



wwPDB EM Validation Summary Report ⓘ

Nov 9, 2024 – 12:03 pm GMT

PDB ID : 5MG3
EMDB ID : EMD-3506
Title : EM fitted model of bacterial holo-translocon
Authors : Schaffitzel, C.; Botte, M.
Deposited on : 2016-11-20
Resolution : 14.00 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.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) : 2.39

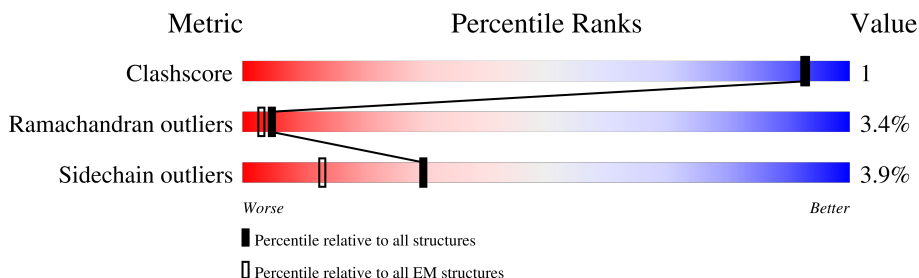
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 14.00 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	Y	458	
2	E	140	
3	G	136	
4	D	622	
5	F	323	
6	C	559	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 26650 atoms, of which 13553 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 Protein translocase subunit SecY.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	Y	443	7004	2259	3581	566	580	18	0	0

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	-14	VAL	-	expression tag	UNP P0AGA2
Y	-13	TRP	-	expression tag	UNP P0AGA2
Y	-12	ASN	-	expression tag	UNP P0AGA2
Y	-11	CYS	-	expression tag	UNP P0AGA2
Y	-10	GLU	-	expression tag	UNP P0AGA2
Y	-9	ARG	-	expression tag	UNP P0AGA2
Y	-8	ILE	-	expression tag	UNP P0AGA2
Y	-7	THR	-	expression tag	UNP P0AGA2
Y	-6	ILE	-	expression tag	UNP P0AGA2
Y	-5	SER	-	expression tag	UNP P0AGA2
Y	-4	HIS	-	expression tag	UNP P0AGA2
Y	-3	ARG	-	expression tag	UNP P0AGA2
Y	-2	LYS	-	expression tag	UNP P0AGA2
Y	-1	GLN	-	expression tag	UNP P0AGA2
Y	0	THR	-	expression tag	UNP P0AGA2

- Molecule 2 is a protein called Protein translocase subunit SecE.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	E	65	1062	332	552	91	86	1	0	0

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	369	MET	-	initiating methionine	UNP P0AG96
E	370	HIS	-	expression tag	UNP P0AG96

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Chain	Residue	Modelled	Actual	Comment	Reference
E	371	HIS	-	expression tag	UNP P0AG96
E	372	HIS	-	expression tag	UNP P0AG96
E	373	HIS	-	expression tag	UNP P0AG96
E	374	HIS	-	expression tag	UNP P0AG96
E	375	HIS	-	expression tag	UNP P0AG96
E	376	ASP	-	expression tag	UNP P0AG96
E	377	ASP	-	expression tag	UNP P0AG96
E	378	ASP	-	expression tag	UNP P0AG96
E	379	ASP	-	expression tag	UNP P0AG96
E	380	LYS	-	expression tag	UNP P0AG96
E	381	ALA	-	expression tag	UNP P0AG96
E	382	MET	-	expression tag	UNP P0AG96
E	383	GLY	-	expression tag	UNP P0AG96

- Molecule 3 is a protein called Protein-export membrane protein SecG.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	G	32	Total	C	H	N	O	S	0	0
			480	151	244	39	44	2		

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	439	VAL	-	expression tag	UNP P0AG99
G	440	GLY	-	expression tag	UNP P0AG99
G	441	THR	-	expression tag	UNP P0AG99
G	442	GLY	-	expression tag	UNP P0AG99
G	443	TRP	-	expression tag	UNP P0AG99
G	444	TYR	-	expression tag	UNP P0AG99
G	445	SER	-	expression tag	UNP P0AG99
G	446	GLY	-	expression tag	UNP P0AG99
G	447	SER	-	expression tag	UNP P0AG99
G	448	PRO	-	expression tag	UNP P0AG99
G	449	GLY	-	expression tag	UNP P0AG99
G	450	ILE	-	expression tag	UNP P0AG99
G	451	LEU	-	expression tag	UNP P0AG99
G	452	TYR	-	expression tag	UNP P0AG99
G	453	HIS	-	expression tag	UNP P0AG99
G	454	TRP	-	expression tag	UNP P0AG99
G	455	PRO	-	expression tag	UNP P0AG99
G	456	GLU	-	expression tag	UNP P0AG99
G	457	VAL	-	expression tag	UNP P0AG99

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Chain	Residue	Modelled	Actual	Comment	Reference
G	458	LEU	-	expression tag	UNP P0AG99
G	459	ARG	-	expression tag	UNP P0AG99
G	460	ILE	-	expression tag	UNP P0AG99
G	461	GLN	-	expression tag	UNP P0AG99
G	462	GLU	-	expression tag	UNP P0AG99
G	463	LEU	-	expression tag	UNP P0AG99
G	464	ILE	-	expression tag	UNP P0AG99

- Molecule 4 is a protein called Protein translocase subunit SecD.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	414	Total	C	H	N	O	S	0	0
			6419	1991	3291	545	582	10		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-6	MET	-	initiating methionine	UNP P0AG90
D	-5	HIS	-	expression tag	UNP P0AG90
D	-4	HIS	-	expression tag	UNP P0AG90
D	-3	HIS	-	expression tag	UNP P0AG90
D	-2	HIS	-	expression tag	UNP P0AG90
D	-1	HIS	-	expression tag	UNP P0AG90
D	0	HIS	-	expression tag	UNP P0AG90
D	1	MET	-	expression tag	UNP P0AG90
D	142	VAL	ALA	conflict	UNP P0AG90

- Molecule 5 is a protein called Protein translocase subunit SecF.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	F	289	Total	C	H	N	O	S	0	0
			4502	1434	2291	366	398	13		

- Molecule 6 is a protein called Membrane protein insertase YidC.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	C	455	Total	C	H	N	O	S	0	0
			7183	2336	3594	582	650	21		

There are 17 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	MET	-	initiating methionine	UNP P25714
C	-3	ASP	-	expression tag	UNP P25714
C	-2	PRO	-	expression tag	UNP P25714
C	-1	SER	-	expression tag	UNP P25714
C	0	SER	-	expression tag	UNP P25714
C	1	ARG	-	expression tag	UNP P25714
C	228	ALA	GLU	conflict	UNP P25714
C	229	ALA	LYS	conflict	UNP P25714
C	231	ALA	GLU	conflict	UNP P25714
C	232	ALA	LYS	conflict	UNP P25714
C	234	ALA	LYS	conflict	UNP P25714
C	549	HIS	-	expression tag	UNP P25714
C	550	HIS	-	expression tag	UNP P25714
C	551	HIS	-	expression tag	UNP P25714
C	552	HIS	-	expression tag	UNP P25714
C	553	HIS	-	expression tag	UNP P25714
C	554	HIS	-	expression tag	UNP P25714

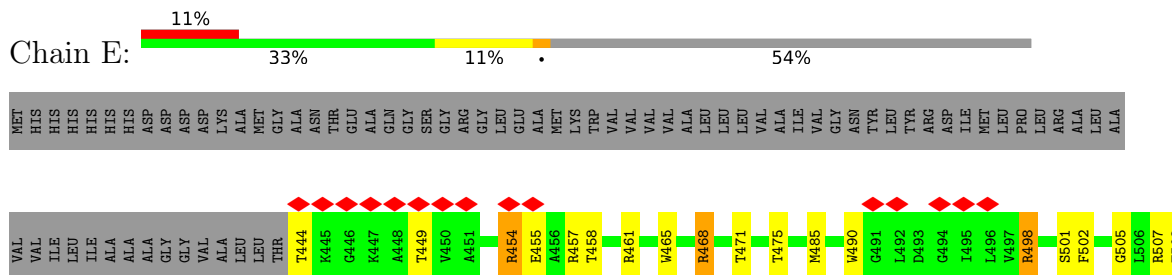
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

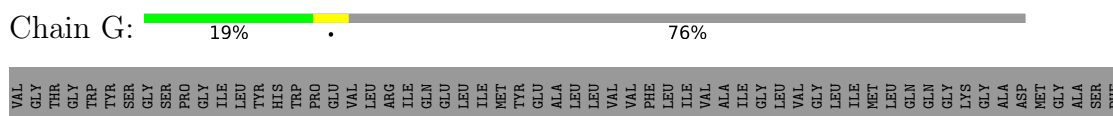
- Molecule 1: Protein translocase subunit SecY

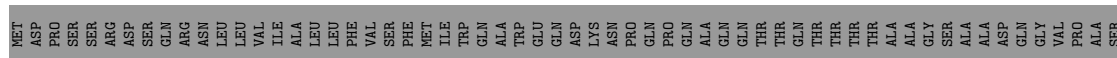


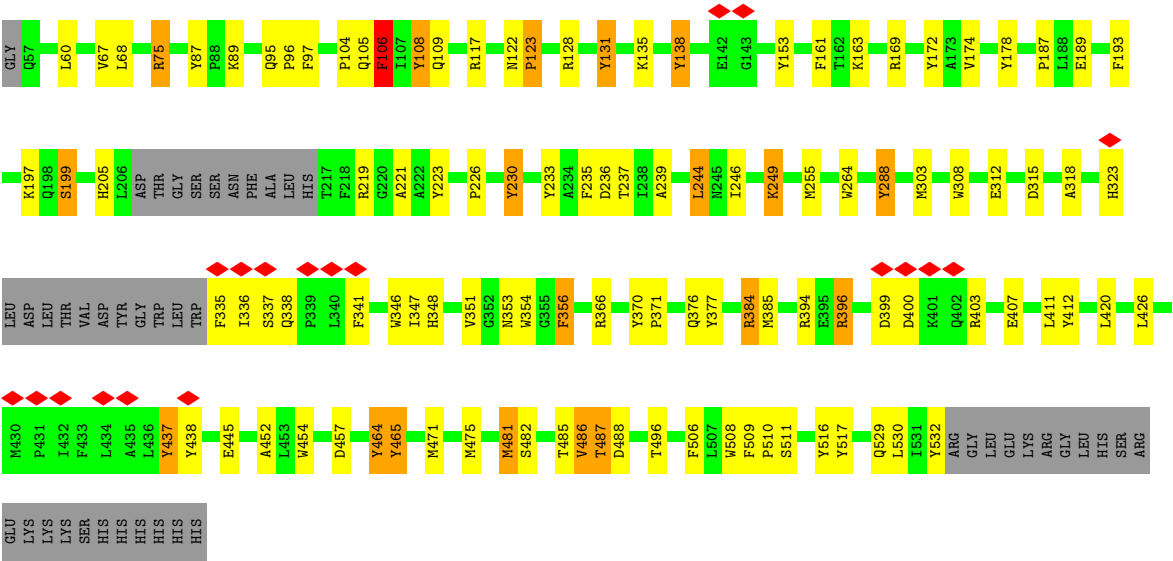
- Molecule 2: Protein translocase subunit SecE



- Molecule 3: Protein-export membrane protein SecG







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	53648	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	100	Depositor
Electron dose ($e^-/\text{\AA}^2$)	10	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON I (4k x 4k)	Depositor
Maximum map value	153.928	Depositor
Minimum map value	-63.993	Depositor
Average map value	1.728	Depositor
Map value standard deviation	15.464	Depositor
Recommended contour level	8.5	Depositor
Map size (\AA)	190.40001, 190.40001, 190.40001	wwPDB
Map dimensions	140, 140, 140	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.36, 1.36, 1.36	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	Y	2.09	27/3501 (0.8%)	2.13	116/4744 (2.4%)
2	E	1.78	6/518 (1.2%)	2.24	19/702 (2.7%)
3	G	1.72	3/238 (1.3%)	1.91	5/320 (1.6%)
4	D	1.62	20/3163 (0.6%)	2.06	82/4288 (1.9%)
5	F	1.59	4/2250 (0.2%)	2.18	77/3049 (2.5%)
6	C	1.62	16/3683 (0.4%)	1.99	97/5013 (1.9%)
All	All	1.76	76/13353 (0.6%)	2.09	396/18116 (2.2%)

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	Y	0	11
2	E	0	3
4	D	0	9
5	F	0	13
6	C	0	21
All	All	0	57

The worst 5 of 76 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Y	317	TYR	CG-CD2	35.73	1.85	1.39
1	Y	317	TYR	CG-CD1	34.43	1.83	1.39
1	Y	317	TYR	CE2-CZ	33.58	1.82	1.38
1	Y	317	TYR	CE1-CZ	33.16	1.81	1.38
1	Y	317	TYR	CD1-CE1	23.16	1.74	1.39

The worst 5 of 396 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	226	ARG	NE-CZ-NH1	28.99	134.80	120.30
4	D	297	ARG	NE-CZ-NH1	22.63	131.61	120.30
1	Y	392	ARG	NE-CZ-NH1	18.04	129.32	120.30
4	D	268	ARG	NE-CZ-NH1	17.26	128.93	120.30
5	F	168	ARG	NE-CZ-NH1	17.14	128.87	120.30

There are no chirality outliers.

5 of 57 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	Y	113	ARG	Sidechain
1	Y	122	TYR	Sidechain
1	Y	22	ARG	Sidechain
1	Y	38	PHE	Sidechain
1	Y	7	LEU	Peptide

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	Y	3423	3581	3583	15	0
2	E	510	552	551	0	0
3	G	236	244	243	1	0
4	D	3128	3291	3292	8	0
5	F	2211	2291	2290	5	0
6	C	3589	3594	3591	8	0
All	All	13097	13553	13550	34	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 1.

The worst 5 of 34 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:Y:317:TYR:CE1	1:Y:317:TYR:CZ	1.81	1.62
1:Y:317:TYR:CG	1:Y:317:TYR:CD1	1.83	1.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:317:TYR:CG	1:Y:317:TYR:CD2	1.85	1.61
1:Y:317:TYR:CZ	1:Y:317:TYR:CE2	1.82	1.59
6:C:486:VAL:HG22	6:C:487:THR:H	1.62	0.64

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	Y	441/458 (96%)	367 (83%)	50 (11%)	24 (5%)	1	15
2	E	63/140 (45%)	57 (90%)	5 (8%)	1 (2%)	8	38
3	G	30/136 (22%)	29 (97%)	1 (3%)	0	100	100
4	D	410/622 (66%)	373 (91%)	25 (6%)	12 (3%)	3	23
5	F	287/323 (89%)	257 (90%)	24 (8%)	6 (2%)	5	30
6	C	449/559 (80%)	395 (88%)	40 (9%)	14 (3%)	3	22
All	All	1680/2238 (75%)	1478 (88%)	145 (9%)	57 (3%)	5	21

5 of 57 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Y	48	VAL
1	Y	71	ALA
1	Y	113	ARG
1	Y	199	LEU
1	Y	305	THR

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	Y	359/374 (96%)	338 (94%)	21 (6%)	17	38
2	E	54/110 (49%)	52 (96%)	2 (4%)	29	49
3	G	27/106 (26%)	27 (100%)	0	100	100
4	D	337/509 (66%)	328 (97%)	9 (3%)	40	58
5	F	237/267 (89%)	227 (96%)	10 (4%)	25	46
6	C	387/475 (82%)	375 (97%)	12 (3%)	35	54
All	All	1401/1841 (76%)	1347 (96%)	54 (4%)	30	48

5 of 54 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	432	PRO
5	F	98	MET
6	C	376	GLN
4	D	438	GLU
5	F	14	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
4	D	404	ASN
5	F	179	HIS
6	C	353	ASN
6	C	348	HIS
4	D	239	ASN

5.3.3 RNA ⓘ

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.

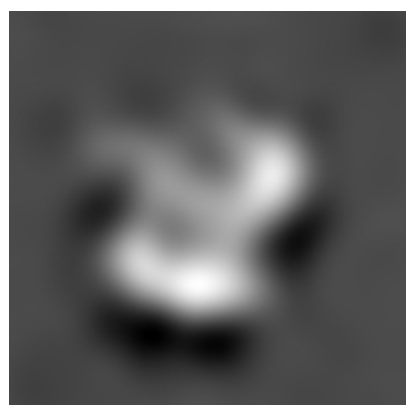
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3506. 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](#)

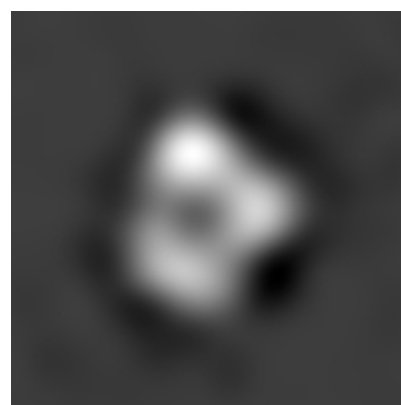
6.1.1 Primary map



X



Y

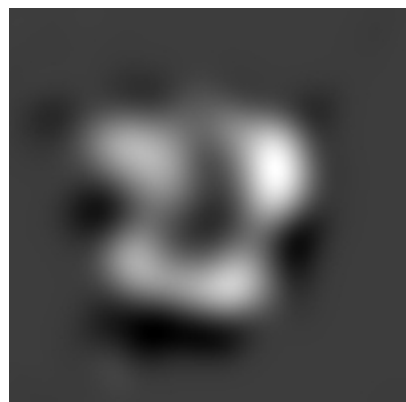


Z

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

6.2 Central slices [i](#)

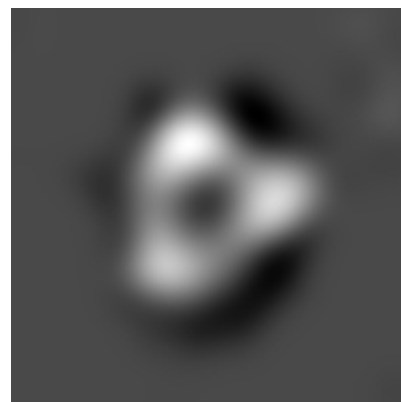
6.2.1 Primary map



X Index: 70



Y Index: 70



Z Index: 70

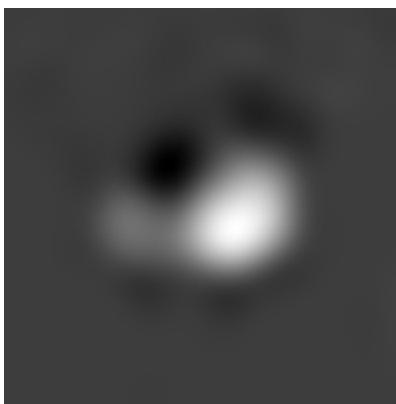
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 61



Y Index: 91

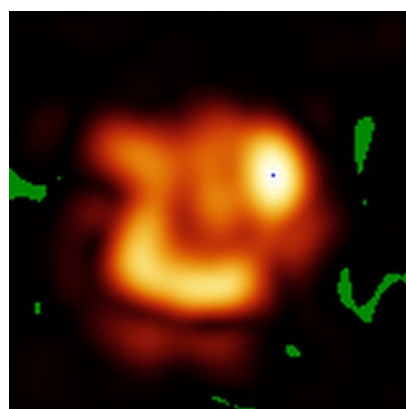


Z Index: 45

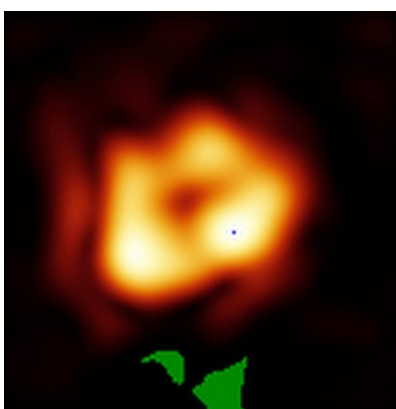
The images above show the largest variance slices of the map in three orthogonal directions.

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

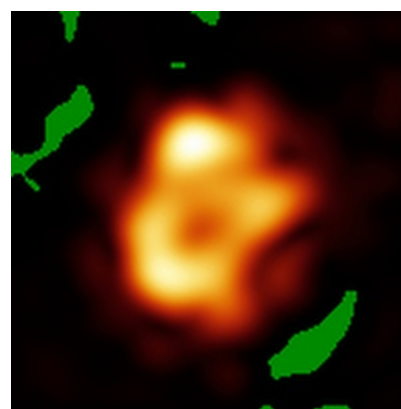
6.4.1 Primary map



X



Y

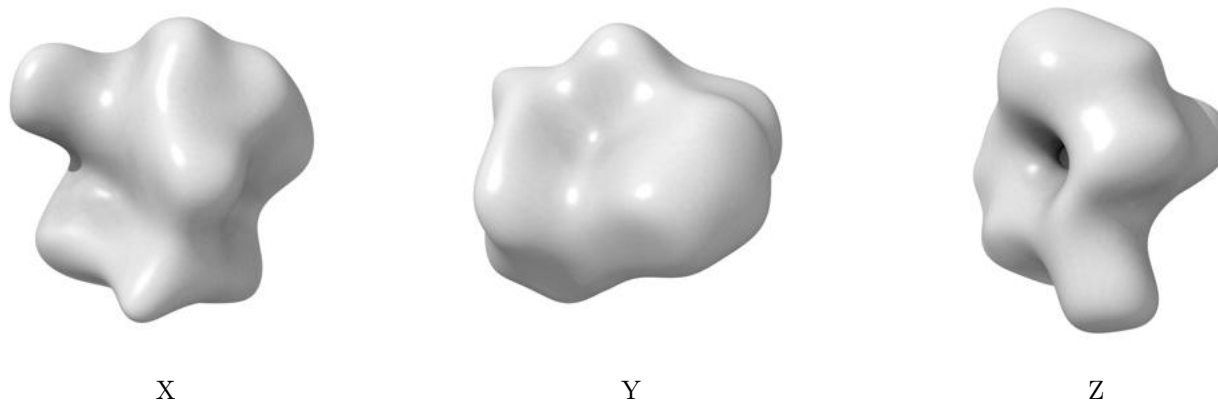


Z

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

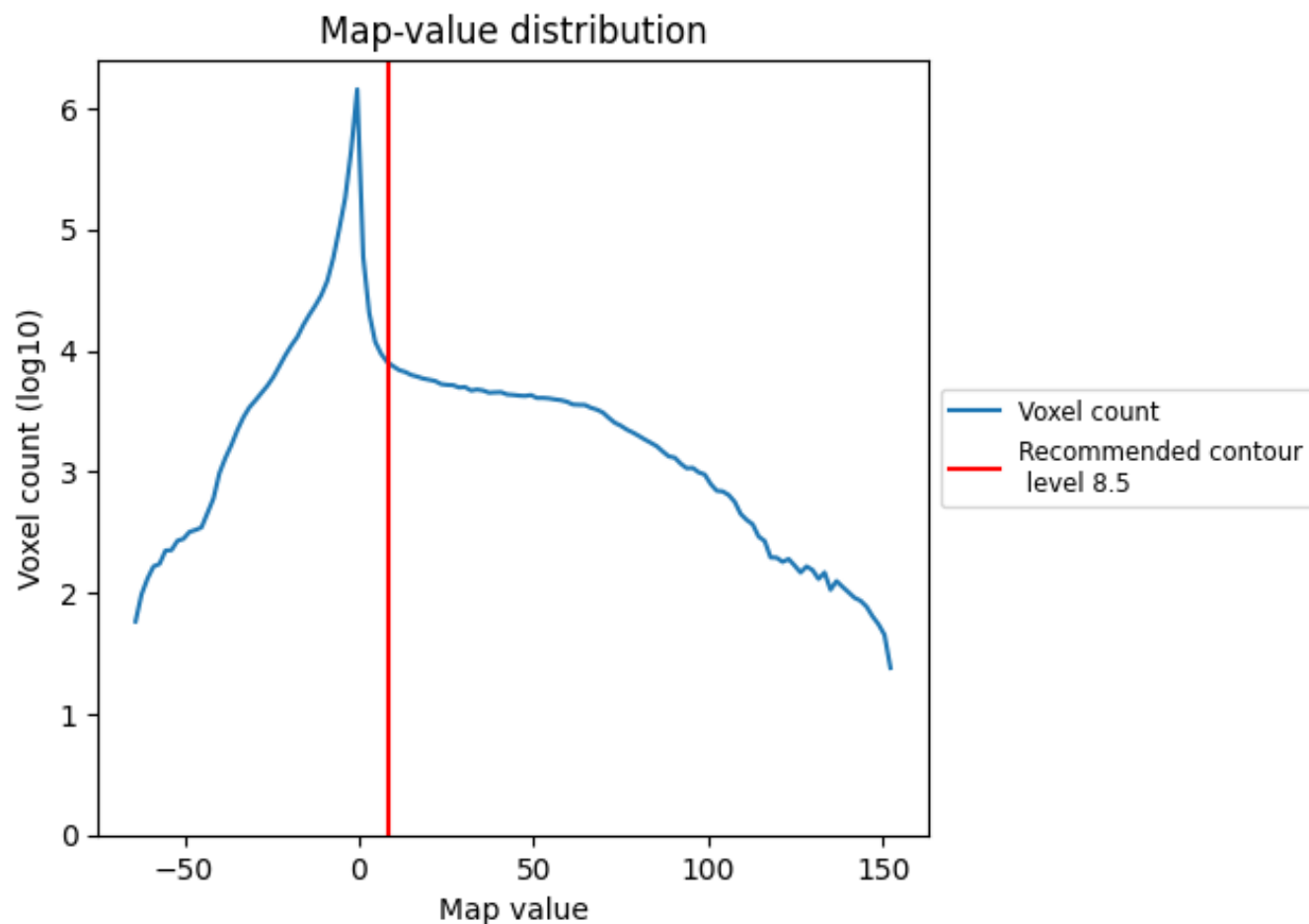
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

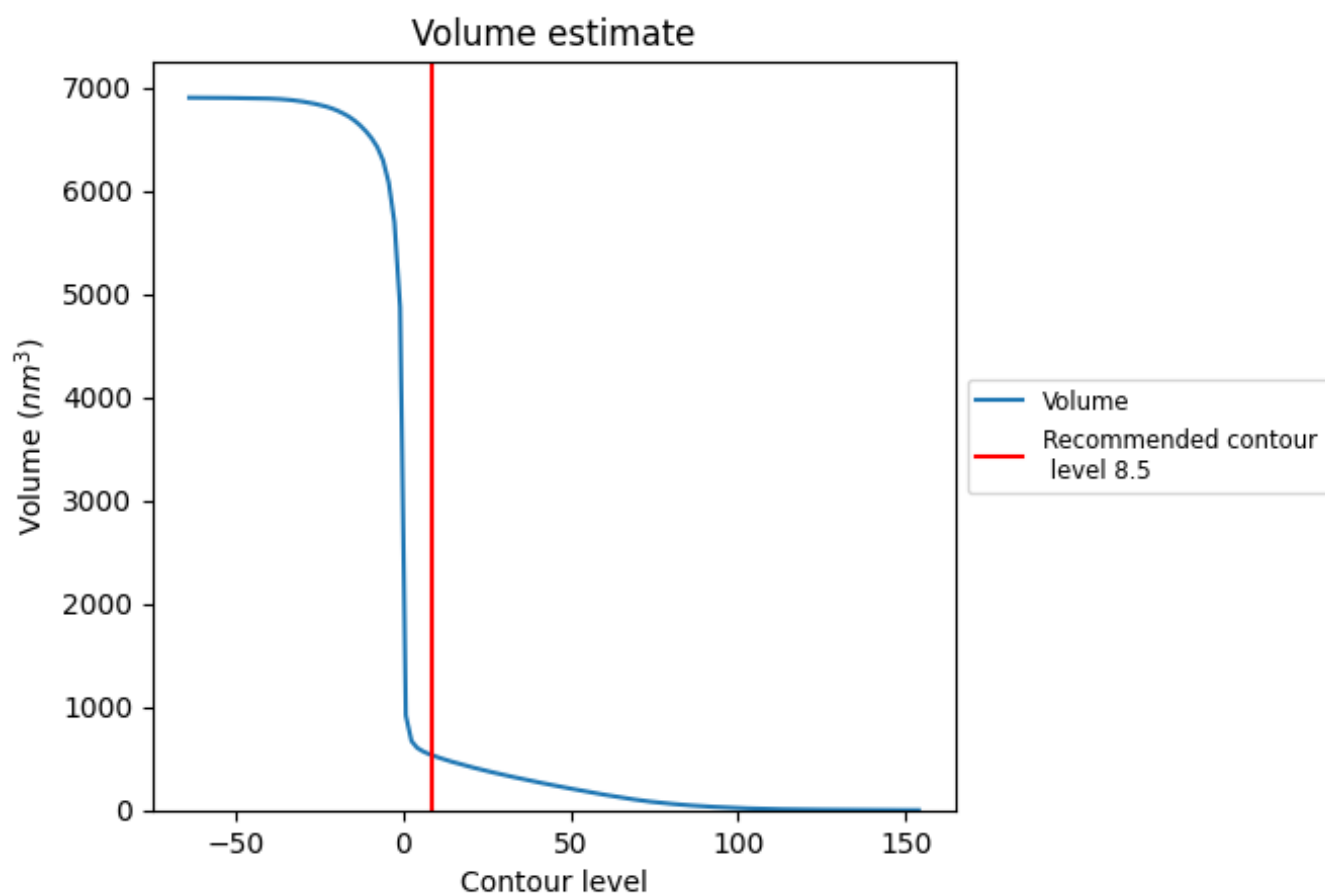
This section contains the results of statistical analysis of the map.

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.

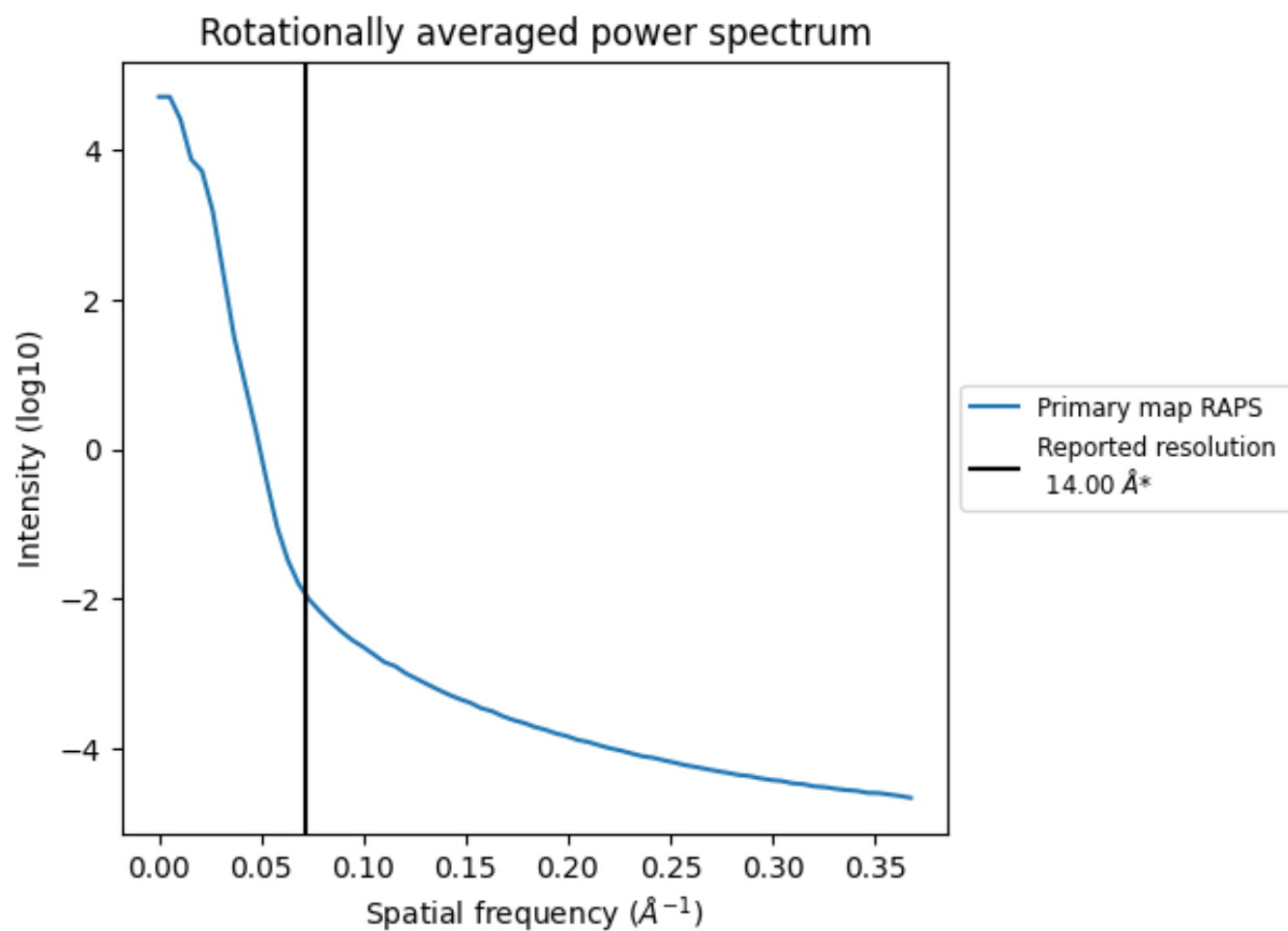
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 533 nm^3 ; this corresponds to an approximate mass of 481 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 ⓘ

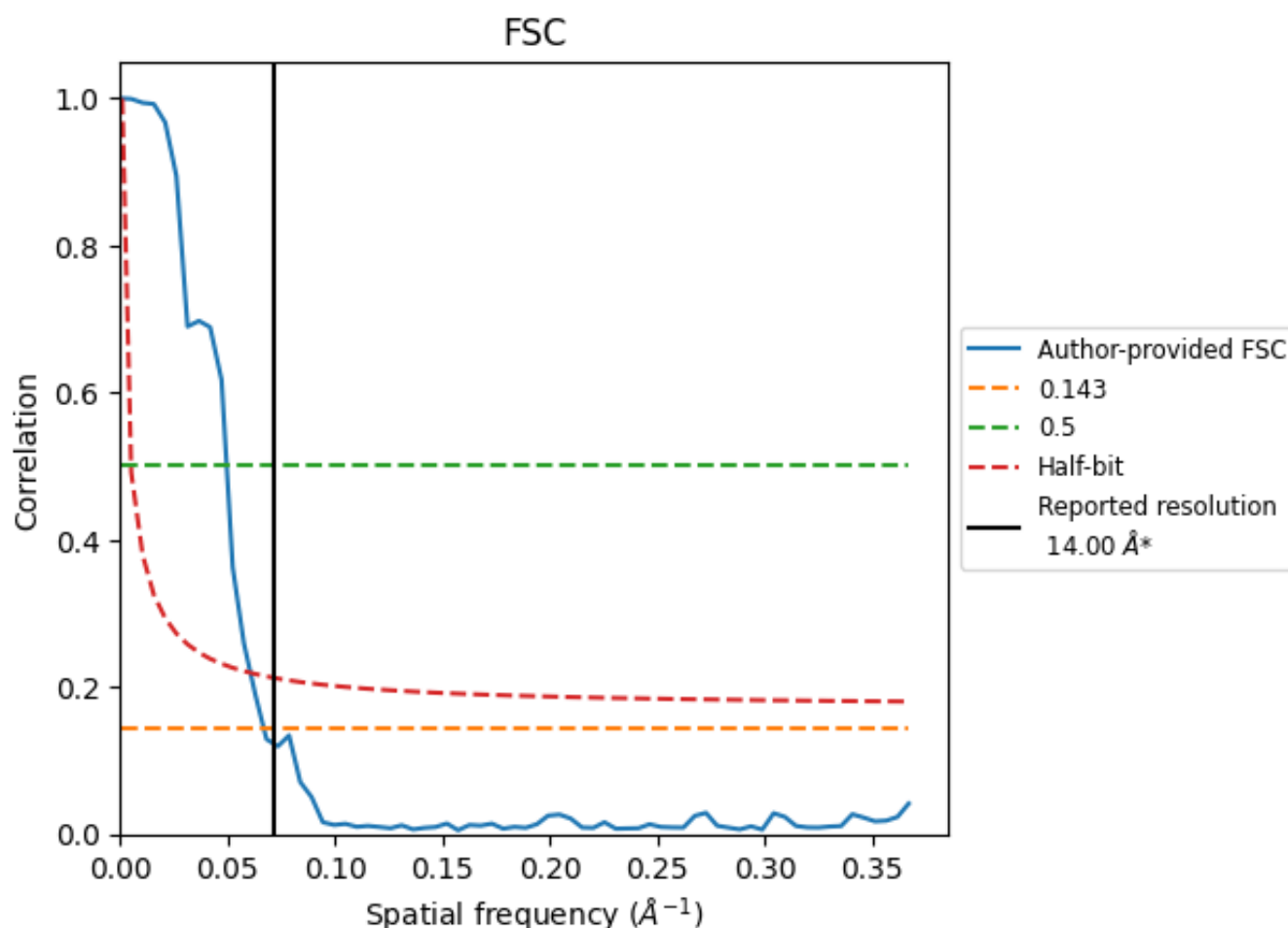


*Reported resolution corresponds to spatial frequency of 0.071 Å⁻¹

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 0.071 Å⁻¹

8.2 Resolution estimates [i](#)

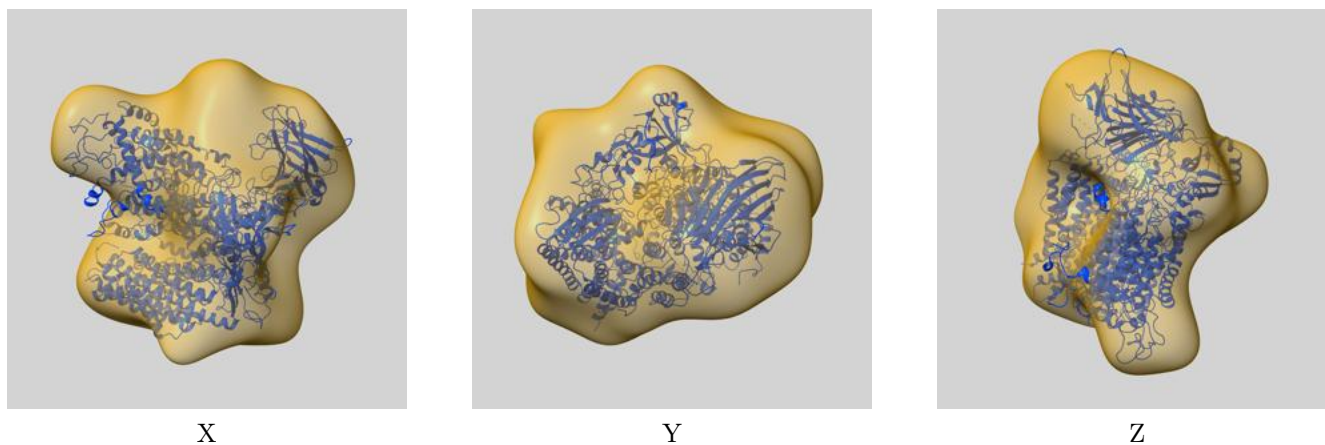
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	14.00	-	-
Author-provided FSC curve	14.95	20.16	16.47
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

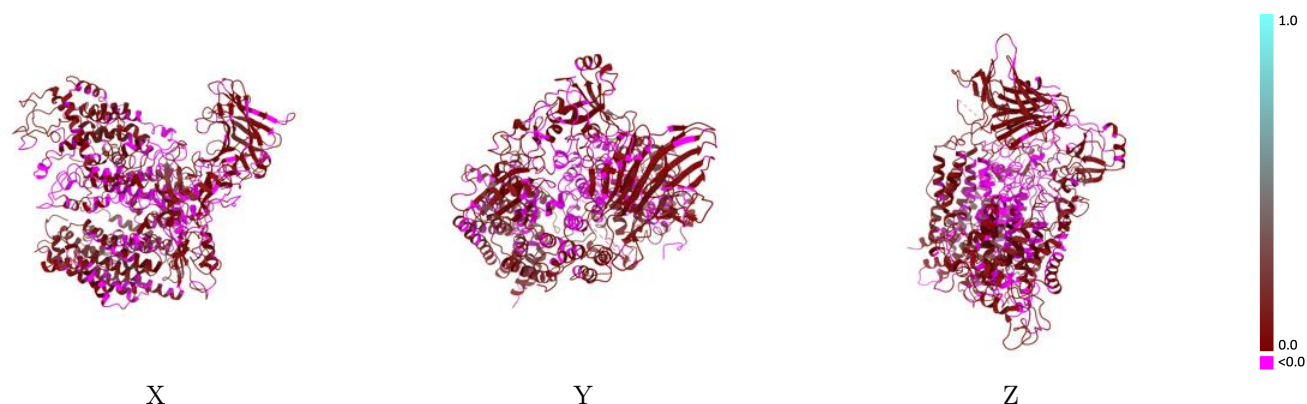
This section contains information regarding the fit between EMDB map EMD-3506 and PDB model 5MG3. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

9.1 Map-model overlay [i](#)



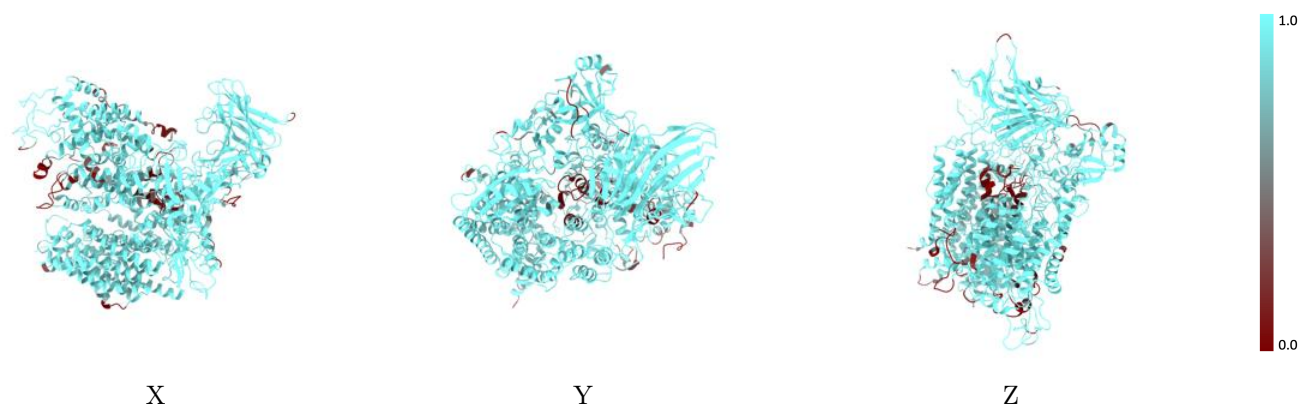
The images above show the 3D surface view of the map at the recommended contour level 8.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



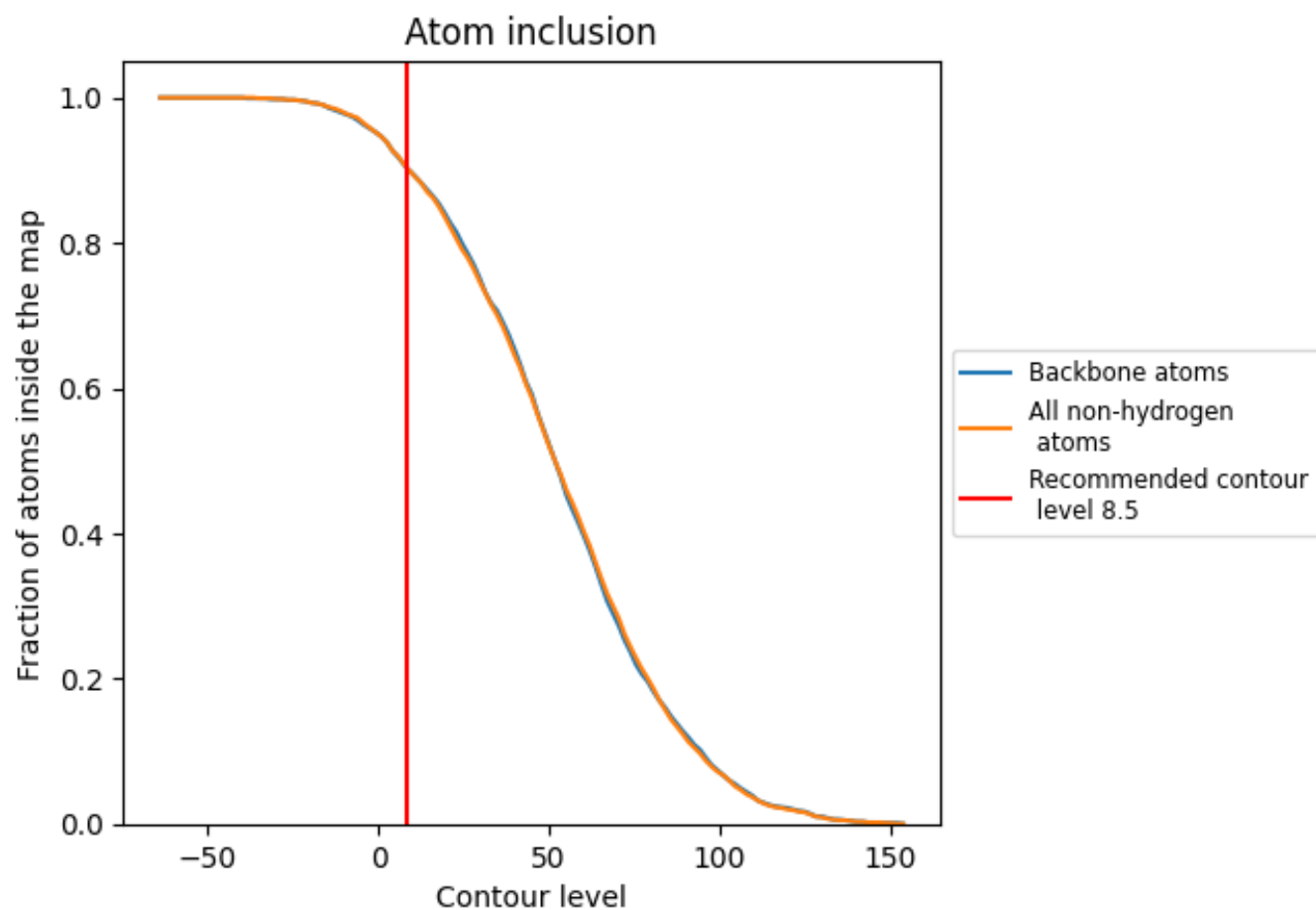
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (8.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 90% 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 (8.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9020	<div></div> 0.0340
C	<div></div> 0.9490	<div></div> 0.0350
D	<div></div> 0.9390	<div></div> 0.0380
E	<div></div> 0.7700	<div></div> 0.0180
F	<div></div> 0.9760	<div></div> 0.0580
G	<div></div> 0.9920	<div></div> -0.0030
Y	<div></div> 0.8100	<div></div> 0.0180

1.0
0.0
-0.0