



Full wwPDB EM Validation Report ⓘ

Aug 30, 2026 – 12:35 am BST

PDB ID : 9SHV / pdb_00009shv
EMDB ID : EMD-54916
Title : Prefusion-stabilized Hendra virus fusion protein in complex with inhibitory nanobody F123
Authors : Kralova, A.; Hanke, L.
Deposited on : 2025-08-28
Resolution : 2.87 Å(reported)
Based on initial model : .

This is a Full wwPDB EM Validation 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:

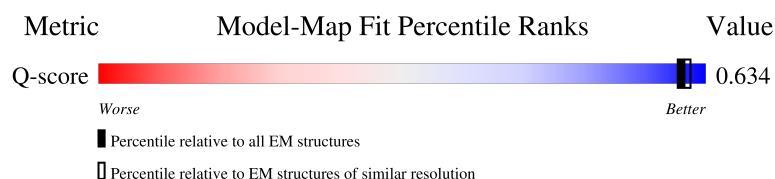
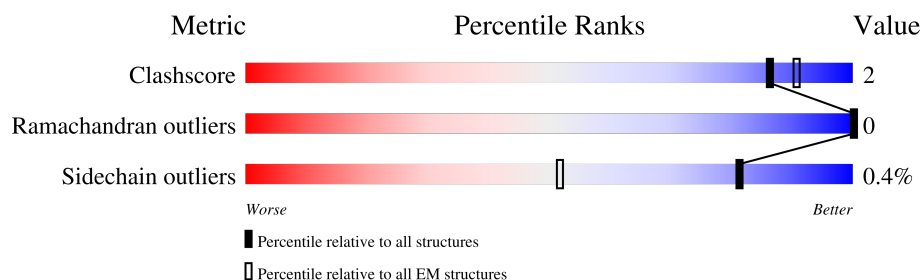
EMDB validation analysis : 0.0.1.dev133
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.87 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	12062 (2.37 - 3.37)

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	Aa	567	
1	Ab	567	
1	Ac	567	
2	Ba	135	

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Mol	Chain	Length	Quality of chain
2	Bb	135	 87% • 11%
2	Bc	135	 84% • 11%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12891 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 Fusion glycoprotein F0.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Aa	441	Total	C	N	O	S	0	0
			3386	2148	550	668	20		
1	Ab	441	Total	C	N	O	S	0	0
			3386	2148	550	668	20		
1	Ac	441	Total	C	N	O	S	0	0
			3386	2148	550	668	20		

There are 252 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Aa	104	CYS	LEU	conflict	UNP O89342
Aa	114	CYS	VAL	conflict	UNP O89342
Aa	172	PHE	LEU	conflict	UNP O89342
Aa	191	PRO	SER	conflict	UNP O89342
Aa	488	MET	-	expression tag	UNP O89342
Aa	489	LYS	-	expression tag	UNP O89342
Aa	490	GLN	-	expression tag	UNP O89342
Aa	491	ILE	-	expression tag	UNP O89342
Aa	492	GLU	-	expression tag	UNP O89342
Aa	493	ASP	-	expression tag	UNP O89342
Aa	494	LYS	-	expression tag	UNP O89342
Aa	495	ILE	-	expression tag	UNP O89342
Aa	496	GLU	-	expression tag	UNP O89342
Aa	497	GLU	-	expression tag	UNP O89342
Aa	498	ILE	-	expression tag	UNP O89342
Aa	499	LEU	-	expression tag	UNP O89342
Aa	500	SER	-	expression tag	UNP O89342
Aa	501	LYS	-	expression tag	UNP O89342
Aa	502	ILE	-	expression tag	UNP O89342
Aa	503	TYR	-	expression tag	UNP O89342
Aa	504	HIS	-	expression tag	UNP O89342
Aa	505	ILE	-	expression tag	UNP O89342
Aa	506	GLU	-	expression tag	UNP O89342
Aa	507	ASN	-	expression tag	UNP O89342

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Chain	Residue	Modelled	Actual	Comment	Reference
Aa	508	GLU	-	expression tag	UNP O89342
Aa	509	ILE	-	expression tag	UNP O89342
Aa	510	ALA	-	expression tag	UNP O89342
Aa	511	ARG	-	expression tag	UNP O89342
Aa	512	ILE	-	expression tag	UNP O89342
Aa	513	LYS	-	expression tag	UNP O89342
Aa	514	LYS	-	expression tag	UNP O89342
Aa	515	LEU	-	expression tag	UNP O89342
Aa	516	ILE	-	expression tag	UNP O89342
Aa	517	GLY	-	expression tag	UNP O89342
Aa	518	GLU	-	expression tag	UNP O89342
Aa	519	ALA	-	expression tag	UNP O89342
Aa	520	PRO	-	expression tag	UNP O89342
Aa	521	GLY	-	expression tag	UNP O89342
Aa	522	GLY	-	expression tag	UNP O89342
Aa	523	ILE	-	expression tag	UNP O89342
Aa	524	GLU	-	expression tag	UNP O89342
Aa	525	GLY	-	expression tag	UNP O89342
Aa	526	ARG	-	expression tag	UNP O89342
Aa	527	LYS	-	expression tag	UNP O89342
Aa	528	LEU	-	expression tag	UNP O89342
Aa	529	HIS	-	expression tag	UNP O89342
Aa	530	HIS	-	expression tag	UNP O89342
Aa	531	HIS	-	expression tag	UNP O89342
Aa	532	HIS	-	expression tag	UNP O89342
Aa	533	HIS	-	expression tag	UNP O89342
Aa	534	HIS	-	expression tag	UNP O89342
Aa	535	HIS	-	expression tag	UNP O89342
Aa	536	HIS	-	expression tag	UNP O89342
Aa	537	SER	-	expression tag	UNP O89342
Aa	538	ALA	-	expression tag	UNP O89342
Aa	539	TRP	-	expression tag	UNP O89342
Aa	540	SER	-	expression tag	UNP O89342
Aa	541	HIS	-	expression tag	UNP O89342
Aa	542	PRO	-	expression tag	UNP O89342
Aa	543	GLN	-	expression tag	UNP O89342
Aa	544	PHE	-	expression tag	UNP O89342
Aa	545	GLU	-	expression tag	UNP O89342
Aa	546	LYS	-	expression tag	UNP O89342
Aa	547	GLY	-	expression tag	UNP O89342
Aa	548	GLY	-	expression tag	UNP O89342
Aa	549	GLY	-	expression tag	UNP O89342

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Chain	Residue	Modelled	Actual	Comment	Reference
Aa	550	SER	-	expression tag	UNP O89342
Aa	551	GLY	-	expression tag	UNP O89342
Aa	552	GLY	-	expression tag	UNP O89342
Aa	553	GLY	-	expression tag	UNP O89342
Aa	554	GLY	-	expression tag	UNP O89342
Aa	555	SER	-	expression tag	UNP O89342
Aa	556	GLY	-	expression tag	UNP O89342
Aa	557	GLY	-	expression tag	UNP O89342
Aa	558	SER	-	expression tag	UNP O89342
Aa	559	ALA	-	expression tag	UNP O89342
Aa	560	TRP	-	expression tag	UNP O89342
Aa	561	SER	-	expression tag	UNP O89342
Aa	562	HIS	-	expression tag	UNP O89342
Aa	563	PRO	-	expression tag	UNP O89342
Aa	564	GLN	-	expression tag	UNP O89342
Aa	565	PHE	-	expression tag	UNP O89342
Aa	566	GLU	-	expression tag	UNP O89342
Aa	567	LYS	-	expression tag	UNP O89342
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Ab	493	ASP	-	expression tag	UNP O89342
Ab	494	LYS	-	expression tag	UNP O89342
Ab	495	ILE	-	expression tag	UNP O89342
Ab	496	GLU	-	expression tag	UNP O89342
Ab	497	GLU	-	expression tag	UNP O89342
Ab	498	ILE	-	expression tag	UNP O89342
Ab	499	LEU	-	expression tag	UNP O89342
Ab	500	SER	-	expression tag	UNP O89342
Ab	501	LYS	-	expression tag	UNP O89342
Ab	502	ILE	-	expression tag	UNP O89342
Ab	503	TYR	-	expression tag	UNP O89342
Ab	504	HIS	-	expression tag	UNP O89342
Ab	505	ILE	-	expression tag	UNP O89342
Ab	506	GLU	-	expression tag	UNP O89342
Ab	507	ASN	-	expression tag	UNP O89342

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Chain	Residue	Modelled	Actual	Comment	Reference
Ab	508	GLU	-	expression tag	UNP O89342
Ab	509	ILE	-	expression tag	UNP O89342
Ab	510	ALA	-	expression tag	UNP O89342
Ab	511	ARG	-	expression tag	UNP O89342
Ab	512	ILE	-	expression tag	UNP O89342
Ab	513	LYS	-	expression tag	UNP O89342
Ab	514	LYS	-	expression tag	UNP O89342
Ab	515	LEU	-	expression tag	UNP O89342
Ab	516	ILE	-	expression tag	UNP O89342
Ab	517	GLY	-	expression tag	UNP O89342
Ab	518	GLU	-	expression tag	UNP O89342
Ab	519	ALA	-	expression tag	UNP O89342
Ab	520	PRO	-	expression tag	UNP O89342
Ab	521	GLY	-	expression tag	UNP O89342
Ab	522	GLY	-	expression tag	UNP O89342
Ab	523	ILE	-	expression tag	UNP O89342
Ab	524	GLU	-	expression tag	UNP O89342
Ab	525	GLY	-	expression tag	UNP O89342
Ab	526	ARG	-	expression tag	UNP O89342
Ab	527	LYS	-	expression tag	UNP O89342
Ab	528	LEU	-	expression tag	UNP O89342
Ab	529	HIS	-	expression tag	UNP O89342
Ab	530	HIS	-	expression tag	UNP O89342
Ab	531	HIS	-	expression tag	UNP O89342
Ab	532	HIS	-	expression tag	UNP O89342
Ab	533	HIS	-	expression tag	UNP O89342
Ab	534	HIS	-	expression tag	UNP O89342
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Ab	540	SER	-	expression tag	UNP O89342
Ab	541	HIS	-	expression tag	UNP O89342
Ab	542	PRO	-	expression tag	UNP O89342
Ab	543	GLN	-	expression tag	UNP O89342
Ab	544	PHE	-	expression tag	UNP O89342
Ab	545	GLU	-	expression tag	UNP O89342
Ab	546	LYS	-	expression tag	UNP O89342
Ab	547	GLY	-	expression tag	UNP O89342
Ab	548	GLY	-	expression tag	UNP O89342
Ab	549	GLY	-	expression tag	UNP O89342

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Ab	552	GLY	-	expression tag	UNP O89342
Ab	553	GLY	-	expression tag	UNP O89342
Ab	554	GLY	-	expression tag	UNP O89342
Ab	555	SER	-	expression tag	UNP O89342
Ab	556	GLY	-	expression tag	UNP O89342
Ab	557	GLY	-	expression tag	UNP O89342
Ab	558	SER	-	expression tag	UNP O89342
Ab	559	ALA	-	expression tag	UNP O89342
Ab	560	TRP	-	expression tag	UNP O89342
Ab	561	SER	-	expression tag	UNP O89342
Ab	562	HIS	-	expression tag	UNP O89342
Ab	563	PRO	-	expression tag	UNP O89342
Ab	564	GLN	-	expression tag	UNP O89342
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Ac	495	ILE	-	expression tag	UNP O89342
Ac	496	GLU	-	expression tag	UNP O89342
Ac	497	GLU	-	expression tag	UNP O89342
Ac	498	ILE	-	expression tag	UNP O89342
Ac	499	LEU	-	expression tag	UNP O89342
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Ac	501	LYS	-	expression tag	UNP O89342
Ac	502	ILE	-	expression tag	UNP O89342
Ac	503	TYR	-	expression tag	UNP O89342
Ac	504	HIS	-	expression tag	UNP O89342
Ac	505	ILE	-	expression tag	UNP O89342
Ac	506	GLU	-	expression tag	UNP O89342
Ac	507	ASN	-	expression tag	UNP O89342

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Chain	Residue	Modelled	Actual	Comment	Reference
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Ac	510	ALA	-	expression tag	UNP O89342
Ac	511	ARG	-	expression tag	UNP O89342
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Ac	524	GLU	-	expression tag	UNP O89342
Ac	525	GLY	-	expression tag	UNP O89342
Ac	526	ARG	-	expression tag	UNP O89342
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Ac	535	HIS	-	expression tag	UNP O89342
Ac	536	HIS	-	expression tag	UNP O89342
Ac	537	SER	-	expression tag	UNP O89342
Ac	538	ALA	-	expression tag	UNP O89342
Ac	539	TRP	-	expression tag	UNP O89342
Ac	540	SER	-	expression tag	UNP O89342
Ac	541	HIS	-	expression tag	UNP O89342
Ac	542	PRO	-	expression tag	UNP O89342
Ac	543	GLN	-	expression tag	UNP O89342
Ac	544	PHE	-	expression tag	UNP O89342
Ac	545	GLU	-	expression tag	UNP O89342
Ac	546	LYS	-	expression tag	UNP O89342
Ac	547	GLY	-	expression tag	UNP O89342
Ac	548	GLY	-	expression tag	UNP O89342
Ac	549	GLY	-	expression tag	UNP O89342

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Chain	Residue	Modelled	Actual	Comment	Reference
Ac	550	SER	-	expression tag	UNP O89342
Ac	551	GLY	-	expression tag	UNP O89342
Ac	552	GLY	-	expression tag	UNP O89342
Ac	553	GLY	-	expression tag	UNP O89342
Ac	554	GLY	-	expression tag	UNP O89342
Ac	555	SER	-	expression tag	UNP O89342
Ac	556	GLY	-	expression tag	UNP O89342
Ac	557	GLY	-	expression tag	UNP O89342
Ac	558	SER	-	expression tag	UNP O89342
Ac	559	ALA	-	expression tag	UNP O89342
Ac	560	TRP	-	expression tag	UNP O89342
Ac	561	SER	-	expression tag	UNP O89342
Ac	562	HIS	-	expression tag	UNP O89342
Ac	563	PRO	-	expression tag	UNP O89342
Ac	564	GLN	-	expression tag	UNP O89342
Ac	565	PHE	-	expression tag	UNP O89342
Ac	566	GLU	-	expression tag	UNP O89342
Ac	567	LYS	-	expression tag	UNP O89342

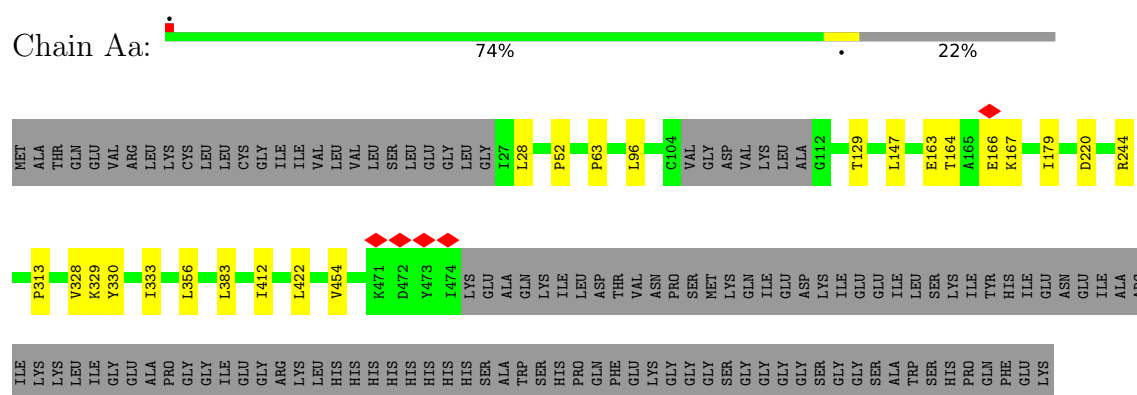
- Molecule 2 is a protein called F123 nanobody.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Ba	120	Total	C	N	O	S	0	0
			911	567	161	177	6		
2	Bb	120	Total	C	N	O	S	0	0
			911	567	161	177	6		
2	Bc	120	Total	C	N	O	S	0	0
			911	567	161	177	6		

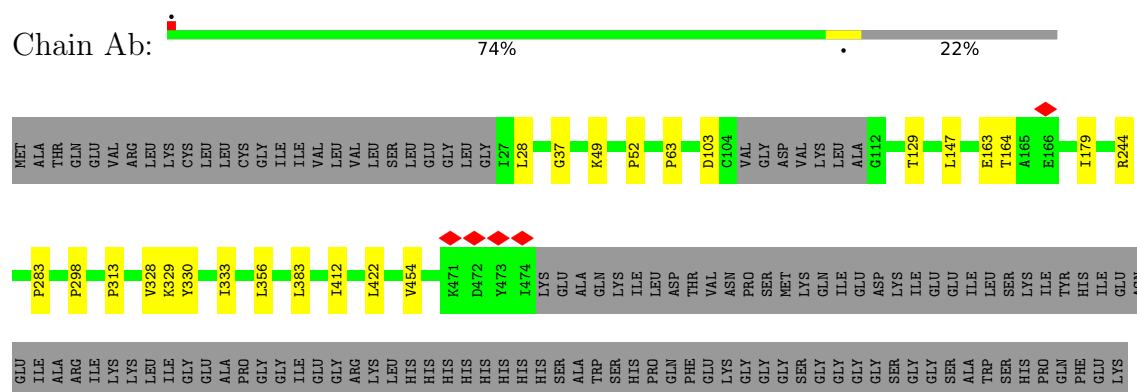
3 Residue-property plots

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.

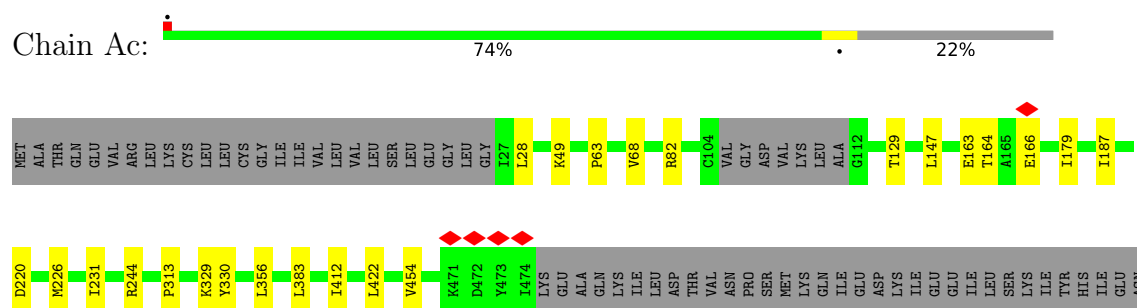
• Molecule 1: Fusion glycoprotein F0



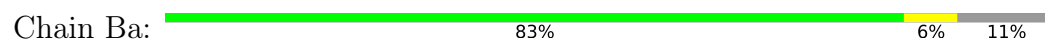
• Molecule 1: Fusion glycoprotein F0



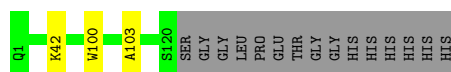
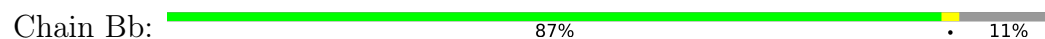
• Molecule 1: Fusion glycoprotein F0



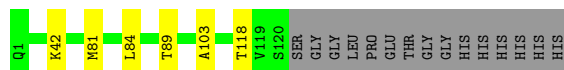
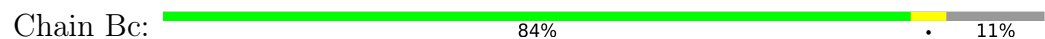
- Molecule 2: F123 nanobody



- Molecule 2: F123 nanobody



- Molecule 2: F123 nanobody



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	494292	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1700	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.368	Depositor
Minimum map value	-0.150	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.0735	Depositor
Map size (Å)	269.568, 269.568, 269.568	wwPDB
Map dimensions	416, 416, 416	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.648, 0.648, 0.648	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	Aa	0.26	0/3435	0.28	0/4670
1	Ab	0.26	0/3435	0.26	0/4670
1	Ac	0.26	0/3435	0.28	0/4670
2	Ba	0.22	0/928	0.33	0/1258
2	Bb	0.22	0/928	0.32	0/1258
2	Bc	0.23	0/928	0.35	0/1258
All	All	0.25	0/13089	0.29	0/17784

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	Aa	3386	0	3444	16	0
1	Ab	3386	0	3444	16	0
1	Ac	3386	0	3444	16	0
2	Ba	911	0	894	6	0
2	Bb	911	0	894	3	0
2	Bc	911	0	894	4	0
All	All	12891	0	13014	53	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 2.

All (53) 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:Aa:147:LEU:HD11	1:Aa:163:GLU:HA	1.76	0.67
1:Ac:147:LEU:HD11	1:Ac:163:GLU:HA	1.78	0.65
1:Aa:244:ARG:HH11	1:Aa:244:ARG:HG3	1.62	0.65
1:Ab:244:ARG:HH11	1:Ab:244:ARG:HG3	1.64	0.63
1:Aa:28:LEU:HD22	1:Aa:356:LEU:HB3	1.81	0.62
1:Ac:244:ARG:HH11	1:Ac:244:ARG:HG3	1.64	0.62
1:Ab:147:LEU:HD11	1:Ab:163:GLU:HA	1.82	0.61
1:Ab:28:LEU:HD22	1:Ab:356:LEU:HB3	1.83	0.61
1:Ac:28:LEU:HD22	1:Ac:356:LEU:HB3	1.83	0.60
1:Ab:383:LEU:HD21	1:Ab:422:LEU:HD11	1.84	0.59
1:Aa:383:LEU:HD21	1:Aa:422:LEU:HD11	1.83	0.58
1:Ac:383:LEU:HD21	1:Ac:422:LEU:HD11	1.84	0.58
2:Bc:89:THR:HG23	2:Bc:118:THR:HA	1.86	0.58
1:Aa:454:VAL:HG11	1:Ac:313:PRO:HD3	1.86	0.57
1:Ab:313:PRO:HD3	1:Ac:454:VAL:HG11	1.87	0.57
1:Aa:313:PRO:HD3	1:Ab:454:VAL:HG11	1.86	0.56
2:Bb:42:LYS:NZ	2:Bb:42:LYS:HB3	2.22	0.55
1:Aa:163:GLU:HG2	1:Aa:164:THR:HG23	1.90	0.53
1:Ac:244:ARG:HG3	1:Ac:244:ARG:NH1	2.24	0.53
1:Ac:129:THR:HG21	2:Bc:103:ALA:HB3	1.90	0.52
2:Bc:42:LYS:NZ	2:Bc:42:LYS:HB3	2.24	0.52
1:Ab:163:GLU:HG2	1:Ab:164:THR:HG23	1.91	0.52
1:Aa:129:THR:HG21	2:Ba:103:ALA:HB3	1.91	0.51
1:Aa:244:ARG:HG3	1:Aa:244:ARG:NH1	2.25	0.51
2:Ba:42:LYS:HB3	2:Ba:42:LYS:NZ	2.27	0.50
2:Ba:89:THR:HG23	2:Ba:118:THR:HA	1.93	0.50
1:Ab:129:THR:HG21	2:Bb:103:ALA:HB3	1.92	0.50
1:Ab:244:ARG:HG3	1:Ab:244:ARG:NH1	2.25	0.50
2:Ba:1:GLN:HA	2:Ba:110:TYR:CZ	2.47	0.49
1:Ac:226:MET:HG2	1:Ac:231:ILE:HG12	1.97	0.46
1:Ab:329:LYS:HE2	1:Ab:330:TYR:CZ	2.49	0.46
1:Ac:166:GLU:N	1:Ac:166:GLU:OE2	2.49	0.46
1:Ab:52:PRO:HD2	2:Bb:100:TRP:CH2	2.51	0.46
1:Ac:329:LYS:HE2	1:Ac:330:TYR:CZ	2.51	0.46
1:Aa:166:GLU:N	1:Aa:166:GLU:OE2	2.48	0.46
1:Ab:328:VAL:HB	1:Ab:333:ILE:HD11	1.97	0.45
2:Ba:63:LYS:HB3	2:Ba:63:LYS:HE2	1.55	0.45
1:Aa:328:VAL:HB	1:Aa:333:ILE:HD11	1.98	0.45
1:Aa:329:LYS:HE2	1:Aa:330:TYR:CZ	2.51	0.45
1:Ac:163:GLU:HG2	1:Ac:164:THR:HG23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Bc:81:MET:HE2	2:Bc:84:LEU:HD21	2.01	0.43
1:Aa:63:PRO:HB2	1:Aa:179:ILE:HD12	2.01	0.43
1:Ab:383:LEU:HD23	1:Ab:412:ILE:HD12	2.01	0.43
1:Ab:63:PRO:HB2	1:Ab:179:ILE:HD12	2.01	0.42
1:Ac:383:LEU:HD23	1:Ac:412:ILE:HD12	2.01	0.42
1:Aa:167:LYS:HB3	1:Aa:167:LYS:HE2	1.84	0.42
1:Ac:68:VAL:HG12	1:Ac:187:ILE:HD13	2.02	0.41
1:Ac:82:ARG:HD2	1:Ac:82:ARG:HA	1.86	0.41
1:Ac:63:PRO:HB2	1:Ac:179:ILE:HD12	2.02	0.41
1:Aa:383:LEU:HD23	1:Aa:412:ILE:HD12	2.02	0.41
1:Aa:52:PRO:HD2	2:Ba:100:TRP:CH2	2.56	0.41
1:Ab:37:GLY:O	1:Ab:298:PRO:HA	2.21	0.41
1:Ab:52:PRO:HA	1:Ab:283:PRO:HA	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	Aa	437/567 (77%)	434 (99%)	3 (1%)	0	100	100
1	Ab	437/567 (77%)	434 (99%)	3 (1%)	0	100	100
1	Ac	437/567 (77%)	433 (99%)	4 (1%)	0	100	100
2	Ba	118/135 (87%)	118 (100%)	0	0	100	100
2	Bb	118/135 (87%)	118 (100%)	0	0	100	100
2	Bc	118/135 (87%)	118 (100%)	0	0	100	100
All	All	1665/2106 (79%)	1655 (99%)	10 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Aa	392/494 (79%)	390 (100%)	2 (0%)	81	93
1	Ab	392/494 (79%)	390 (100%)	2 (0%)	81	93
1	Ac	392/494 (79%)	390 (100%)	2 (0%)	81	93
2	Ba	96/107 (90%)	96 (100%)	0	100	100
2	Bb	96/107 (90%)	96 (100%)	0	100	100
2	Bc	96/107 (90%)	96 (100%)	0	100	100
All	All	1464/1803 (81%)	1458 (100%)	6 (0%)	81	94

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Aa	96	LEU
1	Aa	220	ASP
1	Ab	49	LYS
1	Ab	103	ASP
1	Ac	49	LYS
1	Ac	220	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	Aa	393	GLN
1	Ab	325	ASN
1	Ab	393	GLN
1	Ab	468	GLN
1	Ac	393	GLN
1	Ac	459	GLN
2	Ba	13	GLN
2	Ba	52	ASN
2	Bb	38	GLN
2	Bb	43	GLN
2	Bb	52	ASN

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Mol	Chain	Res	Type
2	Bc	13	GLN
2	Bc	52	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](#)

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.

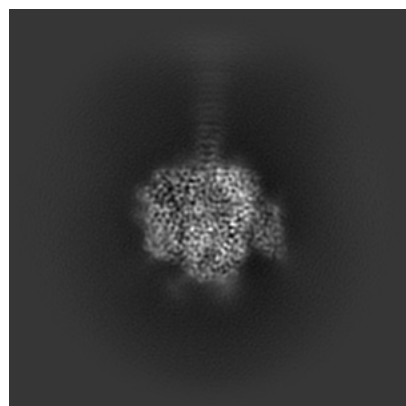
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54916. These allow visual inspection of the internal detail of the map and identification of artifacts.

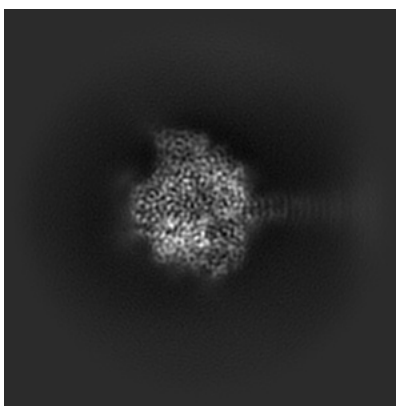
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

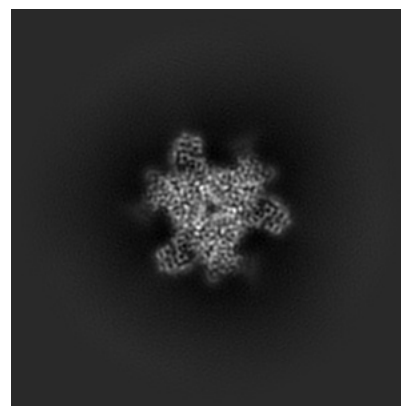
6.1.1 Primary map



X

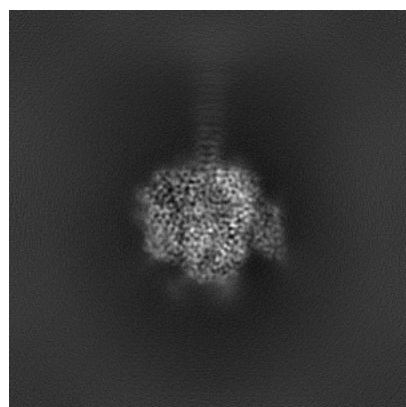


Y

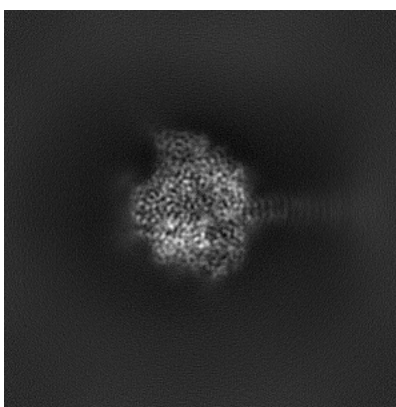


Z

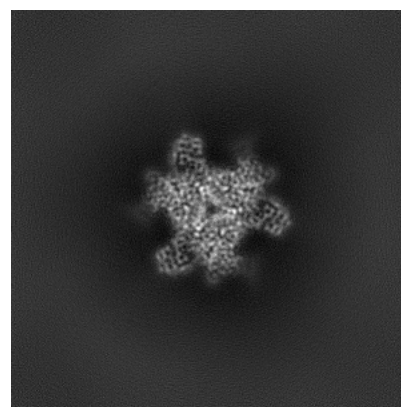
6.1.2 Raw map



X



Y

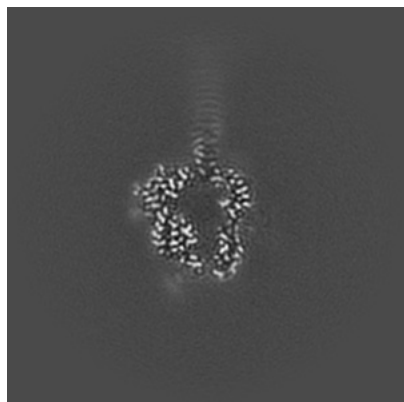


Z

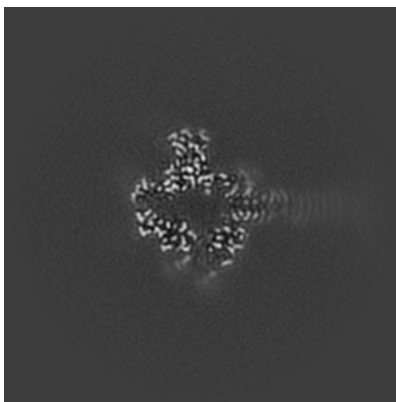
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

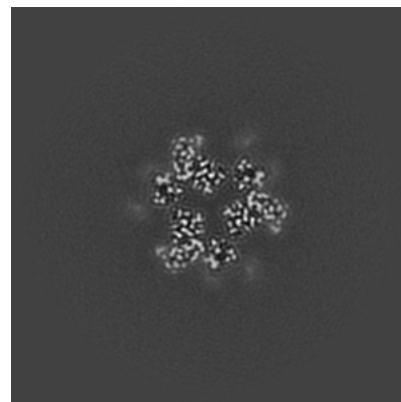
6.2.1 Primary map



X Index: 208

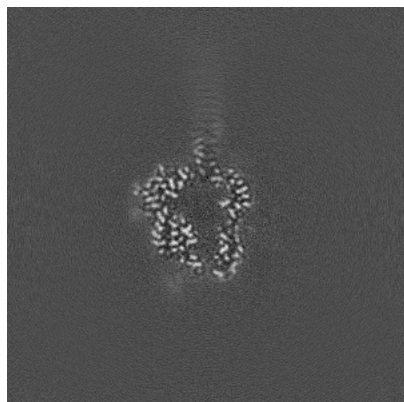


Y Index: 208

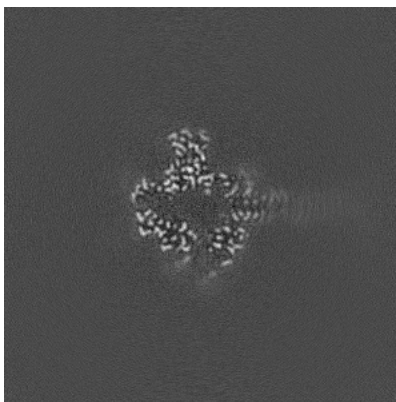


Z Index: 208

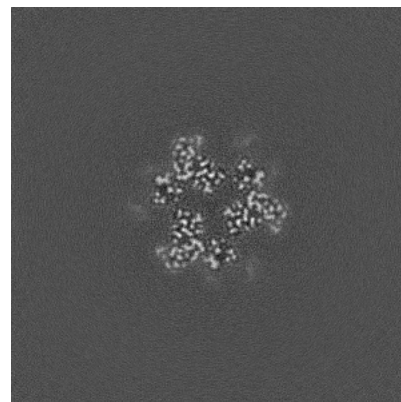
6.2.2 Raw map



X Index: 208



Y Index: 208

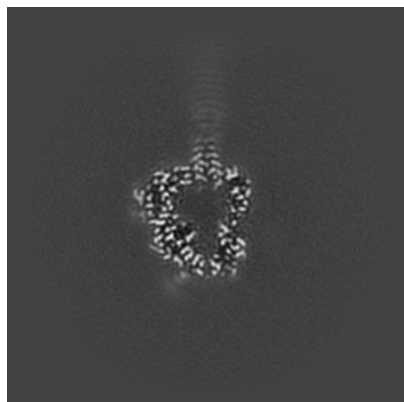


Z Index: 208

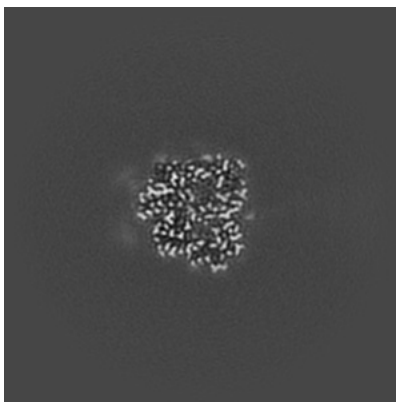
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

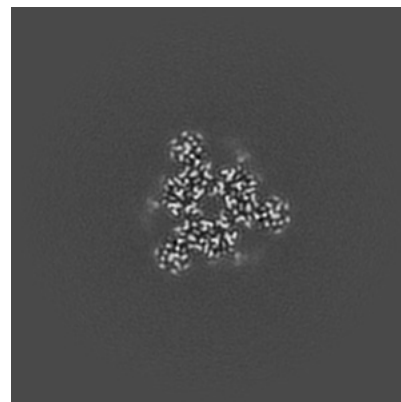
6.3.1 Primary map



X Index: 212

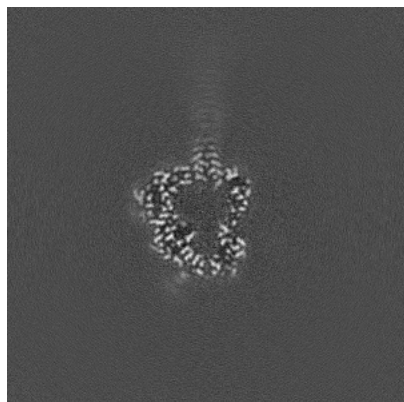


Y Index: 230

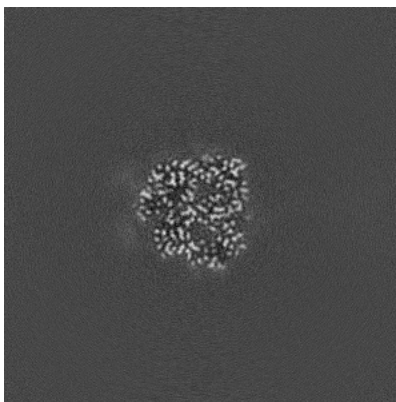


Z Index: 186

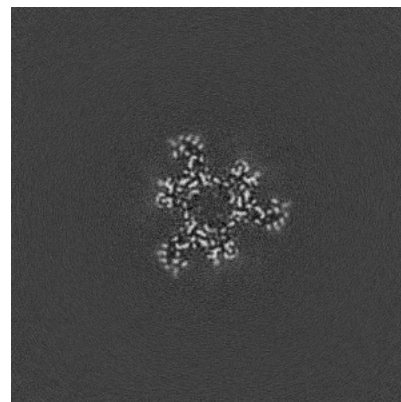
6.3.2 Raw map



X Index: 212



Y Index: 232

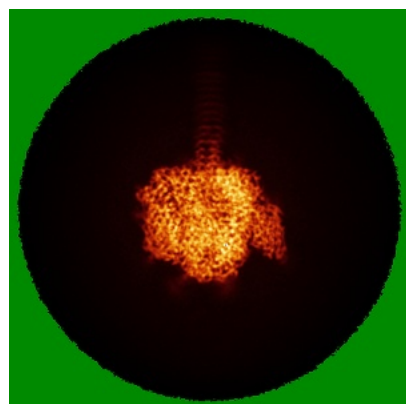


Z Index: 191

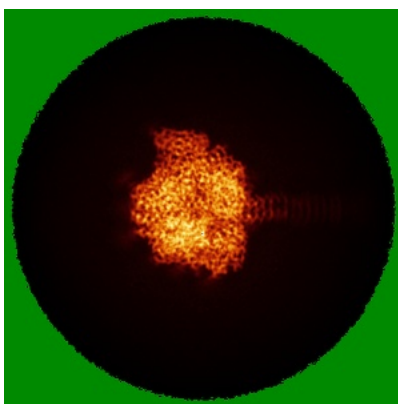
The images above show the largest variance slices of the map in three orthogonal directions.

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

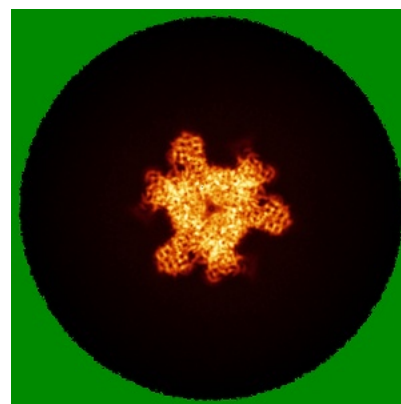
6.4.1 Primary map



X

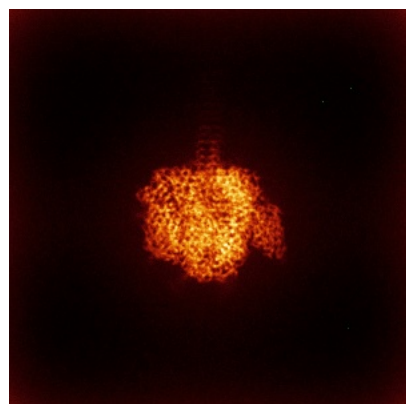


Y

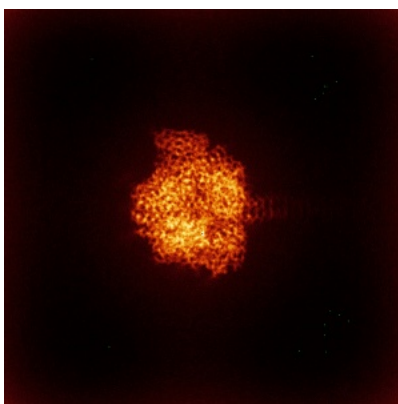


Z

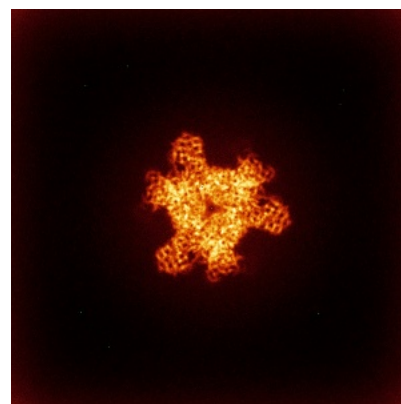
6.4.2 Raw map



X



Y

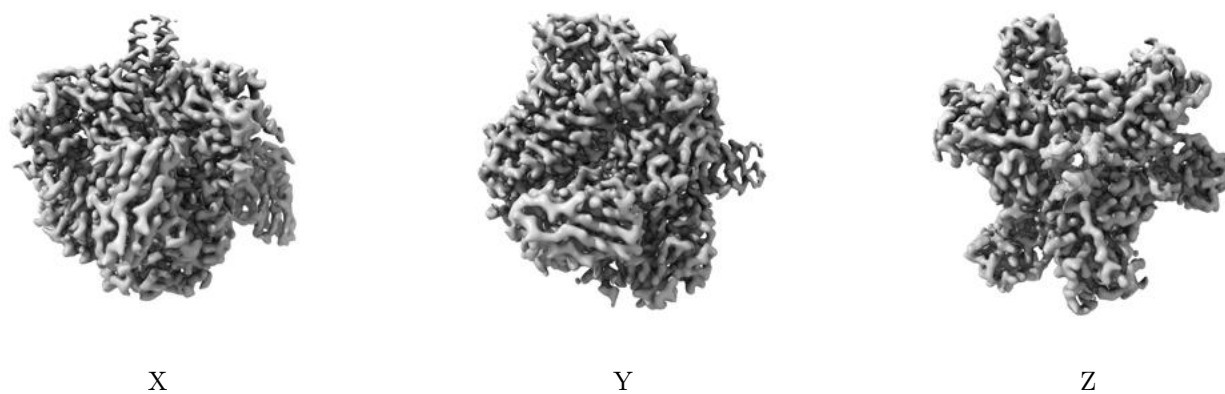


Z

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.

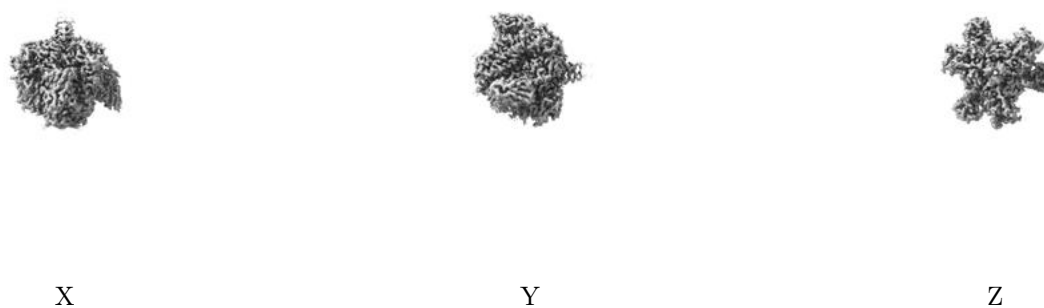
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0735. 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.

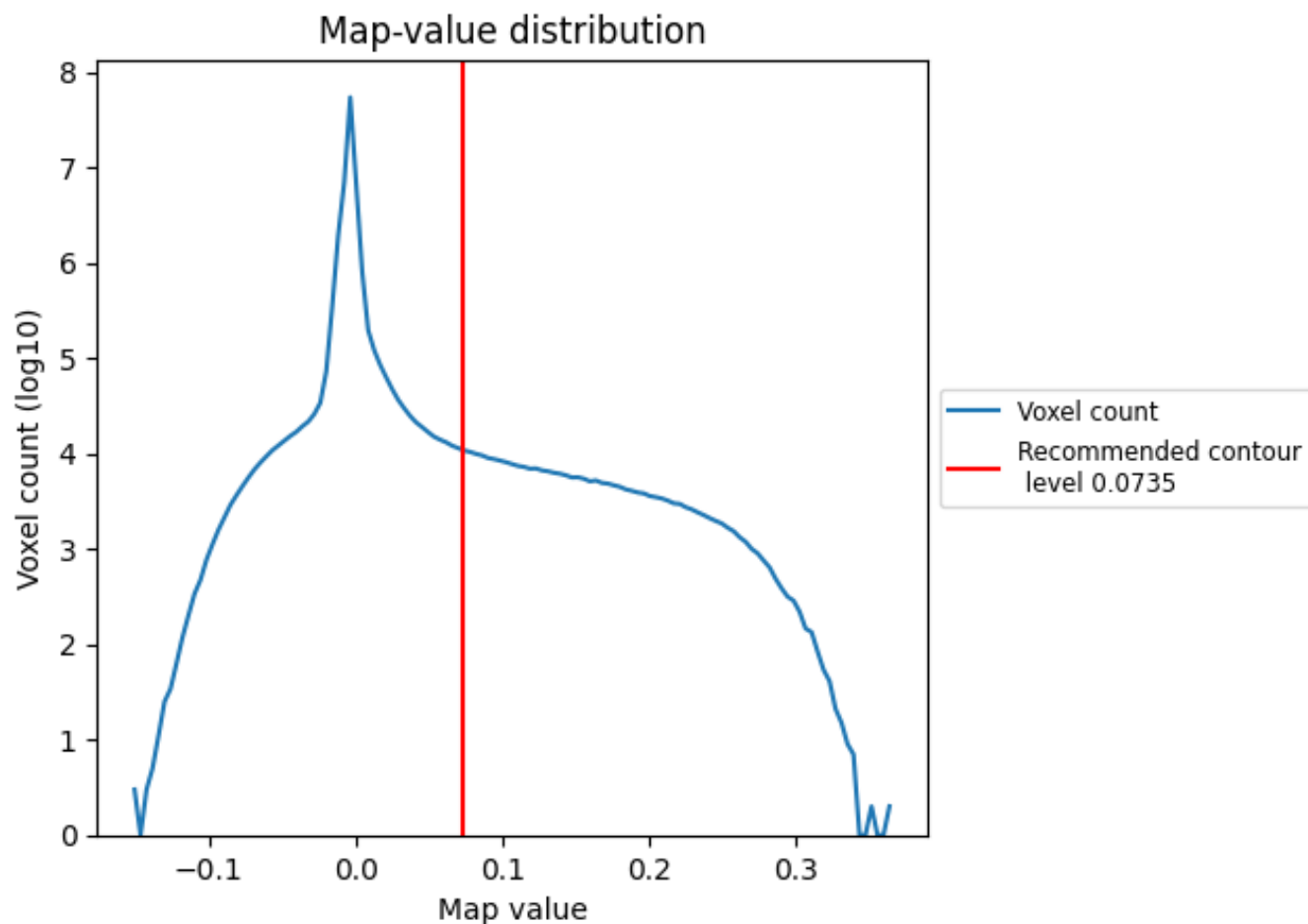
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

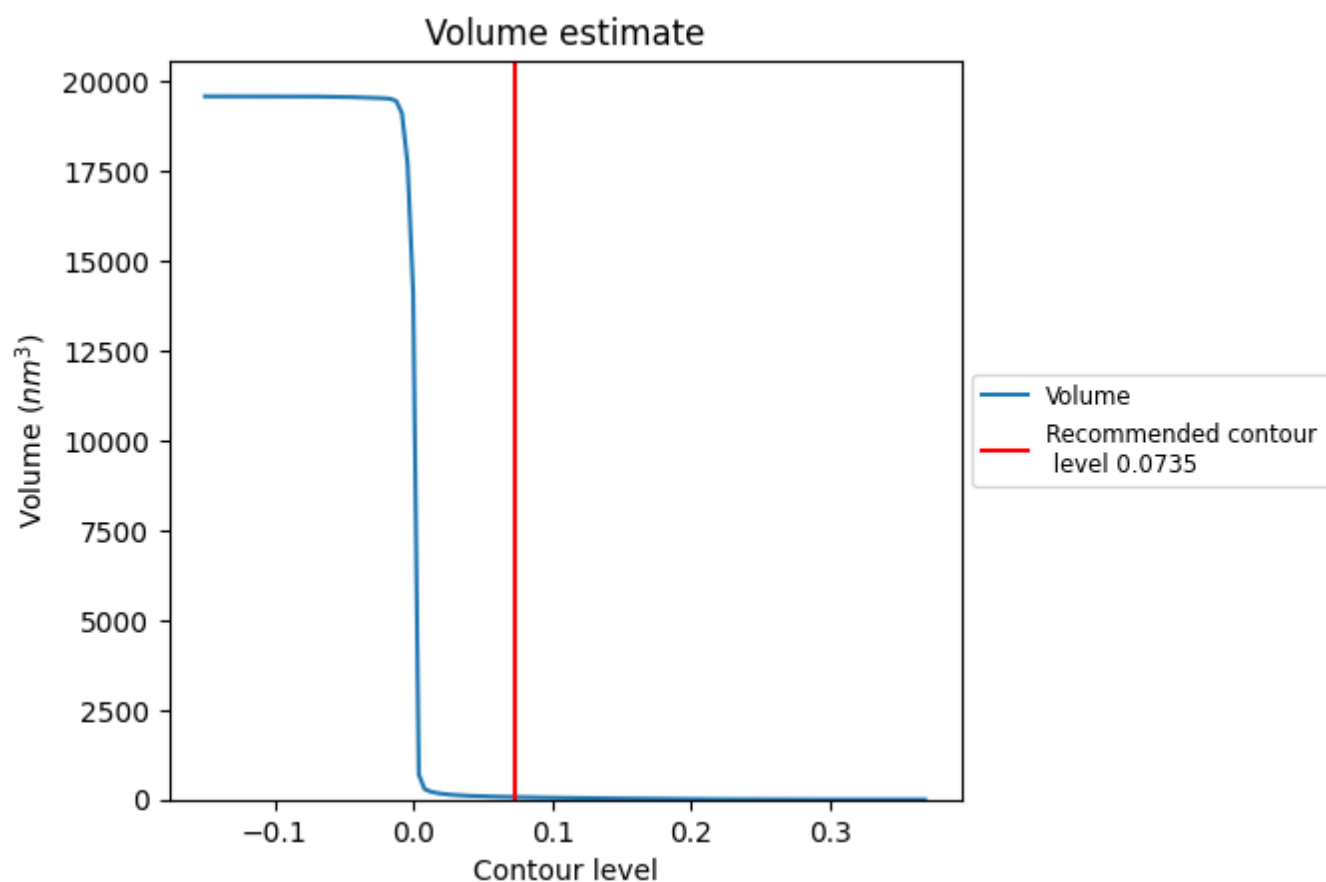
This section contains the results of statistical analysis of the map.

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.

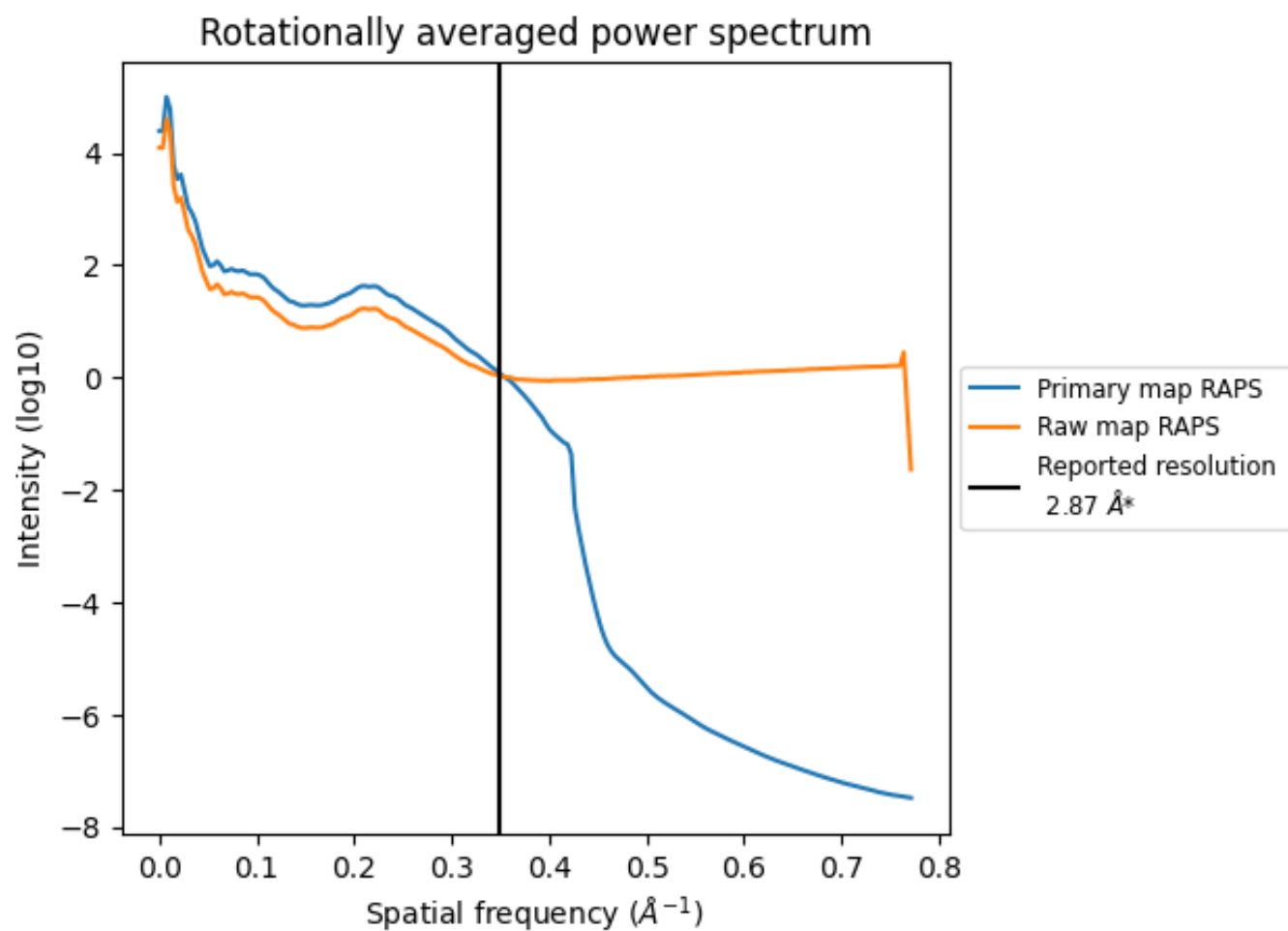
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 69 nm^3 ; this corresponds to an approximate mass of 62 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 ⓘ

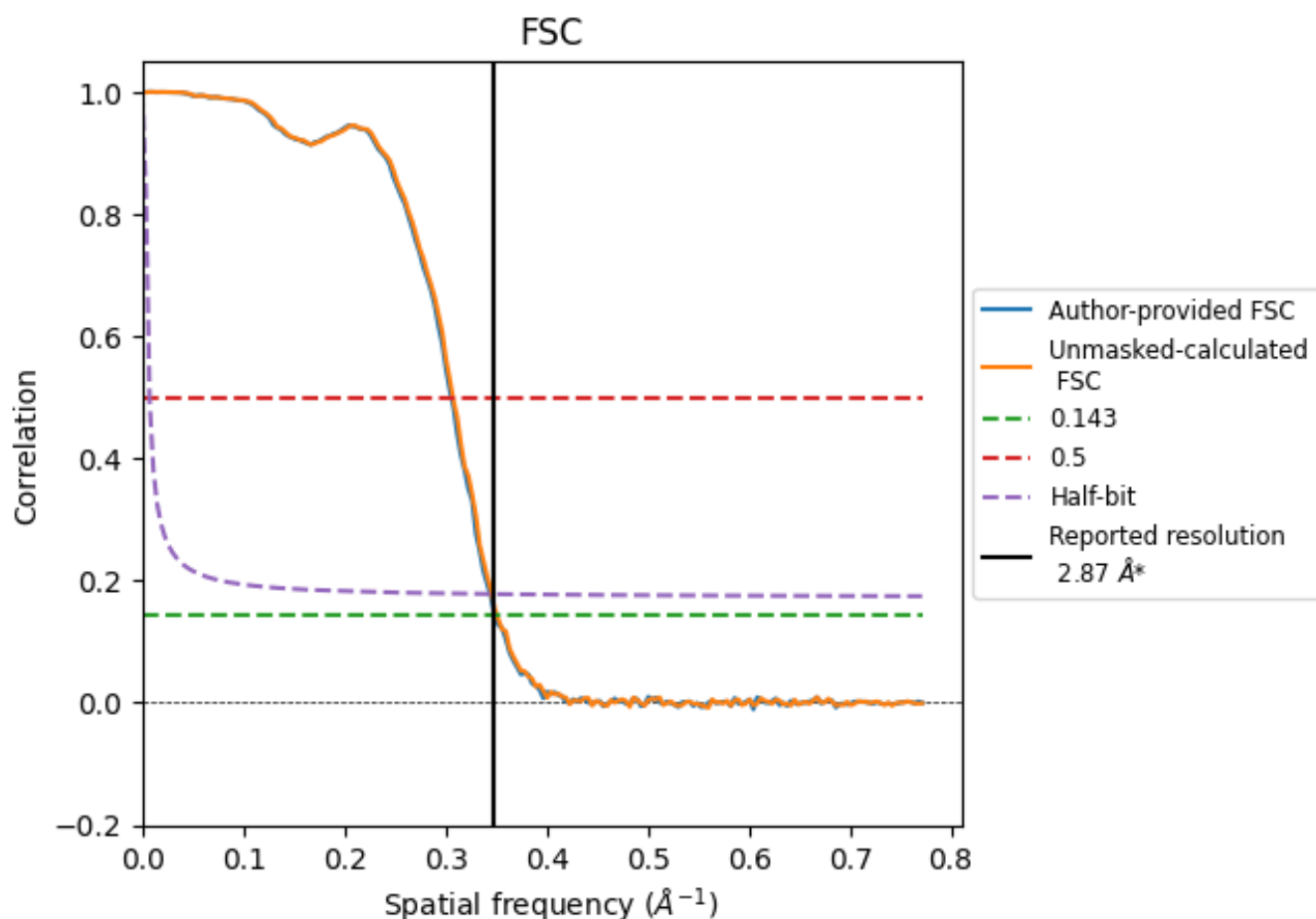


*Reported resolution corresponds to spatial frequency of 0.348 Å⁻¹

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 0.348 Å⁻¹

8.2 Resolution estimates [i](#)

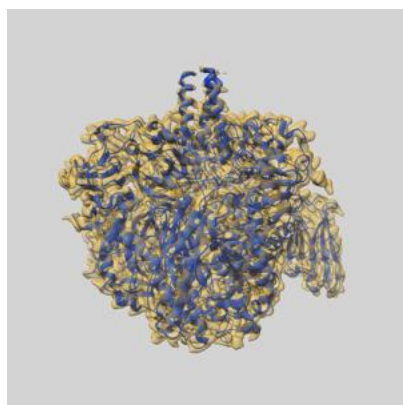
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.87	-	-
Author-provided FSC curve	2.87	3.27	2.91
Unmasked-calculated*	2.85	3.25	2.89

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

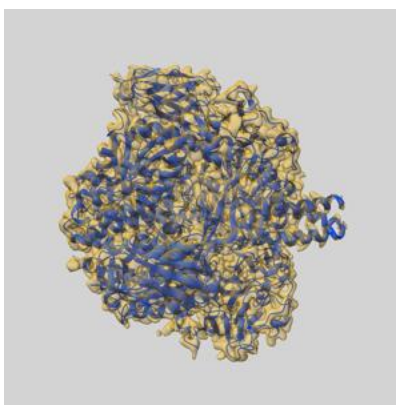
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-54916 and PDB model 9SHV. Per-residue inclusion information can be found in section 3 on page 11.

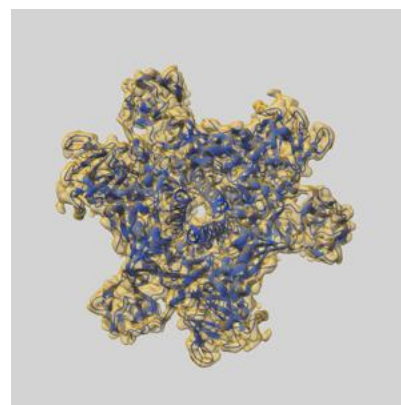
9.1 Map-model overlay [i](#)



X



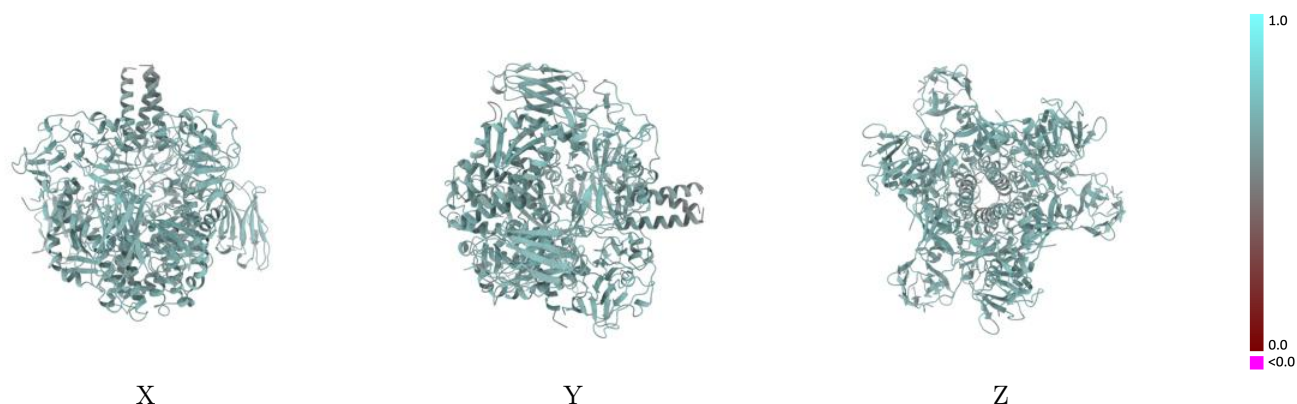
Y



Z

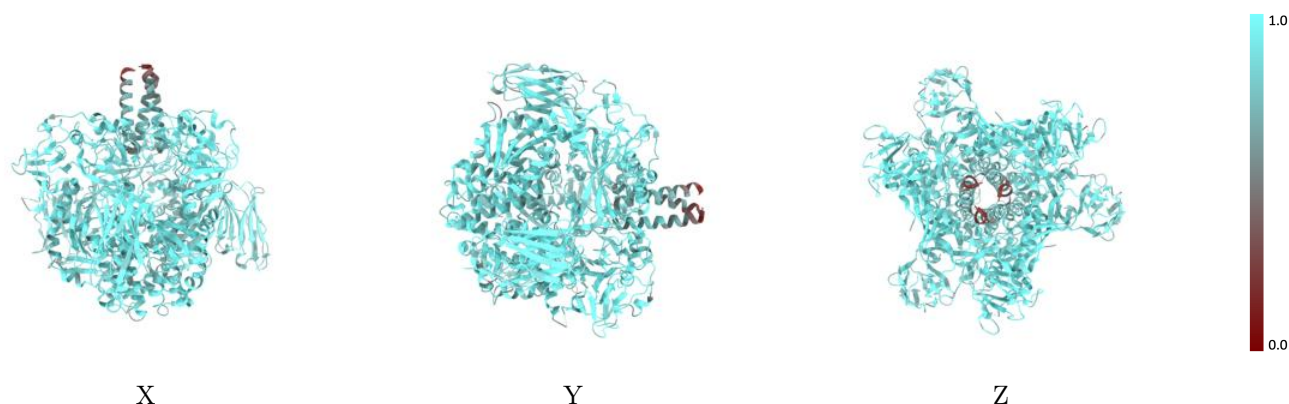
The images above show the 3D surface view of the map at the recommended contour level 0.0735 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



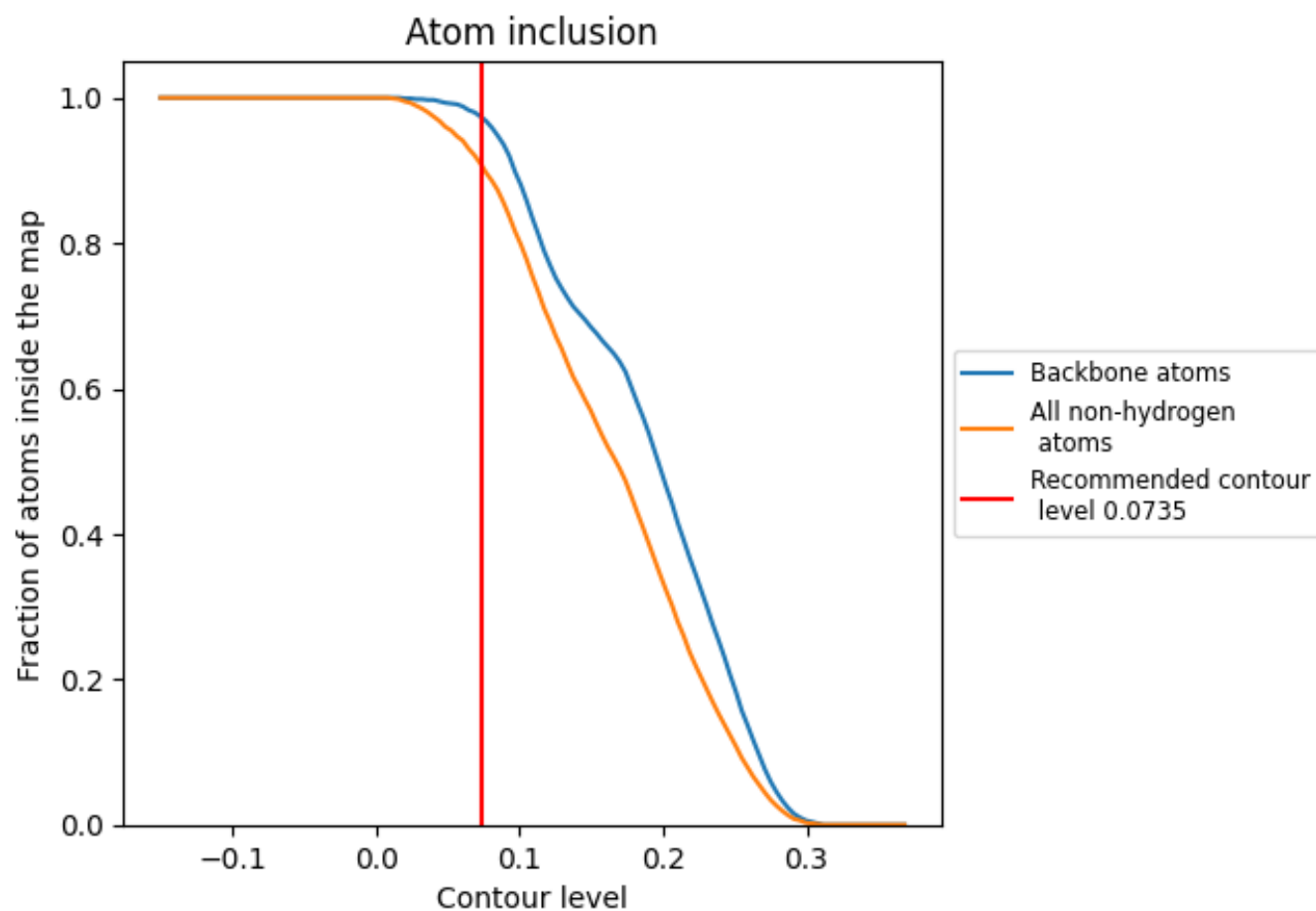
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0735).

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 91% 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 (0.0735) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9070	0.6340
Aa	0.9120	0.6360
Ab	0.9140	0.6380
Ac	0.9130	0.6370
Ba	0.8880	0.6220
Bb	0.8840	0.6250
Bc	0.8840	0.6220

1.0

0.0

<0.0