



Full wwPDB EM Validation Report ⓘ

Nov 2, 2024 – 10:41 pm GMT

PDB ID : 7B3Y
EMDB ID : EMD-11997
Title : Structure of a nanoparticle for a COVID-19 vaccine candidate
Authors : Duyvesteyn, H.M.E.; Stuart, D.I.
Deposited on : 2020-12-01
Resolution : 3.70 Å(reported)
Based on initial model : 5KP9

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/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>.

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

EMDB validation analysis : 0.0.1.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

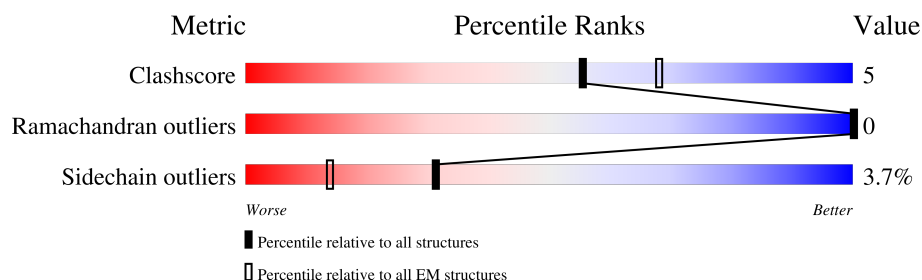
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 $\leq 5\%$. 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	B	341	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1516 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 Fibronectin binding protein,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	202	Total	C	N	O	S	0	0
			1516	987	249	273	7		

There are 45 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-130	MET	-	initiating methionine	UNP A0A0H3BX48
B	-129	GLY	-	expression tag	UNP A0A0H3BX48
B	-128	SER	-	expression tag	UNP A0A0H3BX48
B	-125	THR	ASP	conflict	UNP A0A0H3BX48
B	-118	GLY	SER	conflict	UNP A0A0H3BX48
B	-114	PRO	GLN	conflict	UNP A0A0H3BX48
B	-108	THR	ILE	conflict	UNP A0A0H3BX48
B	-93	GLU	ILE	conflict	UNP A0A0H3BX48
B	-90	ARG	LYS	conflict	UNP A0A0H3BX48
B	-65	HIS	GLN	conflict	UNP A0A0H3BX48
B	-58	TYR	MET	conflict	UNP A0A0H3BX48
B	-41	VAL	ILE	conflict	UNP A0A0H3BX48
B	-38	PRO	ALA	conflict	UNP A0A0H3BX48
B	-36	GLU	THR	conflict	UNP A0A0H3BX48
B	-30	ASP	GLN	conflict	UNP A0A0H3BX48
B	-24	ASP	ASN	conflict	UNP A0A0H3BX48
B	-22	GLU	LYS	conflict	UNP A0A0H3BX48
B	-19	GLU	LYS	conflict	UNP A0A0H3BX48
B	-14	THR	-	linker	UNP A0A0H3BX48
B	-13	GLY	-	linker	UNP A0A0H3BX48
B	-12	GLY	-	linker	UNP A0A0H3BX48
B	-11	SER	-	linker	UNP A0A0H3BX48
B	-10	GLY	-	linker	UNP A0A0H3BX48
B	-9	GLY	-	linker	UNP A0A0H3BX48
B	-8	SER	-	linker	UNP A0A0H3BX48
B	-7	GLY	-	linker	UNP A0A0H3BX48
B	-6	GLY	-	linker	UNP A0A0H3BX48

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	SER	-	linker	UNP A0A0H3BX48
B	-4	GLY	-	linker	UNP A0A0H3BX48
B	-3	GLY	-	linker	UNP A0A0H3BX48
B	-2	SER	-	linker	UNP A0A0H3BX48
B	24	LYS	GLU	conflict	UNP Q9WXS1
B	31	LEU	GLU	conflict	UNP Q9WXS1
B	59	MET	LYS	conflict	UNP Q9WXS1
B	74	ALA	CYS	conflict	UNP Q9WXS1
B	98	ALA	CYS	conflict	UNP Q9WXS1
B	185	VAL	ASP	conflict	UNP Q9WXS1
B	188	ALA	ARG	conflict	UNP Q9WXS1
B	204	GLY	-	expression tag	UNP Q9WXS1
B	205	SER	-	expression tag	UNP Q9WXS1
B	206	GLY	-	expression tag	UNP Q9WXS1
B	207	GLU	-	expression tag	UNP Q9WXS1
B	208	PRO	-	expression tag	UNP Q9WXS1
B	209	GLU	-	expression tag	UNP Q9WXS1
B	210	ALA	-	expression tag	UNP Q9WXS1

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	150785	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	48.1	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	165000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.855	Depositor
Minimum map value	-0.276	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.039	Depositor
Recommended contour level	0.193	Depositor
Map size (\AA)	456.4, 456.4, 456.4	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.63, 1.63, 1.63	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	B	0.72	0/1545	0.68	0/2084

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	B	1516	0	1583	15	0
All	All	1516	0	1583	15	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 5.

All (15) 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:B:2:GLU:HG2	1:B:125:ILE:CD1	1.91	1.01
1:B:2:GLU:HG2	1:B:125:ILE:HD12	1.52	0.90
1:B:29:VAL:HG13	1:B:34:VAL:HB	1.62	0.82
1:B:2:GLU:HG2	1:B:125:ILE:HD11	1.63	0.79
1:B:150:LYS:HD3	1:B:171:LEU:HD13	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:LEU:HD23	1:B:149:VAL:HG13	1.84	0.59
1:B:5:PHE:HE2	1:B:104:PHE:CE2	2.27	0.53
1:B:5:PHE:CE2	1:B:104:PHE:CE2	3.00	0.49
1:B:88:PRO:HA	1:B:127:LYS:HE2	1.95	0.48
1:B:110:MET:HE3	1:B:133:VAL:HG12	1.97	0.46
1:B:110:MET:HE3	1:B:133:VAL:CG1	2.47	0.45
1:B:110:MET:O	1:B:110:MET:HG2	2.19	0.42
1:B:25:LYS:HD3	1:B:180:VAL:HG13	2.01	0.41
1:B:67:THR:HA	1:B:88:PRO:HD3	2.02	0.41
1:B:115:LEU:HD23	1:B:115:LEU:C	2.41	0.41

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	B	200/341 (59%)	196 (98%)	4 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	B	161/269 (60%)	155 (96%)	6 (4%)	29	54

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	6	LYS
1	B	14	LEU
1	B	29	VAL
1	B	47	ASP
1	B	109	VAL
1	B	134	VAL

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 oligosaccharides 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.

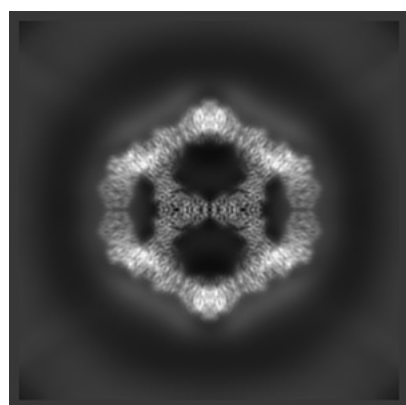
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11997. These allow visual inspection of the internal detail of the map and identification of artifacts.

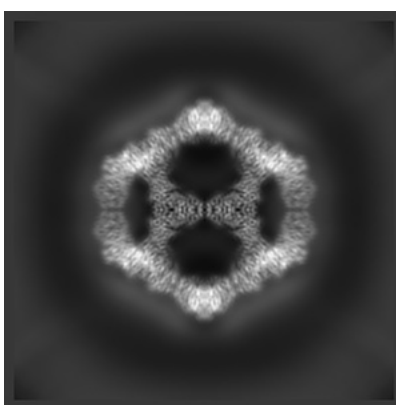
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

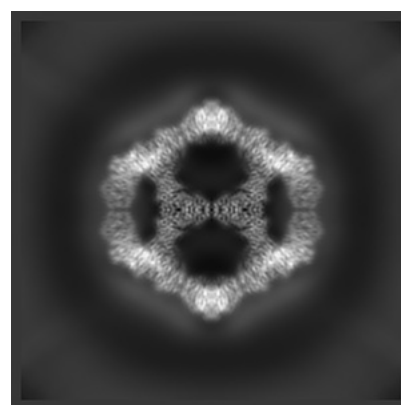
6.1.1 Primary map



X



Y

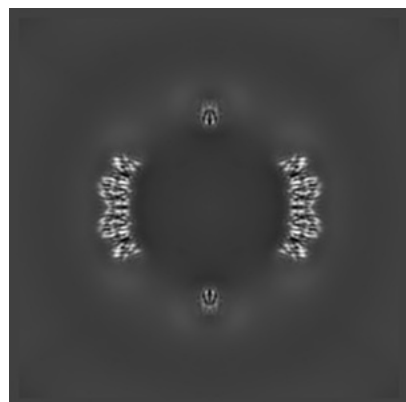


Z

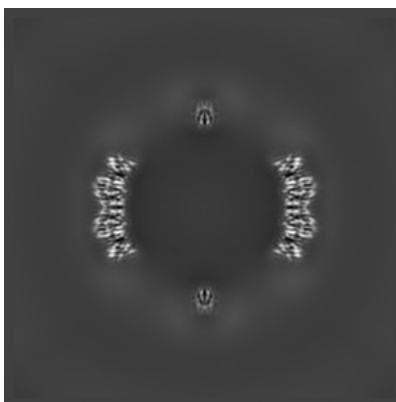
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

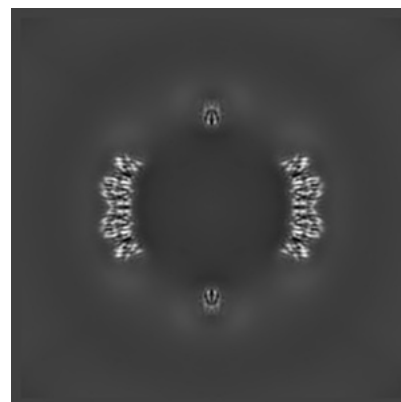
6.2.1 Primary map



X Index: 140



Y Index: 140

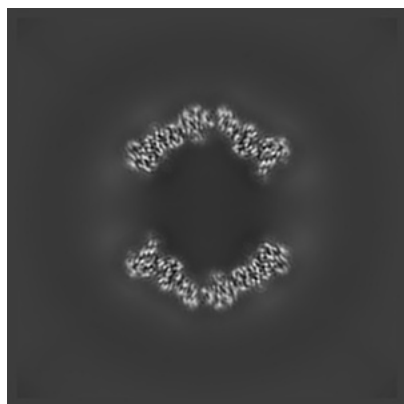


Z Index: 140

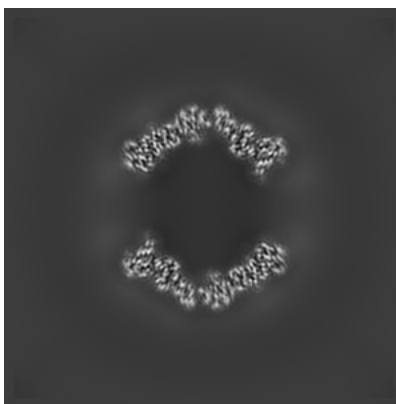
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

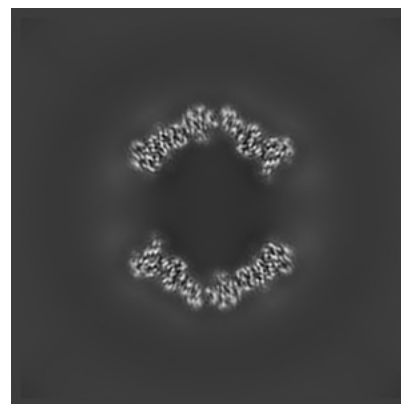
6.3.1 Primary map



X Index: 175



Y Index: 175

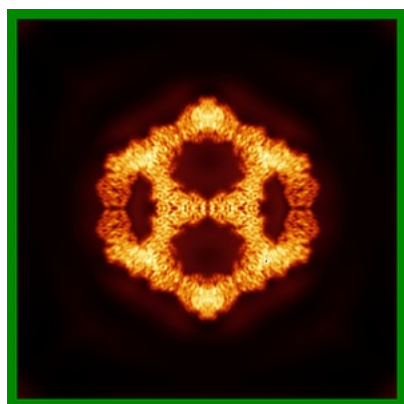


Z Index: 175

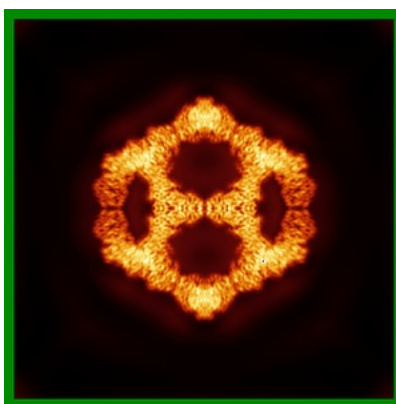
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

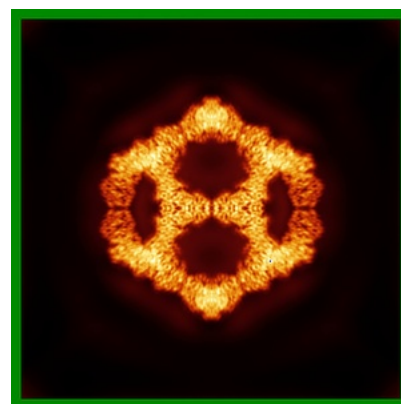
6.4.1 Primary map



X



Y

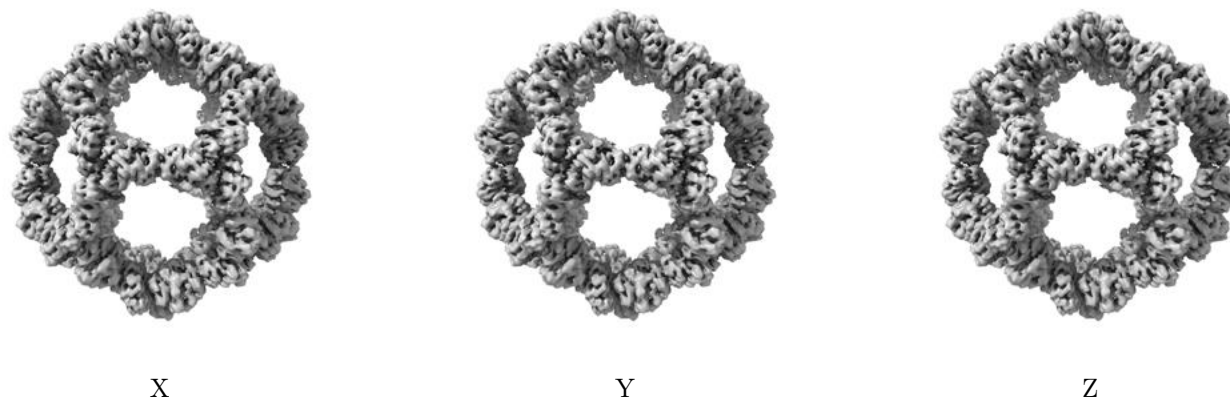


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.193. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

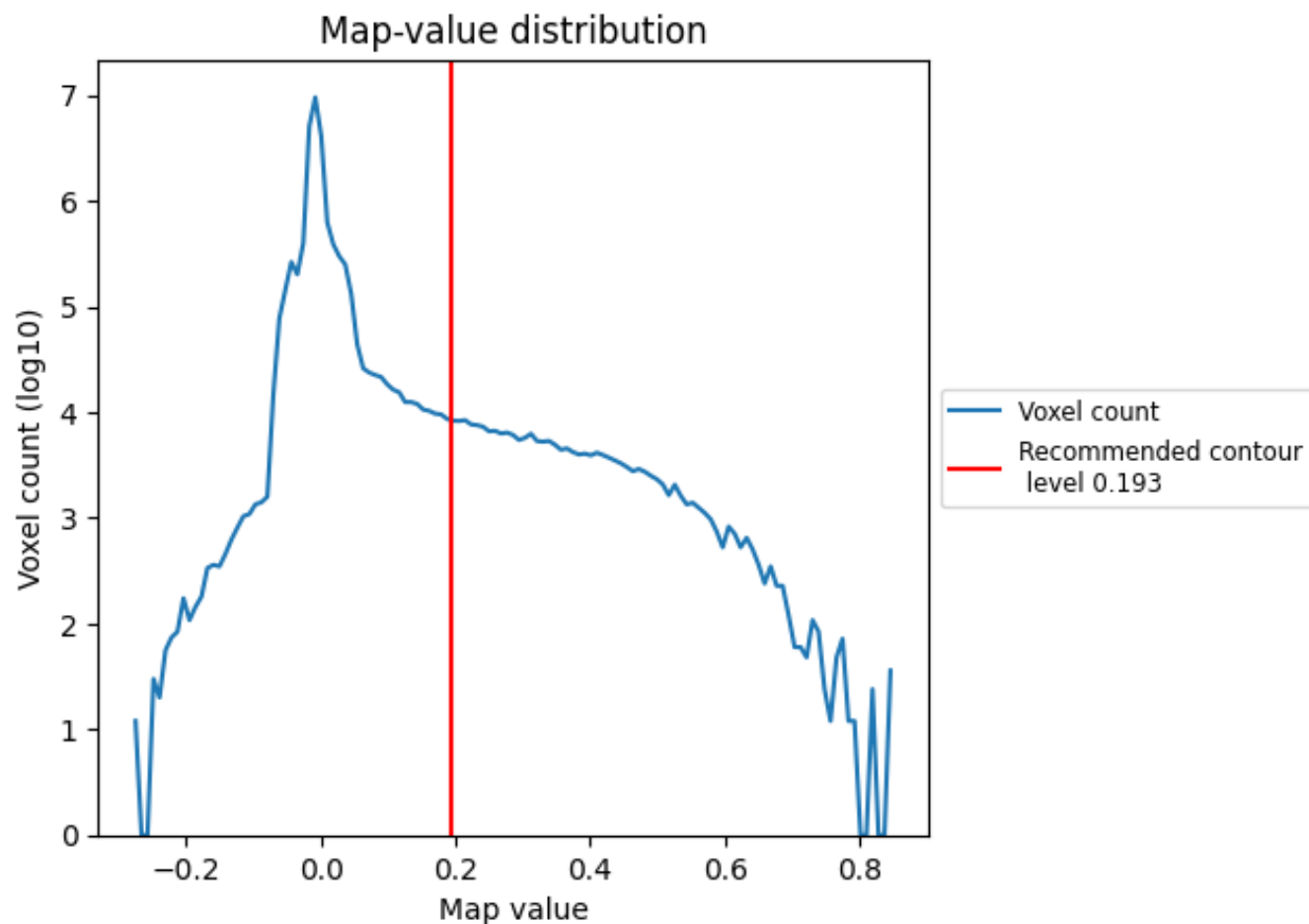
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

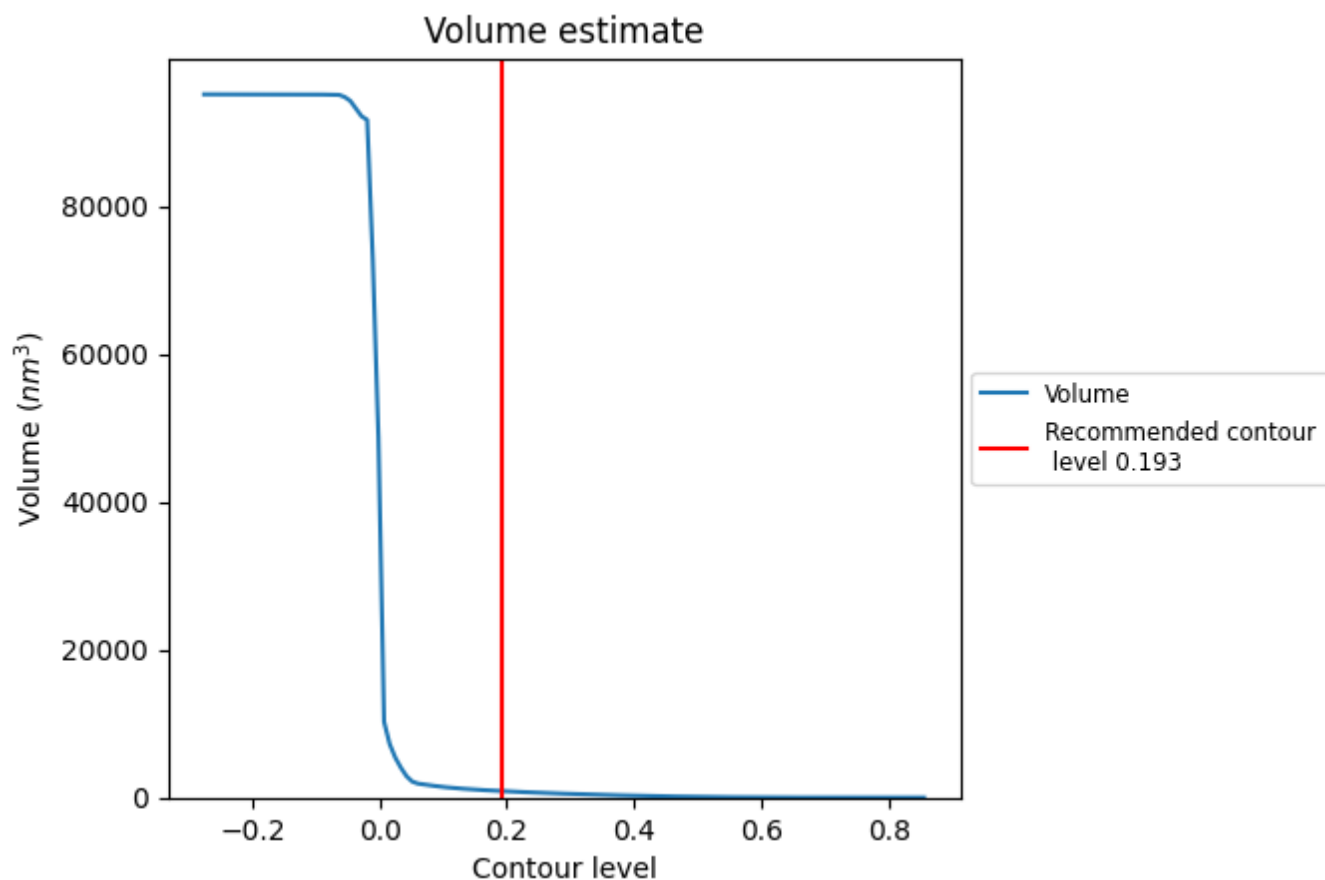
This section contains the results of statistical analysis of the map.

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.

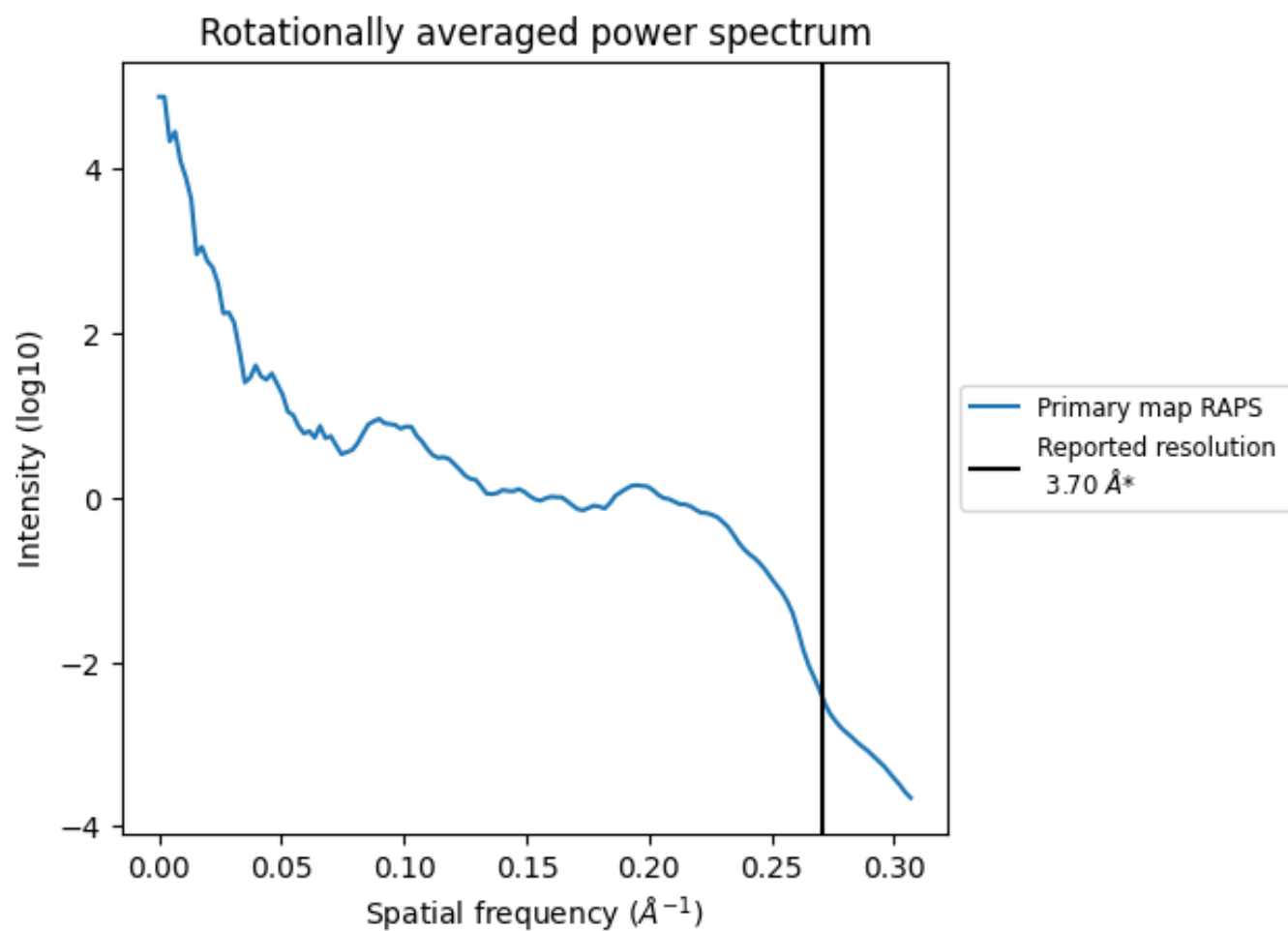
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 872 nm³; this corresponds to an approximate mass of 787 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 0.270 Å⁻¹

8 Fourier-Shell correlation ⓘ

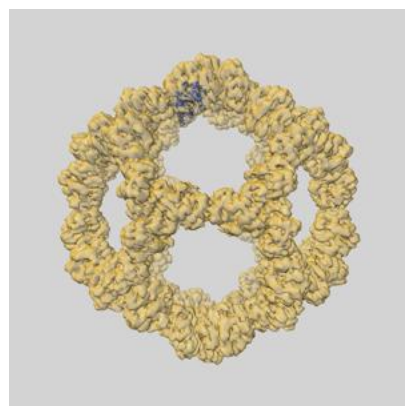
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

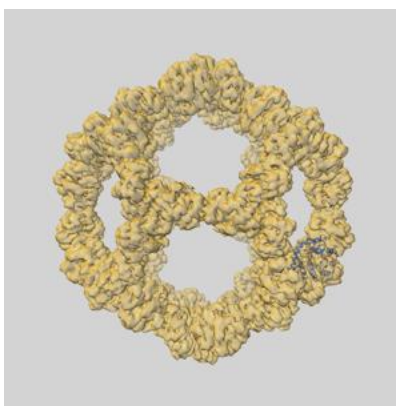
This section contains information regarding the fit between EMDB map EMD-11997 and PDB model 7B3Y. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlays

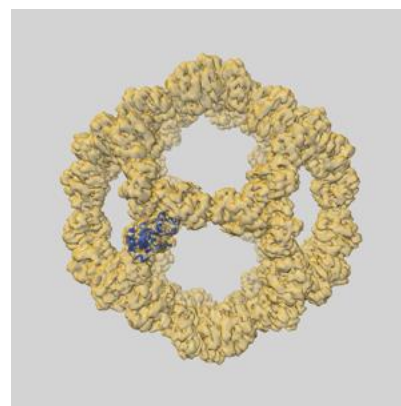
9.1.1 Map-model overlay [i](#)



X

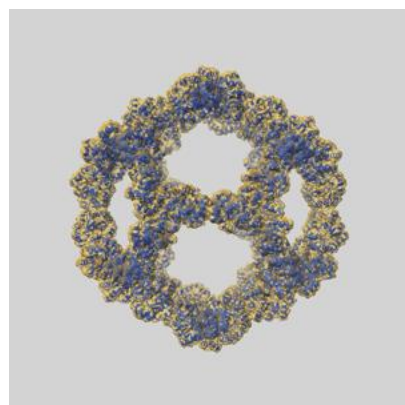


Y

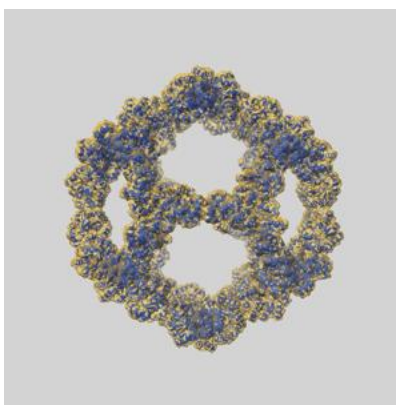


Z

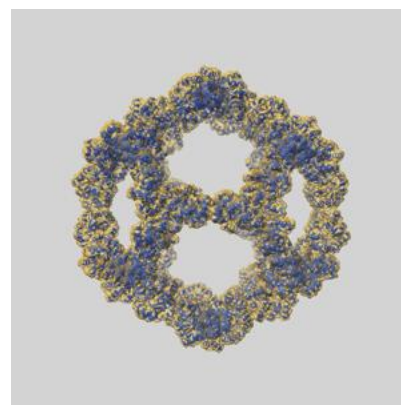
9.1.2 Map-model assembly overlay [i](#)



X



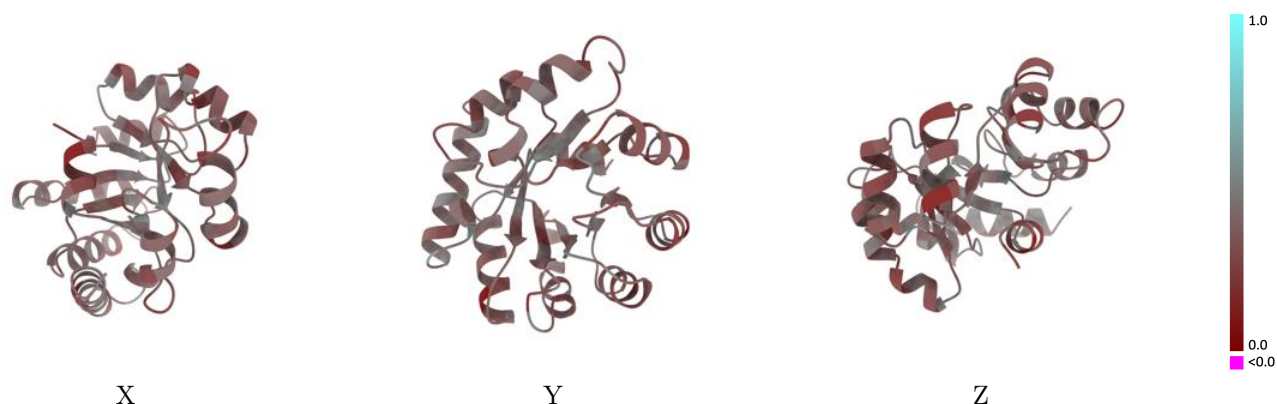
Y



Z

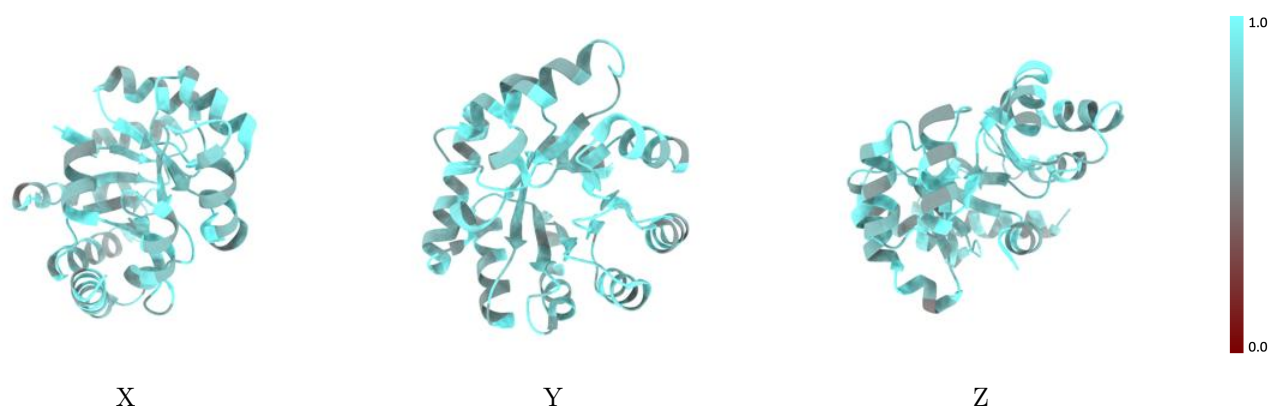
The images above show the 3D surface view of the map at the recommended contour level 0.193 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



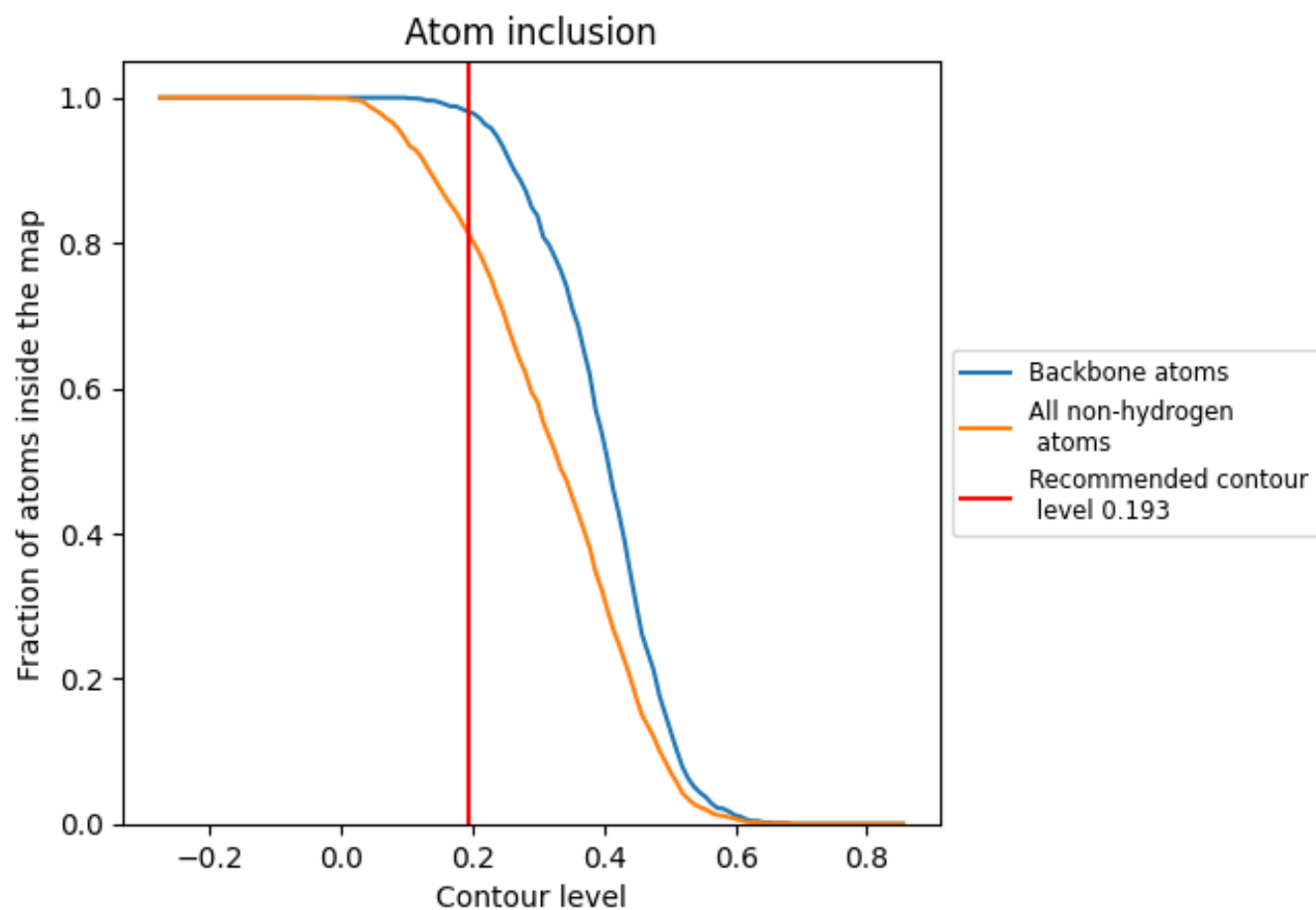
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.193).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 81% 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 (0.193) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.8130	<div><div></div></div> 0.3500
B	<div><div></div></div> 0.8130	<div><div></div></div> 0.3500

