Full wwPDB EM Validation Report (i)

Nov 28, 2022 – 11:56 PM EST

EMDB ID	:	EMD-24080
Title	:	MicroED Structure of Acetaminophen
Authors	:	Powell, S.M.; Novikova, I.V.; Evans, J.E.
Deposited on	:	2021-05-21
Resolution	:	Not provided

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.dev43
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Experimental information (i)

Property	Value	Source
EM reconstruction method	CRYSTALLOGRAPHY	Depositor
Imposed symmetry	Not Provided	
Number of images used	Not provided	
Resolution determination method	DIFFRACTION PATTERN/LAYERLINES	Depositor
CTF correction method	Not provided	
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	0.008	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI CETA (4k x 4k)	Depositor
Maximum map value	12.226	Depositor
Minimum map value	-2.875	Depositor
Average map value	0.002	Depositor
Map value standard deviation	1.054	Depositor
Recommended contour level	1.5	Depositor
Map size (Å)	20.504168, 20.894722, 19.723055	wwPDB
Map dimensions	107, 105, 101	wwPDB
Map angles (°)	90.0, 97.903, 90.0	wwPDB
Pixel spacing (Å)	0.19527778, 0.19527778, 0.19527777	Depositor

2 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-24080. These allow visual inspection of the internal detail of the map and identification of artifacts.

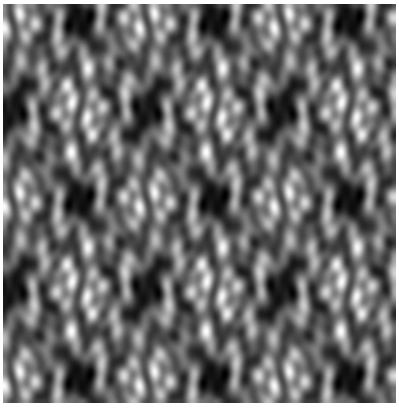
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

2.1 Orthogonal projections (i)

2.1.1 Primary map

X

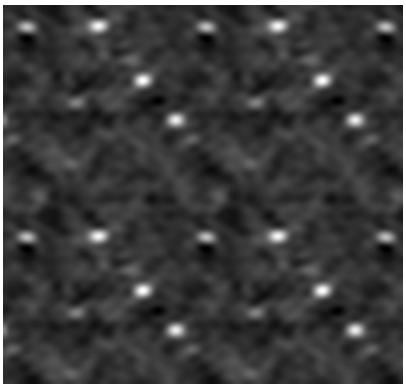
Y

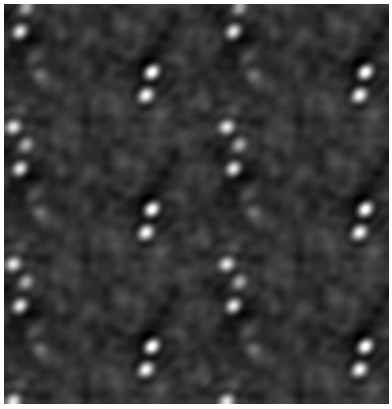

Z

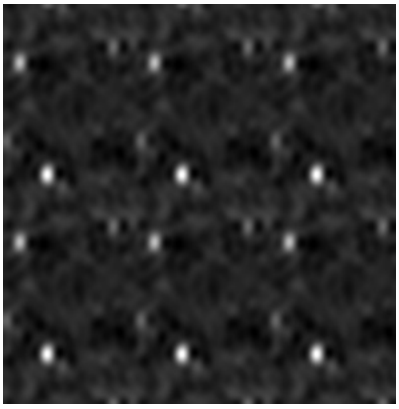
The images above show the map projected in three orthogonal directions.

2.2 Central slices (i)

2.2.1 Primary map


X Index: 52

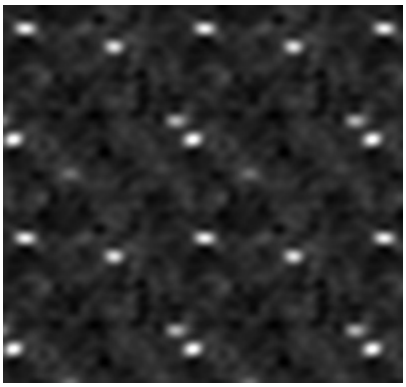

Y Index: 53


Z Index: 50

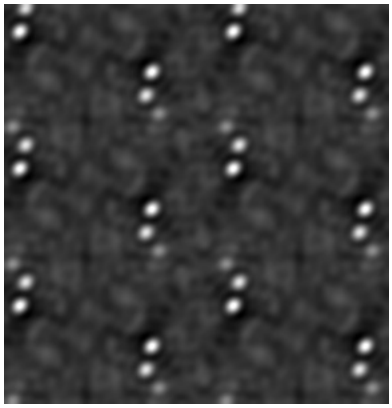
The images above show central slices of the map in three orthogonal directions.

2.3 Largest variance slices (i)

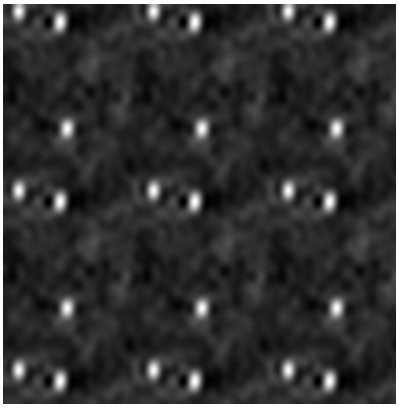
2.3.1 Primary map



X Index: 14



Y Index: 6

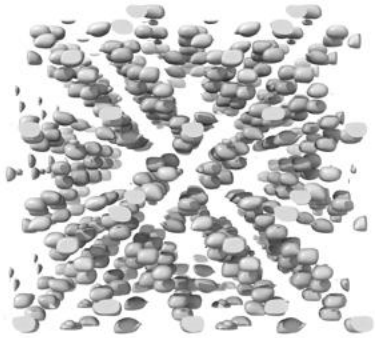


Z Index: 39

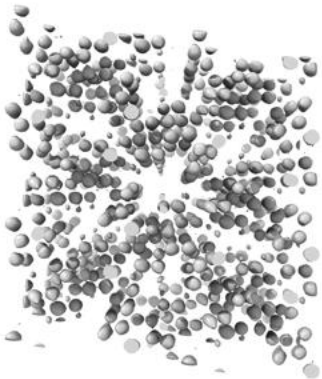
The images above show the largest variance slices of the map in three orthogonal directions.

2.4 Orthogonal surface views (i)

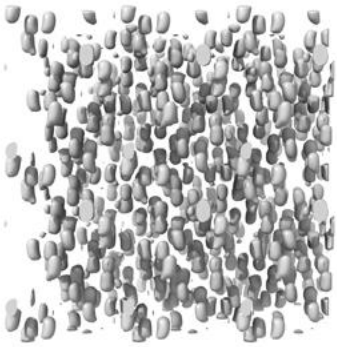
2.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

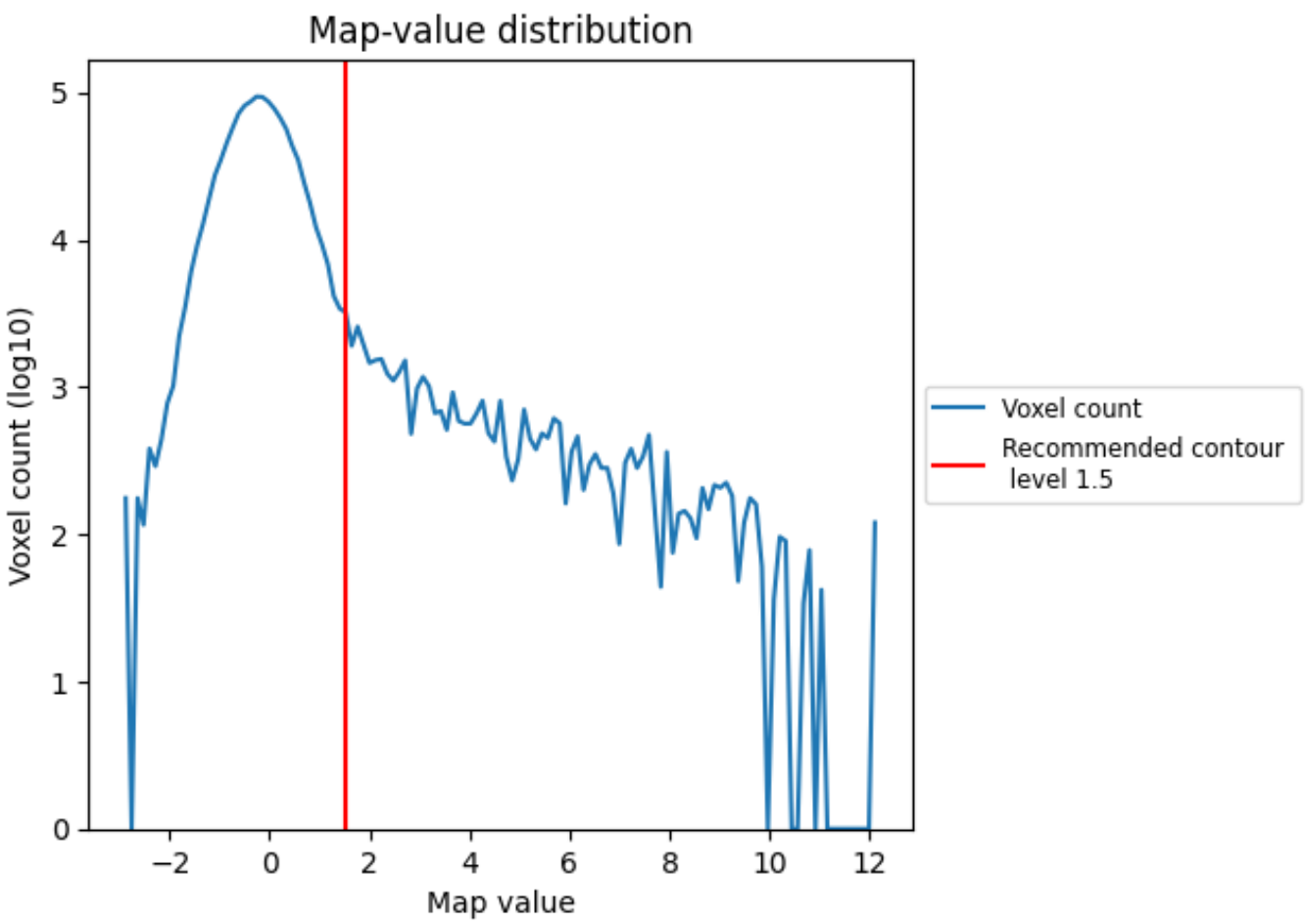
2.5 Mask visualisation (i)

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

3 Map analysis (i)

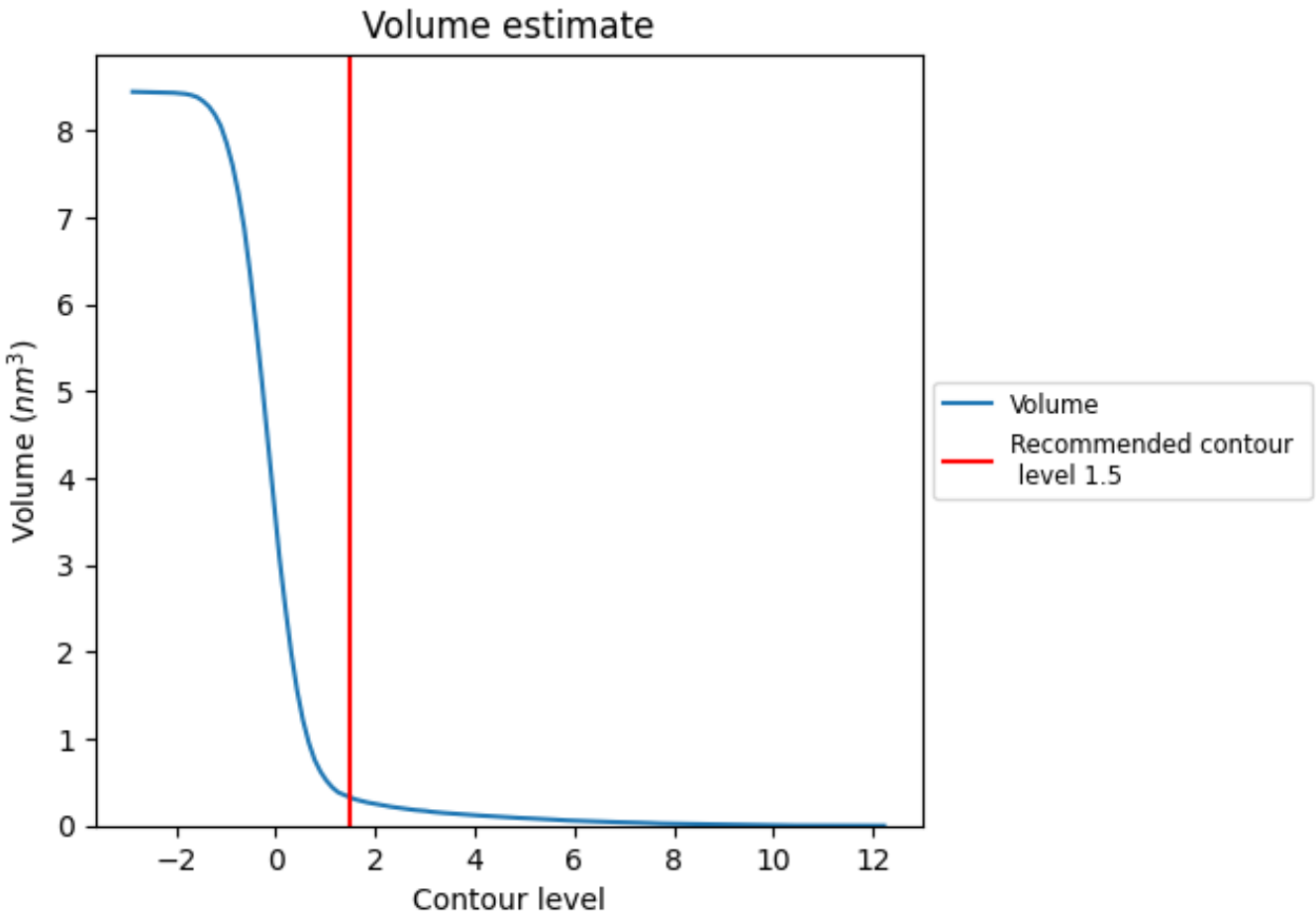
This section contains the results of statistical analysis of the map.

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 0 nm^3; this corresponds to an approximate mass of 0 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)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

4 Fourier-Shell correlation (i)

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