wwPDB EM Validation Summary Report (i)

Mar 31, 2021 – 10:43 am BST

EMDB ID	:	EMD-3500
Title	:	Substrate specificity in plant nitrilase helical assemblies is determined by their twist.
Authors	:	Woodward, J.D.; Trompetter, I.; Sewell, B.T.; Piotrowski, M.
Deposited on	:	2016-11-15
Resolution	:	20.00 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.dev75
Validation Pipeline (wwPDB-VP)	:	2.18

1 Experimental information (i)

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-69°, rise=14.7 Å, axial sym=D2	Depositor
Number of segments used	1824	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	Not provided	
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose (e^-/Å^2)	20.0	Depositor
Minimum defocus (nm)	0.3	Depositor
Maximum defocus (nm)	0.5	Depositor
Magnification	50200.	Depositor
Image detector	GATAN ULTRASCAN 4000 (4k x 4k)	Depositor
Maximum map value	0.102	Depositor
Minimum map value	-0.046	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.0177	Depositor
Map size (Å)	270.08, 270.08, 270.08	wwPDB
Map dimensions	64, 64, 64	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	4.22, 4.22, 4.22	Depositor

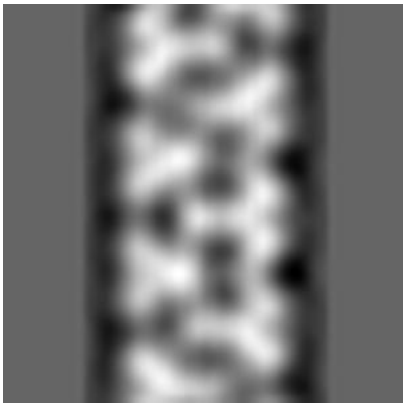
2 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-3500. 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

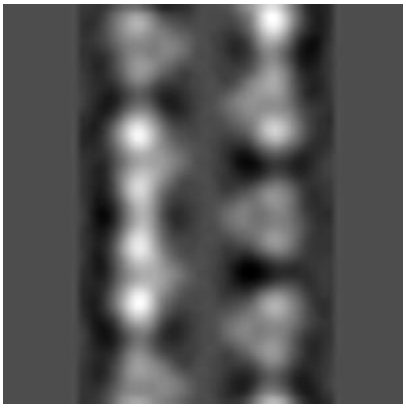
Y

Z

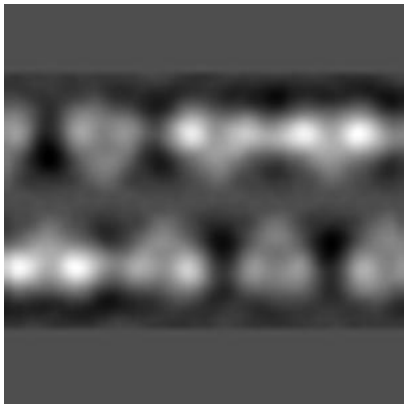
The images above show the map projected in three orthogonal directions.

2.2 Central slices (i)

2.2.1 Primary map



X Index: 32



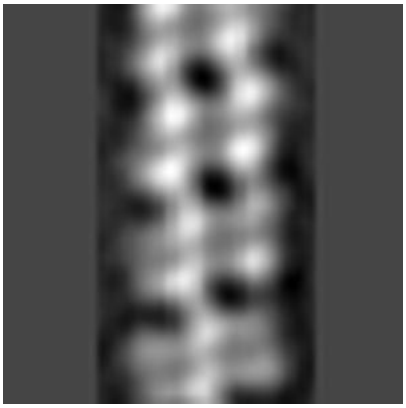
Y Index: 32

Z Index: 32

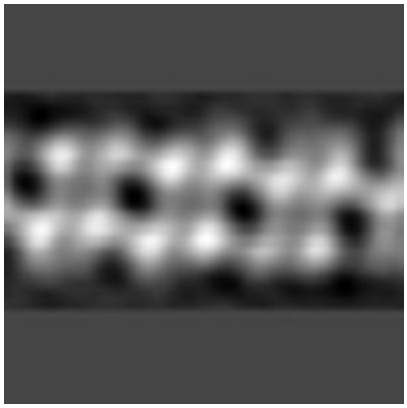
The images above show central slices of the map in three orthogonal directions.

2.3 Largest variance slices (i)

2.3.1 Primary map



X Index: 23



Y Index: 41

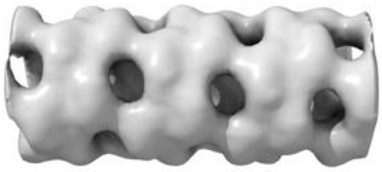
Z Index: 1

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

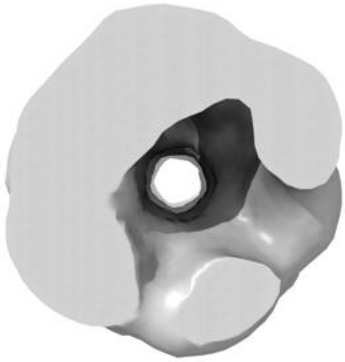
2.4 Orthogonal surface views (i)

2.4.1 Primary map

X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0177. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

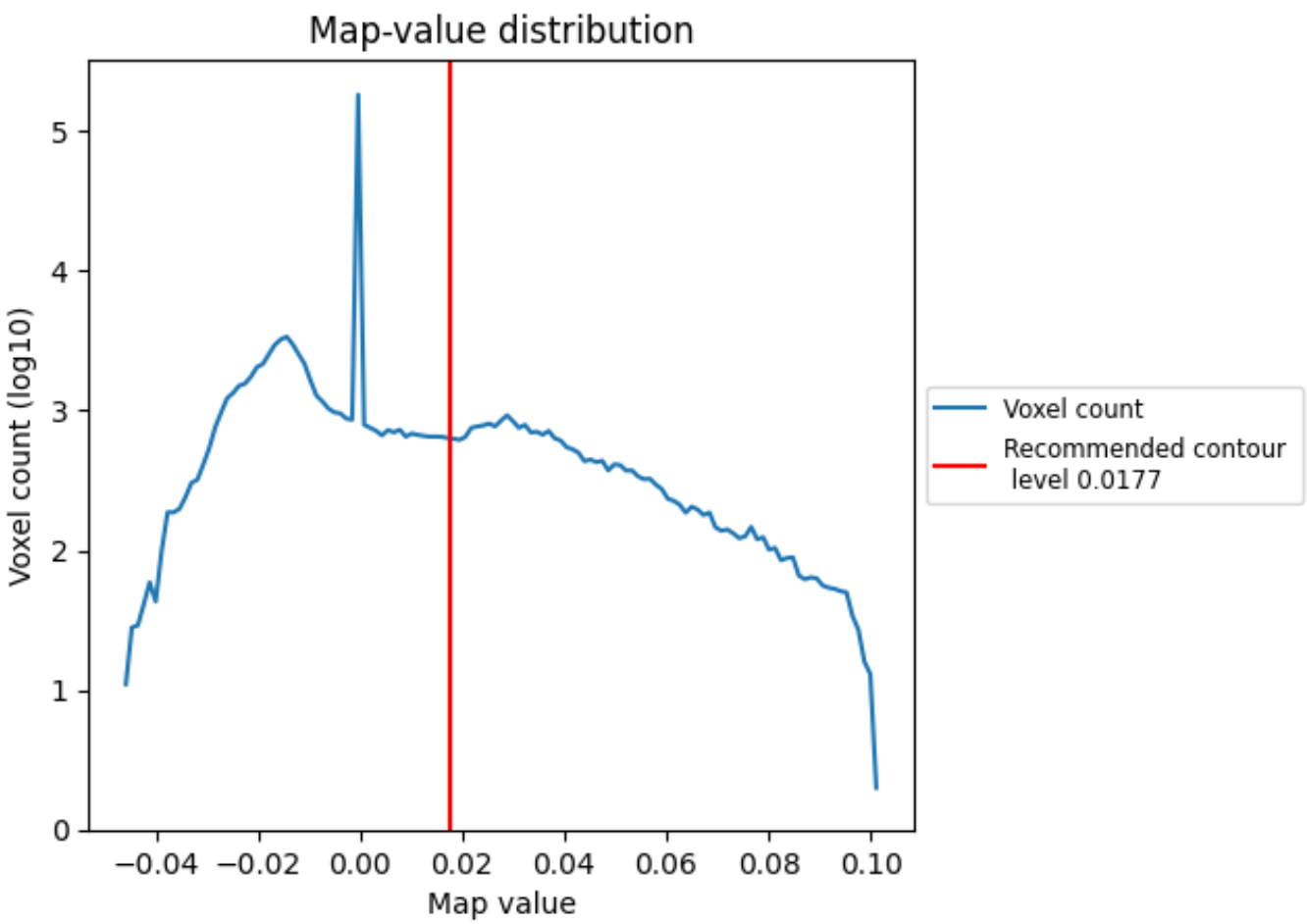
2.5 Mask visualisation (i)

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

3 Map analysis (i)

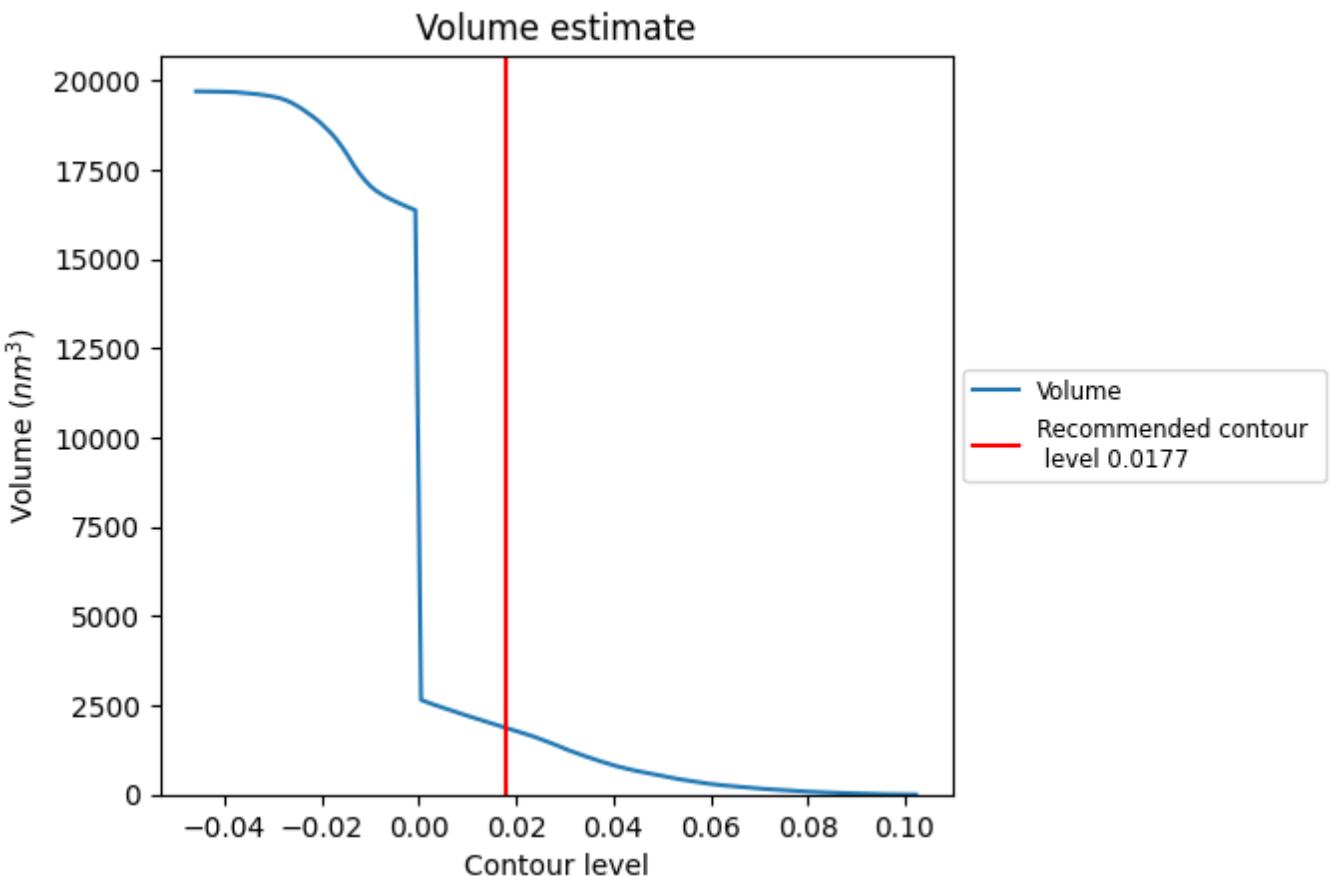
This section contains the results of statistical analysis of the map.

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.

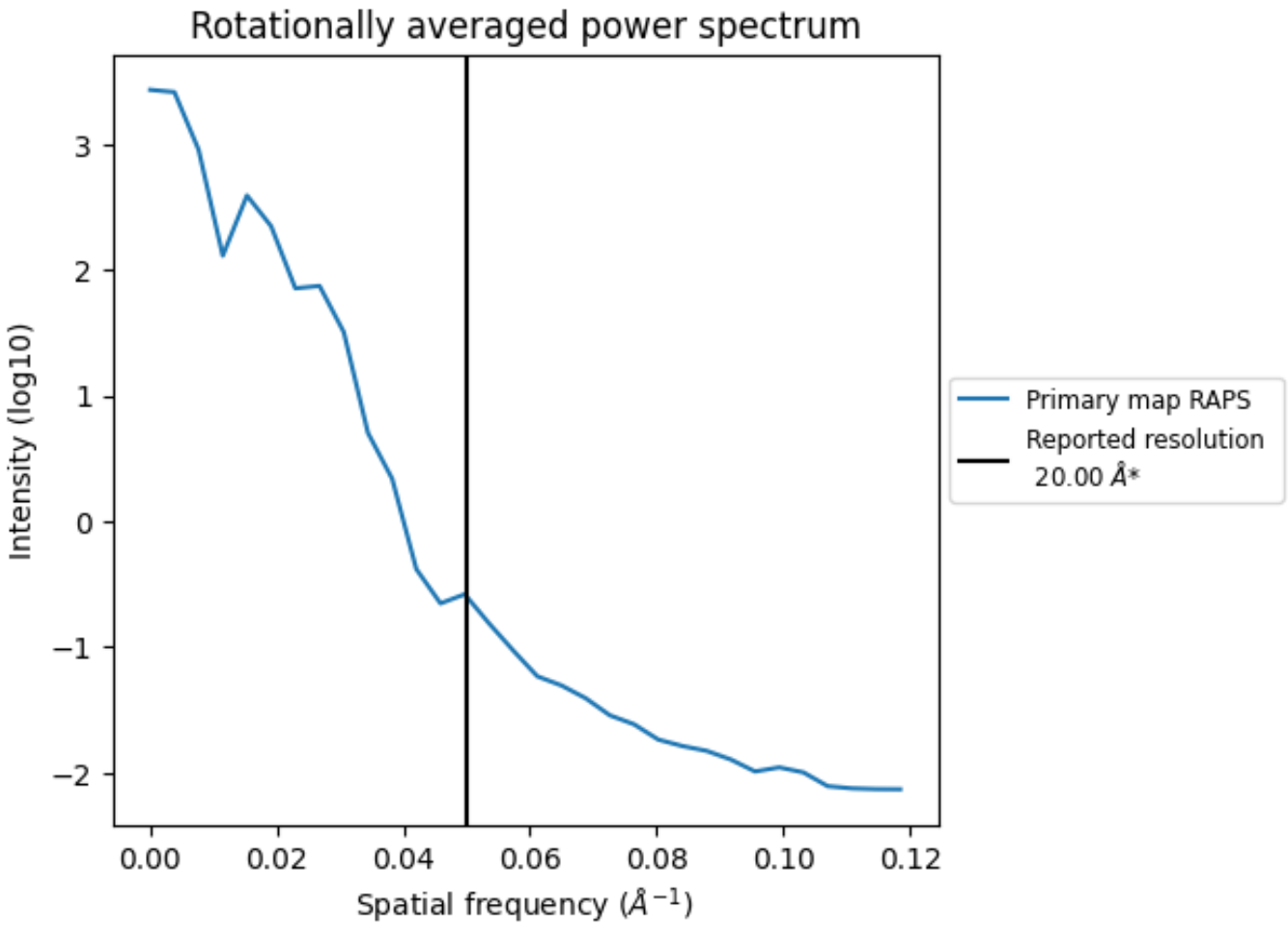
3.2 Volume estimate (i)



The volume at the recommended contour level is 1878 nm^3; this corresponds to an approximate mass of 1697 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 0.050 Å^{-1}

4 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.