



wwPDB EM Validation Summary Report ⓘ

Mar 20, 2023 – 12:44 am GMT

PDB ID : 8A9A
EMDB ID : EMD-15274
Title : Single Particle cryo-EM of the lipid binding protein P116 (MPN213) from Mycoplasma pneumoniae at 3.3 Angstrom resolution.
Authors : Sprankel, L.; Vizarraga, D.
Deposited on : 2022-06-28
Resolution : 3.30 Å(reported)

This is a wwPDB EM Validation Summary 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.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.32.1

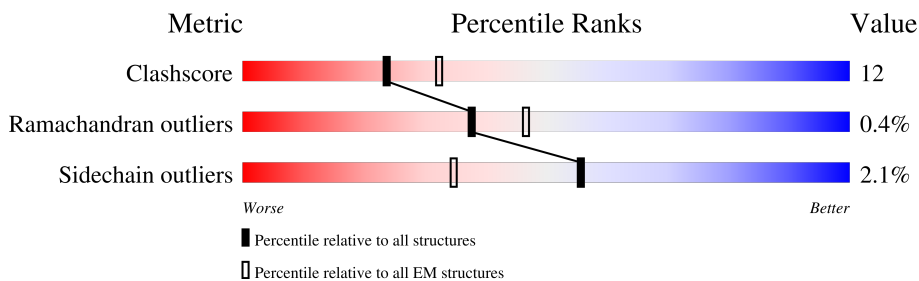
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	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 $\leq 5\%$. 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	1007	<p>50% (Poor fit), 57% (0 outliers), 23% (1 outlier), 20% (2+ outliers)</p>
1	B	1007	<p>22% (Poor fit), 56% (0 outliers), 24% (1 outlier), 20% (2+ outliers)</p>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 12772 atoms, of which 0 are hydrogens and 0 are deuteriums.

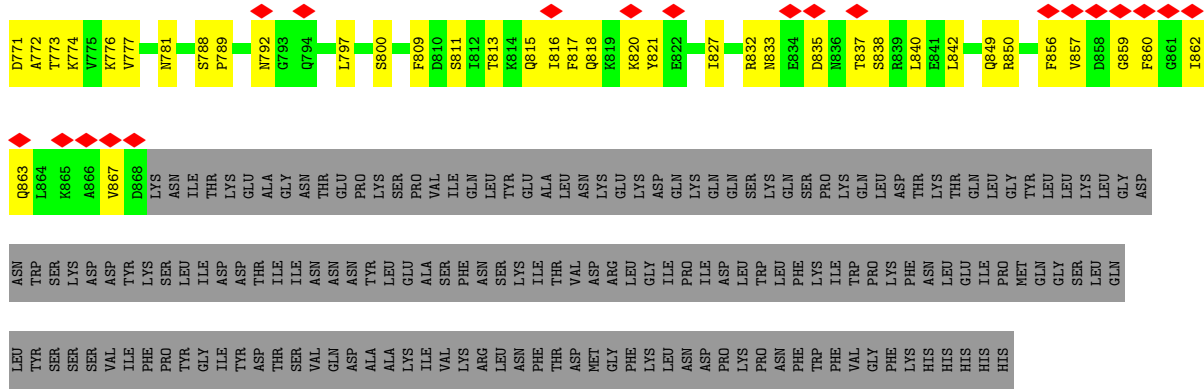
In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Lipid binding protein P116 (MPN213).

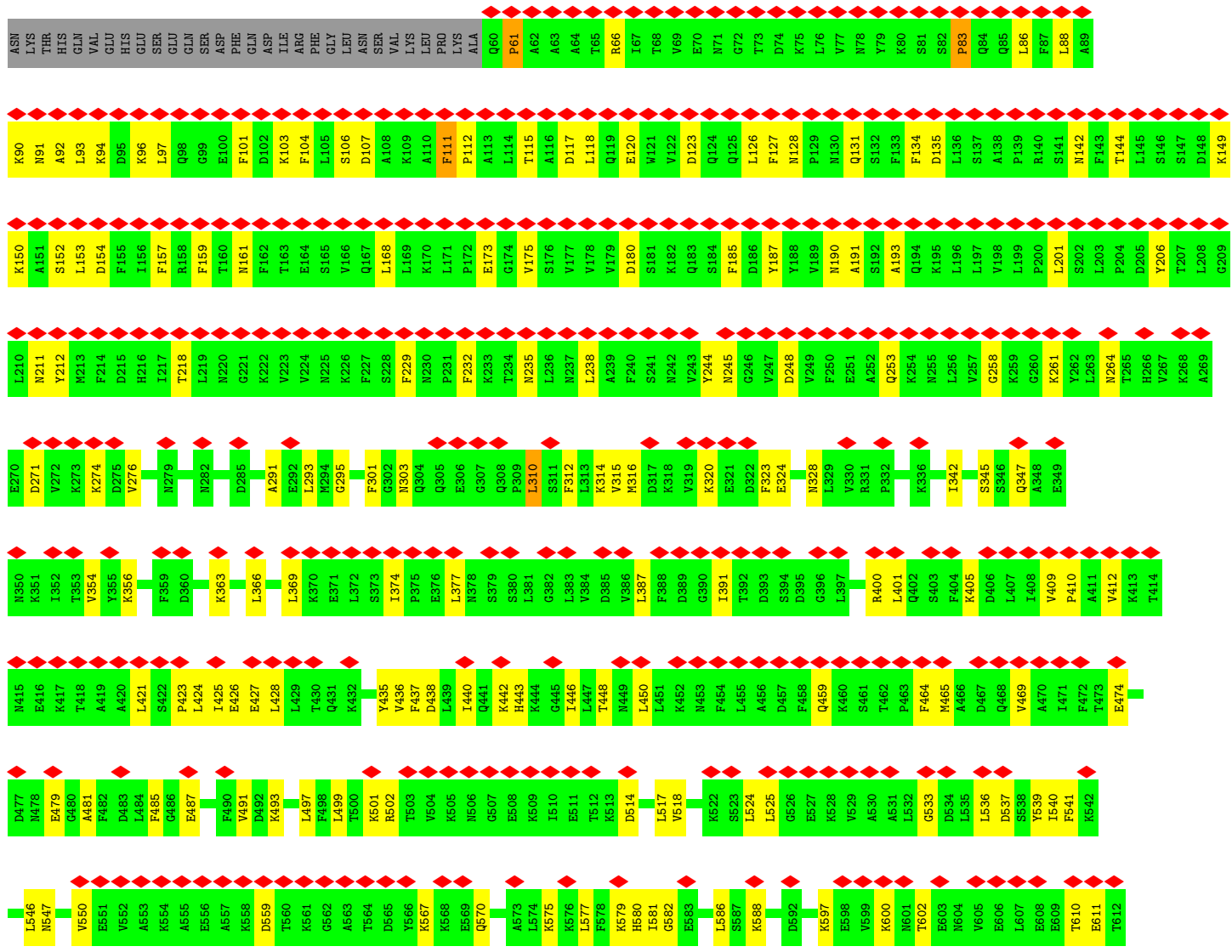
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	B	809	6386	4120	1027	1231	8	0	0
1	A	809	6386	4120	1027	1231	8	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1031	LYS	-	expression tag	UNP P75556
B	1032	HIS	-	expression tag	UNP P75556
B	1033	HIS	-	expression tag	UNP P75556
B	1034	HIS	-	expression tag	UNP P75556
B	1035	HIS	-	expression tag	UNP P75556
B	1036	HIS	-	expression tag	UNP P75556
A	1031	LYS	-	expression tag	UNP P75556
A	1032	HIS	-	expression tag	UNP P75556
A	1033	HIS	-	expression tag	UNP P75556
A	1034	HIS	-	expression tag	UNP P75556
A	1035	HIS	-	expression tag	UNP P75556
A	1036	HIS	-	expression tag	UNP P75556



● Molecule 1: Lipid binding protein P116 (MPN213)



T613	T614	K615	V616	K617	K618	L619	E622	E626	L627	G628	K633	K634	G635	D646	T647	K648	T653	L654	D655	K656	L657	K660	G661	E662	K665	A666	M667	K668	D669	I672	K673	E674	G675	F676	P677	G678	V685	V686	P687	E691	M695	T696	A700	K703	S706	D709	N718	D719	S722	V723	K724	E725	T726	D727	S728	G733	G734	S735	K634	F736	D737	I738	K739	Y740	G741	G742	E743	N744	L745	N746	V747	L748	P749	A750	Y751	Y752	S753	L754	I755	N756	S757	E758	I759	Q762	I763	I764	V686	G765	V766	D767	T768	T769	I770	D771	A772	T773	K774	V775	K776	V777	K780	N781	K782	E783	K787	N792	G793	Q794	F809	D810	S811	I812	T813	K814	Q815	I816	F817	Q818	K819	K820	Y821	E822	F823	K824	D825	N826	I827	Q828	V829	F830	A831	R832	N833	E834	D835	M836	T837	S838	R839	L840	E841	L842	D843	I844	S845	D846	P847	E848	Q849	R850	V851	I852	P853	F854	A855	F856	V857	D858	LYS	LEU	GLY	ASP	ASN	TRP	SER	SER	SER	VAL	ILE	PHE	PRO	TYR	LYS	LEU	ILE	ASN	THR	THR	ASP	THR	ILE	ALA	GLY	ASN	GLN	THR	ASP	ALA	PRO	LYS	SER	ALA	PRO	VAL	LYS	ARG	LEU	GLY	LYS	ILE	ASN	ASP	THR	THR	ASP	VAL	ASP	GLY	MET	GLY	PHE	LYS	LEU	ILE	ASN	PRO	ASP	PRO	TRP	ASN	PHE	TRP	PHE	ILE	VAL	GLY	PHE	LYS	ASN	HIS	HIS	HIS	HIS	PRO	MET	GLN
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	1324330	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	6.498	Depositor
Minimum map value	-4.064	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.033	Depositor
Recommended contour level	0.6	Depositor
Map size (Å)	537.6, 537.6, 537.6	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.26	0/6497	0.49	1/8756 (0.0%)
1	B	0.26	0/6497	0.49	1/8756 (0.0%)
All	All	0.26	0/12994	0.49	2/17512 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	61	PRO	N-CA-CB	6.07	110.58	103.30
1	B	61	PRO	N-CA-CB	6.04	110.55	103.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6386	0	6434	157	0
1	B	6386	0	6434	155	0
All	All	12772	0	12868	309	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 12.

The worst 5 of 309 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:PHE:HB2	1:A:187:TYR:HB3	1.67	0.77
1:B:157:PHE:HB2	1:B:187:TYR:HB3	1.67	0.76
1:B:120:GLU:HG3	1:B:235:ASN:HD21	1.51	0.76
1:A:120:GLU:HG3	1:A:235:ASN:HD21	1.51	0.75
1:B:421:LEU:HD21	1:B:450:LEU:HD21	1.71	0.73

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	807/1007 (80%)	719 (89%)	85 (10%)	3 (0%)	34	66
1	B	807/1007 (80%)	719 (89%)	85 (10%)	3 (0%)	34	66
All	All	1614/2014 (80%)	1438 (89%)	170 (10%)	6 (0%)	38	66

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	92	ALA
1	A	92	ALA
1	B	61	PRO
1	A	61	PRO
1	B	867	VAL

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	700/899 (78%)	685 (98%)	15 (2%)	53	75
1	B	700/899 (78%)	685 (98%)	15 (2%)	53	75
All	All	1400/1798 (78%)	1370 (98%)	30 (2%)	56	75

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	781	ASN
1	A	748	LEU
1	A	107	ASP
1	A	781	ASN
1	A	405	LYS

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

Mol	Chain	Res	Type
1	B	235	ASN
1	A	235	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

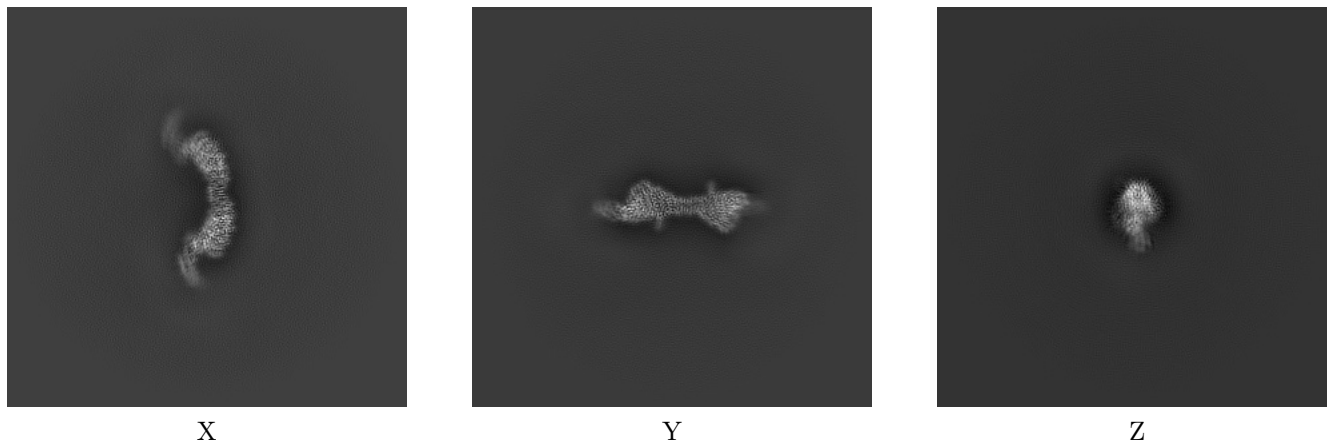
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15274. These allow visual inspection of the internal detail of the map and identification of artifacts.

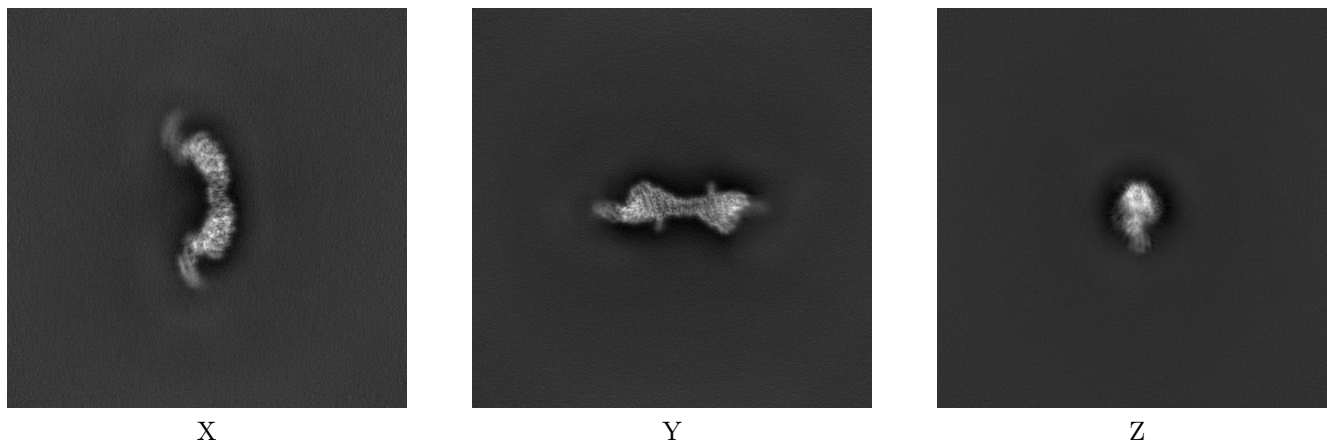
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



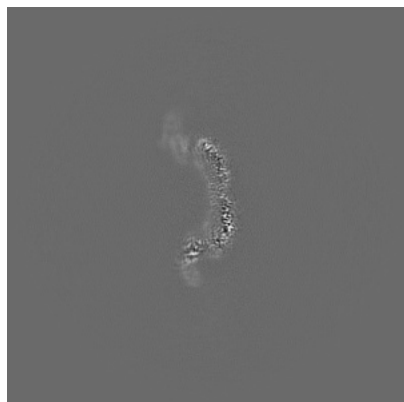
6.1.2 Raw map



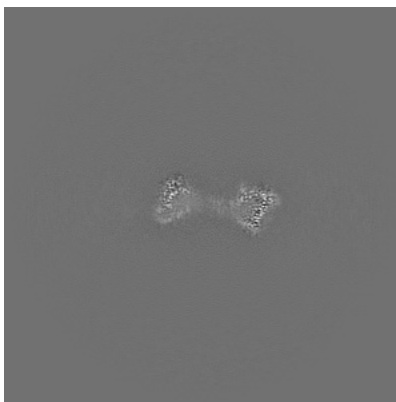
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

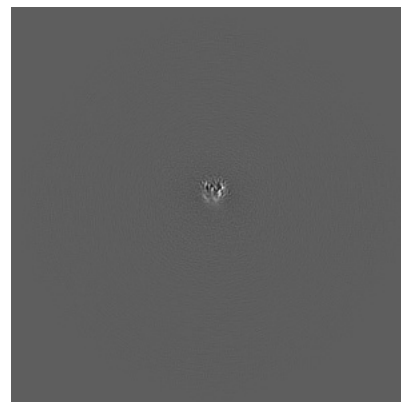
6.2.1 Primary map



X Index: 256



Y Index: 256

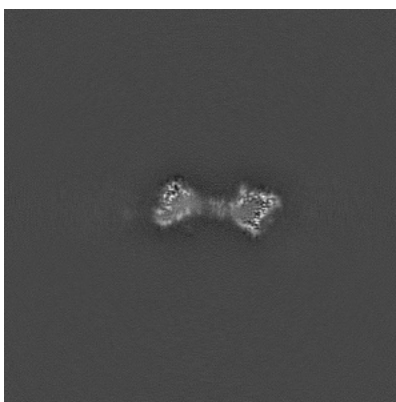


Z Index: 256

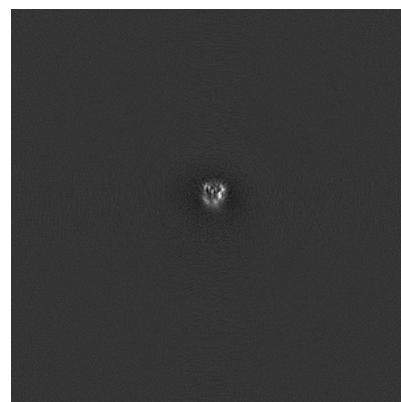
6.2.2 Raw map



X Index: 256



Y Index: 256

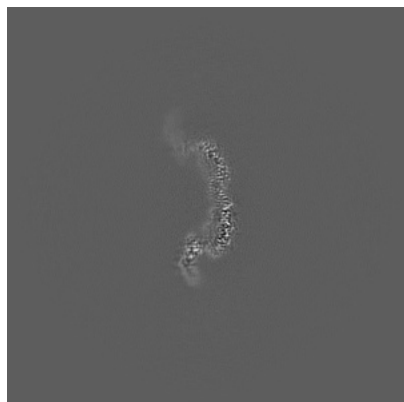


Z Index: 256

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: 253

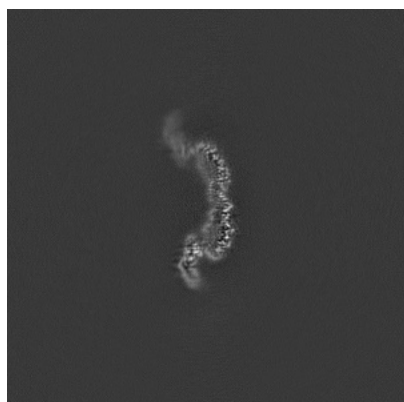


Y Index: 280

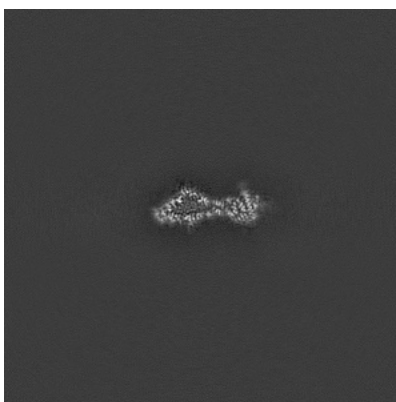


Z Index: 233

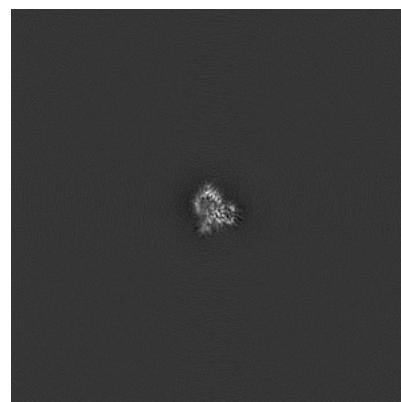
6.3.2 Raw map



X Index: 253



Y Index: 273

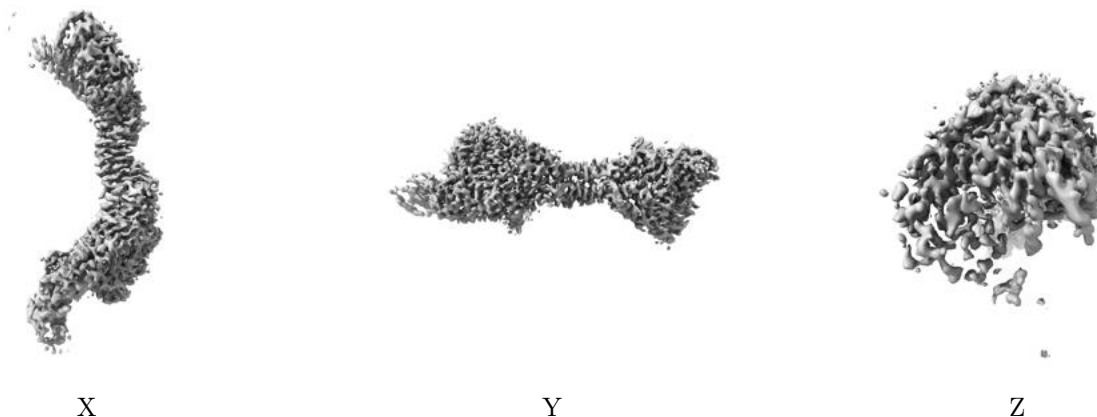


Z Index: 211

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

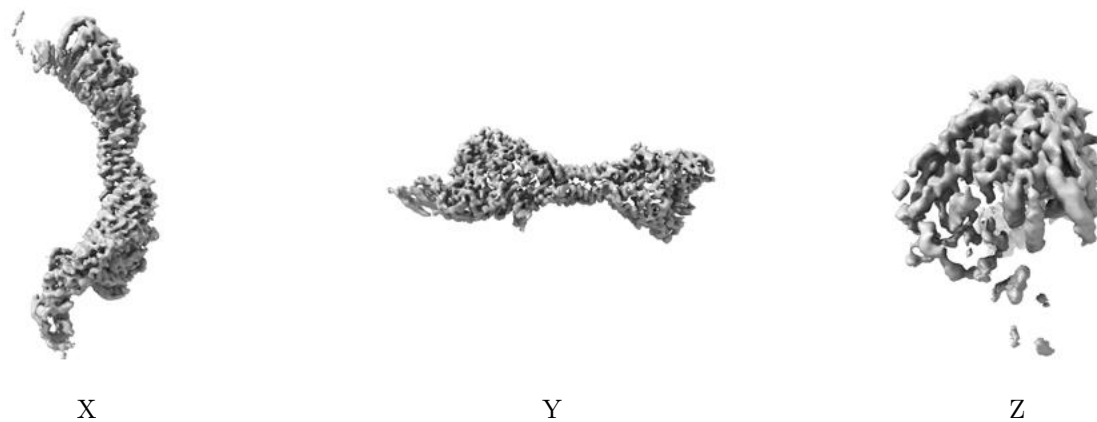
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.6. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

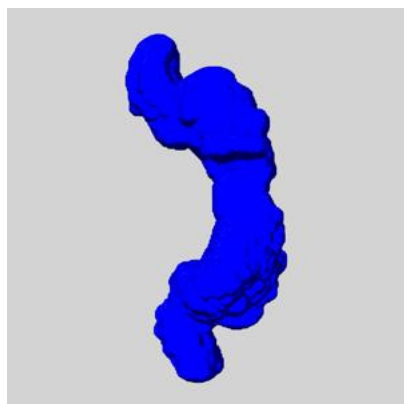
6.5 Mask visualisation [i](#)

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

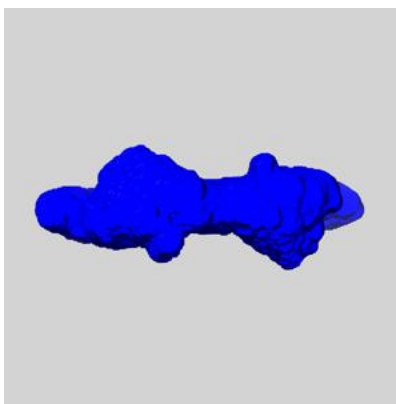
A mask typically either:

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

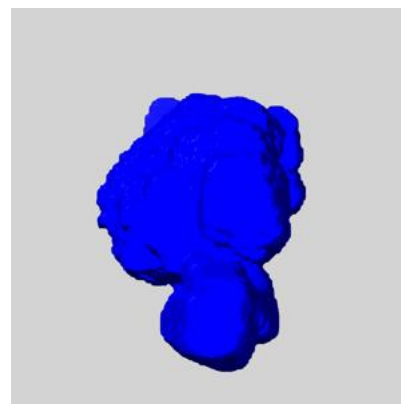
6.5.1 emd_15274_msk_1.map [i](#)



X



Y

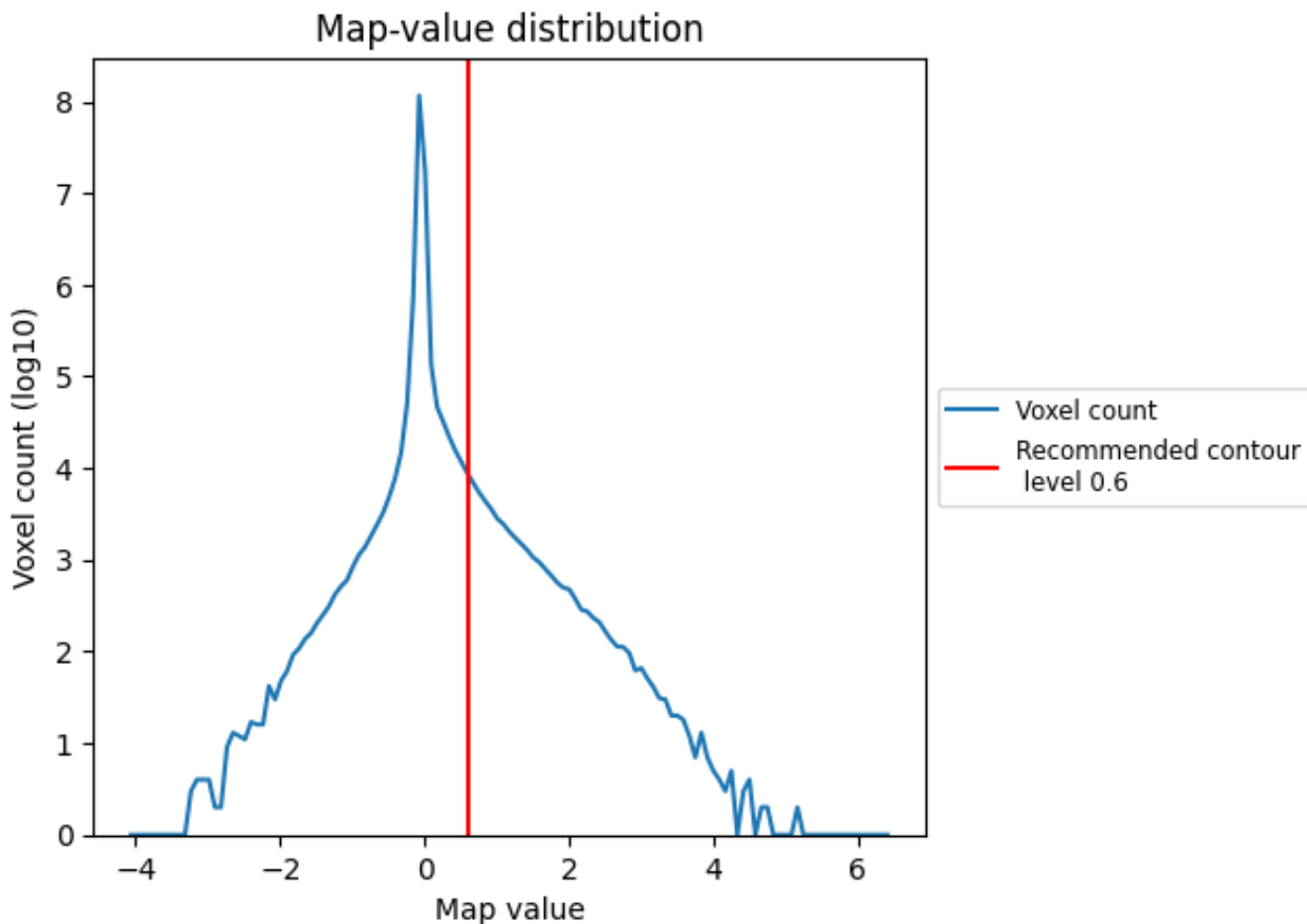


Z

7 Map analysis [i](#)

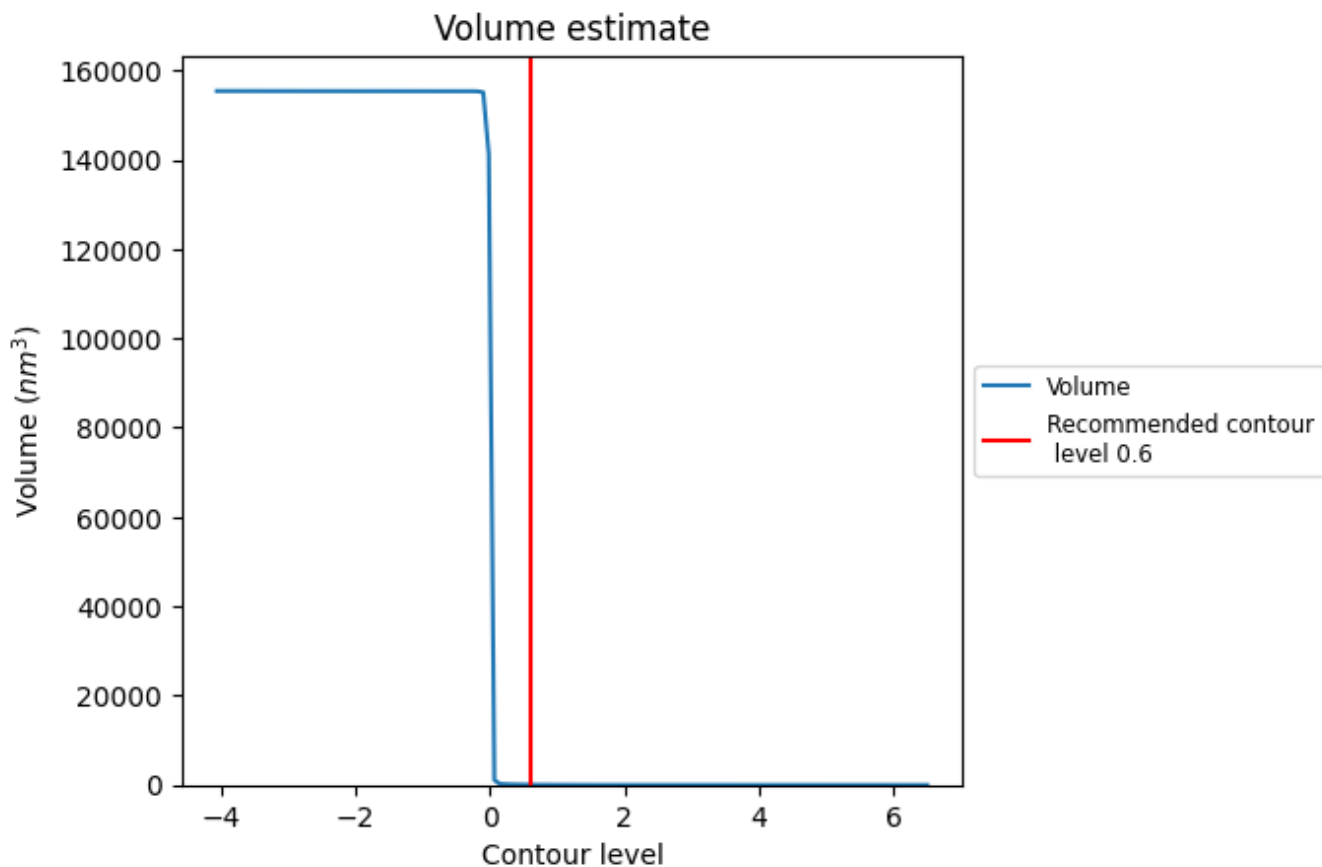
This section contains the results of statistical analysis of the map.

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.

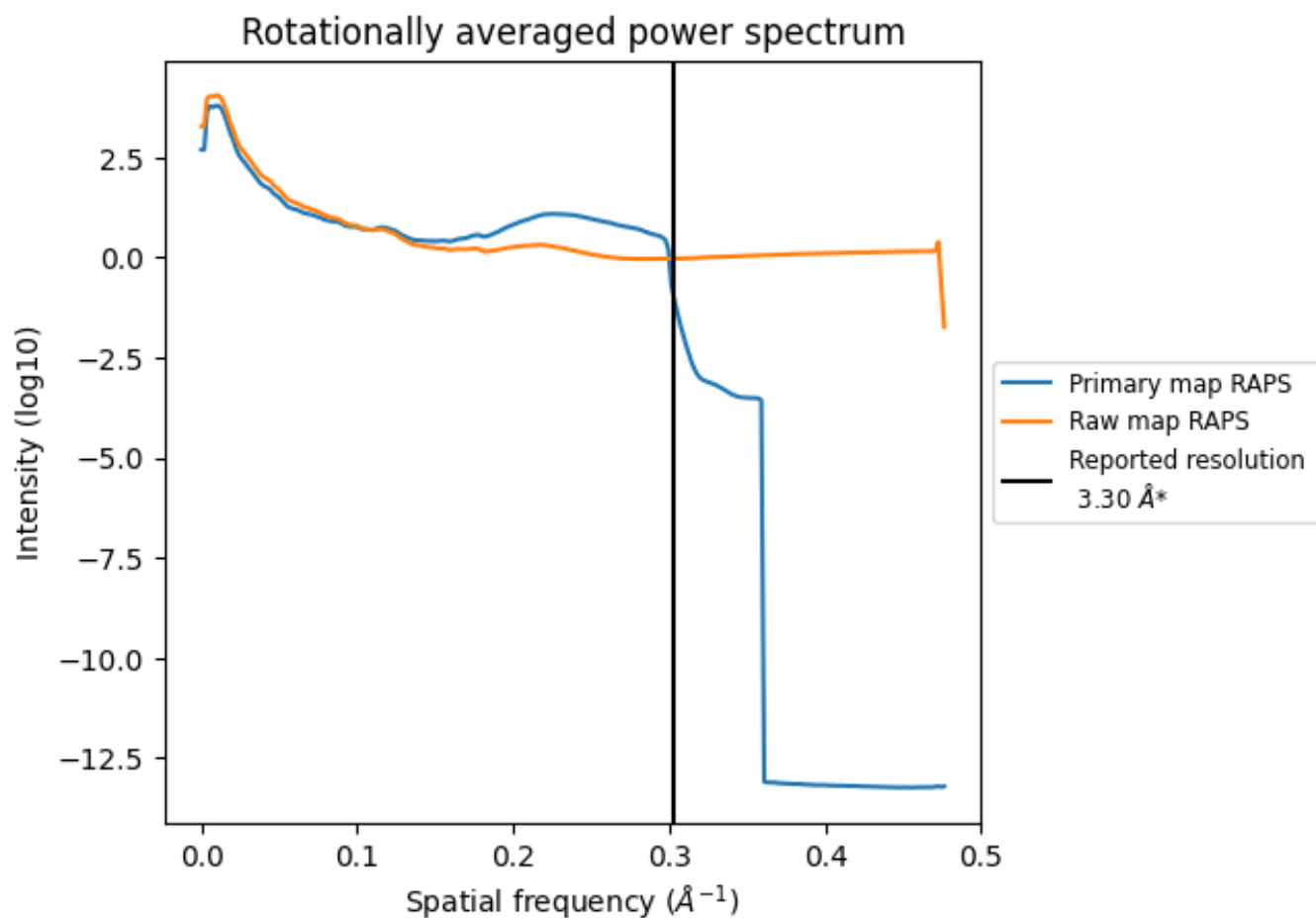
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 56 nm³; this corresponds to an approximate mass of 50 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

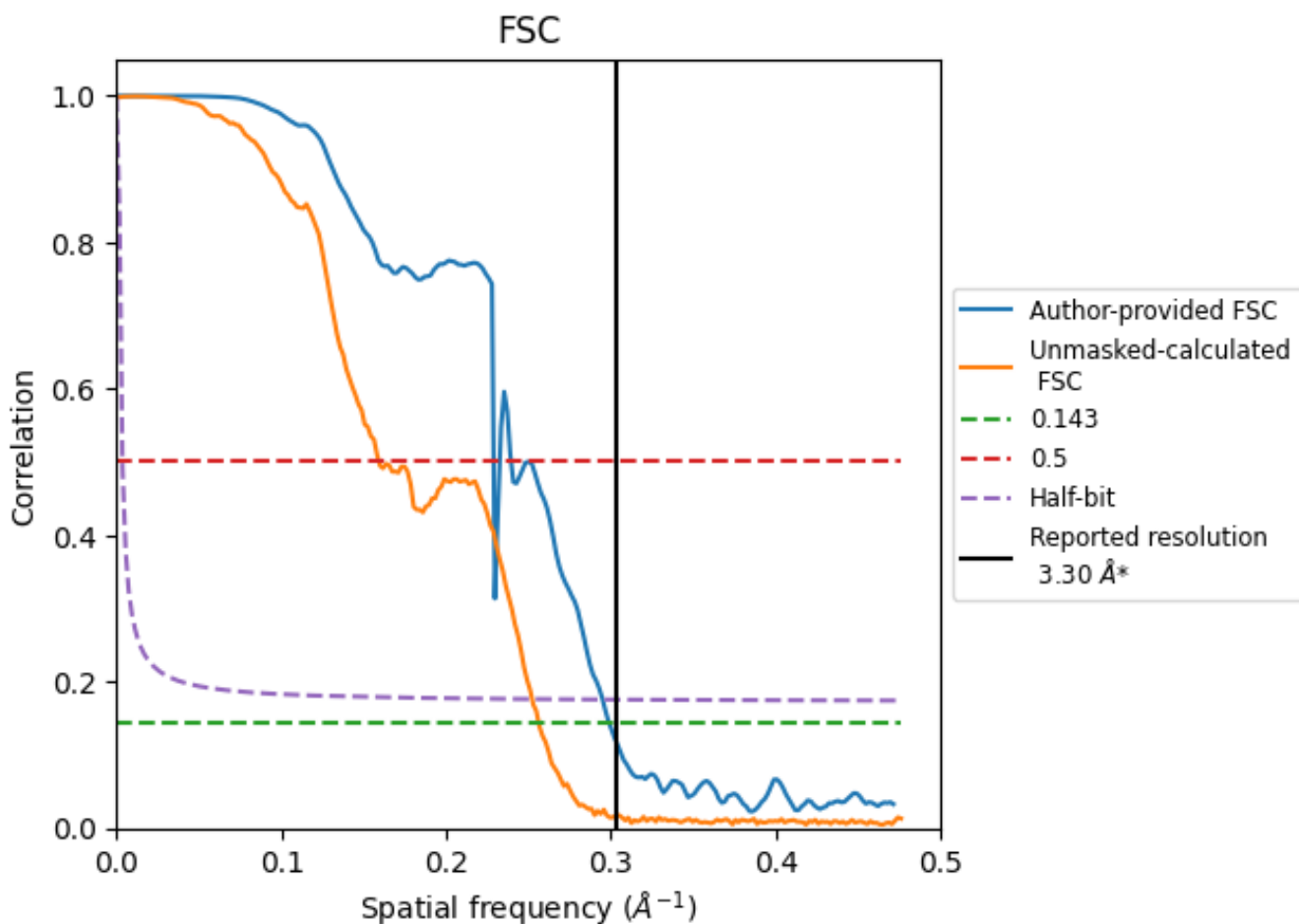


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

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 0.303 Å⁻¹

8.2 Resolution estimates [i](#)

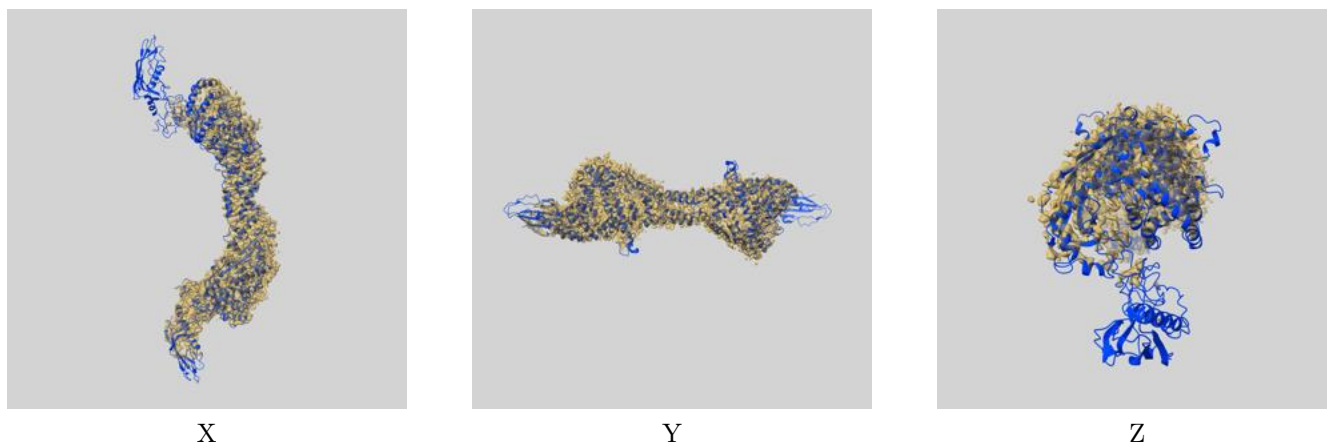
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.34	4.37	3.39
Unmasked-calculated*	3.90	6.28	3.96

*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 3.90 differs from the reported value 3.3 by more than 10 %

9 Map-model fit [i](#)

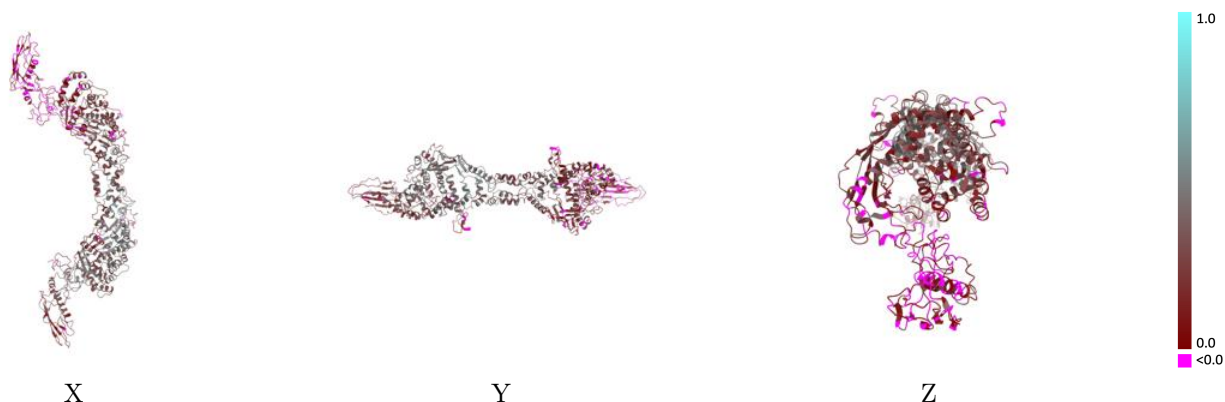
This section contains information regarding the fit between EMDB map EMD-15274 and PDB model 8A9A. Per-residue inclusion information can be found in section [3](#) on page [4](#).

9.1 Map-model overlay [i](#)



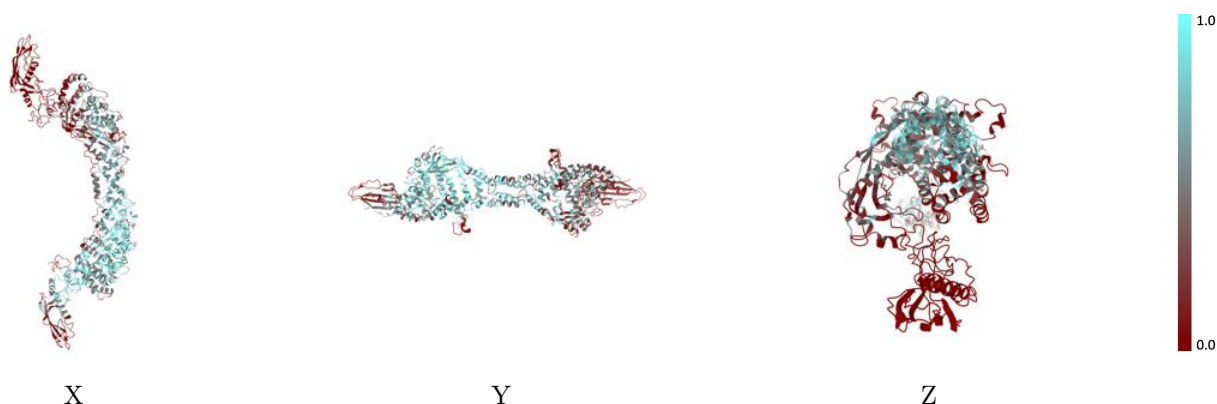
The images above show the 3D surface view of the map at the recommended contour level 0.6 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



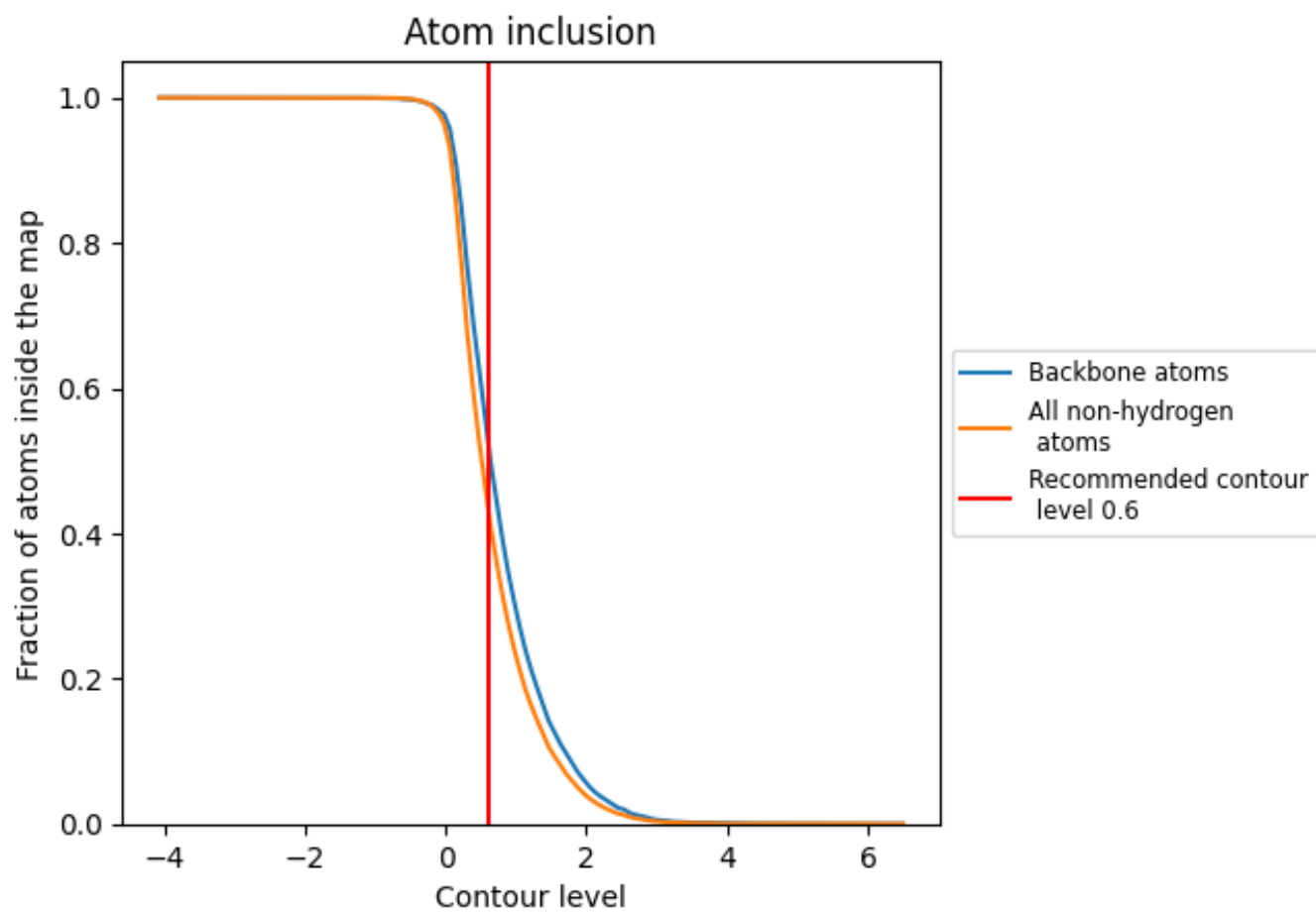
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.6).







9.4 Atom inclusion [i](#)



At the recommended contour level, 53% of all backbone atoms, 44% 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 (0.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4382	 0.2730
A	 0.3031	 0.1890
B	 0.5733	 0.3560

