



wwPDB EM Validation Summary Report ⓘ

Nov 14, 2022 – 04:33 PM EST

PDB ID : 7K8B
EMDB ID : EMD-22725
Title : CryoEM structure of a trehalose monomycolate transporter in lipid nanodiscs
Authors : Su, C.-C.
Deposited on : 2020-09-26
Resolution : 2.94 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.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

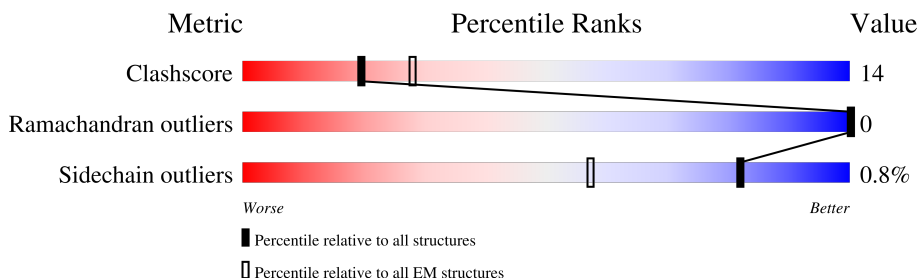
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.94 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	1013	<div> <div>22%</div> <div>49%</div> <div>22%</div> <div>28%</div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5543 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 Drug exporters of the RND superfamily-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	726	5543	3588	919	1008	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: Drug exporters of the RND superfamily-like protein



LEU	ARG	GLU	GLN	ARG	K702
PRO	PRO	SER	GLU	ALA	Y703
ASN	ASN	TRP	GLY	LEU	L704
GLY	GLY	LEU	ASP	VAL	
GLY	GLY	ALA	GLU	VAL	A711
ALA	LEU	ALA	PRO	GLY	L712
PRO	ALA	ARG	THR	ALA	L713
ALA	GLY	GLY	THR	PRO	L714
ASP	ASP	PRO	ARG	PRO	D715
ALA	ALA	ALA	PHE	PRO	
THR	THR	PRO	ALA	PRO	I719
THR	ALA	ALA	MET	PRO	
ALA	LYS	ALA	ALA	ARG	F722
ILE	ASN	ASN	ARG	PRO	L723
PRO	VAL	VAL	ASN	HIS	V724
THR	PRO	PRO	ALA	ASP	
PRO	GLN	VAL	VAL	PRO	F725
PRO	PRO	PRO	ARG	THR	A726
GLN	GLN	PRO	ASN	HIS	V727
ARG	ARG	ALA	ALA	PRO	M728
GLU	GLN	GLN	VAL	ALA	K729
GLU	GLN	PRO	ASN	PRO	L730
GLU	GLU	GLU	SER	GLU	L731
PRO	PRO	ARG	ALA	PRO	
SER	SER	PRO	VAL	VAL	G732
THR	THR	SER	HIS	ARG	D733
GLU	GLU	THR	GLY	PRO	D734
LYS	ASP	ASP	GLY	MET	G735
LEU	THR	THR	ALA	PRO	A736
ASN	ASN	THR	GLY	PRO	M737
THR	THR	ARG	SER	MET	
ARG	ARG	ALA	ALA	ARG	R740
GLU	GLU	MET	ALA	SER	M741
ASP	ASP	PRO	ALA	ASN	K742
ALA	ALA	PRO	PRO	ALA	K743
PRO	PRO	GLN	THR	PRO	
GLU	GLU	GLY	GLU	SER	R744
PRO	ASP	ARG	ARG	ALA	
PRO	PRO	PRO	ALA	ALA	
GLU	GLU	PRO	PRO	GLY	E747
THR	THR	ALA	ARG	THR	K748
LYS	LYS	GLY	PRO	ALA	
ARG	ARG	PRO	GLY	ARG	L751
GLY	GLY	ALA	ILE	ILE	G752
GLY	GLY	ASP	PRO	SER	E753
GLY	GLY	ARG	ALA	THR	I754
MET	MET	GLY	GLN	PRO	E755
SER	SER	ASN	PRO	PRO	
GLU	GLU	GLU	PRO	GLN	L756
GLN	GLN	ASN	ALA	PRO	
ASP	ASP	PRO	PRO	PRO	F757
LEU	LEU	THR	THR	GLN	ASP
LEU	LEU	THR	GLN	PRO	GLU
ARG	ARG	ALA	ARG	PRO	ARG
ARG	ARG	PHE	GLU	PRO	LYS
GLU	GLU	SER	ALA	ALA	ARG
GLY	GLY	THR	ARG	PRO	THR
ARG	ARG	GLN	ILE	GLN	VAL
					ARG
					ARG
					GLU
					SER
					GLU
					THR
					ASP

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	103810	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	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	21.598	Depositor
Minimum map value	-4.106	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.225	Depositor
Recommended contour level	0.4	Depositor
Map size (\AA)	130.68001, 99.36, 96.12	wwPDB
Map dimensions	89, 92, 121	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.08, 1.08, 1.08	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	0.30	1/5654 (0.0%)	0.55	1/7693 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	617	SER	CA-C	-5.39	1.39	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	617	SER	CB-CA-C	-5.93	98.84	110.10

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	5543	0	5713	158	0
All	All	5543	0	5713	158	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 14.

The worst 5 of 158 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:98:VAL:HA	1:A:105:ILE:HD11	1.60	0.84
1:A:683:ALA:HB1	1:A:712:LEU:HD21	1.66	0.77
1:A:413:VAL:HA	1:A:416:ILE:HG12	1.67	0.77
1:A:217:ILE:HG21	1:A:334:LEU:HD21	1.69	0.74
1:A:462:LYS:HB3	1:A:543:GLU:H	1.52	0.74

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	722/1013 (71%)	682 (94%)	40 (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	592/818 (72%)	587 (99%)	5 (1%)	81	93

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	487	PHE
1	A	520	LEU

Continued on next page...

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Mol	Chain	Res	Type
1	A	521	GLU
1	A	613	ASP
1	A	617	SER

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	172	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 monosaccharides 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.

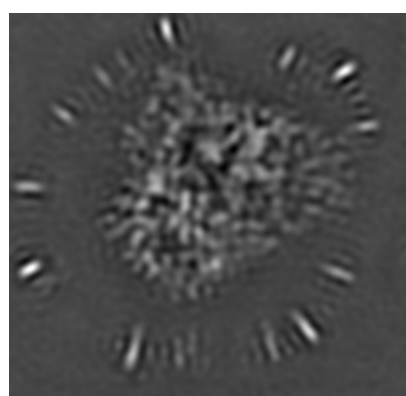
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22725. These allow visual inspection of the internal detail of the map and identification of artifacts.

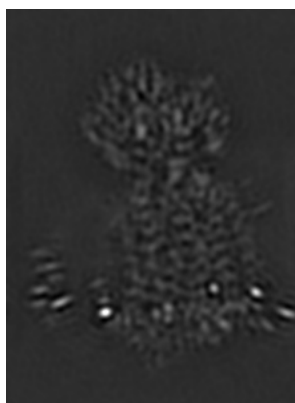
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

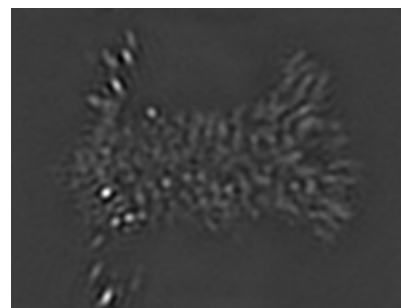
6.1.1 Primary map



X



Y

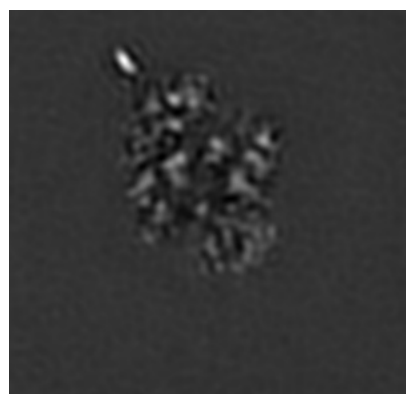


Z

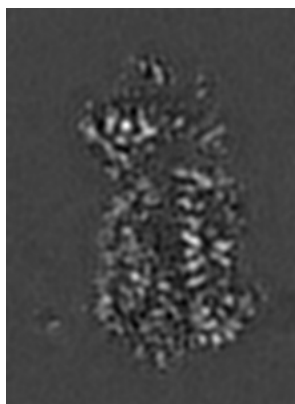
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 60



Y Index: 46

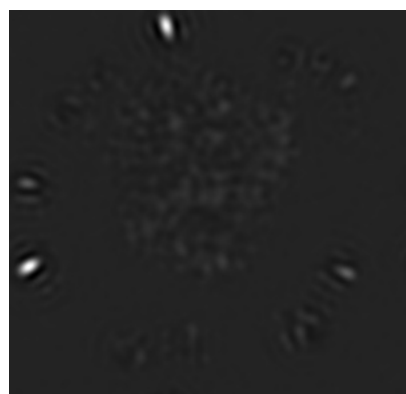


Z Index: 44

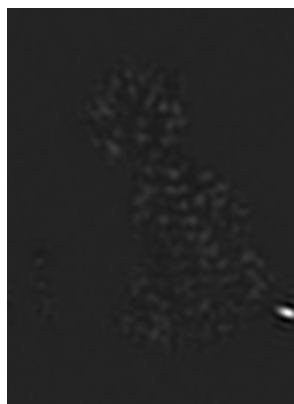
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

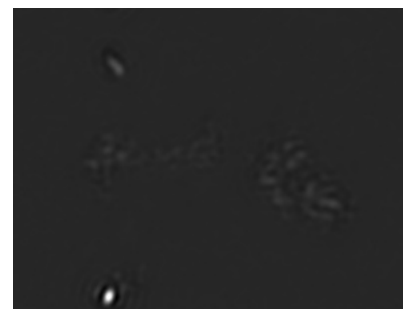
6.3.1 Primary map



X Index: 28



Y Index: 36

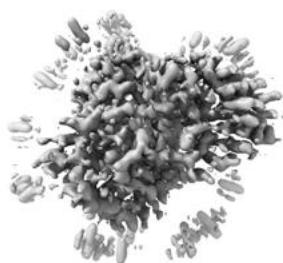


Z Index: 30

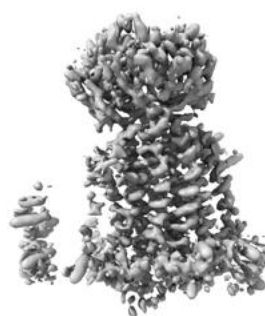
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

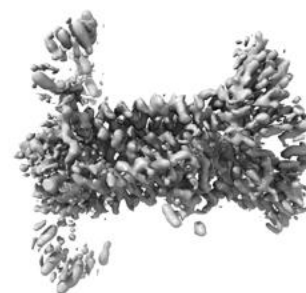
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

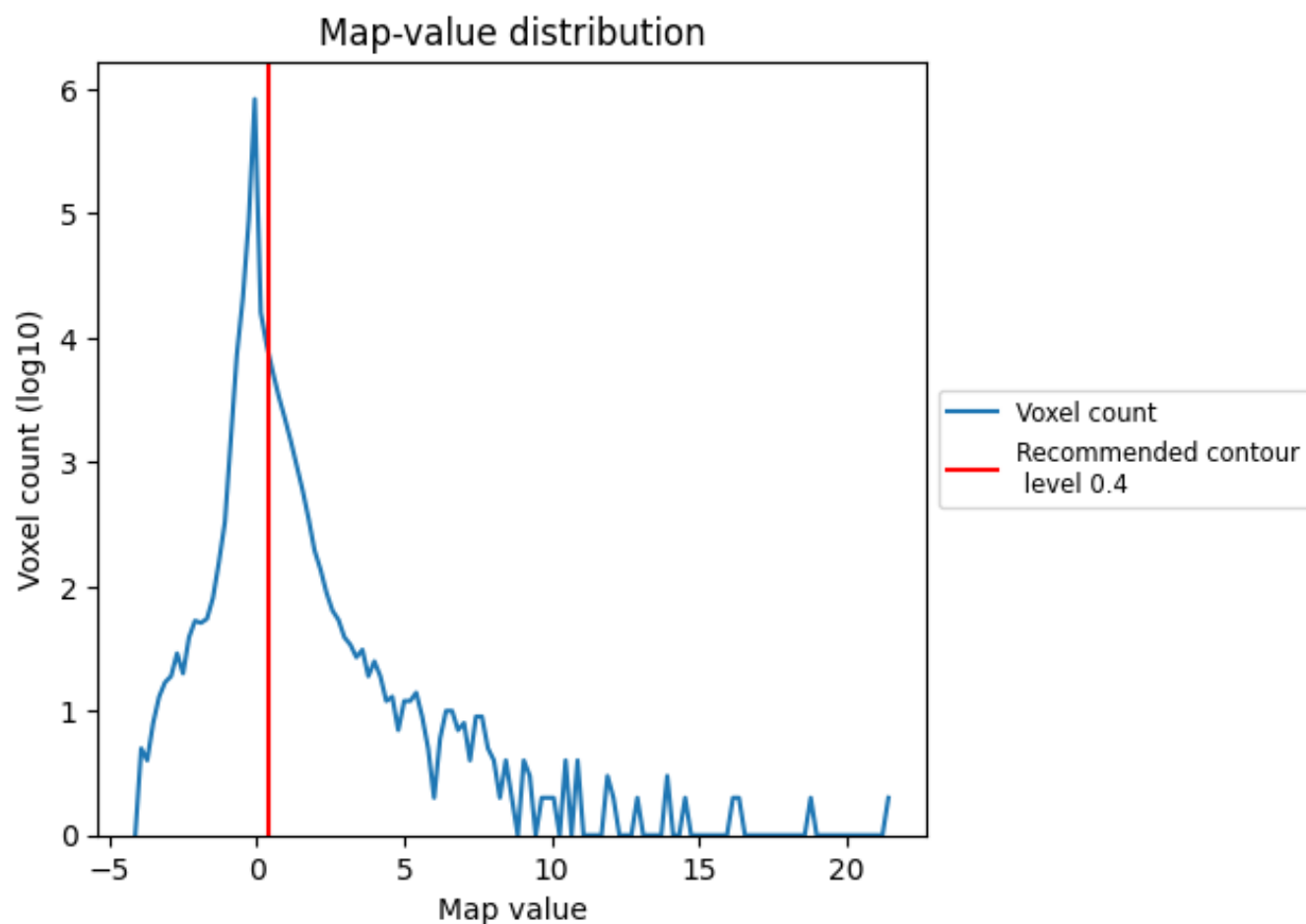
6.5 Mask visualisation

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

7 Map analysis ⓘ

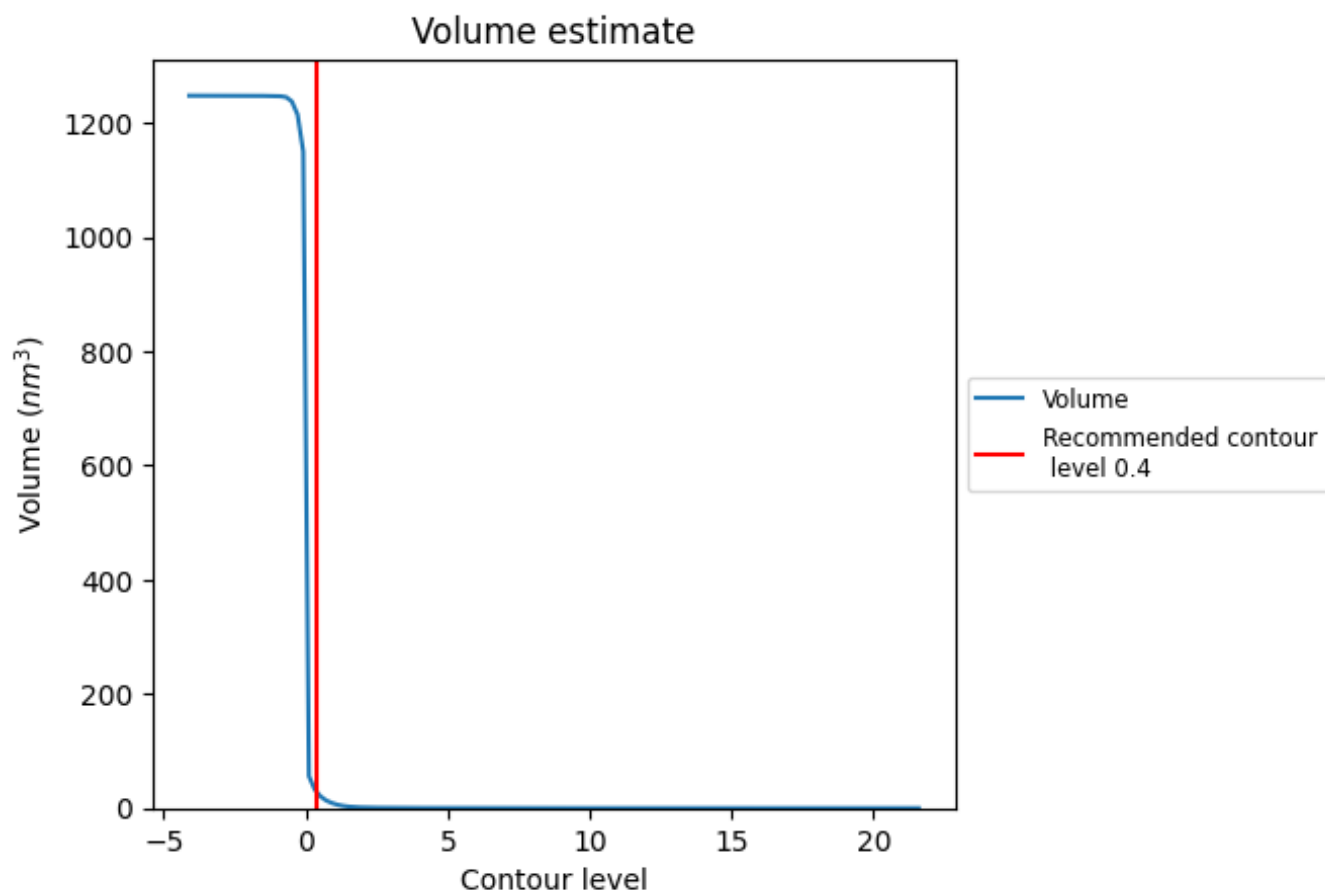
This section contains the results of statistical analysis of the map.

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 28 nm³; this corresponds to an approximate mass of 25 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](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

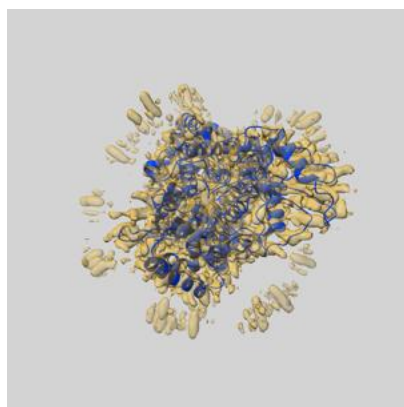
8 Fourier-Shell correlation

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

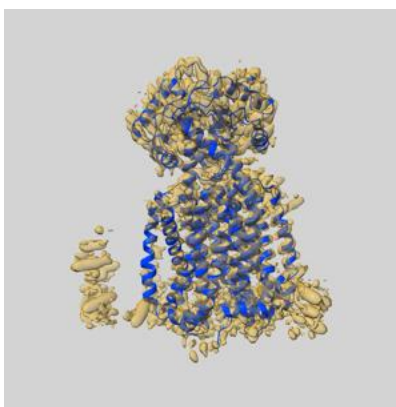
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-22725 and PDB model 7K8B. Per-residue inclusion information can be found in section [3](#) on page [4](#).

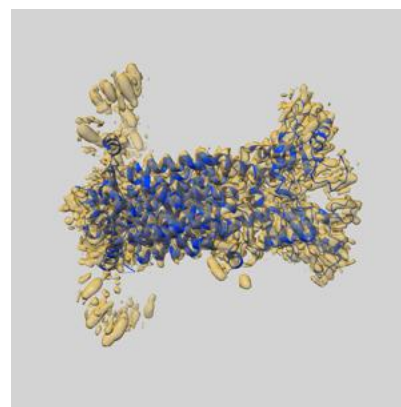
9.1 Map-model overlay [i](#)



X



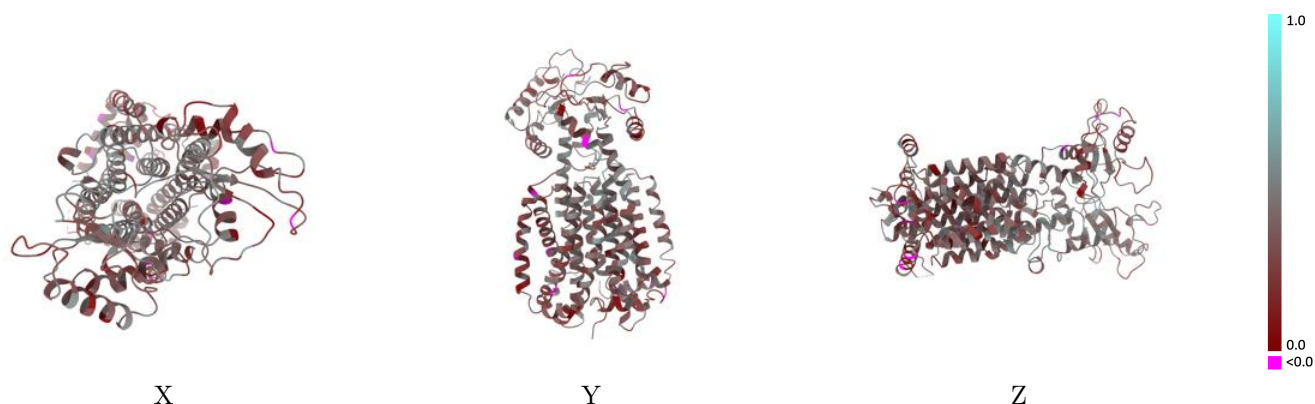
Y



Z

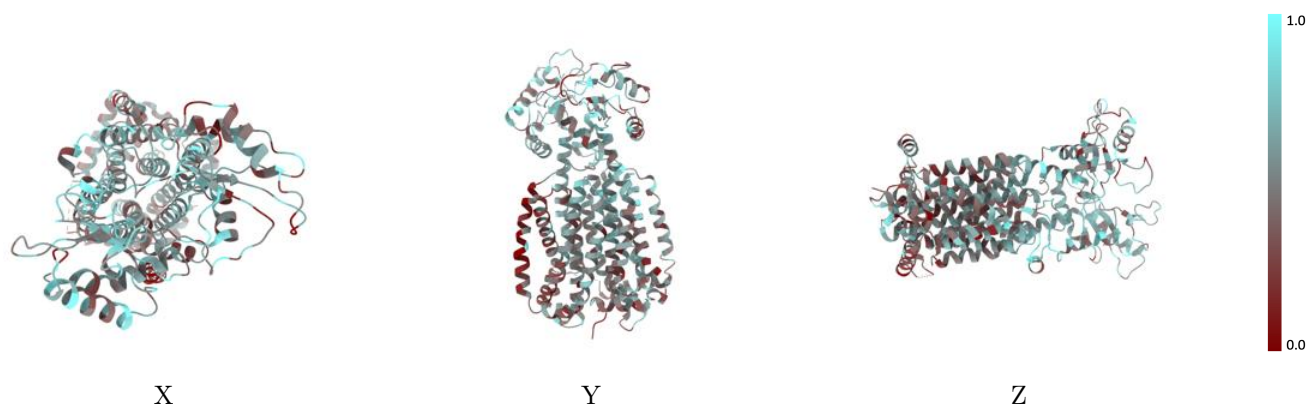
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



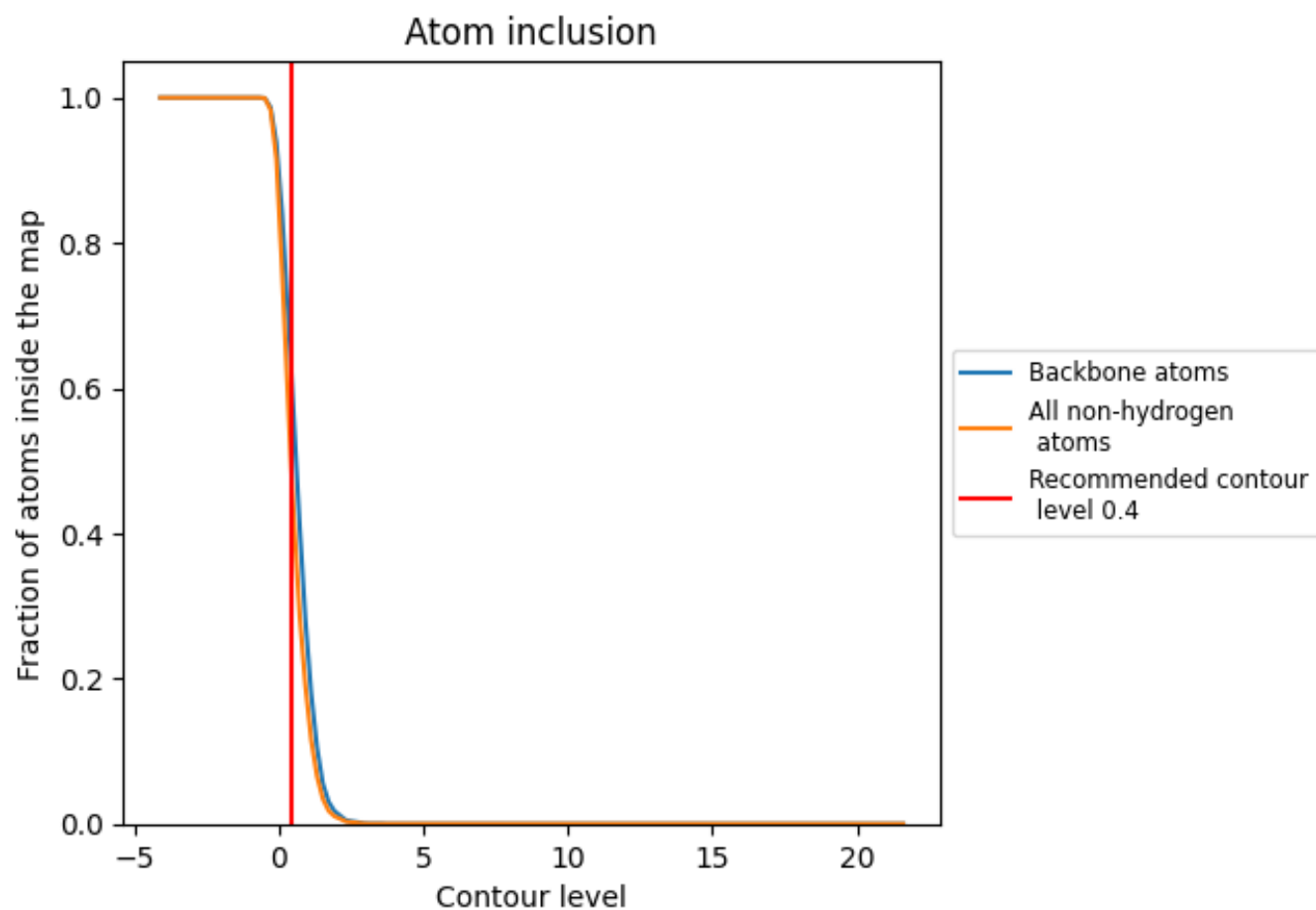
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.4).

9.4 Atom inclusion [i](#)



At the recommended contour level, 64% of all backbone atoms, 51% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.5064	<div></div> 0.3490
A	<div></div> 0.5064	<div></div> 0.3490

