

wwPDB EM Validation Summary Report (i)

Sep 7, 2021 – 01:23 PM BST

EMDB ID : EMD-12024

Title: Programmable icosahedral shell system for virus trapping: DNA-origami T=1

shell (at 25mM MgCl2)

Authors: Sigl, C.; Willner, E.M.; Engelen, W.; Kretzmann, J.A.; Sachenbacher, K.;

Liedl, A.; Kolbe, F.; Wilsch, F.; Aghvami, S.A.; Protzer, U.; Hagan, M.F.;

Fraden, S.; Dietz, H.

Deposited on : 2020-12-03

Resolution : 22.20 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 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.dev97Validation Pipeline (wwPDB-VP) : 2.23.1

1 Experimental information (i)

Property	Value	Source	
EM reconstruction method	SINGLE PARTICLE	Depositor	
Imposed symmetry	POINT, I	Depositor	
Number of particles used	720	Depositor	
Resolution determination method	FSC 0.143 CUT-OFF	Depositor	
CTF correction method	Not provided		
Microscope	FEI TITAN KRIOS	Depositor	
Voltage (kV)	300	Depositor	
Electron dose $(e^-/\text{Å}^2)$	31.3	Depositor	
Minimum defocus (nm)	Not provided		
Maximum defocus (nm)	Not provided		
Magnification	Not provided		
Image detector	FEI FALCON III (4k x 4k)	Depositor	
Maximum map value	0.085	Depositor	
Minimum map value	-0.028	Depositor	
Average map value	0.002	Depositor	
Map value standard deviation	0.011	Depositor	
Recommended contour level	0.0173	Depositor	
Map size (Å)	1709.999, 1709.999, 1709.999	wwPDB	
Map dimensions	374, 374, 374	wwPDB	
Map angles (°)	90.0, 90.0, 90.0	wwPDB	
Pixel spacing (Å)	4.57219, 4.57219, 4.57219	Depositor	



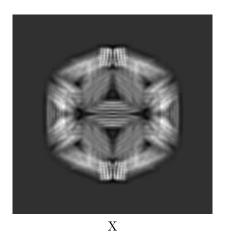
2 Map visualisation (i)

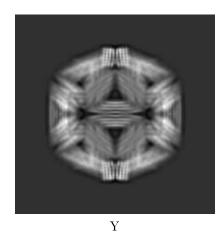
This section contains visualisations of the EMDB entry EMD-12024. These allow visual inspection of the internal detail of the map and identification of artifacts.

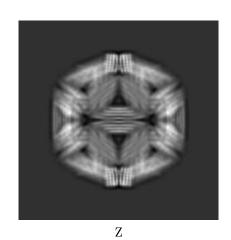
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

2.1 Orthogonal projections (i)

2.1.1 Primary map







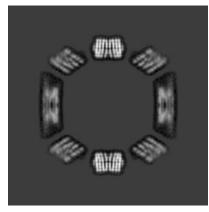
The images above show the map projected in three orthogonal directions.

2.2 Central slices (i)

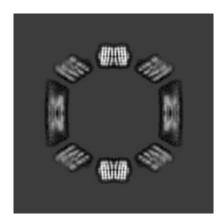
2.2.1 Primary map







Y Index: 187



Z Index: 187

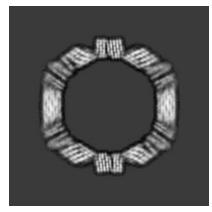


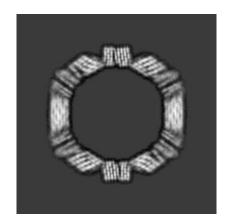
The images above show central slices of the map in three orthogonal directions.

Largest variance slices (i) 2.3

2.3.1Primary map







X Index: 203

Y Index: 203

Z Index: 203

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

2.4 Orthogonal surface views (i)

2.4.1Primary map







The images above show the 3D surface view of the map at the recommended contour level 0.0173. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

Y



2.5 Mask visualisation (i)

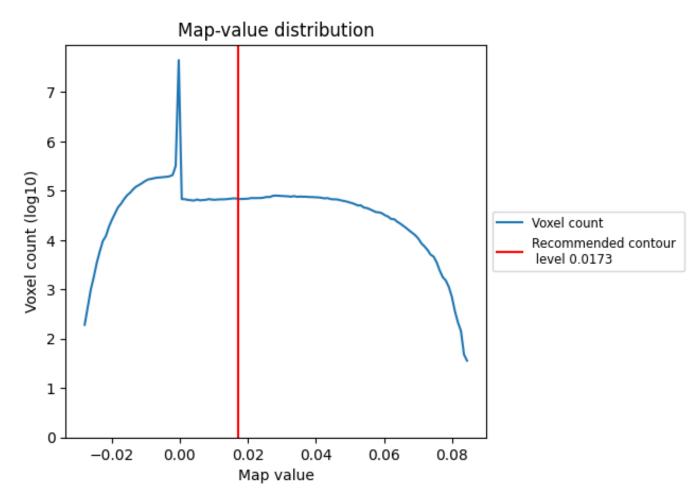
This section was not generated. No masks/segmentation were deposited.



3 Map analysis (i)

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

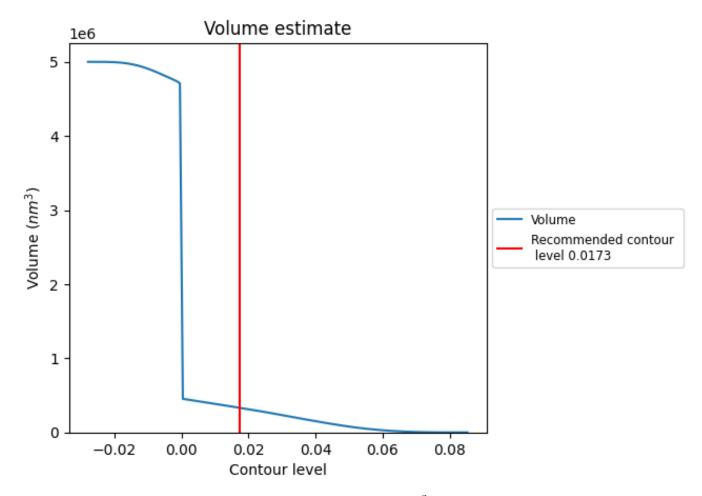
3.1 Map-value distribution (i)



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)

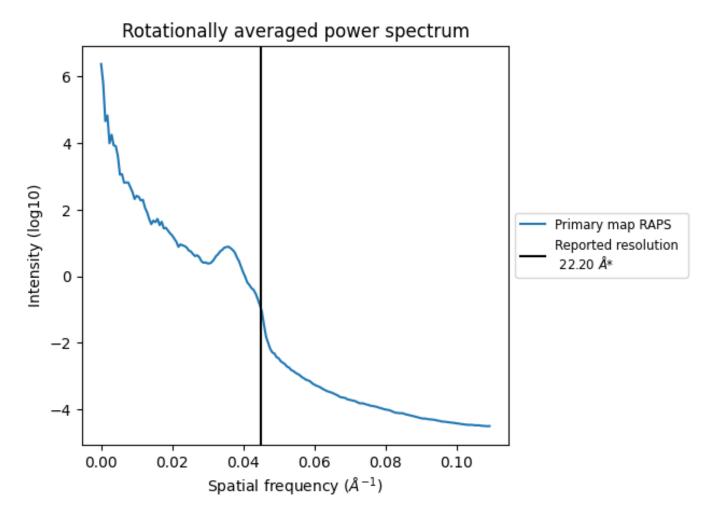


The volume at the recommended contour level is 332039 nm³; this corresponds to an approximate mass of 299939 kDa.

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)



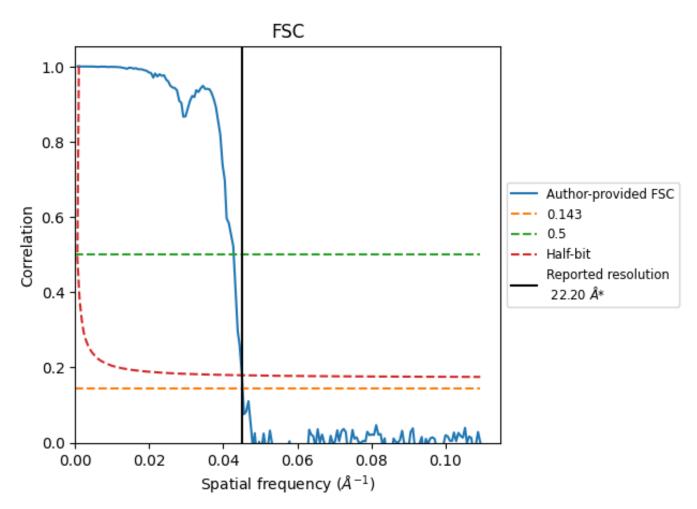
^{*}Reported resolution corresponds to spatial frequency of 0.045 ${\rm \AA}^{-1}$



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 0.045 Å^{-1}



4.2 Resolution estimates (i)

Resolution estimate (Å)	\mid Estimation criterion (FSC cut-off) \mid		
resolution estimate (A)	0.143	0.5	Half-bit
Reported by author	22.20	-	-
Author-provided FSC curve	22.12	23.36	22.17
Unmasked-calculated*	-	-	-

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

