



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 05:10 PM UTC

PDB ID : 8YWX / pdb_00008ywx
EMDB ID : EMD-39646
Title : the complex structure of the H4B6 Fab with the RBD of Omicron BA.5 S protein
Authors : Xia, L.Y.; Zhang, Y.Y.; Zhou, Q.
Deposited on : 2024-04-01
Resolution : 3.40 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

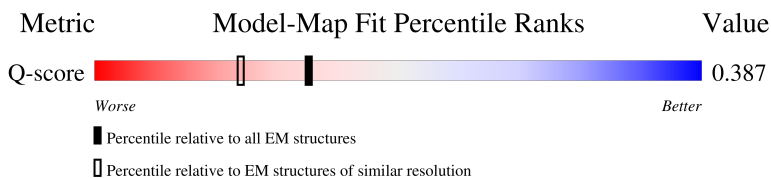
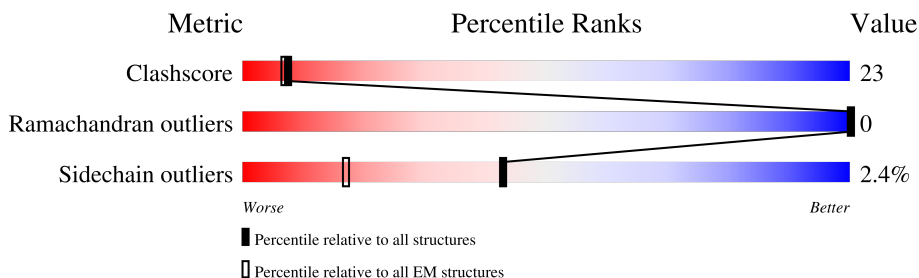
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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	14717 (2.90 - 3.90)

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	E	707	
2	D	214	
3	A	1120	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4803 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 H4B6 Fab's heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	E	218	Total	C	N	O	S	0	0
			1618	1015	278	319	6		

- Molecule 2 is a protein called H4B6 Fab's light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	212	Total	C	N	O	S	0	0
			1645	1028	278	334	5		

- Molecule 3 is a protein called Spike protein S2'.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	193	Total	C	N	O	S	0	0
			1540	992	261	279	8		

There are 31 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	156	ASP	GLU	conflict	UNP P0DTC2
A	339	ASP	GLY	variant	UNP P0DTC2
A	371	PHE	SER	variant	UNP P0DTC2
A	373	PRO	SER	variant	UNP P0DTC2
A	375	PHE	SER	variant	UNP P0DTC2
A	376	ALA	THR	variant	UNP P0DTC2
A	405	ASN	ASP	variant	UNP P0DTC2
A	408	SER	ARG	variant	UNP P0DTC2
A	417	ASN	LYS	variant	UNP P0DTC2
A	440	LYS	ASN	variant	UNP P0DTC2
A	452	ARG	LEU	variant	UNP P0DTC2
A	477	ASN	SER	variant	UNP P0DTC2
A	478	LYS	THR	variant	UNP P0DTC2
A	484	ALA	GLU	variant	UNP P0DTC2
A	486	VAL	PHE	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	498	ARG	GLN	variant	UNP P0DTC2
A	501	TYR	ASN	variant	UNP P0DTC2
A	505	HIS	TYR	variant	UNP P0DTC2
A	614	GLY	ASP	variant	UNP P0DTC2
A	655	TYR	HIS	variant	UNP P0DTC2
A	658	SER	ASN	conflict	UNP P0DTC2
A	764	LYS	ASN	variant	UNP P0DTC2
A	796	TYR	ASP	variant	UNP P0DTC2
A	817	PRO	PHE	conflict	UNP P0DTC2
A	892	PRO	ALA	conflict	UNP P0DTC2
A	899	PRO	ALA	conflict	UNP P0DTC2
A	942	PRO	ALA	conflict	UNP P0DTC2
A	954	HIS	GLN	variant	UNP P0DTC2
A	969	LYS	ASN	variant	UNP P0DTC2
A	986	PRO	LYS	variant	UNP P0DTC2
A	987	PRO	VAL	variant	UNP P0DTC2



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

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	368678	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	6.832	Depositor
Minimum map value	-5.316	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.041	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	434.80002, 434.80002, 434.80002	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.087, 1.087, 1.087	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	E	0.53	2/1655 (0.1%)	1.88	62/2251 (2.8%)
2	D	0.34	1/1679 (0.1%)	1.25	35/2280 (1.5%)
3	A	0.88	2/1586 (0.1%)	1.89	52/2158 (2.4%)
All	All	0.62	5/4920 (0.1%)	1.70	149/6689 (2.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	103	GLY	C-N	-9.22	1.12	1.33
1	E	2	VAL	C-N	-8.51	1.20	1.33
3	A	438	SER	CA-CB	-6.36	1.45	1.52
3	A	349	SER	CA-CB	-5.55	1.44	1.53
2	D	59	PRO	N-CD	5.01	1.54	1.47

The worst 5 of 149 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	24	ALA	CB-CA-C	-22.61	77.60	110.62
1	E	11	LEU	N-CA-C	21.35	144.54	110.17
1	E	10	ASP	N-CA-C	-20.64	80.07	107.73
1	E	11	LEU	CB-CA-C	-17.29	80.28	109.50
1	E	11	LEU	N-CA-CB	-17.10	82.76	110.63

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	103	GLY	Mainchain
1	E	2	VAL	Mainchain
1	E	5	VAL	Mainchain

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	E	1618	0	1593	72	0
2	D	1645	0	1596	51	0
3	A	1540	0	1463	113	0
All	All	4803	0	4652	218	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 23.

The worst 5 of 218 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:A:382:VAL:HG11	3:A:387:LEU:CD2	1.41	1.45
3:A:382:VAL:CG1	3:A:387:LEU:HD21	1.49	1.42
3:A:372:ALA:HB3	3:A:374:PHE:CE1	1.62	1.33
3:A:374:PHE:CD2	3:A:377:PHE:HD2	1.46	1.31
3:A:382:VAL:CG1	3:A:387:LEU:CD2	2.07	1.29

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	E	216/707 (31%)	209 (97%)	7 (3%)	0	100	100
2	D	210/214 (98%)	201 (96%)	9 (4%)	0	100	100
3	A	191/1120 (17%)	186 (97%)	5 (3%)	0	100	100
All	All	617/2041 (30%)	596 (97%)	21 (3%)	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	E	182/590 (31%)	182 (100%)	0	100	100
2	D	187/188 (100%)	186 (100%)	1 (0%)	81	81
3	A	165/972 (17%)	153 (93%)	12 (7%)	13	39
All	All	534/1750 (30%)	521 (98%)	13 (2%)	43	62

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	410	ILE
3	A	433	VAL
3	A	488	CYS
3	A	468	ILE
3	A	472	ILE

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

Mol	Chain	Res	Type
3	A	481	ASN
3	A	505	HIS
2	D	137	ASN

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Mol	Chain	Res	Type
2	D	158	ASN
3	A	414	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	E	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	2:VAL	C	3:GLN	N	1.20
1	E	103:GLY	C	104:GLY	N	1.12

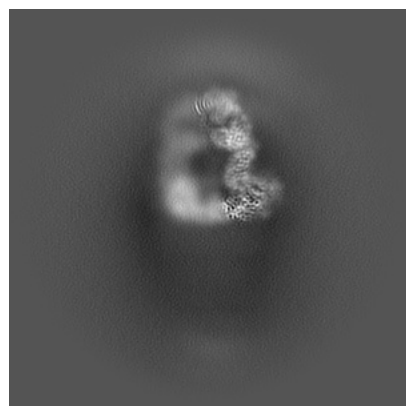
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39646. These allow visual inspection of the internal detail of the map and identification of artifacts.

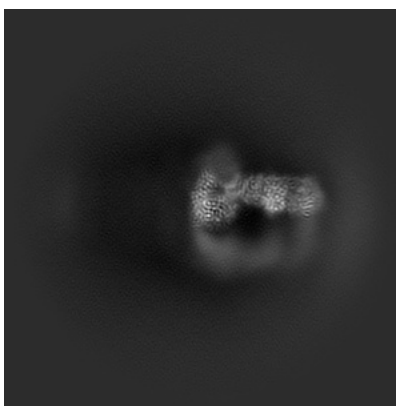
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

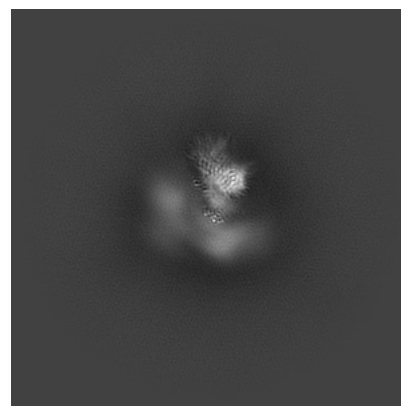
6.1.1 Primary map



X

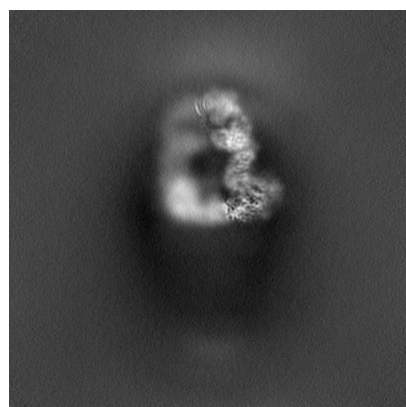


Y

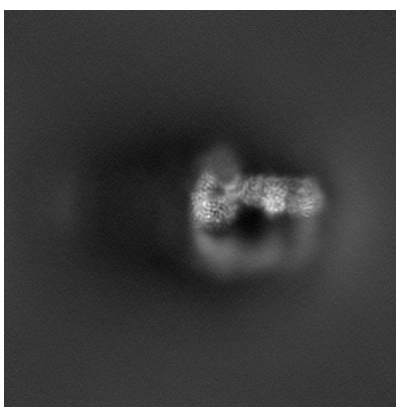


Z

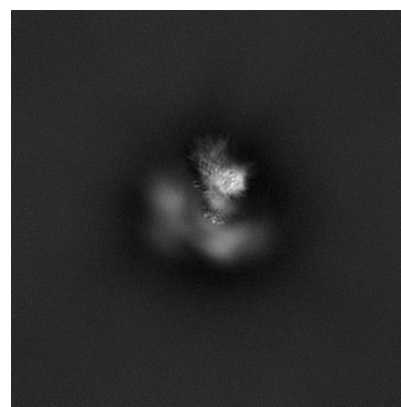
6.1.2 Raw map



X



Y

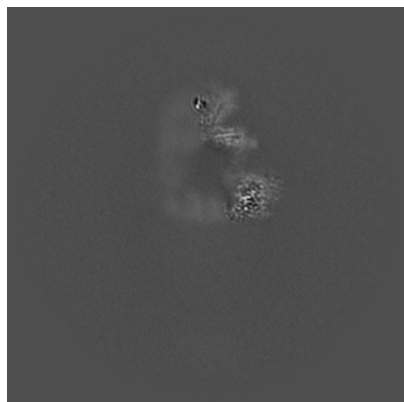


Z

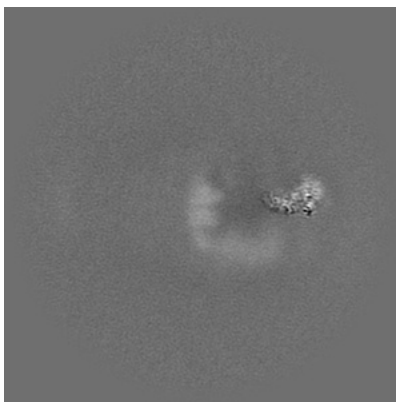
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

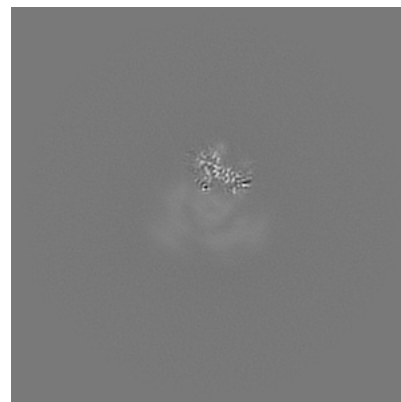
6.2.1 Primary map



X Index: 200

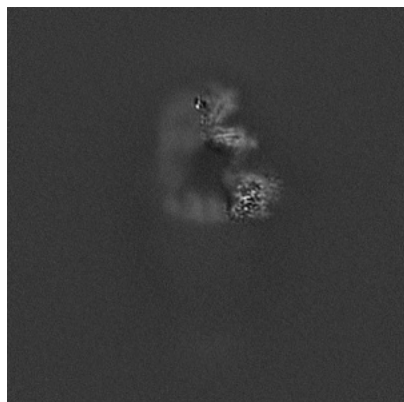


Y Index: 200

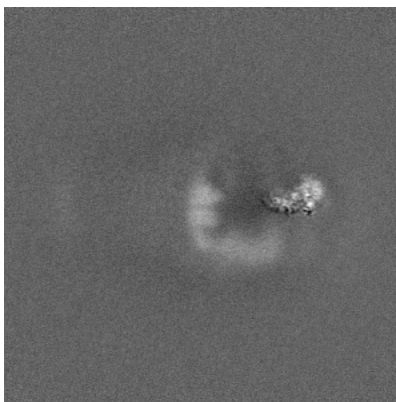


Z Index: 200

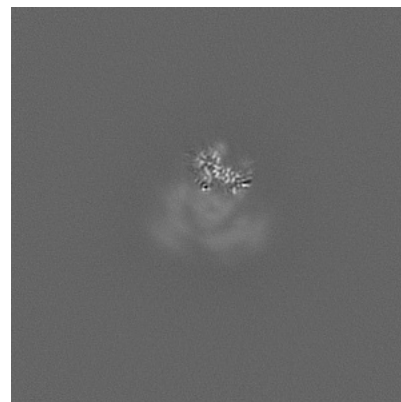
6.2.2 Raw map



X Index: 200



Y Index: 200

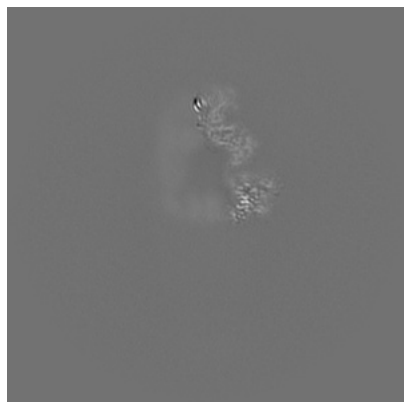


Z Index: 200

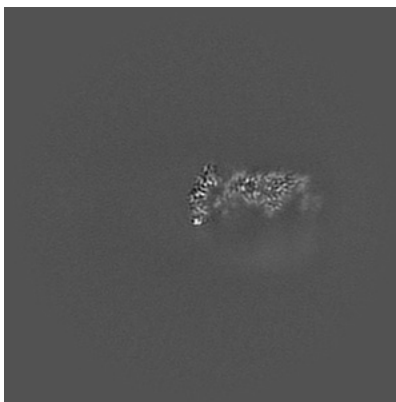
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

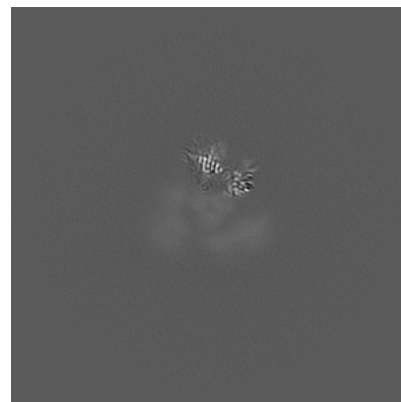
6.3.1 Primary map



X Index: 205

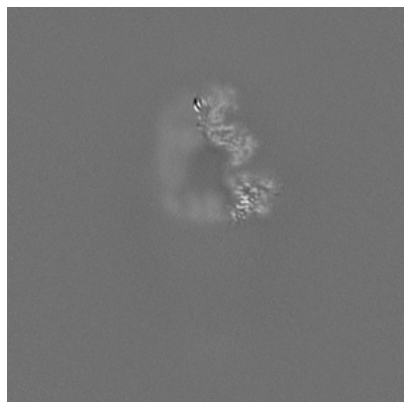


Y Index: 228

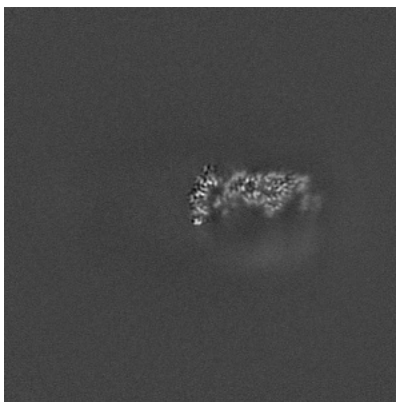


Z Index: 204

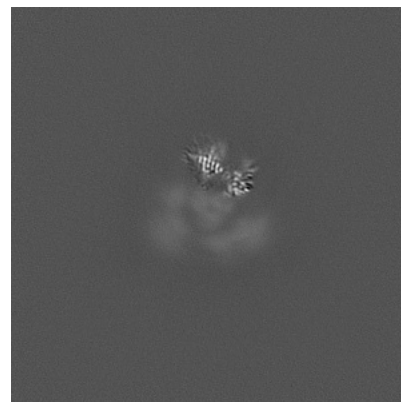
6.3.2 Raw map



X Index: 205



Y Index: 228

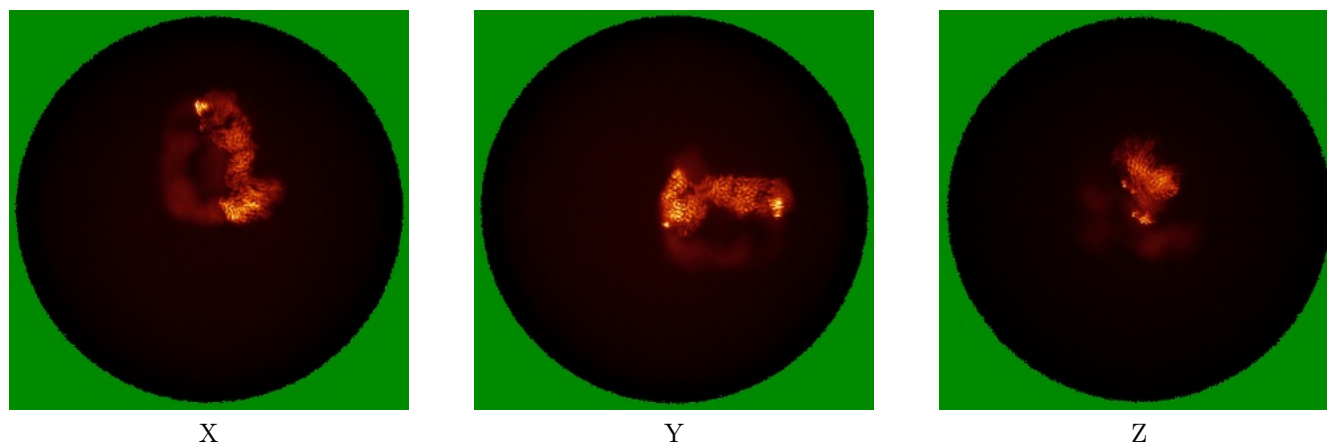


Z Index: 204

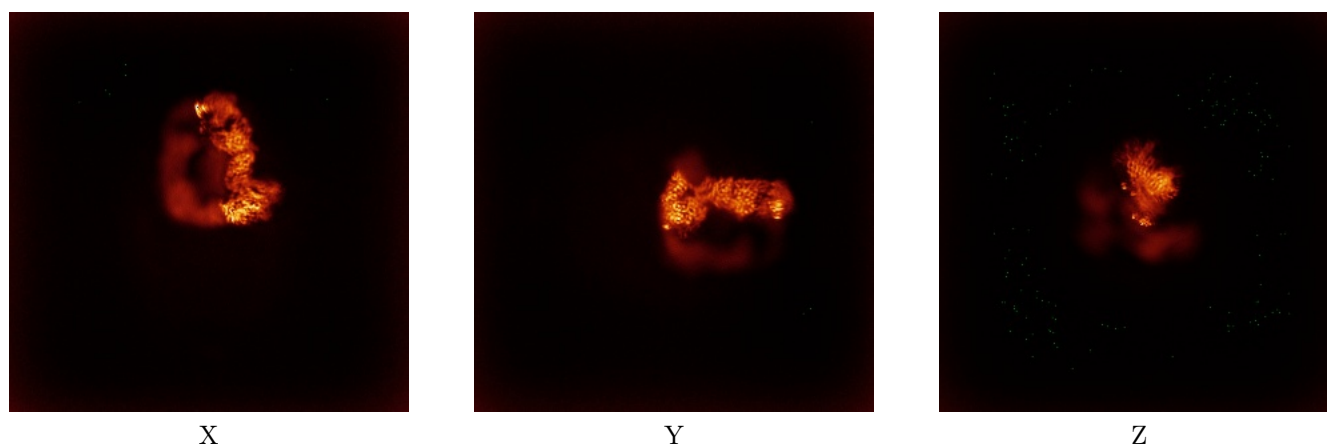
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

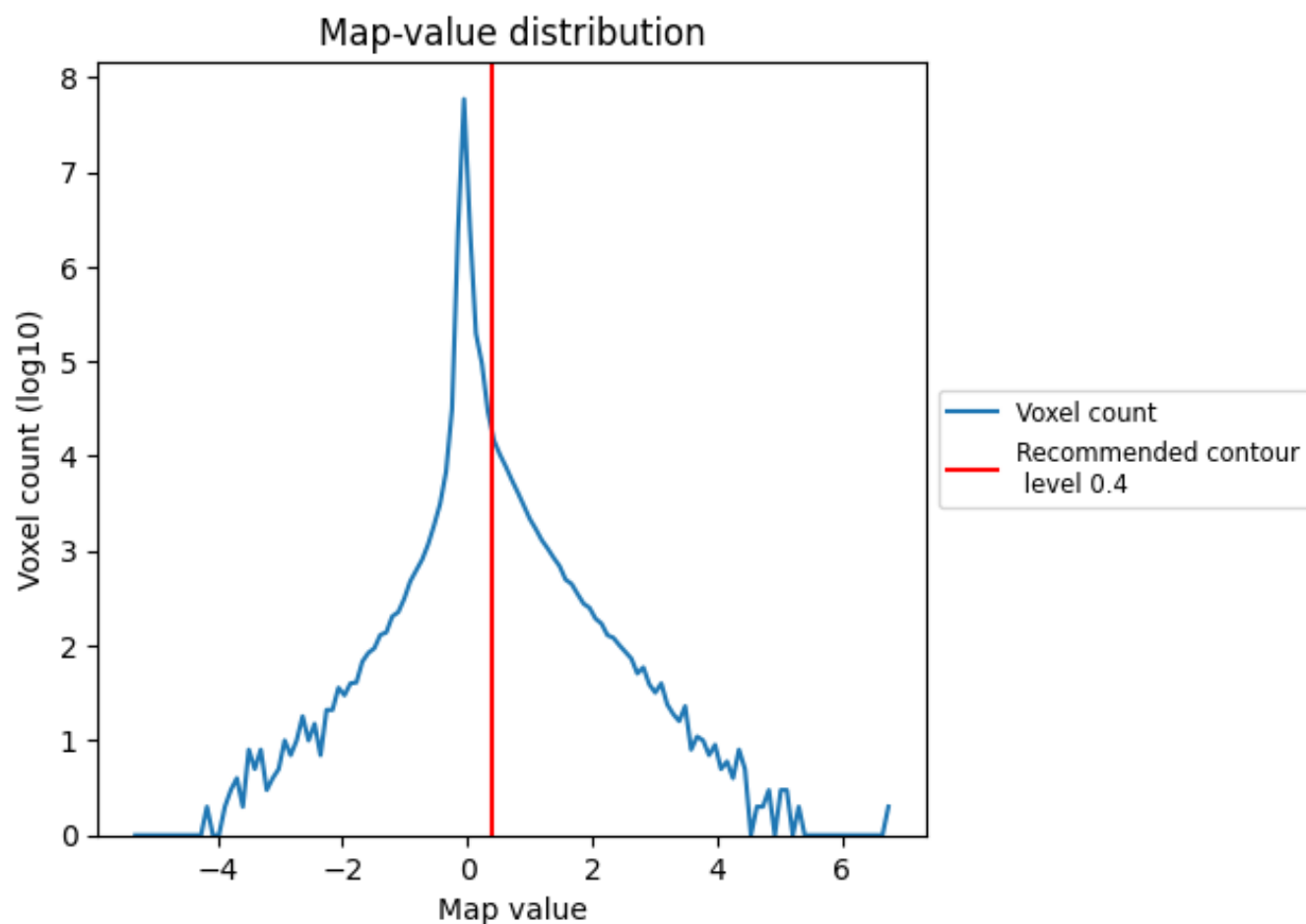
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

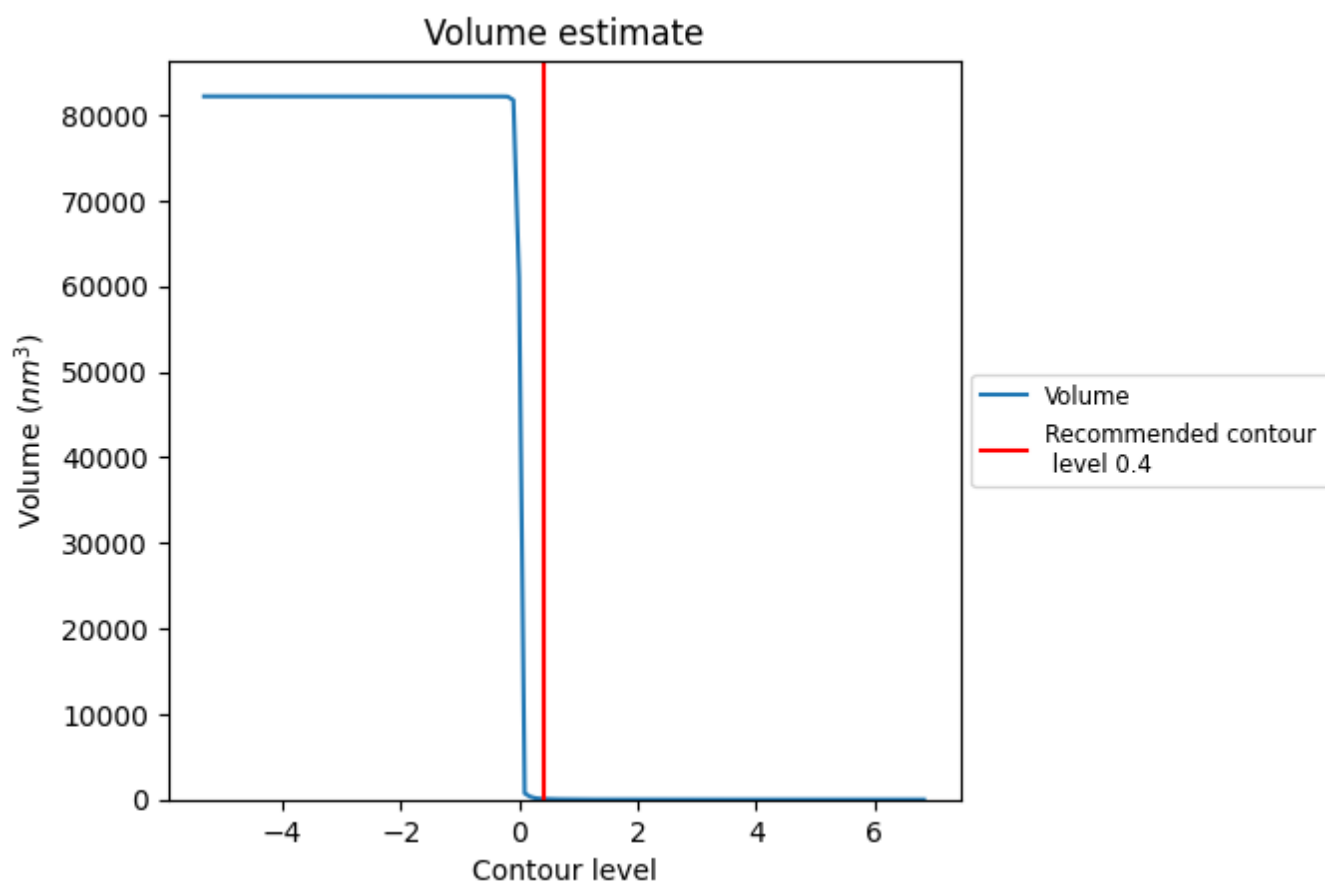
This section contains the results of statistical analysis of the map.

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.

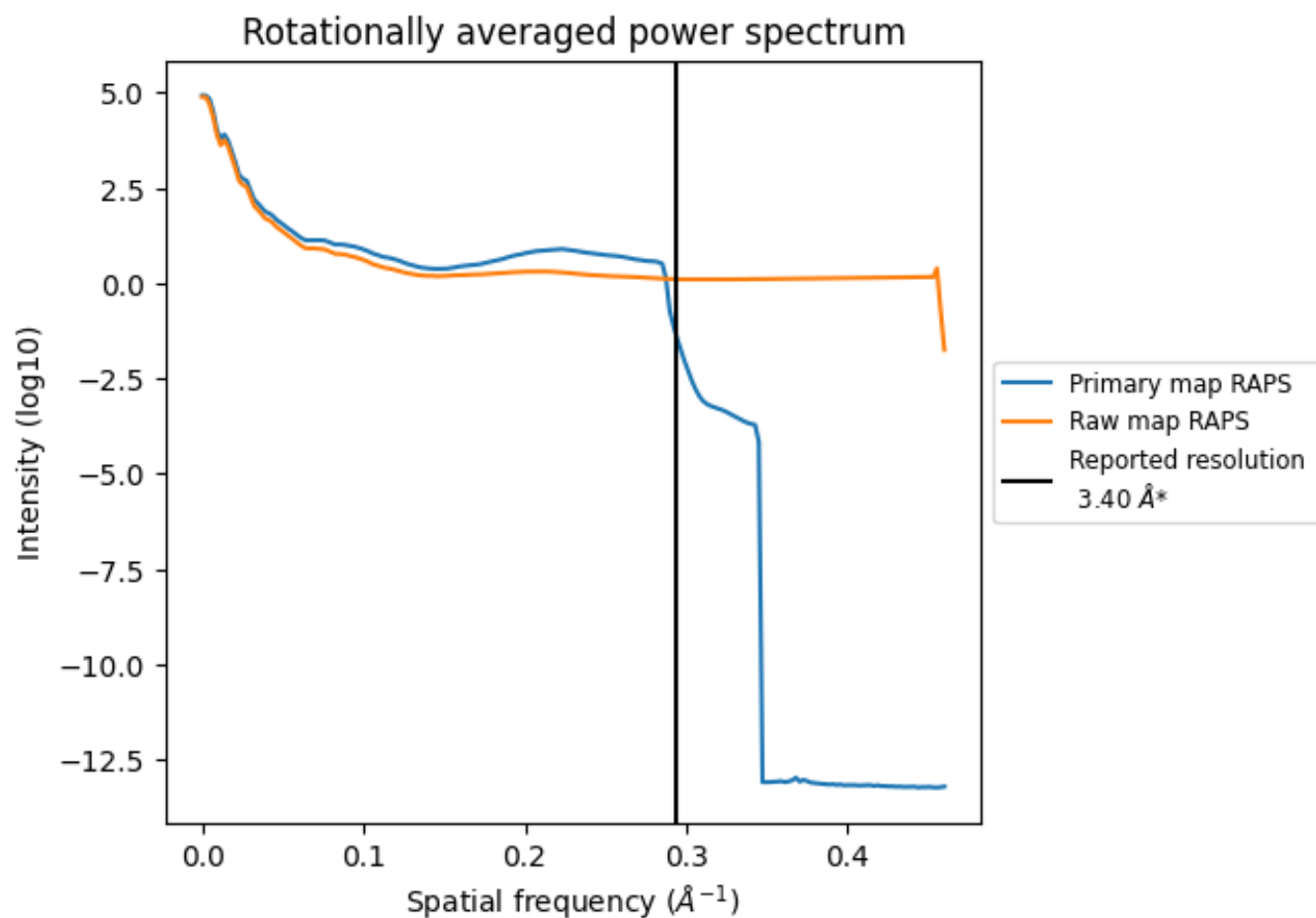
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 80 nm³; this corresponds to an approximate mass of 73 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 ⓘ

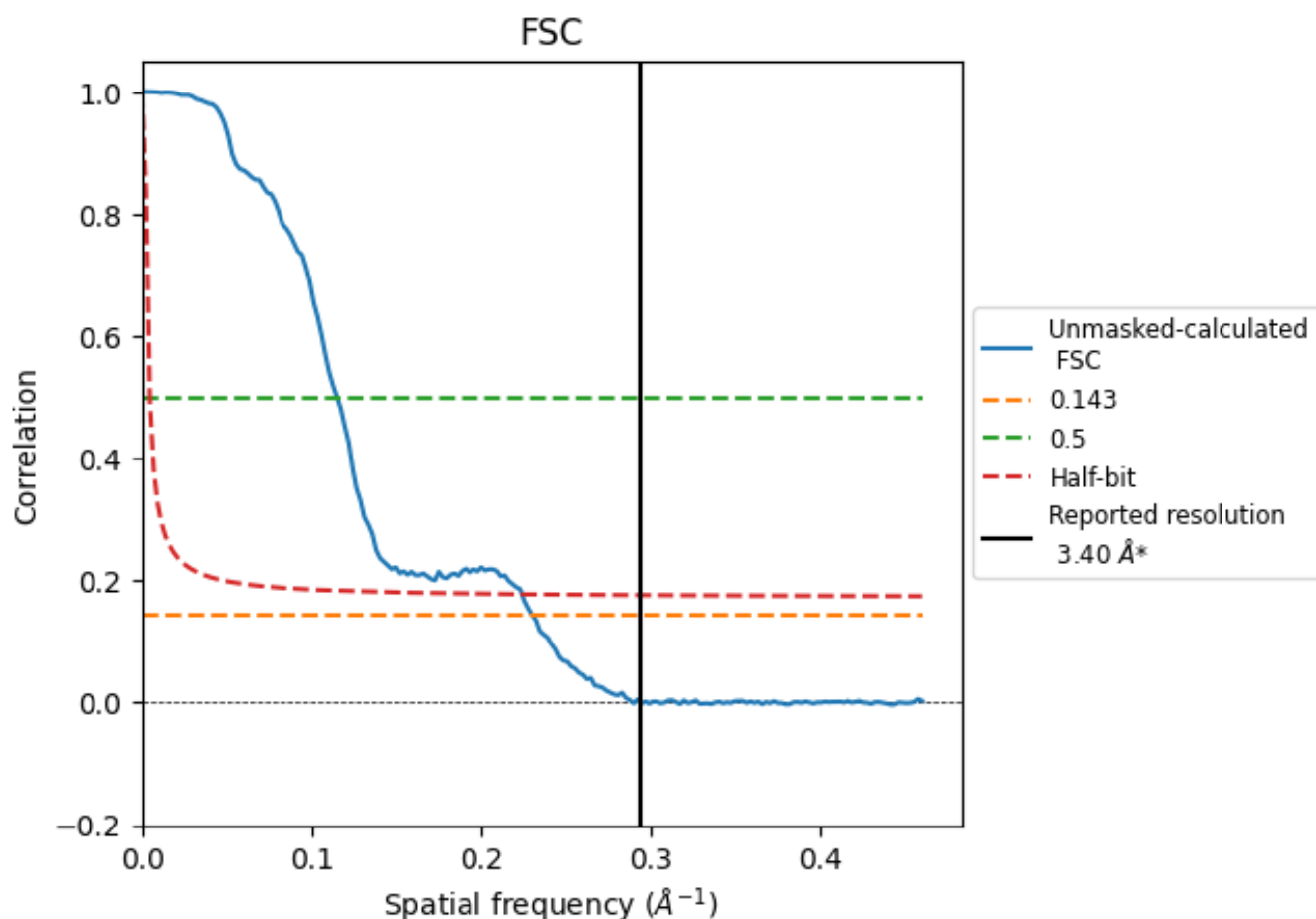


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

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 0.294 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.34	8.70	4.46

*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 4.34 differs from the reported value 3.4 by more than 10 %

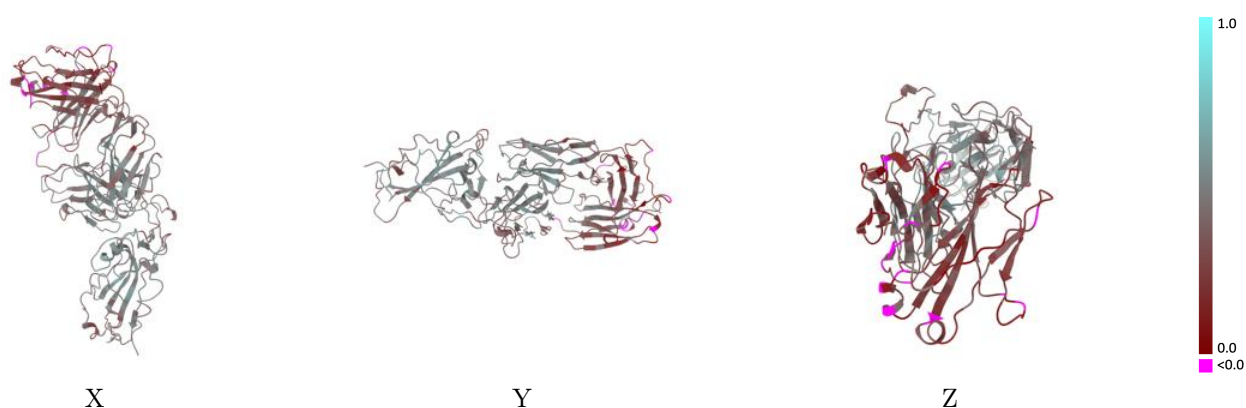
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-39646 and PDB model 8YWX. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay [i](#)

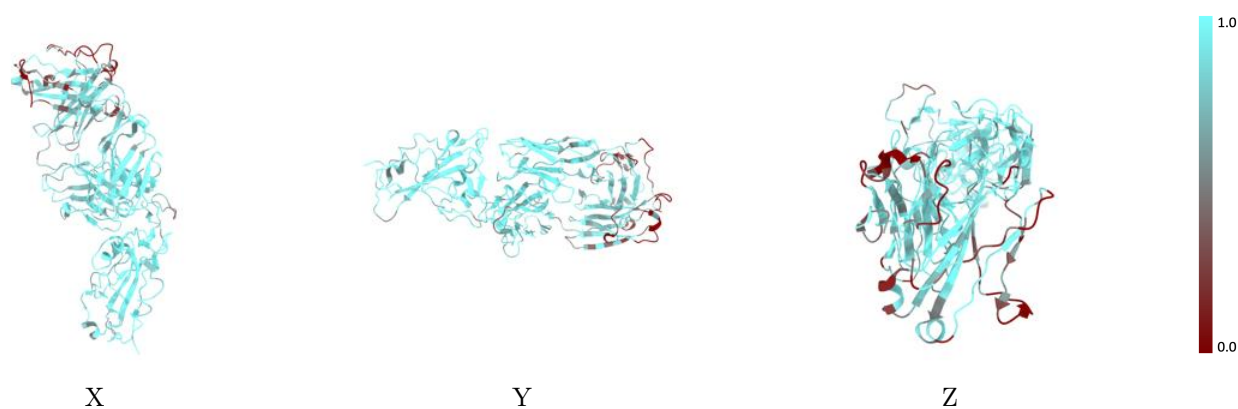
This section was not generated.

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



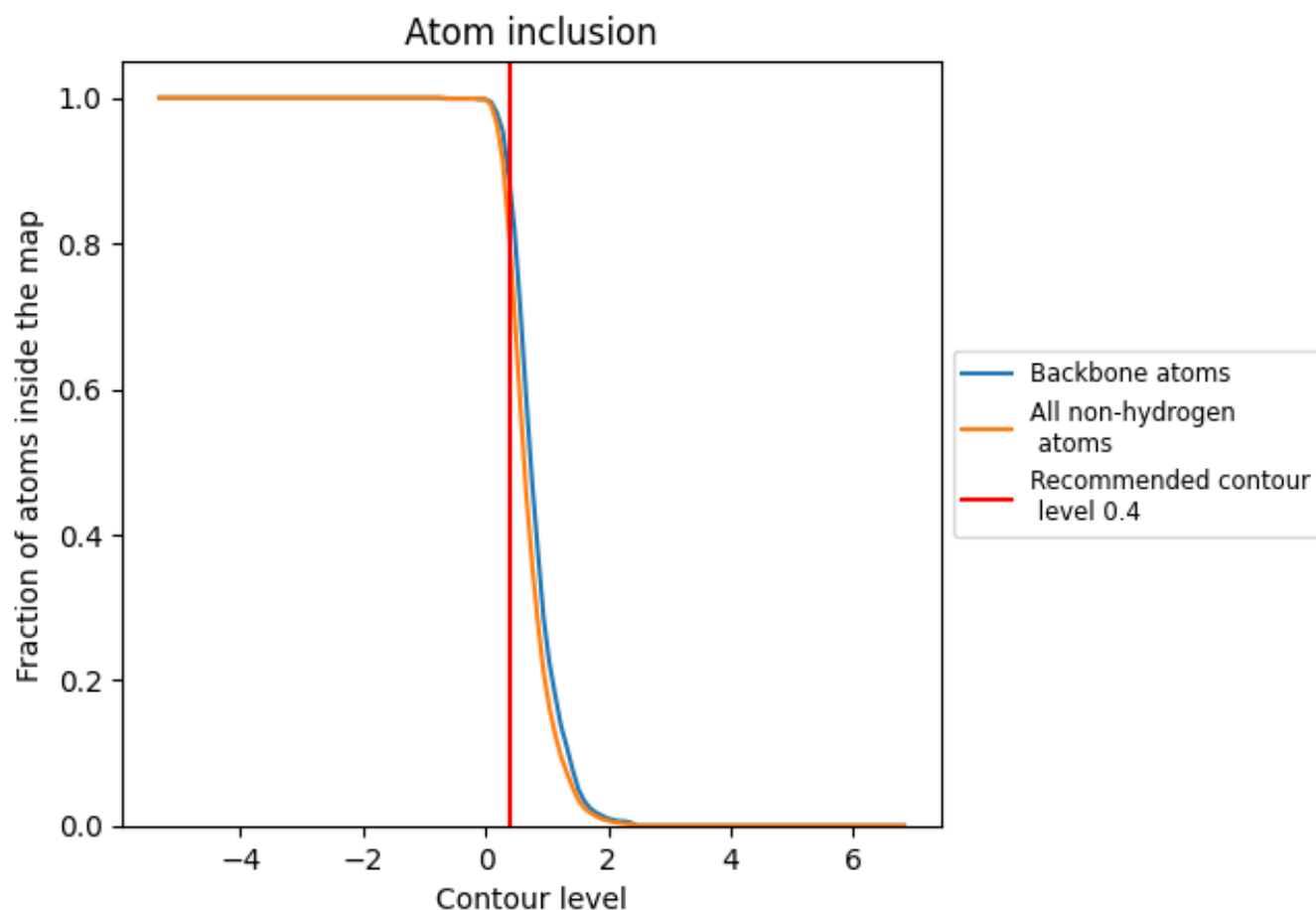
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.4).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 80% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7970	0.3870
A	0.8730	0.4550
D	0.7590	0.3480
E	0.7650	0.3630

