



wwPDB EM Validation Summary Report ⓘ

May 29, 2025 – 04:37 PM EDT

PDB ID : 9NFK / pdb_00009nfk
EMDB ID : EMD-49368
Title : Tuna P-glycoprotein Apo Conformation 3
Authors : Young, M.A.; Rees, S.D.; Nicklisch, S.C.T.; Stowell, M.; Hamdoun, A.; Chang, G.
Deposited on : 2025-02-21
Resolution : 3.99 Å(reported)
Based on initial model : .

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.dev118
MolProbity : 4-5-2 with Phenix2.0rc1
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) : 2.43.1

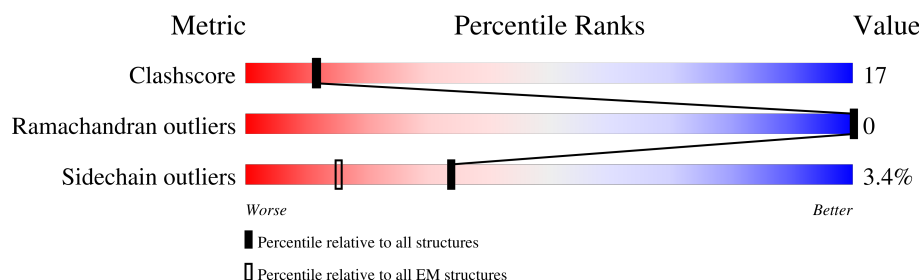
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.99 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	1306	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6975 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 Permeability Glycoprotein (P-gp).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	898	6975	4498	1163	1268	46	0	0

LEU	THR	GLY	ARG	ALA	T915
SER	ILE	GLY	ARG	ASN	
THR	LEU	VAL	GLY	SER	E919
ILE	SER	SER	ASN	PHE	N920
GLN	GLY	GLN	THR	THR	I921
ASN	GLY	GLY	LYS	PRO	
ALA	GLN	PRO	VAL	M1014	Y924
ASP	LYS	VAL	SER		
ARG	GLN	LEU	LYS	K1017	L927
ILE	ARG	PHE	GLY		T928
ALA	ILE	ASP	GLU	M1020	R929
VAL	ALA	CYS	THR	S1021	
PHE	ILE	THR	LEU	A1022	K932
GLN	ALA	LEU	ALA	S1023	F933
ALA	ARG	ALA	LEU	H1024	
GLY	ALA	GLU	VAL	L1025	Q938
VAL	ILE	ASN	GLY		
VAL	VAL	ILE	SER	L1028	L941
VAL	ARG	ALA	SER	M1029	
GLU	ASN	TYR	GLY	M1030	Y945
GLN	PRO	GLY	CYS	R1031	
THR	LYS	ASP	LYS	E1032	S948
THR	LEU	ASN	LYS	PRO	Q949
HIS	LEU	SER	SER	ALA	K950
GLN	LEU	ARG	THR	ILE	
GLN	LEU	THR	THR	ASP	Y954
LEU	ASP	VAL	ILE	ASN	
LEU	GLU	THR	GLN	LEU	T958
ALA	ALA	LEU	LEU	SER	
LYS	THR	GLU	LEU	GLU	F961
LYS	SER	GLU	GLY	GLY	
GLY	ALA	ILE	ARG	GLY	H965
ILE	LEU	GLN	PHE	GLN	
TYR	ASP	ALA	TYR	SER	
THR	THR	ALA	ASP	PRO	F974
MET	GLU	ALA	PRO	ASP	
LEU	SER	LYS	MET	LYS	L980
VAL	GLU	ALA	HIS	PHE	
ASN	LYS	ALA	GLY	ASP	G984
THR	VAL	ASN	LYS	GLY	R985
GLN	VAL	ILE	VAL	ASN	H986
MET	GLN	HIS	VAL	VAL	D987
GLY	GLU	SER	LEU	ARG	A988
HIS	ALA	PHE	ASP	PHE	E989
GLU	LEU	ILE	GLY	GLU	G990
ARG	ASP	GLU	ILE	GLY	V991
ASN	GLN	ASN	ILE	GLY	Y992
THR	ALA	GLN	SER	VAL	L993
ILE	CYS	ALA	LEU	LYS	Y994
ASP	ILE	SER	PRO	PHE	I995
HIS	ARG	GLN	GLY	ASN	S996
HIS	GLY	TYR	LEU	TYR	A997
HIS	ARG	ASN	ILE	PRO	Y999
HIS	THR	ASP	SER	ARG	
HIS	CYS	THR	HIS	TRP	G1001
HIS	ILE	GLN	ALA	GLU	A1002
	VAL	VAL	LEU	VAL	M1003
	VAL	ARG	ARG	PRO	A1004
	ALA	ASP	SER	PRO	V1005
	HIS	LYS	GLN	ILE	G1006
	ARG	ILE	LEU		E1007

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	75691	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	55	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.787	Depositor
Minimum map value	-1.040	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.042	Depositor
Recommended contour level	0.13	Depositor
Map size (Å)	299.2, 299.2, 299.2	wwPDB
Map dimensions	160, 160, 160	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.8700001, 1.8700001, 1.8700001	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	0.19	0/7108	0.33	0/9598

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	6975	0	7086	245	0
All	All	6975	0	7086	245	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 17.

The worst 5 of 245 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:LEU:HD23	1:A:565:LEU:HD11	1.32	1.05
1:A:454:ARG:NH1	1:A:470:ILE:O	2.01	0.93
1:A:284:ARG:NH1	1:A:285:GLU:OE2	2.08	0.86
1:A:332:LEU:O	1:A:336:LYS:N	2.09	0.86
1:A:379:SER:O	1:A:383:ASN:ND2	2.13	0.81

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	890/1306 (68%)	844 (95%)	46 (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	741/1088 (68%)	716 (97%)	25 (3%)	32	54

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	585	LEU
1	A	619	ILE
1	A	933	PHE
1	A	613	PHE
1	A	733	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	165	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	207	GLN
1	A	474	ASN
1	A	614	HIS
1	A	949	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.

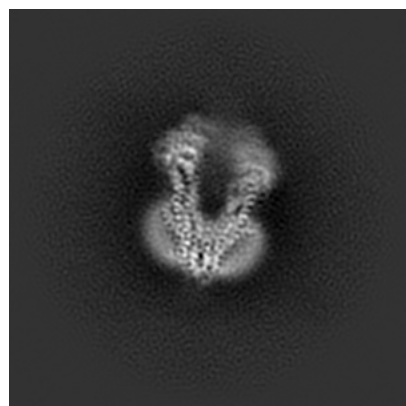
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-49368. These allow visual inspection of the internal detail of the map and identification of artifacts.

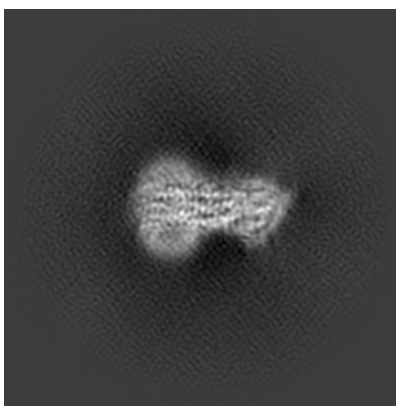
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

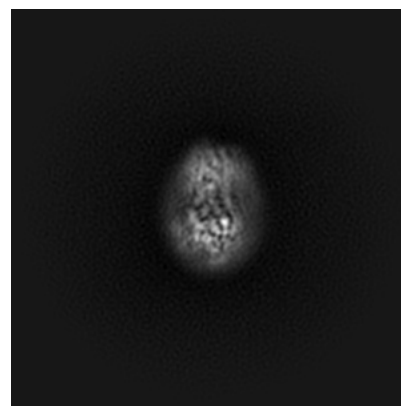
6.1.1 Primary map



X

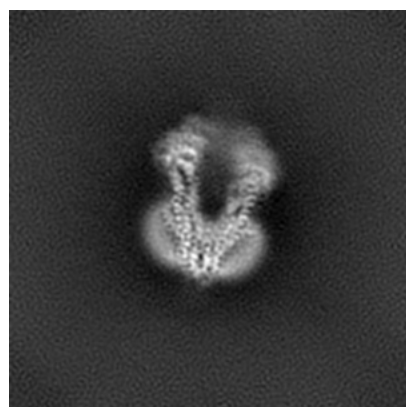


Y

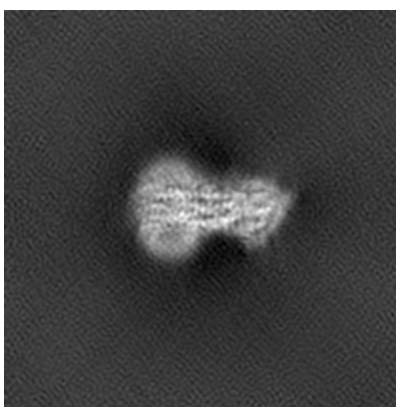


Z

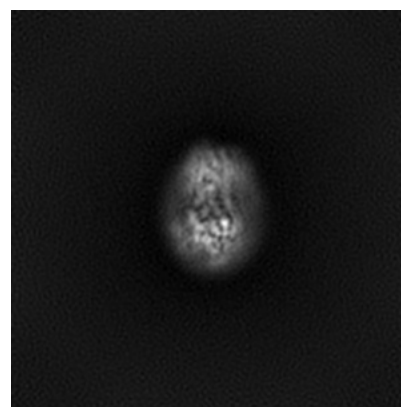
6.1.2 Raw map



X



Y

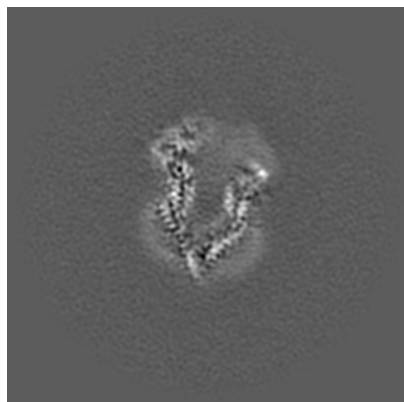


Z

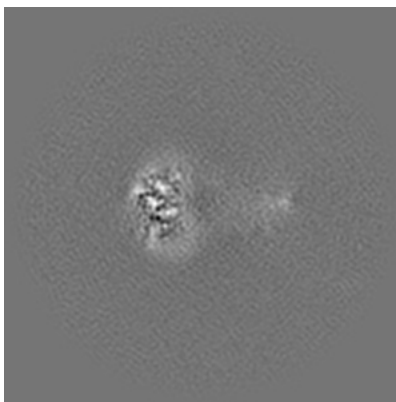
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

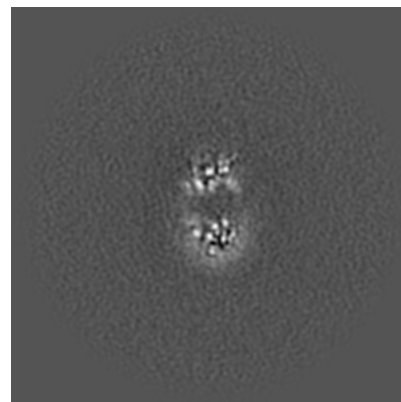
6.2.1 Primary map



X Index: 80

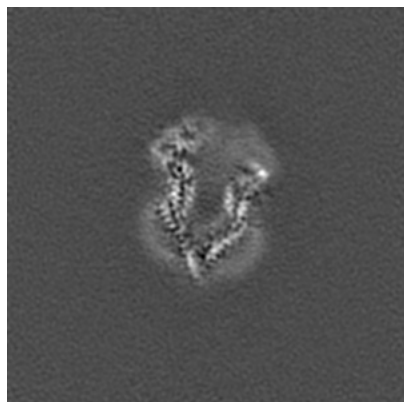


Y Index: 80

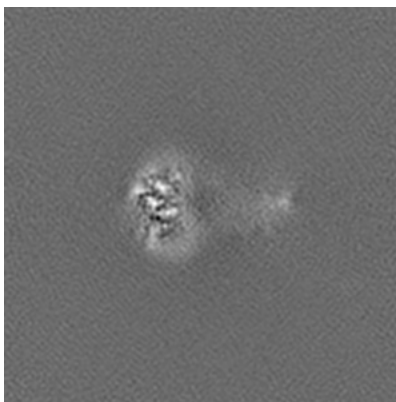


Z Index: 80

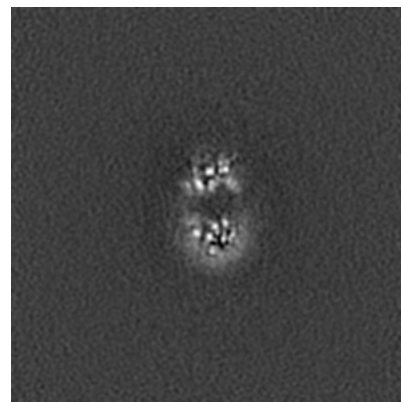
6.2.2 Raw map



X Index: 80



Y Index: 80

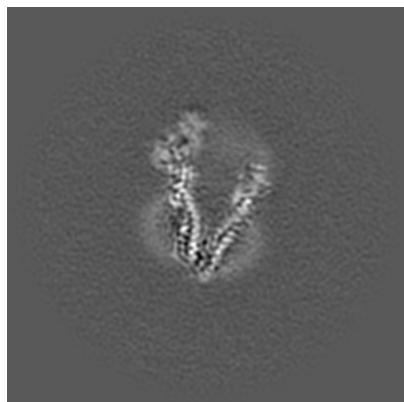


Z Index: 80

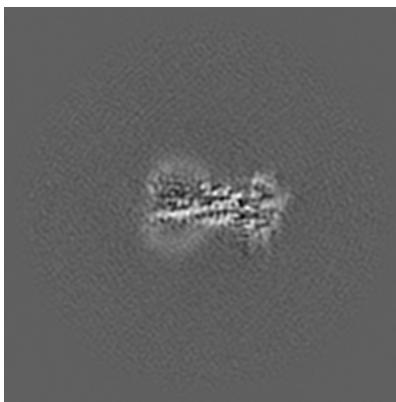
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

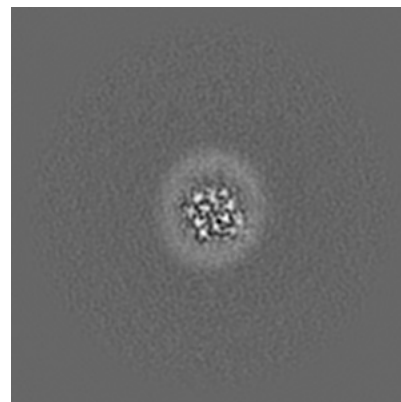
6.3.1 Primary map



X Index: 85

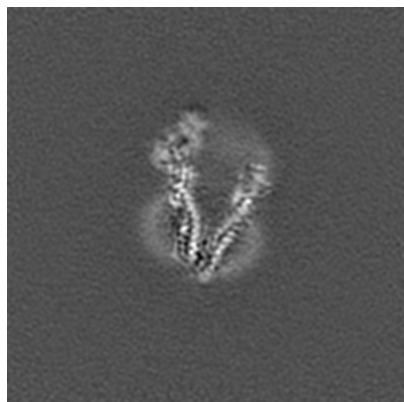


Y Index: 68

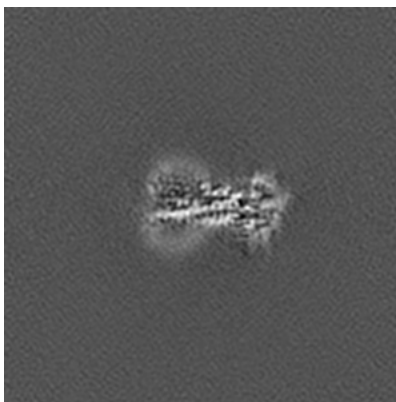


Z Index: 63

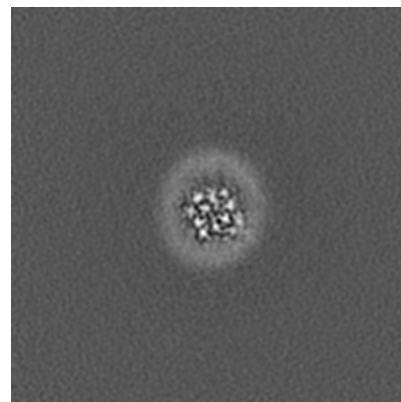
6.3.2 Raw map



X Index: 85



Y Index: 68

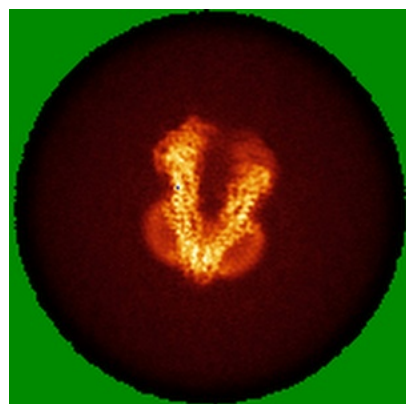


Z Index: 63

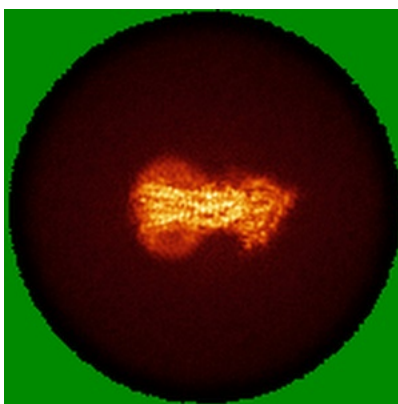
The images above show the largest variance slices of the map in three orthogonal directions.

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

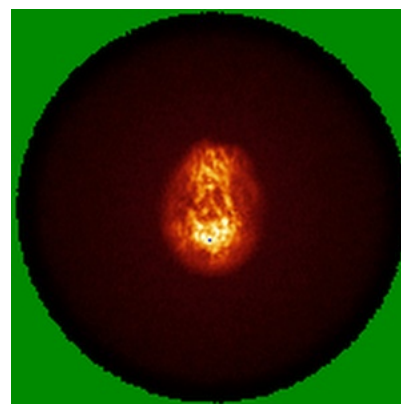
6.4.1 Primary map



X

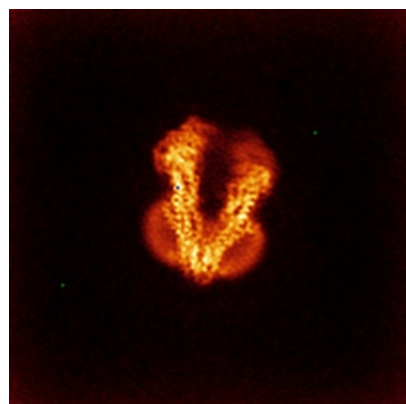


Y

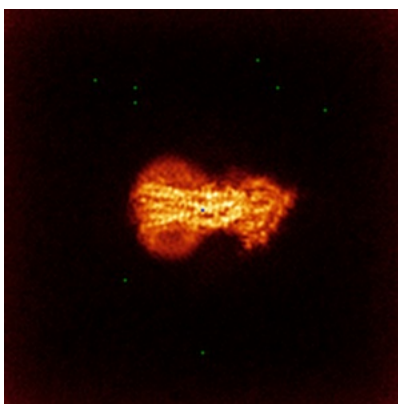


Z

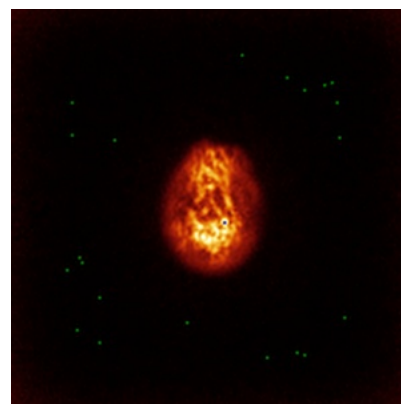
6.4.2 Raw map



X



Y

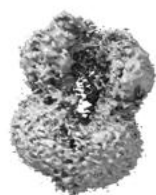


Z

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



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.13. 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



X



Y



Z

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.

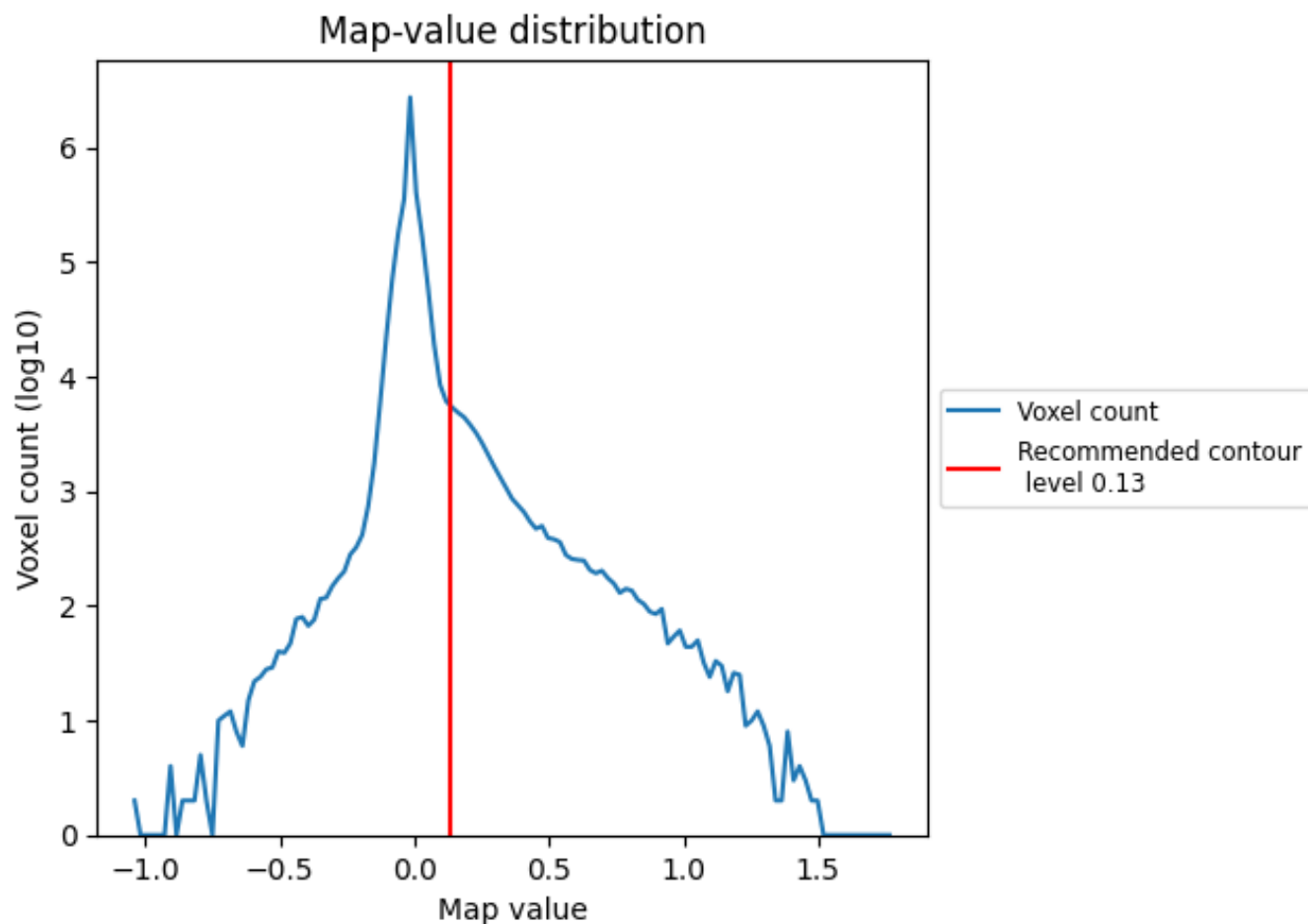
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

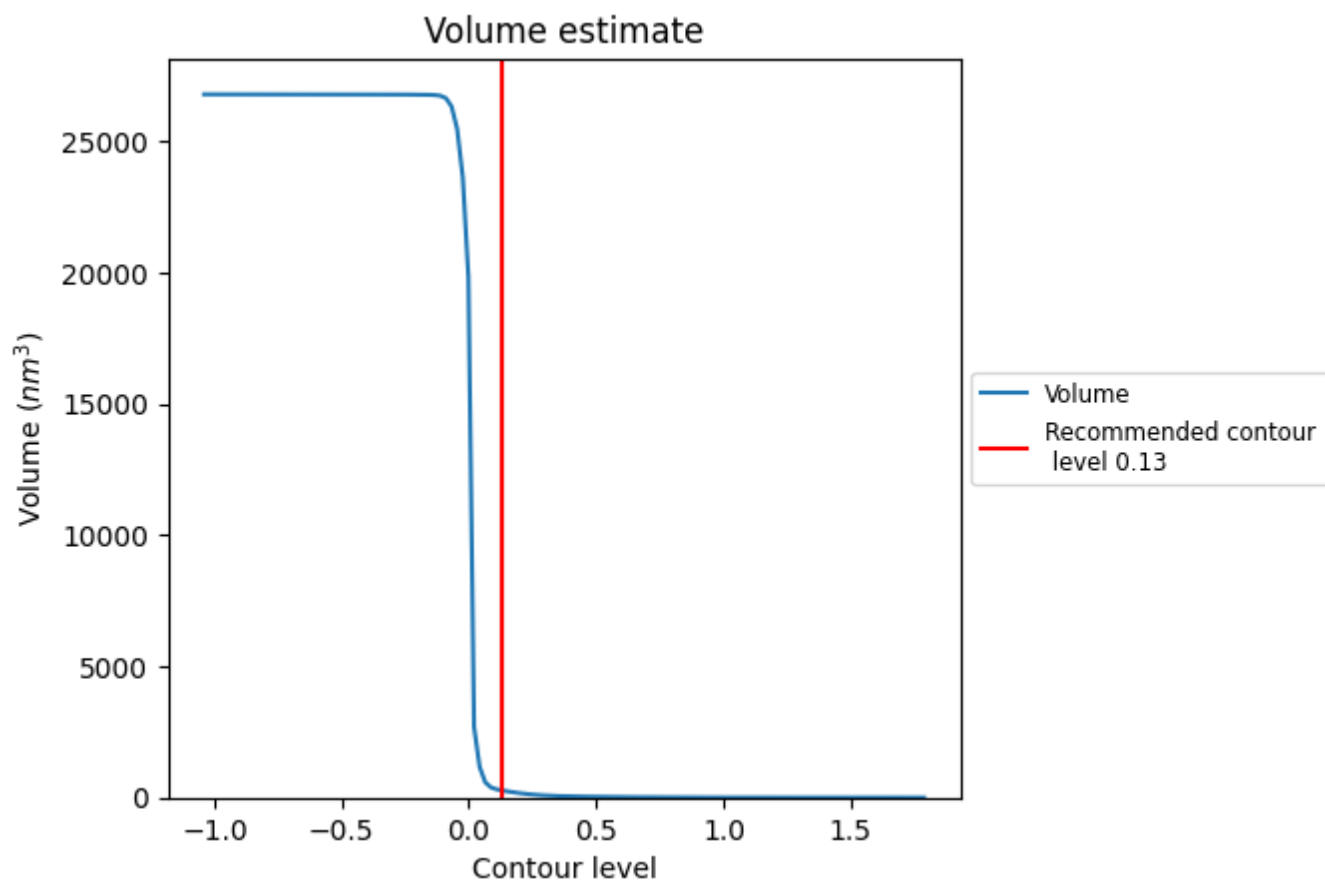
This section contains the results of statistical analysis of the map.

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.

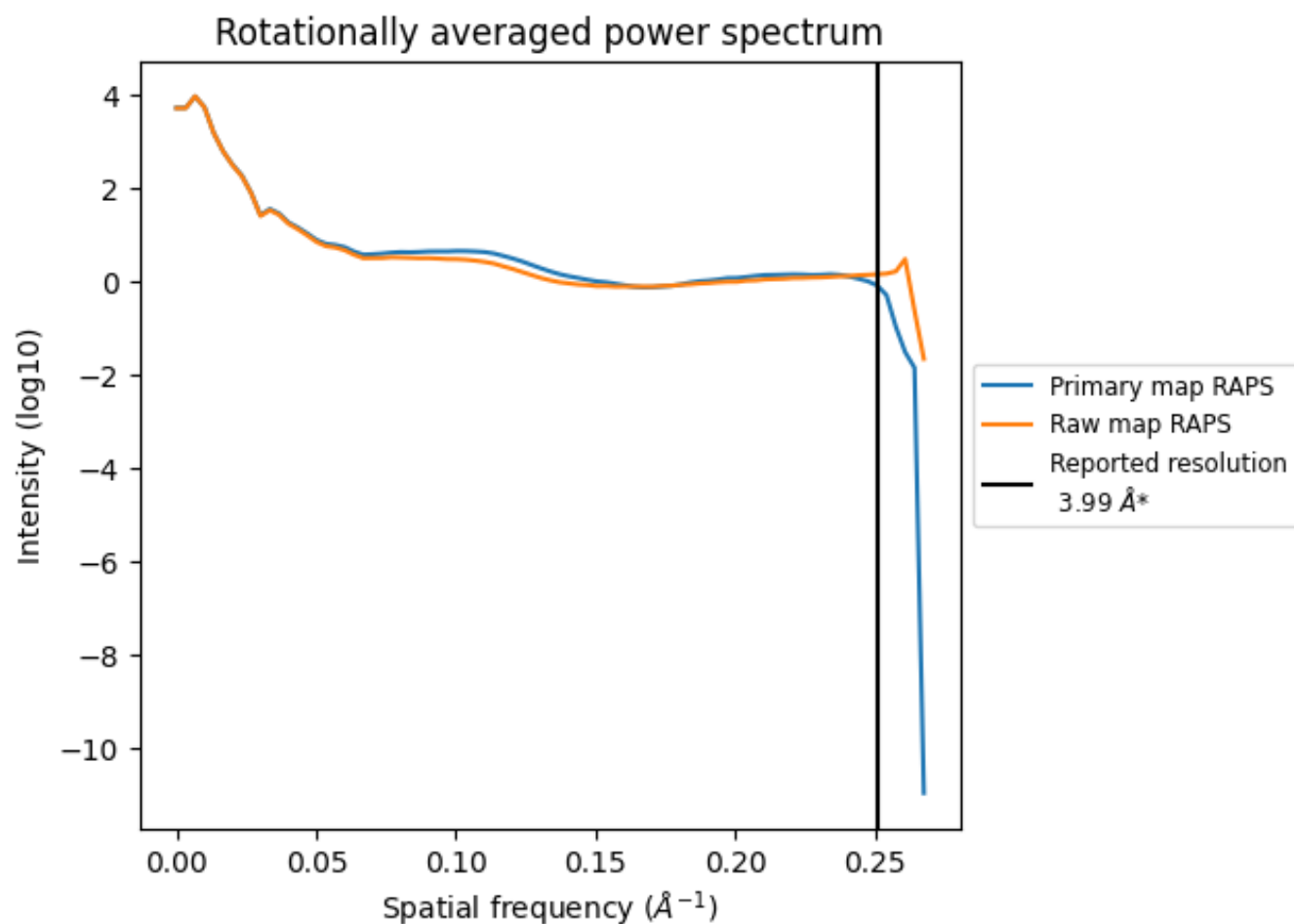
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 273 nm^3 ; this corresponds to an approximate mass of 246 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 ⓘ

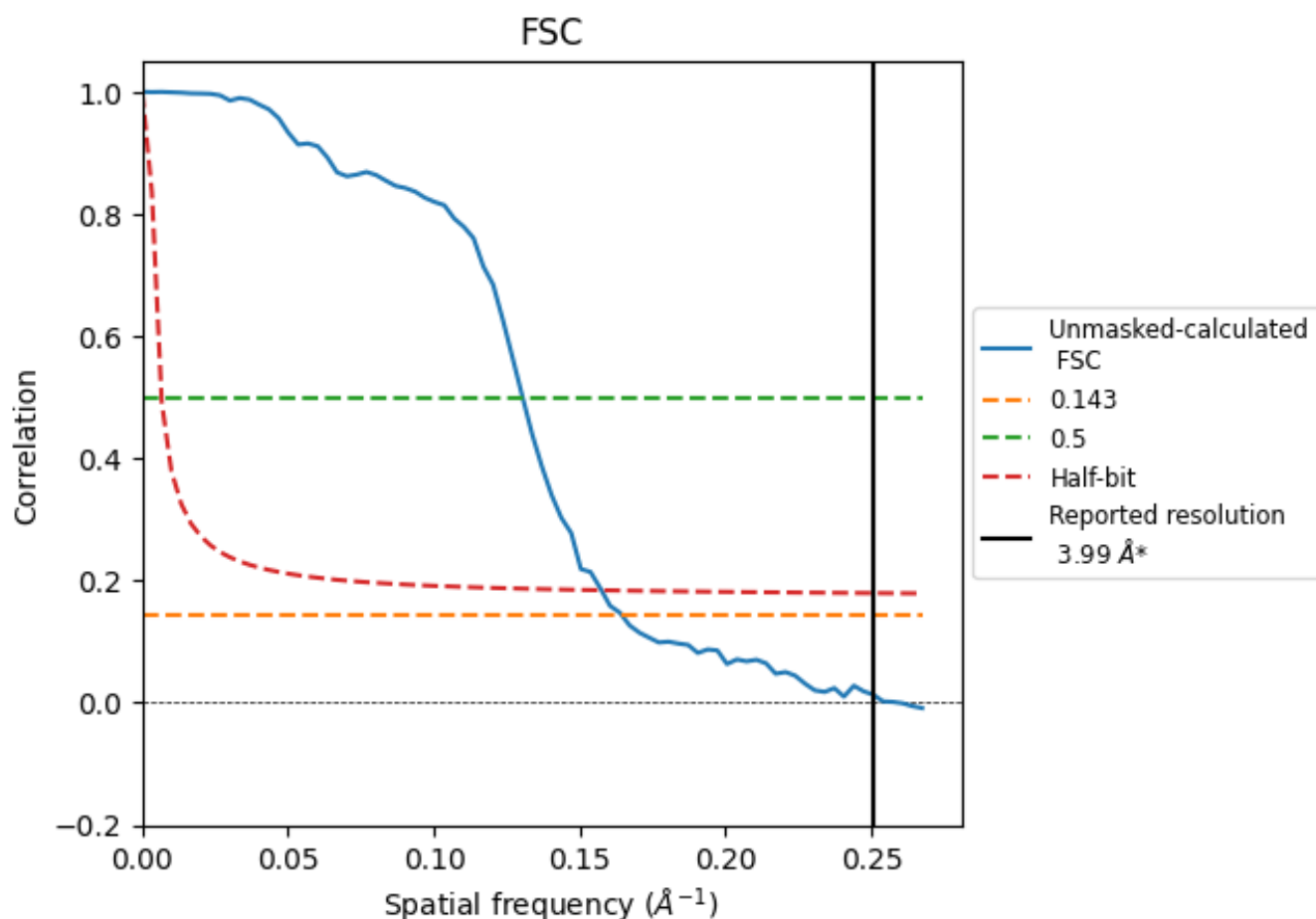


*Reported resolution corresponds to spatial frequency of 0.251 Å⁻¹

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 0.251 Å⁻¹

8.2 Resolution estimates [i](#)

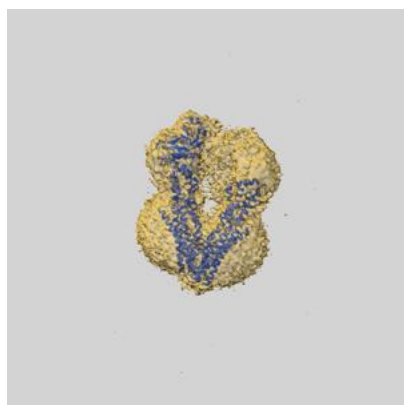
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.99	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.08	7.66	6.35

*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 6.08 differs from the reported value 3.99 by more than 10 %

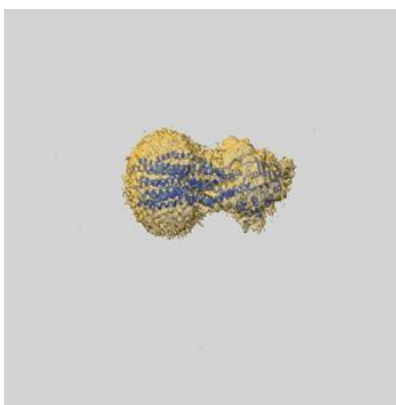
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-49368 and PDB model 9NFK. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

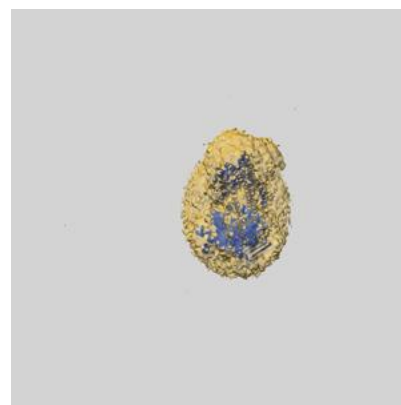
9.1 Map-model overlay [i](#)



X



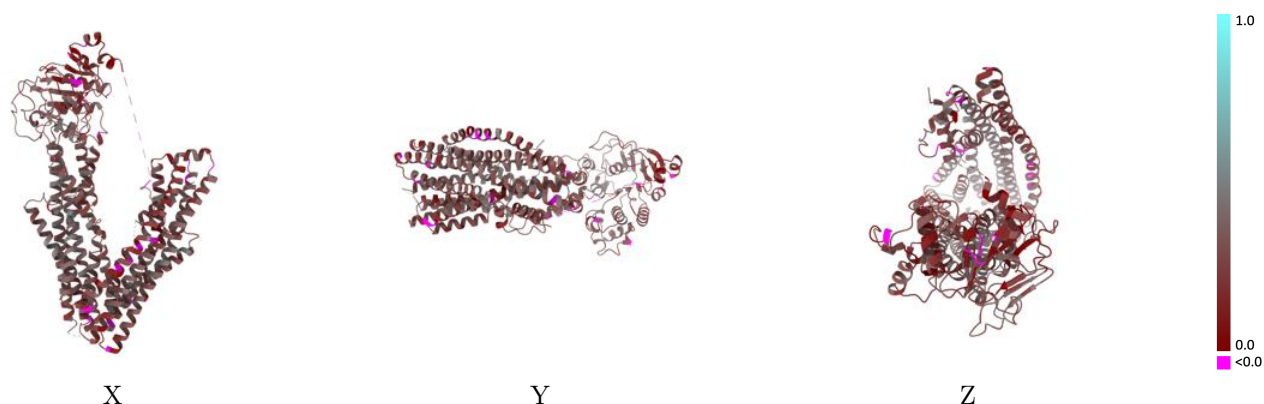
Y



Z

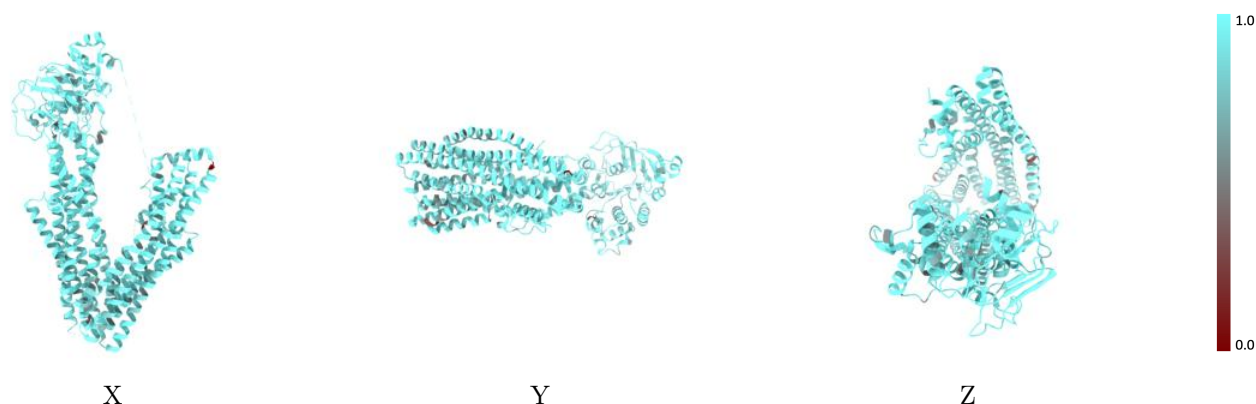
The images above show the 3D surface view of the map at the recommended contour level 0.13 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



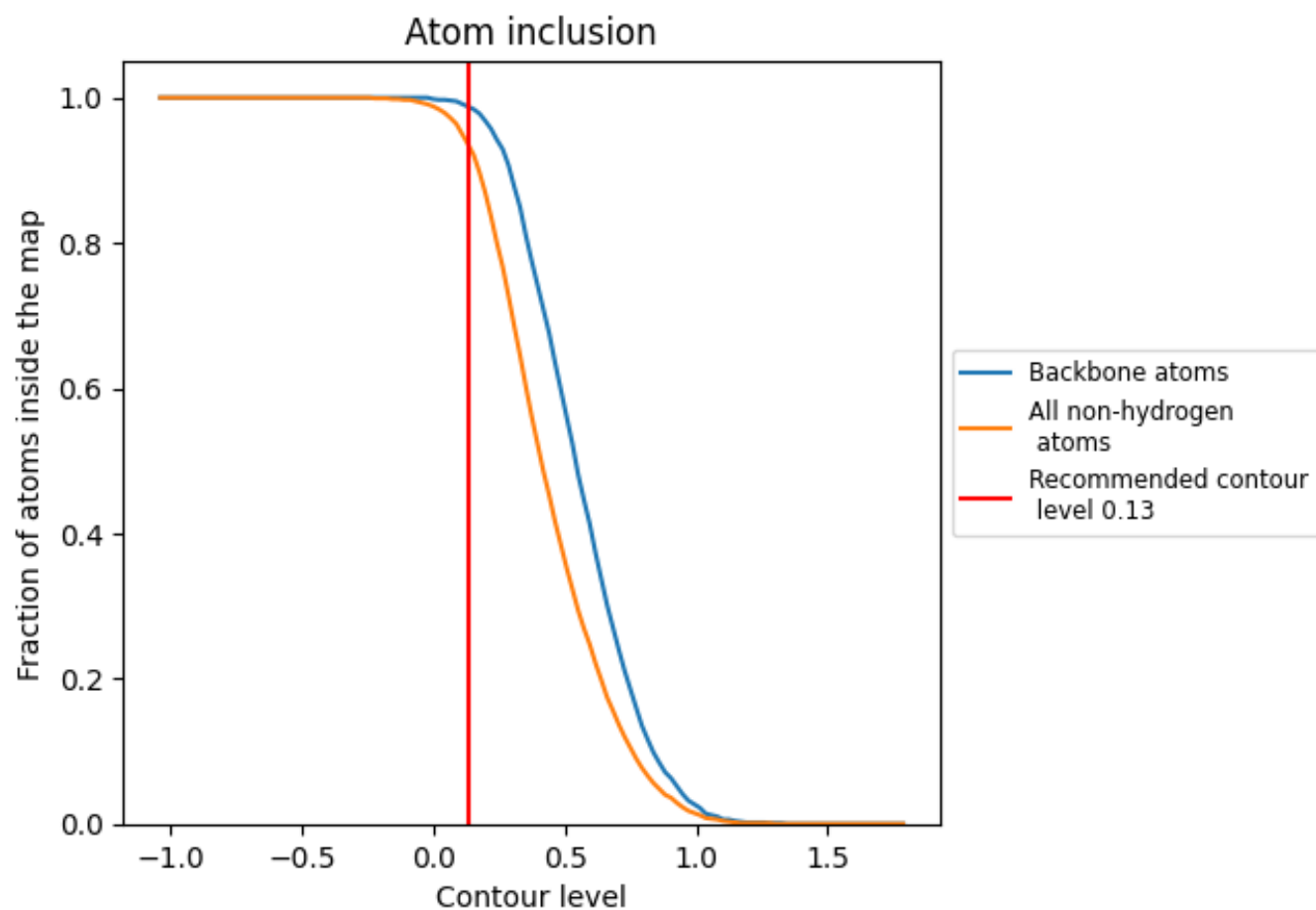
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.13).

9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 94% 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 (0.13) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9370	<div></div> 0.2850
A	<div></div> 0.9370	<div></div> 0.2850

