



wwPDB EM Validation Summary Report ⓘ

Mar 10, 2026 – 11:20 AM UTC

PDB ID : 7PQQ / pdb_00007pqq
EMDB ID : EMD-13596
Title : Structure of thermostabilised human NTCP in complex with Megabody 91
Authors : Goutam, K.; Reyes, N.
Deposited on : 2021-09-18
Resolution : 3.30 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

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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

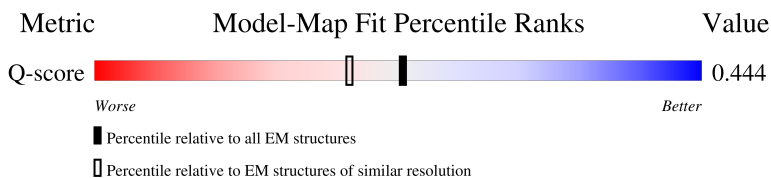
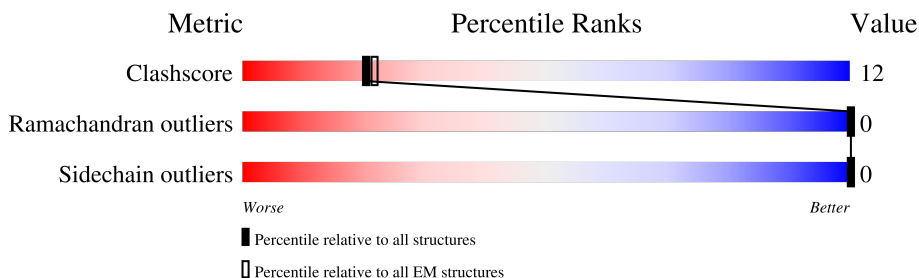
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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	15087 (2.80 - 3.80)

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	333	
2	B	906	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3207 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 Sodium/bile acid cotransporter.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	298	Total	C	N	O	S	0	0
			2279	1519	355	378	27		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	MET	-	initiating methionine	UNP Q14973
A	5	THR	ASN	engineered mutation	UNP Q14973
A	11	THR	ASN	engineered mutation	UNP Q14973
A	33	VAL	PHE	engineered mutation	UNP Q14973
A	37	ILE	PHE	engineered mutation	UNP Q14973
A	86	ASN	LYS	engineered mutation	UNP Q14973
A	95	ILE	VAL	engineered mutation	UNP Q14973
A	107	ILE	VAL	engineered mutation	UNP Q14973
A	129	LEU	CYS	engineered mutation	UNP Q14973
A	221	HIS	LEU	engineered mutation	UNP Q14973
A	329	LEU	-	expression tag	UNP Q14973
A	330	GLU	-	expression tag	UNP Q14973
A	331	VAL	-	expression tag	UNP Q14973
A	332	LEU	-	expression tag	UNP Q14973
A	333	PHE	-	expression tag	UNP Q14973
A	334	GLN	-	expression tag	UNP Q14973

- Molecule 2 is a protein called Anti-RON nanobody,Megabody 91,Glucosidase YgjK.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	119	Total	C	N	O	S	0	0
			928	586	161	177	4		

- Molecule 1: Sodium/bile acid cotransporter



Y865	VAL	VAL	LYS	LYS	S788	L791	S792	C793	A794	A795	S796	S797	M804	A805	W806	Q809	A810	P811	G812	K813	E814	R815	E816	F817	F820	I821	N822	W823	N824	Y825	G826	N827	D832	S833	V834	F838	T839	I840	D843	N844	A845	K846	I847	T848	V849	M853	P858	T861	A862	V863	Y864
HIS	GLY	HIS	THR	ALA	ASP	LYS	PRO	ASP	GLY	ASN	THR	MET	GLY	PHE	GLY	THR	VAL	THR	ILE	THR	GLY	THR	LYS	ILE	THR	ASP	PRO	ARG	ASN	GLY	THR	VAL	TRP	GLY	GLN	LYS	VAL	TRP	GLY	LEU	GLY	THR	LYS	ALA	THR	ILE	ALA	VAL	GLN		
LYS	LEU	THR	ALA	ASP	VAL	ASP	VAL	GLN	LYS	THR	MET	THR	LEU	ARG	THR	ARG	PRO	THR	THR	LYS	LEU	THR	LYS	LYS	THR	ASP	PRO	LEU	ASP	LEU	VAL	TRP	ASP	GLY	GLN	LYS	VAL	LEU	ALA	THR	LYS	GLY	ALA	LEU	VAL	GLN					
GLU	TYR	PRO	ASP	TYR	GLN	ARG	LYS	THR	ILE	THR	ALA	ASP	ARG	GLY	THR	VAL	THR	PHE	GLY	LYS	VAL	GLN	VAL	ALA	THR	ASP	LEU	THR	GLY	ASN	TYR	GLN	VAL	GLY	HIS	LYS	VAL	THR	ASN	ARG	THR	ILE	ALA	HIS	ILE						
ASN	SER	THR	THR	LEU	TYR	THR	THR	THR	TYR	SER	THR	HIS	LEU	LEU	THR	ALA	GLN	GLY	ASP	THR	VAL	SER	GLY	ILE	ARG	ASP	ILE	SER	LEU	ASN	ALA	THR	ARG	ALA	THR	GLN	SER	THR	ASP	ASN	THR	THR	ASN	THR	PRO	GLU					
GLN	THR	ARG	VAL	VAL	LYS	ALA	ALA	ILE	GLN	PHE	THR	LEU	ASN	GLY	ASN	TRP	SER	GLY	VAL	ALA	LYS	PHE	ASN	THR	THR	VAL	THR	PRO	PRO	VAL	THR	SER	THR	ALA	GLY	PRO	TRP	GLU	ASP	THR	THR	PHE	ALA	ASN	PRO	ASP					
ILE	ALA	LYS	ASN	ILE	ARG	ALA	ALA	VAL	GLN	THR	SER	TRP	GLN	ILE	GLN	PRO	GLY	VAL	ARG	PRO	ALA	THR	GLY	PHE	THR	VAL	PRO	ASP	LEU	THR	ASP	PRO	GLY	ARG	ASN	TRP	GLY	ASN	TRP	ASP	THR	LYS	THR	THR	TRP	SER					
VAL	MET	GLU	VAL	TYR	ASN	VAL	VAL	THR	GLN	ASP	LYS	THR	TRP	VAL	ALA	THR	TYR	LYS	VAL	ALA	THR	HIS	ASP	TRP	TRP	LEU	ARG	ASN	GLY	GLY	ASN	GLY	PRO	GLY	VAL	PRO	GLU	ARG	LYS	ALA	HIS	ASN	THR	GLU	SER	GLY	GLY	MET	LEU	PHE	THR

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	184768	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 ($e^-/\text{\AA}^2$)	56.5	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.331	Depositor
Minimum map value	-0.649	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	282.24, 282.24, 282.24	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.008, 1.008, 1.008	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	0.15	0/2328	0.35	0/3157
2	B	0.22	0/946	0.42	0/1282
All	All	0.18	0/3274	0.37	0/4439

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	2279	0	2446	54	0
2	B	928	0	902	33	0
All	All	3207	0	3348	80	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 12.

The worst 5 of 80 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:67:ALA:HA	1:A:71:ILE:HD12	1.70	0.72
1:A:111:ALA:O	1:A:305:TRP:NE1	2.24	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:795:ALA:HB3	2:B:847:ILE:HD12	1.79	0.65
2:B:815:ARG:HD2	2:B:880:THR:HG21	1.78	0.64
2:B:2:VAL:O	2:B:2:VAL:HG12	1.95	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	296/333 (89%)	285 (96%)	11 (4%)	0	100	100
2	B	115/906 (13%)	107 (93%)	8 (7%)	0	100	100
All	All	411/1239 (33%)	392 (95%)	19 (5%)	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	256/287 (89%)	256 (100%)	0	100	100
2	B	97/745 (13%)	97 (100%)	0	100	100
All	All	353/1032 (34%)	353 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	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.

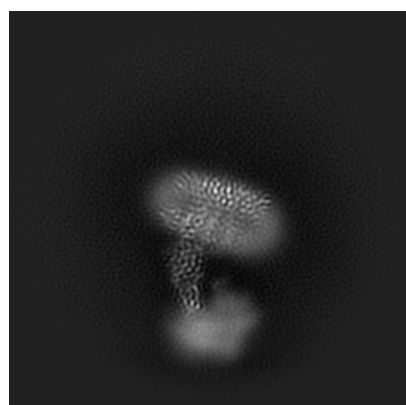
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13596. These allow visual inspection of the internal detail of the map and identification of artifacts.

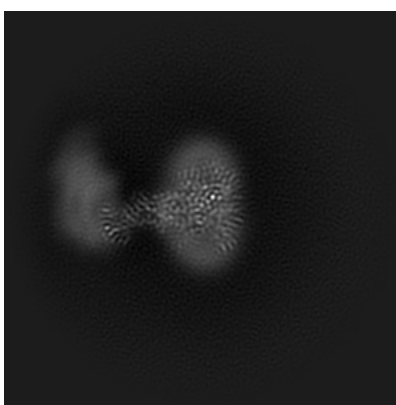
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

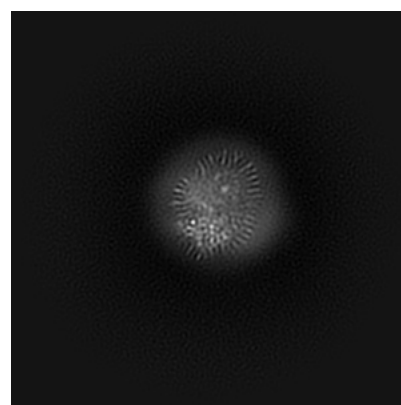
6.1.1 Primary map



X



Y

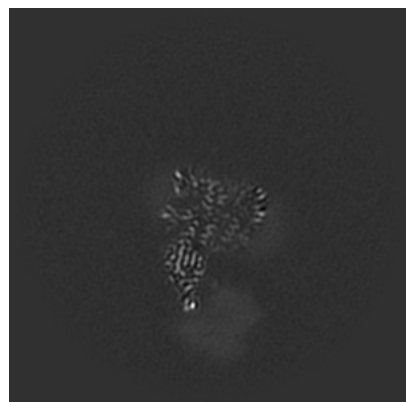


Z

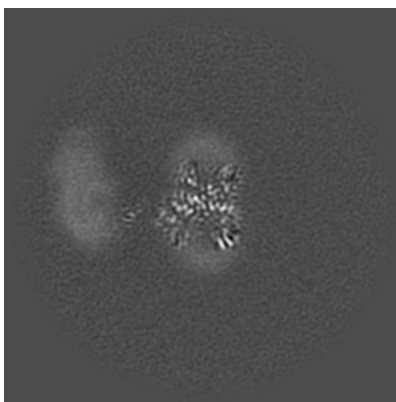
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

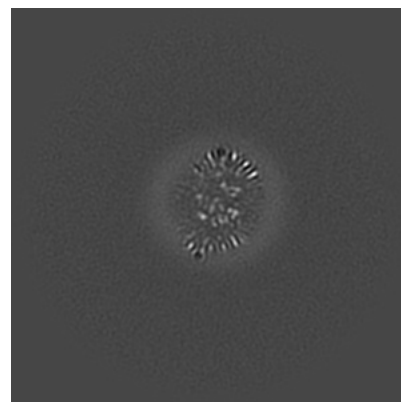
6.2.1 Primary map



X Index: 140



Y Index: 140

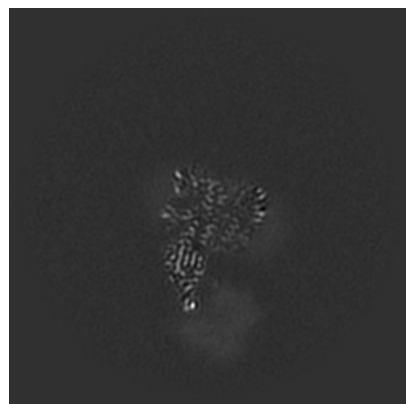


Z Index: 140

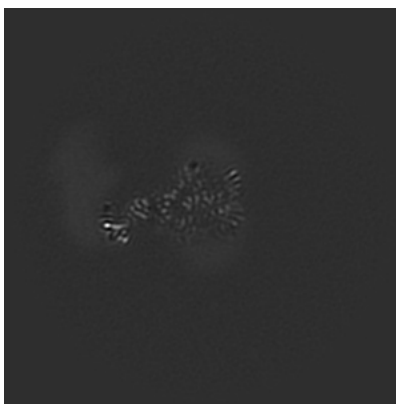
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 140



Y Index: 131



Z Index: 146

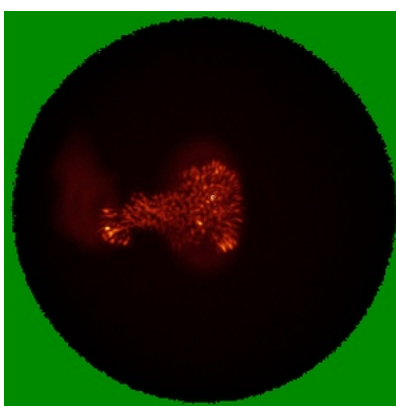
The images above show the largest variance slices of the map in three orthogonal directions.

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

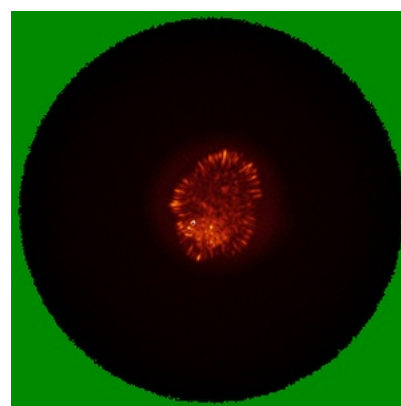
6.4.1 Primary map



X



Y

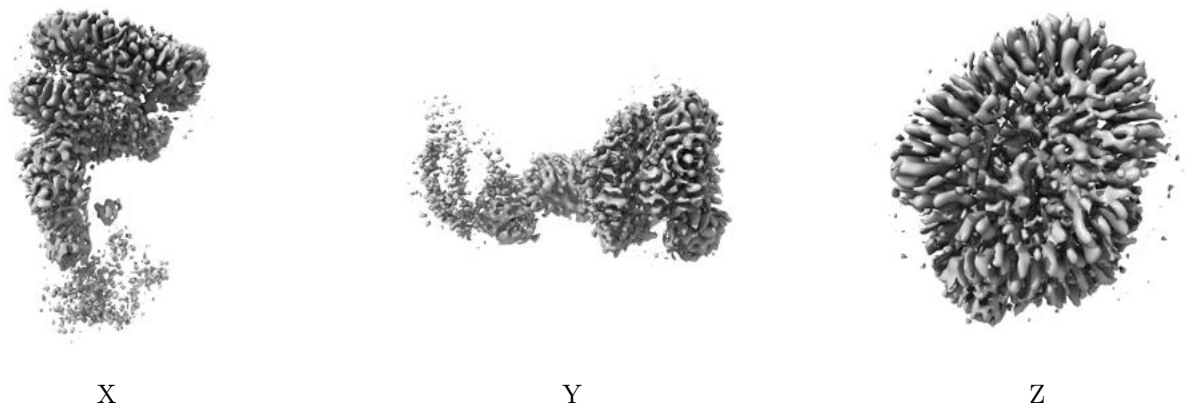


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

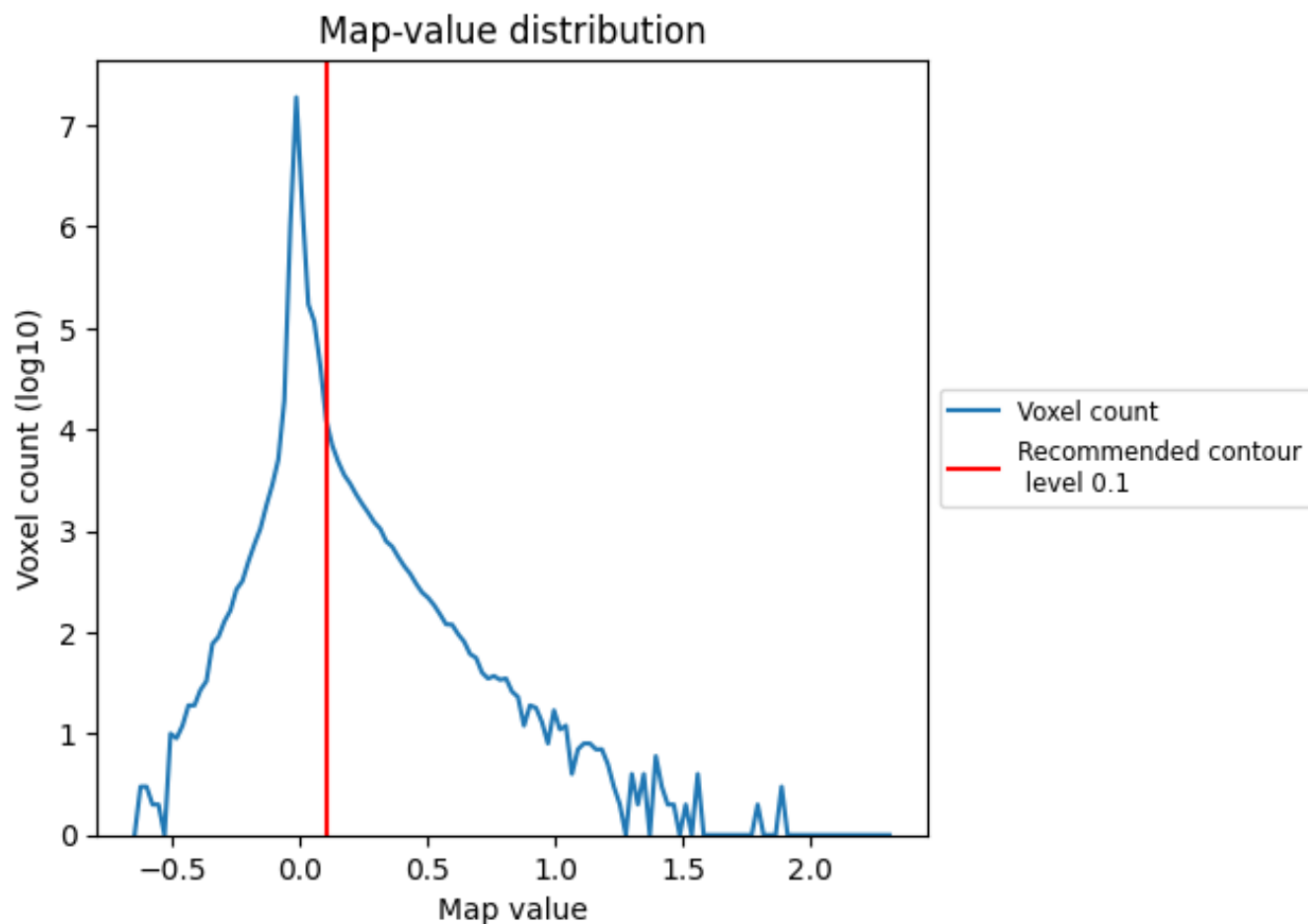
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

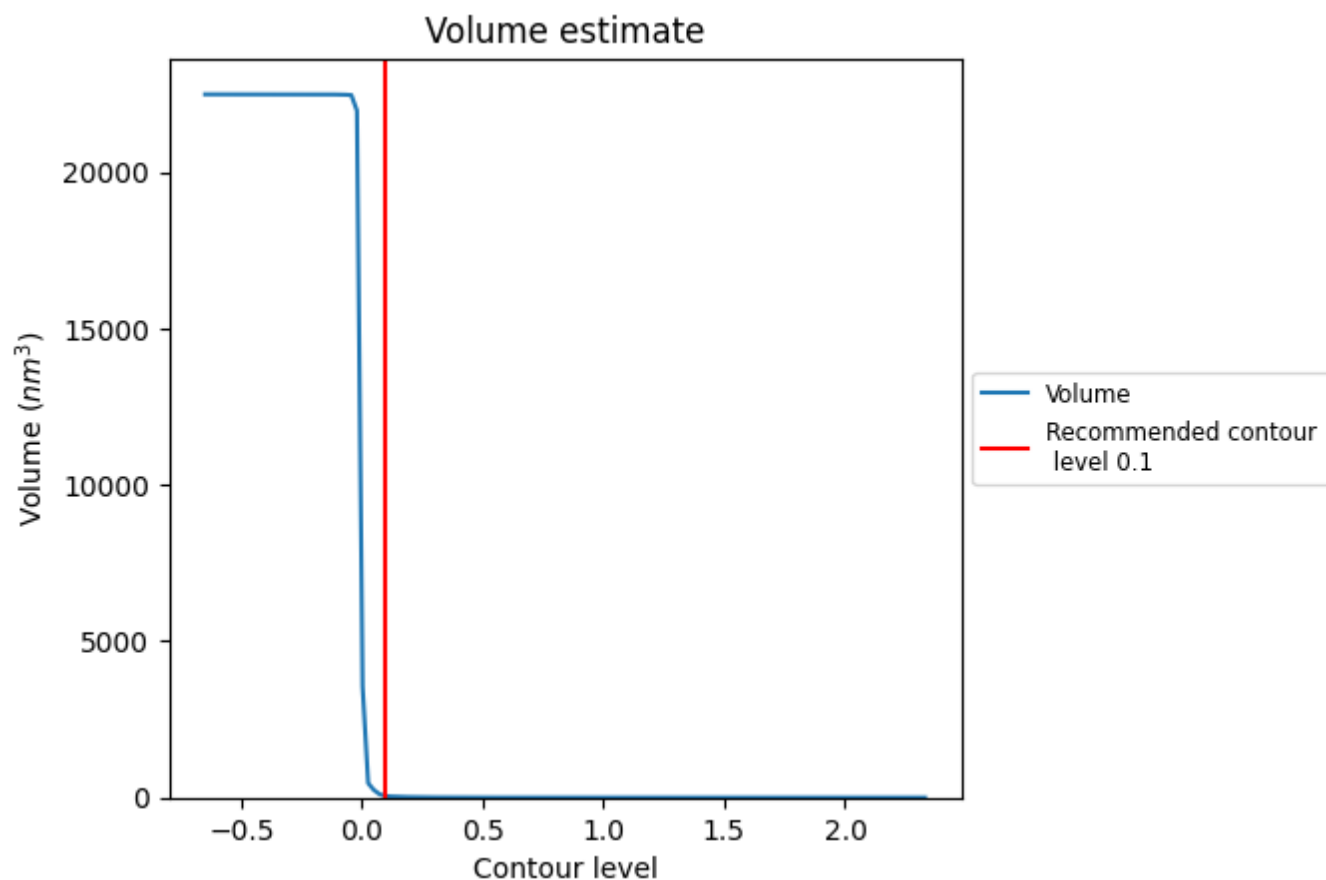
This section contains the results of statistical analysis of the map.

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.

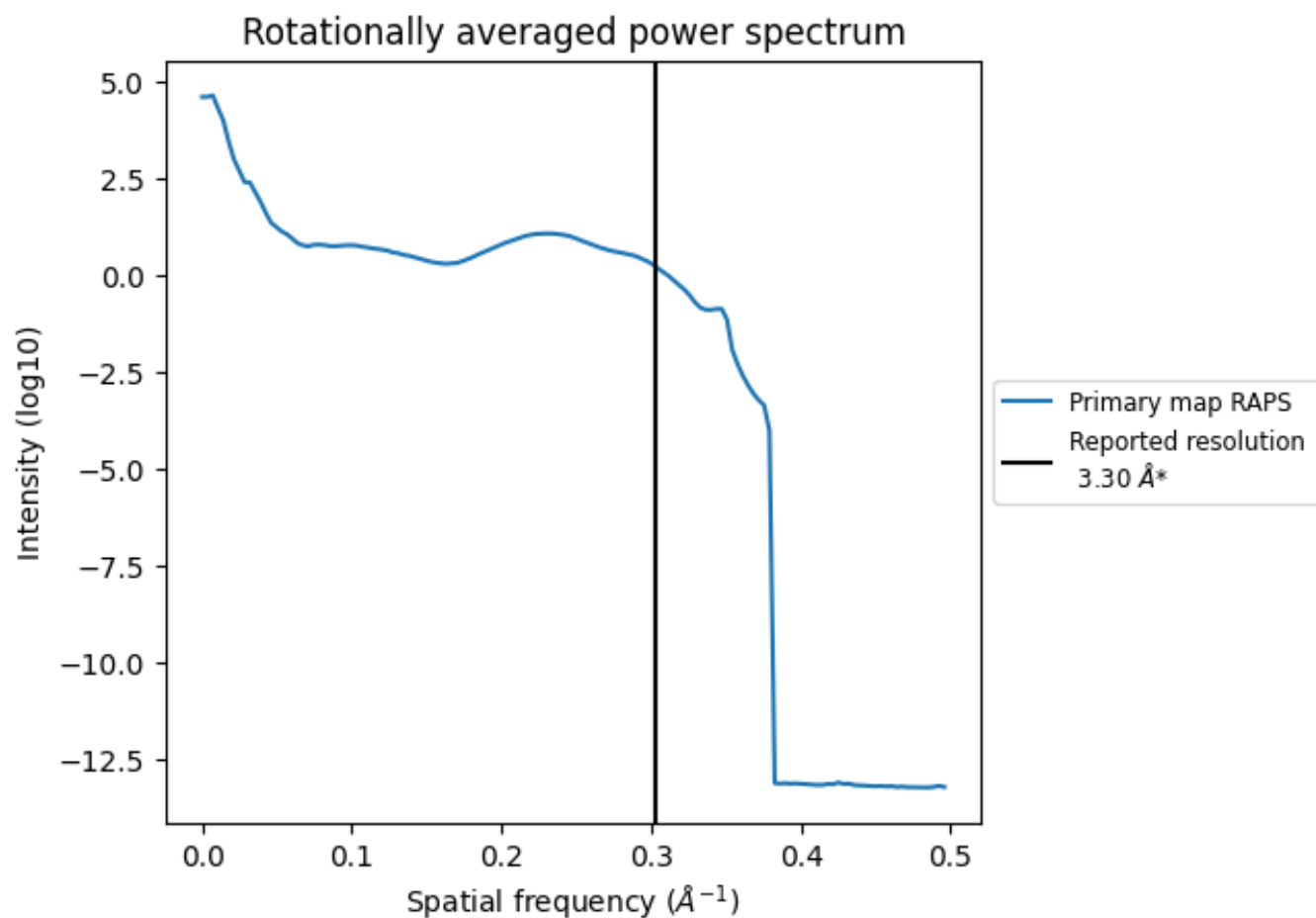
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 48 nm^3 ; this corresponds to an approximate mass of 43 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 0.303 Å⁻¹

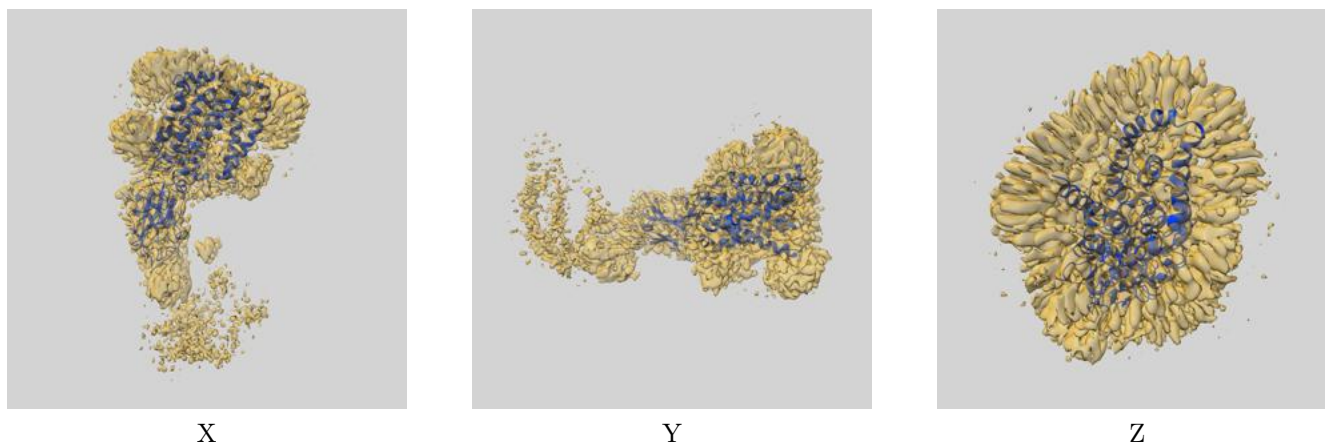
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

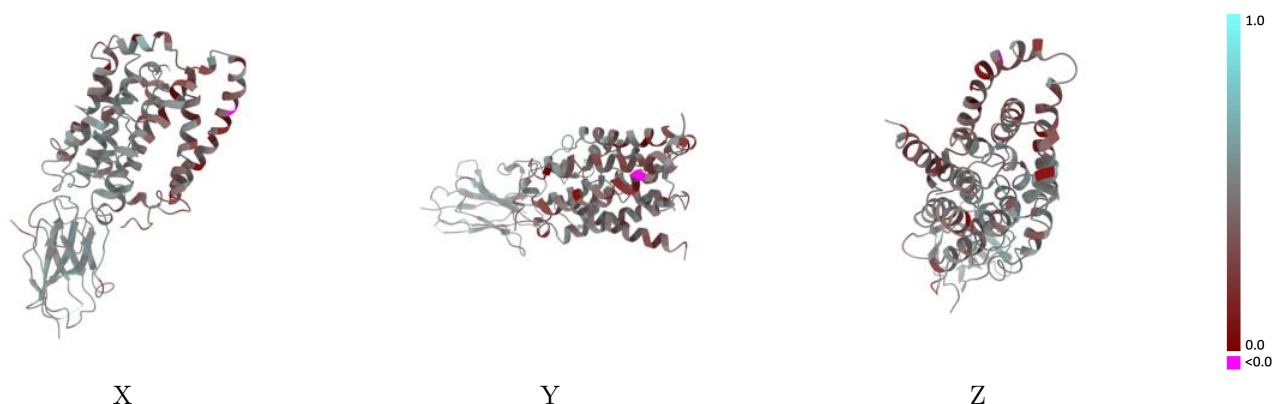
This section contains information regarding the fit between EMDB map EMD-13596 and PDB model 7PQQ. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



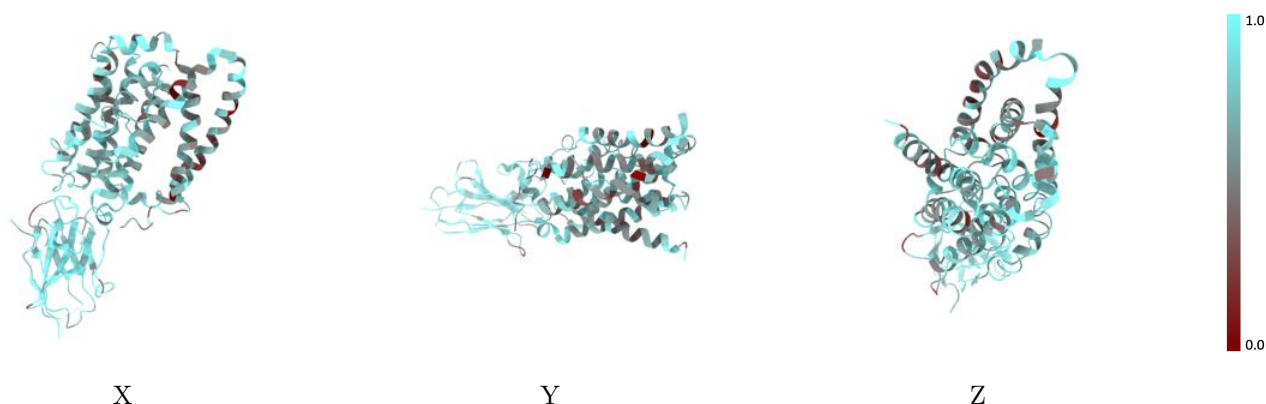
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



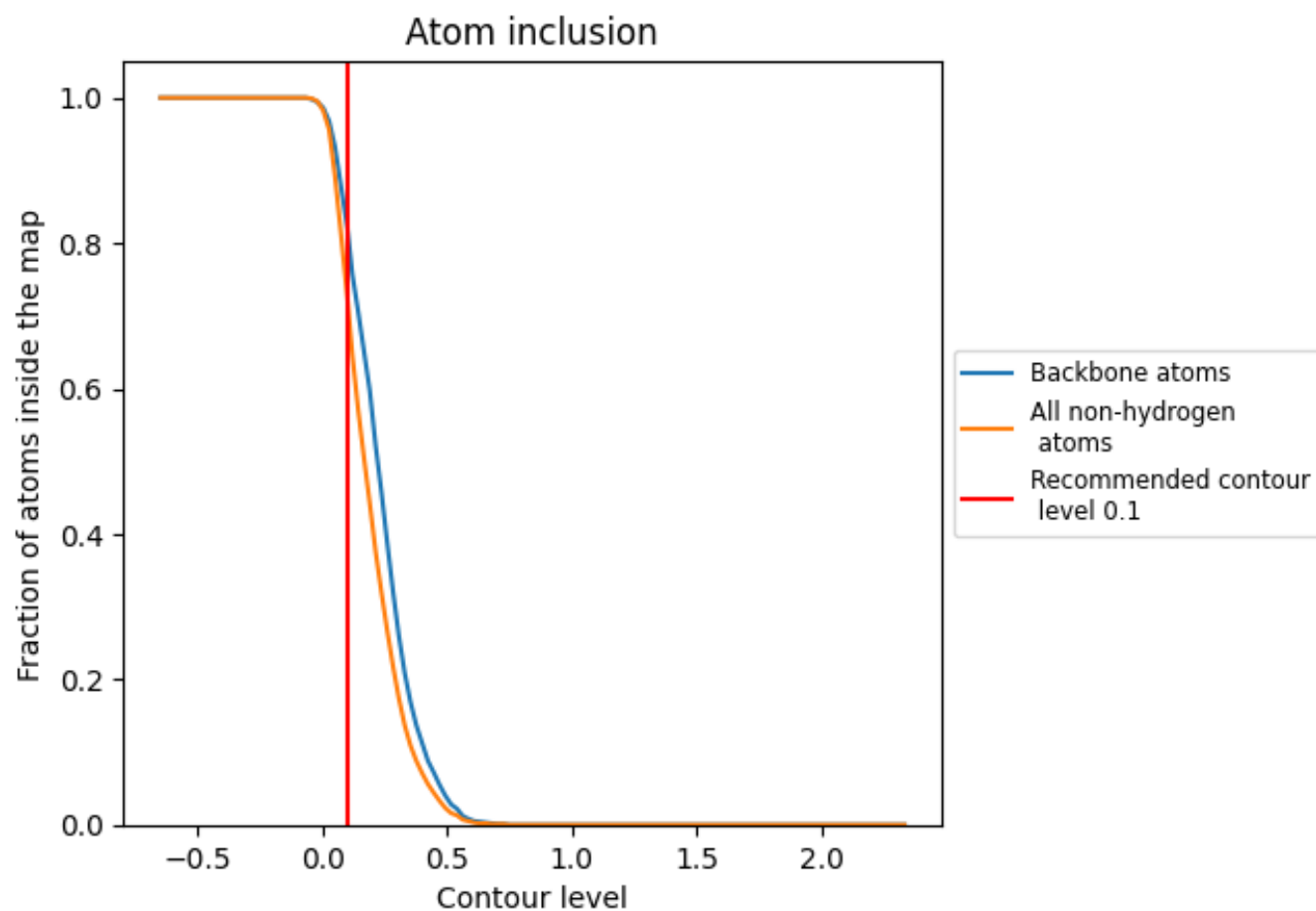
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

9.4 Atom inclusion ⓘ



At the recommended contour level, 82% of all backbone atoms, 72% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7230	0.4440
A	0.6850	0.4250
B	0.8190	0.4890

