



wwPDB EM Validation Summary Report ⓘ

Dec 7, 2024 – 12:36 PM EST

PDB ID : 8VDG
EMDB ID : EMD-43149
Title : Cryo-EM structure of human monoclonal antibody C74 targeting IT4VAR22
CIDRa1.7
Authors : Raghavan, S.S.R.; Ward, A.B.
Deposited on : 2023-12-15
Resolution : 3.35 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.dev113
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) : 2.40

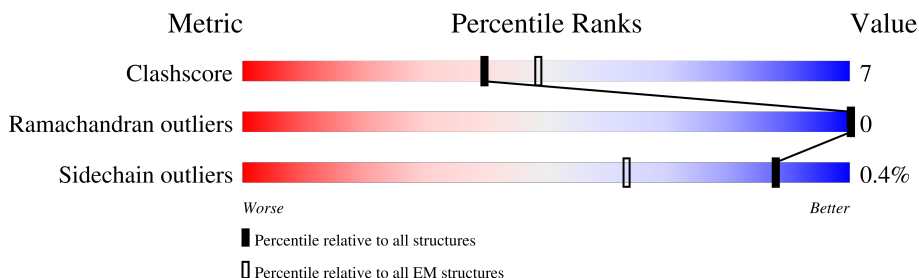
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.35 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	1153	 7% 92%
2	H	121	 80% 18%
3	K	113	 11% 78% 19%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2583 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 Erythrocyte membrane protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	93	Total	C	N	O	S	0	0
			811	533	127	143	8		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	109	GLN	ARG	conflict	UNP A3R6S4
A	329	GLU	GLY	conflict	UNP A3R6S4

- Molecule 2 is a protein called C74 Fab heavy chain.


Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	119	Total	C	N	O	S	0	0
			931	592	157	178	4		

- Molecule 3 is a protein called C74 Fab kappa chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	K	111	Total	C	N	O	S	0	0
			841	528	143	168	2		

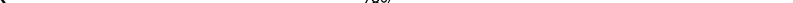
ASP	CYS	LYS	GLU	TRP	PRO	MET	TYR	ARG
ASN	LYS	CYS	TYR	TYR	LYS	CYS	LYS	LEU
ALA	TYR	GLN	GLY	GLN	GLN	ALA	PHE	HIS
ASN	GLU	GLN	GLN	GLN	ARG	ARG	LEU	GLN
PHE	LEU	SER	ARG	SER	SER	TYR	THR	LEU
ILE	TYR	ARG	ASP	ASP	ASP	PHE	ILE	GLU
CYS	ARG	GLY	LEU	LEU	TRP	ASP	ASP	ASP
GLU	LYS	TYR	TYR	GLY	GLU	ALA	SER	GLY
LYS	ALA	THR	GLU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

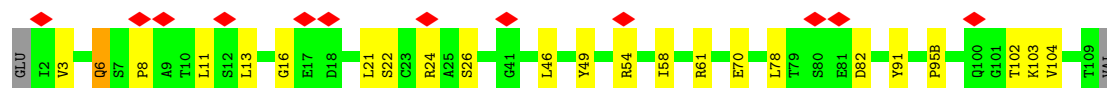
- Molecule 2: C74 Fab heavy chain

Chain H: 



- Molecule 3: C74 Fab kappa chain

Chain K:  11% 78% 19%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	207289	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	51	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.323	Depositor
Minimum map value	-1.049	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.23	Depositor
Map size (\AA)	261.0, 261.0, 261.0	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.725, 0.725, 0.725	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	0.28	0/826	0.43	0/1098
2	H	0.33	0/952	0.59	0/1290
3	K	0.41	0/861	0.62	0/1174
All	All	0.34	0/2639	0.55	0/3562

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	811	0	816	10	0
2	H	931	0	897	15	0
3	K	841	0	817	15	0
All	All	2583	0	2530	35	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 7.

The worst 5 of 35 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:K:13:LEU:HD12	3:K:104:VAL:HG13	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:666:LYS:HD3	2:H:100:LEU:HG	1.85	0.59
3:K:54:ARG:NH1	3:K:58:ILE:O	2.38	0.55
2:H:52(A):LYS:O	2:H:71:ARG:NH1	2.41	0.54
3:K:46:LEU:HD21	3:K:49:TYR:HB3	1.90	0.54

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	83/1153 (7%)	79 (95%)	4 (5%)	0	100	100
2	H	117/121 (97%)	110 (94%)	7 (6%)	0	100	100
3	K	109/113 (96%)	100 (92%)	9 (8%)	0	100	100
All	All	309/1387 (22%)	289 (94%)	20 (6%)	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	92/1030 (9%)	92 (100%)	0	100	100
2	H	99/101 (98%)	99 (100%)	0	100	100
3	K	93/95 (98%)	92 (99%)	1 (1%)	70	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	284/1226 (23%)	283 (100%)	1 (0%)	88	94

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	K	6	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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.

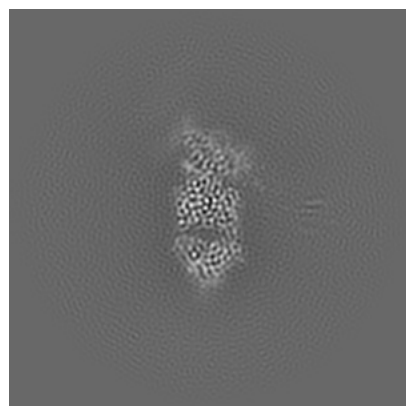
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-43149. These allow visual inspection of the internal detail of the map and identification of artifacts.

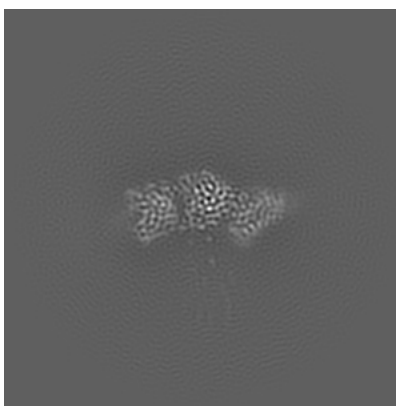
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

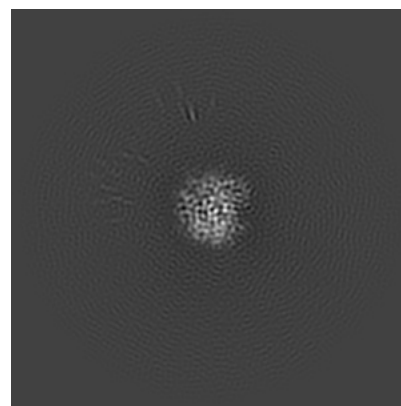
6.1.1 Primary map



X

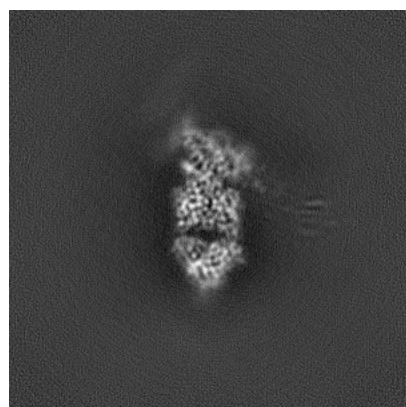


Y

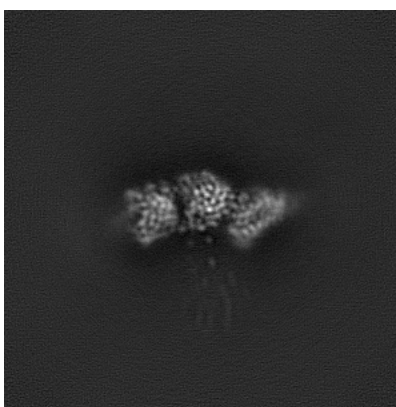


Z

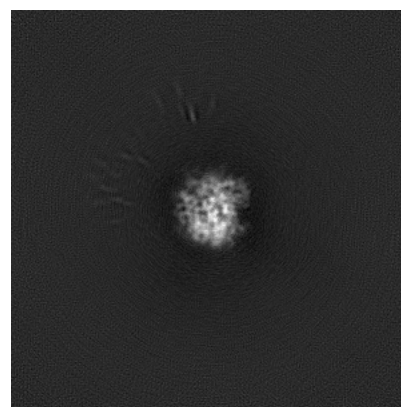
6.1.2 Raw map



X



Y

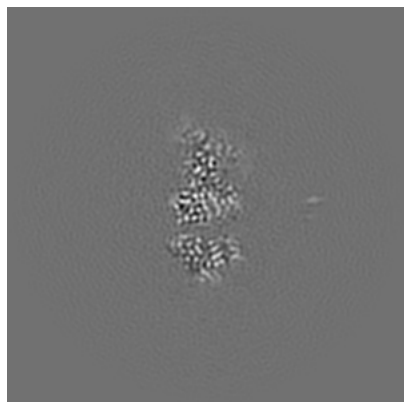


Z

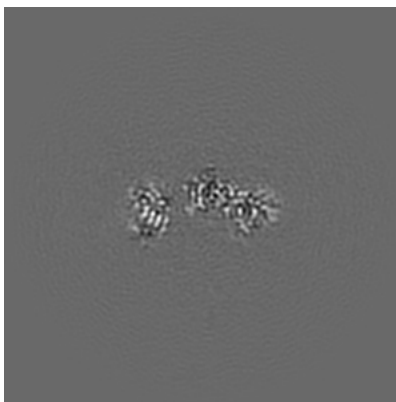
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

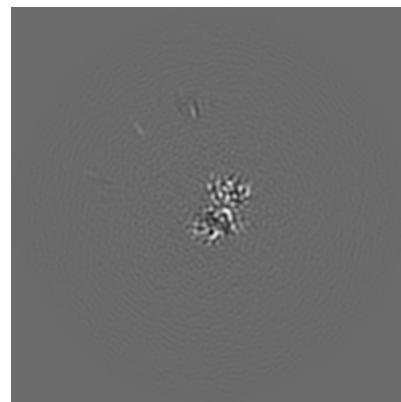
6.2.1 Primary map



X Index: 180

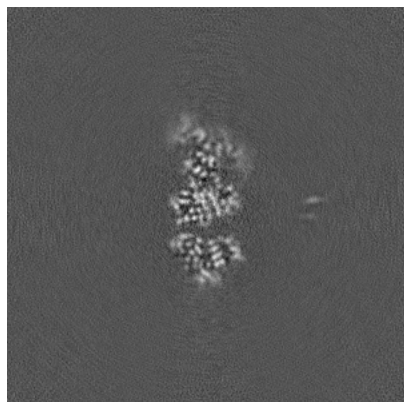


Y Index: 180

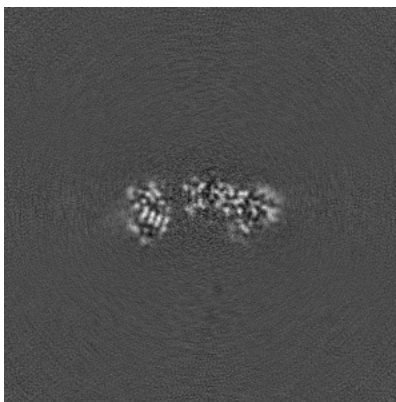


Z Index: 180

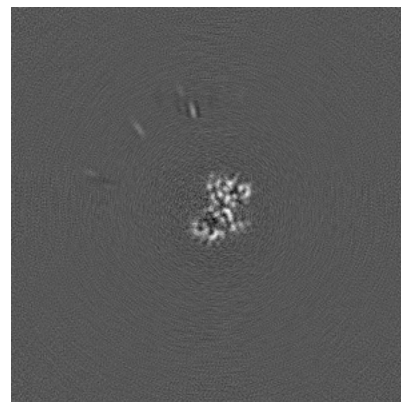
6.2.2 Raw map



X Index: 180



Y Index: 180

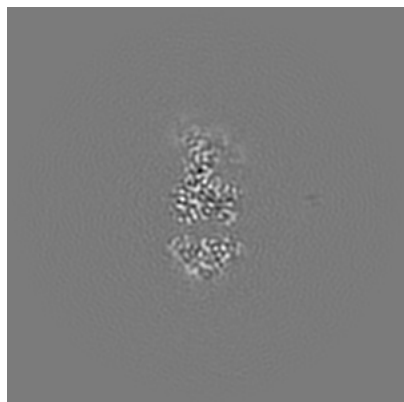


Z Index: 180

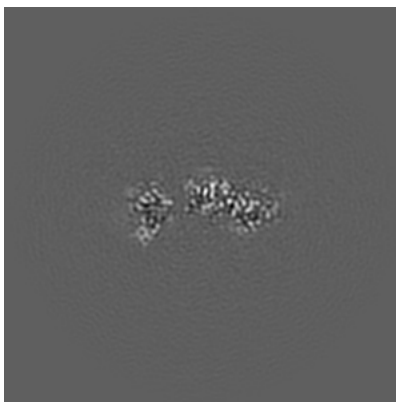
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

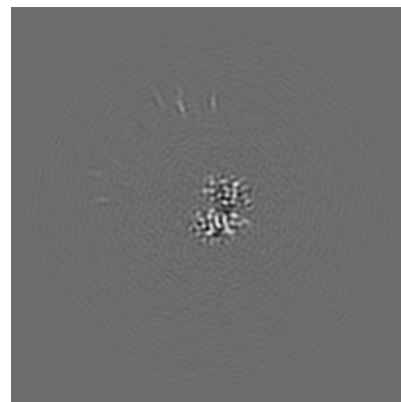
6.3.1 Primary map



X Index: 184

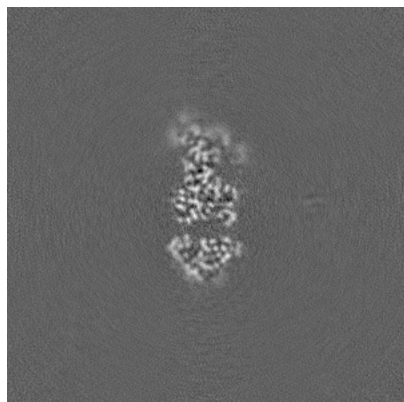


Y Index: 177

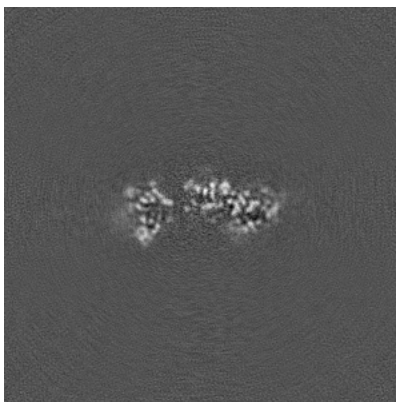


Z Index: 184

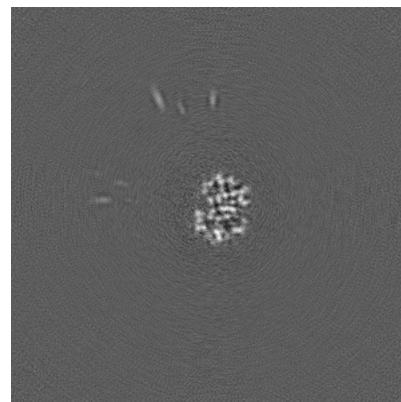
6.3.2 Raw map



X Index: 184



Y Index: 177

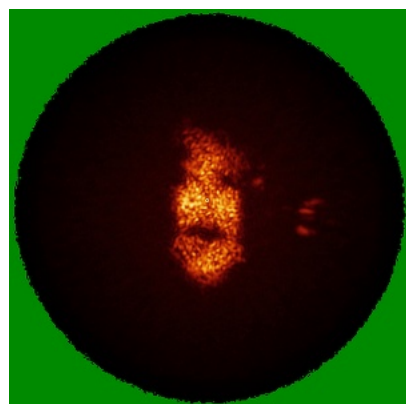


Z Index: 187

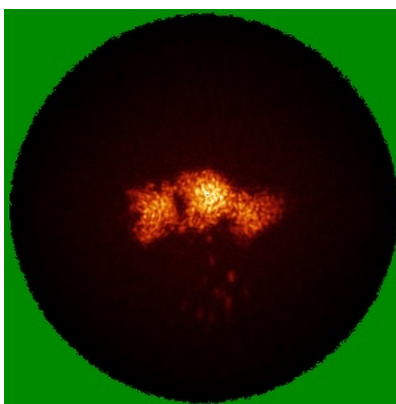
The images above show the largest variance slices of the map in three orthogonal directions.

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

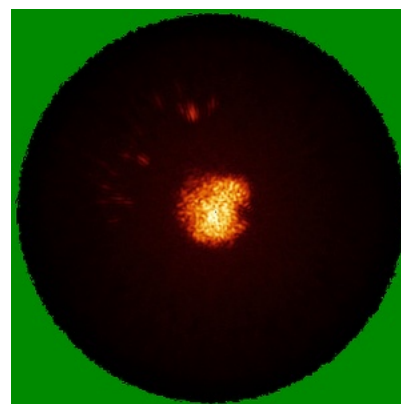
6.4.1 Primary map



X

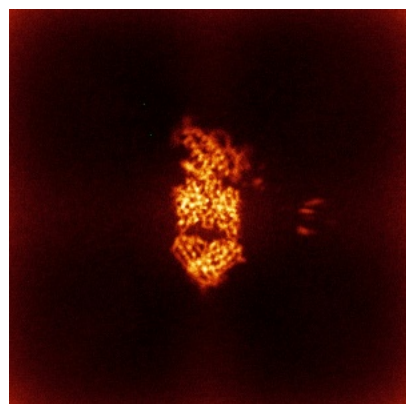


Y

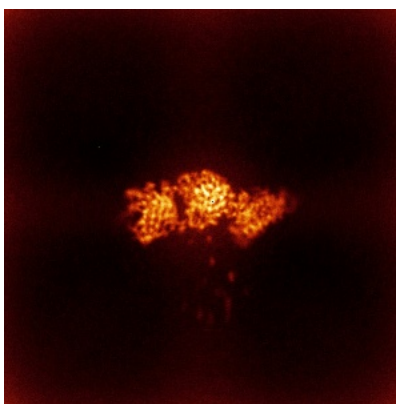


Z

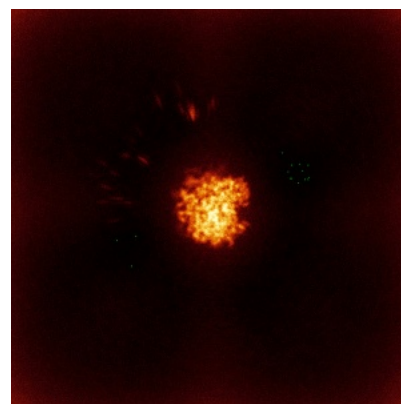
6.4.2 Raw map



X



Y

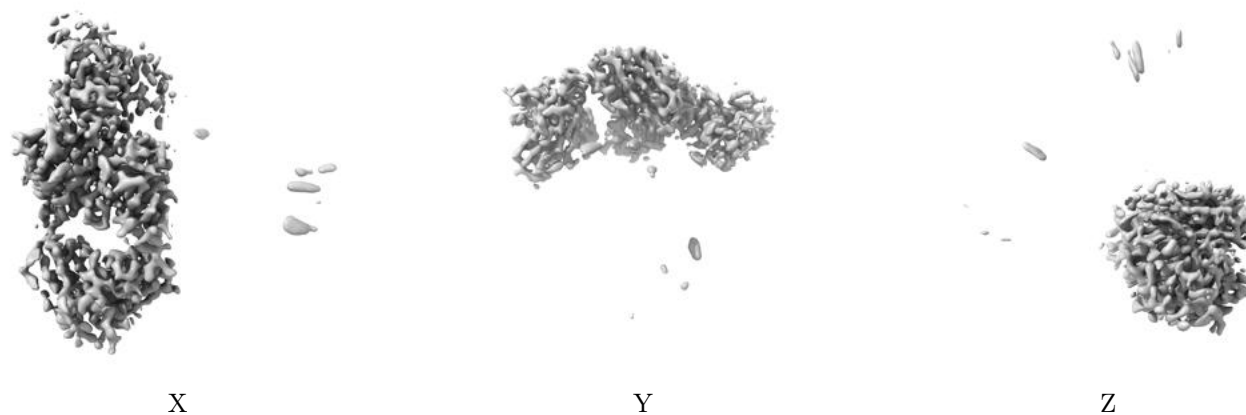


Z

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.

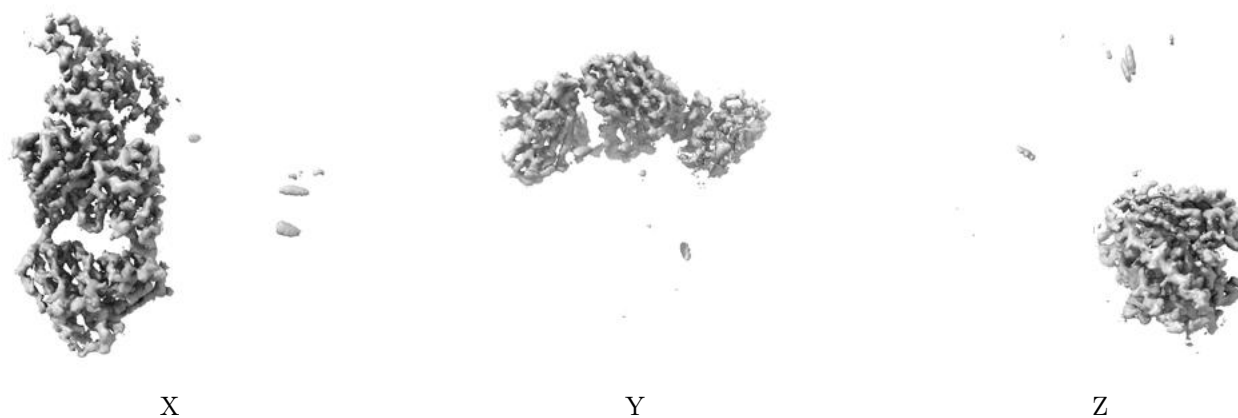
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.23. 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.

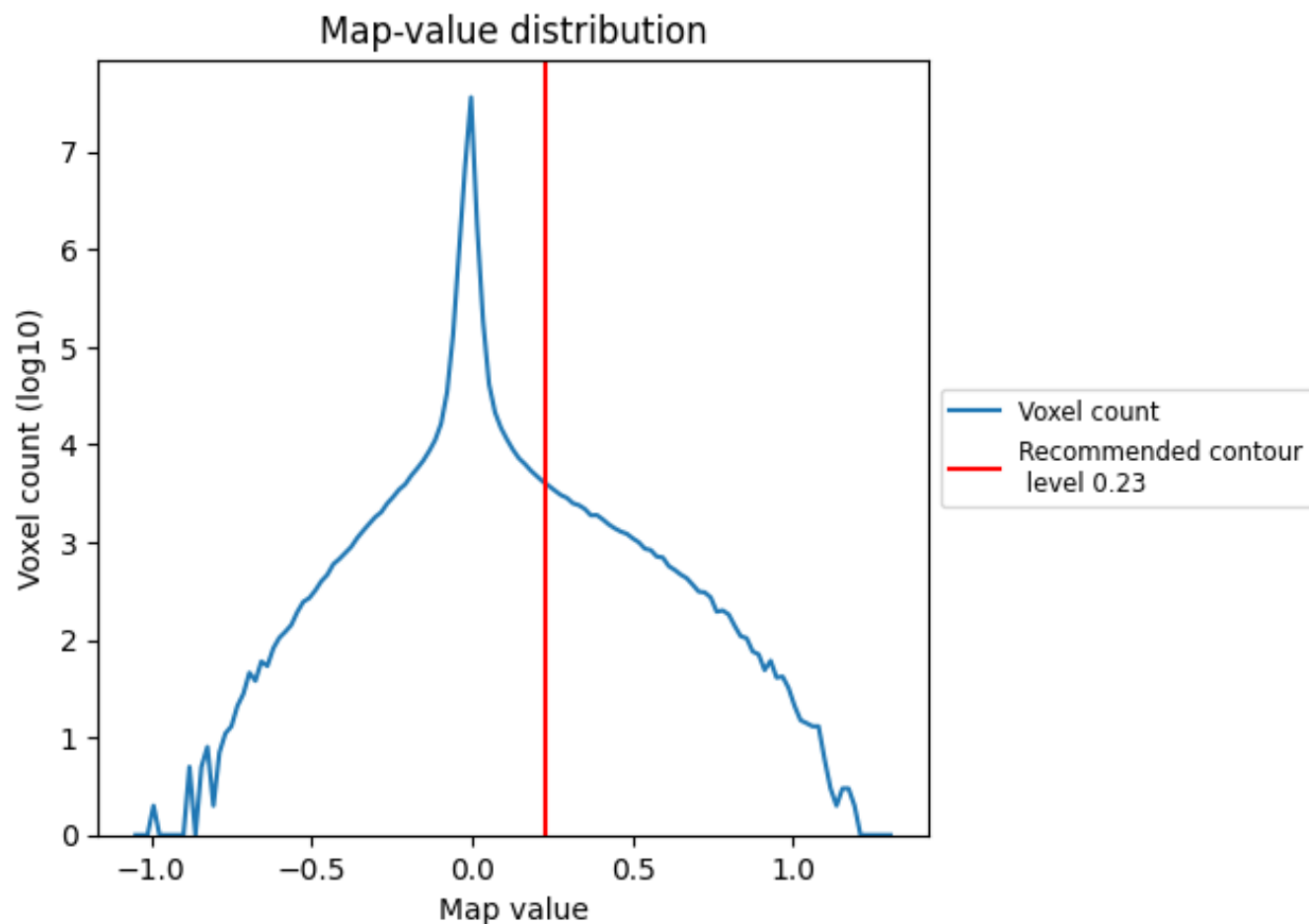
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

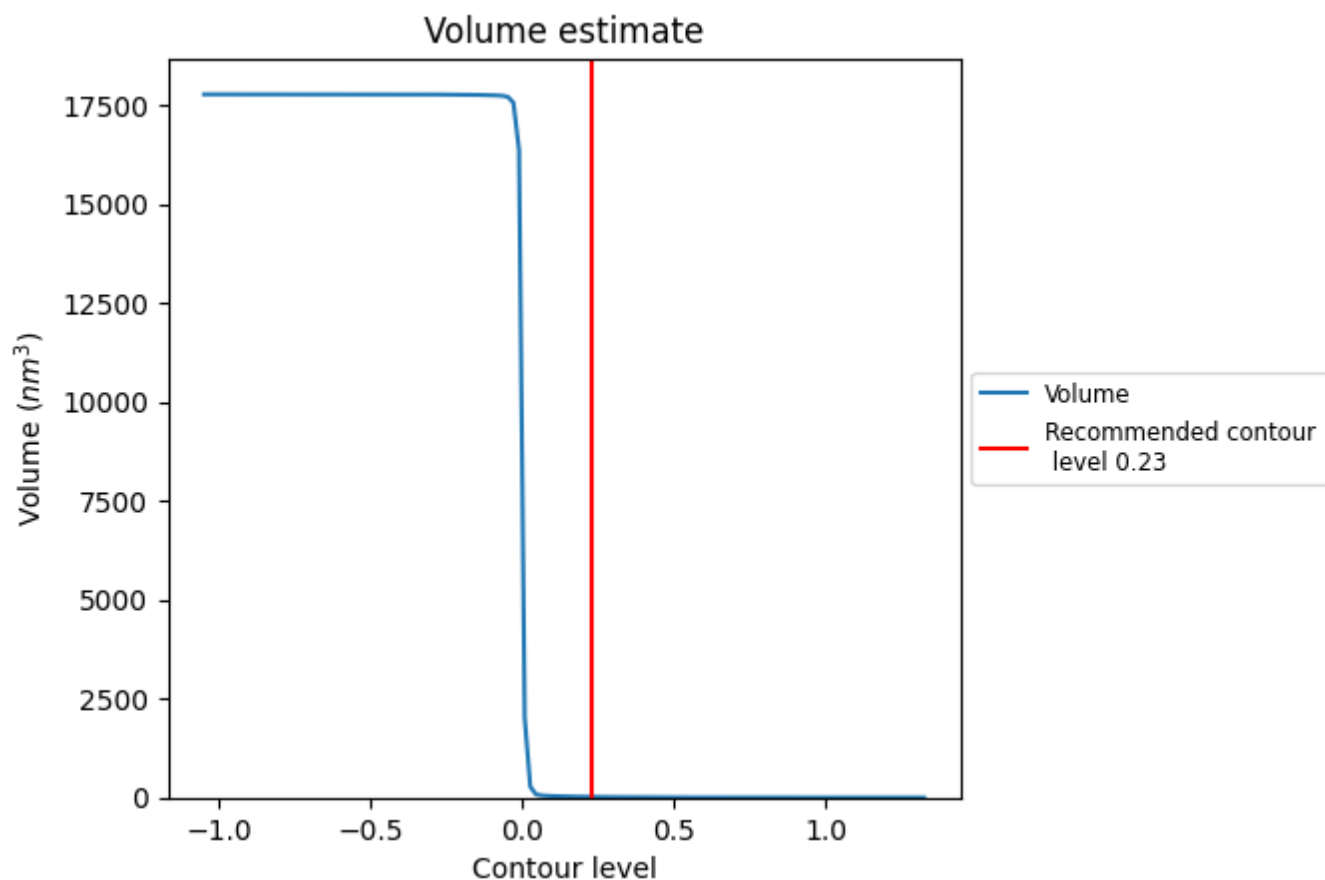
This section contains the results of statistical analysis of the map.

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.

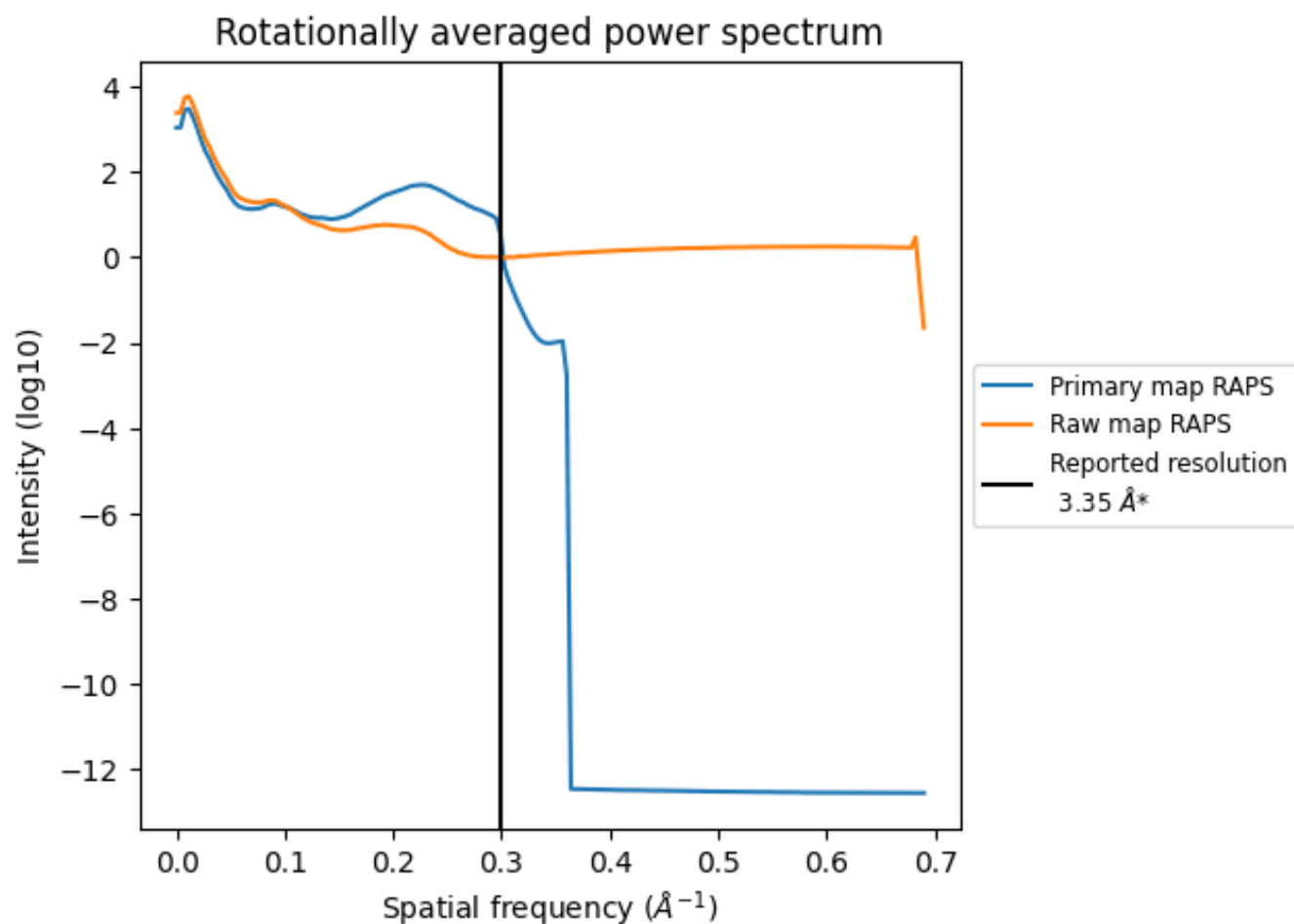
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 16 nm³; this corresponds to an approximate mass of 15 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 ⓘ

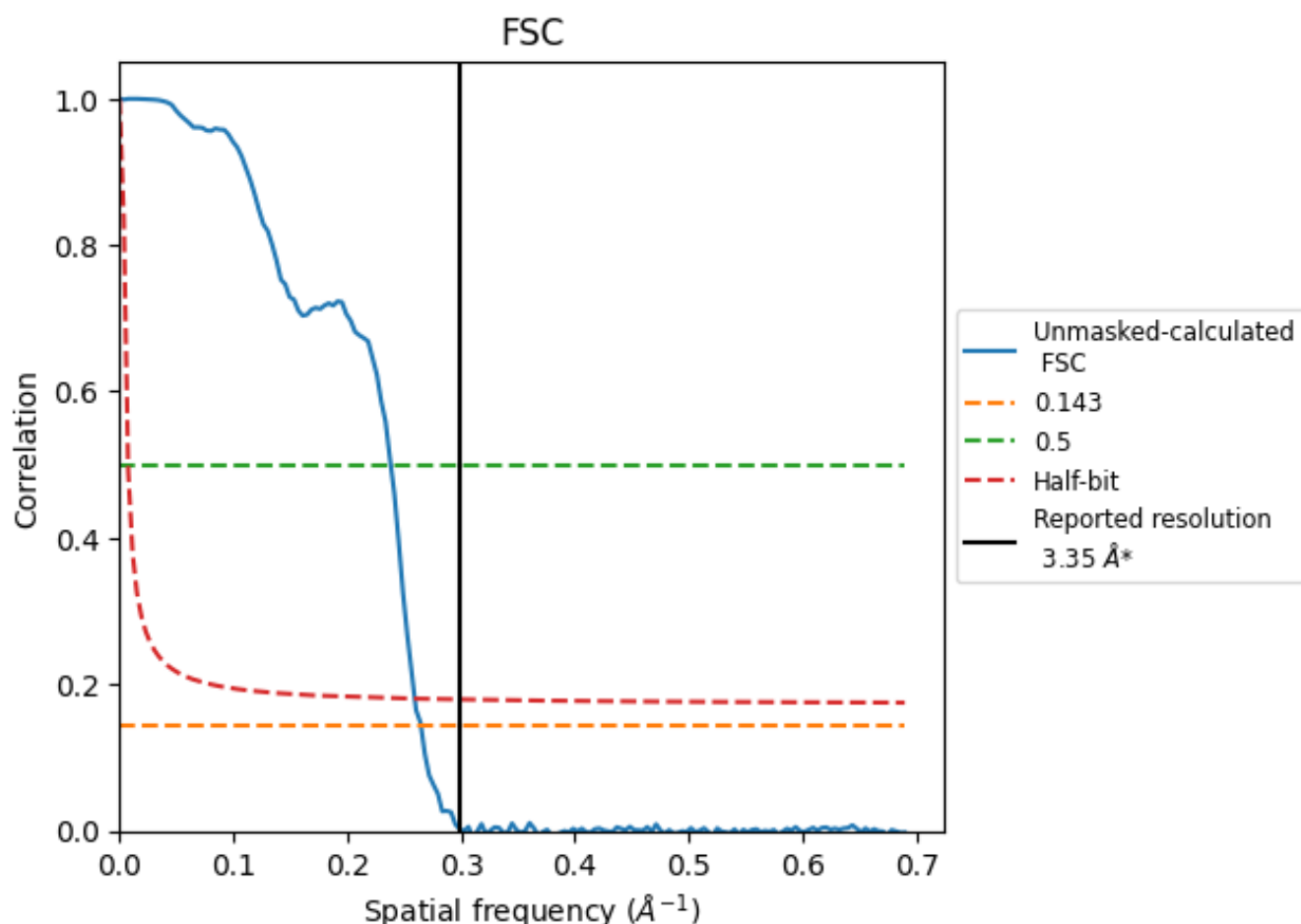


*Reported resolution corresponds to spatial frequency of 0.299 Å⁻¹

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 0.299 Å⁻¹

8.2 Resolution estimates [i](#)

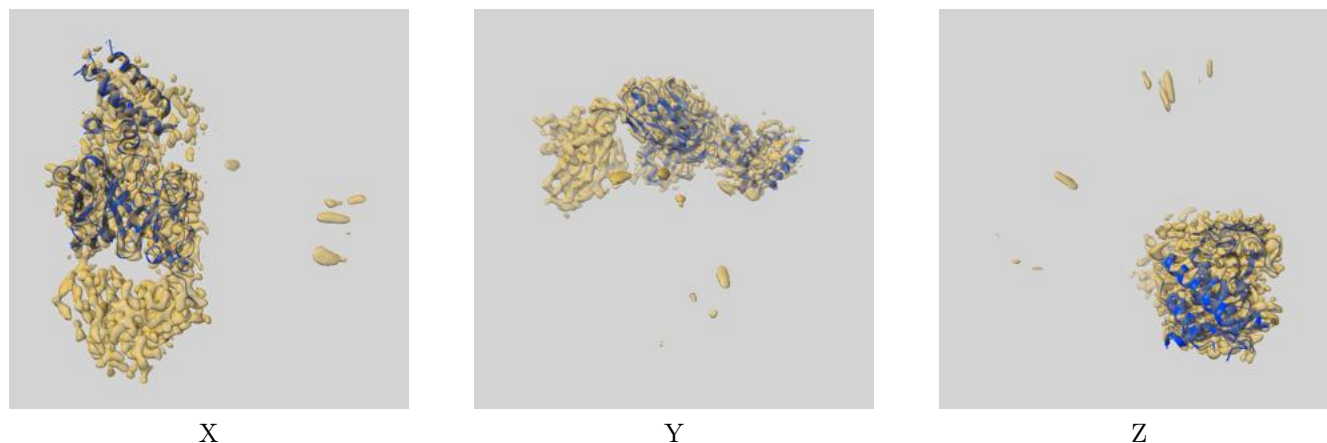
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.35	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.78	4.20	3.86

*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 3.78 differs from the reported value 3.35 by more than 10 %

9 Map-model fit [i](#)

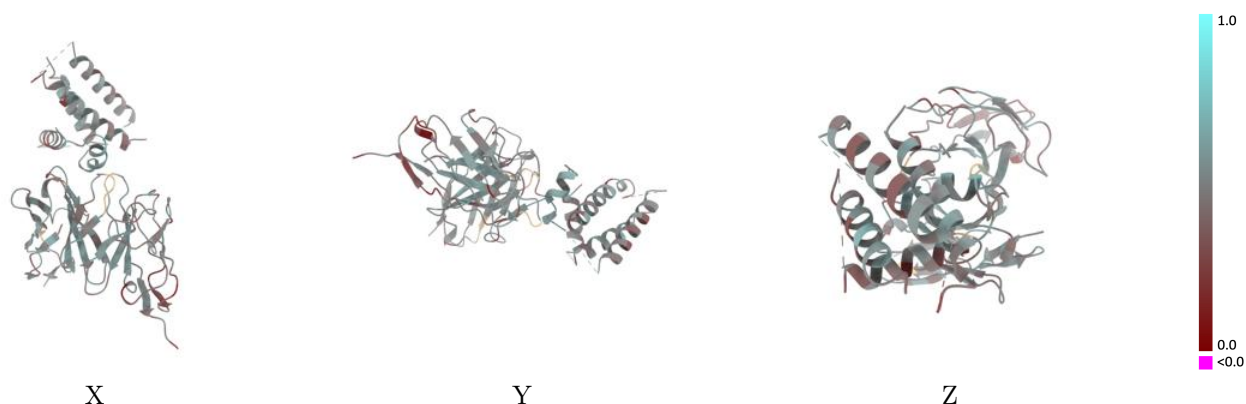
This section contains information regarding the fit between EMDB map EMD-43149 and PDB model 8VDG. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



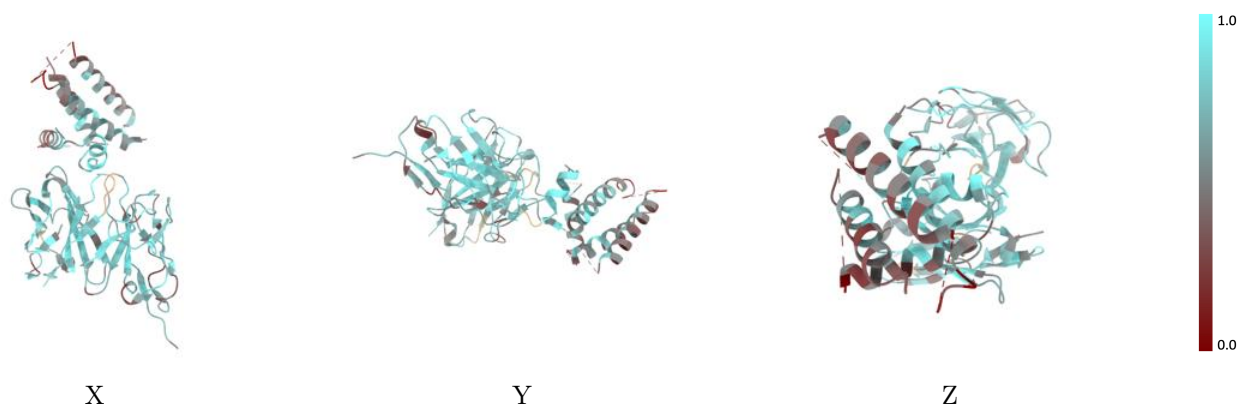
The images above show the 3D surface view of the map at the recommended contour level 0.23 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



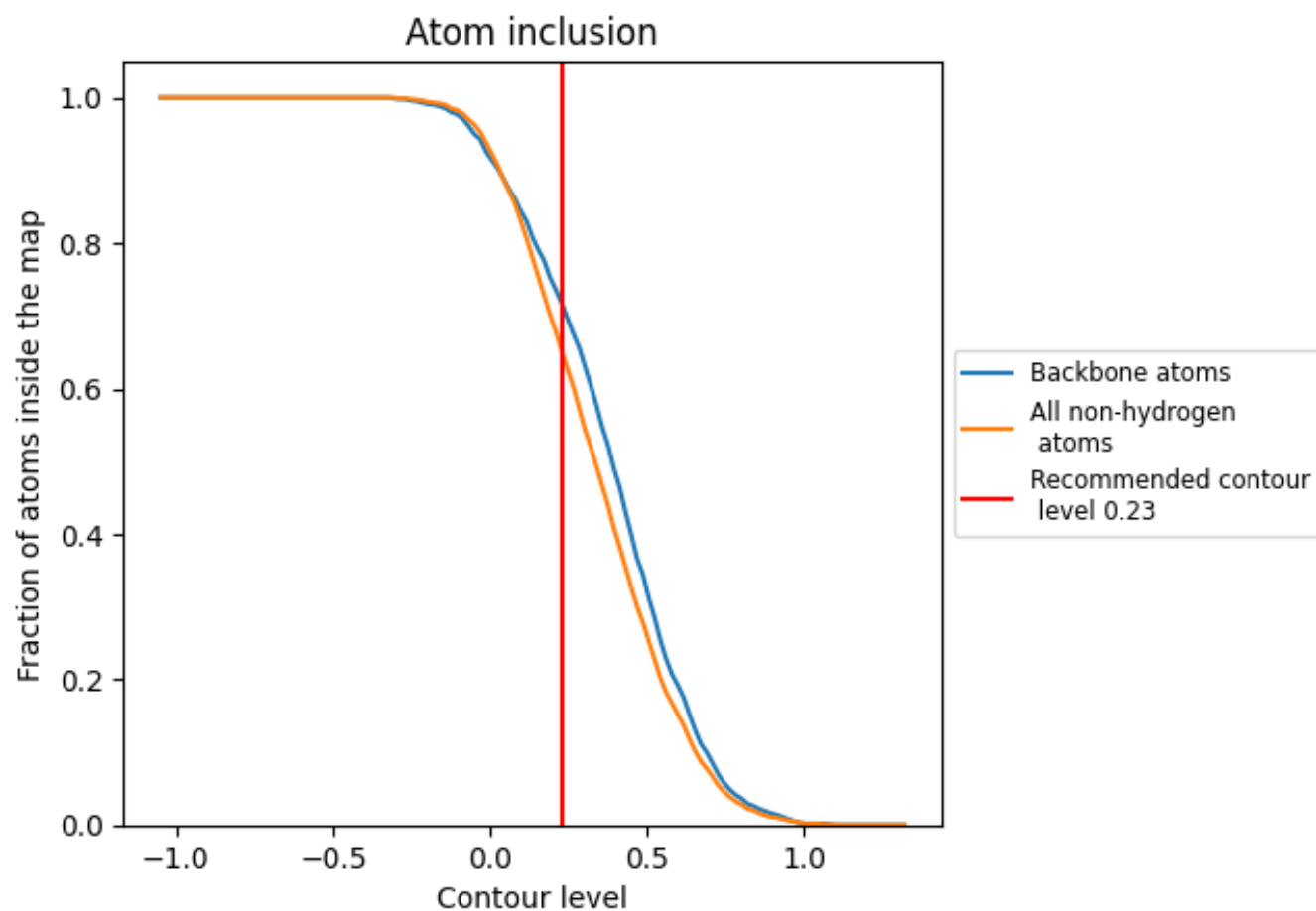
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.23).

9.4 Atom inclusion [i](#)



At the recommended contour level, 72% 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 (0.23) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6510	<div></div> 0.4760
A	<div></div> 0.5550	<div></div> 0.4730
H	<div></div> 0.7140	<div></div> 0.4940
K	<div></div> 0.6750	<div></div> 0.4580

