



wwPDB EM Validation Summary Report ⓘ

Mar 14, 2026 – 06:24 AM UTC

PDB ID : 6SZ9 / pdb_00006sz9
EMDB ID : EMD-10350
Title : Type IV Coupling Complex (T4CC) from *L. pneumophila*.
Authors : Mace, K.; Meir, A.; Lukyanova, N.; Waksman, G.
Deposited on : 2019-10-02
Resolution : 3.70 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:

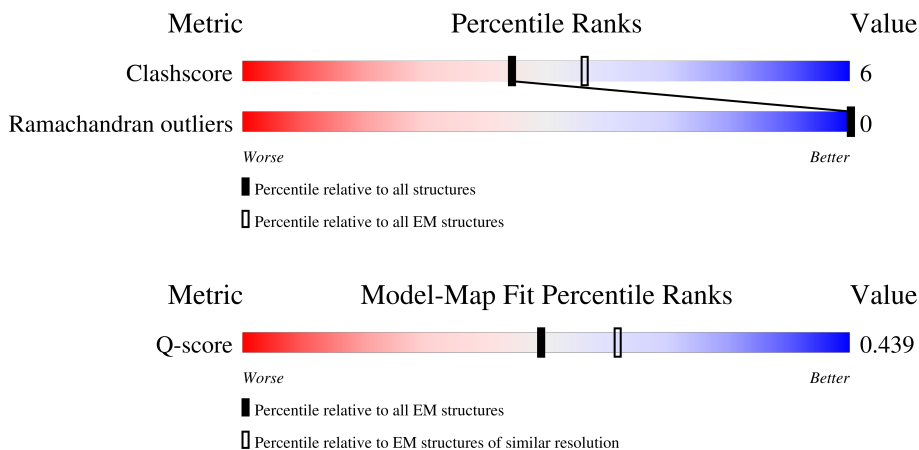
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 3.70 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Q-score	-	25397	11569 (3.20 - 4.20)

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	783	
2	B	380	
3	C	208	
4	D	294	
5	E	230	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10233 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 IcmO (DotL).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	473	Total	C	N	O	S	0	0
			3665	2345	619	684	17		

- Molecule 2 is a protein called IcmP (DotM).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	259	Total	C	N	O	S	0	0
			2085	1326	367	377	15		

- Molecule 3 is a protein called IcmJ (DotN).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	202	Total	C	N	O	S	0	0
			1615	1024	277	304	10		

- Molecule 4 is a protein called DotZ.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	283	Total	C	N	O	S	0	0
			2284	1452	389	441	2		

- Molecule 5 is a protein called DotY.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	73	Total	C	N	O	S	0	0
			583	373	96	110	4		

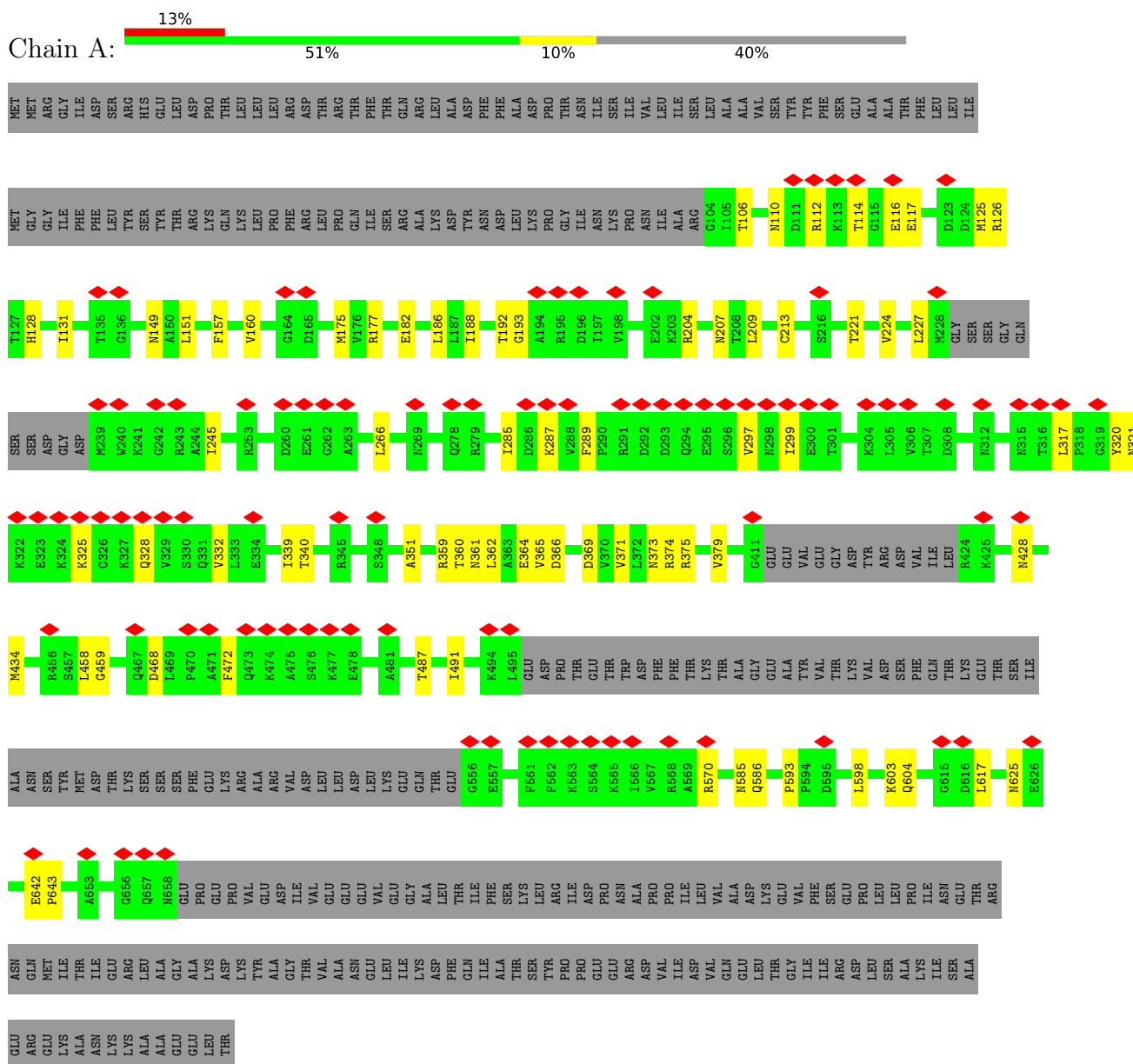
- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
6	C	1	Total 1	Zn 1	0

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: IcmO (DotL)



• Molecule 2: IcmP (DotM)



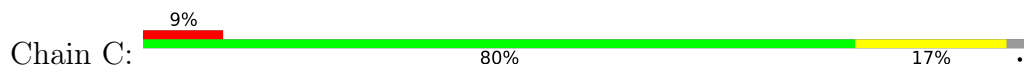
MET
TYR
ILE
GLU
MET
ALA
GLN
GLN
GLN
GLN
SER
GLY
SER
ASP
ASN
SER
MET
ALA
PRO
VAL
TRP
ILE
VAL
GLN
LEU
PHE
PHE
ILE
THR
ALA
TYR
PHE
GLY
TRP
ALA
LEU
ALA
HIS
GLN
TYR
ILE
VAL
SER
PHE
PHE
VAL
PHE
THR
ILE
ASN
ILE
TRP
GLN
ALA
SER
ARG
VAL
ASN
LEU
PHE

LEU
ASN
ASN
GLN
LEU
LEU
ALA
ASN
GLN
TYR
ILE
TYR
MET
GLN
THR
LEU
ASP
PRO
ASN
THR
VAL
TRP
ASP
GLN
MET
VAL
THR
VAL
MET
ARG
TYR
PRO
VAL
ILE
ILE
CYS
ILE
LEU
VAL
VAL
VAL
LEU
ALA
PHE
VAL
LEU
TYR
ASN
SER
ASN
VAL
THR
ASN
LEU
PHE

TYR
R122
K123
T124
Y125
K128
R131
Y145
K146
E147
D148
S151
K156
P158
W159
D183
M191
D199
A200
K201
R202
T205
D213
E216
L225
N234
D253
G254
K255
P256
D257
Y268
H281
I288
Y300
P301
P302
R314
L320

N321
T327
E342
K345
E346
R347
V351
I354
D355
A357
I358
R359
P372
R373
Q374
R375
E376
P380

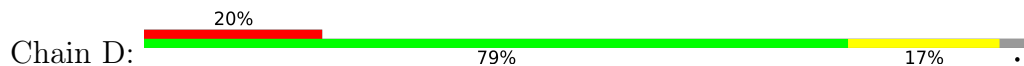
• Molecule 3: IcmJ (DotN)



MET
ALA
ASN
ASN
GLN
GLN
R7
L10
R20
R25
D28
E29
R30
F31
K32
S33
Y34
C46
Q47
F48
C49
G50
L55
D58
D63
G64
D65
N68
N69
R70
V75
I76
A77
C78
C79
F85
S89
Q108
M124
Y128
R137
S138
R142

S143
Q144
I145
I146
E147
G151
E152
Q162
L163
D166
N170
S171
E172
E173
I174
L178
L184
F191
R192
K193
W196
L203
D208

• Molecule 4: DotZ



MET
ASP
GLU
ILE
LYS
ASP
ASP
LEU
S11
Q12
W13
L14
T21
R24
R28
S32
L33
P34
Q35
D36
E37
E40
A41
Y49
Q54
I55
P56
L57
K58
N59
A76
L80
I81
D82
E88
S89
S90
K91
E92
P93
D94
Q96
G97
R101
E102

D106
L111
D126
N127
L128
K146
L147
E148
L151
S152
N155
S156
L157
Y158
K159
N160
N162
S163
K164
I165
K166
K167
N168
A169
K172
K176
A177
F178
I179
H180
C181
D182
K185
D186
Q187
K190
N191
Q194
K198
Q201
T202
L203
A204
V205
S206
V207

E210
L211
K212
I215
L216
T217
N218
L219
E227
T237
D238
R239
T240
N241
R251
V257
I258
I262
I265
P269
K272
I273
D274
Q277
D278
A279
I280
N281
R282
Y286
R289
E293
ARG

• Molecule 5: DotY



MET
PRO
TYR
LYS
T5
D10
L113
R32
F33
E34
L37
T38
K41
L42
L43
P44
P45
N47
D48
E51
K52
I53
K54
E55
Q58
F59
Y60
K61
F62
K63
L64
L65
S66
S67
A68
Q69
Q74
E75
R76
F77
THR
SER
ASP
TYR
GLN
ASN
THR
GLN
GLU
ASN
LYS

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

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

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	219593	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 ($e^-/\text{\AA}^2$)	54	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	42.540	Depositor
Minimum map value	-29.188	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.841	Depositor
Recommended contour level	7	Depositor
Map size (Å)	313.5, 313.5, 313.5	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.045, 1.045, 1.045	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.20	0/3727	0.48	0/5031
2	B	0.22	0/2132	0.47	0/2883
3	C	0.28	0/1646	0.50	0/2213
4	D	0.23	0/2318	0.52	0/3131
5	E	0.16	0/592	0.40	0/796
All	All	0.22	0/10415	0.48	0/14054

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	3665	0	3720	48	0
2	B	2085	0	2098	22	0
3	C	1615	0	1578	38	0
4	D	2284	0	2327	34	0
5	E	583	0	599	6	0
6	C	1	0	0	0	0
All	All	10233	0	10322	132	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 6.

The worst 5 of 132 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)
3:C:10:LEU:HG	3:C:48:PHE:HD2	1.52	0.74
3:C:79:CYS:SG	3:C:191:PHE:CE1	2.86	0.68
1:A:126:ARG:HE	1:A:459:GLY:HA2	1.61	0.64
3:C:10:LEU:HG	3:C:48:PHE:CD2	2.32	0.64
3:C:48:PHE:CZ	3:C:85:PHE:CE2	2.87	0.61

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	465/783 (59%)	448 (96%)	17 (4%)	0	100	100
2	B	257/380 (68%)	251 (98%)	6 (2%)	0	100	100
3	C	200/208 (96%)	194 (97%)	6 (3%)	0	100	100
4	D	281/294 (96%)	271 (96%)	10 (4%)	0	100	100
5	E	71/230 (31%)	69 (97%)	2 (3%)	0	100	100
All	All	1274/1895 (67%)	1233 (97%)	41 (3%)	0	100	100

There are no Ramachandran outliers to report.

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

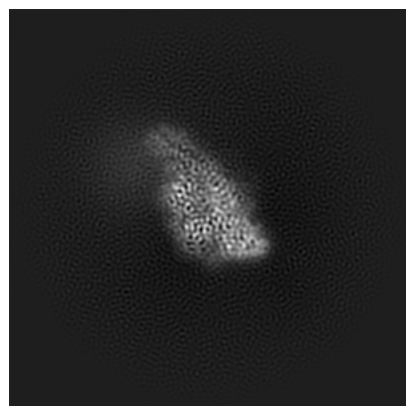
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10350. These allow visual inspection of the internal detail of the map and identification of artifacts.

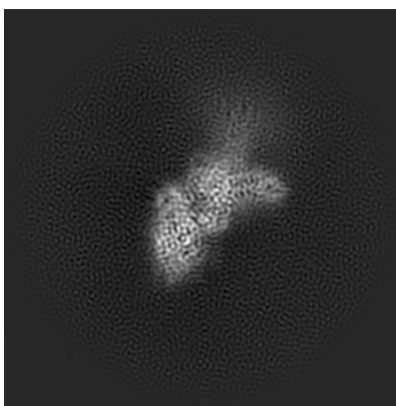
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

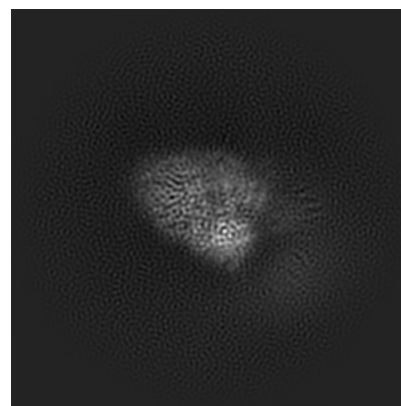
6.1.1 Primary map



X

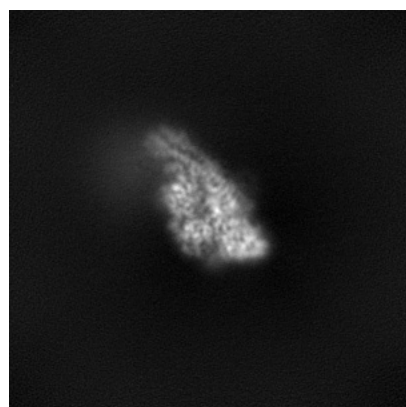


Y

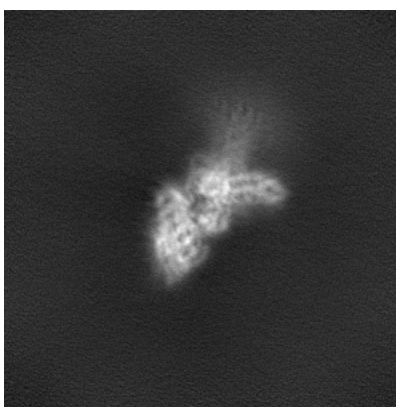


Z

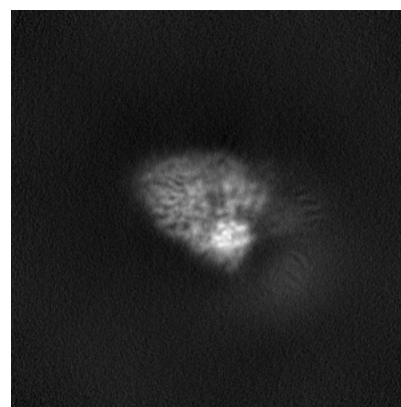
6.1.2 Raw map



X



Y

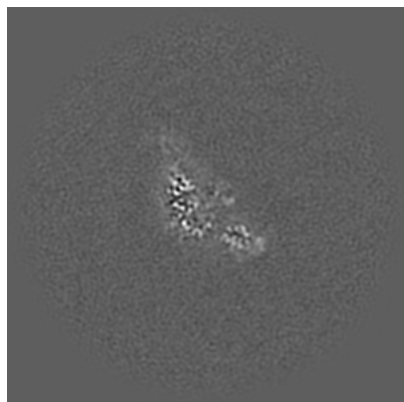


Z

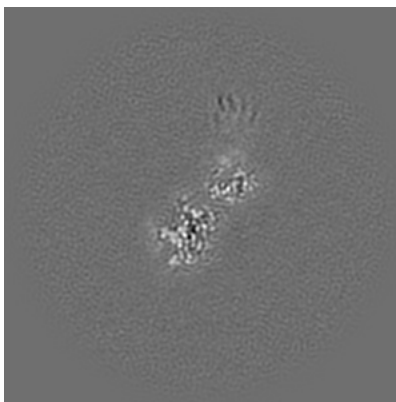
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

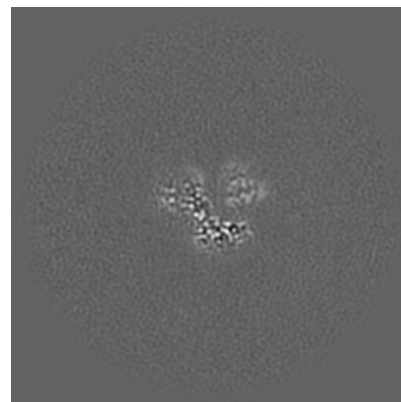
6.2.1 Primary map



X Index: 150



Y Index: 150



Z Index: 150

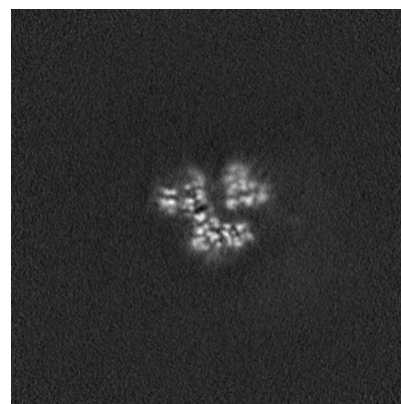
6.2.2 Raw map



X Index: 150



Y Index: 150

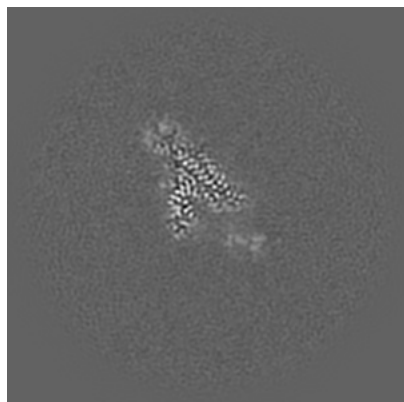


Z Index: 150

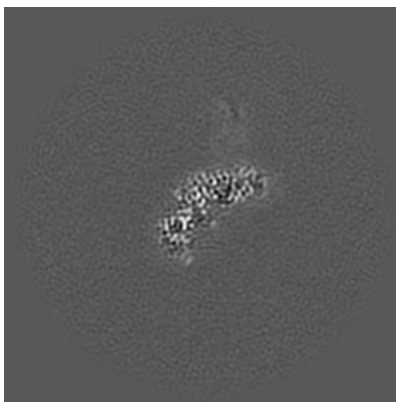
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

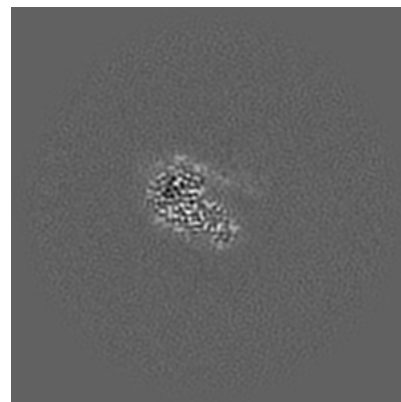
6.3.1 Primary map



X Index: 164

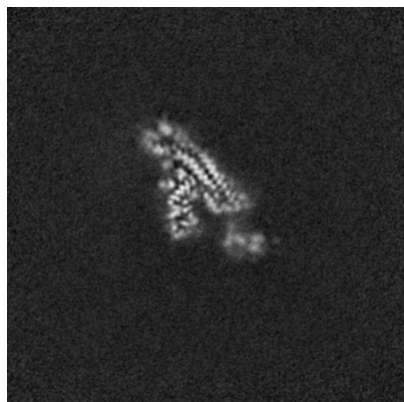


Y Index: 137

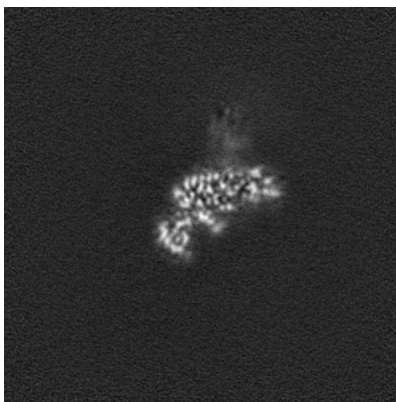


Z Index: 136

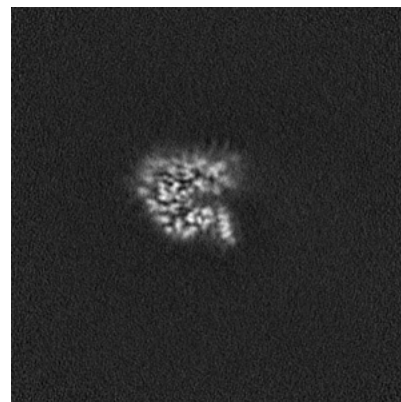
6.3.2 Raw map



X Index: 164



Y Index: 133

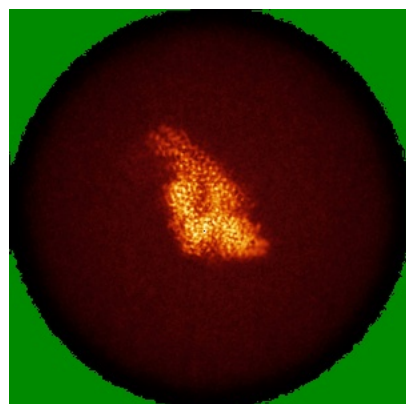


Z Index: 130

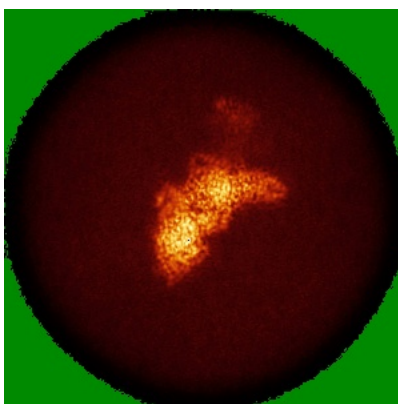
The images above show the largest variance slices of the map in three orthogonal directions.

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

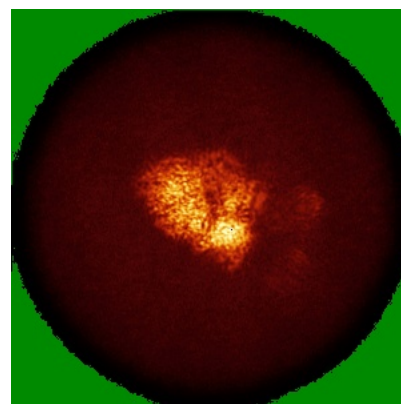
6.4.1 Primary map



X



Y

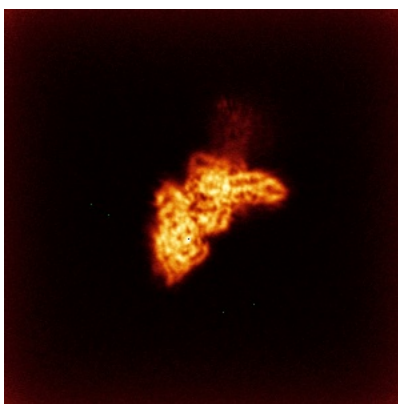


Z

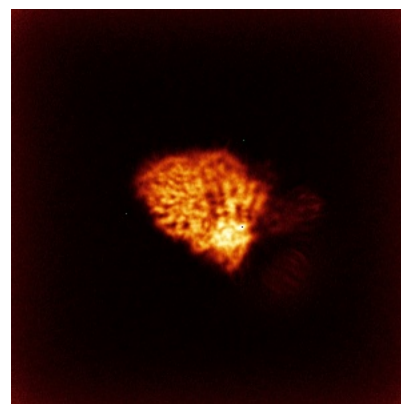
6.4.2 Raw map



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 7.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

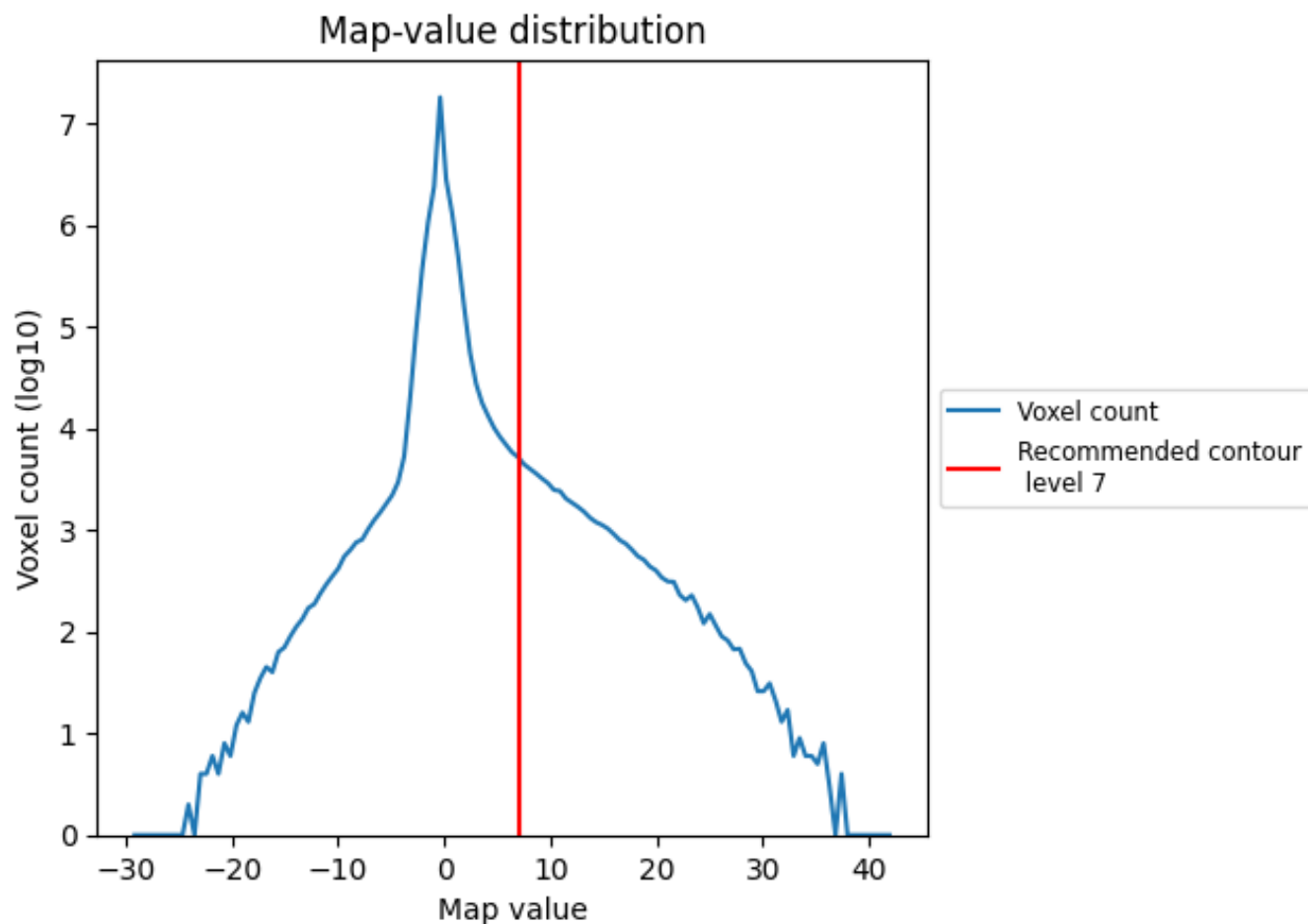
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

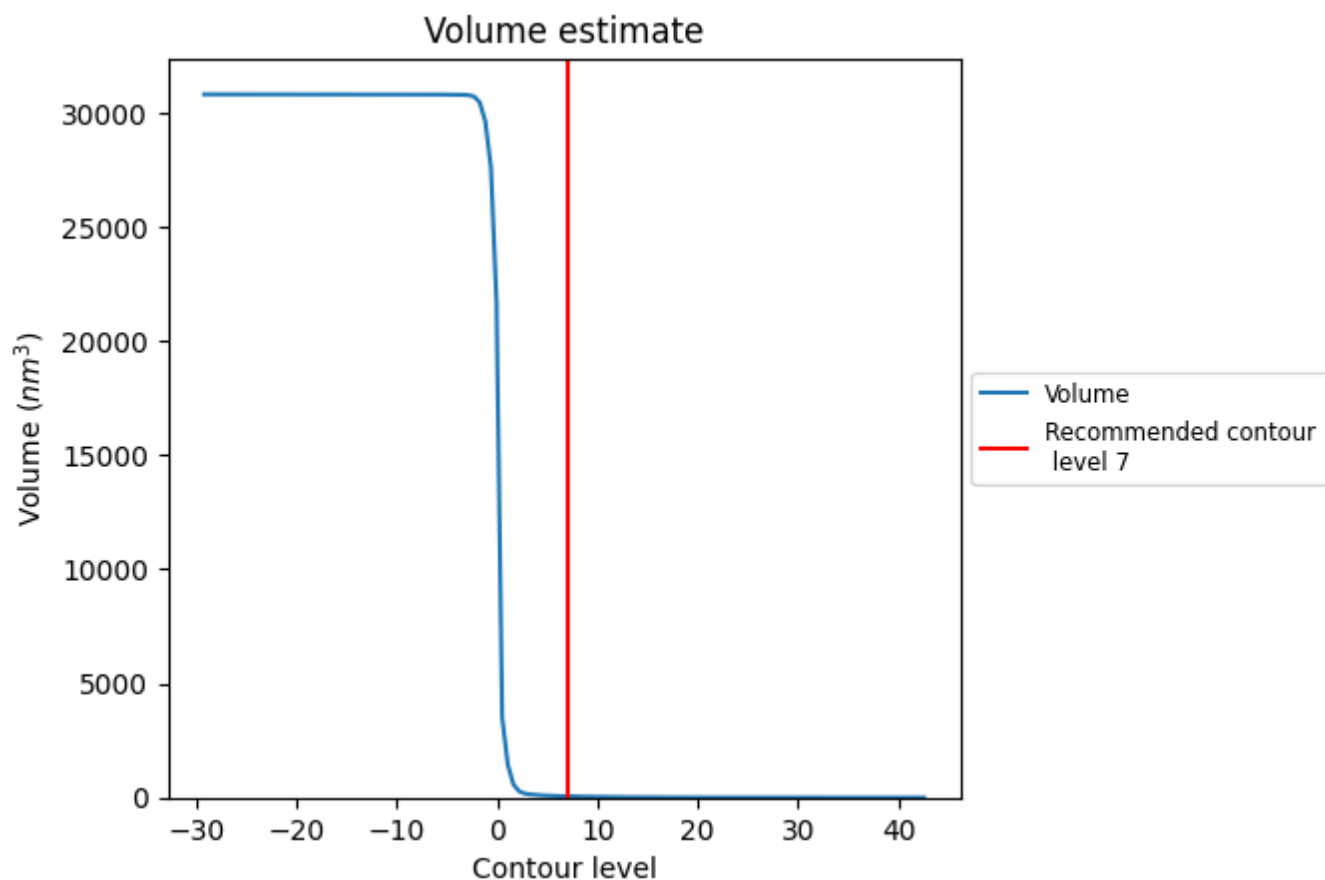
This section contains the results of statistical analysis of the map.

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.

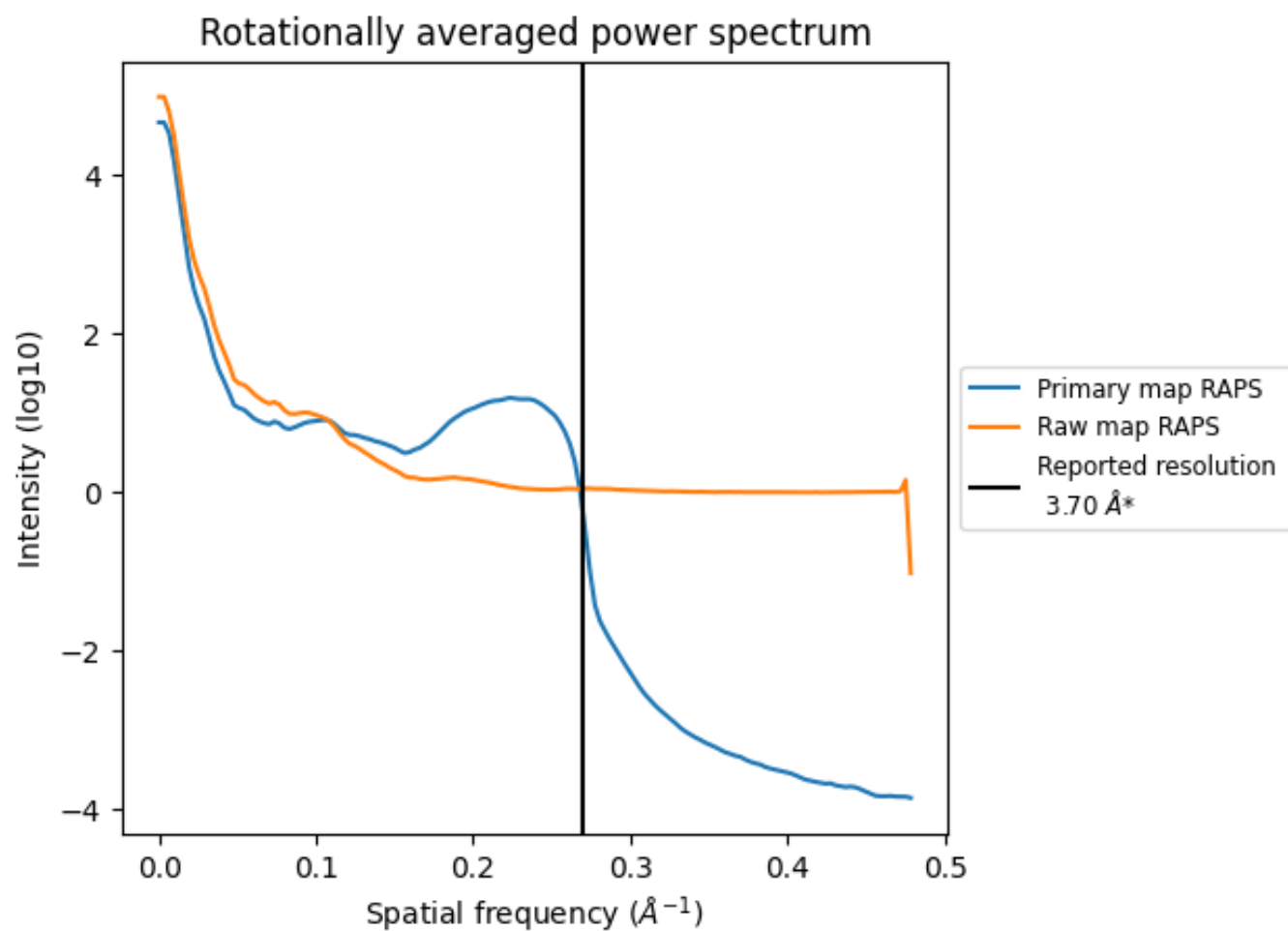
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 54 nm^3 ; this corresponds to an approximate mass of 49 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 ⓘ

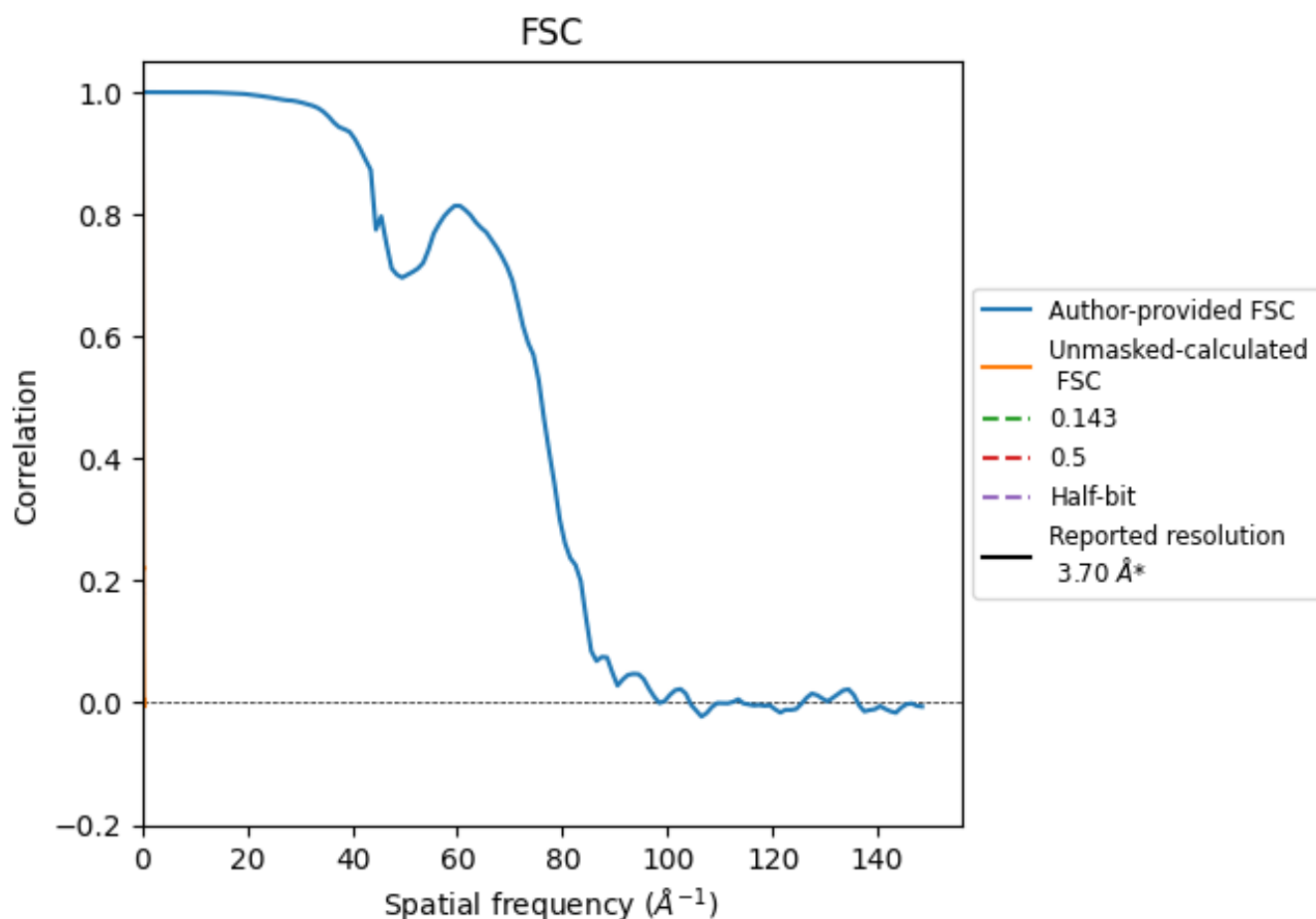


*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

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 0.270 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	0.01	0.01	0.01
Unmasked-calculated*	4.72	7.42	4.88

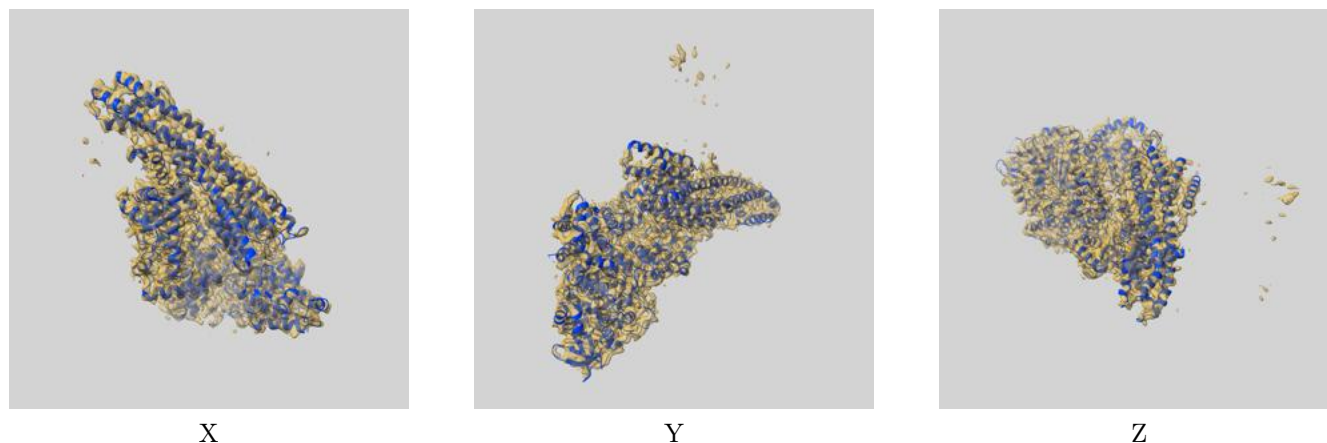
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 0.01 differs from the reported value 3.7 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.72 differs from the reported value 3.7 by more than 10 %

9 Map-model fit [i](#)

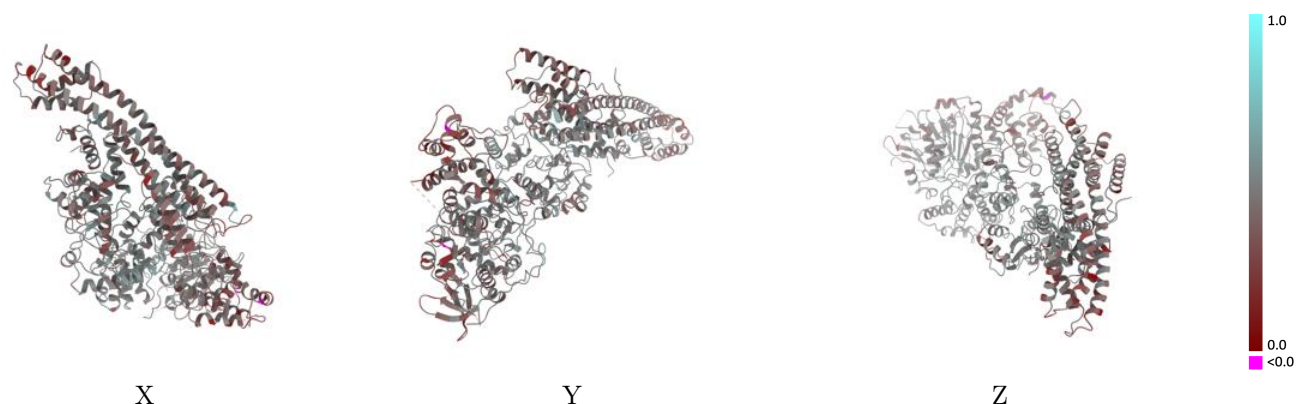
This section contains information regarding the fit between EMDB map EMD-10350 and PDB model 6SZ9. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay [i](#)



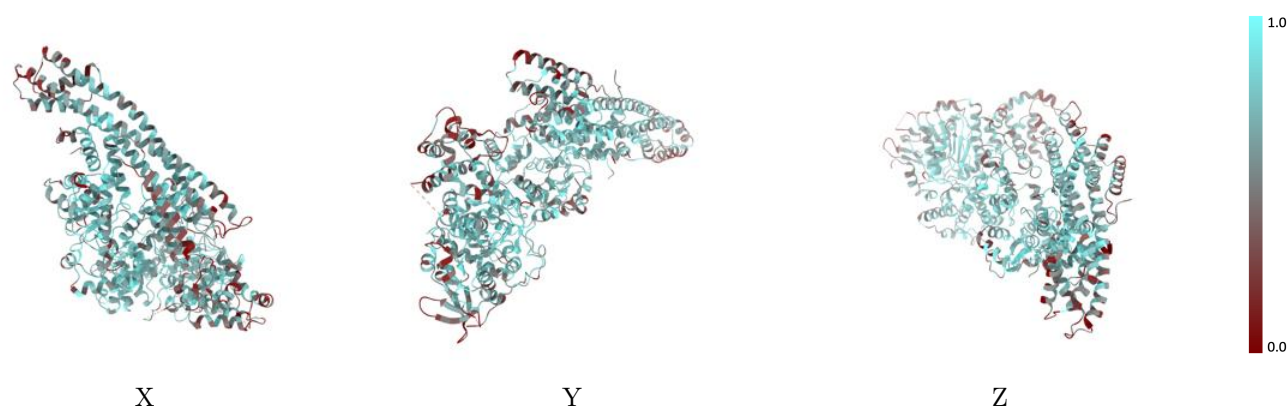
The images above show the 3D surface view of the map at the recommended contour level 7.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



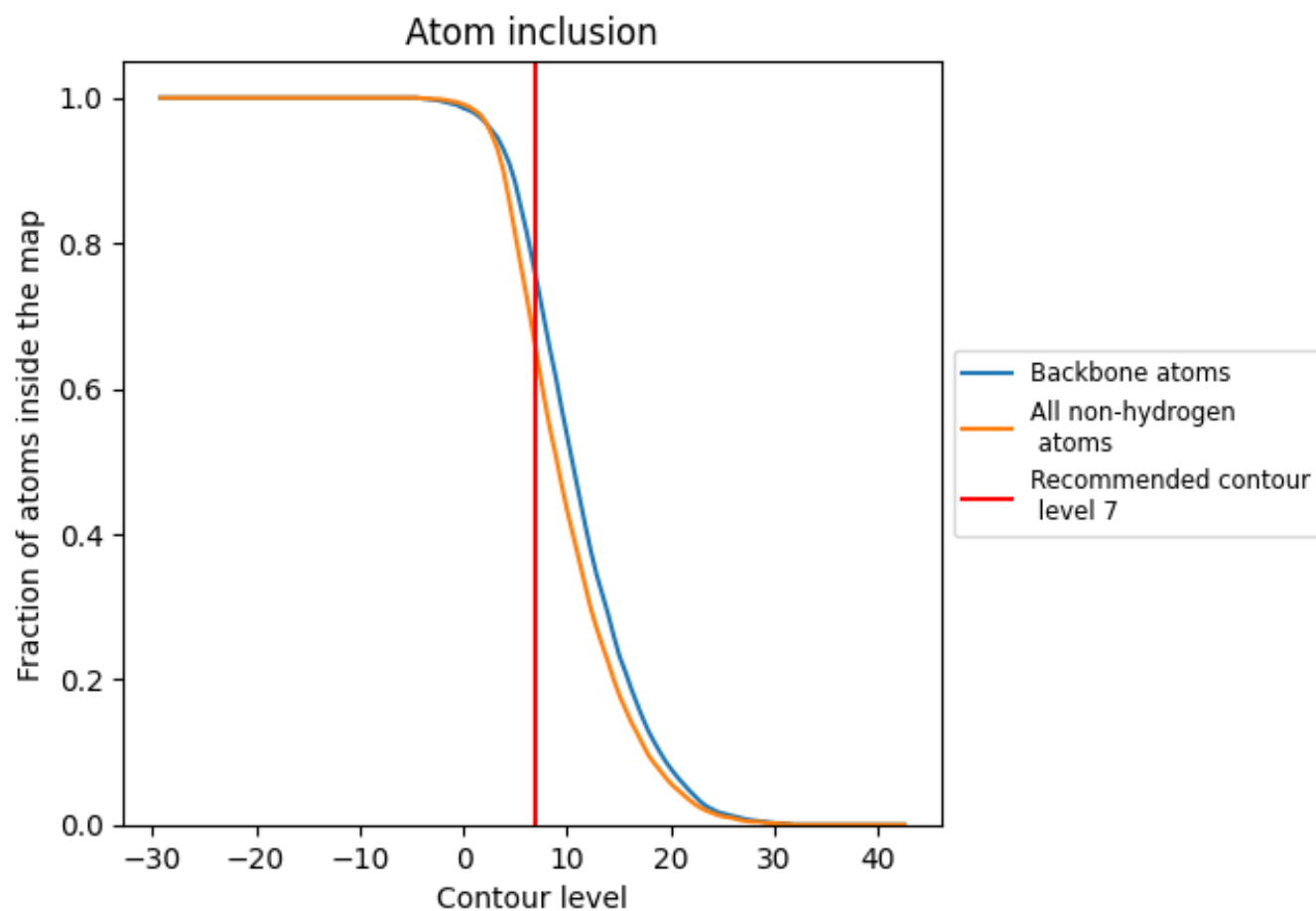
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (7).

9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 65% 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 (7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6520	0.4390
A	0.6200	0.4220
B	0.7300	0.4770
C	0.7410	0.4690
D	0.6070	0.4190
E	0.5140	0.4020

