



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 01:24 AM UTC

PDB ID : 7S1Z / pdb_00007s1z
EMDB ID : EMD-24813
Title : Cryo-EM structure of Human NKCC1 K289NA492EL671C
Authors : Zhao, Y.X.; Cao, E.H.
Deposited on : 2021-09-02
Resolution : 3.30 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

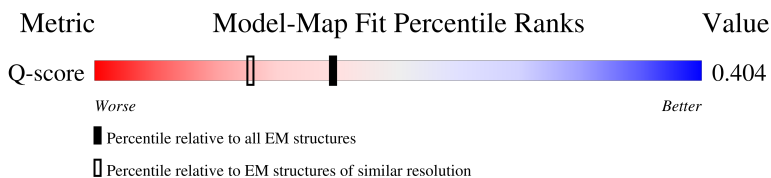
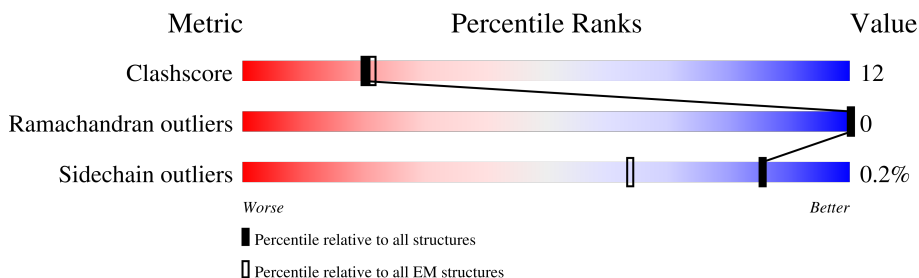
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 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	1216	 29% 9% 61%
1	B	1216	 30% 9% 61%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6416 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 Solute carrier family 12 member 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	472	Total	C	N	O	S	0	0
			3208	2112	517	562	17		
1	B	472	Total	C	N	O	S	0	0
			3208	2112	517	562	17		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP P55011
A	-2	ALA	-	expression tag	UNP P55011
A	-1	MET	-	expression tag	UNP P55011
A	0	GLY	-	expression tag	UNP P55011
A	1	SER	-	expression tag	UNP P55011
A	289	ASN	LYS	engineered mutation	UNP P55011
A	492	GLU	ALA	engineered mutation	UNP P55011
A	518	LEU	ILE	conflict	UNP P55011
A	671	CYS	LEU	engineered mutation	UNP P55011
B	-3	GLY	-	expression tag	UNP P55011
B	-2	ALA	-	expression tag	UNP P55011
B	-1	MET	-	expression tag	UNP P55011
B	0	GLY	-	expression tag	UNP P55011
B	1	SER	-	expression tag	UNP P55011
B	289	ASN	LYS	engineered mutation	UNP P55011
B	492	GLU	ALA	engineered mutation	UNP P55011
B	518	LEU	ILE	conflict	UNP P55011
B	671	CYS	LEU	engineered mutation	UNP P55011

LEU	GLU	ARG	GLU	VAL	LYS
SER	PRO	ALA	ALA	VAL	TRP
LYS	TRP	MET	LYS	VAL	TRP
ASP	ARG	ALA	THR	SER	GLN
LEU	ILE	THR	THR	GLN	ALA
PRO	THR	LEU	PHE	GLU	ASP
PRO	ASP	LEU	GLN	TYR	ASP
ILE	ASN	SER	LYS	SER	MET
LEU	GLU	LYS	LYS	LYS	ASP
LEU	LEU	PHE	GLN	LYS	ASP
VAL	GLU	ARG	GLY	SER	VAL
ARG	LEU	ILE	LYS	ASP	ASP
GLY	TYR	ASP	ASN	LEU	MET
ASN	LYS	PHE	THR	ASP	TYR
HIS	THR	SER	ILE	THR	ASN
GLN	THR	ASP	VAL	SER	ASN
SER	THR	ILE	TRP	PRO	PHE
VAL	ARG	VAL	TRP	LEU	HIS
LEU	GLN	LEU	LEU	SER	ASP
THR	ILE	GLY	PHE	GLU	ALA
PHE	ARG	ASP	ASP	LYS	PHE
TYR	LEU	ILE	ASP	PRO	ASP
SER	ASN	ASN	GLY	ILE	ILE
	GLU	THR	GLY	THR	GLN
	LEU	LYS	LEU	HIS	GLY
	LEU	PRO	THR	LYS	VAL
	LYS	LYS	LEU	VAL	VAL
	GLU	LYS	LEU	GLU	VAL
	HIS	GLU	ILE	GLU	ILE
	SER	ASN	PRO	GLU	ILE
	SER	ILE	TYR	ASP	ASP
	THR	ILE	LEU	GLY	LYS
	ALA	ALA	LEU	LYS	GLU
	ASN	PHE	THR	THR	GLU
	ILE	GLU	LYS	ALA	GLY
	VAL	ILE	LYS	THR	LEU
	MET	ILE	LYS	PRO	GLY
	SEU	GLU	TRP	LEU	SER
	SER	PRO	LYS	LEU	HIS
	PRO	TYR	ASP	LYS	LEU
	VAL	ARG	CYS	LYS	GLN
	ALA	LEU	LYS	GLU	GLY
	ARG	HIS	ILE	SER	GLN
	LYS	GLU	ARG	LYS	GLU
	GLY	ASP	VAL	GLY	GLU
	ALA	ASP	PHE	PRO	GLU
	VAL	LYS	ILE	ILE	LEU
	SER	GLU	GLY	VAL	LEU
	SER	GLN	GLY	PRO	SER
	ALA	ASP	LYS	ASN	GLU
	LEU	ILE	ILE	ASN	LYS
	TYR	ALA	ASN	VAL	LYS
	MET	ASP	ARG	SER	PRO
	ALA	LYS	ILE	ASP	GLY
	TRP	MET	ASP	GLN	THR
	LEU	LYS	HIS	LYS	LYS
	GLU	GLU	ARG	LEU	ASP
	ALA	ASP	ARG	LEU	LYS

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	536763	Depositor
Resolution determination method	DIFFRACTION PATTERN/LAYERLINES	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.175	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	7.275	Depositor
Minimum map value	-5.775	Depositor
Average map value	0.010	Depositor
Map value standard deviation	0.150	Depositor
Recommended contour level	0.6	Depositor
Map size ($\text{\AA}$)	271.36, 271.36, 271.36	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.06, 1.06, 1.06	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	0/3280	0.42	1/4490 (0.0%)
1	B	0.15	0/3280	0.41	0/4490
All	All	0.15	0/6560	0.42	1/8980 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	507	ILE	N-CA-C	-5.77	106.16	112.80

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	3208	0	2984	80	0
1	B	3208	0	2984	72	0
All	All	6416	0	5968	152	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 152 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:B:333:ILE:HG21	1:B:719:GLY:HA3	1.71	0.71
1:A:476:ASN:OD1	1:A:546:ARG:NH1	2.24	0.69
1:A:285:PHE:CE2	1:A:290:GLY:HA3	2.30	0.67
1:A:333:ILE:HG21	1:A:719:GLY:HA3	1.76	0.66
1:A:506:ASN:HD22	1:A:624:LYS:HD2	1.59	0.66

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	470/1216 (39%)	426 (91%)	44 (9%)	0	100	100
1	B	470/1216 (39%)	426 (91%)	44 (9%)	0	100	100
All	All	940/2432 (39%)	852 (91%)	88 (9%)	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	281/985 (28%)	280 (100%)	1 (0%)	84	84
1	B	281/985 (28%)	281 (100%)	0	100	100
All	All	562/1970 (28%)	561 (100%)	1 (0%)	85	88

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

Mol	Chain	Res	Type
1	A	506	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	298	ASN
1	B	298	ASN
1	B	506	ASN
1	B	690	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.

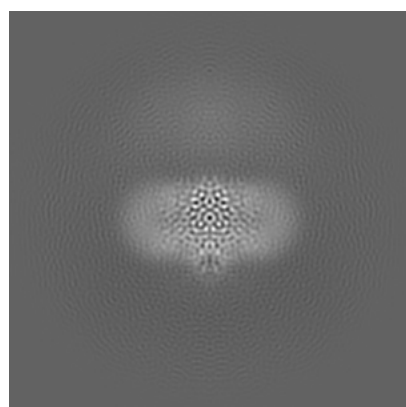
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24813. These allow visual inspection of the internal detail of the map and identification of artifacts.

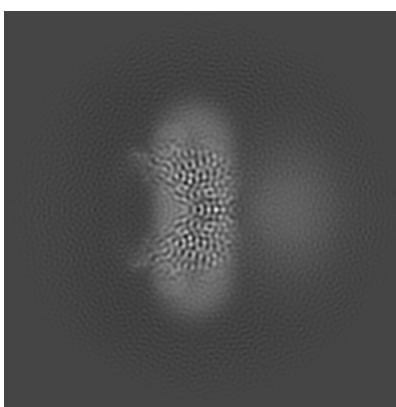
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

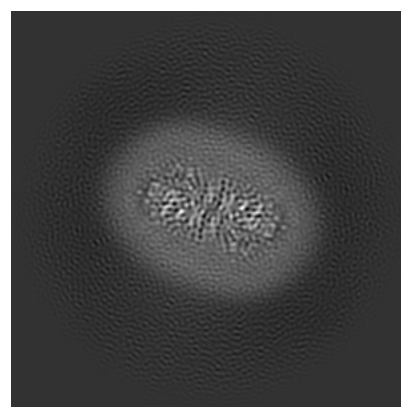
6.1.1 Primary map



X



Y

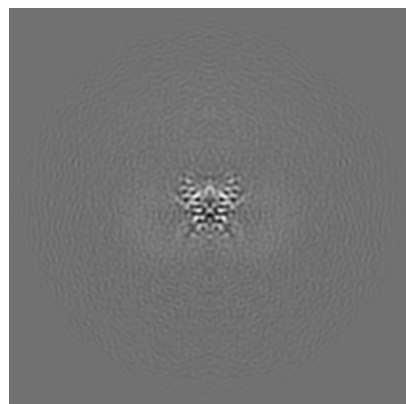


Z

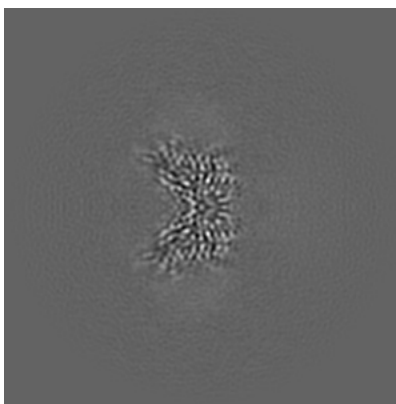
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

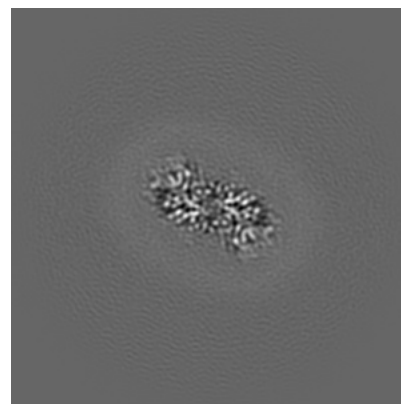
6.2.1 Primary map



X Index: 128



Y Index: 128

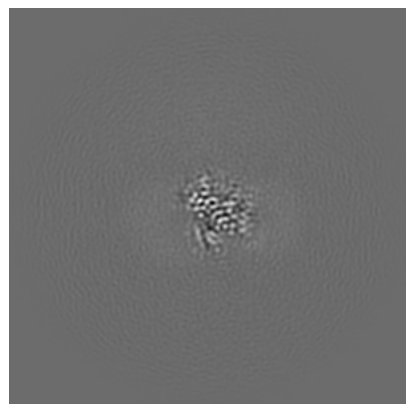


Z Index: 128

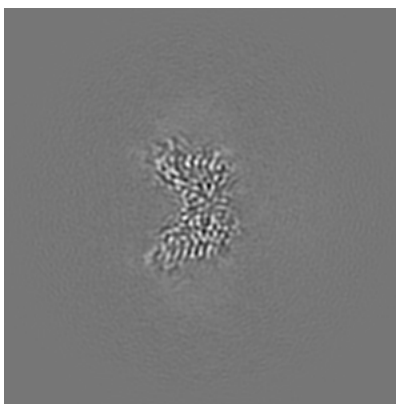
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

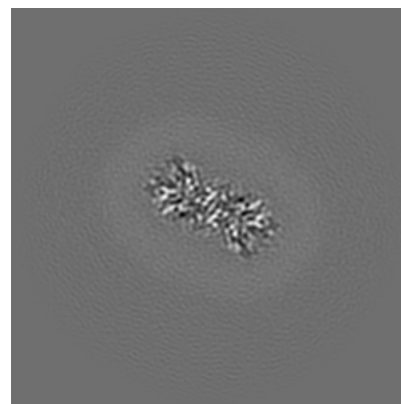
6.3.1 Primary map



X Index: 115



Y Index: 126

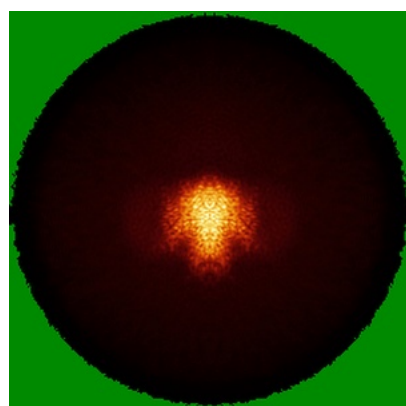


Z Index: 126

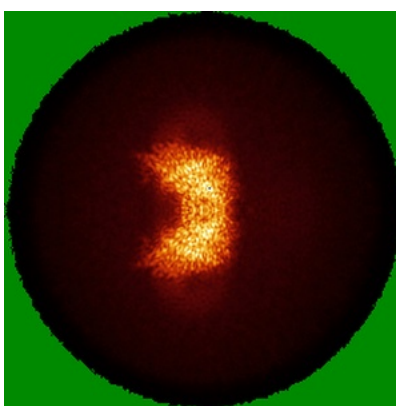
The images above show the largest variance slices of the map in three orthogonal directions.

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

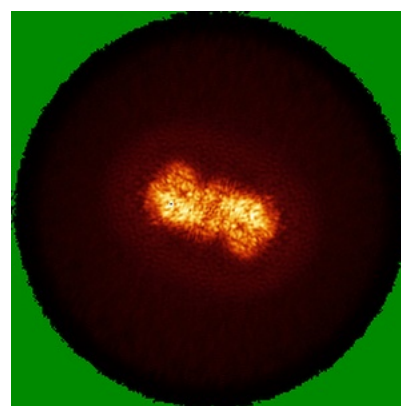
6.4.1 Primary map



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

This section was not generated.

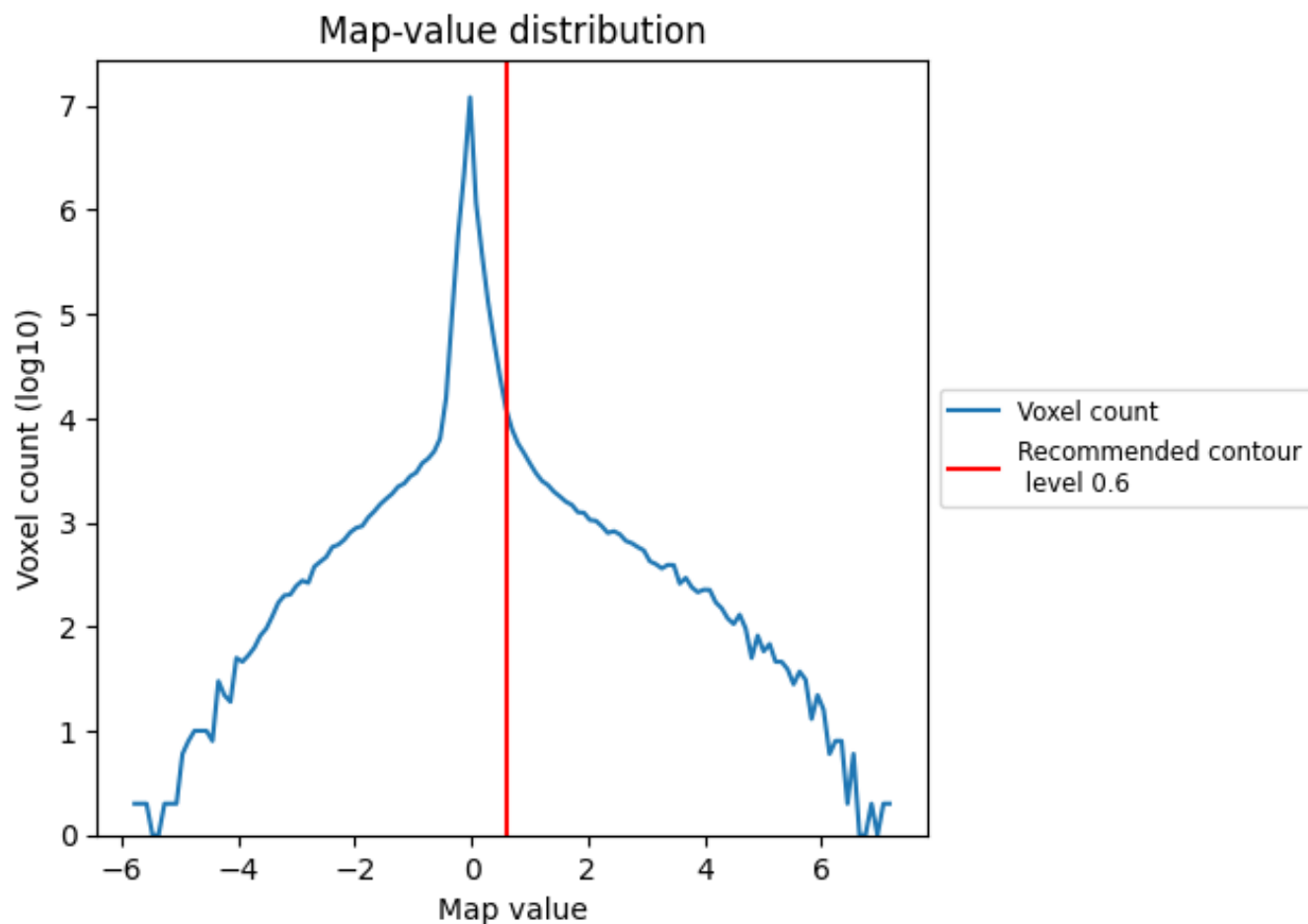
6.6 Mask visualisation

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

7 Map analysis [i](#)

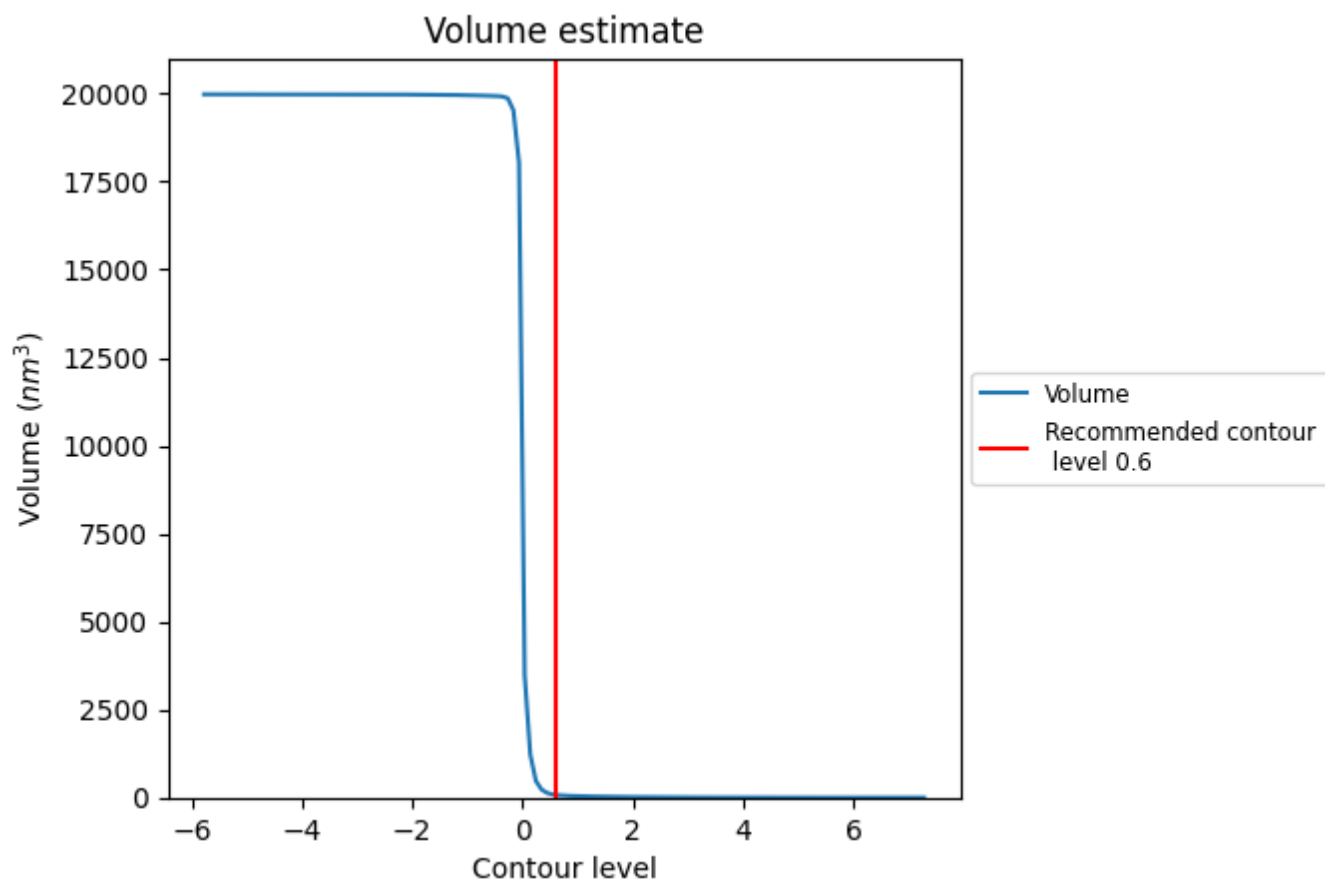
This section contains the results of statistical analysis of the map.

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.

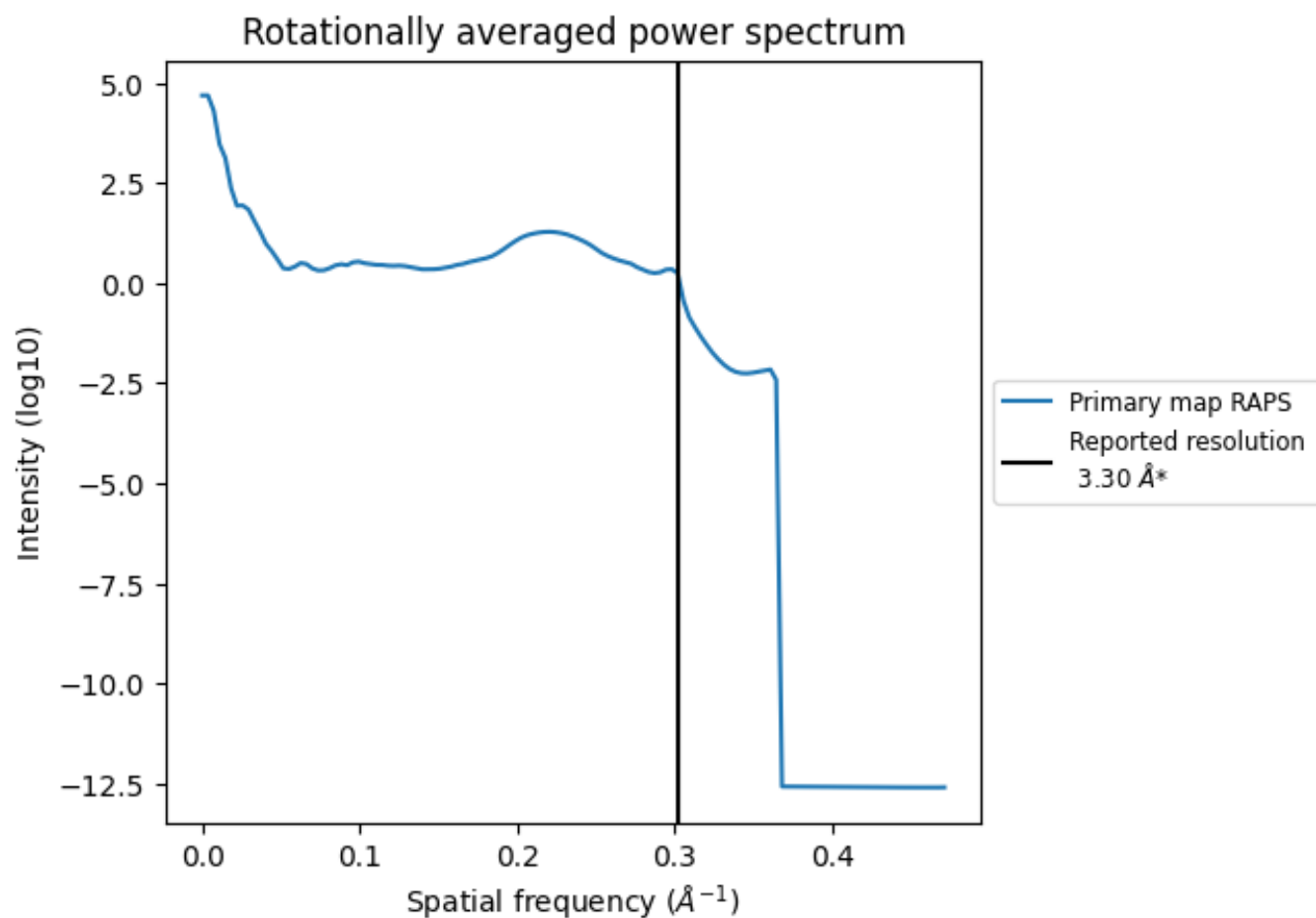
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 77 nm³; this corresponds to an approximate mass of 69 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

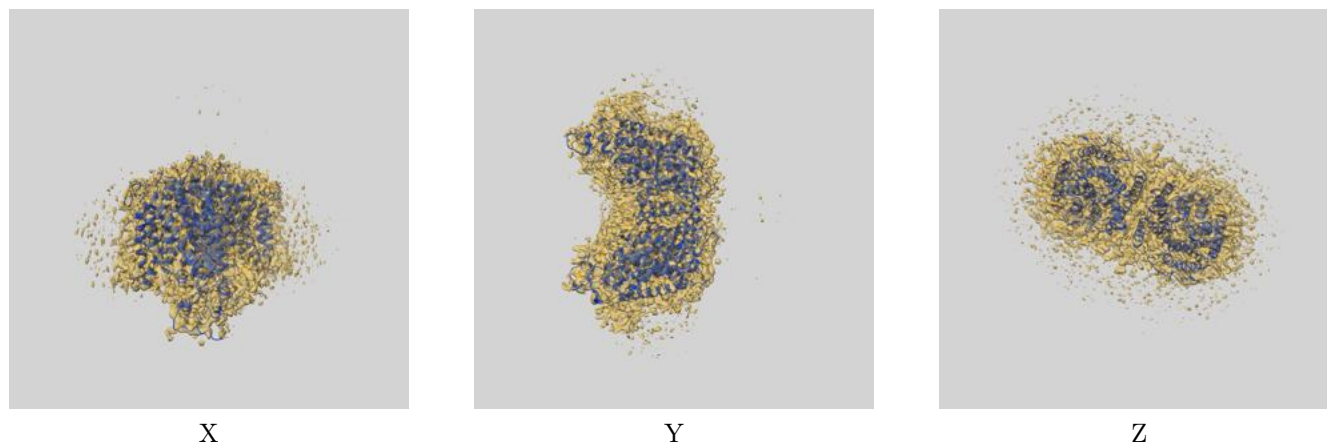
8 Fourier-Shell correlation

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-24813 and PDB model 7S1Z. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



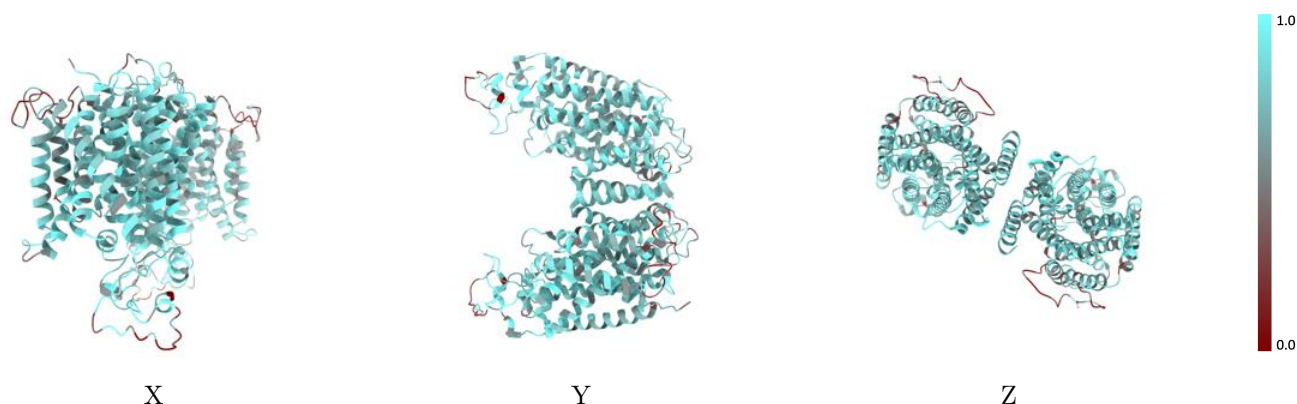
The images above show the 3D surface view of the map at the recommended contour level 0.6 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



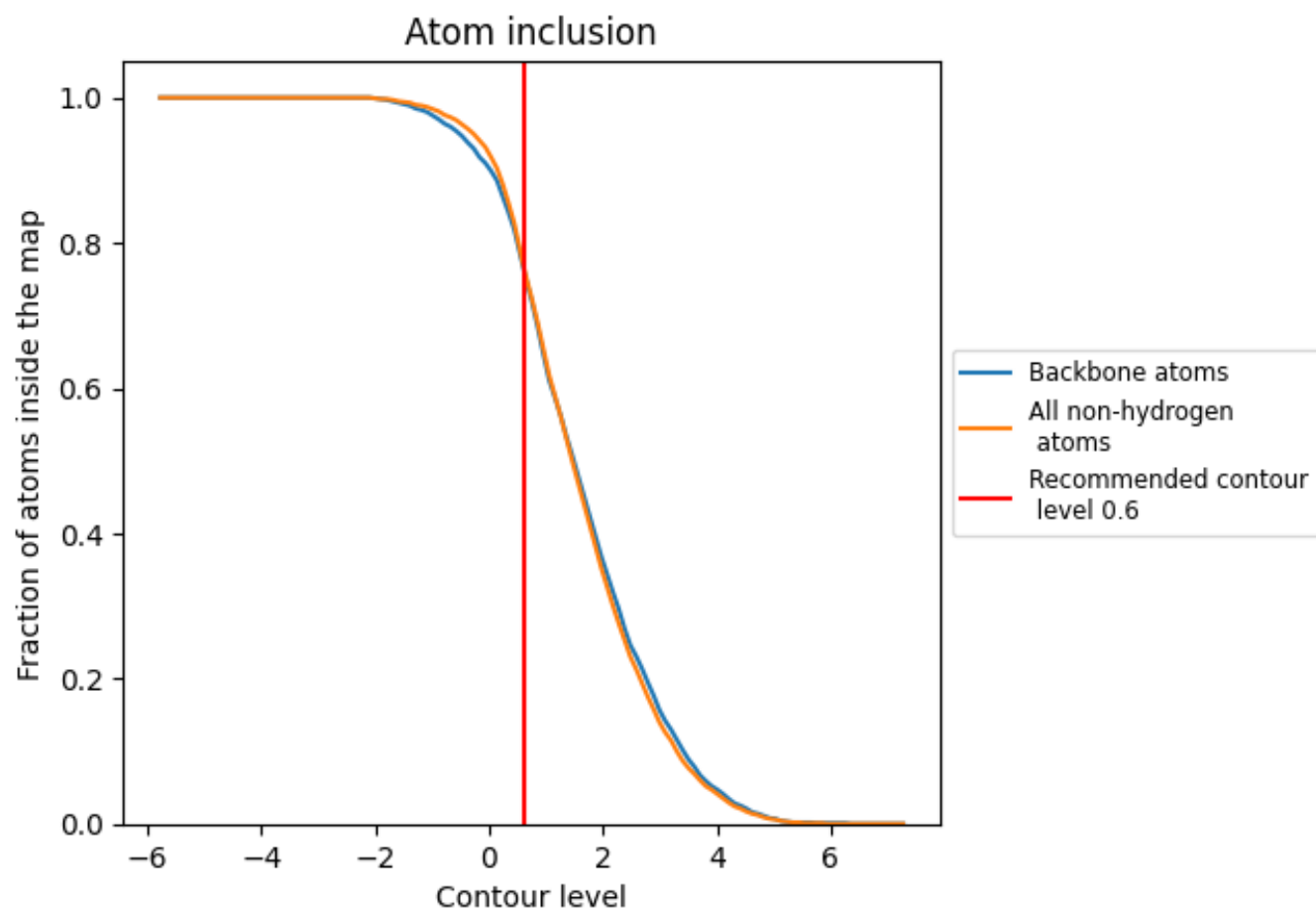
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.6).

9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 77% 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 (0.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7700	0.4040
A	0.7700	0.4050
B	0.7700	0.4030

