



wwPDB EM Validation Summary Report ⓘ

Aug 8, 2026 – 08:40 AM EDT

PDB ID : 11BT / pdb_000011bt
EMDB ID : EMD-75608
Title : C3 Hexon Map of Phage Goslar
Authors : Basu, D.; Gu, Y.; Corbett, K.D.
Deposited on : 2026-02-16
Resolution : 3.57 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:

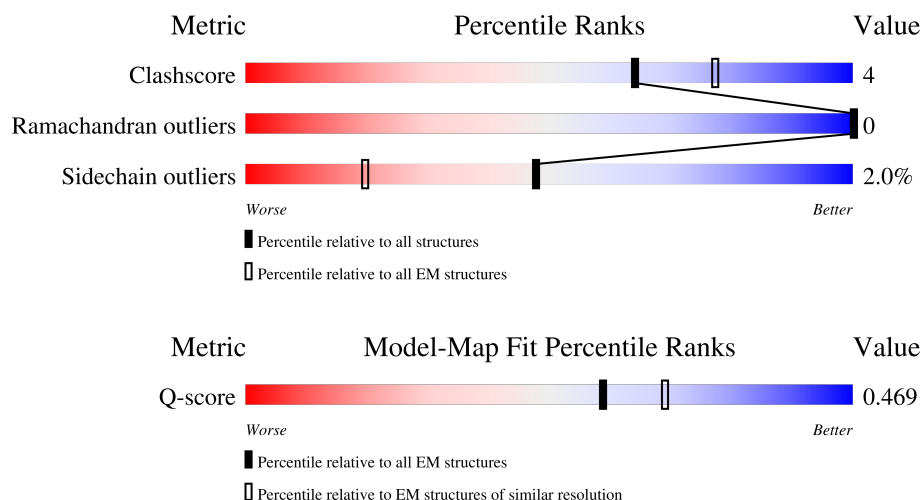
EMDB validation analysis : 0.0.1.dev133
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

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 3.57 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	12682 (3.07 - 4.07)

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	Ar	740	
1	As	740	
1	At	740	
1	Au	740	

Continued on next page...

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Mol	Chain	Length	Quality of chain
1	Av	740	 70% 8% • 21%
1	Aw	740	 69% 9% • 21%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 27906 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 Major capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Ar	583	Total	C	N	O	S	0	0
			4651	2939	809	886	17		
1	As	583	Total	C	N	O	S	0	0
			4651	2939	809	886	17		
1	At	583	Total	C	N	O	S	0	0
			4651	2939	809	886	17		
1	Au	583	Total	C	N	O	S	0	0
			4651	2939	809	886	17		
1	Av	583	Total	C	N	O	S	0	0
			4651	2939	809	886	17		
1	Aw	583	Total	C	N	O	S	0	0
			4651	2939	809	886	17		

- Chain At:



G601	D299	SER	ARG	SER	MET
D614	S300	ASN	SER	ASP	ASN
T623	S307	LYS	IIE	ARG	LYS
D624	T310	THR	THR	LYS	THR
N625	D314	GLU	THR	ALA	LEU
Q629	A315	PRO	PRO	GLN	SER
D634	S352	VAL	GLY	LEU	VAL
G635	L353	ALA	ARG	LEU	ALA
V640	D356	THR	GLU	THR	ALA
V642	F357	ARG	VAL	THR	THR
V649	R358	THR	ASP	LEU	ARG
M655	E373	PHE	SER	GLY	PHE
L656	D377	GLU	ASN	LEU	GLU
R657	V378	THR	PHE	THR	THR
D658	A381	MET	VAL	ALA	ALA
K659	I390	GLY	MET	GLY	ASN
R666	N407	SER	ALA	GLU	SER
G667	V408	CYS	ASP	GLN	ASP
I668	L413	GLY	SER	ARG	ALA
L675	R414	CYS	GLY	GLY	LYS
R707	V415	GLU	GLU	ILE	GLY
N721	D427	LEU	SER	GLU	LEU
E731	Q428	VAL	GLN	THR	THR
N740	R464	LEU	LEU	MET	PHE
	R465		ASN	LEU	ASN
	R466		ALA	ALA	MET
	D473		ARG	ALA	GLU
	F474		ALA	ALA	ASP
	L485		ALA	ASP	LYS
	N517		LEU	PHE	VAL
	R539		IIE	LYS	LYS
	I546		MET	SER	MET
	E547		LEU	LEU	ASP
	G548		HIS	LEU	LYS
	R551		GLY	VAL	ASN
	R555		ASN	PRO	ASN
	N562		VAL	VAL	GLU
	R572		TYR	GLY	GLU
			ALA	THR	MET
			LYS	ASP	ASP
			LYS	VAL	VAL
			GLN	LYS	LYS
			ALA	SER	PHE

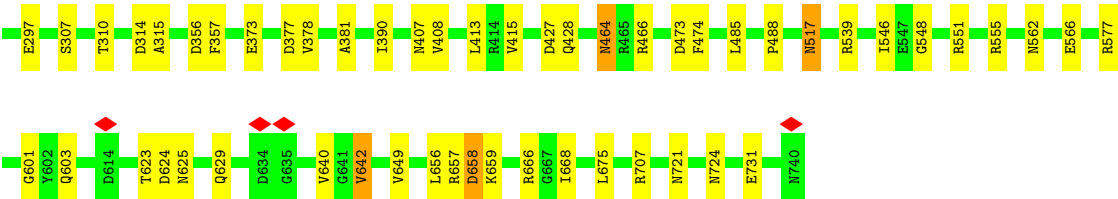
- Chain Au:



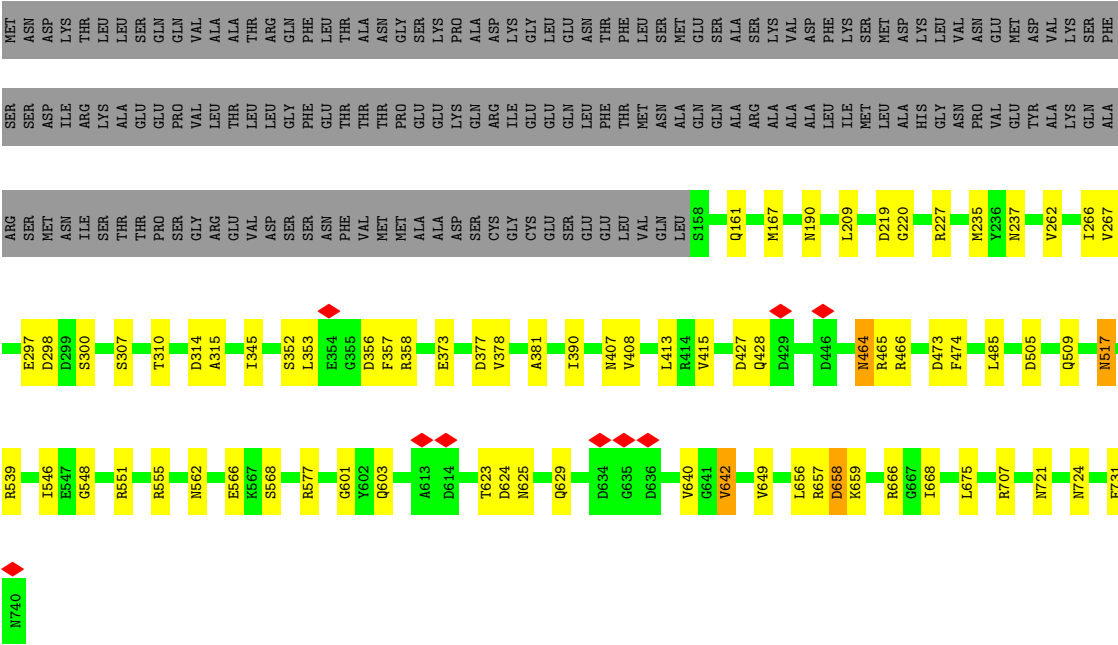
ME1	ASN	ASP	LYS	LEU	SER	GLN	VAL	ALA	ALA	THR	GLN	PHE	LEU	THR	ALA	ASN	GLY	SER	LYS	PRO	ALA	ASP	ARG	LYS	LEU	GLY	LEU	GLU	ASN	THR	PHE	LEU	SER	MET	ALA	GLN	SER	ALA	SER	LYS	VAL	ASP	PHE				
V267	D298	D299	S300	S307	T310	D314	A315	S352	S353	E354	G355	D356	F357	R358	E373	D377	V378	A381	I390	M407	V408	L413	R414	V415	D427	Q428	L443	D446	M464	R465	R466	G469	D473	F474	L485	M517	R539										
E547	G548	R551	B555	M562	R577	G601	T602	Q603	A613	T623	D624	Q629	D634	G635	D636	V640	G641	V642	V649	L656	R657	D688	K659	R666	G667	L668	L675	A690	R707	M721	E731	H740															
SER	SER	ASP	ILE	ARG	THR	ALA	VAL	GLY	THR	GLN	PHE	GLU	THR	ALA	THR	MET	PRO	GLY	GLU	LYS	GLN	ARG	ILE	LYS	GLY	LEU	GLN	PHE	THR	MET	ASN	ALA	GLN	SER	ALA	GLN	ILE	MET	SER	THR	LEU	GLU	TYR	ALA	LYS	GLN	ALA

- Chain Av:

[illegible]



• Molecule 1: Major capsid protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	102070	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	0.623	Depositor
Minimum map value	-0.269	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.034	Depositor
Recommended contour level	0.153	Depositor
Map size (Å)	672.0, 672.0, 672.0	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4, 1.4, 1.4	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	Ar	0.14	0/4735	0.25	0/6411
1	As	0.14	0/4735	0.25	0/6411
1	At	0.15	0/4735	0.25	0/6411
1	Au	0.15	0/4735	0.25	0/6411
1	Av	0.15	0/4735	0.25	0/6411
1	Aw	0.14	0/4735	0.25	0/6411
All	All	0.14	0/28410	0.25	0/38466

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	Ar	4651	0	4633	47	0
1	As	4651	0	4633	47	0
1	At	4651	0	4633	40	0
1	Au	4651	0	4633	42	0
1	Av	4651	0	4633	39	0
1	Aw	4651	0	4633	48	0
All	All	27906	0	27798	226	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 4.

The worst 5 of 226 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:Ar:625:ASN:ND2	1:Aw:603:GLN:OE1	1.98	0.95
1:Ar:629:GLN:HE22	1:Aw:642:VAL:H	1.27	0.81
1:Ar:655:MET:SD	1:Aw:237:ASN:ND2	2.54	0.80
1:As:642:VAL:H	1:At:629:GLN:HE22	1.28	0.79
1:As:603:GLN:OE1	1:At:625:ASN:ND2	2.18	0.75

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	Ar	581/740 (78%)	560 (96%)	21 (4%)	0	100	100
1	As	581/740 (78%)	561 (97%)	20 (3%)	0	100	100
1	At	581/740 (78%)	560 (96%)	21 (4%)	0	100	100
1	Au	581/740 (78%)	560 (96%)	21 (4%)	0	100	100
1	Av	581/740 (78%)	561 (97%)	20 (3%)	0	100	100
1	Aw	581/740 (78%)	561 (97%)	20 (3%)	0	100	100
All	All	3486/4440 (78%)	3363 (96%)	123 (4%)	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	Ar	509/644 (79%)	499 (98%)	10 (2%)	48	66
1	As	509/644 (79%)	499 (98%)	10 (2%)	48	66
1	At	509/644 (79%)	499 (98%)	10 (2%)	48	66
1	Au	509/644 (79%)	499 (98%)	10 (2%)	48	66
1	Av	509/644 (79%)	499 (98%)	10 (2%)	48	66
1	Aw	509/644 (79%)	499 (98%)	10 (2%)	48	66
All	All	3054/3864 (79%)	2994 (98%)	60 (2%)	48	66

5 of 60 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	At	649	VAL
1	Aw	546	ILE
1	Au	546	ILE
1	Aw	517	ASN
1	Aw	658	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	Av	629	GLN
1	Aw	629	GLN
1	As	629	GLN
1	At	367	HIS
1	At	433	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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.

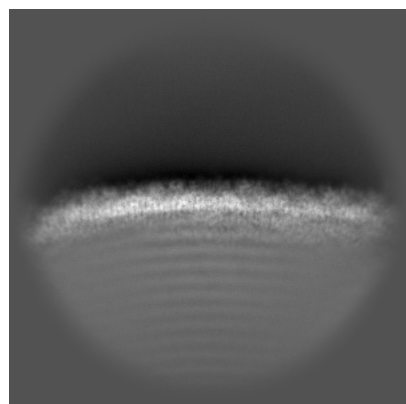
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-75608. These allow visual inspection of the internal detail of the map and identification of artifacts.

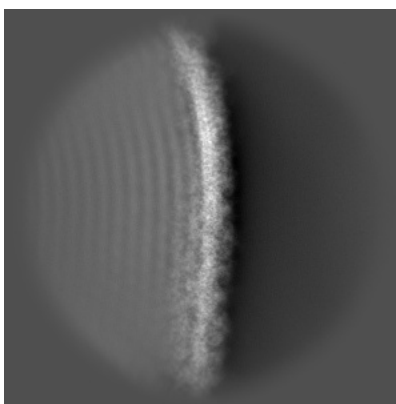
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

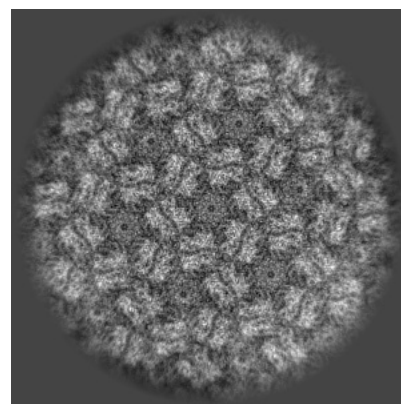
6.1.1 Primary map



X

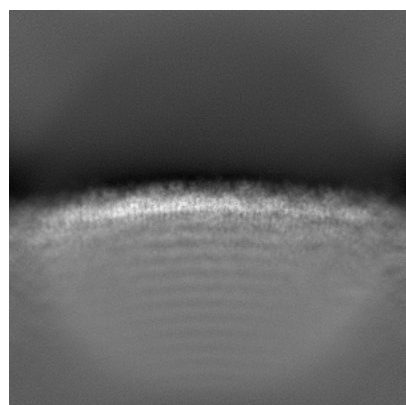


Y

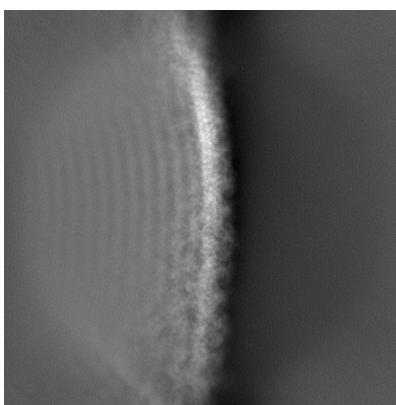


Z

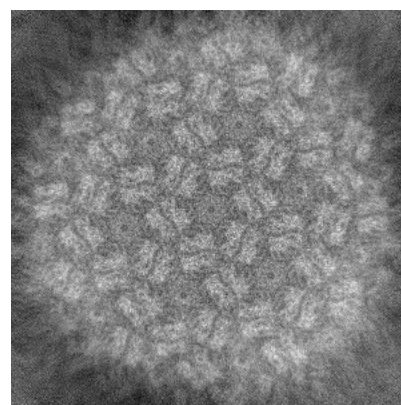
6.1.2 Raw map



X



Y

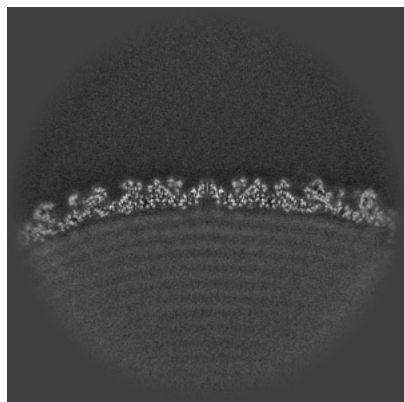


Z

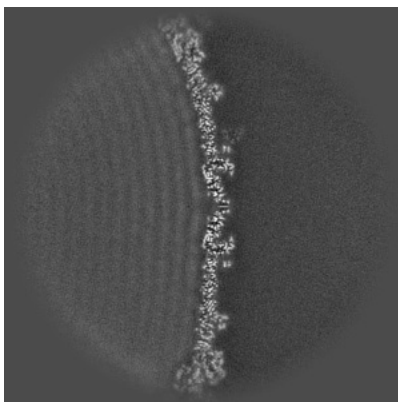
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

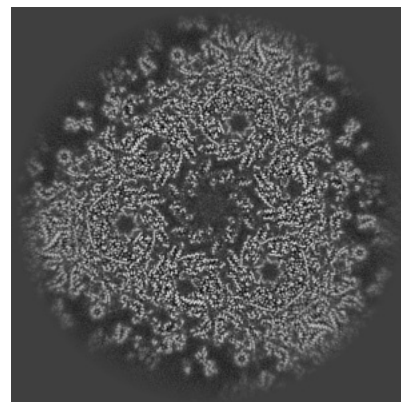
6.2.1 Primary map



X Index: 240

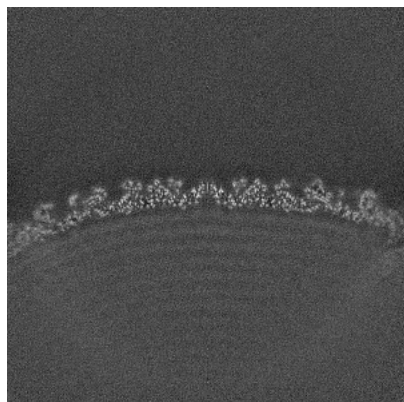


Y Index: 240

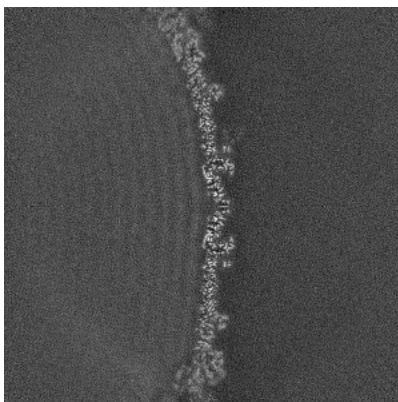


Z Index: 240

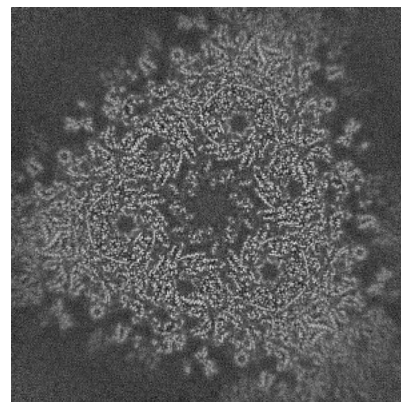
6.2.2 Raw map



X Index: 240



Y Index: 240

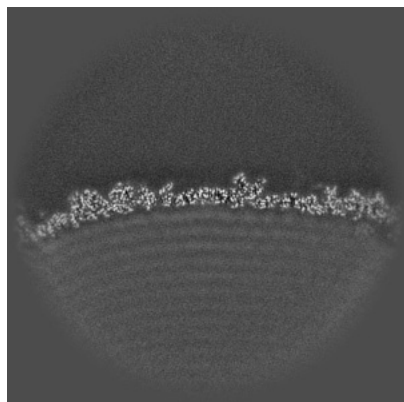


Z Index: 240

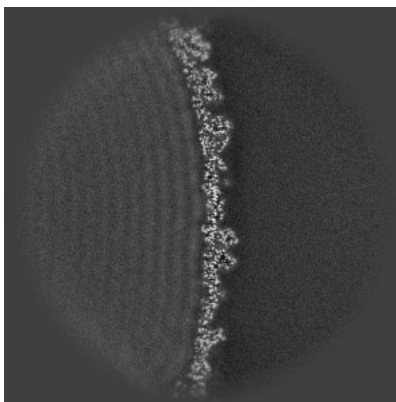
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

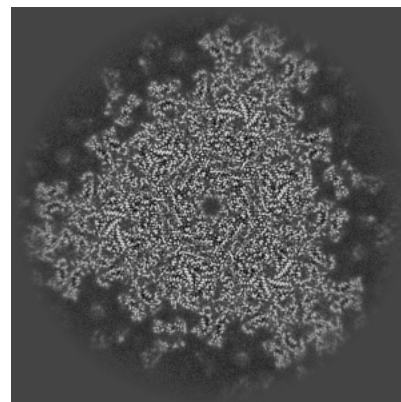
6.3.1 Primary map



X Index: 253

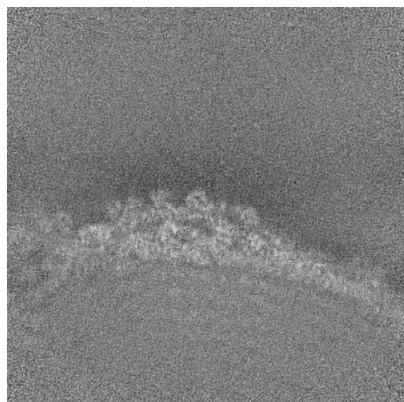


Y Index: 226

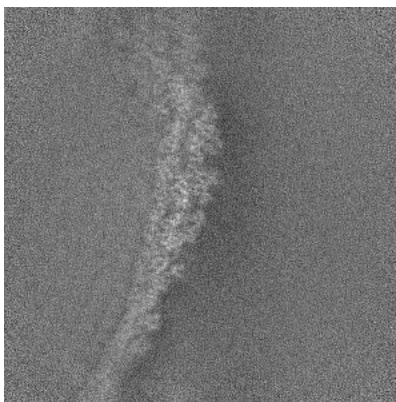


Z Index: 246

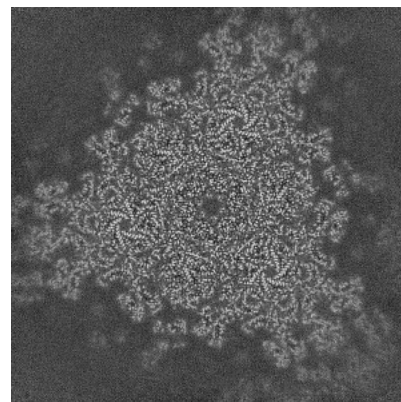
6.3.2 Raw map



X Index: 0



Y Index: 0

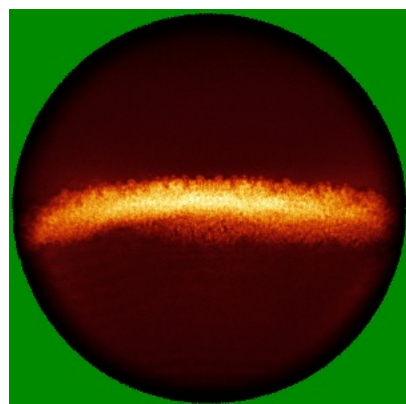


Z Index: 247

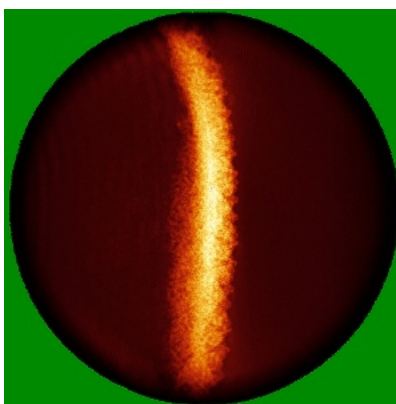
The images above show the largest variance slices of the map in three orthogonal directions.

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

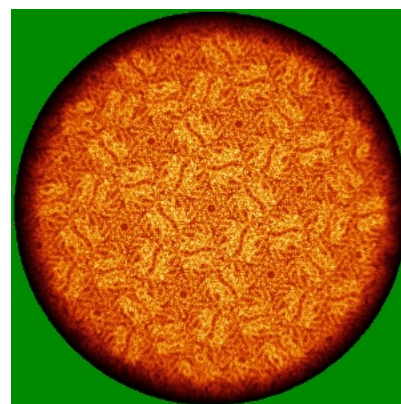
6.4.1 Primary map



X

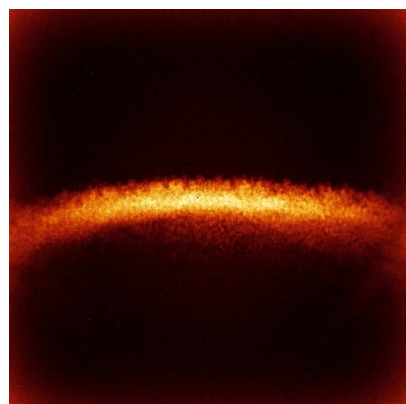


Y

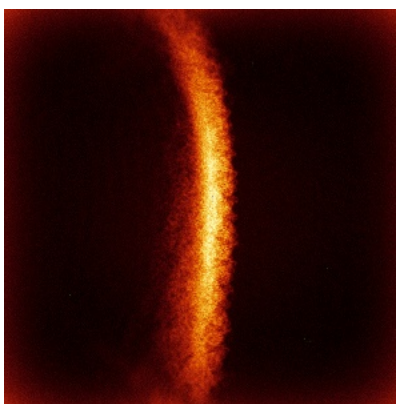


Z

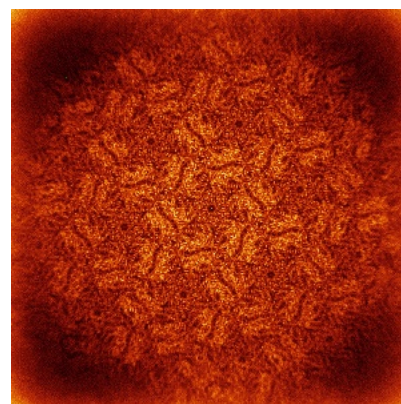
6.4.2 Raw map



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.

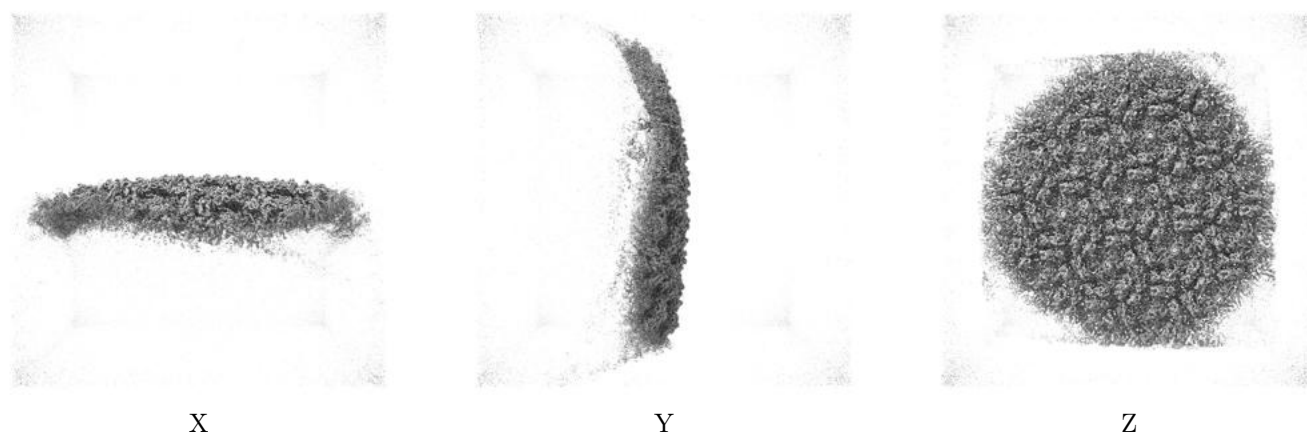
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.153. 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.

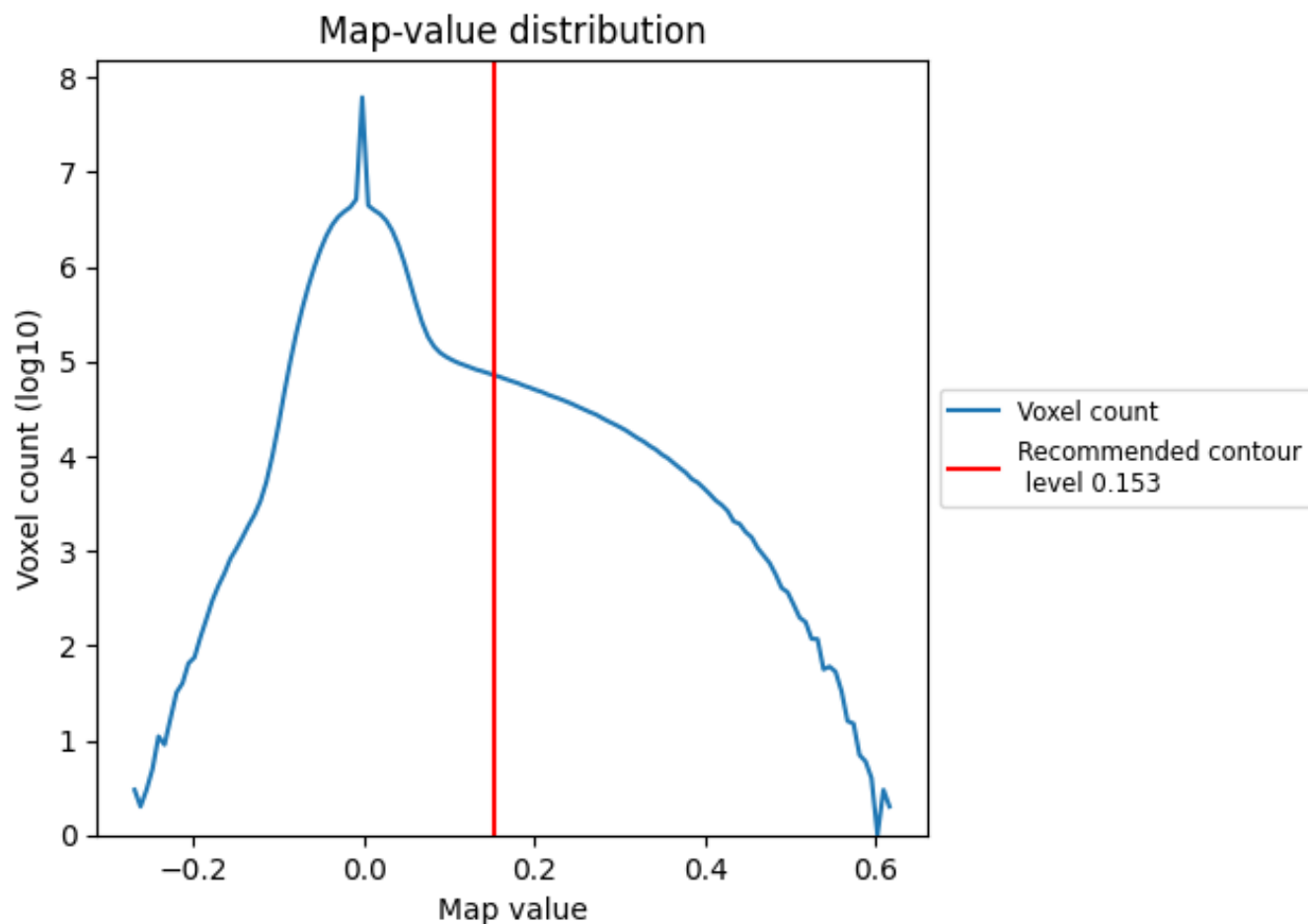
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

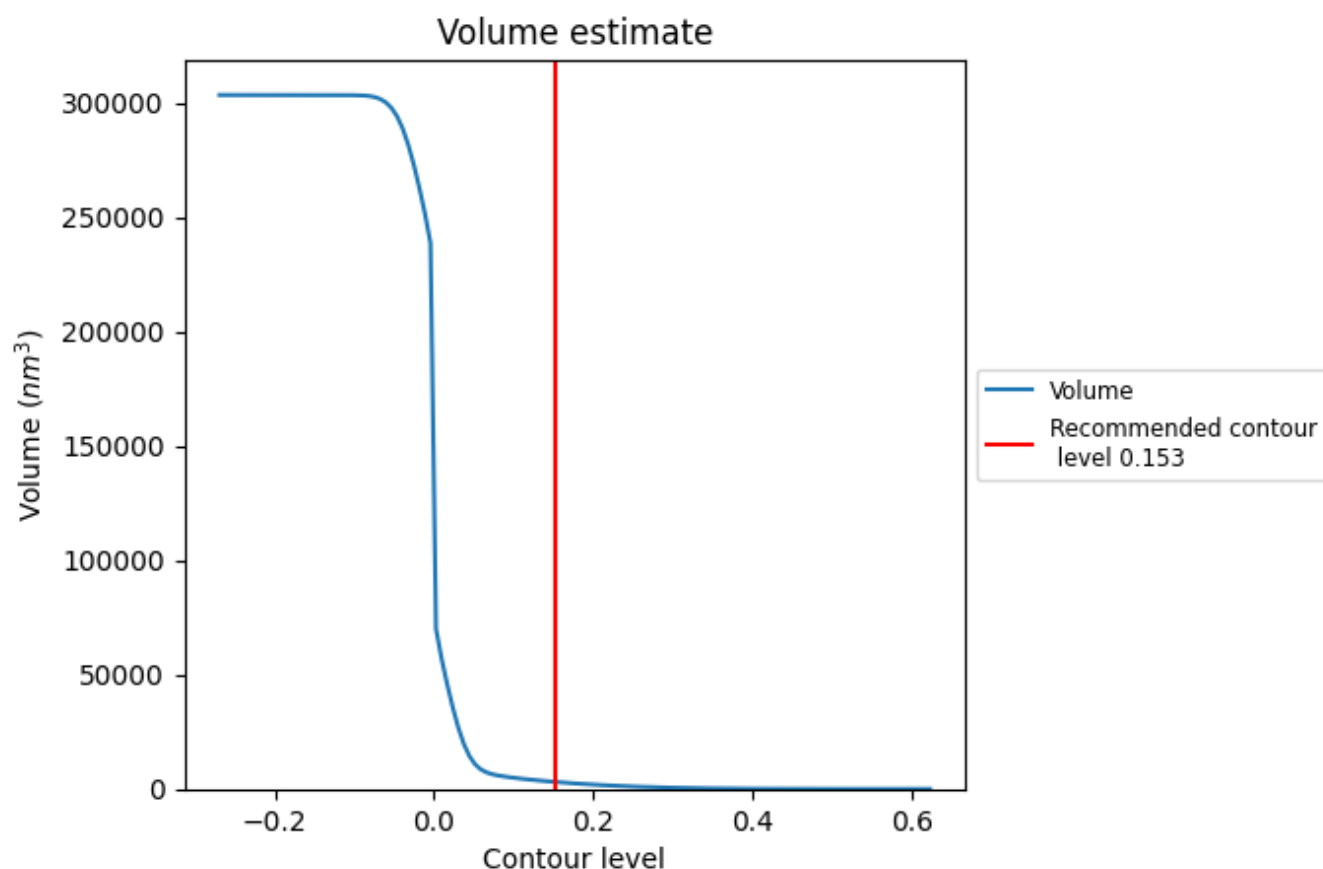
This section contains the results of statistical analysis of the map.

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.

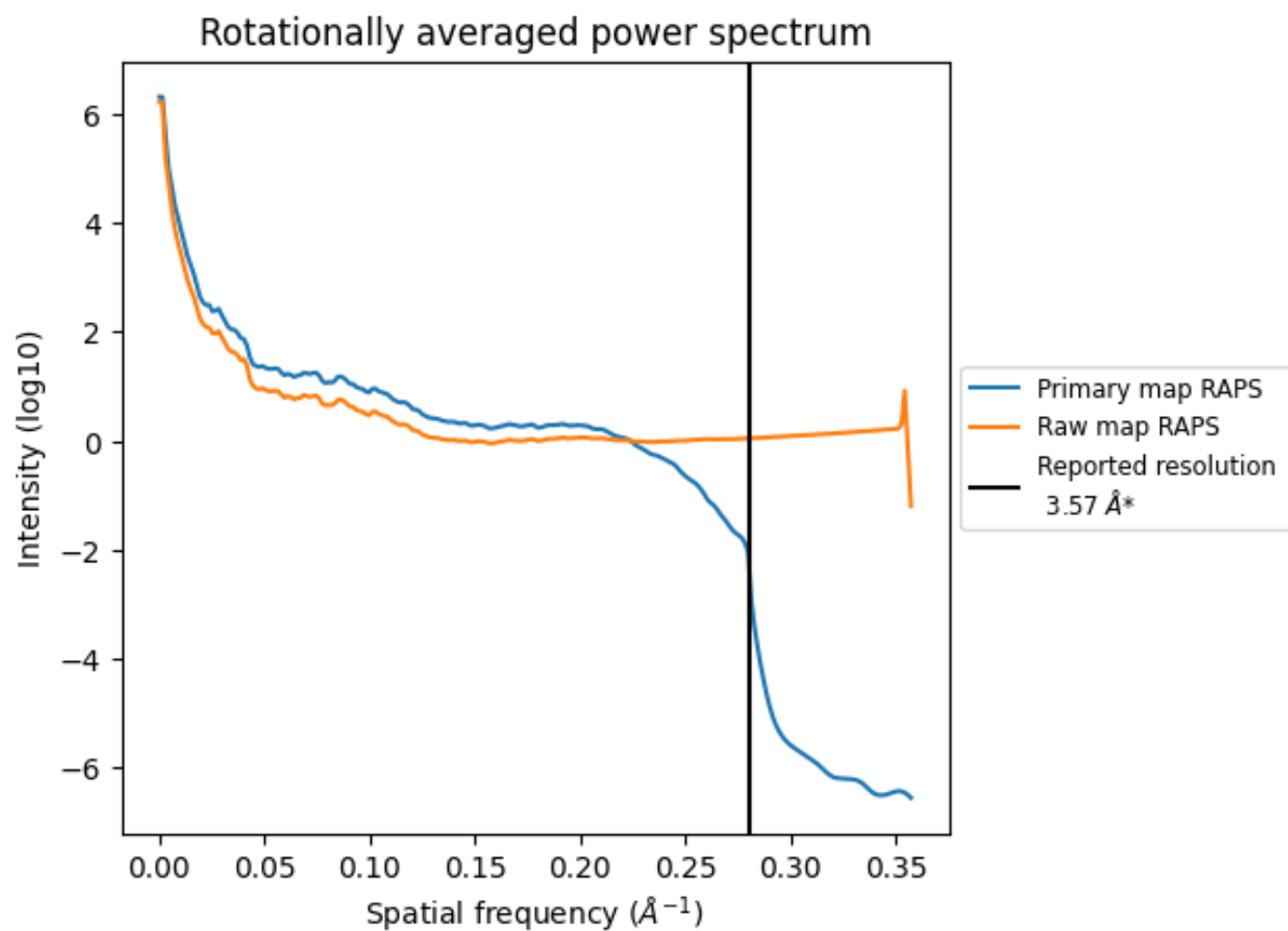
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3048 nm³; this corresponds to an approximate mass of 2753 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 ⓘ

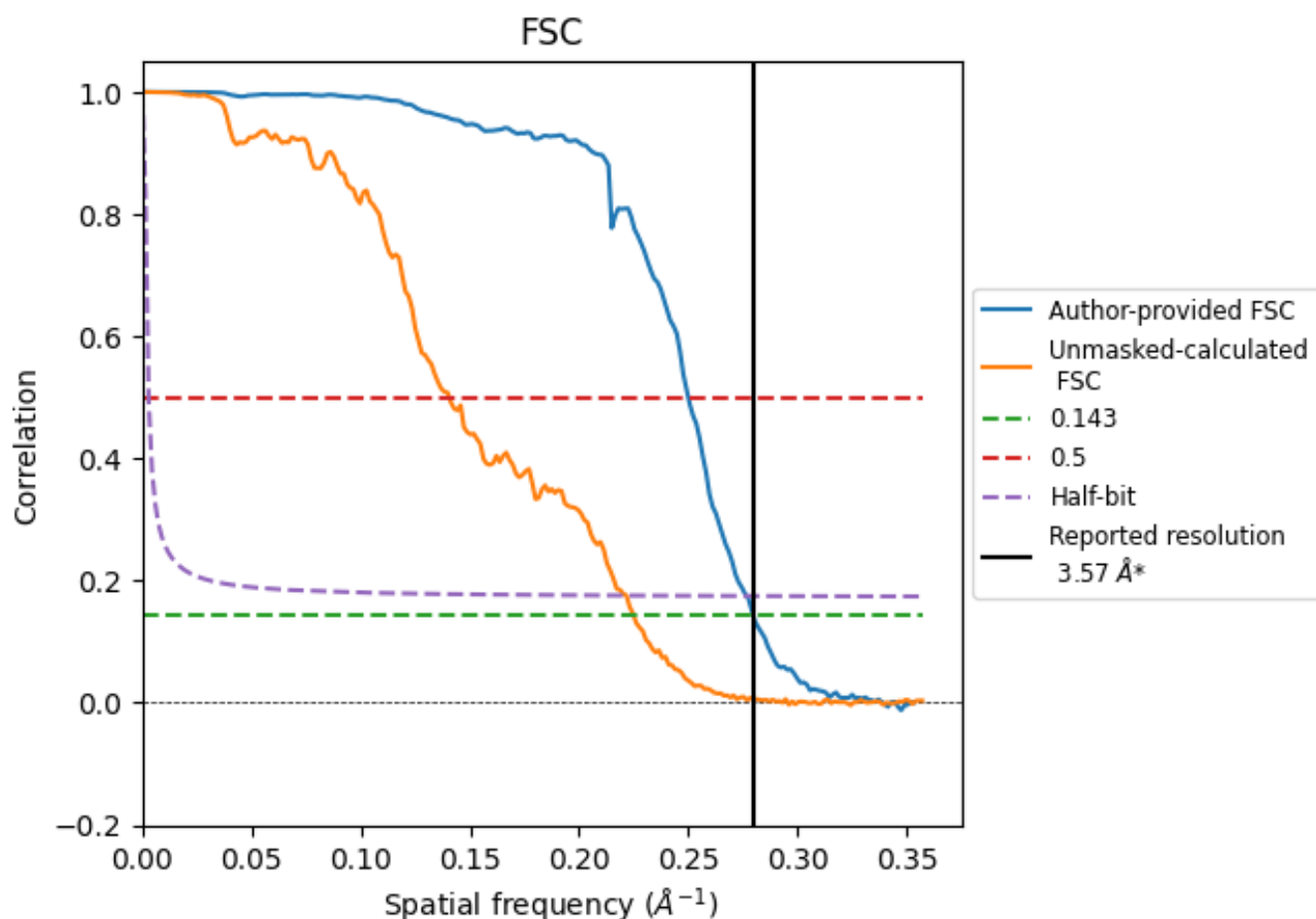


*Reported resolution corresponds to spatial frequency of $0.280 \text{ \AA}^{-1}$

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 0.280 Å⁻¹

8.2 Resolution estimates [i](#)

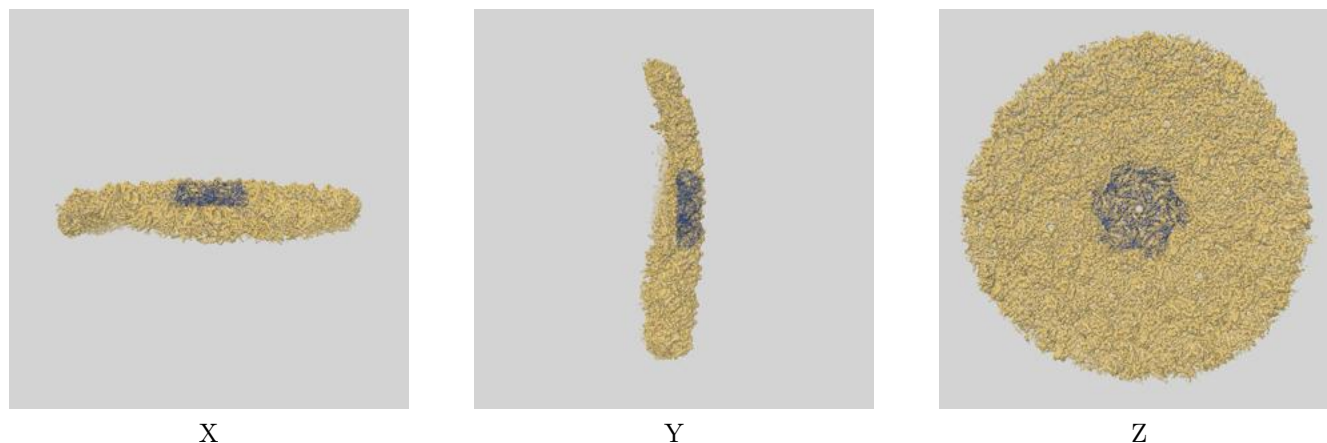
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.57	-	-
Author-provided FSC curve	3.57	4.00	3.61
Unmasked-calculated*	4.44	7.11	4.51

*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 4.44 differs from the reported value 3.57 by more than 10 %

9 Map-model fit [i](#)

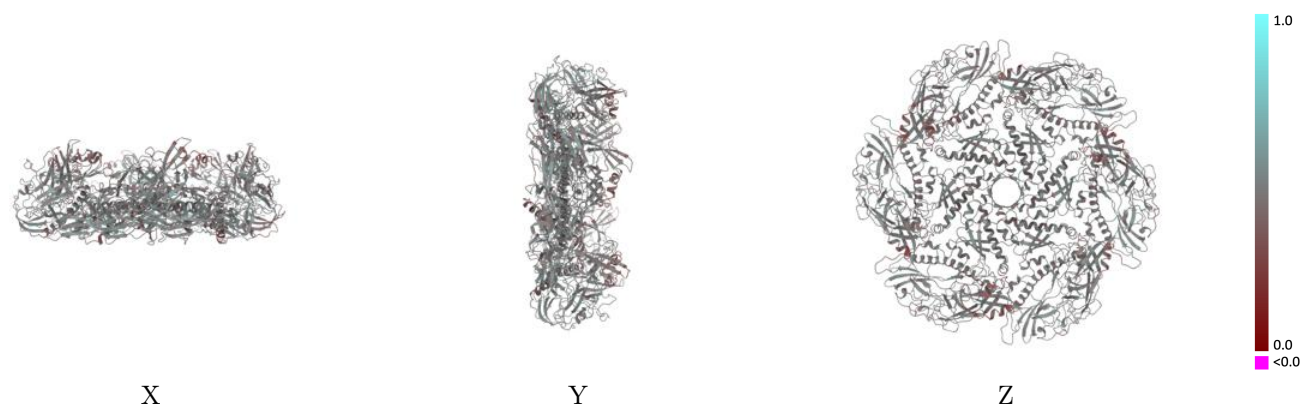
This section contains information regarding the fit between EMDB map EMD-75608 and PDB model 11BT. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

9.1 Map-model overlay [i](#)



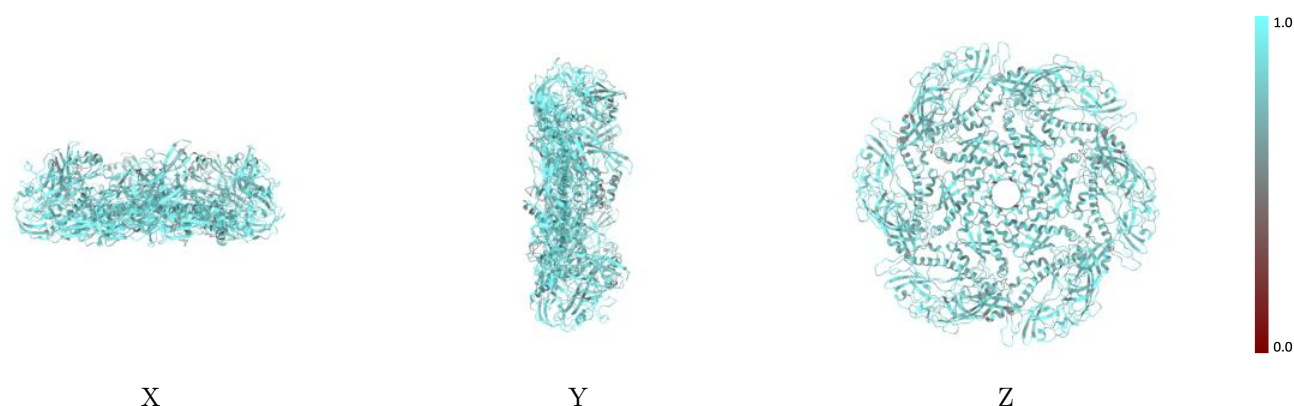
The images above show the 3D surface view of the map at the recommended contour level 0.153 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



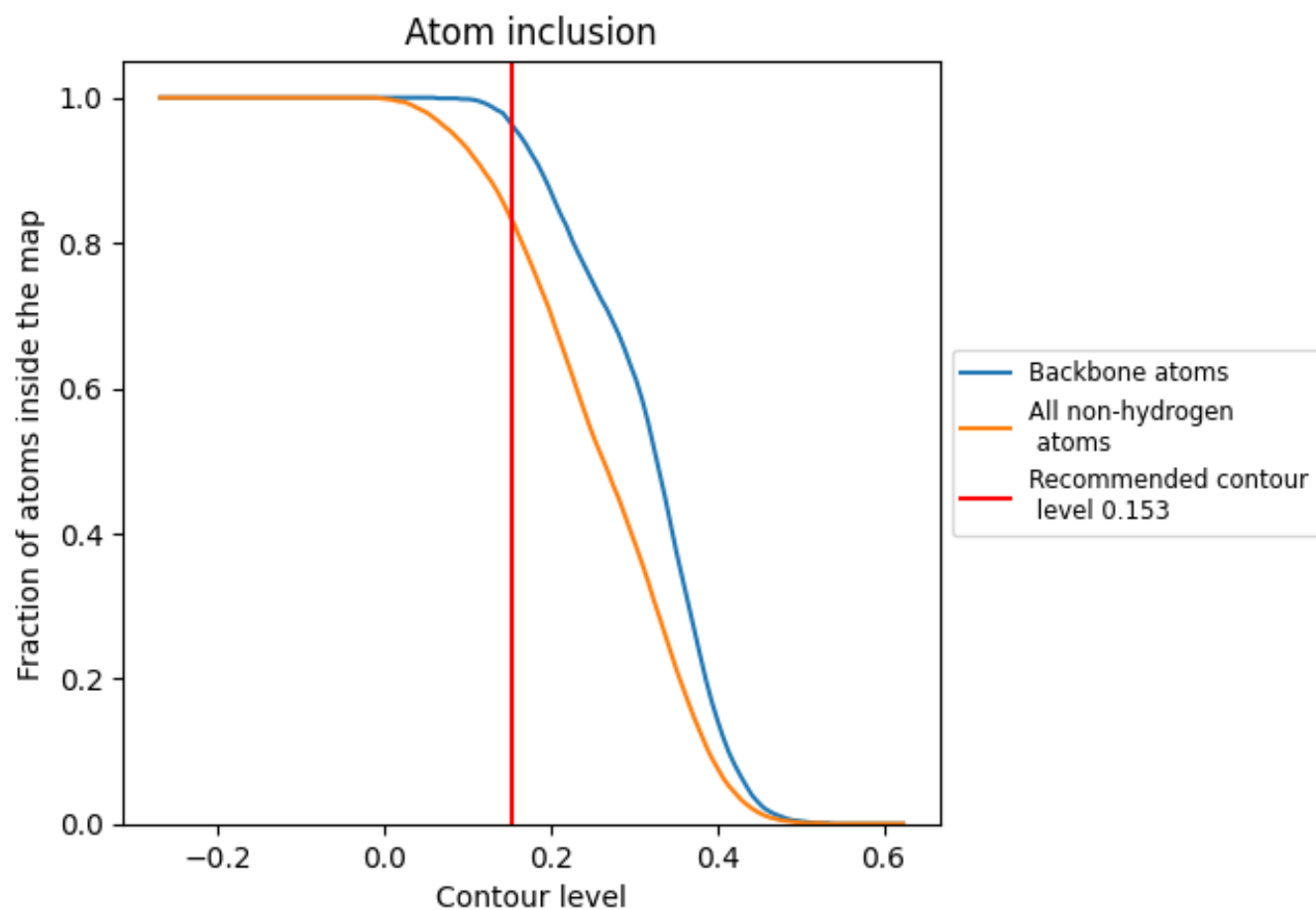
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.153).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 83% 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 (0.153) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8310	0.4690
Ar	0.8300	0.4640
As	0.8240	0.4670
At	0.8420	0.4750
Au	0.8270	0.4670
Av	0.8410	0.4750
Aw	0.8240	0.4660

