



## Full wwPDB EM Validation Report ⓘ

May 2, 2024 – 06:16 PM EDT

PDB ID : 8TOI  
EMDB ID : EMD-41453  
Title : nhTMEM16 lipid scramblase in lipid nanodiscs with MSP1E3 scaffold protein  
in the presence of Ca<sup>2+</sup> (closed state)  
Authors : Feng, Z.; Accardi, A.  
Deposited on : 2023-08-03  
Resolution : 2.64 Å (reported)  
Based on initial model : 6QM9

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev92  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36.2

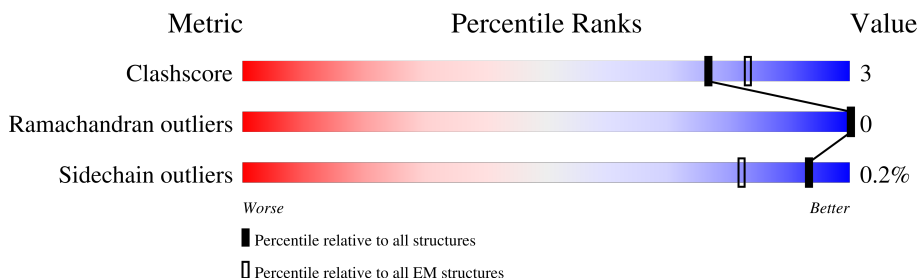
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.64 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	737	
1	B	737	

## 2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 11414 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 Lipid scramblase nhTMEM16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	649	5160	3364	862	914	20	0	0
1	B	649	5160	3364	862	914	20	0	0

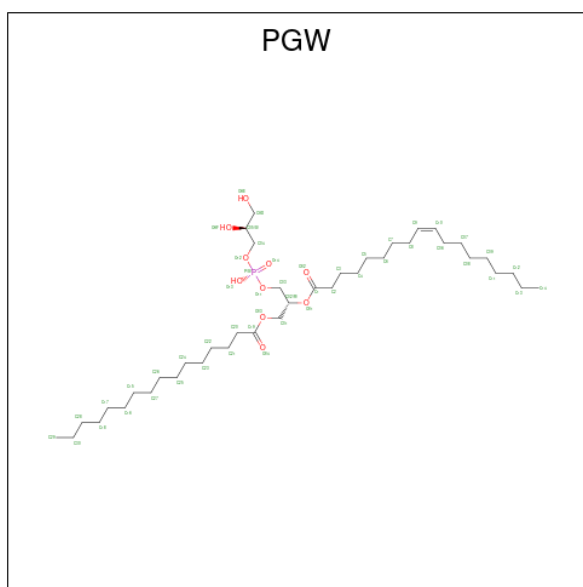
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP C7Z7K1
A	1	PRO	-	expression tag	UNP C7Z7K1
A	736	ALA	-	cloning artifact	UNP C7Z7K1
B	0	GLY	-	expression tag	UNP C7Z7K1
B	1	PRO	-	expression tag	UNP C7Z7K1
B	736	ALA	-	cloning artifact	UNP C7Z7K1

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
2	A	2	Total 2	Ca 2	0
2	B	2	Total 2	Ca 2	0

- Molecule 3 is (1R)-2-[[[S]-[[[2S]-2,3-dihydroxypropyl]oxy](hydroxy)phosphoryl]oxy]-1-[(hexadecanoyloxy)methyl]ethyl (9Z)-octadec-9-enoate (three-letter code: PGW) (formula: C<sub>40</sub>H<sub>77</sub>O<sub>10</sub>P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	O	P	0
			34	25	8	1	
3	A	1	Total	C	O		0
			25	20	5		
3	A	1	Total	C	O	P	0
			30	21	8	1	
3	A	1	Total	C	O	P	0
			29	20	8	1	
3	A	1	Total	C	O	P	0
			26	17	8	1	
3	A	1	Total	C	O	P	0
			23	14	8	1	
3	A	1	Total	C	O	P	0
			26	17	8	1	
3	A	1	Total	C	O	P	0
			28	19	8	1	
3	A	1	Total	C	O	P	0
			30	21	8	1	
3	A	1	Total	C	O	P	0
			29	20	8	1	
3	A	1	Total	C	O	P	0
			35	26	8	1	
3	A	1	Total	C	O	P	0
			27	18	8	1	
3	A	1	Total	C	O	P	0
			39	30	8	1	
3	A	1	Total	C	O	P	0
			33	24	8	1	

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
3	A	1	36	27	8	1	0
3	A	1	36	27	8	1	0
3	A	1	30	21	8	1	0
3	A	1	29	20	8	1	0
3	B	1	34	25	8	1	0
3	B	1	25	20	5		0
3	B	1	30	21	8	1	0
3	B	1	29	20	8	1	0
3	B	1	26	17	8	1	0
3	B	1	23	14	8	1	0
3	B	1	26	17	8	1	0
3	B	1	28	19	8	1	0
3	B	1	30	21	8	1	0
3	B	1	29	20	8	1	0
3	B	1	35	26	8	1	0
3	B	1	27	18	8	1	0
3	B	1	39	30	8	1	0
3	B	1	33	24	8	1	0
3	B	1	36	27	8	1	0
3	B	1	36	27	8	1	0
3	B	1	30	21	8	1	0

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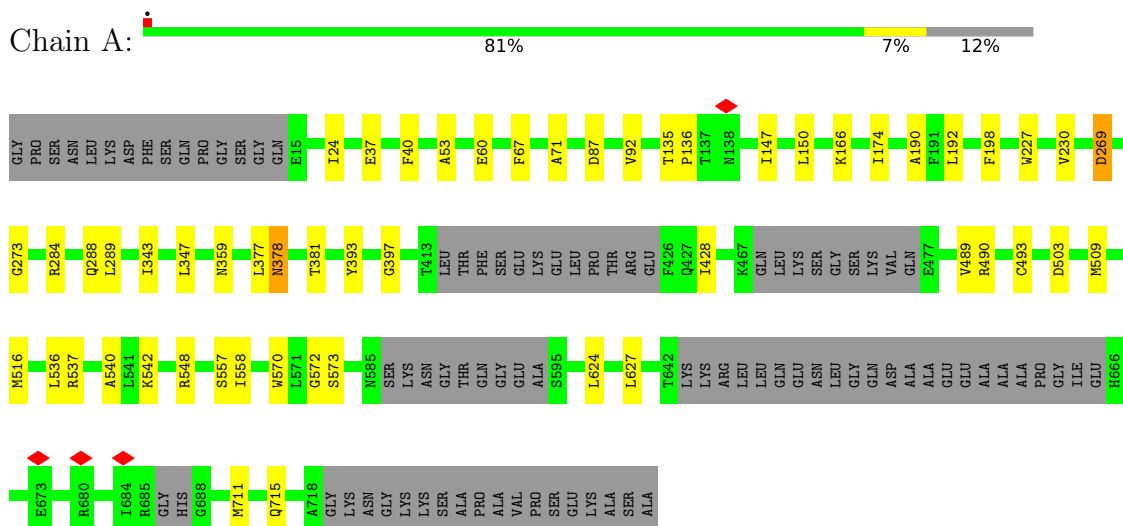
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Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
3	B	1	29	20	8	1	0

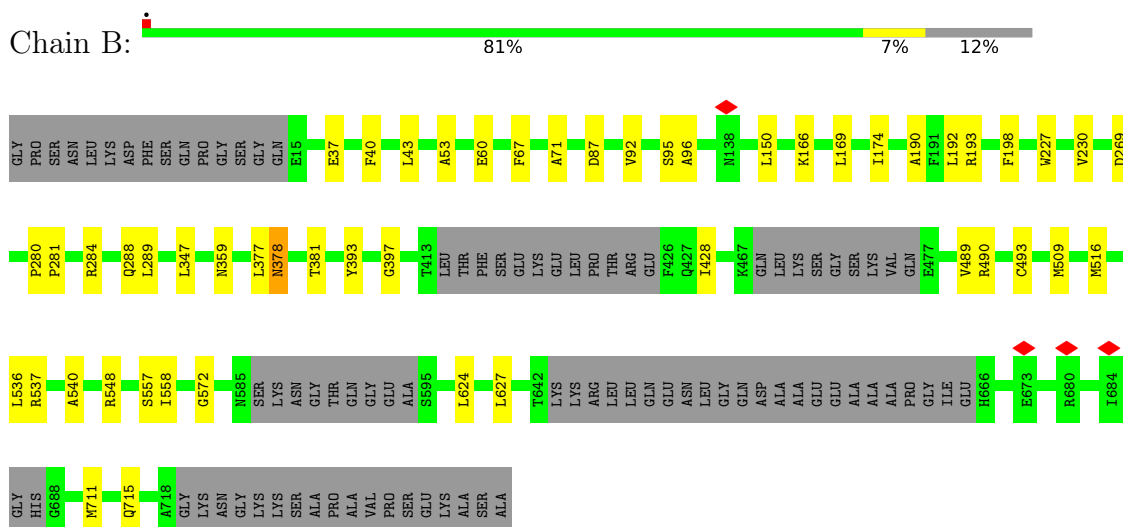
### 3 Residue-property plots

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

- Molecule 1: Lipid scramblase nhTMEM16



- Molecule 1: Lipid scramblase nhTMEM16



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	1017312	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	59.4	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	1900	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	17.543	Depositor
Minimum map value	-6.859	Depositor
Average map value	0.057	Depositor
Map value standard deviation	0.508	Depositor
Recommended contour level	1.1	Depositor
Map size (Å)	211.2, 211.2, 211.2	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.825, 0.825, 0.825	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: PGW, CA

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	0.30	0/5296	0.56	3/7197 (0.0%)
1	B	0.30	0/5296	0.56	3/7197 (0.0%)
All	All	0.30	0/10592	0.56	6/14394 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	509	MET	CB-CG-SD	7.21	134.04	112.40
1	A	509	MET	CB-CG-SD	7.21	134.03	112.40
1	B	509	MET	CG-SD-CE	6.67	110.87	100.20
1	A	509	MET	CG-SD-CE	6.67	110.87	100.20
1	A	269	ASP	CB-CG-OD2	5.15	122.94	118.30
1	B	269	ASP	CB-CG-OD2	5.14	122.93	118.30

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	5160	0	5059	34	0
1	B	5160	0	5059	32	0
2	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2	0	0	0	0
3	A	545	0	594	5	0
3	B	545	0	594	4	0
All	All	11414	0	11306	68	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 (68) 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:A:397:GLY:HA3	1:A:428:ILE:HD11	1.44	0.99
1:B:397:GLY:HA3	1:B:428:ILE:HD11	1.44	0.97
1:B:397:GLY:CA	1:B:428:ILE:HD11	2.21	0.69
1:A:397:GLY:CA	1:A:428:ILE:HD11	2.21	0.68
1:A:397:GLY:HA3	1:A:428:ILE:CD1	2.24	0.64
1:B:397:GLY:HA3	1:B:428:ILE:CD1	2.24	0.62
1:A:711:MET:O	1:A:715:GLN:HB2	2.07	0.55
1:A:53:ALA:HB2	1:A:71:ALA:HB2	1.90	0.54
1:B:711:MET:O	1:B:715:GLN:HB2	2.07	0.54
1:A:150:LEU:HD21	1:A:489:VAL:HG23	1.90	0.54
1:A:230:VAL:HG11	3:A:809:PGW:H5A	1.90	0.53
1:B:53:ALA:HB2	1:B:71:ALA:HB2	1.90	0.53
1:B:230:VAL:HG11	3:B:809:PGW:H5A	1.90	0.53
1:A:537:ARG:O	1:A:540:ALA:HB3	2.10	0.52
1:B:150:LEU:HD21	1:B:489:VAL:HG23	1.90	0.52
1:B:393:TYR:CE2	1:B:428:ILE:HG23	2.45	0.52
1:A:393:TYR:CE2	1:A:428:ILE:HG23	2.45	0.52
1:B:537:ARG:O	1:B:540:ALA:HB3	2.10	0.52
1:A:288:GLN:HB3	3:A:807:PGW:H2A	1.93	0.51
1:B:288:GLN:HB3	3:B:807:PGW:H2A	1.93	0.51
1:A:87:ASP:HB3	1:A:92:VAL:HB	1.93	0.51
1:B:87:ASP:HB3	1:B:92:VAL:HB	1.93	0.51
1:A:37:GLU:O	1:A:40:PHE:HB3	2.12	0.50
1:B:37:GLU:O	1:B:40:PHE:HB3	2.11	0.49
1:B:378:ASN:HA	1:B:381:THR:HG22	1.95	0.49
1:A:60:GLU:HB3	1:A:490:ARG:HD3	1.95	0.48
1:A:166:LYS:O	1:A:537:ARG:NH2	2.45	0.48
1:B:166:LYS:O	1:B:537:ARG:NH2	2.45	0.48
1:B:60:GLU:HB3	1:B:490:ARG:HD3	1.95	0.48
3:B:817:PGW:H24	3:B:817:PGW:H2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:ARG:NE	1:A:359:ASN:O	2.44	0.48
1:A:378:ASN:HA	1:A:381:THR:HG22	1.95	0.48
3:A:817:PGW:H2	3:A:817:PGW:H24	1.95	0.47
1:B:289:LEU:HB3	3:B:813:PGW:H24A	1.95	0.47
1:A:393:TYR:CZ	1:A:428:ILE:HG23	2.50	0.47
1:B:393:TYR:CZ	1:B:428:ILE:HG23	2.50	0.47
1:A:289:LEU:HB3	3:A:813:PGW:H24A	1.95	0.47
1:B:284:ARG:NE	1:B:359:ASN:O	2.44	0.47
1:A:393:TYR:O	1:A:428:ILE:HD13	2.15	0.47
1:B:393:TYR:O	1:B:428:ILE:HD13	2.15	0.46
1:A:503:ASP:OD1	1:A:542:LYS:NZ	2.48	0.45
1:A:347:LEU:HD13	1:A:377:LEU:HD22	1.99	0.45
1:B:493:CYS:O	1:B:548:ARG:NH2	2.51	0.44
1:A:198:PHE:O	1:A:227:TRP:NE1	2.49	0.44
1:B:347:LEU:HD13	1:B:377:LEU:HD22	1.99	0.44
1:B:198:PHE:O	1:B:227:TRP:NE1	2.49	0.43
1:A:493:CYS:O	1:A:548:ARG:NH2	2.51	0.43
1:A:67:PHE:HE1	1:A:489:VAL:HG21	1.84	0.42
1:B:516:MET:HB3	1:B:572:GLY:HA2	2.01	0.42
1:A:516:MET:HB3	1:A:572:GLY:HA2	2.02	0.42
1:B:67:PHE:HE1	1:B:489:VAL:HG21	1.84	0.41
1:B:169:LEU:O	1:B:193:ARG:NH1	2.42	0.41
1:A:135:THR:HA	1:A:136:PRO:HD3	1.86	0.41
1:B:280:PRO:HA	1:B:281:PRO:HD3	1.91	0.41
1:A:24:ILE:HG13	1:A:147:ILE:HG23	2.03	0.41
1:B:557:SER:OG	1:B:558:ILE:N	2.53	0.41
1:A:624:LEU:HA	1:A:627:LEU:HD13	2.02	0.41
1:B:624:LEU:HA	1:B:627:LEU:HD13	2.03	0.41
1:A:557:SER:OG	1:A:558:ILE:N	2.53	0.41
1:A:174:ILE:HG21	1:A:190:ALA:HB2	2.02	0.41
1:A:192:LEU:HG	1:A:536:LEU:HG	2.03	0.41
1:A:343:ILE:HD11	3:A:810:PGW:H22	2.03	0.41
1:A:570:TRP:O	1:A:573:SER:OG	2.35	0.41
1:A:269:ASP:HB2	1:A:273:GLY:H	1.86	0.40
1:B:174:ILE:HG21	1:B:190:ALA:HB2	2.02	0.40
1:B:192:LEU:HG	1:B:536:LEU:HG	2.03	0.40
1:B:40:PHE:O	1:B:43:LEU:HB3	2.22	0.40
1:B:95:SER:OG	1:B:96:ALA:N	2.53	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	637/737 (86%)	614 (96%)	23 (4%)	0	100	100
1	B	637/737 (86%)	614 (96%)	23 (4%)	0	100	100
All	All	1274/1474 (86%)	1228 (96%)	46 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	536/623 (86%)	535 (100%)	1 (0%)	93	97
1	B	536/623 (86%)	535 (100%)	1 (0%)	93	97
All	All	1072/1246 (86%)	1070 (100%)	2 (0%)	93	97

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	378	ASN
1	B	378	ASN

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

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 40 ligands modelled in this entry, 4 are monoatomic - leaving 36 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	PGW	B	808	-	22,22,50	1.38	4 (18%)	26,27,56	1.27	2 (7%)
3	PGW	A	805	-	29,29,50	1.24	4 (13%)	33,34,56	5.49	4 (12%)
3	PGW	B	809	-	25,25,50	1.31	4 (16%)	29,30,56	1.25	2 (6%)
3	PGW	A	820	-	28,28,50	1.23	4 (14%)	32,33,56	1.29	2 (6%)
3	PGW	A	806	-	28,28,50	1.26	4 (14%)	32,33,56	1.30	2 (6%)
3	PGW	A	819	-	29,29,50	1.25	4 (13%)	33,34,56	1.23	2 (6%)
3	PGW	B	806	-	28,28,50	1.26	4 (14%)	32,33,56	1.30	2 (6%)
3	PGW	B	814	-	26,26,50	1.27	4 (15%)	30,31,56	1.22	2 (6%)
3	PGW	B	803	-	33,33,50	1.17	4 (12%)	36,38,56	1.16	2 (5%)
3	PGW	B	811	-	29,29,50	1.23	4 (13%)	33,34,56	1.17	2 (6%)
3	PGW	A	804	-	24,24,50	1.22	3 (12%)	26,26,56	1.31	2 (7%)
3	PGW	B	820	-	28,28,50	1.23	4 (14%)	32,33,56	1.29	2 (6%)
3	PGW	B	804	-	24,24,50	1.21	3 (12%)	26,26,56	1.31	2 (7%)
3	PGW	A	810	-	27,27,50	1.25	4 (14%)	31,32,56	1.21	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	PGW	B	807	-	25,25,50	1.30	4 (16%)	29,30,56	1.23	2 (6%)
3	PGW	A	815	-	38,38,50	1.09	4 (10%)	42,43,56	1.13	2 (4%)
3	PGW	A	817	-	35,35,50	1.11	4 (11%)	39,40,56	1.15	2 (5%)
3	PGW	B	817	-	35,35,50	1.10	4 (11%)	39,40,56	1.15	2 (5%)
3	PGW	B	810	-	27,27,50	1.24	4 (14%)	31,32,56	1.21	2 (6%)
3	PGW	B	813	-	34,34,50	1.14	4 (11%)	38,39,56	1.16	2 (5%)
3	PGW	A	808	-	22,22,50	1.37	4 (18%)	26,27,56	1.27	2 (7%)
3	PGW	B	815	-	38,38,50	1.09	4 (10%)	42,43,56	1.13	2 (4%)
3	PGW	A	816	-	32,32,50	1.16	4 (12%)	36,37,56	1.18	2 (5%)
3	PGW	A	812	-	28,28,50	1.24	4 (14%)	32,33,56	1.21	2 (6%)
3	PGW	A	809	-	25,25,50	1.31	4 (16%)	29,30,56	1.25	2 (6%)
3	PGW	A	814	-	26,26,50	1.27	4 (15%)	30,31,56	1.21	2 (6%)
3	PGW	A	803	-	33,33,50	1.16	4 (12%)	36,38,56	1.16	2 (5%)
3	PGW	A	811	-	29,29,50	1.23	4 (13%)	33,34,56	1.17	2 (6%)
3	PGW	B	812	-	28,28,50	1.24	4 (14%)	32,33,56	1.21	2 (6%)
3	PGW	B	805	-	29,29,50	1.24	4 (13%)	33,34,56	5.49	4 (12%)
3	PGW	B	819	-	29,29,50	1.25	4 (13%)	33,34,56	1.23	2 (6%)
3	PGW	A	813	-	34,34,50	1.15	4 (11%)	38,39,56	1.16	2 (5%)
3	PGW	A	807	-	25,25,50	1.29	4 (16%)	29,30,56	1.23	2 (6%)
3	PGW	B	816	-	32,32,50	1.16	4 (12%)	36,37,56	1.18	2 (5%)
3	PGW	A	818	-	35,35,50	1.14	4 (11%)	39,40,56	1.09	2 (5%)
3	PGW	B	818	-	35,35,50	1.14	4 (11%)	39,40,56	1.09	2 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PGW	B	808	-	-	4/24/24/55	-
3	PGW	A	805	-	-	16/31/31/55	-
3	PGW	B	809	-	-	17/27/27/55	-
3	PGW	A	820	-	-	19/30/30/55	-
3	PGW	A	806	-	-	15/30/30/55	-
3	PGW	A	819	-	-	14/31/31/55	-
3	PGW	B	806	-	-	15/30/30/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PGW	B	814	-	-	13/28/28/55	-
3	PGW	B	803	-	-	12/35/35/55	-
3	PGW	B	811	-	-	18/31/31/55	-
3	PGW	A	804	-	-	7/26/26/55	-
3	PGW	B	820	-	-	19/30/30/55	-
3	PGW	B	804	-	-	7/26/26/55	-
3	PGW	A	810	-	-	12/29/29/55	-
3	PGW	B	807	-	-	18/27/27/55	-
3	PGW	A	815	-	-	20/40/40/55	-
3	PGW	A	817	-	-	16/37/37/55	-
3	PGW	B	817	-	-	16/37/37/55	-
3	PGW	B	810	-	-	12/29/29/55	-
3	PGW	B	813	-	-	15/36/36/55	-
3	PGW	A	808	-	-	4/24/24/55	-
3	PGW	B	815	-	-	20/40/40/55	-
3	PGW	A	816	-	-	16/34/34/55	-
3	PGW	A	812	-	-	21/30/30/55	-
3	PGW	A	809	-	-	17/27/27/55	-
3	PGW	A	814	-	-	13/28/28/55	-
3	PGW	A	803	-	-	12/35/35/55	-
3	PGW	A	811	-	-	18/31/31/55	-
3	PGW	B	812	-	-	21/30/30/55	-
3	PGW	B	805	-	-	16/31/31/55	-
3	PGW	B	819	-	-	14/31/31/55	-
3	PGW	A	813	-	-	15/36/36/55	-
3	PGW	A	807	-	-	18/27/27/55	-
3	PGW	B	816	-	-	16/34/34/55	-
3	PGW	A	818	-	-	22/37/37/55	-
3	PGW	B	818	-	-	22/37/37/55	-

All (142) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	820	PGW	O01-C1	3.18	1.43	1.34
3	A	809	PGW	O01-C1	3.17	1.43	1.34
3	B	820	PGW	O01-C1	3.16	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	809	PGW	O01-C1	3.16	1.43	1.34
3	A	817	PGW	O01-C1	3.12	1.43	1.34
3	A	818	PGW	O01-C1	3.11	1.43	1.34
3	B	818	PGW	O01-C1	3.11	1.43	1.34
3	B	817	PGW	O01-C1	3.10	1.43	1.34
3	A	805	PGW	O01-C1	3.02	1.42	1.34
3	B	805	PGW	O01-C1	3.02	1.42	1.34
3	A	806	PGW	O01-C1	2.99	1.42	1.34
3	B	806	PGW	O01-C1	2.98	1.42	1.34
3	B	819	PGW	O01-C1	2.97	1.42	1.34
3	A	819	PGW	O01-C1	2.95	1.42	1.34
3	B	812	PGW	O01-C1	2.93	1.42	1.34
3	A	812	PGW	O01-C1	2.93	1.42	1.34
3	B	808	PGW	O01-C1	2.93	1.42	1.34
3	B	816	PGW	O01-C1	2.93	1.42	1.34
3	A	804	PGW	O01-C1	2.93	1.42	1.34
3	B	804	PGW	O01-C1	2.93	1.42	1.34
3	B	811	PGW	O01-C1	2.93	1.42	1.34
3	A	803	PGW	O01-C1	2.92	1.42	1.34
3	A	811	PGW	O01-C1	2.92	1.42	1.34
3	B	803	PGW	O01-C1	2.91	1.42	1.34
3	B	813	PGW	O01-C1	2.91	1.42	1.34
3	A	810	PGW	O01-C1	2.90	1.42	1.34
3	A	808	PGW	O01-C1	2.90	1.42	1.34
3	A	816	PGW	O01-C1	2.90	1.42	1.34
3	A	813	PGW	O01-C1	2.89	1.42	1.34
3	B	810	PGW	O01-C1	2.89	1.42	1.34
3	A	815	PGW	O01-C1	2.89	1.42	1.34
3	B	814	PGW	O01-C1	2.88	1.42	1.34
3	B	815	PGW	O01-C1	2.87	1.42	1.34
3	A	814	PGW	O01-C1	2.87	1.42	1.34
3	A	807	PGW	O01-C1	2.85	1.42	1.34
3	B	807	PGW	O01-C1	2.85	1.42	1.34
3	A	805	PGW	O03-C19	2.53	1.40	1.33
3	A	818	PGW	O03-C19	2.53	1.40	1.33
3	B	818	PGW	O03-C19	2.52	1.40	1.33
3	A	809	PGW	O03-C19	2.52	1.40	1.33
3	B	808	PGW	O03-C19	2.51	1.40	1.33
3	B	809	PGW	O03-C19	2.51	1.40	1.33
3	B	805	PGW	O03-C19	2.51	1.40	1.33
3	A	804	PGW	O03-C19	2.50	1.40	1.33
3	B	820	PGW	O03-C19	2.50	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	804	PGW	O03-C19	2.49	1.40	1.33
3	A	808	PGW	O03-C19	2.49	1.40	1.33
3	A	820	PGW	O03-C19	2.48	1.40	1.33
3	A	814	PGW	O03-C19	2.47	1.40	1.33
3	B	806	PGW	O03-C19	2.47	1.40	1.33
3	B	819	PGW	O03-C19	2.46	1.40	1.33
3	B	815	PGW	O03-C19	2.46	1.40	1.33
3	A	815	PGW	O03-C19	2.46	1.40	1.33
3	B	817	PGW	O03-C19	2.46	1.40	1.33
3	A	813	PGW	O03-C19	2.46	1.40	1.33
3	B	813	PGW	O03-C19	2.46	1.40	1.33
3	B	814	PGW	O03-C19	2.45	1.40	1.33
3	A	816	PGW	O03-C19	2.45	1.40	1.33
3	A	811	PGW	O03-C19	2.45	1.40	1.33
3	A	817	PGW	O03-C19	2.44	1.40	1.33
3	A	819	PGW	O03-C19	2.44	1.40	1.33
3	A	803	PGW	O03-C19	2.44	1.40	1.33
3	B	816	PGW	O03-C19	2.44	1.40	1.33
3	A	807	PGW	O03-C19	2.44	1.40	1.33
3	B	811	PGW	O03-C19	2.44	1.40	1.33
3	A	806	PGW	O03-C19	2.43	1.40	1.33
3	A	810	PGW	O03-C19	2.43	1.40	1.33
3	B	807	PGW	O03-C19	2.43	1.40	1.33
3	A	812	PGW	O03-C19	2.42	1.40	1.33
3	B	812	PGW	O03-C19	2.42	1.40	1.33
3	B	803	PGW	O03-C19	2.41	1.40	1.33
3	B	810	PGW	O03-C19	2.40	1.40	1.33
3	B	819	PGW	O03-C01	-2.39	1.39	1.45
3	B	816	PGW	P-O12	2.36	1.64	1.54
3	A	819	PGW	O03-C01	-2.36	1.39	1.45
3	B	803	PGW	P-O12	2.36	1.63	1.54
3	A	813	PGW	P-O12	2.35	1.63	1.54
3	A	816	PGW	P-O12	2.35	1.63	1.54
3	B	809	PGW	P-O12	2.35	1.63	1.54
3	A	809	PGW	P-O12	2.34	1.63	1.54
3	B	815	PGW	P-O12	2.33	1.63	1.54
3	B	813	PGW	P-O12	2.33	1.63	1.54
3	A	820	PGW	P-O12	2.33	1.63	1.54
3	A	803	PGW	P-O12	2.33	1.63	1.54
3	B	820	PGW	P-O12	2.33	1.63	1.54
3	A	814	PGW	P-O12	2.33	1.63	1.54
3	B	819	PGW	P-O12	2.33	1.63	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	807	PGW	P-O12	2.33	1.63	1.54
3	A	819	PGW	P-O12	2.32	1.63	1.54
3	A	812	PGW	P-O12	2.32	1.63	1.54
3	B	812	PGW	P-O12	2.32	1.63	1.54
3	A	810	PGW	P-O12	2.32	1.63	1.54
3	A	805	PGW	P-O12	2.32	1.63	1.54
3	B	814	PGW	P-O12	2.32	1.63	1.54
3	A	806	PGW	P-O12	2.32	1.63	1.54
3	A	811	PGW	P-O12	2.32	1.63	1.54
3	B	805	PGW	P-O12	2.32	1.63	1.54
3	B	808	PGW	P-O12	2.31	1.63	1.54
3	A	808	PGW	P-O12	2.31	1.63	1.54
3	A	815	PGW	P-O12	2.31	1.63	1.54
3	A	818	PGW	P-O12	2.31	1.63	1.54
3	A	807	PGW	P-O12	2.30	1.63	1.54
3	B	810	PGW	P-O12	2.30	1.63	1.54
3	B	818	PGW	P-O12	2.30	1.63	1.54
3	B	806	PGW	P-O12	2.30	1.63	1.54
3	A	813	PGW	O03-C01	-2.30	1.39	1.45
3	B	811	PGW	P-O12	2.29	1.63	1.54
3	B	806	PGW	O03-C01	-2.29	1.39	1.45
3	B	815	PGW	O03-C01	-2.29	1.39	1.45
3	A	810	PGW	O03-C01	-2.29	1.39	1.45
3	B	807	PGW	O03-C01	-2.29	1.39	1.45
3	A	817	PGW	P-O12	2.28	1.63	1.54
3	A	807	PGW	O03-C01	-2.28	1.40	1.45
3	B	817	PGW	P-O12	2.28	1.63	1.54
3	A	803	PGW	O03-C01	-2.28	1.40	1.45
3	A	806	PGW	O03-C01	-2.27	1.40	1.45
3	B	814	PGW	O03-C01	-2.27	1.40	1.45
3	B	804	PGW	O03-C01	-2.27	1.40	1.45
3	B	813	PGW	O03-C01	-2.27	1.40	1.45
3	B	812	PGW	O03-C01	-2.27	1.40	1.45
3	A	814	PGW	O03-C01	-2.27	1.40	1.45
3	A	815	PGW	O03-C01	-2.27	1.40	1.45
3	A	811	PGW	O03-C01	-2.26	1.40	1.45
3	B	803	PGW	O03-C01	-2.26	1.40	1.45
3	A	804	PGW	O03-C01	-2.26	1.40	1.45
3	B	810	PGW	O03-C01	-2.26	1.40	1.45
3	B	811	PGW	O03-C01	-2.25	1.40	1.45
3	A	805	PGW	O03-C01	-2.25	1.40	1.45
3	B	805	PGW	O03-C01	-2.24	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	812	PGW	O03-C01	-2.24	1.40	1.45
3	A	816	PGW	O03-C01	-2.24	1.40	1.45
3	B	816	PGW	O03-C01	-2.23	1.40	1.45
3	B	818	PGW	O03-C01	-2.23	1.40	1.45
3	A	808	PGW	O03-C01	-2.23	1.40	1.45
3	A	820	PGW	O03-C01	-2.22	1.40	1.45
3	A	818	PGW	O03-C01	-2.21	1.40	1.45
3	B	808	PGW	O03-C01	-2.21	1.40	1.45
3	B	817	PGW	O03-C01	-2.20	1.40	1.45
3	B	820	PGW	O03-C01	-2.19	1.40	1.45
3	A	817	PGW	O03-C01	-2.18	1.40	1.45
3	B	809	PGW	O03-C01	-2.15	1.40	1.45
3	A	809	PGW	O03-C01	-2.14	1.40	1.45

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	805	PGW	O01-C1-C2	22.69	160.42	111.50
3	B	805	PGW	O01-C1-C2	22.68	160.38	111.50
3	A	805	PGW	O01-C1-O02	-18.00	80.21	123.70
3	B	805	PGW	O01-C1-O02	-17.98	80.24	123.70
3	B	805	PGW	O02-C1-C2	-11.17	80.14	123.73
3	A	805	PGW	O02-C1-C2	-11.16	80.21	123.73
3	B	806	PGW	O01-C1-C2	4.58	121.36	111.50
3	A	806	PGW	O01-C1-C2	4.56	121.34	111.50
3	B	820	PGW	O01-C1-C2	4.36	120.89	111.50
3	A	820	PGW	O01-C1-C2	4.34	120.86	111.50
3	B	809	PGW	O01-C1-C2	4.22	120.59	111.50
3	A	809	PGW	O01-C1-C2	4.20	120.54	111.50
3	A	807	PGW	O01-C1-C2	4.08	120.30	111.50
3	B	807	PGW	O01-C1-C2	4.08	120.30	111.50
3	B	808	PGW	O01-C1-C2	4.02	120.16	111.50
3	A	808	PGW	O01-C1-C2	4.02	120.16	111.50
3	B	804	PGW	O01-C1-C2	3.98	120.08	111.50
3	A	819	PGW	O01-C1-C2	3.97	120.07	111.50
3	A	804	PGW	O01-C1-C2	3.97	120.06	111.50
3	B	819	PGW	O01-C1-C2	3.96	120.04	111.50
3	B	813	PGW	O01-C1-C2	3.96	120.04	111.50
3	A	813	PGW	O01-C1-C2	3.96	120.03	111.50
3	A	814	PGW	O01-C1-C2	3.95	120.01	111.50
3	A	810	PGW	O01-C1-C2	3.95	120.01	111.50
3	B	814	PGW	O01-C1-C2	3.95	120.01	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	810	PGW	O01-C1-C2	3.95	120.01	111.50
3	A	816	PGW	O01-C1-C2	3.93	119.98	111.50
3	B	816	PGW	O01-C1-C2	3.93	119.97	111.50
3	A	811	PGW	O01-C1-C2	3.91	119.93	111.50
3	B	811	PGW	O01-C1-C2	3.90	119.90	111.50
3	B	812	PGW	O01-C1-C2	3.89	119.89	111.50
3	A	812	PGW	O01-C1-C2	3.89	119.88	111.50
3	A	803	PGW	O01-C1-C2	3.87	119.85	111.50
3	B	803	PGW	O01-C1-C2	3.85	119.81	111.50
3	B	815	PGW	O01-C1-C2	3.85	119.79	111.50
3	A	815	PGW	O01-C1-C2	3.83	119.75	111.50
3	A	817	PGW	O01-C1-C2	3.78	119.65	111.50
3	B	817	PGW	O01-C1-C2	3.77	119.62	111.50
3	A	818	PGW	O01-C1-C2	3.72	119.53	111.50
3	B	818	PGW	O01-C1-C2	3.71	119.50	111.50
3	B	805	PGW	O03-C19-C20	2.88	120.96	111.91
3	A	805	PGW	O03-C19-C20	2.88	120.94	111.91
3	B	812	PGW	O03-C19-C20	2.72	120.44	111.91
3	A	812	PGW	O03-C19-C20	2.70	120.39	111.91
3	B	817	PGW	O03-C19-C20	2.66	120.27	111.91
3	A	817	PGW	O03-C19-C20	2.66	120.26	111.91
3	A	809	PGW	O03-C19-C20	2.66	120.25	111.91
3	A	806	PGW	O03-C19-C20	2.65	120.23	111.91
3	B	809	PGW	O03-C19-C20	2.65	120.22	111.91
3	B	806	PGW	O03-C19-C20	2.64	120.19	111.91
3	A	820	PGW	O03-C19-C20	2.63	120.15	111.91
3	A	815	PGW	O03-C19-C20	2.61	120.11	111.91
3	B	815	PGW	O03-C19-C20	2.61	120.10	111.91
3	B	820	PGW	O03-C19-C20	2.61	120.10	111.91
3	A	808	PGW	O03-C19-C20	2.61	120.09	111.91
3	B	808	PGW	O03-C19-C20	2.60	120.08	111.91
3	B	814	PGW	O03-C19-C20	2.58	120.02	111.91
3	A	814	PGW	O03-C19-C20	2.57	119.99	111.91
3	B	811	PGW	O03-C19-C20	2.57	119.97	111.91
3	A	819	PGW	O03-C19-C20	2.57	119.96	111.91
3	A	811	PGW	O03-C19-C20	2.56	119.94	111.91
3	A	813	PGW	O03-C19-C20	2.56	119.93	111.91
3	B	819	PGW	O03-C19-C20	2.56	119.93	111.91
3	B	813	PGW	O03-C19-C20	2.55	119.92	111.91
3	B	804	PGW	O03-C19-C20	2.55	119.90	111.91
3	A	804	PGW	O03-C19-C20	2.54	119.88	111.91
3	B	816	PGW	O03-C19-C20	2.53	119.85	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	803	PGW	O03-C19-C20	2.53	119.84	111.91
3	A	816	PGW	O03-C19-C20	2.52	119.83	111.91
3	A	810	PGW	O03-C19-C20	2.52	119.82	111.91
3	B	803	PGW	O03-C19-C20	2.52	119.82	111.91
3	B	810	PGW	O03-C19-C20	2.52	119.81	111.91
3	B	818	PGW	O03-C19-C20	2.50	119.76	111.91
3	B	807	PGW	O03-C19-C20	2.50	119.75	111.91
3	A	818	PGW	O03-C19-C20	2.50	119.74	111.91
3	A	807	PGW	O03-C19-C20	2.49	119.72	111.91

There are no chirality outliers.

All (550) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	803	PGW	C03-O11-P-O12
3	A	803	PGW	C03-O11-P-O13
3	A	803	PGW	O02-C1-O01-C02
3	A	803	PGW	O01-C02-C03-O11
3	A	803	PGW	C07-C06-C10-C9
3	A	805	PGW	C03-O11-P-O12
3	A	805	PGW	C03-O11-P-O14
3	A	805	PGW	O02-C1-O01-C02
3	A	806	PGW	C03-O11-P-O12
3	A	806	PGW	C03-O11-P-O13
3	A	806	PGW	C2-C1-O01-C02
3	A	806	PGW	O02-C1-O01-C02
3	A	807	PGW	C03-O11-P-O12
3	A	807	PGW	C03-O11-P-O13
3	A	807	PGW	O02-C1-O01-C02
3	A	808	PGW	C2-C1-O01-C02
3	A	808	PGW	O02-C1-O01-C02
3	A	809	PGW	C03-O11-P-O12
3	A	809	PGW	C03-O11-P-O13
3	A	809	PGW	O02-C1-O01-C02
3	A	810	PGW	C03-O11-P-O12
3	A	810	PGW	C03-O11-P-O13
3	A	810	PGW	O02-C1-O01-C02
3	A	811	PGW	C03-O11-P-O12
3	A	811	PGW	C03-O11-P-O13
3	A	811	PGW	O03-C01-C02-O01
3	A	811	PGW	C2-C1-O01-C02
3	A	811	PGW	C10-C06-C07-C08

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Mol	Chain	Res	Type	Atoms
3	A	812	PGW	C03-O11-P-O12
3	A	812	PGW	C03-O11-P-O13
3	A	813	PGW	C03-O11-P-O12
3	A	813	PGW	C03-O11-P-O13
3	A	813	PGW	O02-C1-O01-C02
3	A	813	PGW	C10-C06-C07-C08
3	A	814	PGW	C03-O11-P-O12
3	A	814	PGW	C03-O11-P-O13
3	A	814	PGW	C2-C1-O01-C02
3	A	815	PGW	C03-O11-P-O12
3	A	815	PGW	C03-O11-P-O13
3	A	815	PGW	O02-C1-O01-C02
3	A	816	PGW	C03-O11-P-O12
3	A	816	PGW	O03-C01-C02-O01
3	A	818	PGW	C03-O11-P-O12
3	A	818	PGW	C03-O11-P-O14
3	A	818	PGW	O02-C1-O01-C02
3	A	819	PGW	C03-O11-P-O12
3	A	819	PGW	C03-O11-P-O13
3	A	819	PGW	C2-C1-O01-C02
3	A	820	PGW	C03-O11-P-O12
3	A	820	PGW	C03-O11-P-O13
3	A	820	PGW	C2-C1-O01-C02
3	B	803	PGW	C03-O11-P-O12
3	B	803	PGW	C03-O11-P-O13
3	B	803	PGW	O02-C1-O01-C02
3	B	803	PGW	O01-C02-C03-O11
3	B	803	PGW	C07-C06-C10-C9
3	B	805	PGW	C03-O11-P-O12
3	B	805	PGW	C03-O11-P-O14
3	B	805	PGW	O02-C1-O01-C02
3	B	806	PGW	C03-O11-P-O12
3	B	806	PGW	C03-O11-P-O13
3	B	806	PGW	C2-C1-O01-C02
3	B	806	PGW	O02-C1-O01-C02
3	B	807	PGW	C03-O11-P-O12
3	B	807	PGW	C03-O11-P-O13
3	B	807	PGW	O02-C1-O01-C02
3	B	808	PGW	C2-C1-O01-C02
3	B	808	PGW	O02-C1-O01-C02
3	B	809	PGW	C03-O11-P-O12
3	B	809	PGW	C03-O11-P-O13

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Mol	Chain	Res	Type	Atoms
3	B	809	PGW	O02-C1-O01-C02
3	B	810	PGW	C03-O11-P-O12
3	B	810	PGW	C03-O11-P-O13
3	B	810	PGW	O02-C1-O01-C02
3	B	811	PGW	C03-O11-P-O12
3	B	811	PGW	C03-O11-P-O13
3	B	811	PGW	O03-C01-C02-O01
3	B	811	PGW	C2-C1-O01-C02
3	B	811	PGW	C10-C06-C07-C08
3	B	812	PGW	C03-O11-P-O12
3	B	812	PGW	C03-O11-P-O13
3	B	813	PGW	C03-O11-P-O12
3	B	813	PGW	C03-O11-P-O13
3	B	813	PGW	O02-C1-O01-C02
3	B	813	PGW	C10-C06-C07-C08
3	B	814	PGW	C03-O11-P-O12
3	B	814	PGW	C03-O11-P-O13
3	B	814	PGW	C2-C1-O01-C02
3	B	815	PGW	C03-O11-P-O12
3	B	815	PGW	C03-O11-P-O13
3	B	815	PGW	O02-C1-O01-C02
3	B	816	PGW	C03-O11-P-O12
3	B	816	PGW	O03-C01-C02-O01
3	B	818	PGW	C03-O11-P-O12
3	B	818	PGW	C03-O11-P-O14
3	B	818	PGW	O02-C1-O01-C02
3	B	819	PGW	C03-O11-P-O12
3	B	819	PGW	C03-O11-P-O13
3	B	819	PGW	C2-C1-O01-C02
3	B	820	PGW	C03-O11-P-O12
3	B	820	PGW	C03-O11-P-O13
3	B	820	PGW	C2-C1-O01-C02
3	A	805	PGW	O04-C19-O03-C01
3	B	805	PGW	O04-C19-O03-C01
3	A	805	PGW	C20-C19-O03-C01
3	B	805	PGW	C20-C19-O03-C01
3	A	809	PGW	O04-C19-O03-C01
3	B	809	PGW	O04-C19-O03-C01
3	A	811	PGW	O02-C1-O01-C02
3	A	814	PGW	O02-C1-O01-C02
3	A	817	PGW	O02-C1-O01-C02
3	A	819	PGW	O02-C1-O01-C02

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Mol	Chain	Res	Type	Atoms
3	A	820	PGW	O02-C1-O01-C02
3	B	811	PGW	O02-C1-O01-C02
3	B	814	PGW	O02-C1-O01-C02
3	B	817	PGW	O02-C1-O01-C02
3	B	819	PGW	O02-C1-O01-C02
3	B	820	PGW	O02-C1-O01-C02
3	A	809	PGW	C20-C19-O03-C01
3	A	820	PGW	C20-C19-O03-C01
3	B	809	PGW	C20-C19-O03-C01
3	B	820	PGW	C20-C19-O03-C01
3	A	803	PGW	C2-C1-O01-C02
3	A	807	PGW	C2-C1-O01-C02
3	A	809	PGW	C2-C1-O01-C02
3	A	810	PGW	C2-C1-O01-C02
3	A	813	PGW	C2-C1-O01-C02
3	A	815	PGW	C2-C1-O01-C02
3	A	817	PGW	C2-C1-O01-C02
3	A	818	PGW	C2-C1-O01-C02
3	B	803	PGW	C2-C1-O01-C02
3	B	807	PGW	C2-C1-O01-C02
3	B	809	PGW	C2-C1-O01-C02
3	B	810	PGW	C2-C1-O01-C02
3	B	813	PGW	C2-C1-O01-C02
3	B	815	PGW	C2-C1-O01-C02
3	B	817	PGW	C2-C1-O01-C02
3	B	818	PGW	C2-C1-O01-C02
3	A	820	PGW	O04-C19-O03-C01
3	B	820	PGW	O04-C19-O03-C01
3	A	806	PGW	C20-C19-O03-C01
3	B	806	PGW	C20-C19-O03-C01
3	A	816	PGW	C2-C1-O01-C02
3	B	816	PGW	C2-C1-O01-C02
3	A	806	PGW	O04-C19-O03-C01
3	B	806	PGW	O04-C19-O03-C01
3	A	819	PGW	C20-C19-O03-C01
3	B	819	PGW	C20-C19-O03-C01
3	A	812	PGW	C20-C19-O03-C01
3	B	812	PGW	C20-C19-O03-C01
3	A	819	PGW	O04-C19-O03-C01
3	B	819	PGW	O04-C19-O03-C01
3	A	816	PGW	O02-C1-O01-C02
3	B	816	PGW	O02-C1-O01-C02

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Mol	Chain	Res	Type	Atoms
3	A	805	PGW	C19-C20-C21-C22
3	A	806	PGW	C1-C2-C3-C4
3	B	805	PGW	C19-C20-C21-C22
3	B	806	PGW	C1-C2-C3-C4
3	A	812	PGW	O04-C19-O03-C01
3	B	812	PGW	O04-C19-O03-C01
3	A	810	PGW	C20-C19-O03-C01
3	B	810	PGW	C20-C19-O03-C01
3	A	817	PGW	C20-C19-O03-C01
3	B	817	PGW	C20-C19-O03-C01
3	A	817	PGW	C19-C20-C21-C22
3	B	817	PGW	C19-C20-C21-C22
3	A	804	PGW	C2-C1-O01-C02
3	A	812	PGW	C2-C1-O01-C02
3	B	804	PGW	C2-C1-O01-C02
3	B	812	PGW	C2-C1-O01-C02
3	A	804	PGW	O02-C1-O01-C02
3	A	812	PGW	O02-C1-O01-C02
3	B	804	PGW	O02-C1-O01-C02
3	B	812	PGW	O02-C1-O01-C02
3	A	815	PGW	C20-C19-O03-C01
3	B	815	PGW	C20-C19-O03-C01
3	A	811	PGW	C6-C7-C8-C9
3	B	811	PGW	C6-C7-C8-C9
3	A	815	PGW	C22-C23-C24-C25
3	A	816	PGW	C23-C24-C25-C26
3	B	815	PGW	C22-C23-C24-C25
3	A	815	PGW	C23-C24-C25-C26
3	B	815	PGW	C23-C24-C25-C26
3	B	816	PGW	C23-C24-C25-C26
3	A	803	PGW	C24-C25-C26-C27
3	A	813	PGW	C24-C25-C26-C27
3	B	803	PGW	C24-C25-C26-C27
3	B	813	PGW	C24-C25-C26-C27
3	A	805	PGW	C01-C02-O01-C1
3	B	805	PGW	C01-C02-O01-C1
3	A	805	PGW	C21-C22-C23-C24
3	A	810	PGW	O04-C19-O03-C01
3	B	810	PGW	O04-C19-O03-C01
3	B	805	PGW	C21-C22-C23-C24
3	A	815	PGW	C19-C20-C21-C22
3	B	815	PGW	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
3	A	817	PGW	O04-C19-O03-C01
3	B	817	PGW	O04-C19-O03-C01
3	A	815	PGW	C10-C06-C07-C08
3	B	815	PGW	C10-C06-C07-C08
3	A	810	PGW	C23-C24-C25-C26
3	A	812	PGW	C21-C22-C23-C24
3	A	815	PGW	C21-C22-C23-C24
3	B	810	PGW	C23-C24-C25-C26
3	B	812	PGW	C21-C22-C23-C24
3	B	815	PGW	C21-C22-C23-C24
3	B	818	PGW	C20-C21-C22-C23
3	A	818	PGW	C20-C21-C22-C23
3	A	803	PGW	C21-C22-C23-C24
3	B	803	PGW	C21-C22-C23-C24
3	A	818	PGW	C19-C20-C21-C22
3	B	818	PGW	C19-C20-C21-C22
3	A	805	PGW	C6-C7-C8-C9
3	A	818	PGW	C10-C06-C07-C08
3	B	805	PGW	C6-C7-C8-C9
3	B	818	PGW	C10-C06-C07-C08
3	A	815	PGW	O04-C19-O03-C01
3	B	815	PGW	O04-C19-O03-C01
3	A	819	PGW	C21-C22-C23-C24
3	B	819	PGW	C21-C22-C23-C24
3	A	819	PGW	C3-C4-C5-C6
3	B	819	PGW	C3-C4-C5-C6
3	A	812	PGW	C19-C20-C21-C22
3	B	812	PGW	C19-C20-C21-C22
3	A	817	PGW	C22-C23-C24-C25
3	B	817	PGW	C22-C23-C24-C25
3	A	803	PGW	C6-C7-C8-C9
3	B	803	PGW	C6-C7-C8-C9
3	A	812	PGW	C22-C23-C24-C25
3	B	812	PGW	C22-C23-C24-C25
3	A	820	PGW	C19-C20-C21-C22
3	B	820	PGW	C19-C20-C21-C22
3	A	806	PGW	C2-C3-C4-C5
3	A	811	PGW	C19-C20-C21-C22
3	B	811	PGW	C19-C20-C21-C22
3	A	820	PGW	C22-C23-C24-C25
3	B	806	PGW	C2-C3-C4-C5
3	B	820	PGW	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
3	A	814	PGW	C21-C22-C23-C24
3	B	814	PGW	C21-C22-C23-C24
3	A	813	PGW	C23-C24-C25-C26
3	A	817	PGW	C24-C25-C26-C27
3	B	813	PGW	C23-C24-C25-C26
3	B	817	PGW	C24-C25-C26-C27
3	A	820	PGW	C1-C2-C3-C4
3	B	820	PGW	C1-C2-C3-C4
3	A	811	PGW	C02-C03-O11-P
3	B	811	PGW	C02-C03-O11-P
3	A	803	PGW	C01-C02-C03-O11
3	A	811	PGW	C01-C02-C03-O11
3	A	820	PGW	C01-C02-C03-O11
3	B	803	PGW	C01-C02-C03-O11
3	B	811	PGW	C01-C02-C03-O11
3	B	820	PGW	C01-C02-C03-O11
3	B	816	PGW	C16-C15-C27-C26
3	A	810	PGW	C22-C23-C24-C25
3	A	816	PGW	C16-C15-C27-C26
3	B	810	PGW	C22-C23-C24-C25
3	A	817	PGW	C15-C16-C17-C18
3	B	817	PGW	C15-C16-C17-C18
3	A	812	PGW	O03-C01-C02-C03
3	A	814	PGW	O03-C01-C02-C03
3	A	815	PGW	O03-C01-C02-C03
3	B	812	PGW	O03-C01-C02-C03
3	B	814	PGW	O03-C01-C02-C03
3	B	815	PGW	O03-C01-C02-C03
3	A	804	PGW	C21-C22-C23-C24
3	B	804	PGW	C21-C22-C23-C24
3	A	816	PGW	C19-C20-C21-C22
3	B	816	PGW	C19-C20-C21-C22
3	A	809	PGW	C21-C22-C23-C24
3	A	812	PGW	C23-C24-C25-C26
3	B	809	PGW	C21-C22-C23-C24
3	B	812	PGW	C23-C24-C25-C26
3	A	816	PGW	C24-C25-C26-C27
3	B	816	PGW	C24-C25-C26-C27
3	A	806	PGW	C21-C22-C23-C24
3	B	806	PGW	C21-C22-C23-C24
3	A	817	PGW	C01-C02-O01-C1
3	A	818	PGW	C01-C02-O01-C1

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Mol	Chain	Res	Type	Atoms
3	A	820	PGW	C03-C02-O01-C1
3	B	817	PGW	C01-C02-O01-C1
3	B	818	PGW	C01-C02-O01-C1
3	B	820	PGW	C03-C02-O01-C1
3	A	803	PGW	C03-O11-P-O14
3	A	806	PGW	C03-O11-P-O14
3	A	809	PGW	C03-O11-P-O14
3	A	810	PGW	C03-O11-P-O14
3	A	811	PGW	C03-O11-P-O14
3	A	812	PGW	C03-O11-P-O14
3	A	813	PGW	C03-O11-P-O14
3	A	814	PGW	C03-O11-P-O14
3	A	815	PGW	C03-O11-P-O14
3	A	819	PGW	C03-O11-P-O14
3	A	820	PGW	C03-O11-P-O14
3	B	803	PGW	C03-O11-P-O14
3	B	806	PGW	C03-O11-P-O14
3	B	809	PGW	C03-O11-P-O14
3	B	810	PGW	C03-O11-P-O14
3	B	811	PGW	C03-O11-P-O14
3	B	812	PGW	C03-O11-P-O14
3	B	813	PGW	C03-O11-P-O14
3	B	814	PGW	C03-O11-P-O14
3	B	815	PGW	C03-O11-P-O14
3	B	819	PGW	C03-O11-P-O14
3	B	820	PGW	C03-O11-P-O14
3	A	810	PGW	O01-C02-C03-O11
3	A	818	PGW	O01-C02-C03-O11
3	B	810	PGW	O01-C02-C03-O11
3	B	818	PGW	O01-C02-C03-O11
3	A	804	PGW	C3-C4-C5-C6
3	B	804	PGW	C3-C4-C5-C6
3	A	814	PGW	O03-C01-C02-O01
3	A	815	PGW	O03-C01-C02-O01
3	B	814	PGW	O03-C01-C02-O01
3	A	815	PGW	C20-C21-C22-C23
3	B	815	PGW	C20-C21-C22-C23
3	A	814	PGW	O03-C19-C20-C21
3	B	814	PGW	O03-C19-C20-C21
3	A	807	PGW	C21-C22-C23-C24
3	B	807	PGW	C21-C22-C23-C24
3	A	810	PGW	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
3	B	810	PGW	C24-C25-C26-C27
3	B	807	PGW	C20-C19-O03-C01
3	A	814	PGW	C23-C24-C25-C26
3	A	815	PGW	C16-C15-C27-C26
3	B	814	PGW	C23-C24-C25-C26
3	B	815	PGW	C16-C15-C27-C26
3	A	810	PGW	C01-C02-C03-O11
3	A	816	PGW	C01-C02-C03-O11
3	B	810	PGW	C01-C02-C03-O11
3	B	816	PGW	C01-C02-C03-O11
3	A	818	PGW	C1-C2-C3-C4
3	B	818	PGW	C1-C2-C3-C4
3	A	807	PGW	C20-C19-O03-C01
3	A	813	PGW	C19-C20-C21-C22
3	B	813	PGW	C19-C20-C21-C22
3	A	816	PGW	C20-C19-O03-C01
3	B	816	PGW	C20-C19-O03-C01
3	A	817	PGW	C16-C17-C18-C28
3	B	817	PGW	C16-C17-C18-C28
3	A	804	PGW	O03-C01-C02-C03
3	B	804	PGW	O03-C01-C02-C03
3	A	818	PGW	C24-C25-C26-C27
3	B	818	PGW	C24-C25-C26-C27
3	A	820	PGW	C2-C3-C4-C5
3	B	820	PGW	C2-C3-C4-C5
3	A	809	PGW	C20-C21-C22-C23
3	B	809	PGW	C20-C21-C22-C23
3	A	820	PGW	O01-C02-C03-O11
3	B	820	PGW	O01-C02-C03-O11
3	A	805	PGW	C3-C4-C5-C6
3	B	805	PGW	C3-C4-C5-C6
3	A	805	PGW	O03-C01-C02-O01
3	A	807	PGW	O03-C01-C02-O01
3	A	820	PGW	O03-C01-C02-O01
3	B	805	PGW	O03-C01-C02-O01
3	B	807	PGW	O03-C01-C02-O01
3	B	815	PGW	O03-C01-C02-O01
3	B	820	PGW	O03-C01-C02-O01
3	A	813	PGW	C21-C22-C23-C24
3	A	817	PGW	C21-C22-C23-C24
3	B	813	PGW	C21-C22-C23-C24
3	B	817	PGW	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
3	A	815	PGW	C3-C4-C5-C6
3	B	815	PGW	C3-C4-C5-C6
3	A	809	PGW	C19-C20-C21-C22
3	B	809	PGW	C19-C20-C21-C22
3	A	820	PGW	C21-C22-C23-C24
3	B	820	PGW	C21-C22-C23-C24
3	A	806	PGW	C01-C02-C03-O11
3	A	819	PGW	C01-C02-C03-O11
3	B	806	PGW	C01-C02-C03-O11
3	B	819	PGW	C01-C02-C03-O11
3	A	816	PGW	C03-O11-P-O13
3	A	818	PGW	C03-O11-P-O13
3	B	816	PGW	C03-O11-P-O13
3	B	818	PGW	C03-O11-P-O13
3	A	813	PGW	C20-C19-O03-C01
3	B	813	PGW	C20-C19-O03-C01
3	A	809	PGW	C01-C02-O01-C1
3	B	809	PGW	C01-C02-O01-C1
3	A	803	PGW	C20-C21-C22-C23
3	B	803	PGW	C20-C21-C22-C23
3	A	805	PGW	O03-C01-C02-C03
3	A	811	PGW	O03-C01-C02-C03
3	A	813	PGW	C02-C03-O11-P
3	B	805	PGW	O03-C01-C02-C03
3	B	811	PGW	O03-C01-C02-C03
3	B	813	PGW	C02-C03-O11-P
3	B	816	PGW	O03-C01-C02-C03
3	A	806	PGW	O01-C02-C03-O11
3	A	816	PGW	O01-C02-C03-O11
3	A	819	PGW	O01-C02-C03-O11
3	B	806	PGW	O01-C02-C03-O11
3	B	816	PGW	O01-C02-C03-O11
3	B	819	PGW	O01-C02-C03-O11
3	A	807	PGW	O04-C19-O03-C01
3	A	816	PGW	O04-C19-O03-C01
3	B	807	PGW	O04-C19-O03-C01
3	B	816	PGW	O04-C19-O03-C01
3	A	812	PGW	O03-C01-C02-O01
3	B	812	PGW	O03-C01-C02-O01
3	A	818	PGW	C23-C24-C25-C26
3	B	818	PGW	C23-C24-C25-C26
3	A	813	PGW	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
3	B	813	PGW	C6-C7-C8-C9
3	A	808	PGW	O03-C19-C20-C21
3	B	808	PGW	O03-C19-C20-C21
3	A	818	PGW	C21-C22-C23-C24
3	B	818	PGW	C21-C22-C23-C24
3	A	818	PGW	C02-C03-O11-P
3	B	818	PGW	C02-C03-O11-P
3	A	813	PGW	O04-C19-O03-C01
3	B	813	PGW	O04-C19-O03-C01
3	A	811	PGW	C20-C19-O03-C01
3	B	811	PGW	C20-C19-O03-C01
3	A	807	PGW	C01-C02-C03-O11
3	B	807	PGW	C01-C02-C03-O11
3	A	807	PGW	C2-C3-C4-C5
3	B	807	PGW	C2-C3-C4-C5
3	A	818	PGW	C2-C3-C4-C5
3	B	818	PGW	C2-C3-C4-C5
3	A	807	PGW	O01-C02-C03-O11
3	A	811	PGW	O01-C02-C03-O11
3	A	812	PGW	O01-C02-C03-O11
3	B	807	PGW	O01-C02-C03-O11
3	B	811	PGW	O01-C02-C03-O11
3	B	812	PGW	O01-C02-C03-O11
3	A	816	PGW	C15-C16-C17-C18
3	B	816	PGW	C15-C16-C17-C18
3	A	816	PGW	O03-C01-C02-C03
3	A	820	PGW	O03-C01-C02-C03
3	B	820	PGW	O03-C01-C02-C03
3	A	809	PGW	O03-C01-C02-O01
3	A	817	PGW	O03-C01-C02-O01
3	B	809	PGW	O03-C01-C02-O01
3	B	817	PGW	O03-C01-C02-O01
3	A	818	PGW	C5-C6-C7-C8
3	B	818	PGW	C5-C6-C7-C8
3	A	807	PGW	C02-C03-O11-P
3	A	809	PGW	C02-C03-O11-P
3	B	807	PGW	C02-C03-O11-P
3	B	809	PGW	C02-C03-O11-P
3	A	811	PGW	O04-C19-O03-C01
3	B	811	PGW	O04-C19-O03-C01
3	A	809	PGW	O01-C1-C2-C3
3	B	809	PGW	O01-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
3	B	805	PGW	C4-C5-C6-C7
3	A	805	PGW	C4-C5-C6-C7
3	A	811	PGW	C3-C4-C5-C6
3	B	811	PGW	C3-C4-C5-C6
3	A	806	PGW	C5-C6-C7-C8
3	B	806	PGW	C5-C6-C7-C8
3	A	812	PGW	C01-C02-C03-O11
3	B	812	PGW	C01-C02-C03-O11
3	A	808	PGW	C03-O11-P-O14
3	A	816	PGW	C03-O11-P-O14
3	B	808	PGW	C03-O11-P-O14
3	B	816	PGW	C03-O11-P-O14
3	A	818	PGW	O04-C19-O03-C01
3	B	818	PGW	O04-C19-O03-C01
3	A	818	PGW	C20-C19-O03-C01
3	B	818	PGW	C20-C19-O03-C01
3	A	809	PGW	C2-C3-C4-C5
3	B	809	PGW	C2-C3-C4-C5
3	A	804	PGW	O03-C01-C02-O01
3	B	804	PGW	O03-C01-C02-O01
3	A	818	PGW	C6-C7-C8-C9
3	B	818	PGW	C6-C7-C8-C9
3	A	811	PGW	C07-C06-C10-C9
3	A	813	PGW	C7-C8-C9-C10
3	B	811	PGW	C07-C06-C10-C9
3	B	813	PGW	C7-C8-C9-C10
3	A	814	PGW	C20-C19-O03-C01
3	B	814	PGW	C20-C19-O03-C01
3	A	815	PGW	C24-C25-C26-C27
3	B	815	PGW	C24-C25-C26-C27
3	A	805	PGW	C22-C23-C24-C25
3	B	805	PGW	C22-C23-C24-C25
3	A	814	PGW	O04-C19-O03-C01
3	B	814	PGW	O04-C19-O03-C01
3	B	812	PGW	C3-C4-C5-C6
3	A	812	PGW	C3-C4-C5-C6
3	A	814	PGW	O04-C19-C20-C21
3	B	814	PGW	O04-C19-C20-C21
3	A	818	PGW	C01-C02-C03-O11
3	B	818	PGW	C01-C02-C03-O11
3	A	806	PGW	C7-C8-C9-C10
3	B	806	PGW	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
3	B	815	PGW	C15-C16-C17-C18
3	A	815	PGW	C15-C16-C17-C18
3	A	805	PGW	C7-C8-C9-C10
3	A	815	PGW	C7-C8-C9-C10
3	B	805	PGW	C7-C8-C9-C10
3	B	815	PGW	C7-C8-C9-C10
3	A	805	PGW	C03-O11-P-O13
3	B	805	PGW	C03-O11-P-O13
3	A	819	PGW	C7-C8-C9-C10
3	B	819	PGW	C7-C8-C9-C10
3	A	809	PGW	C1-C2-C3-C4
3	A	807	PGW	O03-C19-C20-C21
3	B	807	PGW	O03-C19-C20-C21
3	A	807	PGW	C03-O11-P-O14
3	A	809	PGW	O03-C01-C02-C03
3	B	807	PGW	C03-O11-P-O14
3	B	809	PGW	O03-C01-C02-C03
3	B	809	PGW	C1-C2-C3-C4
3	A	819	PGW	C22-C23-C24-C25
3	B	819	PGW	C22-C23-C24-C25
3	A	804	PGW	C7-C8-C9-C10
3	B	804	PGW	C7-C8-C9-C10
3	A	807	PGW	O01-C1-C2-C3
3	B	807	PGW	O01-C1-C2-C3
3	B	820	PGW	O03-C19-C20-C21
3	A	820	PGW	O03-C19-C20-C21
3	A	818	PGW	C7-C8-C9-C10
3	B	818	PGW	C7-C8-C9-C10
3	B	817	PGW	O01-C1-C2-C3
3	A	817	PGW	O01-C1-C2-C3
3	A	812	PGW	C5-C6-C7-C8
3	A	807	PGW	O02-C1-C2-C3
3	B	807	PGW	O02-C1-C2-C3
3	B	812	PGW	C5-C6-C7-C8
3	A	806	PGW	O03-C01-C02-C03
3	A	807	PGW	O03-C01-C02-C03
3	A	817	PGW	O03-C01-C02-C03
3	B	806	PGW	O03-C01-C02-C03
3	B	807	PGW	O03-C01-C02-C03
3	B	817	PGW	O03-C01-C02-C03
3	A	812	PGW	O01-C1-C2-C3
3	B	812	PGW	O01-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
3	A	817	PGW	O02-C1-C2-C3
3	B	817	PGW	O02-C1-C2-C3
3	A	812	PGW	O03-C19-C20-C21
3	B	812	PGW	O03-C19-C20-C21
3	A	807	PGW	O04-C19-C20-C21
3	A	820	PGW	O04-C19-C20-C21
3	B	807	PGW	O04-C19-C20-C21
3	B	820	PGW	O04-C19-C20-C21
3	A	811	PGW	O03-C19-C20-C21
3	B	817	PGW	O03-C19-C20-C21
3	A	817	PGW	O03-C19-C20-C21
3	B	811	PGW	O03-C19-C20-C21
3	A	812	PGW	O02-C1-C2-C3
3	B	812	PGW	O02-C1-C2-C3
3	A	819	PGW	O03-C19-C20-C21
3	B	819	PGW	O03-C19-C20-C21
3	A	812	PGW	O04-C19-C20-C21
3	B	812	PGW	O04-C19-C20-C21

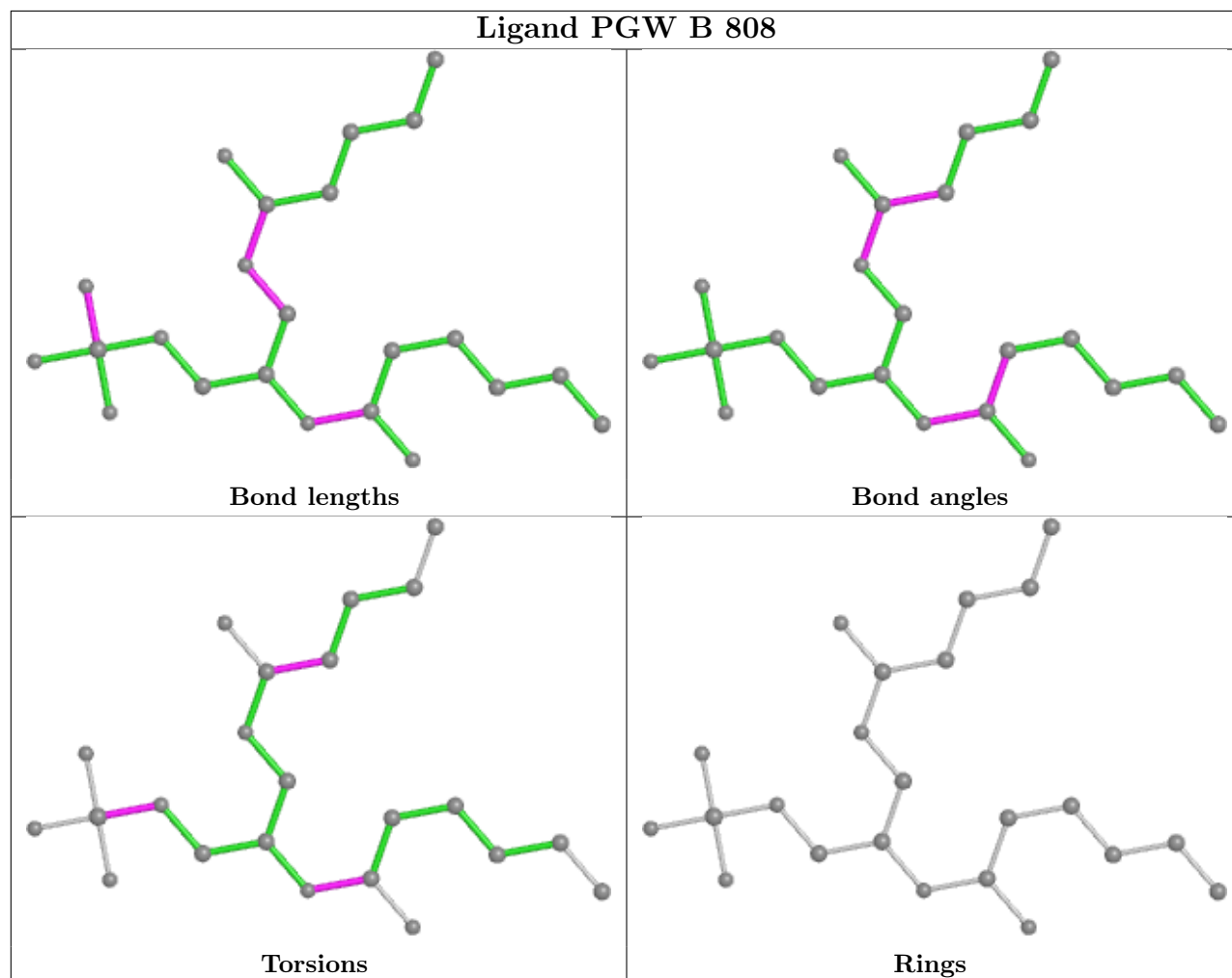
There are no ring outliers.

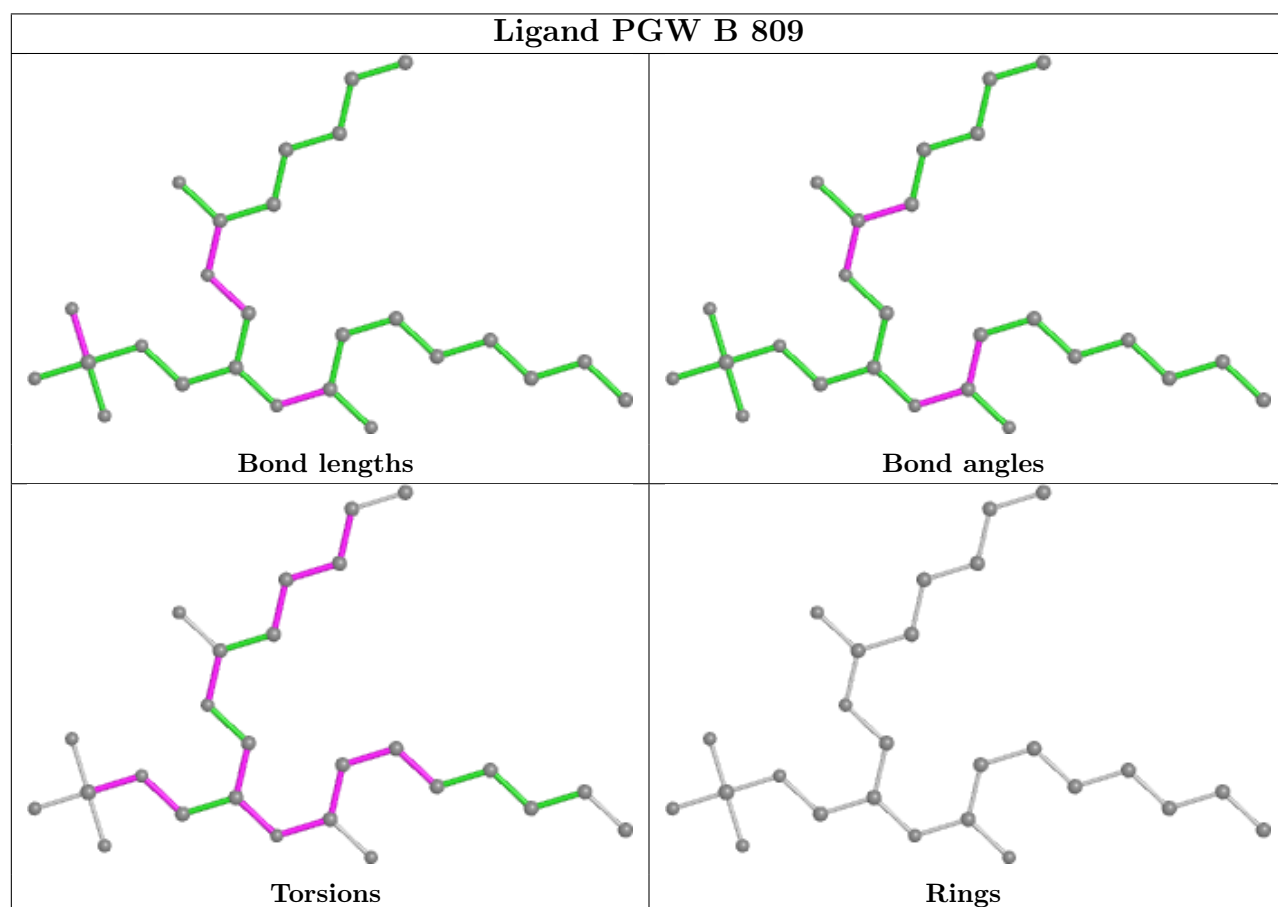
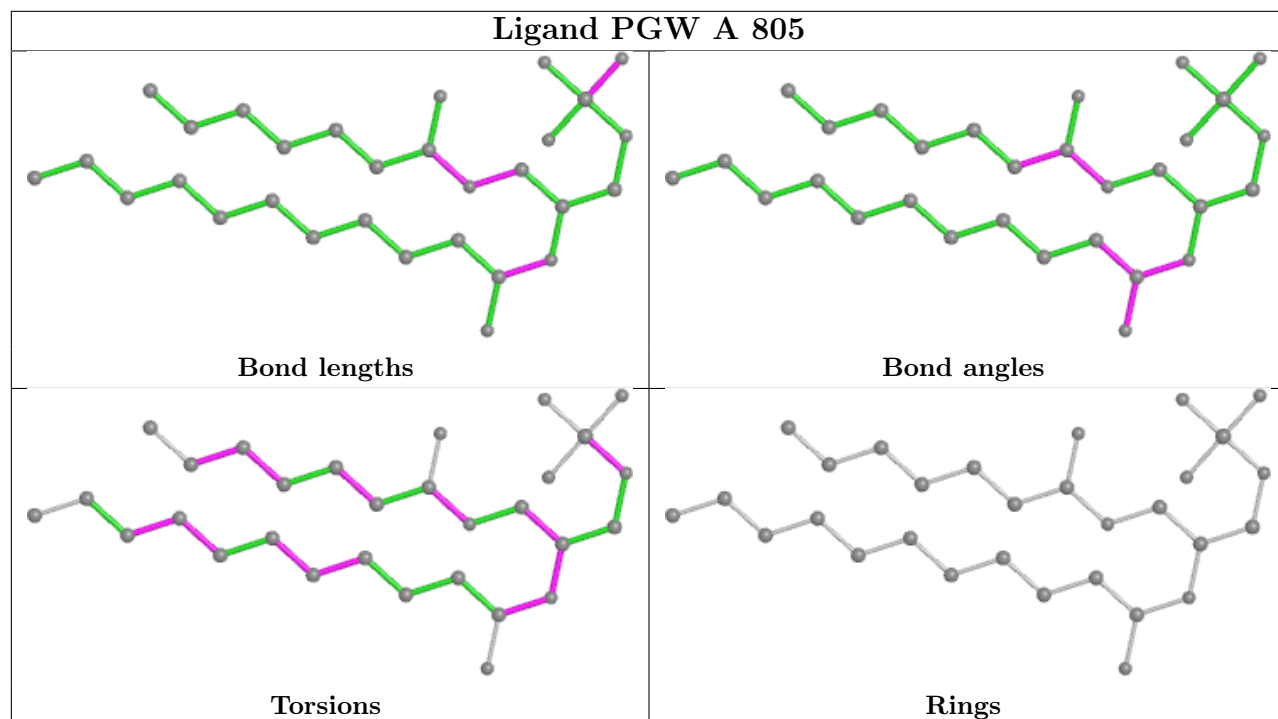
9 monomers are involved in 9 short contacts:

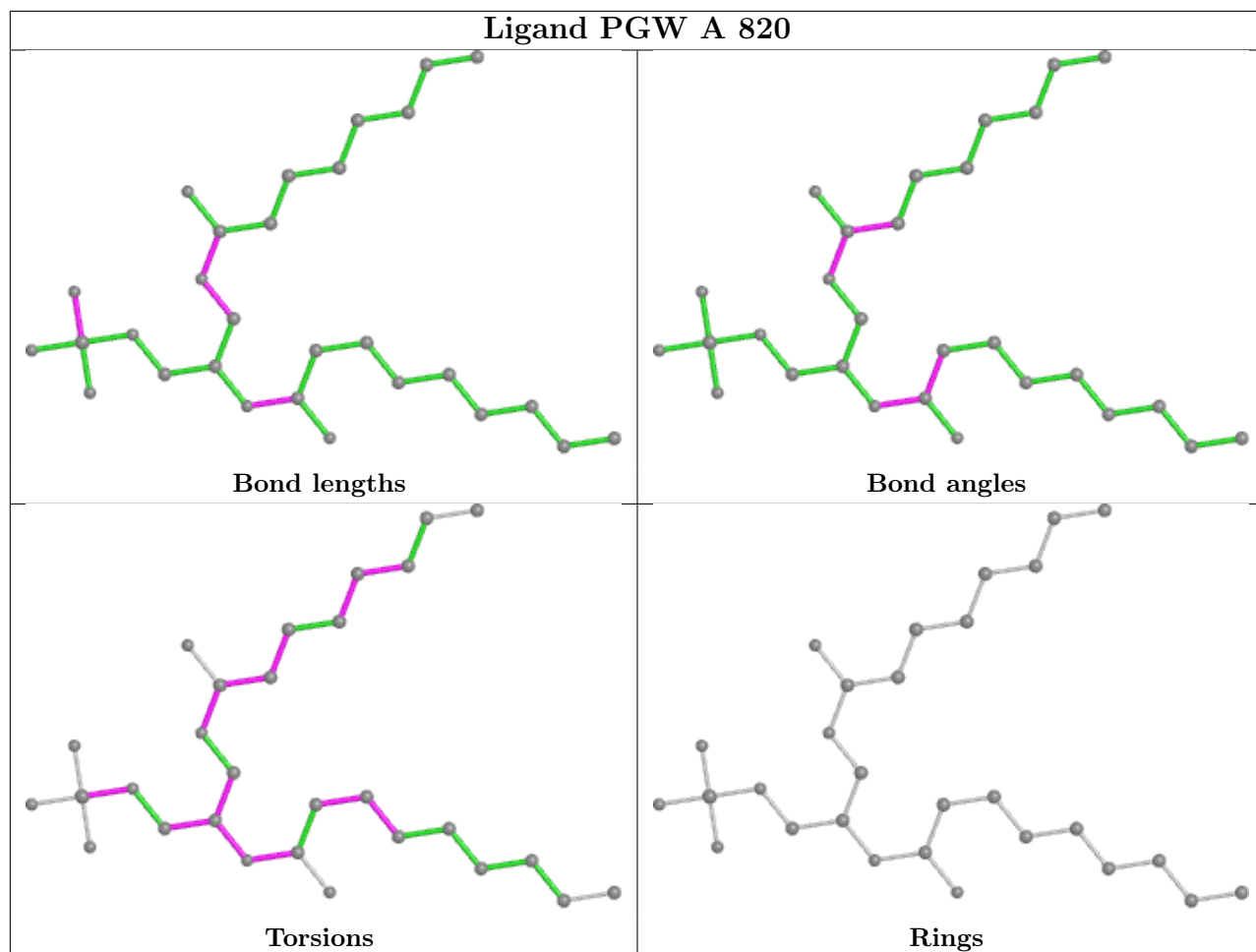
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	809	PGW	1	0
3	A	810	PGW	1	0
3	B	807	PGW	1	0
3	A	817	PGW	1	0
3	B	817	PGW	1	0
3	B	813	PGW	1	0
3	A	809	PGW	1	0
3	A	813	PGW	1	0
3	A	807	PGW	1	0

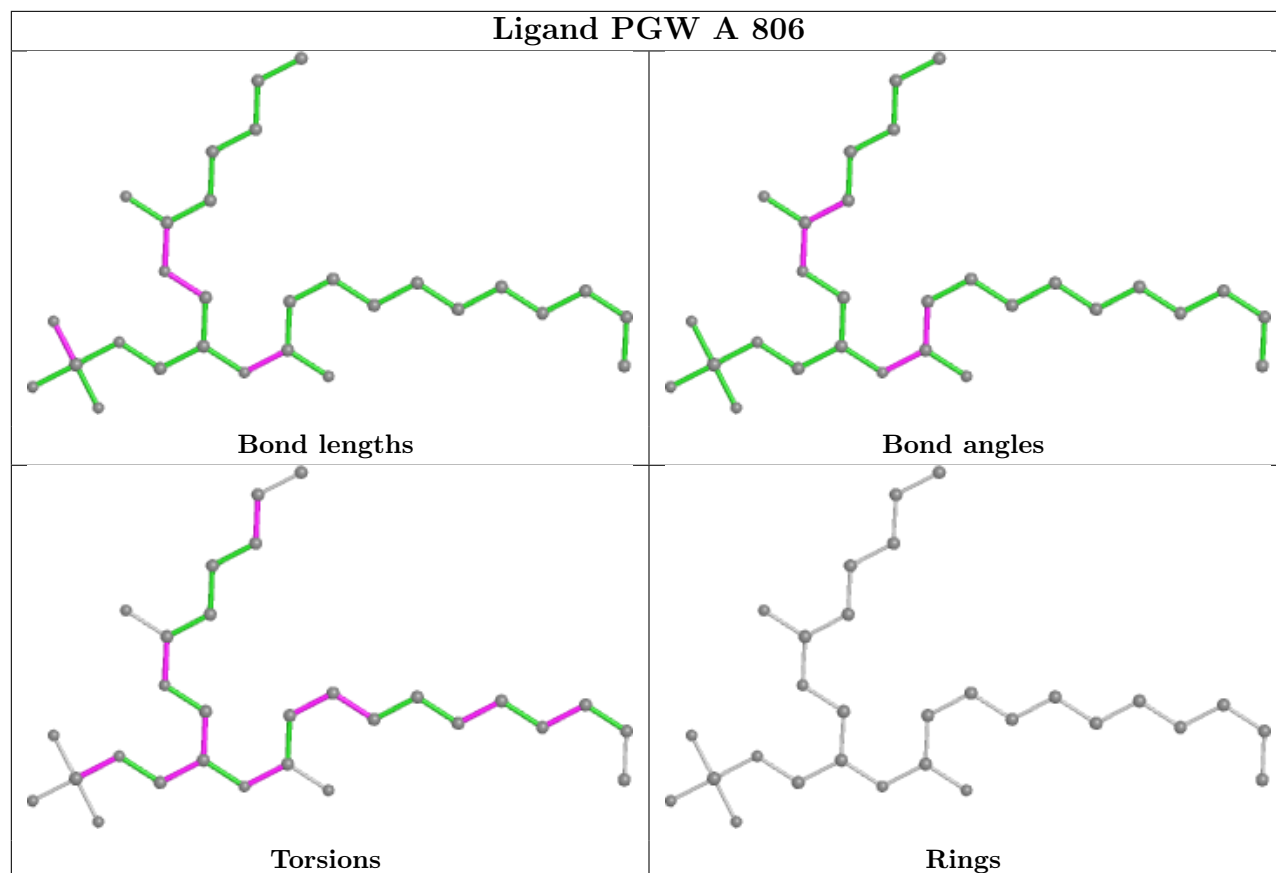
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

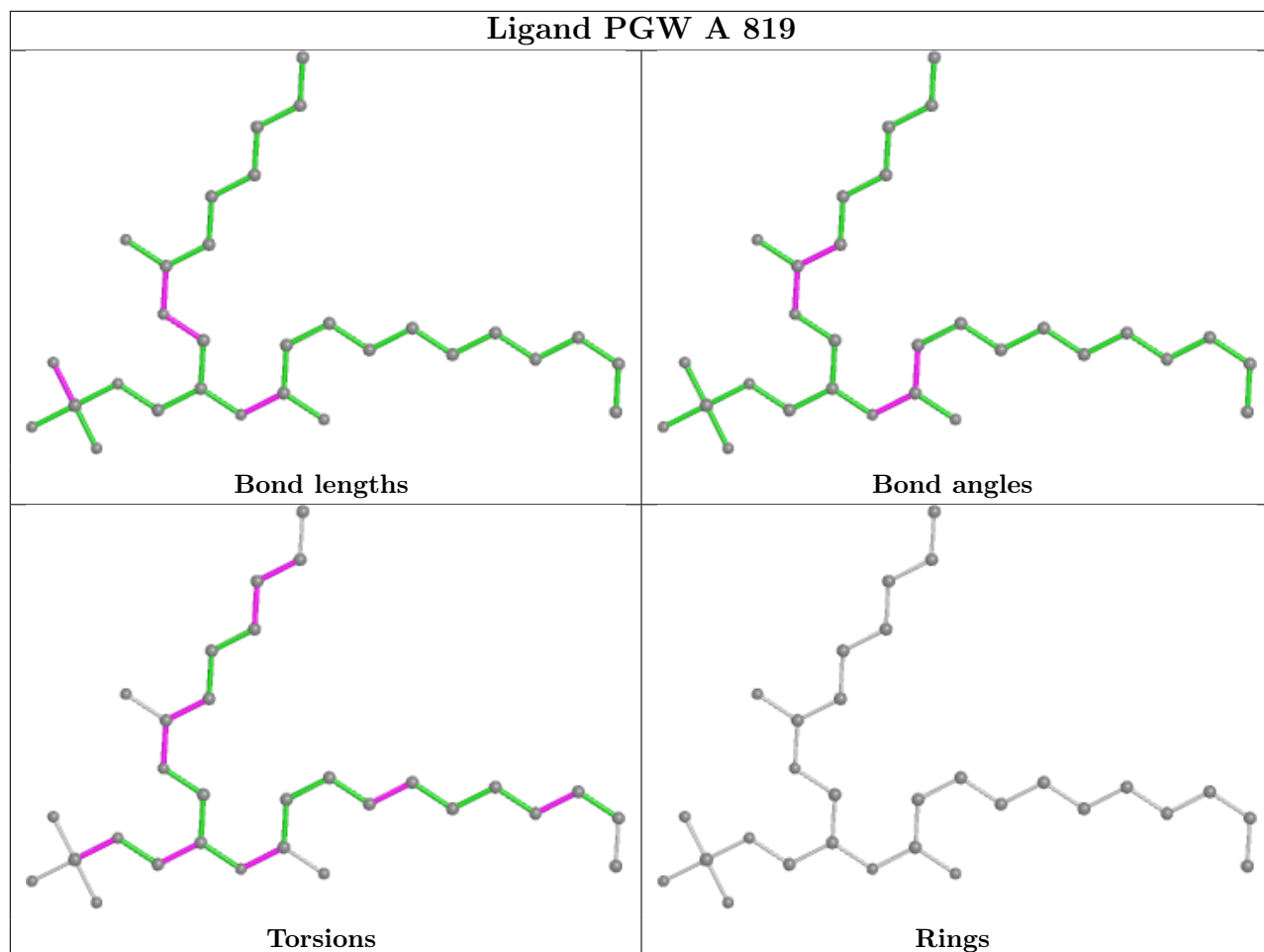
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

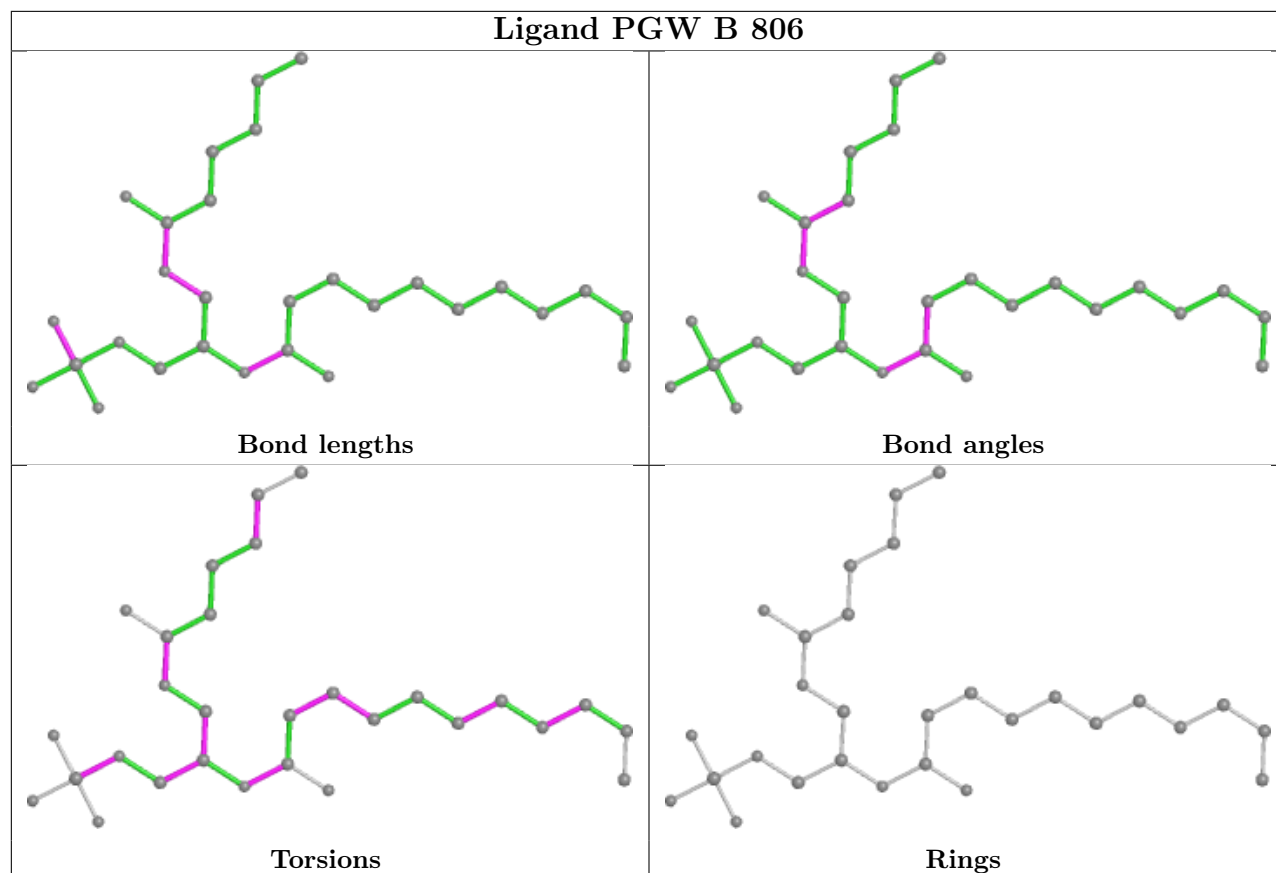




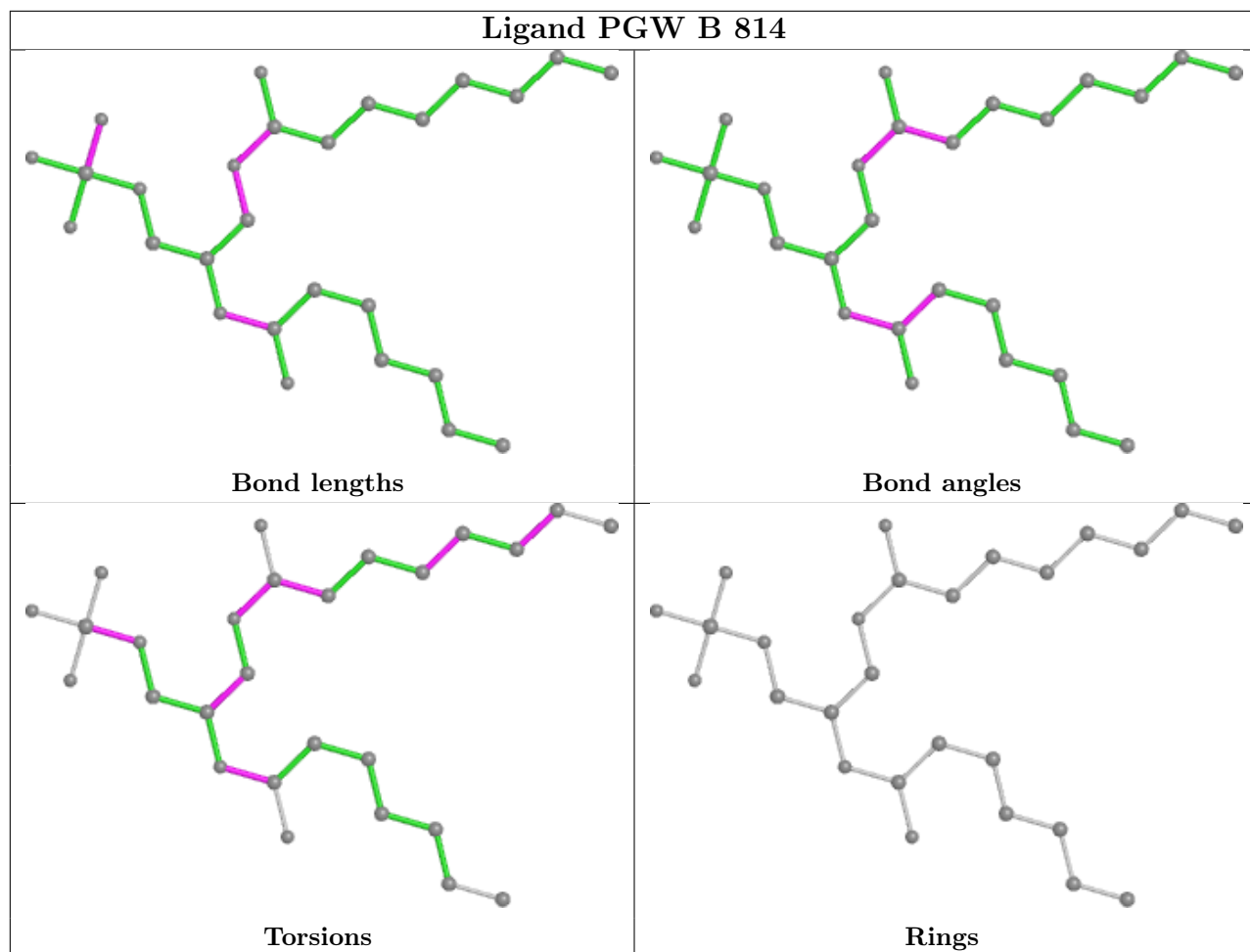


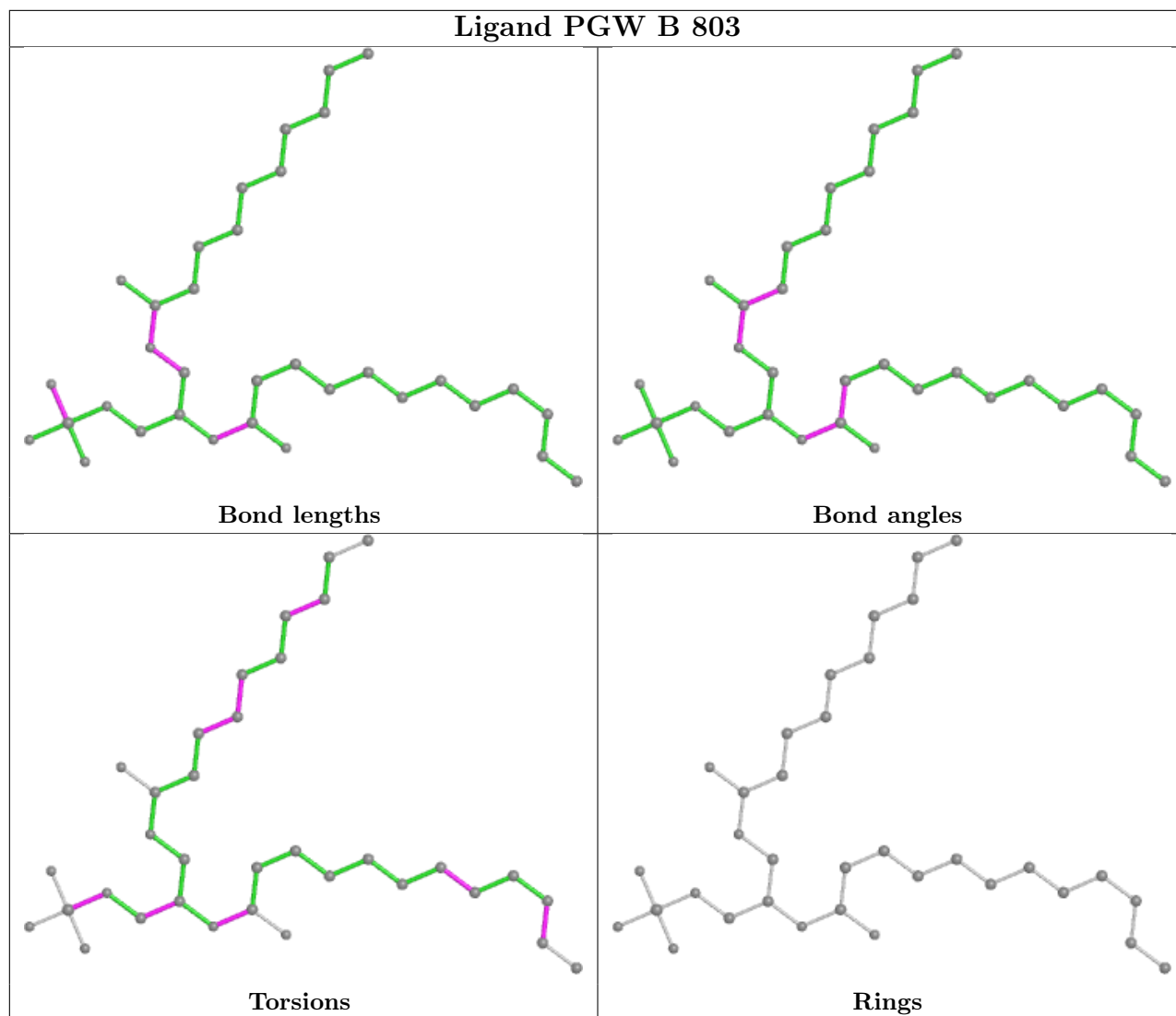


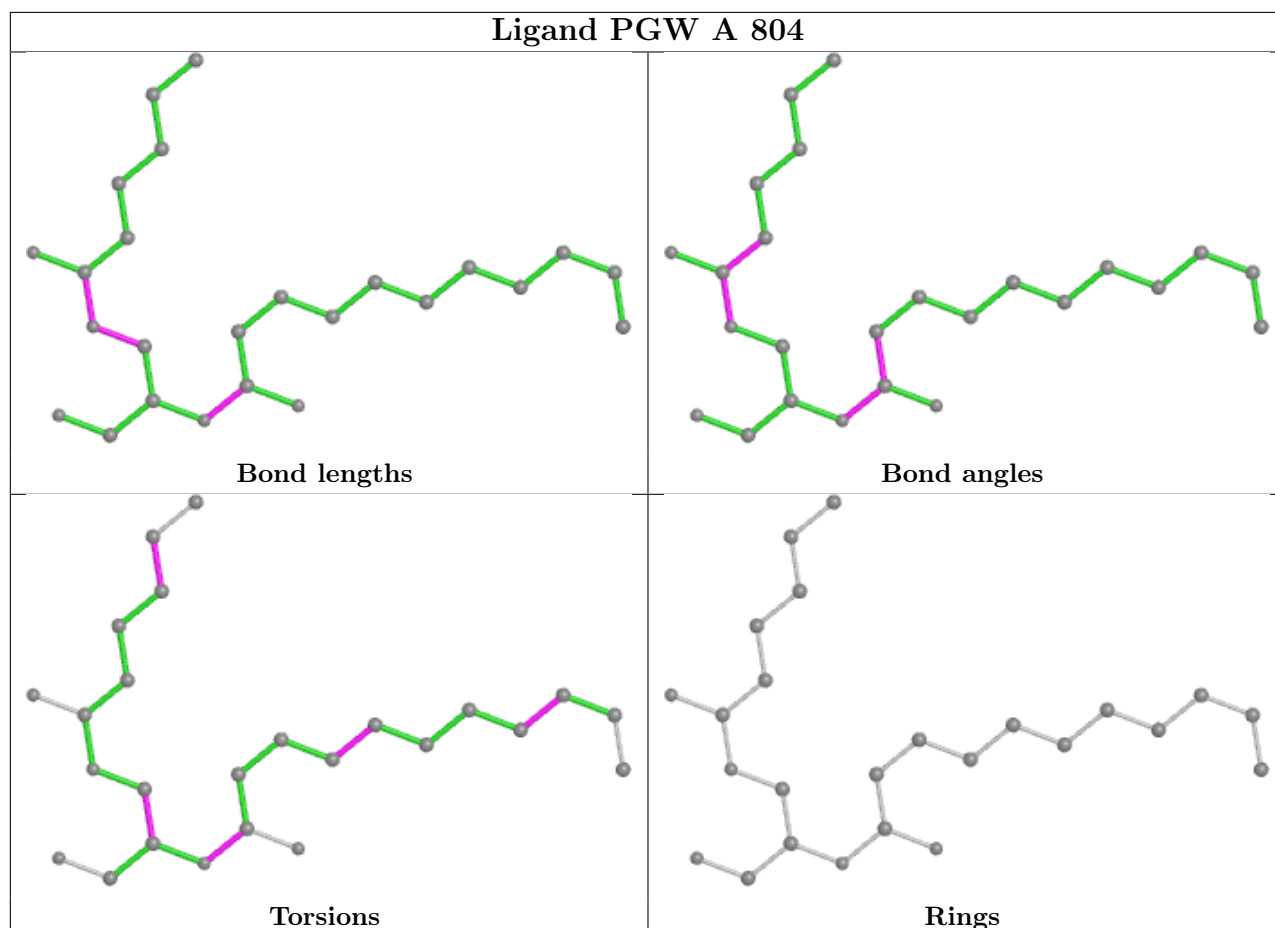
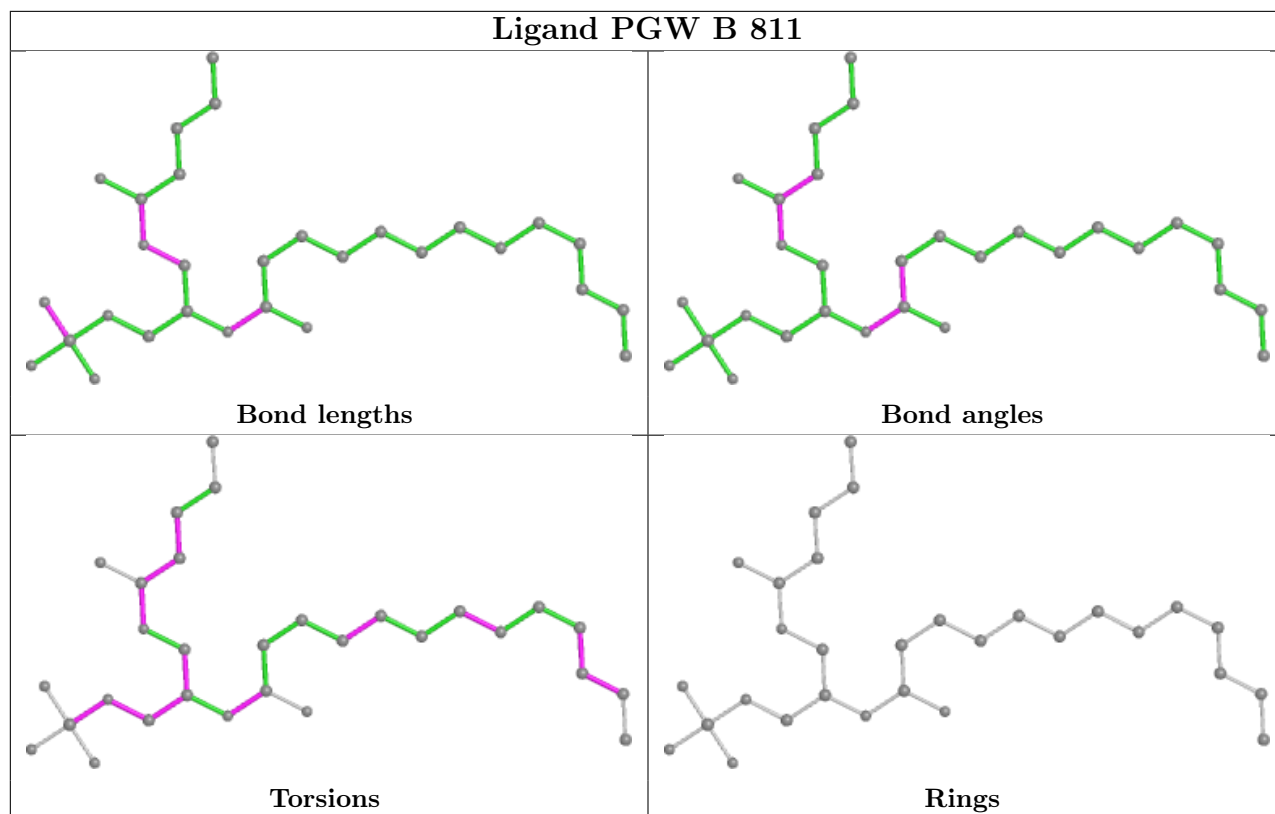


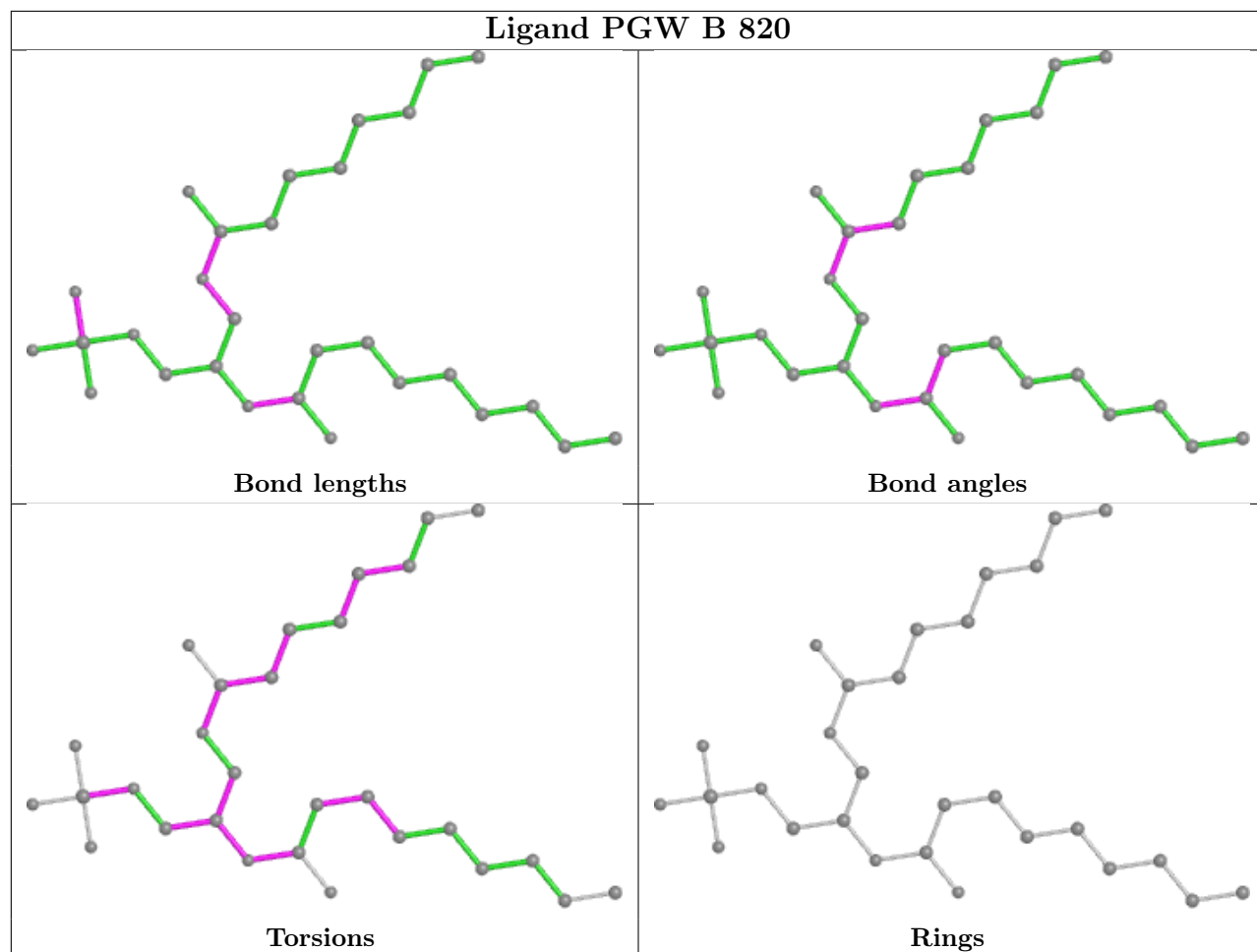


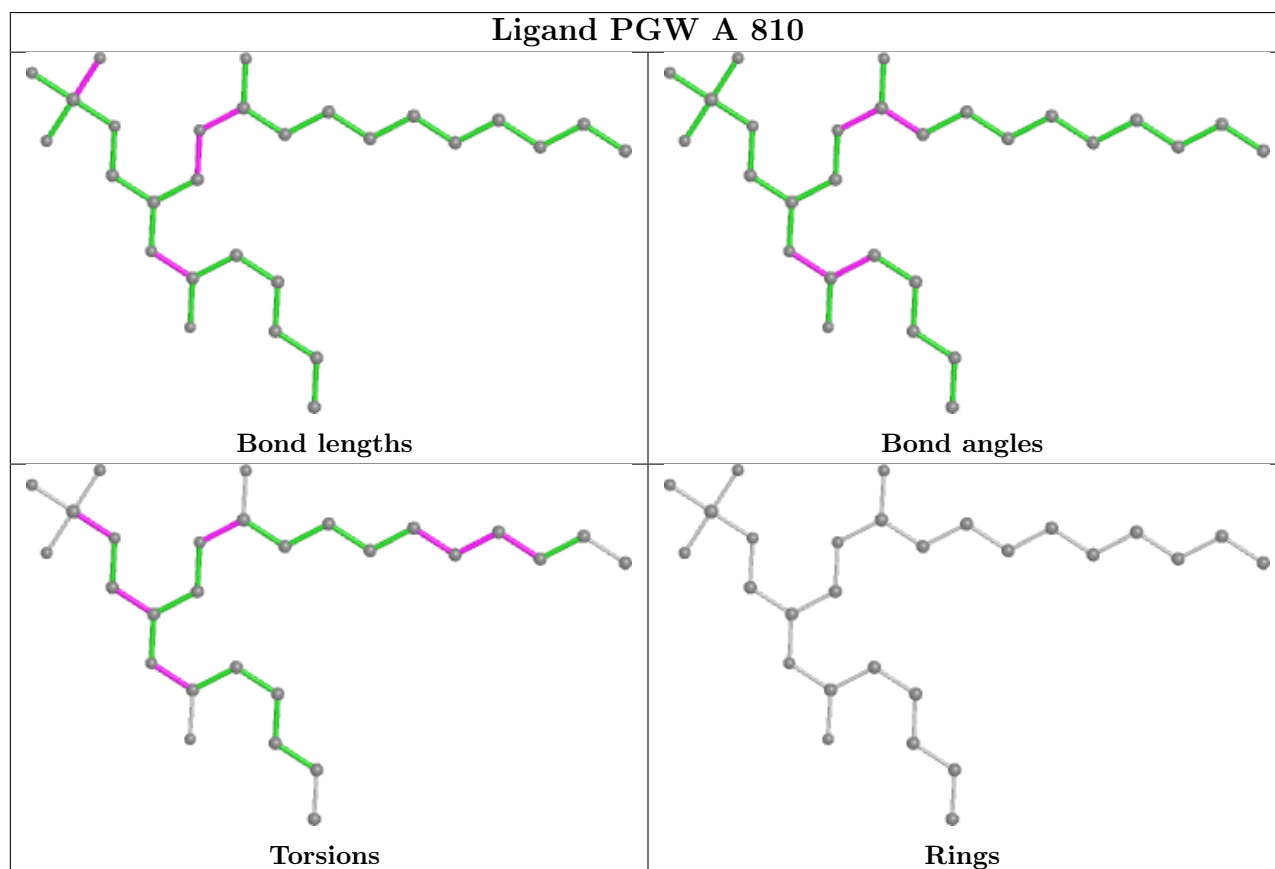
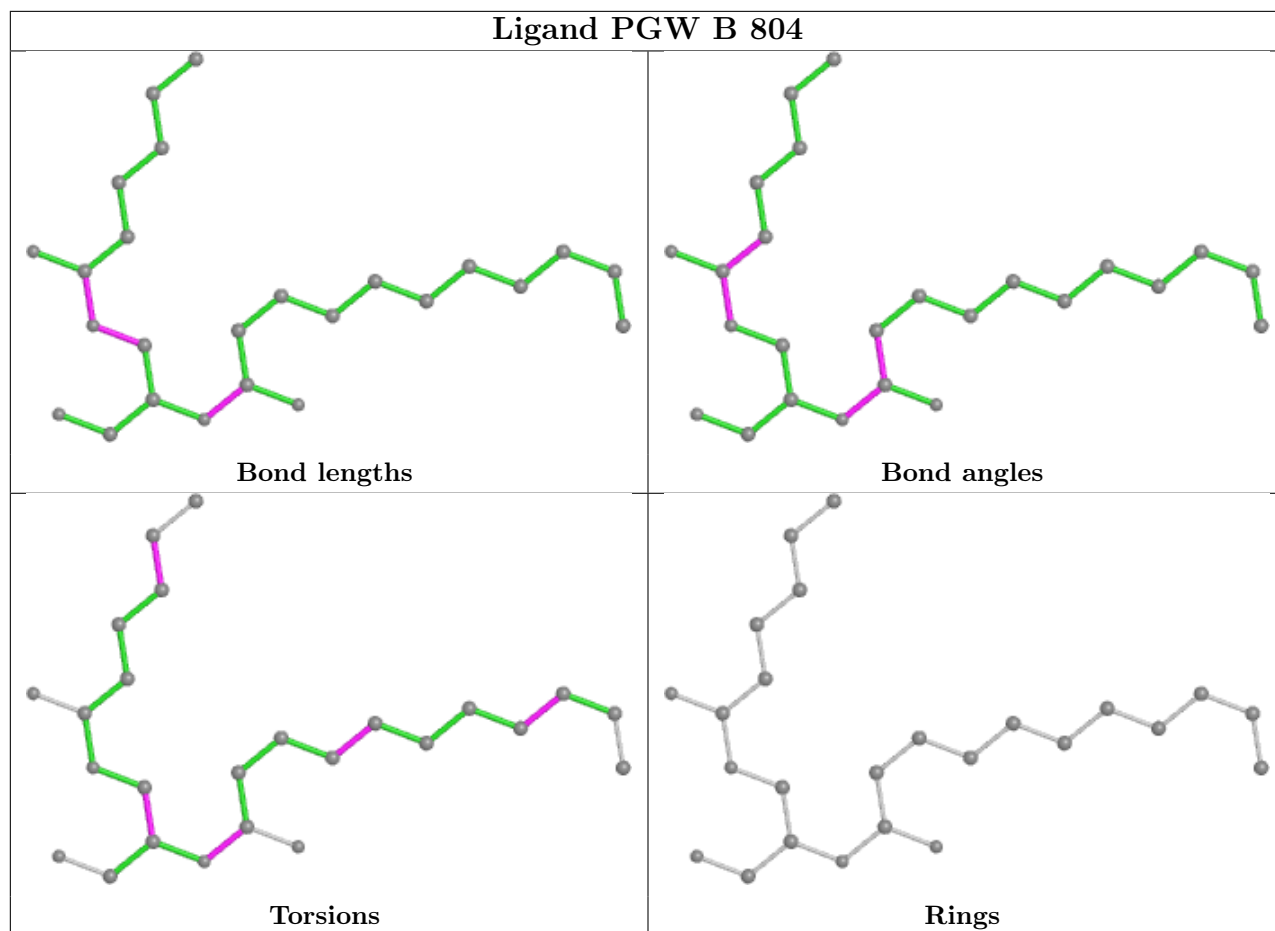


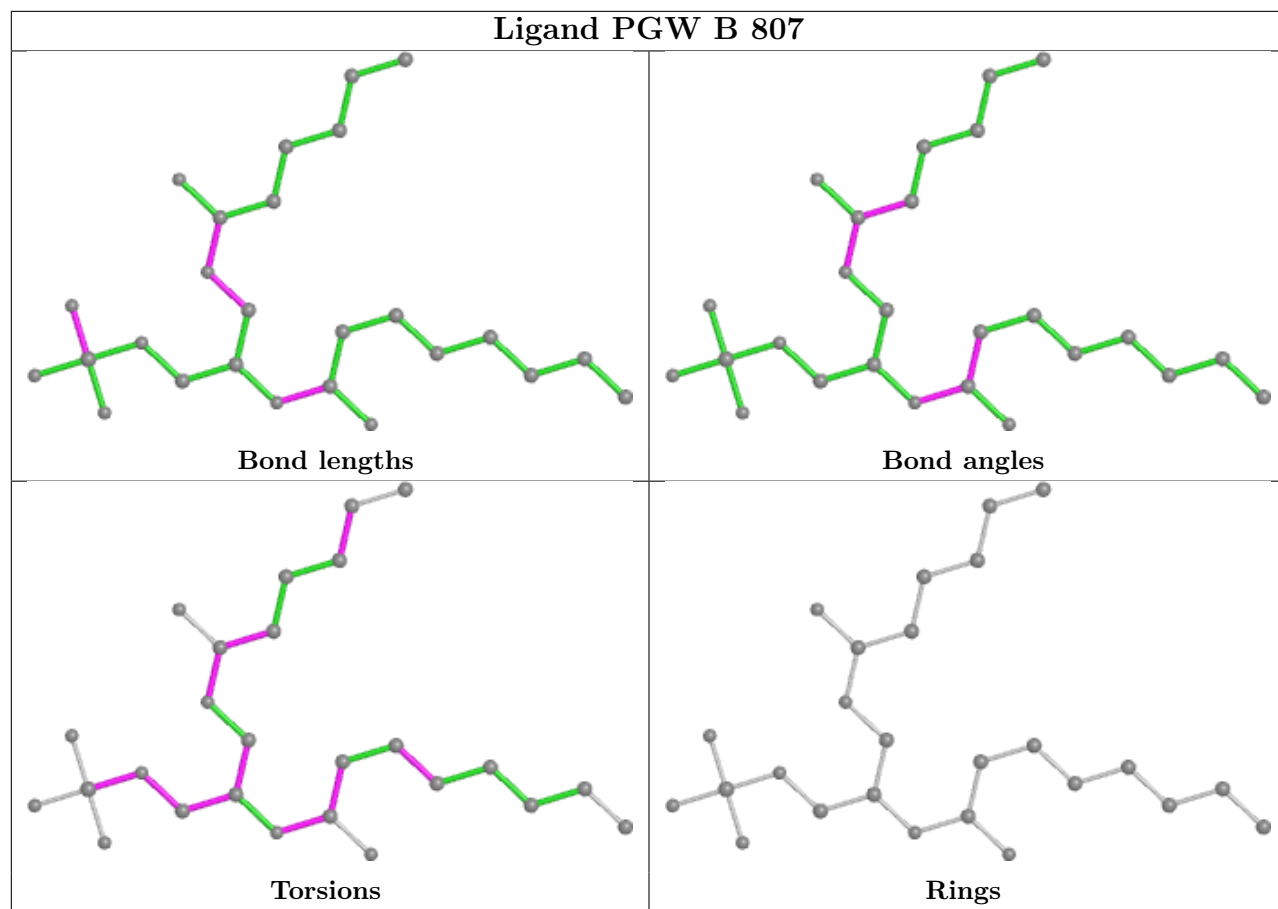


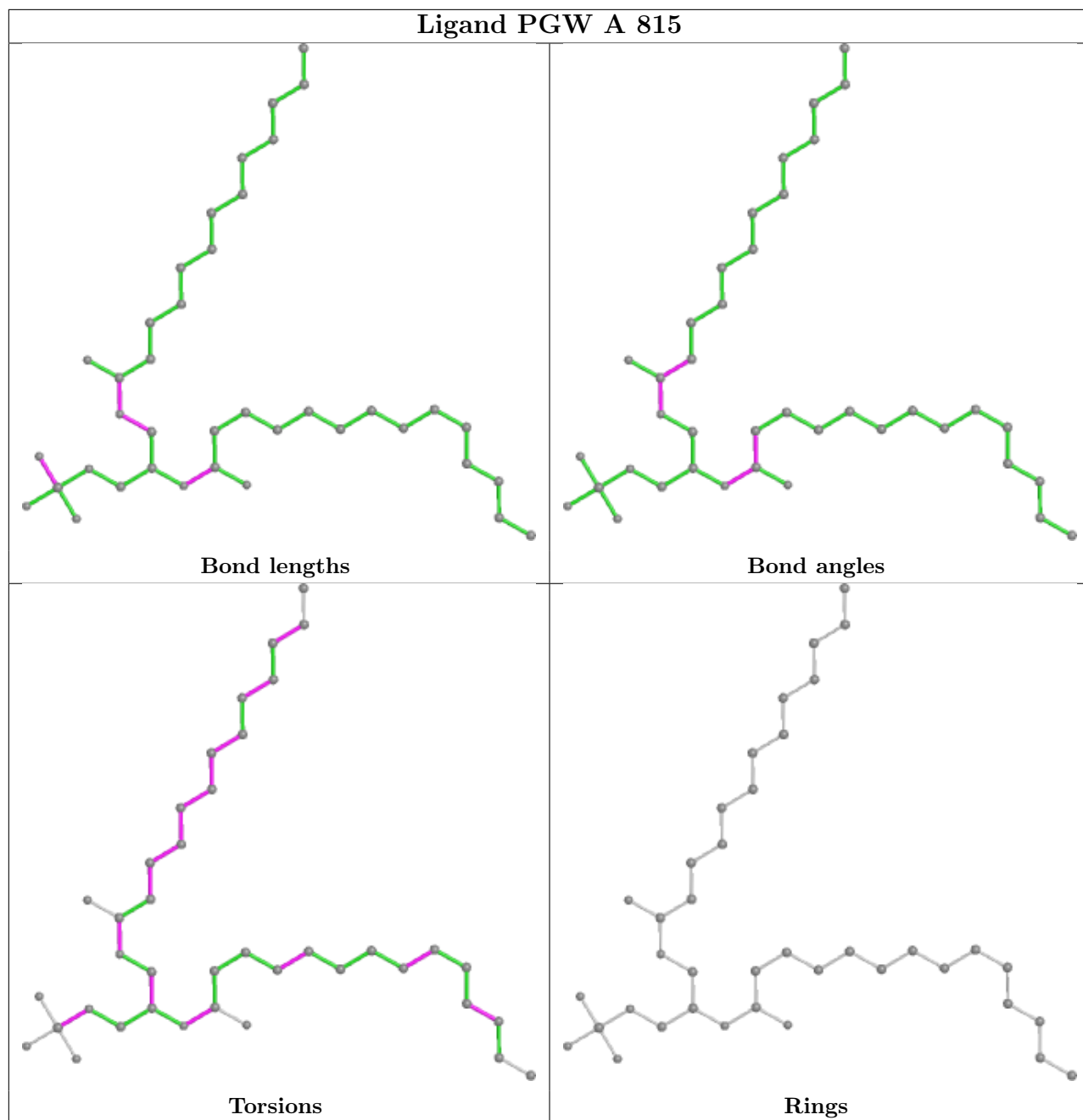


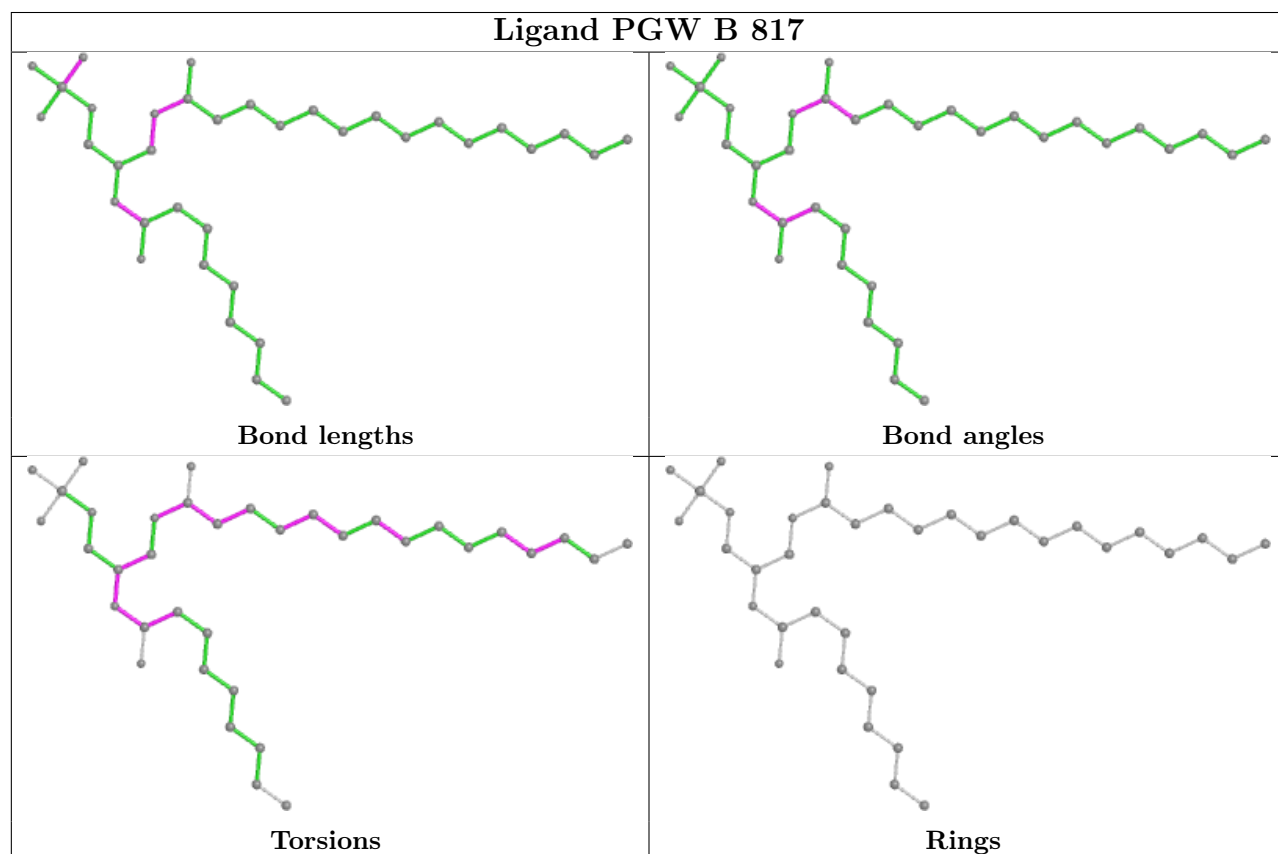
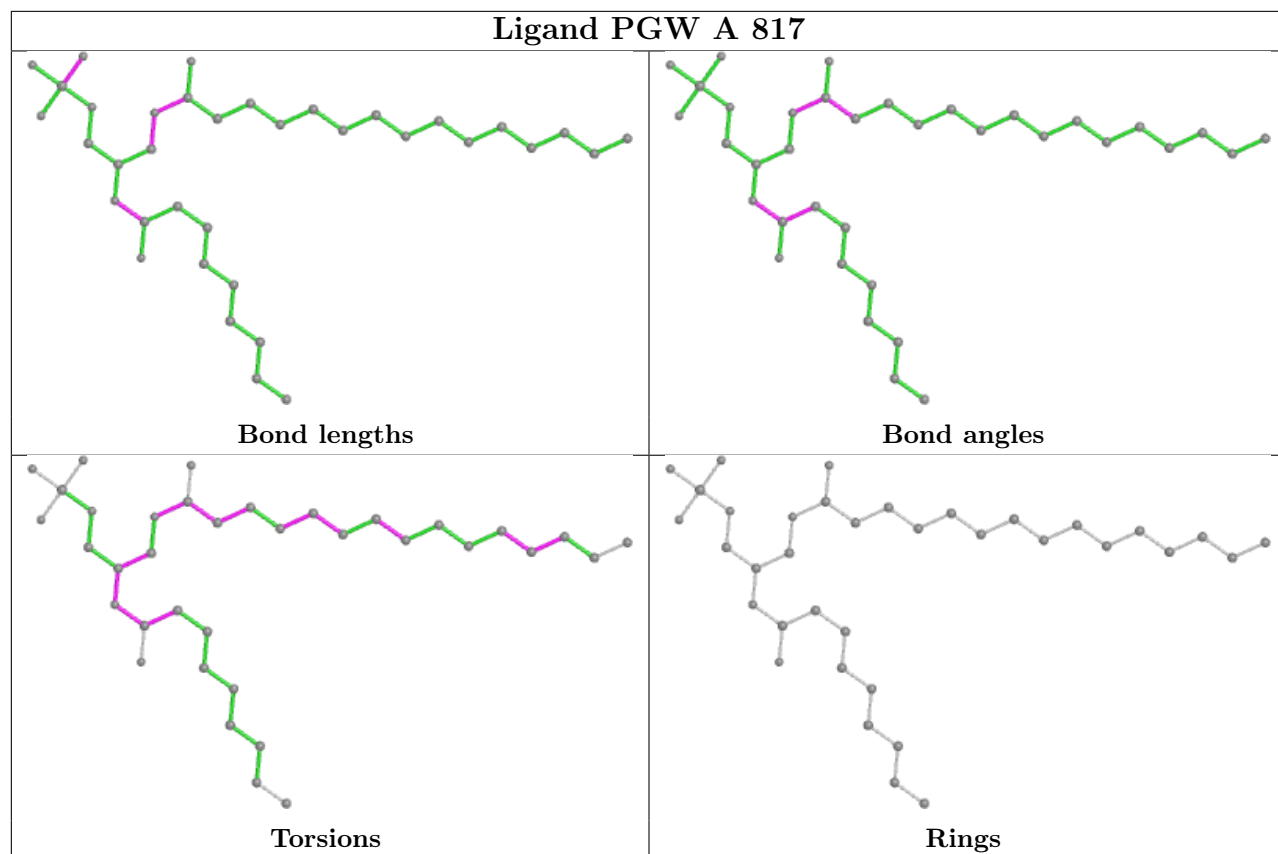




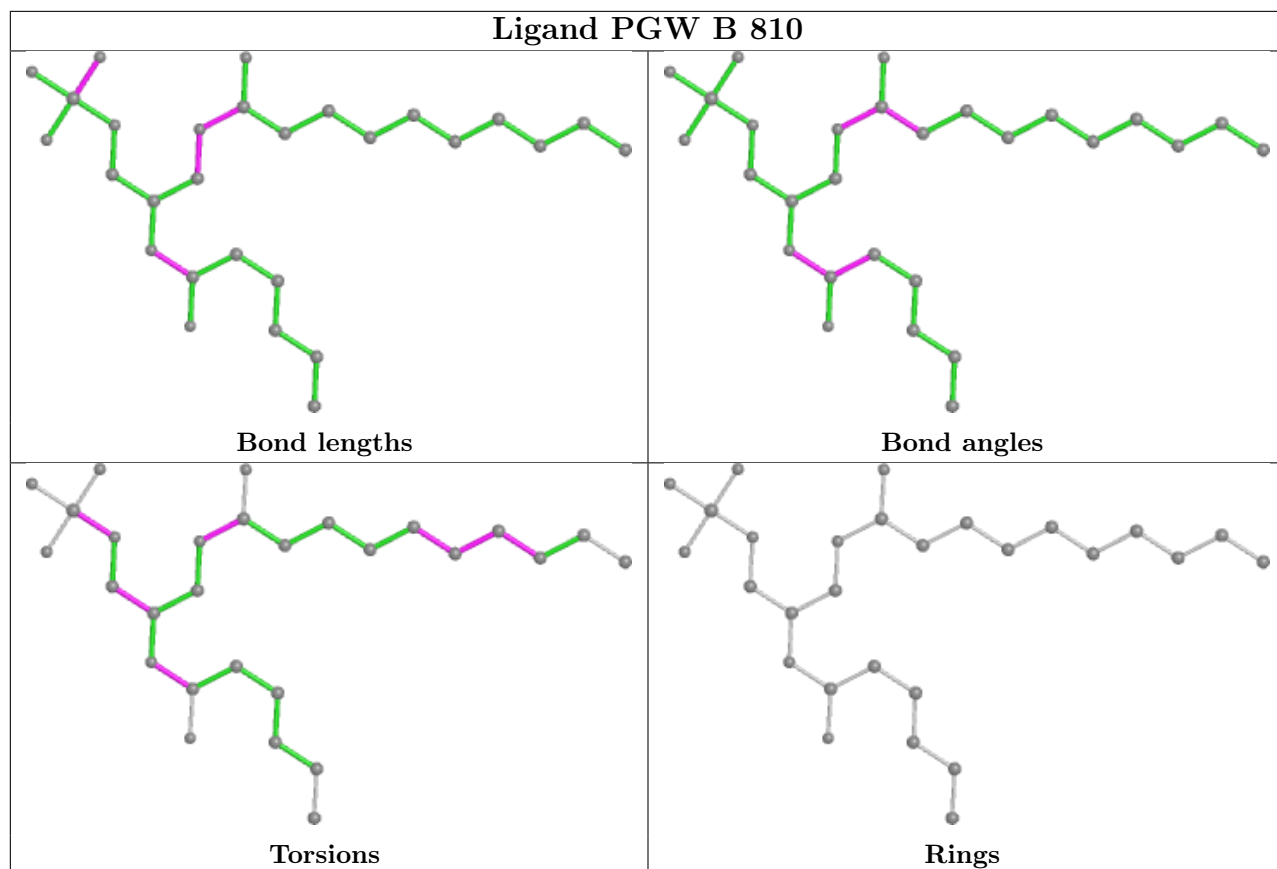


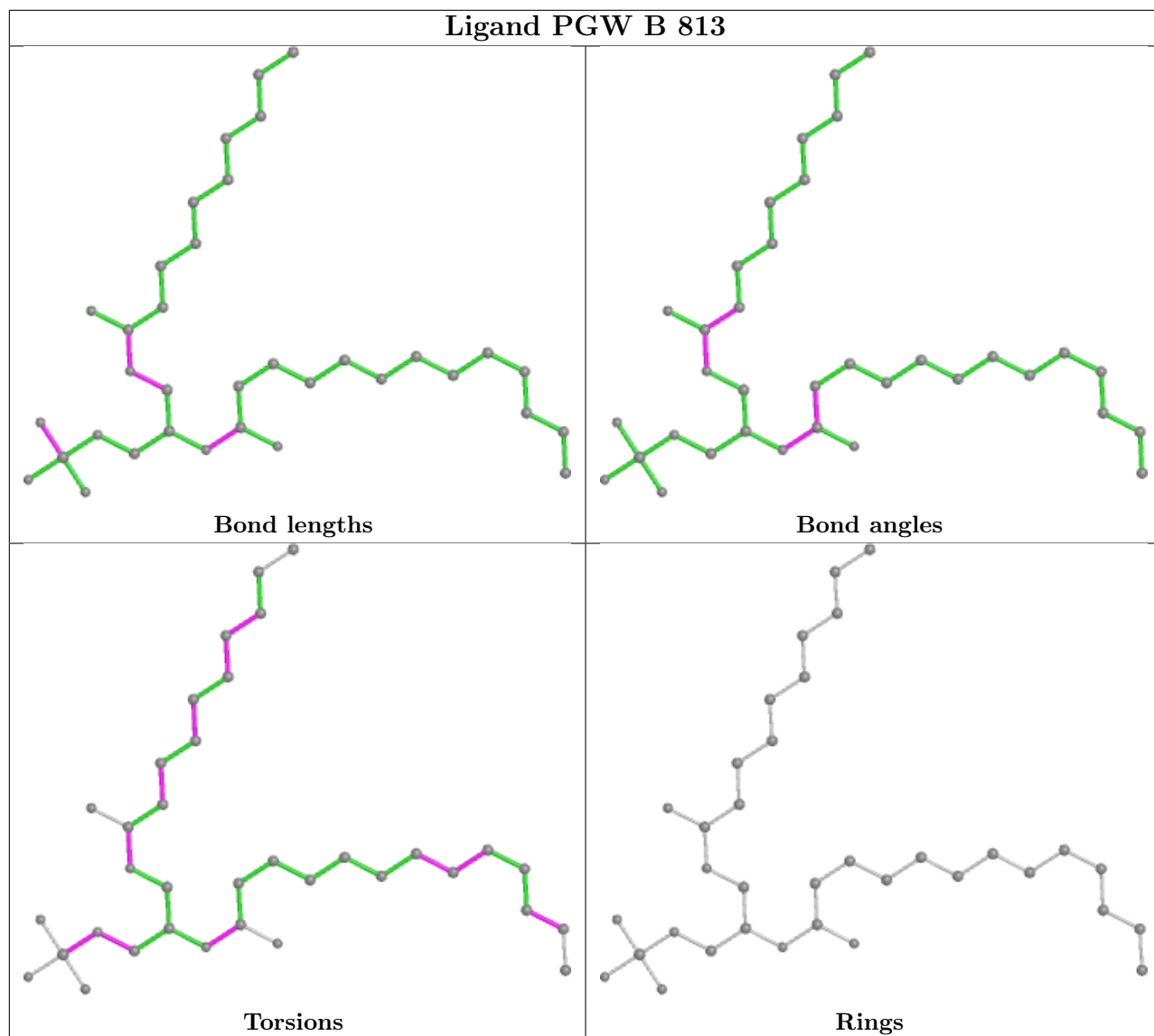


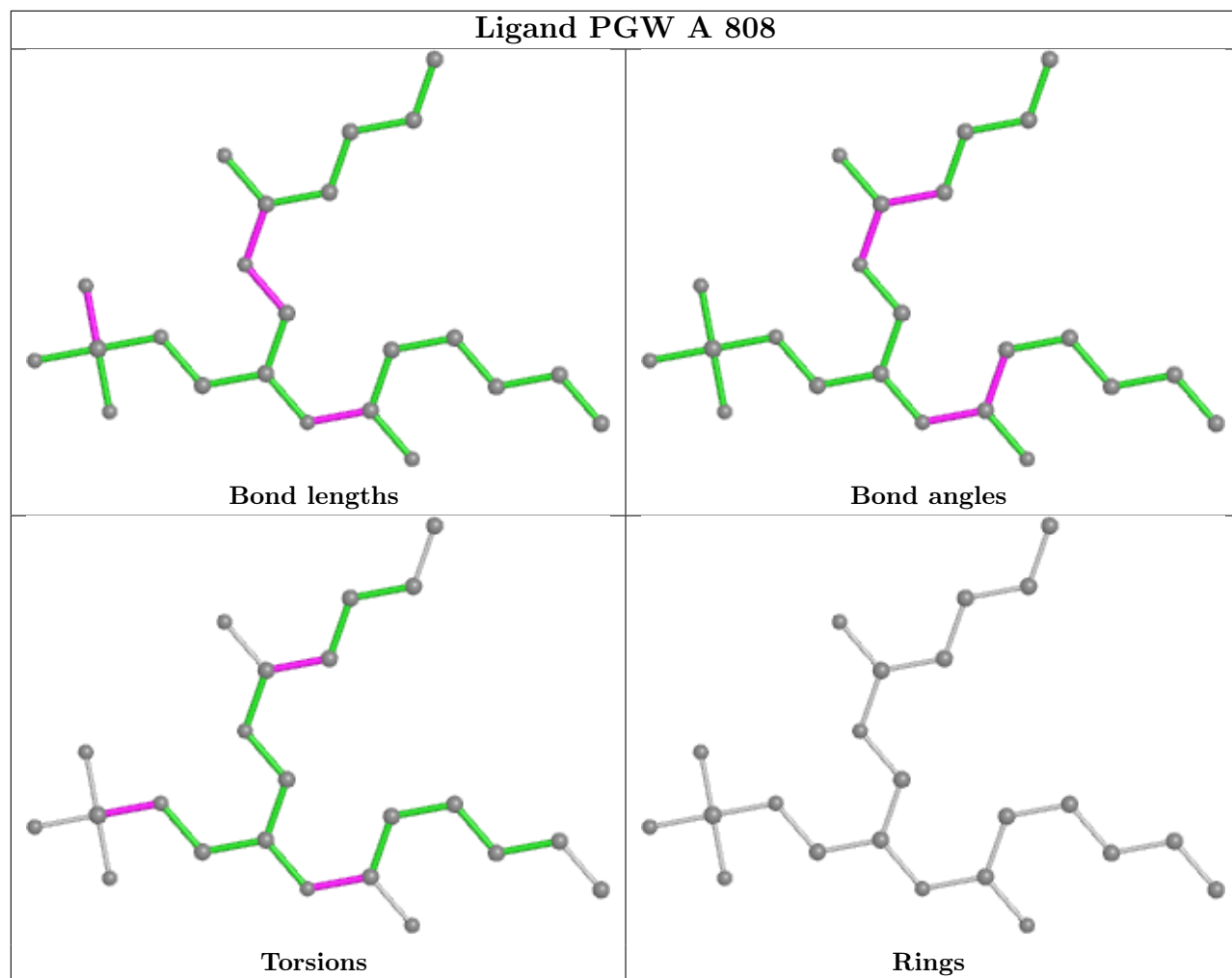


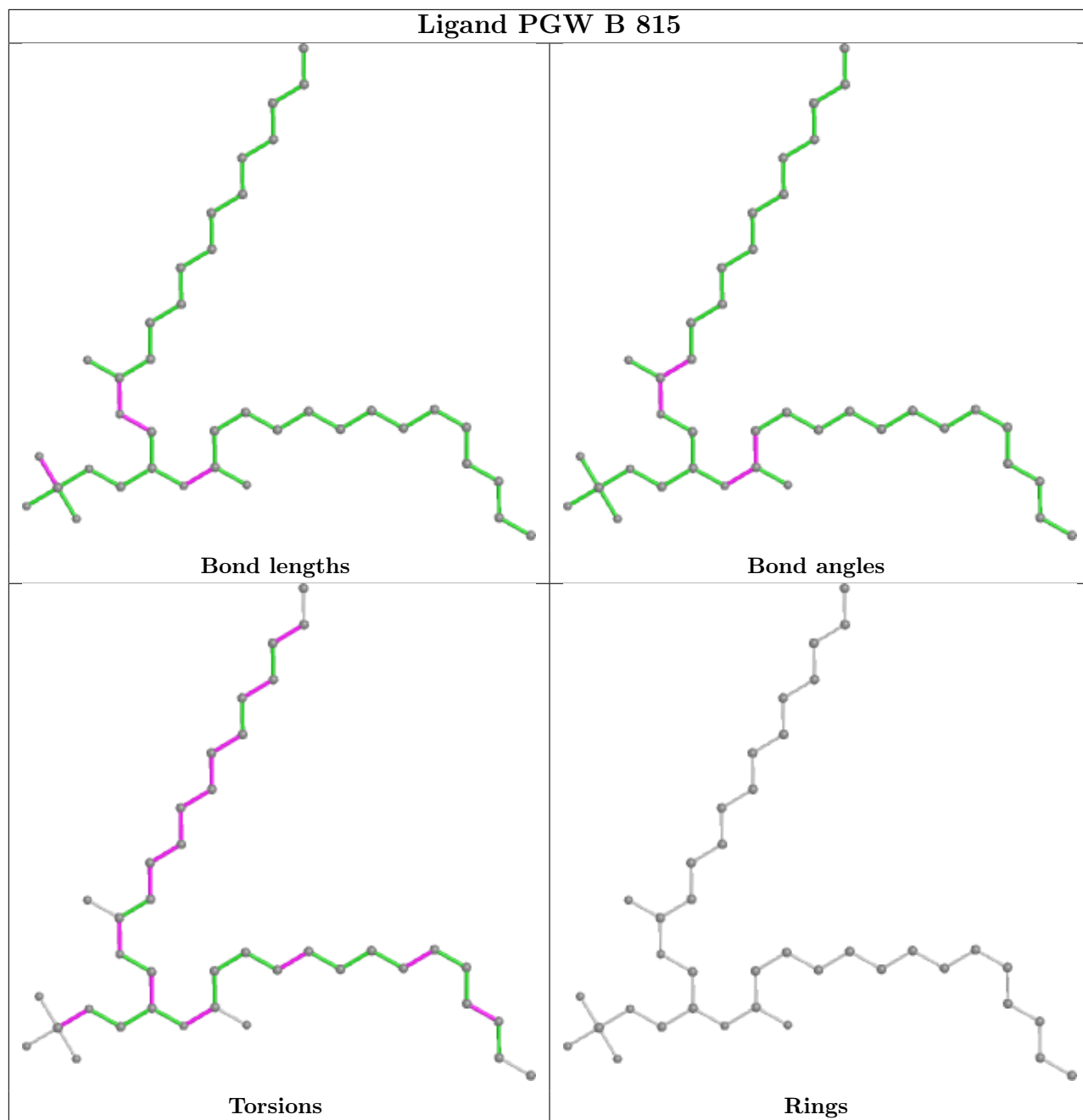


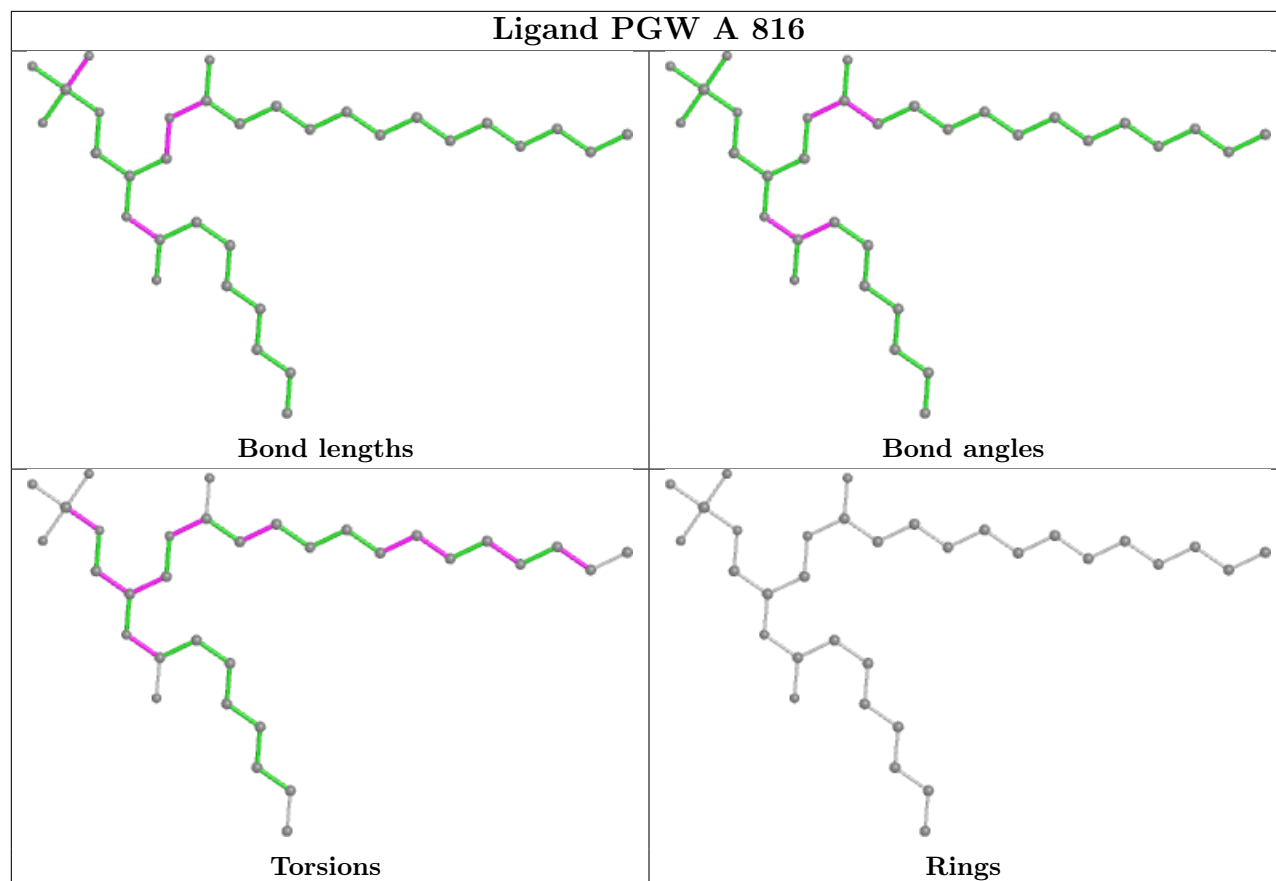


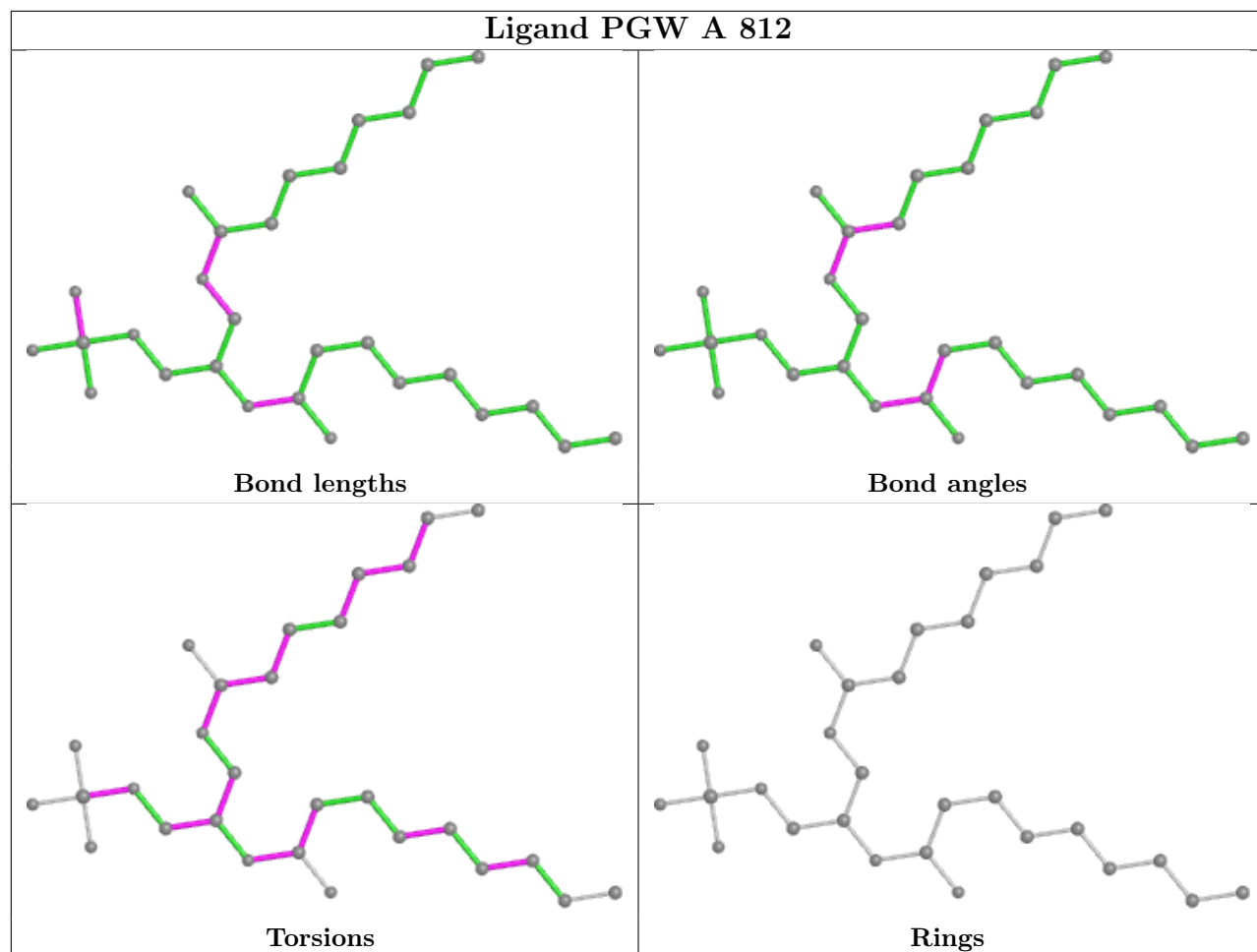


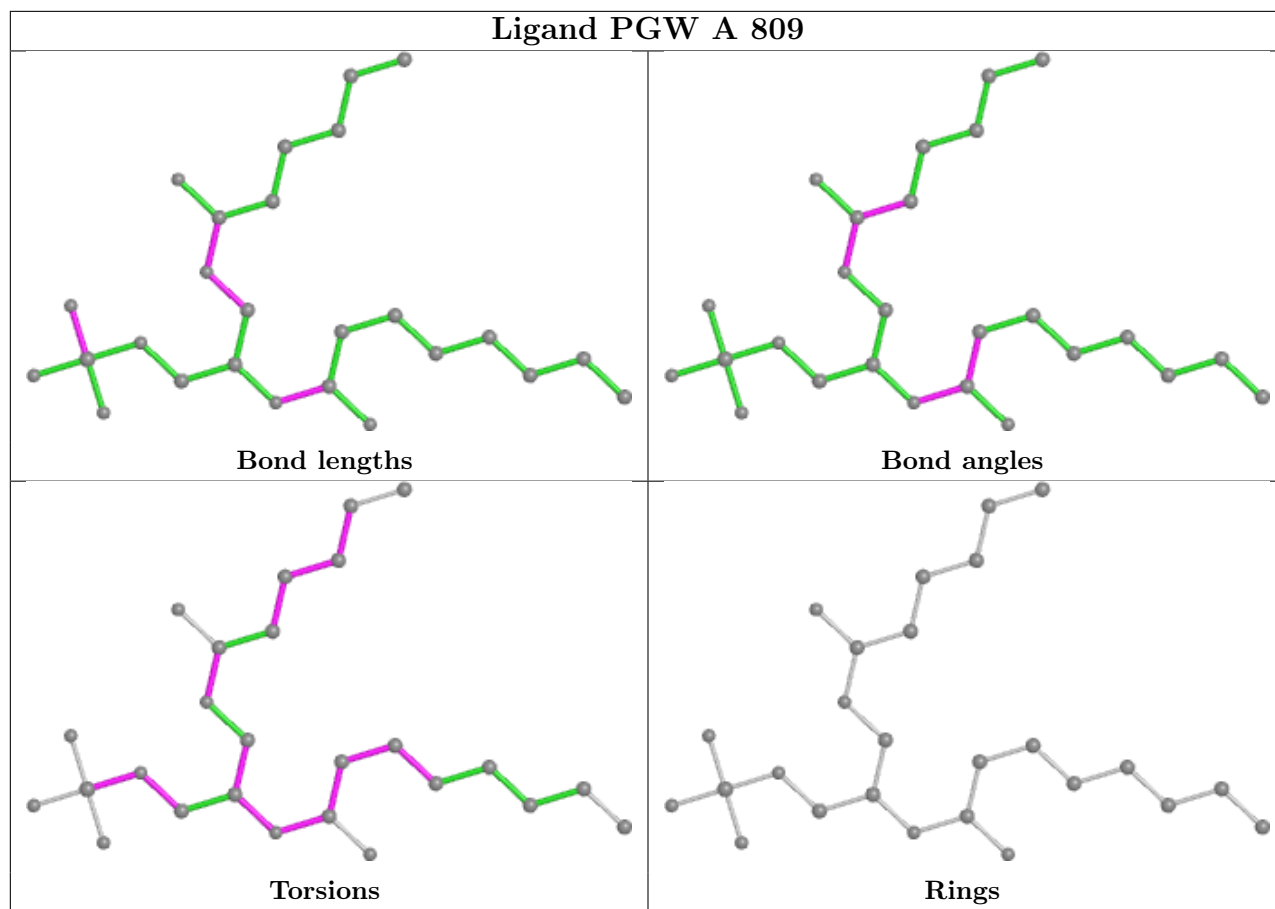


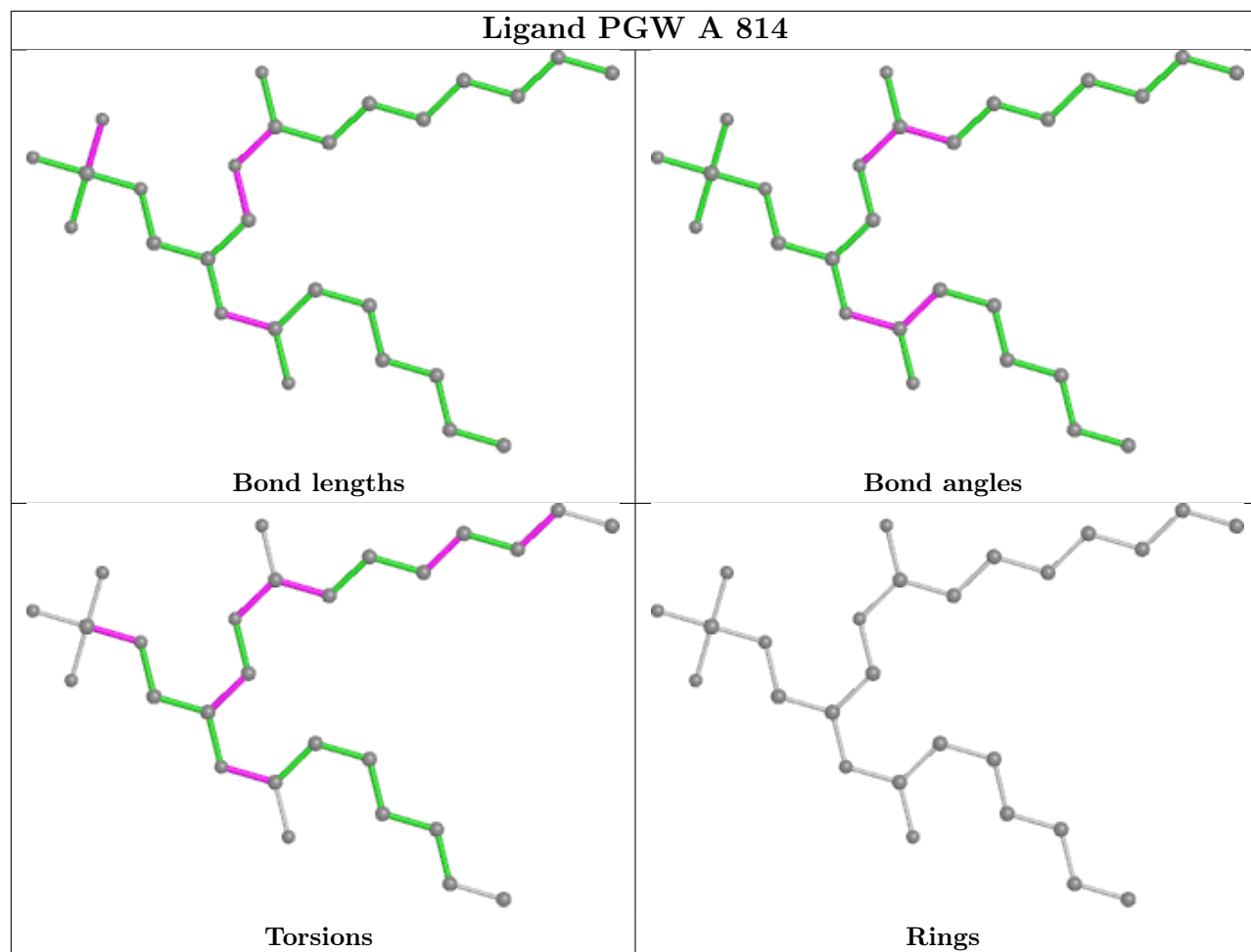




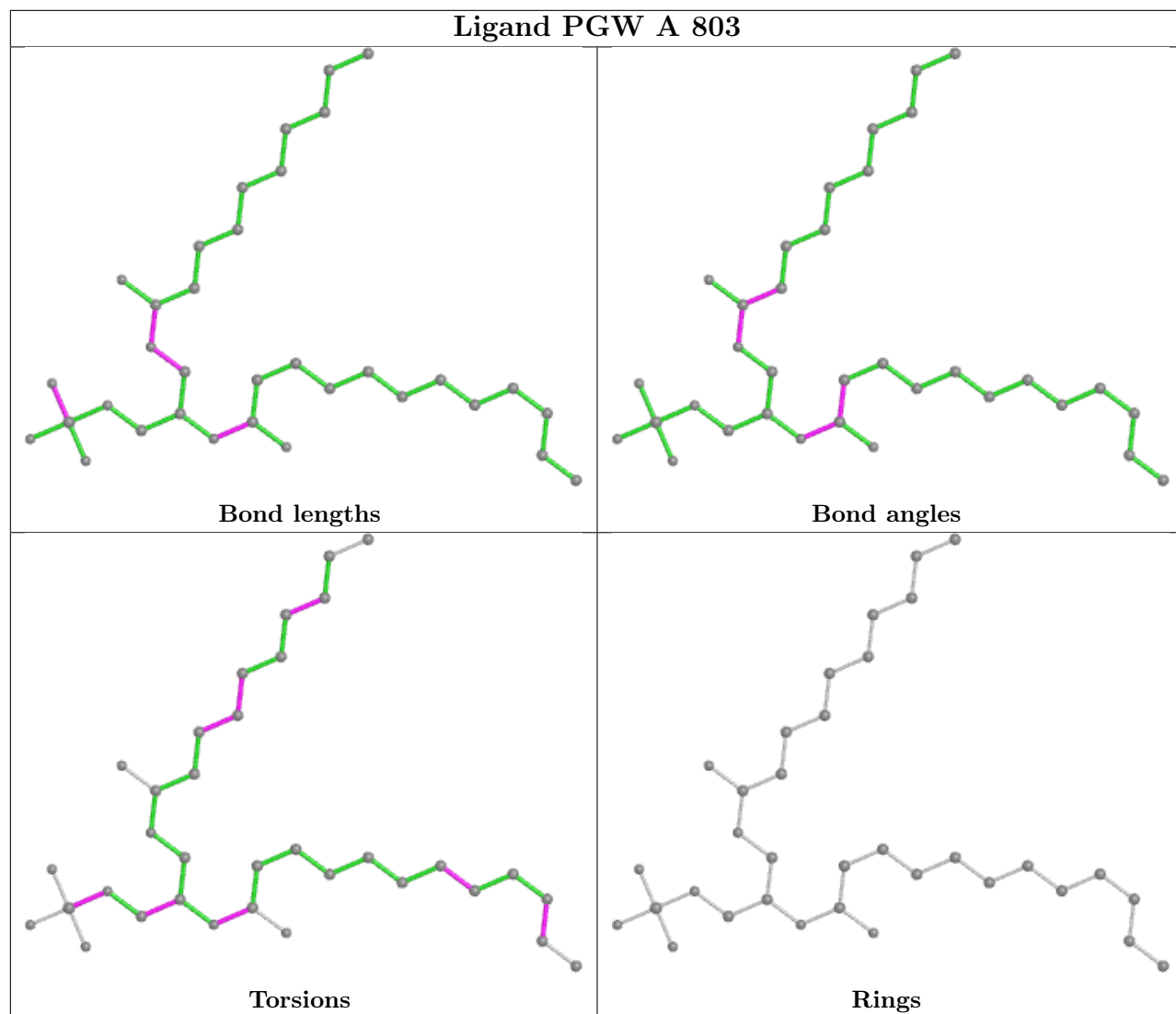


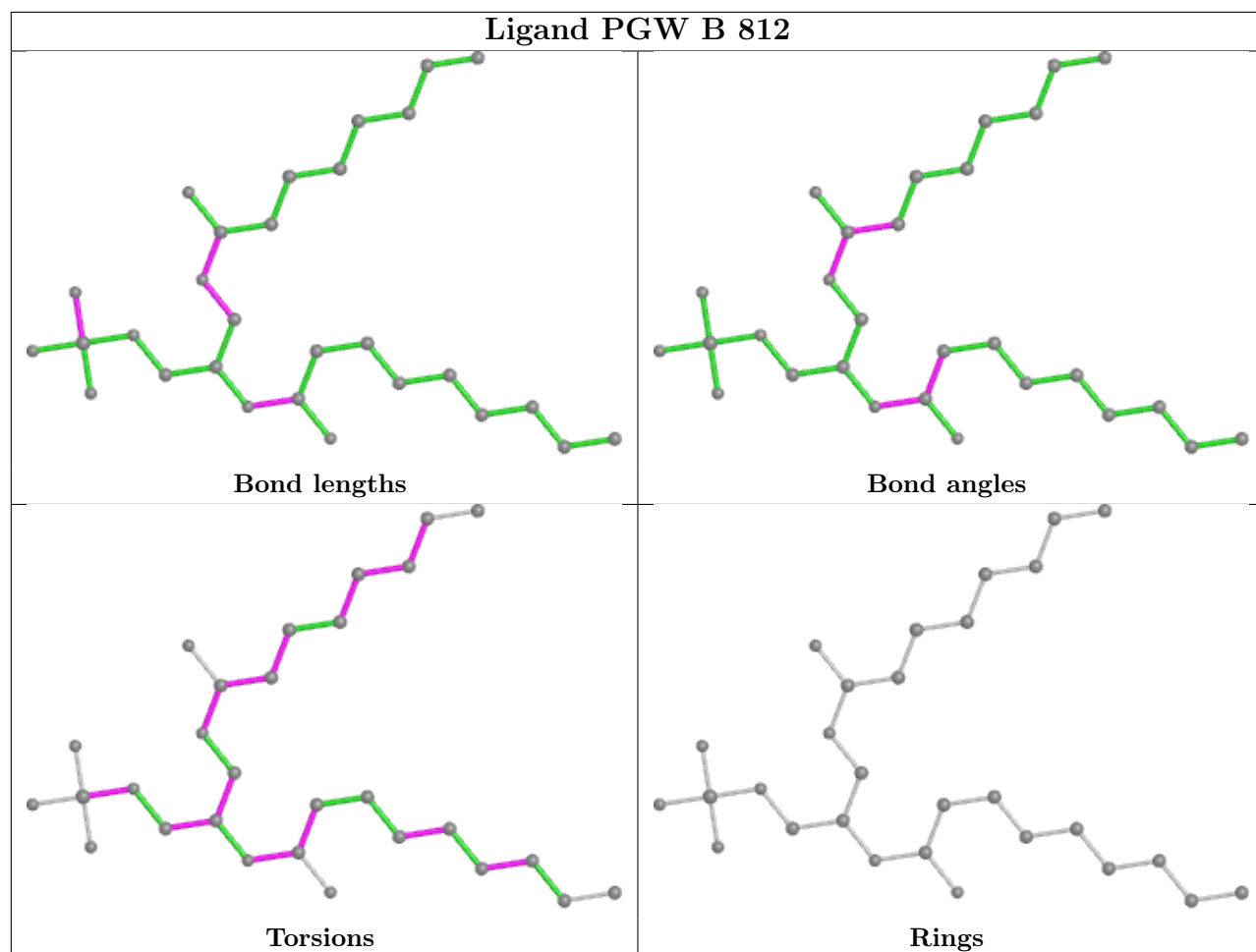
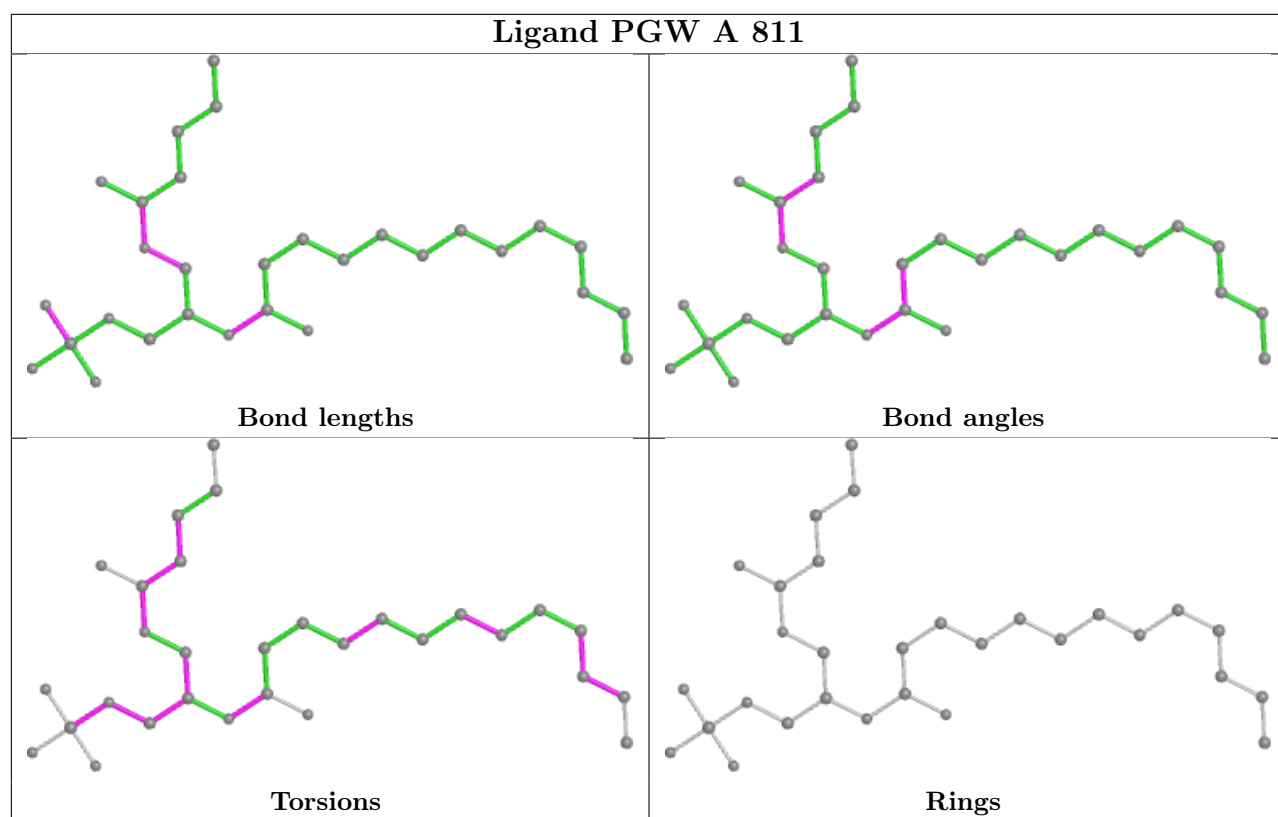


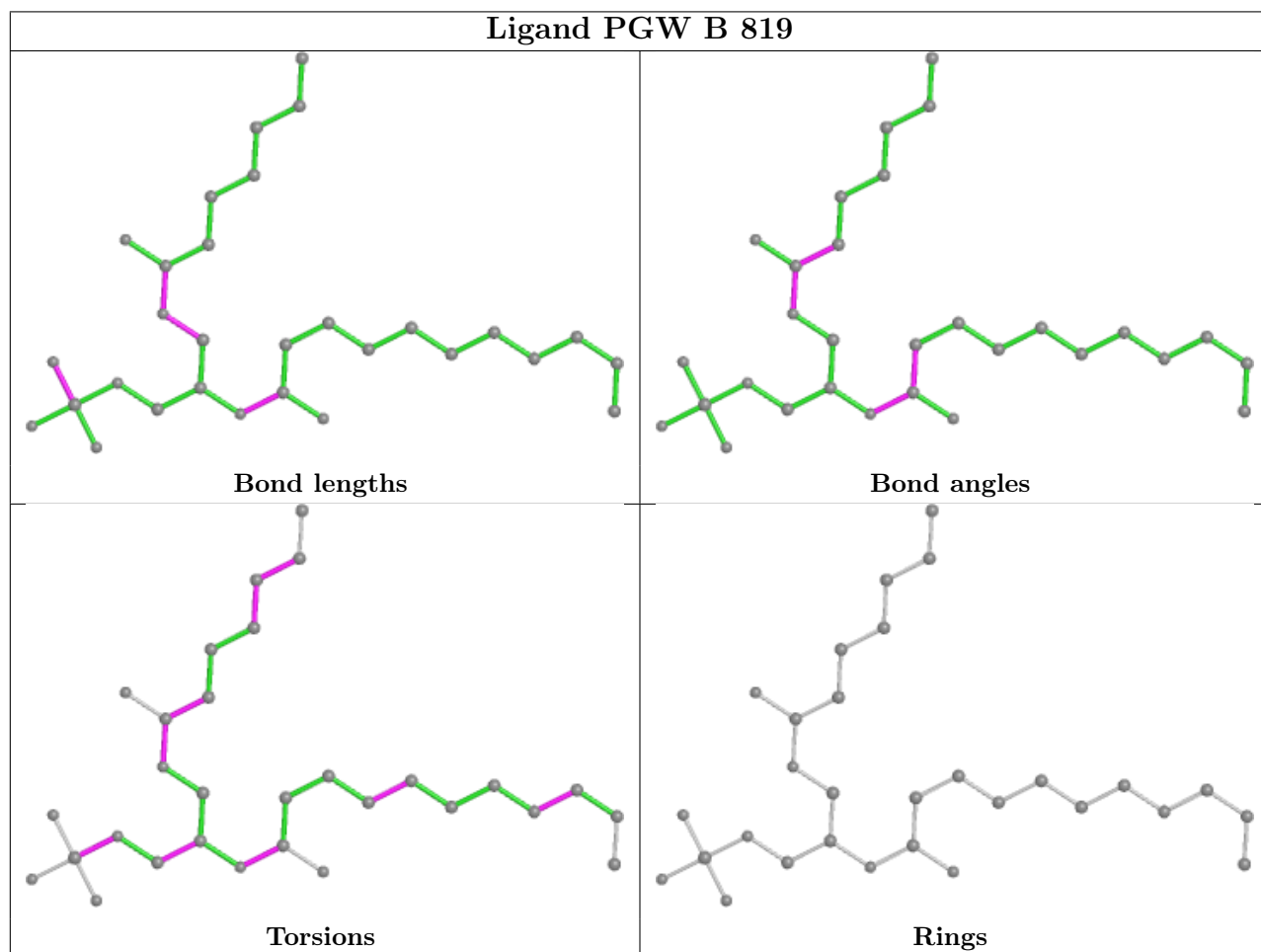
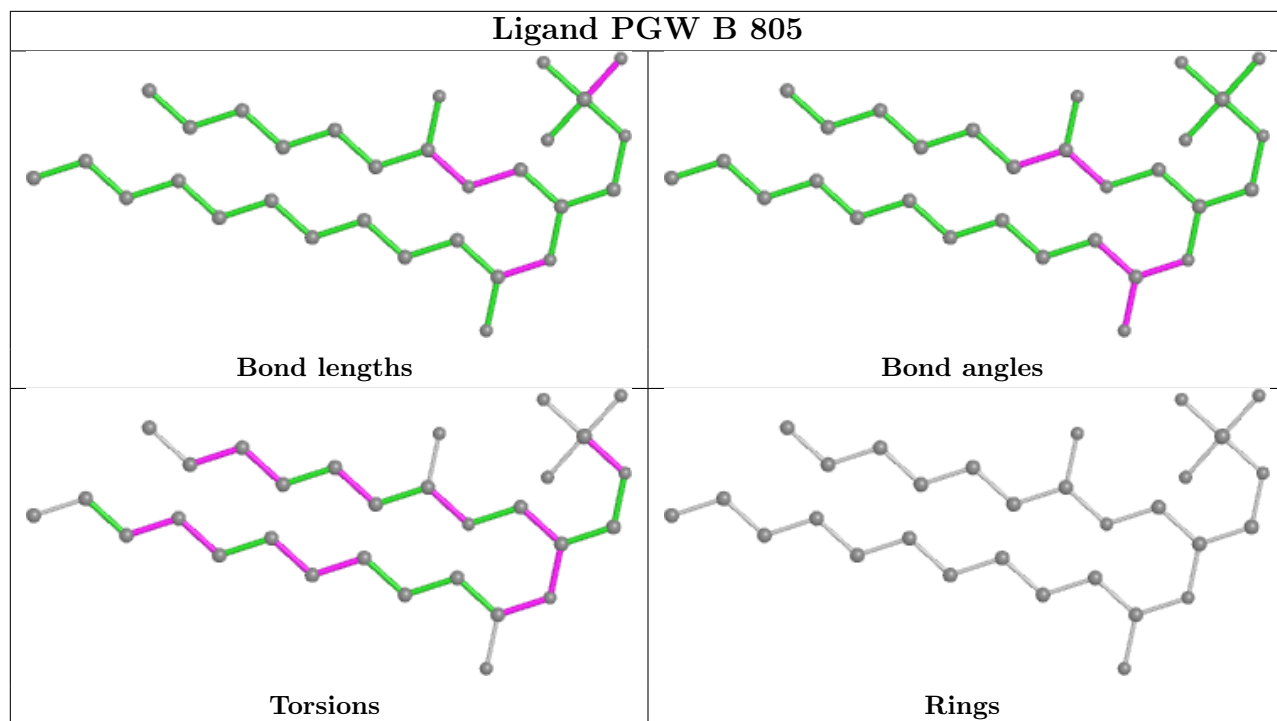


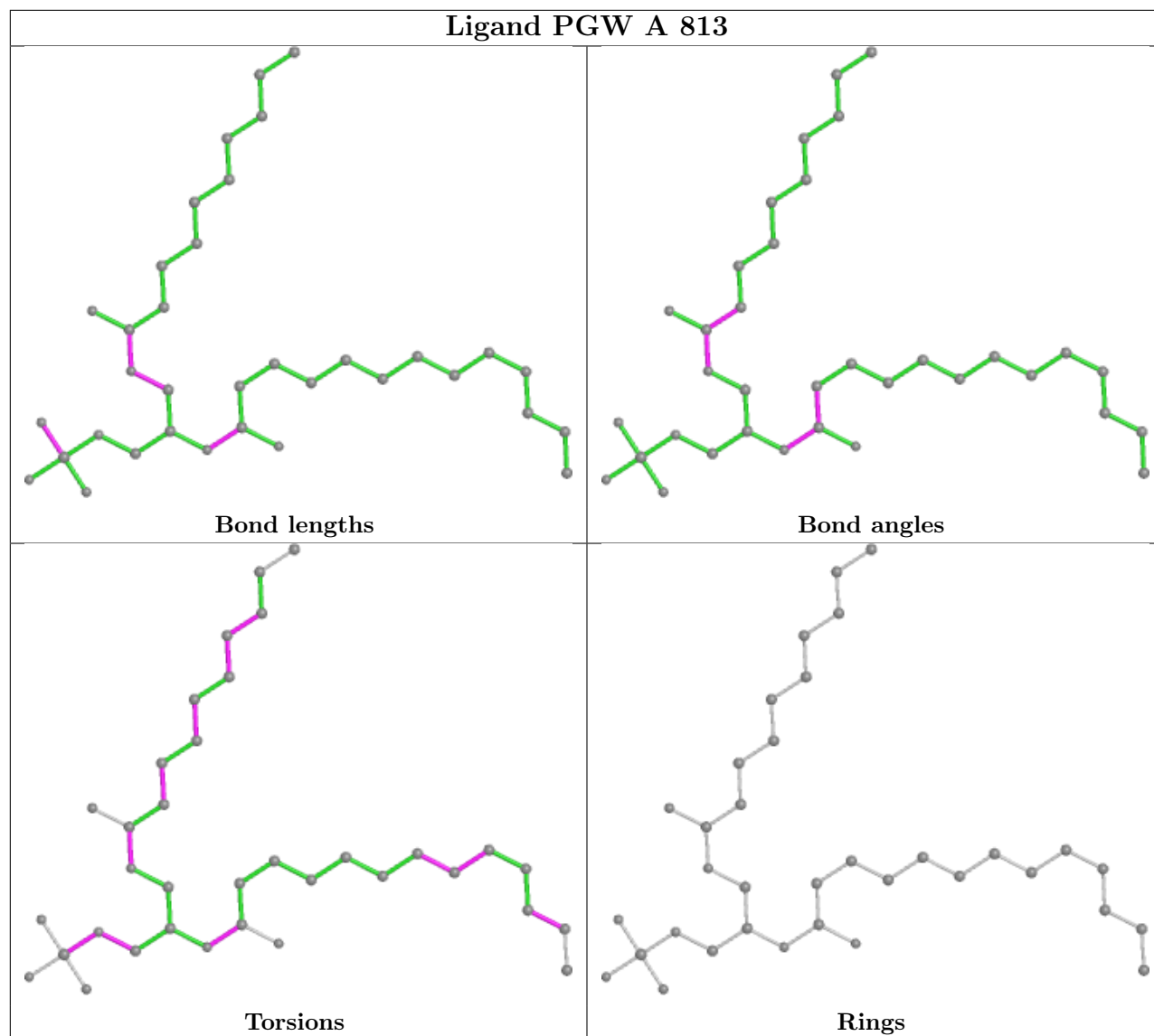


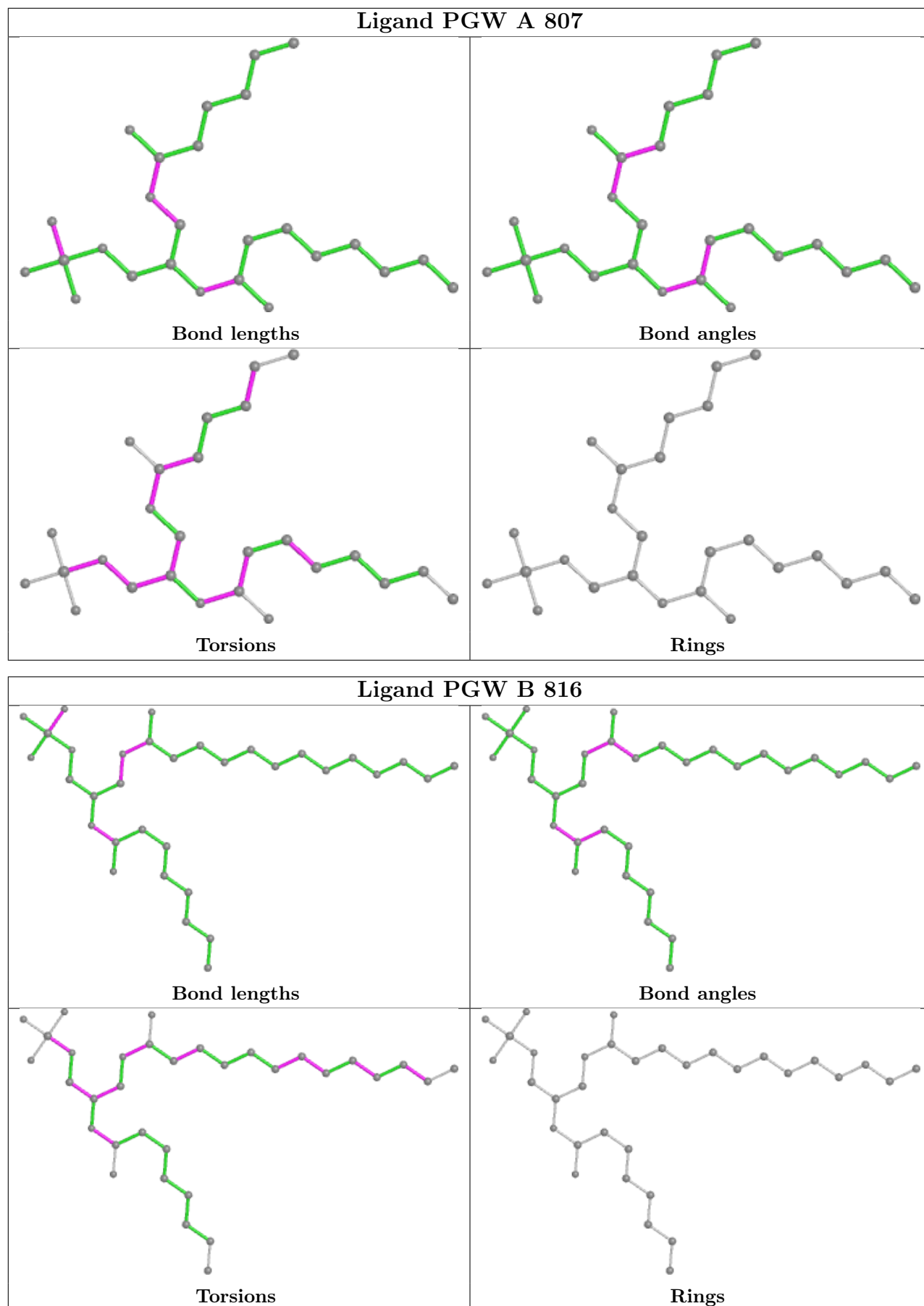


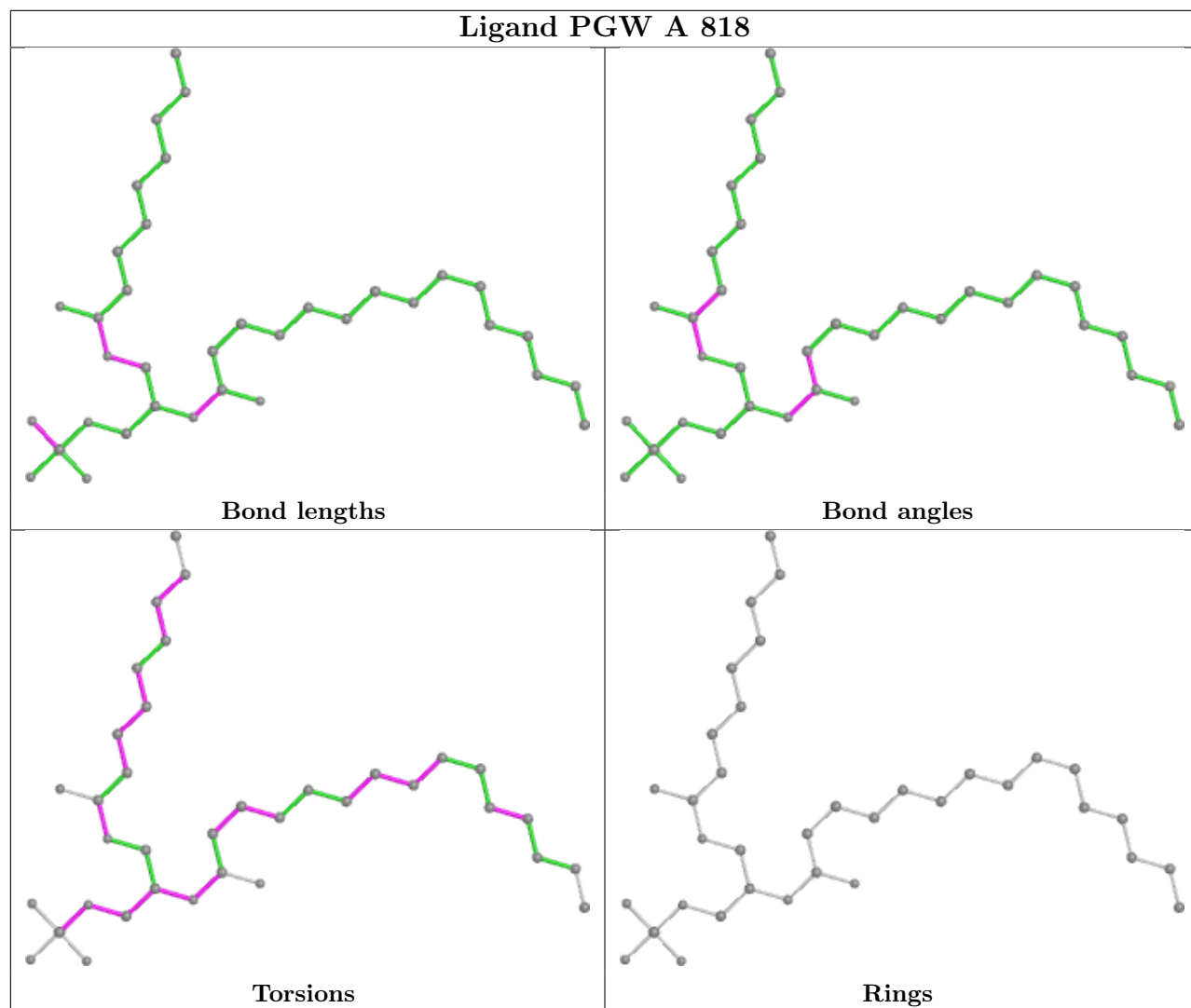


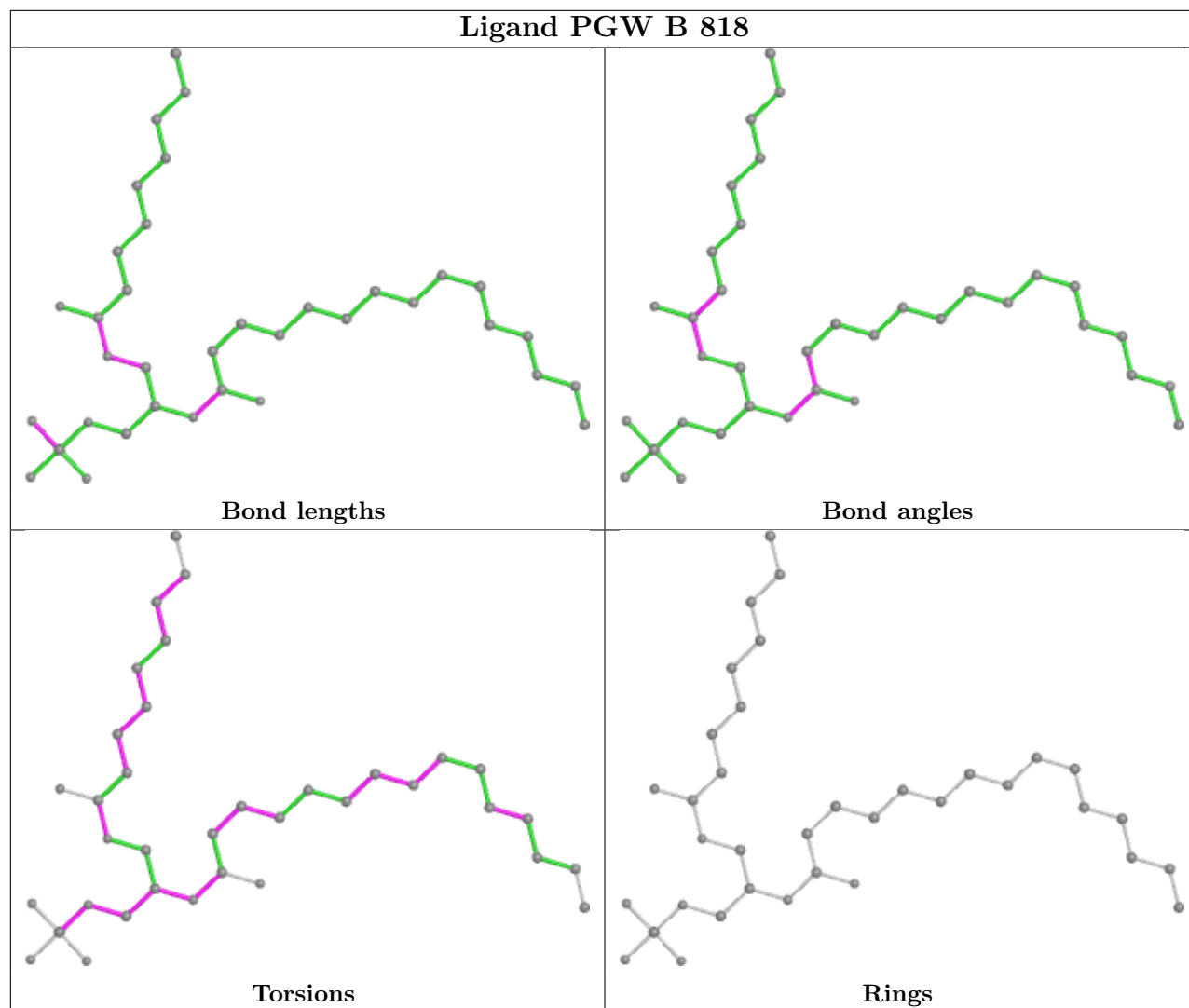












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

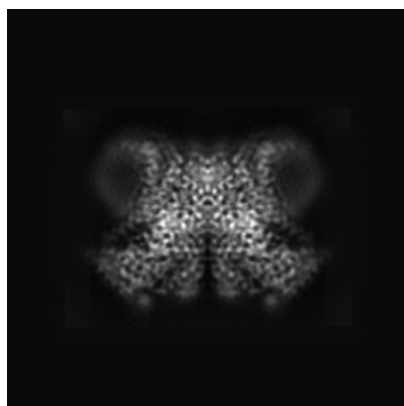
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41453. These allow visual inspection of the internal detail of the map and identification of artifacts.

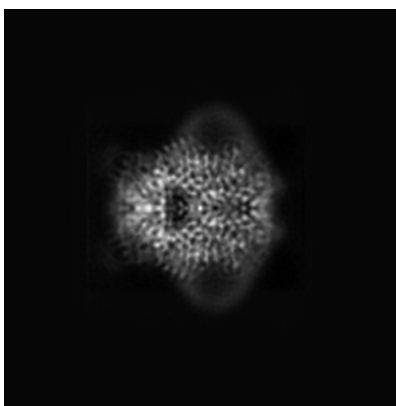
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

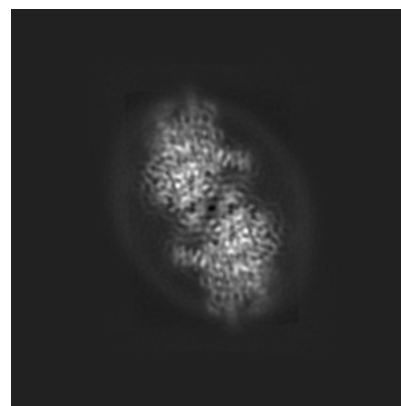
#### 6.1.1 Primary map



X

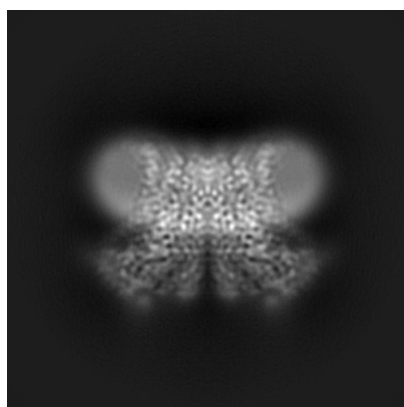


Y

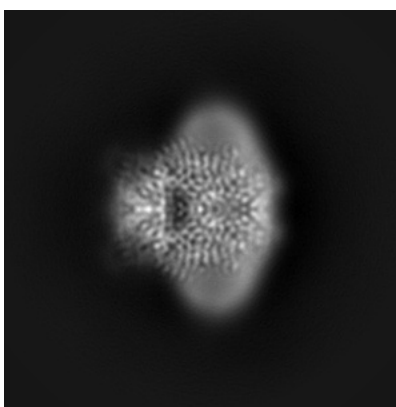


Z

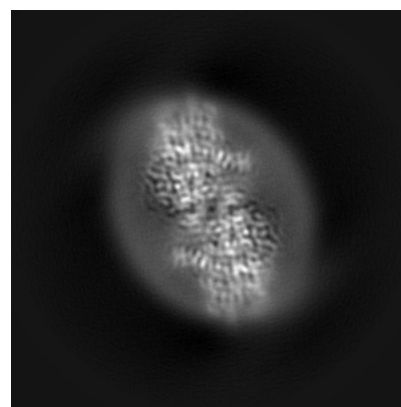
#### 6.1.2 Raw map



X



Y



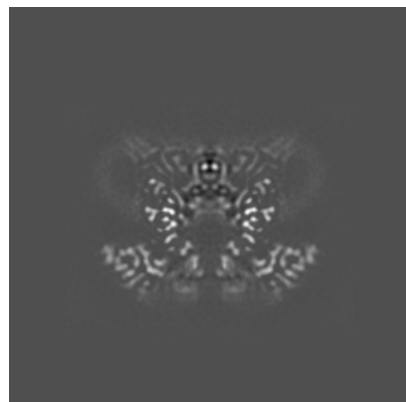
Z

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

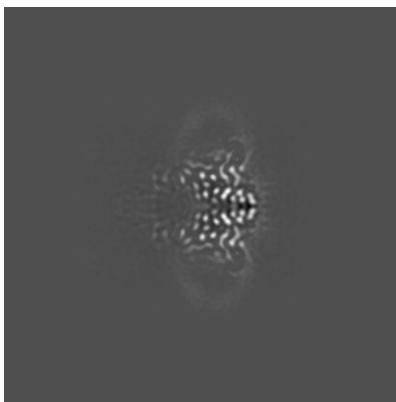


## 6.2 Central slices [i](#)

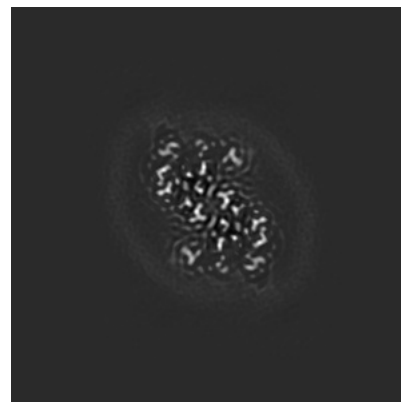
### 6.2.1 Primary map



X Index: 128

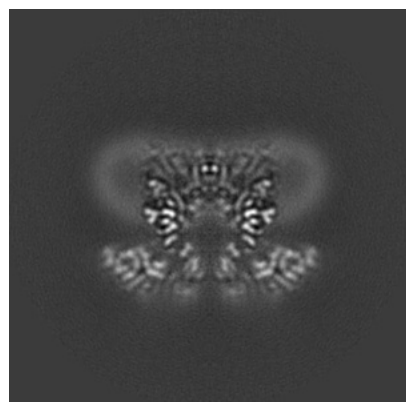


Y Index: 128

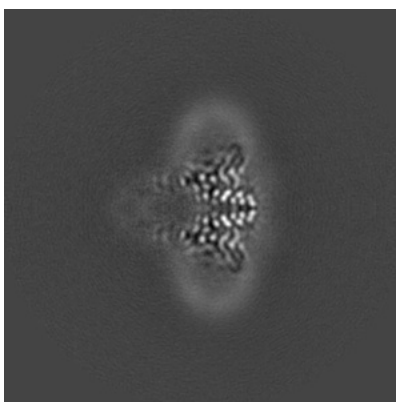


Z Index: 128

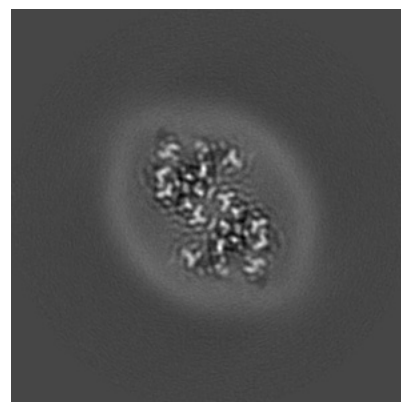
### 6.2.2 Raw map



X Index: 128



Y Index: 128

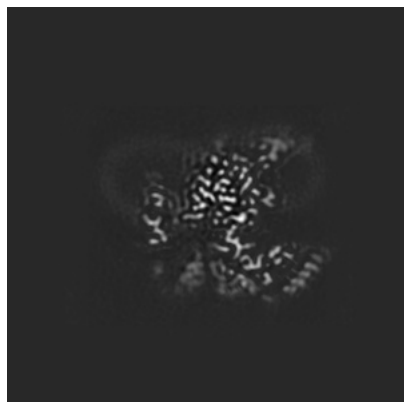


Z Index: 128

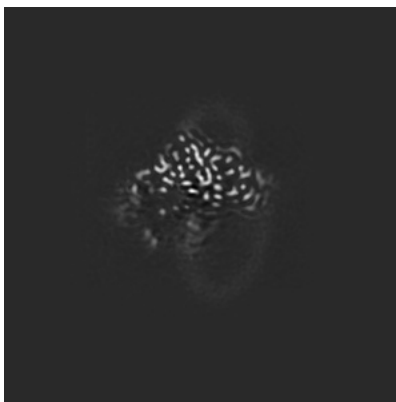
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

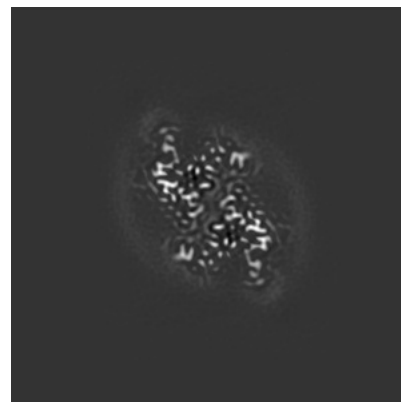
### 6.3.1 Primary map



X Index: 118

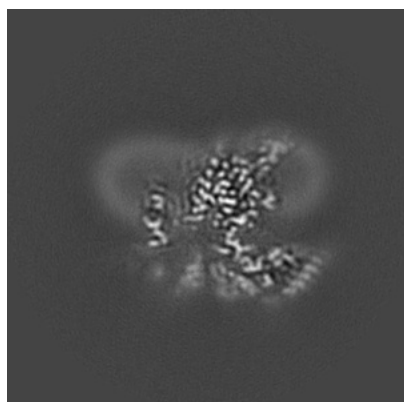


Y Index: 107

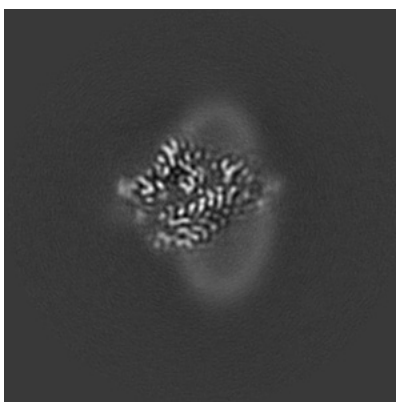


Z Index: 123

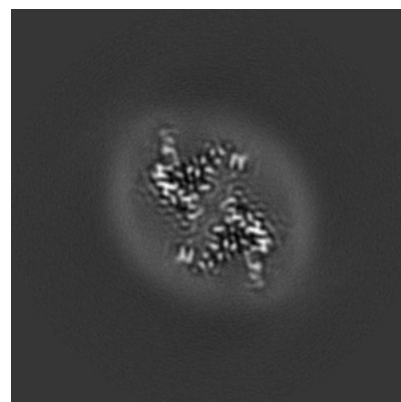
### 6.3.2 Raw map



X Index: 118



Y Index: 100

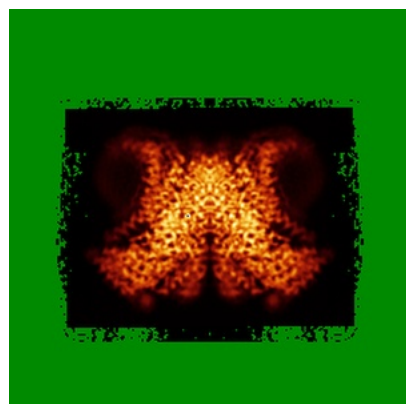


Z Index: 123

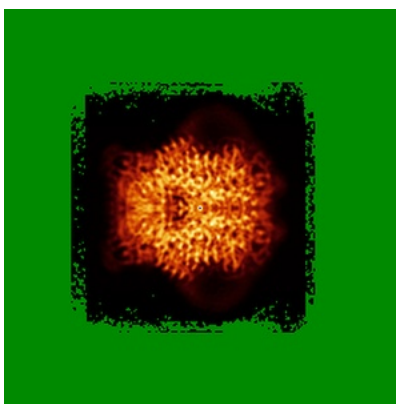
The images above show the largest variance slices of the map in three orthogonal directions.

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

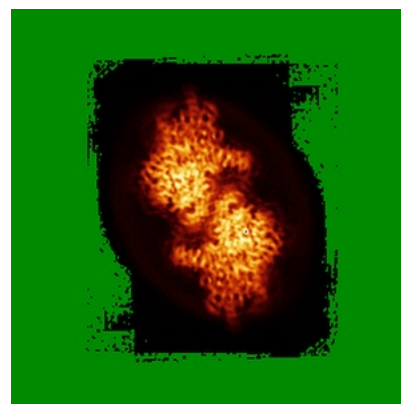
### 6.4.1 Primary map



X

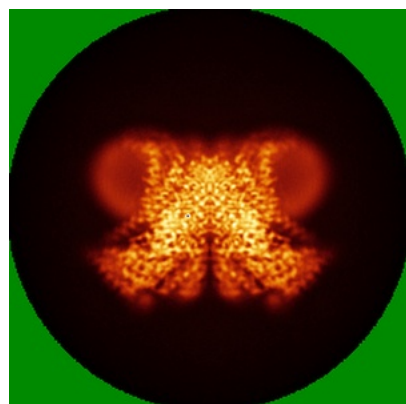


Y

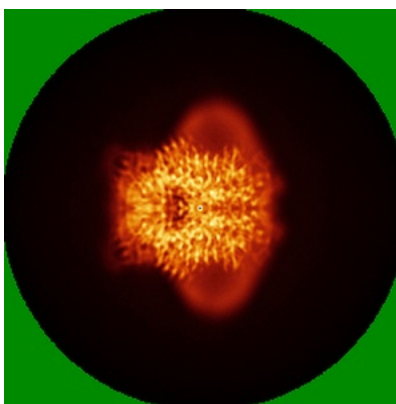


Z

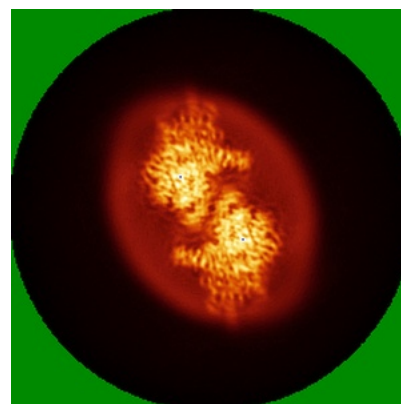
### 6.4.2 Raw map



X



Y

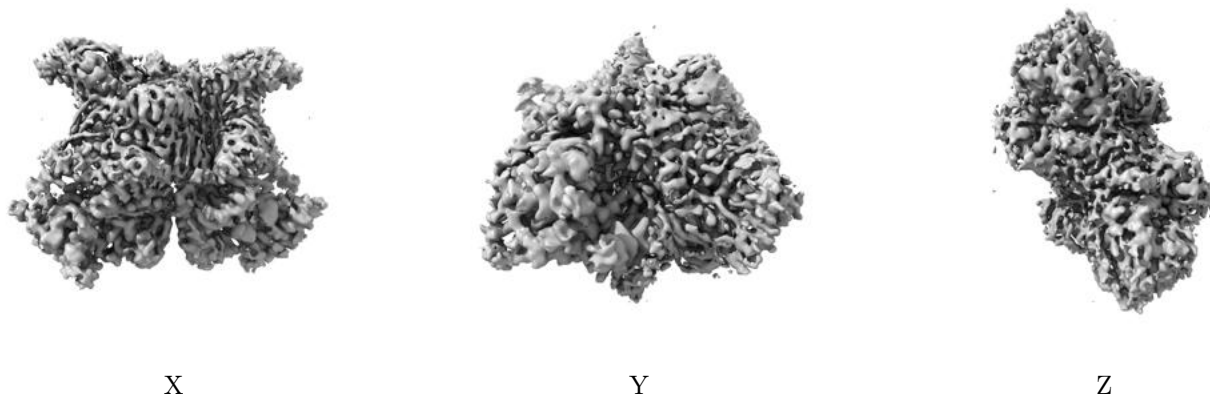


Z

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

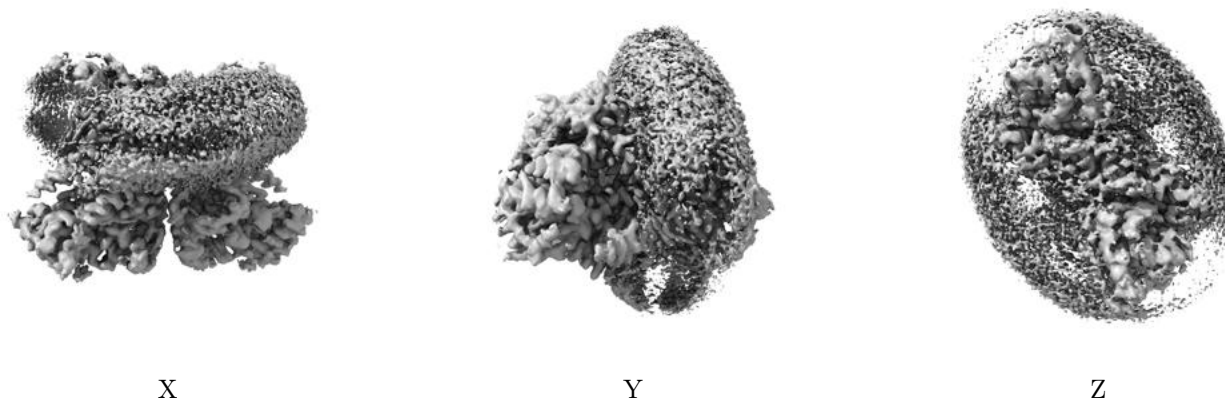
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 1.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

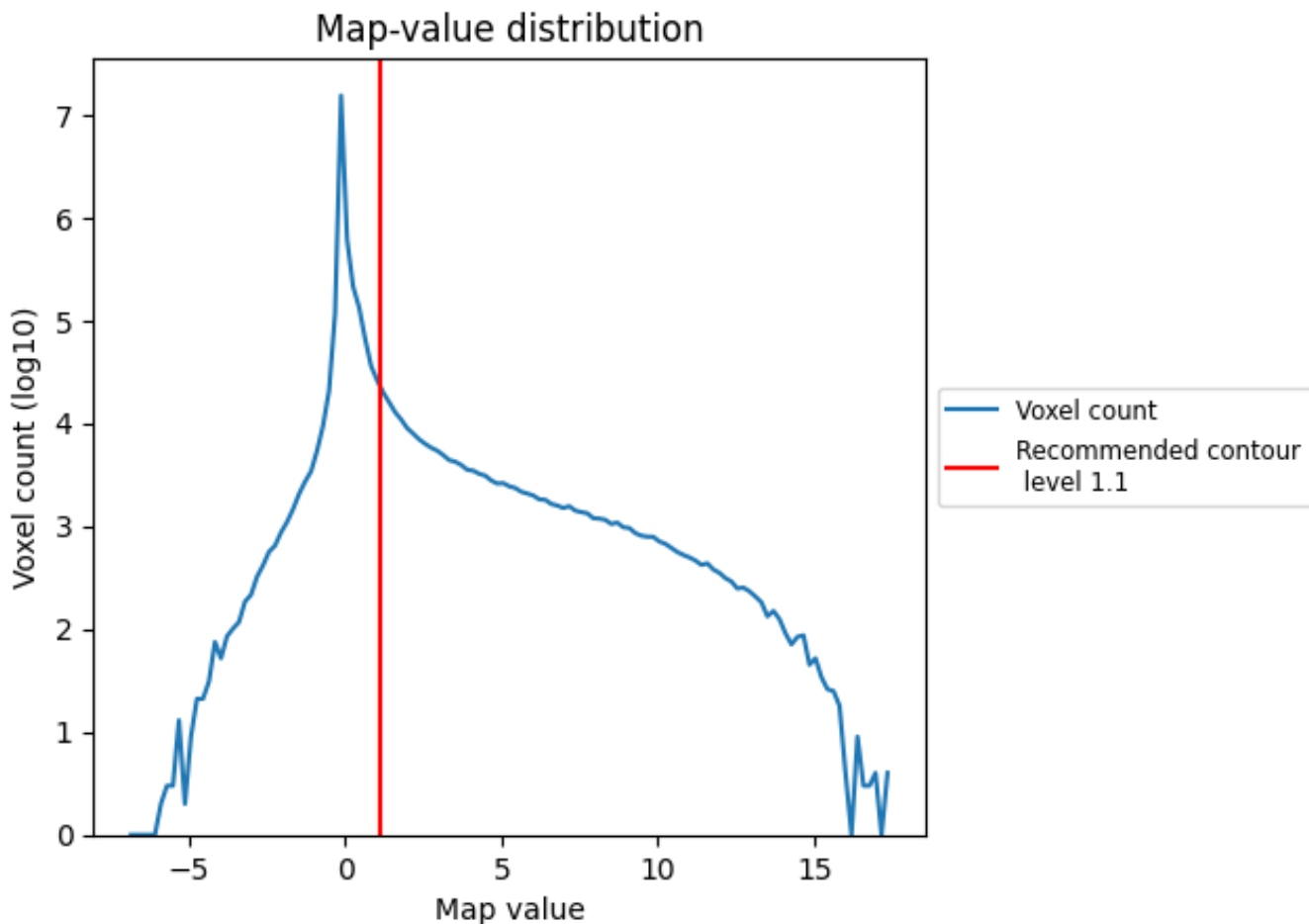
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

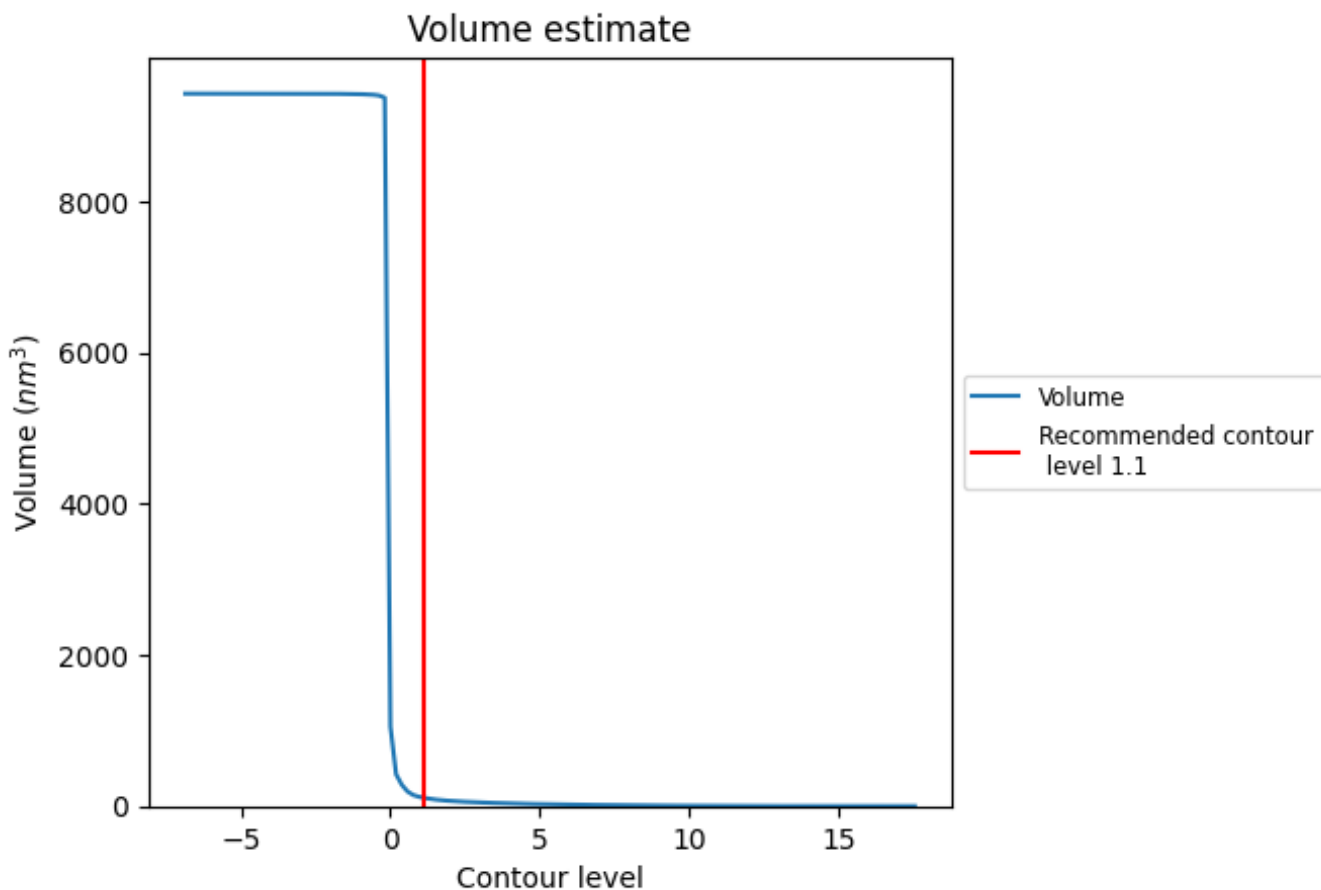
This section contains the results of statistical analysis of the map.

### 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.

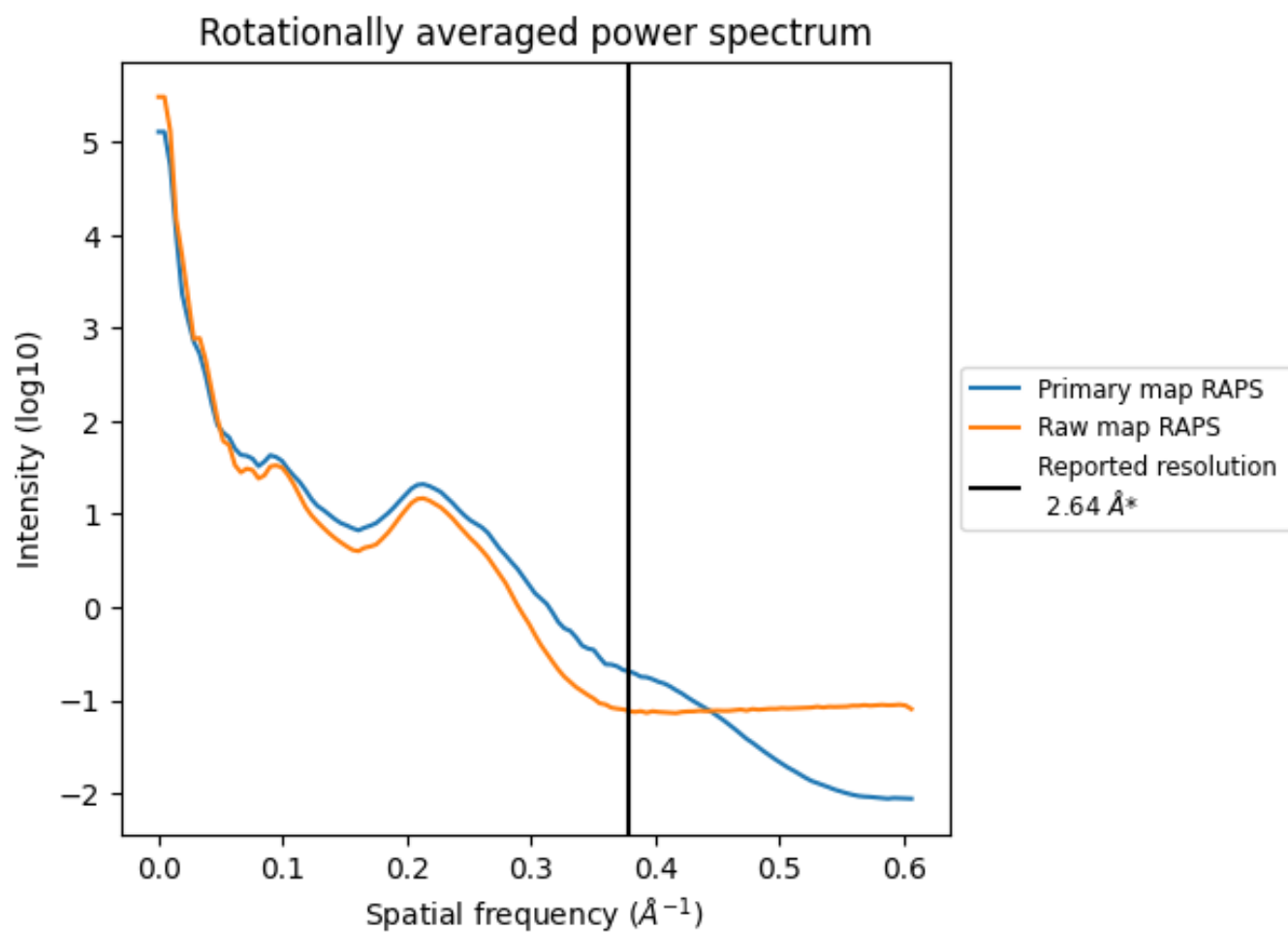
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 112  $\text{nm}^3$ ; this corresponds to an approximate mass of 101 kDa.

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

### 7.3 Rotationally averaged power spectrum i

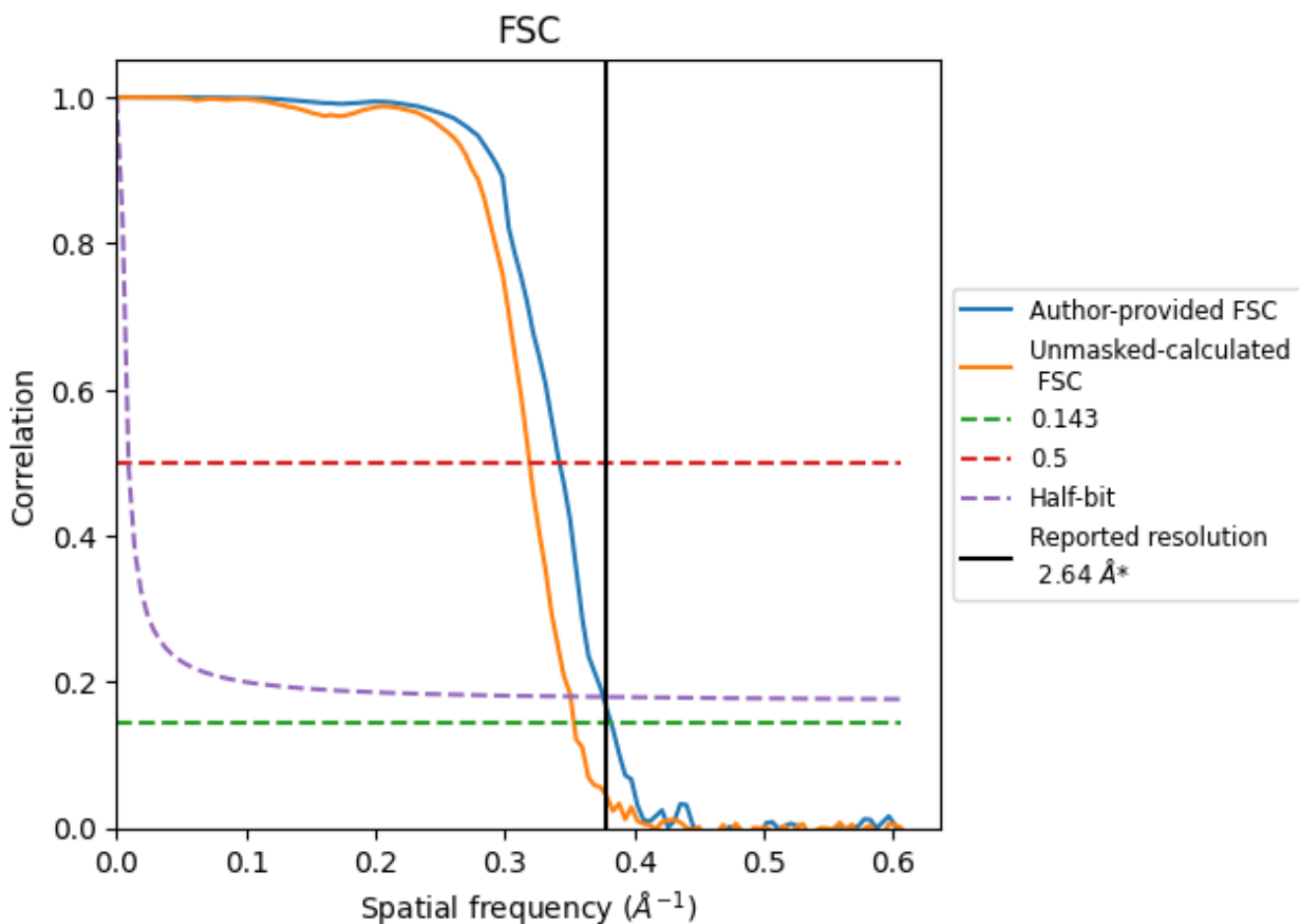


\*Reported resolution corresponds to spatial frequency of  $0.379 \text{ \AA}^{-1}$

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.379  $\text{\AA}^{-1}$



## 8.2 Resolution estimates [i](#)

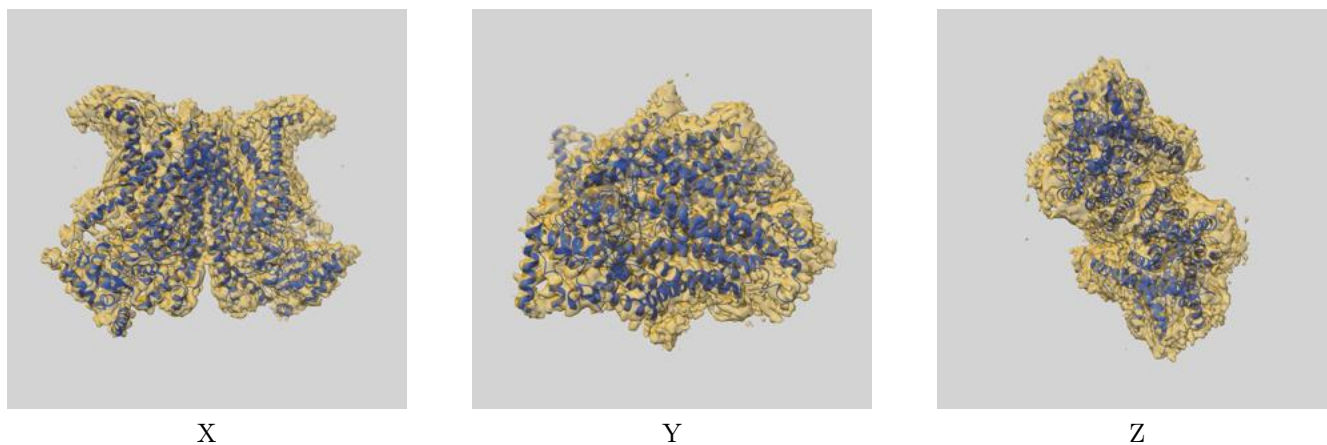
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.64	-	-
Author-provided FSC curve	2.62	2.92	2.66
Unmasked-calculated*	2.83	3.13	2.85

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

## 9 Map-model fit [i](#)

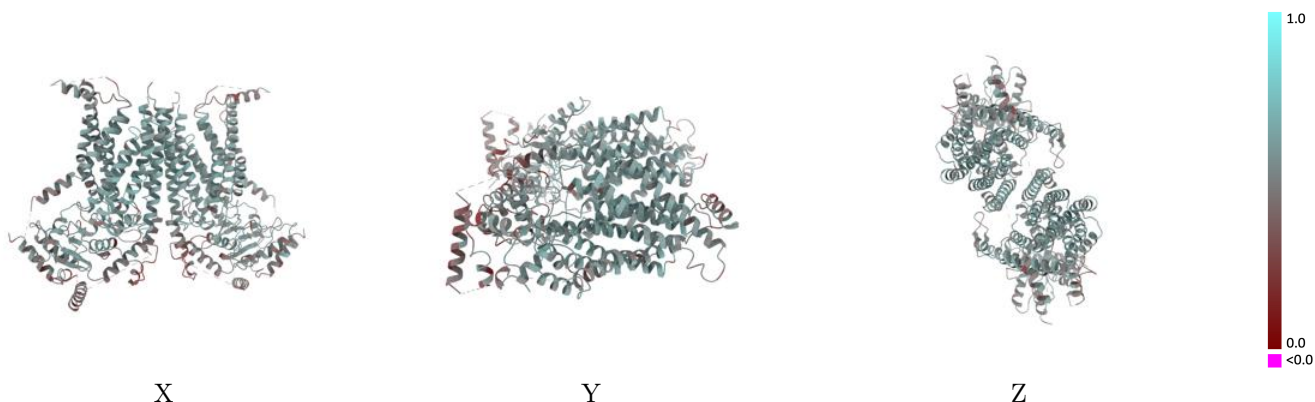
This section contains information regarding the fit between EMDB map EMD-41453 and PDB model 8TOI. Per-residue inclusion information can be found in section 3 on page 7.

### 9.1 Map-model overlay [i](#)



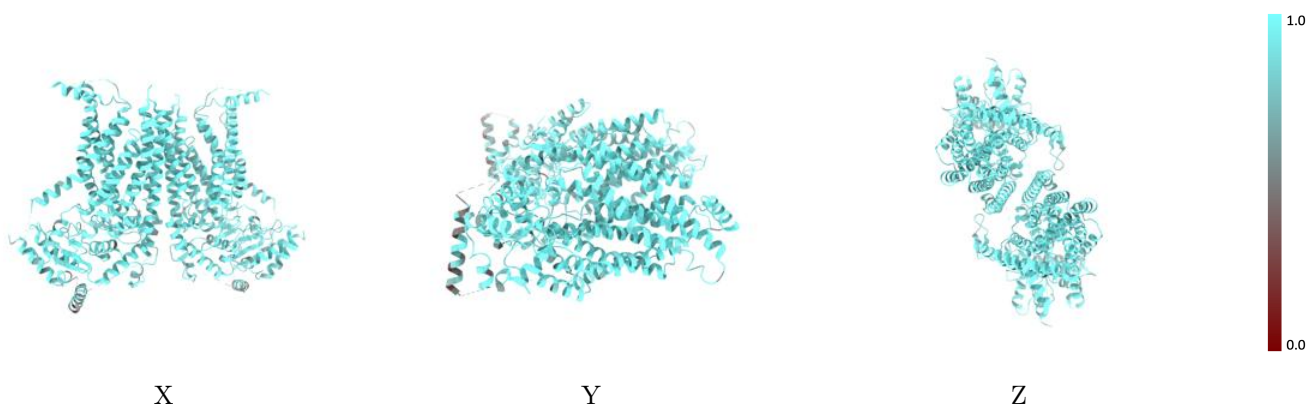
The images above show the 3D surface view of the map at the recommended contour level 1.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



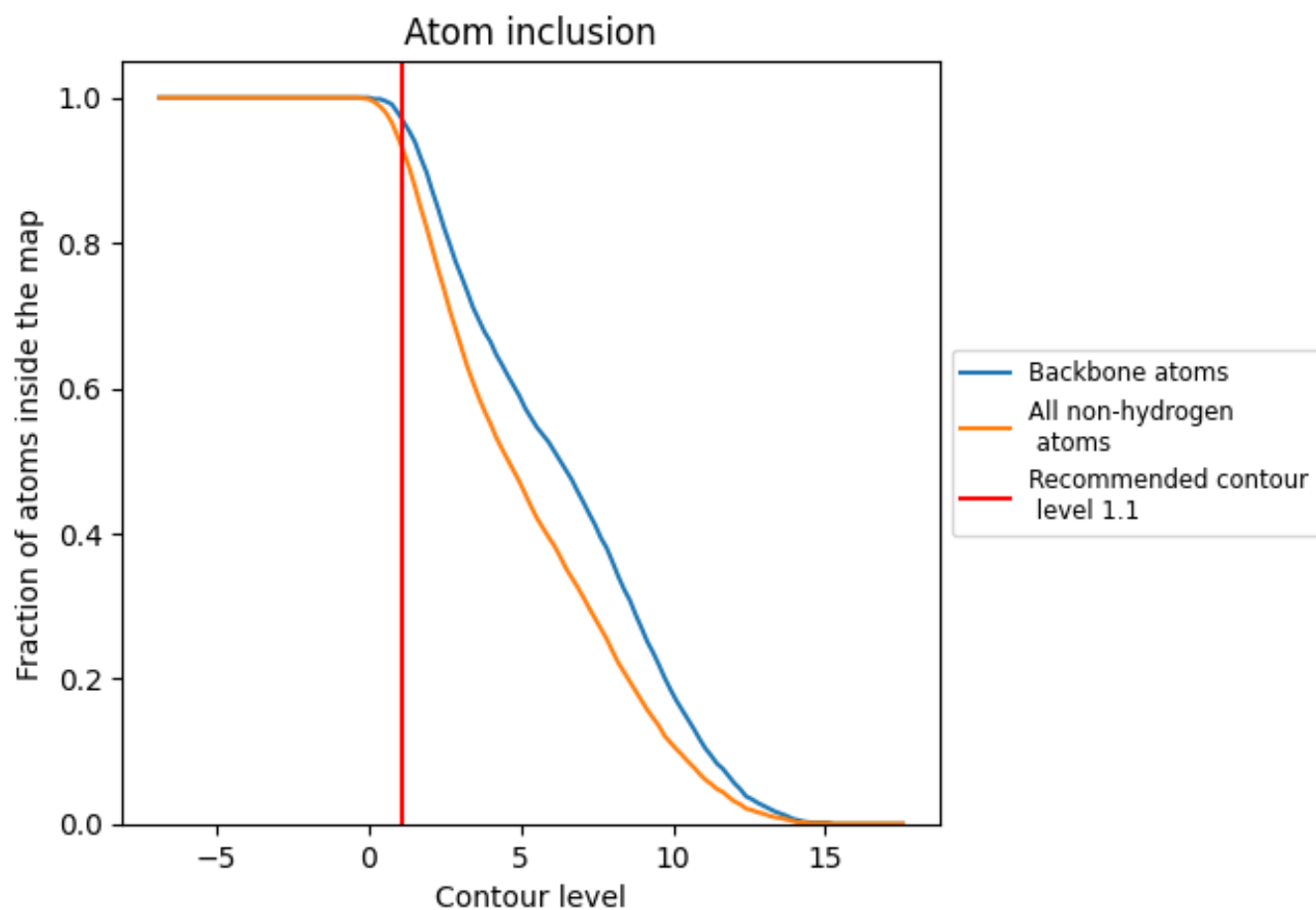
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.1).





## 9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 93% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (1.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9320	 0.5340
A	 0.9320	 0.5340
B	 0.9310	 0.5340

