



wwPDB EM Validation Summary Report ⓘ

Mar 6, 2026 – 02:42 PM UTC

PDB ID : 9E4C / pdb_00009e4c
EMDB ID : EMD-47505
Title : Human ASIC1a at pH 7.5 with partial transmembrane domain
Authors : Hartfield, K.A.; Cahill, J.; Bacongus, I.
Deposited on : 2024-10-24
Resolution : 3.41 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
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

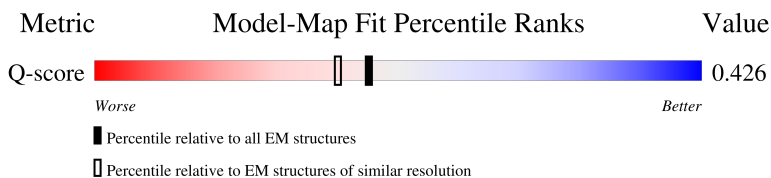
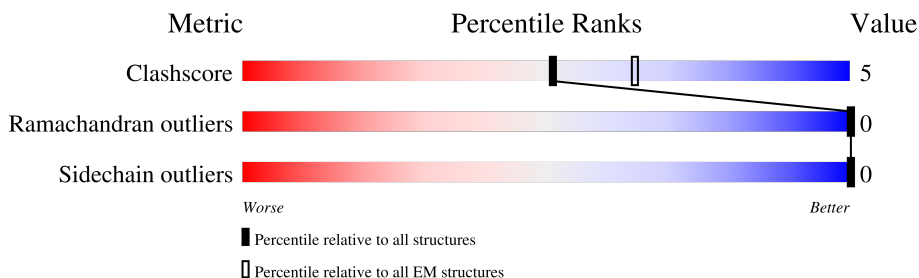
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.41 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	13997 (2.91 - 3.91)

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	531	 6% 68% 8% 24%
1	B	531	 5% 62% 14% 24%
1	C	531	 5% 66% 10% 24%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 9729 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 Acid-sensing ion channel 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	404	Total	C	N	O	S	0	0
			3243	2070	535	609	29		
1	B	404	Total	C	N	O	S	0	0
			3243	2070	535	609	29		
1	C	404	Total	C	N	O	S	0	0
			3243	2070	535	609	29		

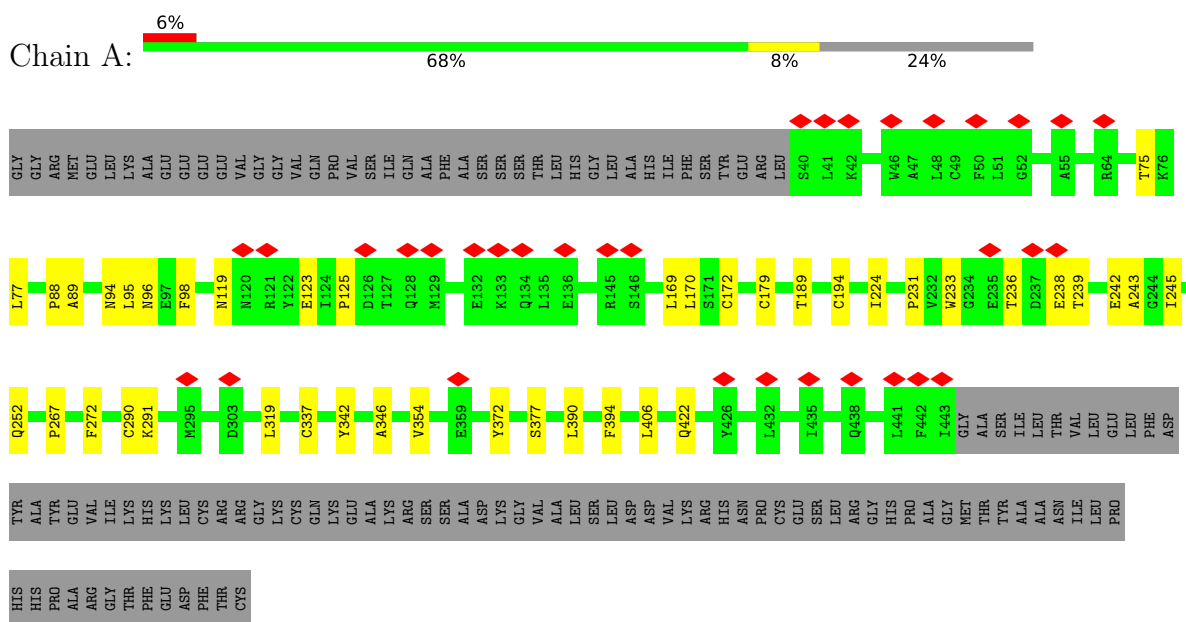
There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P78348
A	-1	GLY	-	expression tag	UNP P78348
A	0	ARG	-	expression tag	UNP P78348
B	-2	GLY	-	expression tag	UNP P78348
B	-1	GLY	-	expression tag	UNP P78348
B	0	ARG	-	expression tag	UNP P78348
C	-2	GLY	-	expression tag	UNP P78348
C	-1	GLY	-	expression tag	UNP P78348
C	0	ARG	-	expression tag	UNP P78348

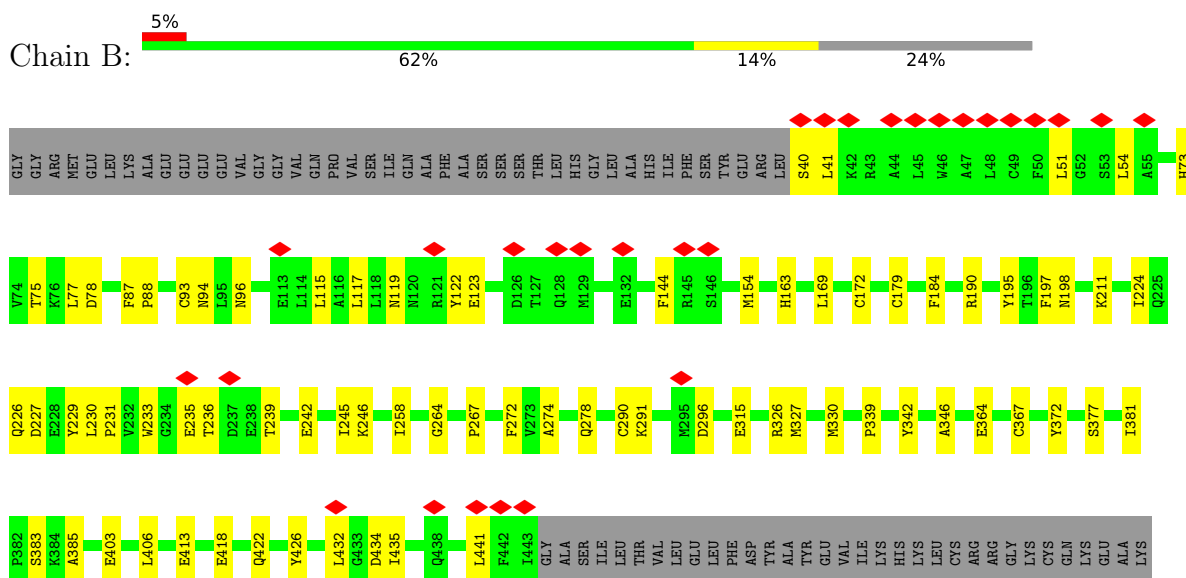
3 Residue-property plots

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: Acid-sensing ion channel 1



• Molecule 1: Acid-sensing ion channel 1



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

● Molecule 1: Acid-sensing ion channel 1



GLY
GLY
ARG
MET
GLU
LEU
LYS
ALA
GLU
GLU
GLU
VAL
GLY
GLY
VAL
GLN
PRO
VAL
SER
ILE
GLN
ALA
PHE
ALA
SER
SER
SER
THR
LEU
HIS
GLY
LEU
ALA
HIS
HIS
ILE
PHE
SER
TYR
GLU
ARG
LEU
S40
L41
K42
R43
A44
L45
W46
A47
L48
C49
F50
L51
G52
S53
L54
Y67
Y68

F69
H70
T75
K76
L77
F87
P88
L95
L115
A116
L117
L118
N119
N120
R121
Y122
E123
Q128
M129
A130
D131
E136
A142
S146
L169
C172
C179
F184
T189
C194
F197
N198
K211
E235
T236
D237
E238
T239
K246
P267

Y282
C290
K291
M296
D296
S297
D298
R326
K330
Y342
A346
P366
C367
N368
L369
Y372
T381
P382
Y389
L390
L406
V414
L415
N416
Q422
Y426
L431
L432
G433
D434
L435
G440
L441
F442
L443
GLY
ALA
SER
ILE
LEU
THR
VAL
LEU
GLU

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

ILE
LEU
PRO
HIS
HIS
PRO
ALA
ARG
GLY
THR
PHE
GLU
ASP
PHE
THR
CYS

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	86378	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 ($e^-/\text{\AA}^2$)	65	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.467	Depositor
Minimum map value	-0.206	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	324.096, 324.096, 324.096	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.84400004, 0.84400004, 0.84400004	Depositor

5 Model quality

5.1 Standard geometry

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	0.12	0/3319	0.31	0/4486
1	B	0.12	0/3319	0.31	0/4486
1	C	0.12	0/3319	0.31	0/4486
All	All	0.12	0/9957	0.31	0/13458

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	3243	0	3139	30	0
1	B	3243	0	3139	54	0
1	C	3243	0	3139	33	0
All	All	9729	0	9417	105	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 5.

The worst 5 of 105 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:169:LEU:HD11	1:A:172:CYS:HB2	1.73	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:422:GLN:NE2	1:B:78:ASP:OD1	2.25	0.70
1:B:169:LEU:HD11	1:B:172:CYS:HB2	1.75	0.68
1:B:115:LEU:HB3	1:B:117:LEU:HD23	1.74	0.68
1:C:236:THR:HB	1:C:239:THR:HG23	1.77	0.65

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	402/531 (76%)	395 (98%)	7 (2%)	0	100	100
1	B	402/531 (76%)	397 (99%)	5 (1%)	0	100	100
1	C	402/531 (76%)	392 (98%)	10 (2%)	0	100	100
All	All	1206/1593 (76%)	1184 (98%)	22 (2%)	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	354/457 (78%)	354 (100%)	0	100	100
1	B	354/457 (78%)	354 (100%)	0	100	100
1	C	354/457 (78%)	354 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1062/1371 (78%)	1062 (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
1	C	70	HIS
1	C	173	HIS
1	B	70	HIS
1	B	96	ASN
1	B	139	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](#)

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.

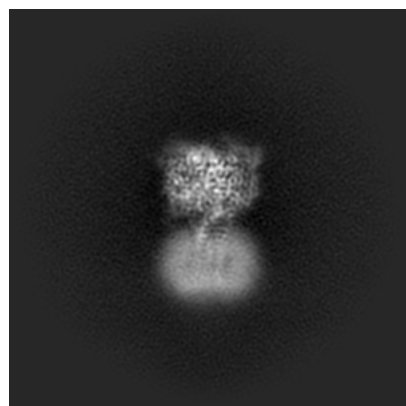
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47505. These allow visual inspection of the internal detail of the map and identification of artifacts.

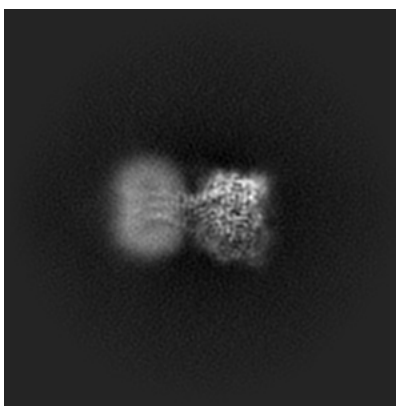
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

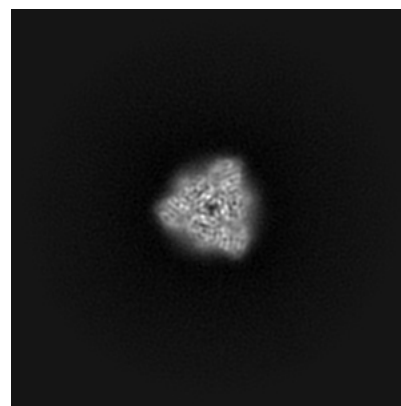
6.1.1 Primary map



X

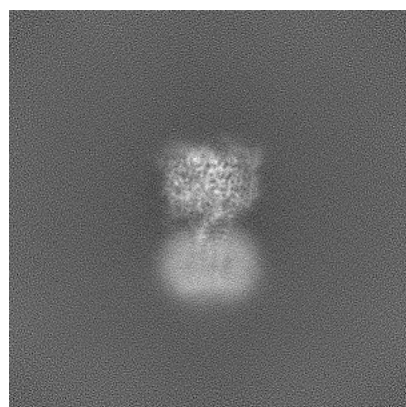


Y

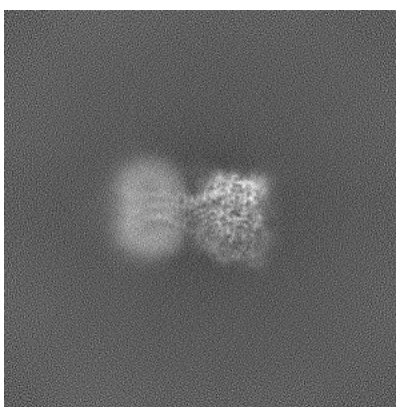


Z

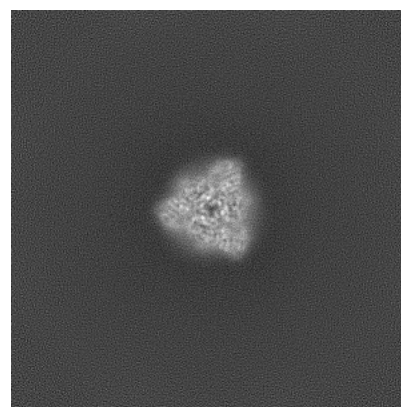
6.1.2 Raw map



X



Y

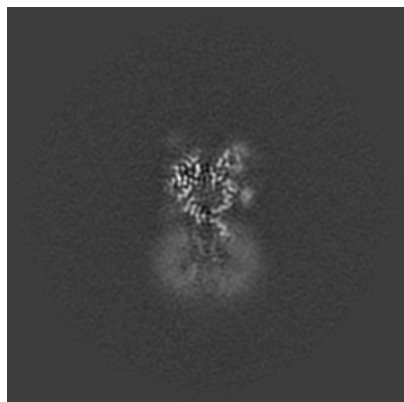


Z

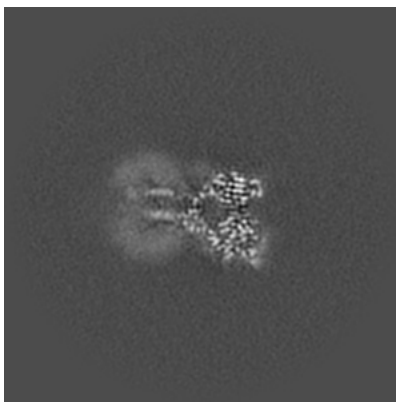
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

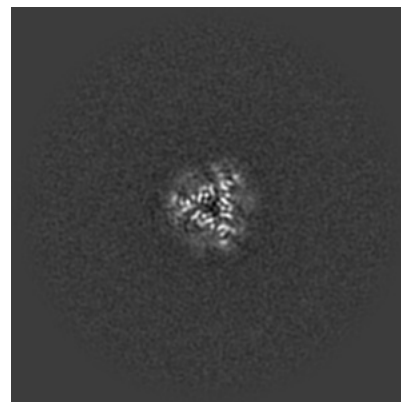
6.2.1 Primary map



X Index: 192



Y Index: 192

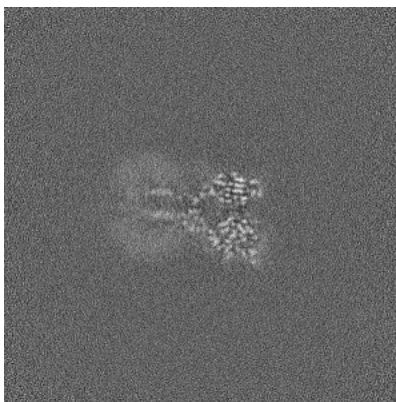


Z Index: 192

6.2.2 Raw map



X Index: 192



Y Index: 192

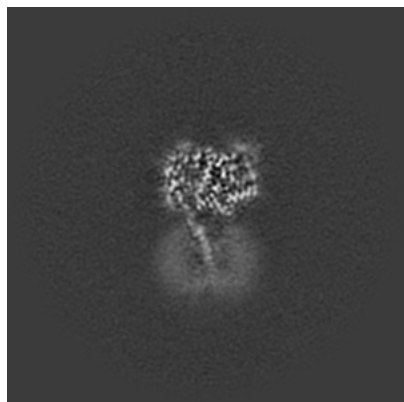


Z Index: 192

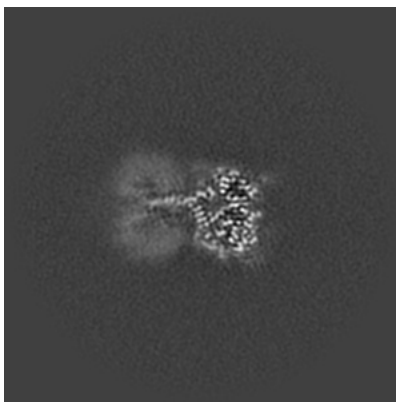
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

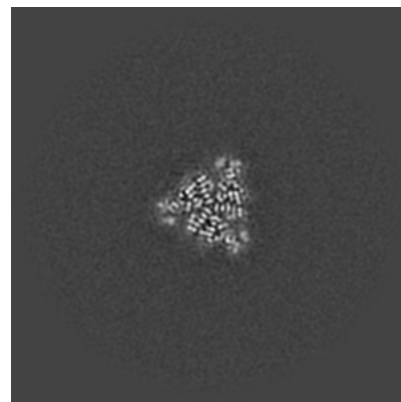
6.3.1 Primary map



X Index: 207

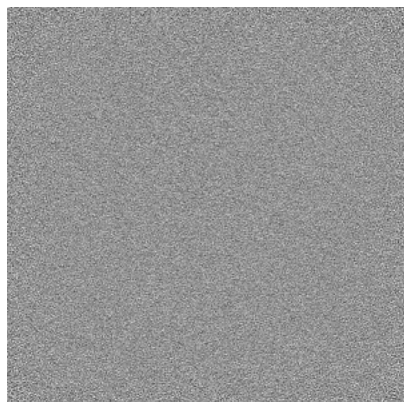


Y Index: 199

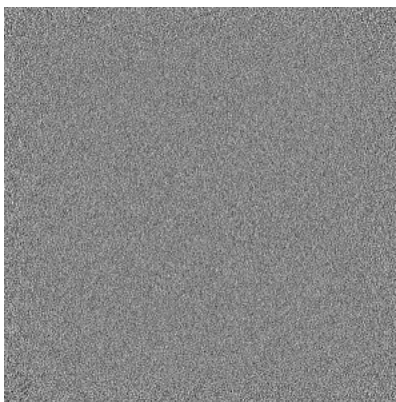


Z Index: 215

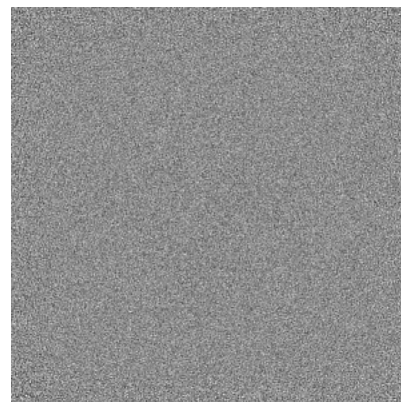
6.3.2 Raw map



X Index: 0



Y Index: 0

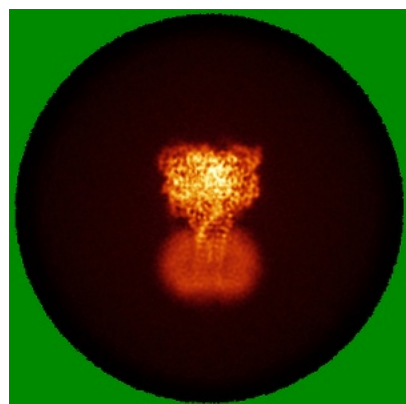


Z Index: 0

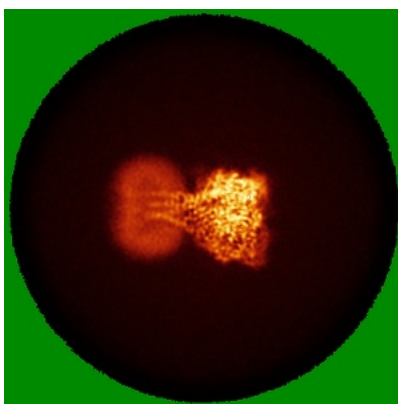
The images above show the largest variance slices of the map in three orthogonal directions.

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

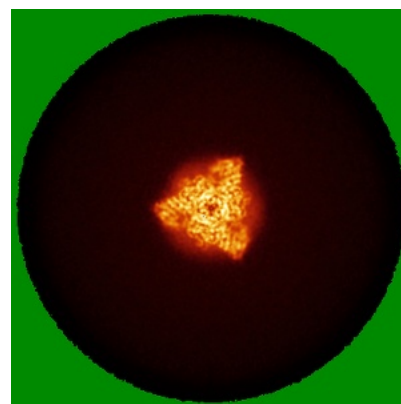
6.4.1 Primary map



X

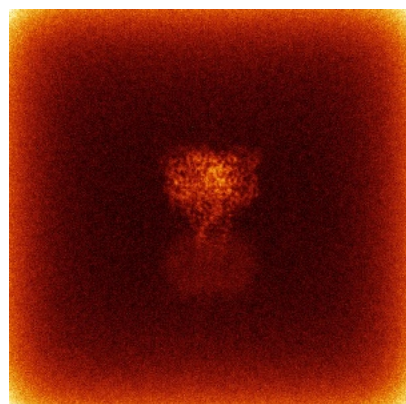


Y

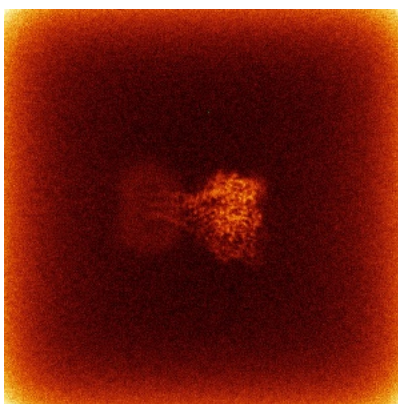


Z

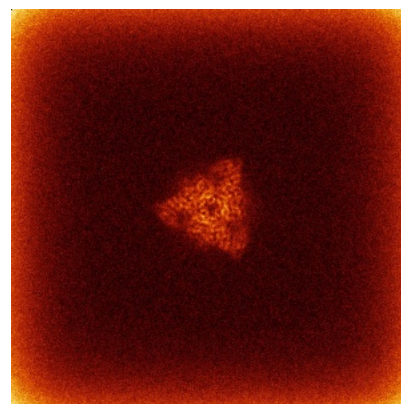
6.4.2 Raw map



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.

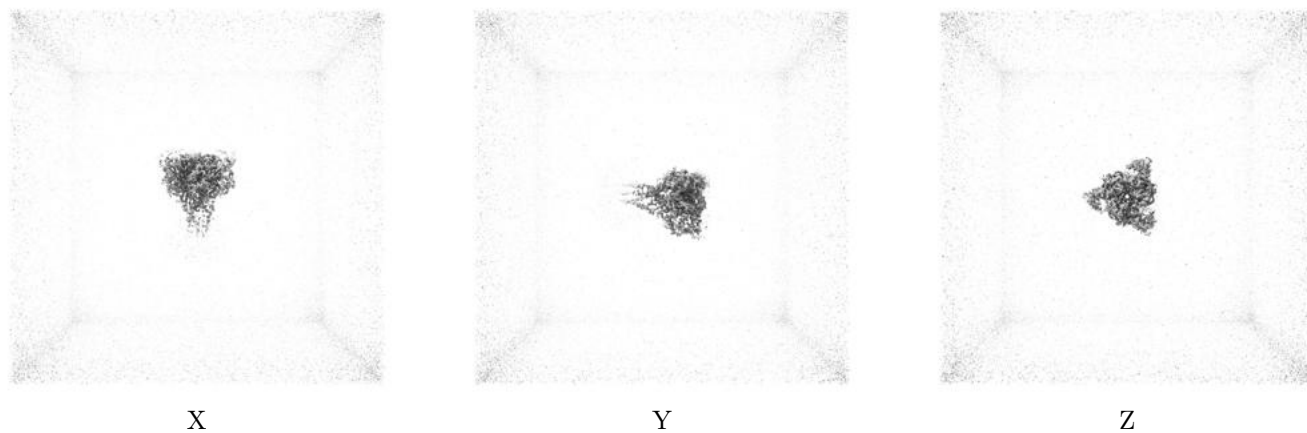
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. 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.

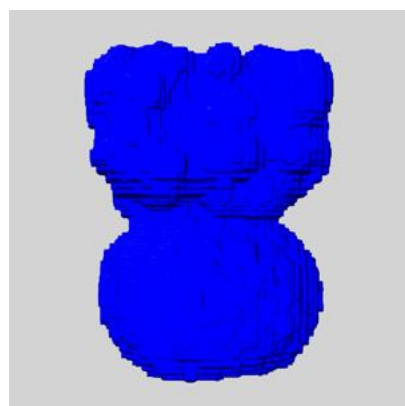
6.6 Mask visualisation [i](#)

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

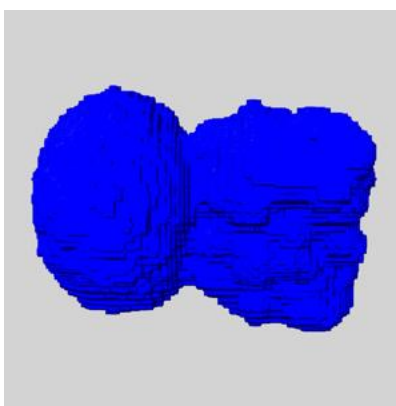
A mask typically either:

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

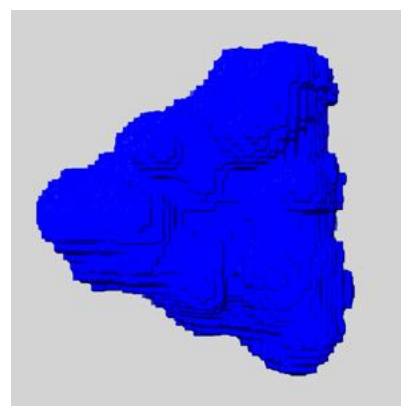
6.6.1 emd_47505_msk_1.map [i](#)



X



Y

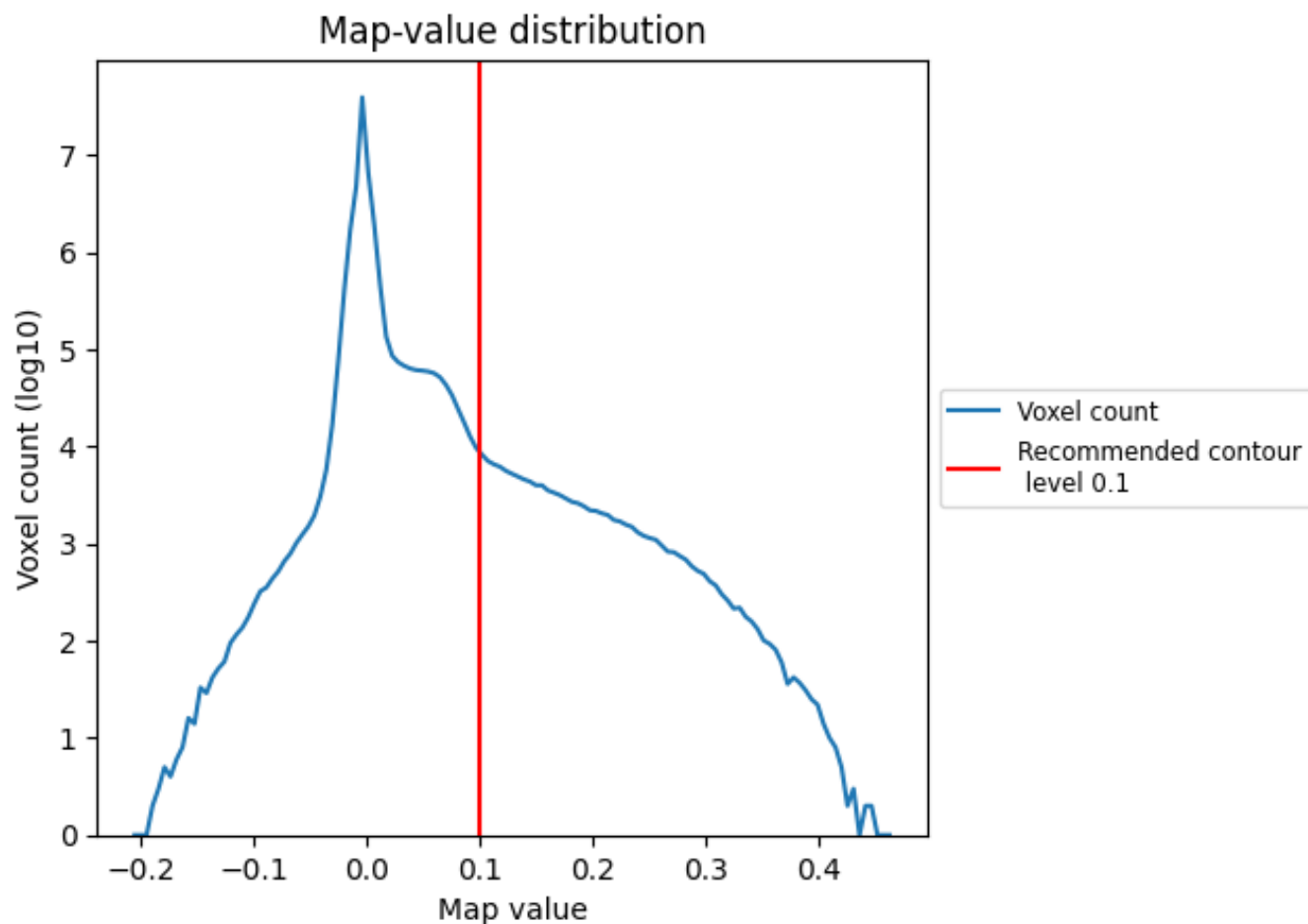


Z

7 Map analysis [i](#)

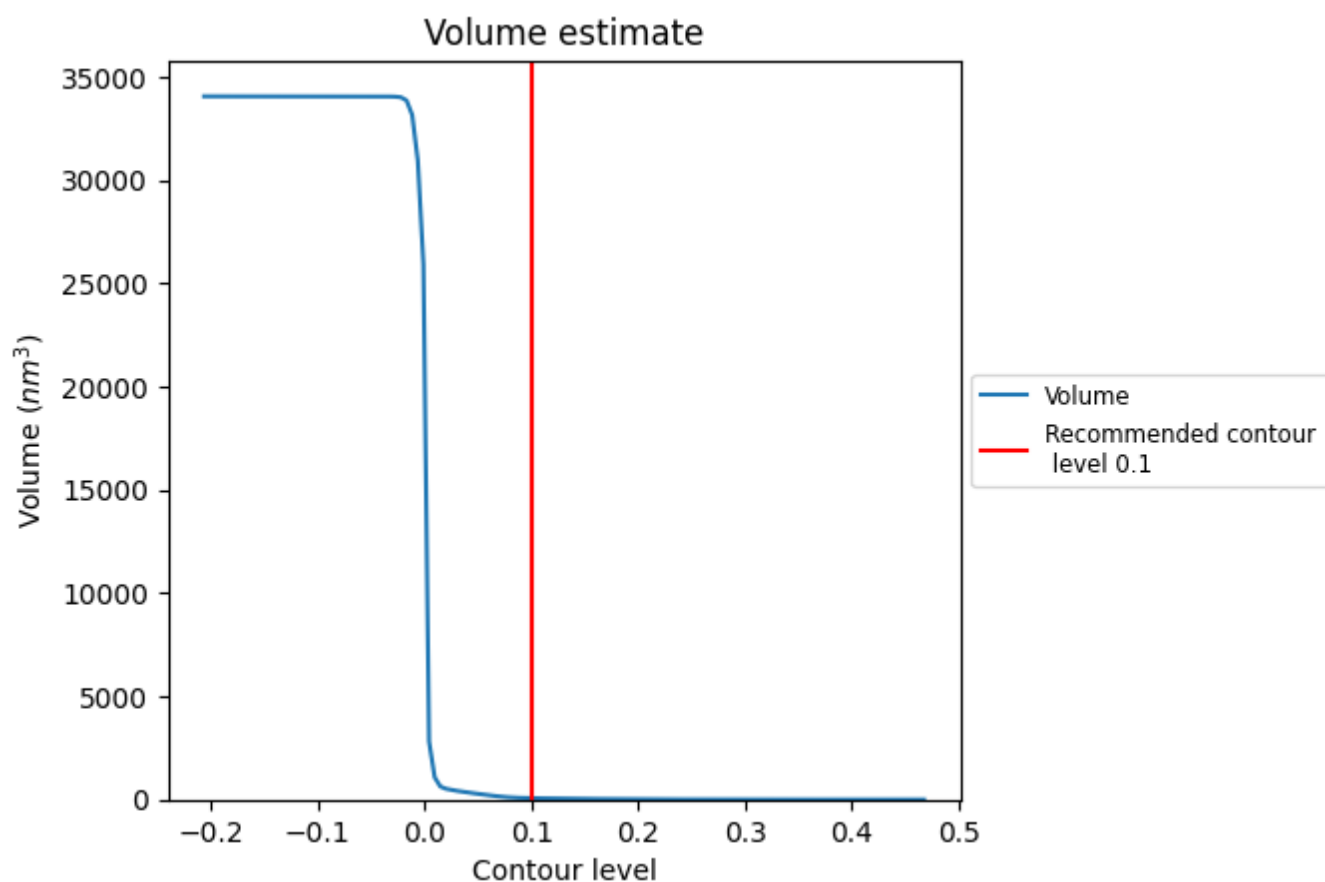
This section contains the results of statistical analysis of the map.

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.

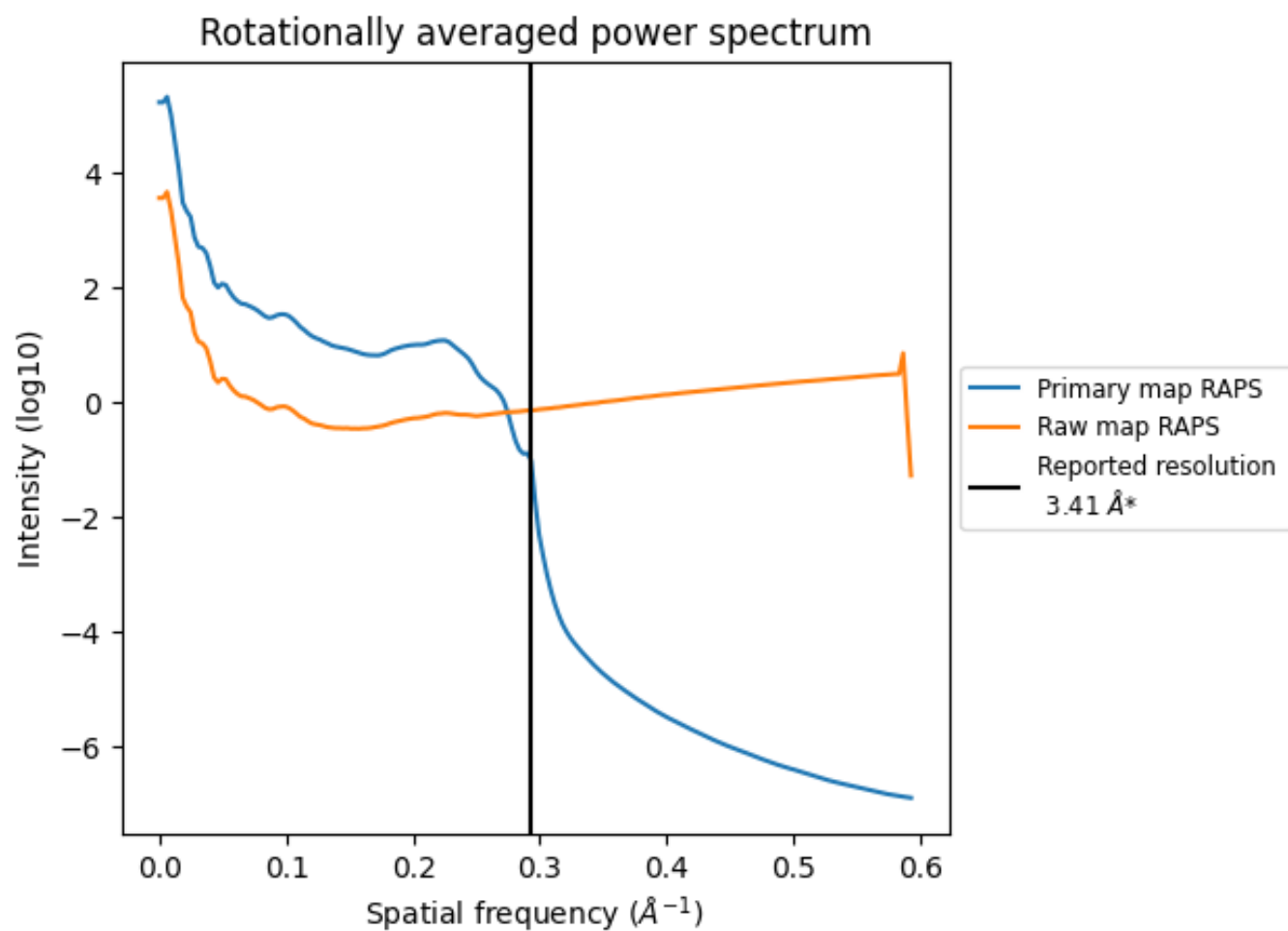
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 68 nm³; this corresponds to an approximate mass of 61 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 ⓘ

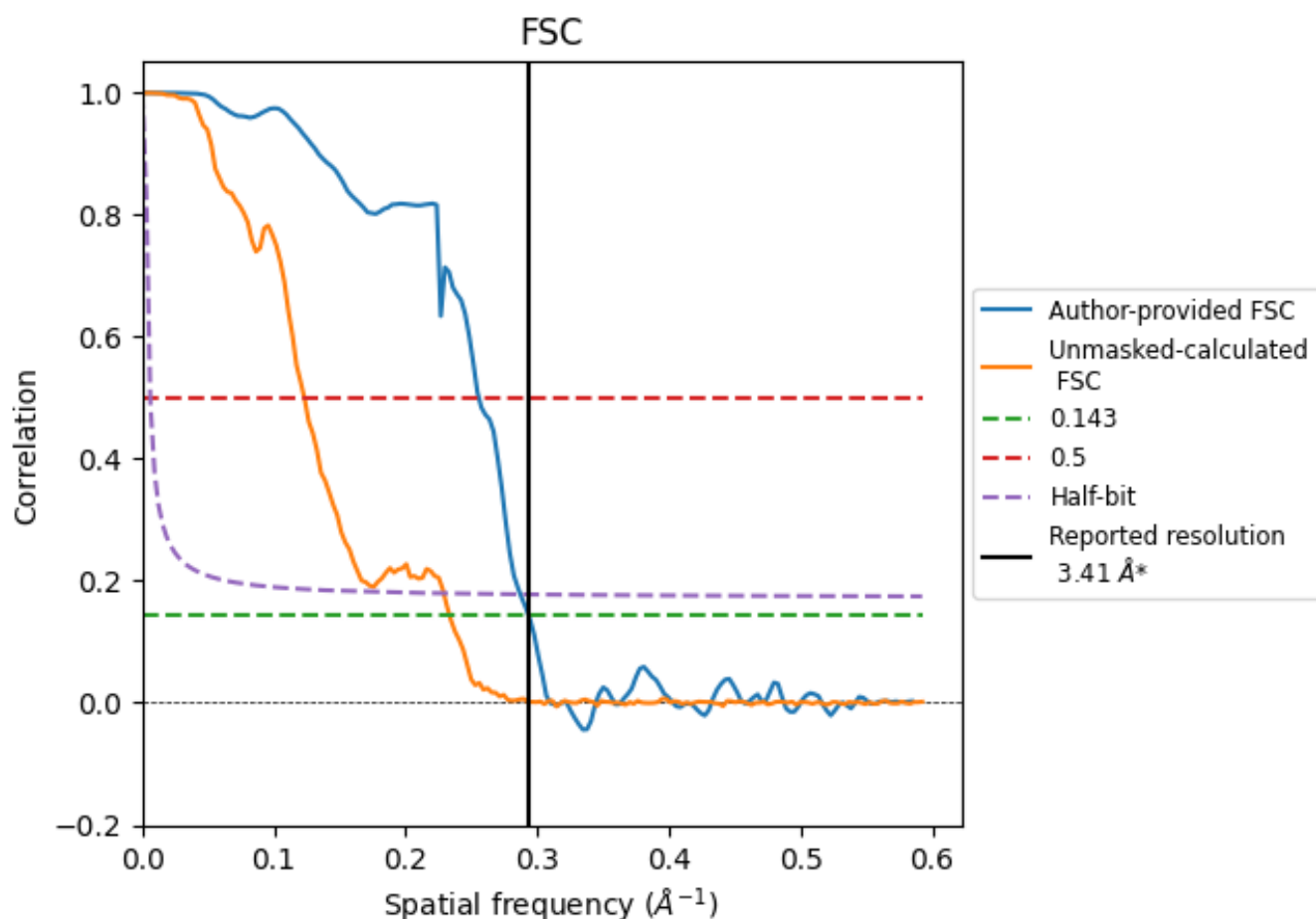


*Reported resolution corresponds to spatial frequency of 0.293 Å⁻¹

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 0.293 Å⁻¹

8.2 Resolution estimates [i](#)

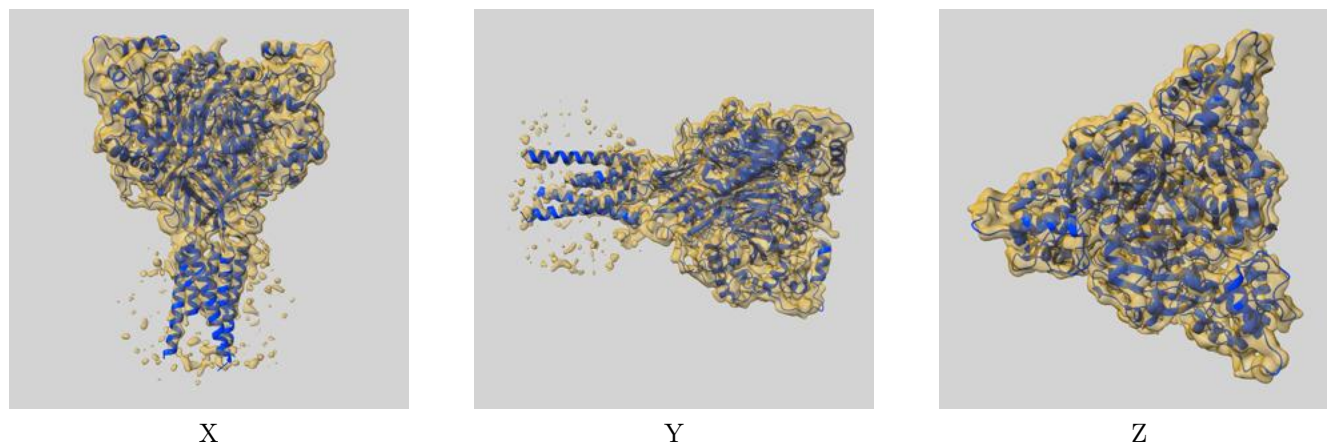
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.41	-	-
Author-provided FSC curve	3.41	3.91	3.48
Unmasked-calculated*	4.28	8.12	4.36

*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 4.28 differs from the reported value 3.41 by more than 10 %

9 Map-model fit [i](#)

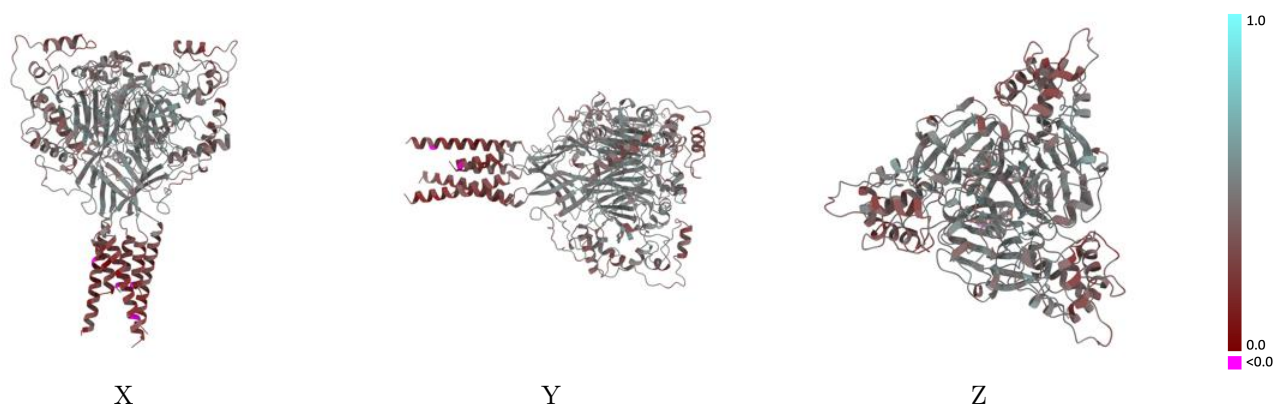
This section contains information regarding the fit between EMDB map EMD-47505 and PDB model 9E4C. Per-residue inclusion information can be found in section [3](#) on page [4](#).

9.1 Map-model overlay [i](#)



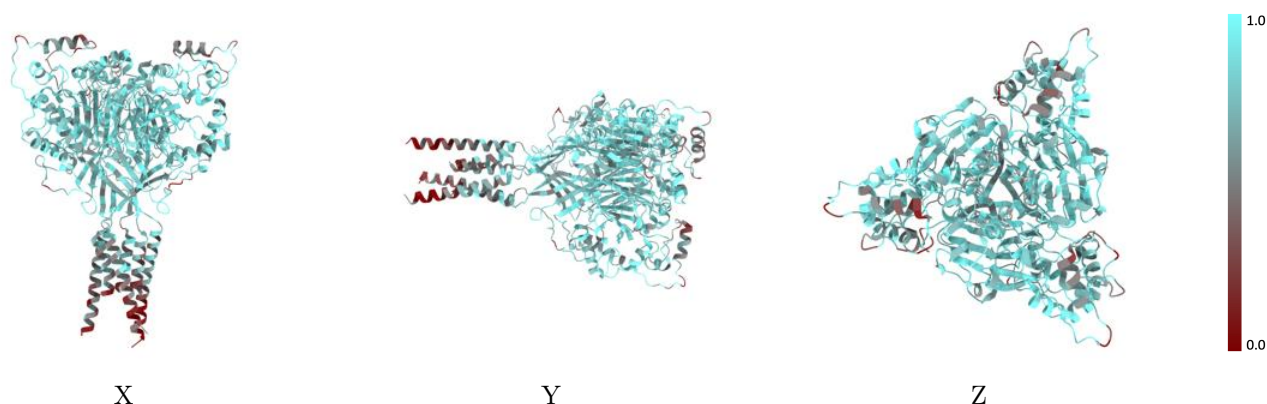
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



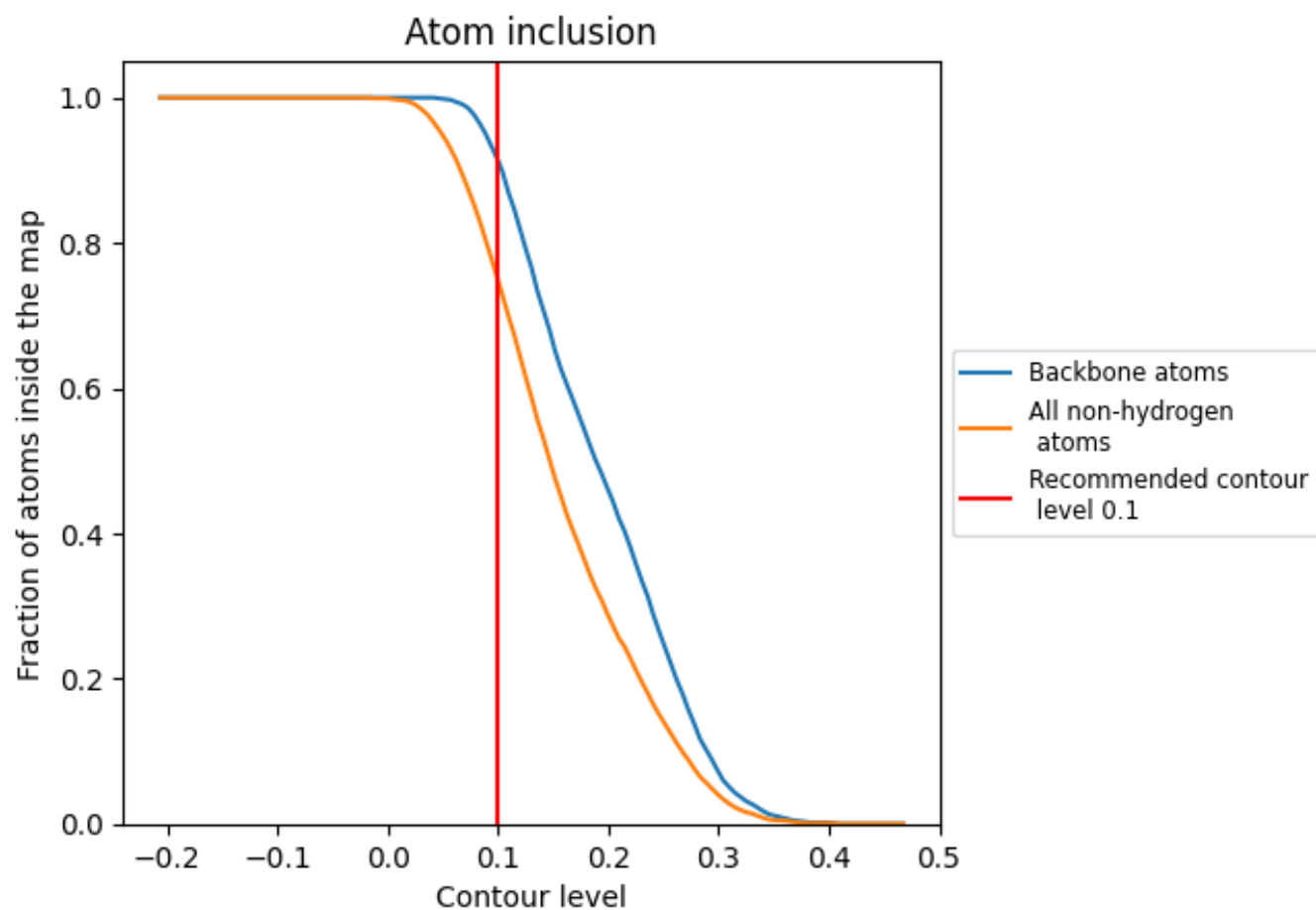
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.7490	<div><div></div></div> 0.4260
A	<div><div></div></div> 0.7410	<div><div></div></div> 0.4200
B	<div><div></div></div> 0.7550	<div><div></div></div> 0.4290
C	<div><div></div></div> 0.7500	<div><div></div></div> 0.4300

