wwPDB EM Validation Summary Report

Nov 9, 2026 – 04:43 pm GMT

PDB ID	:	9R39 / pdb_00009r39
EMDB ID	:	EMD-53552
Title	:	BoNT-NTNH complex from Bacillus toyonensis CH177
Authors	:	Krc, A.; Nowakowska, M.; Stenmark, P.
Deposited on	:	2025-05-03
Resolution	:	2.93 Å(reported)
Based on initial model	:	.

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:

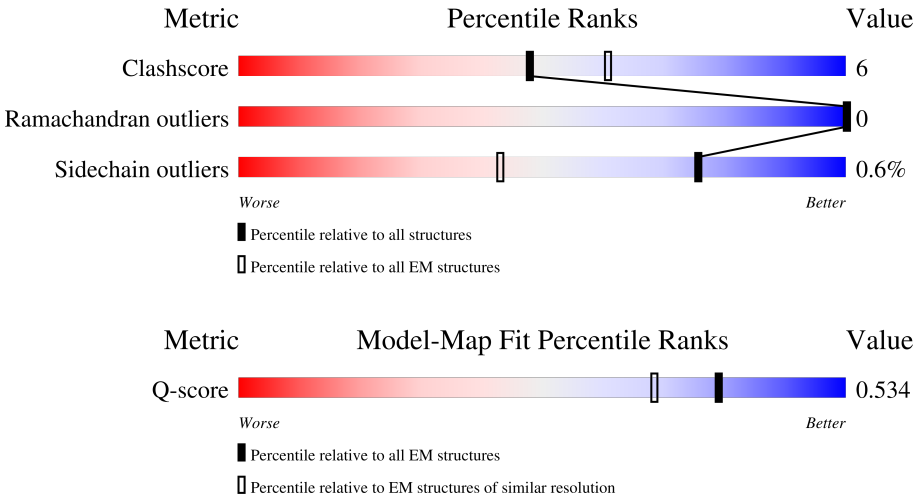
EMDB validation analysis	:	0.0.1.dev133
MolProbity	:	4-5-2 with Phenix2.2
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & 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 2.93 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	13037 (2.43 - 3.43)

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	1239	80% 15% 6%
2	B	1207	76% 15% 9%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 18484 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 BoNT-like toxin from Bacillus toyonensis CH177, BoNT/Bt.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1168	9578	6168	1571	1813	26	0	0

- Molecule 2 is a protein called Non-toxic non-hemagglutinin component from Bacillus toyonensis CH177, NTNH/Bt.

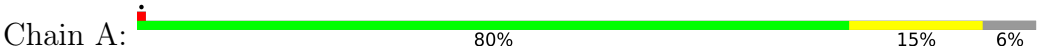
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1094	8906	5704	1451	1721	30	0	0

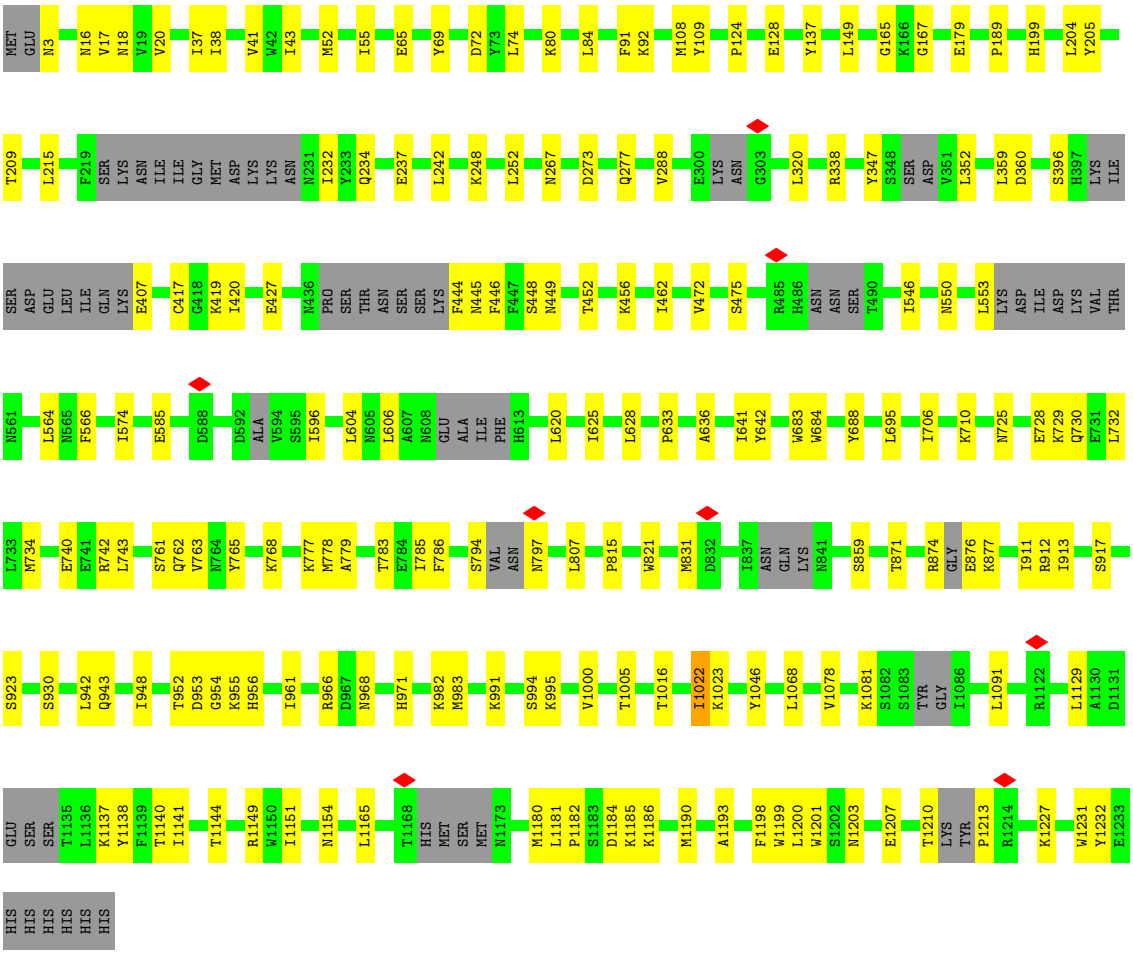
3 Residue-property plots (i)

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: BoNT-like toxin from Bacillus toyonensis CH177, BoNT/Bt

Chain A:

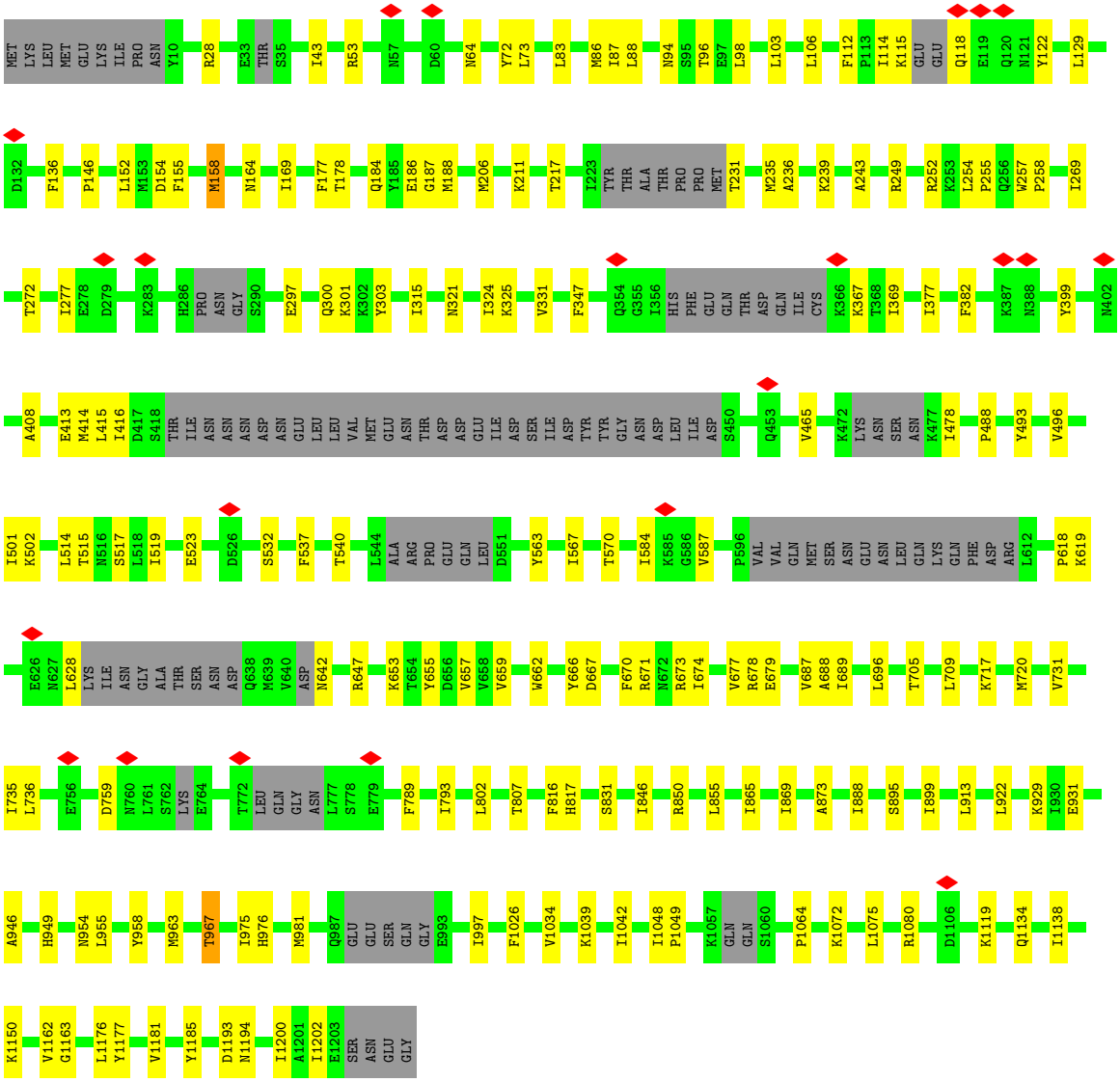




• Molecule 2: Non-toxic non-hemagglutinin component from Bacillus toyonensis CH177, NTNH/Bt

Chain B:




MET LYS LEU MET GLU LYS ILE PRO ASN Y10 R28 E33 THR S35 I43 R53 N57 D60 N64 Y72 L73 L83 M86 I87 L88 N94 S95 T96 E97 L98 L103 L106 F112 P113 I114 K115 GLU GLU Q118 E119 Q120 N121 Y122 L129
D132 F136 P146 L152 M153 D154 F155 M158 N164 I169 F177 T178 Q184 Y185 E186 G187 M188 M206 K211 T217 I223 TYR THR ALA THR PRO PRO MET T231 M235 A236 K239 A243 R249 R252 K253 L254 P255 Q256 W257 P258 I269
T272 I277 E278 D279 K283 H286 PRO ASN GLY S290 E297 Q300 K301 K302 Y303 I315 N321 I324 K325 V331 F347 Q354 G355 I356 HIS PHE GLU GLN THR ASP GLN ILE CYS K366 K367 T368 I369 I377 F382 K387 N388 Y399 N402
A408 E413 M414 L415 I416 D417 S418 THR ILE ASN ASN ASN ASP ASN GLU LEU LEU VAL MET GLU ASN THR ASP ASP GLU ILE ASP SER ILE ASP TYR TYR GLY ASN ASP LEU ILE ASP S450 Q453 V465 K472 LYS ASN SER ASN K477 I478 P488 Y493 V496
I501 K502 L514 T515 N516 S517 L518 I519 E523 D526 S532 F537 T540 L544 ALA ARG PRO GLU GLN LEU D551 Y563 I567 T570 I584 K585 G586 V587 P596 VAL VAL GLN MET SER ASN GLU ASN LEU GLN LYS GLN PHE ASP ARG L612 P618 K619
E626 N627 L628 LYS ILE ASN GLY ALA THR SER ASN ASP Q638 M639 V640 ASP N642 R647 K653 T654 Y655 D656 V657 V658 V659 W662 Y666 D667 F670 R671 N672 R673 I674 V677 R678 E679 V687 A688 I689 L696 T705 L709 K717 M720 V731
I735 L736 E756 D759 N760 L761 S762 LYS E764 T772 LEU GLN GLY ASN L777 S778 E779 F789 I793 L802 T807 F816 H817 S831 I846 R850 L855 I865 I869 A873 I888 S895 I899 L913 L922 K929 I930 E931
A946 H949 N954 L955 Y958 M963 T967 I975 H976 M981 Q987 GLU GLU SER GLN GLY E993 I997 F1026 V1034 K1039 I1042 I1048 P1049 K1057 GLN GLN S1060 P1064 K1072 L1075 R1080 D1106 K1119 Q1134 I1138
K1150 V1162 G1163 L1176 Y1177 V1181 Y1185 D1193 N1194 I1200 A1201 I1202 E1203 SER ASN GLU GLY

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	394398	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; CTF amplitude correction was performed following 3D reconstruction	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	45	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.475	Depositor
Minimum map value	-0.227	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.084	Depositor
Map size (Å)	331.2, 331.2, 331.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.828, 0.828, 0.828	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	A	0.16	0/9790	0.27	0/13213
2	B	0.16	0/9075	0.29	0/12281
All	All	0.16	0/18865	0.28	0/25494

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	A	9578	0	9426	110	0
2	B	8906	0	8835	113	0
All	All	18484	0	18261	215	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 6.

The worst 5 of 215 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:B:514:LEU:HD21	2:B:687:VAL:HG11	1.65	0.78
1:A:1165:LEU:HD11	1:A:1180:MET:HE2	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:415:LEU:HD22	2:B:619:LYS:HB2	1.70	0.74
1:A:706:ILE:HD12	1:A:743:LEU:HB3	1.70	0.72
2:B:677:VAL:HG21	2:B:731:VAL:HG11	1.70	0.72

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	1134/1239 (92%)	1097 (97%)	37 (3%)	0	100	100
2	B	1062/1207 (88%)	1004 (94%)	58 (6%)	0	100	100
All	All	2196/2446 (90%)	2101 (96%)	95 (4%)	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	A	1059/1125 (94%)	1053 (99%)	6 (1%)	78	89
2	B	1013/1117 (91%)	1007 (99%)	6 (1%)	78	89
All	All	2072/2242 (92%)	2060 (99%)	12 (1%)	76	89

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	272	THR
2	B	369	ILE
2	B	1162	VAL
2	B	967	THR
1	A	859	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	339	ASN
2	B	1077	GLN
2	B	690	ASN
2	B	982	GLN
2	B	524	ASN

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.

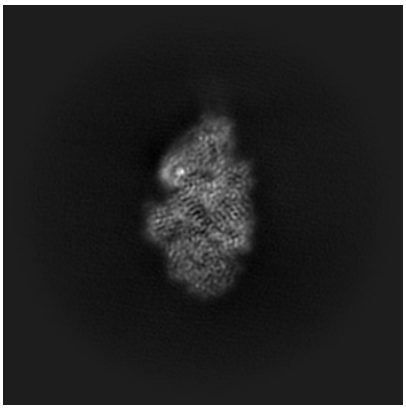
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-53552. These allow visual inspection of the internal detail of the map and identification of artifacts.

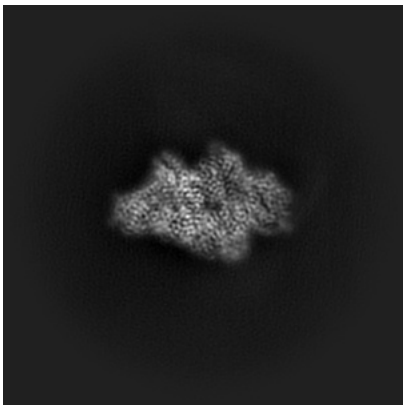
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

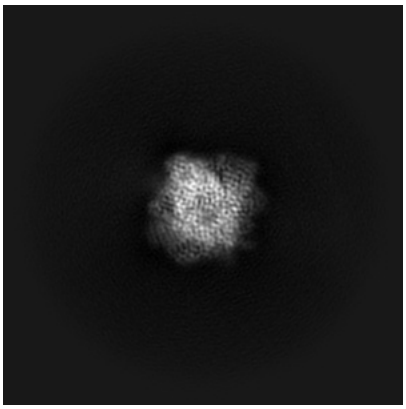
6.1.1 Primary map



X

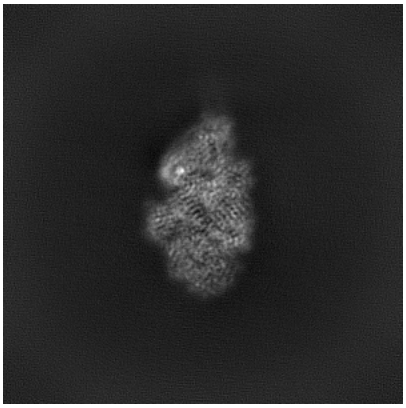


Y

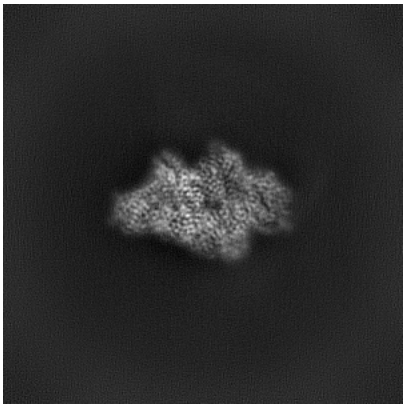


Z

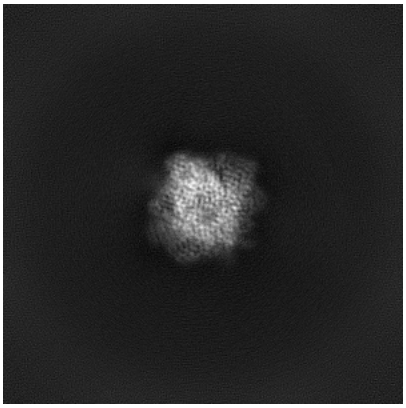
6.1.2 Raw map



X



Y

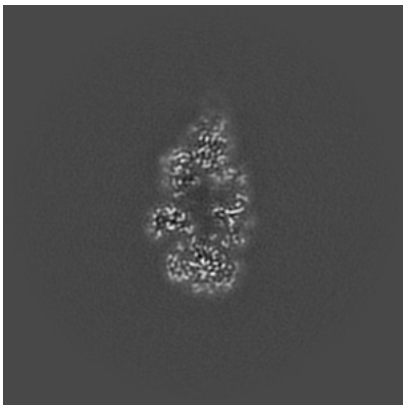


Z

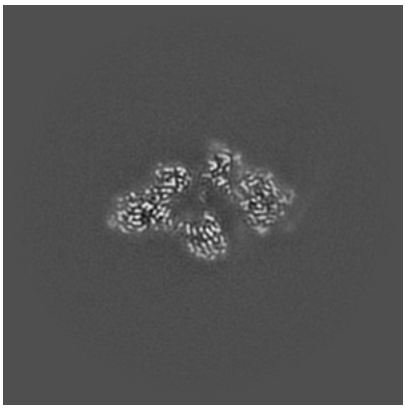
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

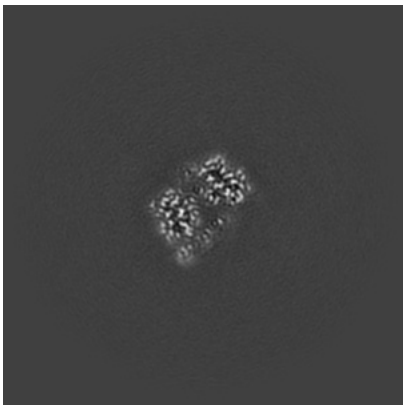
6.2.1 Primary map



X Index: 200

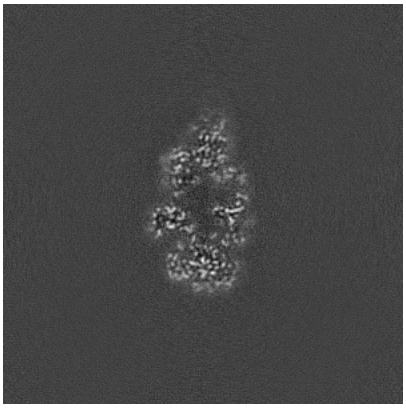


Y Index: 200

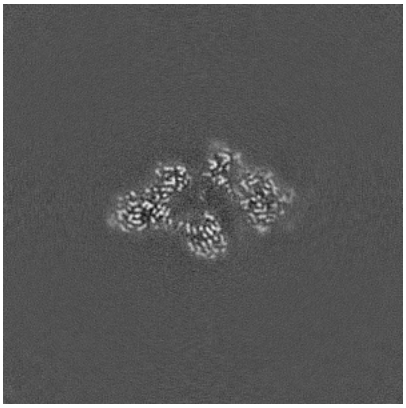


Z Index: 200

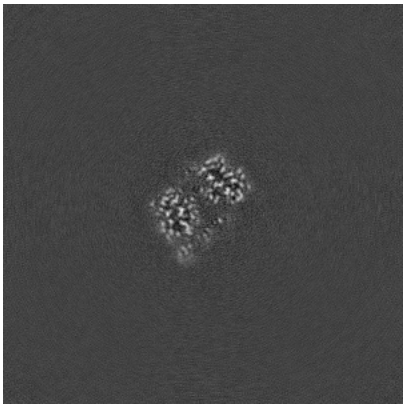
6.2.2 Raw map



X Index: 200



Y Index: 200

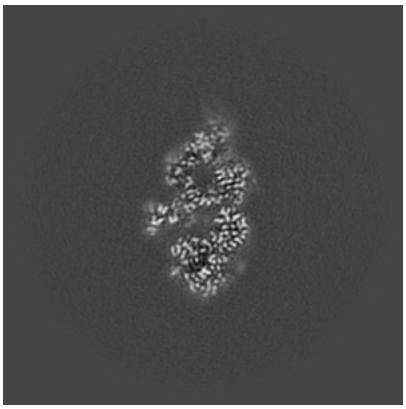


Z Index: 200

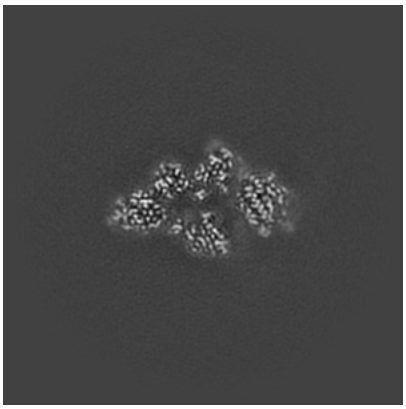
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

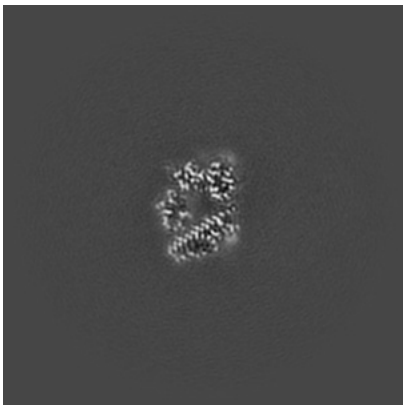
6.3.1 Primary map



X Index: 188

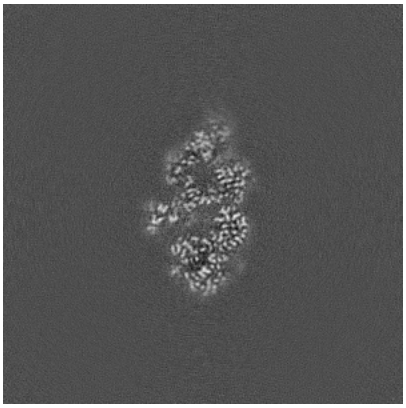


Y Index: 204

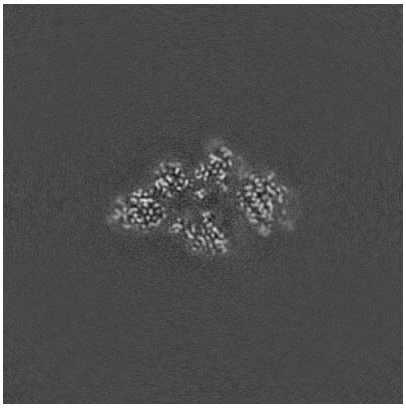


Z Index: 187

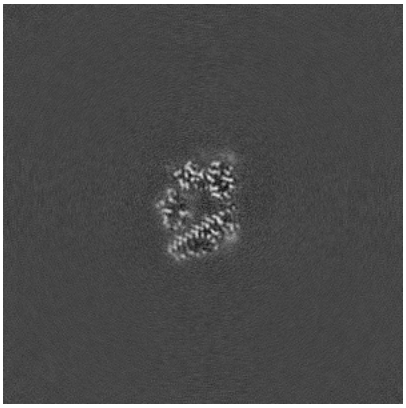
6.3.2 Raw map



X Index: 188



Y Index: 204

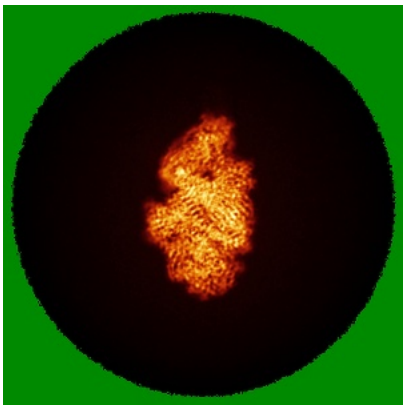


Z Index: 187

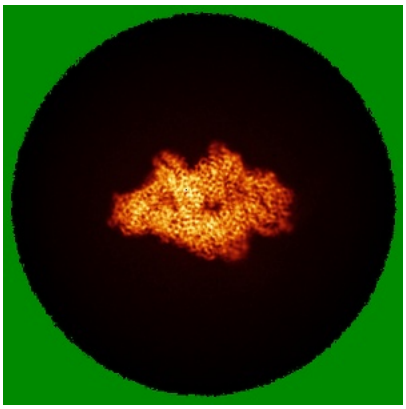
The images above show the largest variance slices of the map in three orthogonal directions.

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

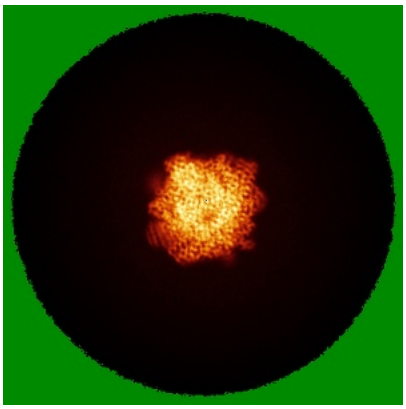
6.4.1 Primary map



X

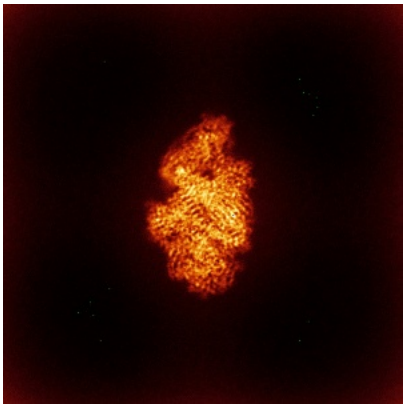


Y

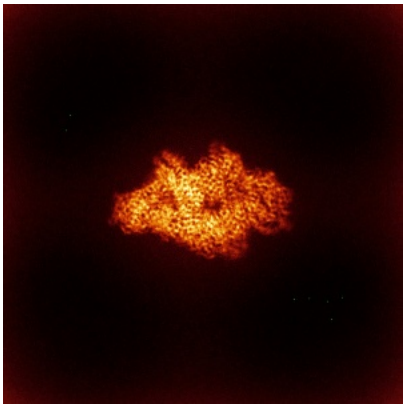


Z

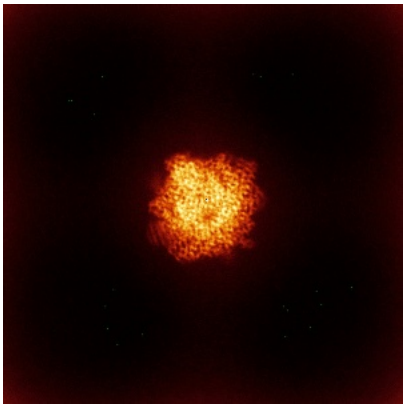
6.4.2 Raw map



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 0.084. 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.

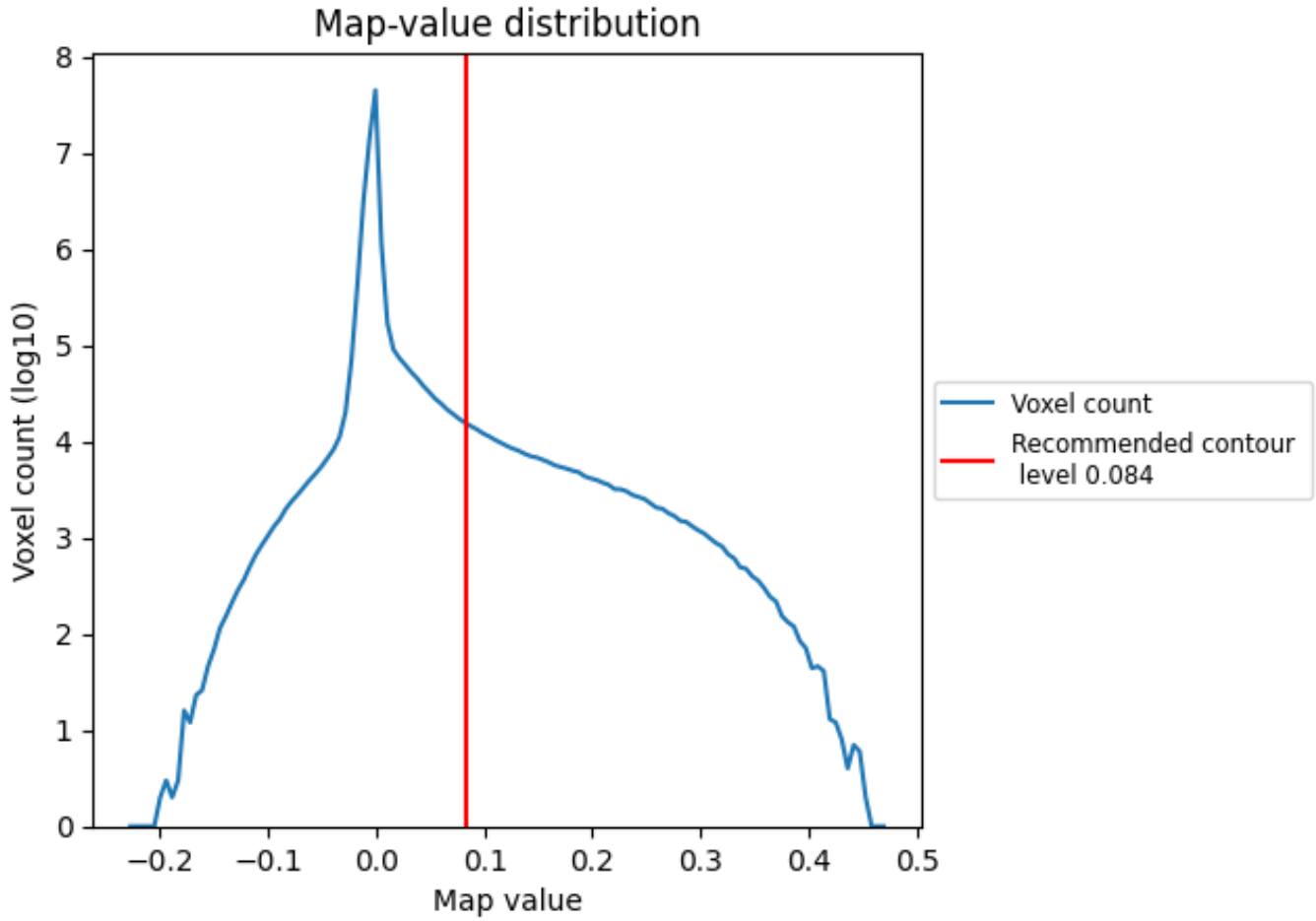
6.6 Mask visualisation (i)

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

7 Map analysis

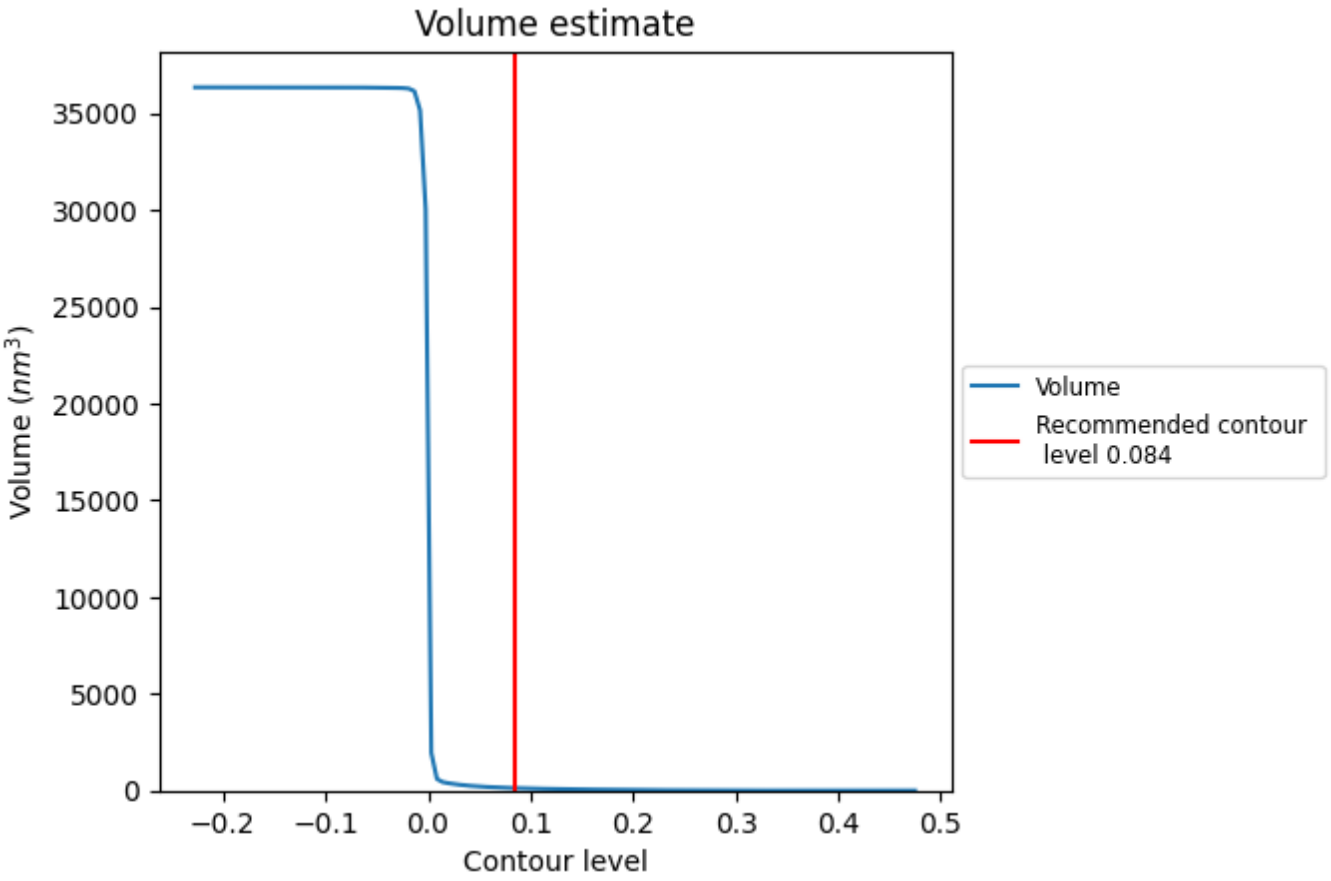
This section contains the results of statistical analysis of the map.

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.

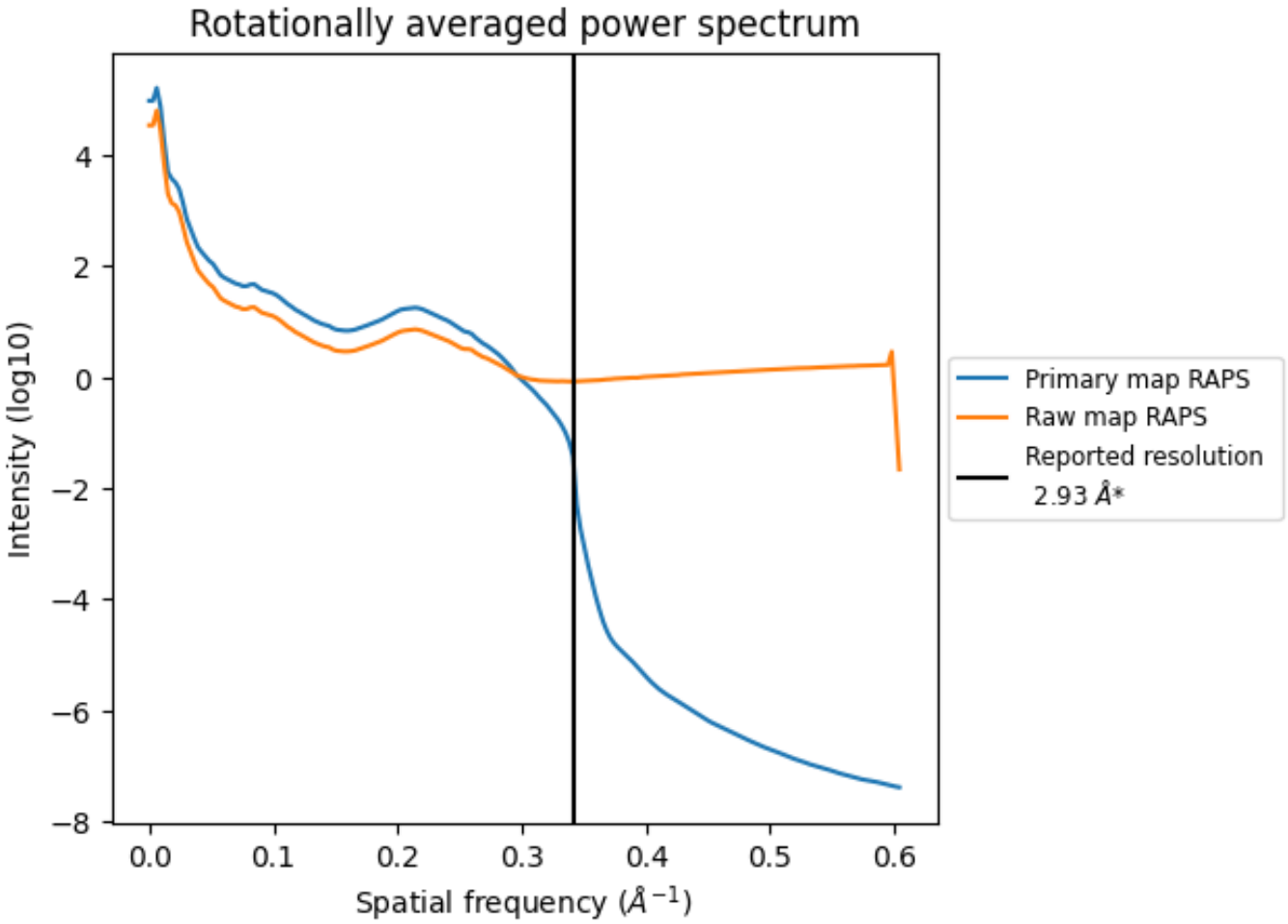
7.2 Volume estimate (i)



The volume at the recommended contour level is 129 nm^3; this corresponds to an approximate mass of 117 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)

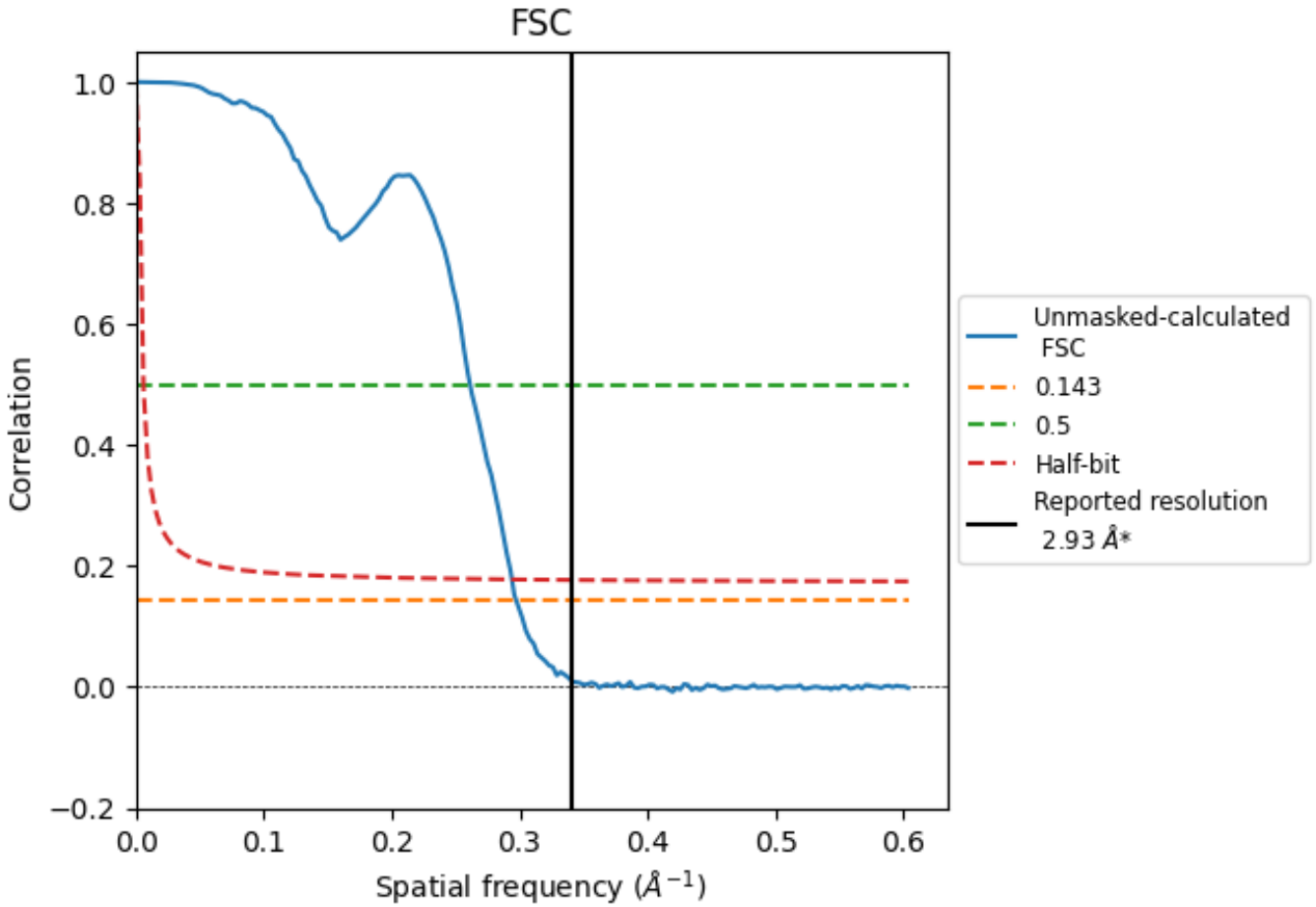


*Reported resolution corresponds to spatial frequency of 0.341 Å^{-1}

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 0.341 Å^{-1}

8.2 Resolution estimates (i)

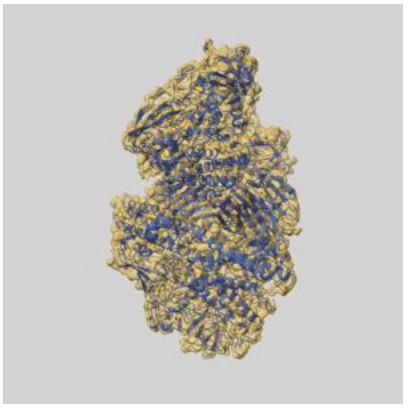
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.93	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.36	3.83	3.40

*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 3.36 differs from the reported value 2.93 by more than 10 %

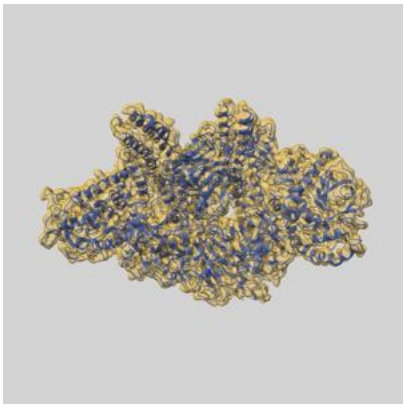
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-53552 and PDB model 9R39. Per-residue inclusion information can be found in section 3 on page 4.

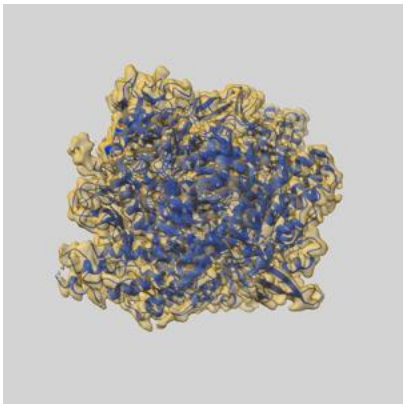
9.1 Map-model overlay



X



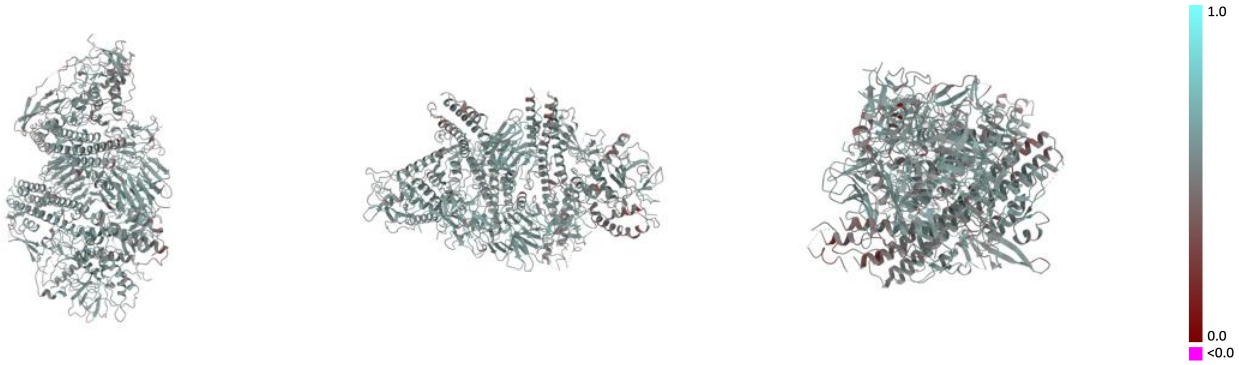
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.084 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.

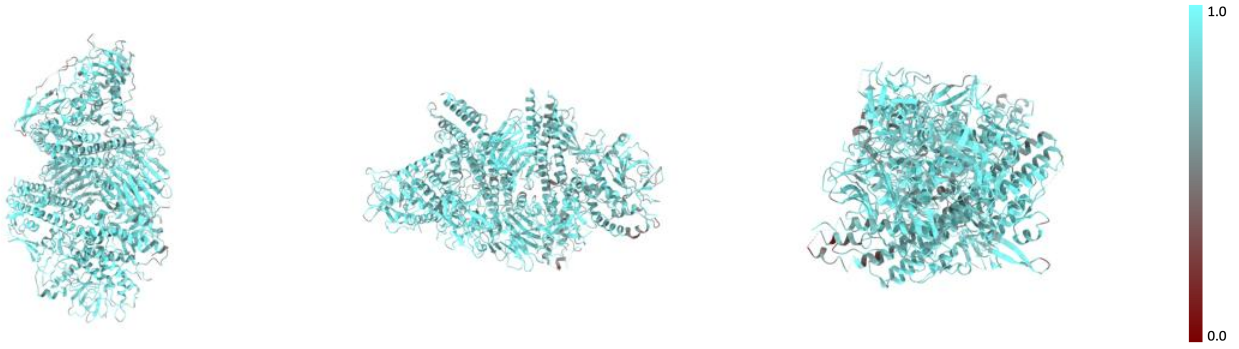
9.2 Q-score mapped to coordinate model



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.

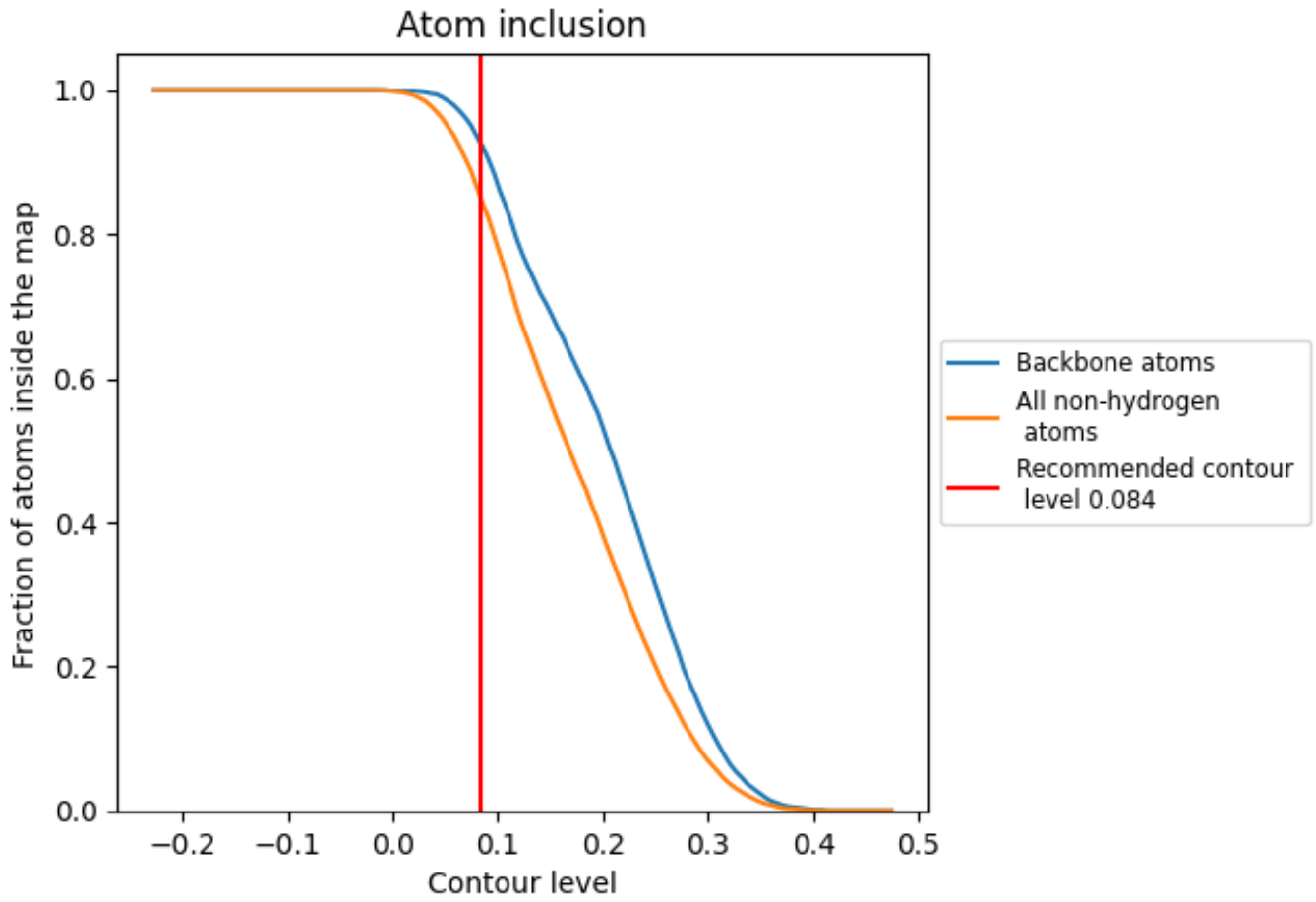
9.3 Atom inclusion mapped to coordinate model



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 (0.084).

9.4 Atom inclusion (i)



At the recommended contour level, 92% of all backbone atoms, 85% 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 (0.084) and Q-score for the entire model and for each chain.



Chain	Atom inclusion	Q-score
All	0.8490	0.5340
A	0.8680	0.5430
B	0.8300	0.5230