



wwPDB EM Validation Summary Report ⓘ

Dec 16, 2024 – 12:32 PM EST

PDB ID : 9BD8
EMDB ID : EMD-44446
Title : ApoB 100 beta barrel bound to LDLR beta propeller
Authors : Dearborn, A.D.; Reimund, M.; Graziano, G.; Lei, H.; Kumar, A.; Neufeld, E.B.; Remaley, A.T.; Marcotrigiano, J.
Deposited on : 2024-04-11
Resolution : 4.80 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
Mogul : 2022.3.0, CSD as543be (2022)
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

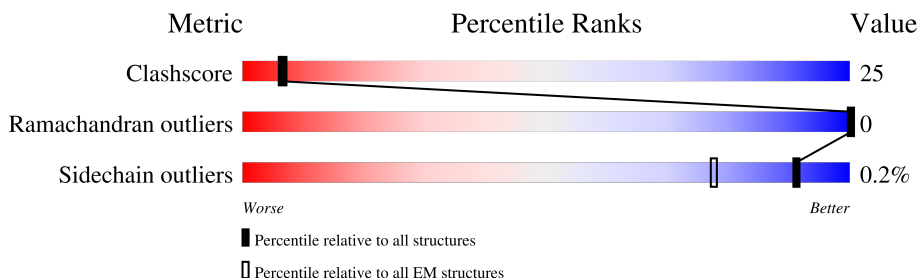
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.80 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	4563	
2	B	860	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 5369 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.

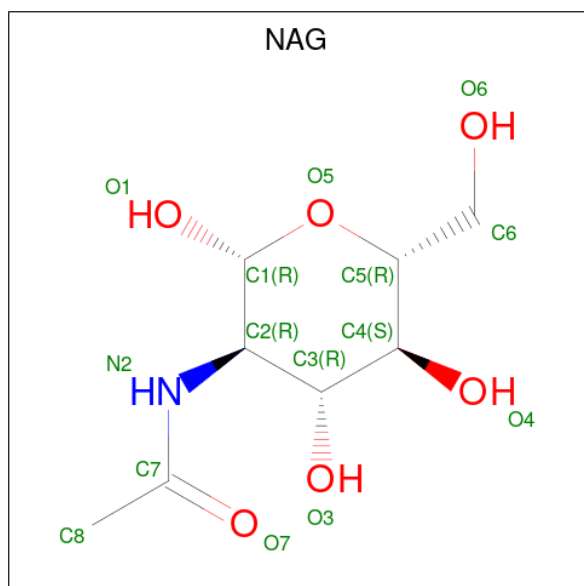
- Molecule 1 is a protein called Apolipoprotein B-100.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	462	Total	C	N	O	S	0	0
			3423	2163	565	680	15		

- Molecule 2 is a protein called Low-density lipoprotein receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	264	Total	C	N	O	S	0	0
			1932	1235	314	378	5		

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			14	8	1	5	







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

- Molecule 2: Low-density lipoprotein receptor

Chain B:  15% 16% 69%

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

[illegible]

V436	A437	S438		I441	Y442	W443	S444	D445	L446	S447		M450	T451	C452	S453	T454	R458	ALA	HIS	GLY	VAL	SER	SER	D465	D466	T467	V468	I469	S470	R471	D472	I473		D477	G478	L479	A480	V481	D482	V483	L484	H485	S486	N487	L488	Y489	W490	T491	D492	S493	V494	L495	G496	T497	V498	S499	V500
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Category	Count
L582	10
H583	10
S584	10
L585	10
S586	10
S587	10
I588	10
G593	10
T597	10
I598	10
L599	10
A606	10
H607	10
P608	10
F609	10
S610	10
L611	10
D616	10
K617	10
V618	10
F619	10
W620	10
T621	10
D622	10
I623	10
I624	10
N625	10
E626	10
A627	10
I628	10
F629	10
S630	10
A631	10
B632	10
R633	10
S637	10
N640	10
L641	10
L642	10
A643	10
L646	10
L647	10
S648	10
P649	10
E650	10
D651	10
M652	10
V653	10
L654	10
F655	10
H656	10

L658	L659	Q660	R661	R662		N665	N666	P667	GLU	ARG	THR	THR	LEU	SER	ASN	GLY	CYS	GLN	TYR	LEU	CYS	PRO	ALA	GLN	ILE	ASN	PRO	HIS	SER	PRO	LYS	PHE	THR	CYS	ALA	CYS	PRO	ASP	GLY	MET	LEU	ALA	ARG	ASP	ARG	MET	SER	CYS	LEU	THR	GLU	ALA	GLU	ALA	ALA
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VAL	ALA	THR	GLU	THR	SER	THR	VAL	ARG	LEU	LYS	VAL	SER	SER	THR	ALA	ALA	VAL	ARG	THR	GLN	HIS	THR	THR	THR	THR	ARG	PRO	PRO	VAL	VAL	PRO	ASP	THR	SER	SER	ARG	LEU	GLY	GLA	GLY	ALA	THR	THR	PRO	PRO	GLU	LEU	THR	THR	THR	VAL	GLU	ILE	LEU	VAL	VAL	THR	MET	SER	HIS	GLN	ALA	ALA	VAL	ALA	GLY	GLY	ARG
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GLY	ASN	GLU	LYS	PRO	SER	SER	VAL	ARG	ALA	LEU	SER	ILE	VAL	LEU	LEU	VAL	VAL	PHE	PHE	LEU	LEU	TRP	LYS	ASN	ASN	TRP	ARG	LEU	LYS	ASN	ASN	PHE	ASP	ASN	VAL	VAL	TYR	GLN	LYS	THR	THR	GLU	ASP	GLU	VAL	VAL	HIS	ILE
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CYS	HIS	ASN	GLN	ASP	GLY	TYR	SER	TYR	PRO	SER	ARG	GLN	MET	VAL	SER	LEU	GLU	ASP	ASP	VAL	ALA
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	522863	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 ($e^-/\text{\AA}^2$)	51.38	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	0.366	Depositor
Minimum map value	-0.134	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	557.76, 557.76, 557.76	wwPDB
Map dimensions	336, 336, 336	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.6600001, 1.6600001, 1.6600001	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.26	0/3483	0.49	0/4744
2	B	0.25	0/1978	0.52	0/2723
All	All	0.26	0/5461	0.50	0/7467

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

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	3423	0	3243	153	0
2	B	1932	0	1728	107	0
3	A	14	0	13	0	0
All	All	5369	0	4984	257	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 25.

The worst 5 of 257 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)
2:B:468:VAL:HG12	2:B:469:ILE:HG12	1.60	0.81
2:B:540:ALA:HB1	2:B:562:TRP:H	1.47	0.80
1:A:294:ILE:HG22	1:A:296:SER:H	1.53	0.74
2:B:480:ALA:HB3	2:B:489:TYR:HB2	1.70	0.74
1:A:238:LEU:HB2	1:A:269:PRO:HD3	1.69	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	446/4563 (10%)	425 (95%)	21 (5%)	0	100	100
2	B	260/860 (30%)	225 (86%)	35 (14%)	0	100	100
All	All	706/5423 (13%)	650 (92%)	56 (8%)	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	366/4080 (9%)	365 (100%)	1 (0%)	91	92
2	B	193/755 (26%)	193 (100%)	0	100	100
All	All	559/4835 (12%)	558 (100%)	1 (0%)	91	94

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

Mol	Chain	Res	Type
1	A	349	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	HIS
1	A	902	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](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	A	4601	1	14,14,15	0.70	0	17,19,21	0.79	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	4601	1	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	4601	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

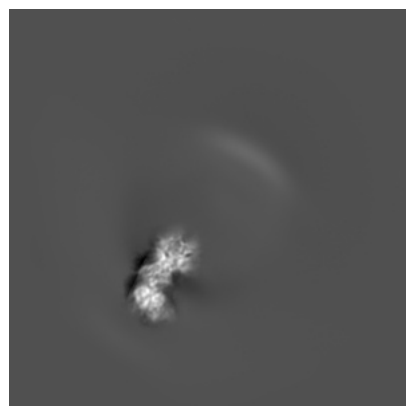
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44446. 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

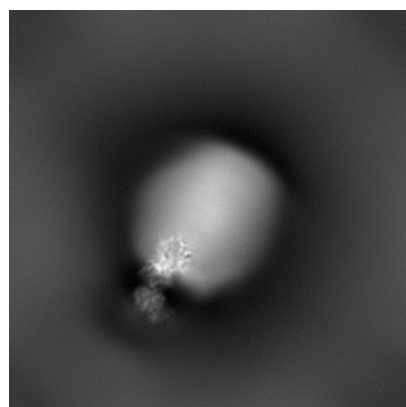


Y

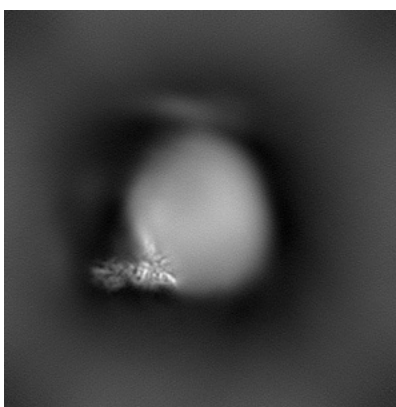


Z

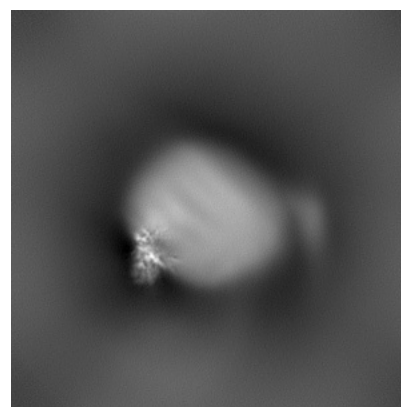
6.1.2 Raw map



X



Y

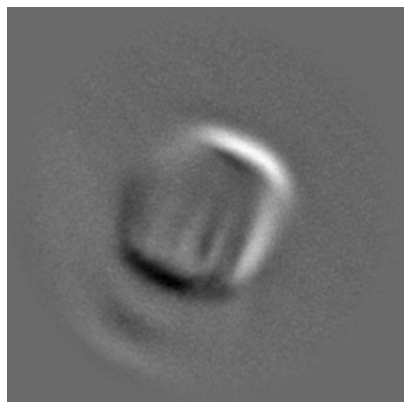


Z

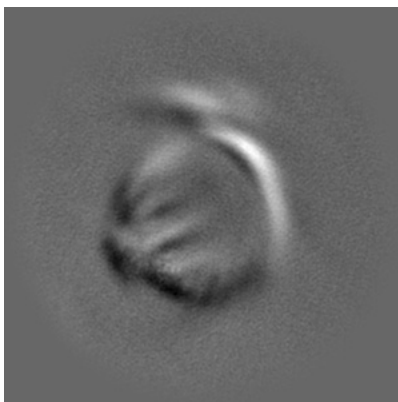
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

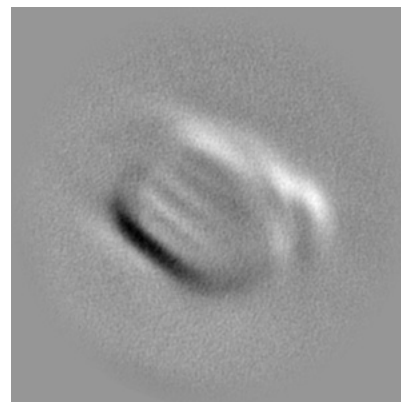
6.2.1 Primary map



X Index: 168

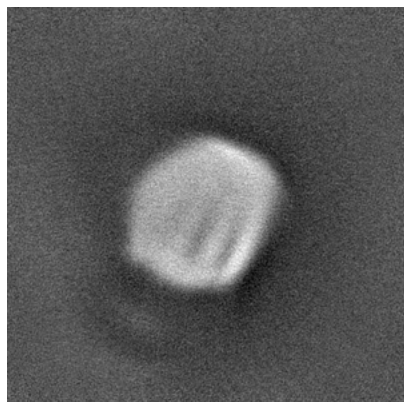


Y Index: 168

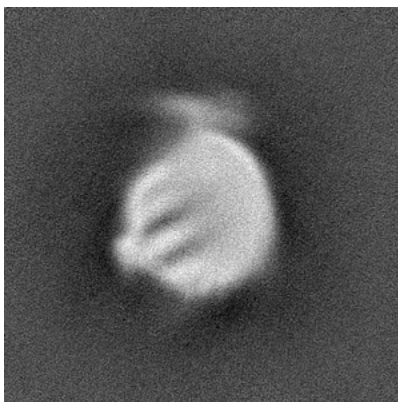


Z Index: 168

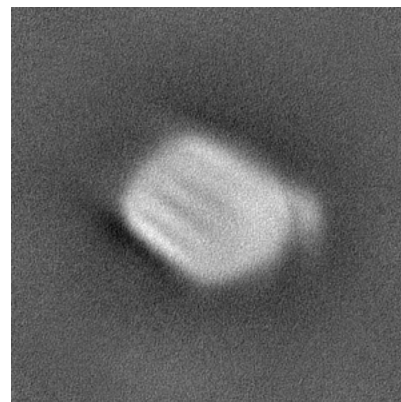
6.2.2 Raw map



X Index: 168



Y Index: 168

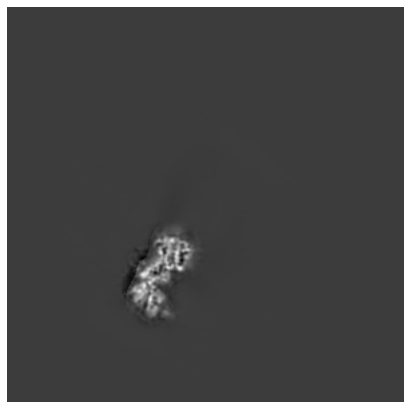


Z Index: 168

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

6.3 Largest variance slices [i](#)

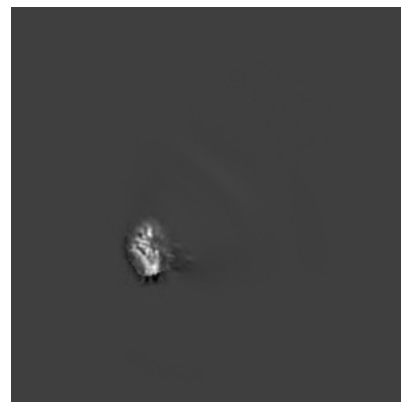
6.3.1 Primary map



X Index: 111

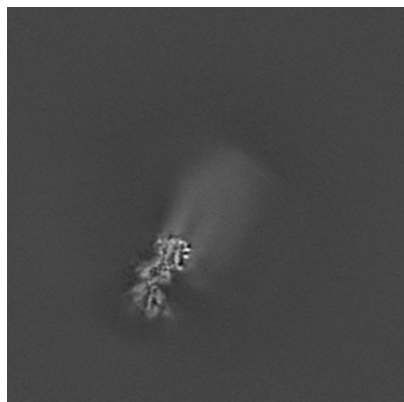


Y Index: 122

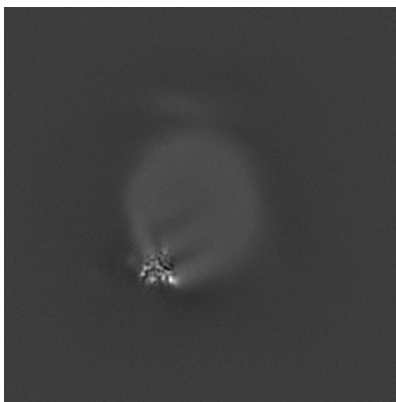


Z Index: 118

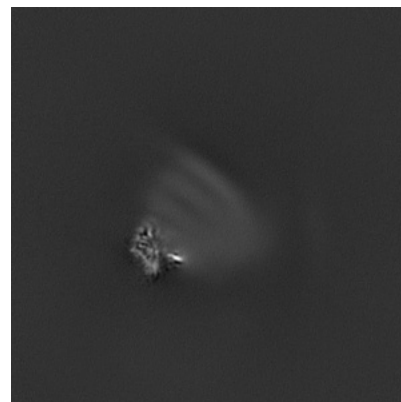
6.3.2 Raw map



X Index: 112



Y Index: 144

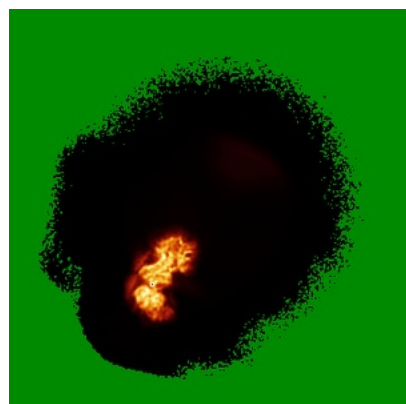


Z Index: 119

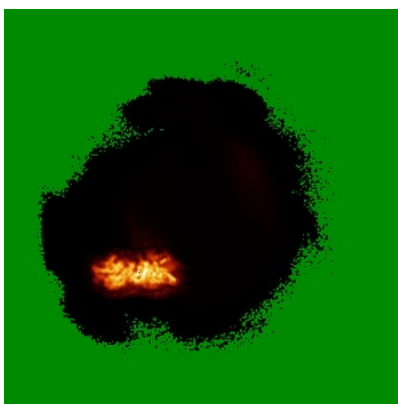
The images above show the largest variance slices of the map in three orthogonal directions.

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

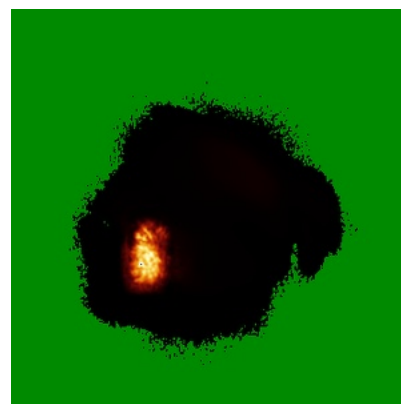
6.4.1 Primary map



X

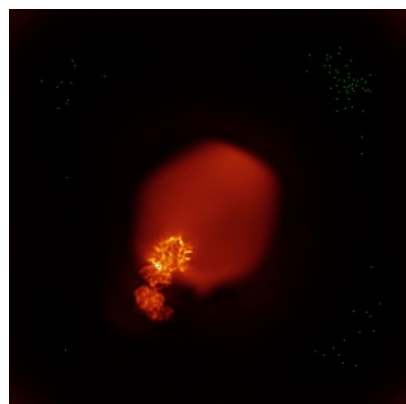


Y

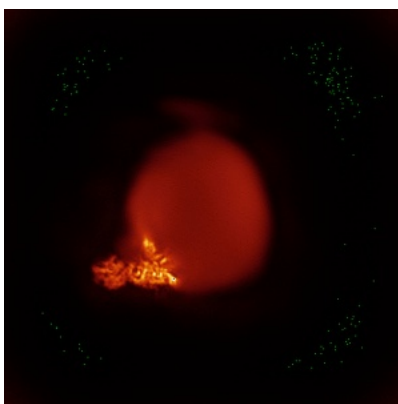


Z

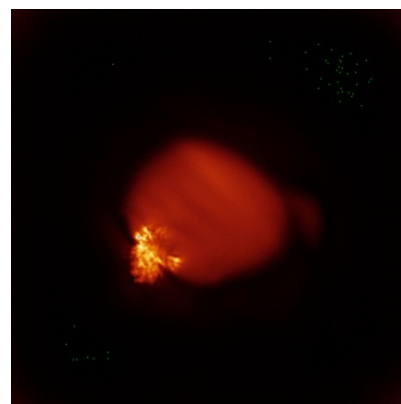
6.4.2 Raw map



X



Y

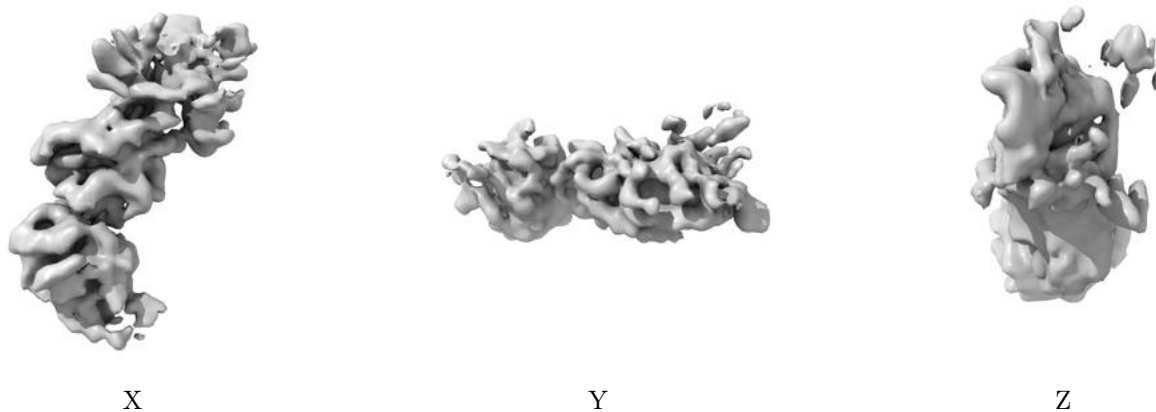


Z

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.

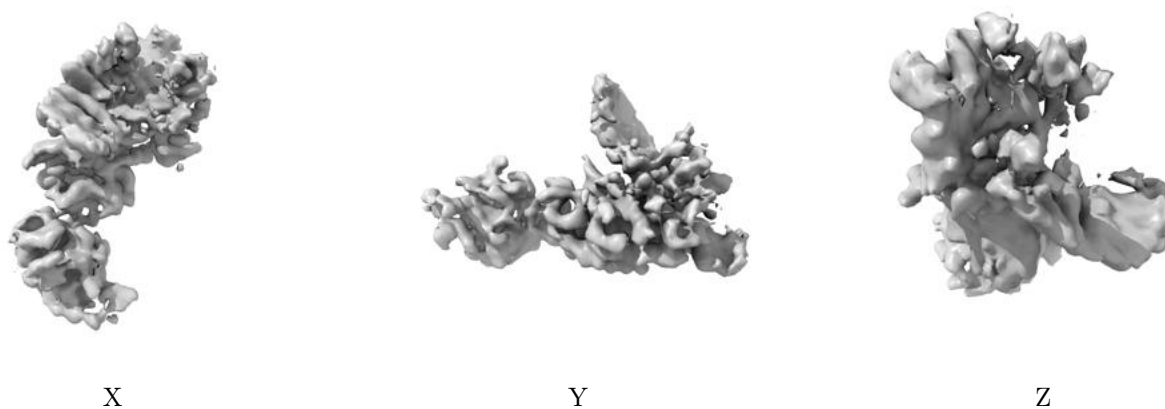
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. 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.

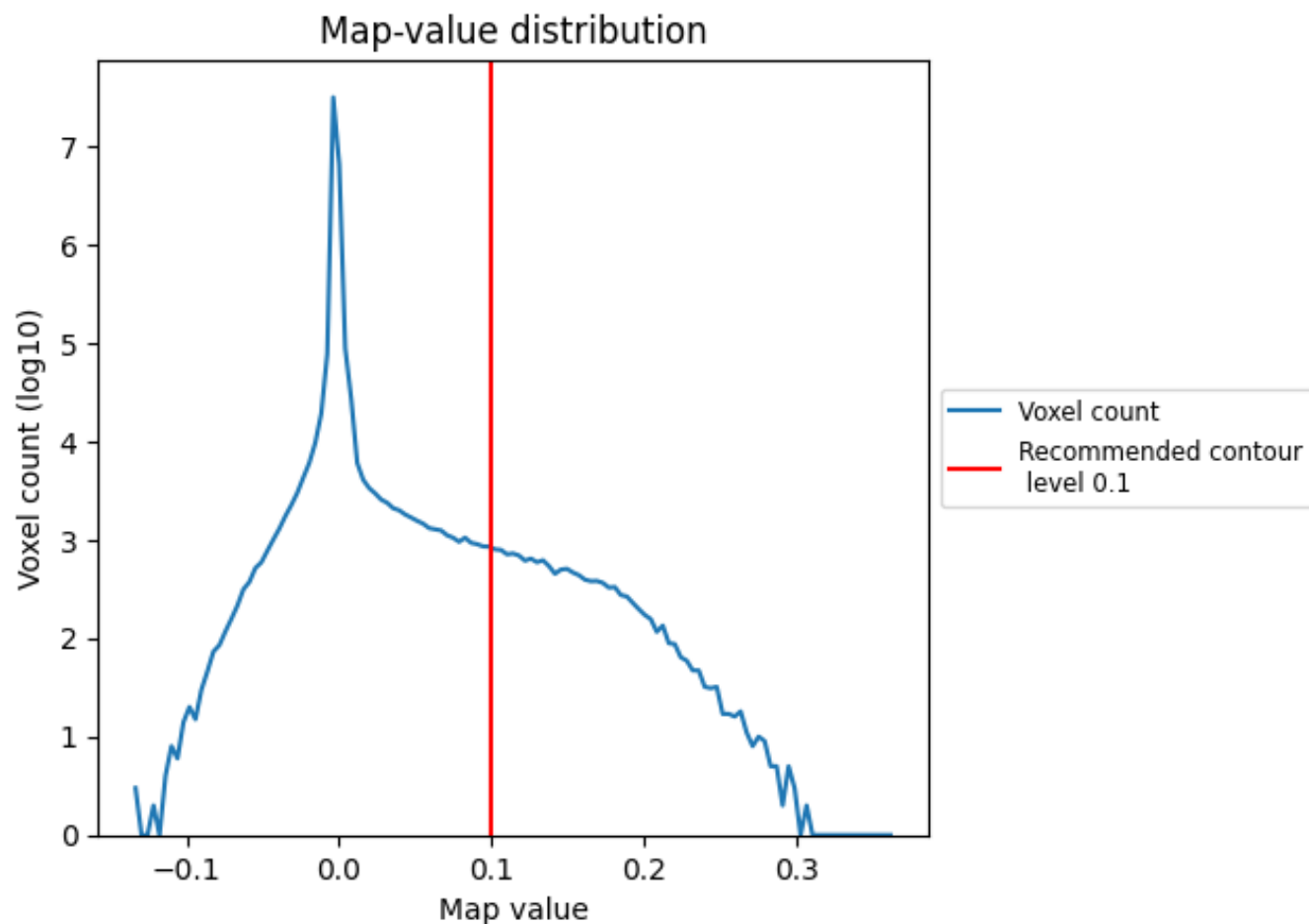
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

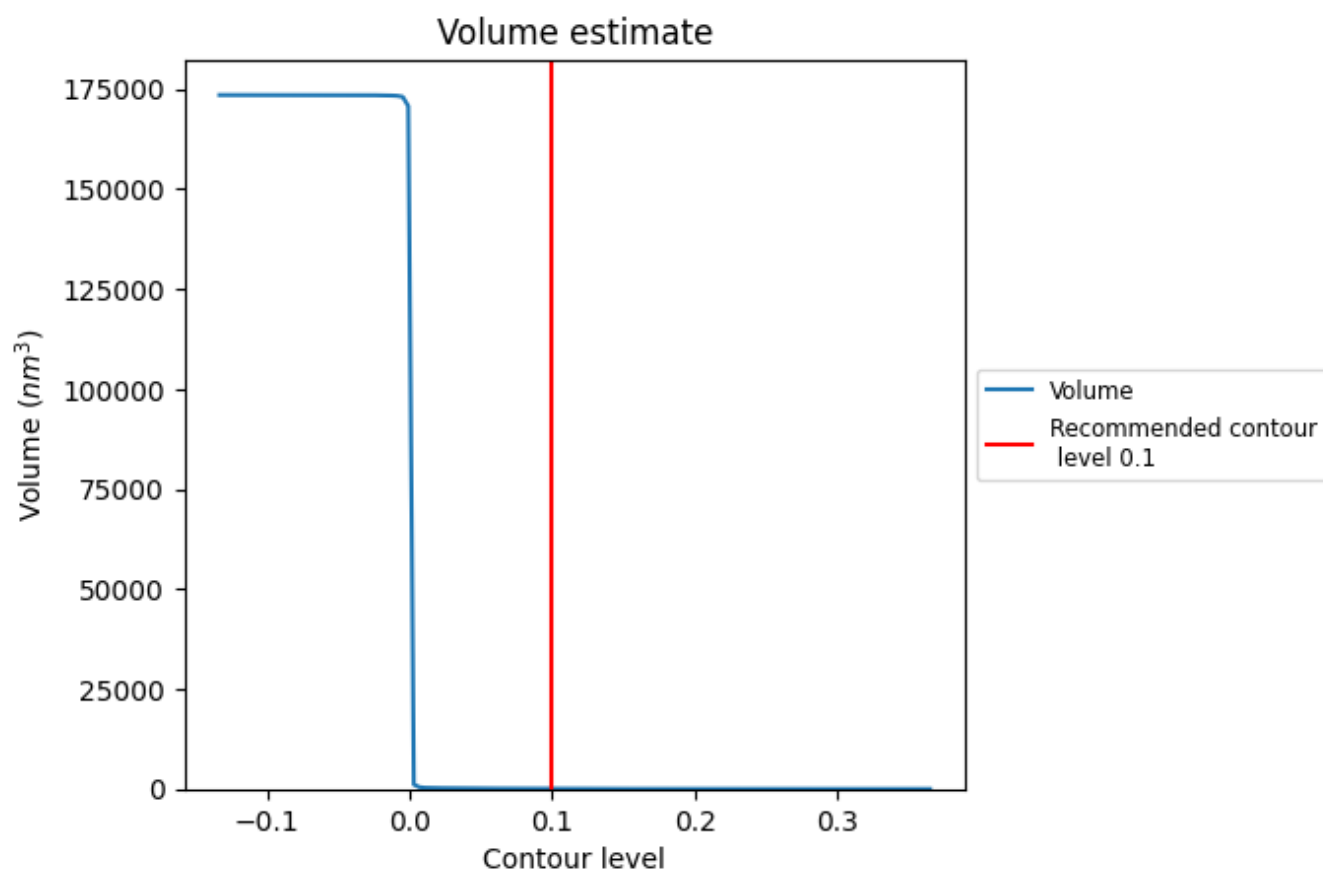
This section contains the results of statistical analysis of the map.

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.

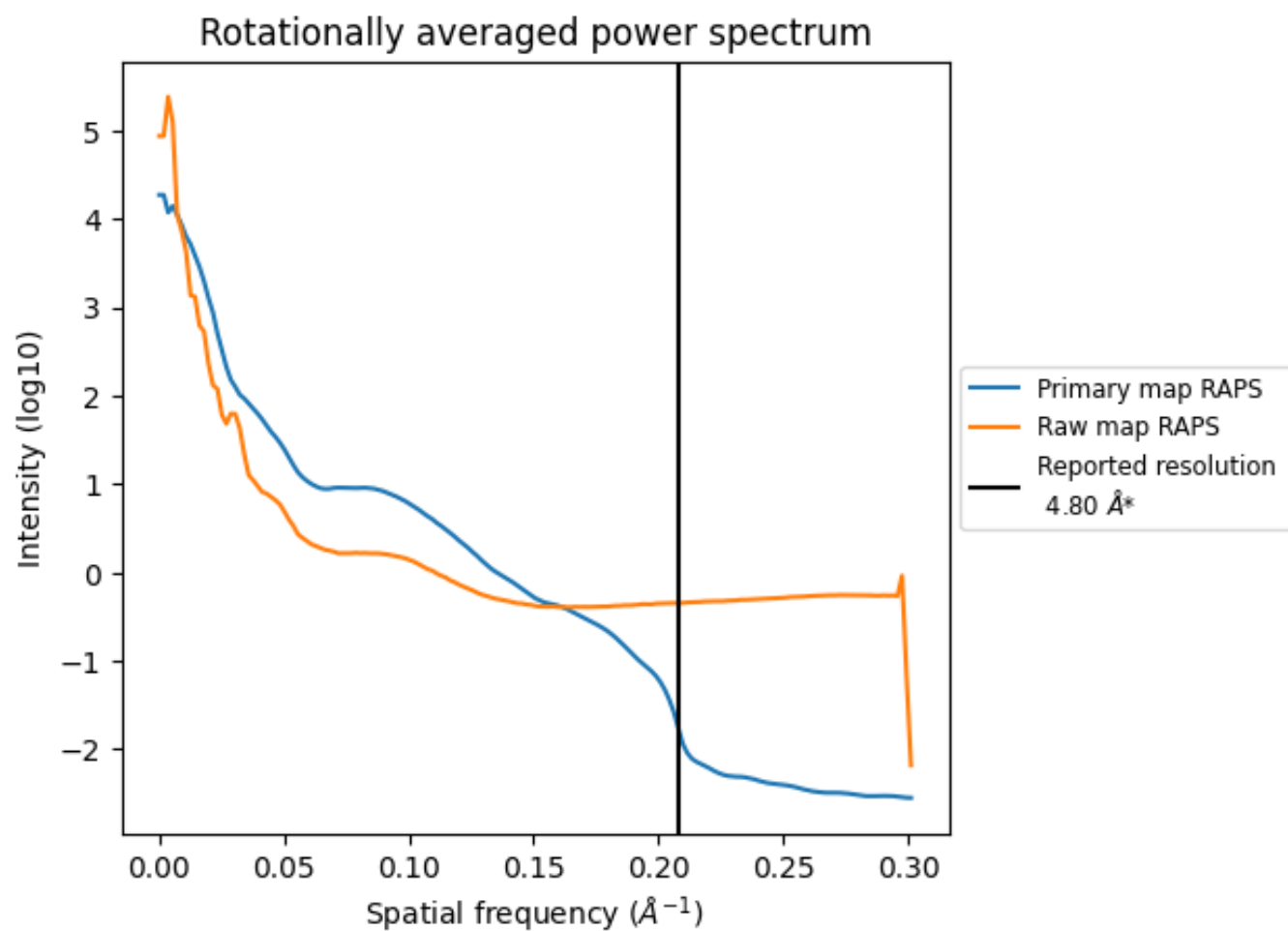
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 63 nm^3 ; this corresponds to an approximate mass of 57 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 ⓘ

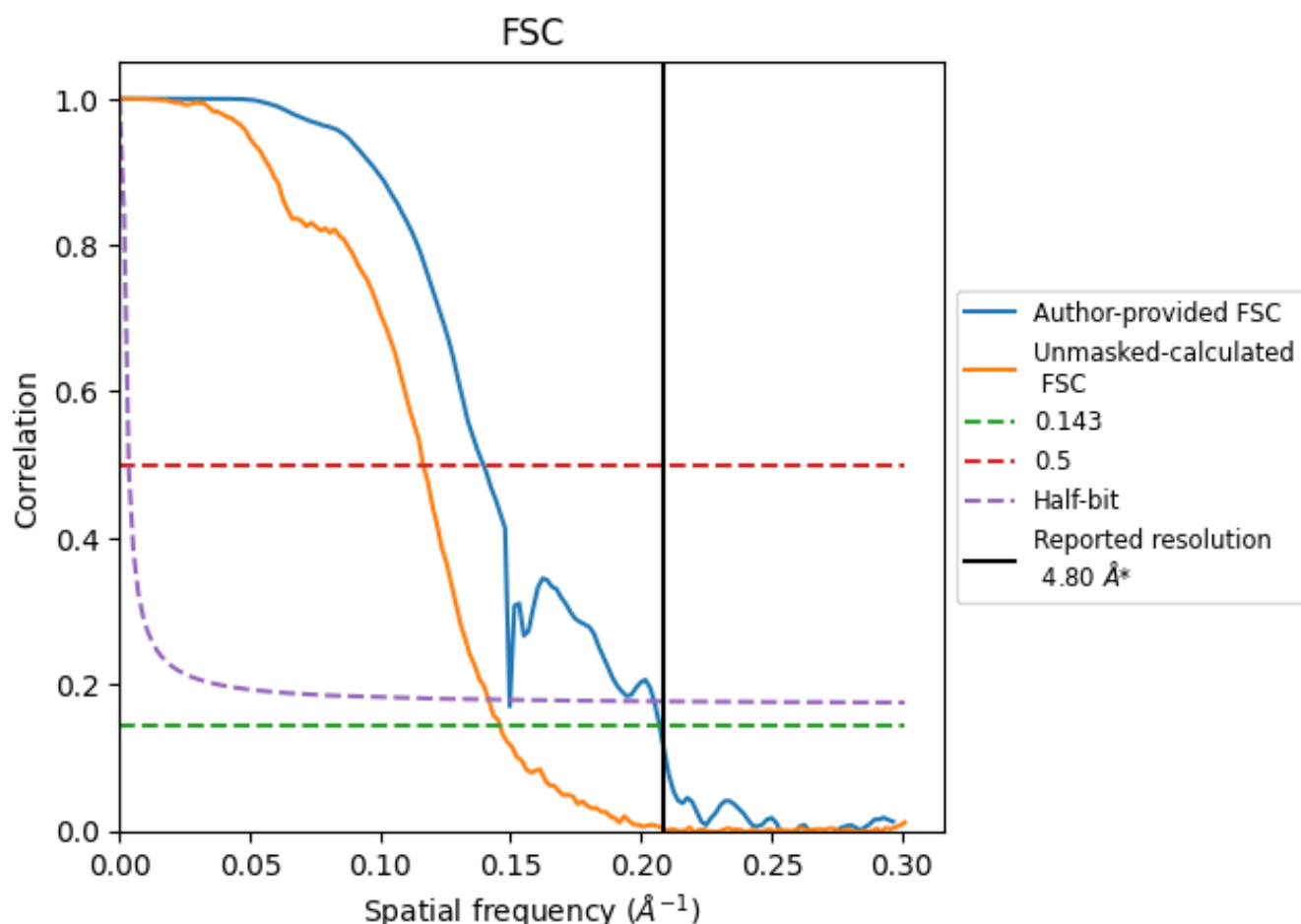


*Reported resolution corresponds to spatial frequency of 0.208 Å⁻¹

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 0.208 \AA^{-1}

8.2 Resolution estimates [i](#)

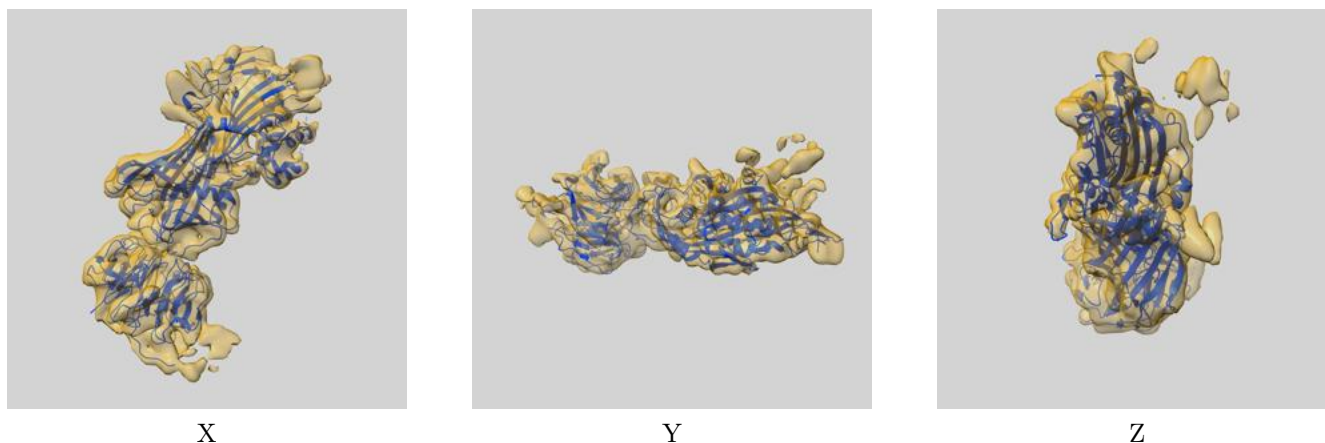
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.80	-	-
Author-provided FSC curve	4.83	7.16	6.68
Unmasked-calculated*	6.85	8.58	7.06

*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 6.85 differs from the reported value 4.8 by more than 10 %

9 Map-model fit [i](#)

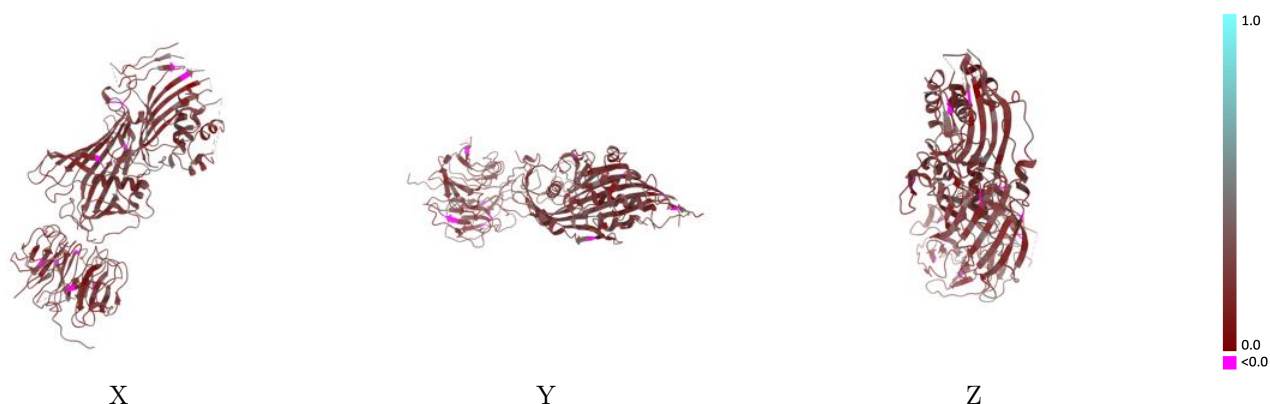
This section contains information regarding the fit between EMDB map EMD-44446 and PDB model 9BD8. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



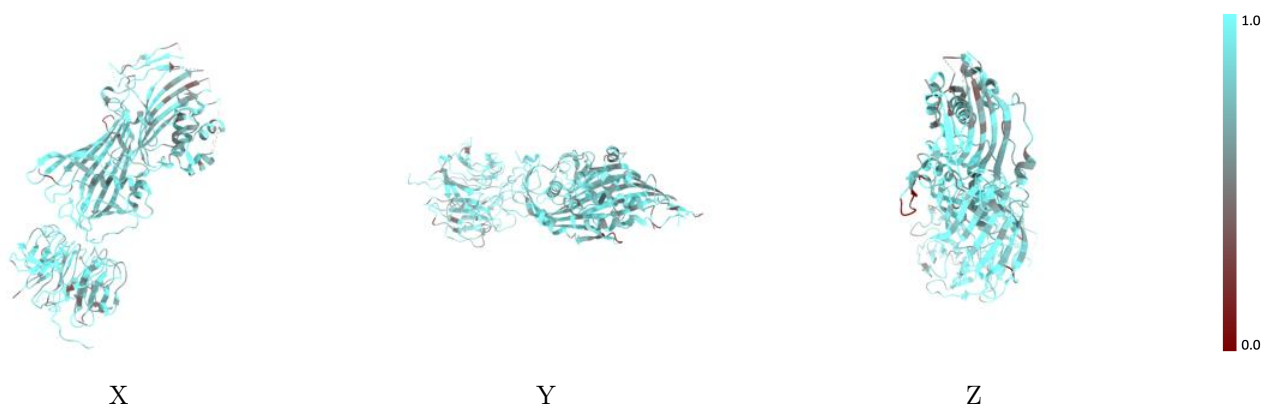
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



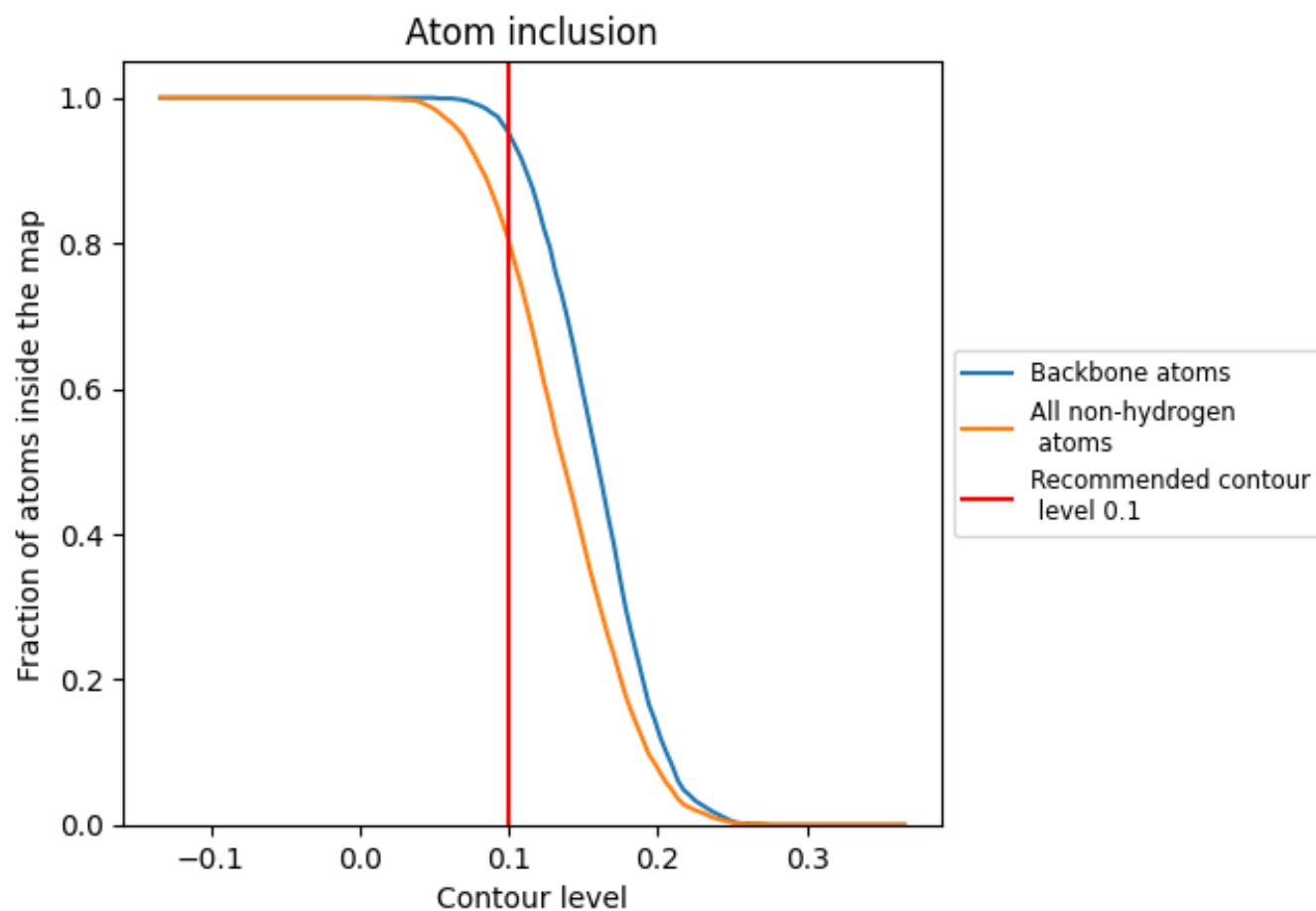
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8040	<div></div> 0.2410
A	<div></div> 0.8000	<div></div> 0.2480
B	<div></div> 0.8100	<div></div> 0.2270

