

Full wwPDB EM Validation Report (i)

May 31, 2022 – 01:42 pm BST

EMDB ID : EMD-13764

Title: Structure of Hedgehog acyltransferase (HHAT) in complex with megabody 177

bound to non-hydrolysable palmitoyl-CoA (Composite Map)

Authors: Coupland, C.; Carrique, L.; Siebold, C.

Deposited on : 2021-10-21

Resolution : 2.70 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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

 $\begin{array}{ccc} EMDB \ validation \ analysis & : & 0.0.1.dev8 \\ Validation \ Pipeline \ (wwPDB-VP) & : & 2.28.1 \end{array}$

$1\quad Experimental\ information\ {\color{red}(\mathbf{i})}$

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	238000	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 $(e^-/\text{Å}^2)$	54.8	Depositor
Minimum defocus (nm)	1.0	Depositor
Maximum defocus (nm)	2.5	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	61.287	Depositor
Minimum map value	-31.064	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	10.8	Depositor
Map size (Å)	331.59, 331.59, 331.59	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1053, 1.1053, 1.1053	Depositor



2 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-13764. 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)

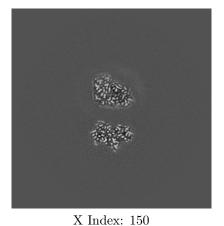
2.1.1 Primary map

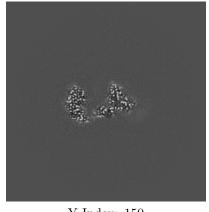


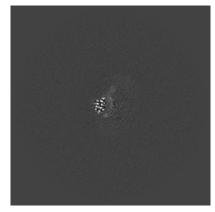
The images above show the map projected in three orthogonal directions.

2.2 Central slices (i)

2.2.1 Primary map







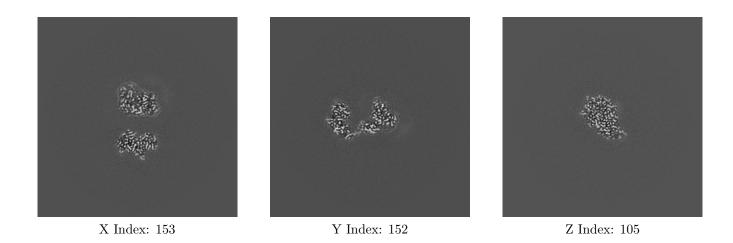
Y Index: 150 Z Index: 150



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

2.3 Largest variance slices (i)

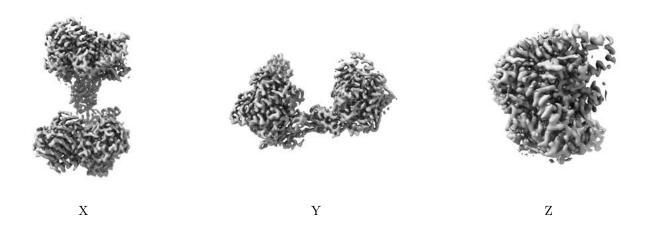
2.3.1 Primary map



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



The images above show the 3D surface view of the map at the recommended contour level 10.8. 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)

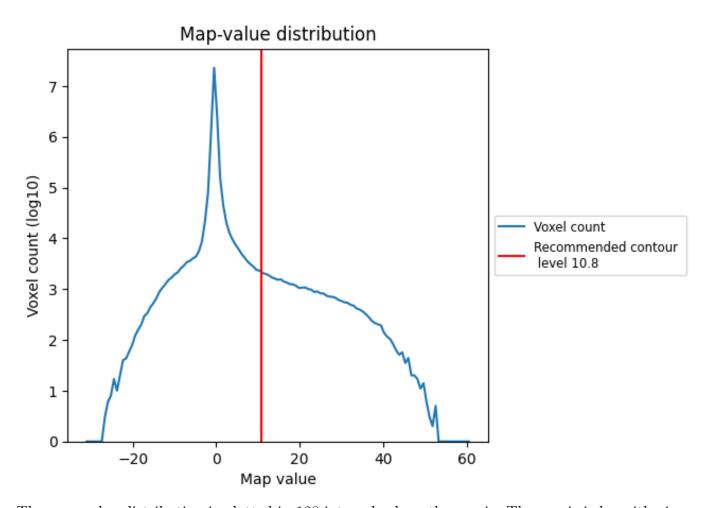
This section was not generated. No masks/segmentation were deposited.



3 Map analysis (i)

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

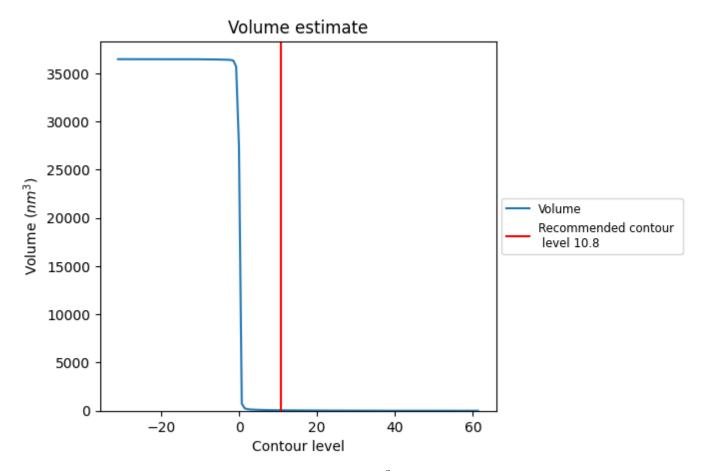
3.1 Map-value distribution (i)



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)

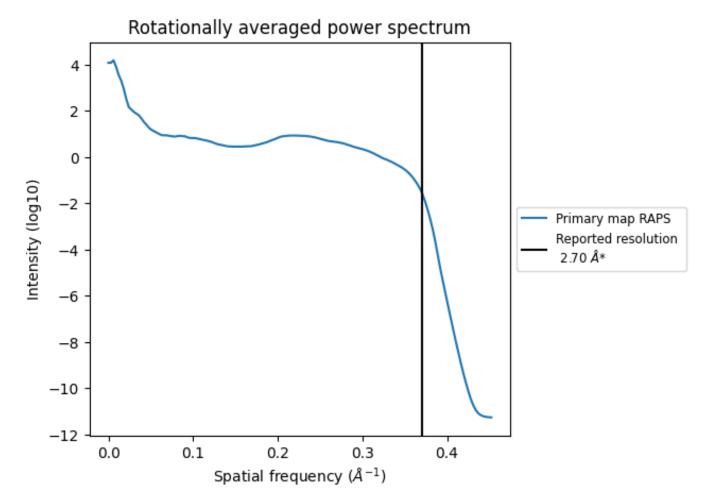


The volume at the recommended contour level is $51~\mathrm{nm^3}$; this corresponds to an approximate mass of $46~\mathrm{kDa}$.

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 0.370 $\rm \mathring{A}^{-1}$



4 Fourier-Shell correlation (i)

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

