



wwPDB EM Validation Summary Report ⓘ

Mar 6, 2026 – 04:07 PM UTC

PDB ID : 7KTV / pdb_00007ktv
EMDB ID : EMD-23031
Title : Cryogenic electron microscopy model of full-length human metavinculin H1' kinked conformation
Authors : Izard, T.; Rangarajan, E.S.
Deposited on : 2020-11-24
Resolution : 4.50 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.dev132
MolProbity : 4-5-2 with Phenix2.0
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) : 2.49

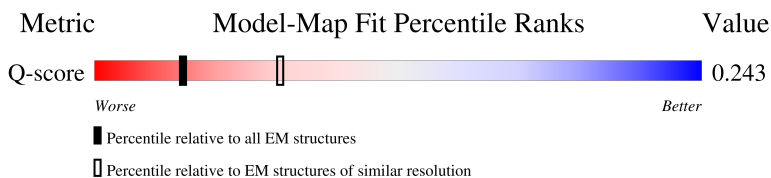
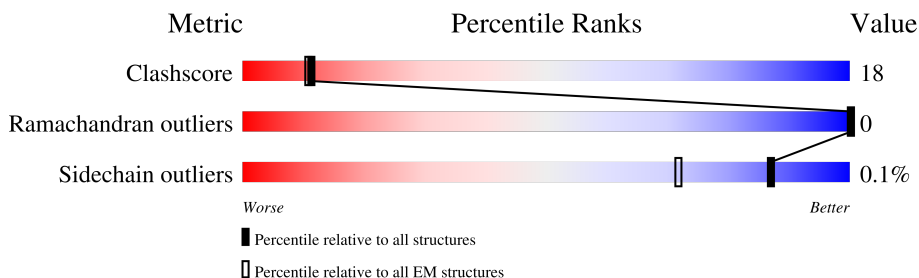
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.50 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	2937 (4.00 - 5.00)

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 $\leq 5\%$. 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	A	1142	 51% 36% 13%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 7577 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 metavinculin.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	995	7577	4671	1373	1490	43	0	0

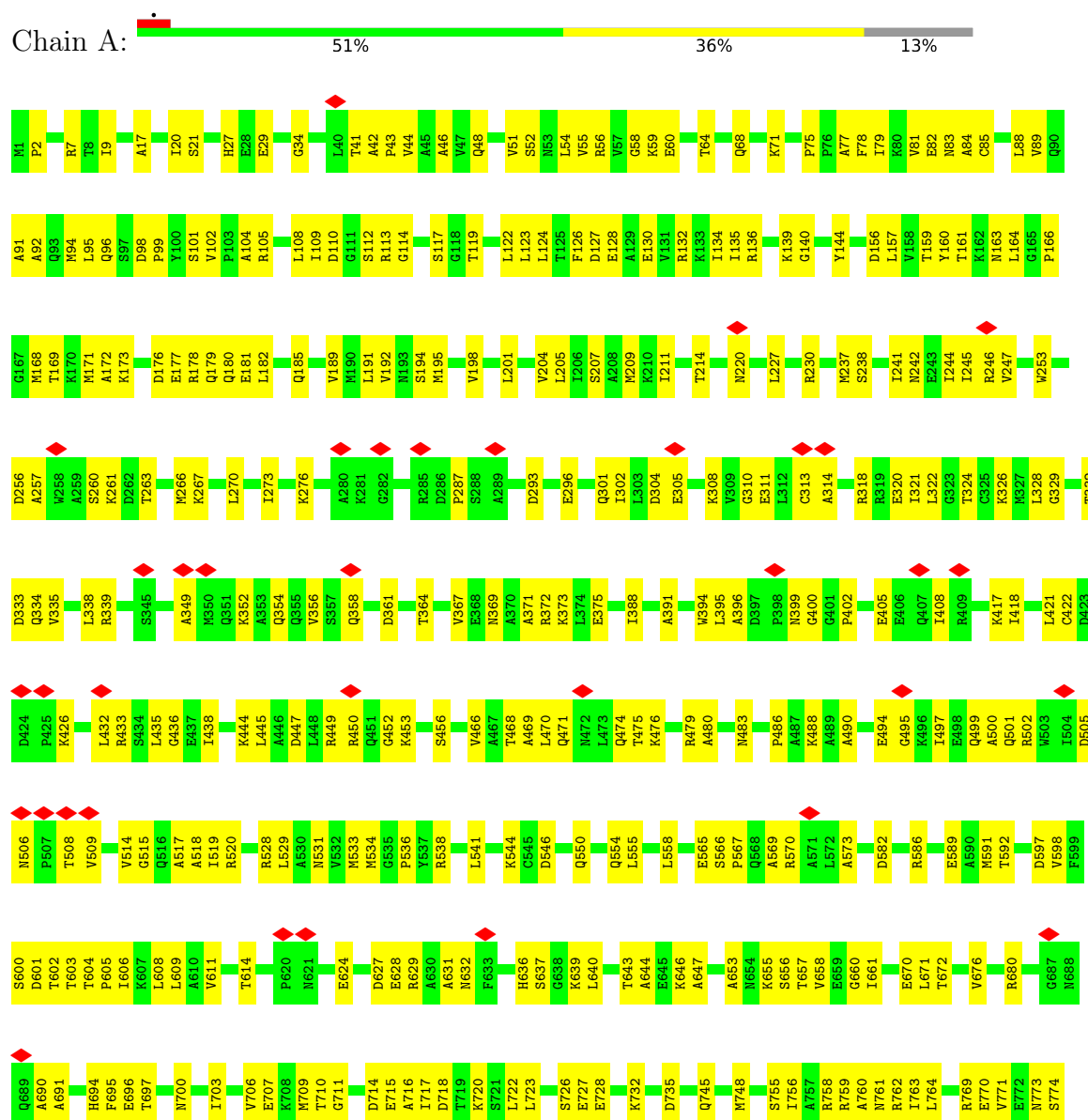
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1135	HIS	-	expression tag	UNP P18206
A	1136	HIS	-	expression tag	UNP P18206
A	1137	HIS	-	expression tag	UNP P18206
A	1138	HIS	-	expression tag	UNP P18206
A	1139	HIS	-	expression tag	UNP P18206
A	1140	HIS	-	expression tag	UNP P18206
A	1141	HIS	-	expression tag	UNP P18206
A	1142	HIS	-	expression tag	UNP P18206

3 Residue-property plots

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: metavinculin



																				M998	S1080	D1081																					M998	G1Y	VAL																					PRO	G1Y	P777																															
																				S1002	R1003	L1004	V1005																					S1002	VAL	VAL																					GLY	GLY	R780																														
																				M1094	A1095																					K1012	ALA	ALA																					PRO	PRO	V783																																
																				L1098	M1099	Q1100																					R1013	ALA	ALA																					ARG	ARG	S787																															
																				E1104	T1105																					L1015	ALA	ALA																					PRO	PRO	L790																																
																				V1106	R1107	E1108																					Q1017	GLY	PHE																					GLY	GLY	S791																															
																																								K1020	PRO	VAL																					GLY	LYS	G812																																		
																																								A1023	PRO	PRO																					ASP	ASP	S816																																		
																																								D1027	ASP	ASP																					GLY	GLY	F817																																		
																																								E1028	MET	MET																					PHE	PHE	I818																																		
																																								V1029	GLU	GLU																					PRO	PRO	D819																																		
																																								T1030	ASP	ASP																					GLY	GLN	S820																																		
																																								R1031	ASP	ASP																					GLN	GLN	R823																																		
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																																								T1041	LEU	LEU																					VAL	VAL	E833																																		
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																																								K1043	VAL	LEU																					GLN	GLN	Q836																																		
																																								R1044	MET	MET																					MET	GLN	P837																																		
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																																								R1046	SER	SER																					MET	MET	E839																																		
																																								T1047	ASN	ASN																					MET	MET	PRO																																		
																																								N1048	GLN	GLN																					ALA	ALA	ASP																																		
																																								L1049	P961	P961																					ALA	ALA	ASP																																		
																																								L1050	Q964	Q964																					ARG	ALA	PHE																																		
																																								Q1051	P965	P965																					GLN	GLN	PRO																																		
																																								V1052	I966	I966																					LEU	LEU	PRO																																		
																																								C1053	L967	L967																					HIS	HIS	PRO																																		
																																								E1054																					ASP	ASP	PRO																																				
																																								R1055																					GLY	GLY	ASP																																				
																																								I1056	A970	A970																					ALA	ALA	LEU																																		
																																								I1059	Q971	Q971																					ARG	GLY	GLU																																		
																																																												LYS	LYS	GLN																																					
																																								L1063	L973	L973																					TRP	TRP	LEU																																		
																																								K1064	H974	H974																					SER	SER	ARG																																		
																																																												LEU	LEU	LEU																																					
																																								S1067	E976	E976																					LYS	LYS	THR																																		
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																																								T1072	K979	K979																					ILE	ILE	LEU																																		
																																								M1073	N980	N980																					PRO	PRO	ALA																																		
																																								L1074	S981	S981																					ALA	ALA	PRO																																		
																																								G1075	S982	S982																					GLY	GLY	LYS																																		
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																																								I1079	R993	R993																					GLY	GLY	PRO																																		
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	413507	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 ($e^-/\text{\AA}^2$)	67.92	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	1400	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.715	Depositor
Minimum map value	-0.396	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.031	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	211.2, 211.2, 211.2	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.825, 0.825, 0.825	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	0.29	0/7654	0.60	0/10325

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	A	7577	0	7762	276	0
All	All	7577	0	7762	276	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 18.

The worst 5 of 276 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:113:ARG:NH2	1:A:1073:MET:SD	2.65	0.70
1:A:75:PRO:HA	1:A:78:PHE:HB3	1.74	0.69
1:A:998:MET:HE3	1:A:1099:MET:HB2	1.76	0.68
1:A:99:PRO:O	1:A:105:ARG:NH2	2.29	0.65
1:A:399:ASN:HD22	1:A:405:GLU:HG2	1.61	0.64

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	991/1142 (87%)	927 (94%)	64 (6%)	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	812/938 (87%)	811 (100%)	1 (0%)	88	88

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	328	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	662	GLN
1	A	654	ASN
1	A	474	GLN
1	A	632	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	399	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-23031. These allow visual inspection of the internal detail of the map and identification of artifacts.

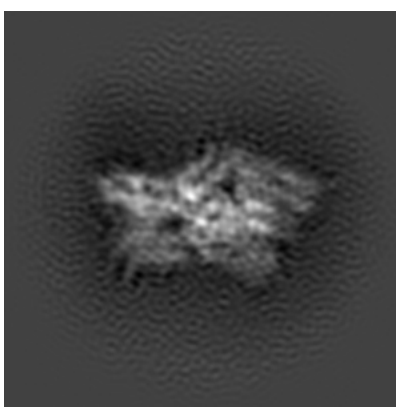
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

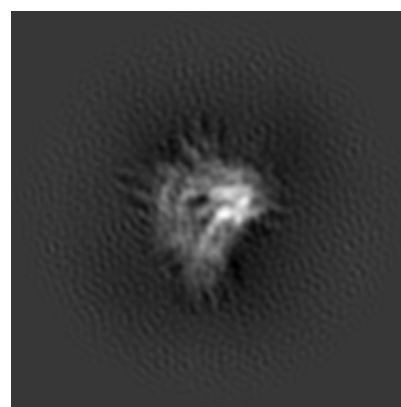
6.1.1 Primary map



X



Y

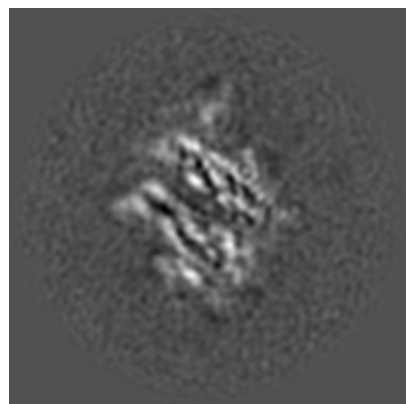


Z

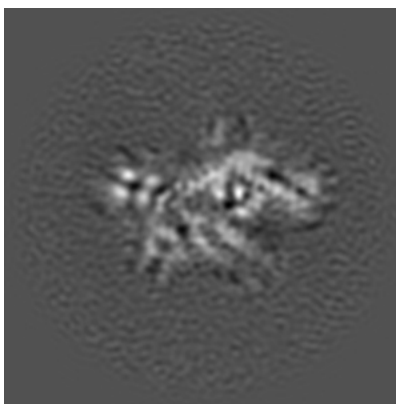
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

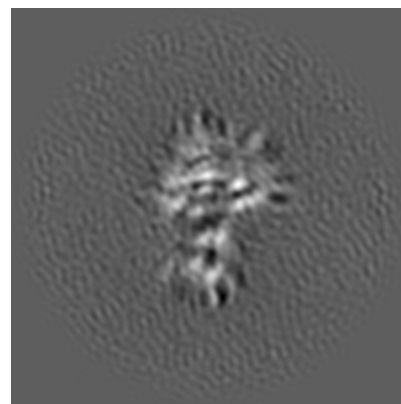
6.2.1 Primary map



X Index: 128



Y Index: 128

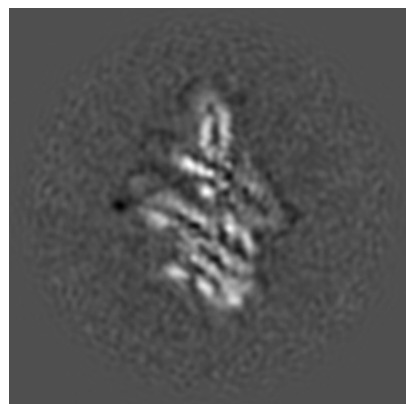


Z Index: 128

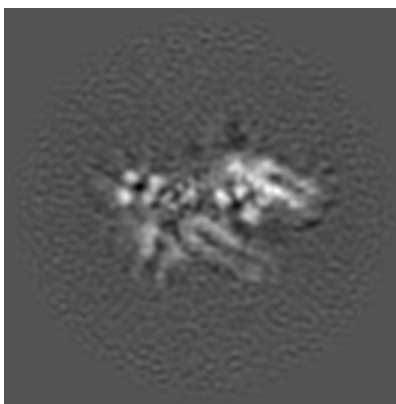
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

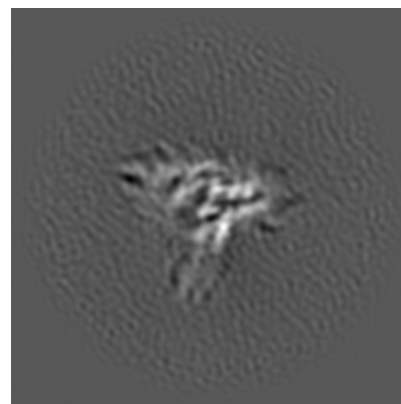
6.3.1 Primary map



X Index: 136



Y Index: 125

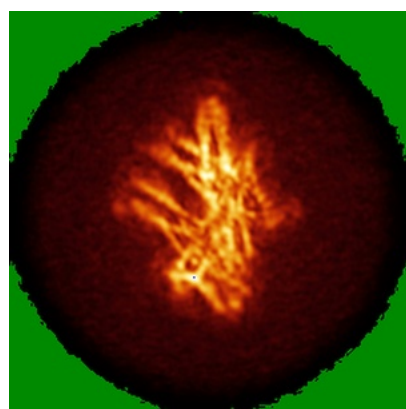


Z Index: 155

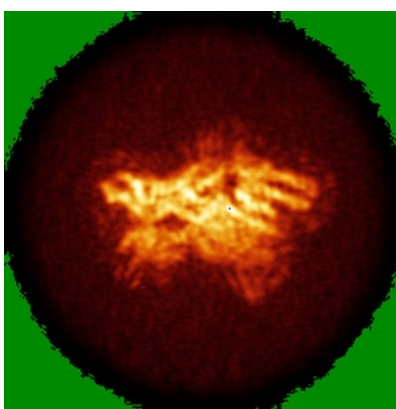
The images above show the largest variance slices of the map in three orthogonal directions.

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

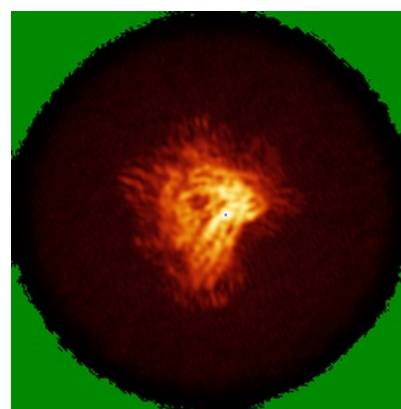
6.4.1 Primary map



X



Y



Z

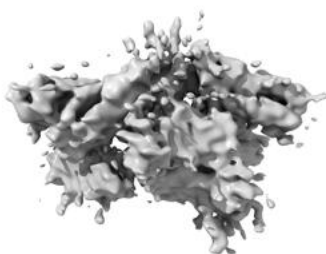
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

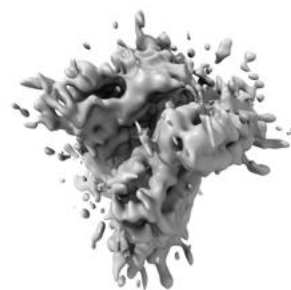
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.12. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

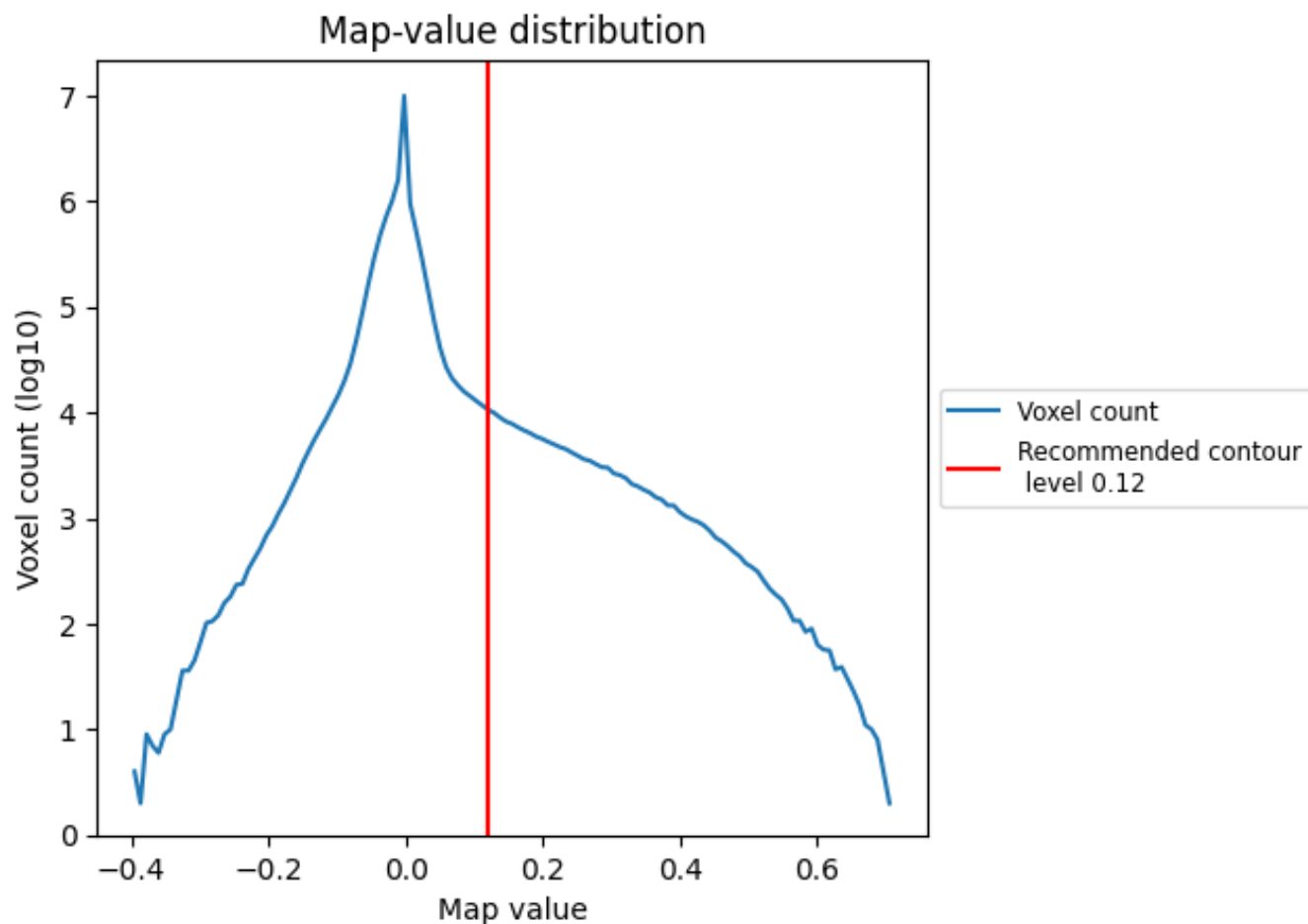
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

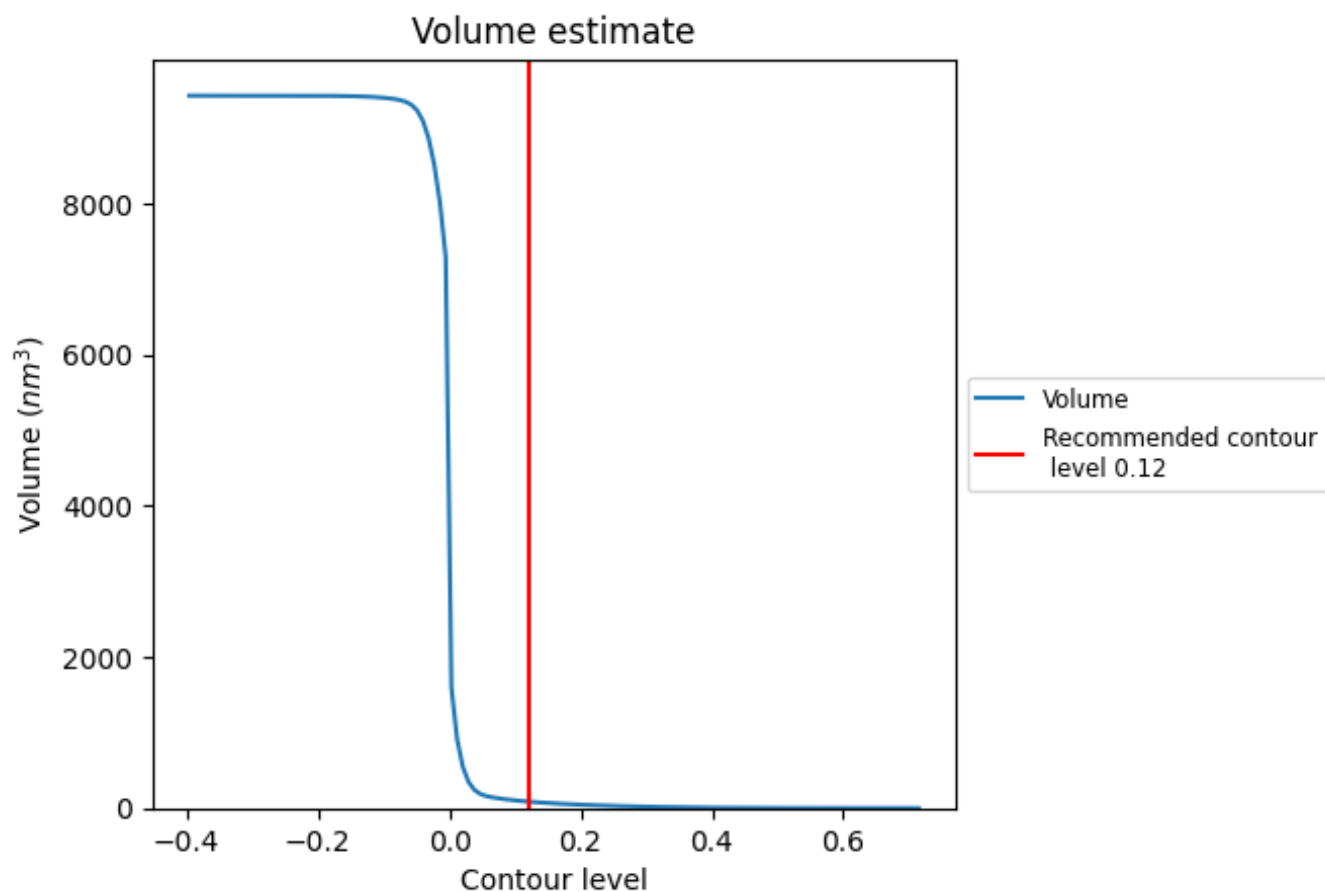
This section contains the results of statistical analysis of the map.

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.

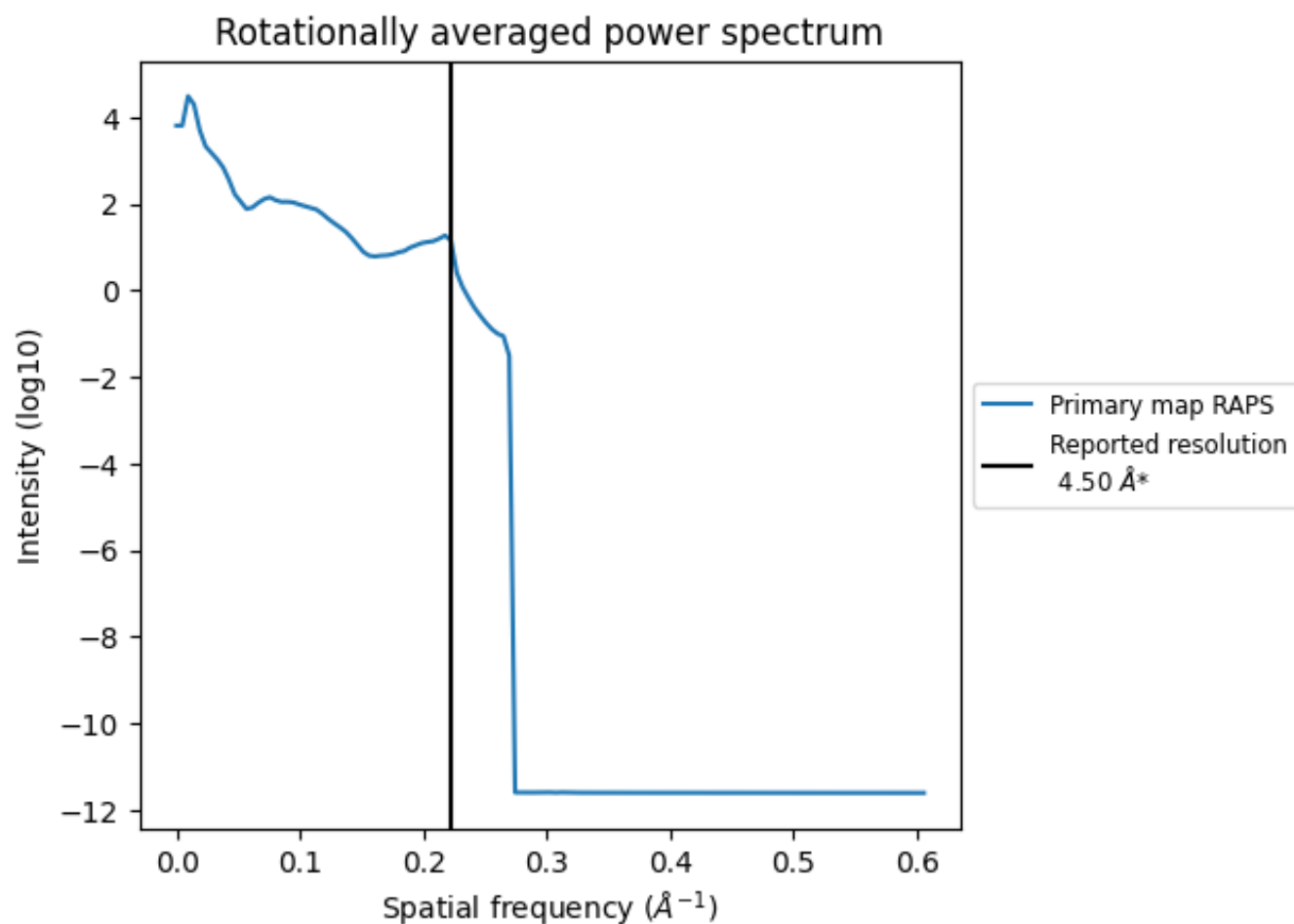
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 87 nm³; this corresponds to an approximate mass of 78 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 $0.222 \text{ \AA}^{-1}$

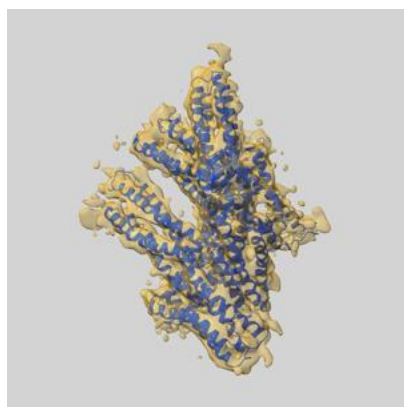
8 Fourier-Shell correlation

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

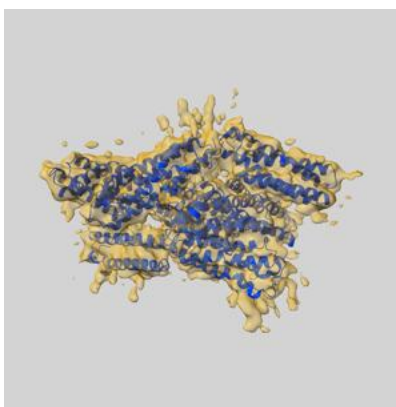
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-23031 and PDB model 7KTV. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

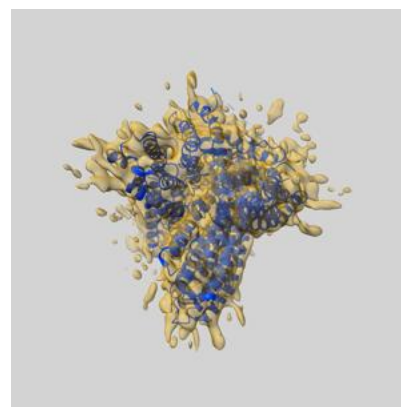
9.1 Map-model overlay [i](#)



X



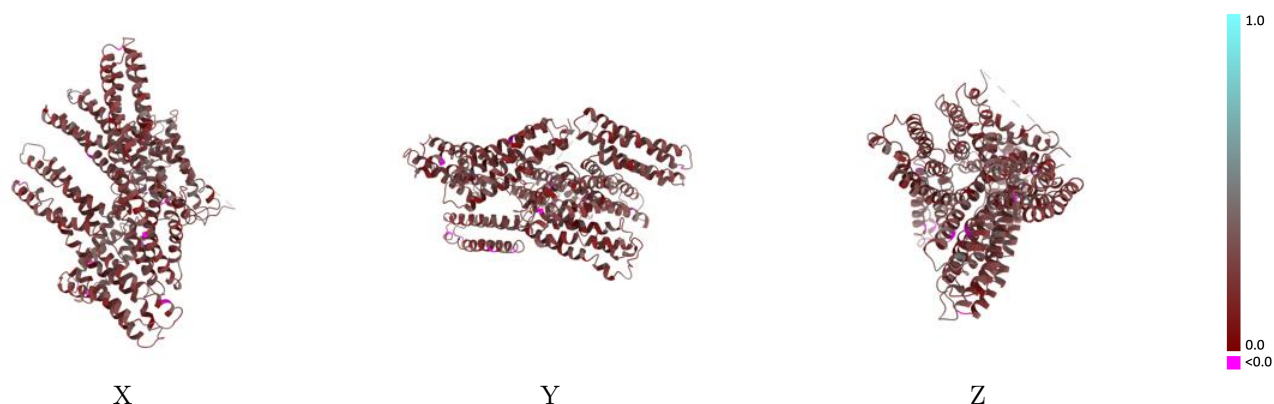
Y



Z

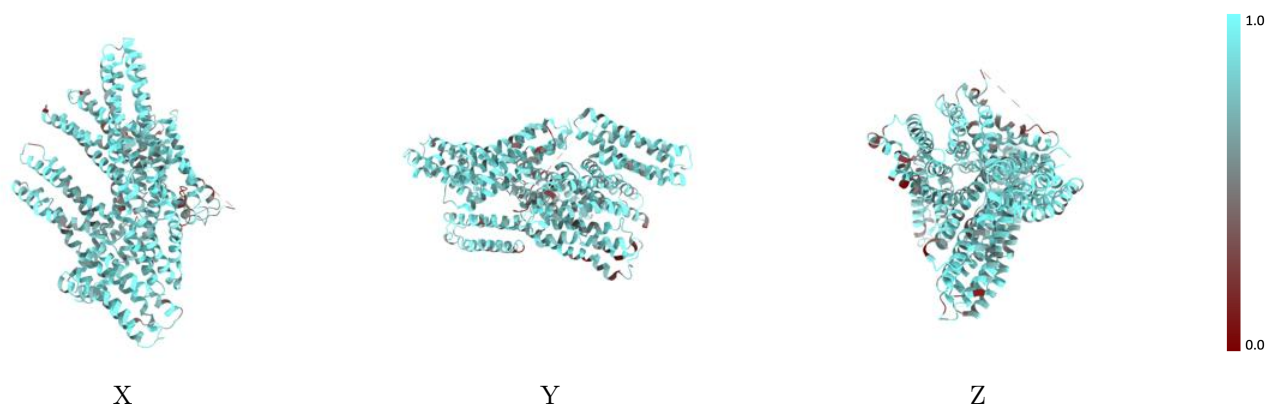
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



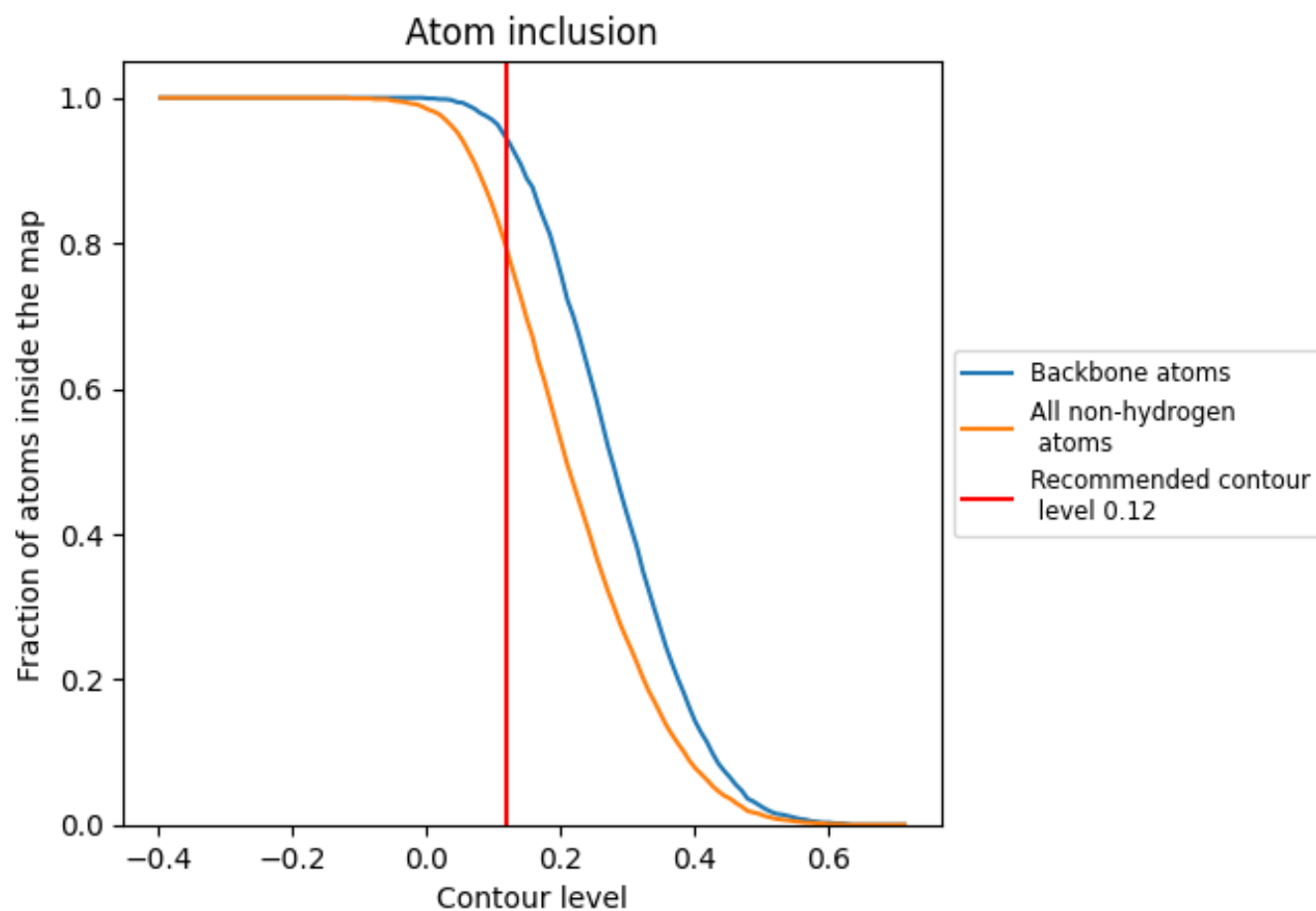
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.12).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 80% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7950	0.2430
A	0.7950	0.2430

