



Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 06:42 PM EST

PDB ID : 3J9J
EMDB ID : EMD-5778
Title : Structure of the capsaicin receptor, TRPV1, determined by single particle electron cryo-microscopy
Authors : Wang, R.Y.-R.; Barad, B.A.; Fraser, J.S.; DiMaio, F.
Deposited on : 2015-02-02
Resolution : 3.27 Å(reported)

This is a Full wwPDB EM Validation 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) : 2.31.3

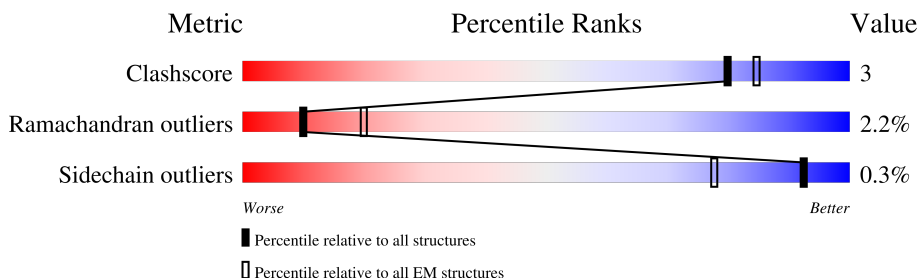
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.27 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	586	
1	B	586	
1	C	586	
1	D	586	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 21068 atoms, of which 10624 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 Transient receptor potential cation channel subfamily V member 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	315	Total	C	H	N	O	S	0	0
			5267	1738	2656	402	451	20		
1	B	315	Total	C	H	N	O	S	0	0
			5267	1738	2656	402	451	20		
1	C	315	Total	C	H	N	O	S	0	0
			5267	1738	2656	402	451	20		
1	D	315	Total	C	H	N	O	S	0	0
			5267	1738	2656	402	451	20		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	273	GLN	ASN	CONFLICT	UNP O35433
B	273	GLN	ASN	CONFLICT	UNP O35433
C	273	GLN	ASN	CONFLICT	UNP O35433
D	273	GLN	ASN	CONFLICT	UNP O35433



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	35645	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	21	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	31000	Depositor
Image detector	GATAN K2 (4k x 4k)	Depositor
Maximum map value	26.520	Depositor
Minimum map value	-13.649	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	7.0	Depositor
Map size (\AA)	311.1936, 311.1936, 311.1936	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.2156, 1.2156, 1.2156	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	0.83	0/2675	0.57	0/3613
1	B	0.83	0/2675	0.57	0/3613
1	C	0.83	0/2675	0.57	0/3613
1	D	0.83	0/2675	0.57	0/3613
All	All	0.83	0/10700	0.57	0/14452

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	2611	2656	2658	19	0
1	B	2611	2656	2658	17	0
1	C	2611	2656	2658	19	0
1	D	2611	2656	2658	18	0
All	All	10444	10624	10632	57	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 3.

All (57) 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:C:156:GLU:OE1	1:C:156:GLU:N	2.27	0.65
1:D:156:GLU:OE1	1:D:156:GLU:N	2.27	0.61
1:B:156:GLU:OE1	1:B:156:GLU:N	2.27	0.59
1:A:156:GLU:OE1	1:A:156:GLU:N	2.27	0.58
1:B:281:GLU:HA	1:B:281:GLU:OE1	2.10	0.52
1:A:281:GLU:HA	1:A:281:GLU:OE1	2.10	0.52
1:C:281:GLU:HA	1:C:281:GLU:OE1	2.10	0.52
1:D:281:GLU:HA	1:D:281:GLU:OE1	2.10	0.51
1:C:189:ILE:HA	1:D:274:MET:HE1	1.94	0.50
1:A:274:MET:HE1	1:B:189:ILE:HA	1.94	0.49
1:B:274:MET:HE1	1:D:189:ILE:HA	1.94	0.49
1:A:189:ILE:HA	1:C:274:MET:HE1	1.95	0.48
1:D:289:GLU:HA	1:D:289:GLU:OE1	2.15	0.47
1:B:289:GLU:HA	1:B:289:GLU:OE1	2.15	0.46
1:B:68:PHE:C	1:B:68:PHE:CD1	2.89	0.46
1:B:68:PHE:CD1	1:B:68:PHE:O	2.69	0.46
1:D:68:PHE:O	1:D:68:PHE:CD1	2.69	0.46
1:C:189:ILE:HG12	1:D:274:MET:SD	2.56	0.46
1:A:68:PHE:CD1	1:A:68:PHE:O	2.69	0.45
1:A:68:PHE:CD1	1:A:68:PHE:C	2.89	0.45
1:A:289:GLU:HA	1:A:289:GLU:OE1	2.15	0.45
1:C:289:GLU:HA	1:C:289:GLU:OE1	2.15	0.45
1:D:68:PHE:CD1	1:D:68:PHE:C	2.89	0.45
1:A:241:MET:HA	1:B:241:MET:SD	2.57	0.45
1:C:241:MET:SD	1:D:241:MET:HA	2.57	0.45
1:C:68:PHE:CD1	1:C:68:PHE:O	2.69	0.44
1:B:241:MET:HA	1:D:241:MET:SD	2.58	0.44
1:A:189:ILE:HG12	1:C:274:MET:SD	2.57	0.44
1:B:274:MET:SD	1:D:189:ILE:HG12	2.57	0.44
1:A:124:LYS:NZ	1:A:133:GLU:OE1	2.52	0.43
1:C:68:PHE:CD1	1:C:68:PHE:C	2.89	0.43
1:D:115:TYR:O	1:D:119:ARG:N	2.52	0.43
1:B:115:TYR:O	1:B:119:ARG:N	2.52	0.43
1:D:124:LYS:NZ	1:D:133:GLU:OE1	2.52	0.43
1:C:115:TYR:O	1:C:119:ARG:N	2.52	0.43
1:A:274:MET:SD	1:B:189:ILE:HG12	2.58	0.43
1:A:241:MET:SD	1:C:241:MET:HA	2.59	0.42
1:C:124:LYS:NZ	1:C:133:GLU:OE1	2.52	0.42
1:A:115:TYR:O	1:A:119:ARG:N	2.52	0.42
1:B:124:LYS:NZ	1:B:133:GLU:OE1	2.52	0.42
1:A:68:PHE:O	1:A:68:PHE:HD1	2.03	0.42
1:B:68:PHE:O	1:B:68:PHE:HD1	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:PHE:CZ	1:D:156:GLU:HA	2.55	0.41
1:D:68:PHE:O	1:D:68:PHE:HD1	2.03	0.41
1:A:252:PHE:CZ	1:B:156:GLU:HA	2.56	0.41
1:C:68:PHE:O	1:C:68:PHE:HD1	2.03	0.41
1:C:224:TYR:O	1:C:230:THR:OG1	2.36	0.41
1:C:236:LYS:HA	1:C:239:ILE:HG12	2.03	0.41
1:D:236:LYS:HA	1:D:239:ILE:HG12	2.03	0.41
1:A:156:GLU:HA	1:C:252:PHE:CZ	2.56	0.40
1:B:180:GLN:O	1:B:181:GLN:HB3	2.21	0.40
1:A:180:GLN:O	1:A:181:GLN:HB3	2.21	0.40
1:A:236:LYS:HA	1:A:239:ILE:HG12	2.03	0.40
1:A:224:TYR:O	1:A:230:THR:OG1	2.36	0.40
1:C:156:GLU:HA	1:D:252:PHE:CZ	2.56	0.40
1:C:180:GLN:O	1:C:181:GLN:HB3	2.21	0.40
1:D:180:GLN:O	1:D:181:GLN:HB3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	313/586 (53%)	295 (94%)	11 (4%)	7 (2%)	6	31
1	B	313/586 (53%)	296 (95%)	10 (3%)	7 (2%)	6	31
1	C	313/586 (53%)	296 (95%)	10 (3%)	7 (2%)	6	31
1	D	313/586 (53%)	296 (95%)	10 (3%)	7 (2%)	6	31
All	All	1252/2344 (53%)	1183 (94%)	41 (3%)	28 (2%)	10	31

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	181	GLN
1	B	181	GLN
1	C	181	GLN
1	D	181	GLN
1	A	129	ASP
1	A	221	ASP
1	B	129	ASP
1	B	221	ASP
1	C	129	ASP
1	C	221	ASP
1	D	129	ASP
1	D	221	ASP
1	A	13	ASN
1	A	287	ALA
1	B	13	ASN
1	B	287	ALA
1	C	13	ASN
1	C	287	ALA
1	D	13	ASN
1	D	287	ALA
1	A	49	PHE
1	B	49	PHE
1	C	49	PHE
1	D	49	PHE
1	A	286	ILE
1	B	286	ILE
1	C	286	ILE
1	D	286	ILE

5.3.2 Protein sidechains ⓘ

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	288/519 (56%)	287 (100%)	1 (0%)	92	96
1	B	288/519 (56%)	287 (100%)	1 (0%)	92	96
1	C	288/519 (56%)	288 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	288/519 (56%)	287 (100%)	1 (0%)	92	96
All	All	1152/2076 (56%)	1149 (100%)	3 (0%)	92	96

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	PHE
1	B	68	PHE
1	D	68	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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.

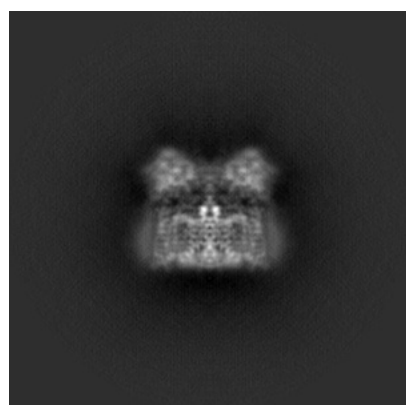
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-5778. These allow visual inspection of the internal detail of the map and identification of artifacts.

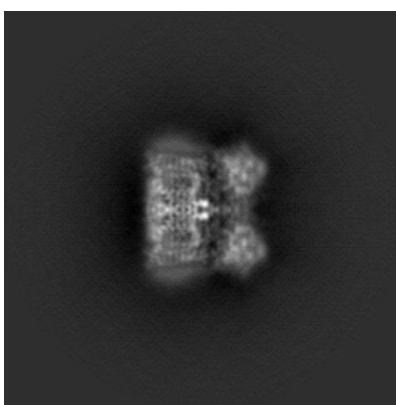
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

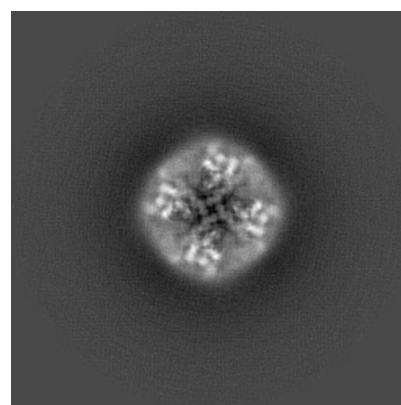
6.1.1 Primary map



X



Y

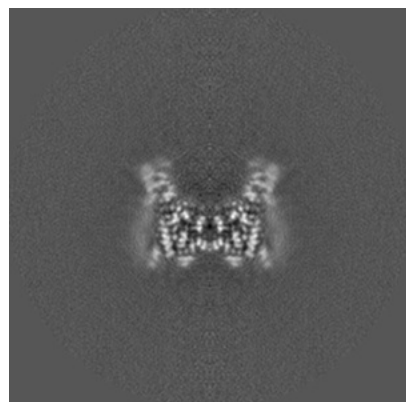


Z

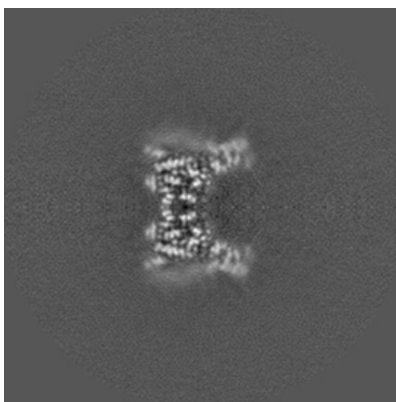
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

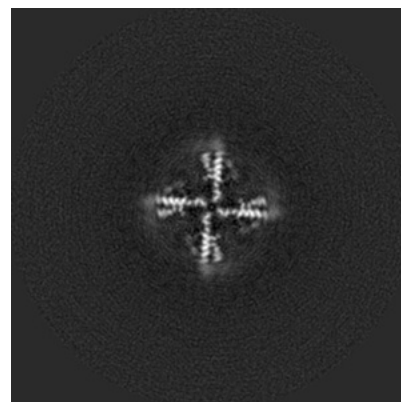
6.2.1 Primary map



X Index: 128



Y Index: 128

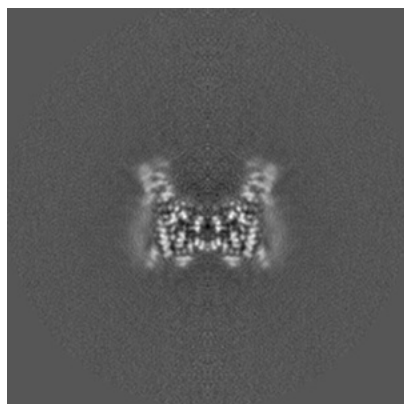


Z Index: 128

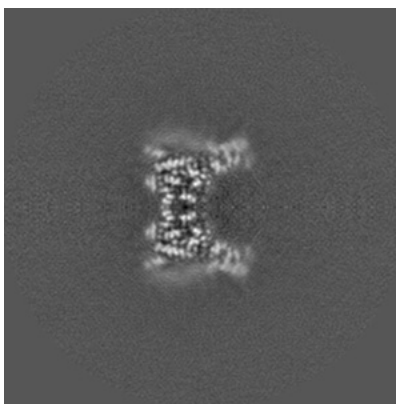
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

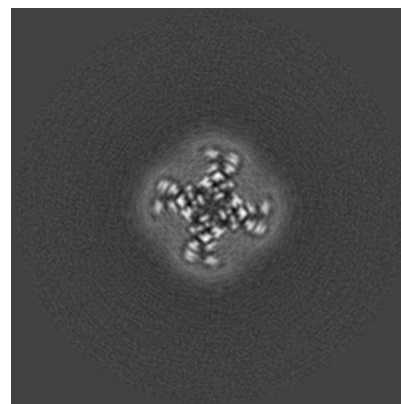
6.3.1 Primary map



X Index: 128



Y Index: 128

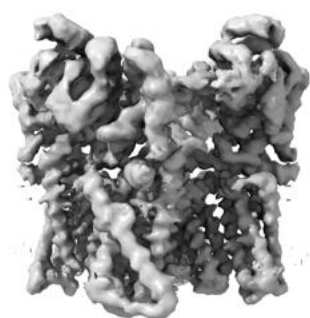


Z Index: 99

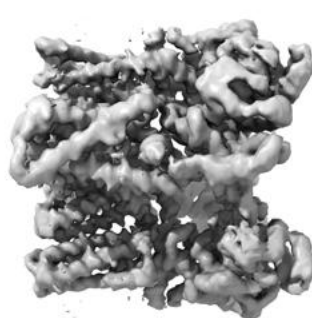
The images above show the largest variance slices of the map in three orthogonal directions.

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 7.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

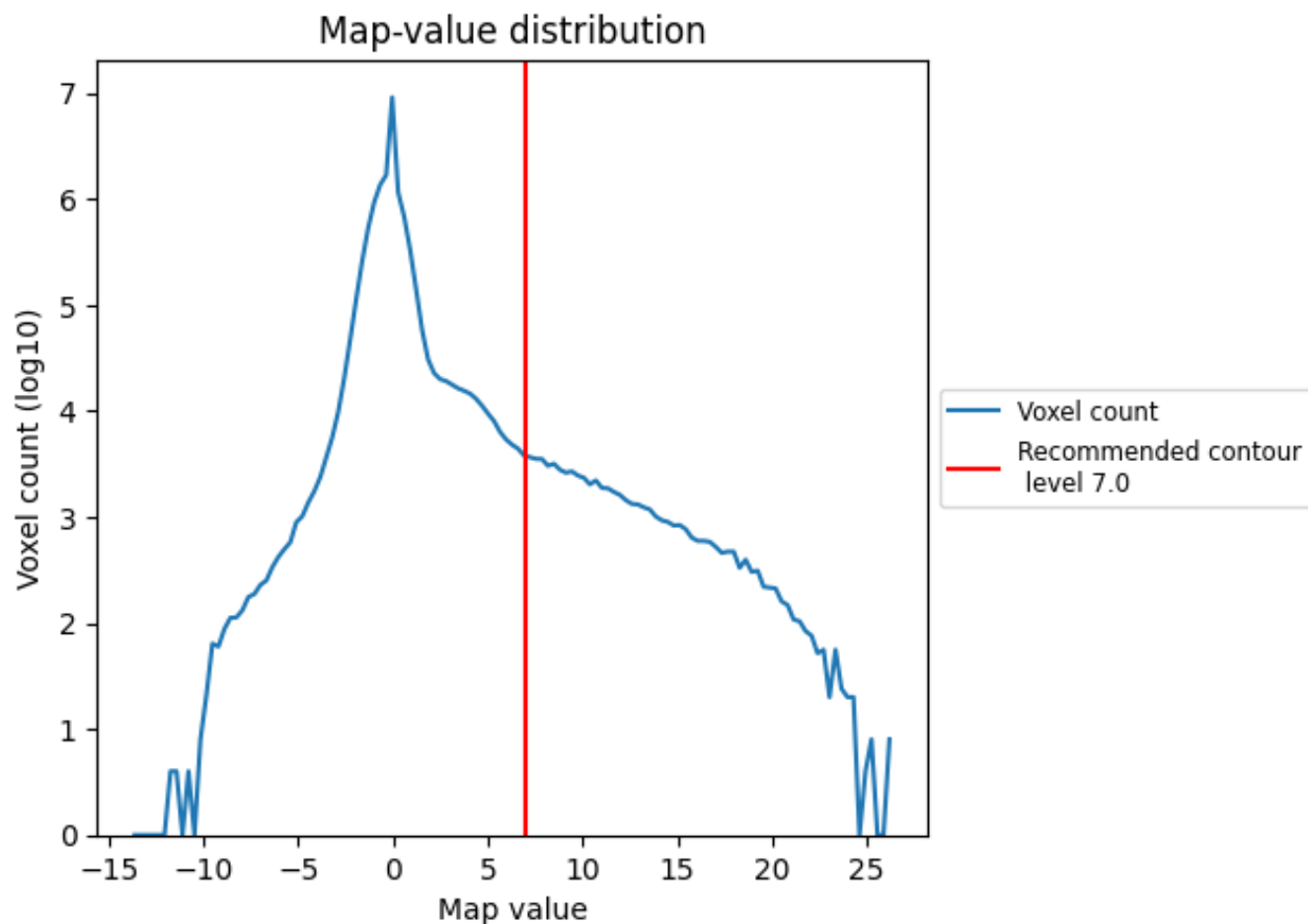
6.5 Mask visualisation

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

7 Map analysis [i](#)

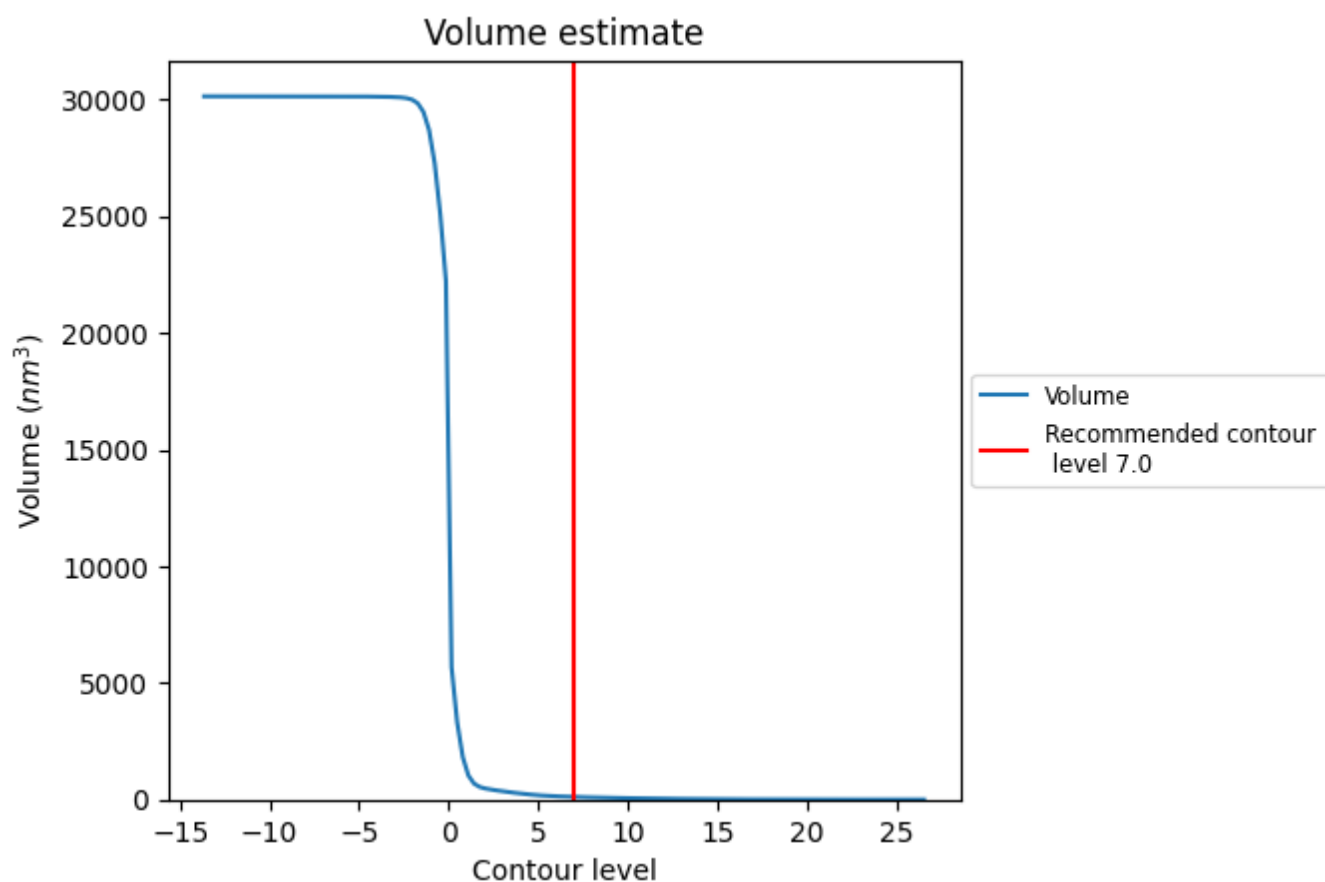
This section contains the results of statistical analysis of the map.

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.

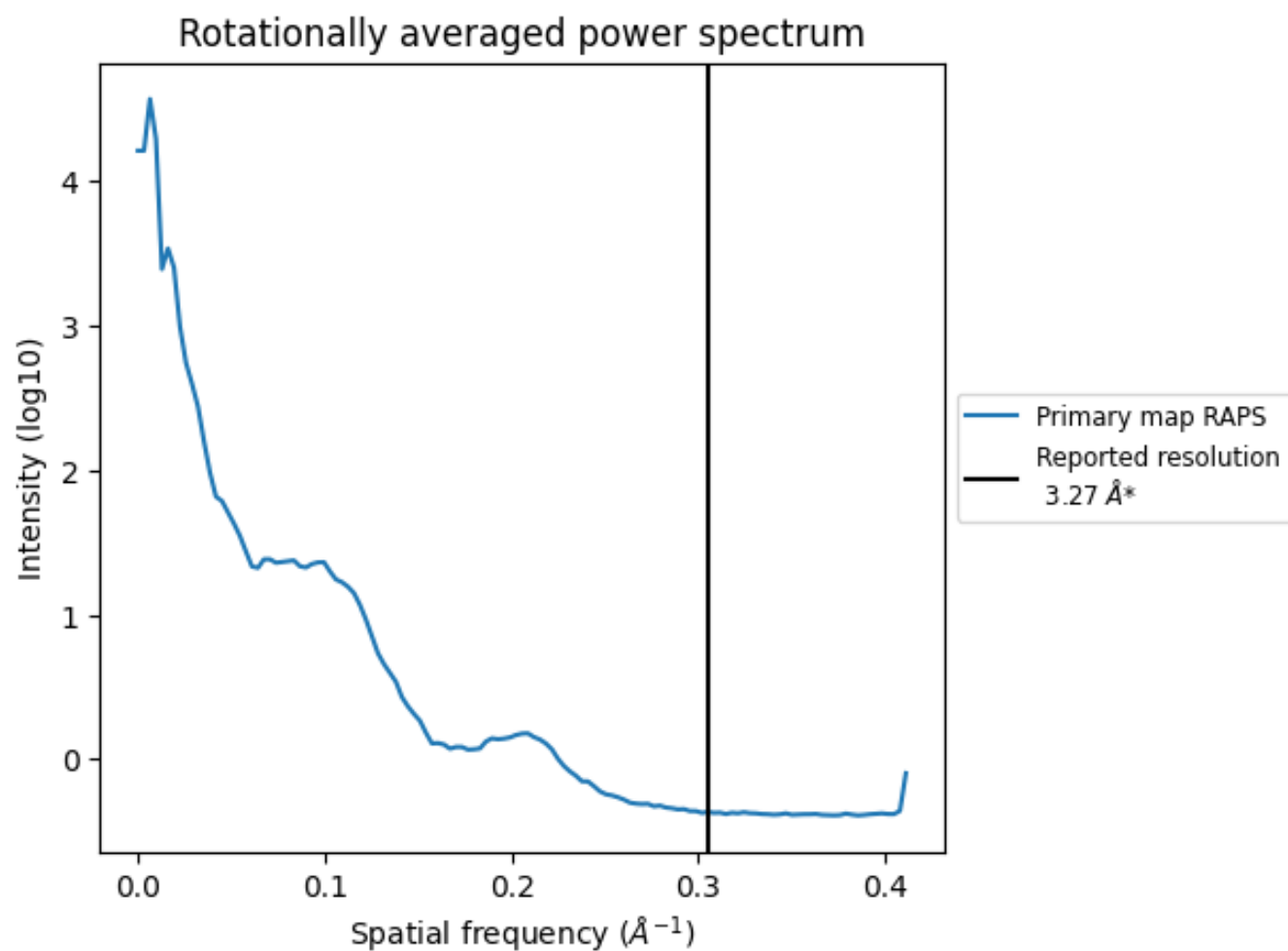
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 113 nm³; this corresponds to an approximate mass of 102 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 0.305 Å⁻¹

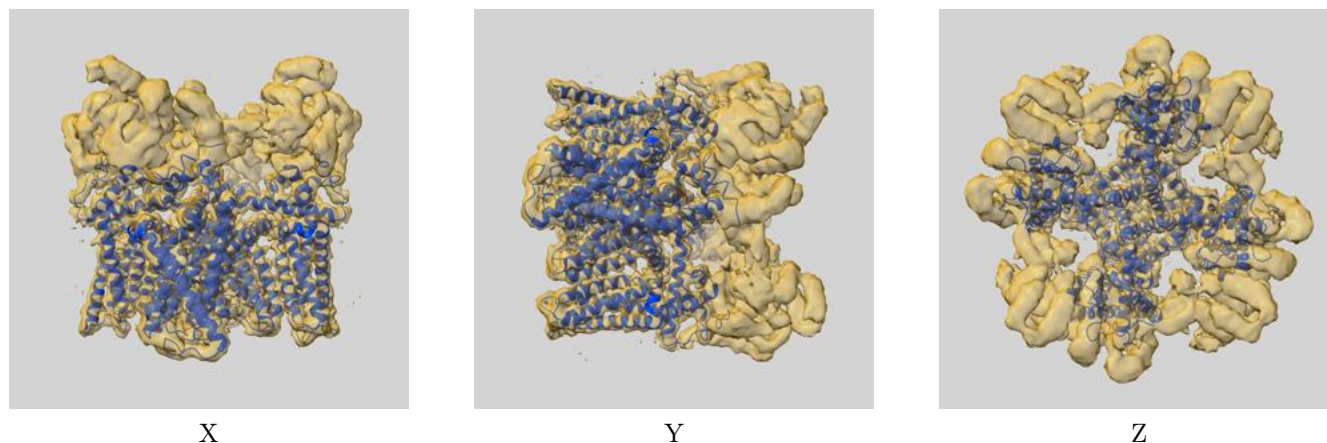
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

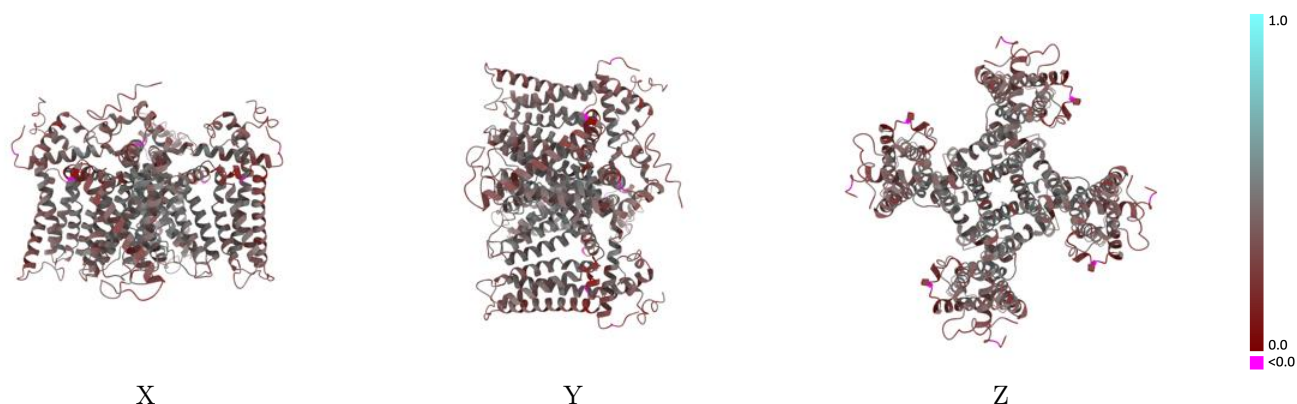
This section contains information regarding the fit between EMDB map EMD-5778 and PDB model 3J9J. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



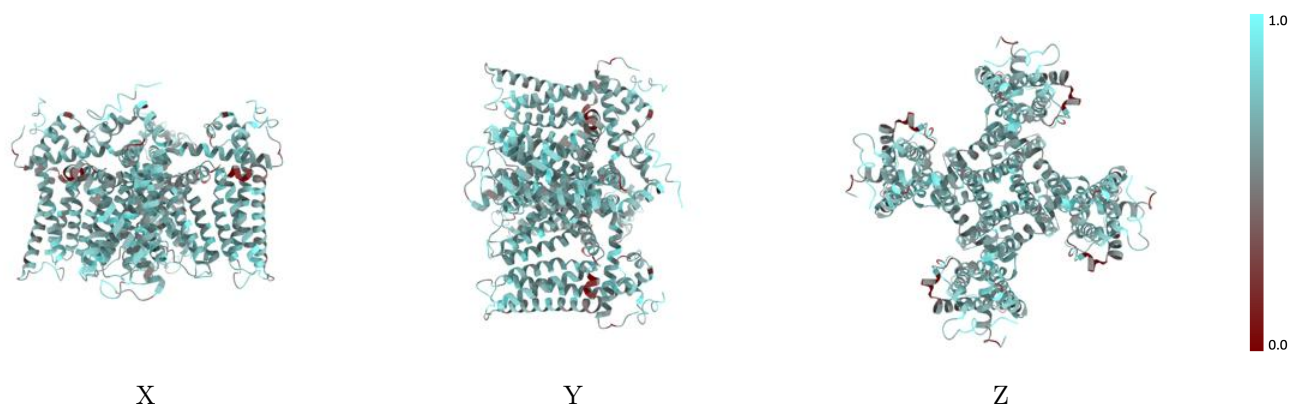
The images above show the 3D surface view of the map at the recommended contour level 7.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



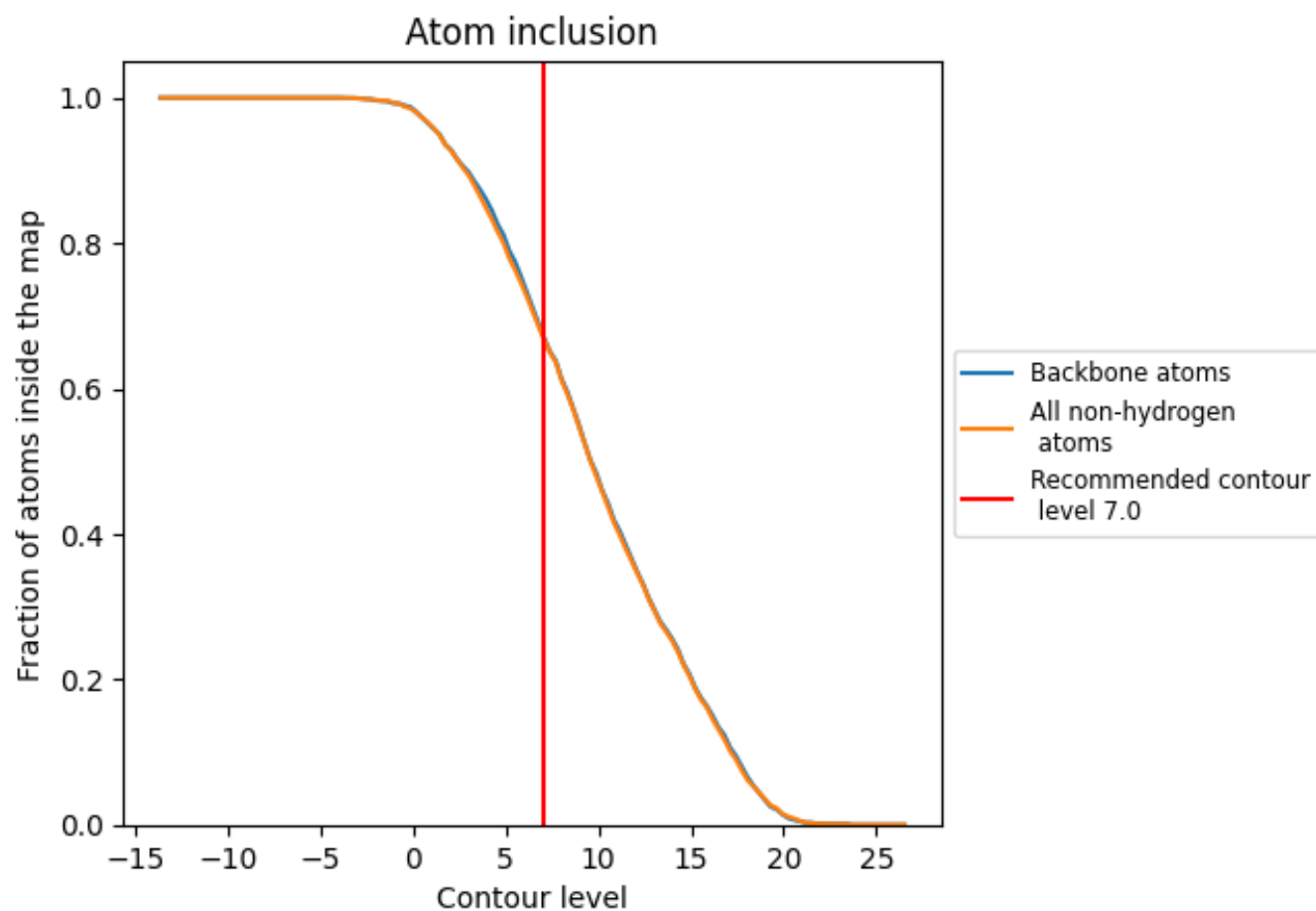
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (7.0).

9.4 Atom inclusion [i](#)



At the recommended contour level, 67% of all backbone atoms, 67% 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 (7.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6703	<div></div> 0.3700
A	<div></div> 0.6806	<div></div> 0.3720
B	<div></div> 0.6806	<div></div> 0.3700
C	<div></div> 0.6802	<div></div> 0.3700
D	<div></div> 0.6806	<div></div> 0.3700

