



wwPDB EM Validation Summary Report ⓘ

Nov 7, 2022 – 02:08 AM EST

PDB ID : 6OCE
EMDB ID : EMD-20017
Title : Structure of the rice hyperosmolality-gated ion channel OSCA1.2
Authors : Maity, K.; Heumann, J.M.; McGrath, A.P.; Chang, G.; Stowell, M.H.
Deposited on : 2019-03-23
Resolution : 4.90 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.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

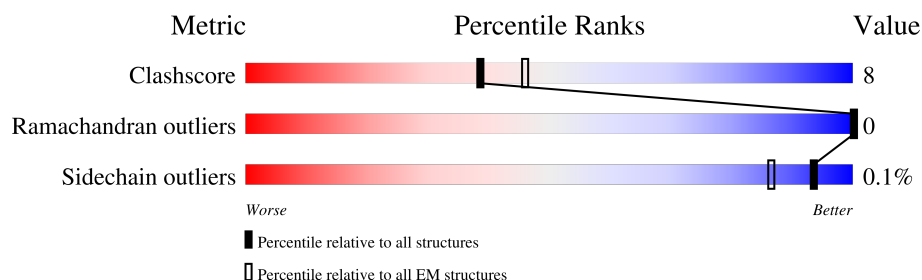
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.90 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	774	<div> <div>42%</div> <div>77%</div> <div>12%</div> <div>11%</div> </div>
1	B	774	<div> <div>40%</div> <div>76%</div> <div>12%</div> <div>11%</div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 11228 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 stress-gated cation channel 1.2.


Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	689	Total	C	N	O	S	0	0
			5614	3716	915	963	20		
1	B	689	Total	C	N	O	S	0	0
			5614	3716	915	963	20		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	767	ILE	-	expression tag	UNP Q5TKG1
A	768	LYS	-	expression tag	UNP Q5TKG1
A	769	PRO	-	expression tag	UNP Q5TKG1
A	770	GLN	-	expression tag	UNP Q5TKG1
A	771	LEU	-	expression tag	UNP Q5TKG1
A	772	GLU	-	expression tag	UNP Q5TKG1
A	773	GLY	-	expression tag	UNP Q5TKG1
A	774	SER	-	expression tag	UNP Q5TKG1
B	767	ILE	-	expression tag	UNP Q5TKG1
B	768	LYS	-	expression tag	UNP Q5TKG1
B	769	PRO	-	expression tag	UNP Q5TKG1
B	770	GLN	-	expression tag	UNP Q5TKG1
B	771	LEU	-	expression tag	UNP Q5TKG1
B	772	GLU	-	expression tag	UNP Q5TKG1
B	773	GLY	-	expression tag	UNP Q5TKG1
B	774	SER	-	expression tag	UNP Q5TKG1

SER	ILE	SER	GLU	ASP	VAL	GLY	MET	GLU	VAL	ILE	VAL	PRO	THR	LYS	ARG	GLN	SER	ARG	ASN	THR	PRO	ALA	GLN	SER	LYS	TYR	GLU	GLY	SER	ASP	THR	LEU	SER	LEU	PRO	GLU	THR	VAL	HIS	GLU	ARG	ILE	LYS	PRO	GLN	LEU	GLY	SER
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• Molecule 1: stress-gated cation channel 1.2

Chain B: 

ILE	VAL	PRO	THR	LYS	GLN	SER	ARG	ARG	ARG	THR	PRO	ALA	GLN	LYS	GLY	SER	ASP	THR	THR	LEU	SER	LEU	PRO	GLU	THR	THR	VAL	HIS	GLU	ARG	ILE	LYS	PRO	LEU	GLY	SER																				
G640	L641	L642	S643	T644	R645	G646	F647	E648	E649	T650	V653	L654	V655	V656	P658	V659	L660	T661	F662	K666	M670	R678	E691	D699	L704	A707	Y708	V712	PHE	LYS	GLY	ARG	GLU	GLU	GLU	ASP	ASN	MET	ILE	SER	GLU	ASP	VAL	GLY	MET	GLU	GLU	VAL								
E552	E553	A554	M555	D556	P557	G558	S559	I560	W564	R568	I569	Y572	L577	V578	Y579	A580	Y581	L585	L586	L587	P588	F589	T590	L591	V592	F593	F594	Y598	R602	I605	Y609	M610	Q611	Q612	Y613	E614	S615	R626	L629	I632	Q635	L636	L637	L638	I639											
G475	T479	G480	S481	A482	L483	D484	Q485	L486	K487	A488	Y489	I490	H491	Q492	S493	A494	M495	E496	I497	P498	R499	T500	L501	G502	V503	A504	M507	R508	A509	T510	Y515	V518	D519	T522	A525	G526	E527	I528	L529	R530	L531	R532	H538	N541	F542	F543	L544	V545	K546	T547	E548					
E399	G400	E402	K403	A404	L405	F406	Q407	L408	K409	P410	L411	I412	K413	I414	D415	V416	I417	K418	S419	F420	I421	F424	L425	P426	G427	I428	K431	V432	F433	L434	I435	L436	L437	P438	T439	I440	F443	F447	E448	G449	L450	I451	L456	E457	I466	F467	L468	F469	F470	F473	L474					
M309	K310	D311	P312	Q313	S314	A315	R326	A329	A330	T342	V343	W344	I345	T346	E347	W348	A349	P350	P352	R353	D354	V355	N358	I362	V365	S366	L367	R370	R371	V376	A377	F378	F379	F383	F384	I387	P388	I389	A390	F391	V392	Q393	S394	L395	A396	S397	L398									
L244	V245	E246	K249	K250	L251	Q252	W253	W254	L255	D256	Y257	Y258	Q259	L260	K261	Y262	E263	R264	N265	P266	S267	K268	R269	P270	T271	T272	K273	T274	G275	F276	L277	G278	C279	F280	G281	S282	E283	D285	V284	A286	L287	E288	Y289	Y290	K291	L294	E295	K296	I297	Q298	K299	E300	E301	E304	R305	Q306
I145	N147	I148	P149	Y150	G151	N152	M153	R154	T157	H158	L159	V160	M161	A162	Y163	A164	T165	T166	F167	W168	Y171	F174	R175	R186	K192	D196	Q197	N204	D208	P209	D210	E211	E215	L222	H228	R231	H232	Q233	N237	A238	N239	K240	A242	D243												
R67	S68	Y69	L70	L73	S74	A78	A79	L80	K81	A91	G92	L93	I101	Y102	L103	G105	I106	K107	I108	F109	V110	P111	I112	S113	I114	A116	S117	L118	V119	L120	F121	P122	V123	M124	W125	T126	M127	D128	T129	L130	D131	S132	M133	K134	V135	V136	H137	S138	K139	I140	L143	S144				
MET	ALA	T3	V4	S5	D6	I7	G8	L9	S10	A11	A12	I13	I14	V15	S16	M17	A18	F21	V24	F25	L28	R29	L30	Q31	D35	R36	F39	P40	K41	W42	TYR	LEU	ARG	GLY	MET	ARG	ASP	SER	PRO	VAL	SER	GLY	ALA	VAL	GLN	LYS	VAL	ASN	L64	N65	N66					

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	64096	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 ($e^-/\text{\AA}^2$)	55	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.097	Depositor
Minimum map value	-0.052	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	331.2, 331.2, 331.2	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.38, 1.38, 1.38	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	1/5771 (0.0%)	0.44	4/7850 (0.1%)
1	B	0.30	1/5771 (0.0%)	0.44	2/7850 (0.0%)
All	All	0.30	2/11542 (0.0%)	0.44	6/15700 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	111	PRO	CB-CG	-6.80	1.16	1.50
1	B	111	PRO	CB-CG	-5.36	1.23	1.50

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	111	PRO	CA-N-CD	-9.79	97.80	111.50
1	B	111	PRO	CA-N-CD	-9.15	98.69	111.50
1	A	110	VAL	C-N-CD	5.72	140.41	128.40
1	A	285	ASP	N-CA-C	5.54	125.95	111.00
1	B	110	VAL	C-N-CD	5.47	139.88	128.40

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	5614	0	5718	78	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	5614	0	5718	101	0
All	All	11228	0	11436	179	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 8.

The worst 5 of 179 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:107:LYS:O	1:A:110:VAL:HG22	1.06	1.23
1:B:107:LYS:O	1:B:110:VAL:CG2	1.87	1.21
1:A:107:LYS:O	1:A:110:VAL:CG2	1.93	1.17
1:B:107:LYS:O	1:B:110:VAL:HG22	0.94	1.11
1:B:395:LEU:HD11	1:B:426:PRO:HB3	1.42	0.97

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	685/774 (88%)	620 (90%)	65 (10%)	0	100	100
1	B	685/774 (88%)	615 (90%)	70 (10%)	0	100	100
All	All	1370/1548 (88%)	1235 (90%)	135 (10%)	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	612/688 (89%)	612 (100%)	0	100	100
1	B	612/688 (89%)	611 (100%)	1 (0%)	93	96
All	All	1224/1376 (89%)	1223 (100%)	1 (0%)	93	96

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

Mol	Chain	Res	Type
1	B	662	PHE

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

Mol	Chain	Res	Type
1	B	336	GLN

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 ⓘ

There are no chain breaks in this entry.

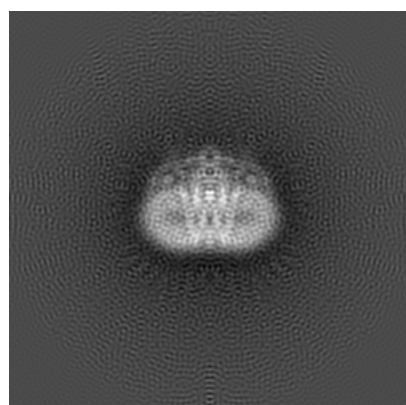
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20017. These allow visual inspection of the internal detail of the map and identification of artifacts.

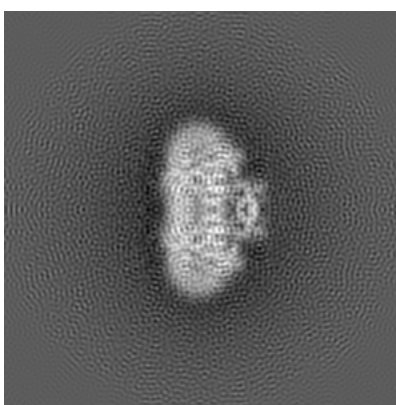
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

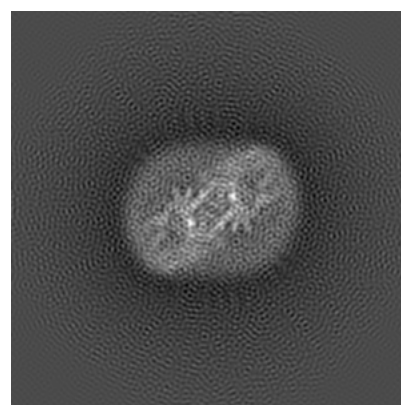
6.1.1 Primary map



X



Y

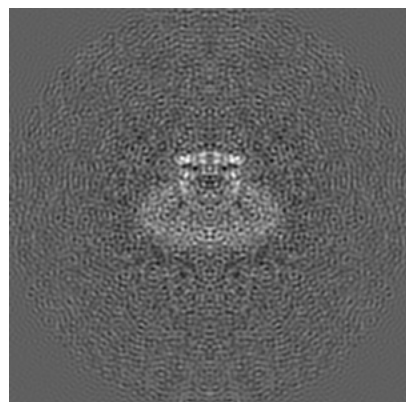


Z

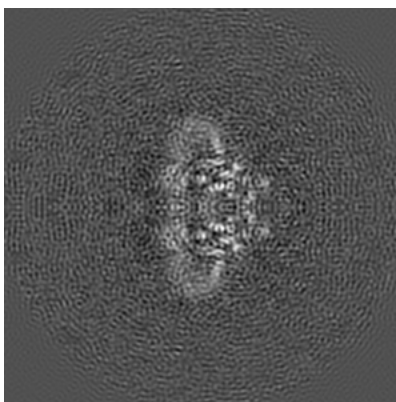
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

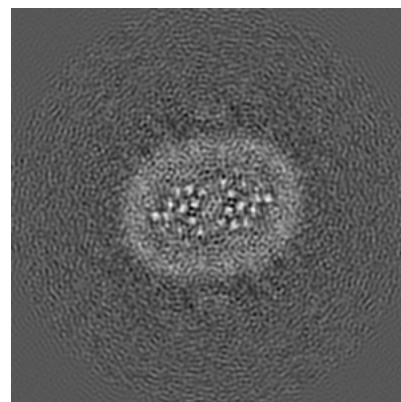
6.2.1 Primary map



X Index: 120



Y Index: 120

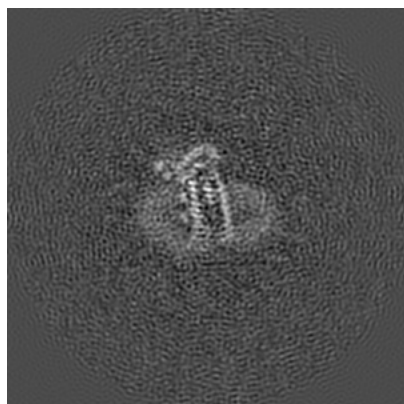


Z Index: 120

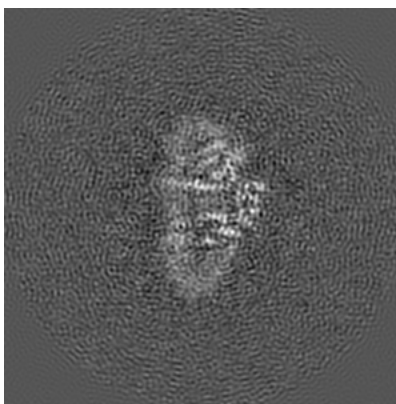
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

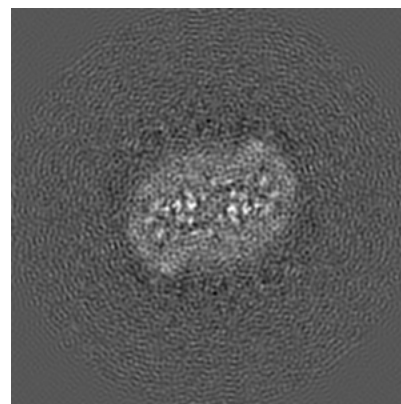
6.3.1 Primary map



X Index: 107



Y Index: 127



Z Index: 130

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

6.4 Orthogonal surface views [i](#)

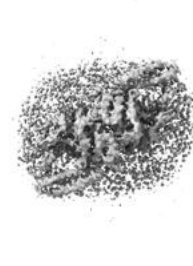
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

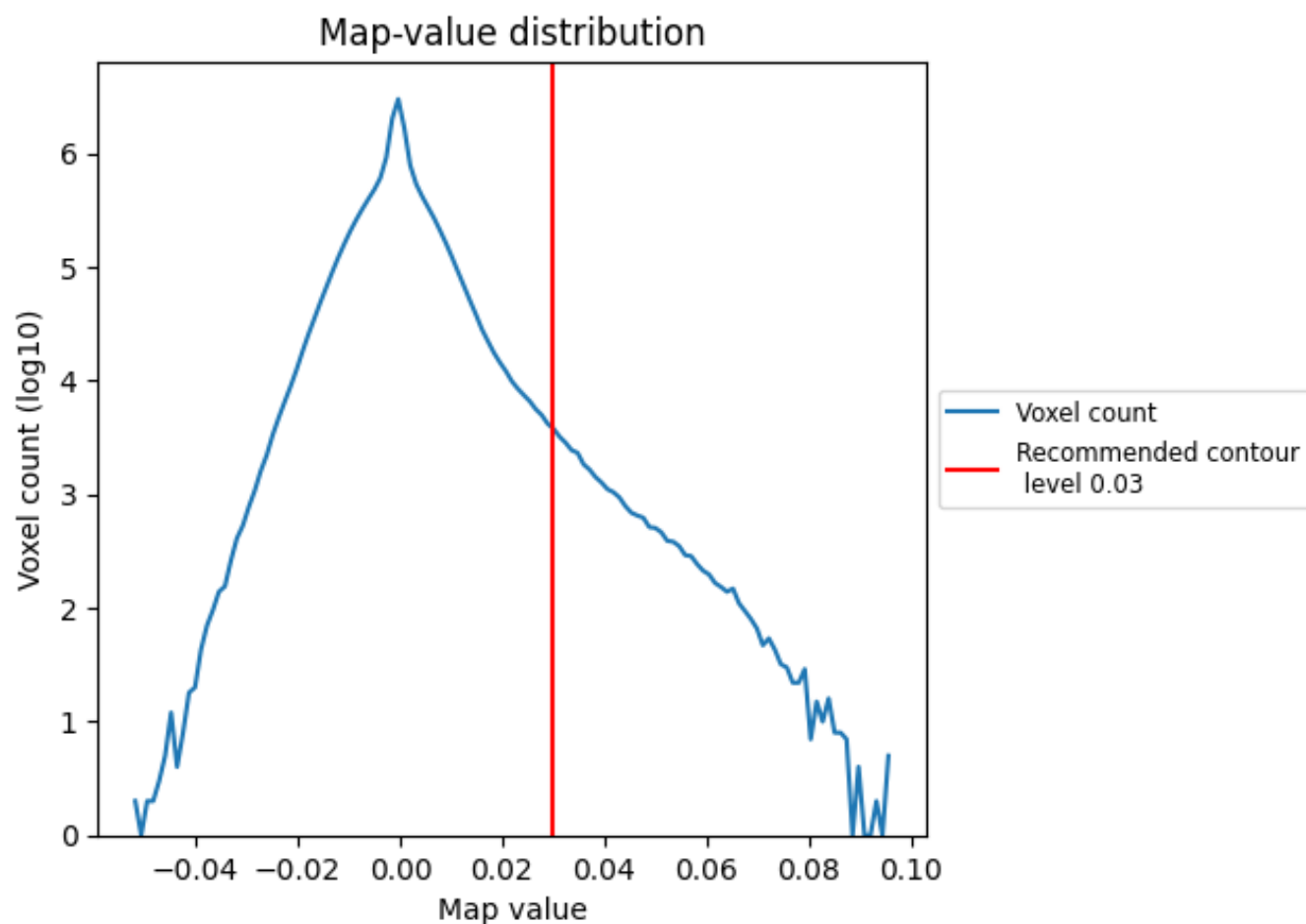
6.5 Mask visualisation

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

7 Map analysis [i](#)

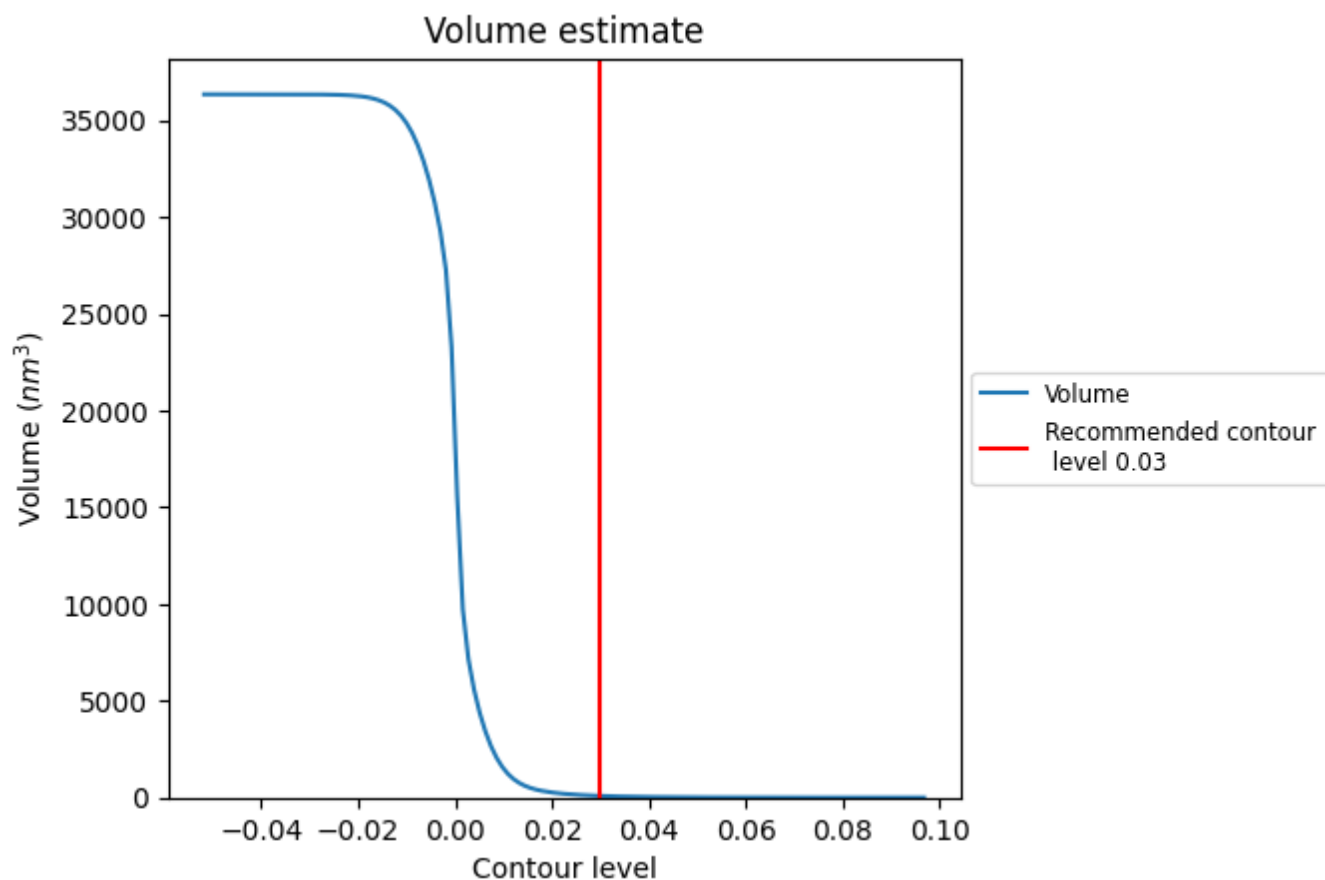
This section contains the results of statistical analysis of the map.

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.

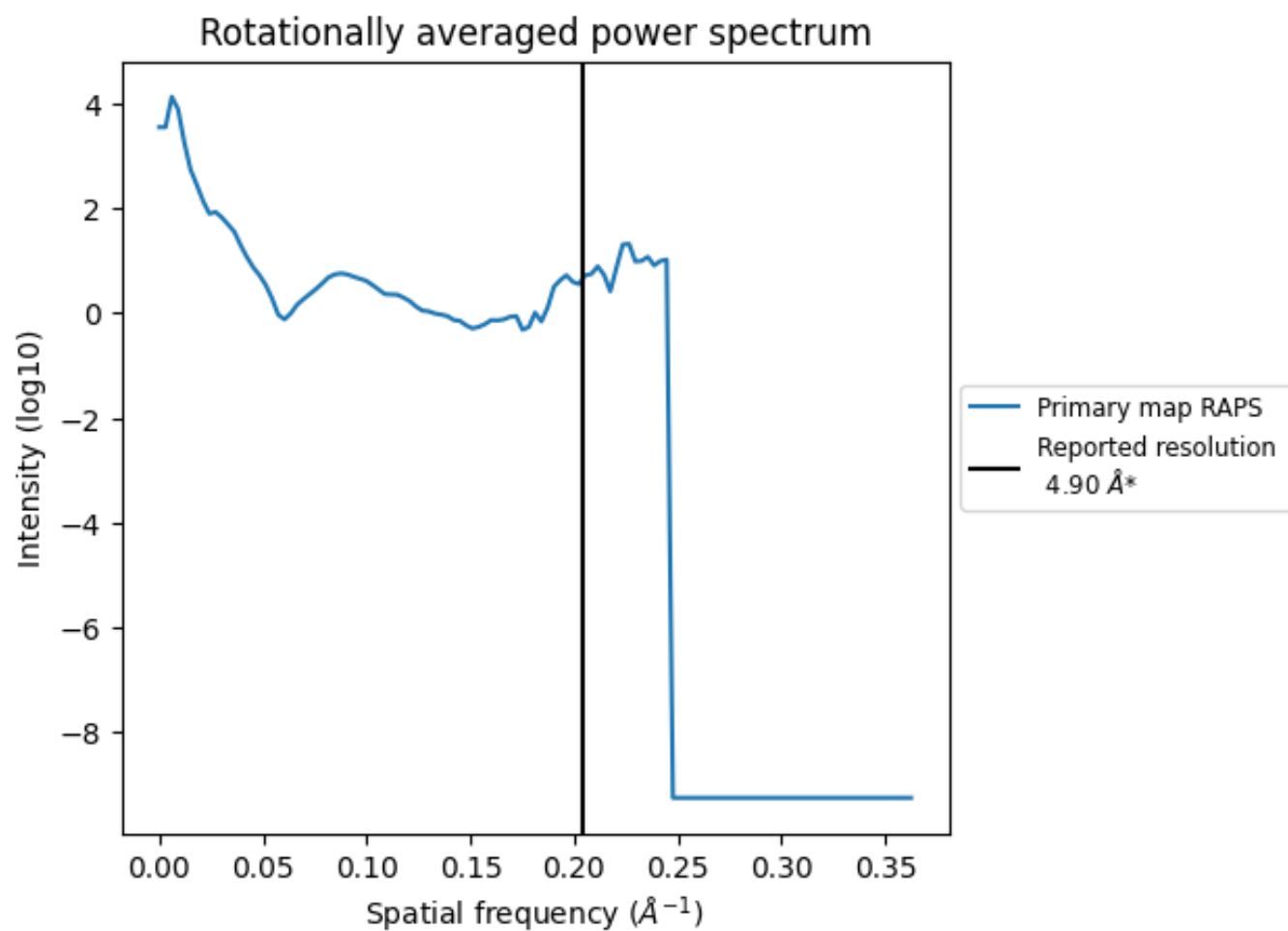
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 84 nm³; this corresponds to an approximate mass of 76 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 0.204 Å⁻¹

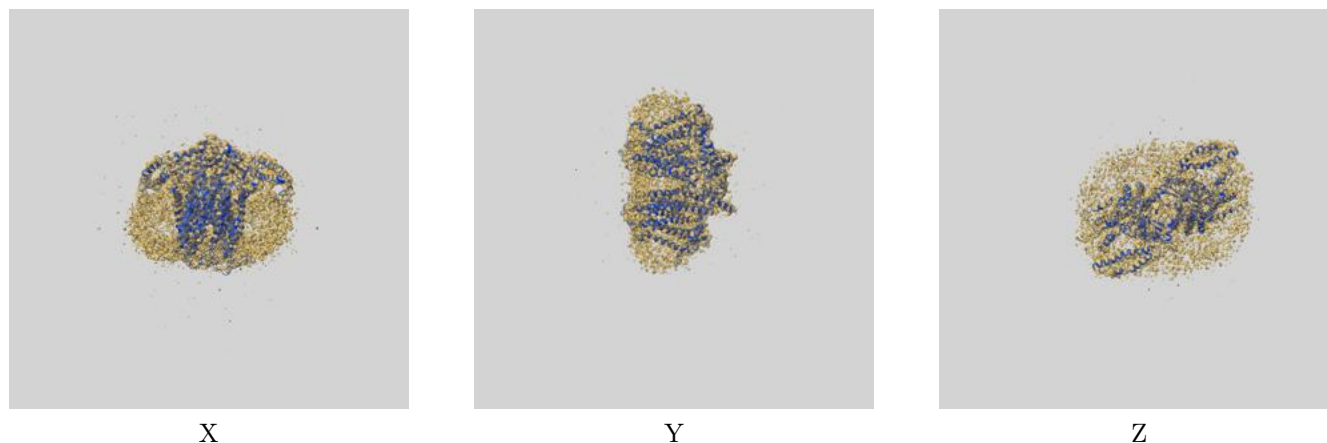
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

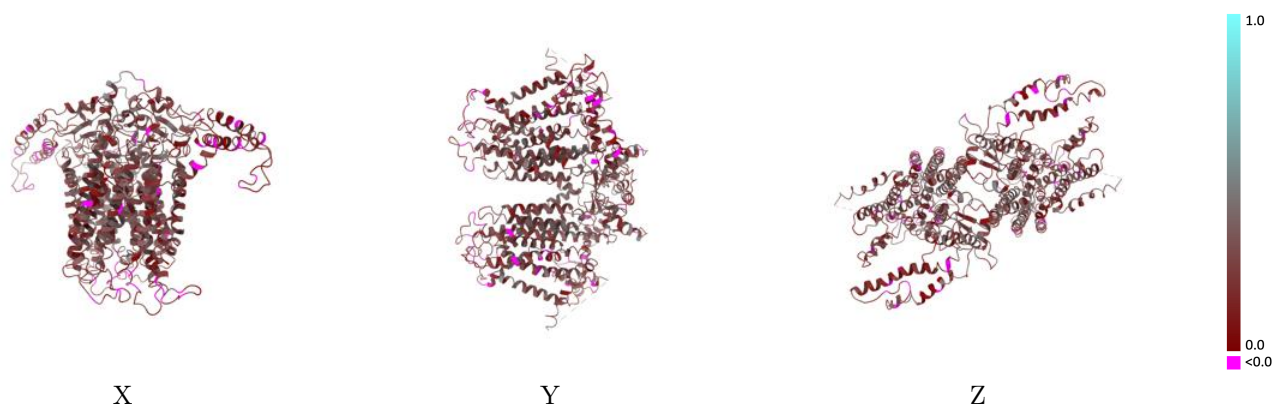
This section contains information regarding the fit between EMDB map EMD-20017 and PDB model 6OCE. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



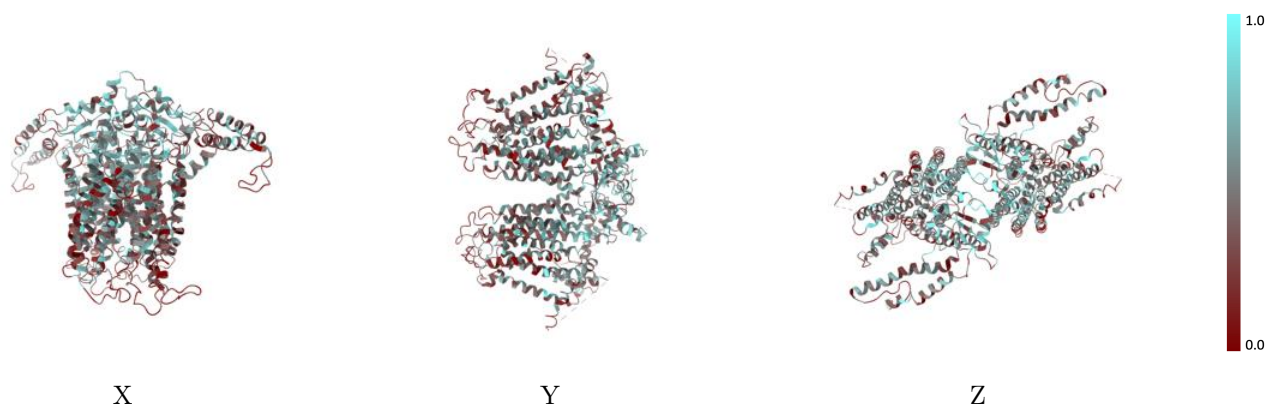
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



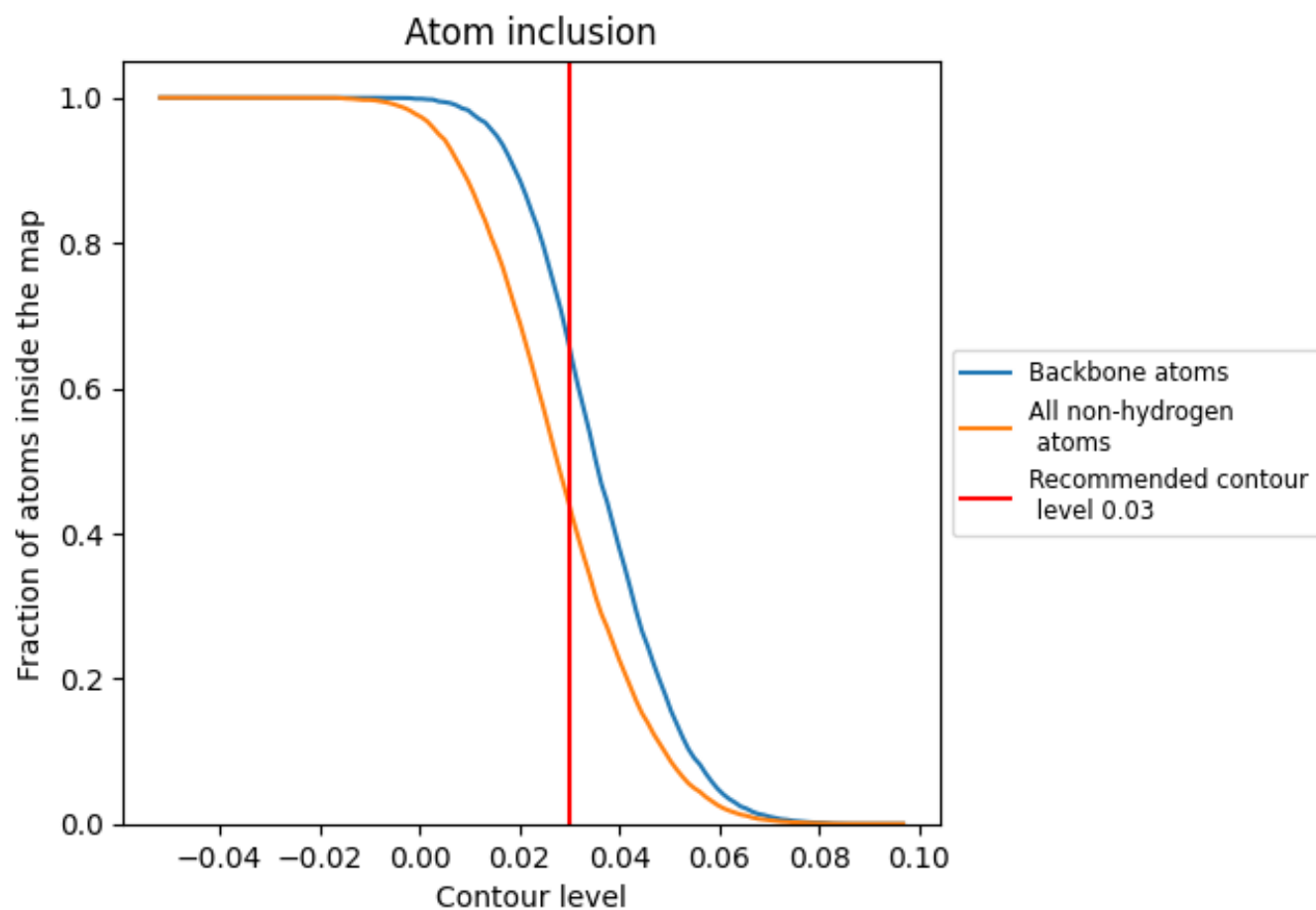
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 66% of all backbone atoms, 44% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.4392	<div></div> 0.2400
A	<div></div> 0.4382	<div></div> 0.2400
B	<div></div> 0.4402	<div></div> 0.2400

