



Full wwPDB EM Validation Report ⓘ

Oct 25, 2022 – 10:24 AM EDT

PDB ID : 8EAV
EMDB ID : EMD-27987
Title : YAR027W and YAR028W in complex with c subunits from yeast VO complex
Authors : Wang, H.; Bueler, S.A.; Rubinstein, J.L.
Deposited on : 2022-08-29
Resolution : 5.70 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.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) : 2.31.2

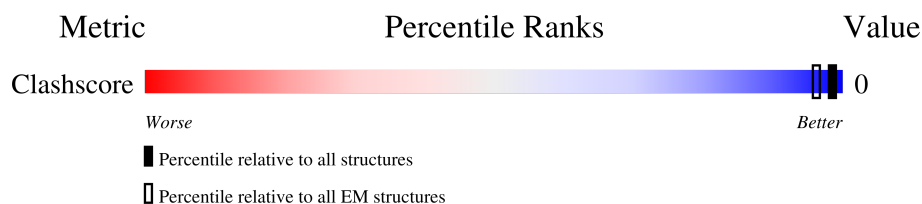
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY


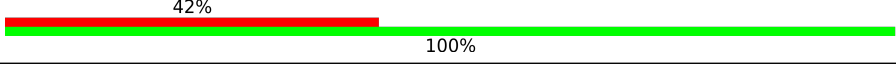
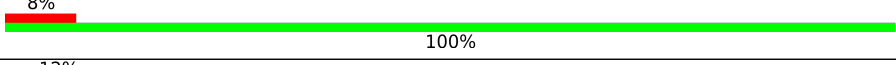
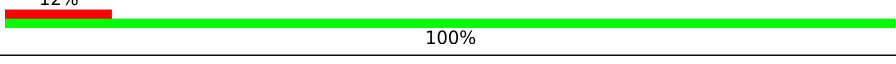
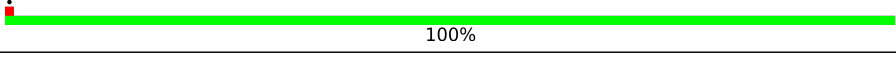
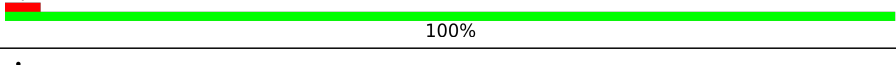
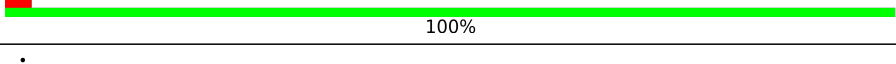
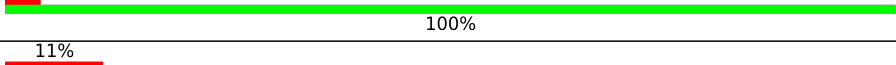
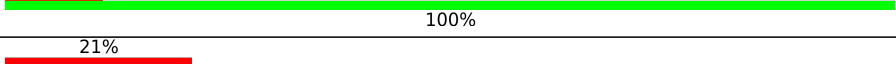
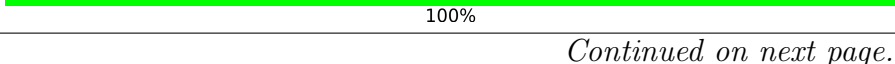
The reported resolution of this entry is 5.70 Å.

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

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	138	
2	Q	178	
3	K	172	
4	L	168	
5	k	145	
6	B	159	
6	C	159	
6	D	159	
6	E	159	
6	F	159	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
6	G	159	<div> <div>21%</div> <div>100%</div> </div>
6	H	159	<div> <div>66%</div> <div>100%</div> </div>
6	M	159	<div> <div>.</div> <div>100%</div> </div>
7	I	187	<div> <div>15%</div> <div>100%</div> </div>
8	J	162	<div> <div>16%</div> <div>99%</div> <div>.</div> </div>
9	N	177	<div> <div>13%</div> <div>100%</div> </div>
10	O	156	<div> <div>15%</div> <div>100%</div> </div>
11	P	135	<div> <div>26%</div> <div>100%</div> </div>

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 14467 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 YAR027W or YAR028W.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	138	Total	C	N	O	0	0
			690	414	138	138		

- Molecule 2 is a protein called YAR027W or YAR028W.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	Q	178	Total	C	N	O	0	0
			891	534	178	179		

- Molecule 3 is a protein called YAR027W or YAR028W.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	K	172	Total	C	N	O	0	0
			861	516	172	173		

- Molecule 4 is a protein called YAR027W or YAR028W.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	L	168	Total	C	N	O	0	0
			841	504	168	169		

- Molecule 5 is a protein called subunit from the c ring of yeast VO complex.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	k	145	Total	C	N	O	0	0
			726	435	145	146		

- Molecule 6 is a protein called subunit from the c ring of yeast VO complex.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	M	159	Total	C	N	O	0	0
			796	477	159	160		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
6	B	159	Total	C	N	O	0	0
			796	477	159	160		
6	C	159	Total	C	N	O	0	0
			796	477	159	160		
6	D	159	Total	C	N	O	0	0
			796	477	159	160		
6	E	159	Total	C	N	O	0	0
			796	477	159	160		
6	F	159	Total	C	N	O	0	0
			796	477	159	160		
6	G	159	Total	C	N	O	0	0
			796	477	159	160		
6	H	159	Total	C	N	O	0	0
			796	477	159	160		

- Molecule 7 is a protein called YAR027W or YAR028W.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	I	187	Total	C	N	O	0	0
			936	561	187	188		

- Molecule 8 is a protein called YAR027W or YAR028W.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	J	162	Total	C	N	O	0	0
			811	486	162	163		

- Molecule 9 is a protein called YAR027W or YAR028W.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	N	177	Total	C	N	O	0	0
			886	531	177	178		

- Molecule 10 is a protein called YAR027W or YAR028W.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	O	156	Total	C	N	O	0	0
			781	468	156	157		

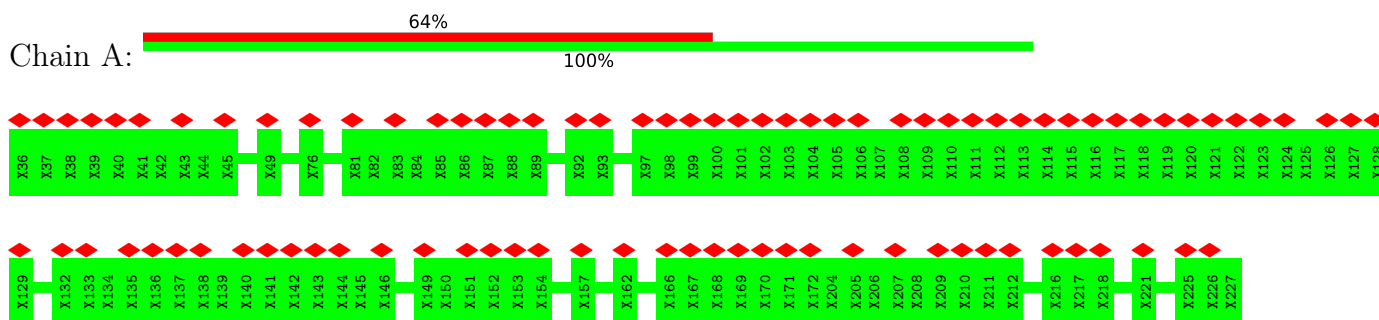
- Molecule 11 is a protein called YAR027W or YAR028W.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	P	135	Total 676	C 405	N 135	O 136	0	0

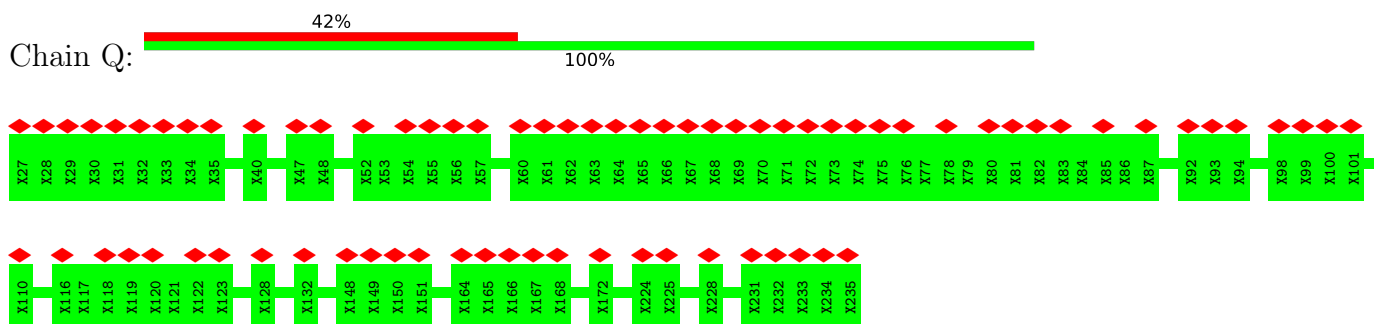
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

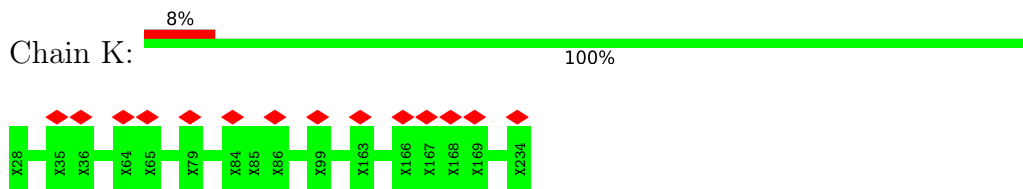
- Molecule 1: YAR027W or YAR028W



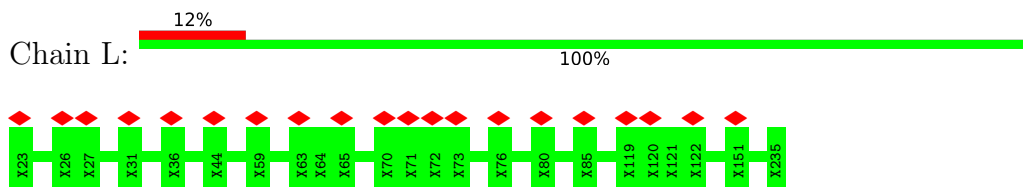
- Molecule 2: YAR027W or YAR028W



- Molecule 3: YAR027W or YAR028W

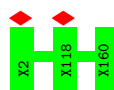


- Molecule 4: YAR027W or YAR028W



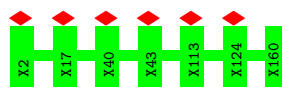
- Molecule 5: subunit from the c ring of yeast VO complex

Chain k:  100%



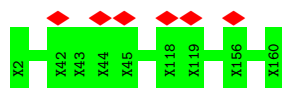
- Molecule 6: subunit from the c ring of yeast VO complex

Chain M:  100%



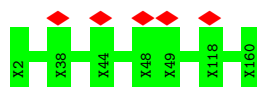
- Molecule 6: subunit from the c ring of yeast VO complex

Chain B:  100%



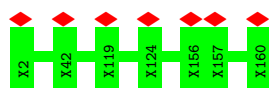
- Molecule 6: subunit from the c ring of yeast VO complex

Chain C:  100%



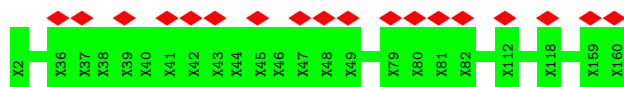
- Molecule 6: subunit from the c ring of yeast VO complex

Chain D:  100%



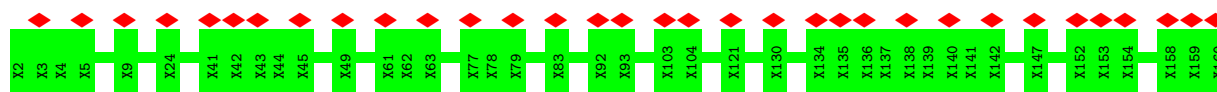
- Molecule 6: subunit from the c ring of yeast VO complex

Chain E:  100%

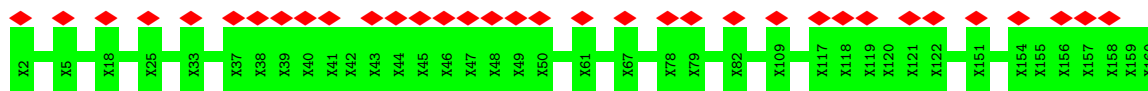


- Molecule 6: subunit from the c ring of yeast VO complex

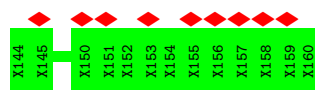
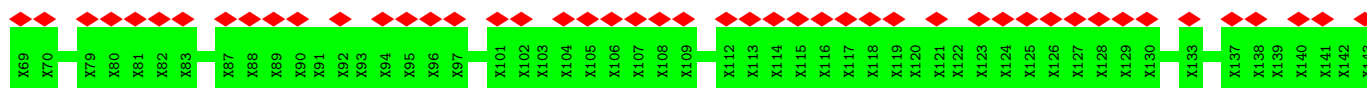
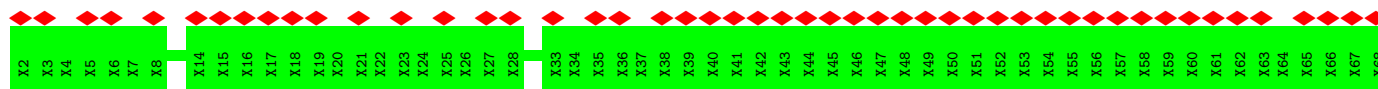
Chain F:  100%



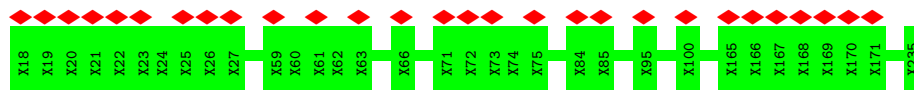
- Molecule 6: subunit from the c ring of yeast VO complex



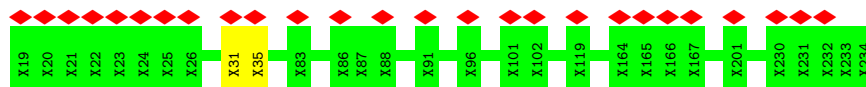
- Molecule 6: subunit from the c ring of yeast VO complex



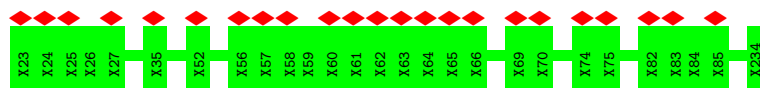
- Molecule 7: YAR027W or YAR028W



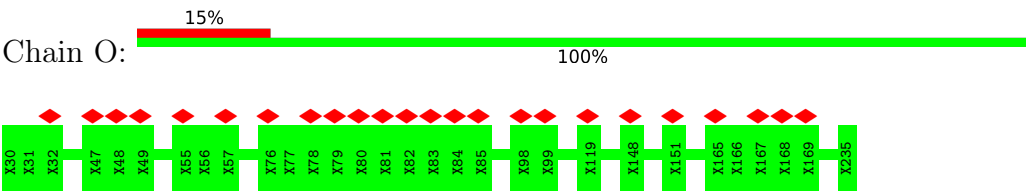
- Molecule 8: YAR027W or YAR028W



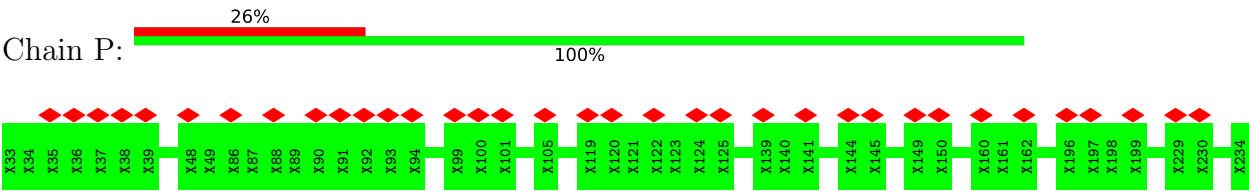
- Molecule 9: YAR027W or YAR028W



- Molecule 10: YAR027W or YAR028W



● Molecule 11: YAR027W or YAR028W



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	19849	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 ($e^-/\text{\AA}^2$)	49	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	4.818	Depositor
Minimum map value	-3.652	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.129	Depositor
Recommended contour level	0.7	Depositor
Map size (Å)	329.59998, 329.59998, 329.59998	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.03, 1.03, 1.03	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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

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	A	690	0	144	0	0
2	Q	891	0	184	0	0
3	K	861	0	185	0	0
4	L	841	0	178	0	0
5	k	726	0	151	0	0
6	B	796	0	164	0	0
6	C	796	0	164	0	0
6	D	796	0	163	0	0
6	E	796	0	163	0	0
6	F	796	0	163	0	0
6	G	796	0	162	0	0
6	H	796	0	162	0	0
6	M	796	0	163	0	0
7	I	936	0	194	0	0
8	J	811	0	171	1	0
9	N	886	0	182	0	0
10	O	781	0	165	0	0
11	P	676	0	149	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	14467	0	3007	1	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 0.

All (1) 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)
8:J:31:UNK:C	8:J:35:UNK:H2	2.31	0.43

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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 [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	L	3
8	J	3
1	A	2
11	P	2
10	O	2
3	K	2
5	k	2
7	I	1
9	N	1
2	Q	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	51:UNK	C	75:UNK	N	32.94
1	I	172:UNK	C	204:UNK	N	22.09
1	P	164:UNK	C	196:UNK	N	18.42
1	P	49:UNK	C	86:UNK	N	18.37
1	L	166:UNK	C	204:UNK	N	18.17
1	N	165:UNK	C	201:UNK	N	15.30
1	O	59:UNK	C	76:UNK	N	14.93
1	A	172:UNK	C	204:UNK	N	14.21
1	J	57:UNK	C	80:UNK	N	14.11
1	Q	172:UNK	C	204:UNK	N	12.44
1	K	169:UNK	C	198:UNK	N	12.25
1	k	78:UNK	C	85:UNK	N	12.00
1	O	169:UNK	C	204:UNK	N	11.51
1	K	68:UNK	C	76:UNK	N	9.24
1	L	94:UNK	C	100:UNK	N	6.77
1	J	169:UNK	C	199:UNK	N	6.34
1	L	46:UNK	C	50:UNK	N	4.61
1	k	42:UNK	C	51:UNK	N	4.49
1	J	31:UNK	C	35:UNK	N	3.17

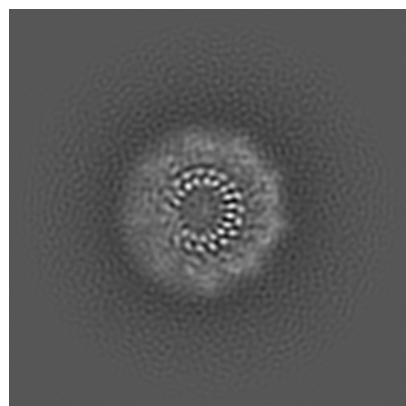
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27987. These allow visual inspection of the internal detail of the map and identification of artifacts.

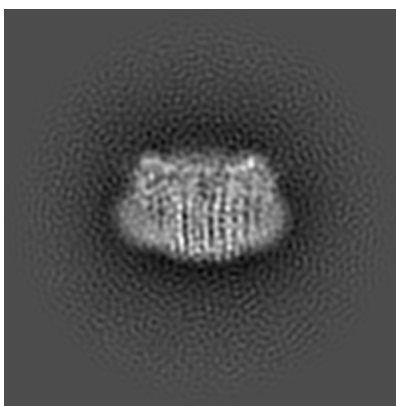
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

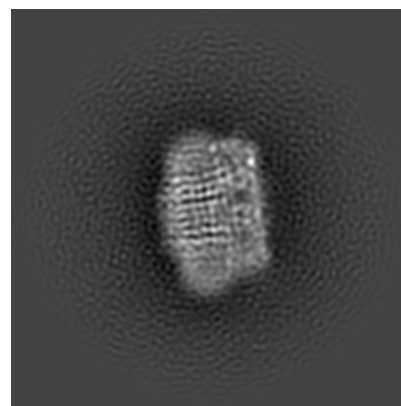
6.1.1 Primary map



X

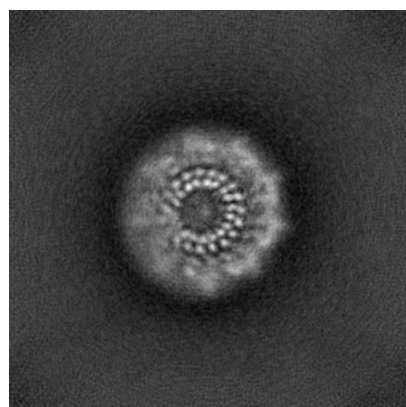


Y

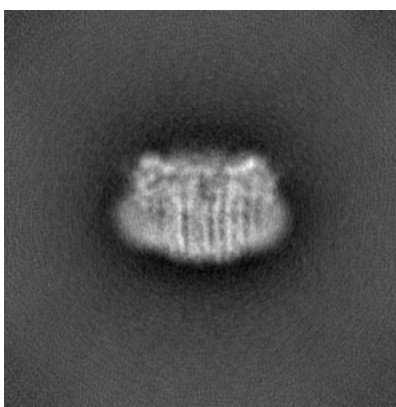


Z

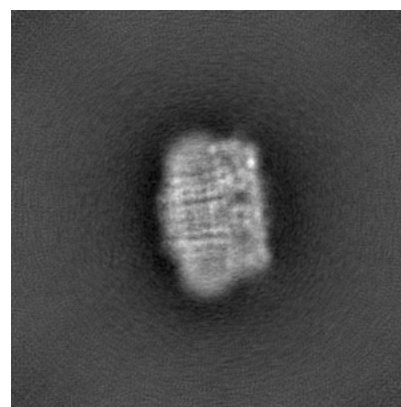
6.1.2 Raw map



X



Y

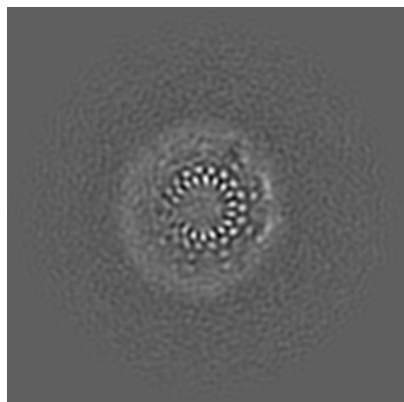


Z

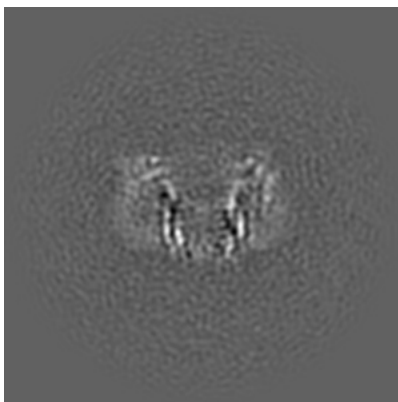
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

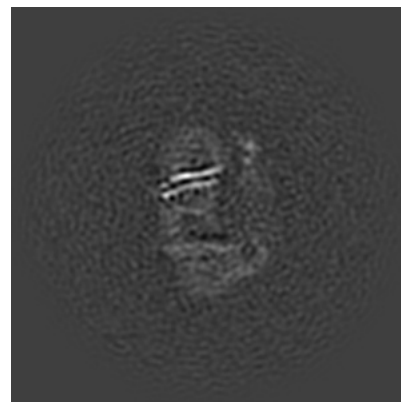
6.2.1 Primary map



X Index: 160

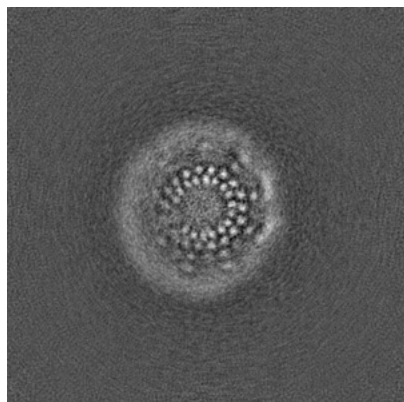


Y Index: 160

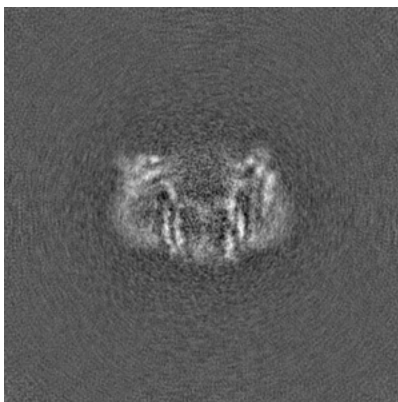


Z Index: 160

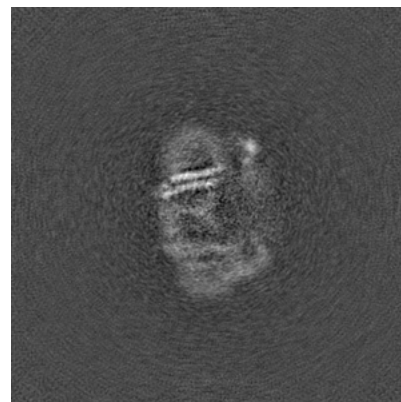
6.2.2 Raw map



X Index: 160



Y Index: 160

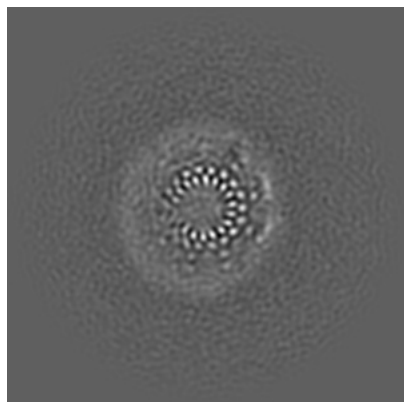


Z Index: 160

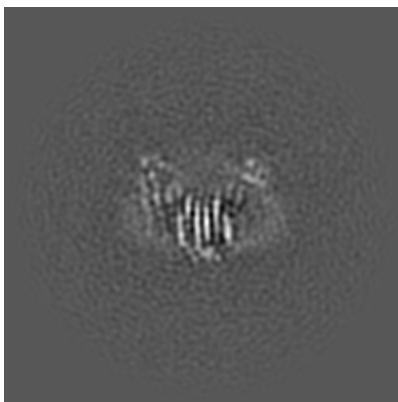
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

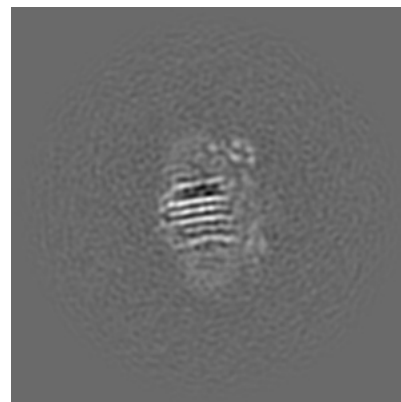
6.3.1 Primary map



X Index: 160

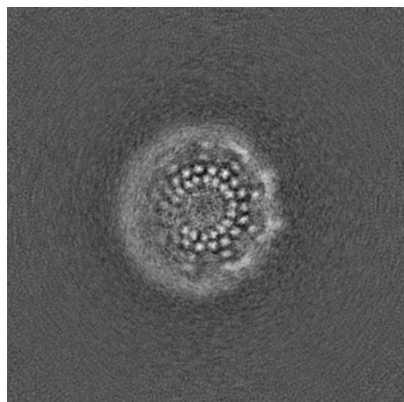


Y Index: 177

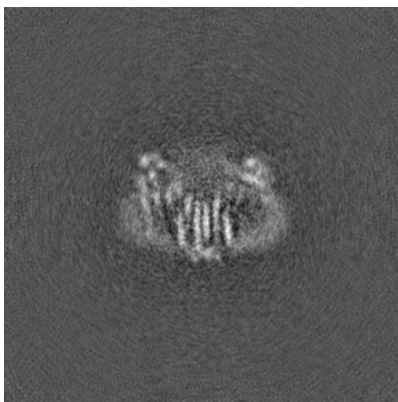


Z Index: 180

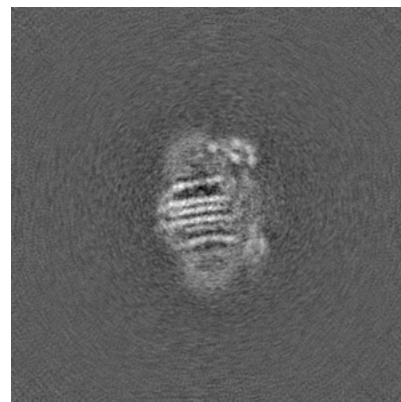
6.3.2 Raw map



X Index: 163



Y Index: 177

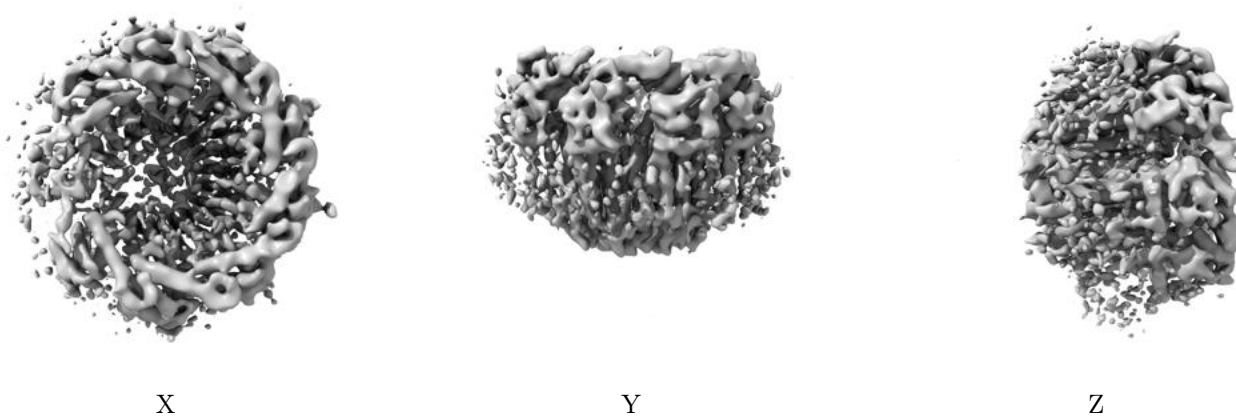


Z Index: 180

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

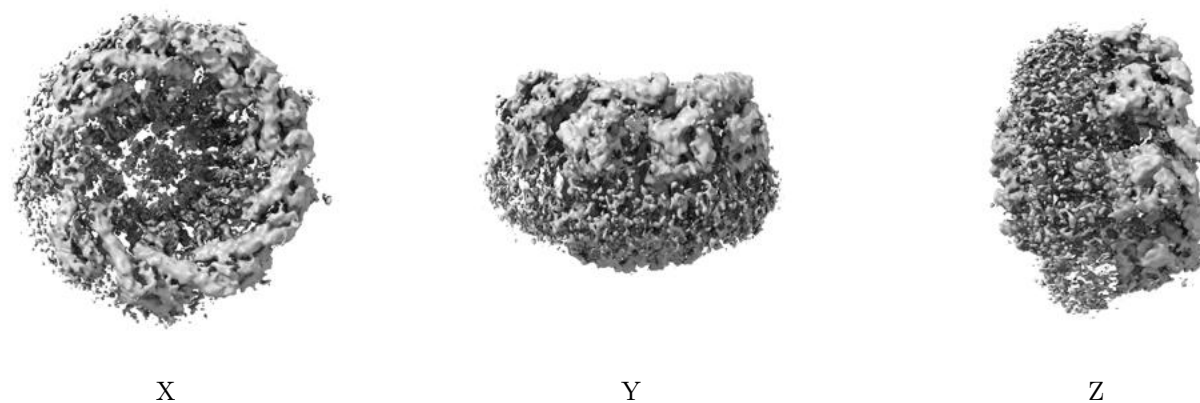
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.7. 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.

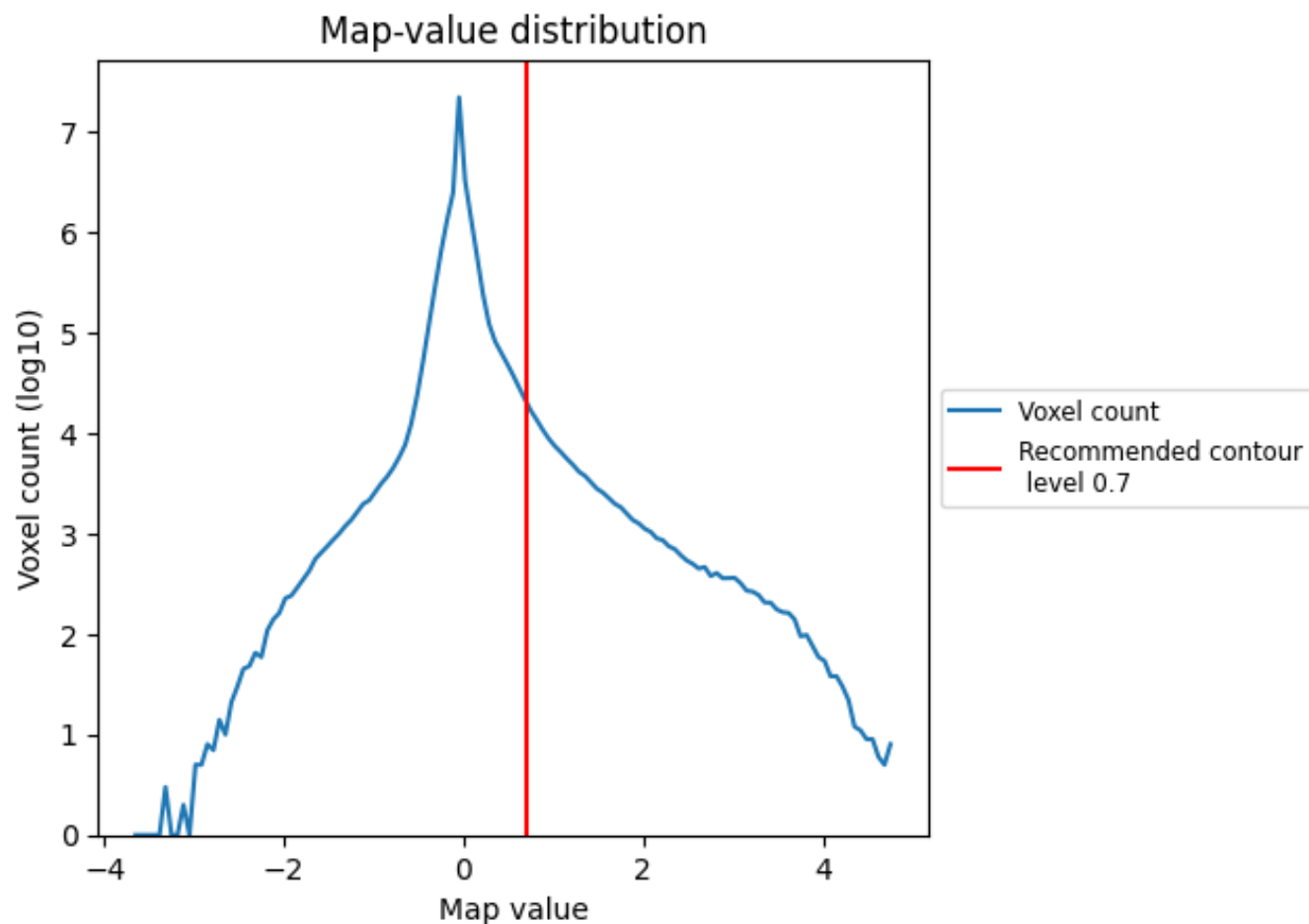
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

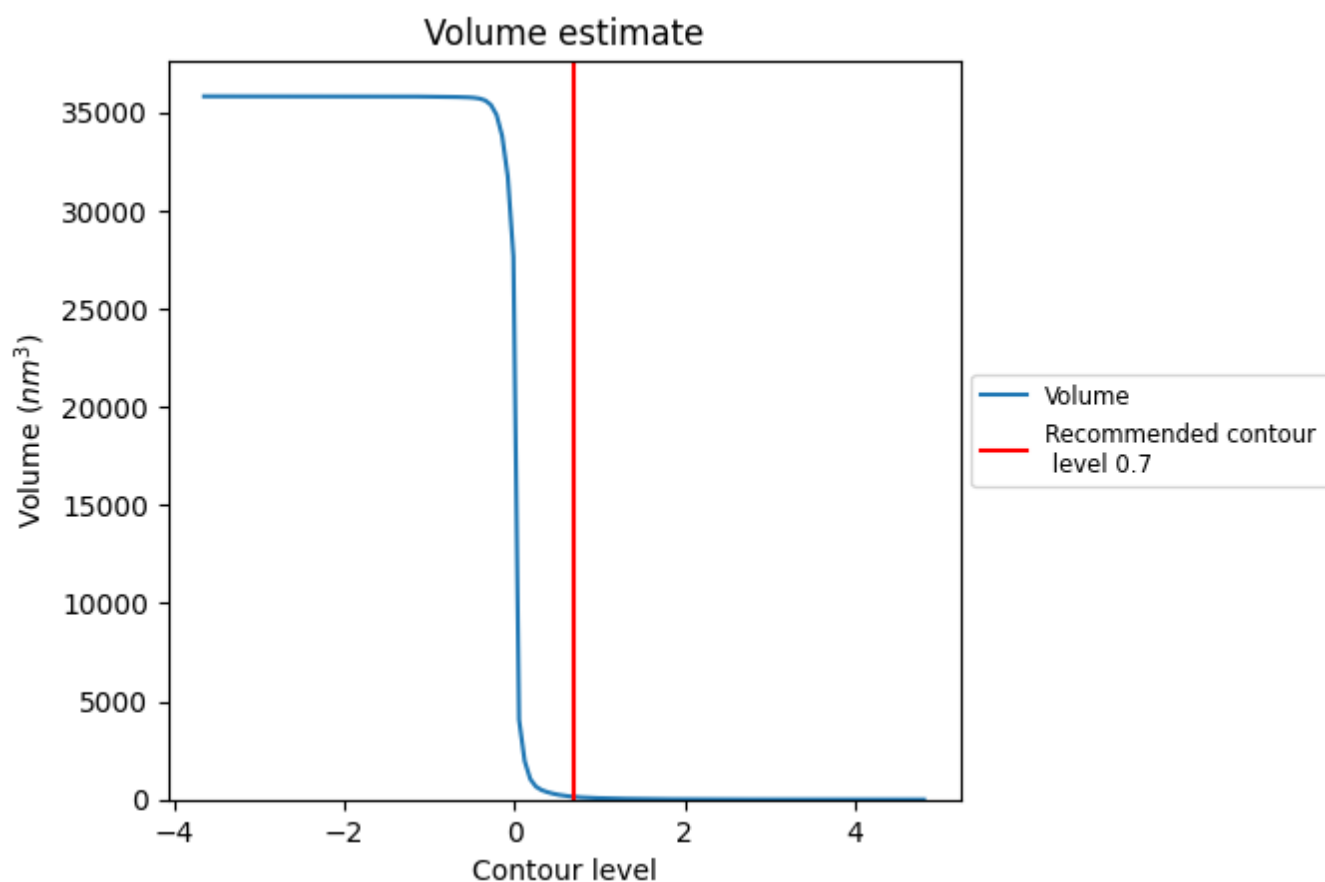
This section contains the results of statistical analysis of the map.

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.

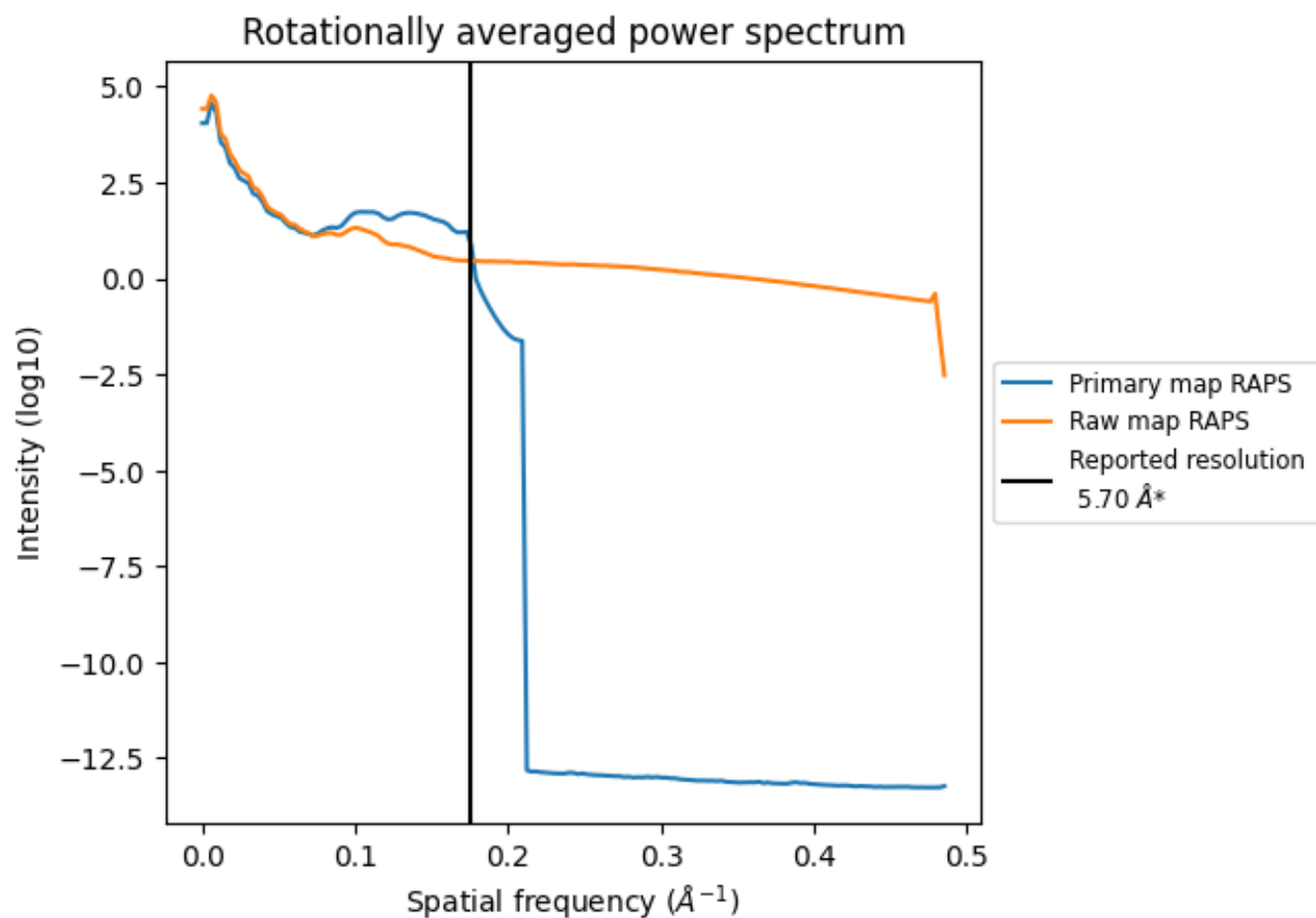
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 141 nm³; this corresponds to an approximate mass of 127 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 ⓘ

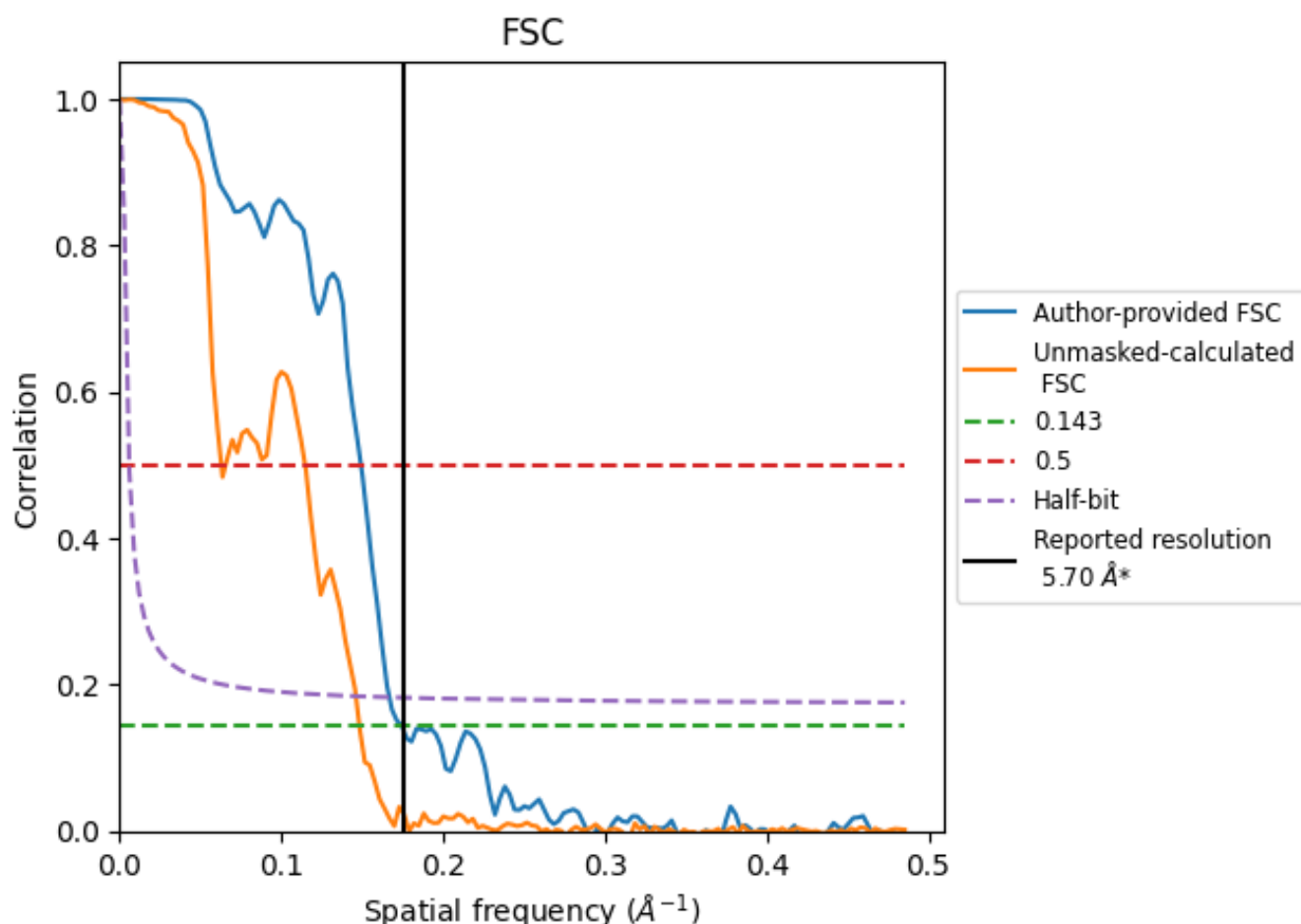


*Reported resolution corresponds to spatial frequency of 0.175 Å⁻¹

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 0.175 \AA^{-1}

8.2 Resolution estimates [i](#)

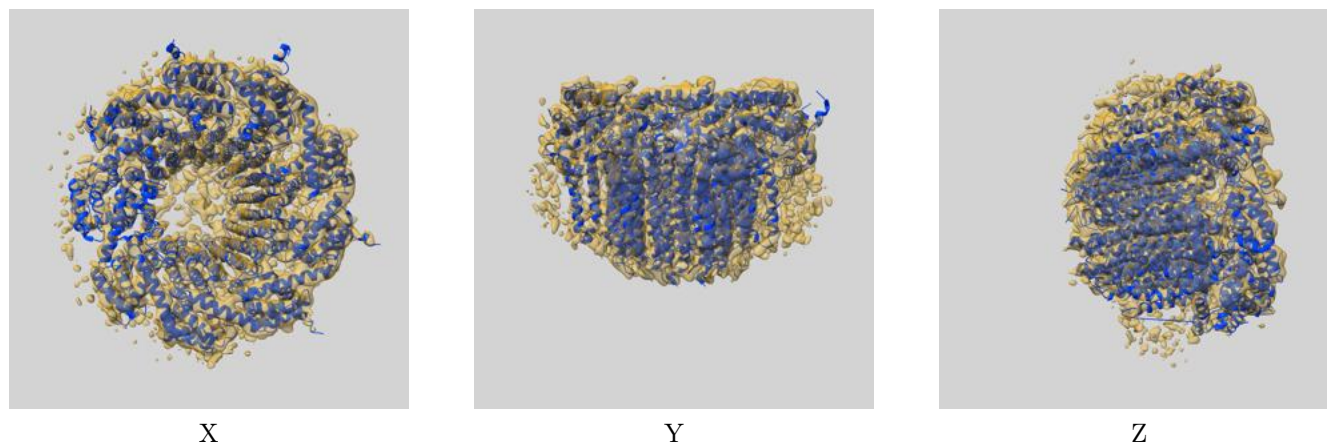
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.70	-	-
Author-provided FSC curve	5.73	6.70	6.00
Unmasked-calculated*	6.74	15.90	6.84

*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 6.74 differs from the reported value 5.7 by more than 10 %

9 Map-model fit [i](#)

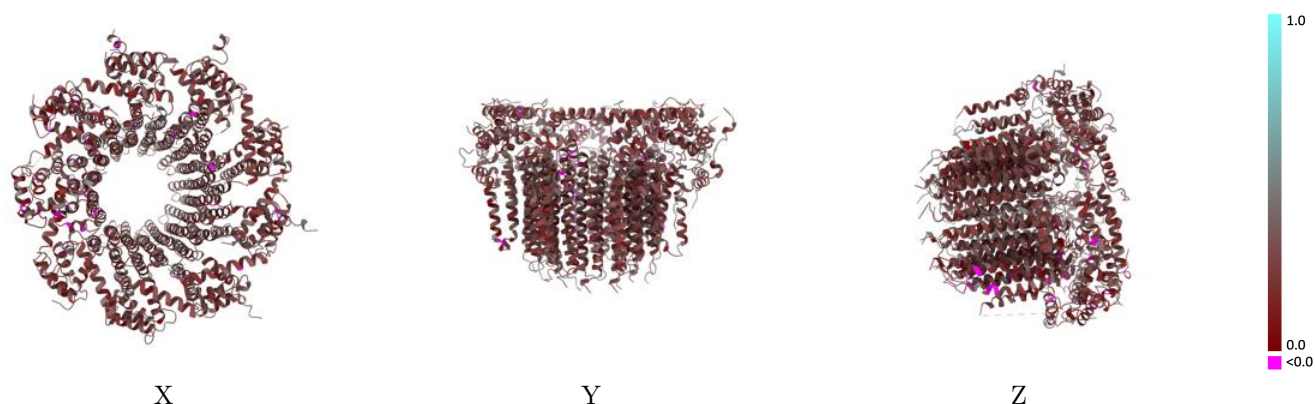
This section contains information regarding the fit between EMDB map EMD-27987 and PDB model 8EAV. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



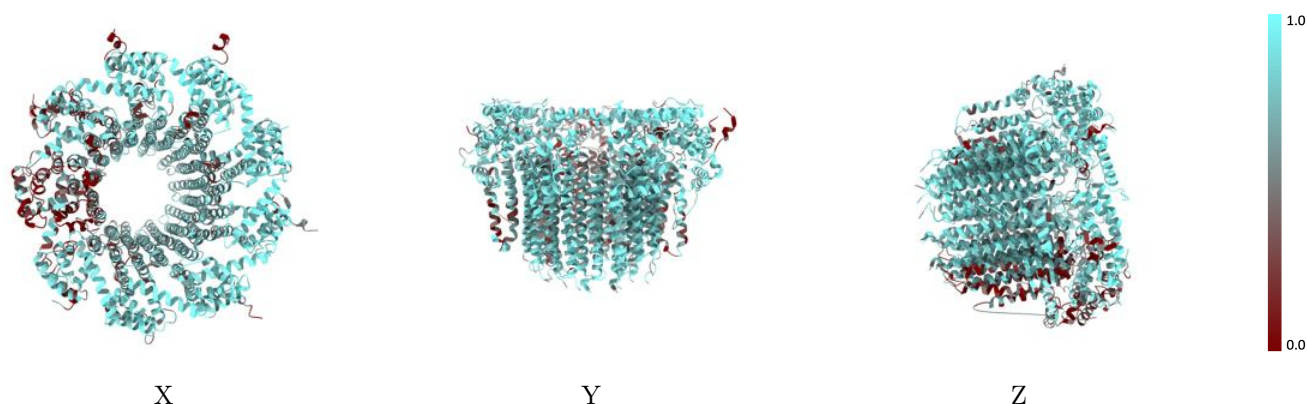
The images above show the 3D surface view of the map at the recommended contour level 0.7 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



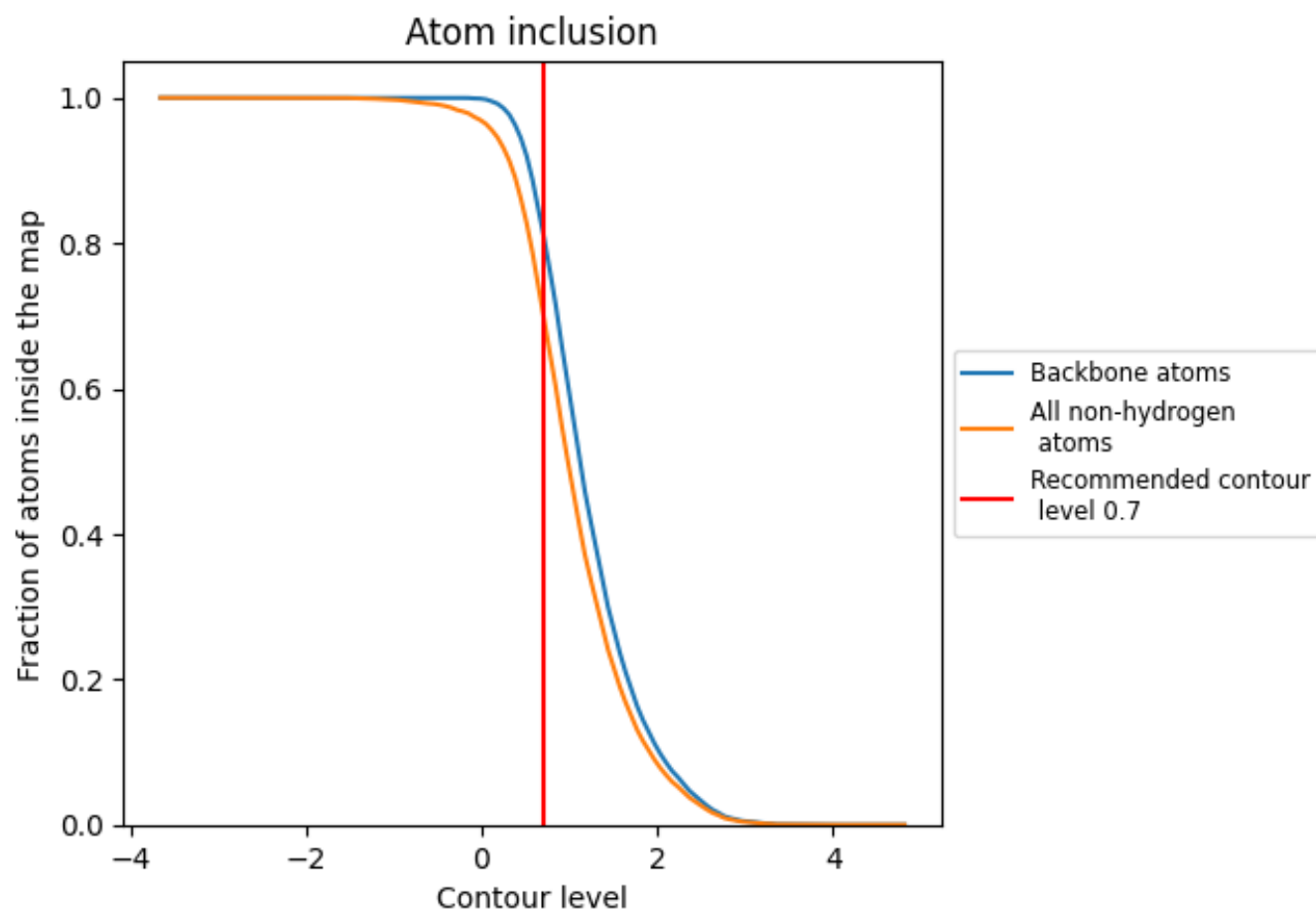
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.7).







































9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 70% 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 (0.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7048	 0.2670
A	 0.3783	 0.2410
B	 0.8103	 0.2700
C	 0.8003	 0.2710
D	 0.7776	 0.2700
E	 0.7525	 0.2570
F	 0.6671	 0.2460
G	 0.6595	 0.2420
H	 0.3769	 0.2110
I	 0.7447	 0.2890
J	 0.7472	 0.2910
K	 0.8107	 0.2850
L	 0.7919	 0.2850
M	 0.7952	 0.2710
N	 0.7494	 0.2780
O	 0.7490	 0.2900
P	 0.6405	 0.2800
Q	 0.5488	 0.2450
k	 0.8375	 0.2840

