



Full wwPDB EM Validation Report ⓘ

Mar 26, 2026 – 11:56 PM UTC

PDB ID : 7OJG / pdb_00007ojg
EMDB ID : EMD-12950
Title : CRYO-EM STRUCTURE OF UNDECAMERIC SLYB FROM ES-
CHERICHIA COLI K12
Authors : Nguyen, V.S.; Remaut, H.
Deposited on : 2021-05-14
Resolution : 3.40 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

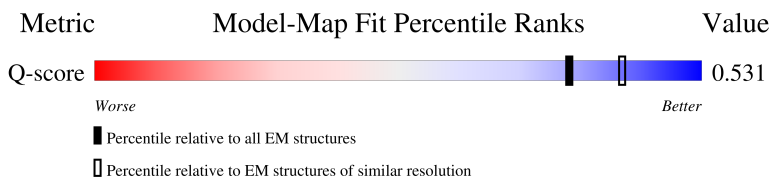
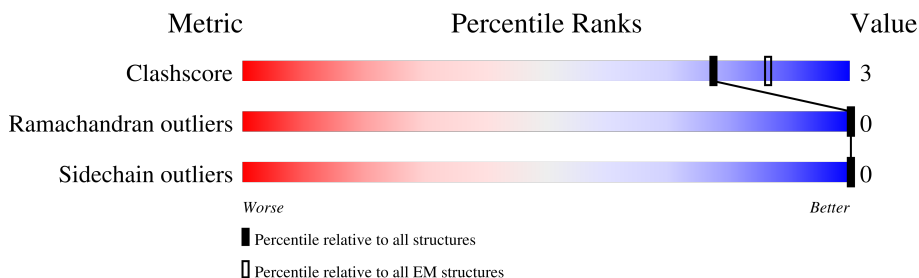
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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.



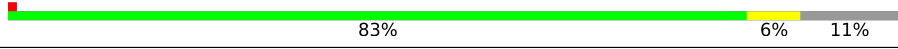
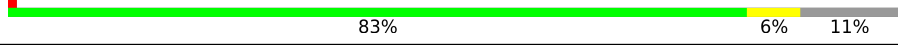
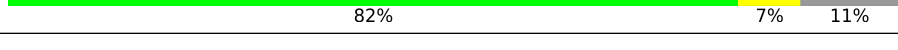
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14717 (2.90 - 3.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	155	
1	B	155	
1	C	155	
1	D	155	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	E	155	 83%6%11%
1	F	155	 81%8%11%
1	G	155	 83%6%11%
1	H	155	 83%6%11%
1	I	155	 83%6%11%
1	J	155	 83%6%11%
1	K	155	 82%7%11%

2 Entry composition

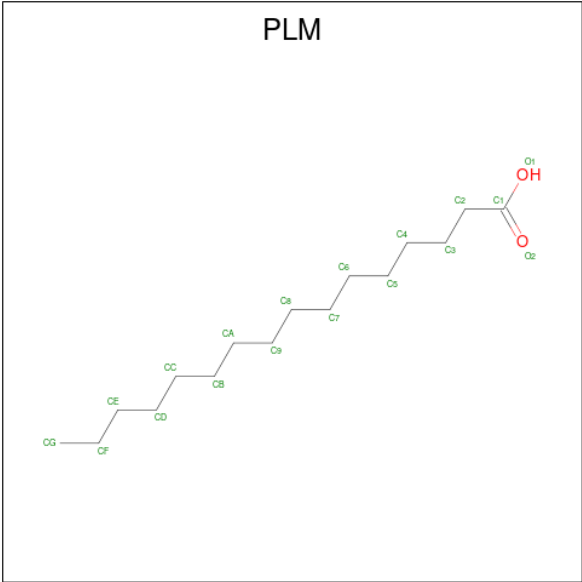
There are 5 unique types of molecules in this entry. The entry contains 13255 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Outer membrane lipoprotein slyB.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	138	Total	C	N	O	S	0	0
			967	584	181	199	3		
1	B	138	Total	C	N	O	S	0	0
			967	584	181	199	3		
1	C	138	Total	C	N	O	S	0	0
			967	584	181	199	3		
1	D	138	Total	C	N	O	S	0	0
			967	584	181	199	3		
1	E	138	Total	C	N	O	S	0	0
			967	584	181	199	3		
1	F	138	Total	C	N	O	S	0	0
			967	584	181	199	3		
1	G	138	Total	C	N	O	S	0	0
			967	584	181	199	3		
1	H	138	Total	C	N	O	S	0	0
			967	584	181	199	3		
1	I	138	Total	C	N	O	S	0	0
			967	584	181	199	3		
1	J	138	Total	C	N	O	S	0	0
			967	584	181	199	3		
1	K	138	Total	C	N	O	S	0	0
			967	584	181	199	3		

- Molecule 2 is PALMITIC ACID (CCD ID: PLM) (formula: $C_{16}H_{32}O_2$) (labeled as "Ligand of Interest" by depositor).



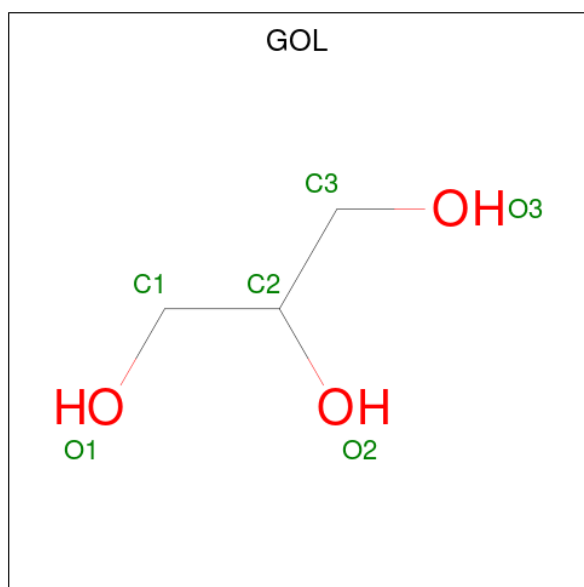
Mol	Chain	Residues	Atoms			AltConf
2	A	1	Total	C	O	0
			17	16	1	
2	A	1	Total	C	O	0
			17	16	1	
2	A	1	Total	C	O	0
			17	16	1	
2	B	1	Total	C	O	0
			17	16	1	
2	B	1	Total	C	O	0
			17	16	1	
2	B	1	Total	C	O	0
			17	16	1	
2	C	1	Total	C	O	0
			17	16	1	
2	C	1	Total	C	O	0
			17	16	1	
2	C	1	Total	C	O	0
			17	16	1	
2	D	1	Total	C	O	0
			17	16	1	
2	D	1	Total	C	O	0
			17	16	1	
2	D	1	Total	C	O	0
			17	16	1	
2	E	1	Total	C	O	0
			17	16	1	
2	E	1	Total	C	O	0
			17	16	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
2	E	1	Total	C	O	0
			17	16	1	
2	F	1	Total	C	O	0
			17	16	1	
2	F	1	Total	C	O	0
			17	16	1	
2	F	1	Total	C	O	0
			17	16	1	
2	G	1	Total	C	O	0
			17	16	1	
2	G	1	Total	C	O	0
			17	16	1	
2	G	1	Total	C	O	0
			17	16	1	
2	H	1	Total	C	O	0
			17	16	1	
2	H	1	Total	C	O	0
			17	16	1	
2	H	1	Total	C	O	0
			17	16	1	
2	I	1	Total	C	O	0
			17	16	1	
2	I	1	Total	C	O	0
			17	16	1	
2	I	1	Total	C	O	0
			17	16	1	
2	J	1	Total	C	O	0
			17	16	1	
2	J	1	Total	C	O	0
			17	16	1	
2	J	1	Total	C	O	0
			17	16	1	
2	K	1	Total	C	O	0
			17	16	1	
2	K	1	Total	C	O	0
			17	16	1	
2	K	1	Total	C	O	0
			17	16	1	

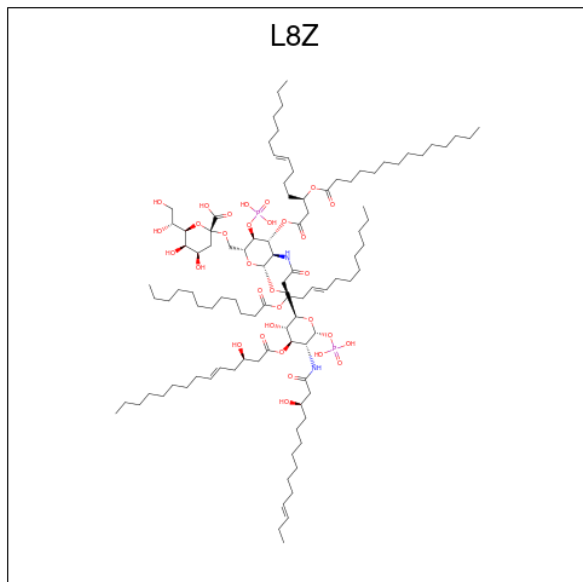
- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
3	A	1	Total	C	O	0
			5	3	2	
3	B	1	Total	C	O	0
			5	3	2	
3	C	1	Total	C	O	0
			5	3	2	
3	D	1	Total	C	O	0
			5	3	2	
3	E	1	Total	C	O	0
			5	3	2	
3	F	1	Total	C	O	0
			5	3	2	
3	G	1	Total	C	O	0
			5	3	2	
3	H	1	Total	C	O	0
			5	3	2	
3	I	1	Total	C	O	0
			5	3	2	
3	J	1	Total	C	O	0
			5	3	2	
3	K	1	Total	C	O	0
			5	3	2	

- Molecule 4 is (2 {R},4 {R},5 {R},6 {R})-6-[(1 {R})-1,2-bis(oxidanyl)ethyl]-2-[[2 {R},3 {S},4 {R},5 {R},6 {R})-5-[({E},3 {R})-3-dodecanoyloxytetradec-5-enoyl]amino]-6-[[2 {R},3 {S},4 {R},5 {R},6 {R})-3-oxidanyl-5-[({E},3 {R})-3-oxidanyltetradec-11-enoyl]amino]-4-[({E},3 {R})-3-oxidanyltetradec-5-enoyl]oxy-6-phosphonoxy-oxan-2-yl]methoxy]-3-phosphonoxy-4-[({E},3 {R})-3-tetradecanoyloxytetradec-7-enoyl]oxy-oxan-2-yl]methoxy]-4,5-bis

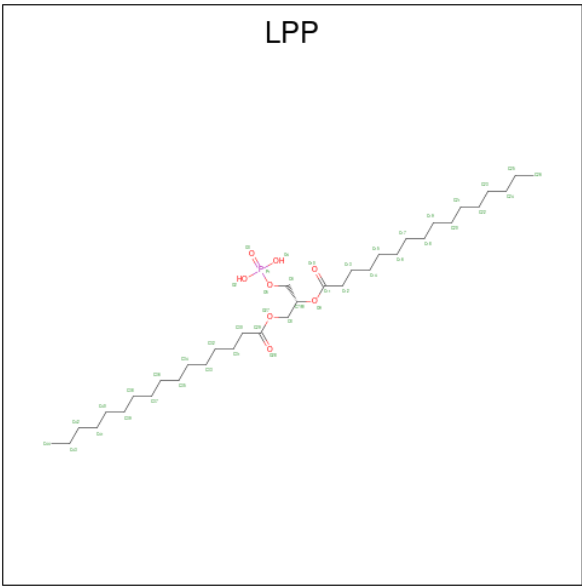
(oxidanyl)oxane-2-carboxylic acid (CCD ID: L8Z) (formula: $C_{102}H_{182}N_2O_{32}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			138	102	2	32	2	
4	B	1	Total	C	N	O	P	0
			138	102	2	32	2	
4	C	1	Total	C	N	O	P	0
			138	102	2	32	2	
4	D	1	Total	C	N	O	P	0
			138	102	2	32	2	
4	E	1	Total	C	N	O	P	0
			138	102	2	32	2	
4	F	1	Total	C	N	O	P	0
			138	102	2	32	2	
4	G	1	Total	C	N	O	P	0
			138	102	2	32	2	
4	H	1	Total	C	N	O	P	0
			138	102	2	32	2	
4	I	1	Total	C	N	O	P	0
			138	102	2	32	2	
4	J	1	Total	C	N	O	P	0
			138	102	2	32	2	
4	K	1	Total	C	N	O	P	0
			138	102	2	32	2	

- Molecule 5 is 2-(HEXADECANOYLOXY)-1-[(PHOSPHONOOXY)METHYL]ETHYL HEXADECANOATE (CCD ID: LPP) (formula: $C_{35}H_{69}O_8P$) (labeled as "Ligand of

Interest" by depositor).

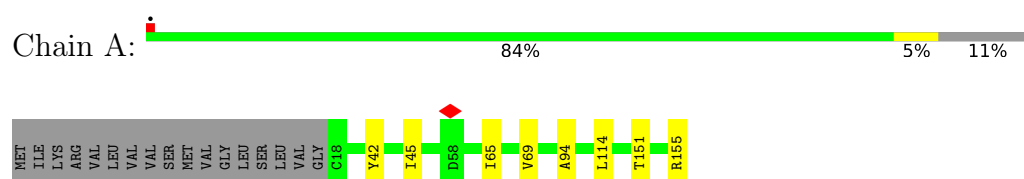


Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	O	P	0
			44	35	8	1	
5	B	1	Total	C	O	P	0
			44	35	8	1	
5	C	1	Total	C	O	P	0
			44	35	8	1	
5	D	1	Total	C	O	P	0
			44	35	8	1	
5	E	1	Total	C	O	P	0
			44	35	8	1	
5	F	1	Total	C	O	P	0
			44	35	8	1	
5	G	1	Total	C	O	P	0
			44	35	8	1	
5	H	1	Total	C	O	P	0
			44	35	8	1	
5	I	1	Total	C	O	P	0
			44	35	8	1	
5	J	1	Total	C	O	P	0
			44	35	8	1	
5	K	1	Total	C	O	P	0
			44	35	8	1	

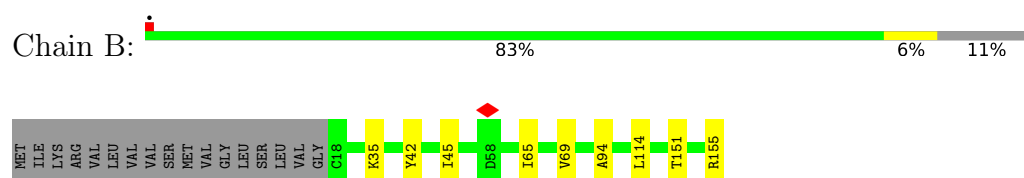
3 Residue-property plots [i](#)

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

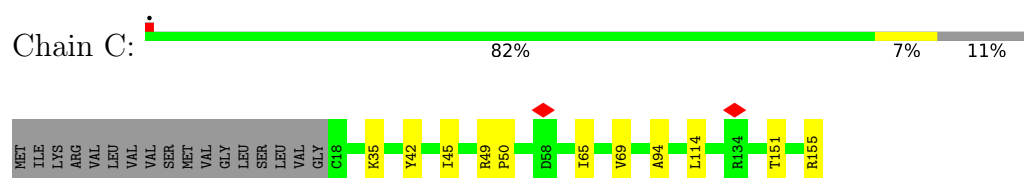
- Molecule 1: Outer membrane lipoprotein slyB



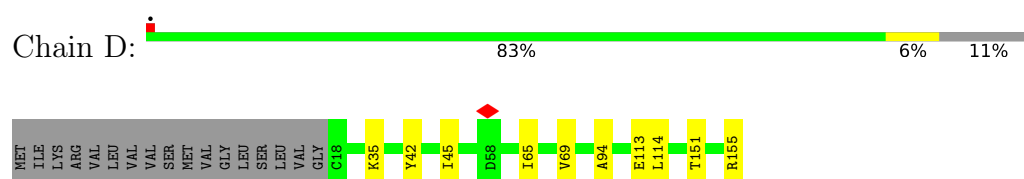
- Molecule 1: Outer membrane lipoprotein slyB



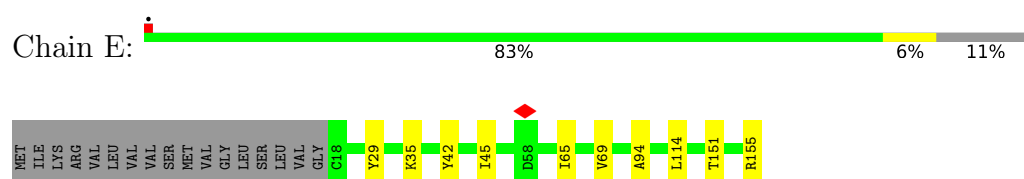
- Molecule 1: Outer membrane lipoprotein slyB



- Molecule 1: Outer membrane lipoprotein slyB



- Molecule 1: Outer membrane lipoprotein slyB



● Molecule 1: Outer membrane lipoprotein slyB

Chain F:  81% 8% 11%

● Molecule 1: Outer membrane lipoprotein slyB

Chain G:  83% 6% 11%

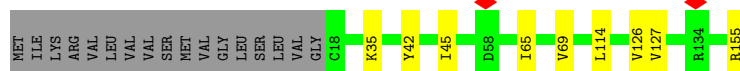
● Molecule 1: Outer membrane lipoprotein slyB

Chain H:  83% 6% 11%

● Molecule 1: Outer membrane lipoprotein slyB

Chain I:  83% 6% 11%

● Molecule 1: Outer membrane lipoprotein slyB

Chain J:  83% 6% 11%

● Molecule 1: Outer membrane lipoprotein slyB

Chain K:  82% 7% 11%

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C11	Depositor
Number of particles used	145472	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	61	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	60000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.047	Depositor
Minimum map value	-0.026	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0085	Depositor
Map size ($\text{\AA}$)	225.79199, 225.79199, 225.79199	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.784, 0.784, 0.784	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PLM, GOL, L8Z, LPP

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	0.21	0/973	0.42	0/1317
1	B	0.22	0/973	0.42	0/1317
1	C	0.22	0/973	0.42	0/1317
1	D	0.21	0/973	0.42	0/1317
1	E	0.22	0/973	0.42	0/1317
1	F	0.21	0/973	0.42	0/1317
1	G	0.22	0/973	0.42	0/1317
1	H	0.21	0/973	0.42	0/1317
1	I	0.21	0/973	0.42	0/1317
1	J	0.21	0/973	0.42	0/1317
1	K	0.22	0/973	0.42	0/1317
All	All	0.22	0/10703	0.42	0/14487

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	967	0	962	5	0
1	B	967	0	962	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	967	0	962	7	0
1	D	967	0	962	7	0
1	E	967	0	962	7	0
1	F	967	0	962	8	0
1	G	967	0	962	7	0
1	H	967	0	962	7	0
1	I	967	0	962	7	0
1	J	967	0	962	7	0
1	K	967	0	962	9	0
2	A	51	0	93	3	0
2	B	51	0	93	2	0
2	C	51	0	93	2	0
2	D	51	0	93	2	0
2	E	51	0	93	2	0
2	F	51	0	93	2	0
2	G	51	0	93	2	0
2	H	51	0	93	2	0
2	I	51	0	93	2	0
2	J	51	0	93	2	0
2	K	51	0	93	1	0
3	A	5	0	3	0	0
3	B	5	0	3	0	0
3	C	5	0	3	0	0
3	D	5	0	3	0	0
3	E	5	0	3	0	0
3	F	5	0	3	0	0
3	G	5	0	3	0	0
3	H	5	0	3	0	0
3	I	5	0	3	0	0
3	J	5	0	3	0	0
3	K	5	0	3	0	0
4	A	138	0	0	0	0
4	B	138	0	0	0	0
4	C	138	0	0	0	0
4	D	138	0	0	0	0
4	E	138	0	0	0	0
4	F	138	0	0	0	0
4	G	138	0	0	0	0
4	H	138	0	0	0	0
4	I	138	0	0	0	0
4	J	138	0	0	1	0
4	K	138	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	44	0	67	0	0
5	B	44	0	67	0	0
5	C	44	0	67	0	0
5	D	44	0	67	0	0
5	E	44	0	67	0	0
5	F	44	0	67	0	0
5	G	44	0	67	0	0
5	H	44	0	67	0	0
5	I	44	0	67	0	0
5	J	44	0	67	0	0
5	K	44	0	67	0	0
All	All	13255	0	12375	73	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 (73) 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:J:127:VAL:HG13	1:K:34:ALA:HA	1.69	0.73
2:A:205:PLM:HF2	1:K:94:ALA:HB2	1.73	0.71
1:J:127:VAL:CG1	1:K:34:ALA:HA	2.34	0.56
1:A:45:ILE:HD11	1:A:114:LEU:HD22	1.88	0.56
1:B:45:ILE:HD11	1:B:114:LEU:HD22	1.88	0.56
1:D:45:ILE:HD11	1:D:114:LEU:HD22	1.88	0.56
1:C:45:ILE:HD11	1:C:114:LEU:HD22	1.88	0.55
1:E:45:ILE:HD11	1:E:114:LEU:HD22	1.88	0.55
1:J:45:ILE:HD11	1:J:114:LEU:HD22	1.88	0.55
1:K:45:ILE:HD11	1:K:114:LEU:HD22	1.88	0.55
1:F:45:ILE:HD11	1:F:114:LEU:HD22	1.88	0.55
1:H:45:ILE:HD11	1:H:114:LEU:HD22	1.88	0.54
1:I:45:ILE:HD11	1:I:114:LEU:HD22	1.88	0.54
1:G:45:ILE:HD11	1:G:114:LEU:HD22	1.88	0.54
1:H:151:THR:HG22	1:I:35:LYS:HE3	1.92	0.52
1:F:151:THR:HG22	1:G:35:LYS:HE3	1.92	0.52
1:G:151:THR:HG22	1:H:35:LYS:HE3	1.92	0.52
1:E:151:THR:HG22	1:F:35:LYS:HE3	1.92	0.52
1:I:151:THR:HG22	1:J:35:LYS:HE3	1.92	0.52
1:A:151:THR:HG22	1:B:35:LYS:HE3	1.92	0.52
1:D:151:THR:HG22	1:E:35:LYS:HE3	1.92	0.52
1:C:151:THR:HG22	1:D:35:LYS:HE3	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:151:THR:HG22	1:C:35:LYS:HE3	1.92	0.51
1:J:126:VAL:HG23	1:K:36:GLN:O	2.11	0.51
1:H:113:GLU:OE2	1:I:29:TYR:OH	2.26	0.48
1:I:65:ILE:O	1:I:69:VAL:HG22	2.17	0.45
1:G:65:ILE:O	1:G:69:VAL:HG22	2.17	0.45
1:A:65:ILE:O	1:A:69:VAL:HG22	2.17	0.45
1:F:65:ILE:O	1:F:69:VAL:HG22	2.17	0.45
1:D:65:ILE:O	1:D:69:VAL:HG22	2.17	0.45
1:K:65:ILE:O	1:K:69:VAL:HG22	2.17	0.45
1:E:65:ILE:O	1:E:69:VAL:HG22	2.17	0.45
1:J:65:ILE:O	1:J:69:VAL:HG22	2.17	0.45
1:C:65:ILE:O	1:C:69:VAL:HG22	2.17	0.45
1:B:65:ILE:O	1:B:69:VAL:HG22	2.17	0.44
1:H:65:ILE:O	1:H:69:VAL:HG22	2.17	0.44
4:J:205:LZ:C30	1:K:70:LEU:HD11	2.47	0.44
1:F:113:GLU:OE2	1:G:29:TYR:OH	2.26	0.43
1:C:42:TYR:HE2	1:C:155:ARG:HH12	1.67	0.43
1:B:42:TYR:HE2	1:B:155:ARG:HH12	1.67	0.43
1:D:42:TYR:HE2	1:D:155:ARG:HH12	1.67	0.42
1:D:94:ALA:HB2	2:E:204:PLM:HF2	2.01	0.42
1:H:94:ALA:HB2	2:I:204:PLM:HF2	2.01	0.42
1:A:42:TYR:HE2	1:A:155:ARG:HH12	1.67	0.42
1:J:42:TYR:HE2	1:J:155:ARG:HH12	1.67	0.42
2:A:205:PLM:H71	2:A:206:PLM:HA1	2.02	0.42
1:F:94:ALA:HB2	2:G:204:PLM:HF2	2.01	0.42
1:I:42:TYR:HE2	1:I:155:ARG:HH12	1.67	0.42
1:E:94:ALA:HB2	2:F:204:PLM:HF2	2.01	0.42
1:I:94:ALA:HB2	2:J:204:PLM:HF2	2.01	0.42
2:B:201:PLM:HA1	2:B:204:PLM:H71	2.02	0.42
2:C:201:PLM:HA1	2:C:204:PLM:H71	2.02	0.42
2:J:201:PLM:HA1	2:J:204:PLM:H71	2.02	0.42
2:K:201:PLM:HA1	2:K:204:PLM:H71	2.02	0.42
1:C:94:ALA:HB2	2:D:204:PLM:HF2	2.01	0.42
2:A:206:PLM:H61	1:K:97:VAL:CG2	2.50	0.41
2:D:201:PLM:HA1	2:D:204:PLM:H71	2.02	0.41
1:H:42:TYR:HE2	1:H:155:ARG:HH12	1.67	0.41
1:B:94:ALA:HB2	2:C:204:PLM:HF2	2.01	0.41
1:E:42:TYR:HE2	1:E:155:ARG:HH12	1.67	0.41
1:F:49:ARG:HA	1:F:50:PRO:HD3	1.91	0.41
1:K:42:TYR:HE2	1:K:155:ARG:HH12	1.67	0.41
2:E:201:PLM:HA1	2:E:204:PLM:H71	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:42:TYR:HE2	1:G:155:ARG:HH12	1.67	0.41
1:G:94:ALA:HB2	2:H:204:PLM:HF2	2.01	0.41
1:F:42:TYR:HE2	1:F:155:ARG:HH12	1.67	0.41
1:A:94:ALA:HB2	2:B:204:PLM:HF2	2.02	0.41
1:C:49:ARG:HA	1:C:50:PRO:HD3	1.91	0.41
2:I:201:PLM:HA1	2:I:204:PLM:H71	2.02	0.41
2:H:201:PLM:HA1	2:H:204:PLM:H71	2.02	0.40
1:D:113:GLU:OE2	1:E:29:TYR:OH	2.26	0.40
2:G:201:PLM:HA1	2:G:204:PLM:H71	2.02	0.40
2:F:201:PLM:HA1	2:F:204:PLM:H71	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	136/155 (88%)	134 (98%)	2 (2%)	0	100	100
1	B	136/155 (88%)	134 (98%)	2 (2%)	0	100	100
1	C	136/155 (88%)	134 (98%)	2 (2%)	0	100	100
1	D	136/155 (88%)	134 (98%)	2 (2%)	0	100	100
1	E	136/155 (88%)	134 (98%)	2 (2%)	0	100	100
1	F	136/155 (88%)	134 (98%)	2 (2%)	0	100	100
1	G	136/155 (88%)	134 (98%)	2 (2%)	0	100	100
1	H	136/155 (88%)	134 (98%)	2 (2%)	0	100	100
1	I	136/155 (88%)	134 (98%)	2 (2%)	0	100	100
1	J	136/155 (88%)	134 (98%)	2 (2%)	0	100	100
1	K	136/155 (88%)	134 (98%)	2 (2%)	0	100	100
All	All	1496/1705 (88%)	1474 (98%)	22 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	102/117 (87%)	102 (100%)	0	100	100
1	B	102/117 (87%)	102 (100%)	0	100	100
1	C	102/117 (87%)	102 (100%)	0	100	100
1	D	102/117 (87%)	102 (100%)	0	100	100
1	E	102/117 (87%)	102 (100%)	0	100	100
1	F	102/117 (87%)	102 (100%)	0	100	100
1	G	102/117 (87%)	102 (100%)	0	100	100
1	H	102/117 (87%)	102 (100%)	0	100	100
1	I	102/117 (87%)	102 (100%)	0	100	100
1	J	102/117 (87%)	102 (100%)	0	100	100
1	K	102/117 (87%)	102 (100%)	0	100	100
All	All	1122/1287 (87%)	1122 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	ASN
1	A	130	GLN
1	A	149	GLN
1	B	130	GLN
1	B	149	GLN
1	C	130	GLN
1	C	149	GLN
1	D	20	ASN
1	D	130	GLN
1	D	149	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	20	ASN
1	E	149	GLN
1	F	149	GLN
1	G	20	ASN
1	G	149	GLN
1	H	20	ASN
1	H	149	GLN
1	I	20	ASN
1	I	130	GLN
1	I	149	GLN
1	J	20	ASN
1	J	130	GLN
1	J	149	GLN
1	K	20	ASN
1	K	130	GLN
1	K	149	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 [i](#)

66 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	L8Z	E	205	-	138,140,140	1.95	27 (19%)	164,176,176	2.13	32 (19%)
4	L8Z	I	205	-	138,140,140	1.95	27 (19%)	164,176,176	2.13	32 (19%)
5	LPP	A	204	-	43,43,43	1.64	3 (6%)	46,48,48	0.97	5 (10%)
2	PLM	K	204	3	15,16,17	0.50	0	14,15,17	0.26	0
2	PLM	F	201	3	15,16,17	0.47	0	14,15,17	0.24	0
4	L8Z	C	205	-	138,140,140	1.95	27 (19%)	164,176,176	2.13	32 (19%)
4	L8Z	H	205	-	138,140,140	1.95	27 (19%)	164,176,176	2.13	32 (19%)
4	L8Z	A	203	-	138,140,140	1.95	27 (19%)	164,176,176	2.12	32 (19%)
2	PLM	B	201	3	15,16,17	0.47	0	14,15,17	0.24	0
3	GOL	H	203	2,1	4,4,5	0.98	0	4,4,5	1.08	0
5	LPP	E	206	-	43,43,43	1.63	3 (6%)	46,48,48	0.97	5 (10%)
2	PLM	H	204	3	15,16,17	0.51	0	14,15,17	0.27	0
2	PLM	K	202	1	15,16,17	0.36	0	14,15,17	0.37	0
4	L8Z	B	205	-	138,140,140	1.95	27 (19%)	164,176,176	2.12	32 (19%)
2	PLM	C	202	1	15,16,17	0.36	0	14,15,17	0.37	0
2	PLM	E	204	3	15,16,17	0.50	0	14,15,17	0.26	0
2	PLM	F	202	1	15,16,17	0.36	0	14,15,17	0.36	0
2	PLM	A	205	3	15,16,17	0.51	0	14,15,17	0.27	0
2	PLM	D	201	3	15,16,17	0.47	0	14,15,17	0.24	0
2	PLM	E	202	1	15,16,17	0.36	0	14,15,17	0.36	0
3	GOL	G	203	2,1	4,4,5	0.97	0	4,4,5	1.08	0
2	PLM	J	201	3	15,16,17	0.47	0	14,15,17	0.24	0
3	GOL	J	203	2,1	4,4,5	0.98	0	4,4,5	1.08	0
4	L8Z	D	205	-	138,140,140	1.95	27 (19%)	164,176,176	2.13	32 (19%)
2	PLM	J	204	3	15,16,17	0.50	0	14,15,17	0.27	0
3	GOL	B	203	2,1	4,4,5	0.97	0	4,4,5	1.08	0
3	GOL	F	203	2,1	4,4,5	0.99	0	4,4,5	1.08	0
3	GOL	C	203	2,1	4,4,5	0.97	0	4,4,5	1.07	0
4	L8Z	K	205	-	138,140,140	1.95	27 (19%)	164,176,176	2.13	32 (19%)
2	PLM	E	201	3	15,16,17	0.47	0	14,15,17	0.24	0
3	GOL	K	203	2,1	4,4,5	0.98	0	4,4,5	1.08	0
2	PLM	I	201	3	15,16,17	0.47	0	14,15,17	0.24	0
2	PLM	C	201	3	15,16,17	0.47	0	14,15,17	0.24	0
2	PLM	I	202	1	15,16,17	0.36	0	14,15,17	0.36	0
5	LPP	I	206	-	43,43,43	1.64	3 (6%)	46,48,48	0.97	5 (10%)
4	L8Z	F	205	-	138,140,140	1.94	27 (19%)	164,176,176	2.12	32 (19%)
3	GOL	D	203	2,1	4,4,5	0.97	0	4,4,5	1.08	0
5	LPP	J	206	-	43,43,43	1.63	3 (6%)	46,48,48	0.97	5 (10%)
5	LPP	H	206	-	43,43,43	1.63	3 (6%)	46,48,48	0.97	5 (10%)
2	PLM	I	204	3	15,16,17	0.50	0	14,15,17	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PLM	H	202	1	15,16,17	0.36	0	14,15,17	0.37	0
2	PLM	C	204	3	15,16,17	0.50	0	14,15,17	0.26	0
3	GOL	A	202	2,1	4,4,5	0.98	0	4,4,5	1.08	0
4	L8Z	J	205	-	138,140,140	1.95	27 (19%)	164,176,176	2.13	32 (19%)
2	PLM	A	201	1	15,16,17	0.36	0	14,15,17	0.37	0
2	PLM	F	204	3	15,16,17	0.51	0	14,15,17	0.26	0
3	GOL	E	203	2,1	4,4,5	0.98	0	4,4,5	1.09	0
2	PLM	G	201	3	15,16,17	0.47	0	14,15,17	0.24	0
2	PLM	B	204	3	15,16,17	0.50	0	14,15,17	0.26	0
3	GOL	I	203	2,1	4,4,5	0.97	0	4,4,5	1.08	0
4	L8Z	G	205	-	138,140,140	1.95	27 (19%)	164,176,176	2.13	32 (19%)
5	LPP	F	206	-	43,43,43	1.63	3 (6%)	46,48,48	0.97	5 (10%)
2	PLM	J	202	1	15,16,17	0.36	0	14,15,17	0.36	0
5	LPP	C	206	-	43,43,43	1.63	3 (6%)	46,48,48	0.97	5 (10%)
5	LPP	K	206	-	43,43,43	1.63	3 (6%)	46,48,48	0.97	5 (10%)
2	PLM	G	204	3	15,16,17	0.50	0	14,15,17	0.26	0
2	PLM	D	202	1	15,16,17	0.36	0	14,15,17	0.36	0
2	PLM	B	202	1	15,16,17	0.36	0	14,15,17	0.36	0
2	PLM	D	204	3	15,16,17	0.51	0	14,15,17	0.27	0
2	PLM	H	201	3	15,16,17	0.47	0	14,15,17	0.24	0
2	PLM	G	202	1	15,16,17	0.36	0	14,15,17	0.36	0
2	PLM	K	201	3	15,16,17	0.47	0	14,15,17	0.24	0
5	LPP	D	206	-	43,43,43	1.63	3 (6%)	46,48,48	0.97	5 (10%)
5	LPP	G	206	-	43,43,43	1.63	3 (6%)	46,48,48	0.97	5 (10%)
2	PLM	A	206	3	15,16,17	0.47	0	14,15,17	0.24	0
5	LPP	B	206	-	43,43,43	1.63	3 (6%)	46,48,48	0.97	5 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	L8Z	E	205	-	-	55/140/199/199	0/3/3/3
4	L8Z	I	205	-	-	55/140/199/199	0/3/3/3
5	LPP	A	204	-	-	17/45/45/45	-
2	PLM	K	204	3	-	2/14/14/15	-
2	PLM	F	201	3	-	5/14/14/15	-
4	L8Z	C	205	-	-	55/140/199/199	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	L8Z	H	205	-	-	55/140/199/199	0/3/3/3
4	L8Z	A	203	-	-	55/140/199/199	0/3/3/3
2	PLM	B	201	3	-	5/14/14/15	-
3	GOL	H	203	2,1	-	0/2/2/4	-
5	LPP	E	206	-	-	17/45/45/45	-
2	PLM	H	204	3	-	2/14/14/15	-
2	PLM	K	202	1	-	0/14/14/15	-
4	L8Z	B	205	-	-	55/140/199/199	0/3/3/3
2	PLM	C	202	1	-	0/14/14/15	-
2	PLM	E	204	3	-	2/14/14/15	-
2	PLM	F	202	1	-	0/14/14/15	-
2	PLM	A	205	3	-	2/14/14/15	-
2	PLM	D	201	3	-	5/14/14/15	-
2	PLM	E	202	1	-	0/14/14/15	-
3	GOL	G	203	2,1	-	0/2/2/4	-
2	PLM	J	201	3	-	5/14/14/15	-
3	GOL	J	203	2,1	-	0/2/2/4	-
4	L8Z	D	205	-	-	55/140/199/199	0/3/3/3
2	PLM	J	204	3	-	2/14/14/15	-
3	GOL	B	203	2,1	-	0/2/2/4	-
3	GOL	F	203	2,1	-	0/2/2/4	-
3	GOL	C	203	2,1	-	0/2/2/4	-
4	L8Z	K	205	-	-	55/140/199/199	0/3/3/3
2	PLM	E	201	3	-	5/14/14/15	-
3	GOL	K	203	2,1	-	0/2/2/4	-
2	PLM	I	201	3	-	5/14/14/15	-
2	PLM	C	201	3	-	5/14/14/15	-
2	PLM	I	202	1	-	0/14/14/15	-
5	LPP	I	206	-	-	17/45/45/45	-
4	L8Z	F	205	-	-	55/140/199/199	0/3/3/3
3	GOL	D	203	2,1	-	0/2/2/4	-
5	LPP	J	206	-	-	17/45/45/45	-
5	LPP	H	206	-	-	17/45/45/45	-
2	PLM	I	204	3	-	2/14/14/15	-
2	PLM	H	202	1	-	0/14/14/15	-
2	PLM	C	204	3	-	2/14/14/15	-
3	GOL	A	202	2,1	-	0/2/2/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	L8Z	J	205	-	-	55/140/199/199	0/3/3/3
2	PLM	A	201	1	-	0/14/14/15	-
2	PLM	F	204	3	-	2/14/14/15	-
3	GOL	E	203	2,1	-	0/2/2/4	-
2	PLM	G	201	3	-	5/14/14/15	-
2	PLM	B	204	3	-	2/14/14/15	-
3	GOL	I	203	2,1	-	0/2/2/4	-
4	L8Z	G	205	-	-	55/140/199/199	0/3/3/3
5	LPP	F	206	-	-	17/45/45/45	-
2	PLM	J	202	1	-	0/14/14/15	-
5	LPP	C	206	-	-	17/45/45/45	-
5	LPP	K	206	-	-	17/45/45/45	-
2	PLM	G	204	3	-	2/14/14/15	-
2	PLM	D	202	1	-	0/14/14/15	-
2	PLM	B	202	1	-	0/14/14/15	-
2	PLM	D	204	3	-	2/14/14/15	-
2	PLM	H	201	3	-	5/14/14/15	-
2	PLM	G	202	1	-	0/14/14/15	-
2	PLM	K	201	3	-	5/14/14/15	-
5	LPP	D	206	-	-	17/45/45/45	-
5	LPP	G	206	-	-	17/45/45/45	-
2	PLM	A	206	3	-	5/14/14/15	-
5	LPP	B	206	-	-	17/45/45/45	-

All (330) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	K	206	LPP	P1-O5	8.45	1.87	1.60
5	A	204	LPP	P1-O5	8.45	1.87	1.60
5	I	206	LPP	P1-O5	8.44	1.87	1.60
5	D	206	LPP	P1-O5	8.43	1.86	1.60
5	G	206	LPP	P1-O5	8.43	1.86	1.60
5	B	206	LPP	P1-O5	8.42	1.86	1.60
5	H	206	LPP	P1-O5	8.42	1.86	1.60
5	J	206	LPP	P1-O5	8.42	1.86	1.60
5	E	206	LPP	P1-O5	8.42	1.86	1.60
5	F	206	LPP	P1-O5	8.42	1.86	1.60
5	C	206	LPP	P1-O5	8.42	1.86	1.60
4	G	205	L8Z	O22-C1A	7.17	1.37	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	205	L8Z	O22-C1A	7.17	1.37	1.23
4	J	205	L8Z	O22-C1A	7.16	1.37	1.23
4	A	203	L8Z	O2-C1	7.16	1.37	1.23
4	F	205	L8Z	O2-C1	7.16	1.37	1.23
4	C	205	L8Z	O2-C1	7.16	1.37	1.23
4	H	205	L8Z	O22-C1A	7.16	1.37	1.23
4	C	205	L8Z	O22-C1A	7.16	1.37	1.23
4	F	205	L8Z	O22-C1A	7.15	1.37	1.23
4	I	205	L8Z	O22-C1A	7.15	1.37	1.23
4	B	205	L8Z	O22-C1A	7.15	1.37	1.23
4	A	203	L8Z	O22-C1A	7.14	1.37	1.23
4	H	205	L8Z	O2-C1	7.14	1.37	1.23
4	J	205	L8Z	O2-C1	7.14	1.37	1.23
4	E	205	L8Z	O22-C1A	7.13	1.37	1.23
4	K	205	L8Z	O2-C1	7.13	1.37	1.23
4	K	205	L8Z	O22-C1A	7.13	1.37	1.23
4	D	205	L8Z	O2-C1	7.13	1.37	1.23
4	I	205	L8Z	O2-C1	7.12	1.37	1.23
4	E	205	L8Z	O2-C1	7.12	1.37	1.23
4	B	205	L8Z	O2-C1	7.12	1.37	1.23
4	G	205	L8Z	O2-C1	7.10	1.37	1.23
4	J	205	L8Z	C2E-C1G	5.60	1.68	1.54
4	K	205	L8Z	C2E-C1G	5.59	1.68	1.54
4	C	205	L8Z	C2E-C1G	5.59	1.68	1.54
4	G	205	L8Z	C2E-C1G	5.58	1.68	1.54
4	I	205	L8Z	C2E-C1G	5.58	1.68	1.54
4	D	205	L8Z	C2E-C1G	5.58	1.68	1.54
4	B	205	L8Z	C2E-C1G	5.57	1.68	1.54
4	E	205	L8Z	C2E-C1G	5.57	1.68	1.54
4	A	203	L8Z	C2E-C1G	5.57	1.68	1.54
4	H	205	L8Z	C2E-C1G	5.56	1.68	1.54
4	F	205	L8Z	C2E-C1G	5.56	1.68	1.54
4	E	205	L8Z	O1-C1B	5.41	1.38	1.22
4	K	205	L8Z	O1-C1B	5.41	1.38	1.22
4	F	205	L8Z	O1-C1B	5.41	1.38	1.22
4	B	205	L8Z	O1-C1B	5.40	1.38	1.22
4	D	205	L8Z	O1-C1B	5.40	1.38	1.22
4	I	205	L8Z	O1-C1B	5.40	1.38	1.22
4	C	205	L8Z	O1-C1B	5.40	1.38	1.22
4	A	203	L8Z	O1-C1B	5.40	1.38	1.22
4	J	205	L8Z	O1-C1B	5.39	1.38	1.22
4	G	205	L8Z	O1-C1B	5.39	1.38	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	205	L8Z	O1-C1B	5.38	1.38	1.22
4	I	205	L8Z	O21-C15	5.00	1.37	1.22
4	G	205	L8Z	O21-C15	5.00	1.37	1.22
4	K	205	L8Z	O21-C15	4.99	1.37	1.22
4	B	205	L8Z	O23-C1C	4.99	1.37	1.22
4	H	205	L8Z	O21-C15	4.98	1.37	1.22
4	J	205	L8Z	O21-C15	4.97	1.37	1.22
4	K	205	L8Z	O23-C1C	4.97	1.37	1.22
4	C	205	L8Z	O21-C15	4.97	1.37	1.22
4	A	203	L8Z	O21-C15	4.97	1.37	1.22
4	I	205	L8Z	O23-C1C	4.97	1.37	1.22
4	D	205	L8Z	O21-C15	4.97	1.37	1.22
4	E	205	L8Z	O21-C15	4.97	1.37	1.22
4	A	203	L8Z	O23-C1C	4.97	1.37	1.22
4	B	205	L8Z	O21-C15	4.97	1.37	1.22
4	F	205	L8Z	O21-C15	4.97	1.37	1.22
4	C	205	L8Z	O23-C1C	4.96	1.37	1.22
4	G	205	L8Z	O23-C1C	4.96	1.37	1.22
4	E	205	L8Z	O23-C1C	4.96	1.37	1.22
4	H	205	L8Z	O23-C1C	4.95	1.37	1.22
4	D	205	L8Z	O23-C1C	4.95	1.37	1.22
4	J	205	L8Z	O23-C1C	4.95	1.37	1.22
4	F	205	L8Z	O23-C1C	4.94	1.37	1.22
4	F	205	L8Z	C62-C52	4.50	1.57	1.31
4	H	205	L8Z	C62-C52	4.50	1.57	1.31
4	A	203	L8Z	C62-C52	4.50	1.57	1.31
4	K	205	L8Z	C62-C52	4.50	1.57	1.31
4	G	205	L8Z	C62-C52	4.49	1.57	1.31
4	I	205	L8Z	C62-C52	4.49	1.57	1.31
4	B	205	L8Z	C62-C52	4.49	1.57	1.31
4	E	205	L8Z	C62-C52	4.49	1.57	1.31
4	J	205	L8Z	C62-C52	4.49	1.57	1.31
4	D	205	L8Z	C62-C52	4.48	1.57	1.31
4	C	205	L8Z	C62-C52	4.48	1.57	1.31
4	D	205	L8Z	C12-C11	4.40	1.56	1.31
4	H	205	L8Z	C12-C11	4.40	1.56	1.31
4	B	205	L8Z	C12-C11	4.40	1.56	1.31
4	C	205	L8Z	C12-C11	4.39	1.56	1.31
4	E	205	L8Z	C12-C11	4.39	1.56	1.31
4	J	205	L8Z	C12-C11	4.39	1.56	1.31
4	F	205	L8Z	C12-C11	4.38	1.56	1.31
4	K	205	L8Z	C12-C11	4.38	1.56	1.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	205	L8Z	C12-C11	4.38	1.56	1.31
4	A	203	L8Z	C12-C11	4.38	1.56	1.31
4	I	205	L8Z	C12-C11	4.38	1.56	1.31
4	J	205	L8Z	O33-C35	-4.35	1.36	1.46
4	G	205	L8Z	O33-C35	-4.34	1.36	1.46
4	F	205	L8Z	C61-C51	4.34	1.56	1.31
4	C	205	L8Z	O33-C35	-4.34	1.36	1.46
4	J	205	L8Z	C61-C51	4.34	1.56	1.31
4	C	205	L8Z	C61-C51	4.33	1.56	1.31
4	B	205	L8Z	C61-C51	4.33	1.56	1.31
4	H	205	L8Z	C61-C51	4.33	1.56	1.31
4	E	205	L8Z	O33-C35	-4.33	1.36	1.46
4	K	205	L8Z	O33-C35	-4.33	1.36	1.46
4	D	205	L8Z	O33-C35	-4.32	1.36	1.46
4	D	205	L8Z	C61-C51	4.32	1.56	1.31
4	G	205	L8Z	C61-C51	4.32	1.56	1.31
4	E	205	L8Z	C61-C51	4.32	1.56	1.31
4	K	205	L8Z	C61-C51	4.32	1.56	1.31
4	I	205	L8Z	C61-C51	4.32	1.56	1.31
4	A	203	L8Z	C61-C51	4.32	1.56	1.31
4	F	205	L8Z	O33-C35	-4.32	1.36	1.46
4	I	205	L8Z	O33-C35	-4.31	1.36	1.46
4	A	203	L8Z	O33-C35	-4.31	1.36	1.46
4	H	205	L8Z	O33-C35	-4.30	1.36	1.46
4	B	205	L8Z	O33-C35	-4.29	1.36	1.46
5	D	206	LPP	C6-C7	4.25	1.64	1.50
5	I	206	LPP	C6-C7	4.25	1.64	1.50
5	H	206	LPP	C6-C7	4.23	1.64	1.50
5	G	206	LPP	C6-C7	4.23	1.64	1.50
5	J	206	LPP	C6-C7	4.23	1.64	1.50
5	A	204	LPP	C6-C7	4.23	1.64	1.50
5	B	206	LPP	C6-C7	4.22	1.64	1.50
5	C	206	LPP	C6-C7	4.22	1.64	1.50
5	E	206	LPP	C6-C7	4.21	1.64	1.50
5	K	206	LPP	C6-C7	4.21	1.64	1.50
5	F	206	LPP	C6-C7	4.20	1.63	1.50
4	H	205	L8Z	C84-C74	4.19	1.55	1.31
4	G	205	L8Z	C84-C74	4.19	1.55	1.31
4	A	203	L8Z	C84-C74	4.18	1.55	1.31
4	B	205	L8Z	C84-C74	4.18	1.55	1.31
4	J	205	L8Z	C84-C74	4.18	1.55	1.31
4	C	205	L8Z	C84-C74	4.18	1.55	1.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	205	L8Z	C84-C74	4.18	1.55	1.31
4	E	205	L8Z	C84-C74	4.18	1.55	1.31
4	I	205	L8Z	C84-C74	4.18	1.55	1.31
4	K	205	L8Z	C84-C74	4.17	1.55	1.31
4	D	205	L8Z	C84-C74	4.17	1.55	1.31
4	G	205	L8Z	O32-C32	-4.14	1.36	1.46
4	C	205	L8Z	O32-C32	-4.13	1.36	1.46
4	I	205	L8Z	O32-C32	-4.13	1.36	1.46
4	E	205	L8Z	O32-C32	-4.13	1.36	1.46
4	H	205	L8Z	O32-C32	-4.12	1.36	1.46
4	K	205	L8Z	O32-C32	-4.10	1.36	1.46
4	J	205	L8Z	O32-C32	-4.09	1.37	1.46
4	B	205	L8Z	O32-C32	-4.09	1.37	1.46
4	D	205	L8Z	O32-C32	-4.09	1.37	1.46
4	F	205	L8Z	O32-C32	-4.08	1.37	1.46
4	A	203	L8Z	O32-C32	-4.08	1.37	1.46
4	G	205	L8Z	C76-C68	3.72	1.60	1.52
4	I	205	L8Z	C76-C68	3.72	1.60	1.52
4	E	205	L8Z	C76-C68	3.72	1.60	1.52
4	C	205	L8Z	C76-C68	3.71	1.60	1.52
4	H	205	L8Z	C76-C68	3.71	1.60	1.52
4	A	203	L8Z	C76-C68	3.71	1.60	1.52
4	J	205	L8Z	C76-C68	3.70	1.60	1.52
4	B	205	L8Z	C76-C68	3.70	1.60	1.52
4	K	205	L8Z	C76-C68	3.70	1.60	1.52
4	D	205	L8Z	C76-C68	3.68	1.60	1.52
4	F	205	L8Z	C76-C68	3.67	1.60	1.52
4	E	205	L8Z	O7-C76	-3.36	1.36	1.43
4	K	205	L8Z	O1B-C1G	-3.36	1.18	1.30
4	I	205	L8Z	O1B-C1G	-3.34	1.18	1.30
4	D	205	L8Z	O7-C76	-3.34	1.36	1.43
4	C	205	L8Z	O1B-C1G	-3.34	1.18	1.30
4	J	205	L8Z	O1B-C1G	-3.34	1.18	1.30
4	A	203	L8Z	O7-C76	-3.34	1.36	1.43
4	K	205	L8Z	O7-C76	-3.34	1.36	1.43
4	A	203	L8Z	O1B-C1G	-3.34	1.18	1.30
4	E	205	L8Z	O1B-C1G	-3.33	1.18	1.30
4	G	205	L8Z	O7-C76	-3.33	1.36	1.43
4	B	205	L8Z	O1B-C1G	-3.33	1.18	1.30
4	D	205	L8Z	O1B-C1G	-3.33	1.18	1.30
4	B	205	L8Z	O7-C76	-3.33	1.36	1.43
4	H	205	L8Z	O1B-C1G	-3.32	1.18	1.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	205	L8Z	O1B-C1G	-3.32	1.18	1.30
4	J	205	L8Z	O7-C76	-3.32	1.36	1.43
4	I	205	L8Z	O7-C76	-3.32	1.36	1.43
4	F	205	L8Z	O1B-C1G	-3.31	1.18	1.30
4	F	205	L8Z	O7-C76	-3.30	1.36	1.43
4	H	205	L8Z	O7-C76	-3.30	1.36	1.43
4	C	205	L8Z	O7-C76	-3.29	1.36	1.43
4	G	205	L8Z	O51-C1F	3.25	1.50	1.41
4	J	205	L8Z	O51-C1F	3.24	1.50	1.41
4	B	205	L8Z	O51-C1F	3.23	1.50	1.41
4	E	205	L8Z	O51-C1F	3.22	1.50	1.41
4	I	205	L8Z	O51-C1F	3.22	1.50	1.41
4	H	205	L8Z	O51-C1F	3.22	1.50	1.41
4	C	205	L8Z	O51-C1F	3.22	1.50	1.41
4	A	203	L8Z	O51-C1F	3.21	1.50	1.41
4	F	205	L8Z	O51-C1F	3.21	1.50	1.41
4	K	205	L8Z	O51-C1F	3.20	1.50	1.41
4	D	205	L8Z	O51-C1F	3.20	1.50	1.41
5	A	204	LPP	O5-C6	-3.11	1.32	1.44
5	I	206	LPP	O5-C6	-3.10	1.32	1.44
5	C	206	LPP	O5-C6	-3.09	1.32	1.44
5	E	206	LPP	O5-C6	-3.08	1.32	1.44
5	G	206	LPP	O5-C6	-3.08	1.32	1.44
5	D	206	LPP	O5-C6	-3.08	1.32	1.44
5	F	206	LPP	O5-C6	-3.08	1.32	1.44
5	B	206	LPP	O5-C6	-3.08	1.32	1.44
5	H	206	LPP	O5-C6	-3.08	1.32	1.44
5	J	206	LPP	O5-C6	-3.08	1.32	1.44
5	K	206	LPP	O5-C6	-3.08	1.32	1.44
4	I	205	L8Z	C2D-N21	2.95	1.50	1.45
4	D	205	L8Z	C2D-N21	2.94	1.50	1.45
4	B	205	L8Z	C2D-N21	2.93	1.50	1.45
4	E	205	L8Z	C2D-N21	2.93	1.50	1.45
4	F	205	L8Z	C2D-N21	2.92	1.50	1.45
4	A	203	L8Z	C2D-N21	2.91	1.50	1.45
4	K	205	L8Z	C2D-N21	2.90	1.50	1.45
4	C	205	L8Z	C2D-N21	2.89	1.50	1.45
4	J	205	L8Z	C2D-N21	2.89	1.50	1.45
4	G	205	L8Z	C2D-N21	2.87	1.50	1.45
4	H	205	L8Z	C2D-N21	2.87	1.50	1.45
4	G	205	L8Z	C3C-C2D	-2.64	1.48	1.53
4	K	205	L8Z	C3C-C2D	-2.63	1.48	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	205	L8Z	C3C-C2D	-2.61	1.48	1.53
4	D	205	L8Z	C3C-C2D	-2.61	1.48	1.53
4	E	205	L8Z	C3C-C2D	-2.60	1.48	1.53
4	A	203	L8Z	C3C-C2D	-2.60	1.48	1.53
4	B	205	L8Z	C3C-C2D	-2.60	1.48	1.53
4	H	205	L8Z	O61-C2E	2.59	1.44	1.40
4	I	205	L8Z	C3C-C2D	-2.58	1.48	1.53
4	I	205	L8Z	O61-C2E	2.58	1.44	1.40
4	J	205	L8Z	C3C-C2D	-2.58	1.49	1.53
4	F	205	L8Z	C3C-C2D	-2.57	1.49	1.53
4	C	205	L8Z	O61-C2E	2.56	1.44	1.40
4	C	205	L8Z	C3C-C2D	-2.56	1.49	1.53
4	F	205	L8Z	O61-C2E	2.55	1.44	1.40
4	D	205	L8Z	C86-C76	2.55	1.58	1.52
4	B	205	L8Z	O61-C2E	2.54	1.44	1.40
4	A	203	L8Z	C86-C76	2.52	1.58	1.52
4	B	205	L8Z	C86-C76	2.52	1.58	1.52
4	H	205	L8Z	C86-C76	2.52	1.58	1.52
4	K	205	L8Z	C86-C76	2.52	1.58	1.52
4	G	205	L8Z	O61-C2E	2.51	1.44	1.40
4	E	205	L8Z	C86-C76	2.51	1.58	1.52
4	C	205	L8Z	C86-C76	2.51	1.58	1.52
4	J	205	L8Z	C86-C76	2.51	1.58	1.52
4	D	205	L8Z	O61-C2E	2.51	1.44	1.40
4	J	205	L8Z	O61-C2E	2.51	1.44	1.40
4	F	205	L8Z	C86-C76	2.50	1.58	1.52
4	E	205	L8Z	O61-C2E	2.50	1.44	1.40
4	K	205	L8Z	O61-C2E	2.50	1.44	1.40
4	I	205	L8Z	C86-C76	2.50	1.58	1.52
4	G	205	L8Z	C86-C76	2.49	1.58	1.52
4	A	203	L8Z	O61-C2E	2.49	1.44	1.40
4	B	205	L8Z	C42-C52	2.29	1.56	1.50
4	K	205	L8Z	C42-C52	2.28	1.56	1.50
4	J	205	L8Z	C42-C52	2.27	1.56	1.50
4	C	205	L8Z	C42-C52	2.27	1.56	1.50
4	D	205	L8Z	C42-C52	2.27	1.56	1.50
4	A	203	L8Z	C42-C52	2.27	1.56	1.50
4	H	205	L8Z	C42-C52	2.27	1.56	1.50
4	G	205	L8Z	C42-C52	2.26	1.56	1.50
4	F	205	L8Z	C42-C52	2.26	1.56	1.50
4	E	205	L8Z	C42-C52	2.25	1.56	1.50
4	I	205	L8Z	C42-C52	2.25	1.56	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	205	L8Z	O31-C31	-2.19	1.37	1.43
4	G	205	L8Z	O31-C31	-2.17	1.37	1.43
4	K	205	L8Z	O31-C31	-2.17	1.37	1.43
4	J	205	L8Z	O31-C31	-2.17	1.37	1.43
4	B	205	L8Z	O31-C31	-2.16	1.37	1.43
4	E	205	L8Z	O31-C31	-2.16	1.37	1.43
4	C	205	L8Z	O31-C31	-2.16	1.37	1.43
4	G	205	L8Z	O3-C3	-2.16	1.37	1.43
4	F	205	L8Z	C58-C68	2.15	1.58	1.52
4	H	205	L8Z	O31-C31	-2.15	1.37	1.43
4	J	205	L8Z	O3-C3	-2.15	1.37	1.43
4	F	205	L8Z	O31-C31	-2.15	1.37	1.43
4	I	205	L8Z	C58-C68	2.15	1.58	1.52
4	B	205	L8Z	O3-C3	-2.15	1.37	1.43
4	F	205	L8Z	O3-C3	-2.15	1.37	1.43
4	A	203	L8Z	O31-C31	-2.15	1.37	1.43
4	D	205	L8Z	O31-C31	-2.15	1.37	1.43
4	A	203	L8Z	O3-C3	-2.15	1.37	1.43
4	K	205	L8Z	C58-C68	2.15	1.58	1.52
4	C	205	L8Z	O3-C3	-2.14	1.37	1.43
4	E	205	L8Z	O3-C3	-2.14	1.37	1.43
4	K	205	L8Z	O3-C3	-2.14	1.37	1.43
4	D	205	L8Z	O3-C3	-2.13	1.37	1.43
4	H	205	L8Z	O3-C3	-2.12	1.37	1.43
4	B	205	L8Z	C58-C68	2.12	1.58	1.52
4	I	205	L8Z	O3-C3	-2.12	1.37	1.43
4	A	203	L8Z	C58-C68	2.12	1.58	1.52
4	E	205	L8Z	C58-C68	2.12	1.58	1.52
4	C	205	L8Z	C58-C68	2.11	1.58	1.52
4	G	205	L8Z	C58-C68	2.11	1.58	1.52
4	D	205	L8Z	C58-C68	2.11	1.58	1.52
4	J	205	L8Z	C58-C68	2.11	1.58	1.52
4	H	205	L8Z	C58-C68	2.10	1.58	1.52
4	D	205	L8Z	O33-C1D	2.09	1.40	1.34
4	H	205	L8Z	O37-C1C	2.08	1.40	1.34
4	A	203	L8Z	O33-C1D	2.08	1.40	1.34
4	G	205	L8Z	O33-C1D	2.08	1.40	1.34
4	J	205	L8Z	O37-C1C	2.08	1.40	1.34
4	E	205	L8Z	O33-C1D	2.08	1.40	1.34
4	H	205	L8Z	O33-C1D	2.08	1.40	1.34
4	A	203	L8Z	O32-C1B	2.08	1.40	1.34
4	C	205	L8Z	O33-C1D	2.07	1.40	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	205	L8Z	O37-C1C	2.07	1.40	1.34
4	G	205	L8Z	O32-C1B	2.07	1.40	1.34
4	J	205	L8Z	O33-C1D	2.07	1.40	1.34
4	F	205	L8Z	O32-C1B	2.07	1.40	1.34
4	F	205	L8Z	O33-C1D	2.07	1.40	1.34
4	B	205	L8Z	O33-C1D	2.07	1.40	1.34
4	H	205	L8Z	O32-C1B	2.07	1.40	1.34
4	I	205	L8Z	O37-C1C	2.06	1.40	1.34
4	B	205	L8Z	O32-C1B	2.06	1.40	1.34
4	B	205	L8Z	O37-C1C	2.06	1.40	1.34
4	C	205	L8Z	O37-C1C	2.06	1.40	1.34
4	E	205	L8Z	O37-C1C	2.06	1.40	1.34
4	E	205	L8Z	O32-C1B	2.05	1.40	1.34
4	K	205	L8Z	O33-C1D	2.05	1.40	1.34
4	A	203	L8Z	O37-C1C	2.05	1.40	1.34
4	I	205	L8Z	O33-C1D	2.04	1.40	1.34
4	K	205	L8Z	O32-C1B	2.04	1.40	1.34
4	F	205	L8Z	O37-C1C	2.04	1.40	1.34
4	K	205	L8Z	O37-C1C	2.04	1.40	1.34
4	C	205	L8Z	O32-C1B	2.04	1.40	1.34
4	I	205	L8Z	O32-C1B	2.04	1.40	1.34
4	D	205	L8Z	O32-C1B	2.04	1.40	1.34
4	J	205	L8Z	O32-C1B	2.03	1.40	1.34
4	G	205	L8Z	O37-C1C	2.03	1.40	1.34

All (407) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	205	L8Z	C22-C1A-N21	7.19	126.07	116.25
4	J	205	L8Z	C22-C1A-N21	7.18	126.06	116.25
4	H	205	L8Z	C22-C1A-N21	7.18	126.06	116.25
4	A	203	L8Z	C22-C1A-N21	7.18	126.05	116.25
4	C	205	L8Z	C22-C1A-N21	7.17	126.05	116.25
4	D	205	L8Z	C22-C1A-N21	7.17	126.04	116.25
4	E	205	L8Z	C22-C1A-N21	7.16	126.04	116.25
4	I	205	L8Z	C22-C1A-N21	7.16	126.03	116.25
4	K	205	L8Z	C22-C1A-N21	7.16	126.02	116.25
4	F	205	L8Z	C22-C1A-N21	7.15	126.02	116.25
4	B	205	L8Z	C22-C1A-N21	7.15	126.01	116.25
4	A	203	L8Z	O22-C1A-C22	-6.51	112.02	121.54
4	H	205	L8Z	O22-C1A-C22	-6.50	112.03	121.54
4	B	205	L8Z	O22-C1A-C22	-6.50	112.03	121.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	205	L8Z	O22-C1A-C22	-6.50	112.04	121.54
4	D	205	L8Z	O22-C1A-C22	-6.50	112.04	121.54
4	F	205	L8Z	O22-C1A-C22	-6.49	112.05	121.54
4	G	205	L8Z	O22-C1A-C22	-6.49	112.05	121.54
4	I	205	L8Z	O22-C1A-C22	-6.48	112.06	121.54
4	C	205	L8Z	O22-C1A-C22	-6.48	112.06	121.54
4	K	205	L8Z	O22-C1A-C22	-6.47	112.08	121.54
4	E	205	L8Z	O22-C1A-C22	-6.45	112.11	121.54
4	I	205	L8Z	O2-C1-C2	-6.45	112.11	121.54
4	E	205	L8Z	O2-C1-C2	-6.44	112.11	121.54
4	D	205	L8Z	O2-C1-C2	-6.44	112.11	121.54
4	J	205	L8Z	O2-C1-C2	-6.44	112.13	121.54
4	G	205	L8Z	O37-C1C-C2A	6.43	122.96	111.43
4	B	205	L8Z	O37-C1C-C2A	6.43	122.95	111.43
4	K	205	L8Z	O37-C1C-C2A	6.43	122.95	111.43
4	A	203	L8Z	O37-C1C-C2A	6.43	122.95	111.43
4	C	205	L8Z	C2-C1-N2	6.43	125.03	116.25
4	E	205	L8Z	O37-C1C-C2A	6.42	122.94	111.43
4	I	205	L8Z	C2-C1-N2	6.42	125.02	116.25
4	C	205	L8Z	O2-C1-C2	-6.42	112.15	121.54
4	C	205	L8Z	O37-C1C-C2A	6.42	122.93	111.43
4	D	205	L8Z	O37-C1C-C2A	6.42	122.93	111.43
4	I	205	L8Z	O37-C1C-C2A	6.41	122.92	111.43
4	E	205	L8Z	C2-C1-N2	6.41	125.01	116.25
4	H	205	L8Z	O37-C1C-C2A	6.41	122.92	111.43
4	K	205	L8Z	O2-C1-C2	-6.41	112.17	121.54
4	J	205	L8Z	O37-C1C-C2A	6.41	122.91	111.43
4	H	205	L8Z	O2-C1-C2	-6.41	112.17	121.54
4	F	205	L8Z	C2-C1-N2	6.40	125.00	116.25
4	D	205	L8Z	C2-C1-N2	6.40	125.00	116.25
4	J	205	L8Z	C2-C1-N2	6.40	124.99	116.25
4	B	205	L8Z	O2-C1-C2	-6.40	112.18	121.54
4	F	205	L8Z	O2-C1-C2	-6.39	112.19	121.54
4	A	203	L8Z	O2-C1-C2	-6.39	112.19	121.54
4	G	205	L8Z	O2-C1-C2	-6.39	112.19	121.54
4	F	205	L8Z	O37-C1C-C2A	6.39	122.88	111.43
4	B	205	L8Z	C2-C1-N2	6.38	124.97	116.25
4	G	205	L8Z	C2-C1-N2	6.38	124.97	116.25
4	A	203	L8Z	C2-C1-N2	6.38	124.96	116.25
4	H	205	L8Z	C2-C1-N2	6.37	124.95	116.25
4	K	205	L8Z	C2-C1-N2	6.37	124.95	116.25
4	C	205	L8Z	O32-C1B-C28	6.34	125.19	111.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	205	L8Z	O32-C1B-C28	6.33	125.18	111.48
4	D	205	L8Z	O32-C1B-C28	6.33	125.17	111.48
4	J	205	L8Z	O32-C1B-C28	6.32	125.16	111.48
4	E	205	L8Z	O32-C1B-C28	6.32	125.15	111.48
4	K	205	L8Z	O32-C1B-C28	6.31	125.14	111.48
4	F	205	L8Z	O32-C1B-C28	6.31	125.13	111.48
4	H	205	L8Z	O32-C1B-C28	6.31	125.12	111.48
4	G	205	L8Z	O32-C1B-C28	6.30	125.12	111.48
4	A	203	L8Z	O32-C1B-C28	6.30	125.11	111.48
4	B	205	L8Z	O32-C1B-C28	6.30	125.11	111.48
4	J	205	L8Z	O36-C15-C21	6.19	122.53	111.43
4	K	205	L8Z	O36-C15-C21	6.19	122.53	111.43
4	D	205	L8Z	O36-C15-C21	6.19	122.52	111.43
4	G	205	L8Z	O36-C15-C21	6.18	122.51	111.43
4	H	205	L8Z	O36-C15-C21	6.18	122.51	111.43
4	E	205	L8Z	O36-C15-C21	6.18	122.50	111.43
4	B	205	L8Z	O36-C15-C21	6.17	122.49	111.43
4	A	203	L8Z	O36-C15-C21	6.17	122.49	111.43
4	I	205	L8Z	O36-C15-C21	6.17	122.49	111.43
4	C	205	L8Z	O36-C15-C21	6.17	122.49	111.43
4	F	205	L8Z	O36-C15-C21	6.15	122.46	111.43
4	H	205	L8Z	C1E-O5-C56	5.96	125.36	113.72
4	E	205	L8Z	C1E-O5-C56	5.95	125.33	113.72
4	K	205	L8Z	C1E-O5-C56	5.94	125.31	113.72
4	J	205	L8Z	C1E-O5-C56	5.93	125.30	113.72
4	G	205	L8Z	C1E-O5-C56	5.93	125.30	113.72
4	F	205	L8Z	C1E-O5-C56	5.93	125.30	113.72
4	D	205	L8Z	C1E-O5-C56	5.93	125.29	113.72
4	I	205	L8Z	C1E-O5-C56	5.92	125.29	113.72
4	A	203	L8Z	C1E-O5-C56	5.92	125.28	113.72
4	B	205	L8Z	C1E-O5-C56	5.92	125.27	113.72
4	C	205	L8Z	C1E-O5-C56	5.91	125.26	113.72
4	I	205	L8Z	P-O14-C1E	-5.86	107.83	123.54
4	H	205	L8Z	P-O14-C1E	-5.85	107.84	123.54
4	J	205	L8Z	P-O14-C1E	-5.85	107.84	123.54
4	G	205	L8Z	P-O14-C1E	-5.85	107.84	123.54
4	E	205	L8Z	P-O14-C1E	-5.85	107.85	123.54
4	F	205	L8Z	P-O14-C1E	-5.85	107.85	123.54
4	D	205	L8Z	P-O14-C1E	-5.85	107.86	123.54
4	K	205	L8Z	P-O14-C1E	-5.84	107.87	123.54
4	A	203	L8Z	P-O14-C1E	-5.84	107.87	123.54
4	C	205	L8Z	P-O14-C1E	-5.84	107.87	123.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	205	L8Z	P-O14-C1E	-5.84	107.89	123.54
4	G	205	L8Z	O21-C15-C21	-5.19	112.59	124.65
4	I	205	L8Z	O21-C15-C21	-5.19	112.60	124.65
4	B	205	L8Z	O21-C15-C21	-5.18	112.61	124.65
4	F	205	L8Z	O21-C15-C21	-5.18	112.61	124.65
4	D	205	L8Z	O21-C15-C21	-5.18	112.61	124.65
4	J	205	L8Z	O21-C15-C21	-5.18	112.61	124.65
4	E	205	L8Z	O21-C15-C21	-5.18	112.62	124.65
4	C	205	L8Z	O21-C15-C21	-5.18	112.62	124.65
4	K	205	L8Z	O21-C15-C21	-5.18	112.62	124.65
4	A	203	L8Z	O21-C15-C21	-5.18	112.62	124.65
4	H	205	L8Z	O21-C15-C21	-5.17	112.63	124.65
4	K	205	L8Z	O23-C1C-C2A	-4.93	113.19	124.65
4	F	205	L8Z	O23-C1C-C2A	-4.93	113.20	124.65
4	G	205	L8Z	O23-C1C-C2A	-4.93	113.20	124.65
4	A	203	L8Z	O23-C1C-C2A	-4.93	113.20	124.65
4	B	205	L8Z	P1-O41-C4B	-4.93	110.28	123.43
4	D	205	L8Z	P1-O41-C4B	-4.92	110.29	123.43
4	C	205	L8Z	O23-C1C-C2A	-4.92	113.22	124.65
4	I	205	L8Z	O23-C1C-C2A	-4.92	113.22	124.65
4	E	205	L8Z	O23-C1C-C2A	-4.92	113.22	124.65
4	E	205	L8Z	P1-O41-C4B	-4.92	110.30	123.43
4	B	205	L8Z	O23-C1C-C2A	-4.92	113.23	124.65
4	D	205	L8Z	O23-C1C-C2A	-4.91	113.24	124.65
4	G	205	L8Z	P1-O41-C4B	-4.91	110.32	123.43
4	I	205	L8Z	P1-O41-C4B	-4.91	110.32	123.43
4	H	205	L8Z	O23-C1C-C2A	-4.91	113.25	124.65
4	F	205	L8Z	P1-O41-C4B	-4.91	110.32	123.43
4	K	205	L8Z	P1-O41-C4B	-4.91	110.33	123.43
4	C	205	L8Z	P1-O41-C4B	-4.91	110.33	123.43
4	J	205	L8Z	O23-C1C-C2A	-4.90	113.26	124.65
4	H	205	L8Z	P1-O41-C4B	-4.90	110.35	123.43
4	J	205	L8Z	P1-O41-C4B	-4.90	110.35	123.43
4	A	203	L8Z	P1-O41-C4B	-4.89	110.38	123.43
4	H	205	L8Z	C3B-O36-C15	4.83	125.44	117.59
4	D	205	L8Z	C3B-O36-C15	4.83	125.44	117.59
4	J	205	L8Z	C3B-O36-C15	4.82	125.43	117.59
4	E	205	L8Z	C3B-O36-C15	4.81	125.41	117.59
4	G	205	L8Z	C3B-O36-C15	4.80	125.39	117.59
4	K	205	L8Z	C3B-O36-C15	4.80	125.39	117.59
4	A	203	L8Z	C3B-O36-C15	4.79	125.38	117.59
4	B	205	L8Z	C3B-O36-C15	4.79	125.37	117.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	205	L8Z	C3B-O36-C15	4.78	125.37	117.59
4	C	205	L8Z	C3B-O36-C15	4.78	125.37	117.59
4	F	205	L8Z	C3B-O36-C15	4.77	125.34	117.59
4	G	205	L8Z	O5-C1E-O14	-4.29	105.75	111.36
4	I	205	L8Z	O5-C1E-O14	-4.29	105.76	111.36
4	H	205	L8Z	O5-C1E-O14	-4.28	105.76	111.36
4	E	205	L8Z	O5-C1E-O14	-4.28	105.77	111.36
4	F	205	L8Z	O5-C1E-O14	-4.28	105.77	111.36
4	A	203	L8Z	O5-C1E-O14	-4.28	105.78	111.36
4	J	205	L8Z	O5-C1E-O14	-4.27	105.78	111.36
4	D	205	L8Z	O5-C1E-O14	-4.27	105.78	111.36
4	K	205	L8Z	O5-C1E-O14	-4.27	105.78	111.36
4	B	205	L8Z	O5-C1E-O14	-4.23	105.83	111.36
4	K	205	L8Z	O1A-C1G-C2E	-4.23	111.05	123.79
4	C	205	L8Z	O5-C1E-O14	-4.22	105.84	111.36
4	G	205	L8Z	O1A-C1G-C2E	-4.22	111.08	123.79
4	D	205	L8Z	O1A-C1G-C2E	-4.22	111.08	123.79
4	B	205	L8Z	O1A-C1G-C2E	-4.21	111.08	123.79
4	E	205	L8Z	O1A-C1G-C2E	-4.21	111.09	123.79
4	J	205	L8Z	O1A-C1G-C2E	-4.21	111.09	123.79
4	C	205	L8Z	O1A-C1G-C2E	-4.21	111.09	123.79
4	I	205	L8Z	O1A-C1G-C2E	-4.21	111.10	123.79
4	A	203	L8Z	O1A-C1G-C2E	-4.21	111.11	123.79
4	H	205	L8Z	O1A-C1G-C2E	-4.21	111.11	123.79
4	F	205	L8Z	O1A-C1G-C2E	-4.19	111.16	123.79
4	D	205	L8Z	O4-C4A-C3B	-4.02	99.62	109.94
4	H	205	L8Z	O4-C4A-C3B	-4.02	99.64	109.94
4	J	205	L8Z	O4-C4A-C3B	-4.00	99.67	109.94
4	F	205	L8Z	O4-C4A-C3B	-4.00	99.67	109.94
4	E	205	L8Z	O4-C4A-C3B	-4.00	99.68	109.94
4	K	205	L8Z	O4-C4A-C3B	-4.00	99.69	109.94
4	B	205	L8Z	O4-C4A-C3B	-4.00	99.70	109.94
4	C	205	L8Z	O4-C4A-C3B	-3.99	99.70	109.94
4	G	205	L8Z	O4-C4A-C3B	-3.99	99.72	109.94
4	I	205	L8Z	O4-C4A-C3B	-3.99	99.72	109.94
4	A	203	L8Z	O4-C4A-C3B	-3.98	99.72	109.94
4	G	205	L8Z	O33-C1D-C2B	3.88	119.88	111.48
4	K	205	L8Z	O33-C1D-C2B	3.87	119.86	111.48
4	I	205	L8Z	O33-C1D-C2B	3.87	119.86	111.48
4	F	205	L8Z	O33-C1D-C2B	3.86	119.83	111.48
4	A	203	L8Z	O33-C1D-C2B	3.86	119.83	111.48
4	E	205	L8Z	O33-C1D-C2B	3.86	119.83	111.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	205	L8Z	O33-C1D-C2B	3.85	119.82	111.48
4	D	205	L8Z	O33-C1D-C2B	3.85	119.81	111.48
4	H	205	L8Z	O33-C1D-C2B	3.85	119.80	111.48
4	J	205	L8Z	O33-C1D-C2B	3.85	119.80	111.48
4	B	205	L8Z	O33-C1D-C2B	3.84	119.78	111.48
4	F	205	L8Z	C2D-N21-C1A	-3.72	117.42	122.90
4	D	205	L8Z	C2D-N21-C1A	-3.70	117.45	122.90
4	A	203	L8Z	C2D-N21-C1A	-3.69	117.47	122.90
4	B	205	L8Z	C2D-N21-C1A	-3.68	117.47	122.90
4	I	205	L8Z	C2D-N21-C1A	-3.67	117.49	122.90
4	C	205	L8Z	C2D-N21-C1A	-3.67	117.49	122.90
4	J	205	L8Z	C2D-N21-C1A	-3.67	117.50	122.90
4	H	205	L8Z	C2D-N21-C1A	-3.66	117.50	122.90
4	K	205	L8Z	C2D-N21-C1A	-3.66	117.50	122.90
4	E	205	L8Z	C2D-N21-C1A	-3.66	117.51	122.90
4	G	205	L8Z	C2D-N21-C1A	-3.64	117.53	122.90
4	H	205	L8Z	O61-C2E-O62	-3.60	100.04	109.97
4	E	205	L8Z	O61-C2E-O62	-3.60	100.04	109.97
4	F	205	L8Z	O61-C2E-O62	-3.59	100.06	109.97
4	G	205	L8Z	O61-C2E-O62	-3.59	100.06	109.97
4	I	205	L8Z	O61-C2E-O62	-3.59	100.06	109.97
4	A	203	L8Z	O61-C2E-O62	-3.59	100.07	109.97
4	B	205	L8Z	O61-C2E-O62	-3.59	100.07	109.97
4	C	205	L8Z	O61-C2E-O62	-3.59	100.08	109.97
4	D	205	L8Z	O61-C2E-O62	-3.59	100.08	109.97
4	K	205	L8Z	O61-C2E-O62	-3.58	100.08	109.97
4	J	205	L8Z	O61-C2E-O62	-3.58	100.08	109.97
4	C	205	L8Z	O1-C1B-C28	-3.46	110.25	123.78
4	E	205	L8Z	O1-C1B-C28	-3.45	110.27	123.78
4	J	205	L8Z	O1-C1B-C28	-3.45	110.28	123.78
4	I	205	L8Z	O1-C1B-C28	-3.45	110.28	123.78
4	D	205	L8Z	O1-C1B-C28	-3.45	110.30	123.78
4	K	205	L8Z	O1-C1B-C28	-3.45	110.30	123.78
4	G	205	L8Z	O1-C1B-C28	-3.45	110.31	123.78
4	H	205	L8Z	O1-C1B-C28	-3.44	110.31	123.78
4	F	205	L8Z	O1-C1B-C28	-3.44	110.32	123.78
4	B	205	L8Z	O1-C1B-C28	-3.44	110.32	123.78
4	A	203	L8Z	O1-C1B-C28	-3.44	110.34	123.78
4	B	205	L8Z	C2C-N2-C1	-3.36	117.95	122.90
4	K	205	L8Z	C2C-N2-C1	-3.35	117.96	122.90
4	J	205	L8Z	C2C-N2-C1	-3.35	117.97	122.90
4	H	205	L8Z	C2C-N2-C1	-3.35	117.97	122.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	205	L8Z	C2C-N2-C1	-3.34	117.97	122.90
4	A	203	L8Z	C2C-N2-C1	-3.34	117.98	122.90
4	G	205	L8Z	C2C-N2-C1	-3.34	117.98	122.90
4	E	205	L8Z	C2C-N2-C1	-3.33	117.99	122.90
4	I	205	L8Z	C2C-N2-C1	-3.33	118.00	122.90
4	C	205	L8Z	C2C-N2-C1	-3.32	118.00	122.90
4	F	205	L8Z	C2C-N2-C1	-3.32	118.01	122.90
5	C	206	LPP	C7-O9-C11	3.08	125.16	117.80
5	A	204	LPP	C7-O9-C11	3.07	125.15	117.80
5	I	206	LPP	C7-O9-C11	3.07	125.15	117.80
5	D	206	LPP	C7-O9-C11	3.07	125.15	117.80
5	B	206	LPP	C7-O9-C11	3.07	125.15	117.80
5	E	206	LPP	C7-O9-C11	3.06	125.11	117.80
5	K	206	LPP	C7-O9-C11	3.06	125.11	117.80
5	F	206	LPP	C7-O9-C11	3.05	125.10	117.80
5	G	206	LPP	C7-O9-C11	3.05	125.09	117.80
5	J	206	LPP	C7-O9-C11	3.05	125.09	117.80
5	H	206	LPP	C7-O9-C11	3.05	125.09	117.80
4	A	203	L8Z	O37-C3C-C4B	2.90	114.02	108.25
4	C	205	L8Z	O37-C3C-C4B	2.90	114.02	108.25
4	B	205	L8Z	O37-C3C-C4B	2.89	114.01	108.25
4	E	205	L8Z	O37-C3C-C4B	2.89	114.00	108.25
4	I	205	L8Z	O37-C3C-C4B	2.88	113.99	108.25
4	J	205	L8Z	O37-C3C-C4B	2.88	113.99	108.25
4	G	205	L8Z	O37-C3C-C4B	2.87	113.97	108.25
4	H	205	L8Z	O37-C3C-C4B	2.87	113.97	108.25
4	G	205	L8Z	C3C-O37-C1C	2.87	122.25	117.59
4	F	205	L8Z	O37-C3C-C4B	2.86	113.94	108.25
4	K	205	L8Z	O37-C3C-C4B	2.86	113.94	108.25
4	D	205	L8Z	O37-C3C-C4B	2.86	113.94	108.25
4	A	203	L8Z	C3C-O37-C1C	2.85	122.22	117.59
4	K	205	L8Z	C3C-O37-C1C	2.84	122.22	117.59
4	E	205	L8Z	C3C-O37-C1C	2.84	122.22	117.59
4	B	205	L8Z	C3C-O37-C1C	2.84	122.21	117.59
4	D	205	L8Z	C3C-O37-C1C	2.84	122.21	117.59
4	A	203	L8Z	C41-C51-C61	-2.84	115.78	126.21
4	H	205	L8Z	C41-C51-C61	-2.83	115.79	126.21
4	B	205	L8Z	C41-C51-C61	-2.83	115.79	126.21
4	F	205	L8Z	C41-C51-C61	-2.83	115.80	126.21
4	I	205	L8Z	C3C-O37-C1C	2.83	122.19	117.59
4	C	205	L8Z	C3C-O37-C1C	2.83	122.19	117.59
4	D	205	L8Z	C41-C51-C61	-2.83	115.81	126.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	205	L8Z	C41-C51-C61	-2.83	115.81	126.21
4	I	205	L8Z	C41-C51-C61	-2.82	115.83	126.21
4	E	205	L8Z	C41-C51-C61	-2.82	115.83	126.21
4	J	205	L8Z	C41-C51-C61	-2.82	115.84	126.21
4	G	205	L8Z	C41-C51-C61	-2.82	115.84	126.21
4	F	205	L8Z	C3C-O37-C1C	2.82	122.17	117.59
4	H	205	L8Z	C3C-O37-C1C	2.82	122.17	117.59
4	J	205	L8Z	C3C-O37-C1C	2.82	122.17	117.59
4	C	205	L8Z	C41-C51-C61	-2.81	115.86	126.21
4	B	205	L8Z	C1E-C2C-C3B	-2.71	105.01	109.92
4	F	205	L8Z	C1E-C2C-C3B	-2.71	105.02	109.92
4	E	205	L8Z	C1E-C2C-C3B	-2.69	105.04	109.92
4	D	205	L8Z	C1E-C2C-C3B	-2.69	105.05	109.92
4	A	203	L8Z	C1E-C2C-C3B	-2.69	105.05	109.92
4	C	205	L8Z	C1E-C2C-C3B	-2.69	105.05	109.92
4	J	205	L8Z	C1E-C2C-C3B	-2.68	105.06	109.92
4	K	205	L8Z	C1E-C2C-C3B	-2.68	105.06	109.92
4	G	205	L8Z	C1E-C2C-C3B	-2.68	105.07	109.92
4	I	205	L8Z	C1E-C2C-C3B	-2.68	105.07	109.92
4	H	205	L8Z	C1E-C2C-C3B	-2.66	105.10	109.92
4	I	205	L8Z	O36-C3B-C2C	2.59	112.69	107.92
4	C	205	L8Z	O36-C3B-C2C	2.58	112.69	107.92
4	H	205	L8Z	O36-C3B-C2C	2.58	112.68	107.92
4	A	203	L8Z	O36-C3B-C2C	2.58	112.68	107.92
4	K	205	L8Z	O36-C3B-C2C	2.58	112.68	107.92
4	F	205	L8Z	O36-C3B-C2C	2.57	112.67	107.92
4	G	205	L8Z	O36-C3B-C2C	2.57	112.67	107.92
4	D	205	L8Z	O36-C3B-C2C	2.56	112.65	107.92
4	J	205	L8Z	O36-C3B-C2C	2.56	112.65	107.92
5	A	204	LPP	O2-P1-O5	-2.56	100.00	106.67
4	B	205	L8Z	O36-C3B-C2C	2.56	112.64	107.92
5	G	206	LPP	O2-P1-O5	-2.55	100.01	106.67
4	E	205	L8Z	O36-C3B-C2C	2.55	112.63	107.92
5	C	206	LPP	O2-P1-O5	-2.55	100.02	106.67
5	B	206	LPP	O2-P1-O5	-2.55	100.02	106.67
5	I	206	LPP	O2-P1-O5	-2.55	100.03	106.67
5	K	206	LPP	O2-P1-O5	-2.55	100.03	106.67
5	H	206	LPP	O2-P1-O5	-2.54	100.04	106.67
5	D	206	LPP	O2-P1-O5	-2.54	100.05	106.67
5	E	206	LPP	O2-P1-O5	-2.54	100.05	106.67
5	J	206	LPP	O2-P1-O5	-2.54	100.05	106.67
5	F	206	LPP	O2-P1-O5	-2.53	100.06	106.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	205	L8Z	O14-C1E-C2C	2.53	112.97	108.40
4	A	203	L8Z	O14-C1E-C2C	2.51	112.94	108.40
4	K	205	L8Z	O14-C1E-C2C	2.51	112.94	108.40
4	I	205	L8Z	O14-C1E-C2C	2.51	112.94	108.40
4	E	205	L8Z	O14-C1E-C2C	2.51	112.94	108.40
4	G	205	L8Z	O14-C1E-C2C	2.50	112.93	108.40
4	C	205	L8Z	O14-C1E-C2C	2.50	112.93	108.40
4	D	205	L8Z	O14-C1E-C2C	2.50	112.92	108.40
4	H	205	L8Z	O14-C1E-C2C	2.50	112.92	108.40
4	J	205	L8Z	O14-C1E-C2C	2.49	112.91	108.40
4	B	205	L8Z	O14-C1E-C2C	2.49	112.90	108.40
4	K	205	L8Z	O61-C2E-C1G	2.44	116.05	109.86
4	E	205	L8Z	O61-C2E-C1G	2.44	116.05	109.86
4	A	203	L8Z	O61-C2E-C1G	2.43	116.04	109.86
4	G	205	L8Z	O61-C2E-C1G	2.43	116.04	109.86
4	C	205	L8Z	O61-C2E-C1G	2.43	116.02	109.86
4	D	205	L8Z	O61-C2E-C1G	2.43	116.02	109.86
4	J	205	L8Z	O61-C2E-C1G	2.42	116.02	109.86
4	H	205	L8Z	O61-C2E-C1G	2.42	116.01	109.86
4	I	205	L8Z	O61-C2E-C1G	2.42	116.00	109.86
4	F	205	L8Z	O61-C2E-C1G	2.42	115.99	109.86
4	B	205	L8Z	O61-C2E-C1G	2.41	115.99	109.86
4	A	203	L8Z	C42-C52-C62	-2.41	117.34	126.21
4	H	205	L8Z	C42-C52-C62	-2.41	117.34	126.21
4	G	205	L8Z	C42-C52-C62	-2.41	117.36	126.21
4	I	205	L8Z	C42-C52-C62	-2.41	117.36	126.21
4	E	205	L8Z	C42-C52-C62	-2.41	117.36	126.21
4	J	205	L8Z	C42-C52-C62	-2.41	117.36	126.21
4	B	205	L8Z	C42-C52-C62	-2.40	117.37	126.21
4	C	205	L8Z	C42-C52-C62	-2.40	117.38	126.21
4	K	205	L8Z	C42-C52-C62	-2.40	117.38	126.21
4	F	205	L8Z	C42-C52-C62	-2.40	117.38	126.21
4	D	205	L8Z	C42-C52-C62	-2.39	117.41	126.21
5	A	204	LPP	O4-P1-O2	2.29	116.40	107.80
5	I	206	LPP	O4-P1-O2	2.29	116.38	107.80
5	E	206	LPP	O4-P1-O2	2.28	116.37	107.80
5	F	206	LPP	O4-P1-O2	2.28	116.36	107.80
5	K	206	LPP	O4-P1-O2	2.28	116.36	107.80
5	J	206	LPP	O4-P1-O2	2.28	116.35	107.80
5	D	206	LPP	O4-P1-O2	2.28	116.34	107.80
5	B	206	LPP	O4-P1-O2	2.28	116.34	107.80
5	G	206	LPP	O4-P1-O2	2.28	116.34	107.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	206	LPP	O4-P1-O2	2.27	116.33	107.80
5	C	206	LPP	O4-P1-O2	2.27	116.33	107.80
5	K	206	LPP	O5-P1-O3	-2.27	100.31	106.44
5	F	206	LPP	O5-P1-O3	-2.27	100.31	106.44
5	I	206	LPP	O5-P1-O3	-2.27	100.31	106.44
5	E	206	LPP	O5-P1-O3	-2.26	100.33	106.44
5	A	204	LPP	O5-P1-O3	-2.26	100.33	106.44
5	J	206	LPP	O5-P1-O3	-2.26	100.34	106.44
5	G	206	LPP	O5-P1-O3	-2.25	100.35	106.44
5	H	206	LPP	O5-P1-O3	-2.25	100.35	106.44
5	D	206	LPP	O5-P1-O3	-2.25	100.36	106.44
5	B	206	LPP	O5-P1-O3	-2.25	100.37	106.44
5	I	206	LPP	O9-C7-C8	2.25	116.40	108.34
5	G	206	LPP	O9-C7-C8	2.24	116.39	108.34
5	C	206	LPP	O5-P1-O3	-2.24	100.38	106.44
5	H	206	LPP	O9-C7-C8	2.23	116.36	108.34
5	J	206	LPP	O9-C7-C8	2.23	116.36	108.34
5	C	206	LPP	O9-C7-C8	2.23	116.35	108.34
5	K	206	LPP	O9-C7-C8	2.23	116.35	108.34
5	D	206	LPP	O9-C7-C8	2.23	116.35	108.34
5	F	206	LPP	O9-C7-C8	2.23	116.34	108.34
5	A	204	LPP	O9-C7-C8	2.23	116.33	108.34
5	B	206	LPP	O9-C7-C8	2.23	116.33	108.34
5	E	206	LPP	O9-C7-C8	2.23	116.33	108.34
4	K	205	L8Z	C3D-C2E-C1G	-2.15	106.52	111.39
4	D	205	L8Z	C3D-C2E-C1G	-2.15	106.52	111.39
4	J	205	L8Z	C3D-C2E-C1G	-2.15	106.53	111.39
4	E	205	L8Z	C3D-C2E-C1G	-2.15	106.53	111.39
4	C	205	L8Z	C3D-C2E-C1G	-2.15	106.54	111.39
4	G	205	L8Z	C3D-C2E-C1G	-2.14	106.55	111.39
4	A	203	L8Z	C3D-C2E-C1G	-2.14	106.55	111.39
4	B	205	L8Z	C3D-C2E-C1G	-2.14	106.56	111.39
4	K	205	L8Z	C3C-C2D-N21	2.13	114.31	110.91
4	E	205	L8Z	C66-O6-C1F	2.13	118.36	113.80
4	C	205	L8Z	C66-O6-C1F	2.13	118.36	113.80
4	I	205	L8Z	C3D-C2E-C1G	-2.13	106.58	111.39
4	H	205	L8Z	C3D-C2E-C1G	-2.12	106.59	111.39
4	F	205	L8Z	C3D-C2E-C1G	-2.12	106.59	111.39
4	B	205	L8Z	C3C-C2D-N21	2.12	114.29	110.91
4	H	205	L8Z	C3C-C2D-N21	2.12	114.29	110.91
4	J	205	L8Z	C66-O6-C1F	2.12	118.34	113.80
4	B	205	L8Z	C66-O6-C1F	2.12	118.34	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	203	L8Z	C3C-C2D-N21	2.12	114.28	110.91
4	G	205	L8Z	C3C-C2D-N21	2.12	114.28	110.91
4	G	205	L8Z	C66-O6-C1F	2.11	118.33	113.80
4	J	205	L8Z	C3C-C2D-N21	2.11	114.28	110.91
4	K	205	L8Z	C66-O6-C1F	2.11	118.32	113.80
4	H	205	L8Z	C66-O6-C1F	2.11	118.32	113.80
4	A	203	L8Z	C66-O6-C1F	2.11	118.31	113.80
4	E	205	L8Z	C3C-C2D-N21	2.10	114.26	110.91
4	F	205	L8Z	C66-O6-C1F	2.10	118.30	113.80
4	D	205	L8Z	C3C-C2D-N21	2.10	114.25	110.91
4	I	205	L8Z	C66-O6-C1F	2.10	118.29	113.80
4	I	205	L8Z	C3C-C2D-N21	2.09	114.25	110.91
4	D	205	L8Z	C66-O6-C1F	2.09	118.28	113.80
4	C	205	L8Z	C3C-C2D-N21	2.09	114.23	110.91
4	F	205	L8Z	C3C-C2D-N21	2.09	114.23	110.91

There are no chirality outliers.

All (869) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	206	PLM	O2-C1-C2-C3
2	B	201	PLM	O2-C1-C2-C3
2	C	201	PLM	O2-C1-C2-C3
2	D	201	PLM	O2-C1-C2-C3
2	E	201	PLM	O2-C1-C2-C3
2	F	201	PLM	O2-C1-C2-C3
2	G	201	PLM	O2-C1-C2-C3
2	H	201	PLM	O2-C1-C2-C3
2	I	201	PLM	O2-C1-C2-C3
2	J	201	PLM	O2-C1-C2-C3
2	K	201	PLM	O2-C1-C2-C3
4	A	203	L8Z	C15-C21-C31-C41
4	A	203	L8Z	C15-C21-C31-O31
4	A	203	L8Z	C21-C31-C41-C51
4	A	203	L8Z	O31-C31-C41-C51
4	A	203	L8Z	C1A-C22-C32-C42
4	A	203	L8Z	C1A-C22-C32-O32
4	A	203	L8Z	O33-C35-C44-C54
4	A	203	L8Z	O5-C1E-O14-P
4	A	203	L8Z	C2C-C3B-O36-C15
4	A	203	L8Z	C4A-C56-C66-O6
4	A	203	L8Z	C2D-C1F-O6-C66

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	A	203	L8Z	O51-C1F-O6-C66
4	A	203	L8Z	C1G-C2E-O61-C67
4	A	203	L8Z	C3D-C2E-O61-C67
4	A	203	L8Z	O62-C2E-O61-C67
4	A	203	L8Z	O1B-C1G-C2E-O61
4	A	203	L8Z	C58-C68-C76-O7
4	A	203	L8Z	C58-C68-C76-C86
4	A	203	L8Z	O62-C68-C76-O7
4	A	203	L8Z	O62-C68-C76-C86
4	A	203	L8Z	O7-C76-C86-O8
4	B	205	L8Z	C15-C21-C31-C41
4	B	205	L8Z	C15-C21-C31-O31
4	B	205	L8Z	C21-C31-C41-C51
4	B	205	L8Z	O31-C31-C41-C51
4	B	205	L8Z	C1A-C22-C32-C42
4	B	205	L8Z	C1A-C22-C32-O32
4	B	205	L8Z	O33-C35-C44-C54
4	B	205	L8Z	O5-C1E-O14-P
4	B	205	L8Z	C2C-C3B-O36-C15
4	B	205	L8Z	C4A-C56-C66-O6
4	B	205	L8Z	C2D-C1F-O6-C66
4	B	205	L8Z	O51-C1F-O6-C66
4	B	205	L8Z	C1G-C2E-O61-C67
4	B	205	L8Z	C3D-C2E-O61-C67
4	B	205	L8Z	O62-C2E-O61-C67
4	B	205	L8Z	O1B-C1G-C2E-O61
4	B	205	L8Z	C58-C68-C76-O7
4	B	205	L8Z	C58-C68-C76-C86
4	B	205	L8Z	O62-C68-C76-O7
4	B	205	L8Z	O62-C68-C76-C86
4	B	205	L8Z	O7-C76-C86-O8
4	C	205	L8Z	C15-C21-C31-C41
4	C	205	L8Z	C15-C21-C31-O31
4	C	205	L8Z	C21-C31-C41-C51
4	C	205	L8Z	O31-C31-C41-C51
4	C	205	L8Z	C1A-C22-C32-C42
4	C	205	L8Z	C1A-C22-C32-O32
4	C	205	L8Z	O33-C35-C44-C54
4	C	205	L8Z	O5-C1E-O14-P
4	C	205	L8Z	C2C-C3B-O36-C15
4	C	205	L8Z	C4A-C56-C66-O6
4	C	205	L8Z	C2D-C1F-O6-C66

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	C	205	L8Z	O51-C1F-O6-C66
4	C	205	L8Z	C1G-C2E-O61-C67
4	C	205	L8Z	C3D-C2E-O61-C67
4	C	205	L8Z	O62-C2E-O61-C67
4	C	205	L8Z	O1B-C1G-C2E-O61
4	C	205	L8Z	C58-C68-C76-O7
4	C	205	L8Z	C58-C68-C76-C86
4	C	205	L8Z	O62-C68-C76-O7
4	C	205	L8Z	O62-C68-C76-C86
4	C	205	L8Z	O7-C76-C86-O8
4	D	205	L8Z	C15-C21-C31-C41
4	D	205	L8Z	C15-C21-C31-O31
4	D	205	L8Z	C21-C31-C41-C51
4	D	205	L8Z	O31-C31-C41-C51
4	D	205	L8Z	C1A-C22-C32-C42
4	D	205	L8Z	C1A-C22-C32-O32
4	D	205	L8Z	O33-C35-C44-C54
4	D	205	L8Z	O5-C1E-O14-P
4	D	205	L8Z	C2C-C3B-O36-C15
4	D	205	L8Z	C4A-C56-C66-O6
4	D	205	L8Z	C2D-C1F-O6-C66
4	D	205	L8Z	O51-C1F-O6-C66
4	D	205	L8Z	C1G-C2E-O61-C67
4	D	205	L8Z	C3D-C2E-O61-C67
4	D	205	L8Z	O62-C2E-O61-C67
4	D	205	L8Z	O1B-C1G-C2E-O61
4	D	205	L8Z	C58-C68-C76-O7
4	D	205	L8Z	C58-C68-C76-C86
4	D	205	L8Z	O62-C68-C76-O7
4	D	205	L8Z	O62-C68-C76-C86
4	D	205	L8Z	O7-C76-C86-O8
4	E	205	L8Z	C15-C21-C31-C41
4	E	205	L8Z	C15-C21-C31-O31
4	E	205	L8Z	C21-C31-C41-C51
4	E	205	L8Z	O31-C31-C41-C51
4	E	205	L8Z	C1A-C22-C32-C42
4	E	205	L8Z	C1A-C22-C32-O32
4	E	205	L8Z	O33-C35-C44-C54
4	E	205	L8Z	O5-C1E-O14-P
4	E	205	L8Z	C2C-C3B-O36-C15
4	E	205	L8Z	C4A-C56-C66-O6
4	E	205	L8Z	C2D-C1F-O6-C66

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	E	205	L8Z	O51-C1F-O6-C66
4	E	205	L8Z	C1G-C2E-O61-C67
4	E	205	L8Z	C3D-C2E-O61-C67
4	E	205	L8Z	O62-C2E-O61-C67
4	E	205	L8Z	O1B-C1G-C2E-O61
4	E	205	L8Z	C58-C68-C76-O7
4	E	205	L8Z	C58-C68-C76-C86
4	E	205	L8Z	O62-C68-C76-O7
4	E	205	L8Z	O62-C68-C76-C86
4	E	205	L8Z	O7-C76-C86-O8
4	F	205	L8Z	C15-C21-C31-C41
4	F	205	L8Z	C15-C21-C31-O31
4	F	205	L8Z	C21-C31-C41-C51
4	F	205	L8Z	O31-C31-C41-C51
4	F	205	L8Z	C1A-C22-C32-C42
4	F	205	L8Z	C1A-C22-C32-O32
4	F	205	L8Z	O33-C35-C44-C54
4	F	205	L8Z	O5-C1E-O14-P
4	F	205	L8Z	C2C-C3B-O36-C15
4	F	205	L8Z	C4A-C56-C66-O6
4	F	205	L8Z	C2D-C1F-O6-C66
4	F	205	L8Z	O51-C1F-O6-C66
4	F	205	L8Z	C1G-C2E-O61-C67
4	F	205	L8Z	C3D-C2E-O61-C67
4	F	205	L8Z	O62-C2E-O61-C67
4	F	205	L8Z	O1B-C1G-C2E-O61
4	F	205	L8Z	C58-C68-C76-O7
4	F	205	L8Z	C58-C68-C76-C86
4	F	205	L8Z	O62-C68-C76-O7
4	F	205	L8Z	O62-C68-C76-C86
4	F	205	L8Z	O7-C76-C86-O8
4	G	205	L8Z	C15-C21-C31-C41
4	G	205	L8Z	C15-C21-C31-O31
4	G	205	L8Z	C21-C31-C41-C51
4	G	205	L8Z	O31-C31-C41-C51
4	G	205	L8Z	C1A-C22-C32-C42
4	G	205	L8Z	C1A-C22-C32-O32
4	G	205	L8Z	O33-C35-C44-C54
4	G	205	L8Z	O5-C1E-O14-P
4	G	205	L8Z	C2C-C3B-O36-C15
4	G	205	L8Z	C4A-C56-C66-O6
4	G	205	L8Z	C2D-C1F-O6-C66

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	G	205	L8Z	O51-C1F-O6-C66
4	G	205	L8Z	C1G-C2E-O61-C67
4	G	205	L8Z	C3D-C2E-O61-C67
4	G	205	L8Z	O62-C2E-O61-C67
4	G	205	L8Z	O1B-C1G-C2E-O61
4	G	205	L8Z	C58-C68-C76-O7
4	G	205	L8Z	C58-C68-C76-C86
4	G	205	L8Z	O62-C68-C76-O7
4	G	205	L8Z	O62-C68-C76-C86
4	G	205	L8Z	O7-C76-C86-O8
4	H	205	L8Z	C15-C21-C31-C41
4	H	205	L8Z	C15-C21-C31-O31
4	H	205	L8Z	C21-C31-C41-C51
4	H	205	L8Z	O31-C31-C41-C51
4	H	205	L8Z	C1A-C22-C32-C42
4	H	205	L8Z	C1A-C22-C32-O32
4	H	205	L8Z	O33-C35-C44-C54
4	H	205	L8Z	O5-C1E-O14-P
4	H	205	L8Z	C2C-C3B-O36-C15
4	H	205	L8Z	C4A-C56-C66-O6
4	H	205	L8Z	C2D-C1F-O6-C66
4	H	205	L8Z	O51-C1F-O6-C66
4	H	205	L8Z	C1G-C2E-O61-C67
4	H	205	L8Z	C3D-C2E-O61-C67
4	H	205	L8Z	O62-C2E-O61-C67
4	H	205	L8Z	O1B-C1G-C2E-O61
4	H	205	L8Z	C58-C68-C76-O7
4	H	205	L8Z	C58-C68-C76-C86
4	H	205	L8Z	O62-C68-C76-O7
4	H	205	L8Z	O62-C68-C76-C86
4	H	205	L8Z	O7-C76-C86-O8
4	I	205	L8Z	C15-C21-C31-C41
4	I	205	L8Z	C15-C21-C31-O31
4	I	205	L8Z	C21-C31-C41-C51
4	I	205	L8Z	O31-C31-C41-C51
4	I	205	L8Z	C1A-C22-C32-C42
4	I	205	L8Z	C1A-C22-C32-O32
4	I	205	L8Z	O33-C35-C44-C54
4	I	205	L8Z	O5-C1E-O14-P
4	I	205	L8Z	C2C-C3B-O36-C15
4	I	205	L8Z	C4A-C56-C66-O6
4	I	205	L8Z	C2D-C1F-O6-C66

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	I	205	L8Z	O51-C1F-O6-C66
4	I	205	L8Z	C1G-C2E-O61-C67
4	I	205	L8Z	C3D-C2E-O61-C67
4	I	205	L8Z	O62-C2E-O61-C67
4	I	205	L8Z	O1B-C1G-C2E-O61
4	I	205	L8Z	C58-C68-C76-O7
4	I	205	L8Z	C58-C68-C76-C86
4	I	205	L8Z	O62-C68-C76-O7
4	I	205	L8Z	O62-C68-C76-C86
4	I	205	L8Z	O7-C76-C86-O8
4	J	205	L8Z	C15-C21-C31-C41
4	J	205	L8Z	C15-C21-C31-O31
4	J	205	L8Z	C21-C31-C41-C51
4	J	205	L8Z	O31-C31-C41-C51
4	J	205	L8Z	C1A-C22-C32-C42
4	J	205	L8Z	C1A-C22-C32-O32
4	J	205	L8Z	O33-C35-C44-C54
4	J	205	L8Z	O5-C1E-O14-P
4	J	205	L8Z	C2C-C3B-O36-C15
4	J	205	L8Z	C4A-C56-C66-O6
4	J	205	L8Z	C2D-C1F-O6-C66
4	J	205	L8Z	O51-C1F-O6-C66
4	J	205	L8Z	C1G-C2E-O61-C67
4	J	205	L8Z	C3D-C2E-O61-C67
4	J	205	L8Z	O62-C2E-O61-C67
4	J	205	L8Z	O1B-C1G-C2E-O61
4	J	205	L8Z	C58-C68-C76-O7
4	J	205	L8Z	C58-C68-C76-C86
4	J	205	L8Z	O62-C68-C76-O7
4	J	205	L8Z	O62-C68-C76-C86
4	J	205	L8Z	O7-C76-C86-O8
4	K	205	L8Z	C15-C21-C31-C41
4	K	205	L8Z	C15-C21-C31-O31
4	K	205	L8Z	C21-C31-C41-C51
4	K	205	L8Z	O31-C31-C41-C51
4	K	205	L8Z	C1A-C22-C32-C42
4	K	205	L8Z	C1A-C22-C32-O32
4	K	205	L8Z	O33-C35-C44-C54
4	K	205	L8Z	O5-C1E-O14-P
4	K	205	L8Z	C2C-C3B-O36-C15
4	K	205	L8Z	C4A-C56-C66-O6
4	K	205	L8Z	C2D-C1F-O6-C66

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	K	205	L8Z	O51-C1F-O6-C66
4	K	205	L8Z	C1G-C2E-O61-C67
4	K	205	L8Z	C3D-C2E-O61-C67
4	K	205	L8Z	O62-C2E-O61-C67
4	K	205	L8Z	O1B-C1G-C2E-O61
4	K	205	L8Z	C58-C68-C76-O7
4	K	205	L8Z	C58-C68-C76-C86
4	K	205	L8Z	O62-C68-C76-O7
4	K	205	L8Z	O62-C68-C76-C86
4	K	205	L8Z	O7-C76-C86-O8
5	A	204	LPP	C6-O5-P1-O3
5	A	204	LPP	C6-O5-P1-O4
5	B	206	LPP	C6-O5-P1-O3
5	B	206	LPP	C6-O5-P1-O4
5	C	206	LPP	C6-O5-P1-O3
5	C	206	LPP	C6-O5-P1-O4
5	D	206	LPP	C6-O5-P1-O3
5	D	206	LPP	C6-O5-P1-O4
5	E	206	LPP	C6-O5-P1-O3
5	E	206	LPP	C6-O5-P1-O4
5	F	206	LPP	C6-O5-P1-O3
5	F	206	LPP	C6-O5-P1-O4
5	G	206	LPP	C6-O5-P1-O3
5	G	206	LPP	C6-O5-P1-O4
5	H	206	LPP	C6-O5-P1-O3
5	H	206	LPP	C6-O5-P1-O4
5	I	206	LPP	C6-O5-P1-O3
5	I	206	LPP	C6-O5-P1-O4
5	J	206	LPP	C6-O5-P1-O3
5	J	206	LPP	C6-O5-P1-O4
5	K	206	LPP	C6-O5-P1-O3
5	K	206	LPP	C6-O5-P1-O4
4	A	203	L8Z	O51-C57-C67-O61
4	B	205	L8Z	O51-C57-C67-O61
4	C	205	L8Z	O51-C57-C67-O61
4	D	205	L8Z	O51-C57-C67-O61
4	E	205	L8Z	O51-C57-C67-O61
4	F	205	L8Z	O51-C57-C67-O61
4	G	205	L8Z	O51-C57-C67-O61
4	H	205	L8Z	O51-C57-C67-O61
4	I	205	L8Z	O51-C57-C67-O61
4	J	205	L8Z	O51-C57-C67-O61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	K	205	L8Z	O51-C57-C67-O61
4	A	203	L8Z	C68-C76-C86-O8
4	B	205	L8Z	C68-C76-C86-O8
4	C	205	L8Z	C68-C76-C86-O8
4	D	205	L8Z	C68-C76-C86-O8
4	E	205	L8Z	C68-C76-C86-O8
4	F	205	L8Z	C68-C76-C86-O8
4	G	205	L8Z	C68-C76-C86-O8
4	H	205	L8Z	C68-C76-C86-O8
4	I	205	L8Z	C68-C76-C86-O8
4	J	205	L8Z	C68-C76-C86-O8
4	K	205	L8Z	C68-C76-C86-O8
4	A	203	L8Z	O5-C56-C66-O6
4	B	205	L8Z	O5-C56-C66-O6
4	C	205	L8Z	O5-C56-C66-O6
4	D	205	L8Z	O5-C56-C66-O6
4	E	205	L8Z	O5-C56-C66-O6
4	F	205	L8Z	O5-C56-C66-O6
4	G	205	L8Z	O5-C56-C66-O6
4	H	205	L8Z	O5-C56-C66-O6
4	I	205	L8Z	O5-C56-C66-O6
4	J	205	L8Z	O5-C56-C66-O6
4	K	205	L8Z	O5-C56-C66-O6
4	A	203	L8Z	C16-C17-C18-C19
4	C	205	L8Z	C16-C17-C18-C19
4	D	205	L8Z	C16-C17-C18-C19
4	F	205	L8Z	C16-C17-C18-C19
4	G	205	L8Z	C16-C17-C18-C19
4	H	205	L8Z	C16-C17-C18-C19
4	I	205	L8Z	C16-C17-C18-C19
4	J	205	L8Z	C16-C17-C18-C19
4	K	205	L8Z	C16-C17-C18-C19
4	B	205	L8Z	C16-C17-C18-C19
4	E	205	L8Z	C16-C17-C18-C19
5	A	204	LPP	C29-C30-C31-C32
5	B	206	LPP	C29-C30-C31-C32
5	C	206	LPP	C29-C30-C31-C32
5	D	206	LPP	C29-C30-C31-C32
5	E	206	LPP	C29-C30-C31-C32
5	F	206	LPP	C29-C30-C31-C32
5	G	206	LPP	C29-C30-C31-C32
5	H	206	LPP	C29-C30-C31-C32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	I	206	LPP	C29-C30-C31-C32
5	J	206	LPP	C29-C30-C31-C32
5	K	206	LPP	C29-C30-C31-C32
4	A	203	L8Z	C94-C36-C37-C38
4	B	205	L8Z	C94-C36-C37-C38
4	C	205	L8Z	C94-C36-C37-C38
4	D	205	L8Z	C94-C36-C37-C38
4	E	205	L8Z	C94-C36-C37-C38
4	F	205	L8Z	C94-C36-C37-C38
4	G	205	L8Z	C94-C36-C37-C38
4	H	205	L8Z	C94-C36-C37-C38
4	I	205	L8Z	C94-C36-C37-C38
4	J	205	L8Z	C94-C36-C37-C38
4	K	205	L8Z	C94-C36-C37-C38
5	B	206	LPP	C11-C12-C13-C14
5	D	206	LPP	C11-C12-C13-C14
5	H	206	LPP	C11-C12-C13-C14
5	K	206	LPP	C11-C12-C13-C14
5	G	206	LPP	C19-C20-C21-C22
5	J	206	LPP	C19-C20-C21-C22
5	A	204	LPP	C19-C20-C21-C22
5	B	206	LPP	C19-C20-C21-C22
5	C	206	LPP	C19-C20-C21-C22
5	D	206	LPP	C19-C20-C21-C22
5	E	206	LPP	C19-C20-C21-C22
5	F	206	LPP	C19-C20-C21-C22
5	H	206	LPP	C19-C20-C21-C22
5	I	206	LPP	C19-C20-C21-C22
5	K	206	LPP	C19-C20-C21-C22
5	G	206	LPP	C11-C12-C13-C14
5	A	204	LPP	C11-C12-C13-C14
5	C	206	LPP	C11-C12-C13-C14
5	E	206	LPP	C11-C12-C13-C14
5	F	206	LPP	C11-C12-C13-C14
5	I	206	LPP	C11-C12-C13-C14
5	J	206	LPP	C11-C12-C13-C14
4	F	205	L8Z	C92-C23-C24-C25
4	G	205	L8Z	C92-C23-C24-C25
4	I	205	L8Z	C92-C23-C24-C25
4	A	203	L8Z	C92-C23-C24-C25
4	B	205	L8Z	C92-C23-C24-C25
4	C	205	L8Z	C92-C23-C24-C25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	D	205	L8Z	C92-C23-C24-C25
4	H	205	L8Z	C92-C23-C24-C25
4	J	205	L8Z	C92-C23-C24-C25
4	E	205	L8Z	C92-C23-C24-C25
4	K	205	L8Z	C92-C23-C24-C25
5	A	204	LPP	C15-C16-C17-C18
5	B	206	LPP	C15-C16-C17-C18
5	C	206	LPP	C15-C16-C17-C18
5	D	206	LPP	C15-C16-C17-C18
5	E	206	LPP	C15-C16-C17-C18
5	F	206	LPP	C15-C16-C17-C18
5	G	206	LPP	C15-C16-C17-C18
5	H	206	LPP	C15-C16-C17-C18
5	I	206	LPP	C15-C16-C17-C18
5	J	206	LPP	C15-C16-C17-C18
5	K	206	LPP	C15-C16-C17-C18
4	G	205	L8Z	C7-C8-C9-C10
4	I	205	L8Z	C7-C8-C9-C10
2	D	201	PLM	C6-C7-C8-C9
2	E	201	PLM	C6-C7-C8-C9
2	F	201	PLM	C6-C7-C8-C9
2	H	201	PLM	C6-C7-C8-C9
4	A	203	L8Z	C7-C8-C9-C10
4	B	205	L8Z	C7-C8-C9-C10
4	C	205	L8Z	C7-C8-C9-C10
4	D	205	L8Z	C7-C8-C9-C10
4	E	205	L8Z	C7-C8-C9-C10
4	F	205	L8Z	C7-C8-C9-C10
4	H	205	L8Z	C7-C8-C9-C10
4	J	205	L8Z	C7-C8-C9-C10
4	K	205	L8Z	C7-C8-C9-C10
2	I	201	PLM	C6-C7-C8-C9
2	A	206	PLM	C6-C7-C8-C9
2	B	201	PLM	C6-C7-C8-C9
2	J	201	PLM	C6-C7-C8-C9
2	K	201	PLM	C6-C7-C8-C9
2	C	201	PLM	C6-C7-C8-C9
2	G	201	PLM	C6-C7-C8-C9
4	A	203	L8Z	C11-C10-C9-C8
4	A	203	L8Z	C44-C54-C64-C74
4	B	205	L8Z	C11-C10-C9-C8
4	B	205	L8Z	C44-C54-C64-C74

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	C	205	L8Z	C11-C10-C9-C8
4	C	205	L8Z	C44-C54-C64-C74
4	D	205	L8Z	C11-C10-C9-C8
4	D	205	L8Z	C44-C54-C64-C74
4	E	205	L8Z	C11-C10-C9-C8
4	E	205	L8Z	C44-C54-C64-C74
4	F	205	L8Z	C11-C10-C9-C8
4	F	205	L8Z	C44-C54-C64-C74
4	G	205	L8Z	C11-C10-C9-C8
4	G	205	L8Z	C44-C54-C64-C74
4	H	205	L8Z	C11-C10-C9-C8
4	H	205	L8Z	C44-C54-C64-C74
4	I	205	L8Z	C11-C10-C9-C8
4	I	205	L8Z	C44-C54-C64-C74
4	J	205	L8Z	C11-C10-C9-C8
4	J	205	L8Z	C44-C54-C64-C74
4	K	205	L8Z	C11-C10-C9-C8
4	K	205	L8Z	C44-C54-C64-C74
2	A	206	PLM	C3-C4-C5-C6
2	D	201	PLM	C3-C4-C5-C6
2	H	201	PLM	C3-C4-C5-C6
2	J	201	PLM	C3-C4-C5-C6
2	C	201	PLM	C3-C4-C5-C6
2	E	201	PLM	C3-C4-C5-C6
2	F	201	PLM	C3-C4-C5-C6
2	G	201	PLM	C3-C4-C5-C6
2	B	201	PLM	C3-C4-C5-C6
2	I	201	PLM	C3-C4-C5-C6
2	K	201	PLM	C3-C4-C5-C6
5	D	206	LPP	C39-C40-C41-C42
5	K	206	LPP	C39-C40-C41-C42
4	C	205	L8Z	C71-C81-C91-C16
4	E	205	L8Z	C71-C81-C91-C16
4	I	205	L8Z	C71-C81-C91-C16
4	J	205	L8Z	C71-C81-C91-C16
5	A	204	LPP	C39-C40-C41-C42
5	B	206	LPP	C39-C40-C41-C42
5	C	206	LPP	C39-C40-C41-C42
5	E	206	LPP	C39-C40-C41-C42
5	F	206	LPP	C39-C40-C41-C42
5	G	206	LPP	C39-C40-C41-C42
5	H	206	LPP	C39-C40-C41-C42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	I	206	LPP	C39-C40-C41-C42
5	J	206	LPP	C39-C40-C41-C42
4	A	203	L8Z	C71-C81-C91-C16
4	B	205	L8Z	C71-C81-C91-C16
4	D	205	L8Z	C71-C81-C91-C16
4	F	205	L8Z	C71-C81-C91-C16
4	G	205	L8Z	C71-C81-C91-C16
4	H	205	L8Z	C71-C81-C91-C16
4	K	205	L8Z	C71-C81-C91-C16
4	A	203	L8Z	C72-C82-C92-C23
4	B	205	L8Z	C72-C82-C92-C23
4	C	205	L8Z	C72-C82-C92-C23
4	D	205	L8Z	C72-C82-C92-C23
4	E	205	L8Z	C72-C82-C92-C23
4	F	205	L8Z	C72-C82-C92-C23
4	G	205	L8Z	C72-C82-C92-C23
4	H	205	L8Z	C72-C82-C92-C23
4	I	205	L8Z	C72-C82-C92-C23
4	J	205	L8Z	C72-C82-C92-C23
4	K	205	L8Z	C72-C82-C92-C23
4	H	205	L8Z	C65-C75-C85-C95
4	A	203	L8Z	C65-C75-C85-C95
4	B	205	L8Z	C65-C75-C85-C95
4	D	205	L8Z	C65-C75-C85-C95
4	E	205	L8Z	C65-C75-C85-C95
4	F	205	L8Z	C65-C75-C85-C95
4	G	205	L8Z	C65-C75-C85-C95
4	I	205	L8Z	C65-C75-C85-C95
4	J	205	L8Z	C65-C75-C85-C95
4	A	203	L8Z	C61-C71-C81-C91
4	A	203	L8Z	C62-C72-C82-C92
4	B	205	L8Z	C61-C71-C81-C91
4	B	205	L8Z	C62-C72-C82-C92
4	C	205	L8Z	C61-C71-C81-C91
4	C	205	L8Z	C62-C72-C82-C92
4	D	205	L8Z	C61-C71-C81-C91
4	D	205	L8Z	C62-C72-C82-C92
4	E	205	L8Z	C61-C71-C81-C91
4	E	205	L8Z	C62-C72-C82-C92
4	F	205	L8Z	C61-C71-C81-C91
4	F	205	L8Z	C62-C72-C82-C92
4	G	205	L8Z	C61-C71-C81-C91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	G	205	L8Z	C62-C72-C82-C92
4	H	205	L8Z	C61-C71-C81-C91
4	H	205	L8Z	C62-C72-C82-C92
4	I	205	L8Z	C61-C71-C81-C91
4	I	205	L8Z	C62-C72-C82-C92
4	J	205	L8Z	C61-C71-C81-C91
4	J	205	L8Z	C62-C72-C82-C92
4	K	205	L8Z	C61-C71-C81-C91
4	K	205	L8Z	C62-C72-C82-C92
4	C	205	L8Z	C65-C75-C85-C95
4	K	205	L8Z	C65-C75-C85-C95
4	C	205	L8Z	C5-C6-C7-C8
4	A	203	L8Z	C5-C6-C7-C8
4	B	205	L8Z	C5-C6-C7-C8
4	D	205	L8Z	C5-C6-C7-C8
4	E	205	L8Z	C5-C6-C7-C8
4	F	205	L8Z	C5-C6-C7-C8
4	G	205	L8Z	C5-C6-C7-C8
4	H	205	L8Z	C5-C6-C7-C8
4	I	205	L8Z	C5-C6-C7-C8
4	J	205	L8Z	C5-C6-C7-C8
4	K	205	L8Z	C5-C6-C7-C8
4	J	205	L8Z	C23-C24-C25-C26
4	K	205	L8Z	C23-C24-C25-C26
4	A	203	L8Z	C23-C24-C25-C26
4	B	205	L8Z	C23-C24-C25-C26
4	C	205	L8Z	C23-C24-C25-C26
4	D	205	L8Z	C23-C24-C25-C26
4	E	205	L8Z	C23-C24-C25-C26
4	F	205	L8Z	C23-C24-C25-C26
4	G	205	L8Z	C23-C24-C25-C26
4	H	205	L8Z	C23-C24-C25-C26
4	I	205	L8Z	C23-C24-C25-C26
4	A	203	L8Z	C2A-C35-C44-C54
4	B	205	L8Z	C2A-C35-C44-C54
4	C	205	L8Z	C2A-C35-C44-C54
4	D	205	L8Z	C2A-C35-C44-C54
4	E	205	L8Z	C2A-C35-C44-C54
4	F	205	L8Z	C2A-C35-C44-C54
4	G	205	L8Z	C2A-C35-C44-C54
4	H	205	L8Z	C2A-C35-C44-C54
4	I	205	L8Z	C2A-C35-C44-C54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	J	205	L8Z	C2A-C35-C44-C54
4	K	205	L8Z	C2A-C35-C44-C54
4	H	205	L8Z	C24-C23-C92-C82
4	A	203	L8Z	C24-C23-C92-C82
4	B	205	L8Z	C24-C23-C92-C82
4	C	205	L8Z	C24-C23-C92-C82
4	D	205	L8Z	C24-C23-C92-C82
4	E	205	L8Z	C24-C23-C92-C82
4	F	205	L8Z	C24-C23-C92-C82
4	G	205	L8Z	C24-C23-C92-C82
4	I	205	L8Z	C24-C23-C92-C82
4	J	205	L8Z	C24-C23-C92-C82
4	K	205	L8Z	C24-C23-C92-C82
4	A	203	L8Z	C36-C37-C38-C39
4	F	205	L8Z	C36-C37-C38-C39
4	G	205	L8Z	C36-C37-C38-C39
4	I	205	L8Z	C36-C37-C38-C39
4	J	205	L8Z	C36-C37-C38-C39
4	K	205	L8Z	C36-C37-C38-C39
4	B	205	L8Z	C36-C37-C38-C39
4	C	205	L8Z	C36-C37-C38-C39
4	D	205	L8Z	C36-C37-C38-C39
4	E	205	L8Z	C36-C37-C38-C39
4	H	205	L8Z	C36-C37-C38-C39
4	A	203	L8Z	C91-C16-C17-C18
4	C	205	L8Z	C91-C16-C17-C18
4	F	205	L8Z	C91-C16-C17-C18
4	J	205	L8Z	C91-C16-C17-C18
4	B	205	L8Z	C91-C16-C17-C18
4	D	205	L8Z	C91-C16-C17-C18
4	E	205	L8Z	C91-C16-C17-C18
4	G	205	L8Z	C91-C16-C17-C18
4	H	205	L8Z	C91-C16-C17-C18
4	I	205	L8Z	C91-C16-C17-C18
4	K	205	L8Z	C91-C16-C17-C18
4	G	205	L8Z	C17-C16-C91-C81
4	J	205	L8Z	C17-C16-C91-C81
4	A	203	L8Z	C17-C16-C91-C81
4	B	205	L8Z	C17-C16-C91-C81
4	D	205	L8Z	C17-C16-C91-C81
4	H	205	L8Z	C17-C16-C91-C81
4	C	205	L8Z	C17-C16-C91-C81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	E	205	L8Z	C17-C16-C91-C81
4	F	205	L8Z	C17-C16-C91-C81
4	I	205	L8Z	C17-C16-C91-C81
4	K	205	L8Z	C17-C16-C91-C81
5	A	204	LPP	C12-C13-C14-C15
5	B	206	LPP	C12-C13-C14-C15
5	D	206	LPP	C12-C13-C14-C15
5	E	206	LPP	C12-C13-C14-C15
5	F	206	LPP	C12-C13-C14-C15
5	G	206	LPP	C12-C13-C14-C15
5	H	206	LPP	C12-C13-C14-C15
5	I	206	LPP	C12-C13-C14-C15
5	K	206	LPP	C12-C13-C14-C15
5	J	206	LPP	C12-C13-C14-C15
5	C	206	LPP	C12-C13-C14-C15
5	A	204	LPP	O9-C7-C8-O27
5	B	206	LPP	O9-C7-C8-O27
5	C	206	LPP	O9-C7-C8-O27
5	D	206	LPP	O9-C7-C8-O27
5	E	206	LPP	O9-C7-C8-O27
5	F	206	LPP	O9-C7-C8-O27
5	G	206	LPP	O9-C7-C8-O27
5	H	206	LPP	O9-C7-C8-O27
5	I	206	LPP	O9-C7-C8-O27
5	J	206	LPP	O9-C7-C8-O27
5	K	206	LPP	O9-C7-C8-O27
4	B	205	L8Z	C53-C63-C73-C83
4	A	203	L8Z	C53-C63-C73-C83
4	D	205	L8Z	C53-C63-C73-C83
4	G	205	L8Z	C53-C63-C73-C83
4	K	205	L8Z	C53-C63-C73-C83
4	C	205	L8Z	C53-C63-C73-C83
4	E	205	L8Z	C53-C63-C73-C83
4	F	205	L8Z	C53-C63-C73-C83
4	H	205	L8Z	C53-C63-C73-C83
4	I	205	L8Z	C53-C63-C73-C83
4	J	205	L8Z	C53-C63-C73-C83
4	A	203	L8Z	C11-C12-C13-C14
4	B	205	L8Z	C11-C12-C13-C14
4	C	205	L8Z	C11-C12-C13-C14
4	D	205	L8Z	C11-C12-C13-C14
4	E	205	L8Z	C11-C12-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	F	205	L8Z	C11-C12-C13-C14
4	G	205	L8Z	C11-C12-C13-C14
4	H	205	L8Z	C11-C12-C13-C14
4	I	205	L8Z	C11-C12-C13-C14
4	J	205	L8Z	C11-C12-C13-C14
4	K	205	L8Z	C11-C12-C13-C14
5	A	204	LPP	O5-C6-C7-O9
5	B	206	LPP	O5-C6-C7-O9
5	C	206	LPP	O5-C6-C7-O9
5	D	206	LPP	O5-C6-C7-O9
5	E	206	LPP	O5-C6-C7-O9
5	F	206	LPP	O5-C6-C7-O9
5	G	206	LPP	O5-C6-C7-O9
5	H	206	LPP	O5-C6-C7-O9
5	I	206	LPP	O5-C6-C7-O9
5	J	206	LPP	O5-C6-C7-O9
5	K	206	LPP	O5-C6-C7-O9
4	A	203	L8Z	C35-C44-C54-C64
4	B	205	L8Z	C35-C44-C54-C64
4	C	205	L8Z	C35-C44-C54-C64
4	E	205	L8Z	C35-C44-C54-C64
4	F	205	L8Z	C35-C44-C54-C64
4	H	205	L8Z	C35-C44-C54-C64
4	I	205	L8Z	C35-C44-C54-C64
4	K	205	L8Z	C35-C44-C54-C64
4	A	203	L8Z	O22-C1A-C22-C32
4	B	205	L8Z	O22-C1A-C22-C32
4	C	205	L8Z	O22-C1A-C22-C32
4	D	205	L8Z	O22-C1A-C22-C32
4	E	205	L8Z	O22-C1A-C22-C32
4	F	205	L8Z	O22-C1A-C22-C32
4	G	205	L8Z	O22-C1A-C22-C32
4	H	205	L8Z	O22-C1A-C22-C32
4	I	205	L8Z	O22-C1A-C22-C32
4	J	205	L8Z	O22-C1A-C22-C32
4	K	205	L8Z	O22-C1A-C22-C32
2	A	205	PLM	C1-C2-C3-C4
2	A	206	PLM	C1-C2-C3-C4
2	B	201	PLM	C1-C2-C3-C4
2	B	204	PLM	C1-C2-C3-C4
2	C	201	PLM	C1-C2-C3-C4
2	C	204	PLM	C1-C2-C3-C4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	D	201	PLM	C1-C2-C3-C4
2	D	204	PLM	C1-C2-C3-C4
2	E	201	PLM	C1-C2-C3-C4
2	E	204	PLM	C1-C2-C3-C4
2	F	201	PLM	C1-C2-C3-C4
2	F	204	PLM	C1-C2-C3-C4
2	G	201	PLM	C1-C2-C3-C4
2	G	204	PLM	C1-C2-C3-C4
2	H	201	PLM	C1-C2-C3-C4
2	H	204	PLM	C1-C2-C3-C4
2	I	201	PLM	C1-C2-C3-C4
2	I	204	PLM	C1-C2-C3-C4
2	J	201	PLM	C1-C2-C3-C4
2	J	204	PLM	C1-C2-C3-C4
2	K	201	PLM	C1-C2-C3-C4
2	K	204	PLM	C1-C2-C3-C4
4	A	203	L8Z	N21-C1A-C22-C32
4	B	205	L8Z	N21-C1A-C22-C32
4	C	205	L8Z	N21-C1A-C22-C32
4	D	205	L8Z	N21-C1A-C22-C32
4	E	205	L8Z	N21-C1A-C22-C32
4	F	205	L8Z	N21-C1A-C22-C32
4	G	205	L8Z	N21-C1A-C22-C32
4	H	205	L8Z	N21-C1A-C22-C32
4	I	205	L8Z	N21-C1A-C22-C32
4	J	205	L8Z	N21-C1A-C22-C32
4	K	205	L8Z	N21-C1A-C22-C32
4	D	205	L8Z	C35-C44-C54-C64
4	G	205	L8Z	C35-C44-C54-C64
4	J	205	L8Z	C35-C44-C54-C64
5	A	204	LPP	O5-C6-C7-C8
5	B	206	LPP	O5-C6-C7-C8
5	C	206	LPP	O5-C6-C7-C8
5	D	206	LPP	O5-C6-C7-C8
5	E	206	LPP	O5-C6-C7-C8
5	G	206	LPP	O5-C6-C7-C8
5	H	206	LPP	O5-C6-C7-C8
5	J	206	LPP	O5-C6-C7-C8
5	K	206	LPP	O5-C6-C7-C8
5	E	206	LPP	C16-C17-C18-C19
5	F	206	LPP	C16-C17-C18-C19
5	H	206	LPP	C16-C17-C18-C19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	J	206	LPP	C16-C17-C18-C19
5	A	204	LPP	C16-C17-C18-C19
5	B	206	LPP	C16-C17-C18-C19
5	I	206	LPP	C16-C17-C18-C19
5	K	206	LPP	C16-C17-C18-C19
5	D	206	LPP	C16-C17-C18-C19
5	C	206	LPP	C16-C17-C18-C19
5	G	206	LPP	C16-C17-C18-C19
4	C	205	L8Z	C4-C5-C6-C7
4	J	205	L8Z	C4-C5-C6-C7
5	A	204	LPP	C6-C7-C8-O27
5	B	206	LPP	C6-C7-C8-O27
5	C	206	LPP	C6-C7-C8-O27
5	D	206	LPP	C6-C7-C8-O27
5	E	206	LPP	C6-C7-C8-O27
5	F	206	LPP	C6-C7-C8-O27
5	G	206	LPP	C6-C7-C8-O27
5	H	206	LPP	C6-C7-C8-O27
5	I	206	LPP	C6-C7-C8-O27
5	J	206	LPP	C6-C7-C8-O27
5	K	206	LPP	C6-C7-C8-O27
4	A	203	L8Z	C4-C5-C6-C7
4	B	205	L8Z	C4-C5-C6-C7
4	D	205	L8Z	C4-C5-C6-C7
4	E	205	L8Z	C4-C5-C6-C7
4	G	205	L8Z	C4-C5-C6-C7
4	H	205	L8Z	C4-C5-C6-C7
4	I	205	L8Z	C4-C5-C6-C7
4	K	205	L8Z	C4-C5-C6-C7
4	F	205	L8Z	C4-C5-C6-C7
4	G	205	L8Z	C1D-C2B-C3A-C45
4	K	205	L8Z	C1D-C2B-C3A-C45
5	A	204	LPP	C8-C7-O9-C11
5	B	206	LPP	C8-C7-O9-C11
5	C	206	LPP	C8-C7-O9-C11
5	D	206	LPP	C8-C7-O9-C11
5	E	206	LPP	C8-C7-O9-C11
5	F	206	LPP	C8-C7-O9-C11
5	G	206	LPP	C8-C7-O9-C11
5	H	206	LPP	C8-C7-O9-C11
5	I	206	LPP	C8-C7-O9-C11
5	J	206	LPP	C8-C7-O9-C11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	K	206	LPP	C8-C7-O9-C11
4	A	203	L8Z	C1D-C2B-C3A-C45
4	B	205	L8Z	C1D-C2B-C3A-C45
4	E	205	L8Z	C1D-C2B-C3A-C45
4	F	205	L8Z	C1D-C2B-C3A-C45
4	H	205	L8Z	C1D-C2B-C3A-C45
5	F	206	LPP	O5-C6-C7-C8
5	I	206	LPP	O5-C6-C7-C8
4	C	205	L8Z	C1D-C2B-C3A-C45
4	D	205	L8Z	C1D-C2B-C3A-C45
4	I	205	L8Z	C1D-C2B-C3A-C45
4	J	205	L8Z	C1D-C2B-C3A-C45
2	B	204	PLM	C3-C4-C5-C6
2	I	204	PLM	C3-C4-C5-C6
2	G	204	PLM	C3-C4-C5-C6
2	H	204	PLM	C3-C4-C5-C6
2	J	204	PLM	C3-C4-C5-C6
2	K	204	PLM	C3-C4-C5-C6
2	A	205	PLM	C3-C4-C5-C6
2	C	204	PLM	C3-C4-C5-C6
2	D	204	PLM	C3-C4-C5-C6
2	E	204	PLM	C3-C4-C5-C6
2	F	204	PLM	C3-C4-C5-C6
5	E	206	LPP	C38-C39-C40-C41
5	H	206	LPP	C38-C39-C40-C41
5	A	204	LPP	C38-C39-C40-C41
5	F	206	LPP	C38-C39-C40-C41
5	B	206	LPP	C38-C39-C40-C41
5	C	206	LPP	C38-C39-C40-C41
5	D	206	LPP	C38-C39-C40-C41
5	G	206	LPP	C38-C39-C40-C41
5	I	206	LPP	C38-C39-C40-C41
5	J	206	LPP	C38-C39-C40-C41
5	K	206	LPP	C38-C39-C40-C41
4	A	203	L8Z	C57-C67-O61-C2E
4	B	205	L8Z	C57-C67-O61-C2E
4	C	205	L8Z	C57-C67-O61-C2E
4	D	205	L8Z	C57-C67-O61-C2E
4	E	205	L8Z	C57-C67-O61-C2E
4	F	205	L8Z	C57-C67-O61-C2E
4	G	205	L8Z	C57-C67-O61-C2E
4	H	205	L8Z	C57-C67-O61-C2E

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	I	205	L8Z	C57-C67-O61-C2E
4	J	205	L8Z	C57-C67-O61-C2E
4	K	205	L8Z	C57-C67-O61-C2E
4	H	205	L8Z	C3-C4-C5-C6
5	C	206	LPP	C34-C35-C36-C37
5	I	206	LPP	C34-C35-C36-C37
5	B	206	LPP	C34-C35-C36-C37
5	D	206	LPP	C34-C35-C36-C37
5	H	206	LPP	C34-C35-C36-C37
5	J	206	LPP	C34-C35-C36-C37
5	G	206	LPP	C34-C35-C36-C37
5	K	206	LPP	C34-C35-C36-C37
5	A	204	LPP	C34-C35-C36-C37
5	E	206	LPP	C34-C35-C36-C37
5	F	206	LPP	C34-C35-C36-C37
4	A	203	L8Z	C3-C4-C5-C6
4	B	205	L8Z	C3-C4-C5-C6
4	C	205	L8Z	C3-C4-C5-C6
4	D	205	L8Z	C3-C4-C5-C6
4	E	205	L8Z	C3-C4-C5-C6
4	F	205	L8Z	C3-C4-C5-C6
4	G	205	L8Z	C3-C4-C5-C6
4	I	205	L8Z	C3-C4-C5-C6
4	J	205	L8Z	C3-C4-C5-C6
4	K	205	L8Z	C3-C4-C5-C6
5	A	204	LPP	C6-O5-P1-O2
5	B	206	LPP	C6-O5-P1-O2
5	C	206	LPP	C6-O5-P1-O2
5	D	206	LPP	C6-O5-P1-O2
5	E	206	LPP	C6-O5-P1-O2
5	F	206	LPP	C6-O5-P1-O2
5	G	206	LPP	C6-O5-P1-O2
5	H	206	LPP	C6-O5-P1-O2
5	I	206	LPP	C6-O5-P1-O2
5	J	206	LPP	C6-O5-P1-O2
5	K	206	LPP	C6-O5-P1-O2
4	A	203	L8Z	C4B-C3C-O37-C1C
4	C	205	L8Z	C4B-C3C-O37-C1C
4	G	205	L8Z	C4B-C3C-O37-C1C
4	B	205	L8Z	C4B-C3C-O37-C1C
4	E	205	L8Z	C4B-C3C-O37-C1C
4	F	205	L8Z	C4B-C3C-O37-C1C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	H	205	L8Z	C4B-C3C-O37-C1C
4	I	205	L8Z	C4B-C3C-O37-C1C
4	J	205	L8Z	C4B-C3C-O37-C1C
4	K	205	L8Z	C4B-C3C-O37-C1C
4	D	205	L8Z	C4B-C3C-O37-C1C
4	A	203	L8Z	C1E-O14-P-O34
4	B	205	L8Z	C1E-O14-P-O34
4	C	205	L8Z	C1E-O14-P-O34
4	D	205	L8Z	C1E-O14-P-O34
4	E	205	L8Z	C1E-O14-P-O34
4	F	205	L8Z	C1E-O14-P-O34
4	G	205	L8Z	C1E-O14-P-O34
4	H	205	L8Z	C1E-O14-P-O34
4	I	205	L8Z	C1E-O14-P-O34
4	J	205	L8Z	C1E-O14-P-O34
4	K	205	L8Z	C1E-O14-P-O34
2	G	201	PLM	CC-CD-CE-CF
2	D	201	PLM	CC-CD-CE-CF
2	J	201	PLM	CC-CD-CE-CF
2	B	201	PLM	CC-CD-CE-CF
2	C	201	PLM	CC-CD-CE-CF
2	E	201	PLM	CC-CD-CE-CF
2	F	201	PLM	CC-CD-CE-CF
2	H	201	PLM	CC-CD-CE-CF
2	K	201	PLM	CC-CD-CE-CF
2	A	206	PLM	CC-CD-CE-CF
2	I	201	PLM	CC-CD-CE-CF
4	K	205	L8Z	C75-C85-C95-C46
4	D	205	L8Z	C75-C85-C95-C46
4	E	205	L8Z	C75-C85-C95-C46
4	I	205	L8Z	C75-C85-C95-C46
4	B	205	L8Z	C75-C85-C95-C46
4	C	205	L8Z	C75-C85-C95-C46
4	F	205	L8Z	C75-C85-C95-C46
4	A	203	L8Z	C75-C85-C95-C46
4	G	205	L8Z	C75-C85-C95-C46
4	H	205	L8Z	C75-C85-C95-C46
4	J	205	L8Z	C75-C85-C95-C46
4	A	203	L8Z	C63-C73-C83-C93
4	F	205	L8Z	C63-C73-C83-C93
4	B	205	L8Z	C63-C73-C83-C93
4	D	205	L8Z	C63-C73-C83-C93

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	K	205	L8Z	C63-C73-C83-C93
4	I	205	L8Z	C63-C73-C83-C93
4	C	205	L8Z	C63-C73-C83-C93
4	H	205	L8Z	C63-C73-C83-C93
4	G	205	L8Z	C63-C73-C83-C93
4	E	205	L8Z	C63-C73-C83-C93
4	J	205	L8Z	C63-C73-C83-C93

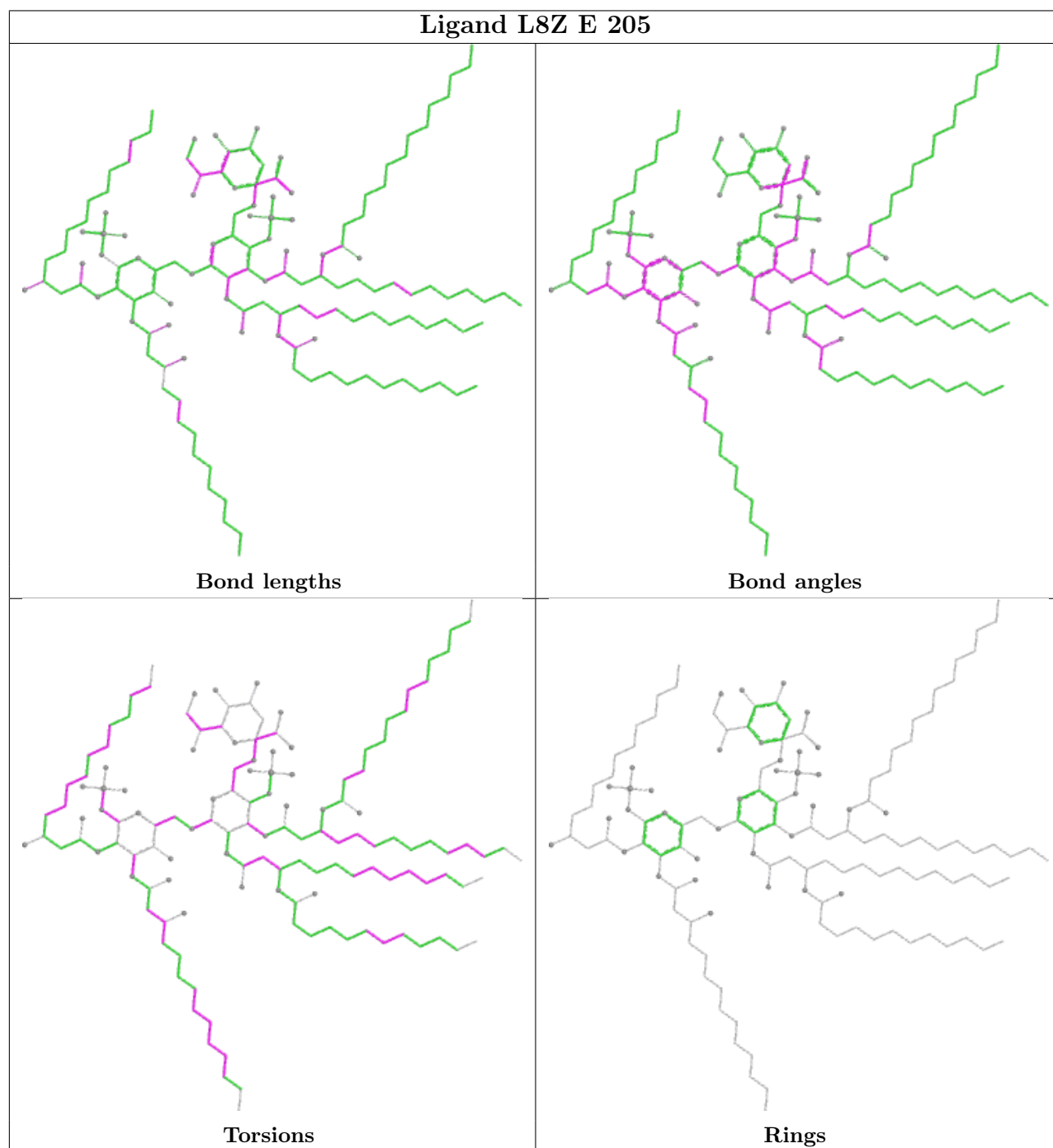
There are no ring outliers.

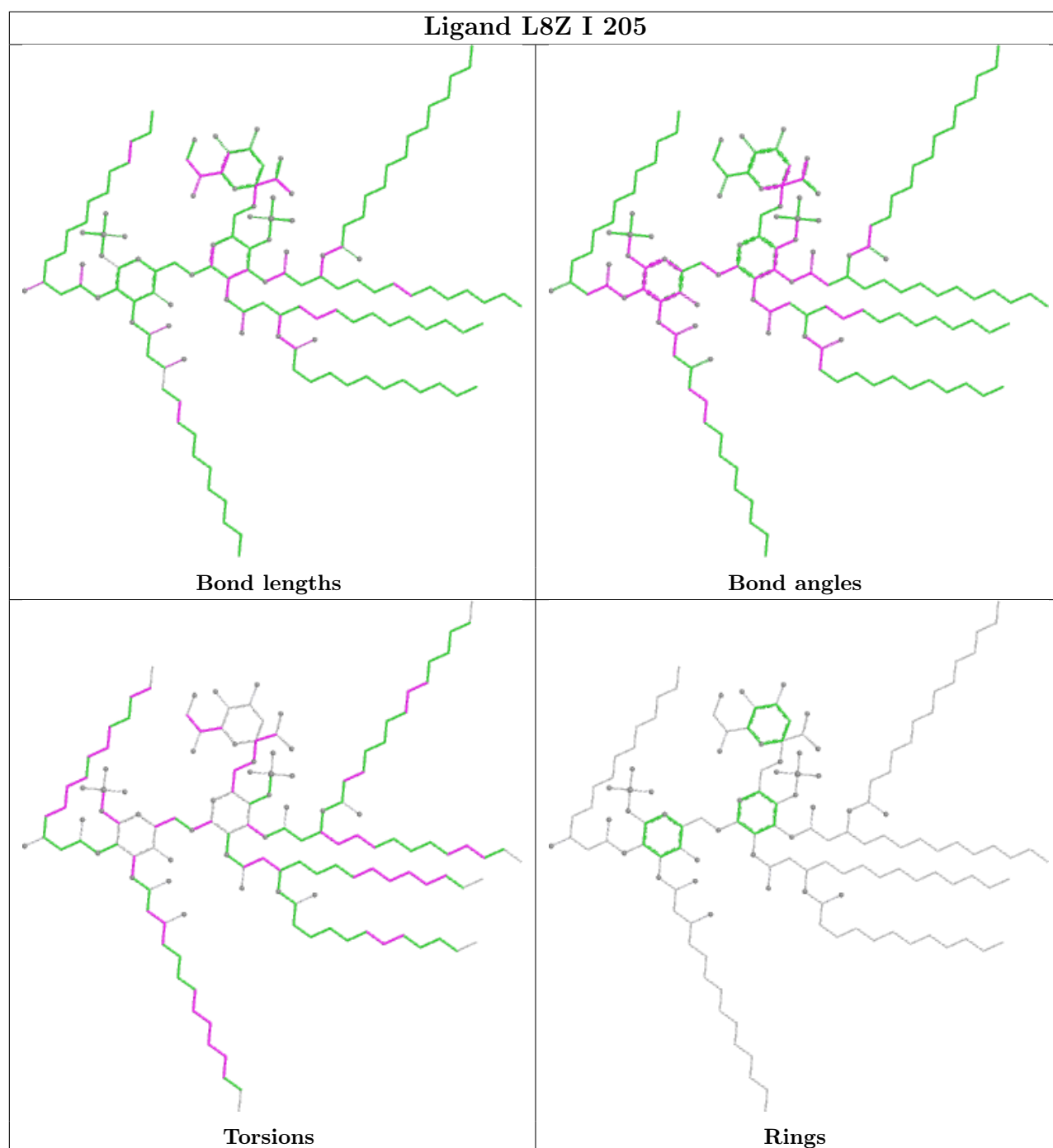
23 monomers are involved in 23 short contacts:

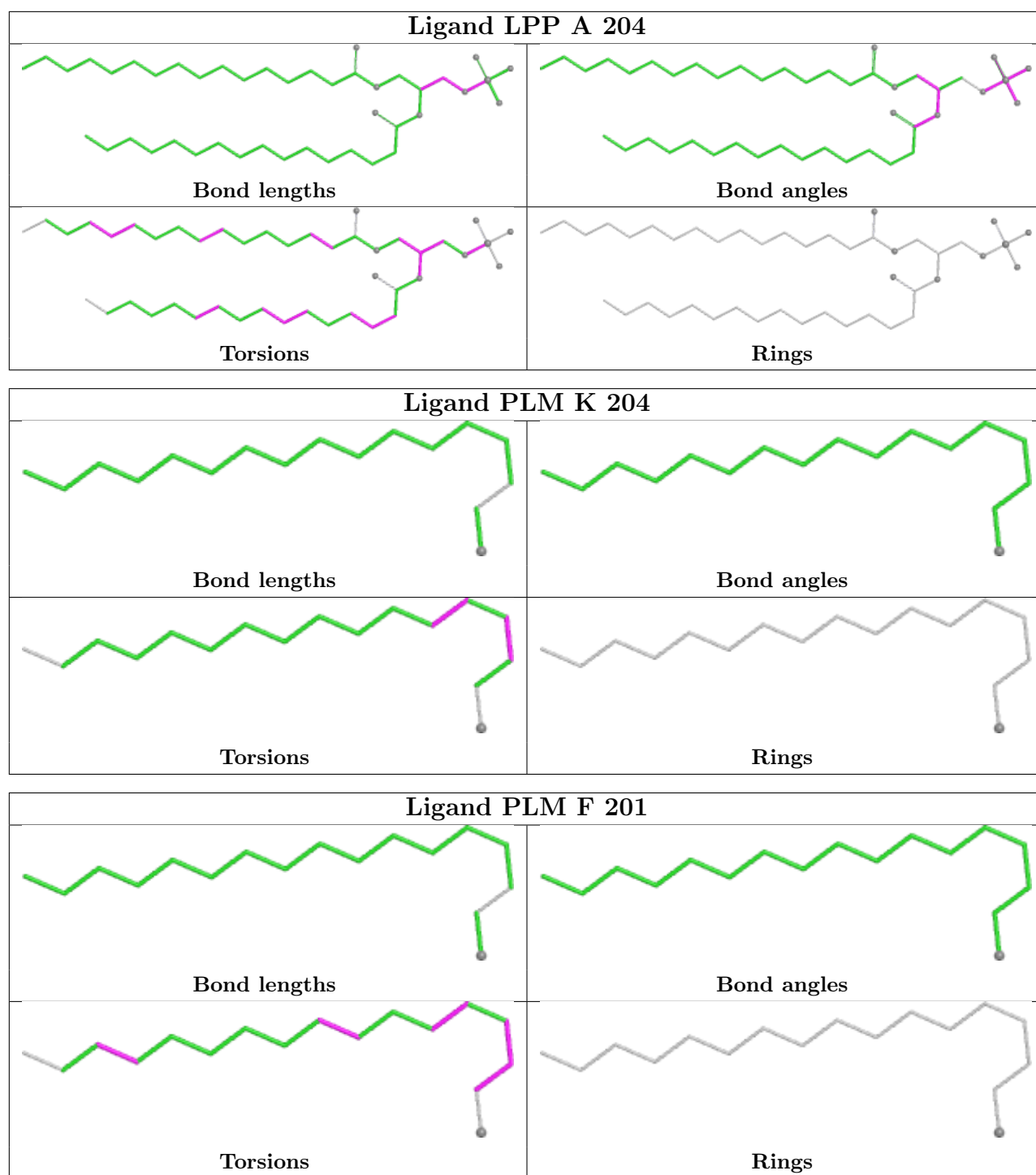
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	K	204	PLM	1	0
2	F	201	PLM	1	0
2	B	201	PLM	1	0
2	H	204	PLM	2	0
2	E	204	PLM	2	0
2	A	205	PLM	2	0
2	D	201	PLM	1	0
2	J	201	PLM	1	0
2	J	204	PLM	2	0
2	E	201	PLM	1	0
2	I	201	PLM	1	0
2	C	201	PLM	1	0
2	I	204	PLM	2	0
2	C	204	PLM	2	0
4	J	205	L8Z	1	0
2	F	204	PLM	2	0
2	G	201	PLM	1	0
2	B	204	PLM	2	0
2	G	204	PLM	2	0
2	D	204	PLM	2	0
2	H	201	PLM	1	0
2	K	201	PLM	1	0
2	A	206	PLM	2	0

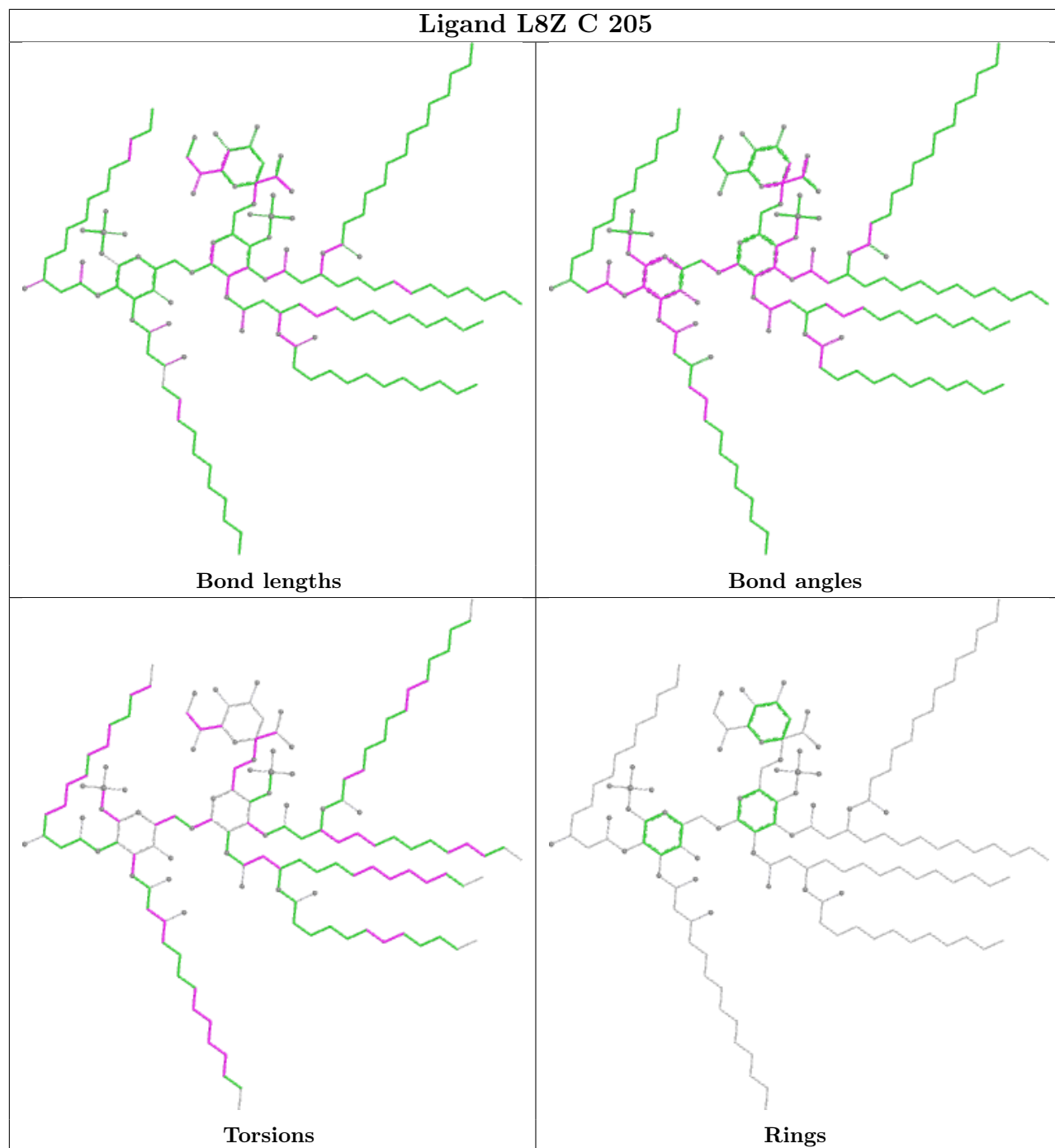
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

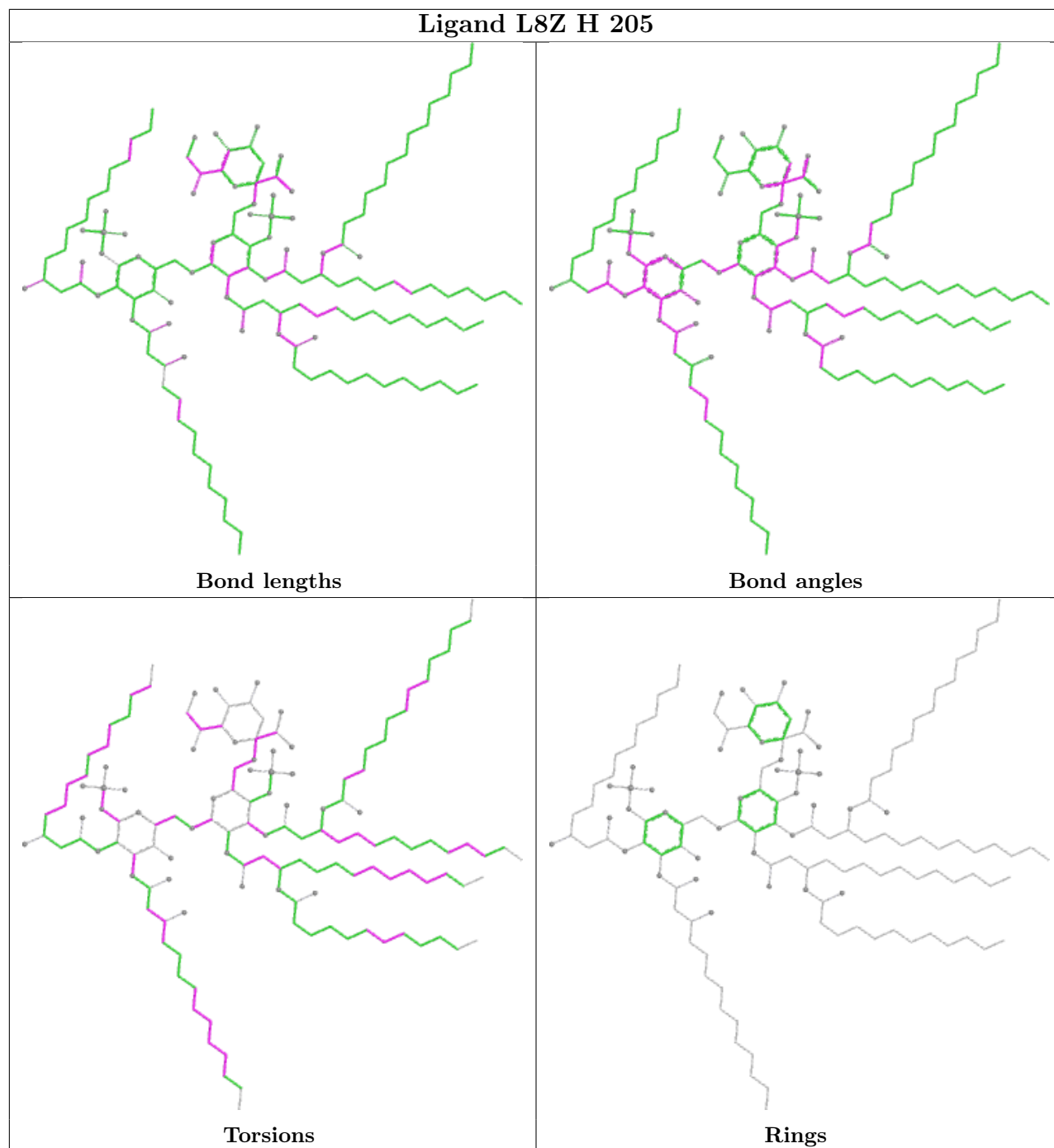
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

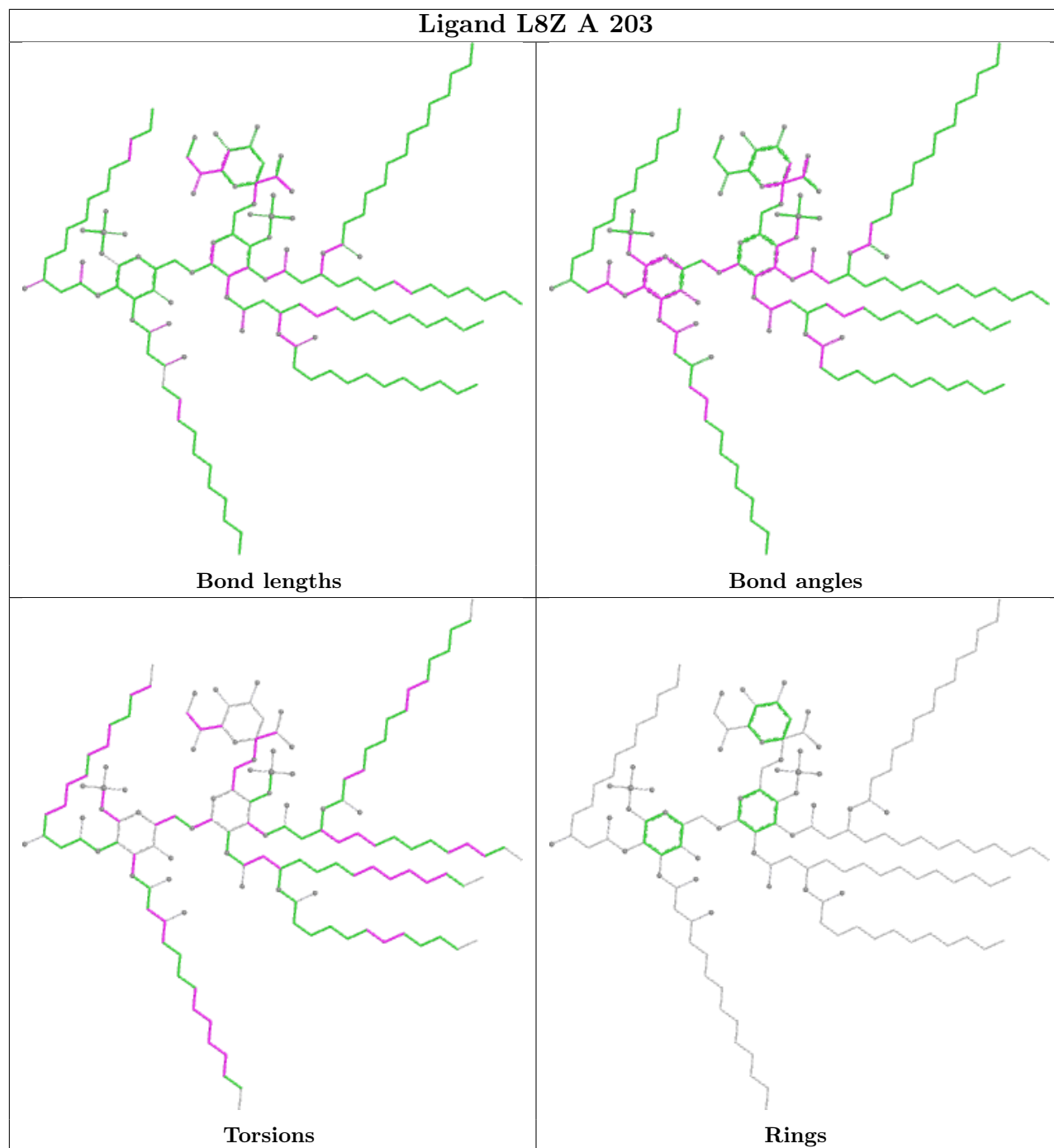


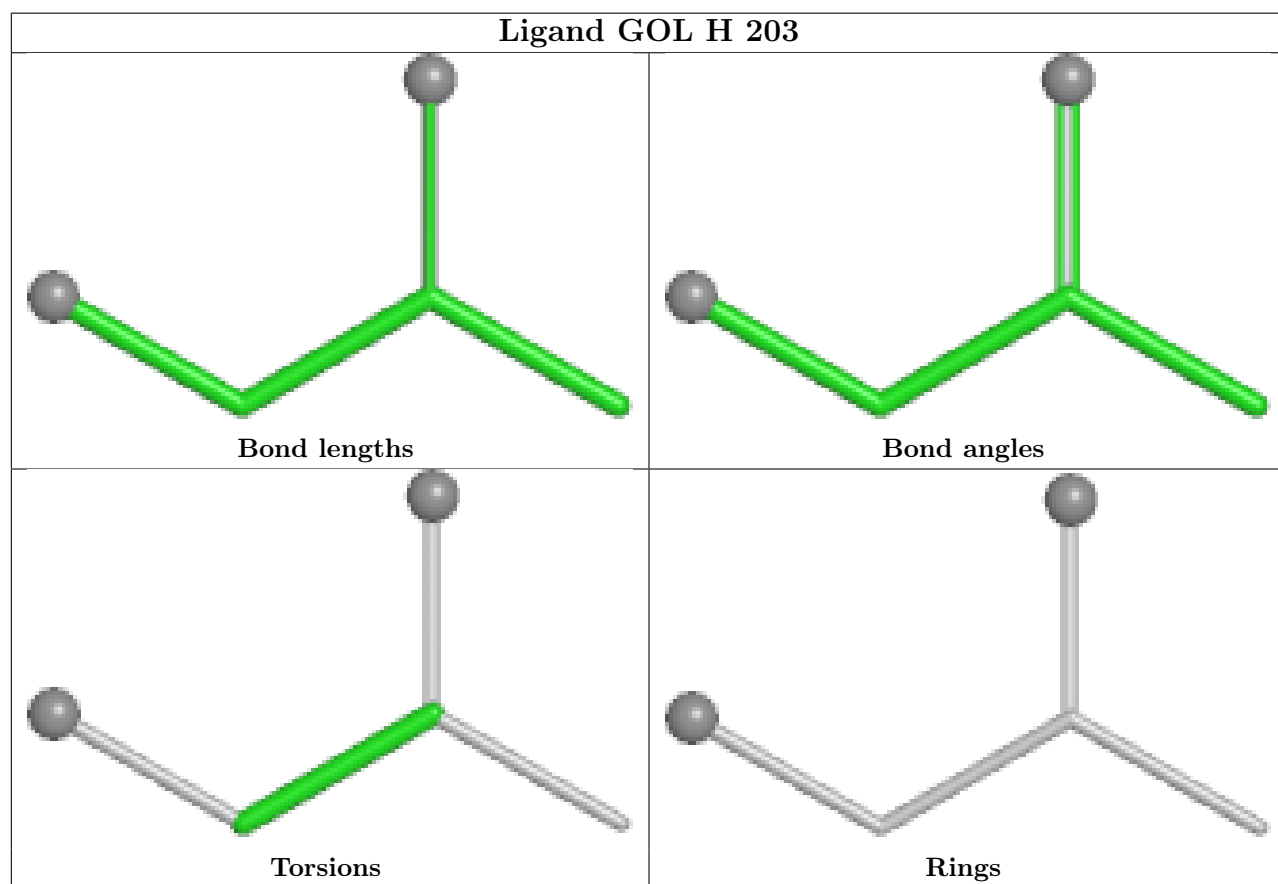
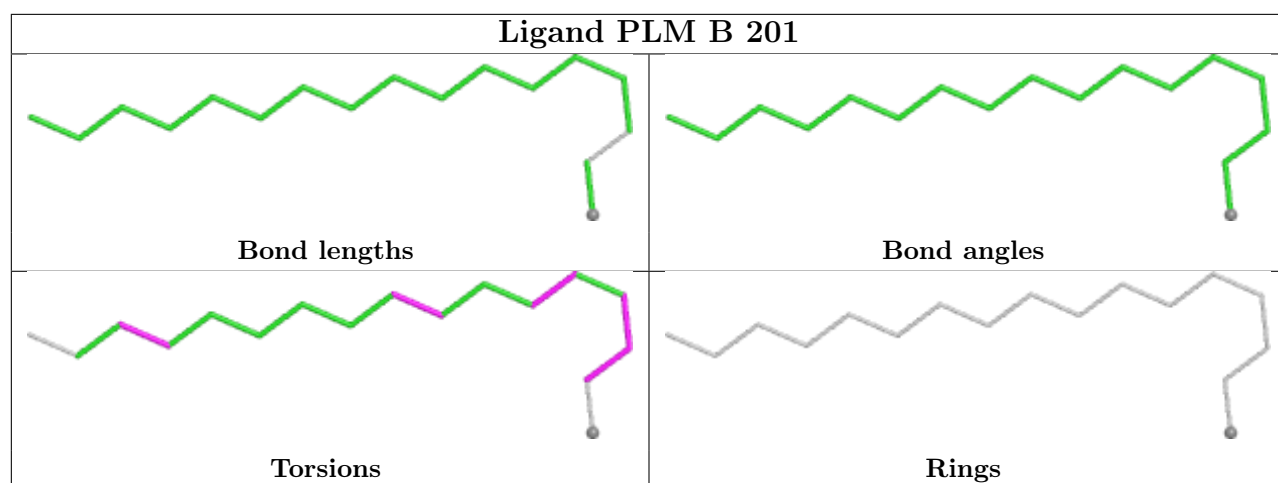


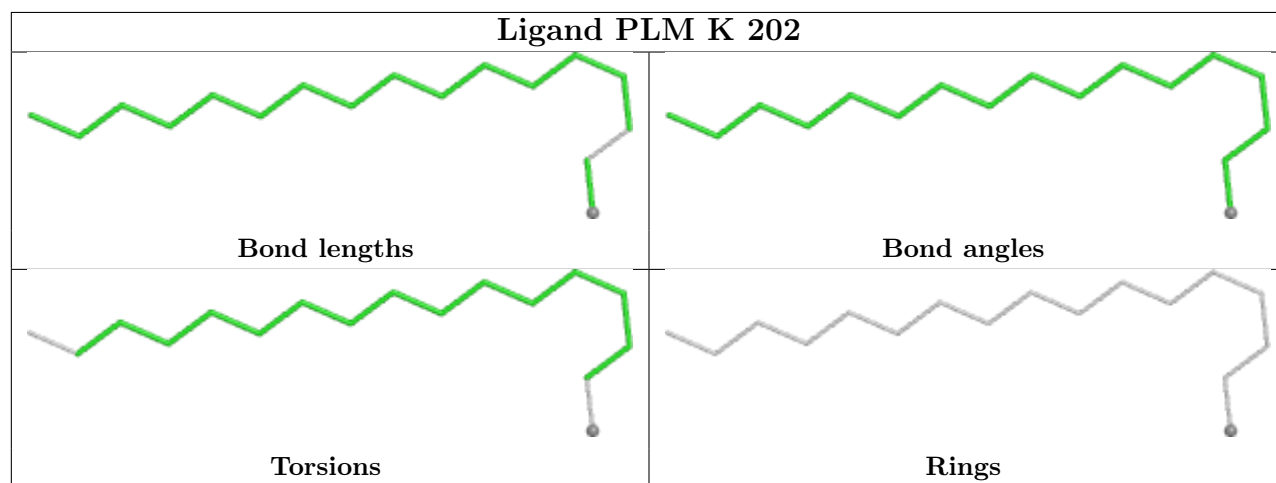
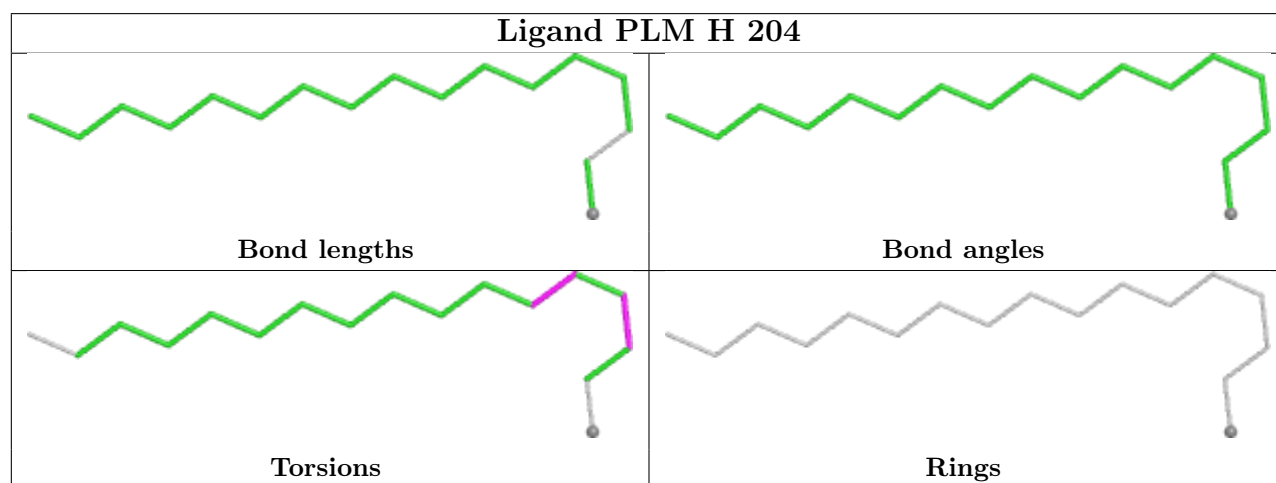
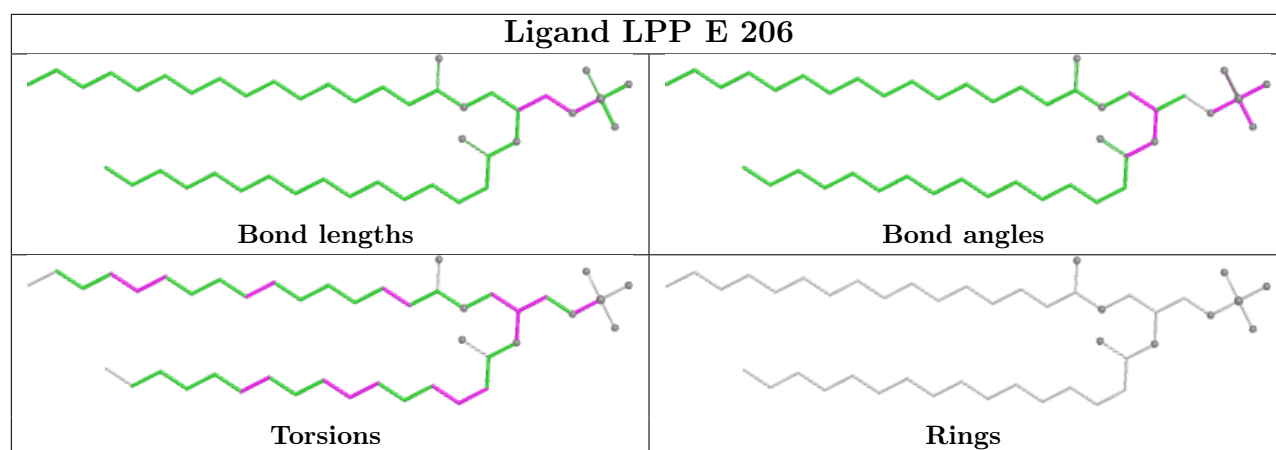


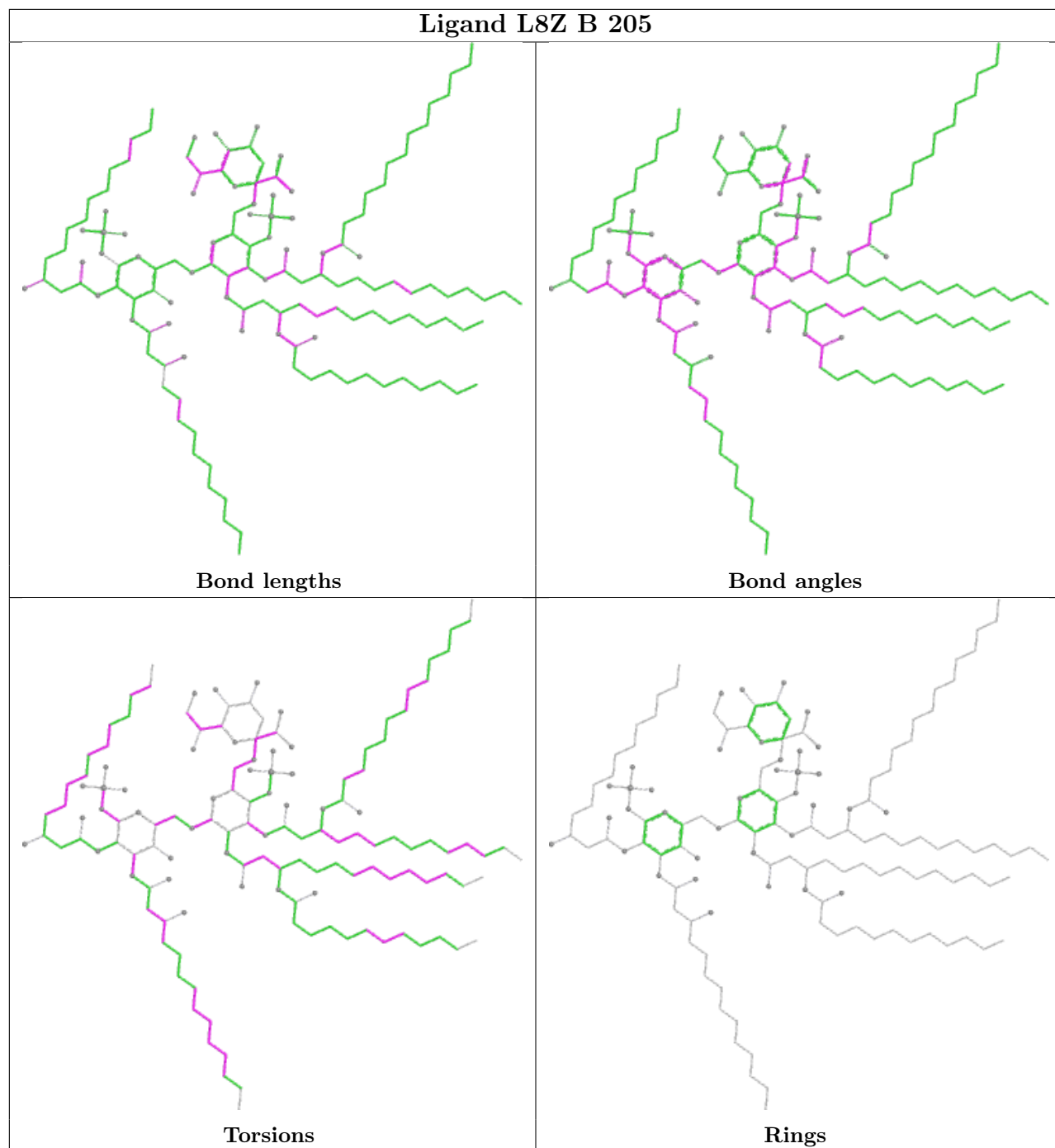


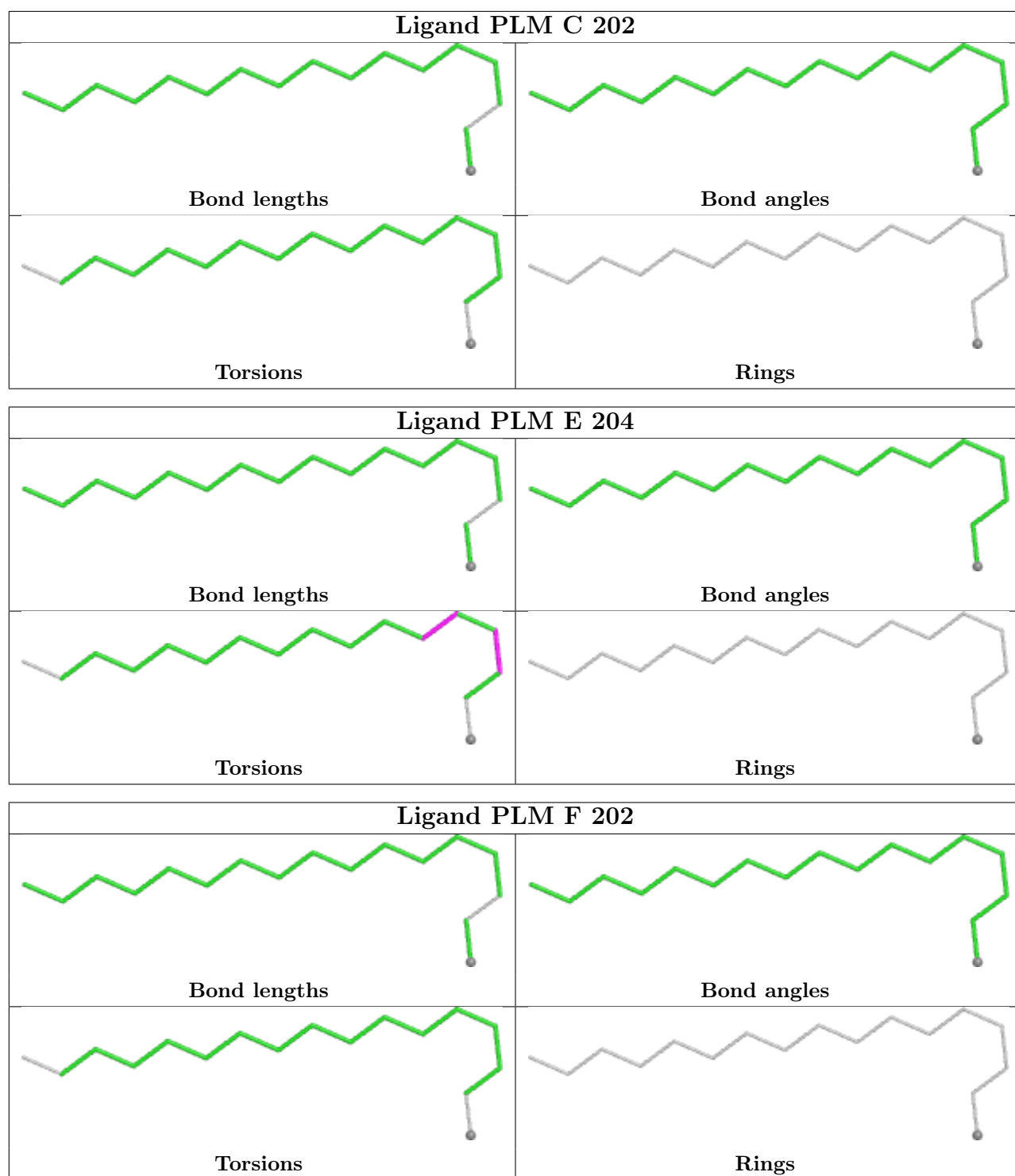


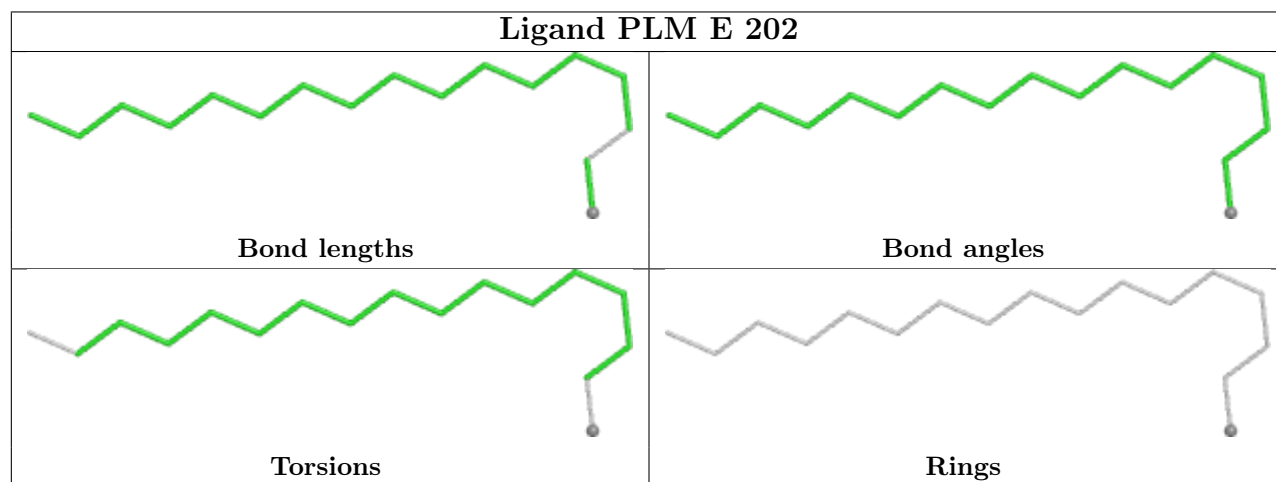
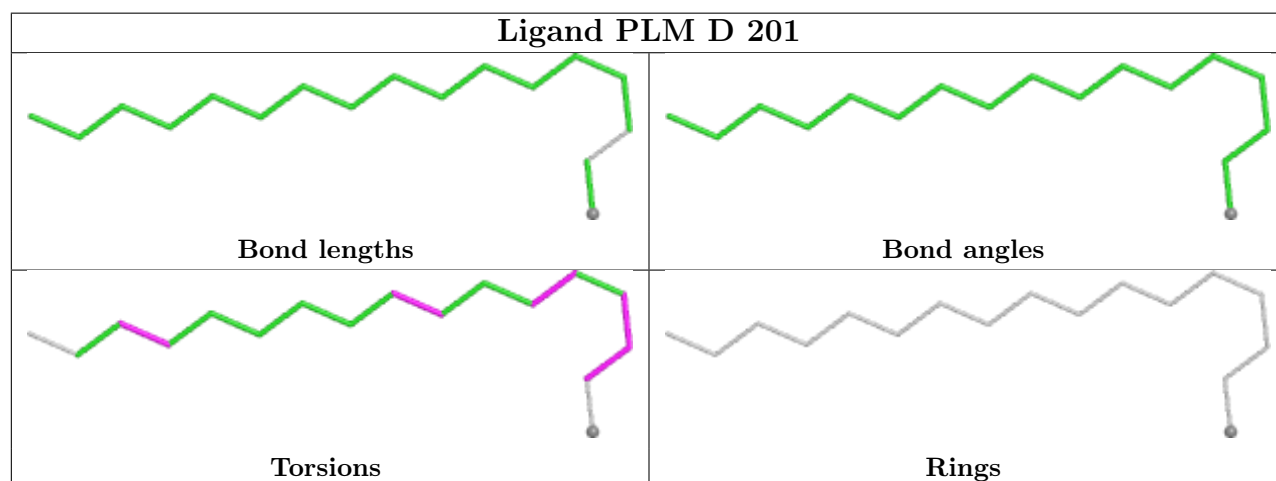
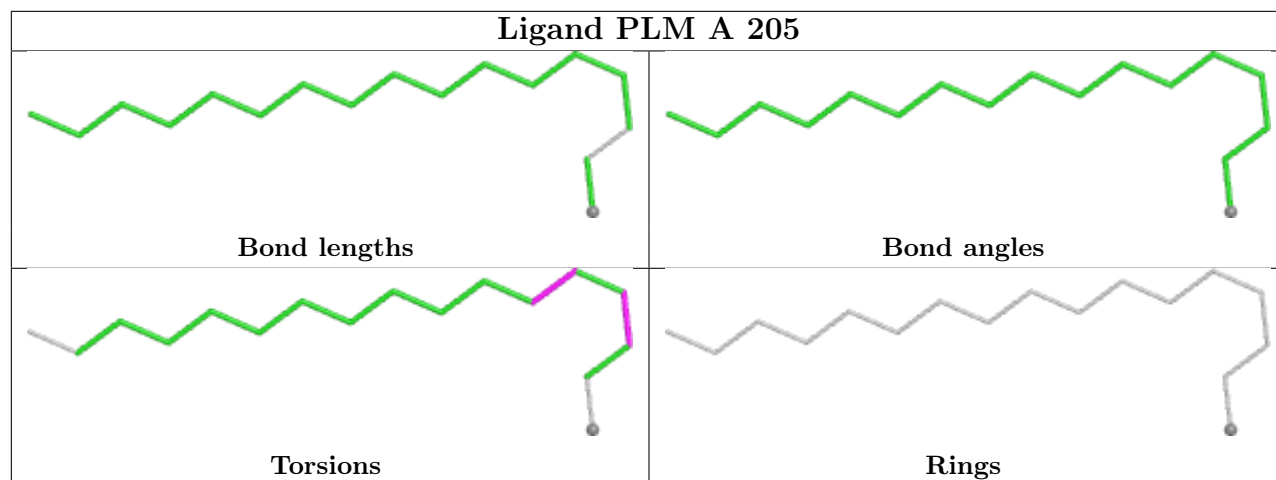


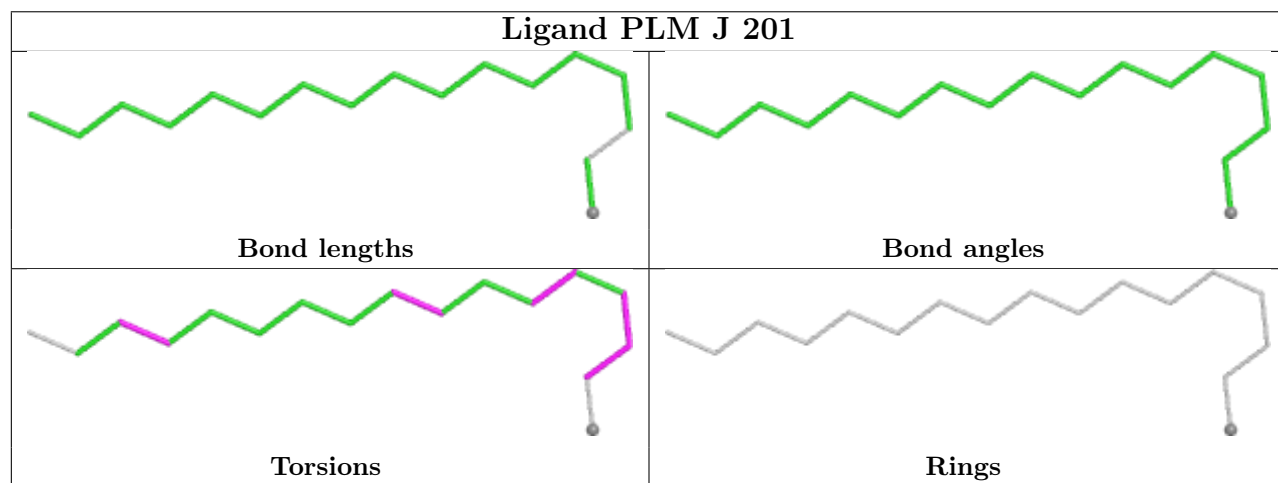
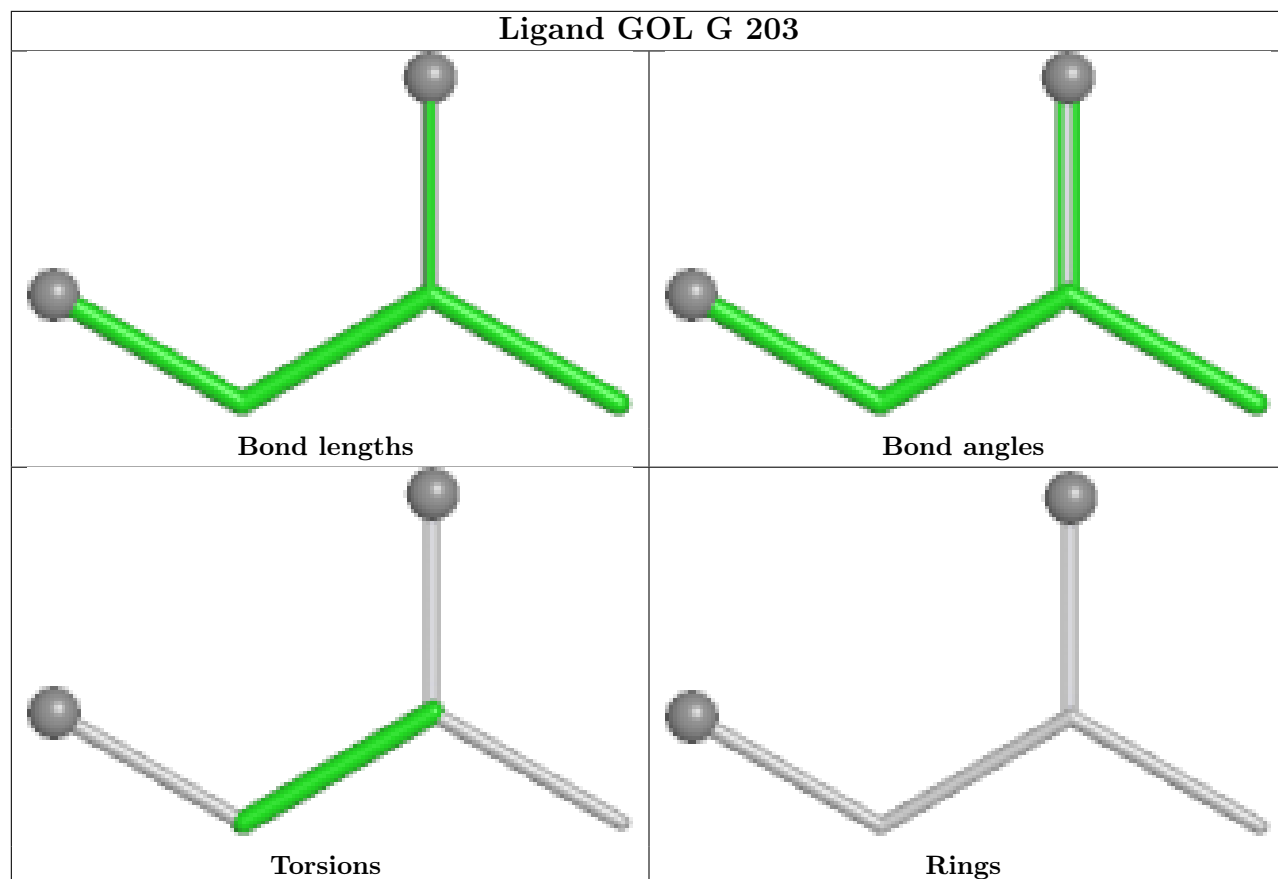


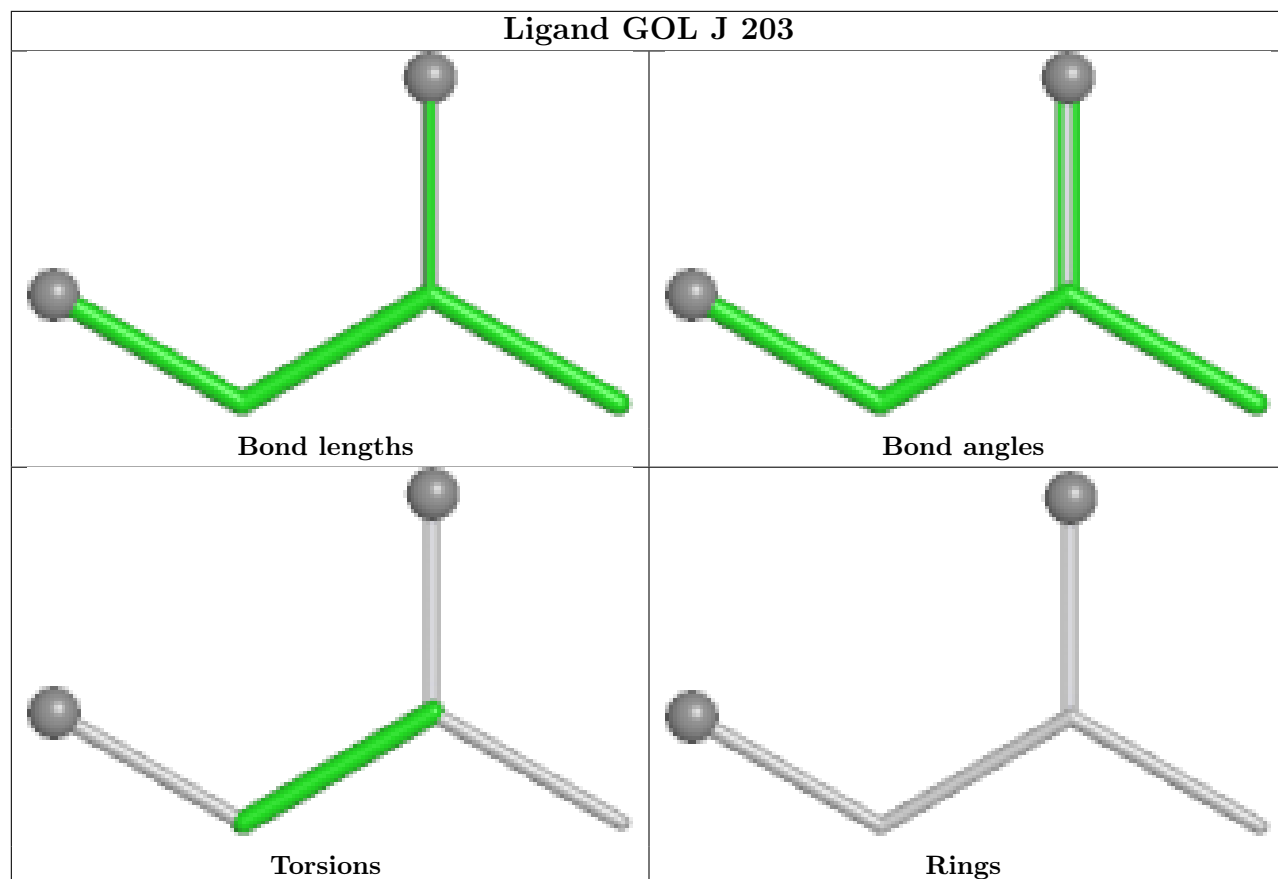


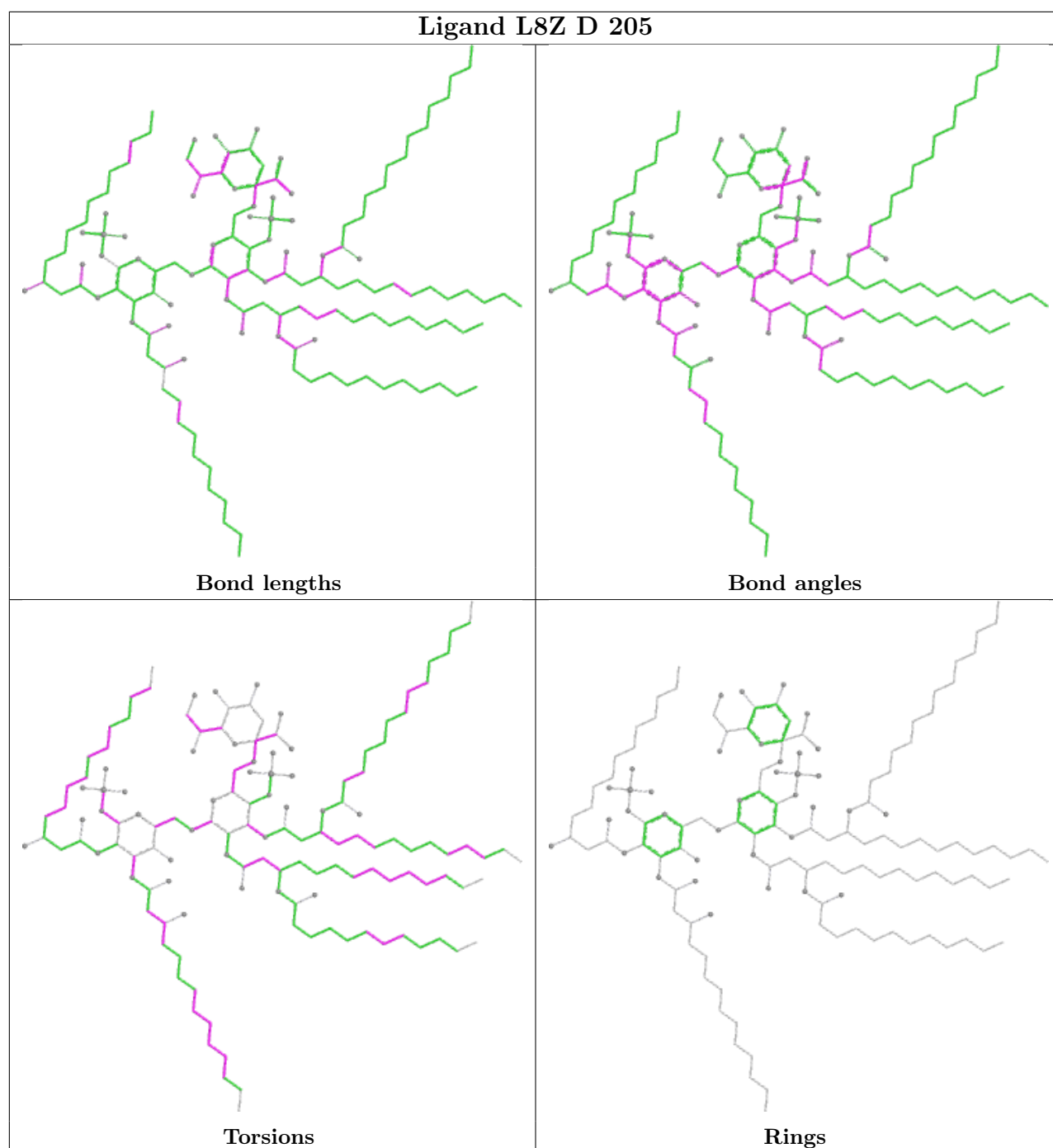


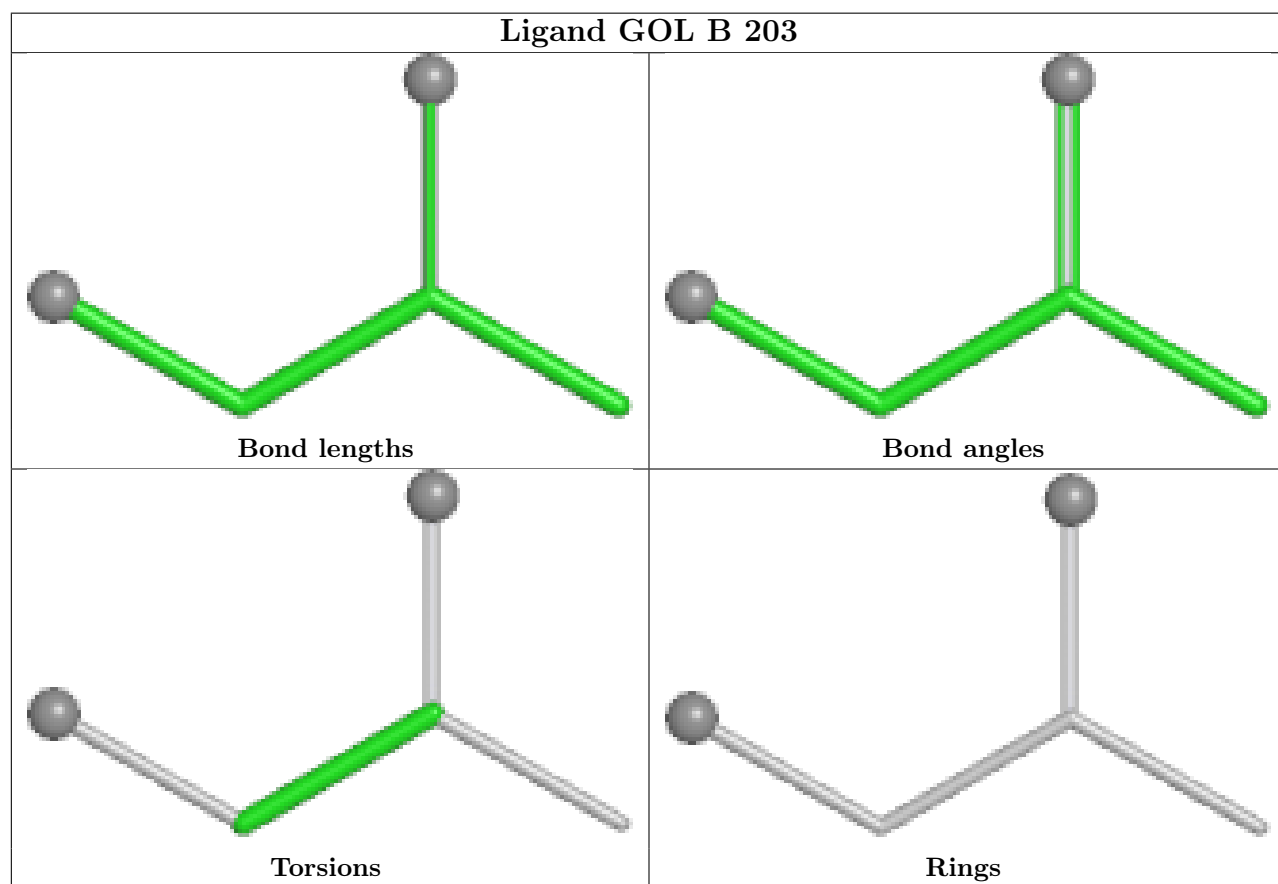
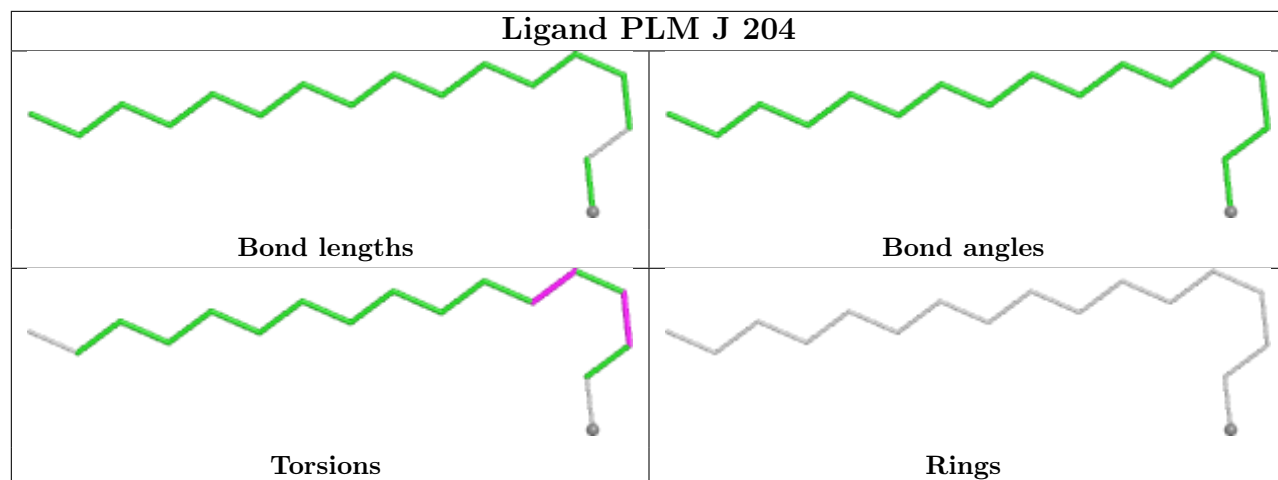


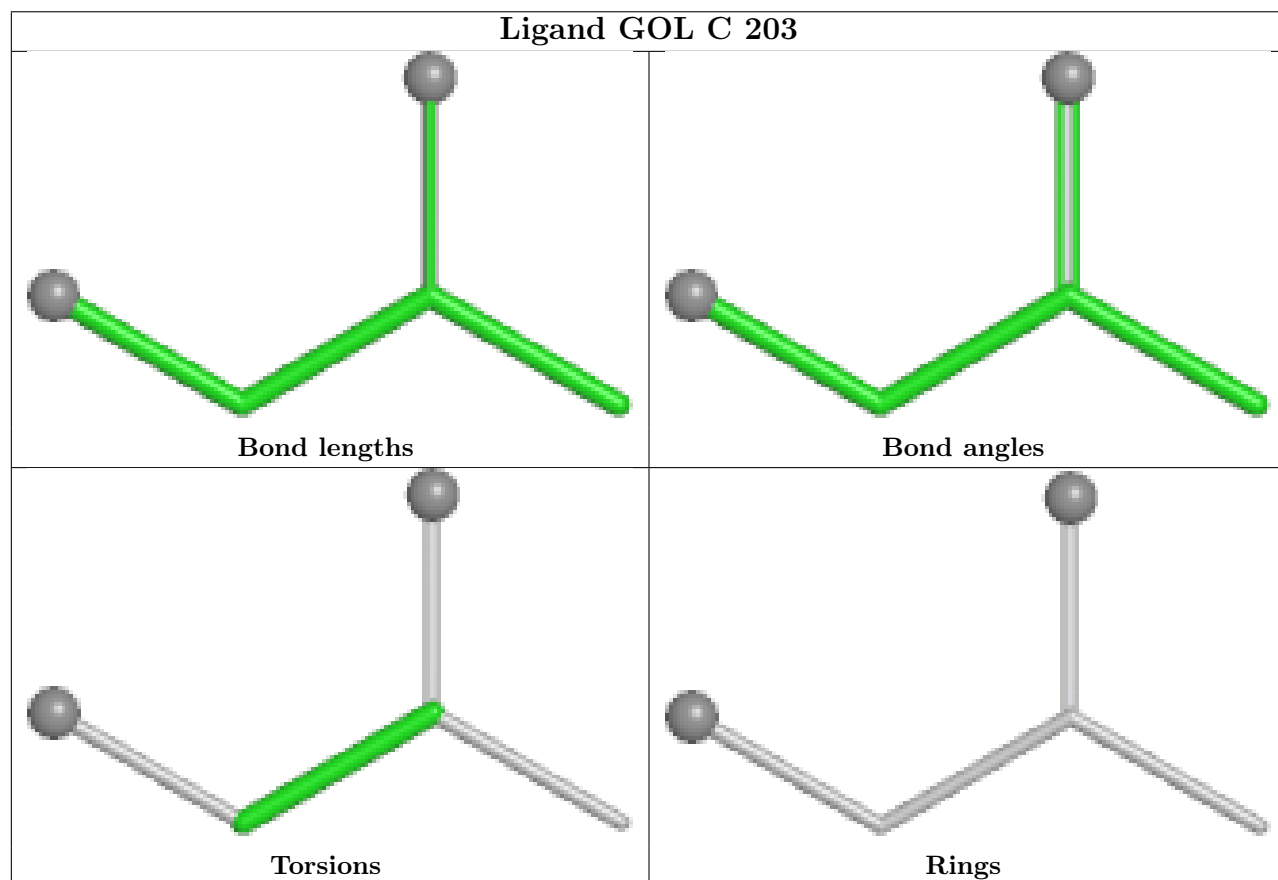
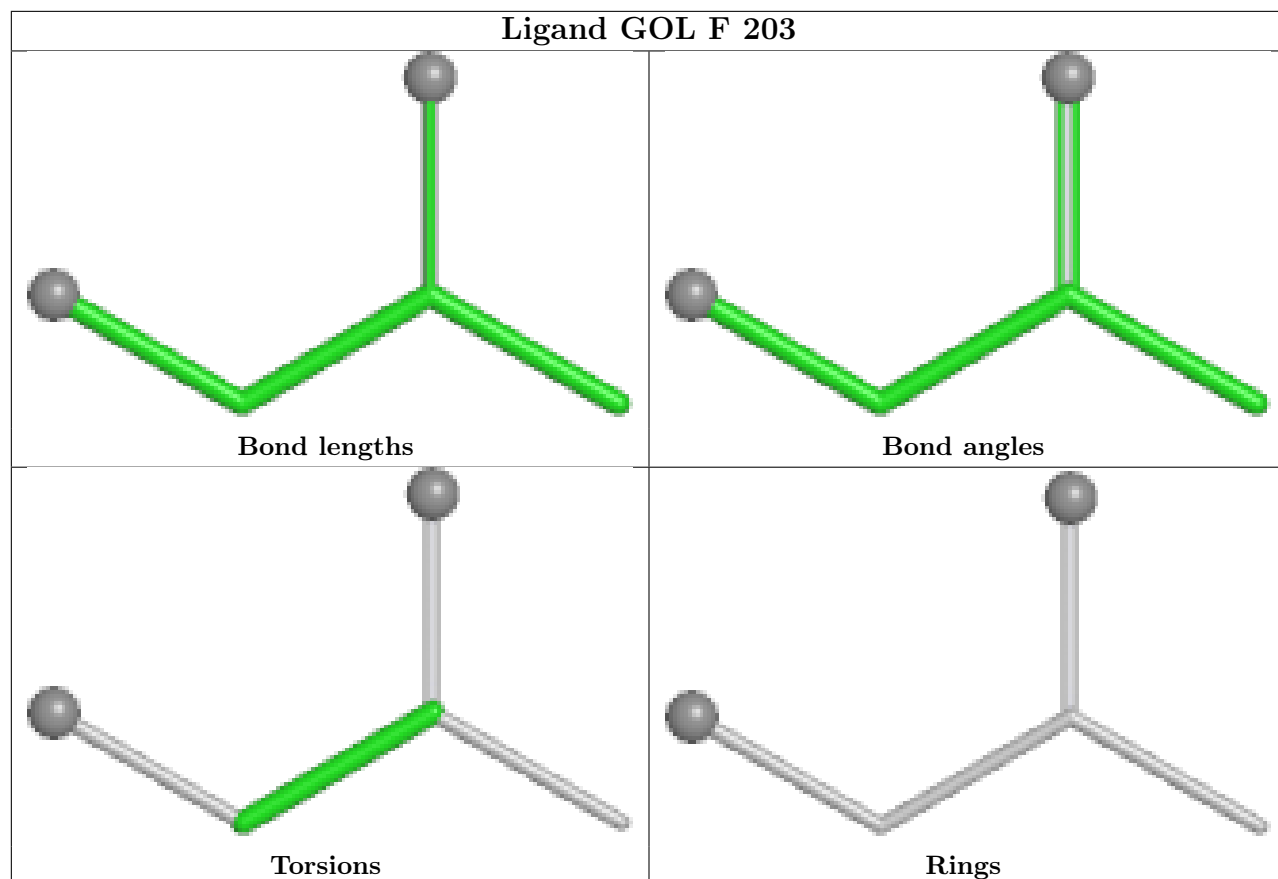


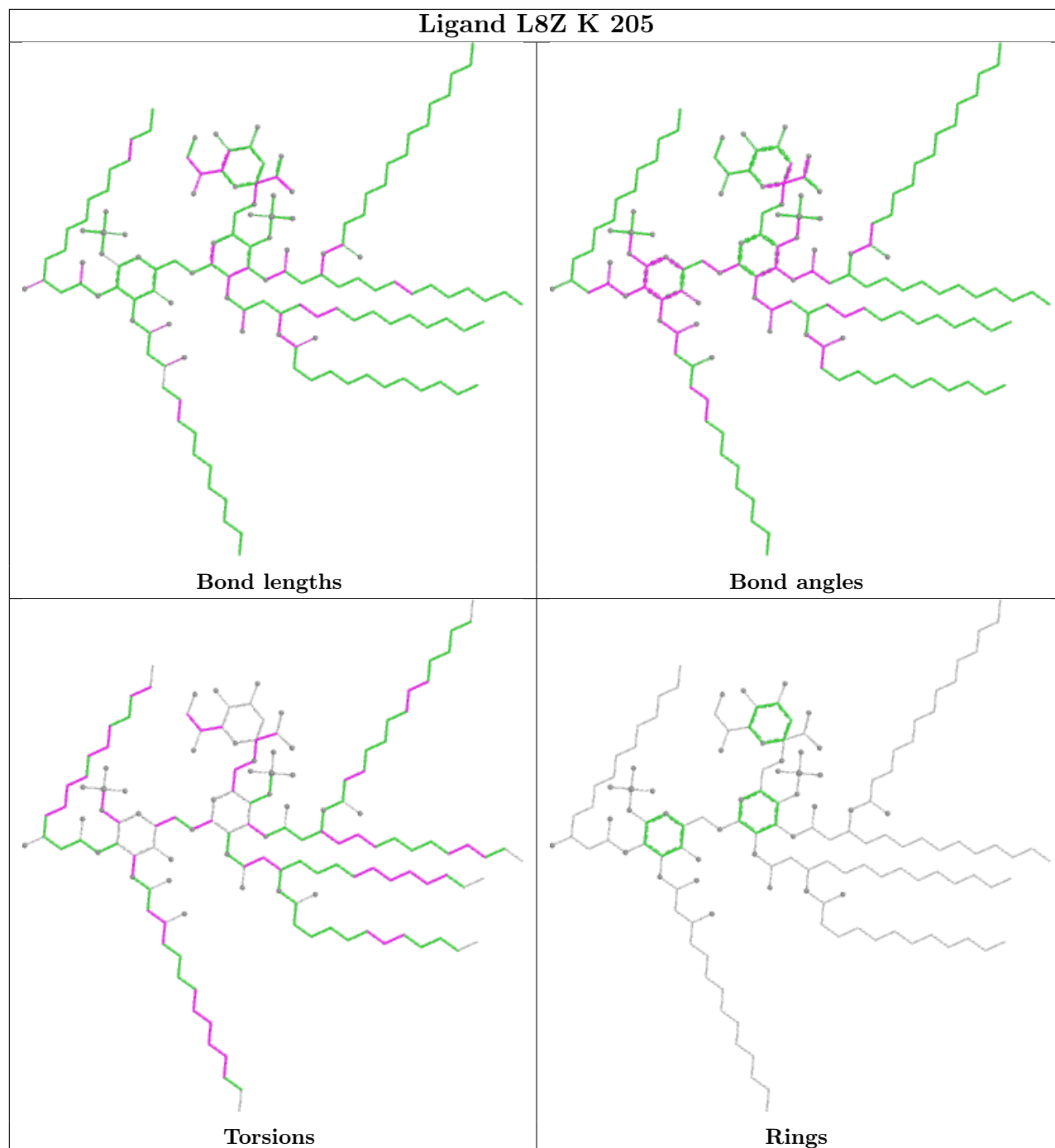


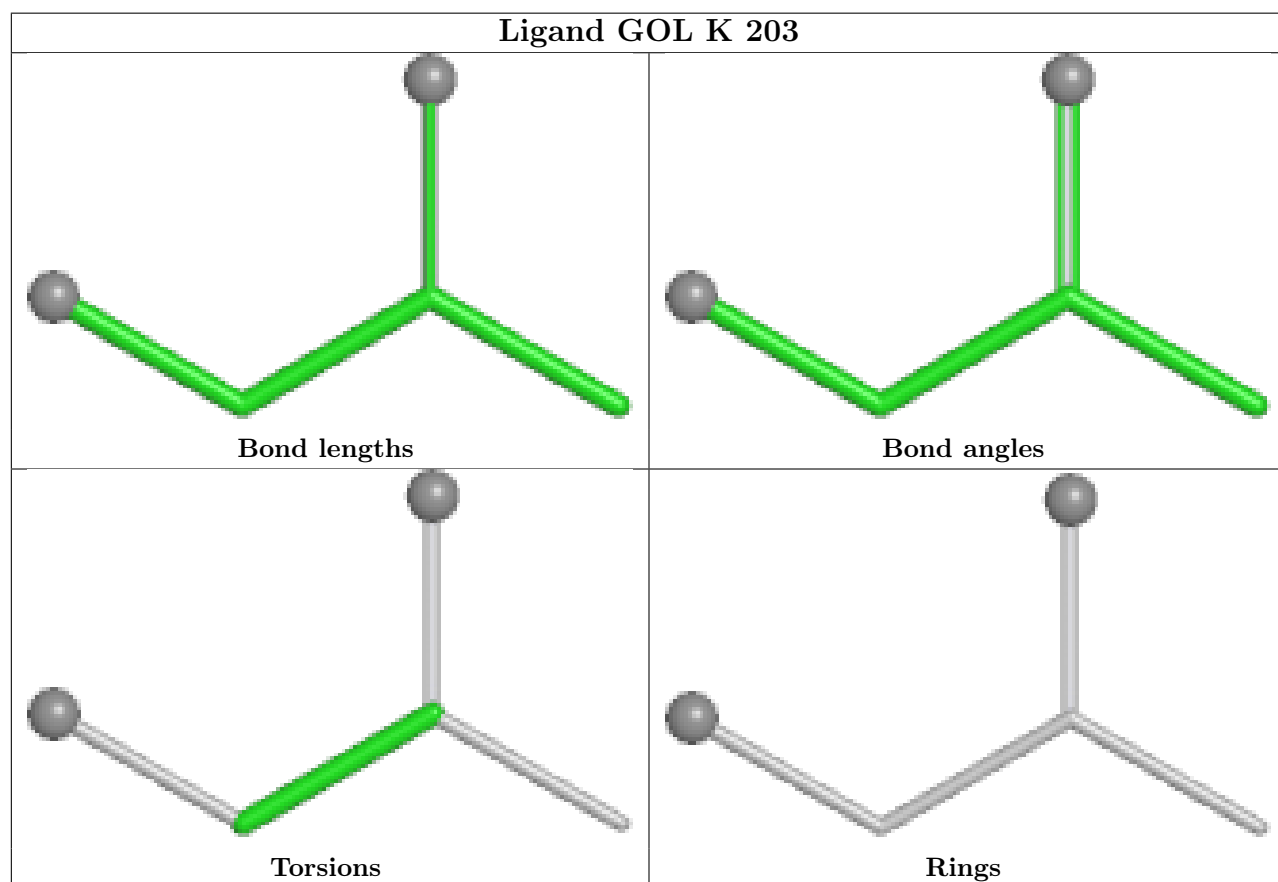
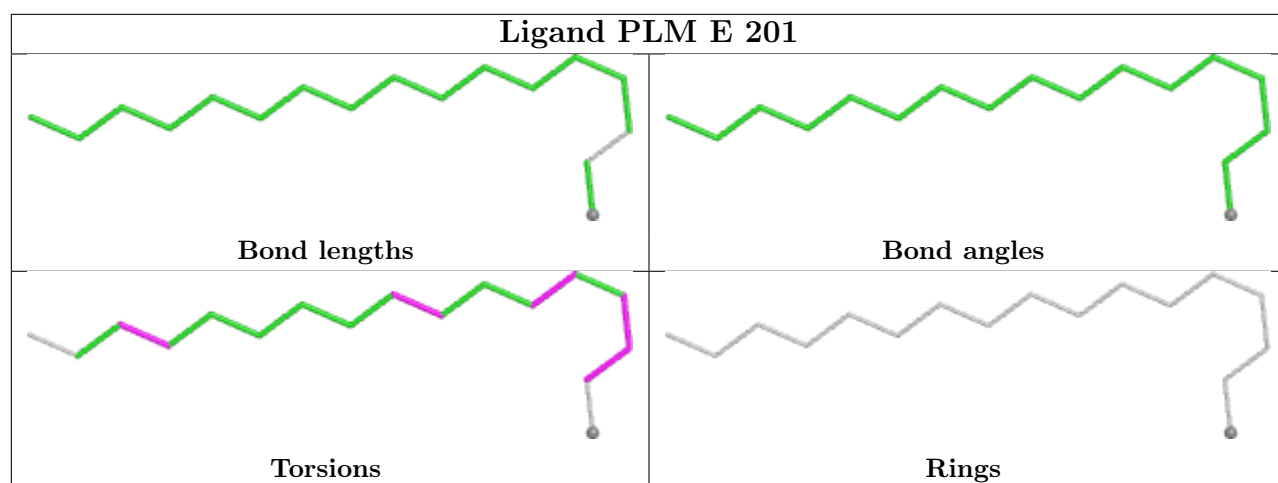


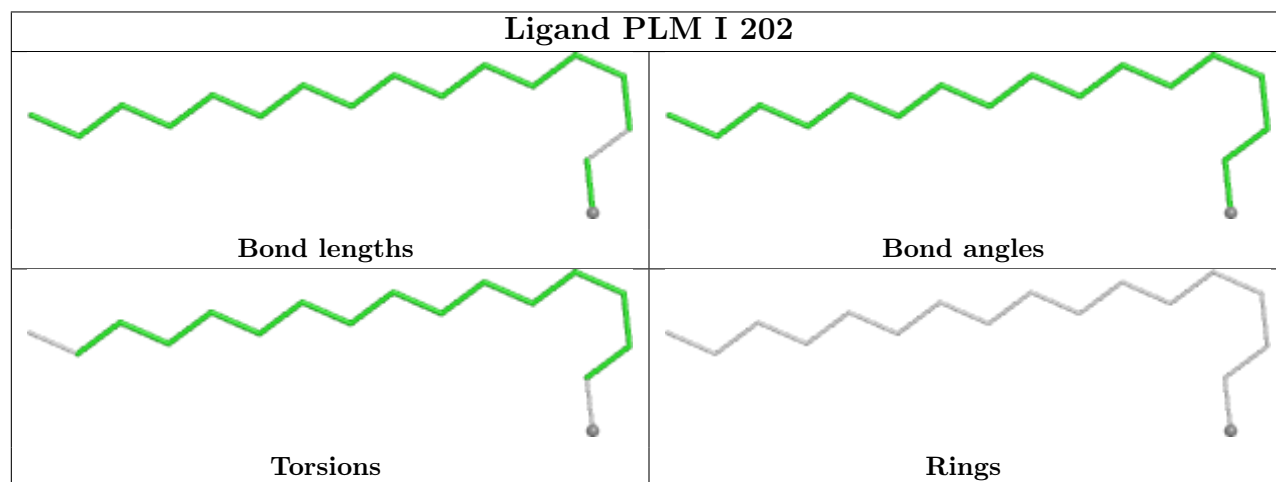
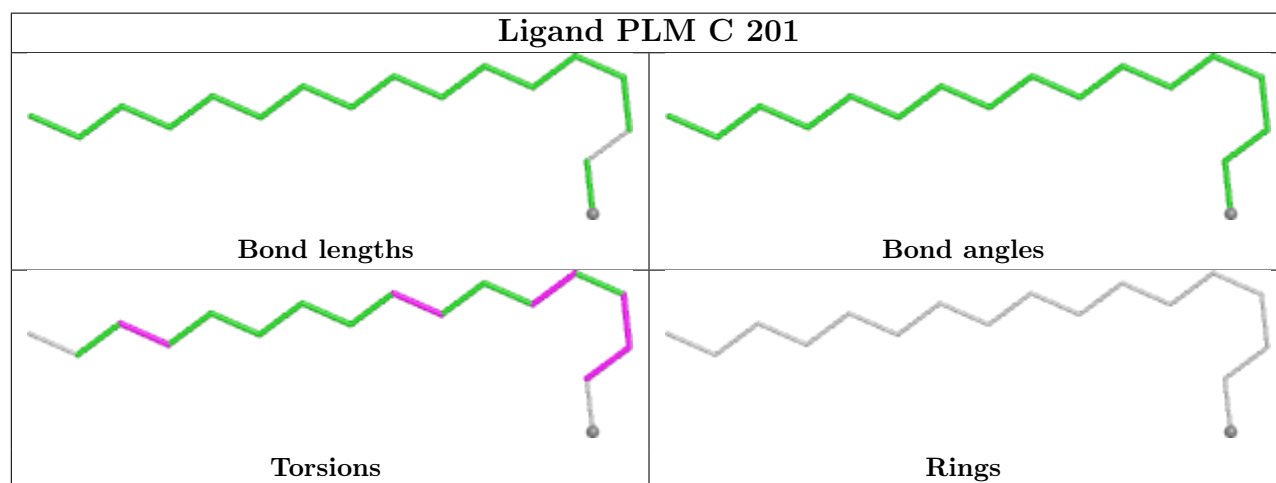
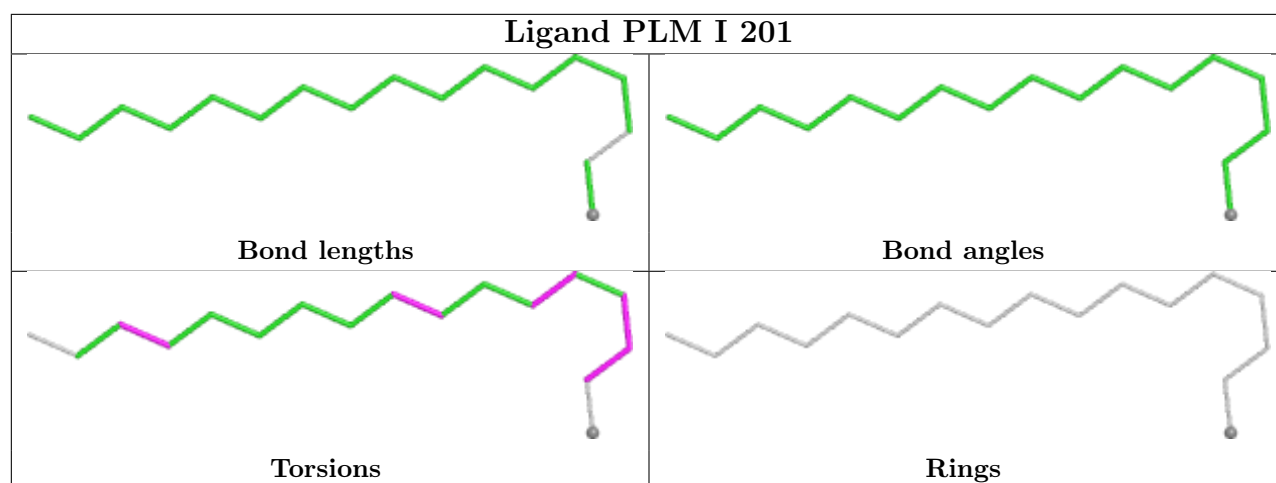


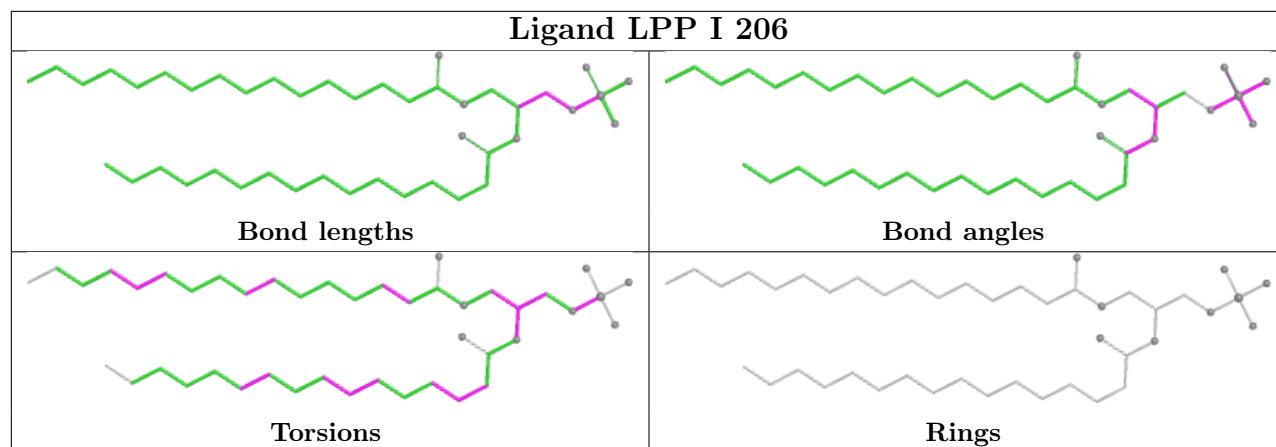


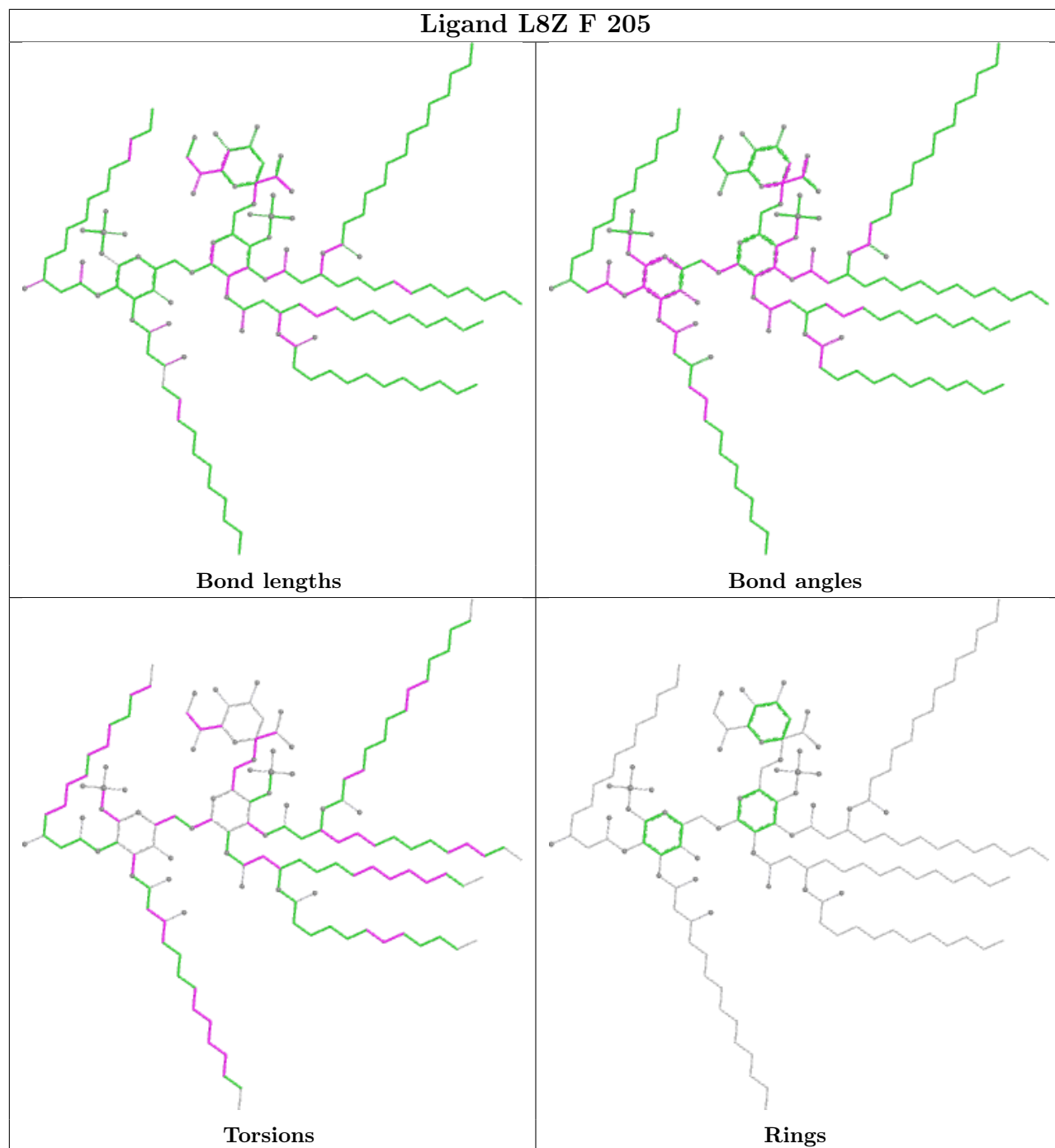


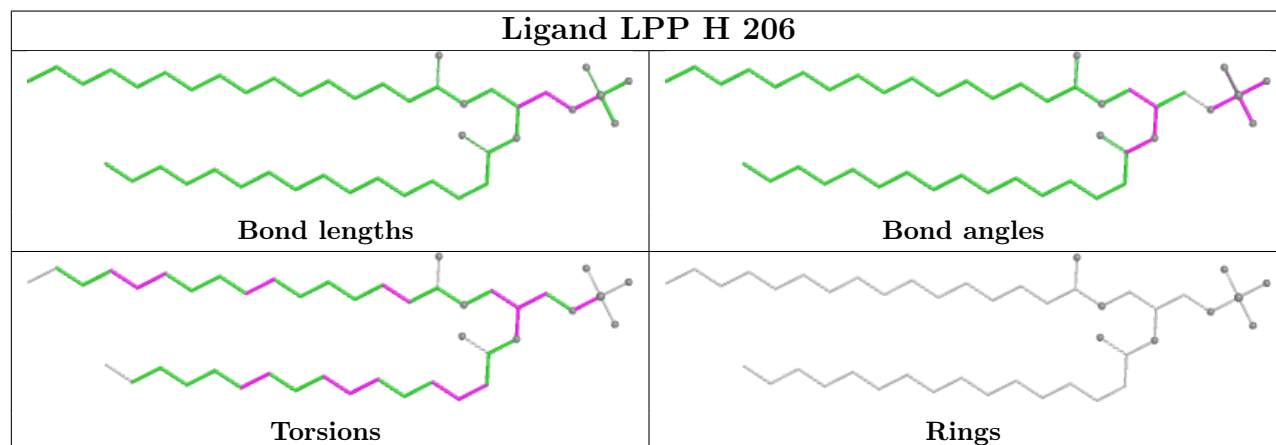
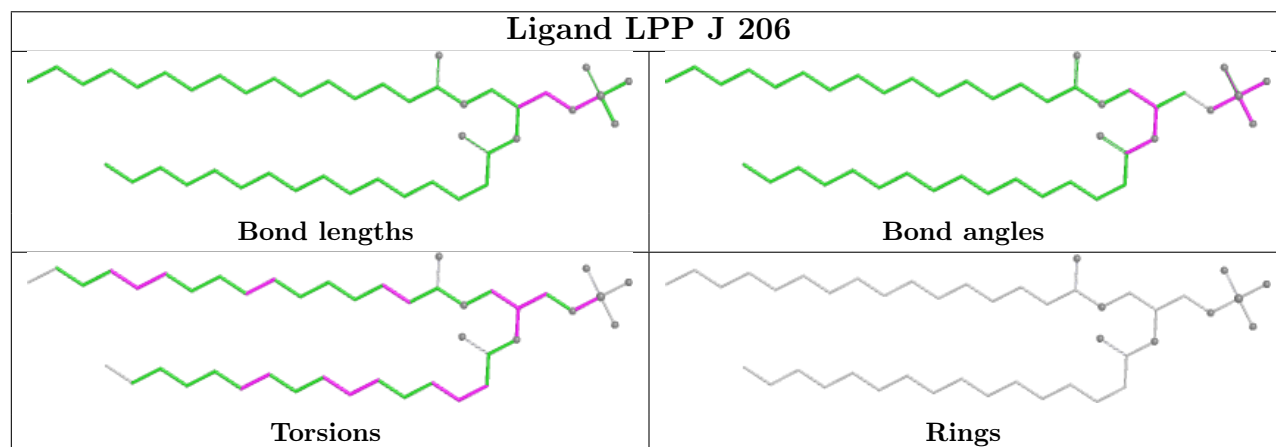
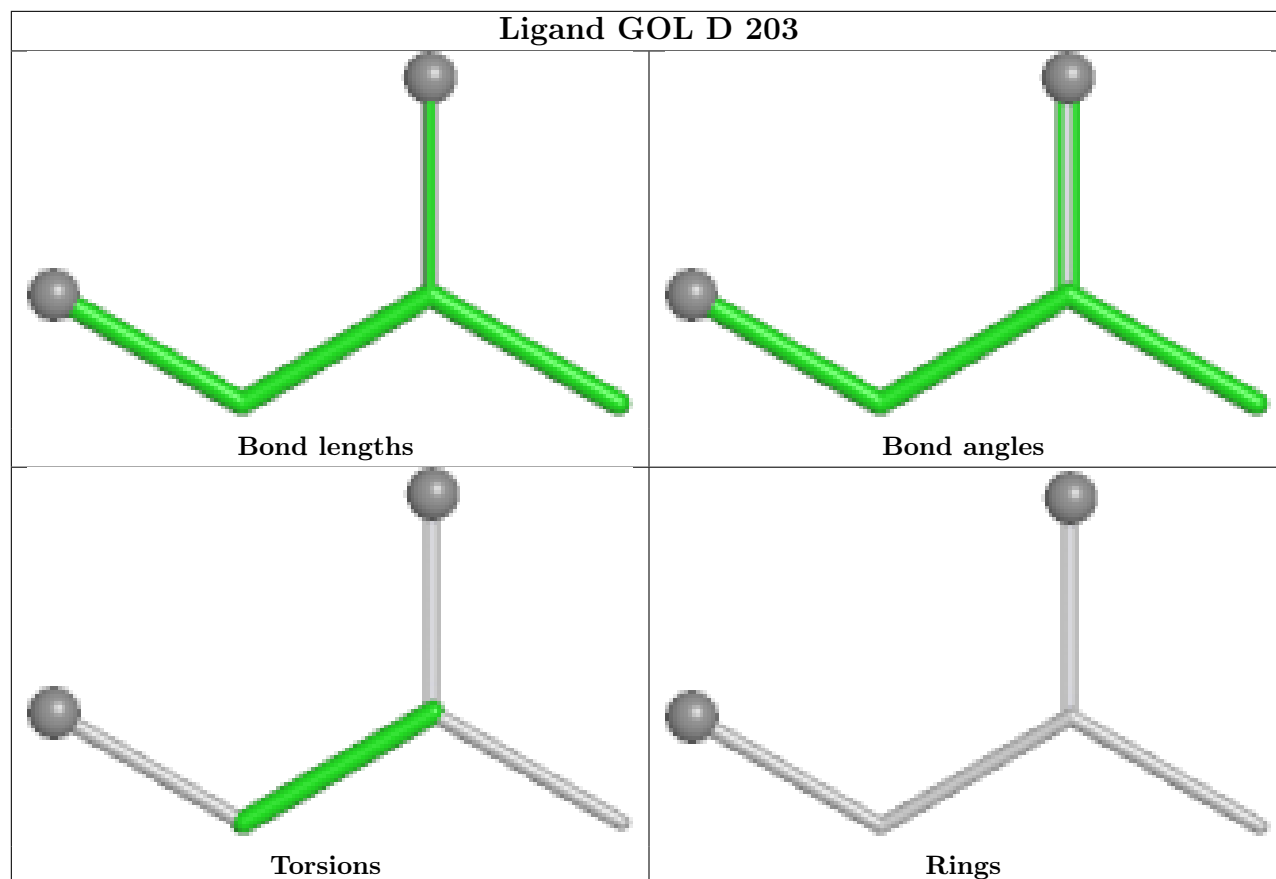


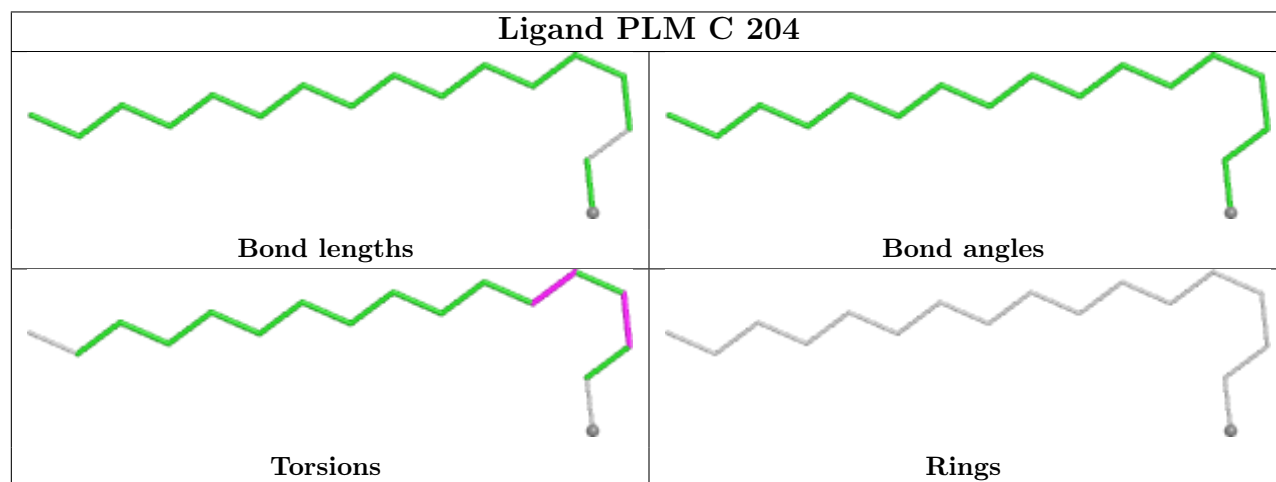
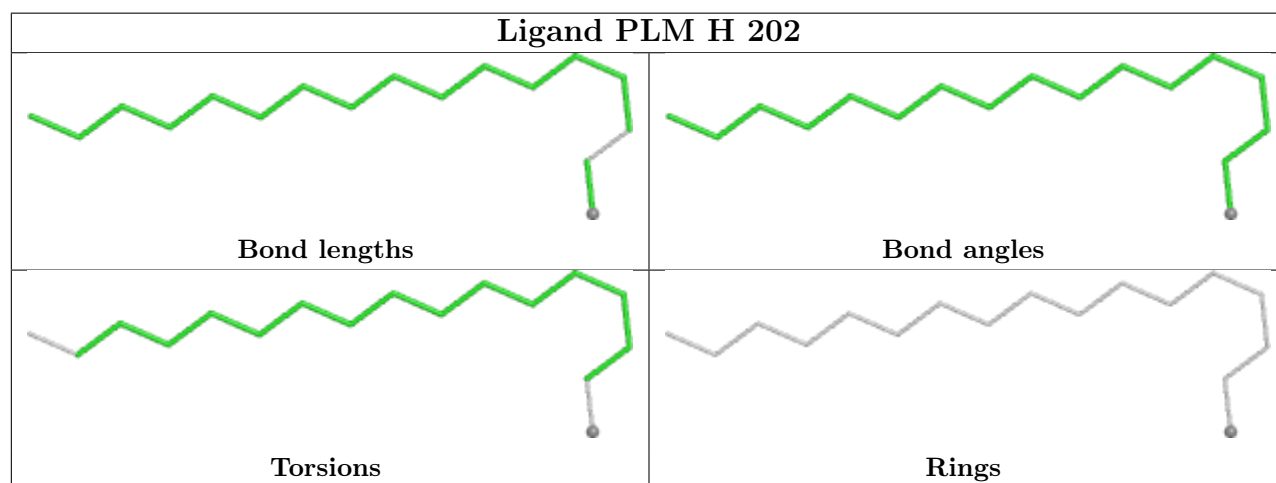
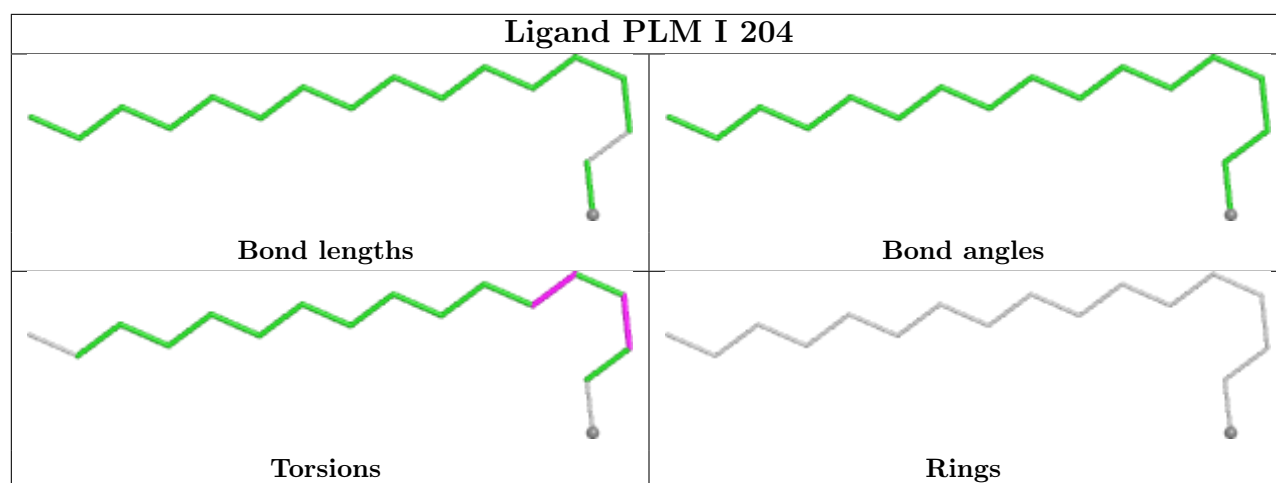


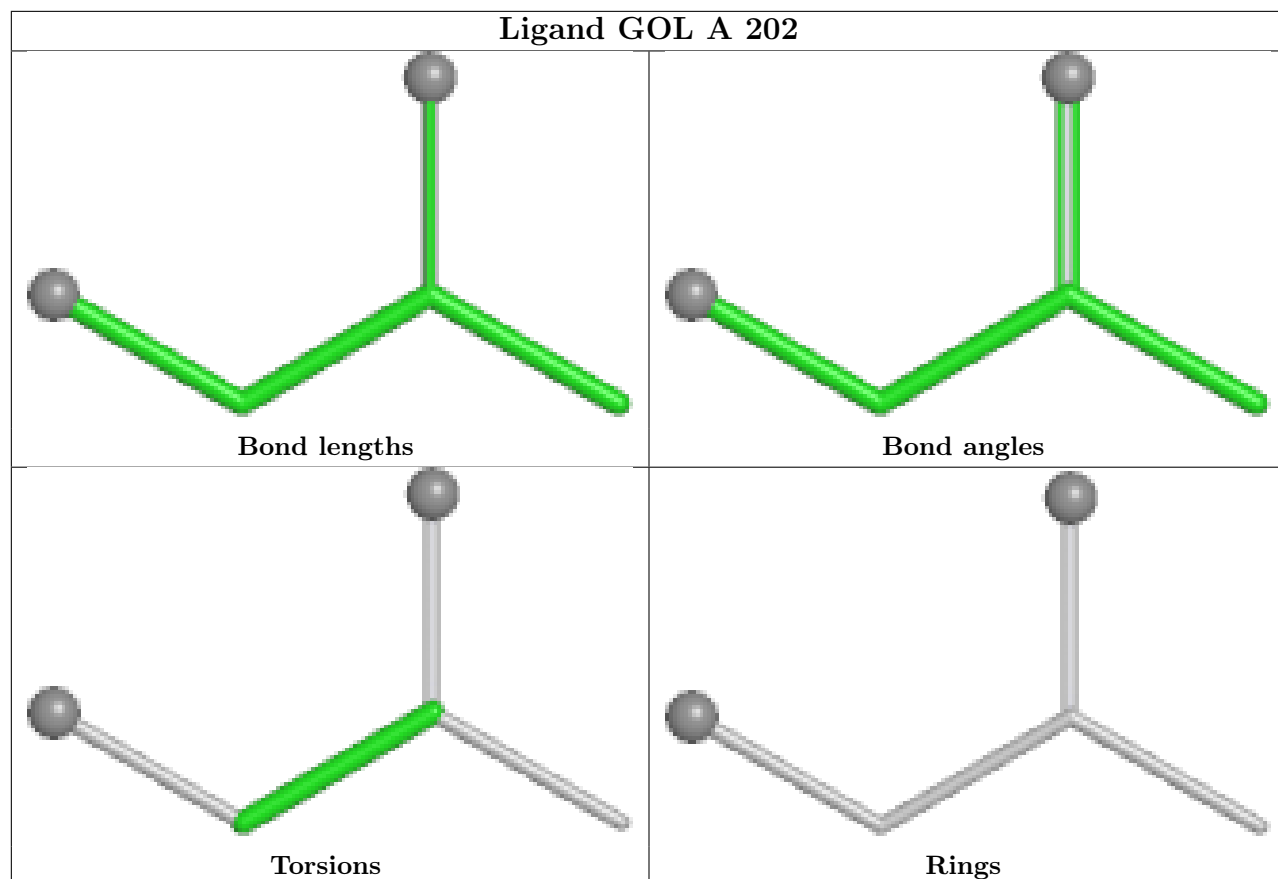


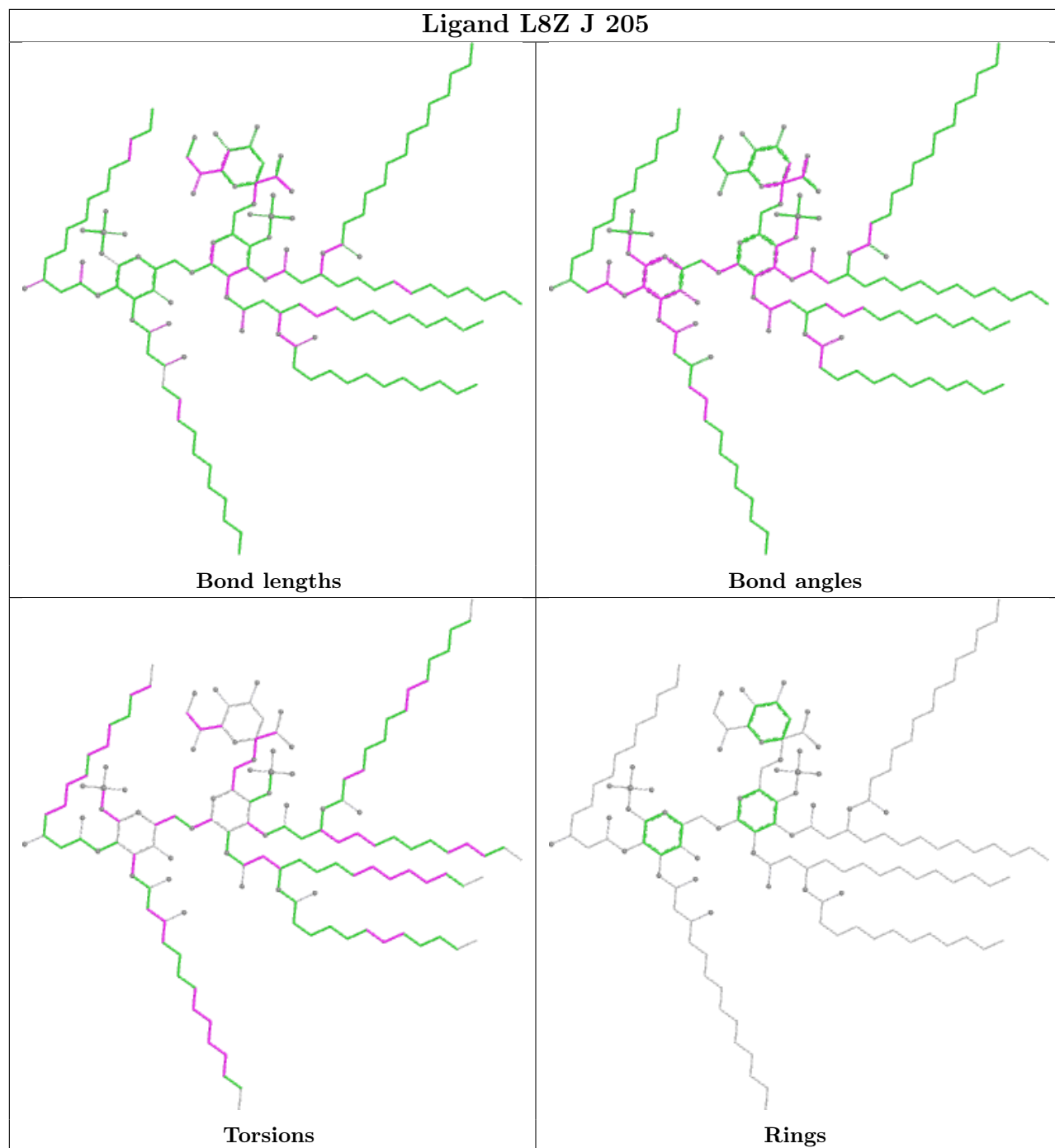


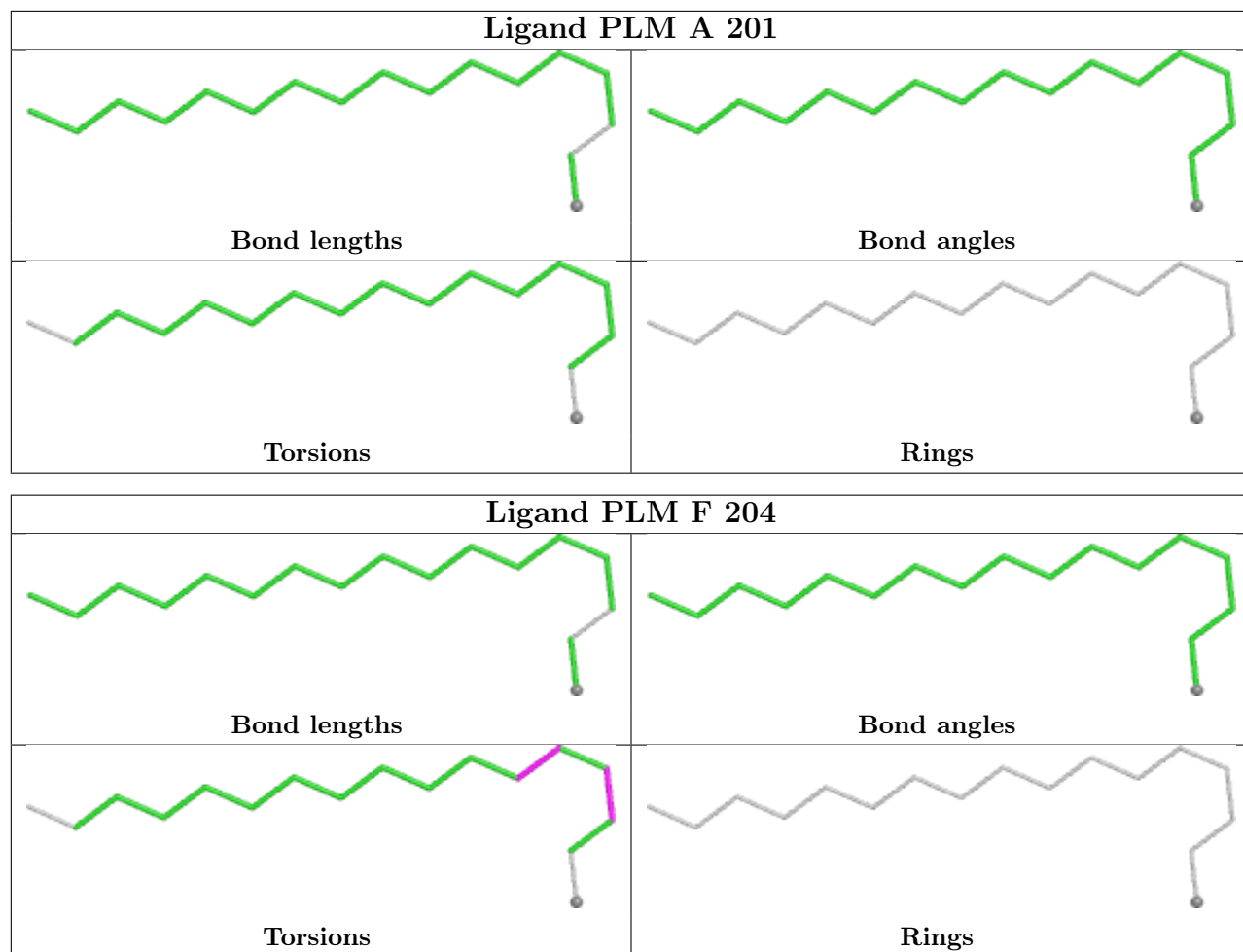


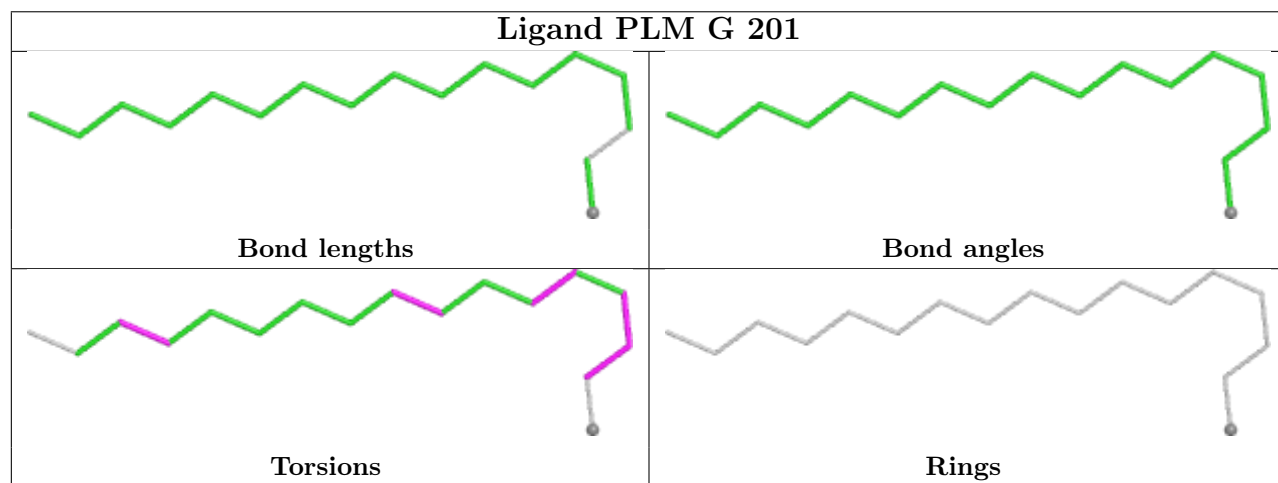
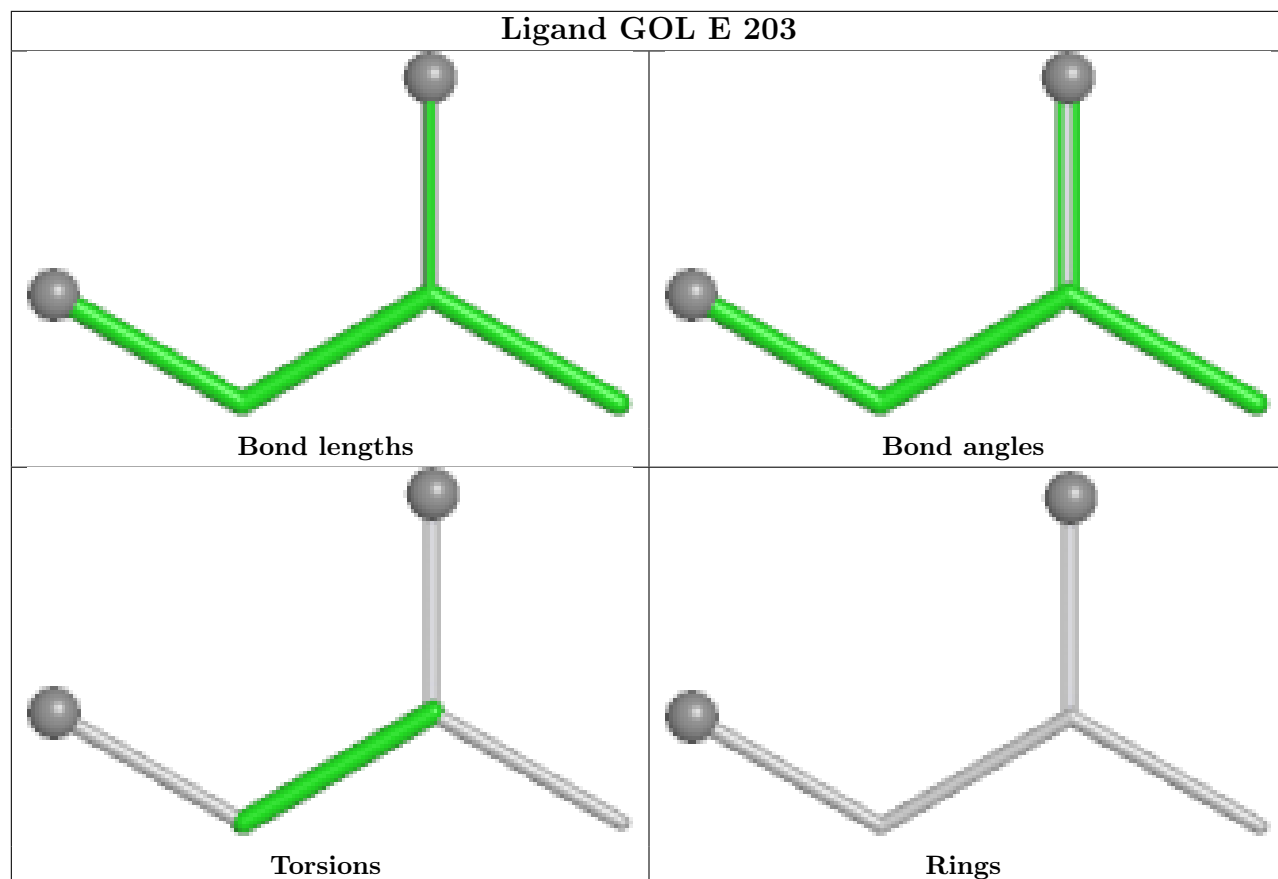


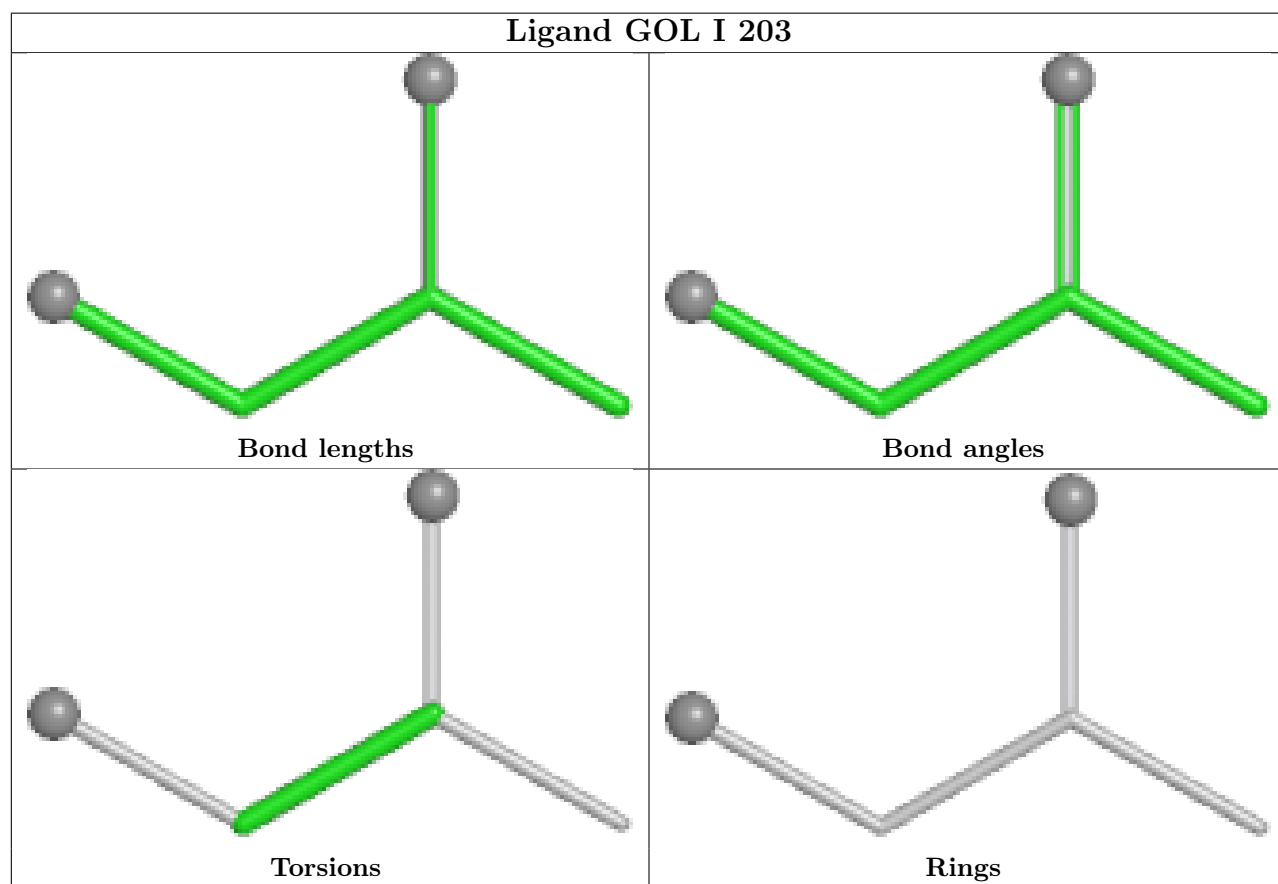
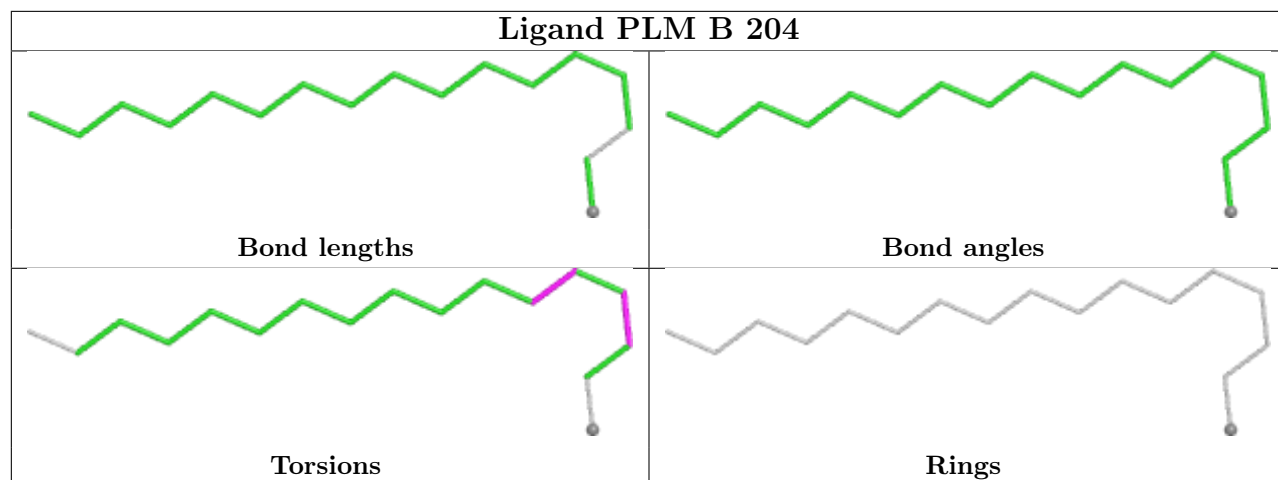


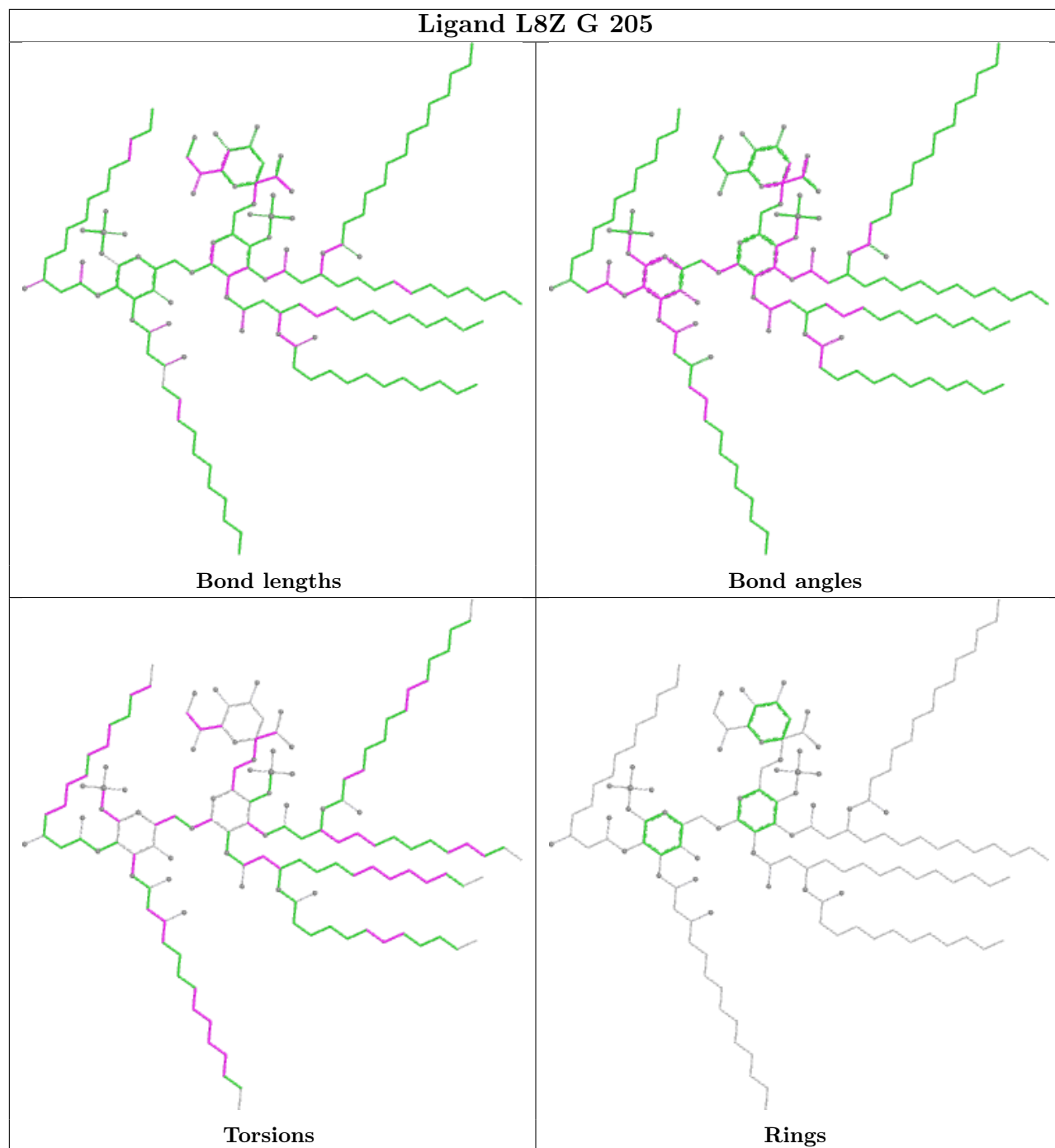


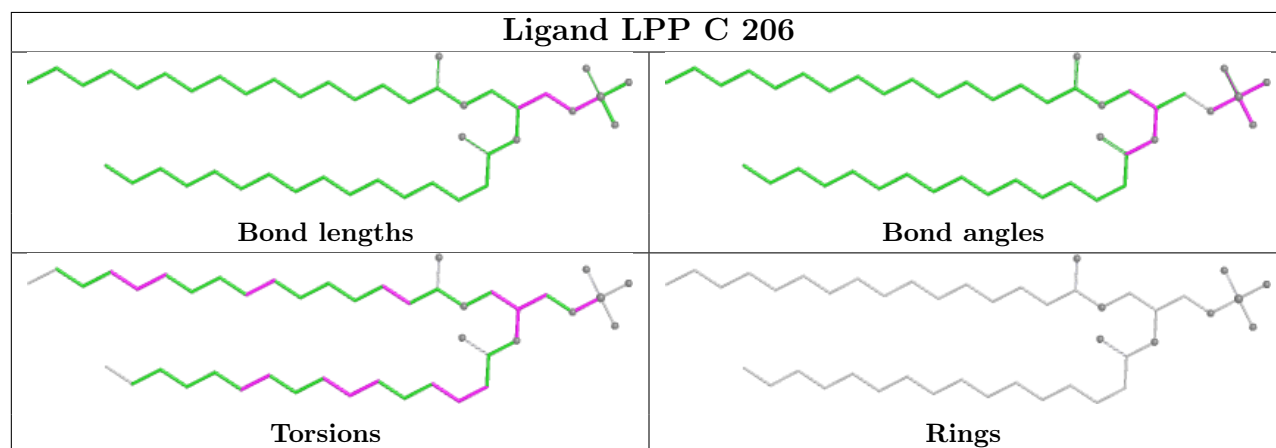
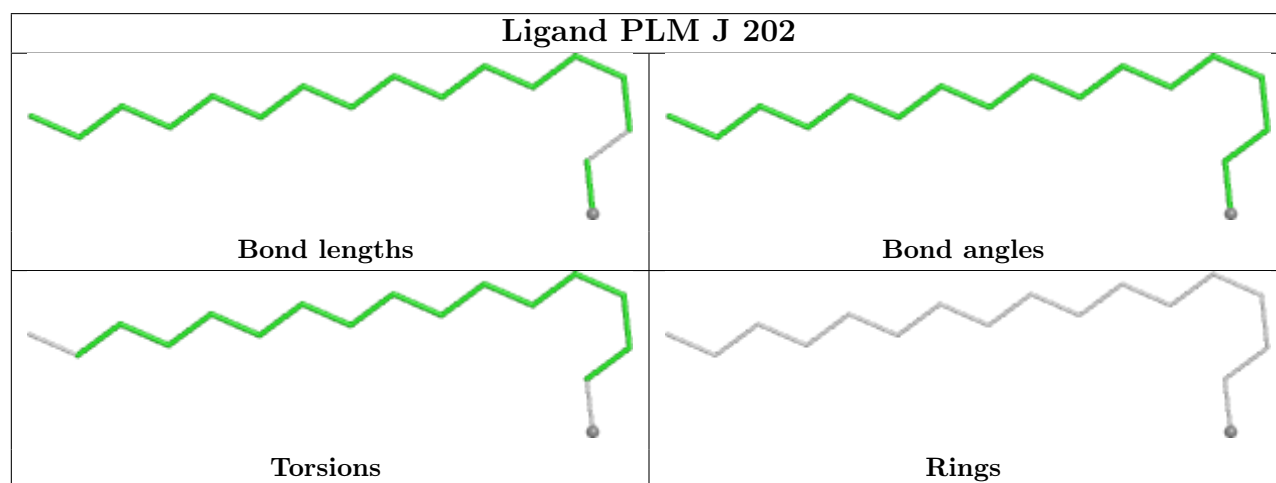
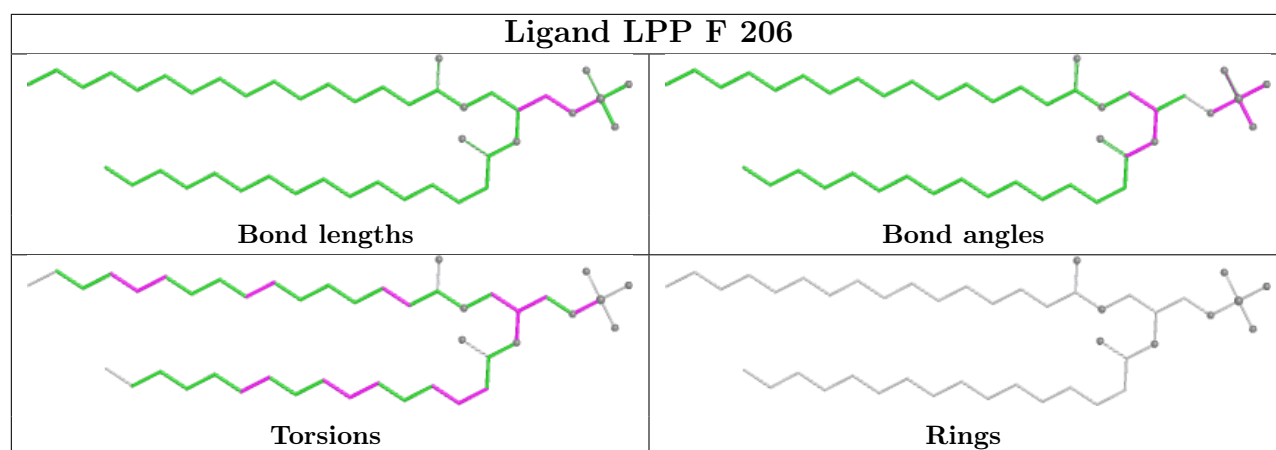


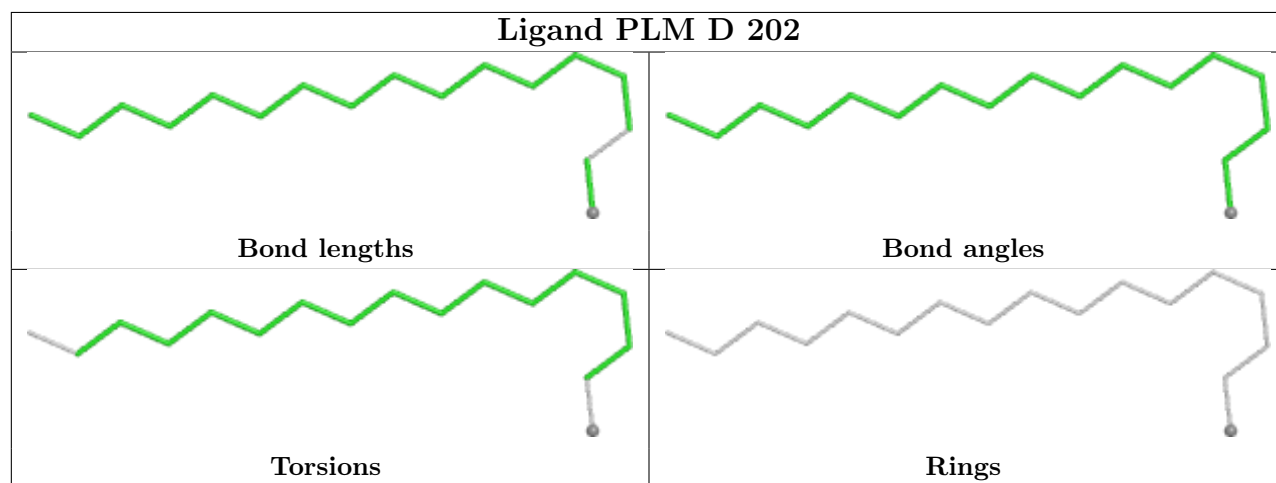
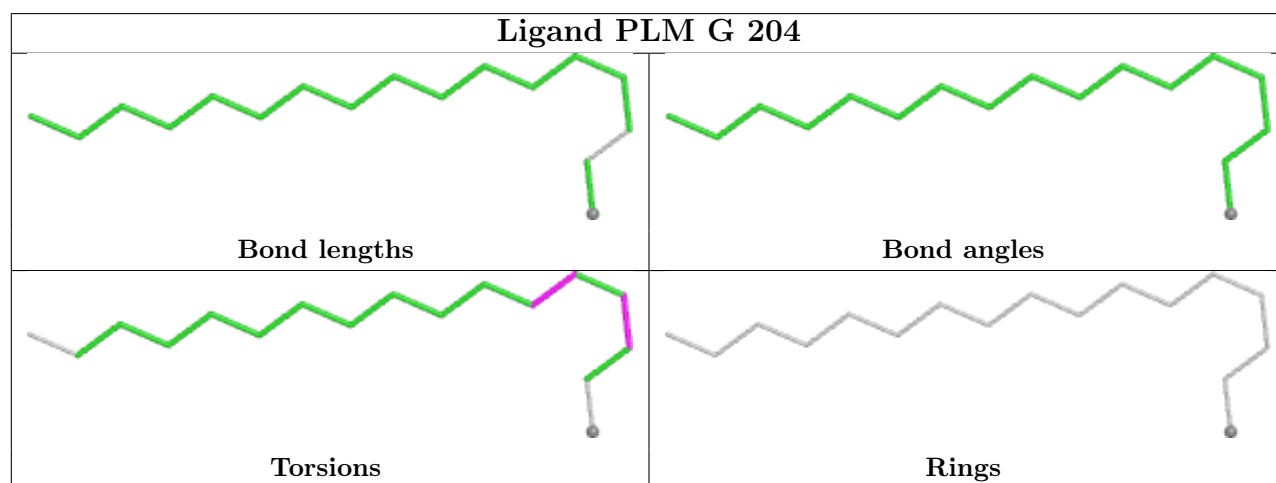
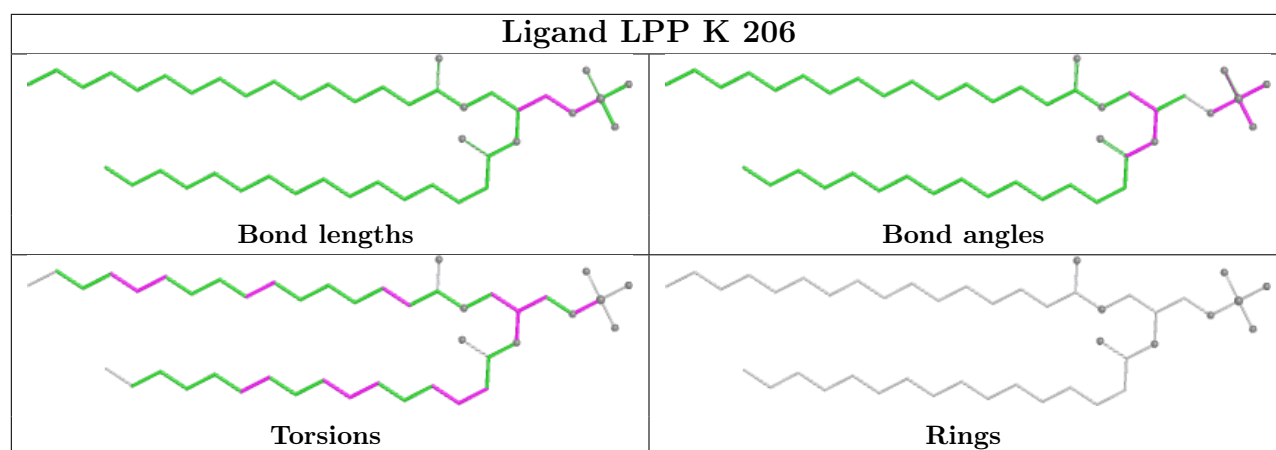


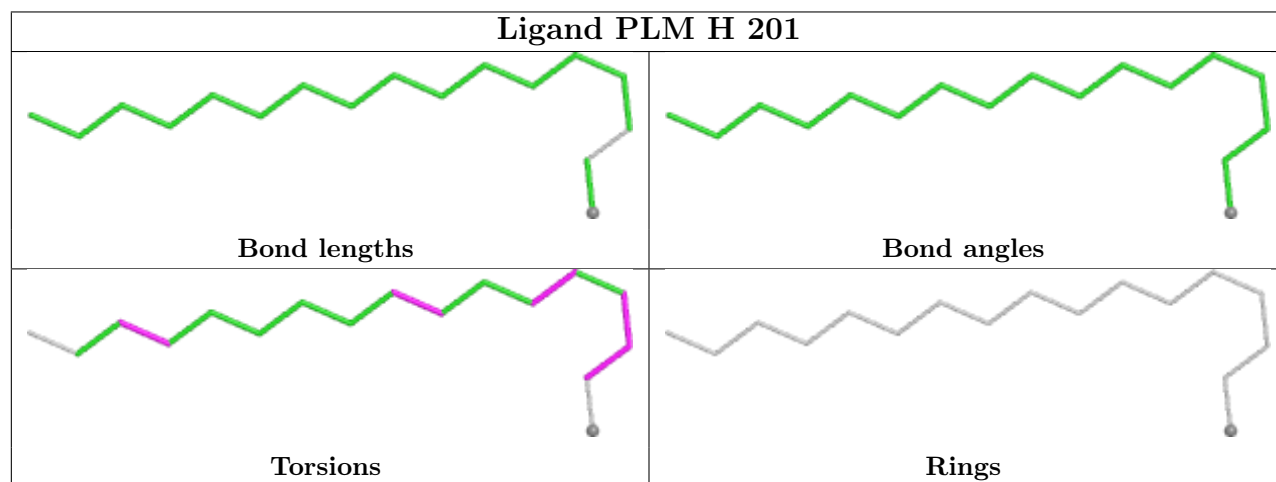
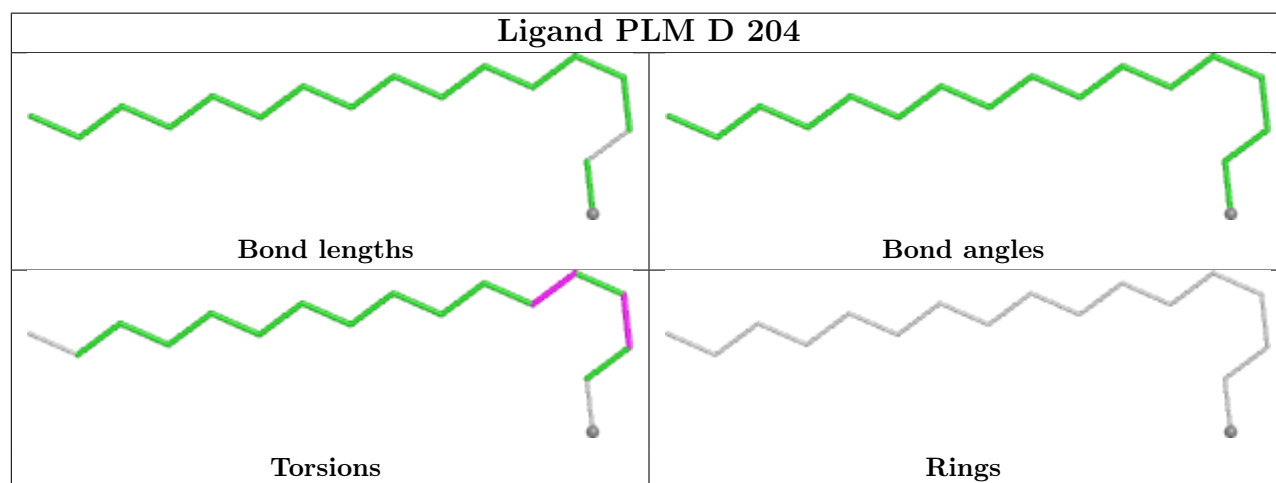
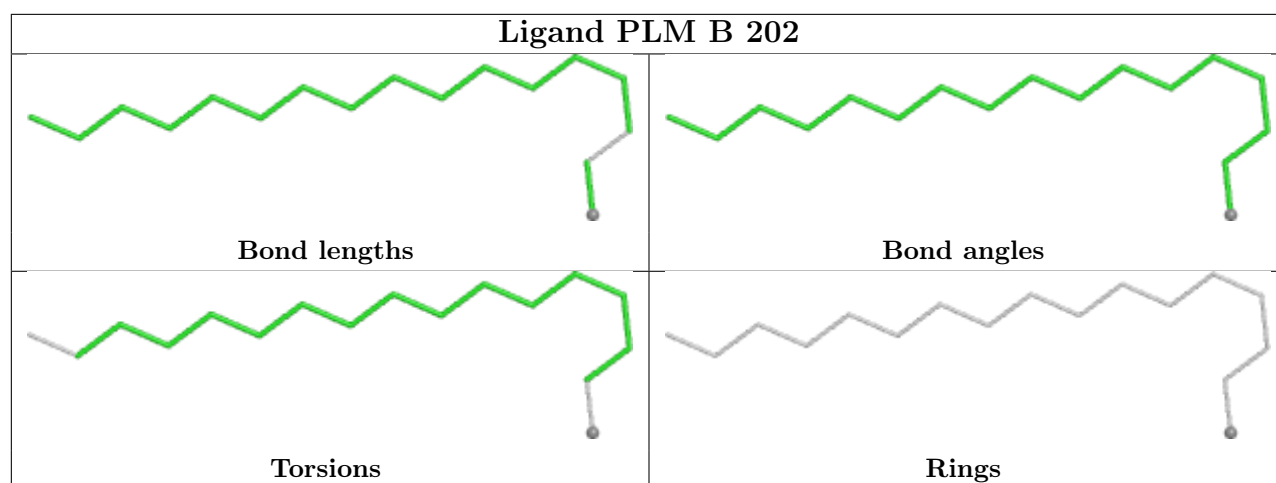


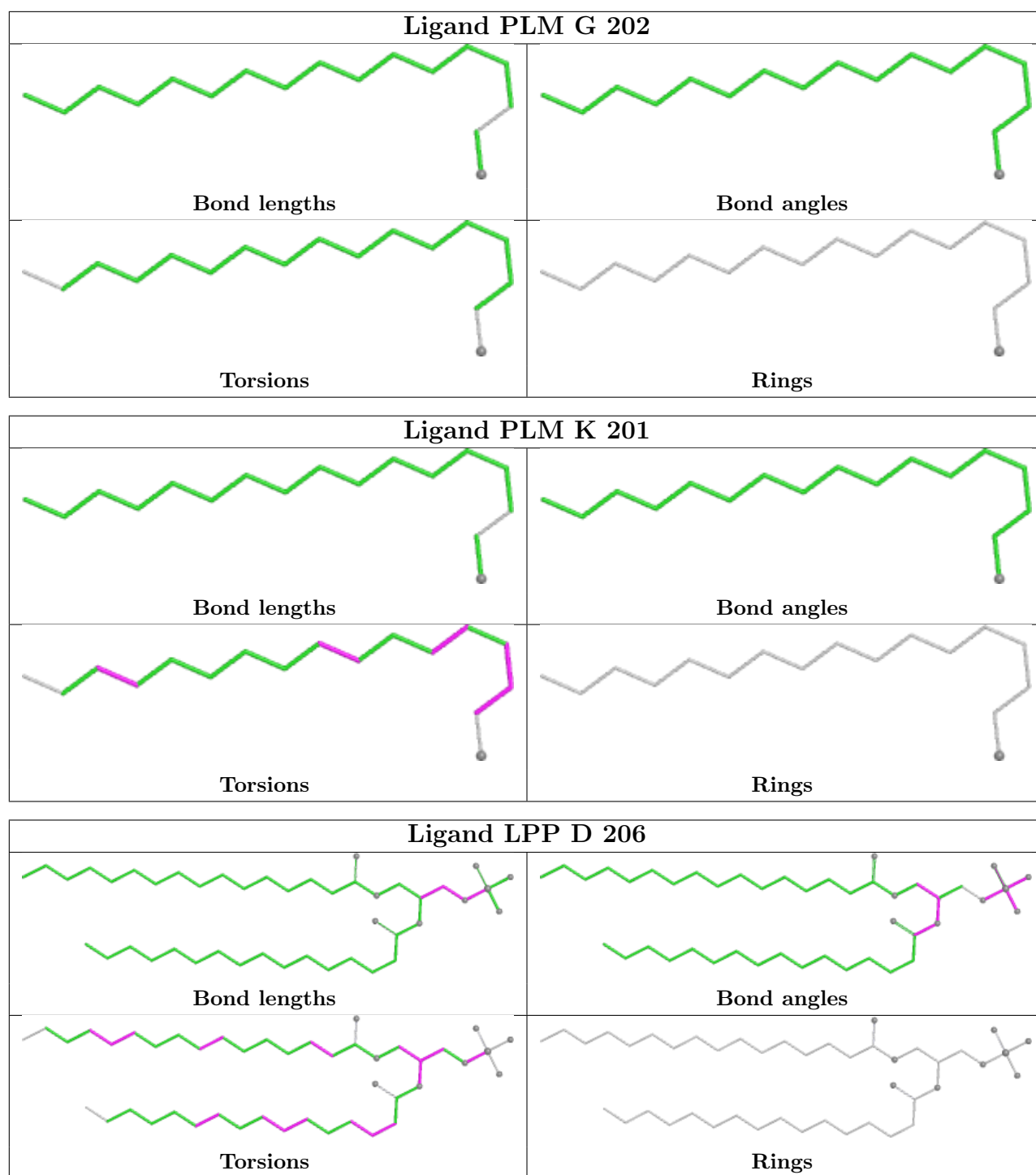


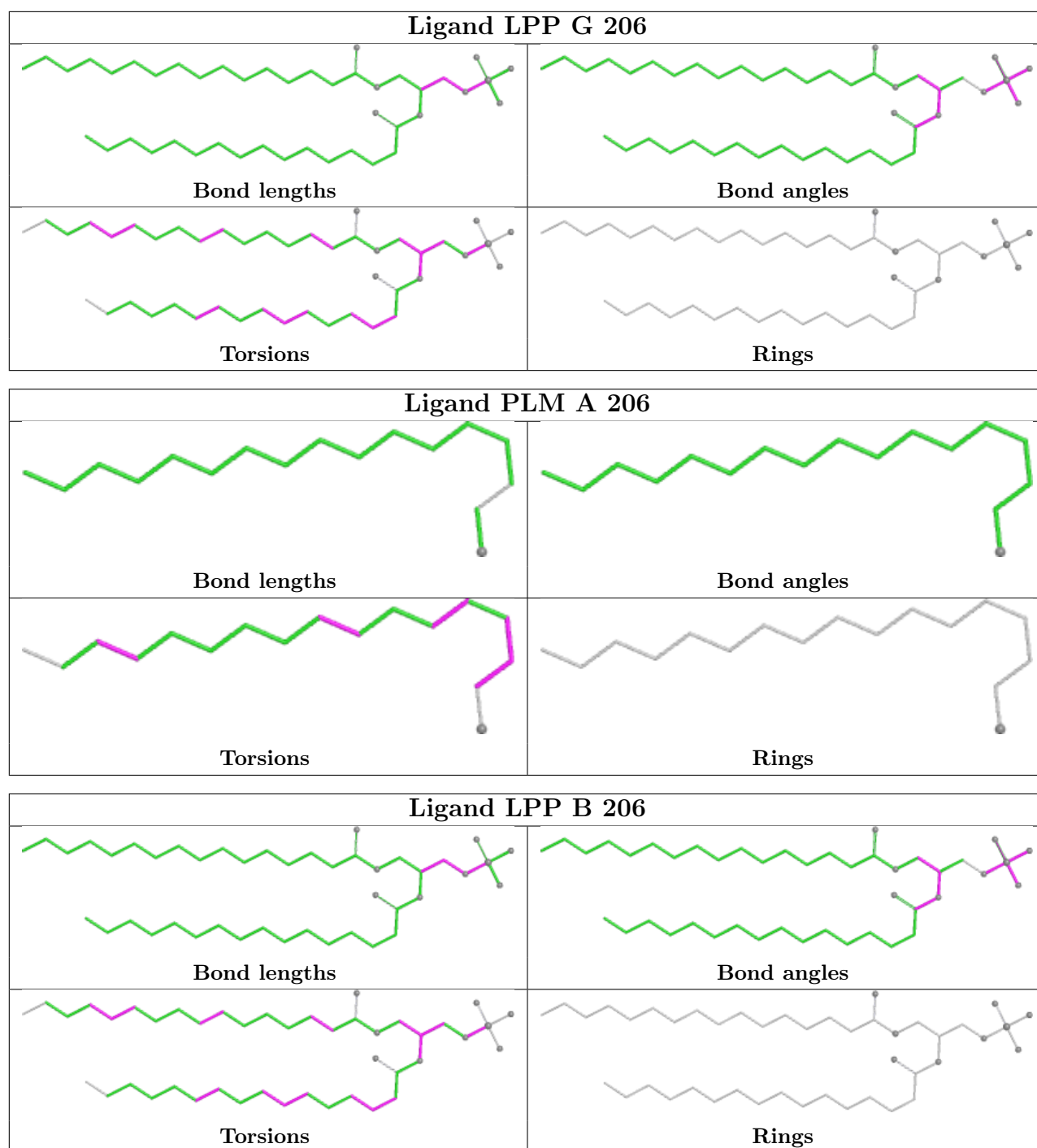












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

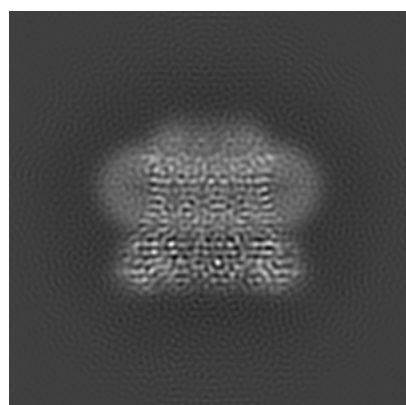
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12950. These allow visual inspection of the internal detail of the map and identification of artifacts.

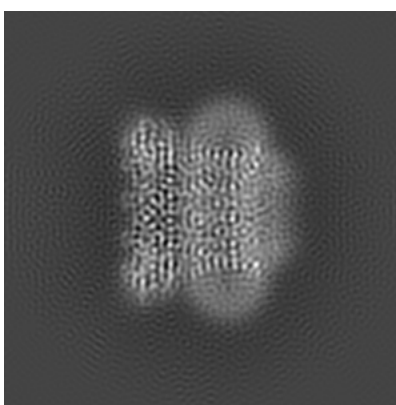
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

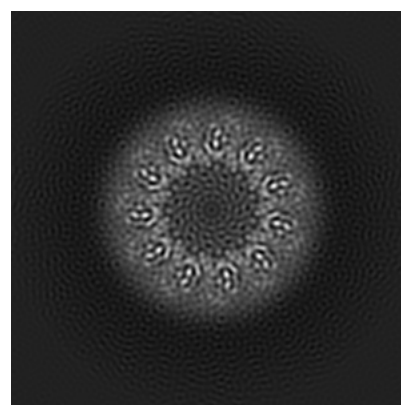
6.1.1 Primary map



X



Y

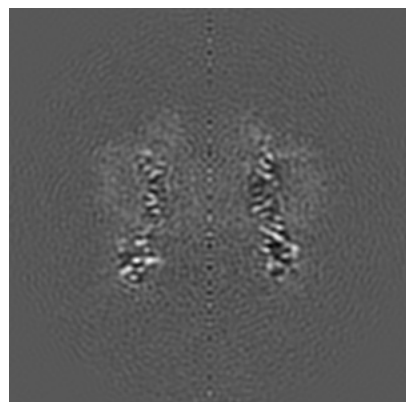


Z

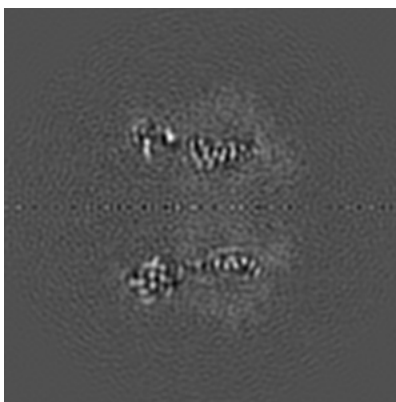
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

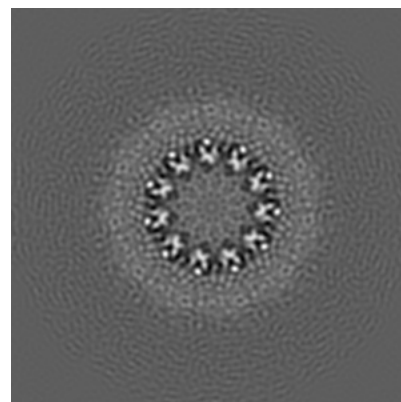
6.2.1 Primary map



X Index: 144



Y Index: 144

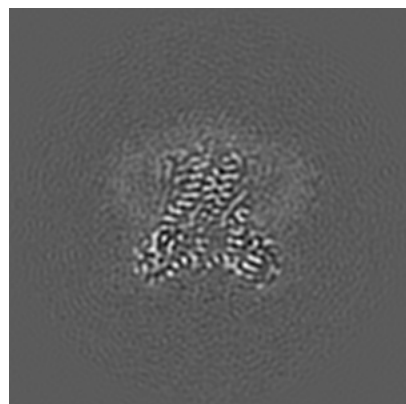


Z Index: 144

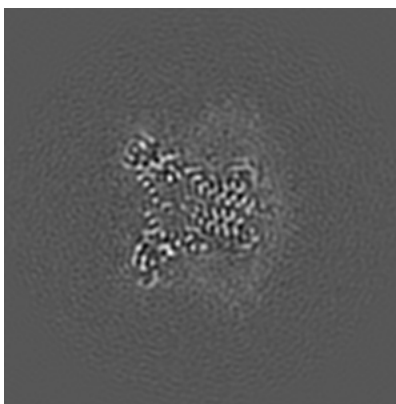
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

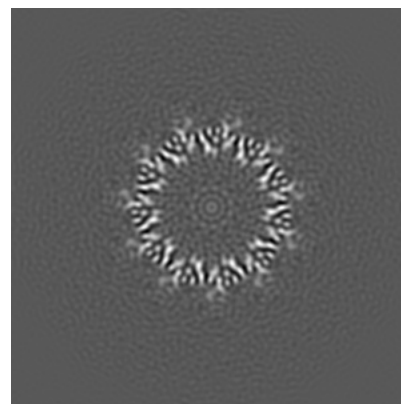
6.3.1 Primary map



X Index: 183



Y Index: 182

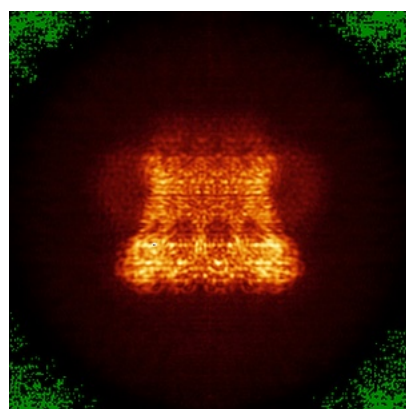


Z Index: 119

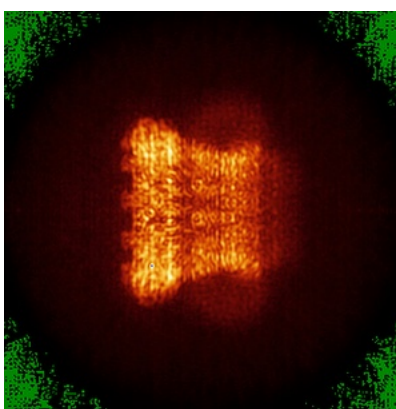
The images above show the largest variance slices of the map in three orthogonal directions.

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

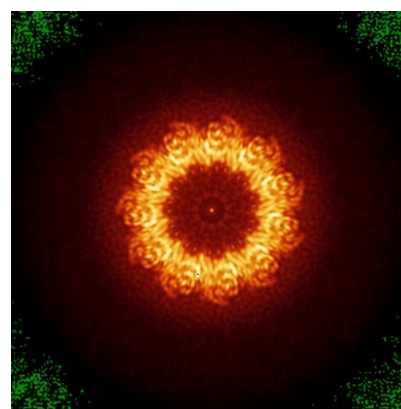
6.4.1 Primary map



X



Y

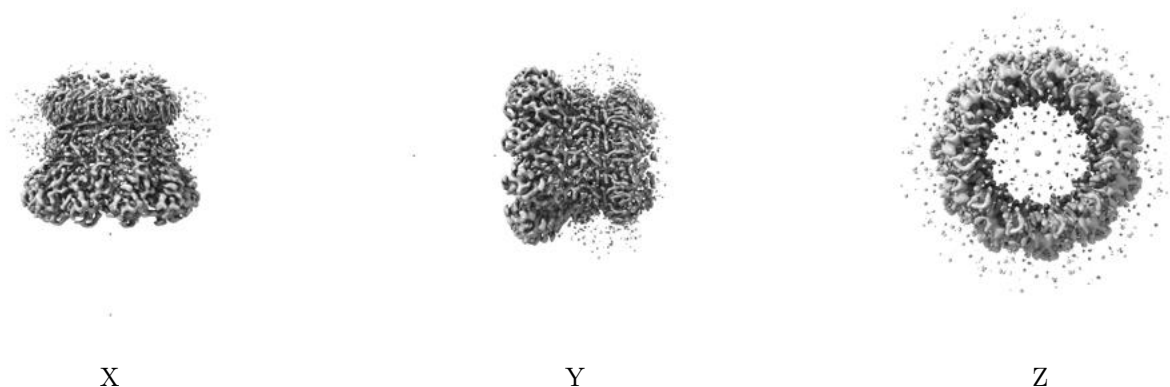


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0085. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

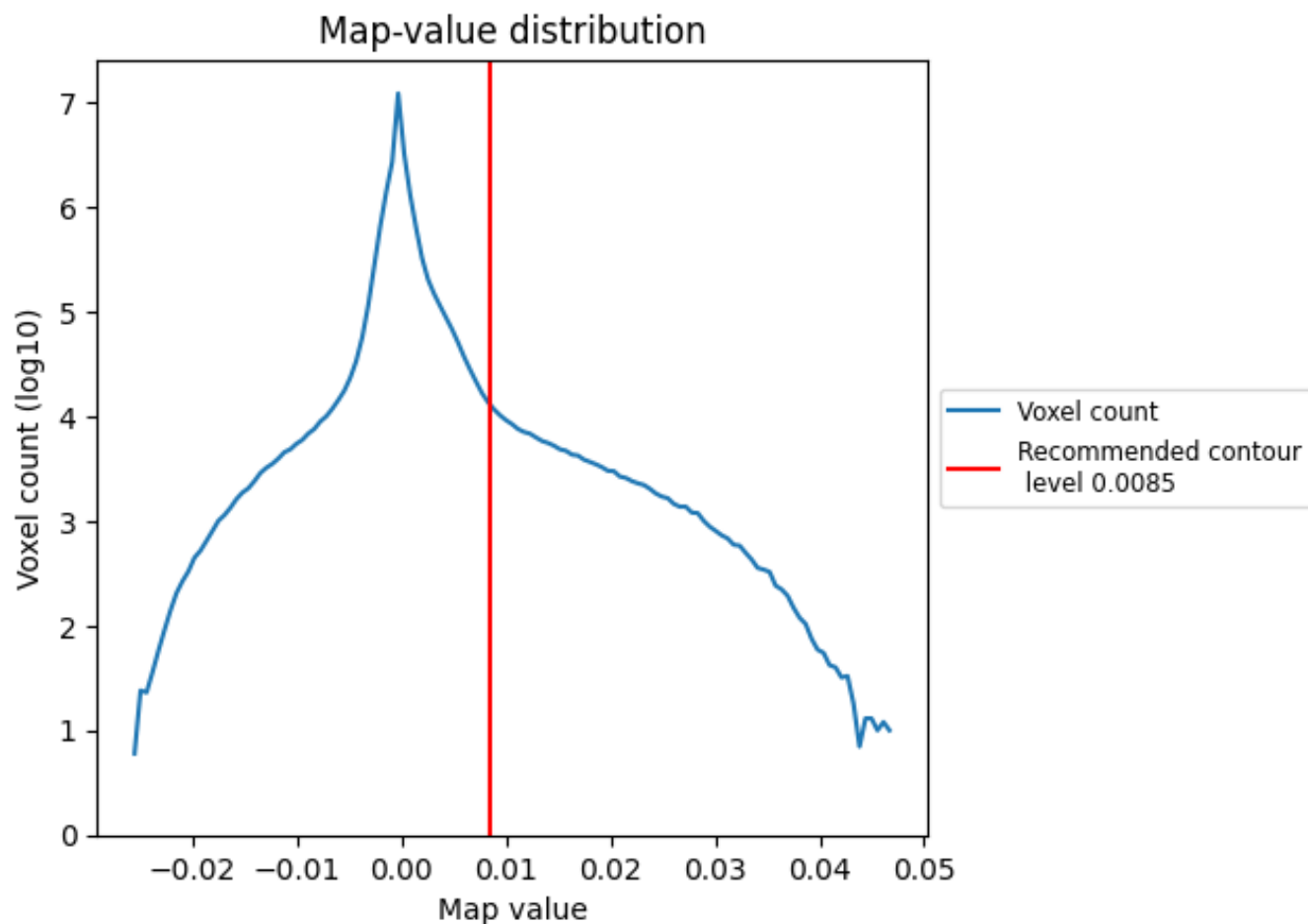
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

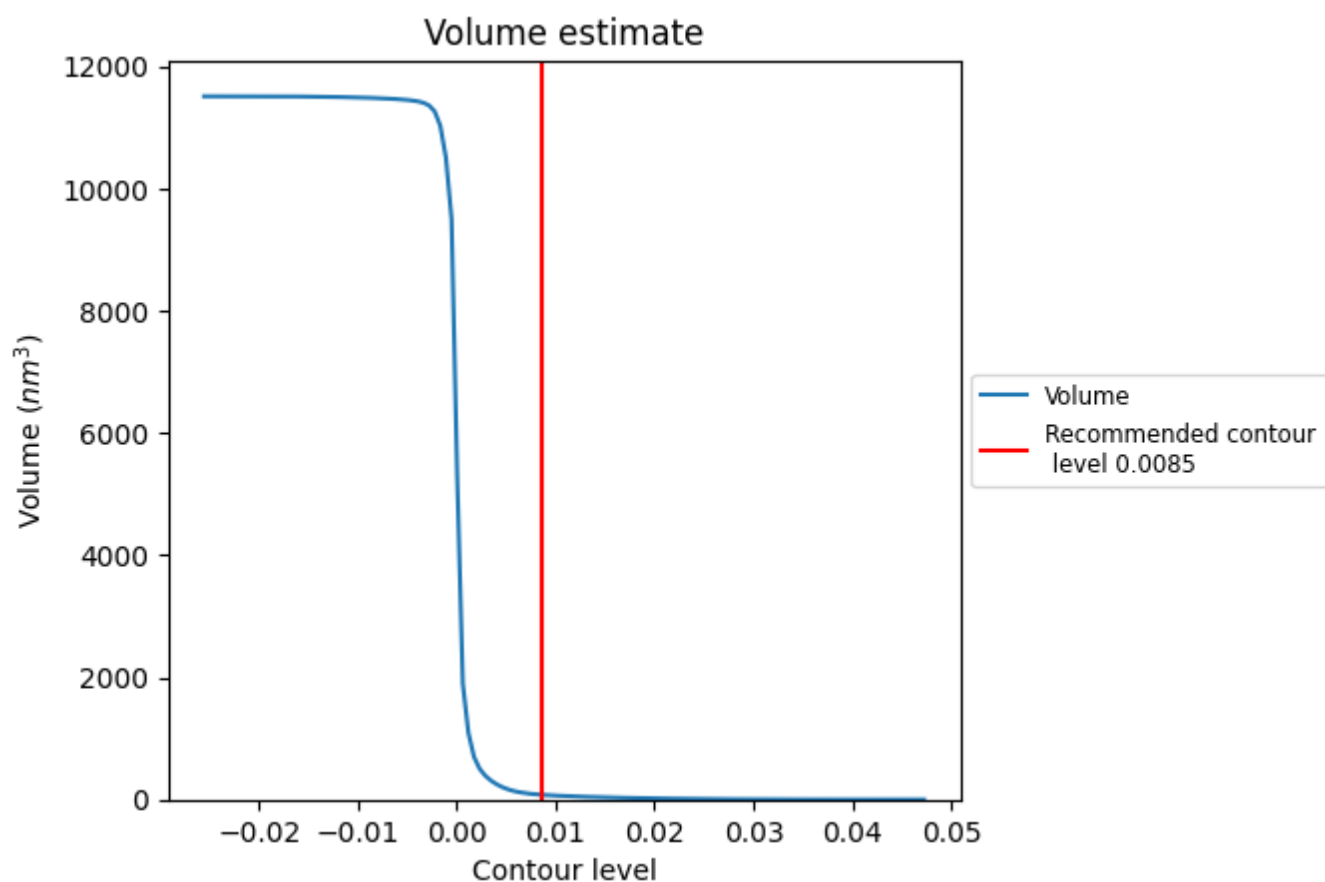
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

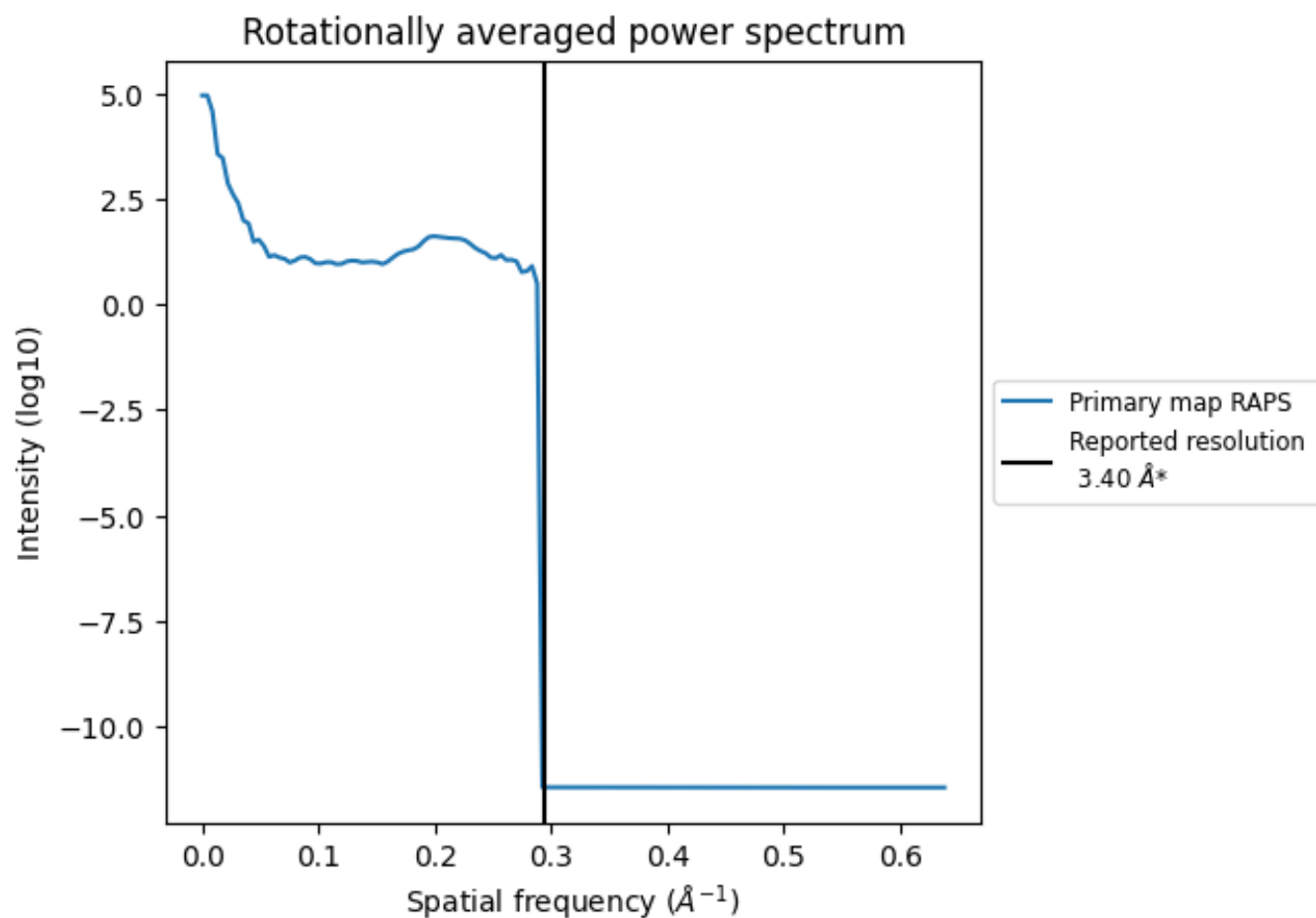
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 79 nm³; this corresponds to an approximate mass of 72 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

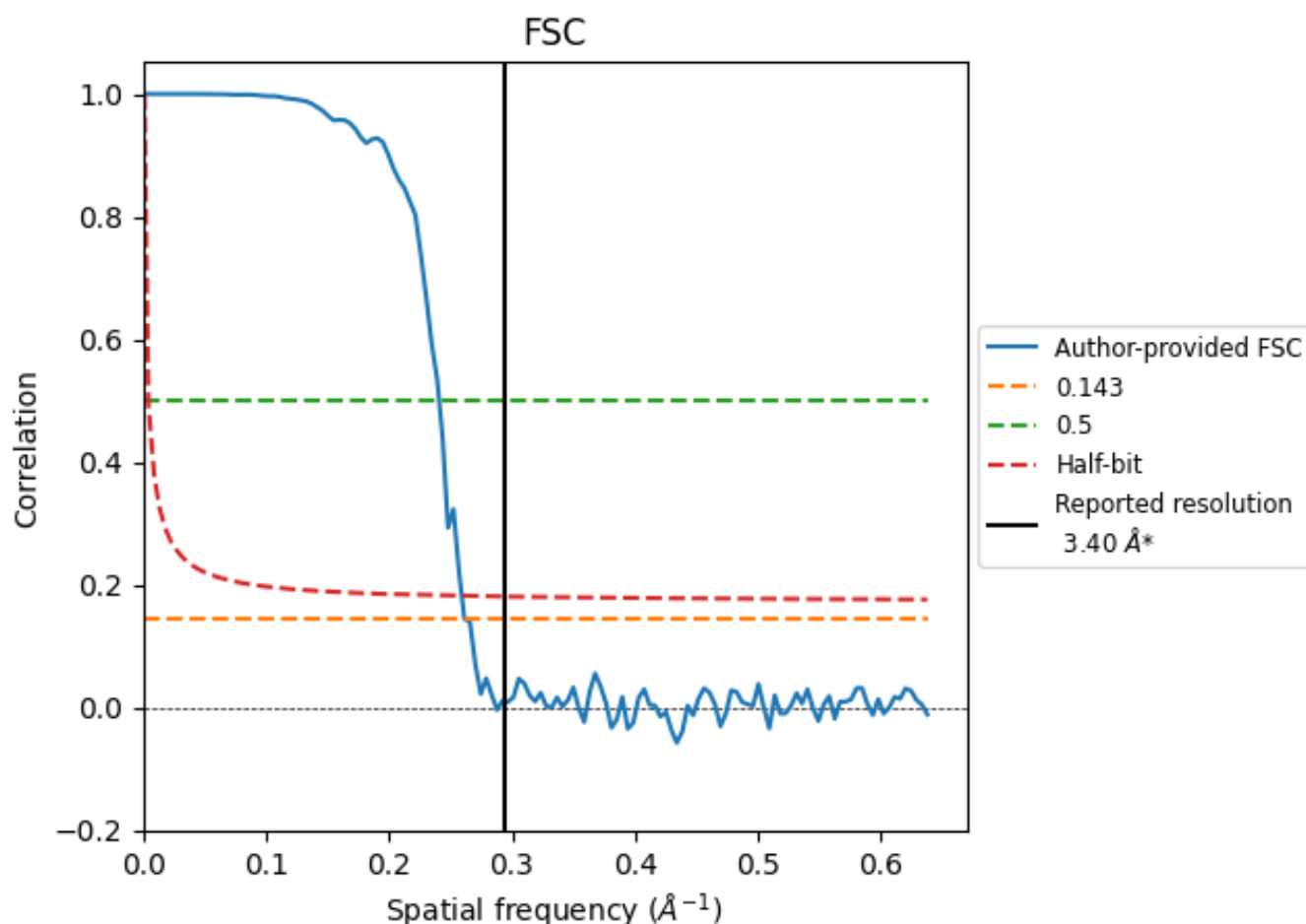


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

8.2 Resolution estimates [i](#)

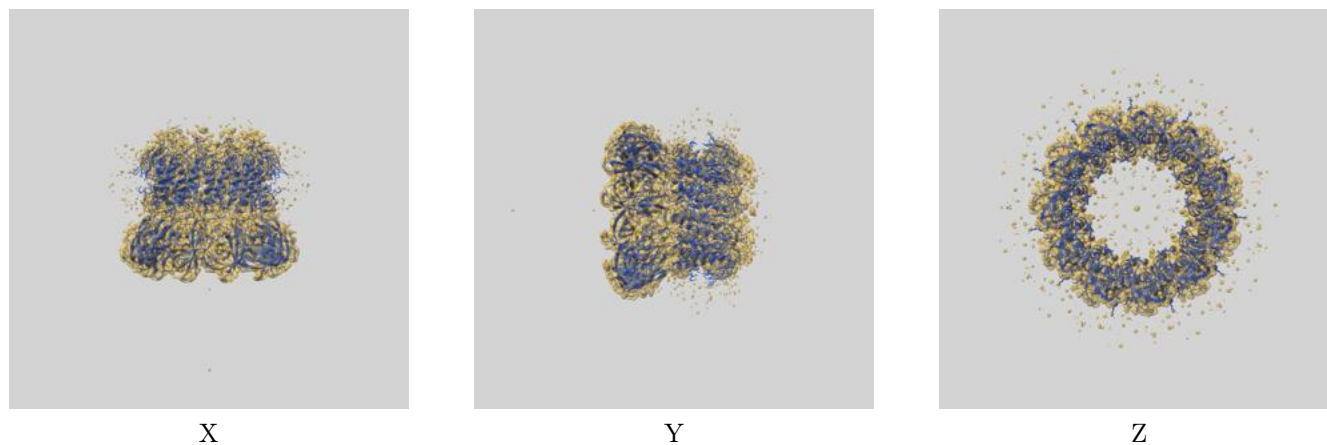
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.82	4.15	3.86
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 3.82 differs from the reported value 3.4 by more than 10 %

9 Map-model fit [i](#)

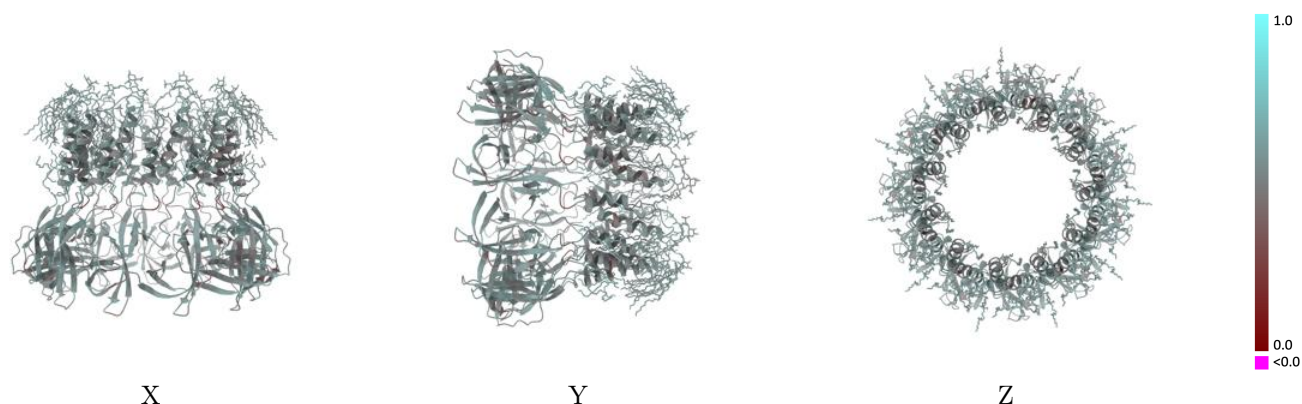
This section contains information regarding the fit between EMDB map EMD-12950 and PDB model 7OJG. Per-residue inclusion information can be found in section [3](#) on page [10](#).

9.1 Map-model overlay [i](#)



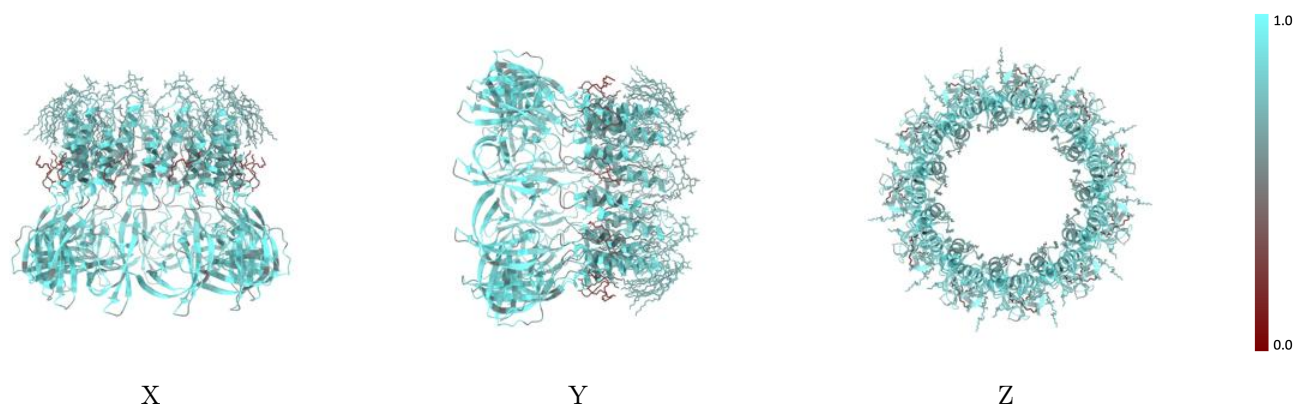
The images above show the 3D surface view of the map at the recommended contour level 0.0085 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



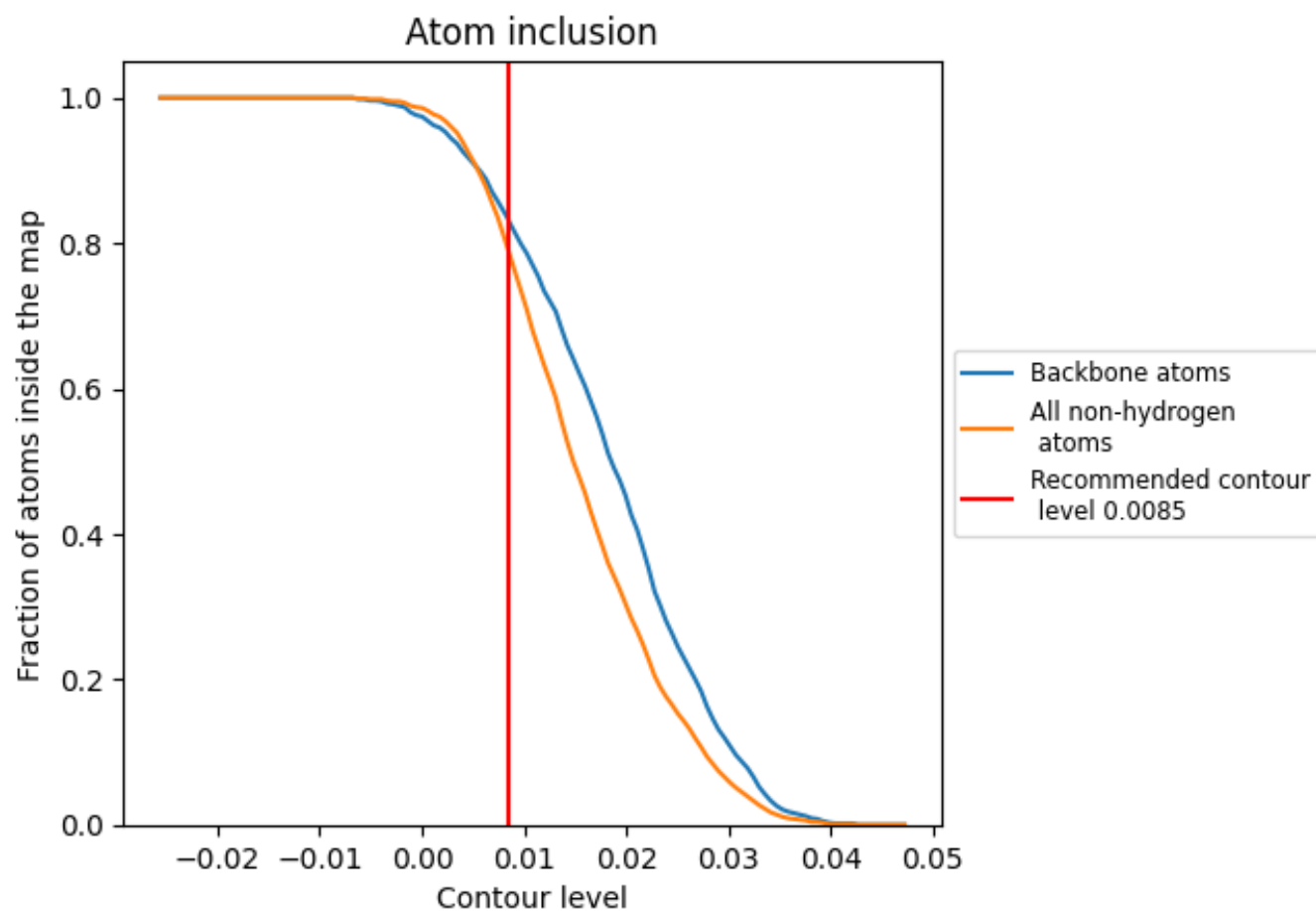
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0085).

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 79% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0085) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7890	0.5310
A	0.7970	0.5350
B	0.7950	0.5340
C	0.7920	0.5320
D	0.7950	0.5330
E	0.7930	0.5330
F	0.7930	0.5350
G	0.7910	0.5340
H	0.7910	0.5350
I	0.7890	0.5360
J	0.7920	0.5360
K	0.7520	0.4980

1.0

0.0

<0.0