



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 19, 2026 – 09:09 PM UTC

PDB ID : 2DB4 / pdb_00002db4
Title : Crystal structure of rotor ring with DCCD 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 : 2005-12-15
Resolution : 2.40 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

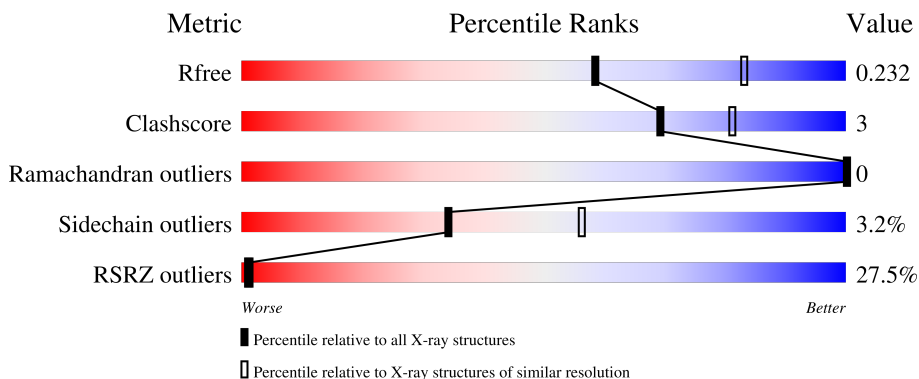
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	
1	B	156	
1	C	156	
1	D	156	

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Mol	Chain	Length	Quality of chain
1	E	156	 25% 94% 5%
1	F	156	 24% 92% 6%
1	G	156	 23% 94% 5%
1	H	156	 20% 94% 5%
1	I	156	 17% 90% 8%
1	J	156	 9% 91% 8%

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
5	UMQ	C	206	X	-	-	-
5	UMQ	F	206	X	-	-	-

2 Entry composition [i](#)

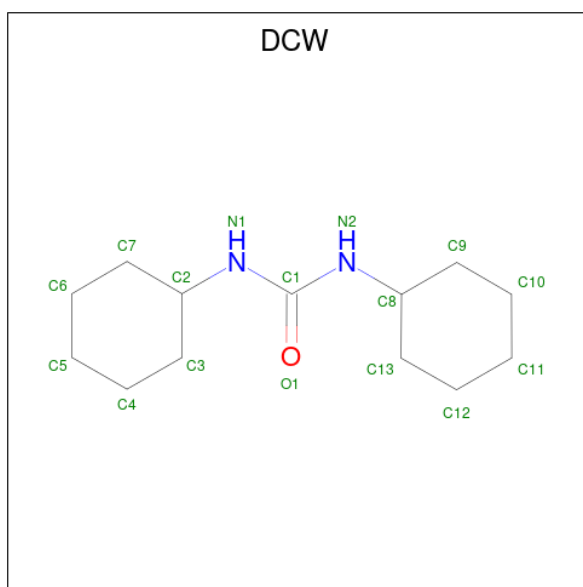
There are 6 unique types of molecules in this entry. The entry contains 12910 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ATPase Subunit K.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	156	1154	760	179	207	8	0	9	0
1	B	156	1154	760	179	207	8	0	9	0
1	C	156	1154	760	179	207	8	0	9	0
1	D	156	1154	760	179	207	8	0	9	0
1	E	156	1154	760	179	207	8	0	9	0
1	F	156	1154	760	179	207	8	0	9	0
1	G	156	1154	760	179	207	8	0	9	0
1	H	156	1154	760	179	207	8	0	9	0
1	I	156	1147	757	178	204	8	0	7	0
1	J	156	1152	759	180	206	7	0	8	0

- Molecule 2 is DICYCLOHEXYLUREA (CCD ID: DCW) (formula: $C_{13}H_{24}N_2O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			16	13	2	1		
2	B	1	Total	C	N	O	0	0
			16	13	2	1		
2	C	1	Total	C	N	O	0	0
			16	13	2	1		
2	D	1	Total	C	N	O	0	0
			16	13	2	1		
2	E	1	Total	C	N	O	0	0
			16	13	2	1		
2	F	1	Total	C	N	O	0	0
			16	13	2	1		
2	G	1	Total	C	N	O	0	0
			16	13	2	1		
2	H	1	Total	C	N	O	0	0
			16	13	2	1		
2	I	1	Total	C	N	O	0	0
			16	13	2	1		
2	J	1	Total	C	N	O	0	0
			16	13	2	1		

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

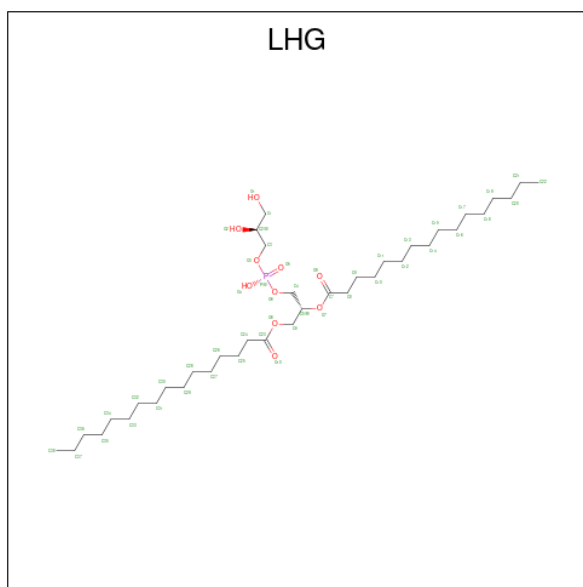
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		
3	B	1	Total	Na	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total Na 1 1	0	0
3	D	1	Total Na 1 1	0	0
3	E	1	Total Na 1 1	0	0
3	F	1	Total Na 1 1	0	0
3	G	1	Total Na 1 1	0	0
3	H	1	Total Na 1 1	0	0
3	I	1	Total Na 1 1	0	0
3	J	1	Total Na 1 1	0	0

- Molecule 4 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



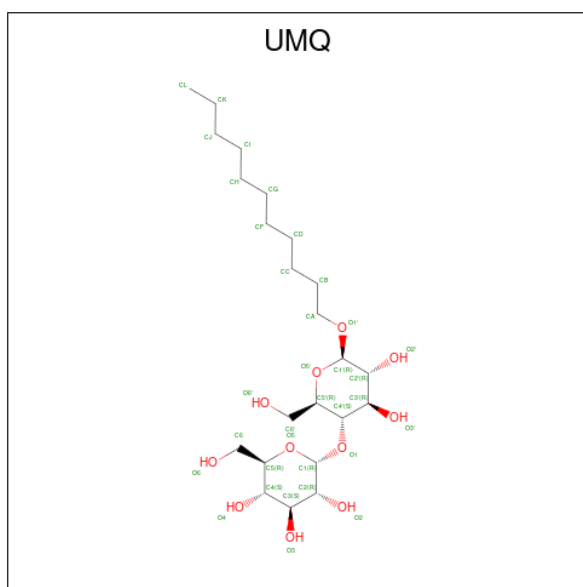
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 40 35 5	0	0
4	A	1	Total C O 40 35 5	0	0
4	B	1	Total C O 40 35 5	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			40	35	5		
4	C	1	Total	C	O	0	0
			40	35	5		
4	C	1	Total	C	O	0	0
			40	35	5		
4	C	1	Total	C	O	0	0
			40	35	5		
4	D	1	Total	C	O	0	0
			40	35	5		
4	D	1	Total	C	O	0	0
			40	35	5		
4	E	1	Total	C	O	0	0
			40	35	5		
4	F	1	Total	C	O	0	0
			40	35	5		
4	F	1	Total	C	O	0	0
			40	35	5		
4	F	1	Total	C	O	0	0
			40	35	5		
4	G	1	Total	C	O	0	0
			40	35	5		
4	G	1	Total	C	O	0	0
			40	35	5		
4	H	1	Total	C	O	0	0
			40	35	5		
4	I	1	Total	C	O	0	0
			40	35	5		
4	I	1	Total	C	O	0	0
			40	35	5		
4	J	1	Total	C	O	0	0
			40	35	5		
4	J	1	Total	C	O	0	0
			40	35	5		

- Molecule 5 is UNDECYL-MALTOSIDE (CCD ID: UMQ) (formula: $C_{23}H_{44}O_{11}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 12 11 1	0	0
5	A	1	Total C O 12 11 1	0	0
5	C	1	Total C O 34 23 11	0	0
5	D	1	Total C O 12 11 1	0	0
5	E	1	Total C O 12 11 1	0	0
5	F	1	Total C O 34 23 11	0	0
5	H	1	Total C O 12 11 1	0	0
5	I	1	Total C O 12 11 1	0	0
5	J	1	Total C O 12 11 1	0	0
5	J	1	Total C O 12 11 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	25	Total O 25 25	0	0
6	B	22	Total O 22 22	0	0

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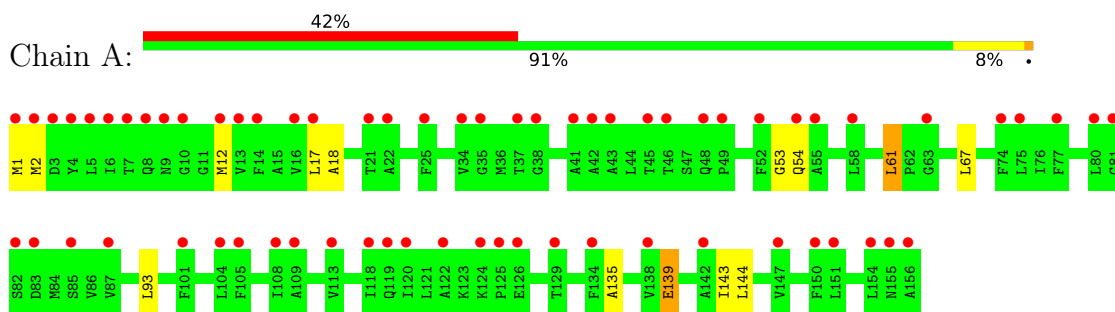
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	14	Total 14	O 14	0	0
6	D	14	Total 14	O 14	0	0
6	E	17	Total 17	O 17	0	0
6	F	20	Total 20	O 20	0	0
6	G	24	Total 24	O 24	0	0
6	H	32	Total 32	O 32	0	0
6	I	47	Total 47	O 47	0	0
6	J	30	Total 30	O 30	0	0

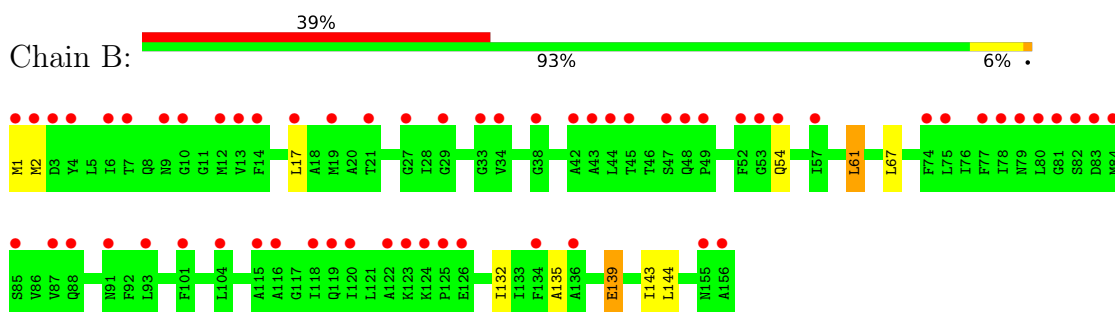
3 Residue-property plots [i](#)

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.

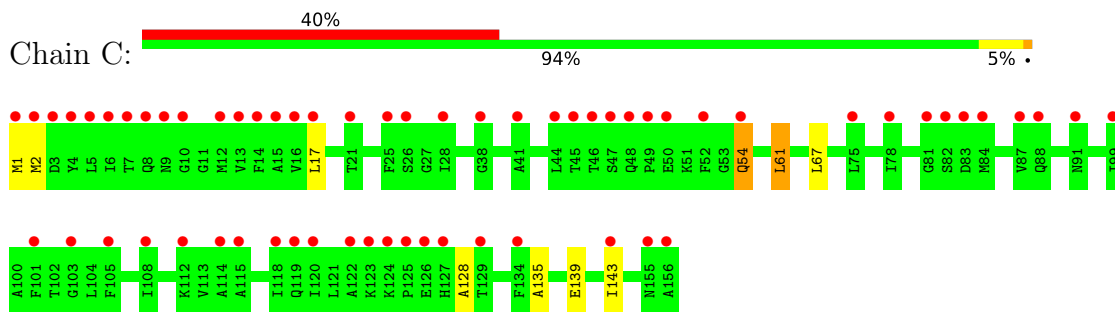
- Molecule 1: V-Type Sodium ATPase Subunit K



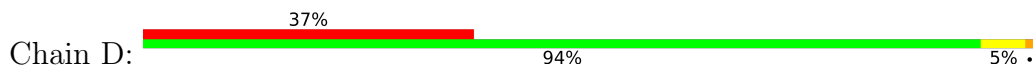
- Molecule 1: V-Type Sodium ATPase Subunit K

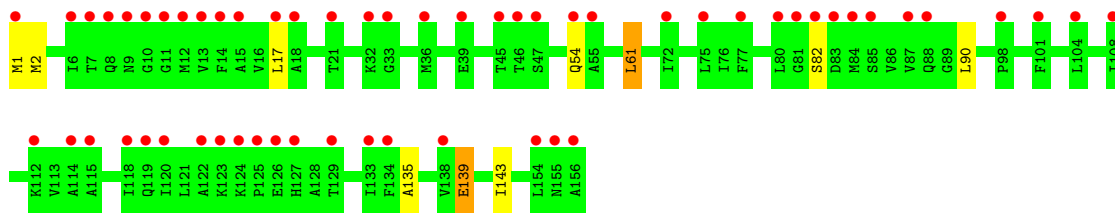


- Molecule 1: V-Type Sodium ATPase Subunit K

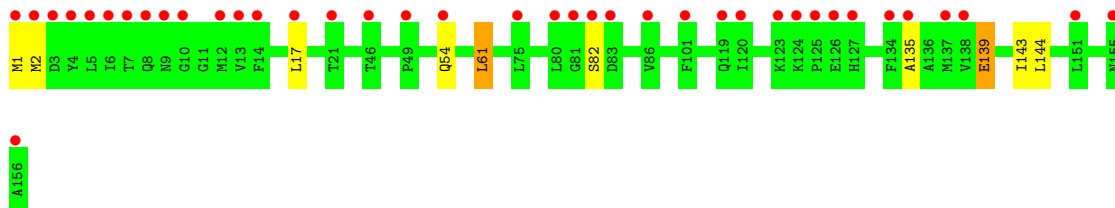


- Molecule 1: V-Type Sodium ATPase Subunit K

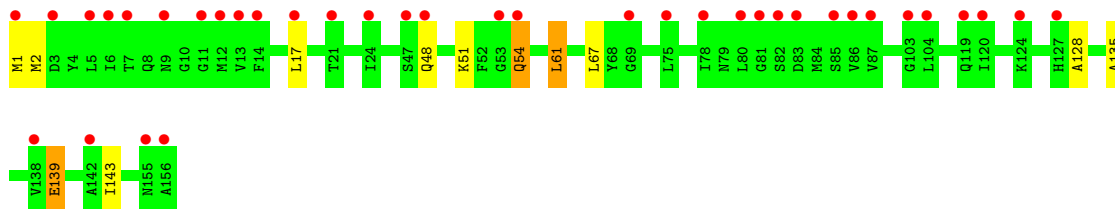
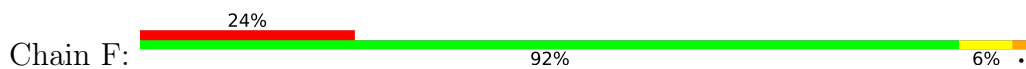




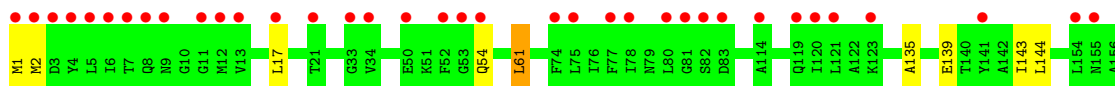
- Molecule 1: V-Type Sodium ATPase Subunit K



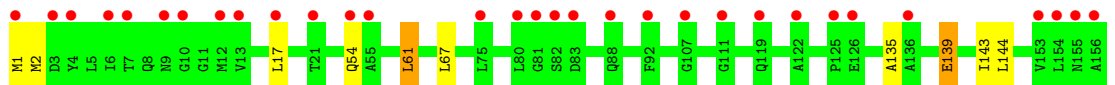
- Molecule 1: V-Type Sodium ATPase Subunit K



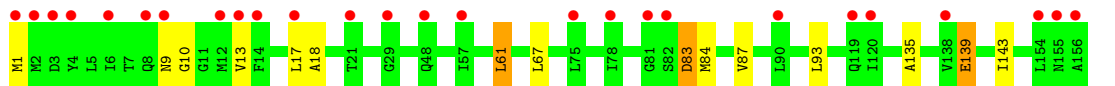
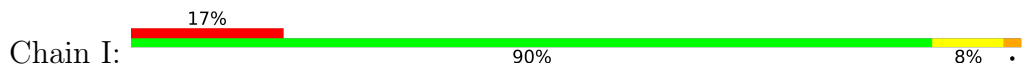
- Molecule 1: V-Type Sodium ATPase Subunit K



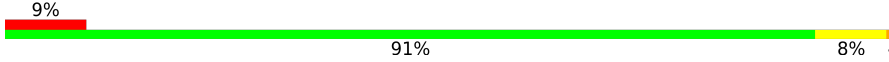
- Molecule 1: V-Type Sodium ATPase Subunit K

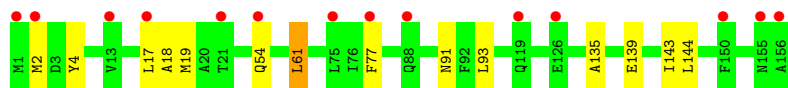


- Molecule 1: V-Type Sodium ATPase Subunit K



● Molecule 1: V-Type Sodium ATPase Subunit K

Chain J:  9% 91% 8%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	120.21Å 125.23Å 211.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	107.83 – 2.40 107.77 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (107.83-2.40) 99.7 (107.77-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 2.39Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.225 , 0.231 0.227 , 0.232	Depositor DCC
R_{free} test set	6272 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	49.3	Xtrriage
Anisotropy	0.315	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 55.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.000 for k,h,-l	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	12910	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.23% 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 i

5.1 Standard geometry i

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.55	0/1218	0.94	1/1647 (0.1%)
1	B	0.55	0/1218	0.95	1/1647 (0.1%)
1	C	0.54	0/1218	0.97	1/1647 (0.1%)
1	D	0.50	0/1218	0.94	1/1647 (0.1%)
1	E	0.52	0/1218	0.95	1/1647 (0.1%)
1	F	0.55	0/1218	0.98	2/1647 (0.1%)
1	G	0.57	0/1218	0.95	1/1647 (0.1%)
1	H	0.58	0/1218	0.94	1/1647 (0.1%)
1	I	0.68	0/1201	0.92	1/1624 (0.1%)
1	J	0.62	0/1211	0.99	1/1638 (0.1%)
All	All	0.57	0/12156	0.95	11/16438 (0.1%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	139	GLU	N-CA-CB	-6.93	99.19	110.14
1	B	139	GLU	N-CA-CB	-6.64	99.64	110.14
1	J	139	GLU	N-CA-CB	-6.57	99.76	110.14
1	C	139	GLU	N-CA-CB	-6.56	99.78	110.14
1	F	139	GLU	N-CA-CB	-6.39	100.38	110.22
1	E	139	GLU	N-CA-CB	-6.20	100.35	110.14
1	H	139	GLU	N-CA-CB	-6.09	100.51	110.14
1	I	139	GLU	N-CA-CB	-6.06	100.56	110.14
1	A	139	GLU	N-CA-CB	-6.04	100.60	110.14
1	D	139	GLU	N-CA-CB	-6.02	100.63	110.14
1	F	139	GLU	CB-CG-CD	-5.07	103.98	112.60

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	A	1154	0	1218	11	0
1	B	1154	0	1218	9	0
1	C	1154	0	1218	9	0
1	D	1154	0	1218	8	0
1	E	1154	0	1218	8	0
1	F	1154	0	1218	11	0
1	G	1154	0	1218	9	0
1	H	1154	0	1218	10	0
1	I	1147	0	1214	12	0
1	J	1152	0	1218	9	0
2	A	16	0	23	0	0
2	B	16	0	23	0	0
2	C	16	0	23	0	0
2	D	16	0	23	0	0
2	E	16	0	23	0	0
2	F	16	0	23	0	0
2	G	16	0	23	0	0
2	H	16	0	23	0	0
2	I	16	0	23	0	0
2	J	16	0	23	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
4	A	80	0	134	7	0
4	B	80	0	134	6	0
4	C	120	0	201	6	0
4	D	80	0	134	6	0
4	E	40	0	67	6	0
4	F	120	0	201	6	0
4	G	80	0	134	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	40	0	67	5	0
4	I	80	0	134	4	0
4	J	80	0	134	4	0
5	A	24	0	46	1	0
5	C	34	0	41	1	0
5	D	12	0	23	0	0
5	E	12	0	23	0	0
5	F	34	0	40	2	0
5	H	12	0	23	0	0
5	I	12	0	23	0	0
5	J	24	0	46	1	0
6	A	25	0	0	0	0
6	B	22	0	0	0	0
6	C	14	0	0	0	0
6	D	14	0	0	0	0
6	E	17	0	0	0	0
6	F	20	0	0	1	0
6	G	24	0	0	0	0
6	H	32	0	0	0	0
6	I	47	0	0	0	0
6	J	30	0	0	0	0
All	All	12910	0	14011	93	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 3.

All (93) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:54[B]:GLN:HE22	5:C:206:UMQ:HA1	1.46	0.80
1:G:2:MET:HG2	1:H:1:MET:HB2	1.73	0.70
1:F:2:MET:HG2	1:G:1:MET:HB2	1.80	0.64
1:A:2:MET:HG2	1:B:1:MET:HB2	1.79	0.64
1:C:2:MET:HG2	1:D:1:MET:HB2	1.81	0.62
1:I:61:LEU:HD23	1:I:135:ALA:HB3	1.83	0.59
4:A:204:LHG:HC62	4:J:204:LHG:HC81	1.82	0.59
4:G:203:LHG:HC81	4:H:203:LHG:HC62	1.84	0.59
1:F:139:GLU:HG2	6:F:320:HOH:O	2.03	0.59
1:F:54[B]:GLN:HE22	5:F:206:UMQ:HA1	1.67	0.59
1:D:2:MET:HG2	1:E:1:MET:HB2	1.86	0.56
1:I:9:ASN:HD21	1:I:83:ASP:HA	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:204:LHG:HC81	4:B:204:LHG:HC62	1.88	0.55
4:A:204:LHG:C6	4:J:204:LHG:HC81	2.37	0.54
1:B:2:MET:HG2	1:C:1:MET:HB2	1.89	0.54
4:G:203:LHG:HC81	4:H:203:LHG:C6	2.38	0.54
1:I:87:VAL:HG23	1:J:4:TYR:CE2	2.43	0.54
1:I:9:ASN:HD21	1:I:84:MET:H	1.56	0.53
4:B:204:LHG:HC81	4:C:204:LHG:HC62	1.92	0.52
4:F:204:LHG:HC81	4:G:203:LHG:HC62	1.91	0.51
1:F:61:LEU:HD23	1:F:135:ALA:HB3	1.92	0.51
1:A:61:LEU:HD23	1:A:135:ALA:HB3	1.92	0.51
1:J:61:LEU:HD23	1:J:135:ALA:HB3	1.93	0.51
1:C:61:LEU:HD23	1:C:135:ALA:HB3	1.92	0.51
1:I:10:GLY:O	1:I:13[A]:VAL:HG22	2.10	0.51
1:E:2:MET:HG2	1:F:1:MET:HB2	1.93	0.50
1:B:61:LEU:HD23	1:B:135:ALA:HB3	1.92	0.50
1:G:61:LEU:HD23	1:G:135:ALA:HB3	1.93	0.50
1:C:17[B]:LEU:HD21	4:C:204:LHG:H192	1.93	0.49
1:D:61:LEU:HD23	1:D:135:ALA:HB3	1.94	0.49
1:I:17[B]:LEU:HD21	4:I:204:LHG:H192	1.94	0.49
4:C:204:LHG:HC81	4:D:203:LHG:HC62	1.94	0.49
5:F:206:UMQ:H6'2	5:F:206:UMQ:H51	1.94	0.49
1:D:17[B]:LEU:HD21	4:D:203:LHG:H192	1.95	0.49
1:A:1:MET:HB2	1:J:2:MET:HG2	1.96	0.48
1:H:61:LEU:HD23	1:H:135:ALA:HB3	1.95	0.48
1:F:17[B]:LEU:HD21	4:F:204:LHG:H192	1.96	0.48
1:A:17[B]:LEU:HD21	4:A:204:LHG:H192	1.96	0.47
4:E:203:LHG:HC81	4:F:204:LHG:HC62	1.95	0.47
1:I:1:MET:HB3	4:I:204:LHG:HC5	1.96	0.47
1:F:17[B]:LEU:HD11	4:F:204:LHG:H171	1.97	0.47
1:I:17[B]:LEU:HD11	4:I:204:LHG:H171	1.95	0.46
1:G:17[B]:LEU:HD21	4:G:203:LHG:H192	1.96	0.46
1:H:17[B]:LEU:HD21	4:H:203:LHG:H192	1.97	0.46
4:I:204:LHG:HC81	4:J:204:LHG:HC62	1.98	0.46
4:C:204:LHG:HC81	4:D:203:LHG:C6	2.46	0.46
4:A:204:LHG:HC81	4:B:204:LHG:C6	2.45	0.46
1:E:61:LEU:HD23	1:E:135:ALA:HB3	1.97	0.45
1:B:17[B]:LEU:HD21	4:B:204:LHG:H192	1.97	0.45
4:F:204:LHG:HC81	4:G:203:LHG:C6	2.46	0.45
1:C:17[B]:LEU:HD11	4:C:204:LHG:H171	1.98	0.45
1:A:1:MET:HB3	4:A:204:LHG:HC5	1.99	0.45
1:E:17[B]:LEU:HD21	4:E:203:LHG:H192	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:144:LEU:HD11	1:F:67:LEU:HD23	1.99	0.45
1:H:1:MET:HB3	4:H:203:LHG:HC5	1.99	0.45
1:H:2:MET:HG2	1:I:1:MET:HB2	1.99	0.44
1:B:144:LEU:HD11	1:C:67:LEU:HD23	1.99	0.44
1:B:17[B]:LEU:HD11	4:B:204:LHG:H171	2.00	0.44
1:A:17[B]:LEU:HD11	4:A:204:LHG:H171	1.99	0.44
1:D:90:LEU:HD22	4:E:203:LHG:H181	1.99	0.44
1:I:9:ASN:ND2	1:I:84:MET:H	2.16	0.44
1:I:18:ALA:HB2	1:I:93:LEU:HA	1.99	0.44
1:D:17[B]:LEU:HD11	4:D:203:LHG:H171	1.99	0.43
1:A:67:LEU:HD23	1:J:144:LEU:HD11	2.00	0.43
1:B:1:MET:HB3	4:B:204:LHG:HC5	2.01	0.43
1:E:1:MET:HB3	4:E:203:LHG:HC5	2.01	0.43
1:E:17[B]:LEU:HD11	4:E:203:LHG:H171	1.99	0.43
1:C:1:MET:HB3	4:C:204:LHG:HC5	2.01	0.43
1:G:1:MET:HB3	4:G:203:LHG:HC5	2.01	0.43
5:J:205:UMQ:HK1	5:J:206:UMQ:HJ2	2.01	0.43
1:G:17[B]:LEU:HD11	4:G:203:LHG:H171	2.01	0.43
1:F:1:MET:HB3	4:F:204:LHG:HC5	2.01	0.43
1:G:2:MET:CG	1:H:1:MET:HB2	2.45	0.43
1:A:144:LEU:HD11	1:B:67:LEU:HD23	2.01	0.43
1:J:17[B]:LEU:HD11	4:J:204:LHG:H171	2.01	0.43
1:D:1:MET:HB3	4:D:203:LHG:HC5	2.00	0.42
1:G:144:LEU:HD11	1:H:67:LEU:HD23	2.01	0.42
1:J:18:ALA:HB2	1:J:93:LEU:HA	2.01	0.42
1:B:61:LEU:HD21	1:B:132:ILE:HA	2.02	0.42
1:H:17[B]:LEU:HD11	4:H:203:LHG:H171	2.01	0.42
1:H:144:LEU:HD11	1:I:67:LEU:HD23	2.01	0.42
1:J:19:MET:CE	1:J:77:PHE:HB2	2.50	0.42
1:J:19:MET:HE3	1:J:77:PHE:HB2	2.02	0.41
4:D:203:LHG:HC81	4:E:203:LHG:HC62	2.03	0.41
1:F:54[B]:GLN:HE21	1:F:128:ALA:HB3	1.86	0.41
1:A:12[A]:MET:HE3	1:J:91:ASN:HD21	1.86	0.40
1:A:53:GLY:HA3	5:A:205:UMQ:HB2	2.04	0.40
1:G:2:MET:SD	1:H:1:MET:HE2	2.61	0.40
1:A:18:ALA:HB2	1:A:93:LEU:HA	2.02	0.40
1:C:54[B]:GLN:HE21	1:C:128:ALA:HB3	1.87	0.40
1:F:48:GLN:OE1	1:F:51:LYS:NZ	2.52	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%)	161 (99%)	2 (1%)	0	100	100
1	B	163/156 (104%)	161 (99%)	2 (1%)	0	100	100
1	C	163/156 (104%)	160 (98%)	3 (2%)	0	100	100
1	D	163/156 (104%)	161 (99%)	2 (1%)	0	100	100
1	E	163/156 (104%)	161 (99%)	2 (1%)	0	100	100
1	F	163/156 (104%)	161 (99%)	2 (1%)	0	100	100
1	G	163/156 (104%)	161 (99%)	2 (1%)	0	100	100
1	H	163/156 (104%)	161 (99%)	2 (1%)	0	100	100
1	I	161/156 (103%)	160 (99%)	1 (1%)	0	100	100
1	J	162/156 (104%)	161 (99%)	1 (1%)	0	100	100
All	All	1627/1560 (104%)	1608 (99%)	19 (1%)	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 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%)	117 (96%)	5 (4%)	27	46
1	B	122/113 (108%)	117 (96%)	5 (4%)	27	46
1	C	122/113 (108%)	118 (97%)	4 (3%)	33	55
1	D	122/113 (108%)	117 (96%)	5 (4%)	27	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	122/113 (108%)	117 (96%)	5 (4%)	27	46
1	F	122/113 (108%)	118 (97%)	4 (3%)	33	55
1	G	122/113 (108%)	118 (97%)	4 (3%)	33	55
1	H	122/113 (108%)	117 (96%)	5 (4%)	27	46
1	I	120/113 (106%)	116 (97%)	4 (3%)	33	55
1	J	121/113 (107%)	117 (97%)	4 (3%)	33	55
All	All	1217/1130 (108%)	1172 (96%)	45 (4%)	34	51

All (45) 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	139	GLU
1	A	143	ILE
1	B	54[A]	GLN
1	B	54[B]	GLN
1	B	61	LEU
1	B	139	GLU
1	B	143	ILE
1	C	54[A]	GLN
1	C	54[B]	GLN
1	C	61	LEU
1	C	143	ILE
1	D	54[A]	GLN
1	D	54[B]	GLN
1	D	61	LEU
1	D	139	GLU
1	D	143	ILE
1	E	54[A]	GLN
1	E	54[B]	GLN
1	E	61	LEU
1	E	139	GLU
1	E	143	ILE
1	F	54[A]	GLN
1	F	54[B]	GLN
1	F	61	LEU
1	F	143	ILE
1	G	54[A]	GLN

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Mol	Chain	Res	Type
1	G	54[B]	GLN
1	G	61	LEU
1	G	143	ILE
1	H	54[A]	GLN
1	H	54[B]	GLN
1	H	61	LEU
1	H	139	GLU
1	H	143	ILE
1	I	61	LEU
1	I	83	ASP
1	I	139	GLU
1	I	143	ILE
1	J	54[A]	GLN
1	J	54[B]	GLN
1	J	61	LEU
1	J	143	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	88	GLN
1	D	88	GLN
1	G	88	GLN
1	I	8	GLN
1	I	9	ASN
1	I	79	ASN
1	J	8	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 50 ligands modelled in this entry, 10 are monoatomic - leaving 40 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
2	DCW	G	201	1	17,17,17	1.18	2 (11%)	21,21,21	1.27	3 (14%)
2	DCW	C	201	1	17,17,17	1.22	2 (11%)	21,21,21	1.35	3 (14%)
2	DCW	F	201	1	17,17,17	1.21	2 (11%)	21,21,21	1.34	3 (14%)
4	LHG	A	203	-	39,39,48	1.08	2 (5%)	41,41,54	1.13	3 (7%)
4	LHG	F	205	-	39,39,48	1.08	2 (5%)	41,41,54	1.12	3 (7%)
5	UMQ	E	204	-	11,11,35	0.25	0	10,10,46	0.57	0
5	UMQ	I	205	-	11,11,35	0.27	0	10,10,46	0.56	0
2	DCW	D	201	1	17,17,17	1.21	2 (11%)	21,21,21	1.36	3 (14%)
4	LHG	G	204	-	39,39,48	1.07	2 (5%)	41,41,54	1.14	3 (7%)
5	UMQ	C	206	-	35,35,35	1.05	2 (5%)	46,46,46	1.64	6 (13%)
5	UMQ	F	206	-	35,35,35	1.10	3 (8%)	46,46,46	1.65	6 (13%)
4	LHG	A	204	-	39,39,48	1.05	2 (5%)	41,41,54	1.06	2 (4%)
4	LHG	D	203	-	39,39,48	1.05	2 (5%)	41,41,54	1.06	2 (4%)
5	UMQ	J	205	-	11,11,35	0.26	0	10,10,46	0.51	0
2	DCW	E	201	1	17,17,17	1.23	2 (11%)	21,21,21	1.40	3 (14%)
2	DCW	H	201	1	17,17,17	1.19	2 (11%)	21,21,21	1.33	3 (14%)
4	LHG	H	203	-	39,39,48	1.05	2 (5%)	41,41,54	1.07	2 (4%)
4	LHG	F	204	-	39,39,48	1.04	2 (5%)	41,41,54	1.06	2 (4%)
4	LHG	B	204	-	39,39,48	1.05	2 (5%)	41,41,54	1.06	2 (4%)
2	DCW	A	201	1	17,17,17	1.21	2 (11%)	21,21,21	1.37	3 (14%)
4	LHG	J	204	-	39,39,48	1.05	2 (5%)	41,41,54	1.02	2 (4%)
4	LHG	C	204	-	39,39,48	1.04	2 (5%)	41,41,54	1.05	2 (4%)
4	LHG	C	205	-	39,39,48	1.07	2 (5%)	41,41,54	1.11	3 (7%)
2	DCW	B	201	1	17,17,17	1.22	2 (11%)	21,21,21	1.37	3 (14%)
4	LHG	D	204	-	39,39,48	1.08	2 (5%)	41,41,54	1.12	3 (7%)
5	UMQ	A	206	-	11,11,35	0.29	0	10,10,46	0.50	0
4	LHG	C	203	-	39,39,48	1.09	2 (5%)	41,41,54	1.10	3 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	LHG	G	203	-	39,39,48	1.04	2 (5%)	41,41,54	1.06	2 (4%)
4	LHG	B	203	-	39,39,48	1.08	2 (5%)	41,41,54	1.13	3 (7%)
4	LHG	E	203	-	39,39,48	1.05	2 (5%)	41,41,54	1.06	2 (4%)
2	DCW	J	201	1	17,17,17	1.23	2 (11%)	21,21,21	1.34	3 (14%)
5	UMQ	A	205	-	11,11,35	0.96	0	10,10,46	0.86	0
4	LHG	I	204	-	39,39,48	1.05	2 (5%)	41,41,54	1.07	2 (4%)
4	LHG	F	203	-	39,39,48	1.08	2 (5%)	41,41,54	1.10	3 (7%)
4	LHG	J	203	-	39,39,48	1.08	2 (5%)	41,41,54	1.12	3 (7%)
5	UMQ	J	206	-	11,11,35	1.31	1 (9%)	10,10,46	1.21	2 (20%)
5	UMQ	H	204	-	11,11,35	0.77	0	10,10,46	0.75	0
4	LHG	I	203	-	39,39,48	1.08	2 (5%)	41,41,54	1.12	3 (7%)
2	DCW	I	201	1	17,17,17	1.28	2 (11%)	21,21,21	1.37	3 (14%)
5	UMQ	D	205	-	11,11,35	0.89	1 (9%)	10,10,46	0.82	0

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	DCW	G	201	1	-	3/8/24/24	0/2/2/2
2	DCW	C	201	1	-	3/8/24/24	0/2/2/2
2	DCW	F	201	1	-	3/8/24/24	0/2/2/2
4	LHG	A	203	-	-	23/41/41/53	-
4	LHG	F	205	-	-	22/41/41/53	-
5	UMQ	E	204	-	-	6/9/9/60	-
5	UMQ	I	205	-	-	6/9/9/60	-
2	DCW	D	201	1	-	3/8/24/24	0/2/2/2
5	UMQ	C	206	-	1/1/10/10	10/20/60/60	0/2/2/2
4	LHG	G	204	-	-	23/41/41/53	-
5	UMQ	F	206	-	1/1/10/10	8/20/60/60	0/2/2/2
4	LHG	A	204	-	-	23/41/41/53	-
4	LHG	D	203	-	-	23/41/41/53	-
5	UMQ	J	205	-	-	4/9/9/60	-
2	DCW	E	201	1	-	3/8/24/24	0/2/2/2
2	DCW	H	201	1	-	3/8/24/24	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	LHG	H	203	-	-	23/41/41/53	-
4	LHG	F	204	-	-	22/41/41/53	-
4	LHG	B	204	-	-	23/41/41/53	-
2	DCW	A	201	1	-	3/8/24/24	0/2/2/2
4	LHG	J	204	-	-	23/41/41/53	-
4	LHG	C	204	-	-	22/41/41/53	-
4	LHG	C	205	-	-	22/41/41/53	-
2	DCW	B	201	1	-	3/8/24/24	0/2/2/2
4	LHG	D	204	-	-	23/41/41/53	-
5	UMQ	A	206	-	-	4/9/9/60	-
4	LHG	C	203	-	-	22/41/41/53	-
4	LHG	G	203	-	-	23/41/41/53	-
4	LHG	B	203	-	-	23/41/41/53	-
4	LHG	E	203	-	-	23/41/41/53	-
2	DCW	J	201	1	-	3/8/24/24	0/2/2/2
5	UMQ	A	205	-	-	5/9/9/60	-
4	LHG	I	204	-	-	22/41/41/53	-
4	LHG	F	203	-	-	23/41/41/53	-
4	LHG	J	203	-	-	23/41/41/53	-
5	UMQ	J	206	-	-	4/9/9/60	-
5	UMQ	H	204	-	-	4/9/9/60	-
4	LHG	I	203	-	-	23/41/41/53	-
2	DCW	I	201	1	-	3/8/24/24	0/2/2/2
5	UMQ	D	205	-	-	3/9/9/60	-

All (67) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	203	LHG	O8-C23	4.60	1.46	1.33
4	F	205	LHG	O8-C23	4.54	1.46	1.33
4	C	203	LHG	O7-C7	4.54	1.47	1.34
4	G	204	LHG	O8-C23	4.53	1.46	1.33
4	C	203	LHG	O8-C23	4.53	1.46	1.33
4	D	204	LHG	O8-C23	4.52	1.46	1.33
4	C	205	LHG	O8-C23	4.50	1.46	1.33
4	B	203	LHG	O8-C23	4.49	1.46	1.33
4	F	203	LHG	O7-C7	4.49	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	203	LHG	O8-C23	4.48	1.46	1.33
4	D	204	LHG	O7-C7	4.48	1.46	1.34
4	J	203	LHG	O7-C7	4.48	1.46	1.34
4	F	203	LHG	O8-C23	4.48	1.46	1.33
4	B	203	LHG	O7-C7	4.47	1.46	1.34
4	J	203	LHG	O8-C23	4.47	1.46	1.33
4	A	203	LHG	O7-C7	4.45	1.46	1.34
4	B	204	LHG	O8-C23	4.42	1.46	1.33
4	H	203	LHG	O8-C23	4.42	1.46	1.33
4	G	204	LHG	O7-C7	4.41	1.46	1.34
4	A	204	LHG	O8-C23	4.41	1.46	1.33
4	E	203	LHG	O8-C23	4.41	1.46	1.33
4	F	205	LHG	O7-C7	4.39	1.46	1.34
4	G	203	LHG	O8-C23	4.39	1.46	1.33
4	I	203	LHG	O7-C7	4.38	1.46	1.34
4	D	203	LHG	O8-C23	4.38	1.46	1.33
4	J	204	LHG	O8-C23	4.37	1.46	1.33
4	C	205	LHG	O7-C7	4.37	1.46	1.34
4	I	204	LHG	O8-C23	4.35	1.46	1.33
4	C	204	LHG	O8-C23	4.35	1.46	1.33
4	F	204	LHG	O8-C23	4.34	1.46	1.33
4	I	204	LHG	O7-C7	4.30	1.46	1.34
4	H	203	LHG	O7-C7	4.26	1.46	1.34
4	E	203	LHG	O7-C7	4.25	1.46	1.34
4	D	203	LHG	O7-C7	4.25	1.46	1.34
4	B	204	LHG	O7-C7	4.23	1.46	1.34
4	A	204	LHG	O7-C7	4.23	1.46	1.34
4	C	204	LHG	O7-C7	4.22	1.46	1.34
4	F	204	LHG	O7-C7	4.21	1.46	1.34
4	J	204	LHG	O7-C7	4.20	1.46	1.34
4	G	203	LHG	O7-C7	4.19	1.46	1.34
5	F	206	UMQ	O3-C3	-4.12	1.32	1.43
5	C	206	UMQ	O3-C3	-4.09	1.32	1.43
5	F	206	UMQ	O2-C2	-3.89	1.33	1.43
5	C	206	UMQ	O2-C2	-3.76	1.33	1.43
2	I	201	DCW	C1-N1	3.61	1.45	1.35
5	J	206	UMQ	CH-CG	3.54	1.69	1.51
2	C	201	DCW	C1-N1	3.49	1.45	1.35
2	E	201	DCW	C1-N1	3.49	1.45	1.35
2	B	201	DCW	C1-N1	3.49	1.45	1.35
2	D	201	DCW	C1-N1	3.46	1.45	1.35
2	J	201	DCW	C1-N1	3.38	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	201	DCW	C1-N1	3.37	1.44	1.35
2	F	201	DCW	C1-N1	3.37	1.44	1.35
2	A	201	DCW	C1-N1	3.36	1.44	1.35
2	H	201	DCW	C1-N1	3.23	1.44	1.35
2	C	201	DCW	C1-N2	2.66	1.42	1.35
2	I	201	DCW	C1-N2	2.64	1.42	1.35
2	A	201	DCW	C1-N2	2.61	1.42	1.35
2	E	201	DCW	C1-N2	2.61	1.42	1.35
2	B	201	DCW	C1-N2	2.60	1.42	1.35
2	J	201	DCW	C1-N2	2.58	1.42	1.35
2	D	201	DCW	C1-N2	2.57	1.42	1.35
2	H	201	DCW	C1-N2	2.55	1.42	1.35
2	F	201	DCW	C1-N2	2.54	1.42	1.35
2	G	201	DCW	C1-N2	2.42	1.42	1.35
5	D	205	UMQ	CL-CK	2.30	1.66	1.50
5	F	206	UMQ	O1'-C1'	2.17	1.43	1.40

All (94) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	206	UMQ	C4-C3-C2	5.45	120.40	110.83
5	C	206	UMQ	C4-C3-C2	5.37	120.26	110.83
5	F	206	UMQ	O2-C2-C1	4.63	121.11	110.08
4	J	203	LHG	O7-C7-C8	4.62	121.48	111.48
4	A	203	LHG	O7-C7-C8	4.60	121.44	111.48
4	B	203	LHG	O7-C7-C8	4.60	121.43	111.48
4	G	204	LHG	O7-C7-C8	4.58	121.39	111.48
4	F	205	LHG	O7-C7-C8	4.52	121.26	111.48
4	F	203	LHG	O7-C7-C8	4.50	121.22	111.48
4	D	204	LHG	O7-C7-C8	4.49	121.19	111.48
4	I	203	LHG	O7-C7-C8	4.48	121.17	111.48
4	C	203	LHG	O7-C7-C8	4.48	121.17	111.48
5	C	206	UMQ	O3-C3-C4	4.42	120.81	110.38
4	C	205	LHG	O7-C7-C8	4.41	121.02	111.48
5	F	206	UMQ	C1-C2-C3	4.24	118.93	110.01
4	I	204	LHG	O7-C7-C8	4.02	120.17	111.48
4	H	203	LHG	O7-C7-C8	3.98	120.09	111.48
5	F	206	UMQ	O3-C3-C4	3.96	119.71	110.38
4	A	204	LHG	O7-C7-C8	3.91	119.95	111.48
4	B	204	LHG	O7-C7-C8	3.91	119.93	111.48
4	C	204	LHG	O7-C7-C8	3.91	119.93	111.48
4	E	203	LHG	O7-C7-C8	3.90	119.92	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	203	LHG	O7-C7-C8	3.90	119.91	111.48
4	F	204	LHG	O7-C7-C8	3.88	119.89	111.48
4	G	203	LHG	O7-C7-C8	3.88	119.87	111.48
5	C	206	UMQ	O2-C2-C1	3.88	119.31	110.08
5	C	206	UMQ	C1-C2-C3	3.80	118.00	110.01
4	J	204	LHG	O7-C7-C8	3.78	119.65	111.48
5	C	206	UMQ	O2-C2-C3	3.68	119.05	110.38
5	F	206	UMQ	O2-C2-C3	3.60	118.85	110.38
5	C	206	UMQ	O3-C3-C2	3.59	118.84	110.38
2	I	201	DCW	C13-C8-N2	-3.56	103.46	110.57
2	H	201	DCW	C13-C8-N2	-3.49	103.61	110.57
2	D	201	DCW	C2-N1-C1	-3.48	115.42	122.92
2	E	201	DCW	C2-N1-C1	-3.48	115.43	122.92
2	B	201	DCW	C2-N1-C1	-3.46	115.46	122.92
2	C	201	DCW	C2-N1-C1	-3.46	115.46	122.92
2	E	201	DCW	C13-C8-N2	-3.46	103.67	110.57
2	F	201	DCW	C2-N1-C1	-3.43	115.53	122.92
2	J	201	DCW	C13-C8-N2	-3.40	103.78	110.57
2	B	201	DCW	C13-C8-N2	-3.37	103.83	110.57
2	C	201	DCW	C13-C8-N2	-3.36	103.85	110.57
2	D	201	DCW	C13-C8-N2	-3.36	103.85	110.57
2	A	201	DCW	C13-C8-N2	-3.36	103.86	110.57
2	J	201	DCW	C2-N1-C1	-3.35	115.71	122.92
2	A	201	DCW	C2-N1-C1	-3.32	115.77	122.92
2	F	201	DCW	C13-C8-N2	-3.22	104.13	110.57
2	G	201	DCW	C13-C8-N2	-3.20	104.18	110.57
2	I	201	DCW	C2-N1-C1	-3.10	116.25	122.92
2	H	201	DCW	C2-N1-C1	-3.05	116.35	122.92
2	G	201	DCW	C2-N1-C1	-3.04	116.37	122.92
2	E	201	DCW	C9-C8-N2	-2.94	104.69	110.57
4	G	204	LHG	O8-C23-C24	2.87	120.60	111.83
2	B	201	DCW	C9-C8-N2	-2.83	104.92	110.57
5	F	206	UMQ	O3-C3-C2	2.83	117.04	110.38
2	A	201	DCW	C9-C8-N2	-2.80	104.97	110.57
4	D	204	LHG	O8-C23-C24	2.79	120.35	111.83
4	C	205	LHG	O8-C23-C24	2.79	120.34	111.83
4	B	204	LHG	O8-C23-C24	2.78	120.31	111.83
4	H	203	LHG	O8-C23-C24	2.77	120.27	111.83
4	D	203	LHG	O8-C23-C24	2.75	120.22	111.83
4	F	205	LHG	O8-C23-C24	2.74	120.20	111.83
4	B	203	LHG	O8-C23-C24	2.74	120.19	111.83
4	A	203	LHG	O8-C23-C24	2.74	120.18	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	204	LHG	O8-C23-C24	2.74	120.17	111.83
4	I	203	LHG	O8-C23-C24	2.73	120.17	111.83
4	E	203	LHG	O8-C23-C24	2.73	120.17	111.83
4	A	204	LHG	O8-C23-C24	2.72	120.14	111.83
4	G	203	LHG	O8-C23-C24	2.72	120.13	111.83
4	C	203	LHG	O8-C23-C24	2.71	120.11	111.83
4	I	204	LHG	O8-C23-C24	2.71	120.10	111.83
2	I	201	DCW	C9-C8-N2	-2.71	105.16	110.57
2	D	201	DCW	C9-C8-N2	-2.70	105.17	110.57
4	J	204	LHG	O8-C23-C24	2.70	120.07	111.83
2	H	201	DCW	C9-C8-N2	-2.70	105.18	110.57
4	C	204	LHG	O8-C23-C24	2.70	120.06	111.83
2	G	201	DCW	C9-C8-N2	-2.59	105.40	110.57
5	J	206	UMQ	CH-CG-CF	-2.59	101.29	114.37
4	F	203	LHG	O8-C23-C24	2.59	119.72	111.83
4	J	203	LHG	O8-C23-C24	2.56	119.63	111.83
2	F	201	DCW	C9-C8-N2	-2.50	105.58	110.57
2	J	201	DCW	C9-C8-N2	-2.41	105.75	110.57
2	C	201	DCW	C9-C8-N2	-2.32	105.93	110.57
5	J	206	UMQ	CI-CH-CG	-2.22	103.14	114.37
4	I	203	LHG	O7-C7-O9	-2.21	118.53	123.70
4	G	204	LHG	O7-C7-O9	-2.21	118.54	123.70
4	D	204	LHG	O7-C7-O9	-2.21	118.54	123.70
4	A	203	LHG	O7-C7-O9	-2.19	118.59	123.70
4	J	203	LHG	O7-C7-O9	-2.18	118.60	123.70
4	B	203	LHG	O7-C7-O9	-2.15	118.68	123.70
4	F	205	LHG	O7-C7-O9	-2.13	118.73	123.70
4	F	203	LHG	O7-C7-O9	-2.13	118.73	123.70
4	C	205	LHG	O7-C7-O9	-2.13	118.73	123.70
4	C	203	LHG	O7-C7-O9	-2.02	118.99	123.70

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	C	206	UMQ	C3
5	F	206	UMQ	C2

All (538) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	201	DCW	N2-C1-N1-C2
2	B	201	DCW	N2-C1-N1-C2

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Mol	Chain	Res	Type	Atoms
2	C	201	DCW	N2-C1-N1-C2
2	D	201	DCW	N2-C1-N1-C2
2	E	201	DCW	N2-C1-N1-C2
2	F	201	DCW	N2-C1-N1-C2
2	G	201	DCW	N2-C1-N1-C2
2	H	201	DCW	N2-C1-N1-C2
2	I	201	DCW	N2-C1-N1-C2
2	J	201	DCW	N2-C1-N1-C2
4	A	203	LHG	O6-C4-C5-O7
4	A	203	LHG	C8-C7-O7-C5
4	B	203	LHG	O6-C4-C5-O7
4	B	203	LHG	C8-C7-O7-C5
4	C	203	LHG	O6-C4-C5-O7
4	C	203	LHG	C8-C7-O7-C5
4	C	205	LHG	O6-C4-C5-O7
4	C	205	LHG	C8-C7-O7-C5
4	D	204	LHG	O6-C4-C5-O7
4	D	204	LHG	C8-C7-O7-C5
4	F	203	LHG	O6-C4-C5-O7
4	F	203	LHG	C8-C7-O7-C5
4	F	205	LHG	O6-C4-C5-O7
4	F	205	LHG	C8-C7-O7-C5
4	G	204	LHG	O6-C4-C5-O7
4	G	204	LHG	C8-C7-O7-C5
4	I	203	LHG	O6-C4-C5-O7
4	I	203	LHG	C8-C7-O7-C5
4	J	203	LHG	O6-C4-C5-O7
4	J	203	LHG	C8-C7-O7-C5
4	J	204	LHG	O9-C7-O7-C5
2	E	201	DCW	O1-C1-N1-C2
2	I	201	DCW	O1-C1-N1-C2
4	A	203	LHG	O9-C7-O7-C5
4	A	204	LHG	O9-C7-O7-C5
4	B	203	LHG	O9-C7-O7-C5
4	B	204	LHG	O9-C7-O7-C5
4	C	203	LHG	O9-C7-O7-C5
4	C	204	LHG	O9-C7-O7-C5
4	C	205	LHG	O9-C7-O7-C5
4	D	203	LHG	O9-C7-O7-C5
4	D	204	LHG	O9-C7-O7-C5
4	E	203	LHG	O9-C7-O7-C5
4	F	203	LHG	O9-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
4	F	204	LHG	O9-C7-O7-C5
4	F	205	LHG	O9-C7-O7-C5
4	G	203	LHG	O9-C7-O7-C5
4	G	204	LHG	O9-C7-O7-C5
4	H	203	LHG	O9-C7-O7-C5
4	I	203	LHG	O9-C7-O7-C5
4	I	204	LHG	O9-C7-O7-C5
4	J	203	LHG	O9-C7-O7-C5
4	A	204	LHG	C8-C7-O7-C5
4	C	204	LHG	C8-C7-O7-C5
4	F	204	LHG	C8-C7-O7-C5
4	I	204	LHG	C8-C7-O7-C5
4	J	204	LHG	C8-C7-O7-C5
2	A	201	DCW	O1-C1-N1-C2
2	B	201	DCW	O1-C1-N1-C2
2	C	201	DCW	O1-C1-N1-C2
2	D	201	DCW	O1-C1-N1-C2
2	F	201	DCW	O1-C1-N1-C2
2	G	201	DCW	O1-C1-N1-C2
2	H	201	DCW	O1-C1-N1-C2
2	J	201	DCW	O1-C1-N1-C2
4	A	204	LHG	C24-C23-O8-C6
4	B	204	LHG	C24-C23-O8-C6
4	C	204	LHG	C24-C23-O8-C6
4	D	203	LHG	C24-C23-O8-C6
4	E	203	LHG	C24-C23-O8-C6
4	F	204	LHG	C24-C23-O8-C6
4	G	203	LHG	C24-C23-O8-C6
4	H	203	LHG	C24-C23-O8-C6
4	I	204	LHG	C24-C23-O8-C6
4	J	204	LHG	C24-C23-O8-C6
5	C	206	UMQ	O5-C5-C6-O6
4	A	204	LHG	O10-C23-O8-C6
4	B	204	LHG	O10-C23-O8-C6
4	C	204	LHG	O10-C23-O8-C6
4	D	203	LHG	O10-C23-O8-C6
4	E	203	LHG	O10-C23-O8-C6
4	F	204	LHG	O10-C23-O8-C6
4	G	203	LHG	O10-C23-O8-C6
4	H	203	LHG	O10-C23-O8-C6
4	I	204	LHG	O10-C23-O8-C6
4	J	204	LHG	O10-C23-O8-C6

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Mol	Chain	Res	Type	Atoms
4	B	204	LHG	C8-C7-O7-C5
4	D	203	LHG	C8-C7-O7-C5
4	E	203	LHG	C8-C7-O7-C5
4	G	203	LHG	C8-C7-O7-C5
4	H	203	LHG	C8-C7-O7-C5
2	A	201	DCW	C3-C2-N1-C1
2	B	201	DCW	C3-C2-N1-C1
2	C	201	DCW	C3-C2-N1-C1
2	D	201	DCW	C3-C2-N1-C1
2	E	201	DCW	C3-C2-N1-C1
2	F	201	DCW	C3-C2-N1-C1
2	G	201	DCW	C3-C2-N1-C1
2	H	201	DCW	C3-C2-N1-C1
2	I	201	DCW	C3-C2-N1-C1
2	J	201	DCW	C3-C2-N1-C1
5	C	206	UMQ	C4-C5-C6-O6
5	C	206	UMQ	O5'-C1'-O1'-CA
5	F	206	UMQ	O5'-C1'-O1'-CA
5	F	206	UMQ	O5-C5-C6-O6
5	F	206	UMQ	C4-C5-C6-O6
5	C	206	UMQ	C2'-C1'-O1'-CA
5	F	206	UMQ	C2'-C1'-O1'-CA
5	C	206	UMQ	O1'-CA-CB-CC
5	F	206	UMQ	O1'-CA-CB-CC
5	J	205	UMQ	CA-CB-CC-CD
4	C	205	LHG	C29-C30-C31-C32
4	D	204	LHG	C31-C32-C33-C34
4	F	205	LHG	C31-C32-C33-C34
4	G	204	LHG	C29-C30-C31-C32
4	G	204	LHG	C31-C32-C33-C34
4	B	203	LHG	C31-C32-C33-C34
4	C	205	LHG	C31-C32-C33-C34
4	D	204	LHG	C34-C35-C36-C37
4	G	204	LHG	C34-C35-C36-C37
4	I	203	LHG	C31-C32-C33-C34
4	J	203	LHG	C31-C32-C33-C34
5	E	204	UMQ	CB-CC-CD-CF
4	A	203	LHG	C31-C32-C33-C34
4	C	203	LHG	C31-C32-C33-C34
4	C	205	LHG	C34-C35-C36-C37
4	F	203	LHG	C31-C32-C33-C34
4	F	205	LHG	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
4	G	203	LHG	C15-C16-C17-C18
4	J	203	LHG	C34-C35-C36-C37
4	A	204	LHG	C10-C11-C12-C13
4	A	204	LHG	C15-C16-C17-C18
4	B	203	LHG	C29-C30-C31-C32
4	B	203	LHG	C34-C35-C36-C37
4	B	204	LHG	C10-C11-C12-C13
4	B	204	LHG	C15-C16-C17-C18
4	C	203	LHG	C29-C30-C31-C32
4	C	204	LHG	C10-C11-C12-C13
4	C	204	LHG	C15-C16-C17-C18
4	D	203	LHG	C15-C16-C17-C18
4	D	204	LHG	C29-C30-C31-C32
4	E	203	LHG	C10-C11-C12-C13
4	E	203	LHG	C15-C16-C17-C18
4	F	204	LHG	C10-C11-C12-C13
4	F	204	LHG	C15-C16-C17-C18
4	F	205	LHG	C29-C30-C31-C32
4	G	203	LHG	C10-C11-C12-C13
4	I	203	LHG	C34-C35-C36-C37
4	I	204	LHG	C15-C16-C17-C18
4	J	203	LHG	C29-C30-C31-C32
4	J	204	LHG	C26-C27-C28-C29
4	A	203	LHG	C34-C35-C36-C37
4	C	203	LHG	C34-C35-C36-C37
4	D	203	LHG	C10-C11-C12-C13
4	H	203	LHG	C10-C11-C12-C13
4	H	203	LHG	C15-C16-C17-C18
4	I	204	LHG	C10-C11-C12-C13
4	J	204	LHG	C10-C11-C12-C13
5	E	204	UMQ	CA-CB-CC-CD
4	A	203	LHG	C29-C30-C31-C32
4	F	203	LHG	C34-C35-C36-C37
4	I	203	LHG	C29-C30-C31-C32
4	J	204	LHG	C15-C16-C17-C18
4	F	203	LHG	C29-C30-C31-C32
4	A	204	LHG	C26-C27-C28-C29
4	C	204	LHG	C26-C27-C28-C29
4	E	203	LHG	C26-C27-C28-C29
4	F	204	LHG	C26-C27-C28-C29
4	I	204	LHG	C26-C27-C28-C29
4	C	203	LHG	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
5	A	205	UMQ	CF-CG-CH-CI
4	B	204	LHG	C26-C27-C28-C29
4	D	203	LHG	C26-C27-C28-C29
4	F	203	LHG	C14-C15-C16-C17
4	H	203	LHG	C26-C27-C28-C29
5	F	206	UMQ	CG-CH-CI-CJ
4	G	203	LHG	C26-C27-C28-C29
4	C	205	LHG	C27-C28-C29-C30
4	D	204	LHG	C27-C28-C29-C30
4	F	205	LHG	C27-C28-C29-C30
4	B	203	LHG	C27-C28-C29-C30
4	G	204	LHG	C14-C15-C16-C17
4	I	203	LHG	C27-C28-C29-C30
4	B	203	LHG	C24-C23-O8-C6
4	C	205	LHG	C24-C23-O8-C6
4	D	204	LHG	C24-C23-O8-C6
4	F	205	LHG	C24-C23-O8-C6
4	G	204	LHG	C24-C23-O8-C6
4	A	203	LHG	C14-C15-C16-C17
4	B	203	LHG	C14-C15-C16-C17
4	C	203	LHG	C27-C28-C29-C30
4	C	205	LHG	C14-C15-C16-C17
4	I	203	LHG	C14-C15-C16-C17
4	J	203	LHG	C14-C15-C16-C17
5	J	205	UMQ	CC-CD-CF-CG
4	A	203	LHG	C27-C28-C29-C30
4	D	204	LHG	C14-C15-C16-C17
4	F	203	LHG	C27-C28-C29-C30
4	G	204	LHG	C27-C28-C29-C30
4	J	203	LHG	C27-C28-C29-C30
4	F	205	LHG	C14-C15-C16-C17
5	D	205	UMQ	CA-CB-CC-CD
4	I	204	LHG	C14-C15-C16-C17
4	A	204	LHG	C14-C15-C16-C17
4	B	204	LHG	C14-C15-C16-C17
4	D	203	LHG	C14-C15-C16-C17
4	G	203	LHG	C14-C15-C16-C17
4	H	203	LHG	C14-C15-C16-C17
4	A	203	LHG	C24-C23-O8-C6
4	E	203	LHG	C14-C15-C16-C17
4	F	204	LHG	C14-C15-C16-C17
4	C	204	LHG	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
4	C	205	LHG	O10-C23-O8-C6
4	D	204	LHG	O10-C23-O8-C6
4	F	205	LHG	O10-C23-O8-C6
4	G	204	LHG	O10-C23-O8-C6
4	J	204	LHG	C14-C15-C16-C17
4	C	203	LHG	C24-C23-O8-C6
4	J	203	LHG	C24-C23-O8-C6
4	B	203	LHG	O10-C23-O8-C6
5	A	205	UMQ	CH-CI-CJ-CK
4	F	203	LHG	C24-C23-O8-C6
4	C	203	LHG	C28-C29-C30-C31
4	F	203	LHG	C28-C29-C30-C31
5	E	204	UMQ	CC-CD-CF-CG
5	E	204	UMQ	CF-CG-CH-CI
4	J	203	LHG	C28-C29-C30-C31
5	C	206	UMQ	CH-CI-CJ-CK
4	A	203	LHG	O10-C23-O8-C6
4	A	203	LHG	C28-C29-C30-C31
4	B	203	LHG	C28-C29-C30-C31
4	I	203	LHG	C28-C29-C30-C31
4	C	205	LHG	C28-C29-C30-C31
4	F	205	LHG	C28-C29-C30-C31
5	J	205	UMQ	CF-CG-CH-CI
4	G	204	LHG	C28-C29-C30-C31
4	D	204	LHG	C28-C29-C30-C31
5	F	206	UMQ	CB-CC-CD-CF
4	F	203	LHG	C25-C26-C27-C28
4	C	203	LHG	C25-C26-C27-C28
4	F	205	LHG	C25-C26-C27-C28
4	I	203	LHG	C25-C26-C27-C28
4	J	203	LHG	C25-C26-C27-C28
4	I	203	LHG	C24-C23-O8-C6
4	A	203	LHG	C25-C26-C27-C28
4	B	203	LHG	C25-C26-C27-C28
4	C	205	LHG	C25-C26-C27-C28
4	D	204	LHG	C25-C26-C27-C28
4	G	204	LHG	C25-C26-C27-C28
4	J	203	LHG	O10-C23-O8-C6
4	C	203	LHG	O10-C23-O8-C6
4	F	203	LHG	O10-C23-O8-C6
5	A	206	UMQ	O1'-CA-CB-CC
5	H	204	UMQ	O1'-CA-CB-CC

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Mol	Chain	Res	Type	Atoms
5	J	206	UMQ	O1'-CA-CB-CC
5	A	205	UMQ	CG-CH-CI-CJ
4	I	203	LHG	O10-C23-O8-C6
4	I	204	LHG	C31-C32-C33-C34
4	J	204	LHG	C31-C32-C33-C34
4	C	204	LHG	C31-C32-C33-C34
4	A	204	LHG	C4-C5-C6-O8
4	B	204	LHG	C4-C5-C6-O8
4	C	204	LHG	C4-C5-C6-O8
4	D	203	LHG	C4-C5-C6-O8
4	E	203	LHG	C4-C5-C6-O8
4	F	204	LHG	C4-C5-C6-O8
4	G	203	LHG	C4-C5-C6-O8
4	H	203	LHG	C4-C5-C6-O8
4	I	204	LHG	C4-C5-C6-O8
4	J	204	LHG	C4-C5-C6-O8
4	A	204	LHG	C31-C32-C33-C34
4	B	204	LHG	C31-C32-C33-C34
4	F	204	LHG	C31-C32-C33-C34
4	G	203	LHG	C31-C32-C33-C34
4	H	203	LHG	C31-C32-C33-C34
4	E	203	LHG	C31-C32-C33-C34
5	C	206	UMQ	CG-CH-CI-CJ
4	D	203	LHG	C31-C32-C33-C34
4	J	204	LHG	C28-C29-C30-C31
4	G	203	LHG	C28-C29-C30-C31
4	H	203	LHG	C28-C29-C30-C31
4	F	204	LHG	C28-C29-C30-C31
4	A	204	LHG	C28-C29-C30-C31
4	B	204	LHG	C28-C29-C30-C31
4	C	204	LHG	C28-C29-C30-C31
4	D	203	LHG	C28-C29-C30-C31
4	E	203	LHG	C28-C29-C30-C31
4	C	203	LHG	C32-C33-C34-C35
4	F	203	LHG	C32-C33-C34-C35
4	I	204	LHG	C28-C29-C30-C31
4	I	203	LHG	C32-C33-C34-C35
5	J	206	UMQ	CI-CJ-CK-CL
4	C	204	LHG	C27-C28-C29-C30
4	F	204	LHG	C27-C28-C29-C30
4	J	203	LHG	C32-C33-C34-C35
4	B	204	LHG	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
4	F	205	LHG	C32-C33-C34-C35
4	H	203	LHG	C27-C28-C29-C30
4	A	203	LHG	C32-C33-C34-C35
4	C	205	LHG	C32-C33-C34-C35
4	G	204	LHG	C32-C33-C34-C35
4	A	204	LHG	C27-C28-C29-C30
4	B	203	LHG	C32-C33-C34-C35
4	D	203	LHG	C27-C28-C29-C30
4	D	204	LHG	C32-C33-C34-C35
4	E	203	LHG	C27-C28-C29-C30
4	G	203	LHG	C27-C28-C29-C30
4	I	204	LHG	C27-C28-C29-C30
5	F	206	UMQ	CI-CJ-CK-CL
4	J	204	LHG	C27-C28-C29-C30
4	I	204	LHG	C35-C36-C37-C38
4	A	204	LHG	C35-C36-C37-C38
4	D	203	LHG	C35-C36-C37-C38
4	E	203	LHG	C35-C36-C37-C38
4	F	204	LHG	C35-C36-C37-C38
4	H	203	LHG	C35-C36-C37-C38
4	F	205	LHG	C23-C24-C25-C26
4	B	204	LHG	C35-C36-C37-C38
4	J	204	LHG	C35-C36-C37-C38
4	C	204	LHG	C35-C36-C37-C38
4	G	203	LHG	C35-C36-C37-C38
5	I	205	UMQ	CH-CI-CJ-CK
4	C	205	LHG	C23-C24-C25-C26
4	D	204	LHG	C23-C24-C25-C26
4	G	204	LHG	C23-C24-C25-C26
4	E	203	LHG	C34-C35-C36-C37
5	H	204	UMQ	CH-CI-CJ-CK
4	D	203	LHG	C34-C35-C36-C37
4	G	203	LHG	C34-C35-C36-C37
4	H	203	LHG	C34-C35-C36-C37
4	B	204	LHG	C34-C35-C36-C37
4	C	204	LHG	C33-C34-C35-C36
4	F	204	LHG	C33-C34-C35-C36
4	A	204	LHG	C34-C35-C36-C37
4	I	204	LHG	C34-C35-C36-C37
4	J	204	LHG	C33-C34-C35-C36
4	F	205	LHG	C24-C25-C26-C27
4	G	204	LHG	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
5	I	205	UMQ	CF-CG-CH-CI
4	B	203	LHG	O6-C4-C5-C6
4	D	204	LHG	O6-C4-C5-C6
4	F	205	LHG	O6-C4-C5-C6
4	J	203	LHG	O6-C4-C5-C6
4	B	203	LHG	C24-C25-C26-C27
4	J	204	LHG	C34-C35-C36-C37
4	B	203	LHG	C23-C24-C25-C26
4	F	203	LHG	C23-C24-C25-C26
4	A	204	LHG	C33-C34-C35-C36
4	G	203	LHG	C33-C34-C35-C36
4	B	204	LHG	C33-C34-C35-C36
4	F	204	LHG	C34-C35-C36-C37
4	I	204	LHG	C33-C34-C35-C36
4	D	204	LHG	C24-C25-C26-C27
4	A	203	LHG	C23-C24-C25-C26
4	C	205	LHG	C24-C25-C26-C27
4	D	203	LHG	C33-C34-C35-C36
4	E	203	LHG	C33-C34-C35-C36
4	H	203	LHG	C33-C34-C35-C36
5	C	206	UMQ	CI-CJ-CK-CL
4	C	204	LHG	C34-C35-C36-C37
4	A	203	LHG	C24-C25-C26-C27
4	J	203	LHG	C24-C25-C26-C27
5	A	205	UMQ	CC-CD-CF-CG
4	F	203	LHG	C24-C25-C26-C27
4	C	203	LHG	C19-C20-C21-C22
4	I	203	LHG	C24-C25-C26-C27
4	C	203	LHG	C23-C24-C25-C26
4	I	203	LHG	C23-C24-C25-C26
4	J	203	LHG	C23-C24-C25-C26
4	D	204	LHG	C19-C20-C21-C22
4	J	203	LHG	C19-C20-C21-C22
4	C	205	LHG	C19-C20-C21-C22
4	A	203	LHG	C19-C20-C21-C22
4	F	205	LHG	C19-C20-C21-C22
4	F	203	LHG	C19-C20-C21-C22
4	C	203	LHG	C24-C25-C26-C27
4	I	203	LHG	C19-C20-C21-C22
4	B	203	LHG	C19-C20-C21-C22
5	J	205	UMQ	CB-CC-CD-CF
4	G	204	LHG	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
5	J	206	UMQ	CD-CF-CG-CH
4	F	204	LHG	C11-C12-C13-C14
4	I	204	LHG	C11-C12-C13-C14
4	C	204	LHG	C11-C12-C13-C14
4	I	204	LHG	O7-C5-C6-O8
4	J	204	LHG	O7-C5-C6-O8
4	G	203	LHG	C11-C12-C13-C14
4	A	204	LHG	C11-C12-C13-C14
4	B	204	LHG	C11-C12-C13-C14
4	D	203	LHG	C11-C12-C13-C14
4	E	203	LHG	C11-C12-C13-C14
4	H	203	LHG	C11-C12-C13-C14
5	A	206	UMQ	CA-CB-CC-CD
4	F	203	LHG	C16-C17-C18-C19
4	C	205	LHG	C26-C27-C28-C29
4	C	203	LHG	C26-C27-C28-C29
4	B	203	LHG	C26-C27-C28-C29
5	H	204	UMQ	CF-CG-CH-CI
4	G	204	LHG	C26-C27-C28-C29
4	F	205	LHG	C26-C27-C28-C29
5	I	205	UMQ	CB-CC-CD-CF
4	D	204	LHG	C26-C27-C28-C29
4	J	204	LHG	C11-C12-C13-C14
4	A	203	LHG	C26-C27-C28-C29
4	A	204	LHG	O7-C5-C6-O8
4	B	204	LHG	O7-C5-C6-O8
4	C	204	LHG	O7-C5-C6-O8
4	D	203	LHG	O7-C5-C6-O8
4	E	203	LHG	O7-C5-C6-O8
4	F	204	LHG	O7-C5-C6-O8
4	G	203	LHG	O7-C5-C6-O8
4	H	203	LHG	O7-C5-C6-O8
4	C	203	LHG	C16-C17-C18-C19
4	J	203	LHG	C26-C27-C28-C29
4	I	203	LHG	C26-C27-C28-C29
4	F	203	LHG	C26-C27-C28-C29
4	J	203	LHG	C16-C17-C18-C19
4	D	204	LHG	C16-C17-C18-C19
5	C	206	UMQ	CF-CG-CH-CI
4	G	204	LHG	C16-C17-C18-C19
5	D	205	UMQ	O1'-CA-CB-CC
4	C	205	LHG	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
4	A	203	LHG	C16-C17-C18-C19
4	F	205	LHG	C16-C17-C18-C19
4	B	203	LHG	C16-C17-C18-C19
4	J	204	LHG	C24-C25-C26-C27
5	A	206	UMQ	CH-CI-CJ-CK
4	A	203	LHG	C6-C5-O7-C7
4	B	203	LHG	C6-C5-O7-C7
4	C	203	LHG	C6-C5-O7-C7
4	C	205	LHG	C6-C5-O7-C7
4	D	204	LHG	C6-C5-O7-C7
4	F	203	LHG	C6-C5-O7-C7
4	F	205	LHG	C6-C5-O7-C7
4	G	204	LHG	C6-C5-O7-C7
4	J	203	LHG	C6-C5-O7-C7
5	I	205	UMQ	O1'-CA-CB-CC
4	A	203	LHG	O6-C4-C5-C6
4	C	205	LHG	O6-C4-C5-C6
4	F	203	LHG	O6-C4-C5-C6
4	G	204	LHG	O6-C4-C5-C6
4	I	203	LHG	O6-C4-C5-C6
4	I	204	LHG	C24-C25-C26-C27
4	A	204	LHG	C24-C25-C26-C27
4	H	203	LHG	C24-C25-C26-C27
4	E	203	LHG	C24-C25-C26-C27
4	G	203	LHG	C24-C25-C26-C27
4	C	204	LHG	C24-C25-C26-C27
4	D	203	LHG	C24-C25-C26-C27
4	B	204	LHG	C24-C25-C26-C27
4	F	204	LHG	C24-C25-C26-C27
5	D	205	UMQ	CG-CH-CI-CJ
4	I	203	LHG	C16-C17-C18-C19
5	I	205	UMQ	CI-CJ-CK-CL
5	H	204	UMQ	CB-CC-CD-CF
5	J	206	UMQ	CA-CB-CC-CD
4	I	203	LHG	C6-C5-O7-C7
5	A	205	UMQ	O1'-CA-CB-CC
4	H	203	LHG	O8-C23-C24-C25
4	A	204	LHG	O8-C23-C24-C25
4	E	203	LHG	O8-C23-C24-C25
4	G	203	LHG	O8-C23-C24-C25
4	B	204	LHG	O8-C23-C24-C25
4	D	203	LHG	O8-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
4	I	203	LHG	C7-C8-C9-C10
4	C	204	LHG	O8-C23-C24-C25
4	F	204	LHG	O8-C23-C24-C25
4	A	204	LHG	O7-C7-C8-C9
4	C	204	LHG	O7-C7-C8-C9
4	G	203	LHG	O7-C7-C8-C9
4	I	204	LHG	O8-C23-C24-C25
4	J	204	LHG	O8-C23-C24-C25
4	E	203	LHG	O7-C7-C8-C9
4	J	204	LHG	O7-C7-C8-C9
5	I	205	UMQ	CA-CB-CC-CD
4	F	204	LHG	O7-C7-C8-C9
4	D	203	LHG	O7-C7-C8-C9
4	H	203	LHG	O7-C7-C8-C9
4	J	204	LHG	C16-C17-C18-C19
4	B	204	LHG	O7-C7-C8-C9
5	E	204	UMQ	CD-CF-CG-CH
4	I	204	LHG	O7-C7-C8-C9
5	A	206	UMQ	CD-CF-CG-CH
4	G	203	LHG	C16-C17-C18-C19
4	A	204	LHG	O10-C23-C24-C25
5	E	204	UMQ	O1'-CA-CB-CC
4	F	204	LHG	O10-C23-C24-C25
4	I	204	LHG	O10-C23-C24-C25
4	J	204	LHG	O10-C23-C24-C25
4	H	203	LHG	C16-C17-C18-C19
4	C	204	LHG	O10-C23-C24-C25
4	E	203	LHG	C16-C17-C18-C19
4	H	203	LHG	O10-C23-C24-C25
4	I	204	LHG	O9-C7-C8-C9
4	B	204	LHG	O10-C23-C24-C25
4	D	203	LHG	O10-C23-C24-C25
4	E	203	LHG	O10-C23-C24-C25
4	B	204	LHG	C16-C17-C18-C19
4	C	204	LHG	O9-C7-C8-C9
4	F	204	LHG	O9-C7-C8-C9
4	G	203	LHG	O10-C23-C24-C25
4	J	204	LHG	O9-C7-C8-C9
4	F	203	LHG	O7-C7-C8-C9
4	I	203	LHG	O7-C7-C8-C9
4	A	204	LHG	C16-C17-C18-C19
4	A	204	LHG	O9-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
4	B	204	LHG	O9-C7-C8-C9
4	D	203	LHG	O9-C7-C8-C9
4	H	203	LHG	O9-C7-C8-C9
4	D	203	LHG	C16-C17-C18-C19
4	A	203	LHG	O7-C7-C8-C9
4	G	204	LHG	O7-C7-C8-C9
4	G	203	LHG	O9-C7-C8-C9
4	B	203	LHG	O7-C7-C8-C9
4	C	205	LHG	O7-C7-C8-C9
4	D	204	LHG	O7-C7-C8-C9
4	F	205	LHG	O7-C7-C8-C9
4	I	203	LHG	O8-C23-C24-C25
4	E	203	LHG	O9-C7-C8-C9
4	F	203	LHG	C7-C8-C9-C10
5	C	206	UMQ	CA-CB-CC-CD
4	C	203	LHG	O7-C7-C8-C9
4	C	205	LHG	O8-C23-C24-C25
4	C	203	LHG	O6-C4-C5-C6
4	A	203	LHG	O8-C23-C24-C25
4	C	203	LHG	O8-C23-C24-C25
4	F	203	LHG	O8-C23-C24-C25
4	F	205	LHG	O8-C23-C24-C25
4	G	204	LHG	O8-C23-C24-C25
4	J	203	LHG	O7-C7-C8-C9
4	J	203	LHG	O10-C23-C24-C25
4	B	203	LHG	O8-C23-C24-C25
4	D	204	LHG	O8-C23-C24-C25
4	J	203	LHG	O8-C23-C24-C25
4	A	203	LHG	O9-C7-C8-C9
4	B	203	LHG	O10-C23-C24-C25
4	D	204	LHG	O10-C23-C24-C25
4	G	204	LHG	O9-C7-C8-C9

There are no ring outliers.

15 monomers are involved in 48 short contacts:

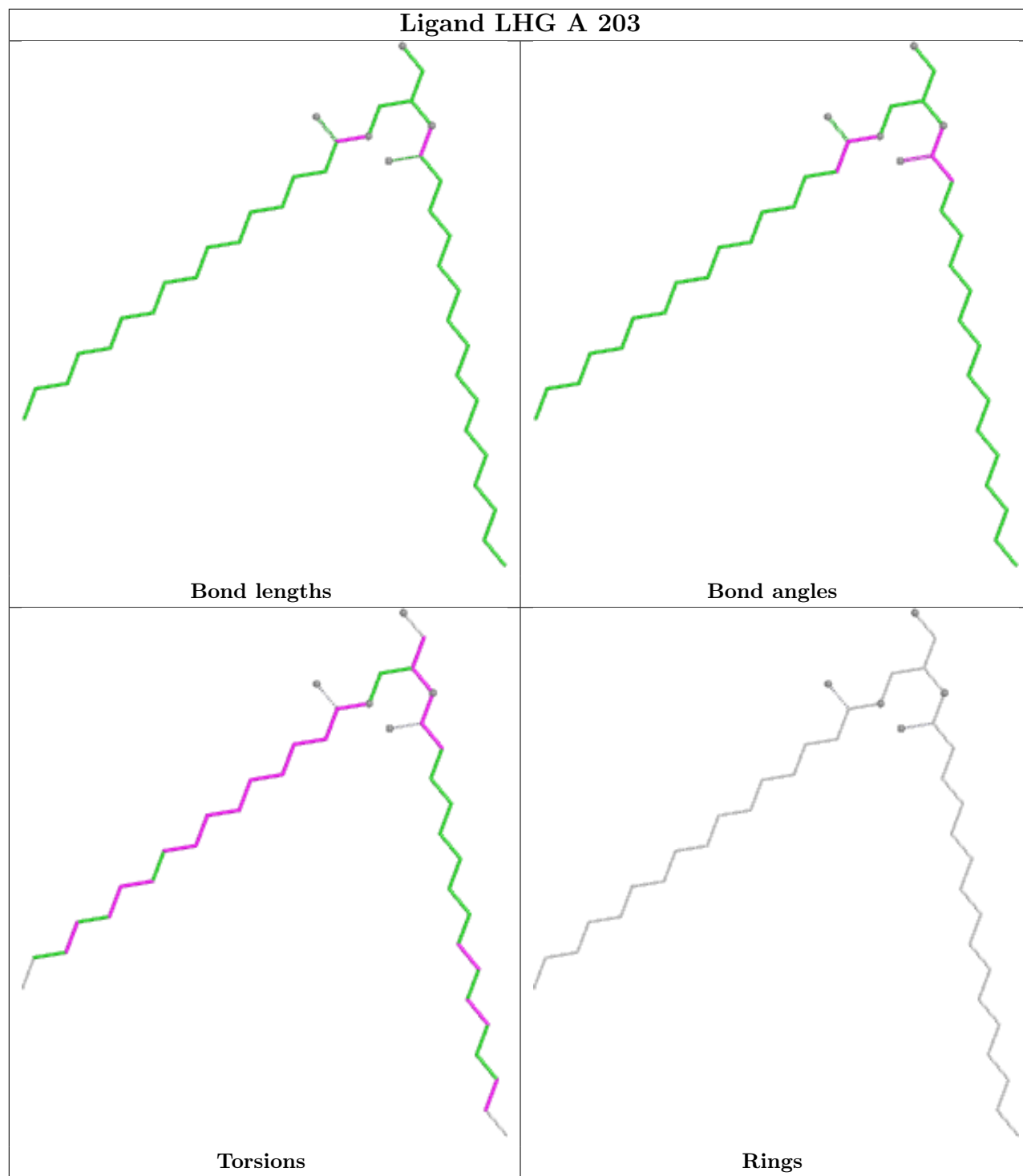
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	206	UMQ	1	0
5	F	206	UMQ	2	0
4	A	204	LHG	7	0
4	D	203	LHG	6	0
5	J	205	UMQ	1	0

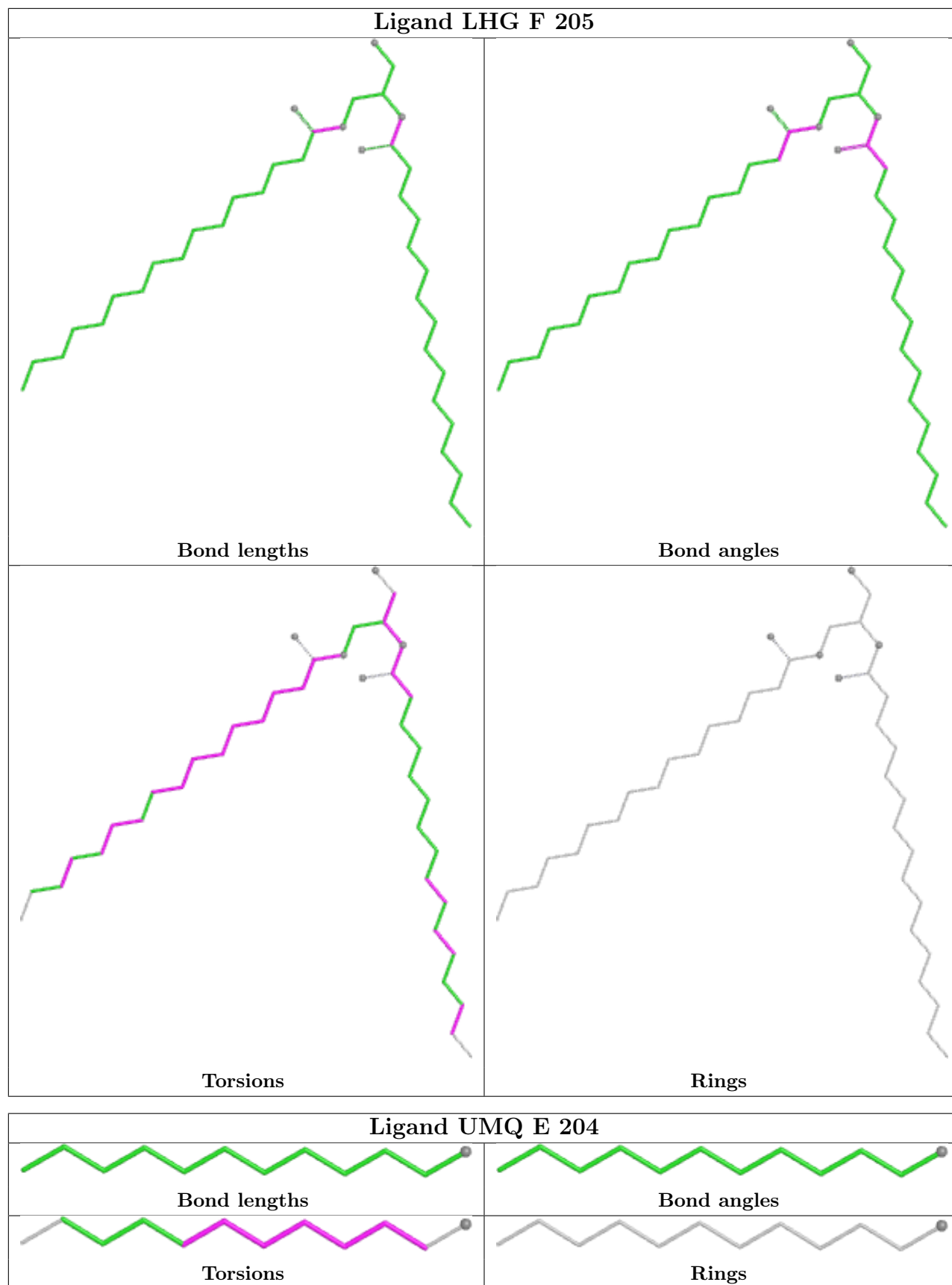
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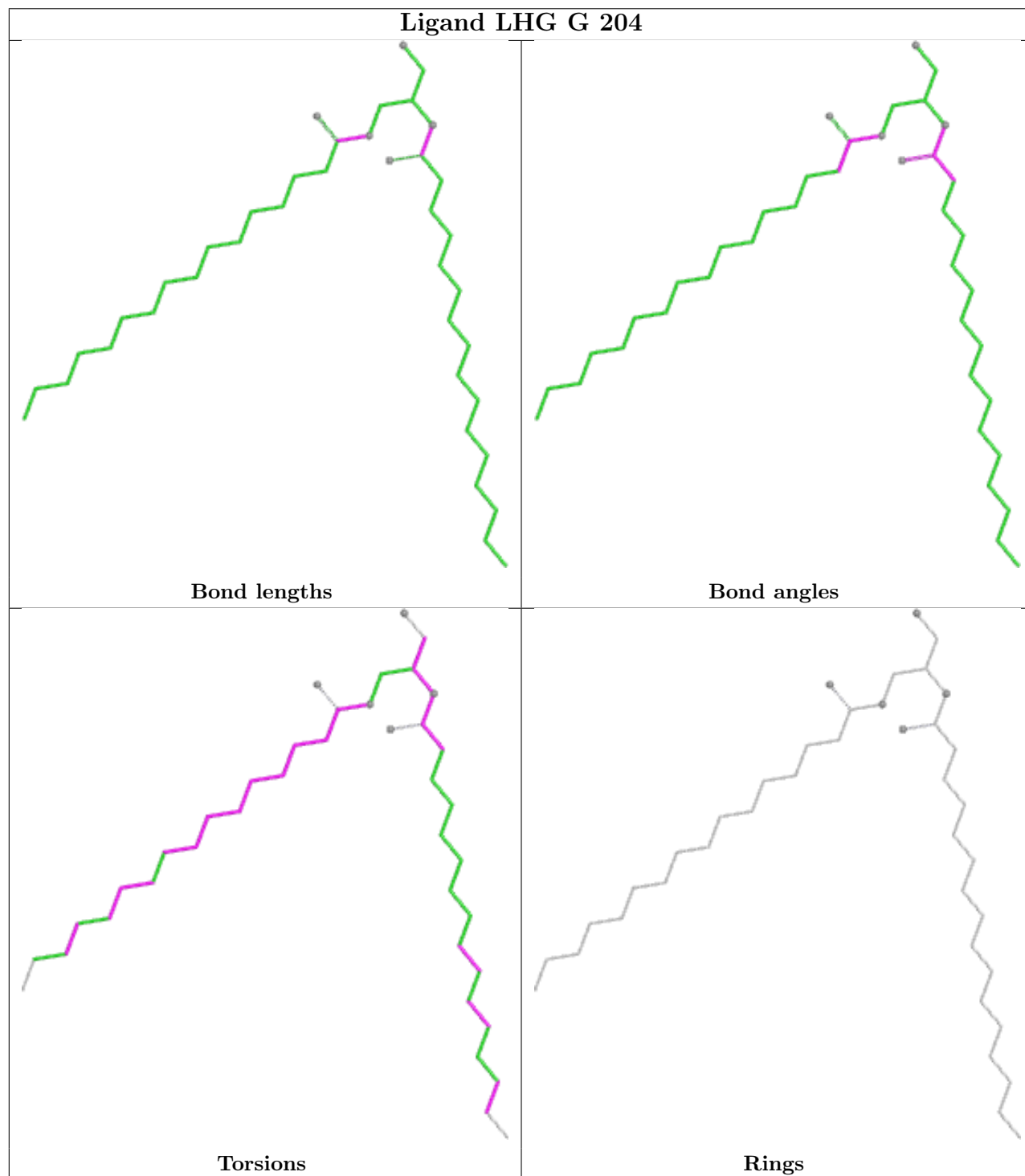
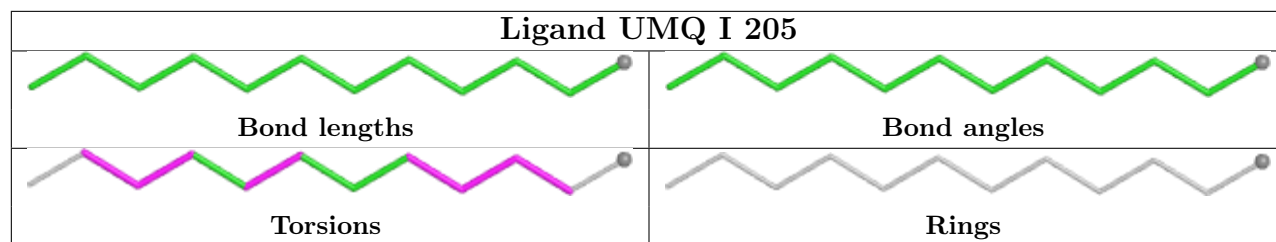
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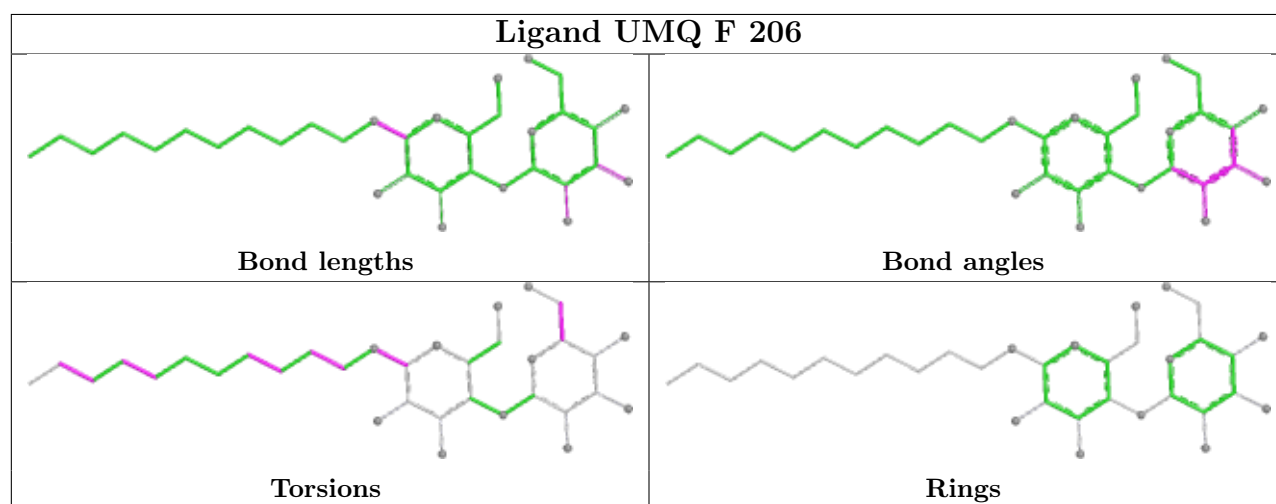
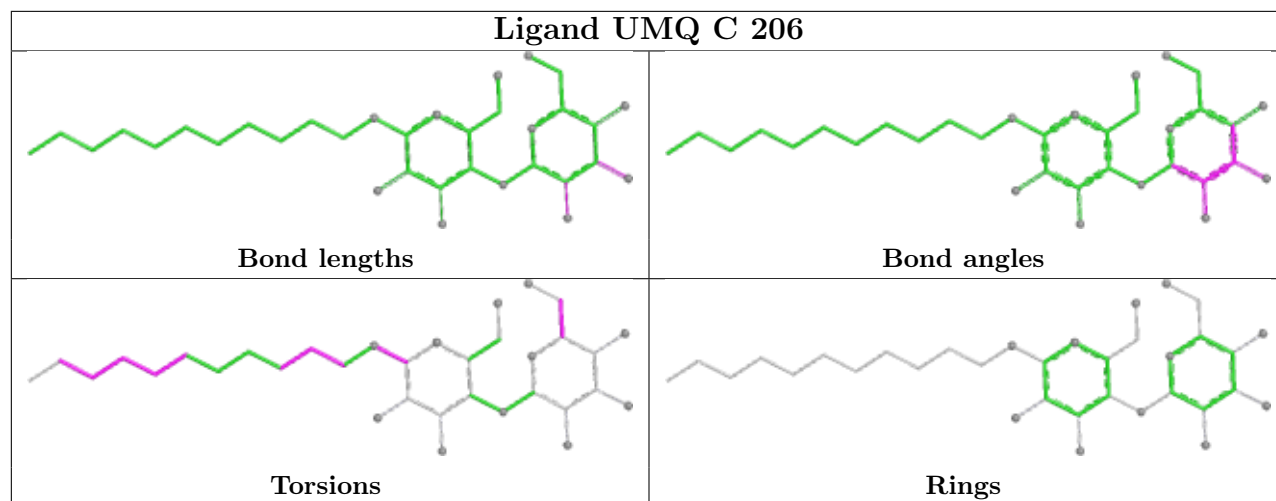
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	203	LHG	5	0
4	F	204	LHG	6	0
4	B	204	LHG	6	0
4	J	204	LHG	4	0
4	C	204	LHG	6	0
4	G	203	LHG	7	0
4	E	203	LHG	6	0
5	A	205	UMQ	1	0
4	I	204	LHG	4	0
5	J	206	UMQ	1	0

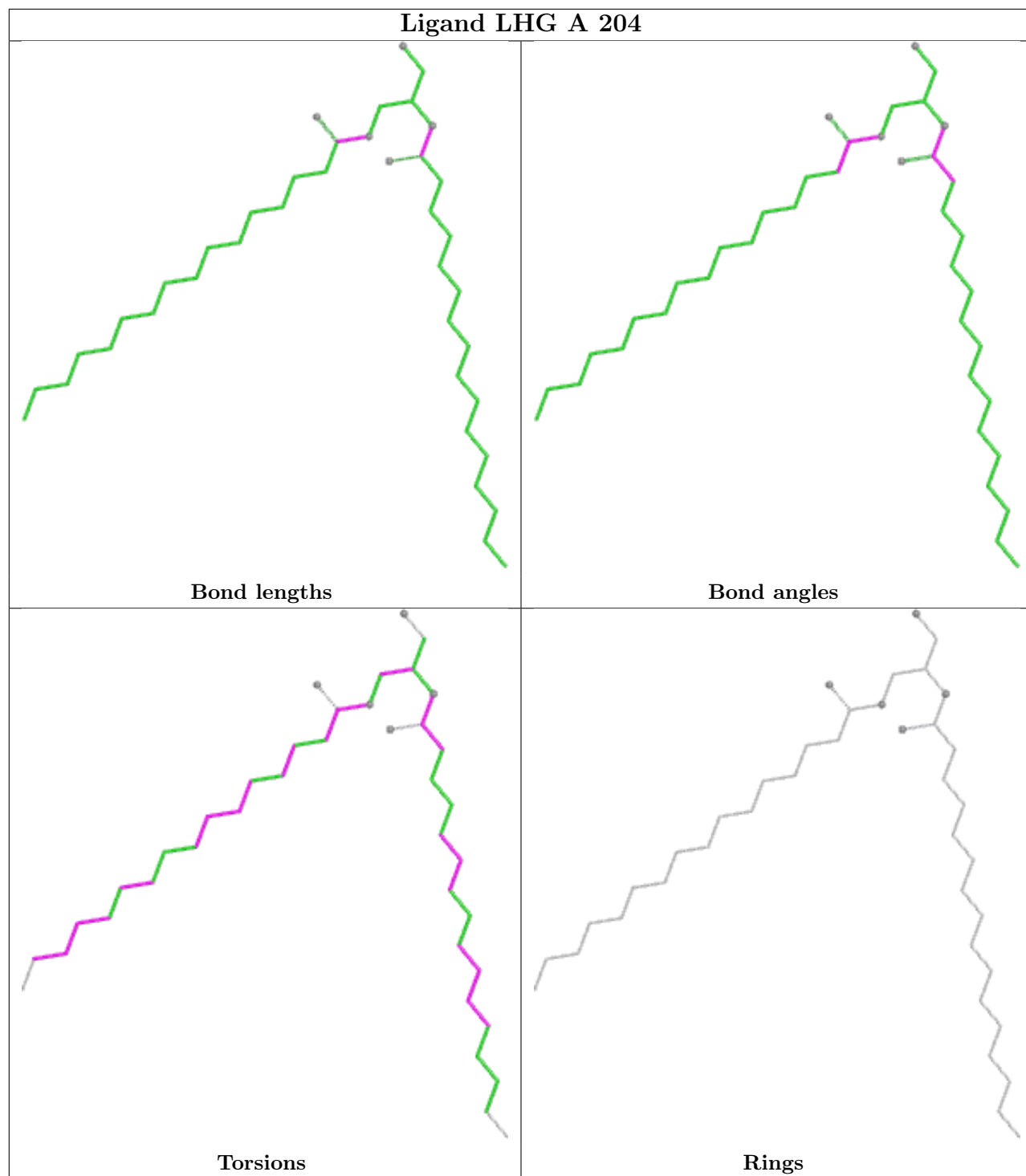
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

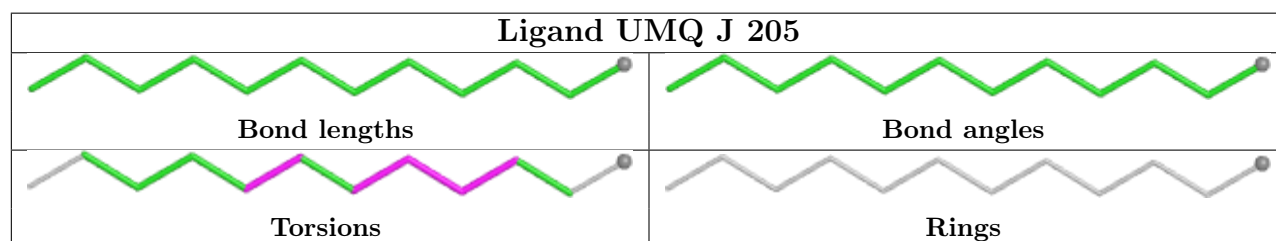
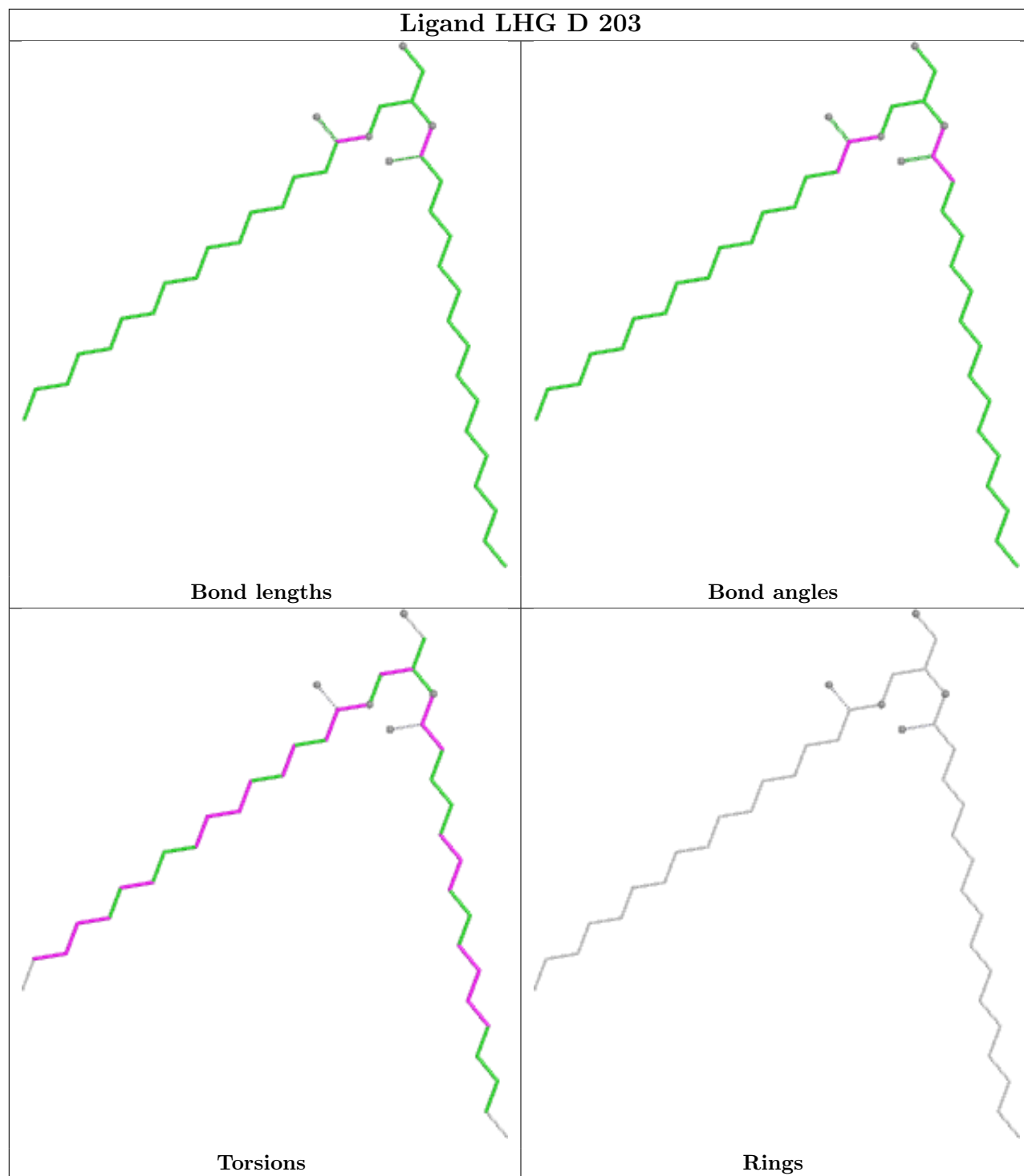


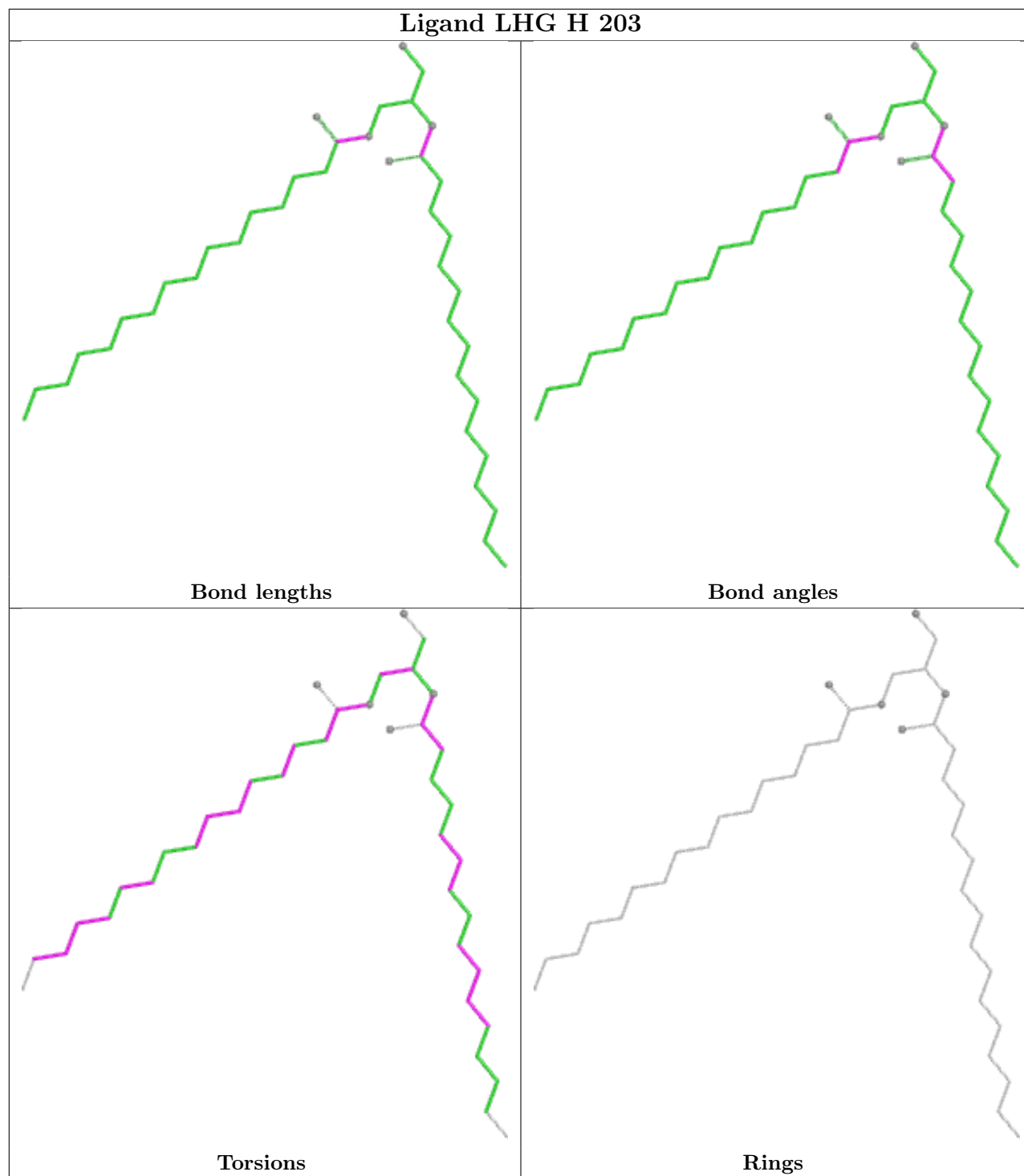


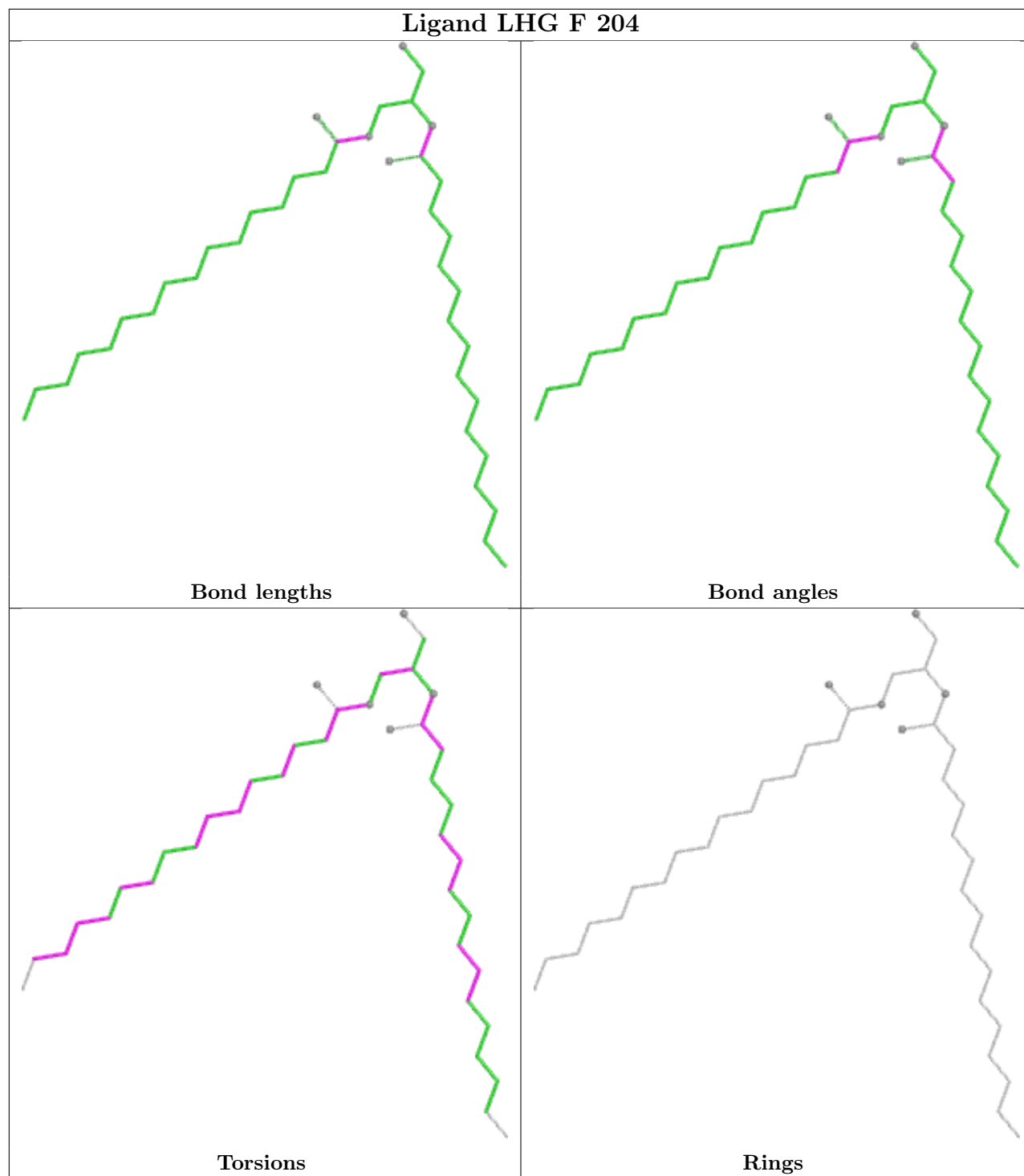


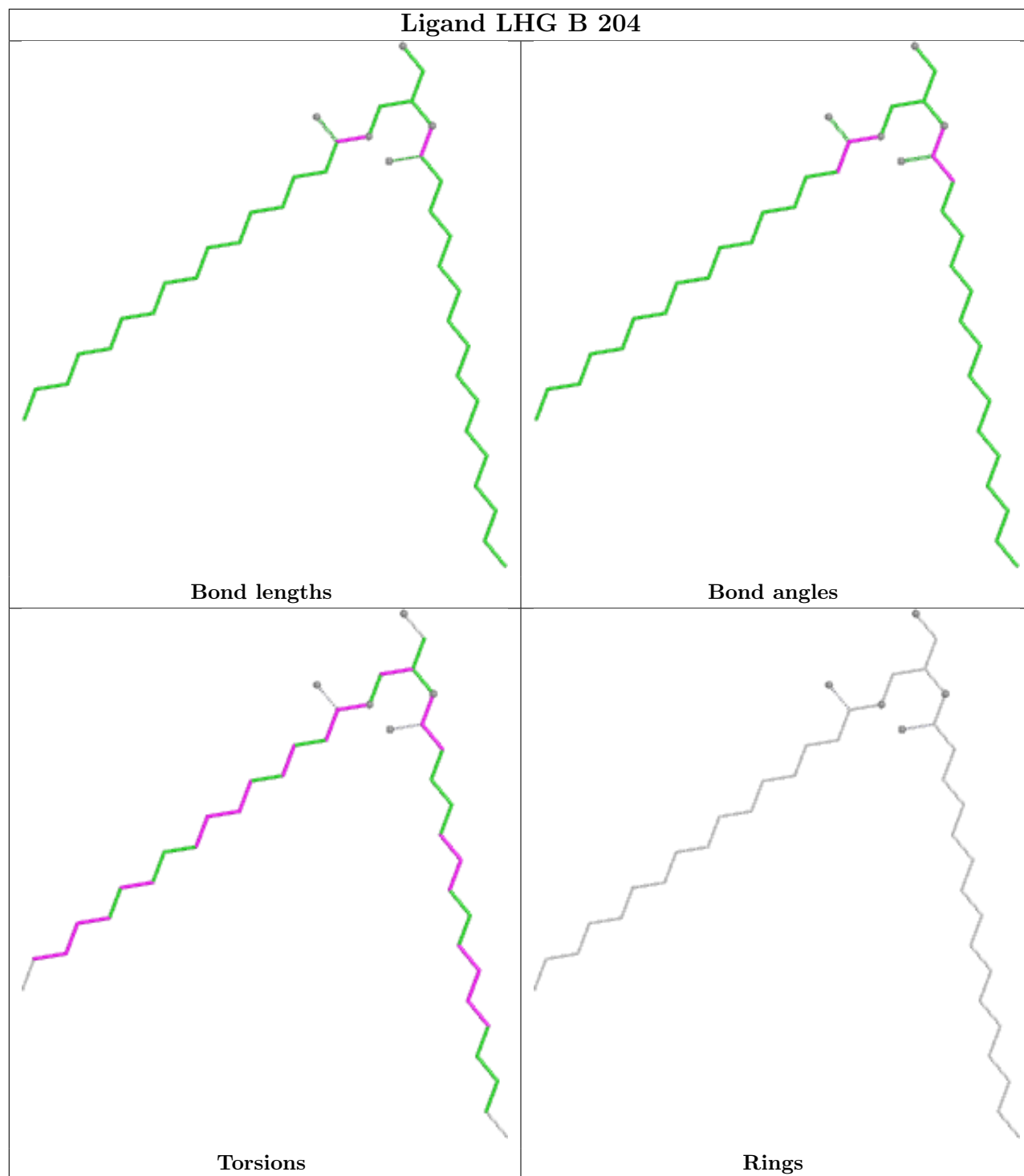


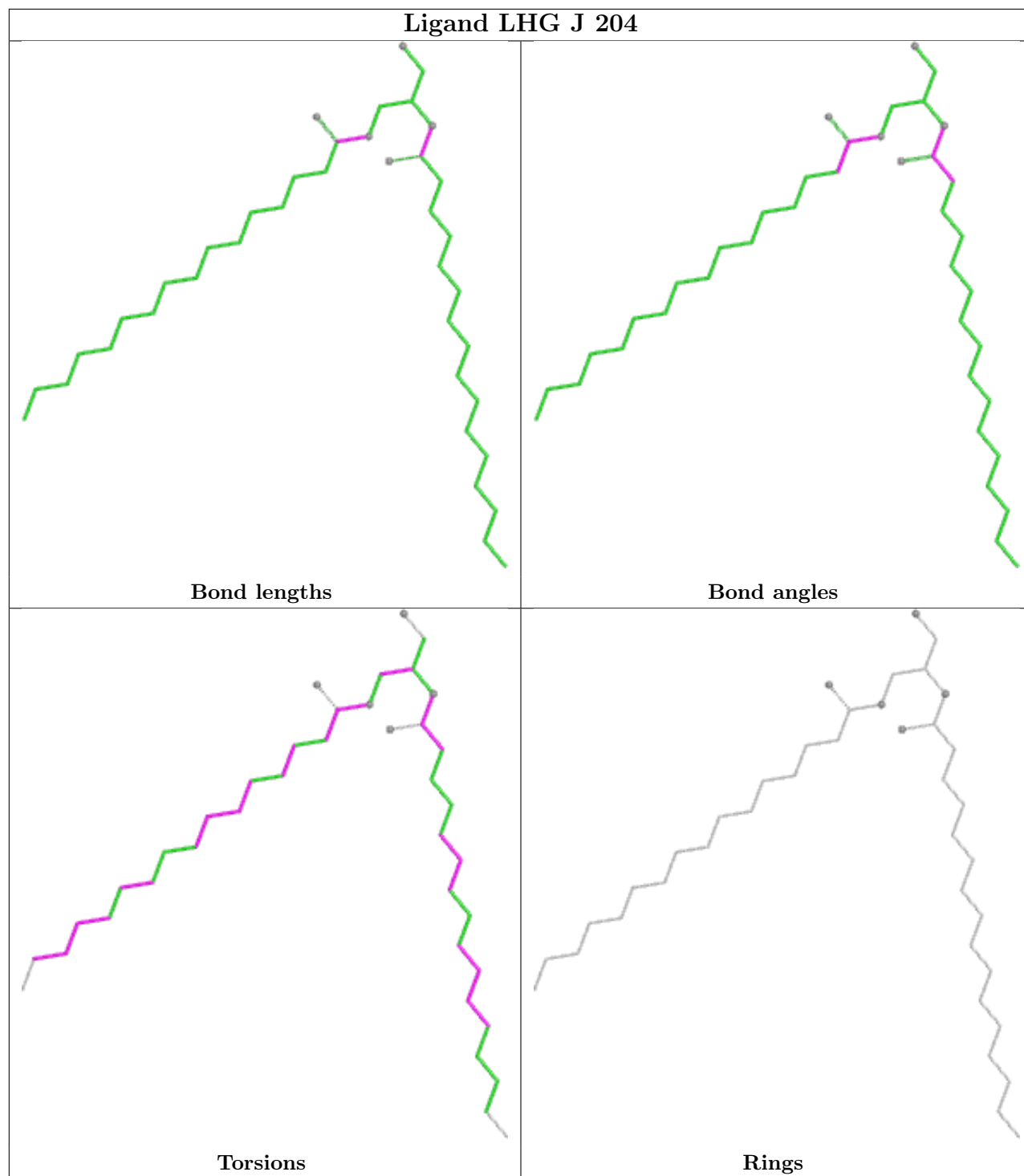


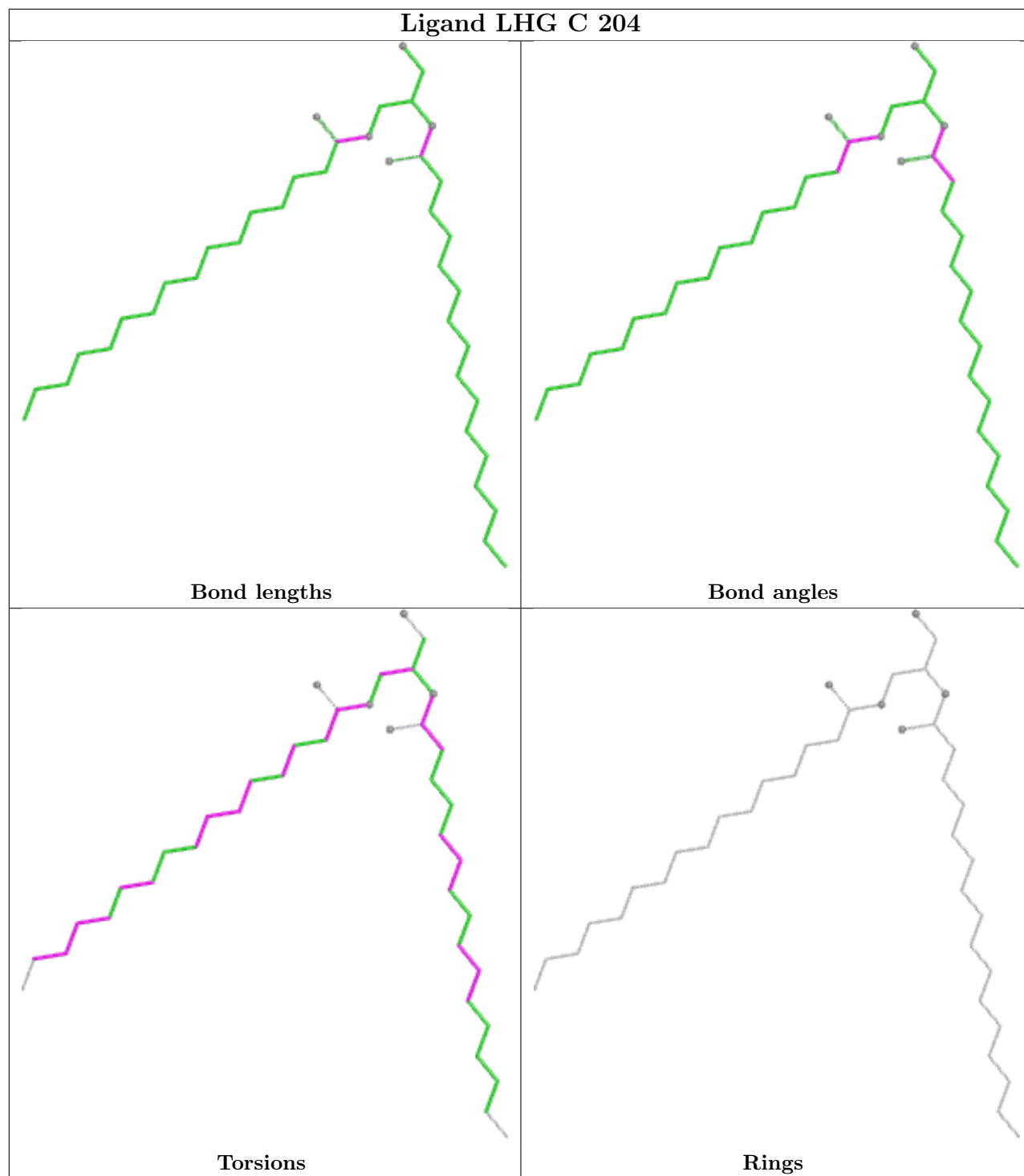


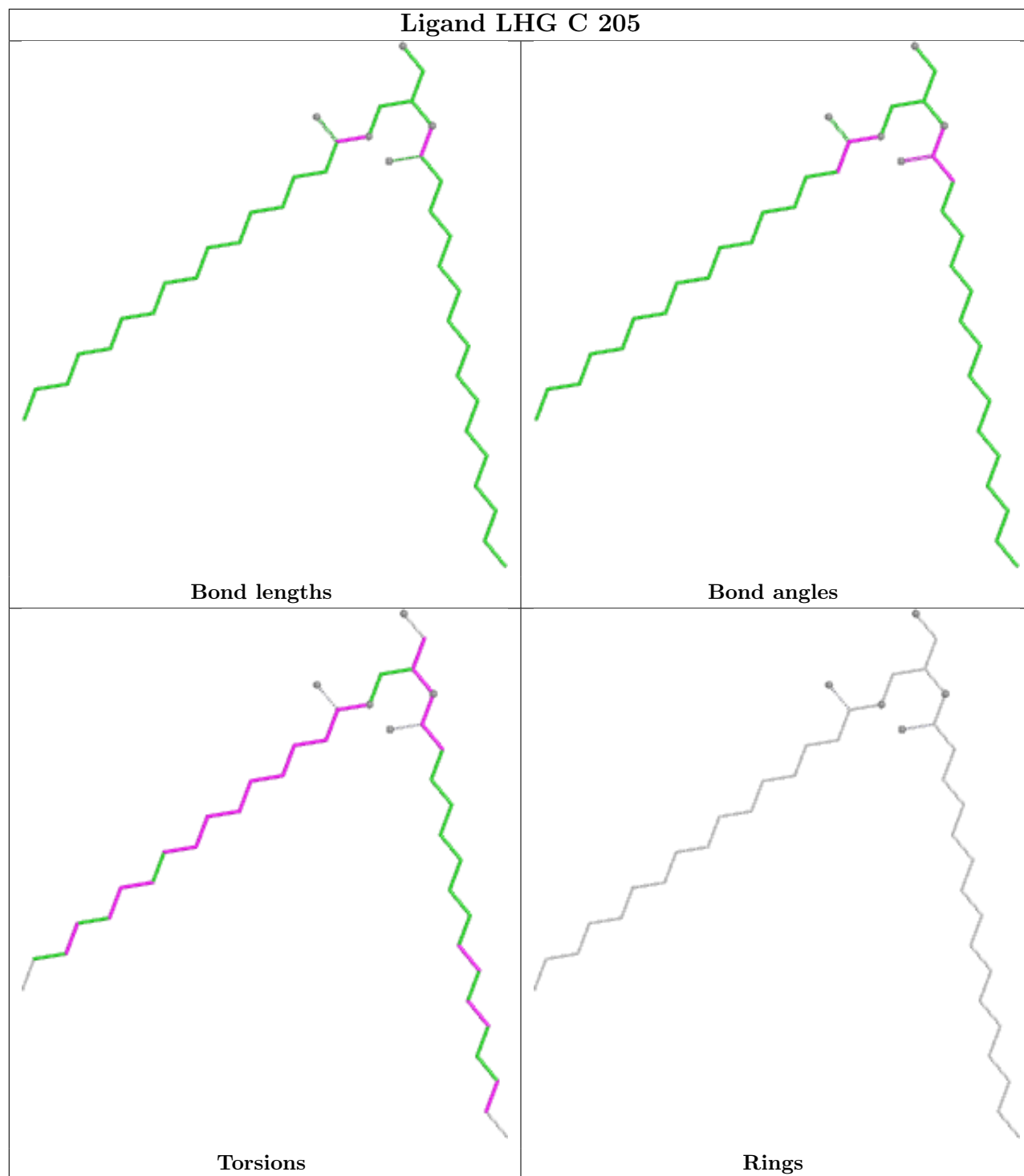


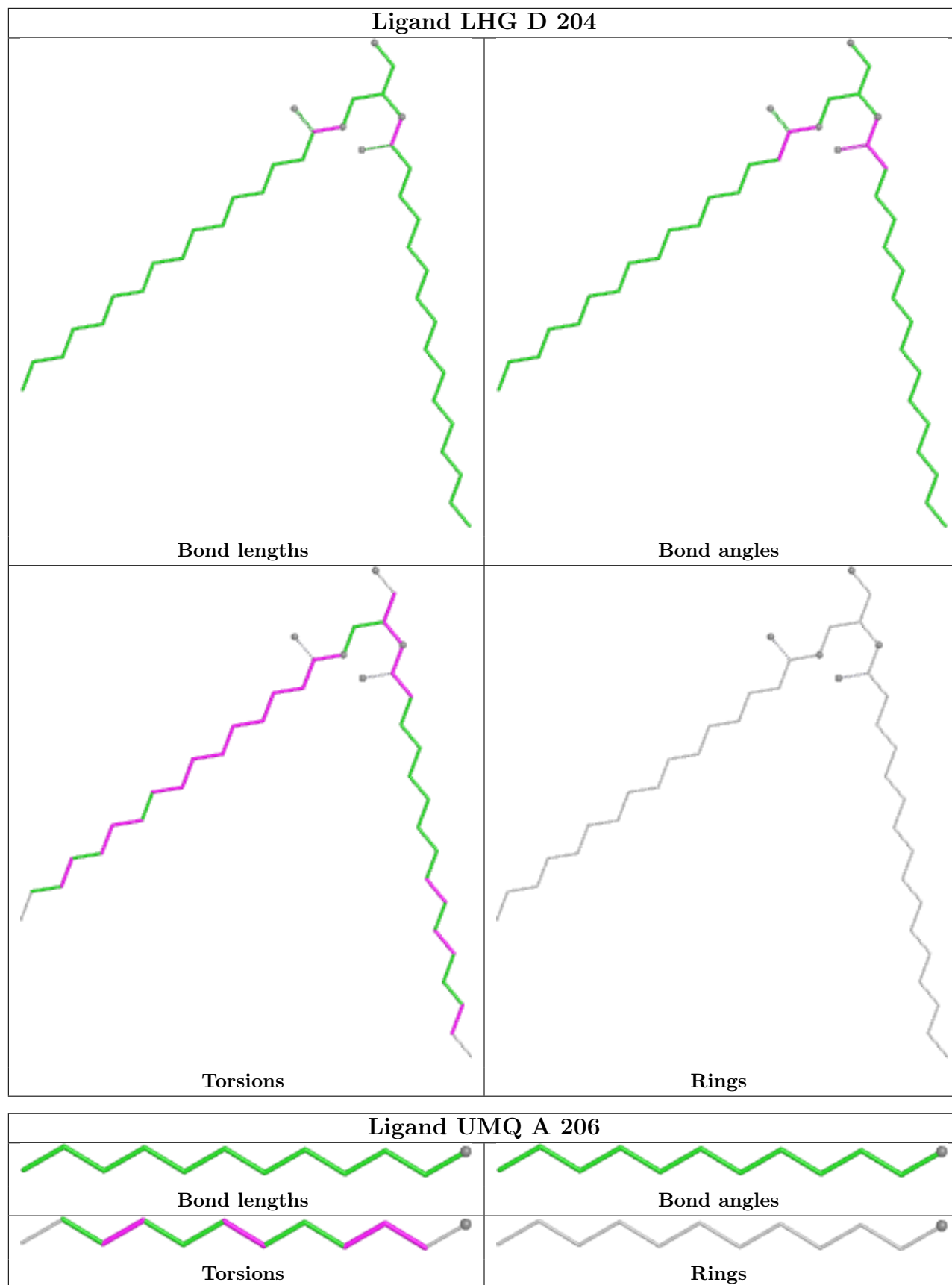


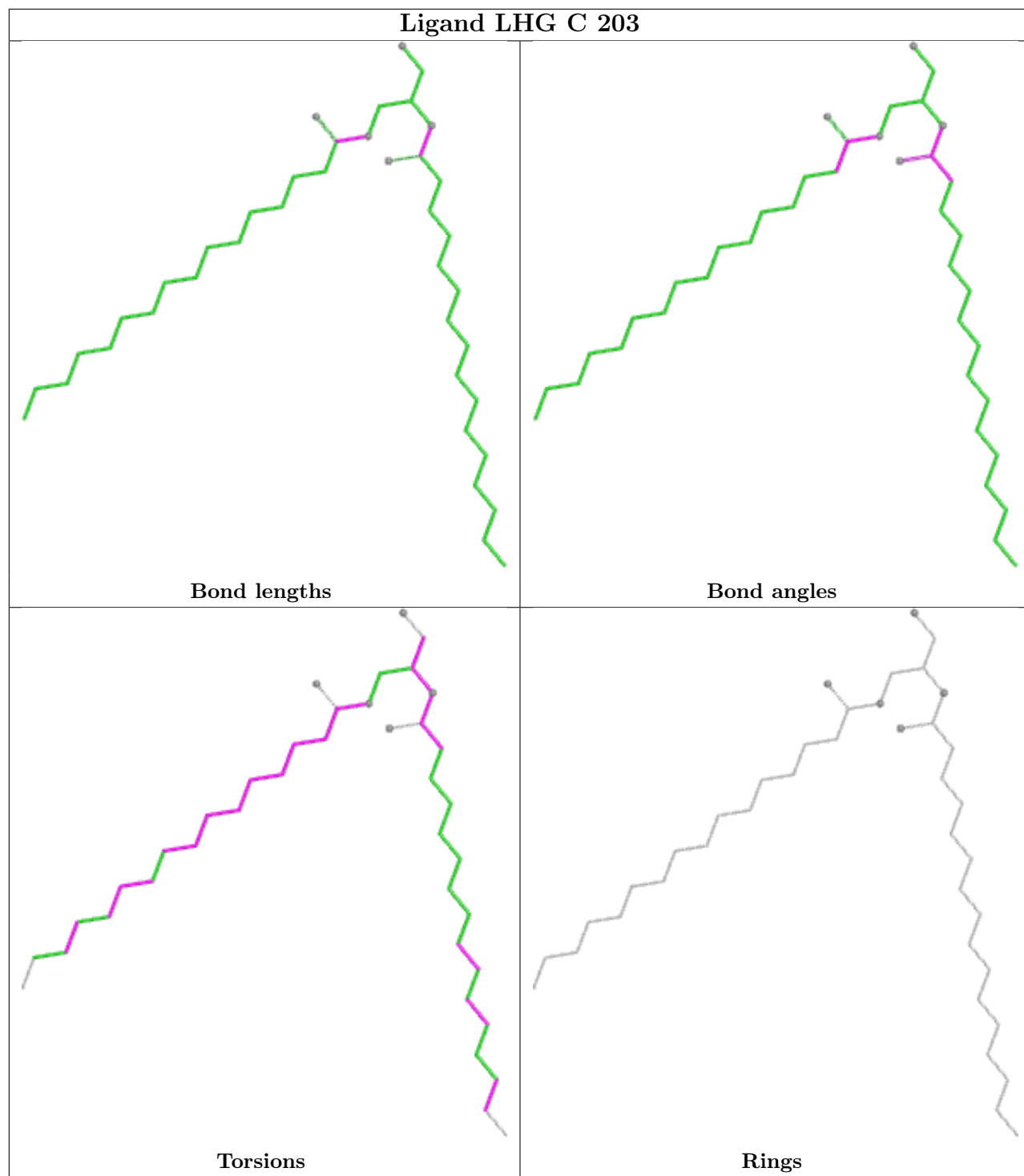


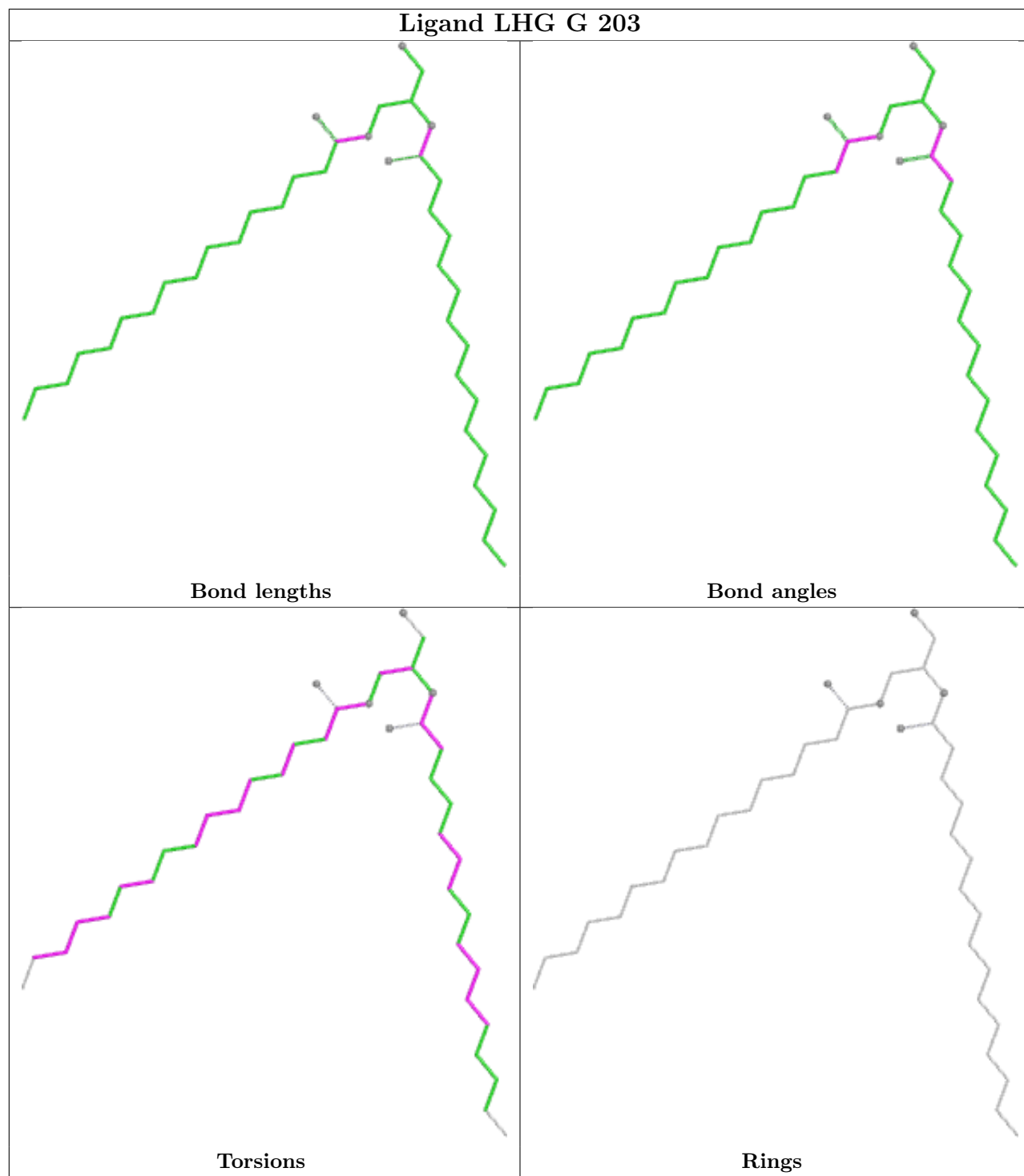


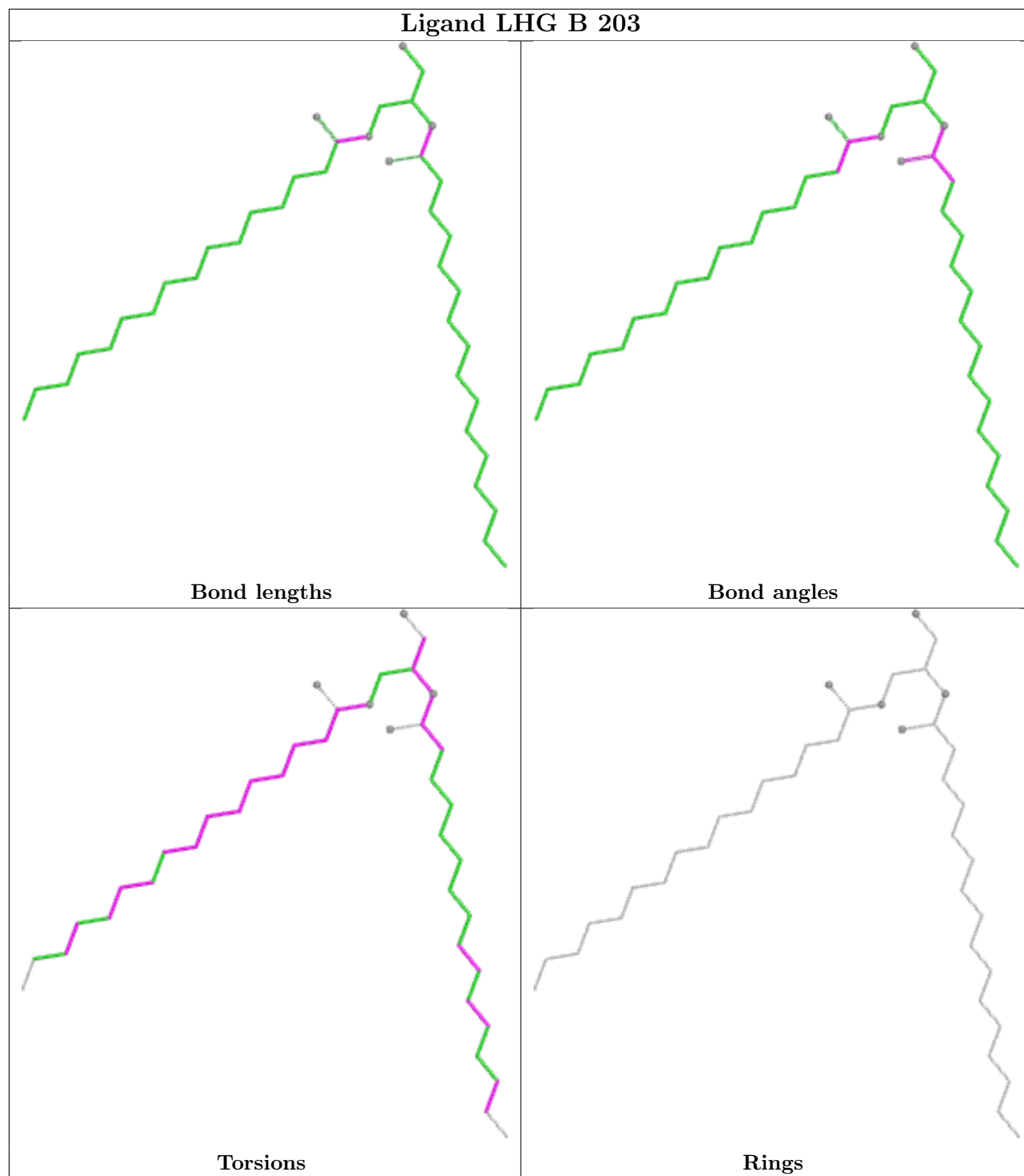


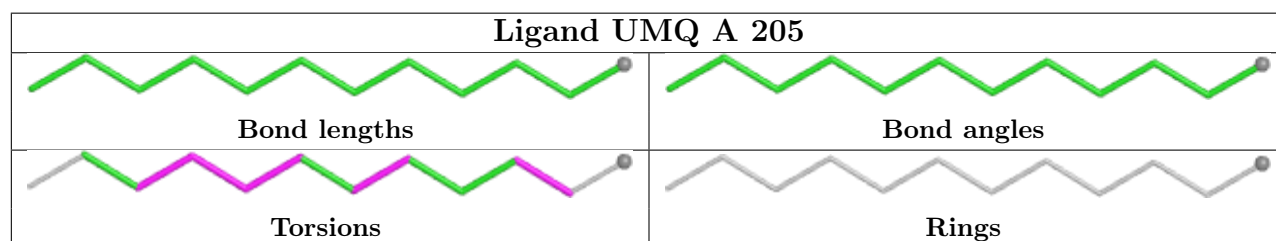
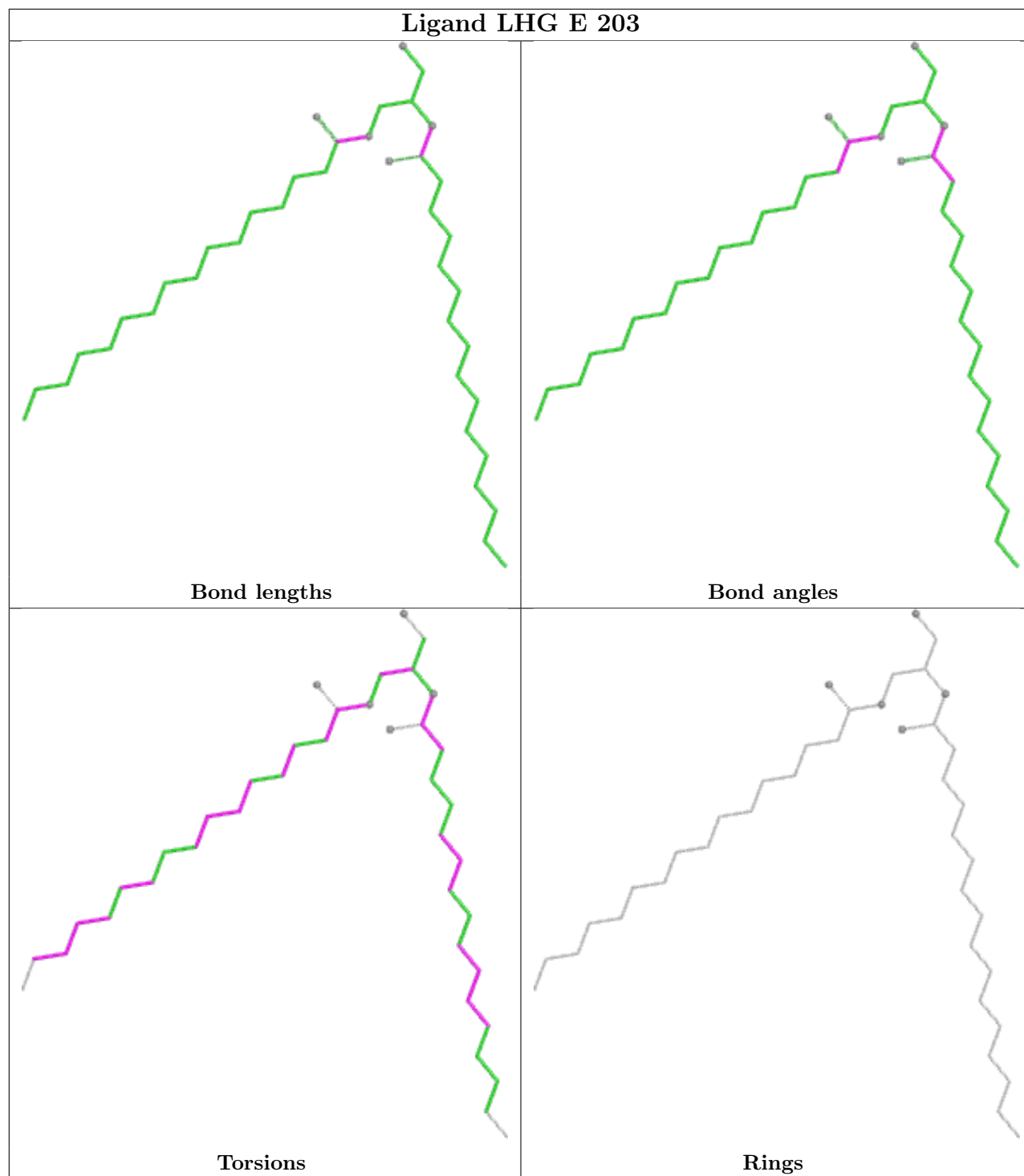


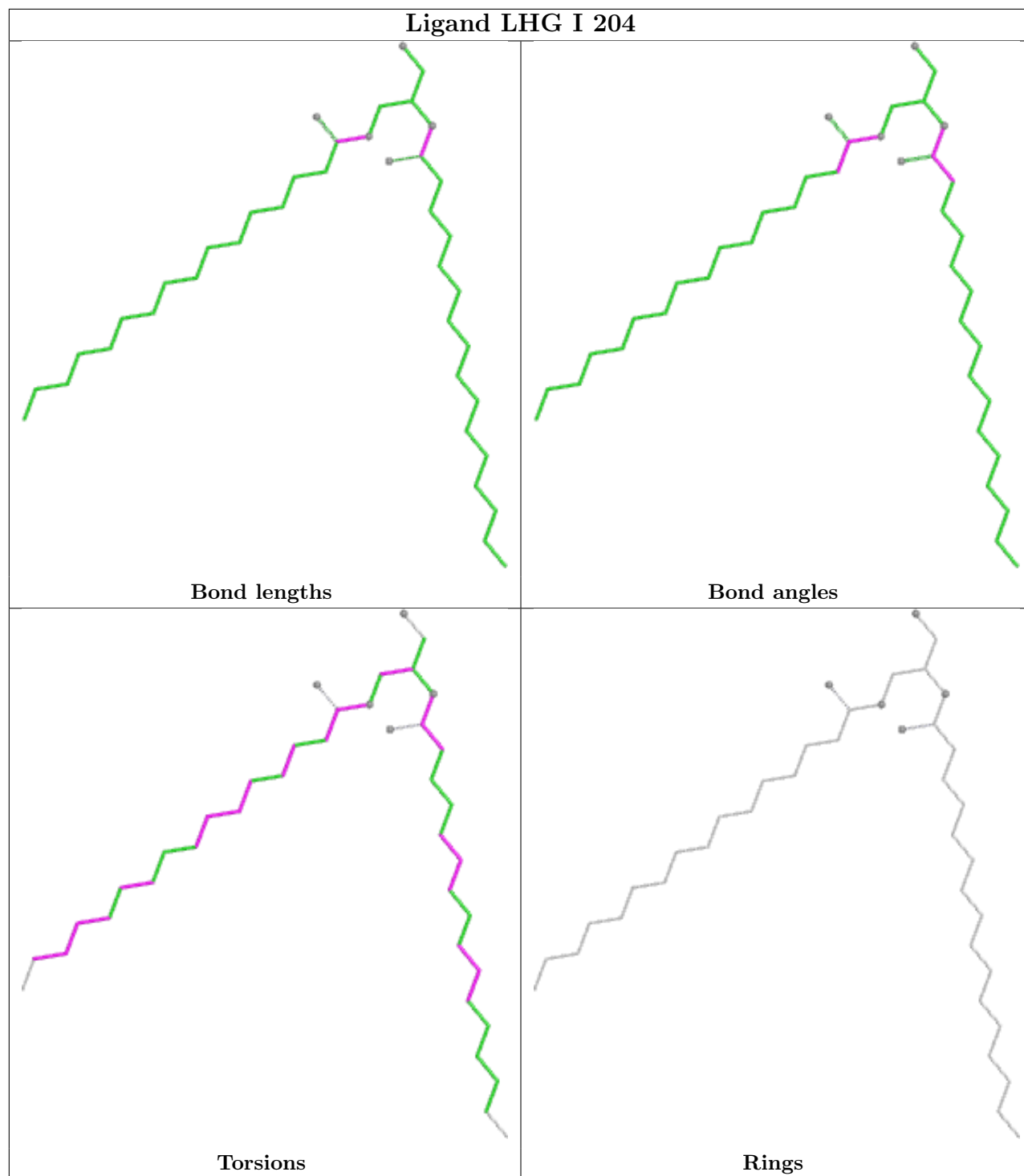


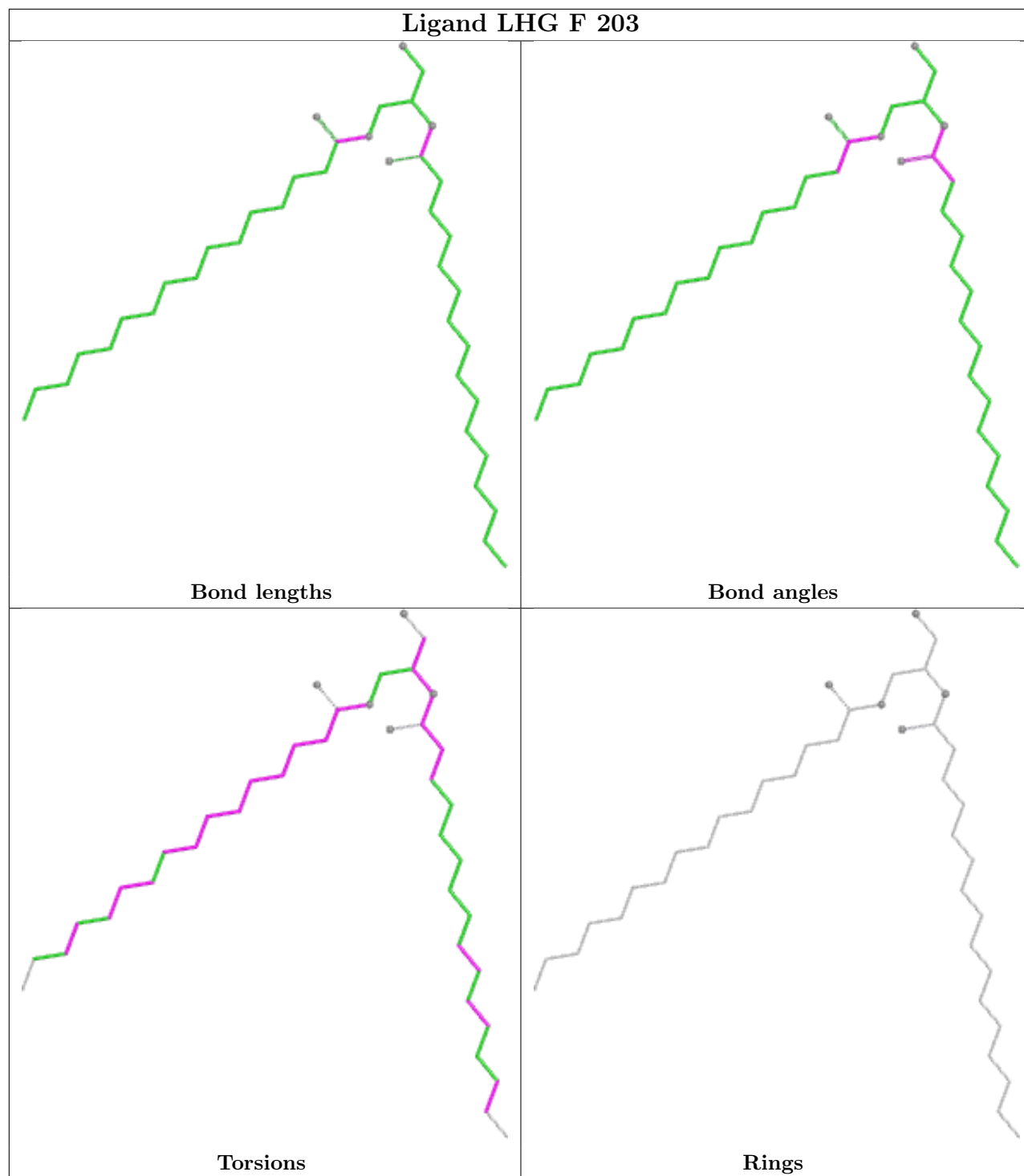


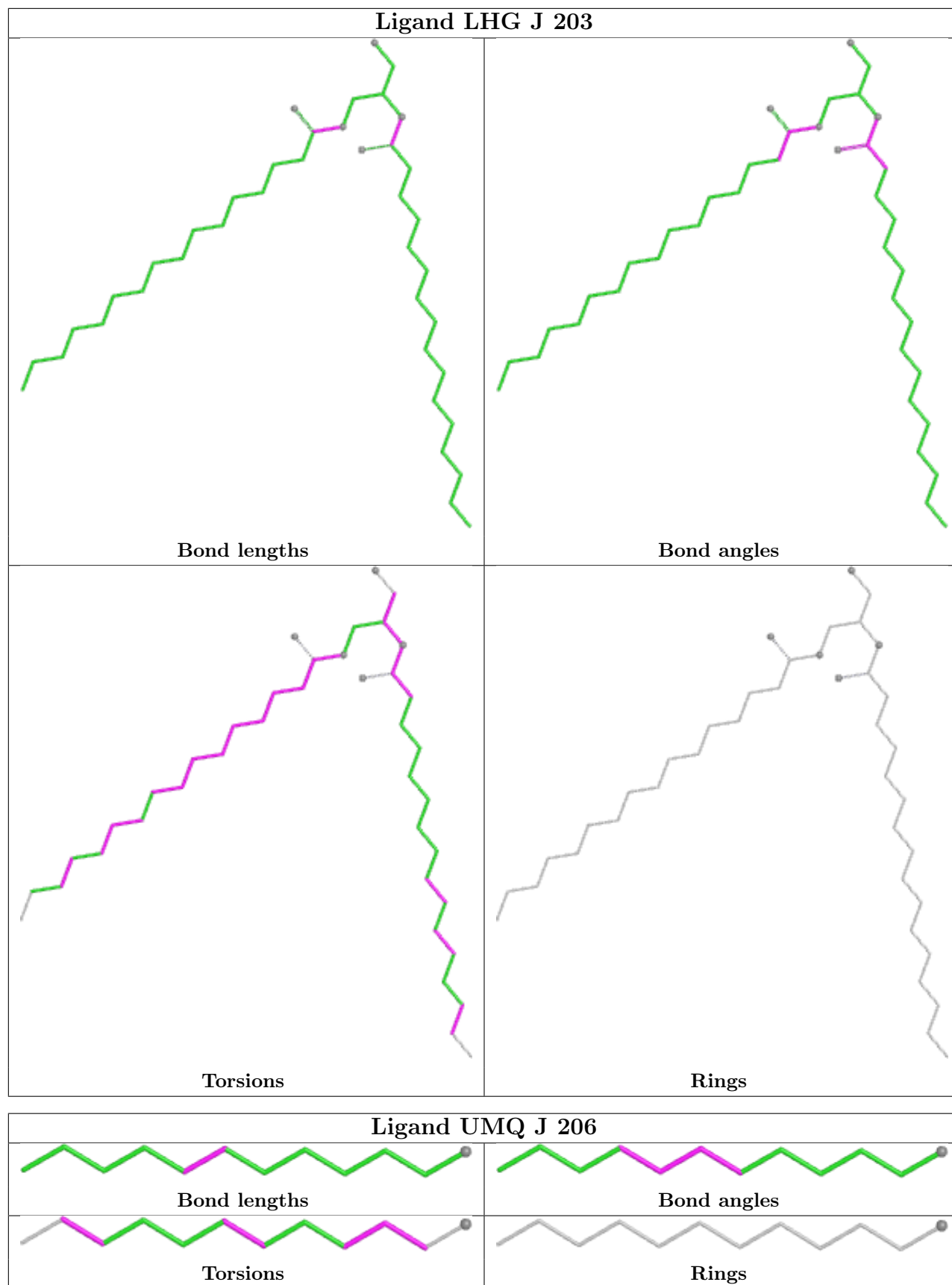


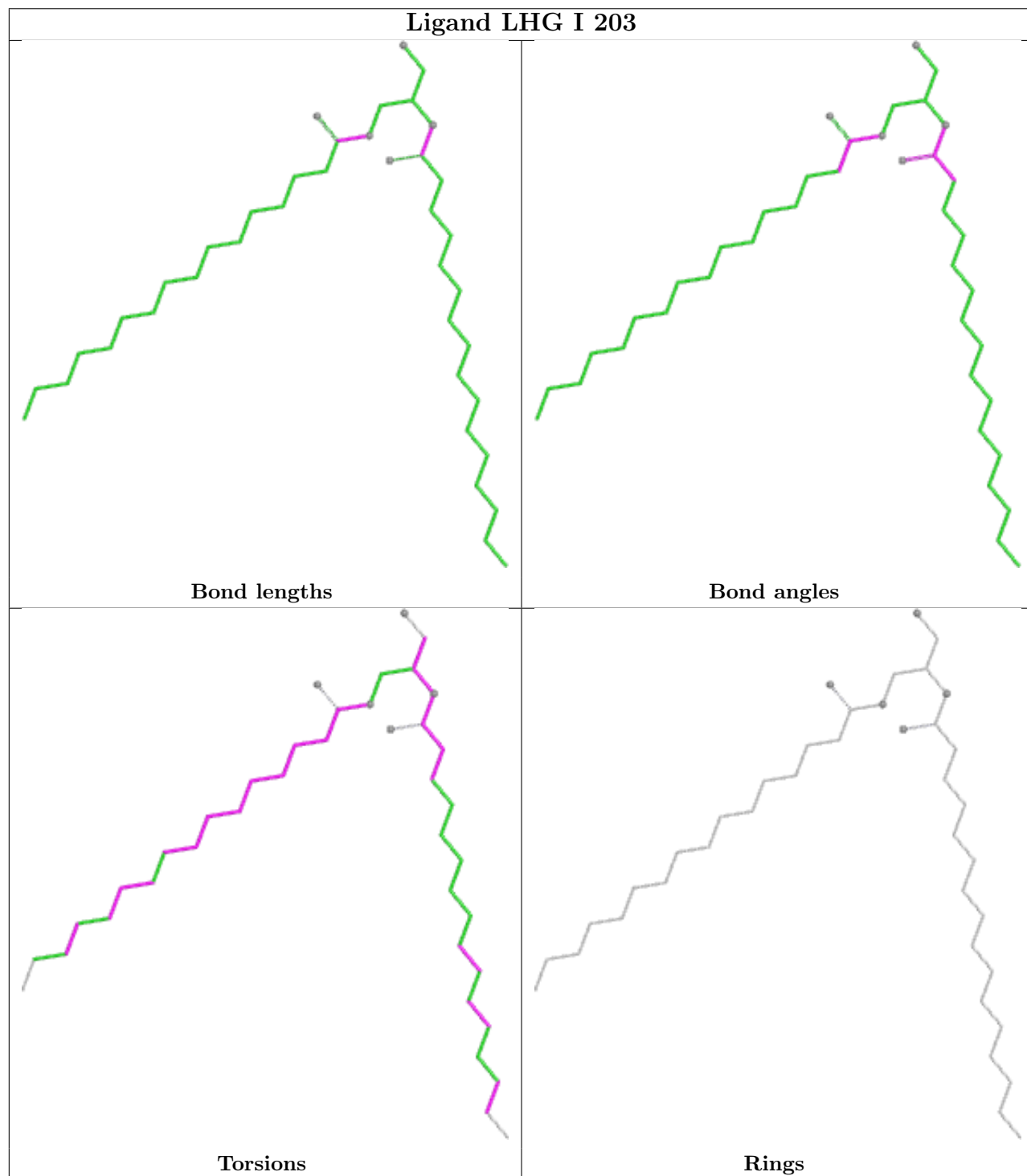
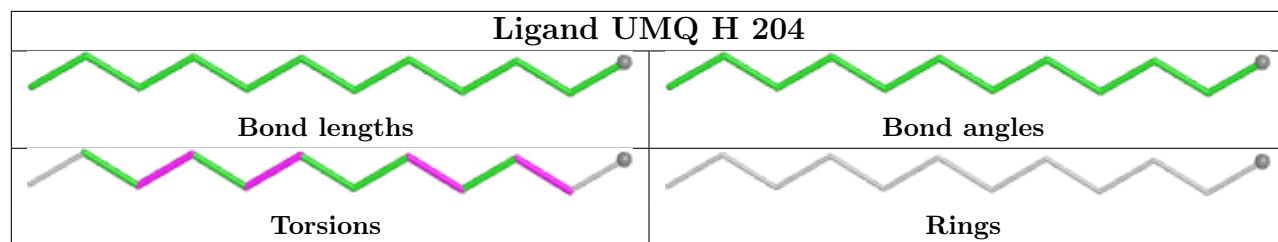


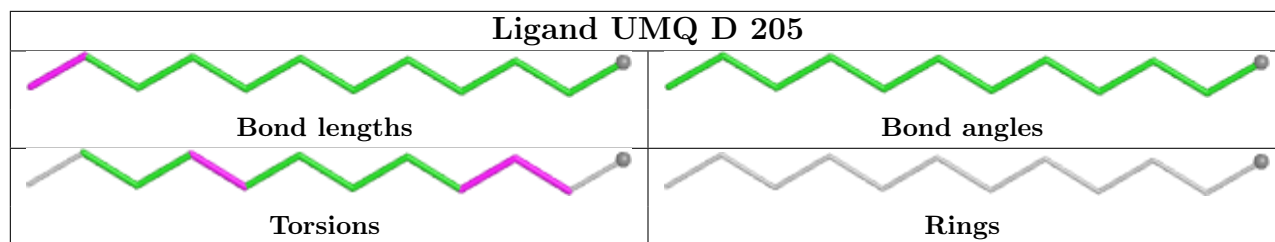












5.7 Other polymers [i](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	2.16	66 (42%) 0 0	23, 51, 69, 81	9 (5%)
1	B	156/156 (100%)	2.18	61 (39%) 1 0	23, 52, 69, 81	9 (5%)
1	C	156/156 (100%)	2.08	62 (39%) 1 0	23, 51, 69, 81	9 (5%)
1	D	156/156 (100%)	2.02	57 (36%) 1 1	23, 52, 69, 81	9 (5%)
1	E	156/156 (100%)	1.81	39 (25%) 2 1	23, 51, 69, 81	9 (5%)
1	F	156/156 (100%)	1.61	37 (23%) 2 1	23, 51, 69, 81	9 (5%)
1	G	156/156 (100%)	1.65	36 (23%) 2 1	23, 51, 69, 81	9 (5%)
1	H	156/156 (100%)	1.48	31 (19%) 3 2	23, 52, 69, 81	9 (5%)
1	I	156/156 (100%)	1.23	26 (16%) 4 3	23, 52, 69, 81	7 (4%)
1	J	156/156 (100%)	1.16	14 (8%) 15 12	23, 51, 60, 72	8 (5%)
All	All	1560/1560 (100%)	1.74	429 (27%) 1 1	23, 51, 69, 81	87 (5%)

All (429) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	81	GLY	10.2
1	D	81	GLY	9.9
1	H	21[A]	THR	9.8
1	E	83[A]	ASP	9.6
1	B	119[A]	GLN	8.9
1	G	81	GLY	8.7
1	F	21[A]	THR	8.5
1	H	12[A]	MET	8.5
1	E	81	GLY	8.5
1	B	82	SER	8.5
1	C	83[A]	ASP	8.4
1	C	17[A]	LEU	8.4
1	G	21[A]	THR	8.4

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Mol	Chain	Res	Type	RSRZ
1	C	12[A]	MET	8.3
1	C	81	GLY	8.2
1	D	21[A]	THR	8.1
1	I	21[A]	THR	8.1
1	A	21[A]	THR	7.9
1	B	21[A]	THR	7.9
1	D	155[A]	ASN	7.8
1	C	21[A]	THR	7.8
1	F	119[A]	GLN	7.8
1	A	119[A]	GLN	7.6
1	E	7	THR	7.6
1	A	6	ILE	7.6
1	J	21[A]	THR	7.6
1	G	12[A]	MET	7.5
1	H	83[A]	ASP	7.5
1	J	75[A]	LEU	7.5
1	A	3	ASP	7.4
1	A	7	THR	7.3
1	C	119[A]	GLN	7.3
1	C	54[A]	GLN	7.2
1	A	81	GLY	7.2
1	A	75[A]	LEU	7.2
1	J	54[A]	GLN	7.1
1	I	155[A]	ASN	7.1
1	B	13[A]	VAL	7.1
1	J	13[A]	VAL	7.0
1	G	82	SER	6.9
1	H	17[A]	LEU	6.9
1	A	83[A]	ASP	6.9
1	H	81	GLY	6.9
1	E	155[A]	ASN	6.8
1	F	83[A]	ASP	6.8
1	E	21[A]	THR	6.8
1	H	119[A]	GLN	6.8
1	B	12[A]	MET	6.7
1	F	81	GLY	6.7
1	D	17[A]	LEU	6.7
1	E	119[A]	GLN	6.7
1	B	17[A]	LEU	6.7
1	C	75[A]	LEU	6.7
1	G	155[A]	ASN	6.6
1	A	155[A]	ASN	6.6

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Mol	Chain	Res	Type	RSRZ
1	E	12[A]	MET	6.6
1	D	83[A]	ASP	6.6
1	F	54[A]	GLN	6.6
1	H	13[A]	VAL	6.5
1	D	12[A]	MET	6.4
1	E	82	SER	6.4
1	B	155[A]	ASN	6.4
1	G	17[A]	LEU	6.3
1	F	17[A]	LEU	6.3
1	J	155[A]	ASN	6.3
1	I	75[A]	LEU	6.3
1	F	12[A]	MET	6.2
1	A	82	SER	6.2
1	H	54[A]	GLN	6.1
1	A	13[A]	VAL	6.1
1	A	17[A]	LEU	6.1
1	G	119[A]	GLN	6.1
1	D	13[A]	VAL	6.1
1	G	7	THR	6.0
1	F	13[A]	VAL	6.0
1	H	75[A]	LEU	6.0
1	I	3	ASP	5.9
1	J	119[A]	GLN	5.9
1	E	8	GLN	5.8
1	E	75[A]	LEU	5.8
1	I	119[A]	GLN	5.8
1	B	83[A]	ASP	5.8
1	I	1	MET	5.8
1	E	17[A]	LEU	5.7
1	E	54[A]	GLN	5.7
1	D	7	THR	5.7
1	D	119[A]	GLN	5.6
1	D	75[A]	LEU	5.5
1	J	17[A]	LEU	5.5
1	A	9	ASN	5.5
1	D	9	ASN	5.5
1	G	78	ILE	5.4
1	G	54[A]	GLN	5.4
1	G	83[A]	ASP	5.3
1	I	13[A]	VAL	5.3
1	A	12[A]	MET	5.3
1	D	54[A]	GLN	5.2

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Mol	Chain	Res	Type	RSRZ
1	F	6	ILE	5.2
1	J	88[A]	GLN	5.2
1	F	75[A]	LEU	5.2
1	H	82	SER	5.2
1	I	17[A]	LEU	5.2
1	G	75[A]	LEU	5.1
1	B	78	ILE	5.1
1	A	54[A]	GLN	5.1
1	E	1	MET	5.0
1	B	75[A]	LEU	5.0
1	G	53	GLY	5.0
1	G	13[A]	VAL	5.0
1	I	12[A]	MET	5.0
1	D	82	SER	4.9
1	C	13[A]	VAL	4.9
1	E	5	LEU	4.9
1	F	82	SER	4.9
1	F	155[A]	ASN	4.9
1	B	77	PHE	4.9
1	B	6	ILE	4.8
1	D	80	LEU	4.8
1	C	3	ASP	4.8
1	C	155[A]	ASN	4.8
1	C	9	ASN	4.7
1	E	124	LYS	4.7
1	A	8	GLN	4.6
1	F	7	THR	4.6
1	G	77	PHE	4.5
1	G	4	TYR	4.4
1	I	2	MET	4.4
1	E	6	ILE	4.4
1	A	154	LEU	4.4
1	D	156	ALA	4.4
1	A	4	TYR	4.3
1	F	3	ASP	4.3
1	A	45	THR	4.3
1	D	115	ALA	4.3
1	E	10	GLY	4.2
1	B	87	VAL	4.2
1	G	9	ASN	4.1
1	B	54[A]	GLN	4.1
1	A	126	GLU	4.1

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Mol	Chain	Res	Type	RSRZ
1	G	6	ILE	4.1
1	E	13[A]	VAL	4.1
1	B	52	PHE	4.1
1	C	156	ALA	4.0
1	G	2	MET	4.0
1	F	14	PHE	3.9
1	H	9	ASN	3.9
1	G	1	MET	3.9
1	A	151	LEU	3.9
1	C	45	THR	3.9
1	C	78	ILE	3.9
1	D	87	VAL	3.9
1	D	122	ALA	3.9
1	C	120	ILE	3.9
1	H	3	ASP	3.9
1	C	88	GLN	3.9
1	D	84	MET	3.8
1	F	80	LEU	3.8
1	B	53	GLY	3.8
1	G	50	GLU	3.8
1	C	8	GLN	3.8
1	A	125	PRO	3.8
1	H	156	ALA	3.8
1	J	156	ALA	3.8
1	C	4	TYR	3.8
1	E	4	TYR	3.8
1	B	125	PRO	3.8
1	F	87	VAL	3.7
1	C	1	MET	3.7
1	B	45	THR	3.7
1	B	42	ALA	3.7
1	C	87	VAL	3.7
1	G	74	PHE	3.7
1	E	120	ILE	3.7
1	B	9	ASN	3.6
1	D	124	LYS	3.6
1	A	5	LEU	3.6
1	G	80	LEU	3.6
1	D	129	THR	3.6
1	A	80	LEU	3.6
1	B	91	ASN	3.6
1	C	7	THR	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	105	PHE	3.5
1	B	79	ASN	3.5
1	B	104	LEU	3.5
1	H	125	PRO	3.5
1	C	124	LYS	3.5
1	A	2	MET	3.5
1	D	15	ALA	3.5
1	G	8	GLN	3.5
1	C	28	ILE	3.5
1	I	9	ASN	3.4
1	F	85	SER	3.4
1	D	126	GLU	3.4
1	C	6	ILE	3.4
1	C	82	SER	3.4
1	I	156	ALA	3.4
1	A	16	VAL	3.4
1	E	80	LEU	3.4
1	A	14	PHE	3.3
1	D	88	GLN	3.3
1	D	125	PRO	3.3
1	A	118	ILE	3.3
1	C	114	ALA	3.3
1	D	11	GLY	3.3
1	C	2	MET	3.2
1	D	32	LYS	3.2
1	D	6	ILE	3.2
1	A	156	ALA	3.2
1	F	9	ASN	3.2
1	B	156	ALA	3.2
1	B	101	PHE	3.2
1	H	136	ALA	3.2
1	E	9	ASN	3.2
1	I	120	ILE	3.2
1	B	116	ALA	3.1
1	C	125	PRO	3.1
1	C	5	LEU	3.1
1	A	43	ALA	3.1
1	C	126	GLU	3.1
1	H	1	MET	3.1
1	E	46	THR	3.1
1	D	10	GLY	3.1
1	H	80	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	7	THR	3.0
1	B	57	ILE	3.0
1	B	120	ILE	3.0
1	B	126	GLU	3.0
1	C	25	PHE	3.0
1	G	3	ASP	3.0
1	D	118	ILE	3.0
1	A	22	ALA	3.0
1	E	156	ALA	3.0
1	B	10	GLY	3.0
1	B	80	LEU	2.9
1	B	88	GLN	2.9
1	D	138	VAL	2.9
1	B	43	ALA	2.9
1	E	14	PHE	2.9
1	D	8	GLN	2.9
1	E	138	VAL	2.9
1	H	122	ALA	2.9
1	G	5	LEU	2.9
1	I	90	LEU	2.9
1	A	134	PHE	2.9
1	E	126	GLU	2.9
1	B	118	ILE	2.9
1	B	124	LYS	2.9
1	C	99	ILE	2.8
1	B	1	MET	2.8
1	H	155[A]	ASN	2.8
1	D	101	PHE	2.8
1	B	4	TYR	2.8
1	H	6	ILE	2.8
1	B	48	GLN	2.8
1	H	92	PHE	2.8
1	F	1	MET	2.7
1	C	48	GLN	2.7
1	C	16	VAL	2.7
1	A	63	GLY	2.7
1	B	33	GLY	2.7
1	G	33	GLY	2.7
1	I	81	GLY	2.7
1	D	134	PHE	2.7
1	D	39	GLU	2.7
1	B	49	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	J	2	MET	2.6
1	B	47	SER	2.6
1	A	48	GLN	2.6
1	B	122	ALA	2.6
1	G	52	PHE	2.6
1	E	2	MET	2.6
1	I	154	LEU	2.6
1	G	34	VAL	2.6
1	I	8	GLN	2.6
1	D	46	THR	2.6
1	D	127	HIS	2.6
1	C	84	MET	2.6
1	C	118	ILE	2.6
1	A	10	GLY	2.5
1	B	29	GLY	2.5
1	I	29	GLY	2.5
1	A	109	ALA	2.5
1	H	7	THR	2.5
1	D	1	MET	2.5
1	H	126	GLU	2.5
1	J	126	GLU	2.5
1	D	154	LEU	2.5
1	E	151	LEU	2.5
1	D	123	LYS	2.5
1	J	1	MET	2.5
1	F	103	GLY	2.5
1	A	74	PHE	2.5
1	D	77	PHE	2.5
1	E	134	PHE	2.5
1	B	115	ALA	2.5
1	B	85	SER	2.5
1	D	85	SER	2.5
1	F	5	LEU	2.5
1	E	127	HIS	2.5
1	C	103	GLY	2.4
1	H	111	GLY	2.4
1	D	112	LYS	2.4
1	F	120	ILE	2.4
1	I	6	ILE	2.4
1	A	25	PHE	2.4
1	F	138	VAL	2.4
1	B	136	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	15	ALA	2.4
1	C	49	PRO	2.4
1	C	14	PHE	2.4
1	A	34	VAL	2.4
1	B	34	VAL	2.4
1	C	115	ALA	2.4
1	F	156	ALA	2.4
1	F	47	SER	2.4
1	B	3	ASP	2.4
1	A	104	LEU	2.4
1	A	42	ALA	2.4
1	A	55	ALA	2.4
1	H	55	ALA	2.4
1	D	33	GLY	2.4
1	E	3	ASP	2.4
1	G	154	LEU	2.4
1	E	101	PHE	2.4
1	I	4	TYR	2.4
1	C	123	LYS	2.4
1	E	135	ALA	2.4
1	C	46	THR	2.3
1	D	47	SER	2.3
1	F	11	GLY	2.3
1	H	88	GLN	2.3
1	H	154	LEU	2.3
1	I	48	GLN	2.3
1	B	14	PHE	2.3
1	A	113	VAL	2.3
1	A	108	ILE	2.3
1	A	120	ILE	2.3
1	A	77	PHE	2.3
1	A	101	PHE	2.3
1	B	123	LYS	2.3
1	C	122	ALA	2.3
1	A	129	THR	2.3
1	D	45	THR	2.3
1	H	10	GLY	2.3
1	C	108	ILE	2.3
1	H	153	VAL	2.3
1	D	55	ALA	2.3
1	A	58	LEU	2.3
1	C	112	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	122	ALA	2.2
1	A	35	GLY	2.2
1	D	36	MET	2.2
1	E	137	MET	2.2
1	A	150	PHE	2.2
1	C	52	PHE	2.2
1	A	49	PRO	2.2
1	A	147	VAL	2.2
1	A	41	ALA	2.2
1	C	41	ALA	2.2
1	A	124	LYS	2.2
1	B	2	MET	2.2
1	G	123	LYS	2.2
1	D	120	ILE	2.2
1	F	78	ILE	2.2
1	C	101	PHE	2.2
1	I	14	PHE	2.2
1	J	77	PHE	2.2
1	E	125	PRO	2.2
1	A	37	THR	2.2
1	G	141	TYR	2.2
1	H	4	TYR	2.2
1	B	27	GLY	2.2
1	B	38	GLY	2.2
1	C	10	GLY	2.2
1	F	69	GLY	2.2
1	A	52	PHE	2.2
1	A	138	VAL	2.2
1	I	138	VAL	2.2
1	D	114	ALA	2.2
1	F	48	GLN	2.2
1	B	44	LEU	2.2
1	E	49	PRO	2.2
1	A	105	PHE	2.2
1	B	134	PHE	2.2
1	F	142	ALA	2.1
1	A	38	GLY	2.1
1	F	53	GLY	2.1
1	F	104	LEU	2.1
1	D	133	ILE	2.1
1	C	47	SER	2.1
1	B	74	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	1	MET	2.1
1	B	19	MET	2.1
1	F	127	HIS	2.1
1	C	129	THR	2.1
1	D	72	ILE	2.1
1	J	150	PHE	2.1
1	A	87	VAL	2.1
1	A	142	ALA	2.1
1	G	114	ALA	2.1
1	D	104	LEU	2.1
1	A	46	THR	2.1
1	D	108	ILE	2.1
1	E	123	LYS	2.1
1	F	124	LYS	2.1
1	D	98	PRO	2.1
1	C	127	HIS	2.1
1	D	14	PHE	2.1
1	B	93	LEU	2.1
1	C	91	ASN	2.1
1	H	107	GLY	2.1
1	I	78	ILE	2.1
1	I	82	SER	2.1
1	B	84	MET	2.1
1	C	44	LEU	2.0
1	C	50	GLU	2.0
1	G	11	GLY	2.0
1	I	57	ILE	2.0
1	A	85	SER	2.0
1	C	134	PHE	2.0
1	E	86	VAL	2.0
1	F	86	VAL	2.0
1	D	18	ALA	2.0
1	G	121	LEU	2.0
1	C	38	GLY	2.0
1	C	143	ILE	2.0
1	F	24	ILE	2.0
1	G	120	ILE	2.0
1	C	26	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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.

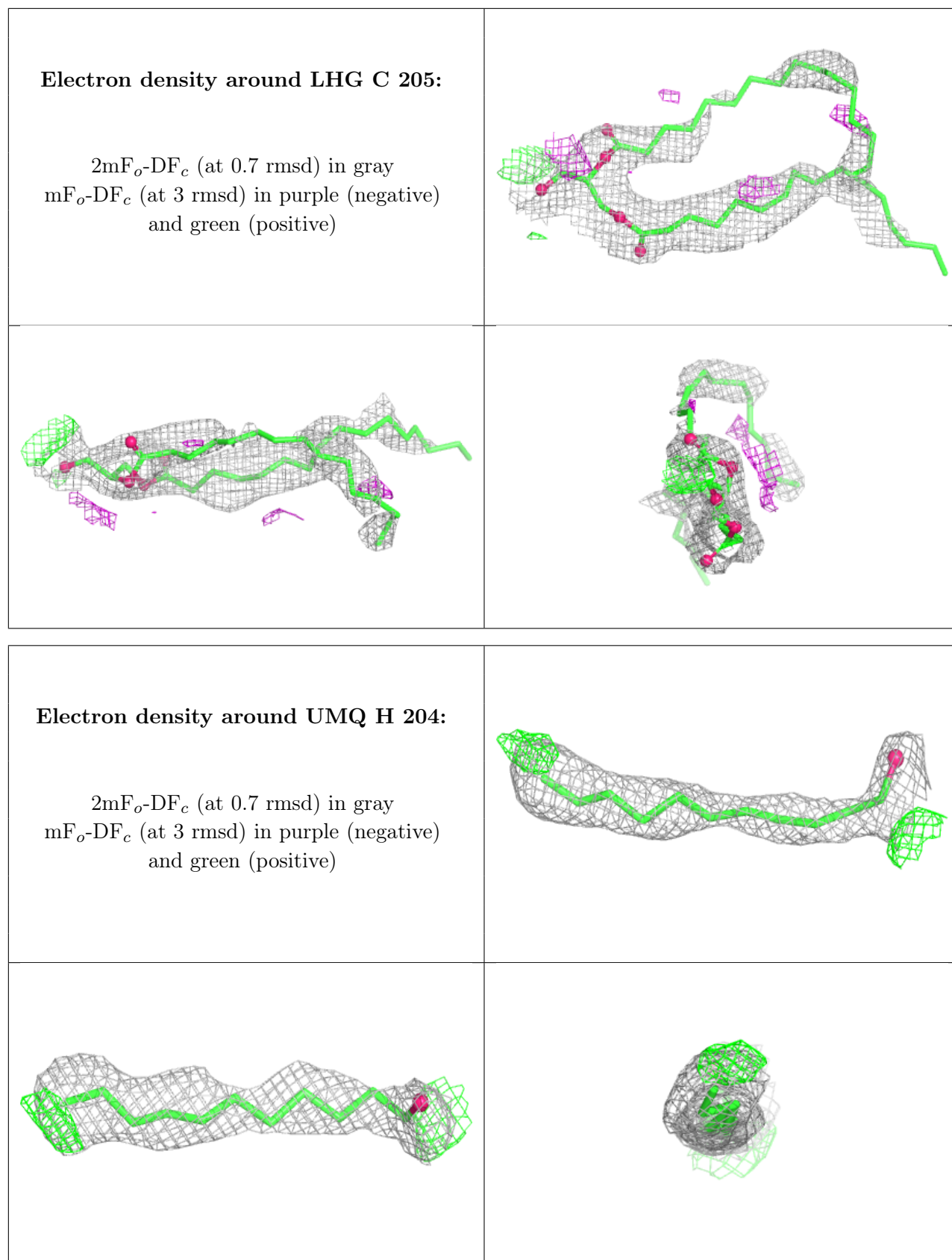
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	LHG	C	205	40/49	0.70	0.36	97,110,121,121	0
5	UMQ	H	204	12/34	0.70	0.36	87,87,89,89	0
5	UMQ	A	206	12/34	0.71	0.38	93,94,95,95	0
4	LHG	C	204	40/49	0.72	0.36	135,142,146,146	0
4	LHG	I	204	40/49	0.72	0.38	135,142,146,146	0
4	LHG	B	204	40/49	0.73	0.34	135,142,146,146	0
5	UMQ	D	205	12/34	0.73	0.37	98,100,102,102	0
4	LHG	A	203	40/49	0.73	0.35	97,110,121,121	0
4	LHG	F	204	40/49	0.74	0.39	135,142,146,146	0
4	LHG	F	205	40/49	0.75	0.34	97,110,121,121	0
4	LHG	C	203	40/49	0.75	0.34	97,110,121,121	0
4	LHG	D	203	40/49	0.75	0.38	135,142,146,146	0
4	LHG	E	203	40/49	0.75	0.37	135,142,146,146	0
4	LHG	B	203	40/49	0.75	0.34	97,110,121,121	0
4	LHG	G	203	40/49	0.76	0.36	135,142,146,146	0
4	LHG	D	204	40/49	0.77	0.31	97,110,121,121	0
4	LHG	H	203	40/49	0.78	0.35	135,142,146,146	0
4	LHG	G	204	40/49	0.78	0.32	97,110,121,121	0
4	LHG	J	204	40/49	0.78	0.37	135,142,146,146	0
4	LHG	F	203	40/49	0.79	0.33	97,110,121,121	0
5	UMQ	J	206	12/34	0.79	0.34	89,90,91,91	0
4	LHG	J	203	40/49	0.80	0.29	97,110,121,121	0
5	UMQ	E	204	12/34	0.80	0.35	95,97,98,98	0
4	LHG	A	204	40/49	0.81	0.34	135,142,146,146	0
5	UMQ	C	206	34/34	0.81	0.20	90,93,96,96	0
2	DCW	D	201	16/16	0.82	0.21	64,65,69,69	0
5	UMQ	F	206	34/34	0.82	0.21	80,87,93,94	0
5	UMQ	A	205	12/34	0.83	0.32	94,96,97,97	0
5	UMQ	I	205	12/34	0.83	0.26	77,78,79,80	0
4	LHG	I	203	40/49	0.83	0.32	97,110,121,121	0
5	UMQ	J	205	12/34	0.84	0.27	93,94,95,95	0
2	DCW	C	201	16/16	0.86	0.20	64,65,69,69	0

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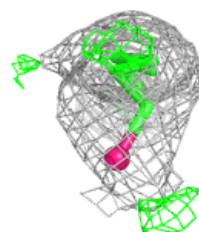
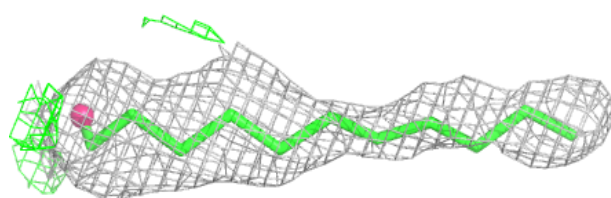
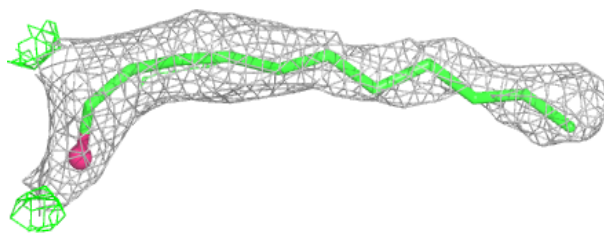
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	DCW	A	201	16/16	0.86	0.20	64,65,69,69	0
3	NA	C	202	1/1	0.86	0.23	62,62,62,62	0
2	DCW	E	201	16/16	0.87	0.19	64,65,69,69	0
3	NA	H	202	1/1	0.87	0.16	62,62,62,62	0
2	DCW	F	201	16/16	0.87	0.19	64,65,69,69	0
2	DCW	G	201	16/16	0.87	0.17	64,65,69,69	0
2	DCW	B	201	16/16	0.88	0.17	64,65,69,69	0
3	NA	F	202	1/1	0.88	0.18	62,62,62,62	0
2	DCW	H	201	16/16	0.88	0.18	63,65,69,69	0
3	NA	D	202	1/1	0.90	0.13	62,62,62,62	0
2	DCW	J	201	16/16	0.92	0.15	64,65,69,69	0
3	NA	E	202	1/1	0.92	0.14	62,62,62,62	0
3	NA	J	202	1/1	0.92	0.14	61,61,61,61	0
3	NA	G	202	1/1	0.93	0.12	62,62,62,62	0
2	DCW	I	201	16/16	0.93	0.13	64,65,69,69	0
3	NA	B	202	1/1	0.93	0.23	62,62,62,62	0
3	NA	A	202	1/1	0.96	0.09	62,62,62,62	0
3	NA	I	202	1/1	0.97	0.12	63,63,63,63	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.

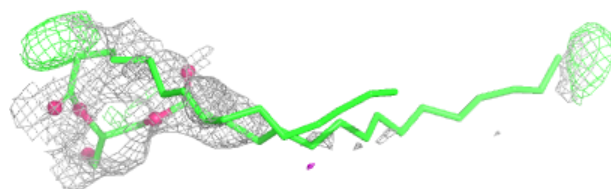
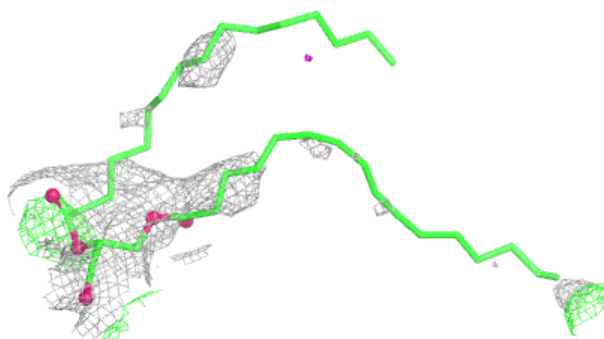


Electron density around UMQ A 206:

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

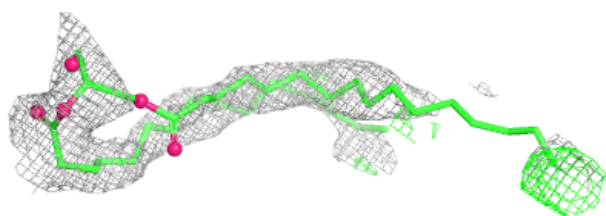
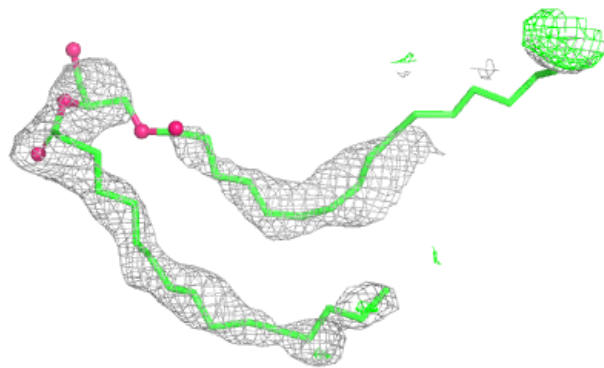
**Electron density around LHG C 204:**

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

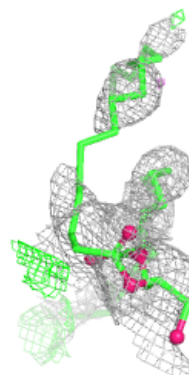
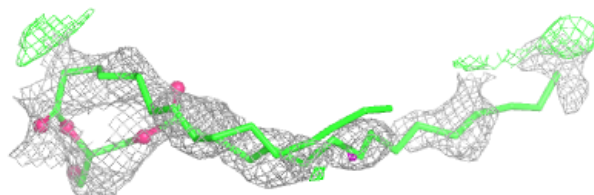
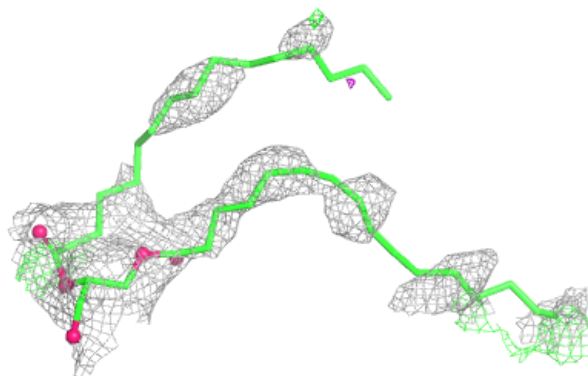


Electron density around LHG I 204:

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

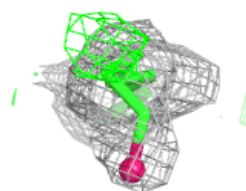
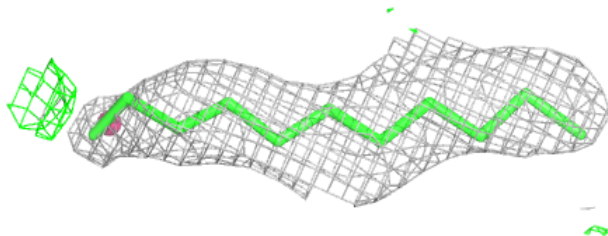
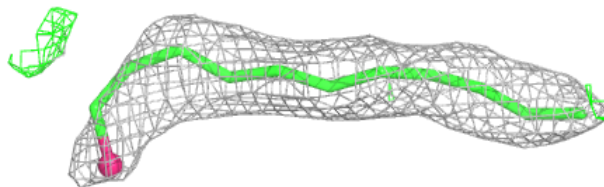
**Electron density around LHG B 204:**

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

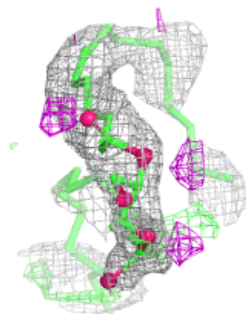
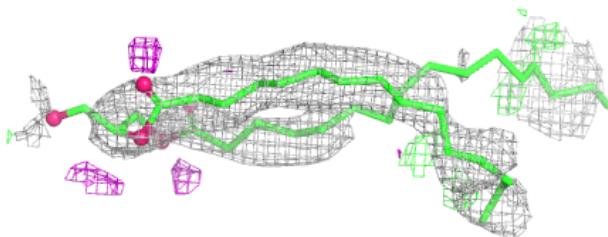
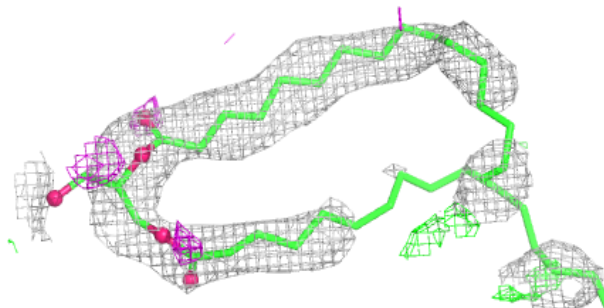


Electron density around UMQ D 205:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

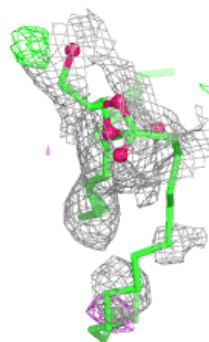
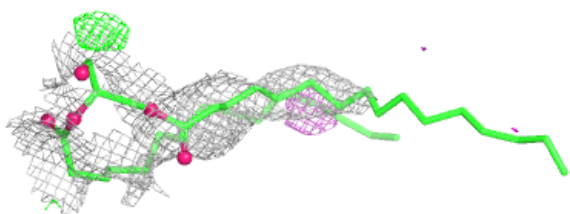
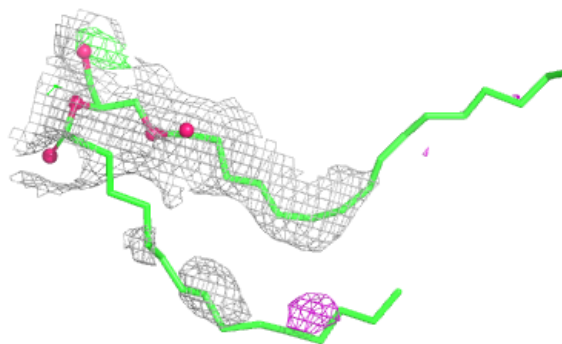
**Electron density around LHG A 203:**

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

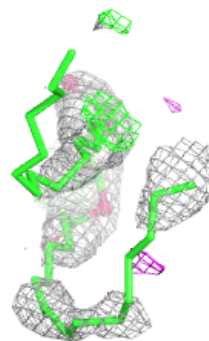
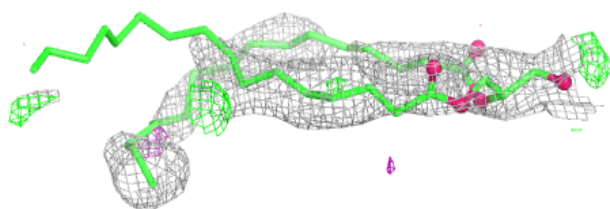
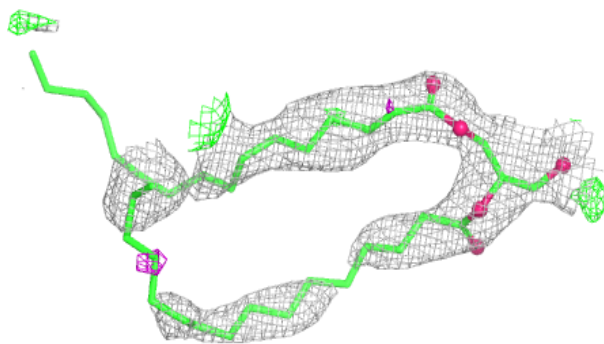


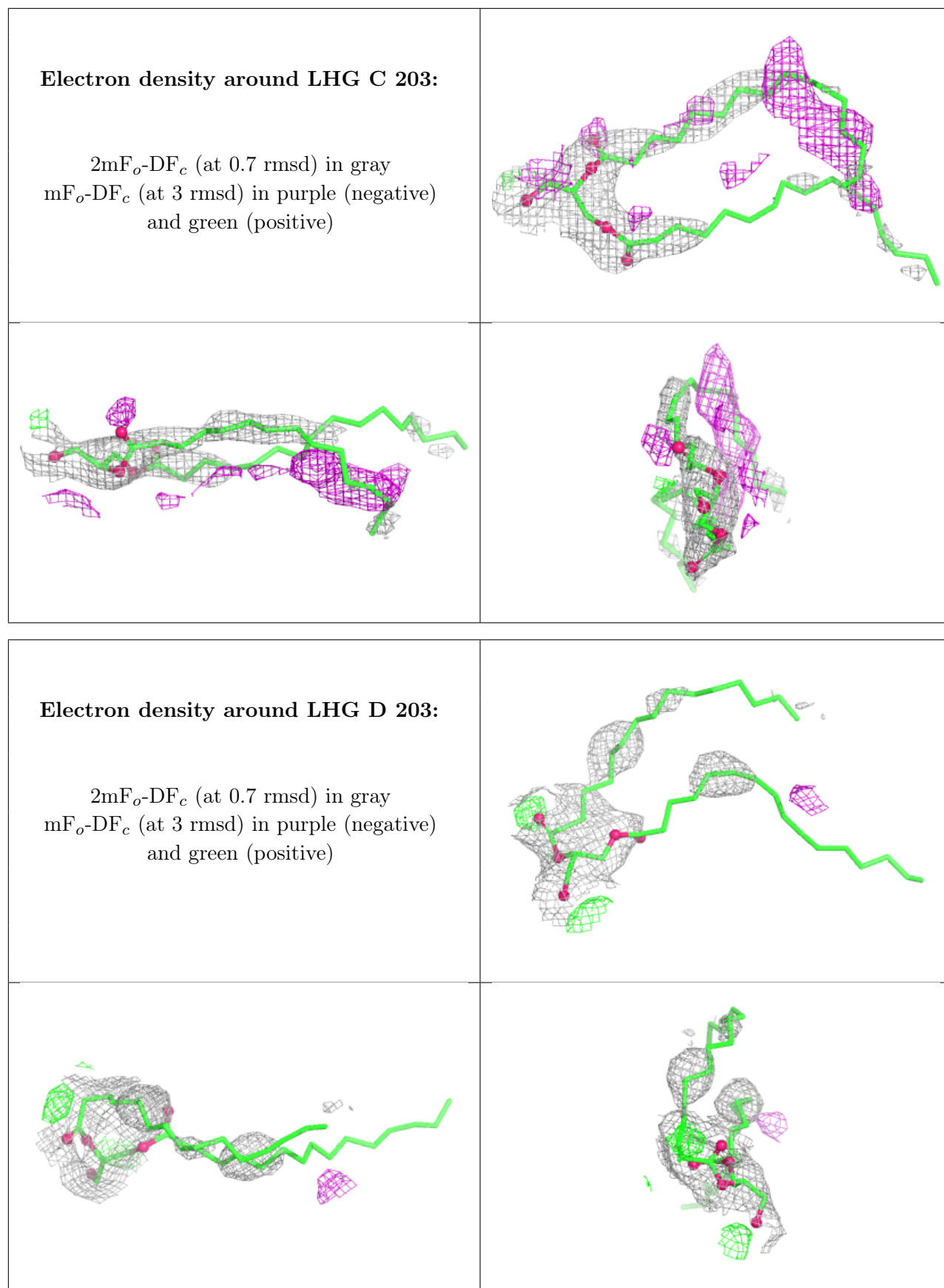
Electron density around LHG F 204:

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

**Electron density around LHG F 205:**

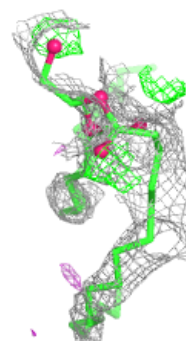
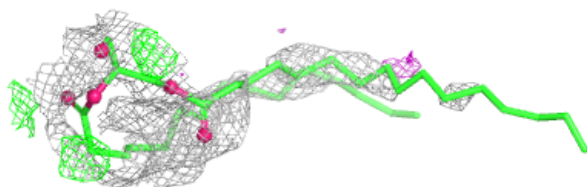
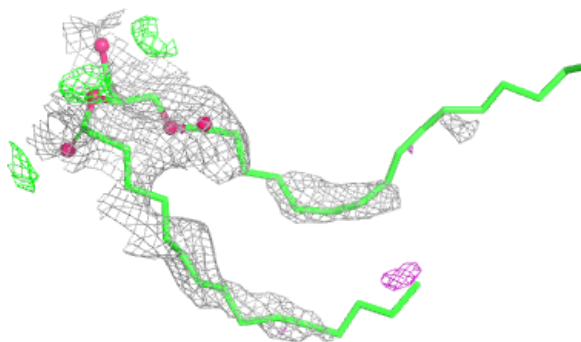
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



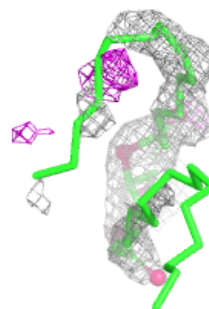
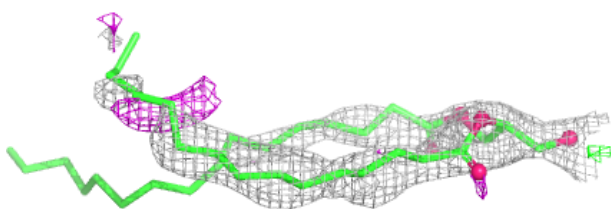
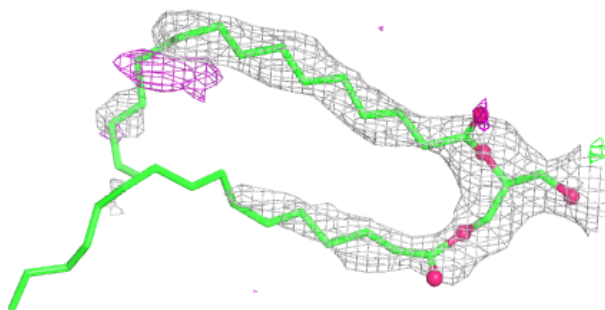


Electron density around LHG E 203:

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

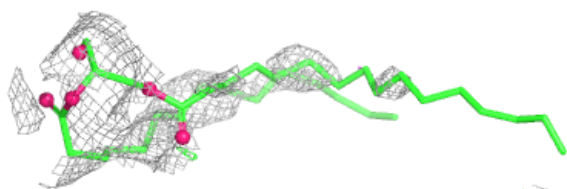
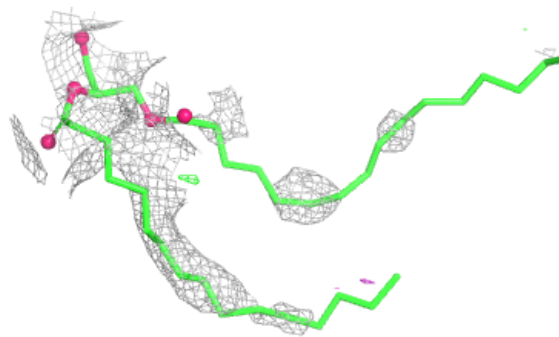
**Electron density around LHG B 203:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

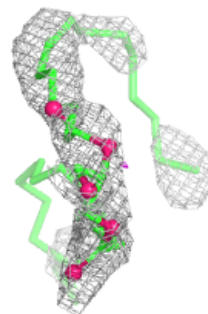
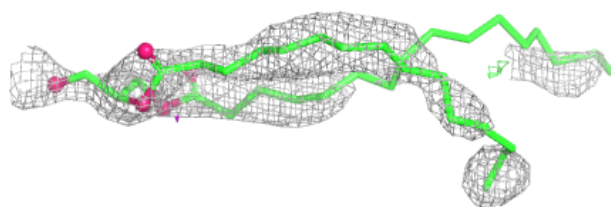
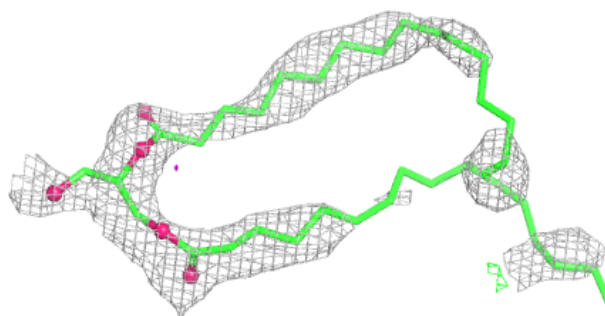


Electron density around LHG G 203:

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

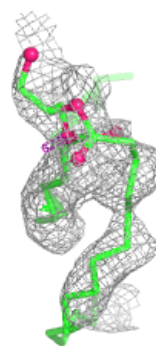
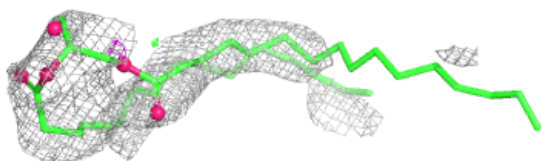
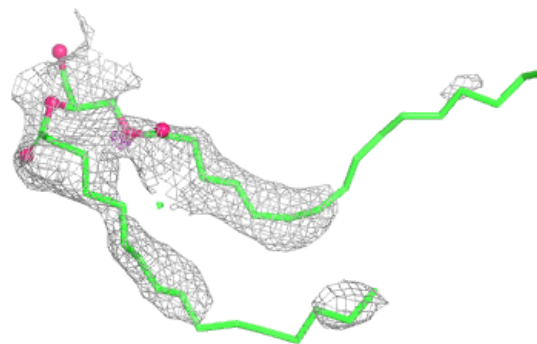
**Electron density around LHG D 204:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

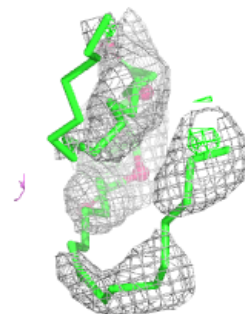
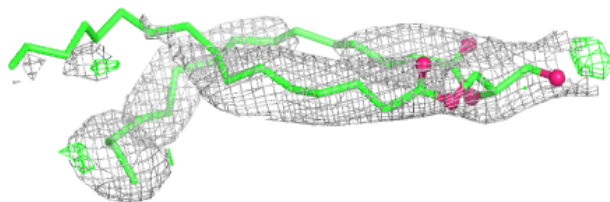
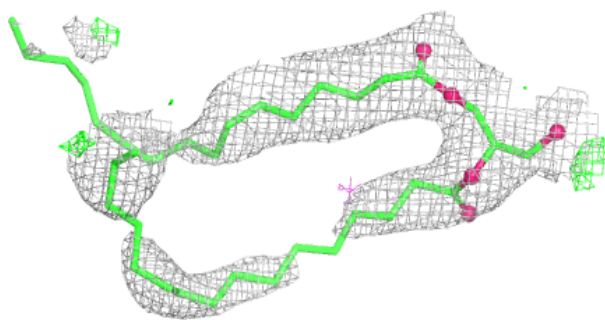


Electron density around LHG H 203:

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

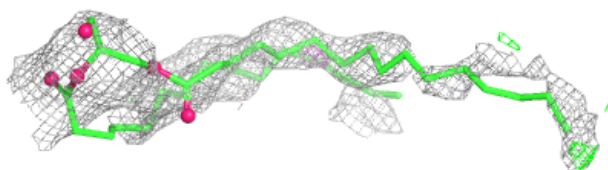
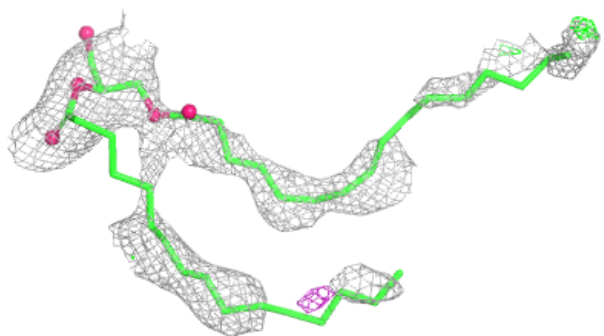
**Electron density around LHG G 204:**

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

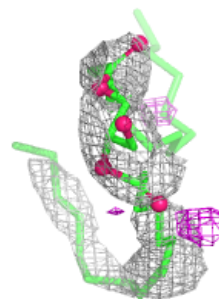
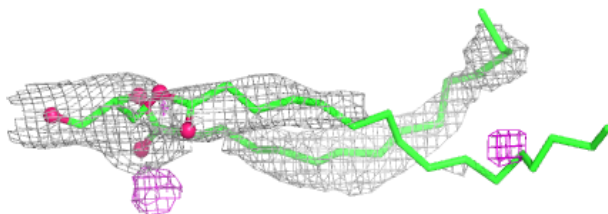
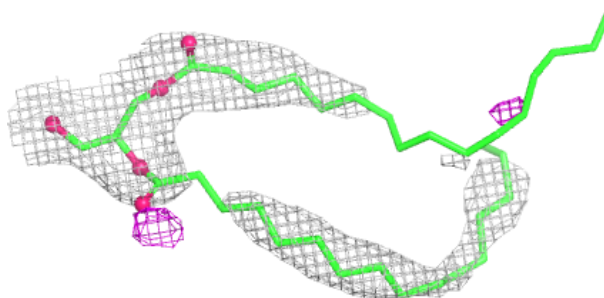


Electron density around LHG J 204:

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

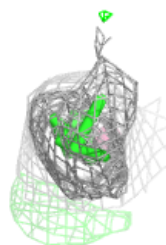
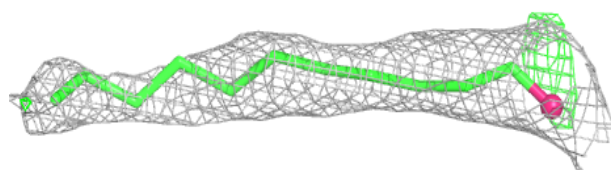
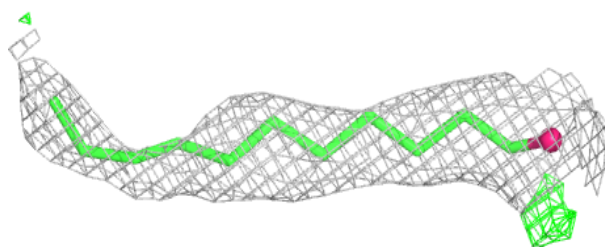
**Electron density around LHG F 203:**

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

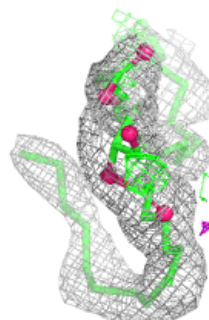
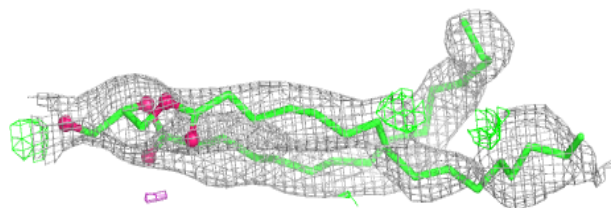
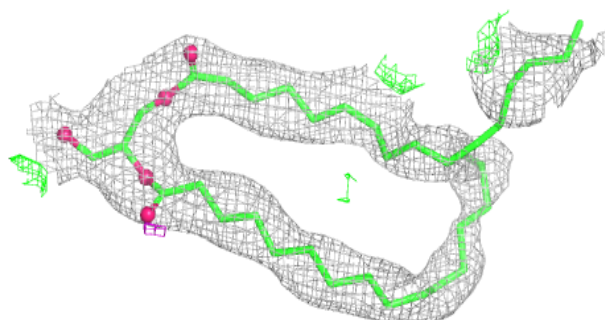


Electron density around UMQ J 206:

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

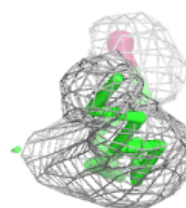
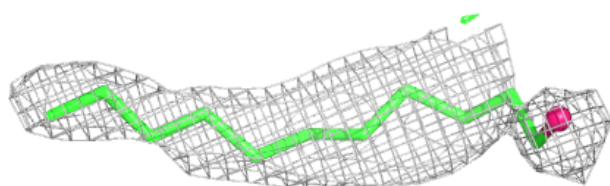
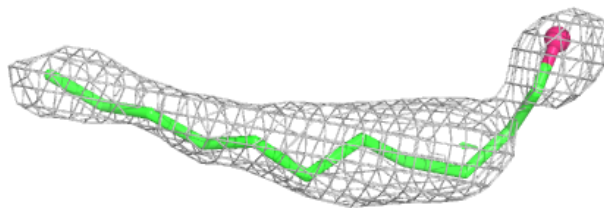
**Electron density around LHG J 203:**

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

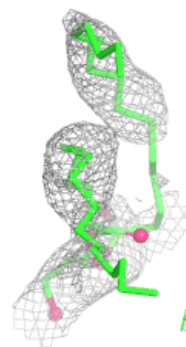
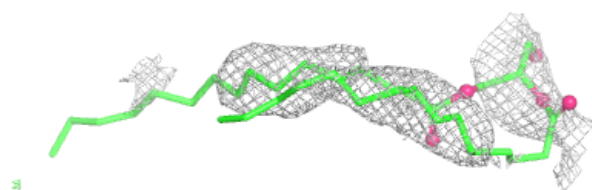
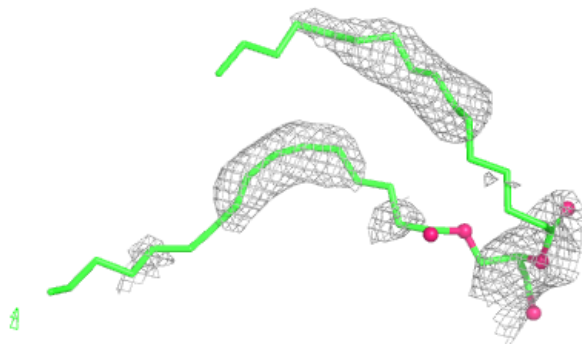


Electron density around UMQ E 204:

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

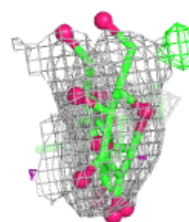
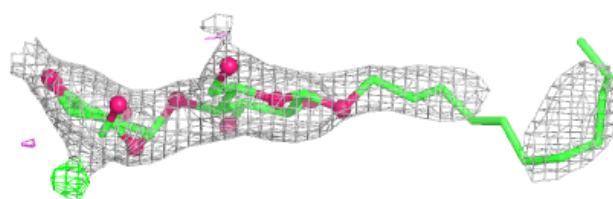
**Electron density around LHG A 204:**

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

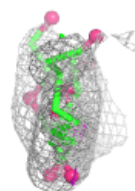
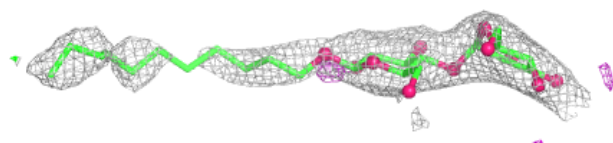
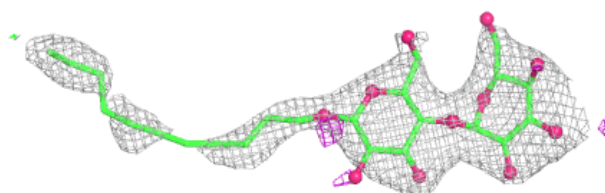


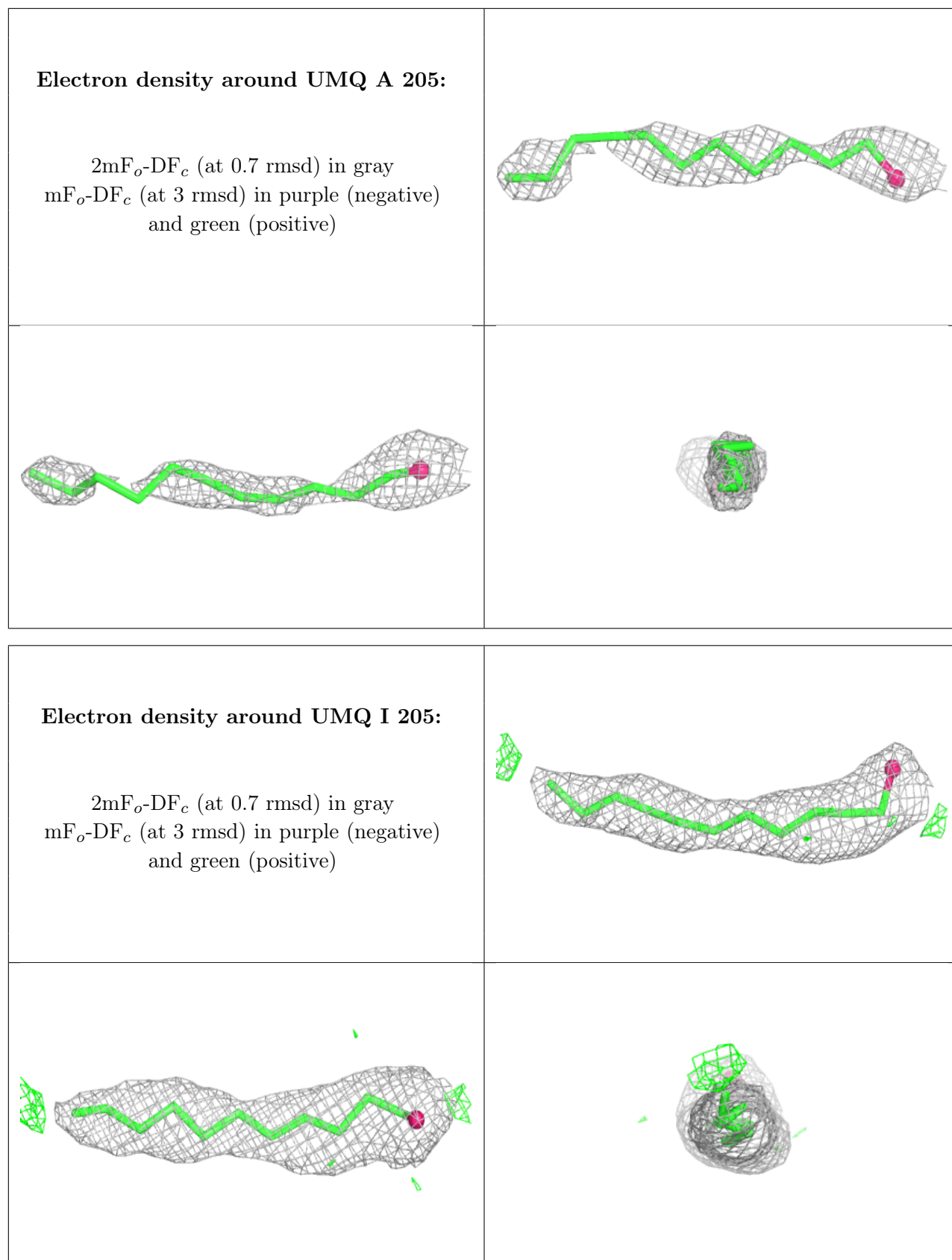
Electron density around UMQ C 206:

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

**Electron density around UMQ F 206:**

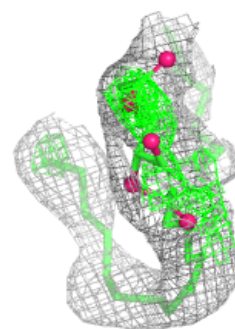
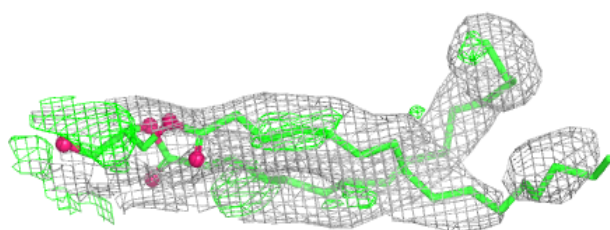
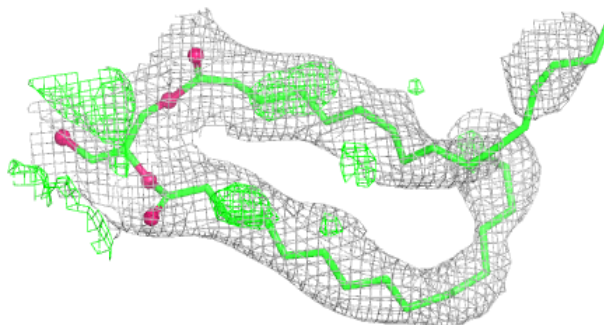
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



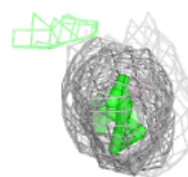
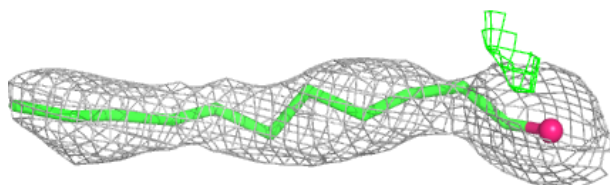
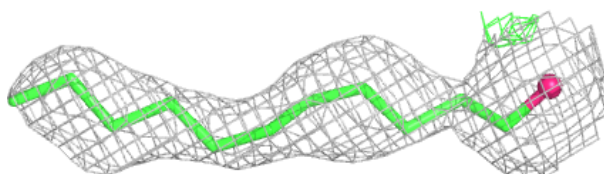


Electron density around LHG I 203:

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

**Electron density around UMQ J 205:**

$2mF_o-DF_c$ (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.