



Full wwPDB EM Validation Report ⓘ

Sep 24, 2023 – 12:20 AM JST

PDB ID : 8IX2
EMDB ID : EMD-35787
Title : Cryo-EM structure of unprotonated LHCII nanodisc at low pH value
Authors : Ruan, M.X.; Ding, W.
Deposited on : 2023-03-31
Resolution : 2.80 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.dev50
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

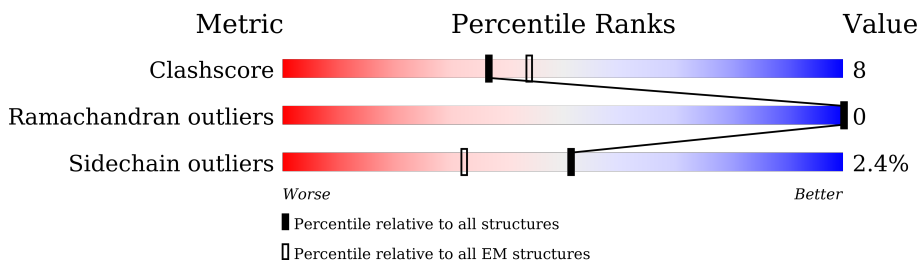
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	 91% 9%
1	N	218	 90% 9%
1	Y	218	 93% 7%

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	302	X	-	-	-
2	CHL	Y	306	X	-	-	-
2	CHL	Y	307	X	-	-	-
2	CHL	Y	308	X	-	-	-
2	CHL	Y	309	X	-	-	-
2	CHL	Y	310	X	-	-	-
3	CLA	G	602	X	-	-	-
3	CLA	G	603	X	-	-	-
3	CLA	G	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	612	X	-	-	-
3	CLA	N	613	X	-	-	-
3	CLA	N	614	X	-	-	-
3	CLA	Y	303	X	-	-	-
3	CLA	Y	304	X	-	-	-
3	CLA	Y	305	X	-	-	-
3	CLA	Y	311	X	-	-	-
3	CLA	Y	313	X	-	-	-
3	CLA	Y	314	X	-	-	-
3	CLA	Y	315	X	-	-	-

2 Entry composition [\(i\)](#)

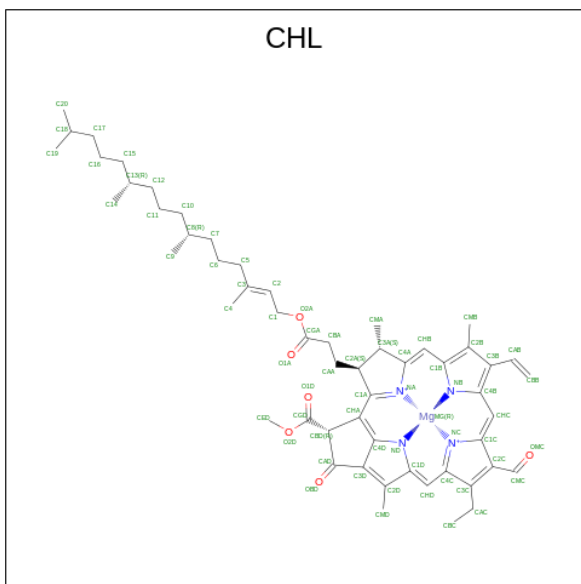
There are 7 unique types of molecules in this entry. The entry contains 8238 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
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 (three-letter code: CHL) (formula: $C_{55}H_{70}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
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	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 (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



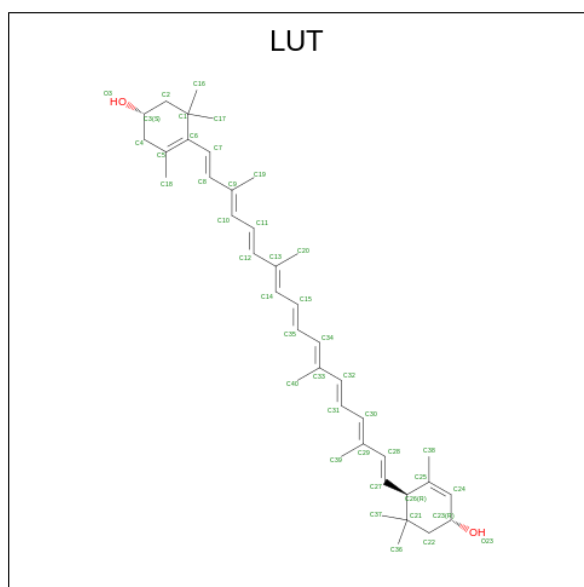
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
3	N	1	65	55	1	4	5	0
3	N	1	65	55	1	4	5	0
3	N	1	62	52	1	4	5	0
3	N	1	65	55	1	4	5	0
3	N	1	65	55	1	4	5	0
3	N	1	65	55	1	4	5	0
3	N	1	65	55	1	4	5	0
3	N	1	49	39	1	4	5	0
3	G	1	65	55	1	4	5	0
3	G	1	65	55	1	4	5	0
3	G	1	62	52	1	4	5	0
3	G	1	65	55	1	4	5	0
3	G	1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

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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 (three-letter code: LUT) (formula: C₄₀H₅₆O₂).



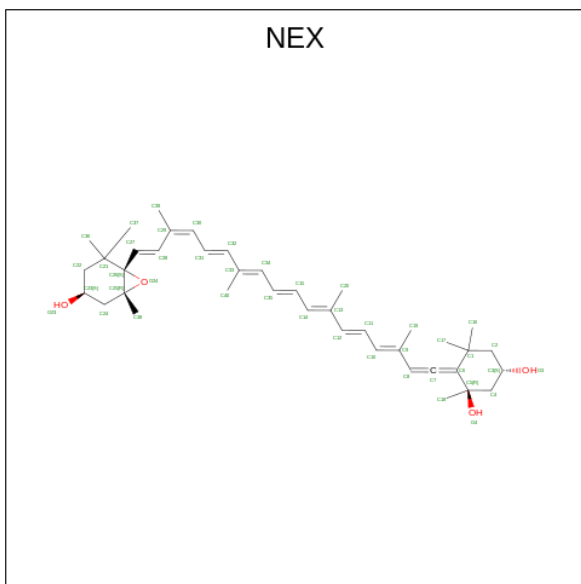
Mol	Chain	Residues	Atoms			AltConf
4	N	1	Total	C	O	0
			42	40	2	

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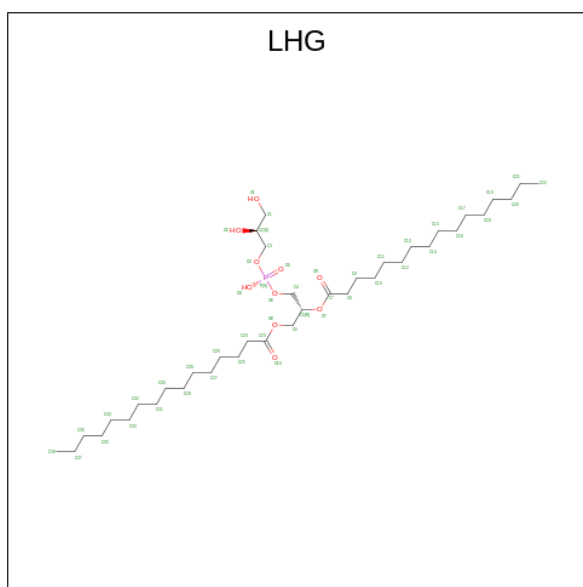
Mol	Chain	Residues	Atoms			AltConf
4	N	1	Total	C	O	0
			42	40	2	
4	G	1	Total	C	O	0
			42	40	2	
4	G	1	Total	C	O	0
			42	40	2	
4	Y	1	Total	C	O	0
			42	40	2	
4	Y	1	Total	C	O	0
			42	40	2	

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



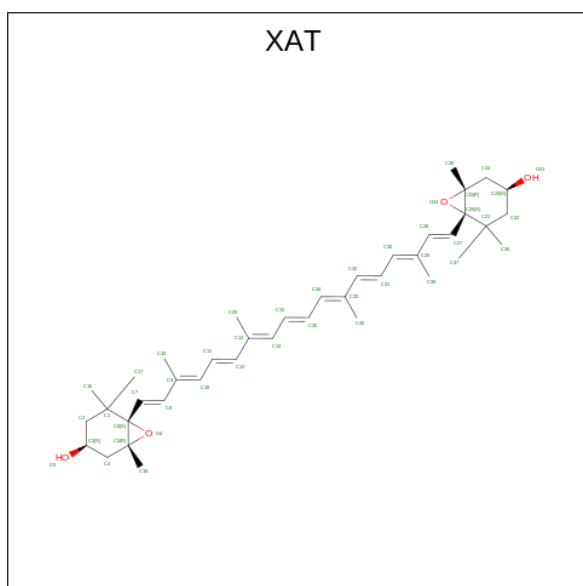
Mol	Chain	Residues	Atoms			AltConf
5	N	1	Total	C	O	0
			44	40	4	
5	G	1	Total	C	O	0
			44	40	4	
5	Y	1	Total	C	O	0
			44	40	4	

- Molecule 6 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



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

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

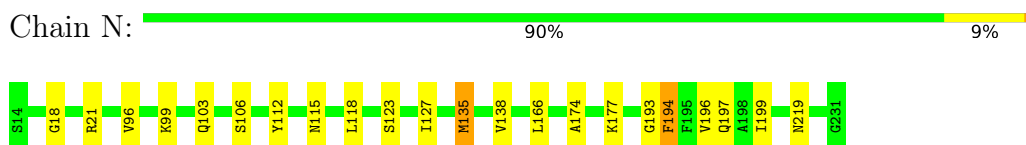


Mol	Chain	Residues	Atoms			AltConf
7	N	1	Total 44	C 40	O 4	0
7	G	1	Total 44	C 40	O 4	0
7	Y	1	Total 44	C 40	O 4	0

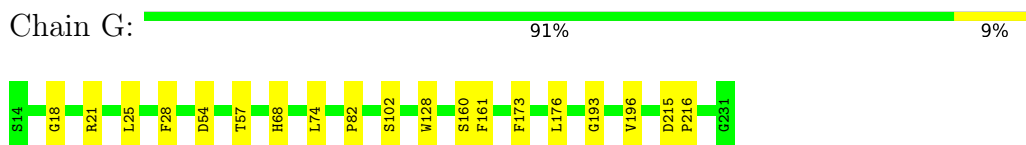
3 Residue-property plots [i](#)

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

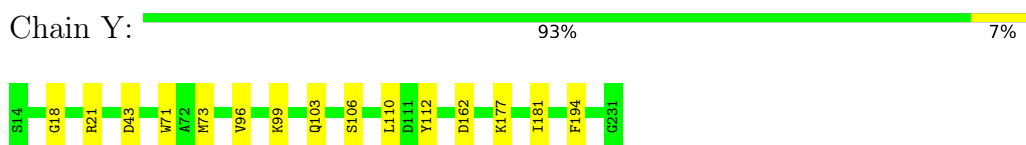
- Molecule 1: Chlorophyll a-b binding protein, chloroplastic



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



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	353360	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	0.453	Depositor
Minimum map value	-0.156	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	220.0, 220.0, 220.0	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	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: LUT, XAT, LHG, NEX, CHL, CLA

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	0.32	0/1713	0.50	0/2333
1	N	0.28	0/1713	0.51	0/2333
1	Y	0.28	0/1713	0.47	0/2333
All	All	0.30	0/5139	0.49	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	1590	11	0
1	N	1661	0	1590	13	0
1	Y	1661	0	1592	8	0
2	G	363	0	350	9	0
2	N	363	0	350	12	0
2	Y	363	0	350	5	0
3	G	501	0	534	27	0
3	N	501	0	534	10	0
3	Y	501	0	534	26	0
4	G	84	0	112	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	N	84	0	112	10	0
4	Y	84	0	112	6	0
5	G	44	0	56	4	0
5	N	44	0	56	4	0
5	Y	44	0	56	4	0
6	G	49	0	74	1	0
6	N	49	0	74	1	0
6	Y	49	0	74	0	0
7	G	44	0	56	4	0
7	N	44	0	56	4	0
7	Y	44	0	56	4	0
All	All	8238	0	8318	138	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (138) 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:610:CLA:H52	4:N:615:LUT:H28	1.64	0.80
3:G:612:CLA:H171	3:G:612:CLA:HMB1	1.70	0.73
3:N:610:CLA:H51	3:N:610:CLA:HBB1	1.73	0.69
1:G:196:VAL:HG11	3:G:613:CLA:HAC2	1.74	0.69
1:G:176:LEU:HG	3:G:610:CLA:HBB	1.77	0.66
3:Y:313:CLA:HMB3	3:Y:313:CLA:H121	1.77	0.66
1:Y:162:ASP:OD2	3:Y:311:CLA:HBD	1.97	0.63
3:G:602:CLA:H52	4:G:616:LUT:H28	1.82	0.61
1:Y:96:VAL:HB	1:Y:99:LYS:HB2	1.84	0.59
3:N:613:CLA:HMB3	4:N:615:LUT:H3	1.83	0.59
3:N:602:CLA:H52	4:N:616:LUT:H28	1.84	0.58
3:G:610:CLA:H72	4:G:615:LUT:H30	1.86	0.58
2:N:601:CHL:H2	2:G:609:CHL:CHC	2.36	0.56
3:Y:303:CLA:H52	4:Y:317:LUT:H28	1.87	0.56
3:Y:311:CLA:H2	3:Y:311:CLA:CHB	2.35	0.56
3:G:610:CLA:H151	4:G:615:LUT:H393	1.89	0.55
3:G:613:CLA:H172	3:G:614:CLA:HBA2	1.88	0.55
1:G:193:GLY:HA3	3:G:613:CLA:HBB1	1.89	0.54
3:Y:311:CLA:H72	4:Y:316:LUT:H30	1.88	0.54
1:N:196:VAL:HG11	3:N:613:CLA:HAC2	1.88	0.54
2:N:607:CHL:H18	2:N:609:CHL:H52	1.89	0.54
2:N:601:CHL:HBA1	2:G:609:CHL:HMB2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:21:ARG:NH2	1:Y:43:ASP:OD2	2.42	0.53
1:G:68:HIS:HE1	3:G:603:CLA:ND	2.05	0.53
1:Y:73:MET:SD	3:Y:311:CLA:HMC3	2.51	0.51
2:G:601:CHL:HMD3	6:G:618:LHG:HC62	1.91	0.51
1:N:174:ALA:HA	1:N:177:LYS:HD2	1.92	0.50
1:N:112:TYR:HB3	1:N:118:LEU:HD23	1.93	0.50
3:N:610:CLA:H2	4:N:615:LUT:H26	1.92	0.50
1:N:193:GLY:O	1:N:197:GLN:HG2	2.12	0.50
3:N:603:CLA:HBC2	2:N:609:CHL:HMD2	1.93	0.50
2:N:601:CHL:H72	2:G:609:CHL:HMC	1.94	0.49
1:G:18:GLY:O	1:G:21:ARG:NH1	2.42	0.49
3:Y:311:CLA:H71	3:Y:313:CLA:HMA1	1.94	0.49
1:Y:162:ASP:OD2	3:Y:311:CLA:HAA1	2.13	0.48
3:G:612:CLA:HMB2	4:G:615:LUT:H32	1.95	0.48
3:G:613:CLA:H2	3:G:613:CLA:H61	1.58	0.48
3:G:613:CLA:HMB3	4:G:615:LUT:H3	1.95	0.48
1:G:176:LEU:HD23	3:G:610:CLA:H3A	1.94	0.47
2:N:608:CHL:H3A	2:N:608:CHL:HBA2	1.69	0.47
3:Y:311:CLA:H121	3:Y:313:CLA:H151	1.95	0.47
3:G:610:CLA:H152	3:G:610:CLA:H111	1.51	0.47
7:Y:301:XAT:H11	7:Y:301:XAT:H191	1.79	0.47
3:G:603:CLA:HBC2	2:G:609:CHL:HMD2	1.97	0.47
3:G:603:CLA:HAC2	2:G:607:CHL:H202	1.96	0.47
3:Y:304:CLA:HBC2	2:Y:310:CHL:HMD2	1.96	0.47
3:G:610:CLA:C2	4:G:615:LUT:H26	2.44	0.47
3:Y:313:CLA:H171	3:Y:313:CLA:HMB1	1.97	0.47
1:N:18:GLY:O	1:N:21:ARG:NH1	2.38	0.46
3:Y:304:CLA:HMD2	2:Y:310:CHL:C3D	2.45	0.46
7:G:619:XAT:H11	7:G:619:XAT:H191	1.81	0.46
3:Y:313:CLA:H8	3:Y:313:CLA:H122	1.35	0.46
1:Y:103:GLN:O	1:Y:106:SER:OG	2.28	0.46
3:N:611:CLA:H93	3:N:611:CLA:H62	1.78	0.45
3:G:612:CLA:H2	3:G:612:CLA:H61	1.74	0.45
3:G:602:CLA:H101	4:G:616:LUT:H371	1.99	0.45
5:N:617:NEX:H35	5:N:617:NEX:H401	1.80	0.45
2:G:609:CHL:H62	2:G:609:CHL:H41	1.87	0.45
7:G:619:XAT:H35	7:G:619:XAT:H401	1.82	0.45
1:G:102:SER:O	1:G:102:SER:OG	2.34	0.45
4:G:616:LUT:H15	4:G:616:LUT:H201	1.83	0.45
5:G:617:NEX:H11	5:G:617:NEX:H191	1.75	0.45
1:Y:18:GLY:O	1:Y:21:ARG:NH1	2.41	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:311:CLA:H92	3:Y:311:CLA:H61	1.84	0.44
3:Y:311:CLA:H52	4:Y:316:LUT:H28	1.98	0.44
3:Y:313:CLA:H111	3:Y:313:CLA:H142	1.65	0.44
3:G:612:CLA:HMC2	4:G:615:LUT:H203	1.99	0.44
4:G:616:LUT:H31	4:G:616:LUT:H391	1.82	0.44
7:Y:301:XAT:H201	7:Y:301:XAT:H15	1.72	0.44
4:N:615:LUT:H35	4:N:615:LUT:H401	1.79	0.44
5:N:617:NEX:H201	5:N:617:NEX:H15	1.74	0.44
1:N:199:ILE:HD12	1:N:199:ILE:HA	1.87	0.44
4:N:615:LUT:H11	4:N:615:LUT:H191	1.85	0.44
1:G:74:LEU:HD23	1:G:74:LEU:HA	1.86	0.44
2:G:608:CHL:H142	2:G:608:CHL:H112	1.88	0.44
2:Y:310:CHL:H91	2:Y:310:CHL:H112	1.87	0.44
5:Y:318:NEX:H201	5:Y:318:NEX:H15	1.75	0.44
1:N:123:SER:O	1:N:127:ILE:HG12	2.18	0.44
5:N:617:NEX:H183	5:N:617:NEX:H192	1.99	0.44
7:N:619:XAT:H35	7:N:619:XAT:H401	1.82	0.44
5:G:617:NEX:H183	5:G:617:NEX:H192	1.99	0.44
1:N:96:VAL:HB	1:N:99:LYS:HB2	2.00	0.43
7:N:619:XAT:H31	7:N:619:XAT:H391	1.83	0.43
3:G:603:CLA:HBB1	2:G:609:CHL:H122	2.01	0.43
4:G:616:LUT:H11	4:G:616:LUT:H191	1.85	0.43
3:G:610:CLA:H92	3:G:610:CLA:H61	1.73	0.43
3:G:604:CLA:HMB3	4:G:616:LUT:H42	1.99	0.43
5:N:617:NEX:H191	5:N:617:NEX:H11	1.78	0.43
2:N:601:CHL:HBA1	2:N:601:CHL:H3A	1.69	0.43
4:Y:317:LUT:H11	4:Y:317:LUT:H191	1.86	0.43
1:N:115:ASN:HB3	1:N:118:LEU:HD13	2.00	0.43
3:Y:311:CLA:H2A	3:Y:311:CLA:O1D	2.19	0.43
1:N:135:MET:HA	1:N:138:VAL:HG22	2.01	0.42
5:Y:318:NEX:H191	5:Y:318:NEX:H11	1.80	0.42
3:N:612:CLA:H122	3:N:612:CLA:H8	1.70	0.42
5:G:617:NEX:H35	5:G:617:NEX:H401	1.75	0.42
7:G:619:XAT:H31	7:G:619:XAT:H391	1.80	0.42
3:Y:311:CLA:H162	3:Y:311:CLA:H141	1.64	0.42
4:N:615:LUT:H15	4:N:615:LUT:H201	1.81	0.42
4:Y:317:LUT:H15	4:Y:317:LUT:H201	1.79	0.42
4:G:615:LUT:H15	4:G:615:LUT:H201	1.78	0.42
1:Y:177:LYS:O	1:Y:181:ILE:HG22	2.19	0.42
7:N:619:XAT:H15	7:N:619:XAT:H201	1.77	0.42
1:N:103:GLN:O	1:N:106:SER:OG	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:313:CLA:H161	3:Y:313:CLA:H192	1.81	0.42
3:G:612:CLA:H112	3:G:612:CLA:H151	1.39	0.42
7:Y:301:XAT:H35	7:Y:301:XAT:H401	1.81	0.42
3:Y:304:CLA:H102	2:Y:310:CHL:H143	2.02	0.42
3:Y:313:CLA:H92	3:Y:313:CLA:H62	1.77	0.42
3:G:611:CLA:H93	3:G:611:CLA:H62	1.84	0.41
3:N:613:CLA:H2	3:N:613:CLA:H61	1.65	0.41
3:G:604:CLA:HBB1	4:G:616:LUT:H183	2.02	0.41
1:N:194:PHE:HE1	4:N:615:LUT:H41	1.85	0.41
2:Y:308:CHL:H93	2:Y:308:CHL:H61	1.86	0.41
2:N:601:CHL:H91	2:N:601:CHL:H112	1.91	0.41
2:N:601:CHL:HMD3	6:N:618:LHG:HC62	2.02	0.41
1:G:25:LEU:HD22	1:G:28:PHE:HB2	2.01	0.41
1:G:54:ASP:O	1:G:57:THR:OG1	2.35	0.41
7:G:619:XAT:H173	7:G:619:XAT:H3	1.89	0.41
3:Y:311:CLA:H162	3:Y:311:CLA:H203	1.73	0.41
4:N:616:LUT:H11	4:N:616:LUT:H191	1.83	0.41
1:G:215:ASP:HA	1:G:216:PRO:HD3	1.92	0.41
3:G:602:CLA:H141	3:G:602:CLA:H161	1.73	0.41
5:Y:318:NEX:H183	5:Y:318:NEX:H192	2.03	0.41
2:N:606:CHL:HBC2	2:N:607:CHL:HHD	2.02	0.41
5:G:617:NEX:H201	5:G:617:NEX:H15	1.76	0.41
1:N:166:LEU:HA	1:N:166:LEU:HD23	1.82	0.40
2:N:607:CHL:H143	2:N:607:CHL:H111	1.91	0.40
4:N:616:LUT:H35	4:N:616:LUT:H401	1.78	0.40
3:Y:312:CLA:H61	3:Y:312:CLA:H2	1.90	0.40
3:Y:312:CLA:H93	3:Y:312:CLA:H62	1.83	0.40
7:N:619:XAT:H11	7:N:619:XAT:H191	1.76	0.40
4:Y:317:LUT:H31	4:Y:317:LUT:H391	1.82	0.40
2:N:608:CHL:H112	2:N:608:CHL:H91	1.78	0.40
7:Y:301:XAT:H3	7:Y:301:XAT:H173	1.86	0.40
3:Y:311:CLA:H92	3:Y:311:CLA:H41	2.03	0.40
3:Y:314:CLA:H2	3:Y:314:CLA:H61	1.64	0.40
5:Y:318:NEX:H401	5:Y:318:NEX:H35	1.76	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%)	208 (96%)	8 (4%)	0	100	100
1	N	216/218 (99%)	210 (97%)	6 (3%)	0	100	100
1	Y	216/218 (99%)	208 (96%)	8 (4%)	0	100	100
All	All	648/654 (99%)	626 (97%)	22 (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%)	163 (97%)	5 (3%)	41	75
1	N	168/168 (100%)	165 (98%)	3 (2%)	59	86
1	Y	168/168 (100%)	164 (98%)	4 (2%)	49	81
All	All	504/504 (100%)	492 (98%)	12 (2%)	51	81

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	135	MET
1	N	194	PHE
1	N	219	ASN
1	G	82	PRO
1	G	128	TRP

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Mol	Chain	Res	Type
1	G	160	SER
1	G	161	PHE
1	G	173	PHE
1	Y	71	TRP
1	Y	110	LEU
1	Y	112	TYR
1	Y	194	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

57 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	CHL	N	605	-	48,56,74	1.71	5 (10%)	51,92,114	1.45	9 (17%)
2	CHL	Y	306	-	48,56,74	1.72	6 (12%)	51,92,114	1.46	9 (17%)
5	NEX	G	617	-	38,46,46	0.91	1 (2%)	50,70,70	2.36	13 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	CHL	N	606	1	51,59,74	1.69	6 (11%)	55,96,114	1.50	10 (18%)
3	CLA	Y	313	-	65,73,73	1.51	7 (10%)	76,113,113	1.38	7 (9%)
2	CHL	N	601	1	66,74,74	1.50	6 (9%)	73,114,114	1.21	9 (12%)
2	CHL	G	601	1	66,74,74	1.50	5 (7%)	73,114,114	1.18	9 (12%)
2	CHL	Y	302	1	66,74,74	1.51	5 (7%)	73,114,114	1.20	9 (12%)
2	CHL	N	609	1	66,74,74	1.46	6 (9%)	73,114,114	1.57	12 (16%)
4	LUT	Y	317	-	42,43,43	0.77	0	51,60,60	1.67	11 (21%)
3	CLA	G	602	1	65,73,73	1.52	5 (7%)	76,113,113	1.23	7 (9%)
3	CLA	N	602	1	65,73,73	1.53	5 (7%)	76,113,113	1.22	8 (10%)
7	XAT	N	619	-	39,47,47	0.93	0	54,74,74	2.69	18 (33%)
3	CLA	Y	314	1	65,73,73	1.51	5 (7%)	76,113,113	1.28	8 (10%)
4	LUT	G	616	-	42,43,43	0.77	0	51,60,60	1.68	11 (21%)
6	LHG	N	618	3	48,48,48	0.96	2 (4%)	51,54,54	1.07	4 (7%)
3	CLA	Y	315	-	49,57,73	1.74	6 (12%)	55,93,113	1.35	8 (14%)
2	CHL	G	607	-	66,74,74	1.49	6 (9%)	73,114,114	1.30	9 (12%)
2	CHL	G	609	1	66,74,74	1.47	6 (9%)	73,114,114	1.42	8 (10%)
3	CLA	N	604	-	62,70,73	1.54	5 (8%)	72,109,113	1.30	7 (9%)
4	LUT	N	616	-	42,43,43	0.77	0	51,60,60	1.74	10 (19%)
3	CLA	N	603	-	65,73,73	1.54	7 (10%)	76,113,113	1.25	8 (10%)
2	CHL	Y	310	1	66,74,74	1.48	5 (7%)	73,114,114	1.49	10 (13%)
2	CHL	N	608	-	66,74,74	1.47	5 (7%)	73,114,114	1.31	10 (13%)
2	CHL	G	608	-	66,74,74	1.49	5 (7%)	73,114,114	1.27	8 (10%)
3	CLA	G	603	-	65,73,73	1.54	7 (10%)	76,113,113	1.21	8 (10%)
3	CLA	Y	304	-	65,73,73	1.55	8 (12%)	76,113,113	1.31	10 (13%)
6	LHG	G	618	3	48,48,48	0.95	2 (4%)	51,54,54	1.07	4 (7%)
7	XAT	Y	301	-	39,47,47	0.93	0	54,74,74	2.69	17 (31%)
2	CHL	G	606	1	51,59,74	1.69	6 (11%)	55,96,114	1.49	11 (20%)
3	CLA	G	614	-	49,57,73	1.72	6 (12%)	55,93,113	1.40	8 (14%)
7	XAT	G	619	-	39,47,47	0.93	0	54,74,74	2.64	17 (31%)
2	CHL	Y	308	-	66,74,74	1.48	6 (9%)	73,114,114	1.32	9 (12%)
3	CLA	N	613	-	65,73,73	1.51	5 (7%)	76,113,113	1.27	8 (10%)
5	NEX	Y	318	-	38,46,46	0.91	1 (2%)	50,70,70	2.38	16 (32%)
3	CLA	Y	303	1	65,73,73	1.54	6 (9%)	76,113,113	1.22	8 (10%)
3	CLA	N	611	6	65,73,73	1.54	5 (7%)	76,113,113	1.24	8 (10%)
2	CHL	Y	309	-	66,74,74	1.49	5 (7%)	73,114,114	1.25	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	CLA	G	610	1	65,73,73	1.55	8 (12%)	76,113,113	1.34	9 (11%)
3	CLA	G	604	-	62,70,73	1.55	5 (8%)	72,109,113	1.32	6 (8%)
3	CLA	G	611	6	65,73,73	1.54	6 (9%)	76,113,113	1.28	9 (11%)
4	LUT	N	615	-	42,43,43	0.78	0	51,60,60	1.57	9 (17%)
3	CLA	N	610	1	65,73,73	1.51	7 (10%)	76,113,113	1.39	8 (10%)
6	LHG	Y	319	3	48,48,48	0.95	2 (4%)	51,54,54	0.99	4 (7%)
2	CHL	Y	307	-	51,59,74	1.66	6 (11%)	55,96,114	1.47	10 (18%)
3	CLA	G	613	-	65,73,73	1.54	5 (7%)	76,113,113	1.27	7 (9%)
3	CLA	G	612	-	65,73,73	1.50	7 (10%)	76,113,113	1.39	8 (10%)
3	CLA	Y	312	6	65,73,73	1.53	5 (7%)	76,113,113	1.27	9 (11%)
3	CLA	Y	305	-	62,70,73	1.55	5 (8%)	72,109,113	1.29	7 (9%)
4	LUT	Y	316	-	42,43,43	0.78	0	51,60,60	1.69	12 (23%)
4	LUT	G	615	-	42,43,43	0.75	0	51,60,60	1.60	9 (17%)
3	CLA	N	612	-	65,73,73	1.49	7 (10%)	76,113,113	1.31	6 (7%)
3	CLA	N	614	-	49,57,73	1.74	5 (10%)	55,93,113	1.38	8 (14%)
2	CHL	G	605	-	48,56,74	1.74	5 (10%)	51,92,114	1.41	9 (17%)
5	NEX	N	617	-	38,46,46	0.89	1 (2%)	50,70,70	2.31	13 (26%)
3	CLA	Y	311	1	65,73,73	1.61	8 (12%)	76,113,113	1.51	11 (14%)
2	CHL	N	607	-	66,74,74	1.49	5 (7%)	73,114,114	1.37	8 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CHL	N	605	-	3/3/16/26	7/18/116/137	-
2	CHL	Y	306	-	3/3/16/26	7/18/116/137	-
5	NEX	G	617	-	-	3/27/83/83	0/3/3/3
2	CHL	N	606	1	3/3/17/26	7/21/119/137	-
3	CLA	Y	313	-	1/1/15/20	16/37/115/115	-
2	CHL	N	601	1	3/3/20/26	12/39/137/137	-
2	CHL	G	601	1	3/3/20/26	14/39/137/137	-
2	CHL	Y	302	1	3/3/20/26	12/39/137/137	-
2	CHL	N	609	1	3/3/20/26	9/39/137/137	-
4	LUT	Y	317	-	-	4/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CLA	G	602	1	1/1/15/20	13/37/115/115	-
3	CLA	N	602	1	1/1/15/20	9/37/115/115	-
7	XAT	N	619	-	-	0/31/93/93	0/4/4/4
3	CLA	Y	314	1	1/1/15/20	11/37/115/115	-
4	LUT	G	616	-	-	6/29/67/67	0/2/2/2
6	LHG	N	618	3	-	10/53/53/53	-
3	CLA	Y	315	-	1/1/11/20	9/18/96/115	-
2	CHL	G	607	-	3/3/20/26	12/39/137/137	-
2	CHL	G	609	1	3/3/20/26	24/39/137/137	-
3	CLA	N	604	-	1/1/14/20	10/34/112/115	-
4	LUT	N	616	-	-	2/29/67/67	0/2/2/2
3	CLA	N	603	-	1/1/15/20	13/37/115/115	-
2	CHL	Y	310	1	3/3/20/26	8/39/137/137	-
2	CHL	N	608	-	3/3/20/26	13/39/137/137	-
2	CHL	G	608	-	3/3/20/26	4/39/137/137	-
3	CLA	G	603	-	1/1/15/20	11/37/115/115	-
3	CLA	Y	304	-	1/1/15/20	16/37/115/115	-
6	LHG	G	618	3	-	14/53/53/53	-
7	XAT	Y	301	-	-	0/31/93/93	0/4/4/4
2	CHL	G	606	1	3/3/17/26	7/21/119/137	-
3	CLA	G	614	-	1/1/11/20	10/18/96/115	-
7	XAT	G	619	-	-	0/31/93/93	0/4/4/4
2	CHL	Y	308	-	3/3/20/26	18/39/137/137	-
3	CLA	N	613	-	1/1/15/20	13/37/115/115	-
5	NEX	Y	318	-	-	3/27/83/83	0/3/3/3
3	CLA	Y	303	1	1/1/15/20	11/37/115/115	-
3	CLA	N	611	6	-	20/37/115/115	-
2	CHL	Y	309	-	3/3/20/26	17/39/137/137	-
3	CLA	G	610	1	1/1/15/20	14/37/115/115	-
3	CLA	G	604	-	1/1/14/20	11/34/112/115	-
3	CLA	G	611	6	-	11/37/115/115	-
4	LUT	N	615	-	-	4/29/67/67	0/2/2/2
3	CLA	N	610	1	1/1/15/20	14/37/115/115	-
6	LHG	Y	319	3	-	10/53/53/53	-
2	CHL	Y	307	-	3/3/17/26	9/21/119/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CLA	G	613	-	1/1/15/20	13/37/115/115	-
3	CLA	G	612	-	1/1/15/20	14/37/115/115	-
3	CLA	Y	312	6	-	10/37/115/115	-
3	CLA	Y	305	-	1/1/14/20	8/34/112/115	-
4	LUT	Y	316	-	-	2/29/67/67	0/2/2/2
4	LUT	G	615	-	-	2/29/67/67	0/2/2/2
3	CLA	N	612	-	1/1/15/20	16/37/115/115	-
3	CLA	N	614	-	1/1/11/20	12/18/96/115	-
2	CHL	G	605	-	3/3/16/26	11/18/116/137	-
5	NEX	N	617	-	-	3/27/83/83	0/3/3/3
3	CLA	Y	311	1	1/1/15/20	19/37/115/115	-
2	CHL	N	607	-	3/3/20/26	13/39/137/137	-

All (253) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Y	311	CLA	C4B-NB	8.26	1.42	1.35
3	G	613	CLA	C4B-NB	7.97	1.42	1.35
3	N	611	CLA	C4B-NB	7.94	1.42	1.35
3	Y	303	CLA	C4B-NB	7.94	1.42	1.35
3	N	602	CLA	C4B-NB	7.88	1.42	1.35
2	Y	302	CHL	C4B-NB	7.88	1.42	1.35
3	G	611	CLA	C4B-NB	7.87	1.42	1.35
3	G	603	CLA	C4B-NB	7.87	1.42	1.35
3	N	603	CLA	C4B-NB	7.81	1.42	1.35
2	G	605	CHL	C4B-NB	7.81	1.42	1.35
3	G	610	CLA	C4B-NB	7.81	1.42	1.35
3	Y	304	CLA	C4B-NB	7.81	1.42	1.35
3	Y	312	CLA	C4B-NB	7.80	1.42	1.35
2	N	606	CHL	C4B-NB	7.80	1.42	1.35
3	N	614	CLA	C4B-NB	7.78	1.42	1.35
2	G	606	CHL	C4B-NB	7.77	1.42	1.35
3	G	604	CLA	C4B-NB	7.75	1.42	1.35
2	G	601	CHL	C4B-NB	7.74	1.42	1.35
3	G	602	CLA	C4B-NB	7.74	1.42	1.35
2	Y	309	CHL	C4B-NB	7.73	1.42	1.35
3	Y	305	CLA	C4B-NB	7.73	1.42	1.35
3	Y	314	CLA	C4B-NB	7.72	1.42	1.35
3	N	604	CLA	C4B-NB	7.71	1.42	1.35
2	N	601	CHL	C4B-NB	7.70	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	607	CHL	C4B-NB	7.68	1.42	1.35
3	N	613	CLA	C4B-NB	7.66	1.42	1.35
2	G	607	CHL	C4B-NB	7.66	1.42	1.35
2	Y	308	CHL	C4B-NB	7.64	1.42	1.35
3	G	614	CLA	C4B-NB	7.64	1.42	1.35
2	G	608	CHL	C4B-NB	7.63	1.42	1.35
2	Y	306	CHL	C4B-NB	7.63	1.42	1.35
3	N	610	CLA	C4B-NB	7.59	1.42	1.35
2	Y	310	CHL	C4B-NB	7.58	1.42	1.35
2	Y	307	CHL	C4B-NB	7.56	1.42	1.35
2	G	609	CHL	C4B-NB	7.53	1.41	1.35
2	N	608	CHL	C4B-NB	7.52	1.41	1.35
3	Y	315	CLA	C4B-NB	7.51	1.41	1.35
2	N	605	CHL	C4B-NB	7.51	1.41	1.35
3	Y	313	CLA	C4B-NB	7.50	1.41	1.35
3	G	612	CLA	C4B-NB	7.45	1.41	1.35
3	N	612	CLA	C4B-NB	7.44	1.41	1.35
2	N	609	CHL	C4B-NB	7.37	1.41	1.35
6	N	618	LHG	O8-C23	4.31	1.45	1.33
6	N	618	LHG	O7-C7	4.27	1.46	1.34
6	G	618	LHG	O8-C23	4.25	1.45	1.33
6	Y	319	LHG	O8-C23	4.25	1.45	1.33
6	G	618	LHG	O7-C7	4.19	1.46	1.34
6	Y	319	LHG	O7-C7	4.19	1.46	1.34
3	Y	304	CLA	C1D-ND	4.10	1.42	1.37
3	G	603	CLA	C1D-ND	4.05	1.42	1.37
3	Y	311	CLA	C1D-ND	4.04	1.42	1.37
3	N	603	CLA	C1D-ND	4.03	1.42	1.37
2	N	608	CHL	C1D-ND	3.99	1.42	1.37
3	Y	315	CLA	C1D-ND	3.97	1.42	1.37
3	G	611	CLA	C1D-ND	3.97	1.42	1.37
2	G	606	CHL	C1D-ND	3.96	1.42	1.37
2	G	605	CHL	C1D-ND	3.94	1.42	1.37
3	G	614	CLA	C1D-ND	3.93	1.42	1.37
3	N	602	CLA	C1D-ND	3.91	1.42	1.37
2	G	601	CHL	C1D-ND	3.91	1.42	1.37
3	N	613	CLA	C1D-ND	3.91	1.42	1.37
2	Y	307	CHL	C1D-ND	3.89	1.42	1.37
2	Y	302	CHL	C1D-ND	3.89	1.42	1.37
2	N	605	CHL	C1D-ND	3.89	1.42	1.37
3	G	604	CLA	C1D-ND	3.88	1.42	1.37
3	Y	303	CLA	C1D-ND	3.88	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	606	CHL	C1D-ND	3.88	1.42	1.37
2	N	601	CHL	C1D-ND	3.88	1.42	1.37
3	G	613	CLA	C1D-ND	3.88	1.42	1.37
3	N	614	CLA	C1D-ND	3.87	1.42	1.37
2	G	608	CHL	C1D-ND	3.87	1.42	1.37
2	G	607	CHL	C1D-ND	3.86	1.42	1.37
2	Y	306	CHL	C1D-ND	3.86	1.42	1.37
3	G	610	CLA	C1D-ND	3.85	1.42	1.37
3	Y	312	CLA	C1D-ND	3.84	1.42	1.37
3	G	602	CLA	C1D-ND	3.84	1.42	1.37
2	Y	309	CHL	C1D-ND	3.83	1.42	1.37
3	Y	305	CLA	C1D-ND	3.82	1.42	1.37
3	N	604	CLA	C1D-ND	3.80	1.42	1.37
2	N	607	CHL	C1D-ND	3.80	1.42	1.37
3	Y	314	CLA	C1D-ND	3.80	1.42	1.37
3	N	611	CLA	C1D-ND	3.79	1.42	1.37
2	Y	308	CHL	C1D-ND	3.77	1.42	1.37
3	N	610	CLA	C1D-ND	3.71	1.42	1.37
2	Y	310	CHL	C1D-ND	3.67	1.42	1.37
3	N	612	CLA	C1D-ND	3.60	1.42	1.37
3	Y	313	CLA	C1D-ND	3.59	1.42	1.37
3	G	612	CLA	C1D-ND	3.57	1.42	1.37
2	N	609	CHL	C1D-ND	3.52	1.42	1.37
2	G	609	CHL	C1D-ND	3.51	1.42	1.37
3	Y	311	CLA	C4D-ND	-3.32	1.33	1.37
2	G	609	CHL	C4D-ND	-3.26	1.33	1.37
2	N	609	CHL	CHC-C1C	3.23	1.43	1.35
3	G	610	CLA	C4D-ND	-3.18	1.33	1.37
2	G	609	CHL	CHC-C1C	3.18	1.43	1.35
2	Y	310	CHL	CHC-C1C	3.18	1.43	1.35
3	Y	313	CLA	C4D-ND	-3.17	1.33	1.37
3	G	612	CLA	C4D-ND	-3.16	1.33	1.37
3	N	612	CLA	C4D-ND	-3.15	1.33	1.37
2	N	609	CHL	C4D-ND	-3.13	1.33	1.37
3	N	610	CLA	C4D-ND	-3.12	1.33	1.37
2	Y	307	CHL	CHC-C1C	3.10	1.42	1.35
2	N	607	CHL	CHC-C1C	3.08	1.42	1.35
2	G	608	CHL	CHC-C1C	3.05	1.42	1.35
3	Y	311	CLA	CHC-C1C	3.04	1.42	1.35
3	G	602	CLA	CHC-C1C	3.04	1.42	1.35
2	N	606	CHL	CHC-C1C	3.03	1.42	1.35
2	N	608	CHL	CHC-C1C	3.02	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	602	CLA	CHC-C1C	3.02	1.42	1.35
3	G	611	CLA	CHC-C1C	3.02	1.42	1.35
2	Y	310	CHL	C4D-ND	-3.02	1.33	1.37
2	G	607	CHL	CHC-C1C	3.02	1.42	1.35
2	Y	309	CHL	CHC-C1C	3.02	1.42	1.35
2	N	601	CHL	CHC-C1C	3.01	1.42	1.35
2	N	605	CHL	CHC-C1C	3.01	1.42	1.35
2	Y	308	CHL	CHC-C1C	3.00	1.42	1.35
3	G	604	CLA	CHC-C1C	3.00	1.42	1.35
3	N	611	CLA	CHC-C1C	3.00	1.42	1.35
3	Y	312	CLA	CHC-C1C	3.00	1.42	1.35
2	G	601	CHL	CHC-C1C	2.99	1.42	1.35
3	Y	305	CLA	CHC-C1C	2.99	1.42	1.35
3	Y	314	CLA	CHC-C1C	2.98	1.42	1.35
3	N	604	CLA	CHC-C1C	2.98	1.42	1.35
3	N	614	CLA	CHC-C1C	2.98	1.42	1.35
3	N	613	CLA	CHC-C1C	2.96	1.42	1.35
3	G	613	CLA	CHC-C1C	2.96	1.42	1.35
3	Y	303	CLA	CHC-C1C	2.96	1.42	1.35
2	G	606	CHL	CHC-C1C	2.96	1.42	1.35
2	G	605	CHL	CHC-C1C	2.95	1.42	1.35
2	N	607	CHL	C4D-ND	-2.95	1.33	1.37
2	Y	302	CHL	CHC-C1C	2.94	1.42	1.35
3	G	614	CLA	CHC-C1C	2.94	1.42	1.35
3	Y	312	CLA	C4D-ND	-2.94	1.33	1.37
3	N	611	CLA	C4D-ND	-2.94	1.33	1.37
2	Y	306	CHL	CHC-C1C	2.93	1.42	1.35
3	N	610	CLA	CHC-C1C	2.93	1.42	1.35
3	N	613	CLA	C4D-ND	-2.92	1.33	1.37
3	Y	315	CLA	C4D-ND	-2.91	1.33	1.37
3	G	610	CLA	CHC-C1C	2.90	1.42	1.35
2	Y	308	CHL	C4D-ND	-2.89	1.33	1.37
3	Y	314	CLA	C4D-ND	-2.89	1.33	1.37
3	Y	315	CLA	CHC-C1C	2.88	1.42	1.35
3	G	603	CLA	CHC-C1C	2.88	1.42	1.35
3	N	604	CLA	C4D-ND	-2.88	1.33	1.37
3	Y	313	CLA	CHC-C1C	2.87	1.42	1.35
3	Y	305	CLA	C4D-ND	-2.86	1.33	1.37
3	N	603	CLA	CHC-C1C	2.86	1.42	1.35
3	G	611	CLA	C4D-ND	-2.86	1.33	1.37
2	G	607	CHL	C4D-ND	-2.85	1.33	1.37
3	G	602	CLA	C4D-ND	-2.85	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	602	CLA	C4D-ND	-2.83	1.33	1.37
3	G	613	CLA	C4D-ND	-2.83	1.33	1.37
3	Y	303	CLA	C4D-ND	-2.82	1.33	1.37
3	Y	311	CLA	CMB-C2B	-2.81	1.45	1.51
3	G	612	CLA	CHC-C1C	2.80	1.42	1.35
2	N	601	CHL	C4D-ND	-2.80	1.33	1.37
3	N	612	CLA	CHC-C1C	2.79	1.42	1.35
5	Y	318	NEX	C7-C8	-2.79	1.27	1.32
3	G	604	CLA	C4D-ND	-2.78	1.33	1.37
5	G	617	NEX	C7-C8	-2.77	1.27	1.32
2	N	606	CHL	C4D-ND	-2.76	1.33	1.37
2	G	608	CHL	C4D-ND	-2.75	1.33	1.37
3	N	614	CLA	C4D-ND	-2.73	1.33	1.37
2	G	601	CHL	C4D-ND	-2.72	1.33	1.37
3	Y	313	CLA	CMB-C2B	-2.72	1.46	1.51
5	N	617	NEX	C7-C8	-2.71	1.27	1.32
3	G	614	CLA	C4D-ND	-2.70	1.34	1.37
2	Y	302	CHL	C4D-ND	-2.69	1.34	1.37
2	G	606	CHL	C4D-ND	-2.69	1.34	1.37
2	Y	309	CHL	C4D-ND	-2.69	1.34	1.37
3	Y	304	CLA	CHC-C1C	2.67	1.41	1.35
2	N	608	CHL	C4D-ND	-2.66	1.34	1.37
2	G	605	CHL	C4D-ND	-2.65	1.34	1.37
3	N	603	CLA	C4D-ND	-2.63	1.34	1.37
2	Y	306	CHL	C4D-ND	-2.63	1.34	1.37
3	G	603	CLA	C4D-ND	-2.62	1.34	1.37
3	Y	304	CLA	C4D-ND	-2.61	1.34	1.37
2	G	609	CHL	CMB-C2B	-2.61	1.46	1.51
2	Y	307	CHL	C4D-ND	-2.59	1.34	1.37
3	G	612	CLA	CMB-C2B	-2.58	1.46	1.51
3	G	610	CLA	CMB-C2B	-2.58	1.46	1.51
3	N	610	CLA	CMB-C2B	-2.57	1.46	1.51
2	N	605	CHL	C4D-ND	-2.56	1.34	1.37
3	N	612	CLA	CMB-C2B	-2.53	1.46	1.51
3	Y	315	CLA	CMB-C2B	-2.50	1.46	1.51
2	G	605	CHL	CMB-C2B	-2.49	1.46	1.51
2	Y	309	CHL	CMB-C2B	-2.47	1.46	1.51
2	N	605	CHL	CMB-C2B	-2.47	1.46	1.51
2	G	607	CHL	CMB-C2B	-2.46	1.46	1.51
2	N	609	CHL	CMB-C2B	-2.46	1.46	1.51
2	Y	306	CHL	CMB-C2B	-2.45	1.46	1.51
2	G	606	CHL	CMB-C2B	-2.45	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	611	CLA	CMB-C2B	-2.45	1.46	1.51
3	Y	303	CLA	CMB-C2B	-2.45	1.46	1.51
3	N	602	CLA	CMB-C2B	-2.45	1.46	1.51
2	Y	308	CHL	CMB-C2B	-2.44	1.46	1.51
2	G	601	CHL	CMB-C2B	-2.44	1.46	1.51
3	N	611	CLA	CMB-C2B	-2.44	1.46	1.51
2	Y	310	CHL	CMB-C2B	-2.43	1.46	1.51
2	N	608	CHL	CMB-C2B	-2.43	1.46	1.51
3	G	602	CLA	CMB-C2B	-2.43	1.46	1.51
2	G	608	CHL	CMB-C2B	-2.43	1.46	1.51
2	N	601	CHL	CMB-C2B	-2.43	1.46	1.51
2	N	607	CHL	CMB-C2B	-2.43	1.46	1.51
3	G	613	CLA	CMB-C2B	-2.43	1.46	1.51
2	Y	302	CHL	CMB-C2B	-2.42	1.46	1.51
3	Y	304	CLA	C3B-C2B	-2.42	1.37	1.40
3	Y	312	CLA	CMB-C2B	-2.41	1.46	1.51
3	N	614	CLA	CMB-C2B	-2.41	1.46	1.51
3	Y	304	CLA	CMB-C2B	-2.41	1.46	1.51
3	G	603	CLA	CMB-C2B	-2.40	1.46	1.51
3	N	613	CLA	CMB-C2B	-2.40	1.46	1.51
3	Y	305	CLA	CMB-C2B	-2.40	1.46	1.51
2	Y	307	CHL	CMB-C2B	-2.40	1.46	1.51
3	Y	314	CLA	CMB-C2B	-2.40	1.46	1.51
3	N	604	CLA	CMB-C2B	-2.39	1.46	1.51
2	N	606	CHL	CMB-C2B	-2.39	1.46	1.51
3	G	614	CLA	CMB-C2B	-2.39	1.46	1.51
3	N	603	CLA	CMB-C2B	-2.39	1.46	1.51
3	G	604	CLA	CMB-C2B	-2.38	1.46	1.51
3	G	612	CLA	C3B-C2B	-2.27	1.37	1.40
3	Y	313	CLA	C3B-C2B	-2.26	1.37	1.40
3	Y	311	CLA	CMC-C2C	-2.25	1.46	1.50
3	Y	311	CLA	C3B-C2B	-2.22	1.37	1.40
3	G	610	CLA	C3B-C2B	-2.18	1.37	1.40
3	G	603	CLA	C3B-C2B	-2.13	1.37	1.40
3	N	610	CLA	C3B-C2B	-2.12	1.37	1.40
3	Y	313	CLA	CMD-C2D	-2.11	1.46	1.50
3	G	603	CLA	CMD-C2D	-2.10	1.46	1.50
3	G	612	CLA	CMD-C2D	-2.09	1.46	1.50
2	G	609	CHL	CMD-C2D	-2.08	1.46	1.50
3	N	612	CLA	CMD-C2D	-2.06	1.46	1.50
3	Y	304	CLA	C4B-CHC	-2.06	1.35	1.41
3	G	610	CLA	CMD-C2D	-2.05	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Y	315	CLA	C3B-C2B	-2.04	1.37	1.40
3	N	612	CLA	C3B-C2B	-2.04	1.37	1.40
2	N	601	CHL	CMD-C2D	-2.03	1.46	1.50
3	Y	304	CLA	CMD-C2D	-2.03	1.46	1.50
3	G	614	CLA	CMD-C2D	-2.03	1.46	1.50
2	Y	307	CHL	CMD-C2D	-2.02	1.46	1.50
2	N	606	CHL	CMD-C2D	-2.02	1.46	1.50
2	G	606	CHL	CMD-C2D	-2.02	1.46	1.50
3	Y	311	CLA	CMD-C2D	-2.02	1.46	1.50
2	Y	306	CHL	CMD-C2D	-2.02	1.46	1.50
3	N	603	CLA	CMD-C2D	-2.01	1.46	1.50
3	G	610	CLA	CMC-C2C	-2.01	1.46	1.50
2	N	609	CHL	CMD-C2D	-2.01	1.46	1.50
3	N	610	CLA	CMD-C2D	-2.01	1.46	1.50
3	Y	303	CLA	C3B-C2B	-2.01	1.37	1.40
2	G	607	CHL	CMD-C2D	-2.00	1.46	1.50
3	G	611	CLA	C3B-C2B	-2.00	1.37	1.40
2	Y	308	CHL	CMD-C2D	-2.00	1.46	1.50
3	N	603	CLA	C3B-C2B	-2.00	1.37	1.40

All (526) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	N	619	XAT	O4-C5-C4	8.54	119.79	113.38
5	Y	318	NEX	O24-C25-C24	8.45	119.73	113.38
5	N	617	NEX	O24-C25-C24	8.41	119.70	113.38
5	G	617	NEX	O24-C25-C24	8.18	119.53	113.38
7	Y	301	XAT	O4-C5-C4	8.01	119.40	113.38
7	G	619	XAT	O4-C5-C4	7.96	119.36	113.38
7	N	619	XAT	O24-C25-C24	7.54	119.05	113.38
7	Y	301	XAT	O24-C25-C24	7.02	118.65	113.38
7	G	619	XAT	O24-C25-C24	6.88	118.55	113.38
7	G	619	XAT	C38-C25-C26	-6.47	111.42	122.26
7	N	619	XAT	C38-C25-C26	-6.45	111.45	122.26
7	Y	301	XAT	C38-C25-C26	-6.39	111.55	122.26
2	N	609	CHL	C4A-NA-C1A	6.39	109.58	106.71
5	Y	318	NEX	C38-C25-C26	-6.28	111.74	122.26
5	N	617	NEX	C38-C25-C26	-6.21	111.85	122.26
7	G	619	XAT	C18-C5-C6	-6.21	111.86	122.26
7	Y	301	XAT	C18-C5-C6	-6.20	111.87	122.26
5	G	617	NEX	C38-C25-C26	-6.18	111.91	122.26
7	N	619	XAT	C18-C5-C6	-6.13	111.99	122.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Y	310	CHL	C4A-NA-C1A	5.85	109.33	106.71
3	G	604	CLA	C4A-NA-C1A	5.68	109.26	106.71
2	G	609	CHL	C4A-NA-C1A	5.23	109.06	106.71
3	Y	311	CLA	C4A-NA-C1A	5.18	109.03	106.71
3	N	612	CLA	C4A-NA-C1A	5.08	108.99	106.71
2	N	607	CHL	C4A-NA-C1A	5.01	108.96	106.71
3	G	611	CLA	C4A-NA-C1A	4.98	108.94	106.71
3	N	604	CLA	C4A-NA-C1A	4.97	108.94	106.71
3	Y	313	CLA	C4A-NA-C1A	4.92	108.92	106.71
3	G	613	CLA	C4A-NA-C1A	4.90	108.91	106.71
3	Y	305	CLA	C4A-NA-C1A	4.90	108.91	106.71
2	N	609	CHL	C1B-CHB-C4A	-4.88	120.45	130.12
3	N	613	CLA	C4A-NA-C1A	4.86	108.89	106.71
7	Y	301	XAT	O24-C25-C38	4.82	120.84	115.06
3	G	602	CLA	C4A-NA-C1A	4.80	108.86	106.71
7	G	619	XAT	O24-C25-C38	4.79	120.80	115.06
3	Y	314	CLA	C4A-NA-C1A	4.77	108.85	106.71
3	N	610	CLA	C4A-NA-C1A	4.71	108.82	106.71
3	Y	312	CLA	C4A-NA-C1A	4.65	108.80	106.71
2	Y	310	CHL	C1B-CHB-C4A	-4.64	120.92	130.12
7	Y	301	XAT	C15-C14-C13	-4.64	120.69	127.31
3	N	611	CLA	C4A-NA-C1A	4.53	108.74	106.71
7	N	619	XAT	O24-C25-C38	4.52	120.47	115.06
2	Y	308	CHL	C4A-NA-C1A	4.49	108.72	106.71
4	G	616	LUT	C35-C34-C33	-4.49	120.91	127.31
5	N	617	NEX	C15-C14-C13	-4.48	120.91	127.31
3	N	602	CLA	C4A-NA-C1A	4.46	108.71	106.71
5	G	617	NEX	C15-C14-C13	-4.43	120.99	127.31
5	G	617	NEX	C35-C34-C33	-4.36	121.09	127.31
5	Y	318	NEX	C27-C28-C29	-4.34	118.80	125.53
3	G	610	CLA	C4A-NA-C1A	4.34	108.66	106.71
3	G	612	CLA	C4A-NA-C1A	4.33	108.65	106.71
5	Y	318	NEX	C15-C14-C13	-4.29	121.18	127.31
3	Y	303	CLA	C4A-NA-C1A	4.27	108.63	106.71
3	Y	311	CLA	CMB-C2B-C1B	-4.26	121.91	128.46
2	G	607	CHL	C4A-NA-C1A	4.24	108.61	106.71
7	G	619	XAT	C15-C14-C13	-4.24	121.26	127.31
7	Y	301	XAT	O4-C5-C18	4.22	120.12	115.06
2	N	606	CHL	C4A-NA-C1A	4.22	108.61	106.71
7	G	619	XAT	O4-C5-C18	4.21	120.10	115.06
2	N	609	CHL	CHD-C1D-ND	-4.20	120.60	124.45
4	Y	317	LUT	C35-C34-C33	-4.17	121.36	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Y	318	NEX	O24-C25-C38	4.16	120.05	115.06
3	G	612	CLA	CMB-C2B-C1B	-4.16	122.07	128.46
2	G	606	CHL	C4A-NA-C1A	4.15	108.57	106.71
5	G	617	NEX	C27-C28-C29	-4.15	119.09	125.53
7	N	619	XAT	C11-C10-C9	-4.14	121.40	127.31
5	G	617	NEX	O24-C25-C38	4.14	120.02	115.06
2	Y	307	CHL	CMB-C2B-C1B	-4.12	122.14	128.46
5	Y	318	NEX	C35-C34-C33	-4.10	121.46	127.31
7	N	619	XAT	C15-C14-C13	-4.10	121.46	127.31
5	N	617	NEX	C27-C28-C29	-4.09	119.19	125.53
5	N	617	NEX	O24-C25-C38	4.08	119.95	115.06
7	N	619	XAT	O4-C5-C18	4.06	119.92	115.06
5	N	617	NEX	C11-C10-C9	-4.05	121.53	127.31
3	N	610	CLA	C1-C2-C3	-4.05	119.04	126.04
3	Y	313	CLA	CMB-C2B-C1B	-4.03	122.28	128.46
5	Y	318	NEX	C11-C10-C9	-4.02	121.57	127.31
2	Y	310	CHL	CHD-C1D-ND	-4.02	120.76	124.45
4	G	615	LUT	C15-C14-C13	-4.01	121.59	127.31
2	G	608	CHL	C4A-NA-C1A	4.00	108.50	106.71
4	N	616	LUT	C35-C34-C33	-4.00	121.60	127.31
2	N	606	CHL	CMB-C2B-C1B	-3.97	122.36	128.46
3	G	612	CLA	C1B-CHB-C4A	-3.96	122.27	130.12
4	Y	316	LUT	C35-C34-C33	-3.93	121.70	127.31
6	N	618	LHG	O7-C7-C8	3.91	119.94	111.50
2	Y	306	CHL	C4A-NA-C1A	3.90	108.46	106.71
3	G	614	CLA	CMB-C2B-C1B	-3.90	122.47	128.46
4	N	616	LUT	C7-C8-C9	-3.89	120.35	126.23
2	G	606	CHL	CMB-C2B-C1B	-3.89	122.49	128.46
7	Y	301	XAT	C11-C10-C9	-3.87	121.79	127.31
3	Y	315	CLA	CMB-C2B-C1B	-3.85	122.55	128.46
7	Y	301	XAT	C31-C30-C29	-3.85	121.82	127.31
2	N	608	CHL	CMB-C2B-C1B	-3.83	122.58	128.46
4	Y	316	LUT	C15-C14-C13	-3.81	121.88	127.31
6	G	618	LHG	O7-C7-C8	3.80	119.69	111.50
3	N	614	CLA	C4A-NA-C1A	3.79	108.41	106.71
3	Y	314	CLA	CMB-C2B-C1B	-3.79	122.64	128.46
3	N	612	CLA	CMB-C2B-C1B	-3.78	122.66	128.46
4	N	615	LUT	C35-C34-C33	-3.76	121.95	127.31
3	G	614	CLA	C4A-NA-C1A	3.75	108.39	106.71
4	N	616	LUT	C11-C10-C9	-3.73	121.98	127.31
3	Y	305	CLA	CMB-C2B-C1B	-3.73	122.73	128.46
5	G	617	NEX	C11-C10-C9	-3.73	121.98	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	615	LUT	C35-C34-C33	-3.70	122.03	127.31
2	G	609	CHL	CMB-C2B-C1B	-3.70	122.78	128.46
4	N	616	LUT	C15-C14-C13	-3.67	122.07	127.31
4	Y	317	LUT	C15-C14-C13	-3.66	122.09	127.31
3	Y	304	CLA	C1B-CHB-C4A	-3.65	122.89	130.12
7	G	619	XAT	C31-C30-C29	-3.63	122.13	127.31
2	N	608	CHL	C1B-CHB-C4A	-3.62	122.94	130.12
3	N	610	CLA	CMB-C2B-C1B	-3.62	122.90	128.46
5	N	617	NEX	C35-C34-C33	-3.62	122.14	127.31
6	Y	319	LHG	O7-C7-C8	3.61	119.29	111.50
2	Y	309	CHL	C4A-NA-C1A	3.61	108.33	106.71
7	Y	301	XAT	C35-C34-C33	-3.61	122.16	127.31
3	N	614	CLA	CMB-C2B-C1B	-3.61	122.92	128.46
4	Y	316	LUT	C31-C30-C29	-3.61	122.16	127.31
3	N	604	CLA	CMB-C2B-C1B	-3.60	122.93	128.46
3	G	612	CLA	CMB-C2B-C3B	3.60	131.41	124.68
4	N	616	LUT	C31-C30-C29	-3.58	122.20	127.31
4	Y	317	LUT	C31-C30-C29	-3.56	122.23	127.31
4	Y	316	LUT	C11-C10-C9	-3.55	122.24	127.31
3	Y	311	CLA	C1B-CHB-C4A	-3.54	123.10	130.12
7	G	619	XAT	C11-C10-C9	-3.53	122.27	127.31
2	G	609	CHL	C1B-CHB-C4A	-3.52	123.15	130.12
2	Y	307	CHL	C4A-NA-C1A	3.50	108.28	106.71
4	G	616	LUT	C7-C8-C9	-3.48	120.97	126.23
3	N	613	CLA	CMB-C2B-C1B	-3.48	123.11	128.46
3	G	611	CLA	CMB-C2B-C1B	-3.48	123.12	128.46
4	N	615	LUT	C15-C14-C13	-3.47	122.36	127.31
4	G	615	LUT	C31-C30-C29	-3.46	122.38	127.31
2	N	607	CHL	C1B-CHB-C4A	-3.45	123.28	130.12
2	Y	307	CHL	CMB-C2B-C3B	3.44	131.11	124.68
3	N	603	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
3	Y	311	CLA	CMB-C2B-C3B	3.43	131.10	124.68
3	Y	311	CLA	C1-C2-C3	-3.43	120.11	126.04
2	Y	308	CHL	CMB-C2B-C1B	-3.43	123.20	128.46
3	Y	304	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
4	G	616	LUT	C31-C30-C29	-3.40	122.46	127.31
3	N	611	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
2	Y	307	CHL	C1B-CHB-C4A	-3.39	123.40	130.12
3	G	604	CLA	CMB-C2B-C1B	-3.39	123.25	128.46
4	G	616	LUT	C11-C10-C9	-3.39	122.47	127.31
2	N	607	CHL	CMB-C2B-C1B	-3.38	123.26	128.46
3	Y	312	CLA	CMB-C2B-C1B	-3.38	123.27	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	605	CHL	C1B-CHB-C4A	-3.36	123.46	130.12
2	N	606	CHL	CMB-C2B-C3B	3.36	130.97	124.68
7	N	619	XAT	C35-C34-C33	-3.36	122.52	127.31
3	Y	313	CLA	C1B-CHB-C4A	-3.35	123.48	130.12
2	G	609	CHL	CHD-C1D-ND	-3.35	121.38	124.45
2	N	605	CHL	CMB-C2B-C1B	-3.35	123.32	128.46
4	Y	317	LUT	C18-C5-C6	-3.34	120.77	124.53
2	G	607	CHL	CMB-C2B-C1B	-3.33	123.34	128.46
3	Y	313	CLA	CMB-C2B-C3B	3.32	130.90	124.68
3	G	610	CLA	CMB-C2B-C1B	-3.32	123.36	128.46
2	G	605	CHL	CMB-C2B-C1B	-3.32	123.36	128.46
2	G	605	CHL	C1B-CHB-C4A	-3.32	123.54	130.12
7	N	619	XAT	C31-C30-C29	-3.32	122.58	127.31
4	Y	316	LUT	C7-C8-C9	-3.32	121.22	126.23
2	Y	302	CHL	CMB-C2B-C1B	-3.32	123.37	128.46
3	N	602	CLA	CMB-C2B-C1B	-3.32	123.37	128.46
2	N	601	CHL	C1B-CHB-C4A	-3.31	123.57	130.12
3	N	610	CLA	C1B-CHB-C4A	-3.30	123.57	130.12
2	Y	310	CHL	CMB-C2B-C1B	-3.30	123.39	128.46
2	N	605	CHL	C4A-NA-C1A	3.30	108.19	106.71
3	G	614	CLA	CMB-C2B-C3B	3.30	130.86	124.68
2	Y	306	CHL	CMB-C2B-C1B	-3.30	123.39	128.46
3	G	613	CLA	CMB-C2B-C1B	-3.30	123.40	128.46
2	G	601	CHL	CMB-C2B-C1B	-3.29	123.41	128.46
2	N	609	CHL	CMB-C2B-C1B	-3.29	123.41	128.46
2	N	601	CHL	CMB-C2B-C1B	-3.29	123.41	128.46
3	G	602	CLA	CMB-C2B-C1B	-3.28	123.42	128.46
3	G	610	CLA	C1B-CHB-C4A	-3.27	123.64	130.12
3	Y	303	CLA	CMB-C2B-C1B	-3.27	123.44	128.46
2	G	606	CHL	CMB-C2B-C3B	3.27	130.79	124.68
2	N	607	CHL	CHD-C1D-ND	-3.27	121.45	124.45
3	G	603	CLA	CMB-C2B-C1B	-3.25	123.47	128.46
2	N	608	CHL	C4A-NA-C1A	3.25	108.17	106.71
4	G	616	LUT	C15-C14-C13	-3.24	122.68	127.31
2	Y	309	CHL	CMB-C2B-C1B	-3.23	123.50	128.46
3	Y	314	CLA	CMB-C2B-C3B	3.23	130.72	124.68
2	G	608	CHL	CMB-C2B-C1B	-3.23	123.50	128.46
4	Y	316	LUT	C18-C5-C6	-3.22	120.91	124.53
7	G	619	XAT	C35-C34-C33	-3.22	122.71	127.31
2	Y	309	CHL	C1B-CHB-C4A	-3.22	123.73	130.12
2	N	608	CHL	CMB-C2B-C3B	3.22	130.71	124.68
3	Y	311	CLA	O2D-CGD-O1D	-3.22	117.54	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Y	311	CLA	CAA-CBA-CGA	-3.21	103.87	113.25
3	N	614	CLA	O2D-CGD-O1D	-3.21	117.57	123.84
4	G	615	LUT	C18-C5-C6	-3.20	120.93	124.53
3	Y	304	CLA	CMB-C2B-C3B	3.20	130.66	124.68
2	G	608	CHL	C1B-CHB-C4A	-3.19	123.80	130.12
3	Y	315	CLA	CMB-C2B-C3B	3.19	130.64	124.68
3	Y	315	CLA	C1B-CHB-C4A	-3.19	123.81	130.12
3	N	612	CLA	CMB-C2B-C3B	3.18	130.63	124.68
3	G	614	CLA	O2D-CGD-O1D	-3.18	117.62	123.84
2	G	607	CHL	C1B-CHB-C4A	-3.16	123.86	130.12
2	Y	302	CHL	C1B-CHB-C4A	-3.15	123.88	130.12
4	Y	317	LUT	C7-C8-C9	-3.14	121.49	126.23
5	Y	318	NEX	C39-C29-C30	-3.14	118.53	122.92
2	Y	306	CHL	C1B-CHB-C4A	-3.14	123.91	130.12
3	Y	305	CLA	CMB-C2B-C3B	3.13	130.53	124.68
4	N	615	LUT	C18-C5-C6	-3.12	121.02	124.53
3	N	603	CLA	C1B-CHB-C4A	-3.12	123.94	130.12
2	Y	308	CHL	C1B-CHB-C4A	-3.11	123.95	130.12
3	N	610	CLA	CMB-C2B-C3B	3.11	130.49	124.68
3	N	614	CLA	CMB-C2B-C3B	3.10	130.48	124.68
3	Y	312	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
3	G	603	CLA	C1B-CHB-C4A	-3.07	124.03	130.12
3	N	603	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
3	N	604	CLA	CMB-C2B-C3B	3.07	130.43	124.68
4	N	615	LUT	C11-C10-C9	-3.07	122.93	127.31
3	G	604	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
2	N	605	CHL	O2D-CGD-O1D	-3.06	117.86	123.84
3	Y	304	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
4	Y	317	LUT	C11-C10-C9	-3.06	122.95	127.31
2	G	605	CHL	C4A-NA-C1A	3.05	108.08	106.71
3	N	611	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
2	Y	308	CHL	O2D-CGD-O1D	-3.05	117.88	123.84
4	N	616	LUT	C18-C5-C6	-3.04	121.11	124.53
3	N	612	CLA	C1B-CHB-C4A	-3.03	124.11	130.12
3	Y	303	CLA	C1B-CHB-C4A	-3.02	124.14	130.12
3	G	611	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
4	N	615	LUT	C31-C30-C29	-3.02	123.01	127.31
2	Y	306	CHL	O2D-CGD-O1D	-3.01	117.95	123.84
3	Y	312	CLA	C1B-CHB-C4A	-3.01	124.15	130.12
2	G	601	CHL	C1B-CHB-C4A	-3.01	124.16	130.12
3	N	603	CLA	CMB-C2B-C3B	3.01	130.30	124.68
3	N	602	CLA	O2D-CGD-O1D	-3.00	117.97	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	N	617	NEX	C39-C29-C30	-3.00	118.72	122.92
2	Y	309	CHL	O2D-CGD-O1D	-3.00	117.97	123.84
2	Y	310	CHL	O2D-CGD-O1D	-3.00	117.97	123.84
2	N	609	CHL	O2D-CGD-O1D	-2.99	117.98	123.84
3	G	614	CLA	C1B-CHB-C4A	-2.99	124.20	130.12
5	G	617	NEX	C19-C9-C10	-2.99	118.74	122.92
3	N	613	CLA	CMB-C2B-C3B	2.98	130.25	124.68
7	Y	301	XAT	C26-C27-C28	-2.97	119.71	125.99
7	N	619	XAT	C7-C8-C9	-2.97	120.93	125.53
2	G	609	CHL	CMB-C2B-C3B	2.97	130.23	124.68
6	Y	319	LHG	O8-C23-C24	2.95	121.18	111.91
4	G	615	LUT	C11-C10-C9	-2.95	123.09	127.31
3	Y	303	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
2	N	608	CHL	O2D-CGD-O1D	-2.95	118.06	123.84
2	Y	308	CHL	CMB-C2B-C3B	2.95	130.20	124.68
3	G	603	CLA	C4A-NA-C1A	2.95	108.03	106.71
3	Y	314	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
3	N	604	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
5	G	617	NEX	C31-C30-C29	-2.94	123.11	127.31
4	G	615	LUT	C7-C8-C9	-2.92	121.82	126.23
2	G	605	CHL	O2D-CGD-O1D	-2.92	118.12	123.84
2	N	606	CHL	C1B-CHB-C4A	-2.92	124.34	130.12
3	G	611	CLA	C1B-CHB-C4A	-2.92	124.34	130.12
3	N	614	CLA	C1B-CHB-C4A	-2.91	124.35	130.12
3	N	602	CLA	C1B-CHB-C4A	-2.91	124.36	130.12
3	N	613	CLA	C1B-CHB-C4A	-2.91	124.36	130.12
4	N	615	LUT	C7-C8-C9	-2.90	121.85	126.23
3	G	602	CLA	C1B-CHB-C4A	-2.90	124.37	130.12
2	N	607	CHL	CMB-C2B-C3B	2.90	130.10	124.68
2	G	607	CHL	O2D-CGD-O1D	-2.90	118.17	123.84
3	N	603	CLA	C4A-NA-C1A	2.90	108.01	106.71
2	G	608	CHL	O2D-CGD-O1D	-2.89	118.19	123.84
3	G	613	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
3	N	611	CLA	C1B-CHB-C4A	-2.88	124.41	130.12
3	G	604	CLA	CMB-C2B-C3B	2.88	130.06	124.68
2	Y	307	CHL	O2D-CGD-O1D	-2.88	118.21	123.84
2	G	607	CHL	CHD-C1D-ND	-2.88	121.81	124.45
2	G	606	CHL	O2D-CGD-O1D	-2.87	118.23	123.84
3	G	603	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
3	G	610	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
7	N	619	XAT	C26-C27-C28	-2.86	119.94	125.99
3	N	613	CLA	O2D-CGD-O1D	-2.86	118.25	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Y	311	CLA	C1D-ND-C4D	-2.86	104.31	106.33
3	G	612	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
2	N	601	CHL	O2D-CGD-O1D	-2.85	118.26	123.84
2	N	607	CHL	O2D-CGD-O1D	-2.85	118.27	123.84
2	N	606	CHL	O2D-CGD-O1D	-2.85	118.27	123.84
2	N	609	CHL	CMB-C2B-C3B	2.84	130.00	124.68
2	G	607	CHL	CMB-C2B-C3B	2.84	130.00	124.68
3	G	610	CLA	C1-C2-C3	-2.84	121.13	126.04
6	N	618	LHG	O8-C23-C24	2.84	120.81	111.91
2	N	605	CHL	CMB-C2B-C3B	2.83	129.98	124.68
7	Y	301	XAT	C7-C8-C9	-2.83	121.14	125.53
3	N	604	CLA	C1B-CHB-C4A	-2.83	124.51	130.12
7	G	619	XAT	C26-C27-C28	-2.83	120.01	125.99
4	G	616	LUT	C18-C5-C6	-2.83	121.35	124.53
3	G	610	CLA	CMB-C2B-C3B	2.83	129.97	124.68
2	N	601	CHL	CMB-C2B-C3B	2.83	129.97	124.68
3	N	603	CLA	CHB-C4A-NA	2.83	128.42	124.51
2	Y	310	CHL	CMB-C2B-C3B	2.82	129.96	124.68
3	G	602	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
5	G	617	NEX	C39-C29-C30	-2.82	118.97	122.92
3	G	611	CLA	CMB-C2B-C3B	2.82	129.95	124.68
2	Y	308	CHL	CHD-C1D-ND	-2.81	121.87	124.45
2	G	601	CHL	O2D-CGD-O1D	-2.81	118.34	123.84
2	Y	302	CHL	O2D-CGD-O1D	-2.81	118.35	123.84
6	G	618	LHG	O8-C23-C24	2.81	120.72	111.91
3	Y	314	CLA	C1B-CHB-C4A	-2.81	124.56	130.12
3	Y	313	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
3	Y	305	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
2	G	606	CHL	C1B-CHB-C4A	-2.80	124.58	130.12
3	Y	305	CLA	C1B-CHB-C4A	-2.79	124.58	130.12
7	G	619	XAT	C24-C23-C22	-2.79	105.38	110.77
3	N	602	CLA	CMB-C2B-C3B	2.79	129.89	124.68
3	G	603	CLA	CMB-C2B-C3B	2.79	129.89	124.68
3	G	613	CLA	CMB-C2B-C3B	2.78	129.89	124.68
2	G	601	CHL	CMB-C2B-C3B	2.78	129.88	124.68
2	Y	302	CHL	CMB-C2B-C3B	2.78	129.88	124.68
3	G	613	CLA	C1B-CHB-C4A	-2.78	124.62	130.12
3	N	611	CLA	CMB-C2B-C3B	2.78	129.87	124.68
3	Y	303	CLA	CMB-C2B-C3B	2.78	129.87	124.68
3	Y	312	CLA	CMB-C2B-C3B	2.77	129.87	124.68
2	Y	306	CHL	CMB-C2B-C3B	2.77	129.85	124.68
3	G	602	CLA	CMB-C2B-C3B	2.76	129.84	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	608	CHL	CHD-C1D-ND	-2.75	121.93	124.45
5	G	617	NEX	C24-C23-C22	-2.75	105.47	110.77
7	Y	301	XAT	C24-C23-C22	-2.73	105.50	110.77
2	G	605	CHL	CMB-C2B-C3B	2.72	129.77	124.68
2	G	608	CHL	CMB-C2B-C3B	2.72	129.77	124.68
6	N	618	LHG	C6-C5-C4	-2.72	105.36	111.79
3	N	612	CLA	O2D-CGD-O1D	-2.72	118.53	123.84
3	N	612	CLA	CHB-C4A-NA	2.71	128.27	124.51
7	G	619	XAT	C7-C8-C9	-2.71	121.32	125.53
2	Y	309	CHL	CMB-C2B-C3B	2.70	129.73	124.68
3	Y	304	CLA	C2A-C1A-CHA	2.69	128.56	123.86
3	Y	315	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
3	N	610	CLA	CHB-C4A-NA	2.68	128.22	124.51
3	Y	313	CLA	CHB-C4A-NA	2.68	128.22	124.51
3	G	603	CLA	CHB-C4A-NA	2.68	128.22	124.51
2	Y	302	CHL	C4A-NA-C1A	2.67	107.91	106.71
2	N	601	CHL	C4A-NA-C1A	2.67	107.91	106.71
2	Y	302	CHL	CHD-C1D-ND	-2.67	122.00	124.45
2	N	606	CHL	C1-C2-C3	-2.64	122.47	126.75
3	Y	315	CLA	C4A-NA-C1A	2.63	107.89	106.71
3	Y	311	CLA	O1D-CGD-CBD	2.63	129.87	124.48
6	G	618	LHG	C5-O7-C7	-2.63	111.31	117.79
7	N	619	XAT	C24-C23-C22	-2.63	105.70	110.77
3	G	612	CLA	CHB-C4A-NA	2.60	128.10	124.51
3	G	604	CLA	C1B-CHB-C4A	-2.59	124.98	130.12
7	Y	301	XAT	C6-C7-C8	-2.59	120.52	125.99
4	N	616	LUT	C38-C25-C24	-2.58	118.03	123.56
5	N	617	NEX	C24-C23-C22	-2.58	105.79	110.77
2	N	601	CHL	CHD-C1D-ND	-2.58	122.09	124.45
7	G	619	XAT	C6-C7-C8	-2.57	120.57	125.99
2	G	606	CHL	C1-C2-C3	-2.56	122.60	126.75
3	N	610	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
4	N	616	LUT	C21-C26-C27	-2.56	109.47	112.70
2	Y	308	CHL	OMC-CMC-C2C	-2.56	119.91	125.69
5	Y	318	NEX	C28-C29-C30	2.55	122.86	118.94
2	G	609	CHL	O2D-CGD-O1D	-2.54	118.87	123.84
3	Y	312	CLA	CHD-C1D-ND	-2.54	122.12	124.45
3	N	613	CLA	CHB-C4A-NA	2.52	128.00	124.51
4	N	615	LUT	C21-C26-C27	-2.52	109.52	112.70
5	Y	318	NEX	C24-C23-C22	-2.47	106.01	110.77
3	G	612	CLA	C1-C2-C3	-2.47	121.78	126.04
4	G	616	LUT	C38-C25-C24	-2.46	118.28	123.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	604	CLA	CHB-C4A-NA	2.46	127.91	124.51
2	N	609	CHL	CHD-C1D-C2D	2.46	130.63	125.48
3	G	611	CLA	CHD-C1D-ND	-2.45	122.20	124.45
2	G	606	CHL	CHB-C4A-NA	2.45	127.91	124.51
2	N	607	CHL	OMC-CMC-C2C	-2.45	120.15	125.69
2	G	601	CHL	CHD-C1D-ND	-2.45	122.21	124.45
3	G	602	CLA	CHB-C4A-NA	2.44	127.89	124.51
4	G	616	LUT	C21-C26-C27	-2.44	109.61	112.70
2	G	606	CHL	OMC-CMC-C2C	-2.43	120.19	125.69
6	G	618	LHG	C6-C5-C4	-2.43	106.04	111.79
2	N	606	CHL	CHB-C4A-NA	2.43	127.87	124.51
2	G	601	CHL	C4A-NA-C1A	2.41	107.79	106.71
3	G	604	CLA	CHB-C4A-NA	2.41	127.85	124.51
2	G	605	CHL	CHD-C1D-ND	-2.41	122.24	124.45
2	Y	310	CHL	OMC-CMC-C2C	-2.41	120.24	125.69
2	G	608	CHL	CHB-C4A-NA	2.41	127.84	124.51
3	G	610	CLA	CHB-C4A-NA	2.41	127.84	124.51
3	Y	305	CLA	CHB-C4A-NA	2.40	127.83	124.51
3	N	602	CLA	CHB-C4A-NA	2.39	127.81	124.51
5	N	617	NEX	C31-C30-C29	-2.39	123.91	127.31
3	G	614	CLA	CHB-C4A-NA	2.39	127.81	124.51
3	G	612	CLA	C2A-C1A-CHA	2.38	128.02	123.86
3	Y	314	CLA	CHD-C1D-ND	-2.38	122.27	124.45
2	Y	307	CHL	C1-C2-C3	-2.38	122.91	126.75
3	Y	314	CLA	CHB-C4A-NA	2.37	127.80	124.51
2	N	605	CHL	CHD-C1D-ND	-2.37	122.28	124.45
4	Y	317	LUT	C18-C5-C4	2.36	118.72	114.36
3	Y	304	CLA	C2C-C1C-NC	2.35	112.18	109.97
7	Y	301	XAT	C27-C28-C29	-2.35	121.88	125.53
3	N	611	CLA	CHD-C1D-ND	-2.35	122.30	124.45
3	Y	303	CLA	CHB-C4A-NA	2.35	127.75	124.51
3	N	611	CLA	CHB-C4A-NA	2.34	127.75	124.51
4	Y	317	LUT	C21-C26-C27	-2.34	109.75	112.70
2	N	606	CHL	CHD-C1D-ND	-2.34	122.31	124.45
2	N	606	CHL	OMC-CMC-C2C	-2.34	120.41	125.69
2	G	607	CHL	OMC-CMC-C2C	-2.33	120.41	125.69
2	G	605	CHL	OMC-CMC-C2C	-2.33	120.41	125.69
5	Y	318	NEX	C2-C1-C6	2.33	111.47	109.21
3	N	614	CLA	CHB-C4A-NA	2.33	127.73	124.51
3	G	610	CLA	O2A-CGA-O1A	-2.32	117.73	123.59
7	G	619	XAT	C4-C3-C2	-2.32	106.29	110.77
2	G	601	CHL	CHB-C4A-NA	2.32	127.72	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	N	619	XAT	C27-C28-C29	-2.31	121.94	125.53
2	Y	309	CHL	CHB-C4A-NA	2.31	127.70	124.51
4	G	615	LUT	C38-C25-C24	-2.31	118.62	123.56
2	Y	306	CHL	OMC-CMC-C2C	-2.31	120.47	125.69
3	G	613	CLA	CHB-C4A-NA	2.30	127.70	124.51
4	Y	317	LUT	C38-C25-C24	-2.30	118.64	123.56
3	G	611	CLA	CHB-C4A-NA	2.30	127.69	124.51
3	Y	312	CLA	O2D-CGD-CBD	2.29	115.34	111.27
4	N	616	LUT	C18-C5-C4	2.29	118.60	114.36
4	N	615	LUT	C38-C25-C24	-2.28	118.67	123.56
3	Y	312	CLA	CHB-C4A-NA	2.28	127.67	124.51
2	N	609	CHL	OMC-CMC-C2C	-2.28	120.54	125.69
7	G	619	XAT	C27-C28-C29	-2.28	122.00	125.53
2	Y	306	CHL	CHD-C1D-ND	-2.27	122.37	124.45
4	Y	316	LUT	C18-C5-C4	2.27	118.56	114.36
3	G	611	CLA	O2D-CGD-CBD	2.26	115.28	111.27
5	G	617	NEX	C26-C27-C28	-2.26	121.22	125.99
3	G	614	CLA	O2A-CGA-O1A	-2.26	117.89	123.59
7	Y	301	XAT	C20-C13-C14	-2.26	119.76	122.92
4	Y	316	LUT	C38-C25-C24	-2.26	118.73	123.56
3	N	613	CLA	CHD-C1D-ND	-2.25	122.38	124.45
2	Y	302	CHL	OMC-CMC-C2C	-2.25	120.61	125.69
2	Y	307	CHL	O2A-CGA-O1A	-2.24	117.93	123.59
7	G	619	XAT	C20-C13-C14	-2.24	119.78	122.92
3	G	602	CLA	CHD-C1D-ND	-2.24	122.40	124.45
2	Y	308	CHL	CHB-C4A-NA	2.24	127.60	124.51
3	Y	305	CLA	CHD-C1D-ND	-2.23	122.40	124.45
2	Y	306	CHL	CHB-C4A-NA	2.23	127.60	124.51
2	Y	309	CHL	O2A-CGA-O1A	-2.23	117.96	123.59
5	N	617	NEX	C28-C29-C30	2.23	122.36	118.94
2	N	606	CHL	O2A-CGA-O1A	-2.23	117.97	123.59
7	N	619	XAT	C20-C13-C14	-2.23	119.80	122.92
3	Y	315	CLA	CHD-C1D-ND	-2.23	122.41	124.45
2	G	606	CHL	O2A-CGA-O1A	-2.22	117.98	123.59
2	Y	306	CHL	O2A-CGA-O1A	-2.22	117.99	123.59
3	G	610	CLA	O1D-CGD-CBD	2.22	129.02	124.48
7	N	619	XAT	C6-C7-C8	-2.22	121.31	125.99
5	Y	318	NEX	C17-C1-C6	-2.22	108.49	110.47
3	Y	311	CLA	CHB-C4A-NA	2.21	127.57	124.51
2	Y	302	CHL	CHB-C4A-NA	2.21	127.57	124.51
5	G	617	NEX	C11-C12-C13	-2.21	120.20	126.42
2	G	609	CHL	OMC-CMC-C2C	-2.21	120.69	125.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	601	CHL	CHB-C4A-NA	2.21	127.56	124.51
2	Y	310	CHL	C1D-CHD-C4C	-2.20	121.32	126.06
2	Y	310	CHL	CHD-C1D-C2D	2.19	130.07	125.48
4	Y	316	LUT	C21-C26-C27	-2.19	109.94	112.70
3	Y	315	CLA	O2A-CGA-O1A	-2.19	118.08	123.59
2	N	605	CHL	CHB-C4A-NA	2.18	127.53	124.51
2	N	601	CHL	OMC-CMC-C2C	-2.18	120.75	125.69
3	N	614	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
2	N	605	CHL	O2A-CGA-O1A	-2.16	118.13	123.59
3	Y	315	CLA	CHB-C4A-NA	2.16	127.50	124.51
3	N	610	CLA	O2A-CGA-O1A	-2.16	118.15	123.59
4	G	616	LUT	C40-C33-C34	-2.16	119.90	122.92
3	G	611	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
3	N	614	CLA	CHD-C1D-ND	-2.15	122.48	124.45
2	G	605	CHL	O2A-CGA-O1A	-2.15	118.17	123.59
2	N	608	CHL	C2A-C1A-CHA	2.15	127.61	123.86
2	N	608	CHL	CHD-C1D-ND	-2.15	122.48	124.45
4	Y	316	LUT	C40-C33-C34	-2.14	119.92	122.92
2	Y	309	CHL	CHD-C1D-ND	-2.14	122.49	124.45
5	Y	318	NEX	C20-C13-C14	-2.14	119.92	122.92
4	Y	317	LUT	C3-C4-C5	-2.14	107.60	111.85
4	G	616	LUT	C18-C5-C4	2.13	118.31	114.36
3	N	602	CLA	CHD-C1D-ND	-2.13	122.50	124.45
2	G	609	CHL	CHB-C4A-NA	2.13	127.46	124.51
7	N	619	XAT	C19-C9-C10	-2.13	119.94	122.92
2	N	608	CHL	OMC-CMC-C2C	-2.13	120.88	125.69
2	N	609	CHL	C1-C2-C3	-2.13	122.36	126.04
3	Y	304	CLA	O2D-CGD-CBD	2.13	115.05	111.27
2	Y	302	CHL	O2A-CGA-O1A	-2.12	118.23	123.59
3	N	613	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
5	N	617	NEX	C26-C27-C28	-2.12	121.52	125.99
2	G	607	CHL	CHB-C4A-NA	2.12	127.44	124.51
3	Y	312	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
2	N	609	CHL	C1D-CHD-C4C	-2.12	121.49	126.06
4	G	615	LUT	C18-C5-C4	2.12	118.27	114.36
2	G	601	CHL	OMC-CMC-C2C	-2.11	120.91	125.69
3	G	614	CLA	CHD-C1D-ND	-2.11	122.51	124.45
3	Y	304	CLA	CHB-C4A-NA	2.11	127.43	124.51
2	G	605	CHL	CHB-C4A-NA	2.11	127.43	124.51
6	N	618	LHG	C5-O7-C7	-2.10	112.62	117.79
2	Y	307	CHL	CHD-C1D-ND	-2.10	122.53	124.45
2	N	601	CHL	O2A-CGA-O1A	-2.10	118.30	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Y	304	CLA	CHA-C1A-NA	-2.09	121.61	126.40
2	N	608	CHL	O2A-CGA-O1A	-2.09	118.32	123.59
2	N	607	CHL	O2A-CGA-O1A	-2.09	118.33	123.59
3	G	603	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
3	Y	313	CLA	CHD-C1D-ND	-2.08	122.54	124.45
7	N	619	XAT	C4-C3-C2	-2.08	106.76	110.77
3	G	613	CLA	CHD-C1D-ND	-2.08	122.55	124.45
3	Y	304	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
2	N	605	CHL	OMC-CMC-C2C	-2.07	121.00	125.69
4	G	616	LUT	C2-C3-C4	-2.07	107.47	110.30
3	Y	311	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
3	G	603	CLA	C2A-C1A-CHA	2.07	127.48	123.86
4	G	615	LUT	C20-C13-C14	-2.07	120.03	122.92
3	Y	314	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
4	Y	316	LUT	C20-C13-C14	-2.07	120.03	122.92
2	G	606	CHL	CHD-C1D-ND	-2.06	122.56	124.45
3	N	604	CLA	CHD-C1D-ND	-2.06	122.56	124.45
4	N	615	LUT	C40-C33-C34	-2.06	120.04	122.92
7	Y	301	XAT	C4-C3-C2	-2.06	106.80	110.77
3	Y	303	CLA	CHD-C1D-ND	-2.06	122.56	124.45
2	G	607	CHL	O2A-CGA-O1A	-2.05	118.42	123.59
2	G	608	CHL	O2A-CGA-O1A	-2.05	118.42	123.59
5	Y	318	NEX	C40-C33-C34	-2.05	120.05	122.92
4	Y	317	LUT	C20-C13-C14	-2.05	120.05	122.92
3	N	603	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
5	Y	318	NEX	C31-C30-C29	-2.05	124.39	127.31
2	Y	307	CHL	C2A-C1A-CHA	2.04	127.43	123.86
4	N	616	LUT	C3-C4-C5	-2.04	107.79	111.85
2	G	601	CHL	O2A-CGA-O1A	-2.04	118.45	123.59
2	N	608	CHL	CHB-C4A-NA	2.04	127.33	124.51
2	Y	307	CHL	CHB-C4A-NA	2.03	127.32	124.51
3	N	603	CLA	CAA-C2A-C3A	-2.02	107.24	112.78
5	Y	318	NEX	C26-C27-C28	-2.02	121.72	125.99
2	Y	310	CHL	O2A-CGA-O1A	-2.02	118.50	123.59
2	G	606	CHL	C2A-C1A-CHA	2.01	127.38	123.86
2	N	609	CHL	C3C-C4C-NC	-2.01	108.31	110.57
2	Y	308	CHL	O2A-CGA-O1A	-2.01	118.51	123.59
6	Y	319	LHG	C6-C5-C4	-2.01	107.03	111.79
4	Y	316	LUT	C39-C29-C30	-2.01	120.11	122.92
2	N	609	CHL	O2A-CGA-O1A	-2.01	118.52	123.59
3	N	611	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
6	Y	319	LHG	O8-C23-O10	-2.01	118.52	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	602	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
3	Y	303	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
5	N	617	NEX	C19-C9-C10	-2.00	120.12	122.92

All (75) chirality outliers are listed below:

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

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Mol	Chain	Res	Type	Atom
2	G	609	CHL	NA
2	Y	302	CHL	NC
2	Y	302	CHL	ND
2	Y	302	CHL	NA
2	Y	306	CHL	NC
2	Y	306	CHL	ND
2	Y	306	CHL	NA
2	Y	307	CHL	NC
2	Y	307	CHL	ND
2	Y	307	CHL	NA
2	Y	308	CHL	NC
2	Y	308	CHL	ND
2	Y	308	CHL	NA
2	Y	309	CHL	NC
2	Y	309	CHL	ND
2	Y	309	CHL	NA
2	Y	310	CHL	NC
2	Y	310	CHL	ND
2	Y	310	CHL	NA
3	N	602	CLA	ND
3	N	603	CLA	ND
3	N	604	CLA	ND
3	N	610	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	303	CLA	ND
3	Y	304	CLA	ND
3	Y	305	CLA	ND
3	Y	311	CLA	ND
3	Y	313	CLA	ND
3	Y	314	CLA	ND
3	Y	315	CLA	ND

All (571) 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	601	CHL	CHA-CBD-CGD-O1D
2	N	601	CHL	CHA-CBD-CGD-O2D
2	N	605	CHL	C1C-C2C-CMC-OMC
2	N	605	CHL	C3C-C2C-CMC-OMC
2	N	606	CHL	C1C-C2C-CMC-OMC
2	N	607	CHL	C1C-C2C-CMC-OMC
2	N	607	CHL	C3C-C2C-CMC-OMC
2	N	608	CHL	C1A-C2A-CAA-CBA
2	N	608	CHL	C3A-C2A-CAA-CBA
2	N	608	CHL	C1C-C2C-CMC-OMC
2	N	608	CHL	C3C-C2C-CMC-OMC
2	N	608	CHL	CBD-CGD-O2D-CED
2	N	609	CHL	C1C-C2C-CMC-OMC
2	N	609	CHL	C3C-C2C-CMC-OMC
2	G	601	CHL	C1C-C2C-CMC-OMC
2	G	601	CHL	C3C-C2C-CMC-OMC
2	G	605	CHL	C1C-C2C-CMC-OMC
2	G	605	CHL	C3C-C2C-CMC-OMC
2	G	606	CHL	C1A-C2A-CAA-CBA
2	G	606	CHL	C3A-C2A-CAA-CBA
2	G	606	CHL	C1C-C2C-CMC-OMC
2	G	606	CHL	C3C-C2C-CMC-OMC
2	G	607	CHL	C1C-C2C-CMC-OMC
2	G	607	CHL	C3C-C2C-CMC-OMC
2	G	608	CHL	C3C-C2C-CMC-OMC
2	G	609	CHL	C1A-C2A-CAA-CBA
2	G	609	CHL	C1C-C2C-CMC-OMC
2	G	609	CHL	C3C-C2C-CMC-OMC
2	Y	302	CHL	C1C-C2C-CMC-OMC
2	Y	302	CHL	C3C-C2C-CMC-OMC
2	Y	306	CHL	C1C-C2C-CMC-OMC
2	Y	306	CHL	C3C-C2C-CMC-OMC
2	Y	307	CHL	C1A-C2A-CAA-CBA
2	Y	307	CHL	C3A-C2A-CAA-CBA
2	Y	307	CHL	C1C-C2C-CMC-OMC
2	Y	308	CHL	C1C-C2C-CMC-OMC
2	Y	308	CHL	C3C-C2C-CMC-OMC
2	Y	309	CHL	C1A-C2A-CAA-CBA
2	Y	309	CHL	C1C-C2C-CMC-OMC
2	Y	309	CHL	C3C-C2C-CMC-OMC
2	Y	309	CHL	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
2	Y	309	CHL	CHA-CBD-CGD-O2D
2	Y	309	CHL	CBD-CGD-O2D-CED
2	Y	310	CHL	C1C-C2C-CMC-OMC
2	Y	310	CHL	C3C-C2C-CMC-OMC
3	N	604	CLA	CHA-CBD-CGD-O1D
3	N	604	CLA	CHA-CBD-CGD-O2D
3	N	611	CLA	CHA-CBD-CGD-O1D
3	N	611	CLA	CHA-CBD-CGD-O2D
3	N	612	CLA	CBD-CGD-O2D-CED
3	N	613	CLA	CBD-CGD-O2D-CED
3	N	614	CLA	C1A-C2A-CAA-CBA
3	N	614	CLA	CHA-CBD-CGD-O1D
3	N	614	CLA	CAD-CBD-CGD-O1D
3	N	614	CLA	CAD-CBD-CGD-O2D
3	G	610	CLA	CBD-CGD-O2D-CED
3	G	613	CLA	CHA-CBD-CGD-O1D
3	G	613	CLA	CHA-CBD-CGD-O2D
3	G	613	CLA	CBD-CGD-O2D-CED
3	G	614	CLA	CHA-CBD-CGD-O1D
3	G	614	CLA	CHA-CBD-CGD-O2D
3	G	614	CLA	CAD-CBD-CGD-O1D
3	G	614	CLA	CAD-CBD-CGD-O2D
3	G	614	CLA	CBD-CGD-O2D-CED
3	Y	303	CLA	CBD-CGD-O2D-CED
3	Y	313	CLA	CBD-CGD-O2D-CED
3	Y	315	CLA	CHA-CBD-CGD-O1D
3	Y	315	CLA	CHA-CBD-CGD-O2D
3	Y	315	CLA	CAD-CBD-CGD-O1D
4	N	615	LUT	C1-C6-C7-C8
4	Y	317	LUT	C1-C6-C7-C8
6	N	618	LHG	C4-O6-P-O4
6	G	618	LHG	C3-O3-P-O5
6	Y	319	LHG	C3-O3-P-O5
6	Y	319	LHG	C4-O6-P-O5
2	Y	309	CHL	O1D-CGD-O2D-CED
2	Y	306	CHL	CBD-CGD-O2D-CED
2	Y	308	CHL	CBD-CGD-O2D-CED
2	Y	310	CHL	CBD-CGD-O2D-CED
3	N	604	CLA	CBD-CGD-O2D-CED
3	G	604	CLA	CBD-CGD-O2D-CED
3	G	612	CLA	CBD-CGD-O2D-CED
3	Y	311	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
3	Y	315	CLA	CBD-CGD-O2D-CED
2	G	606	CHL	O1A-CGA-O2A-C1
3	G	610	CLA	O1D-CGD-O2D-CED
2	N	608	CHL	O1D-CGD-O2D-CED
3	N	612	CLA	O1D-CGD-O2D-CED
3	N	613	CLA	O1D-CGD-O2D-CED
3	G	613	CLA	O1D-CGD-O2D-CED
3	G	614	CLA	O1D-CGD-O2D-CED
3	Y	303	CLA	O1D-CGD-O2D-CED
3	Y	313	CLA	O1D-CGD-O2D-CED
2	G	606	CHL	CBA-CGA-O2A-C1
2	N	601	CHL	CBD-CGD-O2D-CED
3	Y	314	CLA	CBD-CGD-O2D-CED
2	N	606	CHL	O1A-CGA-O2A-C1
2	N	607	CHL	O1A-CGA-O2A-C1
2	G	607	CHL	O1A-CGA-O2A-C1
2	G	609	CHL	O1A-CGA-O2A-C1
2	Y	307	CHL	O1A-CGA-O2A-C1
2	Y	308	CHL	O1A-CGA-O2A-C1
2	N	605	CHL	CBD-CGD-O2D-CED
3	N	604	CLA	C3-C5-C6-C7
3	G	613	CLA	C3-C5-C6-C7
2	N	606	CHL	CBA-CGA-O2A-C1
2	G	609	CHL	CBA-CGA-O2A-C1
2	Y	307	CHL	CBA-CGA-O2A-C1
3	Y	313	CLA	C8-C10-C11-C12
2	G	601	CHL	CBD-CGD-O2D-CED
3	N	614	CLA	CBD-CGD-O2D-CED
3	Y	304	CLA	CBD-CGD-O2D-CED
3	N	610	CLA	CBD-CGD-O2D-CED
2	G	609	CHL	C2A-CAA-CBA-CGA
3	G	604	CLA	C2A-CAA-CBA-CGA
3	Y	305	CLA	C3-C5-C6-C7
2	N	607	CHL	CBA-CGA-O2A-C1
2	G	607	CHL	CBA-CGA-O2A-C1
2	Y	308	CHL	CBA-CGA-O2A-C1
3	G	610	CLA	CBA-CGA-O2A-C1
2	Y	308	CHL	O1D-CGD-O2D-CED
3	N	604	CLA	O1D-CGD-O2D-CED
3	Y	315	CLA	O1D-CGD-O2D-CED
3	G	610	CLA	O1A-CGA-O2A-C1
2	N	607	CHL	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
3	G	612	CLA	O1D-CGD-O2D-CED
3	Y	311	CLA	O1D-CGD-O2D-CED
2	Y	306	CHL	O1D-CGD-O2D-CED
2	G	609	CHL	CBD-CGD-O2D-CED
3	G	604	CLA	O1D-CGD-O2D-CED
3	N	613	CLA	C3-C5-C6-C7
3	G	603	CLA	C3-C5-C6-C7
2	N	608	CHL	C2A-CAA-CBA-CGA
2	G	607	CHL	C2A-CAA-CBA-CGA
2	Y	310	CHL	O1D-CGD-O2D-CED
3	N	614	CLA	CBA-CGA-O2A-C1
3	G	604	CLA	CBA-CGA-O2A-C1
3	G	614	CLA	CBA-CGA-O2A-C1
3	Y	311	CLA	CBA-CGA-O2A-C1
3	Y	315	CLA	CBA-CGA-O2A-C1
6	N	618	LHG	C24-C23-O8-C6
3	G	614	CLA	O1A-CGA-O2A-C1
2	G	609	CHL	C11-C10-C8-C9
2	G	609	CHL	C11-C12-C13-C14
3	N	611	CLA	C6-C7-C8-C9
3	N	612	CLA	C6-C7-C8-C9
3	N	612	CLA	C14-C13-C15-C16
3	G	611	CLA	C6-C7-C8-C9
3	G	612	CLA	C6-C7-C8-C9
3	G	612	CLA	C14-C13-C15-C16
3	Y	311	CLA	C14-C13-C15-C16
3	Y	312	CLA	C6-C7-C8-C9
3	Y	313	CLA	C14-C13-C15-C16
3	N	602	CLA	C10-C11-C12-C13
4	G	616	LUT	C31-C32-C33-C40
4	Y	317	LUT	C31-C32-C33-C40
3	N	611	CLA	C5-C6-C7-C8
3	G	610	CLA	C13-C15-C16-C17
3	Y	314	CLA	O1D-CGD-O2D-CED
3	Y	314	CLA	C3-C5-C6-C7
2	G	605	CHL	CBA-CGA-O2A-C1
3	N	604	CLA	CBA-CGA-O2A-C1
3	N	610	CLA	C5-C6-C7-C8
3	G	603	CLA	C5-C6-C7-C8
3	G	610	CLA	C8-C10-C11-C12
3	Y	305	CLA	CBA-CGA-O2A-C1
2	N	601	CHL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
3	Y	312	CLA	C5-C6-C7-C8
3	N	603	CLA	C6-C7-C8-C10
3	G	612	CLA	C11-C12-C13-C15
3	Y	311	CLA	C11-C12-C13-C15
3	G	604	CLA	O1A-CGA-O2A-C1
3	Y	311	CLA	O1A-CGA-O2A-C1
2	N	608	CHL	C13-C15-C16-C17
2	G	609	CHL	C5-C6-C7-C8
3	Y	303	CLA	C10-C11-C12-C13
3	Y	315	CLA	O1A-CGA-O2A-C1
2	N	605	CHL	O1D-CGD-O2D-CED
3	N	611	CLA	C10-C11-C12-C13
3	G	610	CLA	C5-C6-C7-C8
3	N	614	CLA	O1A-CGA-O2A-C1
6	N	618	LHG	O10-C23-O8-C6
3	N	611	CLA	C8-C10-C11-C12
3	G	612	CLA	C10-C11-C12-C13
3	Y	304	CLA	C8-C10-C11-C12
2	G	601	CHL	O1D-CGD-O2D-CED
3	N	614	CLA	O1D-CGD-O2D-CED
3	Y	304	CLA	O1D-CGD-O2D-CED
2	G	605	CHL	O1A-CGA-O2A-C1
6	G	618	LHG	C8-C7-O7-C5
2	Y	308	CHL	C5-C6-C7-C8
6	N	618	LHG	C4-O6-P-O3
6	G	618	LHG	C4-O6-P-O3
3	Y	311	CLA	C3-C5-C6-C7
3	N	610	CLA	O1D-CGD-O2D-CED
6	G	618	LHG	O9-C7-O7-C5
3	Y	311	CLA	C2A-CAA-CBA-CGA
3	G	610	CLA	C3-C5-C6-C7
2	G	601	CHL	CBA-CGA-O2A-C1
2	Y	309	CHL	CBA-CGA-O2A-C1
3	G	611	CLA	C13-C15-C16-C17
6	Y	319	LHG	C14-C15-C16-C17
3	N	611	CLA	C16-C17-C18-C20
2	Y	302	CHL	CBA-CGA-O2A-C1
6	G	618	LHG	C24-C23-O8-C6
3	G	603	CLA	C15-C16-C17-C18
2	Y	309	CHL	O1A-CGA-O2A-C1
3	G	612	CLA	C4-C3-C5-C6
3	G	613	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
2	N	607	CHL	O1D-CGD-O2D-CED
6	Y	319	LHG	C15-C16-C17-C18
2	N	607	CHL	C2A-CAA-CBA-CGA
2	Y	308	CHL	C2A-CAA-CBA-CGA
3	N	604	CLA	O1A-CGA-O2A-C1
3	Y	305	CLA	O1A-CGA-O2A-C1
3	N	612	CLA	C5-C6-C7-C8
3	Y	304	CLA	C10-C11-C12-C13
6	N	618	LHG	C15-C16-C17-C18
3	Y	311	CLA	C16-C17-C18-C19
6	N	618	LHG	C14-C15-C16-C17
2	G	609	CHL	O1D-CGD-O2D-CED
2	N	606	CHL	C3A-C2A-CAA-CBA
2	G	605	CHL	C3A-C2A-CAA-CBA
3	N	603	CLA	C3A-C2A-CAA-CBA
3	N	614	CLA	C3A-C2A-CAA-CBA
3	Y	304	CLA	C3A-C2A-CAA-CBA
2	G	609	CHL	C16-C17-C18-C19
3	N	611	CLA	C16-C17-C18-C19
2	G	601	CHL	O1A-CGA-O2A-C1
2	Y	302	CHL	O1A-CGA-O2A-C1
3	G	602	CLA	C15-C16-C17-C18
3	Y	313	CLA	C10-C11-C12-C13
6	N	618	LHG	O9-C7-O7-C5
3	N	604	CLA	C2-C1-O2A-CGA
3	Y	305	CLA	C2-C1-O2A-CGA
6	G	618	LHG	O10-C23-O8-C6
4	N	615	LUT	C5-C6-C7-C8
4	G	615	LUT	C1-C6-C7-C8
4	G	615	LUT	C5-C6-C7-C8
4	G	616	LUT	C1-C6-C7-C8
4	G	616	LUT	C5-C6-C7-C8
4	Y	317	LUT	C5-C6-C7-C8
2	N	608	CHL	C5-C6-C7-C8
6	N	618	LHG	C8-C7-O7-C5
2	N	609	CHL	C4-C3-C5-C6
2	Y	309	CHL	C4-C3-C5-C6
3	N	611	CLA	C4-C3-C5-C6
2	N	609	CHL	C2-C3-C5-C6
2	G	601	CHL	C6-C7-C8-C10
2	G	607	CHL	C11-C10-C8-C7
2	Y	309	CHL	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
3	N	611	CLA	C2-C3-C5-C6
3	N	611	CLA	C6-C7-C8-C10
3	N	612	CLA	C12-C13-C15-C16
3	G	612	CLA	C2-C3-C5-C6
3	G	613	CLA	C12-C13-C15-C16
3	Y	312	CLA	C11-C10-C8-C7
3	Y	312	CLA	C12-C13-C15-C16
3	G	612	CLA	C3-C5-C6-C7
2	G	608	CHL	C5-C6-C7-C8
2	Y	308	CHL	C15-C16-C17-C18
3	N	611	CLA	C15-C16-C17-C18
3	G	611	CLA	C5-C6-C7-C8
3	Y	311	CLA	C16-C17-C18-C20
3	N	610	CLA	CBA-CGA-O2A-C1
3	Y	314	CLA	C2A-CAA-CBA-CGA
2	G	607	CHL	C5-C6-C7-C8
3	G	611	CLA	C15-C16-C17-C18
2	N	608	CHL	C3-C5-C6-C7
6	G	618	LHG	C9-C10-C11-C12
3	Y	312	CLA	CBD-CGD-O2D-CED
3	G	612	CLA	C16-C17-C18-C20
2	G	601	CHL	C6-C7-C8-C9
2	G	607	CHL	C11-C10-C8-C9
2	Y	302	CHL	C6-C7-C8-C9
3	N	603	CLA	C6-C7-C8-C9
3	N	610	CLA	C14-C13-C15-C16
3	N	613	CLA	C6-C7-C8-C9
3	G	611	CLA	C11-C10-C8-C9
3	G	612	CLA	C11-C12-C13-C14
3	Y	312	CLA	C11-C10-C8-C9
3	Y	312	CLA	C14-C13-C15-C16
3	Y	313	CLA	C11-C10-C8-C9
2	G	605	CHL	CBD-CGD-O2D-CED
4	N	615	LUT	C11-C12-C13-C20
2	N	606	CHL	C1A-C2A-CAA-CBA
2	G	605	CHL	C1A-C2A-CAA-CBA
3	N	603	CLA	C1A-C2A-CAA-CBA
3	N	604	CLA	C1A-C2A-CAA-CBA
3	G	610	CLA	C1A-C2A-CAA-CBA
3	Y	304	CLA	C1A-C2A-CAA-CBA
3	Y	305	CLA	C1A-C2A-CAA-CBA
3	N	612	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
6	Y	319	LHG	C4-O6-P-O3
3	N	610	CLA	C10-C11-C12-C13
2	G	609	CHL	C4-C3-C5-C6
3	G	602	CLA	C10-C11-C12-C13
3	G	613	CLA	C13-C15-C16-C17
3	Y	313	CLA	C5-C6-C7-C8
3	Y	314	CLA	CBA-CGA-O2A-C1
6	N	618	LHG	C24-C25-C26-C27
3	N	610	CLA	O1A-CGA-O2A-C1
2	N	607	CHL	C15-C16-C17-C18
2	N	608	CHL	CBA-CGA-O2A-C1
3	Y	313	CLA	C16-C17-C18-C20
3	N	611	CLA	CBD-CGD-O2D-CED
3	Y	313	CLA	C13-C15-C16-C17
2	N	607	CHL	C11-C10-C8-C7
2	N	607	CHL	C12-C13-C15-C16
2	N	609	CHL	C12-C13-C15-C16
2	G	607	CHL	C12-C13-C15-C16
2	Y	302	CHL	C6-C7-C8-C10
2	Y	302	CHL	C12-C13-C15-C16
2	Y	308	CHL	C12-C13-C15-C16
3	N	610	CLA	C12-C13-C15-C16
3	N	613	CLA	C6-C7-C8-C10
3	G	602	CLA	C6-C7-C8-C10
3	G	603	CLA	C11-C10-C8-C7
3	G	603	CLA	C12-C13-C15-C16
3	G	611	CLA	C6-C7-C8-C10
3	G	611	CLA	C11-C10-C8-C7
3	G	611	CLA	C12-C13-C15-C16
3	G	613	CLA	C11-C10-C8-C7
3	Y	312	CLA	C6-C7-C8-C10
3	Y	313	CLA	C11-C10-C8-C7
2	N	607	CHL	C14-C13-C15-C16
2	G	607	CHL	C14-C13-C15-C16
2	Y	308	CHL	C11-C10-C8-C9
2	Y	308	CHL	C14-C13-C15-C16
2	Y	309	CHL	C6-C7-C8-C9
3	N	613	CLA	C14-C13-C15-C16
3	G	603	CLA	C11-C10-C8-C9
3	G	611	CLA	C14-C13-C15-C16
3	Y	304	CLA	C6-C7-C8-C9
3	G	602	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
2	Y	310	CHL	C8-C10-C11-C12
2	N	601	CHL	CBA-CGA-O2A-C1
2	N	601	CHL	C3A-C2A-CAA-CBA
2	Y	309	CHL	C3A-C2A-CAA-CBA
3	G	612	CLA	C16-C17-C18-C19
2	N	606	CHL	C3C-C2C-CMC-OMC
2	Y	307	CHL	C3C-C2C-CMC-OMC
2	N	608	CHL	O1A-CGA-O2A-C1
2	G	608	CHL	C2A-CAA-CBA-CGA
3	N	602	CLA	C2A-CAA-CBA-CGA
3	N	613	CLA	C2A-CAA-CBA-CGA
3	Y	314	CLA	O1A-CGA-O2A-C1
2	G	609	CHL	C16-C17-C18-C20
6	Y	319	LHG	C24-C25-C26-C27
3	Y	313	CLA	C16-C17-C18-C19
3	G	602	CLA	C13-C15-C16-C17
3	Y	312	CLA	C15-C16-C17-C18
3	G	604	CLA	C2-C1-O2A-CGA
2	N	607	CHL	C11-C10-C8-C9
2	G	609	CHL	C6-C7-C8-C9
2	G	609	CHL	C14-C13-C15-C16
2	Y	302	CHL	C14-C13-C15-C16
3	N	612	CLA	C11-C12-C13-C14
3	G	602	CLA	C6-C7-C8-C9
3	Y	311	CLA	C11-C10-C8-C9
3	Y	314	CLA	C14-C13-C15-C16
3	G	602	CLA	C2A-CAA-CBA-CGA
2	Y	302	CHL	C3-C5-C6-C7
4	Y	316	LUT	C1-C6-C7-C8
3	G	610	CLA	C15-C16-C17-C18
3	Y	312	CLA	O1D-CGD-O2D-CED
4	Y	317	LUT	C31-C32-C33-C34
2	G	609	CHL	C15-C16-C17-C18
2	N	601	CHL	C12-C13-C15-C16
2	G	601	CHL	C12-C13-C15-C16
2	G	609	CHL	C11-C12-C13-C15
2	Y	308	CHL	C11-C10-C8-C7
2	Y	309	CHL	C6-C7-C8-C10
3	N	602	CLA	C6-C7-C8-C10
3	N	612	CLA	C11-C12-C13-C15
3	N	613	CLA	C12-C13-C15-C16
3	G	602	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
3	G	612	CLA	C6-C7-C8-C10
3	Y	303	CLA	C6-C7-C8-C10
3	Y	304	CLA	C6-C7-C8-C10
3	Y	311	CLA	C11-C10-C8-C7
3	Y	313	CLA	C12-C13-C15-C16
3	Y	314	CLA	C11-C10-C8-C7
3	Y	314	CLA	C12-C13-C15-C16
2	N	606	CHL	CAD-CBD-CGD-O2D
2	G	606	CHL	CAD-CBD-CGD-O2D
2	G	607	CHL	CAD-CBD-CGD-O2D
2	Y	308	CHL	CAD-CBD-CGD-O2D
3	Y	311	CLA	CAD-CBD-CGD-O2D
3	N	611	CLA	O1D-CGD-O2D-CED
3	N	611	CLA	C13-C15-C16-C17
3	Y	304	CLA	C5-C6-C7-C8
2	N	601	CHL	O1A-CGA-O2A-C1
3	Y	313	CLA	C4-C3-C5-C6
2	Y	307	CHL	CBD-CGD-O2D-CED
2	Y	309	CHL	C8-C10-C11-C12
2	G	601	CHL	CHA-CBD-CGD-O1D
3	N	602	CLA	CHA-CBD-CGD-O1D
3	N	602	CLA	CHA-CBD-CGD-O2D
3	N	614	CLA	CHA-CBD-CGD-O2D
3	Y	303	CLA	CHA-CBD-CGD-O1D
3	Y	303	CLA	CHA-CBD-CGD-O2D
2	G	605	CHL	O1D-CGD-O2D-CED
2	N	605	CHL	CBA-CGA-O2A-C1
3	N	612	CLA	C4-C3-C5-C6
2	N	601	CHL	C14-C13-C15-C16
2	N	608	CHL	C11-C10-C8-C9
2	G	601	CHL	C14-C13-C15-C16
3	N	611	CLA	C14-C13-C15-C16
3	N	612	CLA	C11-C10-C8-C9
3	N	613	CLA	C11-C12-C13-C14
3	G	604	CLA	C6-C7-C8-C9
3	Y	314	CLA	C11-C10-C8-C9
4	G	616	LUT	C7-C8-C9-C19
4	G	616	LUT	C31-C32-C33-C34
3	N	613	CLA	CBA-CGA-O2A-C1
3	N	611	CLA	C3-C5-C6-C7
2	G	609	CHL	C2-C3-C5-C6
6	G	618	LHG	C4-O6-P-O4

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Mol	Chain	Res	Type	Atoms
6	Y	319	LHG	C4-O6-P-O4
3	N	614	CLA	O2A-C1-C2-C3
3	G	614	CLA	O2A-C1-C2-C3
3	Y	315	CLA	O2A-C1-C2-C3
3	Y	311	CLA	C5-C6-C7-C8
3	G	613	CLA	CBA-CGA-O2A-C1
3	N	604	CLA	CAD-CBD-CGD-O1D
3	Y	303	CLA	CAD-CBD-CGD-O1D
2	N	605	CHL	O1A-CGA-O2A-C1
2	G	609	CHL	C11-C10-C8-C7
2	G	609	CHL	C12-C13-C15-C16
2	Y	310	CHL	C12-C13-C15-C16
3	N	610	CLA	C11-C10-C8-C7
3	N	611	CLA	C11-C10-C8-C7
3	G	612	CLA	C12-C13-C15-C16
3	N	613	CLA	C13-C15-C16-C17
2	G	608	CHL	C1C-C2C-CMC-OMC
3	N	613	CLA	O1A-CGA-O2A-C1
3	Y	311	CLA	C8-C10-C11-C12
3	G	613	CLA	O1A-CGA-O2A-C1
2	N	609	CHL	C14-C13-C15-C16
3	N	602	CLA	C6-C7-C8-C9
3	G	602	CLA	C11-C12-C13-C14
3	G	613	CLA	C11-C10-C8-C9
3	Y	303	CLA	C6-C7-C8-C9
3	Y	313	CLA	C11-C12-C13-C14
6	Y	319	LHG	C27-C28-C29-C30
2	Y	307	CHL	O1D-CGD-O2D-CED
3	N	602	CLA	C13-C15-C16-C17
3	Y	314	CLA	C13-C15-C16-C17
3	N	614	CLA	C1-C2-C3-C4
3	G	614	CLA	C1-C2-C3-C4
3	Y	315	CLA	C1-C2-C3-C4
3	Y	303	CLA	C2A-CAA-CBA-CGA
3	Y	313	CLA	C2-C1-O2A-CGA
4	Y	316	LUT	C5-C6-C7-C8
3	N	612	CLA	C2-C3-C5-C6
3	Y	313	CLA	C2-C3-C5-C6
6	G	618	LHG	C25-C26-C27-C28
3	G	613	CLA	C2A-CAA-CBA-CGA
6	N	618	LHG	C3-O3-P-O6
6	G	618	LHG	C3-O3-P-O6

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Mol	Chain	Res	Type	Atoms
6	Y	319	LHG	C3-O3-P-O6
3	N	611	CLA	C12-C13-C15-C16
3	N	612	CLA	C6-C7-C8-C10
3	N	613	CLA	C11-C12-C13-C15
3	N	610	CLA	C11-C10-C8-C9
3	G	603	CLA	C14-C13-C15-C16
2	Y	306	CHL	CAA-CBA-CGA-O2A
3	G	602	CLA	C16-C17-C18-C20
6	G	618	LHG	C29-C30-C31-C32
3	G	610	CLA	C10-C11-C12-C13
3	G	603	CLA	C8-C10-C11-C12
6	G	618	LHG	C27-C28-C29-C30
2	Y	309	CHL	C2A-CAA-CBA-CGA
6	Y	319	LHG	C26-C27-C28-C29
2	N	609	CHL	C6-C7-C8-C9
3	G	610	CLA	C6-C7-C8-C9
5	N	617	NEX	C39-C29-C30-C31
5	G	617	NEX	C39-C29-C30-C31
5	Y	318	NEX	C39-C29-C30-C31
3	G	602	CLA	C16-C17-C18-C19
3	N	610	CLA	C13-C15-C16-C17
3	N	603	CLA	C4-C3-C5-C6
2	N	601	CHL	C1A-C2A-CAA-CBA
2	N	609	CHL	C1A-C2A-CAA-CBA
2	Y	308	CHL	C1A-C2A-CAA-CBA
3	N	612	CLA	C11-C10-C8-C7
3	G	604	CLA	C6-C7-C8-C10
3	Y	304	CLA	C12-C13-C15-C16
3	N	603	CLA	C2-C3-C5-C6
3	G	611	CLA	C2-C3-C5-C6
5	N	617	NEX	C28-C29-C30-C31
5	G	617	NEX	C28-C29-C30-C31
5	Y	318	NEX	C28-C29-C30-C31
2	Y	308	CHL	C4-C3-C5-C6
3	G	604	CLA	C4-C3-C5-C6
2	G	605	CHL	C2-C1-O2A-CGA
2	G	609	CHL	C2-C1-O2A-CGA
3	Y	304	CLA	C2-C1-O2A-CGA
3	Y	311	CLA	C11-C12-C13-C14
3	Y	304	CLA	CBA-CGA-O2A-C1
3	Y	304	CLA	O1A-CGA-O2A-C1
4	N	616	LUT	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
3	N	603	CLA	CBA-CGA-O2A-C1
3	G	611	CLA	C4-C3-C5-C6
4	N	615	LUT	C11-C12-C13-C14
4	G	616	LUT	C7-C8-C9-C10
3	N	603	CLA	O1A-CGA-O2A-C1
2	N	605	CHL	CAA-CBA-CGA-O2A
2	Y	309	CHL	C5-C6-C7-C8
2	Y	308	CHL	C2-C3-C5-C6
6	G	618	LHG	O8-C23-C24-C25
2	Y	310	CHL	C14-C13-C15-C16
3	N	611	CLA	C11-C10-C8-C9
3	Y	311	CLA	C6-C7-C8-C9
3	Y	303	CLA	O1A-CGA-O2A-C1
2	Y	306	CHL	CAD-CBD-CGD-O2D
2	Y	307	CHL	CAD-CBD-CGD-O2D
3	G	604	CLA	C2-C3-C5-C6
5	N	617	NEX	O24-C26-C27-C28
5	G	617	NEX	O24-C26-C27-C28
5	Y	318	NEX	O24-C26-C27-C28
3	G	603	CLA	CAA-CBA-CGA-O2A
3	Y	303	CLA	CBA-CGA-O2A-C1
3	N	610	CLA	C2A-CAA-CBA-CGA
3	G	610	CLA	C2A-CAA-CBA-CGA
2	N	609	CHL	CHA-CBD-CGD-O2D
2	G	601	CHL	CHA-CBD-CGD-O2D
2	Y	302	CHL	CHA-CBD-CGD-O1D
2	Y	302	CHL	CHA-CBD-CGD-O2D
3	N	603	CLA	CHA-CBD-CGD-O1D
3	N	603	CLA	CHA-CBD-CGD-O2D
3	G	602	CLA	CHA-CBD-CGD-O1D
3	G	602	CLA	CHA-CBD-CGD-O2D
3	G	603	CLA	CHA-CBD-CGD-O1D
3	G	604	CLA	CHA-CBD-CGD-O1D
3	Y	304	CLA	CHA-CBD-CGD-O1D
3	Y	304	CLA	CHA-CBD-CGD-O2D
3	Y	305	CLA	CHA-CBD-CGD-O1D
2	G	601	CHL	C13-C15-C16-C17
2	G	605	CHL	CAA-CBA-CGA-O2A
3	N	603	CLA	C12-C13-C15-C16
3	N	602	CLA	C11-C12-C13-C14
3	Y	304	CLA	C14-C13-C15-C16
3	Y	305	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
6	G	618	LHG	O10-C23-C24-C25
3	G	603	CLA	CAA-CBA-CGA-O1A
2	N	607	CHL	C1A-C2A-CAA-CBA
2	G	607	CHL	C1A-C2A-CAA-CBA
2	Y	310	CHL	C1A-C2A-CAA-CBA
3	N	610	CLA	C2-C1-O2A-CGA
3	N	612	CLA	C10-C11-C12-C13
2	G	605	CHL	CAA-CBA-CGA-O1A
4	N	616	LUT	C5-C6-C7-C8
3	N	603	CLA	C10-C11-C12-C13
3	Y	311	CLA	C13-C15-C16-C17
2	Y	306	CHL	O1A-CGA-O2A-C1
2	Y	302	CHL	CAA-CBA-CGA-O2A
3	G	610	CLA	CAA-CBA-CGA-O2A
3	Y	311	CLA	C15-C16-C17-C18
2	G	601	CHL	C15-C16-C17-C18
2	G	609	CHL	C3A-C2A-CAA-CBA
2	Y	308	CHL	C3A-C2A-CAA-CBA
3	N	602	CLA	C11-C12-C13-C15
3	Y	305	CLA	C6-C7-C8-C10
3	N	612	CLA	CAA-CBA-CGA-O2A
3	N	603	CLA	C15-C16-C17-C18
2	G	609	CHL	C13-C15-C16-C17
3	N	610	CLA	C8-C10-C11-C12

There are no ring outliers.

45 monomers are involved in 116 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	617	NEX	4	0
2	N	606	CHL	1	0
3	Y	313	CLA	8	0
2	N	601	CHL	6	0
2	G	601	CHL	1	0
2	N	609	CHL	2	0
4	Y	317	LUT	4	0
3	G	602	CLA	3	0
3	N	602	CLA	1	0
7	N	619	XAT	4	0
3	Y	314	CLA	1	0
4	G	616	LUT	7	0
6	N	618	LHG	1	0

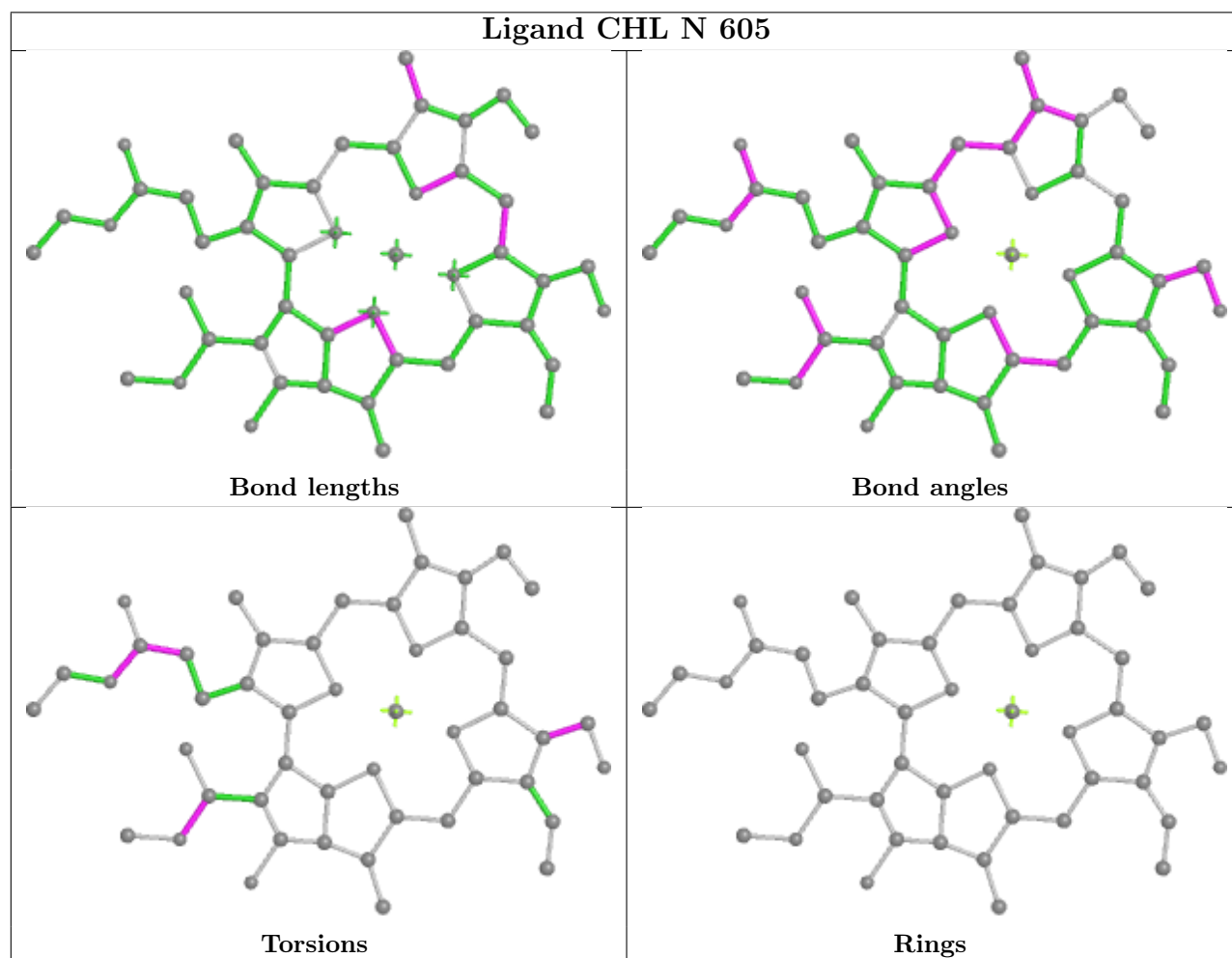
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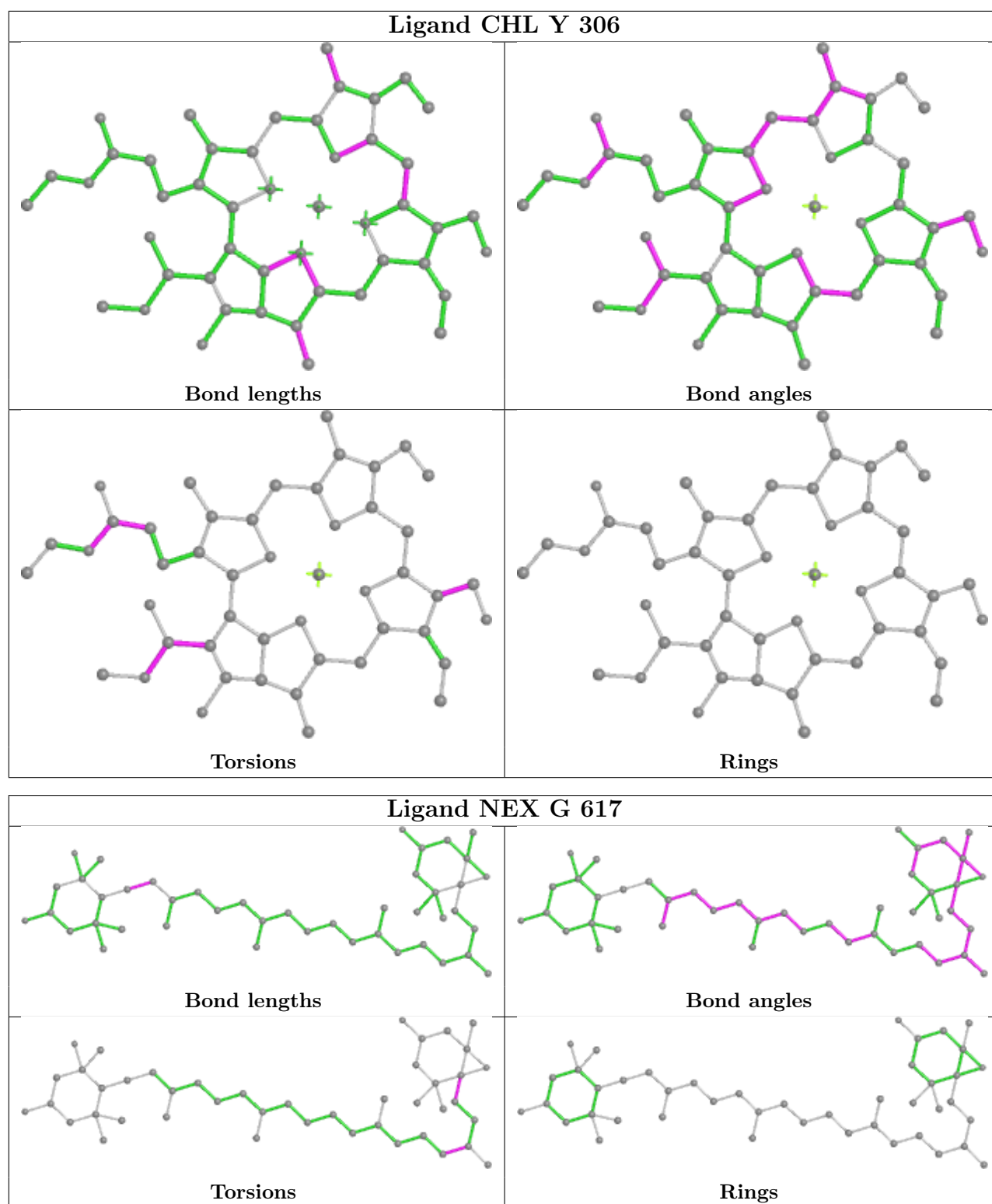
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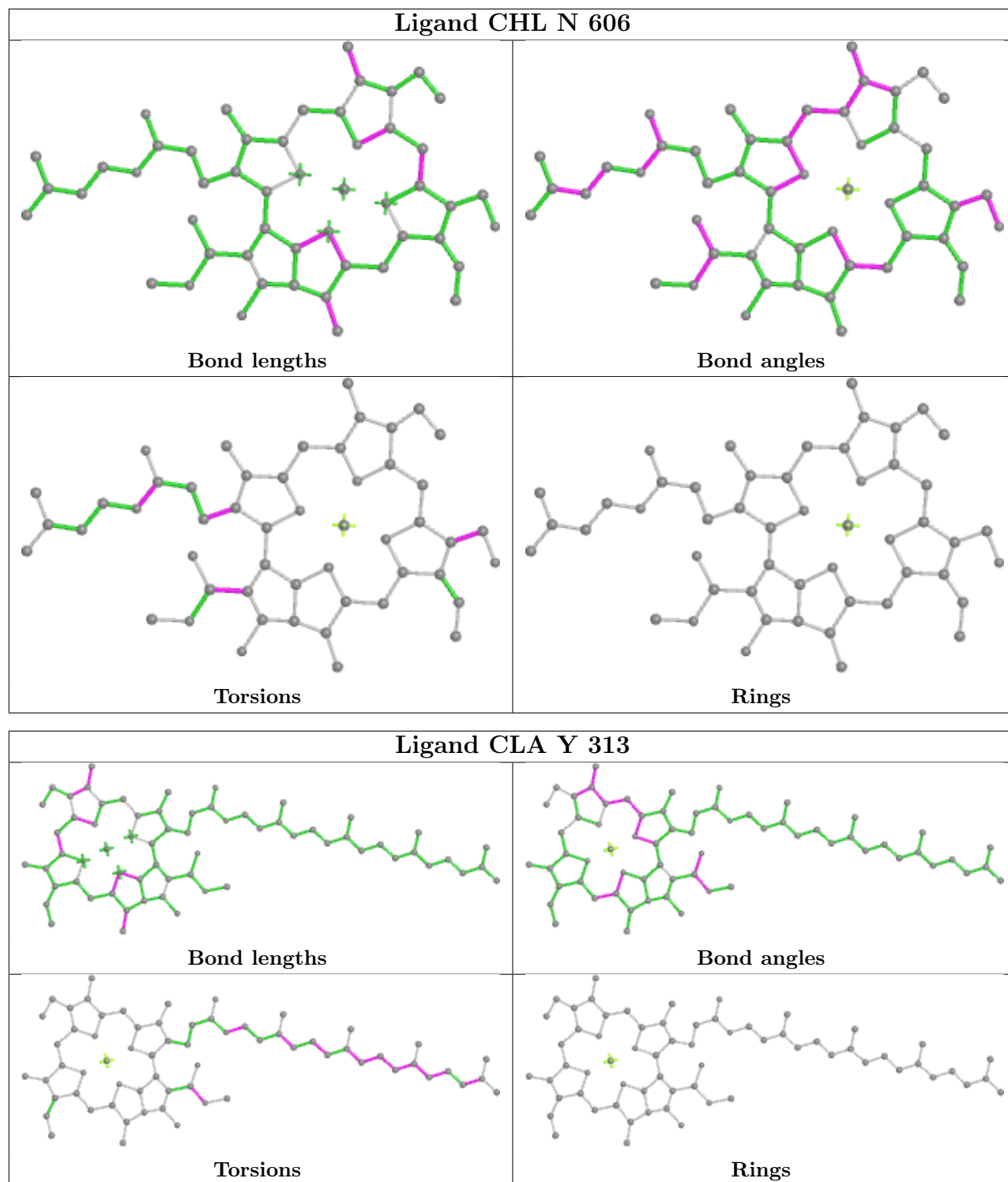
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	607	CHL	1	0
2	G	609	CHL	6	0
4	N	616	LUT	3	0
3	N	603	CLA	1	0
2	Y	310	CHL	4	0
2	N	608	CHL	2	0
2	G	608	CHL	1	0
3	G	603	CLA	4	0
3	Y	304	CLA	3	0
6	G	618	LHG	1	0
7	Y	301	XAT	4	0
3	G	614	CLA	1	0
7	G	619	XAT	4	0
2	Y	308	CHL	1	0
3	N	613	CLA	3	0
5	Y	318	NEX	4	0
3	Y	303	CLA	1	0
3	N	611	CLA	1	0
3	G	610	CLA	7	0
3	G	604	CLA	2	0
3	G	611	CLA	1	0
4	N	615	LUT	7	0
3	N	610	CLA	3	0
3	G	613	CLA	5	0
3	G	612	CLA	5	0
3	Y	312	CLA	2	0
4	Y	316	LUT	2	0
4	G	615	LUT	7	0
3	N	612	CLA	1	0
5	N	617	NEX	4	0
3	Y	311	CLA	13	0
2	N	607	CHL	3	0

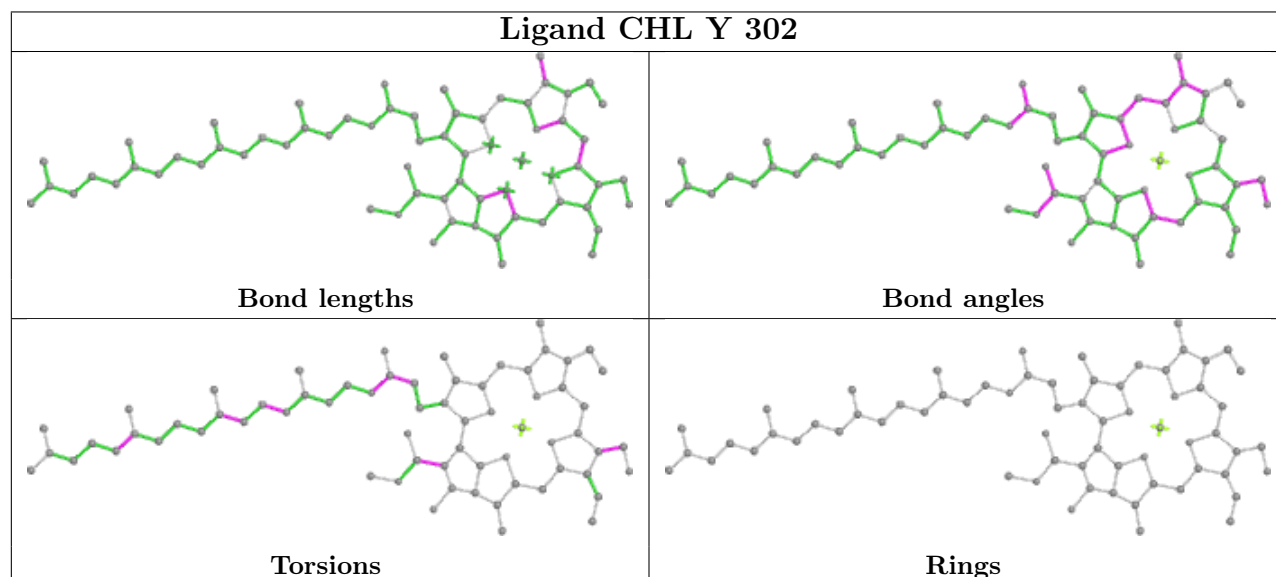
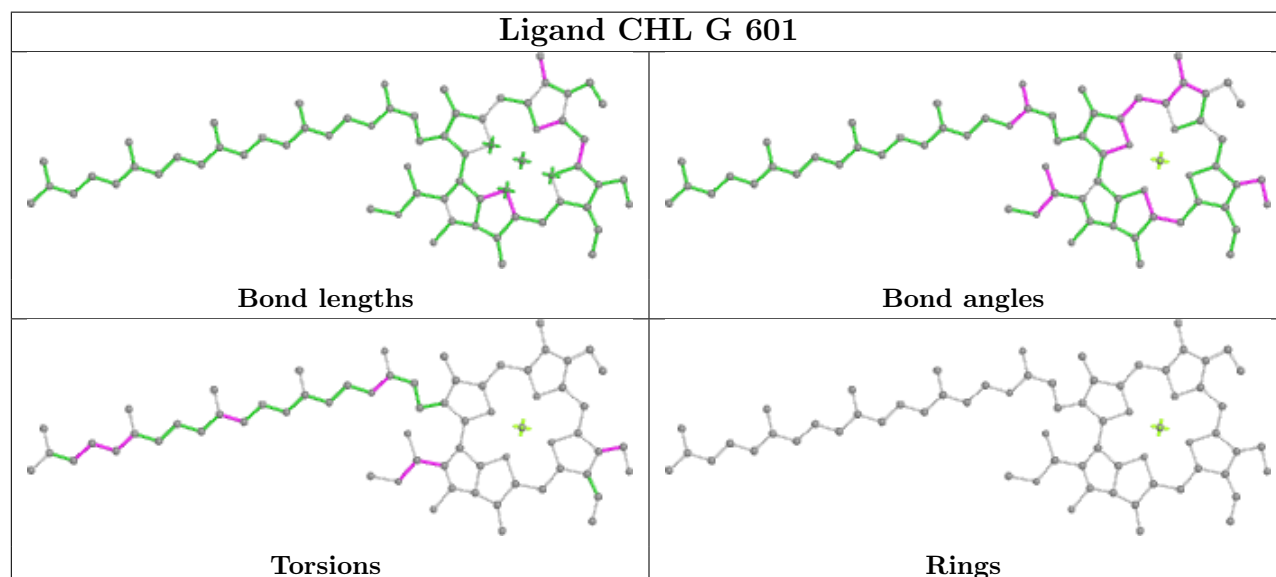
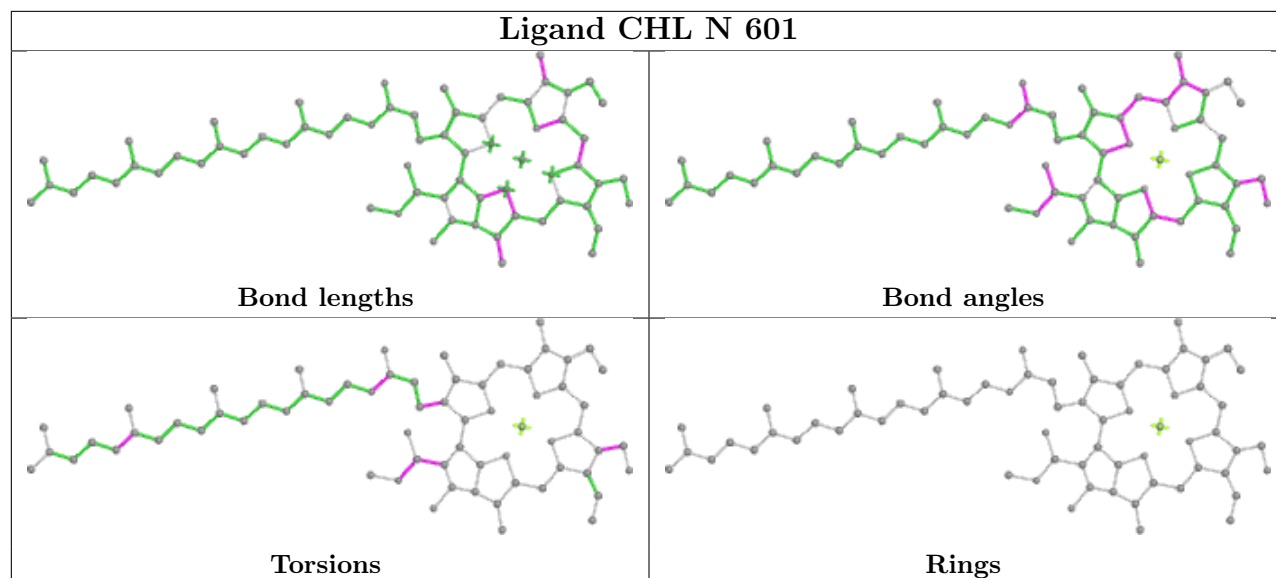
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

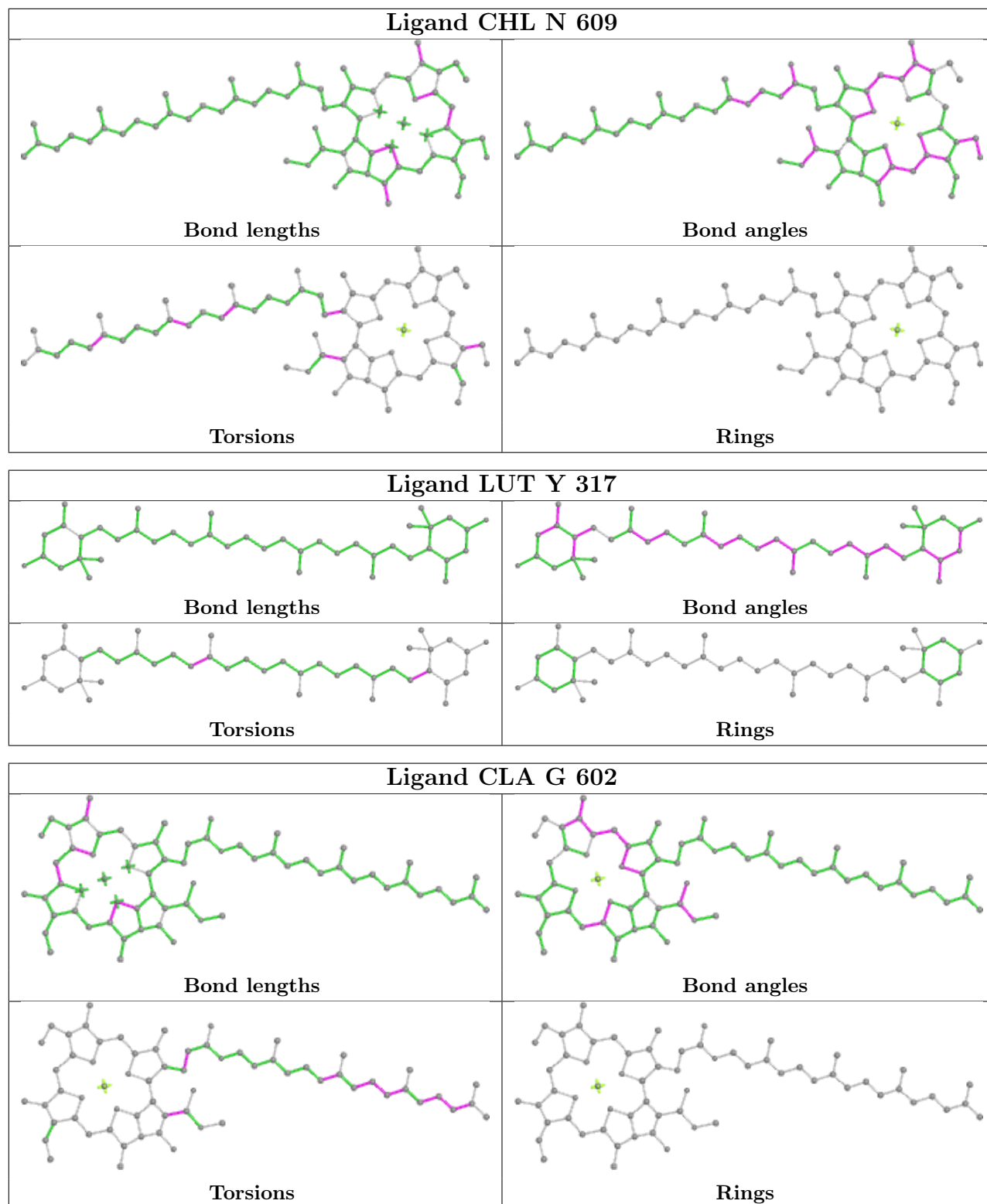
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

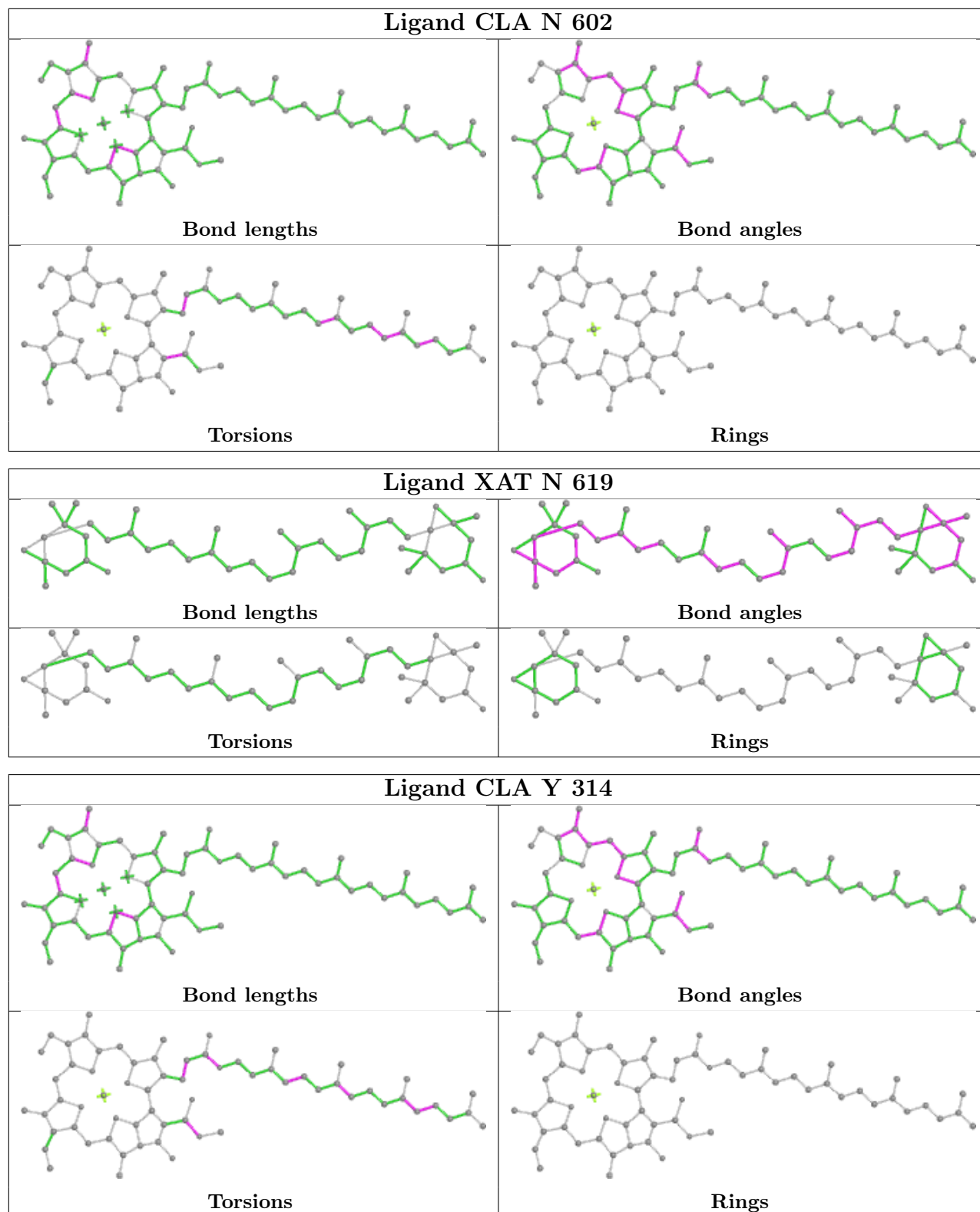


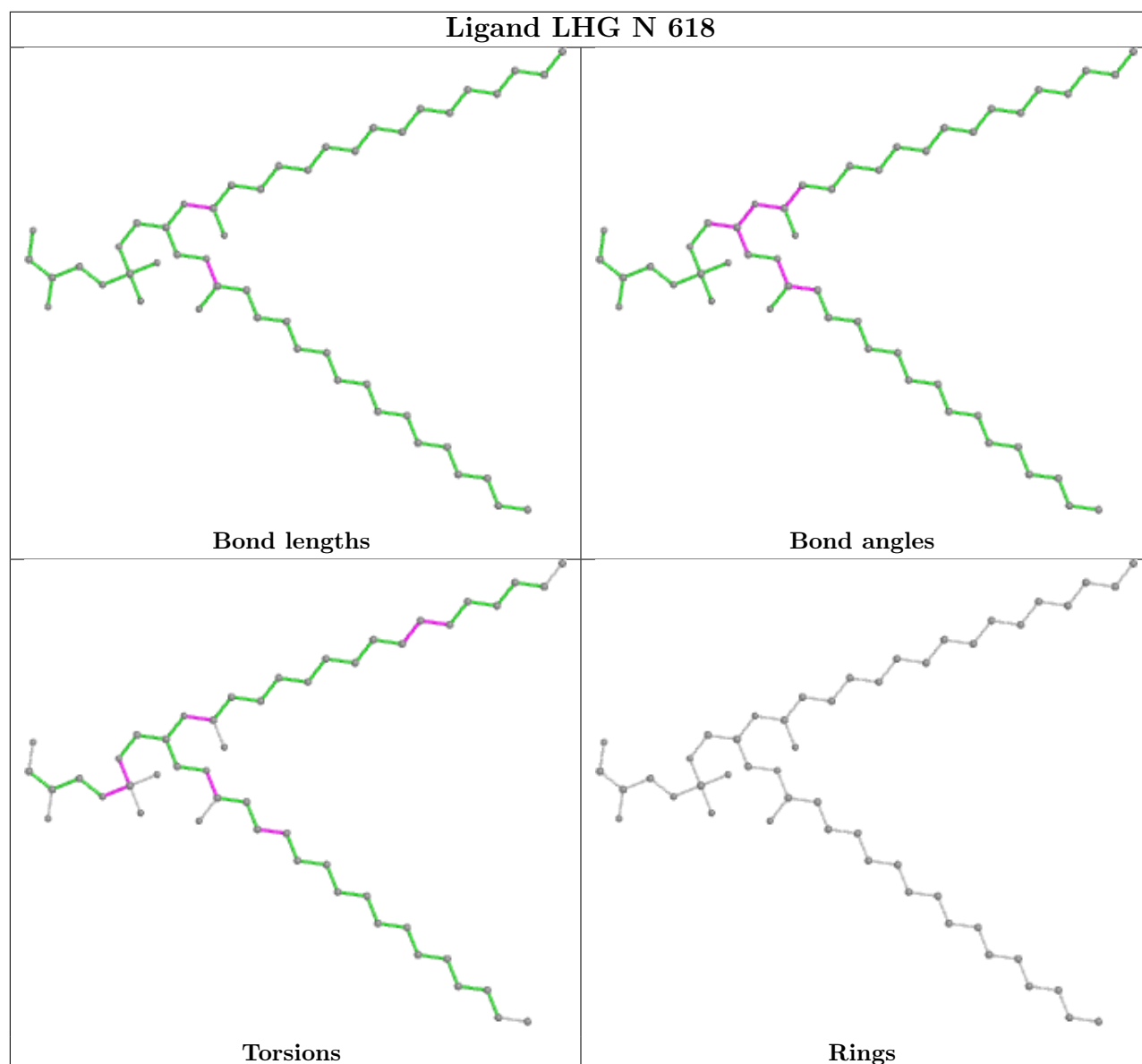
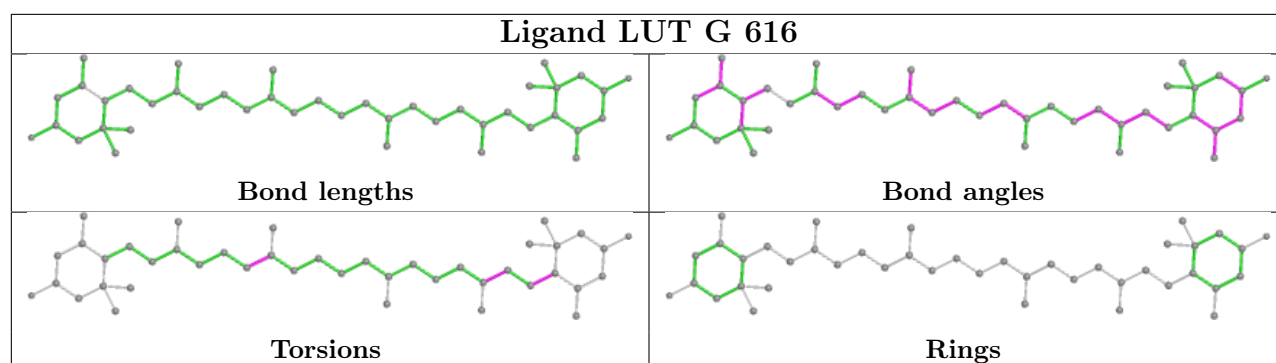


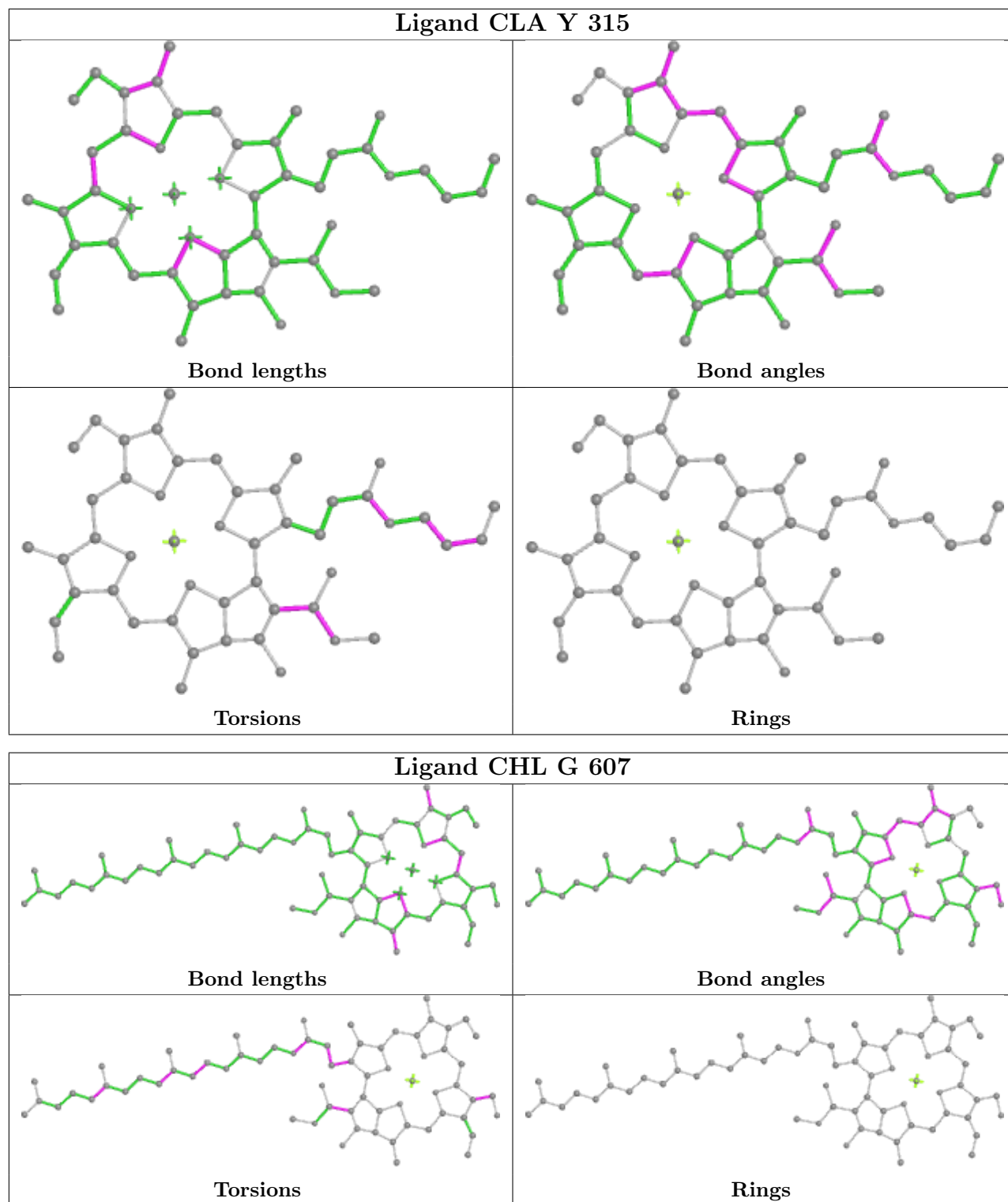


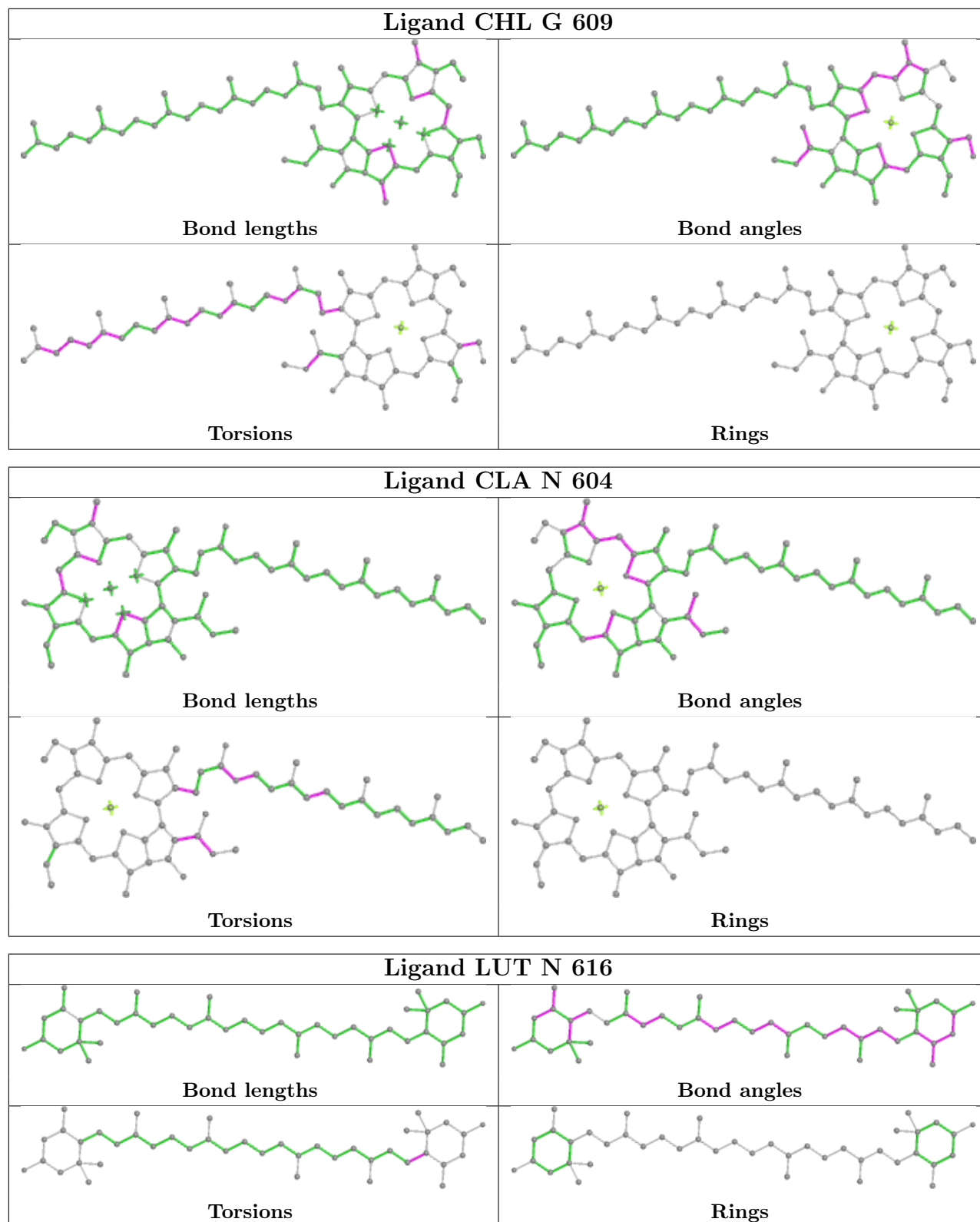


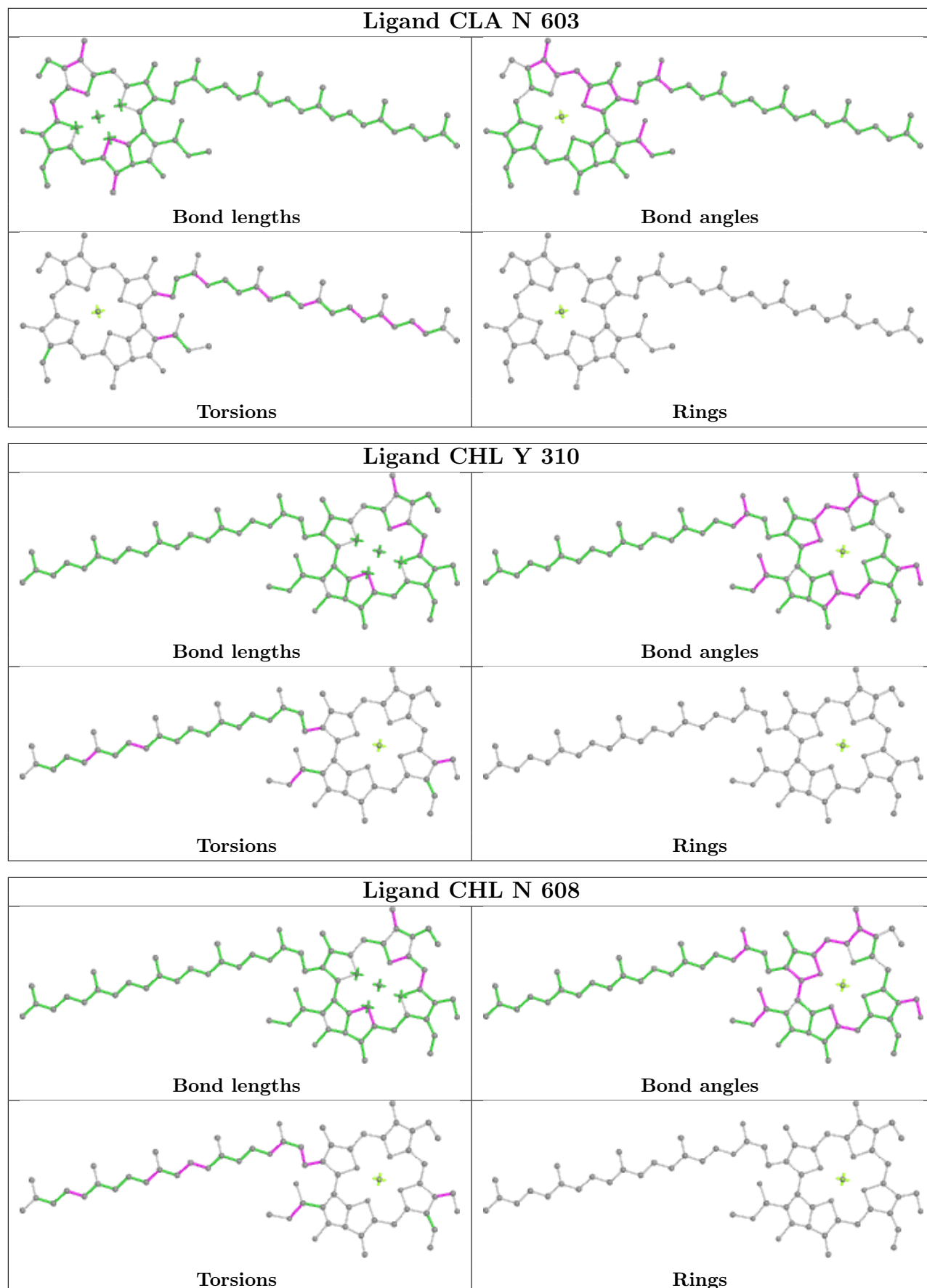


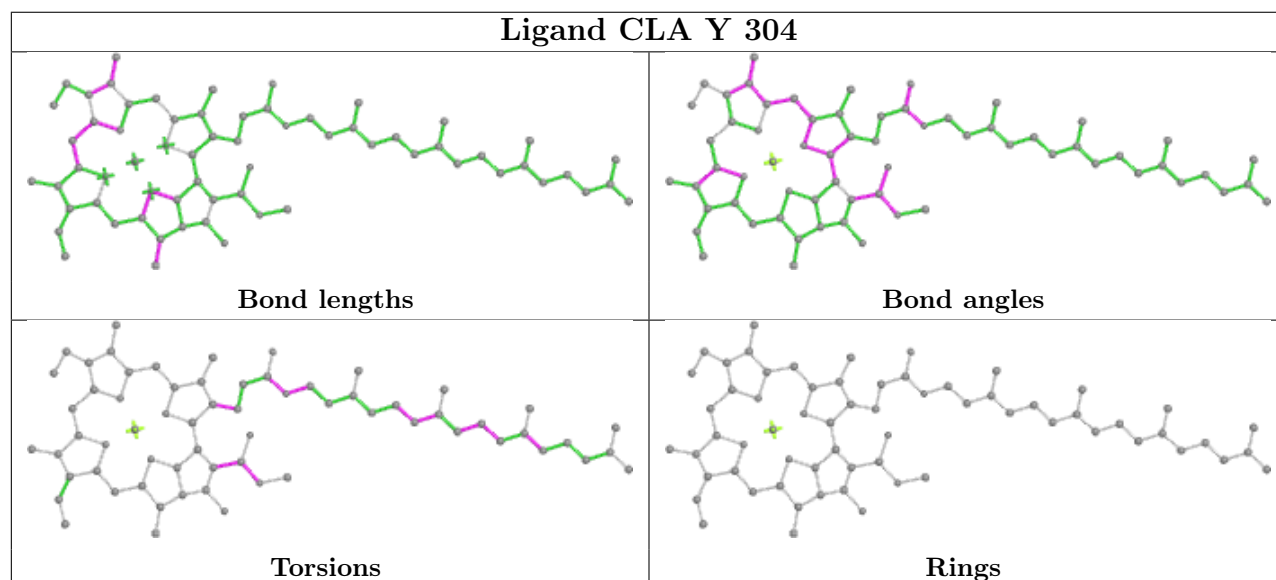
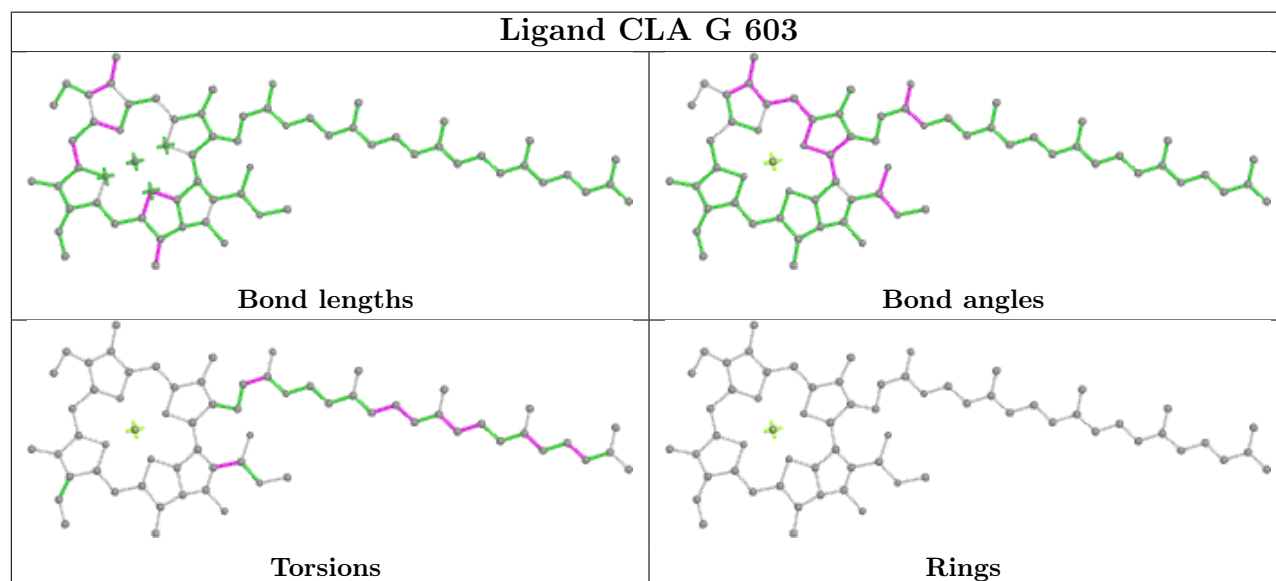
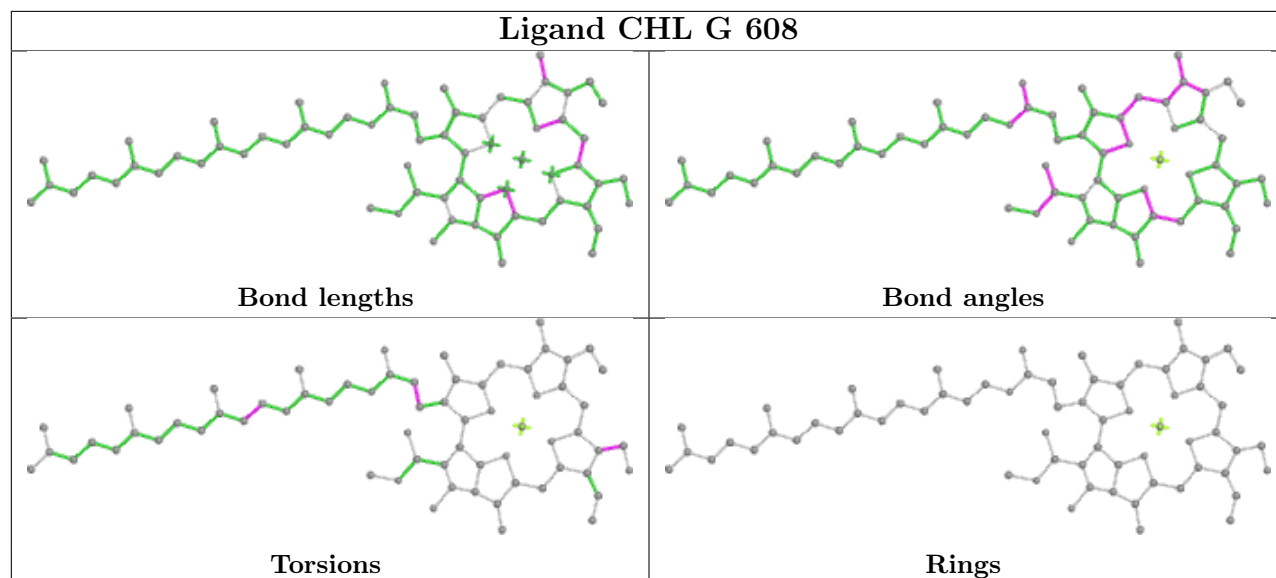


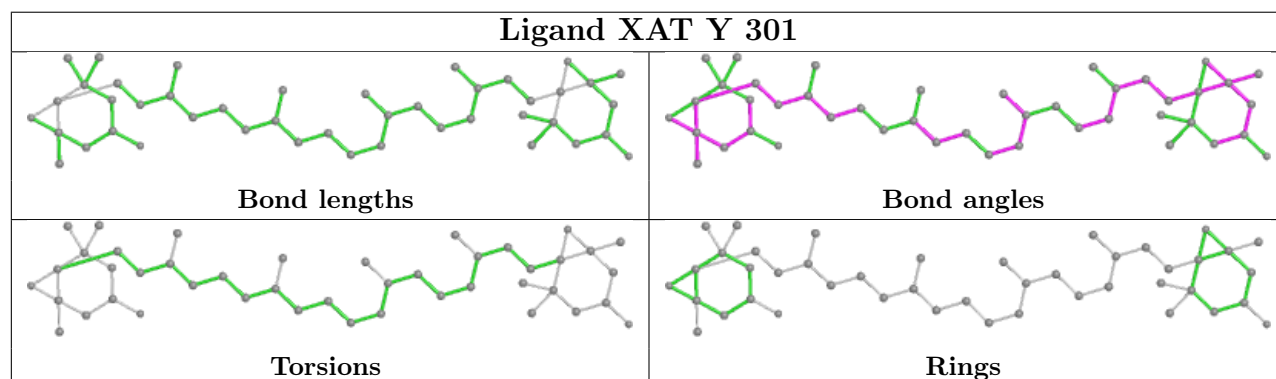
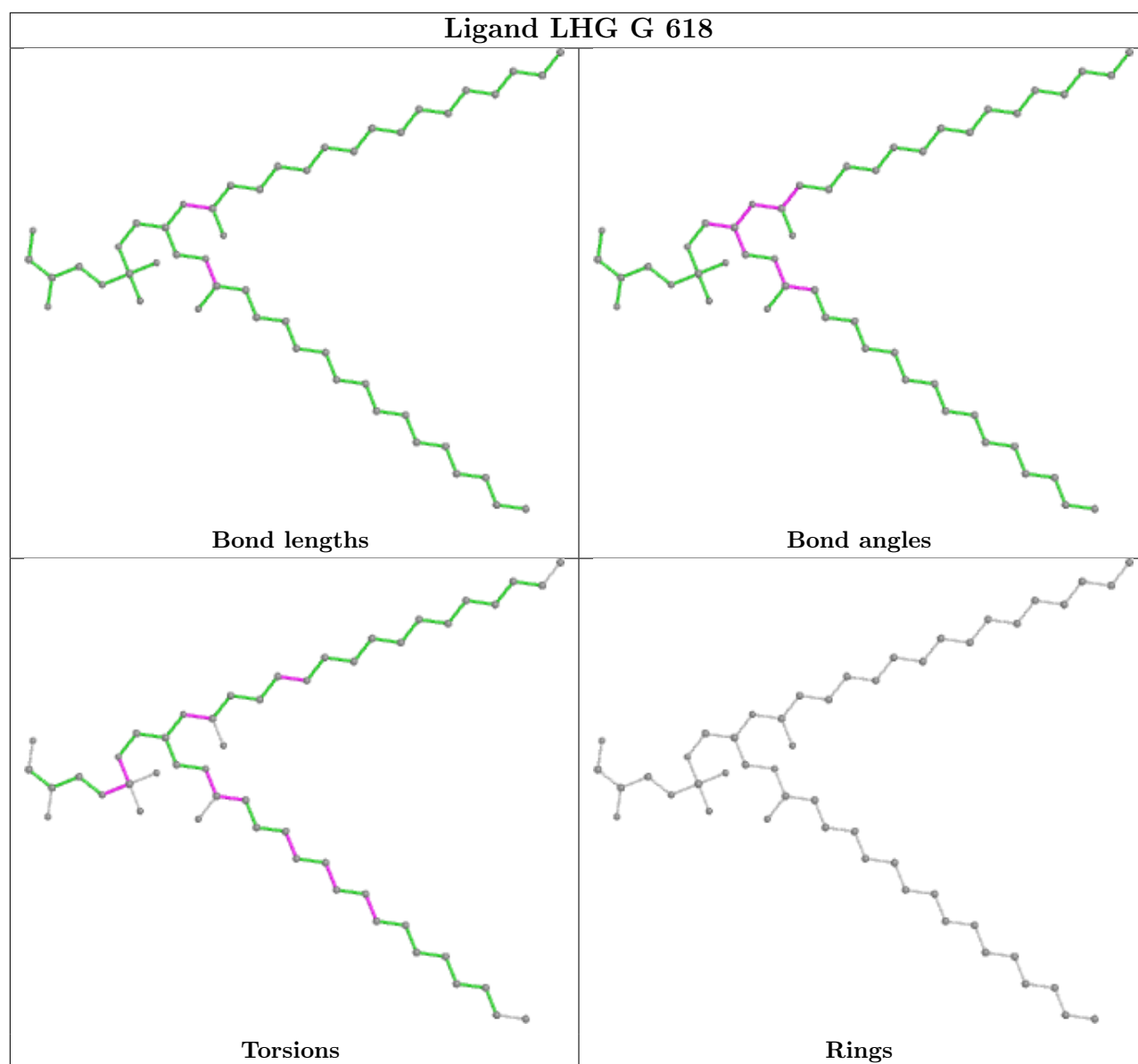


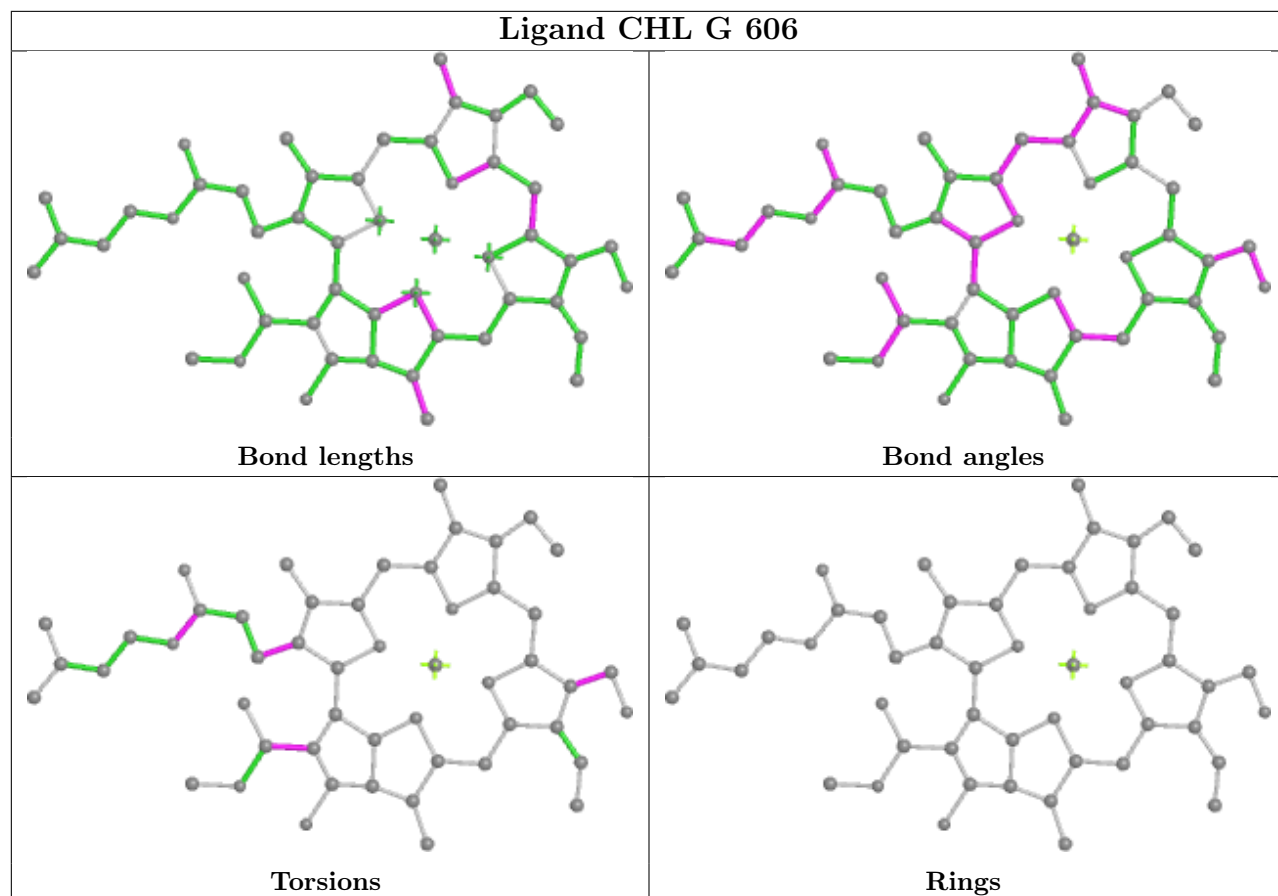


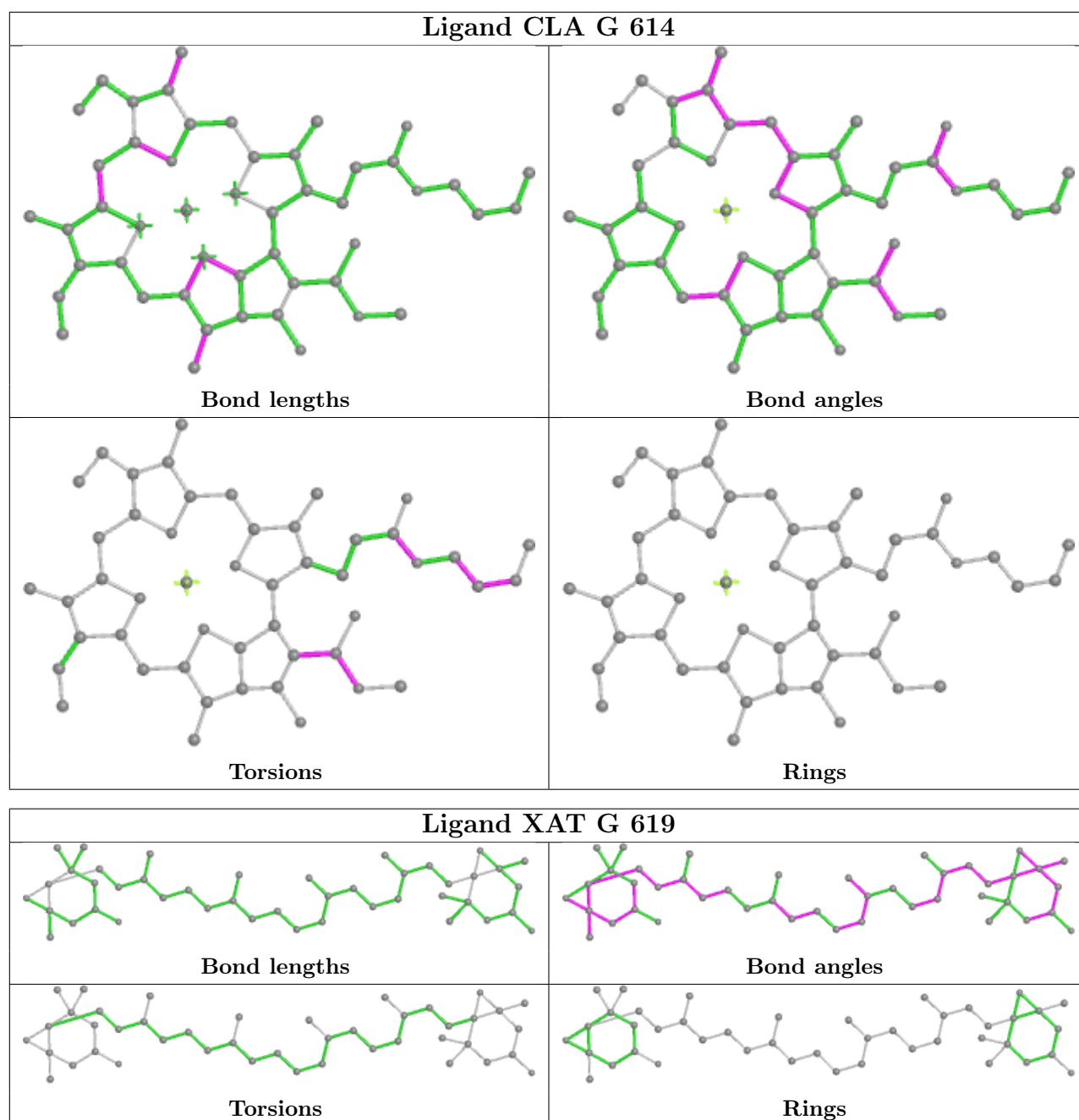


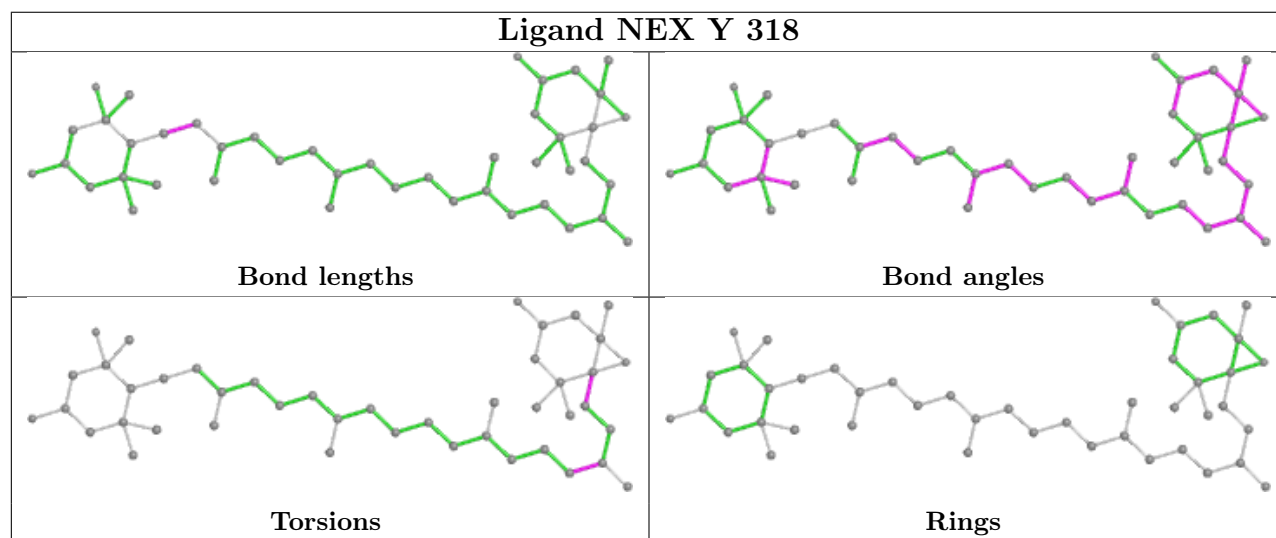
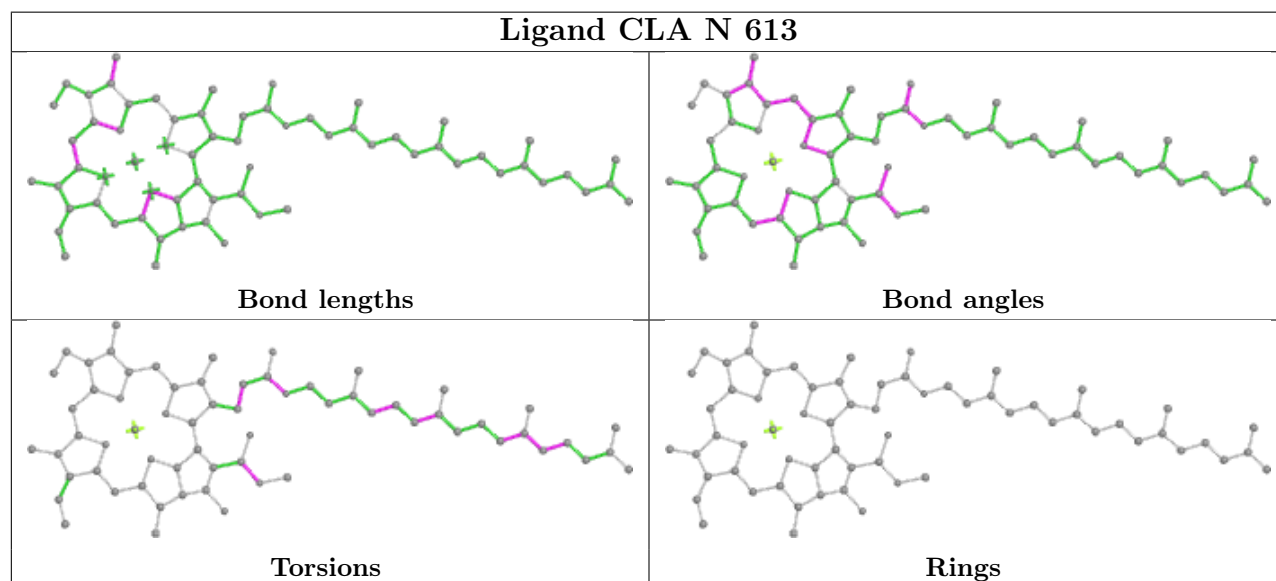
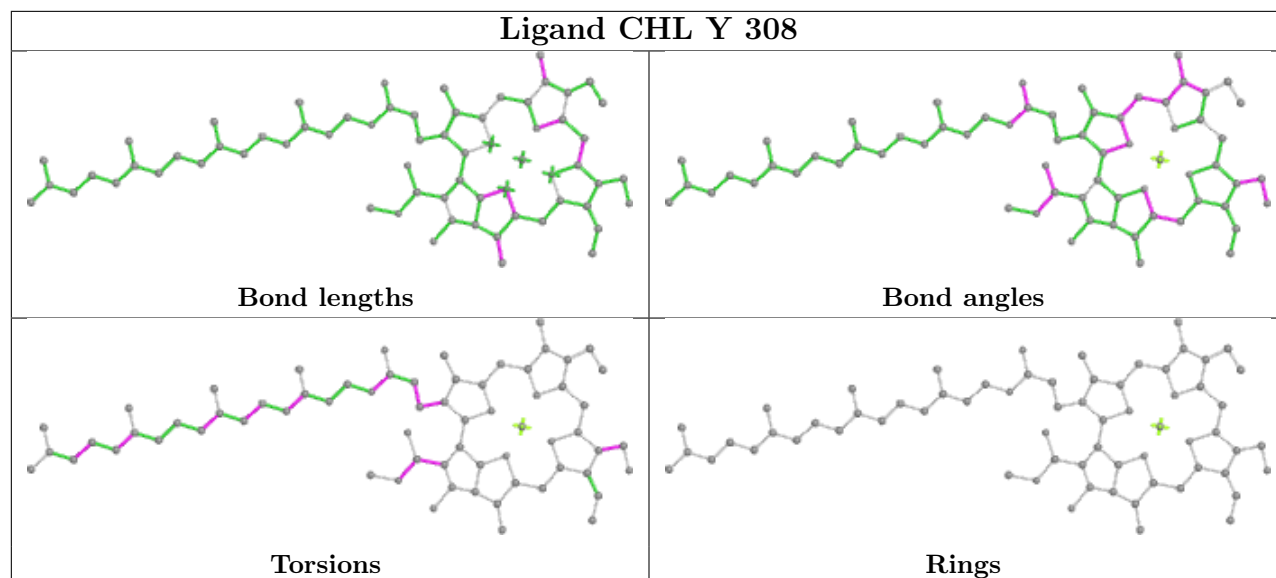


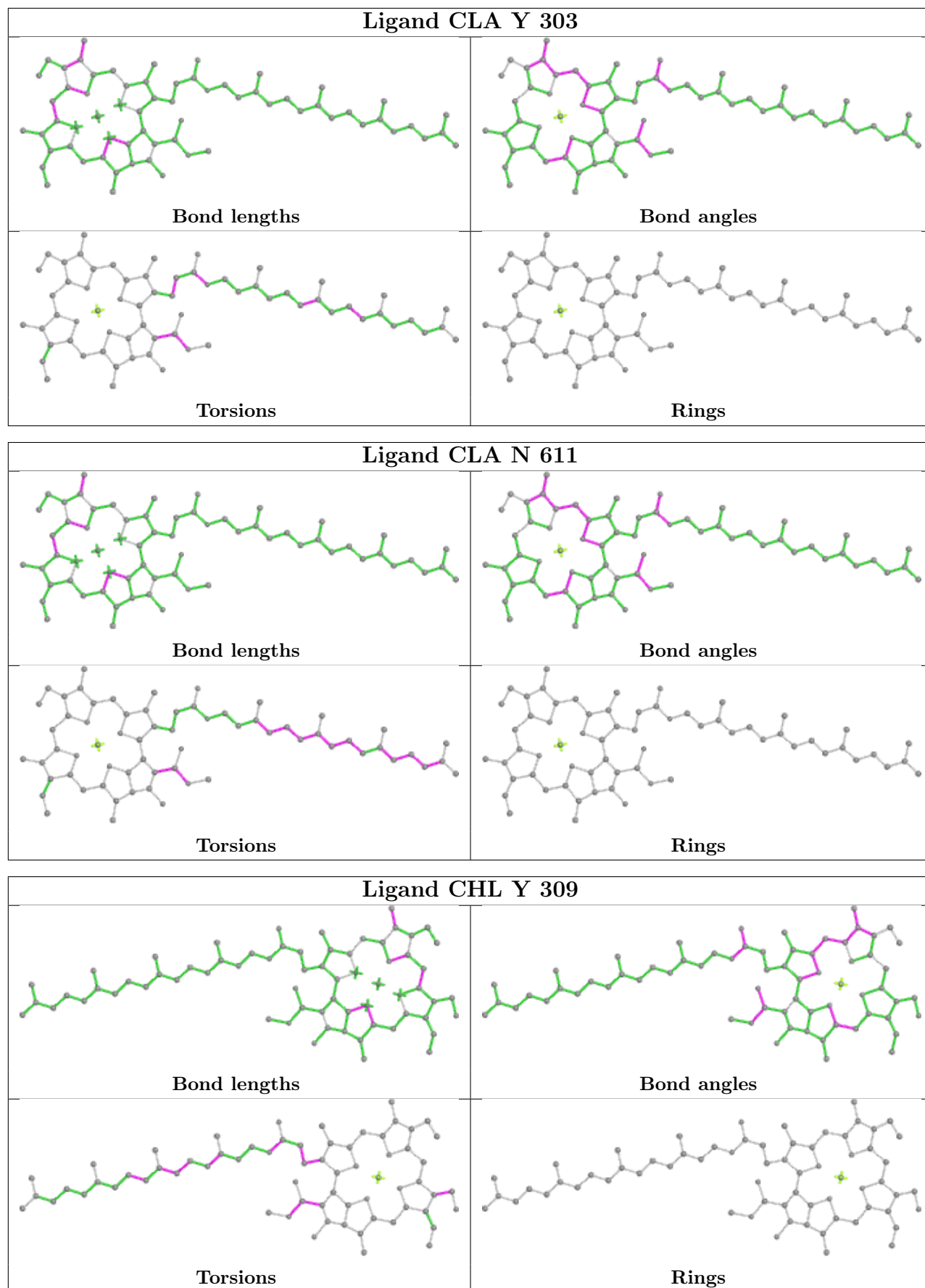


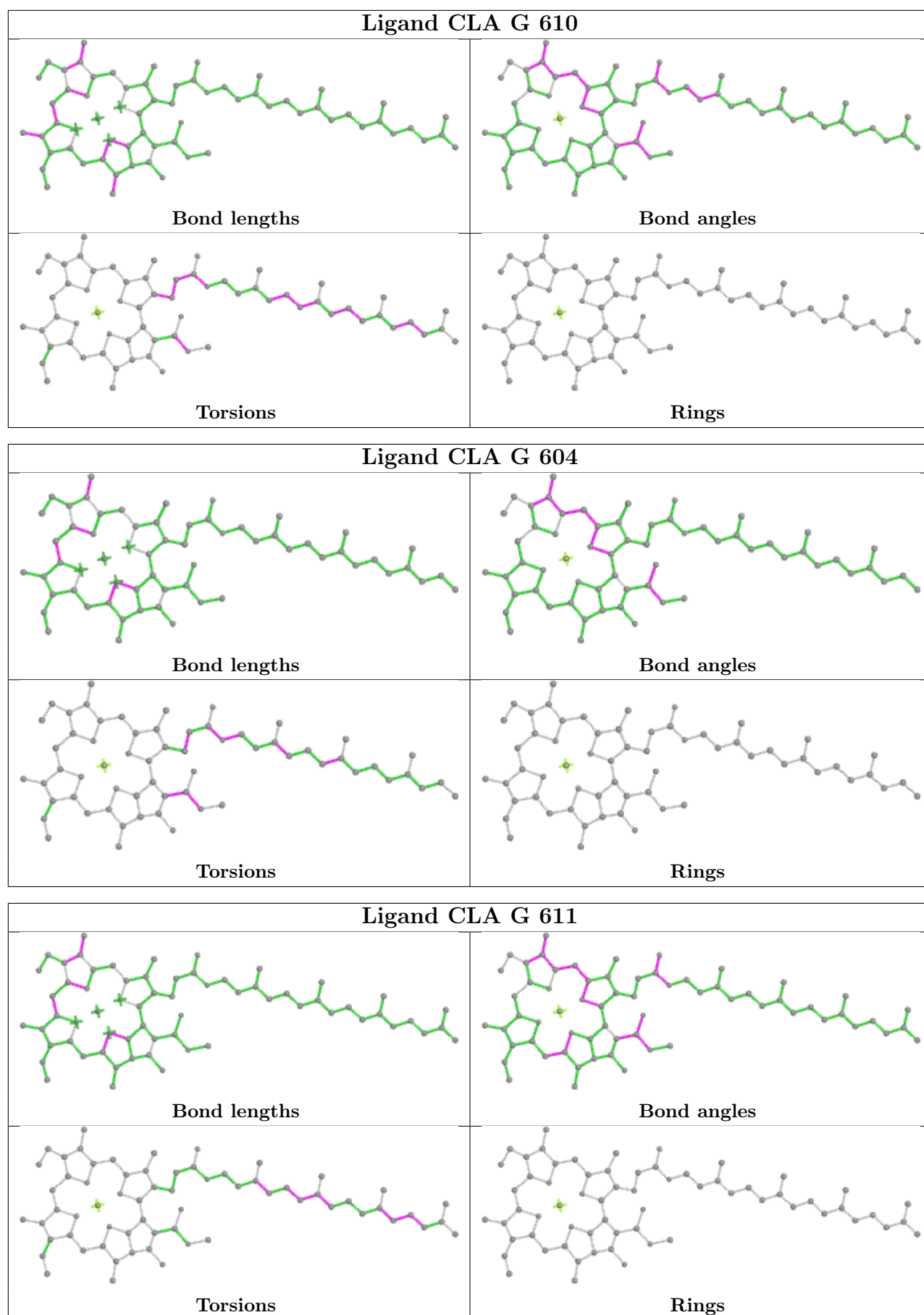


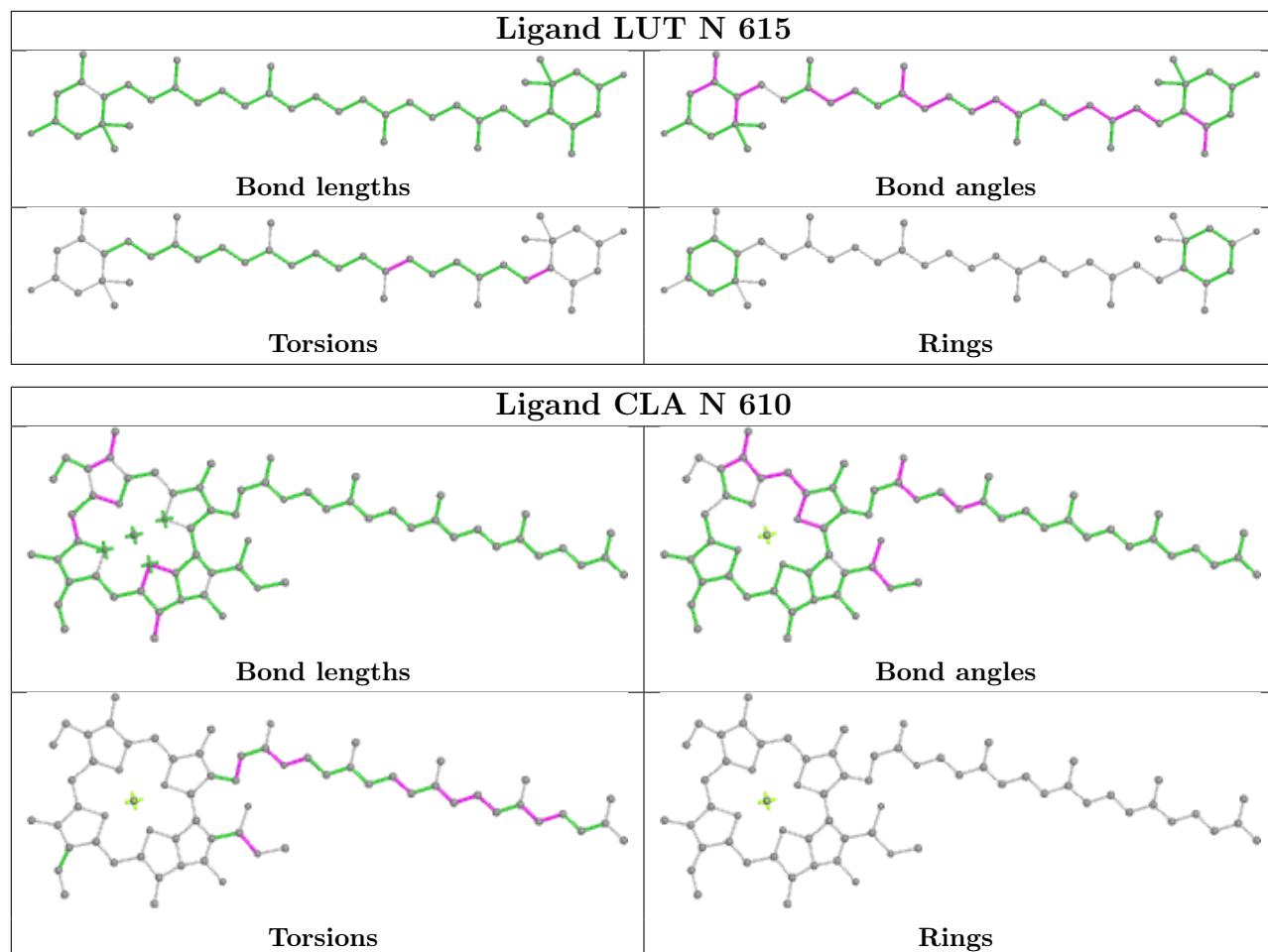


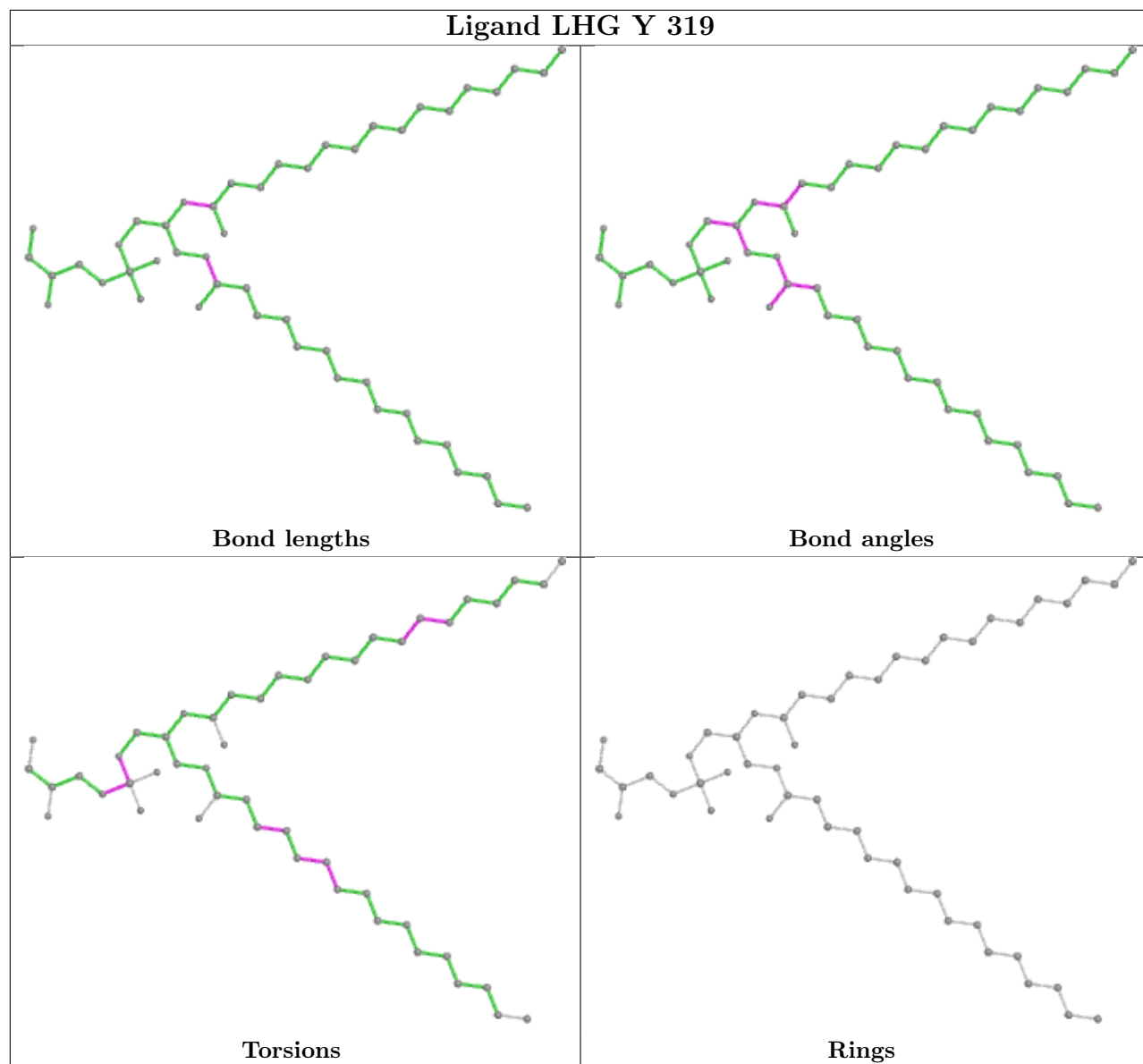


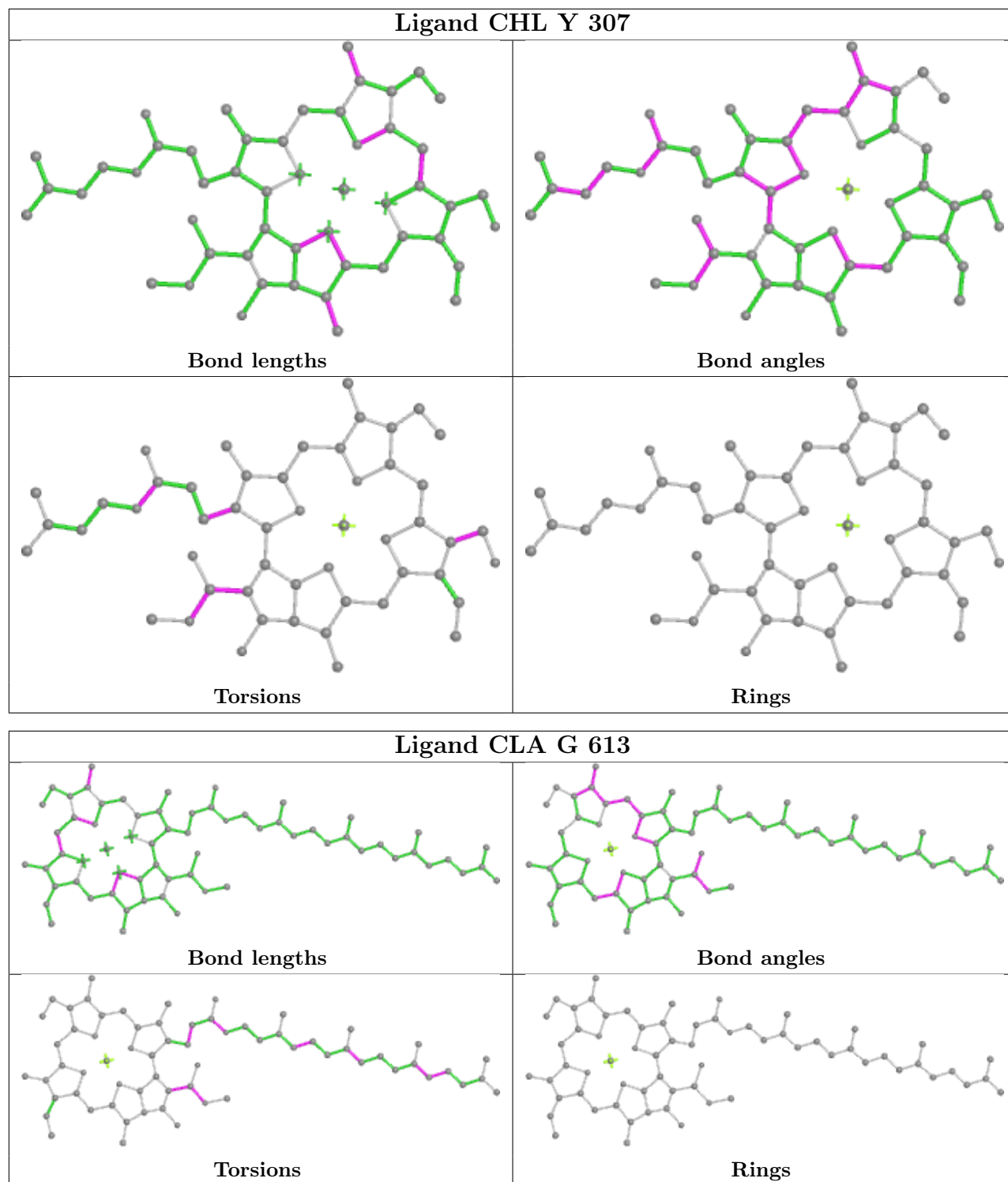


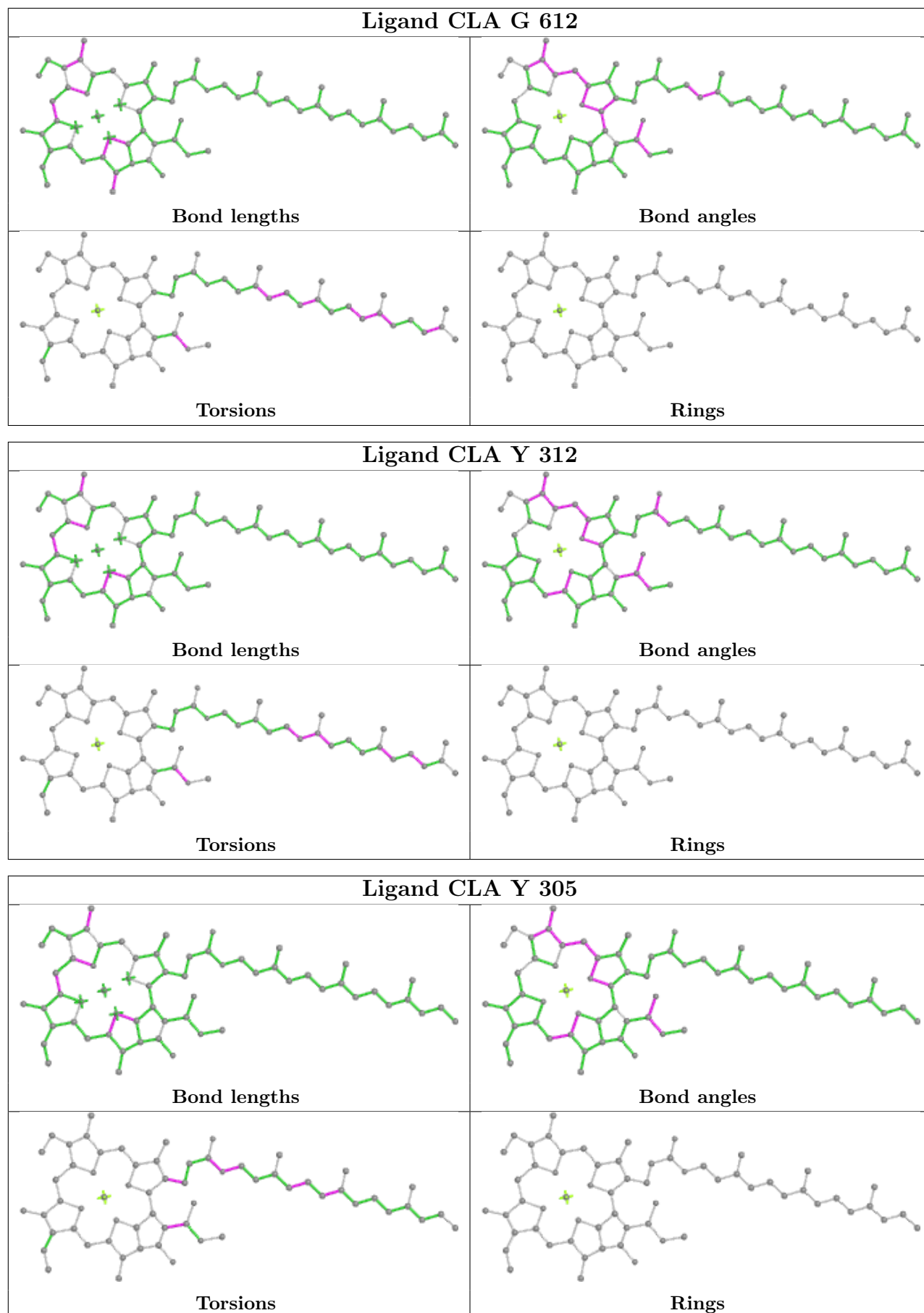


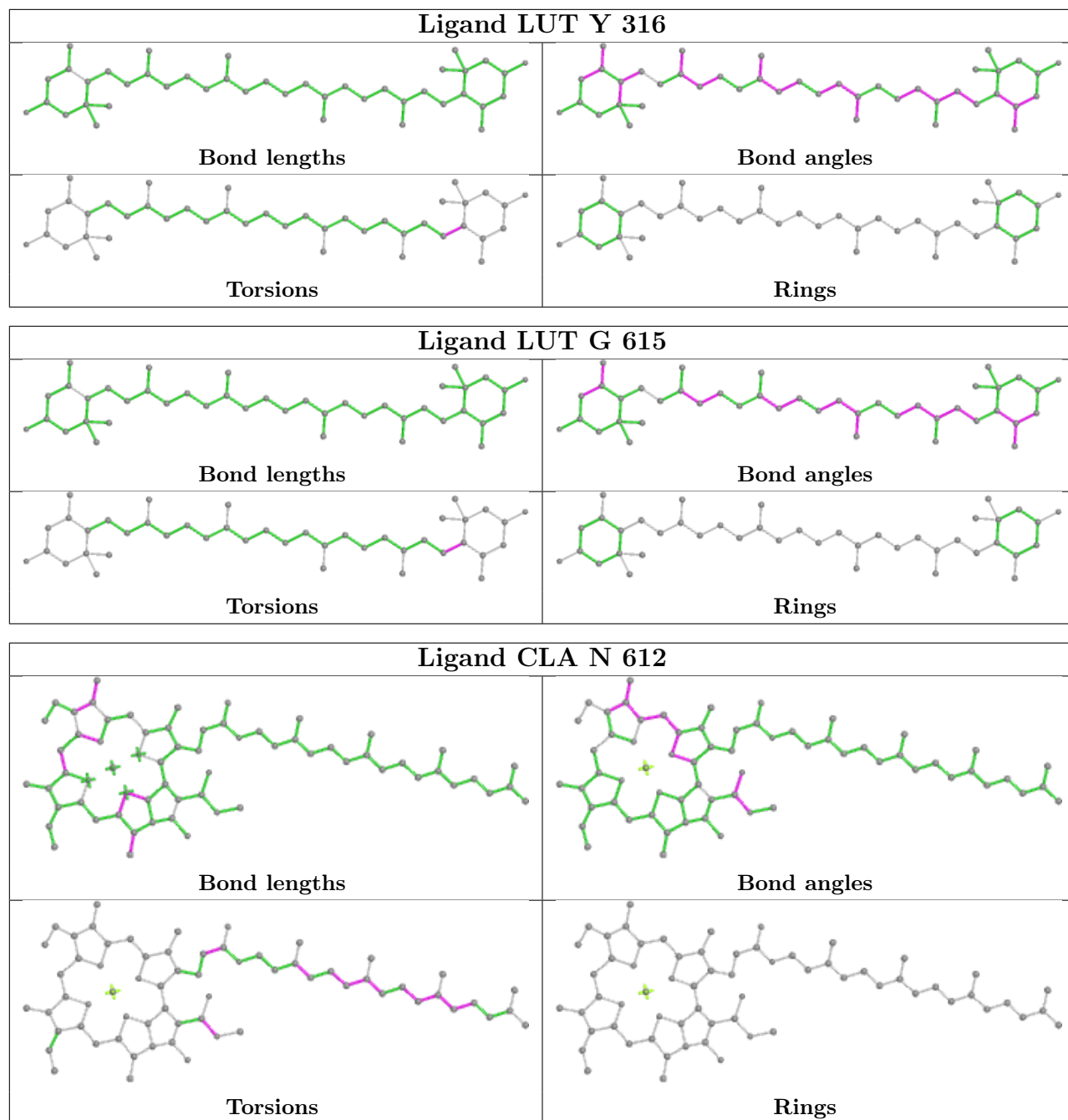


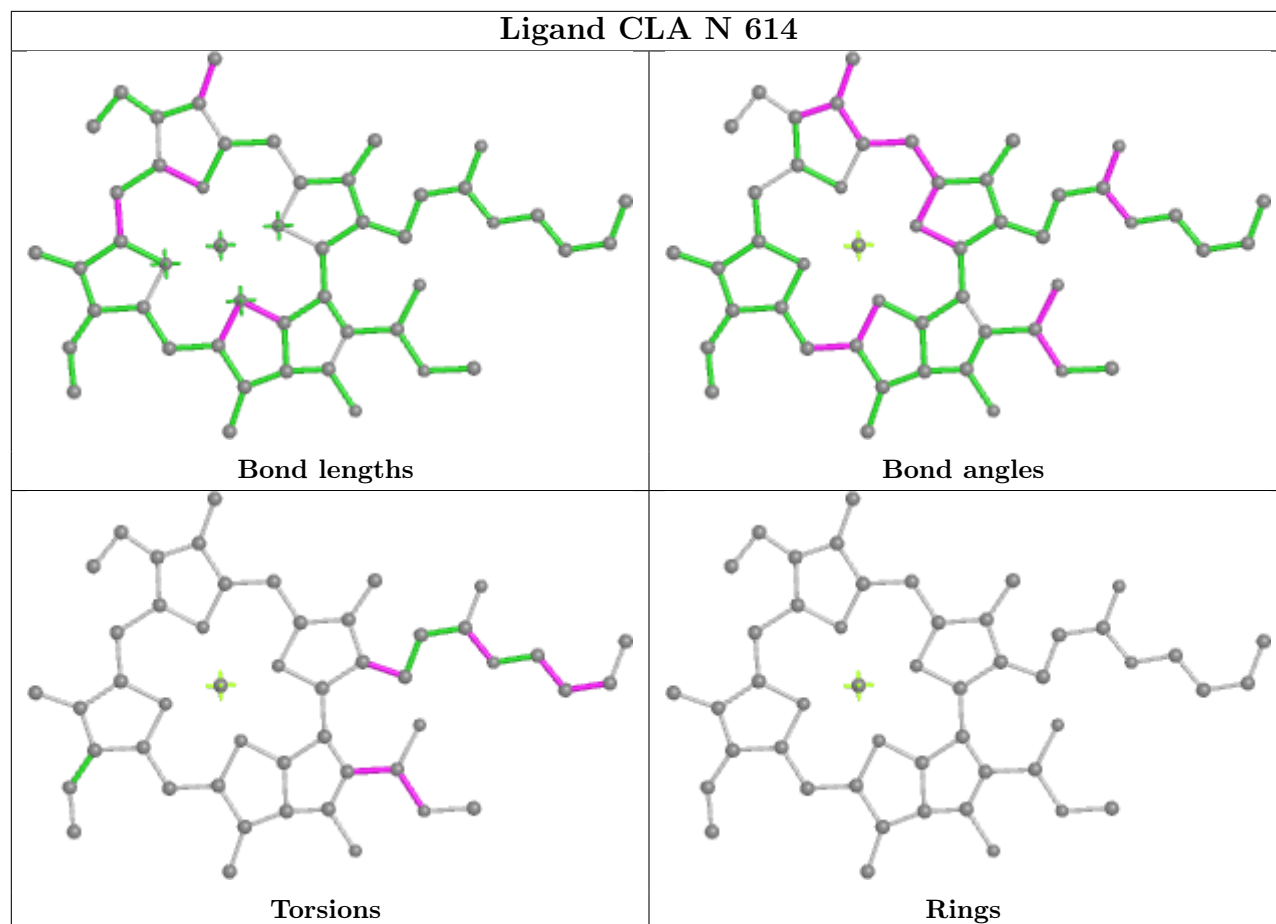


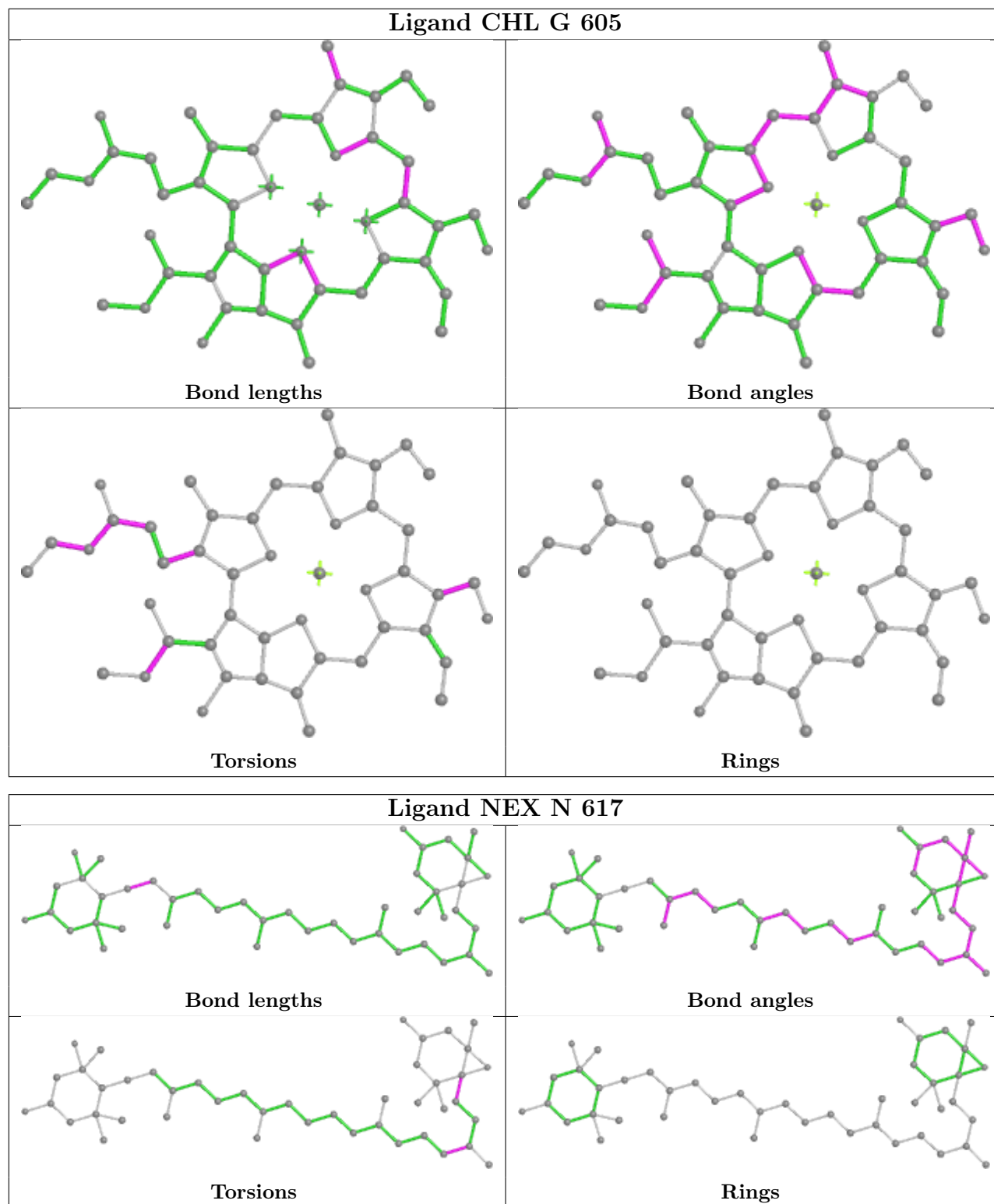


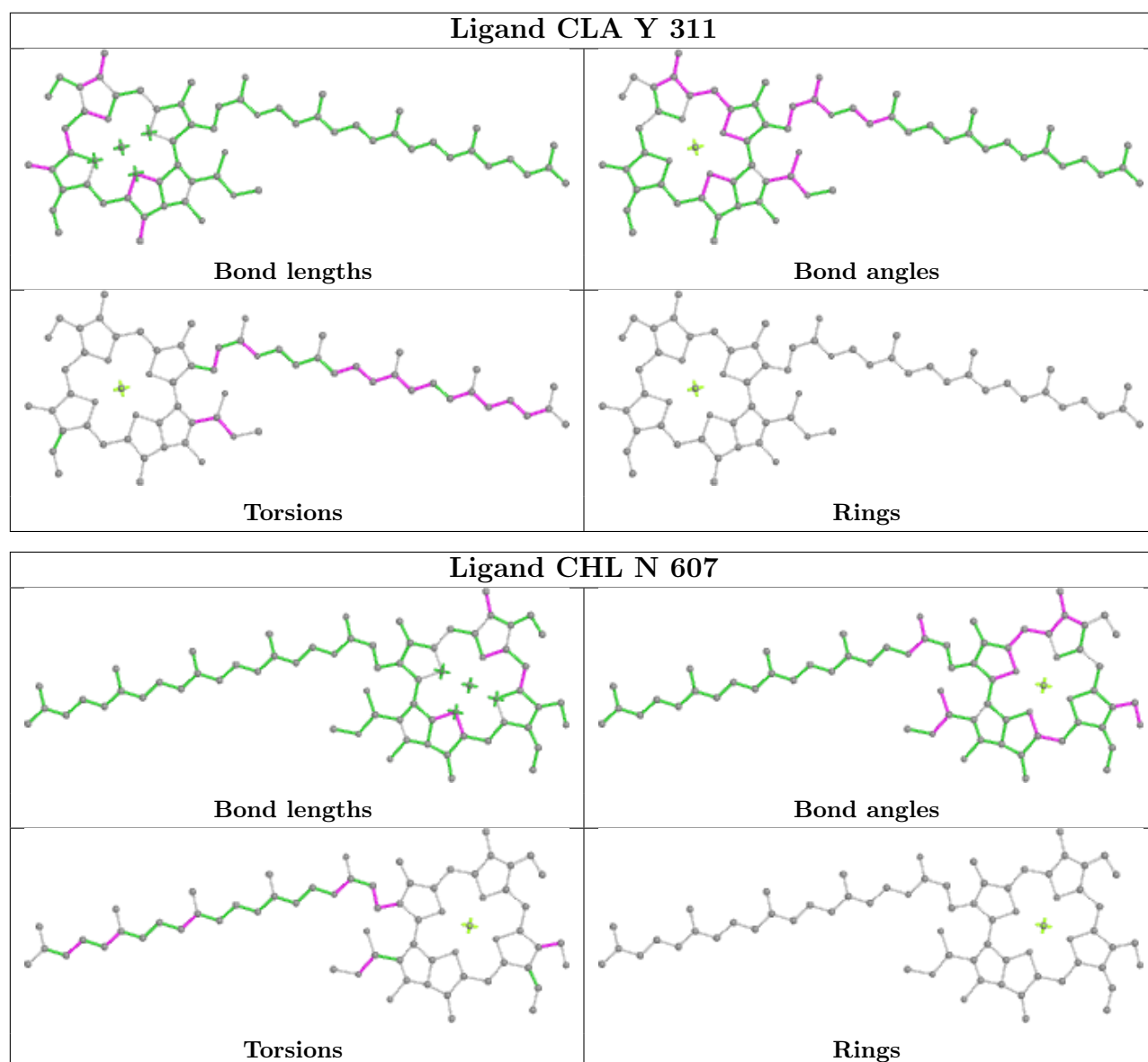












5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

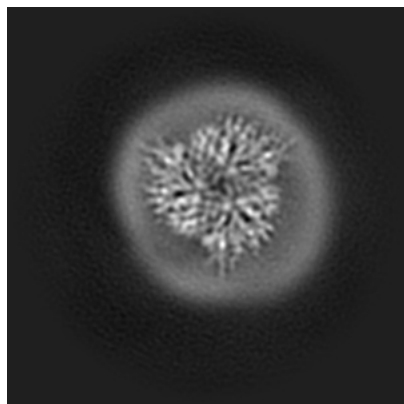
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35787. These allow visual inspection of the internal detail of the map and identification of artifacts.

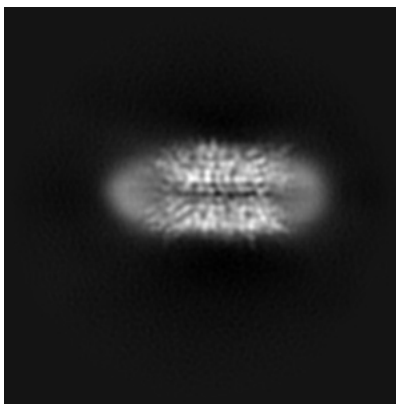
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

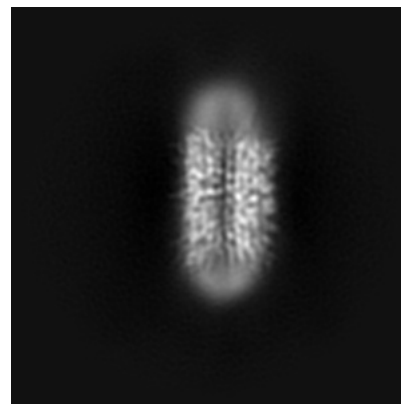
6.1.1 Primary map



X

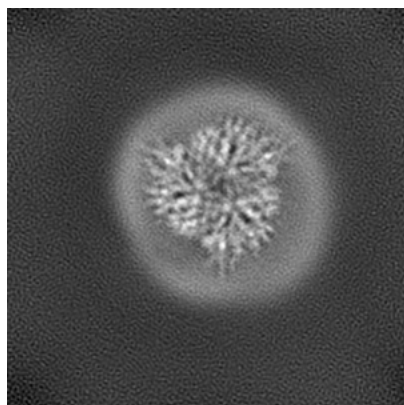


Y

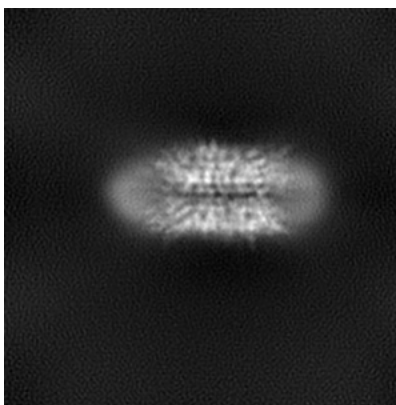


Z

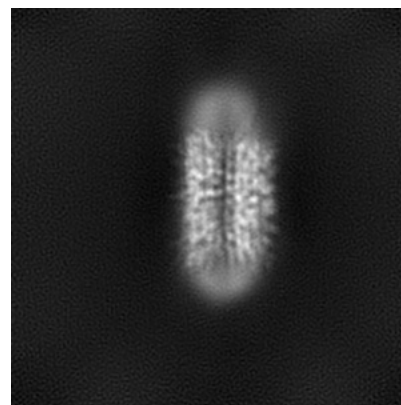
6.1.2 Raw map



X



Y

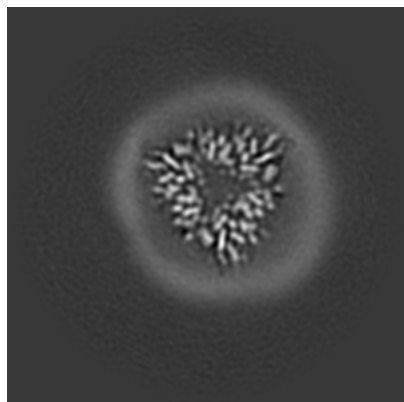


Z

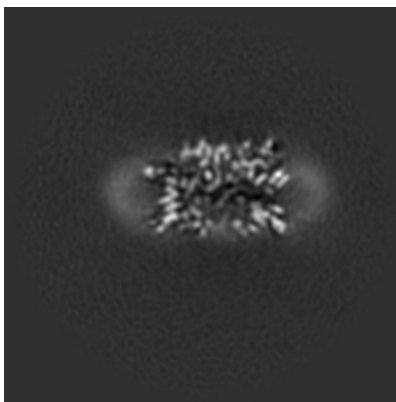
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

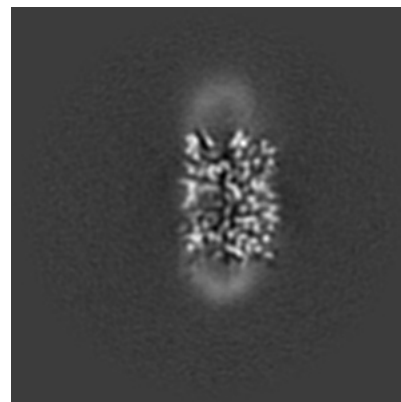
6.2.1 Primary map



X Index: 100

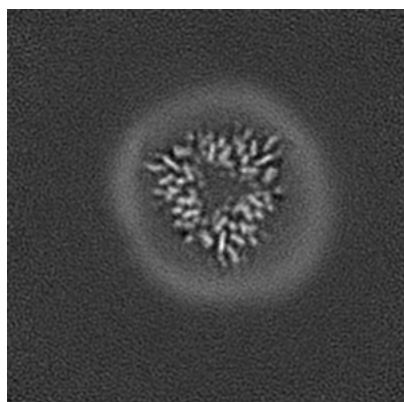


Y Index: 100

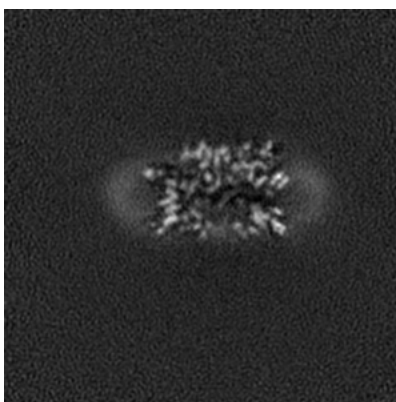


Z Index: 100

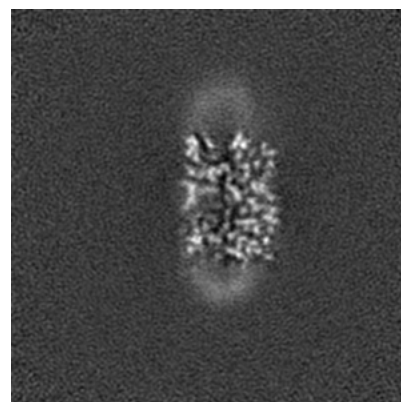
6.2.2 Raw map



X Index: 100



Y Index: 100

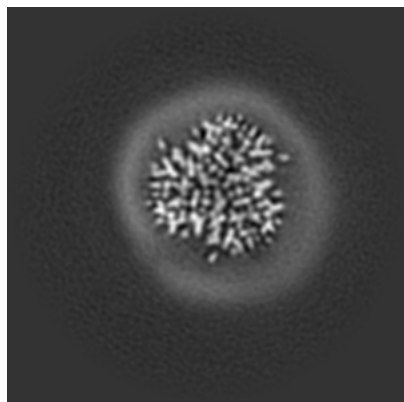


Z Index: 100

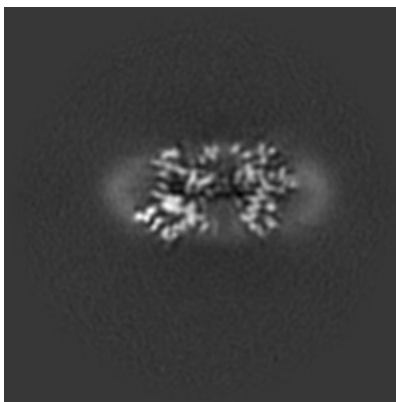
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

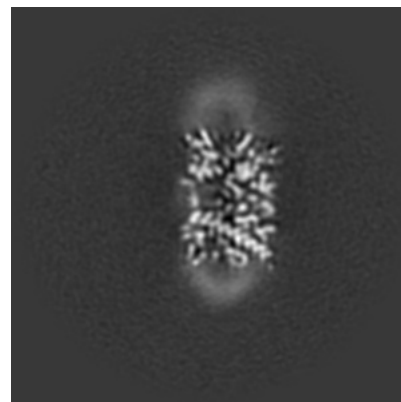
6.3.1 Primary map



X Index: 114

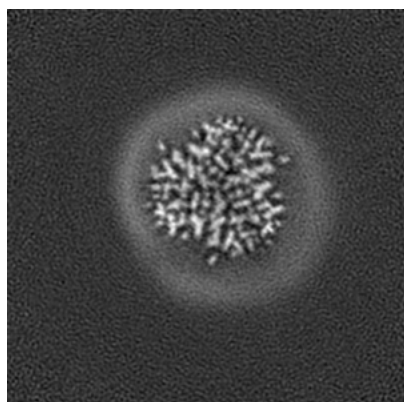


Y Index: 107

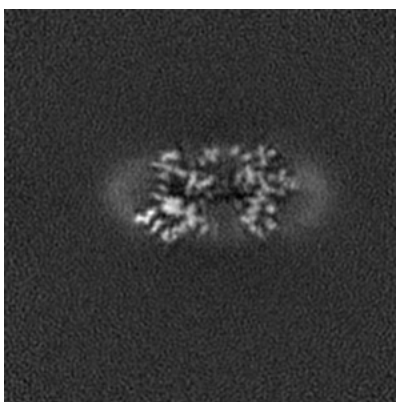


Z Index: 102

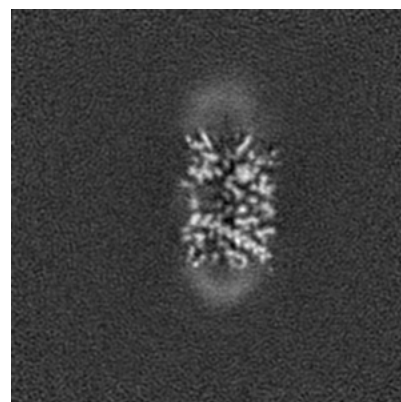
6.3.2 Raw map



X Index: 114



Y Index: 107

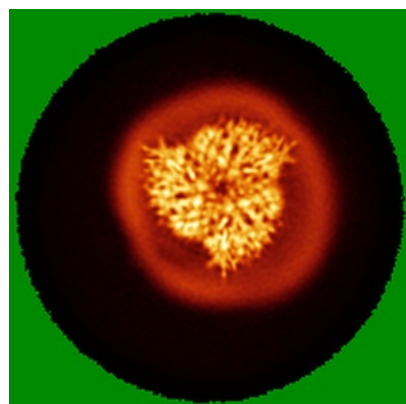


Z Index: 102

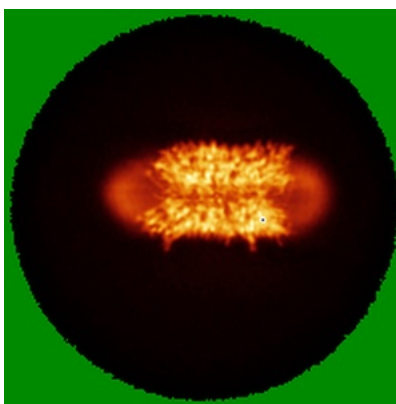
The images above show the largest variance slices of the map in three orthogonal directions.

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

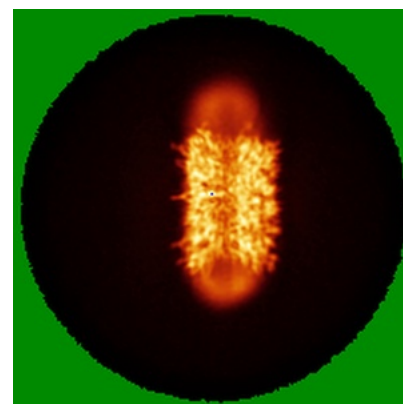
6.4.1 Primary map



X

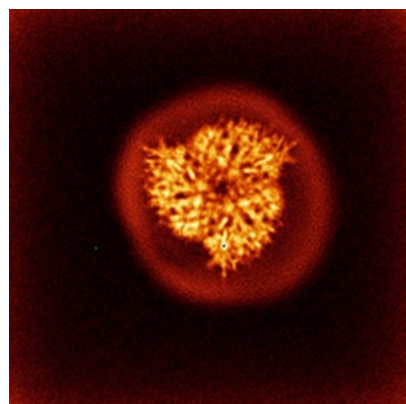


Y

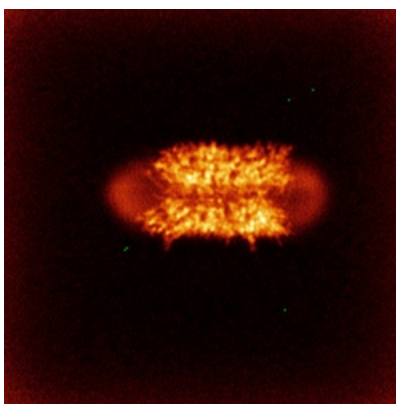


Z

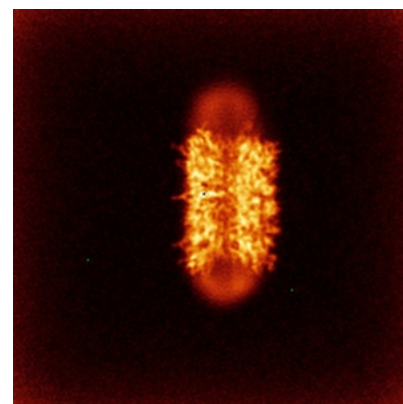
6.4.2 Raw map



X



Y

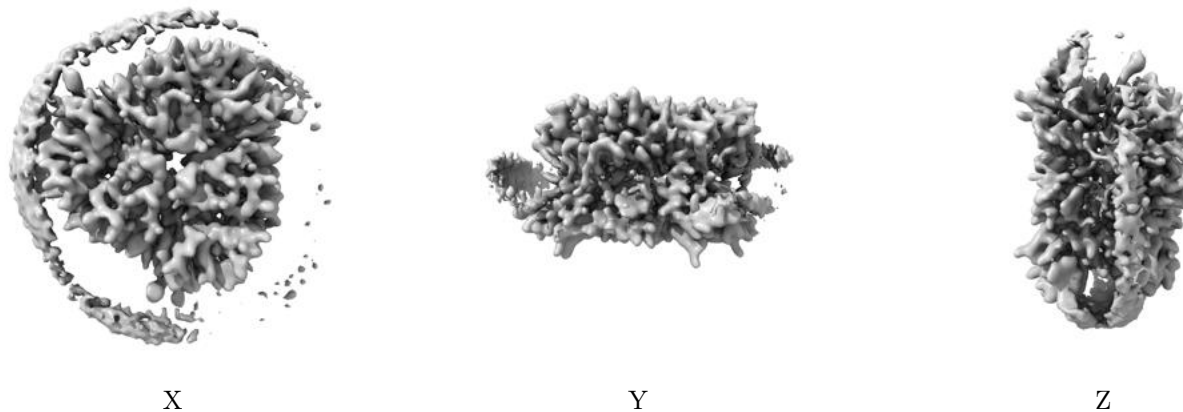


Z

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

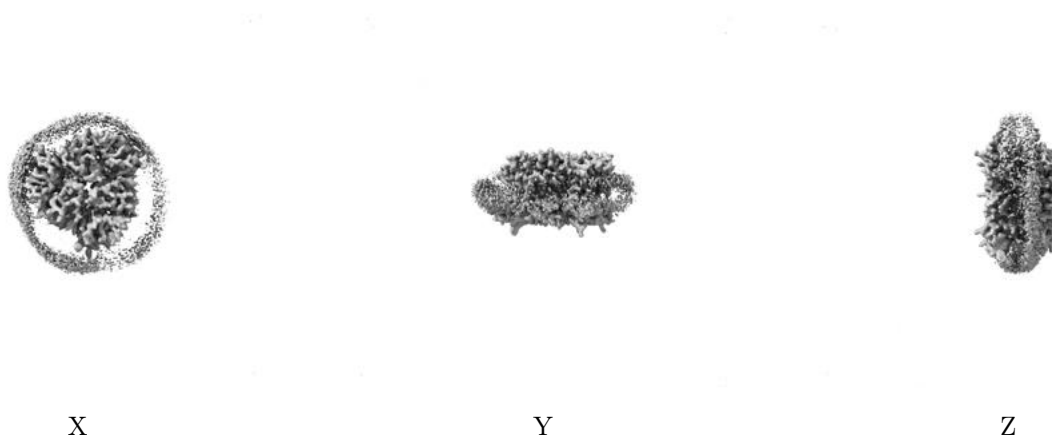
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

6.5.2 Raw map



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.

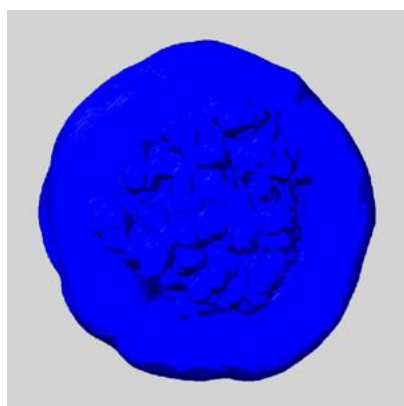
6.6 Mask visualisation [i](#)

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

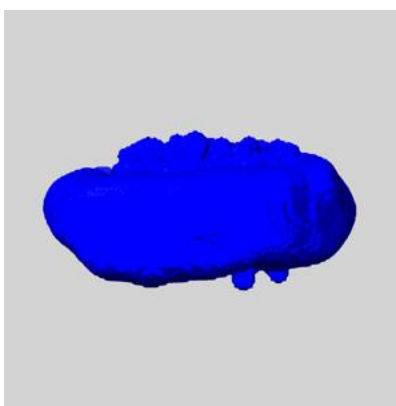
A mask typically either:

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

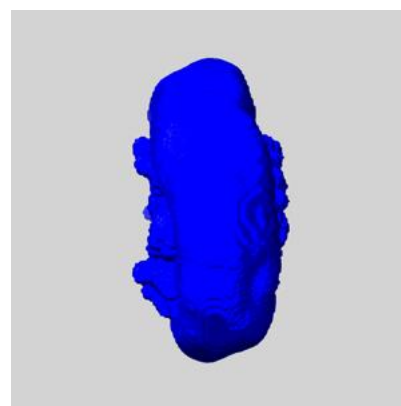
6.6.1 emd_35787_msk_1.map [i](#)



X



Y

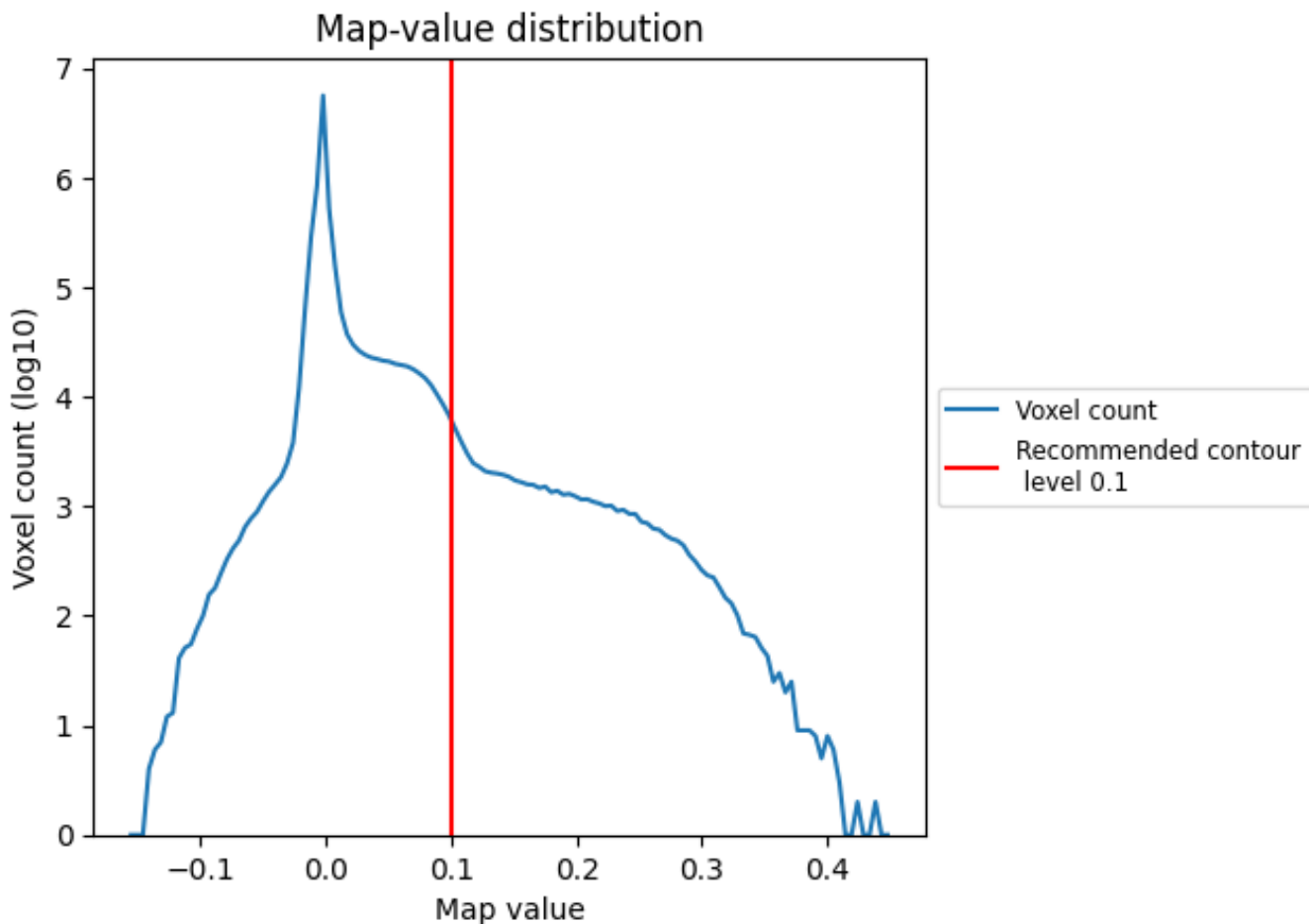


Z

7 Map analysis [i](#)

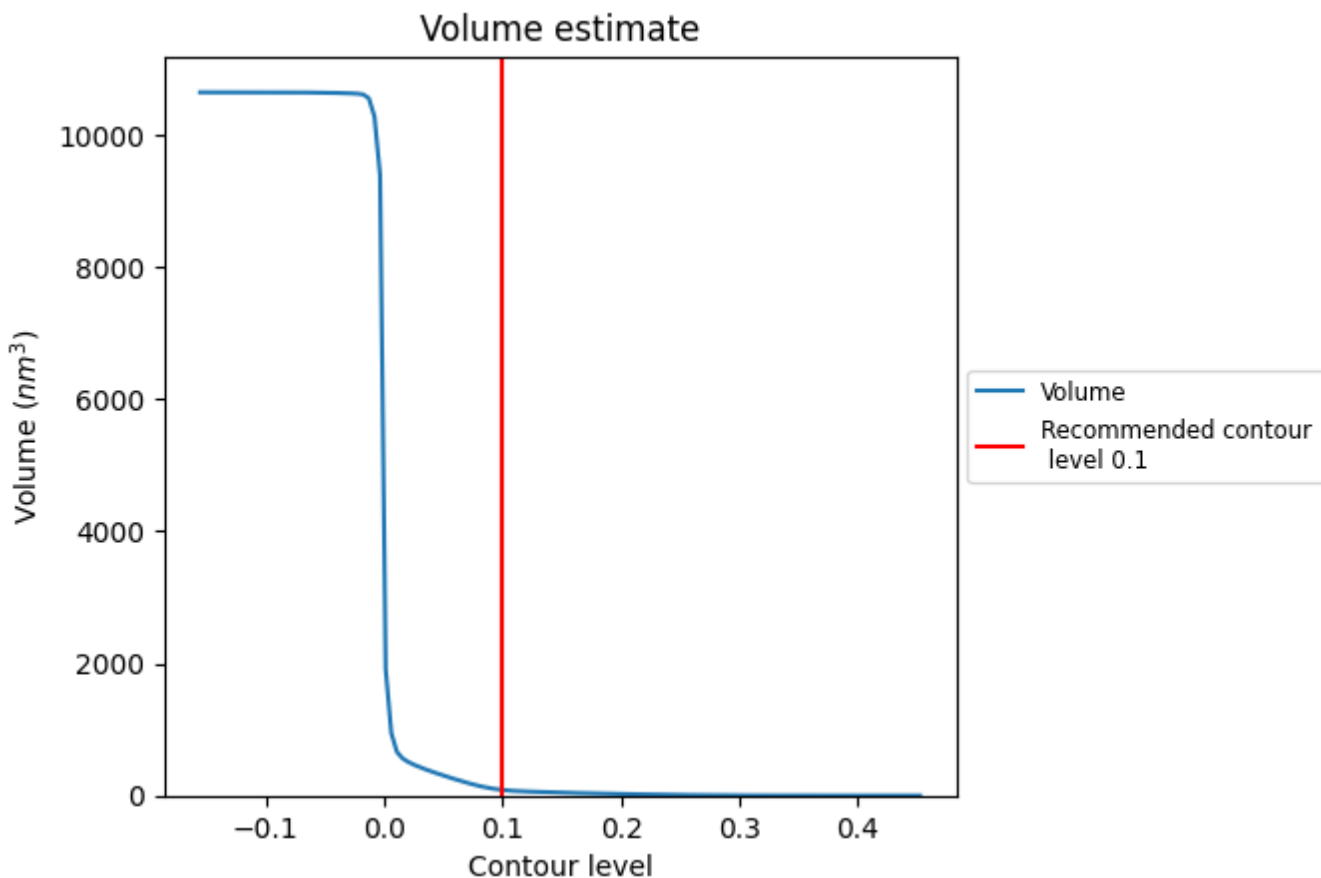
This section contains the results of statistical analysis of the map.

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.

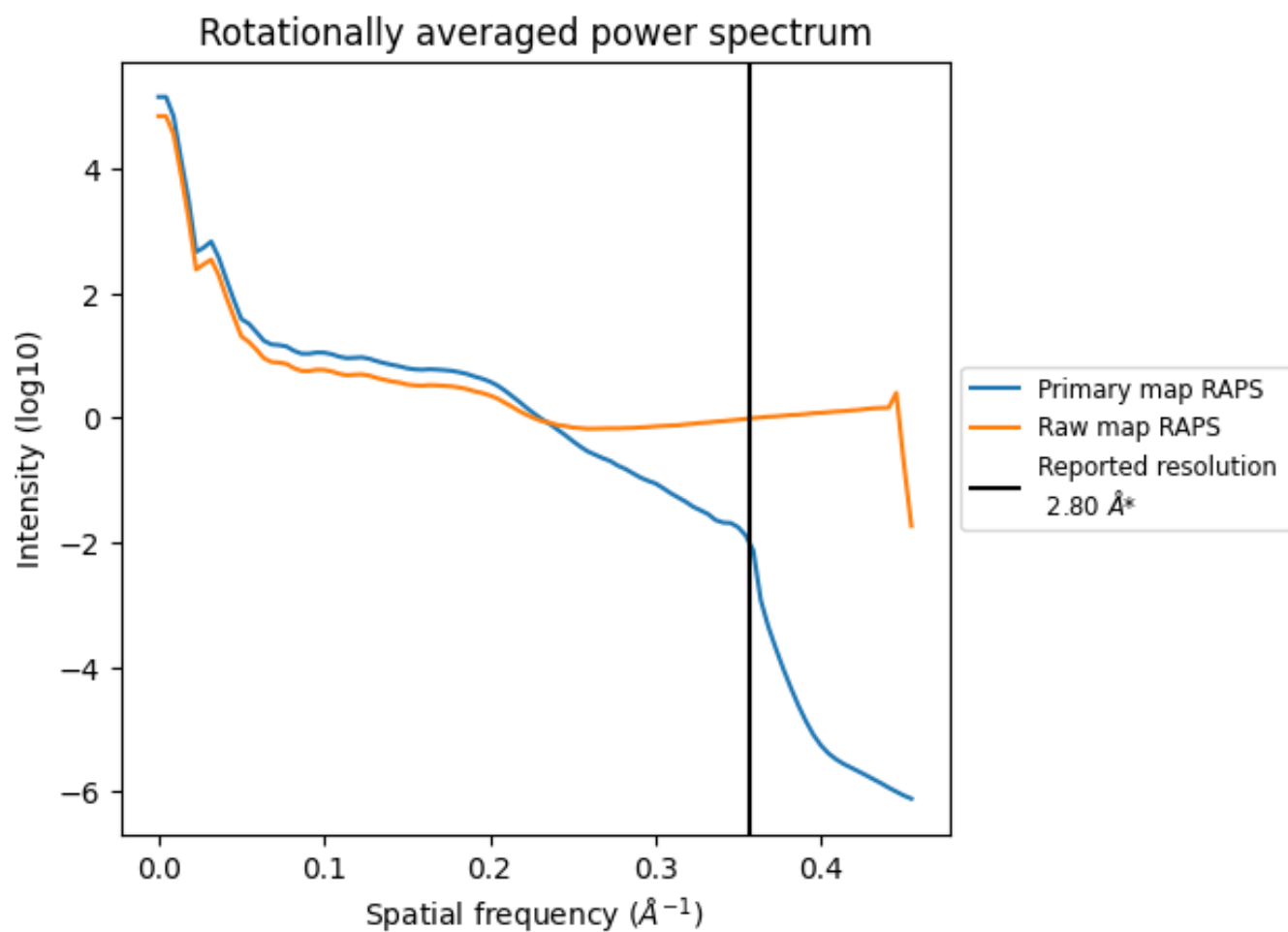
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 85 nm^3 ; this corresponds to an approximate mass of 77 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 i

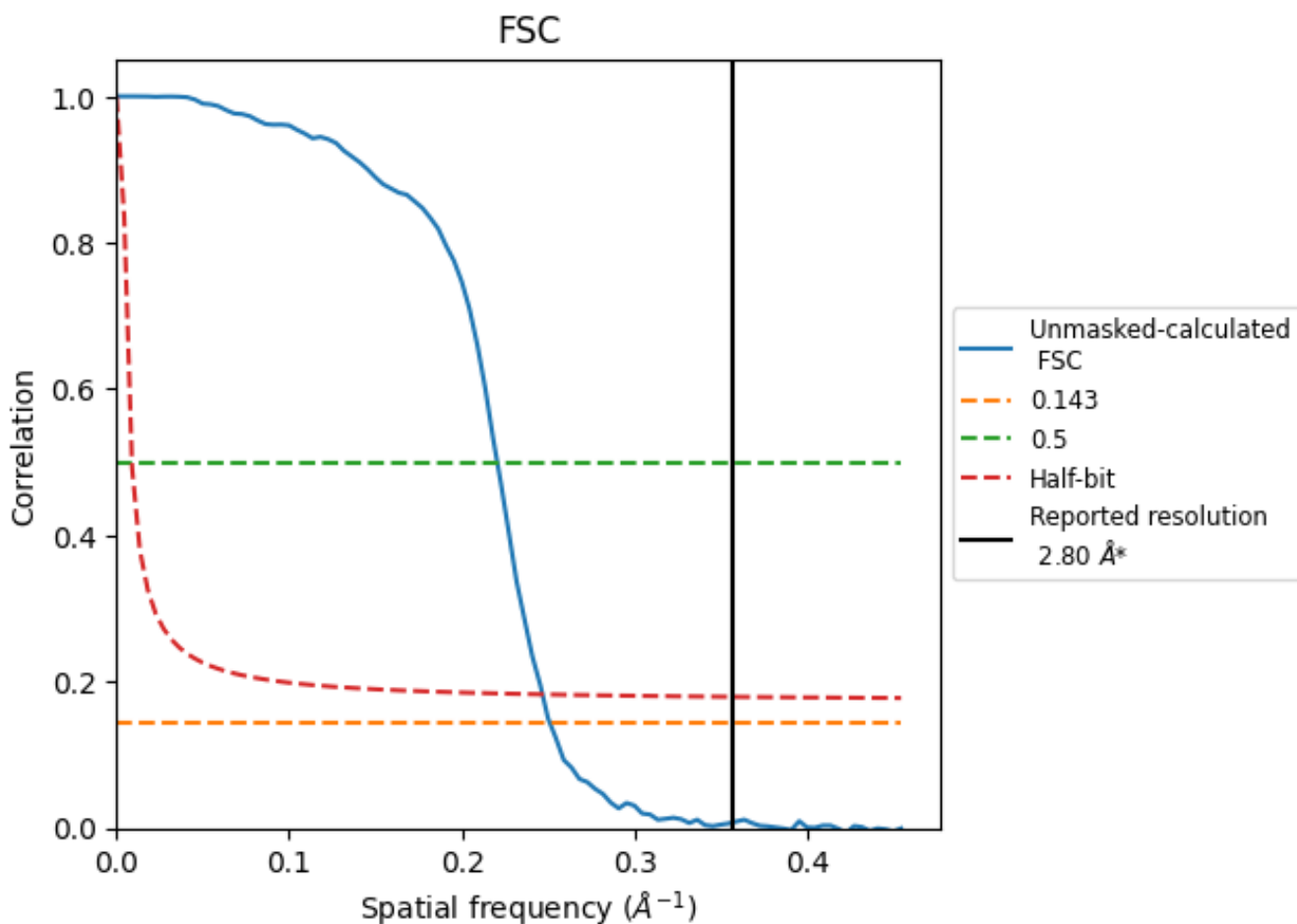


*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

8.2 Resolution estimates [i](#)

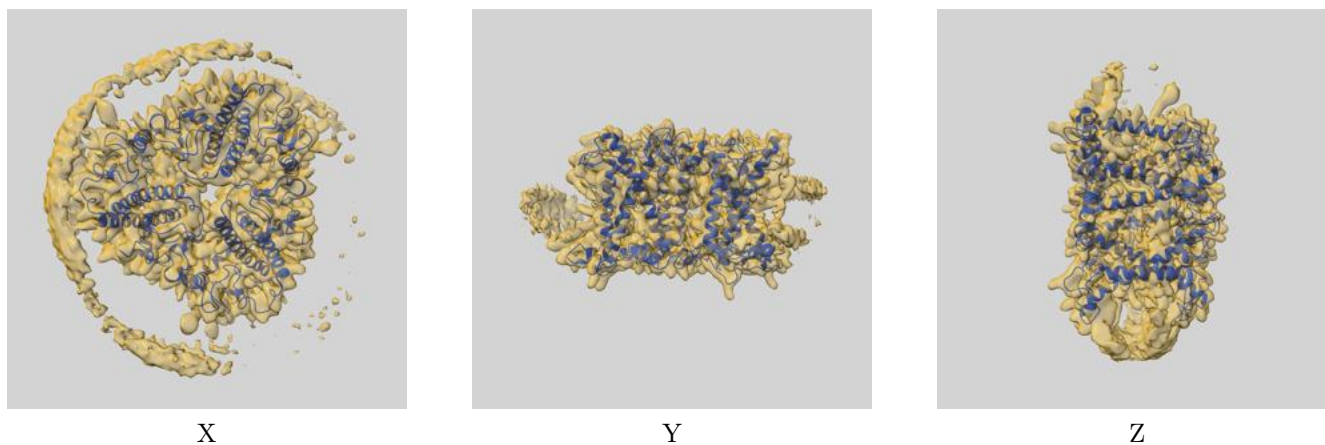
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.98	4.53	4.05

*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 3.98 differs from the reported value 2.8 by more than 10 %

9 Map-model fit [i](#)

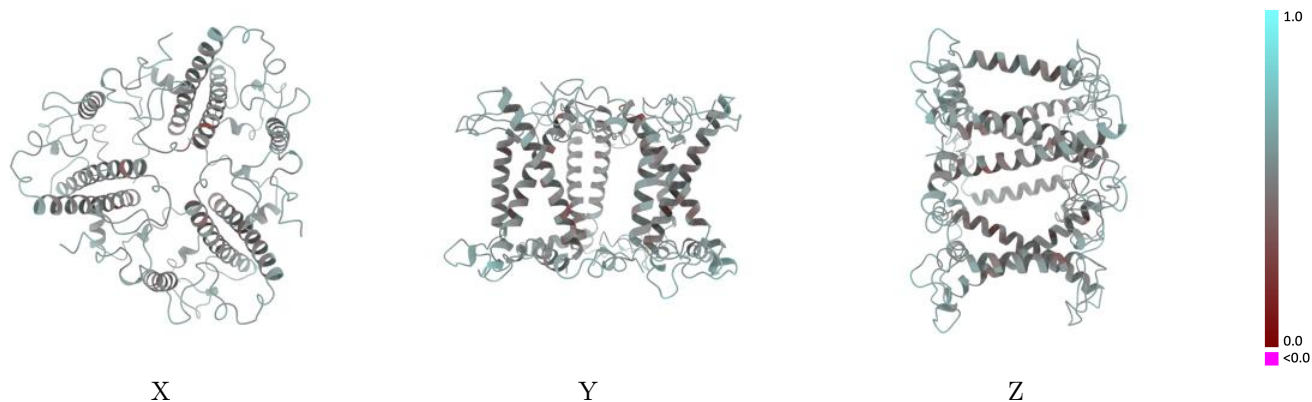
This section contains information regarding the fit between EMDB map EMD-35787 and PDB model 8IX2. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)



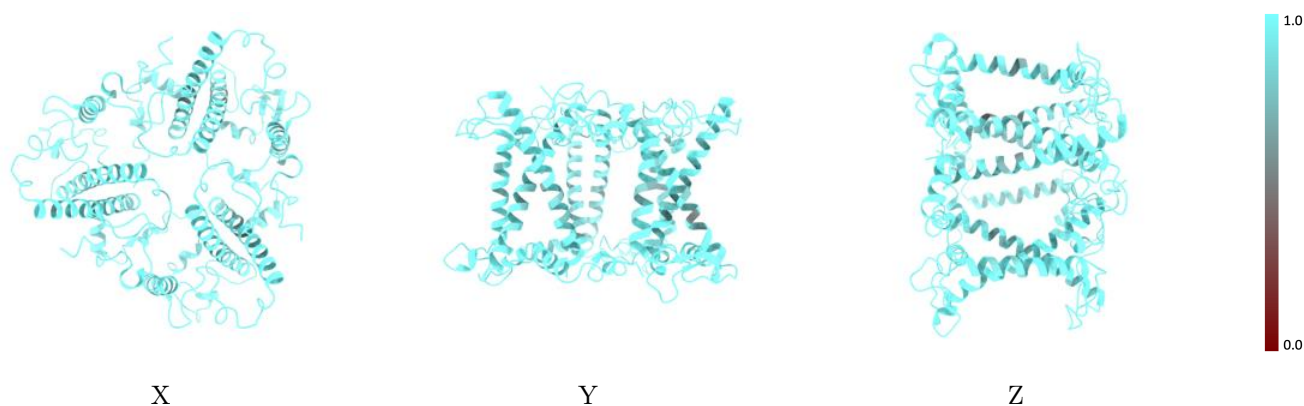
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



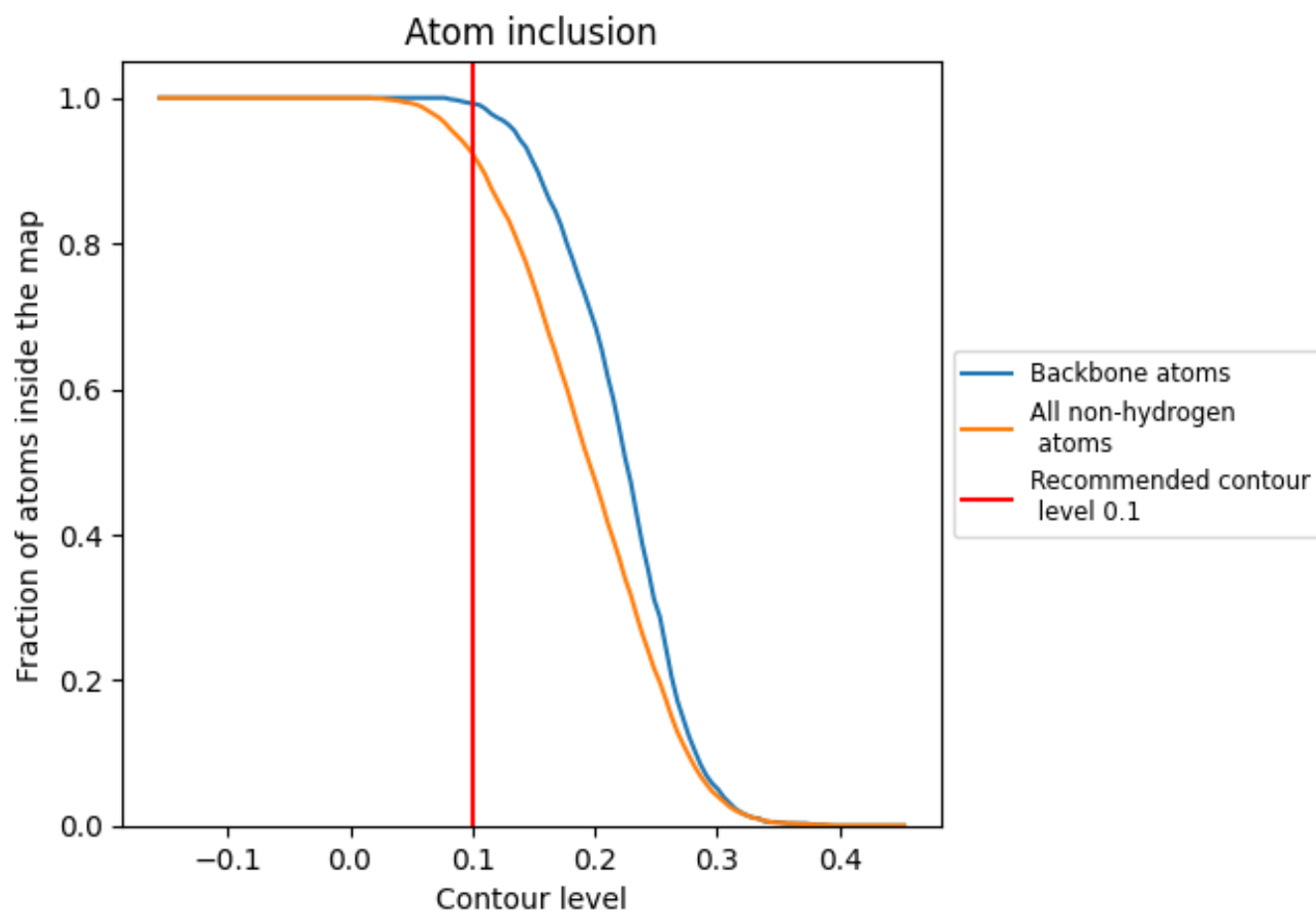
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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









9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 92% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9240	 0.5310
G	 0.9130	 0.5290
N	 0.9250	 0.5330
Y	 0.9330	 0.5310

