



## Full wwPDB EM Validation Report ⓘ

Jun 22, 2026 – 06:44 AM EDT

PDB ID : 9YGR / pdb\_00009ygr  
EMDB ID : EMD-72939  
Title : HCoV-HKU1 C S 2P in complex with H501-022 Fab (local cryoEM)  
Authors : Vasquez, S.; Barnes, C.O.  
Deposited on : 2025-09-29  
Resolution : 3.80 Å (reported)  
Based on initial models : 8Y8A, 5O7P, 7T3M

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132  
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) : 2.49

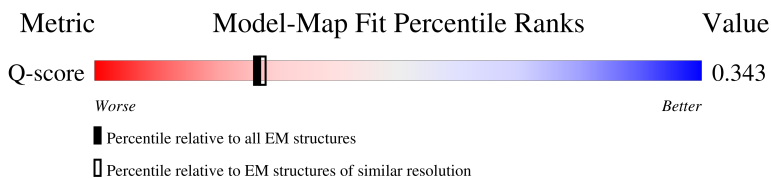
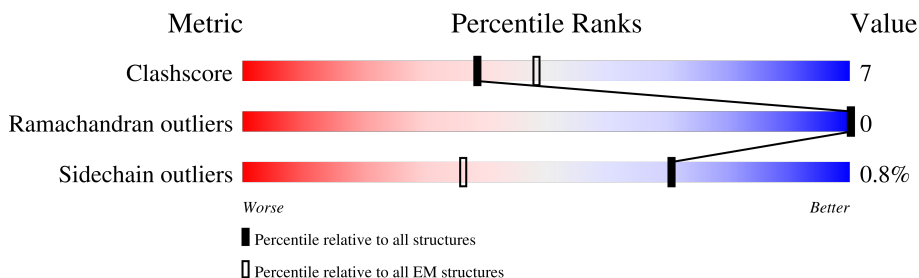
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*


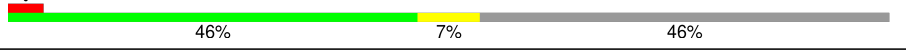

The reported resolution of this entry is 3.80 Å.

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	10198 ( 3.30 - 4.30 )

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  $\geq 3$ , 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	1334	
2	H	228	
3	L	214	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3312 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	204	Total	C	N	O	S	0	0
			1581	995	269	300	17		

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	752	GLY	ARG	engineered mutation	UNP Q0ZME7
A	753	GLY	ARG	engineered mutation	UNP Q0ZME7
A	754	SER	LYS	engineered mutation	UNP Q0ZME7
A	755	GLY	ARG	engineered mutation	UNP Q0ZME7
A	756	SER	ARG	engineered mutation	UNP Q0ZME7
A	1067	PRO	ASN	engineered mutation	UNP Q0ZME7
A	1068	PRO	LEU	engineered mutation	UNP Q0ZME7
A	1278	GLY	-	expression tag	UNP Q0ZME7
A	1279	ARG	-	expression tag	UNP Q0ZME7
A	1280	LEU	-	expression tag	UNP Q0ZME7
A	1281	GLU	-	expression tag	UNP Q0ZME7
A	1282	VAL	-	expression tag	UNP Q0ZME7
A	1283	LEU	-	expression tag	UNP Q0ZME7
A	1284	PHE	-	expression tag	UNP Q0ZME7
A	1285	GLN	-	expression tag	UNP Q0ZME7
A	1286	GLY	-	expression tag	UNP Q0ZME7
A	1287	PRO	-	expression tag	UNP Q0ZME7
A	1288	GLY	-	expression tag	UNP Q0ZME7
A	1289	GLY	-	expression tag	UNP Q0ZME7
A	1290	TYR	-	expression tag	UNP Q0ZME7
A	1291	ILE	-	expression tag	UNP Q0ZME7
A	1292	PRO	-	expression tag	UNP Q0ZME7
A	1293	GLU	-	expression tag	UNP Q0ZME7
A	1294	ALA	-	expression tag	UNP Q0ZME7
A	1295	PRO	-	expression tag	UNP Q0ZME7
A	1296	ARG	-	expression tag	UNP Q0ZME7
A	1297	ASP	-	expression tag	UNP Q0ZME7
A	1298	GLY	-	expression tag	UNP Q0ZME7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1299	GLN	-	expression tag	UNP Q0ZME7
A	1300	ALA	-	expression tag	UNP Q0ZME7
A	1301	TYR	-	expression tag	UNP Q0ZME7
A	1302	VAL	-	expression tag	UNP Q0ZME7
A	1303	ARG	-	expression tag	UNP Q0ZME7
A	1304	LYS	-	expression tag	UNP Q0ZME7
A	1305	ASP	-	expression tag	UNP Q0ZME7
A	1306	GLY	-	expression tag	UNP Q0ZME7
A	1307	GLU	-	expression tag	UNP Q0ZME7
A	1308	TRP	-	expression tag	UNP Q0ZME7
A	1309	VAL	-	expression tag	UNP Q0ZME7
A	1310	LEU	-	expression tag	UNP Q0ZME7
A	1311	LEU	-	expression tag	UNP Q0ZME7
A	1312	SER	-	expression tag	UNP Q0ZME7
A	1313	THR	-	expression tag	UNP Q0ZME7
A	1314	PHE	-	expression tag	UNP Q0ZME7
A	1315	LEU	-	expression tag	UNP Q0ZME7
A	1316	GLY	-	expression tag	UNP Q0ZME7
A	1317	HIS	-	expression tag	UNP Q0ZME7
A	1318	HIS	-	expression tag	UNP Q0ZME7
A	1319	HIS	-	expression tag	UNP Q0ZME7
A	1320	HIS	-	expression tag	UNP Q0ZME7
A	1321	HIS	-	expression tag	UNP Q0ZME7
A	1322	HIS	-	expression tag	UNP Q0ZME7
A	1323	HIS	-	expression tag	UNP Q0ZME7
A	1324	HIS	-	expression tag	UNP Q0ZME7
A	1325	SER	-	expression tag	UNP Q0ZME7
A	1326	ALA	-	expression tag	UNP Q0ZME7
A	1327	TRP	-	expression tag	UNP Q0ZME7
A	1328	SER	-	expression tag	UNP Q0ZME7
A	1329	HIS	-	expression tag	UNP Q0ZME7
A	1330	PRO	-	expression tag	UNP Q0ZME7
A	1331	GLN	-	expression tag	UNP Q0ZME7
A	1332	PHE	-	expression tag	UNP Q0ZME7
A	1333	GLU	-	expression tag	UNP Q0ZME7
A	1334	LYS	-	expression tag	UNP Q0ZME7

- Molecule 2 is a protein called H501-022 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	122	Total	C	N	O	S	0	0
			927	586	154	180	7		

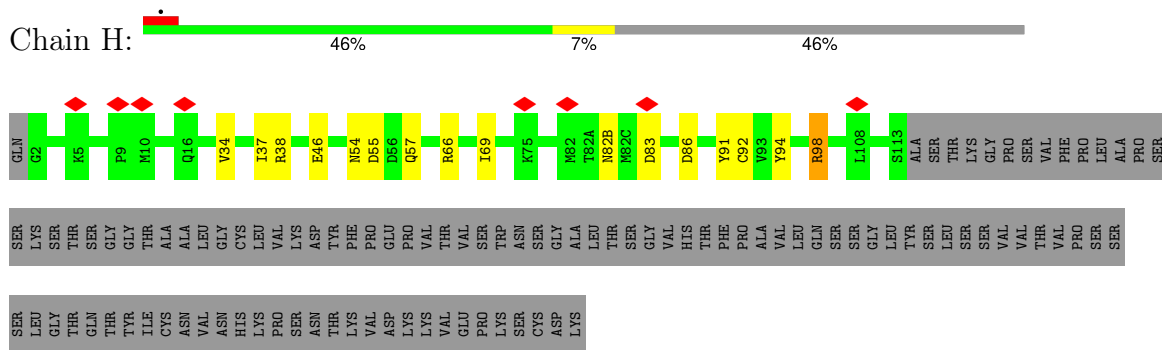
- Molecule 3 is a protein called H501-022 Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	106	Total	C	N	O	S	0	0
			804	504	131	167	2		

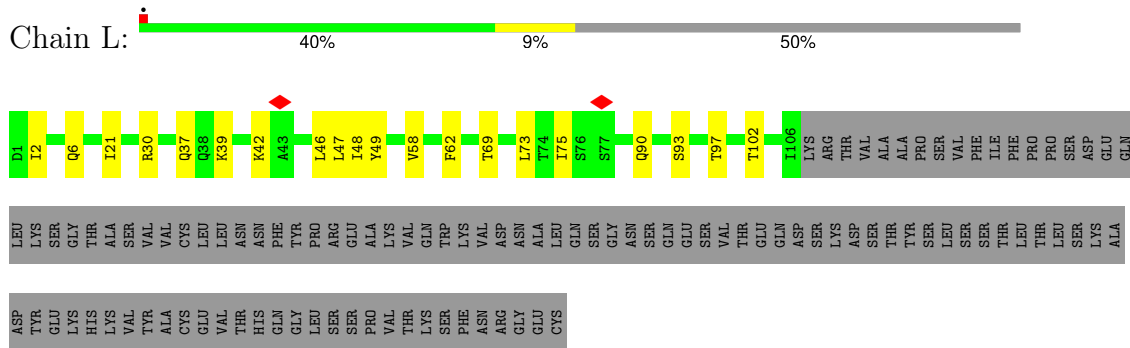


[illegible]

- Molecule 2: H501-022 Fab heavy chain



- Molecule 3: H501-022 Fab light chain



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	139880	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	30	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	130000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.518	Depositor
Minimum map value	-1.764	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.14	Depositor
Map size (Å)	441.6, 441.6, 441.6	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.92, 0.92, 0.92	Depositor



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.17	0/1624	0.41	0/2201
2	H	0.23	0/947	0.48	0/1292
3	L	0.19	0/823	0.45	0/1122
All	All	0.19	0/3394	0.44	0/4615

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	1581	0	1458	28	0
2	H	927	0	927	8	0
3	L	804	0	774	11	0
All	All	3312	0	3159	46	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.

All (46) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:520:CYS:SG	1:A:533:CYS:SG	1.29	1.28

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:LEU:HD12	1:A:403:LEU:O	1.50	1.11
1:A:520:CYS:SG	1:A:533:CYS:CB	2.39	1.09
1:A:370:CYS:HG	1:A:423:CYS:HG	0.88	0.81
1:A:403:LEU:O	1:A:403:LEU:CD1	2.31	0.75
1:A:370:CYS:HG	1:A:423:CYS:CB	2.01	0.72
1:A:401:LEU:HA	1:A:410:GLN:HE22	1.68	0.59
1:A:520:CYS:SG	1:A:533:CYS:HB2	2.39	0.58
1:A:479:PRO:HA	1:A:482:VAL:HG22	1.85	0.58
1:A:339:PRO:HB2	1:A:391:PHE:HA	1.88	0.56
3:L:46:LEU:HD21	3:L:49:TYR:HB3	1.88	0.55
1:A:478:ASP:OD1	1:A:478:ASP:N	2.39	0.52
1:A:369:SER:N	1:A:423:CYS:SG	2.84	0.51
2:H:38:ARG:NH2	2:H:46:GLU:OE2	2.44	0.51
2:H:54:ASN:CG	2:H:55:ASP:H	2.19	0.51
3:L:47:LEU:HA	3:L:58:VAL:HG21	1.92	0.51
1:A:491:PRO:HB2	1:A:557:GLY:HA3	1.94	0.49
1:A:482:VAL:O	1:A:489:LYS:NZ	2.46	0.49
1:A:444:TRP:NE1	1:A:547:PRO:O	2.46	0.49
1:A:495:CYS:SG	1:A:499:THR:OG1	2.72	0.47
2:H:83:ASP:HB3	2:H:86:ASP:HB2	1.97	0.47
1:A:397:ARG:NH2	1:A:400:ASP:OD2	2.48	0.47
2:H:37:ILE:HB	2:H:91:TYR:HB2	1.96	0.47
3:L:39:LYS:HB2	3:L:42:LYS:HB3	1.96	0.47
3:L:2:ILE:HD13	3:L:93:SER:HB2	1.95	0.47
2:H:66:ARG:HE	2:H:82(B):ASN:HB3	1.79	0.47
2:H:98:ARG:HB3	2:H:98:ARG:HH11	1.80	0.47
1:A:387:THR:HB	1:A:593:ILE:HB	1.97	0.47
1:A:370:CYS:N	1:A:423:CYS:SG	2.88	0.46
1:A:523:ASP:OD1	1:A:523:ASP:N	2.47	0.46
3:L:62:PHE:HA	3:L:75:ILE:HG22	1.98	0.46
3:L:21:ILE:HD11	3:L:73:LEU:HD23	1.98	0.45
1:A:370:CYS:SG	1:A:423:CYS:CB	3.05	0.44
1:A:422:SER:HB3	1:A:593:ILE:HG23	1.99	0.44
1:A:370:CYS:SG	1:A:423:CYS:HB3	2.58	0.44
3:L:6:GLN:HE21	3:L:102:THR:HG23	1.81	0.44
3:L:69:THR:HG22	3:L:69:THR:O	2.17	0.43
1:A:448:TYR:OH	1:A:473:PHE:O	2.36	0.43
3:L:37:GLN:HB2	3:L:47:LEU:HD11	2.00	0.43
3:L:90:GLN:HE21	3:L:97:THR:HG22	1.84	0.42
1:A:396:ARG:NH1	1:A:462:TYR:OH	2.52	0.42
1:A:403:LEU:HB3	1:A:424:GLN:HE22	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:57:GLN:NE2	2:H:69:ILE:O	2.52	0.42
1:A:407:GLY:O	1:A:411:SER:OG	2.33	0.41
2:H:34:VAL:HG13	2:H:94:TYR:HE1	1.86	0.40
1:A:536:LYS:HB3	3:L:30:ARG:HD2	2.02	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	192/1334 (14%)	185 (96%)	7 (4%)	0	100	100
2	H	120/228 (53%)	105 (88%)	15 (12%)	0	100	100
3	L	104/214 (49%)	98 (94%)	6 (6%)	0	100	100
All	All	416/1776 (23%)	388 (93%)	28 (7%)	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	183/1192 (15%)	183 (100%)	0	100	100
2	H	107/199 (54%)	105 (98%)	2 (2%)	50	66
3	L	92/189 (49%)	91 (99%)	1 (1%)	65	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	382/1580 (24%)	379 (99%)	3 (1%)	70	76

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

Mol	Chain	Res	Type
2	H	92	CYS
2	H	98	ARG
3	L	48	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	437	ASN
1	A	465	HIS
1	A	552	ASN
2	H	77	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 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 ⓘ

There are no chain breaks in this entry.

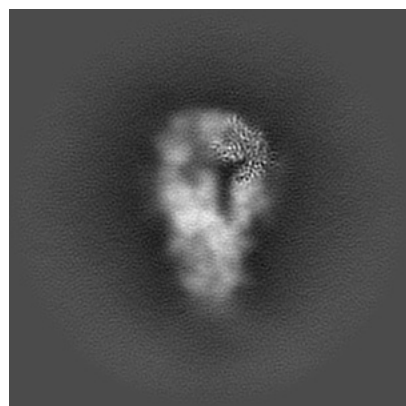
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-72939. These allow visual inspection of the internal detail of the map and identification of artifacts.

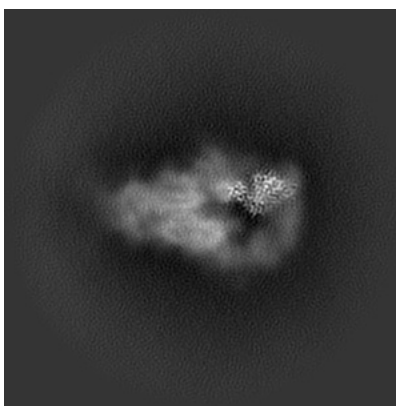
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

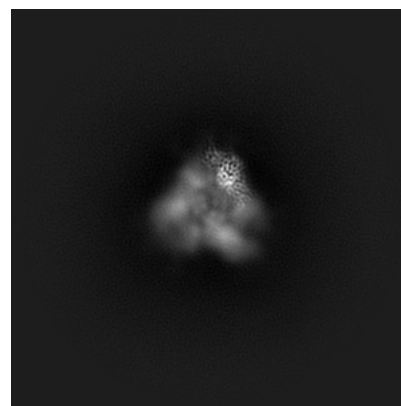
#### 6.1.1 Primary map



X

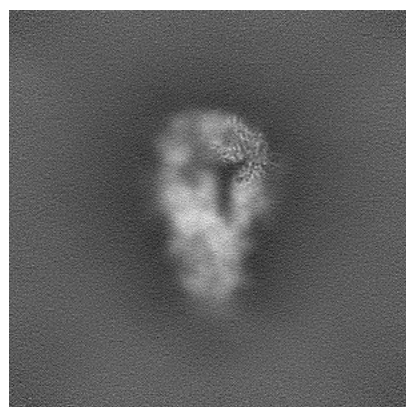


Y

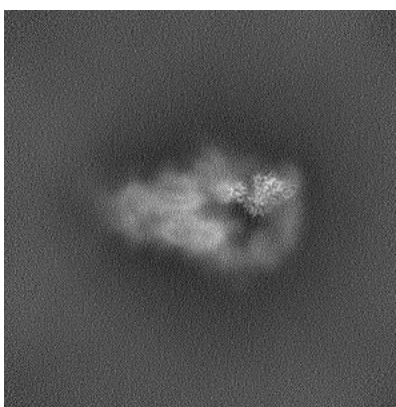


Z

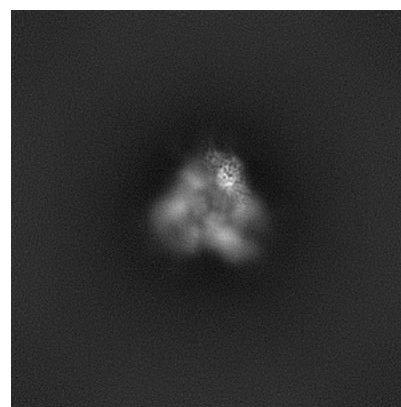
#### 6.1.2 Raw map



X



Y

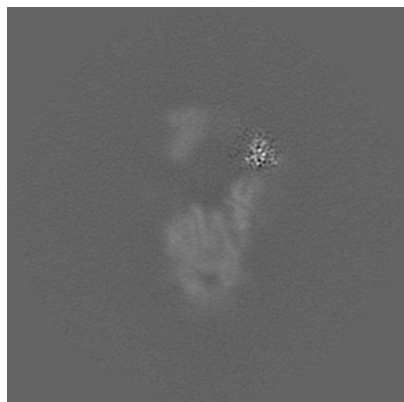


Z

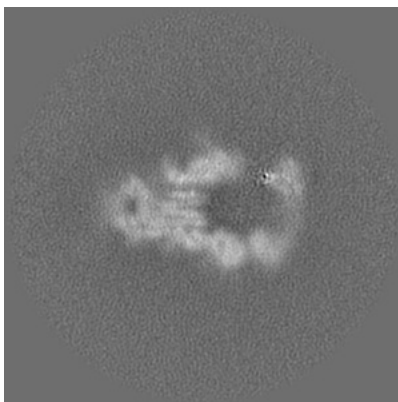
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

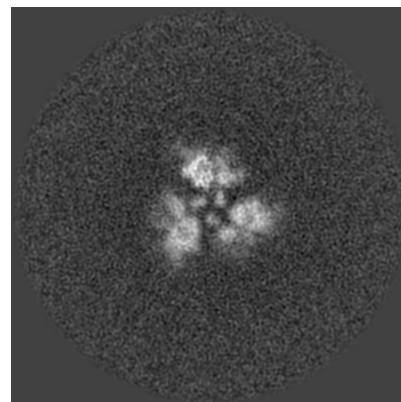
### 6.2.1 Primary map



X Index: 240

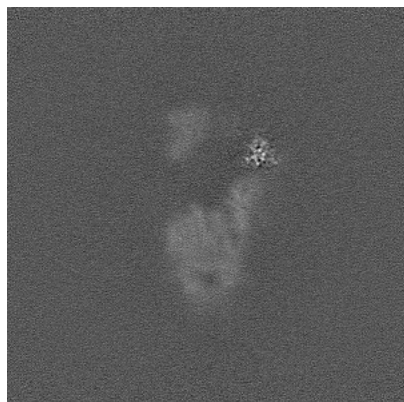


Y Index: 240

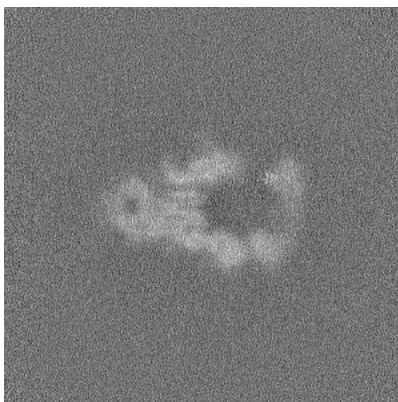


Z Index: 240

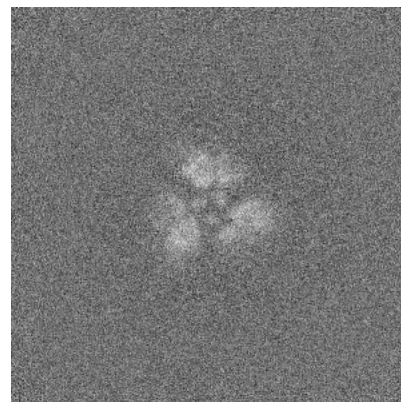
### 6.2.2 Raw map



X Index: 240



Y Index: 240



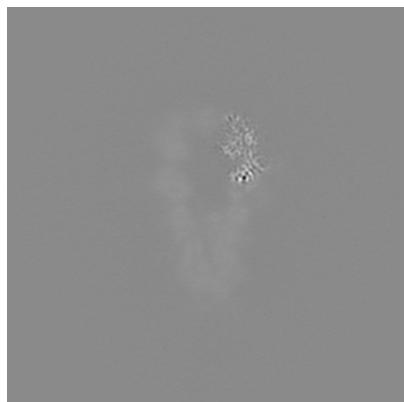
Z Index: 240

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

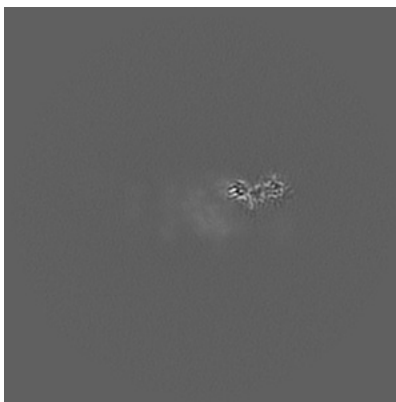


## 6.3 Largest variance slices [i](#)

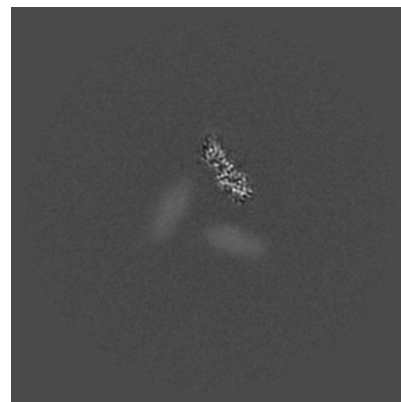
### 6.3.1 Primary map



X Index: 259

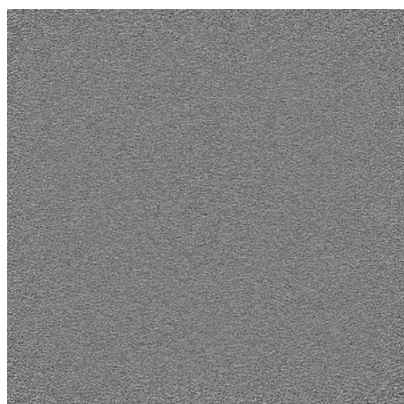


Y Index: 288

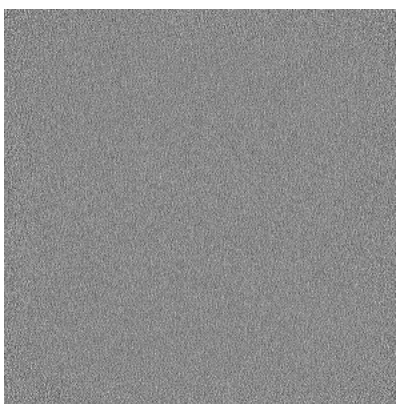


Z Index: 303

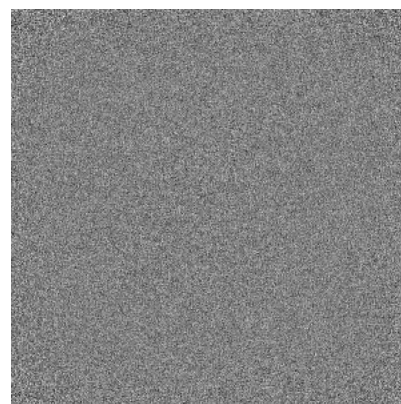
### 6.3.2 Raw map



X Index: 0



Y Index: 0



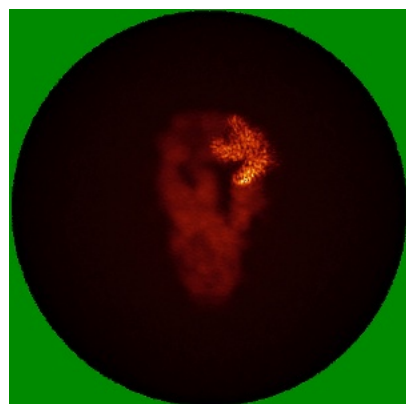
Z Index: 0

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

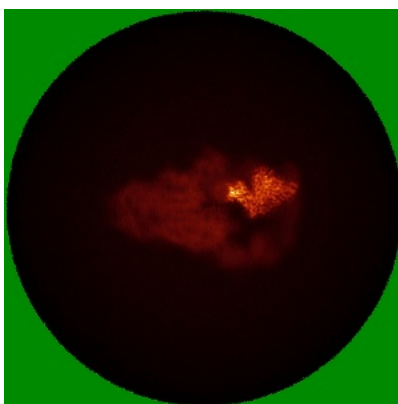


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

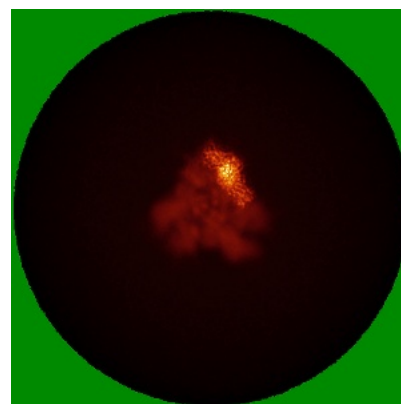
### 6.4.1 Primary map



X



Y

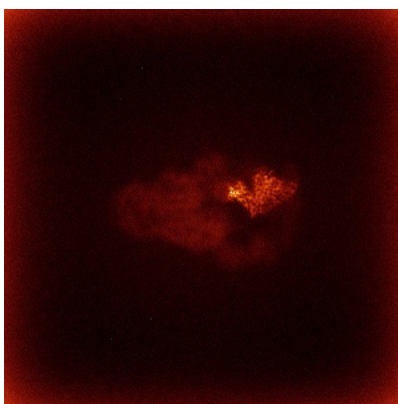


Z

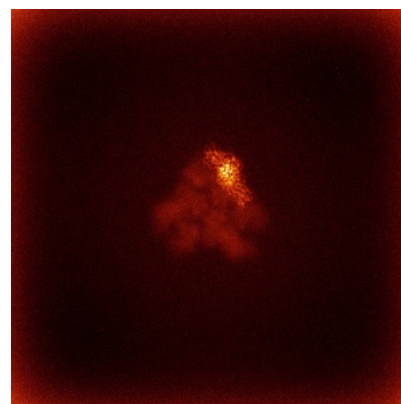
### 6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

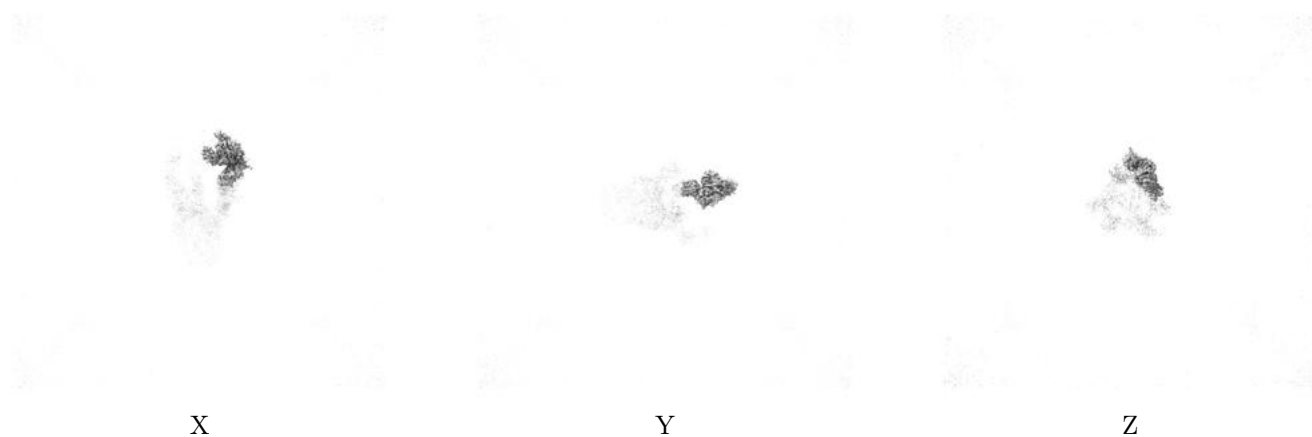
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.14. 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.

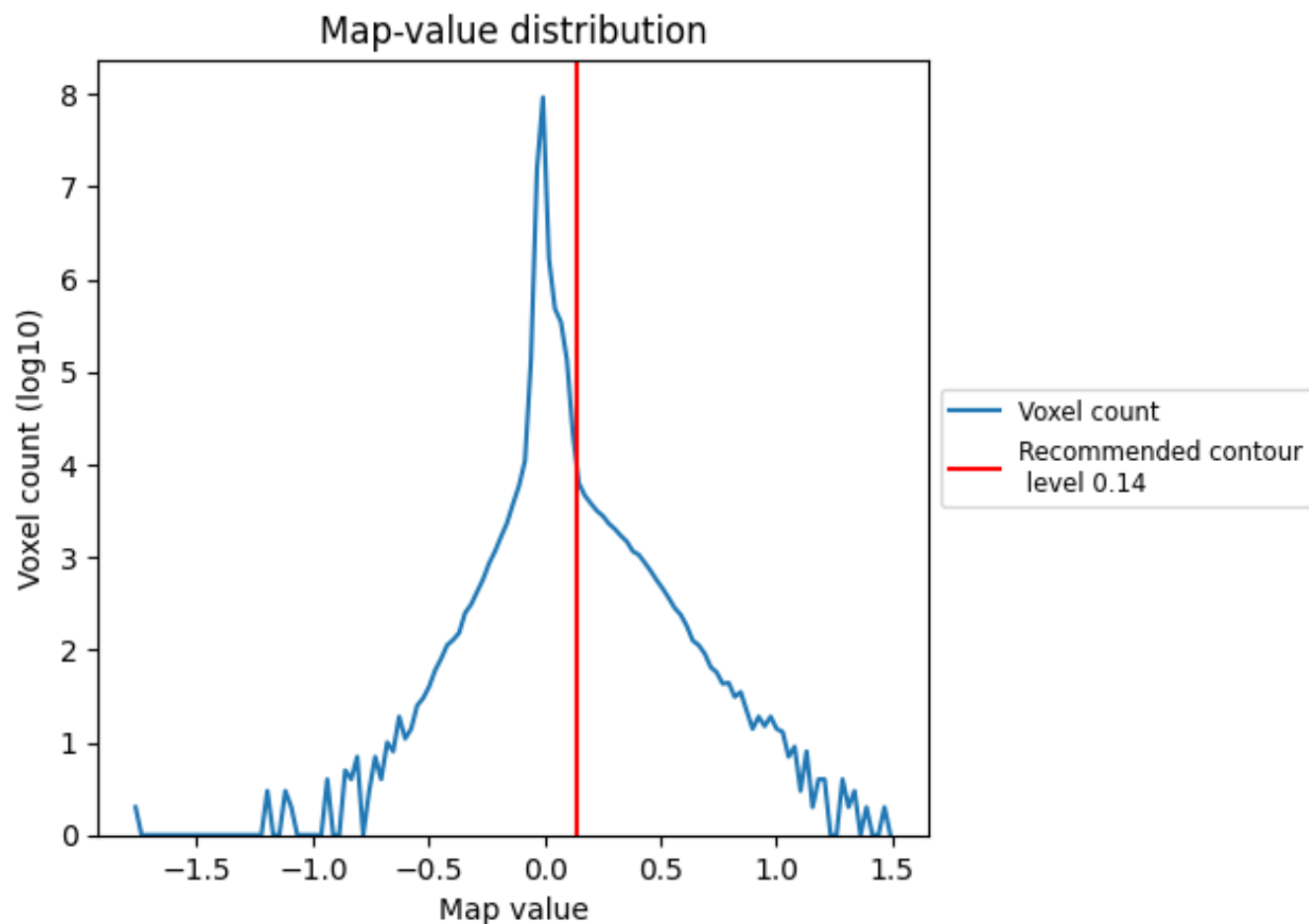
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

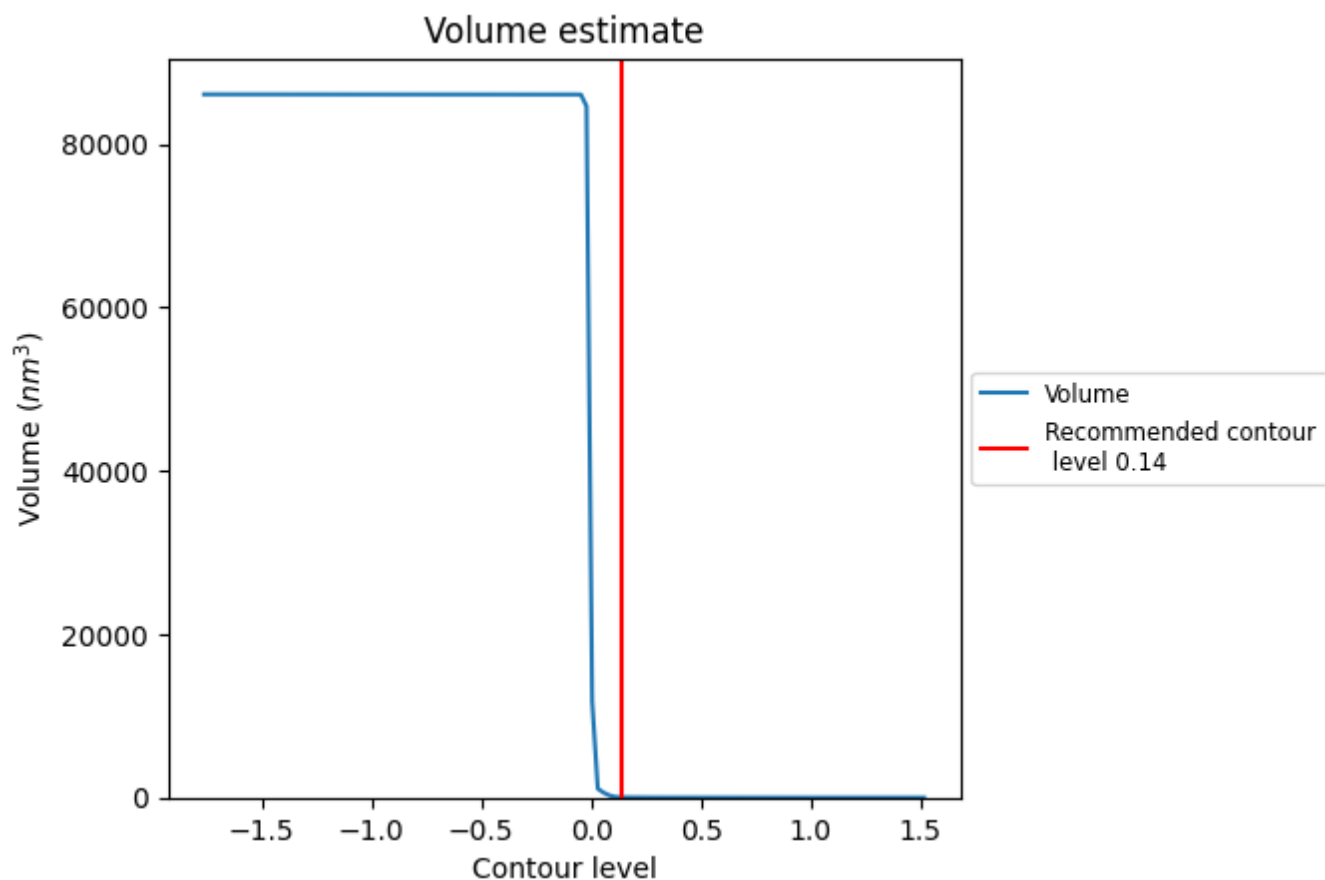
This section contains the results of statistical analysis of the map.

### 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.

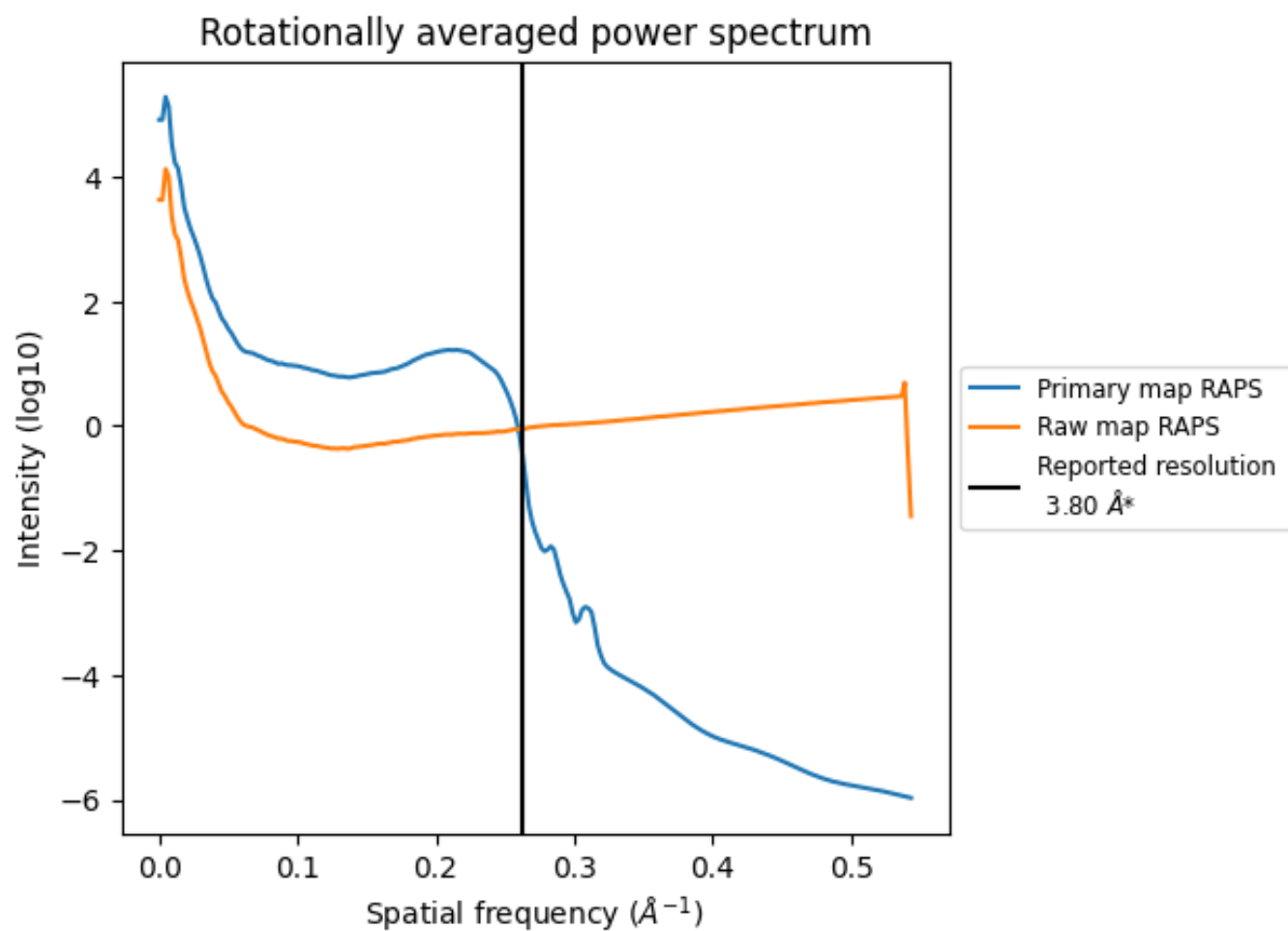
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 31 nm<sup>3</sup>; this corresponds to an approximate mass of 28 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](#)

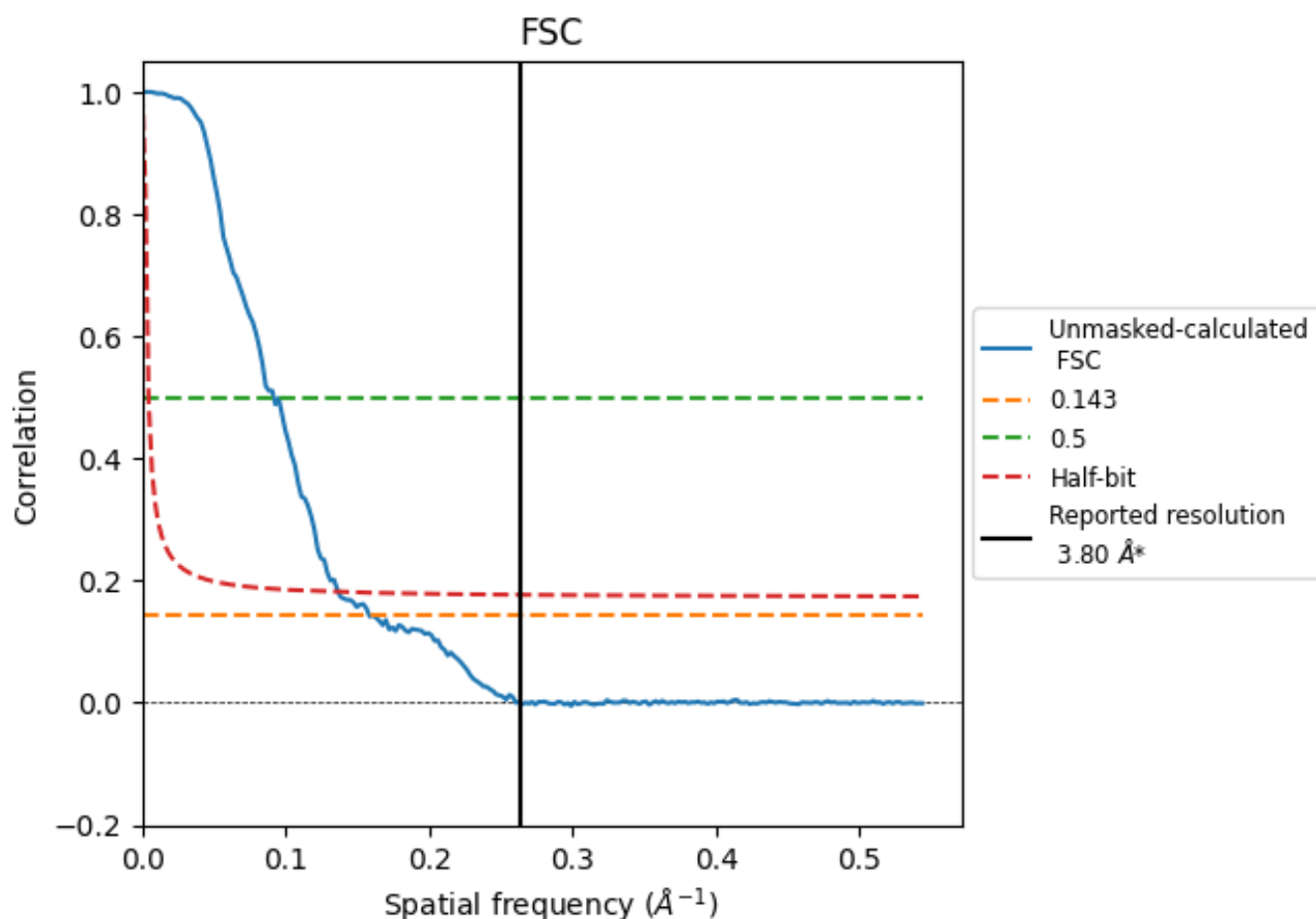


\*Reported resolution corresponds to spatial frequency of 0.263  $\text{\AA}^{-1}$

## 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 0.263 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

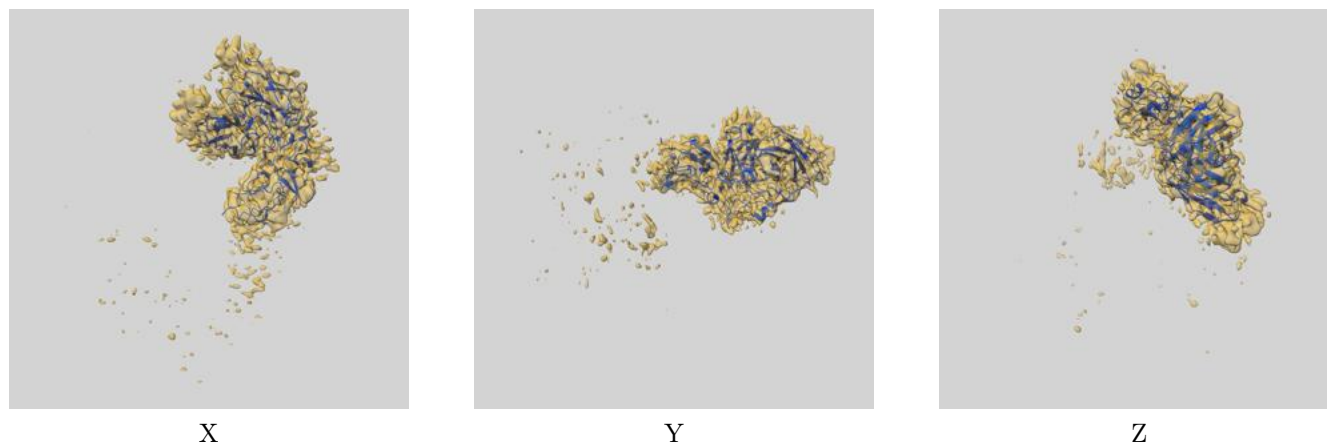
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.32	10.91	7.32

\*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 6.32 differs from the reported value 3.8 by more than 10 %

## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-72939 and PDB model 9YGR. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

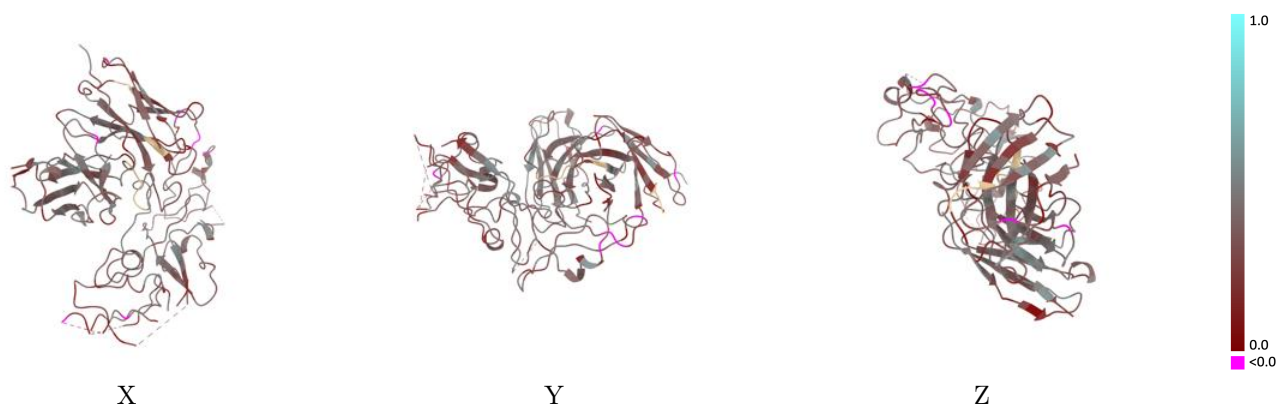
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.14 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.

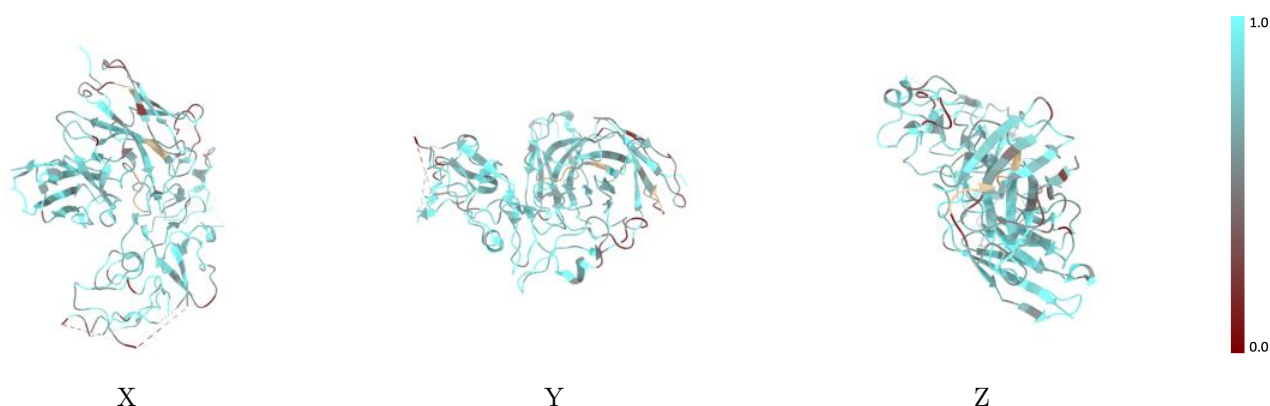


## 9.2 Q-score mapped to coordinate model [i](#)



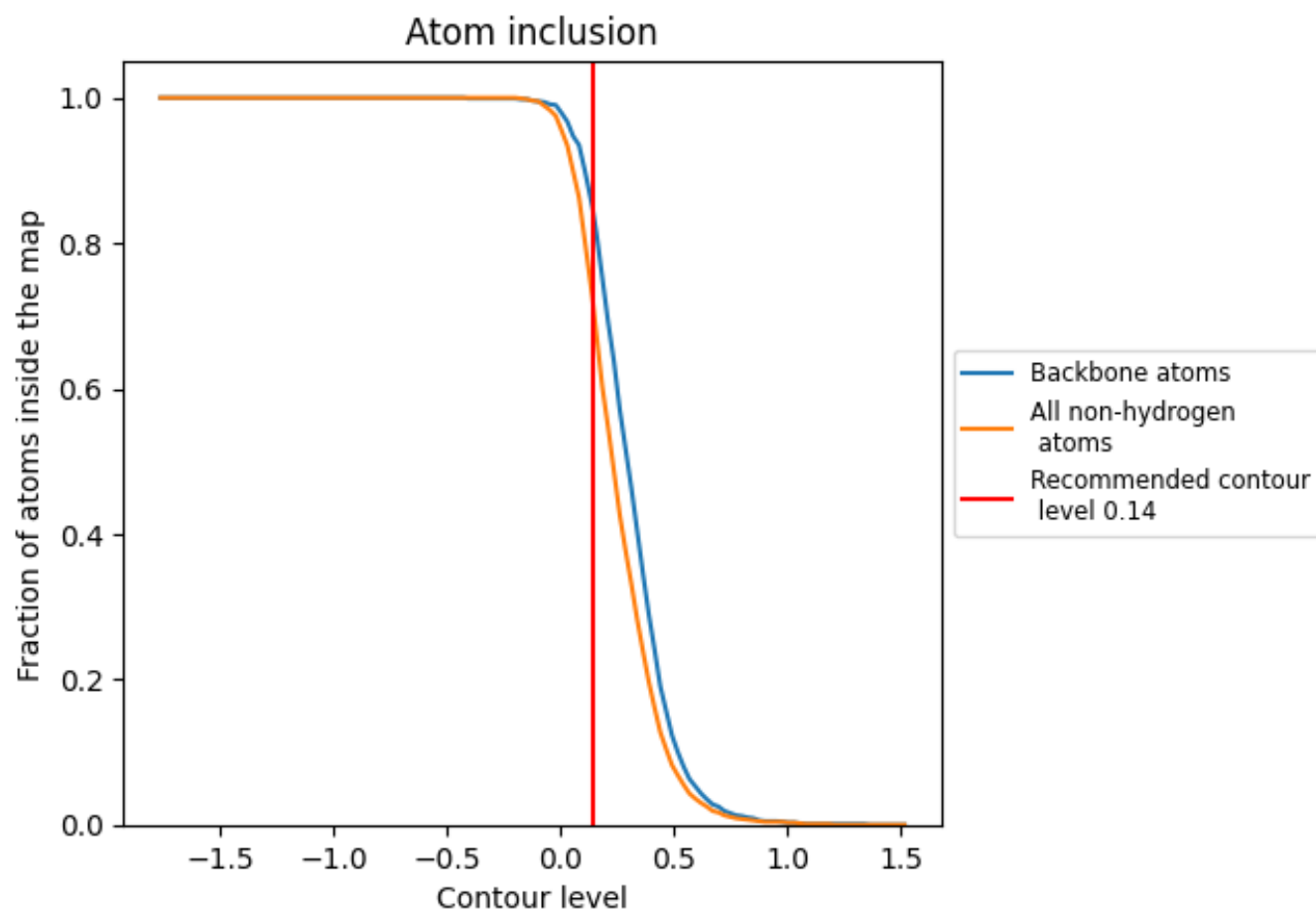
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.14).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 73% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.14) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7270	<div></div> 0.3430
A	<div></div> 0.7250	<div></div> 0.3360
H	<div></div> 0.6790	<div></div> 0.3210
L	<div></div> 0.7870	<div></div> 0.3820

