



Full wwPDB EM Validation Report ⓘ

Sep 10, 2026 – 04:10 pm BST

PDB ID : 9R8M / pdb_00009r8m
EMDB ID : EMD-53831
Title : Structure of human NHE6.1 bound to PIP2
Authors : Hansen, J.S.; Pike, A.C.W.; Chi, G.; Wolf, G.; Ingles-Prieto, A.; Tranberg-Jensen, J.; Ye, M.; Speedman, D.; Goericke, F.; Sauer, D.B.; Beck, H.; Superti-Furga, G.; Huber, K.V.M.
Deposited on : 2025-05-16
Resolution : 2.55 Å(reported)
Based on initial model : .

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.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

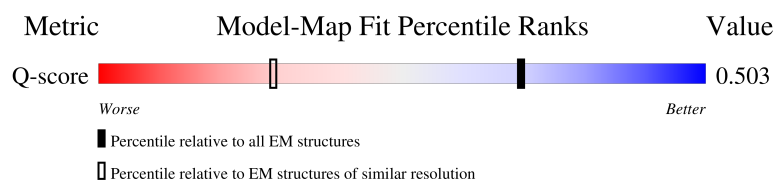
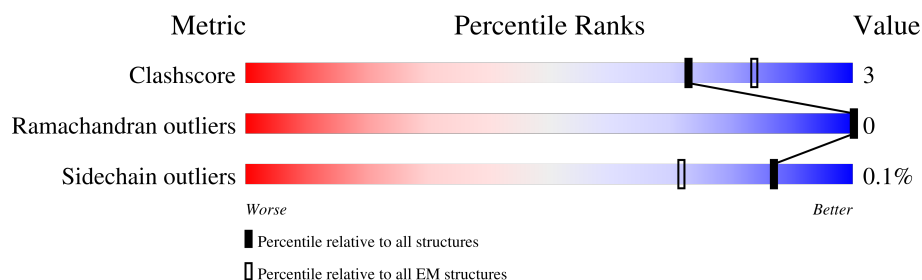
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.55 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7475 (2.05 - 3.05)

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	772	
1	B	772	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8838 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 Isoform 2 of Sodium/hydrogen exchanger 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	539	Total	C	N	O	S	0	0
			4204	2763	681	734	26		
1	B	539	Total	C	N	O	S	0	0
			4204	2763	681	734	26		

There are 142 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	702	ASP	-	expression tag	UNP Q92581
A	703	PRO	-	expression tag	UNP Q92581
A	704	ALA	-	expression tag	UNP Q92581
A	705	PHE	-	expression tag	UNP Q92581
A	706	LEU	-	expression tag	UNP Q92581
A	707	TYR	-	expression tag	UNP Q92581
A	708	LYS	-	expression tag	UNP Q92581
A	709	VAL	-	expression tag	UNP Q92581
A	710	VAL	-	expression tag	UNP Q92581
A	711	ASP	-	expression tag	UNP Q92581
A	712	ILE	-	expression tag	UNP Q92581
A	713	LYS	-	expression tag	UNP Q92581
A	714	ALA	-	expression tag	UNP Q92581
A	715	ALA	-	expression tag	UNP Q92581
A	716	ASP	-	expression tag	UNP Q92581
A	717	ILE	-	expression tag	UNP Q92581
A	718	THR	-	expression tag	UNP Q92581
A	719	SER	-	expression tag	UNP Q92581
A	720	LEU	-	expression tag	UNP Q92581
A	721	TYR	-	expression tag	UNP Q92581
A	722	LYS	-	expression tag	UNP Q92581
A	723	LYS	-	expression tag	UNP Q92581
A	724	VAL	-	expression tag	UNP Q92581
A	725	GLY	-	expression tag	UNP Q92581
A	726	TRP	-	expression tag	UNP Q92581
A	727	SER	-	expression tag	UNP Q92581

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	728	HIS	-	expression tag	UNP Q92581
A	729	PRO	-	expression tag	UNP Q92581
A	730	GLN	-	expression tag	UNP Q92581
A	731	PHE	-	expression tag	UNP Q92581
A	732	GLU	-	expression tag	UNP Q92581
A	733	LYS	-	expression tag	UNP Q92581
A	734	GLY	-	expression tag	UNP Q92581
A	735	GLY	-	expression tag	UNP Q92581
A	736	GLY	-	expression tag	UNP Q92581
A	737	SER	-	expression tag	UNP Q92581
A	738	GLY	-	expression tag	UNP Q92581
A	739	GLY	-	expression tag	UNP Q92581
A	740	GLY	-	expression tag	UNP Q92581
A	741	SER	-	expression tag	UNP Q92581
A	742	GLY	-	expression tag	UNP Q92581
A	743	GLY	-	expression tag	UNP Q92581
A	744	GLY	-	expression tag	UNP Q92581
A	745	SER	-	expression tag	UNP Q92581
A	746	TRP	-	expression tag	UNP Q92581
A	747	SER	-	expression tag	UNP Q92581
A	748	HIS	-	expression tag	UNP Q92581
A	749	PRO	-	expression tag	UNP Q92581
A	750	GLN	-	expression tag	UNP Q92581
A	751	PHE	-	expression tag	UNP Q92581
A	752	GLU	-	expression tag	UNP Q92581
A	753	LYS	-	expression tag	UNP Q92581
A	754	GLY	-	expression tag	UNP Q92581
A	755	THR	-	expression tag	UNP Q92581
A	756	GLU	-	expression tag	UNP Q92581
A	757	LEU	-	expression tag	UNP Q92581
A	758	GLY	-	expression tag	UNP Q92581
A	759	SER	-	expression tag	UNP Q92581
A	760	THR	-	expression tag	UNP Q92581
A	761	MET	-	expression tag	UNP Q92581
A	762	ALA	-	expression tag	UNP Q92581
A	763	SER	-	expression tag	UNP Q92581
A	764	TYR	-	expression tag	UNP Q92581
A	765	PRO	-	expression tag	UNP Q92581
A	766	TYR	-	expression tag	UNP Q92581
A	767	ASP	-	expression tag	UNP Q92581
A	768	VAL	-	expression tag	UNP Q92581
A	769	PRO	-	expression tag	UNP Q92581

Continued on next page...

Continued from previous page...

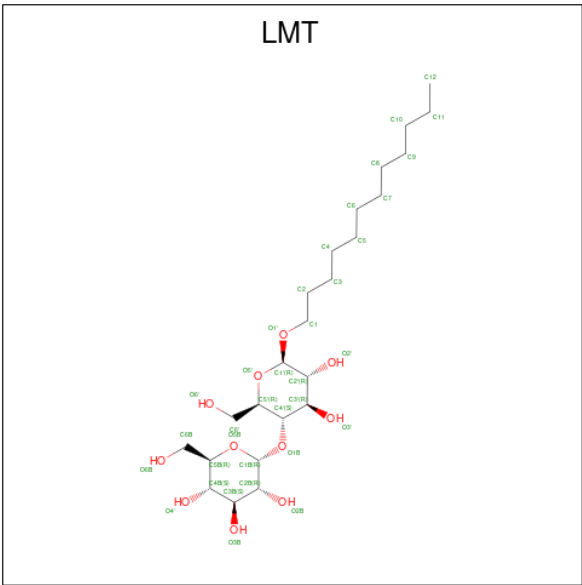
Chain	Residue	Modelled	Actual	Comment	Reference
A	770	ASP	-	expression tag	UNP Q92581
A	771	TYR	-	expression tag	UNP Q92581
A	772	ALA	-	expression tag	UNP Q92581
B	702	ASP	-	expression tag	UNP Q92581
B	703	PRO	-	expression tag	UNP Q92581
B	704	ALA	-	expression tag	UNP Q92581
B	705	PHE	-	expression tag	UNP Q92581
B	706	LEU	-	expression tag	UNP Q92581
B	707	TYR	-	expression tag	UNP Q92581
B	708	LYS	-	expression tag	UNP Q92581
B	709	VAL	-	expression tag	UNP Q92581
B	710	VAL	-	expression tag	UNP Q92581
B	711	ASP	-	expression tag	UNP Q92581
B	712	ILE	-	expression tag	UNP Q92581
B	713	LYS	-	expression tag	UNP Q92581
B	714	ALA	-	expression tag	UNP Q92581
B	715	ALA	-	expression tag	UNP Q92581
B	716	ASP	-	expression tag	UNP Q92581
B	717	ILE	-	expression tag	UNP Q92581
B	718	THR	-	expression tag	UNP Q92581
B	719	SER	-	expression tag	UNP Q92581
B	720	LEU	-	expression tag	UNP Q92581
B	721	TYR	-	expression tag	UNP Q92581
B	722	LYS	-	expression tag	UNP Q92581
B	723	LYS	-	expression tag	UNP Q92581
B	724	VAL	-	expression tag	UNP Q92581
B	725	GLY	-	expression tag	UNP Q92581
B	726	TRP	-	expression tag	UNP Q92581
B	727	SER	-	expression tag	UNP Q92581
B	728	HIS	-	expression tag	UNP Q92581
B	729	PRO	-	expression tag	UNP Q92581
B	730	GLN	-	expression tag	UNP Q92581
B	731	PHE	-	expression tag	UNP Q92581
B	732	GLU	-	expression tag	UNP Q92581
B	733	LYS	-	expression tag	UNP Q92581
B	734	GLY	-	expression tag	UNP Q92581
B	735	GLY	-	expression tag	UNP Q92581
B	736	GLY	-	expression tag	UNP Q92581
B	737	SER	-	expression tag	UNP Q92581
B	738	GLY	-	expression tag	UNP Q92581
B	739	GLY	-	expression tag	UNP Q92581
B	740	GLY	-	expression tag	UNP Q92581

Continued on next page...

Continued from previous page...

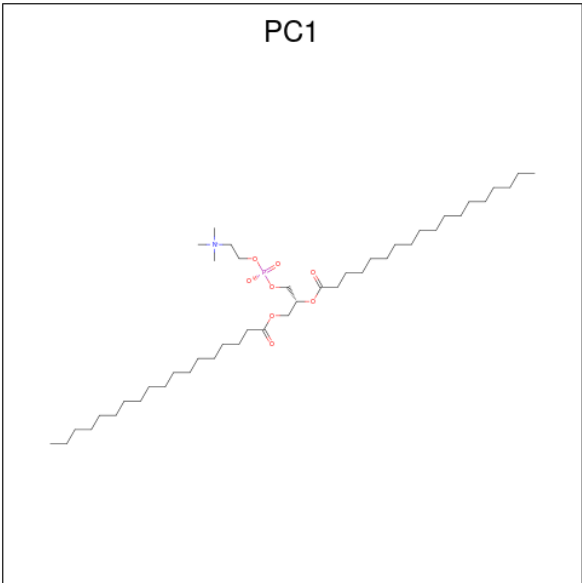
Chain	Residue	Modelled	Actual	Comment	Reference
B	741	SER	-	expression tag	UNP Q92581
B	742	GLY	-	expression tag	UNP Q92581
B	743	GLY	-	expression tag	UNP Q92581
B	744	GLY	-	expression tag	UNP Q92581
B	745	SER	-	expression tag	UNP Q92581
B	746	TRP	-	expression tag	UNP Q92581
B	747	SER	-	expression tag	UNP Q92581
B	748	HIS	-	expression tag	UNP Q92581
B	749	PRO	-	expression tag	UNP Q92581
B	750	GLN	-	expression tag	UNP Q92581
B	751	PHE	-	expression tag	UNP Q92581
B	752	GLU	-	expression tag	UNP Q92581
B	753	LYS	-	expression tag	UNP Q92581
B	754	GLY	-	expression tag	UNP Q92581
B	755	THR	-	expression tag	UNP Q92581
B	756	GLU	-	expression tag	UNP Q92581
B	757	LEU	-	expression tag	UNP Q92581
B	758	GLY	-	expression tag	UNP Q92581
B	759	SER	-	expression tag	UNP Q92581
B	760	THR	-	expression tag	UNP Q92581
B	761	MET	-	expression tag	UNP Q92581
B	762	ALA	-	expression tag	UNP Q92581
B	763	SER	-	expression tag	UNP Q92581
B	764	TYR	-	expression tag	UNP Q92581
B	765	PRO	-	expression tag	UNP Q92581
B	766	TYR	-	expression tag	UNP Q92581
B	767	ASP	-	expression tag	UNP Q92581
B	768	VAL	-	expression tag	UNP Q92581
B	769	PRO	-	expression tag	UNP Q92581
B	770	ASP	-	expression tag	UNP Q92581
B	771	TYR	-	expression tag	UNP Q92581
B	772	ALA	-	expression tag	UNP Q92581

- Molecule 2 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



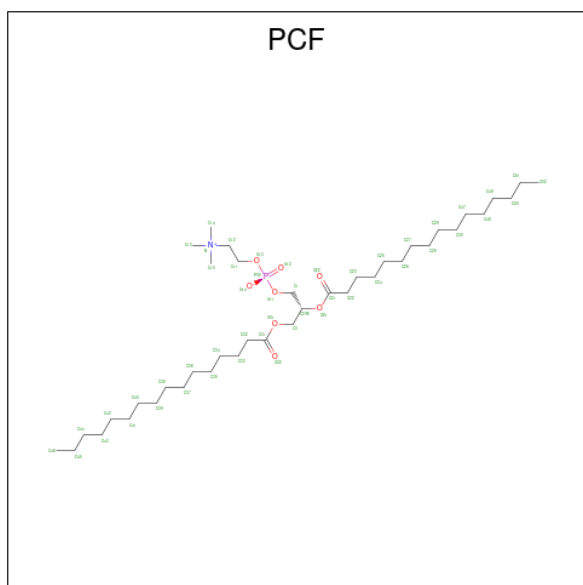
Mol	Chain	Residues	Atoms			AltConf
2	A	1	Total	C	O	0
			35	24	11	
2	B	1	Total	C	O	0
			35	24	11	
2	B	1	Total	C	O	0
			35	24	11	
2	B	1	Total	C	O	0
			35	24	11	

- Molecule 3 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: C₄₄H₈₈NO₈P).



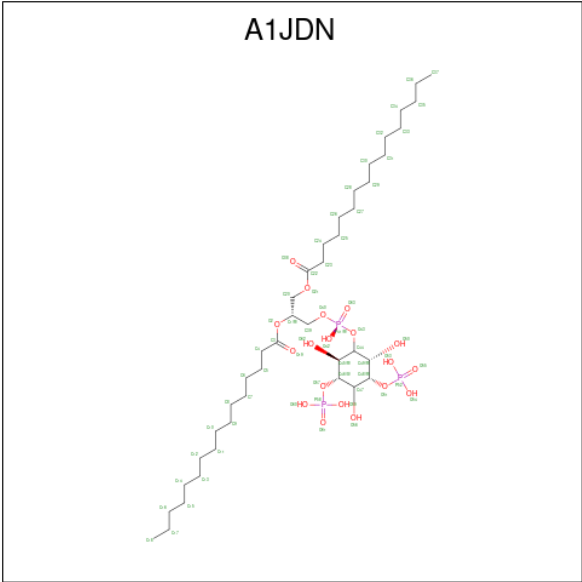
Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			39	29	1	8	1	
3	B	1	Total	C	N	O	P	0
			39	29	1	8	1	

- Molecule 4 is 1,2-DIACYL-SN-GLYCERO-3-PHOSHOCHOLINE (CCD ID: PCF) (formula: $C_{40}H_{80}NO_8P$).

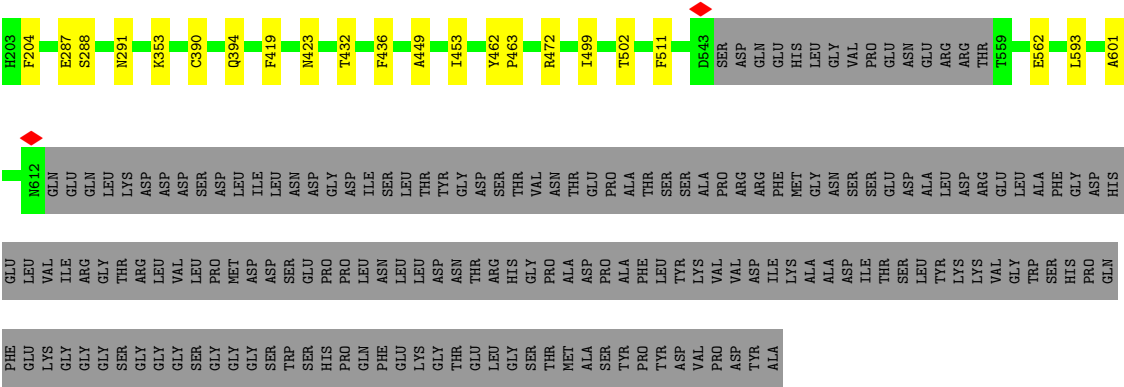


Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			43	33	1	8	1	
4	B	1	Total	C	N	O	P	0
			43	33	1	8	1	

- Molecule 5 is Dipalmitoyl Phosphatidylinositol 3,5-bisphosphate (CCD ID: A1JDN) (formula: $C_{41}H_{81}O_{19}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	O	P	0
			63	41	19	3	
5	B	1	Total	C	O	P	0
			63	41	19	3	



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	586700	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; Patch CTF in cryoSPARC	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	130000	Depositor
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	1.346	Depositor
Minimum map value	-0.544	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.029	Depositor
Recommended contour level	0.22	Depositor
Map size ($\text{\AA}$)	335.52, 335.52, 335.52	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.932, 0.932, 0.932	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PCF, LMT, A1JDN, PC1

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	0.13	0/4311	0.31	0/5861
1	B	0.13	0/4311	0.30	0/5861
All	All	0.13	0/8622	0.31	0/11722

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	4204	0	4200	34	0
1	B	4204	0	4200	26	0
2	A	35	0	46	3	0
2	B	105	0	138	5	0
3	A	39	0	52	3	0
3	B	39	0	52	3	0
4	A	43	0	63	0	0
4	B	43	0	63	0	0
5	A	63	0	0	1	0
5	B	63	0	0	2	0
All	All	8838	0	8814	59	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 (59) 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:562:GLU:HB3	3:B:804:PC1:H143	1.71	0.72
1:A:166:ASN:ND2	1:A:169:ASP:OD1	2.22	0.72
1:A:562:GLU:HB3	3:A:802:PC1:H143	1.73	0.69
1:A:190:PRO:HG3	2:A:801:LMT:H111	1.79	0.65
1:A:182:VAL:HG21	2:A:801:LMT:H6E	1.86	0.58
1:B:202:ARG:HB2	1:B:204:PHE:CE2	2.40	0.56
1:A:88:ILE:HG12	1:A:101:GLU:HG3	1.87	0.56
1:A:143:LEU:HD22	1:B:130:THR:HB	1.88	0.56
1:B:287:GLU:OE2	1:B:291:ASN:ND2	2.39	0.55
1:A:89:TRP:HE1	1:B:353:LYS:HB2	1.71	0.55
1:A:182:VAL:HG13	1:A:186:ILE:HD12	1.89	0.55
5:B:806:A1JDN:O55	5:B:806:A1JDN:O50	2.25	0.55
1:A:202:ARG:HB2	1:A:204:PHE:CE2	2.42	0.55
1:A:87:THR:HB	1:A:104:LEU:HD21	1.89	0.54
1:A:287:GLU:OE2	1:A:291:ASN:ND2	2.40	0.54
1:B:182:VAL:HG13	1:B:186:ILE:HD12	1.91	0.52
1:B:88:ILE:HG12	1:B:101:GLU:HG3	1.91	0.51
1:B:182:VAL:HG21	2:B:802:LMT:H6E	1.93	0.51
1:A:144:VAL:HG21	1:B:142:LEU:HD11	1.93	0.50
1:A:207:ASN:OD1	1:A:472:ARG:NH2	2.41	0.50
1:A:153:TYR:HB3	1:B:153:TYR:HB3	1.93	0.49
1:B:432:THR:HG21	1:B:511:PHE:HZ	1.79	0.47
1:B:472:ARG:HG3	3:B:804:PC1:H132	1.97	0.47
1:B:190:PRO:HG3	2:B:802:LMT:H111	1.96	0.47
2:B:801:LMT:H3'	2:B:801:LMT:H1B	1.72	0.47
1:A:117:ARG:NH1	1:A:434:PHE:O	2.47	0.46
1:A:131:LEU:HD12	1:B:142:LEU:HA	1.97	0.46
2:B:803:LMT:H3'	2:B:803:LMT:H1B	1.70	0.45
5:A:804:A1JDN:O55	5:A:804:A1JDN:O50	2.34	0.45
1:A:472:ARG:HG3	3:A:802:PC1:H132	1.97	0.45
1:B:390:CYS:O	1:B:394:GLN:HG2	2.17	0.45
3:B:804:PC1:H31	3:B:804:PC1:H321	1.55	0.45
1:A:432:THR:HG21	1:A:511:PHE:HZ	1.83	0.44
5:B:806:A1JDN:O42	5:B:806:A1JDN:O62	2.36	0.44
1:A:199:LEU:HA	1:A:204:PHE:CE2	2.53	0.44
1:A:73:ASN:HD21	1:A:175:LYS:HB3	1.82	0.43
1:A:419:PHE:O	1:A:423:ASN:ND2	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:419:PHE:O	1:B:423:ASN:ND2	2.50	0.43
1:A:462:TYR:HB2	1:A:463:PRO:HD3	2.00	0.43
1:A:258:ILE:HG12	1:A:497:LEU:HB3	2.01	0.43
1:B:593:LEU:HD12	1:B:601:ALA:HB2	2.00	0.43
1:A:178:PHE:CD1	2:A:801:LMT:H6D	2.54	0.42
1:A:143:LEU:HB2	1:B:131:LEU:HB2	2.01	0.42
1:A:390:CYS:O	1:A:394:GLN:HG2	2.19	0.42
1:B:288:SER:HA	1:B:291:ASN:ND2	2.35	0.42
1:A:200:LYS:HG2	1:A:201:ARG:HG3	2.00	0.42
1:A:276:VAL:HG22	1:A:540:VAL:HG12	2.01	0.41
1:A:399:TYR:O	1:A:407:GLN:NE2	2.49	0.41
3:A:802:PC1:H321	3:A:802:PC1:H31	1.55	0.41
1:B:436:PHE:HZ	1:B:502:THR:HG21	1.85	0.41
1:B:449:ALA:O	1:B:453:ILE:HG23	2.20	0.41
1:A:449:ALA:O	1:A:453:ILE:HG23	2.21	0.41
1:A:593:LEU:HD12	1:A:601:ALA:HB2	2.02	0.41
1:A:142:LEU:HA	1:B:131:LEU:HD12	2.02	0.41
1:B:462:TYR:HB2	1:B:463:PRO:HD3	2.02	0.41
1:A:353:LYS:HB2	1:B:89:TRP:HE1	1.86	0.40
1:B:70:ASP:OD1	2:B:802:LMT:O4'	2.35	0.40
1:B:180:PRO:HB3	1:B:499:ILE:HG23	2.04	0.40
1:A:124:SER:H	1:A:168:GLN:HB3	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	535/772 (69%)	519 (97%)	16 (3%)	0	100	100
1	B	535/772 (69%)	519 (97%)	16 (3%)	0	100	100
All	All	1070/1544 (69%)	1038 (97%)	32 (3%)	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	448/644 (70%)	448 (100%)	0	100	100
1	B	448/644 (70%)	447 (100%)	1 (0%)	87	93
All	All	896/1288 (70%)	895 (100%)	1 (0%)	87	94

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	160	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	HIS
1	A	408	HIS
1	A	412	GLN
1	B	408	HIS
1	B	412	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

10 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$
5	A1JDN	B	806	-	63,63,63	0.55	1 (1%)	77,81,81	0.62	1 (1%)
4	PCF	A	803	-	42,42,49	0.29	0	48,50,57	0.33	0
2	LMT	B	801	-	36,36,36	0.55	0	47,47,47	0.76	0
3	PC1	B	804	-	38,38,53	0.31	0	44,46,61	0.32	0
2	LMT	B	803	-	36,36,36	0.55	0	47,47,47	0.74	0
5	A1JDN	A	804	-	63,63,63	0.57	2 (3%)	77,81,81	0.66	1 (1%)
2	LMT	B	802	-	36,36,36	0.53	0	47,47,47	1.06	4 (8%)
4	PCF	B	805	-	42,42,49	0.30	0	48,50,57	0.33	0
3	PC1	A	802	-	38,38,53	0.31	0	44,46,61	0.32	0
2	LMT	A	801	-	36,36,36	0.53	0	47,47,47	1.06	4 (8%)

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
5	A1JDN	B	806	-	-	28/60/84/84	0/1/1/1
4	PCF	A	803	-	-	3/46/46/53	-
2	LMT	B	801	-	-	8/21/61/61	0/2/2/2
3	PC1	B	804	-	-	5/42/42/57	-
2	LMT	B	803	-	-	7/21/61/61	0/2/2/2
5	A1JDN	A	804	-	-	27/60/84/84	0/1/1/1
2	LMT	B	802	-	-	11/21/61/61	0/2/2/2
4	PCF	B	805	-	-	2/46/46/53	-
3	PC1	A	802	-	-	5/42/42/57	-
2	LMT	A	801	-	-	11/21/61/61	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	804	A1JDN	P41-O43	2.19	1.66	1.60
5	A	804	A1JDN	P52-O51	2.15	1.63	1.59
5	B	806	A1JDN	P52-O51	2.15	1.63	1.59

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	804	A1JDN	P41-O43-C44	4.06	134.18	119.41
5	B	806	A1JDN	P41-O43-C44	3.69	132.83	119.41
2	B	802	LMT	O5'-C5'-C4'	3.37	116.85	109.75
2	A	801	LMT	O5'-C5'-C4'	3.32	116.74	109.75
2	B	802	LMT	C1'-O5'-C5'	3.03	119.63	113.69
2	A	801	LMT	C1'-O5'-C5'	2.94	119.45	113.69
2	A	801	LMT	C1'-C2'-C3'	-2.60	104.58	110.00
2	B	802	LMT	C1'-C2'-C3'	-2.48	104.83	110.00
2	A	801	LMT	C3'-C4'-C5'	2.42	116.48	110.93
2	B	802	LMT	C3'-C4'-C5'	2.39	116.41	110.93

There are no chirality outliers.

All (107) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	LMT	O5'-C1'-O1'-C1
2	B	802	LMT	O5'-C1'-O1'-C1
3	A	802	PC1	O32-C31-O31-C3
3	A	802	PC1	C32-C31-O31-C3
3	B	804	PC1	O32-C31-O31-C3
3	B	804	PC1	C32-C31-O31-C3
5	A	804	A1JDN	O2-C1-C39-O40
5	A	804	A1JDN	C45-C44-O43-P41
5	A	804	A1JDN	C47-C48-O51-P52
5	A	804	A1JDN	C49-C48-O51-P52
5	A	804	A1JDN	C44-O43-P41-O42
5	B	806	A1JDN	C45-C44-O43-P41
5	B	806	A1JDN	C47-C48-O51-P52
5	B	806	A1JDN	C39-O40-P41-O42
5	B	806	A1JDN	C39-O40-P41-O63
5	B	806	A1JDN	C44-O43-P41-O63
2	B	801	LMT	C3'-C4'-O1B-C1B
2	B	803	LMT	C3'-C4'-O1B-C1B
2	B	801	LMT	C4'-C5'-C6'-O6'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	803	LMT	C4'-C5'-C6'-O6'
5	B	806	A1JDN	C31-C32-C33-C34
2	A	801	LMT	O1'-C1-C2-C3
5	B	806	A1JDN	C3-C4-C5-C6
2	A	801	LMT	C6-C7-C8-C9
2	B	802	LMT	O1'-C1-C2-C3
2	B	802	LMT	C6-C7-C8-C9
2	B	803	LMT	O5'-C5'-C6'-O6'
2	B	801	LMT	O5'-C5'-C6'-O6'
5	B	806	A1JDN	C39-O40-P41-O43
5	B	806	A1JDN	C6-C7-C8-C9
5	A	804	A1JDN	C44-O43-P41-O40
5	B	806	A1JDN	C10-C11-C12-C13
5	A	804	A1JDN	C24-C25-C26-C27
2	A	801	LMT	C2'-C1'-O1'-C1
2	B	802	LMT	C2'-C1'-O1'-C1
5	B	806	A1JDN	C49-C48-O51-P52
5	A	804	A1JDN	C9-C10-C11-C12
5	B	806	A1JDN	C14-C15-C16-C17
5	A	804	A1JDN	C28-C29-C30-C31
5	B	806	A1JDN	C5-C6-C7-C8
5	A	804	A1JDN	C15-C16-C17-C18
5	A	804	A1JDN	C29-C30-C31-C32
5	B	806	A1JDN	C30-C31-C32-C33
2	B	802	LMT	O5'-C5'-C6'-O6'
5	B	806	A1JDN	C28-C29-C30-C31
2	A	801	LMT	O5'-C5'-C6'-O6'
5	A	804	A1JDN	C25-C26-C27-C28
2	B	802	LMT	C1-C2-C3-C4
5	A	804	A1JDN	C30-C31-C32-C33
2	A	801	LMT	C2-C3-C4-C5
5	B	806	A1JDN	C27-C28-C29-C30
2	B	802	LMT	C2-C3-C4-C5
5	B	806	A1JDN	C4-C5-C6-C7
2	A	801	LMT	C1-C2-C3-C4
5	A	804	A1JDN	C20-C1-C39-O40
5	A	804	A1JDN	C39-C1-C20-O21
5	B	806	A1JDN	C11-C10-C9-C8
5	A	804	A1JDN	C3-C4-C5-C6
5	A	804	A1JDN	C4-C5-C6-C7
2	B	801	LMT	C6-C7-C8-C9
2	A	801	LMT	C3-C4-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	A	804	A1JDN	C44-O43-P41-O63
5	B	806	A1JDN	O2-C1-C39-O40
2	B	802	LMT	C3-C4-C5-C6
2	B	803	LMT	C6-C7-C8-C9
4	B	805	PCF	C41-C42-C43-C44
5	B	806	A1JDN	C39-C1-C20-O21
5	A	804	A1JDN	O2-C1-C20-O21
5	B	806	A1JDN	C9-C10-C11-C12
4	A	803	PCF	C41-C42-C43-C44
2	A	801	LMT	C11-C10-C9-C8
2	B	802	LMT	C11-C10-C9-C8
5	B	806	A1JDN	C26-C27-C28-C29
2	B	803	LMT	C7-C8-C9-C10
5	A	804	A1JDN	C11-C10-C9-C8
2	B	801	LMT	O5'-C1'-O1'-C1
2	B	801	LMT	C7-C8-C9-C10
2	B	801	LMT	C9-C10-C11-C12
5	B	806	A1JDN	C44-O43-P41-O40
2	B	803	LMT	C11-C10-C9-C8
2	B	803	LMT	C9-C10-C11-C12
2	B	801	LMT	C11-C10-C9-C8
5	A	804	A1JDN	O21-C22-C23-C24
5	B	806	A1JDN	O2-C1-C20-O21
2	A	801	LMT	C5-C6-C7-C8
4	B	805	PCF	C36-C37-C38-C39
5	B	806	A1JDN	O21-C22-C23-C24
2	B	802	LMT	C7-C8-C9-C10
2	B	802	LMT	C5-C6-C7-C8
5	B	806	A1JDN	C20-C1-C39-O40
2	A	801	LMT	C7-C8-C9-C10
5	A	804	A1JDN	C46-O57-P58-O61
5	A	804	A1JDN	O2-C3-C4-C5
5	A	804	A1JDN	C46-O57-P58-O59
5	A	804	A1JDN	C46-O57-P58-O60
5	B	806	A1JDN	O2-C3-C4-C5
5	A	804	A1JDN	O19-C3-C4-C5
4	A	803	PCF	C37-C38-C39-C40
5	B	806	A1JDN	O19-C3-C4-C5
4	A	803	PCF	C36-C37-C38-C39
3	A	802	PC1	C12-C11-O13-P
3	B	804	PC1	C12-C11-O13-P
5	A	804	A1JDN	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

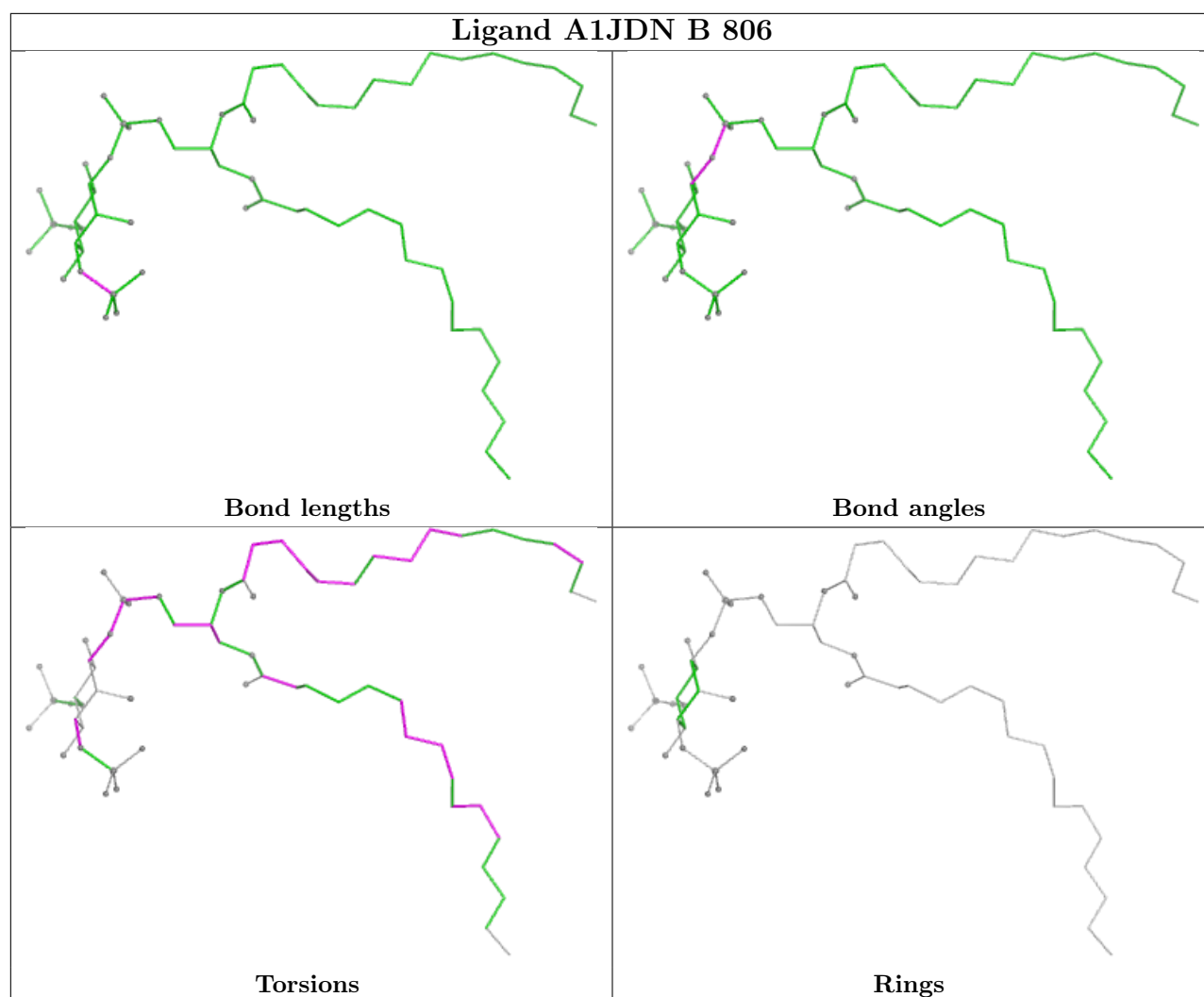
Mol	Chain	Res	Type	Atoms
3	B	804	PC1	O31-C31-C32-C33
3	A	802	PC1	O31-C31-C32-C33
3	A	802	PC1	O32-C31-C32-C33
3	B	804	PC1	O32-C31-C32-C33

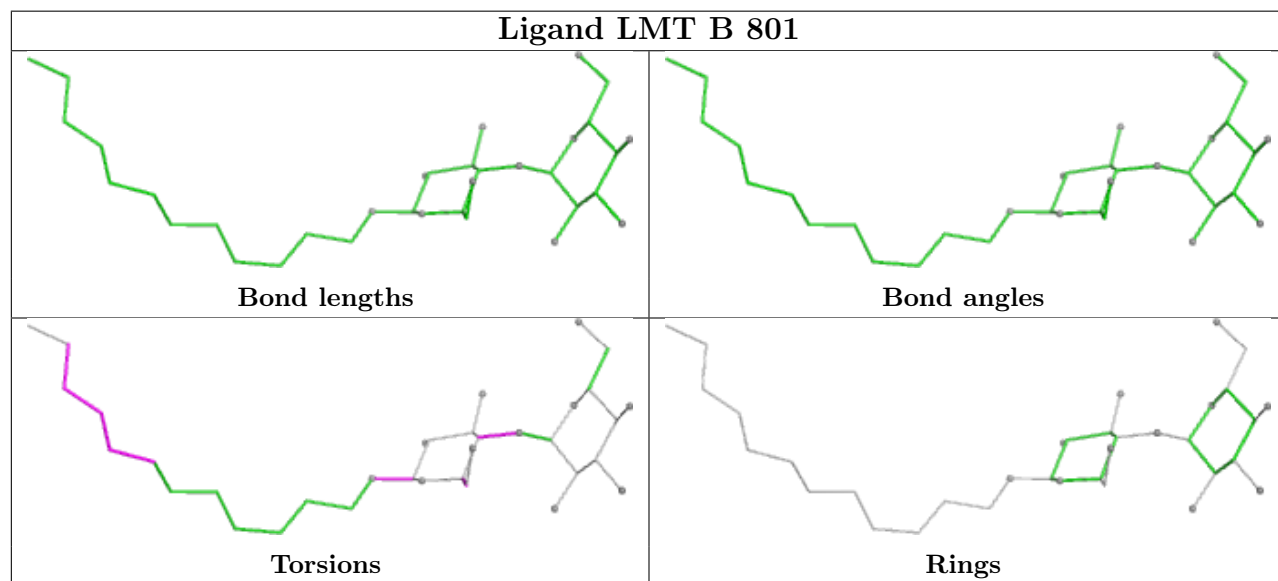
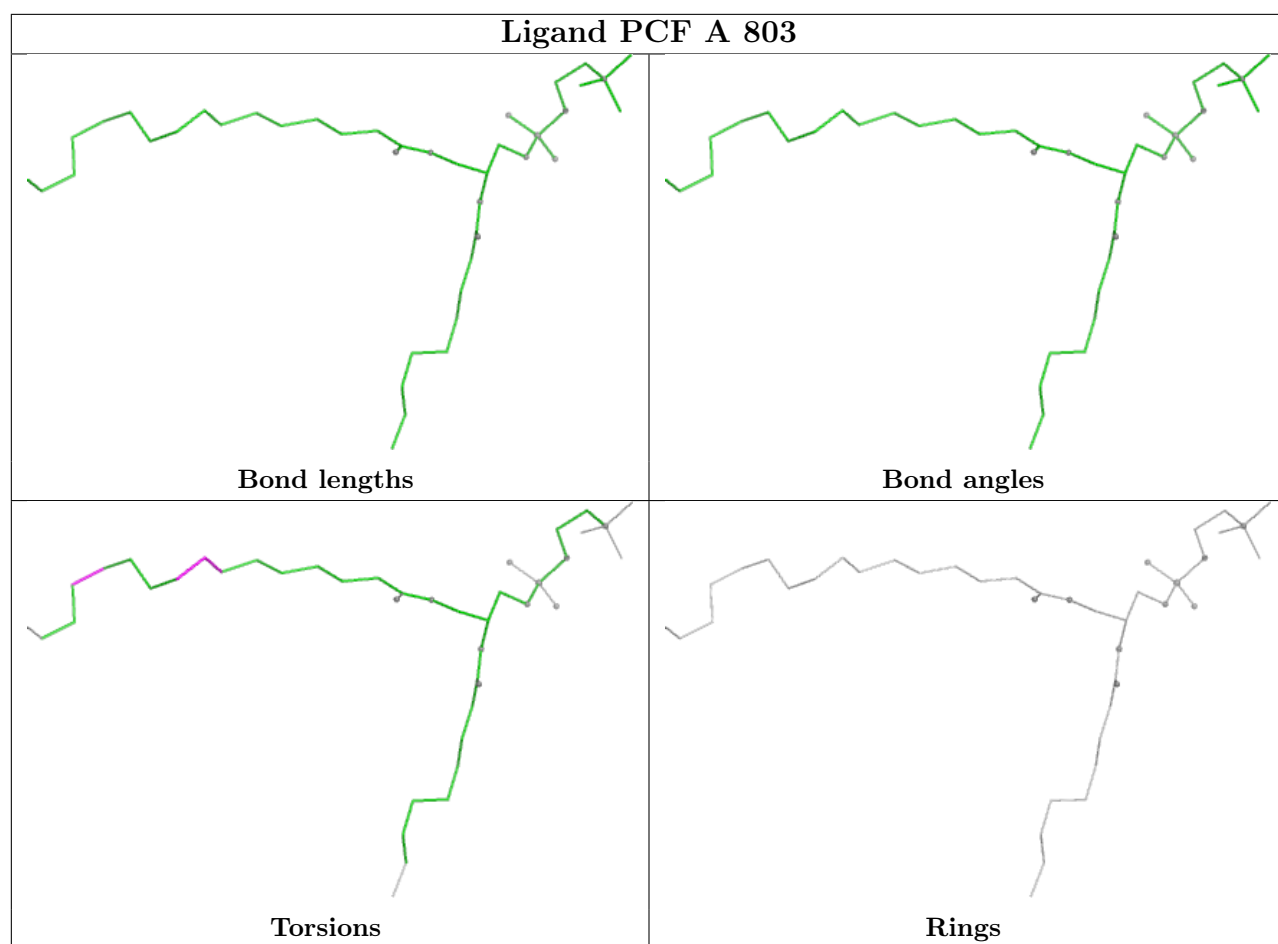
There are no ring outliers.

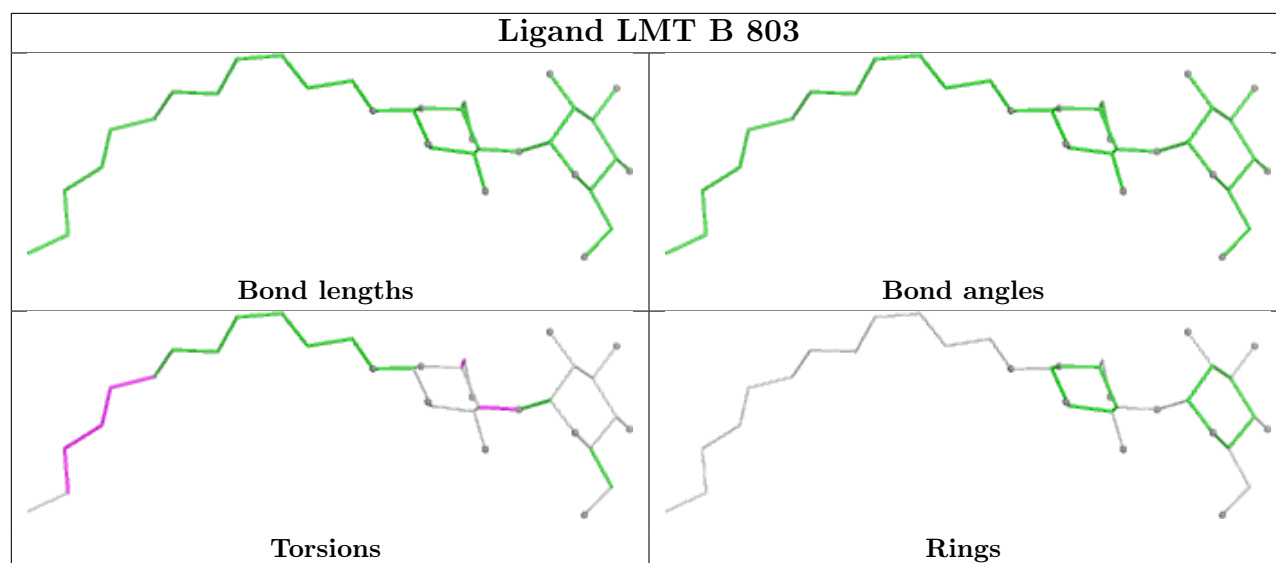
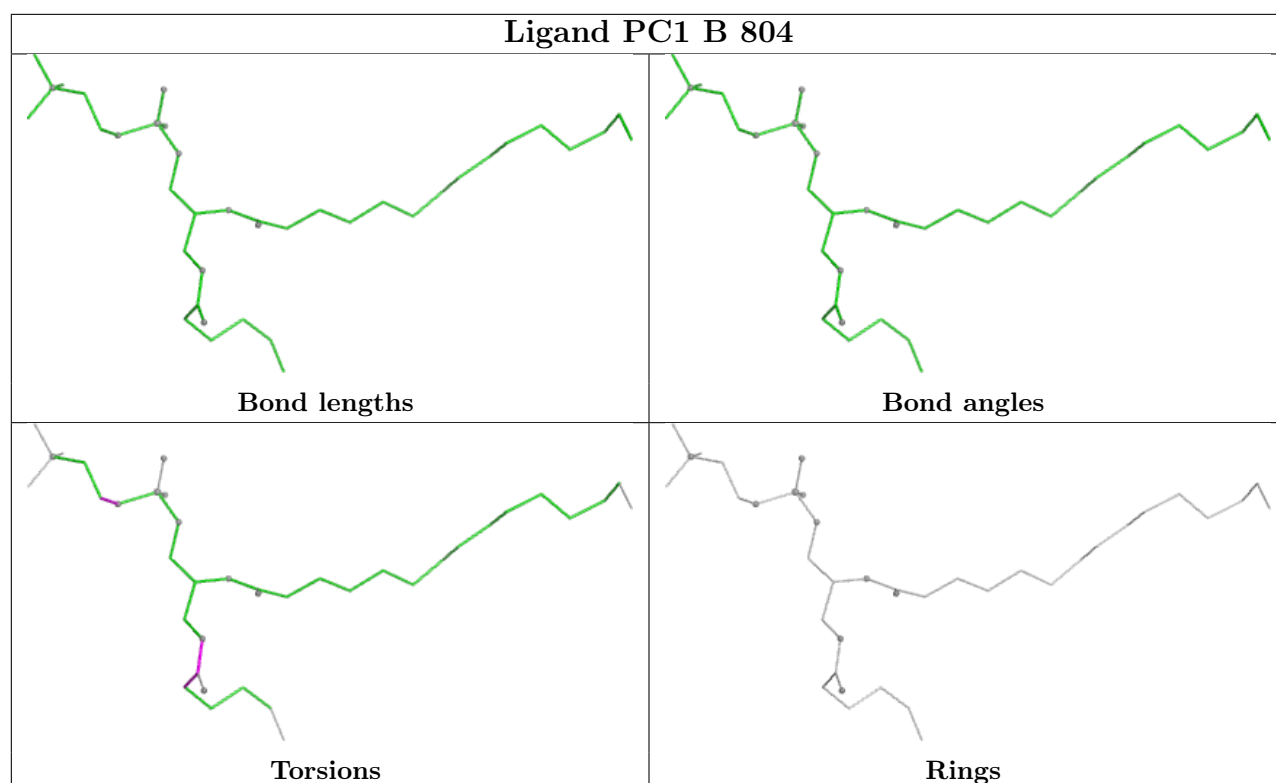
8 monomers are involved in 17 short contacts:

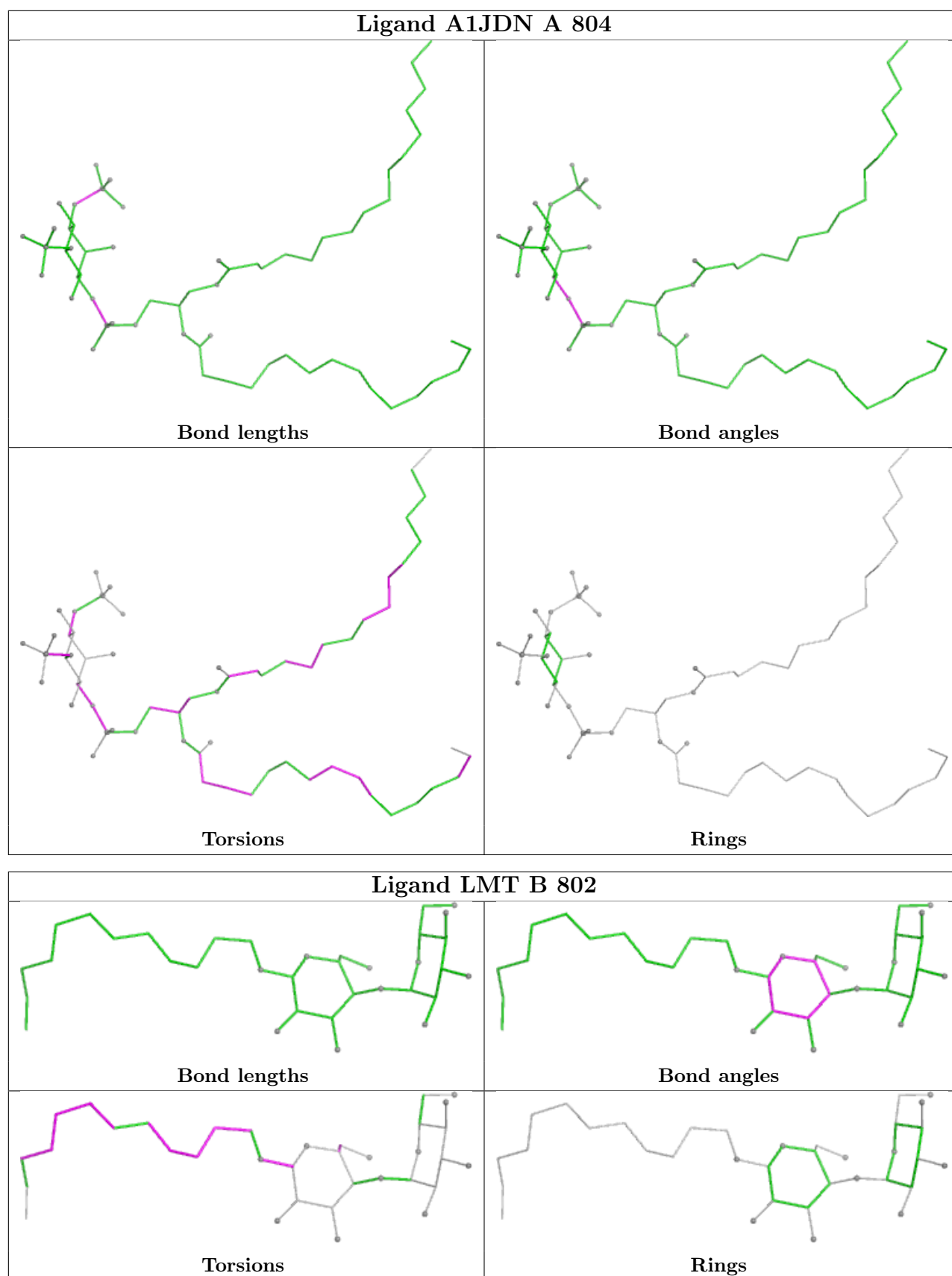
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	806	A1JDN	2	0
2	B	801	LMT	1	0
3	B	804	PC1	3	0
2	B	803	LMT	1	0
5	A	804	A1JDN	1	0
2	B	802	LMT	3	0
3	A	802	PC1	3	0
2	A	801	LMT	3	0

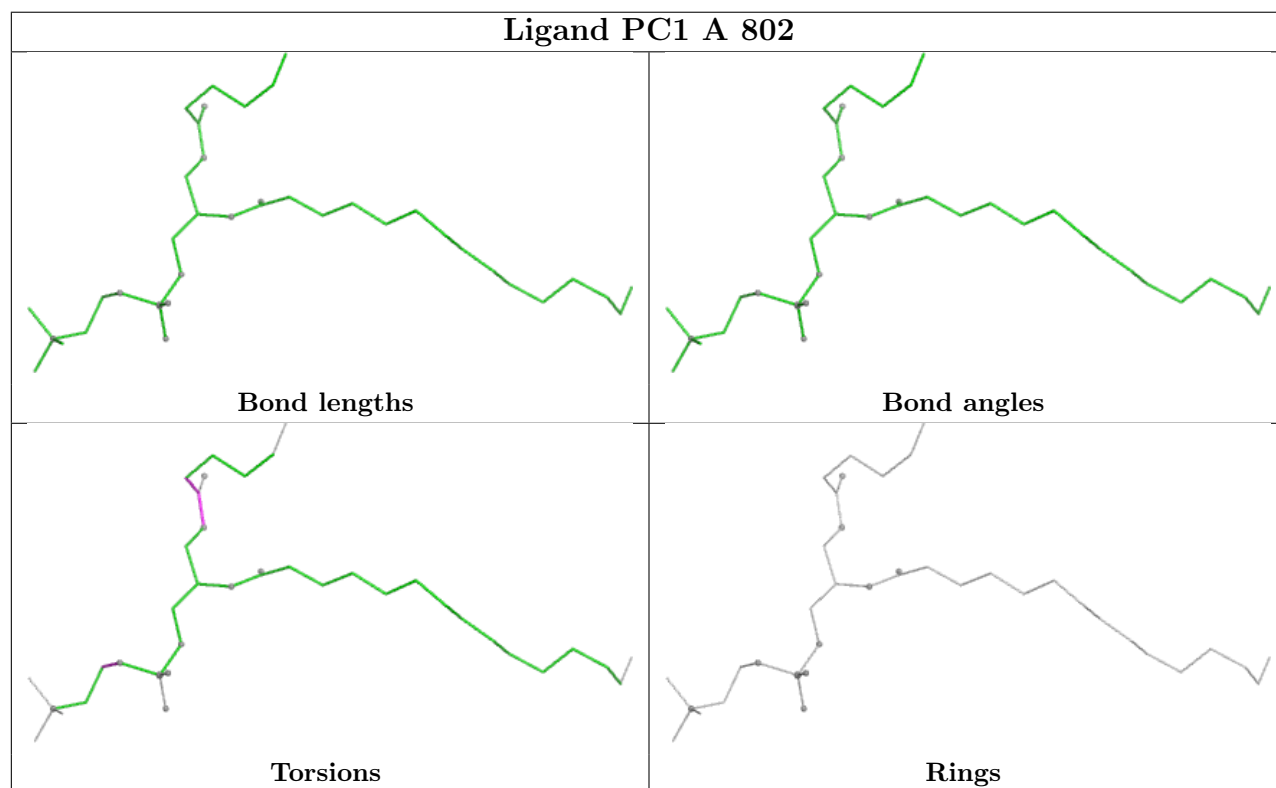
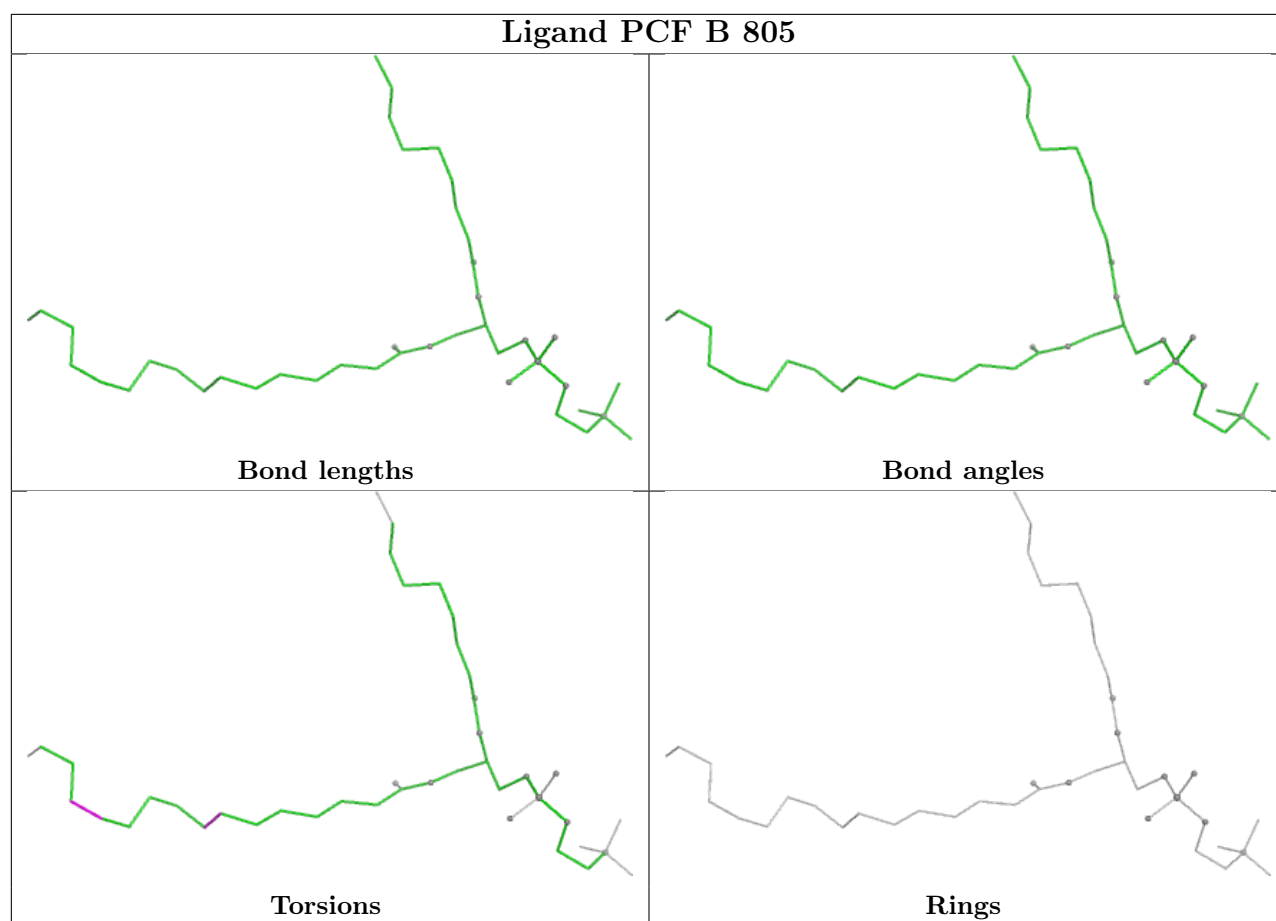
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

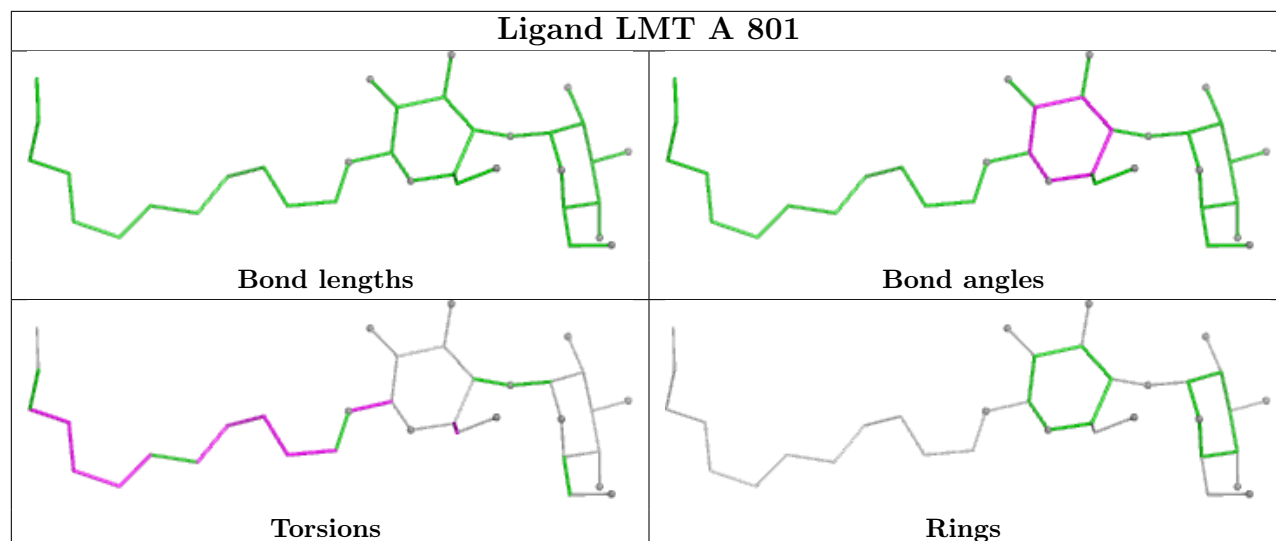












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

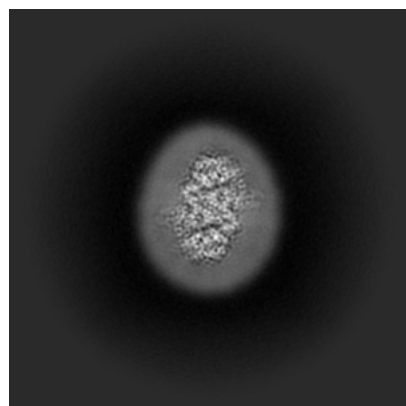
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53831. These allow visual inspection of the internal detail of the map and identification of artifacts.

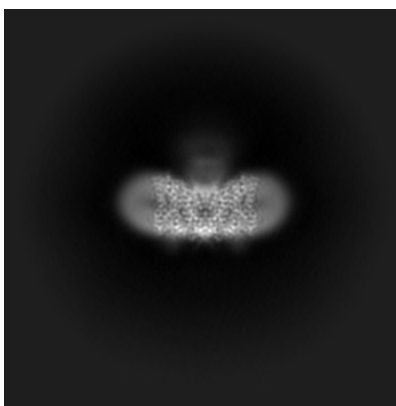
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

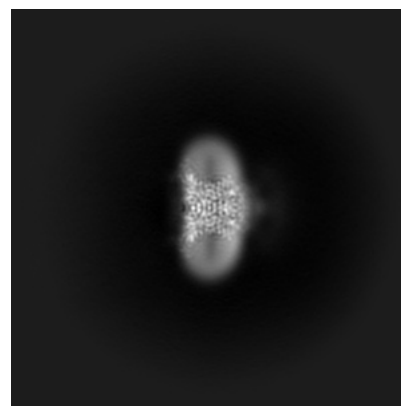
6.1.1 Primary map



X

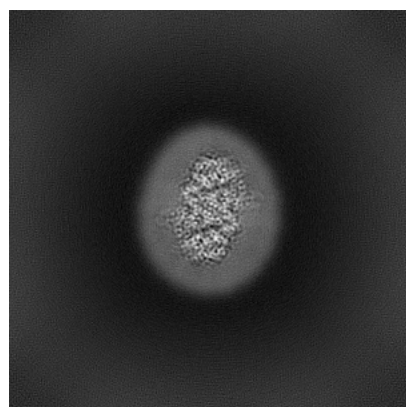


Y

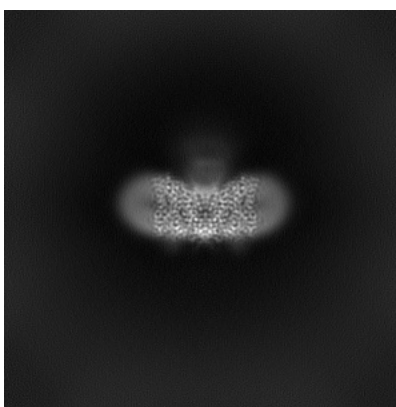


Z

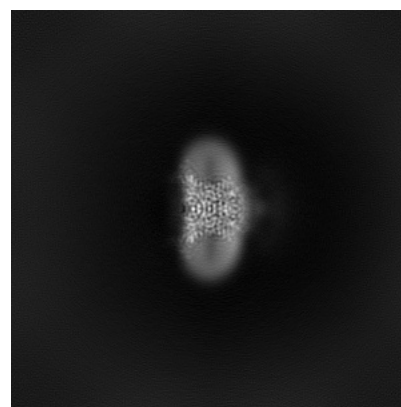
6.1.2 Raw map



X



Y

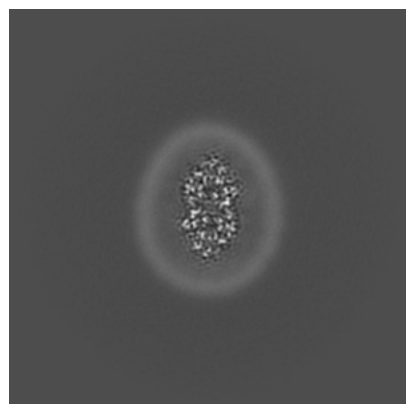


Z

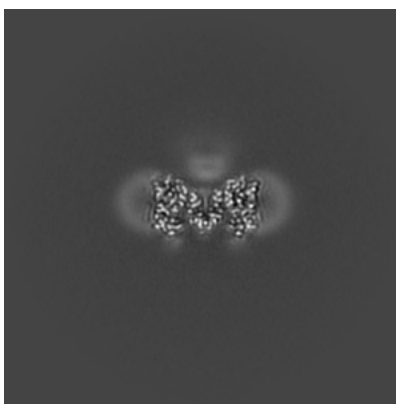
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

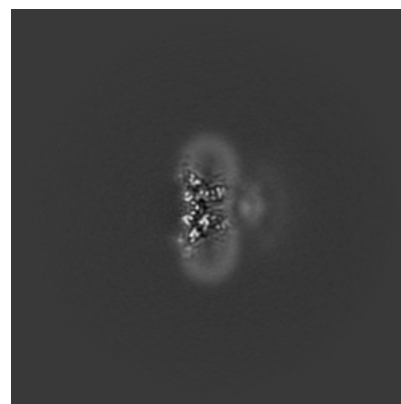
6.2.1 Primary map



X Index: 180

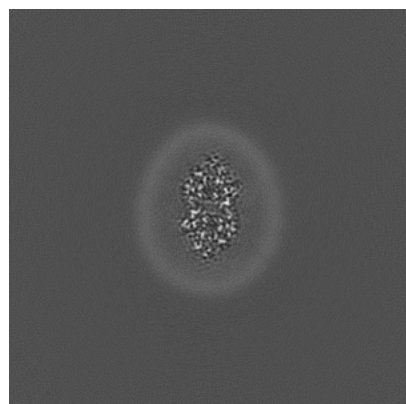


Y Index: 180

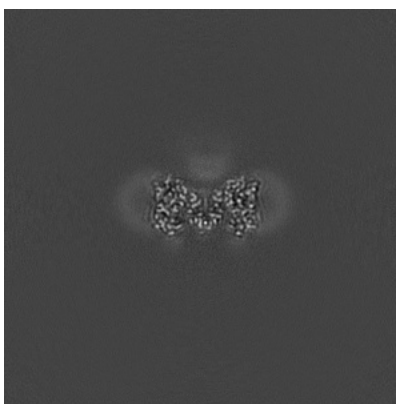


Z Index: 180

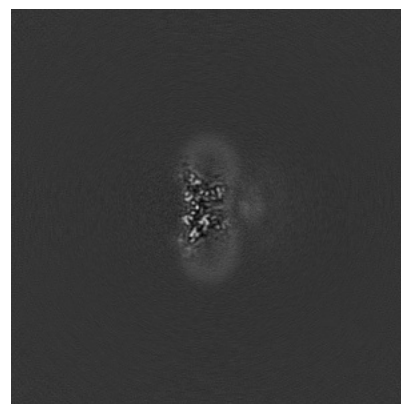
6.2.2 Raw map



X Index: 180



Y Index: 180

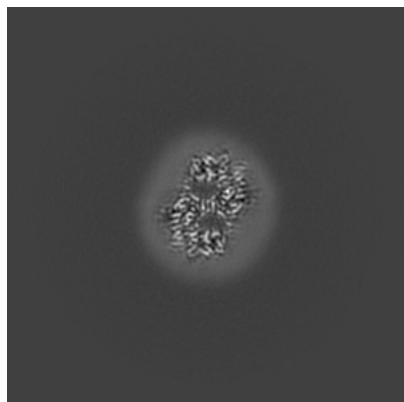


Z Index: 180

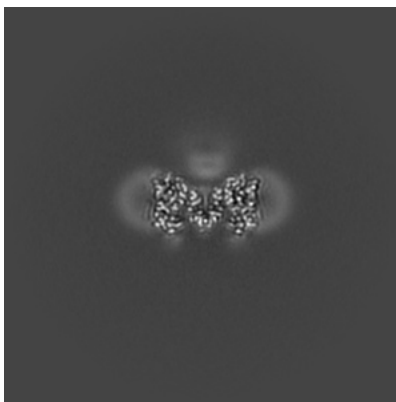
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

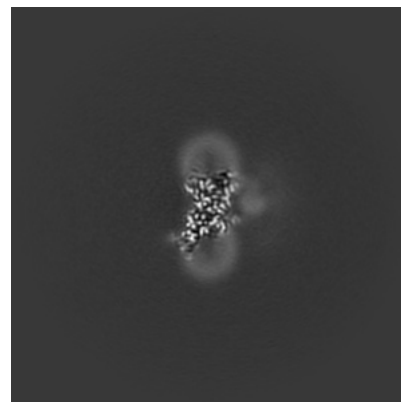
6.3.1 Primary map



X Index: 163

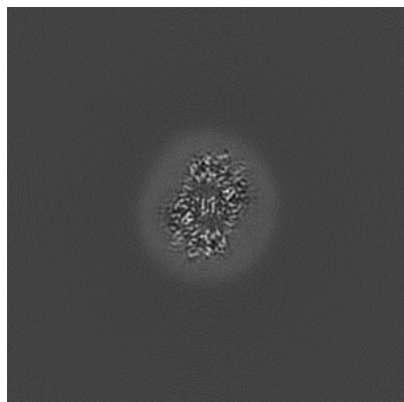


Y Index: 180

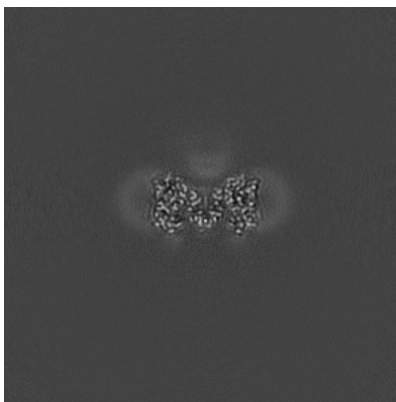


Z Index: 172

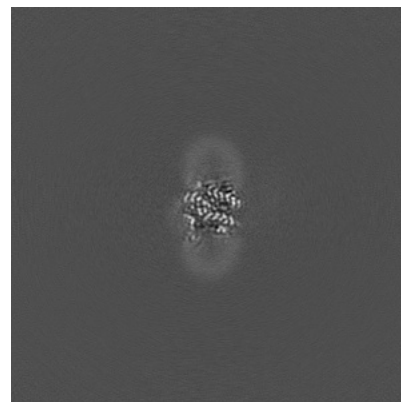
6.3.2 Raw map



X Index: 164



Y Index: 180

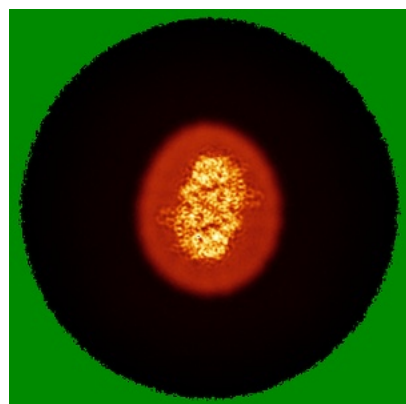


Z Index: 155

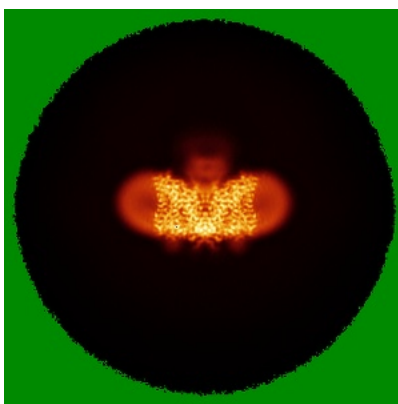
The images above show the largest variance slices of the map in three orthogonal directions.

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

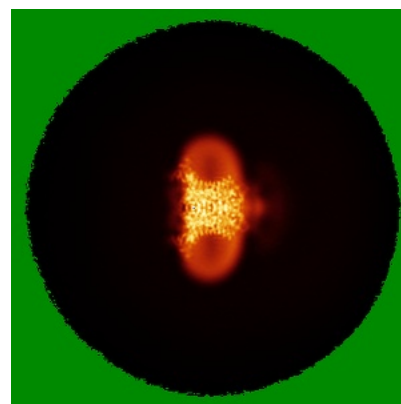
6.4.1 Primary map



X

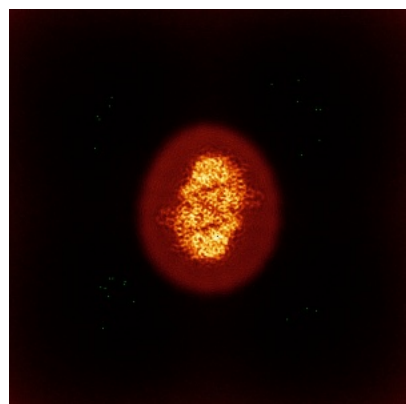


Y

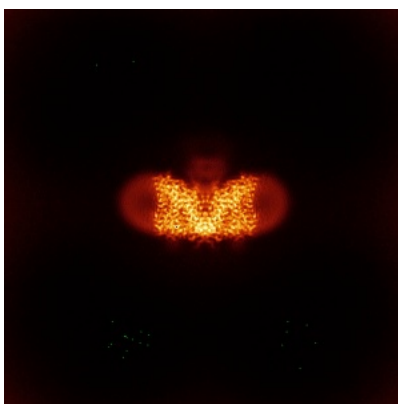


Z

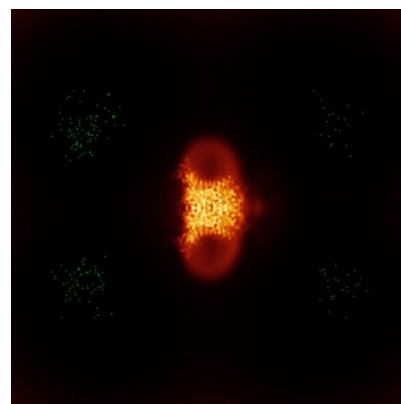
6.4.2 Raw map



X



Y

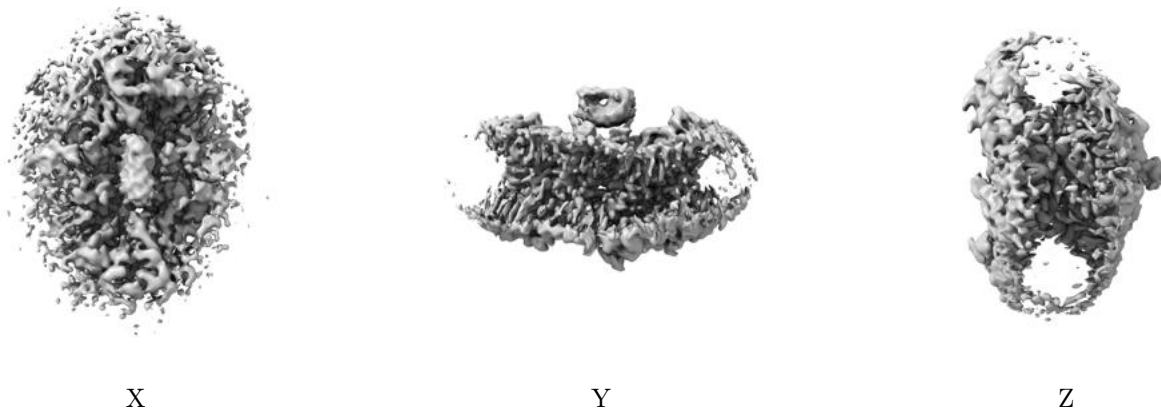


Z

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.

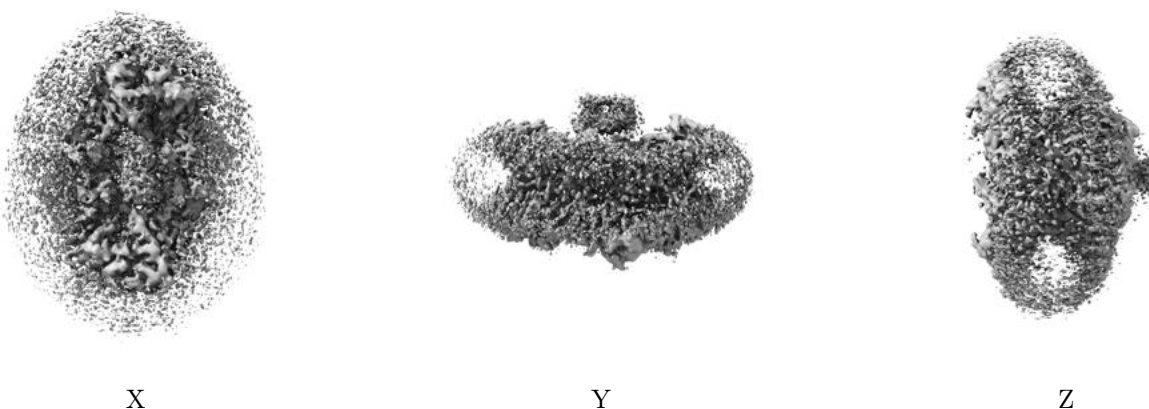
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.22. 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.

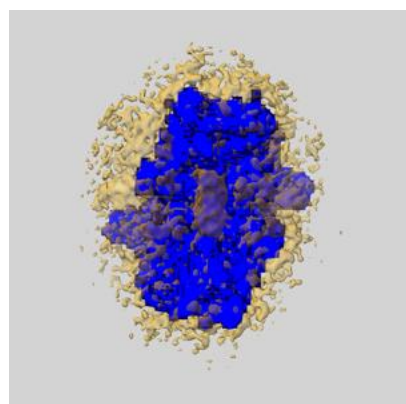
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

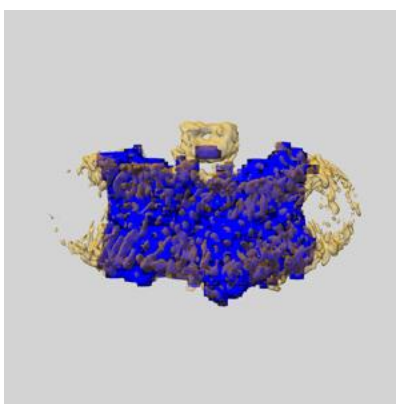
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

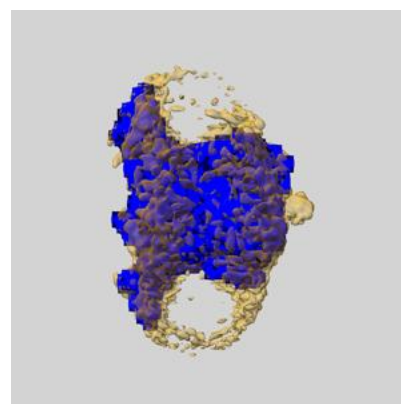
6.6.1 emd_53831_msk_2.map [i](#)



X

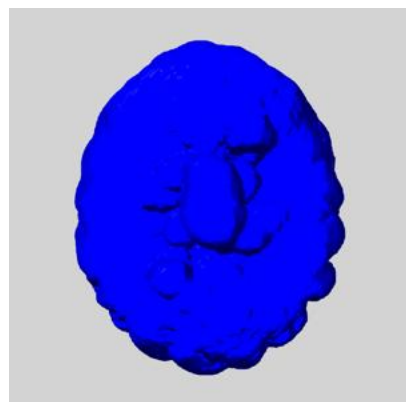


Y

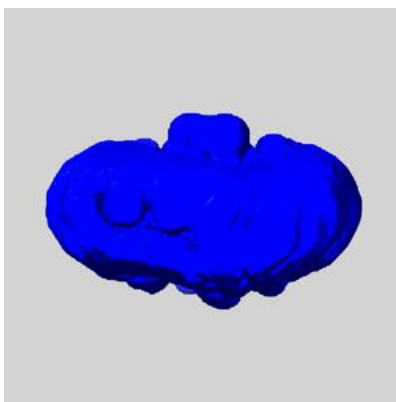


Z

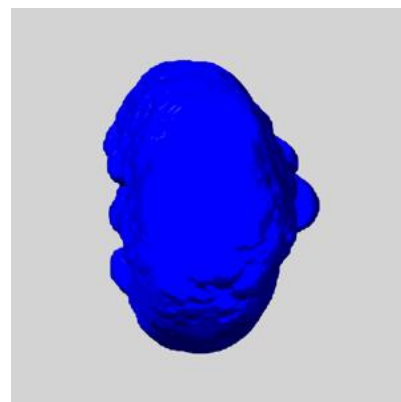
6.6.2 emd_53831_msk_1.map [i](#)



X



Y

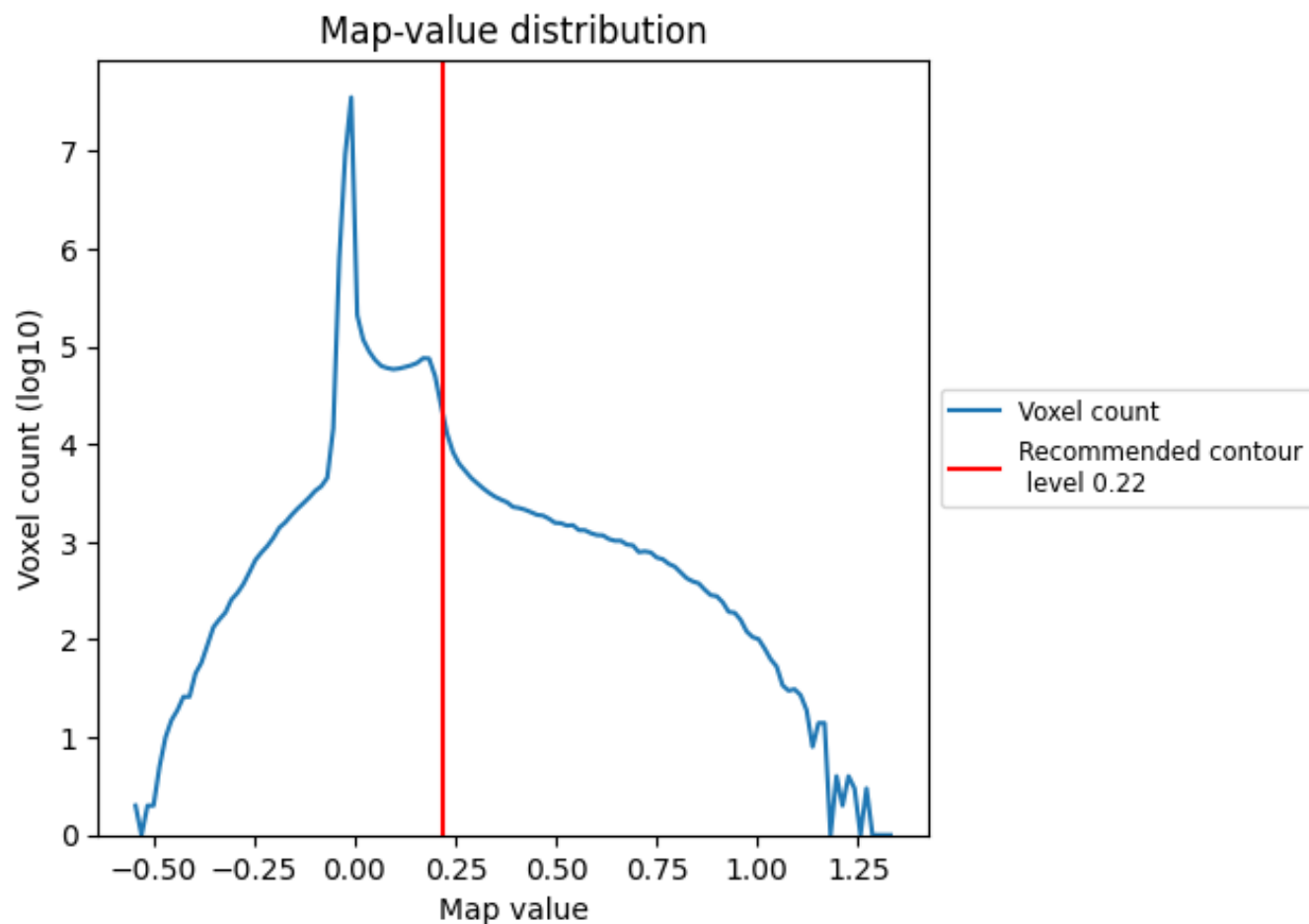


Z

7 Map analysis [i](#)

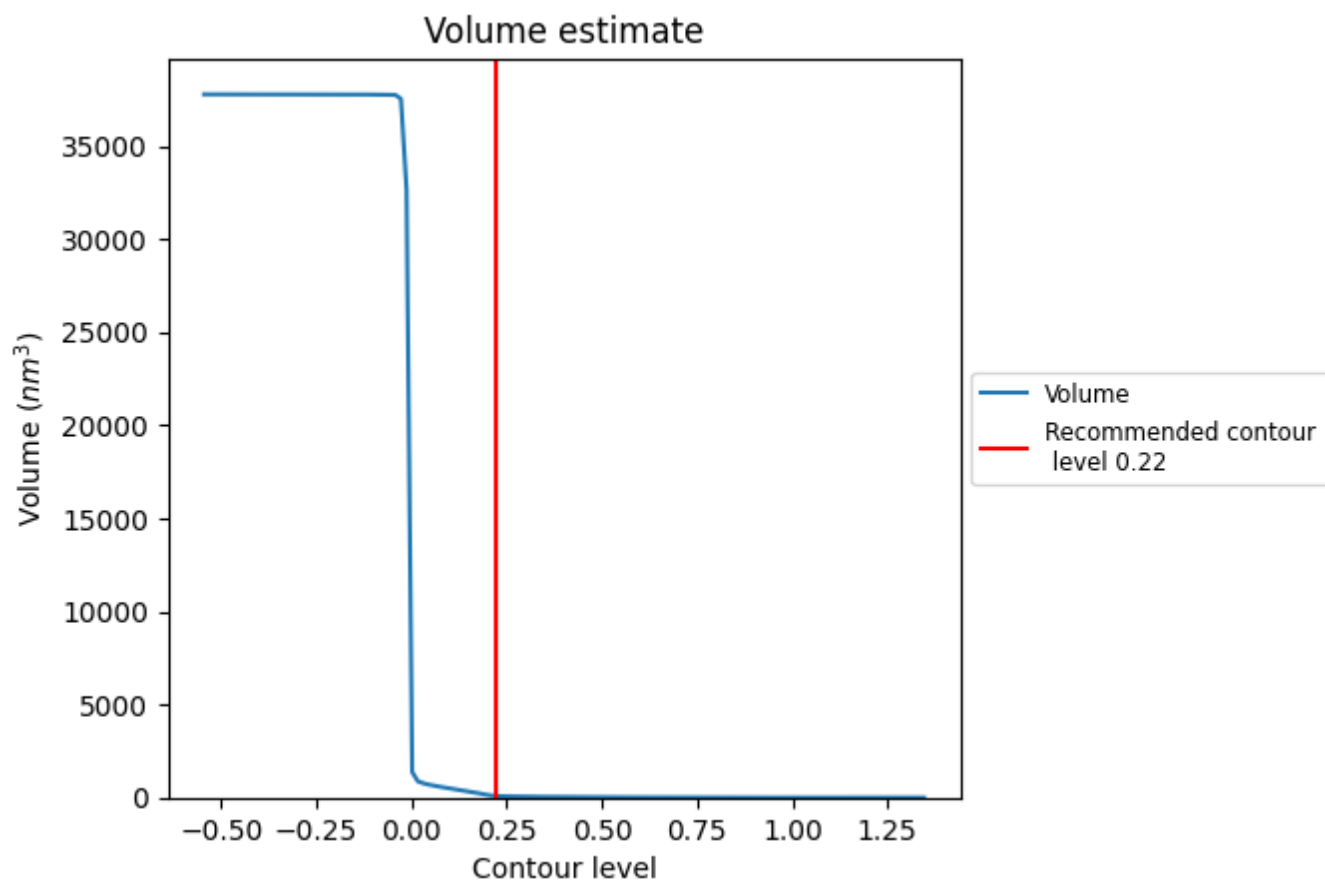
This section contains the results of statistical analysis of the map.

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.

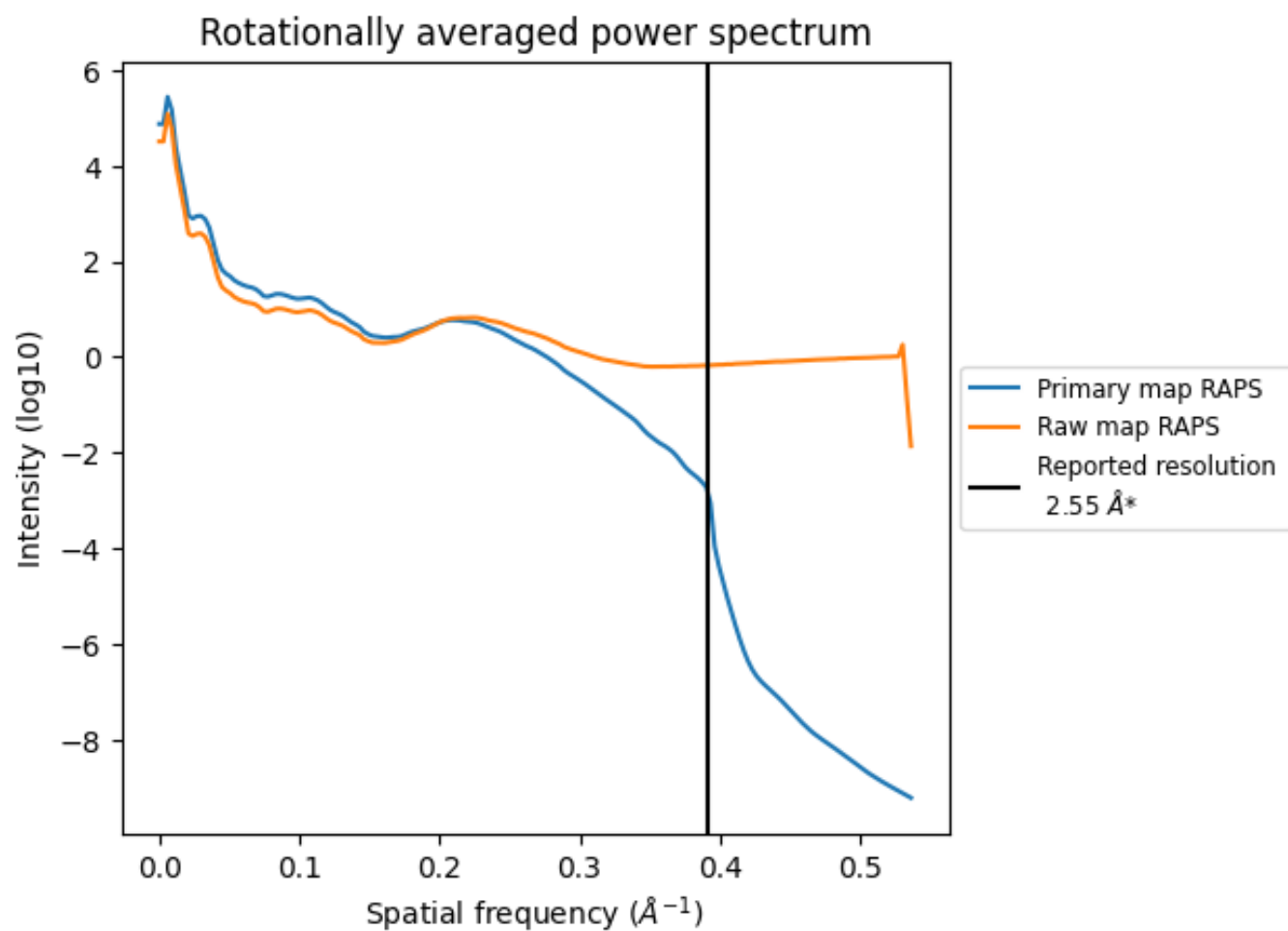
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 91 nm^3 ; this corresponds to an approximate mass of 82 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 ⓘ

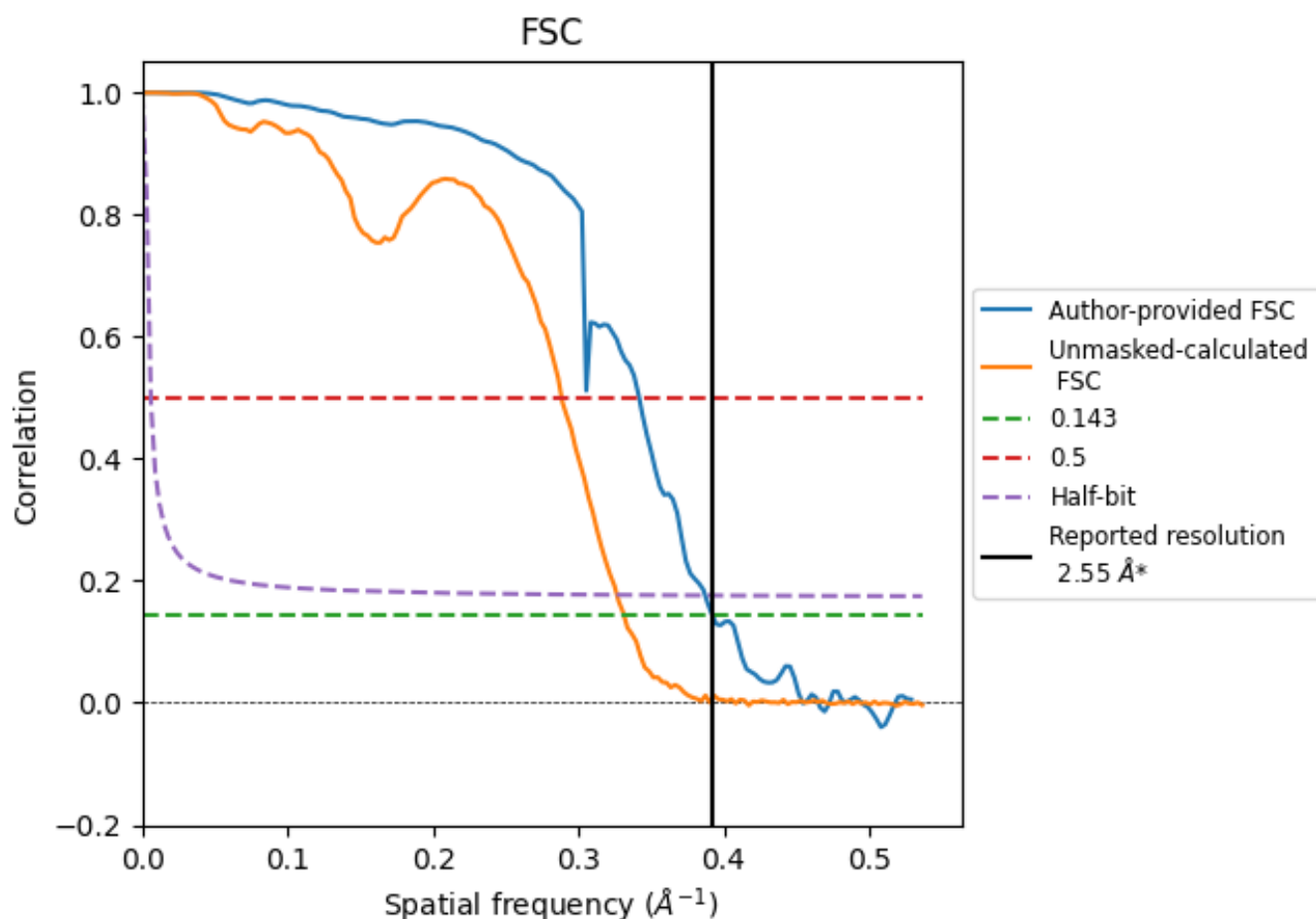


*Reported resolution corresponds to spatial frequency of 0.392 Å⁻¹

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 $0.392 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

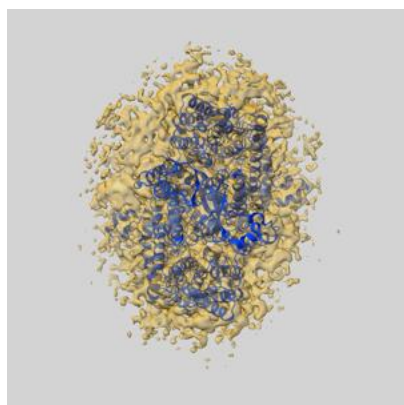
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.55	-	-
Author-provided FSC curve	2.55	2.93	2.58
Unmasked-calculated*	3.02	3.47	3.06

*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 3.02 differs from the reported value 2.55 by more than 10 %

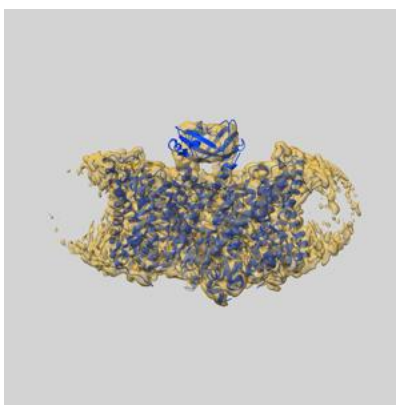
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-53831 and PDB model 9R8M. Per-residue inclusion information can be found in section 3 on page 10.

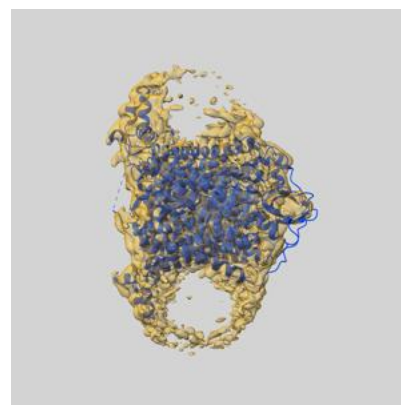
9.1 Map-model overlay [i](#)



X



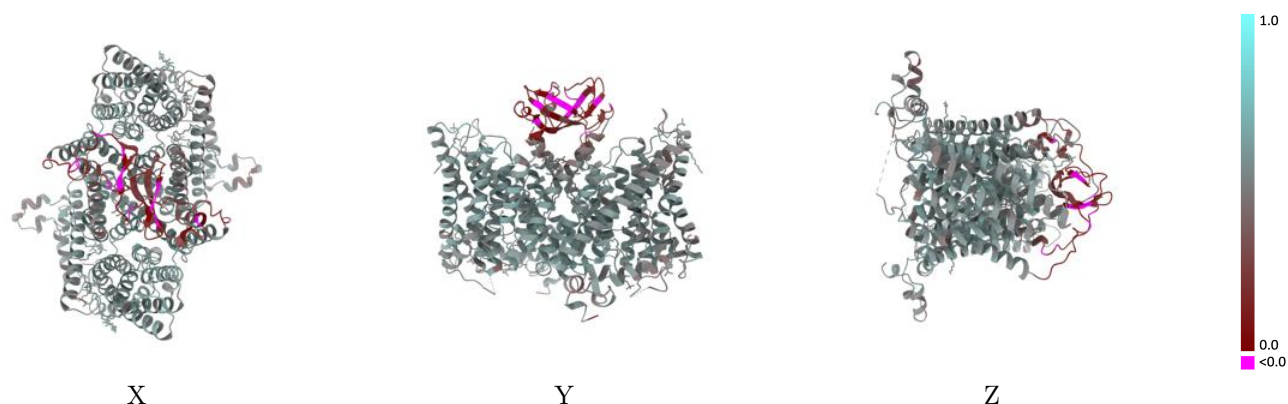
Y



Z

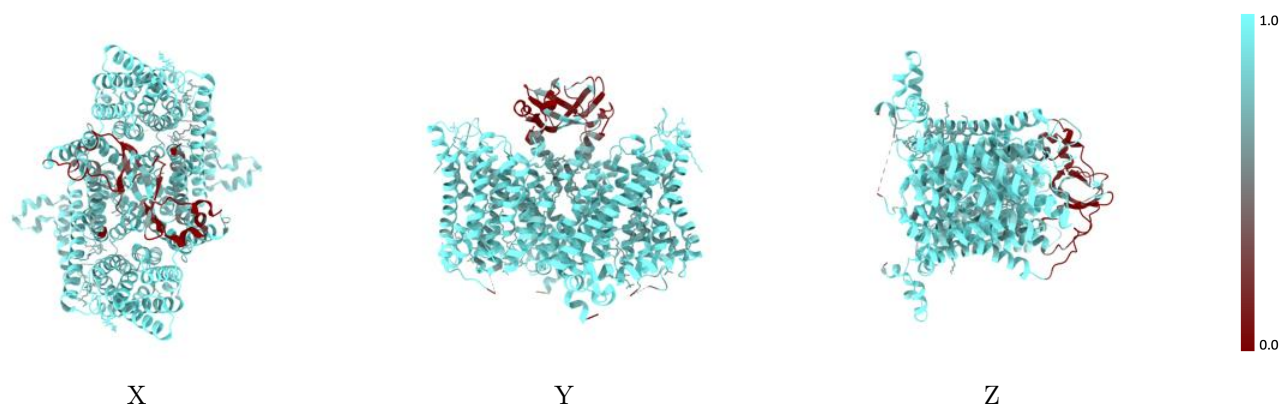
The images above show the 3D surface view of the map at the recommended contour level 0.22 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



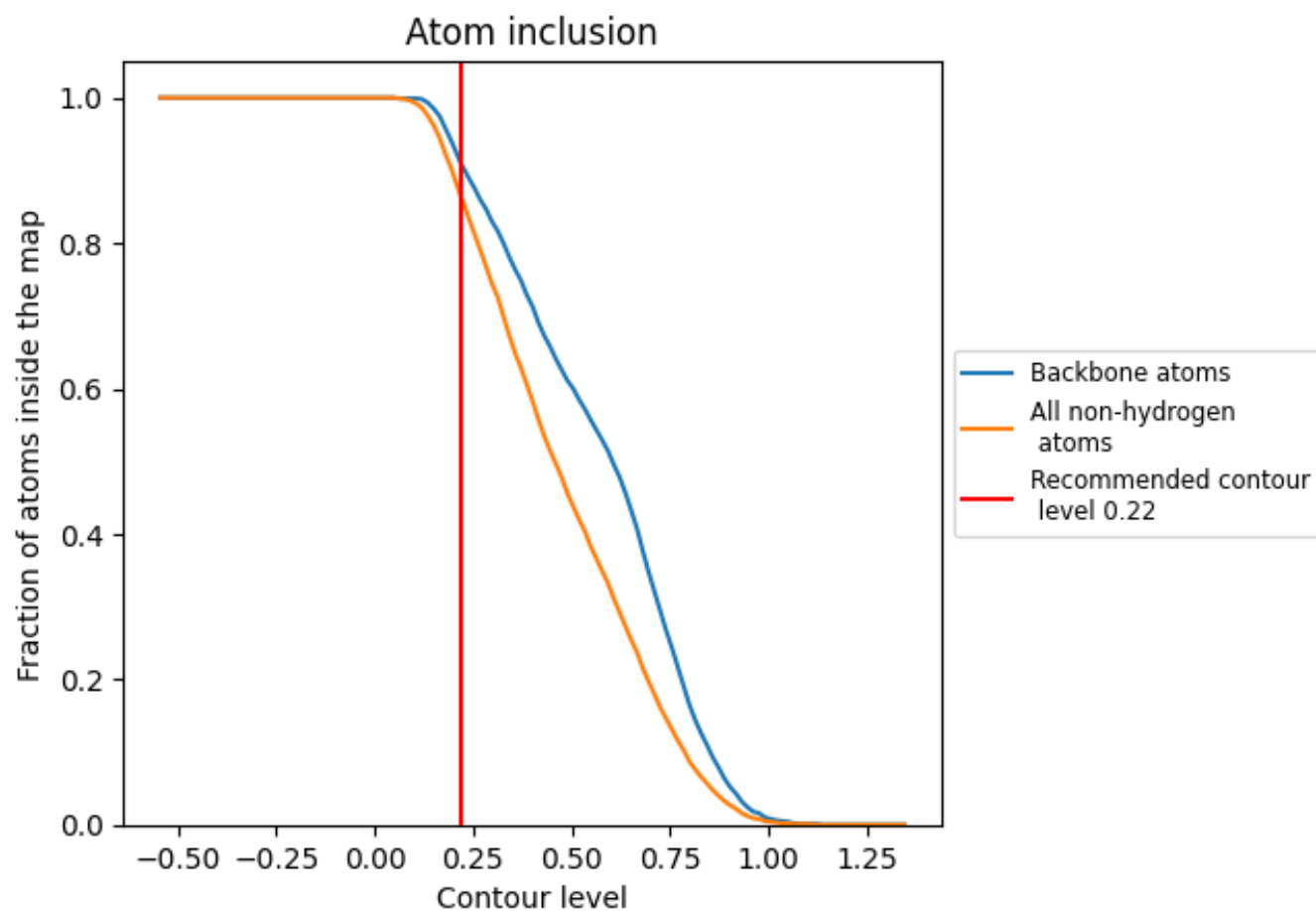
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.22).

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 86% 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 (0.22) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8620	0.5030
A	0.8550	0.4920
B	0.8700	0.5140

