



Full wwPDB EM Validation Report ⓘ

Jan 1, 2025 – 11:25 AM EST

PDB ID : 8U2C
EMDB ID : EMD-41845
Title : Gaussian mixture model based single particle refinement - ABC transporter
(inhibitor-bound ABCG2 from EMPIAR-10374)
Authors : Chen, M.; Pintilie, G.
Deposited on : 2023-09-05
Resolution : 2.50 Å (reported)
Based on initial models : 7FAB, 6ETI

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.dev113
MolProbity : 4.02b-467
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) : 2.40

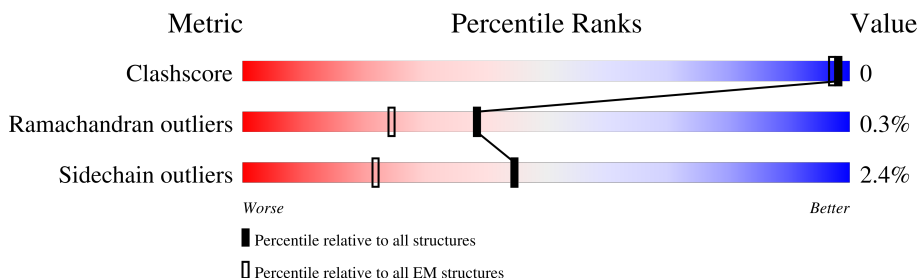
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY





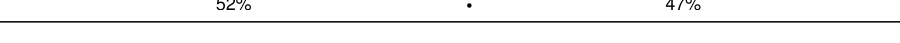
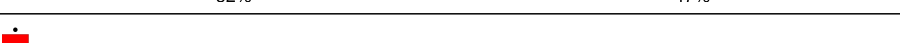


The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	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	655	 83% 14%
1	B	655	 83% 14%
2	C	214	 49% 50%
2	E	214	 49% 50%
3	D	221	 52% 47%
3	F	221	 52% 47%
4	I	217	 39% 59%
4	J	217	 38% 59%

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Mol	Chain	Length	Quality of chain
5	K	210	<div><div><div></div><div></div><div></div></div><div>7%39%5%•55%</div></div>
5	L	210	<div><div><div></div><div></div><div></div></div><div>7%41%•55%</div></div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15042 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 Broad substrate specificity ATP-binding cassette transporter ABCG2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	566	Total	C	N	O	S	0	0
			4405	2859	726	791	29		
1	B	566	Total	C	N	O	S	0	0
			4405	2859	726	791	29		

- Molecule 2 is a protein called 5D3 Fab light chain variable domain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	107	Total	C	N	O	S	0	0
			822	521	137	162	2		
2	E	107	Total	C	N	O	S	0	0
			822	521	137	162	2		

- Molecule 3 is a protein called 5D3 Fab heavy chain variable domain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	118	Total	C	N	O	S	0	0
			928	592	153	180	3		
3	F	118	Total	C	N	O	S	0	0
			928	592	153	180	3		

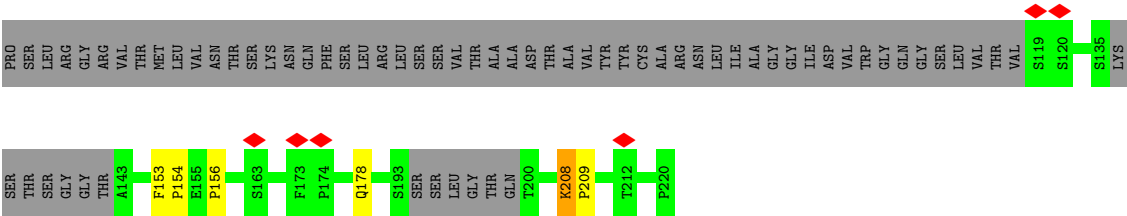
- Molecule 4 is a protein called FAB heavy chain constant domain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	I	89	Total	C	N	O	S	0	0
			650	415	105	128	2		
4	J	89	Total	C	N	O	S	0	0
			650	415	105	128	2		

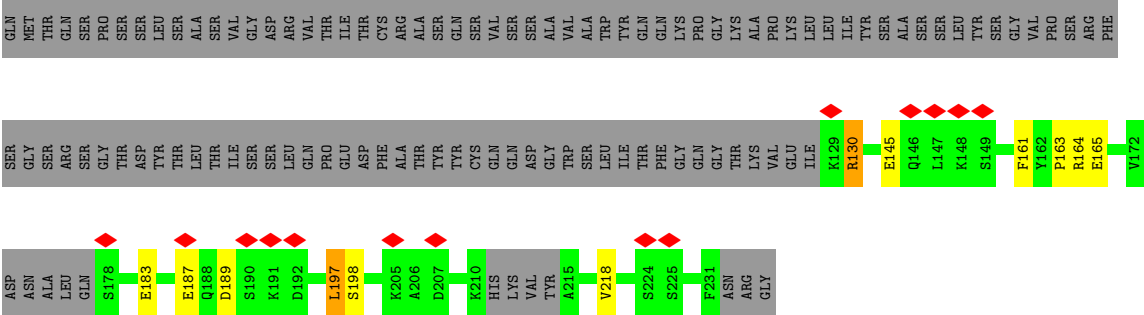
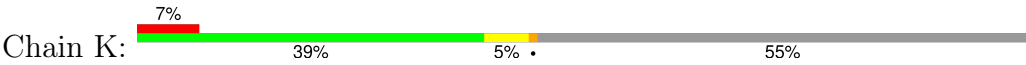
- Molecule 5 is a protein called Fab light chain constant domain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	K	94	Total	C	N	O	S	0	0
			716	448	119	147	2		
5	L	94	Total	C	N	O	S	0	0
			716	448	119	147	2		

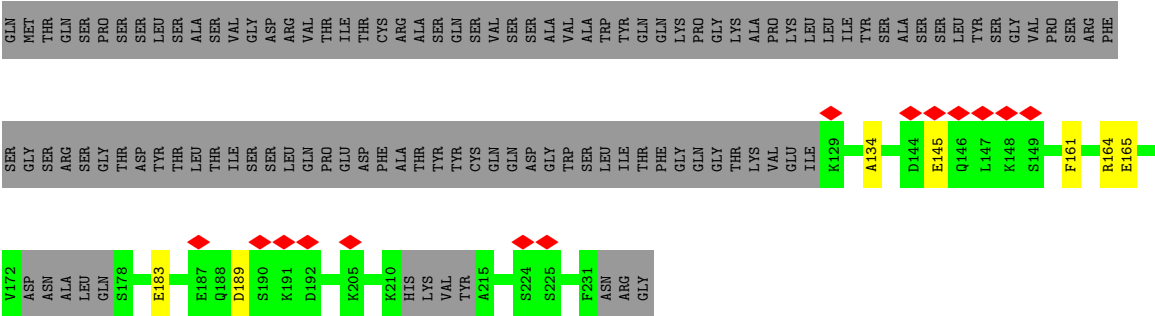
- [illegible]



• Molecule 5: Fab light chain constant domain



• Molecule 5: Fab light chain constant domain



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	284831	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	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	26.854	Depositor
Minimum map value	-9.732	Depositor
Average map value	0.075	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	5	Depositor
Map size (\AA)	268.8, 268.8, 268.8	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.05, 1.05, 1.05	Depositor

5 Model quality

5.1 Standard geometry

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	0.62	0/4497	0.94	6/6085 (0.1%)
1	B	0.62	0/4497	1.01	10/6085 (0.2%)
2	C	0.67	0/842	0.99	1/1144 (0.1%)
2	E	0.67	0/842	0.98	2/1144 (0.2%)
3	D	0.69	0/953	1.03	1/1297 (0.1%)
3	F	0.69	0/953	1.04	3/1297 (0.2%)
4	I	0.61	0/666	1.02	0/911
4	J	0.61	0/666	1.06	0/911
5	K	0.66	0/728	1.07	2/984 (0.2%)
5	L	0.66	0/728	1.03	2/984 (0.2%)
All	All	0.64	0/15372	1.00	27/20842 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
All	All	0	3

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	595	LEU	O-C-N	-20.09	90.55	122.70
1	B	595	LEU	CA-C-N	15.72	151.79	117.20
3	F	84	ARG	NE-CZ-NH2	7.97	124.28	120.30
3	D	84	ARG	NE-CZ-NH2	7.69	124.14	120.30
1	B	595	LEU	C-N-CA	7.17	139.63	121.70
1	B	383	ARG	NE-CZ-NH2	7.00	123.80	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	236	ARG	NE-CZ-NH2	6.95	123.78	120.30
1	A	193	ARG	NE-CZ-NH2	6.62	123.61	120.30
3	F	67	ARG	NE-CZ-NH2	6.47	123.54	120.30
5	K	130	ARG	NE-CZ-NH2	6.46	123.53	120.30
1	B	193	ARG	NE-CZ-NH2	6.38	123.49	120.30
1	B	236	ARG	NE-CZ-NH2	6.21	123.41	120.30
1	A	482	ARG	NE-CZ-NH2	6.04	123.32	120.30
2	C	32	ARG	NE-CZ-NH2	5.91	123.25	120.30
1	B	482	ARG	NE-CZ-NH2	5.74	123.17	120.30
5	L	164	ARG	NE-CZ-NH2	5.68	123.14	120.30
5	K	164	ARG	NE-CZ-NH2	5.68	123.14	120.30
2	E	107	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	B	246	ARG	NE-CZ-NH2	5.31	122.95	120.30
2	E	61	ARG	NE-CZ-NH2	5.27	122.94	120.30
3	F	39	ARG	NE-CZ-NH2	5.24	122.92	120.30
1	A	160	ARG	NE-CZ-NH2	5.24	122.92	120.30
1	A	426	ARG	NE-CZ-NH2	5.22	122.91	120.30
1	B	160	ARG	NE-CZ-NH2	5.18	122.89	120.30
1	B	426	ARG	NE-CZ-NH2	5.13	122.86	120.30
5	L	134	ALA	N-CA-CB	-5.06	103.01	110.10
1	A	383	ARG	NE-CZ-NH2	5.01	122.81	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	459	TYR	Sidechain
1	B	282	TYR	Sidechain
1	B	459	TYR	Sidechain

5.2 Too-close contacts ⓘ

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	4405	0	4482	2	0
1	B	4405	0	4482	2	0
2	C	822	0	801	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	822	0	801	0	0
3	D	928	0	890	0	0
3	F	928	0	890	0	0
4	I	650	0	646	1	0
4	J	650	0	646	2	0
5	K	716	0	699	1	0
5	L	716	0	699	0	0
All	All	15042	0	15036	8	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 0.

All (8) 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)
5:K:197:LEU:HD23	5:K:198:SER:N	2.21	0.56
4:J:153:PHE:CD1	4:J:154:PRO:HA	2.45	0.50
4:J:208:LYS:CB	4:J:209:PRO:HD3	2.48	0.44
4:I:153:PHE:CG	4:I:154:PRO:HA	2.52	0.43
1:B:162:ASN:HA	1:B:165:ILE:HG22	2.03	0.41
1:A:162:ASN:HA	1:A:165:ILE:HG22	2.03	0.41
1:A:596:ASN:OD1	1:A:598:THR:HG23	2.20	0.41
1:B:225:LEU:HD13	1:B:249:ILE:HG23	2.03	0.40

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	558/655 (85%)	545 (98%)	13 (2%)	0	100	100
1	B	558/655 (85%)	546 (98%)	12 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	105/214 (49%)	99 (94%)	6 (6%)	0	100	100
2	E	105/214 (49%)	97 (92%)	8 (8%)	0	100	100
3	D	116/221 (52%)	109 (94%)	7 (6%)	0	100	100
3	F	116/221 (52%)	110 (95%)	6 (5%)	0	100	100
4	I	83/217 (38%)	74 (89%)	8 (10%)	1 (1%)	11	21
4	J	83/217 (38%)	75 (90%)	6 (7%)	2 (2%)	5	8
5	K	88/210 (42%)	81 (92%)	6 (7%)	1 (1%)	12	23
5	L	88/210 (42%)	81 (92%)	6 (7%)	1 (1%)	12	23
All	All	1900/3034 (63%)	1817 (96%)	78 (4%)	5 (0%)	38	56

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	I	156	PRO
5	K	165	GLU
4	J	156	PRO
4	J	208	LYS
5	L	165	GLU

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	482/560 (86%)	472 (98%)	10 (2%)	48	74
1	B	482/560 (86%)	472 (98%)	10 (2%)	48	74
2	C	91/189 (48%)	90 (99%)	1 (1%)	70	87
2	E	91/189 (48%)	89 (98%)	2 (2%)	47	73
3	D	102/193 (53%)	101 (99%)	1 (1%)	73	88
3	F	102/193 (53%)	101 (99%)	1 (1%)	73	88
4	I	78/185 (42%)	76 (97%)	2 (3%)	41	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	J	78/185 (42%)	77 (99%)	1 (1%)	65 85
5	K	84/184 (46%)	75 (89%)	9 (11%)	5 11
5	L	84/184 (46%)	80 (95%)	4 (5%)	21 43
All	All	1674/2622 (64%)	1633 (98%)	41 (2%)	45 70

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	113	ARG
1	A	128	ASP
1	A	242	ILE
1	A	464	TYR
1	A	489	PHE
1	A	585	GLU
1	A	614	LEU
1	A	631	VAL
1	A	653	LYS
1	B	41	ASN
1	B	113	ARG
1	B	128	ASP
1	B	464	TYR
1	B	489	PHE
1	B	585	GLU
1	B	604	ASN
1	B	614	LEU
1	B	631	VAL
1	B	653	LYS
2	C	70	ASP
3	D	65	ARG
2	E	70	ASP
2	E	107	ARG
3	F	65	ARG
4	I	156	PRO
4	I	178	GLN
5	K	130	ARG
5	K	145	GLU
5	K	161	PHE
5	K	163	PRO
5	K	183	GLU
5	K	187	GLU

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Mol	Chain	Res	Type
5	K	189	ASP
5	K	197	LEU
5	K	218	VAL
4	J	178	GLN
5	L	145	GLU
5	L	161	PHE
5	L	183	GLU
5	L	189	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
3	D	36	ASN
3	F	36	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.

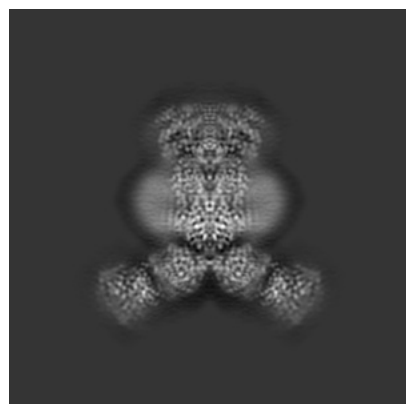
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41845. These allow visual inspection of the internal detail of the map and identification of artifacts.

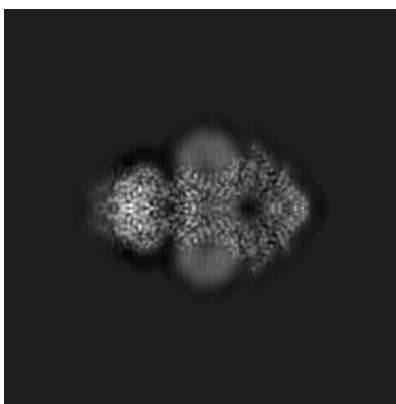
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

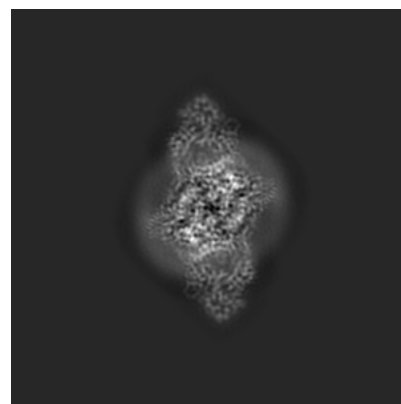
6.1.1 Primary map



X

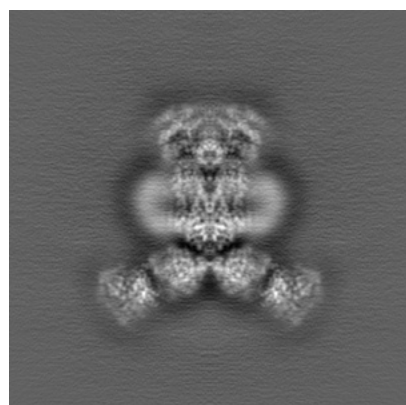


Y

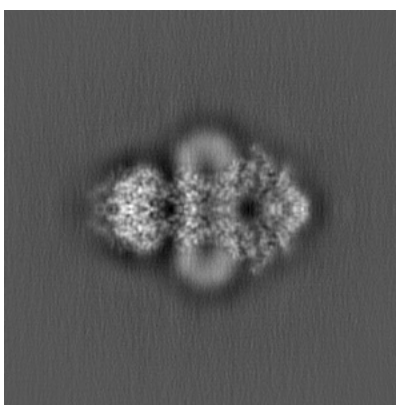


Z

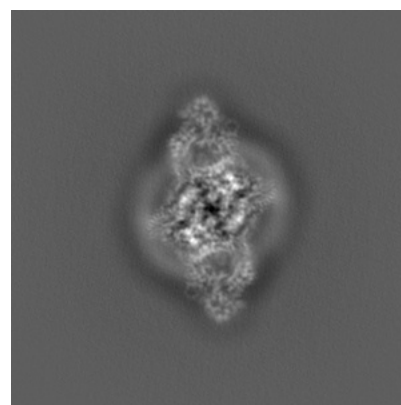
6.1.2 Raw map



X



Y

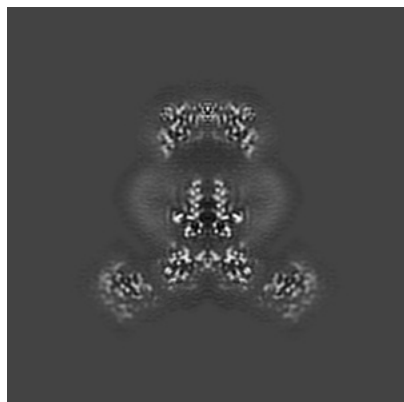


Z

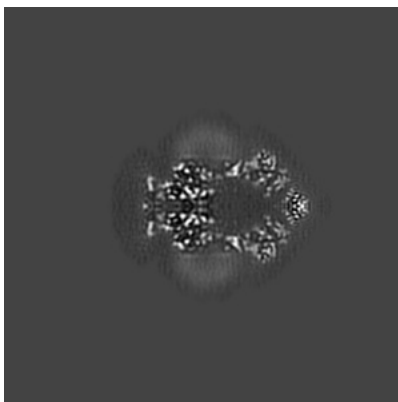
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

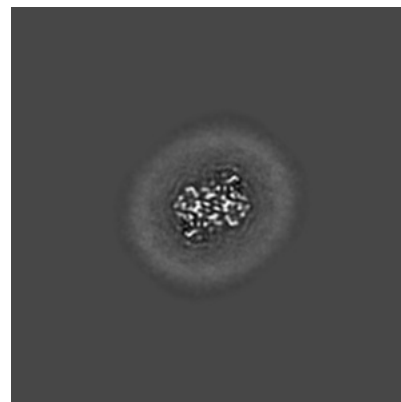
6.2.1 Primary map



X Index: 128

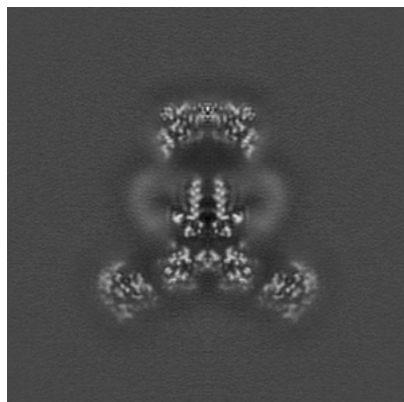


Y Index: 128

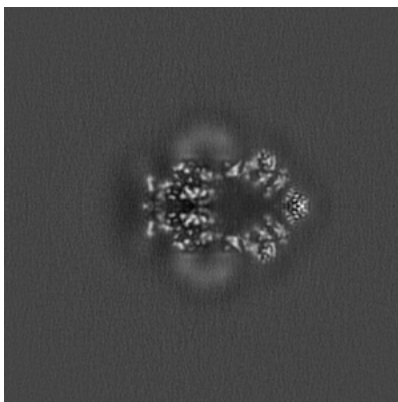


Z Index: 128

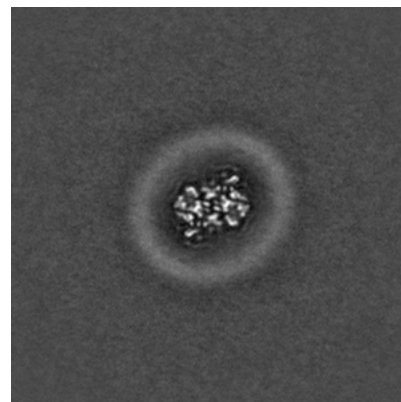
6.2.2 Raw map



X Index: 128



Y Index: 128

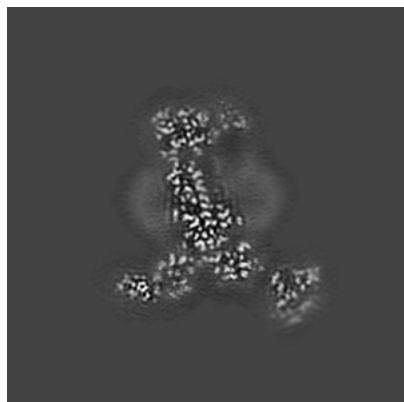


Z Index: 128

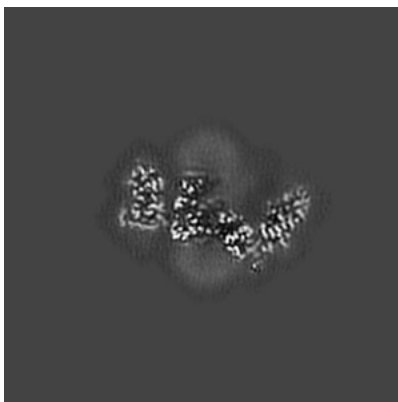
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

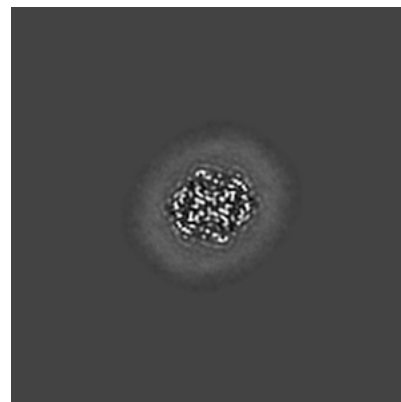
6.3.1 Primary map



X Index: 118

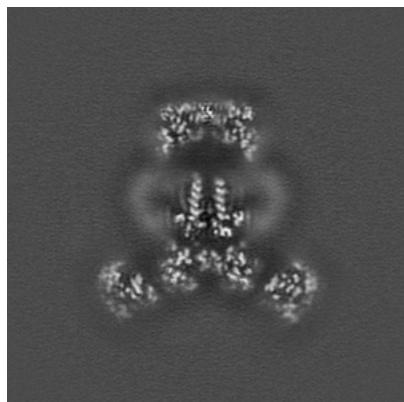


Y Index: 114

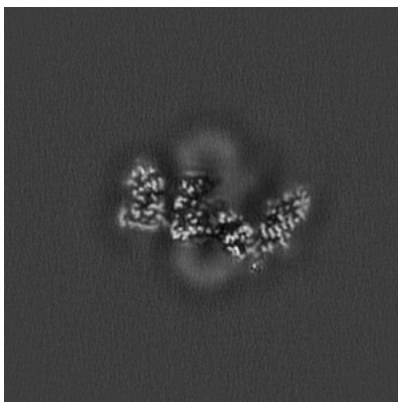


Z Index: 117

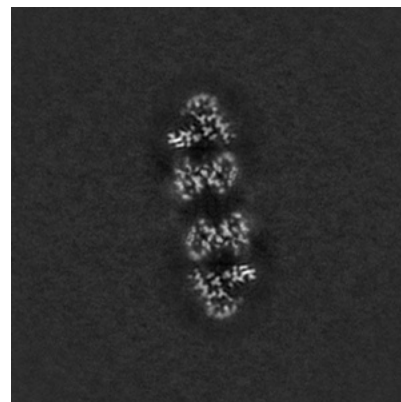
6.3.2 Raw map



X Index: 127



Y Index: 114

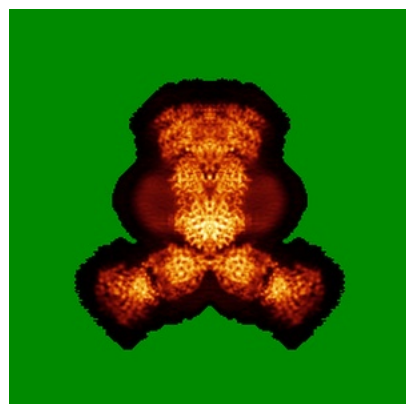


Z Index: 83

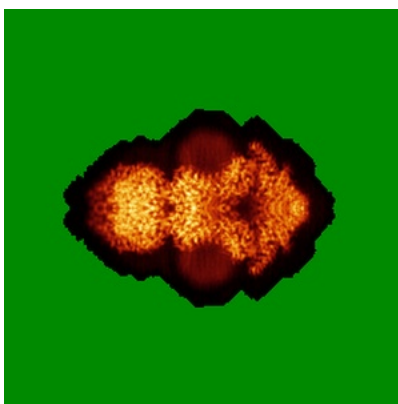
The images above show the largest variance slices of the map in three orthogonal directions.

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

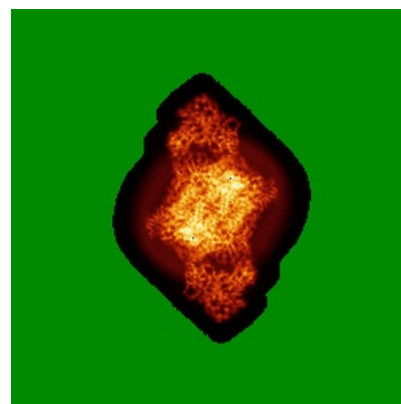
6.4.1 Primary map



X

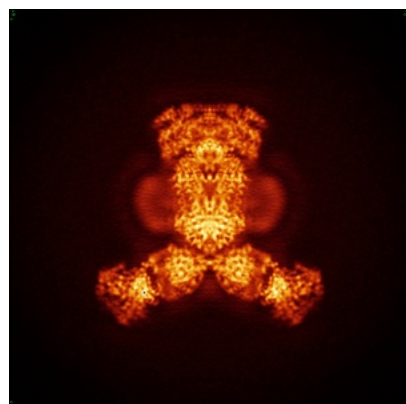


Y

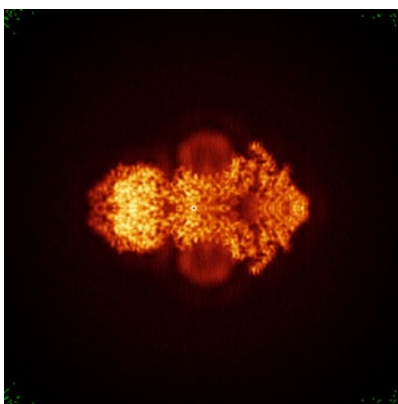


Z

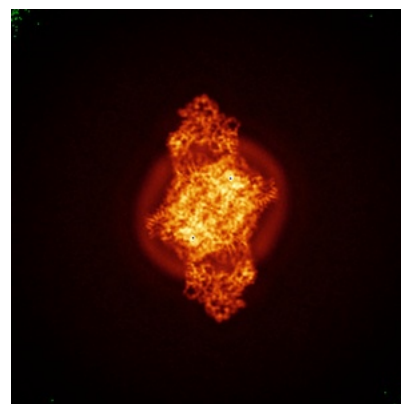
6.4.2 Raw map



X



Y

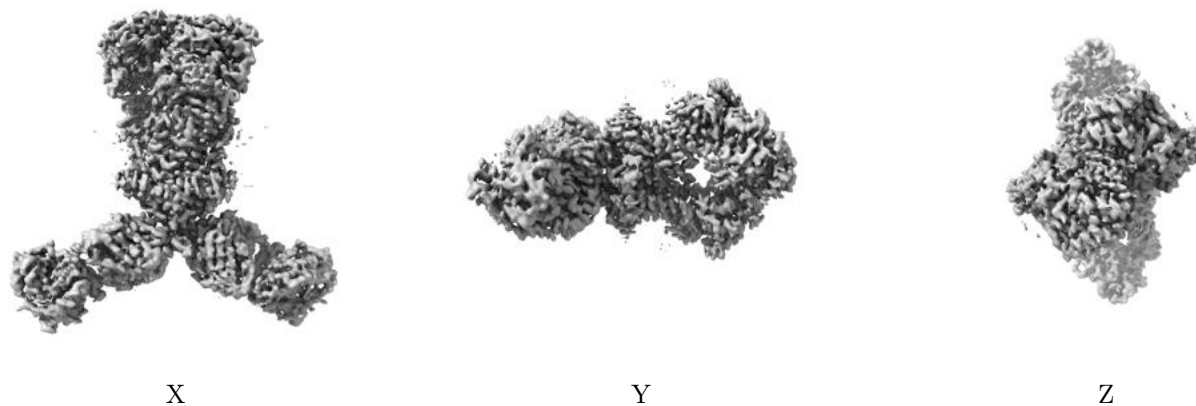


Z

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.

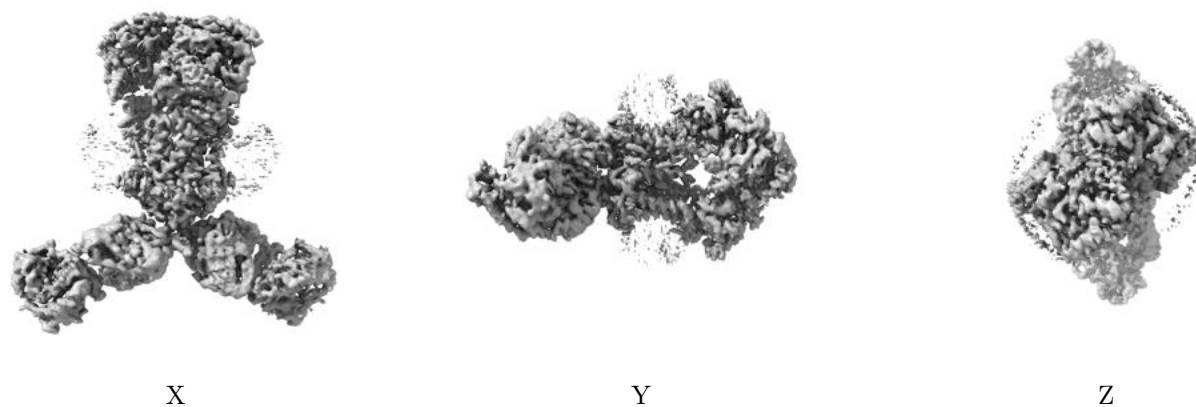
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 5.0. 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.

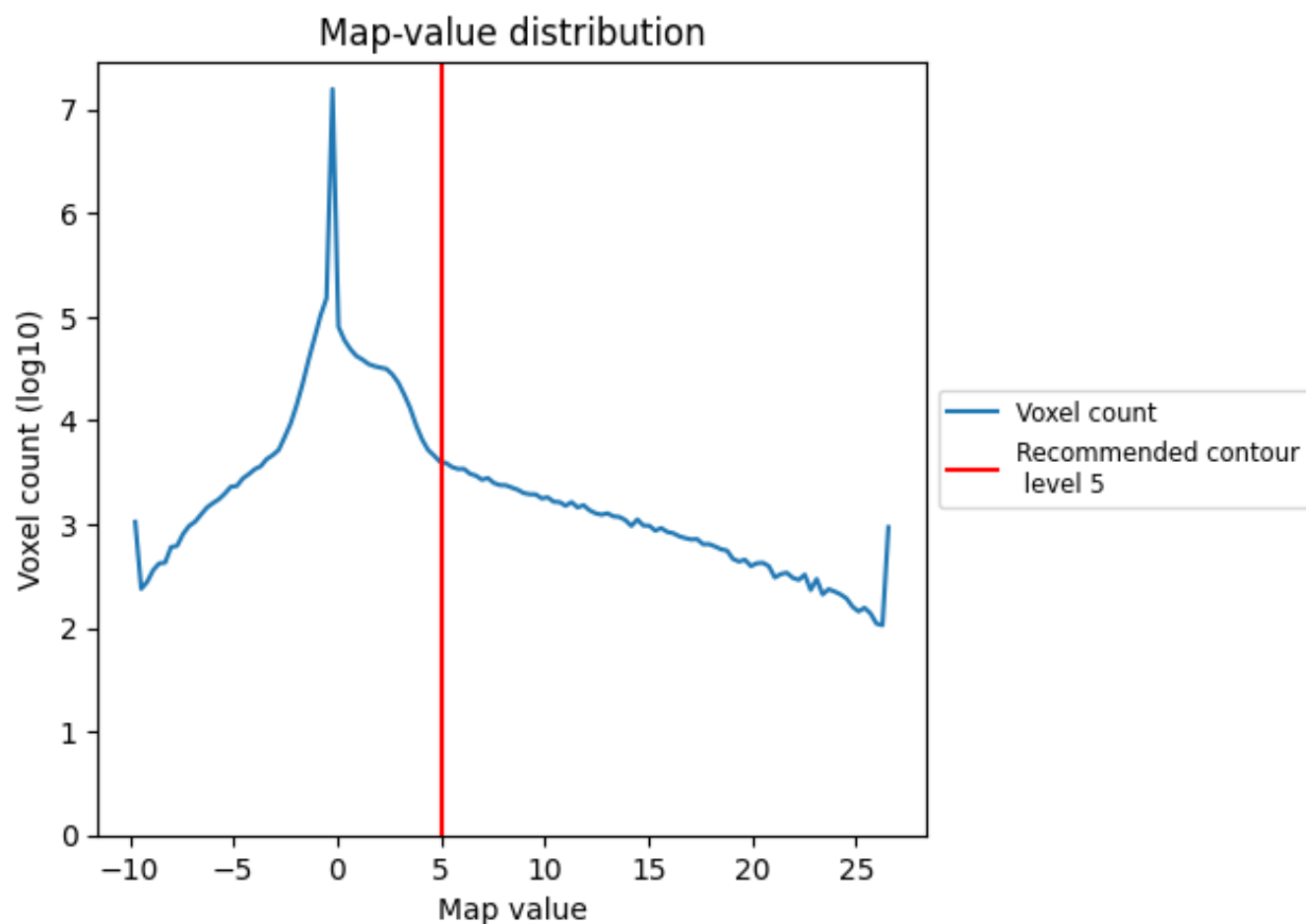
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

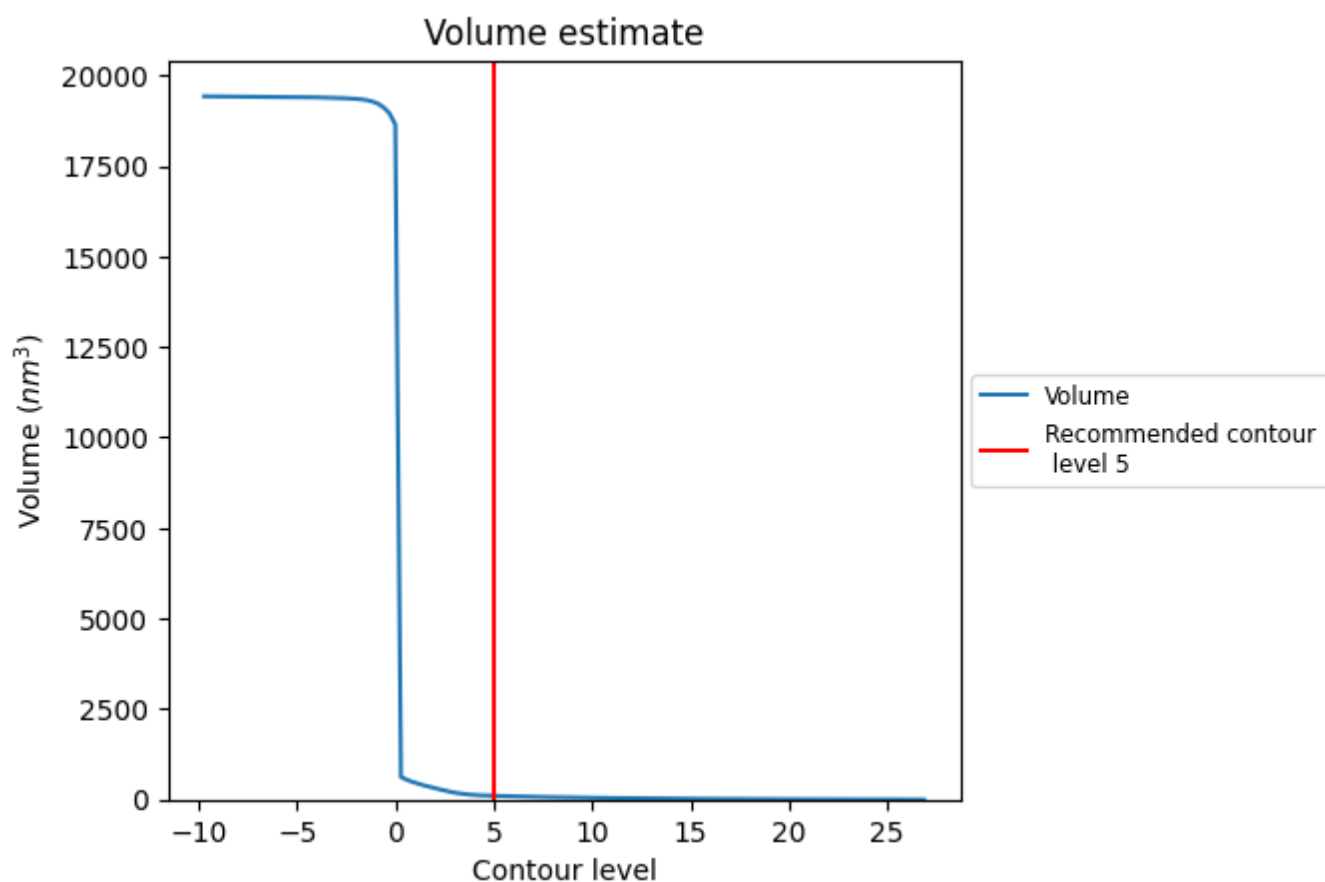
This section contains the results of statistical analysis of the map.

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.

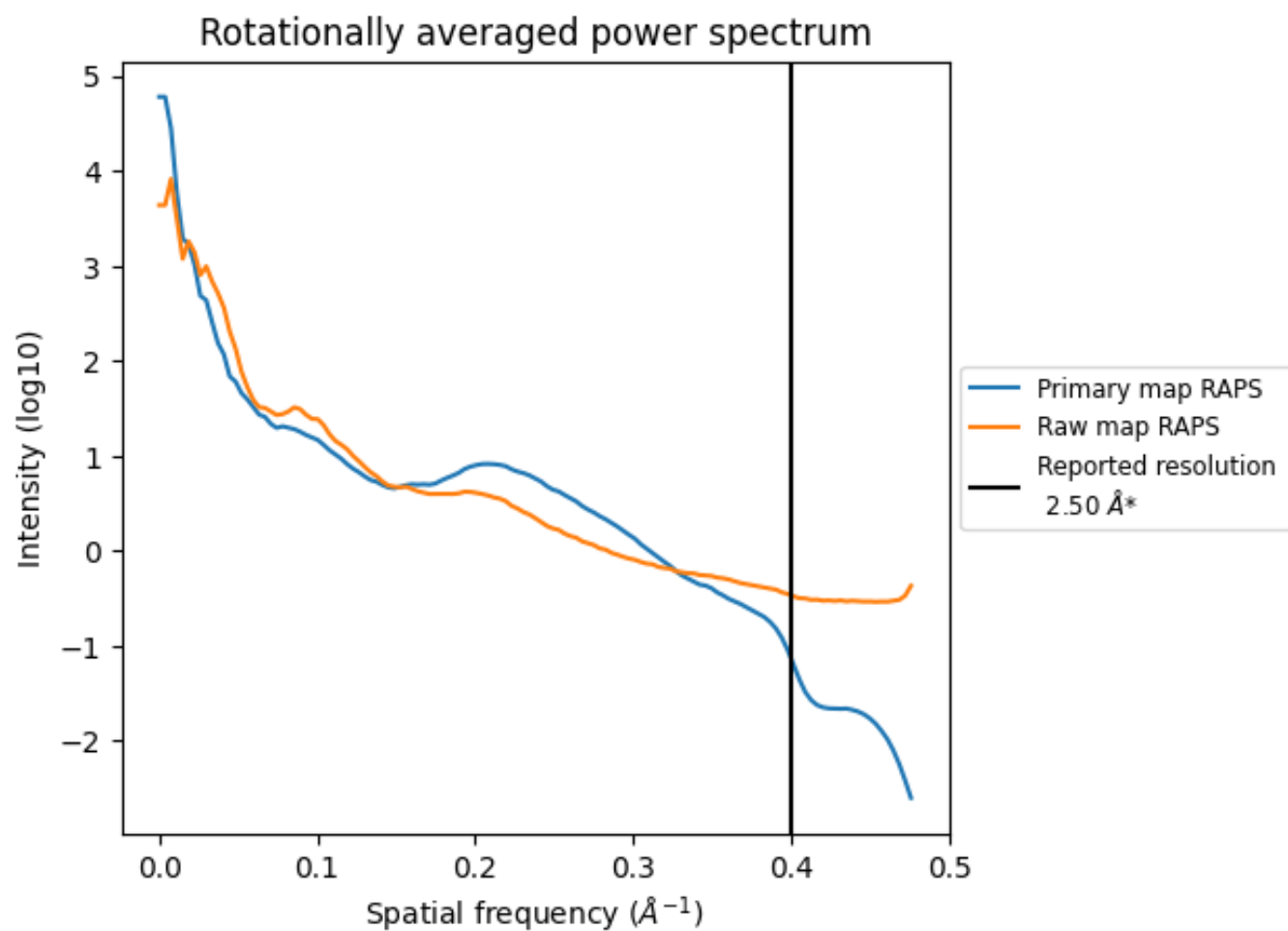
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 104 nm^3 ; this corresponds to an approximate mass of 94 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 ⓘ

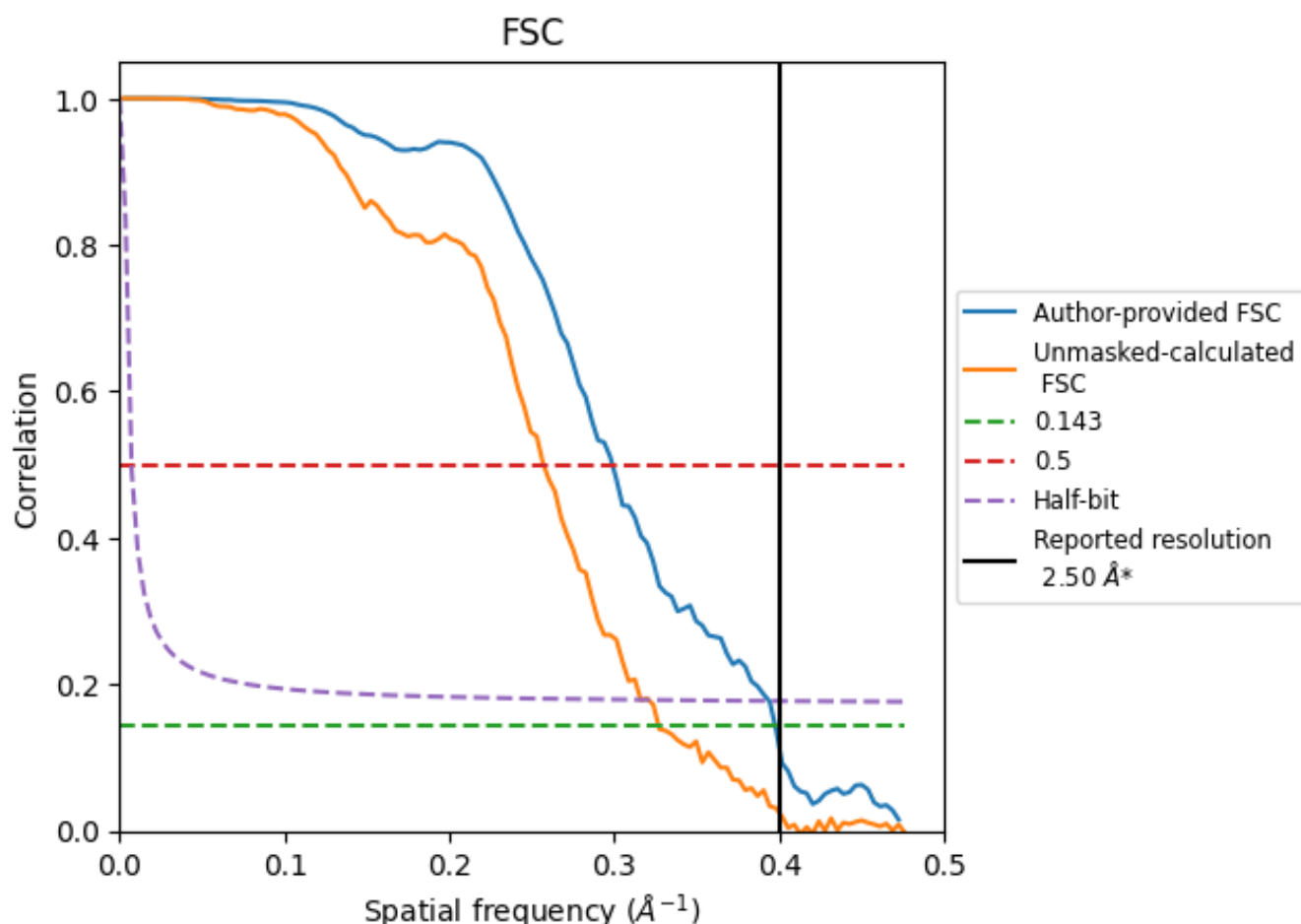


*Reported resolution corresponds to spatial frequency of 0.400 \AA^{-1}

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 0.400 Å⁻¹

8.2 Resolution estimates [i](#)

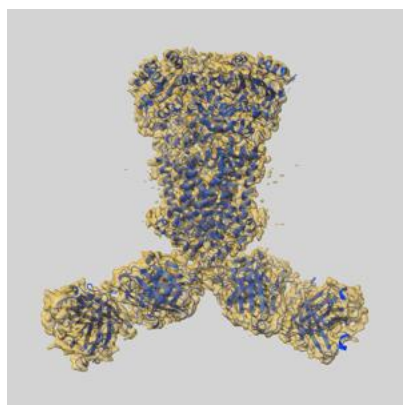
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.50	-	-
Author-provided FSC curve	2.52	3.35	2.54
Unmasked-calculated*	3.06	3.89	3.16

*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 3.06 differs from the reported value 2.5 by more than 10 %

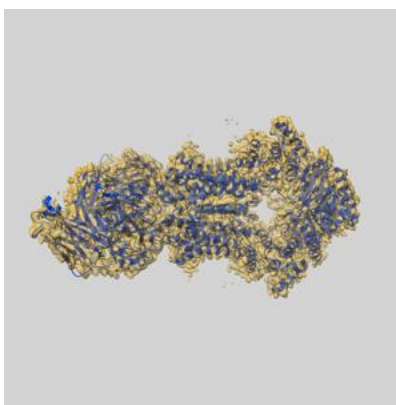
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-41845 and PDB model 8U2C. Per-residue inclusion information can be found in section [3](#) on page [6](#).

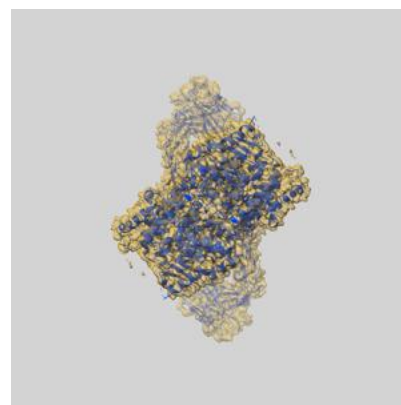
9.1 Map-model overlay [i](#)



X



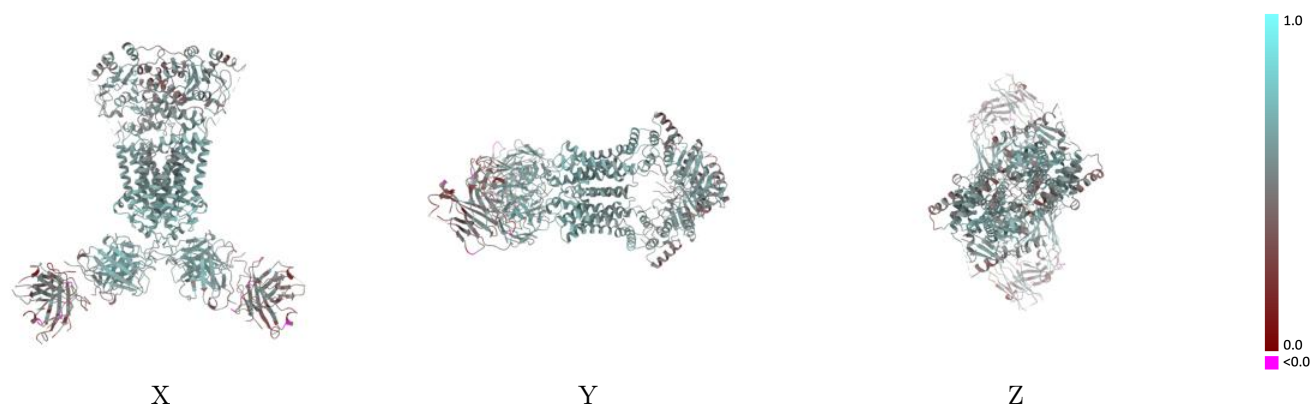
Y



Z

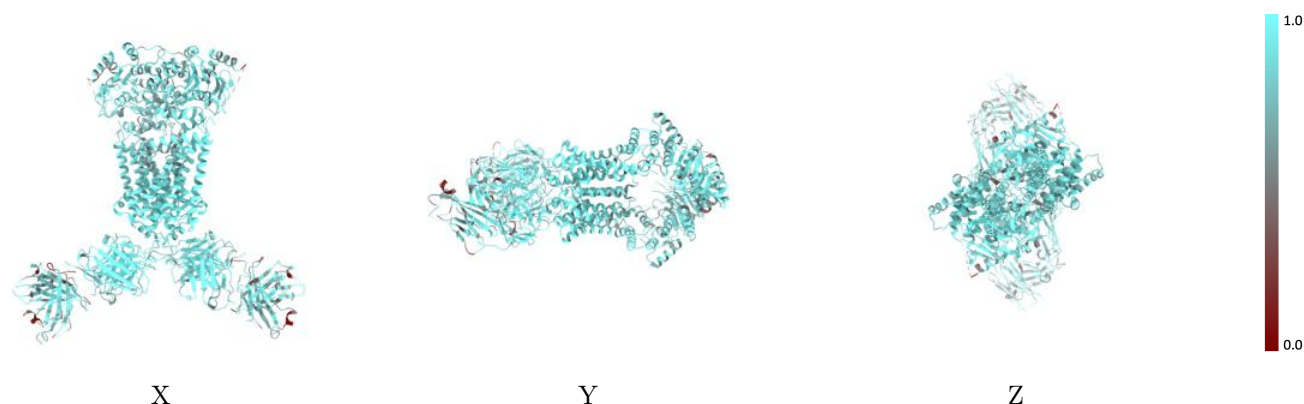
The images above show the 3D surface view of the map at the recommended contour level 5.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



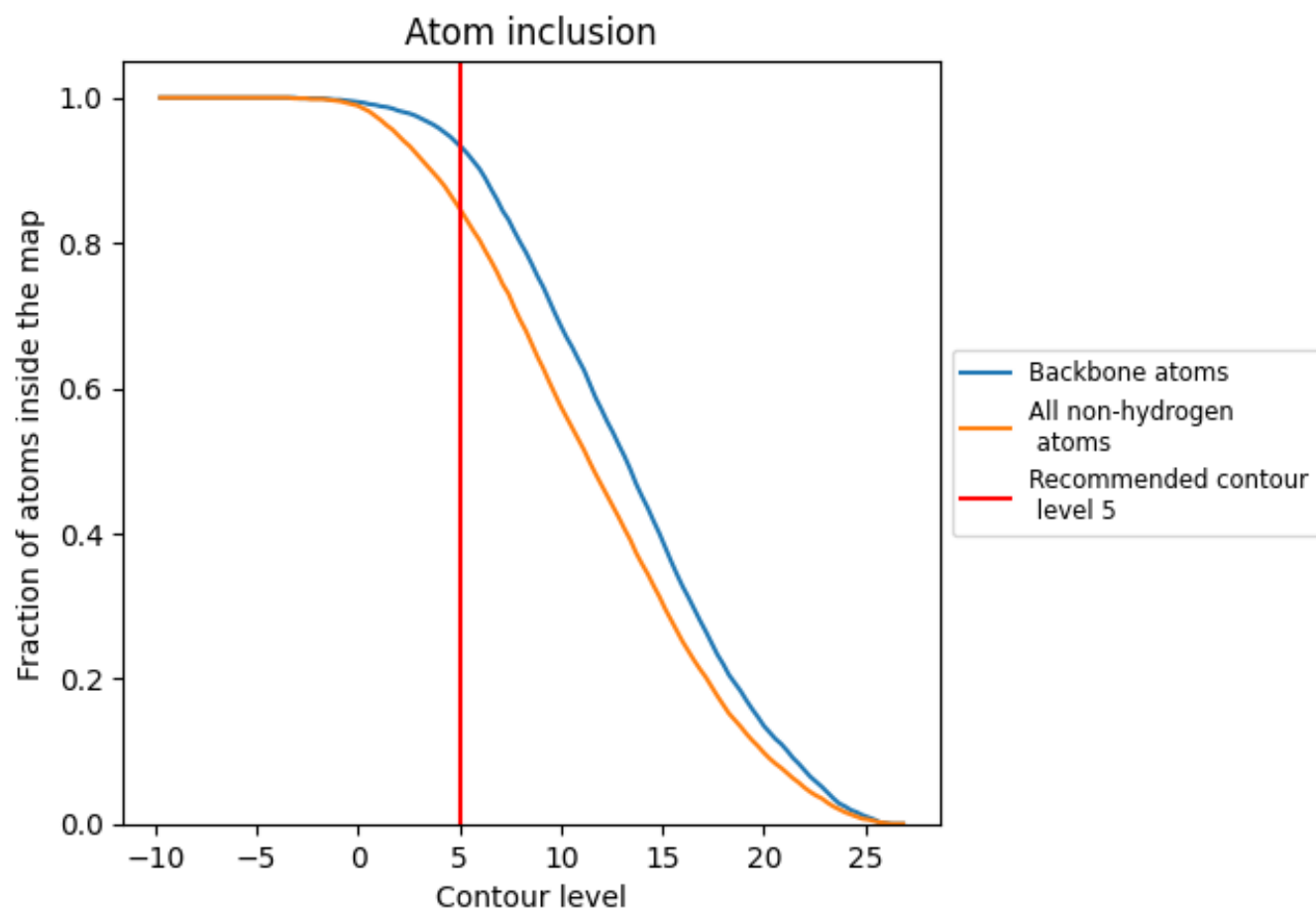
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 85% 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 (5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8470	<div></div> 0.5340
A	<div></div> 0.8700	<div></div> 0.5650
B	<div></div> 0.8700	<div></div> 0.5610
C	<div></div> 0.8770	<div></div> 0.5520
D	<div></div> 0.9070	<div></div> 0.5850
E	<div></div> 0.8770	<div></div> 0.5520
F	<div></div> 0.9060	<div></div> 0.5820
I	<div></div> 0.7600	<div></div> 0.4160
J	<div></div> 0.7650	<div></div> 0.4200
K	<div></div> 0.6780	<div></div> 0.3730
L	<div></div> 0.6810	<div></div> 0.3760

1.0

0.0

<0.0