



Full wwPDB EM Validation Report ⓘ

May 28, 2026 – 12:12 PM EDT

PDB ID : 9NZ2 / pdb_00009nz2
EMDB ID : EMD-49948
Title : Cryo-EM structure of antibody 22F5 in complex with pre-fusion stabilized LayV-F
Authors : May, A.J.; Kumar, U.; Acharya, P.
Deposited on : 2025-03-31
Resolution : 4.46 Å(reported)

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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

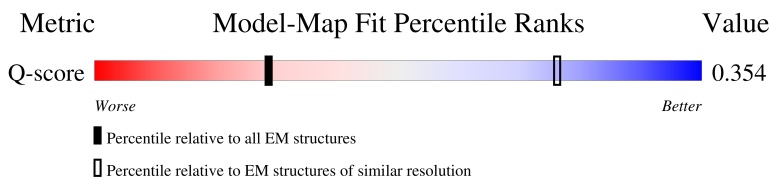
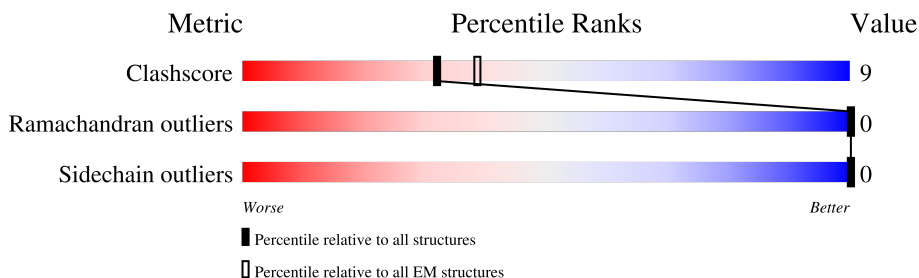
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.46 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.




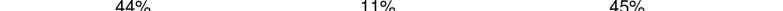



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	3001 (3.96 - 4.96)

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	563	
1	B	563	
1	C	563	
2	D	216	

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Mol	Chain	Length	Quality of chain
2	F	216	
2	I	216	
3	E	219	
3	G	219	
3	H	219	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 31005 atoms, of which 15489 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	A	443	Total	C	H	N	O	S	0	0
			6800	2128	3425	566	661	20		
1	B	443	Total	C	H	N	O	S	0	0
			6800	2128	3425	566	661	20		
1	C	443	Total	C	H	N	O	S	0	0
			6800	2128	3425	566	661	20		

There are 246 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	99	CYS	GLY	engineered mutation	UNP A0AAX3C923
A	109	CYS	ILE	engineered mutation	UNP A0AAX3C923
A	484	GLY	-	expression tag	UNP A0AAX3C923
A	485	SER	-	expression tag	UNP A0AAX3C923
A	486	GLY	-	expression tag	UNP A0AAX3C923
A	487	TYR	-	expression tag	UNP A0AAX3C923
A	488	ILE	-	expression tag	UNP A0AAX3C923
A	489	PRO	-	expression tag	UNP A0AAX3C923
A	490	GLU	-	expression tag	UNP A0AAX3C923
A	491	ALA	-	expression tag	UNP A0AAX3C923
A	492	PRO	-	expression tag	UNP A0AAX3C923
A	493	ARG	-	expression tag	UNP A0AAX3C923
A	494	ASP	-	expression tag	UNP A0AAX3C923
A	495	GLY	-	expression tag	UNP A0AAX3C923
A	496	GLN	-	expression tag	UNP A0AAX3C923
A	497	ALA	-	expression tag	UNP A0AAX3C923
A	498	TYR	-	expression tag	UNP A0AAX3C923
A	499	VAL	-	expression tag	UNP A0AAX3C923
A	500	ARG	-	expression tag	UNP A0AAX3C923
A	501	LYS	-	expression tag	UNP A0AAX3C923
A	502	ASP	-	expression tag	UNP A0AAX3C923
A	503	GLY	-	expression tag	UNP A0AAX3C923
A	504	GLU	-	expression tag	UNP A0AAX3C923
A	505	TRP	-	expression tag	UNP A0AAX3C923

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Chain	Residue	Modelled	Actual	Comment	Reference
A	506	VAL	-	expression tag	UNP A0AAX3C923
A	507	LEU	-	expression tag	UNP A0AAX3C923
A	508	LEU	-	expression tag	UNP A0AAX3C923
A	509	SER	-	expression tag	UNP A0AAX3C923
A	510	THR	-	expression tag	UNP A0AAX3C923
A	511	PHE	-	expression tag	UNP A0AAX3C923
A	512	LEU	-	expression tag	UNP A0AAX3C923
A	513	GLY	-	expression tag	UNP A0AAX3C923
A	514	ARG	-	expression tag	UNP A0AAX3C923
A	515	SER	-	expression tag	UNP A0AAX3C923
A	516	LEU	-	expression tag	UNP A0AAX3C923
A	517	GLU	-	expression tag	UNP A0AAX3C923
A	518	VAL	-	expression tag	UNP A0AAX3C923
A	519	LEU	-	expression tag	UNP A0AAX3C923
A	520	PHE	-	expression tag	UNP A0AAX3C923
A	521	GLN	-	expression tag	UNP A0AAX3C923
A	522	GLY	-	expression tag	UNP A0AAX3C923
A	523	PRO	-	expression tag	UNP A0AAX3C923
A	524	GLY	-	expression tag	UNP A0AAX3C923
A	525	HIS	-	expression tag	UNP A0AAX3C923
A	526	HIS	-	expression tag	UNP A0AAX3C923
A	527	HIS	-	expression tag	UNP A0AAX3C923
A	528	HIS	-	expression tag	UNP A0AAX3C923
A	529	HIS	-	expression tag	UNP A0AAX3C923
A	530	HIS	-	expression tag	UNP A0AAX3C923
A	531	HIS	-	expression tag	UNP A0AAX3C923
A	532	HIS	-	expression tag	UNP A0AAX3C923
A	533	SER	-	expression tag	UNP A0AAX3C923
A	534	ALA	-	expression tag	UNP A0AAX3C923
A	535	TRP	-	expression tag	UNP A0AAX3C923
A	536	SER	-	expression tag	UNP A0AAX3C923
A	537	HIS	-	expression tag	UNP A0AAX3C923
A	538	PRO	-	expression tag	UNP A0AAX3C923
A	539	GLN	-	expression tag	UNP A0AAX3C923
A	540	PHE	-	expression tag	UNP A0AAX3C923
A	541	GLU	-	expression tag	UNP A0AAX3C923
A	542	LYS	-	expression tag	UNP A0AAX3C923
A	543	GLY	-	expression tag	UNP A0AAX3C923
A	544	GLY	-	expression tag	UNP A0AAX3C923
A	545	GLY	-	expression tag	UNP A0AAX3C923
A	546	SER	-	expression tag	UNP A0AAX3C923
A	547	GLY	-	expression tag	UNP A0AAX3C923

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Chain	Residue	Modelled	Actual	Comment	Reference
A	548	GLY	-	expression tag	UNP A0AAX3C923
A	549	GLY	-	expression tag	UNP A0AAX3C923
A	550	GLY	-	expression tag	UNP A0AAX3C923
A	551	SER	-	expression tag	UNP A0AAX3C923
A	552	GLY	-	expression tag	UNP A0AAX3C923
A	553	GLY	-	expression tag	UNP A0AAX3C923
A	554	SER	-	expression tag	UNP A0AAX3C923
A	555	ALA	-	expression tag	UNP A0AAX3C923
A	556	TRP	-	expression tag	UNP A0AAX3C923
A	557	SER	-	expression tag	UNP A0AAX3C923
A	558	HIS	-	expression tag	UNP A0AAX3C923
A	559	PRO	-	expression tag	UNP A0AAX3C923
A	560	GLN	-	expression tag	UNP A0AAX3C923
A	561	PHE	-	expression tag	UNP A0AAX3C923
A	562	GLU	-	expression tag	UNP A0AAX3C923
A	563	LYS	-	expression tag	UNP A0AAX3C923
B	99	CYS	GLY	engineered mutation	UNP A0AAX3C923
B	109	CYS	ILE	engineered mutation	UNP A0AAX3C923
B	484	GLY	-	expression tag	UNP A0AAX3C923
B	485	SER	-	expression tag	UNP A0AAX3C923
B	486	GLY	-	expression tag	UNP A0AAX3C923
B	487	TYR	-	expression tag	UNP A0AAX3C923
B	488	ILE	-	expression tag	UNP A0AAX3C923
B	489	PRO	-	expression tag	UNP A0AAX3C923
B	490	GLU	-	expression tag	UNP A0AAX3C923
B	491	ALA	-	expression tag	UNP A0AAX3C923
B	492	PRO	-	expression tag	UNP A0AAX3C923
B	493	ARG	-	expression tag	UNP A0AAX3C923
B	494	ASP	-	expression tag	UNP A0AAX3C923
B	495	GLY	-	expression tag	UNP A0AAX3C923
B	496	GLN	-	expression tag	UNP A0AAX3C923
B	497	ALA	-	expression tag	UNP A0AAX3C923
B	498	TYR	-	expression tag	UNP A0AAX3C923
B	499	VAL	-	expression tag	UNP A0AAX3C923
B	500	ARG	-	expression tag	UNP A0AAX3C923
B	501	LYS	-	expression tag	UNP A0AAX3C923
B	502	ASP	-	expression tag	UNP A0AAX3C923
B	503	GLY	-	expression tag	UNP A0AAX3C923
B	504	GLU	-	expression tag	UNP A0AAX3C923
B	505	TRP	-	expression tag	UNP A0AAX3C923
B	506	VAL	-	expression tag	UNP A0AAX3C923
B	507	LEU	-	expression tag	UNP A0AAX3C923

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Chain	Residue	Modelled	Actual	Comment	Reference
B	508	LEU	-	expression tag	UNP A0AAX3C923
B	509	SER	-	expression tag	UNP A0AAX3C923
B	510	THR	-	expression tag	UNP A0AAX3C923
B	511	PHE	-	expression tag	UNP A0AAX3C923
B	512	LEU	-	expression tag	UNP A0AAX3C923
B	513	GLY	-	expression tag	UNP A0AAX3C923
B	514	ARG	-	expression tag	UNP A0AAX3C923
B	515	SER	-	expression tag	UNP A0AAX3C923
B	516	LEU	-	expression tag	UNP A0AAX3C923
B	517	GLU	-	expression tag	UNP A0AAX3C923
B	518	VAL	-	expression tag	UNP A0AAX3C923
B	519	LEU	-	expression tag	UNP A0AAX3C923
B	520	PHE	-	expression tag	UNP A0AAX3C923
B	521	GLN	-	expression tag	UNP A0AAX3C923
B	522	GLY	-	expression tag	UNP A0AAX3C923
B	523	PRO	-	expression tag	UNP A0AAX3C923
B	524	GLY	-	expression tag	UNP A0AAX3C923
B	525	HIS	-	expression tag	UNP A0AAX3C923
B	526	HIS	-	expression tag	UNP A0AAX3C923
B	527	HIS	-	expression tag	UNP A0AAX3C923
B	528	HIS	-	expression tag	UNP A0AAX3C923
B	529	HIS	-	expression tag	UNP A0AAX3C923
B	530	HIS	-	expression tag	UNP A0AAX3C923
B	531	HIS	-	expression tag	UNP A0AAX3C923
B	532	HIS	-	expression tag	UNP A0AAX3C923
B	533	SER	-	expression tag	UNP A0AAX3C923
B	534	ALA	-	expression tag	UNP A0AAX3C923
B	535	TRP	-	expression tag	UNP A0AAX3C923
B	536	SER	-	expression tag	UNP A0AAX3C923
B	537	HIS	-	expression tag	UNP A0AAX3C923
B	538	PRO	-	expression tag	UNP A0AAX3C923
B	539	GLN	-	expression tag	UNP A0AAX3C923
B	540	PHE	-	expression tag	UNP A0AAX3C923
B	541	GLU	-	expression tag	UNP A0AAX3C923
B	542	LYS	-	expression tag	UNP A0AAX3C923
B	543	GLY	-	expression tag	UNP A0AAX3C923
B	544	GLY	-	expression tag	UNP A0AAX3C923
B	545	GLY	-	expression tag	UNP A0AAX3C923
B	546	SER	-	expression tag	UNP A0AAX3C923
B	547	GLY	-	expression tag	UNP A0AAX3C923
B	548	GLY	-	expression tag	UNP A0AAX3C923
B	549	GLY	-	expression tag	UNP A0AAX3C923

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Chain	Residue	Modelled	Actual	Comment	Reference
B	550	GLY	-	expression tag	UNP A0AAX3C923
B	551	SER	-	expression tag	UNP A0AAX3C923
B	552	GLY	-	expression tag	UNP A0AAX3C923
B	553	GLY	-	expression tag	UNP A0AAX3C923
B	554	SER	-	expression tag	UNP A0AAX3C923
B	555	ALA	-	expression tag	UNP A0AAX3C923
B	556	TRP	-	expression tag	UNP A0AAX3C923
B	557	SER	-	expression tag	UNP A0AAX3C923
B	558	HIS	-	expression tag	UNP A0AAX3C923
B	559	PRO	-	expression tag	UNP A0AAX3C923
B	560	GLN	-	expression tag	UNP A0AAX3C923
B	561	PHE	-	expression tag	UNP A0AAX3C923
B	562	GLU	-	expression tag	UNP A0AAX3C923
B	563	LYS	-	expression tag	UNP A0AAX3C923
C	99	CYS	GLY	engineered mutation	UNP A0AAX3C923
C	109	CYS	ILE	engineered mutation	UNP A0AAX3C923
C	484	GLY	-	expression tag	UNP A0AAX3C923
C	485	SER	-	expression tag	UNP A0AAX3C923
C	486	GLY	-	expression tag	UNP A0AAX3C923
C	487	TYR	-	expression tag	UNP A0AAX3C923
C	488	ILE	-	expression tag	UNP A0AAX3C923
C	489	PRO	-	expression tag	UNP A0AAX3C923
C	490	GLU	-	expression tag	UNP A0AAX3C923
C	491	ALA	-	expression tag	UNP A0AAX3C923
C	492	PRO	-	expression tag	UNP A0AAX3C923
C	493	ARG	-	expression tag	UNP A0AAX3C923
C	494	ASP	-	expression tag	UNP A0AAX3C923
C	495	GLY	-	expression tag	UNP A0AAX3C923
C	496	GLN	-	expression tag	UNP A0AAX3C923
C	497	ALA	-	expression tag	UNP A0AAX3C923
C	498	TYR	-	expression tag	UNP A0AAX3C923
C	499	VAL	-	expression tag	UNP A0AAX3C923
C	500	ARG	-	expression tag	UNP A0AAX3C923
C	501	LYS	-	expression tag	UNP A0AAX3C923
C	502	ASP	-	expression tag	UNP A0AAX3C923
C	503	GLY	-	expression tag	UNP A0AAX3C923
C	504	GLU	-	expression tag	UNP A0AAX3C923
C	505	TRP	-	expression tag	UNP A0AAX3C923
C	506	VAL	-	expression tag	UNP A0AAX3C923
C	507	LEU	-	expression tag	UNP A0AAX3C923
C	508	LEU	-	expression tag	UNP A0AAX3C923
C	509	SER	-	expression tag	UNP A0AAX3C923

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Chain	Residue	Modelled	Actual	Comment	Reference
C	510	THR	-	expression tag	UNP A0AAX3C923
C	511	PHE	-	expression tag	UNP A0AAX3C923
C	512	LEU	-	expression tag	UNP A0AAX3C923
C	513	GLY	-	expression tag	UNP A0AAX3C923
C	514	ARG	-	expression tag	UNP A0AAX3C923
C	515	SER	-	expression tag	UNP A0AAX3C923
C	516	LEU	-	expression tag	UNP A0AAX3C923
C	517	GLU	-	expression tag	UNP A0AAX3C923
C	518	VAL	-	expression tag	UNP A0AAX3C923
C	519	LEU	-	expression tag	UNP A0AAX3C923
C	520	PHE	-	expression tag	UNP A0AAX3C923
C	521	GLN	-	expression tag	UNP A0AAX3C923
C	522	GLY	-	expression tag	UNP A0AAX3C923
C	523	PRO	-	expression tag	UNP A0AAX3C923
C	524	GLY	-	expression tag	UNP A0AAX3C923
C	525	HIS	-	expression tag	UNP A0AAX3C923
C	526	HIS	-	expression tag	UNP A0AAX3C923
C	527	HIS	-	expression tag	UNP A0AAX3C923
C	528	HIS	-	expression tag	UNP A0AAX3C923
C	529	HIS	-	expression tag	UNP A0AAX3C923
C	530	HIS	-	expression tag	UNP A0AAX3C923
C	531	HIS	-	expression tag	UNP A0AAX3C923
C	532	HIS	-	expression tag	UNP A0AAX3C923
C	533	SER	-	expression tag	UNP A0AAX3C923
C	534	ALA	-	expression tag	UNP A0AAX3C923
C	535	TRP	-	expression tag	UNP A0AAX3C923
C	536	SER	-	expression tag	UNP A0AAX3C923
C	537	HIS	-	expression tag	UNP A0AAX3C923
C	538	PRO	-	expression tag	UNP A0AAX3C923
C	539	GLN	-	expression tag	UNP A0AAX3C923
C	540	PHE	-	expression tag	UNP A0AAX3C923
C	541	GLU	-	expression tag	UNP A0AAX3C923
C	542	LYS	-	expression tag	UNP A0AAX3C923
C	543	GLY	-	expression tag	UNP A0AAX3C923
C	544	GLY	-	expression tag	UNP A0AAX3C923
C	545	GLY	-	expression tag	UNP A0AAX3C923
C	546	SER	-	expression tag	UNP A0AAX3C923
C	547	GLY	-	expression tag	UNP A0AAX3C923
C	548	GLY	-	expression tag	UNP A0AAX3C923
C	549	GLY	-	expression tag	UNP A0AAX3C923
C	550	GLY	-	expression tag	UNP A0AAX3C923
C	551	SER	-	expression tag	UNP A0AAX3C923

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Chain	Residue	Modelled	Actual	Comment	Reference
C	552	GLY	-	expression tag	UNP A0AAX3C923
C	553	GLY	-	expression tag	UNP A0AAX3C923
C	554	SER	-	expression tag	UNP A0AAX3C923
C	555	ALA	-	expression tag	UNP A0AAX3C923
C	556	TRP	-	expression tag	UNP A0AAX3C923
C	557	SER	-	expression tag	UNP A0AAX3C923
C	558	HIS	-	expression tag	UNP A0AAX3C923
C	559	PRO	-	expression tag	UNP A0AAX3C923
C	560	GLN	-	expression tag	UNP A0AAX3C923
C	561	PHE	-	expression tag	UNP A0AAX3C923
C	562	GLU	-	expression tag	UNP A0AAX3C923
C	563	LYS	-	expression tag	UNP A0AAX3C923

- Molecule 2 is a protein called Antibody 22F5 Heavy Chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	D	119	Total	C	H	N	O	S	0	0
			1801	581	878	159	177	6		
2	F	119	Total	C	H	N	O	S	0	0
			1801	581	878	159	177	6		
2	I	119	Total	C	H	N	O	S	0	0
			1801	581	878	159	177	6		

- Molecule 3 is a protein called Antibody 22F5 Kappa Light Chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	E	111	Total	C	H	N	O	S	0	0
			1706	542	846	145	170	3		
3	G	111	Total	C	H	N	O	S	0	0
			1706	542	846	145	170	3		
3	H	111	Total	C	H	N	O	S	0	0
			1706	542	846	145	170	3		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

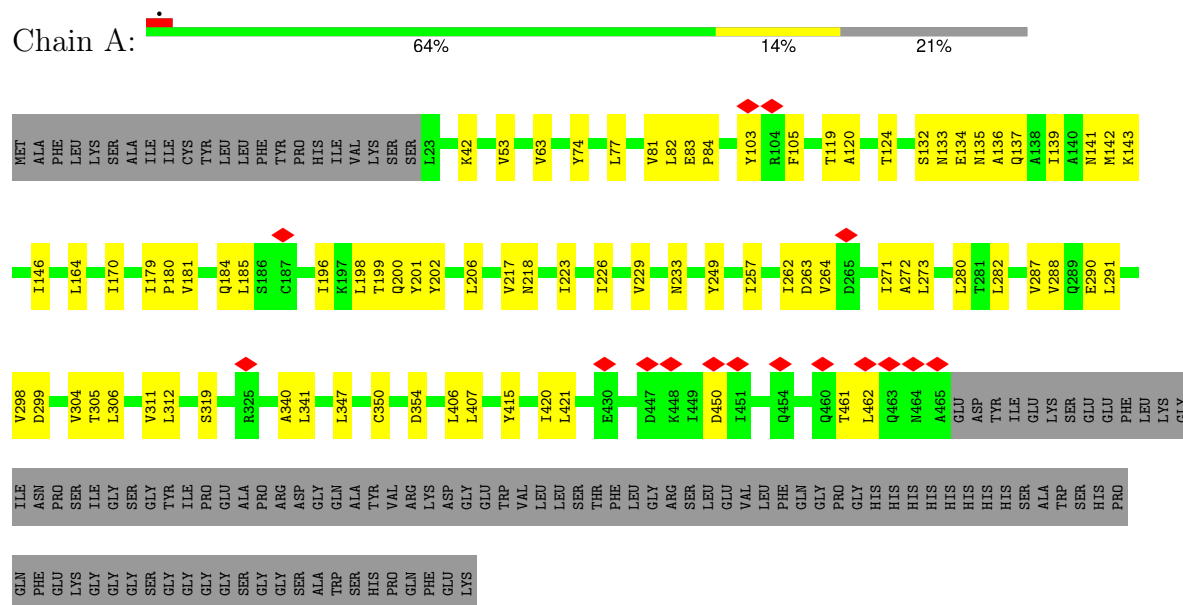


Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	H	N	O	0
			28	8	14	1	5	
4	B	1	Total	C	H	N	O	0
			28	8	14	1	5	
4	C	1	Total	C	H	N	O	0
			28	8	14	1	5	

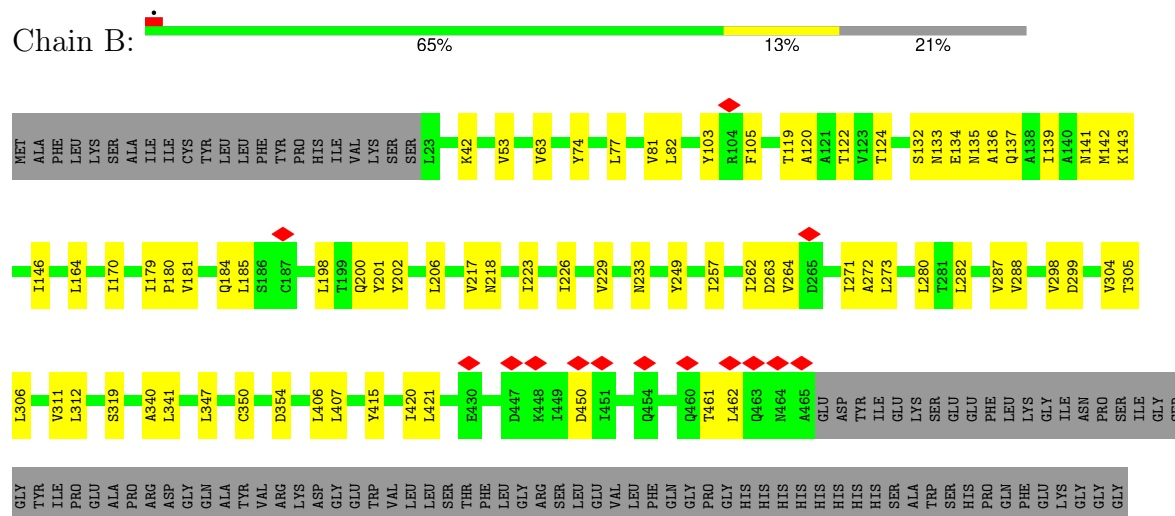
3 Residue-property plots [i](#)

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: Fusion glycoprotein F0



• Molecule 1: Fusion glycoprotein F0



Response	Percentage
Yes, the U.S. is a democracy	47%
No, the U.S. is not a democracy	8%
Don't know	45%

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	245019	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS TUNDRA	Depositor
Voltage (kV)	100	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30.72	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	1.637	Depositor
Minimum map value	-1.148	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.041	Depositor
Recommended contour level	0.324	Depositor
Map size (\AA)	384.0, 384.0, 384.0	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.5, 1.5, 1.5	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.15	0/3420	0.39	0/4653
1	B	0.16	0/3420	0.39	0/4653
1	C	0.16	0/3420	0.39	0/4653
2	D	0.14	0/947	0.40	0/1285
2	F	0.14	0/947	0.40	0/1285
2	I	0.14	0/947	0.40	0/1285
3	E	0.14	0/879	0.40	0/1193
3	G	0.14	0/879	0.40	0/1193
3	H	0.14	0/879	0.40	0/1193
All	All	0.15	0/15738	0.39	0/21393

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	3375	3425	3424	64	0
1	B	3375	3425	3424	63	0
1	C	3375	3425	3424	66	0
2	D	923	878	877	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	923	878	877	14	0
2	I	923	878	877	11	0
3	E	860	846	848	14	0
3	G	860	846	848	13	0
3	H	860	846	848	14	0
4	A	14	14	13	0	0
4	B	14	14	13	0	0
4	C	14	14	13	0	0
All	All	15516	15489	15486	265	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 9.

All (265) 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:C:132:SER:OG	1:C:262:ILE:HD11	1.95	0.67
3:G:20:THR:HG23	3:G:74:THR:HG22	1.77	0.67
1:A:132:SER:OG	1:A:262:ILE:HD11	1.95	0.67
3:E:20:THR:HG23	3:E:74:THR:HG22	1.77	0.66
3:H:20:THR:HG23	3:H:74:THR:HG22	1.77	0.66
1:B:132:SER:OG	1:B:262:ILE:HD11	1.95	0.66
1:C:81:VAL:HG13	1:C:82:LEU:CD2	2.27	0.65
1:A:81:VAL:HG13	1:A:82:LEU:CD2	2.27	0.65
1:B:81:VAL:HG13	1:B:82:LEU:CD2	2.27	0.64
1:A:63:VAL:O	1:A:63:VAL:HG12	2.01	0.61
1:C:461:THR:HG23	1:C:462:LEU:HD23	1.82	0.60
1:B:461:THR:HG23	1:B:462:LEU:HD23	1.82	0.60
1:C:63:VAL:HG12	1:C:63:VAL:O	2.01	0.60
1:A:461:THR:HG23	1:A:462:LEU:HD23	1.82	0.60
1:C:133:ASN:O	1:C:137:GLN:OE1	2.20	0.60
1:B:63:VAL:HG12	1:B:63:VAL:O	2.01	0.60
1:A:133:ASN:O	1:A:137:GLN:OE1	2.20	0.59
1:B:133:ASN:O	1:B:137:GLN:OE1	2.20	0.59
1:B:264:VAL:HG12	1:B:271:ILE:HG22	1.87	0.57
1:A:202:TYR:O	1:A:206:LEU:HD23	2.05	0.56
1:C:81:VAL:HG13	1:C:82:LEU:HD23	1.87	0.56
1:A:81:VAL:HG13	1:A:82:LEU:HD23	1.87	0.56
1:A:202:TYR:CZ	1:A:206:LEU:HD21	2.41	0.56
1:B:202:TYR:O	1:B:206:LEU:HD23	2.05	0.56
1:B:81:VAL:HG13	1:B:82:LEU:HD23	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:VAL:HG12	1:A:271:ILE:HG22	1.87	0.56
1:B:202:TYR:CZ	1:B:206:LEU:HD21	2.41	0.56
1:C:202:TYR:CZ	1:C:206:LEU:HD21	2.41	0.56
1:C:202:TYR:O	1:C:206:LEU:HD23	2.05	0.56
1:C:264:VAL:HG12	1:C:271:ILE:HG22	1.87	0.56
2:F:70:THR:HG22	2:F:71:ARG:N	2.21	0.55
2:I:70:THR:HG22	2:I:71:ARG:N	2.21	0.55
1:A:312:LEU:HD11	1:A:319:SER:HB3	1.89	0.55
2:D:70:THR:HG22	2:D:71:ARG:N	2.21	0.55
1:B:170:ILE:HD11	1:B:201:TYR:CE2	2.42	0.55
1:A:170:ILE:HD11	1:A:201:TYR:CE2	2.41	0.55
1:C:170:ILE:HD11	1:C:201:TYR:CE2	2.41	0.55
1:A:340:ALA:C	1:A:341:LEU:HD22	2.32	0.55
1:C:461:THR:HG23	1:C:462:LEU:CD2	2.37	0.55
1:B:340:ALA:C	1:B:341:LEU:HD22	2.32	0.55
1:C:312:LEU:HD11	1:C:319:SER:HB3	1.89	0.55
2:F:87:THR:HG23	2:F:110:THR:HA	1.89	0.55
2:D:87:THR:HG23	2:D:110:THR:HA	1.89	0.54
1:A:461:THR:HG23	1:A:462:LEU:CD2	2.37	0.54
1:B:312:LEU:HD11	1:B:319:SER:HB3	1.89	0.54
2:I:87:THR:HG23	2:I:110:THR:HA	1.90	0.54
1:C:181:VAL:HG22	1:C:181:VAL:O	2.08	0.54
1:C:340:ALA:C	1:C:341:LEU:HD22	2.32	0.54
1:C:407:LEU:HD22	1:C:415:TYR:CE2	2.43	0.54
1:B:272:ALA:C	1:B:273:LEU:HD22	2.33	0.54
1:B:407:LEU:HD22	1:B:415:TYR:CE2	2.43	0.54
1:B:461:THR:HG23	1:B:462:LEU:CD2	2.37	0.54
1:A:181:VAL:O	1:A:181:VAL:HG22	2.08	0.54
1:B:181:VAL:HG22	1:B:181:VAL:O	2.08	0.54
1:C:272:ALA:C	1:C:273:LEU:HD22	2.33	0.54
2:D:60:VAL:HG12	2:D:62:LYS:H	1.73	0.54
1:A:407:LEU:HD22	1:A:415:TYR:CE2	2.43	0.54
1:C:74:TYR:CE2	1:C:198:LEU:HD11	2.43	0.54
2:F:60:VAL:HG12	2:F:62:LYS:H	1.73	0.54
2:I:60:VAL:HG12	2:I:62:LYS:H	1.73	0.53
1:A:74:TYR:CE2	1:A:198:LEU:HD11	2.43	0.53
1:B:42:LYS:HD2	1:B:280:LEU:HD13	1.91	0.53
1:A:272:ALA:C	1:A:273:LEU:HD22	2.33	0.53
1:B:74:TYR:CD2	1:B:198:LEU:HD11	2.44	0.53
1:A:74:TYR:CD2	1:A:198:LEU:HD11	2.44	0.52
1:A:42:LYS:HD2	1:A:280:LEU:HD13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:TYR:CE2	1:B:198:LEU:HD11	2.43	0.52
1:B:170:ILE:HD12	1:B:170:ILE:H	1.75	0.52
1:C:42:LYS:HD2	1:C:280:LEU:HD13	1.91	0.52
1:A:217:VAL:HG23	1:A:218:ASN:ND2	2.25	0.52
1:B:217:VAL:HG23	1:B:218:ASN:ND2	2.25	0.52
2:F:34:MET:HE3	2:F:92:CYS:HB2	1.92	0.52
1:C:74:TYR:CD2	1:C:198:LEU:HD11	2.44	0.51
1:C:280:LEU:HD12	1:C:280:LEU:O	2.10	0.51
1:A:142:MET:HE2	1:A:142:MET:HA	1.93	0.51
1:B:142:MET:HE2	1:B:142:MET:HA	1.93	0.51
1:C:142:MET:HE2	1:C:142:MET:HA	1.93	0.51
1:C:217:VAL:HG23	1:C:218:ASN:ND2	2.25	0.51
1:C:170:ILE:HD12	1:C:170:ILE:H	1.75	0.51
1:A:170:ILE:H	1:A:170:ILE:HD12	1.75	0.51
1:C:312:LEU:HD12	1:C:312:LEU:C	2.37	0.50
2:D:34:MET:HE3	2:D:92:CYS:HB2	1.92	0.50
1:A:280:LEU:HD12	1:A:280:LEU:O	2.10	0.50
2:I:34:MET:HE3	2:I:92:CYS:HB2	1.92	0.50
1:C:226:ILE:O	1:C:229:VAL:HG22	2.11	0.50
1:A:298:VAL:O	1:A:299:ASP:OD1	2.30	0.50
1:C:179:ILE:N	1:C:180:PRO:HD2	2.27	0.50
1:A:226:ILE:O	1:A:229:VAL:HG22	2.11	0.50
1:B:262:ILE:HG23	1:B:263:ASP:N	2.27	0.50
1:B:280:LEU:O	1:B:280:LEU:HD12	2.10	0.50
1:C:262:ILE:HG23	1:C:263:ASP:N	2.27	0.50
1:C:298:VAL:O	1:C:299:ASP:OD1	2.30	0.50
1:B:312:LEU:C	1:B:312:LEU:HD12	2.36	0.50
1:A:262:ILE:HG23	1:A:263:ASP:N	2.27	0.49
1:B:179:ILE:N	1:B:180:PRO:HD2	2.27	0.49
1:C:119:THR:HG22	1:C:120:ALA:N	2.27	0.49
1:A:120:ALA:O	1:A:124:THR:HG23	2.13	0.49
3:E:8:PRO:O	3:E:101:THR:HG22	2.12	0.49
1:A:119:THR:HG22	1:A:120:ALA:N	2.27	0.49
1:B:226:ILE:O	1:B:229:VAL:HG22	2.11	0.49
1:B:298:VAL:O	1:B:299:ASP:OD1	2.30	0.49
1:B:133:ASN:O	1:B:136:ALA:HB3	2.13	0.49
1:C:77:LEU:O	1:C:81:VAL:HG12	2.13	0.49
1:C:407:LEU:HD13	1:C:415:TYR:CD2	2.48	0.49
3:E:83:LEU:HD11	3:E:105:ILE:HG23	1.95	0.49
1:A:312:LEU:C	1:A:312:LEU:HD12	2.37	0.49
1:A:420:ILE:C	1:A:421:LEU:HD12	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:81:VAL:HG13	1:C:82:LEU:HD22	1.95	0.49
3:G:83:LEU:HD11	3:G:105:ILE:HG23	1.95	0.49
1:A:179:ILE:N	1:A:180:PRO:HD2	2.27	0.49
1:C:120:ALA:O	1:C:124:THR:HG23	2.13	0.49
1:B:120:ALA:O	1:B:124:THR:HG23	2.13	0.49
1:B:280:LEU:HD12	1:B:280:LEU:C	2.37	0.49
1:C:136:ALA:O	1:C:139:ILE:HG22	2.13	0.49
3:H:8:PRO:O	3:H:101:THR:HG22	2.12	0.49
3:H:83:LEU:HD11	3:H:105:ILE:HG23	1.95	0.49
1:A:407:LEU:HD13	1:A:415:TYR:CD2	2.48	0.48
1:B:119:THR:HG22	1:B:120:ALA:N	2.27	0.48
3:G:8:PRO:O	3:G:101:THR:HG22	2.12	0.48
1:B:77:LEU:O	1:B:81:VAL:HG12	2.13	0.48
1:A:133:ASN:O	1:A:136:ALA:HB3	2.13	0.48
1:A:280:LEU:HD12	1:A:280:LEU:C	2.37	0.48
1:A:77:LEU:O	1:A:81:VAL:HG12	2.13	0.48
1:B:420:ILE:C	1:B:421:LEU:HD12	2.38	0.48
1:C:134:GLU:HG2	1:C:135:ASN:N	2.28	0.48
2:D:36:TRP:HB3	2:D:48:MET:HE2	1.96	0.48
1:A:81:VAL:HG13	1:A:82:LEU:HD22	1.95	0.48
3:E:59:PRO:HB2	3:E:61:ARG:HE	1.79	0.48
1:A:53:VAL:HG11	1:A:146:ILE:HD11	1.96	0.48
1:B:134:GLU:HG2	1:B:135:ASN:N	2.28	0.48
1:C:133:ASN:O	1:C:136:ALA:HB3	2.13	0.48
1:C:280:LEU:HD12	1:C:280:LEU:C	2.37	0.48
1:B:407:LEU:HD13	1:B:415:TYR:CD2	2.48	0.48
3:G:59:PRO:HB2	3:G:61:ARG:HE	1.79	0.48
1:B:136:ALA:O	1:B:139:ILE:HG22	2.13	0.48
1:C:53:VAL:HG11	1:C:146:ILE:HD11	1.96	0.48
2:I:36:TRP:HB3	2:I:48:MET:HE2	1.96	0.48
1:A:134:GLU:HG2	1:A:135:ASN:N	2.28	0.48
1:A:184:GLN:C	1:A:185:LEU:HD22	2.39	0.47
1:B:53:VAL:HG11	1:B:146:ILE:HD11	1.96	0.47
1:C:184:GLN:C	1:C:185:LEU:HD22	2.40	0.47
2:F:36:TRP:HB3	2:F:48:MET:HE2	1.96	0.47
3:H:59:PRO:HB2	3:H:61:ARG:HE	1.79	0.47
1:C:420:ILE:C	1:C:421:LEU:HD12	2.38	0.47
1:A:136:ALA:O	1:A:139:ILE:HG22	2.13	0.47
1:B:143:LYS:HA	1:B:146:ILE:HG22	1.96	0.47
2:D:70:THR:HG22	2:D:71:ARG:H	1.79	0.47
3:E:6:GLN:HE21	3:E:101:THR:HG23	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:GLN:C	1:B:185:LEU:HD22	2.40	0.47
2:I:70:THR:HG22	2:I:71:ARG:H	1.79	0.47
1:A:143:LYS:HA	1:A:146:ILE:HG22	1.97	0.47
1:A:200:GLN:HA	1:B:233:ASN:ND2	2.30	0.47
1:C:406:LEU:H	1:C:406:LEU:HD23	1.80	0.47
3:H:6:GLN:HE21	3:H:101:THR:HG23	1.80	0.46
1:A:406:LEU:H	1:A:406:LEU:HD23	1.80	0.46
1:B:406:LEU:HD23	1:B:406:LEU:H	1.80	0.46
1:B:200:GLN:HA	1:C:233:ASN:ND2	2.30	0.46
2:D:67:VAL:CG1	2:D:82:LEU:HD13	2.46	0.46
2:F:21:SER:HG	2:F:79:TYR:HD1	1.61	0.46
2:F:70:THR:HG22	2:F:71:ARG:H	1.79	0.46
3:G:6:GLN:HE21	3:G:101:THR:HG23	1.80	0.46
1:A:282:LEU:C	1:A:282:LEU:HD23	2.41	0.46
1:A:287:VAL:HG22	1:A:288:VAL:N	2.31	0.46
1:C:141:ASN:C	1:C:142:MET:HE2	2.41	0.46
1:C:143:LYS:HA	1:C:146:ILE:HG22	1.97	0.46
1:C:287:VAL:HG22	1:C:288:VAL:N	2.31	0.46
2:F:67:VAL:CG1	2:F:82:LEU:HD13	2.46	0.46
1:A:141:ASN:C	1:A:142:MET:HE2	2.41	0.46
1:B:141:ASN:C	1:B:142:MET:HE2	2.41	0.46
3:G:20:THR:CG2	3:G:74:THR:HG22	2.45	0.46
1:B:81:VAL:HG13	1:B:82:LEU:HD22	1.95	0.46
1:B:282:LEU:C	1:B:282:LEU:HD23	2.41	0.46
1:B:287:VAL:HG22	1:B:288:VAL:N	2.31	0.46
2:I:82:LEU:HD12	2:I:82(A):SER:H	1.81	0.45
1:C:282:LEU:C	1:C:282:LEU:HD23	2.41	0.45
2:I:67:VAL:CG1	2:I:82:LEU:HD13	2.46	0.45
3:H:20:THR:CG2	3:H:74:THR:HG22	2.45	0.45
1:B:223:ILE:HD12	1:B:257:ILE:HG21	1.98	0.45
1:A:223:ILE:HD12	1:A:257:ILE:HG21	1.98	0.45
1:C:264:VAL:HG12	1:C:271:ILE:CG2	2.47	0.45
3:E:10:SER:O	3:E:11:LEU:HD23	2.17	0.45
2:F:82:LEU:HD12	2:F:82(A):SER:H	1.82	0.45
1:A:304:VAL:HG12	1:A:305:THR:N	2.32	0.45
1:C:350:CYS:HA	1:C:354:ASP:O	2.17	0.45
2:D:82:LEU:HD12	2:D:82(A):SER:H	1.82	0.45
3:H:10:SER:O	3:H:11:LEU:HD23	2.17	0.45
1:A:350:CYS:HA	1:A:354:ASP:O	2.17	0.44
1:B:304:VAL:HG12	1:B:305:THR:N	2.32	0.44
2:F:94:ARG:HD2	2:F:95:ALA:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:ASN:ND2	1:C:200:GLN:HA	2.32	0.44
1:C:223:ILE:HD12	1:C:257:ILE:HG21	1.98	0.44
1:B:340:ALA:O	1:B:341:LEU:HD22	2.18	0.44
1:B:350:CYS:HA	1:B:354:ASP:O	2.17	0.44
1:C:304:VAL:HG12	1:C:305:THR:N	2.32	0.44
3:G:10:SER:O	3:G:11:LEU:HD23	2.17	0.44
3:H:96:THR:HG22	3:H:97:PHE:N	2.33	0.44
2:I:94:ARG:HD2	2:I:95:ALA:N	2.33	0.44
1:A:264:VAL:HG12	1:A:271:ILE:CG2	2.47	0.44
1:A:306:LEU:HD23	1:A:306:LEU:H	1.83	0.44
1:B:264:VAL:HG12	1:B:271:ILE:CG2	2.47	0.44
3:E:20:THR:CG2	3:E:74:THR:HG22	2.45	0.44
3:E:27(B):LEU:HD23	3:E:27(B):LEU:H	1.83	0.44
3:G:96:THR:HG22	3:G:97:PHE:N	2.33	0.44
1:A:119:THR:HG22	1:A:120:ALA:H	1.83	0.44
1:C:119:THR:HG22	1:C:120:ALA:H	1.83	0.44
2:D:94:ARG:HD2	2:D:95:ALA:N	2.33	0.44
3:G:27(B):LEU:H	3:G:27(B):LEU:HD23	1.83	0.44
3:H:27(B):LEU:HD23	3:H:27(B):LEU:H	1.83	0.43
3:E:96:THR:HG22	3:E:97:PHE:N	2.33	0.43
1:A:340:ALA:O	1:A:341:LEU:HD22	2.18	0.43
1:C:340:ALA:O	1:C:341:LEU:HD22	2.18	0.43
3:E:6:GLN:NE2	3:E:101:THR:HG23	2.34	0.43
1:A:347:LEU:HD22	1:B:450:ASP:OD1	2.18	0.43
1:B:119:THR:HG22	1:B:120:ALA:H	1.83	0.43
1:C:139:ILE:HD13	1:C:164:LEU:HD13	2.00	0.43
1:B:139:ILE:HD13	1:B:164:LEU:HD13	2.00	0.43
3:H:6:GLN:NE2	3:H:101:THR:HG23	2.34	0.43
1:A:139:ILE:HD13	1:A:164:LEU:HD13	2.00	0.43
3:E:58:VAL:HG12	3:E:59:PRO:O	2.19	0.43
3:G:58:VAL:HG12	3:G:59:PRO:O	2.19	0.43
1:C:306:LEU:HD23	1:C:306:LEU:H	1.83	0.42
3:G:6:GLN:NE2	3:G:101:THR:HG23	2.34	0.42
2:F:100:TRP:O	2:F:100:TRP:CD1	2.72	0.42
1:B:306:LEU:H	1:B:306:LEU:HD23	1.83	0.42
2:D:100:TRP:O	2:D:100:TRP:CD1	2.72	0.42
3:H:58:VAL:HG12	3:H:59:PRO:O	2.19	0.42
2:I:100:TRP:O	2:I:100:TRP:CD1	2.72	0.42
1:A:450:ASP:OD1	1:C:347:LEU:HD22	2.19	0.42
1:A:103:TYR:CZ	1:A:105:PHE:HE1	2.38	0.42
1:B:103:TYR:CZ	1:B:105:PHE:HE1	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:27(B):LEU:HD23	3:G:27(B):LEU:N	2.35	0.42
2:D:68:THR:HG22	2:D:69:MET:N	2.35	0.41
1:A:249:TYR:CD1	1:A:249:TYR:C	2.98	0.41
1:B:249:TYR:CD1	1:B:249:TYR:C	2.98	0.41
1:C:249:TYR:CD1	1:C:249:TYR:C	2.98	0.41
2:I:68:THR:HG22	2:I:69:MET:N	2.35	0.41
2:F:12:LYS:HG3	2:F:18:VAL:HG12	2.03	0.41
1:A:272:ALA:O	1:A:273:LEU:HD22	2.21	0.41
1:B:272:ALA:O	1:B:273:LEU:HD22	2.21	0.41
1:C:103:TYR:CZ	1:C:105:PHE:HE1	2.38	0.41
3:E:27(B):LEU:HD23	3:E:27(B):LEU:N	2.35	0.41
3:H:27(B):LEU:HD23	3:H:27(B):LEU:N	2.35	0.41
1:B:347:LEU:HD22	1:C:450:ASP:OD1	2.21	0.41
3:E:78:VAL:HG22	3:E:79:GLN:N	2.36	0.41
2:D:12:LYS:HG3	2:D:18:VAL:HG12	2.03	0.41
1:A:311:VAL:O	1:A:311:VAL:HG23	2.21	0.41
1:C:50:LYS:C	1:C:51:LEU:HD12	2.46	0.41
1:C:311:VAL:HG23	1:C:311:VAL:O	2.21	0.41
2:F:68:THR:HG22	2:F:69:MET:N	2.35	0.41
1:C:173:GLU:O	1:C:176:ASN:OD1	2.40	0.40
1:C:217:VAL:HG23	1:C:218:ASN:HD22	1.87	0.40
1:A:196:ILE:O	1:A:199:THR:HG22	2.21	0.40
1:C:83:GLU:N	1:C:84:PRO:HD2	2.36	0.40
3:H:8:PRO:CG	3:H:11:LEU:HD21	2.52	0.40
1:A:83:GLU:N	1:A:84:PRO:HD2	2.36	0.40
1:A:290:GLU:HG3	1:A:291:LEU:N	2.37	0.40
1:B:311:VAL:O	1:B:311:VAL:HG23	2.21	0.40
3:E:8:PRO:CG	3:E:11:LEU:HD21	2.52	0.40
2:F:9:ALA:HA	2:F:108:LEU:O	2.22	0.40
3:H:78:VAL:HG22	3:H:79:GLN:N	2.36	0.40
1:B:122:THR:HG22	1:B:218:ASN:OD1	2.22	0.40
1:B:312:LEU:HD12	1:B:312:LEU:O	2.22	0.40
1:C:272:ALA:O	1:C:273:LEU:HD22	2.21	0.40
1:C:290:GLU:HG3	1:C:291:LEU:N	2.37	0.40
3:G:8:PRO:CG	3:G:11:LEU:HD21	2.52	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	A	441/563 (78%)	420 (95%)	21 (5%)	0	100	100
1	B	441/563 (78%)	420 (95%)	21 (5%)	0	100	100
1	C	441/563 (78%)	420 (95%)	21 (5%)	0	100	100
2	D	117/216 (54%)	112 (96%)	5 (4%)	0	100	100
2	F	117/216 (54%)	112 (96%)	5 (4%)	0	100	100
2	I	117/216 (54%)	112 (96%)	5 (4%)	0	100	100
3	E	109/219 (50%)	105 (96%)	4 (4%)	0	100	100
3	G	109/219 (50%)	105 (96%)	4 (4%)	0	100	100
3	H	109/219 (50%)	105 (96%)	4 (4%)	0	100	100
All	All	2001/2994 (67%)	1911 (96%)	90 (4%)	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	A	383/480 (80%)	383 (100%)	0	100	100
1	B	383/480 (80%)	383 (100%)	0	100	100
1	C	383/480 (80%)	383 (100%)	0	100	100
2	D	97/183 (53%)	97 (100%)	0	100	100
2	F	97/183 (53%)	97 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	I	97/183 (53%)	97 (100%)	0	100	100
3	E	97/197 (49%)	97 (100%)	0	100	100
3	G	97/197 (49%)	97 (100%)	0	100	100
3	H	97/197 (49%)	97 (100%)	0	100	100
All	All	1731/2580 (67%)	1731 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	135	ASN
1	A	177	ASN
1	A	214	GLN
1	A	253	HIS
1	A	289	GLN
1	B	177	ASN
1	B	214	GLN
1	B	289	GLN
1	C	135	ASN
1	C	177	ASN
1	C	214	GLN
1	C	253	HIS
1	C	289	GLN
2	D	35	HIS

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

3 ligands are 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	$\# Z > 2$
4	NAG	C	1000	1	14,14,15	0.70	0	17,19,21	0.82	0
4	NAG	A	1000	1	14,14,15	0.69	0	17,19,21	0.82	0
4	NAG	B	1000	1	14,14,15	0.69	0	17,19,21	0.83	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	1000	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1000	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1000	1	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1000	NAG	O5-C5-C6-O6
4	B	1000	NAG	O5-C5-C6-O6
4	C	1000	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

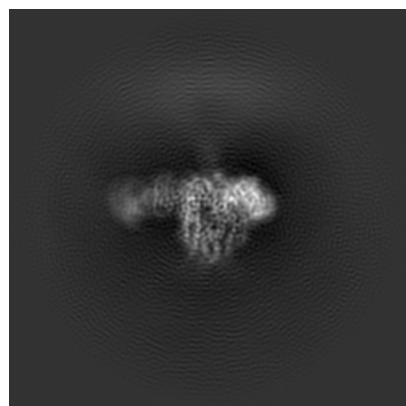
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-49948. These allow visual inspection of the internal detail of the map and identification of artifacts.

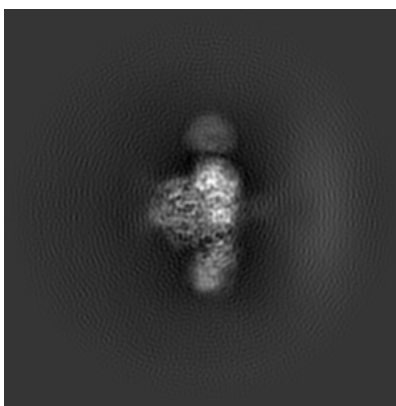
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

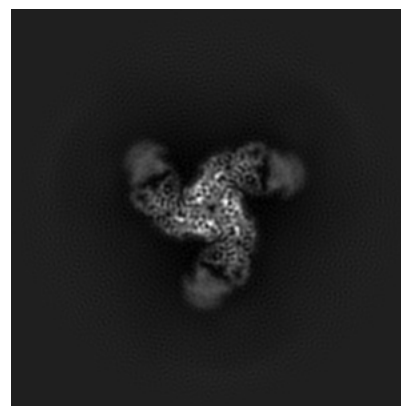
6.1.1 Primary map



X

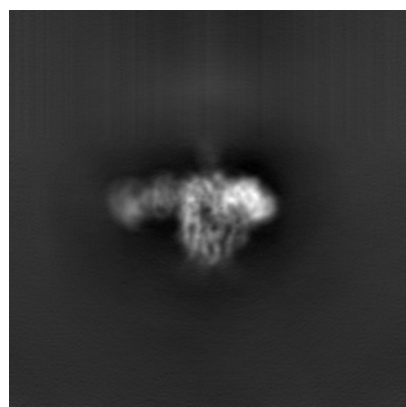


Y

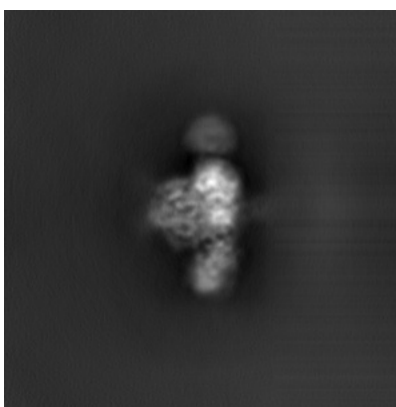


Z

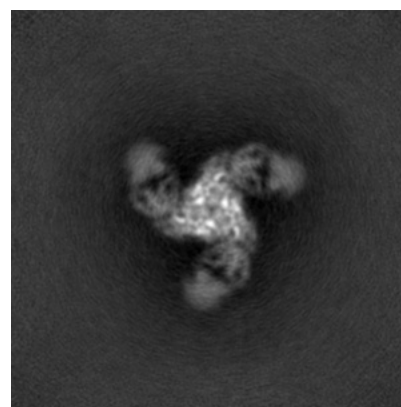
6.1.2 Raw map



X



Y

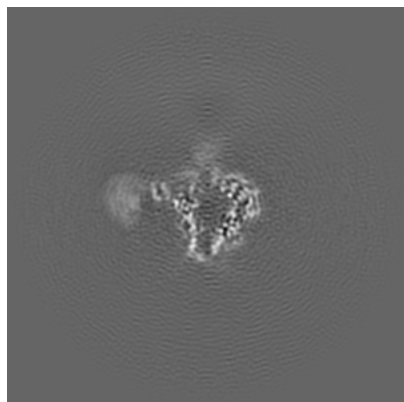


Z

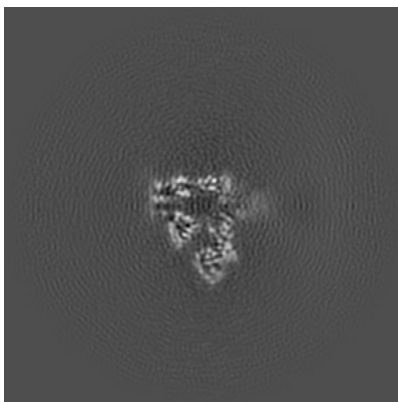
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

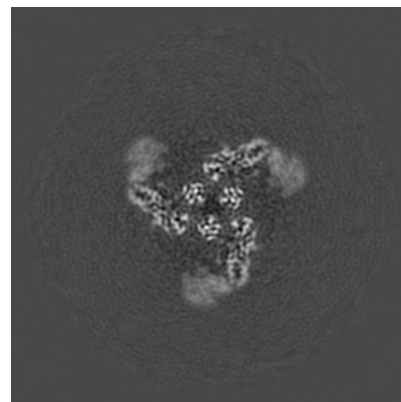
6.2.1 Primary map



X Index: 128

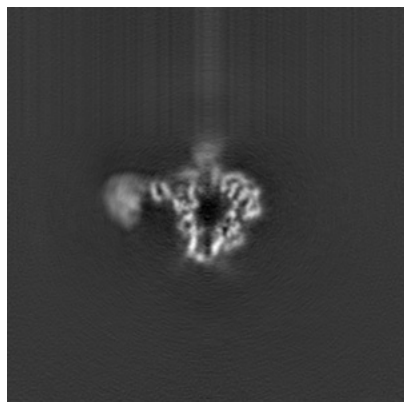


Y Index: 128

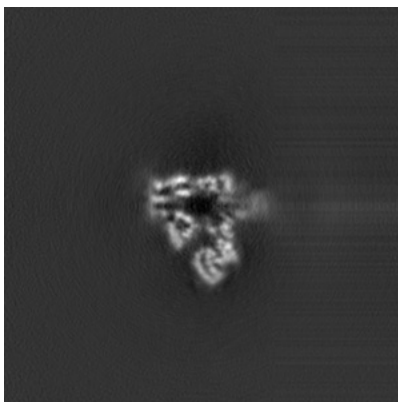


Z Index: 128

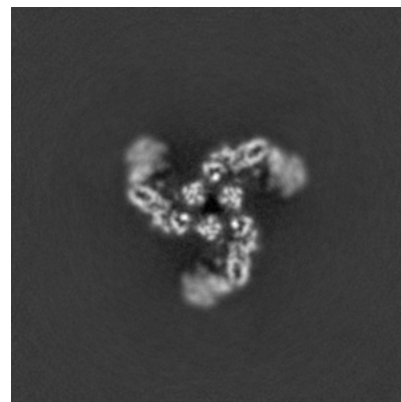
6.2.2 Raw map



X Index: 128



Y Index: 128

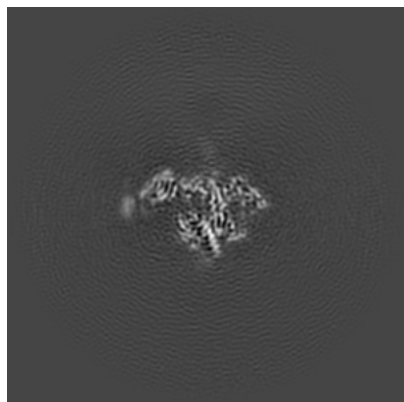


Z Index: 128

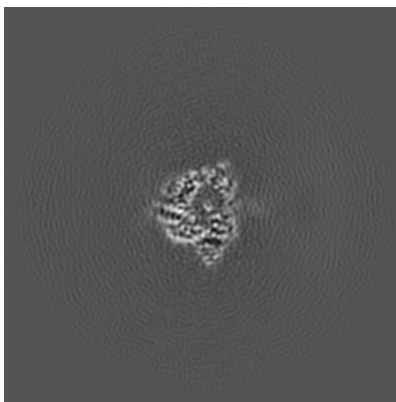
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

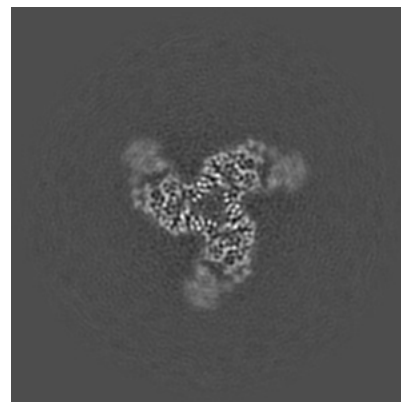
6.3.1 Primary map



X Index: 137

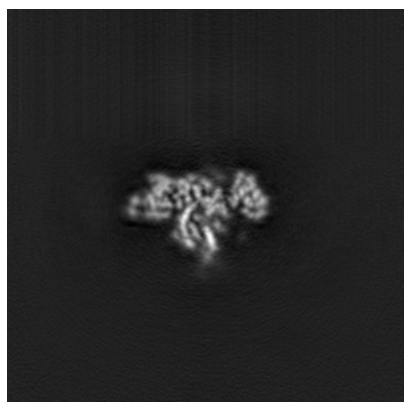


Y Index: 120

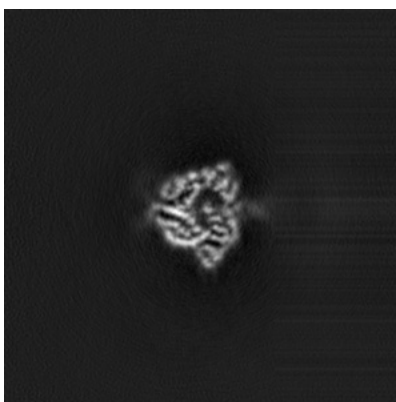


Z Index: 134

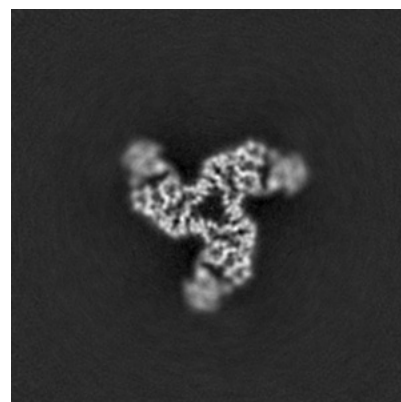
6.3.2 Raw map



X Index: 144



Y Index: 120

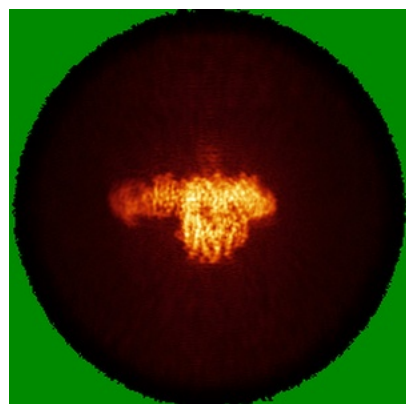


Z Index: 134

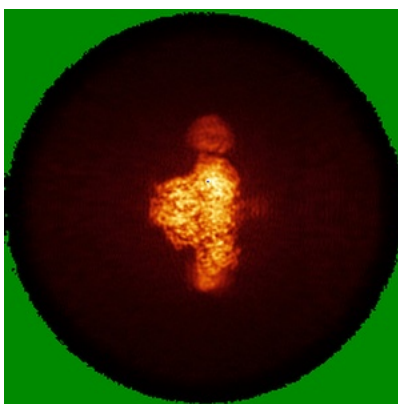
The images above show the largest variance slices of the map in three orthogonal directions.

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

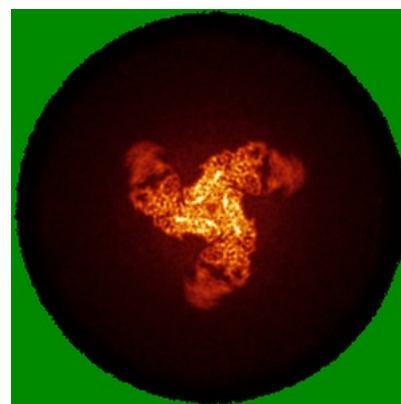
6.4.1 Primary map



X

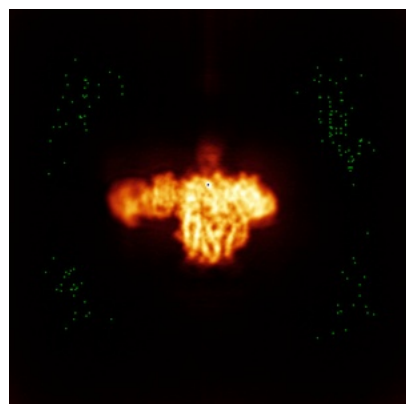


Y

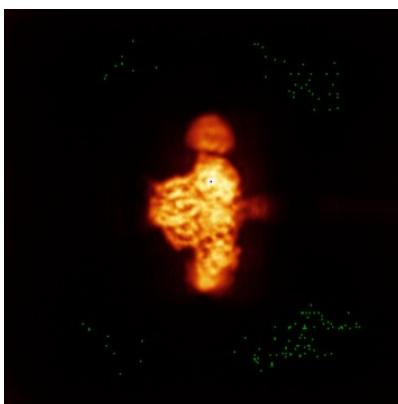


Z

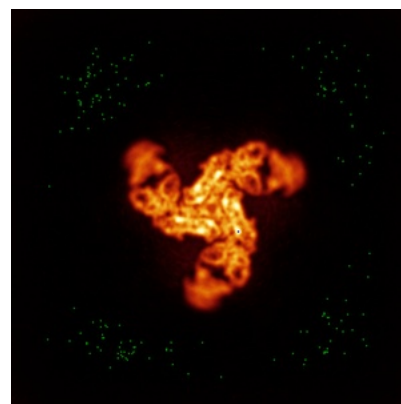
6.4.2 Raw map



X



Y

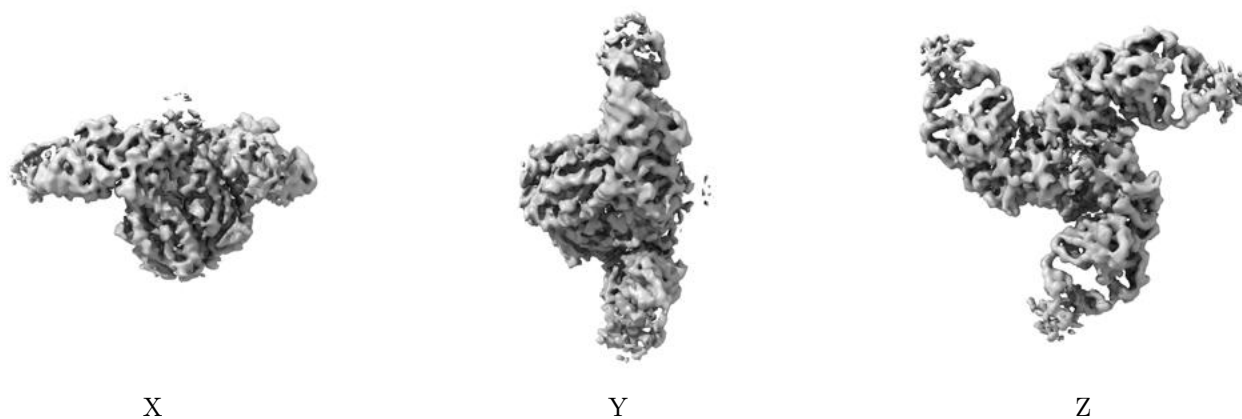


Z

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.

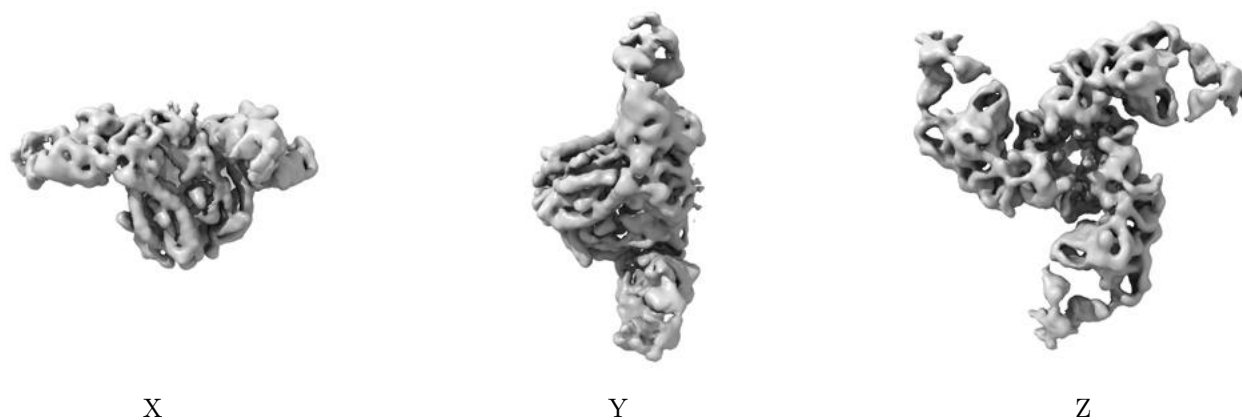
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.324. 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.

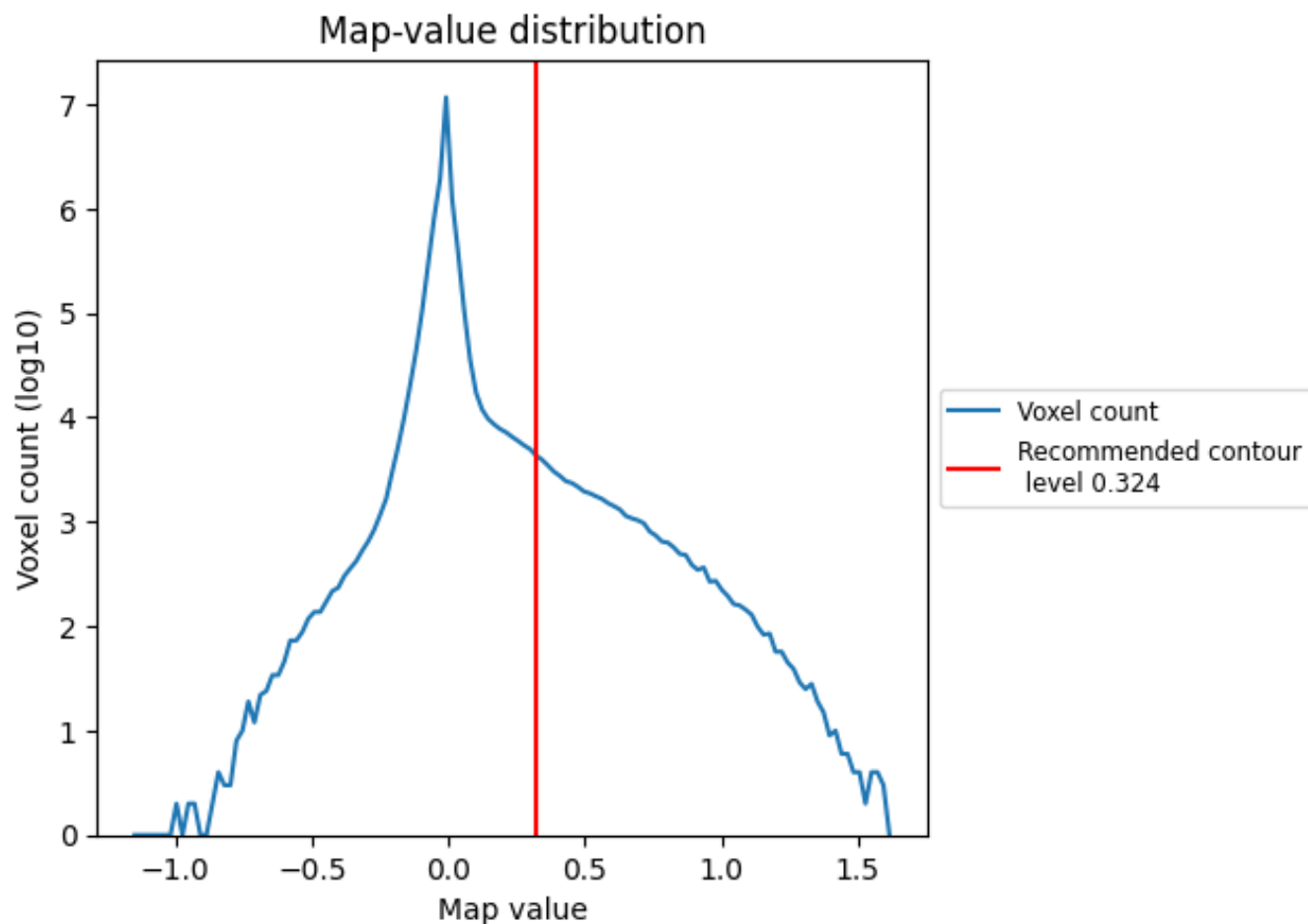
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

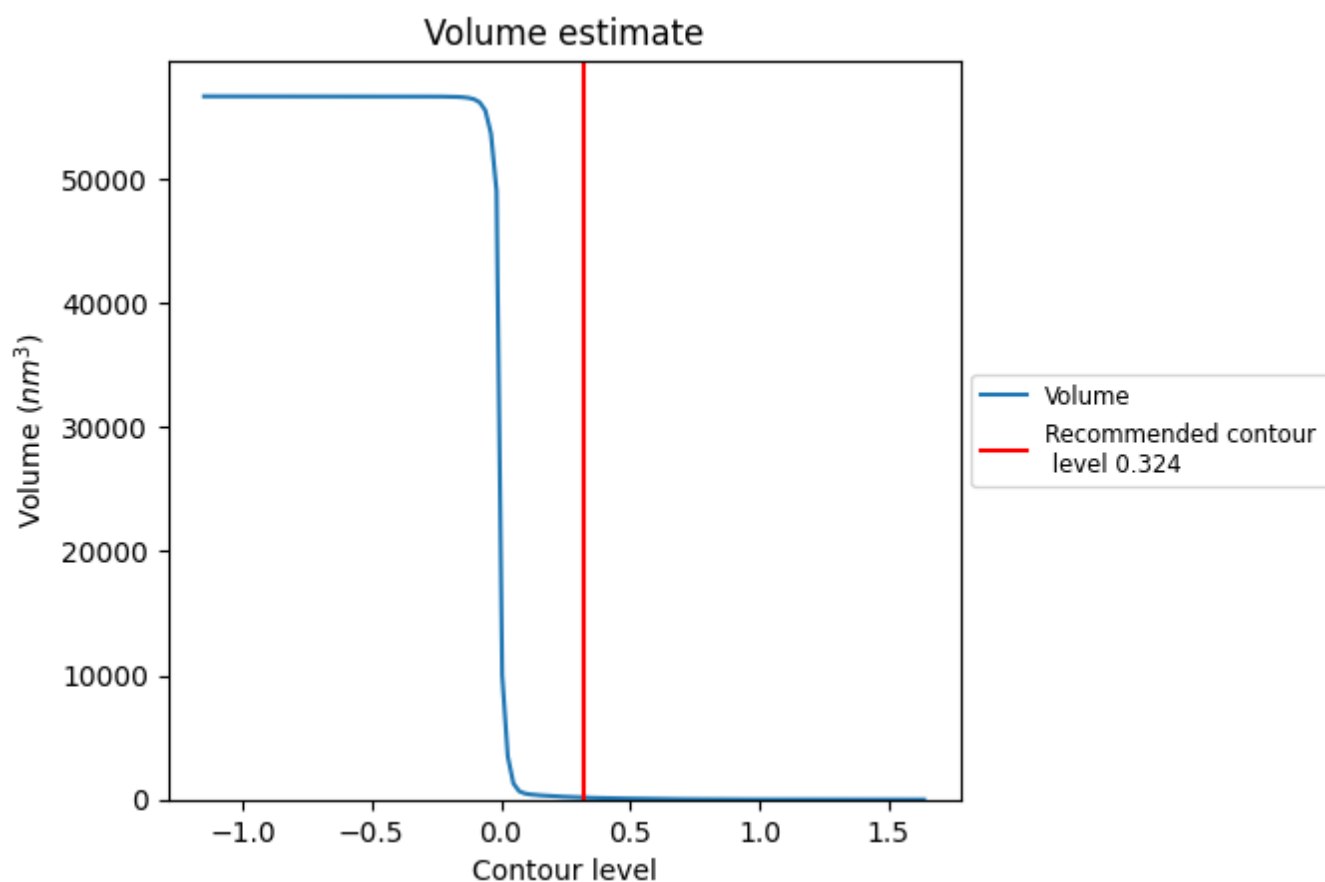
This section contains the results of statistical analysis of the map.

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.

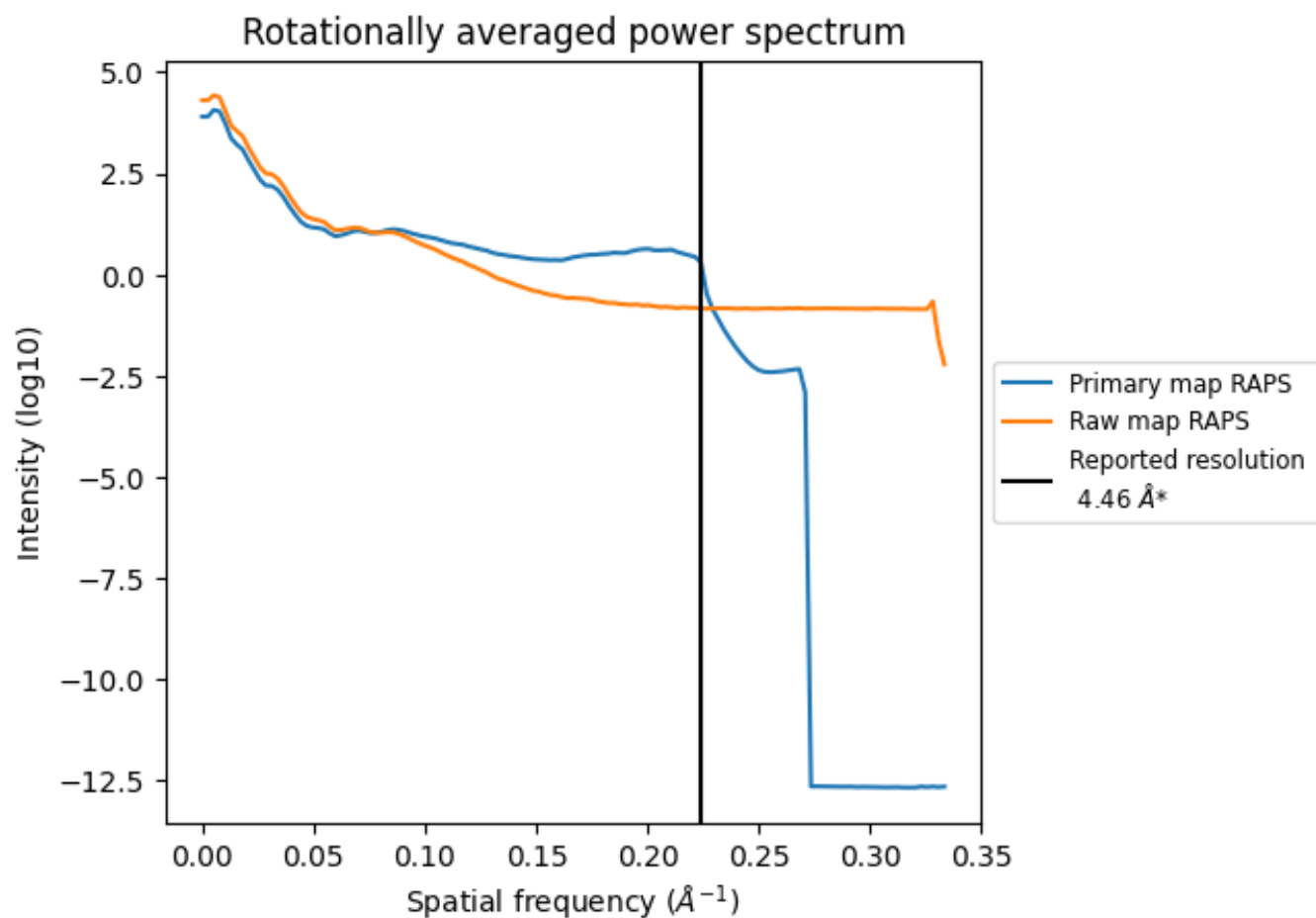
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 160 nm³; this corresponds to an approximate mass of 144 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 ⓘ

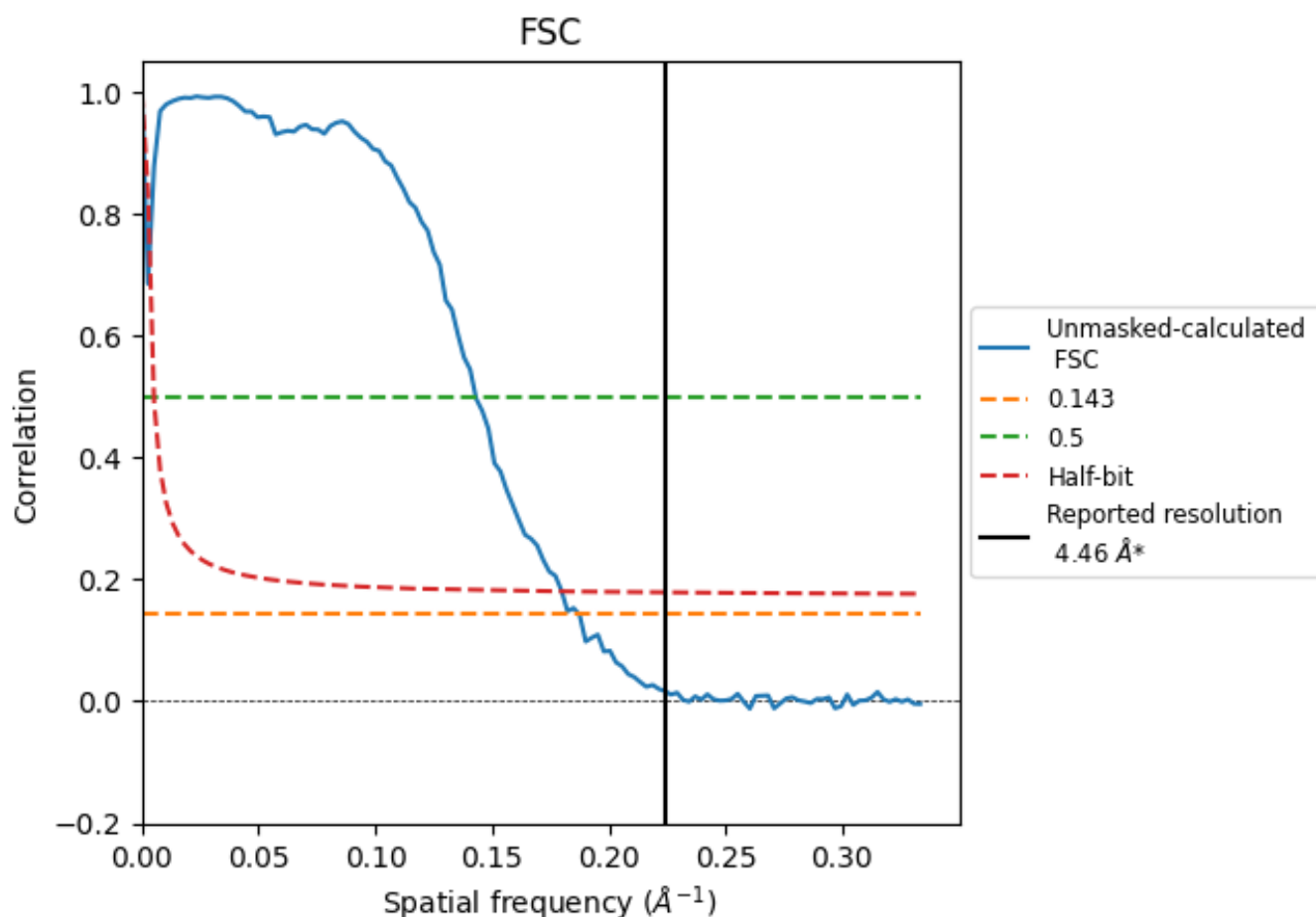


*Reported resolution corresponds to spatial frequency of 0.224 Å⁻¹

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 0.224 Å⁻¹

8.2 Resolution estimates [i](#)

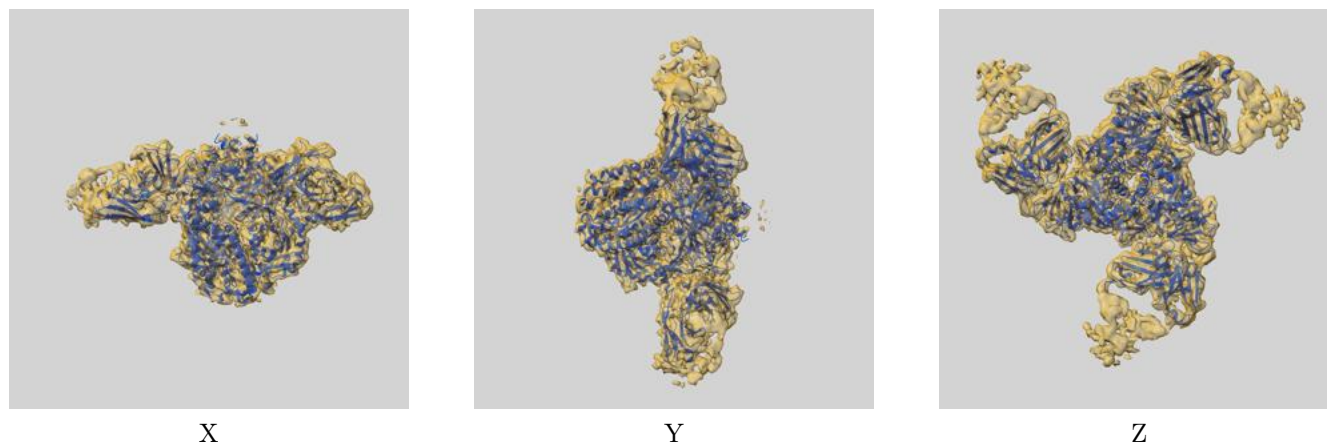
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.46	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	5.34	6.99	303.03

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 5.34 differs from the reported value 4.46 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-49948 and PDB model 9NZ2. Per-residue inclusion information can be found in section [3](#) on page [12](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.324 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](#)



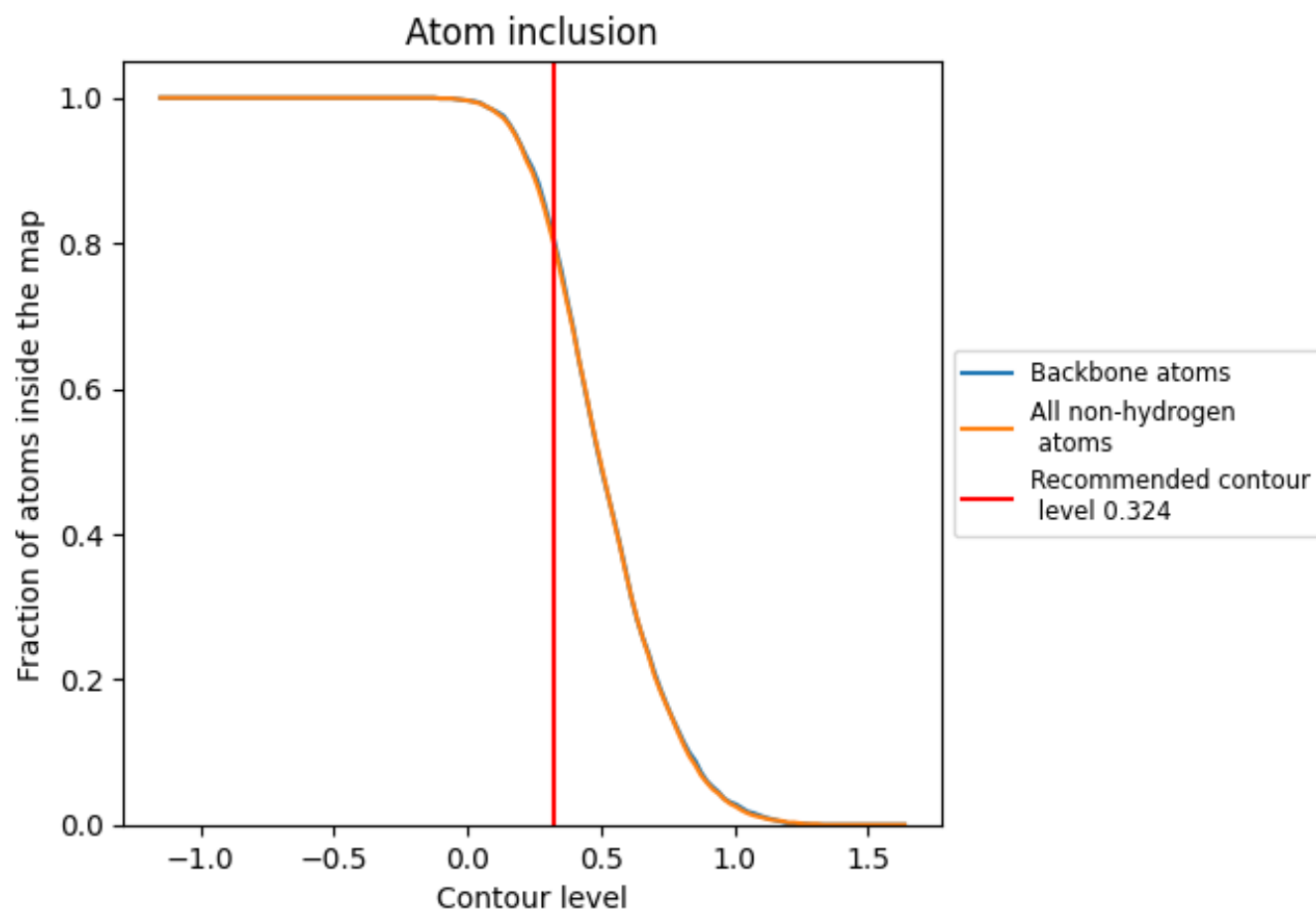
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.324).

9.4 Atom inclusion ⓘ



At the recommended contour level, 81% of all backbone atoms, 80% 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 (0.324) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.7990	<div><div></div></div> 0.3540
A	<div><div></div></div> 0.8020	<div><div></div></div> 0.3660
B	<div><div></div></div> 0.8040	<div><div></div></div> 0.3610
C	<div><div></div></div> 0.8000	<div><div></div></div> 0.3610
D	<div><div></div></div> 0.8410	<div><div></div></div> 0.3560
E	<div><div></div></div> 0.7750	<div><div></div></div> 0.3260
F	<div><div></div></div> 0.8420	<div><div></div></div> 0.3510
G	<div><div></div></div> 0.7680	<div><div></div></div> 0.3230
H	<div><div></div></div> 0.7690	<div><div></div></div> 0.3190
I	<div><div></div></div> 0.8420	<div><div></div></div> 0.3530

1.0

0.0

<0.0