



wwPDB EM Validation Summary Report ⓘ

May 26, 2025 – 12:08 PM EDT

PDB ID : 8GHG / pdb_00008ghg
EMDB ID : EMD-40045
Title : Cryo-EM structure of hSlo1 in digitonin, Ca²⁺-free and EDTA-free
Authors : Tao, X.; Zhao, C.; MacKinnon, R.
Deposited on : 2023-03-10
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.dev118
MolProbity : 4-5-2 with Phenix2.0rc1
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

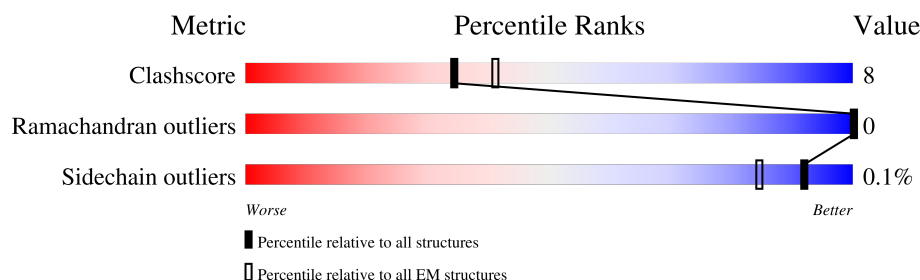
1 Overall quality at a glance

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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	1072	<div> <div>10%</div> <div>58%</div> <div>18%</div> <div>24%</div> </div>
1	B	1072	<div> <div>10%</div> <div>61%</div> <div>15%</div> <div>24%</div> </div>
1	C	1072	<div> <div>12%</div> <div>64%</div> <div>15%</div> <div>20%</div> </div>
1	D	1072	<div> <div>12%</div> <div>64%</div> <div>15%</div> <div>21%</div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 26659 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 Calcium-activated potassium channel subunit alpha-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	816	Total	C	N	O	S	1	0
			6533	4241	1060	1189	43		
1	C	853	Total	C	N	O	S	1	0
			6802	4414	1109	1236	43		
1	B	817	Total	C	N	O	S	1	0
			6549	4254	1062	1190	43		
1	D	849	Total	C	N	O	S	1	0
			6775	4398	1105	1229	43		

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	MET	-	expression tag	UNP Q12791
A	-14	ALA	-	expression tag	UNP Q12791
A	-13	PRO	-	expression tag	UNP Q12791
A	-12	SER	-	expression tag	UNP Q12791
A	-11	ARG	-	expression tag	UNP Q12791
A	-10	LEU	-	expression tag	UNP Q12791
A	-9	GLU	-	expression tag	UNP Q12791
A	-8	GLU	-	expression tag	UNP Q12791
A	-7	GLU	-	expression tag	UNP Q12791
A	-6	LEU	-	expression tag	UNP Q12791
A	-5	ARG	-	expression tag	UNP Q12791
A	-4	ARG	-	expression tag	UNP Q12791
A	-3	ARG	-	expression tag	UNP Q12791
A	-2	LEU	-	expression tag	UNP Q12791
A	-1	THR	-	expression tag	UNP Q12791
A	0	GLU	-	expression tag	UNP Q12791
A	1	PRO	-	expression tag	UNP Q12791
C	-15	MET	-	expression tag	UNP Q12791
C	-14	ALA	-	expression tag	UNP Q12791
C	-13	PRO	-	expression tag	UNP Q12791
C	-12	SER	-	expression tag	UNP Q12791
C	-11	ARG	-	expression tag	UNP Q12791

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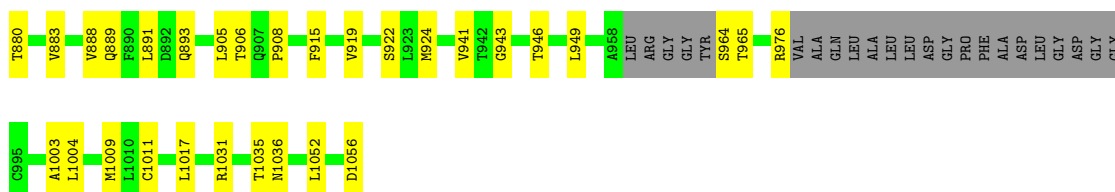
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Chain	Residue	Modelled	Actual	Comment	Reference
C	-10	LEU	-	expression tag	UNP Q12791
C	-9	GLU	-	expression tag	UNP Q12791
C	-8	GLU	-	expression tag	UNP Q12791
C	-7	GLU	-	expression tag	UNP Q12791
C	-6	LEU	-	expression tag	UNP Q12791
C	-5	ARG	-	expression tag	UNP Q12791
C	-4	ARG	-	expression tag	UNP Q12791
C	-3	ARG	-	expression tag	UNP Q12791
C	-2	LEU	-	expression tag	UNP Q12791
C	-1	THR	-	expression tag	UNP Q12791
C	0	GLU	-	expression tag	UNP Q12791
C	1	PRO	-	expression tag	UNP Q12791
B	-15	MET	-	expression tag	UNP Q12791
B	-14	ALA	-	expression tag	UNP Q12791
B	-13	PRO	-	expression tag	UNP Q12791
B	-12	SER	-	expression tag	UNP Q12791
B	-11	ARG	-	expression tag	UNP Q12791
B	-10	LEU	-	expression tag	UNP Q12791
B	-9	GLU	-	expression tag	UNP Q12791
B	-8	GLU	-	expression tag	UNP Q12791
B	-7	GLU	-	expression tag	UNP Q12791
B	-6	LEU	-	expression tag	UNP Q12791
B	-5	ARG	-	expression tag	UNP Q12791
B	-4	ARG	-	expression tag	UNP Q12791
B	-3	ARG	-	expression tag	UNP Q12791
B	-2	LEU	-	expression tag	UNP Q12791
B	-1	THR	-	expression tag	UNP Q12791
B	0	GLU	-	expression tag	UNP Q12791
B	1	PRO	-	expression tag	UNP Q12791
D	-15	MET	-	expression tag	UNP Q12791
D	-14	ALA	-	expression tag	UNP Q12791
D	-13	PRO	-	expression tag	UNP Q12791
D	-12	SER	-	expression tag	UNP Q12791
D	-11	ARG	-	expression tag	UNP Q12791
D	-10	LEU	-	expression tag	UNP Q12791
D	-9	GLU	-	expression tag	UNP Q12791
D	-8	GLU	-	expression tag	UNP Q12791
D	-7	GLU	-	expression tag	UNP Q12791
D	-6	LEU	-	expression tag	UNP Q12791
D	-5	ARG	-	expression tag	UNP Q12791
D	-4	ARG	-	expression tag	UNP Q12791
D	-3	ARG	-	expression tag	UNP Q12791

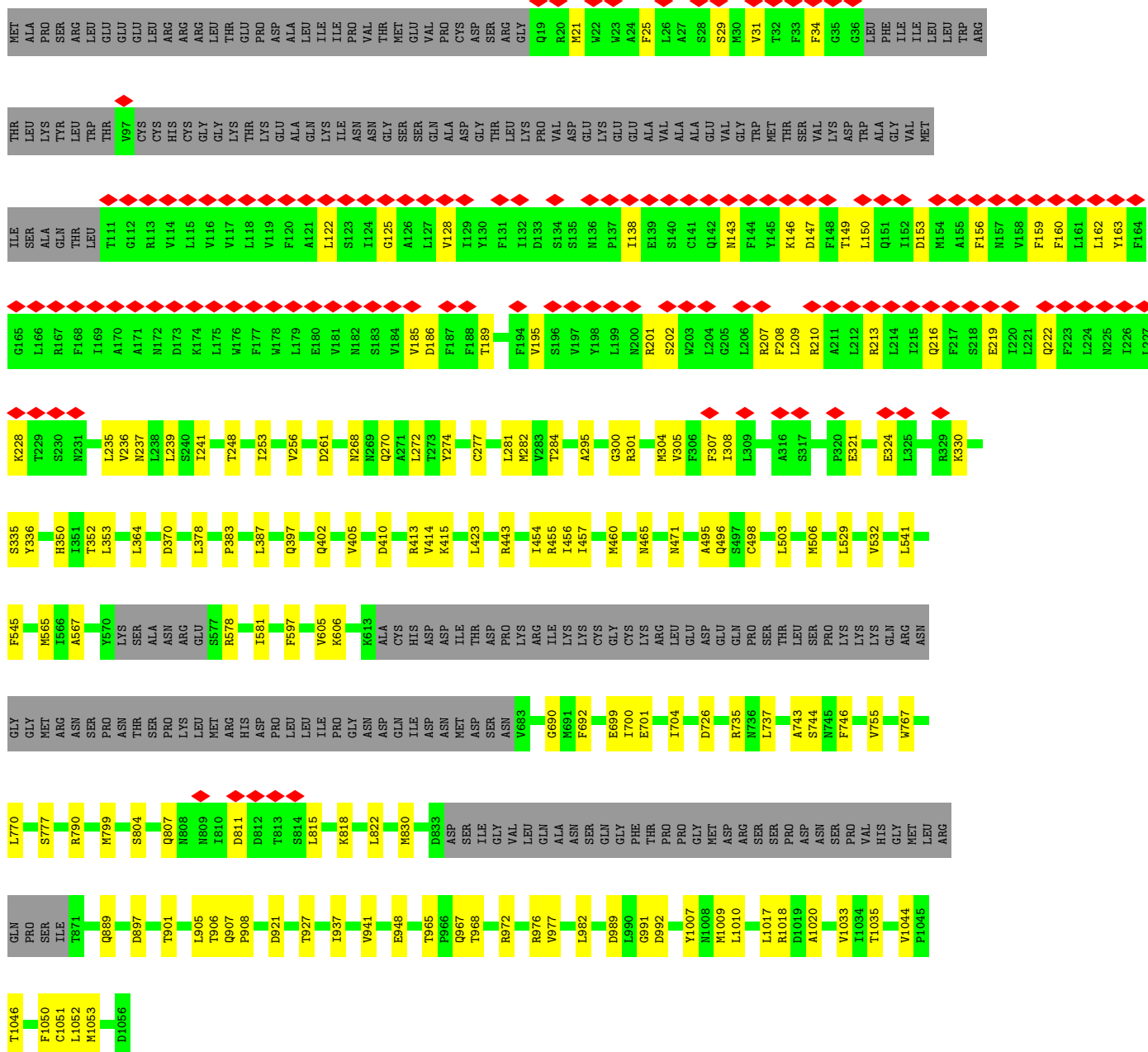
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Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	LEU	-	expression tag	UNP Q12791
D	-1	THR	-	expression tag	UNP Q12791
D	0	GLU	-	expression tag	UNP Q12791
D	1	PRO	-	expression tag	UNP Q12791



• Molecule 1: Calcium-activated potassium channel subunit alpha-1



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W1008	ASN	A743	ARG	M536	R329	S230	R167	SER
M1009	SER	S744	ASN	M561	G341	N231	F168	ALA
L1010	PRO	N745	GLY	L561		S232	I169	GLN
I1014	HIS	F746	MET	K562		T233	A170	T109
R1018	GLY	V755	ARG	L563	N358	K234	A171	L110
	MET	F756	ASN	I566	K361	L235	A172	T111
S1026	LEU	L763	SER			V236	N172	G112
Q1027	ARG	K764	ASN	Y570	K363	N237	D173	R113
C1028	GLN	R765	PRO	LYS	ASP	L238	K174	V114
	PRO		THR	ASP	ASP		L175	V115
V1033	SER	L770	PRO	ALA	V371	S244	L176	L116
I1034	ILE	H771	LYS	ASN		T245	F177	V117
T1035			LEU	ARG	L378	W246	W178	L118
		P774	MET	GLU			L179	V119
V1044			ARG	S577	V414	A249	E180	F120
P1045		S777	HIS		C430	T253	V181	A121
T1046		P783	ASP	F597	I441	H254	N182	L122
F1050	E902	D788	PRO	V605	I445	V256	S183	S123
	L903		LEU	K606				I124
	Y904		ILE	R607	K448	D261	D186	G125
M1053	L905	N808	PRO	C612	N449	F266	F187	A126
	T906	I810	GLY	K613	I454	L272	F188	L127
D1056		D811	ASN	ALA	R455		T189	V128
		D812	GLN	CYS	I456	W282	V190	I129
		T813	ILE	HIS	I457	T287		Y130
	N930	S814	ASP	ASP	M460	T297	F194	D133
	D931		ASN	ILE			V195	S134
N932	N933	K318	MET	THR	N465	T298	S196	S135
N934	L934	L822	ASP	ASP	P473	L299	V197	N136
			ASN	PRO		G300	Y198	N137
				LYS	D482	R301	N200	P137
	I937	D833	V683	ARG	L302	F303	R201	I138
		ASP	F692	ILE	A483	M304	S202	E139
L940	SER	ILE	K698	LYS	I484	V305	L204	S140
V941	ILE	GLY	E699	CYS	L491	F306	G205	C141
E950	GLY	VAL	I700	GLY	Q496	F307	L206	Q142
		LEU	E701	CYS	L503	I308	L207	N143
1953	LEU	GLN	K702	LYS		G310	R207	F144
E956	ALA	ASN	V703	ARG		G311	F208	Y145
	GLN	SER	I704	LEU	M506	L312	L209	K146
R960	ASN	GLN	R707	ASP	F511		R210	D147
	SER	GLY	C722	PRO	I519	A316	A211	F148
R972	THR	THR	D726	THR	K526	S317	L212	T149
	PHE	PRO	S729	LEU		V318	R213	L150
R976	PRO	GLY		SER	L529	V319	L214	Q151
V977	PRO	MET	R735	PRO	E530	P320	I215	I152
	GLY	ARG	N736	LYS	I321	E321	Q216	D153
		SER	L737	LYS	V532	I323	S218	M154
		SER	R742	GLN	S533	E324	E219	A155
	PRO	PRO				L325	I220	F156
						I326	L221	N157
							Q222	V158
							F223	F159
							L224	F160
							N225	L161
							I226	L162
							L227	Y163
							K228	F164
							T229	G165
								L166

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	123286	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 ($e^-/\text{\AA}^2$)	51.4	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.967	Depositor
Minimum map value	-0.314	Depositor
Average map value	0.016	Depositor
Map value standard deviation	0.061	Depositor
Recommended contour level	0.28	Depositor
Map size (\AA)	276.48, 276.48, 276.48	wwPDB
Map dimensions	256, 256, 256	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	0.13	0/6681	0.37	0/9062
1	B	0.14	0/6698	0.39	2/9085 (0.0%)
1	C	0.13	0/6957	0.37	0/9436
1	D	0.12	0/6929	0.34	0/9399
All	All	0.13	0/27265	0.37	2/36982 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	30	MET	CB-CG-SD	5.15	128.15	112.70
1	B	282	MET	CG-SD-CE	5.10	112.12	100.90

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	6533	0	6499	120	0
1	B	6549	0	6512	103	0
1	C	6802	0	6771	104	0
1	D	6775	0	6757	105	0
All	All	26659	0	26539	420	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 420 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:794:ILE:HG21	1:A:827:ILE:HD11	1.64	0.80
1:A:491:LEU:HD12	1:A:737:LEU:HB2	1.67	0.75
1:A:445:ILE:HD13	1:A:472:ILE:HD12	1.69	0.75
1:B:246:TRP:HZ2	1:B:278:VAL:HG13	1.51	0.74
1:B:287:THR:HB	1:D:287:THR:HB	1.71	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	803/1072 (75%)	750 (93%)	53 (7%)	0	100	100
1	B	803/1072 (75%)	761 (95%)	42 (5%)	0	100	100
1	C	843/1072 (79%)	805 (96%)	38 (4%)	0	100	100
1	D	838/1072 (78%)	796 (95%)	42 (5%)	0	100	100
All	All	3287/4288 (77%)	3112 (95%)	175 (5%)	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	724/943 (77%)	723 (100%)	1 (0%)	92	96
1	B	726/943 (77%)	725 (100%)	1 (0%)	92	96
1	C	750/943 (80%)	749 (100%)	1 (0%)	92	96
1	D	747/943 (79%)	747 (100%)	0	100	100
All	All	2947/3772 (78%)	2944 (100%)	3 (0%)	92	96

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

Mol	Chain	Res	Type
1	A	128	VAL
1	C	128	VAL
1	B	329	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 48 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	468	HIS
1	B	1054	GLN
1	B	496	GLN
1	B	893	GLN
1	D	225	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.

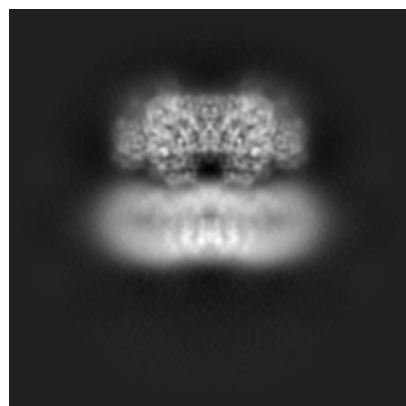
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-40045. These allow visual inspection of the internal detail of the map and identification of artifacts.

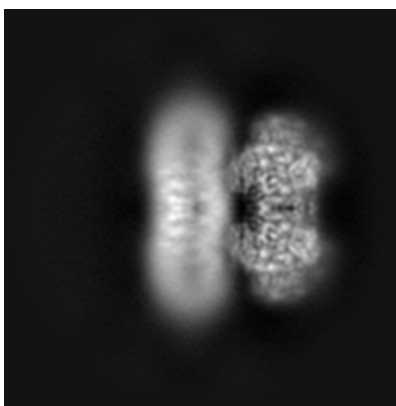
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

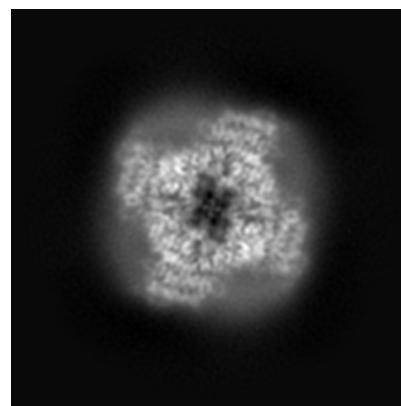
6.1.1 Primary map



X

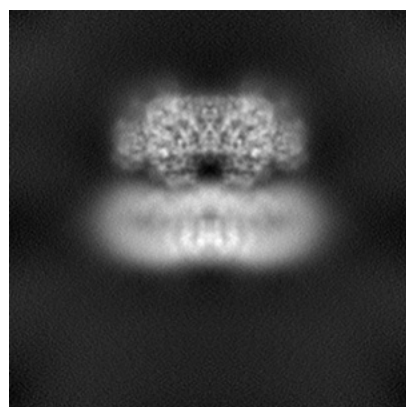


Y

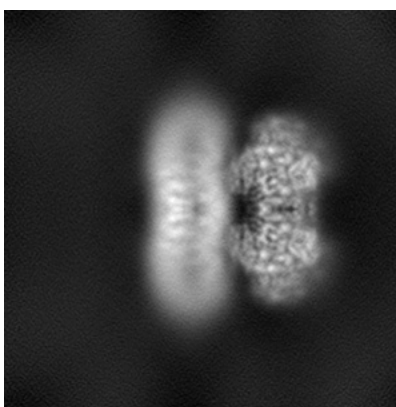


Z

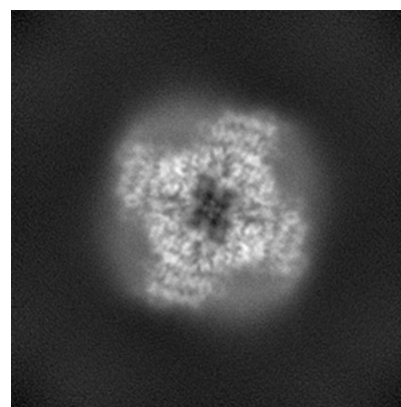
6.1.2 Raw map



X



Y

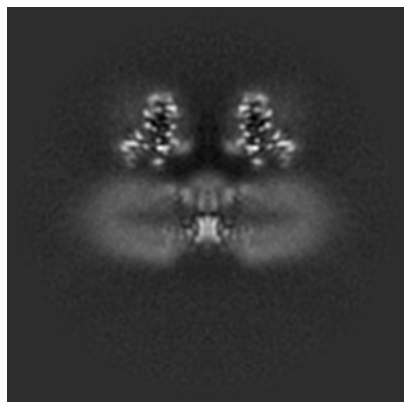


Z

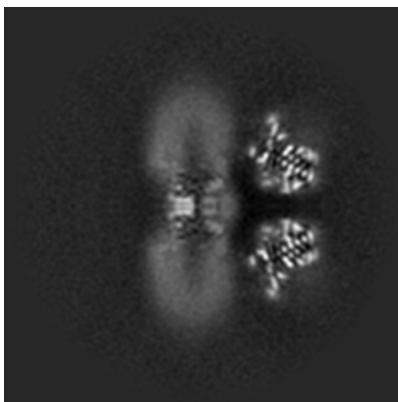
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

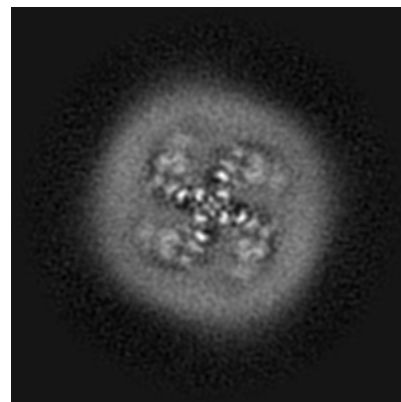
6.2.1 Primary map



X Index: 128

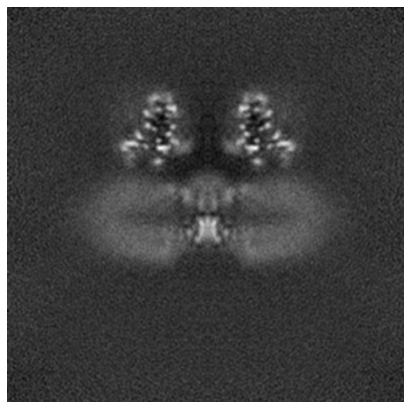


Y Index: 128

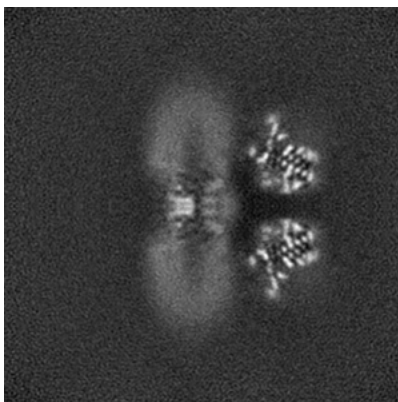


Z Index: 128

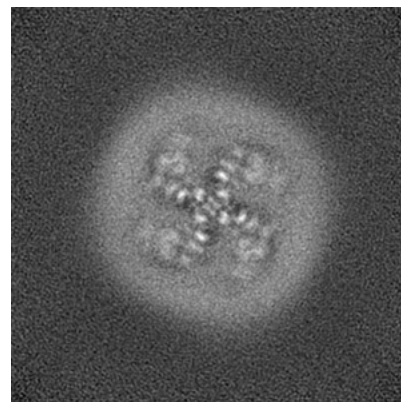
6.2.2 Raw map



X Index: 128



Y Index: 128

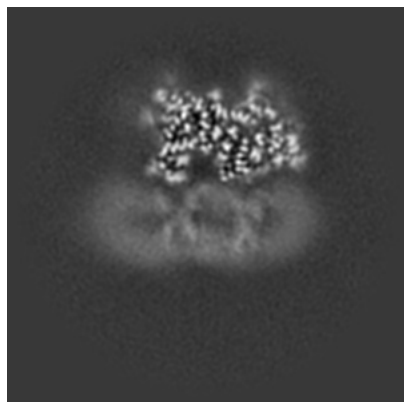


Z Index: 128

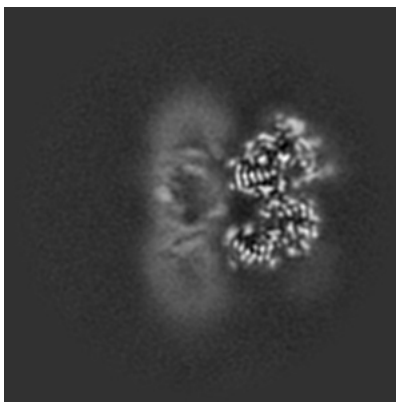
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

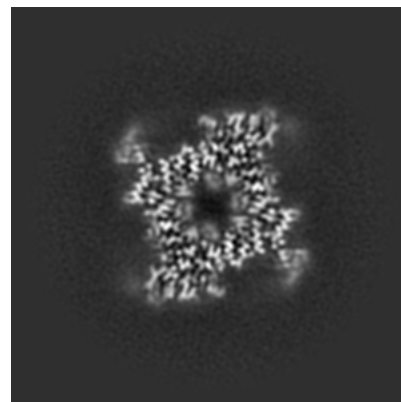
6.3.1 Primary map



X Index: 156

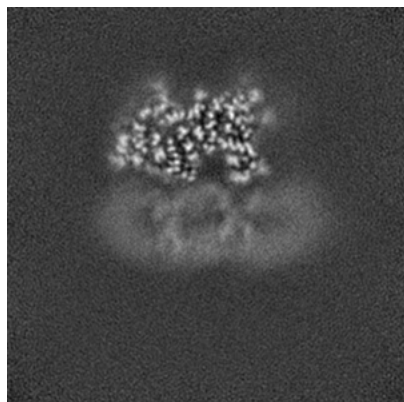


Y Index: 105

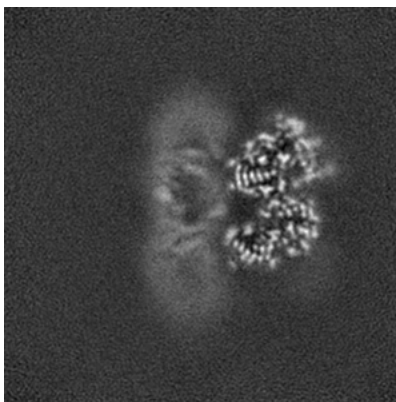


Z Index: 166

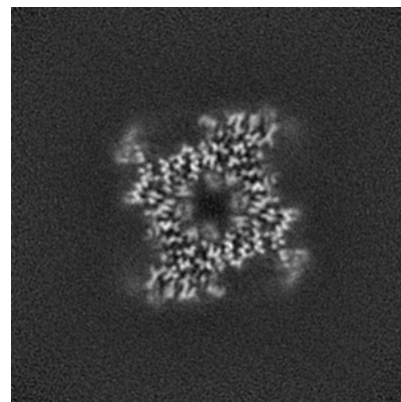
6.3.2 Raw map



X Index: 100



Y Index: 105

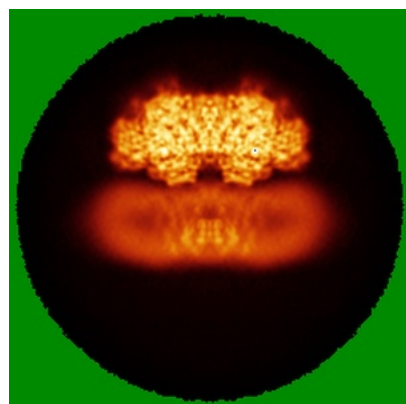


Z Index: 166

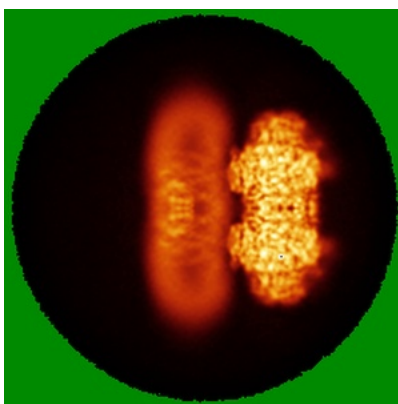
The images above show the largest variance slices of the map in three orthogonal directions.

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

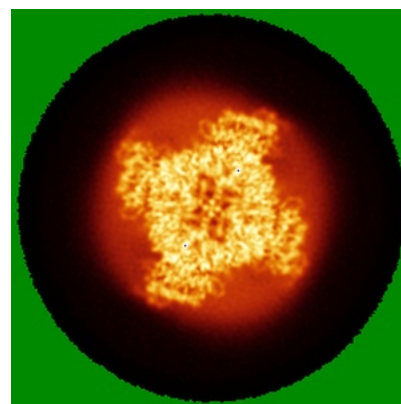
6.4.1 Primary map



X

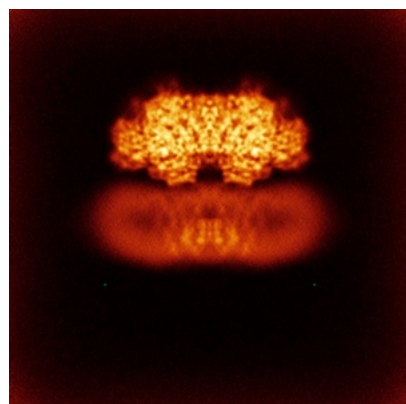


Y

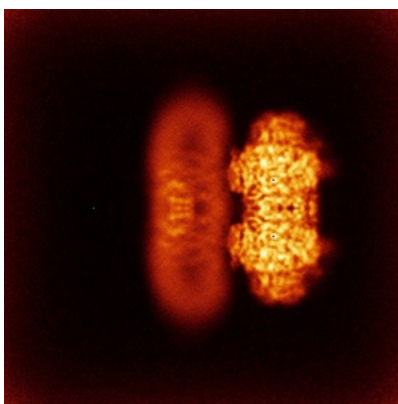


Z

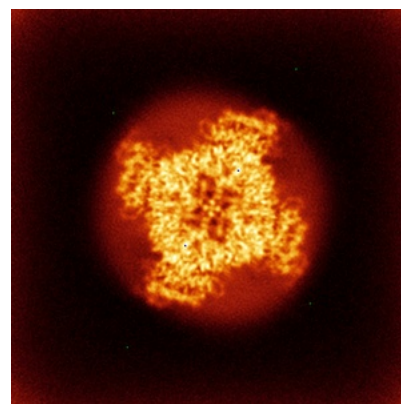
6.4.2 Raw map



X



Y

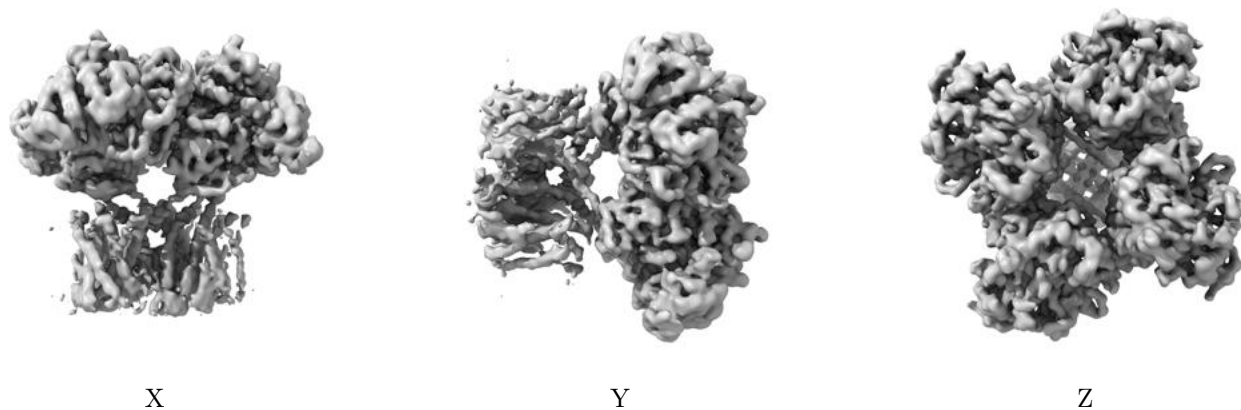


Z

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.

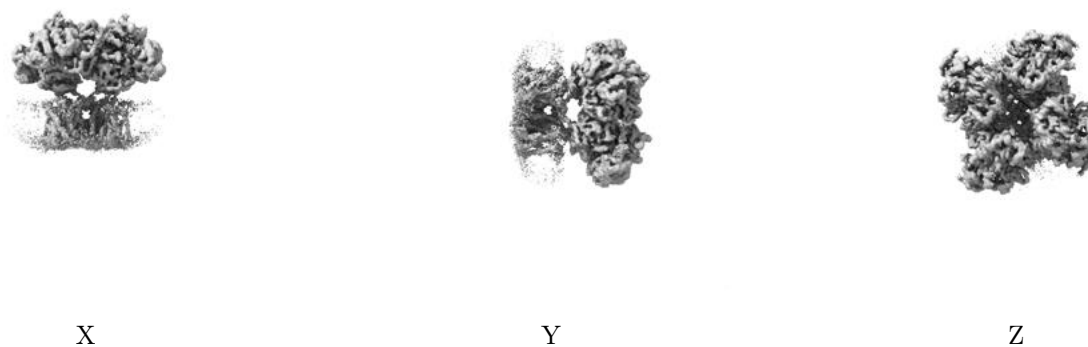
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.28. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

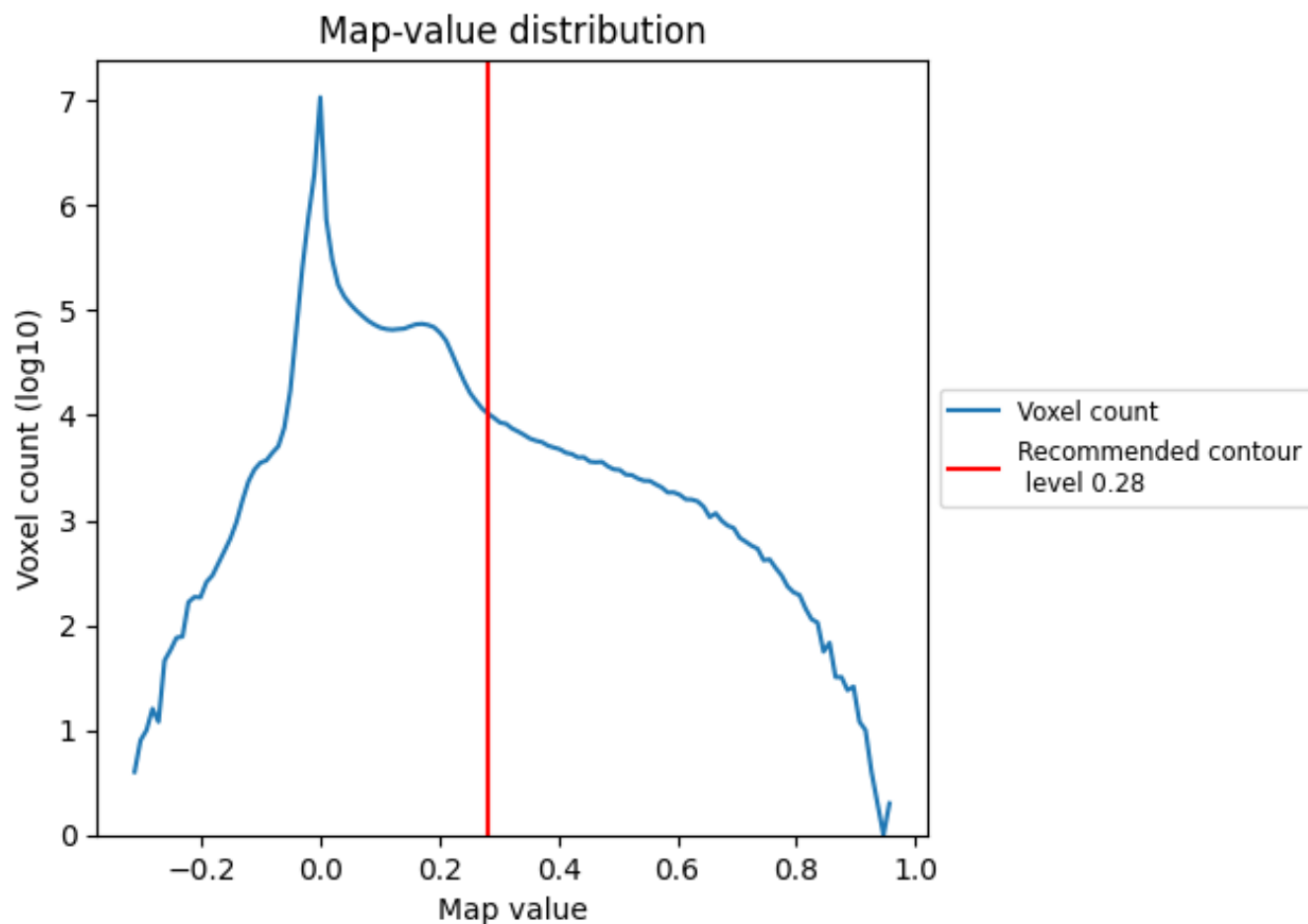
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

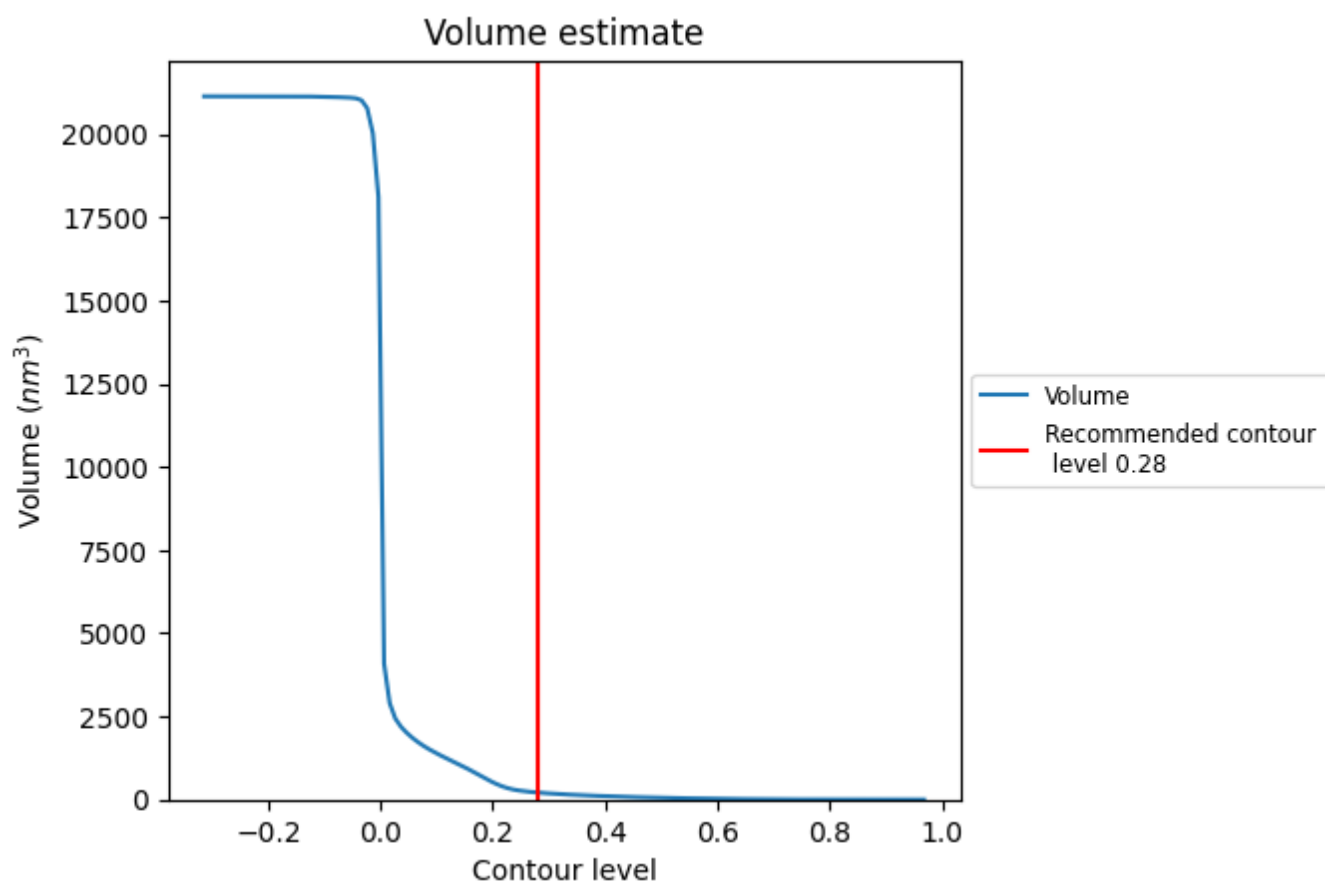
This section contains the results of statistical analysis of the map.

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.

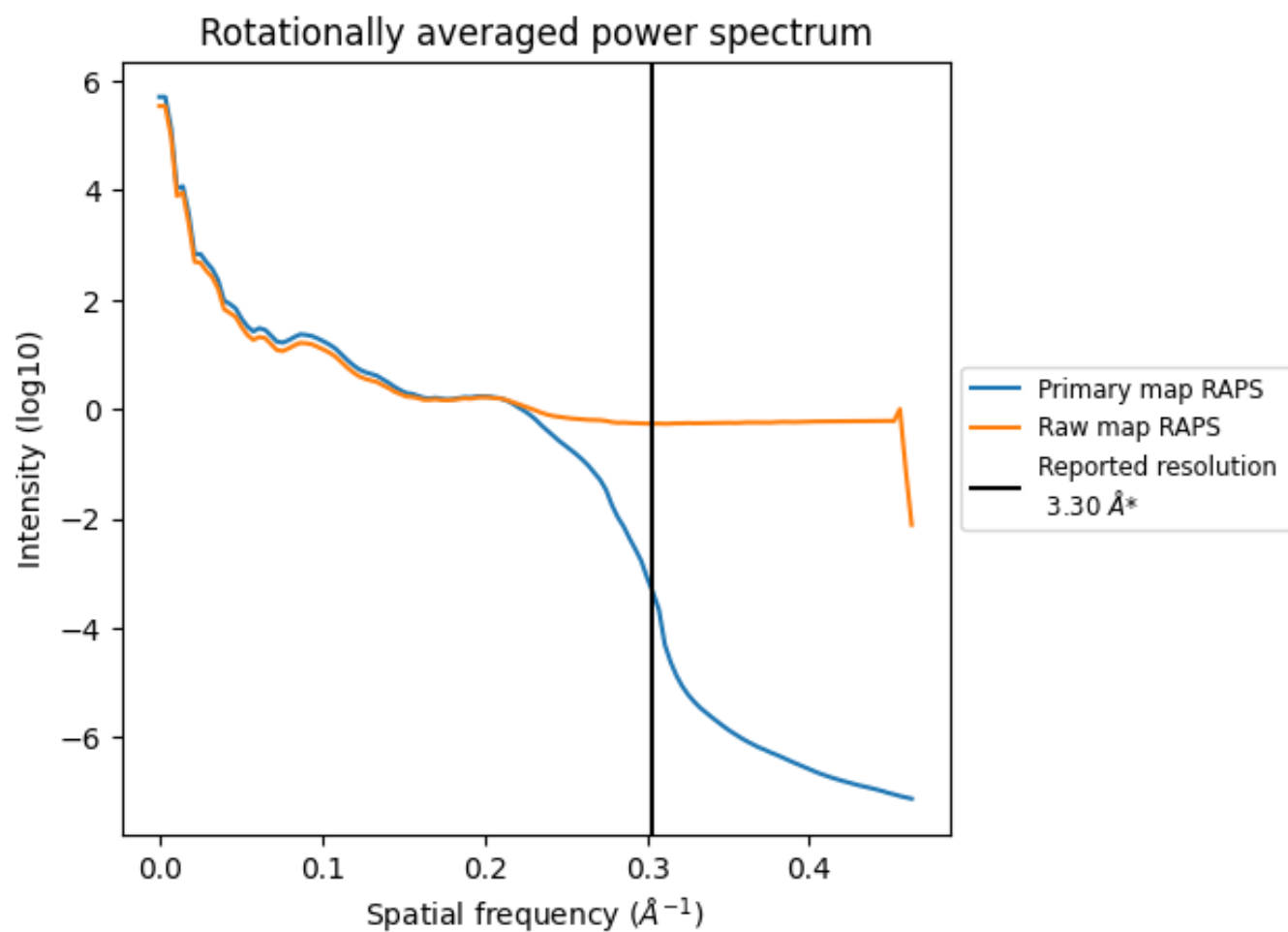
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 210 nm³; this corresponds to an approximate mass of 190 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 ⓘ

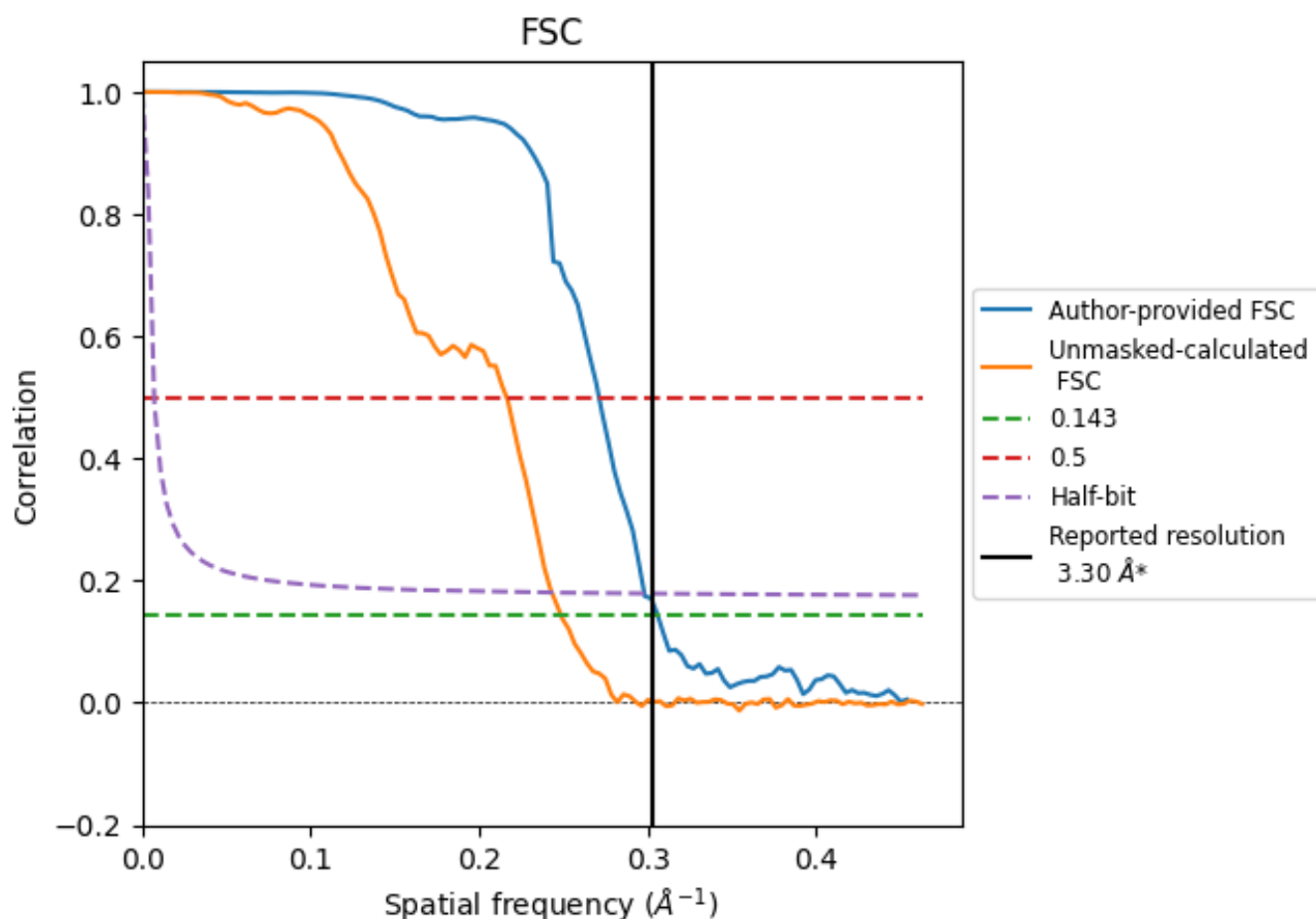


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.303 \AA^{-1}

8.2 Resolution estimates [i](#)

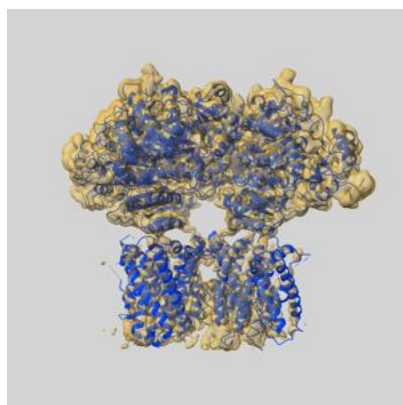
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.27	3.69	3.35
Unmasked-calculated*	4.02	4.62	4.11

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.02 differs from the reported value 3.3 by more than 10 %

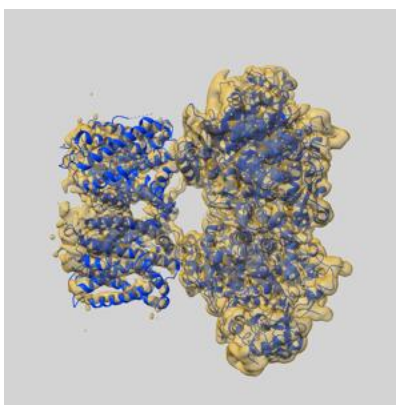
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-40045 and PDB model 8GHG. Per-residue inclusion information can be found in section [3](#) on page [6](#).

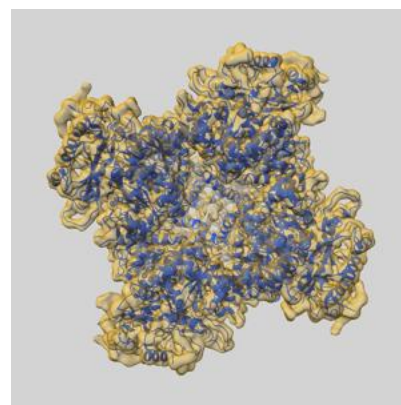
9.1 Map-model overlay [i](#)



X



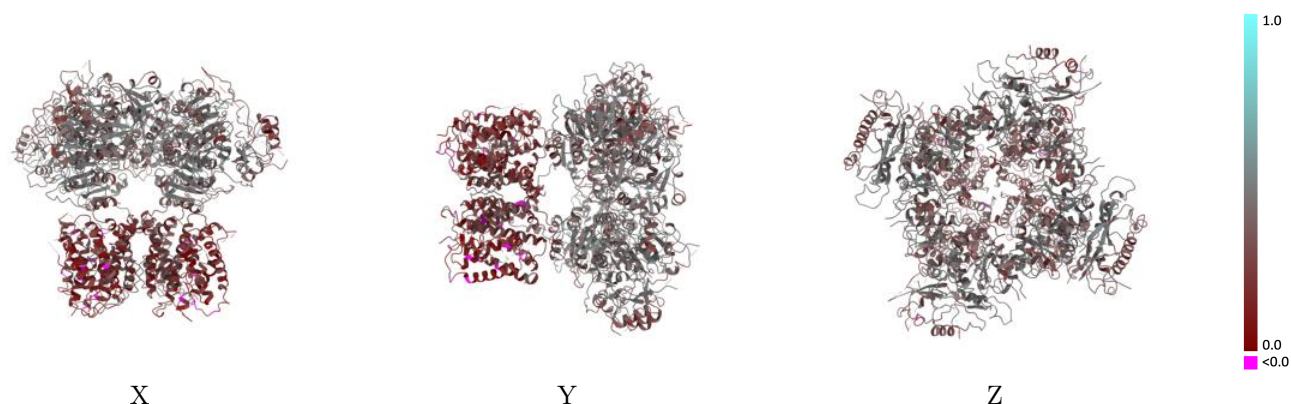
Y



Z

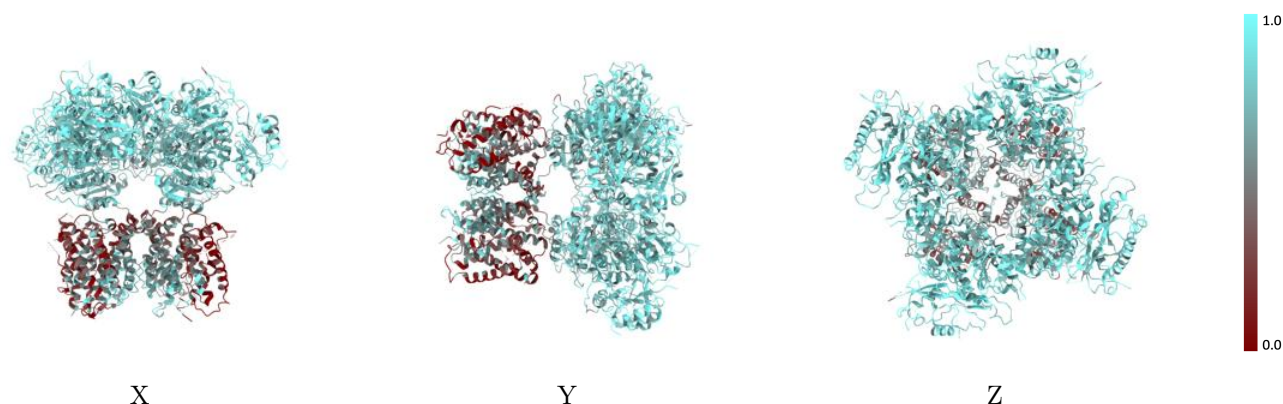
The images above show the 3D surface view of the map at the recommended contour level 0.28 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



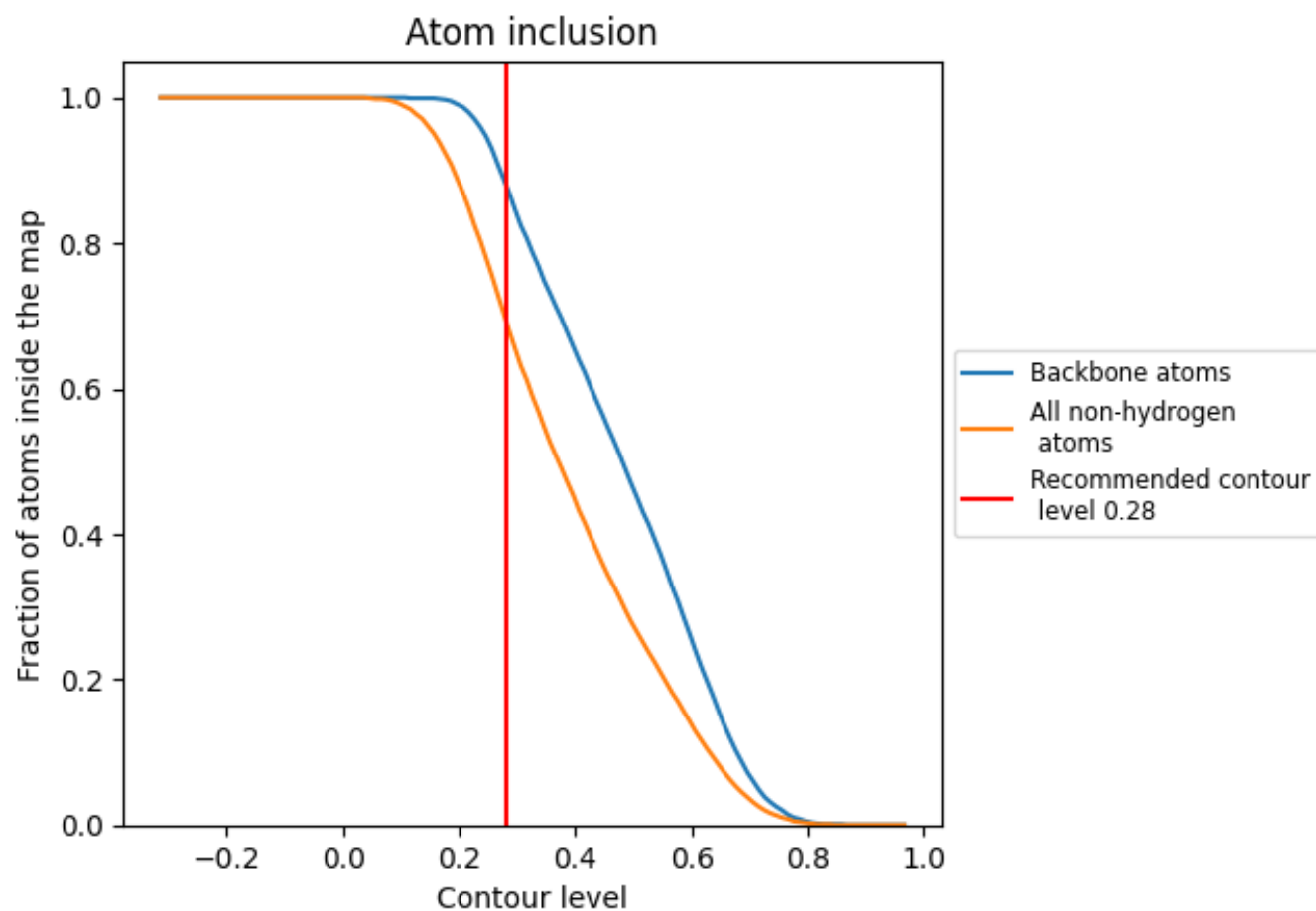
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.28).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 70% 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 (0.28) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6960	<div></div> 0.3570
A	<div></div> 0.7050	<div></div> 0.3560
B	<div></div> 0.6980	<div></div> 0.3540
C	<div></div> 0.6900	<div></div> 0.3580
D	<div></div> 0.6890	<div></div> 0.3580

