



## wwPDB EM Validation Summary Report ⓘ

Jul 15, 2024 – 09:16 pm BST

PDB ID : 7ZRZ  
EMDB ID : EMD-14923  
Title : Structure of the human tRNA splicing endonuclease defines substrate recognition  
Authors : Sekulovski, S.; Trowitzsch, S.  
Deposited on : 2022-05-05  
Resolution : 3.09 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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev92  
MolProbity : 4.02b-467  
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

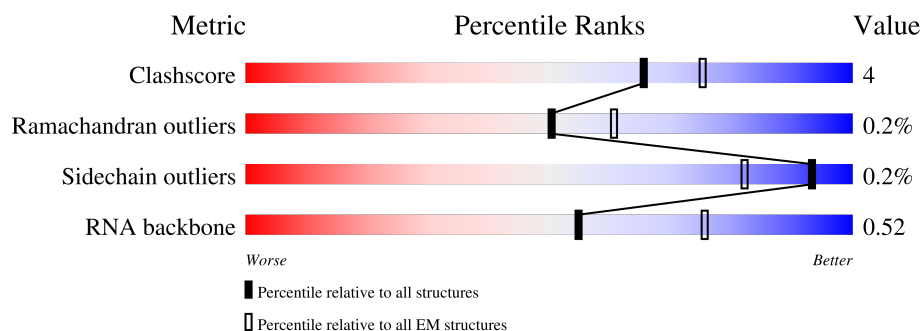
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.09 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
RNA backbone	4643	859

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  $\geq 3$ , 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	AP1	263	
2	BP4	260	
3	CP1	293	
4	DP1	217	
5	ZN1	89	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6580 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 tRNA-splicing endonuclease subunit Sen34.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AP1	184	Total	C	N	O	S	0	0
			1435	923	260	248	4		

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AP1	168	GLY	-	linker	UNP Q9BSV6
AP1	169	GLY	-	linker	UNP Q9BSV6
AP1	170	SER	-	linker	UNP Q9BSV6
AP1	171	GLY	-	linker	UNP Q9BSV6
AP1	172	GLY	-	linker	UNP Q9BSV6
AP1	173	SER	-	linker	UNP Q9BSV6
AP1	174	GLY	-	linker	UNP Q9BSV6
AP1	175	GLY	-	linker	UNP Q9BSV6
AP1	176	SER	-	linker	UNP Q9BSV6
AP1	177	GLY	-	linker	UNP Q9BSV6
AP1	178	GLY	-	linker	UNP Q9BSV6
AP1	179	SER	-	linker	UNP Q9BSV6
AP1	255	PHE	HIS	conflict	UNP Q9BSV6

- Molecule 2 is a protein called tRNA-splicing endonuclease subunit Sen2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	BP4	104	Total	C	N	O	S	0	0
			861	563	146	149	3		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BP4	287	GLY	-	linker	UNP Q8NCE0
BP4	288	GLY	-	linker	UNP Q8NCE0
BP4	289	SER	-	linker	UNP Q8NCE0
BP4	290	GLY	-	linker	UNP Q8NCE0

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Chain	Residue	Modelled	Actual	Comment	Reference
BP4	291	GLY	-	linker	UNP Q8NCE0
BP4	377	PHE	HIS	conflict	UNP Q8NCE0

- Molecule 3 is a protein called tRNA-splicing endonuclease subunit Sen54.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	CP1	220	Total	C	N	O	S	0	0
			1791	1149	313	323	6		

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CP1	412	GLY	-	linker	UNP Q7Z6J9
CP1	413	GLY	-	linker	UNP Q7Z6J9
CP1	414	SER	-	linker	UNP Q7Z6J9
CP1	415	GLY	-	linker	UNP Q7Z6J9
CP1	416	GLY	-	linker	UNP Q7Z6J9
CP1	417	SER	-	linker	UNP Q7Z6J9
CP1	418	GLY	-	linker	UNP Q7Z6J9
CP1	419	GLY	-	linker	UNP Q7Z6J9
CP1	420	SER	-	linker	UNP Q7Z6J9
CP1	421	GLY	-	linker	UNP Q7Z6J9
CP1	422	GLY	-	linker	UNP Q7Z6J9
CP1	423	SER	-	linker	UNP Q7Z6J9
CP1	424	GLY	-	linker	UNP Q7Z6J9

- Molecule 4 is a protein called tRNA-splicing endonuclease subunit Sen15.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	DP1	109	Total	C	N	O	S	0	0
			848	545	133	165	5		

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DP1	-45	MET	-	initiating methionine	UNP Q8WW01
DP1	-44	ASP	-	expression tag	UNP Q8WW01
DP1	-43	GLU	-	expression tag	UNP Q8WW01
DP1	-42	LYS	-	expression tag	UNP Q8WW01
DP1	-41	THR	-	expression tag	UNP Q8WW01
DP1	-40	THR	-	expression tag	UNP Q8WW01
DP1	-39	GLY	-	expression tag	UNP Q8WW01

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Chain	Residue	Modelled	Actual	Comment	Reference
DP1	-38	TRP	-	expression tag	UNP Q8WW01
DP1	-37	ARG	-	expression tag	UNP Q8WW01
DP1	-36	GLY	-	expression tag	UNP Q8WW01
DP1	-35	GLY	-	expression tag	UNP Q8WW01
DP1	-34	HIS	-	expression tag	UNP Q8WW01
DP1	-33	VAL	-	expression tag	UNP Q8WW01
DP1	-32	VAL	-	expression tag	UNP Q8WW01
DP1	-31	GLU	-	expression tag	UNP Q8WW01
DP1	-30	GLY	-	expression tag	UNP Q8WW01
DP1	-29	LEU	-	expression tag	UNP Q8WW01
DP1	-28	ALA	-	expression tag	UNP Q8WW01
DP1	-27	GLY	-	expression tag	UNP Q8WW01
DP1	-26	GLU	-	expression tag	UNP Q8WW01
DP1	-25	LEU	-	expression tag	UNP Q8WW01
DP1	-24	GLU	-	expression tag	UNP Q8WW01
DP1	-23	GLN	-	expression tag	UNP Q8WW01
DP1	-22	LEU	-	expression tag	UNP Q8WW01
DP1	-21	ARG	-	expression tag	UNP Q8WW01
DP1	-20	ALA	-	expression tag	UNP Q8WW01
DP1	-19	ARG	-	expression tag	UNP Q8WW01
DP1	-18	LEU	-	expression tag	UNP Q8WW01
DP1	-17	GLU	-	expression tag	UNP Q8WW01
DP1	-16	HIS	-	expression tag	UNP Q8WW01
DP1	-15	HIS	-	expression tag	UNP Q8WW01
DP1	-14	PRO	-	expression tag	UNP Q8WW01
DP1	-13	GLN	-	expression tag	UNP Q8WW01
DP1	-12	GLY	-	expression tag	UNP Q8WW01
DP1	-11	GLN	-	expression tag	UNP Q8WW01
DP1	-10	ARG	-	expression tag	UNP Q8WW01
DP1	-9	GLU	-	expression tag	UNP Q8WW01
DP1	-8	PRO	-	expression tag	UNP Q8WW01
DP1	-7	GLY	-	expression tag	UNP Q8WW01
DP1	-6	GLU	-	expression tag	UNP Q8WW01
DP1	-5	ASN	-	expression tag	UNP Q8WW01
DP1	-4	LEU	-	expression tag	UNP Q8WW01
DP1	-3	TYR	-	expression tag	UNP Q8WW01
DP1	-2	PHE	-	expression tag	UNP Q8WW01
DP1	-1	GLN	-	expression tag	UNP Q8WW01
DP1	0	GLY	-	expression tag	UNP Q8WW01

- Molecule 5 is a RNA chain called pre-tRNA Arg TCT 3-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	ZN1	77	Total	C	N	O	P	0	0
			1645	735	296	538	76		







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	282863	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	63	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	5.135	Depositor
Minimum map value	-3.450	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.073	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	299.52, 299.52, 299.52	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.78, 0.78, 0.78	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	AP1	0.24	0/1473	0.52	0/2005
2	BP4	0.25	0/885	0.51	0/1196
3	CP1	0.25	0/1838	0.49	0/2486
4	DP1	0.23	0/865	0.46	0/1180
5	ZN1	0.22	0/1839	0.77	0/2864
All	All	0.24	0/6900	0.59	0/9731

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 [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	AP1	1435	0	1451	13	0
2	BP4	861	0	867	7	0
3	CP1	1791	0	1751	16	0
4	DP1	848	0	854	8	0
5	ZN1	1645	0	831	14	0
All	All	6580	0	5754	50	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 4.

The worst 5 of 50 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)
5:ZN1:9:G:H1	5:ZN1:23:C:H41	1.30	0.79
4:DP1:144:VAL:HG12	4:DP1:150:ILE:HG12	1.78	0.65
1:AP1:237:ALA:HB2	1:AP1:245:LEU:HG	1.81	0.63
2:BP4:416:LYS:O	2:BP4:417:GLU:HB2	2.00	0.62
3:CP1:462:ARG:HG2	5:ZN1:82:A:H5"	1.82	0.61

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	AP1	180/263 (68%)	174 (97%)	6 (3%)	0	100	100
2	BP4	100/260 (38%)	93 (93%)	6 (6%)	1 (1%)	15	49
3	CP1	216/293 (74%)	208 (96%)	8 (4%)	0	100	100
4	DP1	107/217 (49%)	101 (94%)	6 (6%)	0	100	100
All	All	603/1033 (58%)	576 (96%)	26 (4%)	1 (0%)	50	79

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	BP4	417	GLU

### 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	AP1	147/208 (71%)	147 (100%)	0	100	100
2	BP4	95/232 (41%)	95 (100%)	0	100	100
3	CP1	192/244 (79%)	191 (100%)	1 (0%)	88	94
4	DP1	98/180 (54%)	98 (100%)	0	100	100
All	All	532/864 (62%)	531 (100%)	1 (0%)	93	97

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

Mol	Chain	Res	Type
3	CP1	111	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
5	ZN1	75/89 (84%)	17 (22%)	1 (1%)

5 of 17 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	ZN1	16	U
5	ZN1	17	G
5	ZN1	18	G
5	ZN1	19	A
5	ZN1	21	A

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	ZN1	24	G

## 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 [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 [i](#)

There are no chain breaks in this entry.

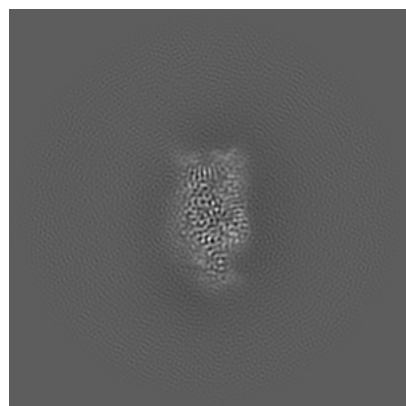
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14923. These allow visual inspection of the internal detail of the map and identification of artifacts.

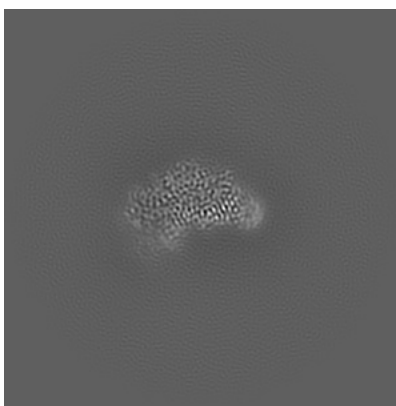
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

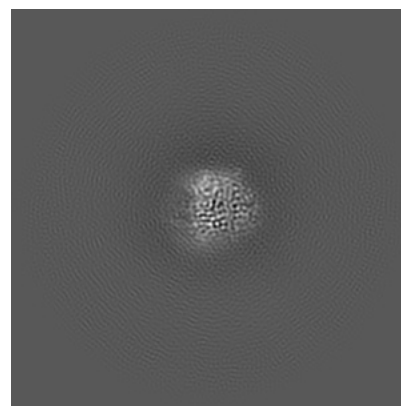
#### 6.1.1 Primary map



X

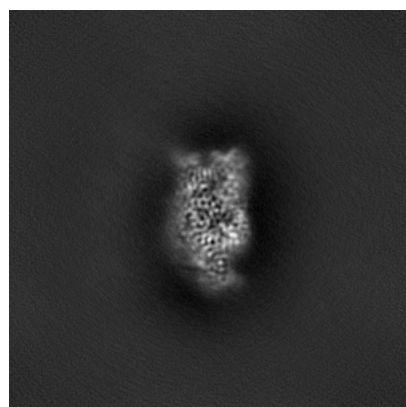


Y

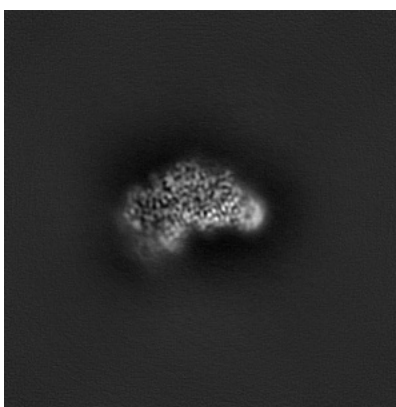


Z

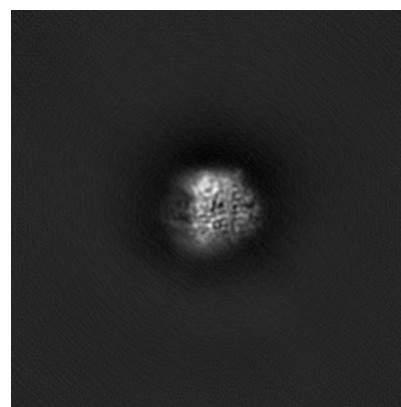
#### 6.1.2 Raw map



X



Y

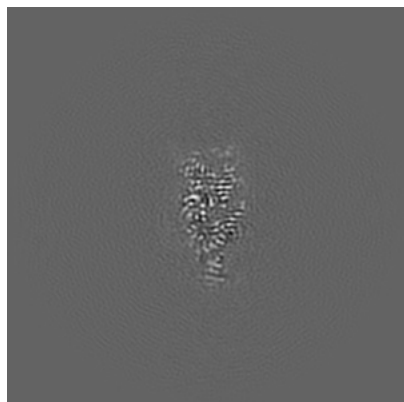


Z

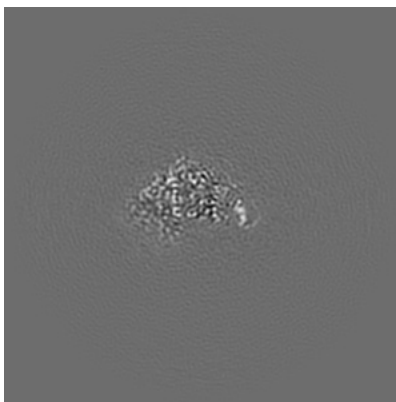
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

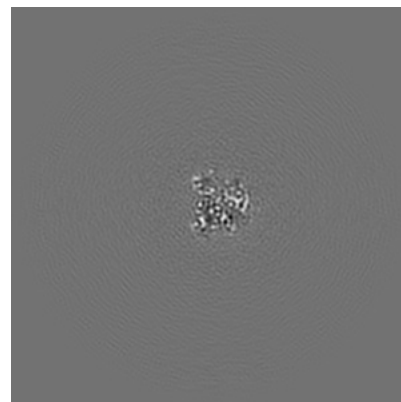
### 6.2.1 Primary map



X Index: 192

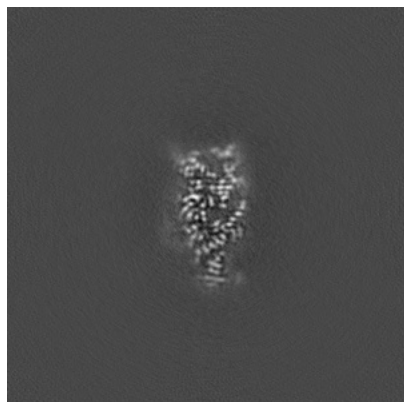


Y Index: 192

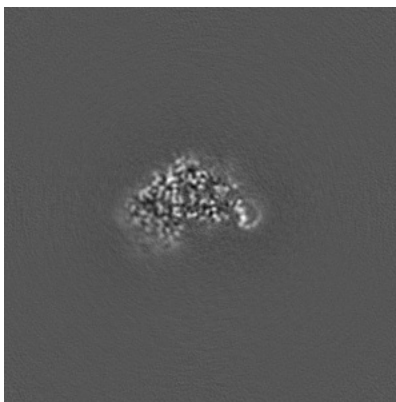


Z Index: 192

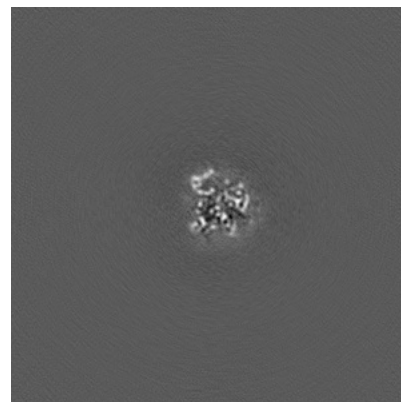
### 6.2.2 Raw map



X Index: 192



Y Index: 192

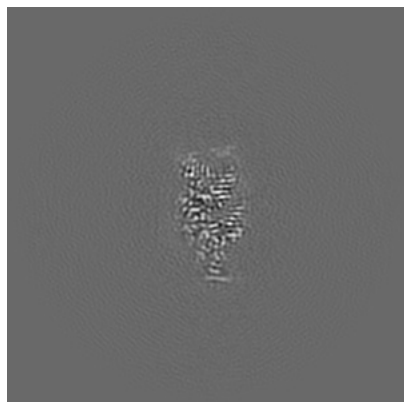


Z Index: 192

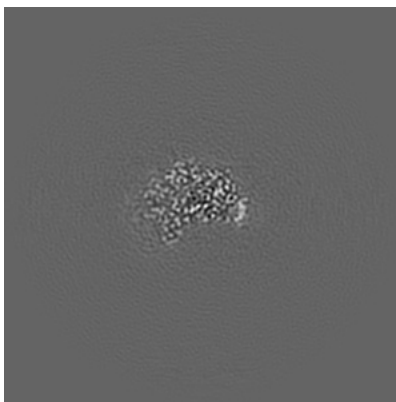
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

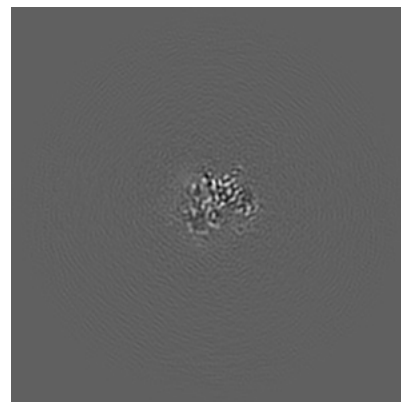
### 6.3.1 Primary map



X Index: 190

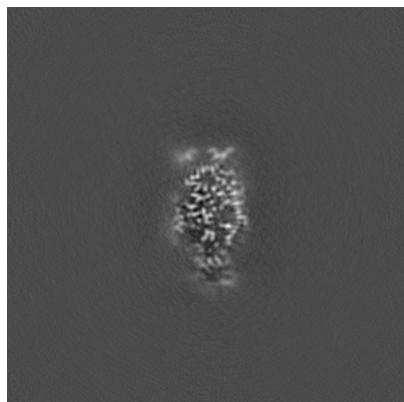


Y Index: 187

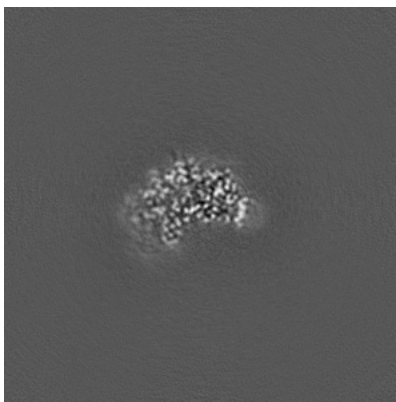


Z Index: 168

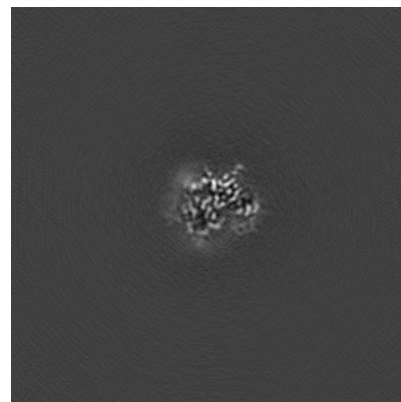
### 6.3.2 Raw map



X Index: 184



Y Index: 187



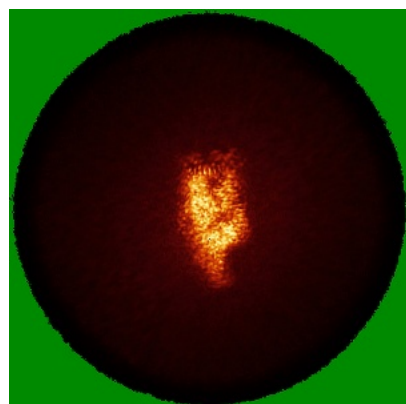
Z Index: 168

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

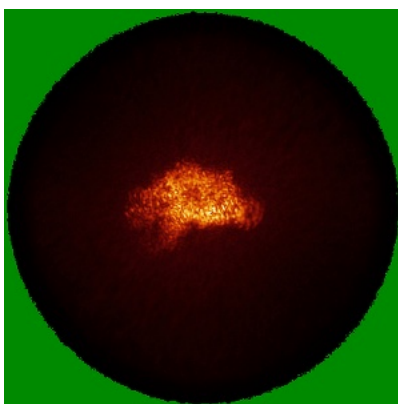


## 6.4 Orthogonal standard-deviation projections (False-color) ⓘ

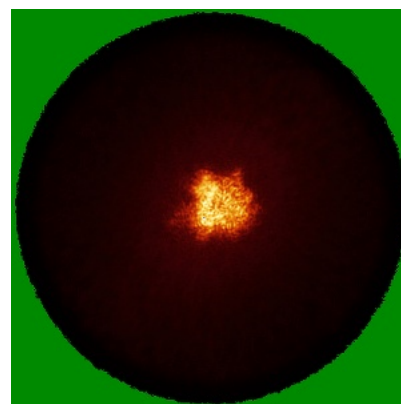
### 6.4.1 Primary map



X

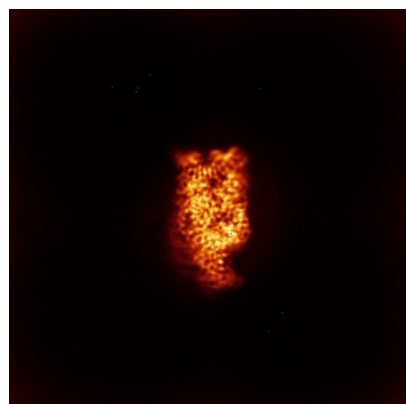


Y

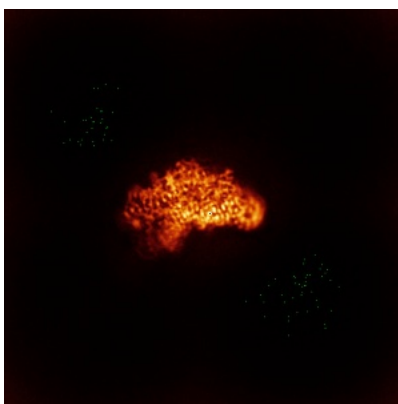


Z

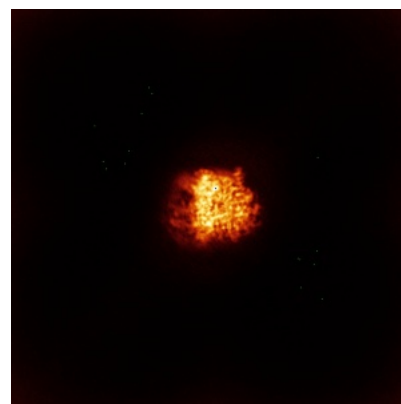
### 6.4.2 Raw map



X



Y

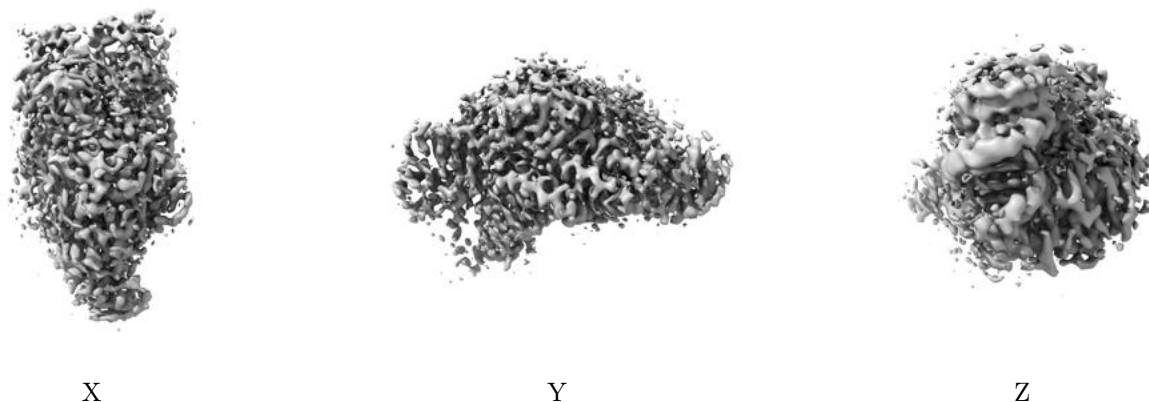


Z

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.

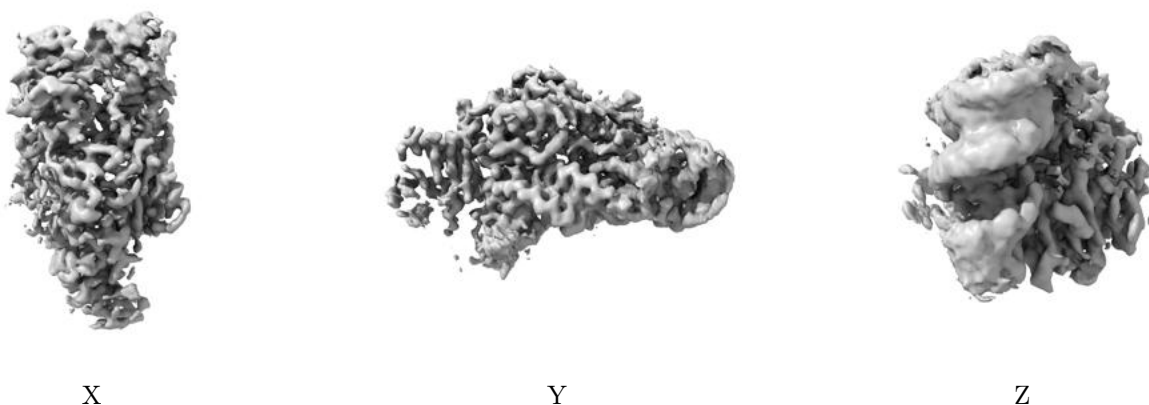
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.5. 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.

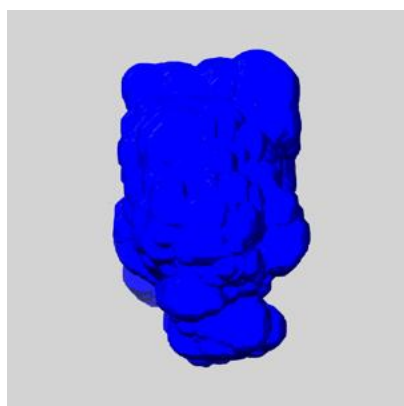
## 6.6 Mask visualisation [i](#)

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

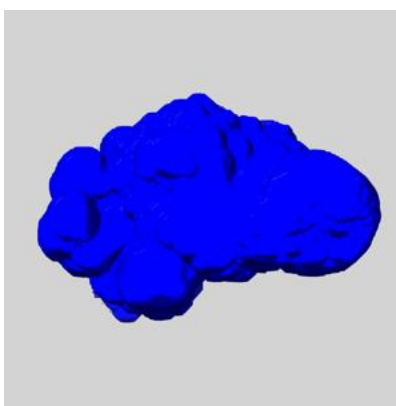
A mask typically either:

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

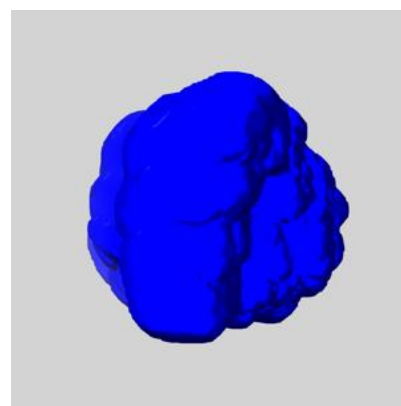
### 6.6.1 emd\_14923\_msk\_1.map [i](#)



X



Y

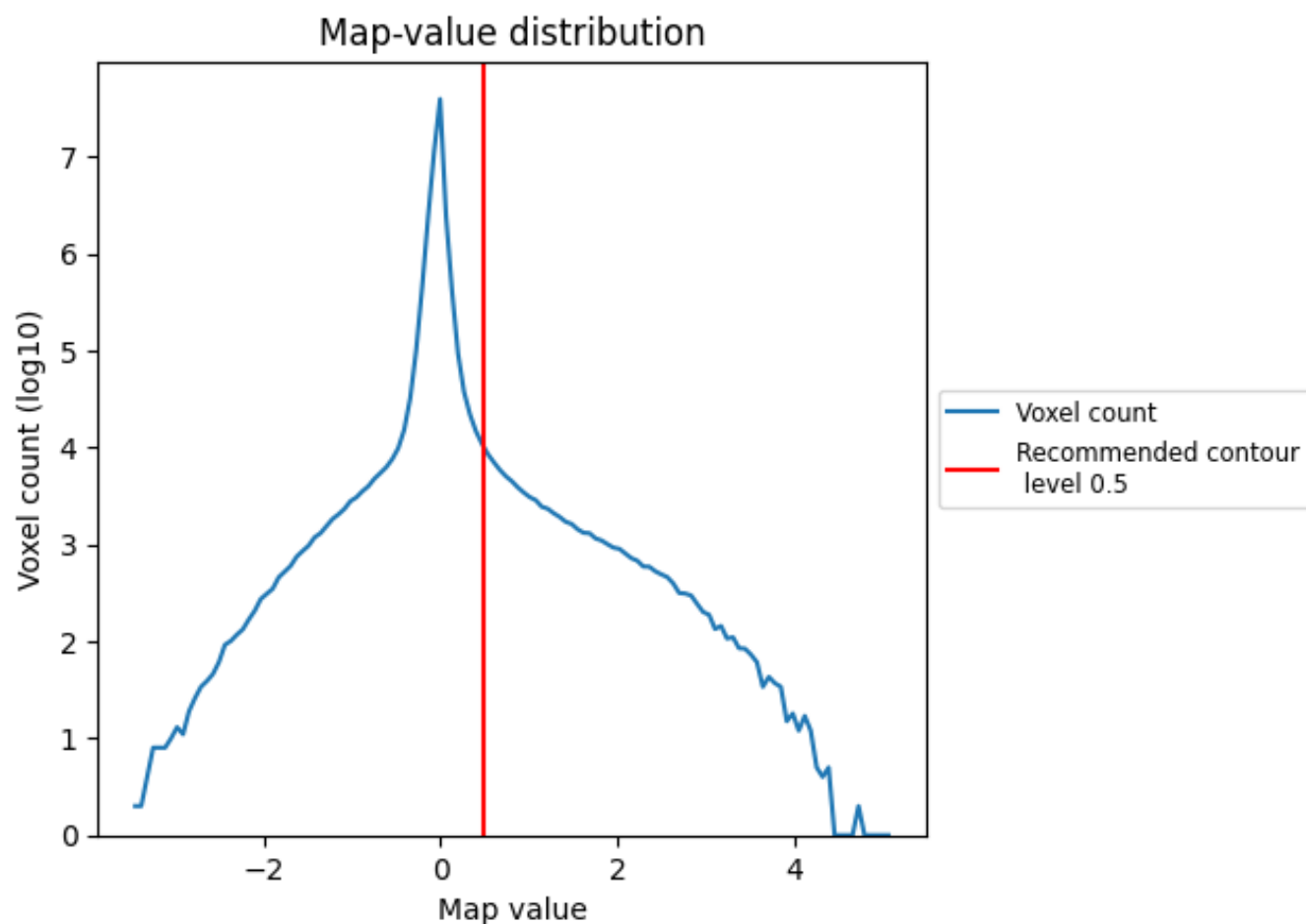


Z

## 7 Map analysis [i](#)

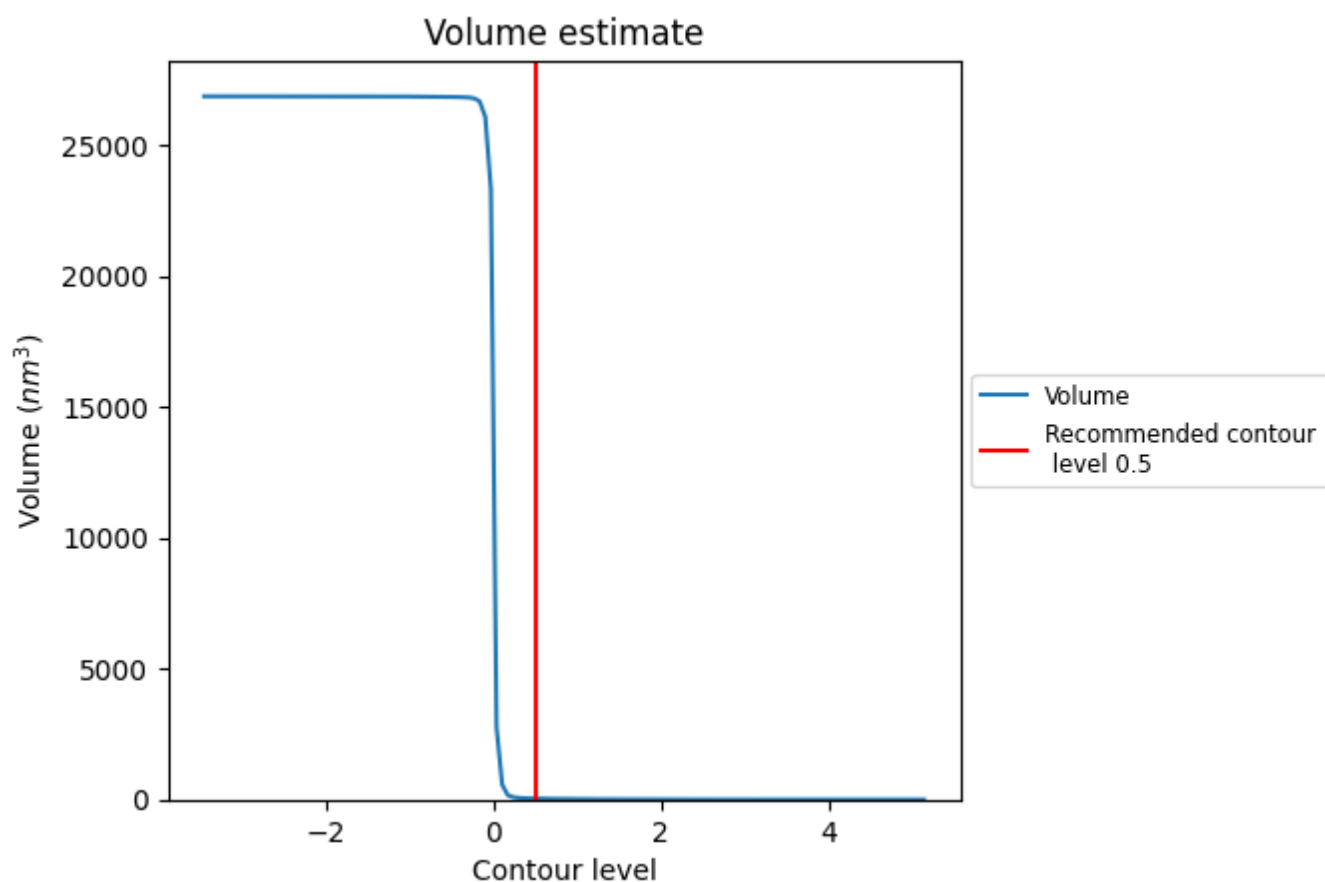
This section contains the results of statistical analysis of the map.

### 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.

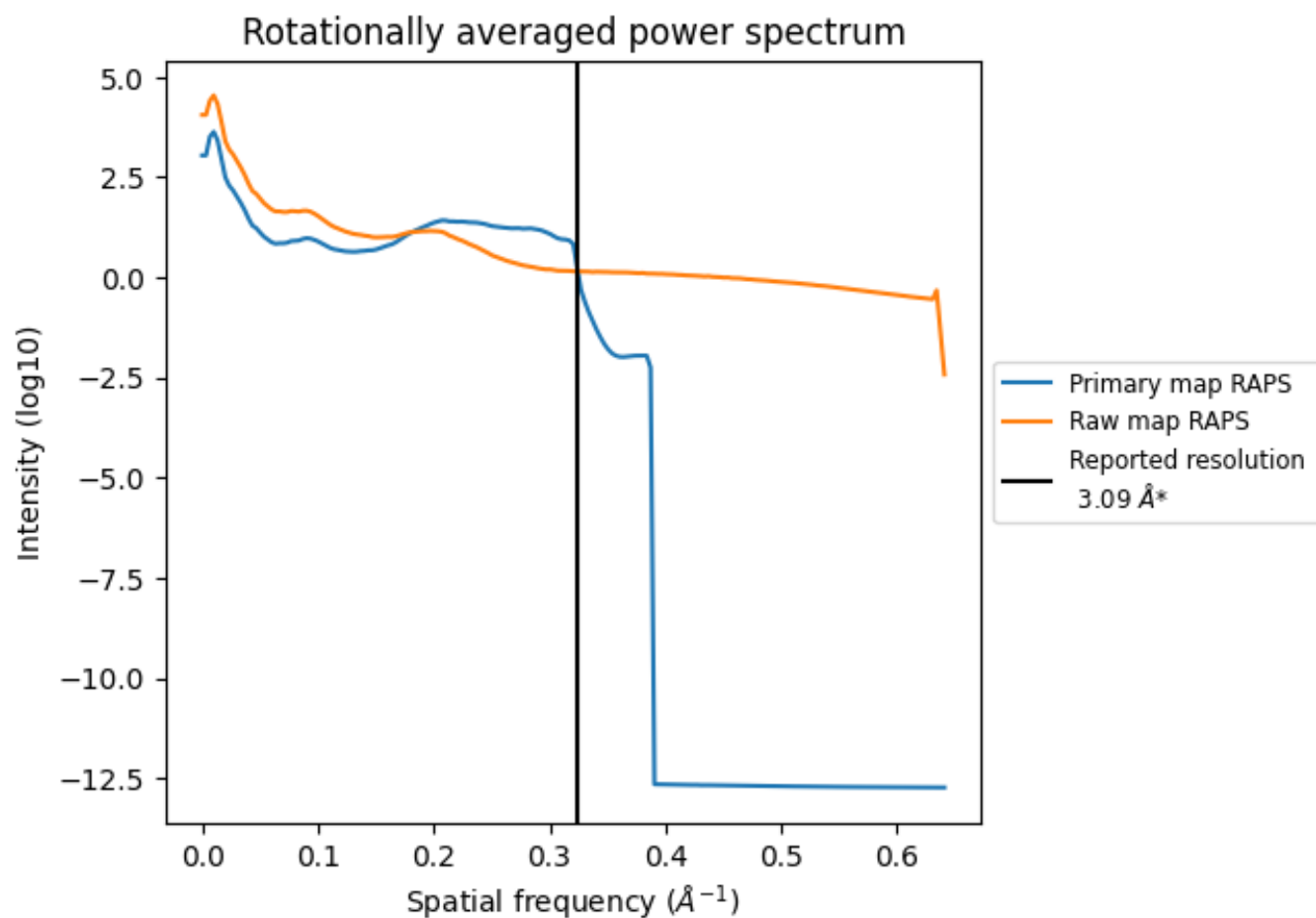
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 38  $\text{nm}^3$ ; this corresponds to an approximate mass of 34 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 ⓘ

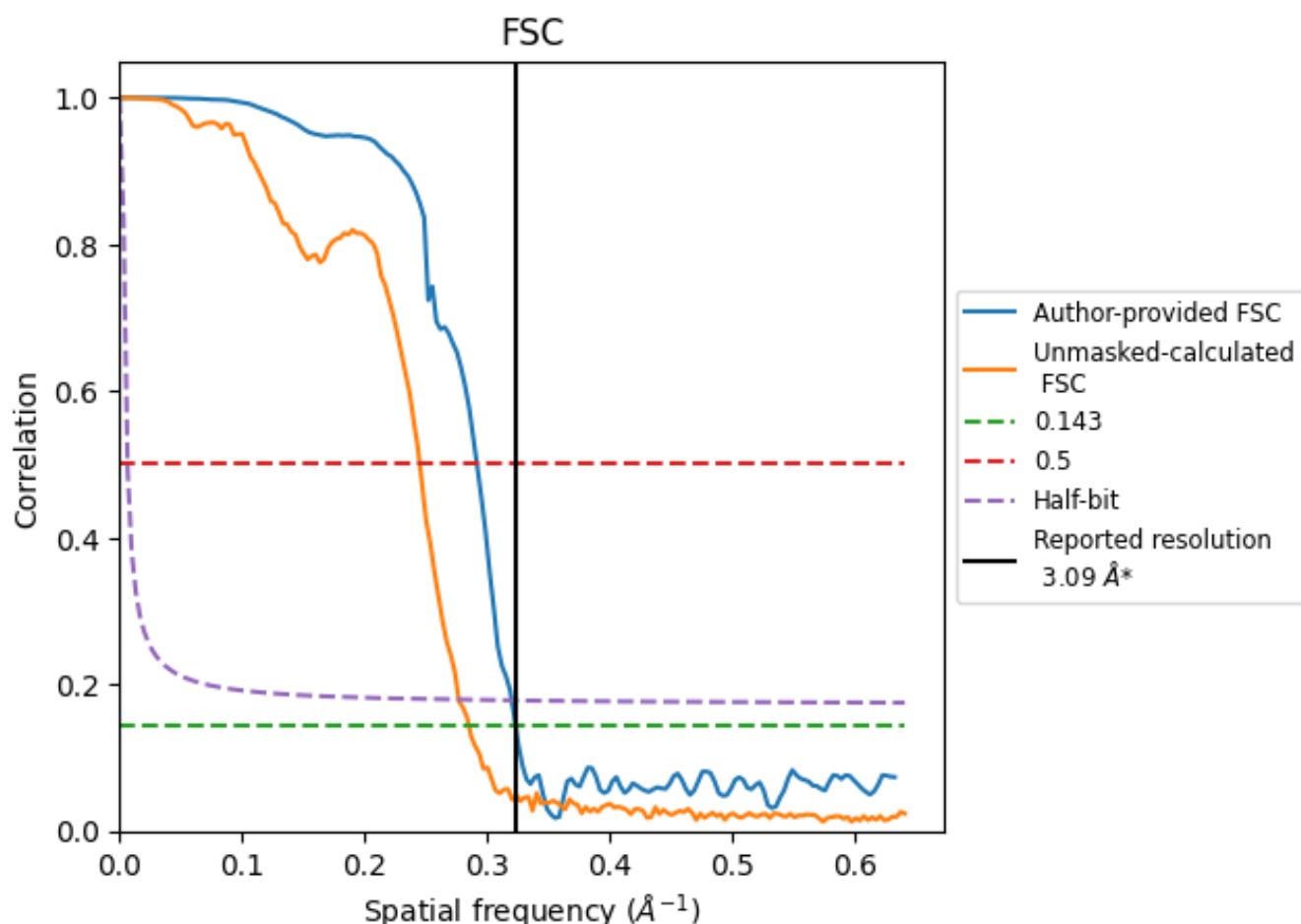


\*Reported resolution corresponds to spatial frequency of 0.324  $\text{\AA}^{-1}$

## 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 0.324  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.09	-	-
Author-provided FSC curve	3.09	3.43	3.12
Unmasked-calculated*	3.51	4.08	3.61

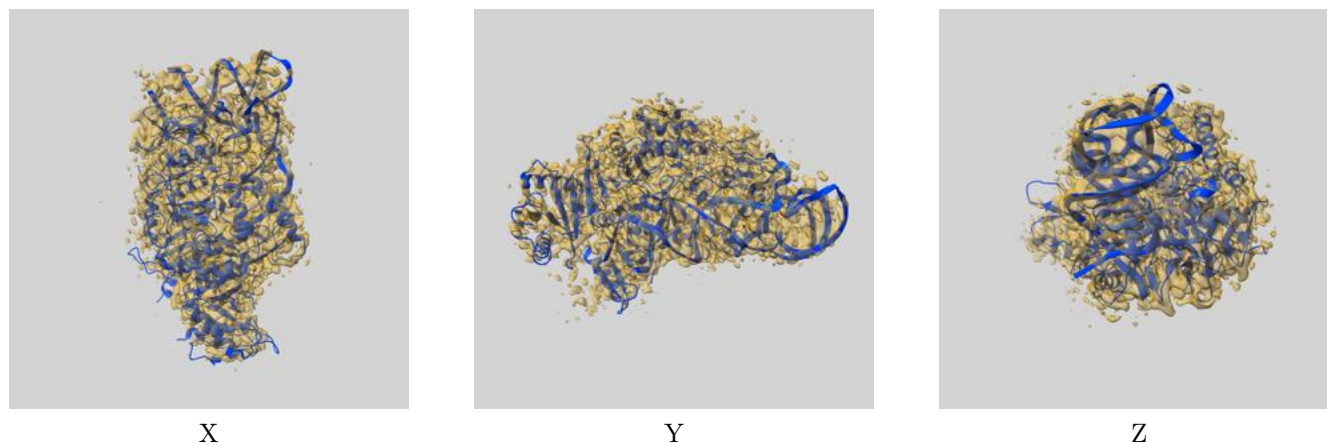
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.51 differs from the reported value 3.09 by more than 10 %



## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-14923 and PDB model 7ZRZ. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

### 9.1 Map-model overlay [i](#)



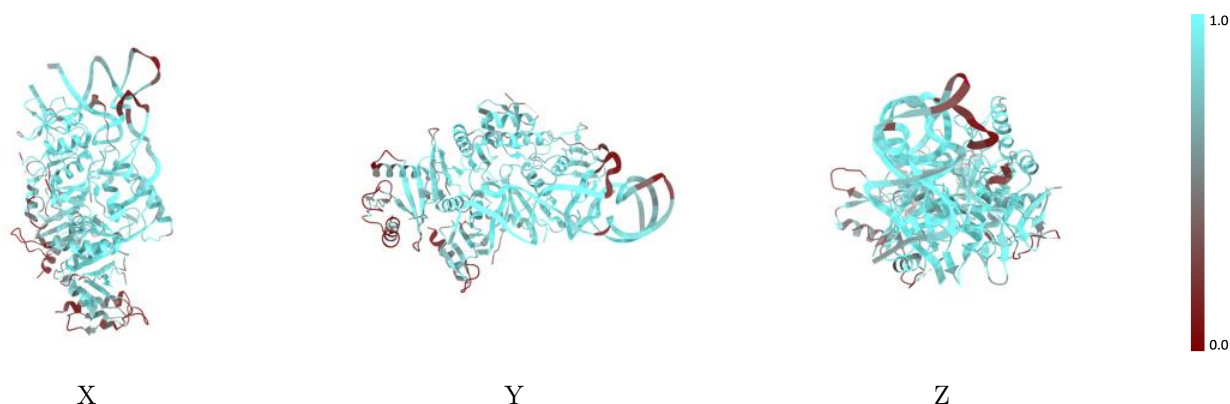
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



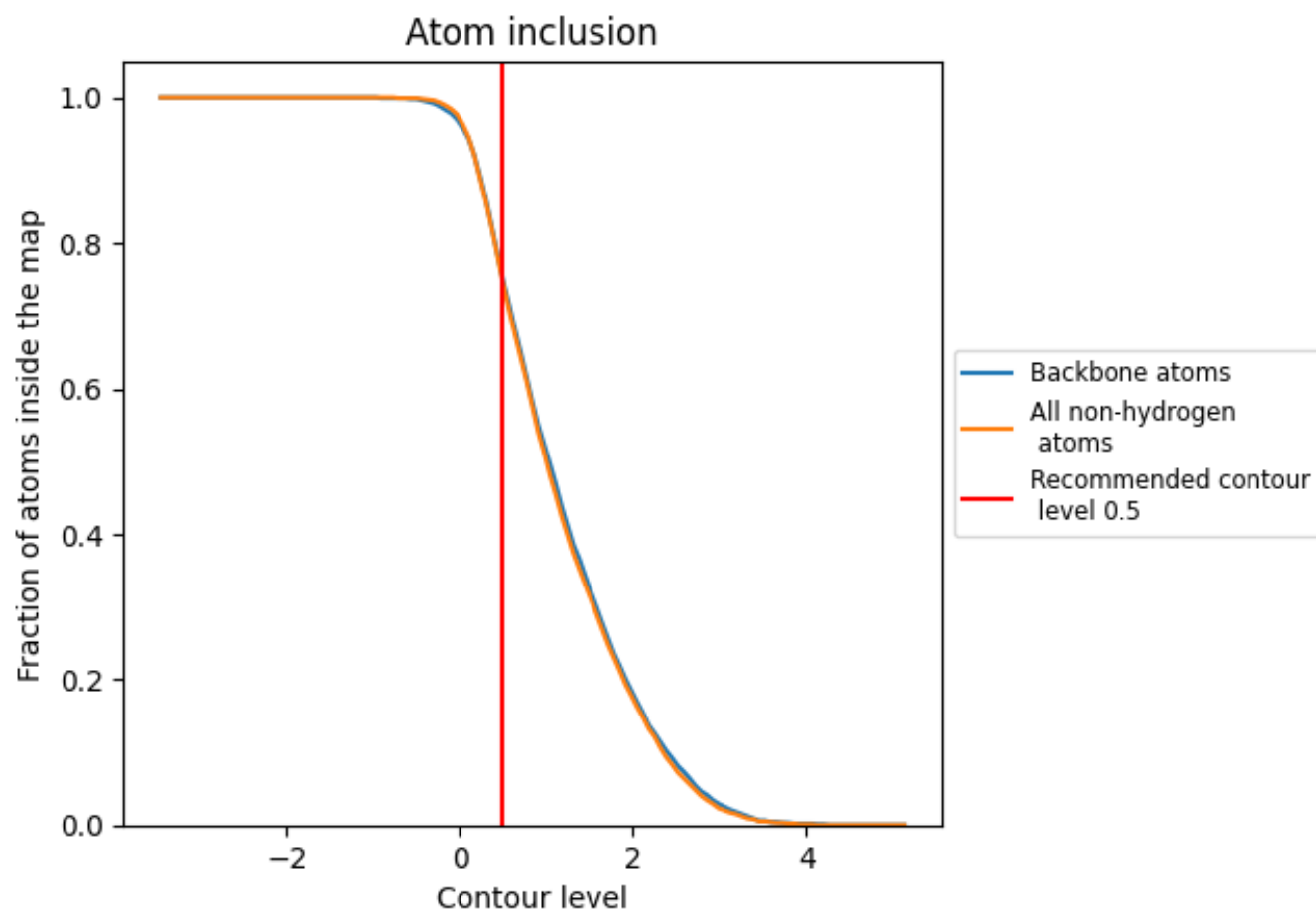
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.5).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 75% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7470	<div></div> 0.5050
AP1	<div></div> 0.8110	<div></div> 0.5510
BP4	<div></div> 0.5950	<div></div> 0.4530
CP1	<div></div> 0.8490	<div></div> 0.5430
DP1	<div></div> 0.4870	<div></div> 0.4150
ZN1	<div></div> 0.7950	<div></div> 0.4950

