



wwPDB EM Validation Summary Report ⓘ

Apr 21, 2026 – 11:01 am BST

PDB ID : 9RIJ / pdb_00009rij
EMDB ID : EMD-53997
Title : EV-A71 (genotype B5) in complex with 16-2-8C Fab
Authors : Zhou, D.; Ren, J.; Stuart, D.I.
Deposited on : 2025-06-11
Resolution : 3.80 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:

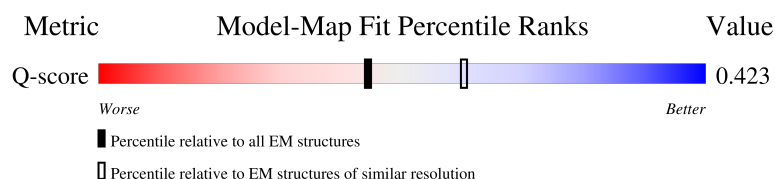
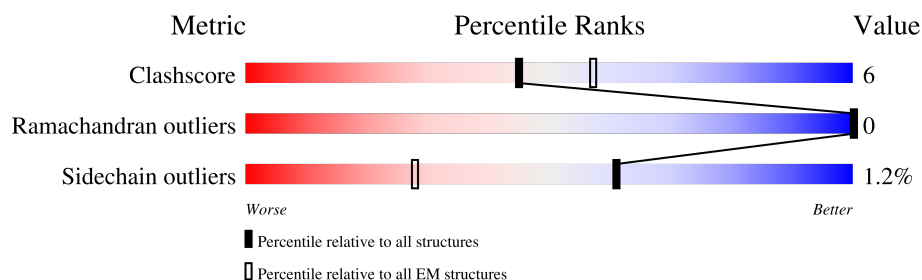
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 ≥ 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	297	 84% 15%
2	B	254	 78% 17% . .
3	C	242	 87% 12%
4	D	69	 62% 20% 17%

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Mol	Chain	Length	Quality of chain
5	H	245	<div><div><div>53%</div><div>44%</div><div>11%</div><div>45%</div></div></div>
6	L	216	<div><div><div>50%</div><div>44%</div><div>6%</div><div>49%</div></div></div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8365 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 Genome polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	296	Total	C	N	O	S	0	0
			2296	1446	393	444	13		

- Molecule 2 is a protein called Genome polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	245	Total	C	N	O	S	0	0
			1900	1216	314	361	9		

- Molecule 3 is a protein called Genome polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	241	Total	C	N	O	S	0	0
			1865	1199	310	344	12		

- Molecule 4 is a protein called Capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	57	Total	C	N	O	S	0	0
			443	276	72	94	1		

- Molecule 5 is a protein called heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	134	Total	C	N	O	S	0	0
			1044	668	168	202	6		

- Molecule 6 is a protein called light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L	110	Total	C	N	O	S	0	0
			796	492	139	163	2		

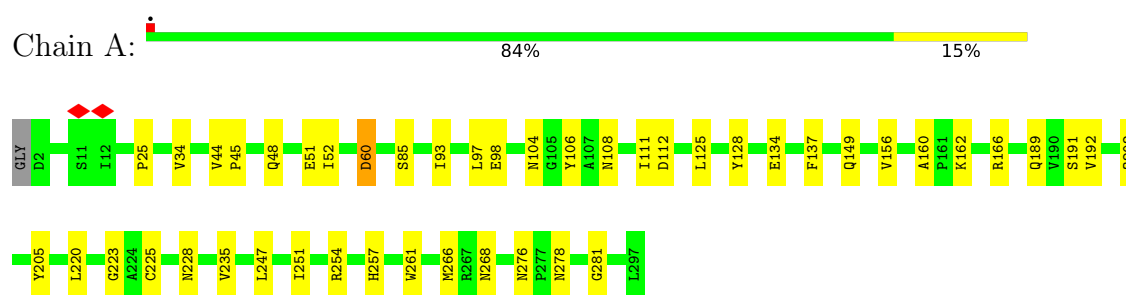
- # SPH

Mol	Chain	Residues	Atoms				AltConf
7	A	1	Total	C	N	O	0
			21	18	1	2	

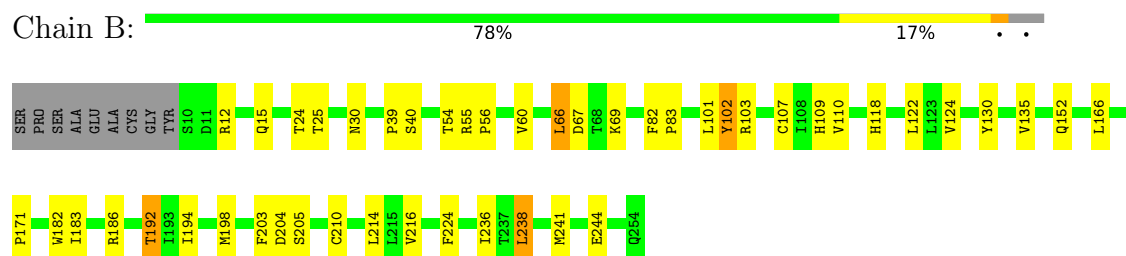
3 Residue-property plots [i](#)

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.

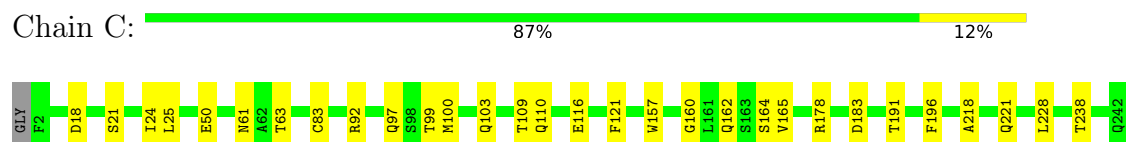
• Molecule 1: Genome polyprotein



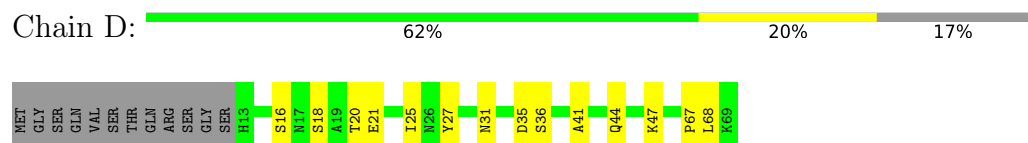
• Molecule 2: Genome polyprotein



• Molecule 3: Genome polyprotein



• Molecule 4: Capsid protein



• Molecule 5: heavy chain



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● Molecule 6: light chain



Q1	S2	V3	L4	T5	Q6	P7	P8	S9	A10	S11	G12	T13	P14	G15	Q16	R17	V18	T19	I20	S21	C22	S23	G24	S25	S26	S27	N28	I29	R30	G31	N32	T33	V34	N35	W36	Y37	Q38	K39	L40	P41	G42	A43	A44	P45	T46	L47	L48	I49	Y50	T51	N52	N53	Q54	R55	P56	S57	G58	V59	P60
D61	R62	F63	S64	G65	S66	K67	S68	G69	T70	S71	A72	S73	L74	A75	I76	S77	G78	L79	Q80	S81	E82	D83	E84	A85	D86	Y87	F88	C89	A90	A91	Y92	D93	G94	S95	L96	N97	A98	V99	V100	F101	G102	G103	G104	T105	K106	L107	T108	V109	L110	GLY	GLN	PRO	LYS	ALA	ASN	PRO	THR	VAL	THR
LEU	PHE	PRO	PRO	SER	GLU	GLU	GLN	ALA	ASN	LYS	ALA	THR	LEU	CYS	LEU	ILE	SER	ASP	PHE	TYR	PRO	GLY	ALA	THR	ALA	TRP	LYS	ALA	ASP	SER	PRO	PRO	VAL	LYS	ALA	GLY	THR	PRO	LYS	GLN	THR	ASN	ASN	LYS	TYR	ALA	ALA	SER	SER	GLY	GLN	PRO	LYS	ALA	ASN	PRO	THR	VAL	THR
TYR	LEU	SER	LEU	THR	PRO	GLU	GLN	THR	LYS	HIS	ARG	SER	TYR	SER	CYS	GLN	VAL	THR	HIS	GLY	THR	VAL	GLU	LYS	THR	ALA	PRO	THR	GLY	VAL	LYS	GLY	THR	GLU	THR	LYS	GLN	THR	ASN	ASN	LYS	TYR	ALA	ALA	SER	SER	GLY	GLN	PRO	LYS	ALA	ASN	PRO	THR	VAL	THR			

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	3665	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	22	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.214	Depositor
Minimum map value	-0.095	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	540.0, 540.0, 540.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.35, 1.35, 1.35	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: SPH

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	0.18	0/2355	0.30	0/3211
2	B	0.18	0/1955	0.30	0/2679
3	C	0.18	0/1920	0.28	0/2626
4	D	0.13	0/452	0.23	0/611
5	H	0.09	0/1076	0.26	0/1472
6	L	0.09	0/812	0.25	0/1107
All	All	0.16	0/8570	0.29	0/11706

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	2296	0	2230	37	0
2	B	1900	0	1834	30	0
3	C	1865	0	1829	19	0
4	D	443	0	420	9	0
5	H	1044	0	1009	19	0
6	L	796	0	774	8	0
7	A	21	0	37	5	0
All	All	8365	0	8133	104	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 6.

The worst 5 of 104 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:128:TYR:HB2	1:A:261:TRP:HB2	1.70	0.73
1:A:125:LEU:HD11	3:C:100:MET:HE1	1.74	0.70
1:A:225:CYS:SG	1:A:228:ASN:ND2	2.64	0.70
6:L:5:THR:HB	6:L:23:SER:HB3	1.75	0.68
1:A:134:GLU:OE1	1:A:254:ARG:NH1	2.28	0.67

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	294/297 (99%)	277 (94%)	17 (6%)	0	100	100
2	B	243/254 (96%)	229 (94%)	14 (6%)	0	100	100
3	C	239/242 (99%)	232 (97%)	7 (3%)	0	100	100
4	D	55/69 (80%)	53 (96%)	2 (4%)	0	100	100
5	H	132/245 (54%)	130 (98%)	2 (2%)	0	100	100
6	L	108/216 (50%)	105 (97%)	3 (3%)	0	100	100
All	All	1071/1323 (81%)	1026 (96%)	45 (4%)	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	253/253 (100%)	250 (99%)	3 (1%)	63	72
2	B	209/215 (97%)	203 (97%)	6 (3%)	37	58
3	C	203/203 (100%)	202 (100%)	1 (0%)	81	81
4	D	48/58 (83%)	47 (98%)	1 (2%)	47	64
5	H	120/217 (55%)	120 (100%)	0	100	100
6	L	88/180 (49%)	88 (100%)	0	100	100
All	All	921/1126 (82%)	910 (99%)	11 (1%)	61	72

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	192	THR
2	B	238	LEU
4	D	25	ILE
3	C	238	THR
2	B	54	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	221	GLN
5	H	60	HIS
2	B	152	GLN
2	B	181	GLN
3	C	48	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	$\# Z > 2$
7	SPH	A	301	-	19,20,20	0.92	1 (5%)	18,21,21	0.85	1 (5%)

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
7	SPH	A	301	-	-	13/21/21/21	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	301	SPH	C4-C5	3.63	1.47	1.31

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	301	SPH	C3-C4-C5	-2.11	120.09	124.79

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	301	SPH	O1-C1-C2-N2

Continued on next page...

Continued from previous page...

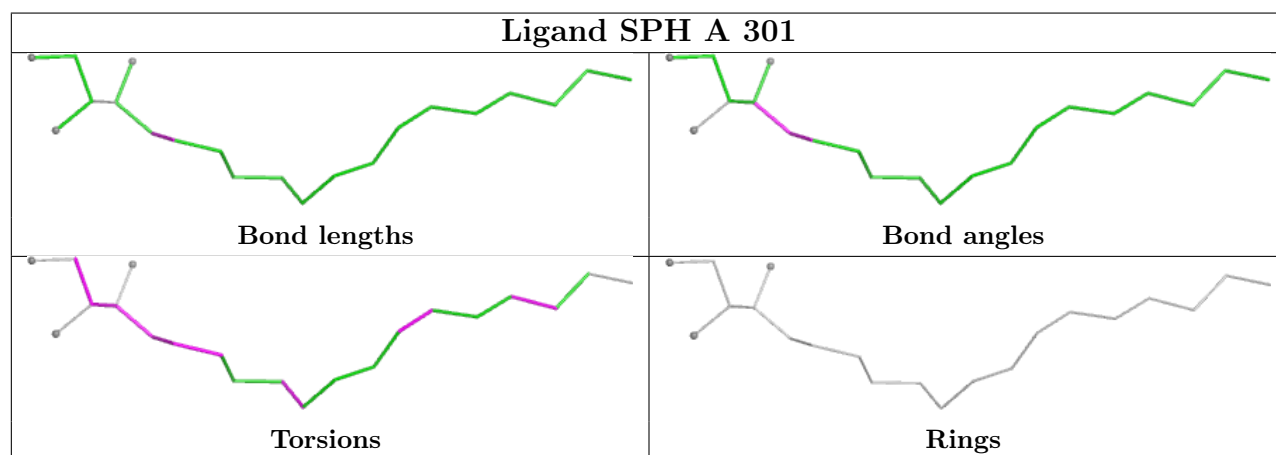
Mol	Chain	Res	Type	Atoms
7	A	301	SPH	O1-C1-C2-C3
7	A	301	SPH	C1-C2-C3-O3
7	A	301	SPH	C1-C2-C3-C4
7	A	301	SPH	N2-C2-C3-C4

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	301	SPH	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.

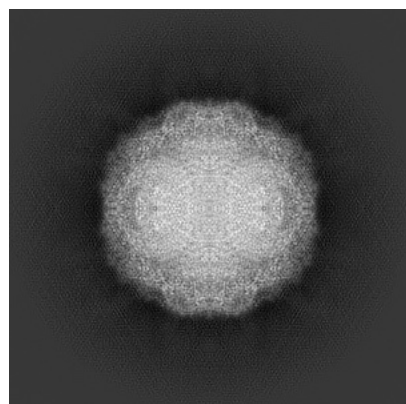
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53997. These allow visual inspection of the internal detail of the map and identification of artifacts.

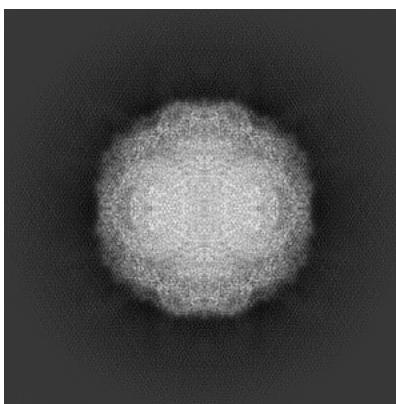
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

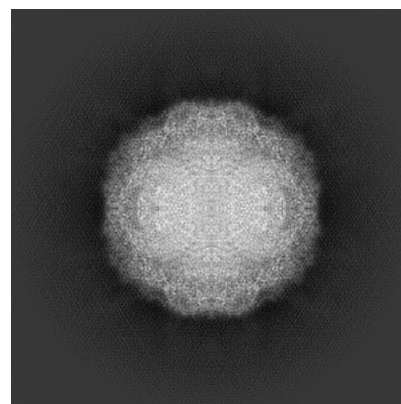
6.1.1 Primary map



X

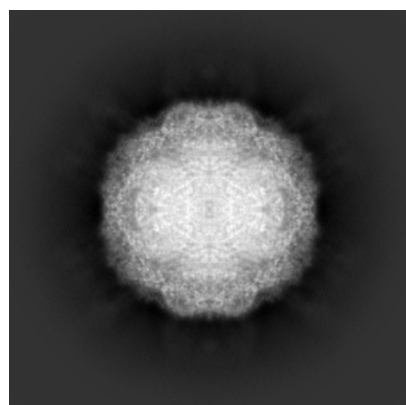


Y

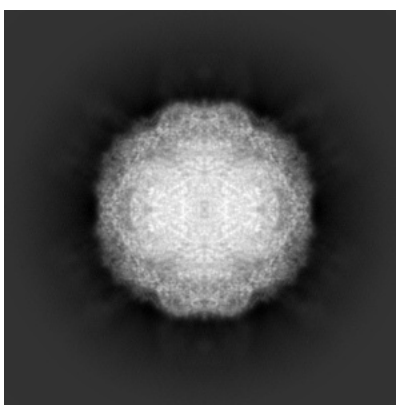


Z

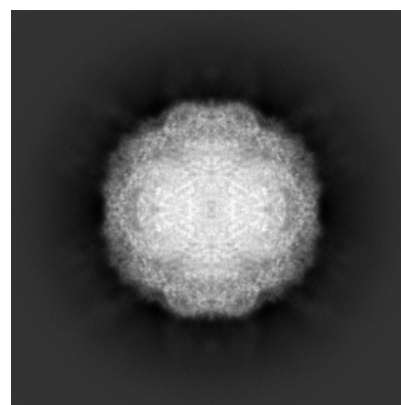
6.1.2 Raw map



X



Y

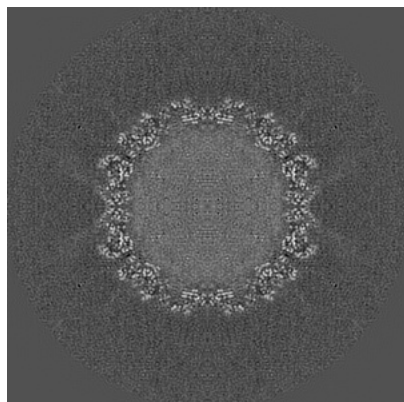


Z

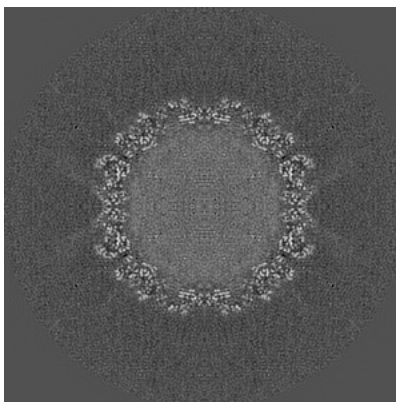
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

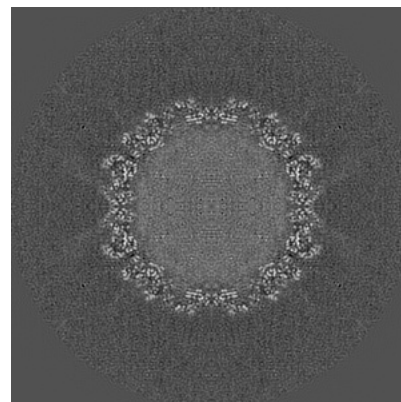
6.2.1 Primary map



X Index: 200

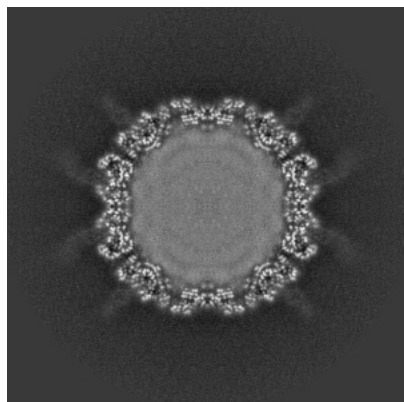


Y Index: 200

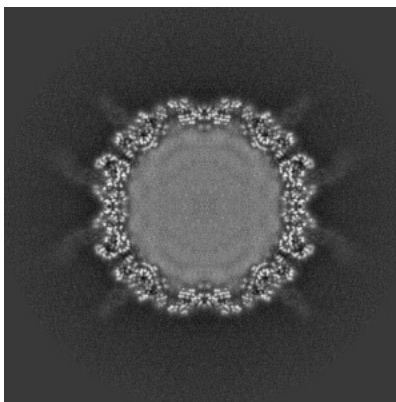


Z Index: 200

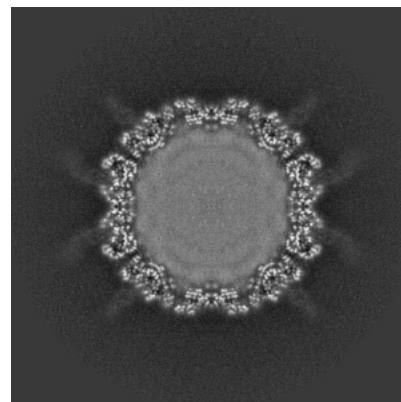
6.2.2 Raw map



X Index: 200



Y Index: 200

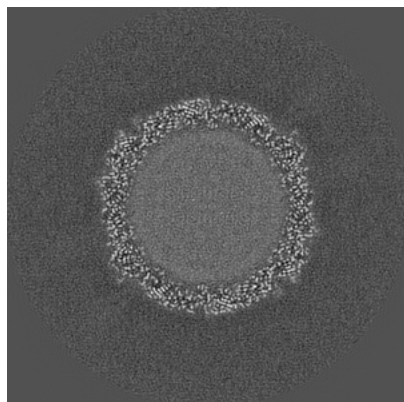


Z Index: 200

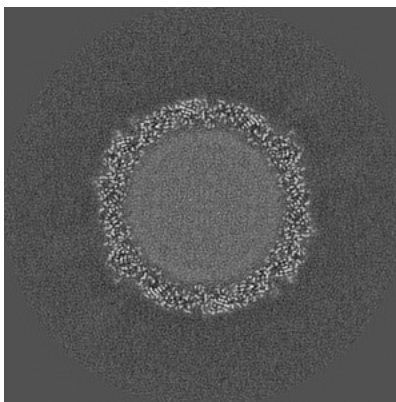
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

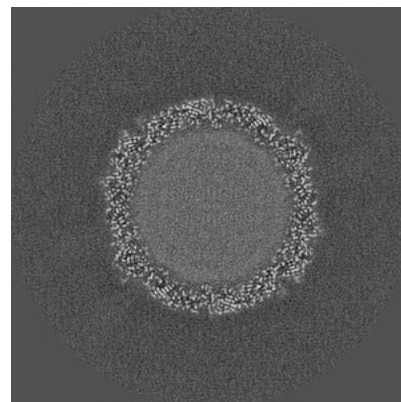
6.3.1 Primary map



X Index: 187

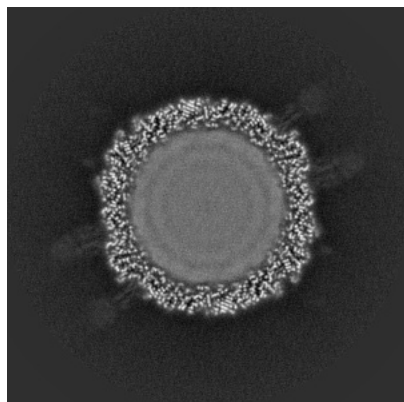


Y Index: 187

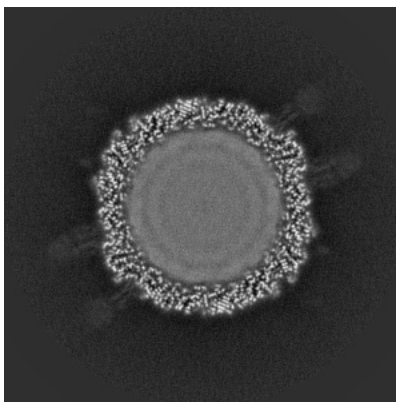


Z Index: 187

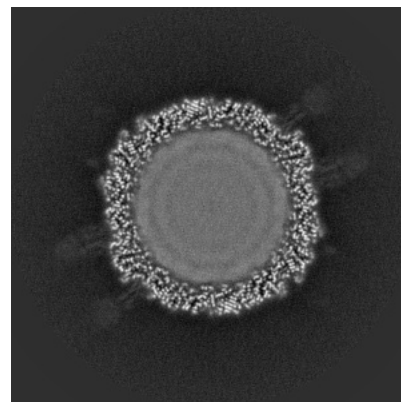
6.3.2 Raw map



X Index: 188



Y Index: 188

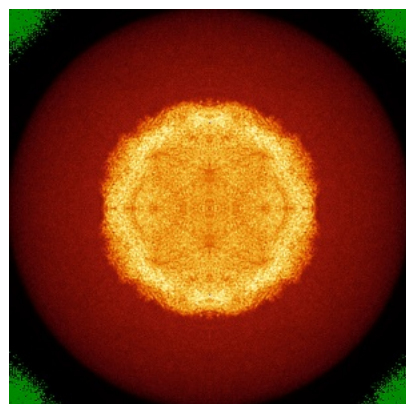


Z Index: 188

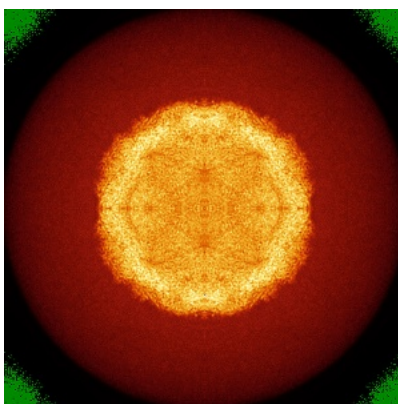
The images above show the largest variance slices of the map in three orthogonal directions.

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

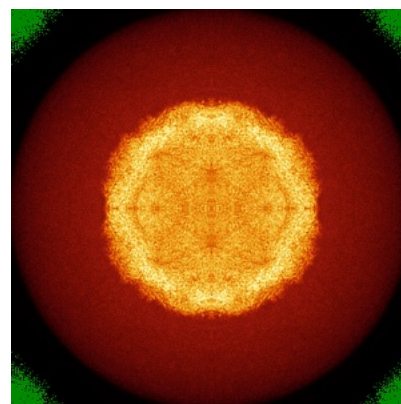
6.4.1 Primary map



X

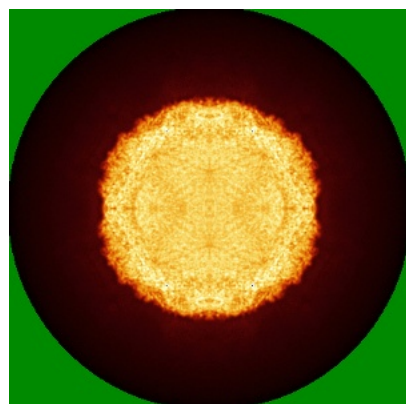


Y

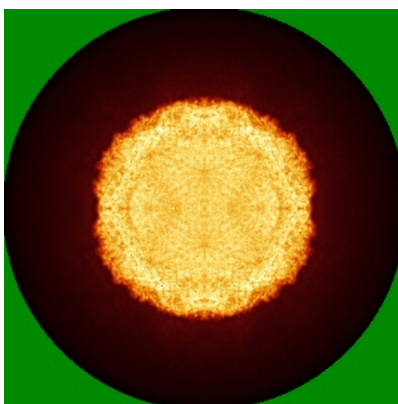


Z

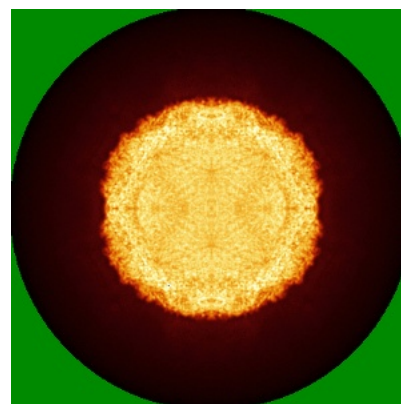
6.4.2 Raw map



X



Y

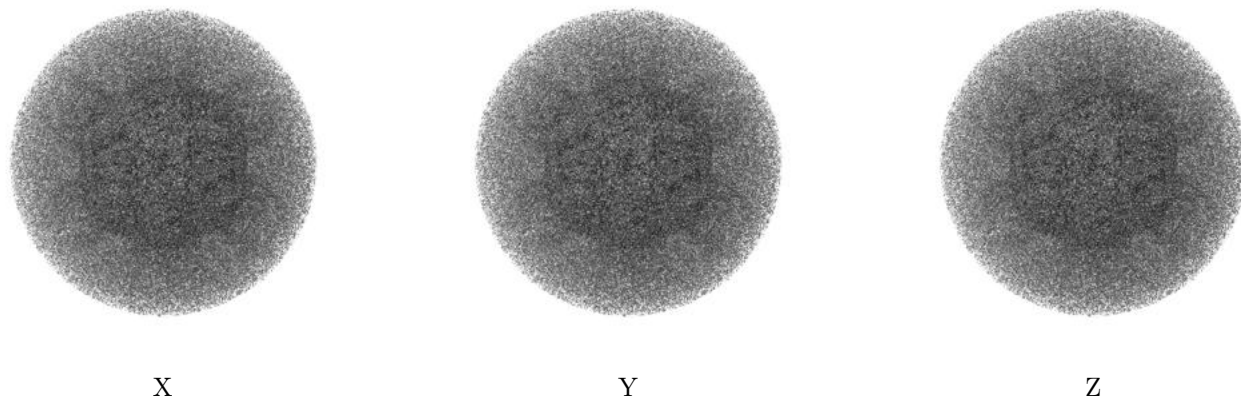


Z

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.

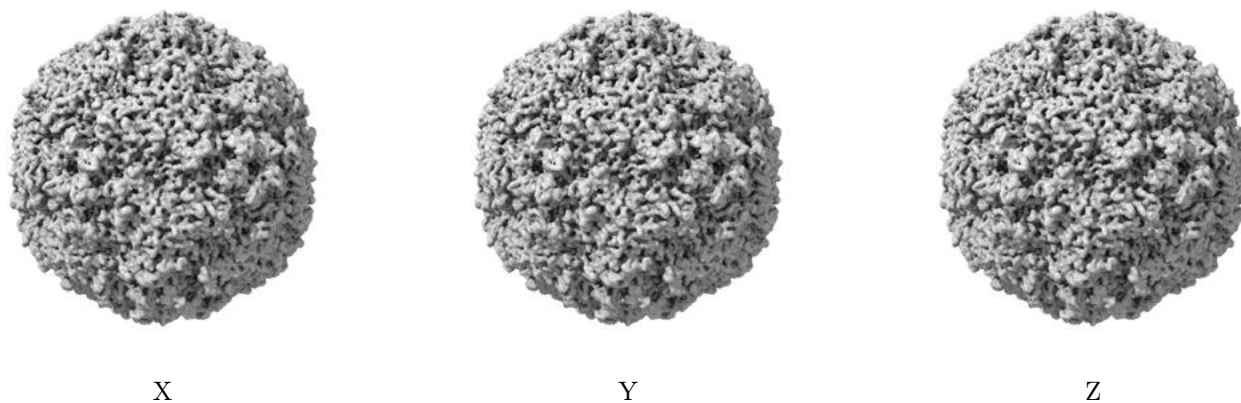
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. 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.

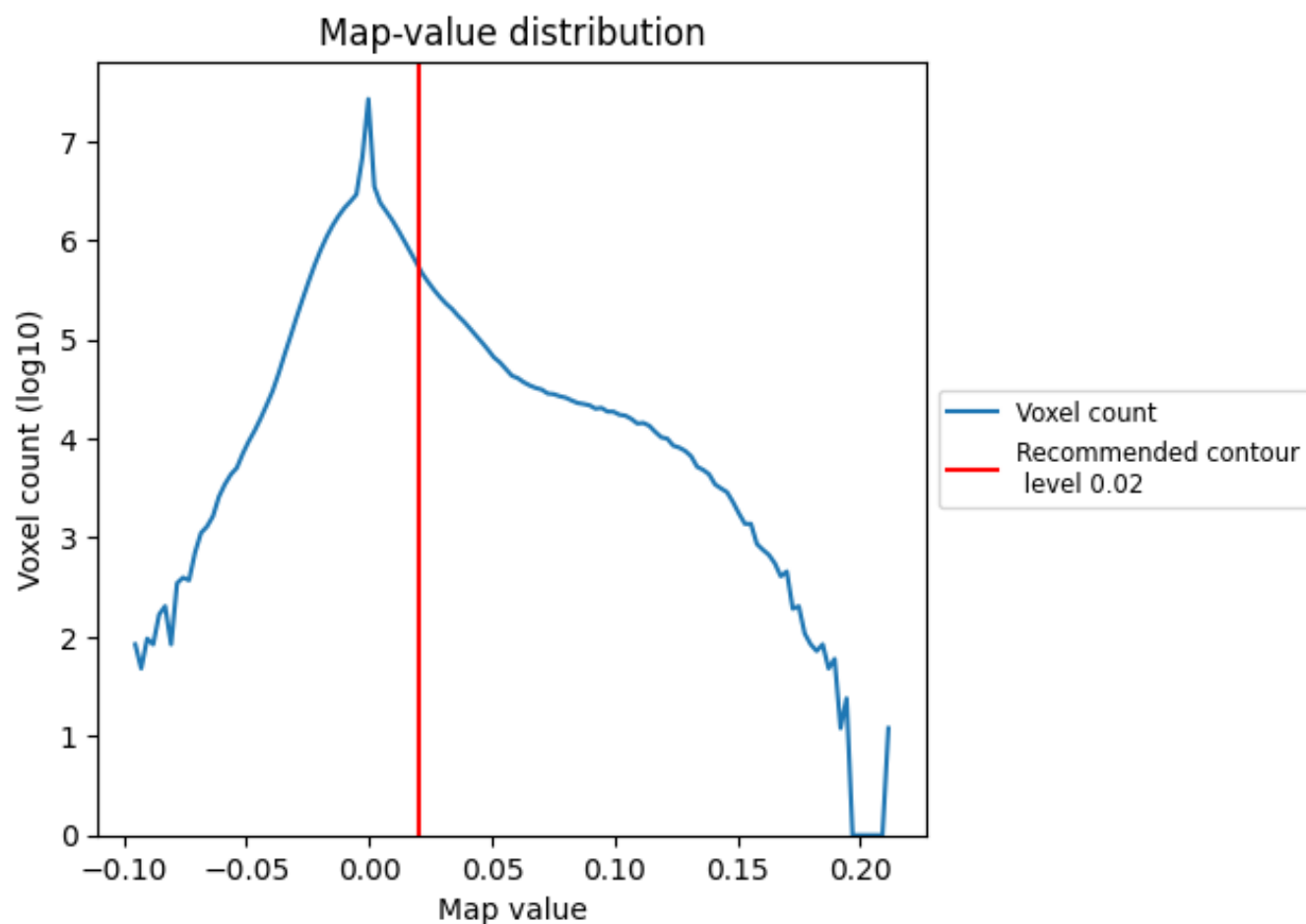
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

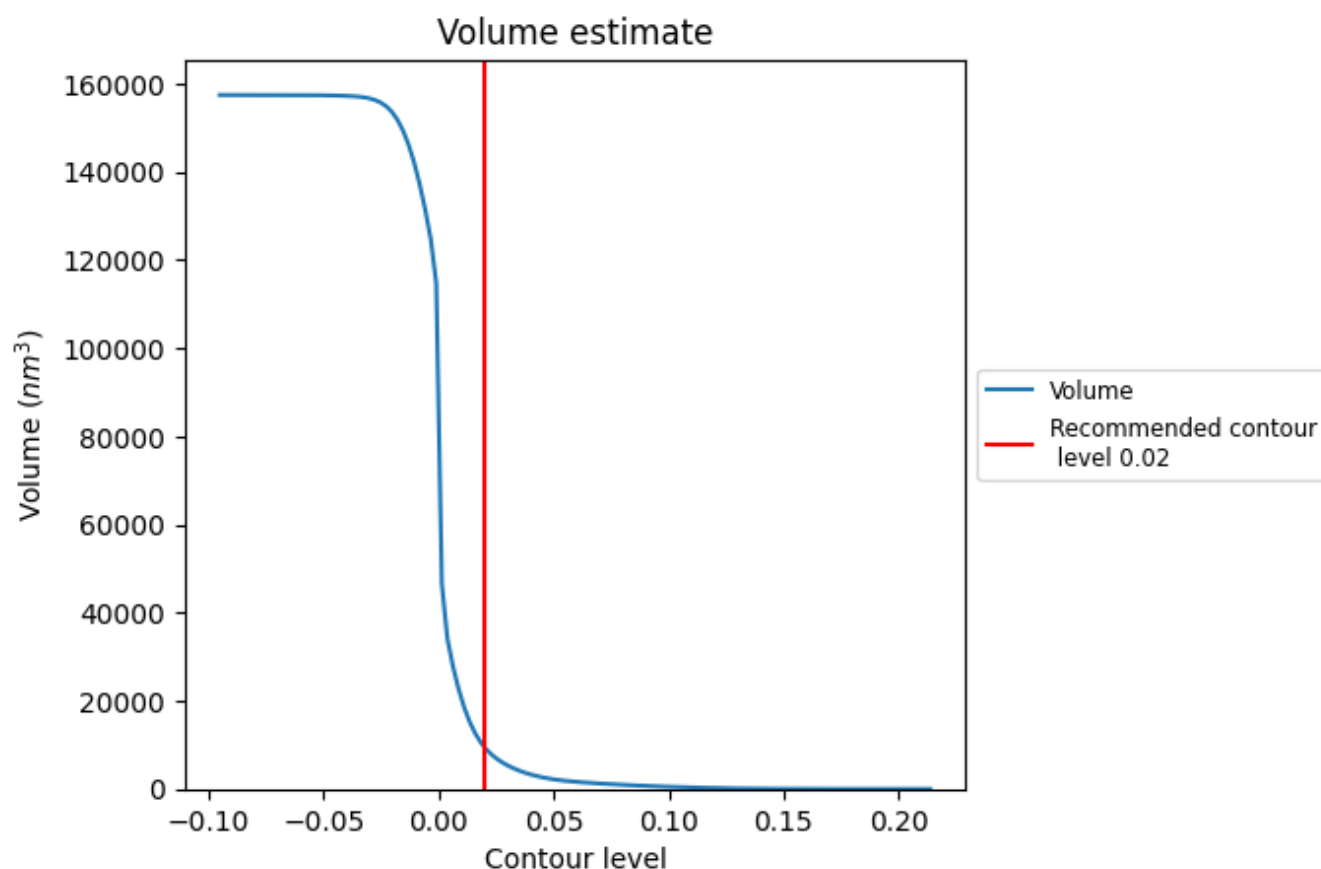
This section contains the results of statistical analysis of the map.

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.

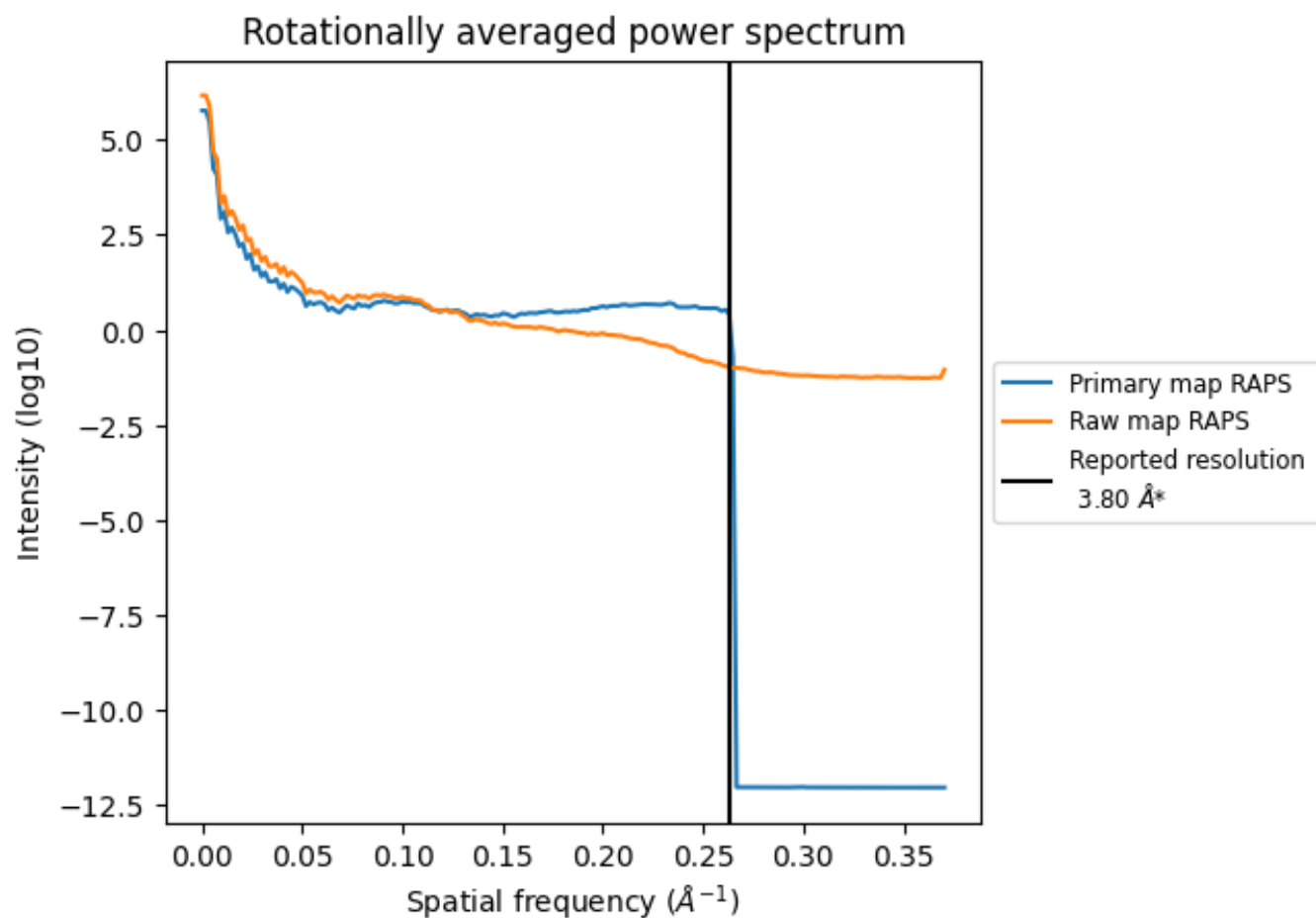
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 9448 nm³; this corresponds to an approximate mass of 8535 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 ⓘ

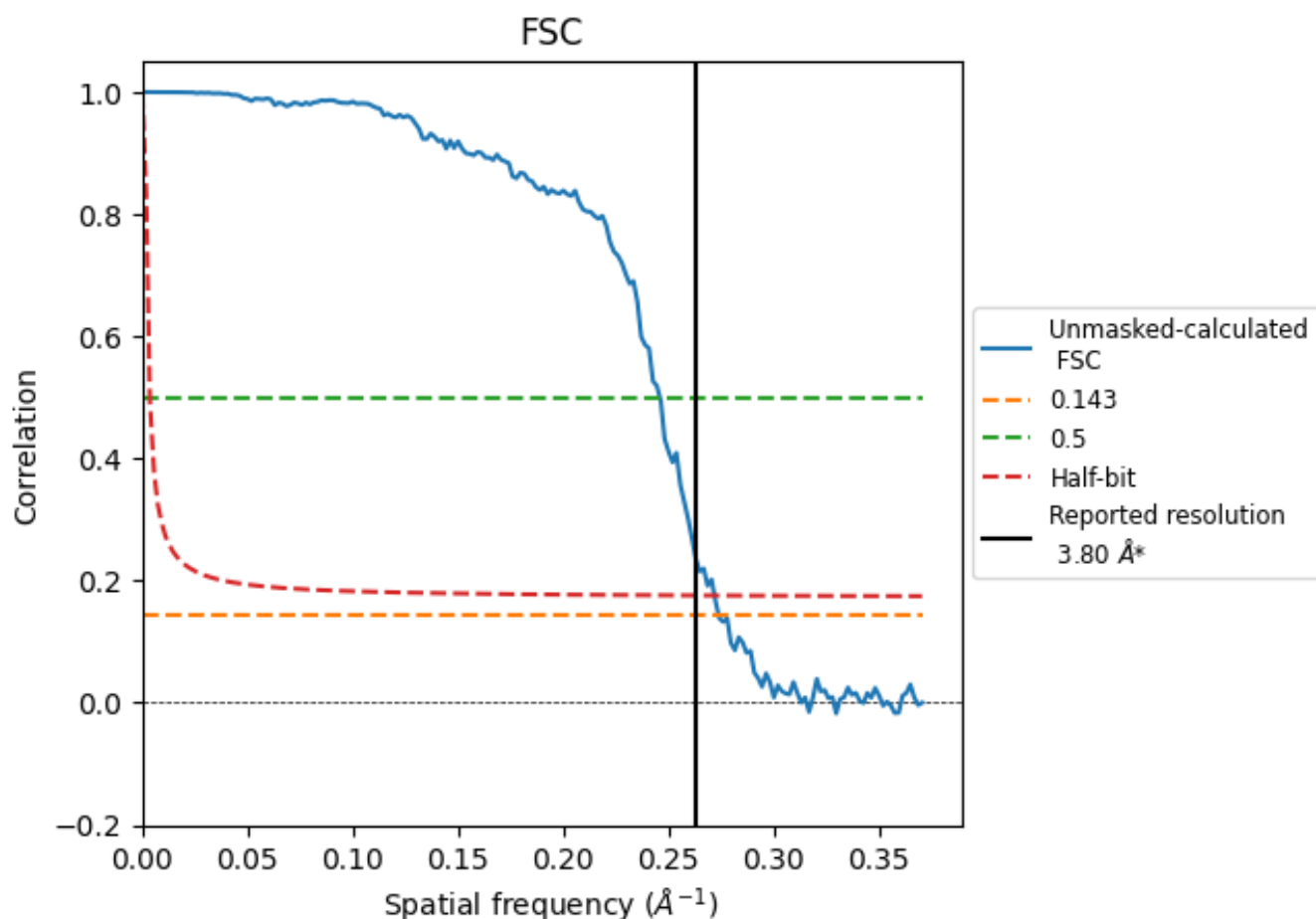


*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

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 0.263 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.65	4.07	3.68

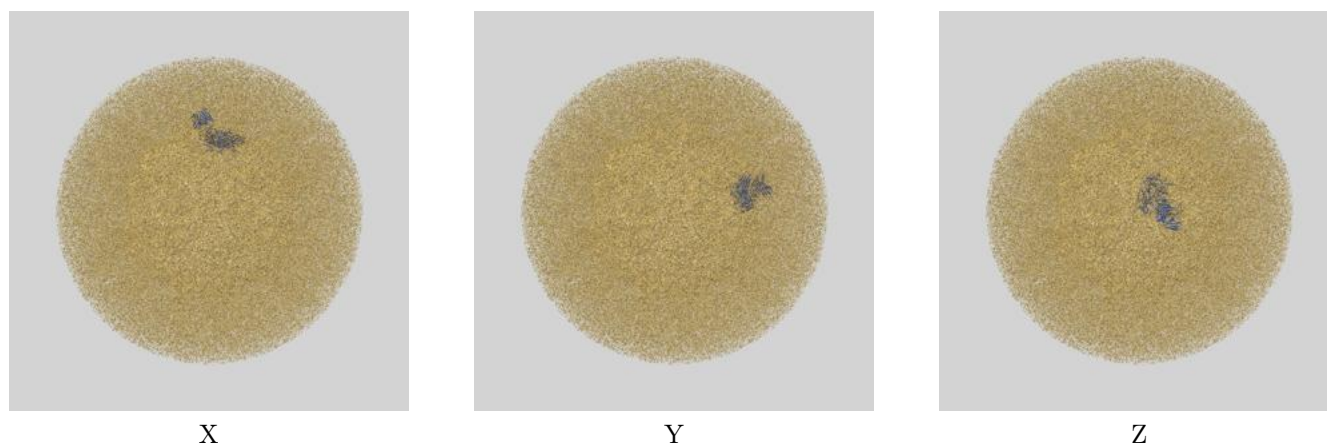
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

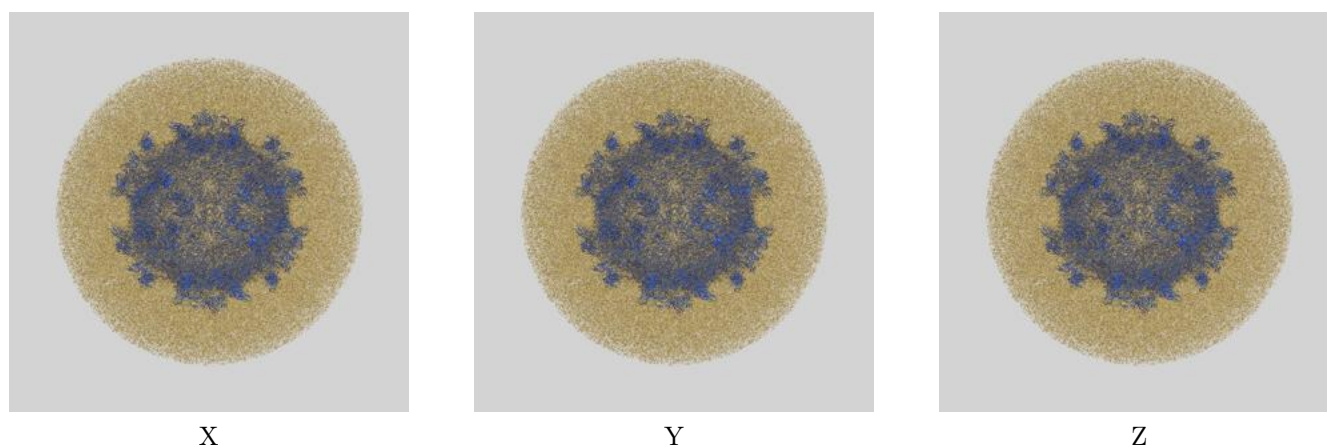
This section contains information regarding the fit between EMDB map EMD-53997 and PDB model 9RIJ. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

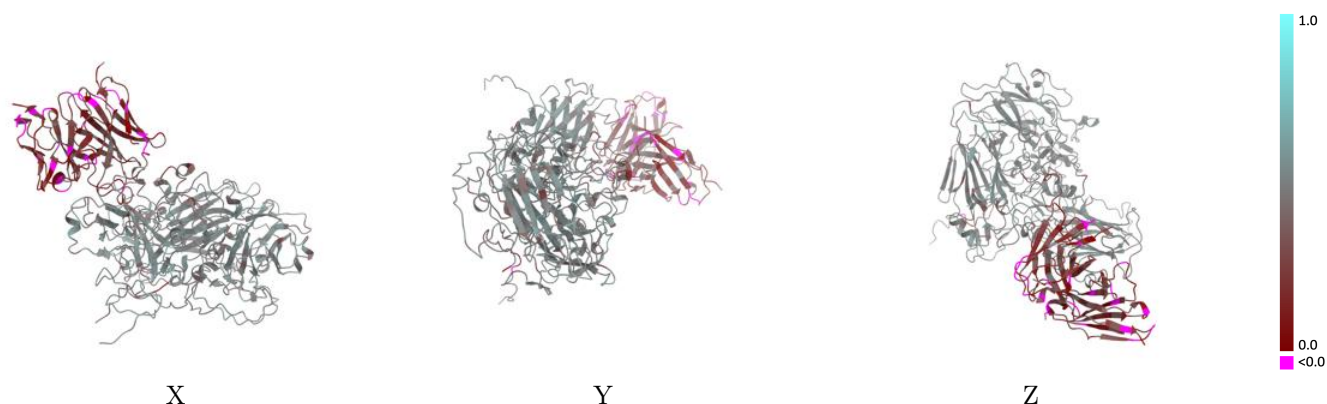


9.1.2 Map-model assembly overlay [i](#)



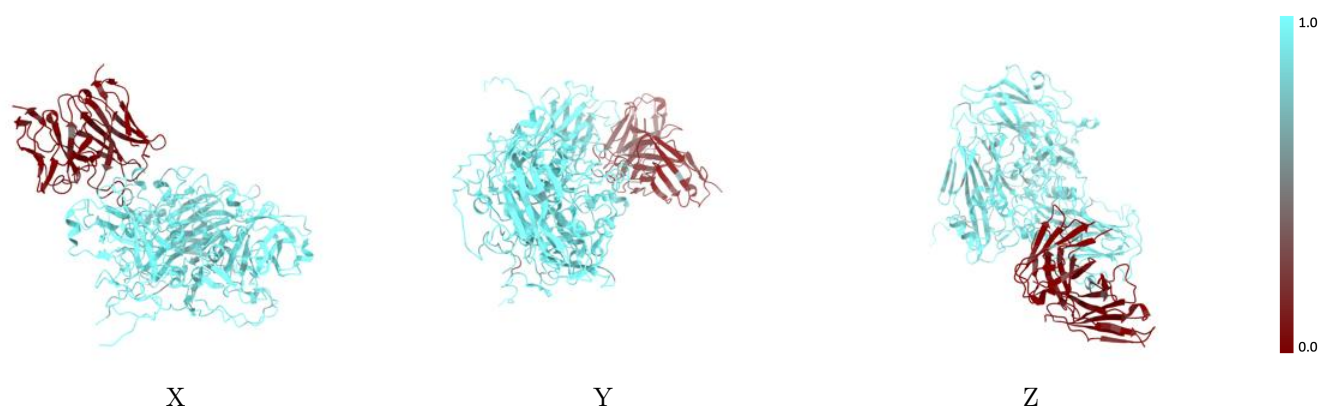
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



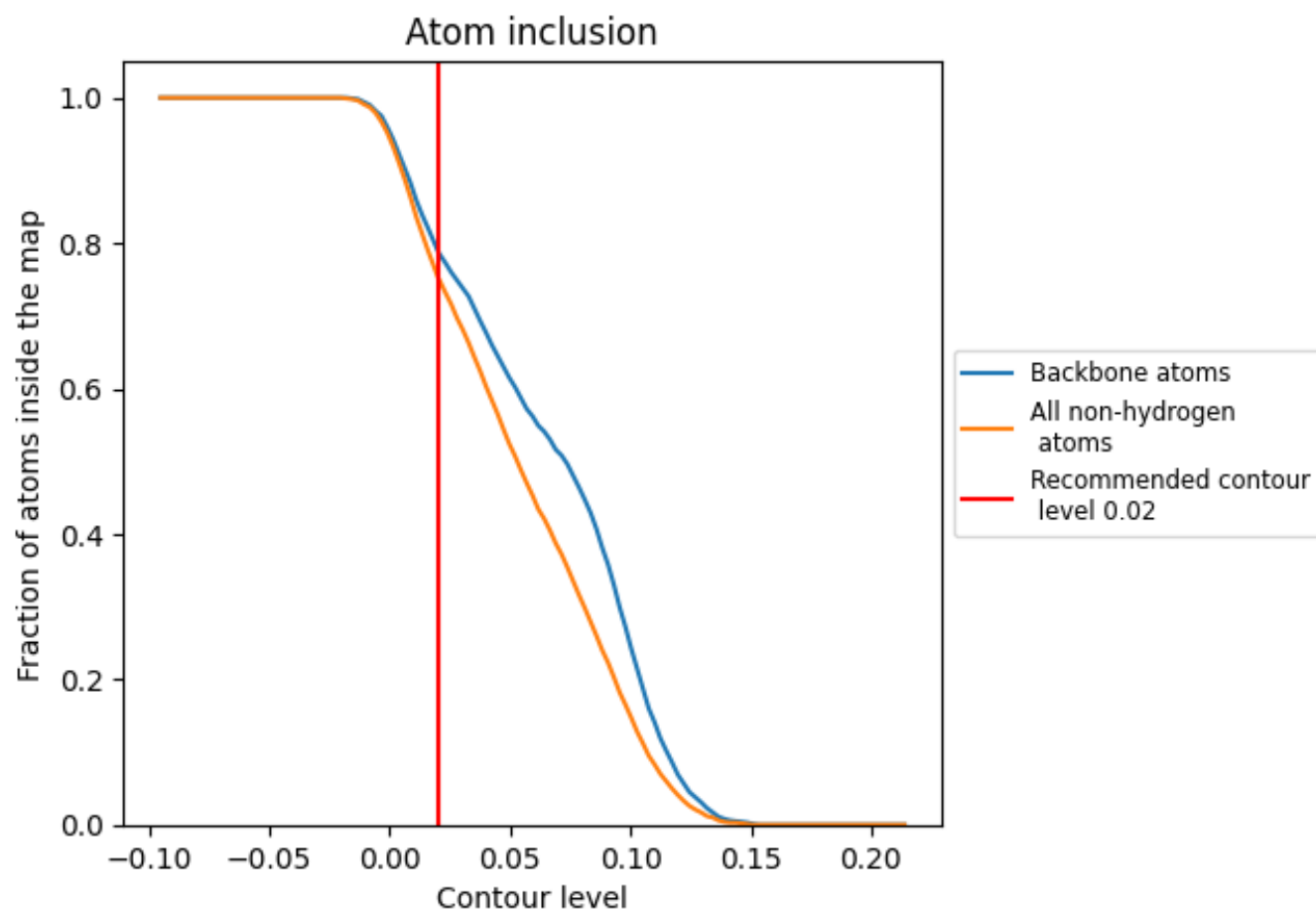
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 75% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7530	<div></div> 0.4230
A	<div></div> 0.9400	<div></div> 0.4840
B	<div></div> 0.9390	<div></div> 0.4850
C	<div></div> 0.9580	<div></div> 0.4930
D	<div></div> 0.9040	<div></div> 0.4580
H	<div></div> 0.0980	<div></div> 0.2090
L	<div></div> 0.0600	<div></div> 0.1940

1.0

0.0

<0.0