wwPDB EM Validation Summary Report (i)

Oct 18, 2026 – 05:30 PM JST

PDB ID	:	21SI / pdb_000021si
EMDB ID	:	EMD-67963
Title	:	cryoEM structure of PROTEIN TANC2 pre-activated
Authors	:	Xue, C.Y.; Liu, Z.M.; Liu, W.; Zhong, D.
Deposited on	:	2025-12-23
Resolution	:	3.70 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:

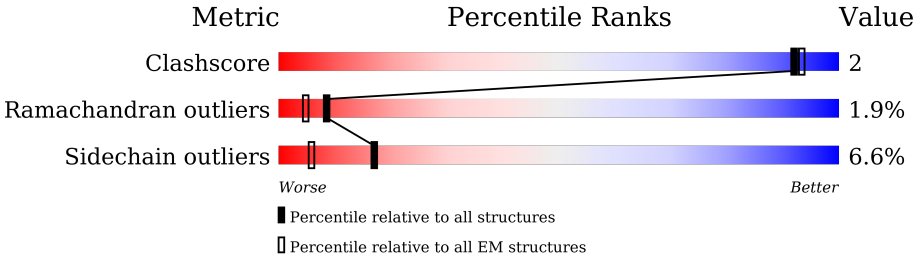
EMDB validation analysis	:	0.0.1.dev133
MolProbity	:	4-5-2 with Phenix2.2
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh &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

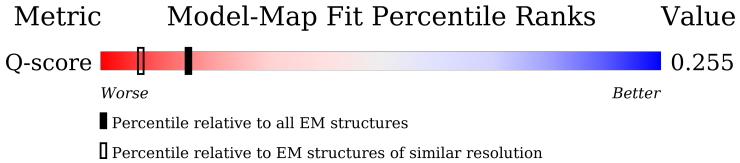
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.70 Å.

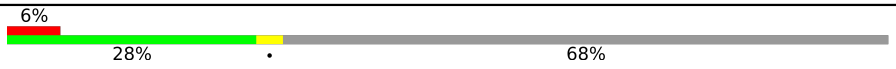
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11569 (3.20 - 4.20)

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	1994	

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 10033 atoms, of which 5044 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 Protein TANC2.

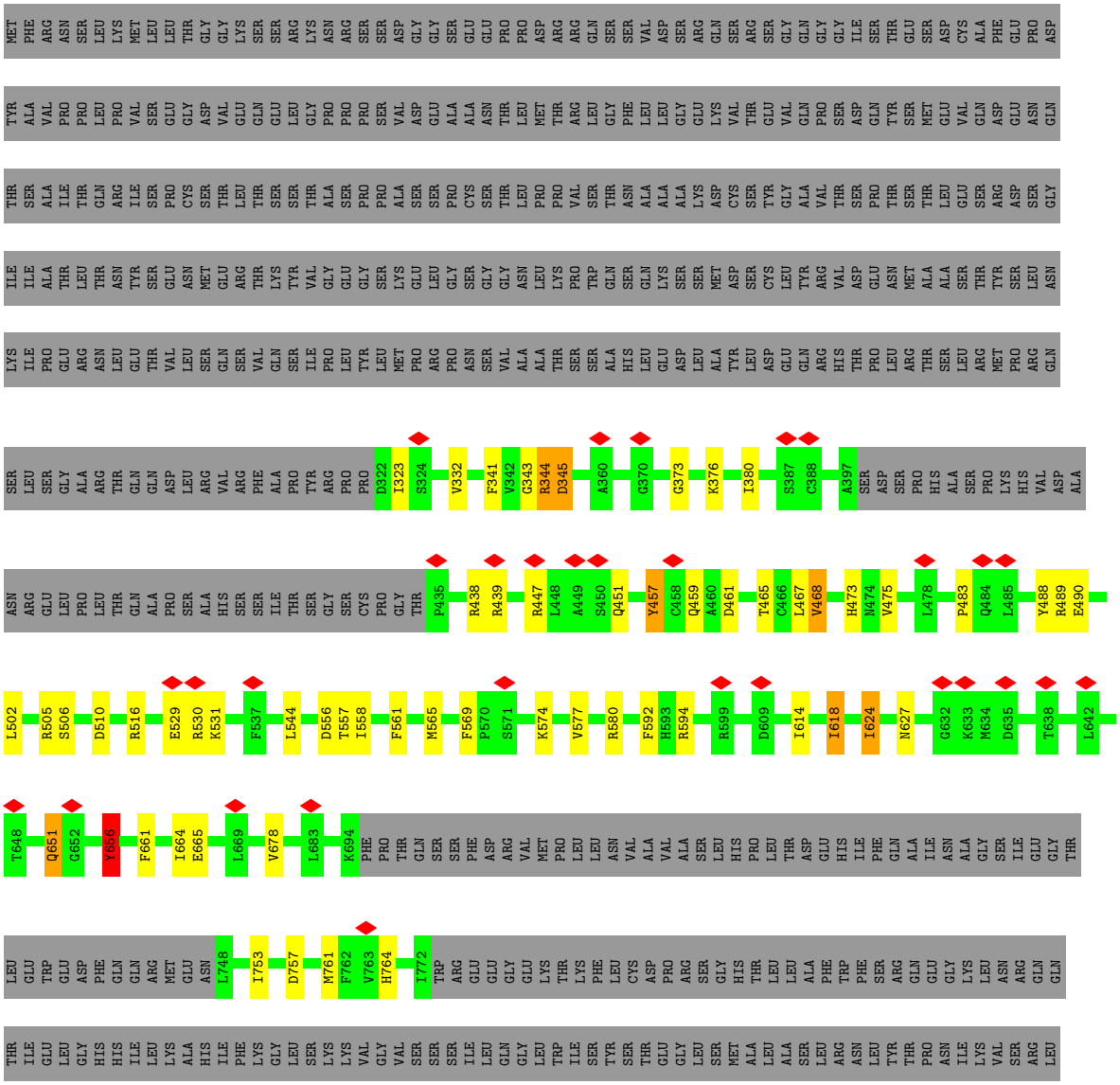
Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	640	10033	3165	5044	872	924	28	0	0

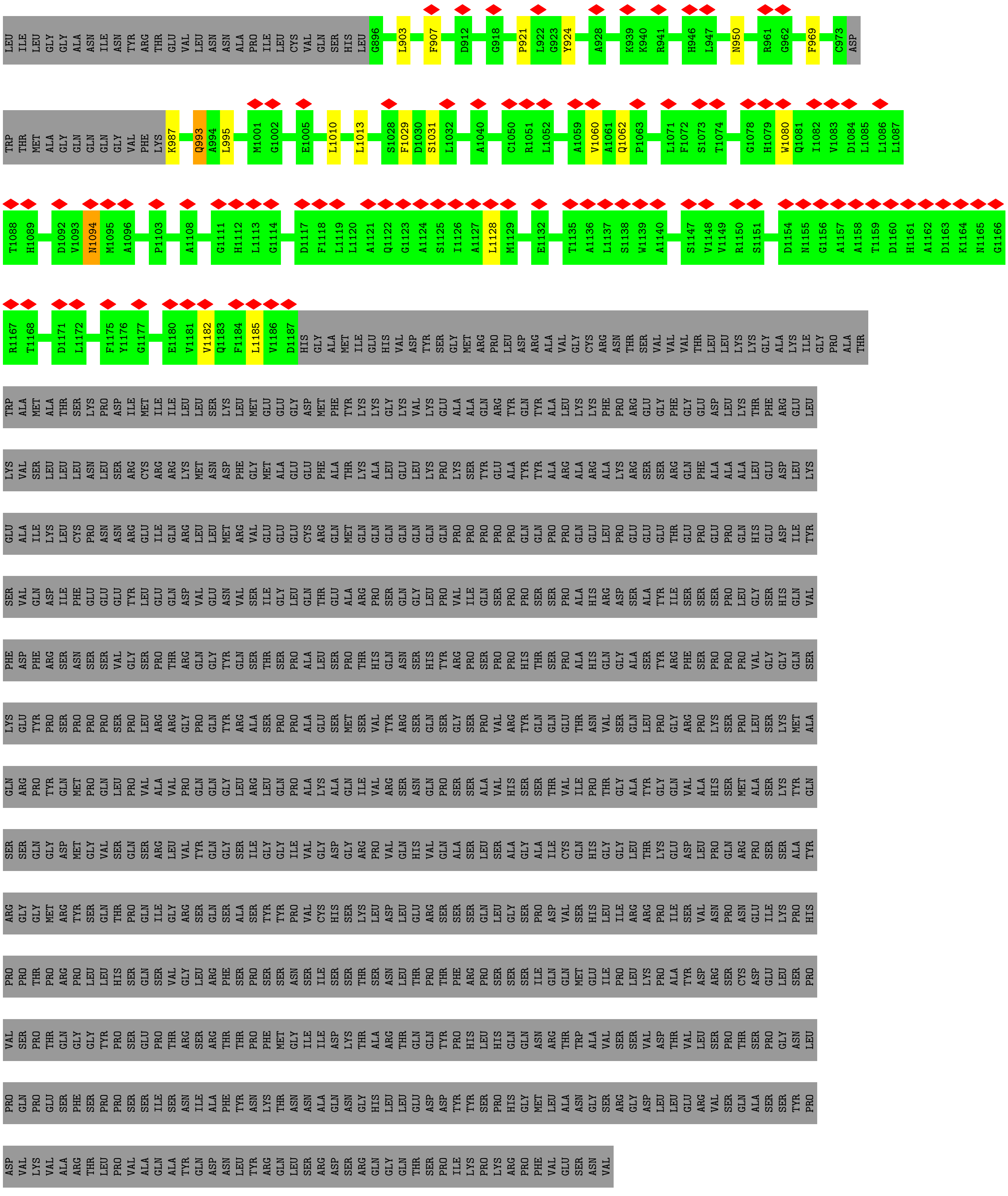
3 Residue-property plots (i)

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: Protein TANC2

Chain A:




LEU ILE LEU GLY GLY ALA ASN ILE ASN TYR ARG THR GLU VAL LEU ASN ASN ALA PRO ILE LEU CYS VAL GLN SER HIS LEU G896 L903 F907 D912 G918 P921 L922 G923 Y924 A928 K939 K940 R941 H946 L947 N950 R961 G962 F969 C973 ASP
TRP THR MET ALA GLY GLN GLN GLN GLY VAL PHE LYS K987 Q993 A994 L995 M1001 G1002 E1005 L1010 L1013 S1028 F1029 D1030 S1031 L1032 A1040 C1050 R1051 L1052 A1059 V1060 A1061 Q1062 P1063 L1071 F1072 S1073 T1074 G1078 H1079 W1080 Q1081 I1082 V1083 D1084 L1085 L1086 L1087
T1088 H1089 D1092 V1093 N1094 M1095 A1096 P1103 A1108 G1111 H1112 L1113 G1114 D1117 F1118 L1119 L1120 A1121 Q1122 G1123 A1124 S1125 I1126 A1127 L1128 M1129 E1132 T1135 A1136 L1137 S1138 W1139 A1140 S1147 V1148 V1149 R1150 S1151 D1154 N1155 G1156 A1157 A1158 T1159 D1160 H1161 A1162 D1163 K1164 N1165 G1166
R1167 T1168 D1171 L1172 F1175 Y1176 G1177 E1180 V1181 V1182 Q1183 F1184 L1185 V1186 D1187 HIS GLY ALA MET ILE GLU HIS VAL ASP TYR SER GLY MET ARG PRO LEU ASP ARG ALA VAL GLY CYS ARG ASN THR SER VAL VAL VAL THR LEU LEU LYS LYS GLY ALA LYS ILE GLY PRO ALA THR
TRP ALA MET ALA THR SER LYS PRO ASP ILE MET ILE ILE LEU LEU SER LYS LEU MET GLU GLU GLY ASP MET PHE TYR LYS LYS GLY LYS VAL LYS GLU ALA ALA GLN ARG TYR GLN TYR ALA LEU LYS LYS PHE PRO ARG GLU GLY PHE GLY GLU ASP LEU LYS THR PHE ARG GLU LEU
LYS VAL SER LEU LEU LEU ASN LEU SER ARG CYS ARG ARG LYS MET ASN ASP PHE GLY MET ALA GLU GLU PHE ALA THR LYS ALA LEU GLU LEU LYS PRO LYS SER TYR GLU ALA TYR TYR ALA ARG ALA ARG ALA LYS ARG SER SER ARG GLN PHE ALA ALA ALA LEU GLU ASP LEU LYS
GLU ALA ILE LYS LEU CYS PRO ASN ASN ARG GLU ILE GLN ARG LEU LEU MET ARG VAL GLU GLU GLU CYS ARG GLN MET GLN GLN GLN GLN GLN GLN GLN PRO PRO PRO PRO PRO GLN GLN PRO PRO GLN GLU LEU PRO GLU GLU GLU THR GLU PRO GLU PRO GLN HIS GLU ASP ILE TYR
SER VAL GLN ASP ILE PHE GLU GLU GLU TYR LEU GLU GLN ASP VAL GLU ASN VAL SER ILE GLY LEU GLN THR GLU ALA ARG PRO SER GLN GLY LEU PRO VAL ILE GLN SER PRO PRO SER SER PRO ALA HIS ARG ASP SER ALA TYR ILE SER SER PRO LEU GLY SER HIS GLN VAL
PHE ASP PHE ARG SER ASN SER SER VAL GLY SER PRO THR ARG GLN GLY TYR GLN SER THR SER PRO ALA LEU SER PRO THR HIS GLN ASN SER HIS TYR ARG PRO SER PRO PRO HIS THR SER PRO ALA HIS GLN GLY ALA SER TYR ARG PHE SER PRO PRO VAL GLY GLN SER
LYS GLU TYR PRO SER PRO PRO PRO SER PRO LEU ARG ARG GLY PRO GLN TYR ARG ALA SER PRO PRO ALA GLU SER MET SER VAL TYR ARG SER GLN SER GLY SER PRO VAL ARG TYR GLN GLN GLU THR ASN VAL SER GLN LEU PRO GLY ARG PRO LYS SER PRO LEU SER LYS MET ALA
GLN ARG PRO TYR GLN MET PRO GLN LEU PRO VAL ALA VAL PRO GLN GLN GLY LEU ARG LEU GLN PRO ALA LYS ALA GLN ILE VAL ARG SER ASN GLN PRO SER SER ALA VAL HIS SER SER THR VAL ILE PRO THR GLY ALA TYR GLY GLN VAL ALA HIS SER MET ALA SER LYS TYR GLN
SER SER GLN GLY ASP MET GLY VAL SER GLN SER ARG LEU VAL TYR GLN GLY SER ILE GLY GLY ILE VAL GLY ASP GLY ARG PRO VAL GLN HIS VAL GLN ALA SER LEU SER ALA GLY ALA ILE CYS GLN HIS GLY GLY LEU THR LYS GLU ASP LEU PRO GLN ARG PRO SER SER ALA TYR
ARG GLY GLY MET ARG TYR SER GLN THR PRO GLN ILE GLY ARG SER GLN SER ALA SER TYR TYR PRO VAL CYS HIS SER LYS LEU ASP LEU GLU ARG SER SER SER GLN LEU GLY SER PRO ASP VAL SER HIS LEU ILE ARG ARG PRO ILE SER VAL ASN PRO ASN GLU ILE LYS PRO HIS
PRO PRO THR PRO ARG PRO LEU LEU HIS SER GLN SER VAL GLY LEU ARG PHE SER PRO SER SER ASN SER ILE SER SER THR SER ASN LEU THR PRO THR PHE ARG PRO SER SER SER ILE GLN GLN MET GLU ILE PRO LEU LYS PRO ALA TYR ASP ARG SER CYS ASP GLU LEU SER PRO
VAL SER PRO THR GLN GLY GLY TYR PRO SER GLU PRO THR ARG SER ARG THR THR PRO PHE MET GLY ILE ILE ASP LYS THR ALA ARG THR GLN GLN TYR PRO HIS LEU HIS GLN GLN ASN ARG THR TRP ALA VAL SER SER VAL ASP THR VAL LEU SER PRO THR SER PRO GLY ASN LEU
PRO GLN PRO GLU SER PHE SER PRO PRO SER SER ILE SER ASN ILE ALA PHE TYR ASN LYS THR ASN ASN ALA GLN ASN GLY HIS LEU LEU GLU ASP ASP TYR TYR SER PRO HIS GLY MET LEU ALA ASN GLY SER ARG GLY ASP LEU LEU GLU ARG VAL SER GLN ALA SER SER TYR PRO
ASP VAL LYS VAL ALA ARG THR LEU PRO VAL ALA GLN ALA TYR GLN ASP ASN LEU TYR ARG GLN LEU SER ARG ASP SER ARG GLN GLY GLN THR SER PRO ILE LYS PRO LYS ARG PRO PHE VAL GLU SER ASN VAL

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, POINT	Depositor
Number of particles used	43365, 43365	Depositor
Resolution determination method	FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION, PHASE FLIPPING AND AMPLITUDE CORRECTION, PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI MORGAGNI	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.367	Depositor
Minimum map value	-1.027	Depositor
Average map value	-0.000	Depositor

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Property	Value	Source
Map value standard deviation	0.025	Depositor
Recommended contour level	0.116	Depositor
Map size (Å)	251.4, 251.4, 251.4	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.838, 0.838, 0.838	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	0.90	3/5076 (0.1%)	1.48	24/6864 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	505	ARG	C-O	-12.66	1.08	1.24
1	A	505	ARG	C-N	-8.42	1.22	1.33
1	A	907	PHE	CA-CB	5.17	1.62	1.53

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	505	ARG	CA-C-N	9.25	139.21	121.54
1	A	505	ARG	C-N-CA	9.25	139.21	121.54
1	A	505	ARG	O-C-N	-6.24	114.30	122.59
1	A	561	PHE	CA-CB-CG	6.00	119.80	113.80
1	A	594	ARG	NE-CZ-NH2	5.92	124.53	119.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	344	ARG	Sidechain
1	A	656	TYR	Sidechain

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	4989	5044	5039	15	0
All	All	4989	5044	5039	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 2.

The worst 5 of 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:A:468:VAL:HG13	1:A:558:ILE:HG23	1.67	0.74
1:A:468:VAL:HG13	1:A:558:ILE:CG2	2.33	0.59
1:A:461:ASP:H	1:A:761:MET:HE1	1.67	0.58
1:A:1128:LEU:HD12	1:A:1128:LEU:H	1.69	0.58
1:A:993:GLN:NE2	1:A:1031:SER:H	2.02	0.57

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	630/1994 (32%)	501 (80%)	117 (19%)	12 (2%)	6 33

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	323	ILE
1	A	483	PRO
1	A	618	ILE
1	A	343	GLY
1	A	506	SER

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	543/1730 (31%)	507 (93%)	36 (7%)	15 42

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	969	PHE
1	A	1185	LEU
1	A	987	LYS
1	A	1062	GLN
1	A	502	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	993	GLN
1	A	1056	GLN
1	A	1161	HIS
1	A	1155	ASN
1	A	627	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 (i)

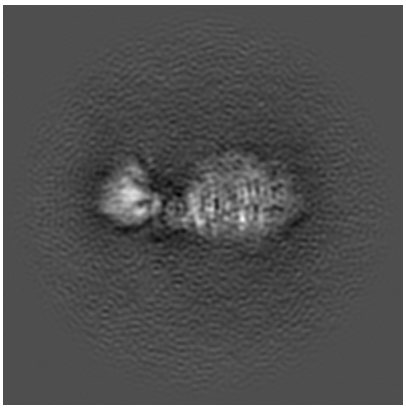
This section contains visualisations of the EMDB entry EMD-67963. These allow visual inspection of the internal detail of the map and identification of artifacts.

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.

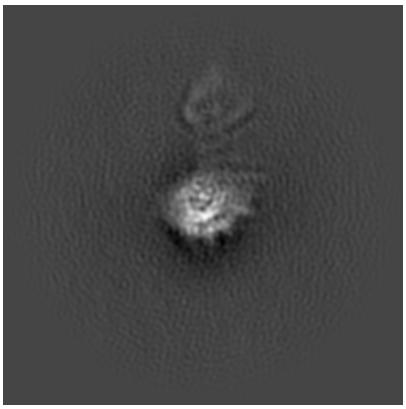
6.1 Orthogonal projections (i)

6.1.1 Primary map

X

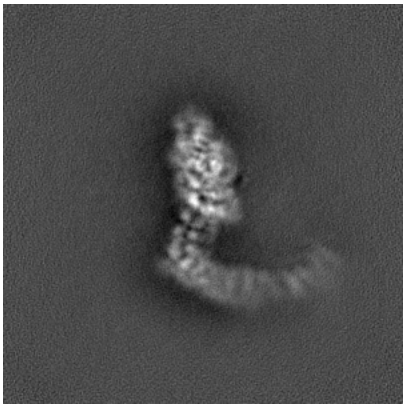


Y



Z

6.1.2 Raw map



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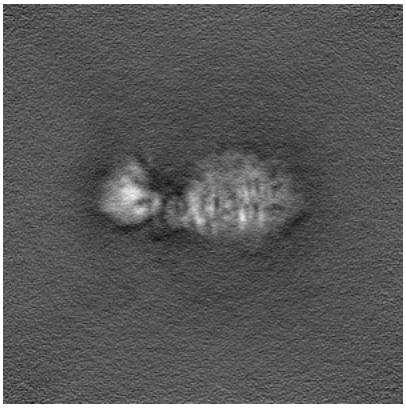

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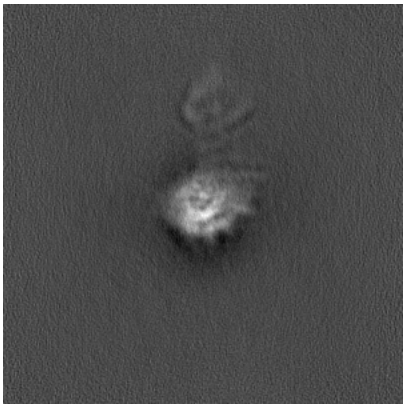
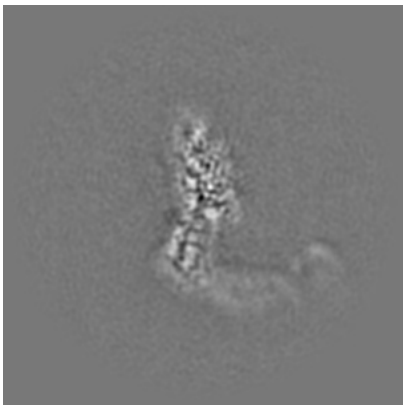


Z

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

6.2 Central slices (i)

6.2.1 Primary map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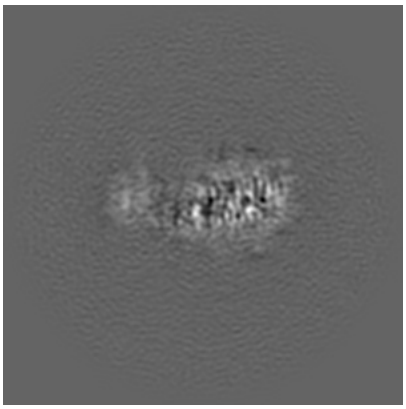
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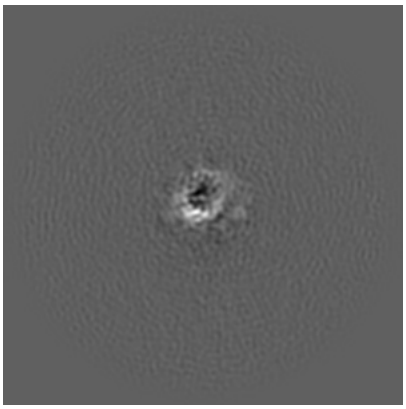
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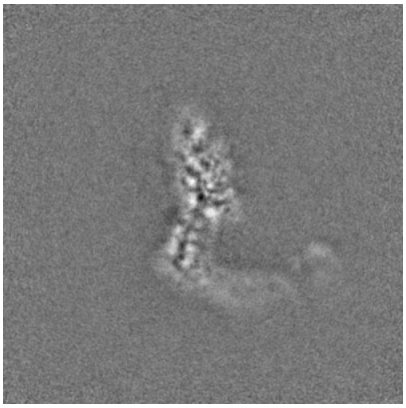
6.2.2 Raw map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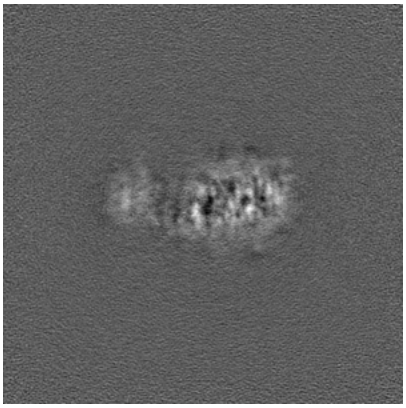
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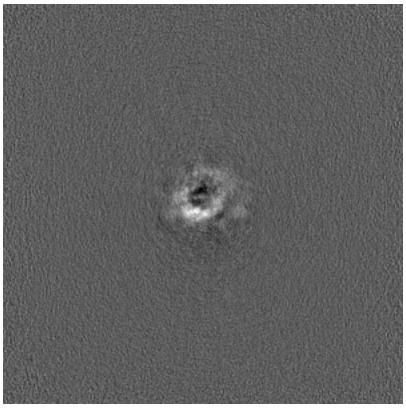
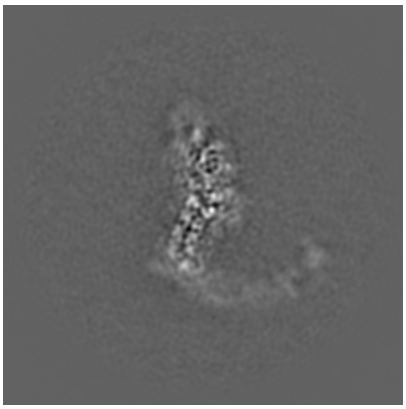

Z Index: 150

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

6.3 Largest variance slices (i)

6.3.1 Primary map



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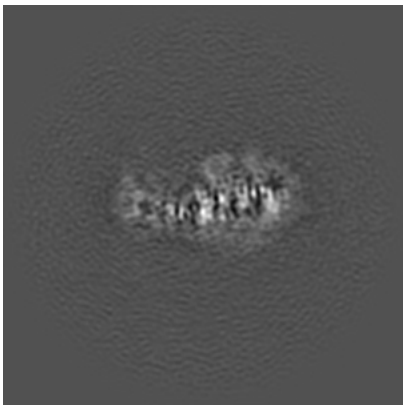

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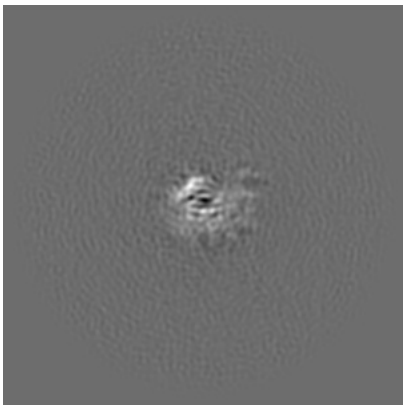
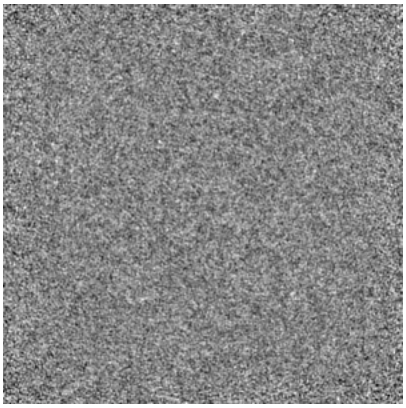
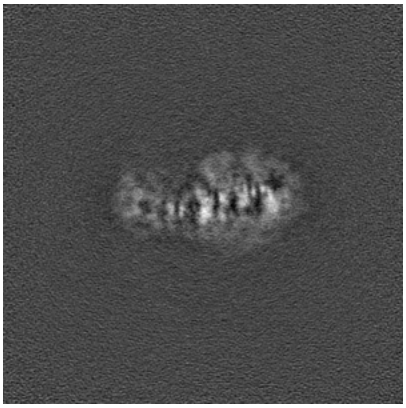


Z Index: 179

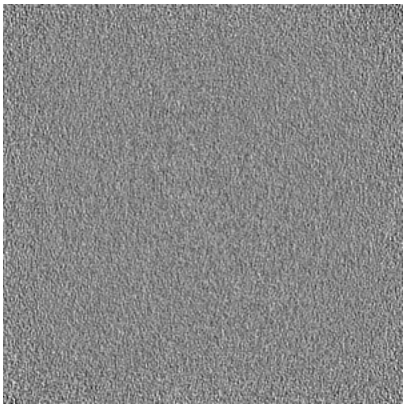
6.3.2 Raw map



X Index: 0



Y Index: 144

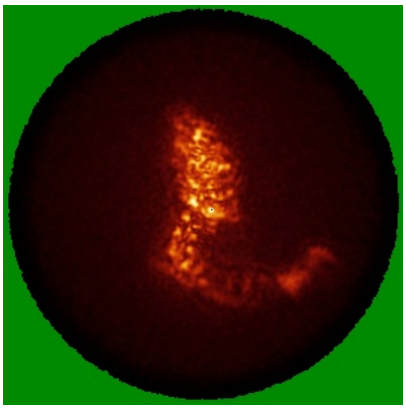


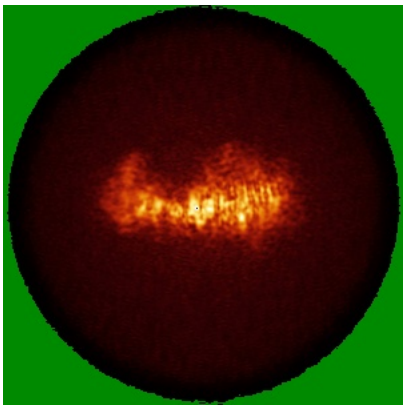
Z Index: 0

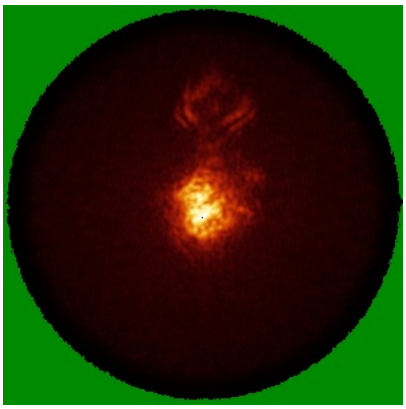
The images above show the largest variance slices of the map in three orthogonal directions.

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

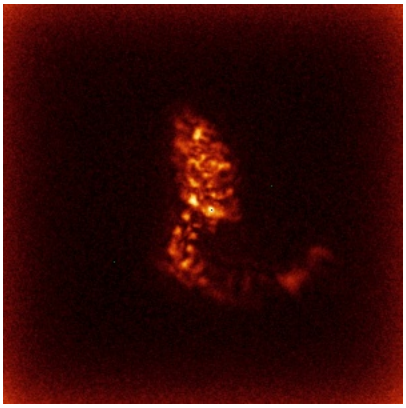
6.4.1 Primary map

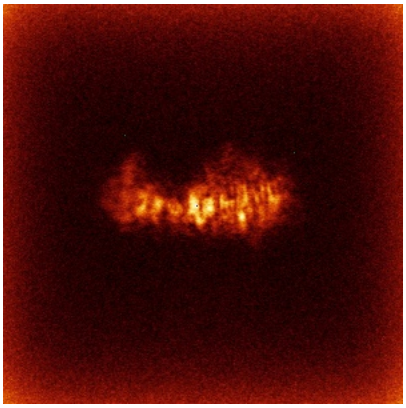

X

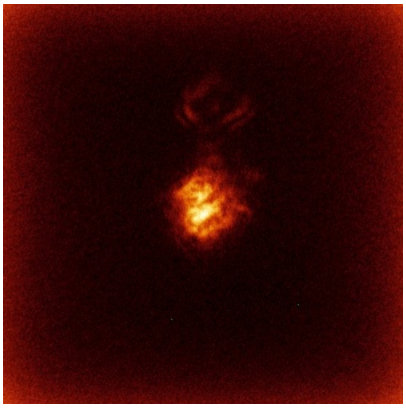

Y


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 0.116. 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.

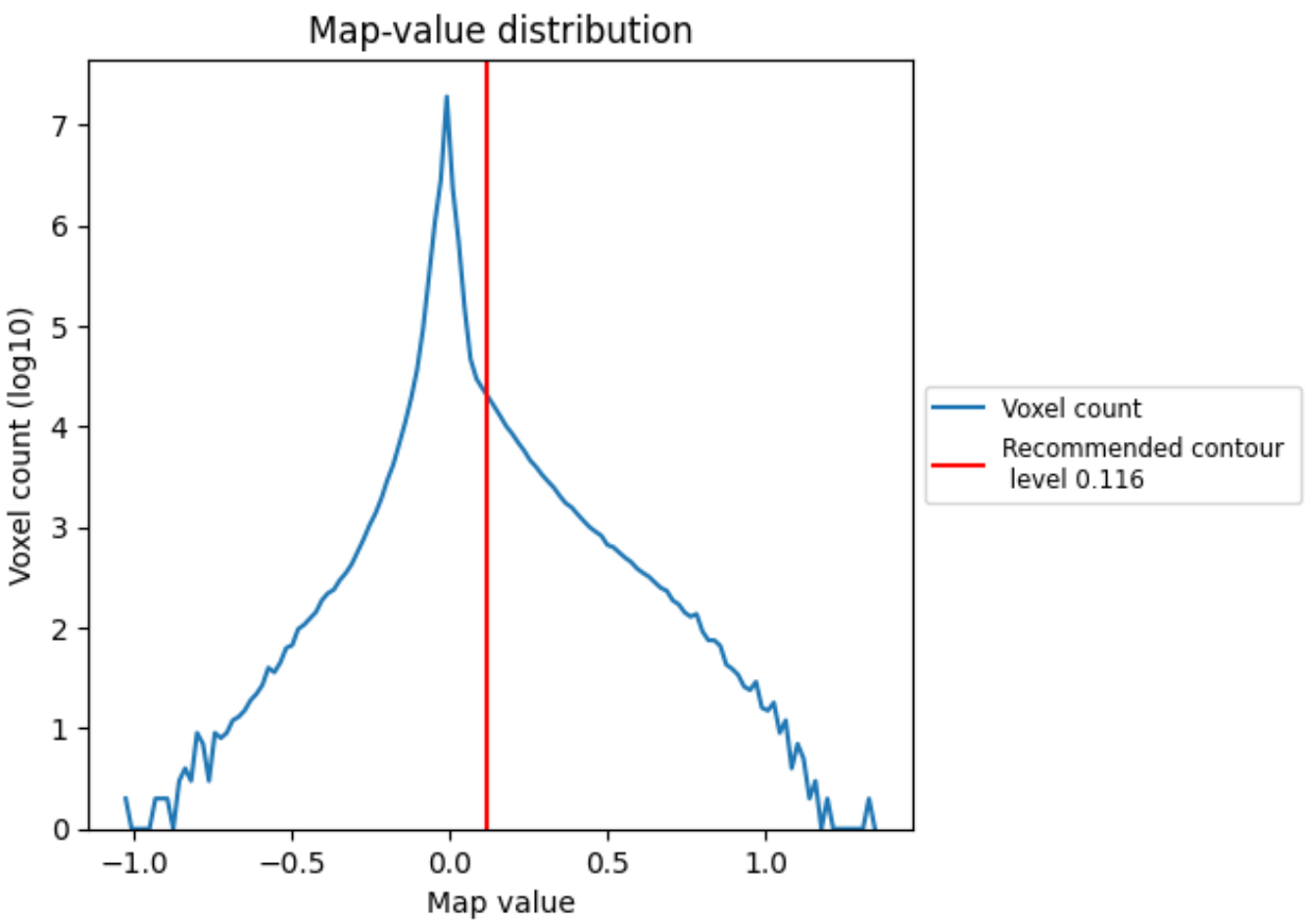
6.6 Mask visualisation (i)

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

7 Map analysis (i)

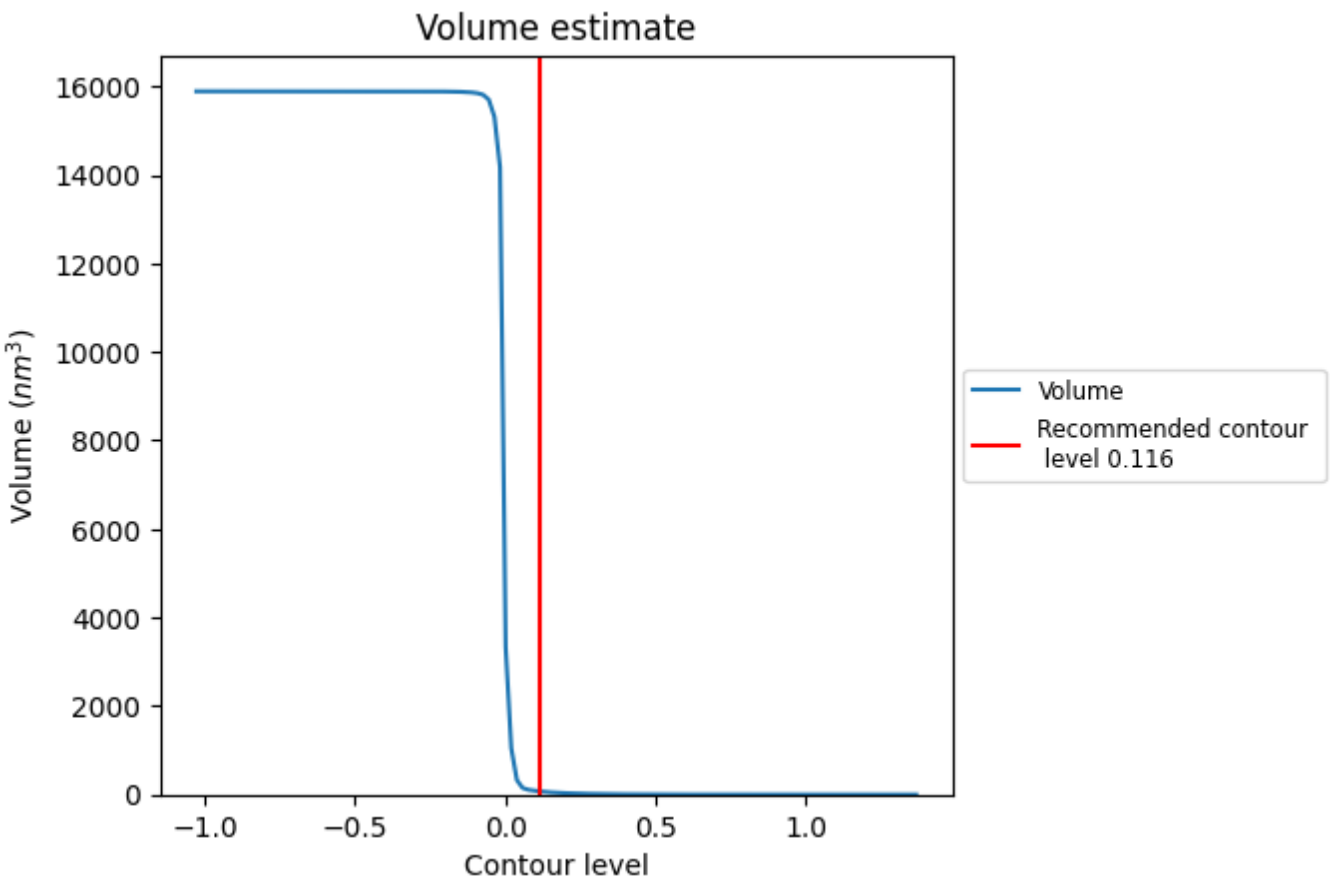
This section contains the results of statistical analysis of the map.

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.

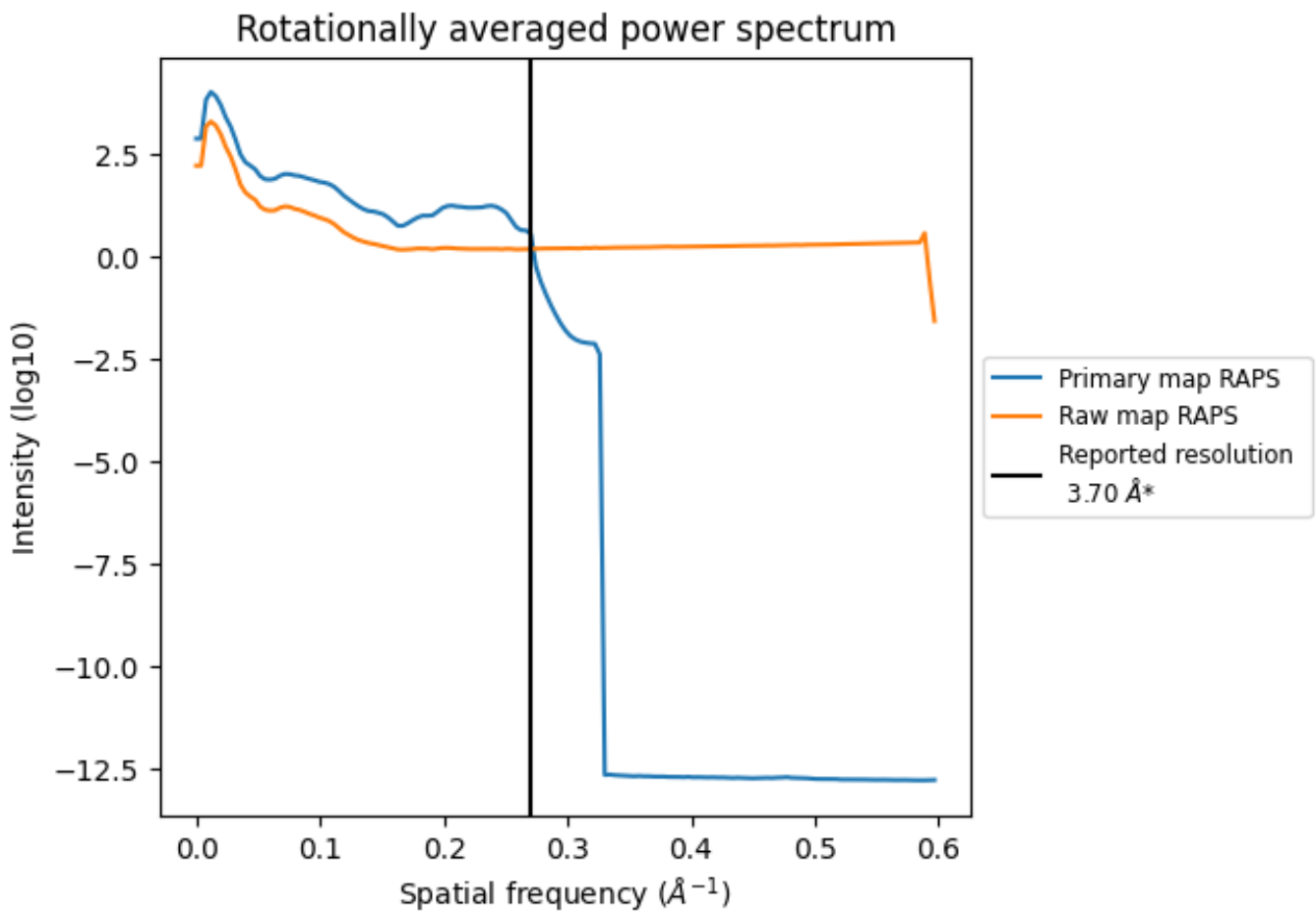
7.2 Volume estimate (i)



The volume at the recommended contour level is 71 nm^3; this corresponds to an approximate mass of 65 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)

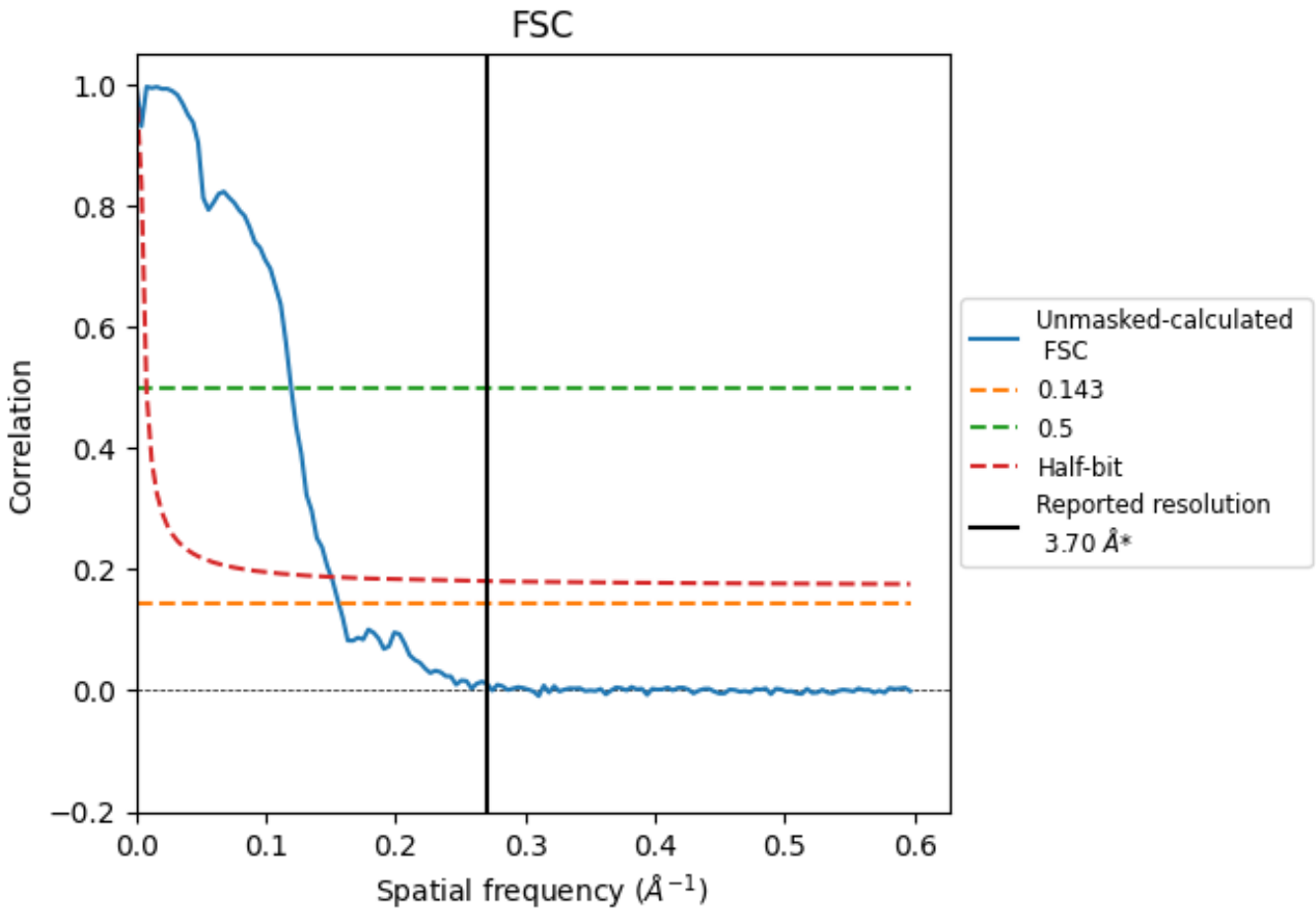


*Reported resolution corresponds to spatial frequency of 0.270 Å^{-1}

8 Fourier-Shell correlation (i)

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 (i)



*Reported resolution corresponds to spatial frequency of 0.270 Å^{-1}

8.2 Resolution estimates (i)

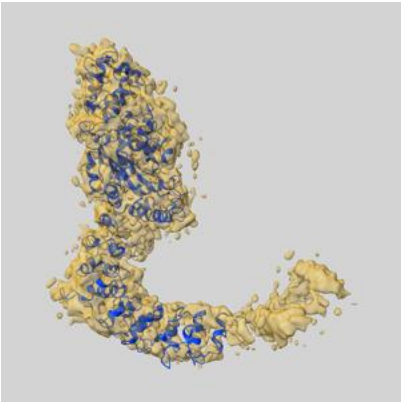
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.40	8.38	6.65

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

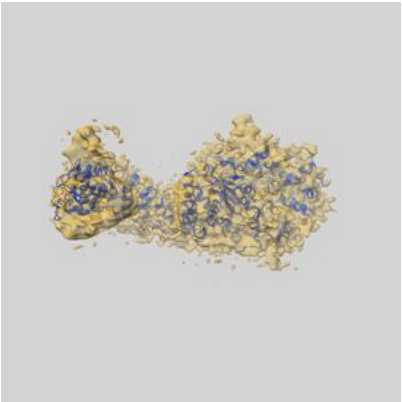
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-67963 and PDB model 21SI. Per-residue inclusion information can be found in section 3 on page 4.

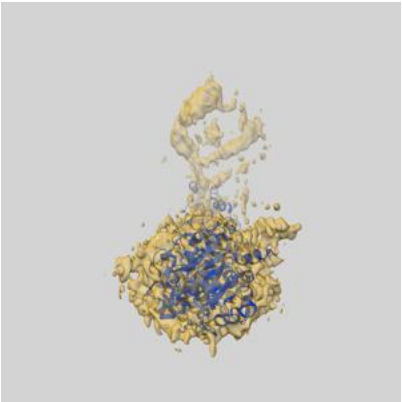
9.1 Map-model overlay (i)



X



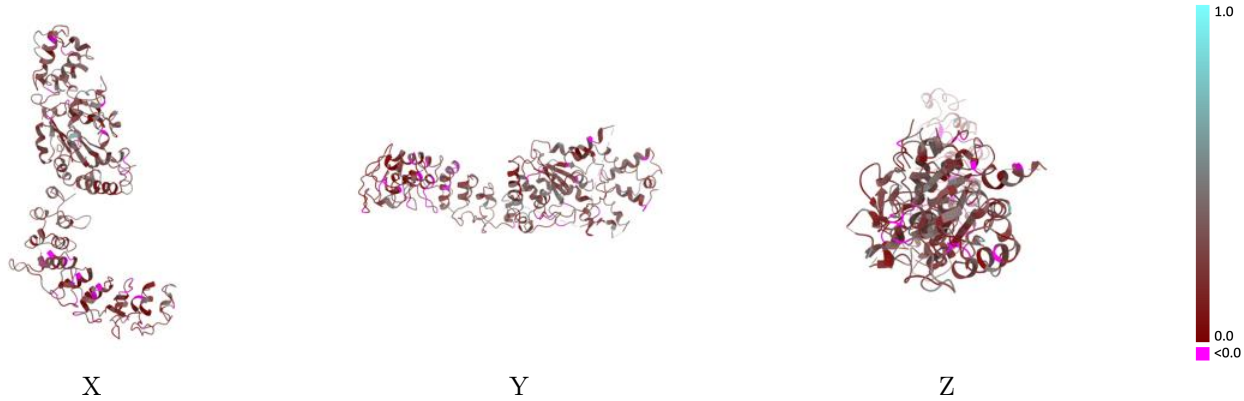
Y



Z

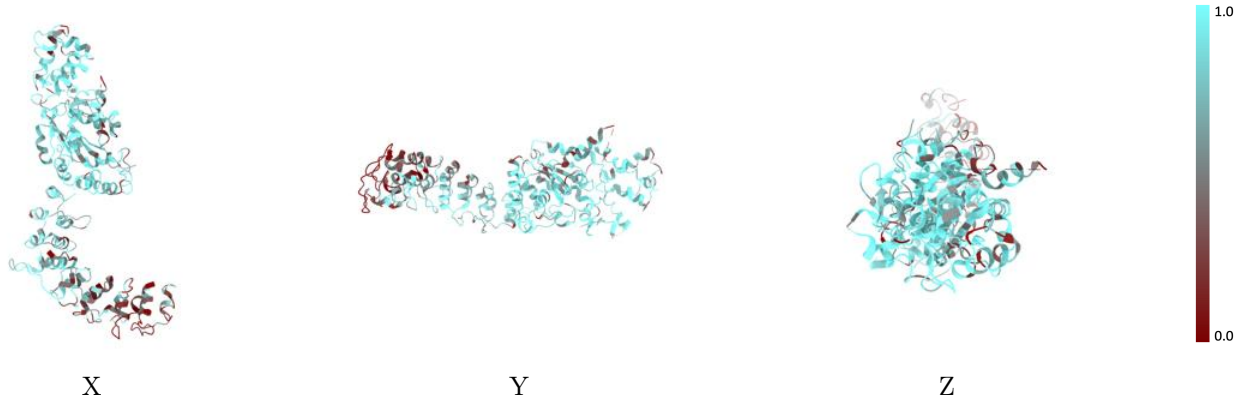
The images above show the 3D surface view of the map at the recommended contour level 0.116 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



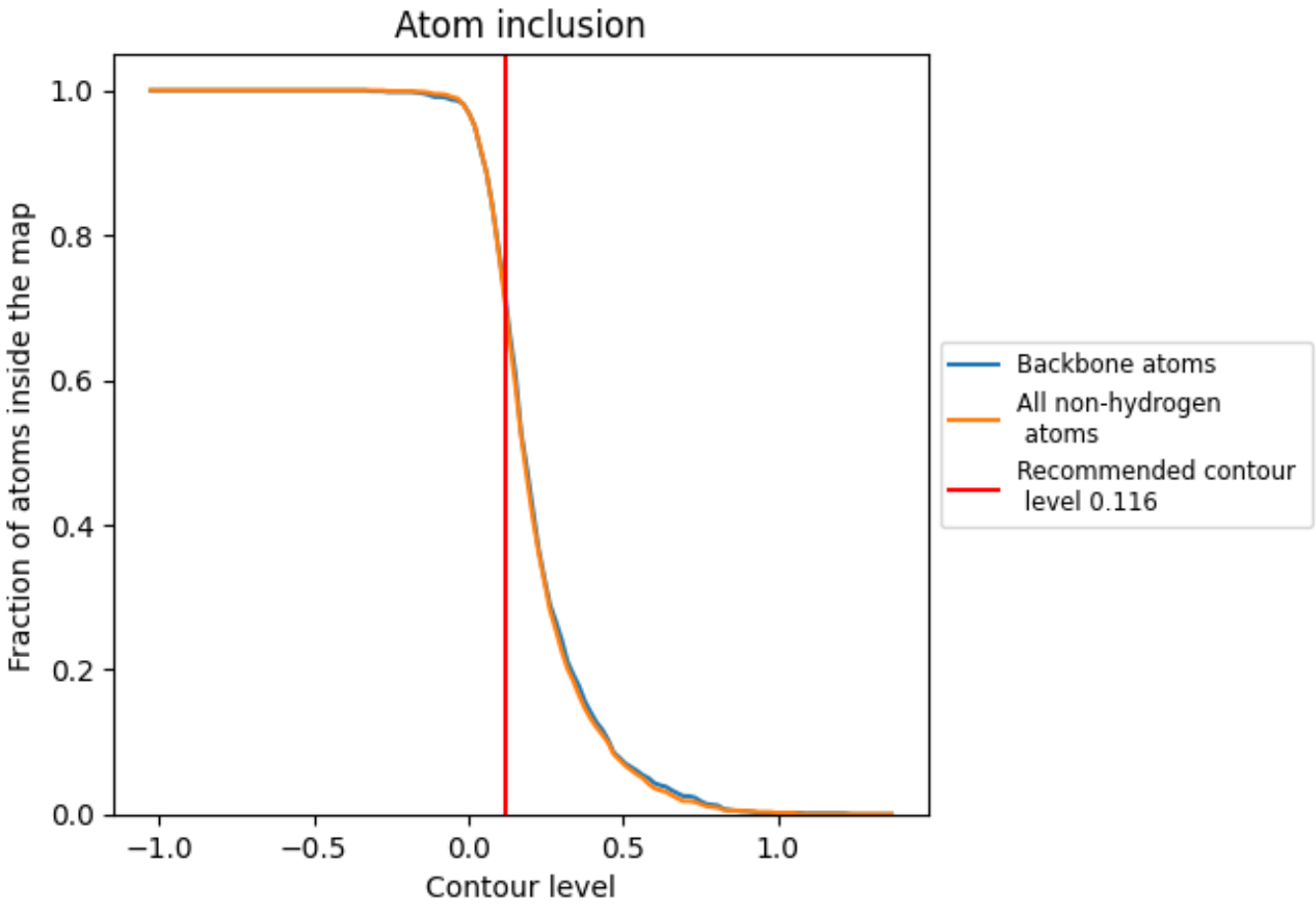
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.116).

9.4 Atom inclusion (i)



At the recommended contour level, 72% of all backbone atoms, 71% 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 (0.116) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7130	0.2550
A	0.7090	0.2550