



wwPDB EM Validation Summary Report ⓘ

Jul 6, 2026 – 02:12 PM EDT

PDB ID : 36AZ / pdb_000036az
EMDB ID : EMD-77344
Title : Structure of BA.1-S-RBD/2130WT/2196-S93Y
Authors : Du, J.; Pallesen, J.
Deposited on : 2026-05-28
Resolution : 3.90 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.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

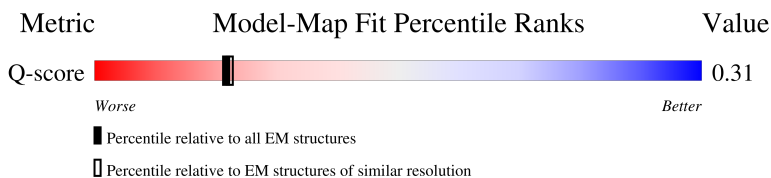
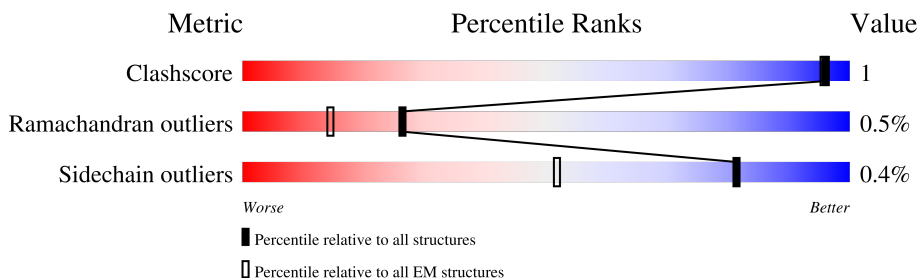
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8855 (3.40 - 4.40)

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	H	480	9% 26% 73%
2	L	239	10% 45% 52%
3	A	223	32% 80% 6% 13%
4	B	236	17% 43% 54%

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Mol	Chain	Length	Quality of chain
5	C	472	5%25%74%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5230 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 2130WT heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	H	130	Total	C	N	O	S	0	0
			996	633	166	193	4		

- Molecule 2 is a protein called 2130WT light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	114	Total	C	N	O	S	0	0
			883	556	146	177	4		

- Molecule 3 is a protein called Spike protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	194	Total	C	N	O	S	0	0
			1558	1004	263	283	8		

There are 41 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	339	ASP	GLY	conflict	UNP P0DTC2
A	371	LEU	SER	conflict	UNP P0DTC2
A	373	PRO	SER	conflict	UNP P0DTC2
A	375	PHE	SER	conflict	UNP P0DTC2
A	417	ASN	LYS	conflict	UNP P0DTC2
A	440	LYS	ASN	conflict	UNP P0DTC2
A	446	SER	GLY	conflict	UNP P0DTC2
A	477	ASN	SER	conflict	UNP P0DTC2
A	478	LYS	THR	conflict	UNP P0DTC2
A	484	ALA	GLU	conflict	UNP P0DTC2
A	493	ARG	GLN	conflict	UNP P0DTC2
A	496	SER	GLY	conflict	UNP P0DTC2
A	498	ARG	GLN	conflict	UNP P0DTC2
A	501	TYR	ASN	conflict	UNP P0DTC2
A	505	HIS	TYR	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	527	GLY	-	expression tag	UNP P0DTC2
A	528	GLY	-	expression tag	UNP P0DTC2
A	529	GLY	-	expression tag	UNP P0DTC2
A	530	LEU	-	expression tag	UNP P0DTC2
A	531	VAL	-	expression tag	UNP P0DTC2
A	532	PRO	-	expression tag	UNP P0DTC2
A	533	GLN	-	expression tag	UNP P0DTC2
A	534	GLN	-	expression tag	UNP P0DTC2
A	535	SER	-	expression tag	UNP P0DTC2
A	536	GLY	-	expression tag	UNP P0DTC2
A	537	GLY	-	expression tag	UNP P0DTC2
A	538	LEU	-	expression tag	UNP P0DTC2
A	539	ASN	-	expression tag	UNP P0DTC2
A	540	ASP	-	expression tag	UNP P0DTC2
A	541	ILE	-	expression tag	UNP P0DTC2
A	542	PHE	-	expression tag	UNP P0DTC2
A	543	GLU	-	expression tag	UNP P0DTC2
A	544	ALA	-	expression tag	UNP P0DTC2
A	545	GLN	-	expression tag	UNP P0DTC2
A	546	LYS	-	expression tag	UNP P0DTC2
A	547	ILE	-	expression tag	UNP P0DTC2
A	548	GLU	-	expression tag	UNP P0DTC2
A	549	TRP	-	expression tag	UNP P0DTC2
A	550	HIS	-	expression tag	UNP P0DTC2
A	551	GLU	-	expression tag	UNP P0DTC2
A	552	GLY	-	expression tag	UNP P0DTC2

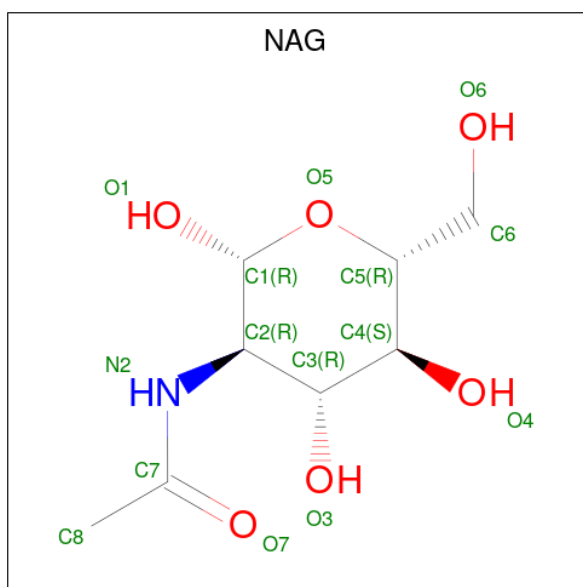
- Molecule 4 is a protein called 2196-S93Y light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	109	Total	C	N	O	S	0	0
			838	528	144	164	2		

- Molecule 5 is a protein called 2196-S93Y heavy chain.

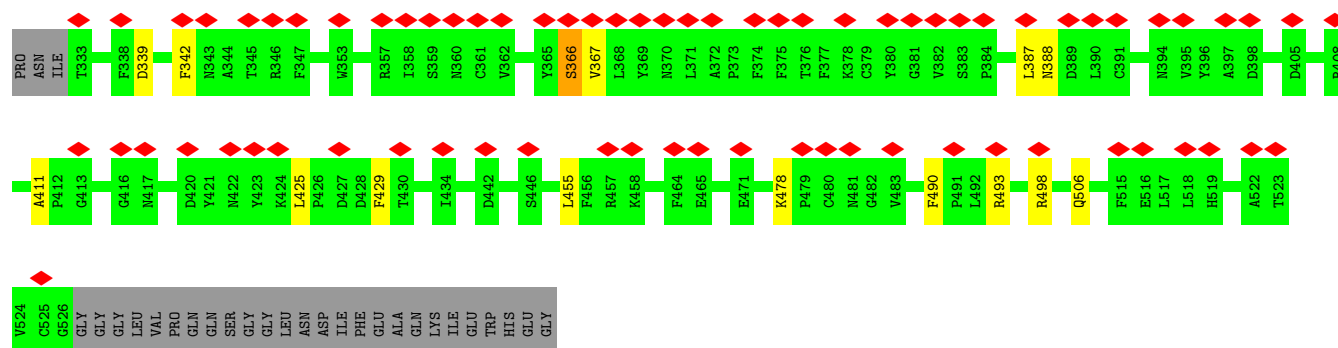
Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	122	Total	C	N	O	S	0	0
			941	588	161	183	9		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

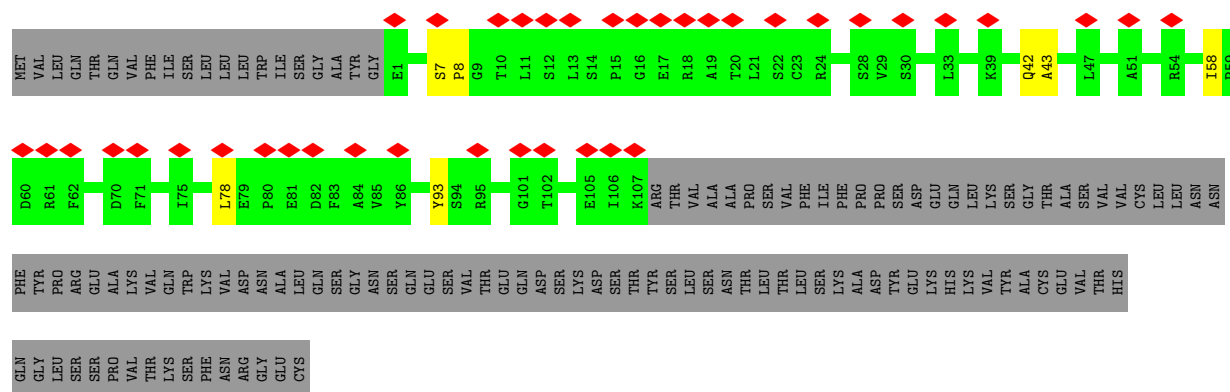


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
6	A	1	14	8	1	5	0

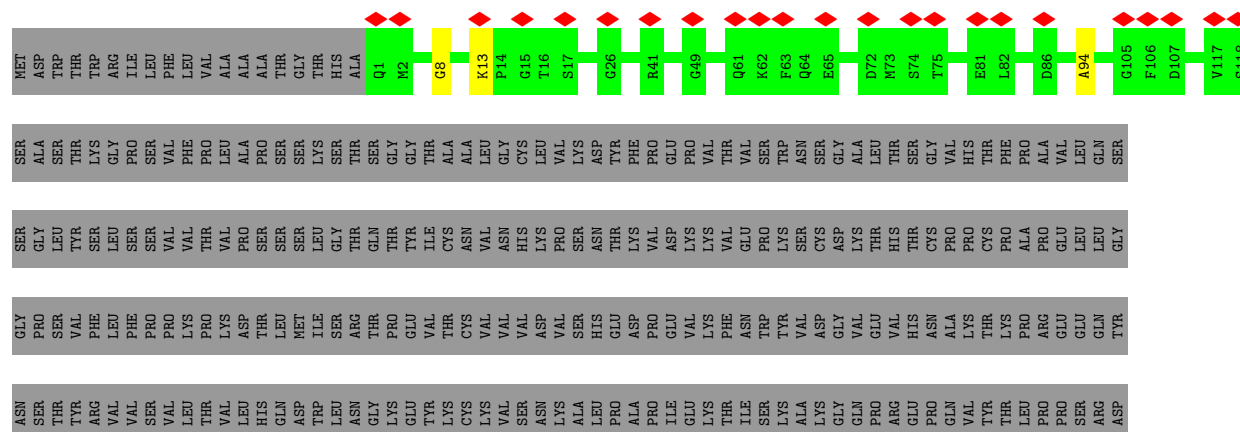
Chain A:



Chain B:



Chain C: 5% 25% 74%



LEU	GLU	THR	LYS	ASN	GLN	VAL	SER	LEU	THR	CYS	LEU	VAL	HIS	LYS	GLY	PHE	LEU	HIS	TYR	PRO	ASN	SER	ASP	ILE	ALA	VAL	GLU	TRP	GLU	SER	ASN	GLY	GLN	PRO	PRO	GLU	ASN	ASN	TYR	LYS	THR	THR	THR	PRO	PRO	VAL	LEU	ASP	SER	ASP	GLY	SER	PHE	PHE	LEU	TYR	SER	LYS	LEU	THR	THR	VAL	ASP	LYS	SER	ARG
TRP	GLN	GLN	GLY	ASN	VAL	PHE	SER	CYS	SER	VAL	MET	HIS	GLU	ALA	LEU	HIS	ASN	HIS	TYR	THR	GLN	LYS	SER	LEU	SER	LEU	SER	PRO	GLY	LYS																																				

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	243248	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	58.6	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	14.242	Depositor
Minimum map value	-0.106	Depositor
Average map value	-0.043	Depositor
Map value standard deviation	0.155	Depositor
Recommended contour level	4.87	Depositor
Map size ($\text{\AA}$)	442.68002, 442.68002, 442.68002	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.054, 1.054, 1.054	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: NAG

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	H	0.61	0/1020	0.93	8/1383 (0.6%)
2	L	0.59	0/902	0.95	6/1223 (0.5%)
3	A	0.59	0/1604	0.97	12/2183 (0.5%)
4	B	0.59	0/859	0.96	5/1165 (0.4%)
5	C	0.58	0/960	0.91	6/1299 (0.5%)
All	All	0.59	0/5345	0.95	37/7253 (0.5%)

There are no bond length outliers.

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	L	42	GLN	CA-C-N	10.05	127.00	119.66
2	L	42	GLN	C-N-CA	10.05	127.00	119.66
5	C	8	GLY	CA-C-N	7.71	127.72	119.78
5	C	8	GLY	C-N-CA	7.71	127.72	119.78
1	H	104	GLY	CA-C-N	7.54	127.17	119.56

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	H	996	0	969	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	L	883	0	859	1	0
3	A	1558	0	1486	6	0
4	B	838	0	810	1	0
5	C	941	0	913	0	0
6	A	14	0	13	2	0
All	All	5230	0	5050	9	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 9 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)
3:A:455:LEU:HD22	3:A:493:ARG:HG3	1.86	0.57
4:B:7:SER:N	4:B:8:PRO:CD	2.76	0.48
3:A:387:LEU:O	3:A:388:ASN:C	2.59	0.45
1:H:61:ALA:N	1:H:62:PRO:CD	2.80	0.44
3:A:342:PHE:CB	6:A:601:NAG:H82	2.47	0.44

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	H	128/480 (27%)	126 (98%)	2 (2%)	0	100	100
2	L	112/239 (47%)	106 (95%)	5 (4%)	1 (1%)	14	47
3	A	192/223 (86%)	185 (96%)	6 (3%)	1 (0%)	24	59
4	B	107/236 (45%)	103 (96%)	3 (3%)	1 (1%)	14	47
5	C	120/472 (25%)	118 (98%)	2 (2%)	0	100	100
All	All	659/1650 (40%)	638 (97%)	18 (3%)	3 (0%)	26	59

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	366	SER
2	L	30(B)	SER
4	B	93	TYR

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	H	105/419 (25%)	105 (100%)	0	100	100
2	L	98/209 (47%)	98 (100%)	0	100	100
3	A	169/191 (88%)	168 (99%)	1 (1%)	78	80
4	B	90/203 (44%)	89 (99%)	1 (1%)	65	74
5	C	104/418 (25%)	104 (100%)	0	100	100
All	All	566/1440 (39%)	564 (100%)	2 (0%)	81	83

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	429	PHE
4	B	78	LEU

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

Mol	Chain	Res	Type
2	L	31	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](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	NAG	A	601	3	14,14,15	0.24	0	17,19,21	0.58	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	A	601	3	-	0/6/23/26	0/1/1/1

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.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	601	NAG	2	0

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.

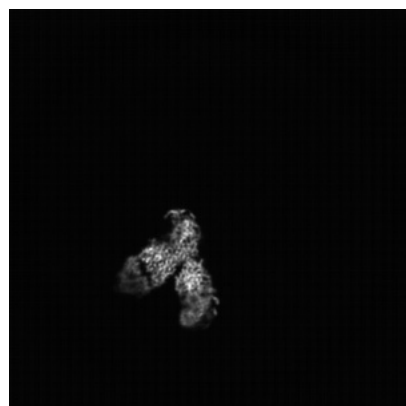
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-77344. These allow visual inspection of the internal detail of the map and identification of artifacts.

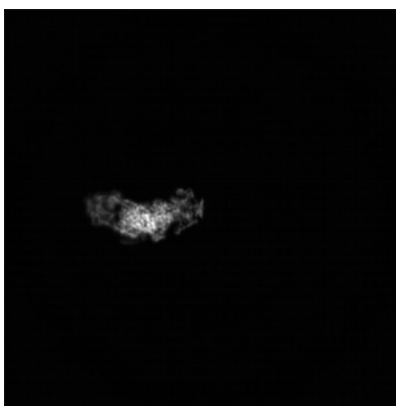
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

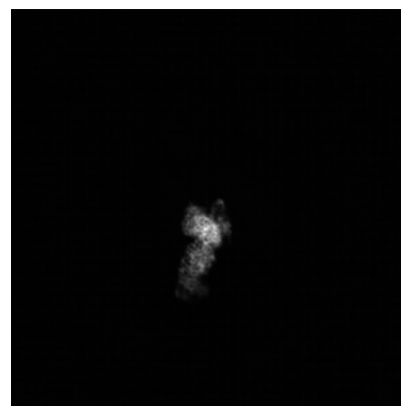
6.1.1 Primary map



X

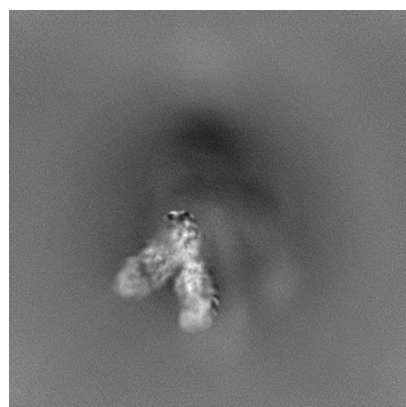


Y

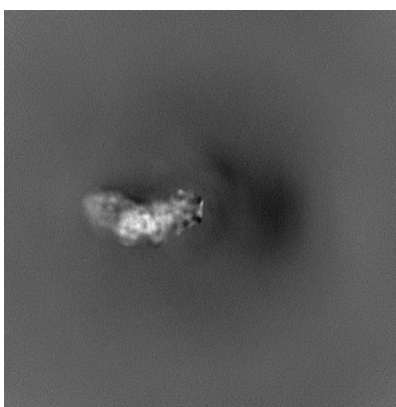


Z

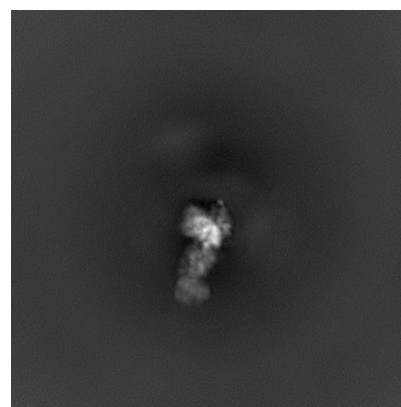
6.1.2 Raw map



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: 210

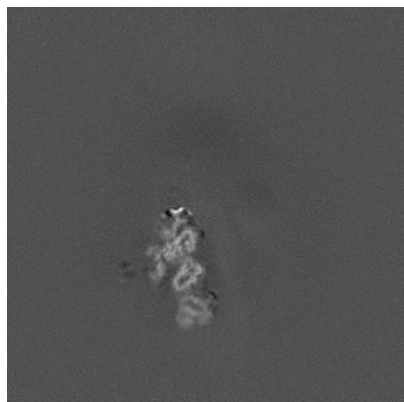


Y Index: 210

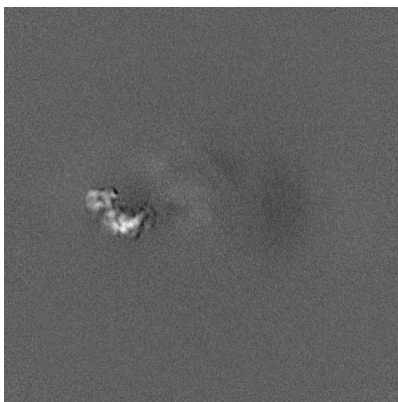


Z Index: 210

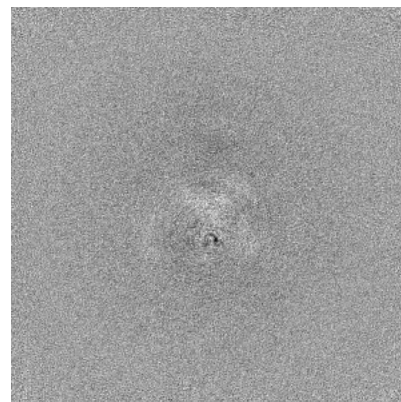
6.2.2 Raw map



X Index: 210



Y Index: 210



Z Index: 210

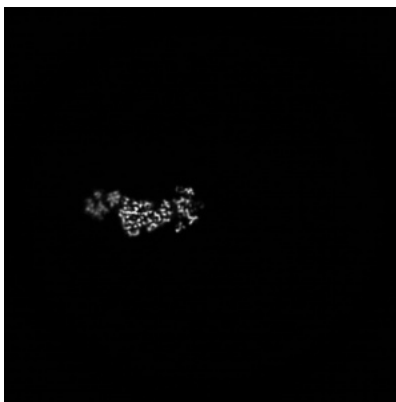
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

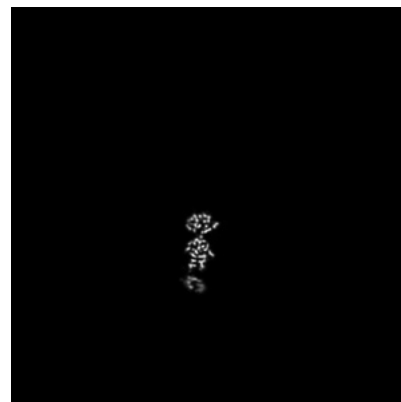
6.3.1 Primary map



X Index: 202



Y Index: 188

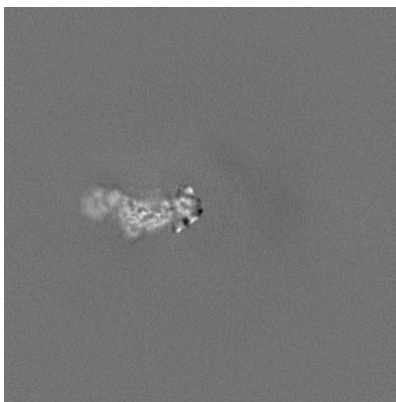


Z Index: 151

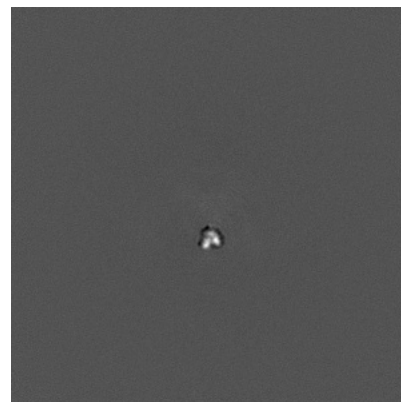
6.3.2 Raw map



X Index: 203



Y Index: 187

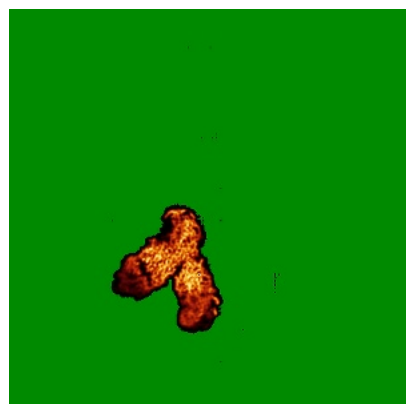


Z Index: 206

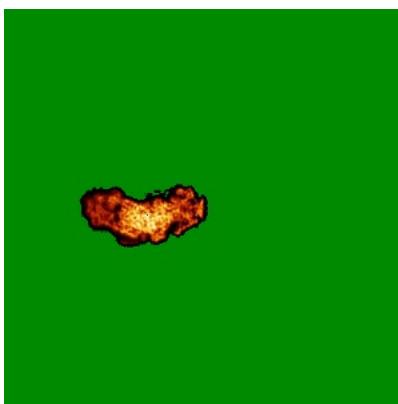
The images above show the largest variance slices of the map in three orthogonal directions.

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

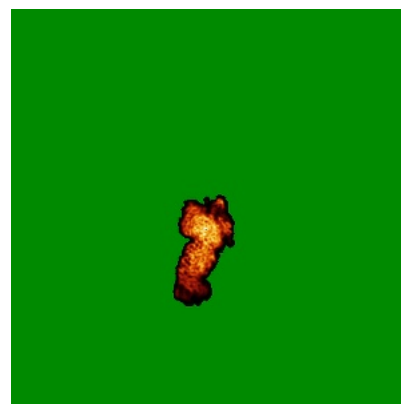
6.4.1 Primary map



X



Y

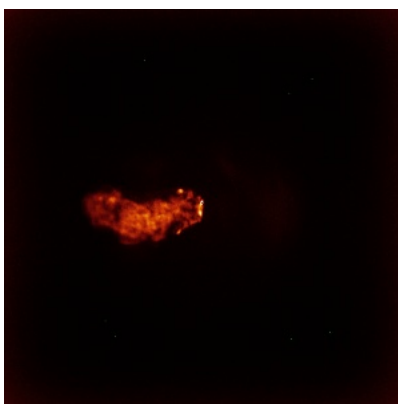


Z

6.4.2 Raw map



X



Y

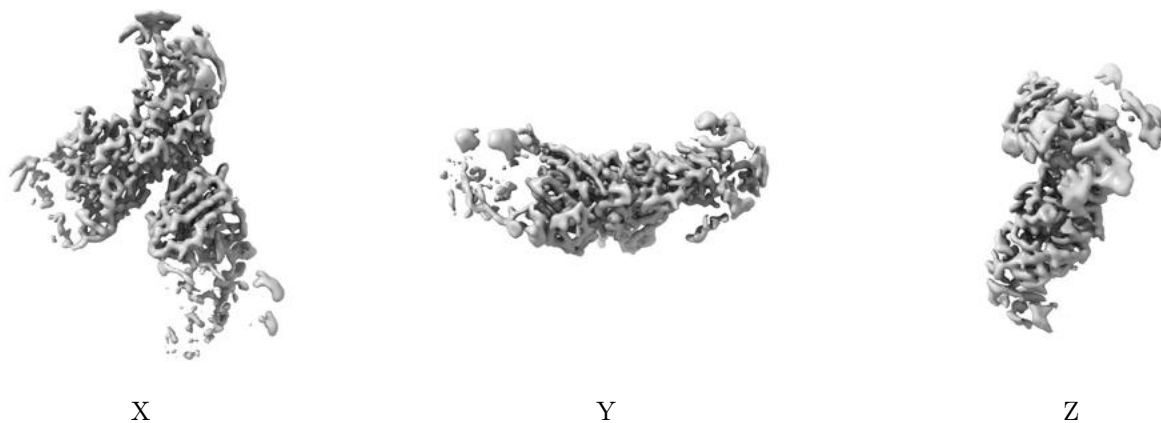


Z

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.

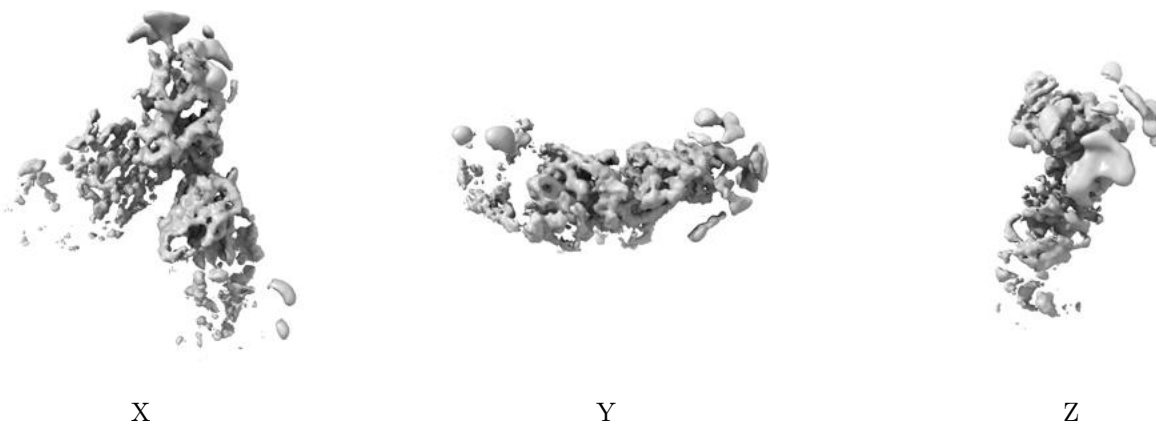
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 4.87. 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.

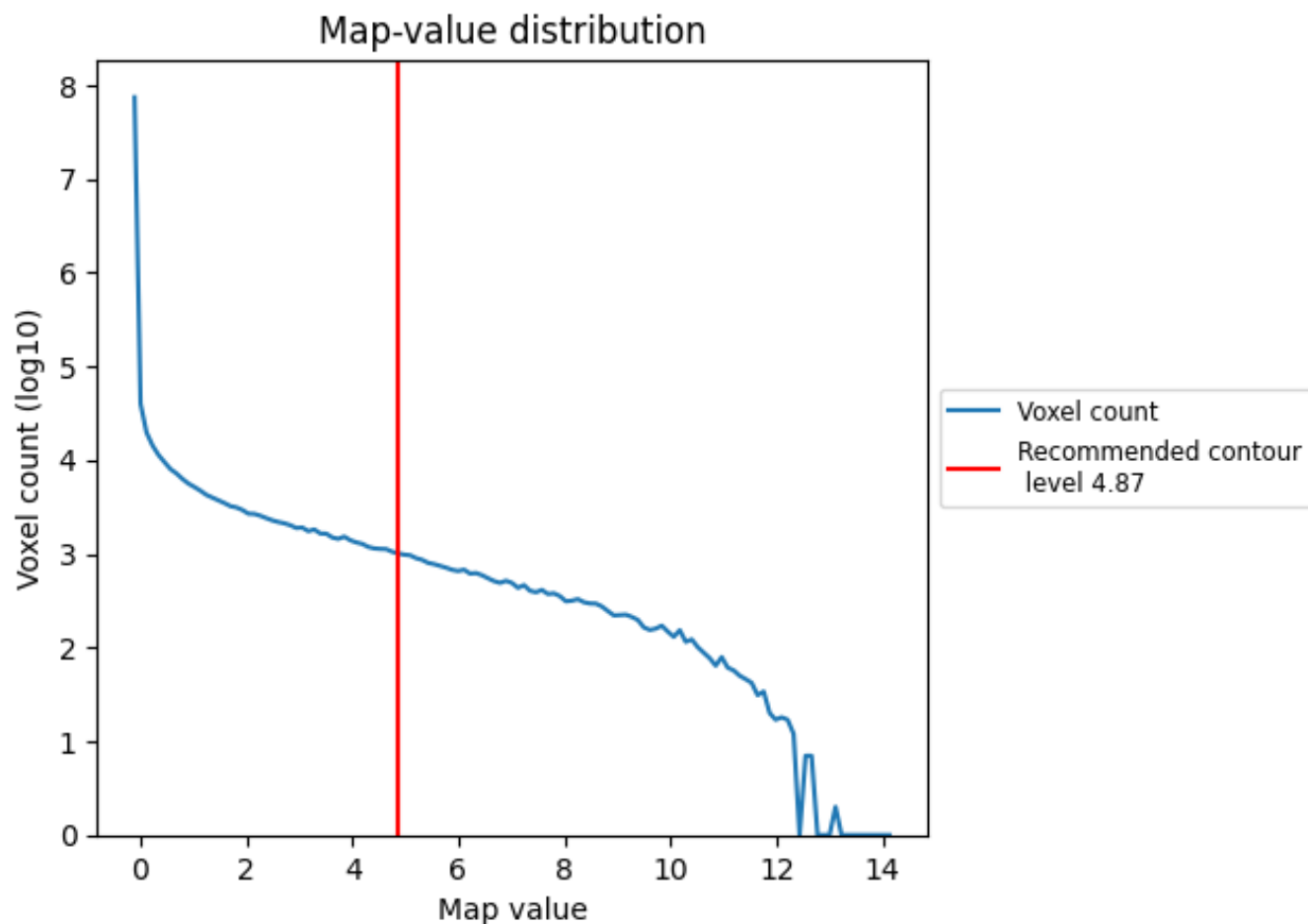
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

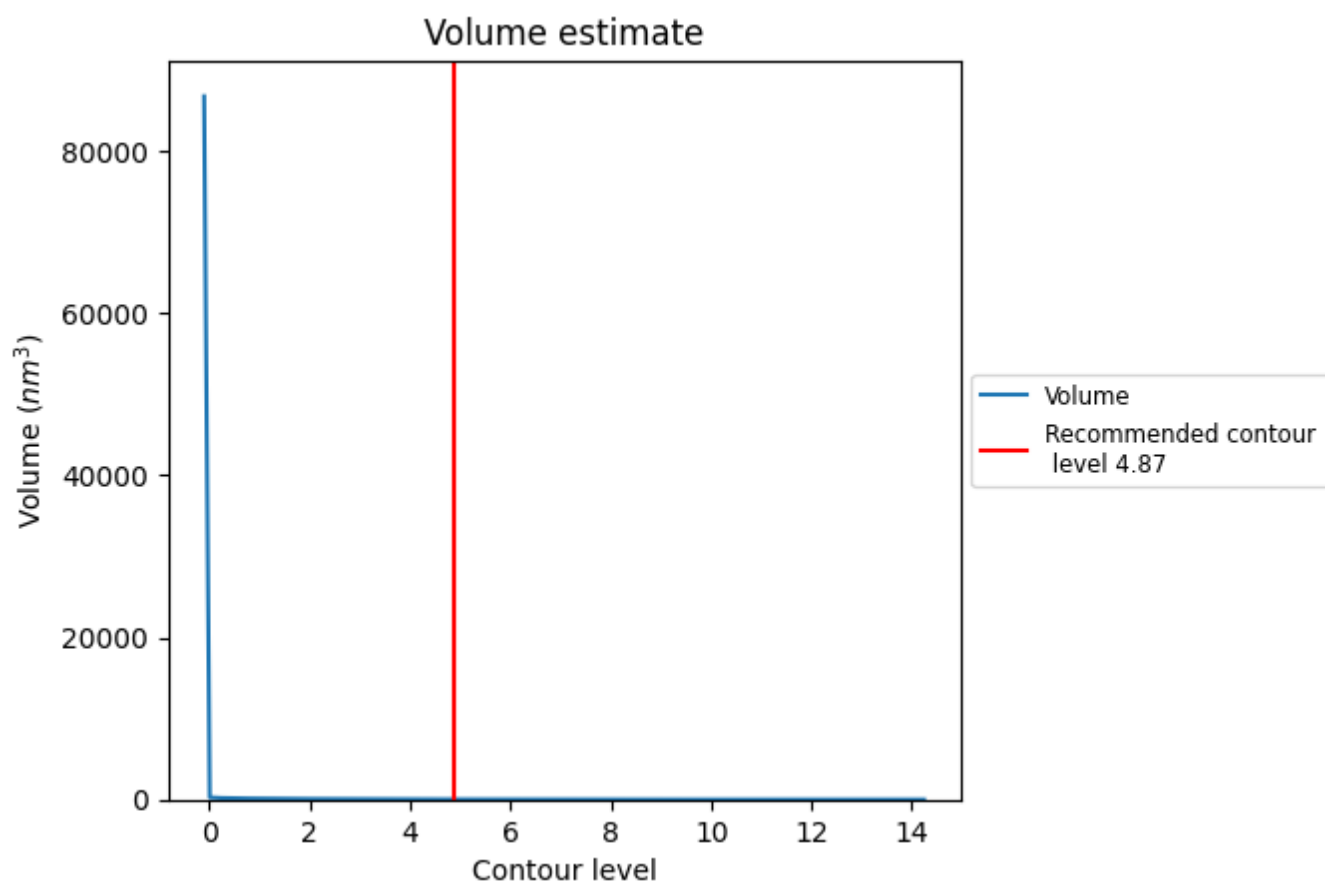
This section contains the results of statistical analysis of the map.

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.

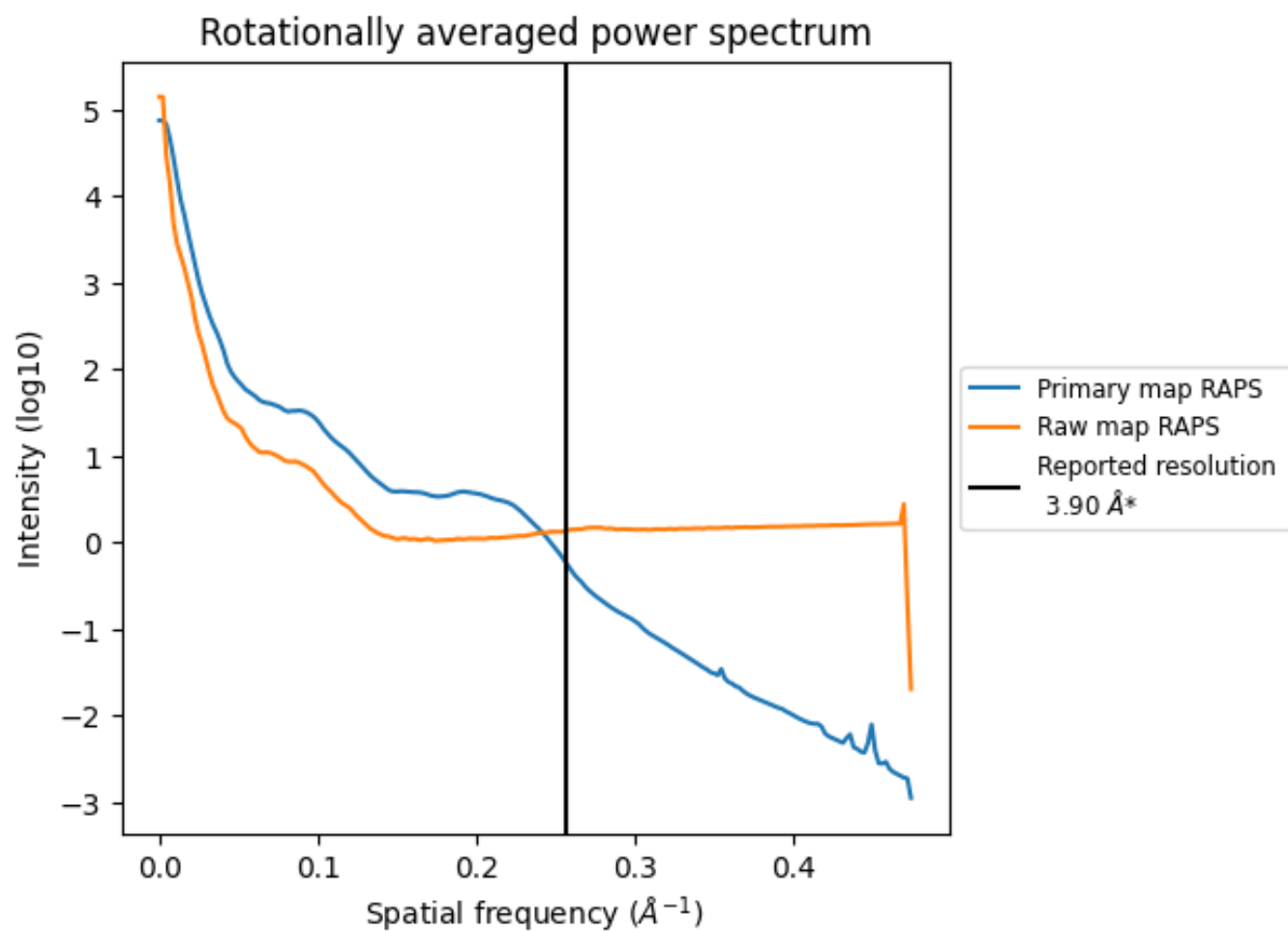
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 27 nm³; this corresponds to an approximate mass of 24 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 ⓘ

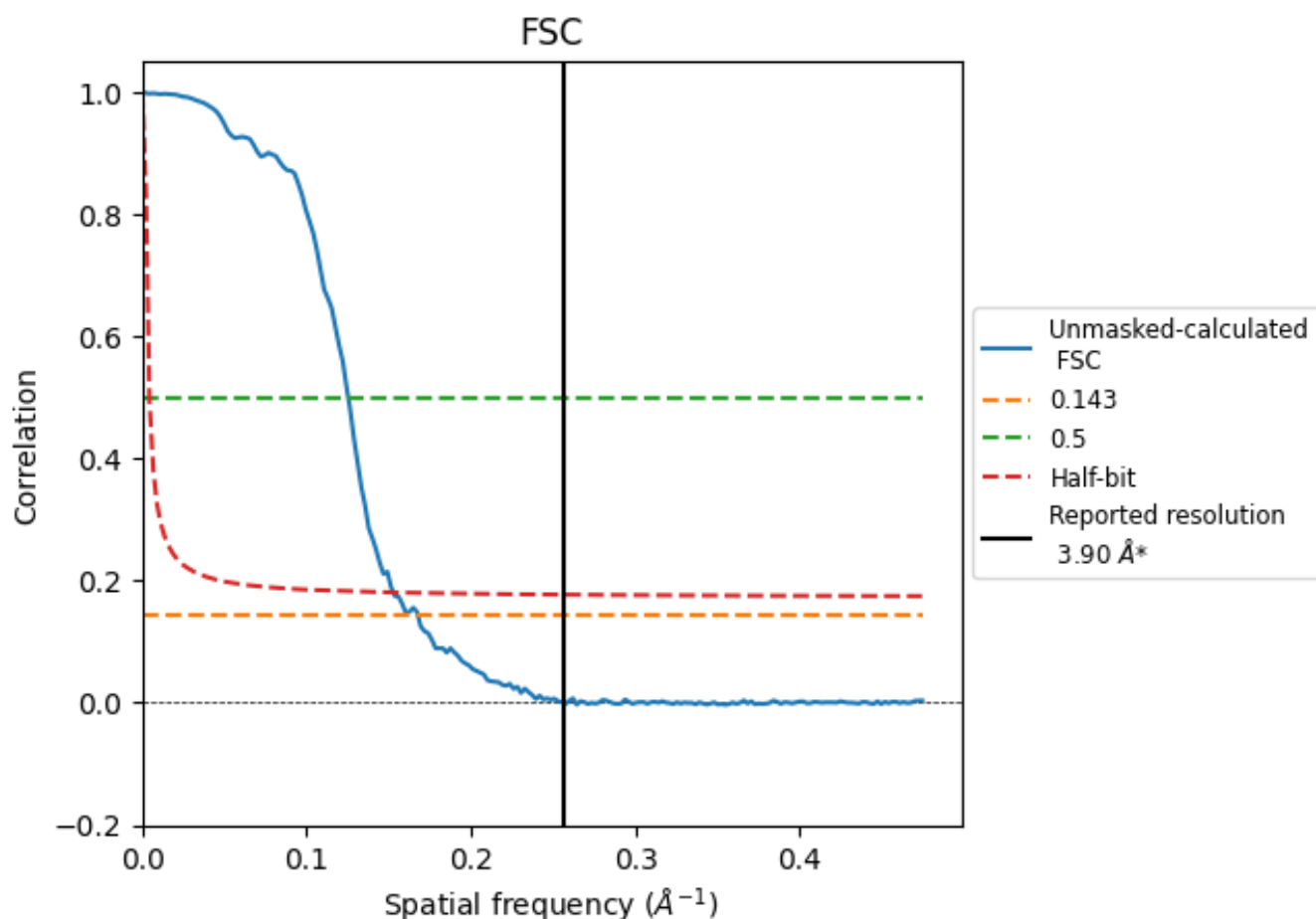


*Reported resolution corresponds to spatial frequency of 0.256 $\text{\AA}^{-1}$

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 0.256 Å⁻¹

8.2 Resolution estimates [i](#)

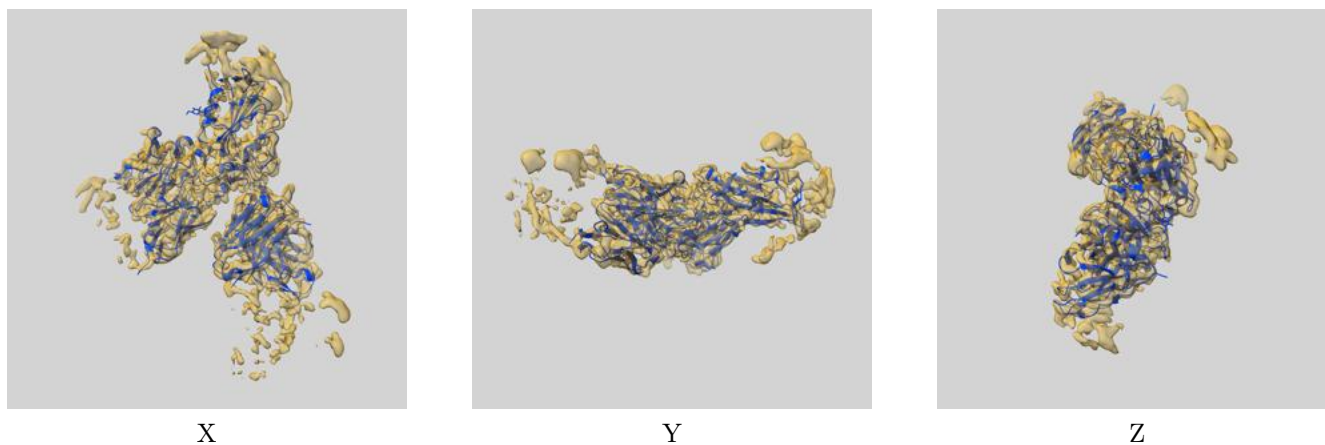
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	5.96	7.98	6.55

*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 5.96 differs from the reported value 3.9 by more than 10 %

9 Map-model fit [i](#)

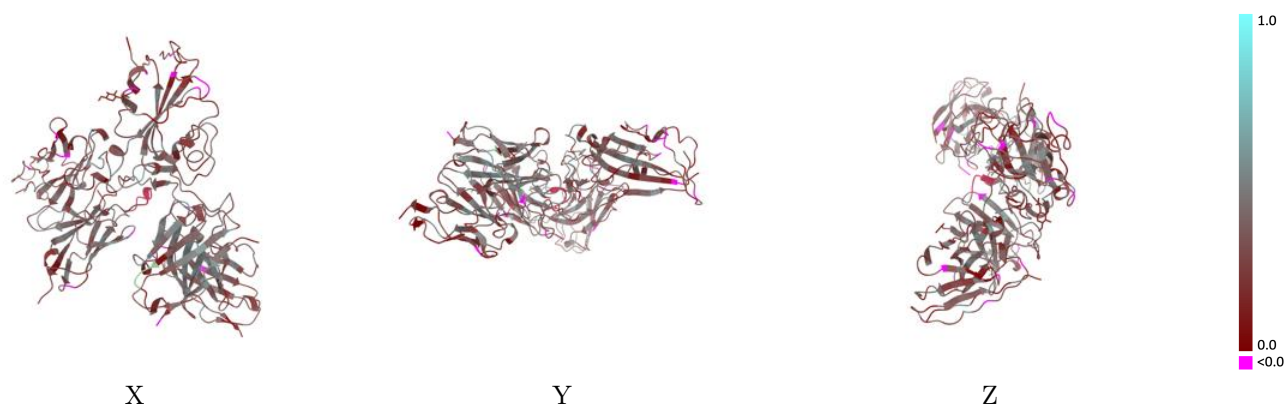
This section contains information regarding the fit between EMDB map EMD-77344 and PDB model 36AZ. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



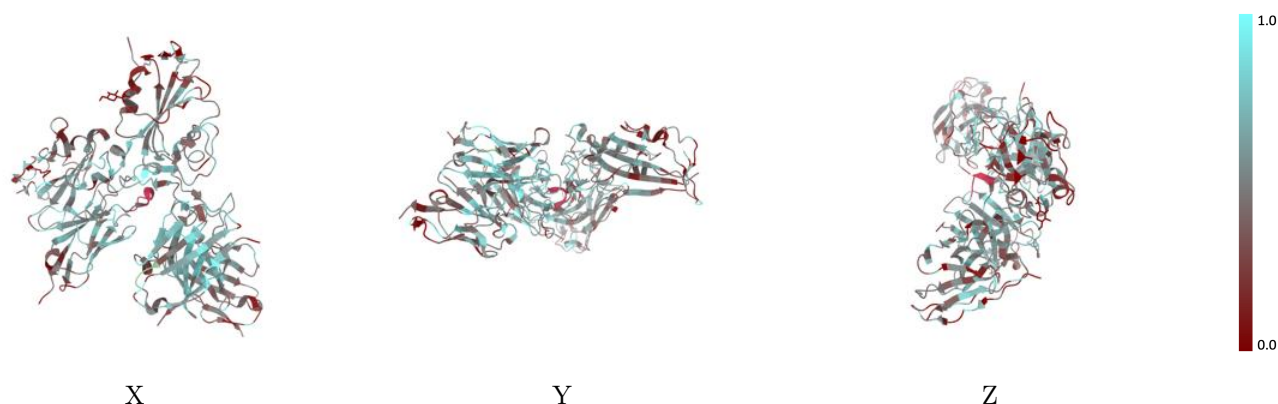
The images above show the 3D surface view of the map at the recommended contour level 4.87 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



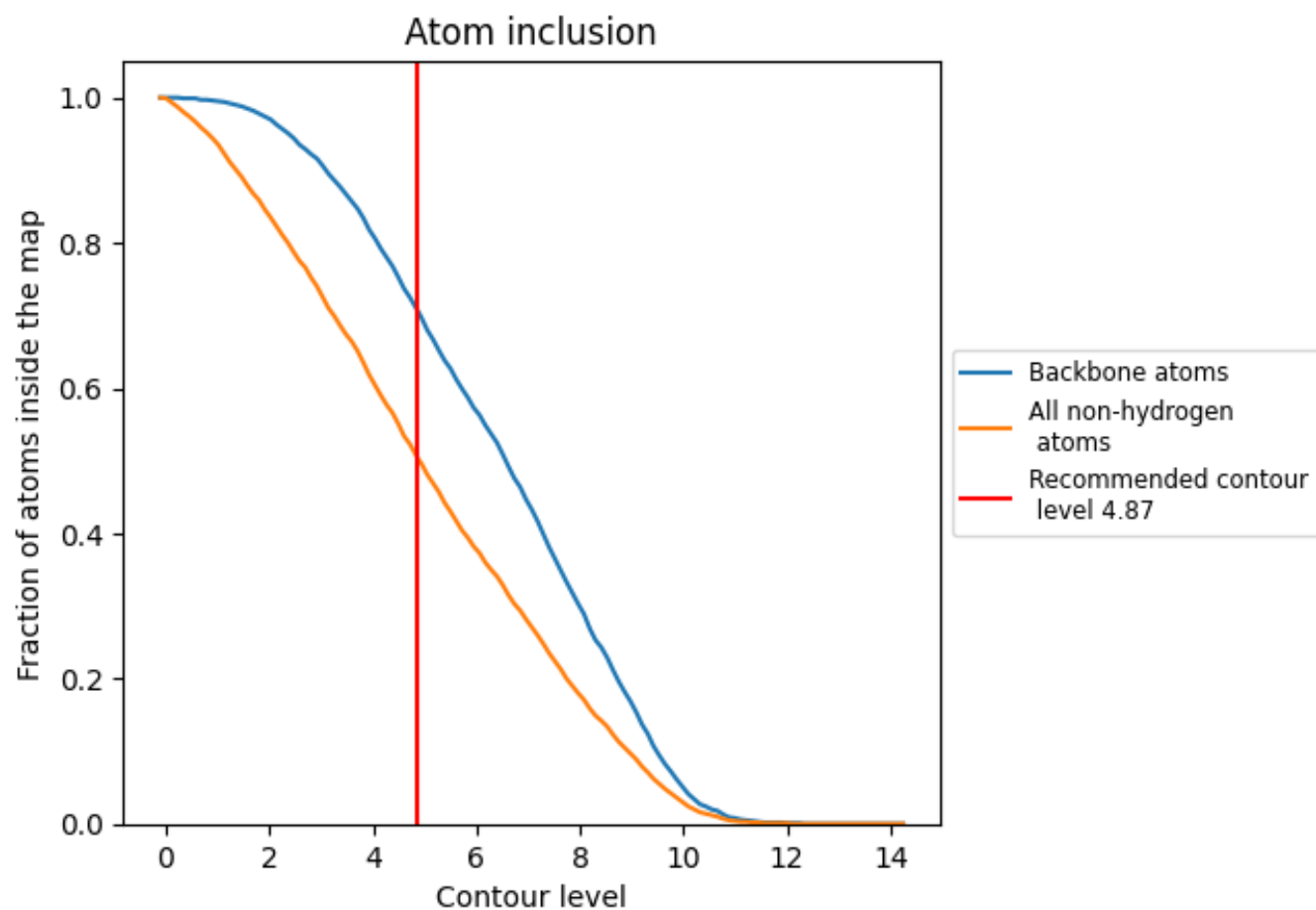
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (4.87).

9.4 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 50% 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 (4.87) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5030	0.3100
A	0.4590	0.2910
B	0.4760	0.2840
C	0.5960	0.3770
H	0.4710	0.2750
L	0.5460	0.3350

