Full wwPDB EM Validation Report (i)

Jun 26, 2023 – 10:53 pm BST

EMDB ID	:	EMD-16144
Title	:	Structure of the SARS-CoV-2 spike glycoprotein in complex with the macrocyclic peptide S1B3inL1
Authors	:	Hurdiss, D.L.; Drulyte, I.
Deposited on	:	2022-11-15
Resolution	:	3.20 Å(reported)

This is a Full wwPDB EM Validation 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/EMMapValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

EMDB validation analysis	:	0.0.1.dev50
Validation Pipeline (wwPDB-VP)	:	2.33

1 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	38457	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	49.0	Depositor
Minimum defocus (nm)	0.75	Depositor
Maximum defocus (nm)	1.5	Depositor
Magnification	130000.0	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.487	Depositor
Minimum map value	-0.345	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.045	Depositor
Map size (Å)	371.52, 371.52, 371.52	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2384, 1.2384, 1.2384	Depositor

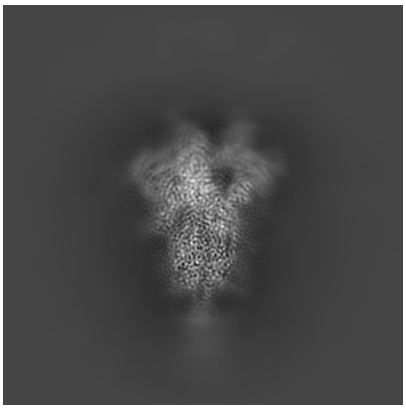
2 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-16144. These allow visual inspection of the internal detail of the map and identification of artifacts.

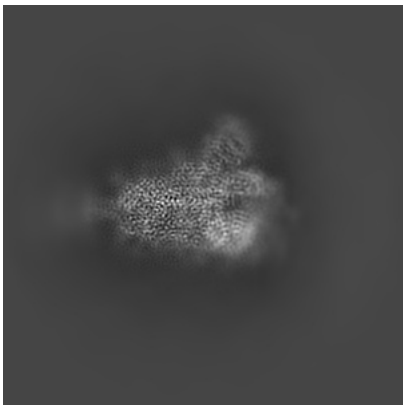
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

2.1 Orthogonal projections (i)

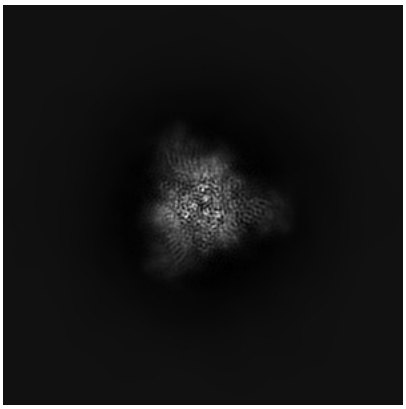
2.1.1 Primary map



X

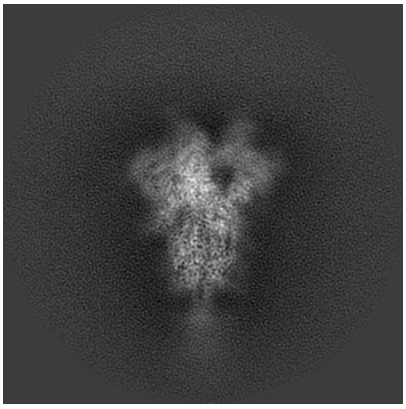


Y



Z

2.1.2 Raw map



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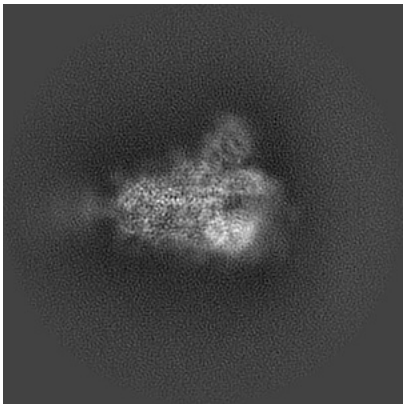
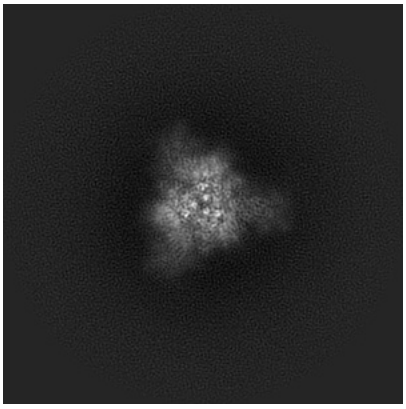


Y



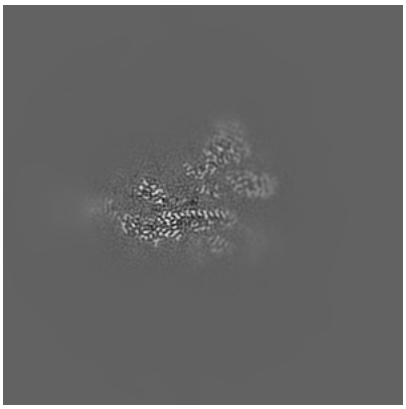
Z

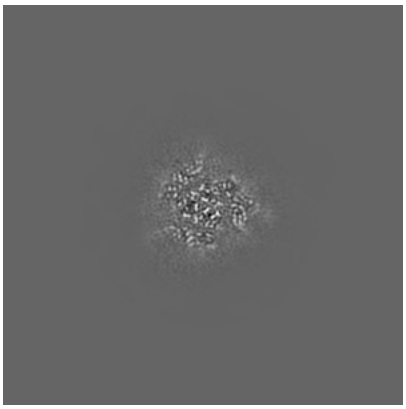
The images above show the map projected in three orthogonal directions.

2.2 Central slices (i)

2.2.1 Primary map

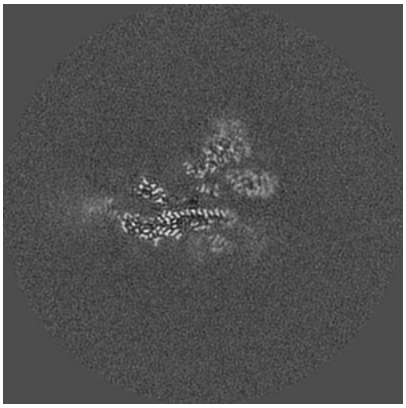
X Index: 150

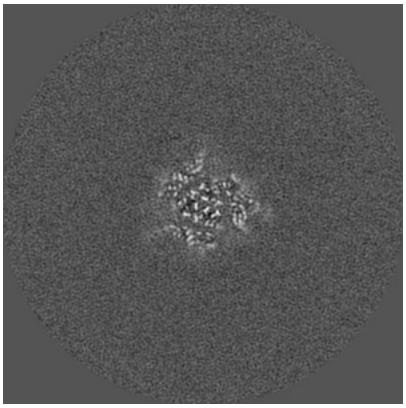

Y Index: 150


Z Index: 150

2.2.2 Raw map

X Index: 150


Y Index: 150


Z Index: 150

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

2.3 Largest variance slices (i)

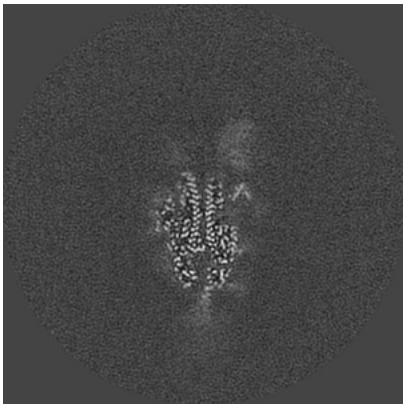
2.3.1 Primary map

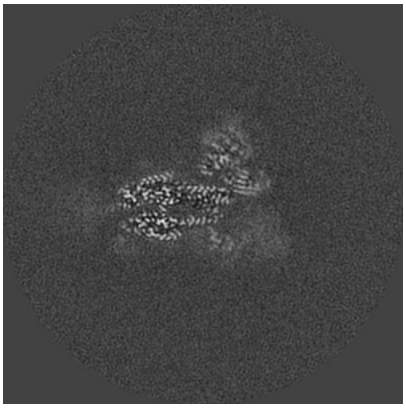
X Index: 153

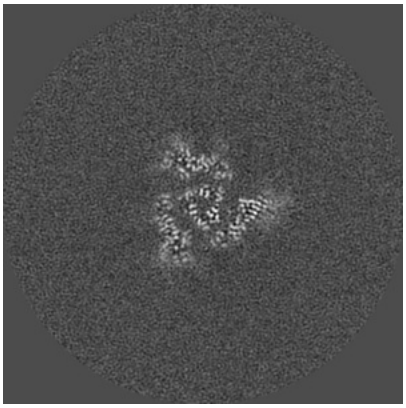
Y Index: 144

Z Index: 120

2.3.2 Raw map


X Index: 152

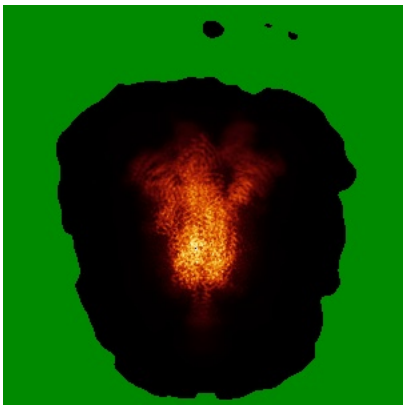

Y Index: 141

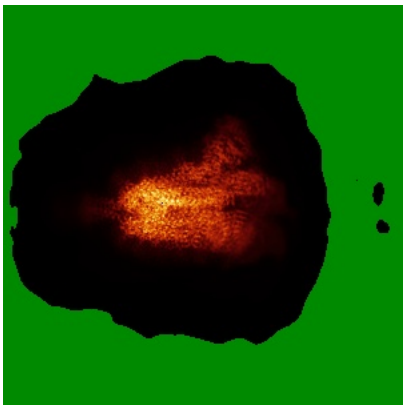

Z Index: 162

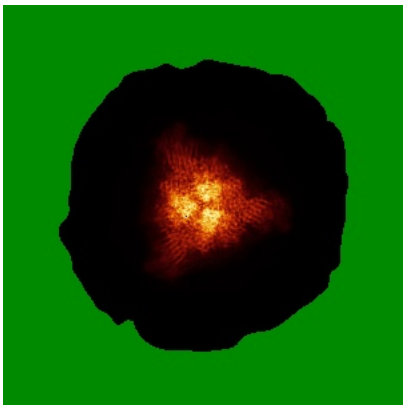
The images above show the largest variance slices of the map in three orthogonal directions.

2.4 Orthogonal standard-deviation projections (False-color) (i)

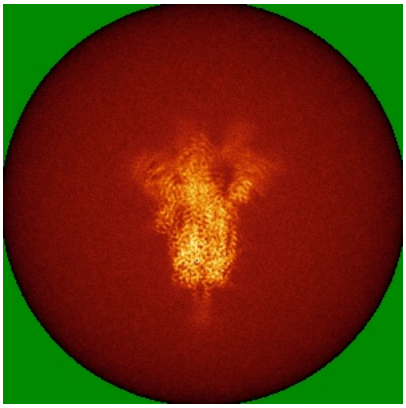
2.4.1 Primary map

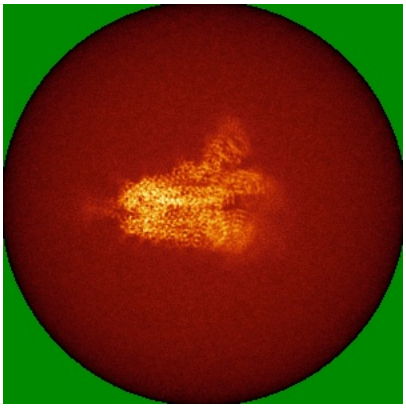

X

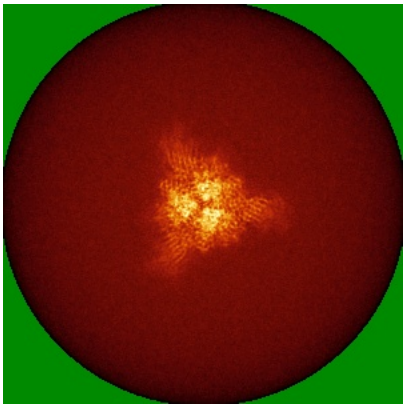

Y


Z

2.4.2 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.

2.5 Orthogonal surface views (i)

2.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.045. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

2.5.2 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.

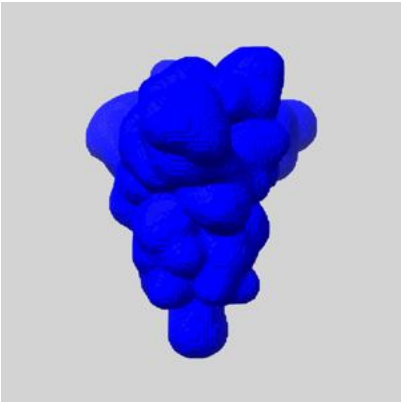
2.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

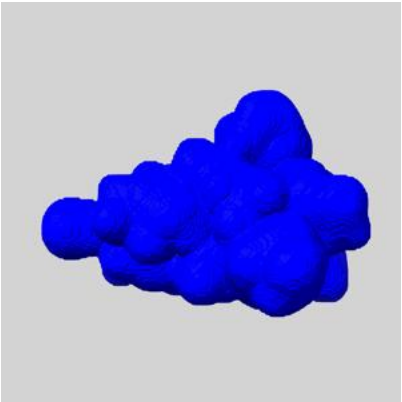
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

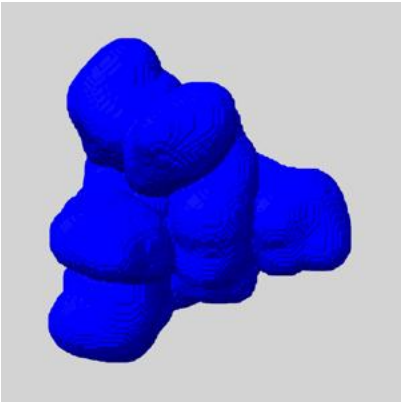
2.6.1 emd_16144_msk_1.map (i)



X



Y

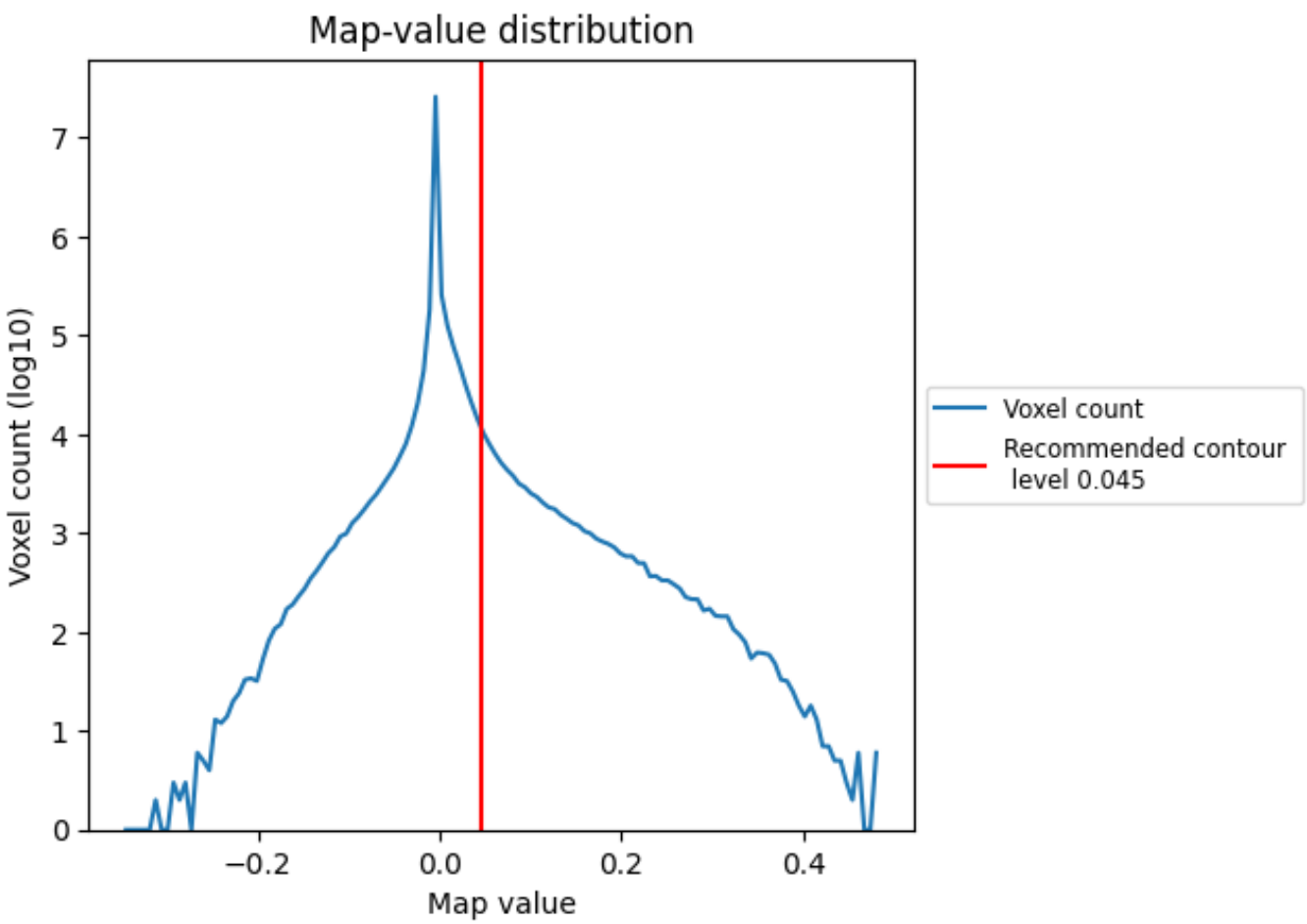


Z

3 Map analysis (i)

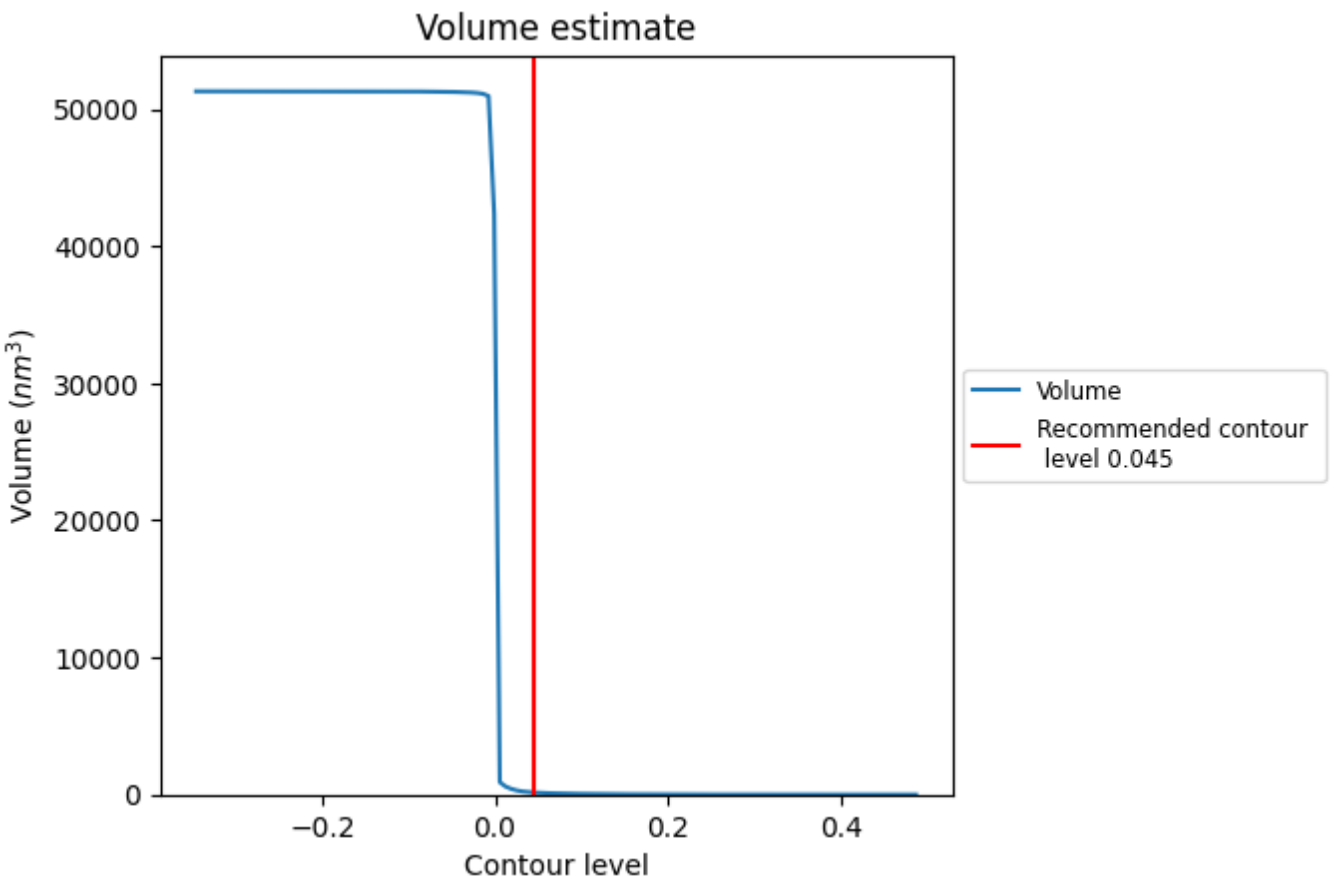
This section contains the results of statistical analysis of the map.

3.1 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.

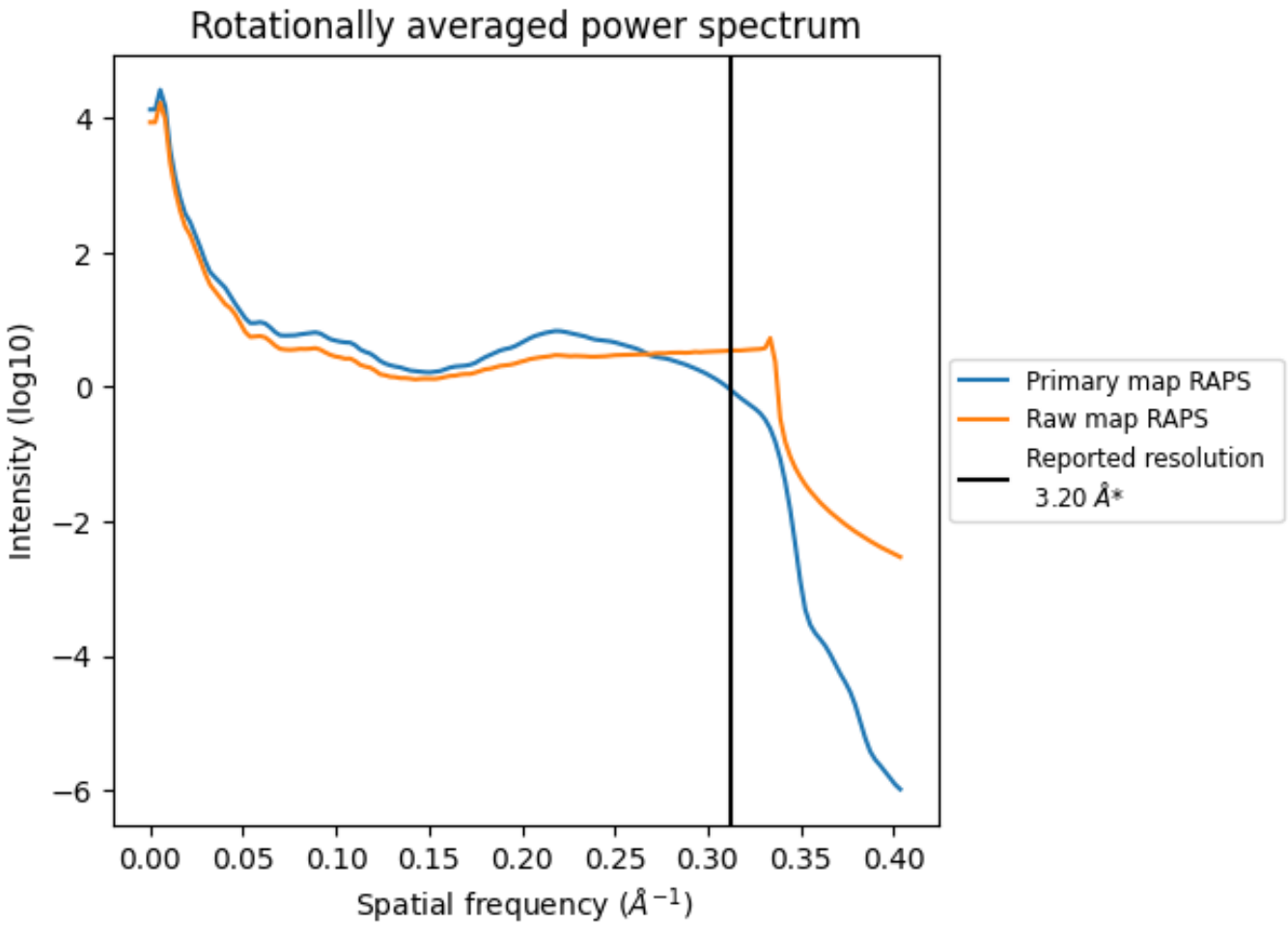
3.2 Volume estimate (i)



The volume at the recommended contour level is 148 nm^3; this corresponds to an approximate mass of 134 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.

3.3 Rotationally averaged power spectrum (i)

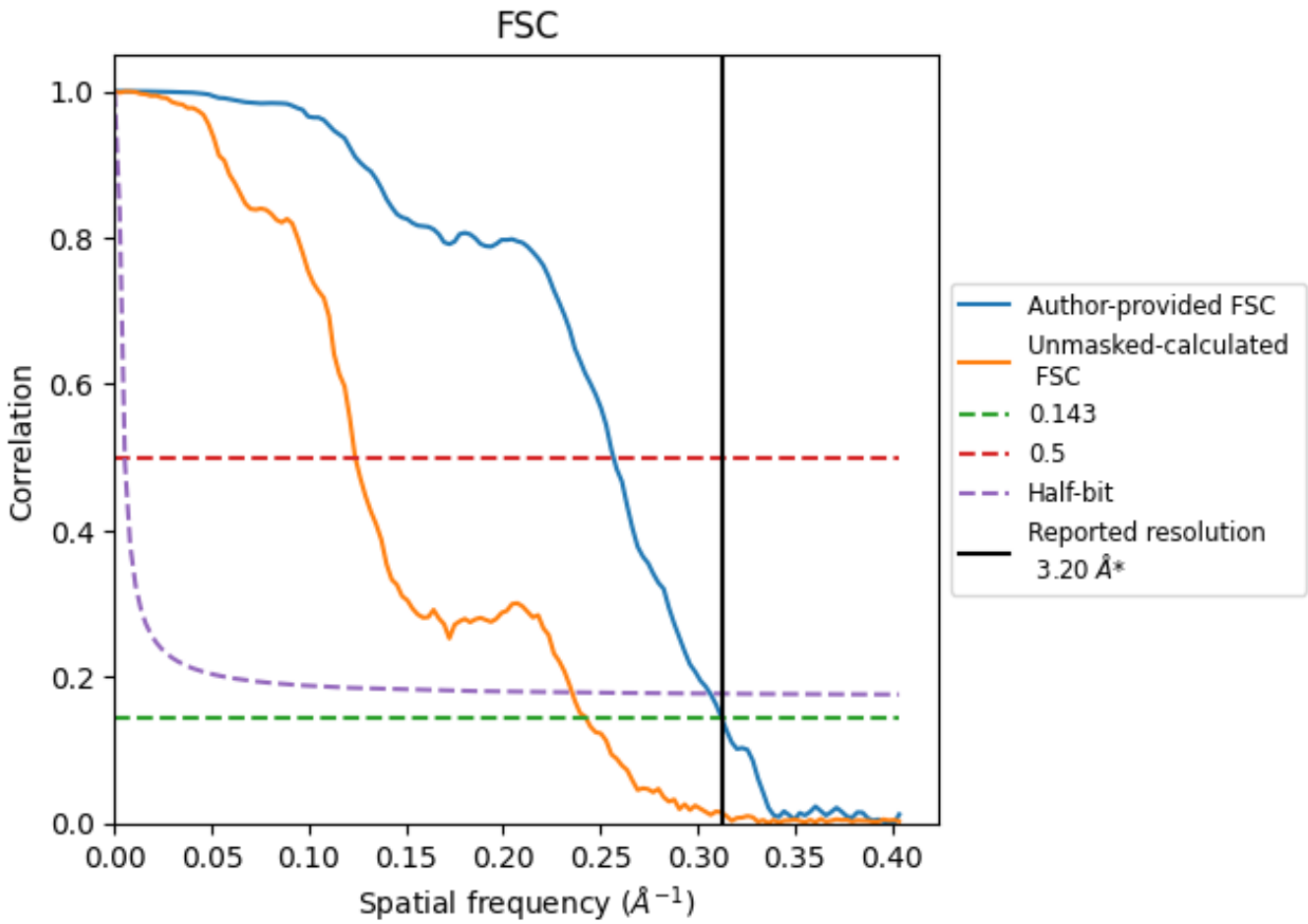


*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

4 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.

4.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

4.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.20	3.90	3.26
Unmasked-calculated*	4.12	8.08	4.25

*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 4.12 differs from the reported value 3.2 by more than 10 %