wwPDB EM Validation Summary Report

Nov 9, 2026 – 01:02 PM JST

PDB ID	:	9XMC / pdb_00009xmc
EMDB ID	:	EMD-67020
Title	:	CryoEM structure of non-structural protein 1 dimer from zika virus complexed with protein binder ZNB6
Authors	:	Jiao, H.Z.; Pan, Q.; Hu, H.L.
Deposited on	:	2025-11-10
Resolution	:	3.50 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 ⓘ 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:

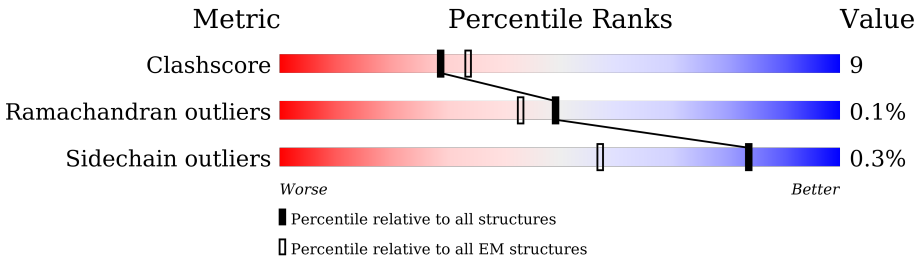
EMDB validation analysis	:	0.0.1.dev133
MolProbity	:	4-5-2 with Phenix2.2
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

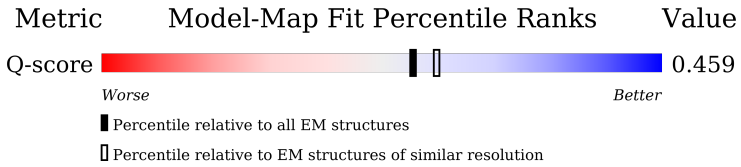
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.50 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13950 (3.00 - 4.00)

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	B	200	18% 28% 10% 62%
2	A	393	8% 70% 19% 10%
2	a	393	11% 65% 19% 16%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 6055 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 de novo designed protein binder ZNB6,Ubiquitin-like protein SMT3,Ubiquitin-like protein SMT3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	77	Total	C	N	O	S	0	0
			610	392	96	120	2		

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	150	THR	ARG	conflict	UNP Q12306
B	157	GLU	ARG	conflict	UNP Q12306
B	185	LYS	-	expression tag	UNP Q12306
B	186	LEU	-	expression tag	UNP Q12306
B	187	ALA	-	expression tag	UNP Q12306
B	188	ALA	-	expression tag	UNP Q12306
B	189	ALA	-	expression tag	UNP Q12306
B	190	LEU	-	expression tag	UNP Q12306
B	191	GLU	-	expression tag	UNP Q12306
B	192	HIS	-	expression tag	UNP Q12306
B	193	HIS	-	expression tag	UNP Q12306
B	194	HIS	-	expression tag	UNP Q12306
B	195	HIS	-	expression tag	UNP Q12306
B	196	HIS	-	expression tag	UNP Q12306
B	197	HIS	-	expression tag	UNP Q12306

- Molecule 2 is a protein called non-structural protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	a	329	Total	C	N	O	S	0	0
			2626	1643	470	493	20		
2	A	352	Total	C	N	O	S	0	0
			2819	1773	506	520	20		

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	-4	HIS	-	expression tag	UNP A0A024B7W1
a	-3	HIS	-	expression tag	UNP A0A024B7W1
a	-2	HIS	-	expression tag	UNP A0A024B7W1
a	-1	HIS	-	expression tag	UNP A0A024B7W1
a	0	HIS	-	expression tag	UNP A0A024B7W1
a	1	HIS	-	expression tag	UNP A0A024B7W1
a	355	LEU	-	expression tag	UNP A0A024B7W1
a	356	VAL	-	expression tag	UNP A0A024B7W1
a	357	PRO	-	expression tag	UNP A0A024B7W1
a	358	ARG	-	expression tag	UNP A0A024B7W1
a	359	GLY	-	expression tag	UNP A0A024B7W1
a	360	SER	-	expression tag	UNP A0A024B7W1
a	361	TRP	-	expression tag	UNP A0A024B7W1
a	362	SER	-	expression tag	UNP A0A024B7W1
a	363	HIS	-	expression tag	UNP A0A024B7W1
a	364	PRO	-	expression tag	UNP A0A024B7W1
a	365	GLN	-	expression tag	UNP A0A024B7W1
a	366	PHE	-	expression tag	UNP A0A024B7W1
a	367	GLU	-	expression tag	UNP A0A024B7W1
a	368	LYS	-	expression tag	UNP A0A024B7W1
a	369	GLY	-	expression tag	UNP A0A024B7W1
a	370	GLY	-	expression tag	UNP A0A024B7W1
a	371	GLY	-	expression tag	UNP A0A024B7W1
a	372	SER	-	expression tag	UNP A0A024B7W1
a	373	GLY	-	expression tag	UNP A0A024B7W1
a	374	GLY	-	expression tag	UNP A0A024B7W1
a	375	GLY	-	expression tag	UNP A0A024B7W1
a	376	SER	-	expression tag	UNP A0A024B7W1
a	377	GLY	-	expression tag	UNP A0A024B7W1
a	378	GLY	-	expression tag	UNP A0A024B7W1
a	379	SER	-	expression tag	UNP A0A024B7W1
a	380	ALA	-	expression tag	UNP A0A024B7W1
a	381	TRP	-	expression tag	UNP A0A024B7W1
a	382	SER	-	expression tag	UNP A0A024B7W1
a	383	HIS	-	expression tag	UNP A0A024B7W1
a	384	PRO	-	expression tag	UNP A0A024B7W1
a	385	GLN	-	expression tag	UNP A0A024B7W1
a	386	PHE	-	expression tag	UNP A0A024B7W1
a	387	GLU	-	expression tag	UNP A0A024B7W1
a	388	LYS	-	expression tag	UNP A0A024B7W1
A	-4	HIS	-	expression tag	UNP A0A024B7W1
A	-3	HIS	-	expression tag	UNP A0A024B7W1
A	-2	HIS	-	expression tag	UNP A0A024B7W1

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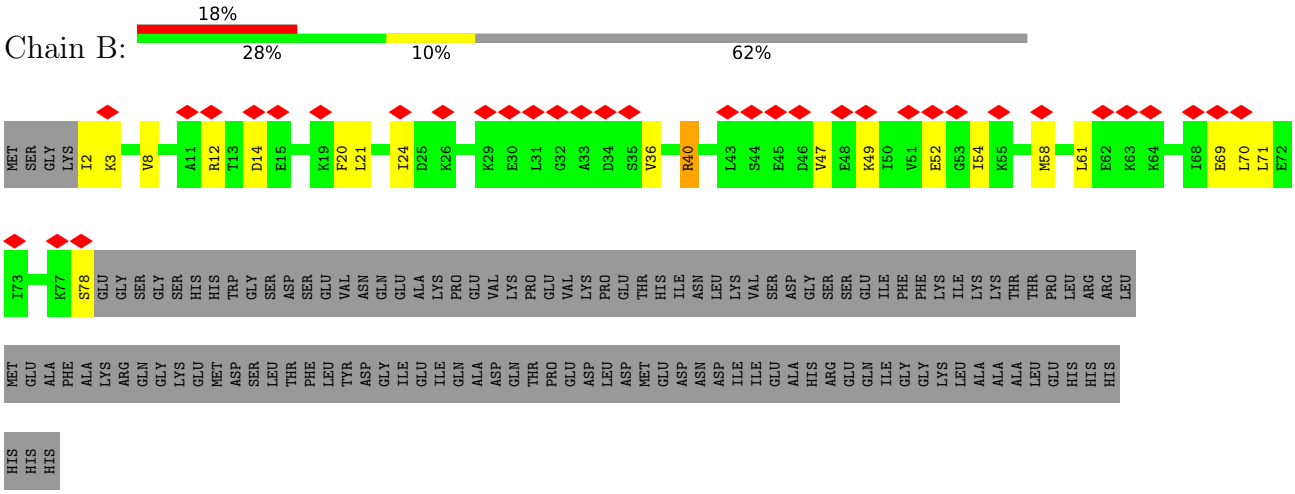
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	HIS	-	expression tag	UNP A0A024B7W1
A	0	HIS	-	expression tag	UNP A0A024B7W1
A	1	HIS	-	expression tag	UNP A0A024B7W1
A	355	LEU	-	expression tag	UNP A0A024B7W1
A	356	VAL	-	expression tag	UNP A0A024B7W1
A	357	PRO	-	expression tag	UNP A0A024B7W1
A	358	ARG	-	expression tag	UNP A0A024B7W1
A	359	GLY	-	expression tag	UNP A0A024B7W1
A	360	SER	-	expression tag	UNP A0A024B7W1
A	361	TRP	-	expression tag	UNP A0A024B7W1
A	362	SER	-	expression tag	UNP A0A024B7W1
A	363	HIS	-	expression tag	UNP A0A024B7W1
A	364	PRO	-	expression tag	UNP A0A024B7W1
A	365	GLN	-	expression tag	UNP A0A024B7W1
A	366	PHE	-	expression tag	UNP A0A024B7W1
A	367	GLU	-	expression tag	UNP A0A024B7W1
A	368	LYS	-	expression tag	UNP A0A024B7W1
A	369	GLY	-	expression tag	UNP A0A024B7W1
A	370	GLY	-	expression tag	UNP A0A024B7W1
A	371	GLY	-	expression tag	UNP A0A024B7W1
A	372	SER	-	expression tag	UNP A0A024B7W1
A	373	GLY	-	expression tag	UNP A0A024B7W1
A	374	GLY	-	expression tag	UNP A0A024B7W1
A	375	GLY	-	expression tag	UNP A0A024B7W1
A	376	SER	-	expression tag	UNP A0A024B7W1
A	377	GLY	-	expression tag	UNP A0A024B7W1
A	378	GLY	-	expression tag	UNP A0A024B7W1
A	379	SER	-	expression tag	UNP A0A024B7W1
A	380	ALA	-	expression tag	UNP A0A024B7W1
A	381	TRP	-	expression tag	UNP A0A024B7W1
A	382	SER	-	expression tag	UNP A0A024B7W1
A	383	HIS	-	expression tag	UNP A0A024B7W1
A	384	PRO	-	expression tag	UNP A0A024B7W1
A	385	GLN	-	expression tag	UNP A0A024B7W1
A	386	PHE	-	expression tag	UNP A0A024B7W1
A	387	GLU	-	expression tag	UNP A0A024B7W1
A	388	LYS	-	expression tag	UNP A0A024B7W1

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.

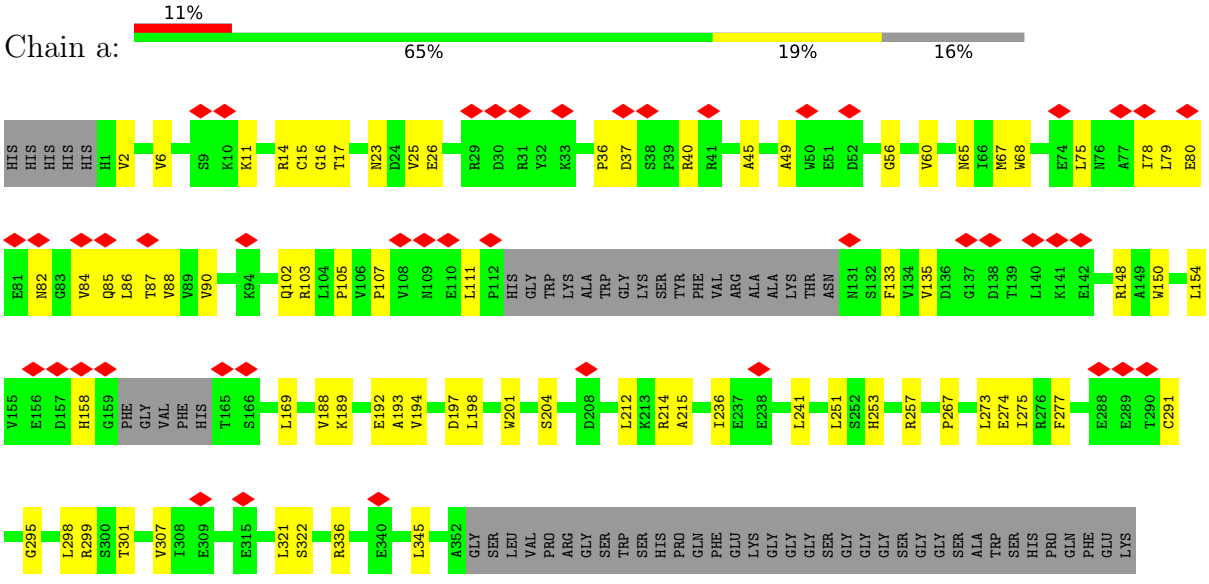
• Molecule 1: de novo designed protein binder ZNB6,Ubiquitin-like protein SMT3,Ubiquitin-like protein SMT3

Chain B:



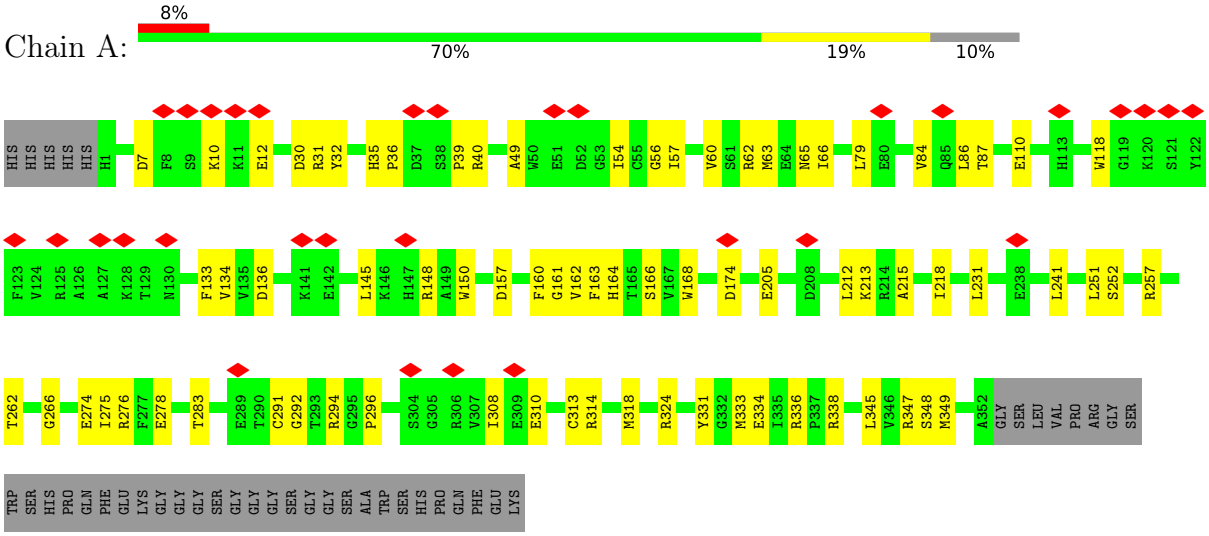
• Molecule 2: non-structural protein 1

Chain a:



• Molecule 2: non-structural protein 1

Chain A:


8%
70%
19%
10%
HIS HIS HIS HIS HIS H1 D7 F8 S9 K10 K11 E12 D30 R31 Y32 H35 P36 D37 S38 P39 R40 A49 W50 E51 D52 G53 I54 C55 G56 I57 V60 S61 R62 M63 E64 N65 I66 L79 E80 V84 Q85 L86 T87 E110 H113 W118 G119 K120 S121 Y122
F123 V124 R125 A126 A127 K128 T129 N130 F133 V134 V135 D136 K141 E142 L145 K146 H147 R148 A149 W150 D157 F160 G161 V162 F163 H164 T165 S166 V167 W168 D174 E205 D208 L212 K213 R214 A215 I218 L231 E238 L241 L251 S252 R257
T262 G266 E274 I275 R276 F277 E278 T283 E289 T290 C291 G292 T293 R294 G295 P296 S304 G305 R306 V307 I308 E309 E310 C313 R314 M318 R324 Y331 G332 M333 E334 I335 R336 P337 R338 L345 V346 R347 S348 M349 A352 GLY SER LEU VAL PRO ARG GLY SER
TRP SER HIS PRO GLN PHE GLU LYS GLY GLY GLY SER GLY GLY GLY SER GLY GLY GLY SER ALA TRP SER HIS PRO GLN PHE GLU LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	107034	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	49	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	58.119	Depositor
Minimum map value	-34.422	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	7.5	Depositor
Map size (Å)	238.0, 238.0, 238.0	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.85, 0.85, 0.85	Depositor

5 Model quality

5.1 Standard geometry

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	0.20	0/614	0.37	0/824
2	A	0.15	0/2897	0.32	0/3928
2	a	0.11	0/2692	0.29	0/3648
All	All	0.14	0/6203	0.31	0/8400

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

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	610	0	647	14	0
2	A	2819	0	2724	59	0
2	a	2626	0	2540	47	0
All	All	6055	0	5911	112	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 9.

The worst 5 of 112 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)
2:A:31:ARG:HG3	2:A:32:TYR:H	1.37	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:39:PRO:HB3	2:A:118:TRP:HE1	1.43	0.83
2:a:193:ALA:HB3	2:a:204:SER:HB2	1.68	0.75
2:A:294:ARG:NH1	2:A:334:GLU:OE2	2.23	0.72
2:A:262:THR:O	2:A:294:ARG:NH2	2.23	0.71

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	75/200 (38%)	74 (99%)	1 (1%)	0	100 100
2	A	350/393 (89%)	309 (88%)	40 (11%)	1 (0%)	36 67
2	a	323/393 (82%)	295 (91%)	28 (9%)	0	100 100
All	All	748/986 (76%)	678 (91%)	69 (9%)	1 (0%)	49 79

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	318	MET

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	69/175 (39%)	67 (97%)	2 (3%)	37 60
2	A	307/337 (91%)	307 (100%)	0	100 100
2	a	290/337 (86%)	290 (100%)	0	100 100
All	All	666/849 (78%)	664 (100%)	2 (0%)	84 83

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	14	ASP
1	B	40	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
2	A	48	GLN
2	A	131	ASN
2	A	164	HIS
2	a	253	HIS
2	a	195	HIS

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.

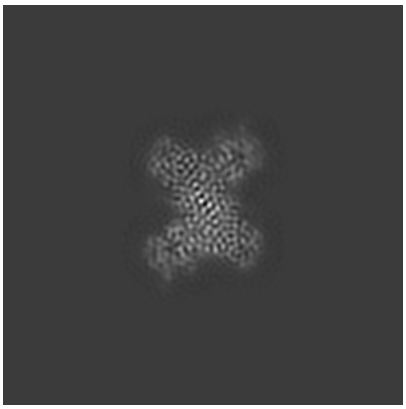
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-67020. These allow visual inspection of the internal detail of the map and identification of artifacts.

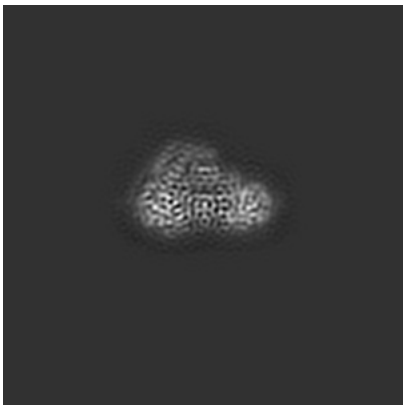
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

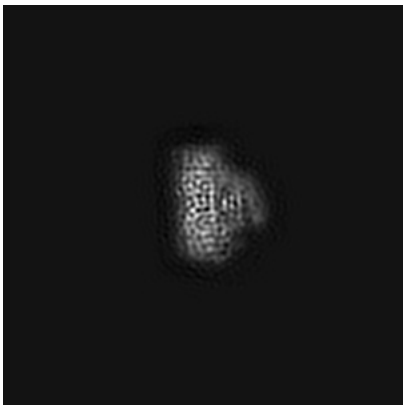
6.1.1 Primary map



X

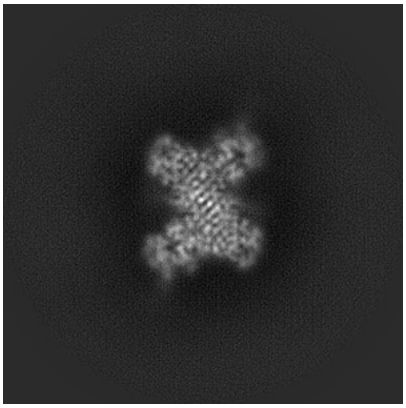


Y

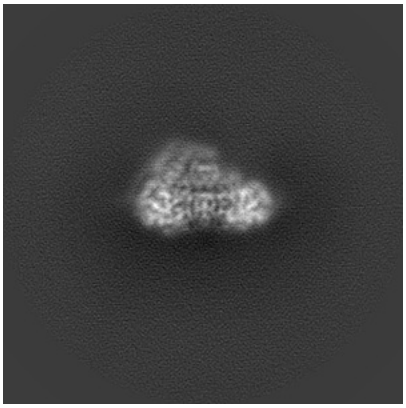


Z

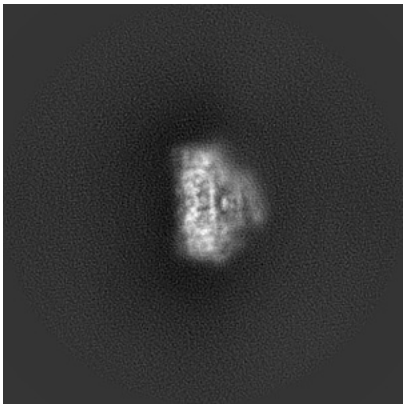
6.1.2 Raw map



X



Y

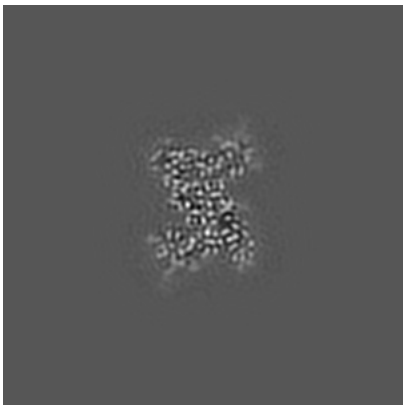


Z

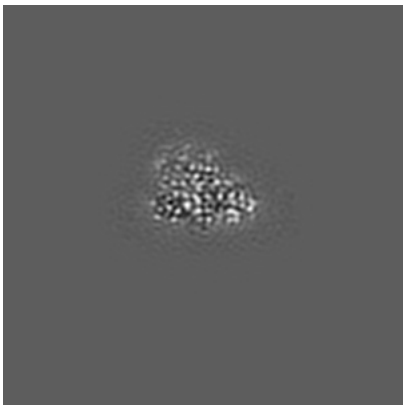
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map



X Index: 140

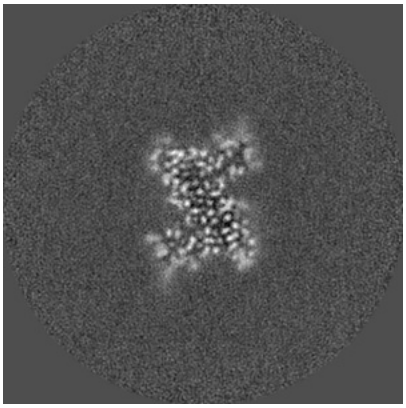


Y Index: 140

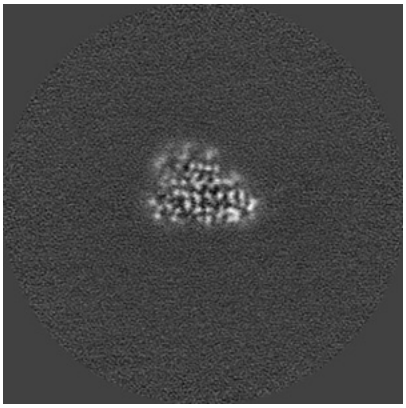


Z Index: 140

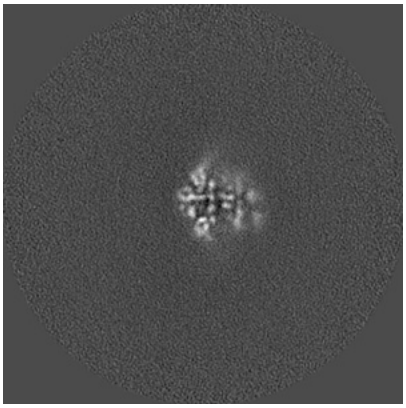
6.2.2 Raw map



X Index: 140



Y Index: 140

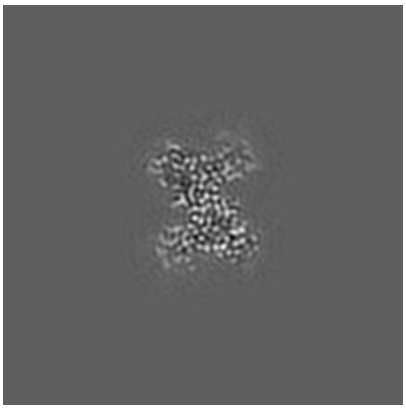


Z Index: 140

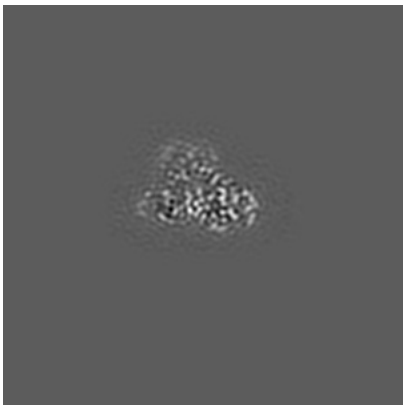
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 136

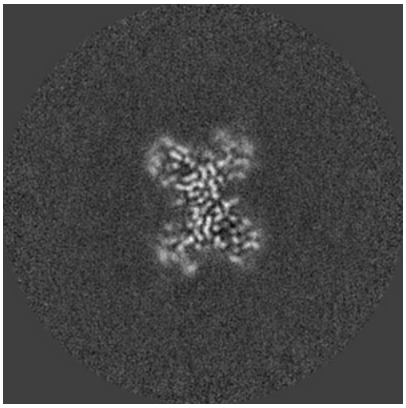


Y Index: 134

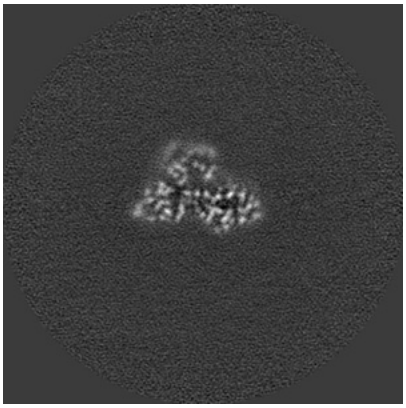


Z Index: 115

6.3.2 Raw map



X Index: 134



Y Index: 131

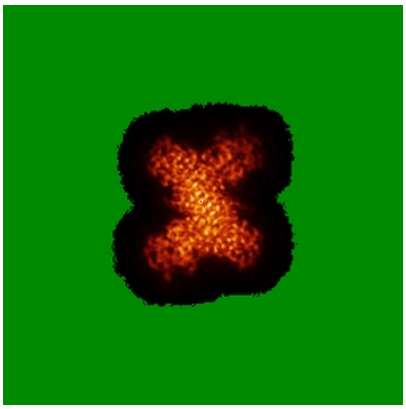


Z Index: 115

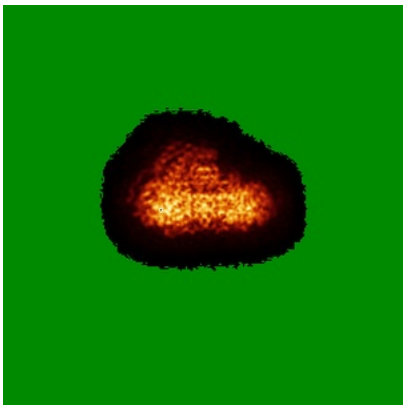
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

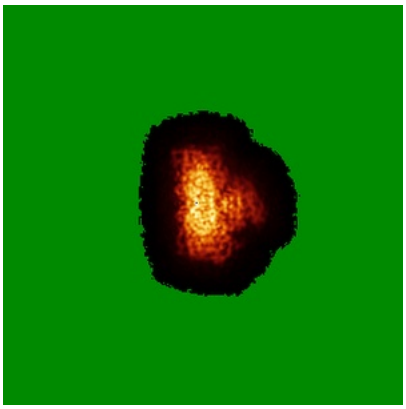
6.4.1 Primary map



X

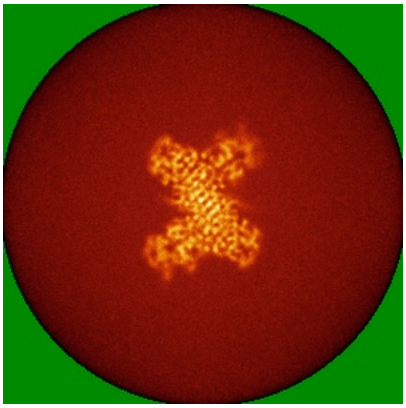


Y

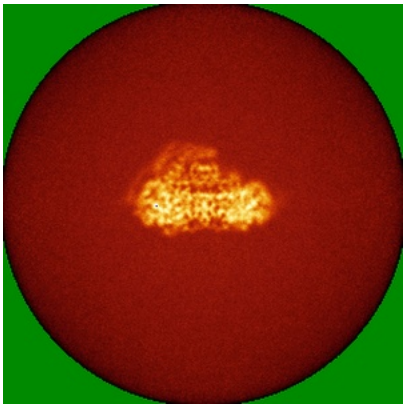


Z

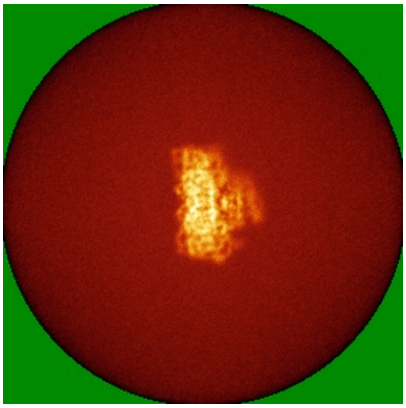
6.4.2 Raw map



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



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 7.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

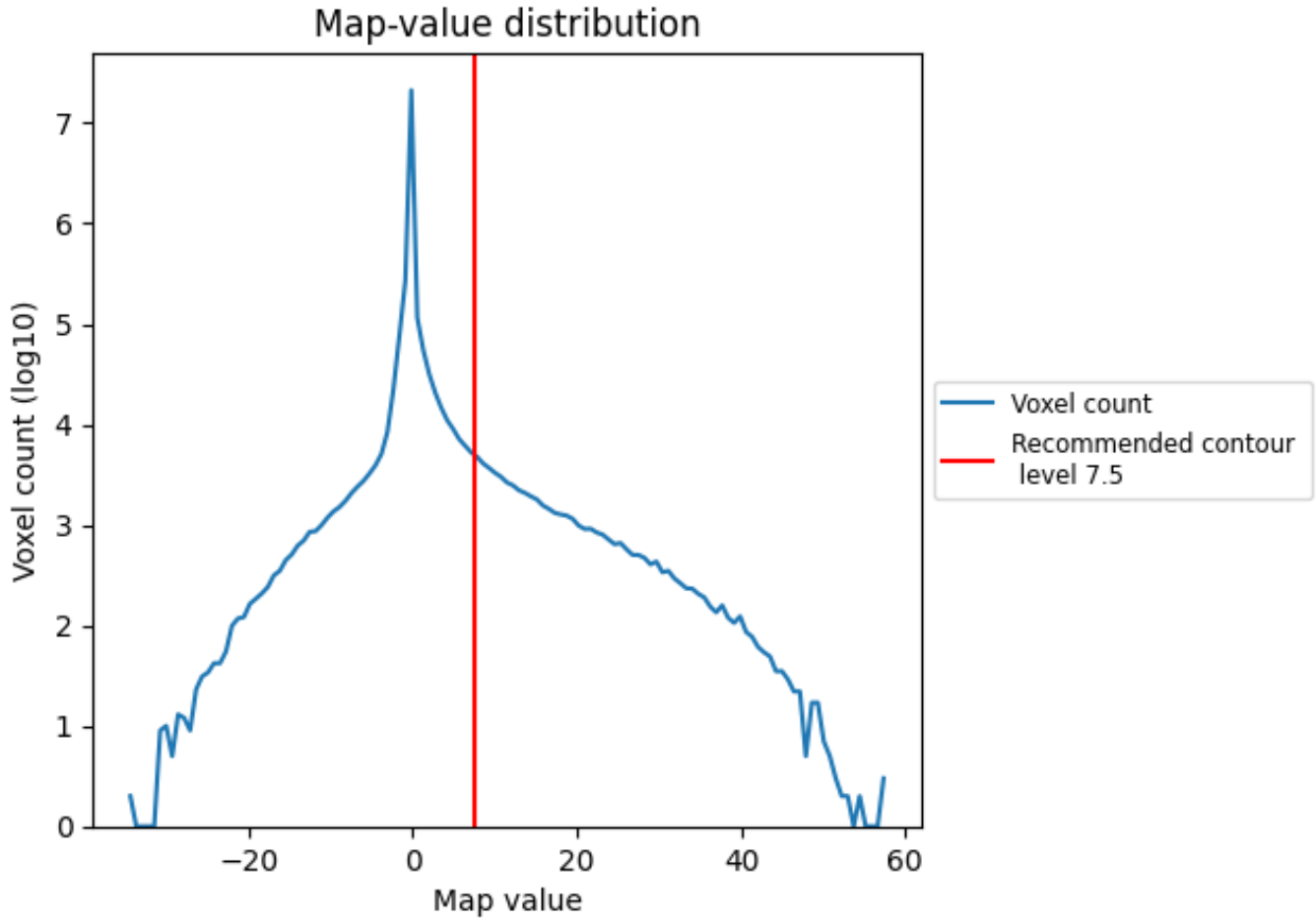
6.6 Mask visualisation (i)

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

7 Map analysis

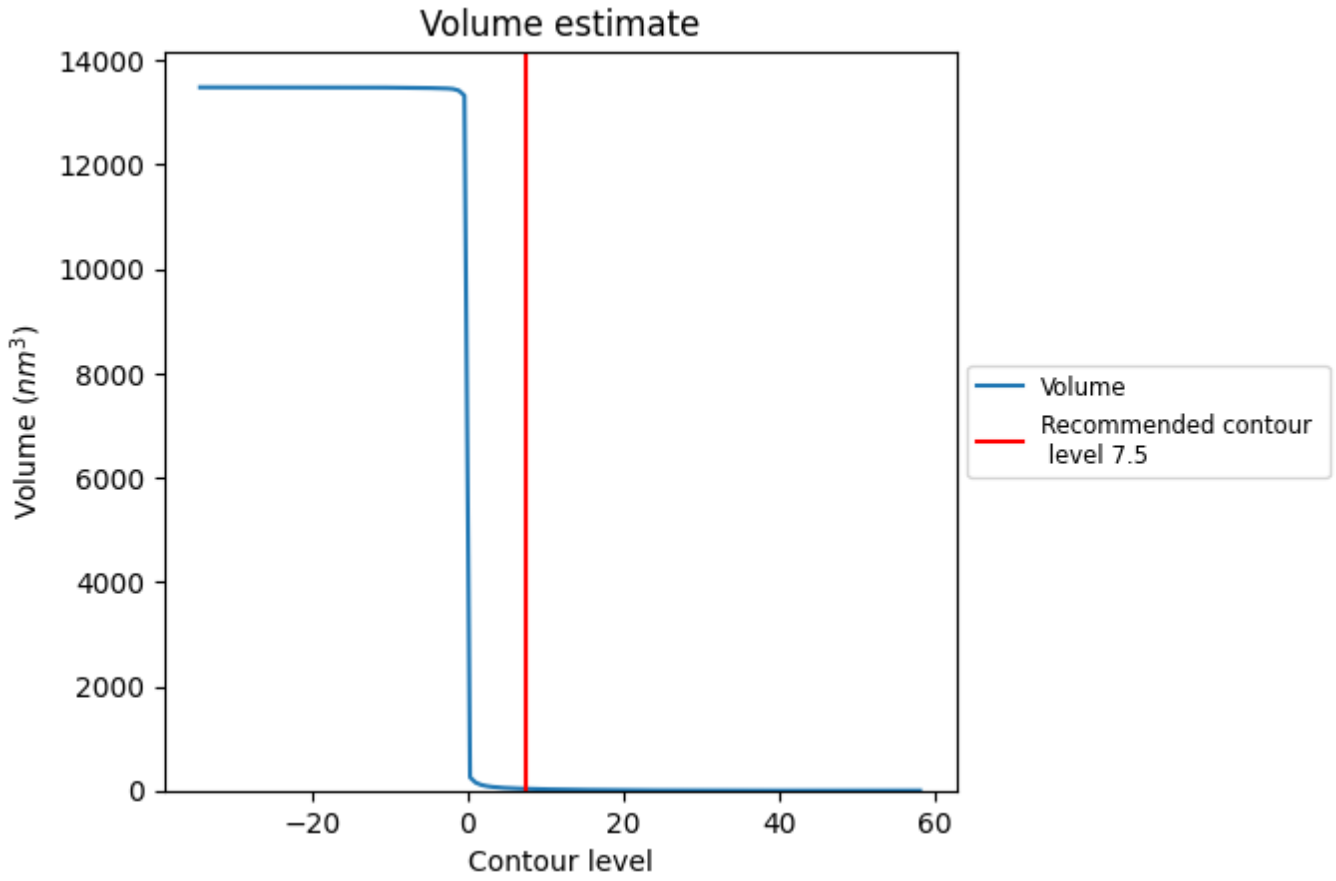
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

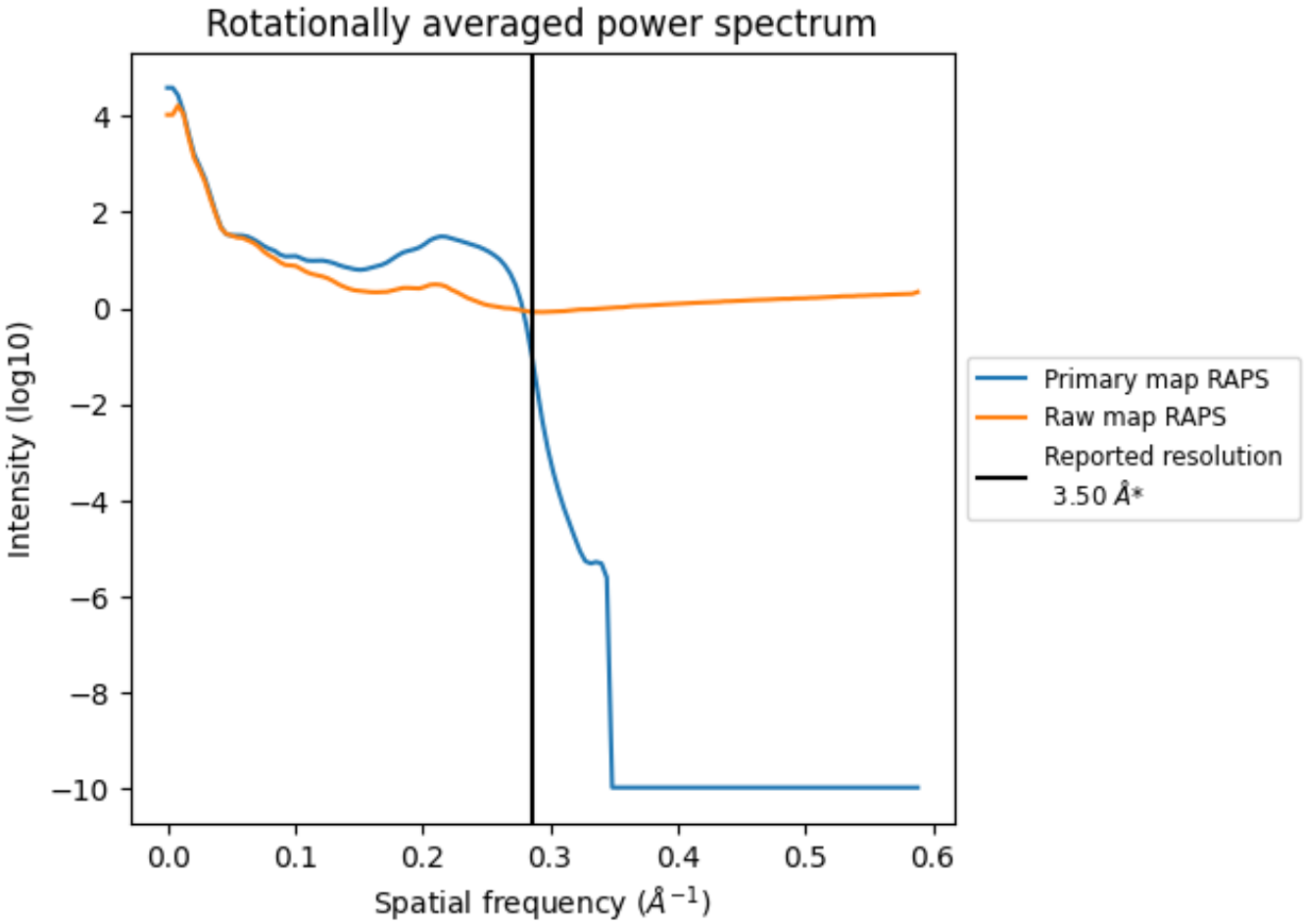
7.2 Volume estimate (i)



The volume at the recommended contour level is 34 nm^3; this corresponds to an approximate mass of 31 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)

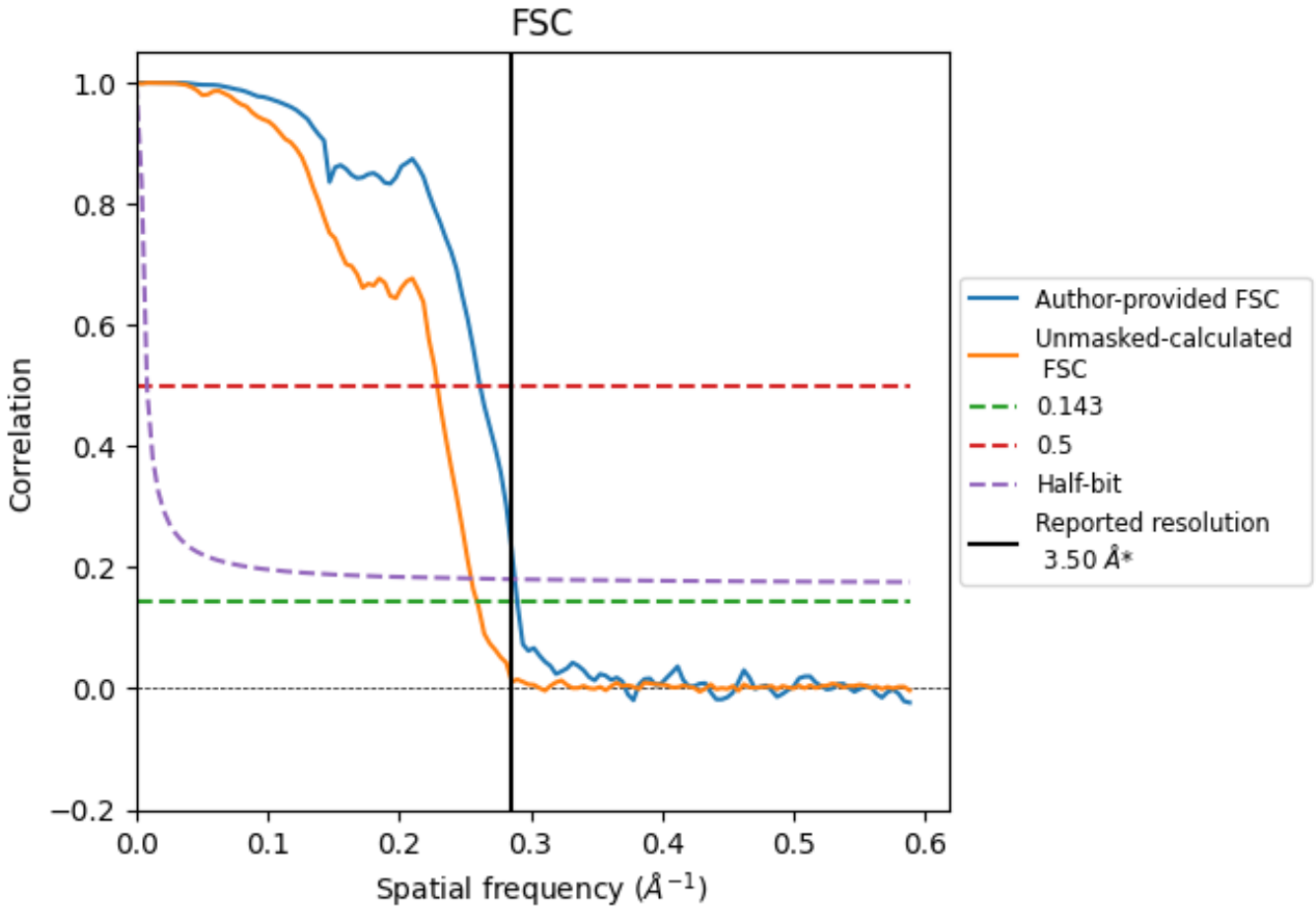


*Reported resolution corresponds to spatial frequency of 0.286 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.286 Å^{-1}

8.2 Resolution estimates (i)

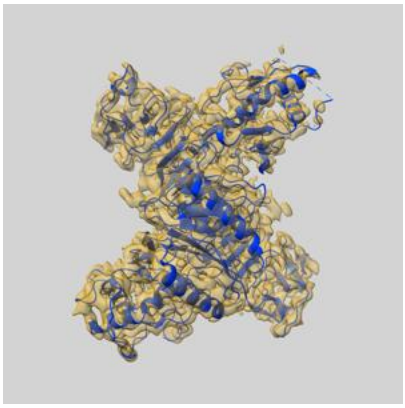
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.45	3.82	3.47
Unmasked-calculated*	3.86	4.37	3.92

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.86 differs from the reported value 3.5 by more than 10 %

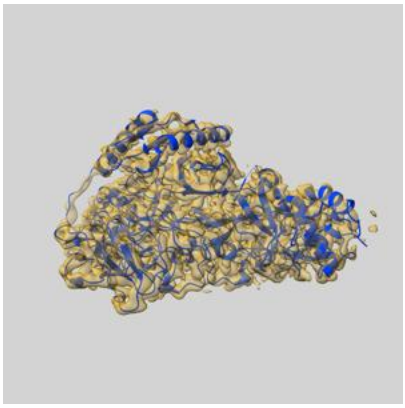
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-67020 and PDB model 9XMC. Per-residue inclusion information can be found in section 3 on page 6.

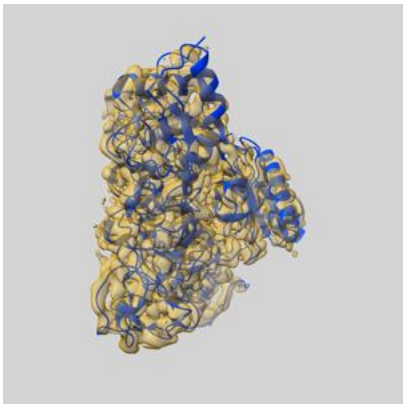
9.1 Map-model overlay



X



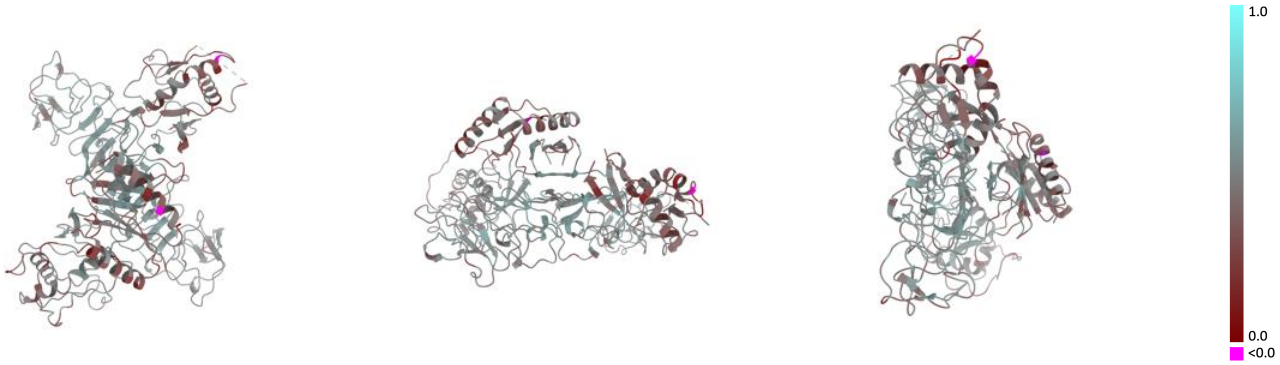
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 7.5 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.

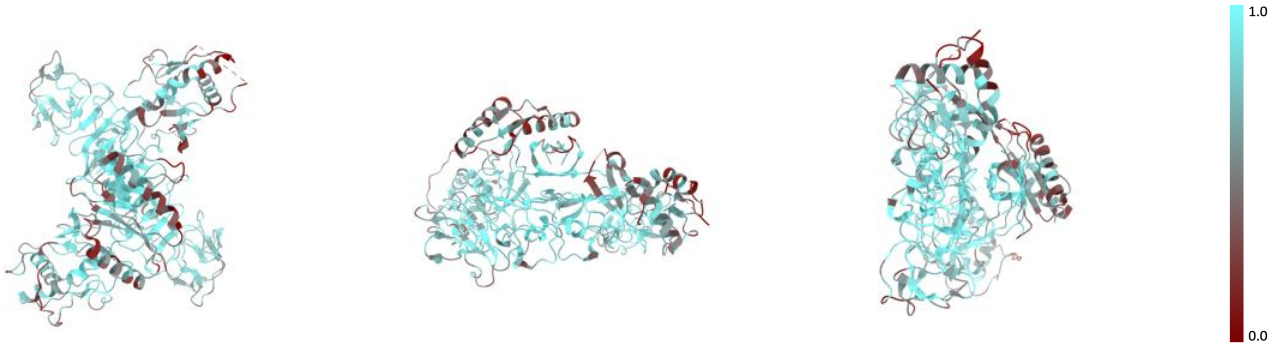
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

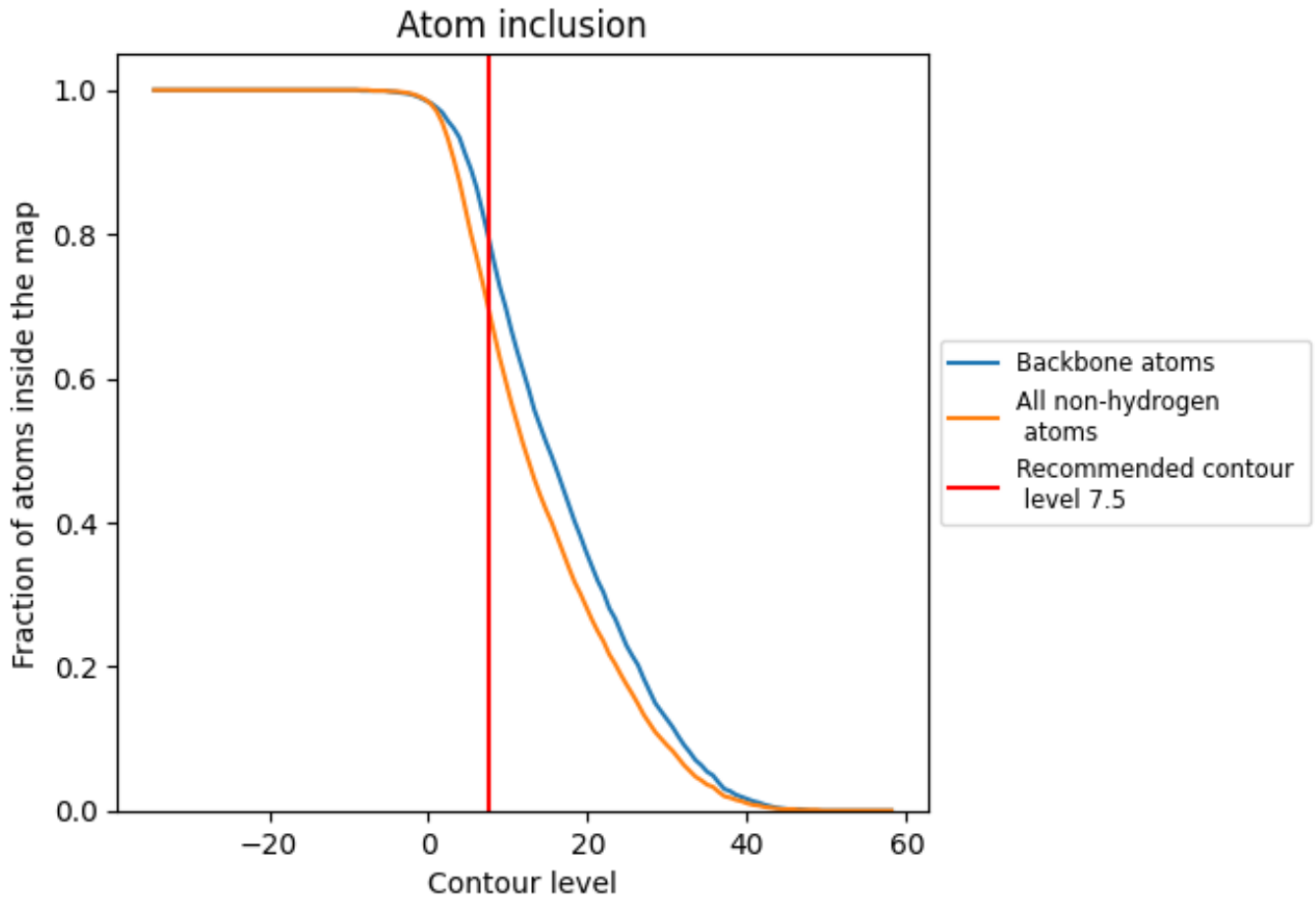
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (7.5).

9.4 Atom inclusion (i)



At the recommended contour level, 80% of all backbone atoms, 70% 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 (7.5) and Q-score for the entire model and for each chain.



Chain	Atom inclusion	Q-score
All	0.6980	0.4590
A	0.7430	0.4760
B	0.4630	0.3630
a	0.7050	0.4640