



Full wwPDB EM Validation Report ⓘ

Jan 15, 2025 – 10:29 AM EST

PDB ID : 8TEH
EMDB ID : EMD-41186
Title : Cryo-EM structure of Arabidopsis thaliana Bor1 in lipid nanodiscs
Authors : Jiang, Y.; Jiang, J.
Deposited on : 2023-07-06
Resolution : 2.30 Å(reported)

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<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.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

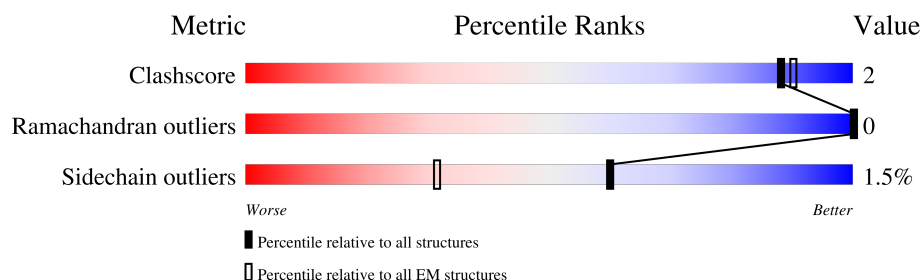
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.30 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	714	<div> <div>8%</div> <div>73%</div> <div>22%</div> </div>
1	B	714	<div> <div>8%</div> <div>74%</div> <div>22%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9816 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.

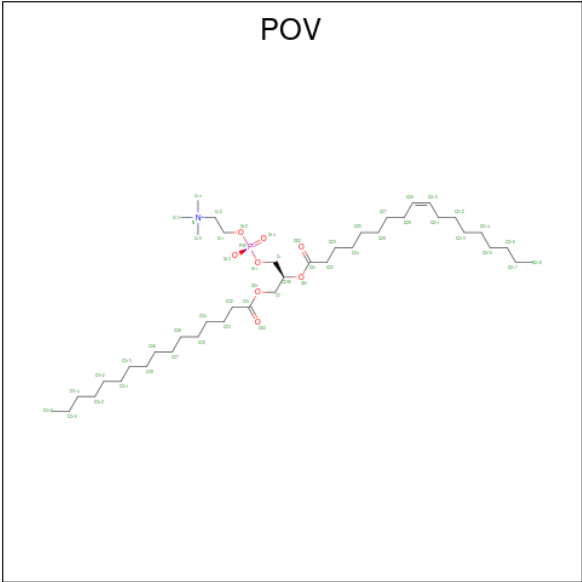
- Molecule 1 is a protein called Boron transporter 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	554	Total	C	N	O	S	0	0
			4374	2889	709	746	30		
1	B	554	Total	C	N	O	S	0	0
			4374	2889	709	746	30		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	705	HIS	-	expression tag	UNP Q8VYR7
A	706	HIS	-	expression tag	UNP Q8VYR7
A	707	HIS	-	expression tag	UNP Q8VYR7
A	708	HIS	-	expression tag	UNP Q8VYR7
A	709	HIS	-	expression tag	UNP Q8VYR7
A	710	HIS	-	expression tag	UNP Q8VYR7
A	711	HIS	-	expression tag	UNP Q8VYR7
A	712	HIS	-	expression tag	UNP Q8VYR7
A	713	HIS	-	expression tag	UNP Q8VYR7
A	714	HIS	-	expression tag	UNP Q8VYR7
B	705	HIS	-	expression tag	UNP Q8VYR7
B	706	HIS	-	expression tag	UNP Q8VYR7
B	707	HIS	-	expression tag	UNP Q8VYR7
B	708	HIS	-	expression tag	UNP Q8VYR7
B	709	HIS	-	expression tag	UNP Q8VYR7
B	710	HIS	-	expression tag	UNP Q8VYR7
B	711	HIS	-	expression tag	UNP Q8VYR7
B	712	HIS	-	expression tag	UNP Q8VYR7
B	713	HIS	-	expression tag	UNP Q8VYR7
B	714	HIS	-	expression tag	UNP Q8VYR7

- Molecule 2 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (three-letter code: POV) (formula: C₄₂H₈₂NO₈P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	O			0
			18	16	2			
2	A	1	Total	C	O			0
			22	20	2			
2	A	1	Total	C	O			0
			38	33	5			
2	A	1	Total	C	N	O	P	0
			51	41	1	8	1	
2	A	1	Total	C	N	O	P	0
			47	37	1	8	1	
2	A	1	Total	C				0
			15	15				
2	A	1	Total	C	O	P		0
			39	31	7	1		
2	A	1	Total	C	N	O	P	0
			39	29	1	8	1	
2	A	1	Total	C	N	O	P	0
			35	25	1	8	1	
2	A	1	Total	C	N	O	P	0
			36	26	1	8	1	
2	A	1	Total	C				0
			15	15				
2	A	1	Total	C	N	O	P	0
			35	25	1	8	1	
2	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	B	1	Total	C	O	P		0
			39	31	7	1		

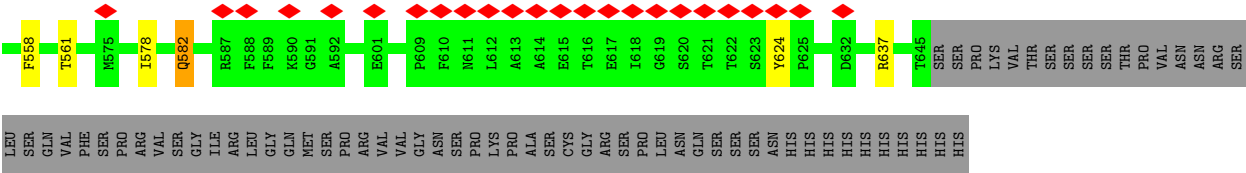
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Mol	Chain	Residues	Atoms					AltConf
2	B	1	Total	C	N	O	P	0
			39	29	1	8	1	
2	B	1	Total	C	N	O	P	0
			35	25	1	8	1	
2	B	1	Total	C	N	O	P	0
			36	26	1	8	1	
2	B	1	Total	C	N	O	P	0
			35	25	1	8	1	
2	B	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	B	1	Total	C	O			0
			18	16	2			
2	B	1	Total	C	O			0
			22	20	2			
2	B	1	Total	C	O			0
			38	33	5			
2	B	1	Total	C	N	O	P	0
			51	41	1	8	1	
2	B	1	Total	C	N	O	P	0
			47	37	1	8	1	

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		AltConf
3	A	107	Total	O	0
			107	107	
3	B	107	Total	O	0
			107	107	



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1012376	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 ($e^-/\text{\AA}^2$)	55	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.254	Depositor
Minimum map value	-0.145	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	239.04, 239.04, 239.04	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: POV

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	0.25	0/4496	0.46	0/6109
1	B	0.25	0/4496	0.46	0/6109
All	All	0.25	0/8992	0.46	0/12218

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4374	0	4463	18	0
1	B	4374	0	4463	17	0
2	A	442	0	629	4	0
2	B	412	0	581	4	0
3	A	107	0	0	4	0
3	B	107	0	0	3	0
All	All	9816	0	10136	35	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 2.

All (35) 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:B:220:LYS:NZ	3:B:903:HOH:O	2.16	0.79
1:A:558:PHE:O	1:A:561:THR:OG1	2.02	0.77
1:A:220:LYS:NZ	3:A:903:HOH:O	2.16	0.77
1:B:558:PHE:O	1:B:561:THR:OG1	2.02	0.77
1:A:502:GLU:OE2	1:B:637:ARG:NH2	2.30	0.65
1:B:463:GLN:O	3:B:902:HOH:O	2.15	0.63
1:A:637:ARG:NH2	1:B:502:GLU:OE2	2.32	0.62
1:A:463:GLN:O	3:A:902:HOH:O	2.16	0.61
1:B:144:ALA:O	1:B:309:TYR:OH	2.23	0.55
1:A:144:ALA:O	1:A:309:TYR:OH	2.23	0.53
2:A:805:POV:P	2:A:805:POV:H14B	2.49	0.53
1:A:173:LYS:HG3	2:A:812:POV:H15A	1.92	0.52
2:B:811:POV:P	2:B:811:POV:H14B	2.49	0.52
1:B:173:LYS:HG3	2:B:805:POV:H15A	1.92	0.51
1:B:180:ARG:NH1	2:B:805:POV:H14A	2.26	0.50
1:B:23:LYS:O	1:B:27:THR:HG23	2.12	0.50
1:A:23:LYS:O	1:A:27:THR:HG23	2.12	0.50
1:A:180:ARG:NH1	2:A:812:POV:H14A	2.26	0.50
1:B:38:ALA:HB3	1:B:39:PRO:HD3	1.95	0.48
1:A:38:ALA:HB3	1:A:39:PRO:HD3	1.95	0.47
1:A:495:TYR:OH	3:A:901:HOH:O	2.10	0.47
1:B:311:ASP:OD2	3:B:904:HOH:O	2.21	0.46
1:B:495:TYR:O	1:B:499:MET:HG3	2.16	0.45
1:B:524:PHE:O	1:B:528:GLU:HG3	2.17	0.45
1:A:516:LEU:HD13	1:A:544:ALA:HA	1.99	0.44
1:B:180:ARG:NE	2:B:806:POV:O22	2.50	0.44
1:A:131:TRP:HB3	1:A:135:MET:HE3	2.00	0.44
1:A:495:TYR:O	1:A:499:MET:HG3	2.16	0.44
1:A:311:ASP:OD2	3:A:904:HOH:O	2.21	0.44
1:B:516:LEU:HD13	1:B:544:ALA:HA	1.99	0.43
1:A:524:PHE:O	1:A:528:GLU:HG3	2.18	0.43
1:A:180:ARG:NE	2:A:813:POV:O22	2.50	0.43
1:B:180:ARG:O	1:B:264:ARG:NH2	2.50	0.42
1:B:578:ILE:O	1:B:582:GLN:NE2	2.53	0.42
1:A:578:ILE:O	1:A:582:GLN:NE2	2.53	0.41

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	548/714 (77%)	539 (98%)	9 (2%)	0	100	100
1	B	548/714 (77%)	539 (98%)	9 (2%)	0	100	100
All	All	1096/1428 (77%)	1078 (98%)	18 (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	468/613 (76%)	461 (98%)	7 (2%)	60	76
1	B	468/613 (76%)	461 (98%)	7 (2%)	60	76
All	All	936/1226 (76%)	922 (98%)	14 (2%)	60	76

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	ASP
1	A	119	ASP
1	A	203	PHE
1	A	463	GLN
1	A	521	SER
1	A	582	GLN
1	A	624	TYR
1	B	25	ASP

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Mol	Chain	Res	Type
1	B	119	ASP
1	B	203	PHE
1	B	463	GLN
1	B	521	SER
1	B	582	GLN
1	B	624	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	595	GLN
1	B	595	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](#)

24 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	POV	A	809	-	34,34,51	0.60	0	40,42,59	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	POV	B	808	-	21,21,51	0.37	0	21,21,59	0.40	0
2	POV	A	806	-	14,14,51	1.04	1 (7%)	13,13,59	0.59	0
2	POV	B	805	-	34,34,51	0.58	0	40,42,59	0.71	1 (2%)
2	POV	A	812	-	34,34,51	0.58	0	40,42,59	0.71	1 (2%)
2	POV	A	804	-	50,50,51	5.18	1 (2%)	56,58,59	0.54	0
2	POV	B	810	-	50,50,51	5.17	1 (2%)	56,58,59	0.54	0
2	POV	B	802	-	38,38,51	0.58	0	44,46,59	0.53	0
2	POV	A	802	-	21,21,51	0.37	0	21,21,59	0.40	0
2	POV	B	803	-	34,34,51	0.59	0	40,42,59	0.56	0
2	POV	A	805	-	46,46,51	0.53	0	52,54,59	0.52	0
2	POV	A	813	-	51,51,51	0.50	0	57,59,59	0.47	0
2	POV	A	807	-	35,38,51	0.41	0	36,41,59	0.34	0
2	POV	A	810	-	35,35,51	0.59	0	41,43,59	0.56	0
2	POV	B	804	-	35,35,51	0.59	0	41,43,59	0.56	0
2	POV	A	811	-	14,14,51	1.03	1 (7%)	13,13,59	0.58	0
2	POV	B	809	-	37,37,51	0.41	0	39,39,59	0.42	0
2	POV	B	807	-	17,17,51	0.97	1 (5%)	17,17,59	0.61	0
2	POV	A	801	-	17,17,51	0.97	1 (5%)	17,17,59	0.61	0
2	POV	B	806	-	51,51,51	0.50	0	57,59,59	0.47	0
2	POV	B	811	-	46,46,51	0.53	0	52,54,59	0.52	0
2	POV	A	803	-	37,37,51	0.41	0	39,39,59	0.42	0
2	POV	B	801	-	35,38,51	0.41	0	36,41,59	0.35	0
2	POV	A	808	-	38,38,51	0.58	0	44,46,59	0.52	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	POV	A	809	-	-	10/38/38/55	-
2	POV	B	808	-	-	7/20/20/55	-
2	POV	A	806	-	-	10/12/12/55	-
2	POV	B	805	-	-	16/38/38/55	-
2	POV	A	812	-	-	16/38/38/55	-
2	POV	A	804	-	-	18/54/54/55	-
2	POV	B	810	-	-	18/54/54/55	-
2	POV	B	802	-	-	15/42/42/55	-
2	POV	A	802	-	-	7/20/20/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	POV	B	803	-	-	10/38/38/55	-
2	POV	A	805	-	-	27/50/50/55	-
2	POV	A	813	-	-	30/55/55/55	-
2	POV	A	807	-	-	18/38/40/55	-
2	POV	A	810	-	-	21/39/39/55	-
2	POV	B	804	-	-	21/39/39/55	-
2	POV	A	811	-	-	10/12/12/55	-
2	POV	B	809	-	-	14/39/39/55	-
2	POV	B	807	-	-	8/15/15/55	-
2	POV	A	801	-	-	8/15/15/55	-
2	POV	B	806	-	-	30/55/55/55	-
2	POV	B	811	-	-	27/50/50/55	-
2	POV	A	803	-	-	14/39/39/55	-
2	POV	B	801	-	-	18/38/40/55	-
2	POV	A	808	-	-	15/42/42/55	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	804	POV	C215-C214	36.42	3.32	1.51
2	B	810	POV	C215-C214	36.41	3.32	1.51
2	B	807	POV	C29-C210	3.77	1.53	1.31
2	A	801	POV	C29-C210	3.77	1.53	1.31
2	A	806	POV	C29-C210	3.76	1.53	1.31
2	A	811	POV	C29-C210	3.74	1.52	1.31

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	805	POV	C2-O21-C21	2.89	124.70	117.80
2	A	812	POV	C2-O21-C21	2.87	124.66	117.80

There are no chirality outliers.

All (388) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	803	POV	C22-C21-O21-C2
2	A	804	POV	C11-O12-P-O13

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Mol	Chain	Res	Type	Atoms
2	A	805	POV	C11-O12-P-O11
2	A	805	POV	C11-O12-P-O13
2	A	805	POV	C11-O12-P-O14
2	A	808	POV	C1-O11-P-O13
2	A	808	POV	C11-O12-P-O13
2	A	808	POV	C22-C21-O21-C2
2	A	809	POV	C1-O11-P-O14
2	A	809	POV	C11-O12-P-O14
2	A	809	POV	O32-C31-O31-C3
2	A	810	POV	C1-O11-P-O12
2	A	810	POV	C11-O12-P-O11
2	A	810	POV	C11-O12-P-O14
2	A	812	POV	C1-O11-P-O12
2	A	812	POV	C11-O12-P-O11
2	A	812	POV	C3-C2-O21-C21
2	A	813	POV	C1-O11-P-O12
2	A	813	POV	C1-O11-P-O13
2	A	813	POV	C1-O11-P-O14
2	A	813	POV	O22-C21-O21-C2
2	B	802	POV	C1-O11-P-O13
2	B	802	POV	C11-O12-P-O13
2	B	802	POV	C22-C21-O21-C2
2	B	803	POV	C1-O11-P-O14
2	B	803	POV	C11-O12-P-O14
2	B	803	POV	O32-C31-O31-C3
2	B	804	POV	C1-O11-P-O12
2	B	804	POV	C11-O12-P-O11
2	B	804	POV	C11-O12-P-O14
2	B	805	POV	C1-O11-P-O12
2	B	805	POV	C11-O12-P-O11
2	B	805	POV	C3-C2-O21-C21
2	B	806	POV	C1-O11-P-O12
2	B	806	POV	C1-O11-P-O13
2	B	806	POV	C1-O11-P-O14
2	B	806	POV	O22-C21-O21-C2
2	B	809	POV	C22-C21-O21-C2
2	B	810	POV	C11-O12-P-O13
2	B	811	POV	C11-O12-P-O11
2	B	811	POV	C11-O12-P-O13
2	B	811	POV	C11-O12-P-O14
2	A	803	POV	O32-C31-O31-C3
2	B	809	POV	O32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
2	A	803	POV	O22-C21-O21-C2
2	A	808	POV	O22-C21-O21-C2
2	B	802	POV	O22-C21-O21-C2
2	B	809	POV	O22-C21-O21-C2
2	A	803	POV	C32-C31-O31-C3
2	A	809	POV	C32-C31-O31-C3
2	B	803	POV	C32-C31-O31-C3
2	B	809	POV	C32-C31-O31-C3
2	A	813	POV	C22-C21-O21-C2
2	B	806	POV	C22-C21-O21-C2
2	A	801	POV	C211-C210-C29-C28
2	B	807	POV	C211-C210-C29-C28
2	A	812	POV	O32-C31-O31-C3
2	B	805	POV	O32-C31-O31-C3
2	A	813	POV	C11-C12-N-C13
2	B	806	POV	C11-C12-N-C13
2	A	807	POV	C22-C21-O21-C2
2	B	801	POV	C22-C21-O21-C2
2	A	812	POV	C32-C31-O31-C3
2	B	805	POV	C32-C31-O31-C3
2	A	805	POV	C2-C1-O11-P
2	B	811	POV	C2-C1-O11-P
2	A	807	POV	O22-C21-O21-C2
2	B	801	POV	O22-C21-O21-C2
2	A	805	POV	C32-C31-O31-C3
2	A	807	POV	C32-C31-O31-C3
2	B	801	POV	C32-C31-O31-C3
2	B	811	POV	C32-C31-O31-C3
2	A	808	POV	C24-C25-C26-C27
2	B	802	POV	C24-C25-C26-C27
2	A	805	POV	O32-C31-O31-C3
2	A	807	POV	O32-C31-O31-C3
2	B	801	POV	O32-C31-O31-C3
2	B	811	POV	O32-C31-O31-C3
2	A	810	POV	C22-C21-O21-C2
2	B	804	POV	C22-C21-O21-C2
2	A	813	POV	C212-C213-C214-C215
2	B	806	POV	C212-C213-C214-C215
2	A	804	POV	C31-C32-C33-C34
2	B	810	POV	C31-C32-C33-C34
2	A	803	POV	C31-C32-C33-C34
2	B	801	POV	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
2	B	809	POV	C31-C32-C33-C34
2	A	801	POV	C21-C22-C23-C24
2	A	807	POV	C31-C32-C33-C34
2	B	807	POV	C21-C22-C23-C24
2	A	812	POV	C31-C32-C33-C34
2	B	805	POV	C31-C32-C33-C34
2	A	810	POV	O22-C21-O21-C2
2	A	812	POV	O22-C21-O21-C2
2	B	804	POV	O22-C21-O21-C2
2	B	805	POV	O22-C21-O21-C2
2	A	804	POV	C22-C21-O21-C2
2	A	812	POV	C22-C21-O21-C2
2	B	805	POV	C22-C21-O21-C2
2	B	810	POV	C22-C21-O21-C2
2	A	804	POV	O22-C21-O21-C2
2	B	810	POV	O22-C21-O21-C2
2	A	806	POV	C211-C210-C29-C28
2	A	811	POV	C211-C210-C29-C28
2	A	805	POV	C21-C22-C23-C24
2	B	811	POV	C21-C22-C23-C24
2	A	810	POV	C32-C31-O31-C3
2	B	804	POV	C32-C31-O31-C3
2	A	812	POV	C36-C37-C38-C39
2	B	805	POV	C36-C37-C38-C39
2	A	805	POV	O21-C2-C3-O31
2	B	811	POV	O21-C2-C3-O31
2	A	813	POV	C11-C12-N-C14
2	A	813	POV	C11-C12-N-C15
2	B	806	POV	C11-C12-N-C14
2	B	806	POV	C11-C12-N-C15
2	A	806	POV	C25-C26-C27-C28
2	A	811	POV	C25-C26-C27-C28
2	A	811	POV	C211-C212-C213-C214
2	A	813	POV	C32-C33-C34-C35
2	B	806	POV	C32-C33-C34-C35
2	A	806	POV	C211-C212-C213-C214
2	A	807	POV	C37-C38-C39-C310
2	A	813	POV	C310-C311-C312-C313
2	B	806	POV	C310-C311-C312-C313
2	B	801	POV	C37-C38-C39-C310
2	A	802	POV	C211-C212-C213-C214
2	A	804	POV	C37-C38-C39-C310

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Mol	Chain	Res	Type	Atoms
2	B	808	POV	C211-C212-C213-C214
2	B	810	POV	C37-C38-C39-C310
2	A	805	POV	C312-C313-C314-C315
2	B	811	POV	C312-C313-C314-C315
2	A	804	POV	C312-C313-C314-C315
2	B	810	POV	C312-C313-C314-C315
2	A	807	POV	C35-C36-C37-C38
2	B	801	POV	C35-C36-C37-C38
2	A	812	POV	C33-C34-C35-C36
2	B	805	POV	C33-C34-C35-C36
2	A	805	POV	C313-C314-C315-C316
2	B	811	POV	C313-C314-C315-C316
2	A	813	POV	C312-C313-C314-C315
2	A	804	POV	C213-C214-C215-C216
2	A	813	POV	C25-C26-C27-C28
2	B	806	POV	C312-C313-C314-C315
2	B	806	POV	C25-C26-C27-C28
2	B	810	POV	C213-C214-C215-C216
2	A	813	POV	C34-C35-C36-C37
2	B	806	POV	C34-C35-C36-C37
2	A	810	POV	O32-C31-O31-C3
2	B	804	POV	O32-C31-O31-C3
2	A	805	POV	C32-C33-C34-C35
2	B	811	POV	C32-C33-C34-C35
2	B	809	POV	C22-C23-C24-C25
2	A	803	POV	C22-C23-C24-C25
2	A	808	POV	C32-C33-C34-C35
2	B	802	POV	C32-C33-C34-C35
2	B	804	POV	C24-C25-C26-C27
2	A	810	POV	C24-C25-C26-C27
2	B	806	POV	C22-C23-C24-C25
2	A	813	POV	C22-C23-C24-C25
2	A	812	POV	C35-C36-C37-C38
2	B	805	POV	C35-C36-C37-C38
2	A	806	POV	C210-C211-C212-C213
2	A	811	POV	C210-C211-C212-C213
2	A	813	POV	C31-C32-C33-C34
2	B	806	POV	C31-C32-C33-C34
2	A	803	POV	C33-C34-C35-C36
2	B	809	POV	C33-C34-C35-C36
2	B	811	POV	C37-C38-C39-C310
2	A	805	POV	C37-C38-C39-C310

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Mol	Chain	Res	Type	Atoms
2	A	805	POV	C34-C35-C36-C37
2	B	811	POV	C310-C311-C312-C313
2	B	811	POV	C34-C35-C36-C37
2	A	805	POV	C310-C311-C312-C313
2	A	805	POV	C31-C32-C33-C34
2	B	811	POV	C31-C32-C33-C34
2	A	803	POV	C37-C38-C39-C310
2	A	805	POV	C35-C36-C37-C38
2	B	811	POV	C35-C36-C37-C38
2	B	809	POV	C37-C38-C39-C310
2	A	807	POV	C25-C26-C27-C28
2	B	801	POV	C25-C26-C27-C28
2	B	805	POV	C22-C23-C24-C25
2	A	812	POV	C22-C23-C24-C25
2	B	811	POV	C311-C310-C39-C38
2	A	805	POV	C311-C310-C39-C38
2	A	803	POV	C210-C211-C212-C213
2	A	813	POV	C26-C27-C28-C29
2	B	806	POV	C26-C27-C28-C29
2	B	809	POV	C210-C211-C212-C213
2	A	805	POV	C1-C2-C3-O31
2	A	807	POV	C1-C2-C3-O31
2	B	801	POV	C1-C2-C3-O31
2	B	811	POV	C1-C2-C3-O31
2	B	801	POV	C24-C25-C26-C27
2	A	807	POV	C24-C25-C26-C27
2	A	805	POV	C22-C23-C24-C25
2	B	811	POV	C22-C23-C24-C25
2	A	803	POV	C213-C214-C215-C216
2	B	809	POV	C213-C214-C215-C216
2	A	804	POV	C212-C213-C214-C215
2	B	810	POV	C212-C213-C214-C215
2	A	807	POV	C32-C33-C34-C35
2	B	801	POV	C32-C33-C34-C35
2	A	813	POV	O21-C2-C3-O31
2	B	806	POV	O21-C2-C3-O31
2	A	806	POV	C26-C27-C28-C29
2	A	811	POV	C26-C27-C28-C29
2	A	808	POV	C37-C38-C39-C310
2	B	802	POV	C37-C38-C39-C310
2	A	813	POV	C39-C310-C311-C312
2	B	806	POV	C39-C310-C311-C312

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Mol	Chain	Res	Type	Atoms
2	A	810	POV	C25-C26-C27-C28
2	B	804	POV	C25-C26-C27-C28
2	B	801	POV	C312-C313-C314-C315
2	A	807	POV	C312-C313-C314-C315
2	A	813	POV	C32-C31-O31-C3
2	B	806	POV	C32-C31-O31-C3
2	A	807	POV	C33-C34-C35-C36
2	B	801	POV	C33-C34-C35-C36
2	A	805	POV	O11-C1-C2-C3
2	B	811	POV	O11-C1-C2-C3
2	A	813	POV	C313-C314-C315-C316
2	B	806	POV	C313-C314-C315-C316
2	B	803	POV	C34-C35-C36-C37
2	A	809	POV	C34-C35-C36-C37
2	A	813	POV	C214-C215-C216-C217
2	B	806	POV	C214-C215-C216-C217
2	A	813	POV	C21-C22-C23-C24
2	B	806	POV	C21-C22-C23-C24
2	A	804	POV	C1-C2-C3-O31
2	A	809	POV	C1-C2-C3-O31
2	A	813	POV	C1-C2-C3-O31
2	B	803	POV	C1-C2-C3-O31
2	B	806	POV	C1-C2-C3-O31
2	B	810	POV	C1-C2-C3-O31
2	A	802	POV	C24-C25-C26-C27
2	B	808	POV	C24-C25-C26-C27
2	A	808	POV	C11-C12-N-C14
2	B	802	POV	C11-C12-N-C14
2	A	802	POV	C25-C26-C27-C28
2	B	808	POV	C25-C26-C27-C28
2	A	810	POV	C22-C23-C24-C25
2	B	804	POV	C22-C23-C24-C25
2	B	801	POV	C34-C35-C36-C37
2	A	805	POV	C33-C34-C35-C36
2	A	807	POV	C34-C35-C36-C37
2	A	809	POV	O21-C2-C3-O31
2	B	803	POV	O21-C2-C3-O31
2	B	811	POV	C33-C34-C35-C36
2	A	804	POV	C36-C37-C38-C39
2	B	810	POV	C36-C37-C38-C39
2	A	807	POV	C39-C310-C311-C312
2	B	801	POV	C39-C310-C311-C312

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Mol	Chain	Res	Type	Atoms
2	A	812	POV	C34-C35-C36-C37
2	B	805	POV	C34-C35-C36-C37
2	A	810	POV	O11-C1-C2-C3
2	B	804	POV	O11-C1-C2-C3
2	A	810	POV	C34-C35-C36-C37
2	B	804	POV	C34-C35-C36-C37
2	A	804	POV	C21-C22-C23-C24
2	A	813	POV	O32-C31-O31-C3
2	B	806	POV	O32-C31-O31-C3
2	B	810	POV	C21-C22-C23-C24
2	B	811	POV	C24-C25-C26-C27
2	A	805	POV	C24-C25-C26-C27
2	A	810	POV	C1-C2-O21-C21
2	B	804	POV	C1-C2-O21-C21
2	A	805	POV	O11-C1-C2-O21
2	A	810	POV	O11-C1-C2-O21
2	B	804	POV	O11-C1-C2-O21
2	B	811	POV	O11-C1-C2-O21
2	A	806	POV	C24-C25-C26-C27
2	A	811	POV	C24-C25-C26-C27
2	A	804	POV	C33-C34-C35-C36
2	B	810	POV	C33-C34-C35-C36
2	A	803	POV	C214-C215-C216-C217
2	B	809	POV	C214-C215-C216-C217
2	A	808	POV	O12-C11-C12-N
2	A	810	POV	O12-C11-C12-N
2	B	802	POV	O12-C11-C12-N
2	B	804	POV	O12-C11-C12-N
2	A	807	POV	C23-C24-C25-C26
2	B	801	POV	C23-C24-C25-C26
2	A	808	POV	C11-C12-N-C15
2	B	802	POV	C11-C12-N-C15
2	A	813	POV	C37-C38-C39-C310
2	B	806	POV	C37-C38-C39-C310
2	A	806	POV	C22-C23-C24-C25
2	A	811	POV	C22-C23-C24-C25
2	A	809	POV	C21-C22-C23-C24
2	B	803	POV	C21-C22-C23-C24
2	A	808	POV	C11-C12-N-C13
2	B	802	POV	C11-C12-N-C13
2	A	807	POV	O21-C2-C3-O31
2	B	801	POV	O21-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
2	B	803	POV	C32-C33-C34-C35
2	A	806	POV	C27-C28-C29-C210
2	A	811	POV	C27-C28-C29-C210
2	A	809	POV	C32-C33-C34-C35
2	A	805	POV	C1-O11-P-O14
2	A	809	POV	C1-O11-P-O12
2	A	810	POV	C1-O11-P-O14
2	A	810	POV	C11-O12-P-O13
2	A	812	POV	C1-O11-P-O14
2	A	812	POV	C11-O12-P-O14
2	A	813	POV	C11-O12-P-O14
2	B	803	POV	C1-O11-P-O12
2	B	804	POV	C1-O11-P-O14
2	B	804	POV	C11-O12-P-O13
2	B	805	POV	C1-O11-P-O14
2	B	805	POV	C11-O12-P-O14
2	B	806	POV	C11-O12-P-O14
2	B	811	POV	C1-O11-P-O14
2	A	812	POV	C2-C1-O11-P
2	B	805	POV	C2-C1-O11-P
2	A	808	POV	O32-C31-O31-C3
2	B	802	POV	O32-C31-O31-C3
2	A	808	POV	C32-C31-O31-C3
2	B	802	POV	C32-C31-O31-C3
2	B	808	POV	C1-C2-O21-C21
2	A	802	POV	C1-C2-O21-C21
2	A	801	POV	C25-C26-C27-C28
2	B	807	POV	C25-C26-C27-C28
2	A	813	POV	C311-C312-C313-C314
2	B	806	POV	C311-C312-C313-C314
2	A	801	POV	C26-C27-C28-C29
2	B	807	POV	C26-C27-C28-C29
2	A	806	POV	C29-C210-C211-C212
2	A	811	POV	C29-C210-C211-C212
2	A	802	POV	C22-C21-O21-C2
2	A	804	POV	C32-C31-O31-C3
2	B	810	POV	C32-C31-O31-C3
2	B	808	POV	C22-C21-O21-C2
2	A	806	POV	C213-C214-C215-C216
2	A	811	POV	C213-C214-C215-C216
2	A	802	POV	O22-C21-O21-C2
2	B	808	POV	O22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
2	B	810	POV	O32-C31-O31-C3
2	A	801	POV	O22-C21-C22-C23
2	B	807	POV	O22-C21-C22-C23
2	A	804	POV	O32-C31-O31-C3
2	A	801	POV	C211-C212-C213-C214
2	B	807	POV	C211-C212-C213-C214
2	A	801	POV	O21-C21-C22-C23
2	B	807	POV	O21-C21-C22-C23
2	A	810	POV	O21-C2-C3-O31
2	B	804	POV	O21-C2-C3-O31
2	A	813	POV	C27-C28-C29-C210
2	B	806	POV	C27-C28-C29-C210
2	A	804	POV	C310-C311-C312-C313
2	B	810	POV	C310-C311-C312-C313
2	A	804	POV	C29-C210-C211-C212
2	B	810	POV	C29-C210-C211-C212
2	B	811	POV	C39-C310-C311-C312
2	A	803	POV	C27-C28-C29-C210
2	A	810	POV	C27-C28-C29-C210
2	B	804	POV	C27-C28-C29-C210
2	B	809	POV	C27-C28-C29-C210
2	A	805	POV	C39-C310-C311-C312
2	A	801	POV	C29-C210-C211-C212
2	A	805	POV	C27-C28-C29-C210
2	B	807	POV	C29-C210-C211-C212
2	B	811	POV	C27-C28-C29-C210
2	A	804	POV	C39-C310-C311-C312
2	B	810	POV	C39-C310-C311-C312
2	B	811	POV	C23-C24-C25-C26
2	A	807	POV	C310-C311-C312-C313
2	A	805	POV	C23-C24-C25-C26
2	B	801	POV	C310-C311-C312-C313
2	A	813	POV	C215-C216-C217-C218
2	B	806	POV	C215-C216-C217-C218
2	B	802	POV	C31-C32-C33-C34
2	B	810	POV	C27-C28-C29-C210
2	A	803	POV	O31-C31-C32-C33
2	B	809	POV	O31-C31-C32-C33
2	B	802	POV	C34-C35-C36-C37
2	A	808	POV	C31-C32-C33-C34
2	A	804	POV	C27-C28-C29-C210
2	A	808	POV	C34-C35-C36-C37

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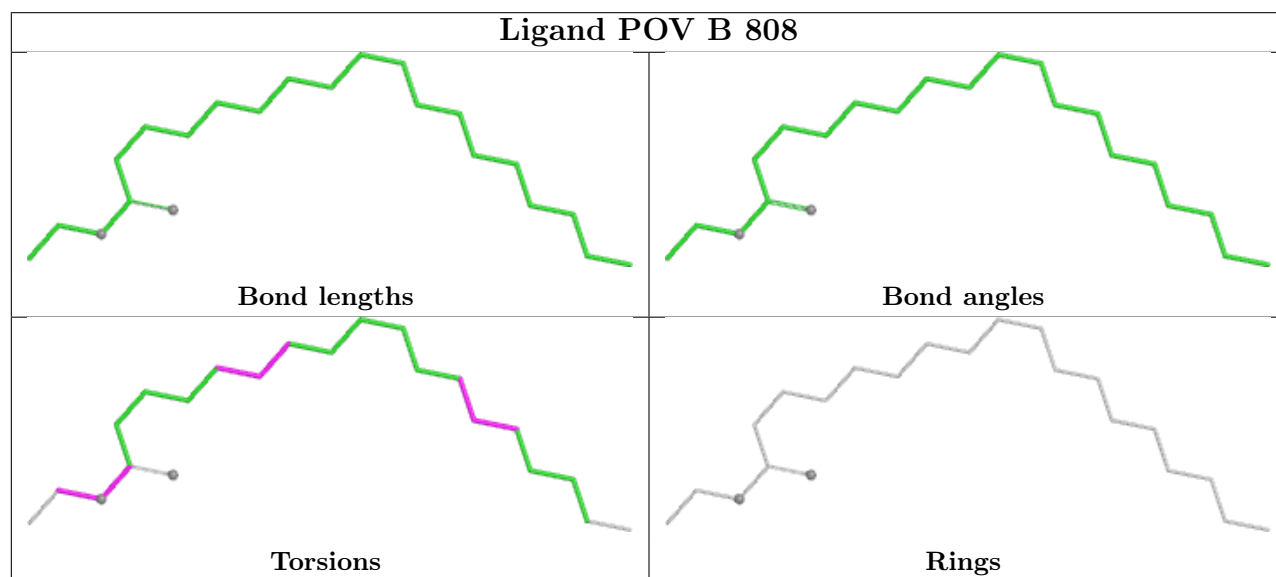
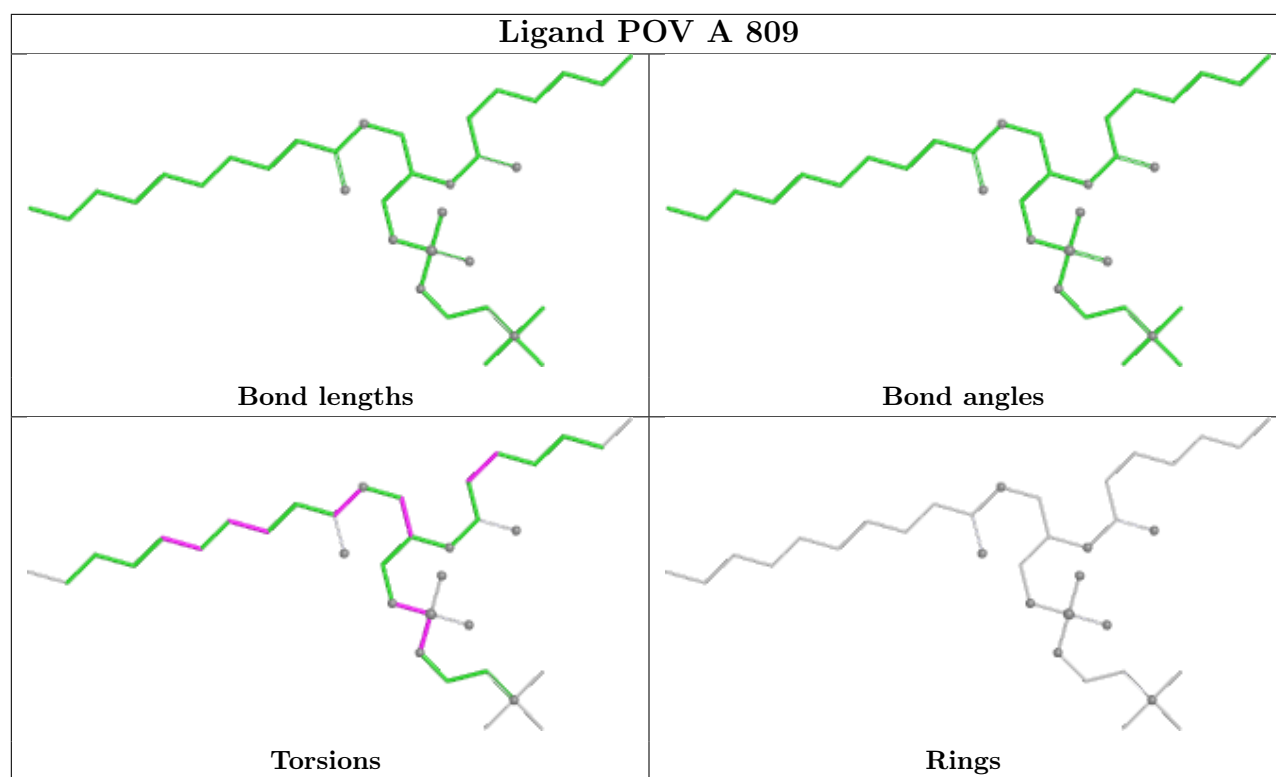
Mol	Chain	Res	Type	Atoms
2	A	802	POV	C212-C213-C214-C215
2	B	808	POV	C212-C213-C214-C215
2	B	804	POV	O31-C31-C32-C33
2	A	810	POV	O31-C31-C32-C33
2	A	803	POV	O32-C31-C32-C33
2	B	809	POV	O32-C31-C32-C33
2	A	810	POV	C21-C22-C23-C24
2	B	804	POV	C21-C22-C23-C24

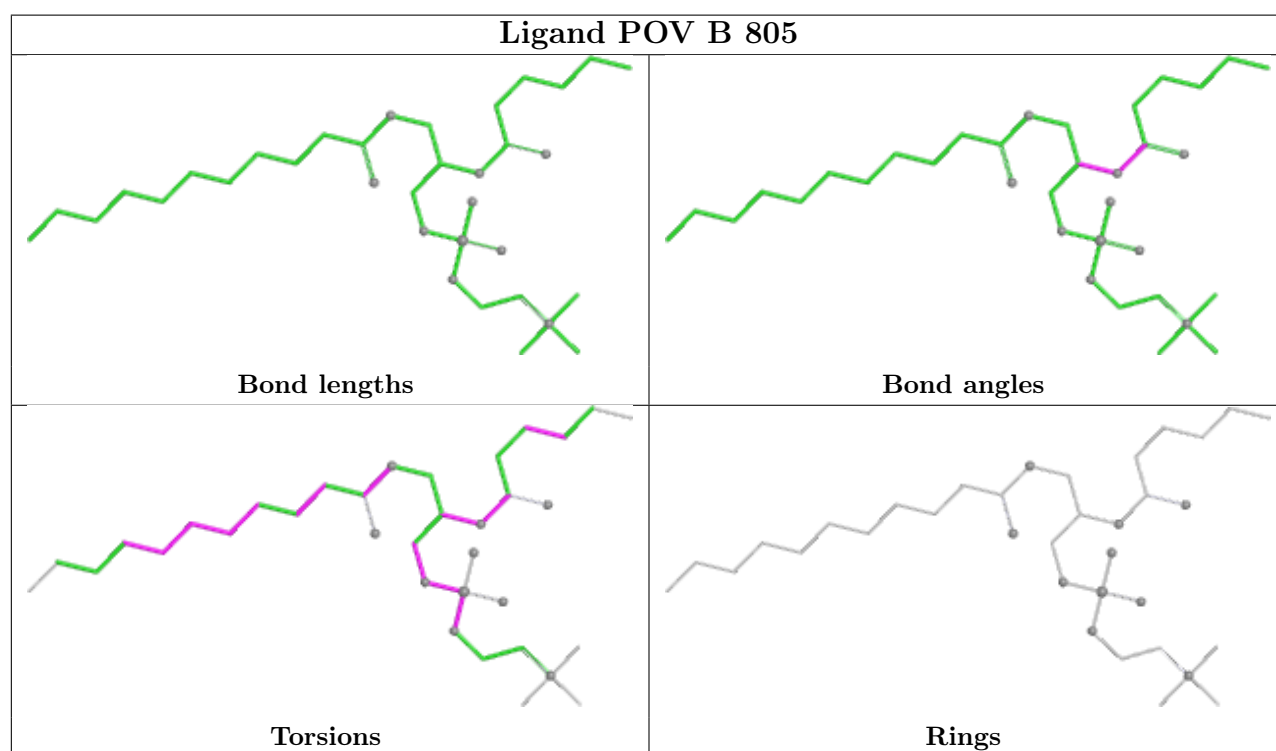
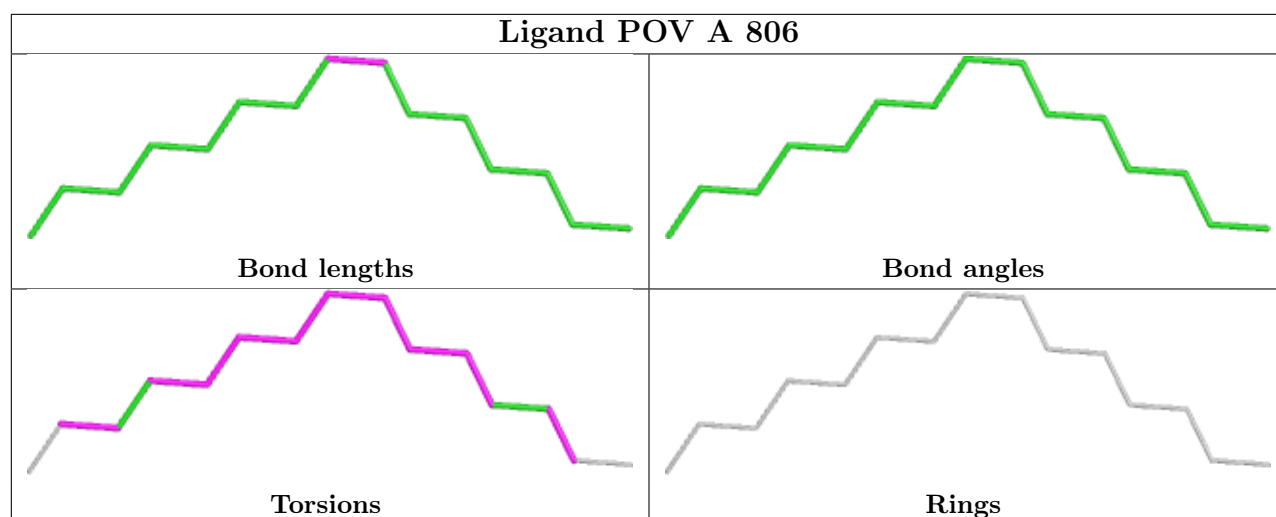
There are no ring outliers.

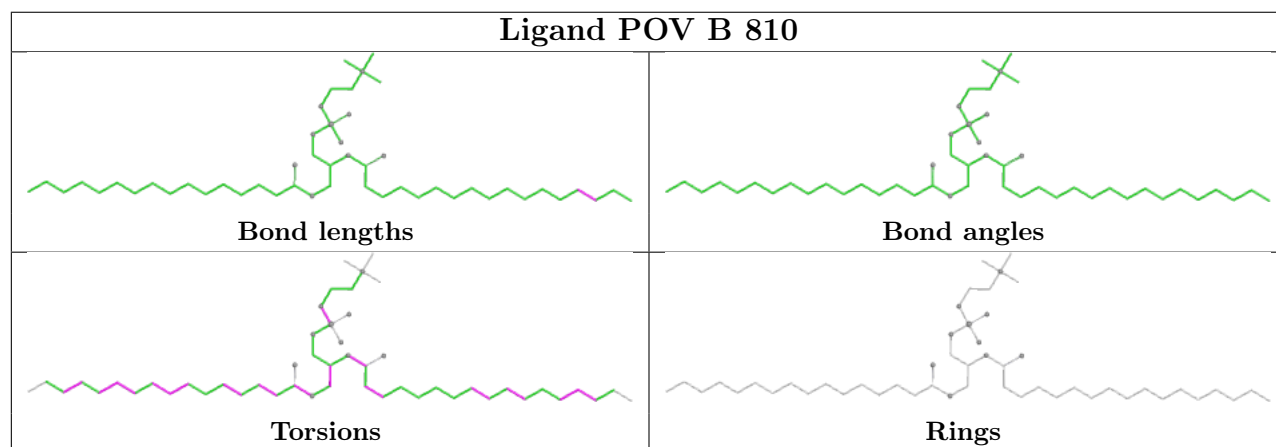
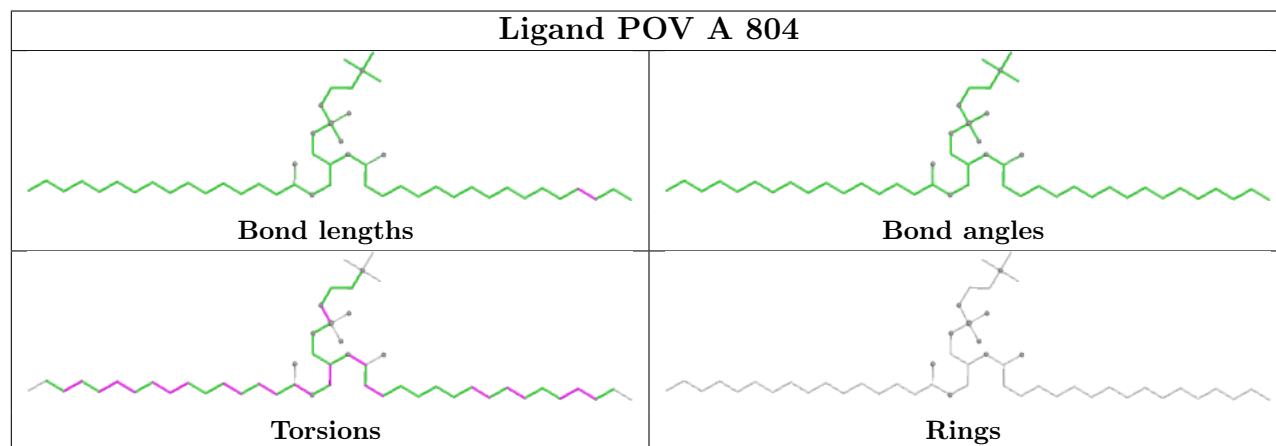
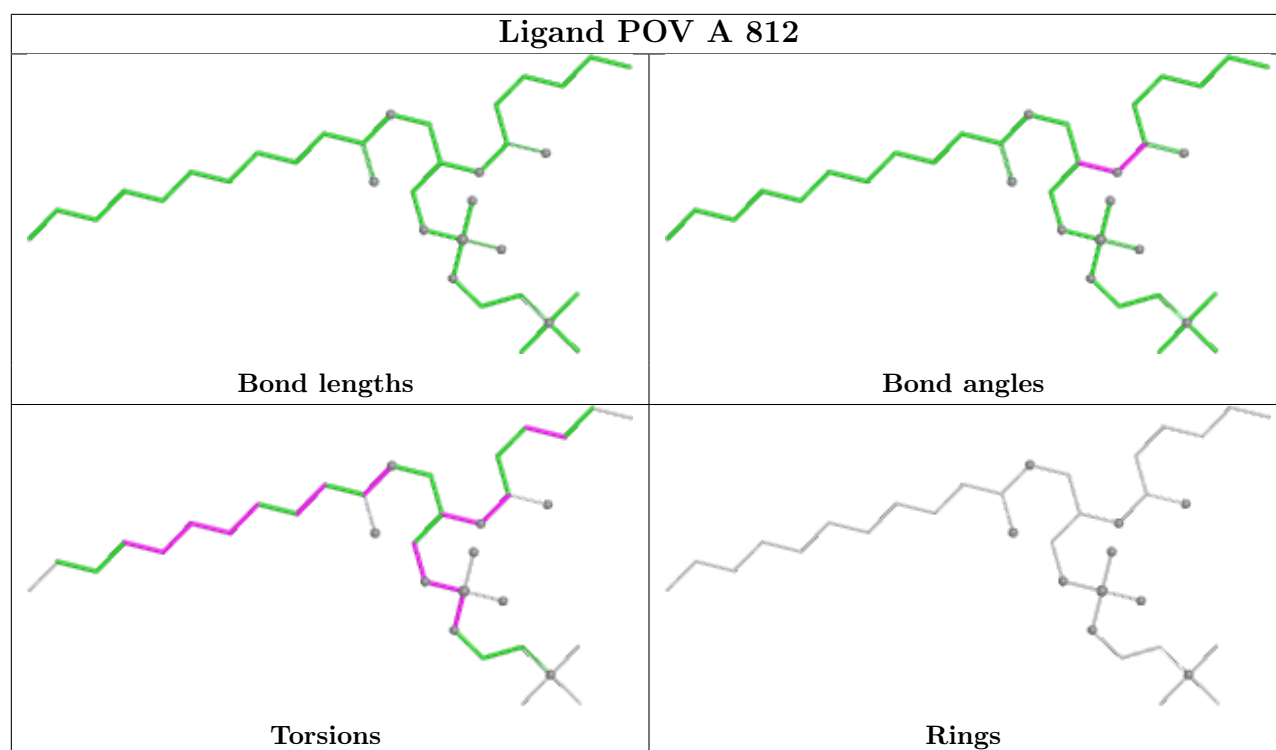
6 monomers are involved in 8 short contacts:

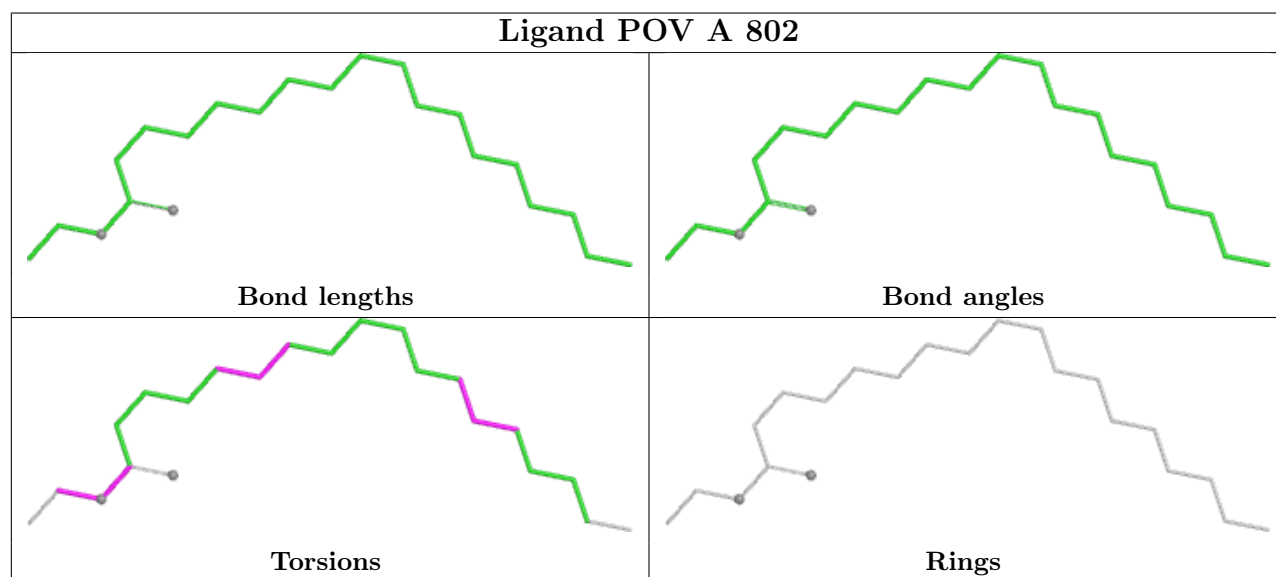
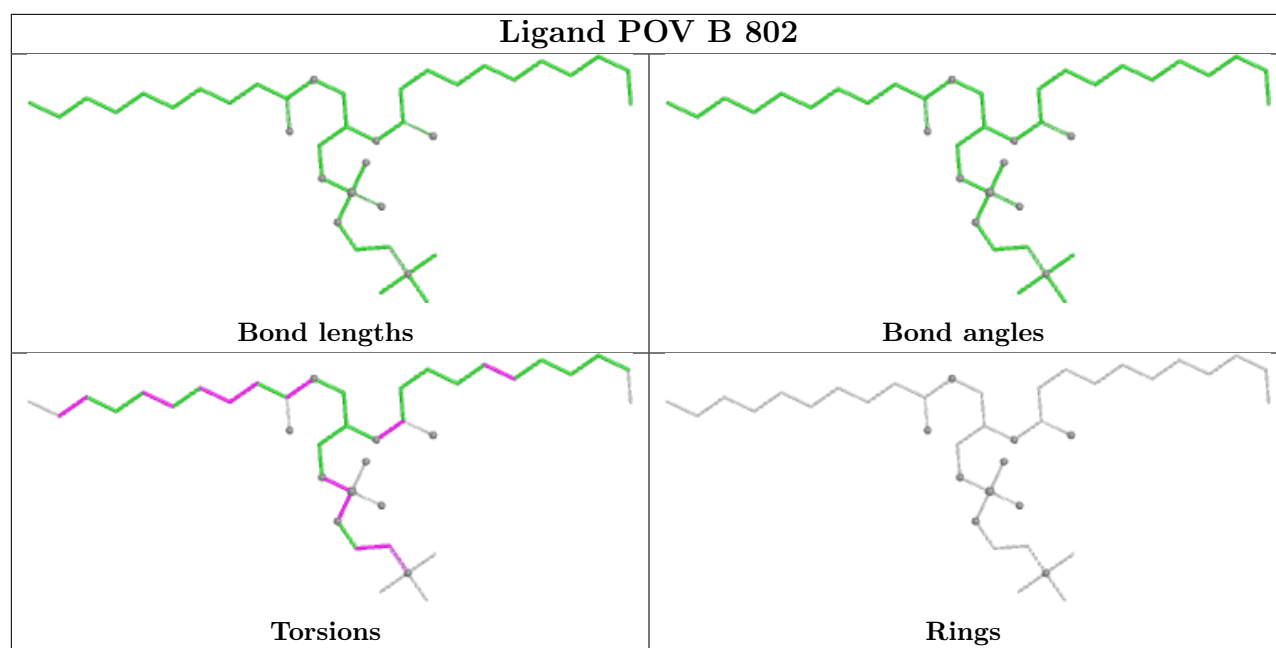
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	805	POV	2	0
2	A	812	POV	2	0
2	A	805	POV	1	0
2	A	813	POV	1	0
2	B	806	POV	1	0
2	B	811	POV	1	0

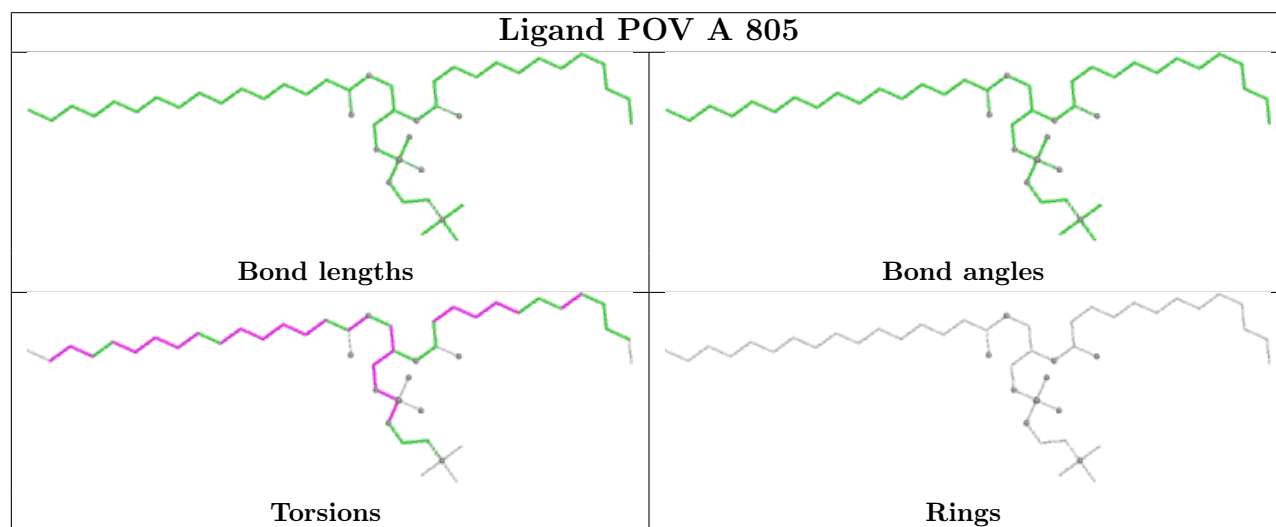
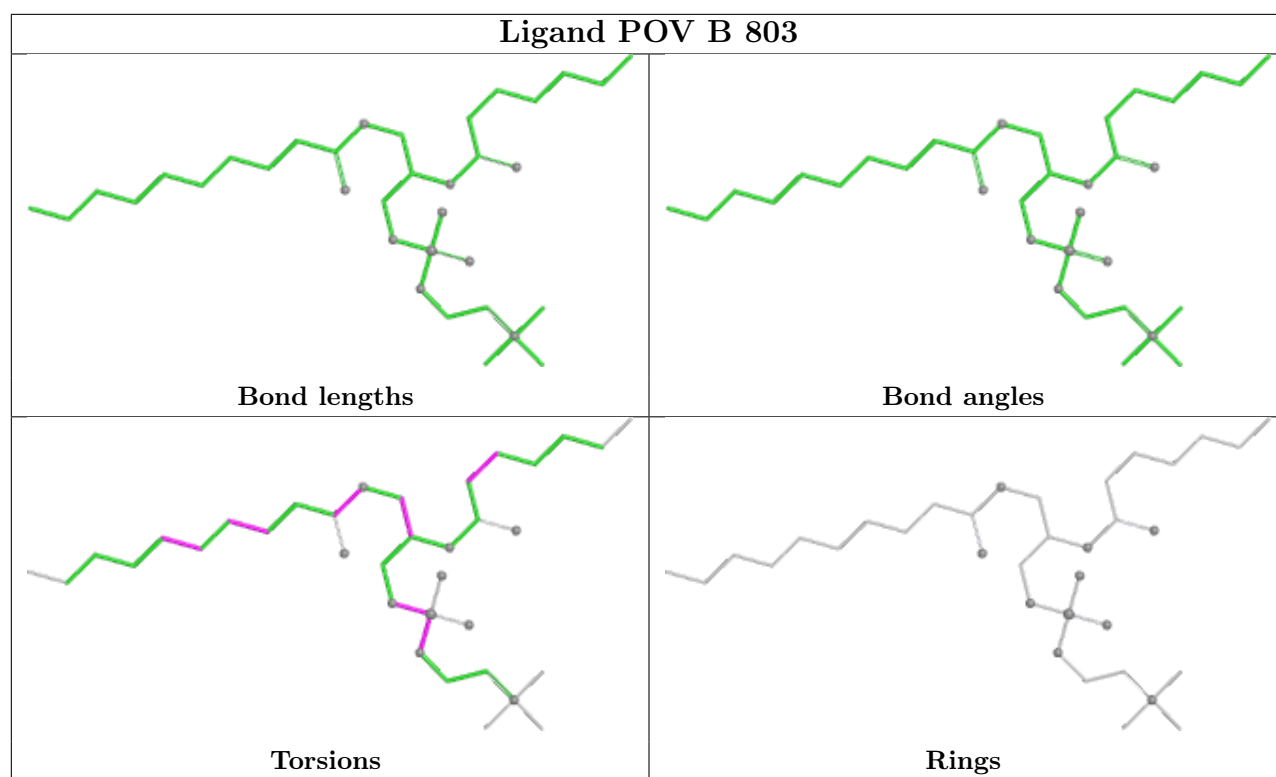
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

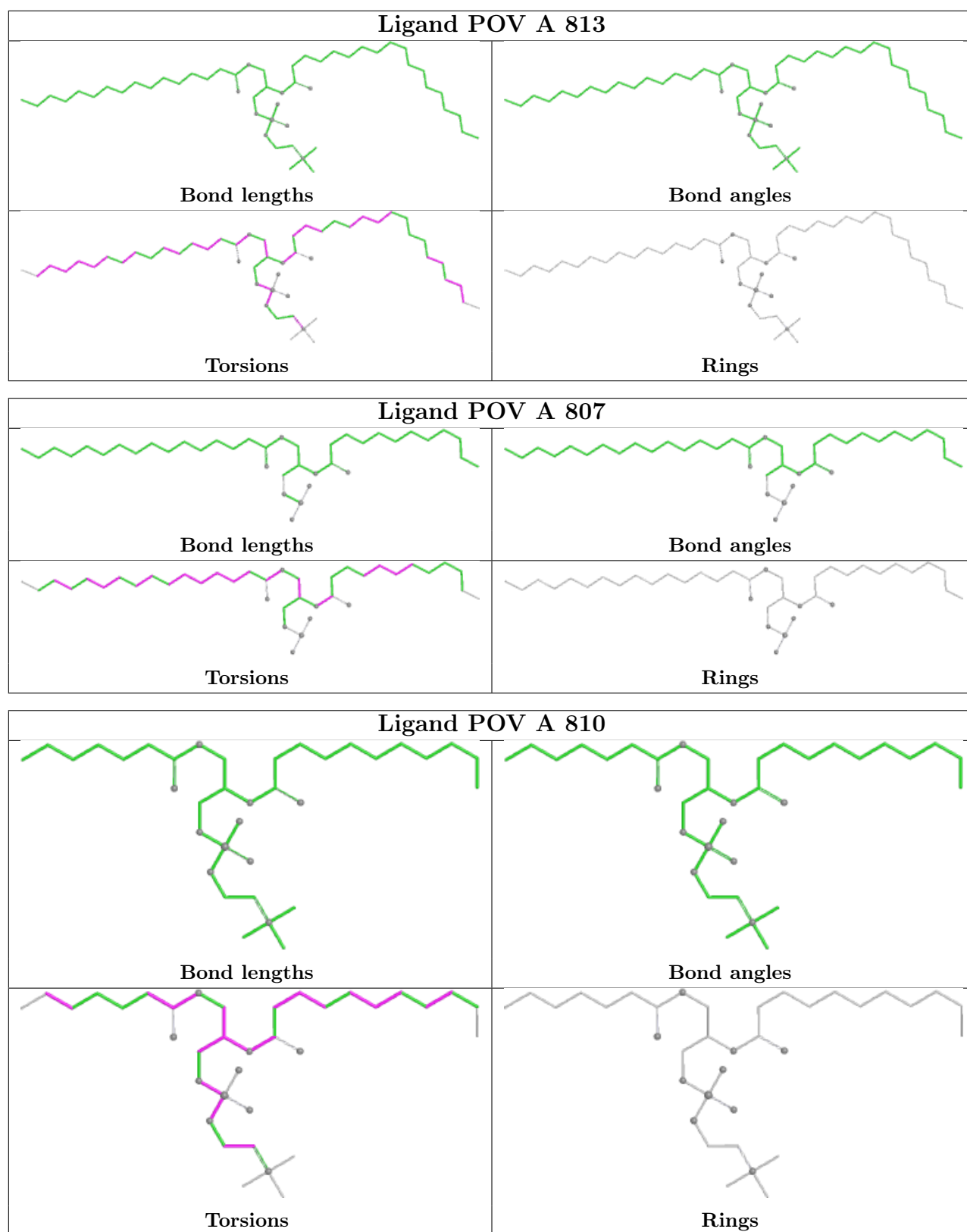


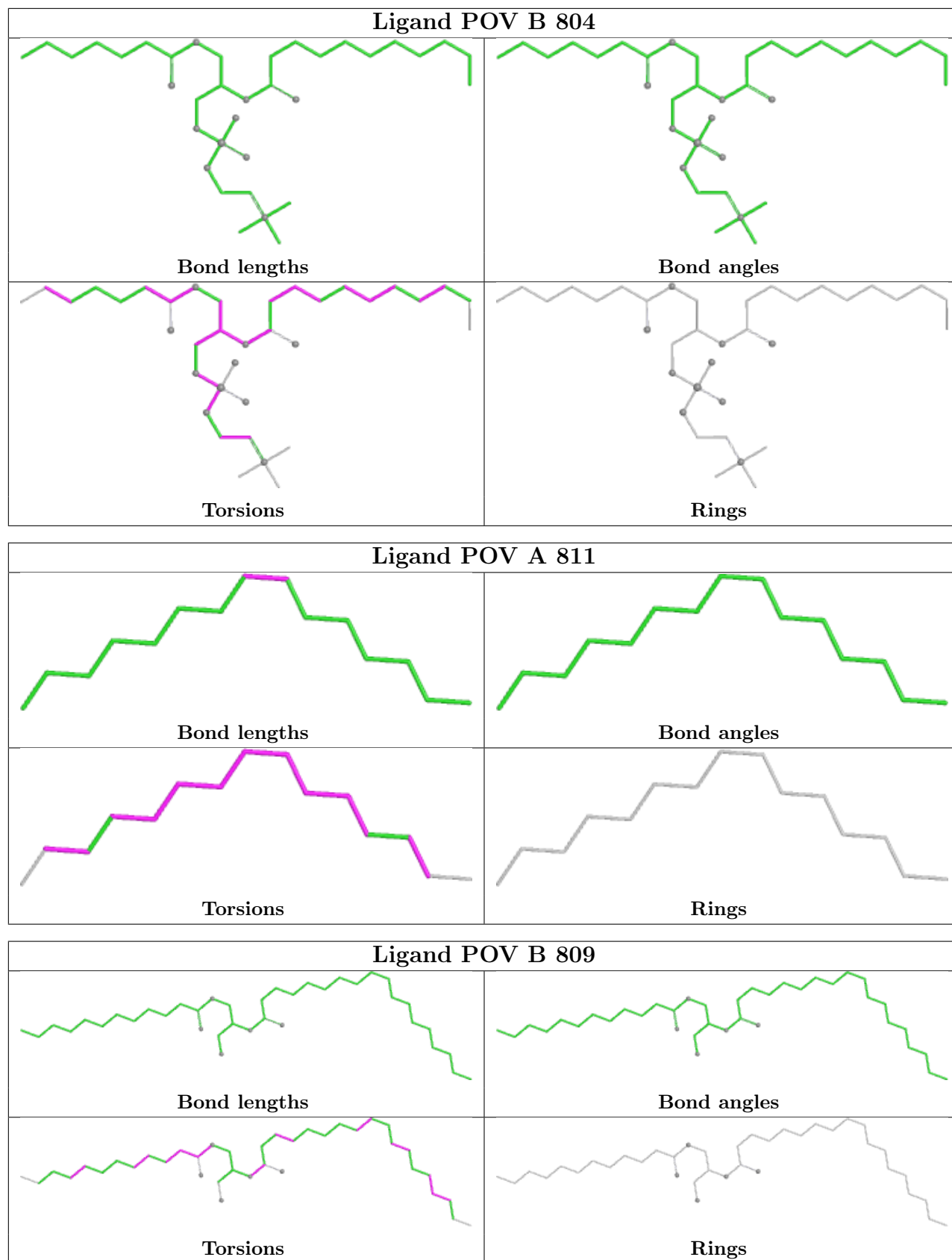


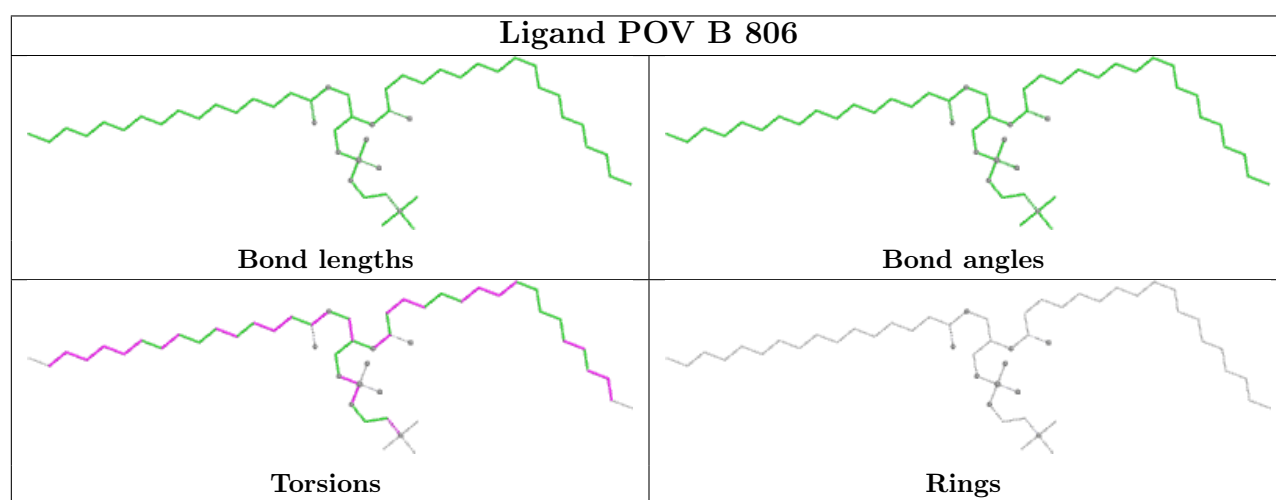
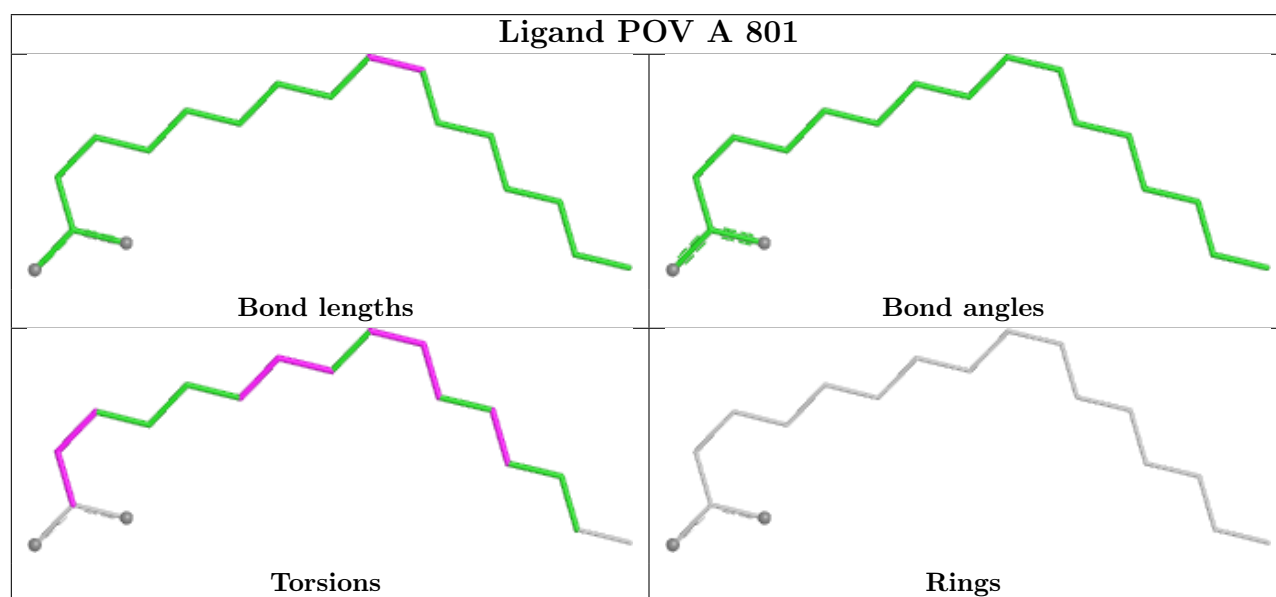
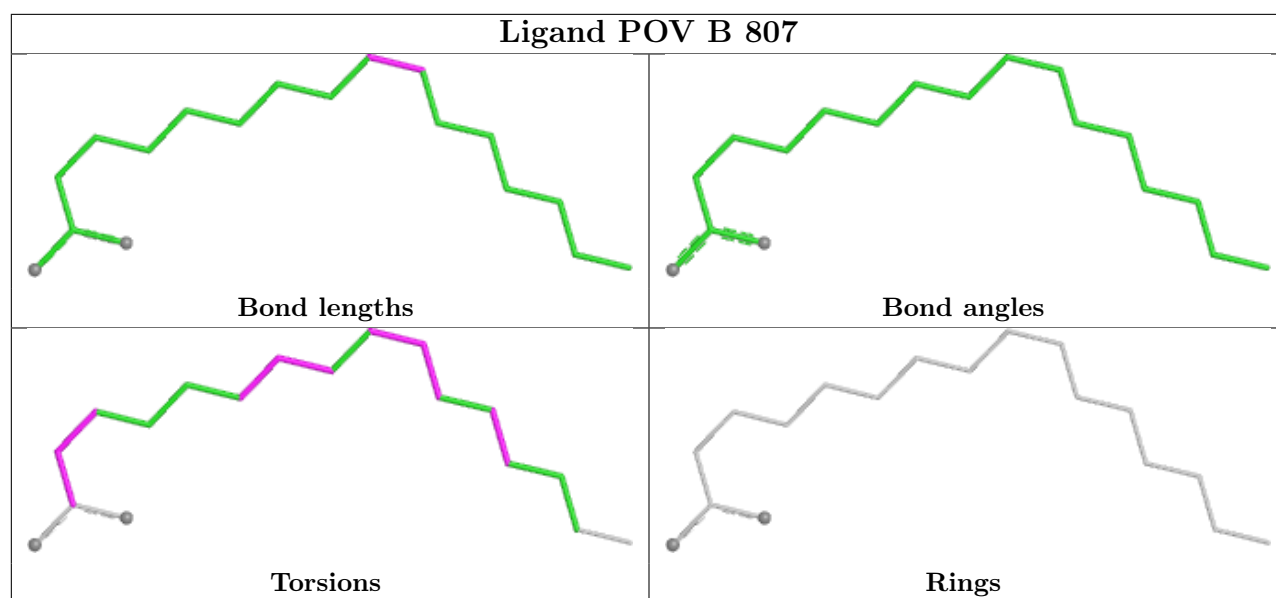


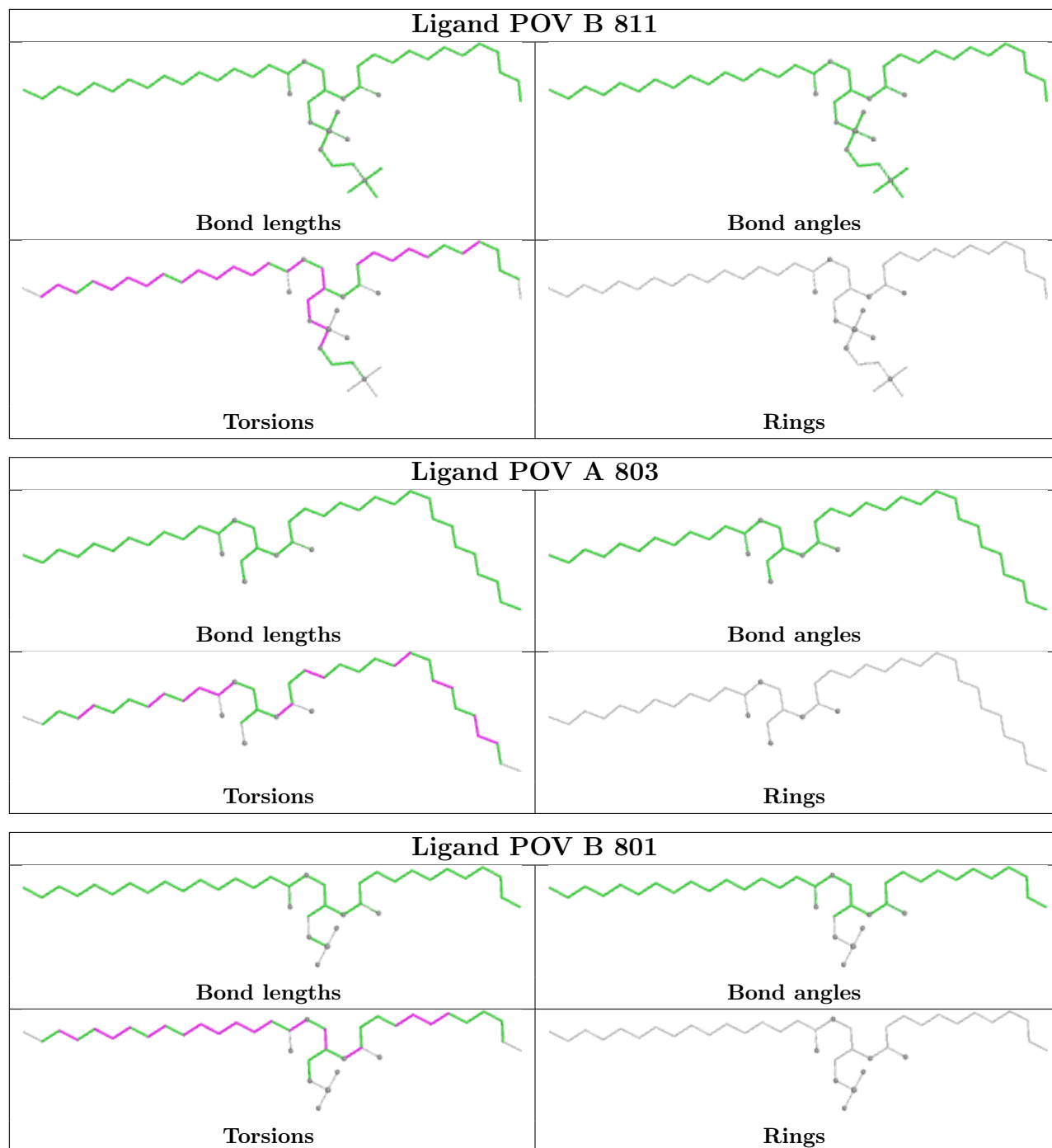


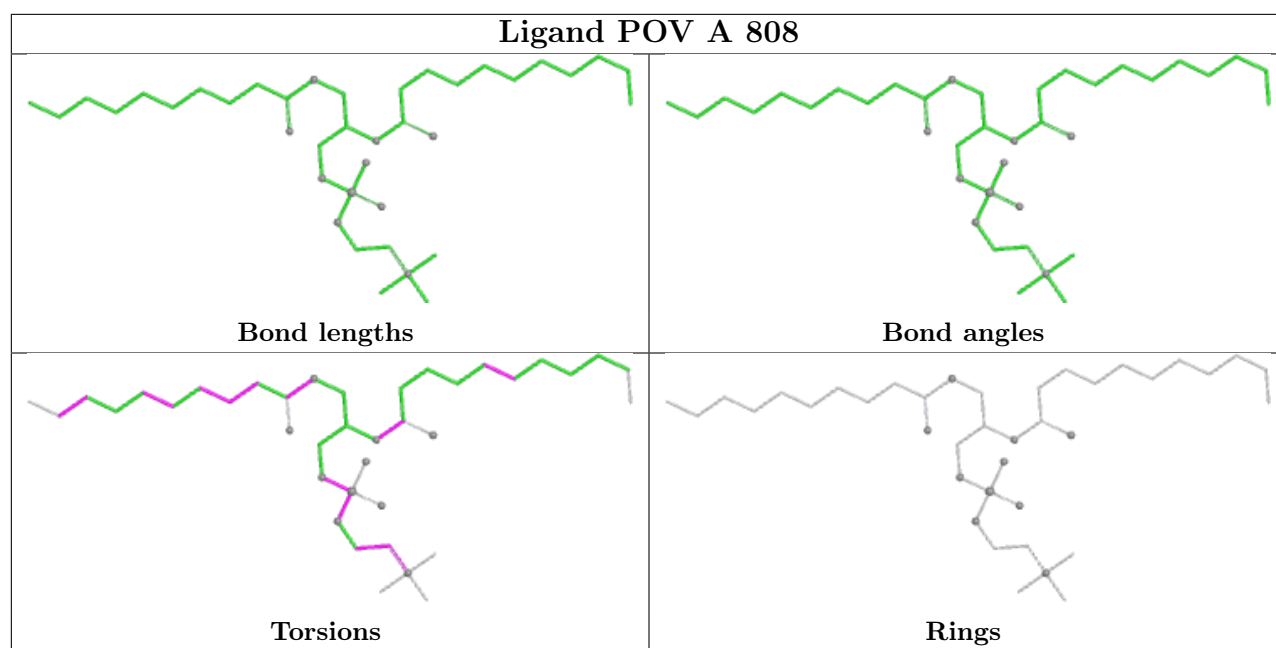












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

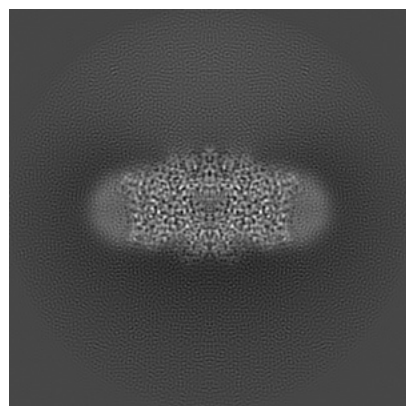
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41186. These allow visual inspection of the internal detail of the map and identification of artifacts.

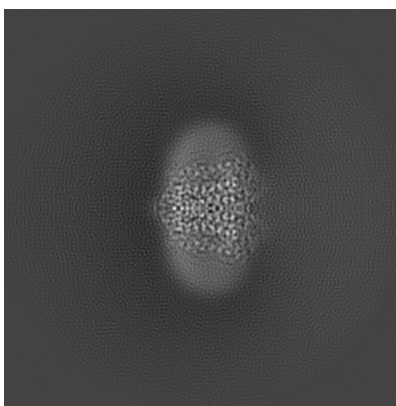
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

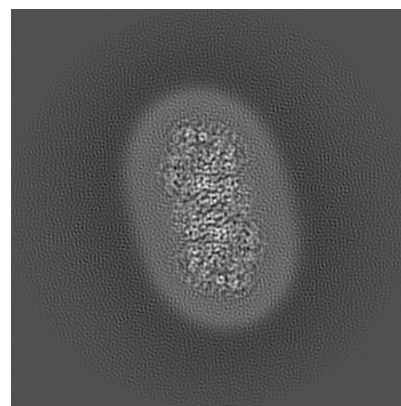
6.1.1 Primary map



X

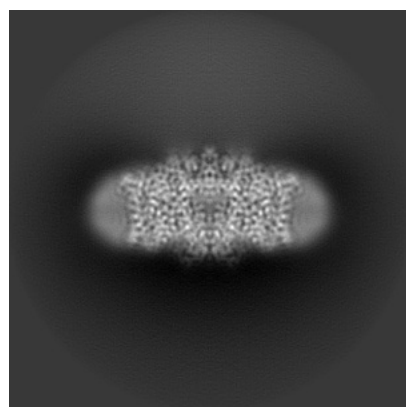


Y

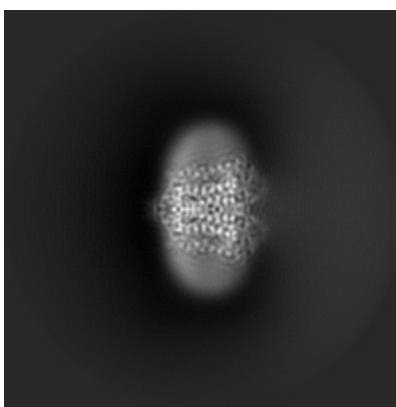


Z

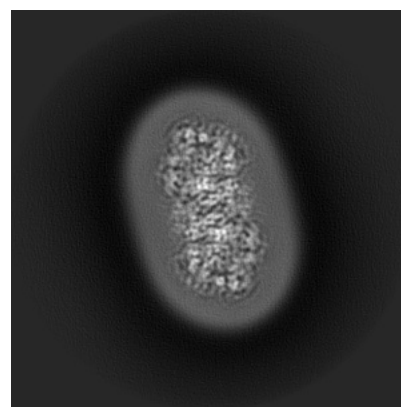
6.1.2 Raw map



X



Y

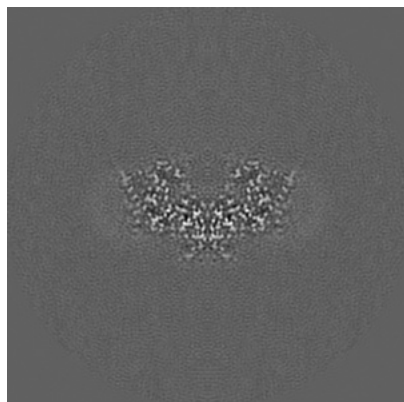


Z

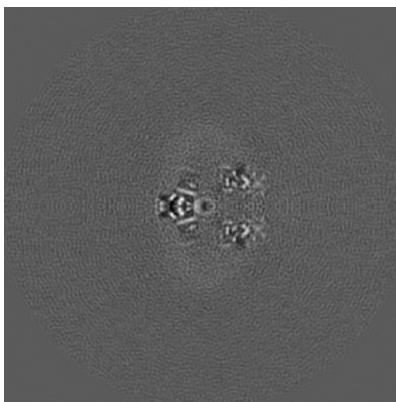
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

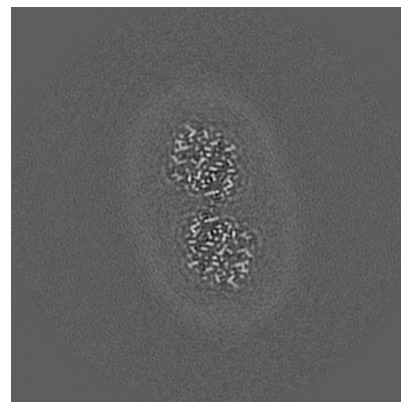
6.2.1 Primary map



X Index: 144

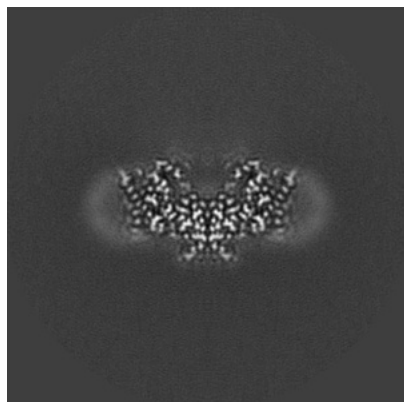


Y Index: 144

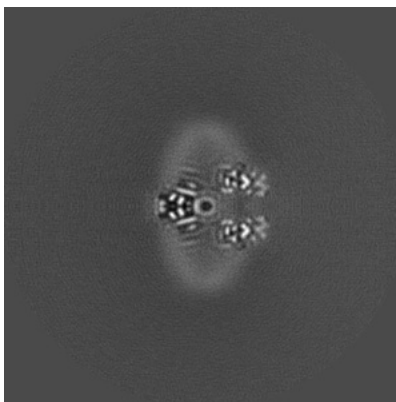


Z Index: 144

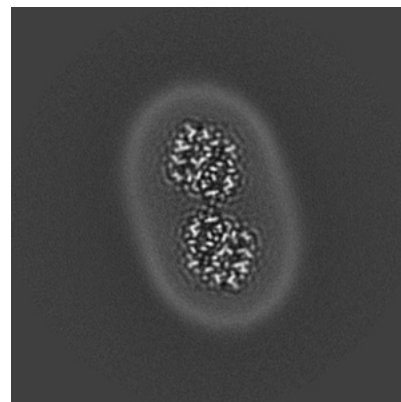
6.2.2 Raw map



X Index: 144



Y Index: 144

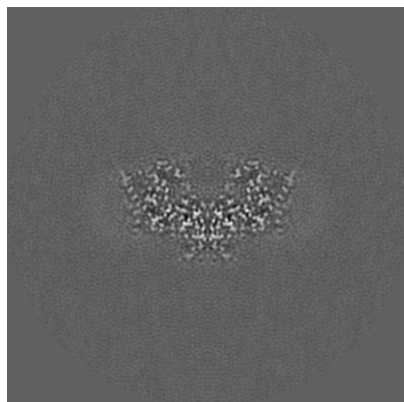


Z Index: 144

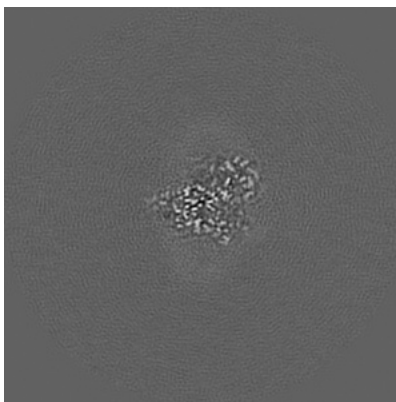
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

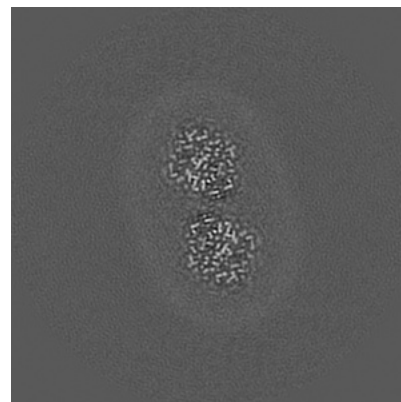
6.3.1 Primary map



X Index: 144

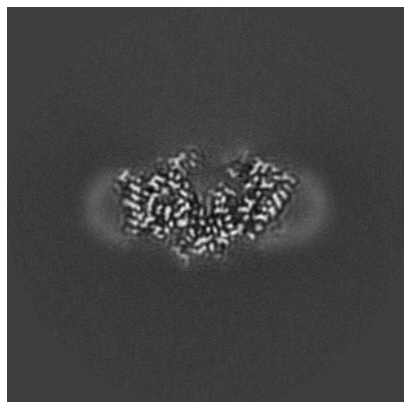


Y Index: 128

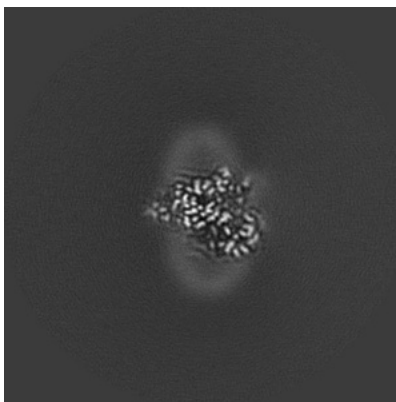


Z Index: 143

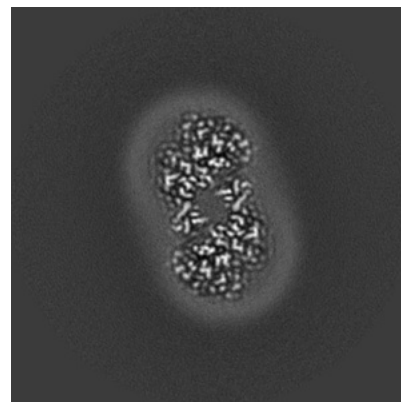
6.3.2 Raw map



X Index: 149



Y Index: 160

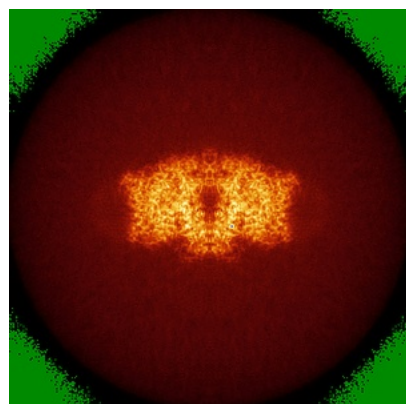


Z Index: 160

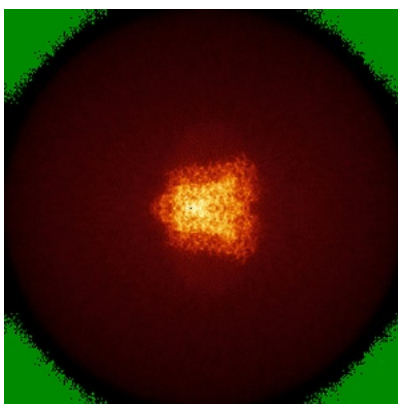
The images above show the largest variance slices of the map in three orthogonal directions.

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

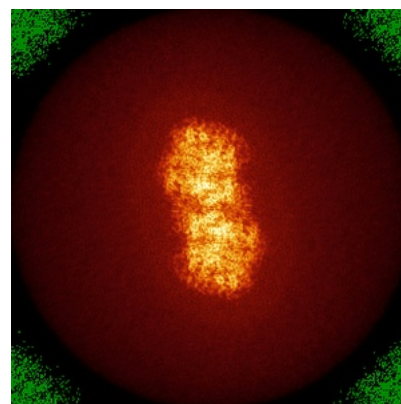
6.4.1 Primary map



X

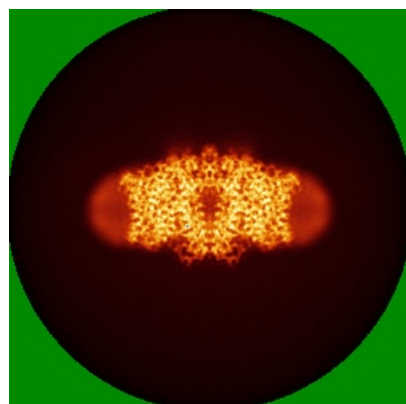


Y

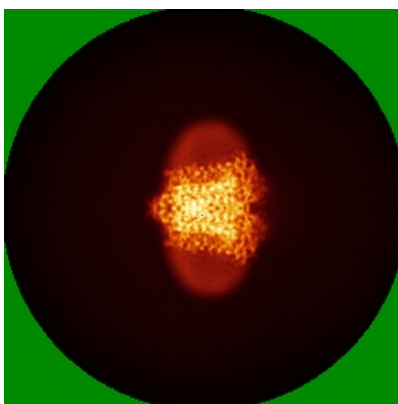


Z

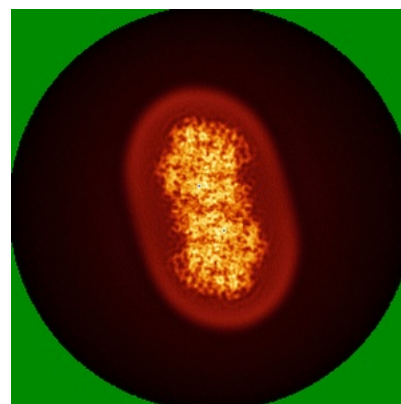
6.4.2 Raw map



X



Y

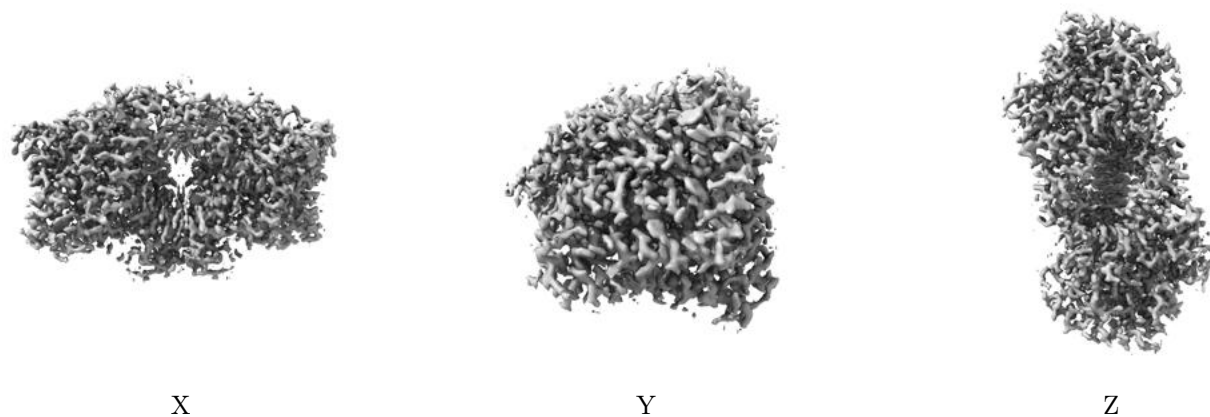


Z

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

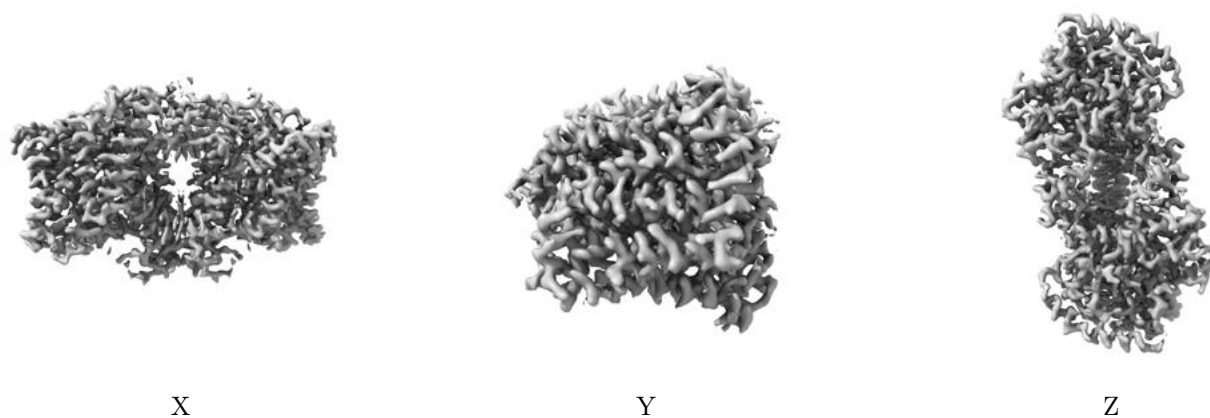
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.05. 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.

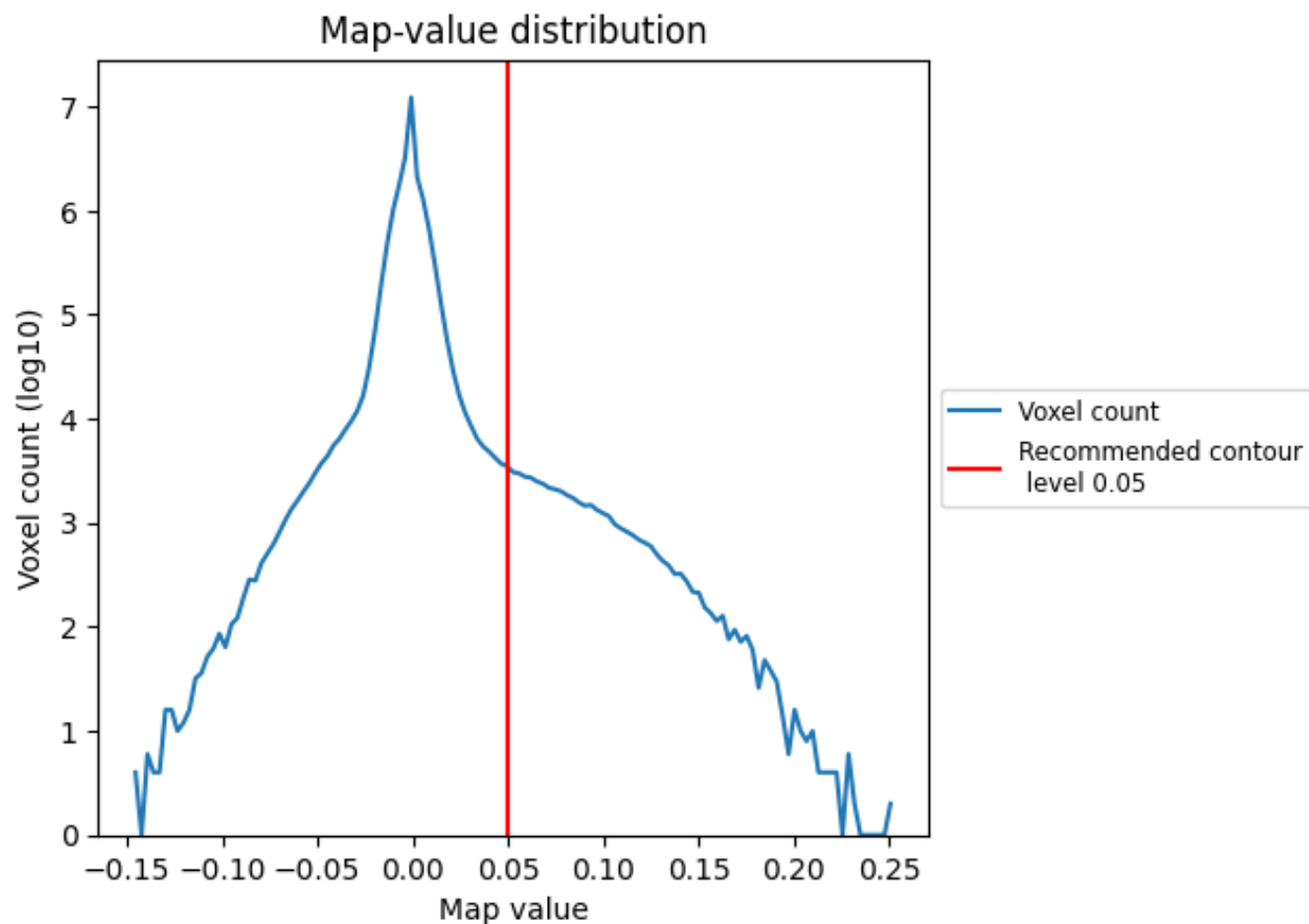
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

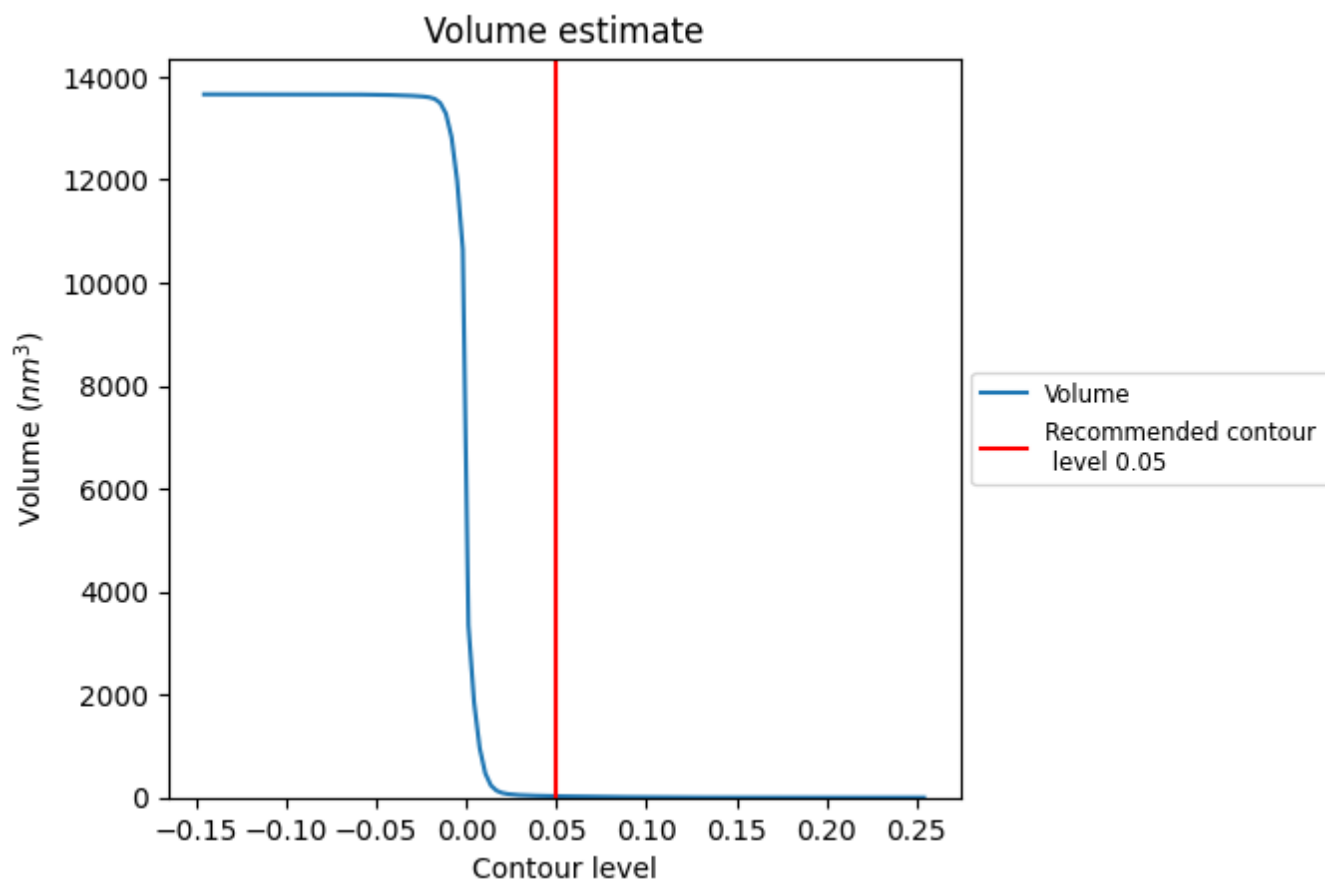
This section contains the results of statistical analysis of the map.

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.

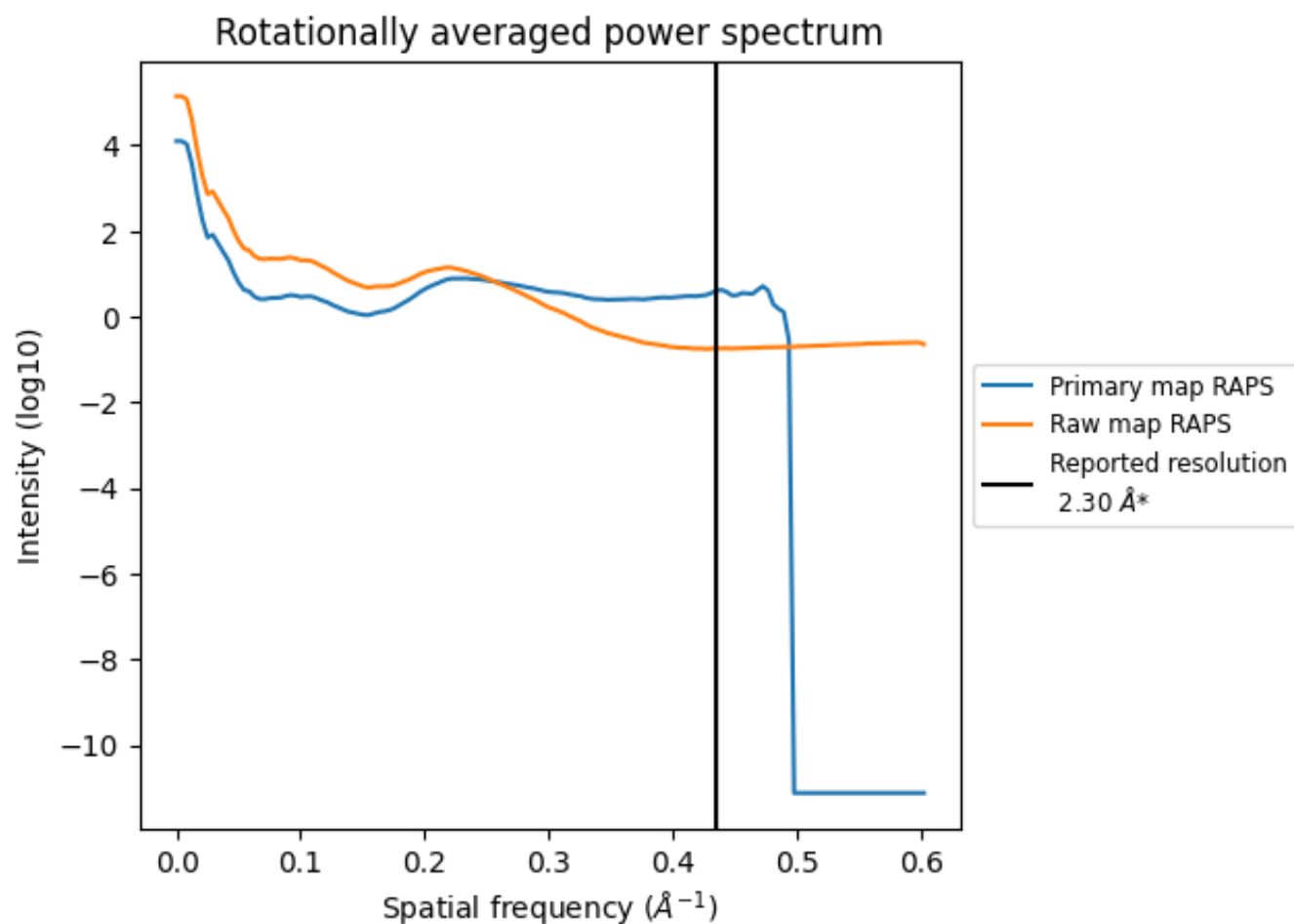
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 27 nm³; this corresponds to an approximate mass of 24 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 ⓘ

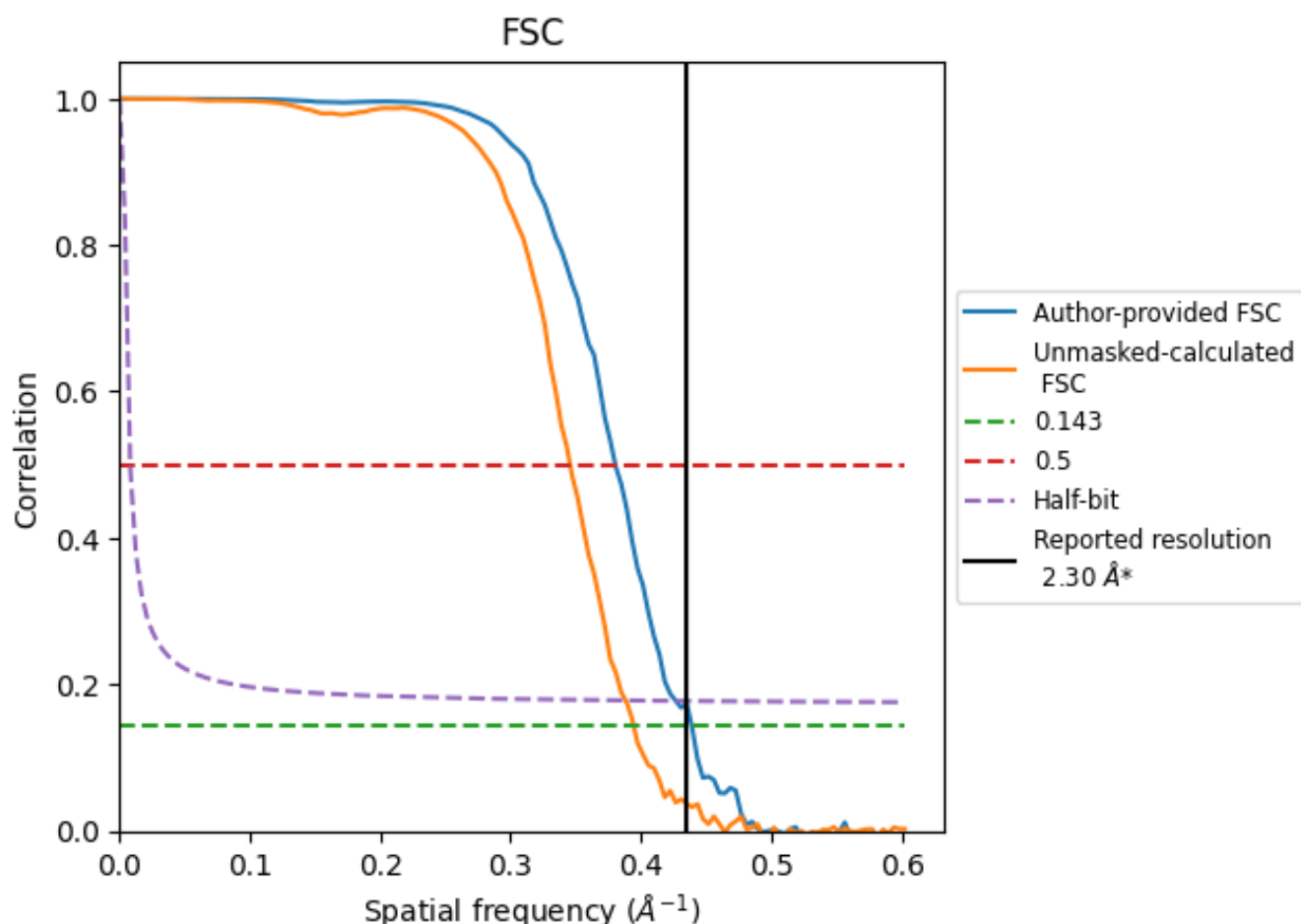


*Reported resolution corresponds to spatial frequency of 0.435 Å⁻¹

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 0.435 \AA^{-1}

8.2 Resolution estimates [i](#)

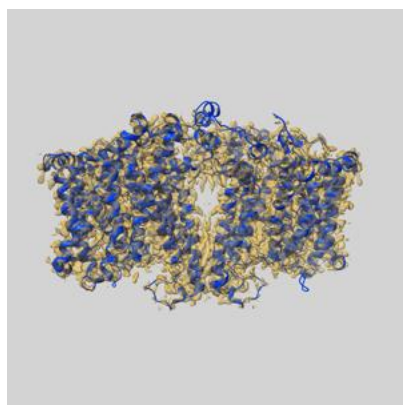
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.30	-	-
Author-provided FSC curve	2.28	2.63	2.34
Unmasked-calculated*	2.53	2.89	2.58

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

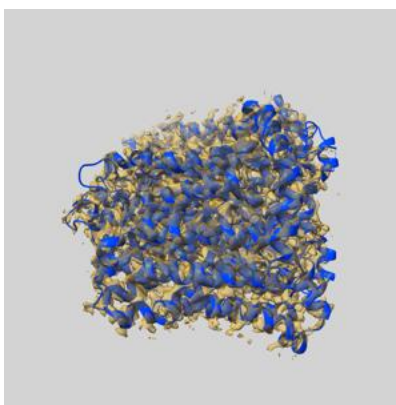
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-41186 and PDB model 8TEH. Per-residue inclusion information can be found in section 3 on page 6.

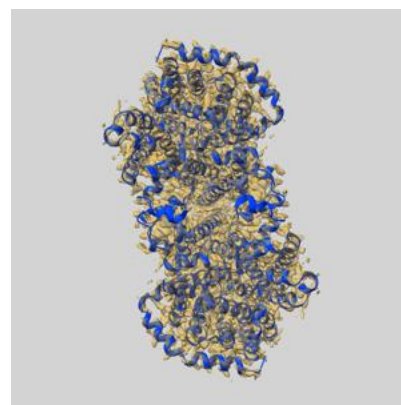
9.1 Map-model overlay [i](#)



X



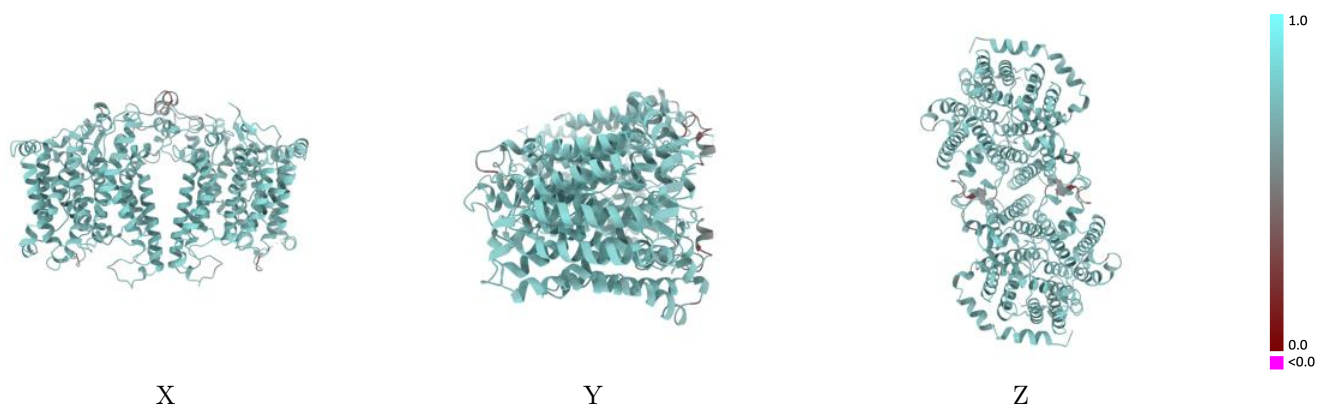
Y



Z

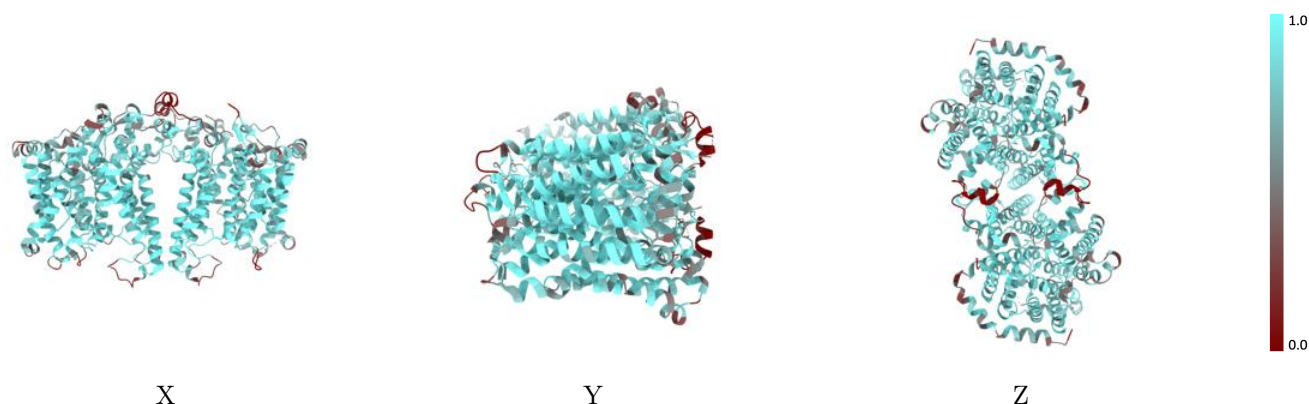
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



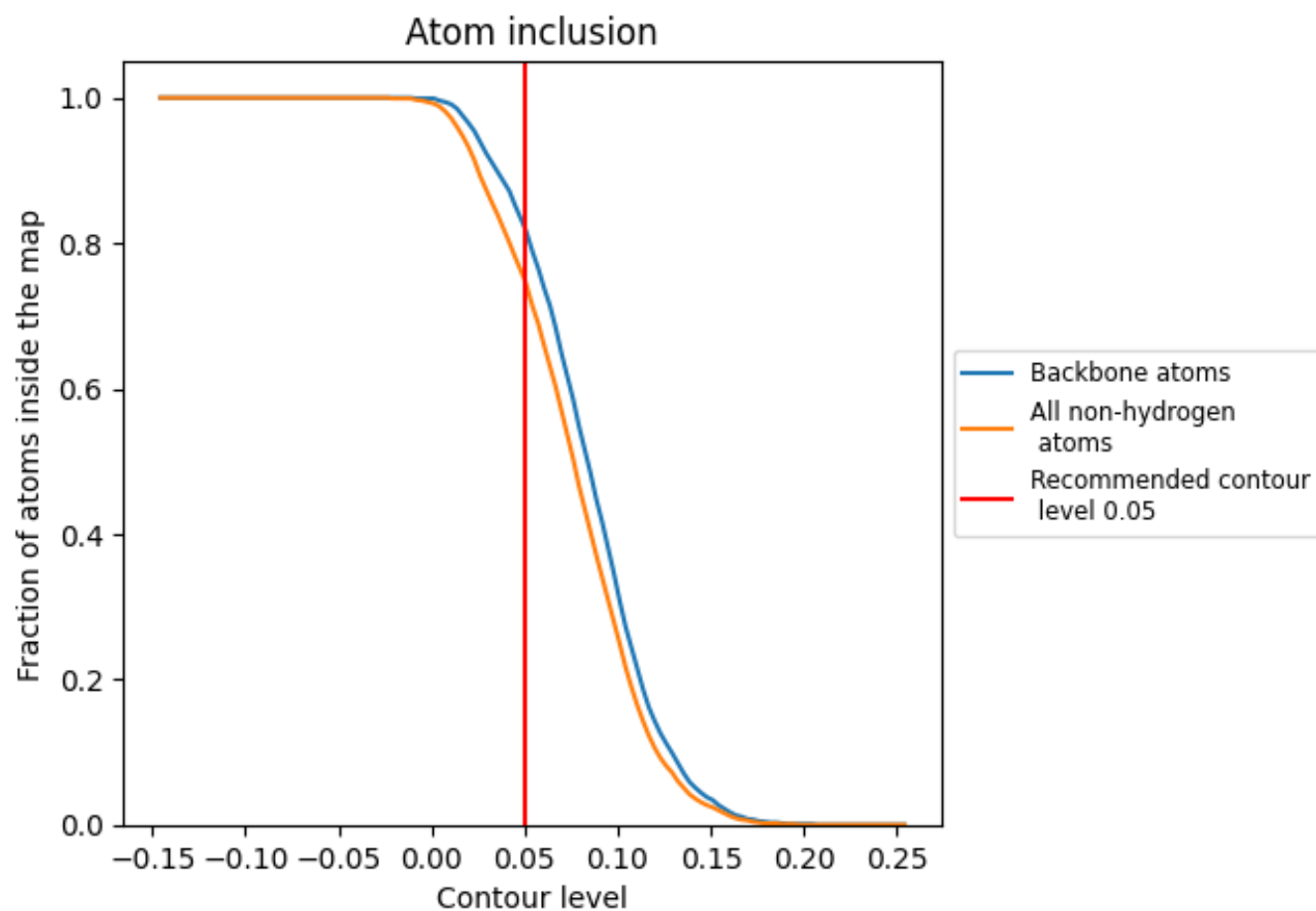
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 75% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7500	<div></div> 0.6820
A	<div></div> 0.7510	<div></div> 0.6810
B	<div></div> 0.7540	<div></div> 0.6830

