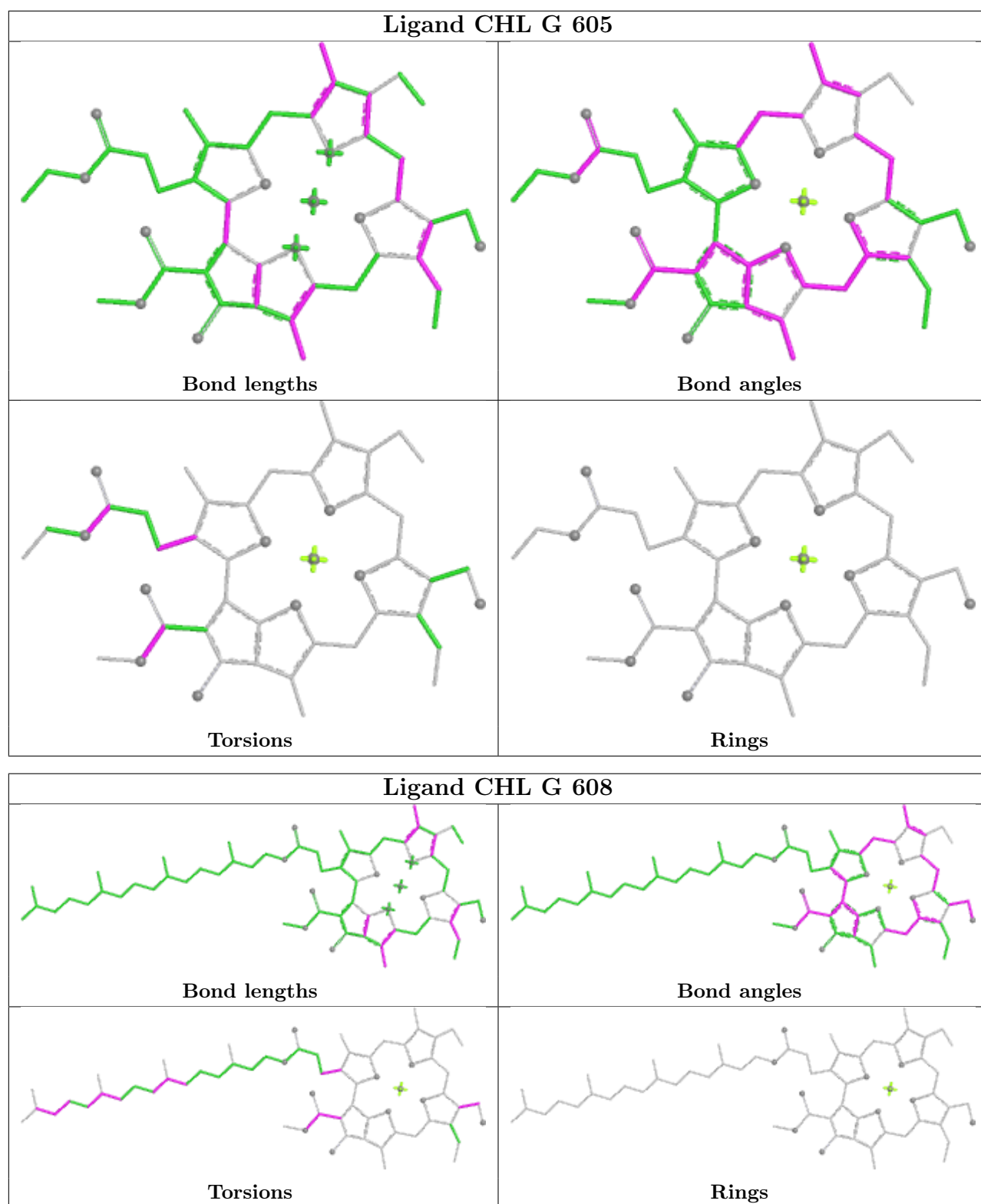


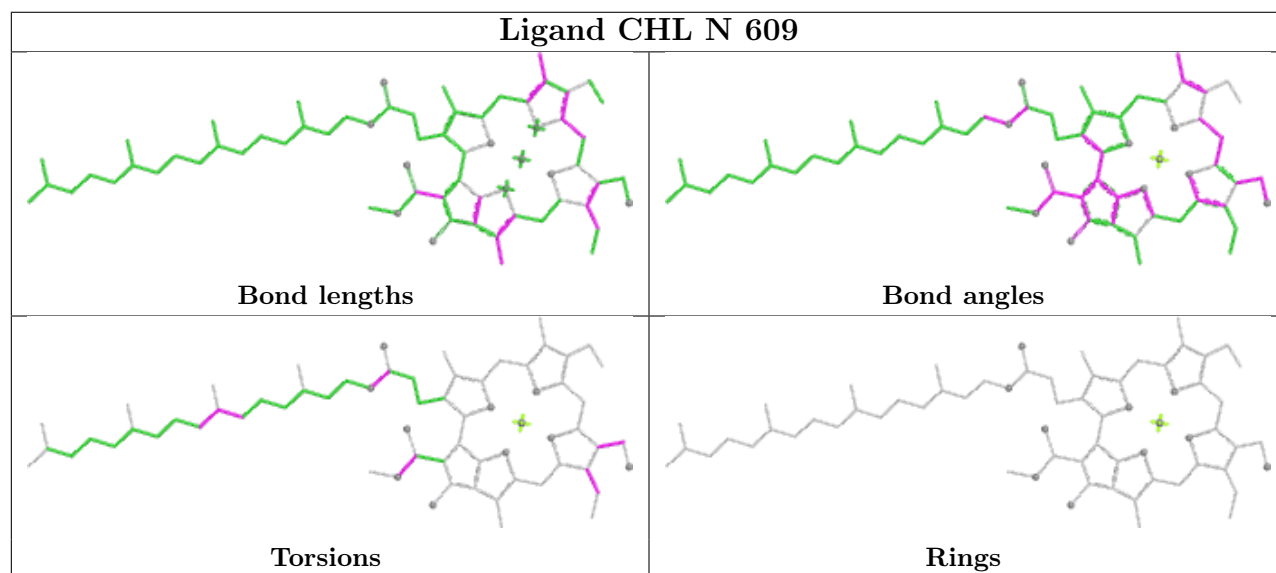
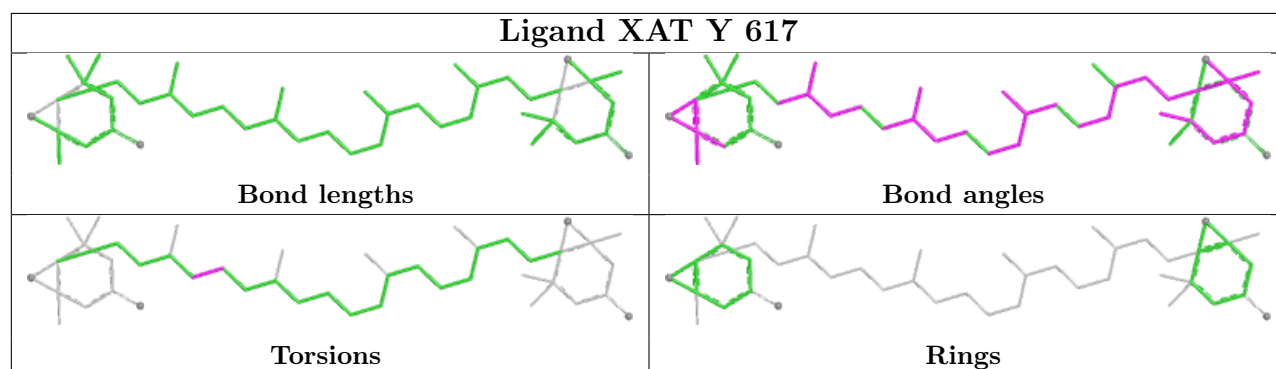
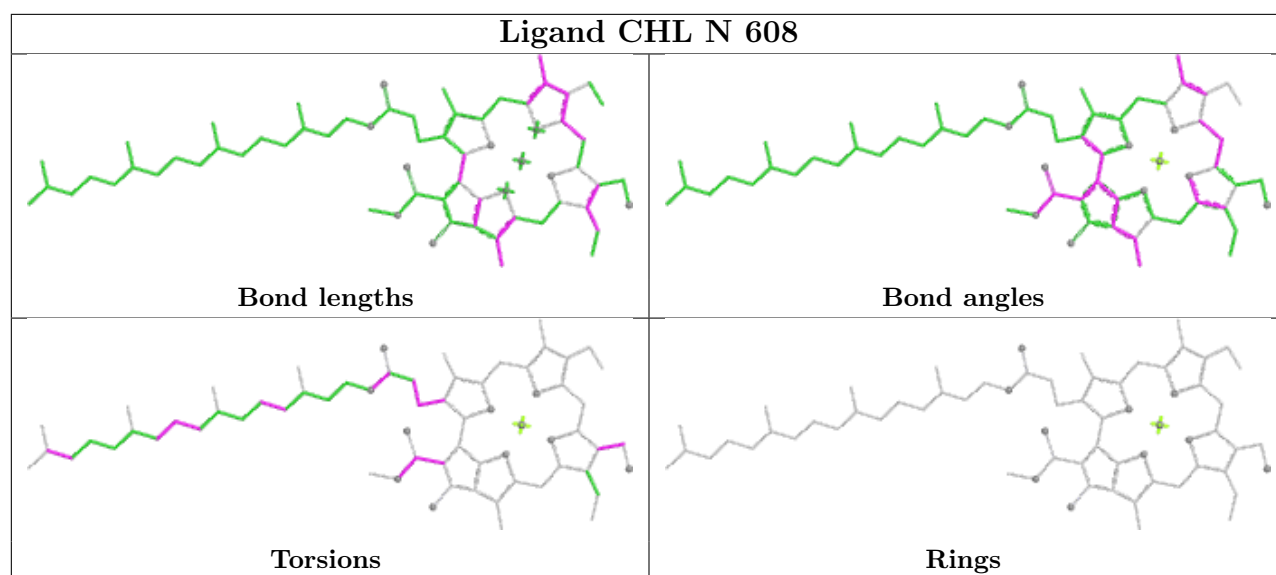


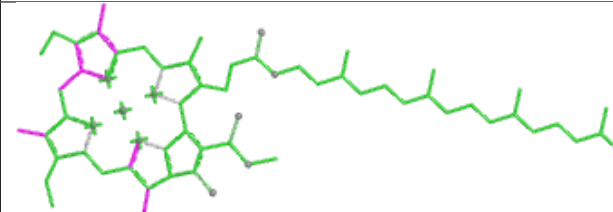
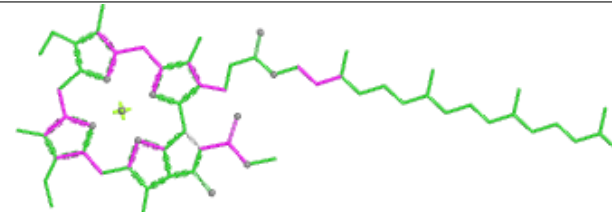
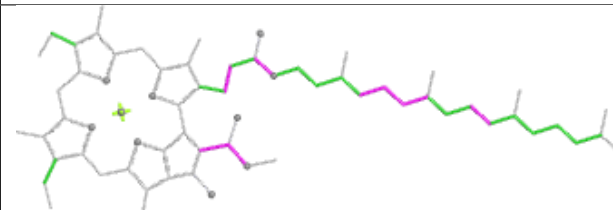
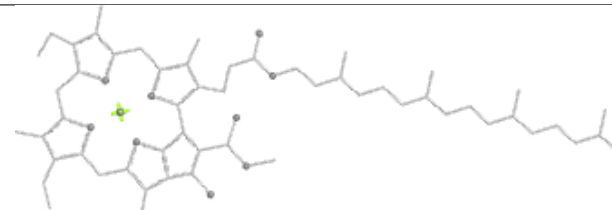


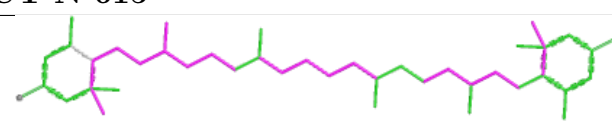
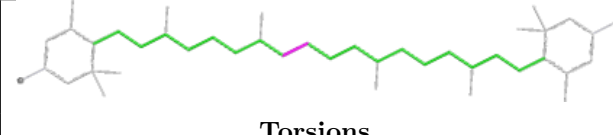
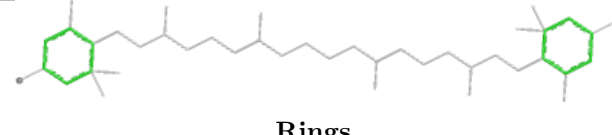


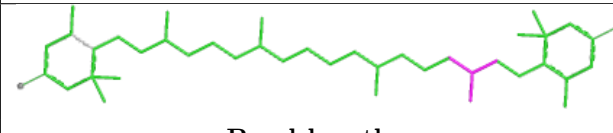
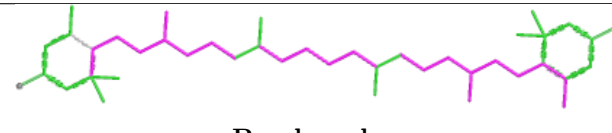
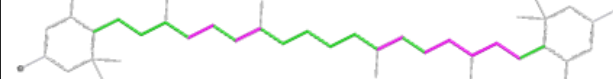
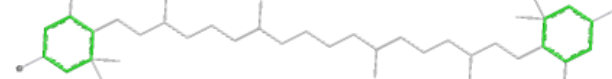


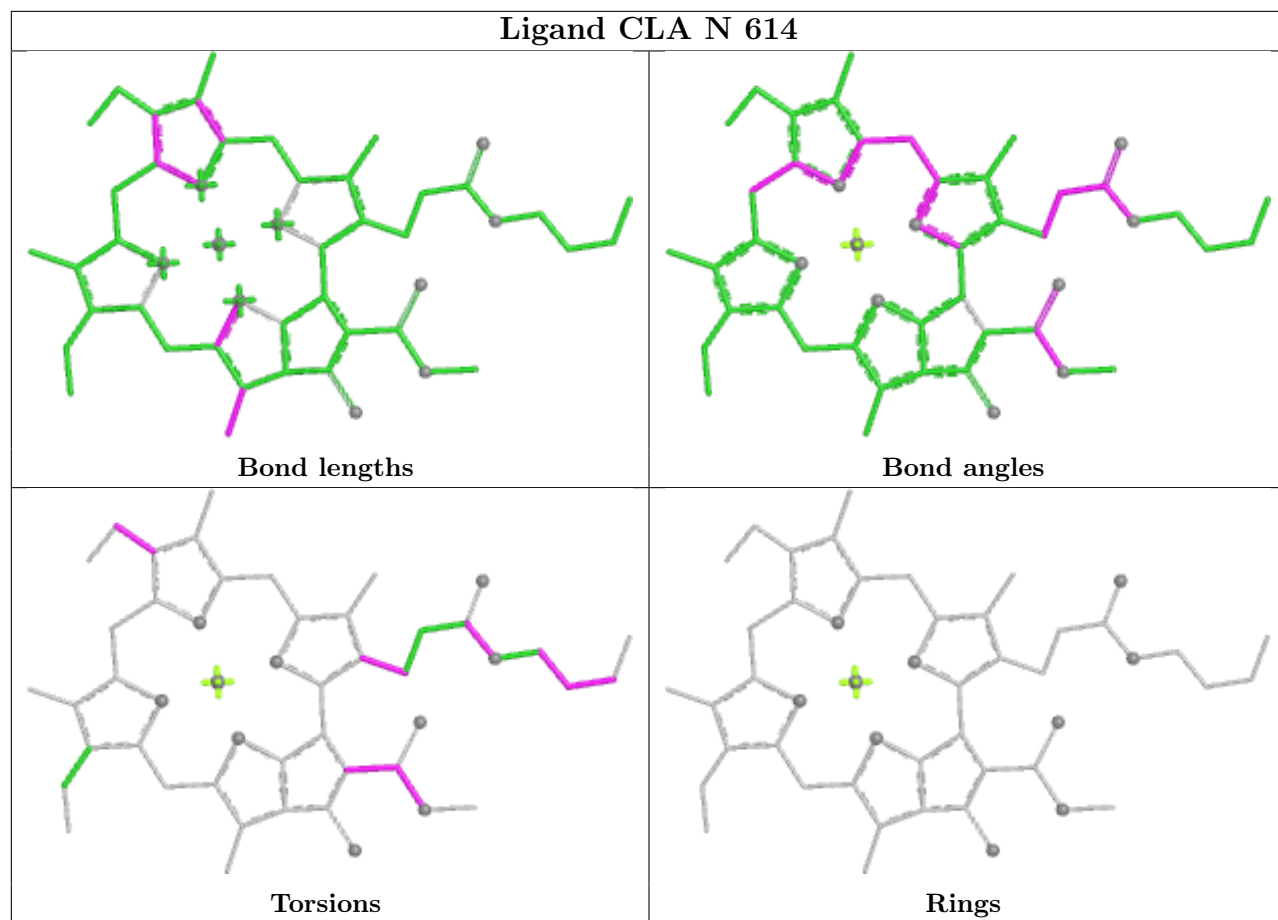


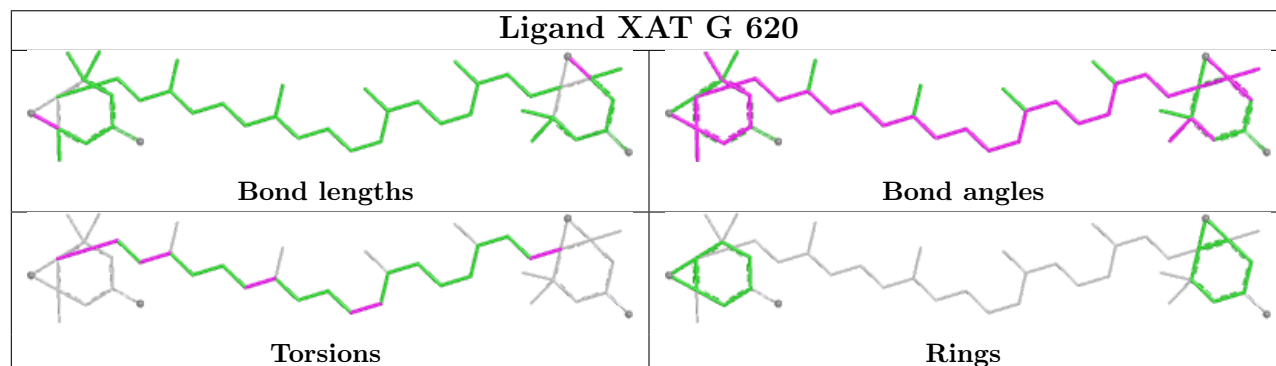
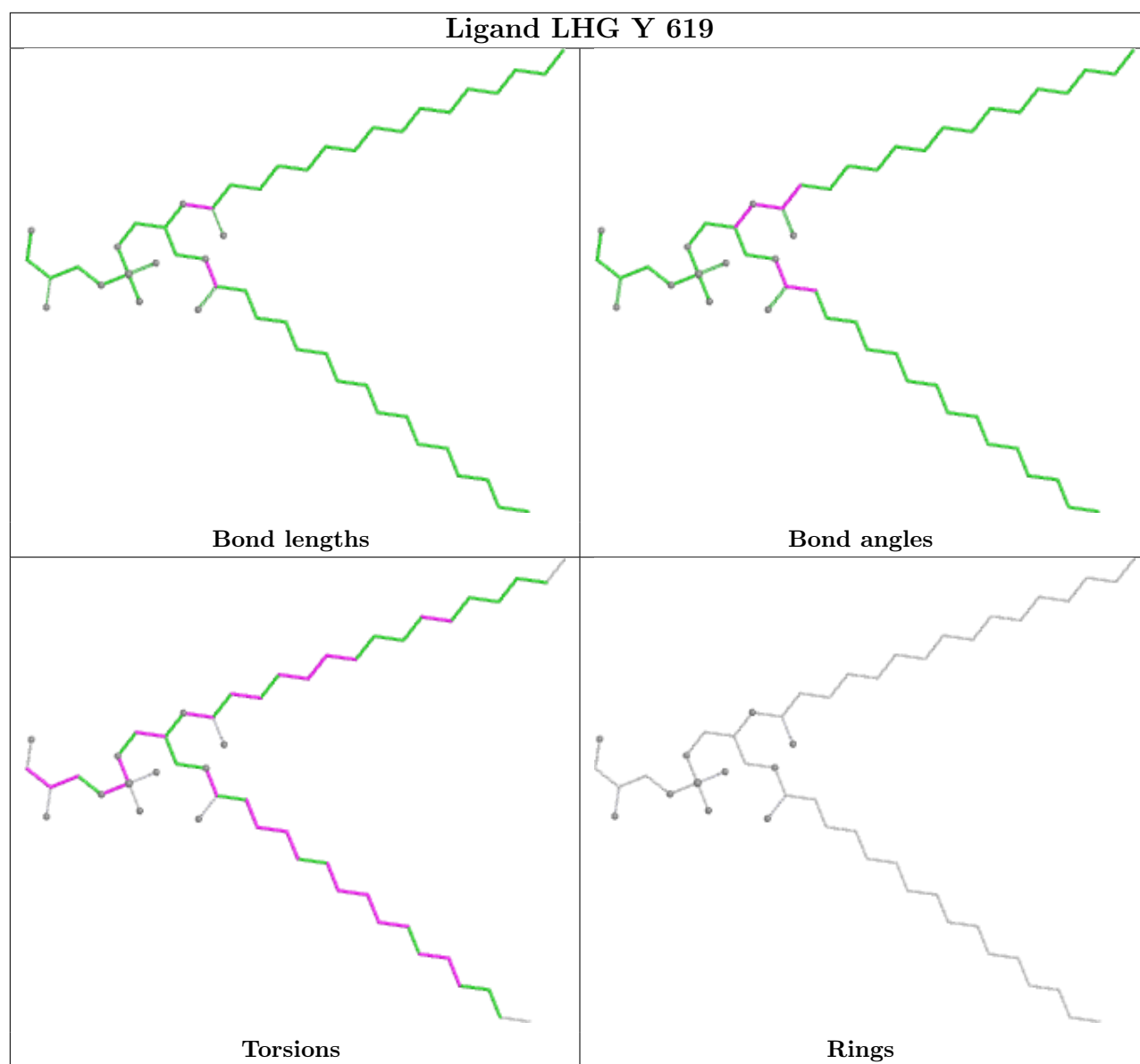


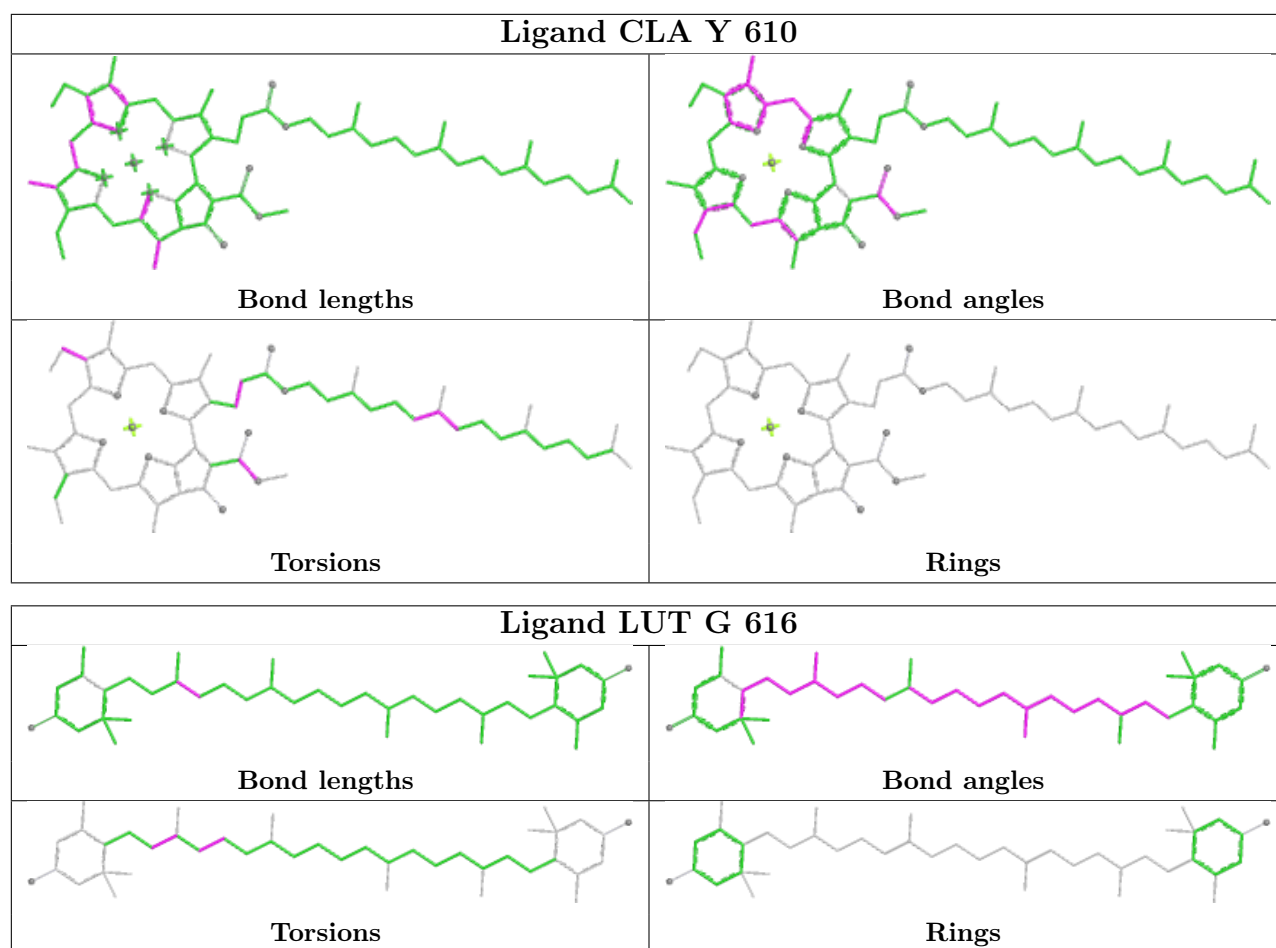
Ligand CLA G 612	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LUT N 615	
	
Bond lengths	Bond angles
	
Torsions	Rings

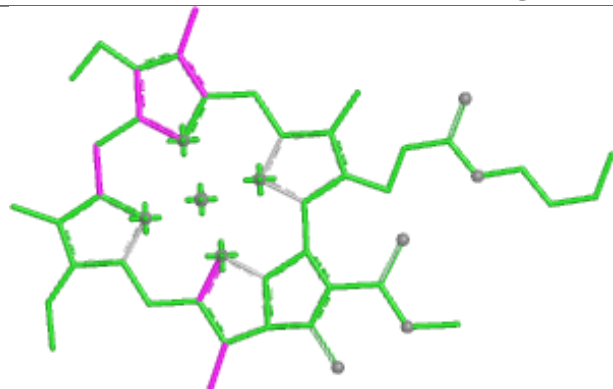
Ligand LUT G 615	
	
Bond lengths	Bond angles
	
Torsions	Rings



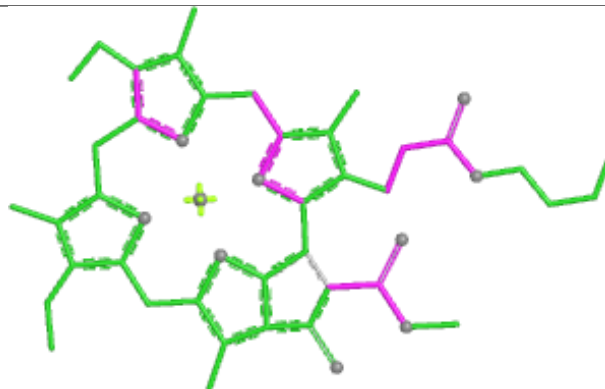




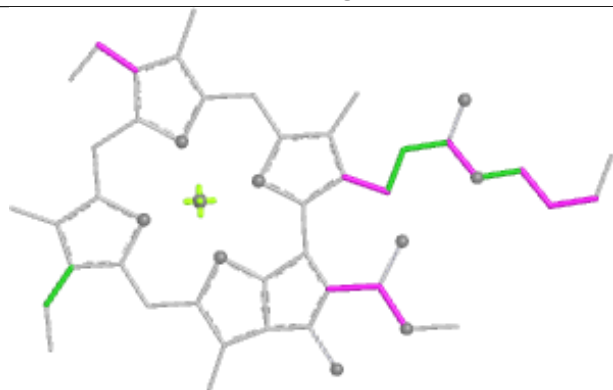
Ligand CLA Y 614



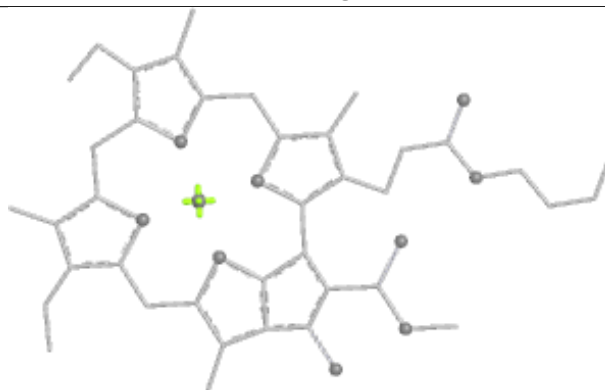
Bond lengths



Bond angles

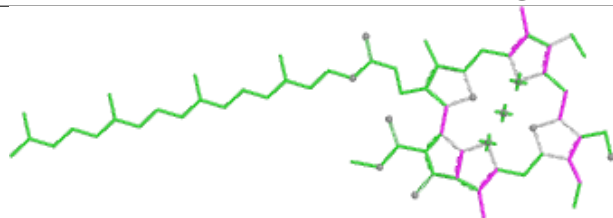


Torsions

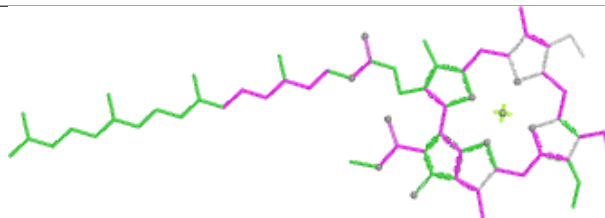


Rings

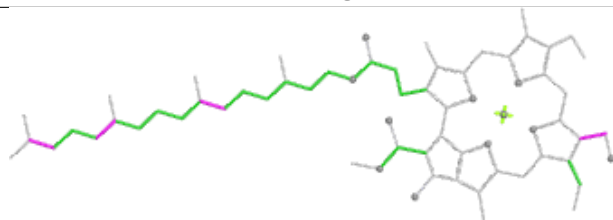
Ligand CHL Y 601



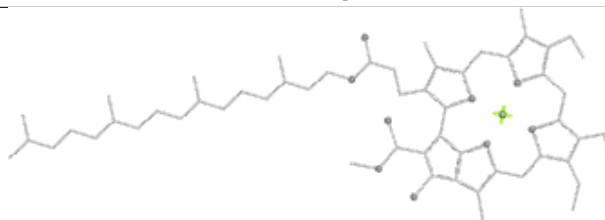
Bond lengths



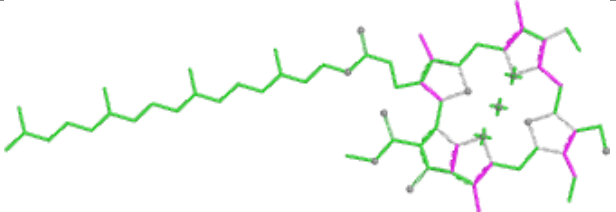
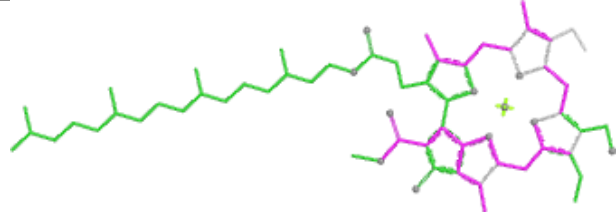
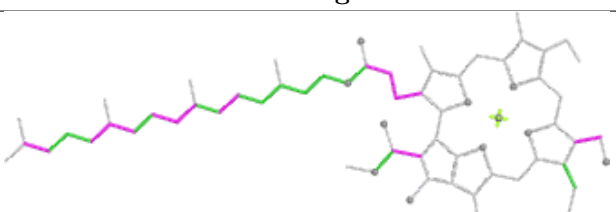
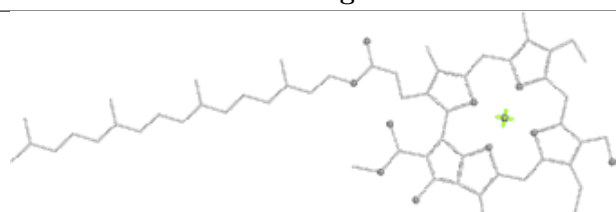
Bond angles

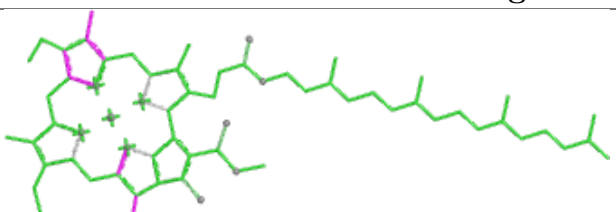
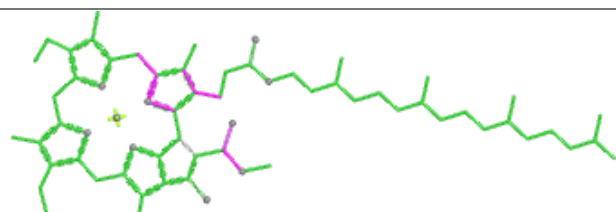
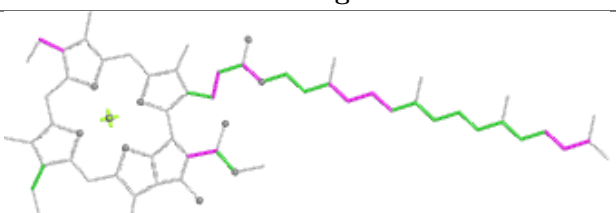
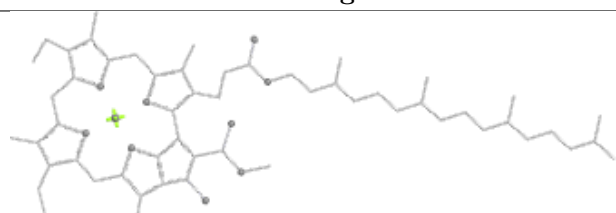


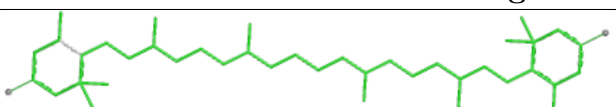
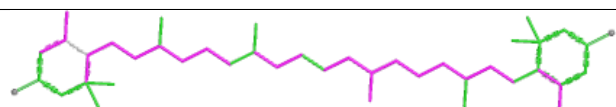
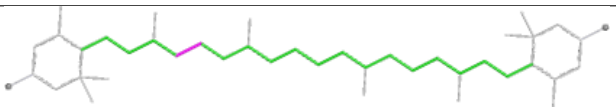
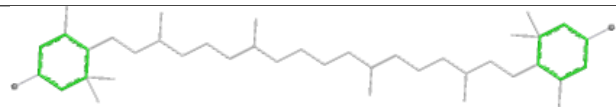
Torsions

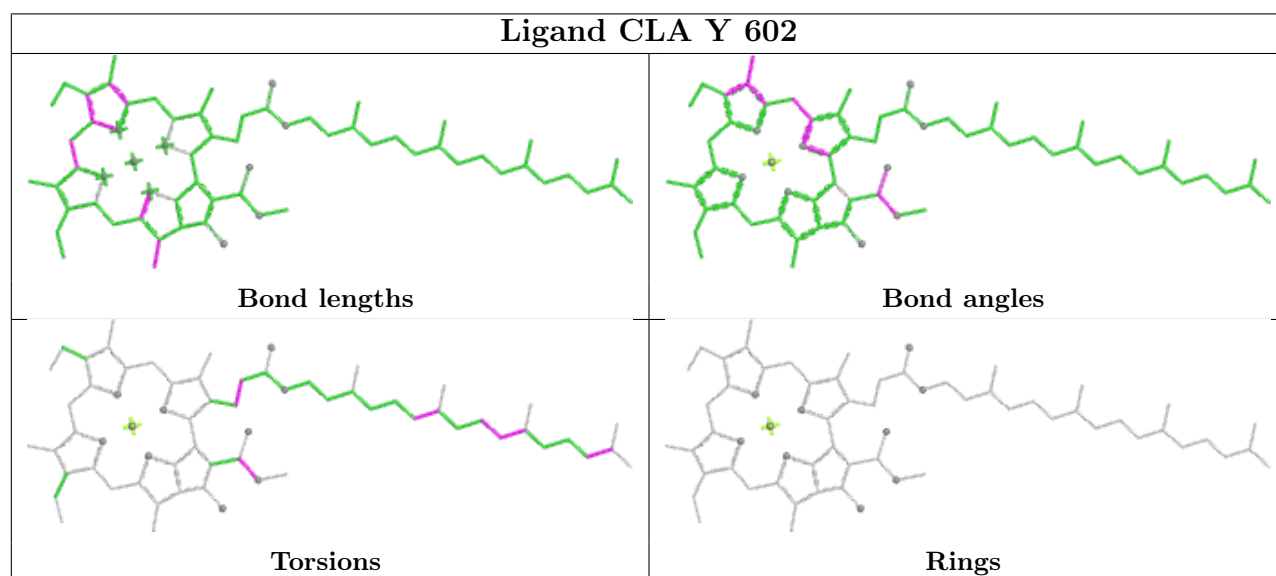
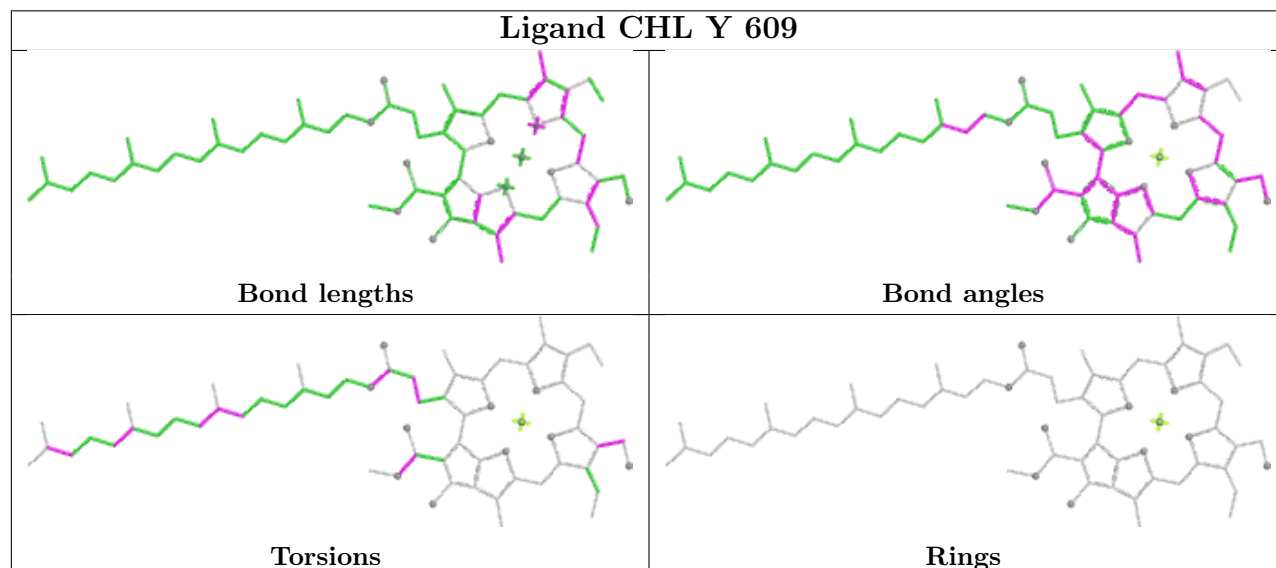
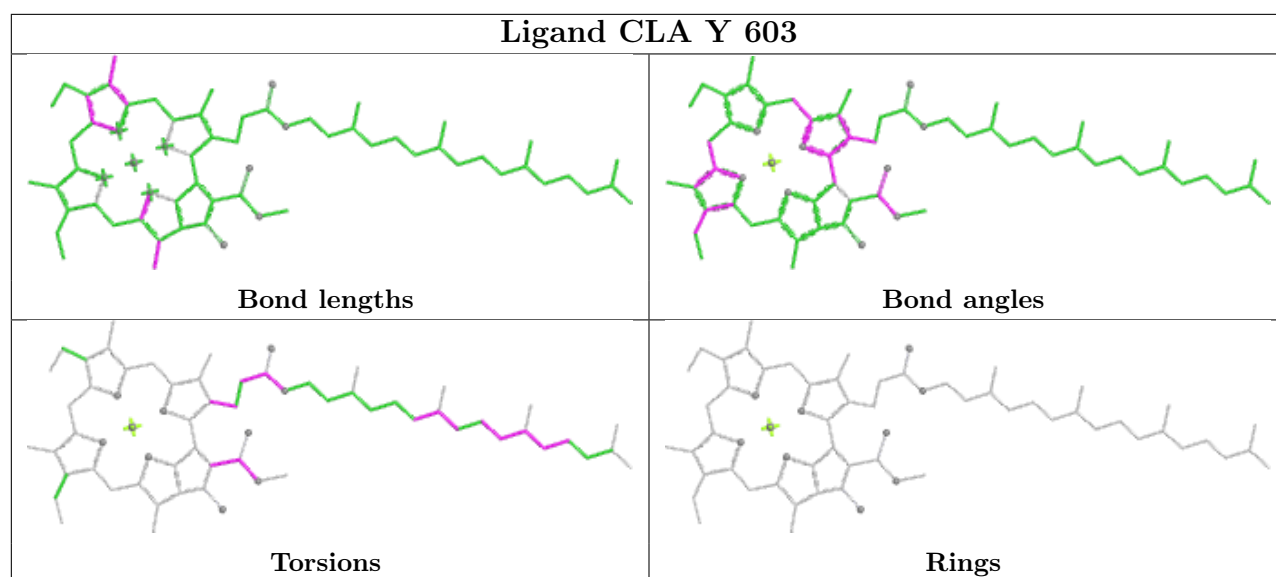


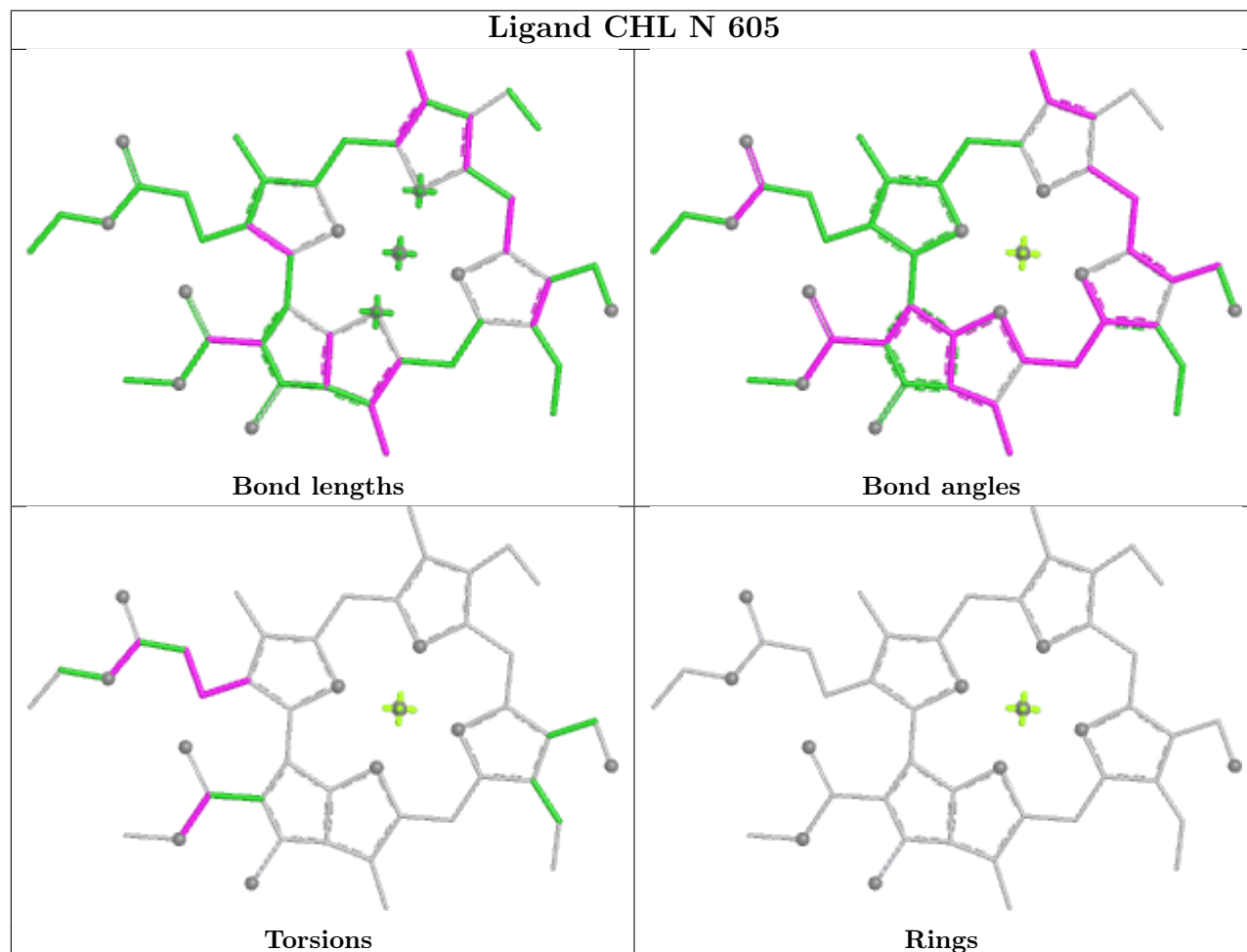
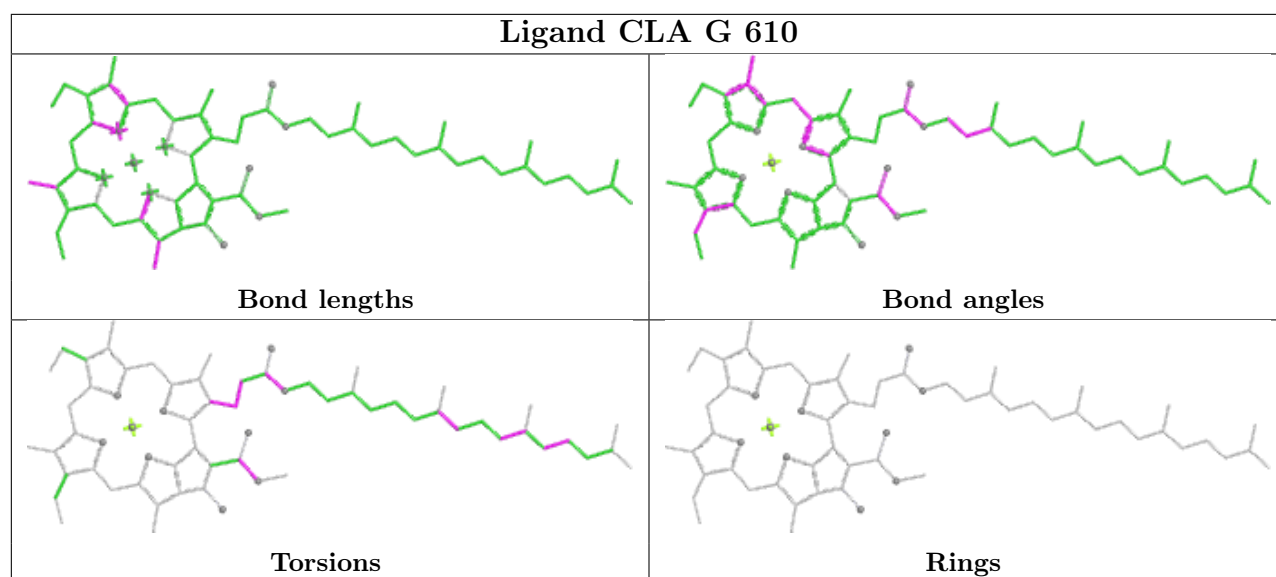
Rings

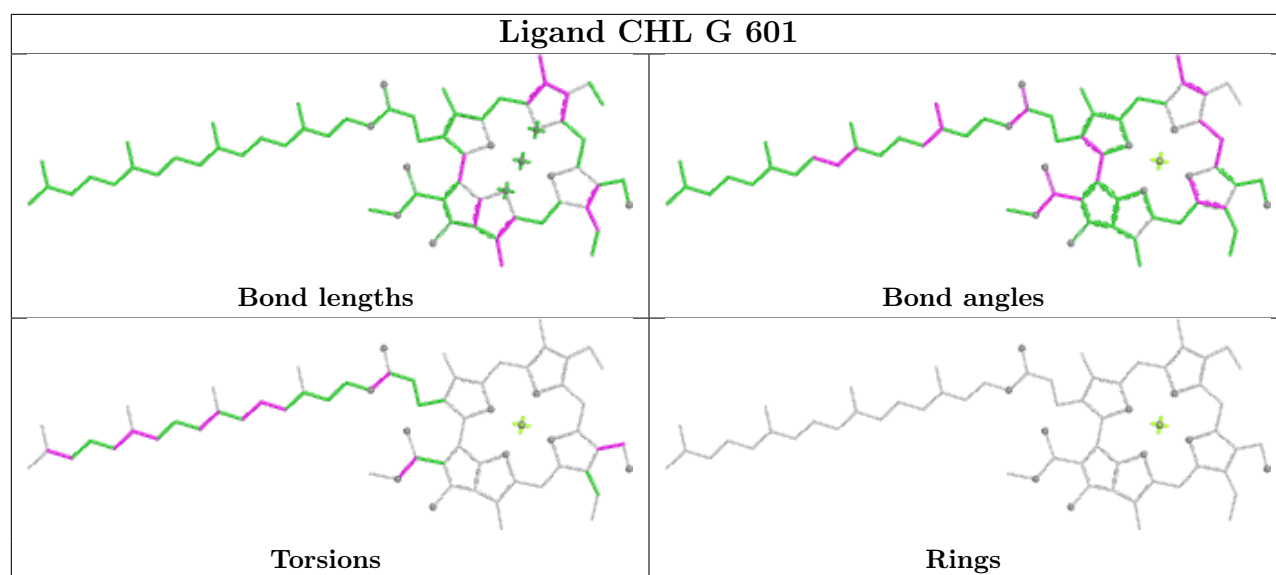
Ligand CHL N 607	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA N 612	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LUT N 616	
	
Bond lengths	Bond angles
	
Torsions	Rings







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.

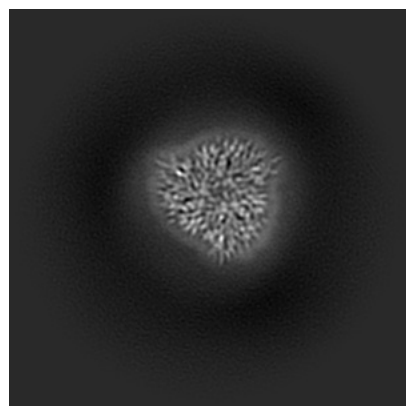
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35783. These allow visual inspection of the internal detail of the map and identification of artifacts.

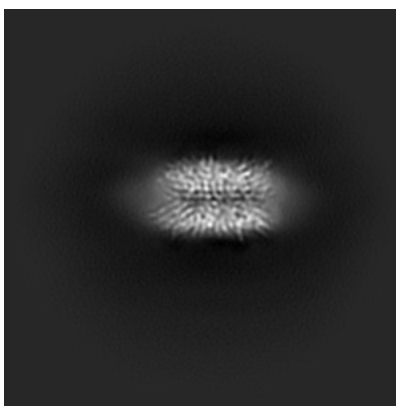
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

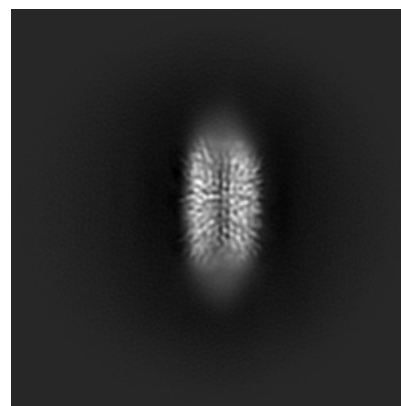
6.1.1 Primary map



X

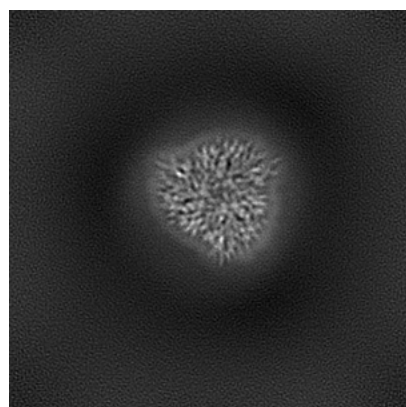


Y

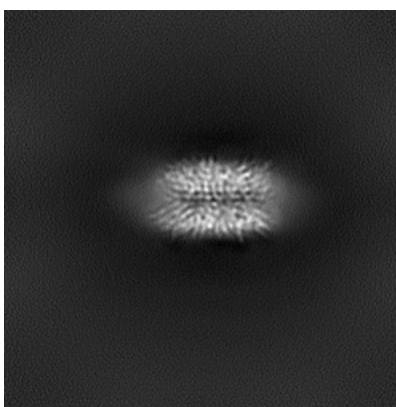


Z

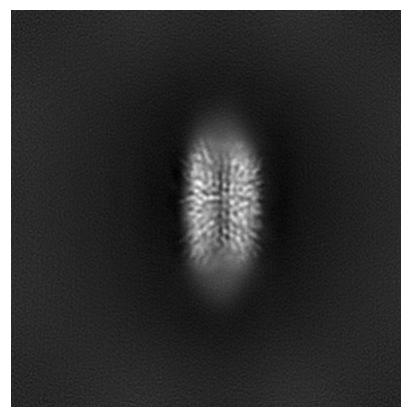
6.1.2 Raw map



X



Y

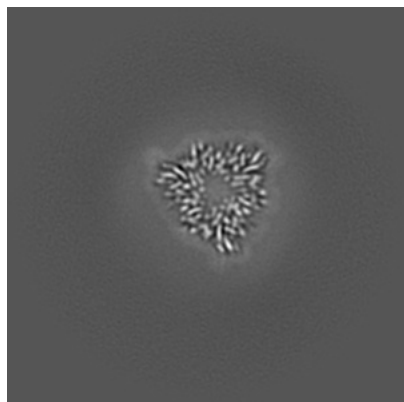


Z

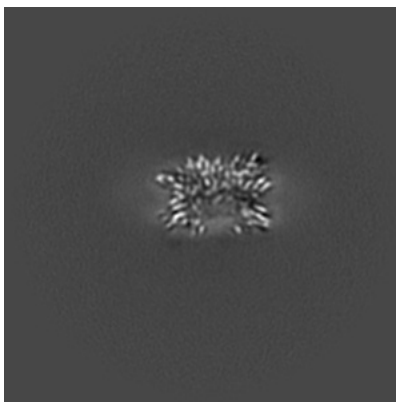
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

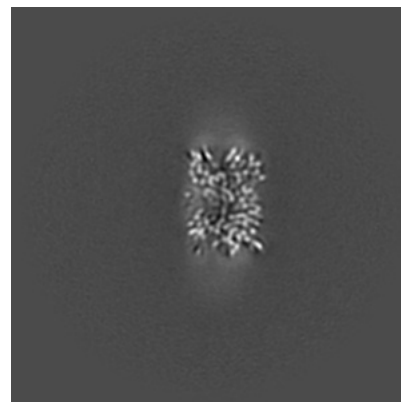
6.2.1 Primary map



X Index: 128

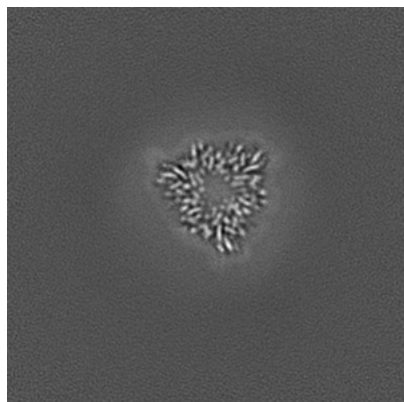


Y Index: 128

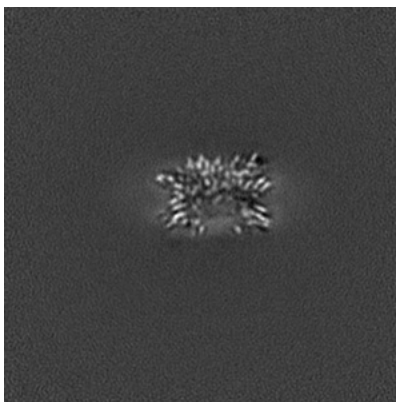


Z Index: 128

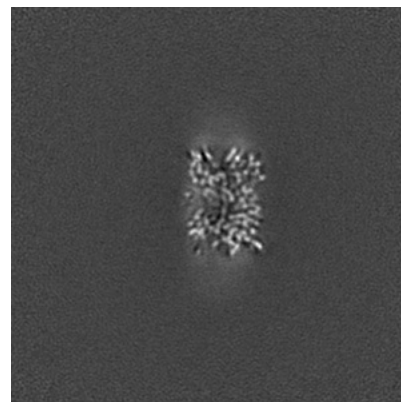
6.2.2 Raw map



X Index: 128



Y Index: 128

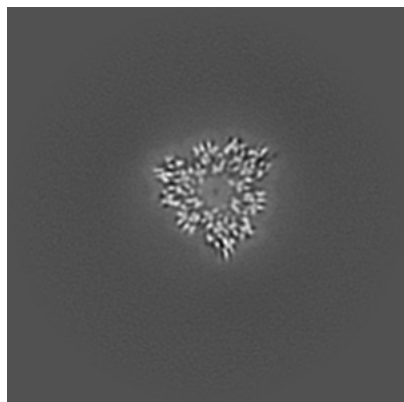


Z Index: 128

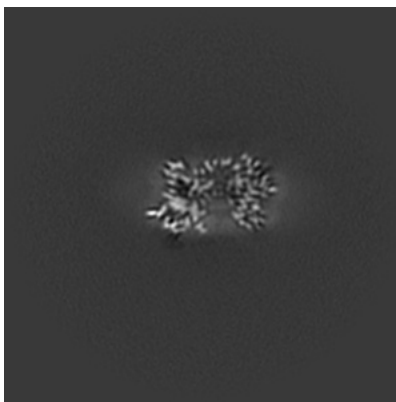
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

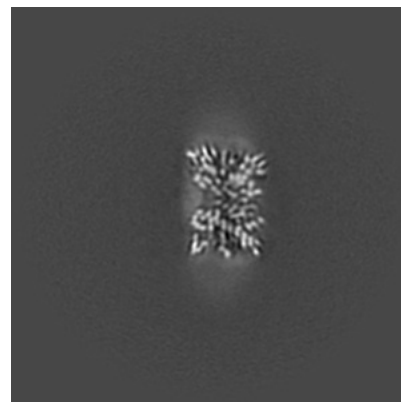
6.3.1 Primary map



X Index: 118

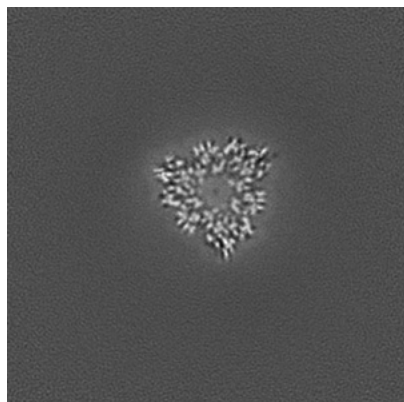


Y Index: 135

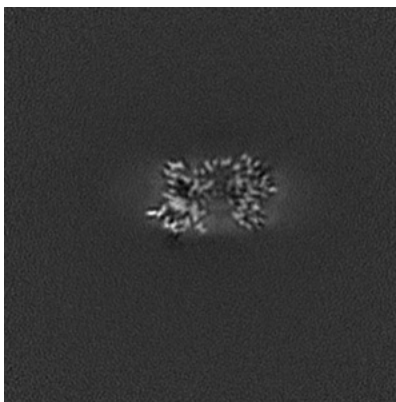


Z Index: 131

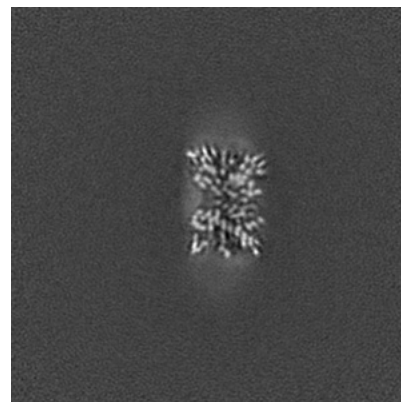
6.3.2 Raw map



X Index: 118



Y Index: 135

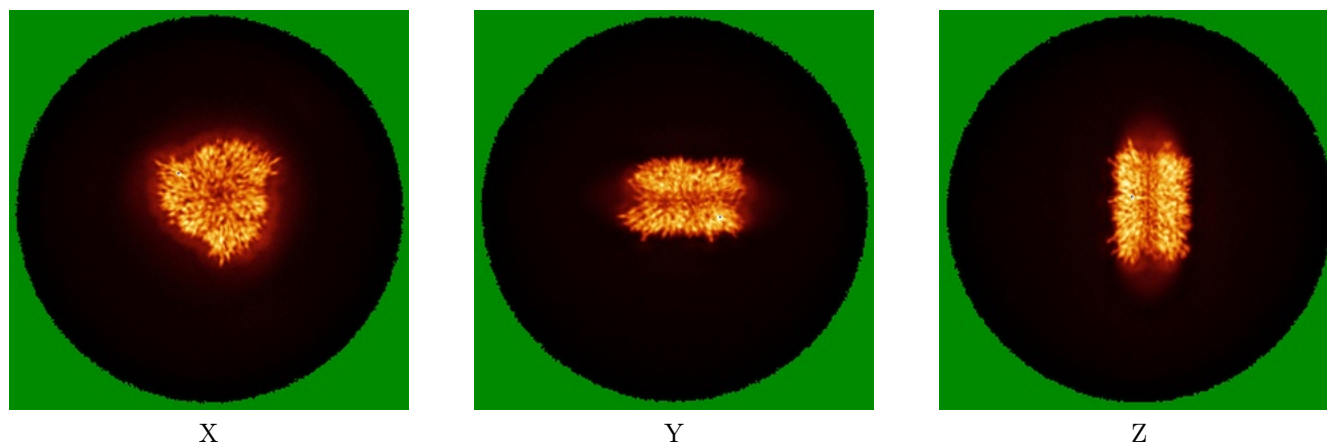


Z Index: 131

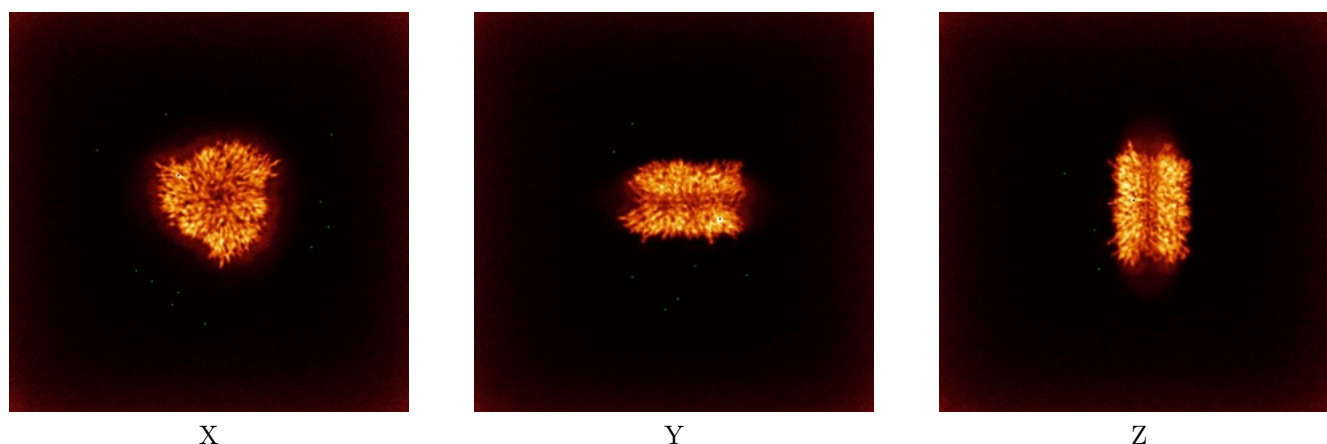
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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

6.5 Orthogonal surface views [i](#)

This section was not generated.

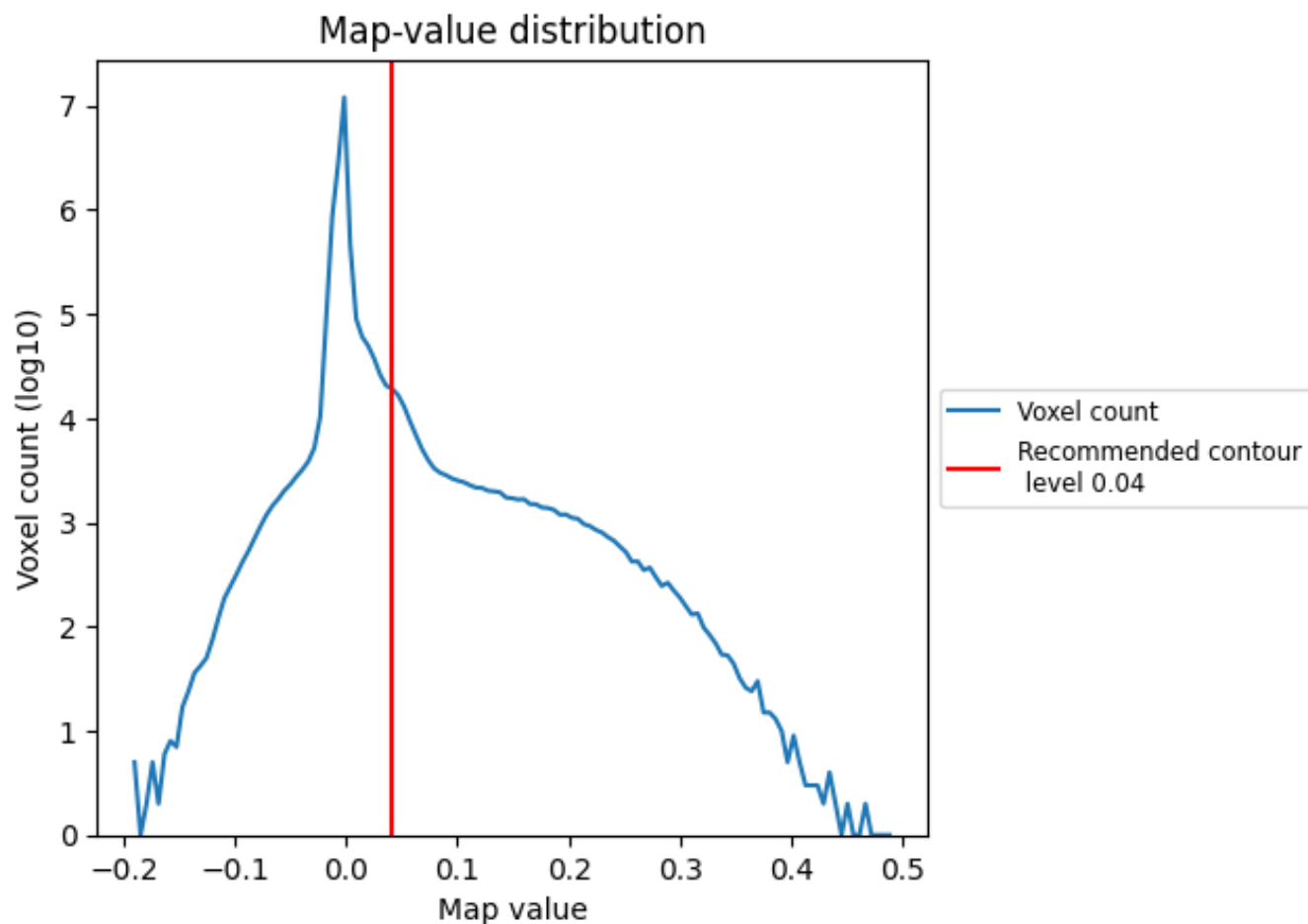
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

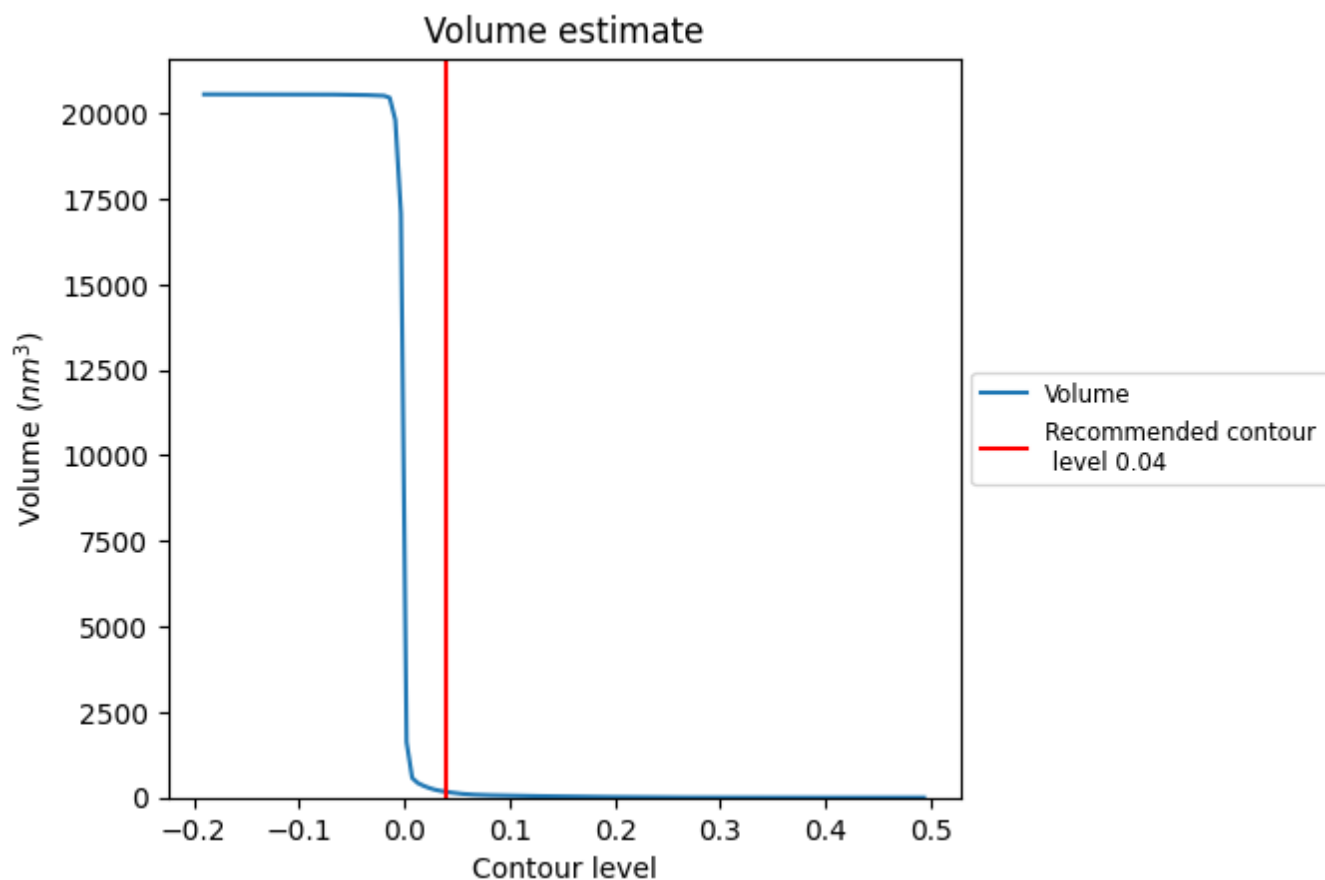
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

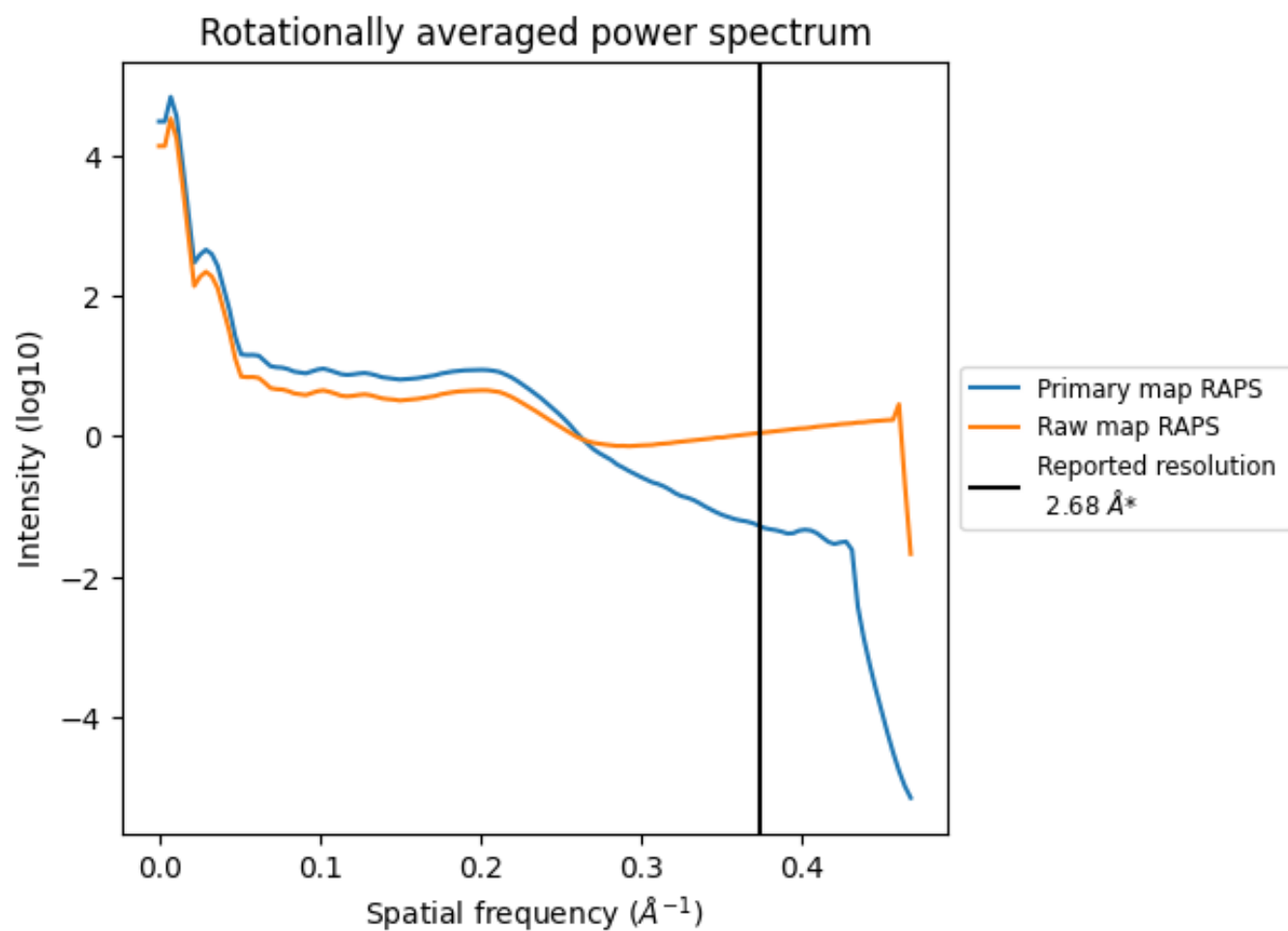
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 167 nm^3 ; this corresponds to an approximate mass of 151 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 ⓘ

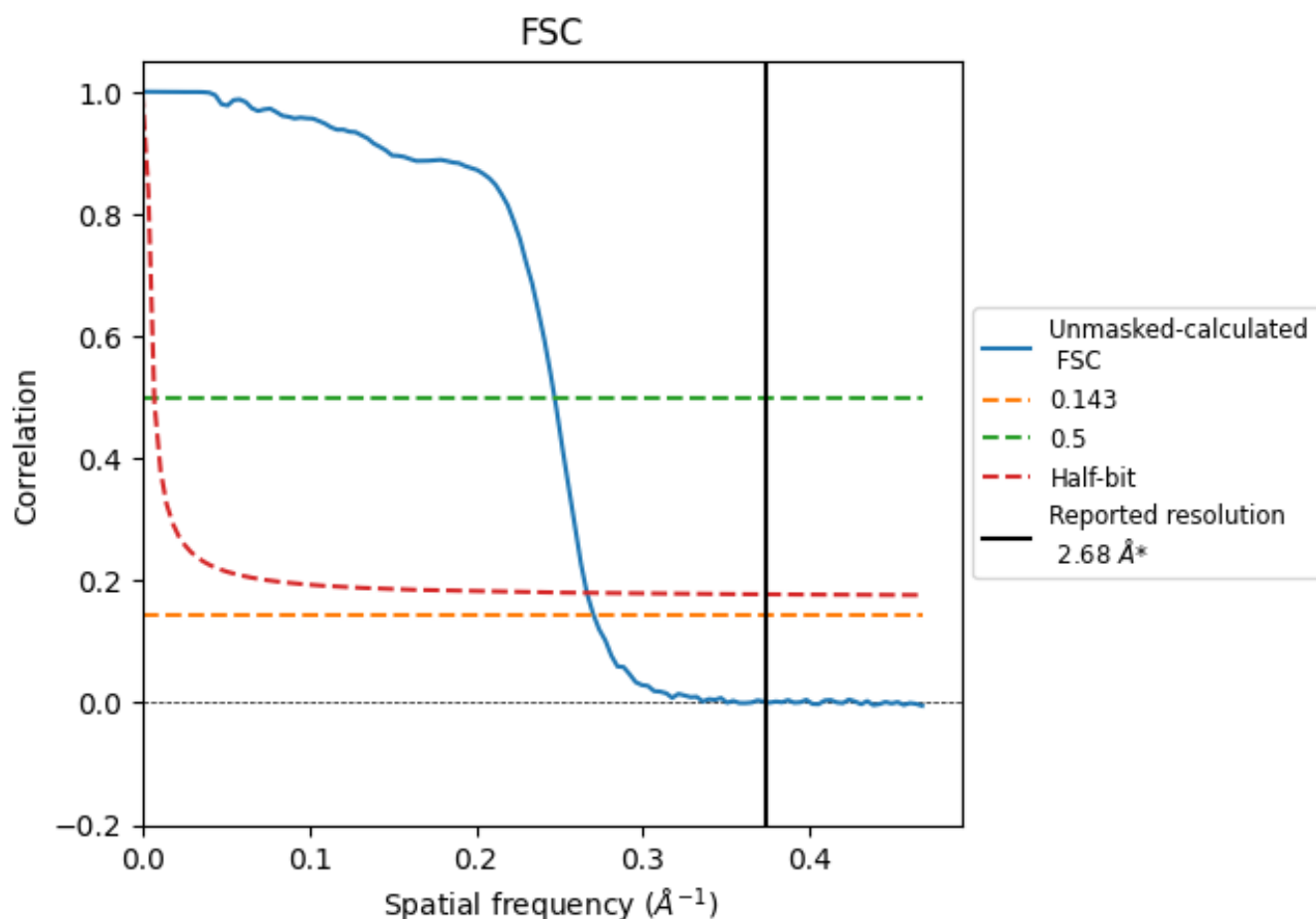


*Reported resolution corresponds to spatial frequency of 0.373 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.373 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.68	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.70	4.05	3.75

*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 3.70 differs from the reported value 2.68 by more than 10 %

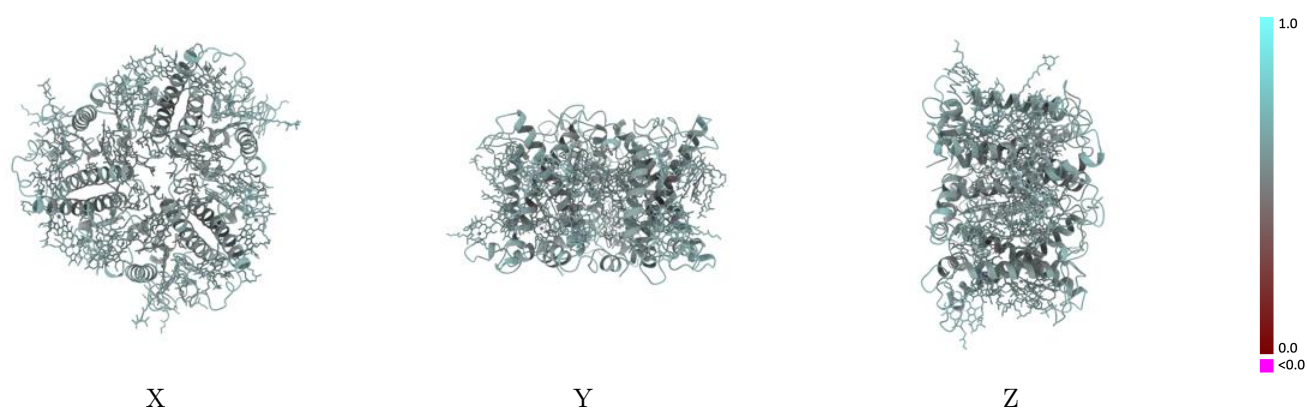
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-35783 and PDB model 8IWY. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)

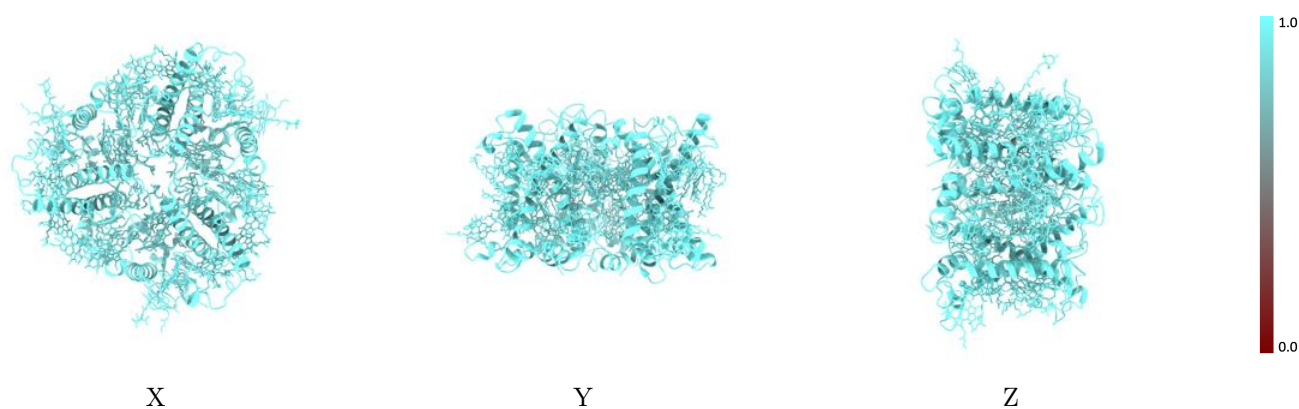
This section was not generated.

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



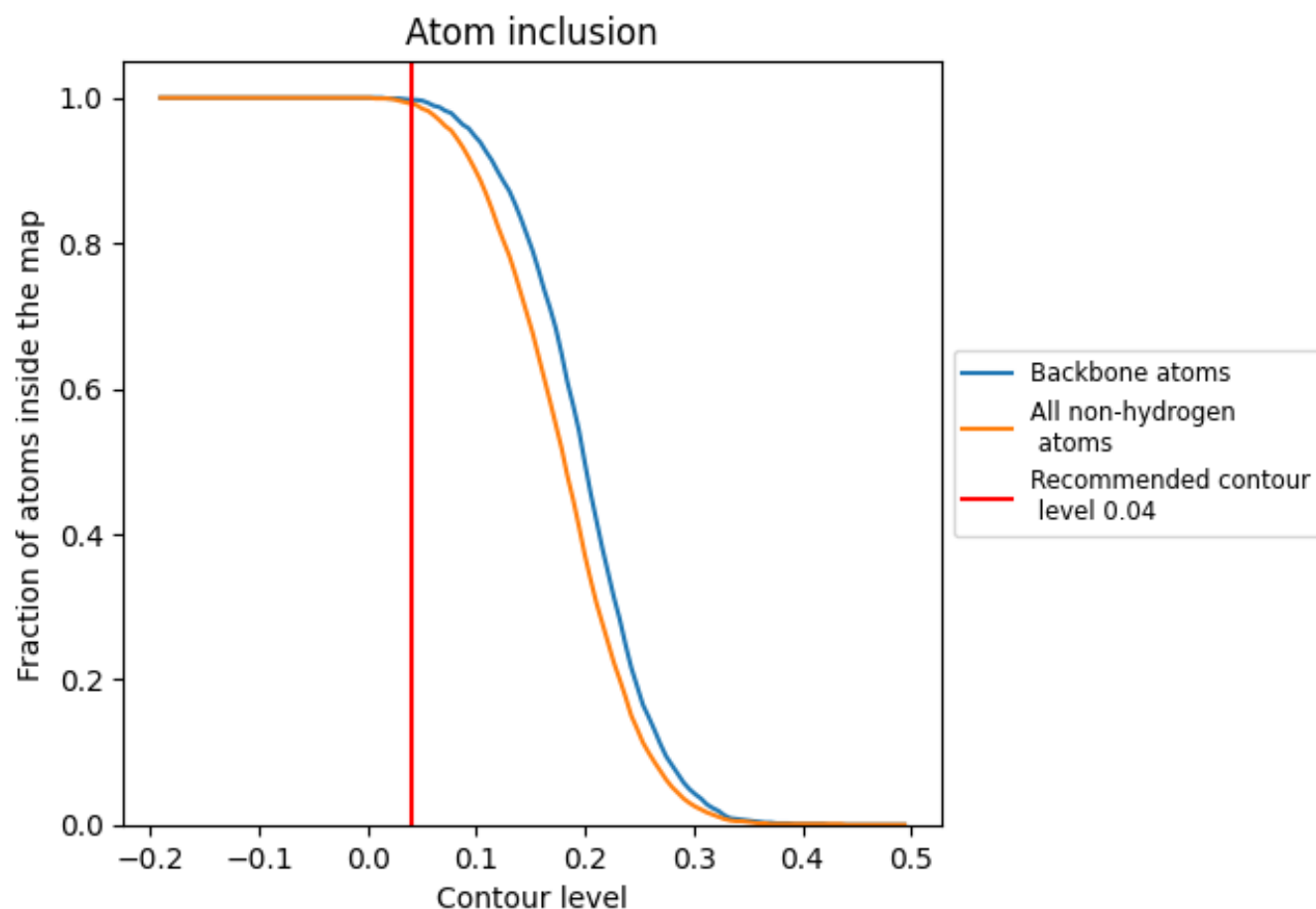
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.04).

9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 99% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9920	0.5720
G	0.9900	0.5730
N	0.9930	0.5710
Y	0.9930	0.5710

