



wwPDB EM Validation Summary Report ⓘ

Feb 19, 2025 – 07:53 PM JST

PDB ID : 9KYY
EMDB ID : EMD-61456
Title : The scaffold tetramer of phage P22
Authors : Liu, H.R.; Xiao, H.
Deposited on : 2024-12-09
Resolution : 6.90 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.dev117
MolProbity : 4.02b-467
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) : 2.41.2

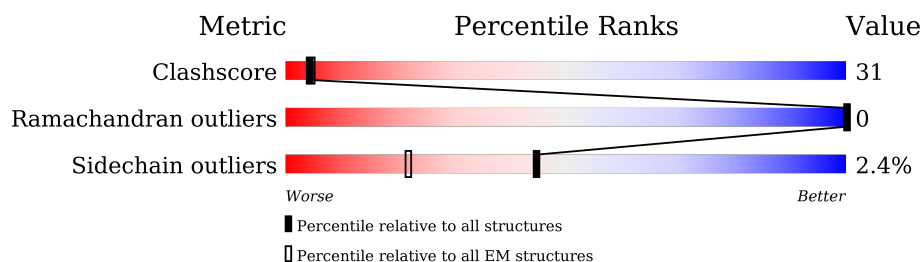
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY



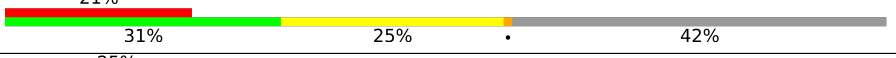
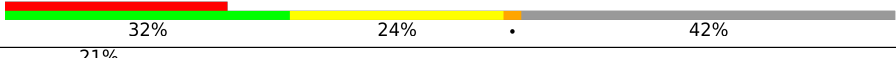
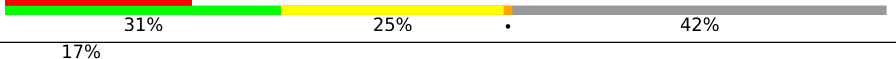

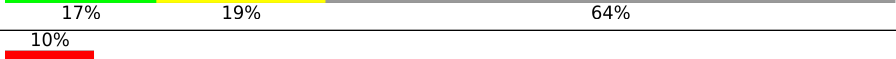
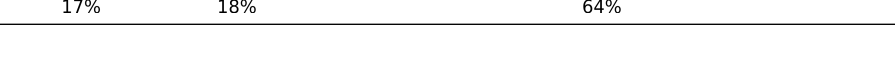
The reported resolution of this entry is 6.90 Å.

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 ≥ 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	303	
1	B	303	
1	C	303	
1	D	303	
1	E	303	
1	F	303	
1	G	303	
1	H	303	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 9112 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 Scaffolding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	176	Total	C	N	O	S	0	0
			1401	870	252	273	6		
1	B	109	Total	C	N	O	S	0	0
			877	548	159	165	5		
1	C	176	Total	C	N	O	S	0	0
			1401	870	252	273	6		
1	D	176	Total	C	N	O	S	0	0
			1401	870	252	273	6		
1	E	176	Total	C	N	O	S	0	0
			1401	870	252	273	6		
1	F	109	Total	C	N	O	S	0	0
			877	548	159	165	5		
1	G	109	Total	C	N	O	S	0	0
			877	548	159	165	5		
1	H	109	Total	C	N	O	S	0	0
			877	548	159	165	5		

GLY
LYS
GLN
ILE
SER
SER
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• Molecule 1: Scaffolding protein

Chain C: 21% 31% 25% 42%

MET
GLU
PRO
THR
THR
GLU
GLN
THR
THR
ASP
GLU
LEU
THR
THR
SER
GLY
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ALA
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F127
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ARG
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R70
R71
R72
Q73
R74
E75
L76
E77
M80
R85
G86
E87
L88
P89
E90
S91
F156
L92
R93
V94
N95
P96
D97
L98
P99
P100
Q101
P102
D103
I104
M105
A106
Y107
L108
S109
E110
E111
G112
L113
A114
K115
Y116
D117
Y118
D119
N120
S121
R122
A123
L124

A125
A126
N128
A129
A130
N131
T132
E133
W134
L135
M136
K137
A138
Q139
D140
A141
R142
S143
N144
A147
K152
T153
E154
VAL
F155
F156
T157
Q158
Q159
S160
Q162
Y163
V164
E165
A166
K169
H170
Y171
A174
E175
E176
L177
P180
D181
Y182
Q183
E184
K185
E186
D187
Q191
L192
V193

P194
P195
A196
V197
D200
L201
R202
L203
F205
P206
E207
K208
S209
A210
A211
L212
W213
Y214
H215
L216
G217
A218
L219
P220
K221
K222
A223
R224
Q225
L226
L227
A228
M229
D230
G231
Q232
S233
A234
L235
E237
L238
T239
R240
L241
S242
E243
R244
L245
THR
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SER
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• Molecule 1: Scaffolding protein

Chain D: 25% 32% 24% 42%

MET
GLU
PRO
THR
THR
GLU
GLN
THR
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R74
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E77
Q78
Q79
M80
V83
K84
R85
G86
L88
P89
E90
S91
F156
T157
Q158
Q159
S160
R93
V94
N95
P96
D97
L98
P99
P100
Q101
P102
D103
I104
M105
A106
Y107
L108
S109
E110
E111
G112
L113
A114
K115
Y116
D117
Y118
D119
N120
S121

R122
A123
L124
A125
A126
F127
N128
A129
A130
N131
T132
E133
W134
L135
M136
K137
A138
D140
A141
R142
S143
N144
A147
K152
T153
E154
Q154
F155
T157
Q158
Q159
S160
A161
Y163
V164
E165
A166
K169
H170
Y171
D172
A173
A174
E175
K176
L177
M178
I179
P180
D181
Y182
Q183
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K185
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D187
A188
F189
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Q191
L192
V193
P195
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V197
G198
A199
D200
L201
R202
L203
F205
P206
E207
S208
A210
A211
L212
P213
Y214
H215
P219
N220
E221
K222
A223
R224
Q225
L226
L227
A228
M229
D230
G231
Q232
S233
A234
L235
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L238
T239
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• Molecule 1: Scaffolding protein

Chain E: 21% 31% 25% 42%

MET
GLU
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GLU
LEU
THR
THR
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LYS
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ASP
GLU
THR
ALA
PRO
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	33180	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	32	Depositor
Minimum defocus (nm)	1600	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	11.942	Depositor
Minimum map value	-6.079	Depositor
Average map value	0.022	Depositor
Map value standard deviation	0.767	Depositor
Recommended contour level	3	Depositor
Map size (\AA)	339.19998, 339.19998, 339.19998	wwPDB
Map dimensions	160, 160, 160	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	2.12, 2.12, 2.12	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	0.35	0/1425	0.64	0/1923
1	B	0.28	0/889	0.62	0/1191
1	C	0.34	0/1425	0.65	0/1923
1	D	0.32	0/1425	0.63	0/1923
1	E	0.31	0/1425	0.64	0/1923
1	F	0.28	0/889	0.62	0/1191
1	G	0.28	0/889	0.62	0/1191
1	H	0.28	0/889	0.62	0/1191
All	All	0.31	0/9256	0.63	0/12456

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	1401	0	1376	107	0
1	B	877	0	880	51	0
1	C	1401	0	1376	102	0
1	D	1401	0	1376	98	0
1	E	1401	0	1376	92	0
1	F	877	0	880	50	0
1	G	877	0	880	54	0
1	H	877	0	880	50	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	9112	0	9024	571	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 31.

The worst 5 of 571 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:C:139:GLN:HG3	1:D:139:GLN:HE22	1.17	1.08
1:A:108:LEU:HD22	1:C:125:ALA:HB2	1.35	1.07
1:D:236:ILE:HG23	1:G:239:THR:HG23	1.36	1.04
1:C:229:MET:HE1	1:C:233:SER:HB3	1.45	0.94
1:D:108:LEU:HD23	1:E:121:SER:HB2	1.50	0.91

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	174/303 (57%)	158 (91%)	16 (9%)	0	100	100
1	B	105/303 (35%)	104 (99%)	1 (1%)	0	100	100
1	C	174/303 (57%)	163 (94%)	11 (6%)	0	100	100
1	D	174/303 (57%)	161 (92%)	13 (8%)	0	100	100
1	E	174/303 (57%)	161 (92%)	13 (8%)	0	100	100
1	F	105/303 (35%)	104 (99%)	1 (1%)	0	100	100
1	G	105/303 (35%)	104 (99%)	1 (1%)	0	100	100
1	H	105/303 (35%)	104 (99%)	1 (1%)	0	100	100
All	All	1116/2424 (46%)	1059 (95%)	57 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	144/244 (59%)	139 (96%)	5 (4%)	31	51
1	B	90/244 (37%)	89 (99%)	1 (1%)	70	80
1	C	144/244 (59%)	140 (97%)	4 (3%)	38	57
1	D	144/244 (59%)	139 (96%)	5 (4%)	31	51
1	E	144/244 (59%)	140 (97%)	4 (3%)	38	57
1	F	90/244 (37%)	89 (99%)	1 (1%)	70	80
1	G	90/244 (37%)	89 (99%)	1 (1%)	70	80
1	H	90/244 (37%)	89 (99%)	1 (1%)	70	80
All	All	936/1952 (48%)	914 (98%)	22 (2%)	45	62

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	240	ARG
1	E	224	ARG
1	E	169	LYS
1	E	240	ARG
1	C	122	ARG

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	G	162	GLN
1	H	162	GLN
1	D	215	HIS
1	D	219	ASN
1	E	158	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.

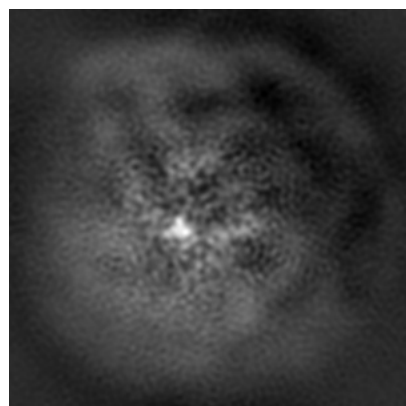
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-61456. These allow visual inspection of the internal detail of the map and identification of artifacts.

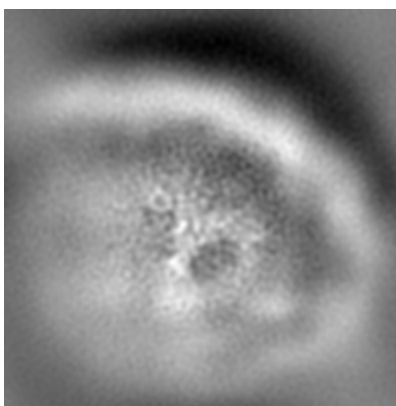
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

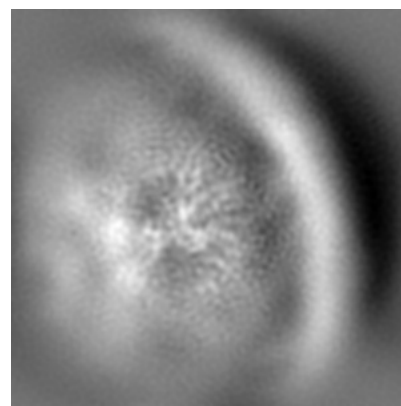
6.1.1 Primary map



X

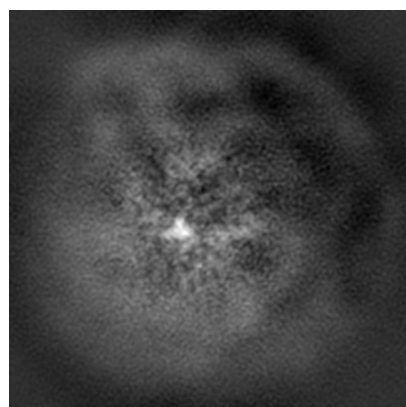


Y

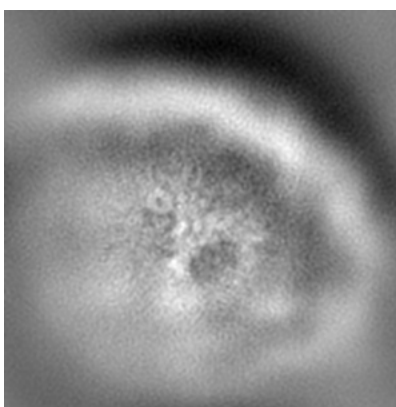


Z

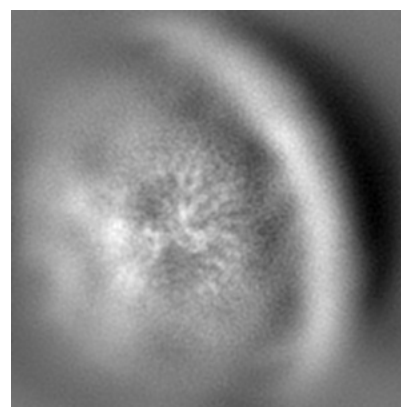
6.1.2 Raw map



X



Y

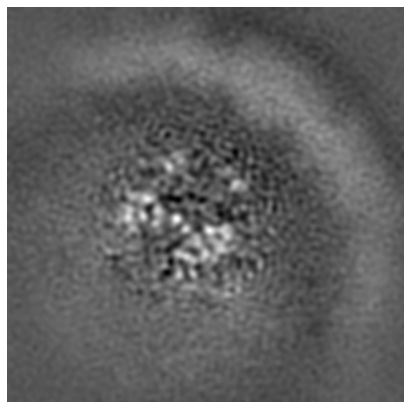


Z

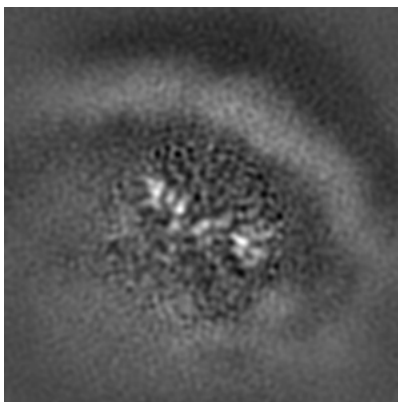
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

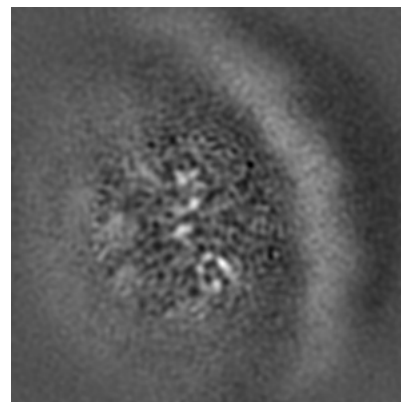
6.2.1 Primary map



X Index: 80

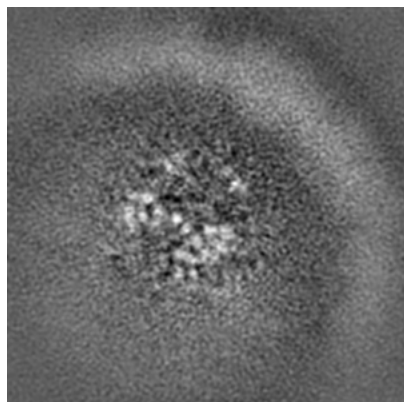


Y Index: 80

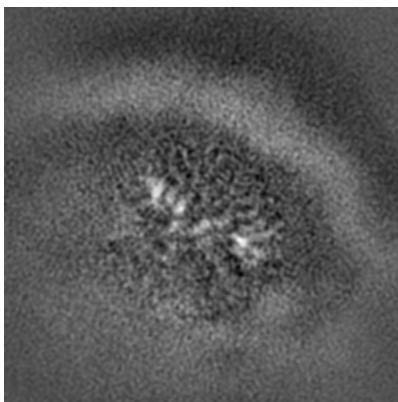


Z Index: 80

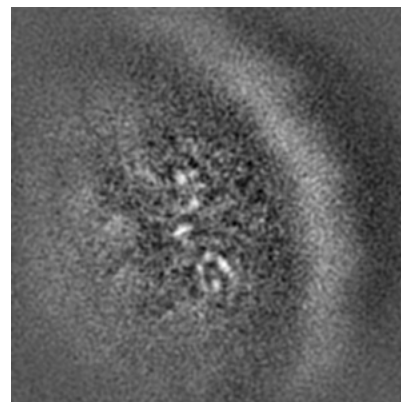
6.2.2 Raw map



X Index: 80



Y Index: 80

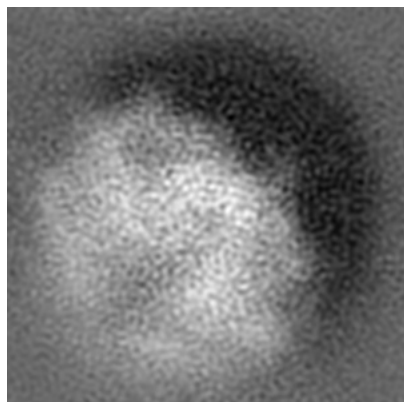


Z Index: 80

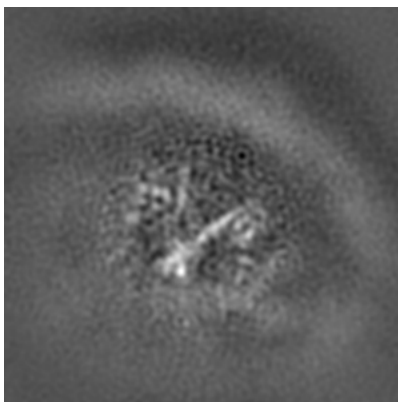
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

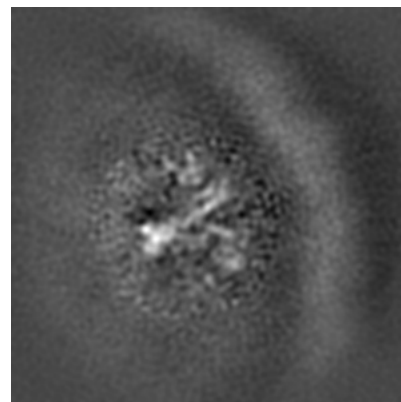
6.3.1 Primary map



X Index: 123

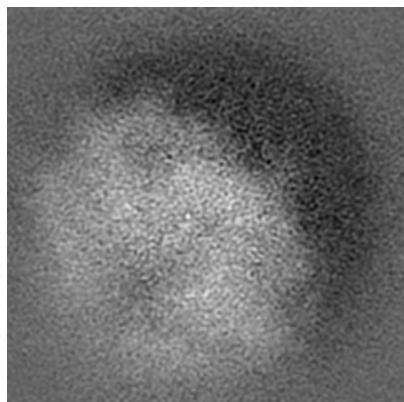


Y Index: 70

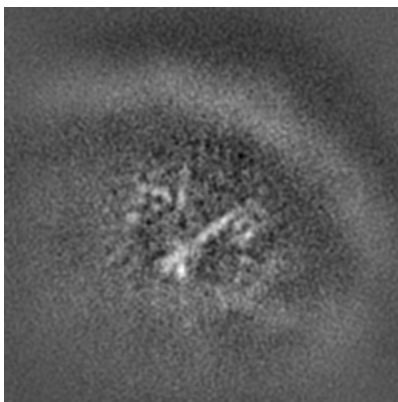


Z Index: 70

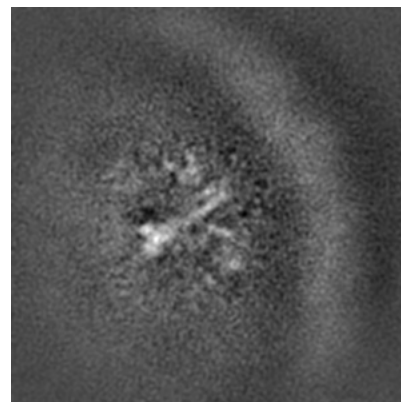
6.3.2 Raw map



X Index: 123



Y Index: 70

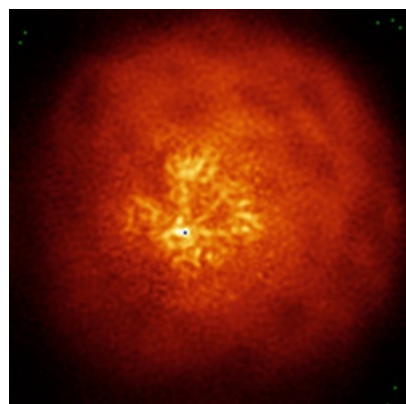


Z Index: 70

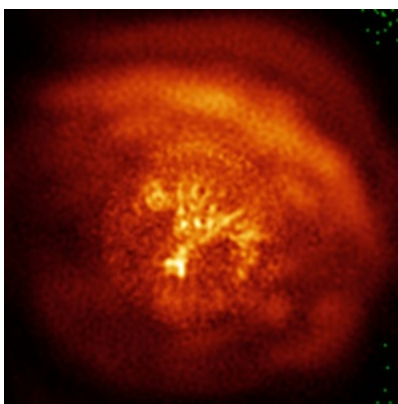
The images above show the largest variance slices of the map in three orthogonal directions.

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

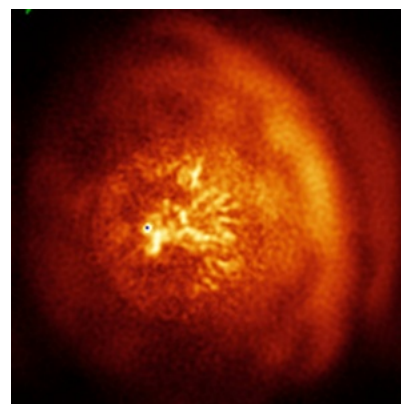
6.4.1 Primary map



X

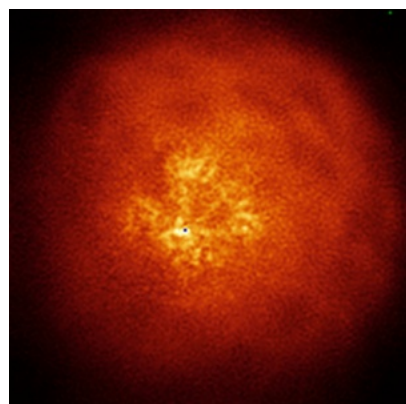


Y

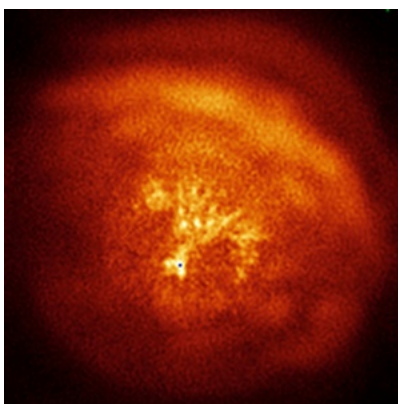


Z

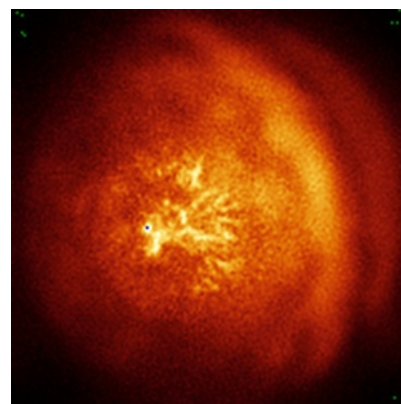
6.4.2 Raw map



X



Y

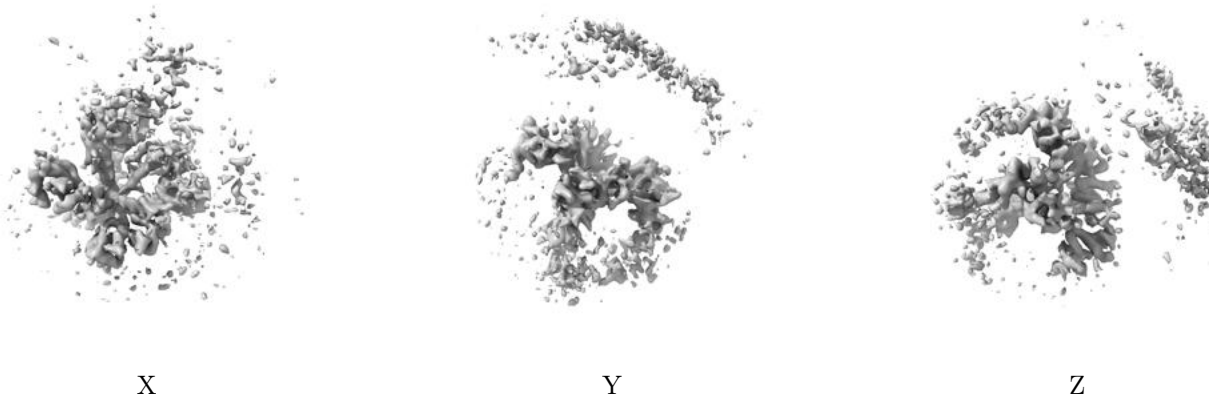


Z

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 3.0. 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.

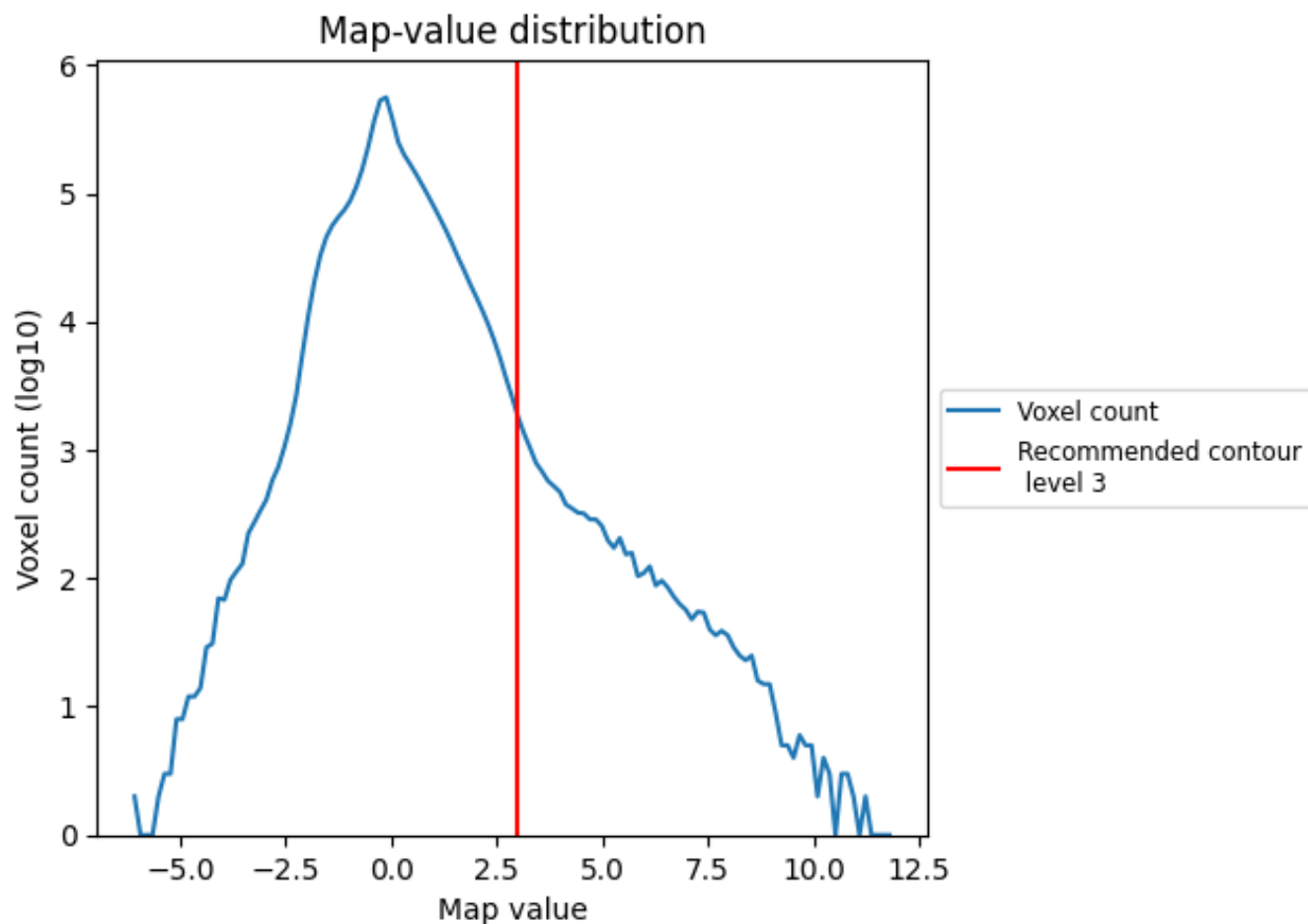
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

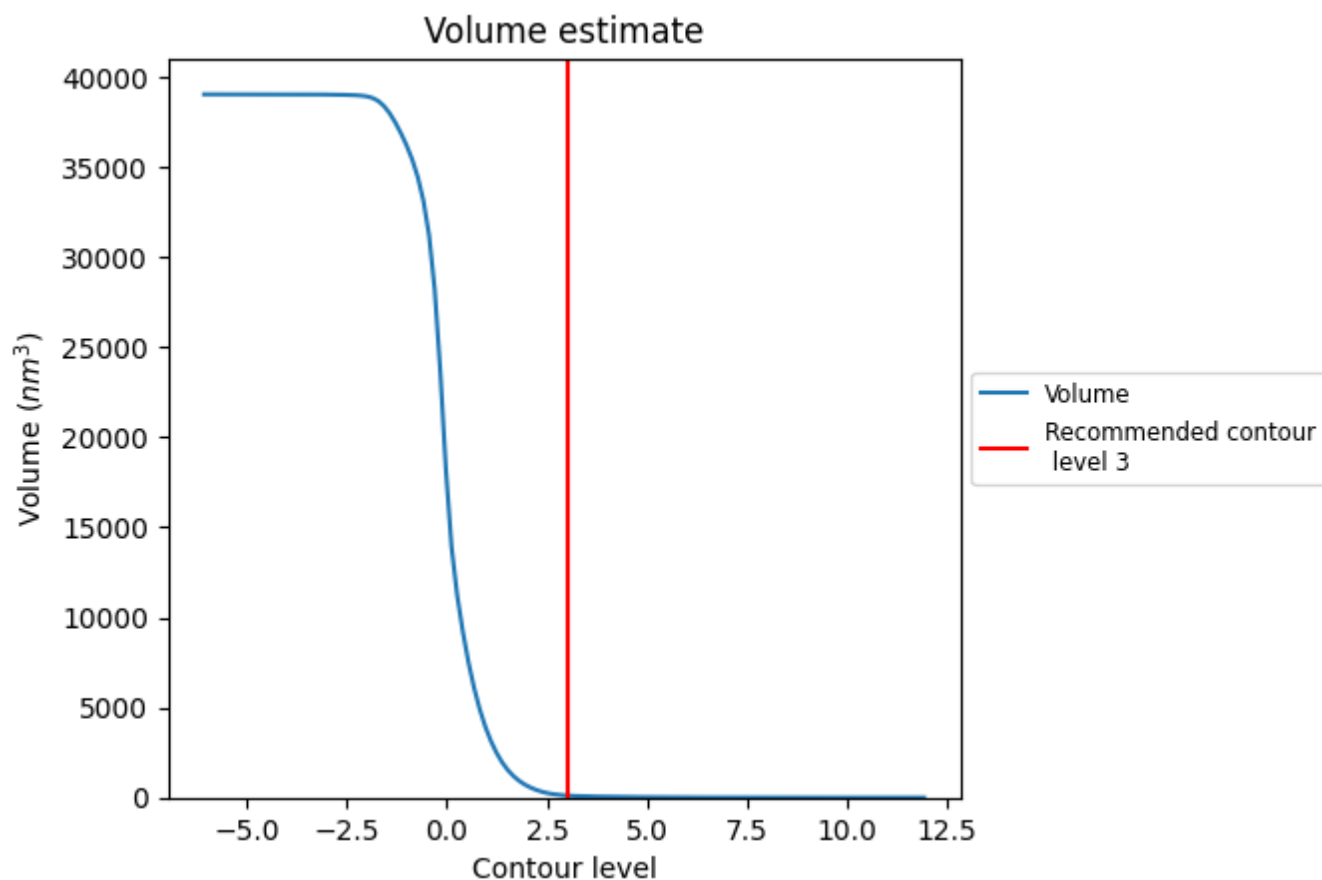
This section contains the results of statistical analysis of the map.

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.

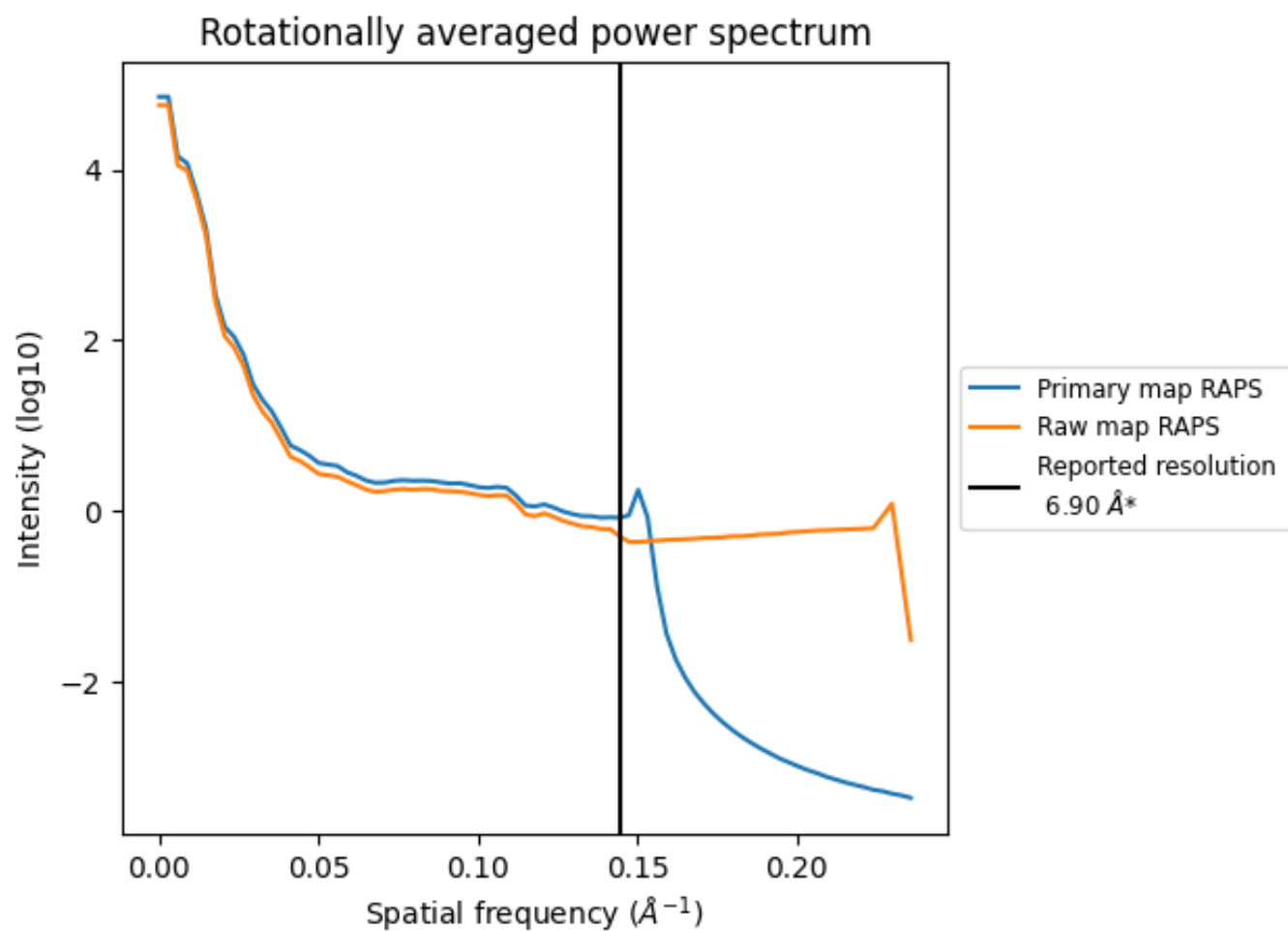
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 113 nm³; this corresponds to an approximate mass of 102 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 ⓘ

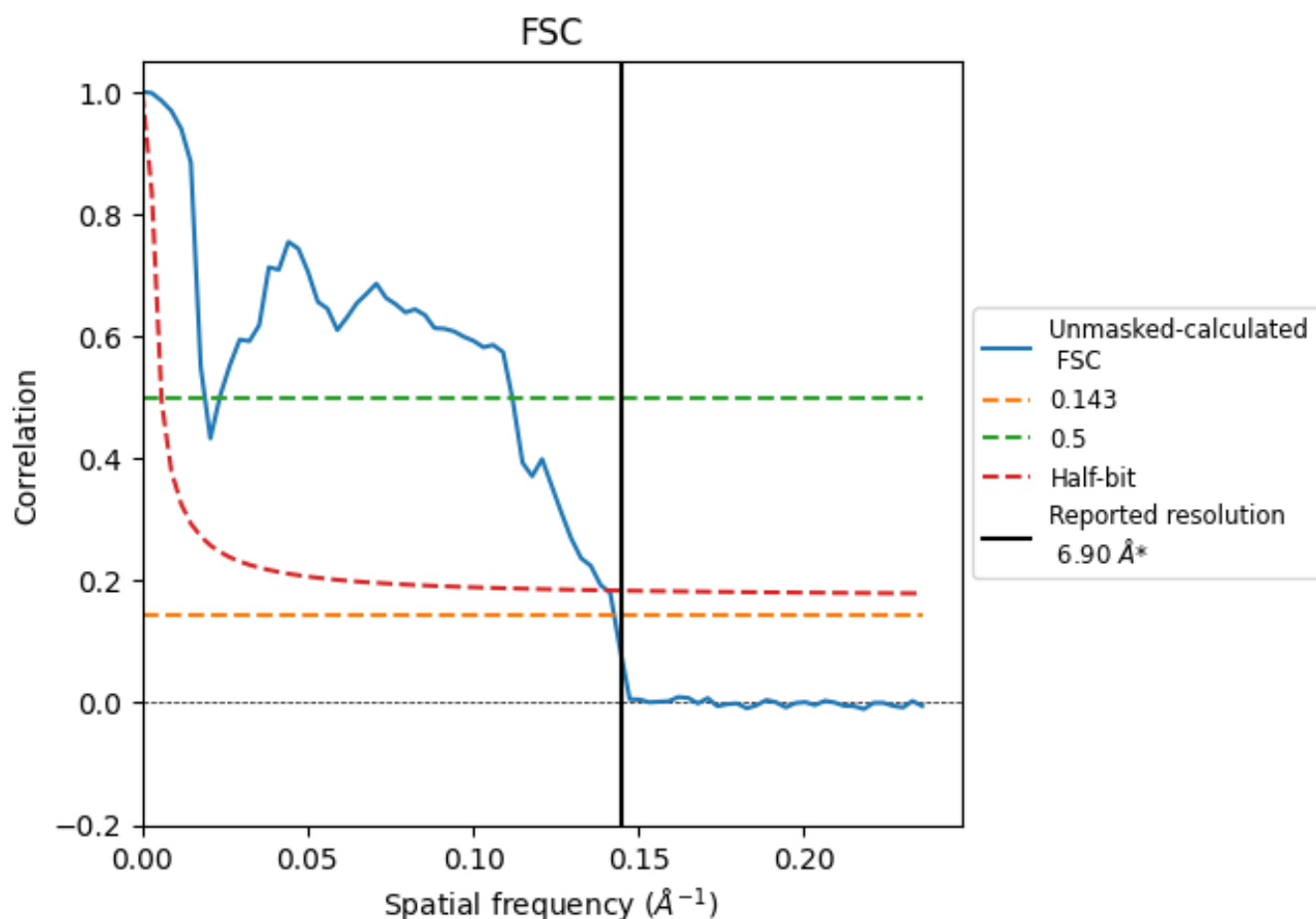


*Reported resolution corresponds to spatial frequency of 0.145 \AA^{-1}

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 0.145 \AA^{-1}

8.2 Resolution estimates [i](#)

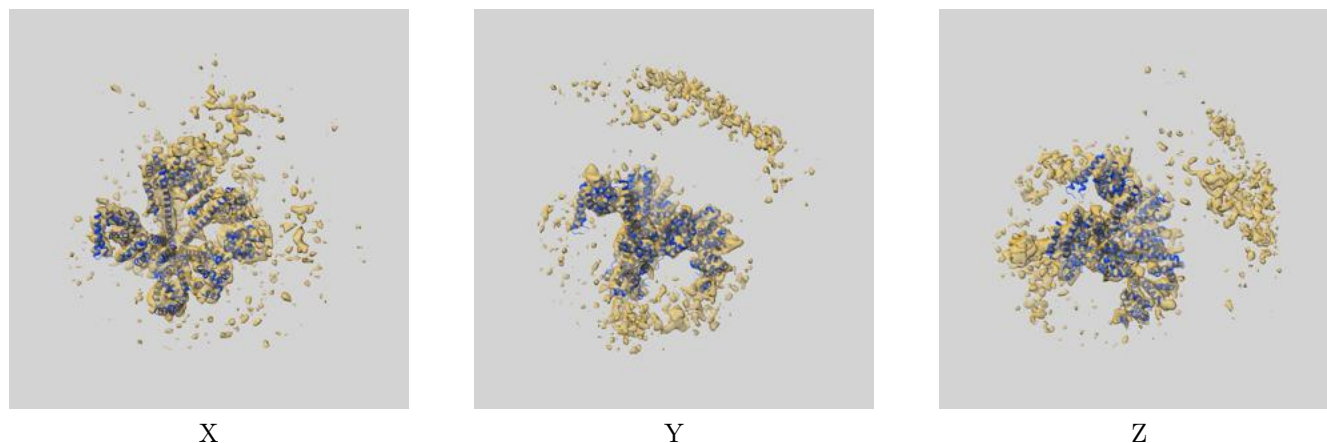
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.01	52.91	7.11

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

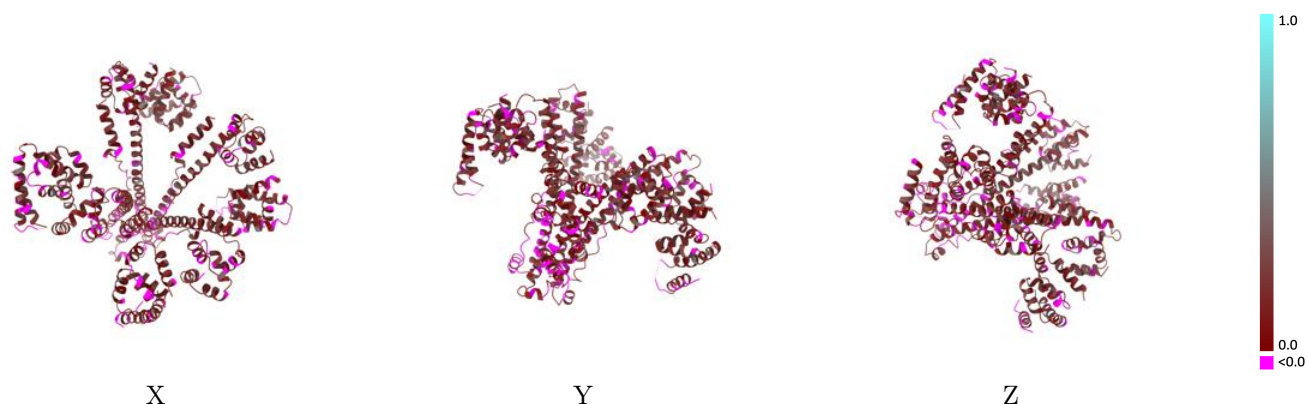
This section contains information regarding the fit between EMDB map EMD-61456 and PDB model 9KYX. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



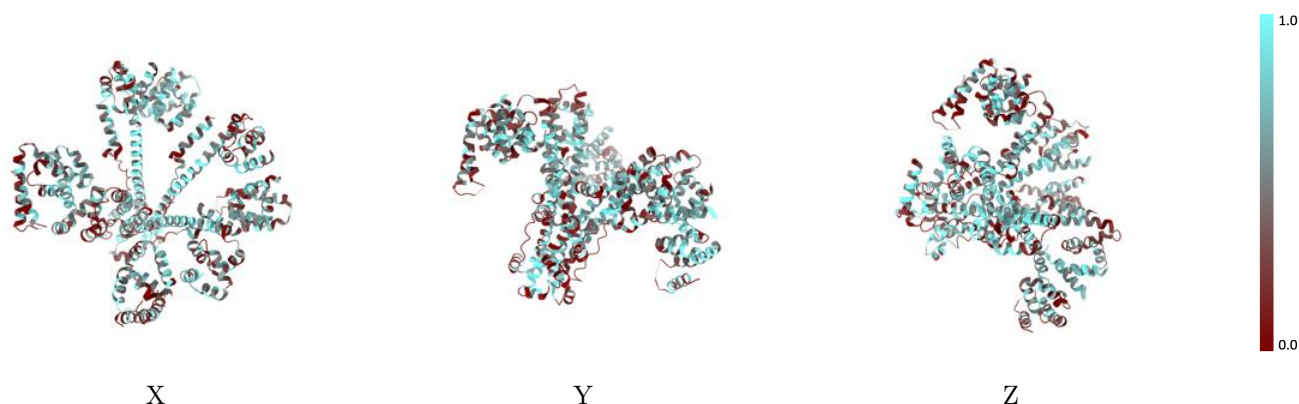
The images above show the 3D surface view of the map at the recommended contour level 3.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



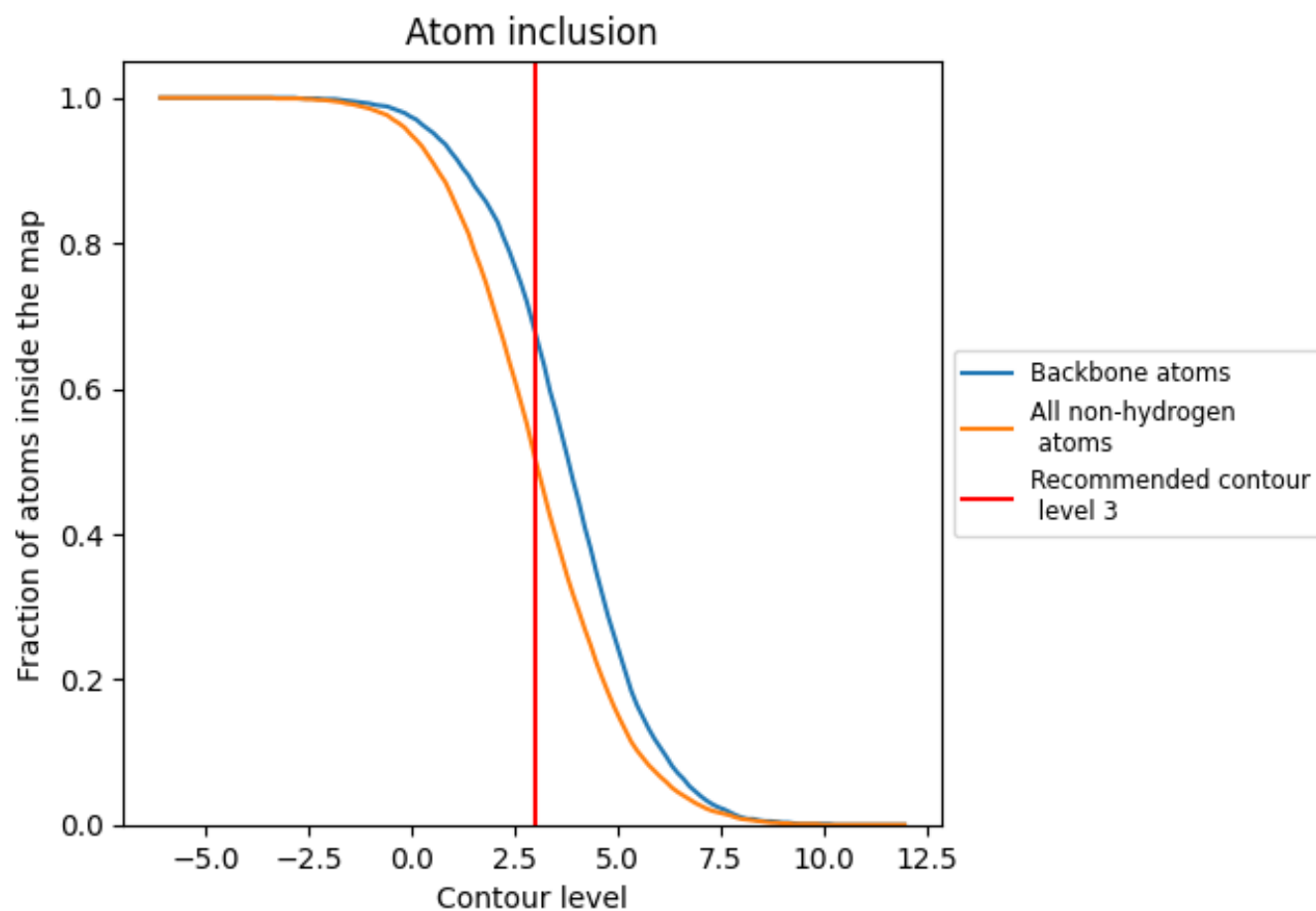
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 68% of all backbone atoms, 50% 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 (3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.5020	<div></div> 0.1290
A	<div></div> 0.5110	<div></div> 0.1470
B	<div></div> 0.4530	<div></div> 0.1430
C	<div></div> 0.5220	<div></div> 0.1150
D	<div></div> 0.4910	<div></div> 0.1240
E	<div></div> 0.5350	<div></div> 0.1300
F	<div></div> 0.4550	<div></div> 0.1240
G	<div></div> 0.4200	<div></div> 0.0890
H	<div></div> 0.6010	<div></div> 0.1560

1.0

0.0

<0.0