# Full wwPDB EM Validation Report (i)

Mar 31, 2021 – 11:01 am BST

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|---|---|---|
| EMDB ID | : | EMD-4406 |
| Title | : | Cryo-EM informed directed evolution of Nitrilase 4 leads to a change in quaternary structure. |
| Authors | : | Mulelu, A.E.; Woodward, J.D. |
| Deposited on | : | 2018-11-08 |
| Resolution | : | 20.00 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 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=-65.59083°, rise=14.52459 Å, axial sym=C2 | Depositor |
| Number of segments used | 10000 | Depositor |
| Resolution determination method | FSC 0.5 CUT-OFF | Depositor |
| CTF correction method | Not provided | |
| Microscope | FEI TECNAI 20 | Depositor |
| Voltage (kV) | 200 | Depositor |
| Electron dose ($e^-$/Å$^2$) | 10.0 | Depositor |
| Minimum defocus (nm) | 0.5 | Depositor |
| Maximum defocus (nm) | 0.5 | Depositor |
| Magnification | 50000. | Depositor |
| Image detector | GATAN ULTRASCAN 4000 (4k x 4k) | Depositor |
| Maximum map value | 4.961 | Depositor |
| Minimum map value | -2.571 | Depositor |
| Average map value | 0.000 | Depositor |
| Map value standard deviation | 1.000 | Depositor |
| Recommended contour level | 2.0 | Depositor |
| Map size (Å) | 328.80002, 328.80002, 328.80002 | wwPDB |
| Map dimensions | 80, 80, 80 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 4.11, 4.11, 4.11 | Depositor |

# 2 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-4406. These allow visual inspection of the internal detail of the map and identification of artifacts.

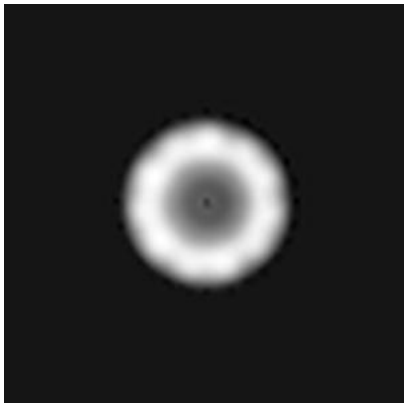
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

## 2.1 Orthogonal projections (i)

### 2.1.1 Primary map

X

Y

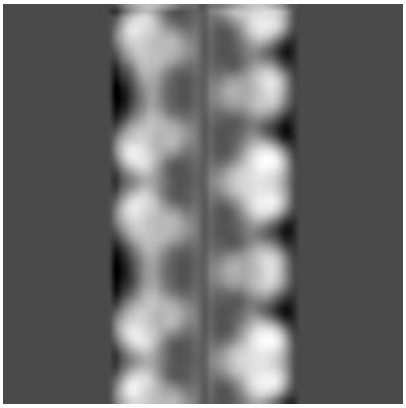


Z

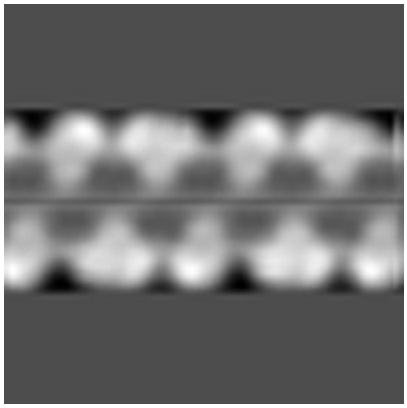
The images above show the map projected in three orthogonal directions.

## 2.2 Central slices (i)

### 2.2.1 Primary map



X Index: 40



Y Index: 40

Z Index: 40

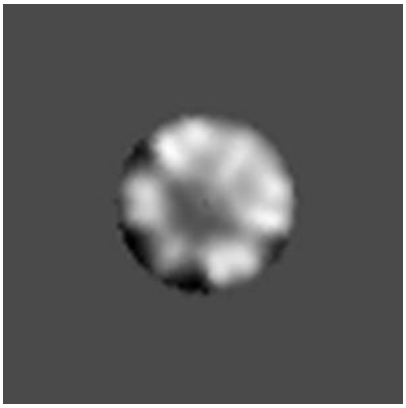
The images above show central slices of the map in three orthogonal directions.

## 2.3 Largest variance slices (i)

### 2.3.1 Primary map

X Index: 29

Y Index: 50



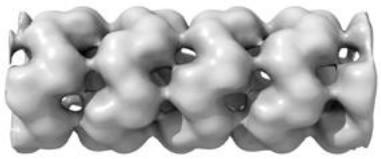
Z Index: 64

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

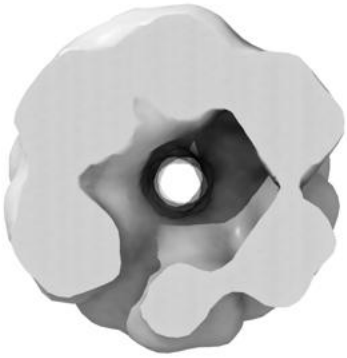
## 2.4 Orthogonal surface views (i)

### 2.4.1 Primary map

X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

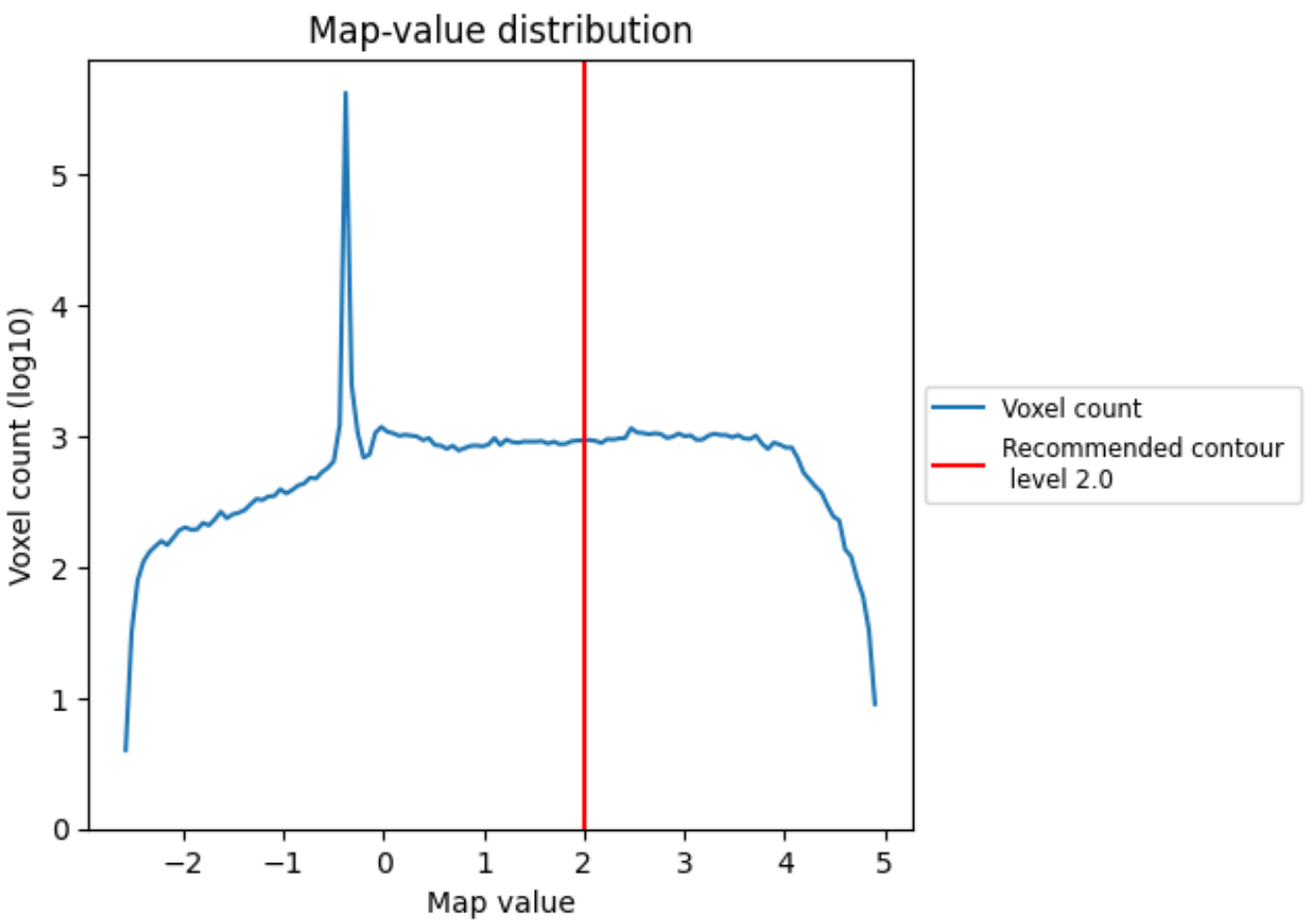
## 2.5 Mask visualisation (i)

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

# 3 Map analysis (i)

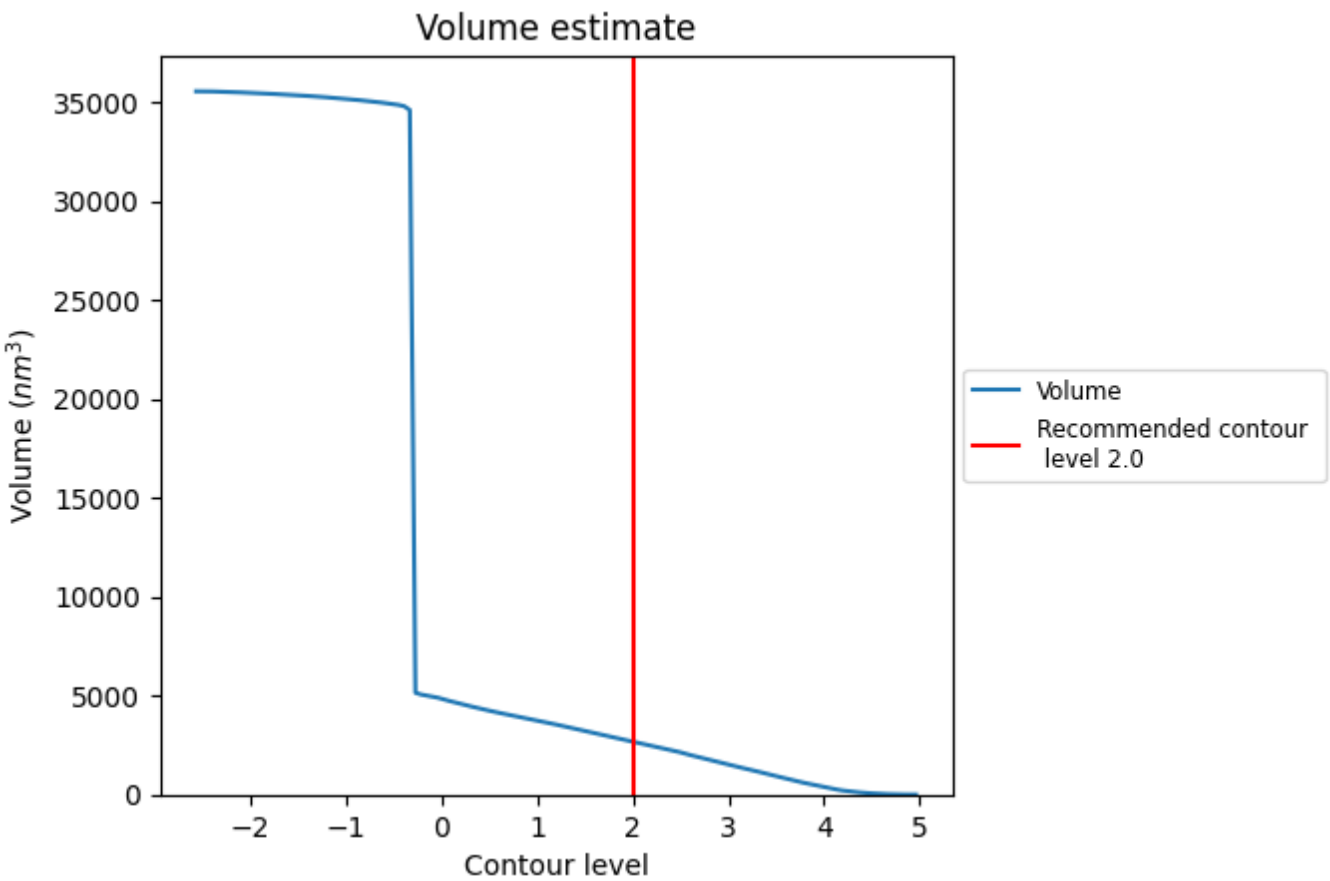
This section contains the results of statistical analysis of the map.

## 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.

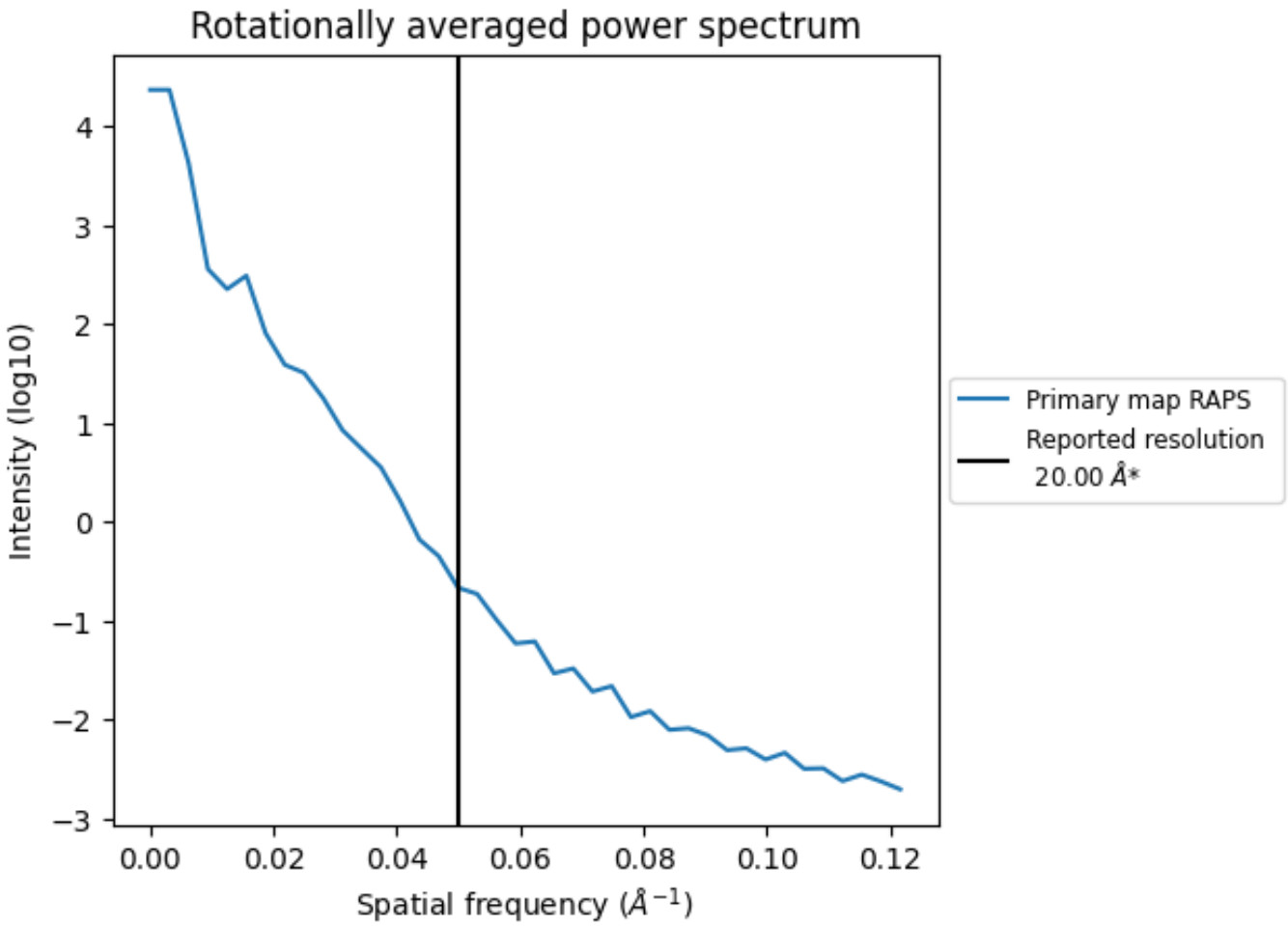
## 3.2 Volume estimate (i)




The volume at the recommended contour level is 2686 $nm^3$; this corresponds to an approximate mass of 2426 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.