wwPDB EM Validation Summary Report (i)

Aug 24, 2021 – 10:01 AM EDT

EMDB ID	:	EMD-24404
Title	:	Covalent inhibition of hAChE by organophosphates causes homodimer dissociation through long-range allosteric effects
Authors	:	Blumenthal, D.K.; Cheng, X.; Fager, M.; Ho, K.Y.; Rohrer, J.; Gerlits, O.; Juneja, P.; Kovalevsky, A.; Radic, Z.
Deposited on	:	2021-07-07
Resolution	:	9.00 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/EMMapValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

EMDB validation analysis	:	0.0.0.dev97
Validation Pipeline (wwPDB-VP)	:	2.23.1

1 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	2744	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	64.56	Depositor
Minimum defocus (nm)	1.5	Depositor
Maximum defocus (nm)	3.0	Depositor
Magnification	130000.0	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.725	Depositor
Minimum map value	-0.252	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.044	Depositor
Recommended contour level	0.281	Depositor
Map size (Å)	270.4, 270.4, 270.4	wwPDB
Map dimensions	260, 260, 260	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

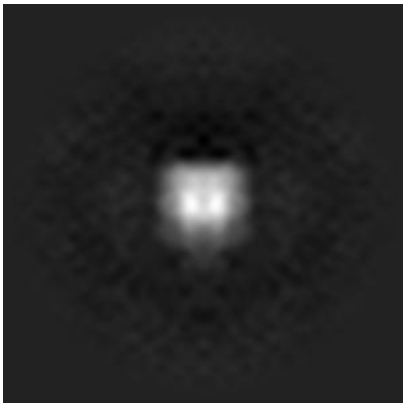
2 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-24404. These allow visual inspection of the internal detail of the map and identification of artifacts.

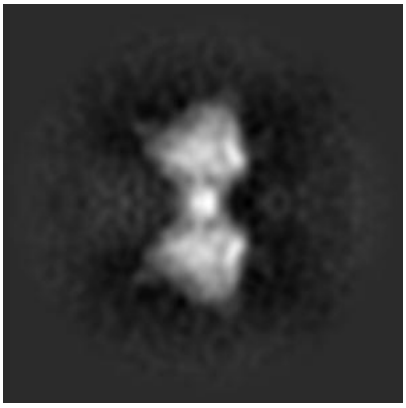
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

2.1 Orthogonal projections (i)

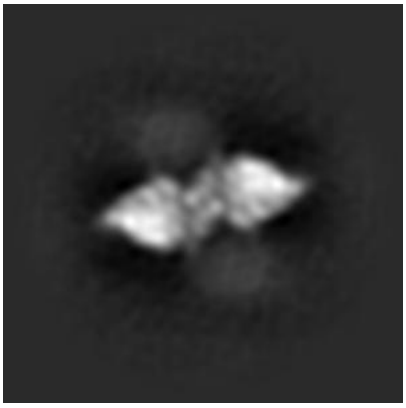
2.1.1 Primary map



X



Y

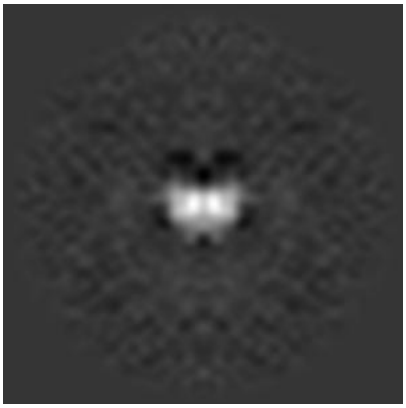


Z

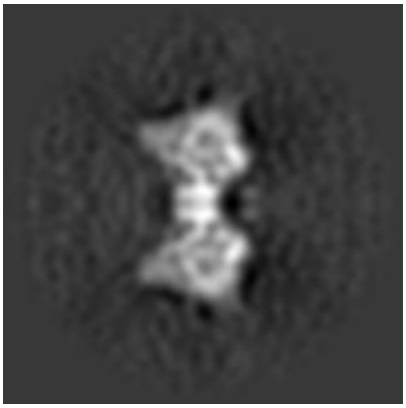
The images above show the map projected in three orthogonal directions.

2.2 Central slices (i)

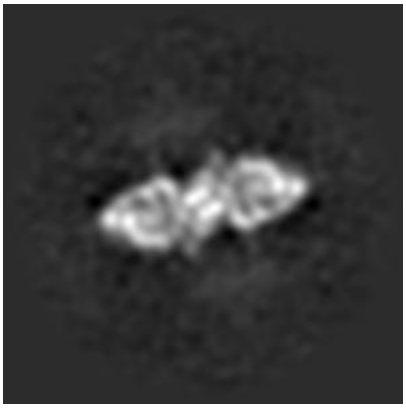
2.2.1 Primary map



X Index: 130



Y Index: 130

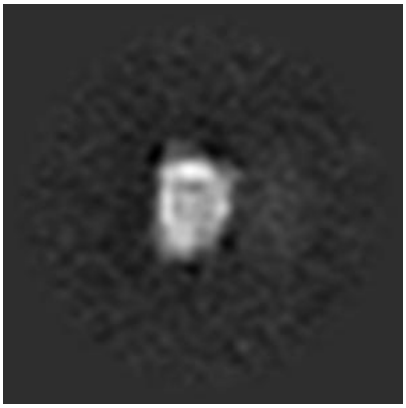


Z Index: 130

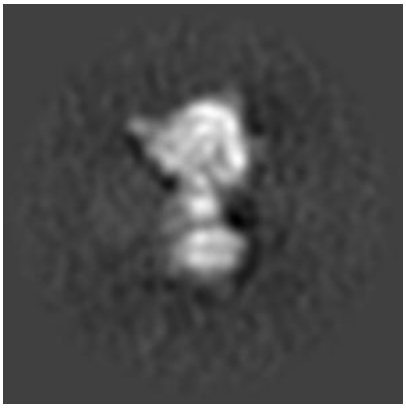
The images above show central slices of the map in three orthogonal directions.

2.3 Largest variance slices (i)

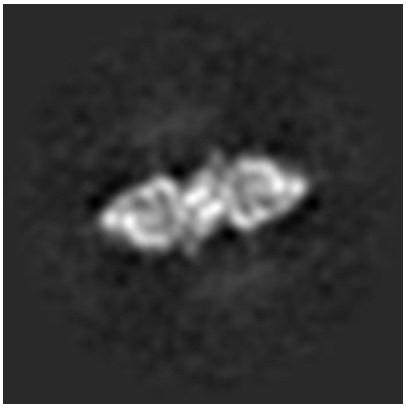
2.3.1 Primary map



X Index: 99



Y Index: 139



Z Index: 129

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

2.4 Orthogonal surface views (i)

2.4.1 Primary map

X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.281. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

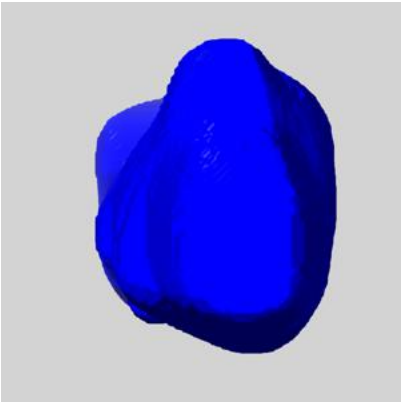
2.5 Mask visualisation (i)

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

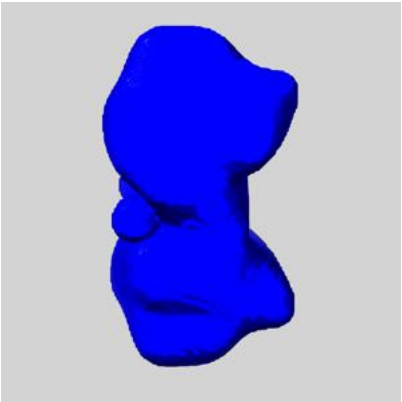
A mask typically either:

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

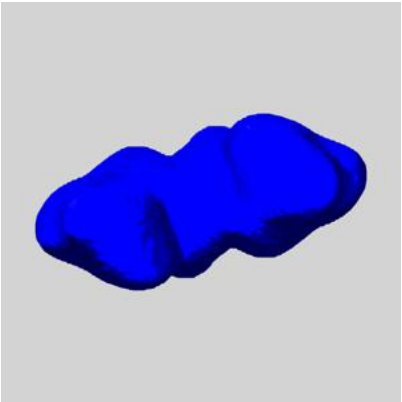
2.5.1 emd_24404_msk_1.map (i)



X



Y

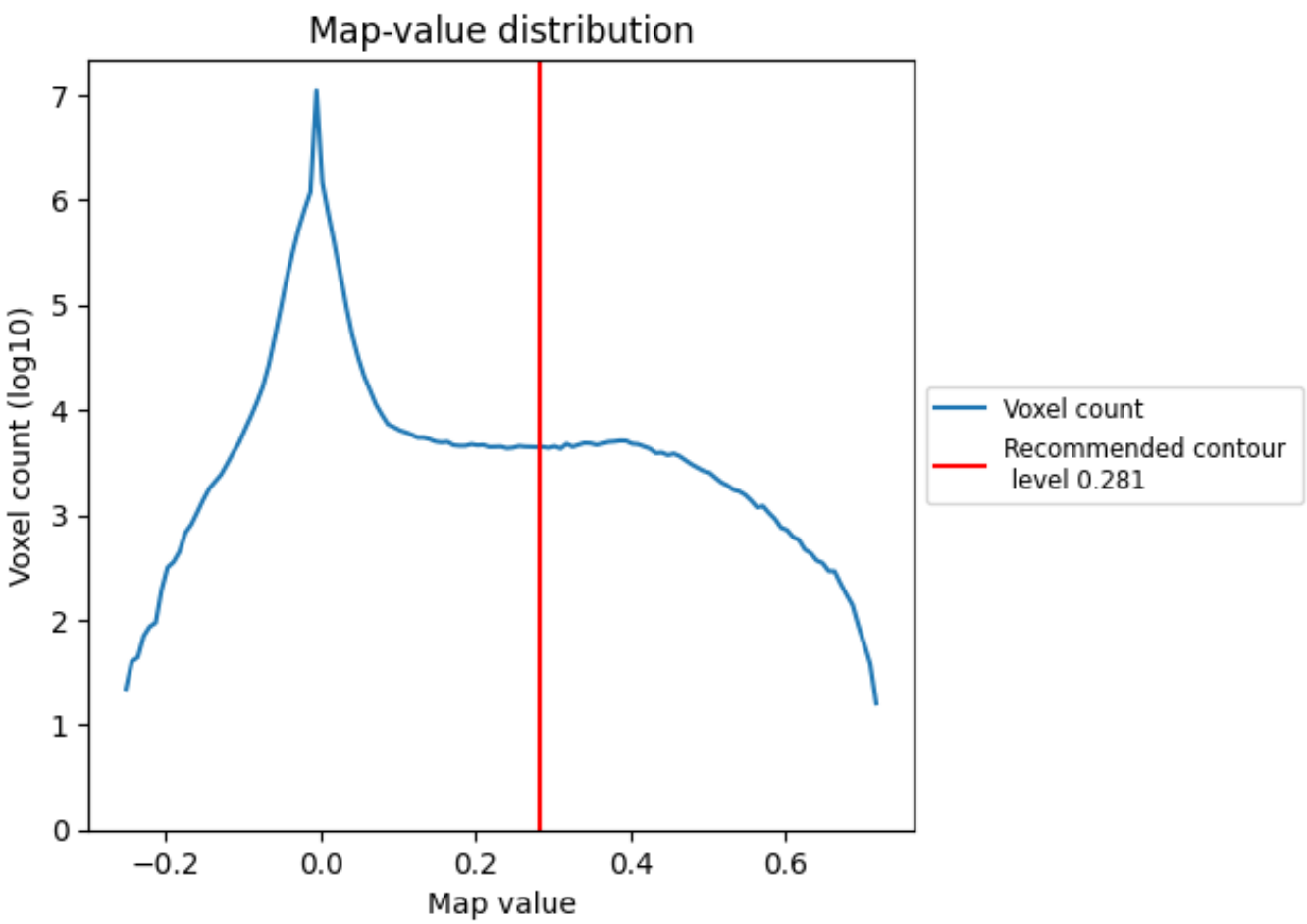


Z

3 Map analysis (i)

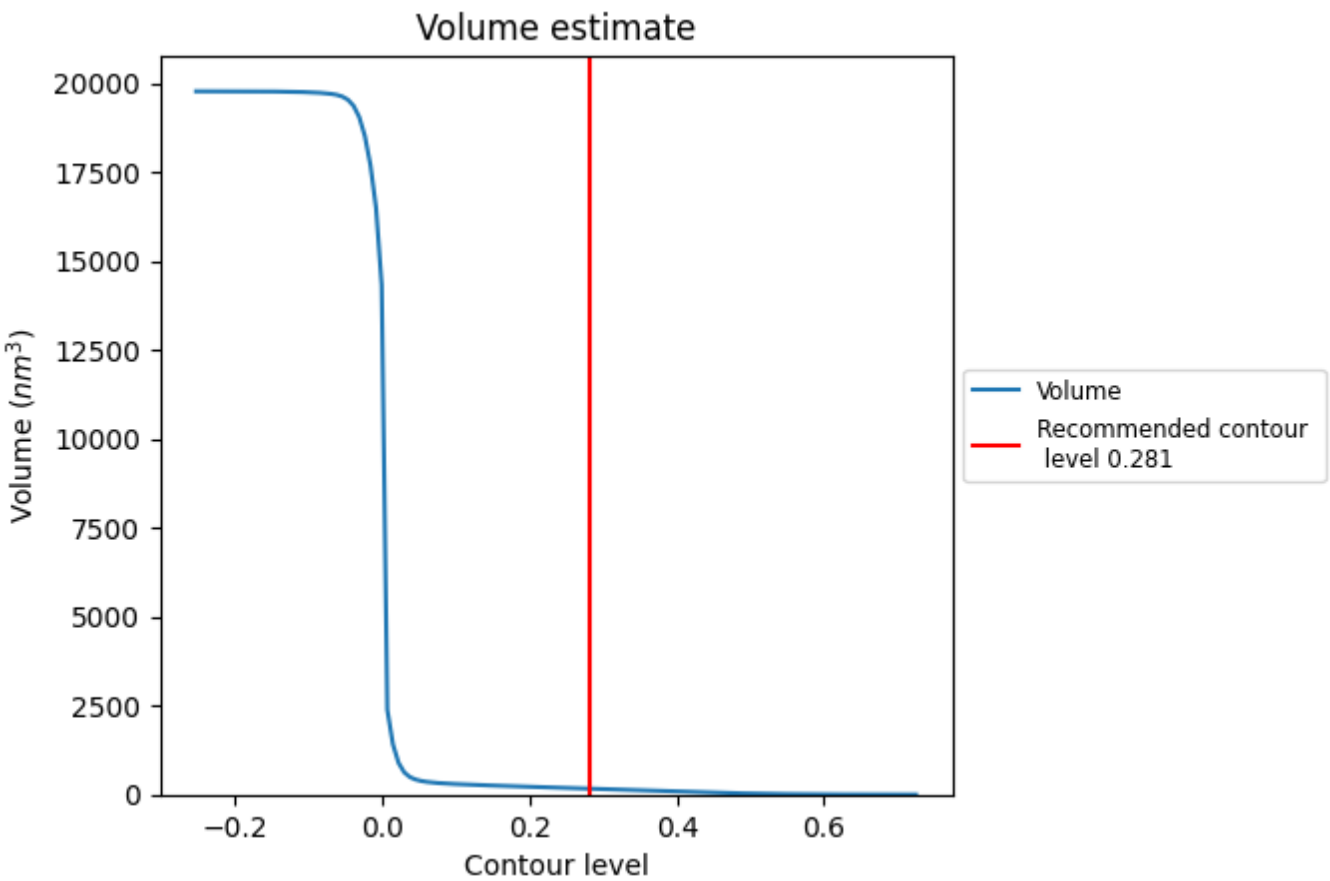
This section contains the results of statistical analysis of the map.

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.

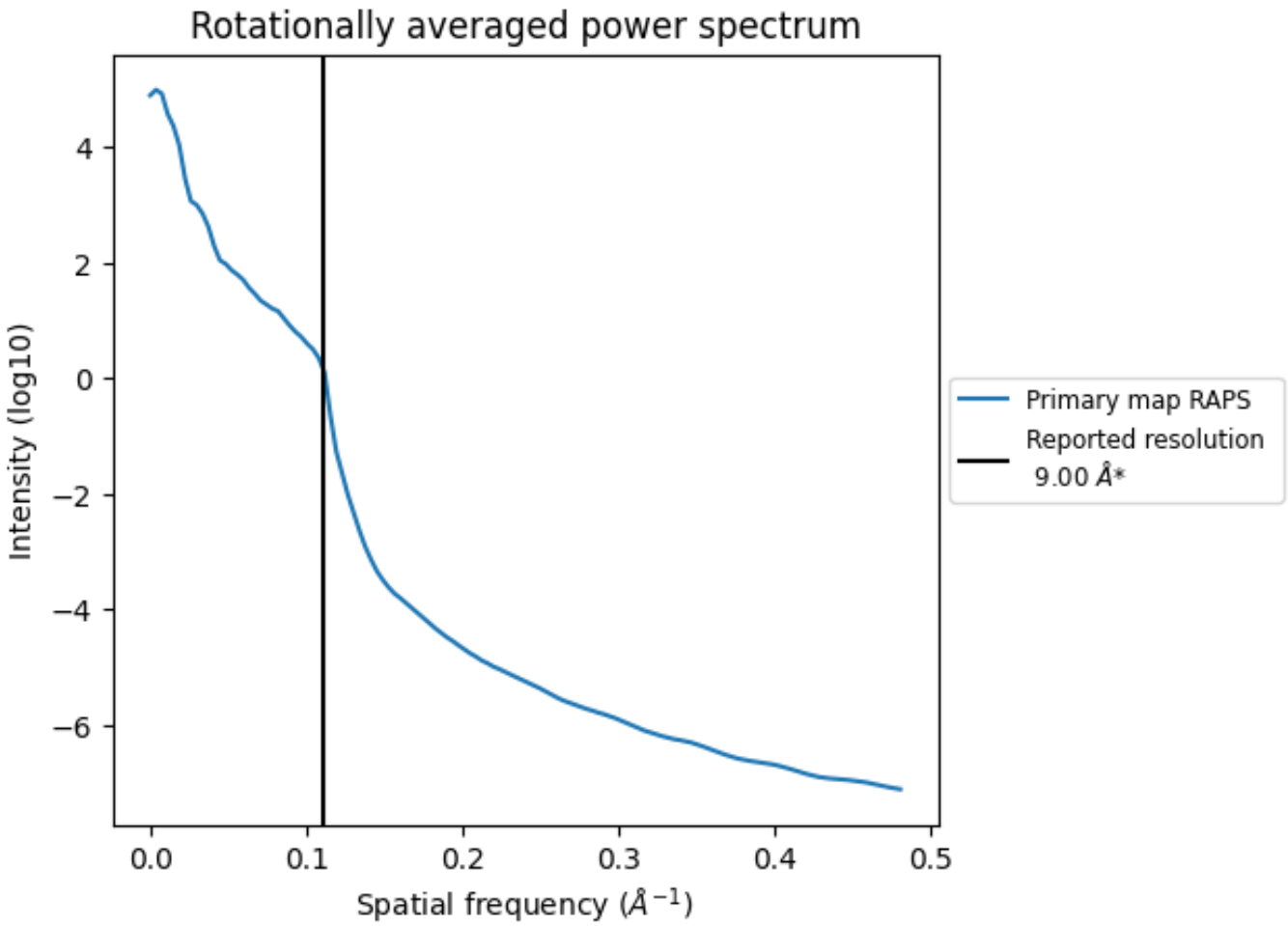
3.2 Volume estimate (i)



The volume at the recommended contour level is 166 nm^3; this corresponds to an approximate mass of 150 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)

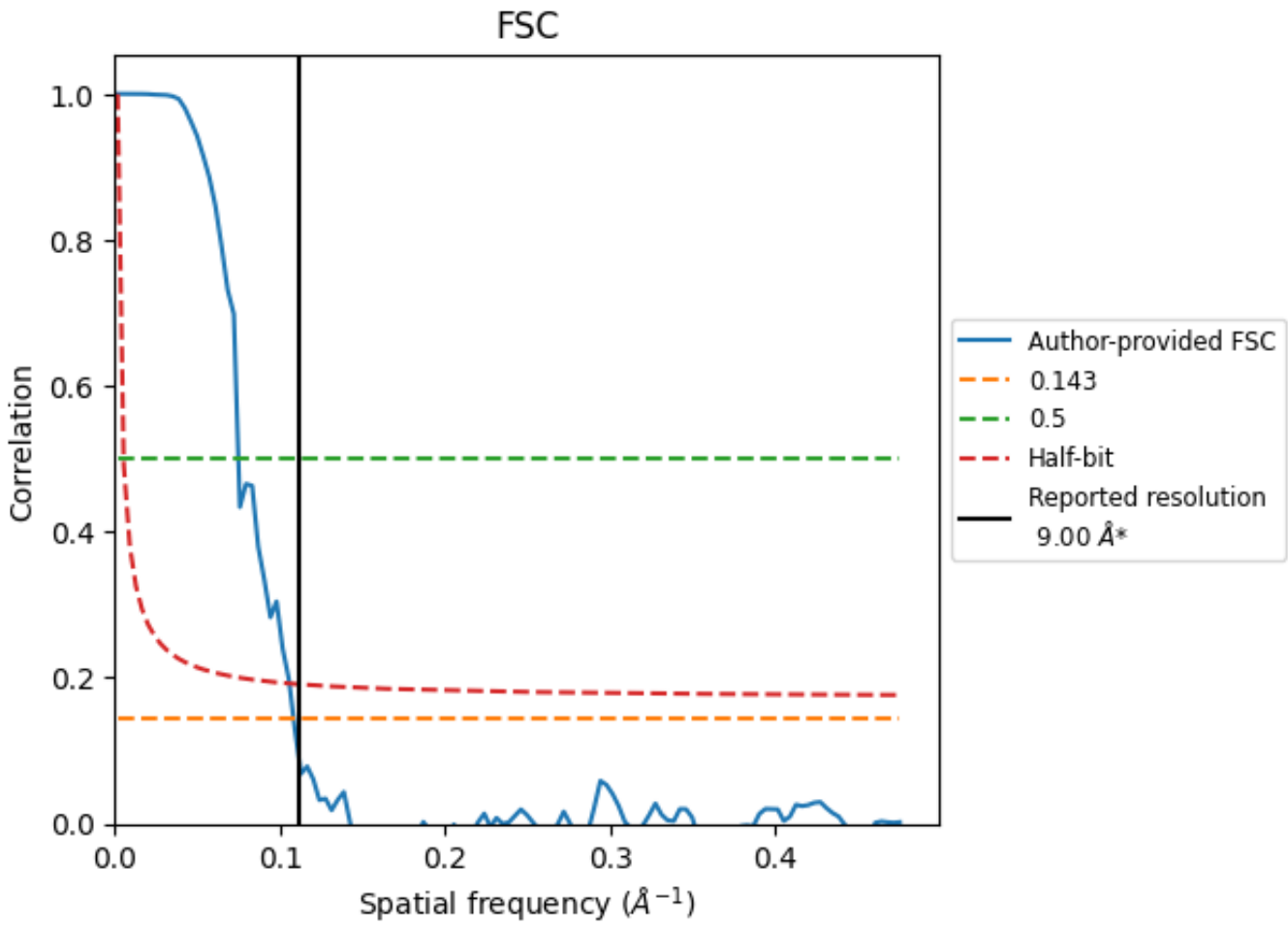


*Reported resolution corresponds to spatial frequency of 0.111 Å^{-1}

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 0.111 Å^{-1}

4.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	9.00	-	-
Author-provided FSC curve	9.23	13.35	9.46
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.