



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 12:23 AM UTC

PDB ID : 8Z6X / pdb_00008z6x
EMDB ID : EMD-39807
Title : Structure of EG.5.1 RBD in complex with antibody CYFN1006-2.
Authors : Wang, Y.J.; Sun, L.
Deposited on : 2024-04-19
Resolution : 2.96 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
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

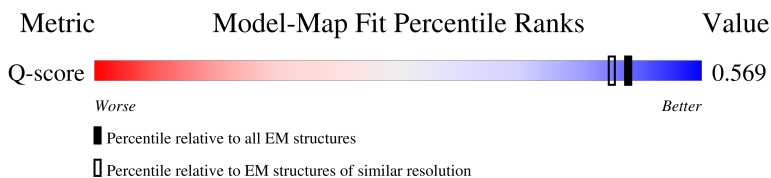
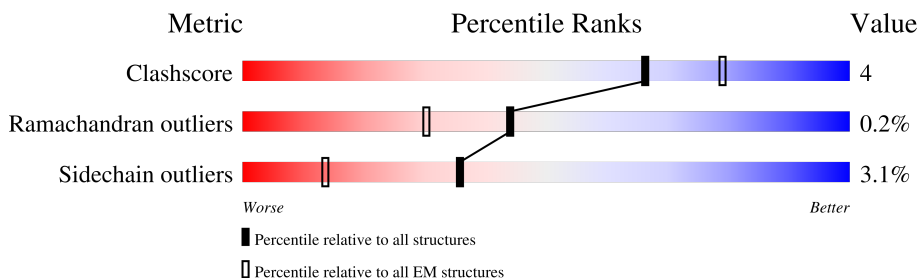
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.96 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	13155 (2.46 - 3.46)

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	1295	
2	C	215	
3	B	451	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4704 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,Fibritin,Expression Tag.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	196	Total	C	N	O	S	0	0
			1553	1001	261	283	8		

There are 79 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	initiating methionine	UNP P0DTC2
A	-5	PRO	-	expression tag	UNP P0DTC2
A	-4	MET	-	expression tag	UNP P0DTC2
A	-3	GLY	-	expression tag	UNP P0DTC2
A	-2	SER	-	expression tag	UNP P0DTC2
A	-1	LEU	-	expression tag	UNP P0DTC2
A	0	GLN	-	expression tag	UNP P0DTC2
A	1	PRO	-	expression tag	UNP P0DTC2
A	2	LEU	-	expression tag	UNP P0DTC2
A	3	ALA	-	expression tag	UNP P0DTC2
A	4	THR	-	expression tag	UNP P0DTC2
A	5	LEU	-	expression tag	UNP P0DTC2
A	6	TYR	-	expression tag	UNP P0DTC2
A	7	LEU	-	expression tag	UNP P0DTC2
A	8	LEU	-	expression tag	UNP P0DTC2
A	9	GLY	-	expression tag	UNP P0DTC2
A	10	MET	-	expression tag	UNP P0DTC2
A	11	LEU	-	expression tag	UNP P0DTC2
A	12	VAL	-	expression tag	UNP P0DTC2
A	13	ALA	-	expression tag	UNP P0DTC2
A	14	SER	-	expression tag	UNP P0DTC2
A	15	VAL	-	expression tag	UNP P0DTC2
A	16	LEU	-	expression tag	UNP P0DTC2
A	17	ALA	-	expression tag	UNP P0DTC2
A	23	ILE	THR	variant	UNP P0DTC2
A	?	-	LEU	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	28	SER	ALA	variant	UNP P0DTC2
A	53	HIS	GLN	variant	UNP P0DTC2
A	84	ALA	VAL	variant	UNP P0DTC2
A	143	ASP	GLY	variant	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	146	GLN	HIS	variant	UNP P0DTC2
A	183	GLU	GLN	variant	UNP P0DTC2
A	213	GLU	VAL	variant	UNP P0DTC2
A	252	VAL	GLY	variant	UNP P0DTC2
A	339	HIS	GLY	variant	UNP P0DTC2
A	346	THR	ARG	variant	UNP P0DTC2
A	368	ILE	LEU	variant	UNP P0DTC2
A	371	PHE	SER	variant	UNP P0DTC2
A	373	PRO	SER	variant	UNP P0DTC2
A	375	PHE	SER	variant	UNP P0DTC2
A	376	ALA	THR	variant	UNP P0DTC2
A	405	ASN	ASP	variant	UNP P0DTC2
A	408	SER	ARG	variant	UNP P0DTC2
A	417	ASN	LYS	variant	UNP P0DTC2
A	440	LYS	ASN	conflict	UNP P0DTC2
A	445	PRO	VAL	variant	UNP P0DTC2
A	446	SER	GLY	variant	UNP P0DTC2
A	456	LEU	PHE	variant	UNP P0DTC2
A	460	LYS	ASN	variant	UNP P0DTC2
A	477	ASN	SER	variant	UNP P0DTC2
A	478	LYS	THR	variant	UNP P0DTC2
A	484	ALA	GLU	variant	UNP P0DTC2
A	486	PRO	PHE	variant	UNP P0DTC2
A	490	SER	PHE	variant	UNP P0DTC2
A	498	ARG	GLN	variant	UNP P0DTC2
A	501	TYR	ASN	variant	UNP P0DTC2
A	505	HIS	TYR	variant	UNP P0DTC2
A	614	GLY	ASP	variant	UNP P0DTC2
A	655	TYR	HIS	variant	UNP P0DTC2
A	679	LYS	ASN	variant	UNP P0DTC2
A	681	HIS	PRO	variant	UNP P0DTC2
A	682	GLY	ARG	conflict	UNP P0DTC2
A	683	SER	ARG	conflict	UNP P0DTC2
A	685	SER	ARG	conflict	UNP P0DTC2
A	764	LYS	ASN	variant	UNP P0DTC2
A	796	TYR	ASP	variant	UNP P0DTC2
A	817	PRO	PHE	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	892	PRO	ALA	conflict	UNP P0DTC2
A	899	PRO	ALA	conflict	UNP P0DTC2
A	942	PRO	ALA	conflict	UNP P0DTC2
A	954	HIS	GLN	variant	UNP P0DTC2
A	969	LYS	ASN	variant	UNP P0DTC2
A	986	PRO	LYS	variant	UNP P0DTC2
A	987	PRO	VAL	variant	UNP P0DTC2
A	1209	GLY	-	linker	UNP P0DTC2
A	1210	SER	-	linker	UNP P0DTC2

- Molecule 2 is a protein called CYFN1006-2 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	203	Total	C	N	O	S	0	0
			1502	938	251	306	7		

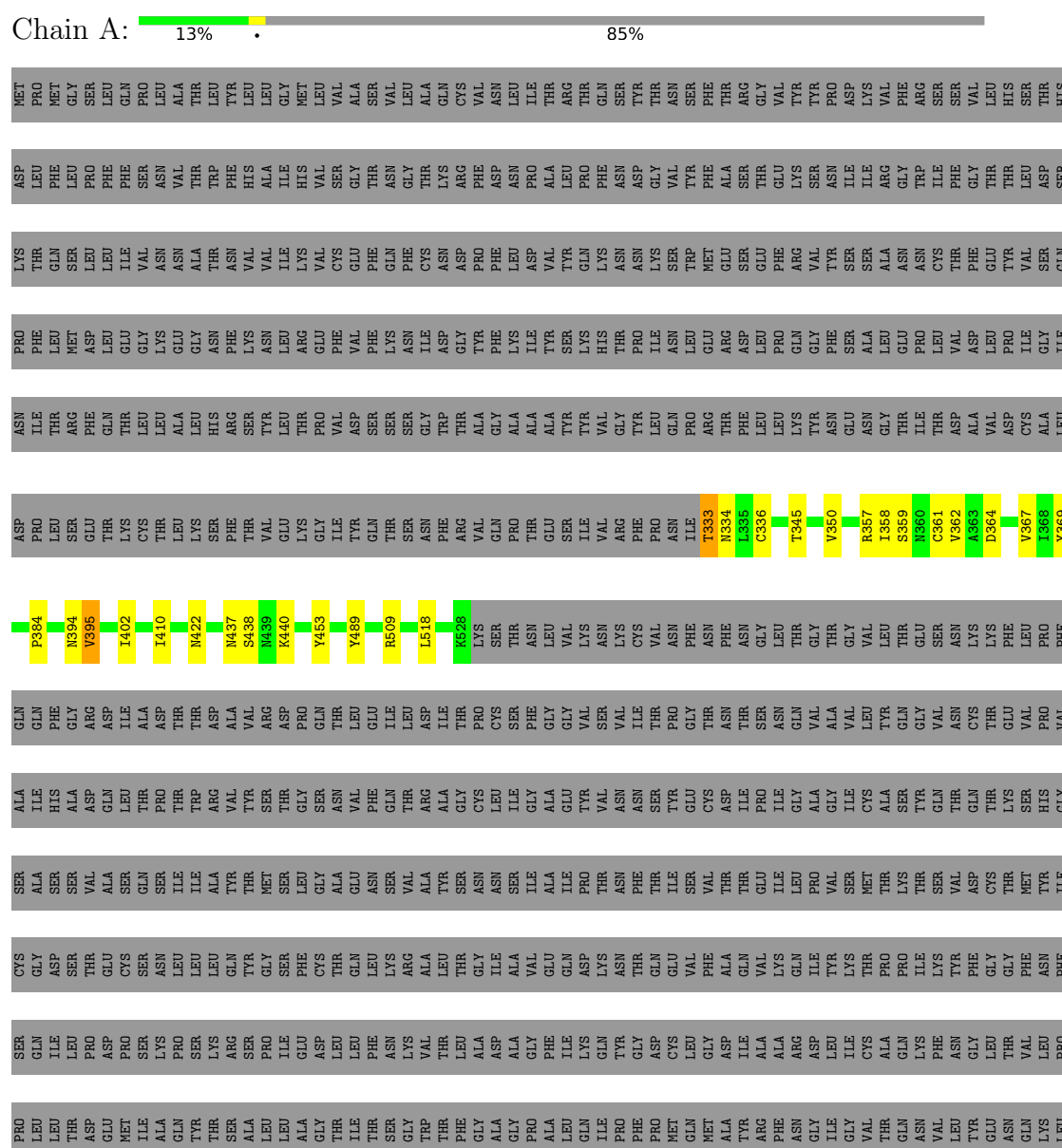
- Molecule 3 is a protein called CYFN1006-2 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	219	Total	C	N	O	S	0	0
			1649	1052	269	320	8		

3 Residue-property plots

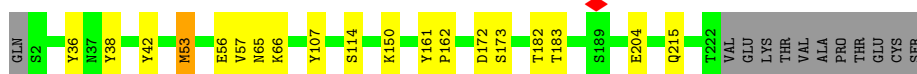
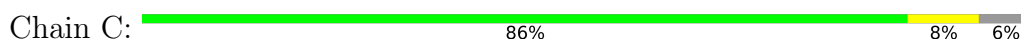
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Spike glycoprotein,Fibritin,Expression Tag

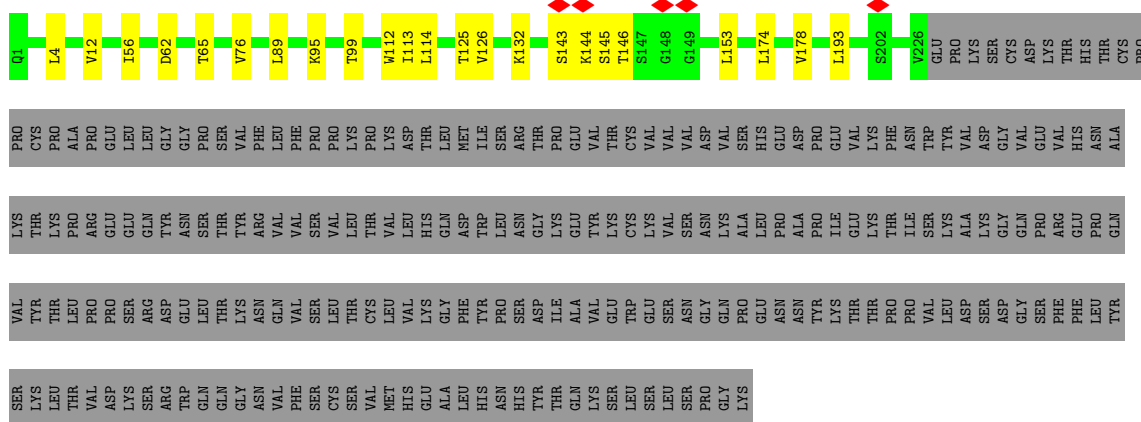


HIS	HIS	TYP	ASP	PHE	CYS	ARG	ILE
	HIS	VAL	VAL	VAL	GLY	LEU	ALA
	HIS	ARG	ASP	THR	LYS	ASN	ASN
	HIS	LYS	GLY	GLN	GLY	PRO	GLN
	HIS	ASP	LEU	ARG	TYR	THR	PHE
HIS	GLY	ASP	ASP	ASN	HIS	GLU	ASN
	GLU	ILE	ILE	PHE	LEU	ALA	SER
	TRP	SER	SER	TYR	MET	GLU	ALA
	VAL	GLY	ILE	GLU	PHE	VAL	ILE
	PHE	ILE	GLY	PRO	SER	GLN	GLY
HIS	LEU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

- Molecule 2: CYFN1006-2 light chain



- Molecule 3: CYFN1006-2 heavy chain



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	244940	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	16.377	Depositor
Minimum map value	-0.140	Depositor
Average map value	-0.031	Depositor
Map value standard deviation	0.144	Depositor
Recommended contour level	2.5	Depositor
Map size (Å)	571.2, 571.2, 571.2	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.19, 1.19, 1.19	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	0.11	0/1601	0.26	0/2182
2	C	0.18	0/1540	0.35	1/2101 (0.0%)
3	B	0.16	0/1694	0.31	0/2307
All	All	0.15	0/4835	0.31	1/6590 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	38	TYR	N-CA-C	-6.15	97.70	110.80

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	1553	0	1488	17	0
2	C	1502	0	1445	10	0
3	B	1649	0	1618	13	0
All	All	4704	0	4551	36	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 4.

The worst 5 of 36 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:B:56:ILE:HG22	3:B:65:THR:HG22	1.64	0.80
1:A:333:THR:OG1	1:A:334:ASN:N	2.27	0.67
2:C:56:GLU:O	2:C:66:LYS:N	2.31	0.63
1:A:334:ASN:O	1:A:362:VAL:HG22	1.97	0.63
2:C:204:GLU:N	2:C:204:GLU:OE1	2.35	0.59

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	194/1295 (15%)	185 (95%)	9 (5%)	0	100	100
2	C	201/215 (94%)	185 (92%)	15 (8%)	1 (0%)	24	49
3	B	217/451 (48%)	197 (91%)	20 (9%)	0	100	100
All	All	612/1961 (31%)	567 (93%)	44 (7%)	1 (0%)	44	66

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	57	VAL

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	169/1118 (15%)	163 (96%)	6 (4%)	31	56
2	C	168/179 (94%)	164 (98%)	4 (2%)	43	67
3	B	184/399 (46%)	178 (97%)	6 (3%)	33	58
All	All	521/1696 (31%)	505 (97%)	16 (3%)	36	59

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	B	146	THR
3	B	145	SER
2	C	150	LYS
3	B	144	LYS
2	C	53	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
3	B	120	GLN
3	B	186	GLN
2	C	45	HIS
2	C	209	HIS
3	B	44	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 [i](#)

There are no chain breaks in this entry.

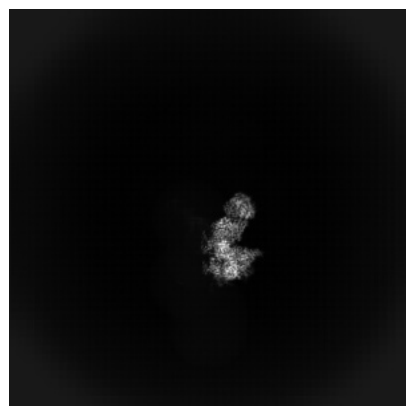
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39807. These allow visual inspection of the internal detail of the map and identification of artifacts.

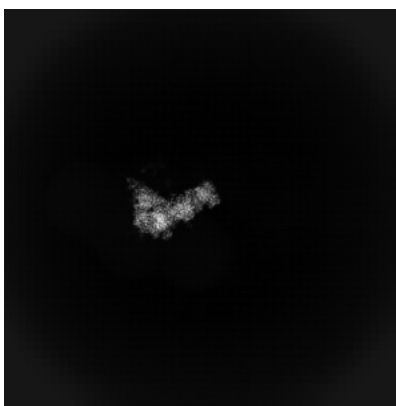
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

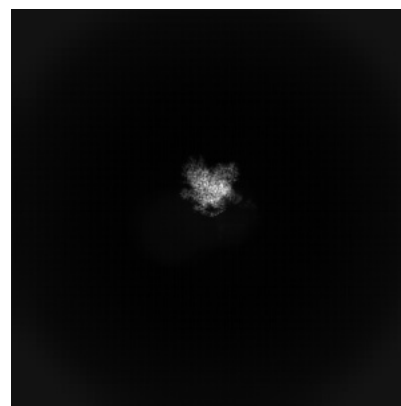
6.1.1 Primary map



X

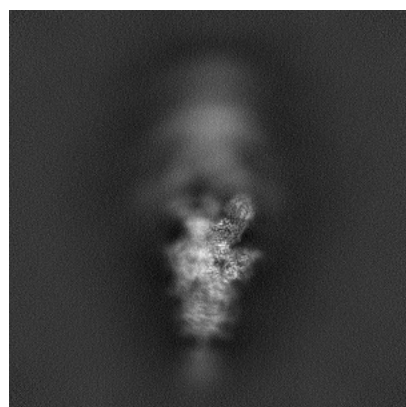


Y

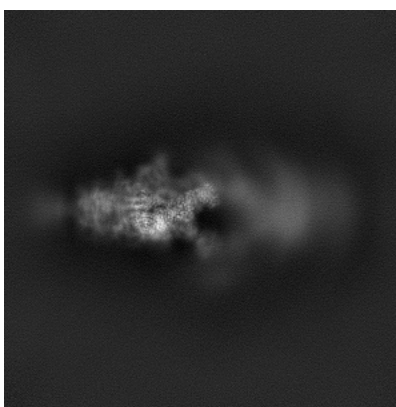


Z

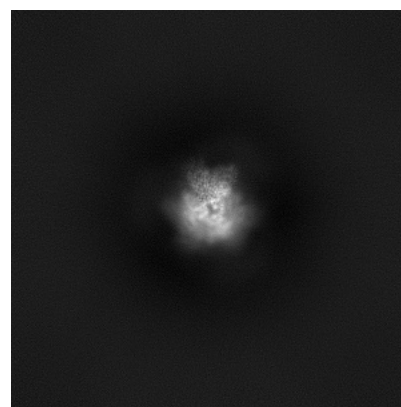
6.1.2 Raw map



X



Y

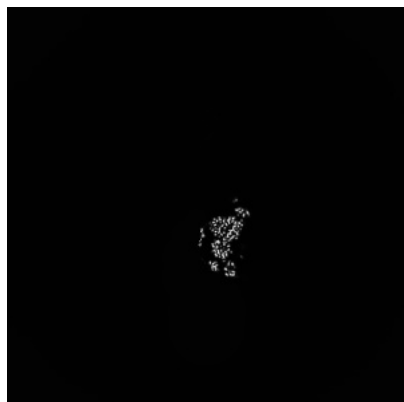


Z

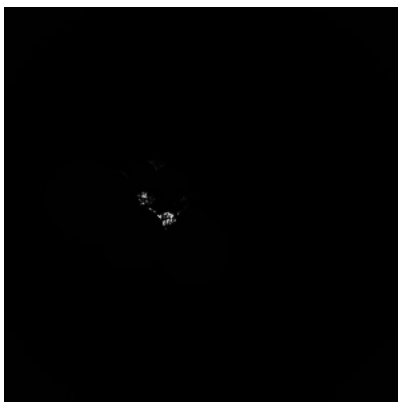
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

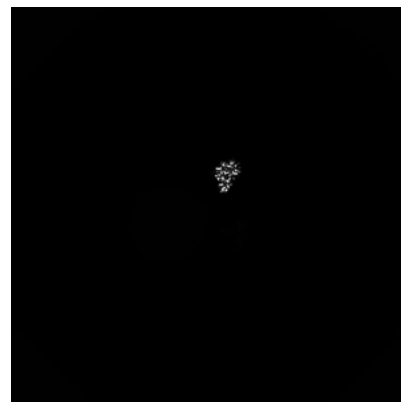
6.2.1 Primary map



X Index: 240

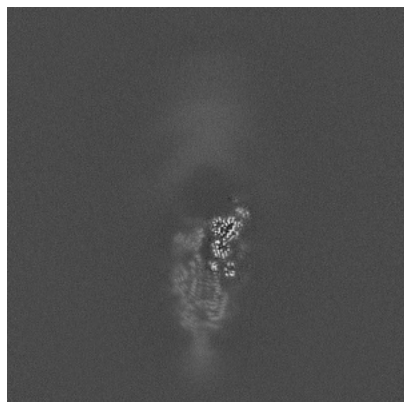


Y Index: 240

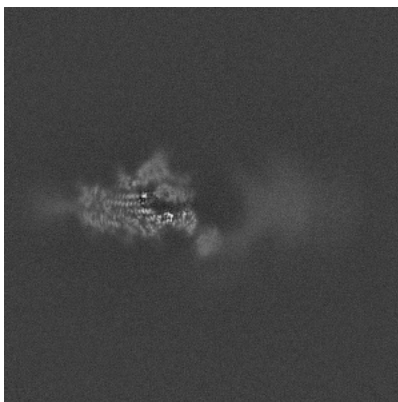


Z Index: 240

6.2.2 Raw map



X Index: 240



Y Index: 240

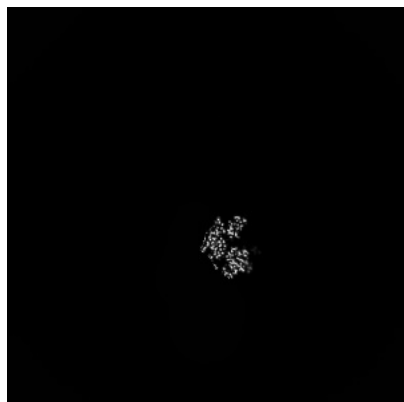


Z Index: 240

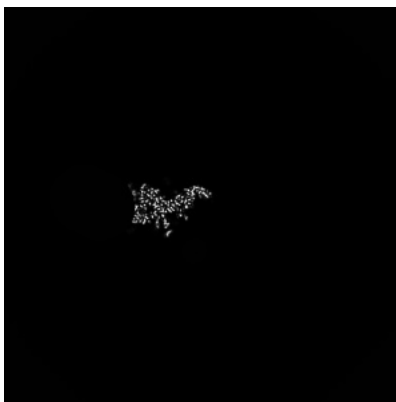
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 232

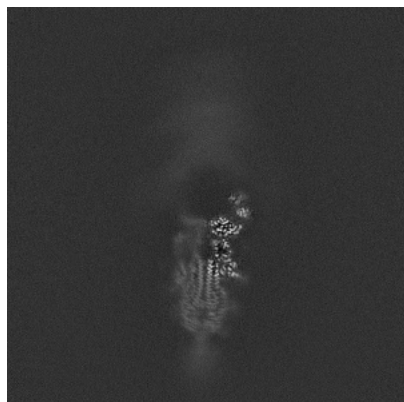


Y Index: 263

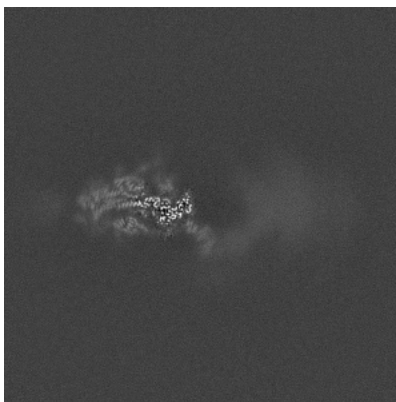


Z Index: 184

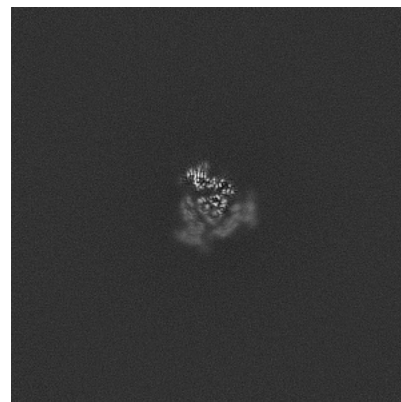
6.3.2 Raw map



X Index: 244



Y Index: 251

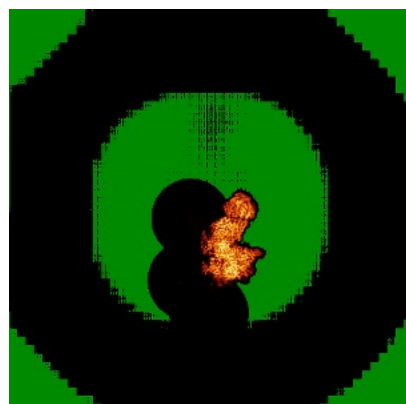


Z Index: 170

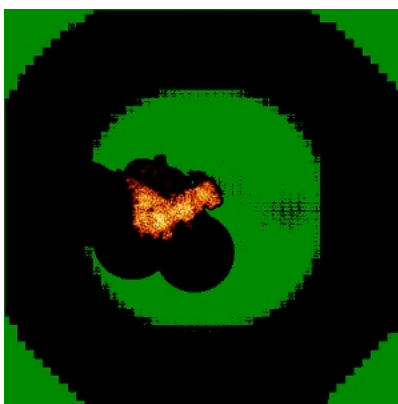
The images above show the largest variance slices of the map in three orthogonal directions.

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

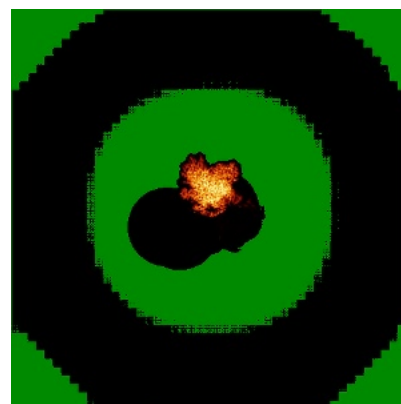
6.4.1 Primary map



X

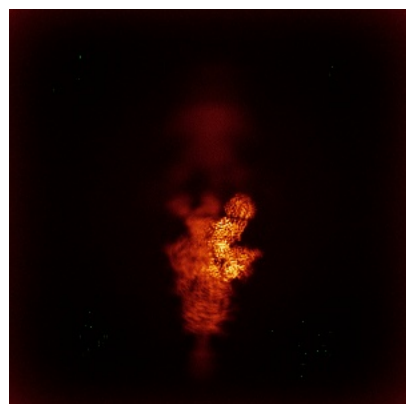


Y

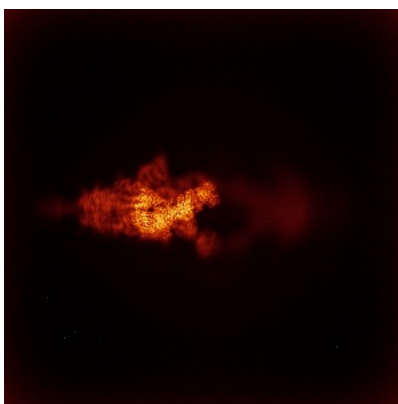


Z

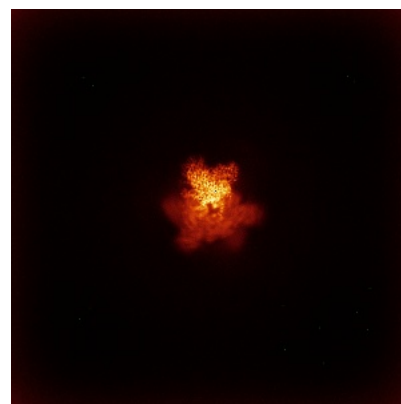
6.4.2 Raw map



X



Y

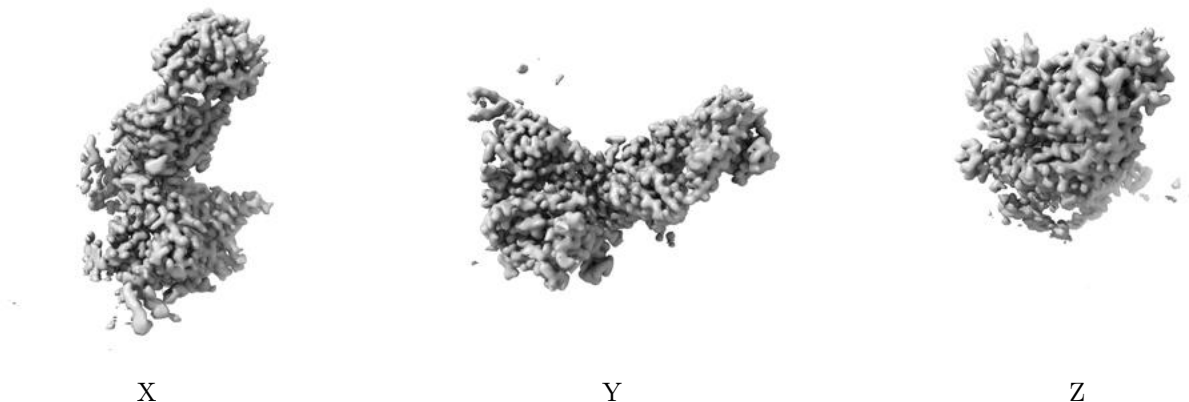


Z

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

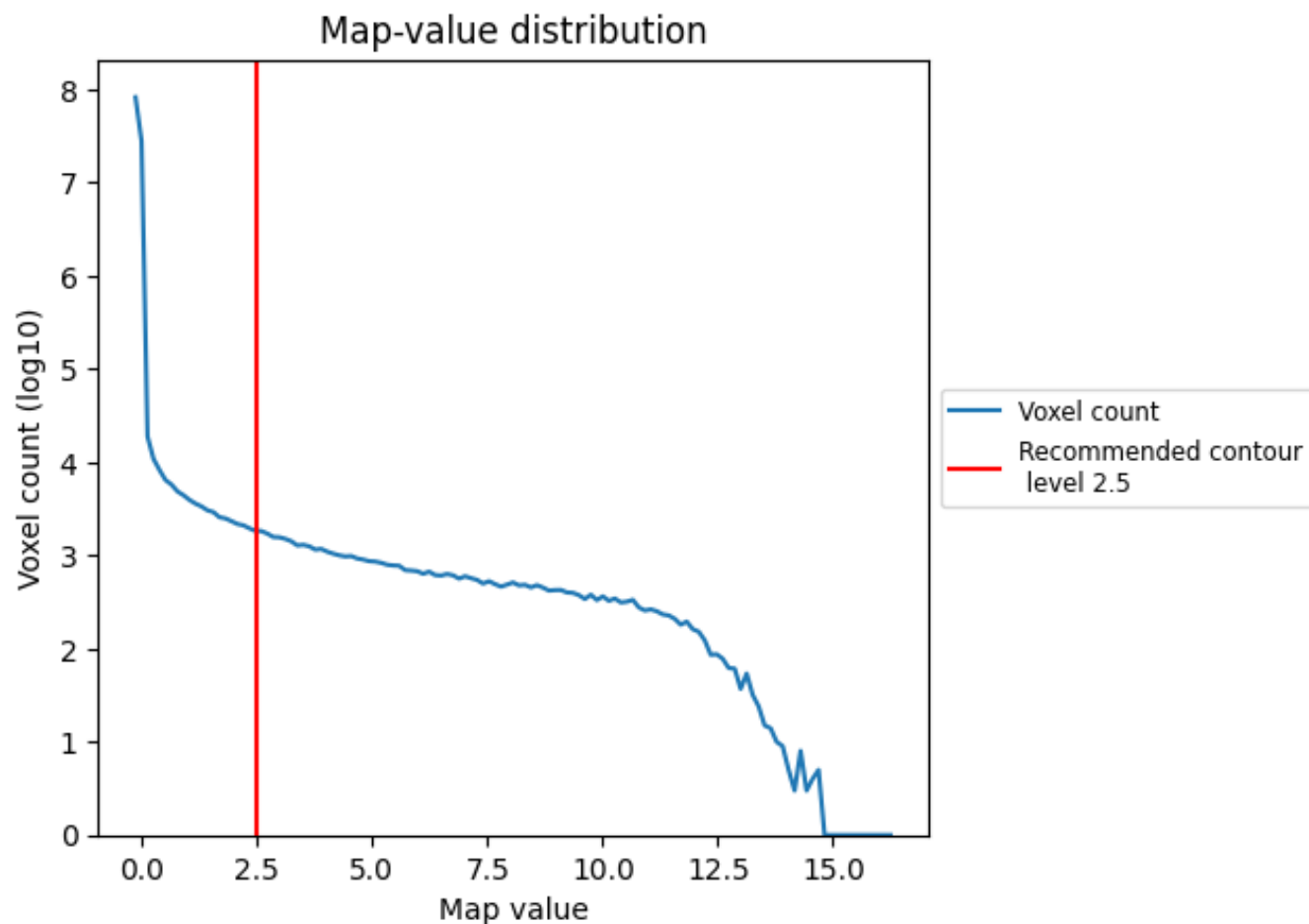
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

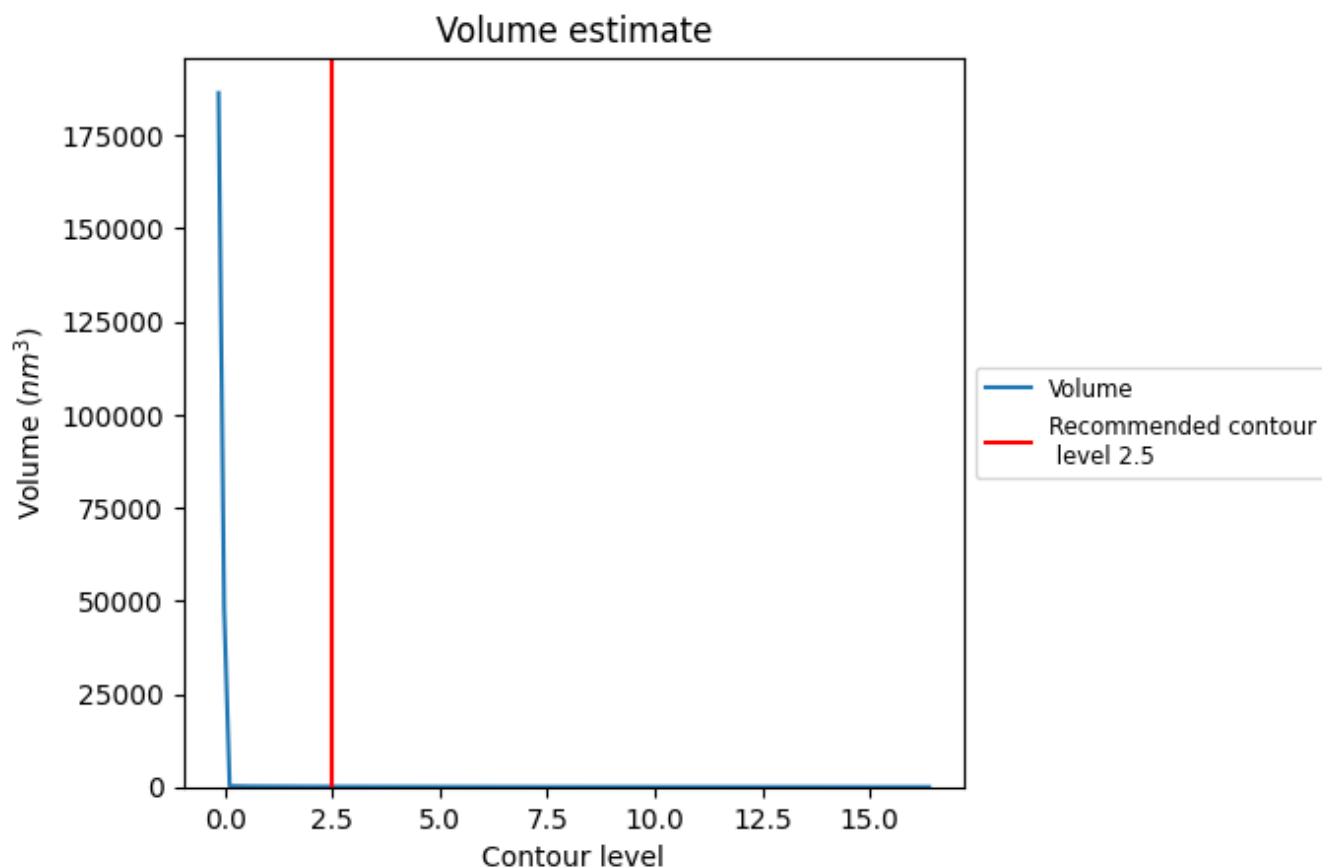
This section contains the results of statistical analysis of the map.

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.

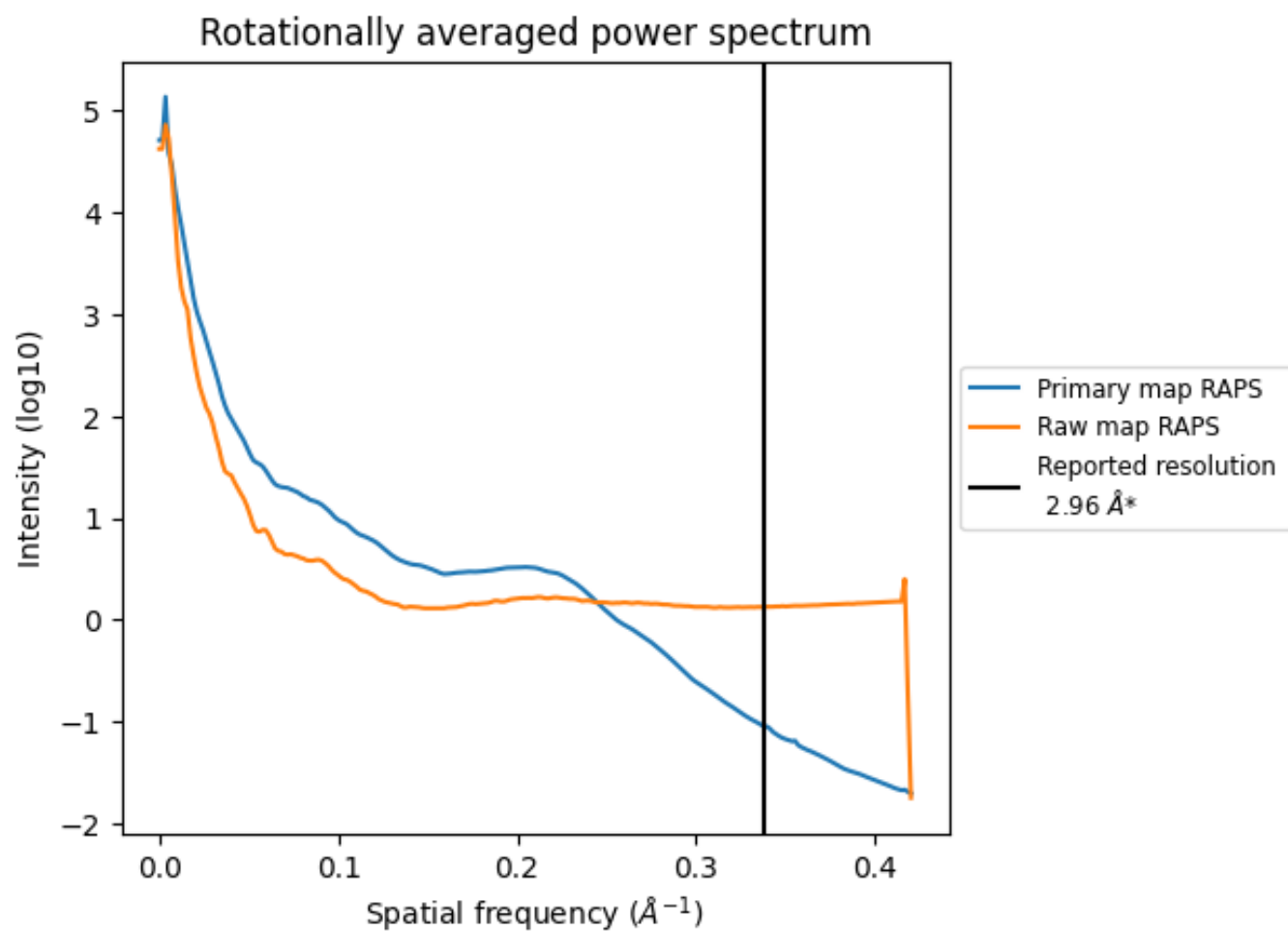
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 86 nm^3 ; this corresponds to an approximate mass of 78 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 ⓘ

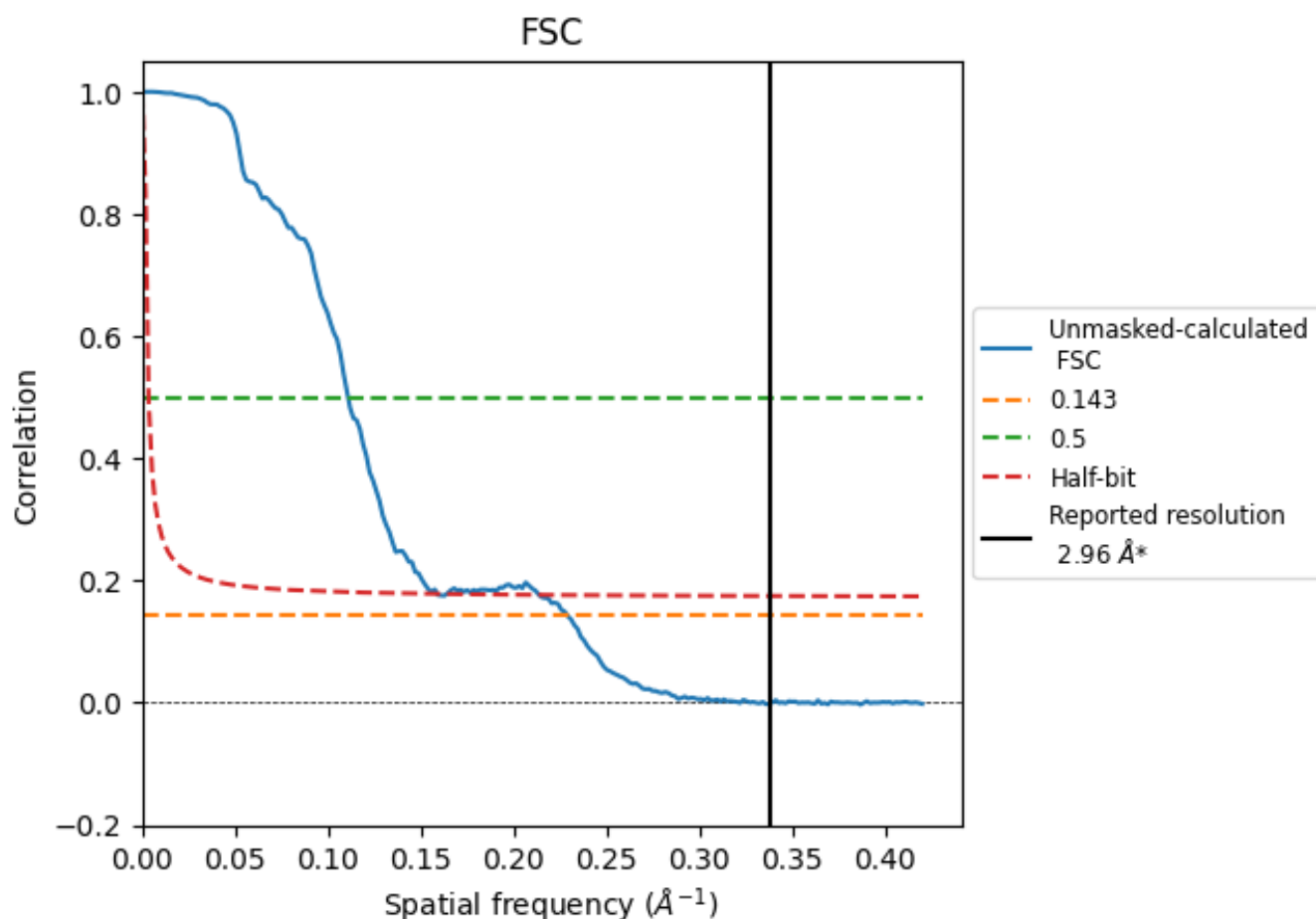


*Reported resolution corresponds to spatial frequency of 0.338 Å⁻¹

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 0.338 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.96	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.37	9.02	6.29

*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 4.37 differs from the reported value 2.96 by more than 10 %

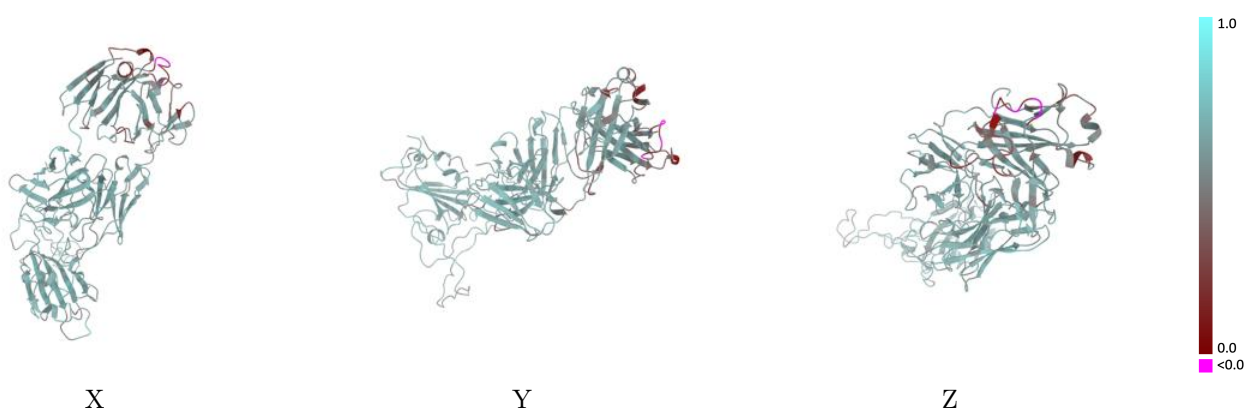
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-39807 and PDB model 8Z6X. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)

This section was not generated.

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

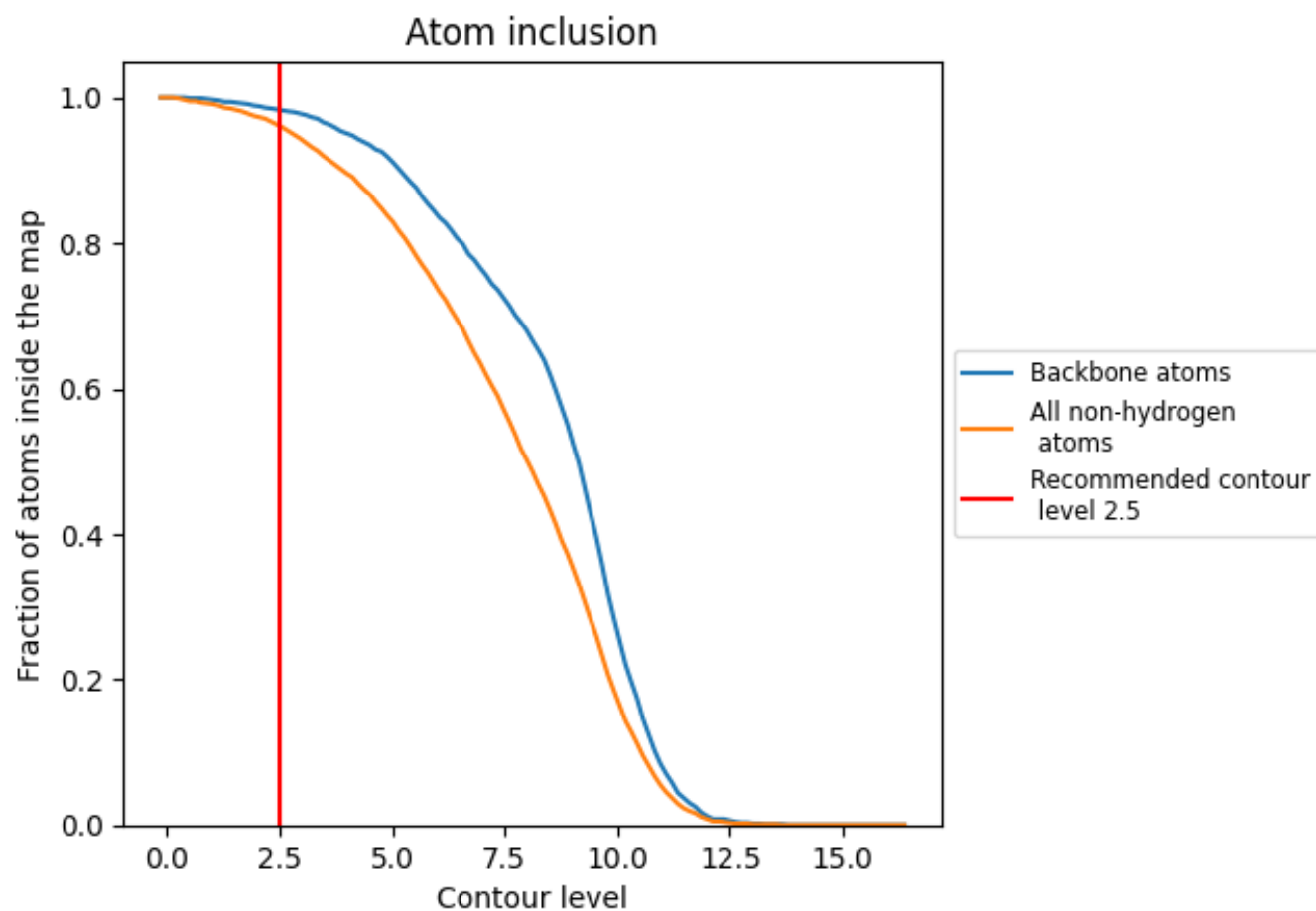


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 96% 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 (2.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9610	0.5690
A	0.9770	0.5980
B	0.9520	0.5640
C	0.9530	0.5440

