



wwPDB EM Validation Summary Report ⓘ

Nov 8, 2022 – 04:52 pm GMT

PDB ID : 8B8J
EMDB ID : EMD-15914
Title : Cryo-EM structure of Ca²⁺-bound mTMEM16F F518H mutant in Digitonin
Authors : Arndt, M.; Alvadia, C.; Straub, M.S.; Clerico Mosina, V.; Paulino, C.; Dutzler, R.
Deposited on : 2022-10-04
Resolution : 2.96 Å (reported)
Based on initial model : 6QP6

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

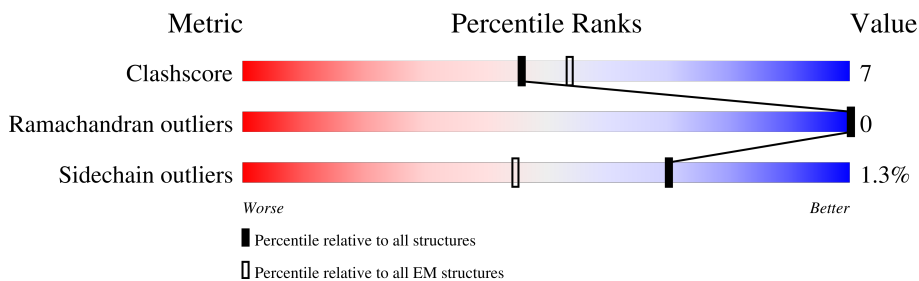
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.96 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	975	 5% 58% 14% 27%
1	B	975	 6% 58% 14% 27%

2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 11686 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 Anoctamin-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	709	Total	C	N	O	S	0	0
			5840	3843	942	1017	38		
1	B	709	Total	C	N	O	S	0	0
			5840	3843	942	1017	38		

There are 130 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	518	HIS	PHE	engineered mutation	UNP Q6P9J9
A	912	ALA	-	expression tag	UNP Q6P9J9
A	913	LEU	-	expression tag	UNP Q6P9J9
A	914	GLU	-	expression tag	UNP Q6P9J9
A	915	VAL	-	expression tag	UNP Q6P9J9
A	916	LEU	-	expression tag	UNP Q6P9J9
A	917	PHE	-	expression tag	UNP Q6P9J9
A	918	GLN	-	expression tag	UNP Q6P9J9
A	919	GLY	-	expression tag	UNP Q6P9J9
A	920	PRO	-	expression tag	UNP Q6P9J9
A	921	GLN	-	expression tag	UNP Q6P9J9
A	922	GLY	-	expression tag	UNP Q6P9J9
A	923	THR	-	expression tag	UNP Q6P9J9
A	924	GLU	-	expression tag	UNP Q6P9J9
A	925	GLN	-	expression tag	UNP Q6P9J9
A	926	LYS	-	expression tag	UNP Q6P9J9
A	927	LEU	-	expression tag	UNP Q6P9J9
A	928	ILE	-	expression tag	UNP Q6P9J9
A	929	SER	-	expression tag	UNP Q6P9J9
A	930	GLU	-	expression tag	UNP Q6P9J9
A	931	GLU	-	expression tag	UNP Q6P9J9
A	932	ASP	-	expression tag	UNP Q6P9J9
A	933	LEU	-	expression tag	UNP Q6P9J9
A	934	ARG	-	expression tag	UNP Q6P9J9
A	935	GLY	-	expression tag	UNP Q6P9J9
A	936	ALA	-	expression tag	UNP Q6P9J9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	937	SER	-	expression tag	UNP Q6P9J9
A	938	MET	-	expression tag	UNP Q6P9J9
A	939	ASP	-	expression tag	UNP Q6P9J9
A	940	GLU	-	expression tag	UNP Q6P9J9
A	941	LYS	-	expression tag	UNP Q6P9J9
A	942	THR	-	expression tag	UNP Q6P9J9
A	943	THR	-	expression tag	UNP Q6P9J9
A	944	GLY	-	expression tag	UNP Q6P9J9
A	945	TRP	-	expression tag	UNP Q6P9J9
A	946	ARG	-	expression tag	UNP Q6P9J9
A	947	GLY	-	expression tag	UNP Q6P9J9
A	948	GLY	-	expression tag	UNP Q6P9J9
A	949	HIS	-	expression tag	UNP Q6P9J9
A	950	VAL	-	expression tag	UNP Q6P9J9
A	951	VAL	-	expression tag	UNP Q6P9J9
A	952	GLU	-	expression tag	UNP Q6P9J9
A	953	GLY	-	expression tag	UNP Q6P9J9
A	954	LEU	-	expression tag	UNP Q6P9J9
A	955	ALA	-	expression tag	UNP Q6P9J9
A	956	GLY	-	expression tag	UNP Q6P9J9
A	957	GLU	-	expression tag	UNP Q6P9J9
A	958	LEU	-	expression tag	UNP Q6P9J9
A	959	GLU	-	expression tag	UNP Q6P9J9
A	960	GLN	-	expression tag	UNP Q6P9J9
A	961	LEU	-	expression tag	UNP Q6P9J9
A	962	ARG	-	expression tag	UNP Q6P9J9
A	963	ALA	-	expression tag	UNP Q6P9J9
A	964	ARG	-	expression tag	UNP Q6P9J9
A	965	LEU	-	expression tag	UNP Q6P9J9
A	966	GLU	-	expression tag	UNP Q6P9J9
A	967	HIS	-	expression tag	UNP Q6P9J9
A	968	HIS	-	expression tag	UNP Q6P9J9
A	969	PRO	-	expression tag	UNP Q6P9J9
A	970	GLN	-	expression tag	UNP Q6P9J9
A	971	GLY	-	expression tag	UNP Q6P9J9
A	972	GLN	-	expression tag	UNP Q6P9J9
A	973	ARG	-	expression tag	UNP Q6P9J9
A	974	GLU	-	expression tag	UNP Q6P9J9
A	975	PRO	-	expression tag	UNP Q6P9J9
B	518	HIS	PHE	engineered mutation	UNP Q6P9J9
B	912	ALA	-	expression tag	UNP Q6P9J9
B	913	LEU	-	expression tag	UNP Q6P9J9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	914	GLU	-	expression tag	UNP Q6P9J9
B	915	VAL	-	expression tag	UNP Q6P9J9
B	916	LEU	-	expression tag	UNP Q6P9J9
B	917	PHE	-	expression tag	UNP Q6P9J9
B	918	GLN	-	expression tag	UNP Q6P9J9
B	919	GLY	-	expression tag	UNP Q6P9J9
B	920	PRO	-	expression tag	UNP Q6P9J9
B	921	GLN	-	expression tag	UNP Q6P9J9
B	922	GLY	-	expression tag	UNP Q6P9J9
B	923	THR	-	expression tag	UNP Q6P9J9
B	924	GLU	-	expression tag	UNP Q6P9J9
B	925	GLN	-	expression tag	UNP Q6P9J9
B	926	LYS	-	expression tag	UNP Q6P9J9
B	927	LEU	-	expression tag	UNP Q6P9J9
B	928	ILE	-	expression tag	UNP Q6P9J9
B	929	SER	-	expression tag	UNP Q6P9J9
B	930	GLU	-	expression tag	UNP Q6P9J9
B	931	GLU	-	expression tag	UNP Q6P9J9
B	932	ASP	-	expression tag	UNP Q6P9J9
B	933	LEU	-	expression tag	UNP Q6P9J9
B	934	ARG	-	expression tag	UNP Q6P9J9
B	935	GLY	-	expression tag	UNP Q6P9J9
B	936	ALA	-	expression tag	UNP Q6P9J9
B	937	SER	-	expression tag	UNP Q6P9J9
B	938	MET	-	expression tag	UNP Q6P9J9
B	939	ASP	-	expression tag	UNP Q6P9J9
B	940	GLU	-	expression tag	UNP Q6P9J9
B	941	LYS	-	expression tag	UNP Q6P9J9
B	942	THR	-	expression tag	UNP Q6P9J9
B	943	THR	-	expression tag	UNP Q6P9J9
B	944	GLY	-	expression tag	UNP Q6P9J9
B	945	TRP	-	expression tag	UNP Q6P9J9
B	946	ARG	-	expression tag	UNP Q6P9J9
B	947	GLY	-	expression tag	UNP Q6P9J9
B	948	GLY	-	expression tag	UNP Q6P9J9
B	949	HIS	-	expression tag	UNP Q6P9J9
B	950	VAL	-	expression tag	UNP Q6P9J9
B	951	VAL	-	expression tag	UNP Q6P9J9
B	952	GLU	-	expression tag	UNP Q6P9J9
B	953	GLY	-	expression tag	UNP Q6P9J9
B	954	LEU	-	expression tag	UNP Q6P9J9
B	955	ALA	-	expression tag	UNP Q6P9J9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	956	GLY	-	expression tag	UNP Q6P9J9
B	957	GLU	-	expression tag	UNP Q6P9J9
B	958	LEU	-	expression tag	UNP Q6P9J9
B	959	GLU	-	expression tag	UNP Q6P9J9
B	960	GLN	-	expression tag	UNP Q6P9J9
B	961	LEU	-	expression tag	UNP Q6P9J9
B	962	ARG	-	expression tag	UNP Q6P9J9
B	963	ALA	-	expression tag	UNP Q6P9J9
B	964	ARG	-	expression tag	UNP Q6P9J9
B	965	LEU	-	expression tag	UNP Q6P9J9
B	966	GLU	-	expression tag	UNP Q6P9J9
B	967	HIS	-	expression tag	UNP Q6P9J9
B	968	HIS	-	expression tag	UNP Q6P9J9
B	969	PRO	-	expression tag	UNP Q6P9J9
B	970	GLN	-	expression tag	UNP Q6P9J9
B	971	GLY	-	expression tag	UNP Q6P9J9
B	972	GLN	-	expression tag	UNP Q6P9J9
B	973	ARG	-	expression tag	UNP Q6P9J9
B	974	GLU	-	expression tag	UNP Q6P9J9
B	975	PRO	-	expression tag	UNP Q6P9J9

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
2	A	3	Total Ca 3 3	0
2	B	3	Total Ca 3 3	0



MET	GLN	THR	ARG	LYS	VAL	LEU	LEU	ASN	ASN	MET	LYS	GLU	LEU	LEU	LEU	GLU	GLU	ASP	ASP	ASP	GLY	ASP	ILE	VAL	LEU	LEU	GLN	THR	ILE	VAL	CYS	PRO	THR	PHE	GLY	SER	LEU	LEU	M43	Q44	Q45	D46	F47	P50	E51	L62	F63	D66	G67	Q68	R69	R70	GLY																	
F73	E78	S81	L85	GLU	ASN	GLU	ASN	ASN	LYS	LYS	G89	K93	R96	K97	R98	Q99	E102	L106	Q111	L112	E113	A114	S117	V118	S119	ASP	D121	K122	F125	V126	K127	V128	P131	K149	PRO	ASN	ASP	ASP	LEU	LYS	THR	ARG	SER	PRO	PHE	GLY	ASN	LEU	ASN	ASP	TRP																			
PHE	THR	LYS	VAL	LEU	ARG	VAL	ASN	GLU	SER	VAL	PRO	ILE	LYS	PRO	GLU	GLN	GLU	PHE	PHE	THR	ALA	PHE	ASN	LYS	SER	ARG	MET	ASN	ASN	ASP	PHE	TYR	ILE	LEU	ASP	ARG	ASP	S202	T212	T216	V220	LYS	TYR	GLN	VAL	MET	ASN	ASN	VAL	ASN	LYS	PHE	GLY	I233	R234	R235	L236													
F246	H249	D250	C251	R252	Y255	E265	R266	L269	Y270	A274	K281	K282	Q283	L287	Y291	E294	Y305	V316	Y325	L326	D327	N330	L347	P357	F358	C365	S368	L371	C372	I373	F374	D375	F382	A383	V384	F385	M386	W397																																
E403	Q414	GLU	GLU	GLN	ALA	PRO	PRO	TYR	GLU	ALA	T509	CYS	ASN	HIS	VAL	VAL	ILE	GLU	ILE	THR	GLN	GLU	GLU	ARG	ILE	PRO	PHE	L326	D327	THR	T446	C447	Q448	K449	R452	V460	I464	F462	I463	V464	F465	S466	T467	T468	LEU	PRO	LYS	ASN	ASN	GLY																				
THR	ASP	PRO	ILE	GLN	LYS	TYR	L503	T504	P505	Q506	M507	A508	T509	S510	I511	T512	A513	I516	S517	H518	I523	T526	F538	E539	L540	P541	R542	Y547	K554	Q559	F560	V561	A571	Y586	L587	L588	G589	K590	Y591	R592	E595	C596	D597	L605	Q623	L627																								
P628	R636	V640	SER	SER	GLU	K645	R649	D653	Y654	K661	L662	F665	Y668	L669	I672	V682	F685	P686	P689	E689	I700	R701	V702	R712	R713	K718	A724	W725	Q726	P727	A745	S748	Y756	Y757	F760	P763	P764																																	
M773	N778	F784	N785	I786	K790	N791	THR	ASP	E795	I799	G800	L801	R808	Y809	F812	Y828	K835	L836	I846	F852	V860	S861	K862	I863	T864	K865	S866	K867	I868	K869	R870	E871	K872	Y873	L874	T875	GLN	LYS	LEU	LEU	LEU	HIS	GLU	SER	HIS	HIS	LYS	ASP																						
LEU	THR	LYS	ASN	MET	VAL	GLY	ILE	ILE	ALA	ALA	GLU	ARG	ILE	GLY	GLY	THR	VAL	ARG	ASN	ASN	SER	VAL	ARG	HIS	PRO	PRO	LYS	LEU	GLU	ALA	LEU	LEU	PHE	GLN	GLY	PRO	GLN	GLY	THR	THR	GLU	GLN	LYS	LEU	ILE	SER	GLU	GLU	ASP	LEU	ARG	ARG	GLY	ALA	ALA	SER	MET	ASP	GLU	LYS	THR	THR	GLY	TRP	ARG					
GLY	GLY	HIS	VAL	VAL	GLU	GLY	LEU	LEU	ALA	ALA	GLU	GLU	LEU	LEU	GLN	LEU	ARG	ALA	ALA	ARG	LEU	LEU	GLU	HIS	HIS	PRO	PRO	LYS	LEU	GLU	GLY	GLN	ALA	LEU	LEU	LEU	LEU	PHE	GLN	GLY	PRO	GLN	GLY	THR	THR	GLU	GLN	LYS	LEU	ILE	SER	GLU	GLU	ASP	LEU	ARG	ARG	GLY	ALA	ALA	SER	MET	ASP	GLU	LYS	THR	THR	GLY	TRP	ARG

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	394821	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 ($e^-/\text{\AA}^2$)	66.6	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.038	Depositor
Minimum map value	-0.415	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.149	Depositor
Map size (\AA)	338.52002, 338.52002, 338.52002	wwPDB
Map dimensions	260, 260, 260	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.302, 1.302, 1.302	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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	0/5999	0.44	0/8133
1	B	0.27	0/5999	0.44	0/8133
All	All	0.27	0/11998	0.44	0/16266

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	5840	0	5829	77	0
1	B	5840	0	5829	78	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
All	All	11686	0	11658	154	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 7.

The worst 5 of 154 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:B:559:GLN:HG3	1:B:669:LEU:HD21	1.67	0.77
1:A:559:GLN:HG3	1:A:669:LEU:HD21	1.67	0.75
1:A:357:PRO:HA	1:A:801:LEU:HD21	1.69	0.73
1:B:357:PRO:HA	1:B:801:LEU:HD21	1.69	0.73
1:B:778:ASN:OD1	1:B:808:ARG:NH1	2.26	0.67

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	691/975 (71%)	675 (98%)	16 (2%)	0	100	100
1	B	691/975 (71%)	674 (98%)	17 (2%)	0	100	100
All	All	1382/1950 (71%)	1349 (98%)	33 (2%)	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	638/878 (73%)	630 (99%)	8 (1%)	69	87
1	B	638/878 (73%)	630 (99%)	8 (1%)	69	87
All	All	1276/1756 (73%)	1260 (99%)	16 (1%)	70	87

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	685	PHE
1	B	597	ASP
1	B	73	PHE
1	B	539	GLU
1	A	763	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	351	GLN
1	B	401	GLN
1	B	814	ASN
1	B	544	GLN
1	A	544	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](#)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

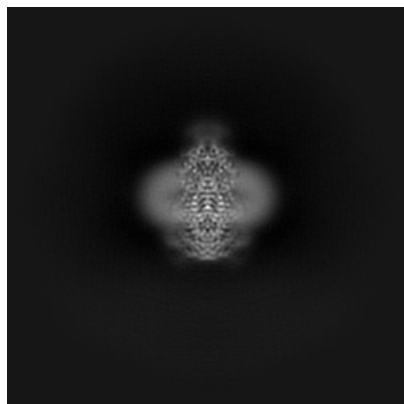
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15914. These allow visual inspection of the internal detail of the map and identification of artifacts.

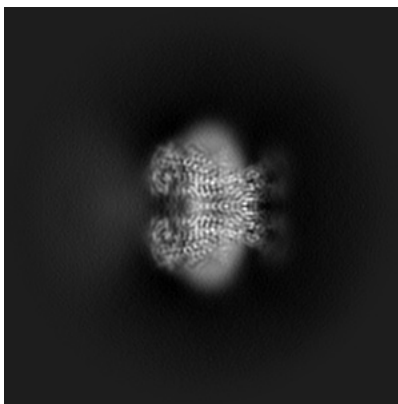
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

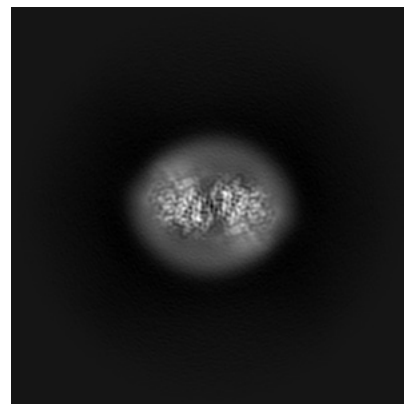
6.1.1 Primary map



X

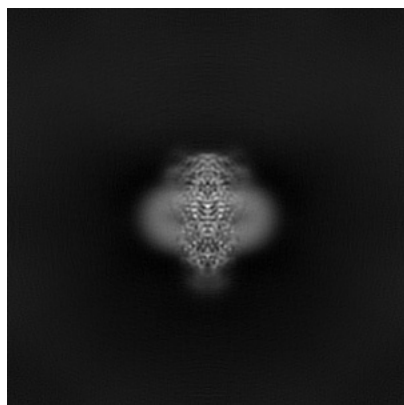


Y

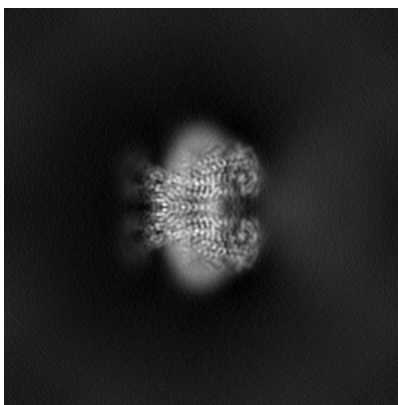


Z

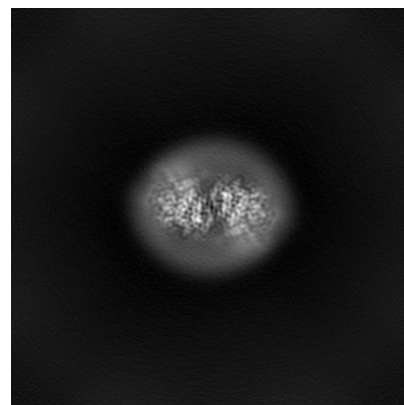
6.1.2 Raw map



X



Y

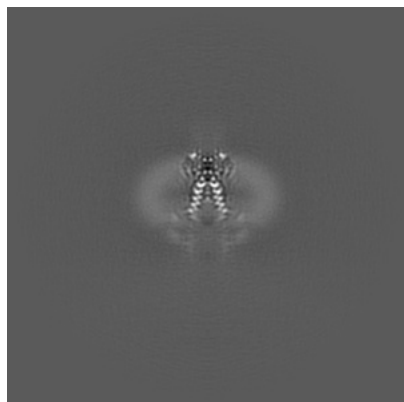


Z

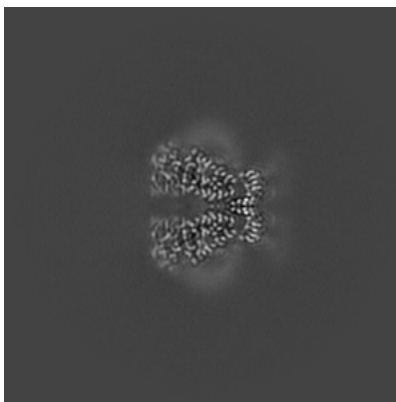
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

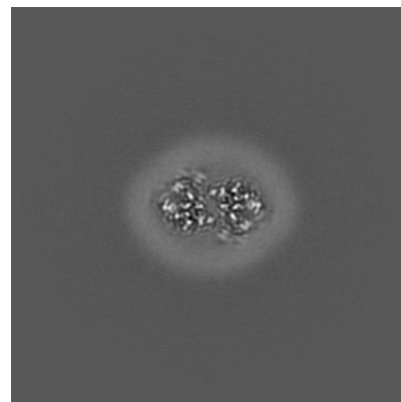
6.2.1 Primary map



X Index: 130

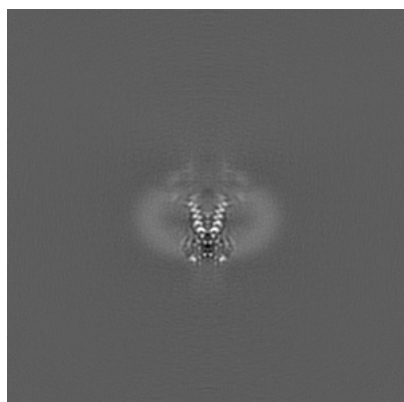


Y Index: 130

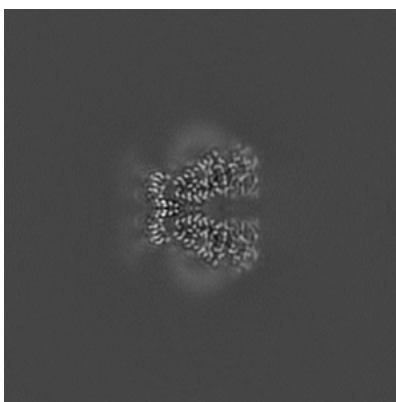


Z Index: 130

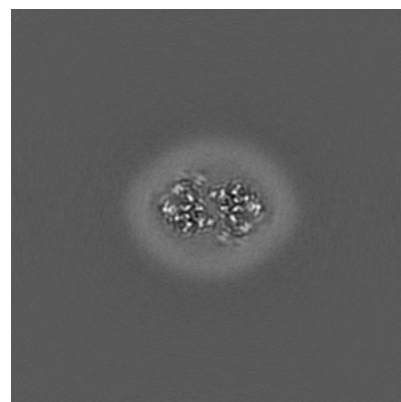
6.2.2 Raw map



X Index: 130



Y Index: 130

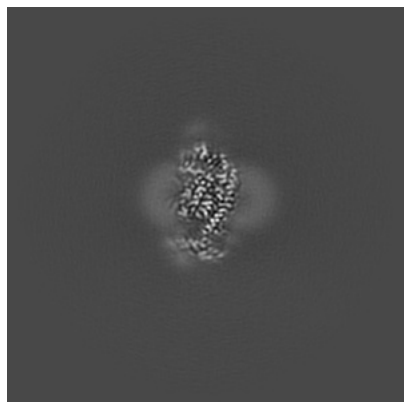


Z Index: 130

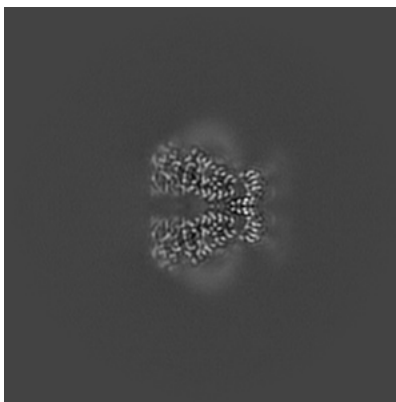
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

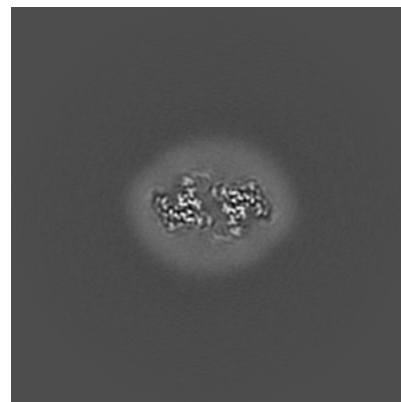
6.3.1 Primary map



X Index: 147

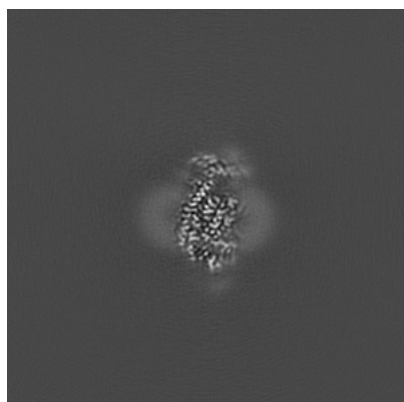


Y Index: 130

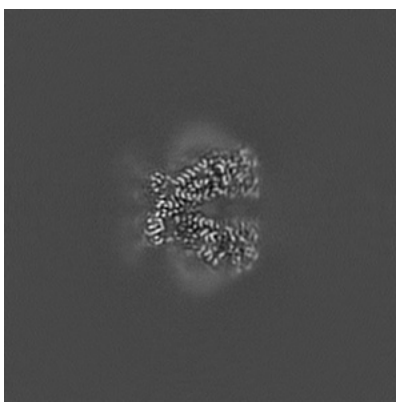


Z Index: 125

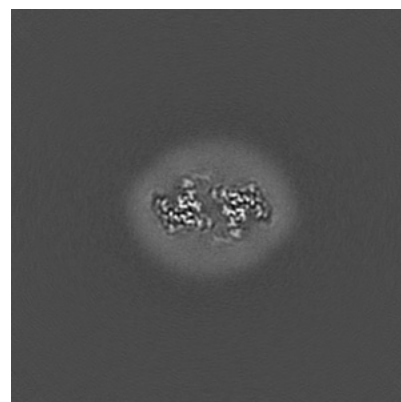
6.3.2 Raw map



X Index: 113



Y Index: 131

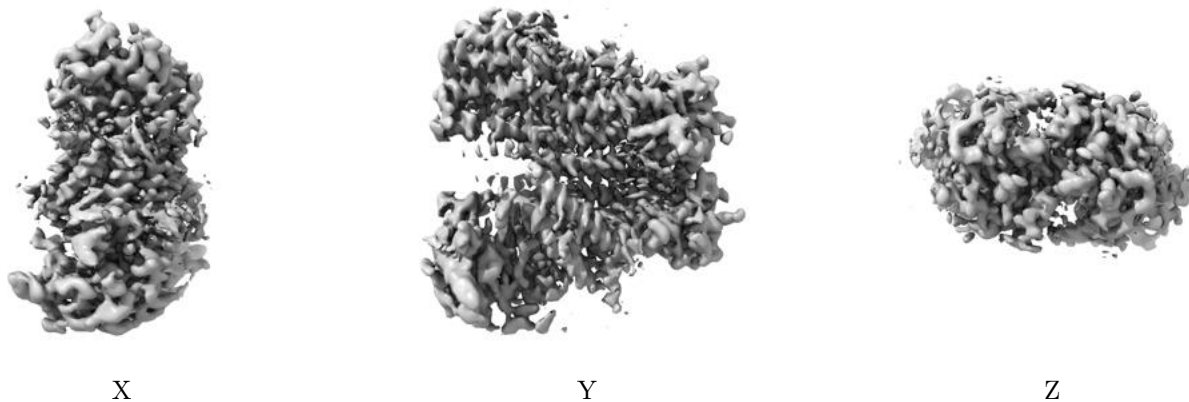


Z Index: 135

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

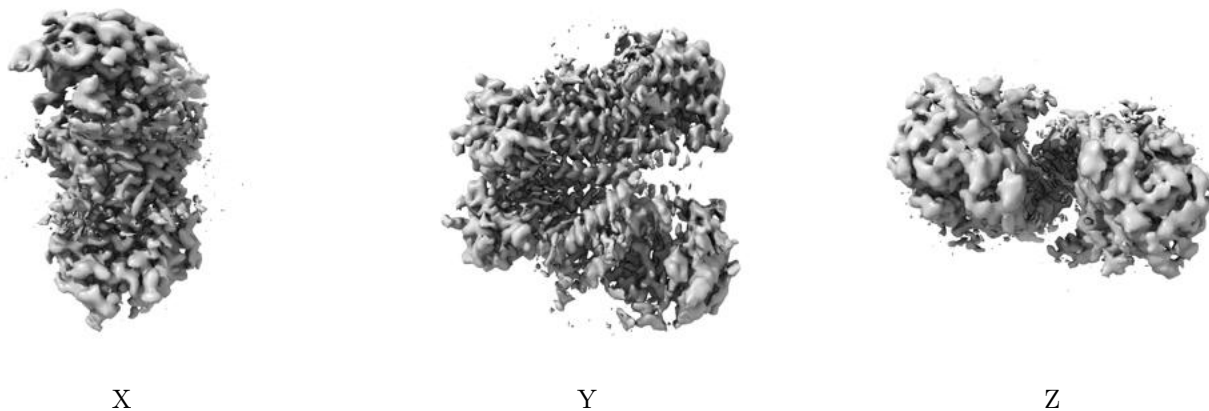
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.149. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

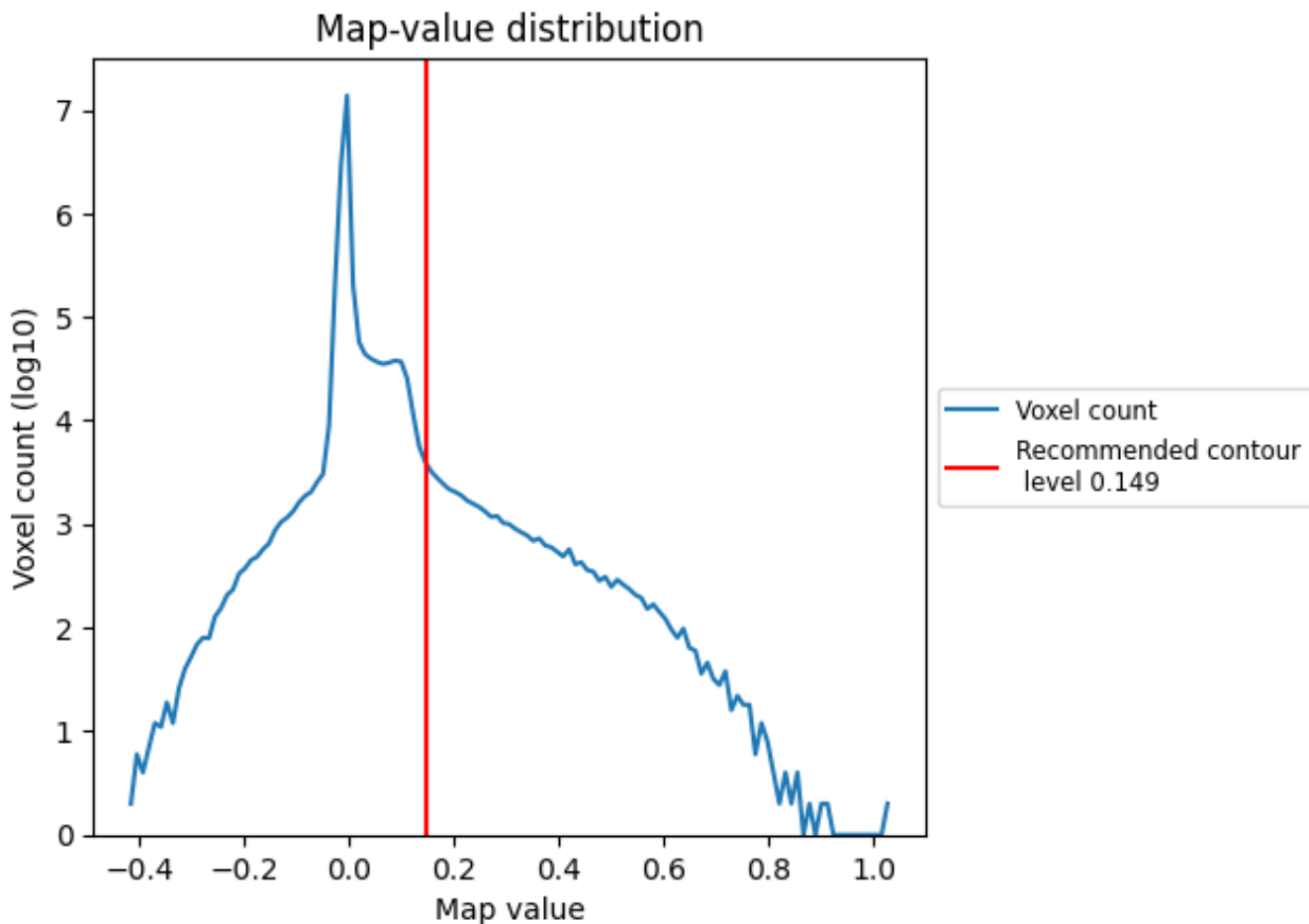
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

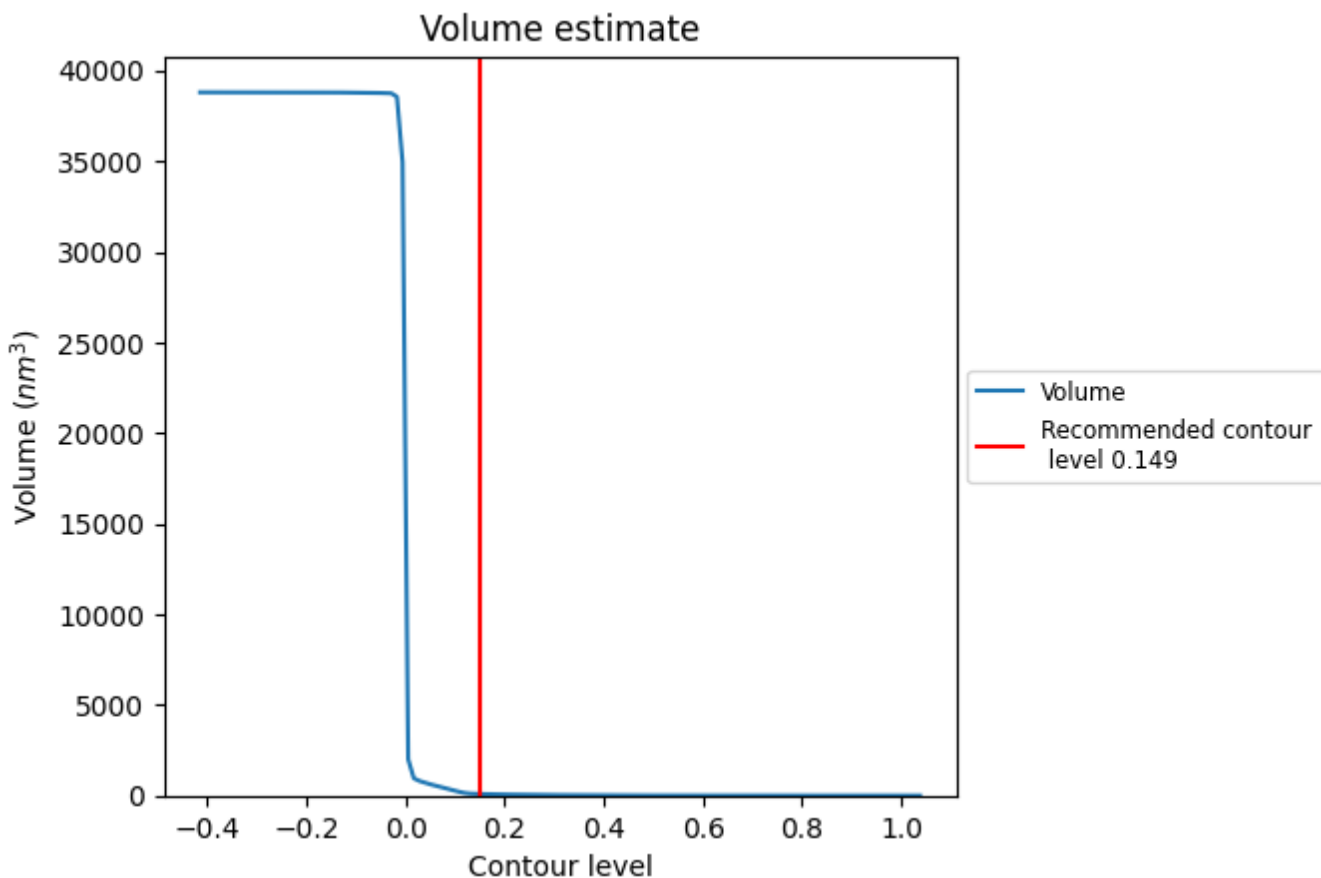
This section contains the results of statistical analysis of the map.

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.

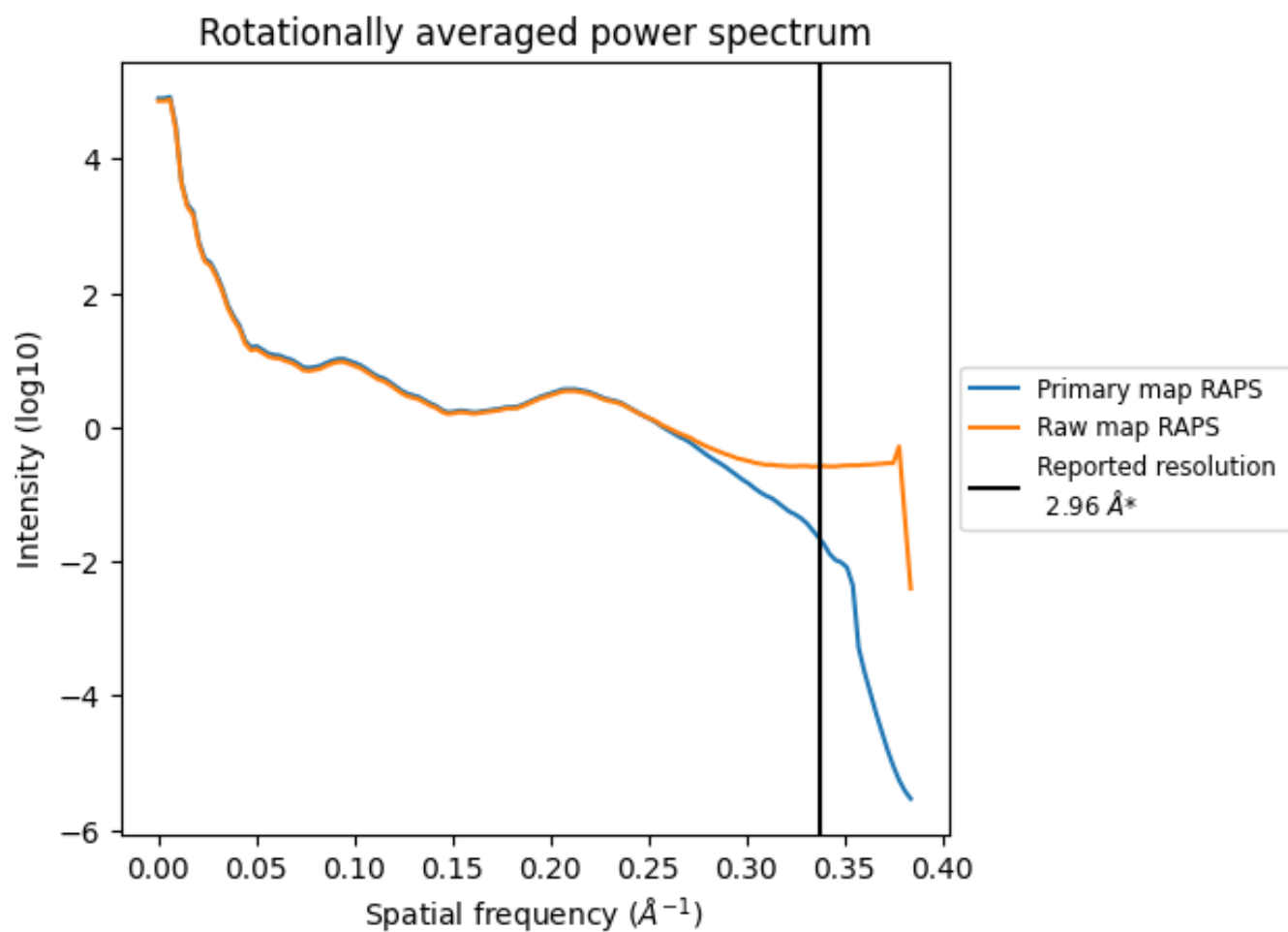
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 87 nm³; this corresponds to an approximate mass of 79 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](#)

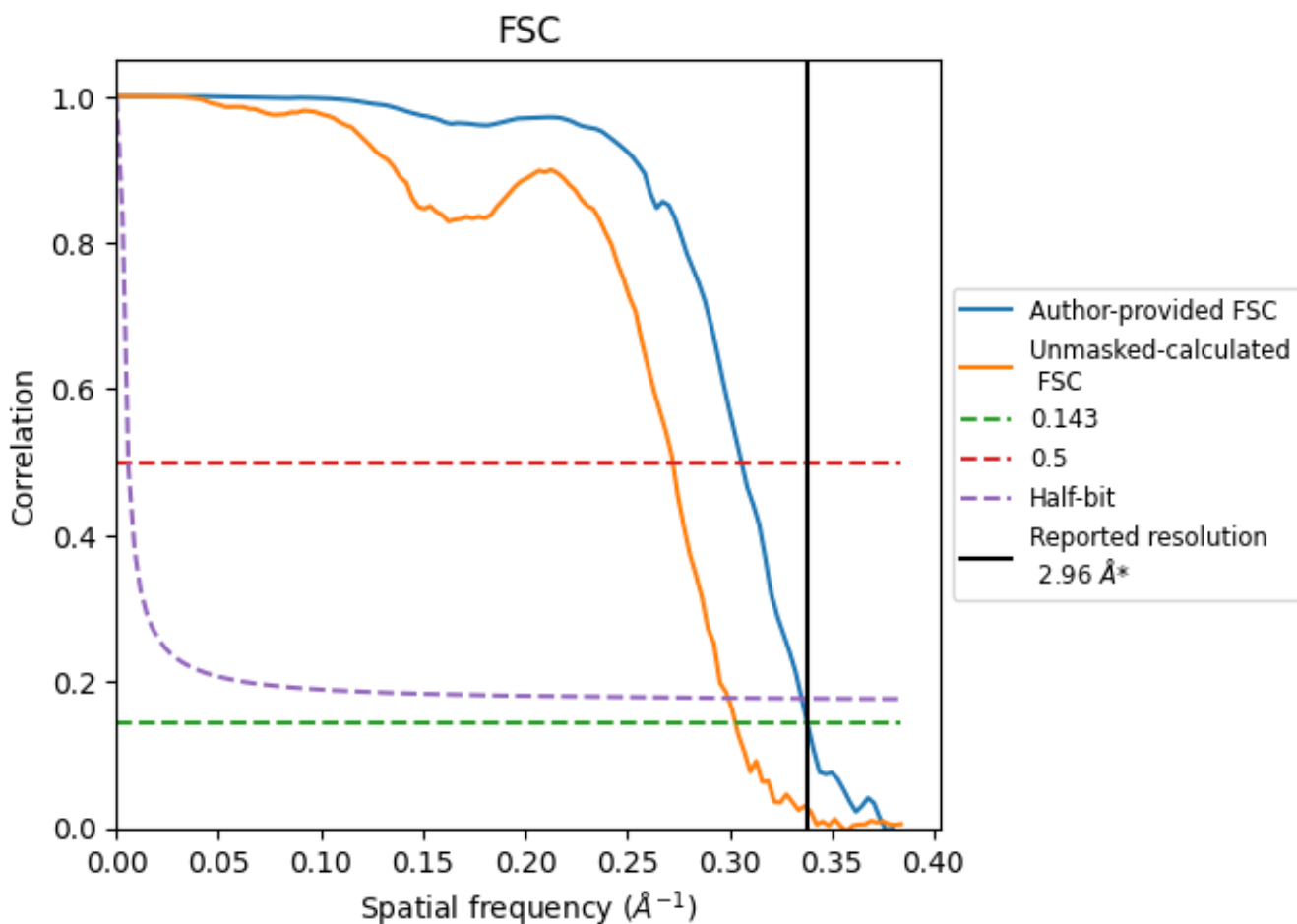


*Reported resolution corresponds to spatial frequency of 0.338 Å⁻¹

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 0.338 Å⁻¹

8.2 Resolution estimates [i](#)

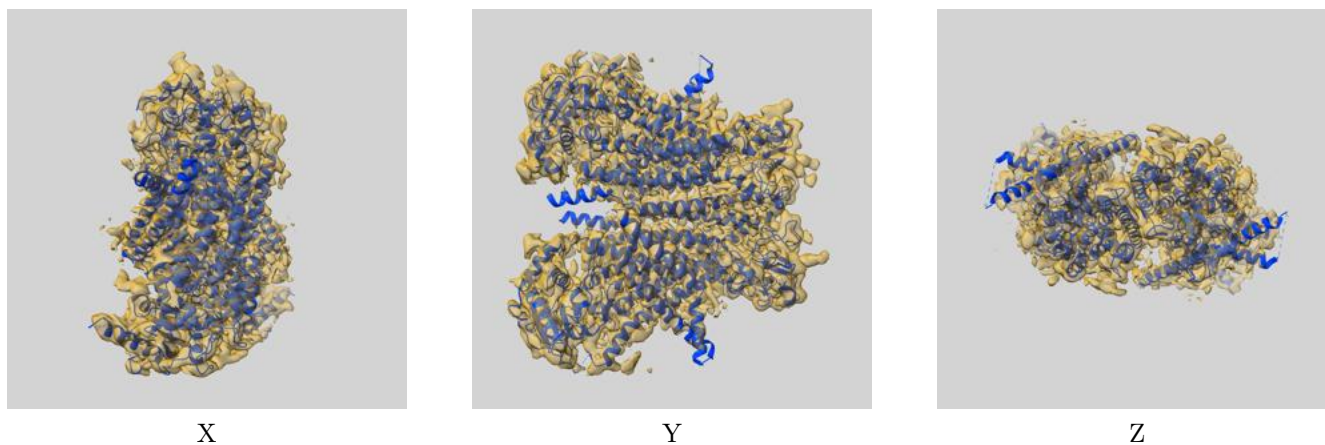
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.96	-	-
Author-provided FSC curve	2.96	3.27	2.98
Unmasked-calculated*	3.30	3.67	3.34

*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 3.30 differs from the reported value 2.96 by more than 10 %

9 Map-model fit [i](#)

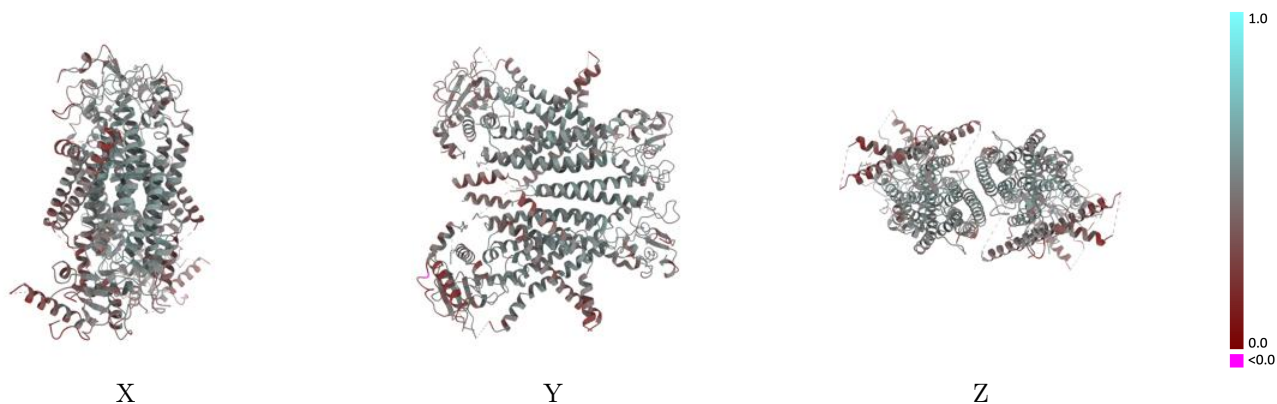
This section contains information regarding the fit between EMDB map EMD-15914 and PDB model 8B8J. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



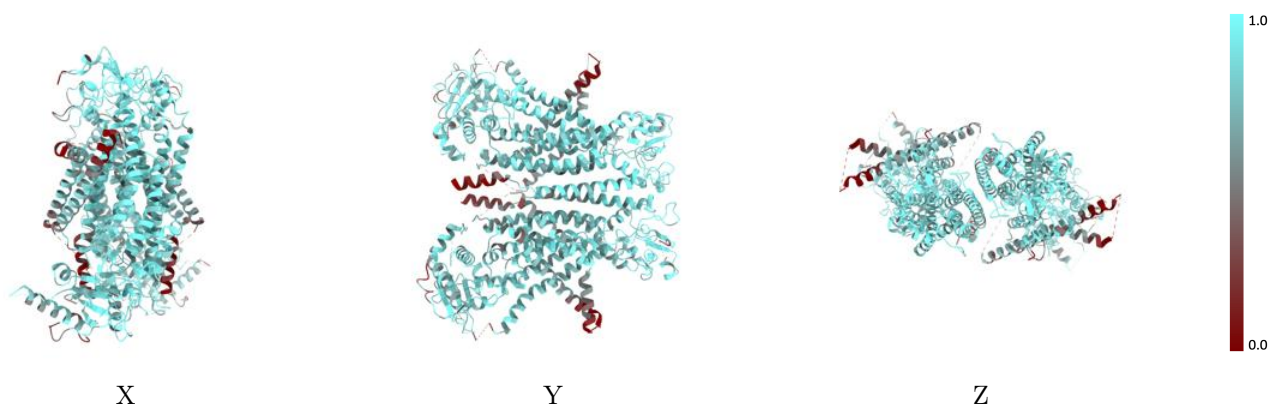
The images above show the 3D surface view of the map at the recommended contour level 0.149 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



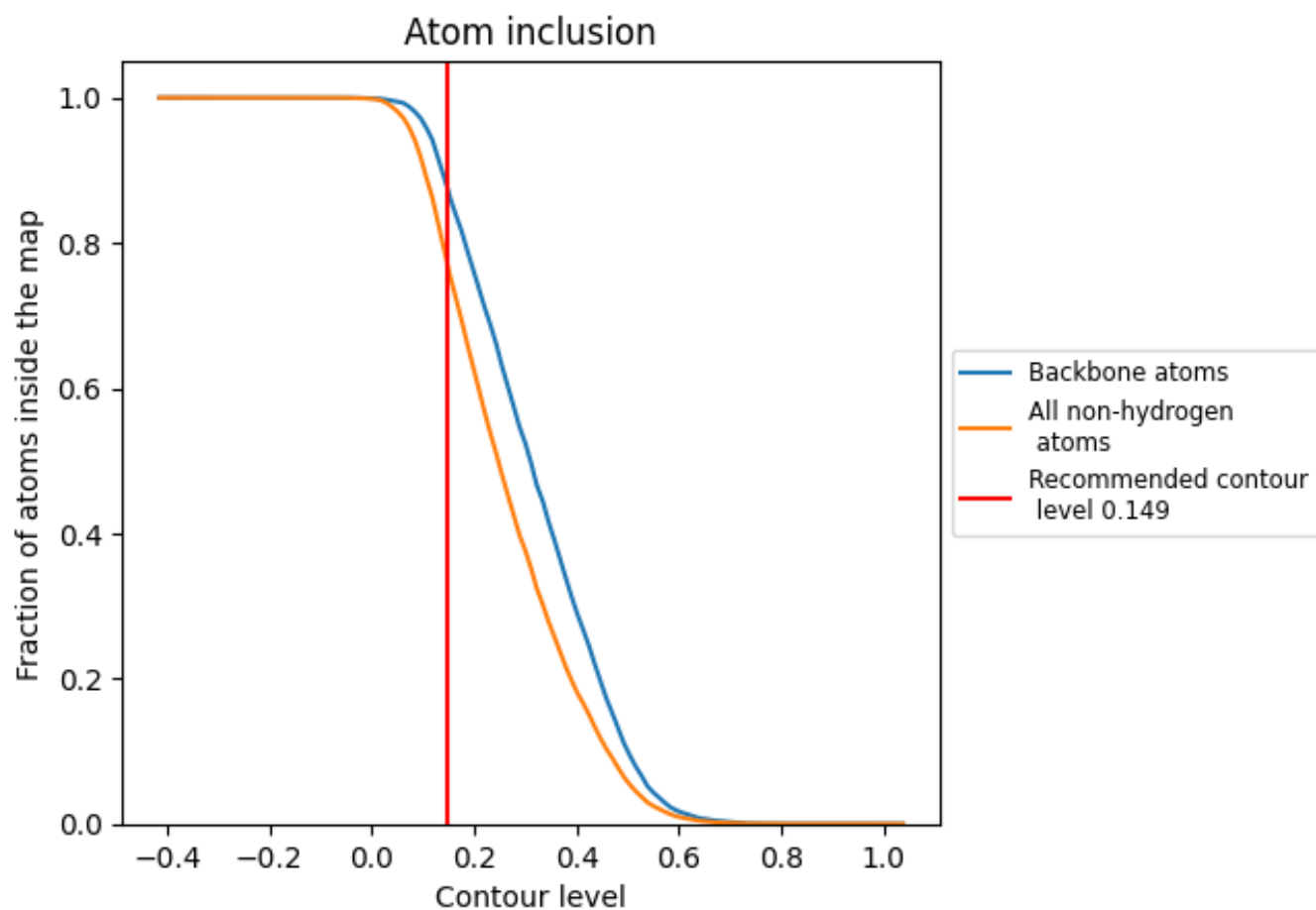
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.149).







9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 77% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.149) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7690	 0.4590
A	 0.7644	 0.4590
B	 0.7735	 0.4590

