



Full wwPDB EM Validation Report ⓘ

Jun 25, 2025 – 12:24 AM JST

PDB ID : 8IWX / pdb_00008iwx
EMDB ID : EMD-35782
Title : Cryo-EM structure of unprotonated LHCII in detergent solution at high pH value
Authors : Ruan, M.X.; Ding, W.
Deposited on : 2023-03-31
Resolution : 2.59 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.dev118
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

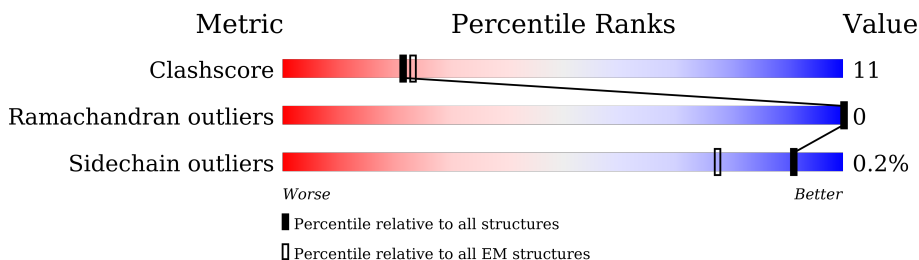
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.59 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	85% 15%
1	N	218	87% 13%
1	Y	218	86% 13%

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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	613	X	-	-	-
3	CLA	Y	614	X	-	-	-

2 Entry composition [i](#)

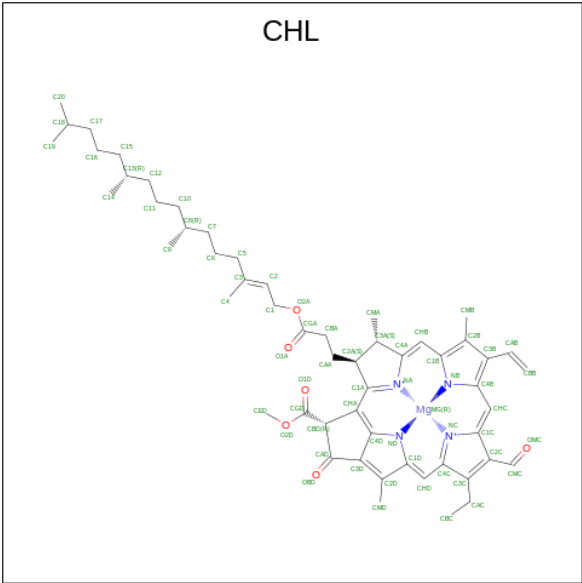
There are 7 unique types of molecules in this entry. The entry contains 8238 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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



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

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

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

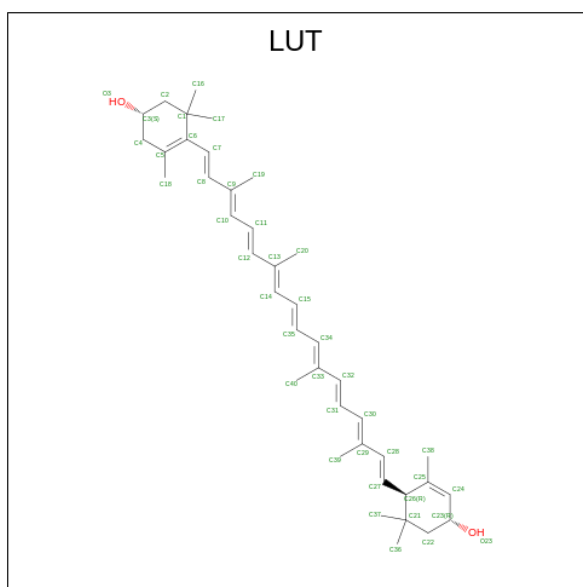


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Mol	Chain	Residues	Atoms					AltConf
3	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	G	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
3	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	Y	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
3	Y	1	Total	C	Mg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

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



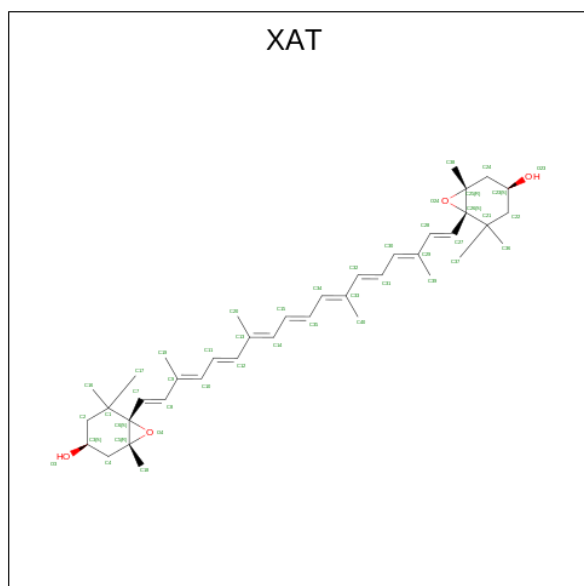
Mol	Chain	Residues	Atoms			AltConf
4	N	1	Total	C	O	0
			42	40	2	

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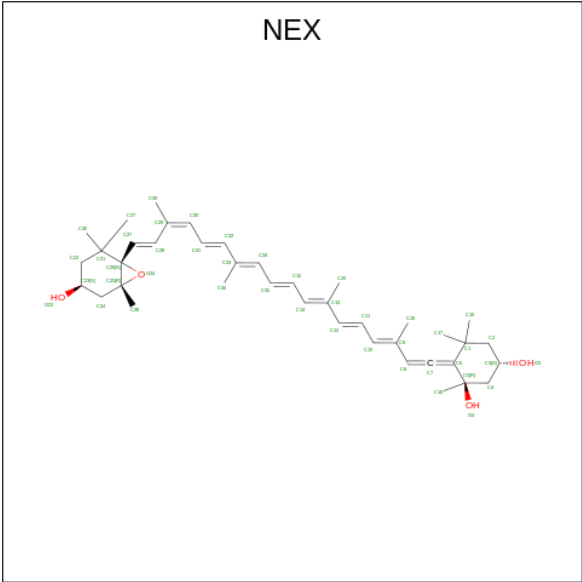
Mol	Chain	Residues	Atoms			AltConf
4	N	1	Total	C	O	0
			42	40	2	
4	G	1	Total	C	O	0
			42	40	2	
4	G	1	Total	C	O	0
			42	40	2	
4	Y	1	Total	C	O	0
			42	40	2	
4	Y	1	Total	C	O	0
			42	40	2	

- Molecule 5 is (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).



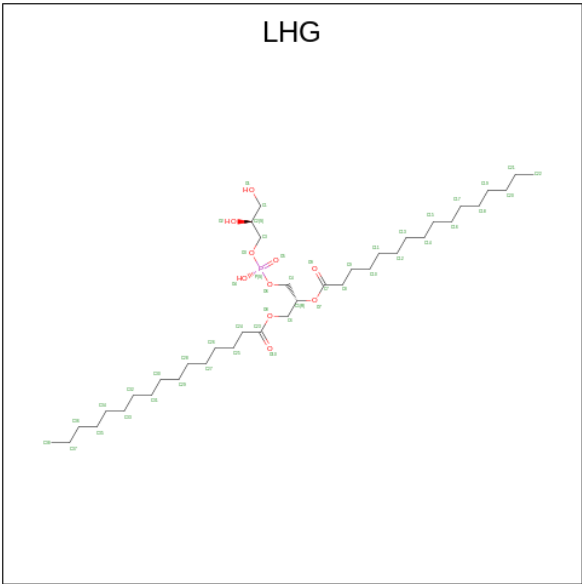
Mol	Chain	Residues	Atoms			AltConf
5	N	1	Total	C	O	0
			44	40	4	
5	N	1	Total	C	O	0
			44	40	4	
5	G	1	Total	C	O	0
			44	40	4	

- 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	N	1	Total	C	O	0
			44	40	4	
6	G	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	N	1	Total 49	C 38	O 10	P 1	0
7	G	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


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

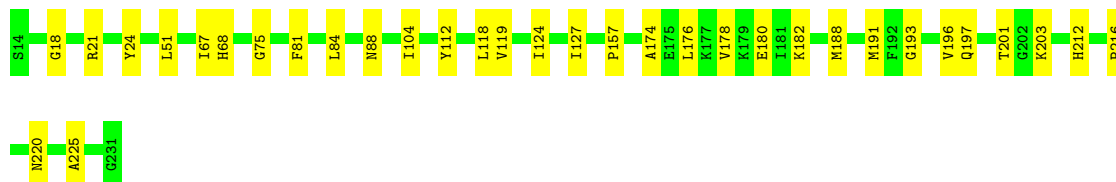
- Molecule 1: Chlorophyll a-b binding protein, chloroplastic

Chain N:  87% 13%




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

Chain G:  85% 15%



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

Chain Y:  86% 13%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	653924	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	0.467	Depositor
Minimum map value	-0.199	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	214.00002, 214.00002, 214.00002	wwPDB
Map dimensions	200, 200, 200	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: CHL, NEX, CLA, LHG, LUT, XAT

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	G	0.28	0/1713	0.55	0/2333
1	N	0.30	0/1713	0.56	0/2333
1	Y	0.29	0/1713	0.55	0/2333
All	All	0.29	0/5139	0.55	0/6999

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	1661	0	1592	28	0
1	N	1661	0	1591	23	0
1	Y	1661	0	1591	27	0
2	G	363	0	350	21	0
2	N	363	0	350	21	0
2	Y	363	0	350	22	0
3	G	501	0	534	22	0
3	N	501	0	534	15	0
3	Y	501	0	534	29	0
4	G	84	0	112	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	N	84	0	112	9	0
4	Y	84	0	112	13	0
5	G	44	0	56	9	0
5	N	88	0	112	11	0
6	G	44	0	56	1	0
6	N	44	0	56	0	0
6	Y	44	0	56	2	0
7	G	49	0	74	3	0
7	N	49	0	74	3	0
7	Y	49	0	74	8	0
All	All	8238	0	8320	190	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (190) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:602:CLA:HAB	4:N:616:LUT:H32	1.55	0.87
1:Y:191:MET:HE2	4:Y:616:LUT:H10	1.62	0.81
3:Y:602:CLA:HAB	4:Y:616:LUT:H32	1.64	0.80
2:G:601:CHL:HAC1	7:G:618:LHG:HC12	1.64	0.77
5:N:617:XAT:H242	2:Y:601:CHL:HMC	1.68	0.74
2:N:601:CHL:HMC	5:N:620:XAT:H242	1.73	0.70
1:G:212:HIS:HD1	3:G:613:CLA:HAA2	1.58	0.68
3:N:610:CLA:H52	4:N:615:LUT:H30	1.76	0.66
1:G:112:TYR:HB2	1:G:119:VAL:HG22	1.79	0.63
3:Y:613:CLA:H8	3:Y:614:CLA:HMD3	1.78	0.63
1:N:112:TYR:HB2	1:N:119:VAL:HG22	1.80	0.61
3:G:602:CLA:H52	4:G:616:LUT:H28	1.82	0.61
2:N:609:CHL:HMC	2:Y:601:CHL:H72	1.83	0.60
1:N:102:SER:HB2	2:N:607:CHL:HED2	1.81	0.60
3:Y:610:CLA:H52	4:Y:615:LUT:H30	1.83	0.60
1:G:84:LEU:O	1:G:88:ASN:ND2	2.34	0.60
1:G:201:THR:HG22	1:G:203:LYS:HG3	1.82	0.60
7:N:619:LHG:HC91	7:N:619:LHG:H282	1.85	0.59
3:G:610:CLA:H52	4:G:615:LUT:H30	1.86	0.58
1:Y:112:TYR:HB2	1:Y:119:VAL:HG22	1.85	0.58
1:Y:161:PHE:HD1	2:Y:608:CHL:H61	1.67	0.58
1:G:24:TYR:HD2	2:G:601:CHL:HAA2	1.68	0.58
1:Y:197:GLN:O	1:Y:201:THR:OG1	2.22	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:112:TYR:HD2	1:N:118:LEU:HD23	1.69	0.57
1:G:178:VAL:O	1:G:182:LYS:HG3	2.04	0.57
2:Y:608:CHL:HAA2	2:Y:608:CHL:H171	1.86	0.57
2:G:607:CHL:H18	2:G:609:CHL:H52	1.86	0.57
7:G:618:LHG:H281	7:G:618:LHG:HC91	1.87	0.56
1:Y:112:TYR:HB3	1:Y:118:LEU:HB3	1.86	0.56
3:Y:611:CLA:H121	3:Y:612:CLA:HBB1	1.87	0.56
2:N:601:CHL:H72	2:G:609:CHL:HMC	1.86	0.56
3:Y:602:CLA:H52	4:Y:616:LUT:H28	1.88	0.55
2:G:601:CHL:H8	5:G:619:XAT:H14	1.88	0.55
2:G:601:CHL:HMC	5:G:619:XAT:H242	1.87	0.55
2:N:606:CHL:HBC2	2:N:607:CHL:HHD	1.89	0.55
1:N:70:ARG:NH1	2:N:608:CHL:OBD	2.40	0.54
1:G:157:PRO:HB3	2:G:608:CHL:HBC2	1.90	0.54
1:G:51:LEU:HD13	3:G:602:CLA:H42	1.89	0.53
1:G:75:GLY:HA2	4:G:616:LUT:H181	1.89	0.53
3:G:604:CLA:O2A	6:G:617:NEX:H241	2.08	0.53
1:Y:51:LEU:HD13	3:Y:602:CLA:H42	1.90	0.53
2:G:608:CHL:HHC	2:G:608:CHL:HBB1	1.91	0.52
3:Y:613:CLA:H151	3:Y:614:CLA:HBA2	1.92	0.52
3:G:610:CLA:HBB1	4:G:615:LUT:H32	1.91	0.52
1:Y:41:PRO:HG2	1:Y:177:LYS:HD2	1.91	0.52
2:Y:606:CHL:HMB1	2:Y:609:CHL:HMC	1.92	0.52
2:N:607:CHL:H18	2:N:609:CHL:H52	1.92	0.51
1:N:115:ASN:HD22	1:N:118:LEU:HD13	1.75	0.51
3:N:613:CLA:H141	3:N:614:CLA:H2	1.91	0.51
1:Y:139:GLU:OE1	1:Y:142:ARG:NH2	2.43	0.51
2:G:607:CHL:H12	2:G:607:CHL:HMA2	1.93	0.51
2:N:608:CHL:H3A	2:N:608:CHL:H151	1.92	0.51
2:N:601:CHL:HHB	2:G:609:CHL:HMB2	1.93	0.50
1:G:188:MET:HE1	3:G:602:CLA:HBB1	1.91	0.50
1:Y:73:MET:HE1	3:Y:610:CLA:HHC	1.93	0.50
1:Y:75:GLY:HA2	4:Y:616:LUT:H181	1.94	0.49
1:N:157:PRO:HB3	2:N:608:CHL:HBC2	1.94	0.49
1:G:104:ILE:HG21	1:G:124:ILE:HD13	1.94	0.49
3:G:610:CLA:CBB	4:G:615:LUT:H32	2.43	0.49
3:N:610:CLA:CBB	4:N:615:LUT:H32	2.42	0.49
2:Y:608:CHL:H11	3:Y:610:CLA:HMD2	1.95	0.49
1:N:134:LEU:HD21	2:N:606:CHL:H43	1.94	0.49
2:N:609:CHL:HMB2	2:Y:601:CHL:HHB	1.95	0.48
1:Y:134:LEU:HD23	6:Y:617:NEX:C14	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:112:TYR:HB3	1:N:118:LEU:HB3	1.95	0.48
1:N:176:LEU:HD23	1:N:179:LYS:HD2	1.95	0.48
5:N:617:XAT:H12	2:Y:601:CHL:H111	1.95	0.48
2:Y:606:CHL:HBC2	2:Y:607:CHL:HHD	1.95	0.48
3:Y:611:CLA:H102	3:Y:611:CLA:H62	1.35	0.48
3:Y:603:CLA:H102	2:Y:609:CHL:H143	1.96	0.48
3:Y:610:CLA:H2	4:Y:615:LUT:H28	1.96	0.48
3:Y:603:CLA:HBB1	2:Y:609:CHL:H122	1.95	0.47
1:G:191:MET:HE2	4:G:616:LUT:H10	1.96	0.47
1:Y:212:HIS:ND1	3:Y:613:CLA:HAA2	2.30	0.47
1:Y:180:GLU:HB2	3:Y:610:CLA:C1B	2.45	0.47
1:G:216:PRO:O	1:G:220:ASN:ND2	2.47	0.47
2:G:606:CHL:HBC2	2:G:607:CHL:HHD	1.97	0.47
1:G:112:TYR:HB3	1:G:118:LEU:HB3	1.96	0.47
2:Y:609:CHL:HBB1	2:Y:609:CHL:HHC	1.97	0.47
1:Y:182:LYS:HB3	3:Y:611:CLA:HMD2	1.96	0.47
7:Y:618:LHG:H172	7:Y:618:LHG:H201	1.54	0.47
1:G:196:VAL:HG11	3:G:613:CLA:HAC2	1.97	0.46
2:N:601:CHL:HBA1	2:N:601:CHL:H3A	1.64	0.46
3:N:611:CLA:H91	3:N:611:CLA:H112	1.60	0.46
1:G:176:LEU:HB3	3:G:610:CLA:HHB	1.96	0.46
1:G:212:HIS:CD2	3:G:614:CLA:NB	2.84	0.46
1:N:18:GLY:O	1:N:21:ARG:NH1	2.39	0.46
3:N:613:CLA:H2	3:N:613:CLA:H61	1.49	0.46
3:N:613:CLA:H93	7:N:619:LHG:H131	1.97	0.46
2:N:609:CHL:CMB	2:Y:601:CHL:HHB	2.46	0.46
3:N:611:CLA:H101	3:N:611:CLA:H62	1.40	0.46
1:G:180:GLU:HG3	3:G:610:CLA:C4B	2.45	0.46
1:N:181:ILE:HG21	1:N:185:ARG:HH21	1.80	0.46
5:N:617:XAT:H35	5:N:617:XAT:H401	1.76	0.46
1:Y:134:LEU:HD23	6:Y:617:NEX:C15	2.45	0.46
3:Y:610:CLA:H61	4:Y:615:LUT:H371	1.97	0.46
5:N:620:XAT:H401	5:N:620:XAT:H35	1.73	0.45
1:G:68:HIS:HB3	1:G:188:MET:SD	2.55	0.45
2:N:608:CHL:H11	3:N:610:CLA:HMD2	1.99	0.45
1:G:81:PHE:HD2	3:G:604:CLA:HHD	1.81	0.45
1:Y:167:ALA:HB1	1:Y:173:PHE:CD2	2.51	0.45
2:G:601:CHL:H111	5:G:619:XAT:H12	1.98	0.45
1:N:175:GLU:O	1:N:179:LYS:HG3	2.16	0.45
1:G:18:GLY:O	1:G:21:ARG:NH1	2.42	0.45
4:Y:616:LUT:H11	4:Y:616:LUT:H191	1.86	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:619:XAT:H35	5:G:619:XAT:H401	1.78	0.45
3:N:610:CLA:H2	4:N:615:LUT:H28	1.99	0.45
1:G:193:GLY:O	1:G:197:GLN:HG3	2.17	0.45
3:Y:611:CLA:HMA3	7:Y:618:LHG:HC32	1.99	0.45
4:G:616:LUT:H15	4:G:616:LUT:H201	1.77	0.45
2:N:606:CHL:HBA2	2:N:606:CHL:H12	1.84	0.45
1:N:182:LYS:HB3	3:N:611:CLA:HMD1	1.99	0.44
2:Y:607:CHL:H92	2:Y:609:CHL:H18	1.99	0.44
1:N:161:PHE:HA	2:N:608:CHL:H72	1.99	0.44
1:Y:115:ASN:HB3	1:Y:118:LEU:HB2	1.99	0.44
2:Y:607:CHL:H12	2:Y:607:CHL:HMA2	1.99	0.44
3:Y:611:CLA:H71	3:Y:612:CLA:ND	2.33	0.44
3:N:604:CLA:H61	3:N:604:CLA:H101	1.81	0.44
1:G:118:LEU:HG	3:G:604:CLA:H102	2.00	0.44
3:N:603:CLA:H72	3:N:603:CLA:H112	1.80	0.44
3:G:611:CLA:H143	3:G:611:CLA:H111	1.83	0.44
1:Y:185:ARG:HB3	7:Y:618:LHG:H252	2.00	0.44
1:N:59:ALA:HA	1:N:62:ARG:CZ	2.48	0.44
1:Y:70:ARG:HG2	3:Y:610:CLA:C3C	2.48	0.44
4:N:616:LUT:H35	4:N:616:LUT:H401	1.83	0.44
1:G:127:ILE:HG12	2:G:605:CHL:HAC1	2.00	0.43
3:G:611:CLA:HBB1	5:G:619:XAT:H221	1.99	0.43
1:Y:52:SER:HB3	1:Y:58:PHE:HD1	1.81	0.43
1:N:178:VAL:HG12	1:N:182:LYS:HE2	1.99	0.43
3:Y:613:CLA:H112	7:Y:618:LHG:H342	1.99	0.43
2:Y:608:CHL:H151	2:Y:608:CHL:H3A	2.00	0.43
1:N:56:GLU:O	1:N:60:LYS:HG2	2.19	0.43
5:N:617:XAT:H10	2:Y:601:CHL:H13	2.00	0.43
5:G:619:XAT:H15	5:G:619:XAT:H201	1.71	0.43
1:Y:110:LEU:HB3	1:Y:121:ALA:HB3	2.00	0.43
2:Y:608:CHL:H201	3:Y:610:CLA:H141	2.00	0.43
2:N:609:CHL:HHC	2:Y:601:CHL:H52	2.01	0.43
7:N:619:LHG:H282	7:N:619:LHG:H312	1.80	0.43
3:G:613:CLA:H61	3:G:613:CLA:H2	1.66	0.43
1:Y:112:TYR:HE2	3:Y:604:CLA:H143	1.84	0.43
4:Y:615:LUT:H31	4:Y:615:LUT:H391	1.92	0.43
3:Y:603:CLA:HBB2	2:Y:609:CHL:H202	2.00	0.43
1:N:139:GLU:HG3	1:N:142:ARG:HH21	1.83	0.43
2:G:601:CHL:H51	5:G:619:XAT:H401	2.00	0.43
4:N:615:LUT:H35	4:N:615:LUT:H401	1.82	0.43
1:Y:118:LEU:HD21	3:Y:604:CLA:H161	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Y:618:LHG:H332	7:Y:618:LHG:H301	1.41	0.43
5:N:617:XAT:H31	5:N:617:XAT:H391	1.86	0.42
2:G:607:CHL:H143	2:G:607:CHL:H111	1.80	0.42
3:Y:611:CLA:H142	3:Y:611:CLA:H111	1.55	0.42
4:Y:616:LUT:H201	4:Y:616:LUT:H15	1.80	0.42
1:N:174:ALA:O	1:N:178:VAL:HG23	2.19	0.42
2:G:601:CHL:C3C	5:G:619:XAT:H362	2.50	0.42
3:Y:603:CLA:H61	3:Y:603:CLA:H2	1.79	0.42
1:G:174:ALA:O	1:G:178:VAL:HG23	2.20	0.42
1:G:225:ALA:HB3	1:Y:105:PHE:HE2	1.85	0.42
2:G:601:CHL:H141	2:G:601:CHL:H162	1.73	0.42
4:Y:615:LUT:H11	4:Y:615:LUT:H191	1.87	0.42
7:Y:618:LHG:H332	7:Y:618:LHG:HC91	2.02	0.42
2:G:607:CHL:H93	2:G:607:CHL:H61	1.83	0.42
4:G:616:LUT:H35	4:G:616:LUT:H401	1.90	0.42
2:G:601:CHL:HMA1	5:G:619:XAT:H403	2.01	0.41
1:N:75:GLY:HA2	4:N:616:LUT:H181	2.02	0.41
2:G:601:CHL:H161	2:G:601:CHL:H202	1.82	0.41
2:G:601:CHL:H13	7:G:618:LHG:H211	2.02	0.41
5:N:620:XAT:H201	5:N:620:XAT:H15	1.67	0.41
3:Y:610:CLA:CBB	4:Y:615:LUT:H32	2.51	0.41
1:N:191:MET:HE2	4:N:616:LUT:H10	2.03	0.41
1:Y:180:GLU:HB2	3:Y:610:CLA:C2B	2.51	0.41
2:N:608:CHL:H162	2:N:608:CHL:H122	1.70	0.41
4:N:616:LUT:H11	4:N:616:LUT:H191	1.87	0.41
3:G:602:CLA:H93	3:G:602:CLA:H111	1.92	0.41
1:N:185:ARG:HH11	3:N:602:CLA:C1D	2.34	0.41
5:N:617:XAT:H28	7:Y:618:LHG:H362	2.02	0.41
5:N:617:XAT:H14	2:Y:601:CHL:H8	2.02	0.41
1:G:67:ILE:HD13	1:G:67:ILE:HA	1.91	0.41
1:Y:17:TYR:HE2	1:Y:174:ALA:HB1	1.86	0.41
2:Y:601:CHL:HBA1	2:Y:601:CHL:H3A	1.71	0.41
1:N:85:LEU:HD23	1:N:85:LEU:HA	1.91	0.40
3:G:610:CLA:H2	4:G:615:LUT:H28	2.02	0.40
7:Y:618:LHG:H271	7:Y:618:LHG:HC62	2.02	0.40
2:N:607:CHL:H12	2:N:607:CHL:HMA2	2.01	0.40
5:N:617:XAT:H15	5:N:617:XAT:H201	1.71	0.40
1:G:112:TYR:HD2	1:G:118:LEU:HD23	1.85	0.40
3:G:602:CLA:H161	3:G:602:CLA:H141	1.84	0.40
1:Y:17:TYR:CE2	1:Y:174:ALA:HB1	2.56	0.40
3:N:603:CLA:H91	2:N:609:CHL:H143	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:610:CLA:H61	4:G:615:LUT:H371	2.03	0.40
3:G:613:CLA:H2A	3:G:613:CLA:HED3	2.02	0.40
4:Y:616:LUT:H31	4:Y:616:LUT:H391	1.93	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	216/218 (99%)	210 (97%)	6 (3%)	0	100	100
1	N	216/218 (99%)	211 (98%)	5 (2%)	0	100	100
1	Y	216/218 (99%)	209 (97%)	7 (3%)	0	100	100
All	All	648/654 (99%)	630 (97%)	18 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	168/168 (100%)	168 (100%)	0	100	100
1	N	168/168 (100%)	168 (100%)	0	100	100
1	Y	168/168 (100%)	167 (99%)	1 (1%)	84	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	504/504 (100%)	503 (100%)	1 (0%)	91	98

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

Mol	Chain	Res	Type
1	Y	182	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	N	115	ASN
1	G	183	ASN
1	Y	131	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

57 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	LUT	G	616	-	42,43,43	0.75	0	51,60,60	1.74	11 (21%)
6	NEX	Y	617	-	38,46,46	1.58	7 (18%)	50,70,70	1.60	10 (20%)
3	CLA	Y	610	1	65,73,73	1.51	8 (12%)	76,113,113	1.24	8 (10%)
3	CLA	Y	612	1	65,73,73	1.50	9 (13%)	76,113,113	1.18	7 (9%)
3	CLA	G	614	-	49,57,73	1.80	7 (14%)	55,93,113	1.35	7 (12%)
4	LUT	N	616	-	42,43,43	0.77	0	51,60,60	1.59	9 (17%)
2	CHL	G	608	-	66,74,74	1.53	7 (10%)	73,114,114	1.27	8 (10%)
3	CLA	G	612	1	65,73,73	1.50	8 (12%)	76,113,113	1.37	8 (10%)
3	CLA	N	604	-	62,70,73	1.55	6 (9%)	72,109,113	1.38	8 (11%)
3	CLA	N	603	-	65,73,73	1.54	6 (9%)	76,113,113	1.34	8 (10%)
3	CLA	N	612	-	65,73,73	1.52	6 (9%)	76,113,113	1.27	7 (9%)
3	CLA	G	604	-	62,70,73	1.54	6 (9%)	72,109,113	1.42	7 (9%)
6	NEX	G	617	-	38,46,46	1.57	7 (18%)	50,70,70	1.60	10 (20%)
2	CHL	G	609	1	66,74,74	1.44	6 (9%)	73,114,114	1.92	16 (21%)
2	CHL	N	606	-	51,59,74	1.70	5 (9%)	55,96,114	1.74	13 (23%)
2	CHL	G	606	-	51,59,74	1.71	6 (11%)	55,96,114	1.71	11 (20%)
3	CLA	N	611	7	65,73,73	1.46	9 (13%)	76,113,113	1.26	6 (7%)
3	CLA	G	611	7	65,73,73	1.54	7 (10%)	76,113,113	1.26	7 (9%)
3	CLA	Y	613	1	65,73,73	1.50	6 (9%)	76,113,113	1.35	8 (10%)
4	LUT	G	615	-	42,43,43	0.76	0	51,60,60	1.68	12 (23%)
3	CLA	Y	604	-	62,70,73	1.53	6 (9%)	72,109,113	1.54	10 (13%)
2	CHL	N	605	-	48,56,74	1.71	6 (12%)	51,92,114	1.57	9 (17%)
3	CLA	G	610	1	65,73,73	1.55	8 (12%)	76,113,113	1.32	11 (14%)
7	LHG	Y	618	3	48,48,48	0.92	2 (4%)	51,54,54	1.07	3 (5%)
2	CHL	G	605	-	48,56,74	1.69	6 (12%)	51,92,114	1.63	10 (19%)
3	CLA	N	610	1	65,73,73	1.48	7 (10%)	76,113,113	1.27	10 (13%)
3	CLA	G	603	-	65,73,73	1.52	6 (9%)	76,113,113	1.32	7 (9%)
2	CHL	Y	607	-	66,74,74	1.45	6 (9%)	73,114,114	1.72	12 (16%)
3	CLA	Y	602	1	65,73,73	1.50	7 (10%)	76,113,113	1.33	6 (7%)
2	CHL	N	601	1	66,74,74	1.46	6 (9%)	73,114,114	1.48	11 (15%)
2	CHL	G	601	-	66,74,74	1.42	7 (10%)	73,114,114	1.37	11 (15%)
2	CHL	Y	601	1	66,74,74	1.48	6 (9%)	73,114,114	1.39	11 (15%)
5	XAT	N	617	-	39,47,47	0.95	2 (5%)	54,74,74	2.67	20 (37%)
5	XAT	N	620	-	39,47,47	0.94	2 (5%)	54,74,74	2.74	22 (40%)
2	CHL	Y	605	-	48,56,74	1.70	5 (10%)	51,92,114	1.52	9 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	CHL	N	607	-	66,74,74	1.46	6 (9%)	73,114,114	1.67	12 (16%)
3	CLA	N	614	-	49,57,73	1.77	6 (12%)	55,93,113	1.44	7 (12%)
2	CHL	Y	609	1	66,74,74	1.51	6 (9%)	73,114,114	1.37	10 (13%)
4	LUT	Y	616	-	42,43,43	0.80	0	51,60,60	1.76	10 (19%)
2	CHL	G	607	-	66,74,74	1.46	6 (9%)	73,114,114	1.72	12 (16%)
3	CLA	N	613	1	65,73,73	1.51	6 (9%)	76,113,113	1.44	8 (10%)
3	CLA	Y	614	-	49,57,73	1.77	7 (14%)	55,93,113	1.37	7 (12%)
6	NEX	N	618	-	38,46,46	1.58	7 (18%)	50,70,70	1.60	10 (20%)
2	CHL	Y	606	-	51,59,74	1.69	5 (9%)	55,96,114	1.83	11 (20%)
3	CLA	Y	611	7	65,73,73	1.45	9 (13%)	76,113,113	1.26	6 (7%)
3	CLA	Y	603	-	65,73,73	1.48	6 (9%)	76,113,113	1.42	9 (11%)
4	LUT	Y	615	-	42,43,43	0.79	0	51,60,60	1.64	12 (23%)
5	XAT	G	619	-	39,47,47	0.95	2 (5%)	54,74,74	2.70	20 (37%)
3	CLA	G	613	1	65,73,73	1.50	6 (9%)	76,113,113	1.43	8 (10%)
7	LHG	N	619	3	48,48,48	0.91	2 (4%)	51,54,54	1.04	2 (3%)
2	CHL	N	609	1	66,74,74	1.48	6 (9%)	73,114,114	1.90	16 (21%)
3	CLA	G	602	1	65,73,73	1.56	6 (9%)	76,113,113	1.24	8 (10%)
4	LUT	N	615	-	42,43,43	0.77	0	51,60,60	1.66	10 (19%)
3	CLA	N	602	1	65,73,73	1.52	6 (9%)	76,113,113	1.39	8 (10%)
7	LHG	G	618	3	48,48,48	0.93	2 (4%)	51,54,54	1.06	3 (5%)
2	CHL	Y	608	-	66,74,74	1.48	7 (10%)	73,114,114	1.33	8 (10%)
2	CHL	N	608	-	66,74,74	1.51	7 (10%)	73,114,114	1.25	9 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	LUT	G	616	-	-	3/29/67/67	0/2/2/2
6	NEX	Y	617	-	-	9/27/83/83	0/3/3/3
3	CLA	Y	610	1	1/1/15/20	2/37/115/115	-
3	CLA	Y	612	1	1/1/15/20	18/37/115/115	-
3	CLA	G	614	-	1/1/11/20	9/18/96/115	-
4	LUT	N	616	-	-	3/29/67/67	0/2/2/2
2	CHL	G	608	-	3/3/20/26	14/39/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CLA	G	612	1	1/1/15/20	19/37/115/115	-
3	CLA	N	604	-	1/1/14/20	13/34/112/115	-
3	CLA	N	603	-	1/1/15/20	18/37/115/115	-
3	CLA	N	612	-	1/1/15/20	16/37/115/115	-
3	CLA	G	604	-	1/1/14/20	12/34/112/115	-
6	NEX	G	617	-	-	9/27/83/83	0/3/3/3
2	CHL	G	609	1	3/3/20/26	13/39/137/137	-
2	CHL	N	606	-	3/3/17/26	8/21/119/137	-
2	CHL	G	606	-	3/3/17/26	6/21/119/137	-
3	CLA	N	611	7	1/1/15/20	15/37/115/115	-
3	CLA	G	611	7	-	12/37/115/115	-
3	CLA	Y	613	1	1/1/15/20	8/37/115/115	-
4	LUT	G	615	-	-	4/29/67/67	0/2/2/2
3	CLA	Y	604	-	1/1/14/20	13/34/112/115	-
2	CHL	N	605	-	3/3/16/26	7/18/116/137	-
3	CLA	G	610	1	1/1/15/20	3/37/115/115	-
7	LHG	Y	618	3	-	35/53/53/53	-
2	CHL	G	605	-	3/3/16/26	6/18/116/137	-
3	CLA	N	610	1	1/1/15/20	4/37/115/115	-
3	CLA	G	603	-	1/1/15/20	16/37/115/115	-
2	CHL	Y	607	-	3/3/20/26	13/39/137/137	-
3	CLA	Y	602	1	1/1/15/20	10/37/115/115	-
2	CHL	N	601	1	3/3/20/26	12/39/137/137	-
2	CHL	G	601	-	3/3/20/26	17/39/137/137	-
2	CHL	Y	601	1	3/3/20/26	11/39/137/137	-
5	XAT	N	617	-	-	7/31/93/93	0/4/4/4
5	XAT	N	620	-	-	7/31/93/93	0/4/4/4
2	CHL	Y	605	-	3/3/16/26	8/18/116/137	-
2	CHL	N	607	-	3/3/20/26	14/39/137/137	-
3	CLA	N	614	-	1/1/11/20	9/18/96/115	-
2	CHL	Y	609	1	3/3/20/26	13/39/137/137	-
4	LUT	Y	616	-	-	3/29/67/67	0/2/2/2
2	CHL	G	607	-	3/3/20/26	14/39/137/137	-
3	CLA	N	613	1	1/1/15/20	12/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CLA	Y	614	-	1/1/11/20	8/18/96/115	-
6	NEX	N	618	-	-	9/27/83/83	0/3/3/3
2	CHL	Y	606	-	3/3/17/26	7/21/119/137	-
3	CLA	Y	611	7	1/1/15/20	13/37/115/115	-
3	CLA	Y	603	-	1/1/15/20	17/37/115/115	-
4	LUT	Y	615	-	-	4/29/67/67	0/2/2/2
5	XAT	G	619	-	-	7/31/93/93	0/4/4/4
3	CLA	G	613	1	1/1/15/20	10/37/115/115	-
7	LHG	N	619	3	-	30/53/53/53	-
2	CHL	N	609	1	3/3/20/26	11/39/137/137	-
3	CLA	G	602	1	1/1/15/20	12/37/115/115	-
4	LUT	N	615	-	-	5/29/67/67	0/2/2/2
3	CLA	N	602	1	1/1/15/20	7/37/115/115	-
7	LHG	G	618	3	-	30/53/53/53	-
2	CHL	Y	608	-	3/3/20/26	17/39/137/137	-
2	CHL	N	608	-	3/3/20/26	13/39/137/137	-

All (306) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	614	CLA	C4B-NB	8.13	1.42	1.35
3	G	611	CLA	C4B-NB	8.06	1.42	1.35
2	N	608	CHL	C4B-NB	8.04	1.42	1.35
3	G	602	CLA	C4B-NB	8.03	1.42	1.35
3	Y	614	CLA	C4B-NB	8.01	1.42	1.35
2	G	608	CHL	C4B-NB	7.98	1.42	1.35
3	N	614	CLA	C4B-NB	7.96	1.42	1.35
3	N	612	CLA	C4B-NB	7.86	1.42	1.35
2	Y	609	CHL	C4B-NB	7.85	1.42	1.35
3	G	610	CLA	C4B-NB	7.81	1.42	1.35
3	N	603	CLA	C4B-NB	7.77	1.42	1.35
2	G	606	CHL	C4B-NB	7.77	1.42	1.35
3	G	603	CLA	C4B-NB	7.76	1.42	1.35
3	G	613	CLA	C4B-NB	7.74	1.42	1.35
2	N	606	CHL	C4B-NB	7.72	1.42	1.35
2	Y	608	CHL	C4B-NB	7.67	1.42	1.35
2	Y	606	CHL	C4B-NB	7.67	1.42	1.35
3	G	604	CLA	C4B-NB	7.67	1.42	1.35
3	N	613	CLA	C4B-NB	7.66	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Y	613	CLA	C4B-NB	7.66	1.42	1.35
3	N	604	CLA	C4B-NB	7.65	1.42	1.35
2	Y	601	CHL	C4B-NB	7.58	1.42	1.35
2	N	601	CHL	C4B-NB	7.55	1.41	1.35
3	Y	603	CLA	C4B-NB	7.52	1.41	1.35
3	Y	612	CLA	C4B-NB	7.52	1.41	1.35
3	Y	604	CLA	C4B-NB	7.51	1.41	1.35
3	Y	610	CLA	C4B-NB	7.44	1.41	1.35
3	N	602	CLA	C4B-NB	7.42	1.41	1.35
3	G	612	CLA	C4B-NB	7.38	1.41	1.35
2	N	605	CHL	C4B-NB	7.36	1.41	1.35
2	Y	605	CHL	C4B-NB	7.34	1.41	1.35
2	N	607	CHL	C4B-NB	7.32	1.41	1.35
2	G	607	CHL	C4B-NB	7.28	1.41	1.35
2	N	609	CHL	C4B-NB	7.22	1.41	1.35
2	Y	607	CHL	C4B-NB	7.19	1.41	1.35
3	N	610	CLA	C4B-NB	7.19	1.41	1.35
3	Y	602	CLA	C4B-NB	7.14	1.41	1.35
2	G	605	CHL	C4B-NB	7.12	1.41	1.35
3	N	611	CLA	C4B-NB	7.08	1.41	1.35
3	Y	611	CLA	C4B-NB	7.04	1.41	1.35
2	G	609	CHL	C4B-NB	6.94	1.41	1.35
2	G	601	CHL	C4B-NB	6.82	1.41	1.35
7	G	618	LHG	O8-C23	4.33	1.46	1.33
3	N	602	CLA	C1D-ND	4.27	1.43	1.37
3	N	613	CLA	C1D-ND	4.23	1.43	1.37
2	Y	608	CHL	C1D-ND	4.13	1.42	1.37
7	Y	618	LHG	O8-C23	4.13	1.45	1.33
7	N	619	LHG	O8-C23	4.13	1.45	1.33
3	N	603	CLA	C1D-ND	4.08	1.42	1.37
2	G	608	CHL	C1D-ND	4.06	1.42	1.37
2	Y	609	CHL	C1D-ND	4.06	1.42	1.37
3	G	614	CLA	C1D-ND	4.02	1.42	1.37
3	N	614	CLA	C1D-ND	4.01	1.42	1.37
3	Y	614	CLA	C1D-ND	3.96	1.42	1.37
2	N	608	CHL	C1D-ND	3.96	1.42	1.37
3	Y	610	CLA	C1D-ND	3.96	1.42	1.37
3	G	611	CLA	C1D-ND	3.96	1.42	1.37
7	N	619	LHG	O7-C7	3.95	1.45	1.34
2	Y	601	CHL	C1D-ND	3.94	1.42	1.37
7	Y	618	LHG	O7-C7	3.94	1.45	1.34
2	Y	605	CHL	C1D-ND	3.93	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	610	CLA	C1D-ND	3.93	1.42	1.37
2	N	605	CHL	C1D-ND	3.92	1.42	1.37
2	G	605	CHL	C1D-ND	3.90	1.42	1.37
3	G	603	CLA	C1D-ND	3.89	1.42	1.37
7	G	618	LHG	O7-C7	3.88	1.45	1.34
3	Y	602	CLA	C1D-ND	3.87	1.42	1.37
6	Y	617	NEX	C14-C13	3.86	1.40	1.35
3	N	604	CLA	C1D-ND	3.84	1.42	1.37
2	N	606	CHL	C1D-ND	3.82	1.42	1.37
3	N	610	CLA	C1D-ND	3.81	1.42	1.37
3	G	602	CLA	C1D-ND	3.81	1.42	1.37
6	N	618	NEX	C14-C13	3.80	1.40	1.35
6	N	618	NEX	C30-C29	3.80	1.40	1.35
6	G	617	NEX	C30-C29	3.79	1.40	1.35
6	Y	617	NEX	C30-C29	3.78	1.40	1.35
6	Y	617	NEX	C34-C33	3.77	1.40	1.35
3	Y	613	CLA	C1D-ND	3.77	1.42	1.37
3	N	612	CLA	C1D-ND	3.76	1.42	1.37
3	Y	603	CLA	C1D-ND	3.76	1.42	1.37
6	G	617	NEX	C14-C13	3.74	1.40	1.35
2	N	601	CHL	C1D-ND	3.74	1.42	1.37
2	Y	606	CHL	C1D-ND	3.73	1.42	1.37
3	G	613	CLA	C1D-ND	3.73	1.42	1.37
6	N	618	NEX	C34-C33	3.72	1.40	1.35
6	G	617	NEX	C34-C33	3.72	1.40	1.35
3	G	612	CLA	C1D-ND	3.70	1.42	1.37
3	G	604	CLA	C1D-ND	3.68	1.42	1.37
2	G	606	CHL	C1D-ND	3.66	1.42	1.37
2	Y	607	CHL	C1D-ND	3.57	1.42	1.37
3	Y	612	CLA	C1D-ND	3.56	1.42	1.37
2	N	609	CHL	C4D-ND	-3.53	1.32	1.37
2	G	609	CHL	C4D-ND	-3.52	1.32	1.37
3	Y	604	CLA	C1D-ND	3.50	1.42	1.37
2	G	607	CHL	C1D-ND	3.50	1.42	1.37
2	N	607	CHL	C1D-ND	3.44	1.42	1.37
2	N	609	CHL	C1D-ND	3.37	1.41	1.37
2	G	609	CHL	C1D-ND	3.35	1.41	1.37
2	N	607	CHL	CHC-C1C	3.34	1.43	1.35
3	Y	611	CLA	C4D-ND	-3.31	1.33	1.37
2	G	605	CHL	CHC-C1C	3.30	1.43	1.35
2	N	605	CHL	CHC-C1C	3.30	1.43	1.35
2	G	601	CHL	C1D-ND	3.29	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	611	CLA	C4D-ND	-3.28	1.33	1.37
2	G	607	CHL	CHC-C1C	3.28	1.43	1.35
2	Y	607	CHL	CHC-C1C	3.24	1.43	1.35
2	G	608	CHL	CHC-C1C	3.24	1.43	1.35
2	Y	605	CHL	CHC-C1C	3.21	1.43	1.35
2	N	608	CHL	CHC-C1C	3.21	1.43	1.35
3	G	610	CLA	CHC-C1C	3.20	1.43	1.35
3	G	614	CLA	CHC-C1C	3.20	1.43	1.35
2	N	609	CHL	CHC-C1C	3.18	1.43	1.35
2	Y	606	CHL	CHC-C1C	3.18	1.43	1.35
2	N	606	CHL	CHC-C1C	3.16	1.43	1.35
2	G	607	CHL	C4D-ND	-3.15	1.33	1.37
6	N	618	NEX	C10-C9	3.15	1.40	1.35
2	N	607	CHL	C4D-ND	-3.15	1.33	1.37
6	G	617	NEX	C10-C9	3.14	1.39	1.35
2	Y	601	CHL	CHC-C1C	3.14	1.43	1.35
2	G	601	CHL	CHC-C1C	3.13	1.43	1.35
3	G	602	CLA	CHC-C1C	3.13	1.43	1.35
2	G	609	CHL	CHC-C1C	3.13	1.43	1.35
2	N	609	CHL	CMB-C2B	-3.12	1.45	1.51
6	Y	617	NEX	C10-C9	3.10	1.39	1.35
2	Y	606	CHL	C4D-ND	-3.09	1.33	1.37
3	G	604	CLA	CHC-C1C	3.08	1.42	1.35
3	Y	602	CLA	C4D-ND	-3.08	1.33	1.37
3	G	603	CLA	CHC-C1C	3.06	1.42	1.35
3	N	602	CLA	CHC-C1C	3.06	1.42	1.35
3	N	613	CLA	CHC-C1C	3.06	1.42	1.35
2	N	601	CHL	CHC-C1C	3.05	1.42	1.35
3	Y	602	CLA	CHC-C1C	3.05	1.42	1.35
3	N	611	CLA	C1D-ND	3.04	1.41	1.37
3	N	610	CLA	CHC-C1C	3.03	1.42	1.35
3	N	614	CLA	CHC-C1C	3.03	1.42	1.35
3	N	603	CLA	CHC-C1C	3.03	1.42	1.35
3	Y	612	CLA	C4D-ND	-3.03	1.33	1.37
3	Y	613	CLA	C4D-ND	-3.03	1.33	1.37
3	G	602	CLA	C4D-ND	-3.01	1.33	1.37
3	N	612	CLA	CHC-C1C	3.00	1.42	1.35
3	Y	614	CLA	CHC-C1C	3.00	1.42	1.35
3	Y	610	CLA	CHC-C1C	2.99	1.42	1.35
3	G	611	CLA	CHC-C1C	2.97	1.42	1.35
2	Y	607	CHL	C4D-ND	-2.97	1.33	1.37
3	Y	604	CLA	C4D-ND	-2.96	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	613	CLA	CHC-C1C	2.95	1.42	1.35
3	Y	611	CLA	C1D-ND	2.95	1.41	1.37
2	N	606	CHL	C4D-ND	-2.94	1.33	1.37
2	G	606	CHL	C4D-ND	-2.94	1.33	1.37
2	G	606	CHL	CHC-C1C	2.93	1.42	1.35
3	N	610	CLA	C4D-ND	-2.93	1.33	1.37
3	Y	613	CLA	CHC-C1C	2.92	1.42	1.35
3	Y	604	CLA	CMB-C2B	-2.91	1.45	1.51
2	G	601	CHL	C4D-ND	-2.91	1.33	1.37
3	N	604	CLA	CHC-C1C	2.90	1.42	1.35
3	Y	604	CLA	CHC-C1C	2.90	1.42	1.35
3	G	611	CLA	C4D-ND	-2.90	1.33	1.37
3	N	604	CLA	C4D-ND	-2.90	1.33	1.37
2	Y	608	CHL	CHC-C1C	2.90	1.42	1.35
3	G	613	CLA	C4D-ND	-2.88	1.33	1.37
3	N	613	CLA	C4D-ND	-2.88	1.33	1.37
2	Y	609	CHL	C4D-ND	-2.86	1.33	1.37
3	G	604	CLA	C4D-ND	-2.85	1.33	1.37
2	G	609	CHL	CMB-C2B	-2.85	1.45	1.51
2	Y	609	CHL	CMB-C2B	-2.85	1.45	1.51
3	Y	610	CLA	C4D-ND	-2.85	1.33	1.37
3	N	602	CLA	C4D-ND	-2.83	1.33	1.37
3	Y	603	CLA	CHC-C1C	2.82	1.42	1.35
3	G	612	CLA	C4D-ND	-2.80	1.33	1.37
3	N	612	CLA	C4D-ND	-2.79	1.33	1.37
3	G	612	CLA	CMB-C2B	-2.79	1.45	1.51
3	G	614	CLA	C4D-ND	-2.77	1.33	1.37
3	N	603	CLA	C4D-ND	-2.77	1.33	1.37
2	G	606	CHL	CMB-C2B	-2.77	1.45	1.51
3	Y	611	CLA	CHC-C1C	2.76	1.42	1.35
3	N	611	CLA	CHC-C1C	2.76	1.42	1.35
3	N	614	CLA	C4D-ND	-2.76	1.33	1.37
5	G	619	XAT	O4-C5	-2.73	1.42	1.46
3	G	603	CLA	C4D-ND	-2.72	1.33	1.37
3	Y	612	CLA	CHC-C1C	2.72	1.41	1.35
3	G	604	CLA	CMB-C2B	-2.70	1.46	1.51
2	N	608	CHL	C4D-ND	-2.69	1.34	1.37
3	G	610	CLA	C4D-ND	-2.69	1.34	1.37
5	N	617	XAT	O4-C5	-2.68	1.42	1.46
3	Y	603	CLA	C4D-ND	-2.67	1.34	1.37
3	Y	612	CLA	CMB-C2B	-2.66	1.46	1.51
2	N	601	CHL	C4D-ND	-2.66	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Y	609	CHL	CHC-C1C	2.63	1.41	1.35
3	G	612	CLA	CHC-C1C	2.63	1.41	1.35
3	N	604	CLA	CMB-C2B	-2.63	1.46	1.51
2	N	605	CHL	C4D-ND	-2.63	1.34	1.37
2	Y	608	CHL	C4D-ND	-2.63	1.34	1.37
2	Y	601	CHL	C4D-ND	-2.61	1.34	1.37
2	G	605	CHL	C4D-ND	-2.61	1.34	1.37
2	Y	608	CHL	CMB-C2B	-2.59	1.46	1.51
3	Y	614	CLA	C4D-ND	-2.59	1.34	1.37
3	N	603	CLA	CMB-C2B	-2.58	1.46	1.51
2	G	608	CHL	CMB-C2B	-2.57	1.46	1.51
2	G	608	CHL	CMD-C2D	-2.56	1.45	1.50
2	G	608	CHL	C4D-ND	-2.56	1.34	1.37
3	Y	611	CLA	CMB-C2B	-2.55	1.46	1.51
3	N	611	CLA	CMB-C2B	-2.54	1.46	1.51
3	N	610	CLA	CMB-C2B	-2.54	1.46	1.51
2	Y	605	CHL	C4D-ND	-2.53	1.34	1.37
3	Y	613	CLA	CMB-C2B	-2.53	1.46	1.51
2	G	601	CHL	CMB-C2B	-2.52	1.46	1.51
2	Y	606	CHL	CMB-C2B	-2.50	1.46	1.51
2	N	608	CHL	CMB-C2B	-2.50	1.46	1.51
3	G	610	CLA	CMB-C2B	-2.49	1.46	1.51
5	N	620	XAT	O4-C5	-2.49	1.42	1.46
3	Y	611	CLA	CMD-C2D	-2.48	1.45	1.50
3	Y	603	CLA	CMB-C2B	-2.47	1.46	1.51
2	N	605	CHL	CMB-C2B	-2.47	1.46	1.51
3	N	612	CLA	CMB-C2B	-2.47	1.46	1.51
3	G	614	CLA	CMB-C2B	-2.46	1.46	1.51
2	Y	605	CHL	CMB-C2B	-2.46	1.46	1.51
3	G	603	CLA	CMB-C2B	-2.45	1.46	1.51
2	G	607	CHL	CMB-C2B	-2.44	1.46	1.51
2	Y	607	CHL	CMB-C2B	-2.44	1.46	1.51
3	Y	614	CLA	CMB-C2B	-2.43	1.46	1.51
2	G	601	CHL	CMD-C2D	-2.43	1.45	1.50
3	Y	610	CLA	CMB-C2B	-2.42	1.46	1.51
3	G	611	CLA	CMB-C2B	-2.42	1.46	1.51
6	G	617	NEX	C32-C33	-2.41	1.40	1.45
3	N	614	CLA	CMB-C2B	-2.41	1.46	1.51
2	N	606	CHL	CMB-C2B	-2.40	1.46	1.51
6	N	618	NEX	C32-C33	-2.40	1.40	1.45
6	N	618	NEX	C28-C29	-2.40	1.40	1.45
3	G	602	CLA	CMB-C2B	-2.40	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Y	601	CHL	CMB-C2B	-2.39	1.46	1.51
2	N	601	CHL	CMB-C2B	-2.39	1.46	1.51
2	G	605	CHL	CMB-C2B	-2.39	1.46	1.51
2	N	607	CHL	CMB-C2B	-2.38	1.46	1.51
6	Y	617	NEX	C28-C29	-2.38	1.40	1.45
6	G	617	NEX	C28-C29	-2.38	1.40	1.45
6	Y	617	NEX	C32-C33	-2.38	1.40	1.45
3	Y	602	CLA	CMB-C2B	-2.38	1.46	1.51
3	G	610	CLA	C3B-C2B	-2.38	1.37	1.40
3	N	611	CLA	CMD-C2D	-2.37	1.45	1.50
3	N	602	CLA	CMB-C2B	-2.35	1.46	1.51
5	N	617	XAT	O24-C25	-2.35	1.42	1.46
2	N	601	CHL	CMD-C2D	-2.34	1.45	1.50
6	Y	617	NEX	C12-C13	-2.33	1.40	1.45
5	G	619	XAT	O24-C25	-2.33	1.42	1.46
3	Y	612	CLA	C3B-C2B	-2.33	1.37	1.40
3	G	613	CLA	CMB-C2B	-2.33	1.46	1.51
6	N	618	NEX	C12-C13	-2.32	1.41	1.45
2	Y	601	CHL	CMD-C2D	-2.32	1.45	1.50
3	G	612	CLA	C3B-C2B	-2.32	1.37	1.40
3	N	613	CLA	CMB-C2B	-2.31	1.46	1.51
3	N	611	CLA	C3B-C2B	-2.31	1.37	1.40
6	G	617	NEX	C12-C13	-2.30	1.41	1.45
3	Y	610	CLA	C3B-C2B	-2.30	1.37	1.40
2	G	608	CHL	C3B-C2B	-2.28	1.37	1.40
5	N	620	XAT	O24-C25	-2.28	1.43	1.46
2	N	609	CHL	MG-ND	-2.28	2.01	2.05
2	G	609	CHL	MG-ND	-2.27	2.01	2.05
3	G	612	CLA	MG-NA	2.26	2.11	2.06
3	Y	614	CLA	CMD-C2D	-2.25	1.46	1.50
3	Y	604	CLA	CMD-C2D	-2.25	1.46	1.50
3	G	614	CLA	C3B-C2B	-2.24	1.37	1.40
2	N	608	CHL	C3B-C2B	-2.24	1.37	1.40
3	N	610	CLA	C3B-C2B	-2.22	1.37	1.40
2	G	607	CHL	CMD-C2D	-2.19	1.46	1.50
3	Y	612	CLA	CMC-C2C	-2.17	1.46	1.50
3	G	614	CLA	CMD-C2D	-2.16	1.46	1.50
2	Y	608	CHL	C3B-C2B	-2.14	1.37	1.40
3	Y	610	CLA	C3B-CAB	-2.13	1.43	1.47
3	Y	611	CLA	C3B-C2B	-2.13	1.37	1.40
2	Y	607	CHL	CMD-C2D	-2.13	1.46	1.50
3	Y	603	CLA	CMD-C2D	-2.11	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	602	CLA	C3B-C2B	-2.11	1.37	1.40
3	N	614	CLA	CMD-C2D	-2.10	1.46	1.50
3	G	613	CLA	CMD-C2D	-2.10	1.46	1.50
3	G	612	CLA	C4B-CHC	-2.09	1.35	1.41
3	Y	602	CLA	C3B-CAB	-2.09	1.43	1.47
3	Y	612	CLA	CMD-C2D	-2.08	1.46	1.50
3	N	603	CLA	C3B-C2B	-2.08	1.37	1.40
3	Y	614	CLA	C3B-C2B	-2.08	1.37	1.40
3	G	603	CLA	CMD-C2D	-2.08	1.46	1.50
3	Y	613	CLA	CMD-C2D	-2.07	1.46	1.50
2	Y	608	CHL	CMD-C2D	-2.07	1.46	1.50
3	N	612	CLA	CMD-C2D	-2.07	1.46	1.50
3	N	610	CLA	CMD-C2D	-2.07	1.46	1.50
2	G	606	CHL	CMD-C2D	-2.06	1.46	1.50
2	G	605	CHL	CMD-C2D	-2.05	1.46	1.50
2	Y	609	CHL	C3B-C2B	-2.05	1.37	1.40
2	N	608	CHL	CMD-C2D	-2.05	1.46	1.50
3	N	602	CLA	C1D-C2D	2.05	1.49	1.45
3	N	611	CLA	CMC-C2C	-2.05	1.46	1.50
3	G	604	CLA	CMD-C2D	-2.05	1.46	1.50
3	Y	611	CLA	C3B-CAB	-2.04	1.43	1.47
3	G	610	CLA	CMD-C2D	-2.04	1.46	1.50
3	Y	610	CLA	CMD-C2D	-2.03	1.46	1.50
3	Y	602	CLA	CMD-C2D	-2.03	1.46	1.50
2	G	601	CHL	C3B-CAB	-2.03	1.43	1.47
2	N	607	CHL	CMD-C2D	-2.03	1.46	1.50
3	N	604	CLA	CMD-C2D	-2.03	1.46	1.50
3	N	611	CLA	MG-ND	-2.03	2.01	2.05
3	N	613	CLA	CMD-C2D	-2.02	1.46	1.50
3	Y	611	CLA	MG-ND	-2.02	2.01	2.05
2	N	605	CHL	CMD-C2D	-2.02	1.46	1.50
3	G	611	CLA	CMC-C2C	-2.01	1.46	1.50
3	Y	612	CLA	C4B-CHC	-2.01	1.35	1.41
3	G	611	CLA	CMD-C2D	-2.01	1.46	1.50
3	G	610	CLA	C3B-CAB	-2.00	1.43	1.47

All (549) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	609	CHL	C4A-NA-C1A	8.31	110.44	106.71
5	G	619	XAT	O24-C25-C24	7.76	119.22	113.38
2	Y	607	CHL	C4A-NA-C1A	7.56	110.10	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	607	CHL	C4A-NA-C1A	7.48	110.07	106.71
5	N	620	XAT	O24-C25-C24	7.44	118.97	113.38
2	Y	606	CHL	C4A-NA-C1A	7.20	109.94	106.71
5	N	617	XAT	O24-C25-C24	7.10	118.72	113.38
5	N	620	XAT	O4-C5-C4	6.99	118.63	113.38
5	N	617	XAT	O4-C5-C4	6.94	118.60	113.38
2	N	609	CHL	C4A-NA-C1A	6.83	109.78	106.71
5	G	619	XAT	O4-C5-C4	6.76	118.46	113.38
2	N	607	CHL	C4A-NA-C1A	6.67	109.70	106.71
2	N	606	CHL	C4A-NA-C1A	6.66	109.70	106.71
2	G	609	CHL	C1B-CHB-C4A	-6.56	117.12	130.12
2	G	606	CHL	C4A-NA-C1A	6.43	109.60	106.71
3	G	613	CLA	C4A-NA-C1A	6.35	109.56	106.71
2	G	607	CHL	C1B-CHB-C4A	-6.17	117.90	130.12
3	Y	613	CLA	C4A-NA-C1A	6.10	109.45	106.71
2	N	609	CHL	C1B-CHB-C4A	-6.02	118.20	130.12
2	N	607	CHL	C1B-CHB-C4A	-5.86	118.51	130.12
5	N	620	XAT	C15-C14-C13	-5.84	118.98	127.31
2	Y	607	CHL	C1B-CHB-C4A	-5.77	118.68	130.12
2	N	609	CHL	CMB-C2B-C1B	-5.76	119.61	128.46
5	N	617	XAT	C15-C14-C13	-5.57	119.37	127.31
3	Y	603	CLA	C4A-NA-C1A	5.54	109.19	106.71
5	G	619	XAT	C15-C14-C13	-5.42	119.57	127.31
3	N	613	CLA	C4A-NA-C1A	5.37	109.12	106.71
3	N	603	CLA	C4A-NA-C1A	5.31	109.09	106.71
3	G	604	CLA	CMB-C2B-C1B	-5.20	120.47	128.46
3	Y	604	CLA	CMB-C2B-C1B	-5.16	120.53	128.46
5	N	620	XAT	O24-C25-C38	5.05	121.11	115.06
3	Y	611	CLA	C4A-NA-C1A	5.00	108.95	106.71
3	Y	604	CLA	C4A-NA-C1A	4.99	108.95	106.71
3	G	611	CLA	C4A-NA-C1A	4.96	108.94	106.71
3	G	604	CLA	C4A-NA-C1A	4.94	108.93	106.71
3	N	611	CLA	C4A-NA-C1A	4.92	108.92	106.71
3	N	613	CLA	CMB-C2B-C1B	-4.91	120.92	128.46
2	Y	608	CHL	C4A-NA-C1A	4.90	108.91	106.71
2	N	601	CHL	C4A-NA-C1A	4.89	108.90	106.71
5	N	617	XAT	O24-C25-C38	4.85	120.87	115.06
3	G	603	CLA	C4A-NA-C1A	4.83	108.88	106.71
3	N	612	CLA	C4A-NA-C1A	4.82	108.87	106.71
3	N	614	CLA	C4A-NA-C1A	4.77	108.85	106.71
3	N	602	CLA	C4A-NA-C1A	4.72	108.83	106.71
2	G	605	CHL	C1B-CHB-C4A	-4.71	120.79	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	N	620	XAT	C35-C34-C33	-4.71	120.59	127.31
5	G	619	XAT	O24-C25-C38	4.64	120.62	115.06
5	G	619	XAT	O4-C5-C18	4.64	120.61	115.06
3	N	604	CLA	CMB-C2B-C1B	-4.62	121.37	128.46
5	N	617	XAT	C35-C34-C33	-4.57	120.79	127.31
3	N	604	CLA	C4A-NA-C1A	4.52	108.74	106.71
4	G	616	LUT	C2-C3-C4	-4.51	104.12	110.30
5	G	619	XAT	C11-C10-C9	-4.49	120.90	127.31
5	N	620	XAT	C11-C10-C9	-4.44	120.97	127.31
2	G	609	CHL	CMB-C2B-C1B	-4.43	121.66	128.46
3	G	612	CLA	CMB-C2B-C1B	-4.42	121.67	128.46
5	N	620	XAT	C18-C5-C6	-4.42	114.86	122.26
5	G	619	XAT	C18-C5-C6	-4.36	114.94	122.26
5	N	617	XAT	O4-C5-C18	4.32	120.24	115.06
2	Y	606	CHL	CMB-C2B-C1B	-4.28	121.89	128.46
2	N	609	CHL	CHD-C1D-ND	-4.28	120.52	124.45
4	Y	616	LUT	C15-C14-C13	-4.27	121.21	127.31
2	Y	605	CHL	C1B-CHB-C4A	-4.24	121.72	130.12
3	G	613	CLA	CMB-C2B-C1B	-4.24	121.95	128.46
5	G	619	XAT	C35-C34-C33	-4.23	121.28	127.31
4	G	616	LUT	C15-C14-C13	-4.22	121.29	127.31
2	N	608	CHL	C4A-NA-C1A	4.21	108.60	106.71
2	G	609	CHL	CHD-C1D-ND	-4.21	120.58	124.45
3	Y	602	CLA	CMB-C2B-C1B	-4.19	122.02	128.46
3	N	613	CLA	CMB-C2B-C3B	4.18	132.50	124.68
5	N	620	XAT	O4-C5-C18	4.18	120.07	115.06
4	Y	616	LUT	C31-C30-C29	-4.18	121.35	127.31
2	N	609	CHL	CMB-C2B-C3B	4.18	132.49	124.68
5	N	617	XAT	C18-C5-C6	-4.17	115.27	122.26
3	N	602	CLA	CMB-C2B-C1B	-4.14	122.10	128.46
2	N	605	CHL	C1B-CHB-C4A	-4.13	121.94	130.12
5	N	620	XAT	C38-C25-C26	-4.09	115.40	122.26
5	G	619	XAT	C38-C25-C26	-4.09	115.40	122.26
4	N	615	LUT	C7-C8-C9	-4.09	120.06	126.23
5	N	617	XAT	C11-C10-C9	-4.08	121.49	127.31
5	N	617	XAT	C38-C25-C26	-4.07	115.43	122.26
6	Y	617	NEX	C39-C29-C30	-4.05	117.24	122.92
2	Y	606	CHL	C1B-CHB-C4A	-4.05	122.10	130.12
3	G	604	CLA	CMB-C2B-C3B	4.04	132.24	124.68
6	N	618	NEX	C39-C29-C30	-4.04	117.26	122.92
3	N	610	CLA	C4A-NA-C1A	4.03	108.52	106.71
6	G	617	NEX	C39-C29-C30	-4.01	117.31	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	606	CHL	CMB-C2B-C1B	-3.99	122.33	128.46
2	G	606	CHL	CMB-C2B-C1B	-3.98	122.34	128.46
3	G	602	CLA	C4A-NA-C1A	3.98	108.50	106.71
4	G	616	LUT	C31-C30-C29	-3.97	121.64	127.31
4	N	615	LUT	C35-C34-C33	-3.97	121.65	127.31
3	Y	604	CLA	C4-C3-C5	3.97	121.94	115.27
3	Y	613	CLA	CMB-C2B-C1B	-3.96	122.38	128.46
4	N	615	LUT	C15-C14-C13	-3.92	121.71	127.31
2	Y	601	CHL	C4A-NA-C1A	3.92	108.47	106.71
3	Y	604	CLA	CMB-C2B-C3B	3.91	131.99	124.68
6	G	617	NEX	C35-C15-C14	3.90	131.47	123.47
2	Y	609	CHL	CMB-C2B-C1B	-3.90	122.47	128.46
6	N	618	NEX	C35-C15-C14	3.89	131.44	123.47
6	Y	617	NEX	C35-C15-C14	3.89	131.44	123.47
3	G	614	CLA	C4A-NA-C1A	3.88	108.45	106.71
3	Y	602	CLA	CMB-C2B-C3B	3.88	131.93	124.68
4	G	615	LUT	C35-C34-C33	-3.86	121.80	127.31
2	N	605	CHL	C4A-NA-C1A	3.85	108.44	106.71
3	Y	602	CLA	C4A-NA-C1A	3.80	108.41	106.71
3	G	612	CLA	CMB-C2B-C3B	3.77	131.74	124.68
2	G	608	CHL	C4A-NA-C1A	3.76	108.40	106.71
4	N	615	LUT	C11-C10-C9	-3.76	121.94	127.31
5	N	620	XAT	C26-C27-C28	-3.75	118.06	125.99
4	Y	615	LUT	C11-C10-C9	-3.74	121.97	127.31
2	Y	609	CHL	C4A-NA-C1A	3.74	108.39	106.71
2	G	601	CHL	CMB-C2B-C1B	-3.72	122.75	128.46
7	Y	618	LHG	O7-C7-C8	3.71	119.51	111.50
3	G	610	CLA	CAC-C3C-C4C	3.68	129.59	124.81
2	N	605	CHL	CMB-C2B-C1B	-3.68	122.80	128.46
3	Y	610	CLA	C1B-CHB-C4A	-3.68	122.83	130.12
3	G	610	CLA	C1B-CHB-C4A	-3.68	122.83	130.12
5	G	619	XAT	C26-C27-C28	-3.67	118.22	125.99
2	N	601	CHL	C1B-CHB-C4A	-3.67	122.84	130.12
2	G	605	CHL	CMB-C2B-C1B	-3.65	122.85	128.46
3	N	604	CLA	CMB-C2B-C3B	3.65	131.50	124.68
3	N	602	CLA	CMB-C2B-C3B	3.65	131.50	124.68
3	G	603	CLA	CMB-C2B-C1B	-3.64	122.87	128.46
2	Y	608	CHL	CMB-C2B-C1B	-3.63	122.88	128.46
2	N	607	CHL	CMB-C2B-C1B	-3.62	122.91	128.46
3	G	611	CLA	CMB-C2B-C1B	-3.59	122.94	128.46
3	N	610	CLA	CMB-C2B-C1B	-3.58	122.96	128.46
4	G	615	LUT	C21-C26-C27	-3.57	108.19	112.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	607	CHL	CHD-C1D-ND	-3.56	121.18	124.45
3	G	613	CLA	CMB-C2B-C3B	3.56	131.34	124.68
5	G	619	XAT	C17-C1-C2	-3.56	102.80	108.98
3	Y	603	CLA	CMB-C2B-C1B	-3.55	123.01	128.46
2	Y	606	CHL	CMB-C2B-C3B	3.54	131.31	124.68
7	G	618	LHG	O8-C23-C24	3.54	123.03	111.91
2	N	606	CHL	C1B-CHB-C4A	-3.52	123.14	130.12
3	Y	612	CLA	C4A-NA-C1A	3.52	108.29	106.71
3	N	610	CLA	C1B-CHB-C4A	-3.52	123.14	130.12
5	N	617	XAT	C17-C1-C2	-3.52	102.87	108.98
2	G	607	CHL	CHD-C1D-ND	-3.51	121.22	124.45
2	N	601	CHL	CMB-C2B-C1B	-3.51	123.07	128.46
3	Y	612	CLA	CMB-C2B-C1B	-3.51	123.07	128.46
4	N	616	LUT	C21-C26-C27	-3.50	108.28	112.70
2	G	605	CHL	C4A-NA-C1A	3.50	108.28	106.71
4	Y	616	LUT	C21-C26-C27	-3.49	108.29	112.70
5	N	617	XAT	C26-C27-C28	-3.49	118.62	125.99
6	G	617	NEX	C40-C33-C34	-3.49	118.04	122.92
6	G	617	NEX	C15-C35-C34	3.48	130.61	123.47
6	Y	617	NEX	C15-C35-C34	3.48	130.60	123.47
3	G	610	CLA	CMB-C2B-C1B	-3.48	123.12	128.46
6	N	618	NEX	C15-C35-C34	3.48	130.60	123.47
6	N	618	NEX	C40-C33-C34	-3.47	118.06	122.92
6	Y	617	NEX	C40-C33-C34	-3.47	118.06	122.92
2	G	606	CHL	C1B-CHB-C4A	-3.47	123.25	130.12
3	Y	611	CLA	CMB-C2B-C1B	-3.46	123.15	128.46
2	Y	607	CHL	CMB-C2B-C1B	-3.45	123.15	128.46
6	Y	617	NEX	C20-C13-C14	-3.45	118.09	122.92
2	Y	609	CHL	C1B-CHB-C4A	-3.45	123.29	130.12
6	G	617	NEX	C20-C13-C14	-3.45	118.10	122.92
6	N	618	NEX	C20-C13-C14	-3.44	118.10	122.92
5	N	620	XAT	C11-C12-C13	-3.44	116.76	126.42
3	N	612	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
2	N	608	CHL	C1B-CHB-C4A	-3.40	123.37	130.12
3	N	611	CLA	CMB-C2B-C1B	-3.38	123.27	128.46
3	Y	614	CLA	CMB-C2B-C1B	-3.37	123.28	128.46
2	G	609	CHL	CMB-C2B-C3B	3.37	130.98	124.68
4	G	616	LUT	C7-C8-C9	-3.37	121.14	126.23
4	N	616	LUT	C35-C34-C33	-3.37	122.50	127.31
2	N	606	CHL	CMB-C2B-C3B	3.36	130.97	124.68
3	Y	614	CLA	C4A-NA-C1A	3.36	108.22	106.71
2	Y	605	CHL	CMB-C2B-C1B	-3.36	123.30	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	N	615	LUT	C21-C26-C27	-3.35	108.46	112.70
5	N	617	XAT	C31-C30-C29	-3.35	122.53	127.31
3	N	614	CLA	CMB-C2B-C1B	-3.35	123.32	128.46
4	Y	616	LUT	C35-C34-C33	-3.34	122.54	127.31
4	N	616	LUT	C15-C14-C13	-3.33	122.55	127.31
2	G	601	CHL	C1B-CHB-C4A	-3.33	123.52	130.12
3	G	614	CLA	CMB-C2B-C1B	-3.33	123.34	128.46
4	N	616	LUT	C31-C30-C29	-3.33	122.56	127.31
2	G	607	CHL	CMB-C2B-C1B	-3.32	123.36	128.46
4	Y	615	LUT	C15-C14-C13	-3.31	122.58	127.31
4	G	615	LUT	C11-C10-C9	-3.31	122.58	127.31
3	G	602	CLA	CMB-C2B-C1B	-3.31	123.37	128.46
2	N	608	CHL	CMB-C2B-C1B	-3.30	123.39	128.46
5	N	617	XAT	C11-C12-C13	-3.30	117.14	126.42
3	Y	610	CLA	CMB-C2B-C1B	-3.30	123.40	128.46
2	Y	601	CHL	CMB-C2B-C1B	-3.28	123.42	128.46
4	Y	616	LUT	C7-C8-C9	-3.28	121.28	126.23
4	G	615	LUT	C15-C14-C13	-3.28	122.63	127.31
2	N	607	CHL	CMB-C2B-C3B	3.28	130.81	124.68
3	Y	602	CLA	C1B-CHB-C4A	-3.27	123.65	130.12
2	Y	607	CHL	CHD-C1D-ND	-3.26	121.46	124.45
2	Y	605	CHL	C4A-NA-C1A	3.26	108.17	106.71
5	N	620	XAT	C17-C1-C2	-3.25	103.33	108.98
3	Y	613	CLA	CMB-C2B-C3B	3.25	130.76	124.68
5	N	620	XAT	C18-C5-C4	3.23	117.91	114.28
3	N	611	CLA	C1B-CHB-C4A	-3.23	123.73	130.12
4	Y	616	LUT	C11-C10-C9	-3.22	122.71	127.31
5	G	619	XAT	C11-C12-C13	-3.22	117.37	126.42
4	N	616	LUT	C11-C10-C9	-3.22	122.72	127.31
5	G	619	XAT	C31-C30-C29	-3.20	122.74	127.31
3	Y	604	CLA	O2D-CGD-O1D	-3.20	117.58	123.84
4	G	615	LUT	C7-C8-C9	-3.18	121.42	126.23
2	Y	606	CHL	CHD-C1D-ND	-3.17	121.55	124.45
6	G	617	NEX	C32-C33-C34	3.16	123.79	118.94
2	Y	609	CHL	CHD-C1D-ND	-3.16	121.55	124.45
6	N	618	NEX	C32-C33-C34	3.15	123.77	118.94
2	Y	605	CHL	O2D-CGD-O1D	-3.15	117.69	123.84
6	Y	617	NEX	C32-C33-C34	3.14	123.76	118.94
3	G	611	CLA	O2D-CGD-O1D	-3.14	117.71	123.84
3	G	610	CLA	CMB-C2B-C3B	3.14	130.54	124.68
2	N	606	CHL	CHD-C1D-ND	-3.13	121.58	124.45
3	Y	610	CLA	C4A-NA-C1A	3.13	108.11	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	610	CLA	O2D-CGD-O1D	-3.12	117.74	123.84
2	G	608	CHL	CMB-C2B-C1B	-3.12	123.67	128.46
2	Y	601	CHL	C1B-CHB-C4A	-3.12	123.94	130.12
3	N	603	CLA	CMB-C2B-C1B	-3.12	123.67	128.46
2	G	605	CHL	C2A-C1A-CHA	3.11	129.29	123.86
6	G	617	NEX	C12-C13-C14	3.11	123.71	118.94
2	Y	607	CHL	CMB-C2B-C3B	3.11	130.49	124.68
2	G	606	CHL	O2D-CGD-O1D	-3.11	117.77	123.84
3	Y	614	CLA	C1B-CHB-C4A	-3.10	123.97	130.12
2	N	601	CHL	CMB-C2B-C3B	3.10	130.49	124.68
2	G	601	CHL	CMB-C2B-C3B	3.10	130.47	124.68
3	N	602	CLA	O2D-CGD-O1D	-3.09	117.79	123.84
6	Y	617	NEX	C12-C13-C14	3.09	123.68	118.94
6	N	618	NEX	C12-C13-C14	3.08	123.67	118.94
3	N	602	CLA	C1B-CHB-C4A	-3.08	124.02	130.12
2	G	607	CHL	CMB-C2B-C3B	3.07	130.43	124.68
3	N	604	CLA	C1B-CHB-C4A	-3.07	124.03	130.12
4	Y	615	LUT	C7-C8-C9	-3.07	121.60	126.23
3	Y	611	CLA	C1B-CHB-C4A	-3.06	124.05	130.12
2	N	605	CHL	O2D-CGD-O1D	-3.06	117.86	123.84
4	Y	615	LUT	C35-C34-C33	-3.05	122.95	127.31
3	G	611	CLA	C1B-CHB-C4A	-3.05	124.08	130.12
3	G	604	CLA	C1B-CHB-C4A	-3.04	124.09	130.12
2	Y	601	CHL	CMB-C2B-C3B	3.04	130.36	124.68
3	Y	604	CLA	C1B-CHB-C4A	-3.03	124.11	130.12
3	G	603	CLA	CMB-C2B-C3B	3.03	130.35	124.68
3	Y	610	CLA	CMB-C2B-C3B	3.03	130.35	124.68
3	G	614	CLA	C1B-CHB-C4A	-3.02	124.13	130.12
5	N	620	XAT	C5-C4-C3	-3.02	106.77	112.75
6	Y	617	NEX	C19-C9-C10	-3.02	118.69	122.92
6	N	618	NEX	C19-C9-C10	-3.01	118.71	122.92
3	N	610	CLA	CMB-C2B-C3B	3.00	130.30	124.68
7	N	619	LHG	O7-C7-C8	3.00	117.97	111.50
2	G	607	CHL	C2A-C1A-CHA	3.00	129.10	123.86
3	G	612	CLA	CAA-C2A-C3A	-3.00	104.57	112.78
6	G	617	NEX	C19-C9-C10	-2.99	118.73	122.92
5	G	619	XAT	C18-C5-C4	2.99	117.64	114.28
3	G	602	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
3	G	610	CLA	C4A-NA-C1A	2.98	108.05	106.71
3	Y	603	CLA	O2D-CGD-O1D	-2.97	118.02	123.84
3	G	602	CLA	C1B-CHB-C4A	-2.97	124.24	130.12
5	N	617	XAT	C18-C5-C4	2.97	117.62	114.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	609	CHL	O2D-CGD-O1D	-2.97	118.04	123.84
3	Y	611	CLA	CMB-C2B-C3B	2.96	130.22	124.68
3	G	612	CLA	C4A-NA-C1A	2.96	108.03	106.71
2	G	605	CHL	O2D-CGD-O1D	-2.95	118.06	123.84
3	Y	603	CLA	CMB-C2B-C3B	2.95	130.21	124.68
5	N	620	XAT	C6-C7-C8	-2.95	119.75	125.99
6	N	618	NEX	C28-C29-C30	2.95	123.47	118.94
6	Y	617	NEX	C28-C29-C30	2.95	123.47	118.94
3	N	604	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
2	Y	601	CHL	CHD-C1D-ND	-2.94	121.75	124.45
2	N	605	CHL	CMB-C2B-C3B	2.94	130.19	124.68
3	Y	603	CLA	CAA-C2A-C3A	-2.94	104.73	112.78
3	Y	614	CLA	CMB-C2B-C3B	2.93	130.16	124.68
4	G	616	LUT	C21-C26-C27	-2.93	109.00	112.70
6	G	617	NEX	C28-C29-C30	2.93	123.43	118.94
2	Y	601	CHL	O2D-CGD-O1D	-2.91	118.14	123.84
3	G	612	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
2	G	606	CHL	CMB-C2B-C3B	2.91	130.13	124.68
2	Y	607	CHL	C2A-C1A-CHA	2.91	128.95	123.86
3	Y	603	CLA	CHB-C4A-NA	2.91	128.53	124.51
3	N	614	CLA	O2D-CGD-O1D	-2.91	118.16	123.84
2	Y	608	CHL	C1B-CHB-C4A	-2.91	124.36	130.12
2	G	605	CHL	CMB-C2B-C3B	2.90	130.10	124.68
2	N	609	CHL	O2D-CGD-CBD	2.90	116.42	111.27
2	N	607	CHL	C2A-C1A-CHA	2.90	128.93	123.86
3	G	612	CLA	C1B-CHB-C4A	-2.89	124.39	130.12
2	G	609	CHL	O2D-CGD-O1D	-2.89	118.19	123.84
2	G	609	CHL	C1D-ND-C4D	2.88	108.38	106.33
3	Y	614	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
3	N	611	CLA	CMB-C2B-C3B	2.87	130.05	124.68
3	Y	604	CLA	C5-C3-C2	-2.87	115.32	121.12
5	N	620	XAT	C7-C8-C9	-2.87	121.08	125.53
3	G	610	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
3	N	603	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
3	N	612	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
3	N	613	CLA	C1B-CHB-C4A	-2.84	124.48	130.12
3	G	614	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
2	G	601	CHL	O2D-CGD-O1D	-2.83	118.31	123.84
2	G	606	CHL	CHD-C1D-ND	-2.82	121.86	124.45
3	Y	602	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
4	N	616	LUT	C7-C8-C9	-2.82	121.98	126.23
2	N	607	CHL	O2D-CGD-O1D	-2.80	118.36	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Y	609	CHL	O2D-CGD-O1D	-2.80	118.36	123.84
3	Y	613	CLA	C1B-CHB-C4A	-2.80	124.57	130.12
3	Y	603	CLA	C1B-CHB-C4A	-2.80	124.57	130.12
2	N	601	CHL	CHD-C1D-ND	-2.80	121.88	124.45
3	N	603	CLA	CAA-C2A-C3A	-2.80	105.12	112.78
3	G	611	CLA	CMB-C2B-C3B	2.80	129.91	124.68
3	G	613	CLA	C1B-CHB-C4A	-2.80	124.58	130.12
3	Y	610	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
2	N	606	CHL	O2D-CGD-O1D	-2.78	118.40	123.84
4	Y	615	LUT	C21-C26-C27	-2.78	109.19	112.70
2	G	601	CHL	OMC-CMC-C2C	-2.78	119.41	125.69
2	Y	608	CHL	CMB-C2B-C3B	2.78	129.87	124.68
3	N	603	CLA	C1B-CHB-C4A	-2.77	124.64	130.12
2	N	609	CHL	CHD-C1D-C2D	2.77	131.28	125.48
2	G	608	CHL	C1B-CHB-C4A	-2.77	124.64	130.12
2	G	601	CHL	C3C-C4C-NC	-2.77	107.47	110.57
7	G	618	LHG	O7-C7-C8	2.76	117.45	111.50
2	G	609	CHL	CHD-C1D-C2D	2.76	131.26	125.48
4	G	616	LUT	C11-C10-C9	-2.76	123.37	127.31
5	N	617	XAT	C5-C4-C3	-2.75	107.30	112.75
3	N	603	CLA	CHB-C4A-NA	2.75	128.31	124.51
3	N	612	CLA	CMB-C2B-C3B	2.75	129.82	124.68
5	G	619	XAT	C5-C4-C3	-2.73	107.35	112.75
2	Y	608	CHL	O2D-CGD-O1D	-2.73	118.50	123.84
2	G	606	CHL	O2D-CGD-CBD	2.73	116.11	111.27
3	N	613	CLA	O2A-CGA-O1A	-2.72	116.72	123.59
2	G	608	CHL	O2D-CGD-O1D	-2.72	118.52	123.84
3	G	613	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
3	N	614	CLA	C1B-CHB-C4A	-2.72	124.73	130.12
3	G	603	CLA	C1B-CHB-C4A	-2.72	124.73	130.12
3	G	603	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
3	N	614	CLA	CMB-C2B-C3B	2.70	129.73	124.68
3	G	602	CLA	CMB-C2B-C3B	2.70	129.73	124.68
2	G	606	CHL	C2A-C1A-CHA	2.69	128.56	123.86
3	N	611	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
2	Y	609	CHL	CAC-C3C-C4C	2.69	128.30	124.81
3	G	614	CLA	CMB-C2B-C3B	2.69	129.70	124.68
3	N	611	CLA	CHB-C4A-NA	2.68	128.21	124.51
3	Y	613	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
2	Y	605	CHL	CMB-C2B-C3B	2.66	129.66	124.68
2	G	609	CHL	C2D-C1D-ND	-2.66	108.14	110.10
2	Y	606	CHL	C1-C2-C3	-2.66	122.45	126.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Y	611	CLA	CHB-C4A-NA	2.65	128.18	124.51
2	Y	607	CHL	O2D-CGD-O1D	-2.65	118.66	123.84
3	N	602	CLA	CHD-C1D-ND	-2.64	122.02	124.45
3	N	613	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
3	G	603	CLA	CHB-C4A-NA	2.63	128.15	124.51
3	Y	614	CLA	CHB-C4A-NA	2.63	128.14	124.51
5	N	617	XAT	C27-C28-C29	-2.63	121.46	125.53
2	N	605	CHL	C2A-C1A-CHA	2.62	128.45	123.86
5	N	617	XAT	C15-C35-C34	-2.62	118.10	123.47
5	N	620	XAT	C31-C30-C29	-2.61	123.58	127.31
2	N	609	CHL	C1D-ND-C4D	2.61	108.19	106.33
3	N	610	CLA	CHB-C4A-NA	2.61	128.12	124.51
2	Y	605	CHL	C2A-C1A-CHA	2.60	128.41	123.86
2	N	609	CHL	C2D-C1D-ND	-2.60	108.19	110.10
2	N	601	CHL	O2D-CGD-O1D	-2.60	118.75	123.84
4	Y	616	LUT	C35-C15-C14	-2.60	118.16	123.47
3	G	613	CLA	CHB-C4A-NA	2.59	128.09	124.51
2	N	608	CHL	O2D-CGD-O1D	-2.59	118.78	123.84
5	G	619	XAT	C7-C8-C9	-2.58	121.52	125.53
3	N	612	CLA	C1B-CHB-C4A	-2.58	125.00	130.12
2	N	606	CHL	C1-C2-C3	-2.58	122.58	126.75
2	N	608	CHL	CMB-C2B-C3B	2.58	129.50	124.68
4	Y	616	LUT	C38-C25-C24	-2.57	118.05	123.56
2	Y	606	CHL	CBA-CAA-C2A	-2.57	106.27	113.86
5	G	619	XAT	C15-C35-C34	-2.57	118.21	123.47
7	Y	618	LHG	O8-C23-C24	2.57	119.96	111.91
4	G	615	LUT	C18-C5-C6	-2.56	121.65	124.53
3	N	612	CLA	CHB-C4A-NA	2.56	128.05	124.51
3	Y	610	CLA	CHB-C4A-NA	2.55	128.04	124.51
4	G	616	LUT	C38-C25-C24	-2.55	118.09	123.56
2	Y	609	CHL	CMB-C2B-C3B	2.55	129.46	124.68
3	N	614	CLA	CHB-C4A-NA	2.55	128.04	124.51
3	Y	611	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
3	G	612	CLA	CHB-C4A-NA	2.53	128.01	124.51
2	G	609	CHL	O2D-CGD-CBD	2.53	115.77	111.27
2	Y	606	CHL	O2D-CGD-O1D	-2.53	118.89	123.84
2	G	608	CHL	CHD-C1D-ND	-2.53	122.13	124.45
3	N	602	CLA	CHB-C4A-NA	2.52	128.00	124.51
2	Y	606	CHL	C2A-C1A-CHA	2.52	128.26	123.86
3	Y	602	CLA	CHB-C4A-NA	2.51	127.99	124.51
2	G	608	CHL	C2D-C1D-ND	-2.51	108.26	110.10
4	G	615	LUT	C38-C25-C24	-2.51	118.19	123.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	616	LUT	C16-C1-C6	-2.50	106.25	110.30
4	Y	615	LUT	C2-C3-C4	2.50	113.72	110.30
2	Y	601	CHL	C2D-C1D-ND	-2.50	108.27	110.10
2	N	601	CHL	C1-C2-C3	-2.49	121.73	126.04
3	Y	612	CLA	CAA-C2A-C3A	-2.49	105.96	112.78
3	G	604	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
2	Y	609	CHL	C16-C15-C13	-2.49	107.88	115.92
3	G	604	CLA	CHB-C4A-NA	2.48	127.95	124.51
3	Y	612	CLA	O2D-CGD-O1D	-2.48	118.99	123.84
3	G	610	CLA	CHB-C4A-NA	2.48	127.94	124.51
2	G	605	CHL	C3C-C4C-NC	-2.48	107.79	110.57
2	Y	608	CHL	C2A-C1A-CHA	2.47	128.18	123.86
4	G	615	LUT	C35-C15-C14	-2.47	118.42	123.47
7	N	619	LHG	O8-C23-C24	2.47	119.65	111.91
3	Y	612	CLA	C1B-CHB-C4A	-2.46	125.24	130.12
3	Y	612	CLA	CMB-C2B-C3B	2.46	129.27	124.68
4	G	615	LUT	C30-C31-C32	-2.45	115.56	123.22
3	G	613	CLA	CHD-C1D-ND	-2.45	122.20	124.45
6	Y	617	NEX	C27-C28-C29	-2.45	121.73	125.53
5	N	617	XAT	C7-C8-C9	-2.44	121.74	125.53
3	N	603	CLA	CMB-C2B-C3B	2.44	129.24	124.68
3	Y	613	CLA	CHB-C4A-NA	2.43	127.88	124.51
2	G	609	CHL	OMC-CMC-C2C	-2.43	120.19	125.69
6	G	617	NEX	C27-C28-C29	-2.43	121.76	125.53
2	G	609	CHL	C2A-C1A-CHA	2.42	128.10	123.86
4	Y	615	LUT	C18-C5-C6	-2.42	121.81	124.53
5	N	617	XAT	C6-C7-C8	-2.42	120.88	125.99
6	N	618	NEX	C27-C28-C29	-2.42	121.78	125.53
2	Y	601	CHL	OMC-CMC-C2C	-2.41	120.23	125.69
2	G	607	CHL	O2D-CGD-O1D	-2.41	119.13	123.84
3	N	604	CLA	C1-C2-C3	-2.40	121.89	126.04
2	G	609	CHL	O2A-CGA-O1A	-2.40	117.54	123.59
5	G	619	XAT	C6-C7-C8	-2.39	120.93	125.99
3	Y	604	CLA	CHB-C4A-NA	2.39	127.81	124.51
2	Y	607	CHL	CAA-C2A-C3A	-2.38	106.27	112.78
2	G	607	CHL	C1D-CHD-C4C	-2.37	120.94	126.06
3	N	613	CLA	CHD-C1D-ND	-2.37	122.28	124.45
3	G	610	CLA	CMC-C2C-C1C	2.36	128.64	125.04
3	G	602	CLA	CHB-C4A-NA	2.36	127.78	124.51
2	Y	608	CHL	CHB-C4A-NA	2.36	127.78	124.51
3	N	604	CLA	CHD-C1D-ND	-2.36	122.29	124.45
4	N	615	LUT	C35-C15-C14	-2.35	118.66	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	607	CHL	OMC-CMC-C2C	-2.34	120.39	125.69
3	G	613	CLA	O2A-CGA-O1A	-2.34	117.68	123.59
3	G	610	CLA	CAC-C3C-C2C	-2.34	123.53	127.53
4	N	615	LUT	C22-C23-C24	-2.34	109.08	111.74
3	N	613	CLA	CHB-C4A-NA	2.33	127.73	124.51
5	N	620	XAT	C15-C35-C34	-2.33	118.71	123.47
2	N	606	CHL	C2A-C1A-CHA	2.33	127.93	123.86
2	G	601	CHL	O2A-CGA-O1A	-2.32	117.75	123.59
2	Y	607	CHL	OMC-CMC-C2C	-2.31	120.46	125.69
2	G	608	CHL	CMB-C2B-C3B	2.30	128.99	124.68
4	N	615	LUT	C30-C31-C32	-2.30	116.04	123.22
5	G	619	XAT	C27-C28-C29	-2.29	121.97	125.53
2	N	609	CHL	OMC-CMC-C2C	-2.29	120.50	125.69
3	G	602	CLA	CHD-C1D-ND	-2.29	122.35	124.45
3	G	611	CLA	O2D-CGD-CBD	2.29	115.33	111.27
3	N	610	CLA	O2A-CGA-O1A	-2.29	117.83	123.59
3	N	604	CLA	CHB-C4A-NA	2.28	127.67	124.51
2	G	601	CHL	C2A-C1A-CHA	2.28	127.84	123.86
7	G	618	LHG	O8-C23-O10	-2.27	117.85	123.59
2	G	608	CHL	CHB-C4A-NA	2.27	127.66	124.51
4	Y	615	LUT	C38-C25-C24	-2.27	118.71	123.56
5	N	620	XAT	C27-C28-C29	-2.26	122.02	125.53
4	N	616	LUT	C38-C25-C24	-2.26	118.72	123.56
2	Y	601	CHL	C1-C2-C3	-2.26	122.13	126.04
5	N	620	XAT	O3-C3-C2	-2.26	105.32	109.80
2	N	606	CHL	O2D-CGD-CBD	2.25	115.27	111.27
2	N	607	CHL	CHA-C1A-NA	-2.25	121.24	126.40
2	Y	605	CHL	O2A-CGA-O1A	-2.25	117.91	123.59
3	N	602	CLA	O2D-CGD-CBD	2.25	115.26	111.27
3	G	614	CLA	CHD-C1D-ND	-2.24	122.39	124.45
4	Y	615	LUT	C8-C7-C6	-2.24	120.92	127.20
2	G	607	CHL	CHA-C1A-NA	-2.23	121.29	126.40
3	Y	603	CLA	C1-C2-C3	-2.23	122.19	126.04
3	Y	604	CLA	O2D-CGD-CBD	2.23	115.22	111.27
2	N	605	CHL	C3C-C4C-NC	-2.22	108.08	110.57
2	N	608	CHL	CHB-C4A-NA	2.22	127.59	124.51
3	G	611	CLA	CHB-C4A-NA	2.22	127.58	124.51
2	G	605	CHL	C2D-C1D-ND	-2.21	108.47	110.10
5	G	619	XAT	O3-C3-C2	-2.21	105.40	109.80
2	Y	606	CHL	C3A-C2A-C1A	2.21	104.65	101.34
3	G	604	CLA	CHD-C1D-ND	-2.21	122.42	124.45
4	N	616	LUT	C16-C1-C6	-2.21	106.72	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	615	LUT	C22-C23-C24	-2.21	109.23	111.74
2	Y	608	CHL	CHD-C1D-ND	-2.20	122.43	124.45
4	Y	615	LUT	C22-C23-C24	-2.20	109.23	111.74
3	N	614	CLA	CHD-C1D-ND	-2.20	122.43	124.45
2	Y	606	CHL	O2A-CGA-O1A	-2.20	118.05	123.59
2	G	609	CHL	C3C-C4C-NC	-2.20	108.11	110.57
2	G	607	CHL	CAA-C2A-C3A	-2.20	106.77	112.78
2	N	601	CHL	OMC-CMC-C2C	-2.20	120.72	125.69
3	N	612	CLA	CAA-C2A-C3A	-2.19	106.77	112.78
2	N	609	CHL	O2A-CGA-O1A	-2.19	118.06	123.59
2	G	605	CHL	CHD-C1D-ND	-2.19	122.44	124.45
3	Y	610	CLA	CHD-C1D-ND	-2.19	122.44	124.45
2	N	609	CHL	C2A-C1A-CHA	2.19	127.68	123.86
2	N	609	CHL	C3C-C4C-NC	-2.19	108.12	110.57
2	N	607	CHL	C1D-CHD-C4C	-2.18	121.35	126.06
3	Y	613	CLA	CHD-C1D-ND	-2.18	122.45	124.45
3	Y	604	CLA	C1-C2-C3	-2.18	122.27	126.04
2	N	607	CHL	CAA-C2A-C3A	-2.18	106.81	112.78
2	Y	605	CHL	CHD-C1D-ND	-2.17	122.46	124.45
2	Y	609	CHL	O2A-CGA-O1A	-2.17	118.13	123.59
2	N	609	CHL	C1D-CHD-C4C	-2.16	121.39	126.06
4	Y	616	LUT	C1-C2-C3	2.16	118.53	113.64
2	G	601	CHL	C2D-C1D-ND	-2.16	108.51	110.10
5	N	620	XAT	C40-C33-C34	-2.16	119.90	122.92
2	N	608	CHL	OMC-CMC-C2C	-2.16	120.81	125.69
3	G	610	CLA	C1-C2-C3	-2.16	122.31	126.04
2	G	605	CHL	CHA-C1A-NA	-2.15	121.47	126.40
2	G	609	CHL	CHD-C4C-C3C	2.15	128.00	124.84
2	N	601	CHL	C16-C15-C13	-2.15	108.97	115.92
2	Y	601	CHL	CHD-C1D-C2D	2.15	129.99	125.48
2	Y	607	CHL	CHA-C1A-NA	-2.15	121.48	126.40
2	G	607	CHL	CHD-C1D-C2D	2.14	129.98	125.48
2	Y	605	CHL	C3C-C4C-NC	-2.14	108.17	110.57
3	G	612	CLA	C2C-C1C-NC	2.13	111.97	109.97
3	G	610	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
2	G	606	CHL	O2A-CGA-O1A	-2.13	118.22	123.59
3	Y	614	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
2	N	605	CHL	O2A-CGA-O1A	-2.12	118.23	123.59
4	G	616	LUT	C35-C34-C33	-2.12	124.28	127.31
7	Y	618	LHG	C5-O7-C7	-2.12	112.57	117.79
4	G	616	LUT	C15-C35-C34	-2.12	119.13	123.47
4	Y	615	LUT	C31-C30-C29	-2.12	124.29	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	606	CHL	CBA-CAA-C2A	-2.12	107.62	113.86
2	N	607	CHL	CHD-C1D-C2D	2.12	129.92	125.48
4	G	615	LUT	C2-C3-C4	2.11	113.19	110.30
3	Y	612	CLA	CHB-C4A-NA	2.11	127.43	124.51
2	N	601	CHL	C2D-C1D-ND	-2.11	108.55	110.10
4	Y	616	LUT	C2-C3-C4	2.10	113.19	110.30
2	G	609	CHL	C1D-CHD-C4C	-2.10	121.52	126.06
2	N	601	CHL	C7-C6-C5	-2.10	107.67	113.36
4	N	615	LUT	C38-C25-C24	-2.10	119.08	123.56
3	Y	613	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
4	G	616	LUT	C3-C4-C5	-2.09	107.69	111.85
4	G	615	LUT	C8-C7-C6	-2.09	121.34	127.20
5	N	617	XAT	C24-C23-C22	-2.09	106.74	110.77
2	Y	607	CHL	CHD-C1D-C2D	2.09	129.86	125.48
4	Y	615	LUT	C35-C15-C14	-2.08	119.20	123.47
2	Y	601	CHL	O1D-CGD-CBD	2.08	128.75	124.48
2	Y	607	CHL	C1D-CHD-C4C	-2.08	121.56	126.06
2	N	606	CHL	O2A-CGA-O1A	-2.08	118.35	123.59
2	N	608	CHL	C2A-C1A-CHA	2.07	127.49	123.86
3	G	614	CLA	CHB-C4A-NA	2.07	127.37	124.51
4	N	616	LUT	C35-C15-C14	-2.06	119.24	123.47
3	G	602	CLA	O2D-CGD-CBD	2.06	114.93	111.27
2	N	608	CHL	CHD-C1D-ND	-2.06	122.56	124.45
2	G	601	CHL	C1-C2-C3	-2.06	122.48	126.04
2	Y	609	CHL	CHB-C4A-NA	2.06	127.36	124.51
2	N	606	CHL	C3A-C2A-C1A	2.06	104.42	101.34
2	N	607	CHL	O2D-CGD-CBD	2.06	114.92	111.27
3	N	610	CLA	CMC-C2C-C1C	2.06	128.17	125.04
2	N	609	CHL	CHD-C4C-C3C	2.05	127.86	124.84
2	N	606	CHL	CHB-C4A-NA	2.04	127.33	124.51
3	N	610	CLA	C1-C2-C3	-2.03	122.52	126.04
3	Y	610	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
2	G	606	CHL	C1-C2-C3	-2.03	123.47	126.75
2	G	606	CHL	CHB-C4A-NA	2.03	127.32	124.51
5	N	620	XAT	C25-C24-C23	-2.03	108.74	112.75
3	N	603	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
3	Y	603	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
2	N	605	CHL	CHD-C1D-ND	-2.02	122.60	124.45
2	G	601	CHL	O2D-CGD-CBD	2.01	114.84	111.27
3	N	610	CLA	CAC-C3C-C4C	2.01	127.42	124.81
3	G	603	CLA	CHA-C1A-NA	-2.01	121.80	126.40
4	N	615	LUT	C16-C1-C6	-2.00	107.05	110.30

All (77) chirality outliers are listed below:

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

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Mol	Chain	Res	Type	Atom
2	Y	606	CHL	NA
2	Y	606	CHL	ND
2	Y	606	CHL	NC
2	Y	607	CHL	NA
2	Y	607	CHL	ND
2	Y	607	CHL	NC
2	Y	608	CHL	NA
2	Y	608	CHL	ND
2	Y	608	CHL	NC
2	Y	609	CHL	NA
2	Y	609	CHL	ND
2	Y	609	CHL	NC
3	N	602	CLA	ND
3	N	603	CLA	ND
3	N	604	CLA	ND
3	N	610	CLA	ND
3	N	611	CLA	ND
3	N	612	CLA	ND
3	N	613	CLA	ND
3	N	614	CLA	ND
3	G	602	CLA	ND
3	G	603	CLA	ND
3	G	604	CLA	ND
3	G	610	CLA	ND
3	G	612	CLA	ND
3	G	613	CLA	ND
3	G	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	613	CLA	ND
3	Y	614	CLA	ND

All (645) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	N	601	CHL	C1C-C2C-CMC-OMC
2	N	601	CHL	C3C-C2C-CMC-OMC
2	N	605	CHL	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
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	608	CHL	C1C-C2C-CMC-OMC
2	N	608	CHL	C3C-C2C-CMC-OMC
2	N	609	CHL	C1C-C2C-CMC-OMC
2	N	609	CHL	C3C-C2C-CMC-OMC
2	G	601	CHL	C1C-C2C-CMC-OMC
2	G	601	CHL	C3C-C2C-CMC-OMC
2	G	607	CHL	C2A-CAA-CBA-CGA
2	G	607	CHL	C1C-C2C-CMC-OMC
2	G	607	CHL	C3C-C2C-CMC-OMC
2	G	608	CHL	C3C-C2C-CMC-OMC
2	G	608	CHL	CBD-CGD-O2D-CED
2	G	609	CHL	C1C-C2C-CMC-OMC
2	G	609	CHL	C3C-C2C-CMC-OMC
2	Y	601	CHL	C1C-C2C-CMC-OMC
2	Y	601	CHL	C3C-C2C-CMC-OMC
2	Y	601	CHL	CHA-CBD-CGD-O1D
2	Y	601	CHL	CHA-CBD-CGD-O2D
2	Y	605	CHL	CBD-CGD-O2D-CED
2	Y	606	CHL	CBA-CGA-O2A-C1
2	Y	606	CHL	C1C-C2C-CMC-OMC
2	Y	606	CHL	C3C-C2C-CMC-OMC
2	Y	607	CHL	C2A-CAA-CBA-CGA
2	Y	607	CHL	C1C-C2C-CMC-OMC
2	Y	607	CHL	C3C-C2C-CMC-OMC
2	Y	608	CHL	C1C-C2C-CMC-OMC
2	Y	608	CHL	C3C-C2C-CMC-OMC
2	Y	609	CHL	C1C-C2C-CMC-OMC
2	Y	609	CHL	C3C-C2C-CMC-OMC
3	N	602	CLA	CHA-CBD-CGD-O2D
3	N	611	CLA	CHA-CBD-CGD-O1D
3	N	611	CLA	CHA-CBD-CGD-O2D
3	N	614	CLA	CHA-CBD-CGD-O1D
3	N	614	CLA	CHA-CBD-CGD-O2D
3	G	604	CLA	C1A-C2A-CAA-CBA
3	G	613	CLA	CBD-CGD-O2D-CED
3	G	614	CLA	CBD-CGD-O2D-CED
3	Y	602	CLA	CBD-CGD-O2D-CED
3	Y	604	CLA	C1A-C2A-CAA-CBA
3	Y	611	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
4	N	615	LUT	C27-C28-C29-C39
4	G	615	LUT	C27-C28-C29-C30
4	G	615	LUT	C27-C28-C29-C39
4	Y	615	LUT	C27-C28-C29-C39
5	N	617	XAT	O4-C6-C7-C8
5	N	617	XAT	C7-C8-C9-C10
5	N	617	XAT	C7-C8-C9-C19
5	N	620	XAT	O4-C6-C7-C8
5	N	620	XAT	C7-C8-C9-C10
5	N	620	XAT	C7-C8-C9-C19
5	N	620	XAT	C31-C32-C33-C34
5	N	620	XAT	C31-C32-C33-C40
5	G	619	XAT	O4-C6-C7-C8
5	G	619	XAT	C7-C8-C9-C10
5	G	619	XAT	C7-C8-C9-C19
5	G	619	XAT	O24-C26-C27-C28
5	G	619	XAT	C31-C32-C33-C34
5	G	619	XAT	C31-C32-C33-C40
6	N	618	NEX	C11-C10-C9-C8
6	N	618	NEX	C11-C10-C9-C19
6	N	618	NEX	C10-C11-C12-C13
6	G	617	NEX	C11-C10-C9-C8
6	G	617	NEX	C11-C10-C9-C19
6	G	617	NEX	C10-C11-C12-C13
6	Y	617	NEX	C11-C10-C9-C8
6	Y	617	NEX	C11-C10-C9-C19
6	Y	617	NEX	C10-C11-C12-C13
7	G	618	LHG	C3-O3-P-O5
7	G	618	LHG	C4-O6-P-O4
7	Y	618	LHG	O1-C1-C2-C3
7	Y	618	LHG	C2-C3-O3-P
7	Y	618	LHG	C3-O3-P-O4
7	Y	618	LHG	C4-O6-P-O3
3	Y	604	CLA	O1D-CGD-O2D-CED
2	N	605	CHL	CBD-CGD-O2D-CED
2	G	601	CHL	CBD-CGD-O2D-CED
3	N	610	CLA	CBD-CGD-O2D-CED
3	G	603	CLA	CBD-CGD-O2D-CED
3	Y	603	CLA	CBD-CGD-O2D-CED
3	Y	604	CLA	CBD-CGD-O2D-CED
3	Y	613	CLA	CBD-CGD-O2D-CED
3	Y	614	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
2	N	606	CHL	O1A-CGA-O2A-C1
2	Y	606	CHL	O1A-CGA-O2A-C1
3	G	613	CLA	O1D-CGD-O2D-CED
3	G	614	CLA	O1D-CGD-O2D-CED
3	Y	602	CLA	O1D-CGD-O2D-CED
2	N	606	CHL	CBA-CGA-O2A-C1
2	N	607	CHL	CBD-CGD-O2D-CED
3	N	613	CLA	CBD-CGD-O2D-CED
3	N	614	CLA	CBD-CGD-O2D-CED
3	G	612	CLA	CBD-CGD-O2D-CED
3	Y	612	CLA	CBD-CGD-O2D-CED
2	N	607	CHL	O1A-CGA-O2A-C1
2	G	606	CHL	O1A-CGA-O2A-C1
2	G	607	CHL	O1A-CGA-O2A-C1
2	Y	607	CHL	O1A-CGA-O2A-C1
3	Y	614	CLA	O1A-CGA-O2A-C1
7	N	619	LHG	O10-C23-O8-C6
7	G	618	LHG	O10-C23-O8-C6
7	Y	618	LHG	O10-C23-O8-C6
2	G	608	CHL	O1D-CGD-O2D-CED
2	Y	605	CHL	O1D-CGD-O2D-CED
2	Y	601	CHL	CBD-CGD-O2D-CED
3	N	604	CLA	CBD-CGD-O2D-CED
3	Y	613	CLA	O1D-CGD-O2D-CED
3	Y	611	CLA	C3-C5-C6-C7
2	G	606	CHL	CBA-CGA-O2A-C1
2	G	607	CHL	CBA-CGA-O2A-C1
7	G	618	LHG	C24-C23-O8-C6
7	Y	618	LHG	C24-C23-O8-C6
2	N	606	CHL	CBD-CGD-O2D-CED
2	N	607	CHL	C2A-CAA-CBA-CGA
2	G	607	CHL	C3-C5-C6-C7
3	G	604	CLA	C3-C5-C6-C7
3	Y	612	CLA	C3-C5-C6-C7
2	N	607	CHL	CBA-CGA-O2A-C1
2	Y	607	CHL	CBA-CGA-O2A-C1
3	Y	614	CLA	CBA-CGA-O2A-C1
7	N	619	LHG	C24-C23-O8-C6
2	N	605	CHL	O1D-CGD-O2D-CED
3	N	610	CLA	O1D-CGD-O2D-CED
3	G	610	CLA	CBD-CGD-O2D-CED
3	Y	610	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
3	Y	603	CLA	O1D-CGD-O2D-CED
4	G	616	LUT	C29-C30-C31-C32
2	G	601	CHL	C3-C5-C6-C7
3	N	614	CLA	CBA-CGA-O2A-C1
3	N	603	CLA	CBD-CGD-O2D-CED
7	Y	618	LHG	C15-C16-C17-C18
3	N	614	CLA	O1A-CGA-O2A-C1
3	Y	614	CLA	O1D-CGD-O2D-CED
2	Y	607	CHL	C3-C5-C6-C7
3	N	604	CLA	C3-C5-C6-C7
3	N	611	CLA	C3-C5-C6-C7
3	G	612	CLA	C3-C5-C6-C7
7	Y	618	LHG	C33-C34-C35-C36
3	G	614	CLA	CBA-CGA-O2A-C1
7	Y	618	LHG	C17-C18-C19-C20
3	G	603	CLA	O1D-CGD-O2D-CED
2	G	601	CHL	O1D-CGD-O2D-CED
7	N	619	LHG	C28-C29-C30-C31
3	G	612	CLA	O1D-CGD-O2D-CED
3	N	613	CLA	O1D-CGD-O2D-CED
3	G	614	CLA	O1A-CGA-O2A-C1
3	N	614	CLA	O1D-CGD-O2D-CED
2	N	601	CHL	CBD-CGD-O2D-CED
2	G	601	CHL	C15-C16-C17-C18
3	Y	613	CLA	C13-C15-C16-C17
2	G	608	CHL	C11-C12-C13-C14
2	Y	608	CHL	C11-C12-C13-C14
2	Y	609	CHL	C6-C7-C8-C9
2	Y	609	CHL	C11-C12-C13-C14
3	N	611	CLA	C11-C10-C8-C9
3	Y	612	CLA	O1D-CGD-O2D-CED
2	Y	601	CHL	C15-C16-C17-C18
3	Y	611	CLA	C10-C11-C12-C13
5	N	617	XAT	C11-C12-C13-C20
3	N	611	CLA	C10-C11-C12-C13
3	Y	611	CLA	C15-C16-C17-C18
3	N	603	CLA	C13-C15-C16-C17
3	G	603	CLA	C5-C6-C7-C8
7	Y	618	LHG	O1-C1-C2-O2
3	G	602	CLA	C10-C11-C12-C13
3	Y	612	CLA	CBA-CGA-O2A-C1
2	N	607	CHL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
2	G	607	CHL	C5-C6-C7-C8
7	Y	618	LHG	C23-C24-C25-C26
3	Y	611	CLA	C5-C6-C7-C8
3	N	604	CLA	O1D-CGD-O2D-CED
2	N	608	CHL	C12-C13-C15-C16
2	G	608	CHL	C12-C13-C15-C16
3	N	611	CLA	C6-C7-C8-C10
3	N	612	CLA	C11-C10-C8-C7
3	Y	611	CLA	C6-C7-C8-C10
3	G	613	CLA	C3-C5-C6-C7
2	Y	608	CHL	C2A-CAA-CBA-CGA
2	Y	607	CHL	C5-C6-C7-C8
3	G	612	CLA	C8-C10-C11-C12
3	N	612	CLA	C3-C5-C6-C7
3	N	611	CLA	C5-C6-C7-C8
3	N	611	CLA	C8-C10-C11-C12
3	G	603	CLA	C10-C11-C12-C13
3	G	603	CLA	C15-C16-C17-C18
3	Y	611	CLA	C8-C10-C11-C12
7	N	619	LHG	C4-O6-P-O3
7	G	618	LHG	C4-O6-P-O3
7	Y	618	LHG	C3-O3-P-O6
7	N	619	LHG	C23-C24-C25-C26
3	N	612	CLA	CBA-CGA-O2A-C1
3	G	612	CLA	CBA-CGA-O2A-C1
3	G	604	CLA	C13-C15-C16-C17
2	N	601	CHL	C15-C16-C17-C18
3	N	611	CLA	C13-C15-C16-C17
2	N	608	CHL	C2A-CAA-CBA-CGA
3	G	611	CLA	C3-C5-C6-C7
3	Y	604	CLA	CBA-CGA-O2A-C1
2	Y	601	CHL	O1D-CGD-O2D-CED
2	N	606	CHL	O1D-CGD-O2D-CED
6	N	618	NEX	C20-C13-C14-C15
6	N	618	NEX	C39-C29-C30-C31
6	G	617	NEX	C20-C13-C14-C15
6	G	617	NEX	C39-C29-C30-C31
6	Y	617	NEX	C20-C13-C14-C15
6	Y	617	NEX	C39-C29-C30-C31
7	N	619	LHG	C25-C26-C27-C28
7	Y	618	LHG	C32-C33-C34-C35
2	N	608	CHL	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
7	Y	618	LHG	C30-C31-C32-C33
3	G	610	CLA	O1D-CGD-O2D-CED
3	Y	610	CLA	O1D-CGD-O2D-CED
7	G	618	LHG	C9-C10-C11-C12
6	N	618	NEX	C12-C13-C14-C15
6	N	618	NEX	C28-C29-C30-C31
6	G	617	NEX	C12-C13-C14-C15
6	G	617	NEX	C28-C29-C30-C31
6	Y	617	NEX	C12-C13-C14-C15
6	Y	617	NEX	C28-C29-C30-C31
3	G	612	CLA	O1A-CGA-O2A-C1
3	Y	612	CLA	O1A-CGA-O2A-C1
2	N	609	CHL	C4-C3-C5-C6
7	Y	618	LHG	C24-C25-C26-C27
2	N	609	CHL	C2-C3-C5-C6
2	G	608	CHL	C6-C7-C8-C9
2	Y	609	CHL	C11-C10-C8-C9
3	N	613	CLA	C11-C12-C13-C14
3	Y	612	CLA	C11-C10-C8-C9
3	Y	603	CLA	C2A-CAA-CBA-CGA
3	Y	604	CLA	O1A-CGA-O2A-C1
7	N	619	LHG	C15-C16-C17-C18
4	N	615	LUT	C27-C28-C29-C30
3	N	613	CLA	C3-C5-C6-C7
7	G	618	LHG	C23-C24-C25-C26
7	G	618	LHG	C32-C33-C34-C35
7	G	618	LHG	C14-C15-C16-C17
7	Y	618	LHG	C14-C15-C16-C17
3	Y	613	CLA	C3-C5-C6-C7
2	N	605	CHL	CBA-CGA-O2A-C1
2	N	605	CHL	C3A-C2A-CAA-CBA
2	N	606	CHL	C3A-C2A-CAA-CBA
2	G	601	CHL	C3A-C2A-CAA-CBA
2	G	605	CHL	C3A-C2A-CAA-CBA
2	G	606	CHL	C3A-C2A-CAA-CBA
2	Y	606	CHL	C3A-C2A-CAA-CBA
3	N	603	CLA	C3A-C2A-CAA-CBA
3	G	604	CLA	C3A-C2A-CAA-CBA
3	Y	603	CLA	C3A-C2A-CAA-CBA
3	Y	603	CLA	C10-C11-C12-C13
3	N	612	CLA	O1A-CGA-O2A-C1
7	N	619	LHG	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
3	N	612	CLA	CBD-CGD-O2D-CED
3	N	604	CLA	CBA-CGA-O2A-C1
3	G	611	CLA	CBA-CGA-O2A-C1
2	G	601	CHL	C2A-CAA-CBA-CGA
7	Y	618	LHG	C13-C14-C15-C16
3	N	604	CLA	C13-C15-C16-C17
3	Y	604	CLA	C2-C1-O2A-CGA
3	G	613	CLA	C13-C15-C16-C17
7	G	618	LHG	C25-C26-C27-C28
7	Y	618	LHG	C11-C10-C9-C8
4	G	615	LUT	C1-C6-C7-C8
4	G	615	LUT	C5-C6-C7-C8
4	Y	615	LUT	C1-C6-C7-C8
4	Y	615	LUT	C5-C6-C7-C8
7	G	618	LHG	C29-C30-C31-C32
3	N	603	CLA	O1D-CGD-O2D-CED
2	N	609	CHL	C12-C13-C15-C16
2	G	608	CHL	C6-C7-C8-C10
2	Y	608	CHL	C11-C12-C13-C15
3	N	611	CLA	C12-C13-C15-C16
3	N	613	CLA	C11-C12-C13-C15
3	G	602	CLA	C6-C7-C8-C10
3	G	603	CLA	C12-C13-C15-C16
3	Y	612	CLA	C11-C10-C8-C7
2	N	605	CHL	O1A-CGA-O2A-C1
3	N	604	CLA	O1A-CGA-O2A-C1
3	G	611	CLA	O1A-CGA-O2A-C1
7	N	619	LHG	O9-C7-O7-C5
7	G	618	LHG	O9-C7-O7-C5
7	G	618	LHG	C28-C29-C30-C31
7	N	619	LHG	C8-C7-O7-C5
7	G	618	LHG	C8-C7-O7-C5
7	Y	618	LHG	C8-C7-O7-C5
7	N	619	LHG	C14-C15-C16-C17
2	N	601	CHL	C13-C15-C16-C17
3	N	611	CLA	C15-C16-C17-C18
3	G	612	CLA	C15-C16-C17-C18
2	G	606	CHL	CBD-CGD-O2D-CED
3	G	603	CLA	C3-C5-C6-C7
3	Y	602	CLA	C15-C16-C17-C18
2	N	607	CHL	C14-C13-C15-C16
2	N	609	CHL	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
2	Y	607	CHL	C14-C13-C15-C16
3	N	602	CLA	C6-C7-C8-C9
3	N	603	CLA	C6-C7-C8-C9
3	N	612	CLA	C11-C10-C8-C9
3	G	602	CLA	C6-C7-C8-C9
3	G	603	CLA	C11-C10-C8-C9
3	G	603	CLA	C14-C13-C15-C16
3	G	611	CLA	C14-C13-C15-C16
3	G	612	CLA	C11-C10-C8-C9
3	Y	602	CLA	C2A-CAA-CBA-CGA
2	N	606	CHL	C1A-C2A-CAA-CBA
2	N	609	CHL	C1A-C2A-CAA-CBA
2	G	601	CHL	C1A-C2A-CAA-CBA
2	G	605	CHL	C1A-C2A-CAA-CBA
2	G	606	CHL	C1A-C2A-CAA-CBA
2	G	608	CHL	C1A-C2A-CAA-CBA
2	Y	606	CHL	C1A-C2A-CAA-CBA
3	N	603	CLA	C1A-C2A-CAA-CBA
3	N	604	CLA	C1A-C2A-CAA-CBA
3	Y	602	CLA	C1A-C2A-CAA-CBA
3	Y	603	CLA	C1A-C2A-CAA-CBA
3	Y	614	CLA	C1A-C2A-CAA-CBA
3	G	612	CLA	C16-C17-C18-C20
7	Y	618	LHG	O9-C7-O7-C5
7	G	618	LHG	C10-C11-C12-C13
2	N	607	CHL	C15-C16-C17-C18
3	N	612	CLA	C8-C10-C11-C12
3	N	612	CLA	C10-C11-C12-C13
3	Y	612	CLA	C10-C11-C12-C13
3	G	611	CLA	C8-C10-C11-C12
7	Y	618	LHG	C11-C12-C13-C14
2	G	608	CHL	C5-C6-C7-C8
7	G	618	LHG	C33-C34-C35-C36
7	Y	618	LHG	C35-C36-C37-C38
7	G	618	LHG	C27-C28-C29-C30
2	G	609	CHL	C4-C3-C5-C6
3	G	602	CLA	C15-C16-C17-C18
2	G	605	CHL	C2A-CAA-CBA-CGA
3	G	612	CLA	C16-C17-C18-C19
7	N	619	LHG	C24-C25-C26-C27
7	Y	618	LHG	C31-C32-C33-C34
2	N	607	CHL	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
2	G	607	CHL	C12-C13-C15-C16
2	G	609	CHL	C2-C3-C5-C6
2	Y	607	CHL	C12-C13-C15-C16
3	N	602	CLA	C6-C7-C8-C10
3	N	603	CLA	C6-C7-C8-C10
3	N	603	CLA	C11-C12-C13-C15
3	N	603	CLA	C12-C13-C15-C16
3	G	603	CLA	C11-C10-C8-C7
3	G	611	CLA	C12-C13-C15-C16
3	G	612	CLA	C11-C10-C8-C7
3	G	612	CLA	C11-C12-C13-C15
3	G	612	CLA	C12-C13-C15-C16
3	G	613	CLA	C12-C13-C15-C16
3	Y	603	CLA	C6-C7-C8-C10
3	Y	612	CLA	C11-C12-C13-C15
3	Y	604	CLA	C3-C5-C6-C7
2	N	608	CHL	C14-C13-C15-C16
2	G	607	CHL	C14-C13-C15-C16
2	G	609	CHL	C14-C13-C15-C16
2	Y	607	CHL	C11-C10-C8-C9
2	Y	609	CHL	C14-C13-C15-C16
3	N	611	CLA	C14-C13-C15-C16
3	N	613	CLA	C6-C7-C8-C9
3	G	612	CLA	C11-C12-C13-C14
3	G	612	CLA	C14-C13-C15-C16
3	G	613	CLA	C14-C13-C15-C16
3	Y	603	CLA	C6-C7-C8-C9
3	Y	611	CLA	C6-C7-C8-C9
3	Y	611	CLA	C11-C10-C8-C9
3	Y	612	CLA	C11-C12-C13-C14
3	Y	603	CLA	C8-C10-C11-C12
4	Y	615	LUT	C27-C28-C29-C30
7	G	618	LHG	C26-C27-C28-C29
3	Y	612	CLA	C4-C3-C5-C6
7	G	618	LHG	C15-C16-C17-C18
2	N	601	CHL	C3A-C2A-CAA-CBA
3	Y	604	CLA	C3A-C2A-CAA-CBA
3	N	602	CLA	C10-C11-C12-C13
3	Y	612	CLA	C8-C10-C11-C12
3	N	612	CLA	O1D-CGD-O2D-CED
2	Y	605	CHL	C3C-C2C-CMC-OMC
7	N	619	LHG	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
2	N	608	CHL	O1D-CGD-O2D-CED
7	Y	618	LHG	O6-C4-C5-O7
2	N	601	CHL	O1D-CGD-O2D-CED
7	Y	618	LHG	C34-C35-C36-C37
7	N	619	LHG	O7-C5-C6-O8
2	G	609	CHL	C2-C1-O2A-CGA
3	Y	612	CLA	C2-C3-C5-C6
2	N	607	CHL	C10-C11-C12-C13
3	G	611	CLA	C13-C15-C16-C17
2	N	608	CHL	C11-C10-C8-C9
3	N	604	CLA	C11-C12-C13-C14
3	N	611	CLA	C6-C7-C8-C9
3	G	611	CLA	C11-C10-C8-C9
3	G	602	CLA	C2A-CAA-CBA-CGA
4	N	615	LUT	C1-C6-C7-C8
4	N	615	LUT	C5-C6-C7-C8
4	G	616	LUT	C1-C6-C7-C8
4	G	616	LUT	C5-C6-C7-C8
4	Y	616	LUT	C1-C6-C7-C8
5	N	617	XAT	C11-C12-C13-C14
3	N	613	CLA	C16-C17-C18-C20
7	G	618	LHG	O6-C4-C5-C6
7	Y	618	LHG	O6-C4-C5-C6
2	N	607	CHL	C11-C10-C8-C7
2	G	607	CHL	C11-C10-C8-C7
2	G	609	CHL	C12-C13-C15-C16
2	Y	607	CHL	C11-C10-C8-C7
3	N	604	CLA	C11-C12-C13-C15
3	N	613	CLA	C6-C7-C8-C10
3	G	611	CLA	C11-C10-C8-C7
3	Y	602	CLA	C11-C12-C13-C15
3	Y	611	CLA	C11-C10-C8-C7
4	Y	616	LUT	C29-C30-C31-C32
3	Y	603	CLA	CBA-CGA-O2A-C1
7	N	619	LHG	C29-C30-C31-C32
7	N	619	LHG	C30-C31-C32-C33
2	N	609	CHL	CBA-CGA-O2A-C1
3	G	603	CLA	C13-C15-C16-C17
2	N	605	CHL	CAD-CBD-CGD-O2D
2	Y	606	CHL	CAD-CBD-CGD-O2D
3	N	612	CLA	CAD-CBD-CGD-O2D
3	Y	603	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
3	Y	614	CLA	CAD-CBD-CGD-O2D
2	G	606	CHL	O1D-CGD-O2D-CED
2	Y	608	CHL	C3-C5-C6-C7
7	N	619	LHG	C4-C5-C6-O8
7	G	618	LHG	C4-C5-C6-O8
3	N	614	CLA	O2A-C1-C2-C3
3	G	614	CLA	O2A-C1-C2-C3
2	G	609	CHL	CBA-CGA-O2A-C1
2	N	601	CHL	CHA-CBD-CGD-O1D
2	N	601	CHL	CHA-CBD-CGD-O2D
2	G	601	CHL	CHA-CBD-CGD-O1D
2	G	601	CHL	CHA-CBD-CGD-O2D
2	Y	609	CHL	CHA-CBD-CGD-O1D
3	N	602	CLA	CHA-CBD-CGD-O1D
3	G	602	CLA	CHA-CBD-CGD-O1D
3	G	614	CLA	CHA-CBD-CGD-O1D
3	G	614	CLA	CHA-CBD-CGD-O2D
3	Y	604	CLA	CHA-CBD-CGD-O1D
3	Y	604	CLA	CHA-CBD-CGD-O2D
3	Y	603	CLA	O1A-CGA-O2A-C1
7	G	618	LHG	O7-C5-C6-O8
7	Y	618	LHG	O7-C5-C6-O8
7	N	619	LHG	O1-C1-C2-O2
7	G	618	LHG	O1-C1-C2-O2
2	N	607	CHL	C11-C10-C8-C9
2	G	607	CHL	C11-C10-C8-C9
3	G	604	CLA	O1A-CGA-O2A-C1
3	G	612	CLA	C10-C11-C12-C13
2	Y	609	CHL	C16-C17-C18-C20
3	G	604	CLA	C2A-CAA-CBA-CGA
2	G	609	CHL	C1A-C2A-CAA-CBA
2	Y	609	CHL	C1A-C2A-CAA-CBA
3	N	610	CLA	C1A-C2A-CAA-CBA
3	G	602	CLA	C1A-C2A-CAA-CBA
3	G	610	CLA	C1A-C2A-CAA-CBA
2	Y	605	CHL	CBA-CGA-O2A-C1
3	G	604	CLA	CBA-CGA-O2A-C1
7	G	618	LHG	C30-C31-C32-C33
5	N	620	XAT	C9-C10-C11-C12
7	G	618	LHG	C3-O3-P-O6
7	N	619	LHG	C4-O6-P-O4
7	Y	618	LHG	C4-O6-P-O4

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Mol	Chain	Res	Type	Atoms
7	N	619	LHG	O6-C4-C5-C6
3	N	614	CLA	CAD-CBD-CGD-O1D
3	G	614	CLA	CAD-CBD-CGD-O1D
3	Y	612	CLA	C5-C6-C7-C8
2	N	601	CHL	C11-C10-C8-C7
2	N	608	CHL	C11-C10-C8-C7
2	Y	608	CHL	C6-C7-C8-C10
3	N	611	CLA	C11-C10-C8-C7
3	N	613	CLA	C12-C13-C15-C16
3	G	604	CLA	C12-C13-C15-C16
3	Y	613	CLA	C12-C13-C15-C16
7	G	618	LHG	O6-C4-C5-O7
2	N	609	CHL	C2C-C3C-CAC-CBC
4	N	616	LUT	C29-C30-C31-C32
7	N	619	LHG	C13-C14-C15-C16
2	G	608	CHL	C1C-C2C-CMC-OMC
2	Y	605	CHL	C1C-C2C-CMC-OMC
7	Y	618	LHG	C4-C5-C6-O8
2	Y	605	CHL	O1A-CGA-O2A-C1
2	Y	601	CHL	C13-C15-C16-C17
3	Y	611	CLA	C4-C3-C5-C6
2	G	601	CHL	C6-C7-C8-C9
3	N	603	CLA	C14-C13-C15-C16
3	Y	602	CLA	C6-C7-C8-C9
3	Y	602	CLA	C11-C12-C13-C14
7	Y	618	LHG	C12-C13-C14-C15
3	G	603	CLA	C8-C10-C11-C12
3	Y	603	CLA	C5-C6-C7-C8
3	N	614	CLA	C1-C2-C3-C4
3	G	614	CLA	C1-C2-C3-C4
3	Y	614	CLA	C1-C2-C3-C4
7	Y	618	LHG	C4-C5-O7-C7
2	G	608	CHL	C2A-CAA-CBA-CGA
3	N	604	CLA	C2-C1-O2A-CGA
3	G	611	CLA	C2-C1-O2A-CGA
7	N	619	LHG	O6-C4-C5-O7
4	Y	616	LUT	C5-C6-C7-C8
3	G	602	CLA	C8-C10-C11-C12
7	N	619	LHG	C3-O3-P-O6
2	Y	609	CHL	C12-C13-C15-C16
3	G	602	CLA	C11-C12-C13-C15
3	Y	602	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
2	G	608	CHL	C14-C13-C15-C16
3	N	603	CLA	C11-C12-C13-C14
3	N	613	CLA	C14-C13-C15-C16
3	G	604	CLA	C14-C13-C15-C16
2	G	601	CHL	C13-C15-C16-C17
5	N	617	XAT	C9-C10-C11-C12
2	G	609	CHL	C2C-C3C-CAC-CBC
2	G	601	CHL	CBA-CGA-O2A-C1
3	N	610	CLA	C5-C6-C7-C8
2	N	609	CHL	O1A-CGA-O2A-C1
6	N	618	NEX	C30-C31-C32-C33
6	G	617	NEX	C30-C31-C32-C33
6	Y	617	NEX	C30-C31-C32-C33
2	G	601	CHL	C2-C1-O2A-CGA
2	Y	601	CHL	C2-C1-O2A-CGA
3	N	613	CLA	C16-C17-C18-C19
2	G	607	CHL	C15-C16-C17-C18
3	N	602	CLA	C2A-CAA-CBA-CGA
3	Y	613	CLA	C2A-CAA-CBA-CGA
2	N	609	CHL	C4C-C3C-CAC-CBC
2	Y	601	CHL	C3A-C2A-CAA-CBA
2	Y	605	CHL	C3A-C2A-CAA-CBA
5	G	619	XAT	C9-C10-C11-C12
3	Y	611	CLA	C2-C3-C5-C6
2	G	607	CHL	C6-C7-C8-C9
2	Y	607	CHL	C6-C7-C8-C9
3	Y	604	CLA	C11-C12-C13-C14
2	N	608	CHL	C16-C17-C18-C20
2	G	608	CHL	C16-C17-C18-C19
7	N	619	LHG	C4-C5-O7-C7
3	N	612	CLA	C4-C3-C5-C6
2	N	601	CHL	C1A-C2A-CAA-CBA
2	Y	601	CHL	C1A-C2A-CAA-CBA
2	Y	605	CHL	C1A-C2A-CAA-CBA
3	N	612	CLA	C11-C12-C13-C15
3	Y	603	CLA	C12-C13-C15-C16
6	G	617	NEX	C33-C34-C35-C15
3	G	613	CLA	C15-C16-C17-C18
3	G	613	CLA	C2A-CAA-CBA-CGA
3	N	612	CLA	C5-C6-C7-C8
2	Y	608	CHL	C4-C3-C5-C6
3	G	604	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
2	G	605	CHL	O1D-CGD-O2D-CED
6	N	618	NEX	C33-C34-C35-C15
6	Y	617	NEX	C33-C34-C35-C15
2	G	609	CHL	C16-C17-C18-C19
3	Y	612	CLA	C16-C17-C18-C20
7	Y	618	LHG	C27-C28-C29-C30
3	N	603	CLA	C10-C11-C12-C13
3	G	612	CLA	C4-C3-C5-C6
2	N	606	CHL	C2-C1-O2A-CGA
3	G	604	CLA	C2-C1-O2A-CGA
2	G	601	CHL	O1A-CGA-O2A-C1
3	N	603	CLA	O1A-CGA-O2A-C1
4	N	616	LUT	C1-C6-C7-C8
7	G	618	LHG	O1-C1-C2-C3
3	N	612	CLA	C2-C3-C5-C6
2	G	609	CHL	C4C-C3C-CAC-CBC
7	N	619	LHG	C34-C35-C36-C37
3	G	602	CLA	C13-C15-C16-C17
2	G	601	CHL	C6-C7-C8-C10
3	Y	612	CLA	C16-C17-C18-C19
3	Y	613	CLA	C15-C16-C17-C18
2	G	605	CHL	CBA-CGA-O2A-C1
2	Y	608	CHL	C2-C3-C5-C6
3	G	612	CLA	C2-C3-C5-C6
2	Y	608	CHL	C16-C17-C18-C19
2	N	601	CHL	C11-C10-C8-C9
2	Y	608	CHL	C6-C7-C8-C9
3	G	602	CLA	C11-C12-C13-C14
3	Y	613	CLA	C14-C13-C15-C16
3	N	603	CLA	CAD-CBD-CGD-O2D
3	G	603	CLA	CAD-CBD-CGD-O2D
3	Y	612	CLA	CAD-CBD-CGD-O2D
7	N	619	LHG	C6-C5-O7-C7
7	G	618	LHG	C4-C5-O7-C7
7	G	618	LHG	C6-C5-O7-C7
2	N	607	CHL	C5-C6-C7-C8
2	Y	608	CHL	CAA-CBA-CGA-O2A
3	G	603	CLA	C16-C17-C18-C20
3	G	612	CLA	C5-C6-C7-C8
3	G	604	CLA	C2-C3-C5-C6
2	G	609	CHL	O1A-CGA-O2A-C1
5	N	620	XAT	O24-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
2	N	608	CHL	CAA-CBA-CGA-O2A
3	Y	614	CLA	O2A-C1-C2-C3
2	N	608	CHL	O2A-C1-C2-C3
2	G	608	CHL	O2A-C1-C2-C3
2	Y	608	CHL	O2A-C1-C2-C3
2	Y	609	CHL	O2A-C1-C2-C3
2	Y	608	CHL	CHA-CBD-CGD-O1D
2	Y	608	CHL	CHA-CBD-CGD-O2D
2	Y	609	CHL	CHA-CBD-CGD-O2D
3	N	604	CLA	CHA-CBD-CGD-O1D
3	G	602	CLA	CHA-CBD-CGD-O2D
3	G	603	CLA	CHA-CBD-CGD-O1D
3	N	611	CLA	C4-C3-C5-C6
3	Y	603	CLA	CAA-CBA-CGA-O2A
3	N	603	CLA	C2A-CAA-CBA-CGA
3	N	603	CLA	CBA-CGA-O2A-C1
7	Y	618	LHG	O8-C23-C24-C25
2	Y	609	CHL	C6-C7-C8-C10
3	G	603	CLA	C16-C17-C18-C19
3	N	612	CLA	C11-C12-C13-C14
7	G	618	LHG	O8-C23-C24-C25
7	N	619	LHG	O1-C1-C2-C3
5	N	617	XAT	C31-C32-C33-C34
3	G	613	CLA	CBA-CGA-O2A-C1
3	Y	602	CLA	C13-C15-C16-C17
3	G	611	CLA	C16-C17-C18-C20
7	N	619	LHG	C3-O3-P-O5
4	N	616	LUT	C5-C6-C7-C8
2	N	608	CHL	CAA-CBA-CGA-O1A
3	Y	603	CLA	CAA-CBA-CGA-O1A
2	G	605	CHL	O1A-CGA-O2A-C1
7	N	619	LHG	O8-C23-C24-C25
2	Y	608	CHL	CAA-CBA-CGA-O1A
3	N	604	CLA	C4-C3-C5-C6
2	Y	608	CHL	CAD-CBD-CGD-O1D
3	N	604	CLA	CAD-CBD-CGD-O1D
7	Y	618	LHG	C6-C5-O7-C7
3	Y	603	CLA	C14-C13-C15-C16
7	Y	618	LHG	O10-C23-C24-C25
7	N	619	LHG	C9-C10-C11-C12
3	G	613	CLA	C8-C10-C11-C12
3	N	603	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
3	Y	612	CLA	CAA-CBA-CGA-O2A
2	G	607	CHL	C6-C7-C8-C10
2	Y	607	CHL	C6-C7-C8-C10
3	N	602	CLA	C11-C12-C13-C15
3	Y	611	CLA	C11-C12-C13-C15
3	Y	604	CLA	CAA-CBA-CGA-O2A
4	N	615	LUT	C29-C30-C31-C32
3	N	613	CLA	C13-C15-C16-C17
3	N	603	CLA	CAA-CBA-CGA-O1A
3	Y	604	CLA	CAA-CBA-CGA-O1A
3	G	611	CLA	C10-C11-C12-C13
3	N	612	CLA	CAA-CBA-CGA-O2A

There are no ring outliers.

51 monomers are involved in 151 short contacts:

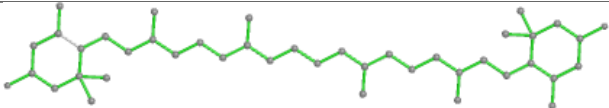
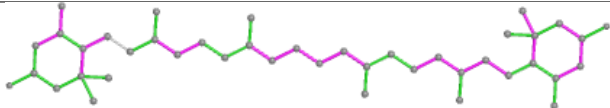
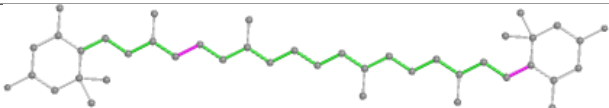
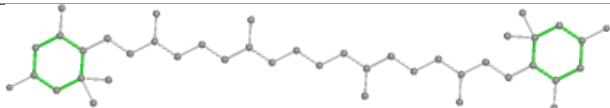
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	616	LUT	5	0
6	Y	617	NEX	2	0
3	Y	610	CLA	10	0
3	Y	612	CLA	2	0
3	G	614	CLA	1	0
4	N	616	LUT	5	0
2	G	608	CHL	2	0
3	N	604	CLA	1	0
3	N	603	CLA	2	0
3	G	604	CLA	3	0
6	G	617	NEX	1	0
2	G	609	CHL	3	0
2	N	606	CHL	3	0
2	G	606	CHL	1	0
3	N	611	CLA	3	0
3	G	611	CLA	2	0
3	Y	613	CLA	4	0
4	G	615	LUT	5	0
3	Y	604	CLA	2	0
3	G	610	CLA	7	0
7	Y	618	LHG	8	0
2	G	605	CHL	1	0
3	N	610	CLA	4	0
2	Y	607	CHL	3	0
3	Y	602	CLA	3	0

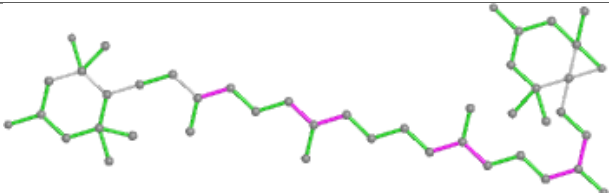
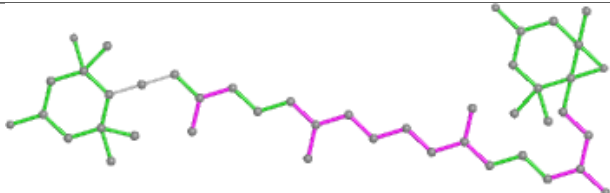
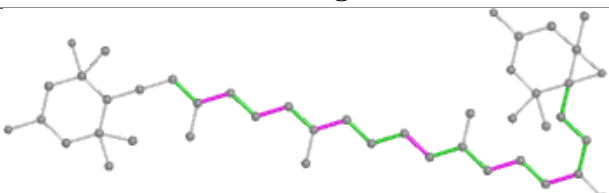

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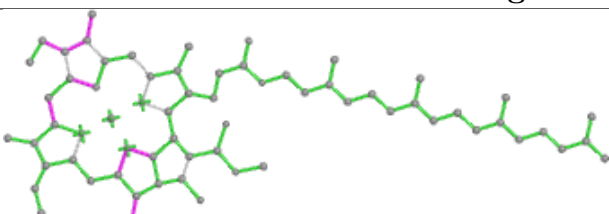
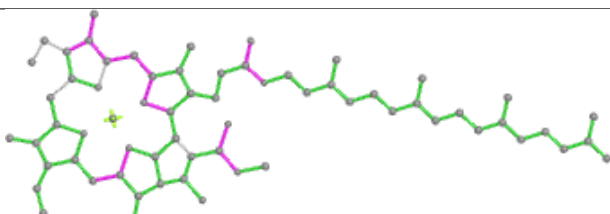
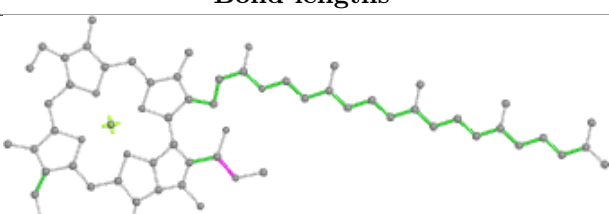
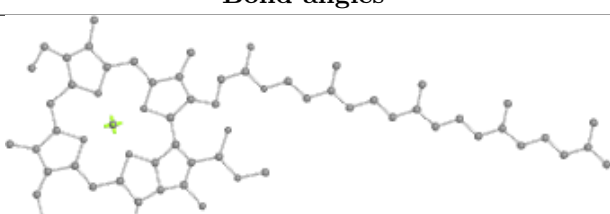
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	N	601	CHL	4	0
2	G	601	CHL	11	0
2	Y	601	CHL	9	0
5	N	617	XAT	8	0
5	N	620	XAT	3	0
2	N	607	CHL	4	0
3	N	614	CLA	1	0
2	Y	609	CHL	6	0
4	Y	616	LUT	7	0
2	G	607	CHL	5	0
3	N	613	CLA	3	0
3	Y	614	CLA	2	0
2	Y	606	CHL	2	0
3	Y	611	CLA	6	0
3	Y	603	CLA	4	0
4	Y	615	LUT	6	0
5	G	619	XAT	9	0
3	G	613	CLA	4	0
7	N	619	LHG	3	0
2	N	609	CHL	6	0
3	G	602	CLA	5	0
4	N	615	LUT	4	0
3	N	602	CLA	2	0
7	G	618	LHG	3	0
2	Y	608	CHL	5	0
2	N	608	CHL	6	0

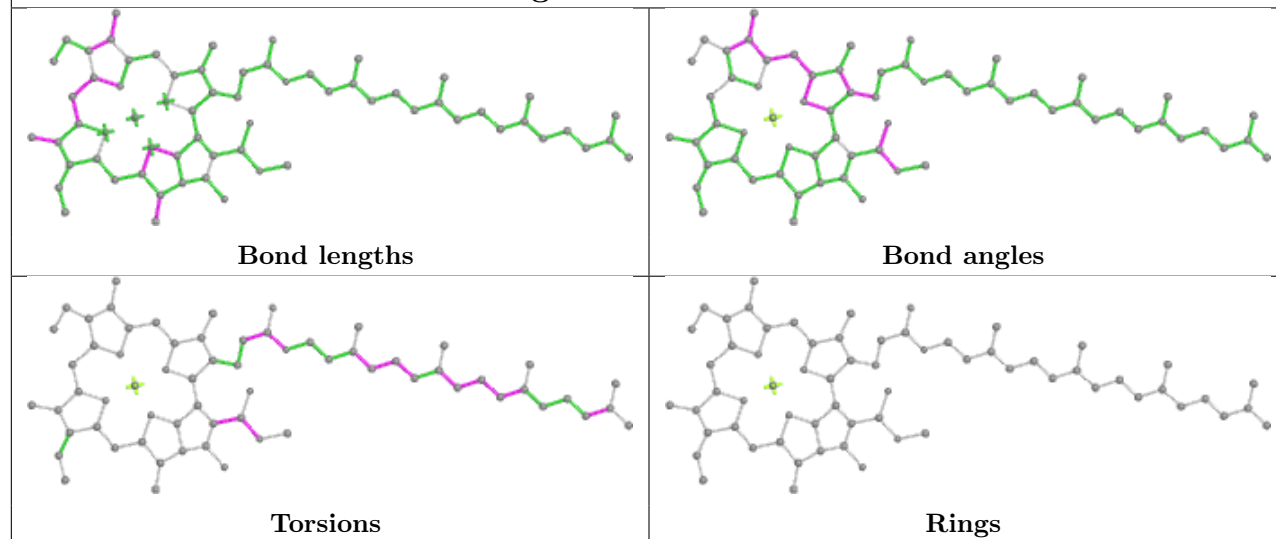
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 LUT G 616	
	
Bond lengths	Bond angles
	
Torsions	Rings

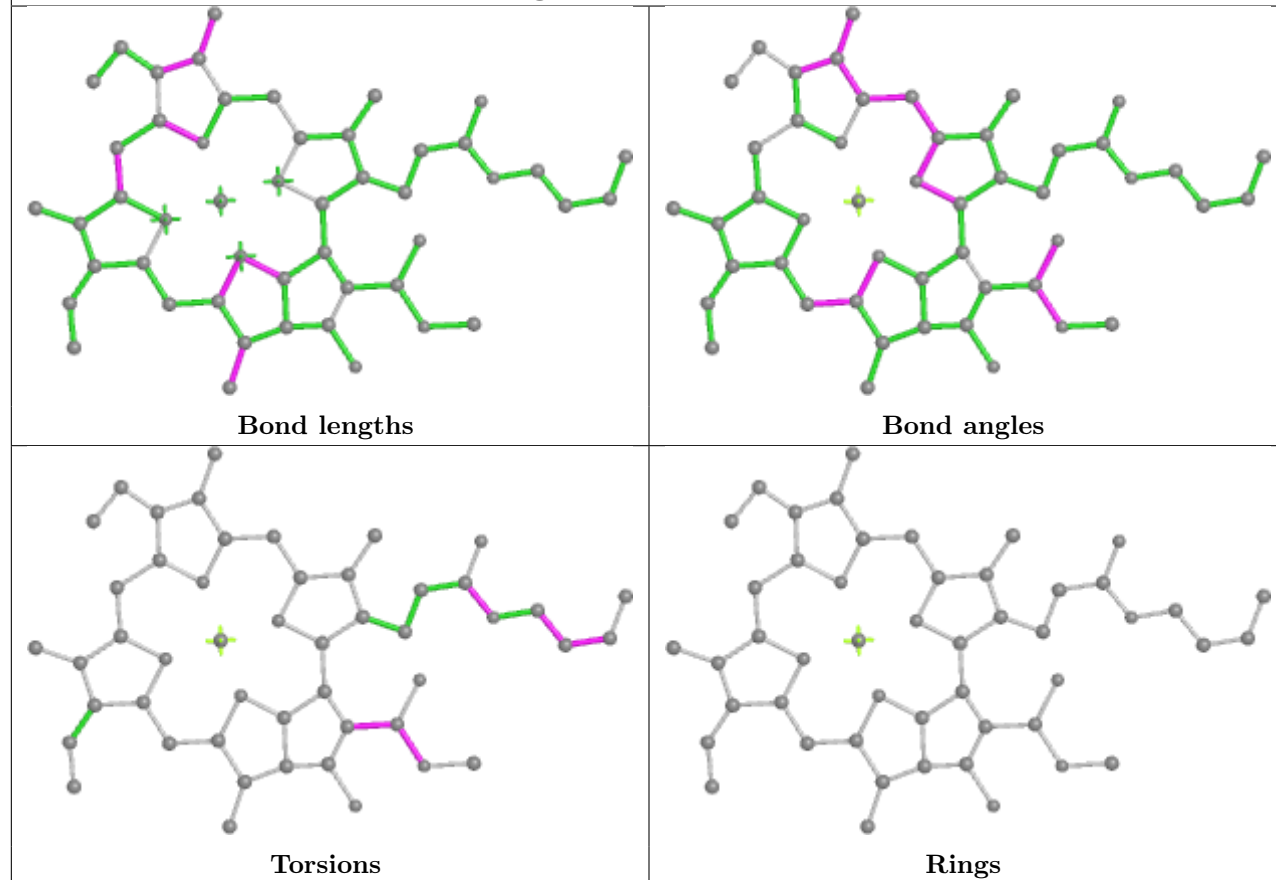
Ligand NEX Y 617	
	
Bond lengths	Bond angles
	
Torsions	Rings

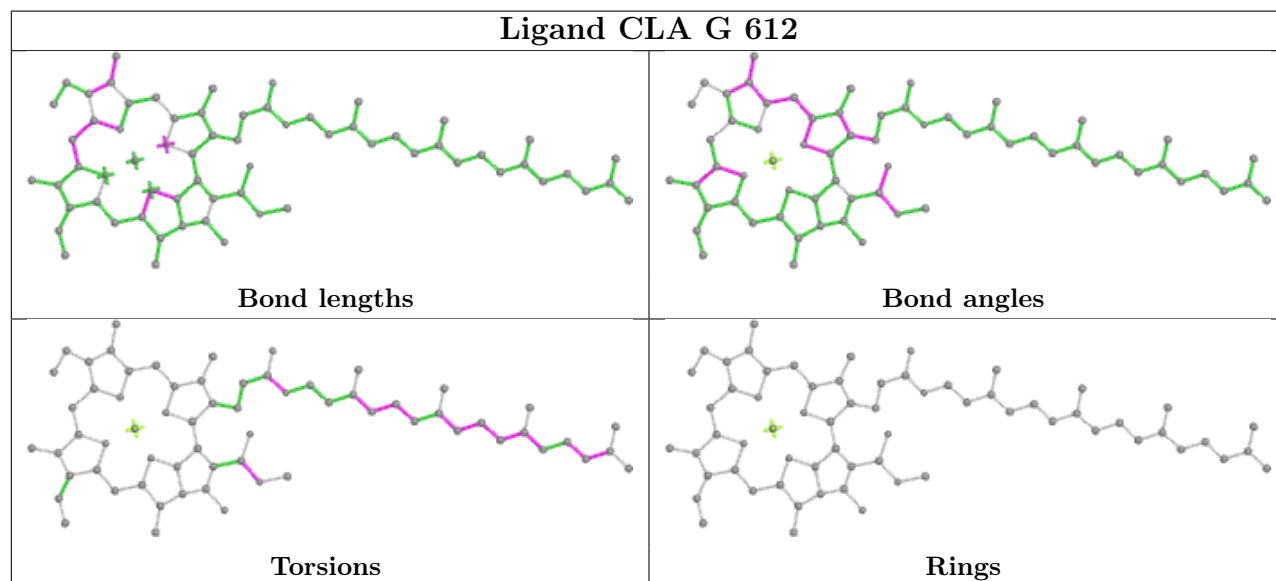
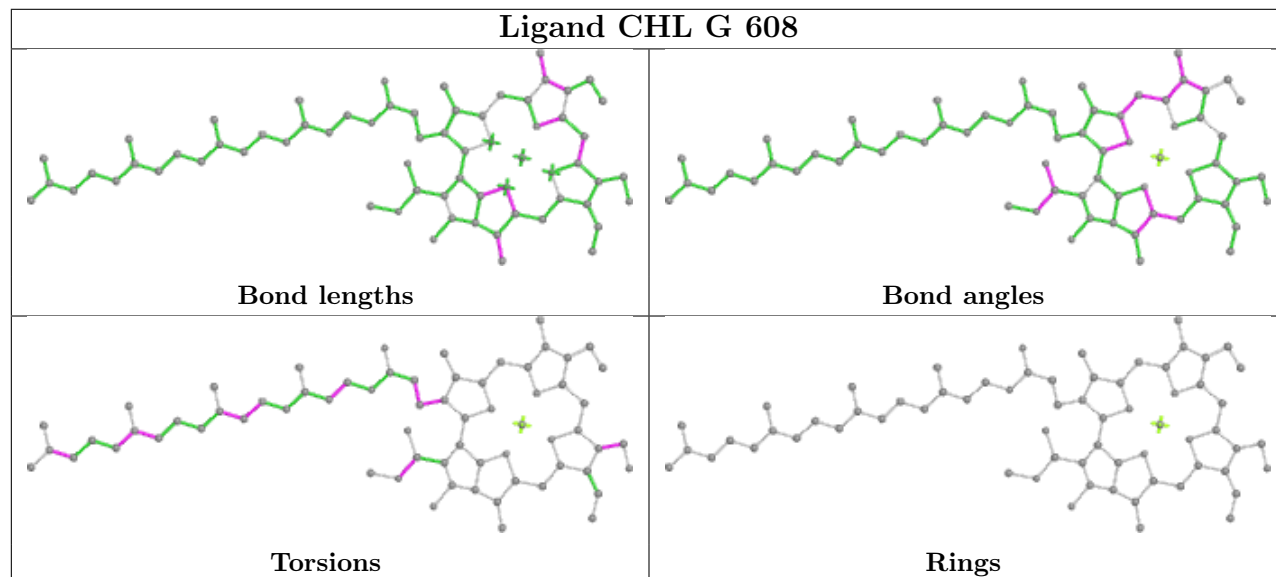
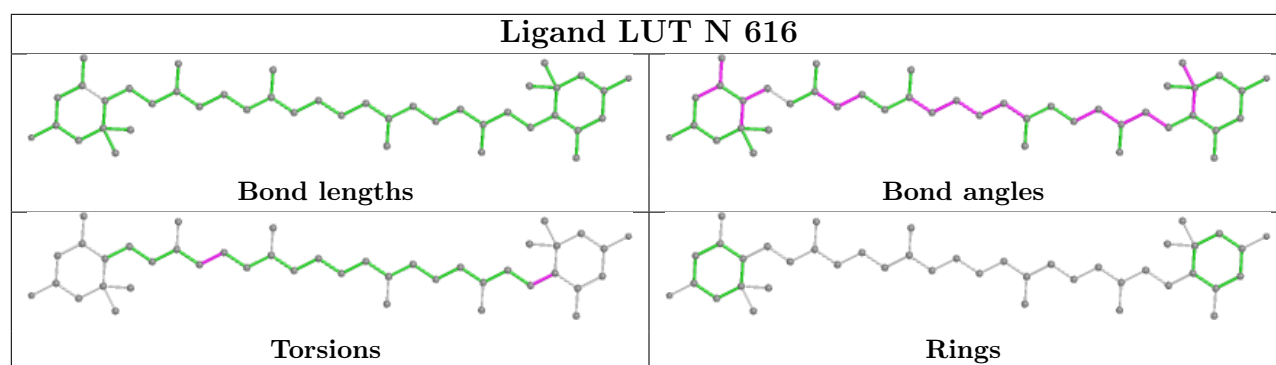
Ligand CLA Y 610	
	
Bond lengths	Bond angles
	
Torsions	Rings

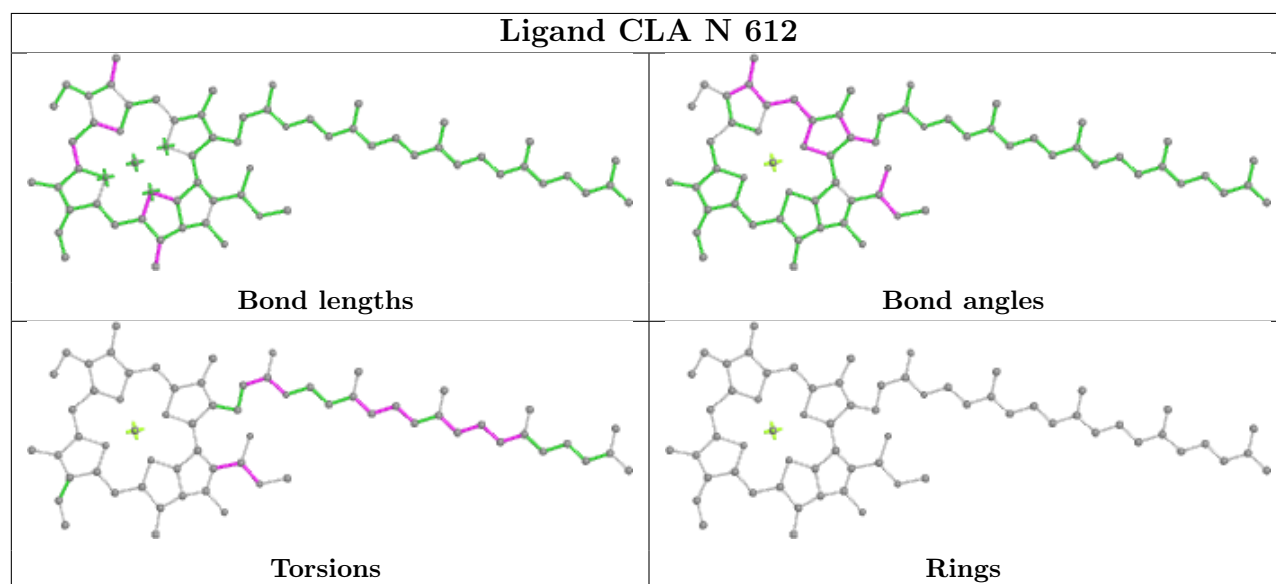
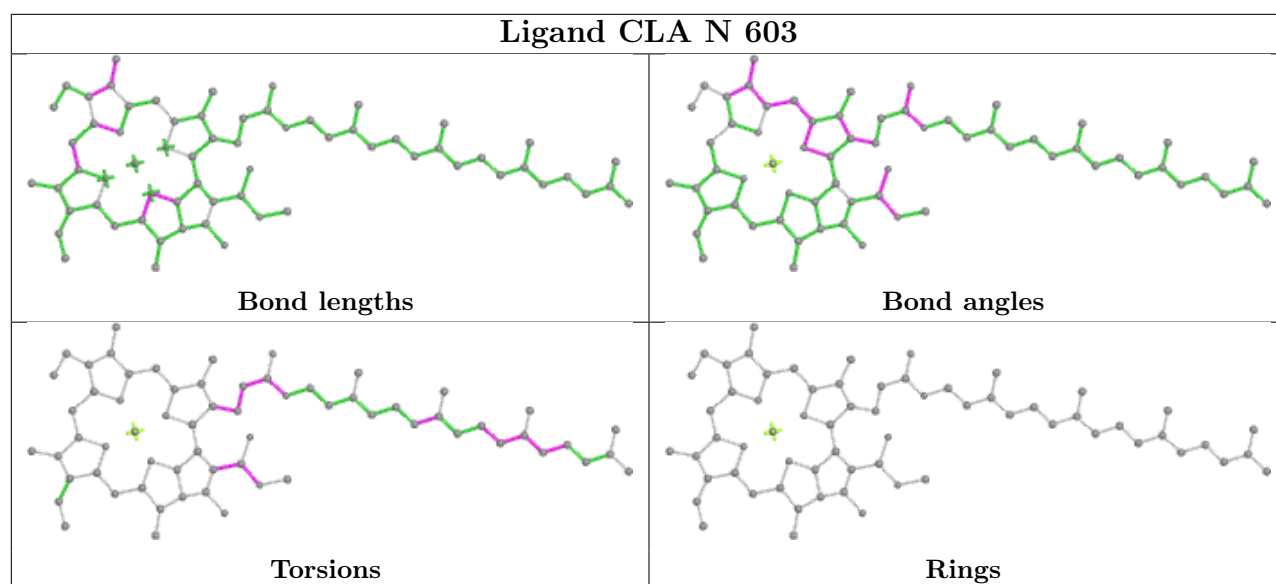
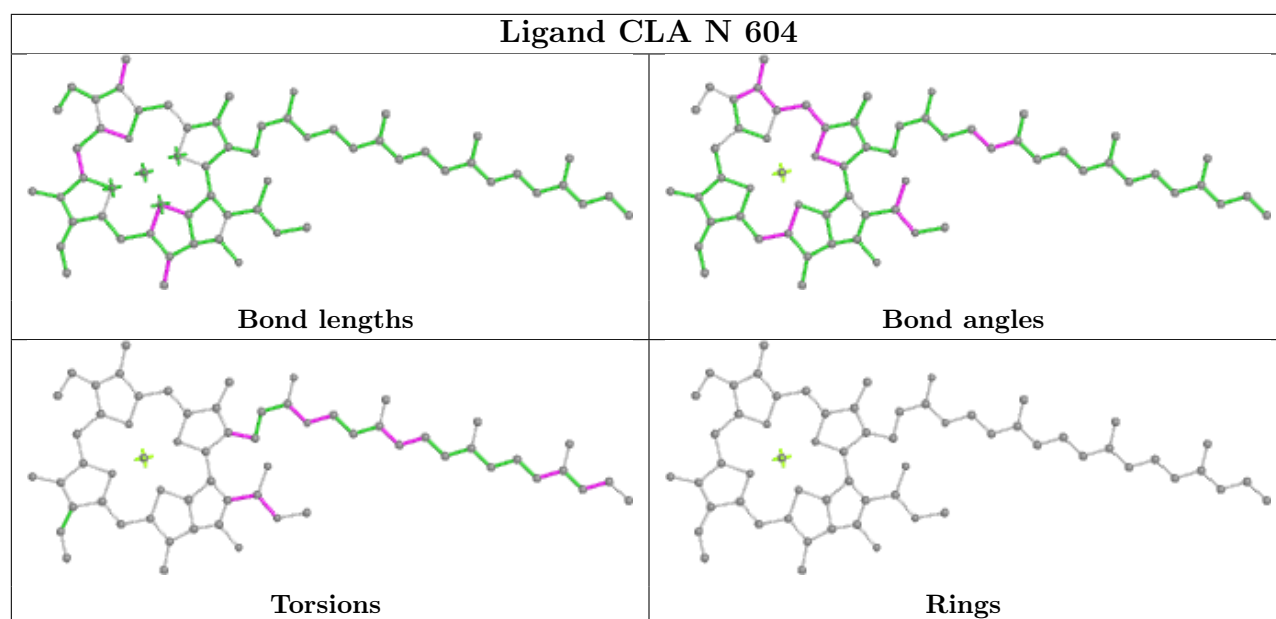
Ligand CLA Y 612

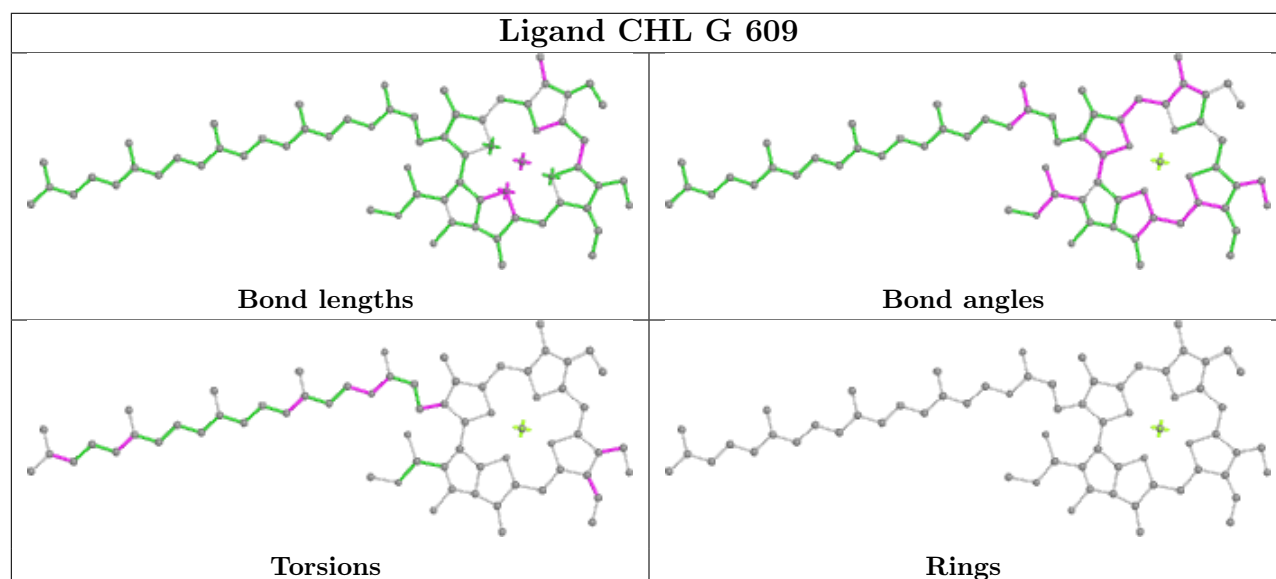
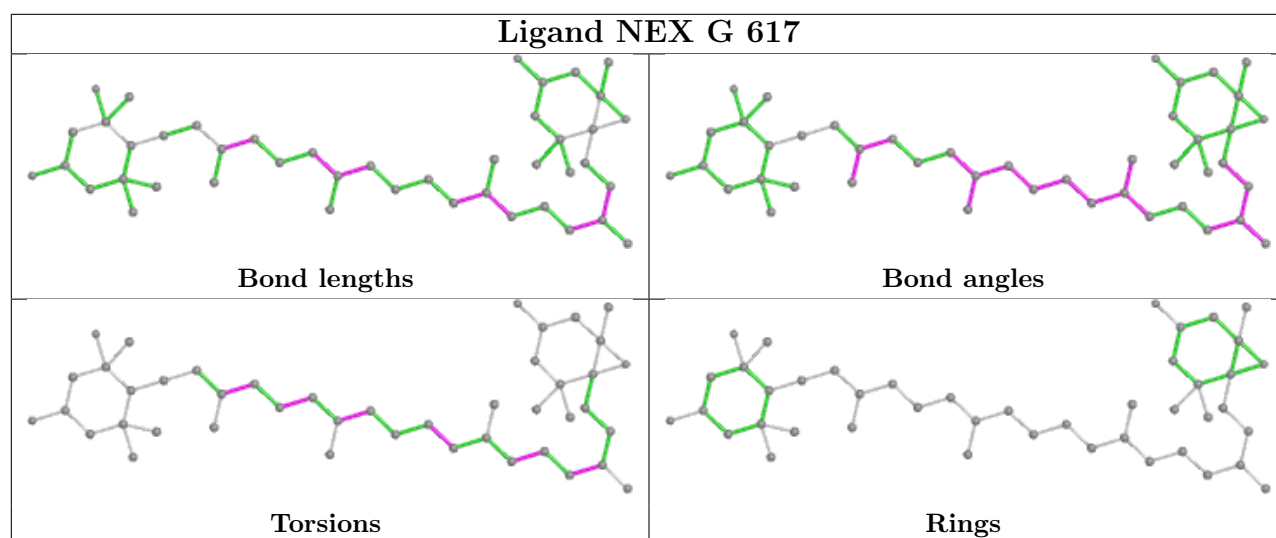
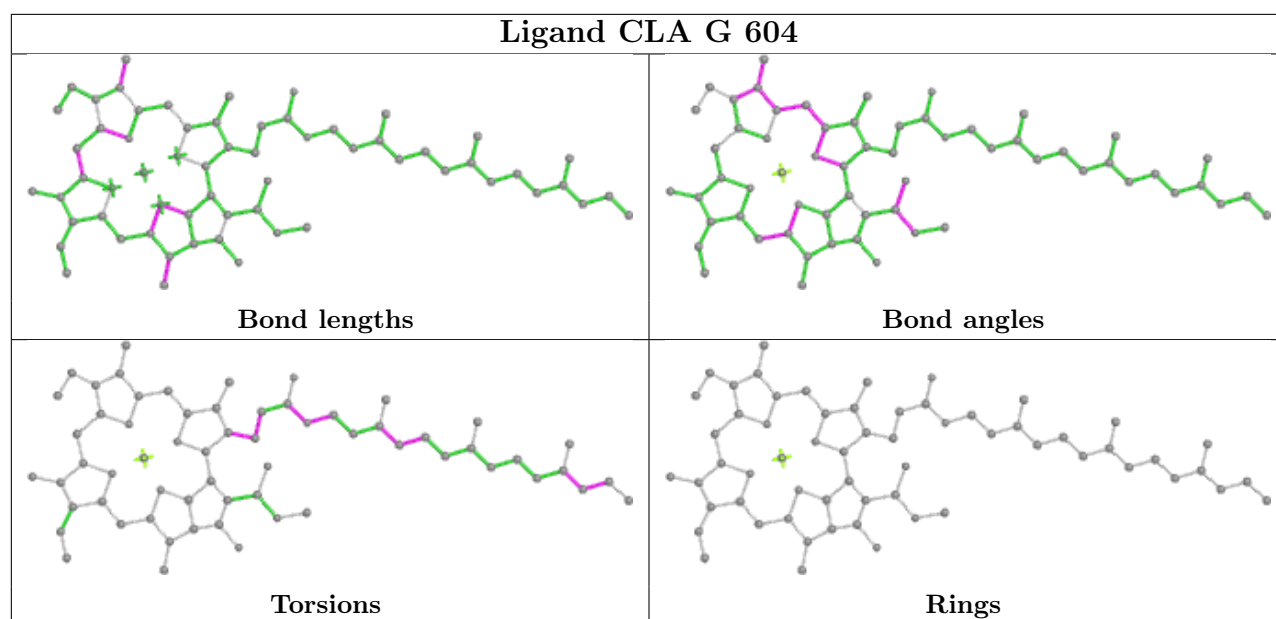


Ligand CLA G 614

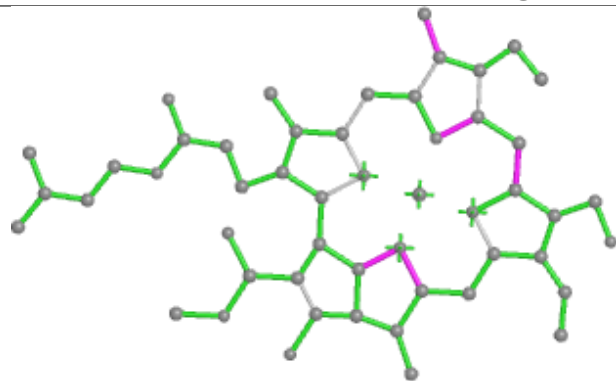




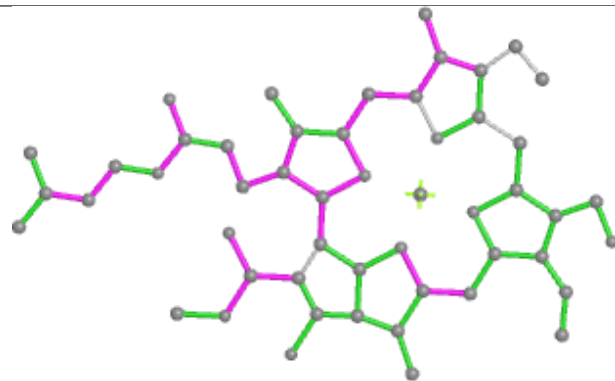




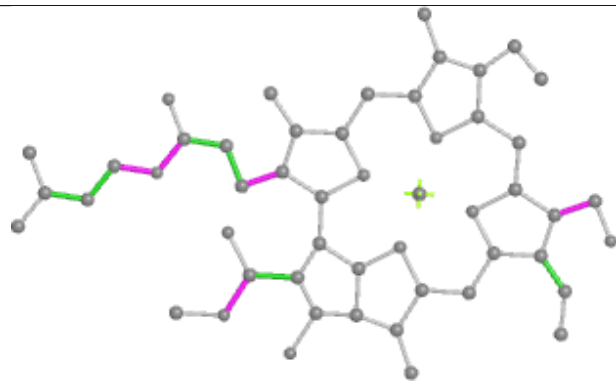
Ligand CHL N 606



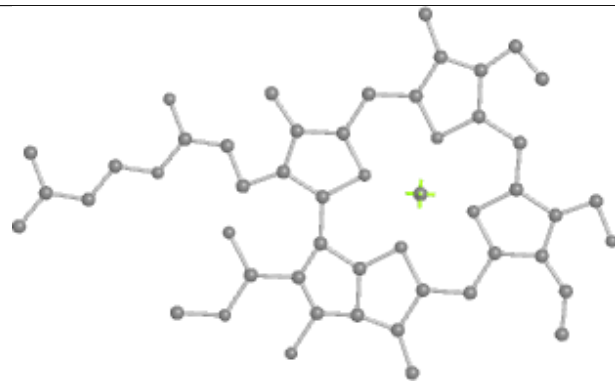
Bond lengths



Bond angles

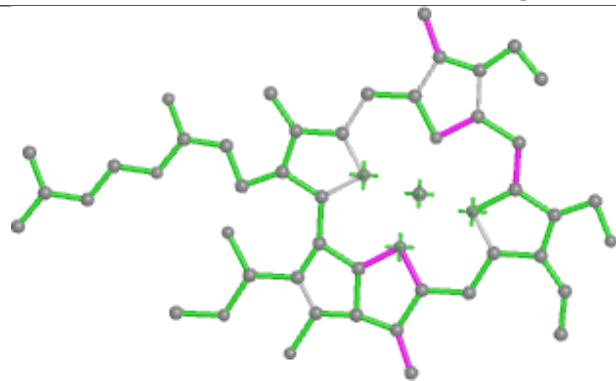


Torsions

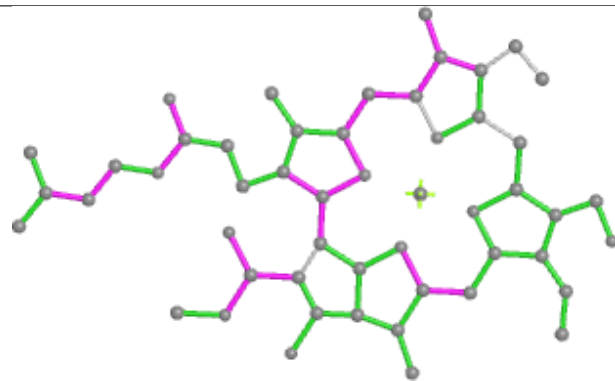


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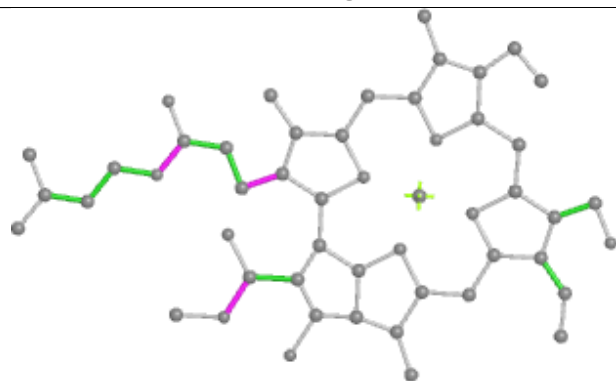
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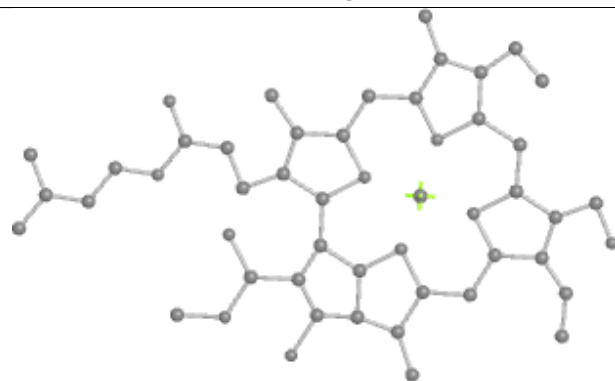
Bond lengths



Bond angles

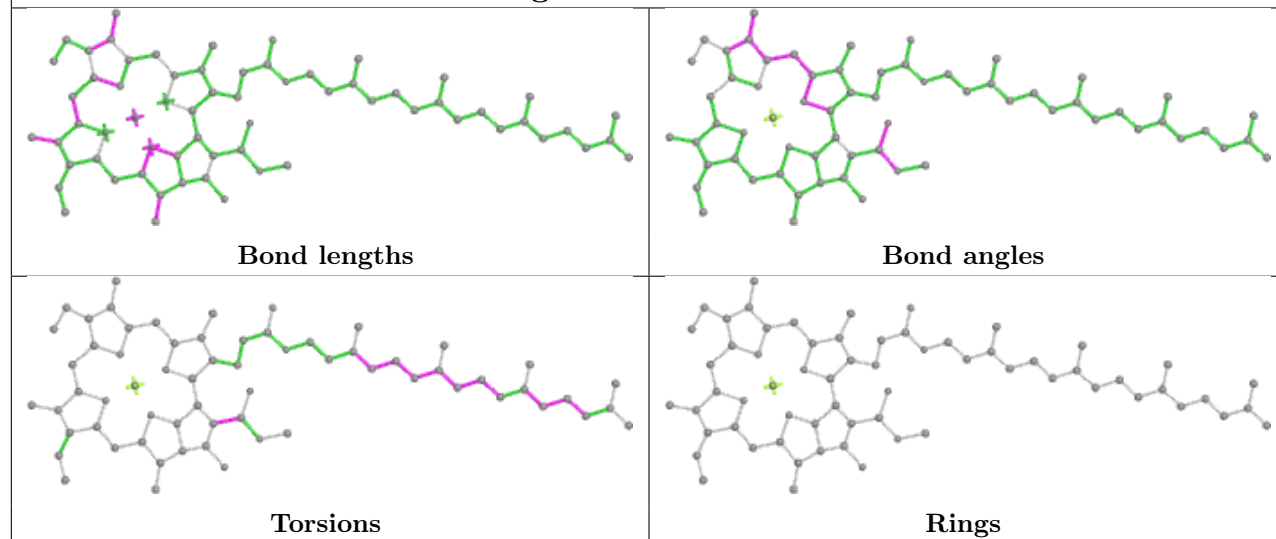


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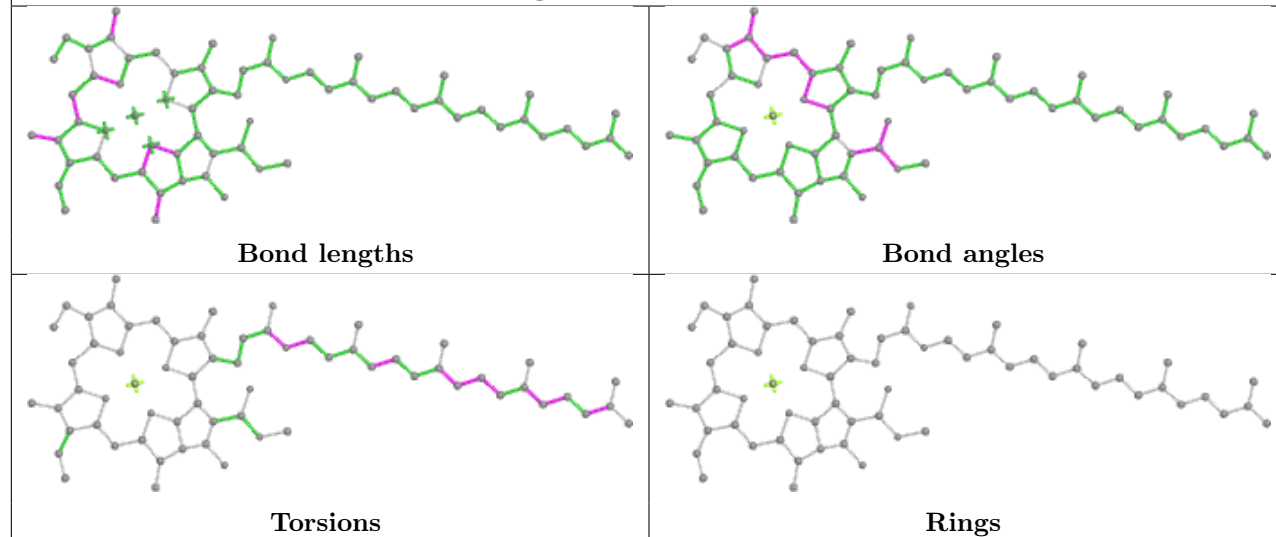


Rings

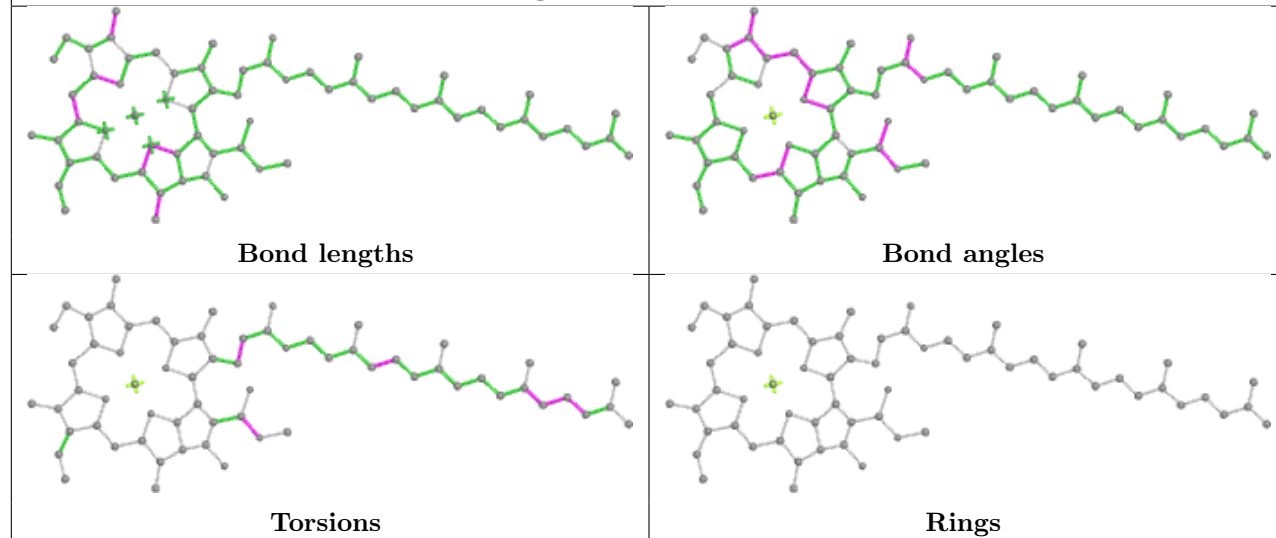
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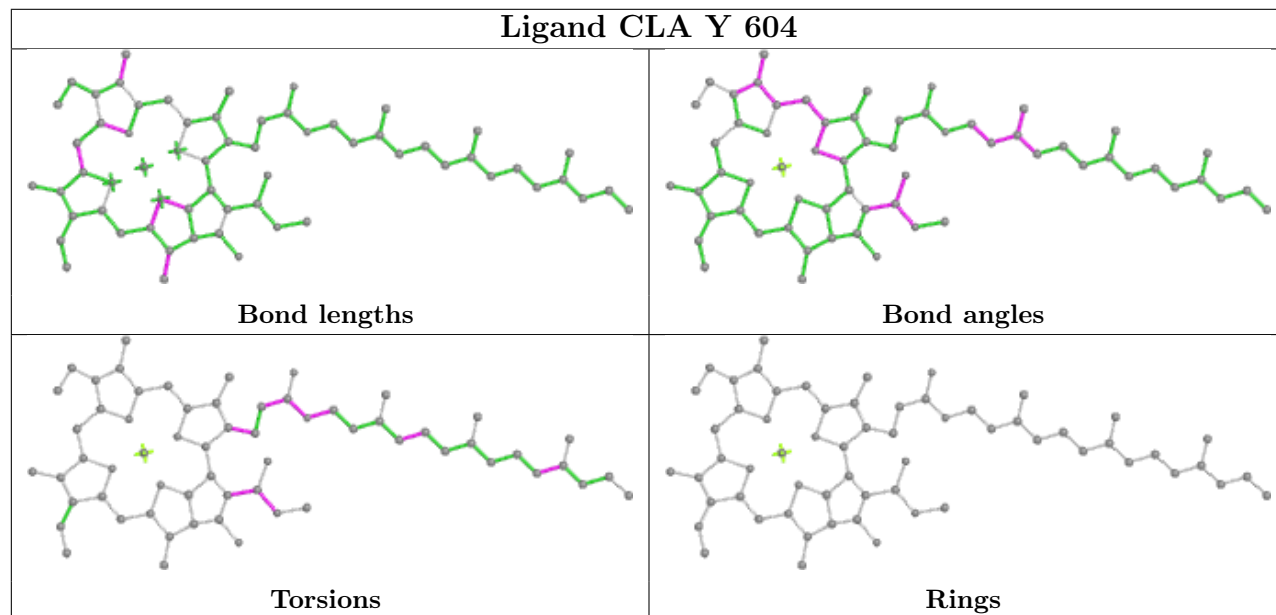
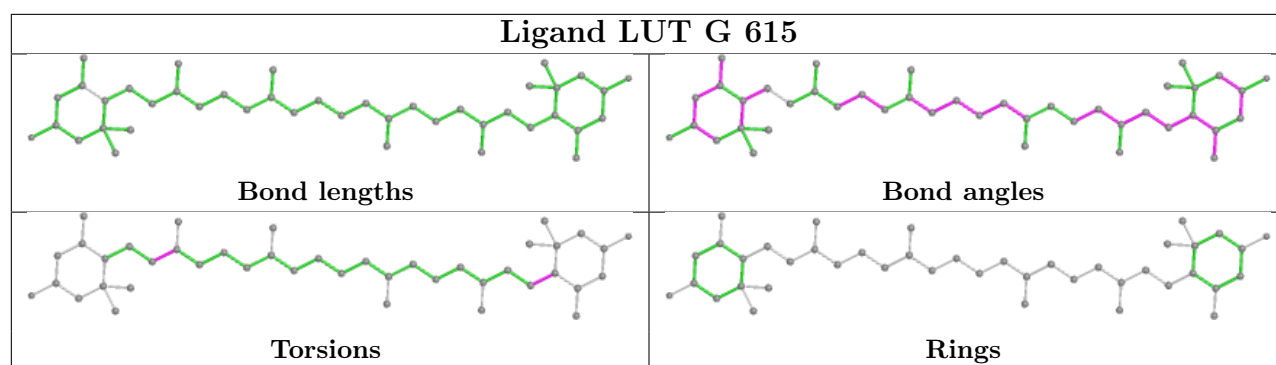


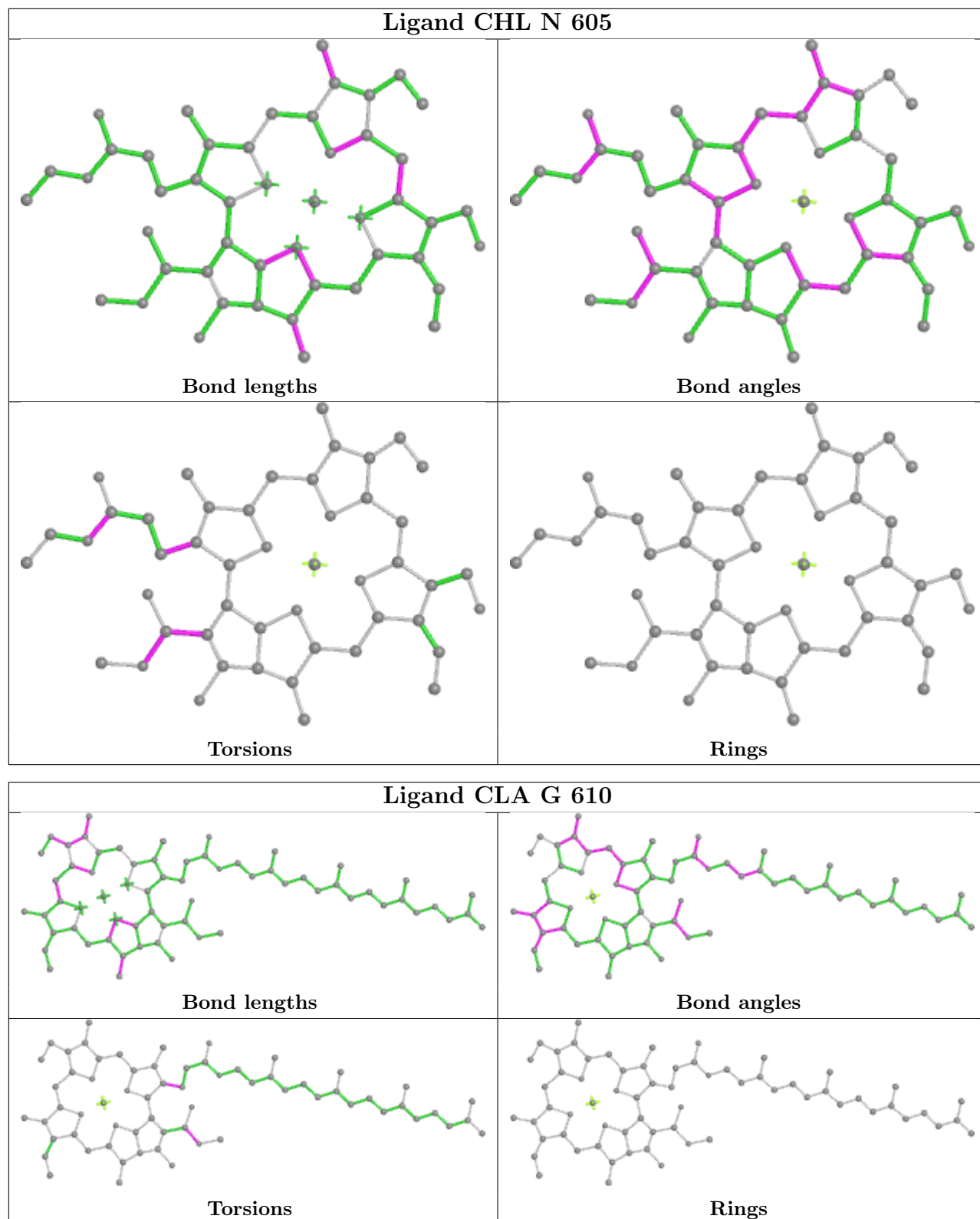
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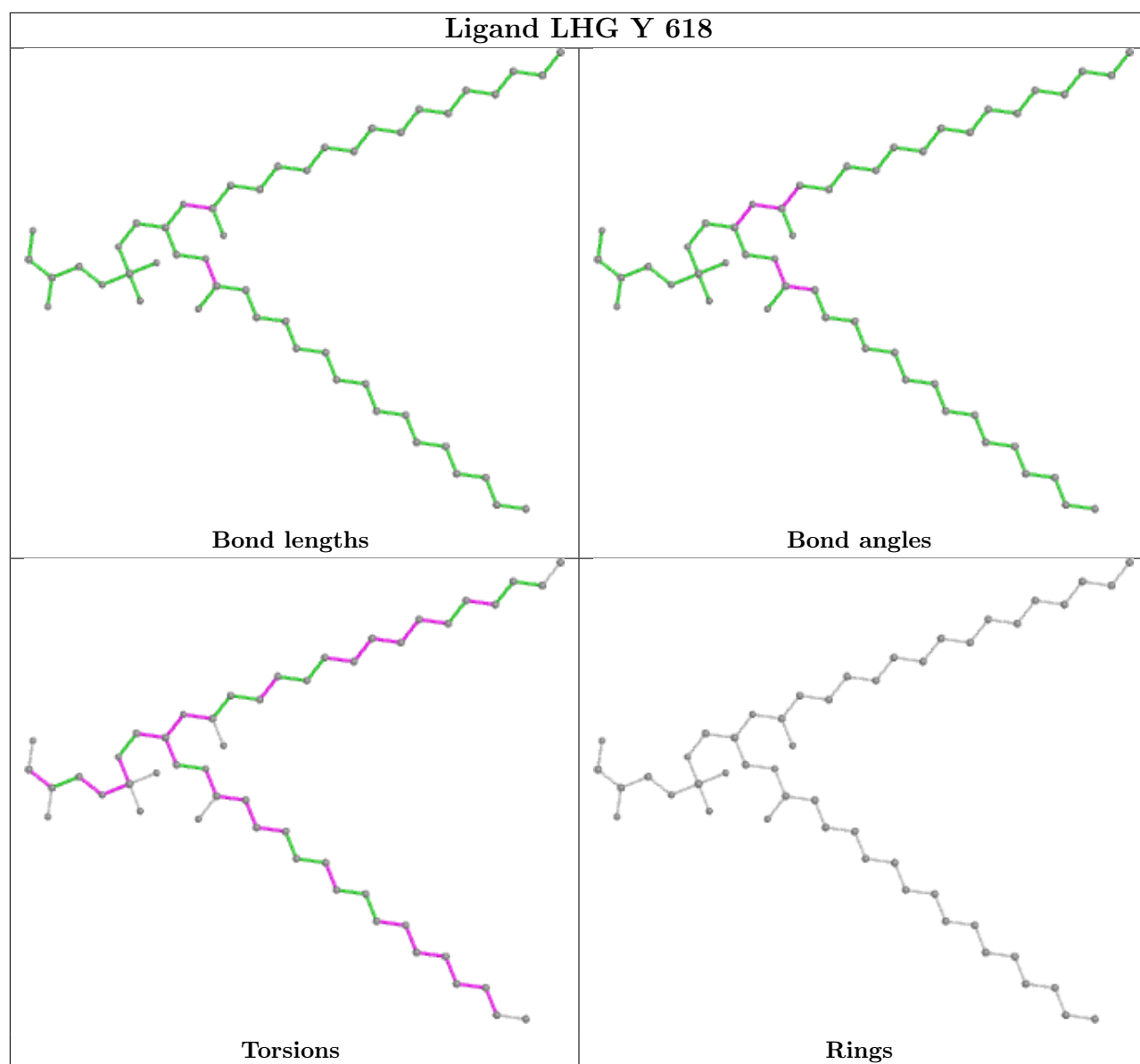


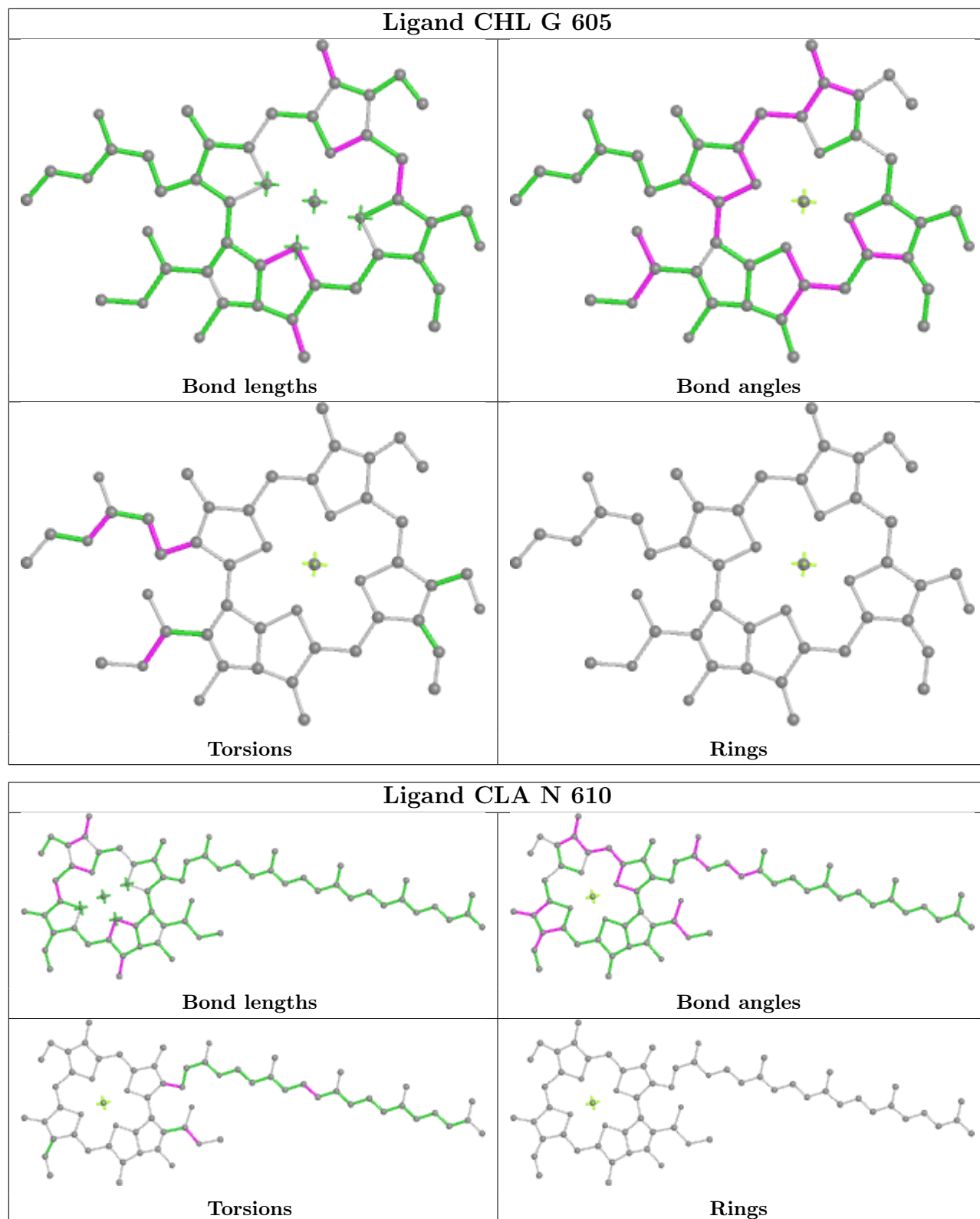
Ligand CLA Y 613

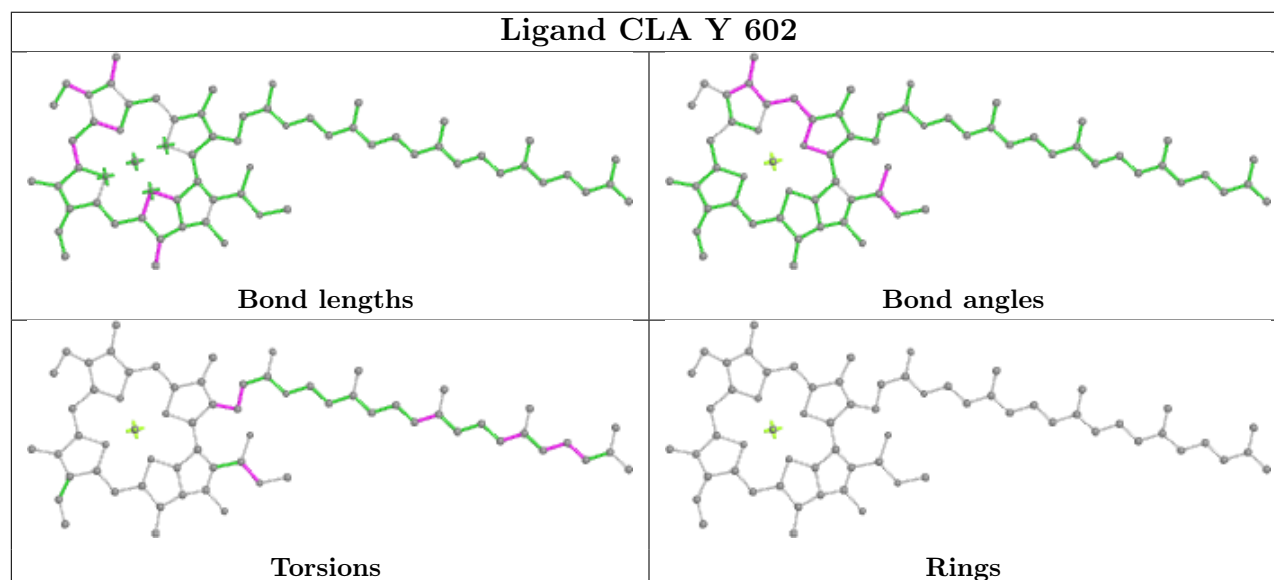
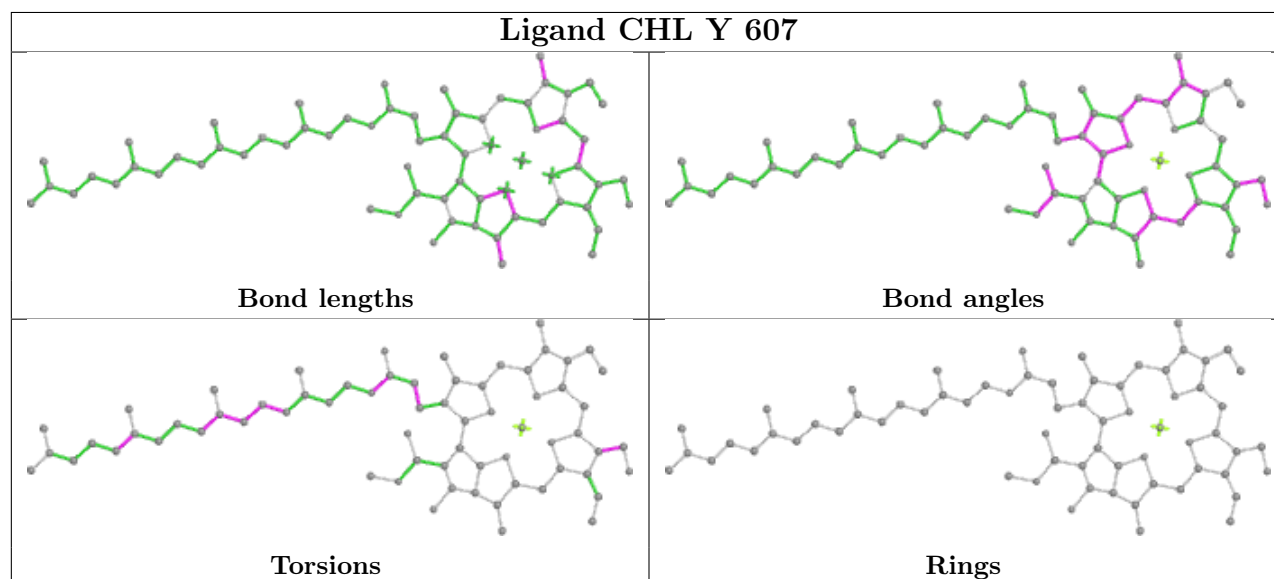
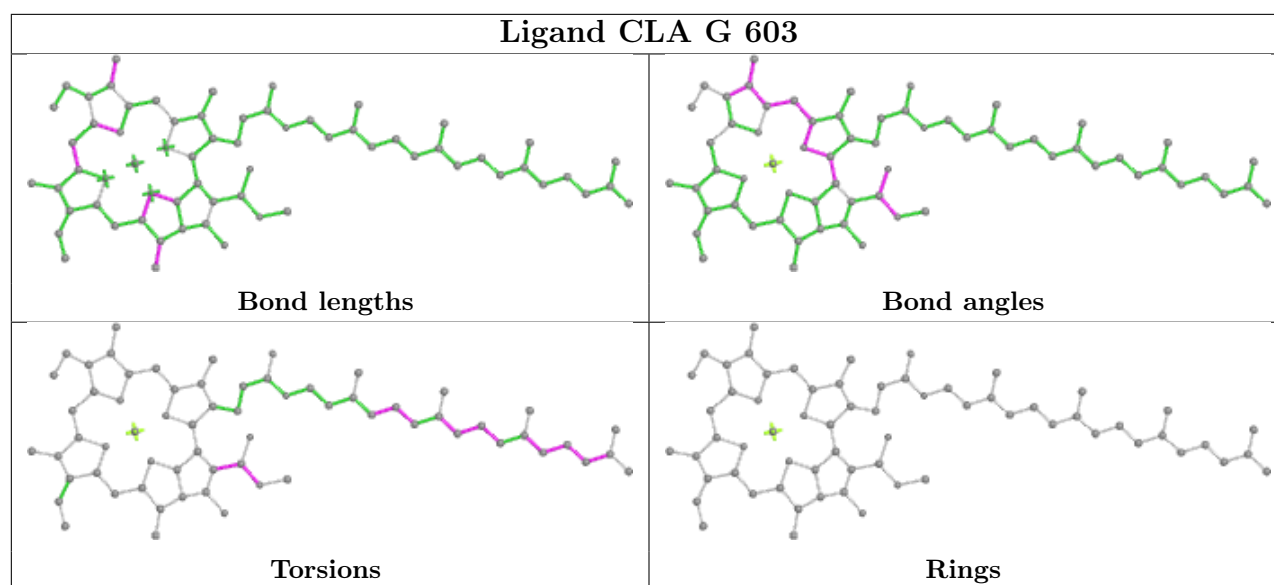


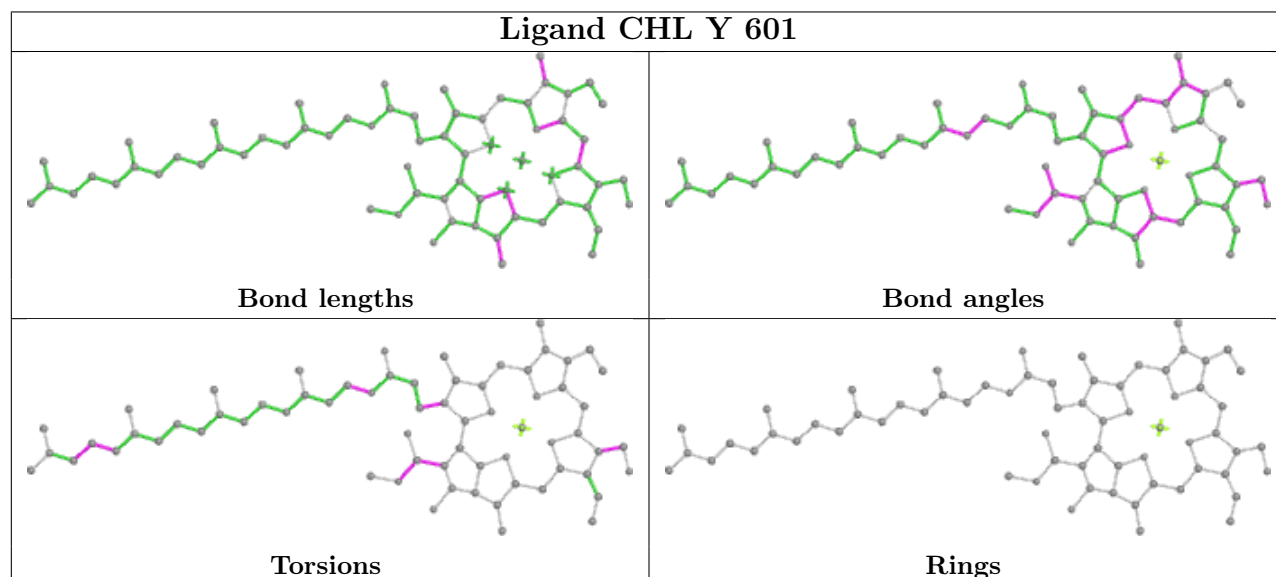
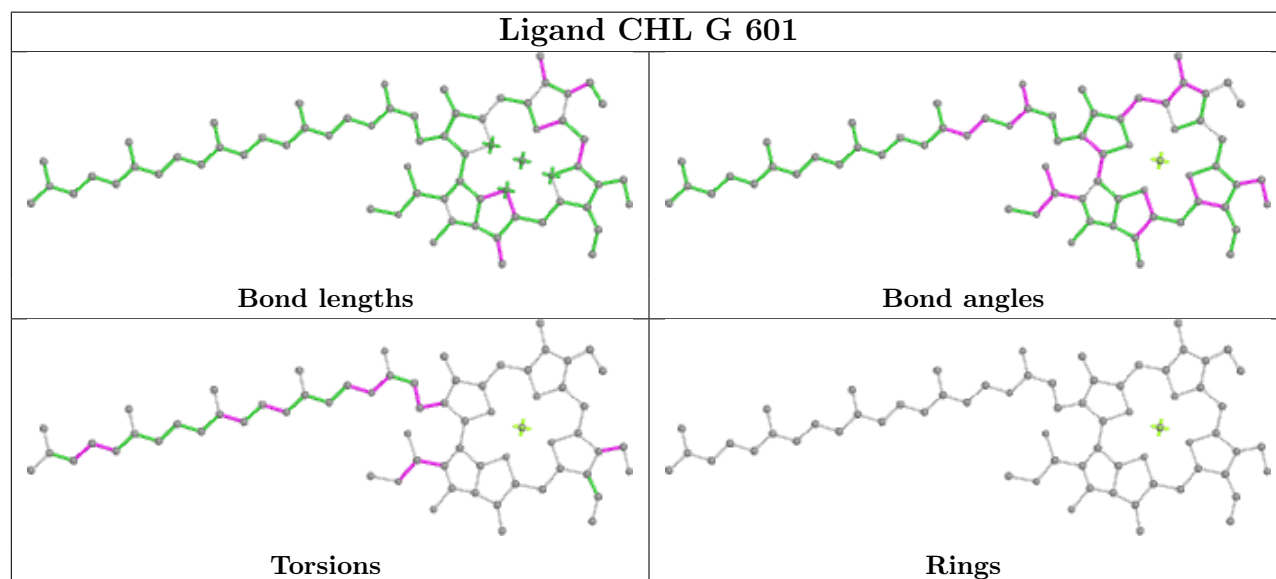
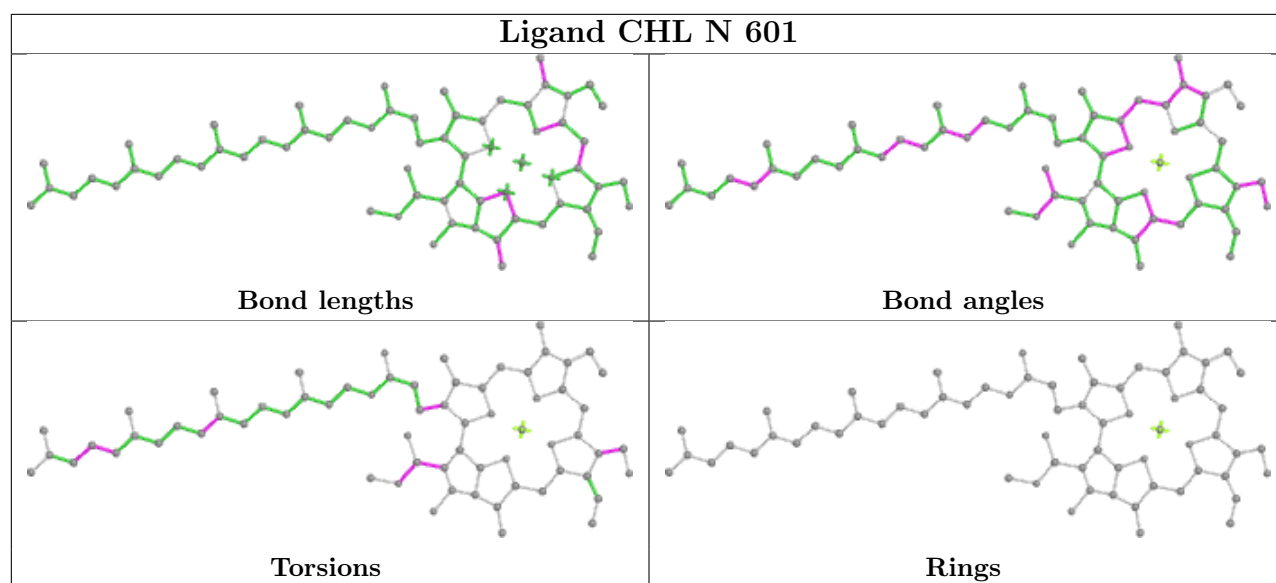


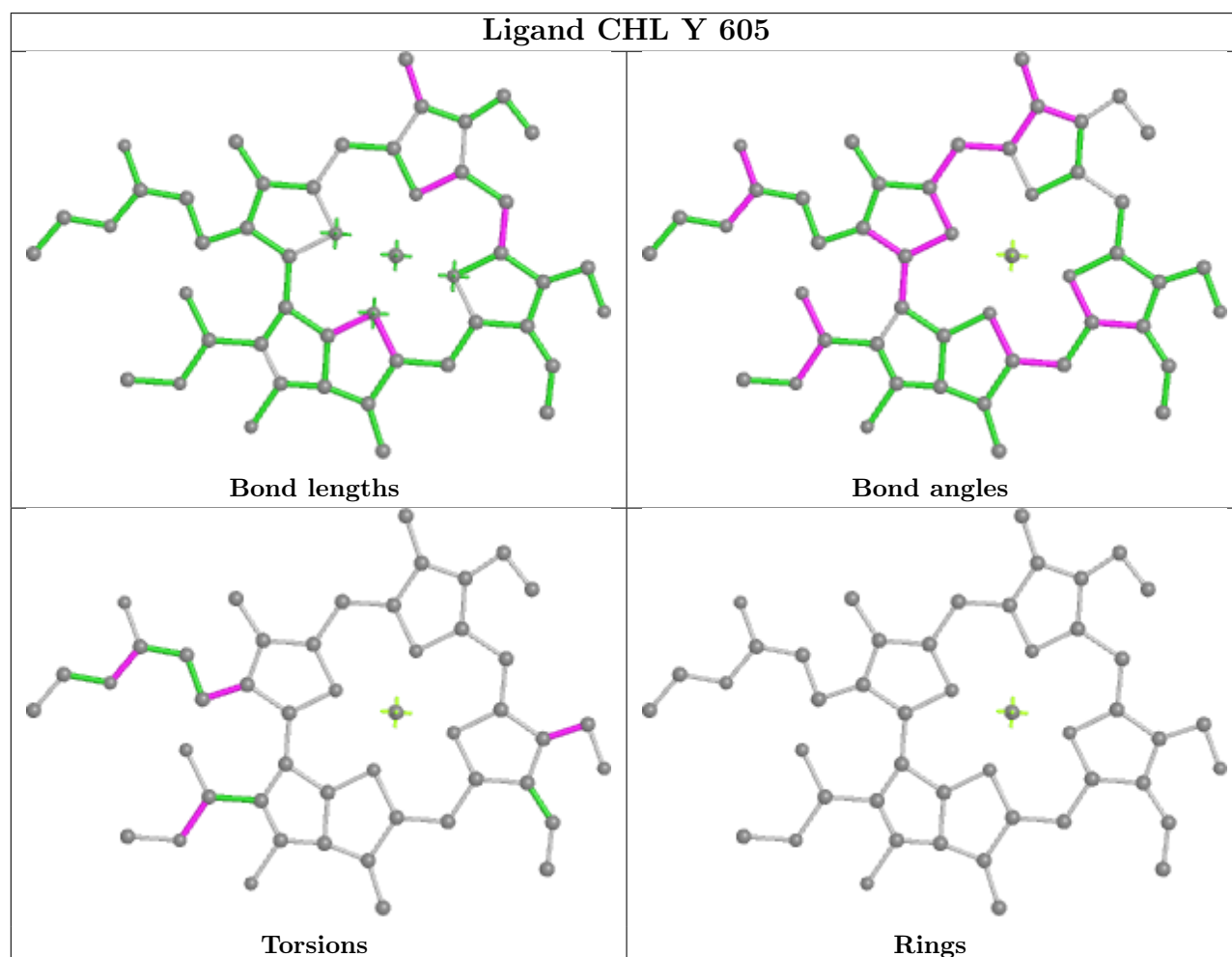
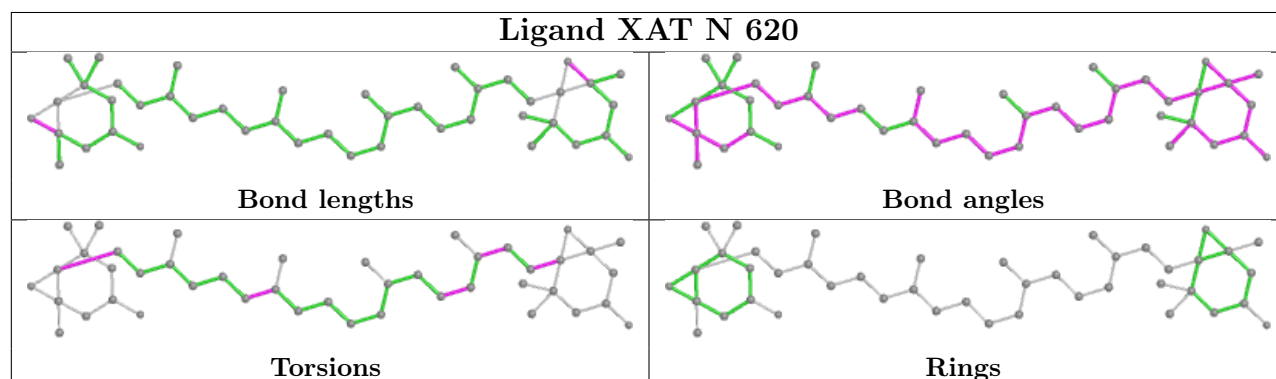
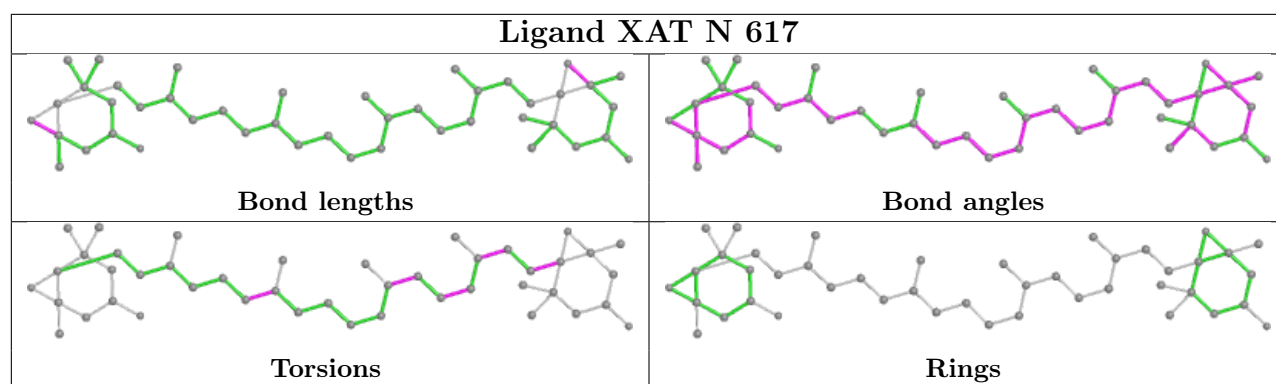


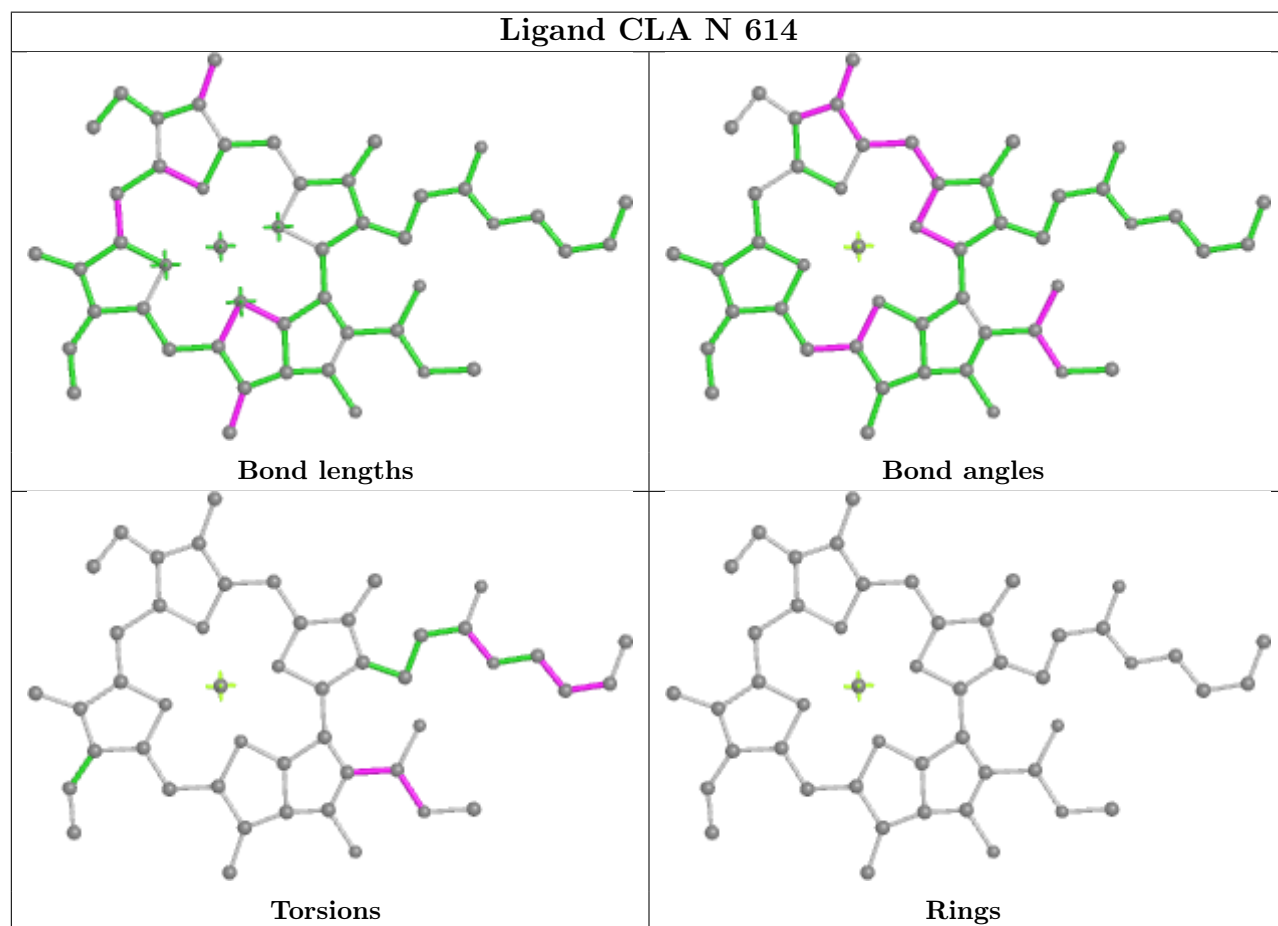
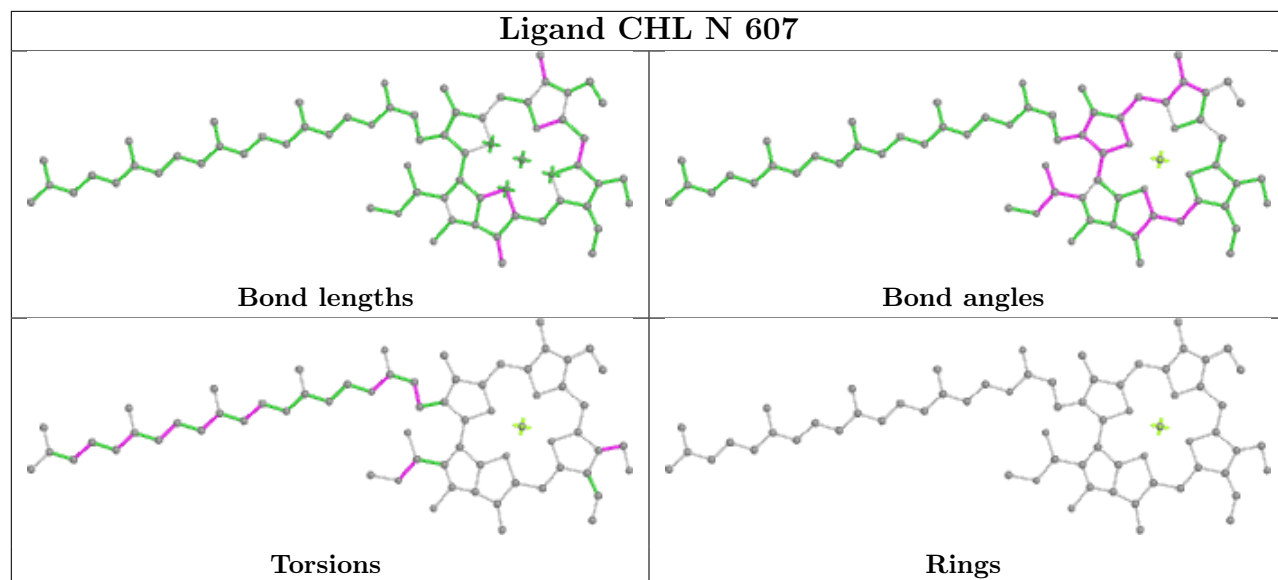


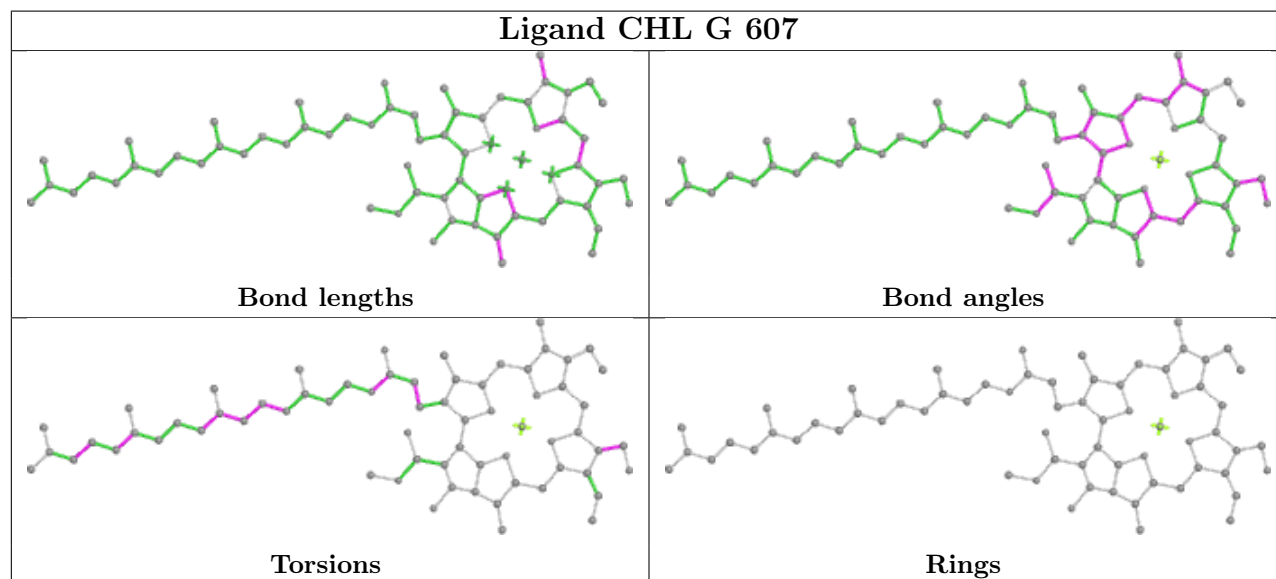
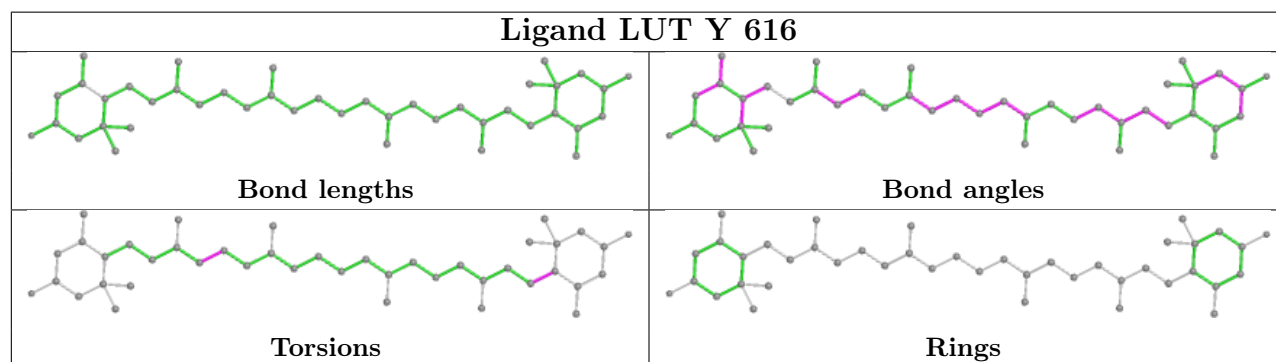
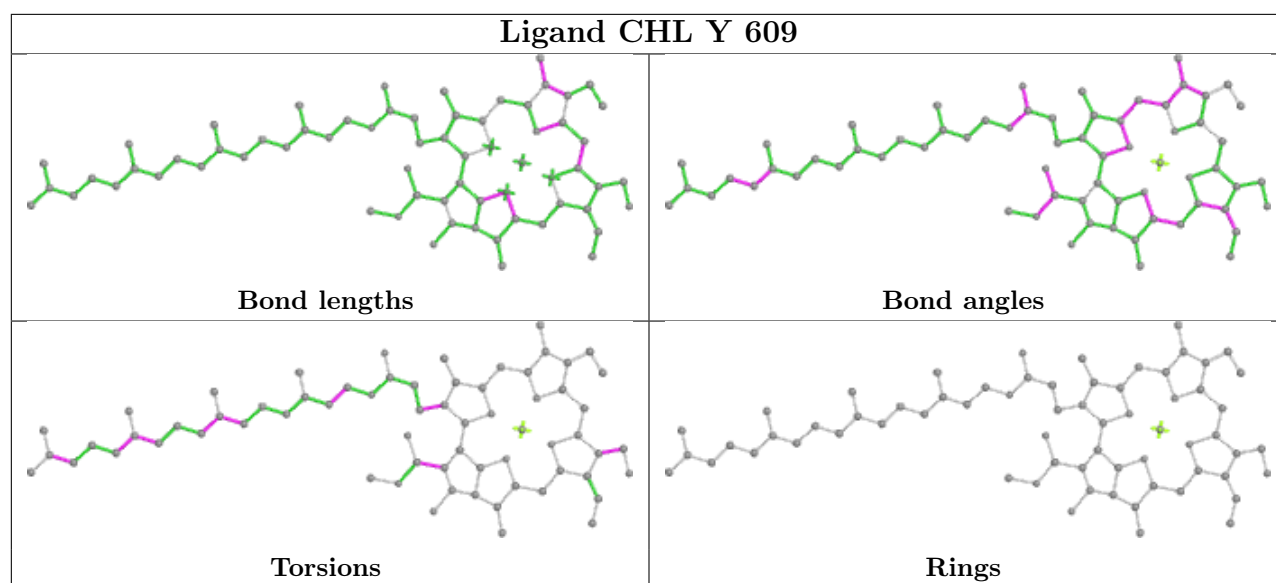




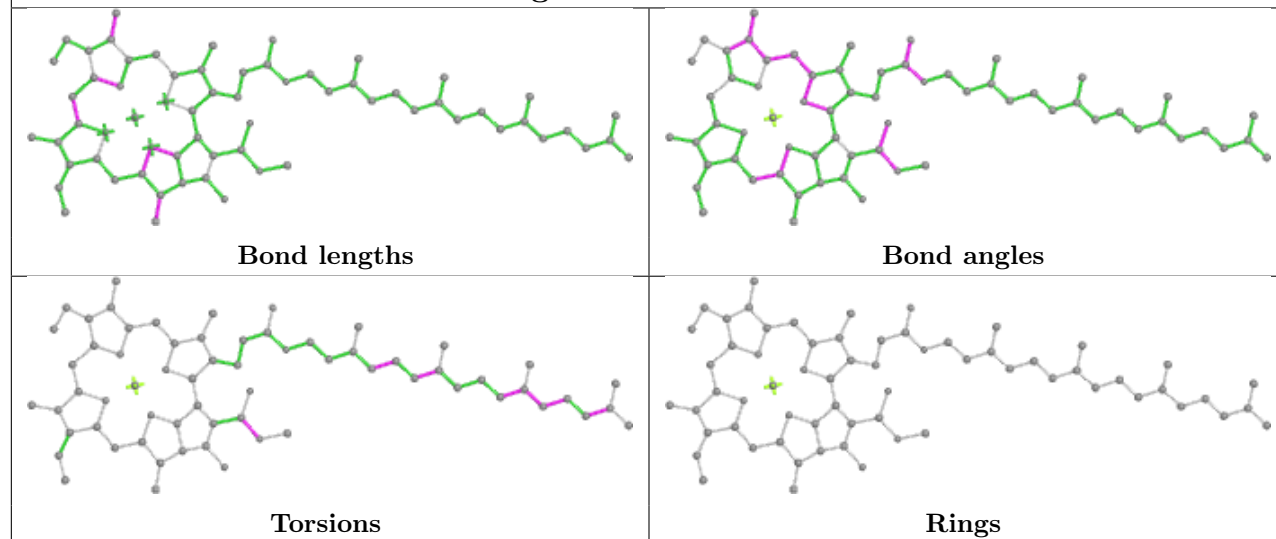




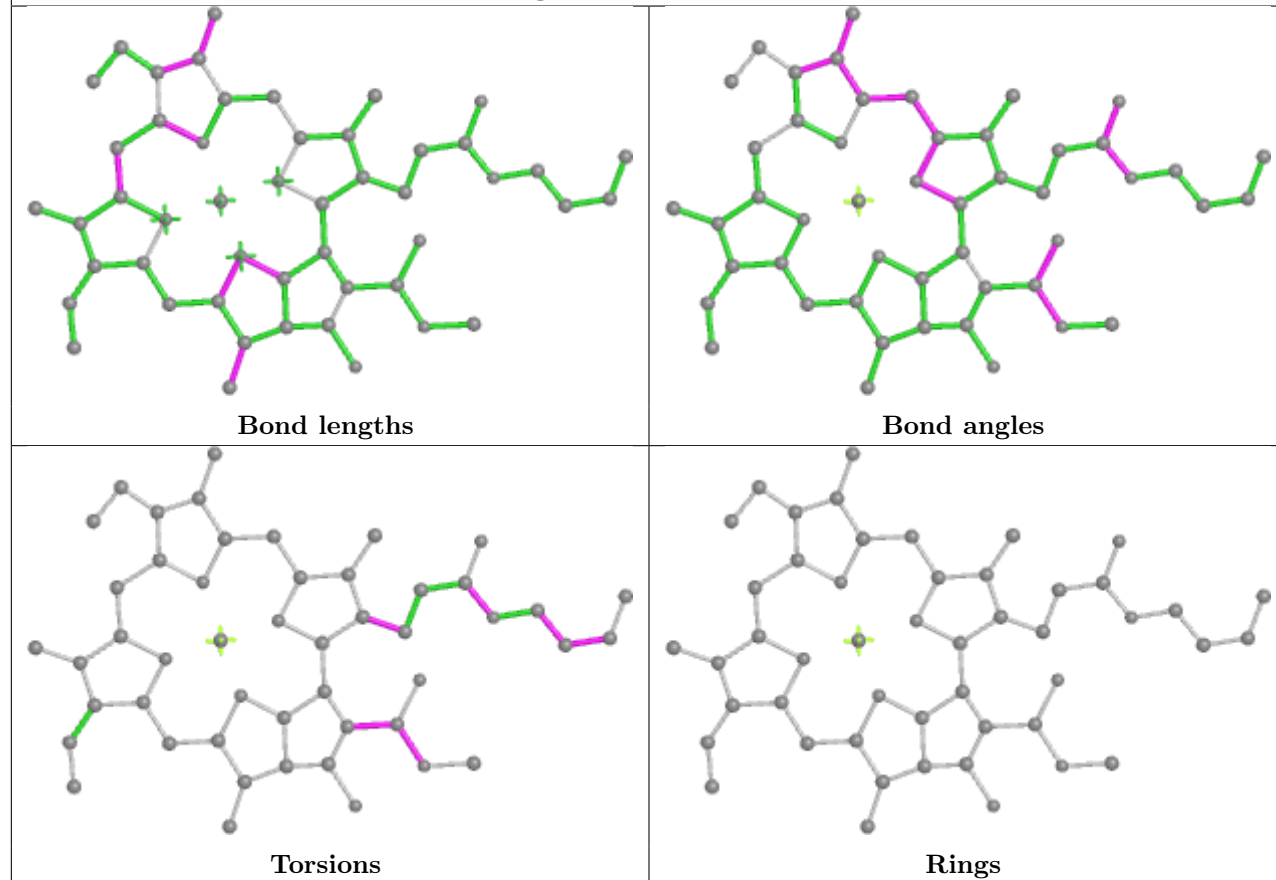


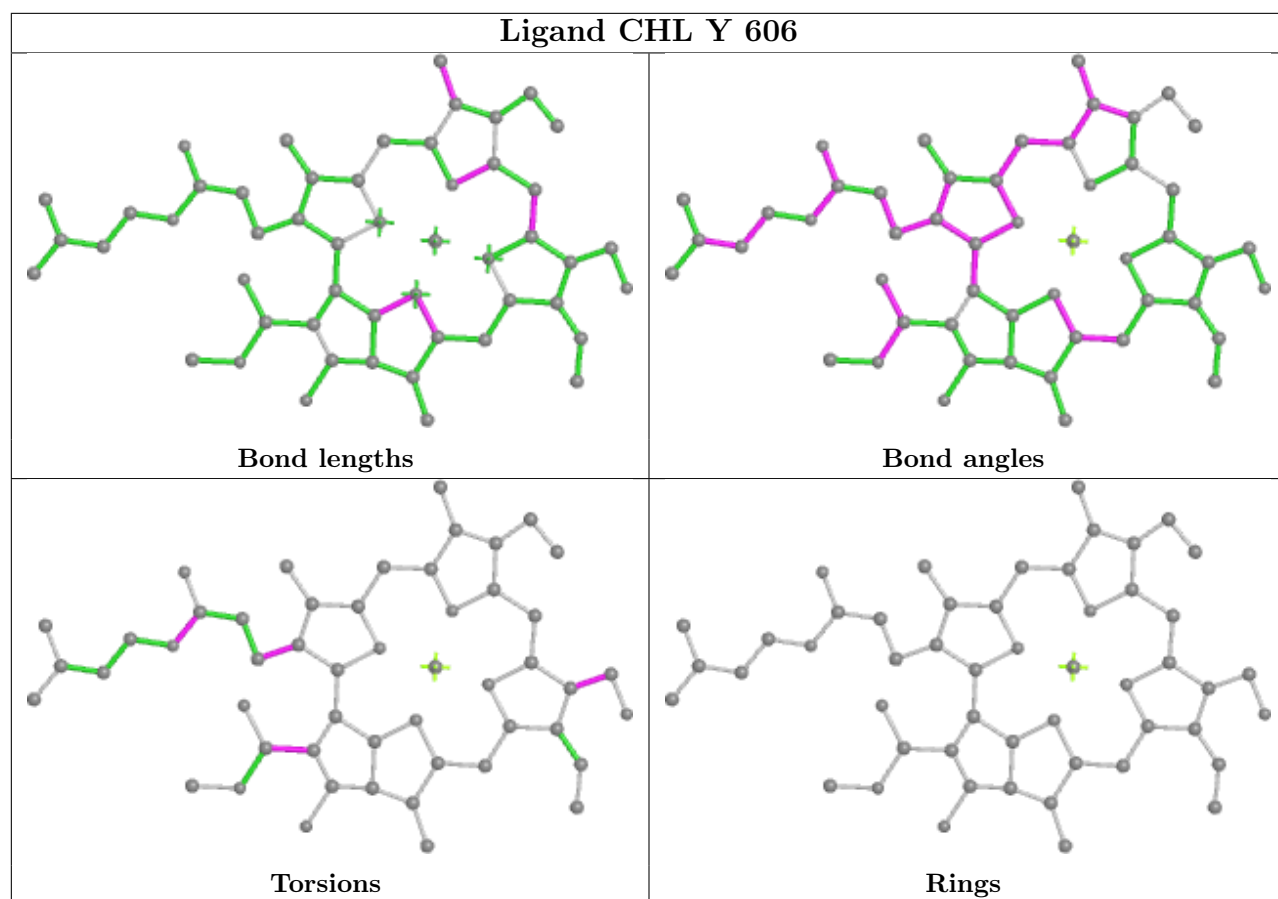
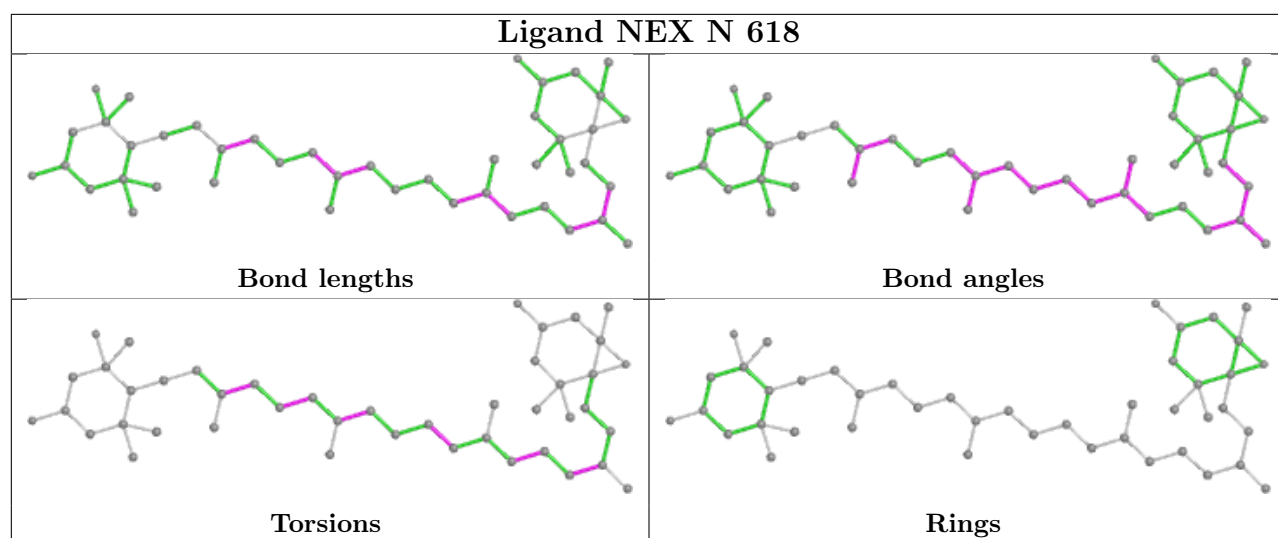


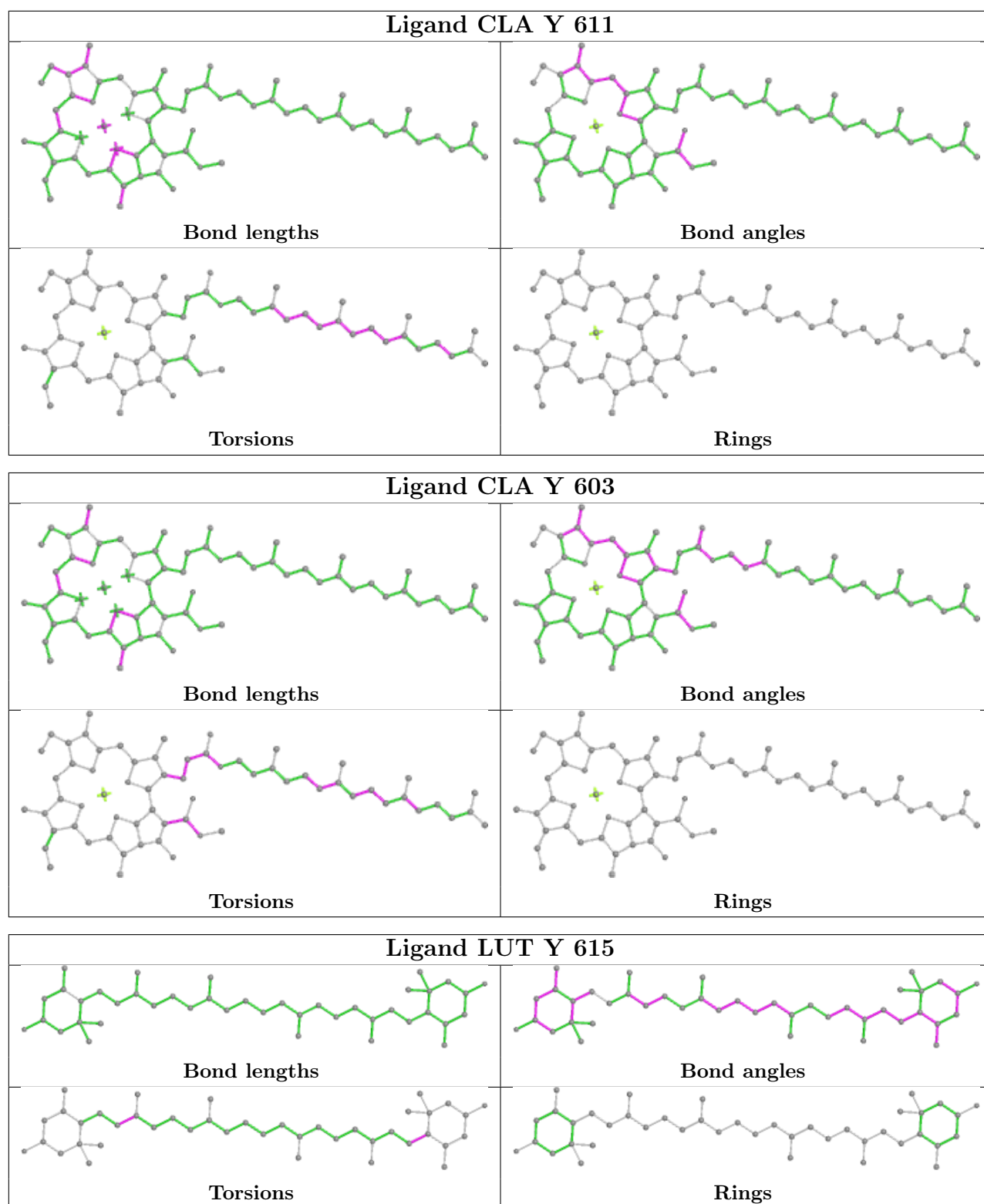
Ligand CLA N 613

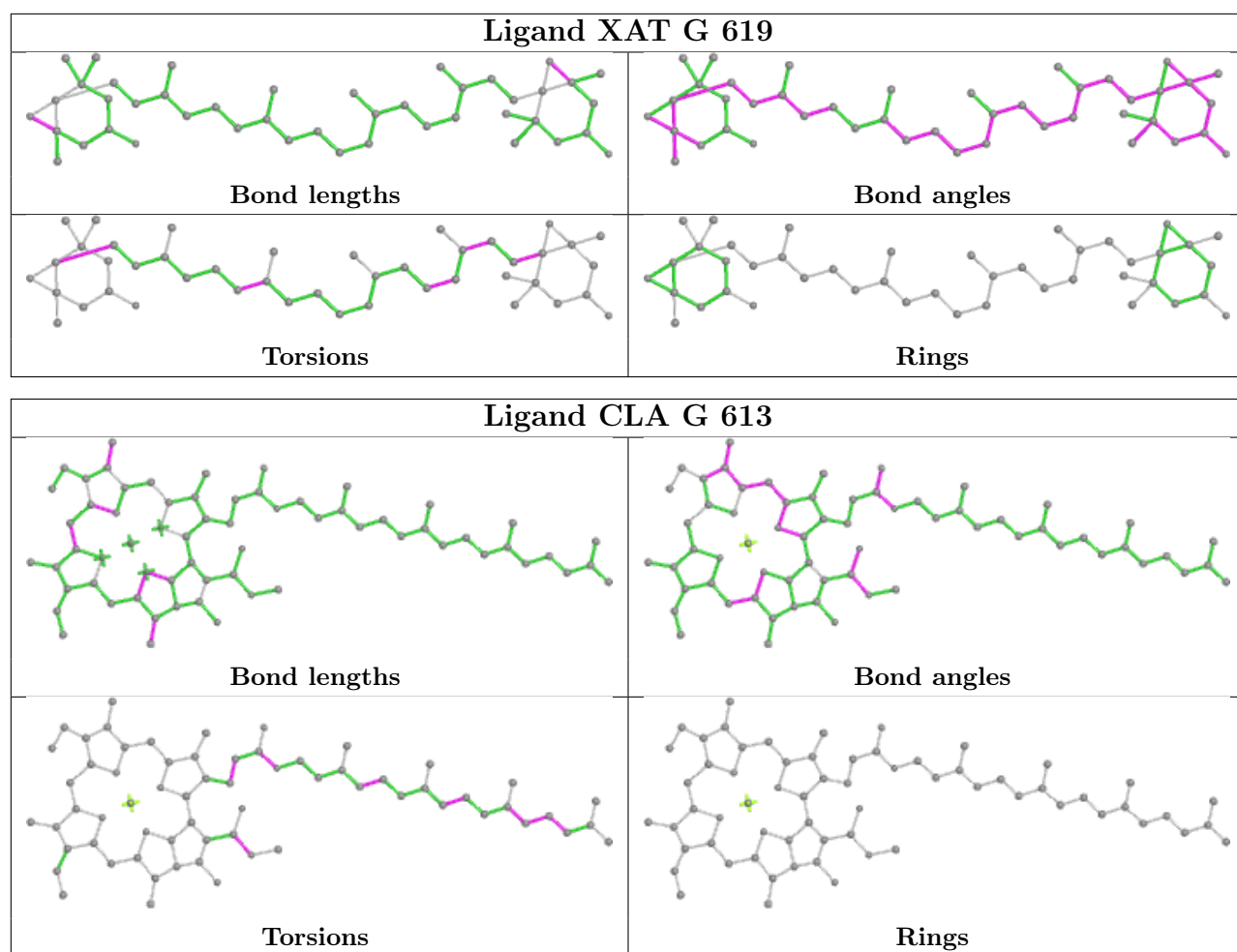


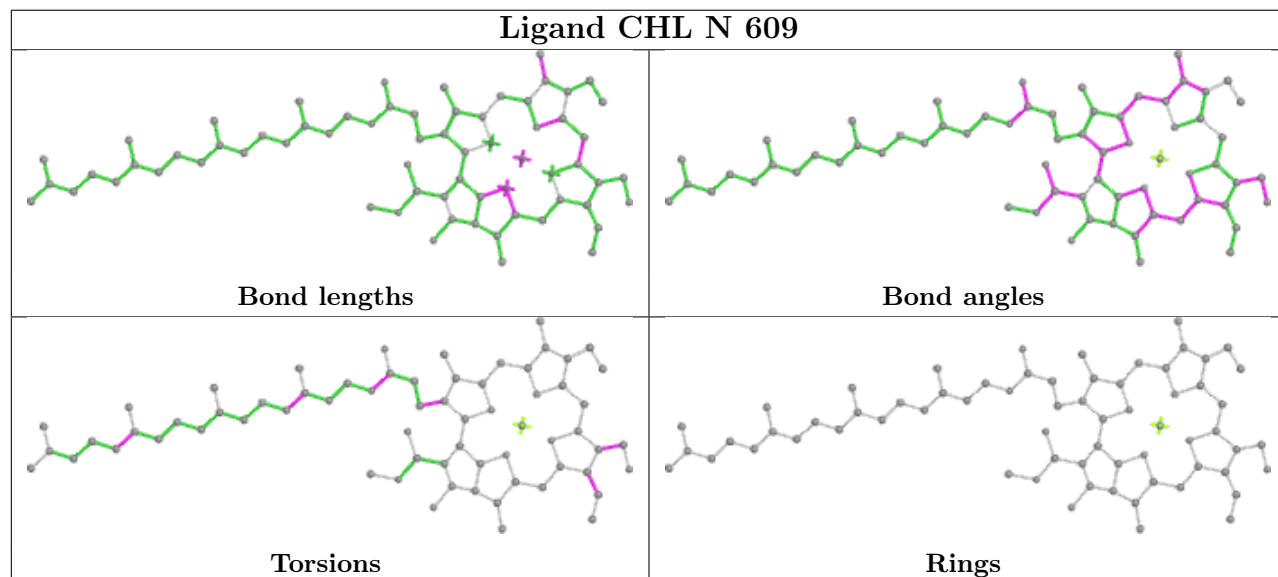
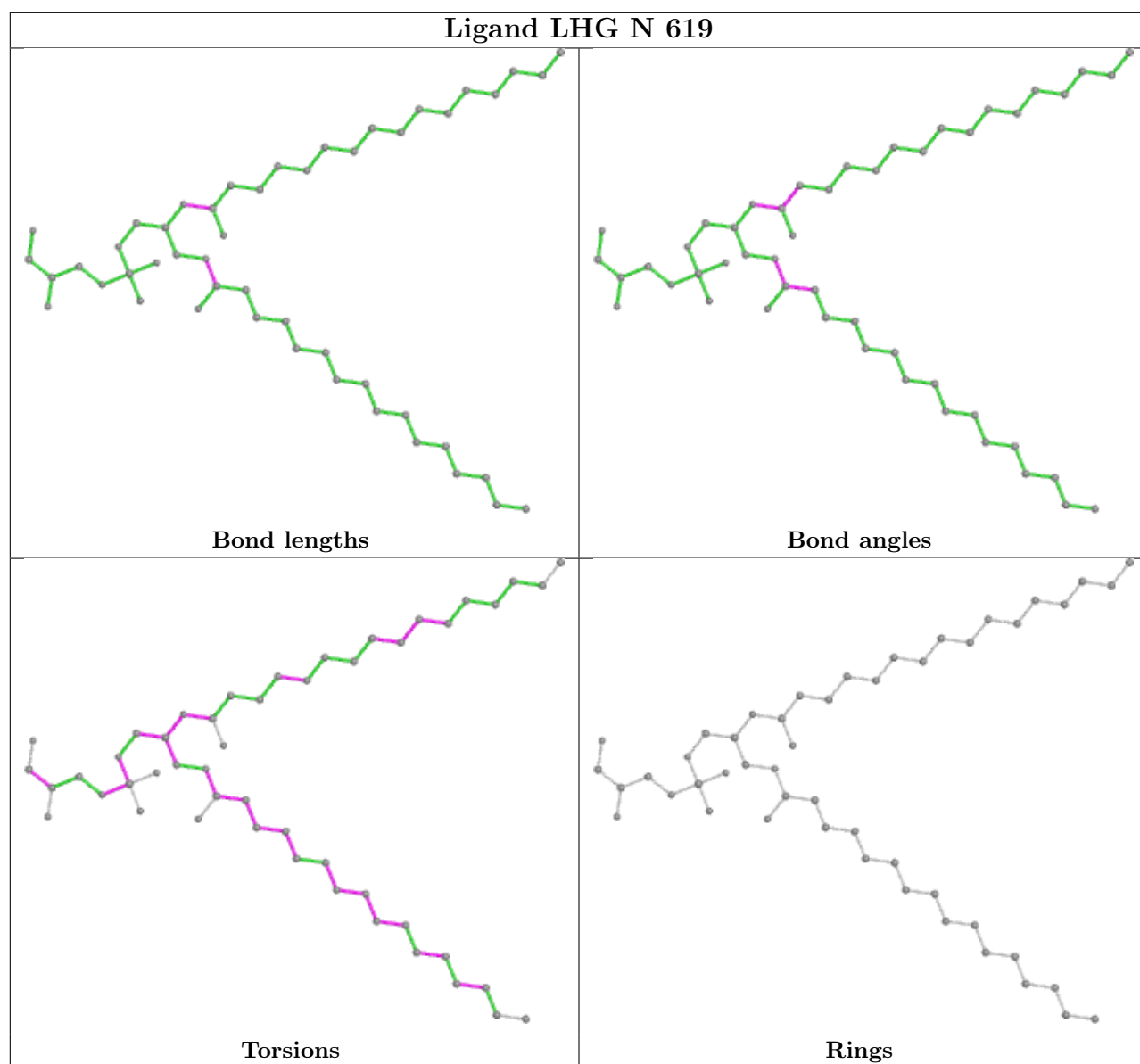
Ligand CLA Y 614

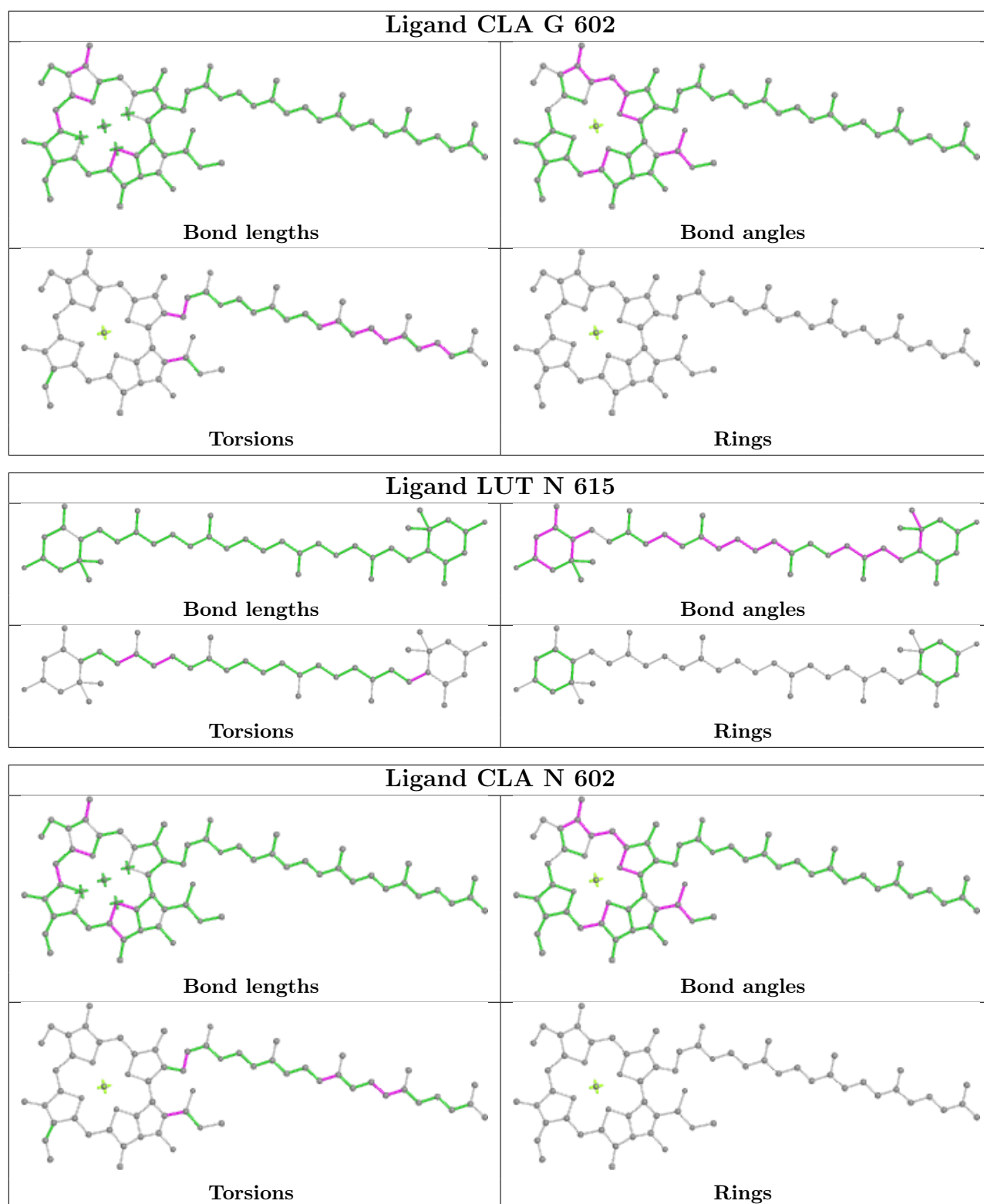


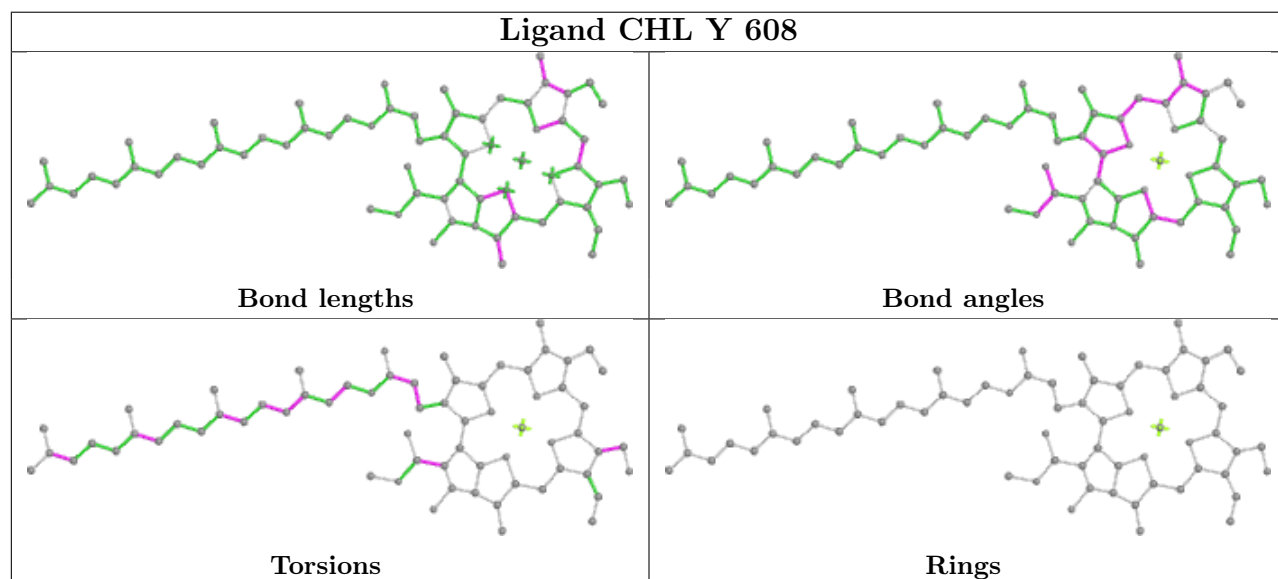
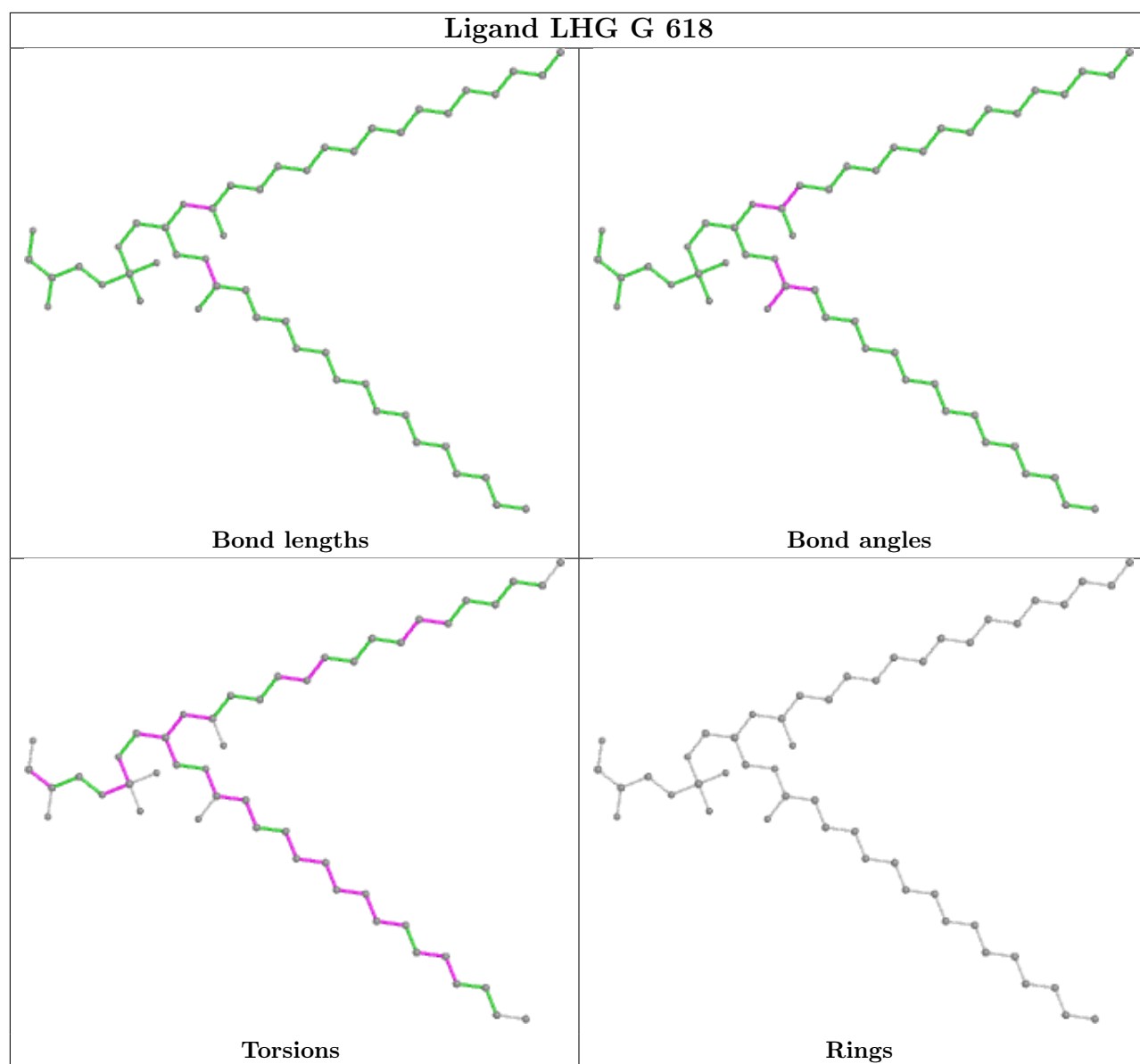


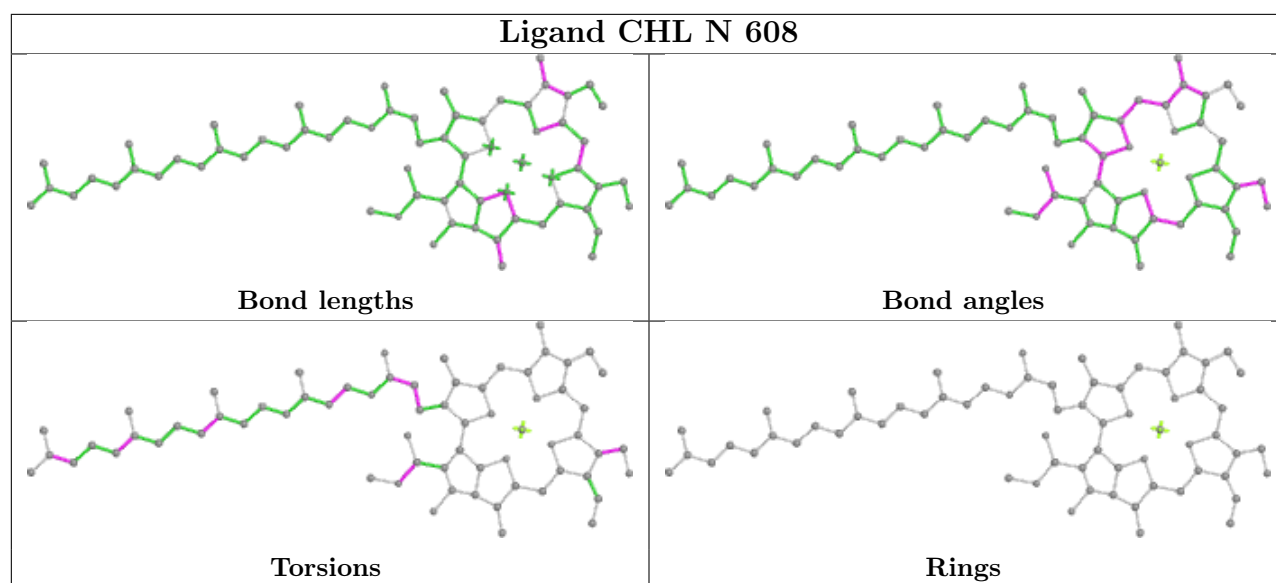












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

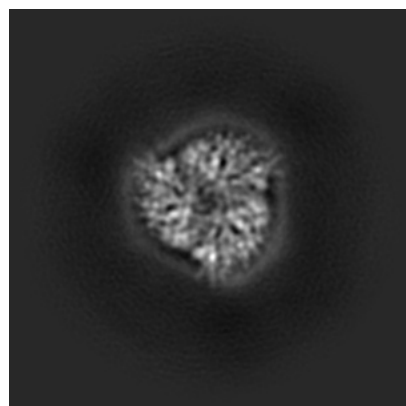
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35782. These allow visual inspection of the internal detail of the map and identification of artifacts.

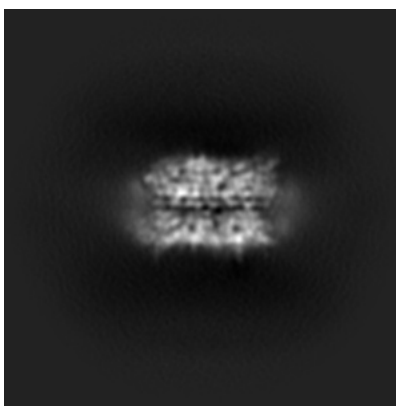
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

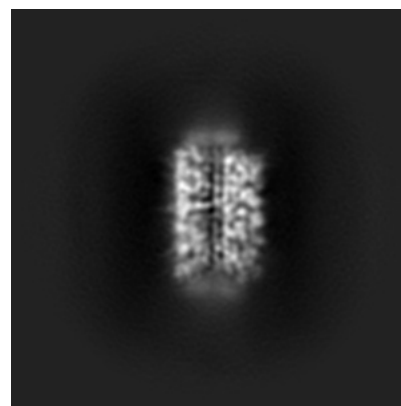
6.1.1 Primary map



X

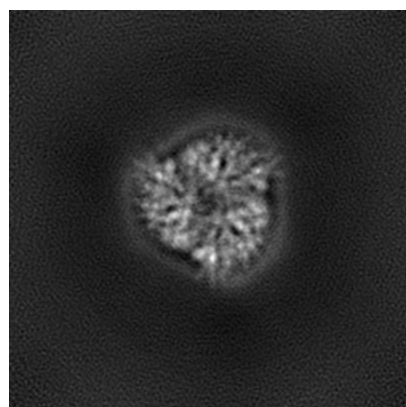


Y

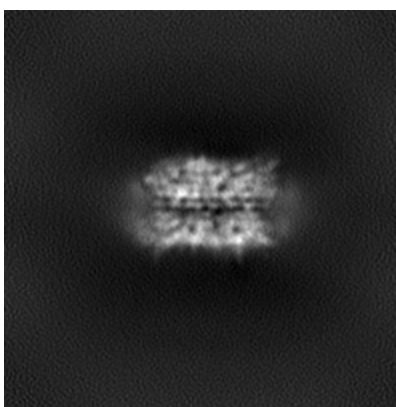


Z

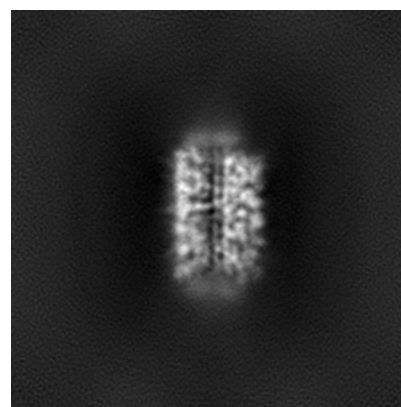
6.1.2 Raw map



X



Y

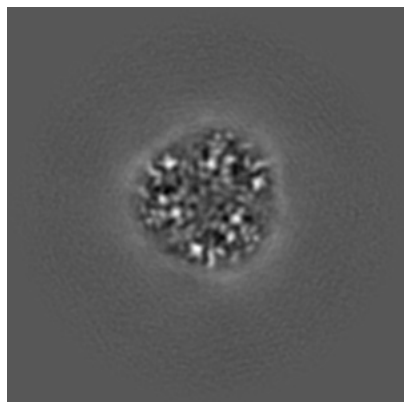


Z

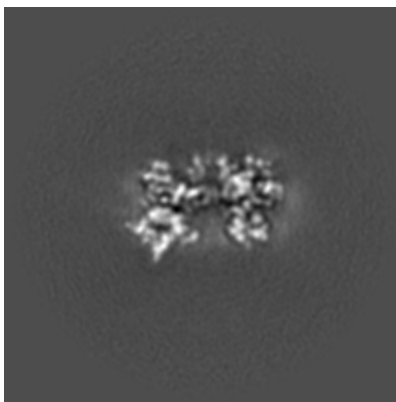
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

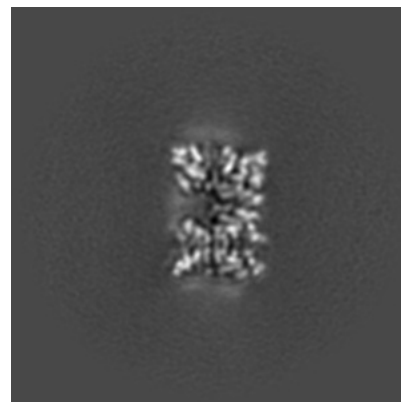
6.2.1 Primary map



X Index: 100

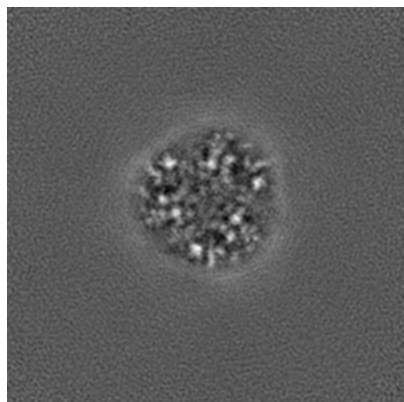


Y Index: 100

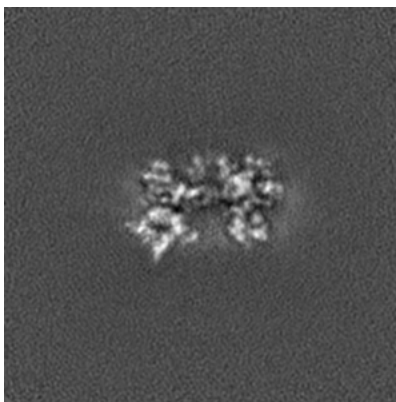


Z Index: 100

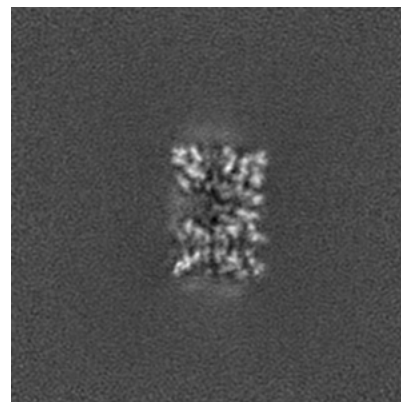
6.2.2 Raw map



X Index: 100



Y Index: 100

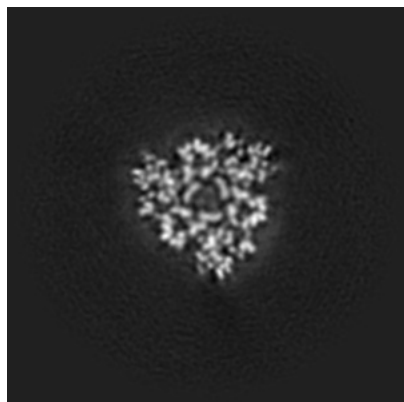


Z Index: 100

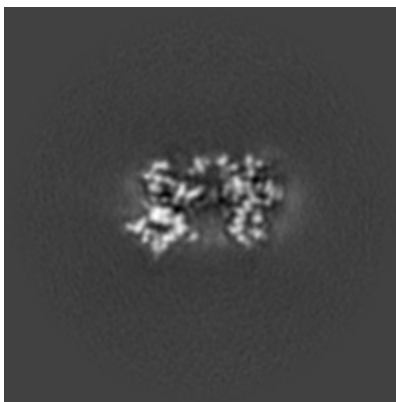
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

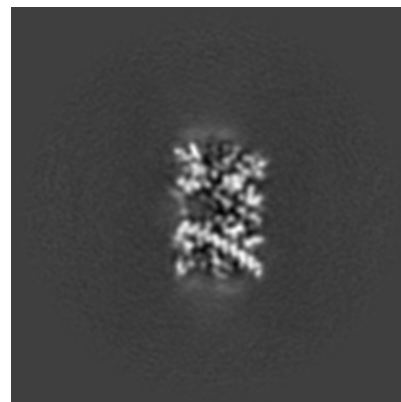
6.3.1 Primary map



X Index: 85

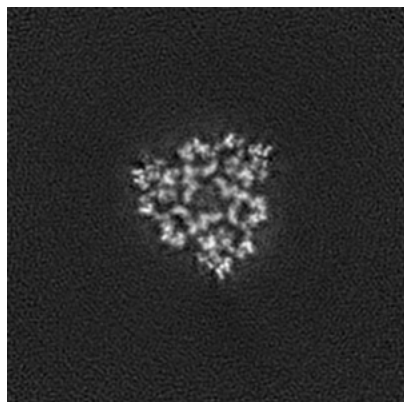


Y Index: 101

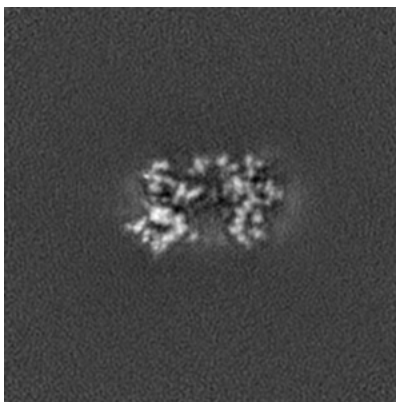


Z Index: 97

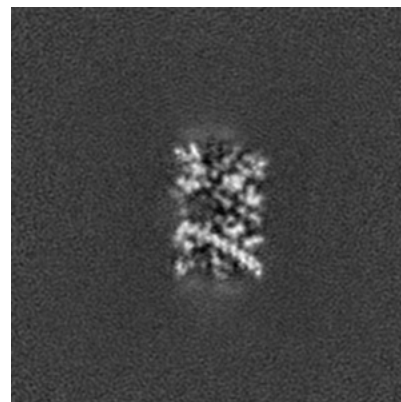
6.3.2 Raw map



X Index: 84



Y Index: 101

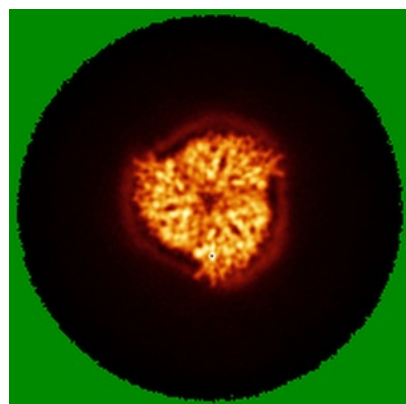


Z Index: 97

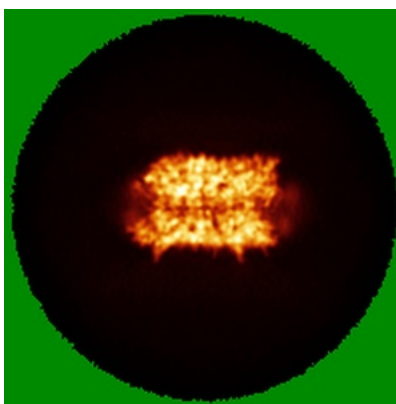
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X

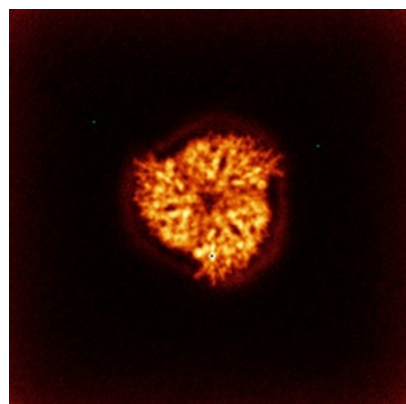


Y

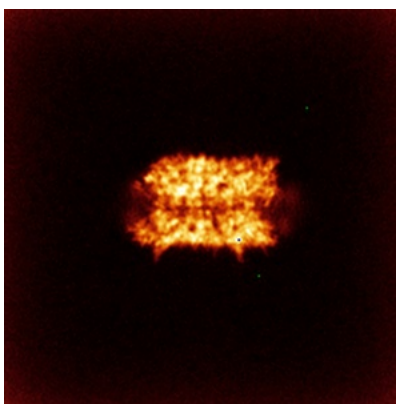


Z

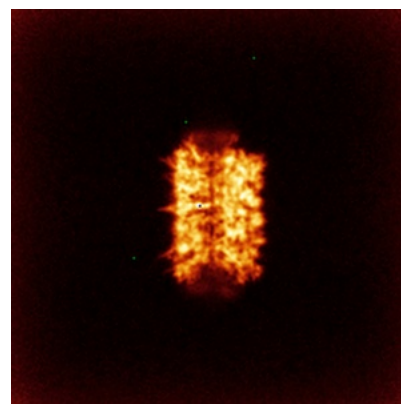
6.4.2 Raw map



X



Y

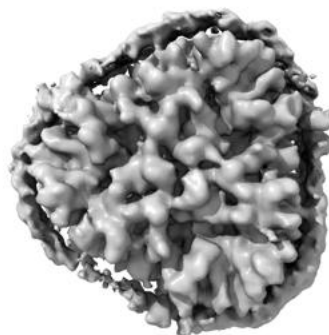


Z

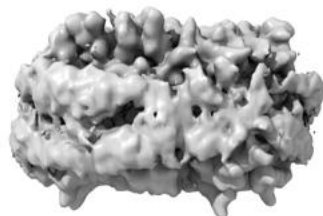
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

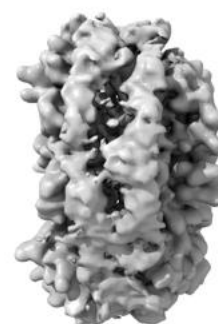
6.5.1 Primary map



X



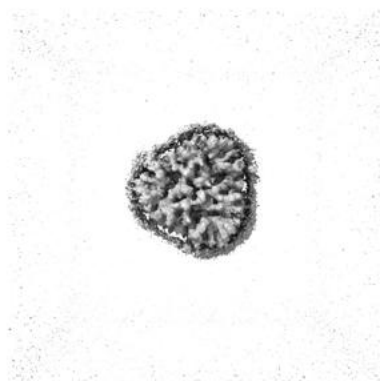
Y



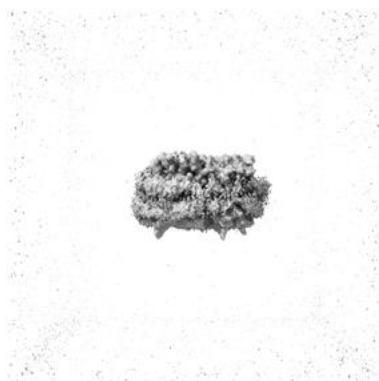
Z

The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

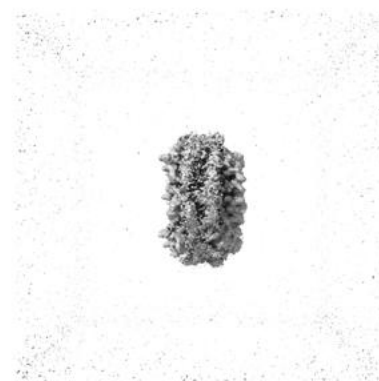
6.5.2 Raw map



X



Y



Z

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

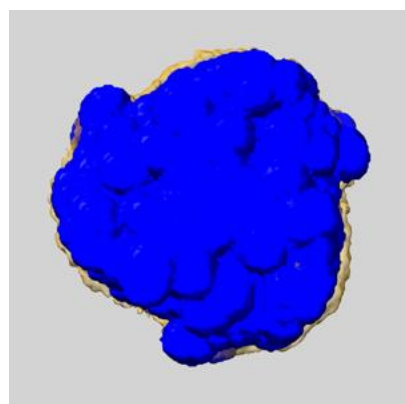
6.6 Mask visualisation [i](#)

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

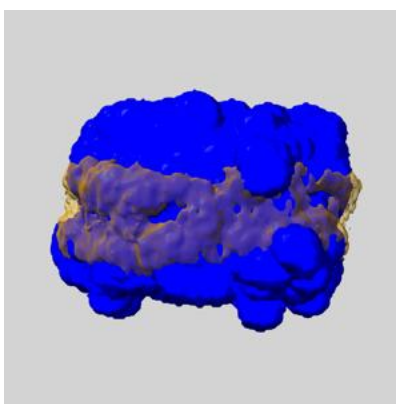
A mask typically either:

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

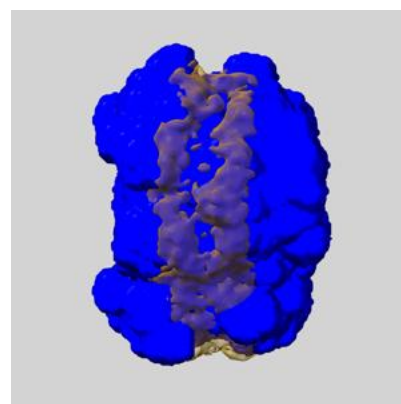
6.6.1 emd_35782_msk_1.map [i](#)



X



Y

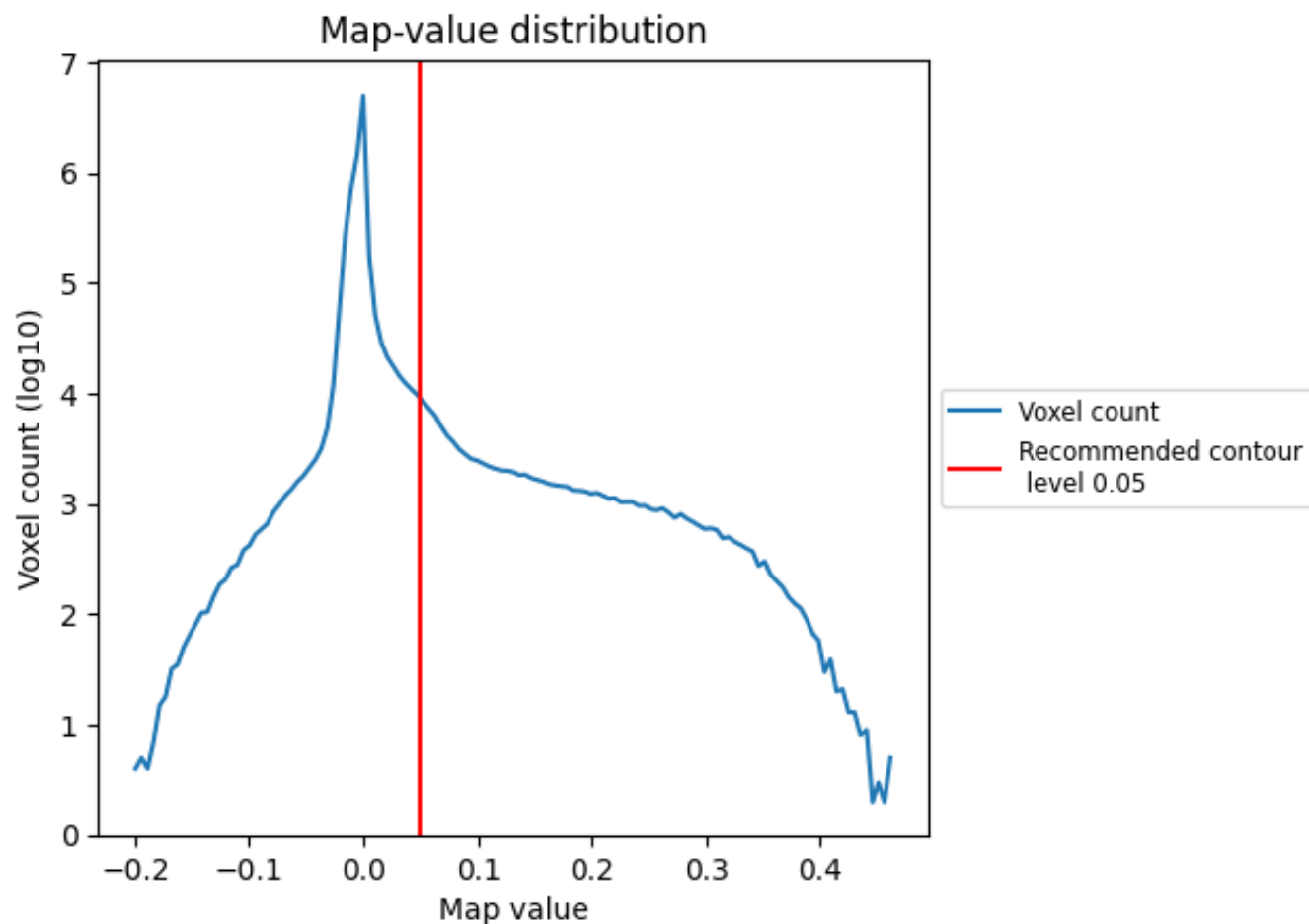


Z

7 Map analysis [i](#)

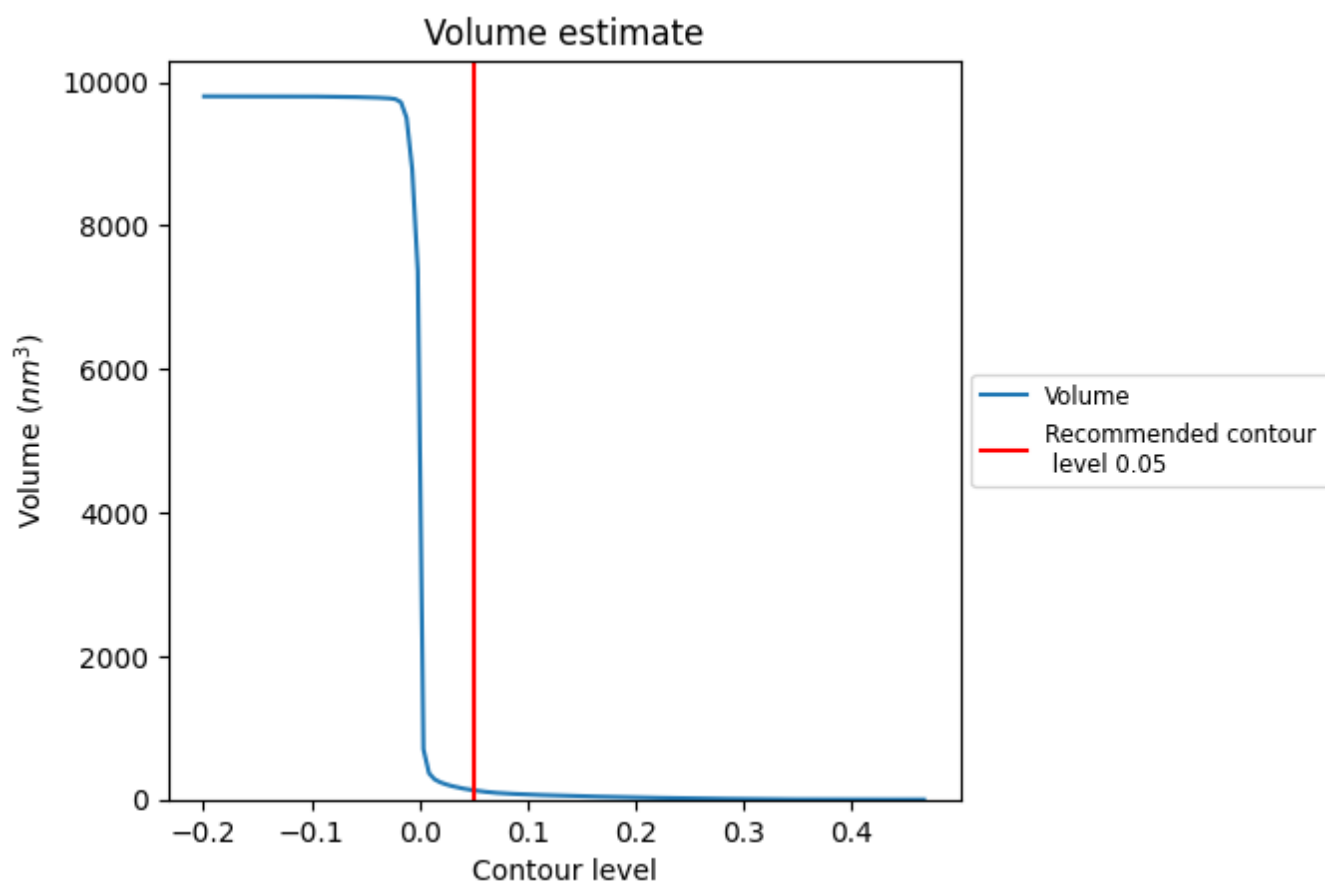
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

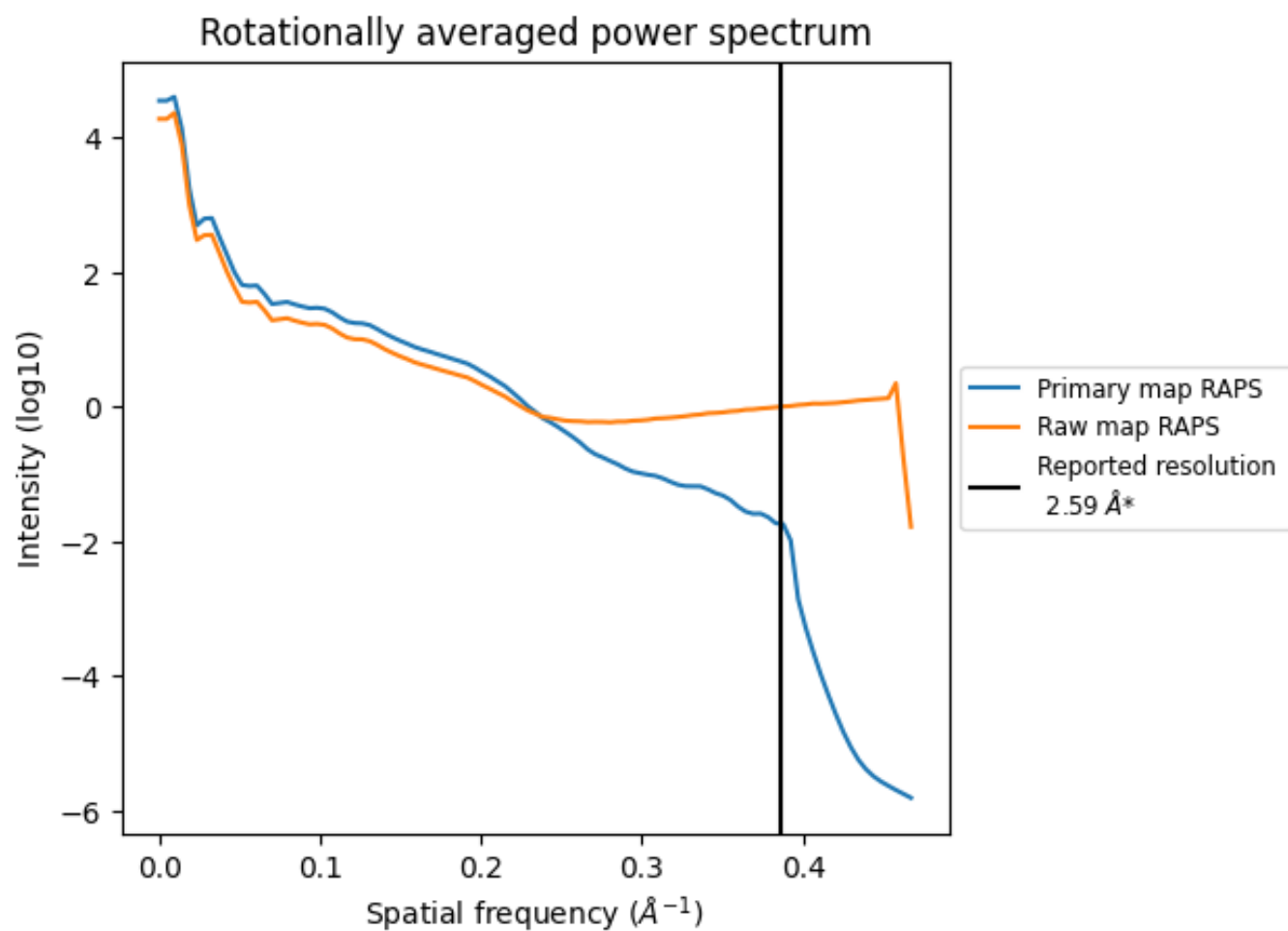
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 129 nm³; this corresponds to an approximate mass of 117 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 ⓘ

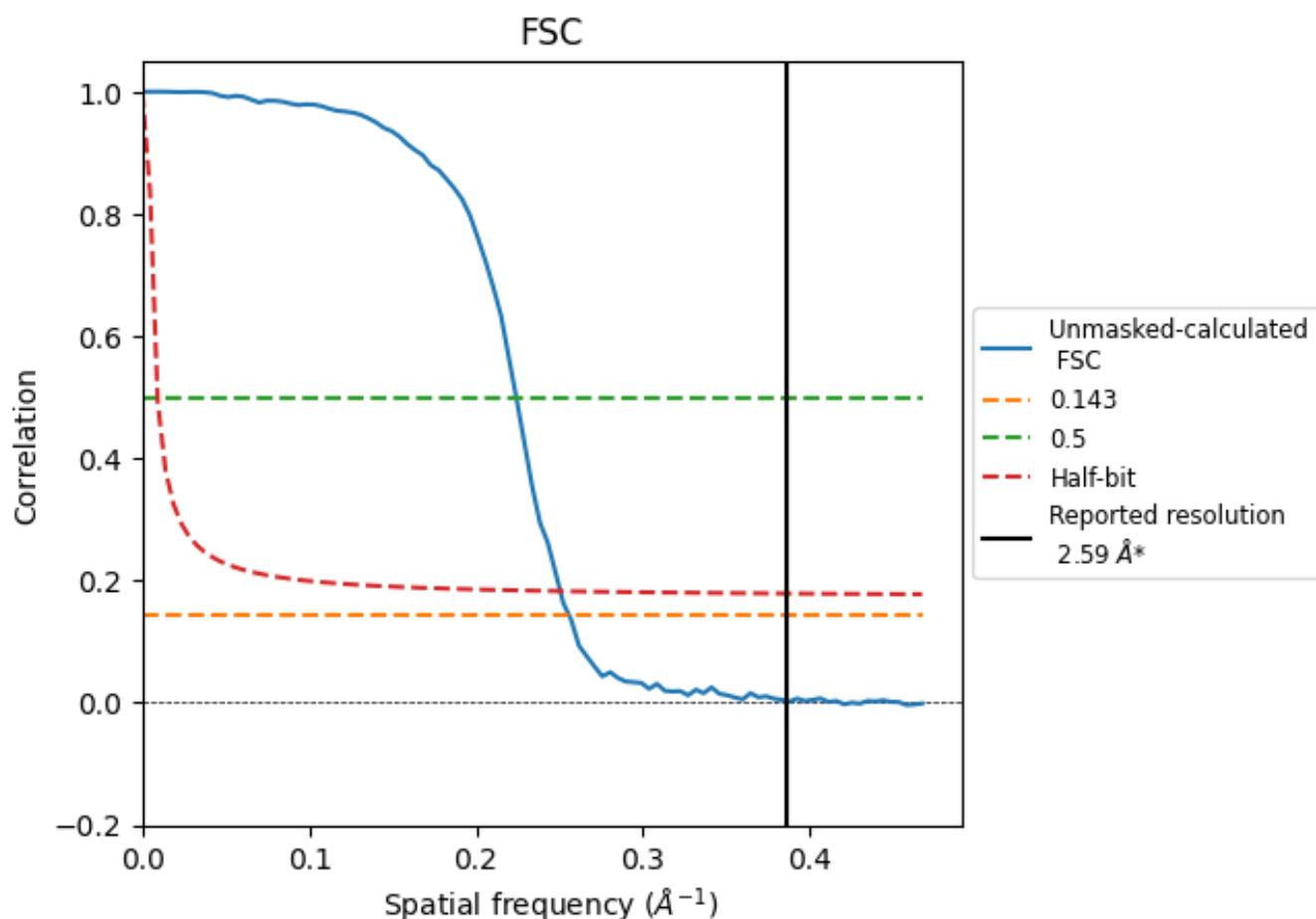


*Reported resolution corresponds to spatial frequency of 0.386 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.386 \AA^{-1}

8.2 Resolution estimates [i](#)

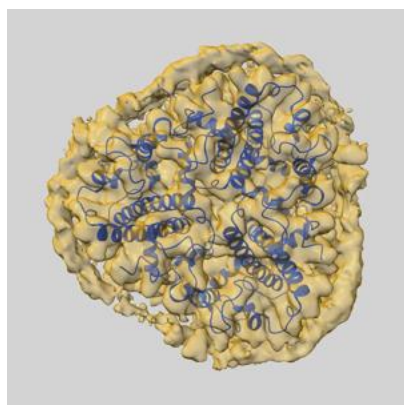
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.59	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.91	4.46	3.99

*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 3.91 differs from the reported value 2.59 by more than 10 %

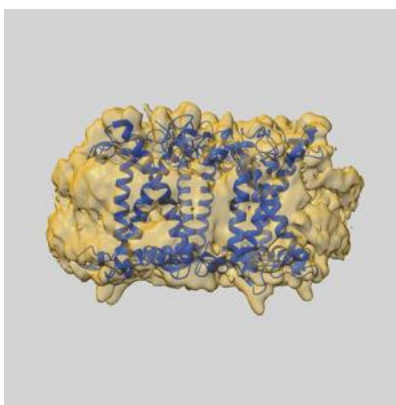
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-35782 and PDB model 8IWX. Per-residue inclusion information can be found in section 3 on page 11.

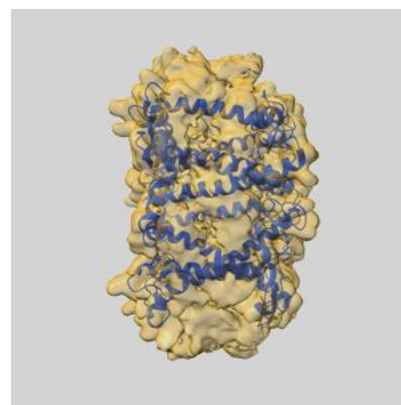
9.1 Map-model overlay [i](#)



X



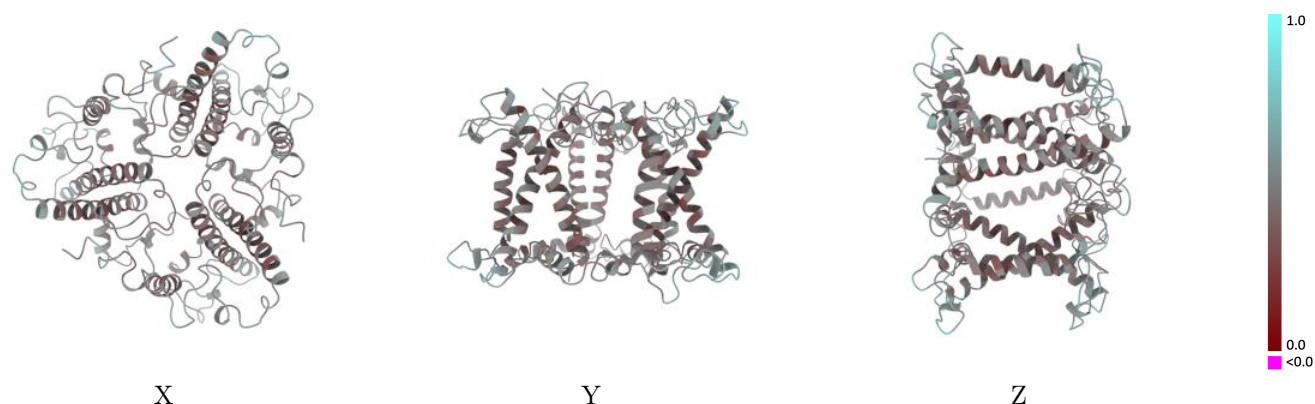
Y



Z

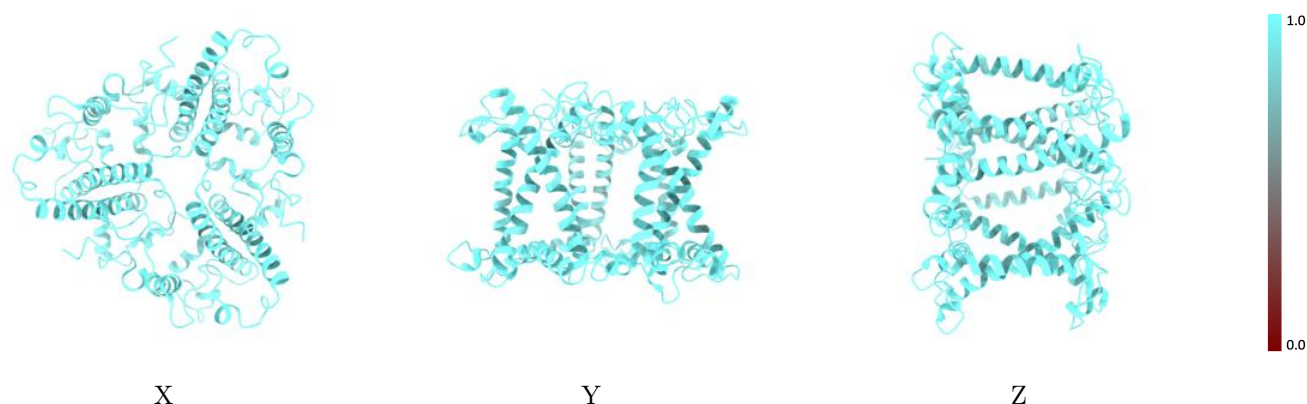
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



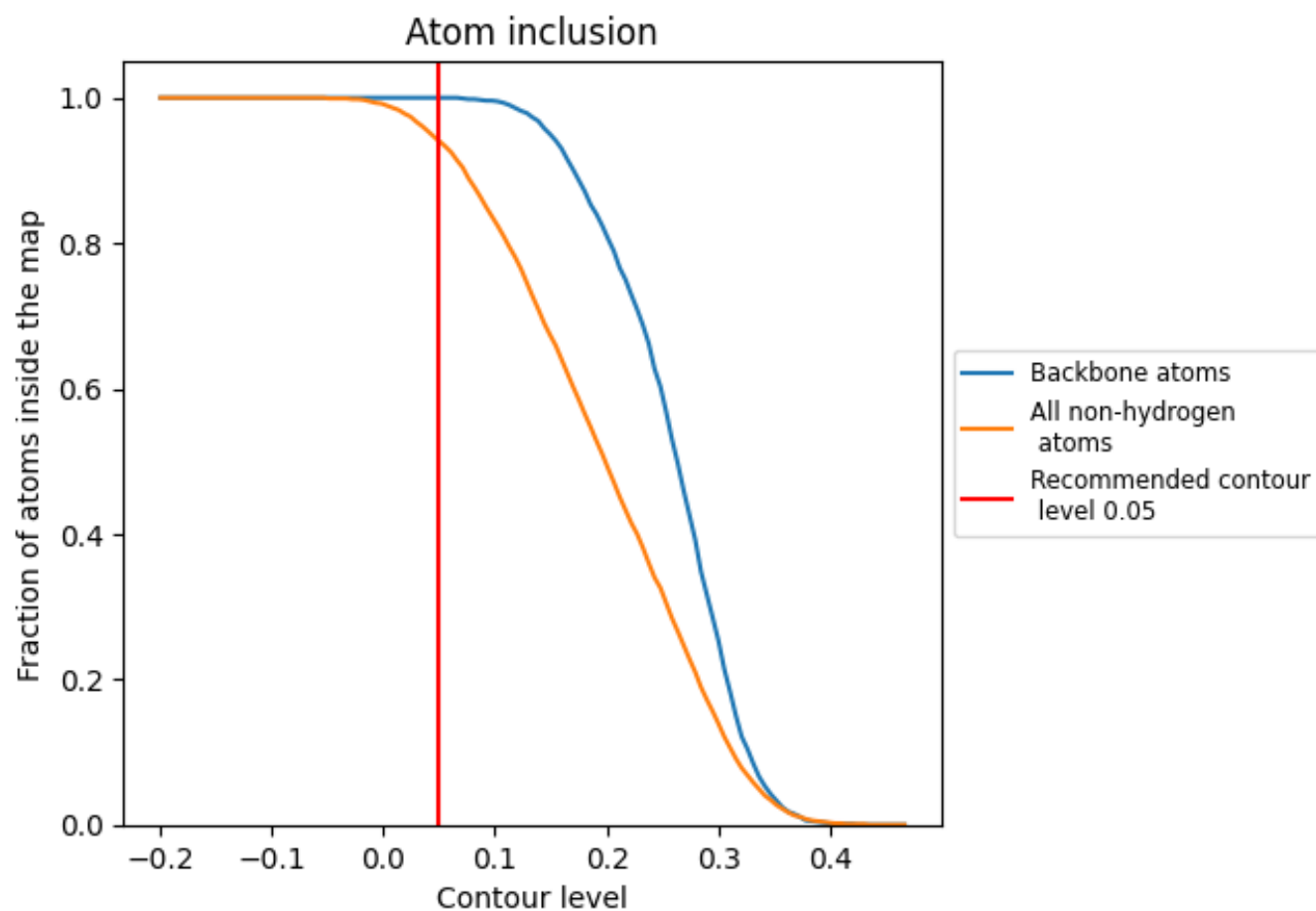
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.05).

9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 94% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9400	<div></div> 0.4660
G	<div></div> 0.9320	<div></div> 0.4690
N	<div></div> 0.9430	<div></div> 0.4640
Y	<div></div> 0.9450	<div></div> 0.4660

