



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 02:08 PM UTC

PDB ID : 8UWC / pdb_00008uwc
EMDB ID : EMD-42661
Title : Site-one protease without SPRING
Authors : Kober, D.L.
Deposited on : 2023-11-06
Resolution : 2.27 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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
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) : 2.49

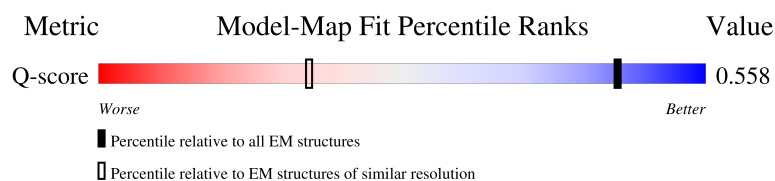
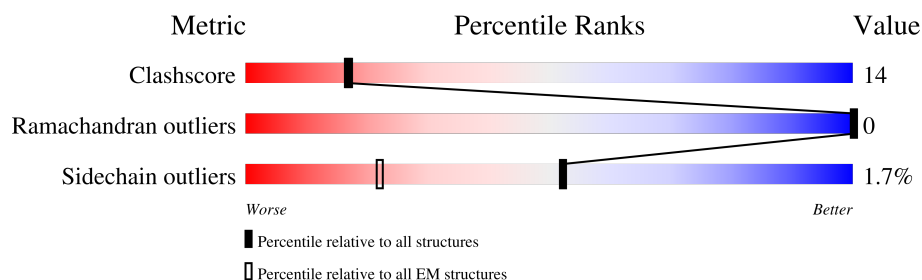
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.27 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	3593 (1.77 - 2.77)

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	1014	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7781 atoms, of which 3835 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 Membrane-bound transcription factor site-1 protease.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	494	Total	C	H	N	O	S	0	0
			7656	2451	3821	654	714	16		

There are 39 discrepancies between the modelled and reference sequences:

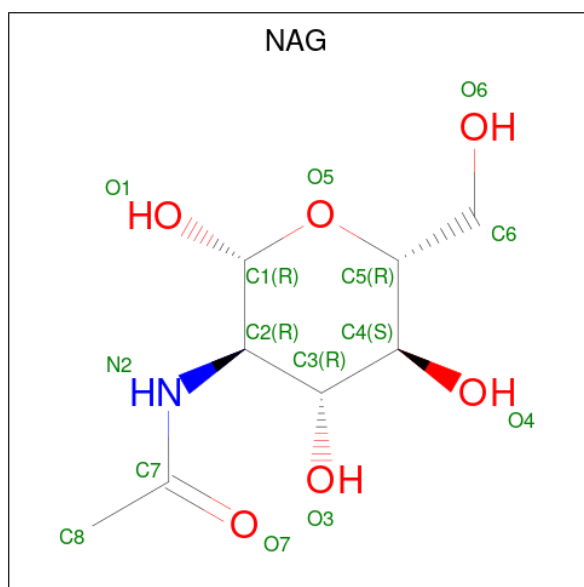
Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	MET	-	initiating methionine	UNP Q14703
A	-4	GLU	-	expression tag	UNP Q14703
A	-3	THR	-	expression tag	UNP Q14703
A	-2	ASP	-	expression tag	UNP Q14703
A	-1	THR	-	expression tag	UNP Q14703
A	0	LEU	-	expression tag	UNP Q14703
A	1	LEU	-	expression tag	UNP Q14703
A	2	LEU	-	expression tag	UNP Q14703
A	3	TRP	-	expression tag	UNP Q14703
A	4	VAL	-	expression tag	UNP Q14703
A	5	LEU	-	expression tag	UNP Q14703
A	6	LEU	-	expression tag	UNP Q14703
A	7	LEU	-	expression tag	UNP Q14703
A	8	TRP	-	expression tag	UNP Q14703
A	9	VAL	-	expression tag	UNP Q14703
A	10	PRO	-	expression tag	UNP Q14703
A	11	GLY	-	expression tag	UNP Q14703
A	12	SER	-	expression tag	UNP Q14703
A	13	THR	-	expression tag	UNP Q14703
A	14	GLY	-	expression tag	UNP Q14703
A	15	ASP	-	expression tag	UNP Q14703
A	16	TYR	-	expression tag	UNP Q14703
A	17	LYS	-	expression tag	UNP Q14703
A	18	ASP	-	expression tag	UNP Q14703
A	19	ASP	-	expression tag	UNP Q14703
A	20	ASP	-	expression tag	UNP Q14703
A	21	ASP	-	expression tag	UNP Q14703
A	22	LYS	-	expression tag	UNP Q14703

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Chain	Residue	Modelled	Actual	Comment	Reference
A	23	ASP	-	expression tag	UNP Q14703
A	999	HIS	-	expression tag	UNP Q14703
A	1000	HIS	-	expression tag	UNP Q14703
A	1001	HIS	-	expression tag	UNP Q14703
A	1002	HIS	-	expression tag	UNP Q14703
A	1003	HIS	-	expression tag	UNP Q14703
A	1004	HIS	-	expression tag	UNP Q14703
A	1005	HIS	-	expression tag	UNP Q14703
A	1006	HIS	-	expression tag	UNP Q14703
A	1007	HIS	-	expression tag	UNP Q14703
A	1008	HIS	-	expression tag	UNP Q14703

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	H	N	O	0
			28	8	14	1	5	

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		AltConf
3	A	97	Total	O	0
			97	97	

HIS	ASN	LEU	THR
HIS	GLU	SER	ALA
HIS	THR	SER	VAL
HIS	ALA	GLY	VAL
HIS	PRO	GLY	ASN
HIS	SER	ARG	VAL
HIS	ASN	ARG	PRO
HIS	LEU	GLN	ILE
HIS	TRP	PRO	LEU
HIS	LYS	PRO	GLY
HIS	HIS	SER	LEU
HIS	GLN	GLY	TYR
HIS	LYS	ALA	GLN
HIS	LEU	GLY	ILE
HIS	LEU	SER	PRO
HIS	SER	SER	ALA
HIS	ILE	VAL	GLU
HIS	ASP	THR	GLY
HIS	LEU	PRO	GLY
HIS	ASP	GLU	TYR
HIS	LYS	GLY	GLY
HIS	VAL	MET	ASP
HIS	VAL	ARG	ILE
HIS	LEU	GLY	VAL
HIS	PRO	ASN	LEU
HIS	ASN	HIS	TYR
HIS	PHE	LEU	GLY
HIS	ARG	HIS	ASP
HIS	SER	ARG	SER
HIS	ASN	TYR	ASN
HIS	ARG	SER	CYS
HIS	PRO	LYS	LEU
HIS	GLN	VAL	ASP
HIS	VAL	LEU	ASP
HIS	ARG	GLU	SER
HIS	PRO	ALA	HIS
HIS	LEU	HIS	ARG
HIS	SER	LEU	GLN
HIS	PRO	GLY	LYS
HIS	GLY	ASP	CYS
HIS	GLU	PRO	ASP
HIS	SER	LYS	PHE
HIS	GLY	PRO	TRP
HIS	ALA	ARG	LEU
HIS	TRP	PRO	LEU
HIS	ASP	LEU	ASP
HIS	ILE	PRO	ALA
HIS	PRO	ALA	LEU
HIS	GLY	CYS	LEU
HIS	GLY	PRO	GLN
HIS	ILE	ARG	TYR
HIS	ILE	LEU	THR
HIS	MET	SER	SER
HIS	PRO	SER	TYR
HIS	GLY	TRP	GLY
HIS	ARG	ALA	VAL
HIS	TYR	LYS	THR
HIS	ASN	PRO	PRO
HIS	GLN	GLN	THR
HIS	GLU	PRO	PRO
HIS	VAL	LEU	SER

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	659523	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	55	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	1.377	Depositor
Minimum map value	-0.964	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.25	Depositor
Map size (Å)	295.19998, 295.19998, 295.19998	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.738, 0.738, 0.738	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.36	0/3923	0.54	0/5329

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	3835	3821	3816	106	0
2	A	14	14	13	3	0
3	A	97	0	0	17	0
All	All	3946	3835	3829	107	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 14.

The worst 5 of 107 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:234:ARG:NH1	1:A:244:ASP:OD1	1.98	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:562:LEU:HG	3:A:1205:HOH:O	1.69	0.91
1:A:427:LEU:O	1:A:430:THR:OG1	1.91	0.89
1:A:297:ILE:HA	3:A:1265:HOH:O	1.76	0.84
1:A:114:LEU:HD12	1:A:126:VAL:HG21	1.67	0.77

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	484/1014 (48%)	458 (95%)	26 (5%)	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	418/875 (48%)	411 (98%)	7 (2%)	53	70

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	214	VAL
1	A	259	SER

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Mol	Chain	Res	Type
1	A	494	CYS
1	A	469	LEU
1	A	195	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	352	GLN
1	A	366	ASN
1	A	541	ASN
1	A	461	GLN
1	A	204	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	NAG	A	1101	1	14,14,15	0.18	0	17,19,21	0.70	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	1101	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1101	NAG	C1-O5-C5	2.46	115.49	112.19

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1101	NAG	O5-C5-C6-O6
2	A	1101	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1101	NAG	3	0

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.

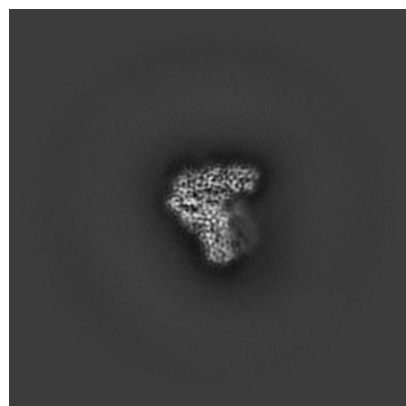
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42661. These allow visual inspection of the internal detail of the map and identification of artifacts.

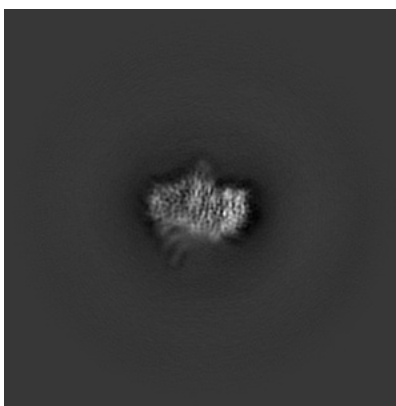
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

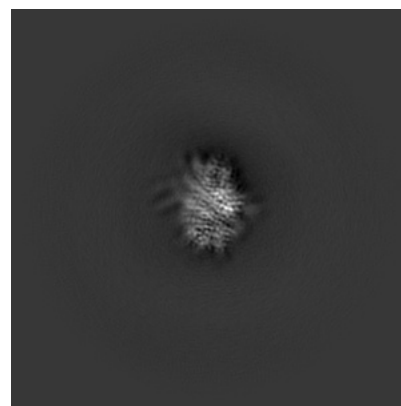
6.1.1 Primary map



X

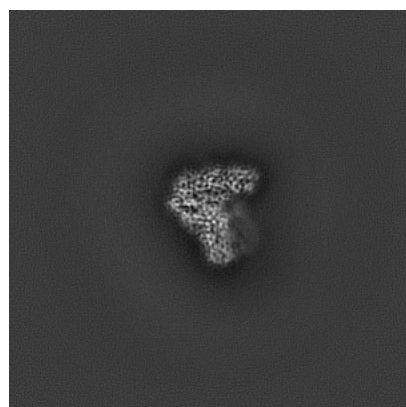


Y

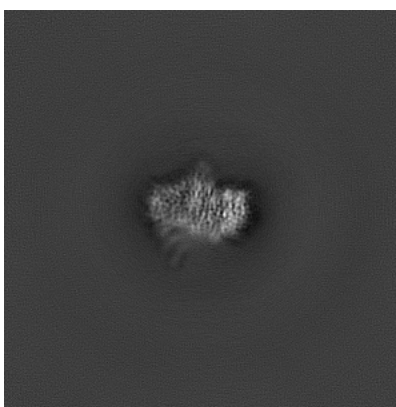


Z

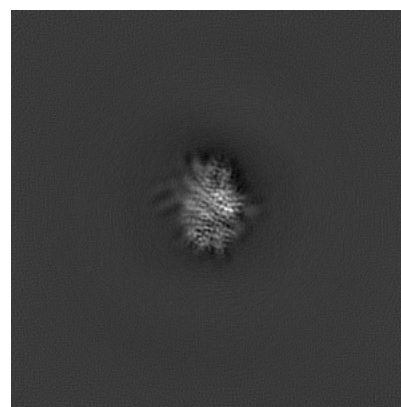
6.1.2 Raw map



X



Y

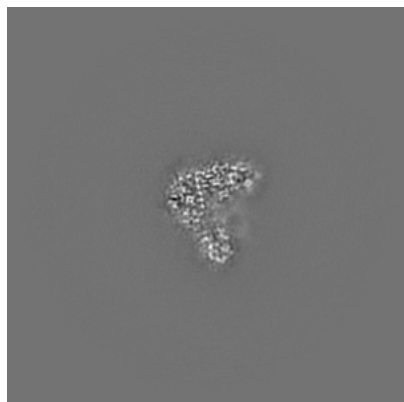


Z

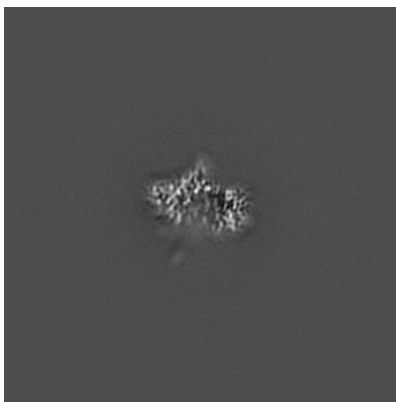
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

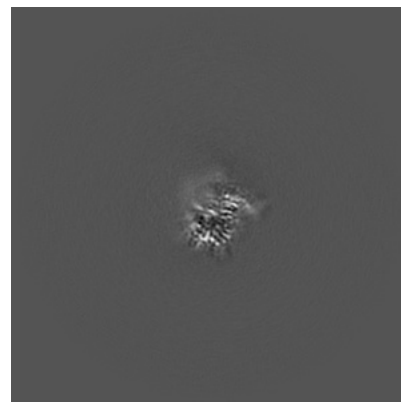
6.2.1 Primary map



X Index: 200

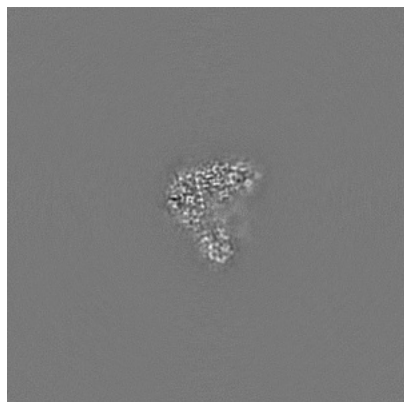


Y Index: 200

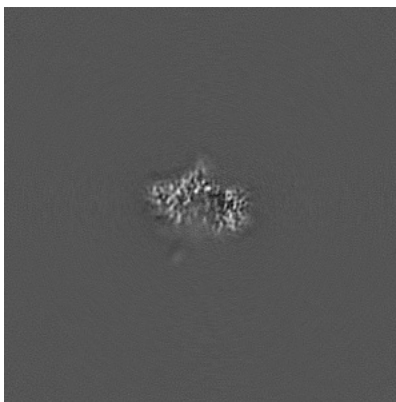


Z Index: 200

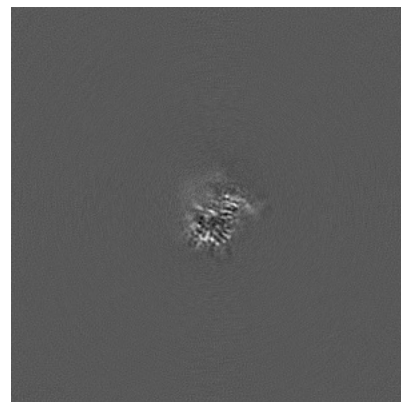
6.2.2 Raw map



X Index: 200



Y Index: 200

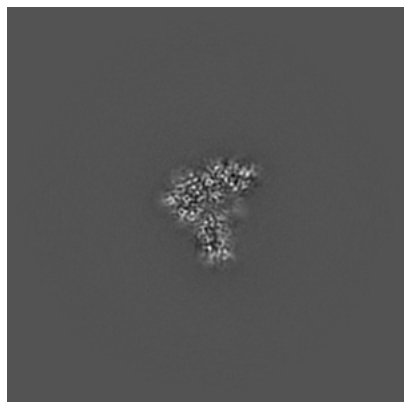


Z Index: 200

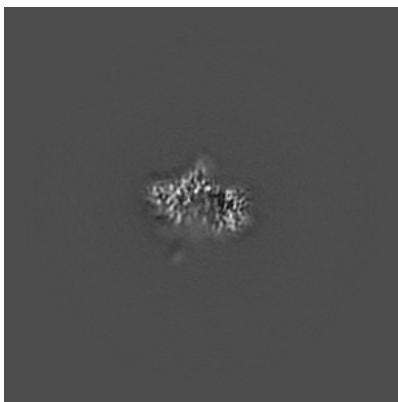
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

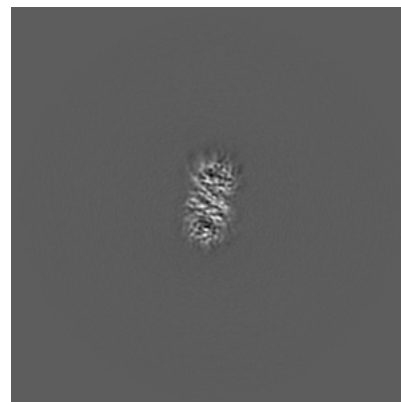
6.3.1 Primary map



X Index: 209

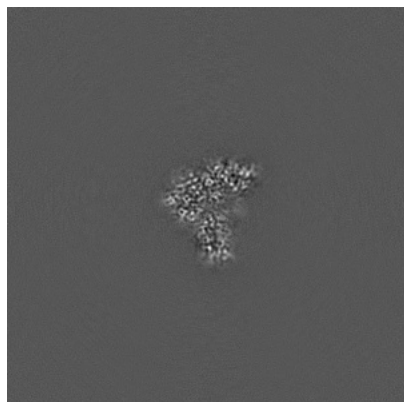


Y Index: 200

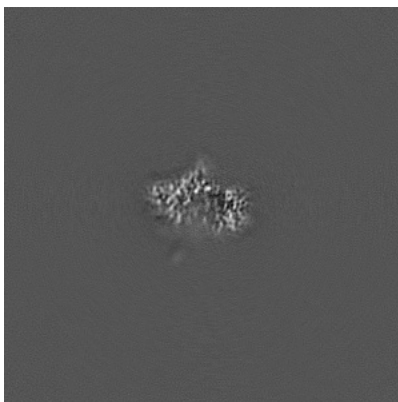


Z Index: 226

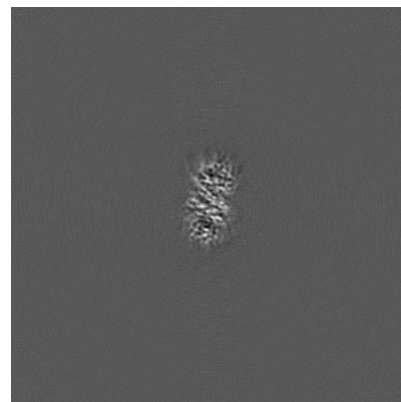
6.3.2 Raw map



X Index: 209



Y Index: 200



Z Index: 226

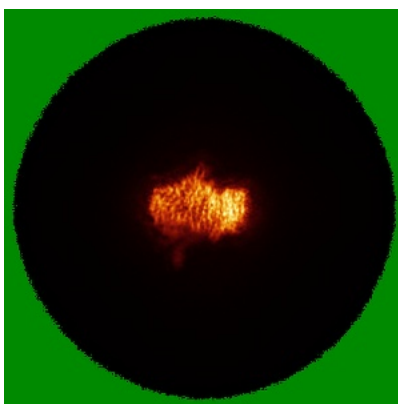
The images above show the largest variance slices of the map in three orthogonal directions.

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

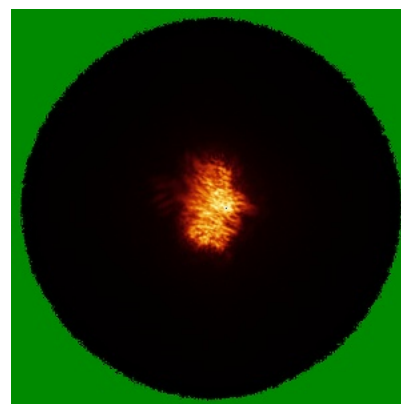
6.4.1 Primary map



X

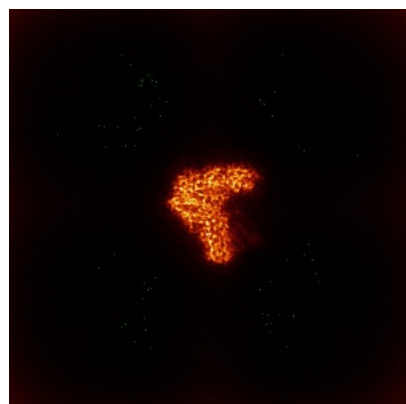


Y

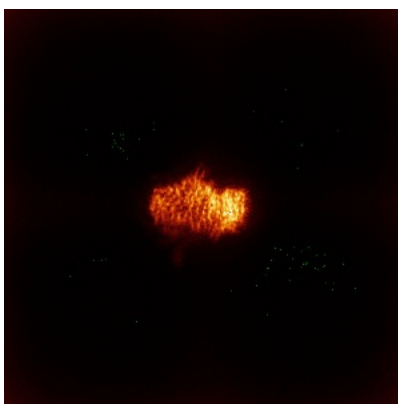


Z

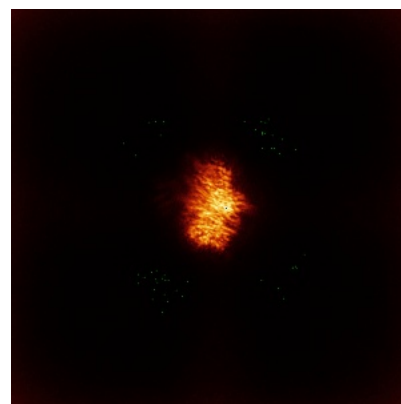
6.4.2 Raw map



X



Y

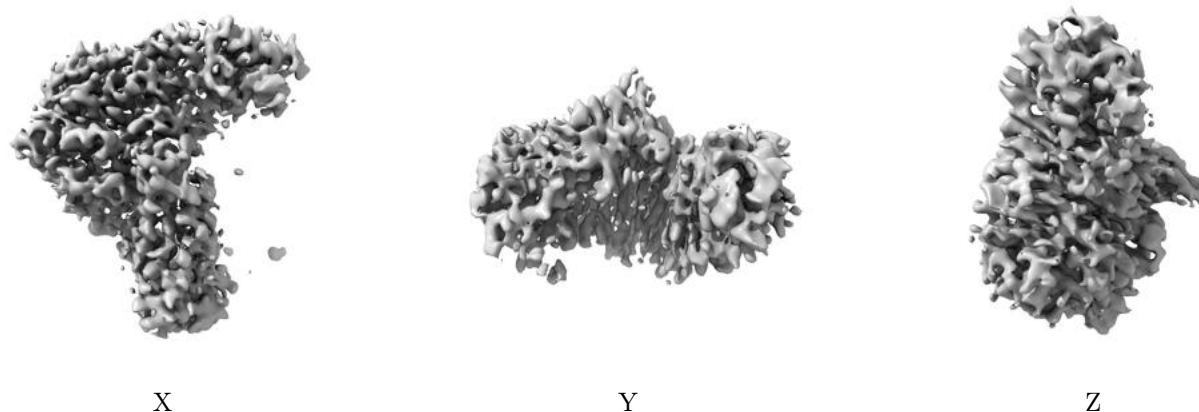


Z

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 0.25. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

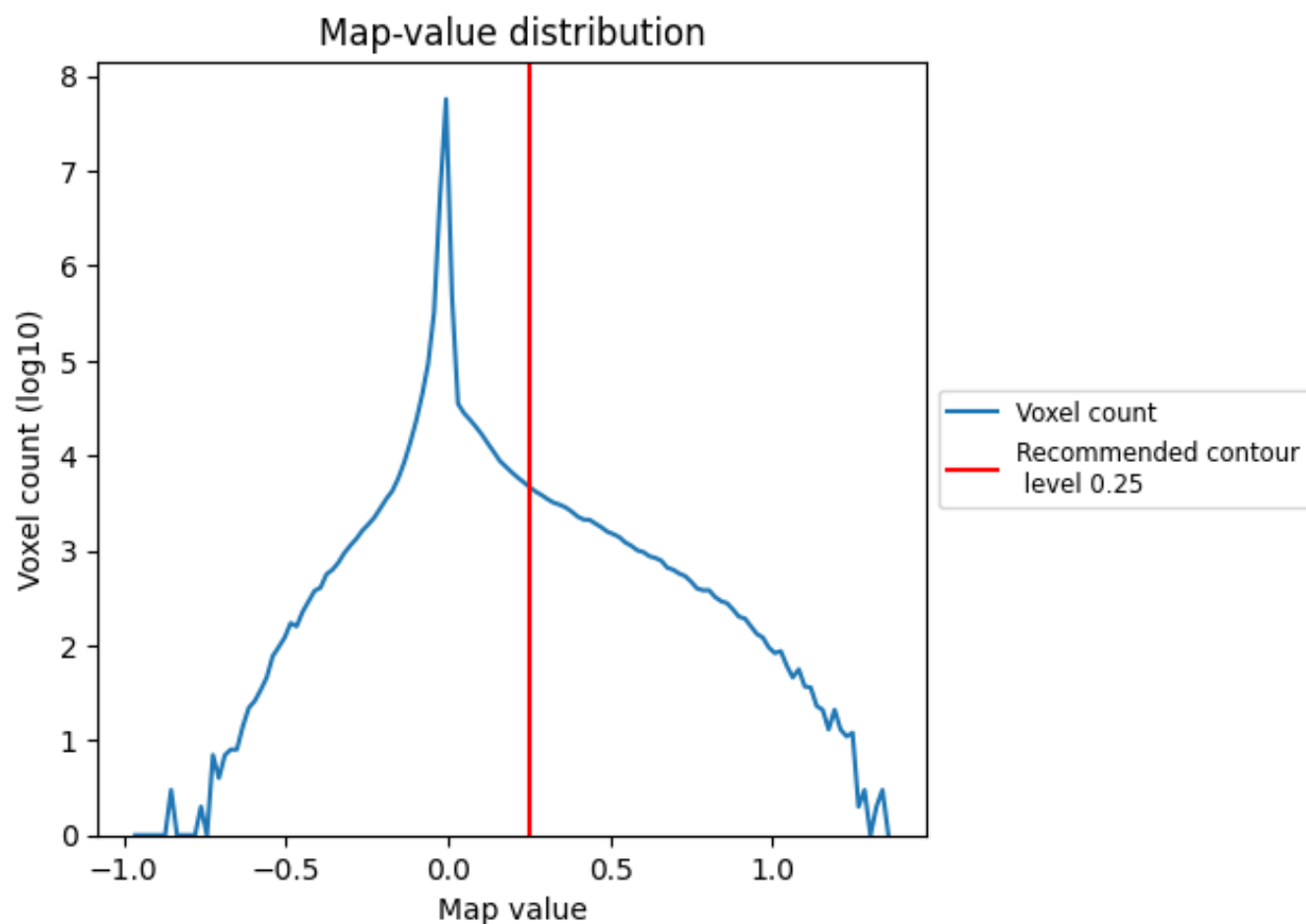
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

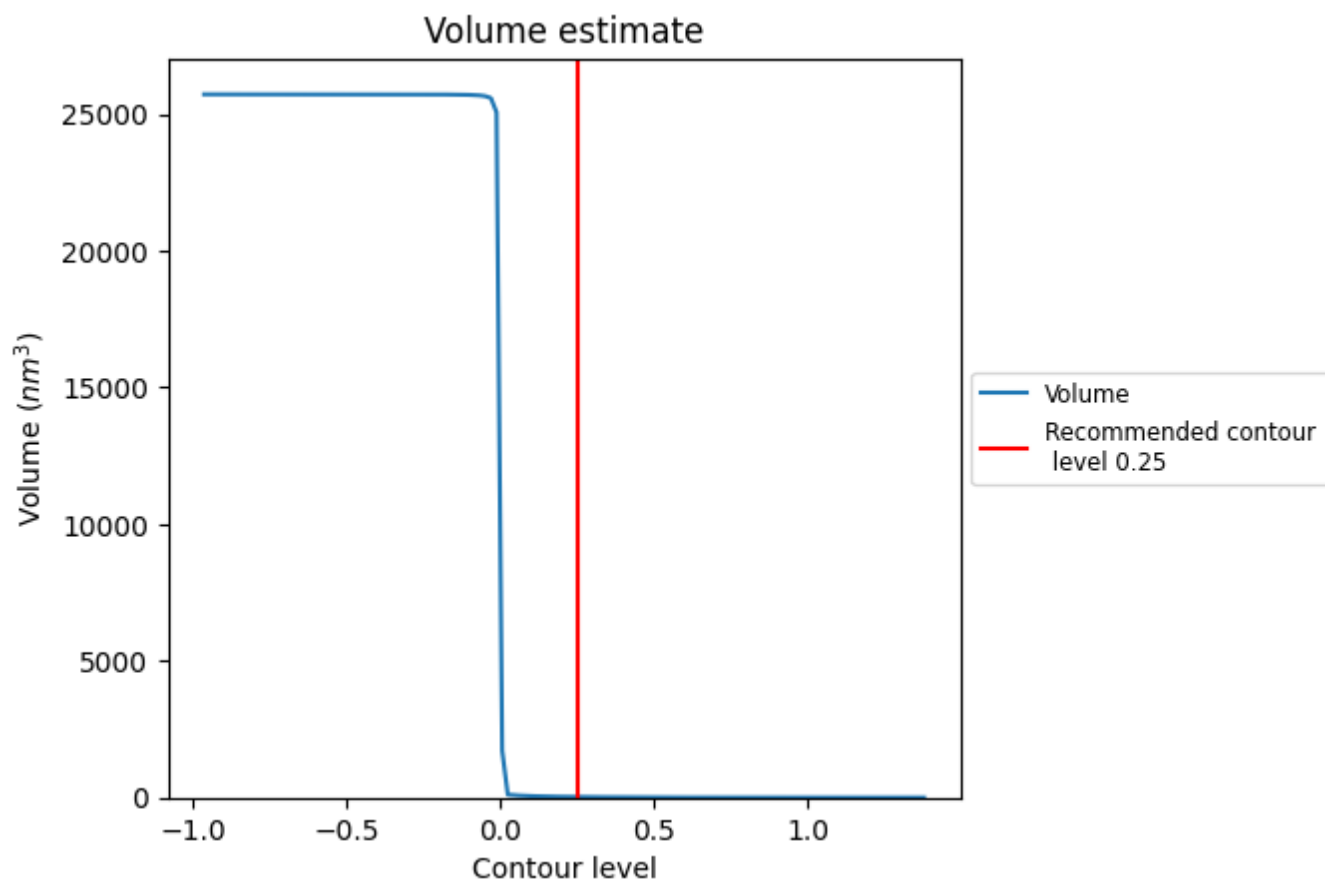
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

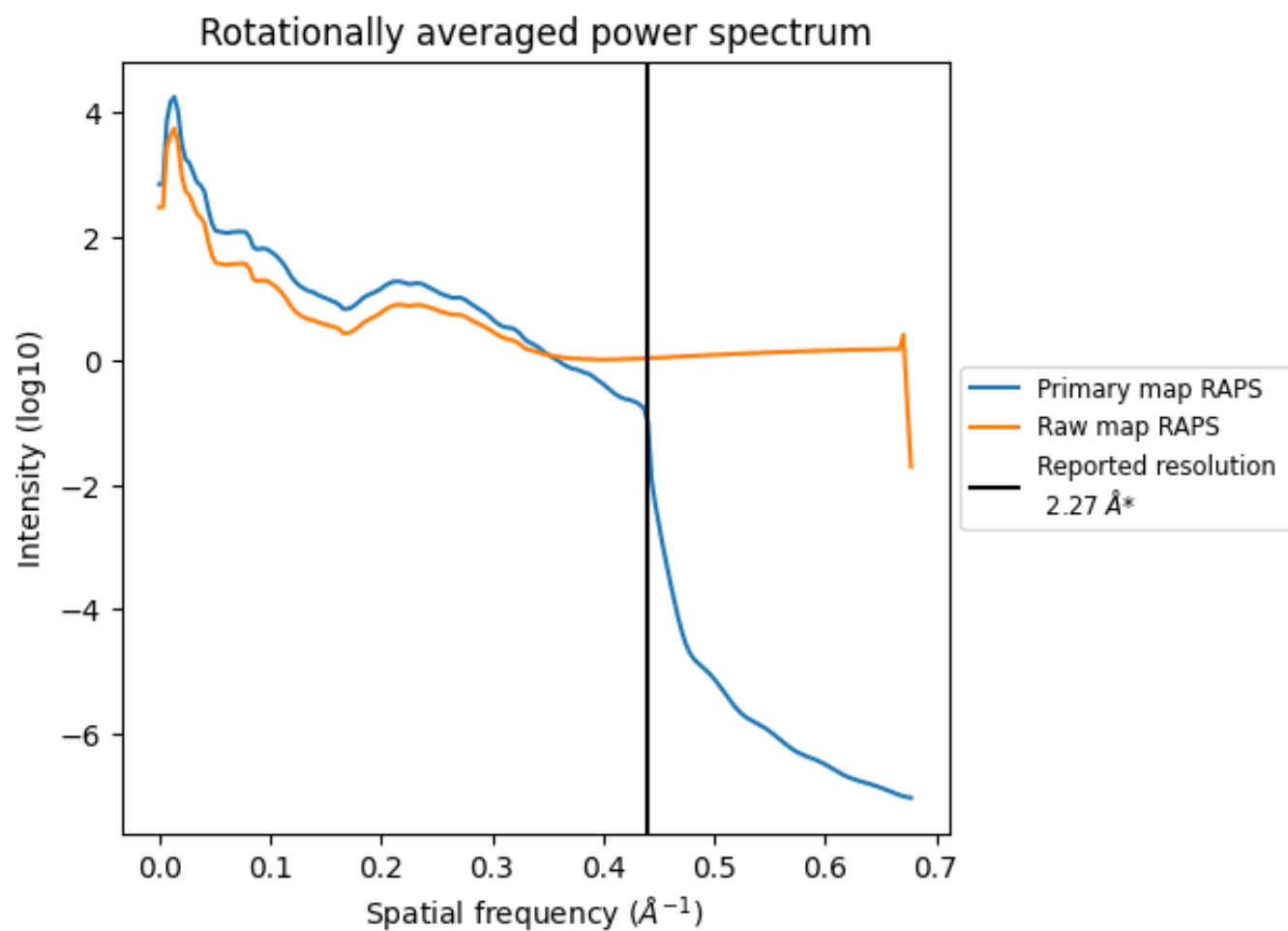
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 23 nm³; this corresponds to an approximate mass of 21 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 ⓘ

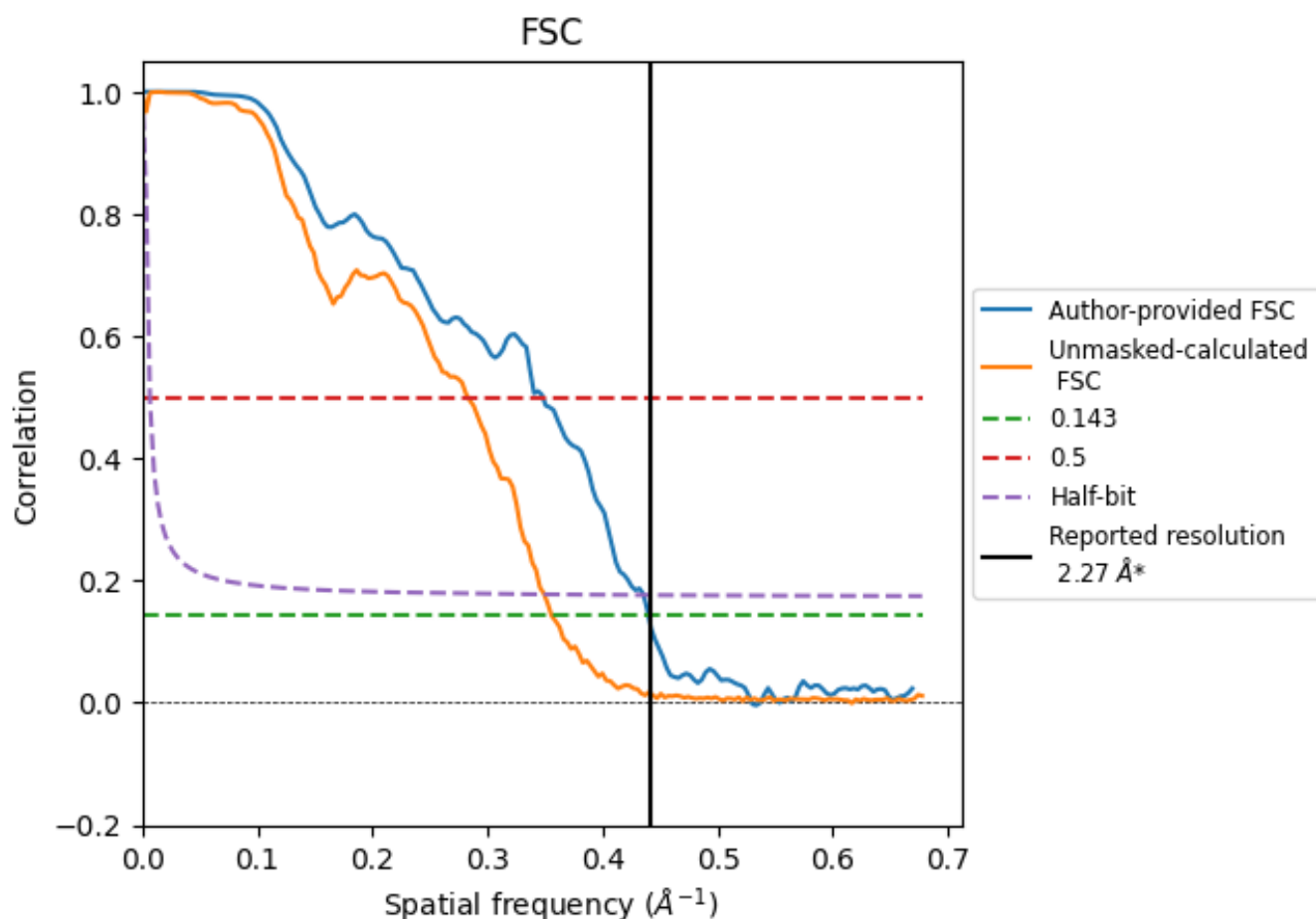


*Reported resolution corresponds to spatial frequency of 0.441 Å⁻¹

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 $0.441 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

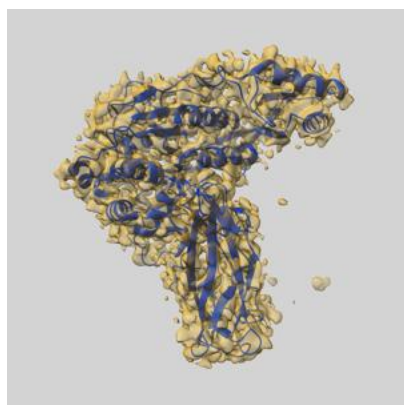
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.27	-	-
Author-provided FSC curve	2.27	2.87	2.30
Unmasked-calculated*	2.81	3.53	2.86

*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 2.81 differs from the reported value 2.27 by more than 10 %

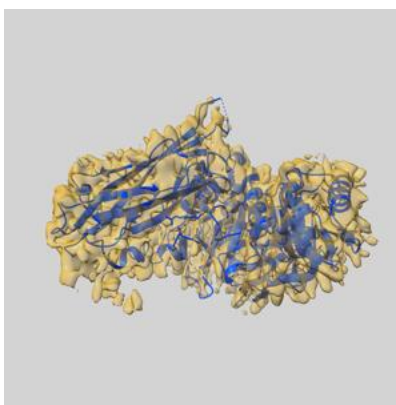
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-42661 and PDB model 8UWC. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

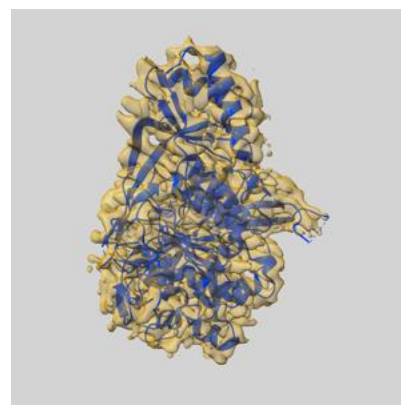
9.1 Map-model overlay [i](#)



X



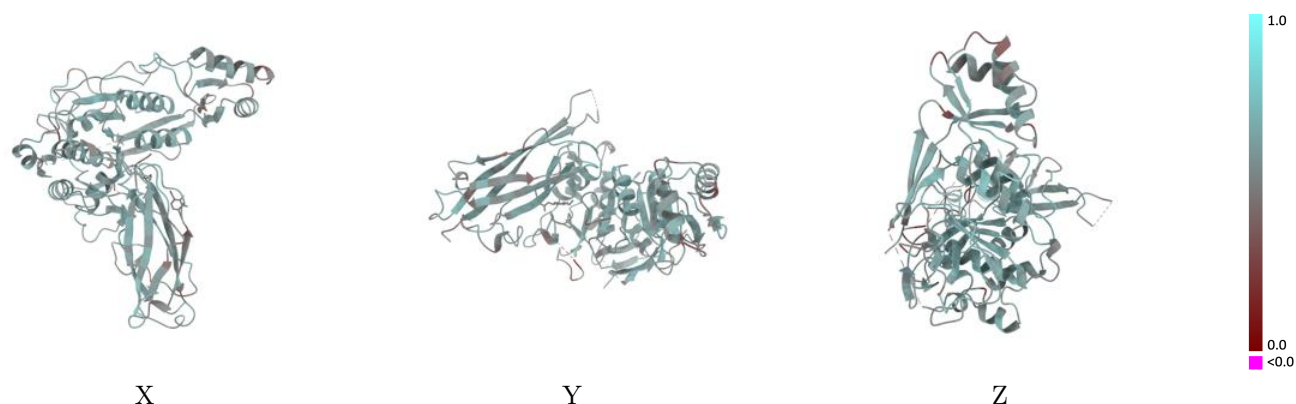
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.25 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](#)

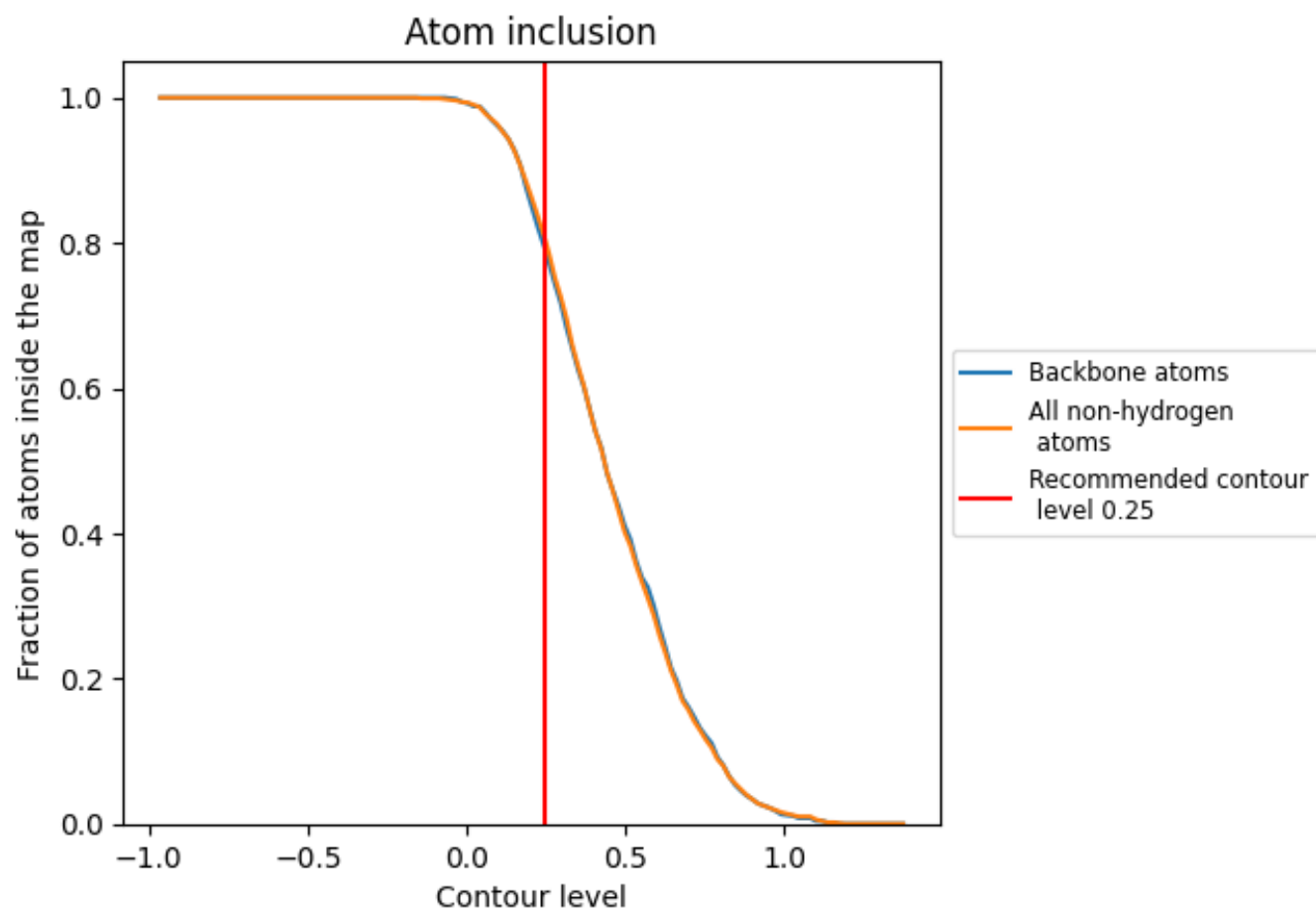


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 80% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8030	0.5580
A	0.8220	0.5580

