



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:23 PM UTC

PDB ID : 2CYD / pdb_00002cyd
Title : Crystal structure of Lithium bound rotor ring of the V-ATPase from *Enterococcus hirae*
Authors : Murata, T.; Yamato, I.; Kakinuma, Y.; Shirouzu, M.; Walker, J.E.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2005-07-06
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

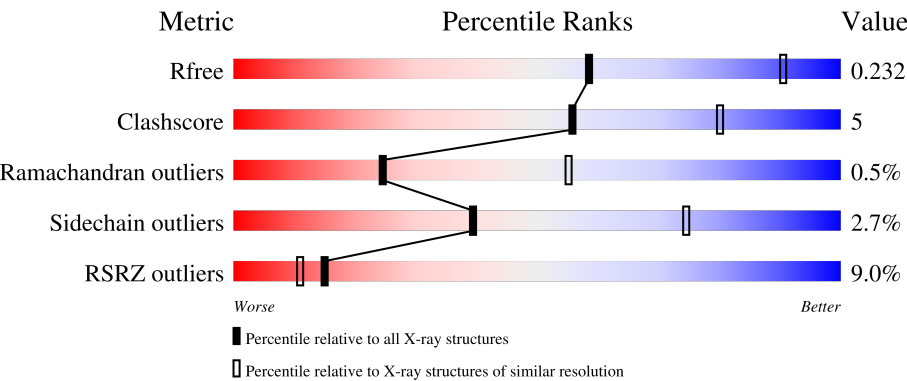
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

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.



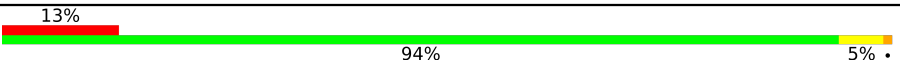
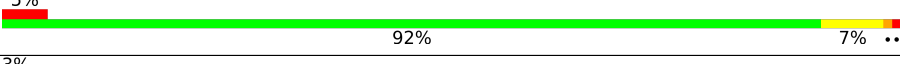
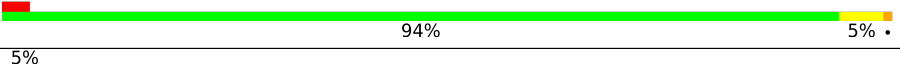
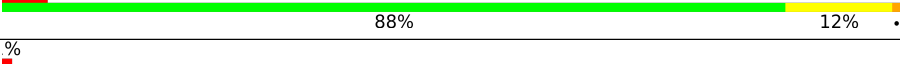
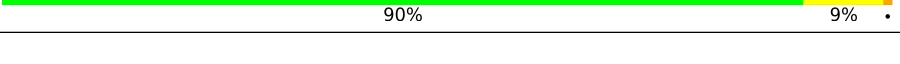
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	156	10% 92% 7% ..
1	B	156	12% 92% 7% ..
1	C	156	19% 88% 11% ..
1	D	156	10% 94% 5% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	E	156	
1	F	156	
1	G	156	
1	H	156	
1	I	156	
1	J	156	

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
4	UMQ	C	1001	X	-	-	-
4	UMQ	F	1002	X	-	-	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 12831 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 V-type sodium ATP synthase subunit K.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	156	Total	C	N	O	S	0	9	0
			1155	760	179	208	8			
1	B	156	Total	C	N	O	S	0	9	0
			1155	760	179	208	8			
1	C	156	Total	C	N	O	S	0	9	0
			1155	760	179	208	8			
1	D	156	Total	C	N	O	S	0	9	0
			1155	760	179	208	8			
1	E	156	Total	C	N	O	S	0	9	0
			1155	760	179	208	8			
1	F	156	Total	C	N	O	S	0	9	0
			1155	760	179	208	8			
1	G	156	Total	C	N	O	S	0	9	0
			1155	760	179	208	8			
1	H	156	Total	C	N	O	S	0	9	0
			1155	760	179	208	8			
1	I	156	Total	C	N	O	S	0	7	0
			1148	757	178	205	8			
1	J	156	Total	C	N	O	S	0	8	0
			1153	759	180	207	7			

- Molecule 2 is LITHIUM ION (CCD ID: LI) (formula: Li).

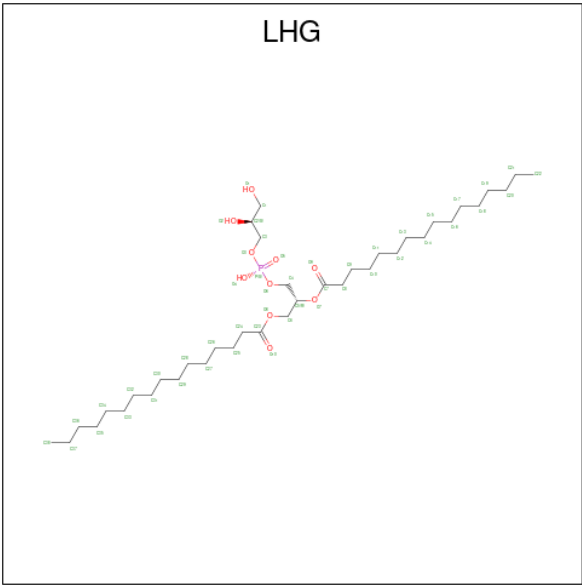
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Li	0	0
			1	1		
2	B	1	Total	Li	0	0
			1	1		
2	C	1	Total	Li	0	0
			1	1		
2	D	1	Total	Li	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	1	Total	Li	0	0
			1	1		
2	F	1	Total	Li	0	0
			1	1		
2	G	1	Total	Li	0	0
			1	1		
2	H	1	Total	Li	0	0
			1	1		
2	I	1	Total	Li	0	0
			1	1		
2	J	1	Total	Li	0	0
			1	1		

- Molecule 3 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



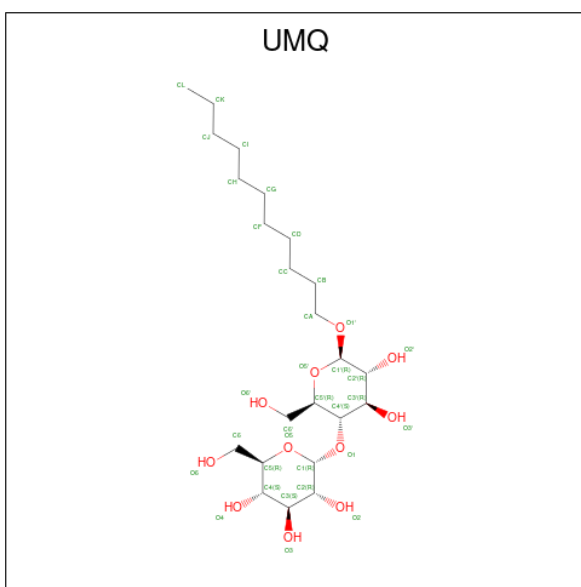
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			49	38	10	1		
3	A	1	Total	C	O		0	0
			40	35	5			
3	B	1	Total	C	O	P	0	0
			49	38	10	1		
3	B	1	Total	C	O		0	0
			40	35	5			
3	C	1	Total	C	O	P	0	0
			49	38	10	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total C O 40 35 5	0	0
3	D	1	Total C O P 49 38 10 1	0	0
3	D	1	Total C O 40 35 5	0	0
3	E	1	Total C O P 49 38 10 1	0	0
3	E	1	Total C O 40 35 5	0	0
3	F	1	Total C O P 49 38 10 1	0	0
3	F	1	Total C O 40 35 5	0	0
3	G	1	Total C O P 49 38 10 1	0	0
3	G	1	Total C O 40 35 5	0	0
3	H	1	Total C O P 49 38 10 1	0	0
3	H	1	Total C O 40 35 5	0	0
3	I	1	Total C O P 49 38 10 1	0	0
3	I	1	Total C O 40 35 5	0	0
3	J	1	Total C O P 49 38 10 1	0	0
3	J	1	Total C O 40 35 5	0	0

- Molecule 4 is UNDECYL-MALTOSIDE (CCD ID: UMQ) (formula: C₂₃H₄₄O₁₁).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total 34	C 23	O 11	0	0
4	F	1	Total 34	C 23	O 11	0	0

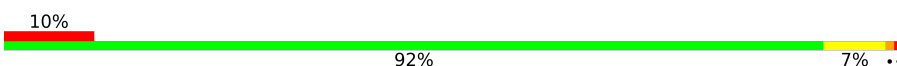
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	29	Total O 29 29	0	0
5	B	29	Total O 29 29	0	0
5	C	19	Total O 19 19	0	0
5	D	24	Total O 24 24	0	0
5	E	25	Total O 25 25	0	0
5	F	32	Total O 32 32	0	0
5	G	35	Total O 35 35	0	0
5	H	37	Total O 37 37	0	0
5	I	57	Total O 57 57	0	0
5	J	35	Total O 35 35	0	0

3 Residue-property plots [i](#)

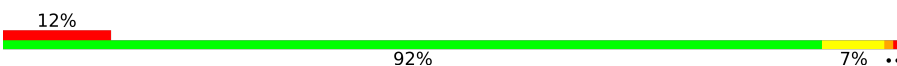
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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: V-type sodium ATP synthase subunit K

Chain A: 



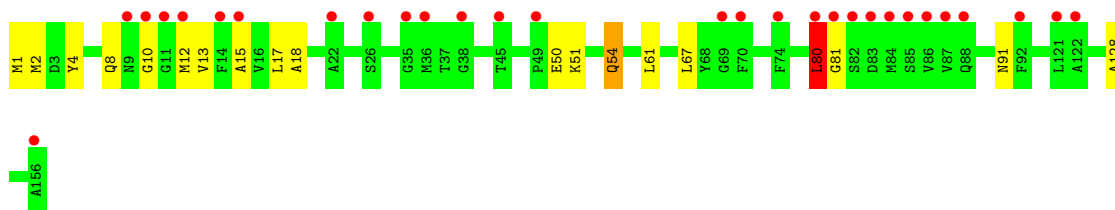
- Molecule 1: V-type sodium ATP synthase subunit K

Chain B: 

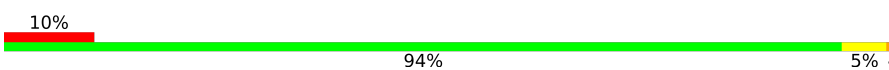


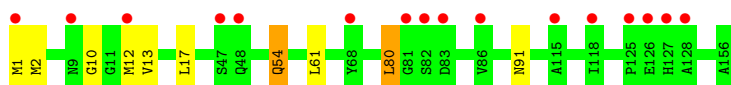
- Molecule 1: V-type sodium ATP synthase subunit K

Chain C: 

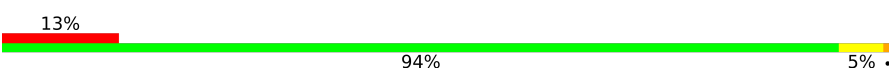


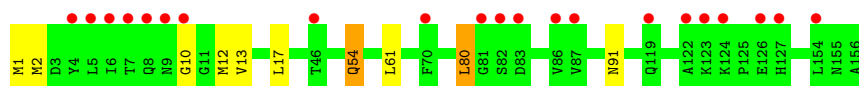
- Molecule 1: V-type sodium ATP synthase subunit K

Chain D: 

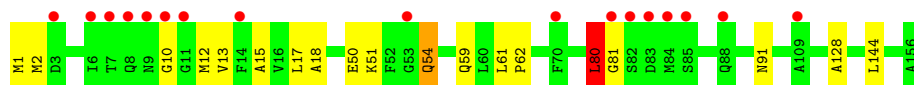
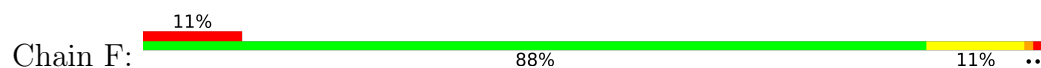


- Molecule 1: V-type sodium ATP synthase subunit K

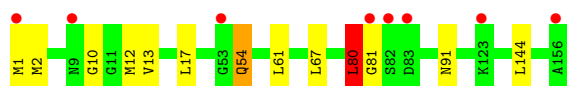
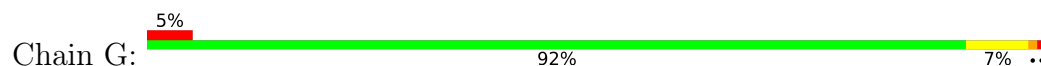
Chain E: 



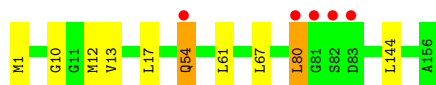
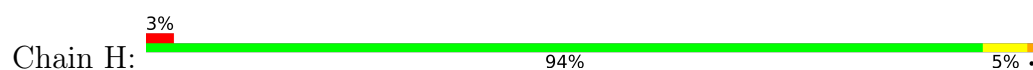
- Molecule 1: V-type sodium ATP synthase subunit K



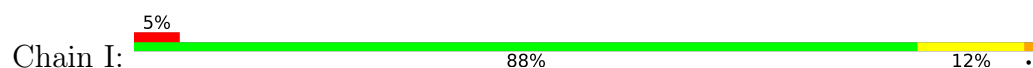
- Molecule 1: V-type sodium ATP synthase subunit K



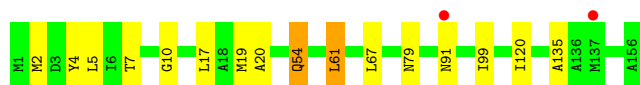
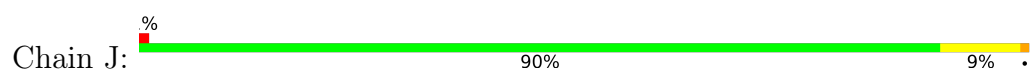
- Molecule 1: V-type sodium ATP synthase subunit K



- Molecule 1: V-type sodium ATP synthase subunit K



- Molecule 1: V-type sodium ATP synthase subunit K



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	119.65Å 125.78Å 210.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	107.80 – 2.80 107.80 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.1 (107.80-2.80) 98.1 (107.80-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.208 , 0.218 (Not available) , 0.232	Depositor DCC
R_{free} test set	3890 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	62.0	Xtriage
Anisotropy	0.222	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 59.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	12831	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.54% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, UMQ, LI

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	A	0.56	0/1219	0.84	0/1649
1	B	0.57	0/1219	0.89	0/1649
1	C	0.58	0/1219	0.90	0/1649
1	D	0.54	0/1219	0.88	0/1649
1	E	0.55	0/1219	0.86	0/1649
1	F	0.58	0/1219	0.87	0/1649
1	G	0.56	0/1219	0.88	0/1649
1	H	0.59	0/1219	0.86	0/1649
1	I	0.66	0/1202	0.87	0/1626
1	J	0.64	0/1212	0.93	0/1640
All	All	0.58	0/12166	0.88	0/16458

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

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	A	1155	0	1218	13	0
1	B	1155	0	1218	13	0
1	C	1155	0	1218	16	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1155	0	1218	11	0
1	E	1155	0	1218	10	0
1	F	1155	0	1218	16	0
1	G	1155	0	1218	14	0
1	H	1155	0	1218	10	0
1	I	1148	0	1214	16	0
1	J	1153	0	1217	15	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
3	A	89	0	141	7	0
3	B	89	0	141	5	0
3	C	89	0	141	6	0
3	D	89	0	141	7	0
3	E	89	0	141	5	0
3	F	89	0	141	6	0
3	G	89	0	141	8	0
3	H	89	0	141	6	0
3	I	89	0	141	4	0
3	J	89	0	141	8	0
4	C	34	0	41	0	0
4	F	34	0	42	0	0
5	A	29	0	0	0	0
5	B	29	0	0	0	0
5	C	19	0	0	0	0
5	D	24	0	0	0	0
5	E	25	0	0	0	0
5	F	32	0	0	0	0
5	G	35	0	0	0	0
5	H	37	0	0	0	0
5	I	57	0	0	0	0
5	J	35	0	0	0	0
All	All	12831	0	13668	124	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 5.

All (124) 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:A:559:LHG:HC62	3:J:9159:LHG:HC81	1.59	0.84
3:G:6159:LHG:HC81	3:H:7159:LHG:HC62	1.65	0.79
3:F:5159:LHG:HC81	3:G:6159:LHG:HC62	1.64	0.78
3:C:2159:LHG:HC81	3:D:3159:LHG:HC62	1.68	0.76
3:A:559:LHG:HC81	3:B:1159:LHG:HC62	1.71	0.71
3:E:4159:LHG:HC81	3:F:5159:LHG:HC62	1.73	0.69
3:I:8159:LHG:HC81	3:J:9159:LHG:HC62	1.75	0.68
3:D:3159:LHG:HC81	3:E:4159:LHG:HC62	1.77	0.67
3:B:1159:LHG:HC81	3:C:2159:LHG:HC62	1.78	0.65
1:I:10:GLY:O	1:I:13[A]:VAL:HG22	1.98	0.64
1:F:2:MET:HG2	1:G:1:MET:HB2	1.79	0.62
1:I:1:MET:HB3	3:I:8159:LHG:HC5	1.83	0.61
3:A:559:LHG:C6	3:J:9159:LHG:HC81	2.32	0.59
1:G:2:MET:HG2	1:H:1:MET:HB2	1.84	0.59
1:I:9:ASN:HD21	1:I:83:ASP:HA	1.68	0.58
1:A:1:MET:HB3	3:A:559:LHG:HC5	1.86	0.57
1:B:1:MET:HB3	3:B:1159:LHG:HC5	1.87	0.57
1:A:2:MET:HG2	1:B:1:MET:HB2	1.86	0.57
1:J:17[B]:LEU:HD21	3:J:9159:LHG:H192	1.87	0.56
3:H:7159:LHG:HC81	3:I:8159:LHG:HC62	1.87	0.56
1:B:17[B]:LEU:HD21	3:B:1159:LHG:H192	1.87	0.55
1:C:2:MET:HG2	1:D:1:MET:HB2	1.88	0.55
1:D:1:MET:HB3	3:D:3159:LHG:HC5	1.89	0.55
1:H:1:MET:HB3	3:H:7159:LHG:HC5	1.88	0.55
1:F:1:MET:HB3	3:F:5159:LHG:HC5	1.88	0.54
1:C:1:MET:HB3	3:C:2159:LHG:HC5	1.88	0.54
1:E:1:MET:HB3	3:E:4159:LHG:HC5	1.90	0.54
3:G:6159:LHG:HC81	3:H:7159:LHG:C6	2.36	0.53
1:F:17[B]:LEU:HD21	3:F:5159:LHG:H192	1.90	0.53
1:A:17[B]:LEU:HD21	3:A:559:LHG:H192	1.90	0.53
1:G:17[B]:LEU:HD21	3:G:6159:LHG:H192	1.91	0.53
1:E:17[B]:LEU:HD21	3:E:4159:LHG:H192	1.90	0.53
3:A:559:LHG:H341	3:J:9159:LHG:H212	1.91	0.52
1:F:50:GLU:HG2	1:F:51:LYS:HG3	1.90	0.52
1:G:1:MET:HB3	3:G:6159:LHG:HC5	1.89	0.52
1:H:17[B]:LEU:HD21	3:H:7159:LHG:H192	1.89	0.52
1:G:2:MET:CG	1:H:1:MET:HB2	2.40	0.52
1:F:2:MET:CG	1:G:1:MET:HB2	2.40	0.52
1:D:17[B]:LEU:HD21	3:D:3159:LHG:H192	1.92	0.51
1:C:17[B]:LEU:HD21	3:C:2159:LHG:H192	1.91	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:12[A]:MET:SD	1:I:80:LEU:HD22	2.52	0.50
1:E:91:ASN:HD21	1:F:12[A]:MET:HE3	1.75	0.50
3:F:5159:LHG:HC81	3:G:6159:LHG:C6	2.38	0.50
1:A:12[A]:MET:HE3	1:J:91:ASN:HD21	1.76	0.49
1:C:50:GLU:HG2	1:C:51:LYS:HG3	1.95	0.49
1:E:2:MET:HG2	1:F:1:MET:HB2	1.93	0.49
1:B:91:ASN:HD21	1:C:12[A]:MET:HE3	1.77	0.48
1:I:9:ASN:HD21	1:I:84:MET:H	1.61	0.48
1:C:2:MET:CG	1:D:1:MET:HB2	2.44	0.47
1:I:144:LEU:HD11	1:J:67:LEU:HD23	1.96	0.47
1:F:91:ASN:HD21	1:G:12[A]:MET:HE3	1.80	0.47
1:I:4:TYR:CD1	1:I:8:GLN:HG3	2.50	0.47
3:C:2159:LHG:HC81	3:D:3159:LHG:C6	2.40	0.47
1:A:2:MET:CG	1:B:1:MET:HB2	2.45	0.46
1:A:80:LEU:HB3	1:A:81:GLY:H	1.65	0.46
1:D:2:MET:HG2	1:E:1:MET:HB2	1.98	0.46
1:I:4:TYR:CE1	1:I:8:GLN:HG3	2.50	0.46
1:A:91:ASN:HD21	1:B:12[A]:MET:HE3	1.81	0.46
1:G:91:ASN:HD21	1:H:12[A]:MET:HE3	1.80	0.45
3:D:3159:LHG:HC81	3:E:4159:LHG:C6	2.46	0.45
1:D:10:GLY:O	1:D:13[A]:VAL:HG22	2.18	0.44
1:C:10:GLY:O	1:C:13[A]:VAL:HG22	2.17	0.44
1:F:10:GLY:O	1:F:13[A]:VAL:HG22	2.17	0.44
1:I:12[A]:MET:HE2	1:I:12[A]:MET:HB2	1.81	0.44
1:D:2:MET:CG	1:E:1:MET:HB2	2.48	0.43
1:I:17[B]:LEU:HD21	3:I:8159:LHG:H192	2.00	0.43
3:G:6159:LHG:H212	3:H:7159:LHG:H341	2.00	0.43
1:D:91:ASN:HD21	1:E:12[A]:MET:HE3	1.82	0.43
1:J:2:MET:HE1	3:J:9159:LHG:H121	2.01	0.43
1:B:10:GLY:O	1:B:13[A]:VAL:HG22	2.18	0.43
1:E:10:GLY:O	1:E:13[A]:VAL:HG22	2.19	0.43
3:A:559:LHG:HC81	3:B:1159:LHG:C6	2.45	0.43
1:B:80:LEU:HB3	1:B:81:GLY:H	1.67	0.43
1:B:144:LEU:HD11	1:C:67:LEU:HD23	2.01	0.43
1:A:1:MET:HB2	1:J:2:MET:HG2	2.00	0.43
1:A:144:LEU:HD11	1:B:67:LEU:HD23	2.01	0.43
1:C:80:LEU:HB3	1:C:81:GLY:H	1.66	0.43
3:F:5159:LHG:H212	3:G:6159:LHG:H341	2.01	0.43
1:H:10:GLY:O	1:H:13[A]:VAL:HG22	2.19	0.43
1:H:144:LEU:HD11	1:I:67:LEU:HD23	2.00	0.43
1:F:144:LEU:HD11	1:G:67:LEU:HD23	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:GLY:O	1:A:13[A]:VAL:HG22	2.19	0.42
1:F:59:GLN:O	1:F:62:PRO:HD2	2.19	0.42
1:J:2:MET:CE	3:J:9159:LHG:H121	2.49	0.42
1:J:5:LEU:HD22	1:J:10:GLY:HA3	2.00	0.42
1:B:2:MET:HG2	1:C:1:MET:HB2	2.00	0.42
1:F:15:ALA:O	1:F:18:ALA:HB3	2.19	0.42
1:A:46:THR:HG22	1:J:120:ILE:HA	2.01	0.42
1:I:87:VAL:HG23	1:J:4:TYR:CE2	2.55	0.42
1:I:152:LEU:HD21	1:J:19:MET:SD	2.59	0.42
1:F:54[B]:GLN:NE2	1:F:128:ALA:HB3	2.34	0.42
1:G:144:LEU:HD11	1:H:67:LEU:HD23	2.02	0.42
1:G:80:LEU:HB3	1:G:81:GLY:H	1.66	0.41
1:J:61:LEU:HD23	1:J:135:ALA:HB3	2.02	0.41
1:C:15:ALA:O	1:C:18:ALA:HB3	2.20	0.41
1:I:9:ASN:ND2	1:I:84:MET:H	2.18	0.41
3:J:9158:LHG:H251	3:J:9158:LHG:HC82	2.03	0.41
3:C:2159:LHG:H212	3:D:3159:LHG:H341	2.03	0.41
1:G:10:GLY:O	1:G:13[A]:VAL:HG22	2.21	0.41
1:I:98:PRO:HG3	1:J:20:ALA:HA	2.03	0.41
1:I:19:MET:CE	1:I:77:PHE:HB2	2.51	0.41
1:C:54[B]:GLN:NE2	1:C:128:ALA:HB3	2.36	0.40
1:F:80:LEU:HB3	1:F:81:GLY:H	1.65	0.40
1:C:4:TYR:CE1	1:C:8:GLN:HG3	2.56	0.40
1:C:91:ASN:HD21	1:D:12[A]:MET:HE3	1.86	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 X-ray entries followed by that with respect to entries of similar resolution.

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	A	163/156 (104%)	162 (99%)	0	1 (1%)	21 51

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	163/156 (104%)	161 (99%)	1 (1%)	1 (1%)	21	51
1	C	163/156 (104%)	162 (99%)	0	1 (1%)	21	51
1	D	163/156 (104%)	161 (99%)	1 (1%)	1 (1%)	21	51
1	E	163/156 (104%)	161 (99%)	1 (1%)	1 (1%)	21	51
1	F	163/156 (104%)	162 (99%)	0	1 (1%)	21	51
1	G	163/156 (104%)	161 (99%)	1 (1%)	1 (1%)	21	51
1	H	163/156 (104%)	161 (99%)	1 (1%)	1 (1%)	21	51
1	I	161/156 (103%)	160 (99%)	1 (1%)	0	100	100
1	J	162/156 (104%)	160 (99%)	2 (1%)	0	100	100
All	All	1627/1560 (104%)	1611 (99%)	8 (0%)	8 (0%)	24	55

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	80	LEU
1	B	80	LEU
1	C	80	LEU
1	E	80	LEU
1	F	80	LEU
1	G	80	LEU
1	H	80	LEU
1	D	80	LEU

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	A	122/113 (108%)	118 (97%)	4 (3%)	33	69
1	B	122/113 (108%)	118 (97%)	4 (3%)	33	69
1	C	122/113 (108%)	118 (97%)	4 (3%)	33	69
1	D	122/113 (108%)	118 (97%)	4 (3%)	33	69

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	122/113 (108%)	118 (97%)	4 (3%)	33	69
1	F	122/113 (108%)	118 (97%)	4 (3%)	33	69
1	G	122/113 (108%)	118 (97%)	4 (3%)	33	69
1	H	122/113 (108%)	118 (97%)	4 (3%)	33	69
1	I	120/113 (106%)	118 (98%)	2 (2%)	53	83
1	J	121/113 (107%)	116 (96%)	5 (4%)	27	62
All	All	1217/1130 (108%)	1178 (97%)	39 (3%)	39	70

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54[A]	GLN
1	A	54[B]	GLN
1	A	61	LEU
1	A	80	LEU
1	B	54[A]	GLN
1	B	54[B]	GLN
1	B	61	LEU
1	B	80	LEU
1	C	54[A]	GLN
1	C	54[B]	GLN
1	C	61	LEU
1	C	80	LEU
1	D	54[A]	GLN
1	D	54[B]	GLN
1	D	61	LEU
1	D	80	LEU
1	E	54[A]	GLN
1	E	54[B]	GLN
1	E	61	LEU
1	E	80	LEU
1	F	54[A]	GLN
1	F	54[B]	GLN
1	F	61	LEU
1	F	80	LEU
1	G	54[A]	GLN
1	G	54[B]	GLN
1	G	61	LEU
1	G	80	LEU
1	H	54[A]	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	54[B]	GLN
1	H	61	LEU
1	H	80	LEU
1	I	61	LEU
1	I	83	ASP
1	J	7	THR
1	J	54[A]	GLN
1	J	54[B]	GLN
1	J	61	LEU
1	J	99	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	ASN
1	B	91	ASN
1	C	91	ASN
1	D	91	ASN
1	E	91	ASN
1	F	91	ASN
1	I	8	GLN
1	I	9	ASN
1	I	79	ASN
1	J	8	GLN
1	J	91	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 32 ligands modelled in this entry, 10 are monoatomic - leaving 22 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	LHG	E	4159	-	39,39,48	1.06	2 (5%)	41,41,54	1.08	2 (4%)
3	LHG	G	6159	-	39,39,48	1.07	2 (5%)	41,41,54	1.07	2 (4%)
3	LHG	F	5159	-	39,39,48	1.06	2 (5%)	41,41,54	1.09	2 (4%)
3	LHG	J	9159	-	39,39,48	1.08	2 (5%)	41,41,54	1.00	2 (4%)
3	LHG	J	9158	-	48,48,48	0.98	2 (4%)	51,54,54	1.05	4 (7%)
3	LHG	H	7159	-	39,39,48	1.06	2 (5%)	41,41,54	1.08	2 (4%)
3	LHG	G	6158	-	48,48,48	1.02	2 (4%)	51,54,54	1.01	4 (7%)
3	LHG	B	1158	-	48,48,48	1.01	2 (4%)	51,54,54	0.99	3 (5%)
3	LHG	H	7158	-	48,48,48	1.00	2 (4%)	51,54,54	1.03	4 (7%)
3	LHG	A	558	-	48,48,48	1.00	2 (4%)	51,54,54	1.02	4 (7%)
3	LHG	D	3158	-	48,48,48	1.00	2 (4%)	51,54,54	1.01	3 (5%)
3	LHG	I	8158	-	48,48,48	1.01	2 (4%)	51,54,54	1.01	4 (7%)
3	LHG	A	559	-	39,39,48	1.07	2 (5%)	41,41,54	1.08	2 (4%)
3	LHG	C	2159	-	39,39,48	1.06	2 (5%)	41,41,54	1.08	2 (4%)
3	LHG	F	5158	-	48,48,48	1.02	2 (4%)	51,54,54	1.04	4 (7%)
4	UMQ	F	1002	-	35,35,35	1.16	3 (8%)	46,46,46	1.39	6 (13%)
3	LHG	E	4158	-	48,48,48	0.99	2 (4%)	51,54,54	1.02	4 (7%)
3	LHG	B	1159	-	39,39,48	1.07	2 (5%)	41,41,54	1.08	2 (4%)
3	LHG	I	8159	-	39,39,48	1.08	2 (5%)	41,41,54	1.10	2 (4%)
3	LHG	C	2158	-	48,48,48	1.03	2 (4%)	51,54,54	0.97	3 (5%)
3	LHG	D	3159	-	39,39,48	1.07	2 (5%)	41,41,54	1.08	2 (4%)
4	UMQ	C	1001	-	35,35,35	1.17	3 (8%)	46,46,46	1.69	9 (19%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LHG	E	4159	-	-	23/41/41/53	-
3	LHG	G	6159	-	-	23/41/41/53	-
3	LHG	F	5159	-	-	23/41/41/53	-
3	LHG	J	9159	-	-	24/41/41/53	-
3	LHG	J	9158	-	-	25/53/53/53	-
3	LHG	H	7159	-	-	23/41/41/53	-
3	LHG	G	6158	-	-	26/53/53/53	-
3	LHG	B	1158	-	-	27/53/53/53	-
3	LHG	H	7158	-	-	27/53/53/53	-
3	LHG	A	558	-	-	25/53/53/53	-
3	LHG	D	3158	-	-	26/53/53/53	-
3	LHG	I	8158	-	-	24/53/53/53	-
3	LHG	A	559	-	-	23/41/41/53	-
3	LHG	C	2159	-	-	23/41/41/53	-
3	LHG	F	5158	-	-	25/53/53/53	-
4	UMQ	F	1002	-	1/1/10/10	12/20/60/60	0/2/2/2
3	LHG	E	4158	-	-	25/53/53/53	-
3	LHG	B	1159	-	-	23/41/41/53	-
3	LHG	I	8159	-	-	24/41/41/53	-
3	LHG	C	2158	-	-	25/53/53/53	-
3	LHG	D	3159	-	-	23/41/41/53	-
4	UMQ	C	1001	-	1/1/10/10	11/20/60/60	0/2/2/2

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	9159	LHG	O7-C7	4.56	1.47	1.34
3	C	2158	LHG	O7-C7	4.54	1.47	1.34
3	I	8159	LHG	O7-C7	4.53	1.47	1.34
3	A	559	LHG	O8-C23	4.53	1.46	1.33
3	D	3158	LHG	O8-C23	4.50	1.46	1.33
3	B	1158	LHG	O8-C23	4.50	1.46	1.33
3	H	7158	LHG	O8-C23	4.49	1.46	1.33
3	H	7159	LHG	O8-C23	4.49	1.46	1.33
3	D	3159	LHG	O8-C23	4.48	1.46	1.33
3	G	6158	LHG	O8-C23	4.48	1.46	1.33
3	G	6159	LHG	O8-C23	4.47	1.46	1.33
3	B	1159	LHG	O8-C23	4.47	1.46	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2158	LHG	O8-C23	4.47	1.46	1.33
3	E	4159	LHG	O8-C23	4.46	1.46	1.33
3	I	8158	LHG	O8-C23	4.45	1.46	1.33
3	G	6158	LHG	O7-C7	4.44	1.46	1.34
3	F	5158	LHG	O8-C23	4.41	1.46	1.33
3	F	5158	LHG	O7-C7	4.41	1.46	1.34
3	E	4158	LHG	O8-C23	4.40	1.46	1.33
3	C	2159	LHG	O8-C23	4.40	1.46	1.33
3	I	8159	LHG	O8-C23	4.40	1.46	1.33
3	F	5159	LHG	O8-C23	4.38	1.46	1.33
3	A	558	LHG	O8-C23	4.38	1.46	1.33
3	D	3159	LHG	O7-C7	4.36	1.46	1.34
3	B	1159	LHG	O7-C7	4.35	1.46	1.34
3	C	2159	LHG	O7-C7	4.33	1.46	1.34
3	G	6159	LHG	O7-C7	4.32	1.46	1.34
3	B	1158	LHG	O7-C7	4.31	1.46	1.34
3	J	9159	LHG	O8-C23	4.30	1.45	1.33
3	F	5159	LHG	O7-C7	4.30	1.46	1.34
4	F	1002	UMQ	O3-C3	-4.29	1.32	1.43
3	E	4159	LHG	O7-C7	4.29	1.46	1.34
3	J	9158	LHG	O8-C23	4.29	1.45	1.33
3	A	559	LHG	O7-C7	4.28	1.46	1.34
3	J	9158	LHG	O7-C7	4.27	1.46	1.34
3	H	7159	LHG	O7-C7	4.27	1.46	1.34
3	A	558	LHG	O7-C7	4.26	1.46	1.34
3	E	4158	LHG	O7-C7	4.26	1.46	1.34
3	H	7158	LHG	O7-C7	4.22	1.46	1.34
3	I	8158	LHG	O7-C7	4.20	1.46	1.34
3	D	3158	LHG	O7-C7	4.17	1.46	1.34
4	F	1002	UMQ	O2-C2	-4.12	1.32	1.43
4	C	1001	UMQ	O3-C3	-4.10	1.32	1.43
4	C	1001	UMQ	O2-C2	-4.09	1.32	1.43
4	C	1001	UMQ	O1'-C1'	2.24	1.43	1.40
4	F	1002	UMQ	O1'-C1'	2.20	1.43	1.40

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1001	UMQ	C4-C3-C2	5.25	120.05	110.83
3	J	9158	LHG	O7-C7-C8	4.69	121.62	111.48
3	D	3158	LHG	O7-C7-C8	4.42	121.04	111.48
3	E	4158	LHG	O7-C7-C8	4.41	121.02	111.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	558	LHG	O7-C7-C8	4.41	121.01	111.48
3	G	6158	LHG	O7-C7-C8	4.40	121.00	111.48
3	H	7158	LHG	O7-C7-C8	4.39	120.97	111.48
3	F	5158	LHG	O7-C7-C8	4.39	120.97	111.48
4	C	1001	UMQ	C1-C2-C3	4.38	119.23	110.01
4	C	1001	UMQ	O3-C3-C4	4.36	120.64	110.38
3	B	1158	LHG	O7-C7-C8	4.33	120.85	111.48
3	I	8158	LHG	O7-C7-C8	4.26	120.69	111.48
3	I	8159	LHG	O7-C7-C8	4.22	120.61	111.48
3	B	1159	LHG	O7-C7-C8	4.21	120.59	111.48
3	D	3159	LHG	O7-C7-C8	4.20	120.57	111.48
3	C	2158	LHG	O7-C7-C8	4.14	120.44	111.48
3	G	6159	LHG	O7-C7-C8	4.11	120.37	111.48
3	F	5159	LHG	O7-C7-C8	4.10	120.36	111.48
3	H	7159	LHG	O7-C7-C8	4.08	120.30	111.48
3	E	4159	LHG	O7-C7-C8	4.06	120.27	111.48
3	C	2159	LHG	O7-C7-C8	4.05	120.25	111.48
3	A	559	LHG	O7-C7-C8	4.05	120.24	111.48
3	J	9159	LHG	O7-C7-C8	3.96	120.05	111.48
4	F	1002	UMQ	C4-C3-C2	3.82	117.53	110.83
4	C	1001	UMQ	O2-C2-C1	3.76	119.04	110.08
4	C	1001	UMQ	O3-C3-C2	3.74	119.19	110.38
4	F	1002	UMQ	C1-C2-C3	3.40	117.16	110.01
4	F	1002	UMQ	O3-C3-C4	3.28	118.12	110.38
4	F	1002	UMQ	O2-C2-C1	3.26	117.84	110.08
3	F	5158	LHG	O8-C23-C24	3.22	121.64	111.83
3	H	7158	LHG	O8-C23-C24	3.09	121.25	111.83
3	I	8158	LHG	O8-C23-C24	3.04	121.12	111.83
3	E	4158	LHG	O8-C23-C24	2.99	120.96	111.83
4	C	1001	UMQ	O1'-C1'-C2'	2.93	112.73	108.27
3	A	558	LHG	O8-C23-C24	2.92	120.73	111.83
3	D	3158	LHG	O8-C23-C24	2.91	120.70	111.83
3	G	6158	LHG	O8-C23-C24	2.89	120.65	111.83
3	J	9158	LHG	O8-C23-C24	2.86	120.56	111.83
3	B	1158	LHG	O8-C23-C24	2.85	120.53	111.83
3	C	2158	LHG	O8-C23-C24	2.84	120.50	111.83
3	C	2159	LHG	O8-C23-C24	2.84	120.50	111.83
3	H	7159	LHG	O8-C23-C24	2.84	120.49	111.83
3	A	559	LHG	O8-C23-C24	2.84	120.48	111.83
3	E	4159	LHG	O8-C23-C24	2.82	120.42	111.83
3	F	5159	LHG	O8-C23-C24	2.81	120.39	111.83
3	D	3159	LHG	O8-C23-C24	2.77	120.29	111.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	6159	LHG	O8-C23-C24	2.77	120.29	111.83
3	B	1159	LHG	O8-C23-C24	2.77	120.28	111.83
3	I	8159	LHG	O8-C23-C24	2.71	120.10	111.83
4	C	1001	UMQ	O2-C2-C3	2.64	116.60	110.38
3	J	9159	LHG	O8-C23-C24	2.62	119.83	111.83
3	J	9158	LHG	O7-C7-O9	-2.58	117.67	123.70
3	I	8158	LHG	O7-C7-O9	-2.53	117.80	123.70
3	H	7158	LHG	O7-C7-O9	-2.45	117.97	123.70
4	F	1002	UMQ	O2-C2-C3	2.45	116.16	110.38
3	A	558	LHG	O7-C7-O9	-2.40	118.09	123.70
3	D	3158	LHG	O7-C7-O9	-2.37	118.16	123.70
3	F	5158	LHG	O8-C23-O10	-2.36	117.72	123.63
3	I	8158	LHG	O8-C23-O10	-2.33	117.80	123.63
3	A	558	LHG	O8-C23-O10	-2.33	117.81	123.63
3	F	5158	LHG	O7-C7-O9	-2.29	118.35	123.70
3	E	4158	LHG	O7-C7-O9	-2.28	118.38	123.70
3	B	1158	LHG	O7-C7-O9	-2.27	118.39	123.70
3	J	9158	LHG	O8-C23-O10	-2.24	118.02	123.63
4	C	1001	UMQ	C3'-C4'-C5'	-2.22	106.02	110.93
3	G	6158	LHG	O7-C7-O9	-2.19	118.58	123.70
3	G	6158	LHG	O8-C23-O10	-2.19	118.16	123.63
3	H	7158	LHG	O8-C23-O10	-2.16	118.23	123.63
3	E	4158	LHG	O8-C23-O10	-2.16	118.23	123.63
4	C	1001	UMQ	O5-C5-C6	2.13	111.72	106.44
4	F	1002	UMQ	O3-C3-C2	2.03	115.16	110.38
3	C	2158	LHG	O7-C7-O9	-2.01	119.01	123.70

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	C	1001	UMQ	C3
4	F	1002	UMQ	C2

All (510) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	558	LHG	O1-C1-C2-O2
3	A	558	LHG	C4-O6-P-O3
3	A	558	LHG	C4-O6-P-O4
3	A	558	LHG	C4-O6-P-O5
3	A	558	LHG	C8-C7-O7-C5
3	A	559	LHG	C8-C7-O7-C5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	B	1158	LHG	C4-O6-P-O3
3	B	1158	LHG	C4-O6-P-O4
3	B	1158	LHG	C4-O6-P-O5
3	B	1158	LHG	C8-C7-O7-C5
3	B	1159	LHG	C8-C7-O7-C5
3	C	2158	LHG	O1-C1-C2-O2
3	C	2158	LHG	C4-O6-P-O3
3	C	2158	LHG	C4-O6-P-O4
3	C	2158	LHG	C4-O6-P-O5
3	C	2158	LHG	C8-C7-O7-C5
3	C	2159	LHG	C8-C7-O7-C5
3	D	3158	LHG	C4-O6-P-O3
3	D	3158	LHG	C4-O6-P-O4
3	D	3158	LHG	C4-O6-P-O5
3	D	3158	LHG	C8-C7-O7-C5
3	D	3159	LHG	C8-C7-O7-C5
3	E	4158	LHG	C4-O6-P-O3
3	E	4158	LHG	C4-O6-P-O4
3	E	4158	LHG	C4-O6-P-O5
3	E	4158	LHG	C8-C7-O7-C5
3	E	4159	LHG	C8-C7-O7-C5
3	F	5158	LHG	O1-C1-C2-O2
3	F	5158	LHG	C4-O6-P-O3
3	F	5158	LHG	C4-O6-P-O4
3	F	5158	LHG	C4-O6-P-O5
3	F	5158	LHG	C8-C7-O7-C5
3	F	5159	LHG	C8-C7-O7-C5
3	G	6158	LHG	C4-O6-P-O3
3	G	6158	LHG	C4-O6-P-O4
3	G	6158	LHG	C4-O6-P-O5
3	G	6158	LHG	C8-C7-O7-C5
3	G	6159	LHG	C8-C7-O7-C5
3	H	7158	LHG	C4-O6-P-O3
3	H	7158	LHG	C4-O6-P-O4
3	H	7158	LHG	C8-C7-O7-C5
3	H	7159	LHG	C8-C7-O7-C5
3	I	8158	LHG	C4-O6-P-O3
3	I	8158	LHG	C4-O6-P-O4
3	I	8158	LHG	C8-C7-O7-C5
3	I	8159	LHG	C8-C7-O7-C5
3	J	9158	LHG	C4-O6-P-O3
3	J	9158	LHG	C4-O6-P-O4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	J	9158	LHG	C4-O6-P-O5
3	J	9158	LHG	C8-C7-O7-C5
3	J	9159	LHG	C8-C7-O7-C5
3	A	558	LHG	O9-C7-O7-C5
3	A	559	LHG	O9-C7-O7-C5
3	B	1158	LHG	O9-C7-O7-C5
3	B	1159	LHG	O9-C7-O7-C5
3	C	2158	LHG	O9-C7-O7-C5
3	C	2159	LHG	O9-C7-O7-C5
3	D	3158	LHG	O9-C7-O7-C5
3	D	3159	LHG	O9-C7-O7-C5
3	E	4158	LHG	O9-C7-O7-C5
3	E	4159	LHG	O9-C7-O7-C5
3	F	5158	LHG	O9-C7-O7-C5
3	F	5159	LHG	O9-C7-O7-C5
3	G	6158	LHG	O9-C7-O7-C5
3	G	6159	LHG	O9-C7-O7-C5
3	H	7158	LHG	O9-C7-O7-C5
3	H	7159	LHG	O9-C7-O7-C5
3	I	8158	LHG	O9-C7-O7-C5
3	I	8159	LHG	O9-C7-O7-C5
3	J	9158	LHG	O9-C7-O7-C5
3	J	9159	LHG	O9-C7-O7-C5
3	A	559	LHG	C24-C23-O8-C6
3	B	1159	LHG	C24-C23-O8-C6
3	C	2159	LHG	C24-C23-O8-C6
3	D	3159	LHG	C24-C23-O8-C6
3	E	4159	LHG	C24-C23-O8-C6
3	F	5159	LHG	C24-C23-O8-C6
3	G	6159	LHG	C24-C23-O8-C6
3	H	7159	LHG	C24-C23-O8-C6
3	I	8159	LHG	C24-C23-O8-C6
3	J	9159	LHG	C24-C23-O8-C6
3	C	2159	LHG	O10-C23-O8-C6
3	F	5159	LHG	O10-C23-O8-C6
3	B	1159	LHG	O10-C23-O8-C6
3	D	3159	LHG	O10-C23-O8-C6
3	I	8159	LHG	O10-C23-O8-C6
4	C	1001	UMQ	O5'-C1'-O1'-CA
4	C	1001	UMQ	C4'-C5'-C6'-O6'
3	A	559	LHG	O10-C23-O8-C6
3	E	4159	LHG	O10-C23-O8-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	G	6159	LHG	O10-C23-O8-C6
3	H	7159	LHG	O10-C23-O8-C6
3	J	9159	LHG	O10-C23-O8-C6
4	F	1002	UMQ	C4-C5-C6-O6
3	A	558	LHG	C24-C23-O8-C6
3	B	1158	LHG	C24-C23-O8-C6
3	C	2158	LHG	C24-C23-O8-C6
3	D	3158	LHG	C24-C23-O8-C6
3	E	4158	LHG	C24-C23-O8-C6
3	F	5158	LHG	C24-C23-O8-C6
3	G	6158	LHG	C24-C23-O8-C6
3	H	7158	LHG	C24-C23-O8-C6
3	I	8158	LHG	C24-C23-O8-C6
3	J	9158	LHG	C24-C23-O8-C6
4	F	1002	UMQ	C4'-C5'-C6'-O6'
4	C	1001	UMQ	C2'-C1'-O1'-CA
3	F	5158	LHG	O10-C23-O8-C6
3	H	7158	LHG	O10-C23-O8-C6
4	C	1001	UMQ	O5'-C5'-C6'-O6'
3	A	558	LHG	O10-C23-O8-C6
3	C	2158	LHG	O10-C23-O8-C6
3	D	3158	LHG	O10-C23-O8-C6
3	E	4158	LHG	O10-C23-O8-C6
3	G	6158	LHG	O10-C23-O8-C6
3	I	8158	LHG	O10-C23-O8-C6
3	J	9158	LHG	O10-C23-O8-C6
3	B	1158	LHG	O10-C23-O8-C6
3	B	1158	LHG	O1-C1-C2-O2
3	D	3158	LHG	O1-C1-C2-O2
3	E	4158	LHG	O1-C1-C2-O2
3	G	6158	LHG	O1-C1-C2-O2
3	H	7158	LHG	O1-C1-C2-O2
4	F	1002	UMQ	O5'-C5'-C6'-O6'
4	C	1001	UMQ	O1'-CA-CB-CC
4	F	1002	UMQ	O5-C5-C6-O6
4	F	1002	UMQ	O1'-CA-CB-CC
3	A	558	LHG	O1-C1-C2-C3
3	B	1158	LHG	O1-C1-C2-C3
3	C	2158	LHG	O1-C1-C2-C3
3	D	3158	LHG	O1-C1-C2-C3
3	E	4158	LHG	O1-C1-C2-C3
3	F	5158	LHG	O1-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	G	6158	LHG	O1-C1-C2-C3
3	H	7158	LHG	O1-C1-C2-C3
3	I	8158	LHG	O1-C1-C2-C3
3	J	9158	LHG	O1-C1-C2-C3
3	I	8159	LHG	C14-C15-C16-C17
3	J	9159	LHG	C10-C11-C12-C13
3	A	559	LHG	C10-C11-C12-C13
3	D	3159	LHG	C10-C11-C12-C13
3	H	7159	LHG	C10-C11-C12-C13
3	J	9159	LHG	C14-C15-C16-C17
3	B	1159	LHG	C10-C11-C12-C13
3	C	2159	LHG	C14-C15-C16-C17
3	E	4159	LHG	C10-C11-C12-C13
3	G	6159	LHG	C10-C11-C12-C13
3	G	6159	LHG	C14-C15-C16-C17
3	I	8158	LHG	C31-C32-C33-C34
3	J	9159	LHG	C26-C27-C28-C29
3	A	558	LHG	C31-C32-C33-C34
3	B	1158	LHG	C31-C32-C33-C34
3	C	2158	LHG	C31-C32-C33-C34
3	C	2159	LHG	C10-C11-C12-C13
3	D	3159	LHG	C14-C15-C16-C17
3	E	4158	LHG	C31-C32-C33-C34
3	E	4159	LHG	C14-C15-C16-C17
3	F	5158	LHG	C31-C32-C33-C34
3	F	5159	LHG	C10-C11-C12-C13
3	H	7158	LHG	C31-C32-C33-C34
3	I	8159	LHG	C10-C11-C12-C13
3	J	9158	LHG	C31-C32-C33-C34
3	I	8158	LHG	O1-C1-C2-O2
3	J	9158	LHG	O1-C1-C2-O2
3	A	559	LHG	C14-C15-C16-C17
3	B	1159	LHG	C14-C15-C16-C17
3	D	3158	LHG	C31-C32-C33-C34
3	F	5159	LHG	C14-C15-C16-C17
3	G	6158	LHG	C31-C32-C33-C34
3	H	7159	LHG	C14-C15-C16-C17
3	F	5159	LHG	C26-C27-C28-C29
4	C	1001	UMQ	CH-CI-CJ-CK
3	A	559	LHG	C26-C27-C28-C29
3	G	6159	LHG	C26-C27-C28-C29
3	C	2159	LHG	C26-C27-C28-C29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	I	8159	LHG	C26-C27-C28-C29
3	H	7158	LHG	C29-C30-C31-C32
3	E	4159	LHG	C26-C27-C28-C29
3	B	1159	LHG	C26-C27-C28-C29
3	D	3158	LHG	C29-C30-C31-C32
3	D	3159	LHG	C26-C27-C28-C29
3	E	4158	LHG	C29-C30-C31-C32
3	H	7159	LHG	C26-C27-C28-C29
3	G	6158	LHG	C29-C30-C31-C32
3	J	9158	LHG	C29-C30-C31-C32
3	A	558	LHG	C29-C30-C31-C32
3	B	1158	LHG	C29-C30-C31-C32
3	F	5158	LHG	C29-C30-C31-C32
3	C	2158	LHG	C29-C30-C31-C32
3	I	8158	LHG	C29-C30-C31-C32
4	F	1002	UMQ	CD-CF-CG-CH
4	F	1002	UMQ	CH-CI-CJ-CK
3	B	1159	LHG	C15-C16-C17-C18
3	H	7159	LHG	C15-C16-C17-C18
3	J	9159	LHG	C31-C32-C33-C34
3	D	3159	LHG	C15-C16-C17-C18
3	E	4159	LHG	C15-C16-C17-C18
3	F	5159	LHG	C15-C16-C17-C18
3	G	6159	LHG	C15-C16-C17-C18
3	C	2159	LHG	C15-C16-C17-C18
3	C	2159	LHG	C31-C32-C33-C34
3	I	8159	LHG	C31-C32-C33-C34
3	A	559	LHG	C31-C32-C33-C34
3	C	2158	LHG	C28-C29-C30-C31
3	E	4159	LHG	C31-C32-C33-C34
3	F	5159	LHG	C31-C32-C33-C34
3	J	9158	LHG	C28-C29-C30-C31
3	A	559	LHG	C15-C16-C17-C18
3	B	1159	LHG	C31-C32-C33-C34
3	D	3159	LHG	C31-C32-C33-C34
3	H	7159	LHG	C31-C32-C33-C34
3	G	6159	LHG	C31-C32-C33-C34
3	I	8159	LHG	C15-C16-C17-C18
3	F	5158	LHG	C28-C29-C30-C31
3	J	9159	LHG	C15-C16-C17-C18
3	A	558	LHG	C28-C29-C30-C31
3	B	1158	LHG	C27-C28-C29-C30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	B	1158	LHG	C28-C29-C30-C31
3	G	6158	LHG	C28-C29-C30-C31
3	I	8158	LHG	C28-C29-C30-C31
3	E	4158	LHG	C27-C28-C29-C30
3	I	8158	LHG	C27-C28-C29-C30
3	A	558	LHG	C27-C28-C29-C30
3	D	3158	LHG	C27-C28-C29-C30
3	D	3158	LHG	C28-C29-C30-C31
3	E	4158	LHG	C28-C29-C30-C31
3	G	6158	LHG	C27-C28-C29-C30
3	H	7158	LHG	C28-C29-C30-C31
3	H	7158	LHG	C27-C28-C29-C30
3	C	2158	LHG	C27-C28-C29-C30
3	J	9158	LHG	C27-C28-C29-C30
3	F	5158	LHG	C27-C28-C29-C30
4	C	1001	UMQ	CB-CC-CD-CF
3	B	1158	LHG	C25-C26-C27-C28
3	G	6158	LHG	C25-C26-C27-C28
3	E	4158	LHG	C25-C26-C27-C28
4	C	1001	UMQ	CG-CH-CI-CJ
3	J	9158	LHG	C25-C26-C27-C28
3	A	558	LHG	C25-C26-C27-C28
3	H	7158	LHG	C25-C26-C27-C28
3	I	8158	LHG	C25-C26-C27-C28
3	D	3158	LHG	C25-C26-C27-C28
3	F	5158	LHG	C25-C26-C27-C28
3	C	2158	LHG	C25-C26-C27-C28
3	C	2159	LHG	C28-C29-C30-C31
3	F	5159	LHG	C28-C29-C30-C31
3	A	559	LHG	C28-C29-C30-C31
3	G	6159	LHG	C28-C29-C30-C31
3	E	4159	LHG	C28-C29-C30-C31
3	J	9159	LHG	C28-C29-C30-C31
3	B	1159	LHG	C28-C29-C30-C31
3	D	3159	LHG	C28-C29-C30-C31
3	I	8158	LHG	C23-C24-C25-C26
3	J	9158	LHG	C23-C24-C25-C26
3	H	7159	LHG	C28-C29-C30-C31
3	I	8159	LHG	C28-C29-C30-C31
4	F	1002	UMQ	CB-CC-CD-CF
3	J	9158	LHG	C34-C35-C36-C37
3	A	558	LHG	C23-C24-C25-C26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	I	8158	LHG	C34-C35-C36-C37
3	E	4159	LHG	C35-C36-C37-C38
3	G	6159	LHG	C35-C36-C37-C38
3	F	5159	LHG	C11-C12-C13-C14
3	C	2158	LHG	C34-C35-C36-C37
3	H	7158	LHG	C34-C35-C36-C37
3	B	1159	LHG	C35-C36-C37-C38
3	D	3159	LHG	C35-C36-C37-C38
3	H	7159	LHG	C35-C36-C37-C38
3	I	8159	LHG	C35-C36-C37-C38
3	A	558	LHG	C34-C35-C36-C37
3	D	3158	LHG	C34-C35-C36-C37
3	I	8159	LHG	C11-C12-C13-C14
3	A	559	LHG	C35-C36-C37-C38
3	B	1158	LHG	C14-C15-C16-C17
3	I	8158	LHG	C14-C15-C16-C17
3	C	2159	LHG	C11-C12-C13-C14
3	E	4159	LHG	C11-C12-C13-C14
3	F	5158	LHG	C34-C35-C36-C37
3	G	6158	LHG	C34-C35-C36-C37
3	C	2158	LHG	C23-C24-C25-C26
3	C	2158	LHG	C12-C13-C14-C15
3	D	3158	LHG	C14-C15-C16-C17
3	A	559	LHG	C11-C12-C13-C14
3	E	4158	LHG	C34-C35-C36-C37
3	J	9159	LHG	C35-C36-C37-C38
3	C	2159	LHG	C35-C36-C37-C38
3	F	5159	LHG	C35-C36-C37-C38
3	B	1159	LHG	C11-C12-C13-C14
3	F	5158	LHG	C23-C24-C25-C26
3	D	3159	LHG	C11-C12-C13-C14
3	H	7159	LHG	C11-C12-C13-C14
4	C	1001	UMQ	CI-CJ-CK-CL
3	E	4158	LHG	C14-C15-C16-C17
3	A	558	LHG	C14-C15-C16-C17
3	B	1158	LHG	C34-C35-C36-C37
3	G	6158	LHG	C23-C24-C25-C26
3	H	7158	LHG	C23-C24-C25-C26
3	G	6159	LHG	C11-C12-C13-C14
3	F	5158	LHG	C12-C13-C14-C15
3	J	9158	LHG	C14-C15-C16-C17
4	F	1002	UMQ	C2'-C1'-O1'-CA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	H	7158	LHG	C14-C15-C16-C17
3	G	6158	LHG	C14-C15-C16-C17
3	D	3158	LHG	C23-C24-C25-C26
3	J	9159	LHG	C11-C12-C13-C14
3	C	2159	LHG	C27-C28-C29-C30
3	I	8159	LHG	C4-C5-C6-O8
3	F	5159	LHG	C27-C28-C29-C30
3	H	7159	LHG	C27-C28-C29-C30
3	A	559	LHG	C27-C28-C29-C30
3	D	3159	LHG	C27-C28-C29-C30
3	E	4159	LHG	C27-C28-C29-C30
3	G	6159	LHG	C27-C28-C29-C30
3	I	8159	LHG	C27-C28-C29-C30
3	C	2158	LHG	C14-C15-C16-C17
3	A	558	LHG	C12-C13-C14-C15
3	H	7158	LHG	C12-C13-C14-C15
3	B	1159	LHG	C27-C28-C29-C30
3	F	5158	LHG	C14-C15-C16-C17
3	I	8158	LHG	C12-C13-C14-C15
3	B	1158	LHG	C12-C13-C14-C15
3	G	6158	LHG	C12-C13-C14-C15
3	I	8158	LHG	C24-C25-C26-C27
3	J	9159	LHG	C27-C28-C29-C30
3	B	1158	LHG	C23-C24-C25-C26
3	E	4158	LHG	C23-C24-C25-C26
4	F	1002	UMQ	CF-CG-CH-CI
3	J	9158	LHG	C12-C13-C14-C15
3	E	4158	LHG	C12-C13-C14-C15
3	D	3158	LHG	C12-C13-C14-C15
3	I	8159	LHG	C34-C35-C36-C37
3	I	8158	LHG	C19-C20-C21-C22
3	E	4159	LHG	C34-C35-C36-C37
3	G	6159	LHG	C34-C35-C36-C37
3	A	559	LHG	C34-C35-C36-C37
3	H	7159	LHG	C34-C35-C36-C37
3	B	1159	LHG	C34-C35-C36-C37
3	D	3159	LHG	C34-C35-C36-C37
3	A	559	LHG	C4-C5-C6-O8
3	B	1159	LHG	C4-C5-C6-O8
3	D	3159	LHG	C4-C5-C6-O8
3	E	4159	LHG	C4-C5-C6-O8
3	F	5159	LHG	C4-C5-C6-O8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	G	6159	LHG	C4-C5-C6-O8
3	H	7159	LHG	C4-C5-C6-O8
3	D	3158	LHG	C24-C25-C26-C27
3	J	9158	LHG	C19-C20-C21-C22
3	C	2159	LHG	C34-C35-C36-C37
3	H	7158	LHG	C24-C25-C26-C27
3	F	5159	LHG	C34-C35-C36-C37
3	B	1158	LHG	C24-C25-C26-C27
3	C	2158	LHG	C24-C25-C26-C27
3	J	9158	LHG	C2-C3-O3-P
4	C	1001	UMQ	CD-CF-CG-CH
3	A	558	LHG	C19-C20-C21-C22
3	F	5158	LHG	C19-C20-C21-C22
3	E	4158	LHG	C24-C25-C26-C27
3	G	6158	LHG	C24-C25-C26-C27
3	A	558	LHG	C24-C25-C26-C27
3	F	5158	LHG	C24-C25-C26-C27
3	D	3158	LHG	C19-C20-C21-C22
3	I	8159	LHG	C33-C34-C35-C36
3	J	9159	LHG	C34-C35-C36-C37
3	J	9158	LHG	C24-C25-C26-C27
3	B	1158	LHG	C2-C3-O3-P
3	D	3158	LHG	C2-C3-O3-P
3	E	4158	LHG	C2-C3-O3-P
3	H	7158	LHG	C2-C3-O3-P
3	I	8158	LHG	C2-C3-O3-P
3	E	4158	LHG	C19-C20-C21-C22
3	A	559	LHG	C33-C34-C35-C36
3	E	4158	LHG	C26-C27-C28-C29
3	C	2159	LHG	C33-C34-C35-C36
3	D	3158	LHG	C26-C27-C28-C29
3	G	6158	LHG	C26-C27-C28-C29
3	J	9159	LHG	C33-C34-C35-C36
3	A	559	LHG	O7-C5-C6-O8
3	B	1159	LHG	O7-C5-C6-O8
3	C	2159	LHG	O7-C5-C6-O8
3	D	3159	LHG	O7-C5-C6-O8
3	E	4159	LHG	O7-C5-C6-O8
3	F	5159	LHG	O7-C5-C6-O8
3	G	6159	LHG	O7-C5-C6-O8
3	H	7159	LHG	O7-C5-C6-O8
3	I	8159	LHG	O7-C5-C6-O8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	J	9159	LHG	O7-C5-C6-O8
3	H	7159	LHG	C33-C34-C35-C36
3	F	5159	LHG	C33-C34-C35-C36
3	C	2159	LHG	C4-C5-C6-O8
3	J	9159	LHG	C4-C5-C6-O8
3	G	6159	LHG	C33-C34-C35-C36
3	H	7158	LHG	C26-C27-C28-C29
3	B	1158	LHG	C26-C27-C28-C29
3	H	7158	LHG	C19-C20-C21-C22
3	B	1159	LHG	C33-C34-C35-C36
4	F	1002	UMQ	O5'-C1'-O1'-CA
3	C	2158	LHG	C19-C20-C21-C22
3	D	3159	LHG	C33-C34-C35-C36
3	H	7158	LHG	C4-O6-P-O5
3	B	1158	LHG	C19-C20-C21-C22
3	A	558	LHG	C2-C3-O3-P
3	C	2158	LHG	C2-C3-O3-P
3	F	5158	LHG	C2-C3-O3-P
3	G	6158	LHG	C2-C3-O3-P
3	G	6158	LHG	C19-C20-C21-C22
3	A	558	LHG	C26-C27-C28-C29
3	E	4159	LHG	C33-C34-C35-C36
3	I	8159	LHG	C18-C19-C20-C21
3	I	8158	LHG	C26-C27-C28-C29
3	F	5158	LHG	C26-C27-C28-C29
3	J	9158	LHG	C26-C27-C28-C29
4	C	1001	UMQ	CF-CG-CH-CI
3	C	2158	LHG	C26-C27-C28-C29
3	A	558	LHG	C4-C5-C6-O8
3	C	2158	LHG	C4-C5-C6-O8
3	E	4158	LHG	C4-C5-C6-O8
3	F	5158	LHG	C4-C5-C6-O8
3	H	7158	LHG	C4-C5-C6-O8
3	I	8158	LHG	C4-C5-C6-O8
3	J	9158	LHG	C4-C5-C6-O8
4	F	1002	UMQ	CI-CJ-CK-CL
3	B	1158	LHG	C4-C5-O7-C7
3	C	2158	LHG	C6-C5-O7-C7
3	F	5158	LHG	C6-C5-O7-C7
3	G	6158	LHG	C6-C5-O7-C7
3	J	9158	LHG	C6-C5-O7-C7
3	I	8159	LHG	C16-C17-C18-C19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	559	LHG	C18-C19-C20-C21
3	C	2159	LHG	C18-C19-C20-C21
3	J	9159	LHG	C18-C19-C20-C21
3	E	4159	LHG	C18-C19-C20-C21
3	H	7159	LHG	C18-C19-C20-C21
3	B	1158	LHG	C4-C5-C6-O8
3	D	3158	LHG	C4-C5-C6-O8
3	G	6158	LHG	C4-C5-C6-O8
3	G	6159	LHG	C18-C19-C20-C21
3	B	1159	LHG	C18-C19-C20-C21
3	J	9159	LHG	C12-C13-C14-C15
3	D	3159	LHG	C16-C17-C18-C19
3	E	4159	LHG	C16-C17-C18-C19
3	F	5159	LHG	C18-C19-C20-C21
3	B	1159	LHG	C16-C17-C18-C19
3	H	7159	LHG	C16-C17-C18-C19
3	G	6159	LHG	C16-C17-C18-C19
3	A	558	LHG	C4-C5-O7-C7
3	A	558	LHG	C6-C5-O7-C7
3	C	2158	LHG	C4-C5-O7-C7
3	D	3158	LHG	C4-C5-O7-C7
3	D	3158	LHG	C6-C5-O7-C7
3	E	4158	LHG	C4-C5-O7-C7
3	E	4158	LHG	C6-C5-O7-C7
3	G	6158	LHG	C4-C5-O7-C7
3	H	7158	LHG	C6-C5-O7-C7
3	I	8158	LHG	C4-C5-O7-C7
3	I	8158	LHG	C6-C5-O7-C7
3	A	559	LHG	C16-C17-C18-C19
3	J	9159	LHG	C24-C25-C26-C27
3	D	3159	LHG	C18-C19-C20-C21
3	A	559	LHG	O8-C23-C24-C25
3	B	1159	LHG	O7-C7-C8-C9
3	H	7159	LHG	O7-C7-C8-C9
3	I	8159	LHG	O7-C7-C8-C9
3	B	1159	LHG	O8-C23-C24-C25
3	D	3159	LHG	O7-C7-C8-C9
3	E	4159	LHG	O7-C7-C8-C9
3	E	4159	LHG	O8-C23-C24-C25
3	G	6159	LHG	O7-C7-C8-C9
3	H	7159	LHG	O8-C23-C24-C25
3	J	9159	LHG	O8-C23-C24-C25

Continued on next page...

Continued from previous page...

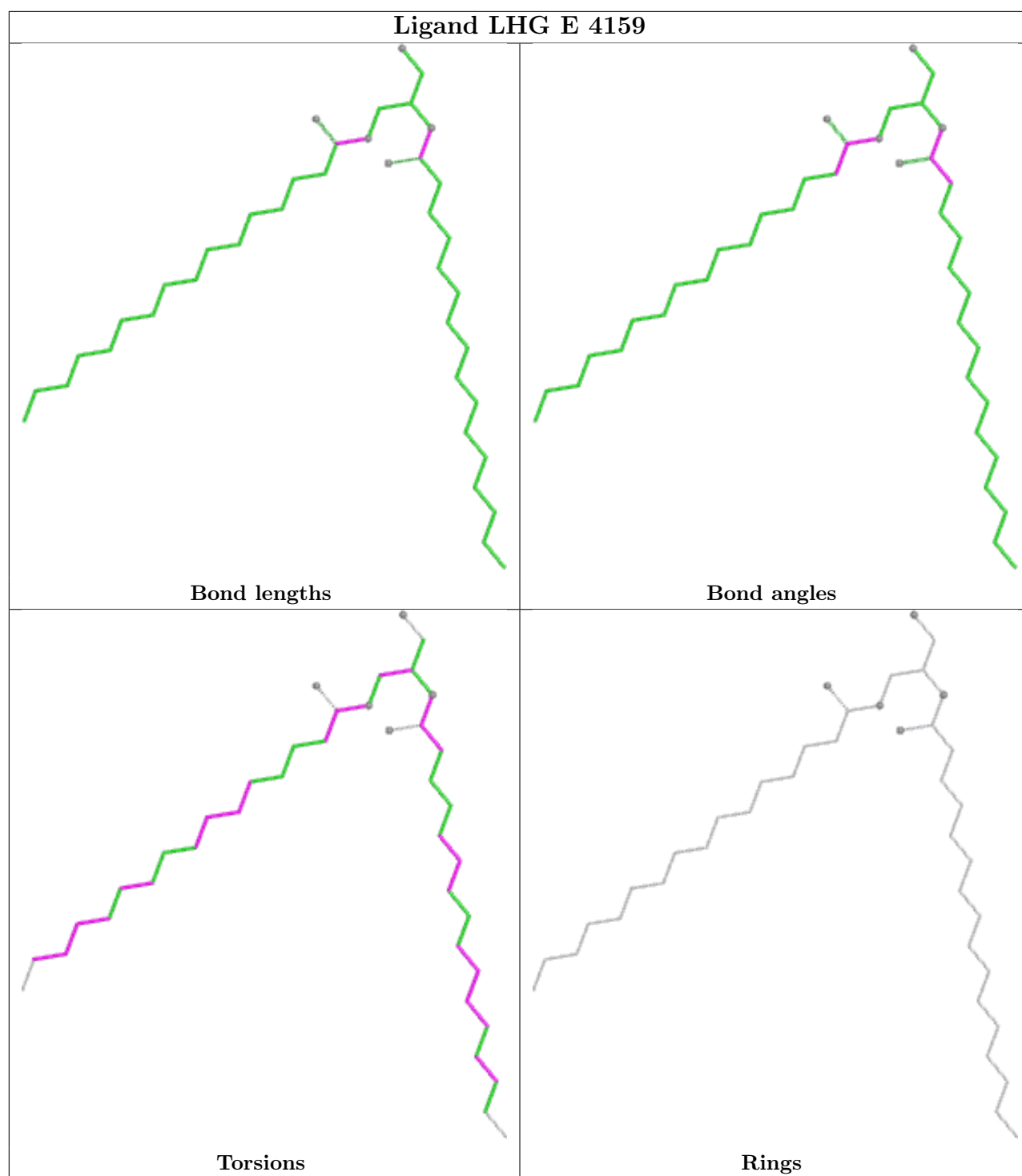
Mol	Chain	Res	Type	Atoms
3	A	559	LHG	O7-C7-C8-C9
3	D	3159	LHG	O8-C23-C24-C25
3	J	9159	LHG	O7-C7-C8-C9
3	C	2159	LHG	O8-C23-C24-C25
3	F	5159	LHG	O7-C7-C8-C9
3	G	6159	LHG	O8-C23-C24-C25
3	F	5159	LHG	O8-C23-C24-C25
3	C	2159	LHG	O7-C7-C8-C9
3	I	8159	LHG	O8-C23-C24-C25
3	C	2159	LHG	C16-C17-C18-C19
3	I	8159	LHG	C12-C13-C14-C15
3	F	5159	LHG	C16-C17-C18-C19
3	B	1158	LHG	C6-C5-O7-C7
3	F	5158	LHG	C4-C5-O7-C7
3	H	7158	LHG	C4-C5-O7-C7
3	J	9158	LHG	C4-C5-O7-C7
3	B	1158	LHG	C10-C11-C12-C13
3	A	559	LHG	O10-C23-C24-C25
3	C	2159	LHG	O9-C7-C8-C9
3	C	2159	LHG	O10-C23-C24-C25
3	F	5159	LHG	O10-C23-C24-C25
3	J	9159	LHG	O9-C7-C8-C9
3	D	3158	LHG	C10-C11-C12-C13
3	I	8159	LHG	O10-C23-C24-C25
3	D	3159	LHG	O9-C7-C8-C9
3	F	5159	LHG	O9-C7-C8-C9
3	G	6159	LHG	O10-C23-C24-C25
3	H	7159	LHG	O9-C7-C8-C9
3	A	559	LHG	O9-C7-C8-C9
3	E	4159	LHG	O9-C7-C8-C9
3	G	6159	LHG	O9-C7-C8-C9
3	B	1159	LHG	O9-C7-C8-C9
3	D	3159	LHG	O10-C23-C24-C25
3	I	8159	LHG	O9-C7-C8-C9
3	H	7158	LHG	C10-C11-C12-C13
3	B	1159	LHG	O10-C23-C24-C25
3	E	4159	LHG	O10-C23-C24-C25
3	H	7159	LHG	O10-C23-C24-C25
3	J	9159	LHG	O10-C23-C24-C25
3	G	6158	LHG	C10-C11-C12-C13
3	B	1158	LHG	O7-C7-C8-C9
3	H	7158	LHG	O7-C7-C8-C9

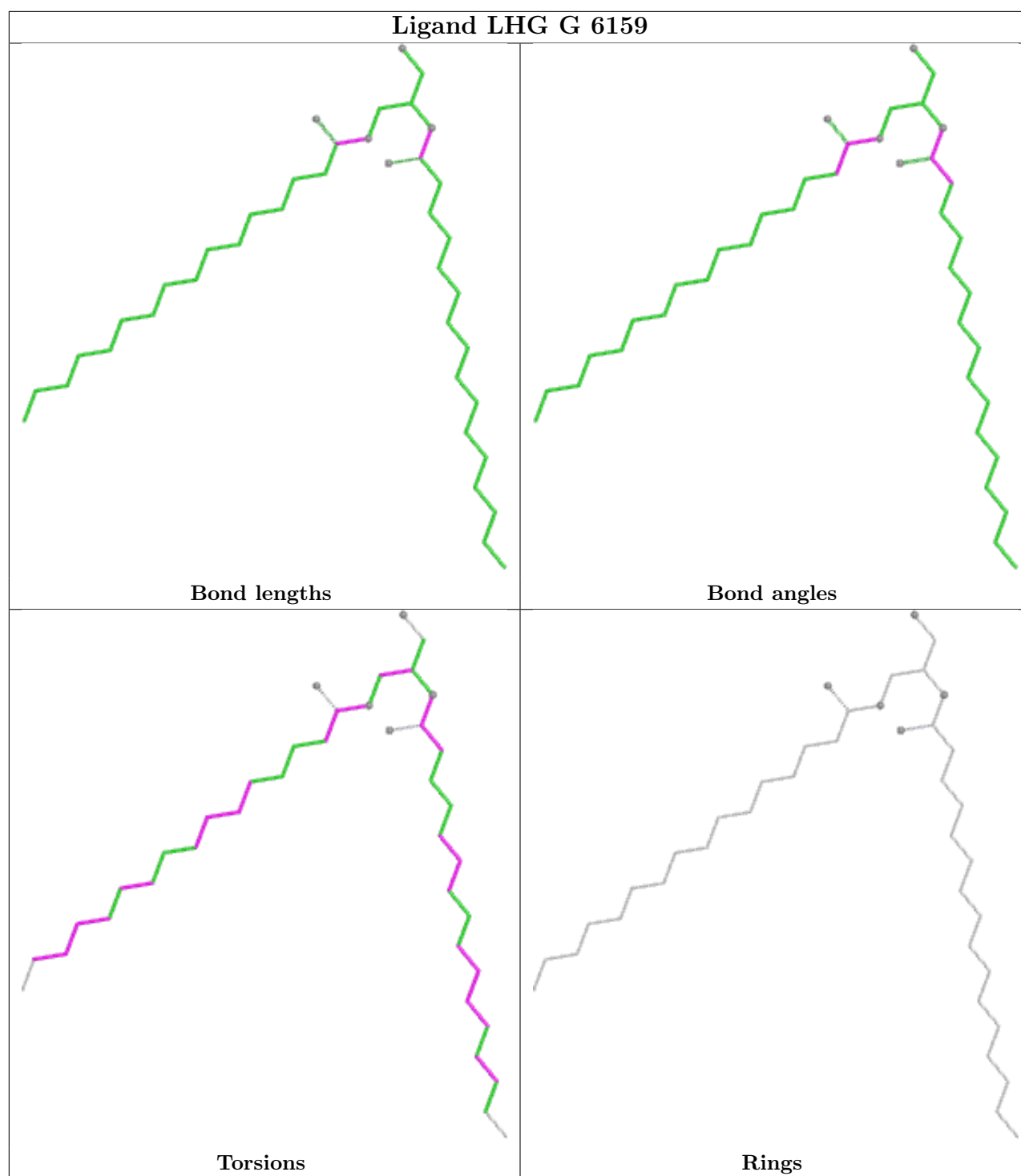
There are no ring outliers.

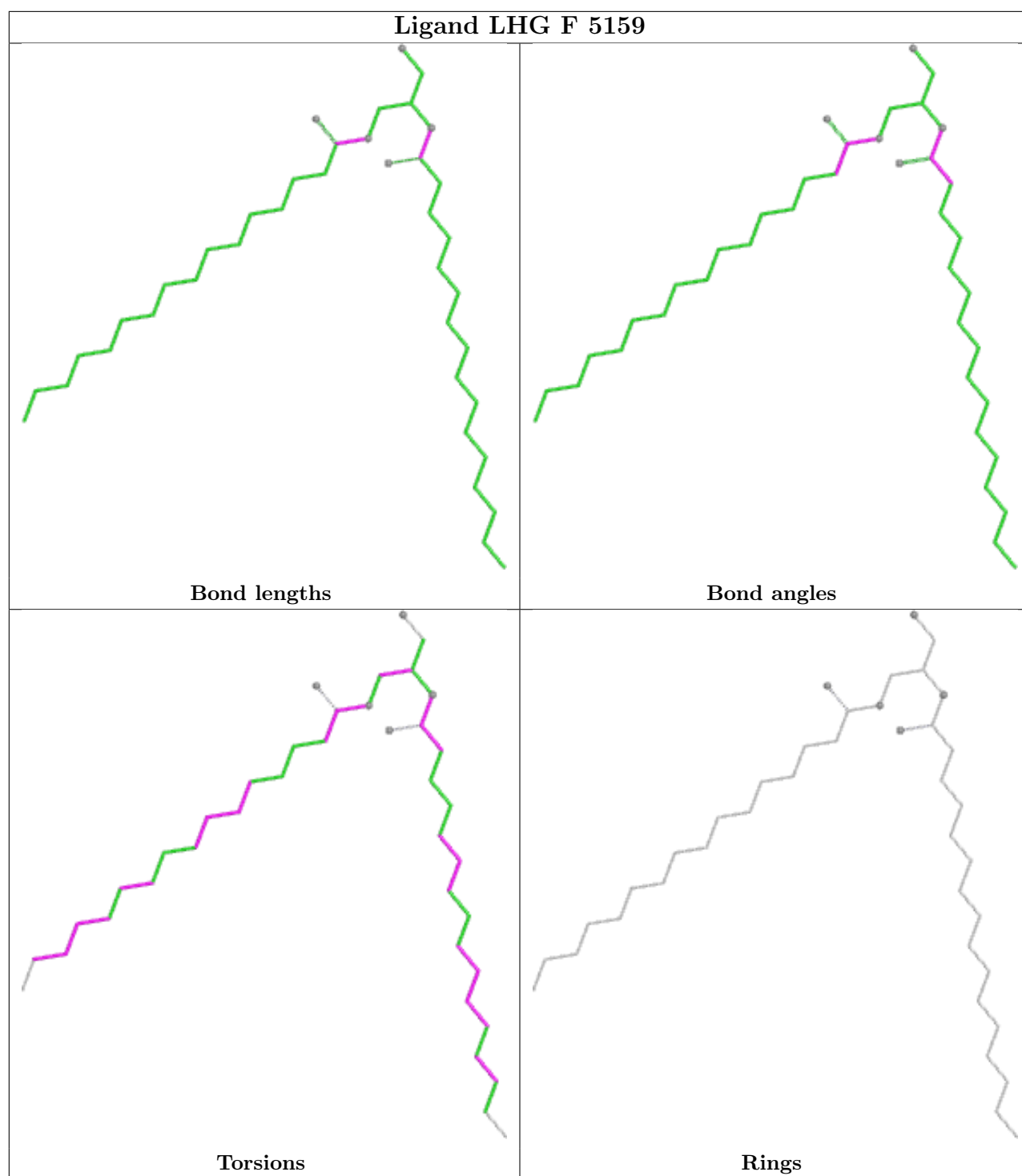
11 monomers are involved in 42 short contacts:

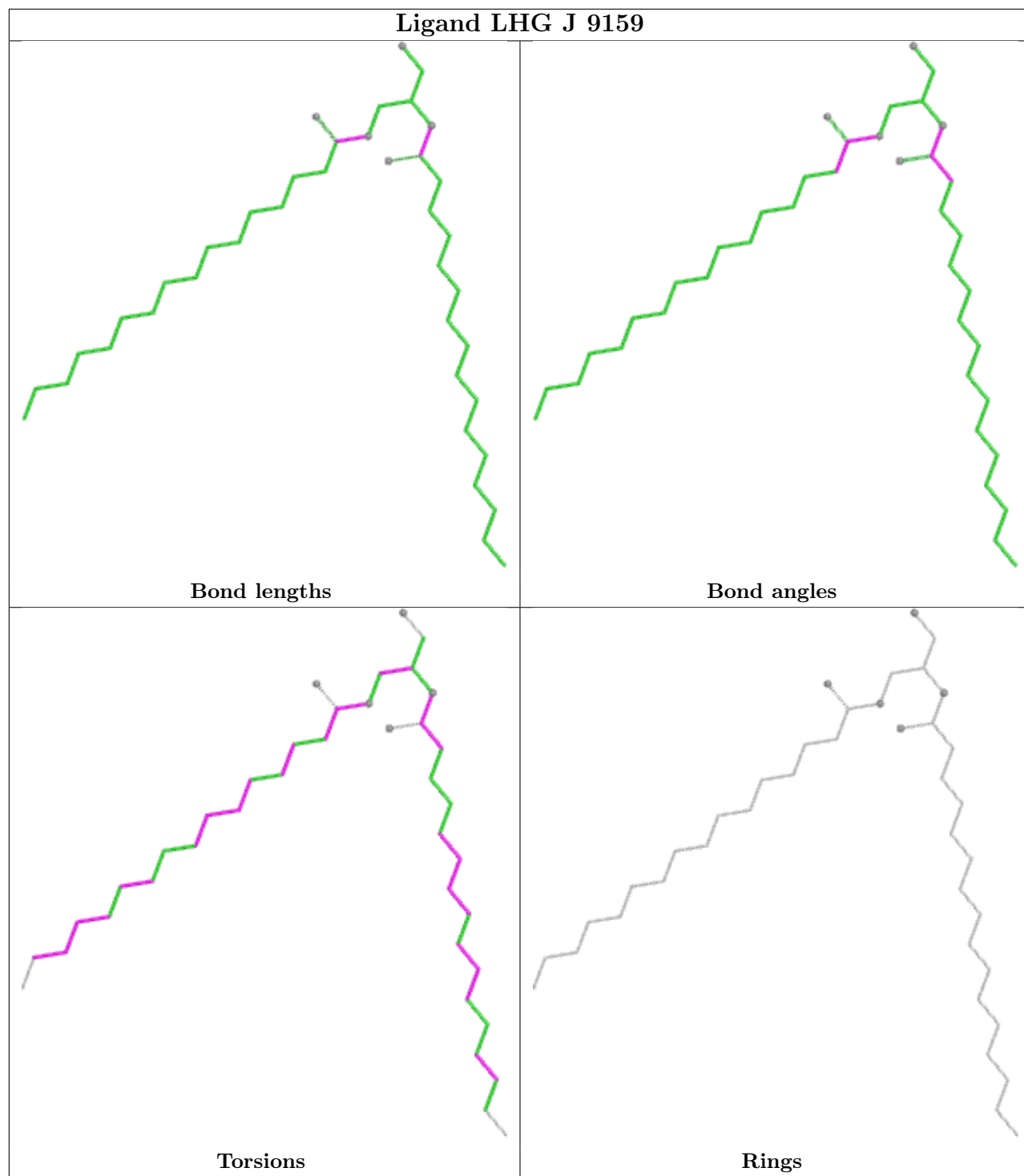
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	4159	LHG	5	0
3	G	6159	LHG	8	0
3	F	5159	LHG	6	0
3	J	9159	LHG	7	0
3	J	9158	LHG	1	0
3	H	7159	LHG	6	0
3	A	559	LHG	7	0
3	C	2159	LHG	6	0
3	B	1159	LHG	5	0
3	I	8159	LHG	4	0
3	D	3159	LHG	7	0

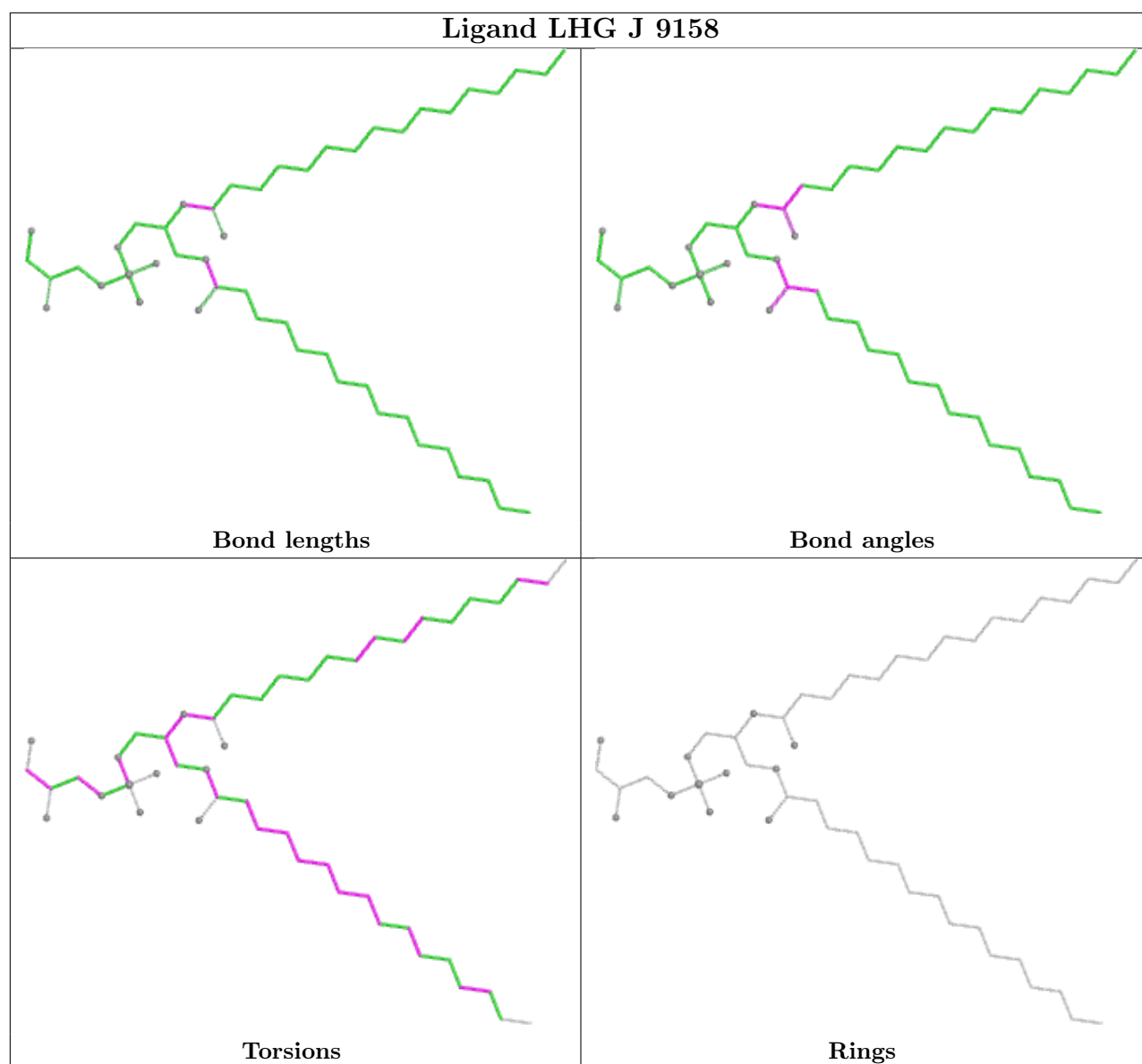
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

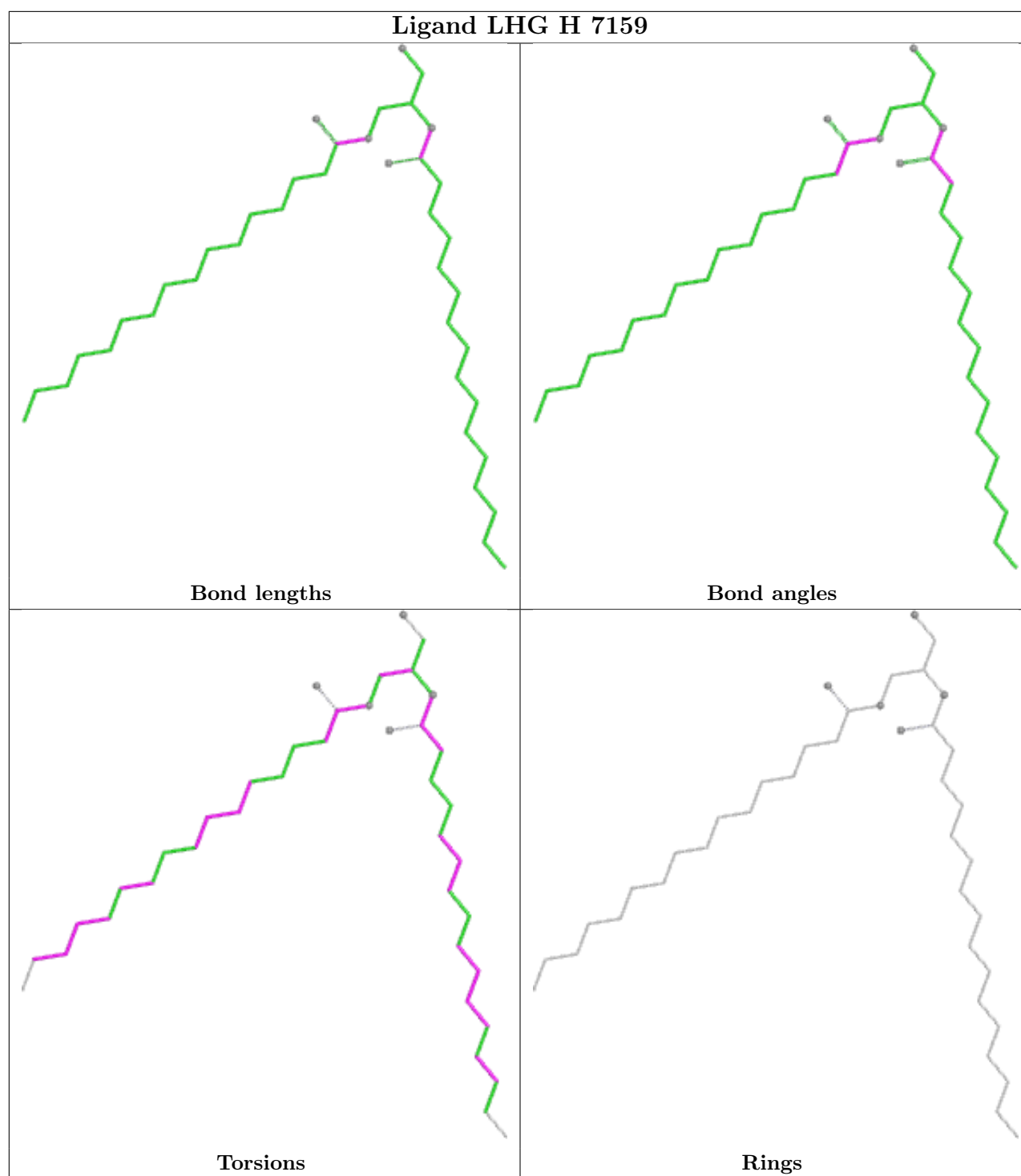


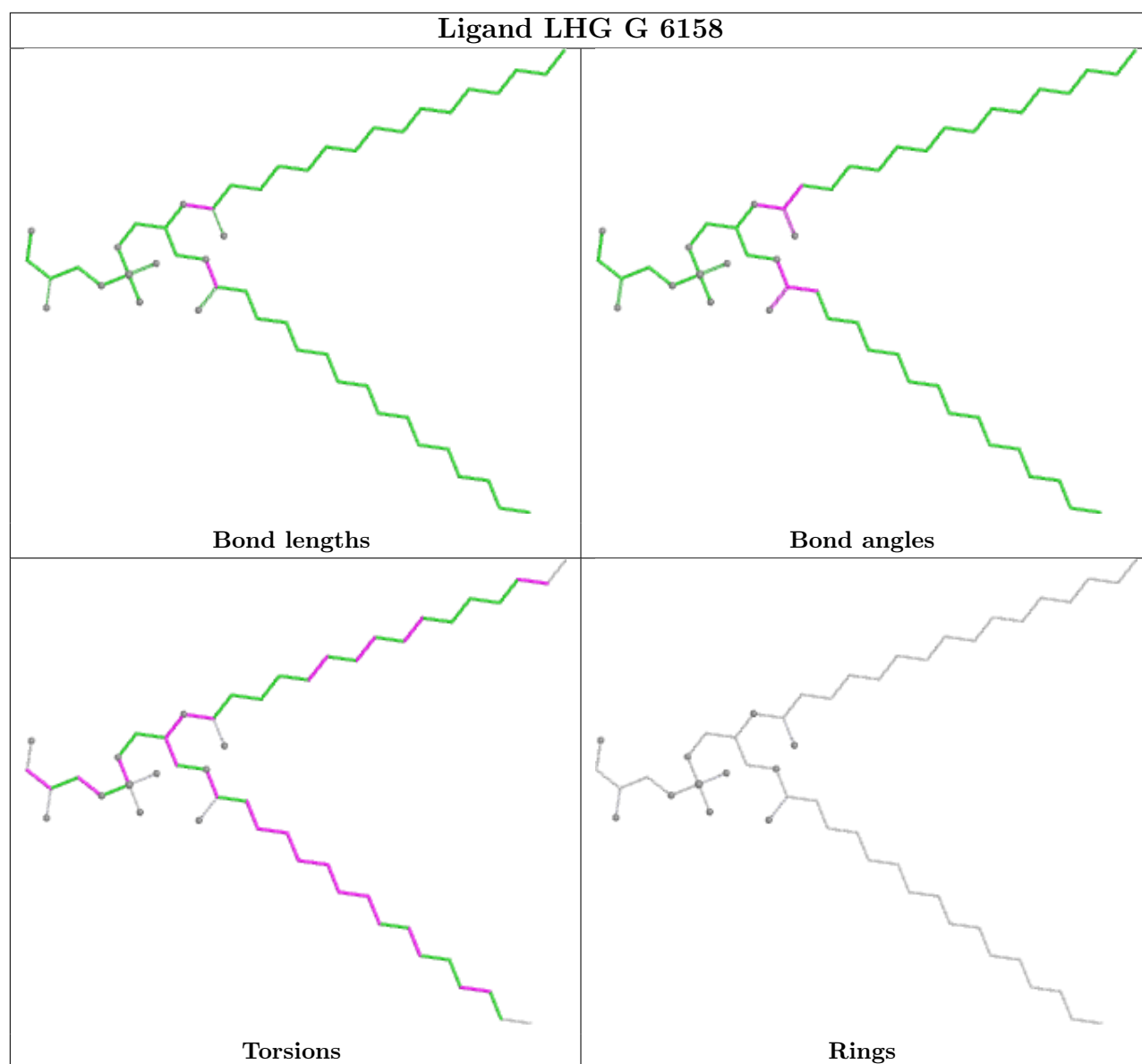


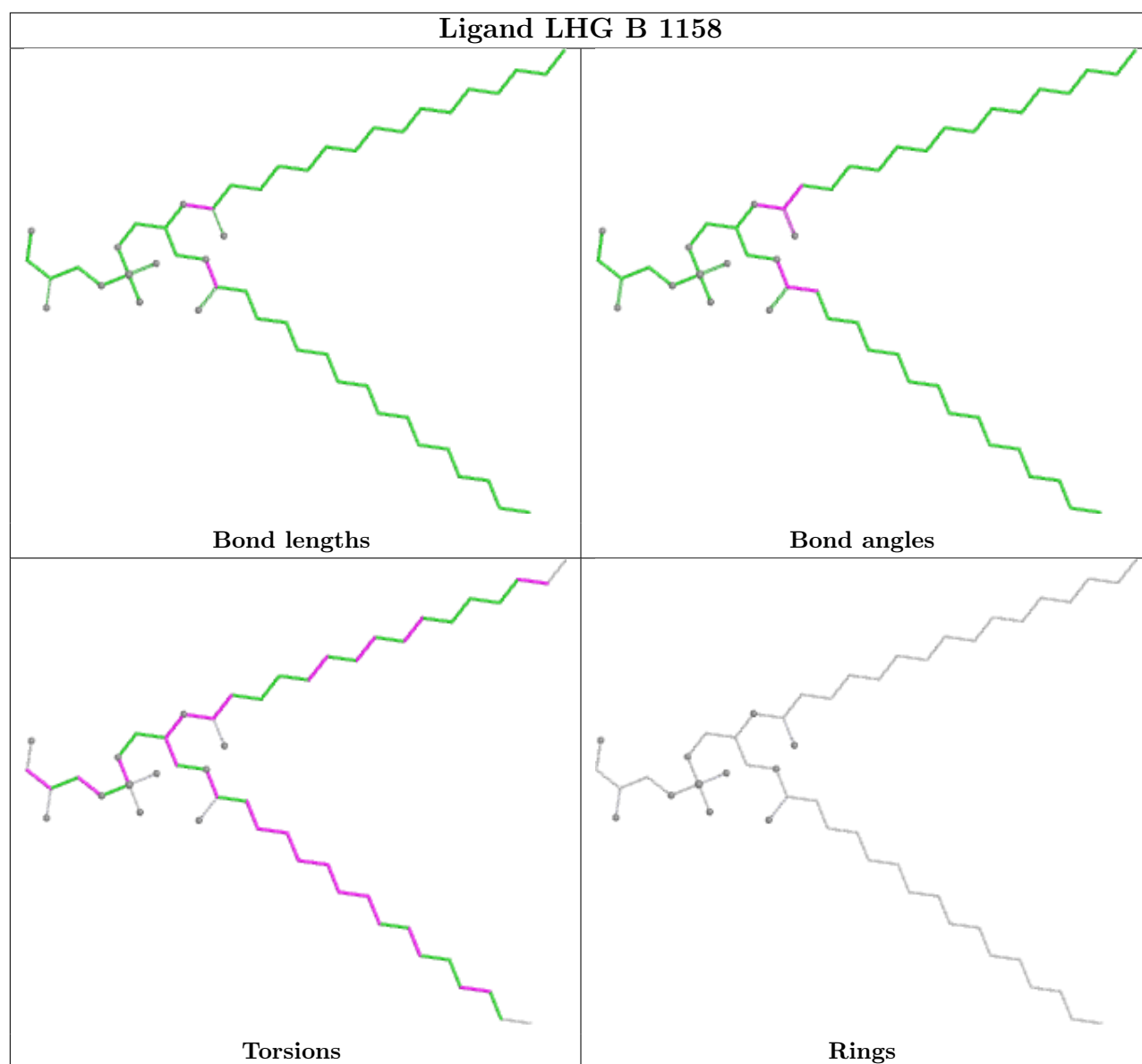


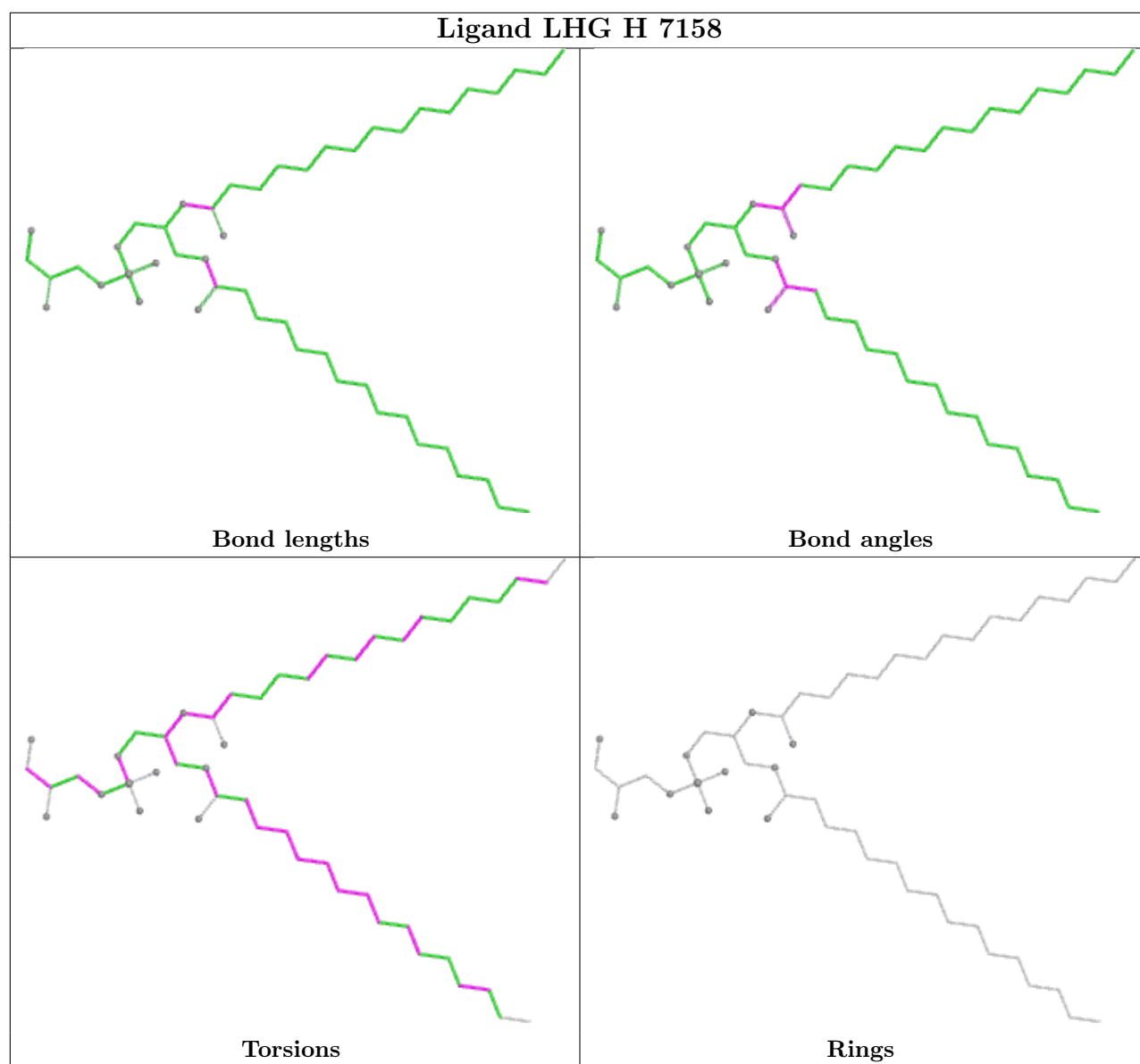


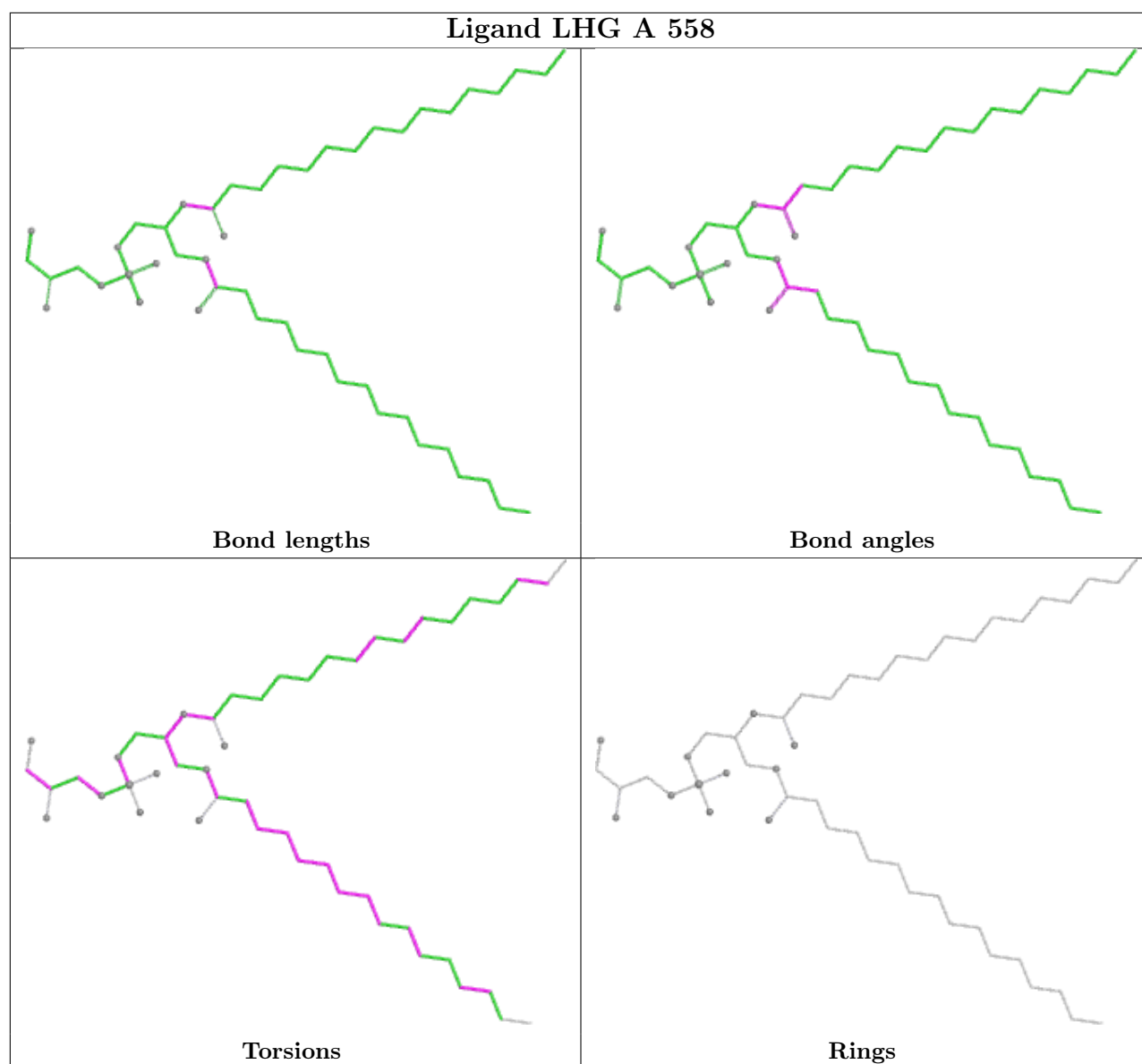


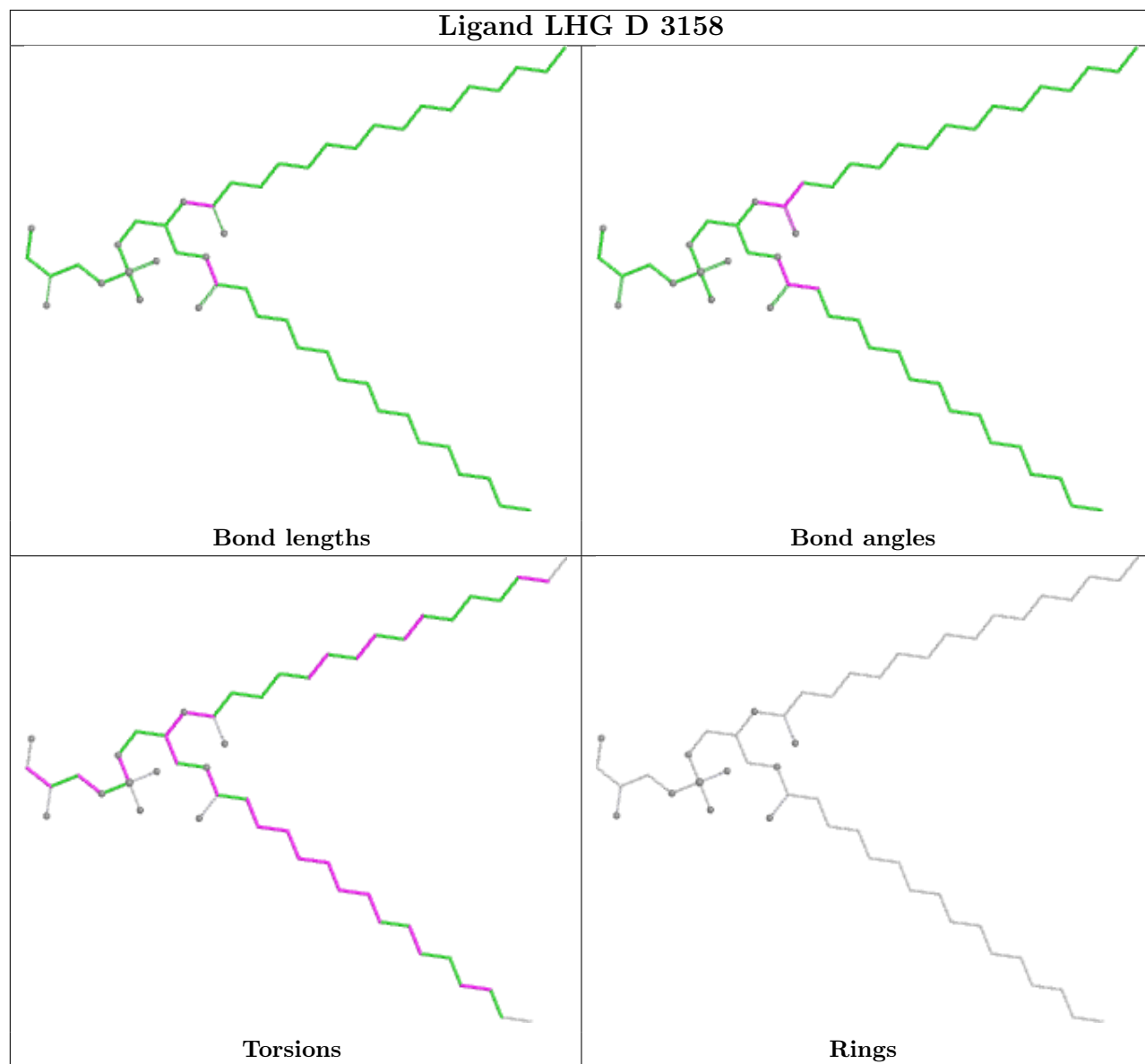


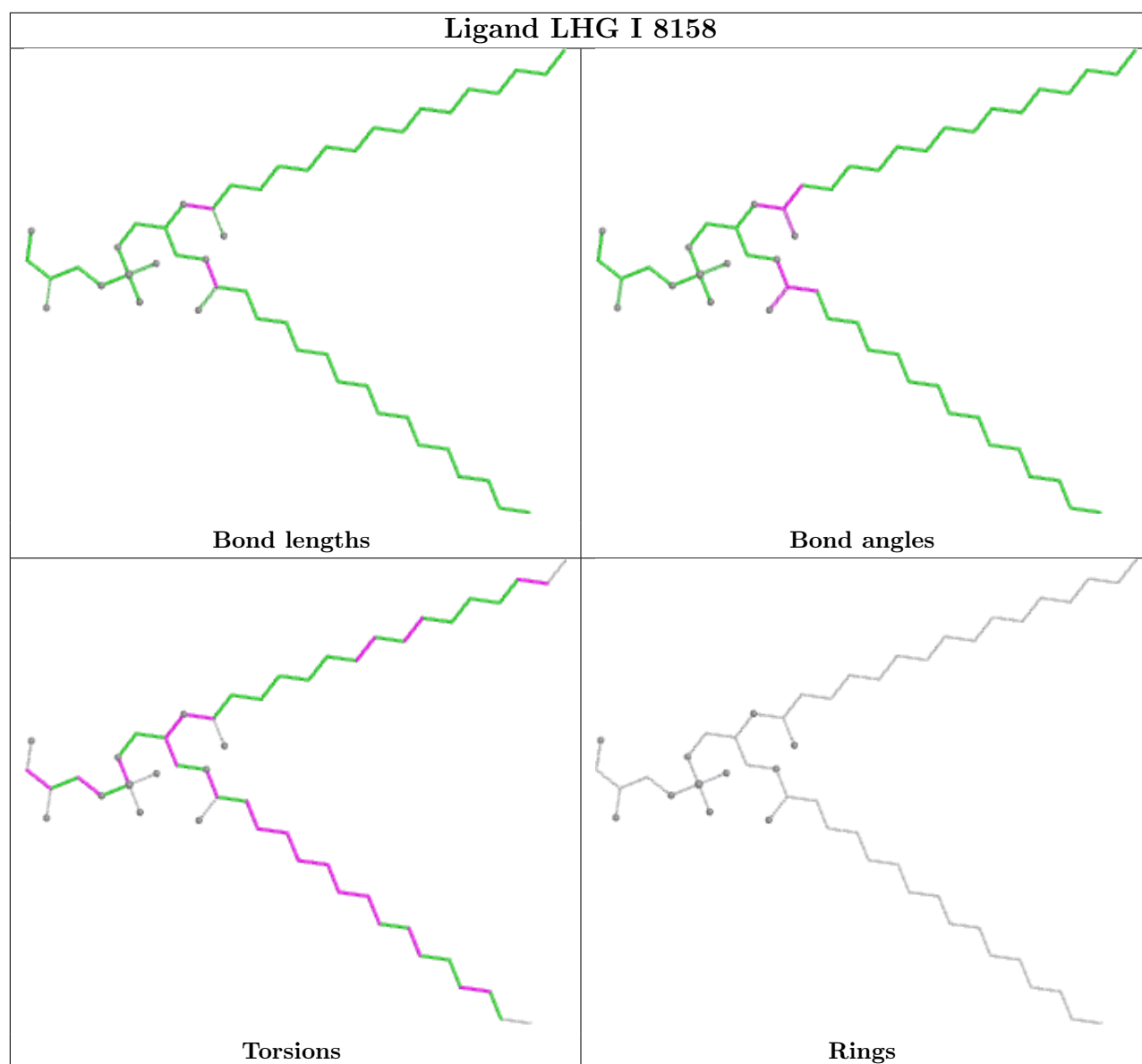


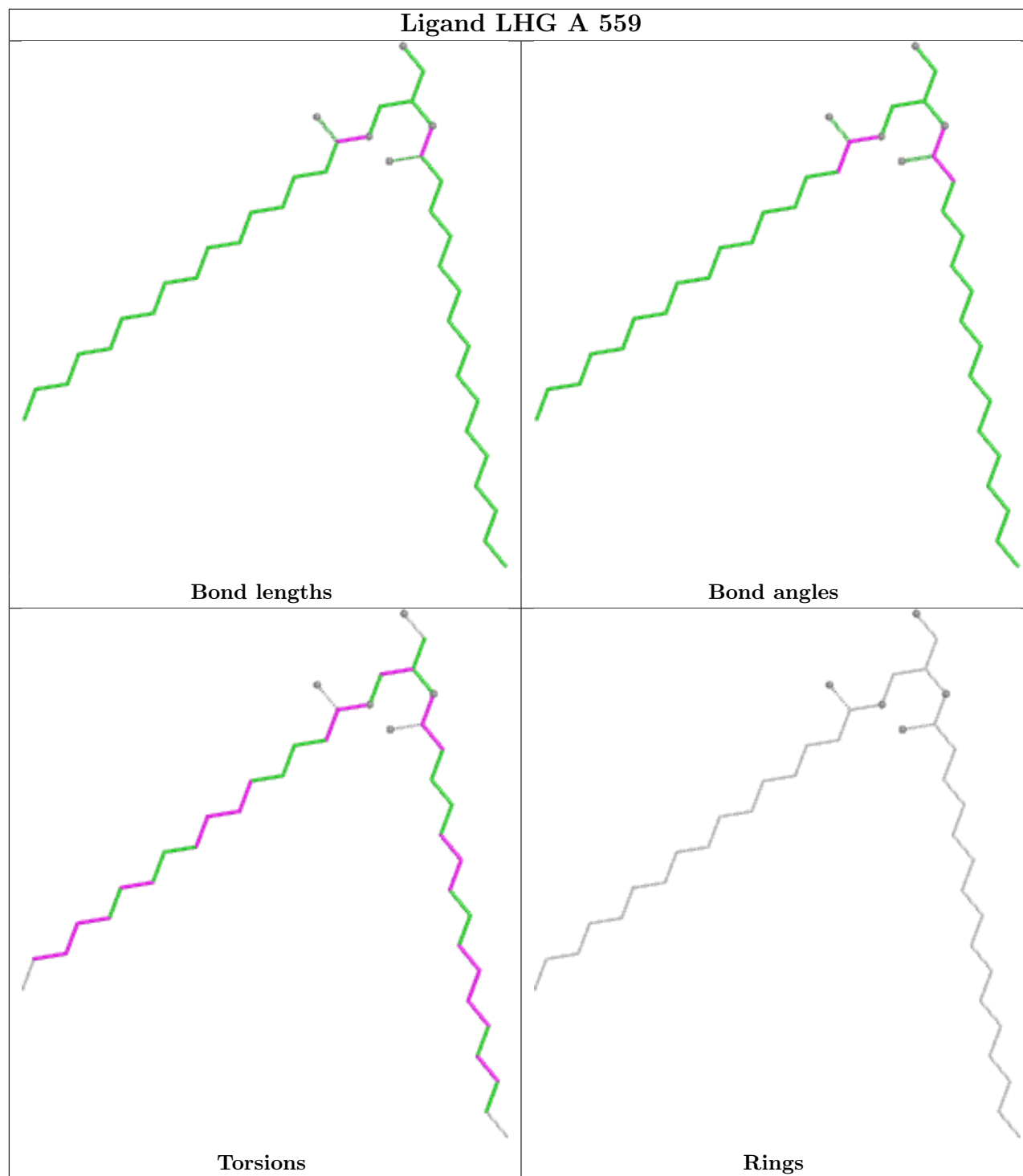


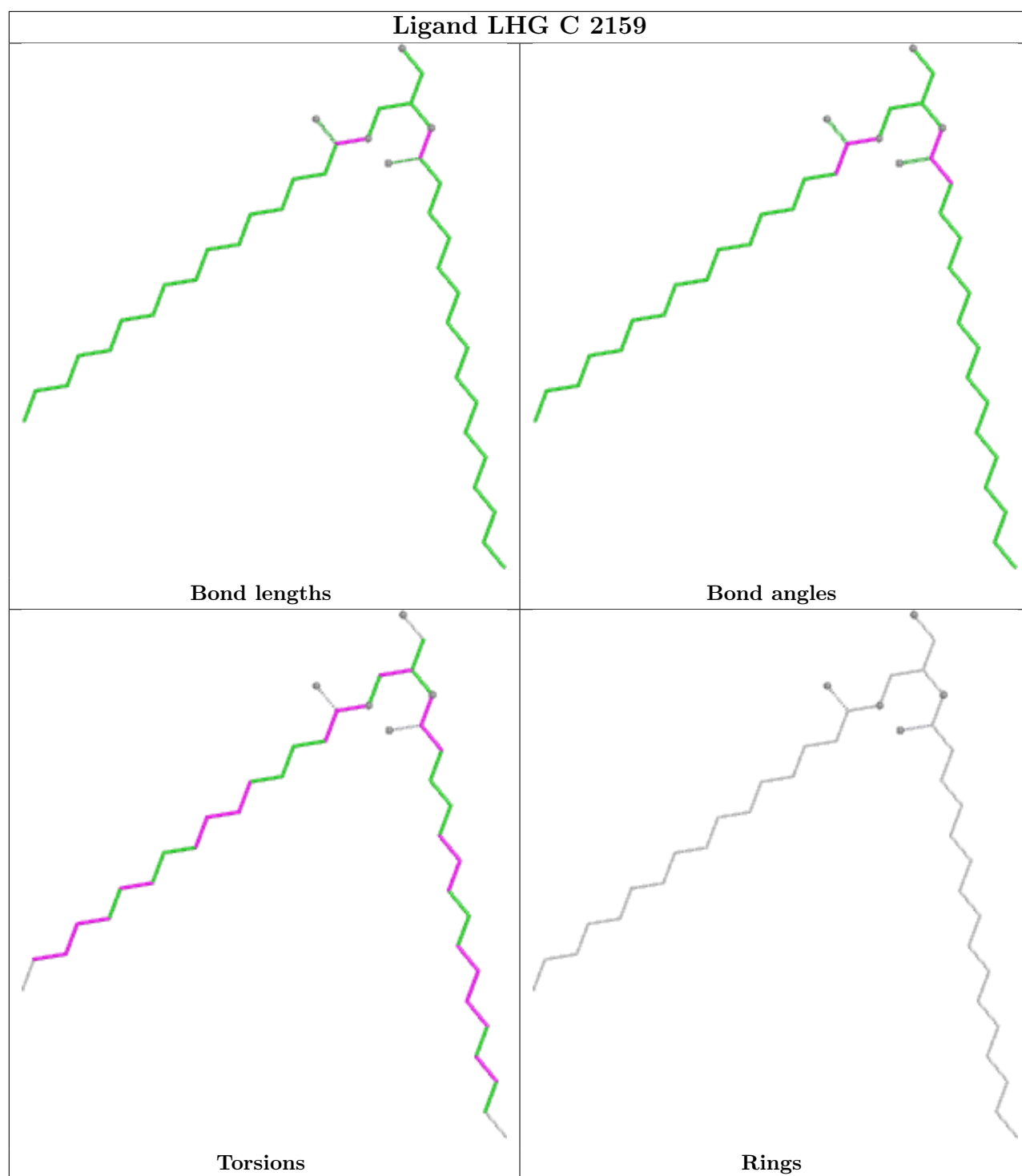


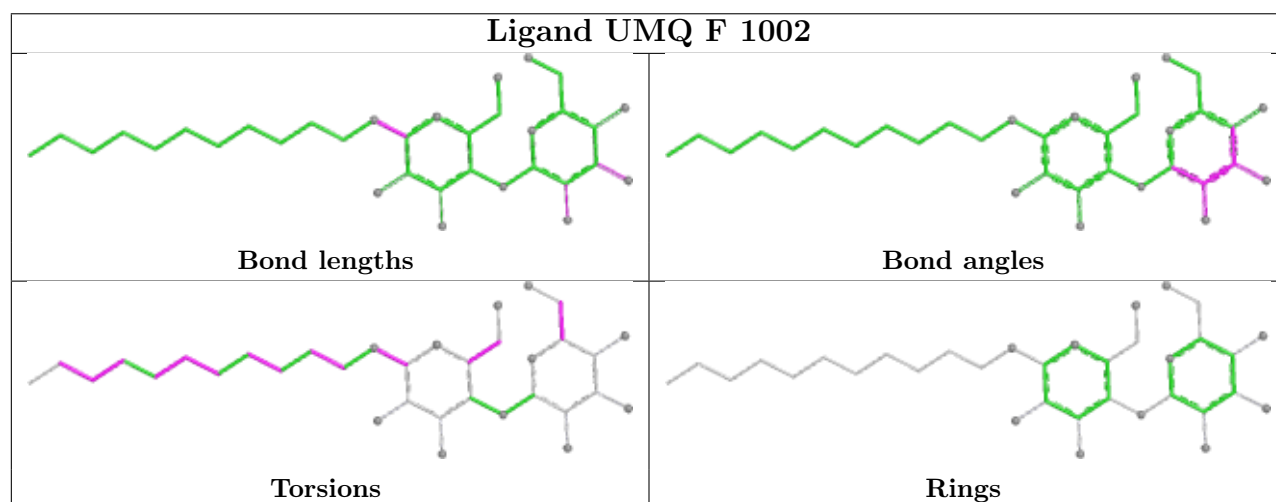
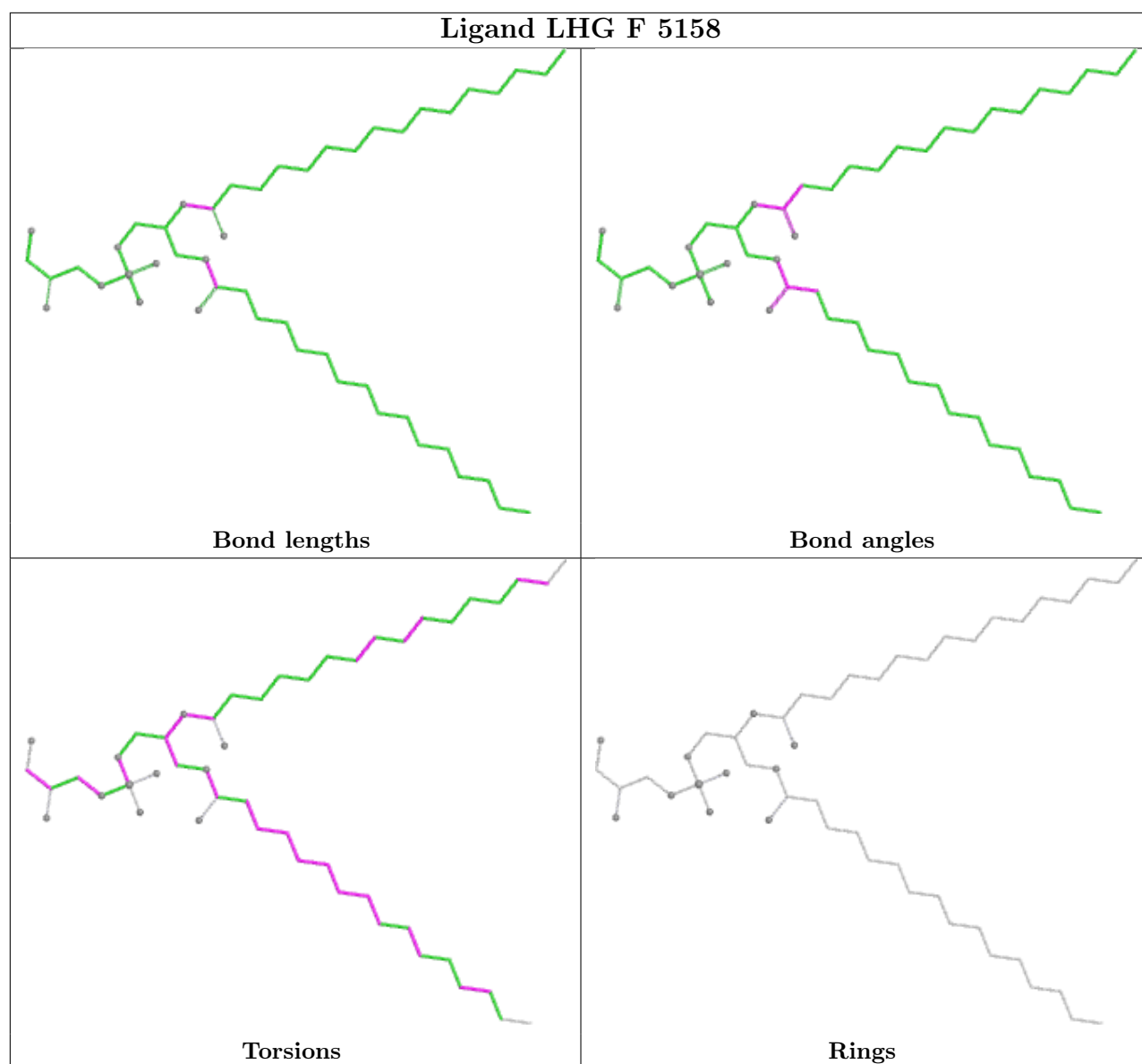


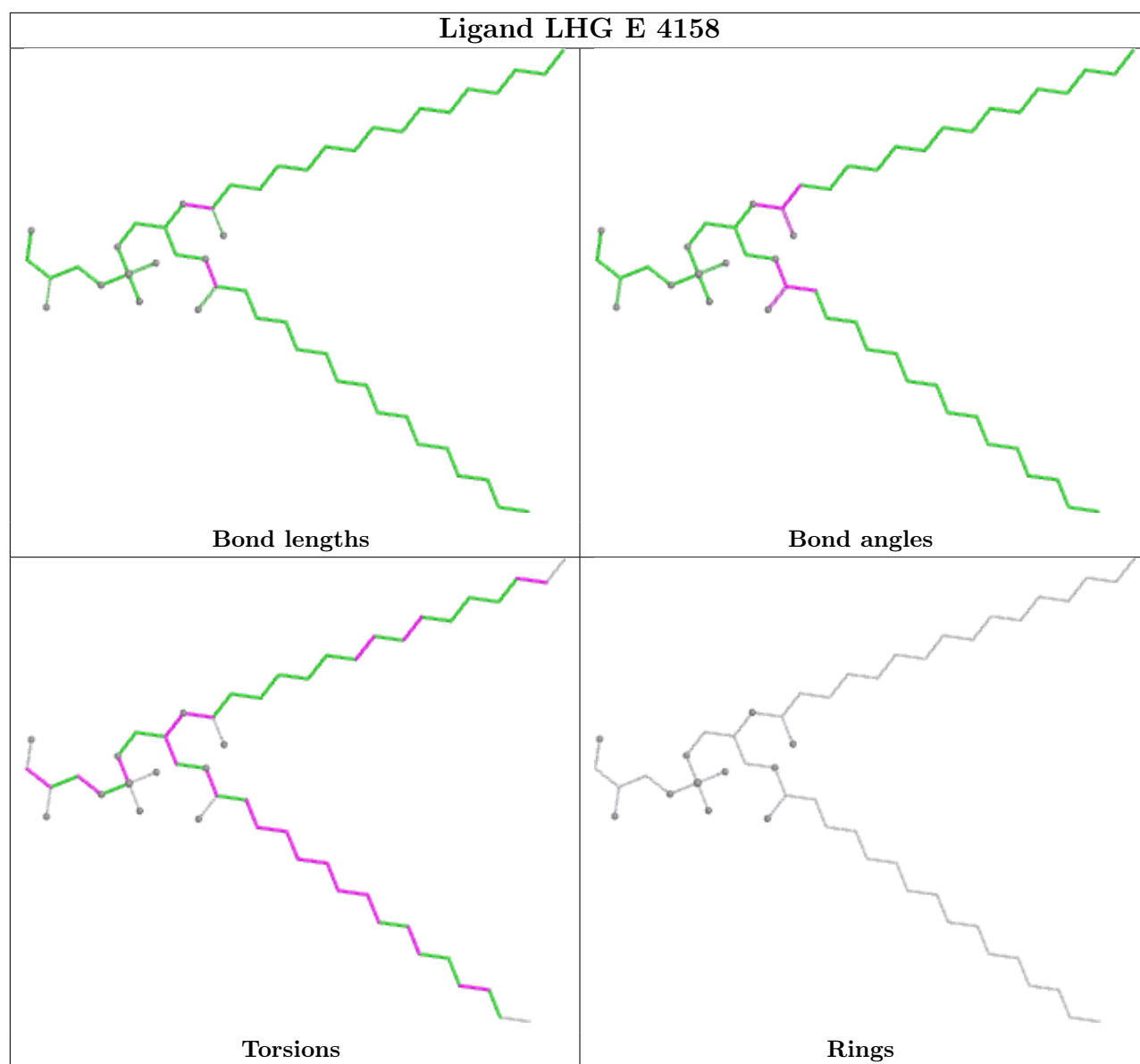


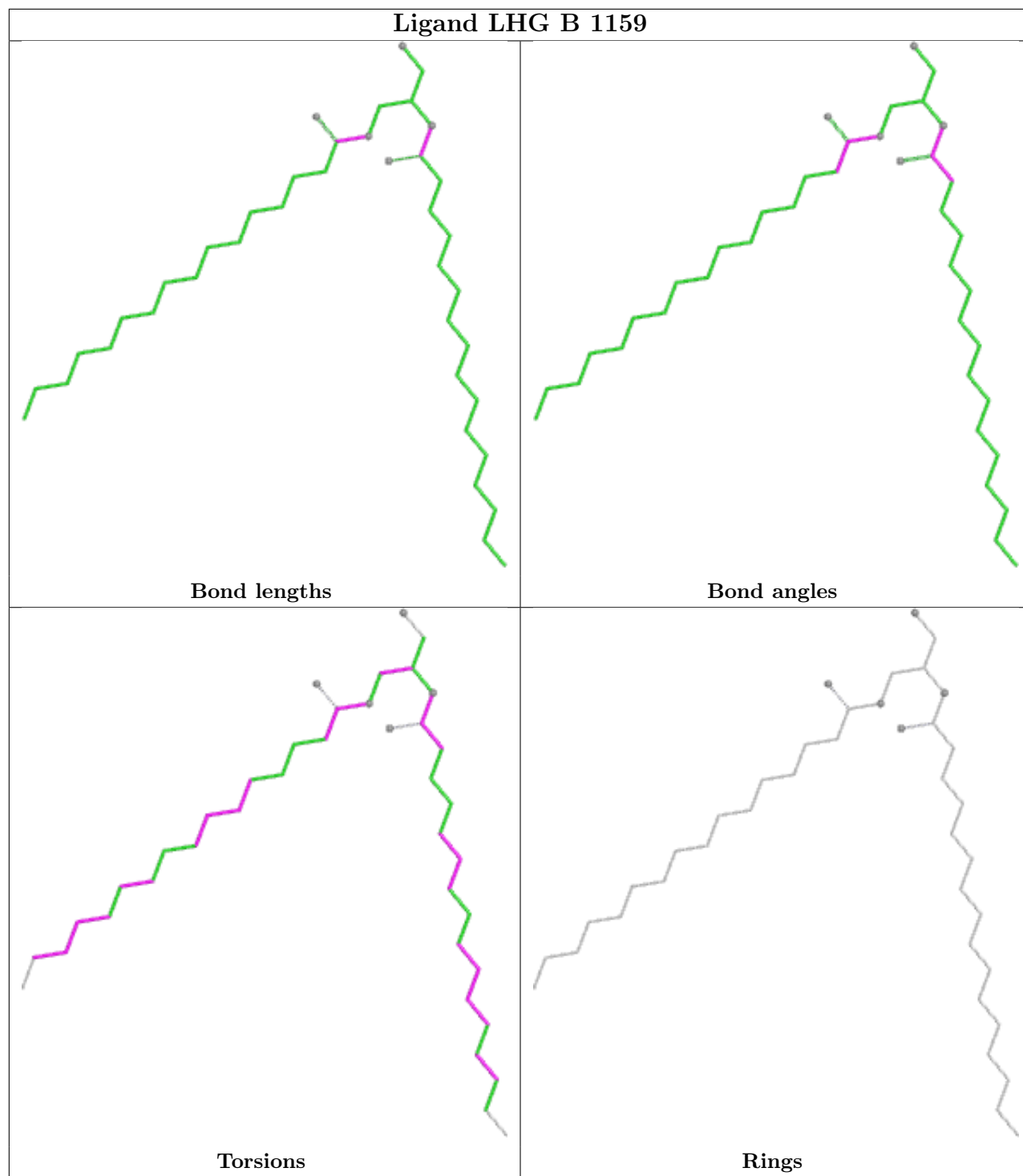


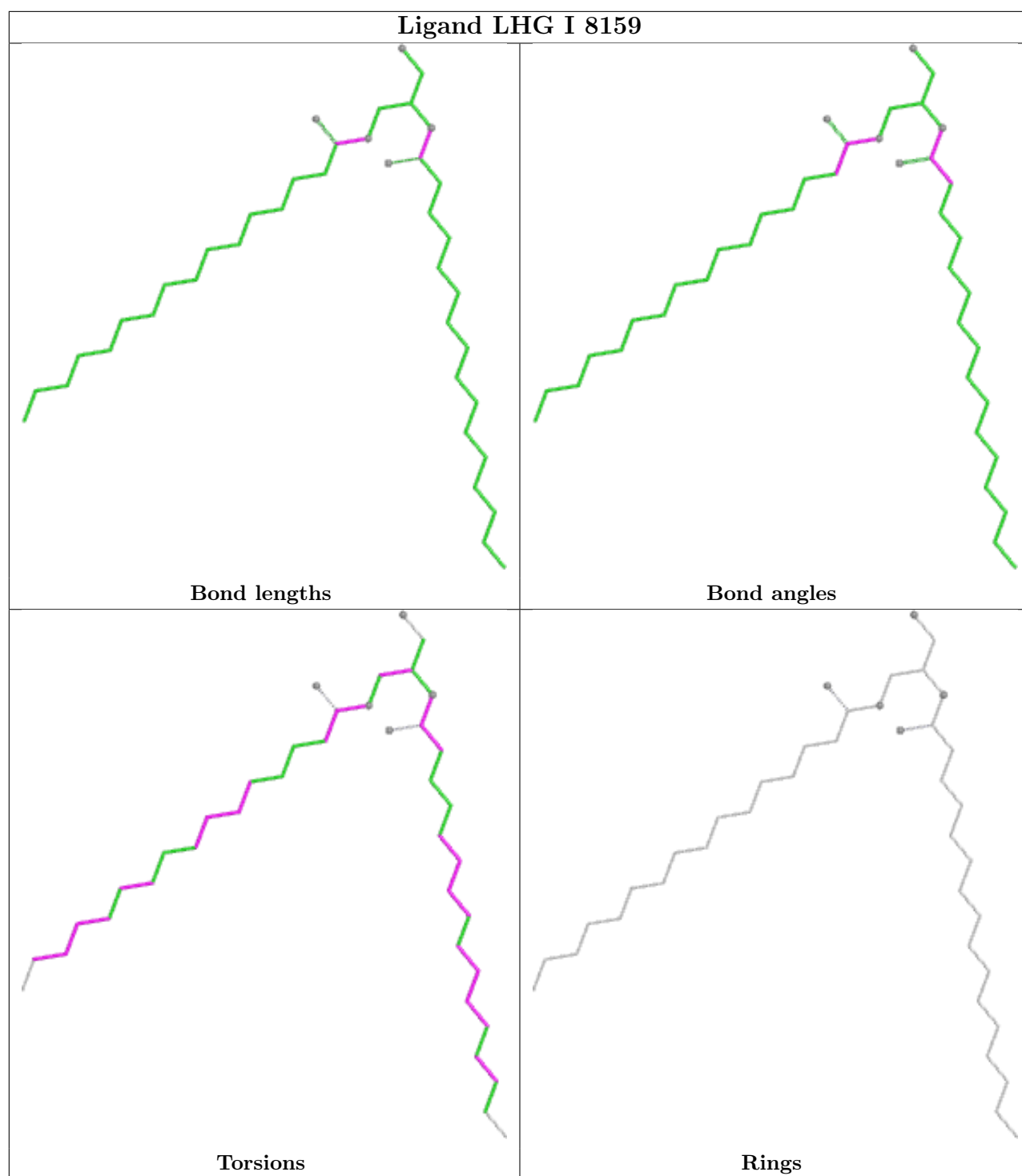


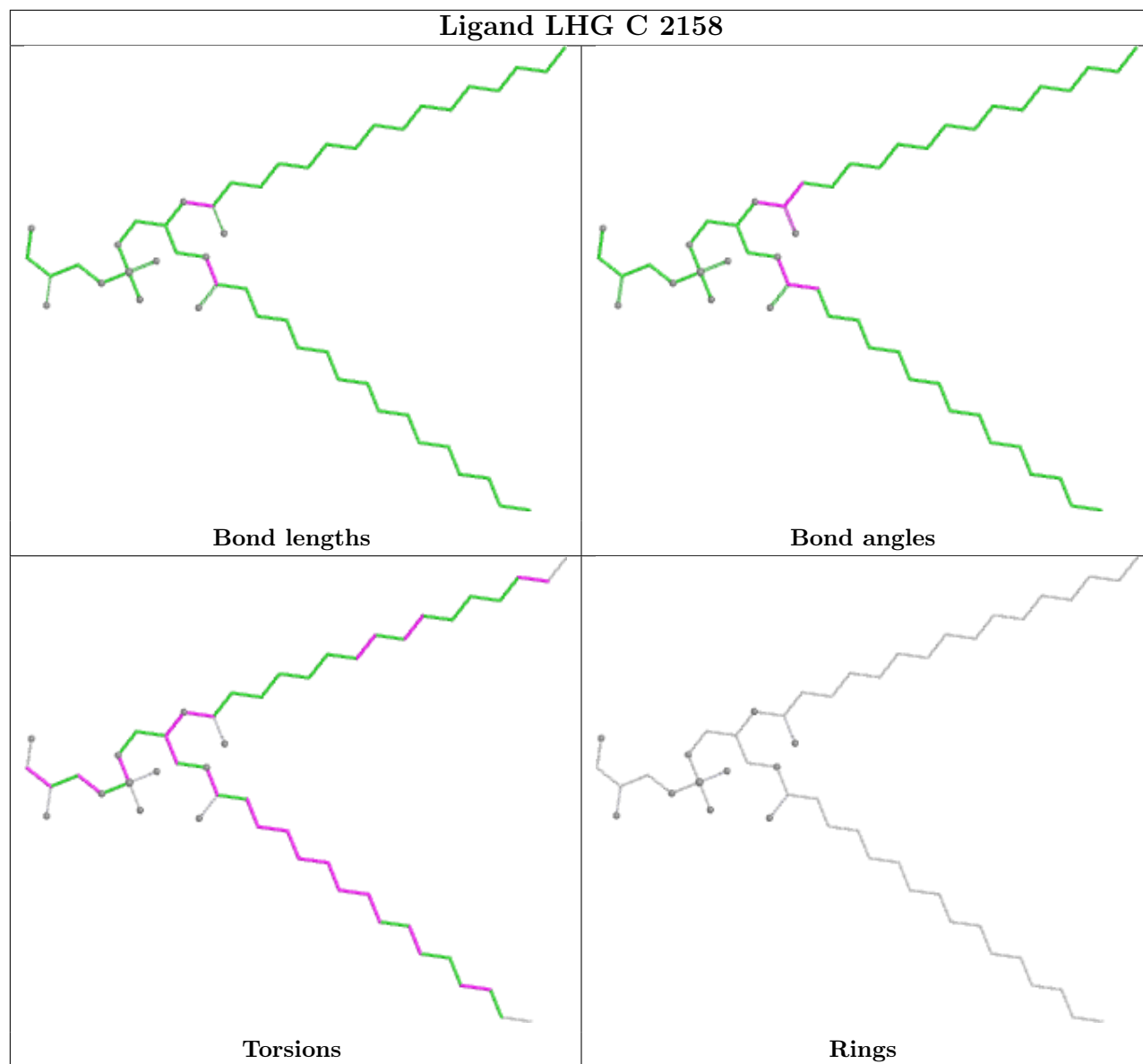


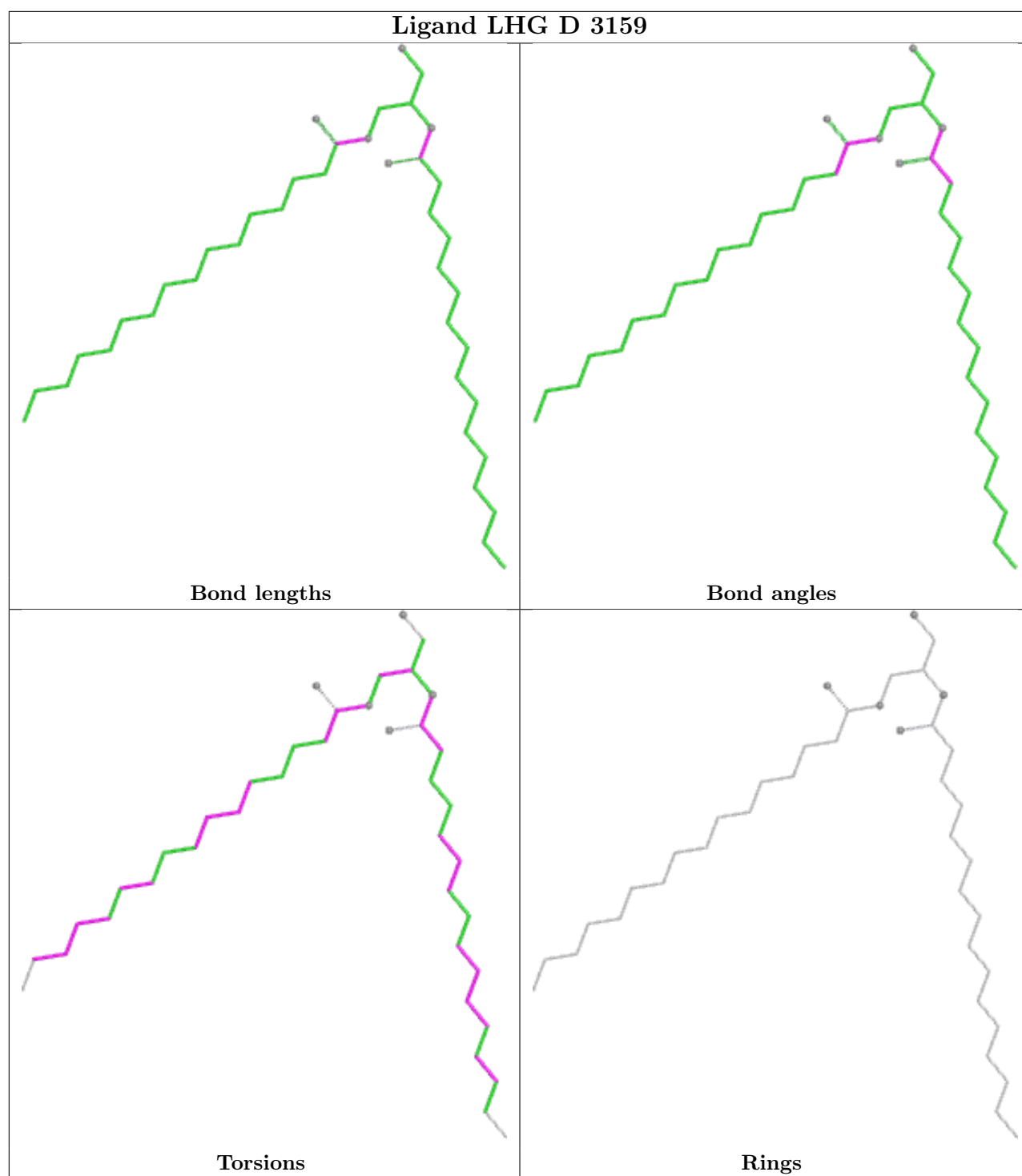


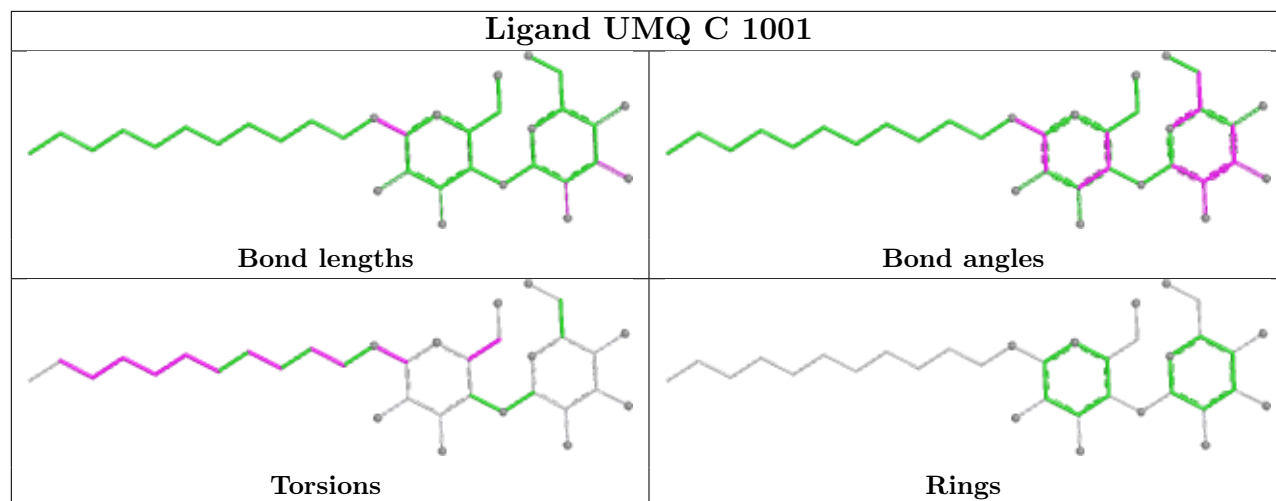












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	156/156 (100%)	0.88	16 (10%) 12 9	33, 49, 68, 86	9 (5%)
1	B	156/156 (100%)	0.92	19 (12%) 8 6	33, 49, 68, 86	9 (5%)
1	C	156/156 (100%)	1.17	29 (18%) 3 2	33, 49, 68, 86	9 (5%)
1	D	156/156 (100%)	0.81	16 (10%) 12 9	33, 49, 68, 86	9 (5%)
1	E	156/156 (100%)	0.87	21 (13%) 7 5	33, 49, 68, 86	9 (5%)
1	F	156/156 (100%)	0.80	17 (10%) 10 8	33, 49, 68, 86	9 (5%)
1	G	156/156 (100%)	0.33	8 (5%) 33 25	33, 49, 68, 86	9 (5%)
1	H	156/156 (100%)	0.29	5 (3%) 50 40	33, 49, 68, 86	9 (5%)
1	I	156/156 (100%)	0.25	8 (5%) 33 25	33, 49, 66, 86	7 (4%)
1	J	156/156 (100%)	0.25	2 (1%) 75 66	33, 49, 59, 72	8 (5%)
All	All	1560/1560 (100%)	0.66	141 (9%) 15 11	33, 49, 68, 86	87 (5%)

All (141) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	81	GLY	9.8
1	F	82	SER	7.8
1	C	83[A]	ASP	7.5
1	E	7	THR	7.5
1	B	82	SER	7.3
1	E	9	ASN	7.2
1	C	82	SER	6.6
1	F	83[A]	ASP	6.5
1	E	8	GLN	6.5
1	A	83[A]	ASP	6.4
1	A	81	GLY	6.1
1	H	81	GLY	6.1
1	F	9	ASN	6.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	81	GLY	5.9
1	E	82	SER	5.8
1	C	81	GLY	5.8
1	D	82	SER	5.6
1	F	10	GLY	5.3
1	B	83[A]	ASP	5.3
1	C	156	ALA	5.2
1	A	82	SER	5.1
1	D	81	GLY	4.7
1	A	9	ASN	4.6
1	E	46	THR	4.4
1	H	83[A]	ASP	4.4
1	E	83[A]	ASP	4.3
1	E	5	LEU	4.3
1	E	10	GLY	4.1
1	C	10	GLY	4.1
1	D	9	ASN	4.1
1	C	84	MET	4.1
1	H	82	SER	4.1
1	G	156	ALA	4.0
1	B	9	ASN	4.0
1	A	156	ALA	4.0
1	B	57	ILE	4.0
1	B	81	GLY	3.9
1	C	85	SER	3.8
1	E	4	TYR	3.8
1	G	53	GLY	3.7
1	A	123	LYS	3.7
1	A	12[A]	MET	3.6
1	E	6	ILE	3.5
1	A	8	GLN	3.5
1	B	1	MET	3.5
1	D	83[A]	ASP	3.4
1	B	126	GLU	3.4
1	D	126	GLU	3.4
1	D	128	ALA	3.3
1	F	11	GLY	3.3
1	C	45	THR	3.3
1	G	82	SER	3.3
1	C	35	GLY	3.2
1	A	15	ALA	3.2
1	B	156	ALA	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	126	GLU	3.2
1	C	87	VAL	3.1
1	F	8	GLN	3.1
1	I	153	VAL	3.1
1	F	3	ASP	3.0
1	B	12[A]	MET	3.0
1	G	123	LYS	3.0
1	B	54[A]	GLN	3.0
1	F	7	THR	2.9
1	A	13[A]	VAL	2.9
1	B	150	PHE	2.9
1	F	53	GLY	2.8
1	C	70	PHE	2.8
1	C	121	LEU	2.8
1	D	12[A]	MET	2.8
1	B	46	THR	2.8
1	H	54[A]	GLN	2.8
1	F	109	ALA	2.8
1	F	88	GLN	2.7
1	F	70	PHE	2.7
1	B	60	LEU	2.7
1	G	1	MET	2.7
1	C	88	GLN	2.7
1	I	52	PHE	2.7
1	C	69	GLY	2.7
1	I	1	MET	2.6
1	C	12[A]	MET	2.6
1	J	137	MET	2.6
1	B	10	GLY	2.6
1	A	84	MET	2.6
1	E	126	GLU	2.5
1	B	154	LEU	2.5
1	C	11	GLY	2.5
1	D	115	ALA	2.5
1	E	70	PHE	2.5
1	B	53	GLY	2.4
1	C	15	ALA	2.4
1	C	22	ALA	2.4
1	E	122	ALA	2.4
1	I	108	ILE	2.4
1	E	127	HIS	2.4
1	I	3	ASP	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	118	ILE	2.4
1	B	52	PHE	2.3
1	C	49	PRO	2.3
1	E	86	VAL	2.3
1	E	87	VAL	2.3
1	I	28	ILE	2.3
1	D	68	TYR	2.3
1	H	80	LEU	2.2
1	B	119[A]	GLN	2.2
1	A	45	THR	2.2
1	D	48	GLN	2.2
1	D	127	HIS	2.2
1	I	104	LEU	2.2
1	D	86	VAL	2.2
1	A	137	MET	2.2
1	C	80	LEU	2.2
1	G	9	ASN	2.1
1	C	86	VAL	2.1
1	A	7	THR	2.1
1	C	38	GLY	2.1
1	C	14	PHE	2.1
1	I	54	GLN	2.1
1	D	125	PRO	2.1
1	F	84	MET	2.1
1	G	81	GLY	2.1
1	C	122	ALA	2.1
1	F	6	ILE	2.1
1	E	123	LYS	2.1
1	G	83[A]	ASP	2.1
1	C	26	SER	2.1
1	B	14	PHE	2.1
1	C	74	PHE	2.1
1	C	92	PHE	2.1
1	J	91	ASN	2.0
1	F	14	PHE	2.0
1	A	6	ILE	2.0
1	E	124	LYS	2.0
1	D	47	SER	2.0
1	E	119[A]	GLN	2.0
1	F	85	SER	2.0
1	E	154	LEU	2.0
1	C	9	ASN	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	36	MET	2.0
1	D	1	MET	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

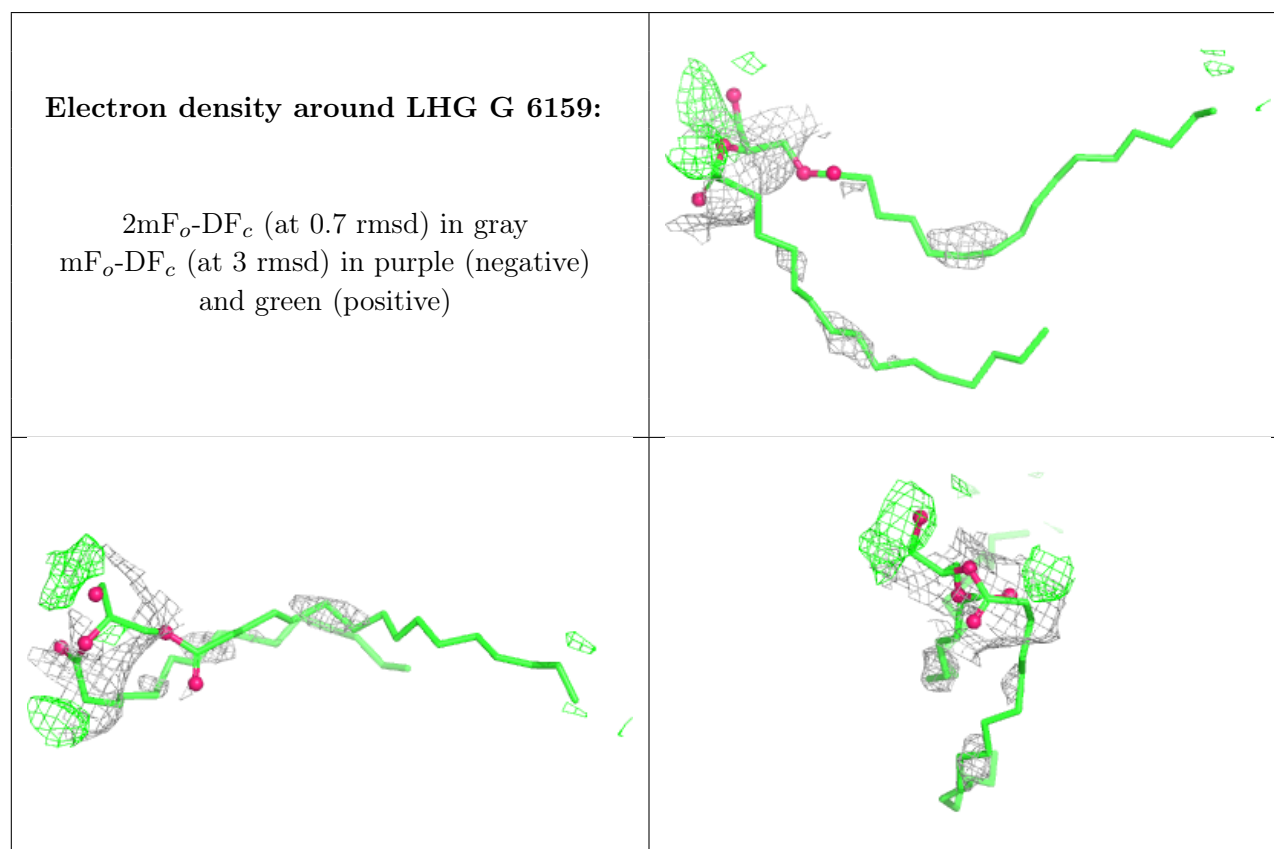
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	LI	I	157	1/1	0.51	0.19	47,47,47,47	0
2	LI	J	157	1/1	0.74	0.21	47,47,47,47	0
3	LHG	G	6159	40/49	0.79	0.36	116,128,142,143	0
3	LHG	D	3158	49/49	0.80	0.31	87,106,123,124	0
3	LHG	B	1159	40/49	0.80	0.34	116,128,142,143	0
3	LHG	F	5158	49/49	0.81	0.32	87,106,122,124	0
3	LHG	H	7158	49/49	0.82	0.31	87,106,123,124	0
3	LHG	D	3159	40/49	0.83	0.33	116,128,142,143	0
3	LHG	E	4159	40/49	0.84	0.31	116,128,142,143	0
2	LI	D	157	1/1	0.84	0.13	47,47,47,47	0
3	LHG	C	2158	49/49	0.84	0.30	87,106,123,124	0
3	LHG	E	4158	49/49	0.84	0.29	87,106,123,124	0
3	LHG	J	9159	40/49	0.84	0.33	116,128,142,143	0
3	LHG	F	5159	40/49	0.85	0.32	116,128,142,143	0
3	LHG	G	6158	49/49	0.85	0.28	87,106,123,124	0
3	LHG	C	2159	40/49	0.85	0.31	116,128,142,143	0
3	LHG	A	558	49/49	0.85	0.29	87,106,123,124	0
3	LHG	I	8158	49/49	0.85	0.29	87,106,122,124	0
3	LHG	B	1158	49/49	0.85	0.30	87,106,123,124	0
3	LHG	A	559	40/49	0.86	0.31	116,128,142,143	0
3	LHG	I	8159	40/49	0.86	0.32	116,128,142,143	0

Continued on next page...

Continued from previous page...

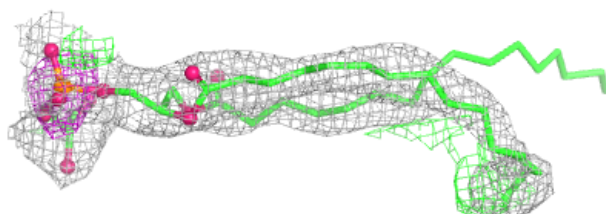
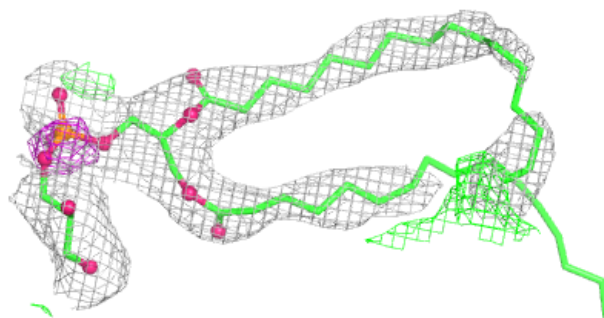
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	LHG	H	7159	40/49	0.86	0.33	116,128,142,143	0
4	UMQ	F	1002	34/34	0.86	0.18	77,88,90,90	0
4	UMQ	C	1001	34/34	0.87	0.19	91,97,98,99	0
2	LI	C	157	1/1	0.87	0.17	47,47,47,47	0
3	LHG	J	9158	49/49	0.88	0.25	87,106,123,124	0
2	LI	E	157	1/1	0.88	0.09	47,47,47,47	0
2	LI	B	157	1/1	0.90	0.09	47,47,47,47	0
2	LI	H	157	1/1	0.91	0.16	47,47,47,47	0
2	LI	F	157	1/1	0.92	0.13	47,47,47,47	0
2	LI	G	157	1/1	0.93	0.08	47,47,47,47	0
2	LI	A	157	1/1	0.97	0.10	47,47,47,47	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

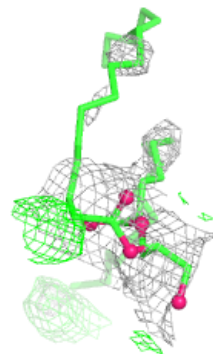
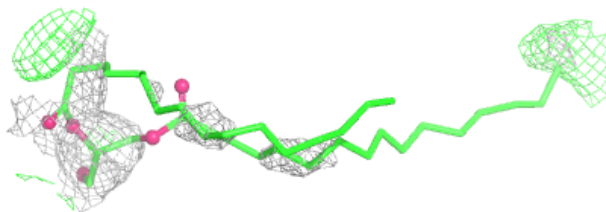
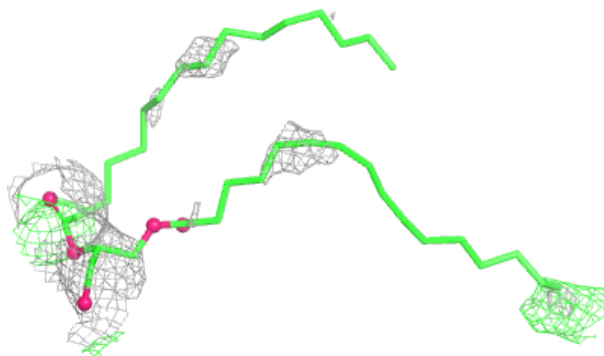


Electron density around LHG D 3158:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

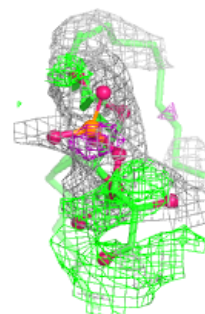
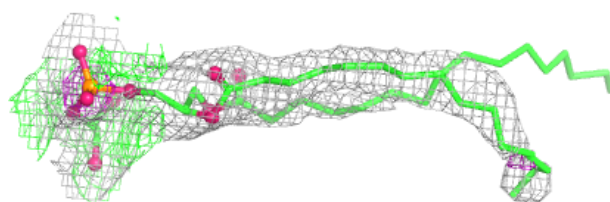
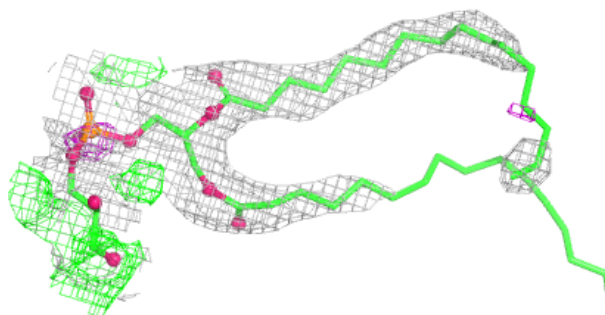
**Electron density around LHG B 1159:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

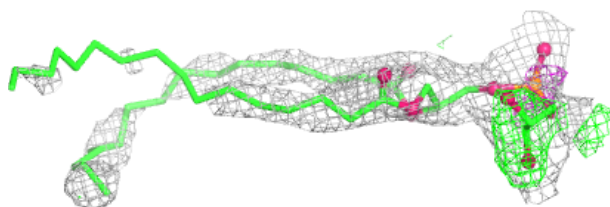
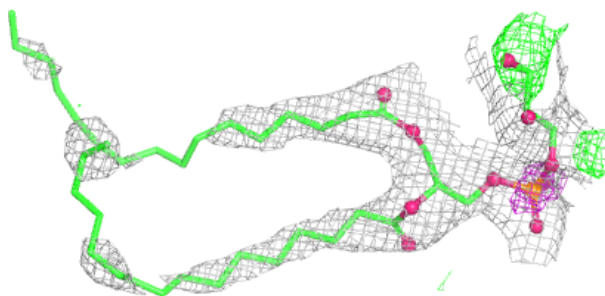


Electron density around LHG F 5158:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

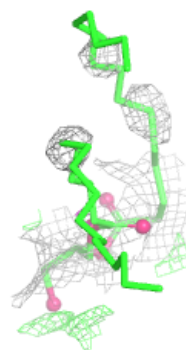
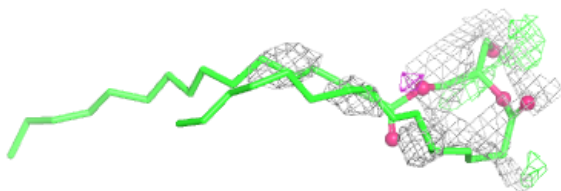
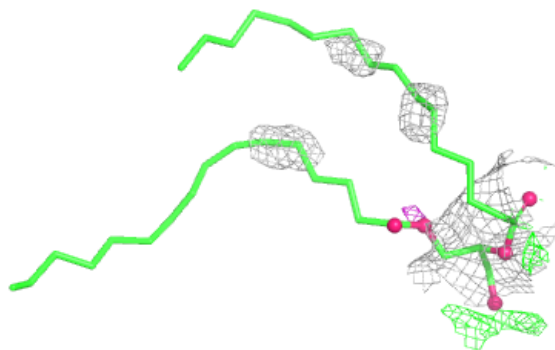
**Electron density around LHG H 7158:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

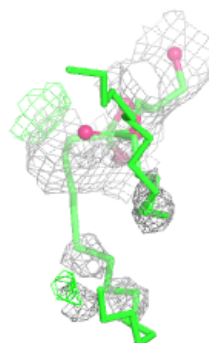
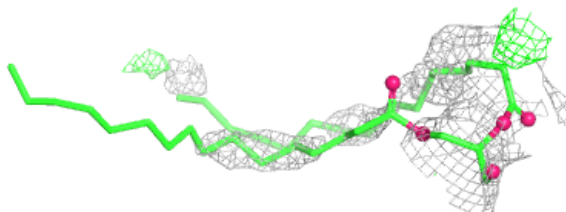
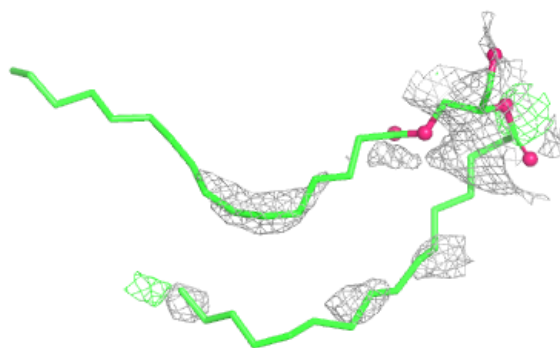


Electron density around LHG D 3159:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

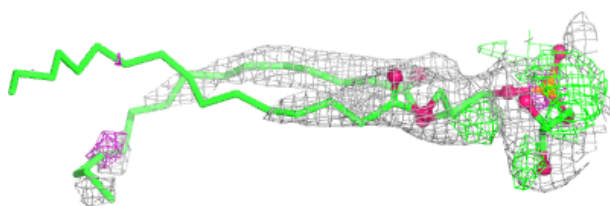
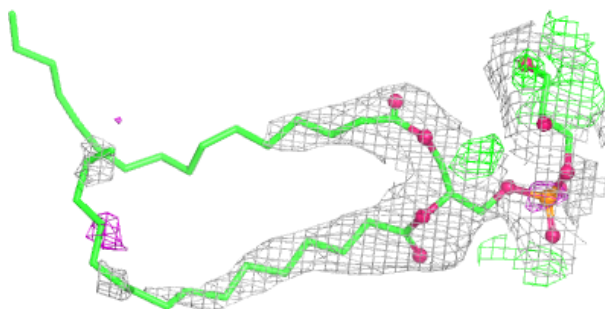
**Electron density around LHG E 4159:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

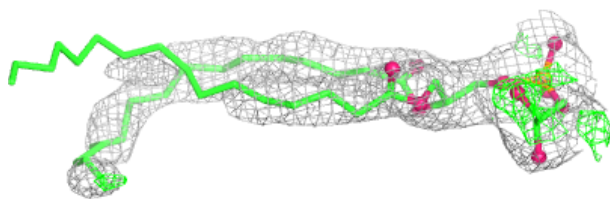
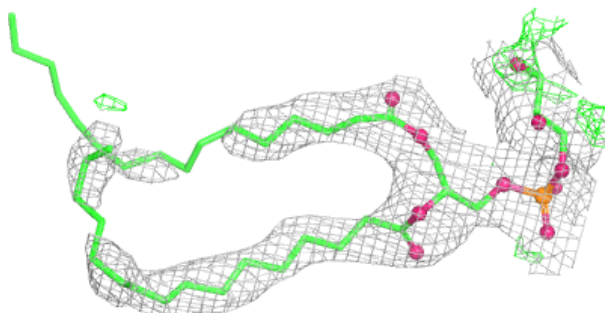


Electron density around LHG C 2158:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

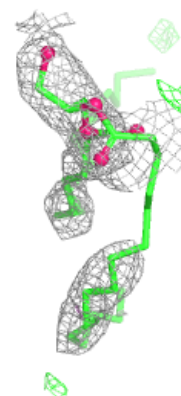
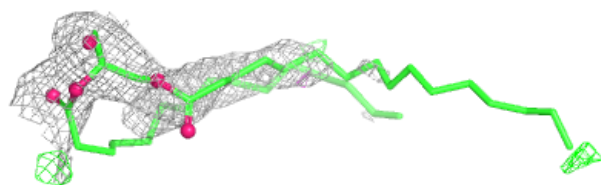
**Electron density around LHG E 4158:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

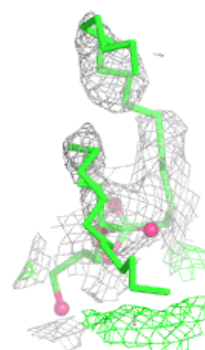
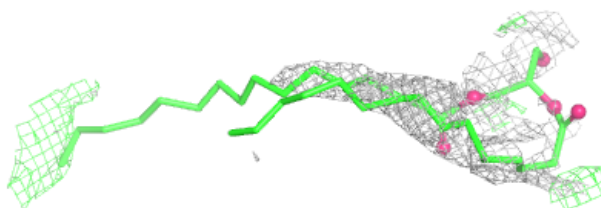
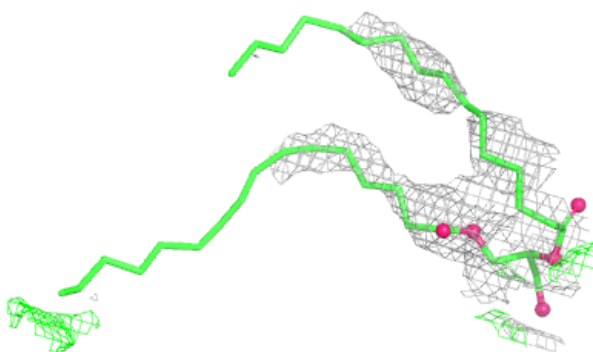


Electron density around LHG J 9159:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

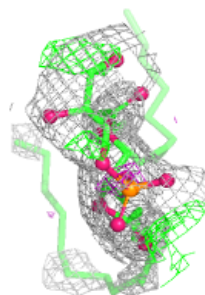
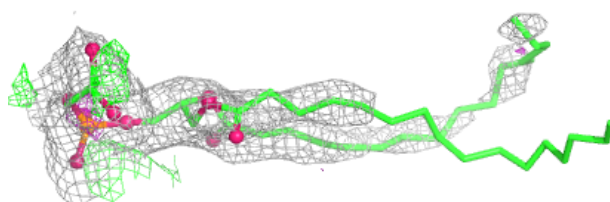
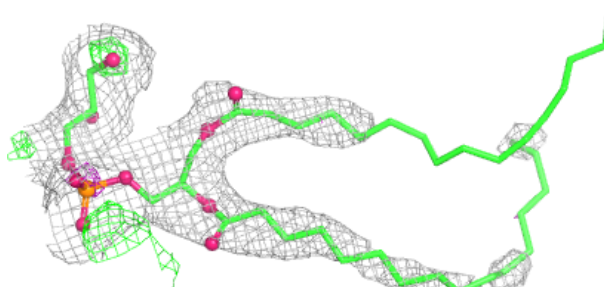
**Electron density around LHG F 5159:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

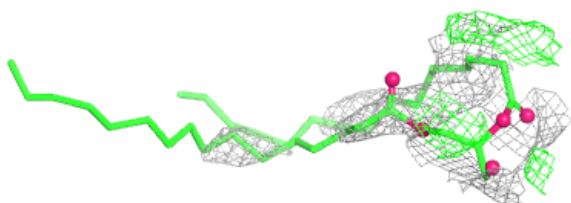
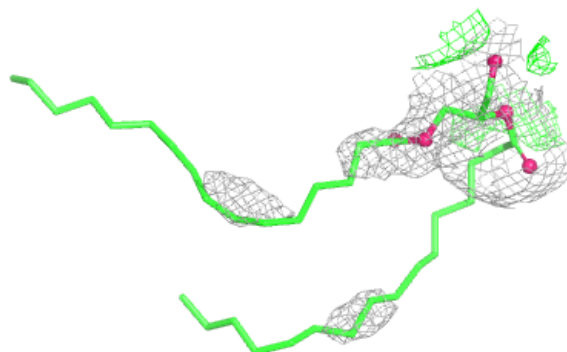


Electron density around LHG G 6158:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

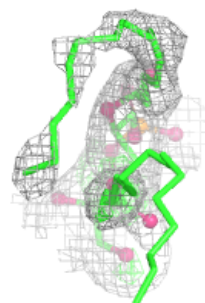
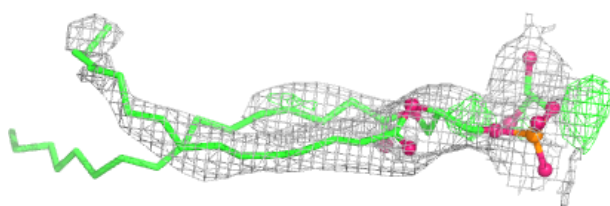
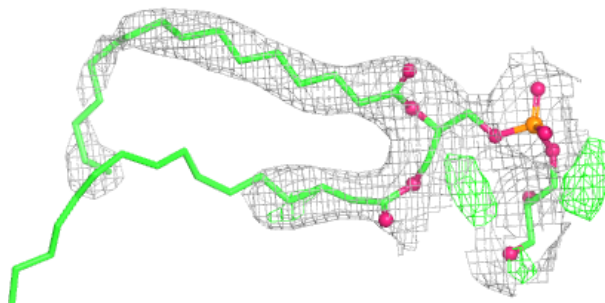
**Electron density around LHG C 2159:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

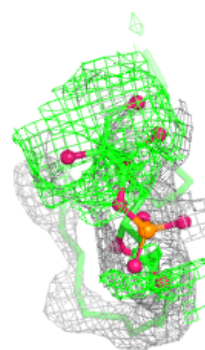
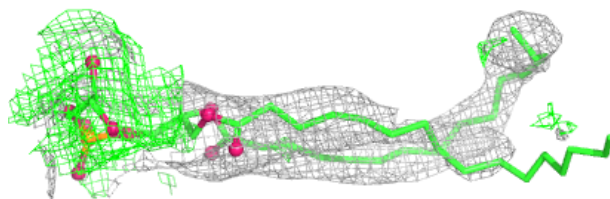
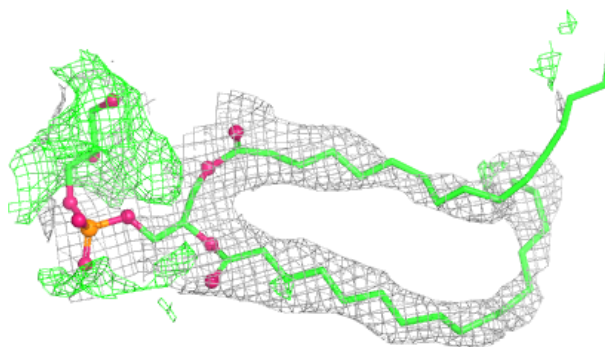


Electron density around LHG A 558:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

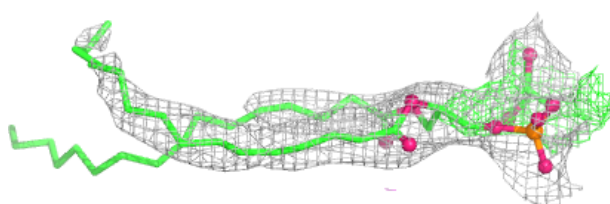
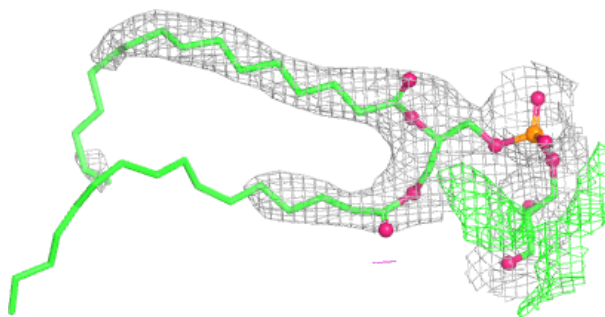
**Electron density around LHG I 8158:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

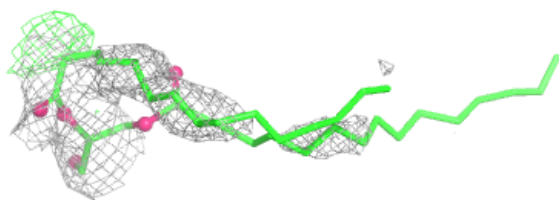
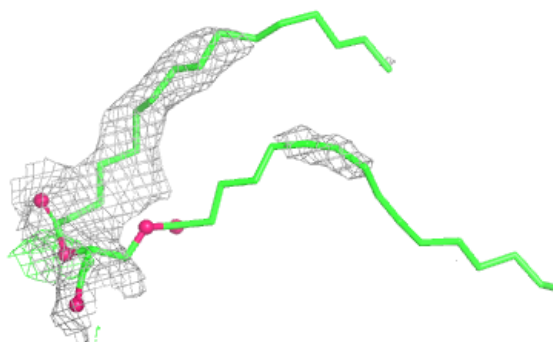


Electron density around LHG B 1158:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

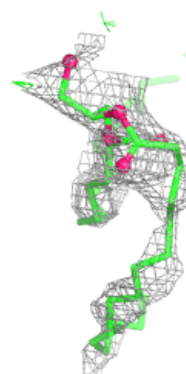
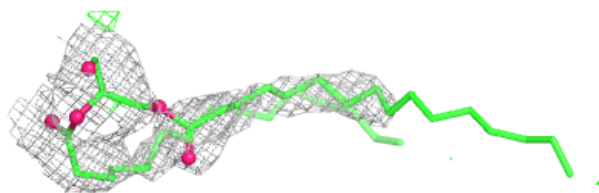
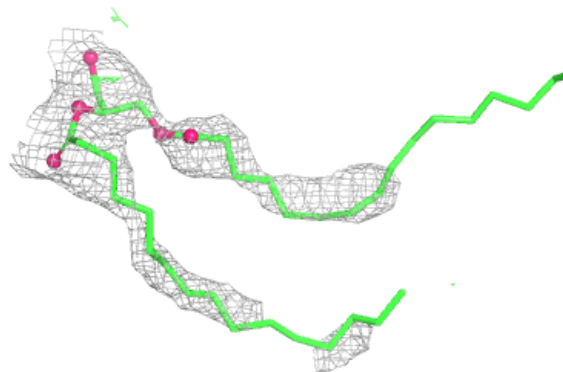
**Electron density around LHG A 559:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

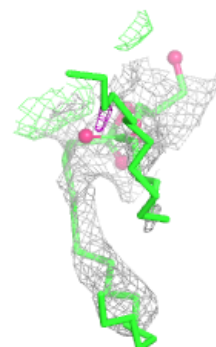
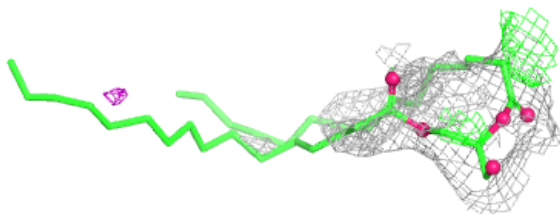
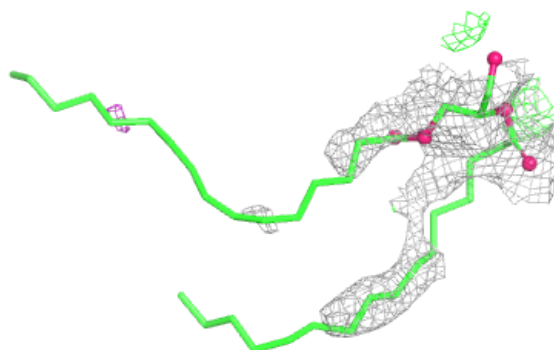


Electron density around LHG I 8159:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

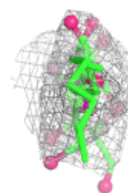
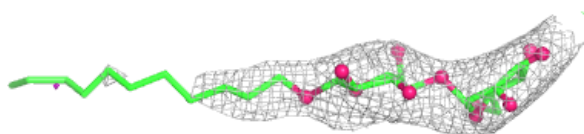
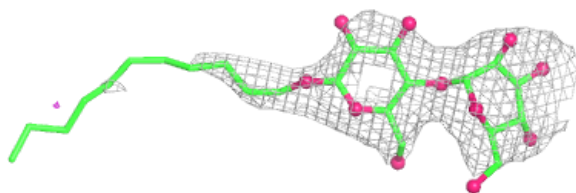
**Electron density around LHG H 7159:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

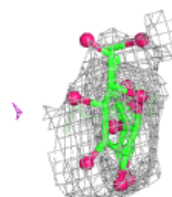
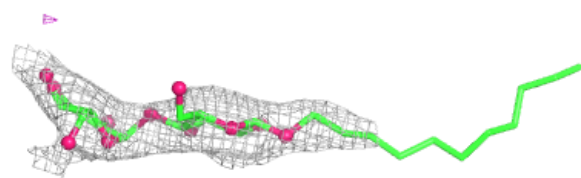
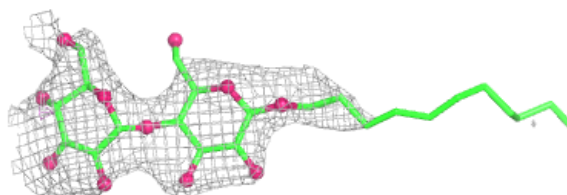


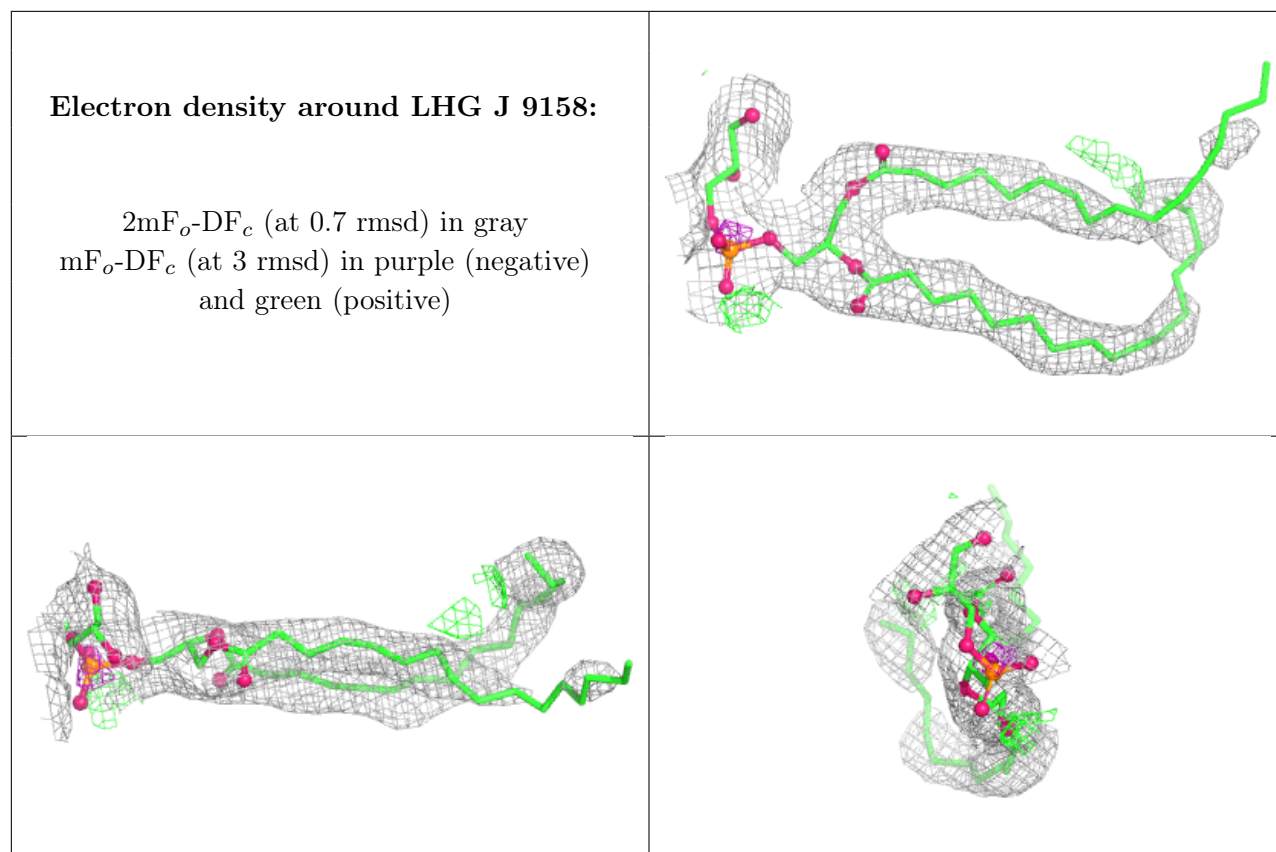
Electron density around UMQ F 1002:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around UMQ C 1001:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.