wwPDB EM Validation Summary Report (i)

Dec 12, 2022 – 05:57 PM EST

PDB ID	:	3JB8
EMDB ID	:	EMD-6382
Title	:	Insight into Three-dimensional structure of Maize Chlorotic Mottle Virus Revealed by Single Particle Analysis
Authors	:	Wang, C.Y.; Zhang, Q.F.; Gao, Y.Z.; Zhou, X.P.; Ji, G.; Huang, X.J.; Hong, J.; Zhang, C.X.
Deposited on	:	2015-08-04
Resolution	:	3.60 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/EMValidationReportHelp
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 (i)) were used in the production of this report:

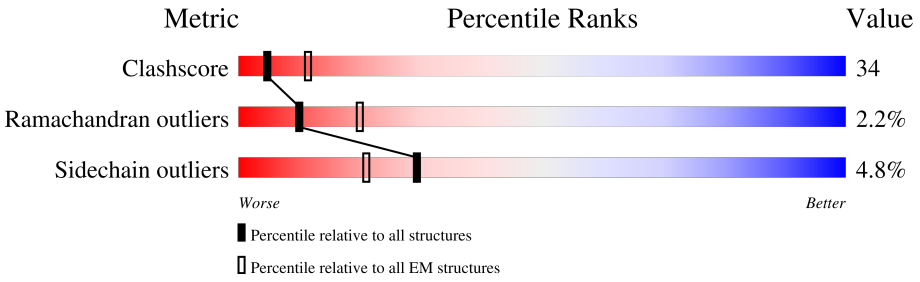
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 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
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 >=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 <=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	185	100% 64% 30% 6%
1	B	185	98% 61% 32% 6% •
1	C	185	99% 62% 31% 6% •

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 4098 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 Coat protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	185	1378	881	231	257	9	0	0
1	B	182	1356	865	228	254	9	0	0
1	C	183	1364	871	229	255	9	0	0

3 Residue-property plots (i)

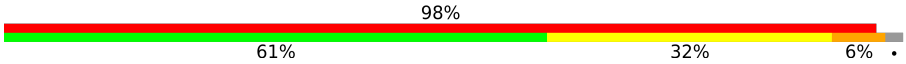
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Coat protein

Chain A:

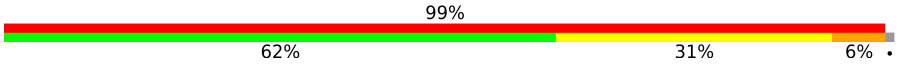
- Molecule 1: Coat protein

Chain B:



- Molecule 1: Coat protein

Chain C:


99%
62%
31%
6%

G45 T46 T47 C48 S49 M50 S51 E52 I53 L54 L55 A56 V57 S58 A59 T60 T61 A62 D63 Q64 I65 L66 E67 I68 P69 V70 C71 A72 G73 I74 D75 F76 P77 A78 G79 T80 P81 P82 R83 Y84 I85 G86 A87 A88 K89 W90 L91 A92 A93 Q94 S95 Q96 M97 W98 N99 T100 I101 V102 F103 N104
S105 V106 R107 I108 T109 W110 E111 T112 F113 T114 A115 D116 T117 T118 S119 G120 Y121 I122 S123 M124 A125 F126 L127 S128 D129 Y130 M131 L132 S133 L134 P135 T136 G137 V138 E139 D140 V141 A142 R143 I144 V145 P146 S147 A148 T149 I150 A151 L152 K153 N154 R155 G156 P157 S158 I159 V160 M161 P162 Q163 N164
R165 T166 A167 F168 R169 C170 I171 Q172 A173 G174 Q175 F176 A177 A178 L179 G180 S181 A182 A183 D184 K185 Q186 M187 Y188 S189 P190 G191 R192 F193 I194 V195 A196 I197 P198 K199 A200 S201 A202 T203 Q204 A205 V206 G207 Q208 I209 K210 I211 S212 Y213 S214 V215 S216 Y217 R218 G219 A220 A221 I222 L223 Q224
P225 A226 L227 VAL PRO

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	53600	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 ($e^-/Å^2$)	Not provided	
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN ULTRASCAN 4000 (4k x 4k)	Depositor
Maximum map value	12.205	Depositor
Minimum map value	-6.675	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	2.0	Depositor
Map size (Å)	358.8, 358.8, 358.8	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.196, 1.196, 1.196	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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.51	0/1408	0.59	1/1922 (0.1%)
1	B	0.51	0/1385	0.60	1/1889 (0.1%)
1	C	0.51	0/1393	0.60	1/1900 (0.1%)
All	All	0.51	0/4186	0.60	3/5711 (0.1%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	145	VAL	C-N-CD	-5.95	107.51	120.60
1	A	145	VAL	C-N-CD	-5.94	107.54	120.60
1	C	145	VAL	C-N-CD	-5.94	107.54	120.60

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	1378	0	1397	103	0
1	B	1356	0	1370	106	0
1	C	1364	0	1381	109	0
All	All	4098	0	4148	279	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 34.

The worst 5 of 279 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:145:VAL:HG13	1:A:146:PRO:CD	1.08	1.54
1:B:145:VAL:HG13	1:B:146:PRO:CD	1.08	1.53
1:C:145:VAL:HG13	1:C:146:PRO:CD	1.08	1.50
1:B:145:VAL:CG1	1:B:146:PRO:CD	1.93	1.45
1:C:145:VAL:CG1	1:C:146:PRO:CD	1.93	1.44

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	183/185 (99%)	161 (88%)	18 (10%)	4 (2%)	6 39
1	B	180/185 (97%)	158 (88%)	18 (10%)	4 (2%)	6 39
1	C	181/185 (98%)	159 (88%)	18 (10%)	4 (2%)	6 39
All	All	544/555 (98%)	478 (88%)	54 (10%)	12 (2%)	10 39

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	155	ARG
1	B	155	ARG
1	C	155	ARG
1	A	74	ILE
1	A	146	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM

entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	146/146 (100%)	139 (95%)	7 (5%)	25	60
1	B	143/146 (98%)	136 (95%)	7 (5%)	25	59
1	C	144/146 (99%)	137 (95%)	7 (5%)	25	59
All	All	433/438 (99%)	412 (95%)	21 (5%)	29	60

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	50	MET
1	C	143	ARG
1	C	153	LYS
1	C	144	ILE
1	C	103	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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.

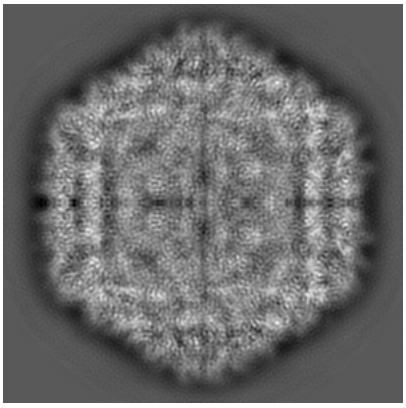
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-6382. These allow visual inspection of the internal detail of the map and identification of artifacts.

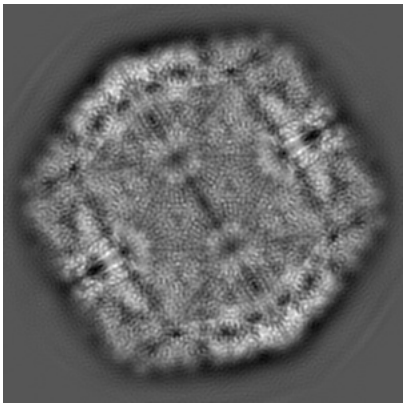
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

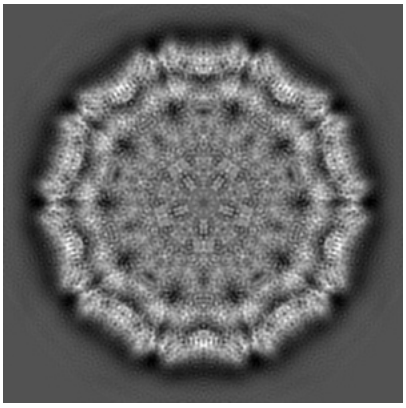
6.1.1 Primary map



X



Y

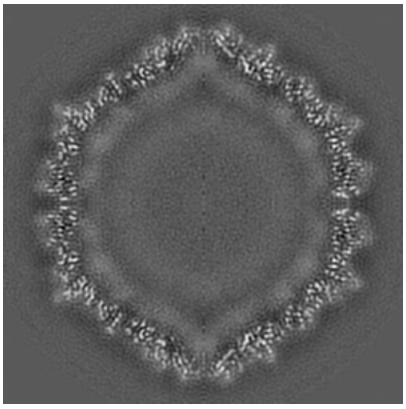


Z

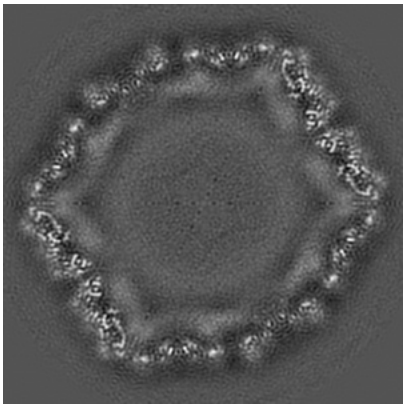
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

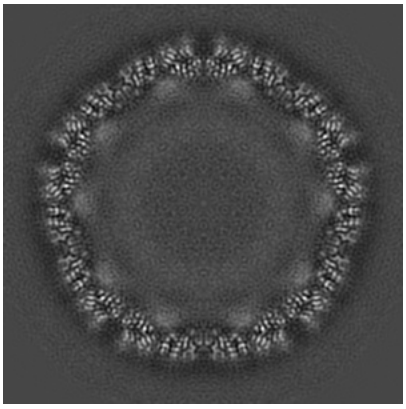
6.2.1 Primary map



X Index: 150



Y Index: 150

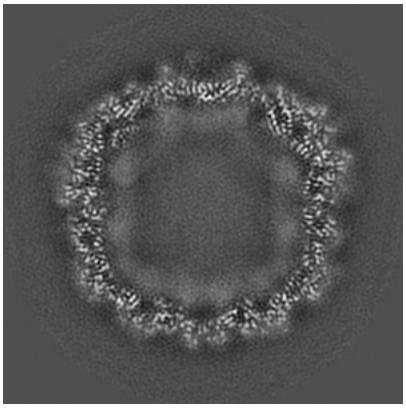


Z Index: 150

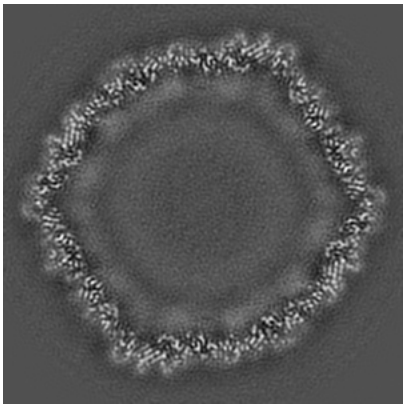
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

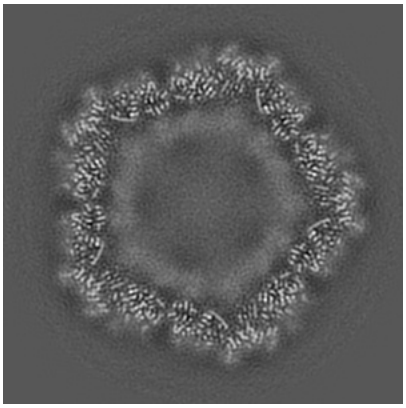
6.3.1 Primary map



X Index: 210



Y Index: 164

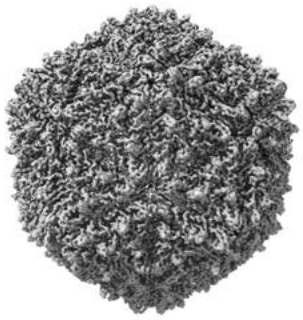


Z Index: 214

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

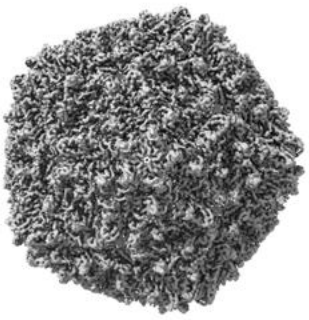
6.4 Orthogonal surface views (i)

6.4.1 Primary map



X

Y



Z

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

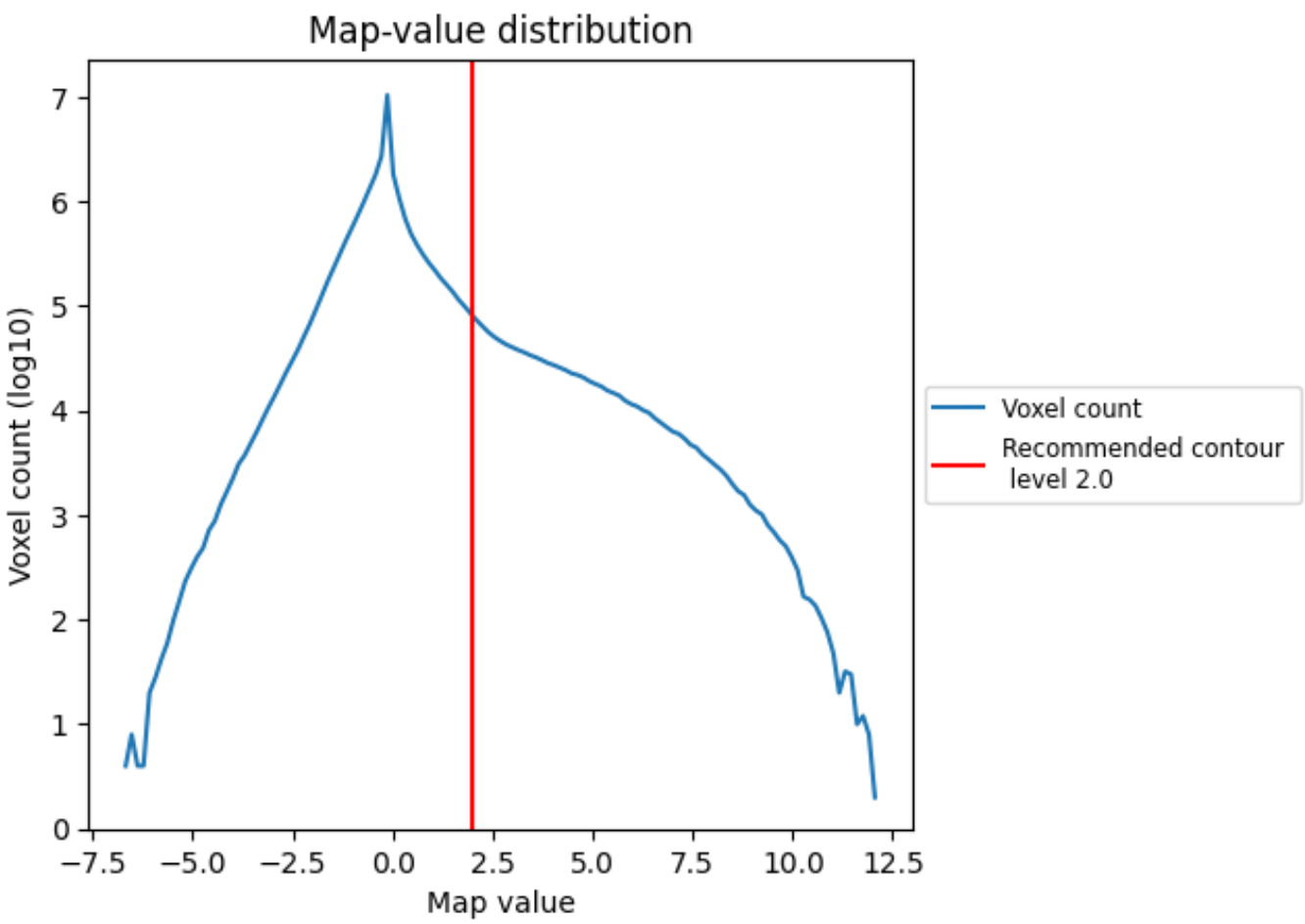
6.5 Mask visualisation (i)

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

7 Map analysis (i)

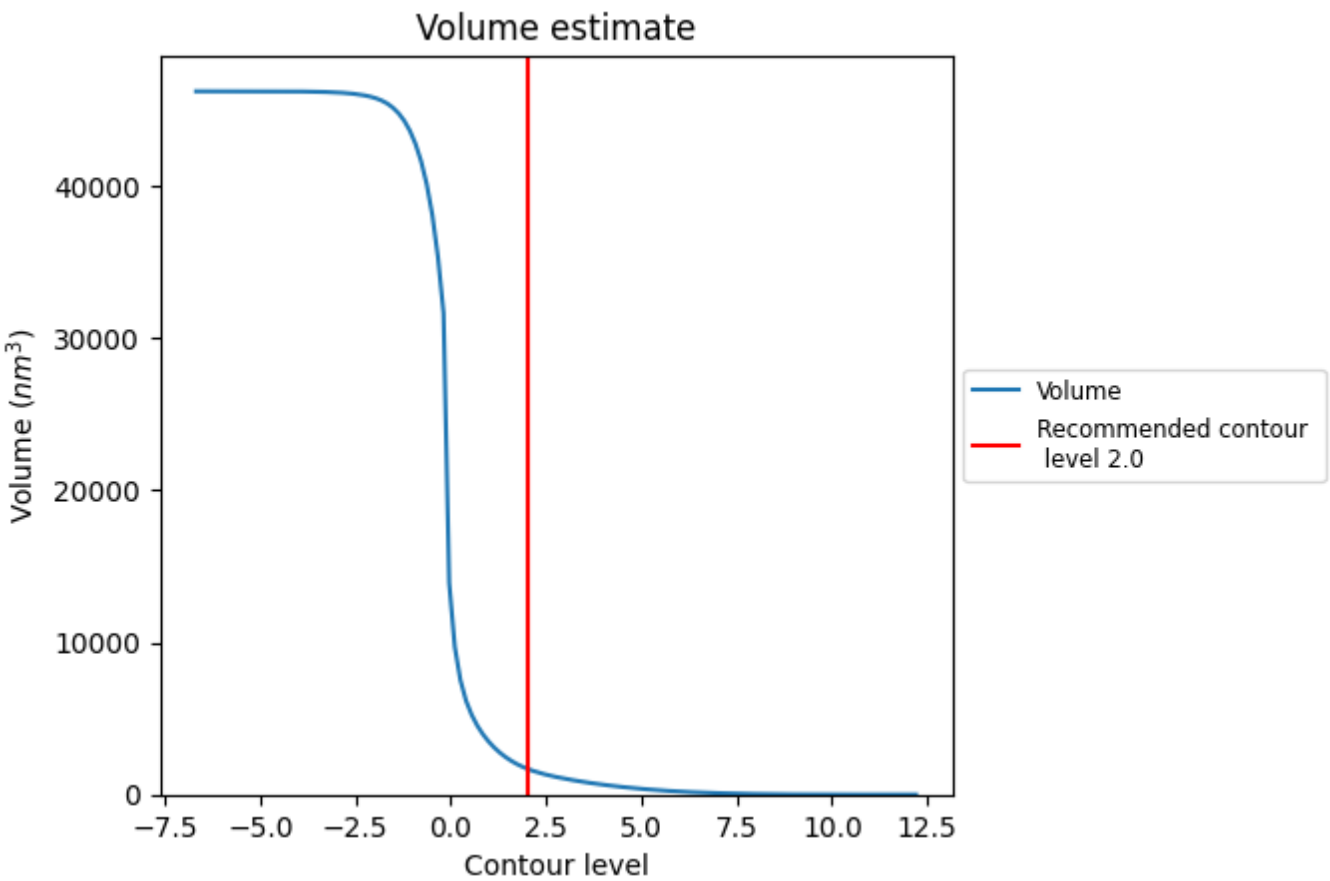
This section contains the results of statistical analysis of the map.

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.

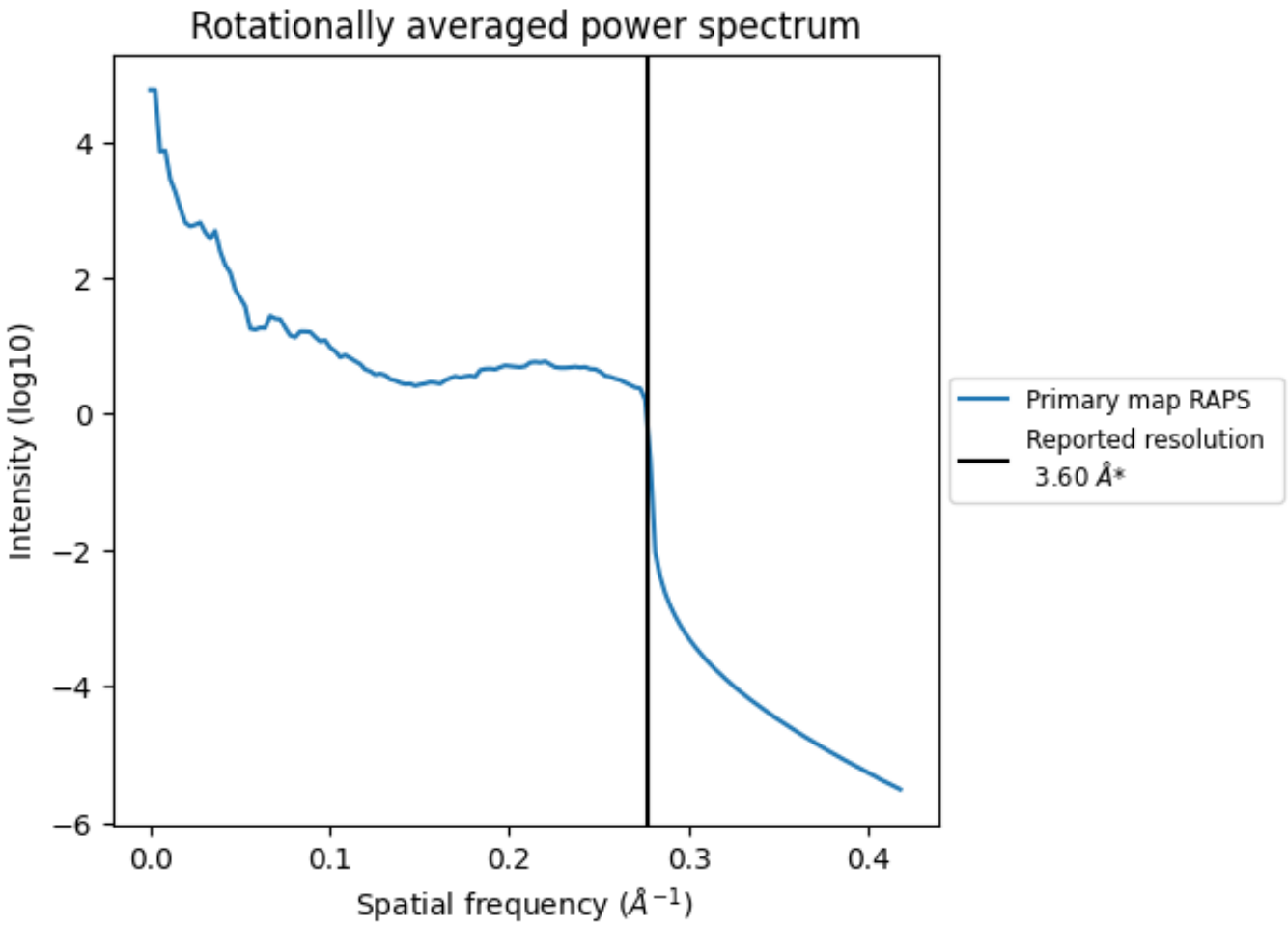
7.2 Volume estimate (i)



The volume at the recommended contour level is 1707 nm^3; this corresponds to an approximate mass of 1542 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 (i)



*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

8 Fourier-Shell correlation (i)

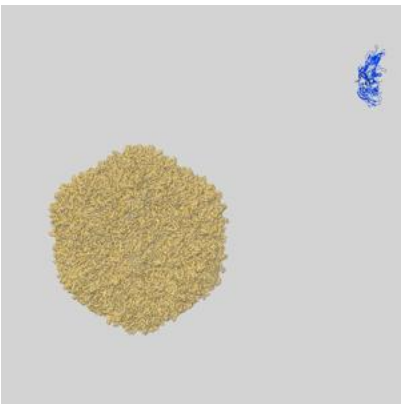
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit (i)

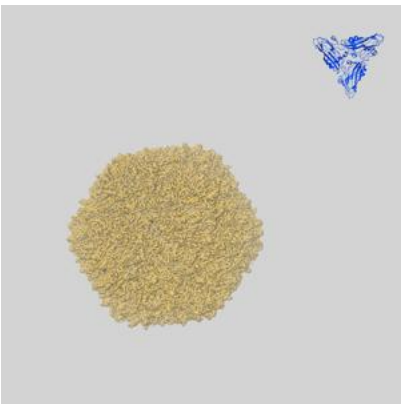
This section contains information regarding the fit between EMDB map EMD-6382 and PDB model 3JB8. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlays

9.1.1 Map-model overlay (i)



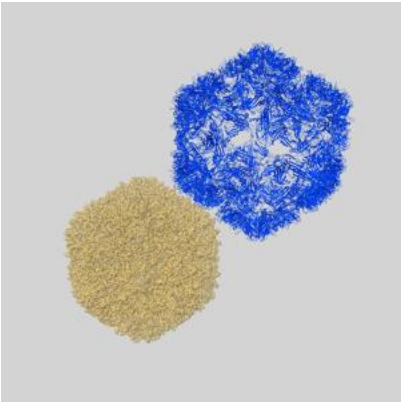
X



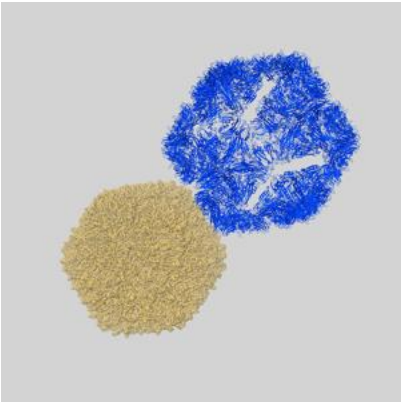
Y

Z

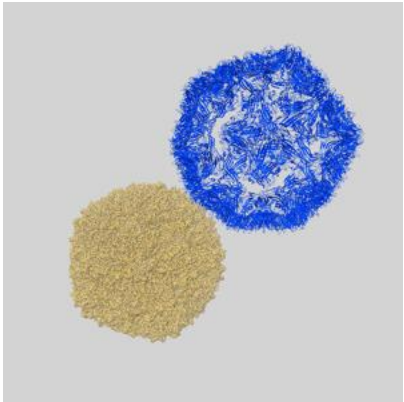
9.1.2 Map-model assembly overlay (i)



X



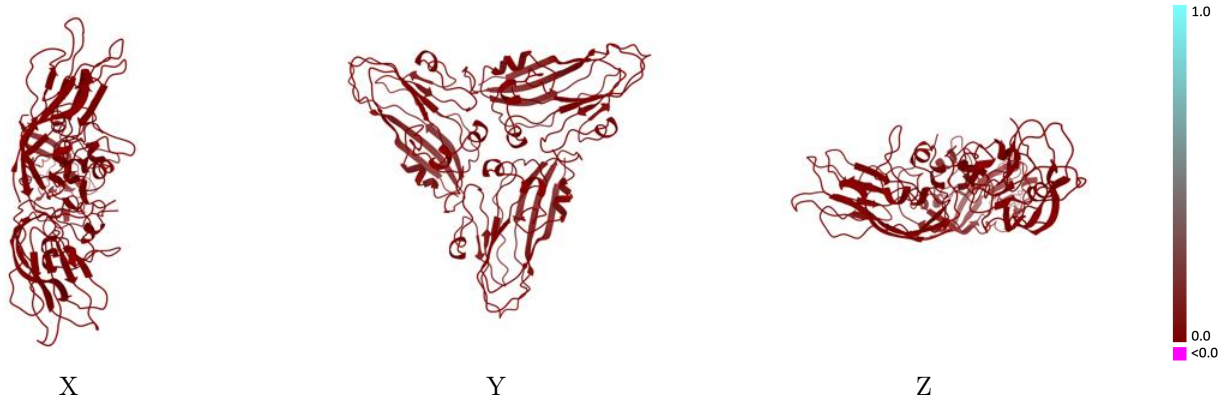
Y



Z

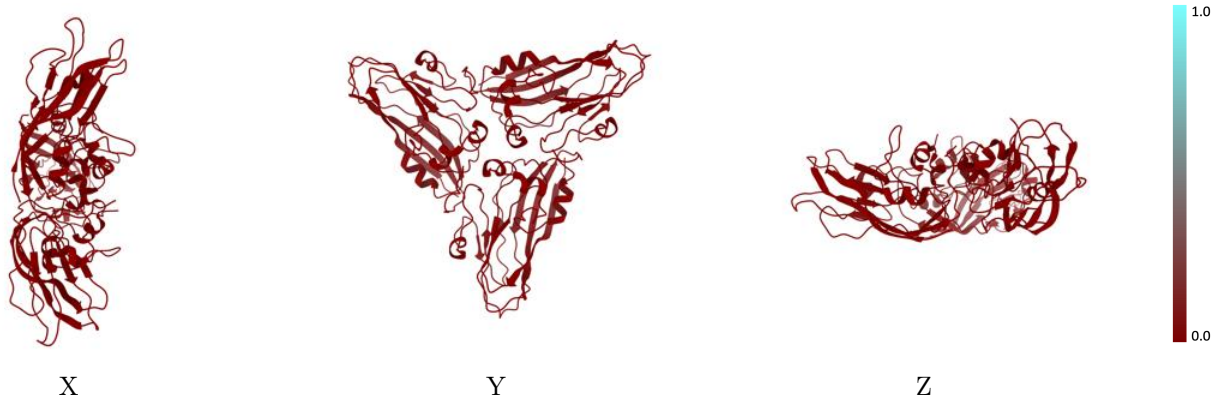
The images above show the 3D surface view of the map at the recommended contour level 2.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



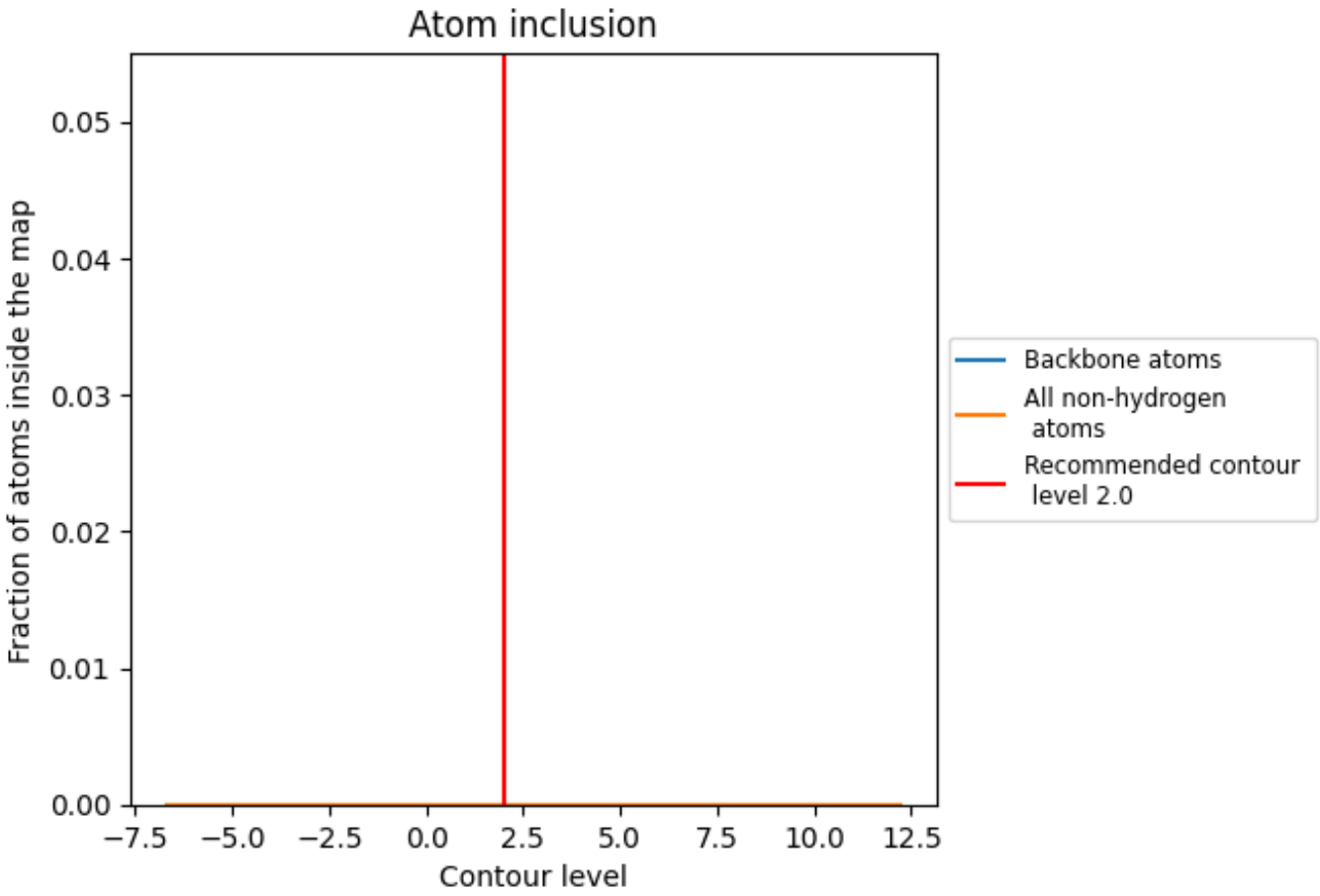
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (2.0).

9.4 Atom inclusion (i)



At the recommended contour level, 0% of all backbone atoms, 0% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (2.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.0000	0.0000
A	0.0000	0.0000
B	0.0000	0.0000
C	0.0000	0.0000