



## wwPDB EM Validation Summary Report ⓘ

Nov 19, 2022 – 07:21 PM EST

PDB ID : 3CNF  
EMDB ID : EMD-1508  
Title : 3.88 Angstrom structure of cytoplasmic polyhedrosis virus by cryo-electron microscopy  
Authors : Yu, X.; Jin, L.; Zhou, Z.H.  
Deposited on : 2008-03-25  
Resolution : 3.88 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev43  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3

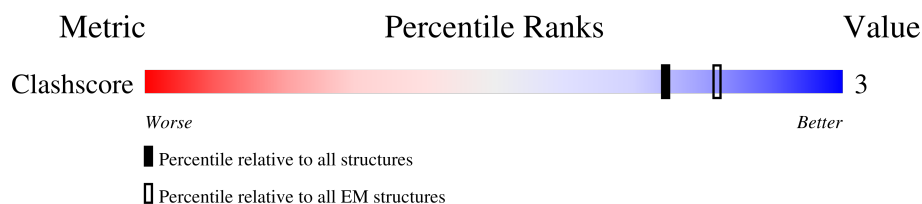
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*




The reported resolution of this entry is 3.88 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1333	 69%                      31%
1	B	1333	 69%                      31%
2	T	1057	 34%                      66%

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2199 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called VP1.

Mol	Chain	Residues	Atoms		AltConf	Trace
1	A	920	Total 920	C 920	0	920
1	B	924	Total 924	C 924	0	924

- Molecule 2 is a protein called VP3.

Mol	Chain	Residues	Atoms		AltConf	Trace
2	T	355	Total 355	C 355	0	355





SER	LEU	THR	TYR	PHE	ALA	ALA
	VAL	GLN	VAL	LYS	LEU	ALA
	GLU	MET	VAL	GLY	SER	ALA
	ALA	ASP	ILE	ARG	GLN	VAL
	ASP	ILE	PRO	THR	LYS	PHE
	THR	ARG	ALA	ARG	SER	PRO
	LEU	ASN	THR	GLU	TYR	PHE
	MET	VAL	ARG	PHE	CYS	THR
	LEU	ALA	ILE	SER	SER	TYR
	THR	THR	THR	GLU	GLY	ASN
ASP	ALA	THR	ILE	ALA	SER	
ILE	MET	LEU	HIS	THR	ALA	
GLY	LEU	THR	ARG	TRP	ILE	
ILE	THR	GLN	GLU	THR	ILE	
THR	ARG	GLU	VAL	ARG	ASN	
HIS	THR	LYS	PHE	VAL	ASN	
GLU	ASN	LYS	ILE	ASP	TYR	
ILE	CYS	ASN	ILE	SER	MET	
VAL	VAL	ILE	HIS	ASP	THR	
ARG	ALA	GLU	LYS	ASP	ALA	
PRO	TYR	VAL	LEU	ASN	VAL	
SER	ILE	GLN	MET	LEU	ALA	
THR	SER	SER	THR	VAL	ASP	
PRO	PHE	ARG	TYR	ASN	ASP	
GLU	TYR	PRO	ALA	ILE	GLU	
LEU	GLU	PHE	LEU	ILE	THR	
ILE	ALA	SER	ILE	ALA	PRO	
ASN	GLY	PHE	GLU	ARG	ILE	
ALA	ILE	ASP	GLU	ILE	ILE	
CYS	ILE	ALA	GLN	ASP	PRO	
TYR	THR	ALA	ASN	LEU	SER	
ASN	ARG	ASN	SER	PRO	THR	
GLY	LEU	MET	THR	ARG	HIS	
SER	HIS	SER	GLN	ARG	THR	
THR	LYS	ILE	VAL	THR	SER	
GLY	THR	TYR	VAL	ARG	ASN	
GLY	ILE	LEU	SER	SER	THR	
ALA	ARG	PHE	ILE	ASN	TYR	
VAL	VAL	ILE	GLY	THR	PRO	
LEU	GLU	VAL	ARG	ALA	GLY	
ASP	GLU	ILE	ASN	TYR	LEU	
PHE	ARG	MET	LEU	HIS	PHE	
ASN	LEU	ASN	ALA	GLY	CYS	
HIS	LYS	GLU	ASP	TYR	GLY	
TYR	VAL	PRO	ILE	GLN	CYS	
SER	ALA	ASN	SER	ARG	ILE	
PRO	ASN	GLY	VAL	TYR	ASP	
VAL	TYR	ALA	PRO	VAL	VAL	
ILE	VAL	ALA	PRO	GLN	SER	
LYS	PRO	THR	LEU	ASN	ALA	
LEU	VAL	PRO	ASN	GLY	ALA	
ARG	ASP	THR	MET	LEU	PRO	
VAL	THR	ARG	TYR	CYS	PHE	

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	12814	Depositor
Resolution determination method	Not provided	
CTF correction method	CTF CORRECTION OF EACH PARTICLE	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	20	Depositor
Minimum defocus (nm)	150.00	Depositor
Maximum defocus (nm)	1300.00	Depositor
Magnification	154380	Depositor
Image detector	GENERIC TVIPS	Depositor
Maximum map value	8.028	Depositor
Minimum map value	0.000	Depositor
Average map value	0.090	Depositor
Map value standard deviation	0.387	Depositor
Recommended contour level	0.644	Depositor
Map size (Å)	747.87, 747.87, 747.87	wwPDB
Map dimensions	771, 771, 771	wwPDB
Map angles (°)	90, 90, 90	wwPDB
Pixel spacing (Å)	0.97, 0.97, 0.97	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	920	0	0	2	0
1	B	924	0	0	5	0
2	T	355	0	0	0	0
All	All	2199	0	0	7	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

The worst 5 of 7 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:568:PHE:CA	1:A:713:MET:CA	2.64	0.76
1:B:511:VAL:CA	1:B:512:LEU:CA	2.72	0.67
1:B:897:TYR:CA	1:B:898:GLN:CA	2.84	0.55
1:B:604:MET:CA	1:B:605:ARG:CA	2.89	0.51
1:B:1266:ASP:CA	1:B:1267:THR:CA	2.89	0.51



There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

### 5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

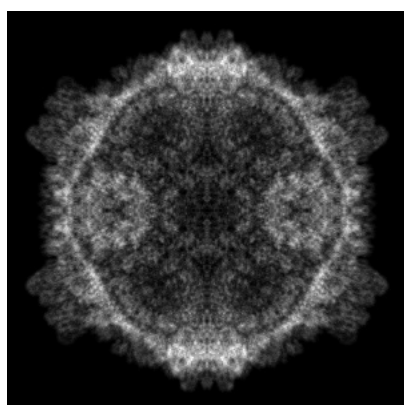
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-1508. These allow visual inspection of the internal detail of the map and identification of artifacts.

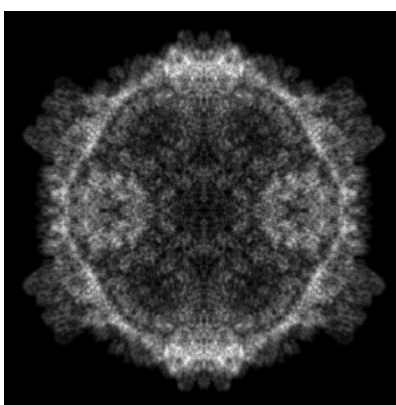
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

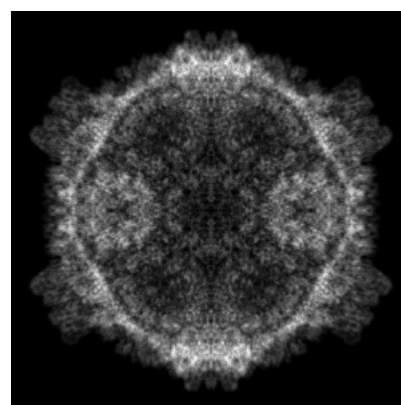
#### 6.1.1 Primary map



X



Y



Z

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

### 6.2 Central slices [i](#)

#### 6.2.1 Primary map



X Index: 385



Y Index: 385



Z Index: 385

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

## 6.3 Largest variance slices [i](#)

### 6.3.1 Primary map



X Index: 353



Y Index: 353

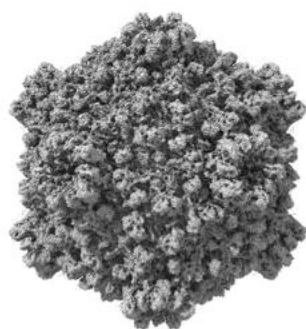


Z Index: 417

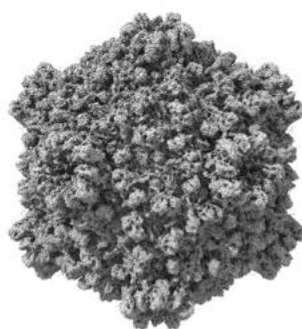
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views [i](#)

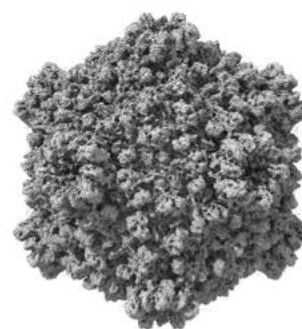
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.644. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

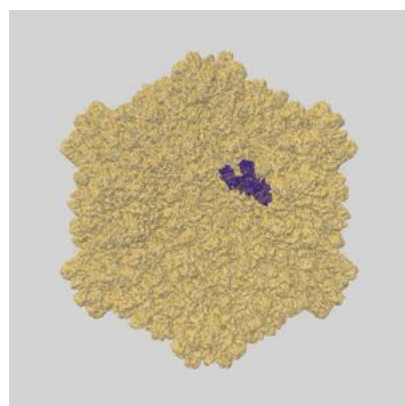
## 6.5 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

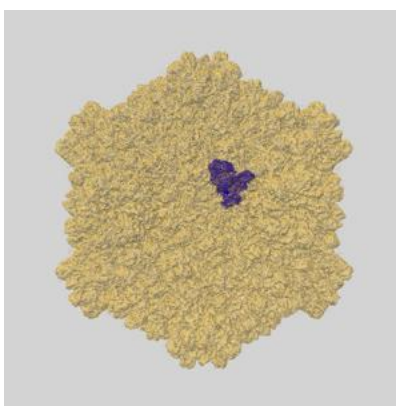
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

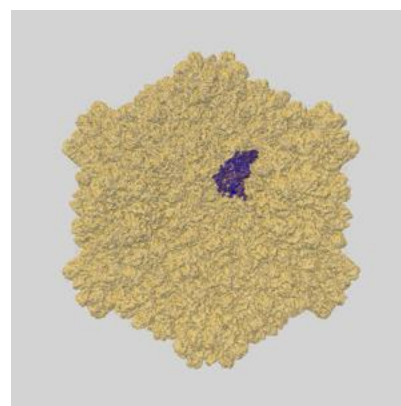
### 6.5.1 emd\_1508\_msk.map [i](#)



X



Y

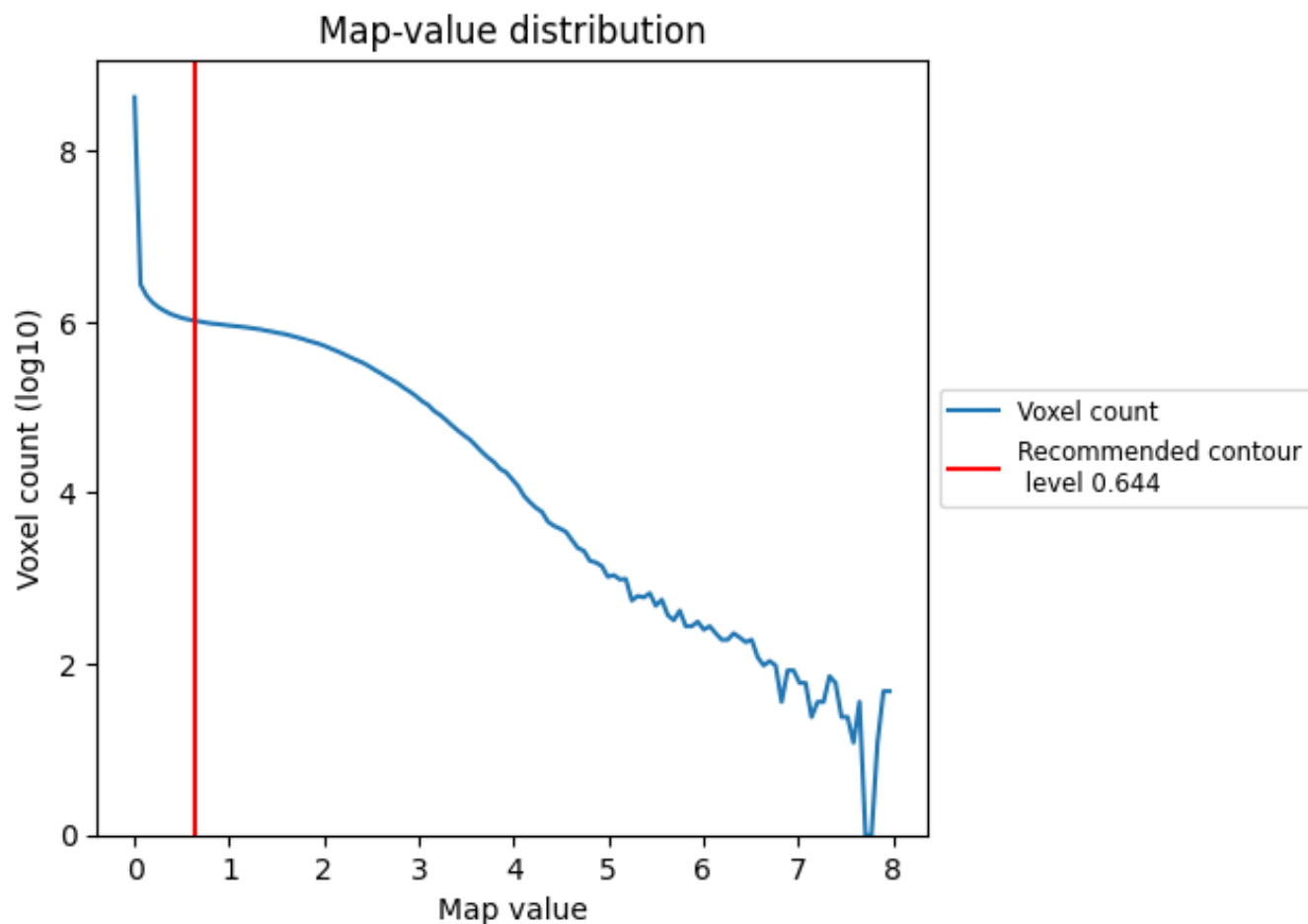


Z

## 7 Map analysis [i](#)

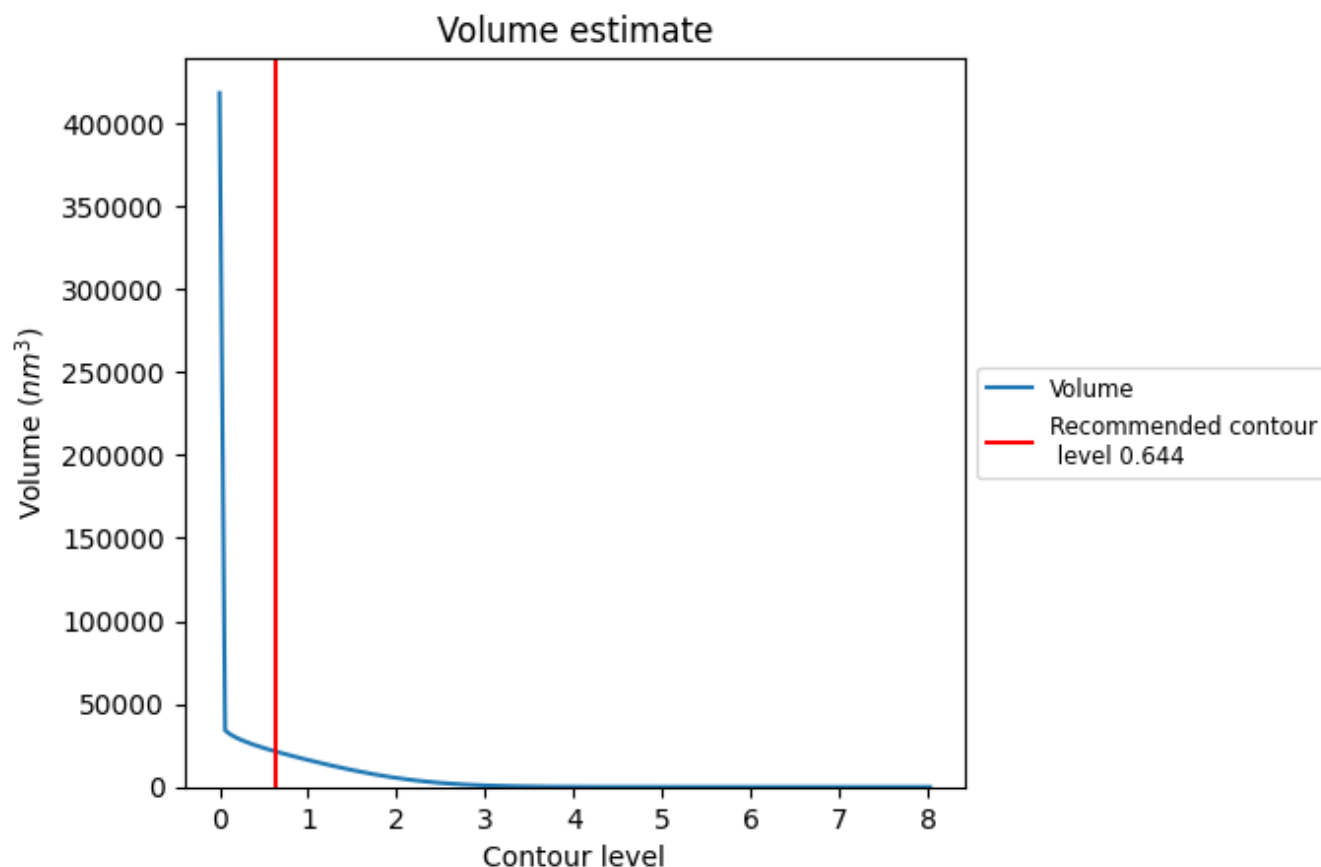
This section contains the results of statistical analysis of the map.

### 7.1 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.

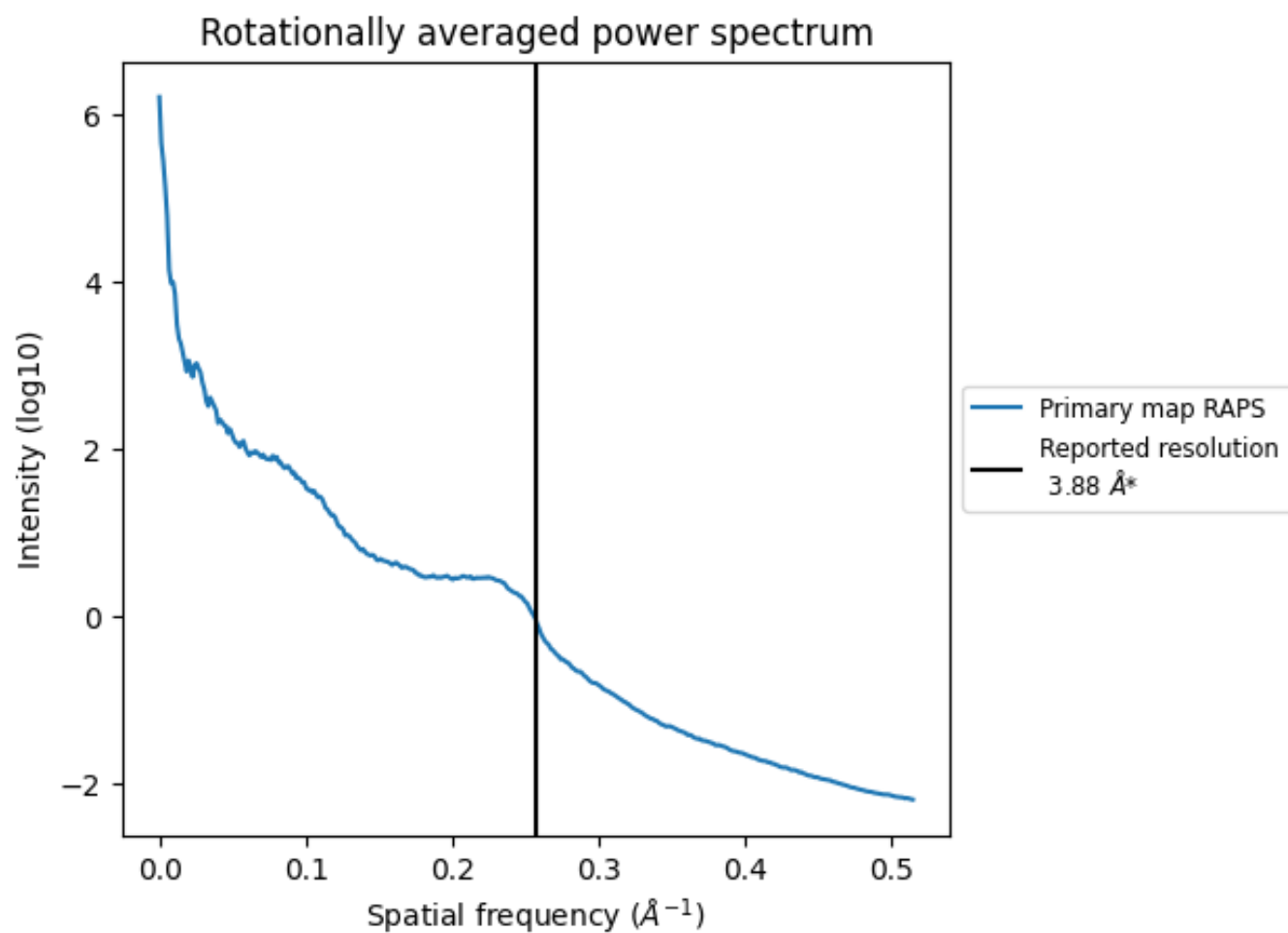
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 21237  $\text{nm}^3$ ; this corresponds to an approximate mass of 19184 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.

### 7.3 Rotationally averaged power spectrum ⓘ



\*Reported resolution corresponds to spatial frequency of 0.258 Å<sup>-1</sup>

## 8 Fourier-Shell correlation ⓘ

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

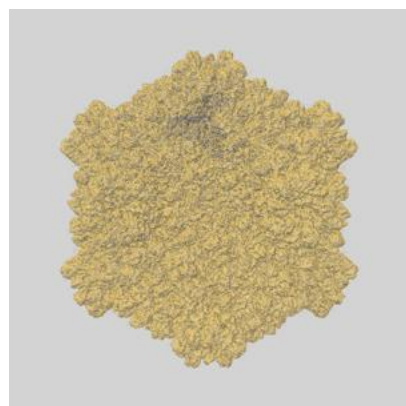


## 9 Map-model fit [i](#)

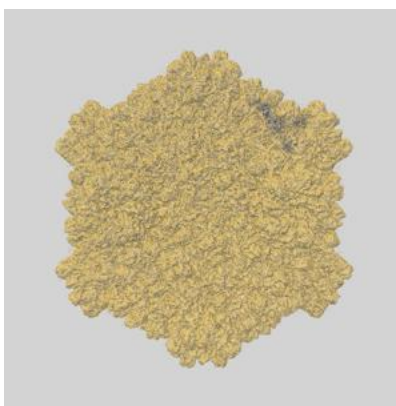
This section contains information regarding the fit between EMDB map EMD-1508 and PDB model 3CNF. Per-residue inclusion information can be found in section 3 on page 4.

### 9.1 Map-model overlays

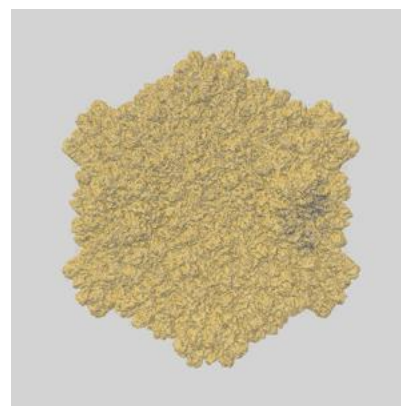
#### 9.1.1 Map-model overlay [i](#)



X

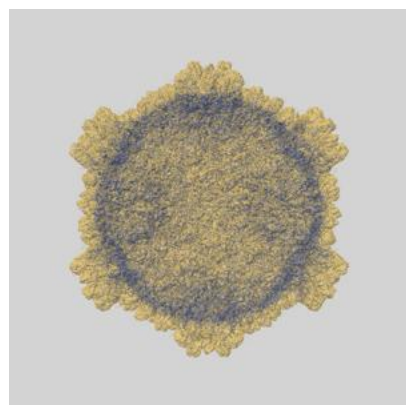


Y

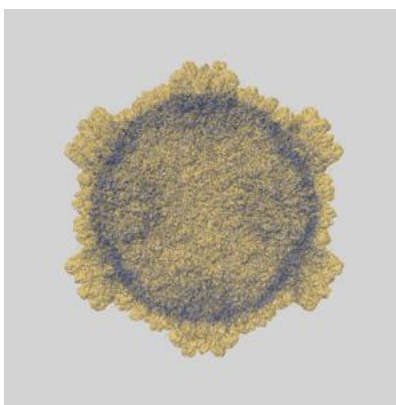


Z

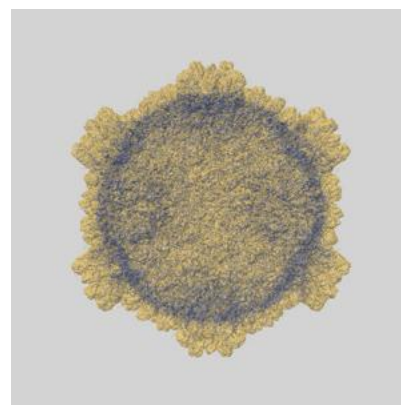
#### 9.1.2 Map-model assembly overlay [i](#)



X



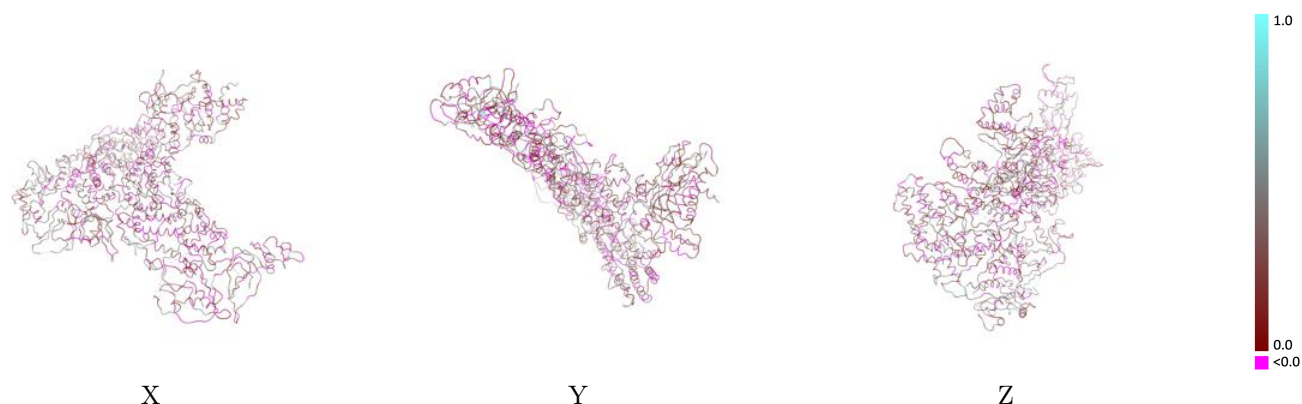
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.644 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



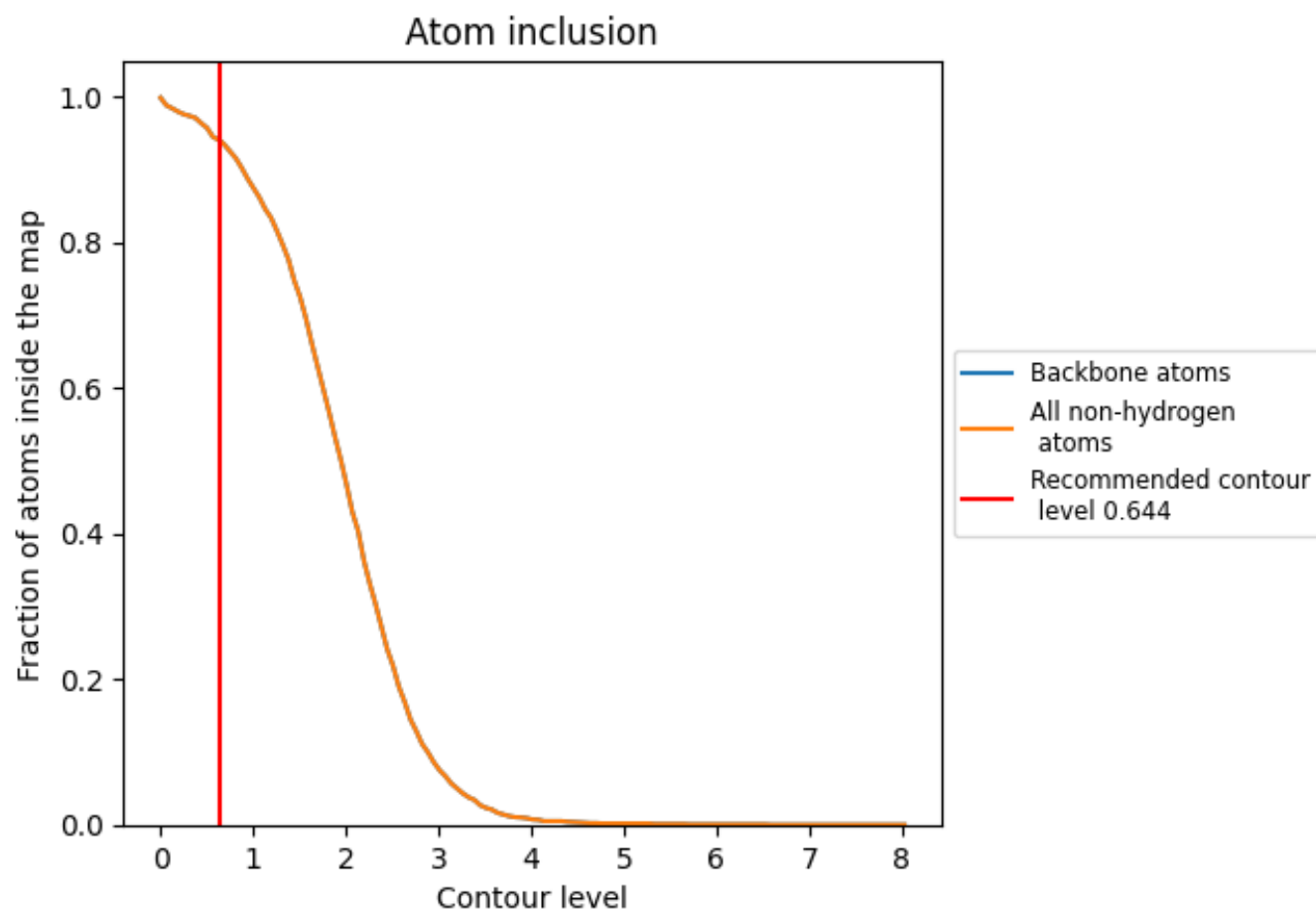
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.644).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 94% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.644) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9391	<div></div> 0.2280
A	<div></div> 0.9370	<div></div> 0.2460
B	<div></div> 0.9232	<div></div> 0.2080
T	<div></div> 0.9859	<div></div> 0.2340

