Full wwPDB EM Validation Report ⓘ

Jul 1, 2024 – 12:23 PM EDT

PDB ID	:	8TEI
EMDB ID	:	EMD-41187
Title	:	Cryo-EM structure of Arabidopsis thaliana Bor1 in lauryl maltose neopentyl glycol (LMNG)
Authors	:	Jiang, Y.; Jiang, J.
Deposited on	:	2023-07-06
Resolution	:	2.58 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

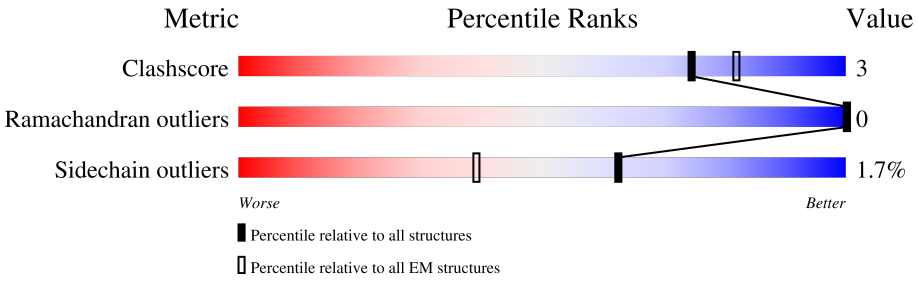
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.58 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 >=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 <=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	8% 71% 7% 22%
1	B	714	8% 71% 6% 22%

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.

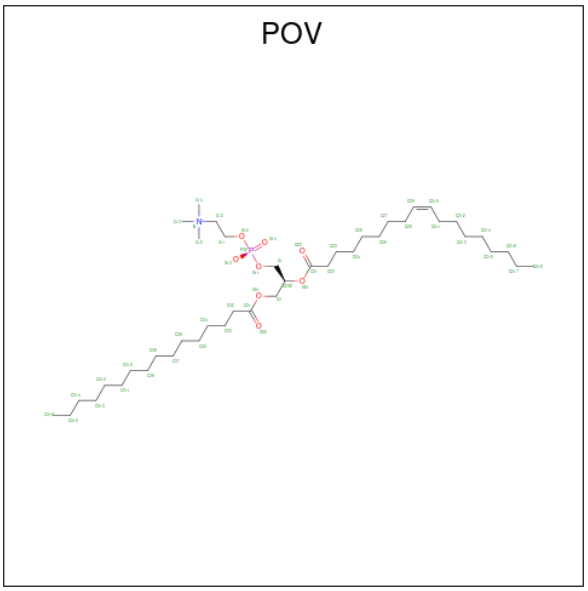
- Molecule 1 is a protein called Boron transporter 1.

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

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: $C_{42}H_{82}NO_8P$) (labeled as "Ligand of Interest" by depositor).



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

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

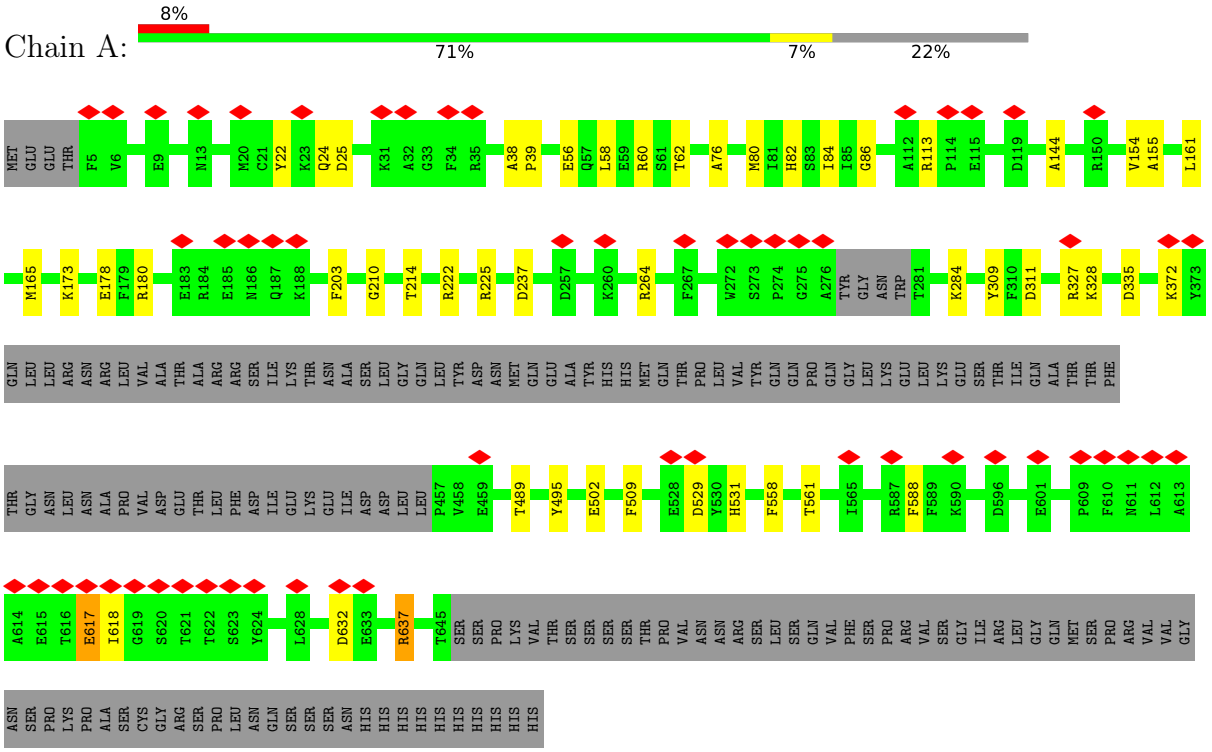
- Molecule 3 is water.

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

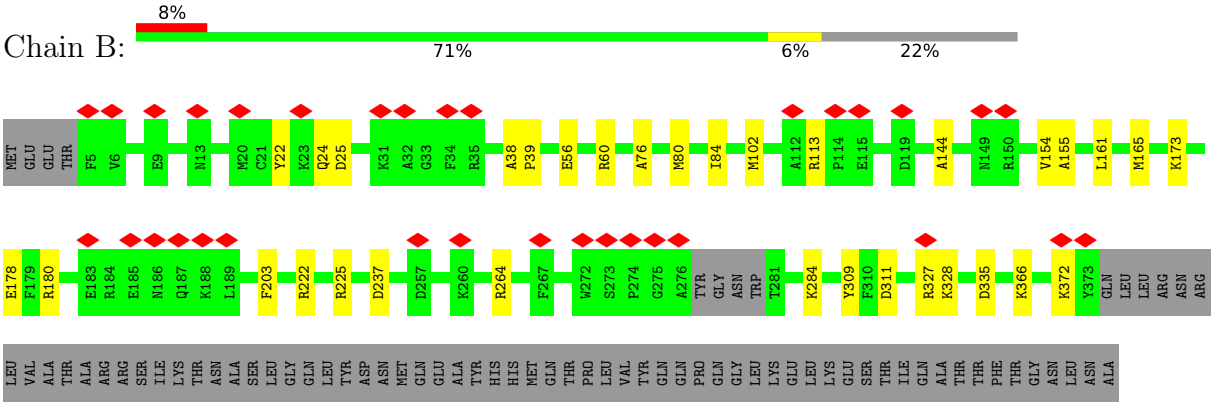
3 Residue-property plots (i)

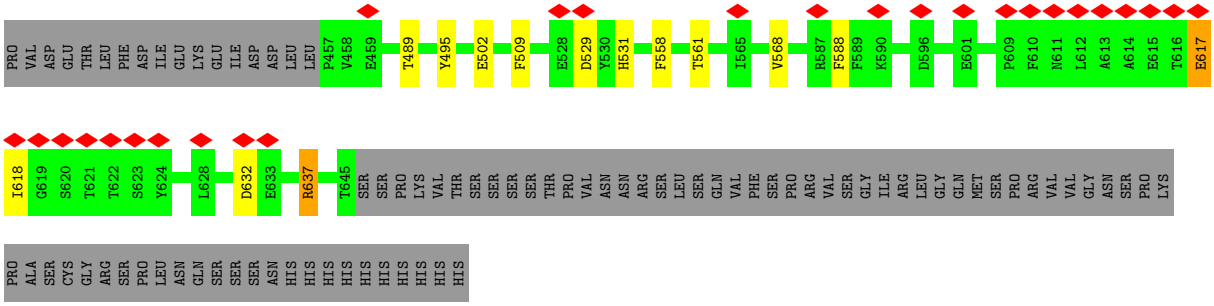
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Boron transporter 1



• Molecule 1: Boron transporter 1




PRO VAL ASP GLU THR LEU PHE ASP ILE GLU LYS GLU ILE ASP ASP LEU LEU P457 V458 E459 T489 Y495 E502 F509 E528 D529 Y530 H531 F558 T561 I565 V568 R587 F588 F589 K590 D596 E601 P609 F610 N611 L612 A613 A614 E615 T616 E617
I618 G619 S620 T621 T622 S623 Y624 L628 D632 E633 R637 T645 SER SER PRO LYS VAL THR SER SER SER SER THR PRO VAL ASN ASN ARG SER LEU SER GLN VAL PHE SER PRO ARG VAL SER GLY ILE ARG LEU GLY GLN MET SER PRO ARG VAL VAL GLY ASN SER PRO LYS
PRO ALA SER CYS GLY ARG SER PRO LEU ASN GLN SER SER SER ASN HIS HIS HIS HIS HIS HIS HIS HIS HIS HIS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	156604	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 ($e^-/Å^2$)	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	0.091	Depositor
Minimum map value	-0.052	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	265.6, 265.6, 265.6	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83000004, 0.83000004, 0.83000004	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	0.47	0/6109
1	B	0.25	0/4496	0.47	0/6109
All	All	0.25	0/8992	0.47	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	33	0
1	B	4374	0	4463	31	0
2	A	427	0	605	5	0
2	B	427	0	605	5	0
3	A	107	0	0	5	0
3	B	107	0	0	5	0
All	All	9816	0	10136	63	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 (63) 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:25:ASP:OD1	1:B:328:LYS:NZ	2.12	0.82
1:A:25:ASP:OD1	1:A:328:LYS:NZ	2.12	0.81
1:B:558:PHE:O	1:B:561:THR:OG1	2.03	0.75
1:A:558:PHE:O	1:A:561:THR:OG1	2.03	0.74
1:A:311:ASP:OD2	3:A:901:HOH:O	2.05	0.74
1:B:311:ASP:OD2	3:B:901:HOH:O	2.05	0.72
1:A:144:ALA:O	1:A:309:TYR:OH	2.12	0.68
1:A:502:GLU:OE2	1:B:637:ARG:NH1	2.27	0.67
1:A:60:ARG:HH22	1:A:489:THR:HG21	1.60	0.67
1:B:60:ARG:HH22	1:B:489:THR:HG21	1.60	0.67
1:B:144:ALA:O	1:B:309:TYR:OH	2.12	0.66
1:B:180:ARG:NE	2:B:807:POV:O22	2.31	0.64
1:A:637:ARG:NH1	1:B:502:GLU:OE2	2.31	0.64
1:A:180:ARG:NE	2:A:812:POV:O22	2.31	0.63
1:B:178:GLU:OE2	1:B:489:THR:OG1	2.19	0.60
1:B:495:TYR:OH	3:B:902:HOH:O	2.10	0.60
1:A:178:GLU:OE2	1:A:489:THR:OG1	2.19	0.58
1:B:25:ASP:OD2	3:B:903:HOH:O	2.17	0.58
1:A:25:ASP:OD2	3:A:903:HOH:O	2.17	0.57
1:A:222:ARG:NH1	1:B:632:ASP:OD2	2.39	0.56
1:B:335:ASP:OD2	3:B:904:HOH:O	2.18	0.55
1:A:632:ASP:OD2	1:B:222:ARG:NH1	2.41	0.54
1:A:335:ASP:OD2	3:A:904:HOH:O	2.19	0.53
1:A:22:TYR:OH	1:A:84:ILE:O	2.14	0.52
1:B:173:LYS:HG3	2:B:806:POV:H13B	1.91	0.52
1:A:173:LYS:HG3	2:A:811:POV:H13B	1.90	0.52
1:B:222:ARG:NH2	1:B:237:ASP:OD2	2.42	0.52
2:A:805:POV:P	2:A:805:POV:H14B	2.52	0.50
1:A:180:ARG:O	1:A:264:ARG:NH2	2.41	0.50
1:B:180:ARG:O	1:B:264:ARG:NH2	2.41	0.49
1:A:58:LEU:O	1:A:62:THR:OG1	2.25	0.49
1:B:161:LEU:O	1:B:165:MET:HG3	2.13	0.49
2:B:812:POV:P	2:B:812:POV:H14B	2.52	0.49
1:A:495:TYR:OH	3:A:902:HOH:O	2.10	0.49
1:A:161:LEU:O	1:A:165:MET:HG3	2.13	0.48
1:A:222:ARG:NH2	1:A:237:ASP:OD2	2.42	0.48
1:B:22:TYR:OH	1:B:84:ILE:O	2.14	0.48
1:A:632:ASP:OD1	1:B:366:LYS:NZ	2.30	0.48
1:B:38:ALA:HB3	1:B:39:PRO:HD3	1.96	0.48
1:A:173:LYS:HG2	2:A:811:POV:H15A	1.97	0.47
1:A:38:ALA:HB3	1:A:39:PRO:HD3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:173:LYS:HG2	2:B:806:POV:H15A	1.97	0.47
1:B:225:ARG:NH2	3:B:911:HOH:O	2.38	0.47
1:A:154:VAL:HG13	1:A:155:ALA:N	2.31	0.46
1:A:225:ARG:NH2	3:A:911:HOH:O	2.38	0.45
1:B:154:VAL:HG13	1:B:155:ALA:N	2.31	0.45
1:B:102:MET:HE1	1:B:568:VAL:HG22	2.00	0.44
1:B:588:PHE:N	1:B:588:PHE:CD2	2.86	0.44
1:A:56:GLU:OE1	1:A:60:ARG:NH1	2.51	0.43
1:A:588:PHE:N	1:A:588:PHE:CD2	2.86	0.43
1:A:76:ALA:O	1:A:80:MET:HG3	2.19	0.42
1:A:161:LEU:HD12	1:A:509:PHE:CD2	2.54	0.42
1:B:56:GLU:OE1	1:B:60:ARG:NH1	2.51	0.42
1:A:210:GLY:O	1:A:214:THR:OG1	2.29	0.42
1:A:529:ASP:O	1:A:531:HIS:ND1	2.53	0.42
1:B:529:ASP:O	1:B:531:HIS:ND1	2.53	0.42
1:A:82:HIS:O	1:A:86:GLY:N	2.51	0.42
1:B:161:LEU:HD12	1:B:509:PHE:CD2	2.54	0.42
2:B:806:POV:H13A	2:B:806:POV:O12	2.21	0.41
1:B:76:ALA:O	1:B:80:MET:HG3	2.19	0.41
1:B:617:GLU:OE1	1:B:618:ILE:N	2.54	0.41
2:A:811:POV:H13A	2:A:811:POV:O12	2.21	0.41
1:A:617:GLU:OE1	1:A:618:ILE:N	2.54	0.41

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	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 (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	468/613 (76%)	460 (98%)	8 (2%)	60	79
1	B	468/613 (76%)	460 (98%)	8 (2%)	60	79
All	All	936/1226 (76%)	920 (98%)	16 (2%)	62	79

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	113	ARG
1	A	203	PHE
1	A	284	LYS
1	A	327	ARG
1	A	372	LYS
1	A	617	GLU
1	A	637	ARG
1	B	24	GLN
1	B	113	ARG
1	B	203	PHE
1	B	284	LYS
1	B	327	ARG
1	B	372	LYS
1	B	617	GLU
1	B	637	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	595	GLN
1	B	24	GLN
1	B	595	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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	B	801	-	36,38,51	0.46	0	36,41,59	0.36	0
2	POV	B	810	-	37,37,51	0.41	0	39,39,59	0.39	0
2	POV	A	803	-	37,37,51	0.41	0	39,39,59	0.39	0
2	POV	B	812	-	46,46,51	0.53	0	52,54,59	0.51	0
2	POV	A	808	-	34,34,51	0.59	0	40,42,59	0.58	0
2	POV	A	809	-	35,35,51	0.59	0	41,43,59	0.56	0
2	POV	B	806	-	34,34,51	0.59	0	40,42,59	0.52	0
2	POV	A	802	-	21,21,51	0.37	0	21,21,59	0.38	0
2	POV	A	805	-	46,46,51	0.52	0	52,54,59	0.51	0
2	POV	B	811	-	50,50,51	4.46	1 (2%)	56,58,59	0.57	1 (1%)
2	POV	B	808	-	17,17,51	0.93	1 (5%)	17,17,59	0.62	0
2	POV	B	807	-	51,51,51	0.50	0	57,59,59	0.47	0
2	POV	B	803	-	34,34,51	0.59	0	40,42,59	0.58	0
2	POV	A	807	-	38,38,51	0.57	0	44,46,59	0.52	0
2	POV	B	809	-	21,21,51	0.37	0	21,21,59	0.38	0
2	POV	A	804	-	50,50,51	4.46	1 (2%)	56,58,59	0.57	1 (1%)
2	POV	B	802	-	38,38,51	0.57	0	44,46,59	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	POV	A	801	-	17,17,51	0.93	1 (5%)	17,17,59	0.61	0
2	POV	A	812	-	51,51,51	0.50	0	57,59,59	0.47	0
2	POV	B	805	-	14,14,51	1.01	1 (7%)	13,13,59	0.56	0
2	POV	A	811	-	34,34,51	0.59	0	40,42,59	0.53	0
2	POV	A	810	-	14,14,51	1.01	1 (7%)	13,13,59	0.56	0
2	POV	B	804	-	35,35,51	0.59	0	41,43,59	0.56	0
2	POV	A	806	-	36,38,51	0.46	0	36,41,59	0.36	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	B	801	-	-	15/38/40/55	-
2	POV	B	810	-	-	18/39/39/55	-
2	POV	A	803	-	-	18/39/39/55	-
2	POV	B	812	-	-	27/50/50/55	-
2	POV	A	808	-	-	12/38/38/55	-
2	POV	A	809	-	-	18/39/39/55	-
2	POV	B	806	-	-	12/38/38/55	-
2	POV	A	802	-	-	3/20/20/55	-
2	POV	A	805	-	-	27/50/50/55	-
2	POV	B	811	-	-	18/54/54/55	-
2	POV	B	808	-	-	9/15/15/55	-
2	POV	B	807	-	-	32/55/55/55	-
2	POV	B	803	-	-	12/38/38/55	-
2	POV	A	807	-	-	14/42/42/55	-
2	POV	B	809	-	-	3/20/20/55	-
2	POV	A	804	-	-	18/54/54/55	-
2	POV	B	802	-	-	14/42/42/55	-
2	POV	A	801	-	-	9/15/15/55	-
2	POV	A	812	-	-	32/55/55/55	-
2	POV	B	805	-	-	6/12/12/55	-
2	POV	A	811	-	-	12/38/38/55	-
2	POV	A	810	-	-	6/12/12/55	-
2	POV	B	804	-	-	18/39/39/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	POV	A	806	-	-	15/38/40/55	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	804	POV	C215-C214	31.35	3.27	1.51
2	B	811	POV	C215-C214	31.33	3.27	1.51
2	A	810	POV	C29-C210	3.66	1.53	1.31
2	B	805	POV	C29-C210	3.66	1.53	1.31
2	A	801	POV	C29-C210	3.64	1.52	1.31
2	B	808	POV	C29-C210	3.64	1.52	1.31

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	804	POV	C215-C214-C213	-2.09	103.81	114.42
2	B	811	POV	C215-C214-C213	-2.09	103.83	114.42

There are no chirality outliers.

All (368) 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
2	A	805	POV	C11-O12-P-O13
2	A	806	POV	C22-C21-O21-C2
2	A	807	POV	O12-C11-C12-N
2	A	807	POV	C22-C21-O21-C2
2	A	808	POV	C1-O11-P-O13
2	A	808	POV	C1-O11-P-O14
2	A	809	POV	C1-O11-P-O12
2	A	809	POV	C1-O11-P-O14
2	A	809	POV	C11-O12-P-O14
2	A	811	POV	C1-O11-P-O13
2	A	811	POV	C11-O12-P-O14
2	A	812	POV	C1-O11-P-O12
2	A	812	POV	C1-O11-P-O13
2	A	812	POV	C1-O11-P-O14
2	A	812	POV	C11-O12-P-O14
2	A	812	POV	O22-C21-O21-C2
2	B	801	POV	C22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
2	B	802	POV	O12-C11-C12-N
2	B	802	POV	C22-C21-O21-C2
2	B	803	POV	C1-O11-P-O13
2	B	803	POV	C1-O11-P-O14
2	B	804	POV	C1-O11-P-O12
2	B	804	POV	C1-O11-P-O14
2	B	804	POV	C11-O12-P-O14
2	B	806	POV	C1-O11-P-O13
2	B	806	POV	C11-O12-P-O14
2	B	807	POV	C1-O11-P-O12
2	B	807	POV	C1-O11-P-O13
2	B	807	POV	C1-O11-P-O14
2	B	807	POV	C11-O12-P-O14
2	B	807	POV	O22-C21-O21-C2
2	B	810	POV	C22-C21-O21-C2
2	B	811	POV	C11-O12-P-O13
2	B	812	POV	C11-O12-P-O13
2	A	803	POV	O22-C21-O21-C2
2	A	806	POV	O22-C21-O21-C2
2	A	807	POV	O22-C21-O21-C2
2	B	801	POV	O22-C21-O21-C2
2	B	802	POV	O22-C21-O21-C2
2	B	810	POV	O22-C21-O21-C2
2	A	803	POV	C32-C31-O31-C3
2	A	811	POV	C32-C31-O31-C3
2	B	806	POV	C32-C31-O31-C3
2	B	810	POV	C32-C31-O31-C3
2	A	812	POV	C22-C21-O21-C2
2	B	807	POV	C22-C21-O21-C2
2	A	808	POV	O32-C31-O31-C3
2	B	803	POV	O32-C31-O31-C3
2	A	801	POV	C211-C210-C29-C28
2	B	808	POV	C211-C210-C29-C28
2	A	803	POV	O32-C31-O31-C3
2	A	811	POV	O32-C31-O31-C3
2	B	806	POV	O32-C31-O31-C3
2	B	810	POV	O32-C31-O31-C3
2	A	808	POV	C32-C31-O31-C3
2	B	803	POV	C32-C31-O31-C3
2	A	809	POV	C22-C21-O21-C2
2	B	804	POV	C22-C21-O21-C2
2	A	806	POV	C32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
2	B	801	POV	C32-C31-O31-C3
2	A	806	POV	O32-C31-O31-C3
2	B	801	POV	O32-C31-O31-C3
2	B	807	POV	C212-C213-C214-C215
2	A	812	POV	C212-C213-C214-C215
2	A	811	POV	C31-C32-C33-C34
2	B	806	POV	C31-C32-C33-C34
2	A	810	POV	C211-C210-C29-C28
2	B	805	POV	C211-C210-C29-C28
2	A	801	POV	C21-C22-C23-C24
2	A	803	POV	C31-C32-C33-C34
2	A	804	POV	C21-C22-C23-C24
2	B	808	POV	C21-C22-C23-C24
2	B	810	POV	C31-C32-C33-C34
2	B	811	POV	C21-C22-C23-C24
2	A	805	POV	C2-C1-O11-P
2	B	812	POV	C2-C1-O11-P
2	A	809	POV	O22-C21-O21-C2
2	B	804	POV	O22-C21-O21-C2
2	A	805	POV	C11-O12-P-O11
2	A	808	POV	C1-O11-P-O12
2	A	809	POV	C11-O12-P-O11
2	B	803	POV	C1-O11-P-O12
2	B	804	POV	C11-O12-P-O11
2	B	812	POV	C11-O12-P-O11
2	A	812	POV	C11-C12-N-C13
2	B	807	POV	C11-C12-N-C13
2	A	805	POV	C32-C31-O31-C3
2	B	812	POV	C32-C31-O31-C3
2	A	810	POV	C210-C211-C212-C213
2	B	805	POV	C210-C211-C212-C213
2	A	807	POV	C32-C33-C34-C35
2	A	810	POV	C24-C25-C26-C27
2	A	812	POV	C22-C23-C24-C25
2	A	812	POV	C32-C33-C34-C35
2	B	802	POV	C32-C33-C34-C35
2	B	805	POV	C24-C25-C26-C27
2	B	807	POV	C32-C33-C34-C35
2	A	805	POV	C35-C36-C37-C38
2	A	810	POV	C211-C212-C213-C214
2	B	805	POV	C211-C212-C213-C214
2	B	807	POV	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
2	B	812	POV	C35-C36-C37-C38
2	A	804	POV	C213-C214-C215-C216
2	A	805	POV	C310-C311-C312-C313
2	A	805	POV	C312-C313-C314-C315
2	B	811	POV	C213-C214-C215-C216
2	B	812	POV	C310-C311-C312-C313
2	B	812	POV	C312-C313-C314-C315
2	A	812	POV	C31-C32-C33-C34
2	B	807	POV	C31-C32-C33-C34
2	A	802	POV	C211-C212-C213-C214
2	A	810	POV	C25-C26-C27-C28
2	B	805	POV	C25-C26-C27-C28
2	B	809	POV	C211-C212-C213-C214
2	A	806	POV	C35-C36-C37-C38
2	B	801	POV	C35-C36-C37-C38
2	A	804	POV	C31-C32-C33-C34
2	B	811	POV	C31-C32-C33-C34
2	A	803	POV	C22-C23-C24-C25
2	B	810	POV	C22-C23-C24-C25
2	A	811	POV	C35-C36-C37-C38
2	B	806	POV	C35-C36-C37-C38
2	A	804	POV	C37-C38-C39-C310
2	A	805	POV	C37-C38-C39-C310
2	A	812	POV	C25-C26-C27-C28
2	A	812	POV	C34-C35-C36-C37
2	B	807	POV	C25-C26-C27-C28
2	B	807	POV	C34-C35-C36-C37
2	B	811	POV	C37-C38-C39-C310
2	B	812	POV	C37-C38-C39-C310
2	A	809	POV	C24-C25-C26-C27
2	B	804	POV	C24-C25-C26-C27
2	A	806	POV	C31-C32-C33-C34
2	B	801	POV	C31-C32-C33-C34
2	A	803	POV	C33-C34-C35-C36
2	B	810	POV	C33-C34-C35-C36
2	A	807	POV	C24-C25-C26-C27
2	B	802	POV	C24-C25-C26-C27
2	A	806	POV	C37-C38-C39-C310
2	B	801	POV	C37-C38-C39-C310
2	A	812	POV	C312-C313-C314-C315
2	B	807	POV	C312-C313-C314-C315
2	A	804	POV	C312-C313-C314-C315

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Mol	Chain	Res	Type	Atoms
2	B	811	POV	C312-C313-C314-C315
2	A	812	POV	C21-C22-C23-C24
2	B	807	POV	C21-C22-C23-C24
2	A	805	POV	O32-C31-O31-C3
2	B	812	POV	O32-C31-O31-C3
2	A	811	POV	C33-C34-C35-C36
2	B	806	POV	C33-C34-C35-C36
2	A	812	POV	C11-C12-N-C14
2	A	812	POV	C11-C12-N-C15
2	B	807	POV	C11-C12-N-C14
2	B	807	POV	C11-C12-N-C15
2	A	804	POV	C212-C213-C214-C215
2	A	805	POV	C34-C35-C36-C37
2	B	811	POV	C212-C213-C214-C215
2	B	812	POV	C34-C35-C36-C37
2	A	805	POV	C313-C314-C315-C316
2	B	812	POV	C313-C314-C315-C316
2	A	803	POV	C213-C214-C215-C216
2	B	810	POV	C213-C214-C215-C216
2	B	810	POV	C32-C33-C34-C35
2	A	804	POV	C22-C21-O21-C2
2	B	811	POV	C22-C21-O21-C2
2	A	803	POV	C32-C33-C34-C35
2	A	805	POV	C33-C34-C35-C36
2	B	812	POV	C33-C34-C35-C36
2	A	804	POV	O22-C21-O21-C2
2	B	811	POV	O22-C21-O21-C2
2	B	801	POV	C24-C25-C26-C27
2	B	807	POV	C11-O12-P-O11
2	A	806	POV	C24-C25-C26-C27
2	B	808	POV	C25-C26-C27-C28
2	A	801	POV	C25-C26-C27-C28
2	A	809	POV	C32-C31-O31-C3
2	B	804	POV	C32-C31-O31-C3
2	A	803	POV	C210-C211-C212-C213
2	B	810	POV	C210-C211-C212-C213
2	A	803	POV	C37-C38-C39-C310
2	B	810	POV	C37-C38-C39-C310
2	A	806	POV	C1-C2-C3-O31
2	B	801	POV	C1-C2-C3-O31
2	A	806	POV	C32-C33-C34-C35
2	B	801	POV	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
2	A	805	POV	C24-C25-C26-C27
2	B	812	POV	C24-C25-C26-C27
2	A	812	POV	C310-C311-C312-C313
2	B	807	POV	C310-C311-C312-C313
2	A	801	POV	C213-C214-C215-C216
2	B	808	POV	C213-C214-C215-C216
2	B	803	POV	C32-C33-C34-C35
2	A	805	POV	O11-C1-C2-O21
2	B	812	POV	O11-C1-C2-O21
2	A	808	POV	C32-C33-C34-C35
2	A	809	POV	O32-C31-O31-C3
2	B	804	POV	O32-C31-O31-C3
2	A	805	POV	O21-C2-C3-O31
2	B	812	POV	O21-C2-C3-O31
2	A	809	POV	O11-C1-C2-C3
2	B	804	POV	O11-C1-C2-C3
2	A	807	POV	C31-C32-C33-C34
2	B	802	POV	C31-C32-C33-C34
2	A	805	POV	C21-C22-C23-C24
2	B	812	POV	C21-C22-C23-C24
2	A	805	POV	C1-C2-C3-O31
2	A	808	POV	C1-C2-C3-O31
2	A	812	POV	C1-C2-C3-O31
2	B	803	POV	C1-C2-C3-O31
2	B	807	POV	C1-C2-C3-O31
2	B	812	POV	C1-C2-C3-O31
2	B	811	POV	C310-C311-C312-C313
2	A	804	POV	C310-C311-C312-C313
2	A	812	POV	C214-C215-C216-C217
2	B	807	POV	C214-C215-C216-C217
2	A	806	POV	C25-C26-C27-C28
2	B	801	POV	C25-C26-C27-C28
2	A	812	POV	C11-O12-P-O11
2	A	805	POV	C23-C24-C25-C26
2	B	812	POV	C23-C24-C25-C26
2	A	801	POV	C22-C23-C24-C25
2	B	808	POV	C22-C23-C24-C25
2	B	801	POV	C34-C35-C36-C37
2	A	802	POV	C25-C26-C27-C28
2	A	806	POV	C34-C35-C36-C37
2	A	809	POV	C22-C23-C24-C25
2	B	804	POV	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
2	B	809	POV	C25-C26-C27-C28
2	A	804	POV	C39-C310-C311-C312
2	B	811	POV	C39-C310-C311-C312
2	A	809	POV	O11-C1-C2-O21
2	B	804	POV	O11-C1-C2-O21
2	A	803	POV	O21-C2-C3-O31
2	A	809	POV	O21-C2-C3-O31
2	B	804	POV	O21-C2-C3-O31
2	B	810	POV	O21-C2-C3-O31
2	A	811	POV	C22-C23-C24-C25
2	B	806	POV	C22-C23-C24-C25
2	A	812	POV	C26-C27-C28-C29
2	B	807	POV	C26-C27-C28-C29
2	A	809	POV	C34-C35-C36-C37
2	B	804	POV	C34-C35-C36-C37
2	A	807	POV	C11-O12-P-O11
2	A	811	POV	C1-O11-P-O12
2	A	811	POV	C11-O12-P-O11
2	B	802	POV	C11-O12-P-O11
2	B	806	POV	C1-O11-P-O12
2	B	806	POV	C11-O12-P-O11
2	A	804	POV	C11-O12-P-O14
2	A	809	POV	C11-O12-P-O13
2	A	812	POV	C11-O12-P-O13
2	B	802	POV	C11-O12-P-O13
2	B	804	POV	C11-O12-P-O13
2	B	807	POV	C11-O12-P-O13
2	B	811	POV	C11-O12-P-O14
2	A	808	POV	C12-C11-O12-P
2	B	803	POV	C12-C11-O12-P
2	A	808	POV	O21-C2-C3-O31
2	A	812	POV	O21-C2-C3-O31
2	B	803	POV	O21-C2-C3-O31
2	B	807	POV	O21-C2-C3-O31
2	B	809	POV	C24-C25-C26-C27
2	A	802	POV	C24-C25-C26-C27
2	A	812	POV	C313-C314-C315-C316
2	B	807	POV	C313-C314-C315-C316
2	A	805	POV	O11-C1-C2-C3
2	B	812	POV	O11-C1-C2-C3
2	A	806	POV	O21-C2-C3-O31
2	B	801	POV	O21-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
2	A	804	POV	C11-O12-P-O11
2	A	805	POV	C1-O11-P-O12
2	A	808	POV	C11-O12-P-O11
2	B	803	POV	C11-O12-P-O11
2	B	811	POV	C11-O12-P-O11
2	B	812	POV	C1-O11-P-O12
2	A	803	POV	C1-C2-C3-O31
2	B	810	POV	C1-C2-C3-O31
2	A	806	POV	C23-C24-C25-C26
2	B	801	POV	C23-C24-C25-C26
2	A	810	POV	C29-C210-C211-C212
2	B	805	POV	C29-C210-C211-C212
2	A	804	POV	C27-C28-C29-C210
2	B	811	POV	C27-C28-C29-C210
2	A	801	POV	O22-C21-C22-C23
2	B	808	POV	O22-C21-C22-C23
2	A	804	POV	C29-C210-C211-C212
2	A	809	POV	C1-C2-O21-C21
2	B	804	POV	C1-C2-O21-C21
2	B	811	POV	C29-C210-C211-C212
2	A	812	POV	C37-C38-C39-C310
2	B	807	POV	C37-C38-C39-C310
2	A	801	POV	O21-C21-C22-C23
2	B	808	POV	O21-C21-C22-C23
2	A	803	POV	C27-C28-C29-C210
2	B	810	POV	C27-C28-C29-C210
2	A	811	POV	C34-C35-C36-C37
2	B	806	POV	C34-C35-C36-C37
2	A	805	POV	C311-C310-C39-C38
2	B	812	POV	C311-C310-C39-C38
2	A	812	POV	C39-C310-C311-C312
2	B	812	POV	C32-C33-C34-C35
2	A	805	POV	C32-C33-C34-C35
2	B	807	POV	C39-C310-C311-C312
2	A	804	POV	O11-C1-C2-O21
2	B	811	POV	O11-C1-C2-O21
2	A	808	POV	C22-C23-C24-C25
2	B	803	POV	C22-C23-C24-C25
2	A	804	POV	O11-C1-C2-C3
2	B	811	POV	O11-C1-C2-C3
2	A	809	POV	C2-C1-O11-P
2	B	804	POV	C2-C1-O11-P

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Mol	Chain	Res	Type	Atoms
2	A	805	POV	C27-C28-C29-C210
2	B	812	POV	C27-C28-C29-C210
2	A	801	POV	C26-C27-C28-C29
2	B	808	POV	C26-C27-C28-C29
2	A	801	POV	C29-C210-C211-C212
2	B	808	POV	C29-C210-C211-C212
2	A	812	POV	C29-C210-C211-C212
2	B	807	POV	C29-C210-C211-C212
2	A	804	POV	C32-C33-C34-C35
2	A	803	POV	O31-C31-C32-C33
2	B	810	POV	O31-C31-C32-C33
2	A	807	POV	C11-C12-N-C13
2	A	807	POV	C11-C12-N-C15
2	B	802	POV	C11-C12-N-C13
2	B	802	POV	C11-C12-N-C15
2	A	809	POV	C25-C26-C27-C28
2	B	811	POV	C32-C33-C34-C35
2	A	805	POV	O21-C21-C22-C23
2	B	812	POV	O21-C21-C22-C23
2	B	804	POV	C25-C26-C27-C28
2	A	812	POV	C27-C28-C29-C210
2	B	807	POV	C27-C28-C29-C210
2	A	807	POV	C37-C38-C39-C310
2	B	802	POV	C11-C12-N-C14
2	B	802	POV	C37-C38-C39-C310
2	A	812	POV	C23-C24-C25-C26
2	B	807	POV	C23-C24-C25-C26
2	A	807	POV	C11-C12-N-C14
2	A	803	POV	O32-C31-C32-C33
2	B	810	POV	O32-C31-C32-C33
2	A	812	POV	C35-C36-C37-C38
2	B	807	POV	C35-C36-C37-C38
2	A	805	POV	C1-O11-P-O14
2	A	807	POV	C1-O11-P-O13
2	A	807	POV	C11-O12-P-O13
2	A	808	POV	C11-O12-P-O14
2	A	811	POV	C1-O11-P-O14
2	B	802	POV	C1-O11-P-O13
2	B	803	POV	C11-O12-P-O14
2	B	806	POV	C1-O11-P-O14
2	B	812	POV	C1-O11-P-O14
2	A	805	POV	O22-C21-C22-C23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	812	POV	O22-C21-C22-C23
2	A	807	POV	C12-C11-O12-P
2	B	802	POV	C12-C11-O12-P
2	A	805	POV	C31-C32-C33-C34
2	B	812	POV	C31-C32-C33-C34
2	A	803	POV	O21-C21-C22-C23
2	B	810	POV	O21-C21-C22-C23
2	A	803	POV	O22-C21-C22-C23
2	A	812	POV	C311-C312-C313-C314
2	B	807	POV	C311-C312-C313-C314
2	A	806	POV	C310-C311-C312-C313
2	B	810	POV	O22-C21-C22-C23
2	B	801	POV	C310-C311-C312-C313

There are no ring outliers.

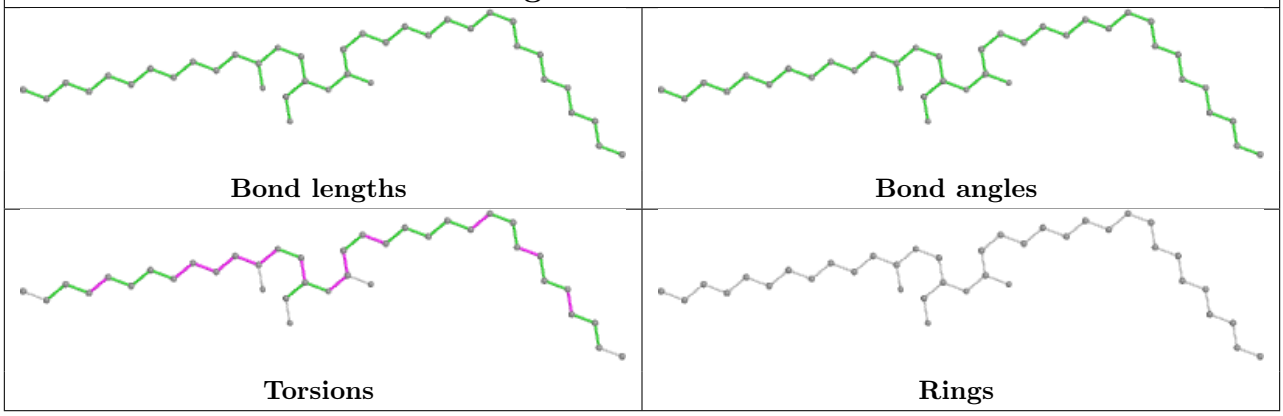
6 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	812	POV	1	0
2	B	806	POV	3	0
2	A	805	POV	1	0
2	B	807	POV	1	0
2	A	812	POV	1	0
2	A	811	POV	3	0

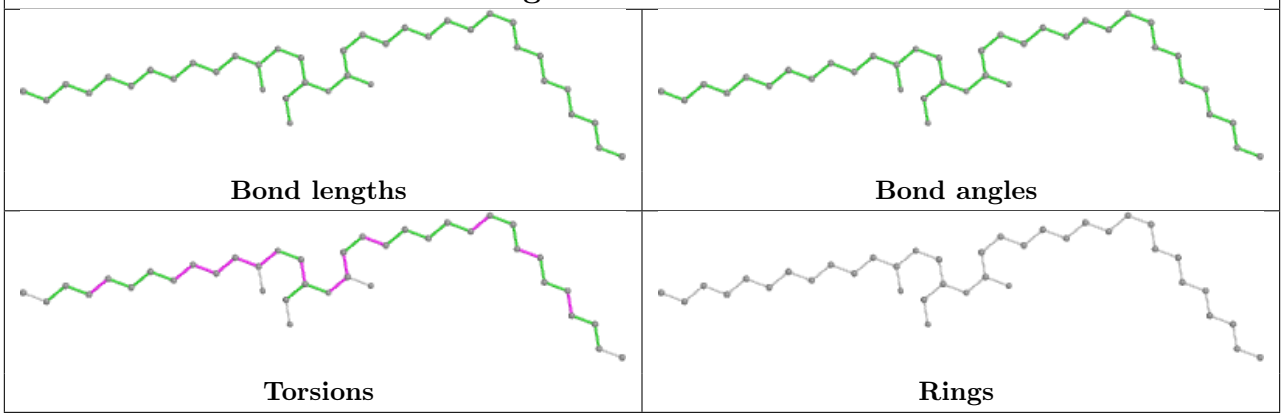
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand POV B 801

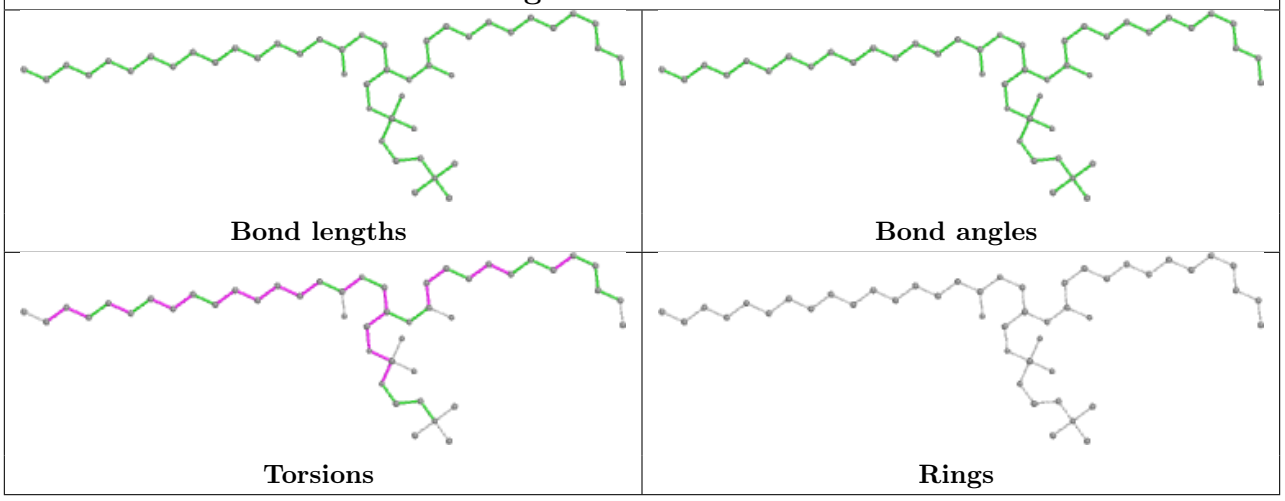
Ligand POV B 810



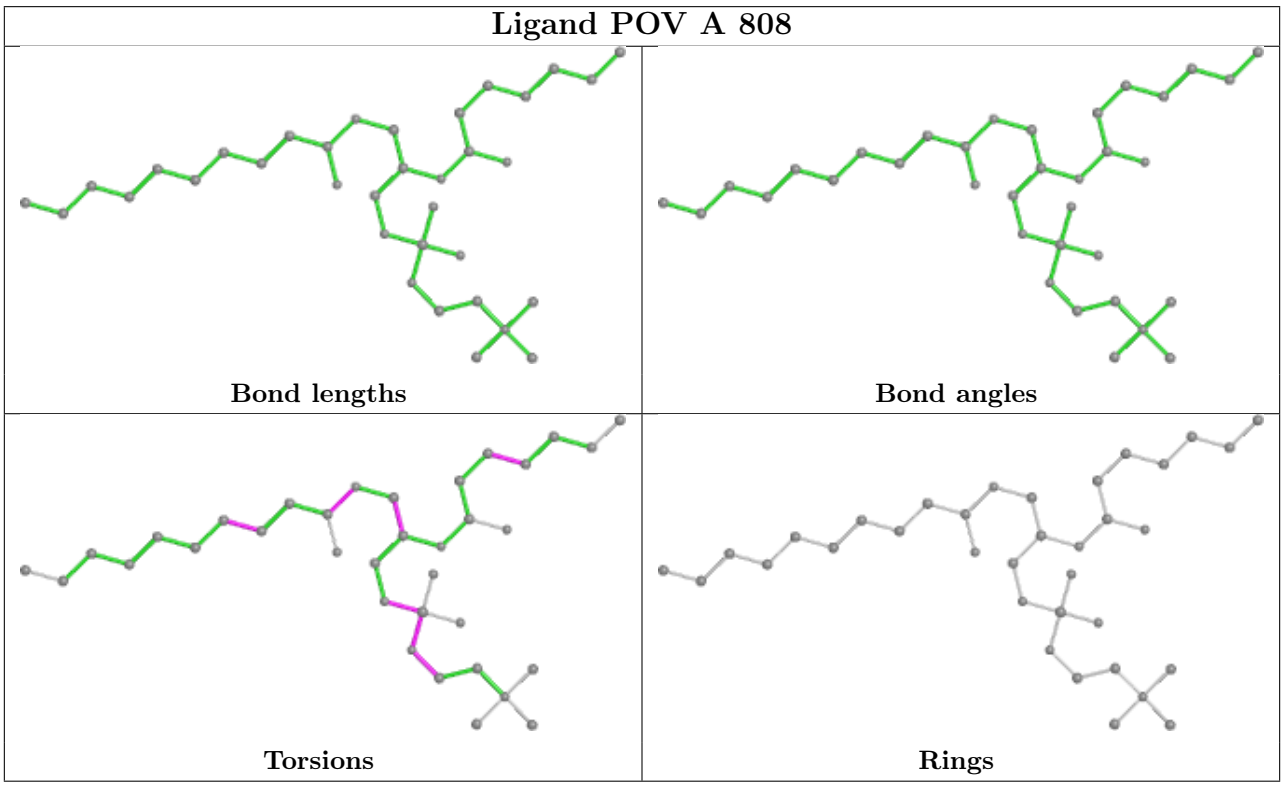
Ligand POV A 803



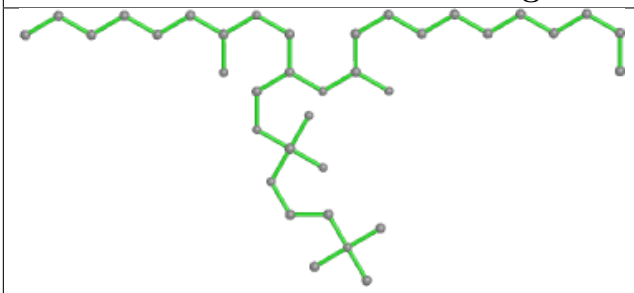
Ligand POV B 812



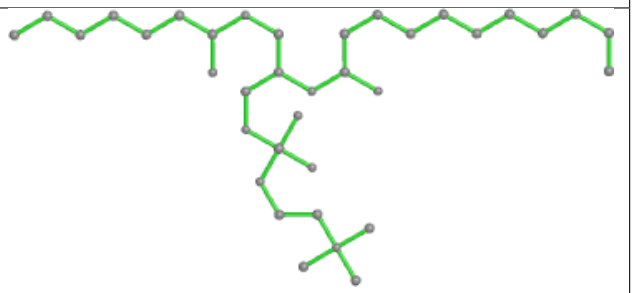
Ligand POV A 808



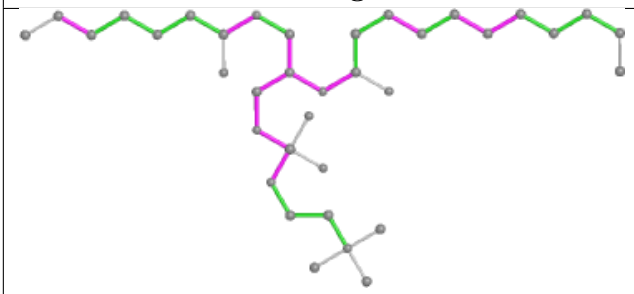
Ligand POV A 809



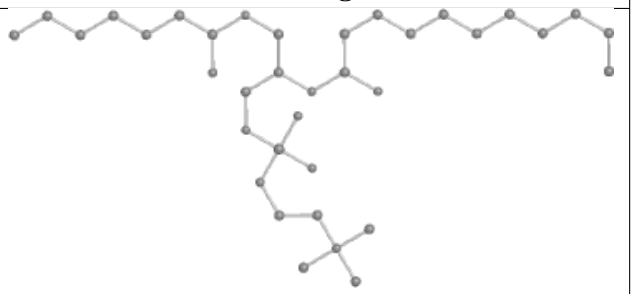
Bond lengths



Bond angles

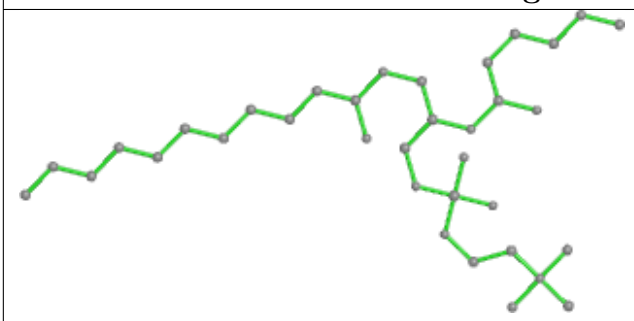


Torsions

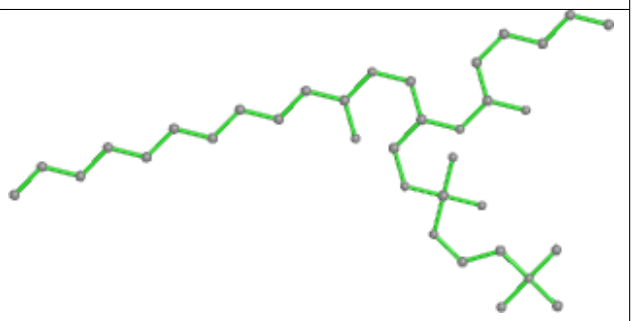


Rings

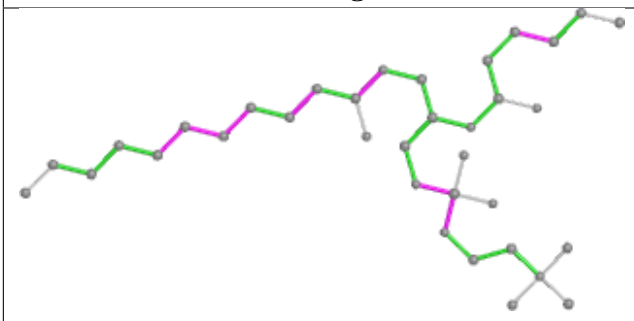
Ligand POV B 806



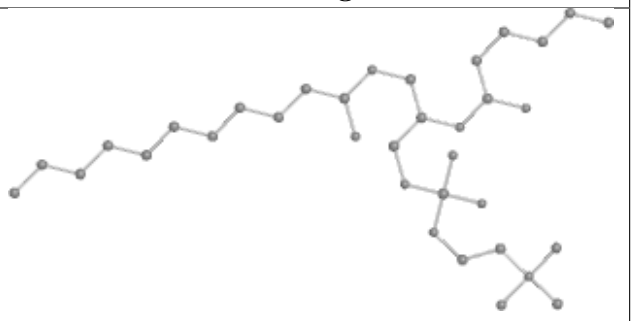
Bond lengths



Bond angles

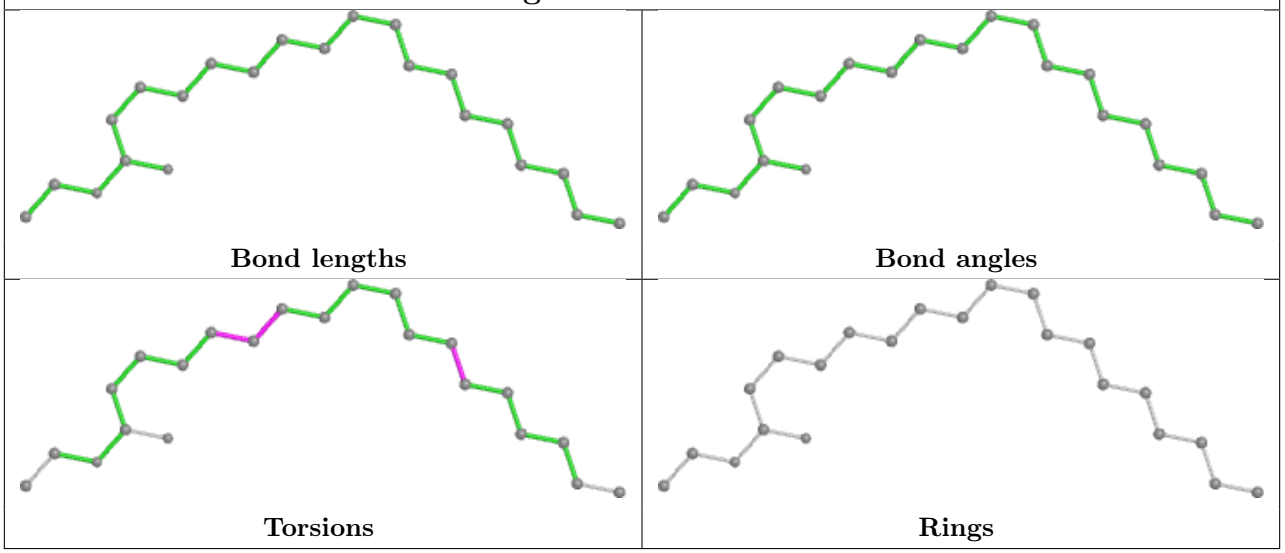


Torsions

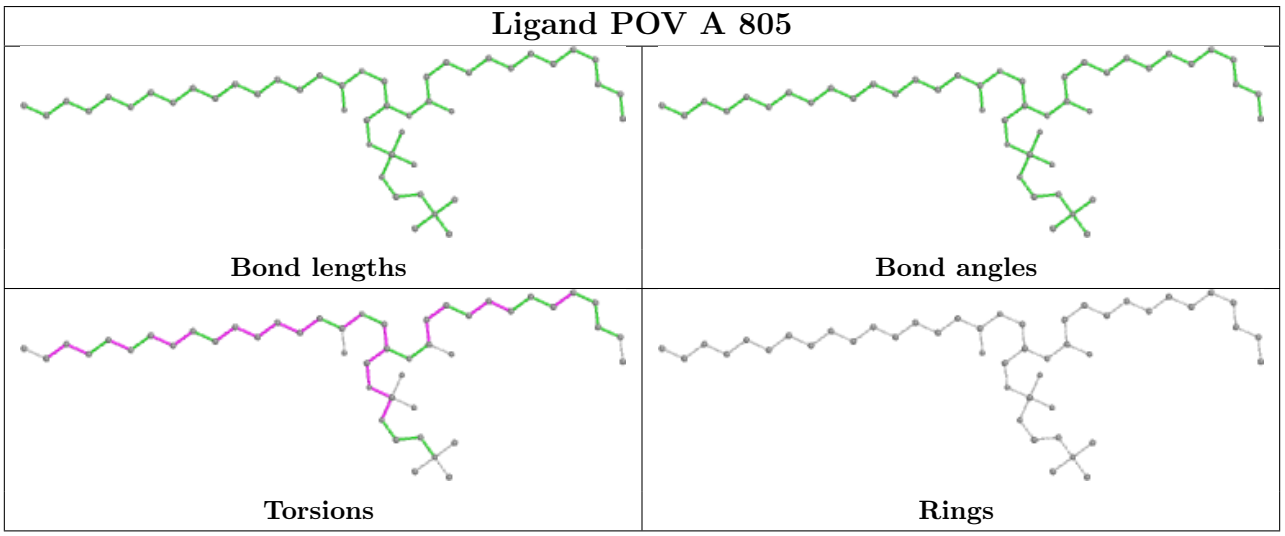


Rings

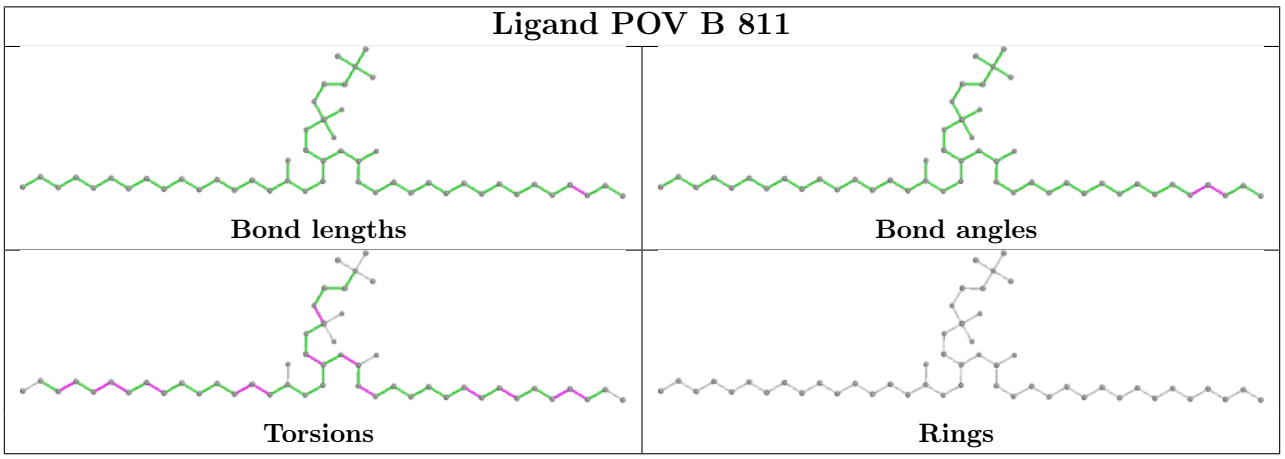
Ligand POV A 802



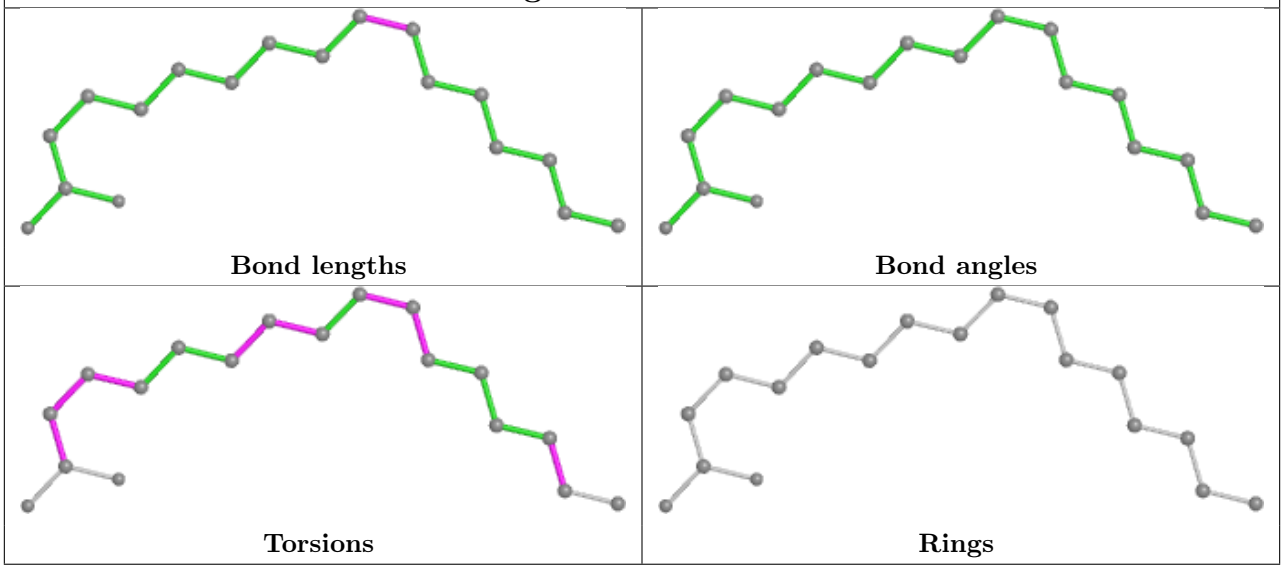
Ligand POV A 805



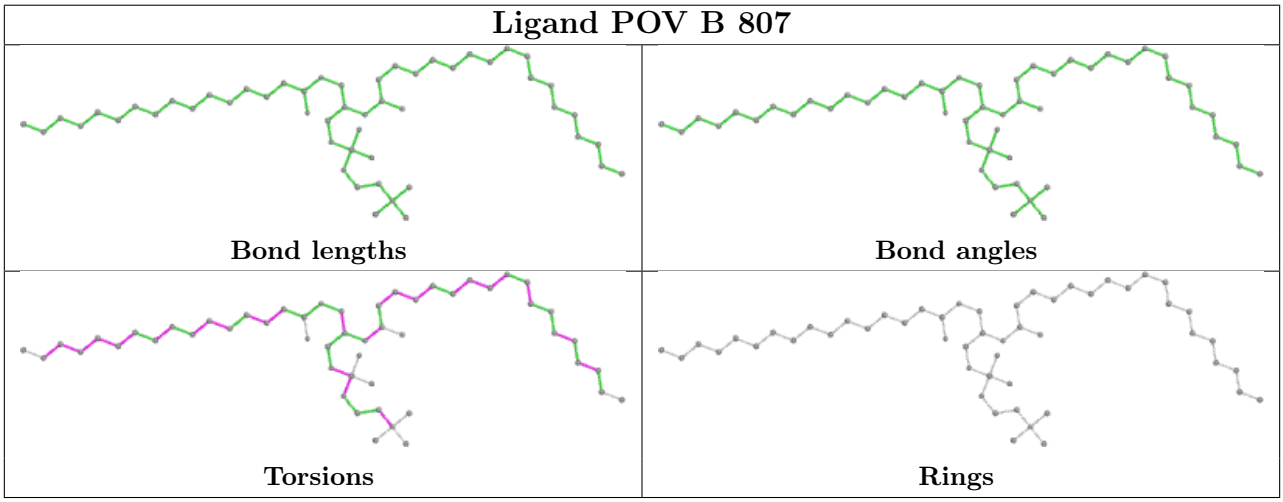
Ligand POV B 811



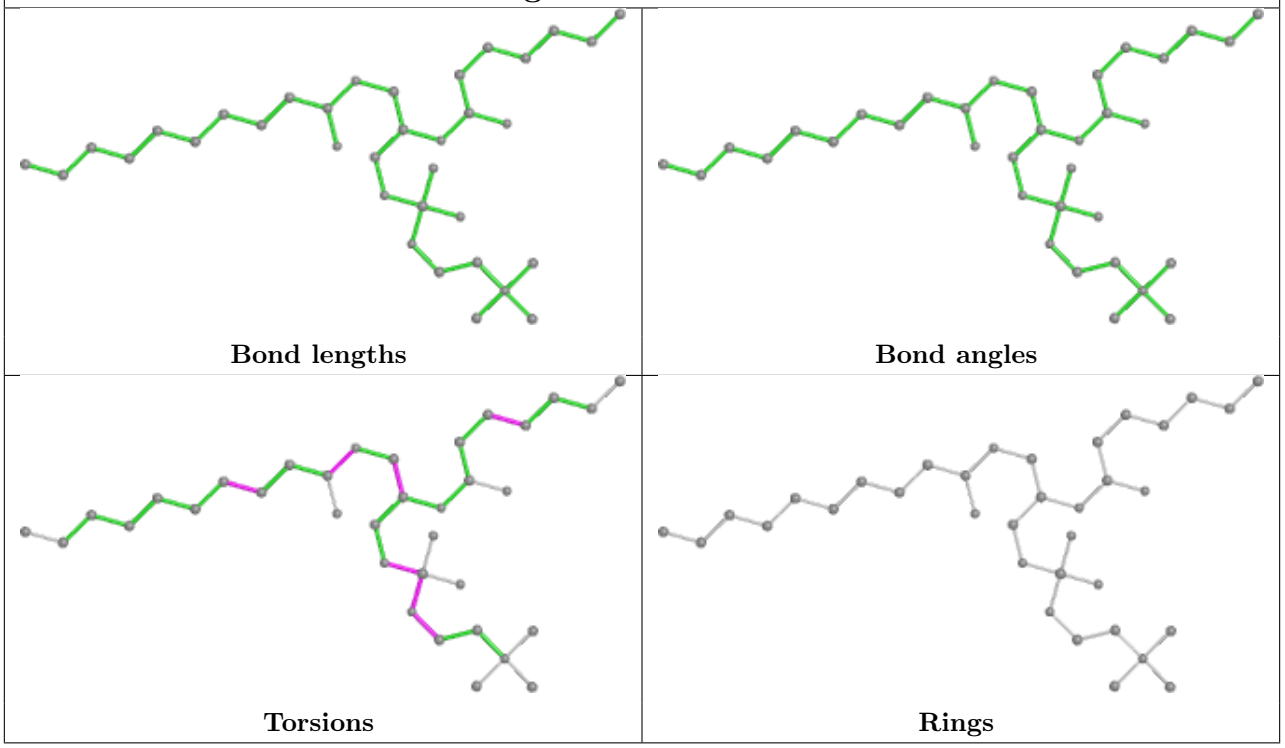
Ligand POV B 808



Ligand POV B 807



Ligand POV B 803



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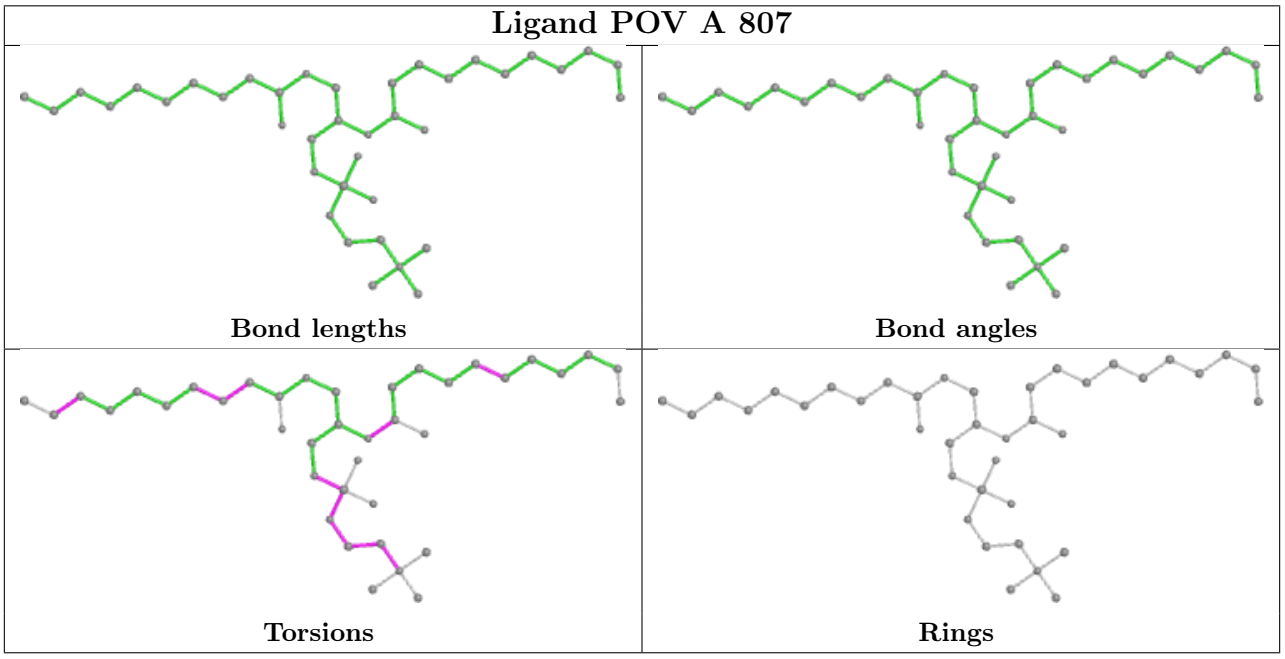
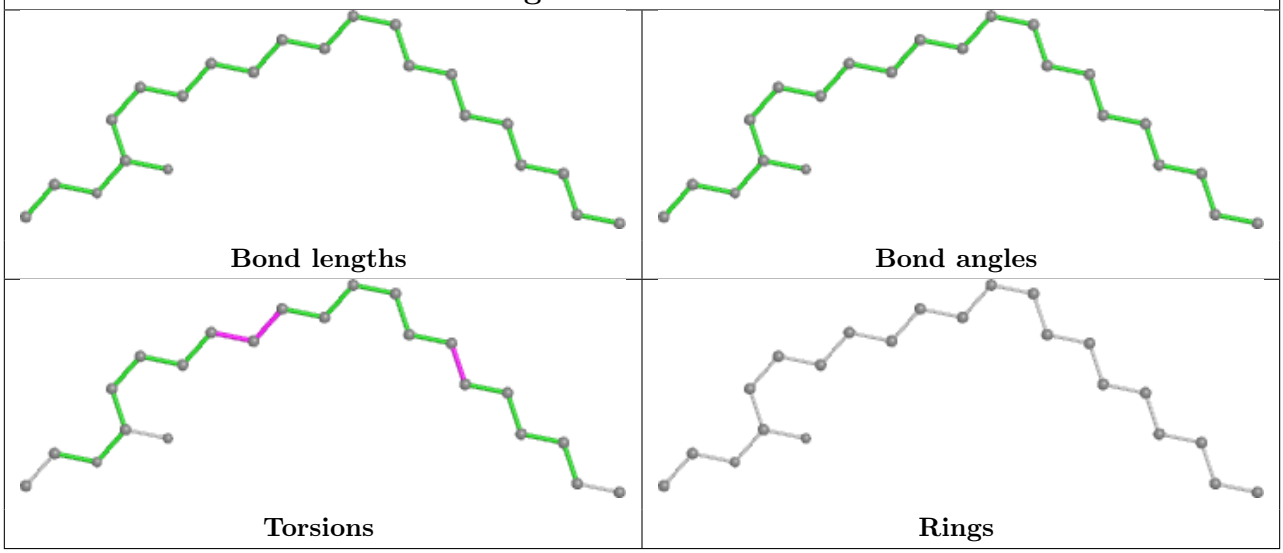


Ligand POV B 809



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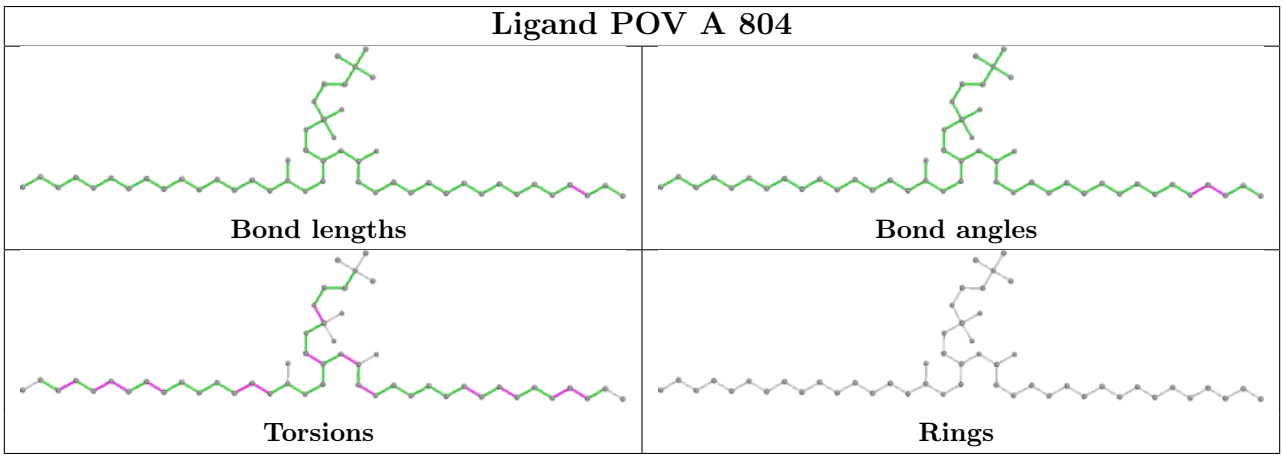
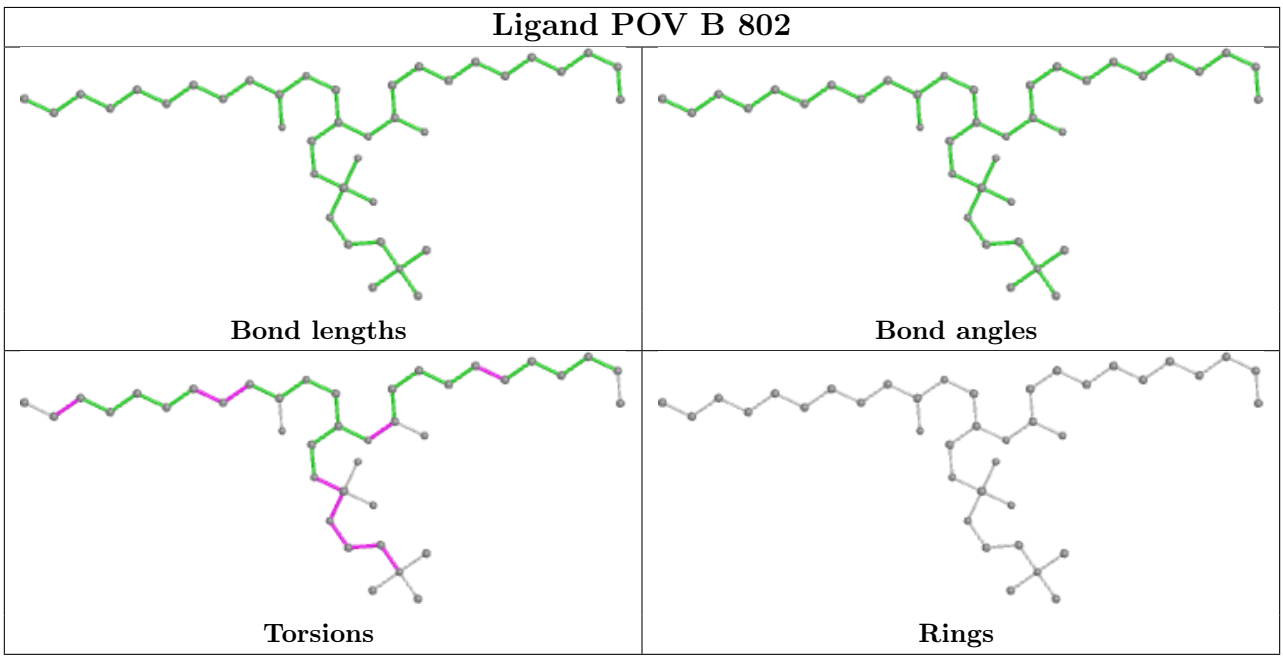
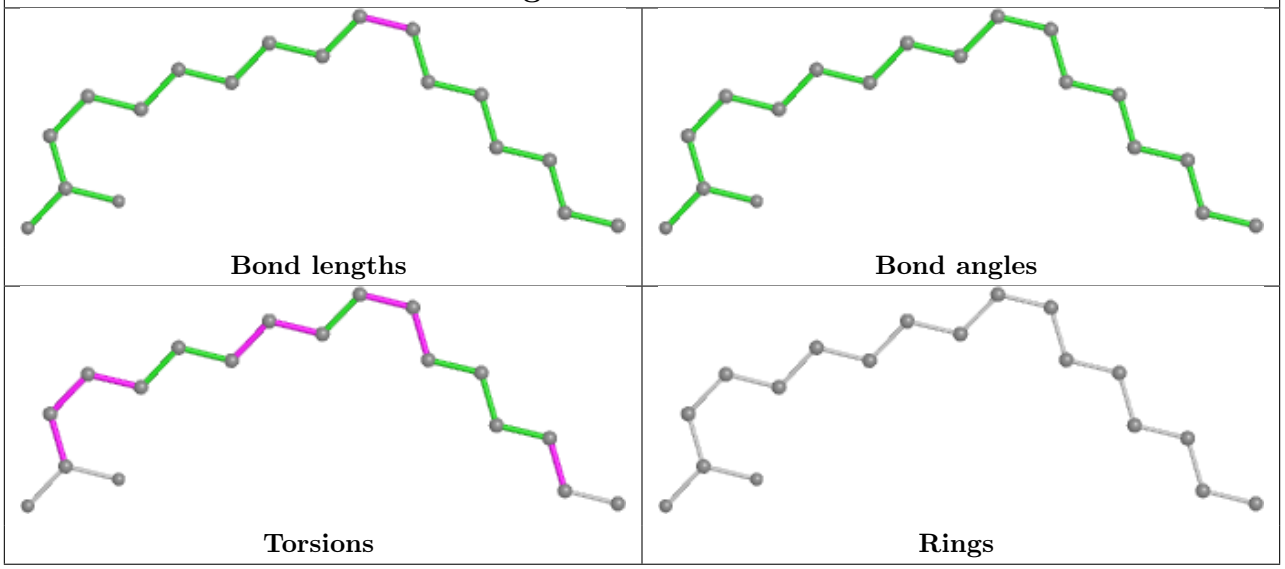


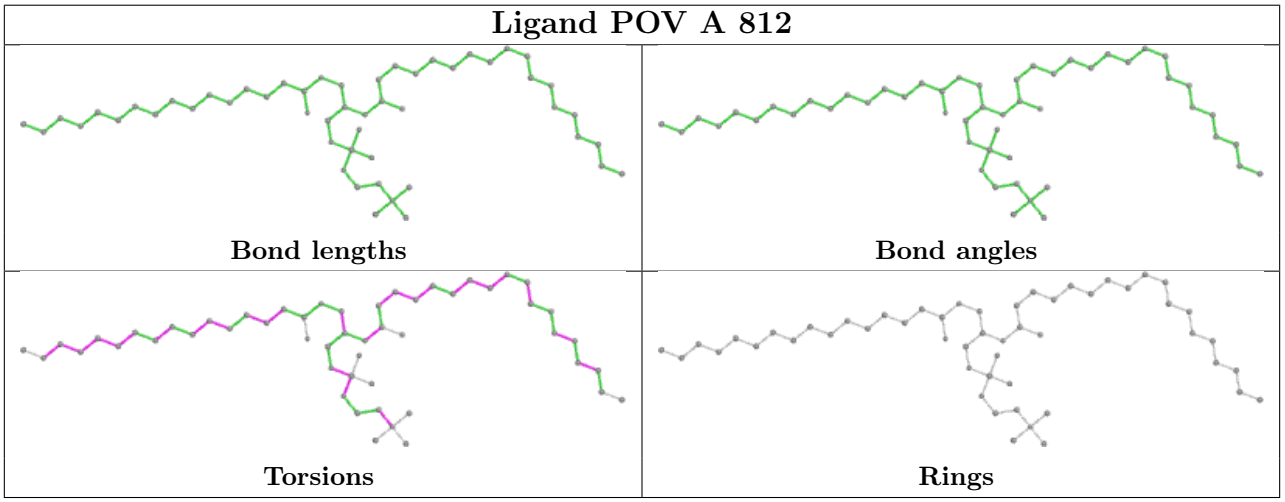
Ligand POV B 802



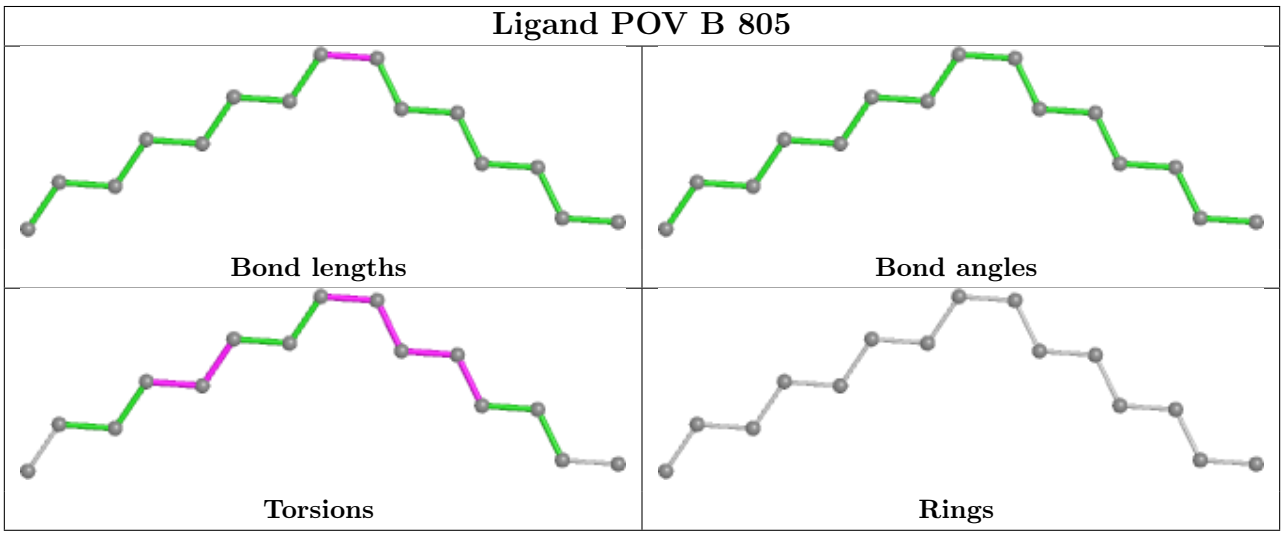
Ligand POV A 801



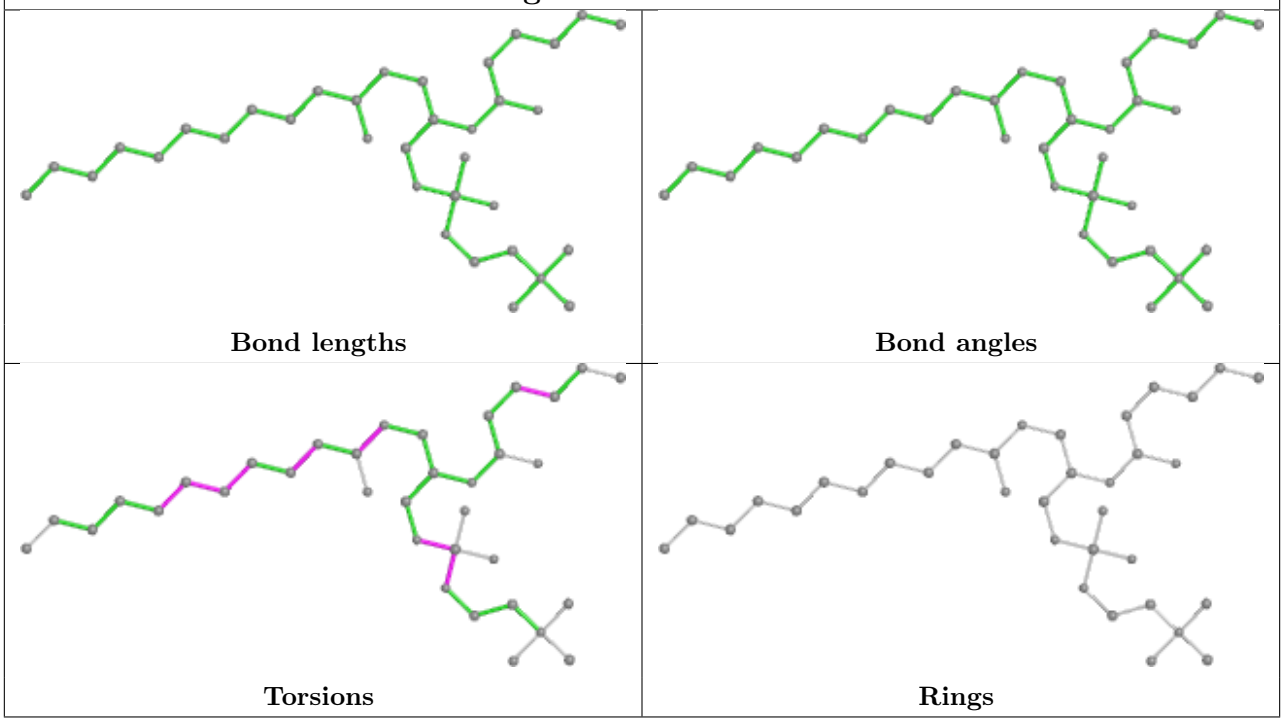
Ligand POV A 812



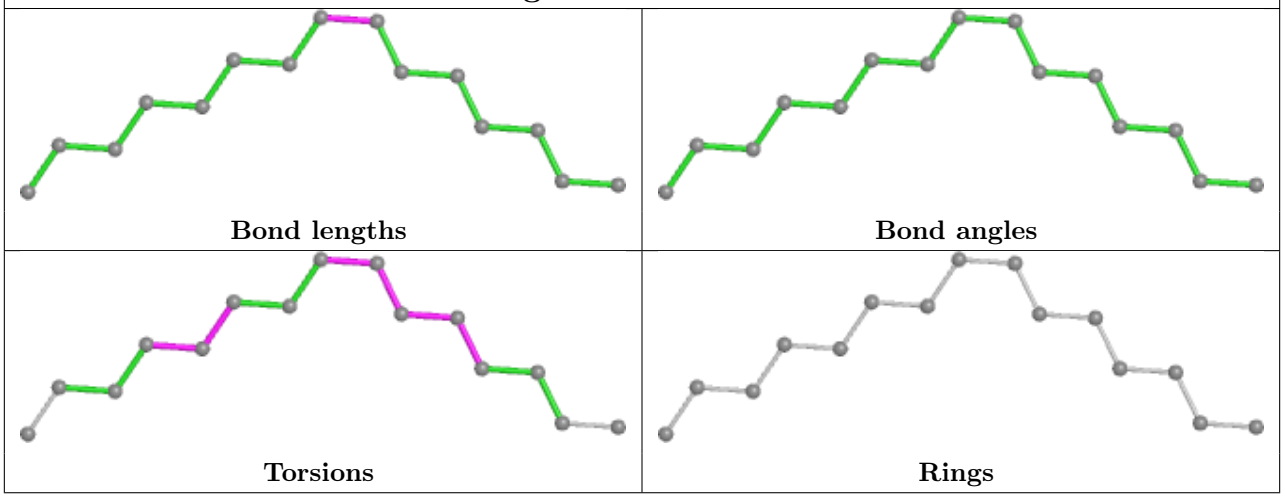
Ligand POV B 805

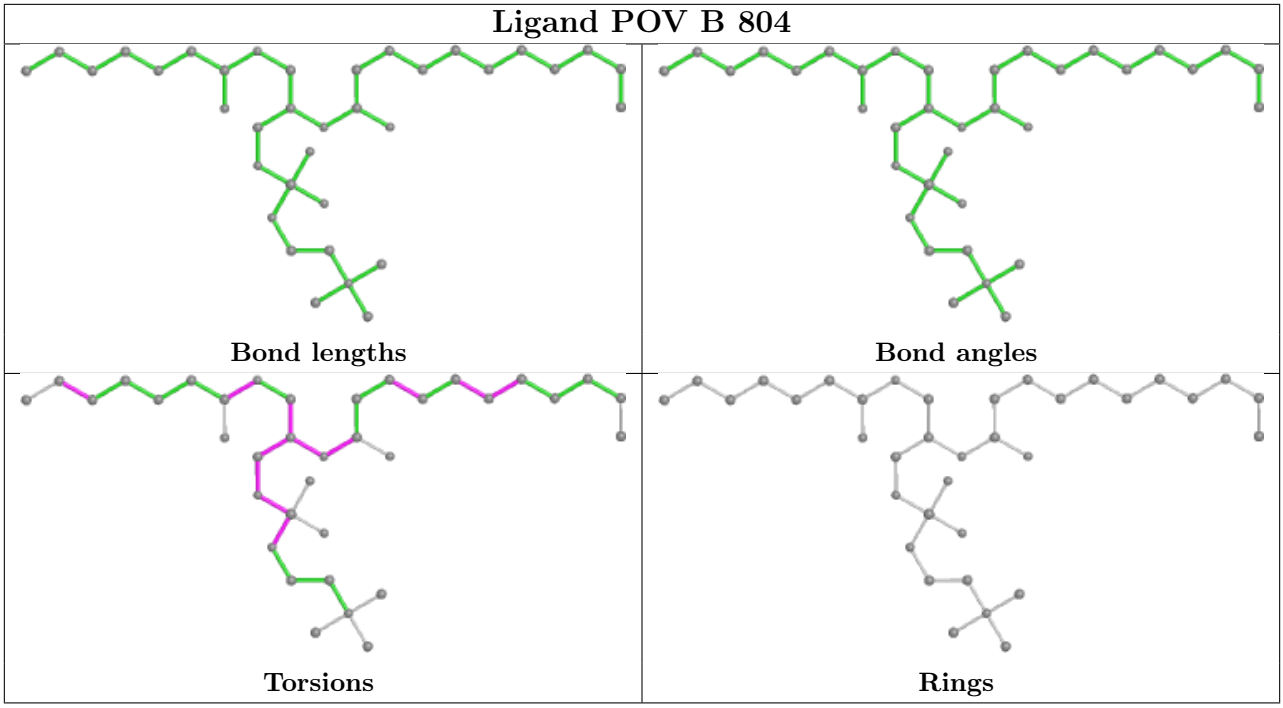


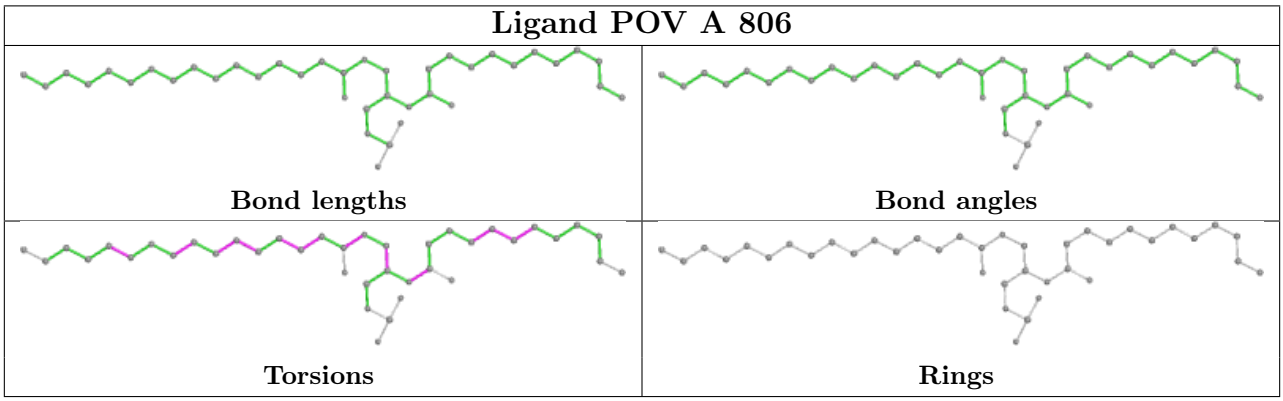
Ligand POV A 811



Ligand POV A 810







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.

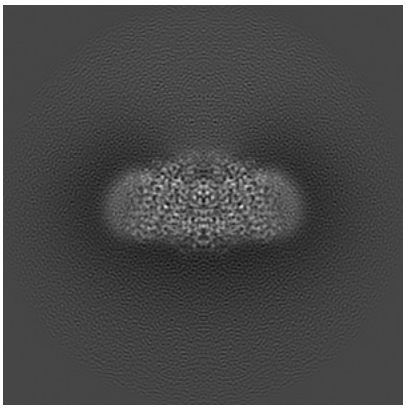
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-41187. These allow visual inspection of the internal detail of the map and identification of artifacts.

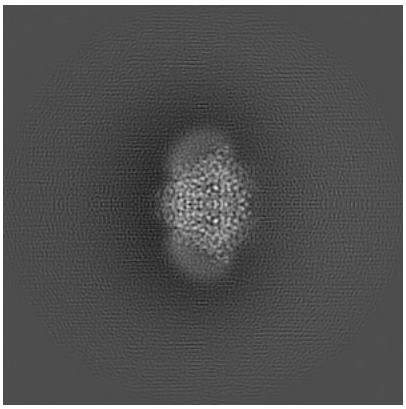
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

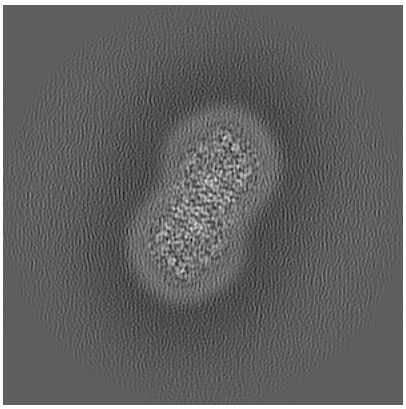
6.1.1 Primary map



X

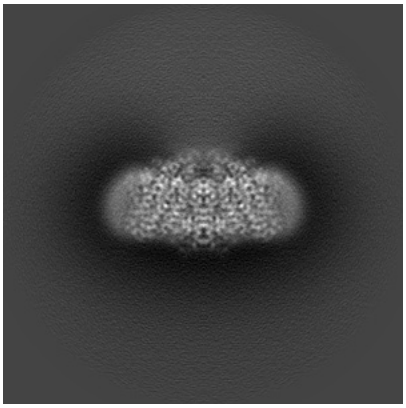


Y

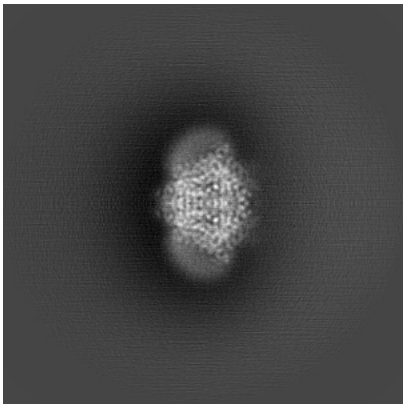


Z

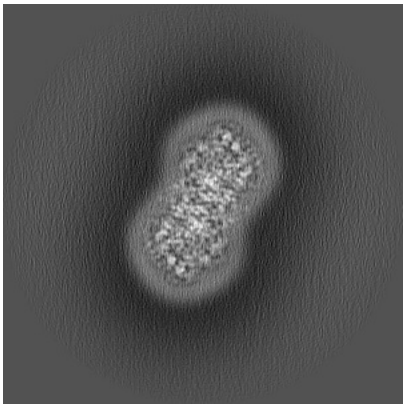
6.1.2 Raw map



X



Y

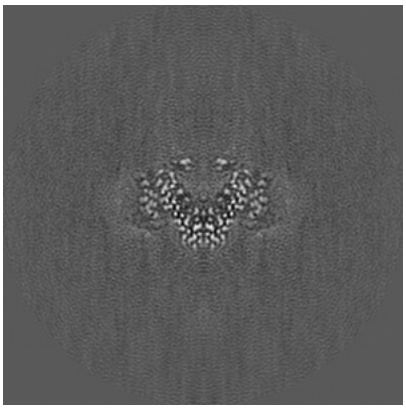


Z

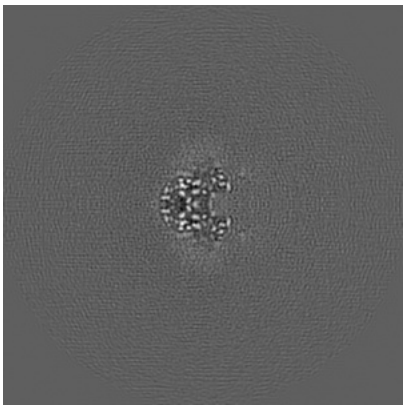
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

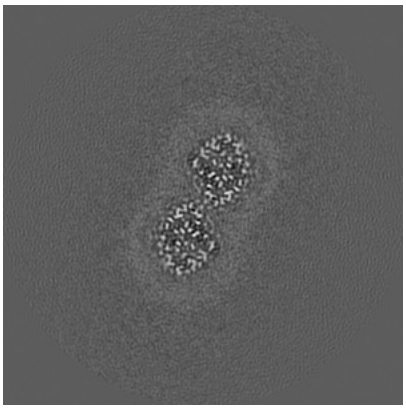
6.2.1 Primary map



X Index: 160

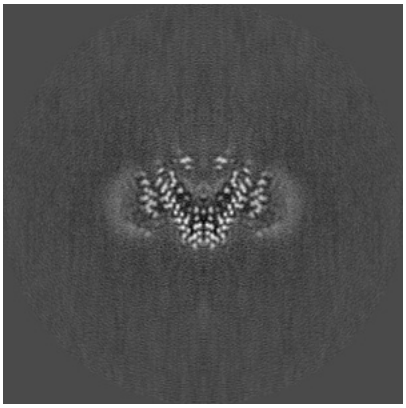


Y Index: 160

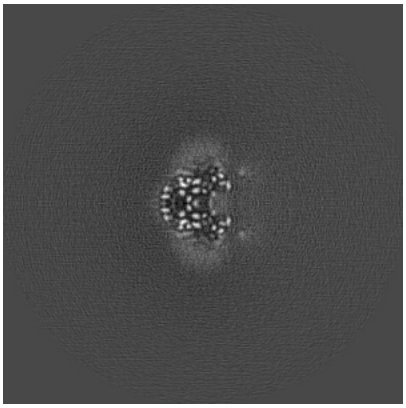


Z Index: 160

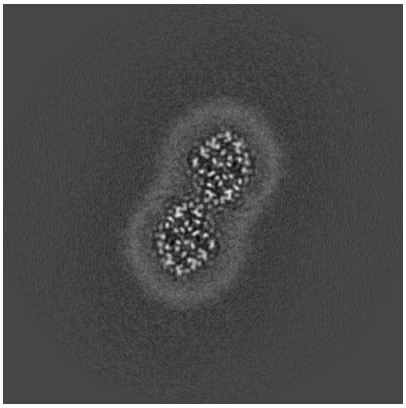
6.2.2 Raw map



X Index: 160



Y Index: 160

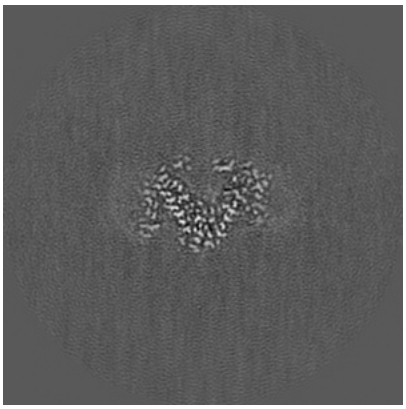


Z Index: 160

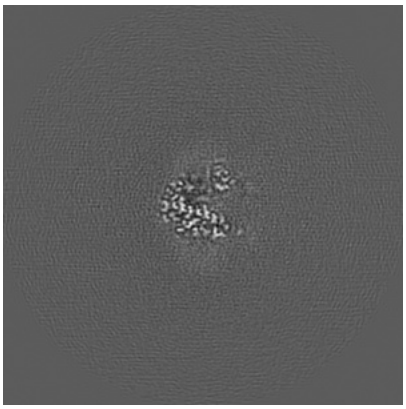
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

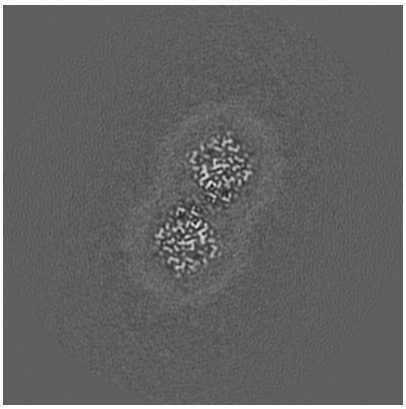
6.3.1 Primary map



X Index: 158

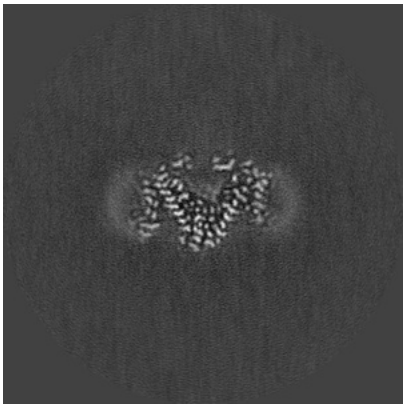


Y Index: 157

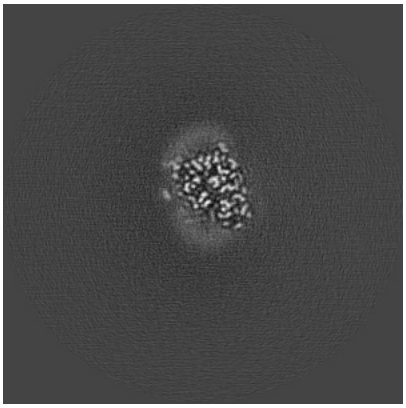


Z Index: 158

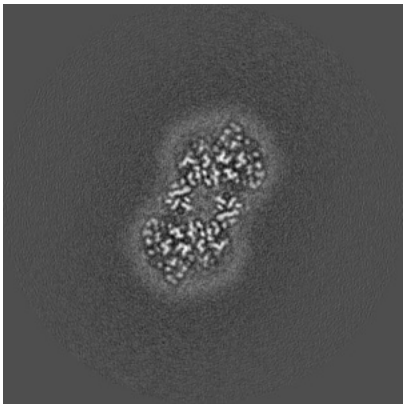
6.3.2 Raw map



X Index: 158



Y Index: 184

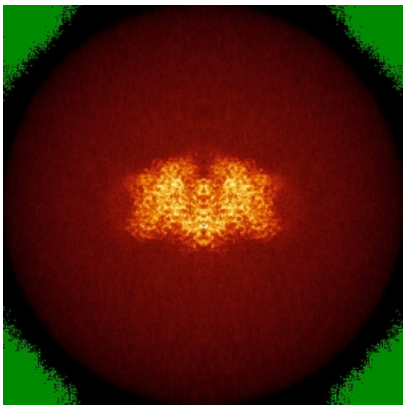


Z Index: 175

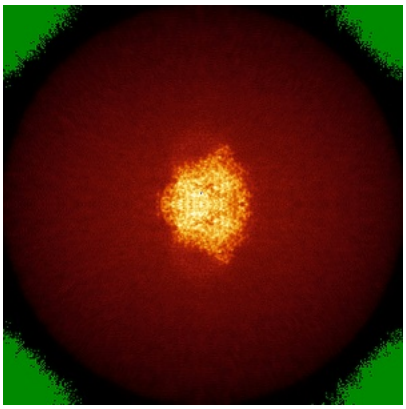
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

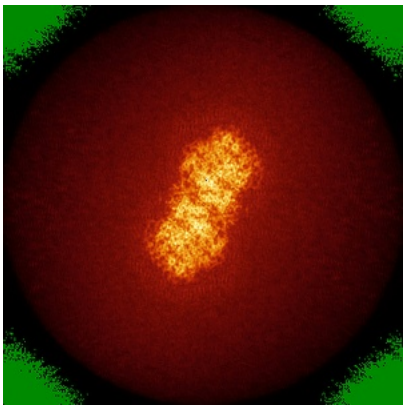
6.4.1 Primary map



X

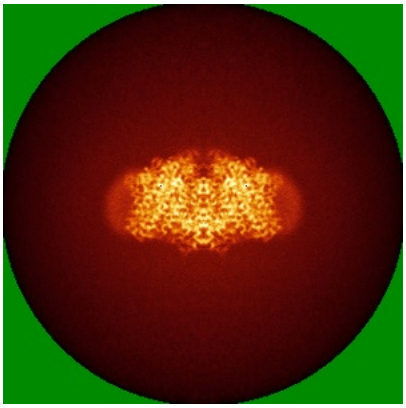


Y

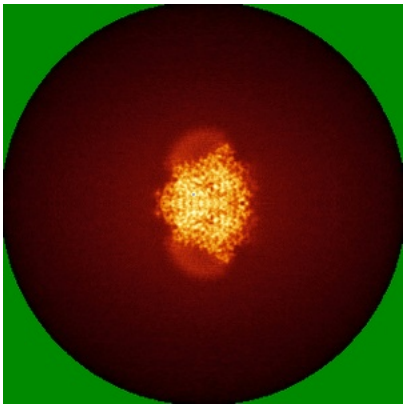


Z

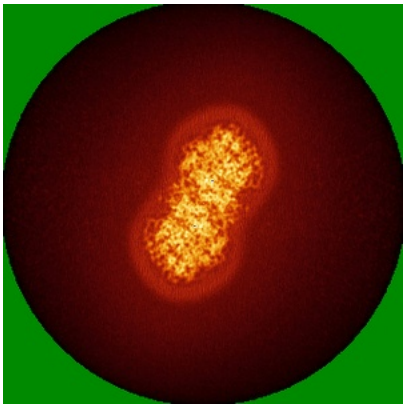
6.4.2 Raw map



X



Y

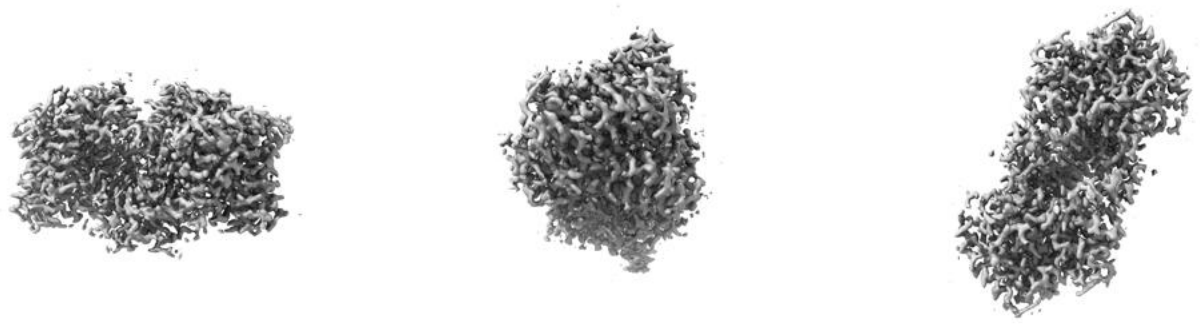


Z

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



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. 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

X Y Z

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.

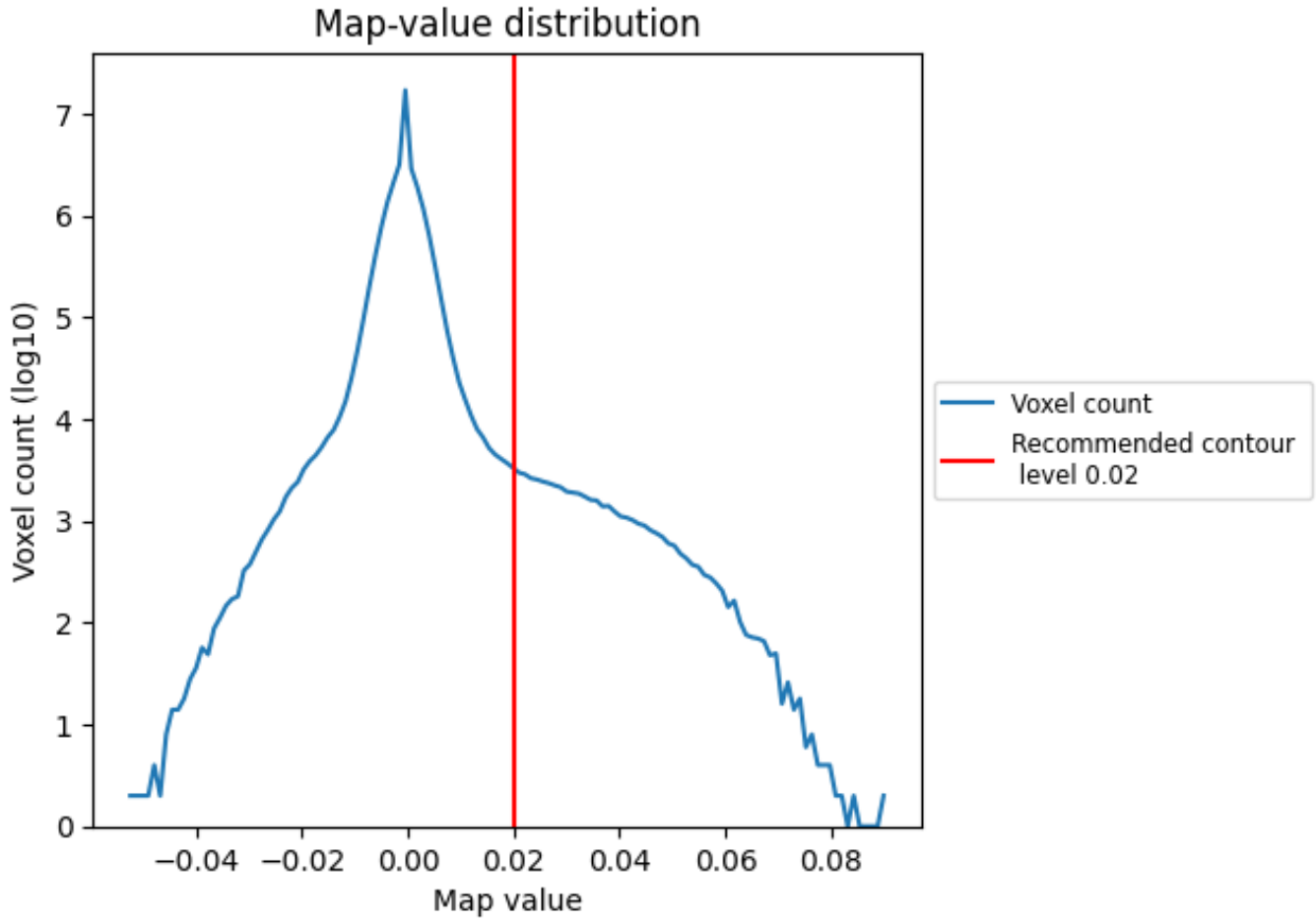
6.6 Mask visualisation (i)

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

7 Map analysis

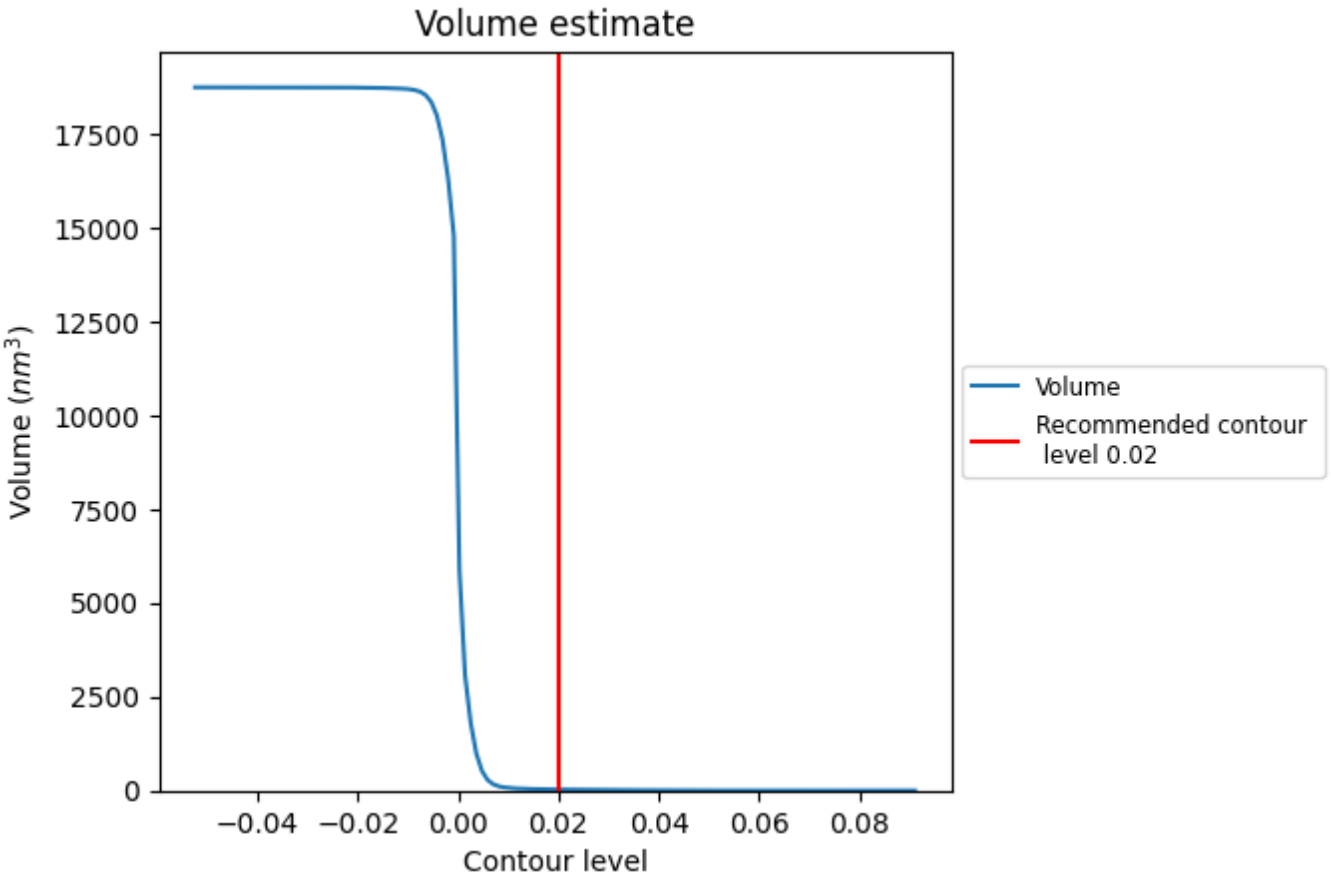
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

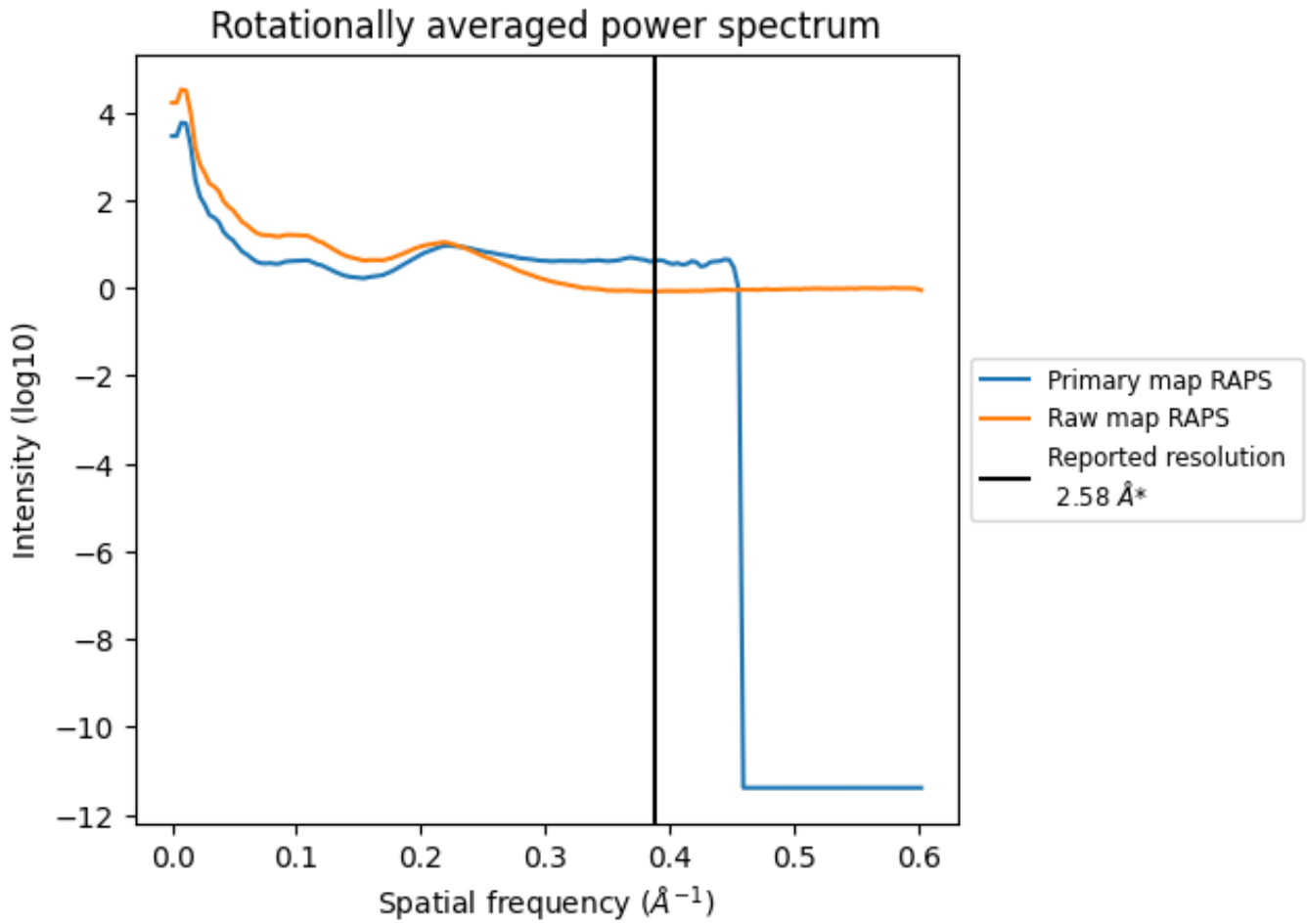
7.2 Volume estimate (i)



The volume at the recommended contour level is 29 nm^3; this corresponds to an approximate mass of 26 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)

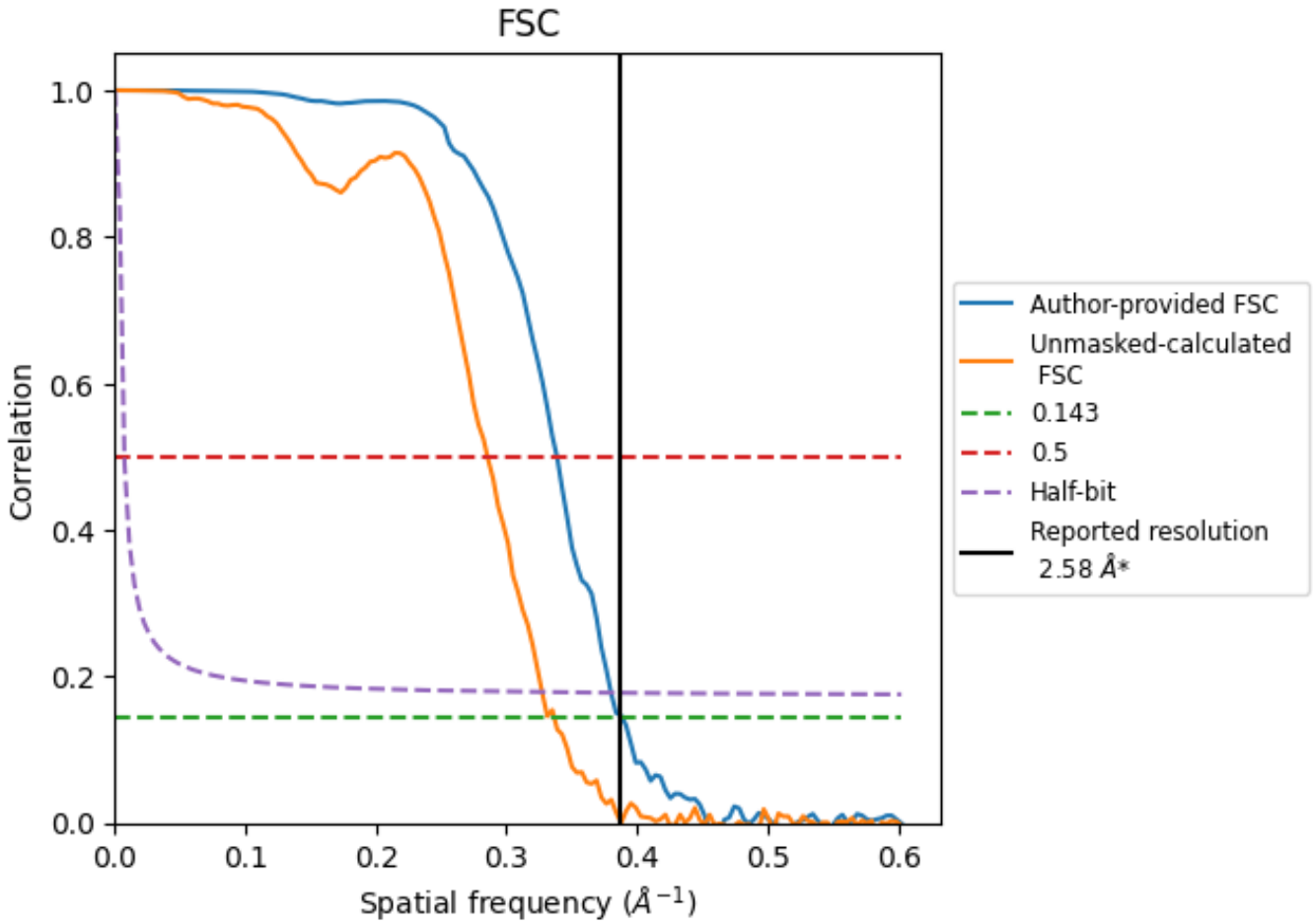


*Reported resolution corresponds to spatial frequency of 0.388 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.388 Å^{-1}

8.2 Resolution estimates (i)

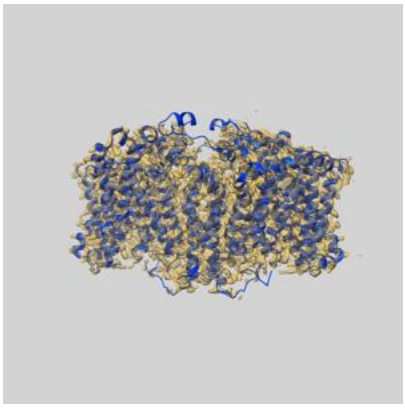
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.58	-	-
Author-provided FSC curve	2.57	2.95	2.63
Unmasked-calculated*	2.97	3.50	3.06

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.97 differs from the reported value 2.58 by more than 10 %

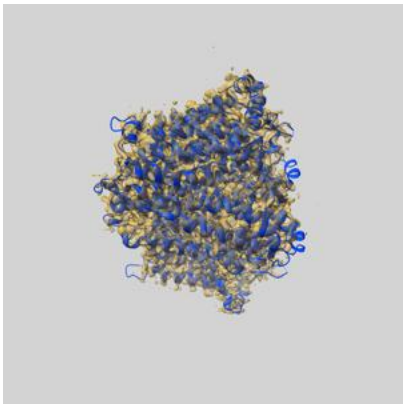
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-41187 and PDB model 8TEI. Per-residue inclusion information can be found in section 3 on page 6.

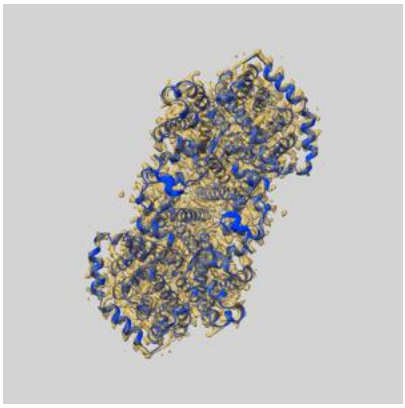
9.1 Map-model overlay



X



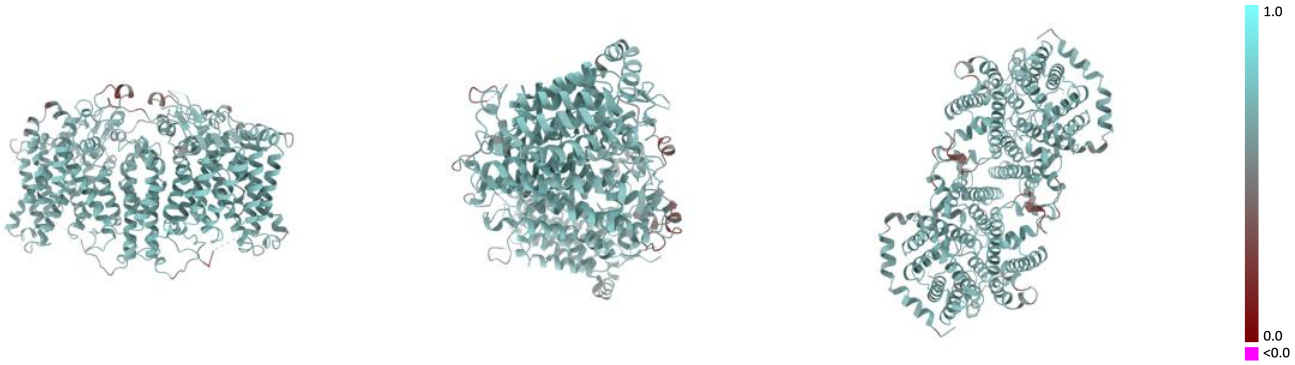
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02 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.

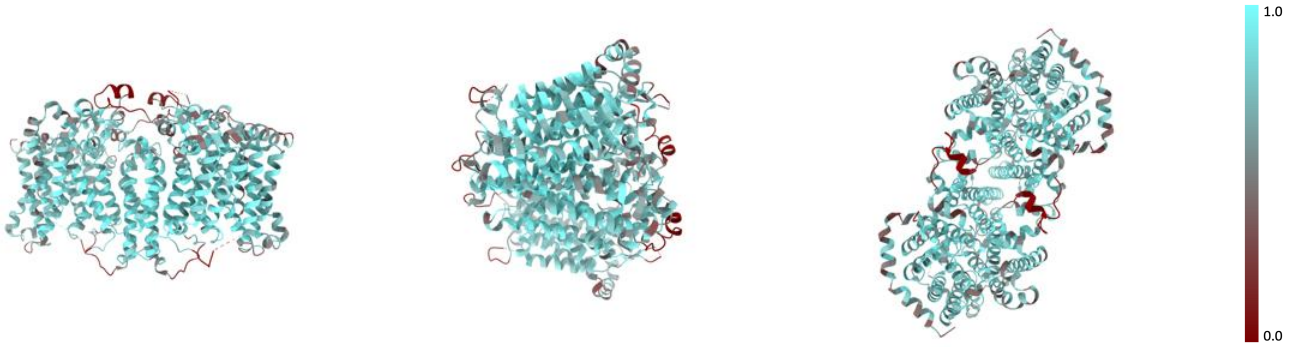
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

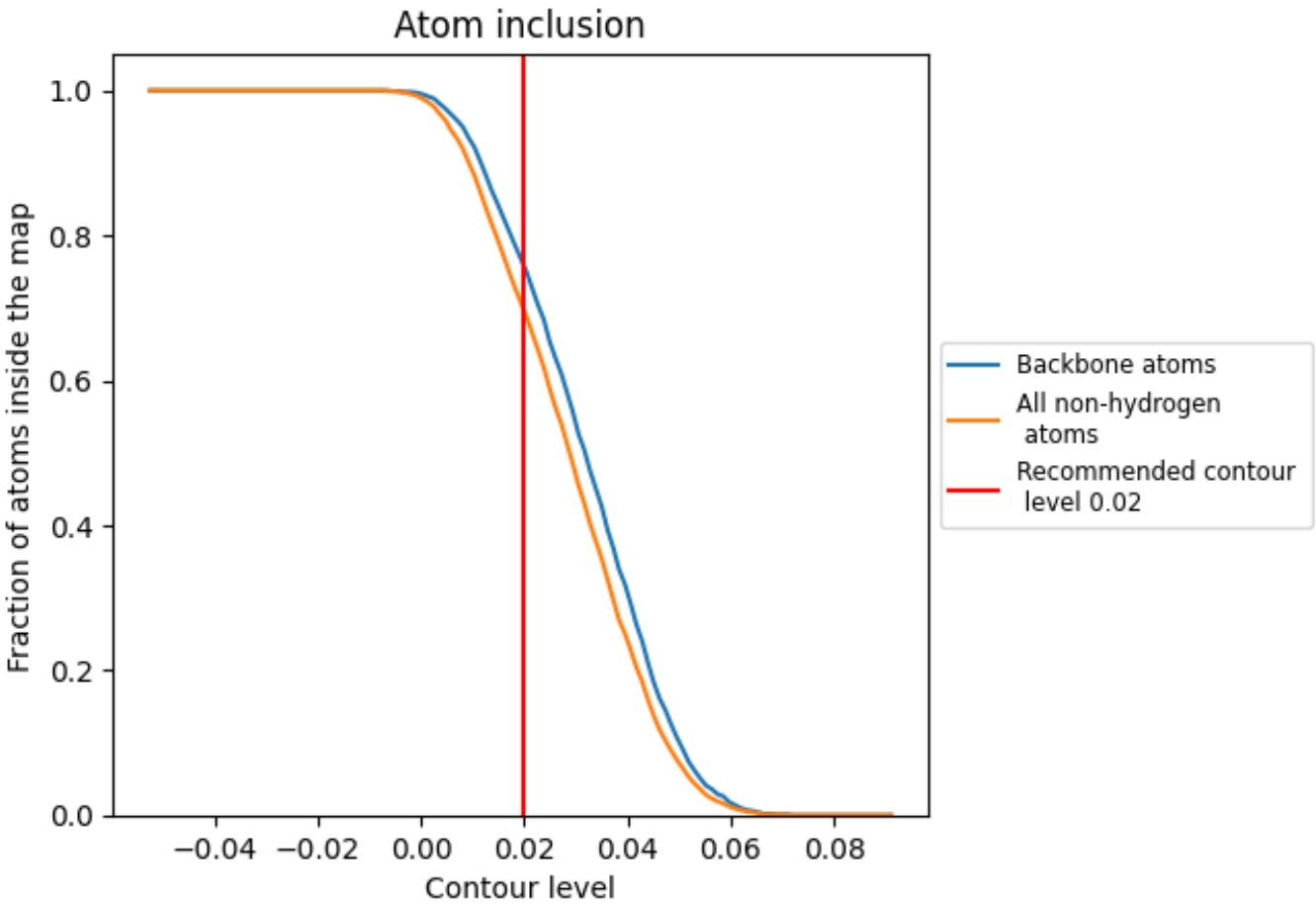
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.02).

9.4 Atom inclusion (i)



At the recommended contour level, 76% of all backbone atoms, 70% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6960	0.6290
A	0.6990	0.6290
B	0.6980	0.6290