



## wwPDB EM Validation Summary Report ⓘ

Apr 5, 2026 – 08:45 PM UTC

PDB ID : 9YJW / pdb\_00009yjwt  
EMDB ID : EMD-73037  
Title : Transferrin Binding Protein A  
Authors : Dubey, S.; Noinaj, N.  
Deposited on : 2025-10-05  
Resolution : 4.20 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](mailto: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>.

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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

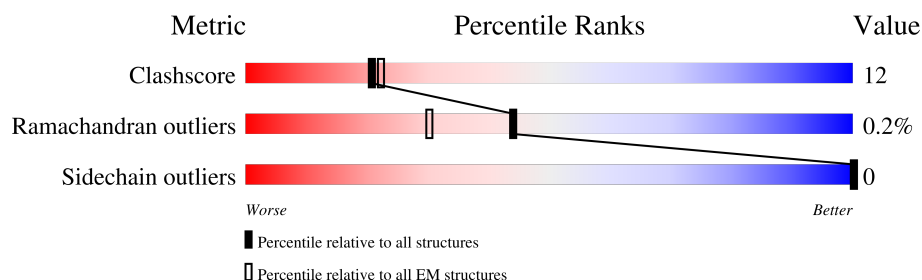
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.20 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	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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  $\geq 3$ , 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	915	<div> <div>77%</div> <div>66%26%8%</div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6609 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 Transferrin-binding protein A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	842	Total	C	N	O	S	0	0
			6609	4130	1196	1268	15		

There are 29 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q9JPJ0
A	2	SER	-	expression tag	UNP Q9JPJ0
A	3	ASN	-	expression tag	UNP Q9JPJ0
A	4	HIS	-	expression tag	UNP Q9JPJ0
A	5	HIS	-	expression tag	UNP Q9JPJ0
A	6	HIS	-	expression tag	UNP Q9JPJ0
A	7	HIS	-	expression tag	UNP Q9JPJ0
A	8	HIS	-	expression tag	UNP Q9JPJ0
A	9	HIS	-	expression tag	UNP Q9JPJ0
A	10	HIS	-	expression tag	UNP Q9JPJ0
A	11	HIS	-	expression tag	UNP Q9JPJ0
A	12	HIS	-	expression tag	UNP Q9JPJ0
A	13	HIS	-	expression tag	UNP Q9JPJ0
A	14	GLU	-	expression tag	UNP Q9JPJ0
A	15	ASN	-	expression tag	UNP Q9JPJ0
A	16	LEU	-	expression tag	UNP Q9JPJ0
A	17	TYR	-	expression tag	UNP Q9JPJ0
A	18	PHE	-	expression tag	UNP Q9JPJ0
A	19	GLN	-	expression tag	UNP Q9JPJ0
A	20	GLY	-	expression tag	UNP Q9JPJ0
A	21	ALA	-	expression tag	UNP Q9JPJ0
A	22	MET	-	expression tag	UNP Q9JPJ0
A	23	ASP	-	expression tag	UNP Q9JPJ0
A	24	ILE	-	expression tag	UNP Q9JPJ0
A	490	ALA	THR	conflict	UNP Q9JPJ0
A	499	MET	VAL	conflict	UNP Q9JPJ0
A	510	MET	LEU	conflict	UNP Q9JPJ0
A	764	MET	VAL	conflict	UNP Q9JPJ0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	870	MET	LEU	conflict	UNP Q9JPJ0



H859	F860	T861	L862	R863	A864	G865	V866	Y867	N868	L869	W870	N871	Y872	R873	Y874	V875	T876	W877	E878	N879	V880	R881	Q882	T883	A884	G885	G886	A887	V888	N889	Q890	H891	K892	N893	V894	G895	V896	Y897	N898	R899	Y900	A901	A902	P903	G904	R905	N906	Y907	T908	F909	S910	L911	E912	N913	K914	F915			
Q799	P800	E801	G802	K803	W804	G805	V806	N807	G808	W809	L810	T811	Y812	S813	K814	A815	K816	E817	I818	THR	GLU	LEU	GLY	SER	ARG	ALA	LEU	LEU	ASN	GLY	ASN	SER	ARG	ASN	THR	LYS	ALA	ALA	THR	ALA	R840	R841	T842	R843	P844	W845	Y846	I847	V848	D849	V850	S851	G852	Y853	Y854	T855	V856	K857	K858
L739	G740	K741	I742	D743	W744	N745	G746	V747	W748	D749	K750	L751	P752	E753	G754	W755	Y756	S757	T758	F759	A760	Y761	N762	R763	W764	R765	V766	R767	D768	I769	K770	K771	R772	A773	D774	R775	I776	D777	I778	Q779	S780	H781	L782	F783	D784	A785	I786	Q787	P788	S789	R790	Y791	V792	V793	G794	L795	G796	Y797	D798
N677	K678	E679	I682	V683	F684	K685	G686	D687	F688	G689	N690	L691	E692	A693	S694	W695	F696	N697	N698	R701	D702	L703	I704	V705	R706	G707	Y708	E709	A710	F648	Q711	I712	K713	D714	G715	K716	E717	E718	A719	K720	G721	D722	P723	A724	Y725	L726	N727	A728	Q729	S730	A731	R732	I733	T734	G735	I736	N737	I738	
V616	S617	T618	G619	T620	H621	R622	T623	L624	S625	W626	N627	I630	V631	L632	K633	P634	T635	D636	W637	L638	D639	L640	T641	Y642	R643	T644	S645	T646	G647	F648	R649	L650	P651	S652	F653	A654	E655	M656	Y657	G658	W659	R660	A661	G662	V663	Q664	S665	K666	A667	V668	K669	I670	D671	P672	E673	K674	S675	F676	
G552	R553	G554	N555	V556	V557	T558	G559	Q560	I561	C562	R563	L564	G565	N566	N567	T568	Y569	T570	D571	C572	T573	P574	R575	S576	I577	N578	G579	K580	S581	Y582	Y583	A584	A585	V586	N589	V590	R591	L592	G593	R594	V595	A596	D597	L602	R603	Y604	D605	Y606	R607	S608	T609	H610	S611	D612	G614	S615			

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	66000	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 ( $e^-/\text{\AA}^2$ )	56	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.532	Depositor
Minimum map value	-0.280	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.186	Depositor
Map size (Å)	261.12, 261.12, 261.12	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.02, 1.02, 1.02	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	0.22	0/6760	0.38	0/9139

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	6609	0	6323	155	0
All	All	6609	0	6323	155	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 12.

The worst 5 of 155 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:160:VAL:HA	1:A:603:ARG:HD2	1.58	0.85
1:A:108:ARG:HH11	1:A:649:ARG:HH22	1.30	0.80
1:A:167:LEU:HD11	1:A:675:SER:HB3	1.63	0.79
1:A:799:GLN:HE22	1:A:804:TRP:HB2	1.51	0.74
1:A:232:ALA:HB1	1:A:901:ALA:HB3	1.68	0.73



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	838/915 (92%)	755 (90%)	81 (10%)	2 (0%)	43 77

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	613	ASP
1	A	815	ALA

### 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	680/749 (91%)	680 (100%)	0	100 100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	799	GLN
1	A	477	HIS
1	A	416	ASN
1	A	374	HIS

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Mol	Chain	Res	Type
1	A	439	ASN

### 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.

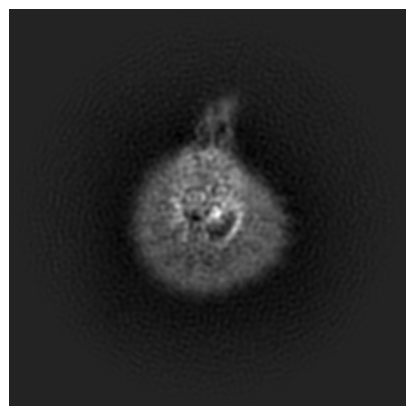
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-73037. These allow visual inspection of the internal detail of the map and identification of artifacts.

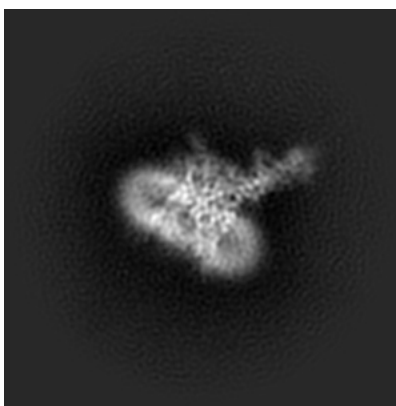
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

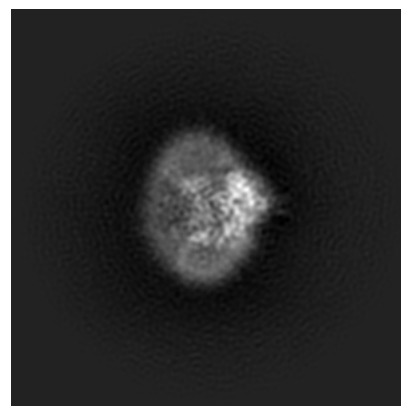
#### 6.1.1 Primary map



X

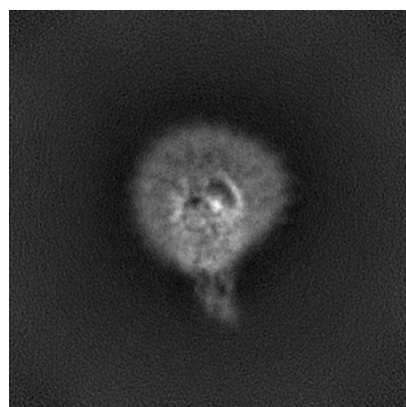


Y

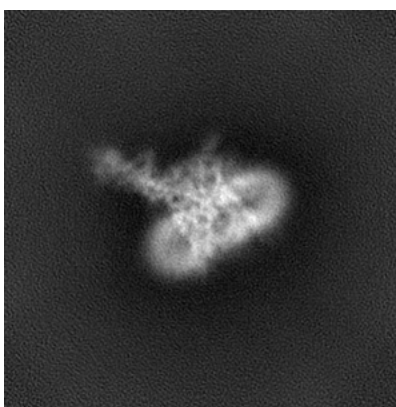


Z

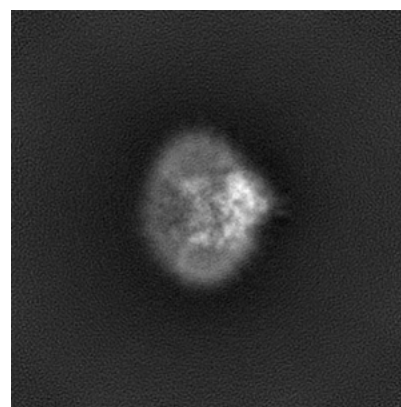
#### 6.1.2 Raw map



X



Y

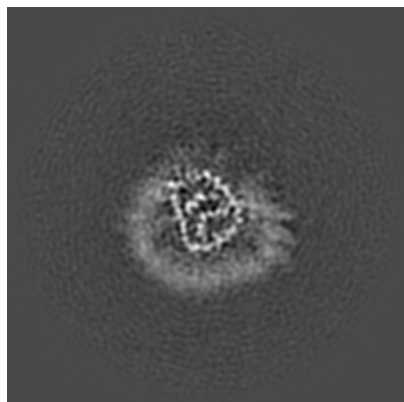


Z

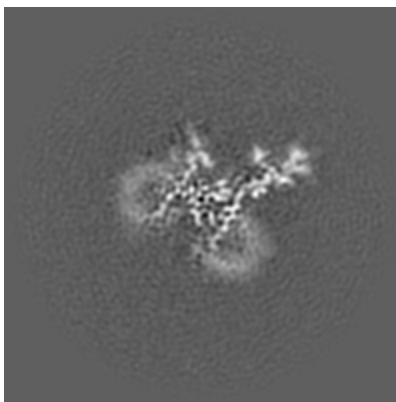
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

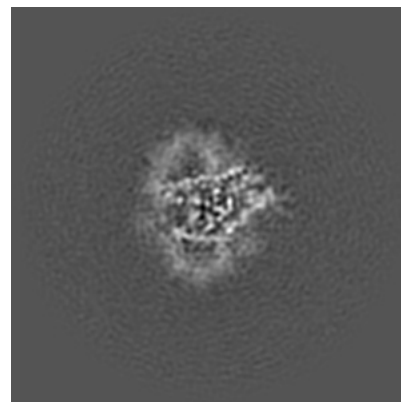
### 6.2.1 Primary map



X Index: 128

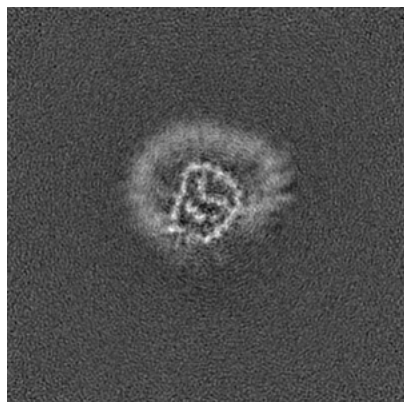


Y Index: 128

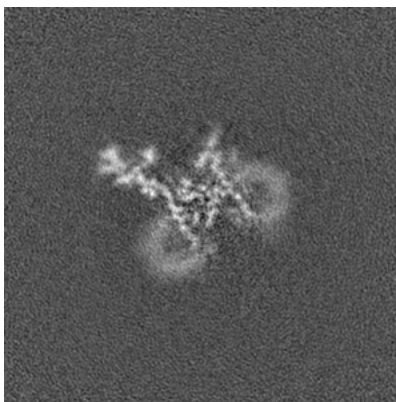


Z Index: 128

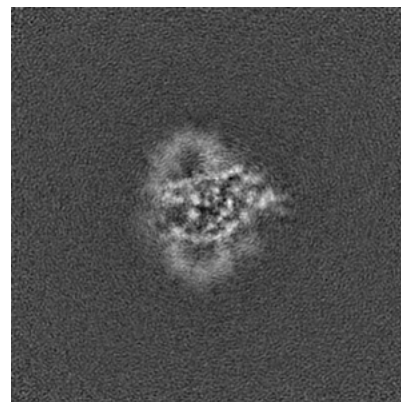
### 6.2.2 Raw map



X Index: 128



Y Index: 128

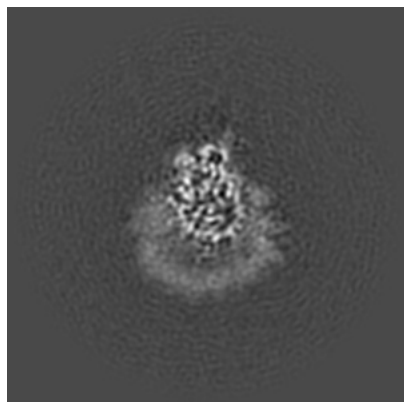


Z Index: 128

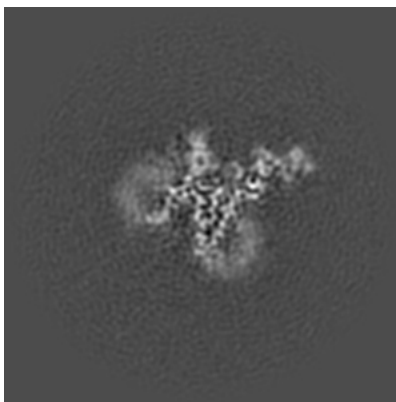
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

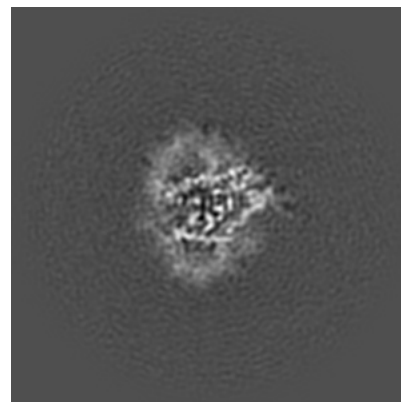
### 6.3.1 Primary map



X Index: 138

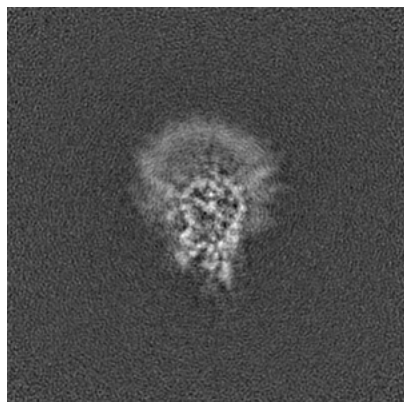


Y Index: 133

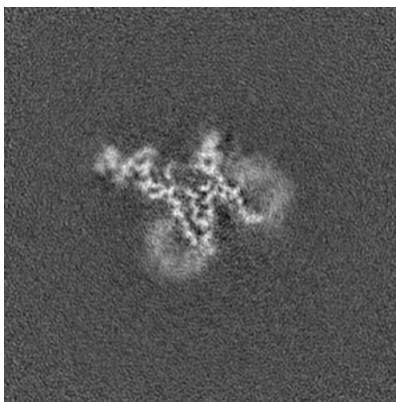


Z Index: 129

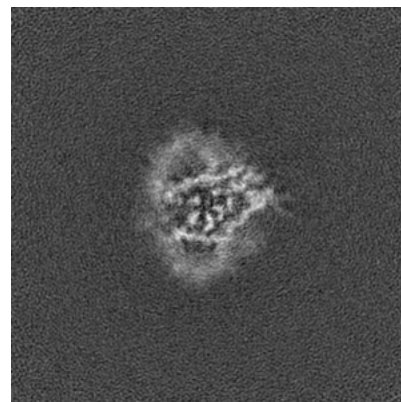
### 6.3.2 Raw map



X Index: 140



Y Index: 132



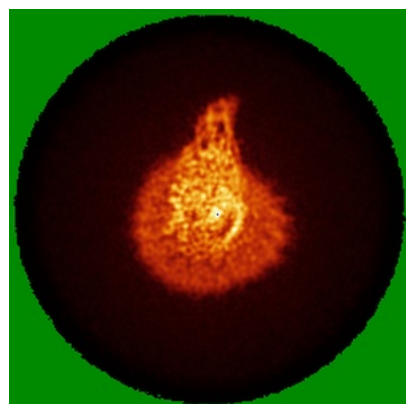
Z Index: 126

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

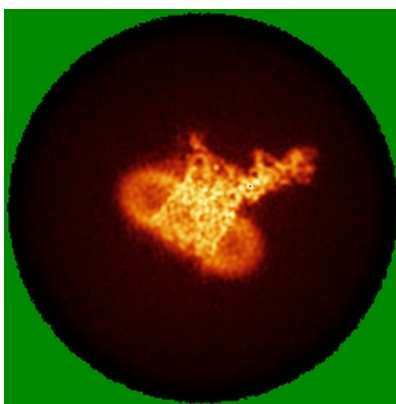


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

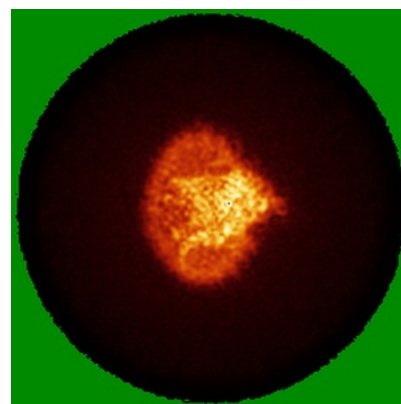
### 6.4.1 Primary map



X

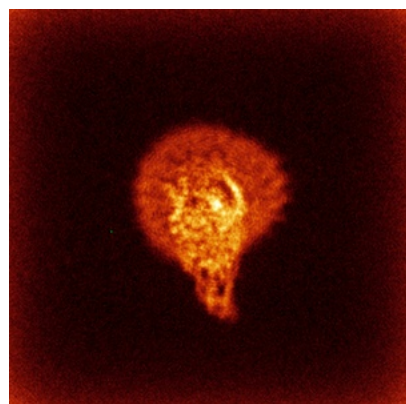


Y

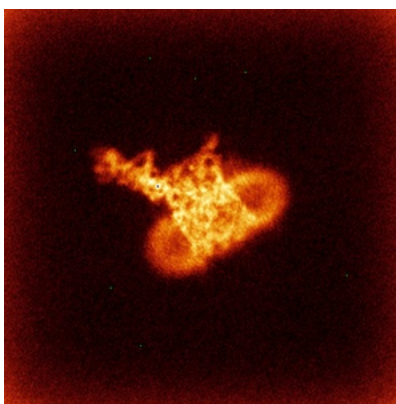


Z

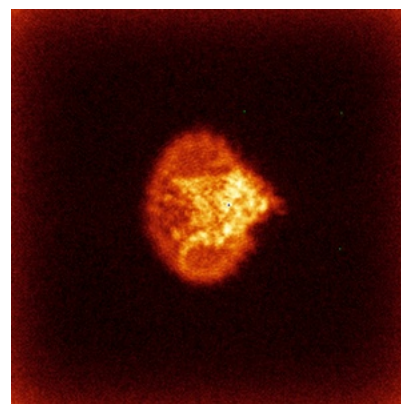
### 6.4.2 Raw map



X



Y

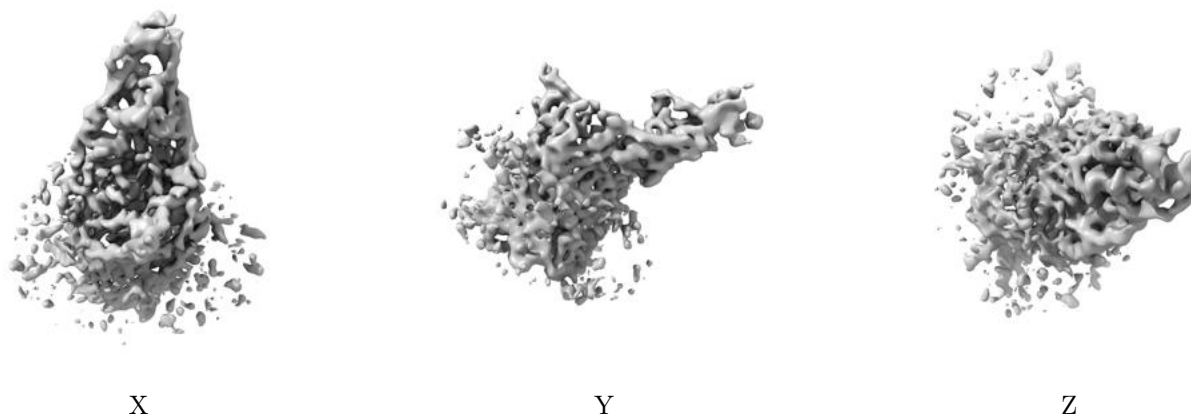


Z

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 0.186. 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.

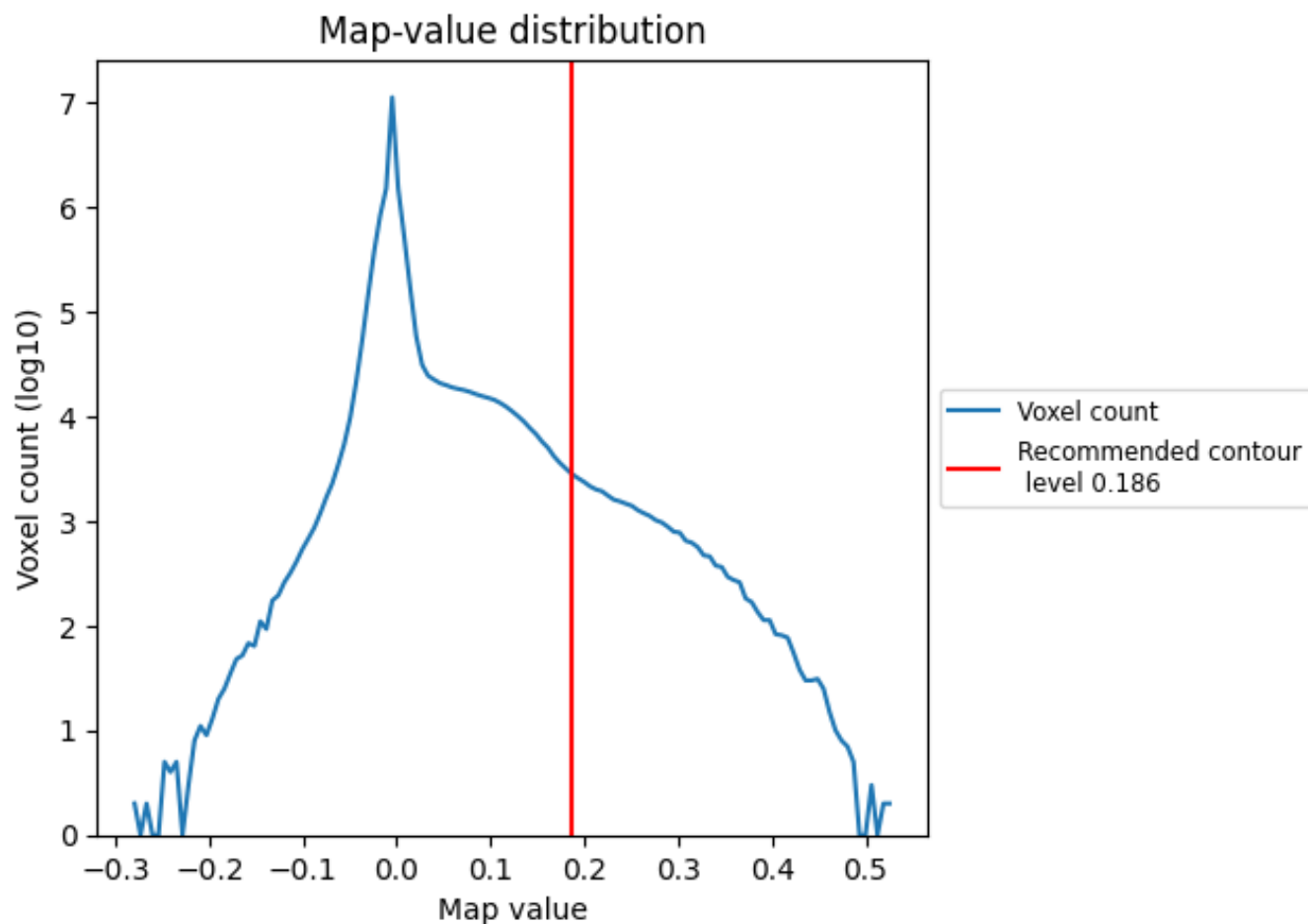
## 6.6 Mask visualisation [i](#)

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.

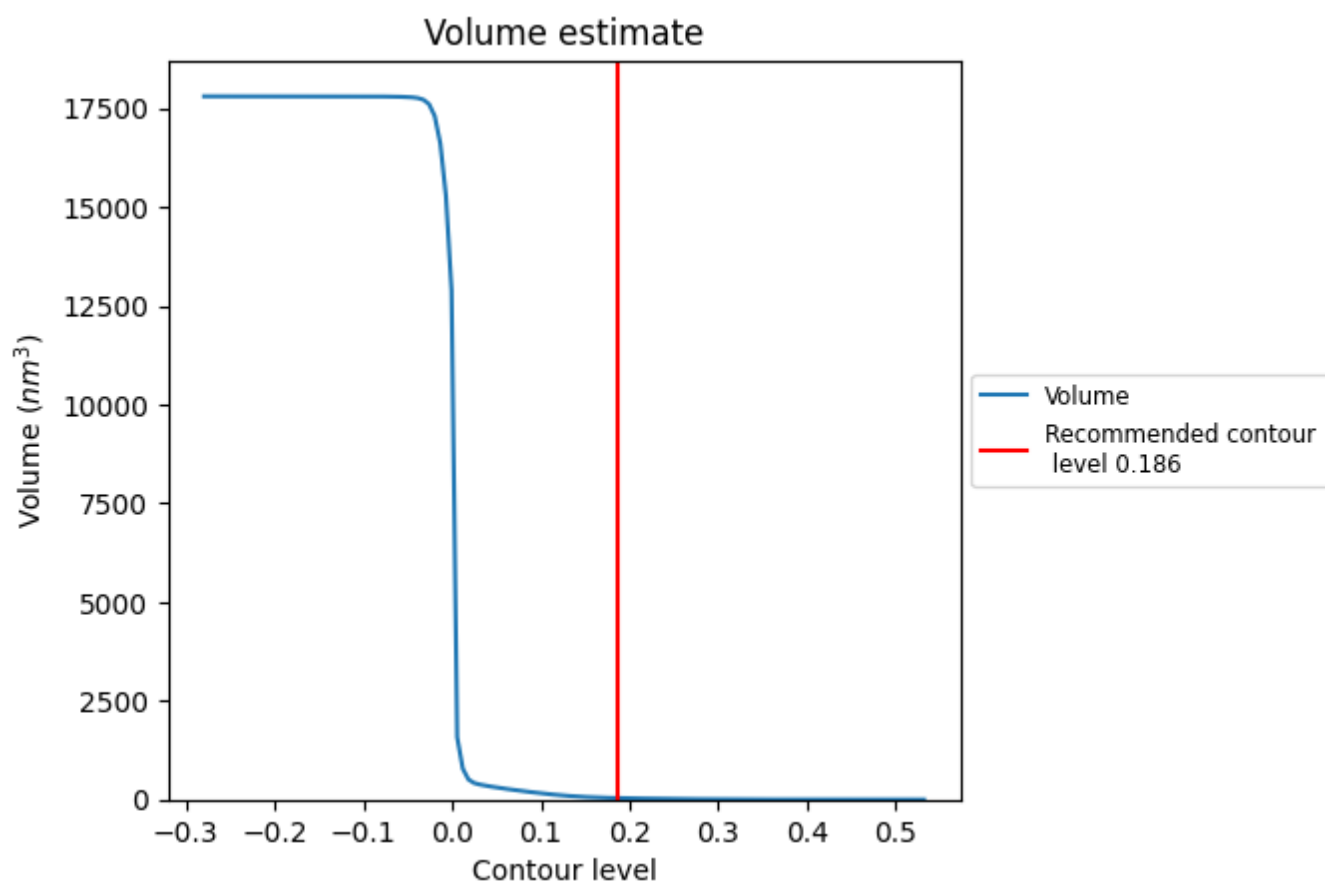
### 7.1 Map-value distribution [i](#)



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.



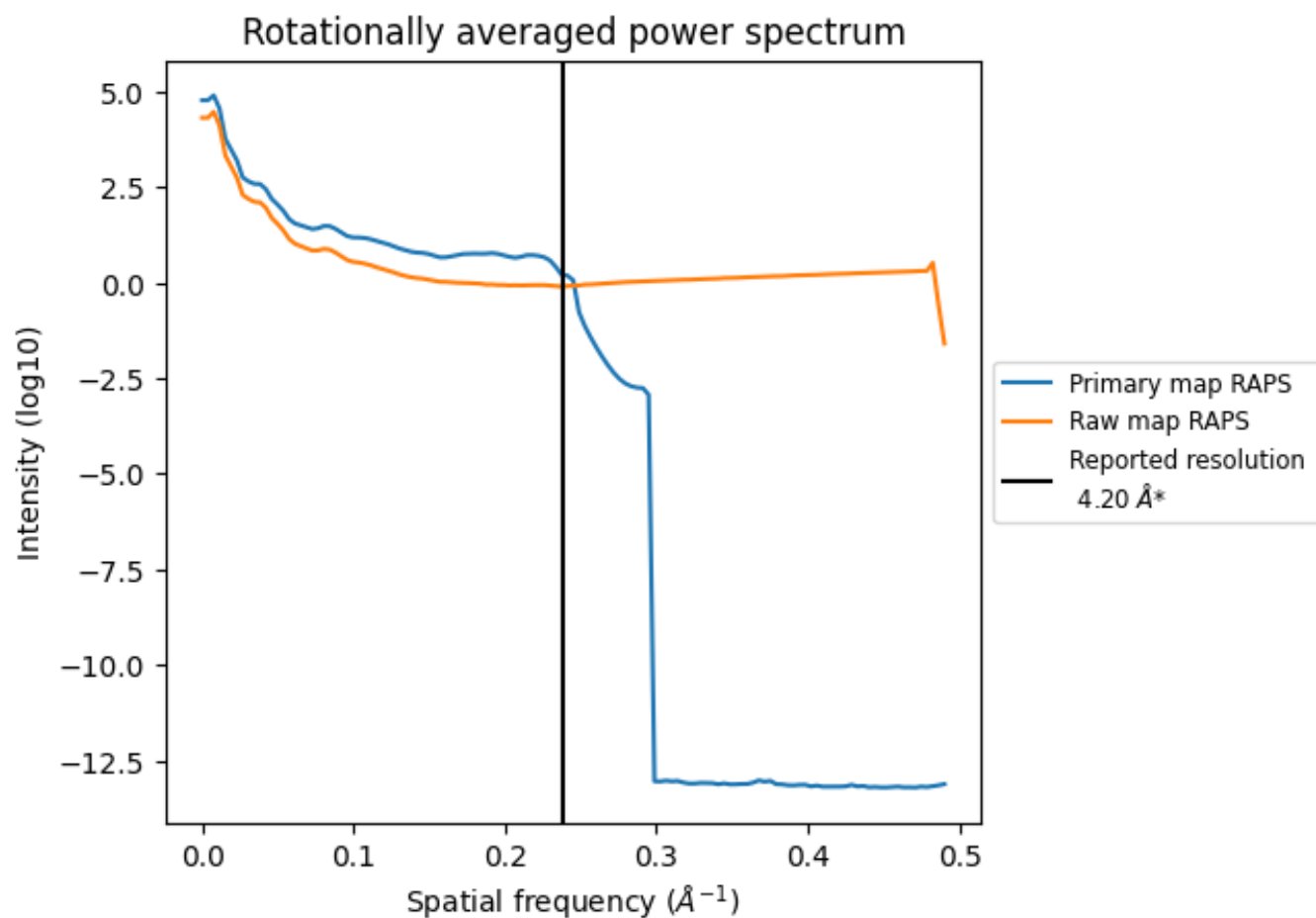
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 38 nm<sup>3</sup>; this corresponds to an approximate mass of 34 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 ⓘ

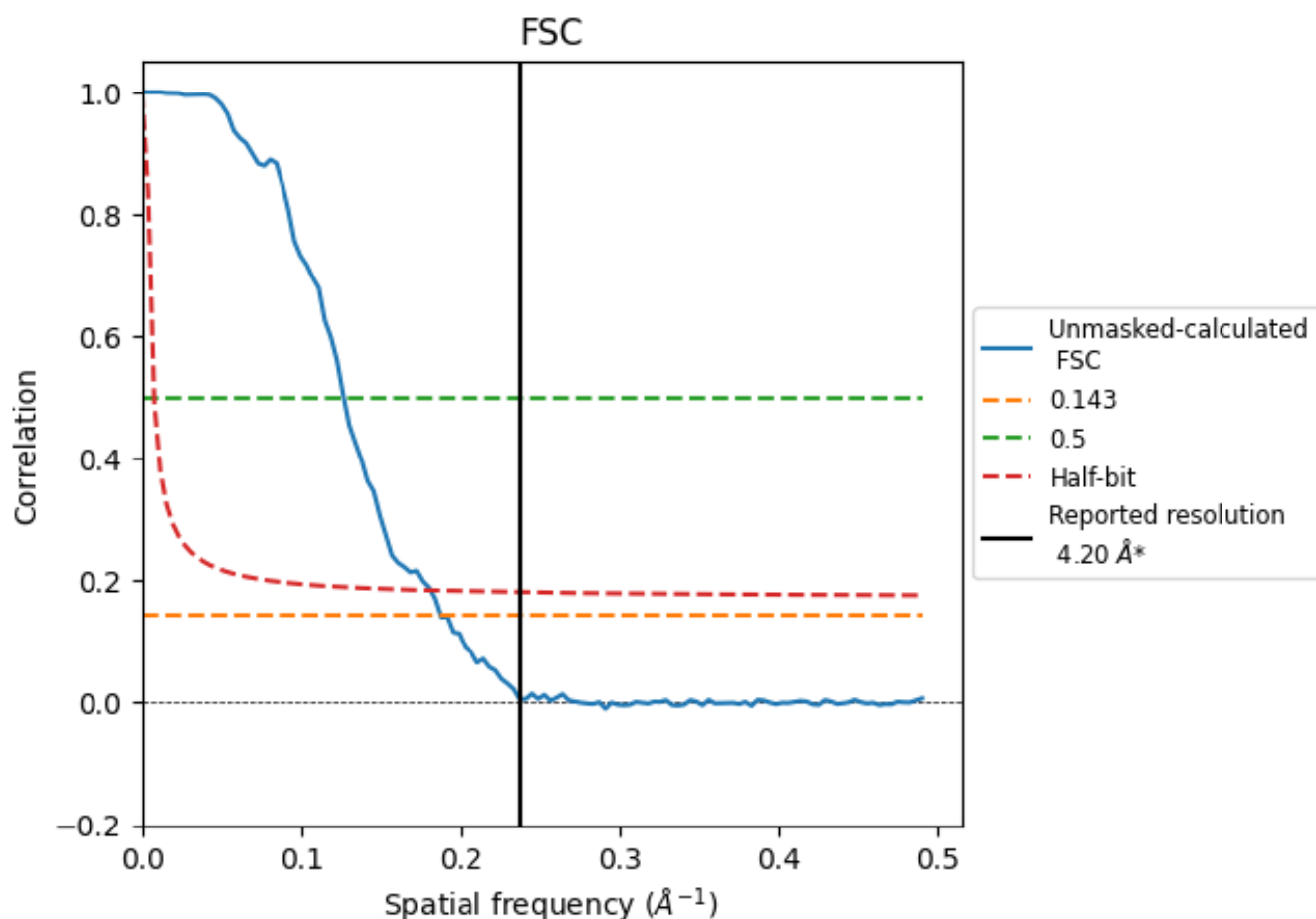


\*Reported resolution corresponds to spatial frequency of 0.238 Å<sup>-1</sup>

## 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 0.238 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

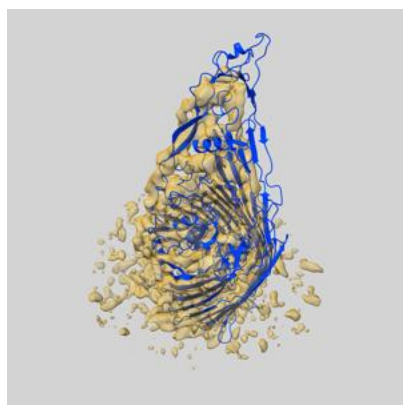
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	5.34	7.89	5.52

\*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 5.34 differs from the reported value 4.2 by more than 10 %

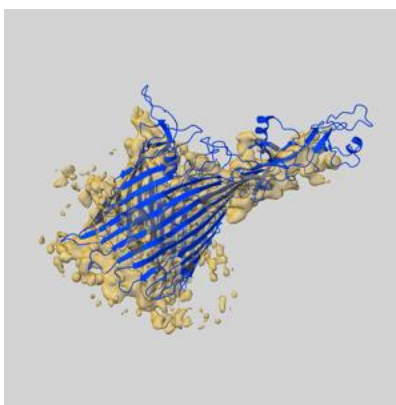
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-73037 and PDB model 9YJW. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

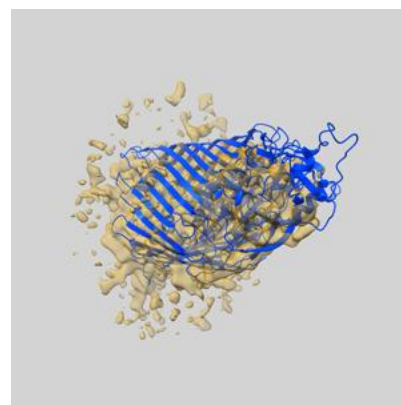
### 9.1 Map-model overlay [i](#)



X



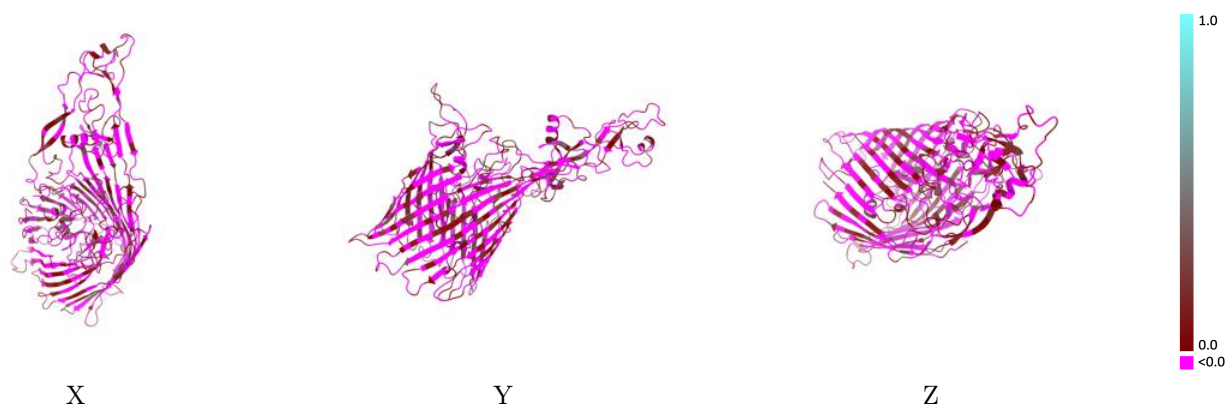
Y



Z

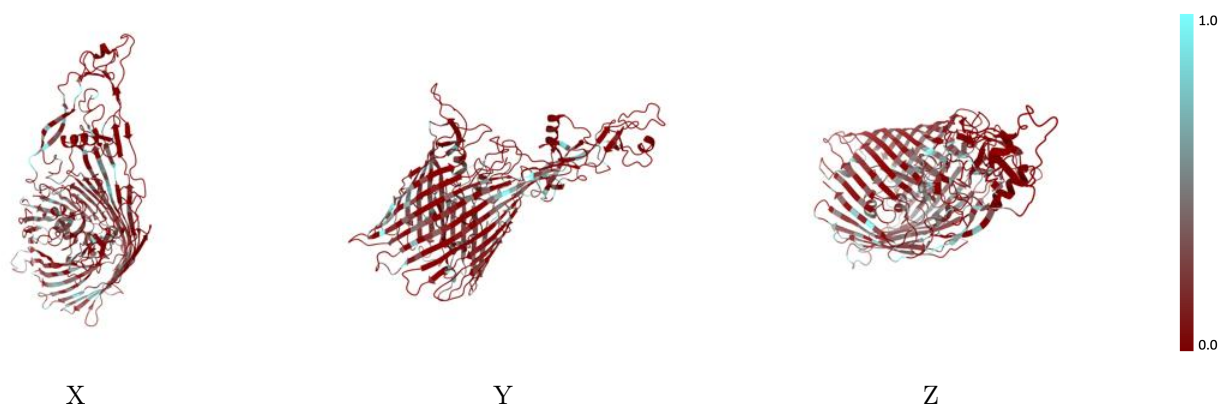
The images above show the 3D surface view of the map at the recommended contour level 0.186 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



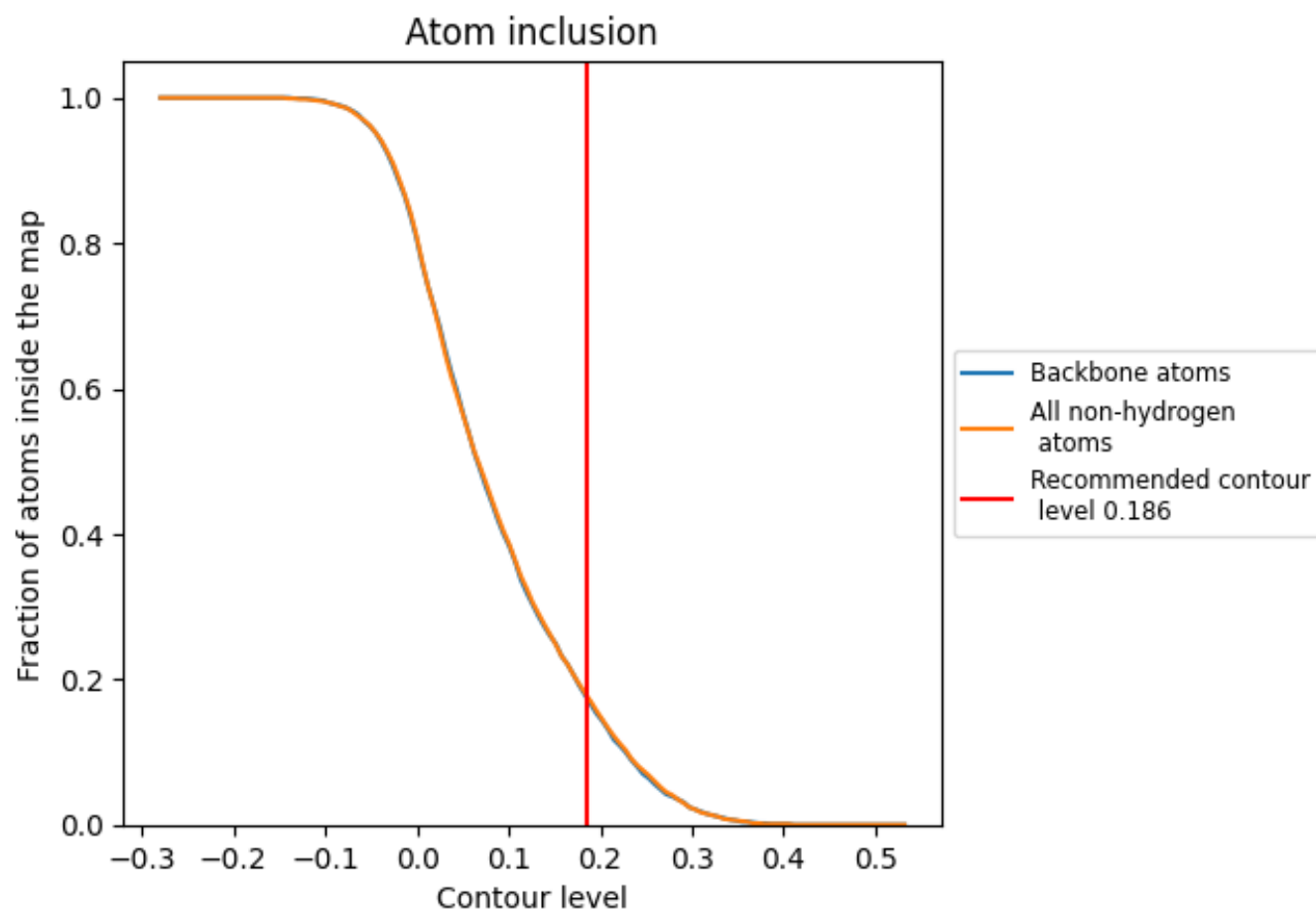
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.186).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 17% of all backbone atoms, 18% 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 (0.186) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.1760	<div></div> -0.0260
A	<div></div> 0.1760	<div></div> -0.0260

