



## wwPDB EM Validation Summary Report ⓘ

Nov 17, 2022 – 08:03 AM EST

PDB ID : 7LF6  
EMDB ID : EMD-23300  
Title : Structure of lysosomal membrane protein  
Authors : Shen, C.; Fu, T.M.; Wang, L.F.; Rawson, S.; Wu, H.  
Deposited on : 2021-01-15  
Resolution : 3.50 Å(reported)

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

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<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>.

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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

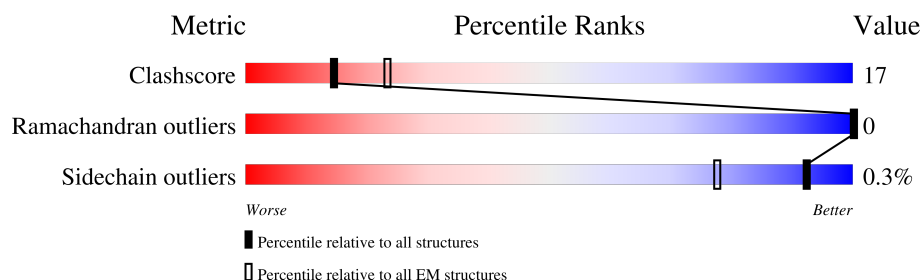
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.50 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)
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  $\geq 3$ , 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	504	<div> <div>12%</div> <div>52%</div> <div>29%</div> <div>19%</div> </div>
1	B	504	<div> <div>13%</div> <div>49%</div> <div>32%</div> <div>19%</div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6288 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.

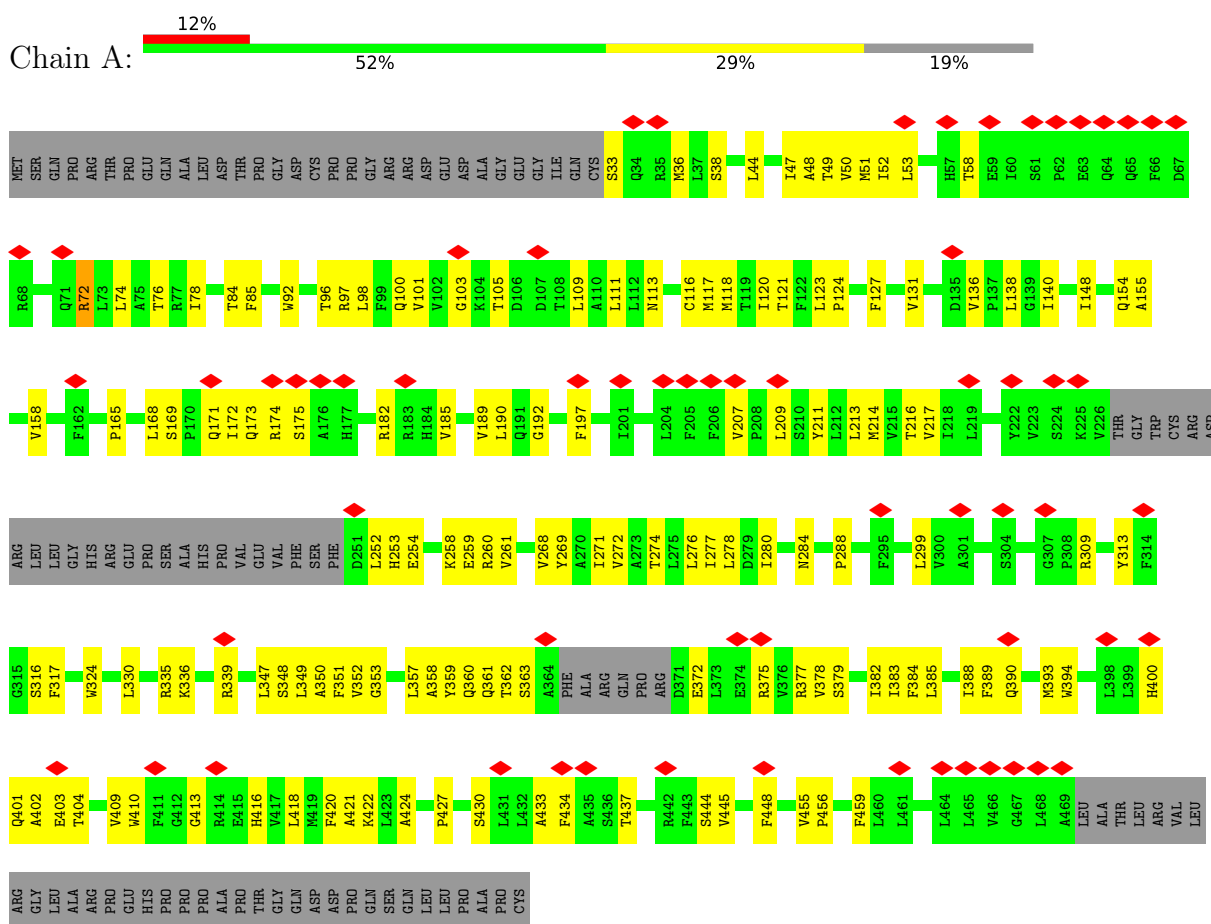
- Molecule 1 is a protein called Endosomal/lysosomal potassium channel TMEM175.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	407	Total	C	N	O	S	0	0
			3144	2082	508	534	20		
1	B	407	Total	C	N	O	S	0	0
			3144	2082	508	534	20		

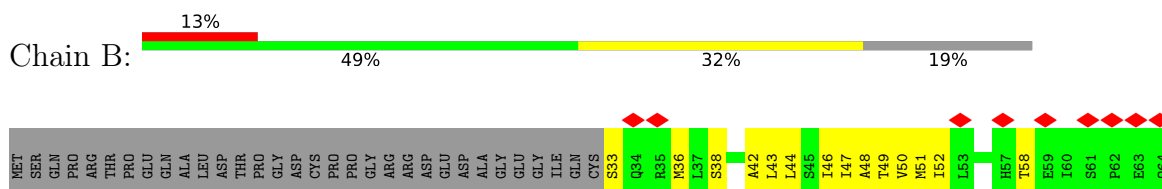
### 3 Residue-property plots

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: Endosomal/lysosomal potassium channel TMEM175



- Molecule 1: Endosomal/lysosomal potassium channel TMEM175



Q65	F66	D67	R68	Q71	R72	L73	L74	A75	T76	R77	I78	T84	F85	T89	W92	T96	R97	L98	F99	Q100	V101	V102	G103	K104	T105	D106	D107	T108	L109	A110	L111	L112	N113	C116	M117	M118	T119	I120	T121	F122	L123	P124	F127	V131	T132	F133	P134	D135	V136	F137	L138	
G139	I140	I148	A149	I150	Q154	A155	V158	F162	H163	F164	P165	L168	S169	P170	Q171	I172	Q173	R174	S175	A176	H177	R182	R183	H184	V185	V189	L190	F197	A198	A199	F202	S203	L204	F205	F206	V207	P208	L209	S210	Y211	L212	L213	M214	V215	T216	V217	I218	L219	L220	P221		
Y222	V223	S224	K225	V226	THR	GLY	TRP	CYS	ARG	ASP	ARG	LEU	LEU	GLY	HIS	ARG	GLU	PRO	SER	ALA	PHE	PHE	D251	L252	H253	E254	K258	E259	R260	V261	V268	Y269	A270	I271	V272	A273	T274	L275	L276	I277	L278	D279	I280	N284	R294	E295	A301					
S304	G307	P308	R309	F310	L311	A312	Y313	F314	G315	S316	F317	W324	L330	R335	K336	R339	L343	T346	L347	S348	L349	A350	F351	V352	G353	L357	A358	Y359	Q360	Q361	T362	S363	A364	PHE	ALA	ARG	GLN	PRO	ARG	D371	E372	L373	E374	R375	V376	R377	V378	S379	I382	I383		
F384	L385	I388	F389	Q390	M393	W394	L398	L399	H400	Q401	A402	E403	T404	V409	W410	F411	G412	G413	R414	E415	H416	V417	L418	W419	F420	A421	K422	L423	A424	P427	C428	A429	S430	L431	L432	A433	F434	A435	S436	T437	C438	L439	L440	S441	R442	F443	S444	V445	F448	A454	V455	P456
C457	A458	F459	L460	L461	L464	L465	V466	G467	L468	A469	LEU	ALA	THR	LEU	ARG	VAL	LEU	ARG	GLY	LEU	ALA	ARG	PRO	GLU	HIS	PRO	PRO	PRO	ALA	ALA	PRO	THR	GLY	GLN	ASP	PRO	PRO	GLN	SER	GLN	LEU	LEU	PRO	PRO	ALA	ALA	PRO	CYS				

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	117539	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 ( $e^-/\text{\AA}^2$ )	66.5	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	1.785	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.161	Depositor
Map size ( $\text{\AA}$ )	264.0, 264.0, 264.0	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	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	0.27	0/3221	0.49	0/4396
1	B	0.27	0/3221	0.49	0/4396
All	All	0.27	0/6442	0.49	0/8792

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	3144	0	3232	114	0
1	B	3144	0	3232	120	0
All	All	6288	0	6464	217	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 17.

The worst 5 of 217 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:359:TYR:HA	1:A:362:THR:HG22	1.66	0.76
1:A:101:VAL:HG23	1:A:172:ILE:HG13	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:359:TYR:HA	1:B:362:THR:HG22	1.66	0.75
1:B:101:VAL:HG23	1:B:172:ILE:HG13	1.67	0.74
1:A:278:LEU:HD13	1:B:50:VAL:HG23	1.70	0.72

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	401/504 (80%)	388 (97%)	13 (3%)	0	100	100
1	B	401/504 (80%)	388 (97%)	13 (3%)	0	100	100
All	All	802/1008 (80%)	776 (97%)	26 (3%)	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	340/426 (80%)	339 (100%)	1 (0%)	92	97
1	B	340/426 (80%)	339 (100%)	1 (0%)	92	97
All	All	680/852 (80%)	678 (100%)	2 (0%)	92	97

All (2) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	A	72	ARG
1	B	72	ARG

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	416	HIS

### 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.

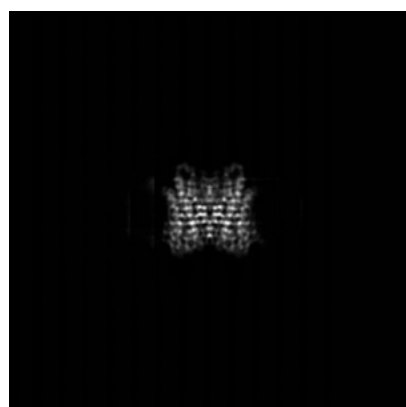
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23300. These allow visual inspection of the internal detail of the map and identification of artifacts.

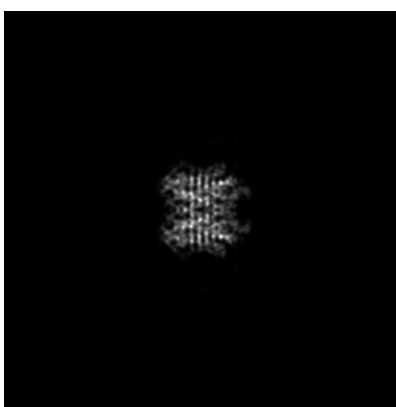
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

#### 6.1.1 Primary map



X



Y

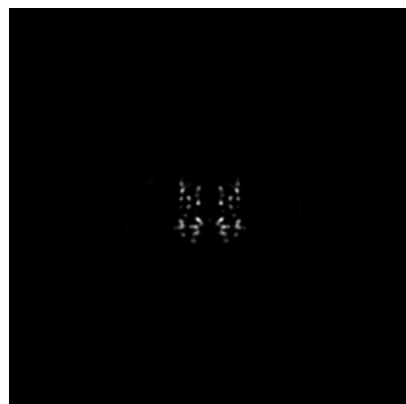


Z

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

### 6.2 Central slices [i](#)

#### 6.2.1 Primary map



X Index: 160



Y Index: 160

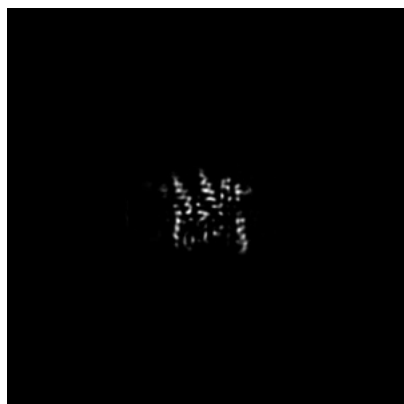


Z Index: 160

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

## 6.3 Largest variance slices [i](#)

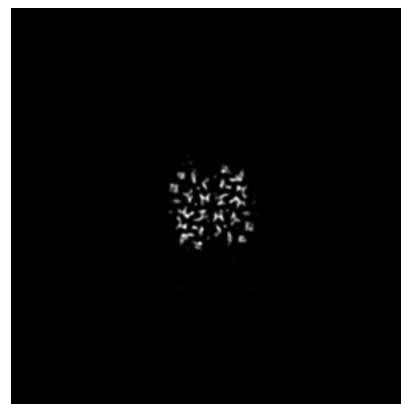
### 6.3.1 Primary map



X Index: 139



Y Index: 144

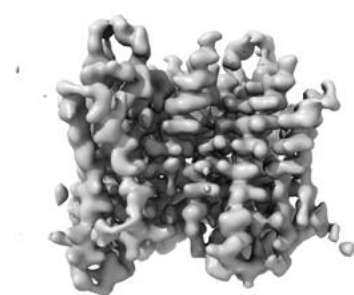


Z Index: 156

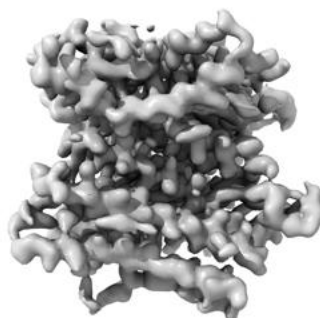
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views [i](#)

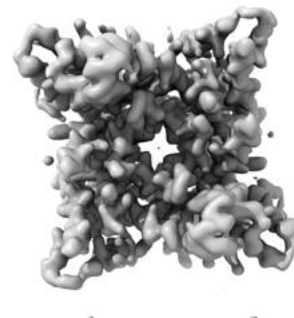
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.161. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

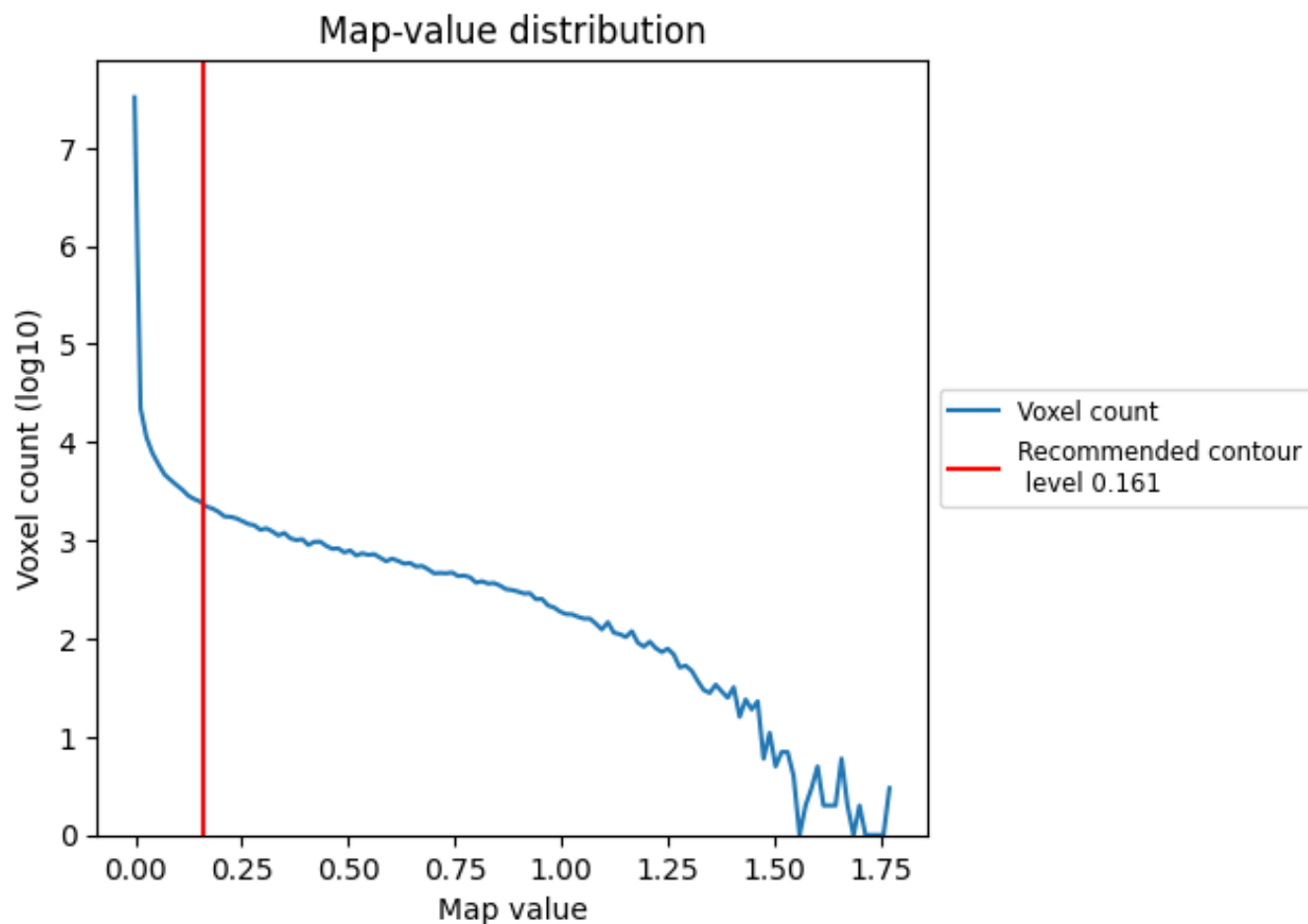
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

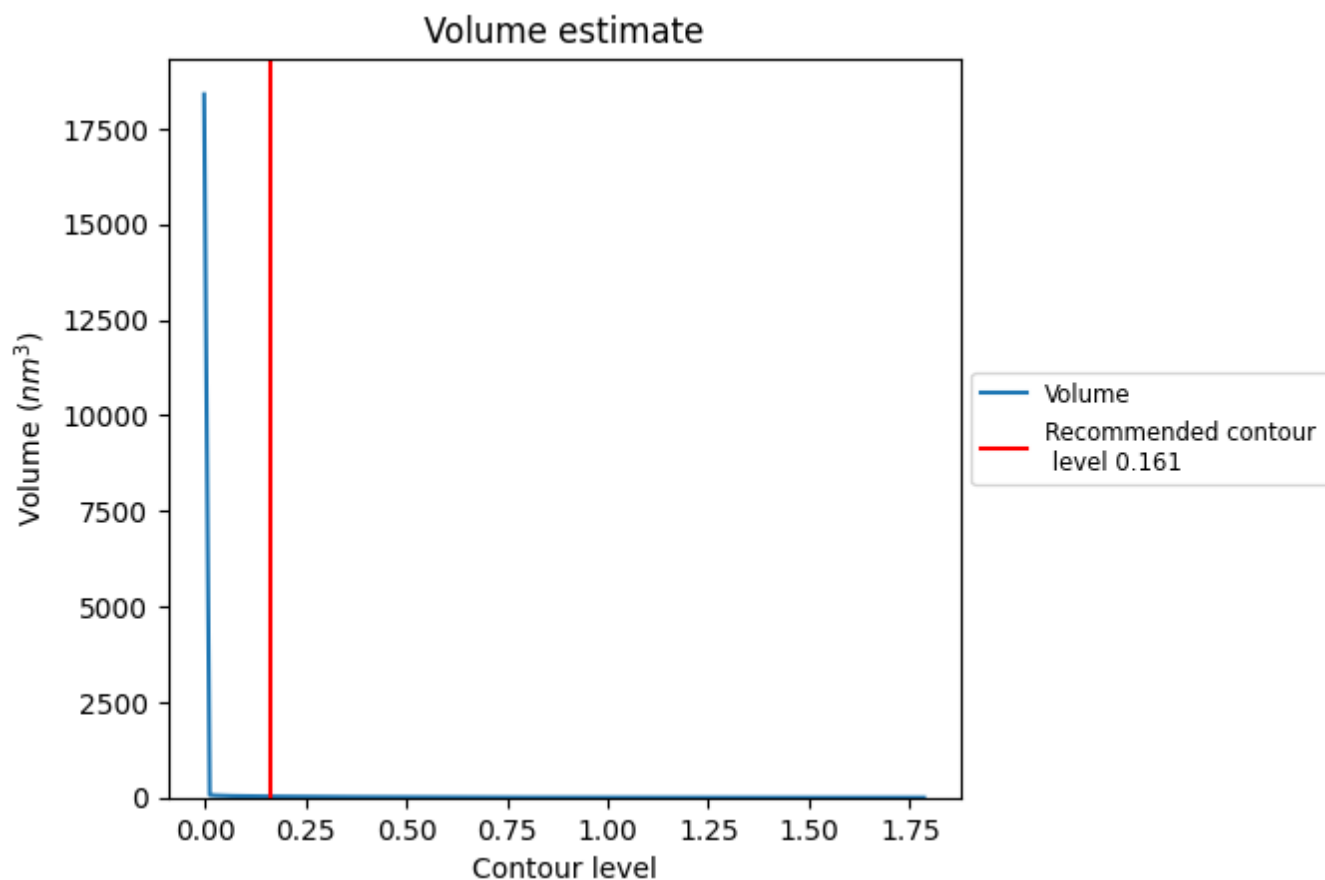
This section contains the results of statistical analysis of the map.

### 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.

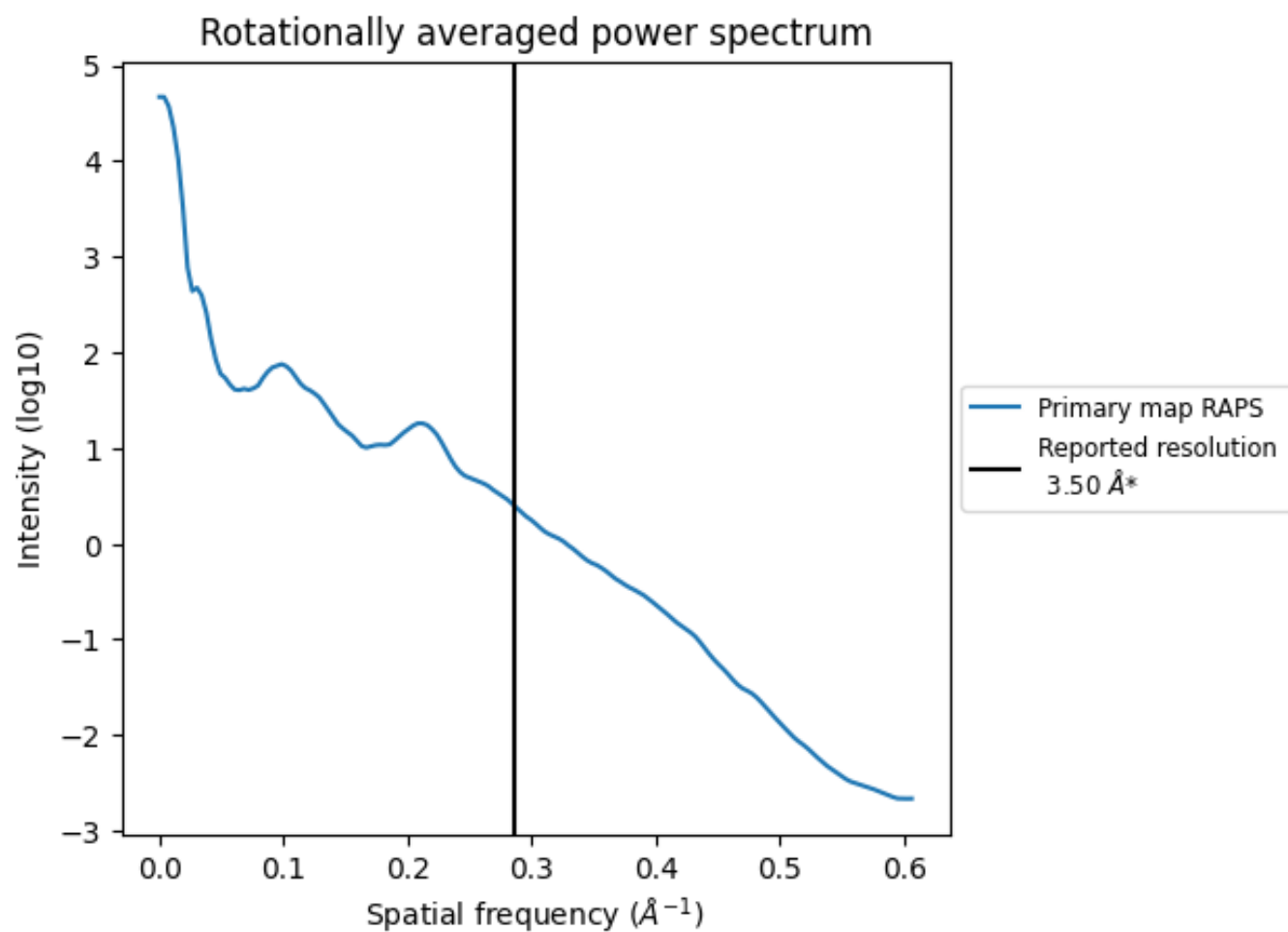
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 29 nm<sup>3</sup>; this corresponds to an approximate mass of 26 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 0.286 Å<sup>-1</sup>

## 8 Fourier-Shell correlation

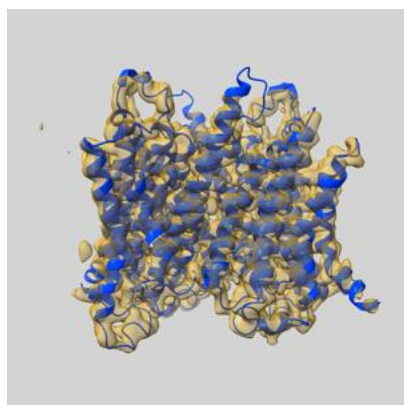
This section was not generated. No FSC curve or half-maps provided.



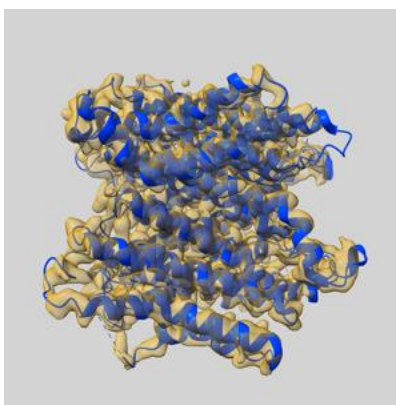
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-23300 and PDB model 7LF6. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

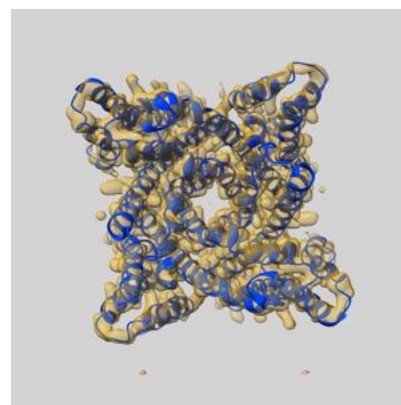
### 9.1 Map-model overlay [i](#)



X



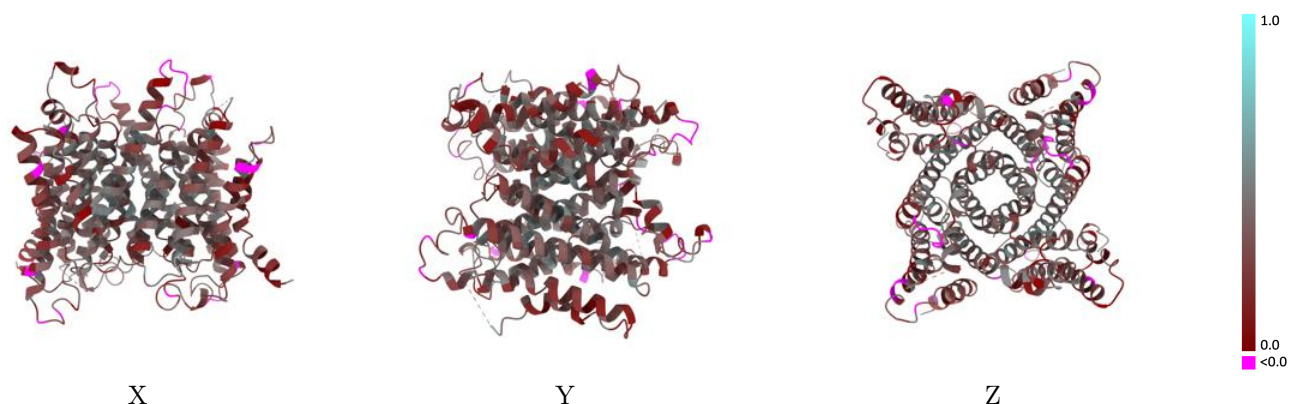
Y



Z

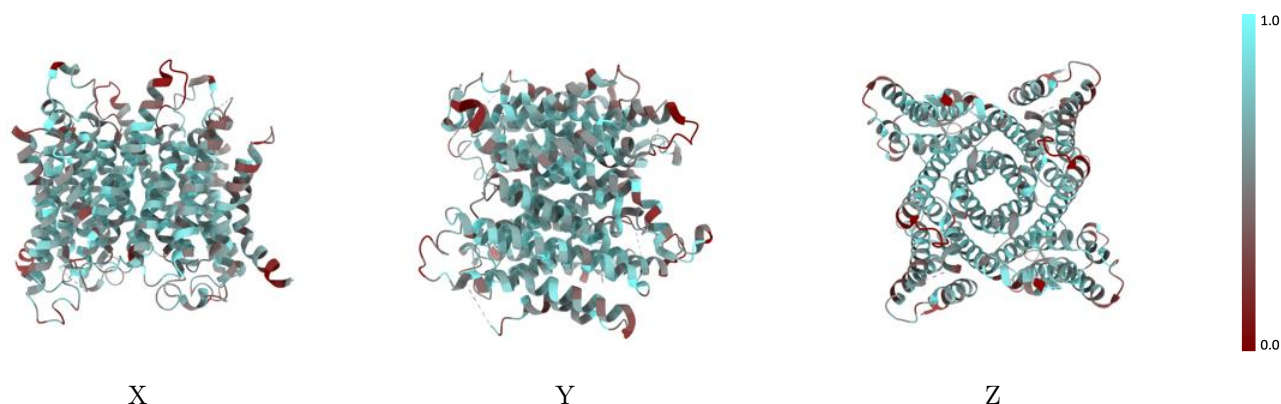
The images above show the 3D surface view of the map at the recommended contour level 0.161 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



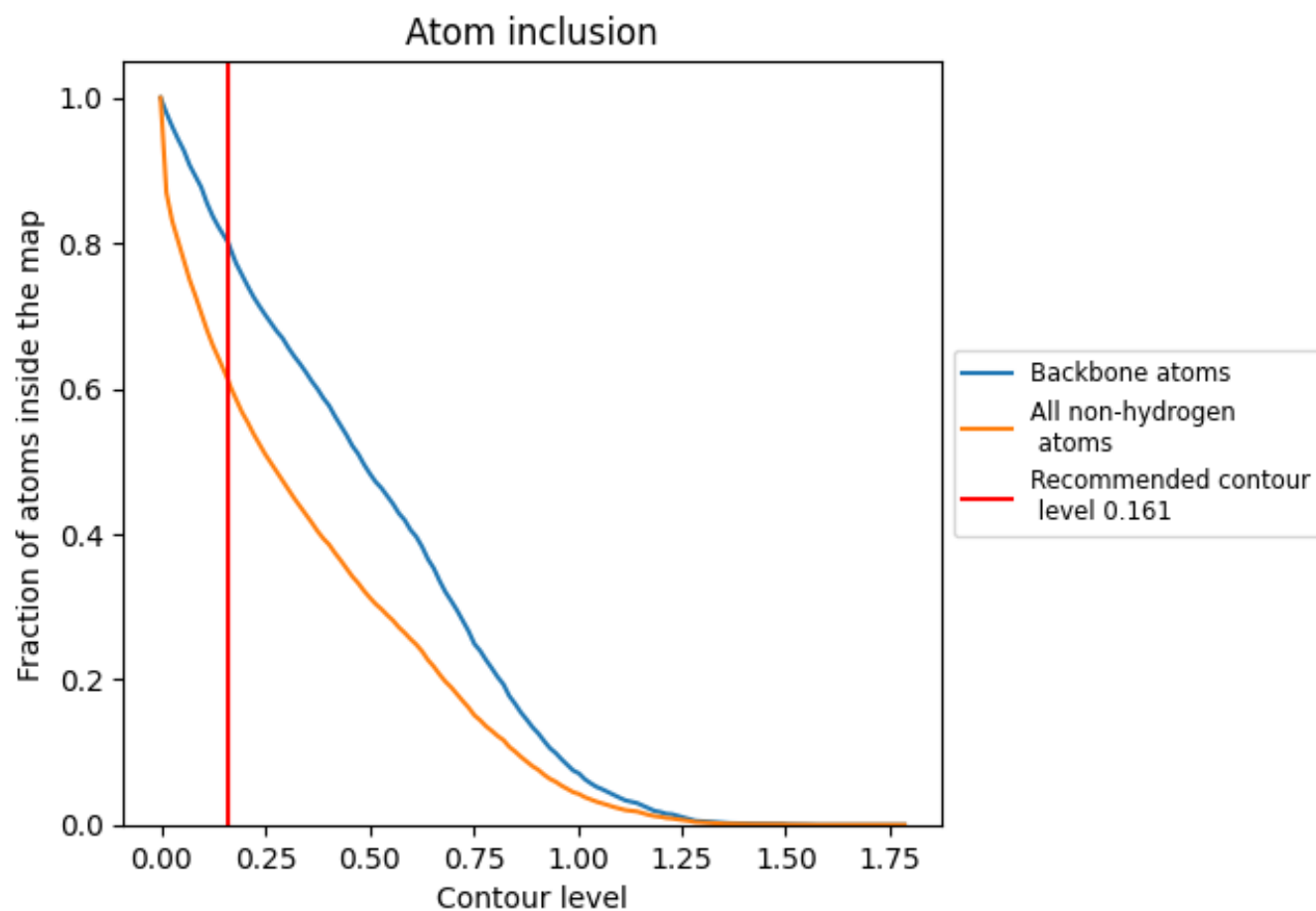
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.161).

## 9.4 Atom inclusion ⓘ



At the recommended contour level, 80% of all backbone atoms, 61% 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 (0.161) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6109	<div></div> 0.3070
A	<div></div> 0.6117	<div></div> 0.3060
B	<div></div> 0.6101	<div></div> 0.3070

