



## wwPDB EM Validation Summary Report ⓘ

May 4, 2025 – 12:55 PM EDT

PDB ID : 8V91 / pdb\_00008v91  
EMDB ID : EMD-43047  
Title : Structure of human AQP4 with a pathogenic autoantibody- rAB 58  
Authors : Gupta, M.; Khandelwal, N.K.; Stroud, R.M.  
Deposited on : 2023-12-07  
Resolution : 2.60 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>.

---

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

EMDB validation analysis : 0.0.1.dev118  
MolProbity : 4-5-2 with Phenix2.0rc1  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

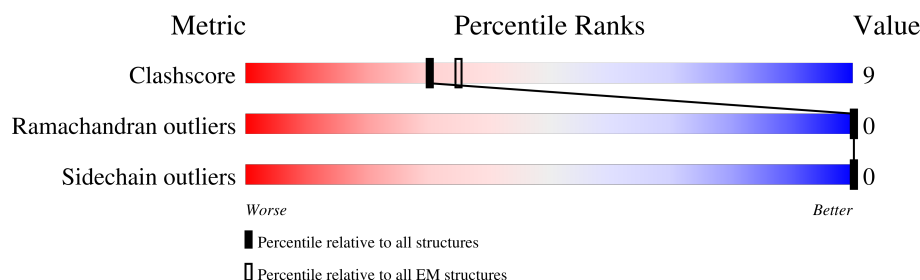
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*


The reported resolution of this entry is 2.60 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	A	323	
1	B	323	
1	C	323	
1	D	323	
2	I	214	
3	J	223	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9913 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 Aquaporin-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	223	Total	C	N	O	S	0	0
			1654	1092	265	284	13		
1	B	223	Total	C	N	O	S	0	0
			1654	1092	265	284	13		
1	C	223	Total	C	N	O	S	0	0
			1654	1092	265	284	13		
1	D	223	Total	C	N	O	S	0	0
			1654	1092	265	284	13		

- Molecule 2 is a protein called rAB 58 Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	I	212	Total	C	N	O	S	0	0
			1626	1021	274	326	5		

- Molecule 3 is a protein called rAB 58 Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	J	216	Total	C	N	O	S	0	0
			1584	997	267	315	5		

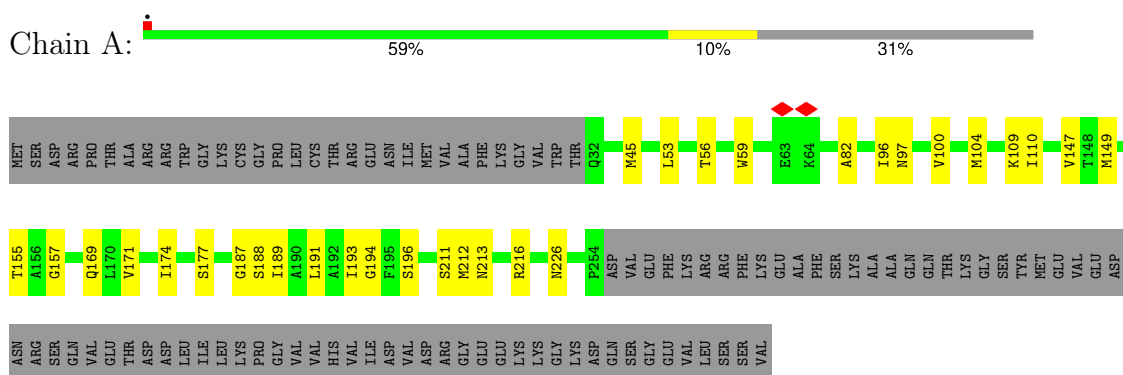
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		AltConf
4	A	21	Total	O	0
			21	21	
4	B	23	Total	O	0
			23	23	
4	C	22	Total	O	0
			22	22	
4	D	21	Total	O	0
			21	21	

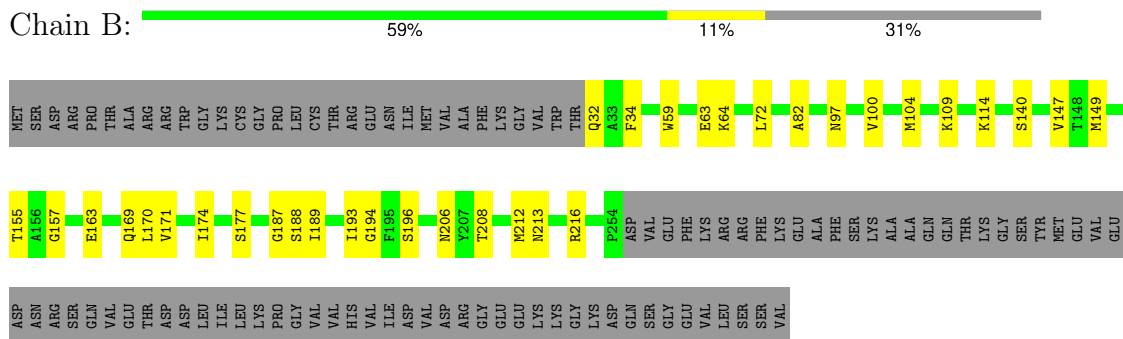
### 3 Residue-property plots

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.

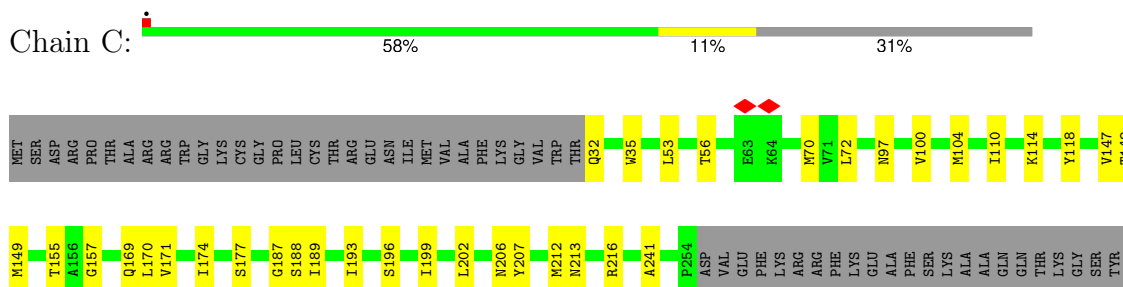
#### • Molecule 1: Aquaporin-4



#### • Molecule 1: Aquaporin-4



#### • Molecule 1: Aquaporin-4



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

• Molecule 1: Aquaporin-4

Chain D:  54% 15% 31%


MET  
SER  
ASP  
ARG  
PRO  
THR  
ALA  
ARG  
GLN  
VAL  
GLU  
THR  
LYS  
CYS  
GLY  
PRO  
LEU  
ILE  
CYS  
LYS  
THR  
ARG  
GLU  
ASN  
VAL  
HIS  
MET  
VAL  
ALA  
PHE  
LYS  
GLY  
VAL  
ASP  
TRP  
THR  
Q32  
A33  
F34  
W35  
K36  
E41  
A44  
M45  
L53  
T56  
E63  
K64  
M70  
A82  
F88  
S92  
T96  
N97

V100  
M104  
K109  
K114  
A126  
G146  
G147  
T143  
M153  
L154  
T155  
A156  
G157  
E163  
Q169  
L170  
V171  
I174  
S177  
K181  
G187  
S188  
I189  
I193  
G194  
F195  
S196  
T199  
G200  
H201  
L202  
I205  
N206  
T207  
T208  
S211  
M212  
N213  
R216  
P254  
ASP  
VAL

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

GLY  
GLU  
VAL  
LEU  
SER  
SER  
VAL

• Molecule 2: rAB 58 Light Chain

Chain I:  18% 84% 15%

D1  
M4  
D17  
T18  
R24  
R30  
S31  
A34  
Q37  
L47  
S76  
D81  
Q89  
H90  
Y91  
N92  
S93  
Y96  
R107  
P113  
F116  
D122  
E123  
Q124  
L125  
K126  
S127  
G128  
T129  
A130  
S131  
L135  
F139  
R142  
E143  
A144  
K145  
V146  
Q147  
V150  
D151

M152  
A153  
L154  
Q155  
S156  
G157  
M158  
S159  
Q160  
V163  
S168  
K169  
ASP  
S171  
L175  
L181  
S182  
K183  
A184  
D185  
Y186  
E187  
K188  
H189  
K190  
L201  
S202  
S203  
T206  
N210  
R211  
G212  
E213  
CYS

• Molecule 3: rAB 58 Heavy Chain

Chain J:  13% 77% 20%

Q1  
V12  
F29  
R30  
A33  
W36  
V37  
R38  
E46  
S52  
I70  
T71  
D73  
N74  
S75  
K76  
L86  
R87  
A88  
D89  
D90  
Y94  
A97  
D100  
Y101  
V102  
F103  
T119  
K120  
G121  
P122  
S123  
V124  
F125  
P126  
S130  
S131  
K132  
S133  
T134  
S135  
G136  
G137  
T138  
A139  
A140

L141  
G142  
C143  
L144  
V145  
K146  
D147  
N158  
S159  
G160  
A161  
A171  
S175  
L178  
L181  
V184  
S189  
S190  
S191  
L192  
G193  
T194  
Q195  
T196  
V201  
N207  
T208  
K209  
V210  
D211  
K212  
K213  
V214  
E215  
P216  
LYS  
SER  
CYS  
ASP  
LYS  
THR  
HIS

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	323342	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	60	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	OTHER	Depositor
Maximum map value	2.848	Depositor
Minimum map value	-1.519	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.051	Depositor
Recommended contour level	0.55	Depositor
Map size ( $\text{\AA}$ )	326.928, 326.928, 326.928	wwPDB
Map dimensions	392, 392, 392	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.83400005, 0.83400005, 0.83400005	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	0.11	0/1697	0.31	0/2317
1	B	0.11	0/1697	0.29	0/2317
1	C	0.10	0/1697	0.27	0/2317
1	D	0.11	0/1697	0.30	0/2317
2	I	0.11	0/1663	0.30	0/2260
3	J	0.11	0/1622	0.27	0/2213
All	All	0.11	0/10073	0.29	0/13741

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	1654	0	1692	24	0
1	B	1654	0	1692	25	0
1	C	1654	0	1692	30	0
1	D	1654	0	1692	48	0
2	I	1626	0	1566	30	0
3	J	1584	0	1536	33	0
4	A	21	0	0	0	0
4	B	23	0	0	1	0
4	C	22	0	0	0	0
4	D	21	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	9913	0	9870	174	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 9.

The worst 5 of 174 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:D:32:GLN:HB3	1:D:35:TRP:CD1	1.71	1.25
1:D:32:GLN:N	1:D:35:TRP:HE1	1.54	1.04
3:J:86:LEU:HD23	3:J:90:ASP:OD2	1.66	0.93
1:D:32:GLN:O	1:D:35:TRP:CD1	2.22	0.92
1:D:32:GLN:HB3	1:D:35:TRP:HD1	1.06	0.88

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	221/323 (68%)	212 (96%)	9 (4%)	0	100	100
1	B	221/323 (68%)	215 (97%)	6 (3%)	0	100	100
1	C	221/323 (68%)	216 (98%)	5 (2%)	0	100	100
1	D	221/323 (68%)	216 (98%)	5 (2%)	0	100	100
2	I	208/214 (97%)	201 (97%)	7 (3%)	0	100	100
3	J	214/223 (96%)	210 (98%)	4 (2%)	0	100	100
All	All	1306/1729 (76%)	1270 (97%)	36 (3%)	0	100	100

There are no Ramachandran outliers to report.



### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	174/261 (67%)	174 (100%)	0	100	100
1	B	174/261 (67%)	174 (100%)	0	100	100
1	C	174/261 (67%)	174 (100%)	0	100	100
1	D	174/261 (67%)	174 (100%)	0	100	100
2	I	182/187 (97%)	182 (100%)	0	100	100
3	J	174/183 (95%)	174 (100%)	0	100	100
All	All	1052/1414 (74%)	1052 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
2	I	199	GLN
3	J	35	ASN
2	I	3	GLN
2	I	79	GLN
2	I	89	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

There are no ligands in this entry.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

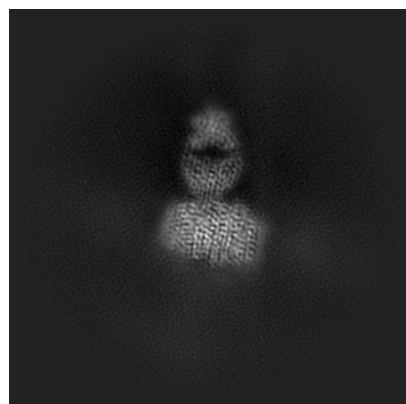
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-43047. These allow visual inspection of the internal detail of the map and identification of artifacts.

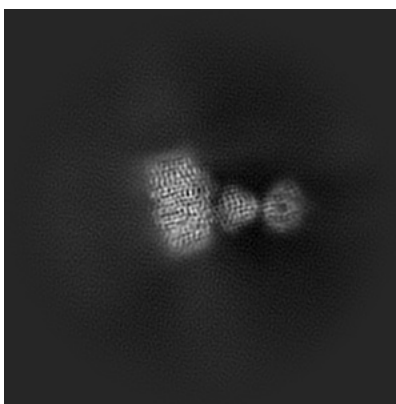
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

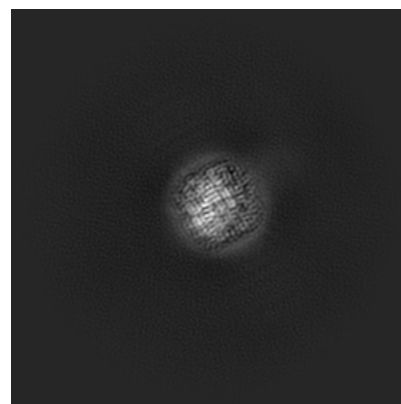
#### 6.1.1 Primary map



X

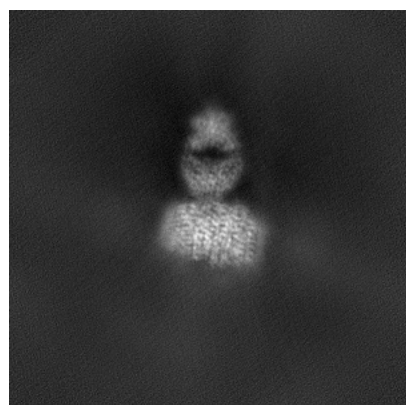


Y

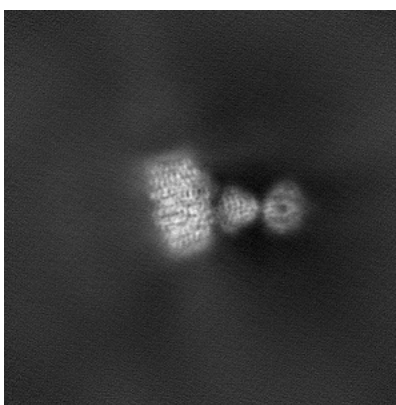


Z

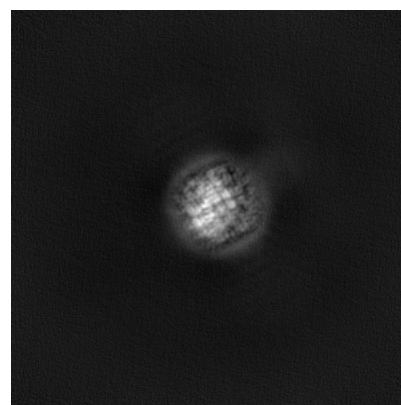
#### 6.1.2 Raw map



X



Y

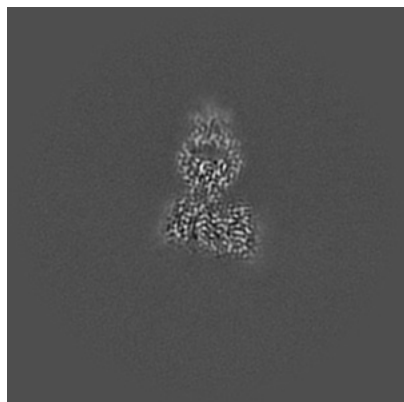


Z

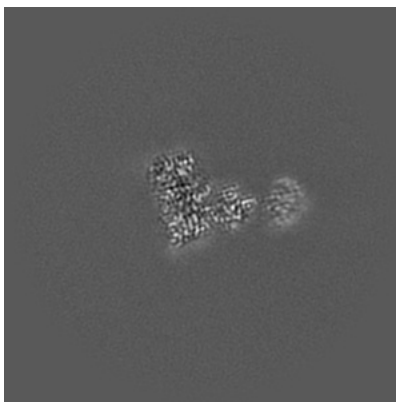
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

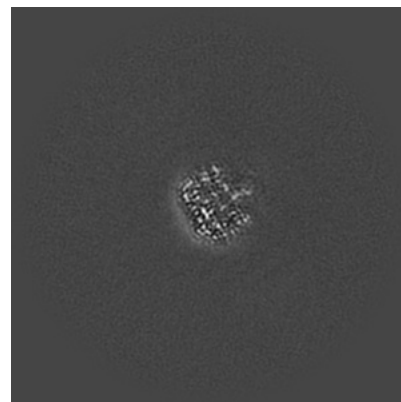
### 6.2.1 Primary map



X Index: 196

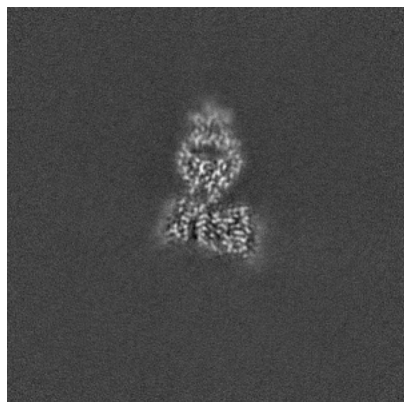


Y Index: 196

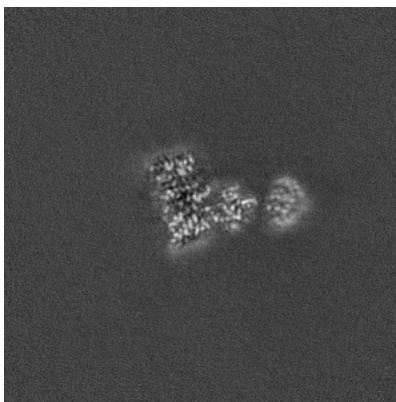


Z Index: 196

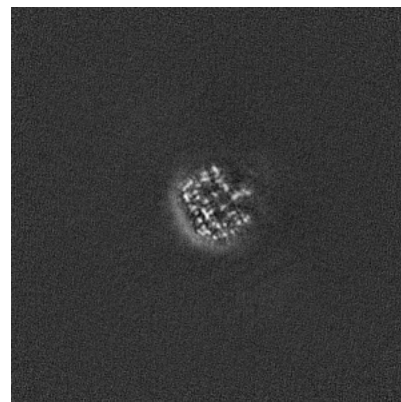
### 6.2.2 Raw map



X Index: 196



Y Index: 196

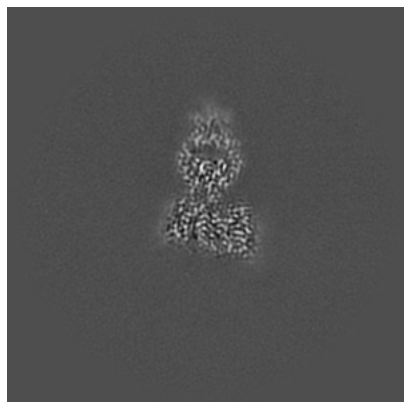


Z Index: 196

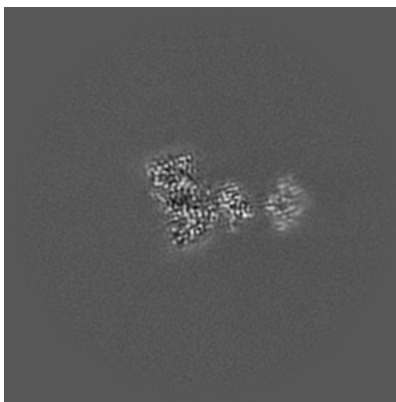
The images above show central slices of the map in three orthogonal directions.

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

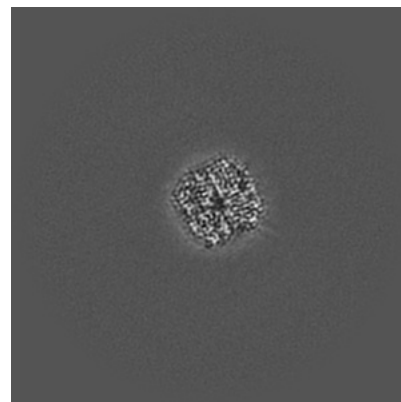
### 6.3.1 Primary map



X Index: 196

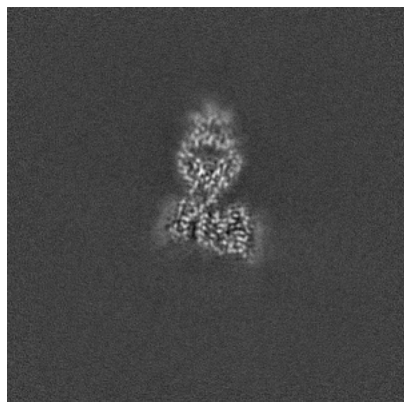


Y Index: 199

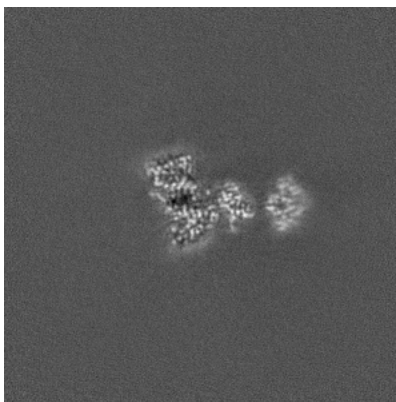


Z Index: 177

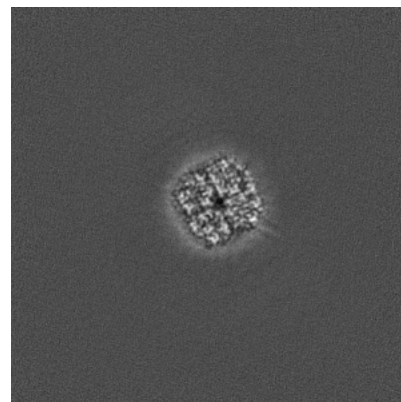
### 6.3.2 Raw map



X Index: 195



Y Index: 199

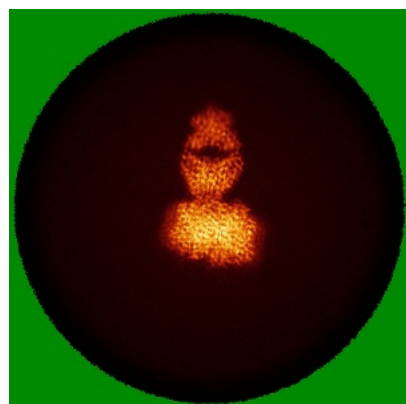


Z Index: 177

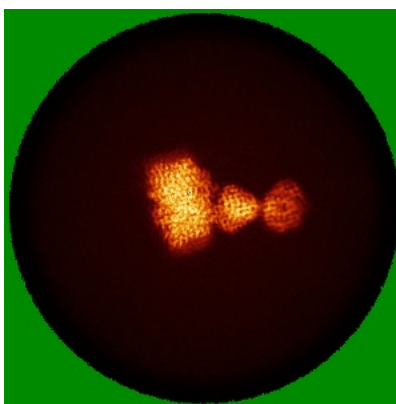
The images above show the largest variance slices of the map in three orthogonal directions.

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

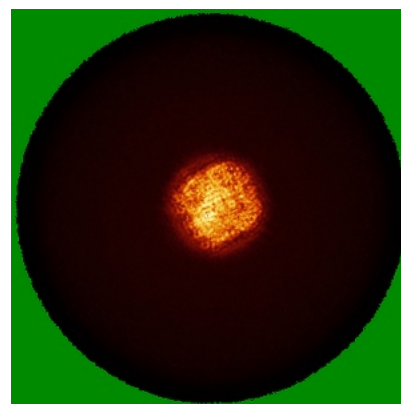
### 6.4.1 Primary map



X

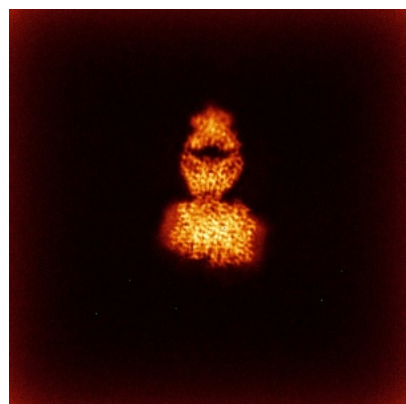


Y

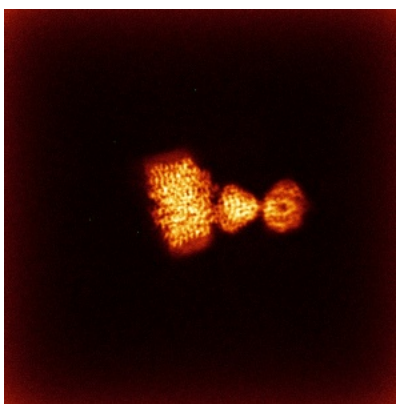


Z

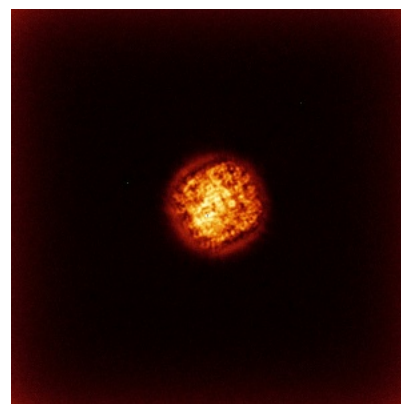
### 6.4.2 Raw map



X



Y



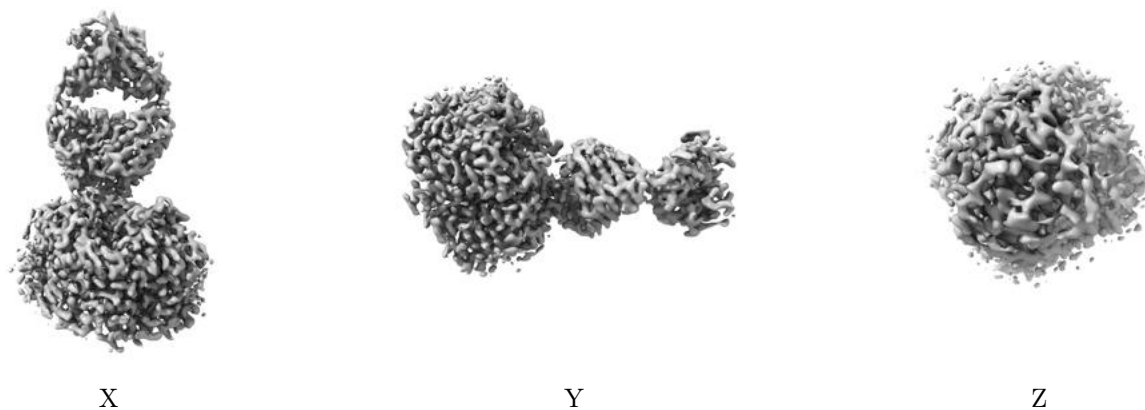
Z

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.



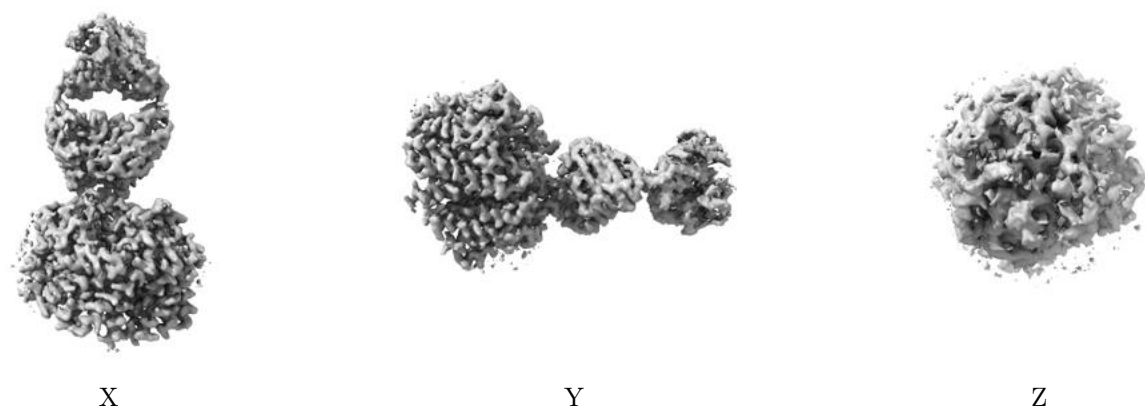
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.55. 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.

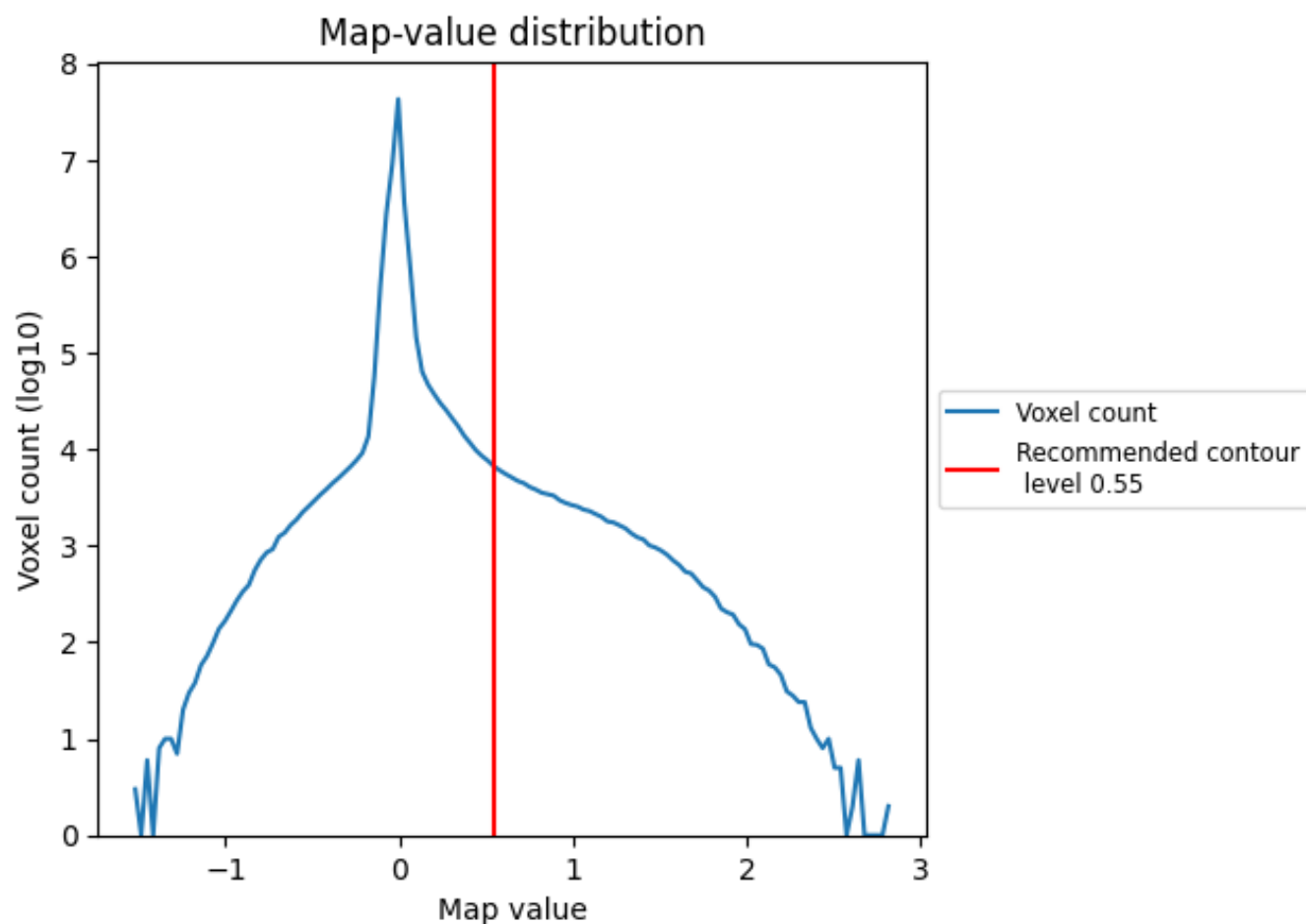
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

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

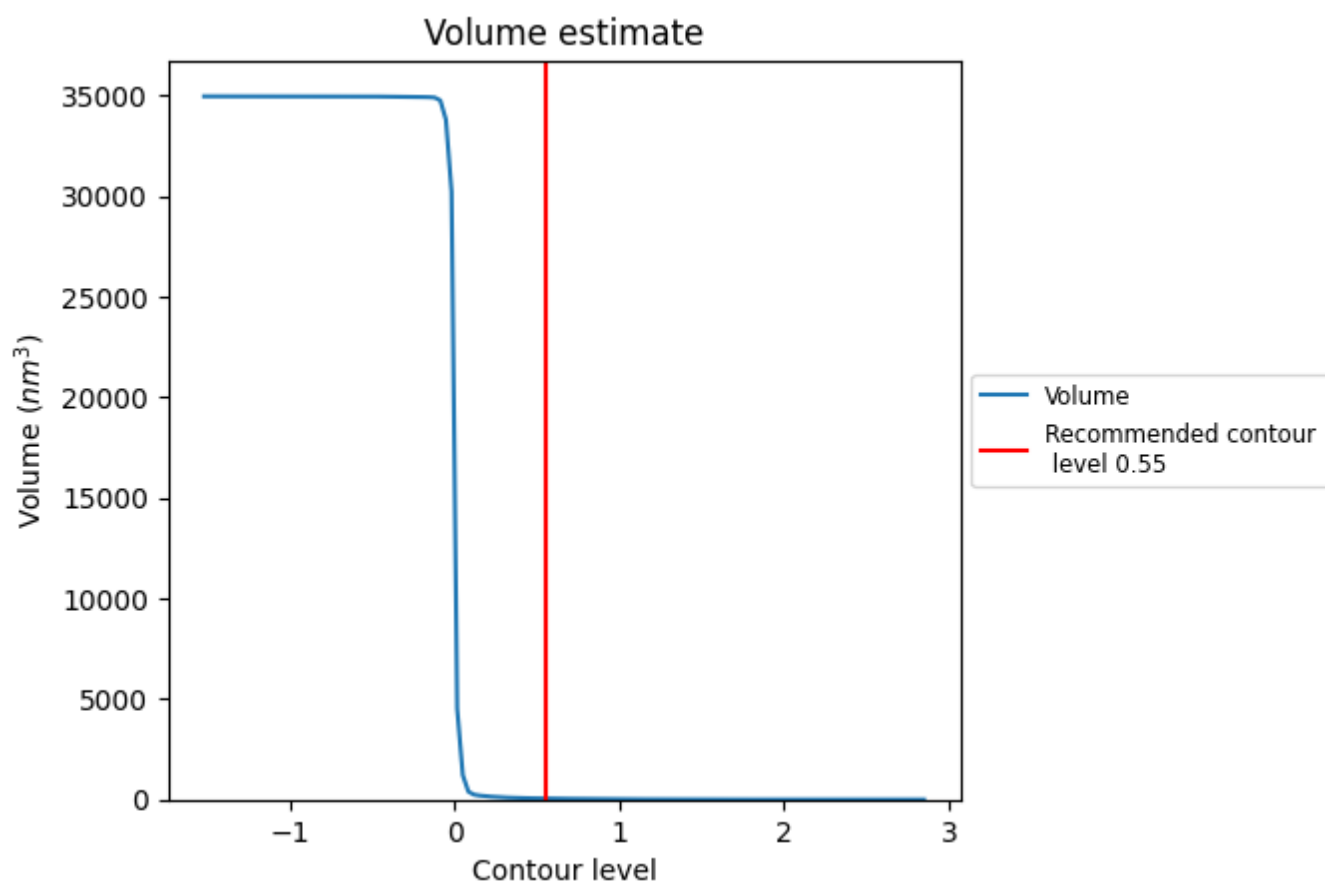
### 7.1 Map-value distribution [i](#)



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.



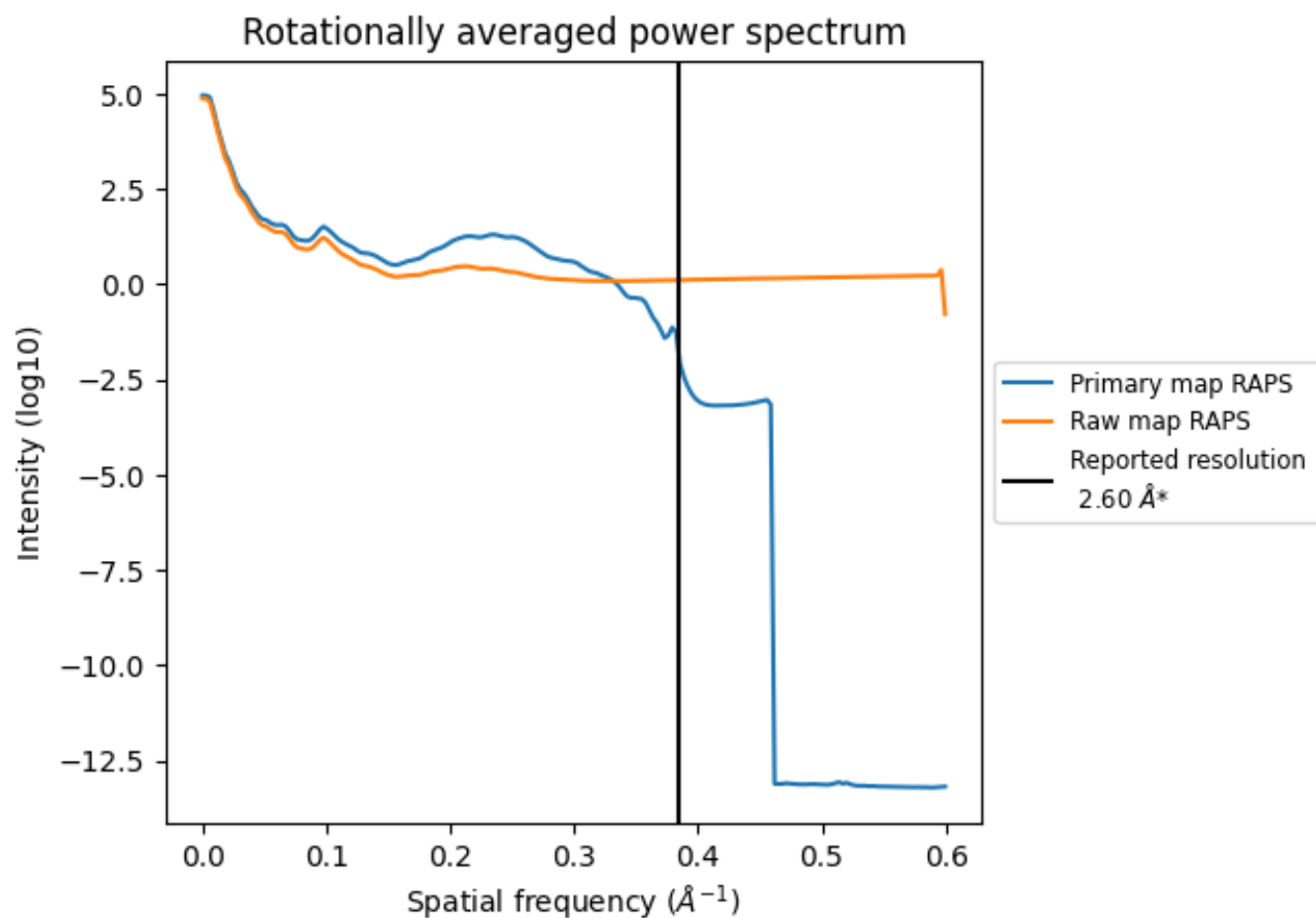
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 52 nm<sup>3</sup>; this corresponds to an approximate mass of 47 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 ⓘ

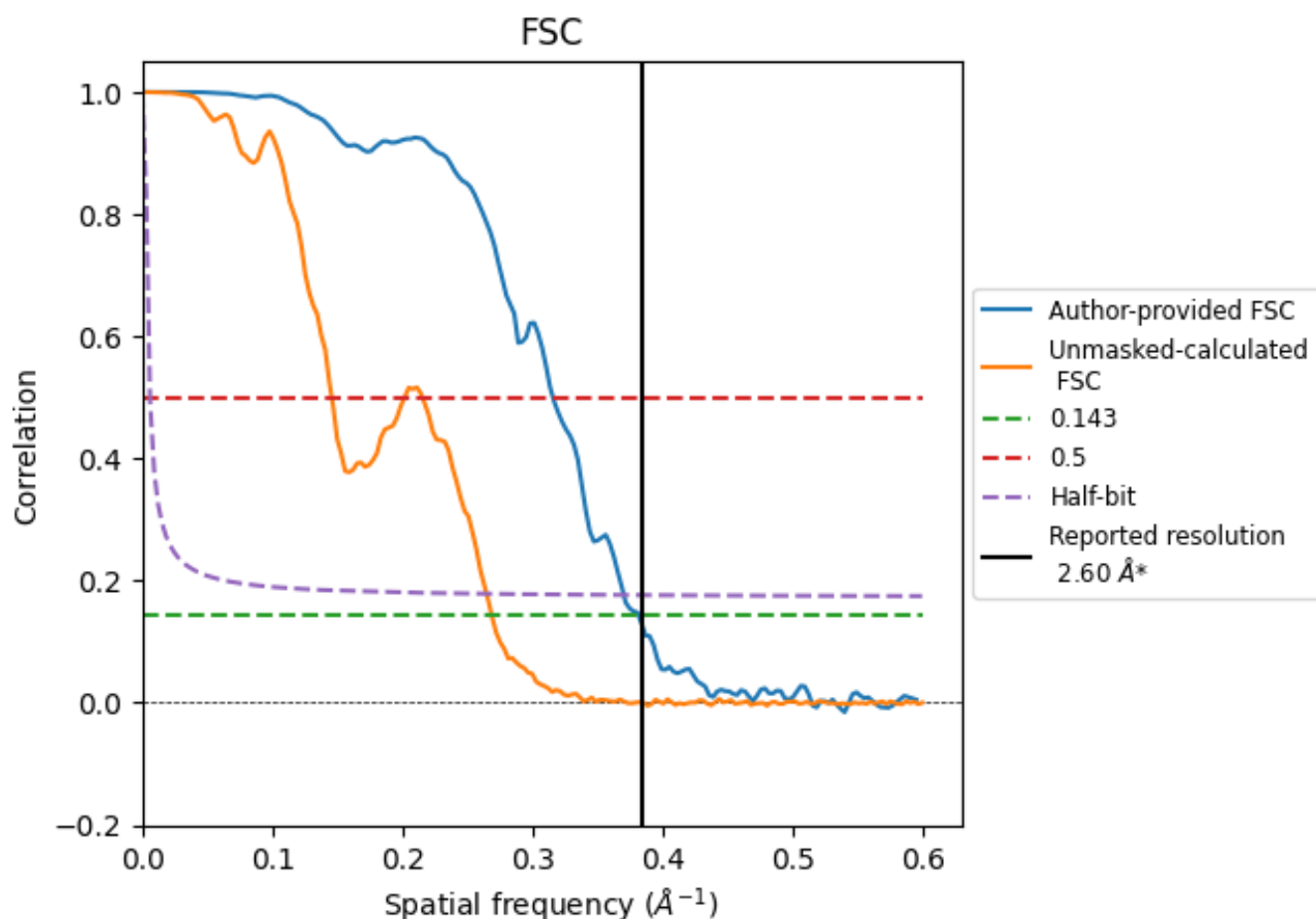


\*Reported resolution corresponds to spatial frequency of 0.385  $\text{\AA}^{-1}$

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

## 8.2 Resolution estimates [i](#)

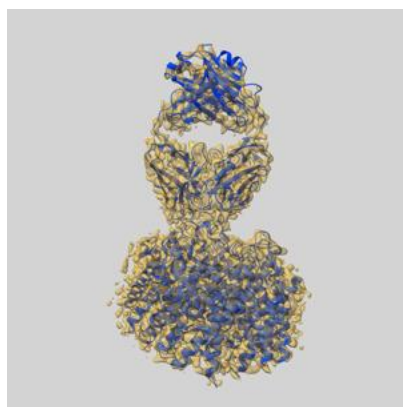
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	2.62	3.17	2.70
Unmasked-calculated*	3.72	6.86	3.78

\*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 3.72 differs from the reported value 2.6 by more than 10 %

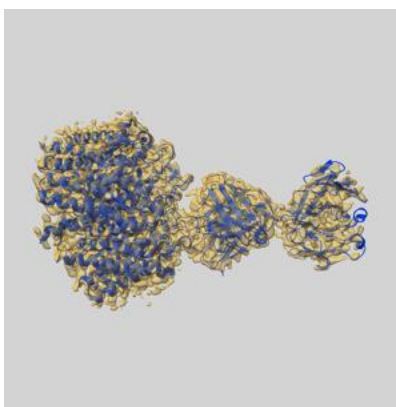
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-43047 and PDB model 8V91. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

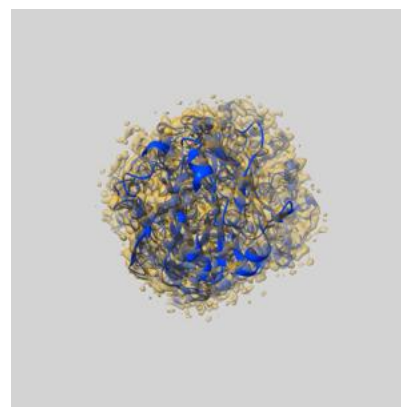
### 9.1 Map-model overlay [i](#)



X



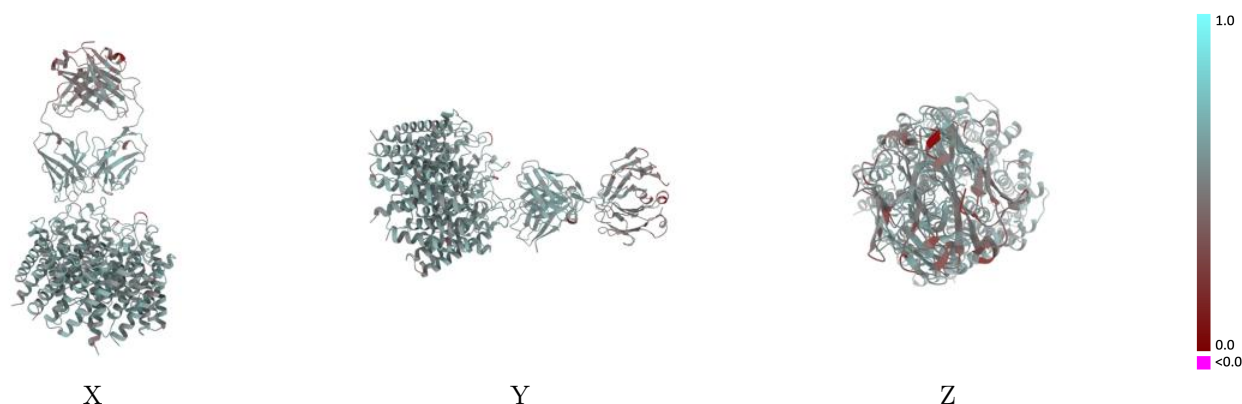
Y



Z

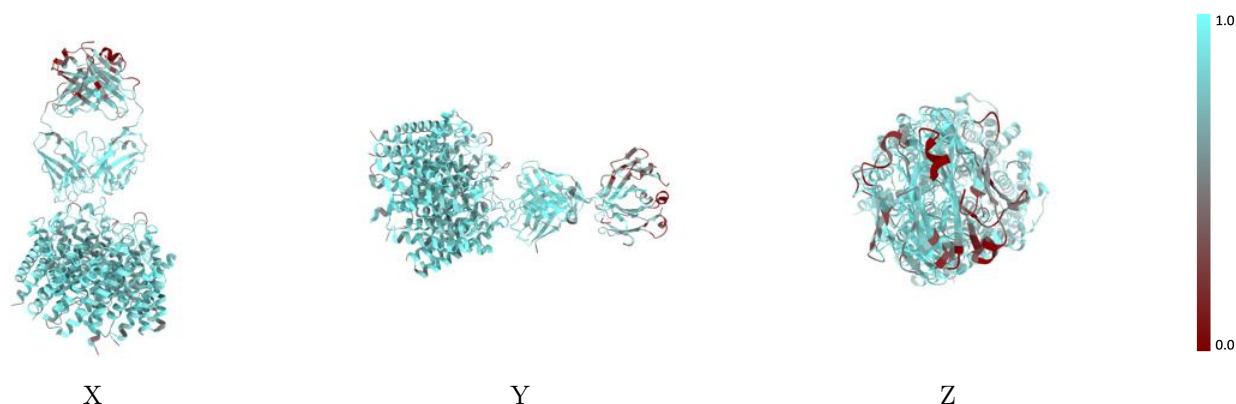
The images above show the 3D surface view of the map at the recommended contour level 0.55 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



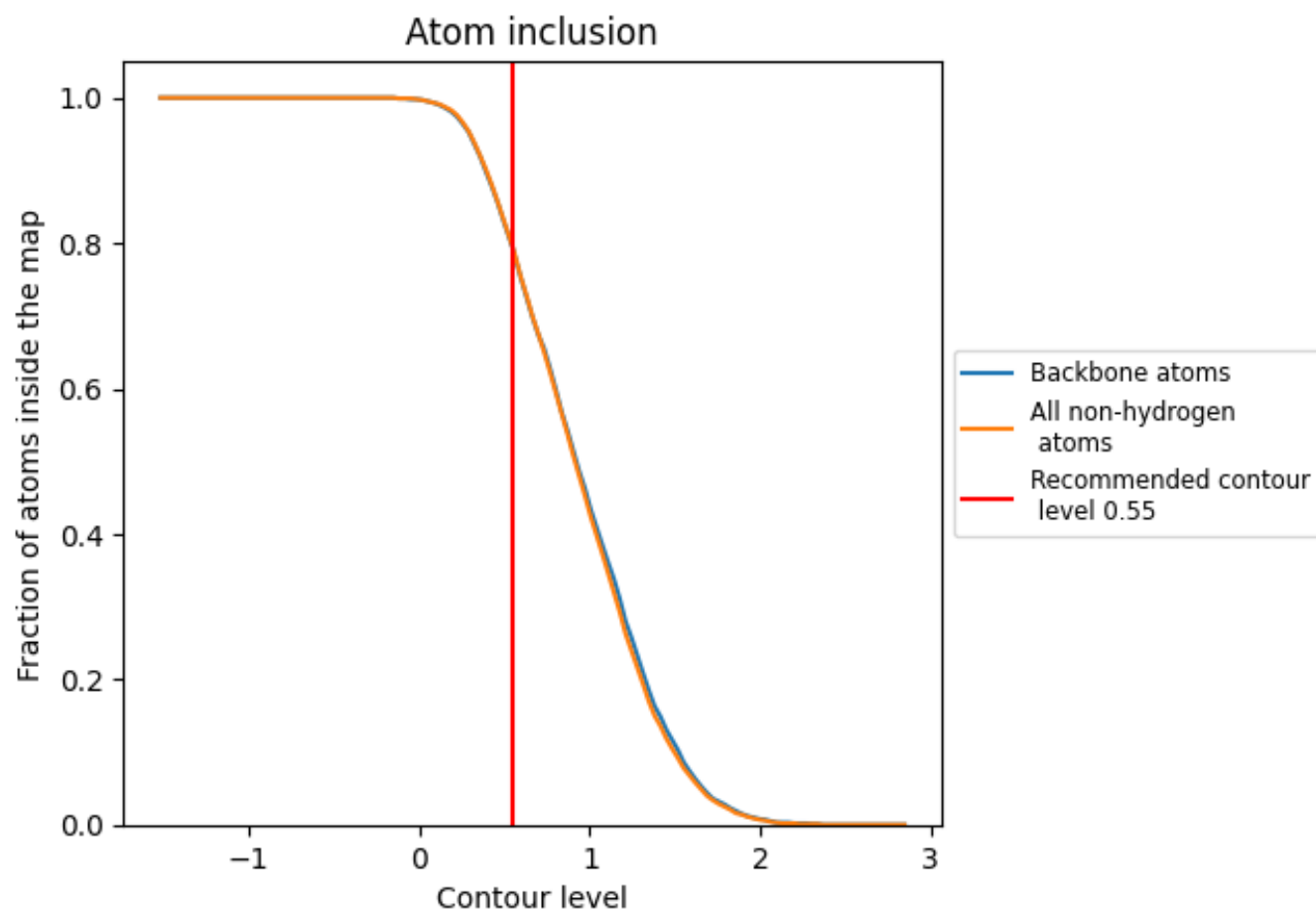
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.55).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 79% 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 (0.55) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.7930	<div><div></div></div> 0.5460
A	<div><div></div></div> 0.8300	<div><div></div></div> 0.5630
B	<div><div></div></div> 0.8500	<div><div></div></div> 0.5670
C	<div><div></div></div> 0.8450	<div><div></div></div> 0.5660
D	<div><div></div></div> 0.8270	<div><div></div></div> 0.5610
I	<div><div></div></div> 0.6860	<div><div></div></div> 0.5100
J	<div><div></div></div> 0.7330	<div><div></div></div> 0.5060

1.0

0.0

<0.0