



## wwPDB EM Validation Summary Report ⓘ

Apr 15, 2026 – 02:27 AM UTC

PDB ID : 9Q71 / pdb\_00009q71  
EMDB ID : EMD-72283  
Title : Structure of the Measles Virus Fusion Glycoprotein Ectodomain in Postfusion Conformation Bound to Neutralizing Antibody H8  
Authors : Zyla, D.; Niemeyer, G.; Porotto, M.; Saphire, E.O.  
Deposited on : 2025-08-22  
Resolution : 2.80 Å (reported)  
Based on initial models : ., 8UTF

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev132  
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

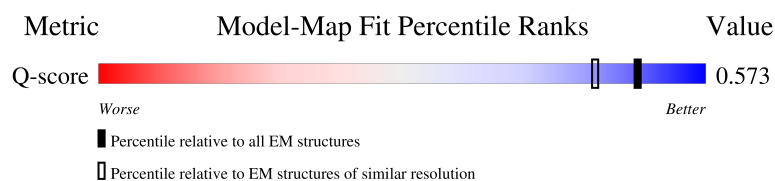
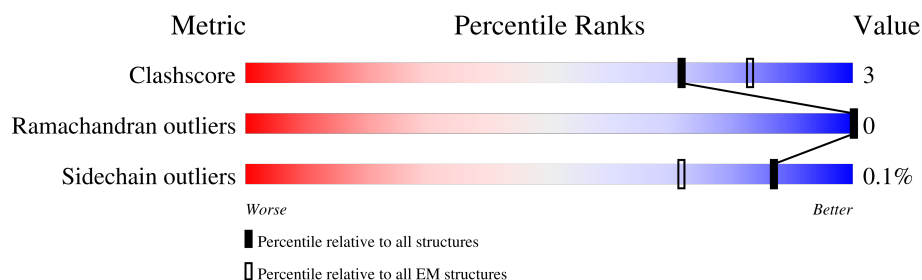
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.











Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11806 ( 2.30 - 3.30 )

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	532	13% 86%
1	B	532	59% 6% 36%
1	C	532	11% 86%
1	D	532	59% 6% 36%

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Mol	Chain	Length	Quality of chain
1	E	532	 13% 86%
1	F	532	 60% 36%
2	G	476	 21% 76%
2	I	476	 23% 75%
2	K	476	 22% 76%
3	H	236	 39% 7% 53%
3	J	236	 40% 6% 53%
3	L	236	 40% 6% 53%

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14828 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	A	72	Total	C	N	O	S	0	0
			565	356	105	100	4		
1	B	342	Total	C	N	O	S	0	0
			2608	1646	439	510	13		
1	C	72	Total	C	N	O	S	0	0
			565	356	105	100	4		
1	D	342	Total	C	N	O	S	0	0
			2608	1646	439	510	13		
1	E	72	Total	C	N	O	S	0	0
			565	356	105	100	4		
1	F	342	Total	C	N	O	S	0	0
			2608	1646	439	510	13		

There are 234 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	170	GLY	GLU	conflict	UNP Q786F3
A	455	GLY	GLU	conflict	UNP Q786F3
A	496	GLY	-	expression tag	UNP Q786F3
A	497	VAL	-	expression tag	UNP Q786F3
A	498	ASP	-	expression tag	UNP Q786F3
A	499	ASP	-	expression tag	UNP Q786F3
A	500	ASP	-	expression tag	UNP Q786F3
A	501	ASP	-	expression tag	UNP Q786F3
A	502	LYS	-	expression tag	UNP Q786F3
A	503	ALA	-	expression tag	UNP Q786F3
A	504	GLY	-	expression tag	UNP Q786F3
A	505	TRP	-	expression tag	UNP Q786F3
A	506	SER	-	expression tag	UNP Q786F3
A	507	HIS	-	expression tag	UNP Q786F3
A	508	PRO	-	expression tag	UNP Q786F3
A	509	GLN	-	expression tag	UNP Q786F3
A	510	PHE	-	expression tag	UNP Q786F3
A	511	GLU	-	expression tag	UNP Q786F3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	512	LYS	-	expression tag	UNP Q786F3
A	513	GLY	-	expression tag	UNP Q786F3
A	514	GLY	-	expression tag	UNP Q786F3
A	515	GLY	-	expression tag	UNP Q786F3
A	516	SER	-	expression tag	UNP Q786F3
A	517	GLY	-	expression tag	UNP Q786F3
A	518	GLY	-	expression tag	UNP Q786F3
A	519	GLY	-	expression tag	UNP Q786F3
A	520	SER	-	expression tag	UNP Q786F3
A	521	GLY	-	expression tag	UNP Q786F3
A	522	GLY	-	expression tag	UNP Q786F3
A	523	GLY	-	expression tag	UNP Q786F3
A	524	SER	-	expression tag	UNP Q786F3
A	525	TRP	-	expression tag	UNP Q786F3
A	526	SER	-	expression tag	UNP Q786F3
A	527	HIS	-	expression tag	UNP Q786F3
A	528	PRO	-	expression tag	UNP Q786F3
A	529	GLN	-	expression tag	UNP Q786F3
A	530	PHE	-	expression tag	UNP Q786F3
A	531	GLU	-	expression tag	UNP Q786F3
A	532	LYS	-	expression tag	UNP Q786F3
B	170	GLY	GLU	conflict	UNP Q786F3
B	455	GLY	GLU	conflict	UNP Q786F3
B	496	GLY	-	expression tag	UNP Q786F3
B	497	VAL	-	expression tag	UNP Q786F3
B	498	ASP	-	expression tag	UNP Q786F3
B	499	ASP	-	expression tag	UNP Q786F3
B	500	ASP	-	expression tag	UNP Q786F3
B	501	ASP	-	expression tag	UNP Q786F3
B	502	LYS	-	expression tag	UNP Q786F3
B	503	ALA	-	expression tag	UNP Q786F3
B	504	GLY	-	expression tag	UNP Q786F3
B	505	TRP	-	expression tag	UNP Q786F3
B	506	SER	-	expression tag	UNP Q786F3
B	507	HIS	-	expression tag	UNP Q786F3
B	508	PRO	-	expression tag	UNP Q786F3
B	509	GLN	-	expression tag	UNP Q786F3
B	510	PHE	-	expression tag	UNP Q786F3
B	511	GLU	-	expression tag	UNP Q786F3
B	512	LYS	-	expression tag	UNP Q786F3
B	513	GLY	-	expression tag	UNP Q786F3
B	514	GLY	-	expression tag	UNP Q786F3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	515	GLY	-	expression tag	UNP Q786F3
B	516	SER	-	expression tag	UNP Q786F3
B	517	GLY	-	expression tag	UNP Q786F3
B	518	GLY	-	expression tag	UNP Q786F3
B	519	GLY	-	expression tag	UNP Q786F3
B	520	SER	-	expression tag	UNP Q786F3
B	521	GLY	-	expression tag	UNP Q786F3
B	522	GLY	-	expression tag	UNP Q786F3
B	523	GLY	-	expression tag	UNP Q786F3
B	524	SER	-	expression tag	UNP Q786F3
B	525	TRP	-	expression tag	UNP Q786F3
B	526	SER	-	expression tag	UNP Q786F3
B	527	HIS	-	expression tag	UNP Q786F3
B	528	PRO	-	expression tag	UNP Q786F3
B	529	GLN	-	expression tag	UNP Q786F3
B	530	PHE	-	expression tag	UNP Q786F3
B	531	GLU	-	expression tag	UNP Q786F3
B	532	LYS	-	expression tag	UNP Q786F3
C	170	GLY	GLU	conflict	UNP Q786F3
C	455	GLY	GLU	conflict	UNP Q786F3
C	496	GLY	-	expression tag	UNP Q786F3
C	497	VAL	-	expression tag	UNP Q786F3
C	498	ASP	-	expression tag	UNP Q786F3
C	499	ASP	-	expression tag	UNP Q786F3
C	500	ASP	-	expression tag	UNP Q786F3
C	501	ASP	-	expression tag	UNP Q786F3
C	502	LYS	-	expression tag	UNP Q786F3
C	503	ALA	-	expression tag	UNP Q786F3
C	504	GLY	-	expression tag	UNP Q786F3
C	505	TRP	-	expression tag	UNP Q786F3
C	506	SER	-	expression tag	UNP Q786F3
C	507	HIS	-	expression tag	UNP Q786F3
C	508	PRO	-	expression tag	UNP Q786F3
C	509	GLN	-	expression tag	UNP Q786F3
C	510	PHE	-	expression tag	UNP Q786F3
C	511	GLU	-	expression tag	UNP Q786F3
C	512	LYS	-	expression tag	UNP Q786F3
C	513	GLY	-	expression tag	UNP Q786F3
C	514	GLY	-	expression tag	UNP Q786F3
C	515	GLY	-	expression tag	UNP Q786F3
C	516	SER	-	expression tag	UNP Q786F3
C	517	GLY	-	expression tag	UNP Q786F3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	518	GLY	-	expression tag	UNP Q786F3
C	519	GLY	-	expression tag	UNP Q786F3
C	520	SER	-	expression tag	UNP Q786F3
C	521	GLY	-	expression tag	UNP Q786F3
C	522	GLY	-	expression tag	UNP Q786F3
C	523	GLY	-	expression tag	UNP Q786F3
C	524	SER	-	expression tag	UNP Q786F3
C	525	TRP	-	expression tag	UNP Q786F3
C	526	SER	-	expression tag	UNP Q786F3
C	527	HIS	-	expression tag	UNP Q786F3
C	528	PRO	-	expression tag	UNP Q786F3
C	529	GLN	-	expression tag	UNP Q786F3
C	530	PHE	-	expression tag	UNP Q786F3
C	531	GLU	-	expression tag	UNP Q786F3
C	532	LYS	-	expression tag	UNP Q786F3
D	170	GLY	GLU	conflict	UNP Q786F3
D	455	GLY	GLU	conflict	UNP Q786F3
D	496	GLY	-	expression tag	UNP Q786F3
D	497	VAL	-	expression tag	UNP Q786F3
D	498	ASP	-	expression tag	UNP Q786F3
D	499	ASP	-	expression tag	UNP Q786F3
D	500	ASP	-	expression tag	UNP Q786F3
D	501	ASP	-	expression tag	UNP Q786F3
D	502	LYS	-	expression tag	UNP Q786F3
D	503	ALA	-	expression tag	UNP Q786F3
D	504	GLY	-	expression tag	UNP Q786F3
D	505	TRP	-	expression tag	UNP Q786F3
D	506	SER	-	expression tag	UNP Q786F3
D	507	HIS	-	expression tag	UNP Q786F3
D	508	PRO	-	expression tag	UNP Q786F3
D	509	GLN	-	expression tag	UNP Q786F3
D	510	PHE	-	expression tag	UNP Q786F3
D	511	GLU	-	expression tag	UNP Q786F3
D	512	LYS	-	expression tag	UNP Q786F3
D	513	GLY	-	expression tag	UNP Q786F3
D	514	GLY	-	expression tag	UNP Q786F3
D	515	GLY	-	expression tag	UNP Q786F3
D	516	SER	-	expression tag	UNP Q786F3
D	517	GLY	-	expression tag	UNP Q786F3
D	518	GLY	-	expression tag	UNP Q786F3
D	519	GLY	-	expression tag	UNP Q786F3
D	520	SER	-	expression tag	UNP Q786F3

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Chain	Residue	Modelled	Actual	Comment	Reference
D	521	GLY	-	expression tag	UNP Q786F3
D	522	GLY	-	expression tag	UNP Q786F3
D	523	GLY	-	expression tag	UNP Q786F3
D	524	SER	-	expression tag	UNP Q786F3
D	525	TRP	-	expression tag	UNP Q786F3
D	526	SER	-	expression tag	UNP Q786F3
D	527	HIS	-	expression tag	UNP Q786F3
D	528	PRO	-	expression tag	UNP Q786F3
D	529	GLN	-	expression tag	UNP Q786F3
D	530	PHE	-	expression tag	UNP Q786F3
D	531	GLU	-	expression tag	UNP Q786F3
D	532	LYS	-	expression tag	UNP Q786F3
E	170	GLY	GLU	conflict	UNP Q786F3
E	455	GLY	GLU	conflict	UNP Q786F3
E	496	GLY	-	expression tag	UNP Q786F3
E	497	VAL	-	expression tag	UNP Q786F3
E	498	ASP	-	expression tag	UNP Q786F3
E	499	ASP	-	expression tag	UNP Q786F3
E	500	ASP	-	expression tag	UNP Q786F3
E	501	ASP	-	expression tag	UNP Q786F3
E	502	LYS	-	expression tag	UNP Q786F3
E	503	ALA	-	expression tag	UNP Q786F3
E	504	GLY	-	expression tag	UNP Q786F3
E	505	TRP	-	expression tag	UNP Q786F3
E	506	SER	-	expression tag	UNP Q786F3
E	507	HIS	-	expression tag	UNP Q786F3
E	508	PRO	-	expression tag	UNP Q786F3
E	509	GLN	-	expression tag	UNP Q786F3
E	510	PHE	-	expression tag	UNP Q786F3
E	511	GLU	-	expression tag	UNP Q786F3
E	512	LYS	-	expression tag	UNP Q786F3
E	513	GLY	-	expression tag	UNP Q786F3
E	514	GLY	-	expression tag	UNP Q786F3
E	515	GLY	-	expression tag	UNP Q786F3
E	516	SER	-	expression tag	UNP Q786F3
E	517	GLY	-	expression tag	UNP Q786F3
E	518	GLY	-	expression tag	UNP Q786F3
E	519	GLY	-	expression tag	UNP Q786F3
E	520	SER	-	expression tag	UNP Q786F3
E	521	GLY	-	expression tag	UNP Q786F3
E	522	GLY	-	expression tag	UNP Q786F3
E	523	GLY	-	expression tag	UNP Q786F3

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Chain	Residue	Modelled	Actual	Comment	Reference
E	524	SER	-	expression tag	UNP Q786F3
E	525	TRP	-	expression tag	UNP Q786F3
E	526	SER	-	expression tag	UNP Q786F3
E	527	HIS	-	expression tag	UNP Q786F3
E	528	PRO	-	expression tag	UNP Q786F3
E	529	GLN	-	expression tag	UNP Q786F3
E	530	PHE	-	expression tag	UNP Q786F3
E	531	GLU	-	expression tag	UNP Q786F3
E	532	LYS	-	expression tag	UNP Q786F3
F	170	GLY	GLU	conflict	UNP Q786F3
F	455	GLY	GLU	conflict	UNP Q786F3
F	496	GLY	-	expression tag	UNP Q786F3
F	497	VAL	-	expression tag	UNP Q786F3
F	498	ASP	-	expression tag	UNP Q786F3
F	499	ASP	-	expression tag	UNP Q786F3
F	500	ASP	-	expression tag	UNP Q786F3
F	501	ASP	-	expression tag	UNP Q786F3
F	502	LYS	-	expression tag	UNP Q786F3
F	503	ALA	-	expression tag	UNP Q786F3
F	504	GLY	-	expression tag	UNP Q786F3
F	505	TRP	-	expression tag	UNP Q786F3
F	506	SER	-	expression tag	UNP Q786F3
F	507	HIS	-	expression tag	UNP Q786F3
F	508	PRO	-	expression tag	UNP Q786F3
F	509	GLN	-	expression tag	UNP Q786F3
F	510	PHE	-	expression tag	UNP Q786F3
F	511	GLU	-	expression tag	UNP Q786F3
F	512	LYS	-	expression tag	UNP Q786F3
F	513	GLY	-	expression tag	UNP Q786F3
F	514	GLY	-	expression tag	UNP Q786F3
F	515	GLY	-	expression tag	UNP Q786F3
F	516	SER	-	expression tag	UNP Q786F3
F	517	GLY	-	expression tag	UNP Q786F3
F	518	GLY	-	expression tag	UNP Q786F3
F	519	GLY	-	expression tag	UNP Q786F3
F	520	SER	-	expression tag	UNP Q786F3
F	521	GLY	-	expression tag	UNP Q786F3
F	522	GLY	-	expression tag	UNP Q786F3
F	523	GLY	-	expression tag	UNP Q786F3
F	524	SER	-	expression tag	UNP Q786F3
F	525	TRP	-	expression tag	UNP Q786F3
F	526	SER	-	expression tag	UNP Q786F3

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Chain	Residue	Modelled	Actual	Comment	Reference
F	527	HIS	-	expression tag	UNP Q786F3
F	528	PRO	-	expression tag	UNP Q786F3
F	529	GLN	-	expression tag	UNP Q786F3
F	530	PHE	-	expression tag	UNP Q786F3
F	531	GLU	-	expression tag	UNP Q786F3
F	532	LYS	-	expression tag	UNP Q786F3

- Molecule 2 is a protein called mAb H8 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	113	Total	C	N	O	S	0	0
			871	556	146	166	3		
2	I	118	Total	C	N	O	S	0	0
			905	575	151	176	3		
2	K	116	Total	C	N	O	S	0	0
			893	569	149	172	3		

- Molecule 3 is a protein called mAb H8 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	110	Total	C	N	O	S	0	0
			838	531	140	165	2		
3	J	110	Total	C	N	O	S	0	0
			838	531	140	165	2		
3	L	110	Total	C	N	O	S	0	0
			838	531	140	165	2		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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





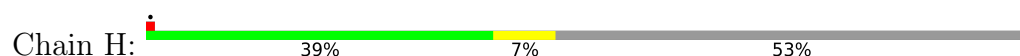




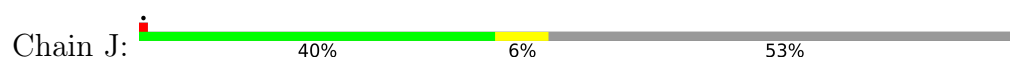


[illegible]

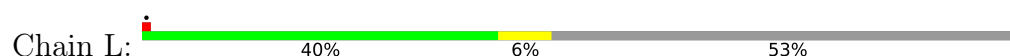
- Molecule 3: mAb H8 light chain

[illegible]

- Molecule 3: mAb H8 light chain

[illegible]

- Molecule 3: mAb H8 light chain



LEU	SER	SER	THR	THR	THR	SER	LEU	LYS	ASP	TYR	GLU	LYS	HIS	VAL	VAL	ALA	CYS	THR	HIS	THR	GLN	GLY	THR	HIS	VAL	GLY	THR	ALA	VAL	GLN	ASP	LEU	SER	GLY	THR	ASP	THR	VAL	THR	VAL	ALA	PRO	SER						
VAL	PHE	ILE	PHE	PRO	SER	GLU	GLN	LEU	LYS	SER	VAL	ALA	VAL	VAL	VAL	VAL	CYS	LEU	ASN	PHE	THR	PRO	ARG	GLU	ALA	LYS	VAL	GLN	TRP	LYS	VAL	ASP	ASN	ALA	LEU	SER	GLY	ASN	SER	GLN	GLU	VAL	THR	ARG	THR	VAL	ALA	ALA	PRO
MET	GLY	TRP	SER	CYS	ILE	ILE	LEU	PHE	VAL	ALA	THR	ALA	HIS	VAL	SER	GLY	THR	ASN	GLY	ASN	L15	A19	T20	T21	Q41	Q42	K43	L51	L77	M78	I79	E84	E85	T88	H94	S95	W96	T100	I109	K110	ARG	THR	VAL	ALA	ALA	PRO			

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	312000	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 ( $e^-/\text{\AA}^2$ )	70	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.702	Depositor
Minimum map value	-0.452	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.0519	Depositor
Map size (Å)	513.92, 513.92, 513.92	wwPDB
Map dimensions	584, 584, 584	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.88, 0.88, 0.88	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	0.11	0/572	0.24	0/773
1	B	0.12	0/2648	0.27	0/3595
1	C	0.11	0/572	0.22	0/773
1	D	0.11	0/2648	0.26	0/3595
1	E	0.10	0/572	0.23	0/773
1	F	0.11	0/2648	0.25	0/3595
2	G	0.10	0/894	0.23	0/1210
2	I	0.11	0/929	0.24	0/1259
2	K	0.10	0/917	0.25	0/1243
3	H	0.12	0/860	0.29	0/1170
3	J	0.10	0/860	0.26	0/1170
3	L	0.11	0/860	0.29	0/1170
All	All	0.11	0/14980	0.26	0/20326

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	565	0	595	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2608	0	2627	24	0
1	C	565	0	595	10	0
1	D	2608	0	2627	26	0
1	E	565	0	595	5	0
1	F	2608	0	2627	20	0
2	G	871	0	837	6	0
2	I	905	0	868	5	0
2	K	893	0	858	6	0
3	H	838	0	813	9	0
3	J	838	0	813	8	0
3	L	838	0	813	9	0
4	A	42	0	39	0	0
4	C	42	0	39	1	0
4	E	42	0	39	0	0
All	All	14828	0	14785	101	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 3.

The worst 5 of 101 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:B:252:SER:H	1:B:255:ASP:HB2	1.52	0.75
1:D:448:LEU:HD11	1:F:202:LEU:HD13	1.76	0.67
2:I:100:GLY:HA3	2:I:106:TYR:HB2	1.80	0.64
1:D:459:VAL:HG12	1:F:179:GLN:HG3	1.82	0.60
3:H:41:GLN:HB2	3:H:51:LEU:HD11	1.83	0.60

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	70/532 (13%)	67 (96%)	3 (4%)	0	100	100
1	B	340/532 (64%)	333 (98%)	7 (2%)	0	100	100
1	C	70/532 (13%)	68 (97%)	2 (3%)	0	100	100
1	D	340/532 (64%)	333 (98%)	7 (2%)	0	100	100
1	E	70/532 (13%)	66 (94%)	4 (6%)	0	100	100
1	F	340/532 (64%)	333 (98%)	7 (2%)	0	100	100
2	G	109/476 (23%)	106 (97%)	3 (3%)	0	100	100
2	I	116/476 (24%)	110 (95%)	6 (5%)	0	100	100
2	K	114/476 (24%)	111 (97%)	3 (3%)	0	100	100
3	H	108/236 (46%)	100 (93%)	8 (7%)	0	100	100
3	J	108/236 (46%)	103 (95%)	5 (5%)	0	100	100
3	L	108/236 (46%)	101 (94%)	7 (6%)	0	100	100
All	All	1893/5328 (36%)	1831 (97%)	62 (3%)	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	64/442 (14%)	64 (100%)	0	100	100
1	B	291/442 (66%)	291 (100%)	0	100	100
1	C	64/442 (14%)	64 (100%)	0	100	100
1	D	291/442 (66%)	291 (100%)	0	100	100
1	E	64/442 (14%)	64 (100%)	0	100	100
1	F	291/442 (66%)	291 (100%)	0	100	100
2	G	91/417 (22%)	91 (100%)	0	100	100
2	I	96/417 (23%)	95 (99%)	1 (1%)	68	88
2	K	94/417 (22%)	94 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	H	93/204 (46%)	93 (100%)	0	100	100
3	J	93/204 (46%)	93 (100%)	0	100	100
3	L	93/204 (46%)	93 (100%)	0	100	100
All	All	1625/4515 (36%)	1624 (100%)	1 (0%)	87	97

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	I	82	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	385	ASN
3	H	93	GLN
3	H	41	GLN
3	H	94	HIS
1	D	158	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](#)

9 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	A	603	1	14,14,15	0.72	0	17,19,21	0.88	0
4	NAG	C	603	1	14,14,15	0.72	0	17,19,21	0.89	0
4	NAG	C	602	1	14,14,15	0.72	0	17,19,21	0.85	0
4	NAG	E	603	1	14,14,15	0.70	0	17,19,21	1.32	1 (5%)
4	NAG	E	601	1	14,14,15	0.72	0	17,19,21	0.78	0
4	NAG	E	602	1	14,14,15	0.72	0	17,19,21	0.84	0
4	NAG	C	601	1	14,14,15	0.72	0	17,19,21	0.82	0
4	NAG	A	601	1	14,14,15	0.71	0	17,19,21	0.87	0
4	NAG	A	602	1	14,14,15	0.71	0	17,19,21	0.85	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	603	1	-	0/6/23/26	0/1/1/1
4	NAG	C	603	1	-	0/6/23/26	0/1/1/1
4	NAG	C	602	1	-	0/6/23/26	0/1/1/1
4	NAG	E	603	1	-	2/6/23/26	0/1/1/1
4	NAG	E	601	1	-	0/6/23/26	0/1/1/1
4	NAG	E	602	1	-	0/6/23/26	0/1/1/1
4	NAG	C	601	1	-	0/6/23/26	0/1/1/1
4	NAG	A	601	1	-	2/6/23/26	0/1/1/1
4	NAG	A	602	1	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	603	NAG	C2-N2-C7	3.36	127.40	122.90
4	A	602	NAG	O5-C1-C2	-2.01	108.19	111.29

There are no chirality outliers.

All (5) torsion outliers are listed below:



Mol	Chain	Res	Type	Atoms
4	A	601	NAG	C8-C7-N2-C2
4	A	601	NAG	O7-C7-N2-C2
4	A	602	NAG	O5-C5-C6-O6
4	E	603	NAG	C1-C2-N2-C7
4	E	603	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	603	NAG	1	0

## 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.

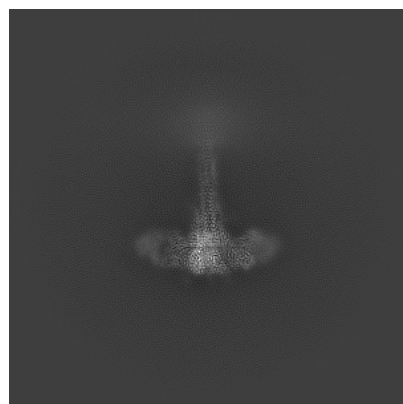
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-72283. These allow visual inspection of the internal detail of the map and identification of artifacts.

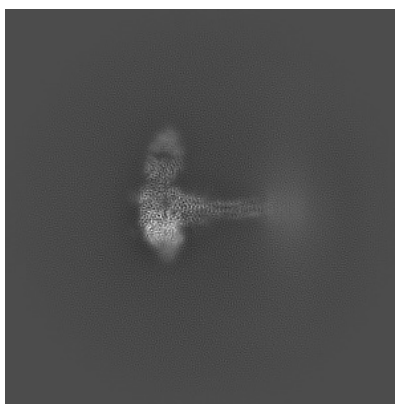
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

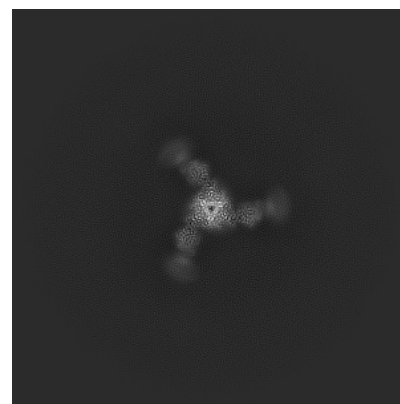
#### 6.1.1 Primary map



X

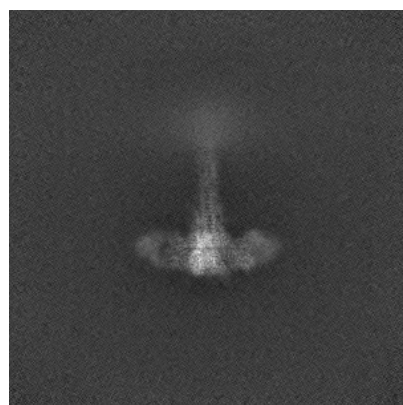


Y



Z

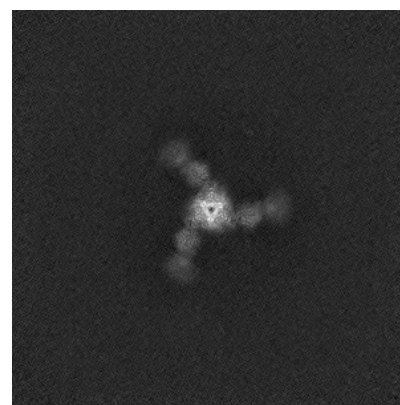
#### 6.1.2 Raw map



X



Y

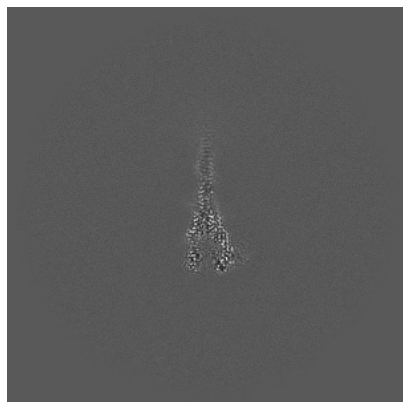


Z

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

## 6.2 Central slices [i](#)

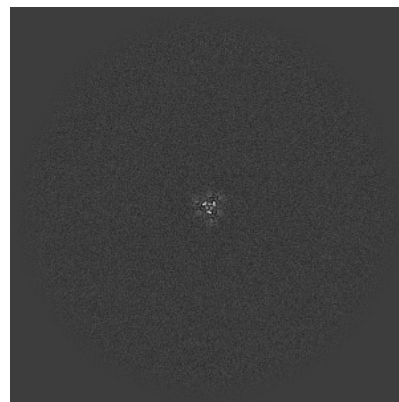
### 6.2.1 Primary map



X Index: 292

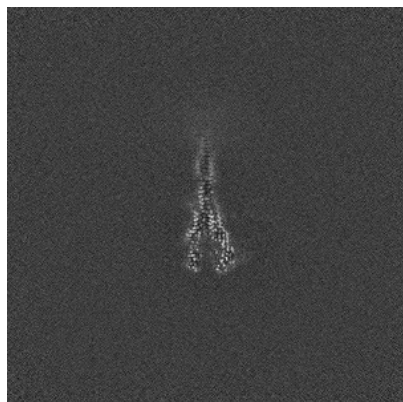


Y Index: 292



Z Index: 292

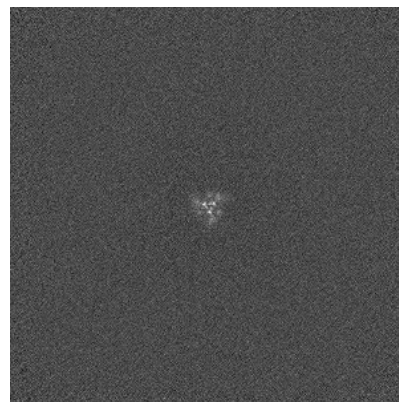
### 6.2.2 Raw map



X Index: 292



Y Index: 292



Z Index: 292

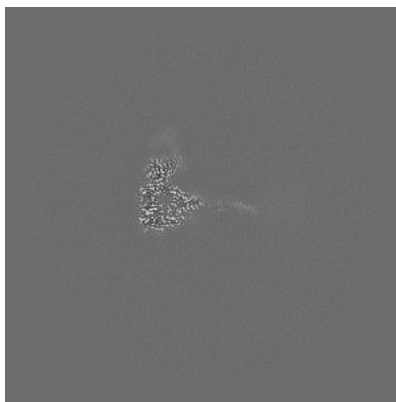
The images above show central slices of the map in three orthogonal directions.

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

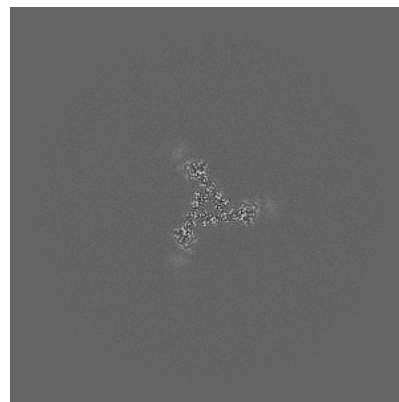
### 6.3.1 Primary map



X Index: 284

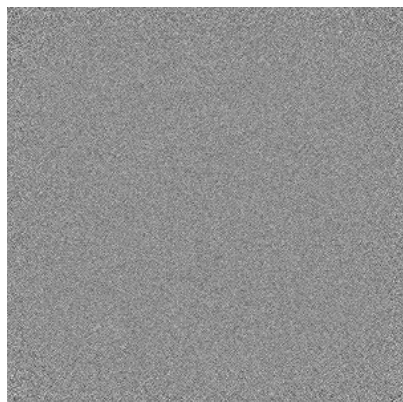


Y Index: 278

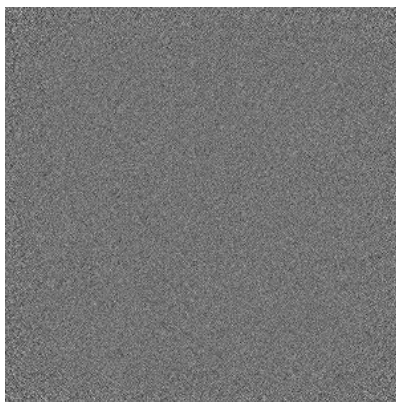


Z Index: 219

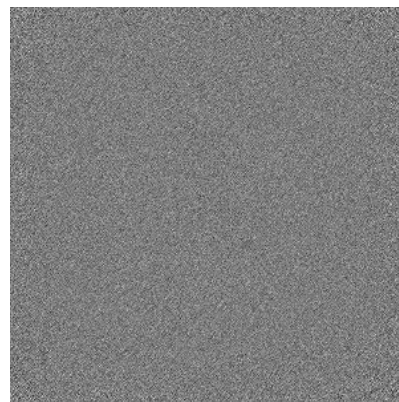
### 6.3.2 Raw map



X Index: 0



Y Index: 0



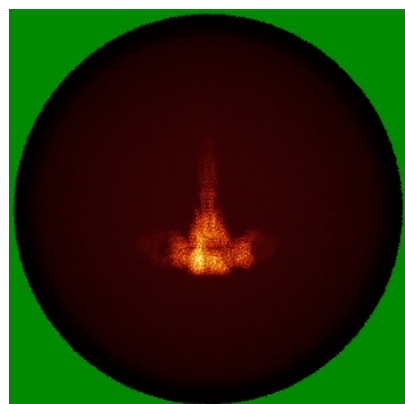
Z Index: 583

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

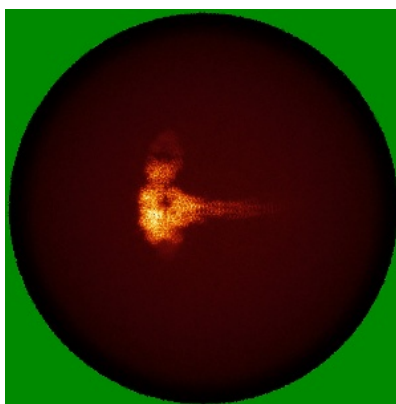


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

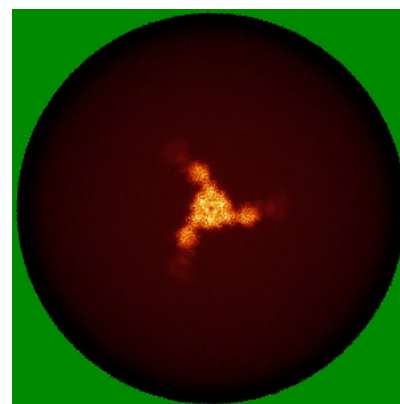
### 6.4.1 Primary map



X

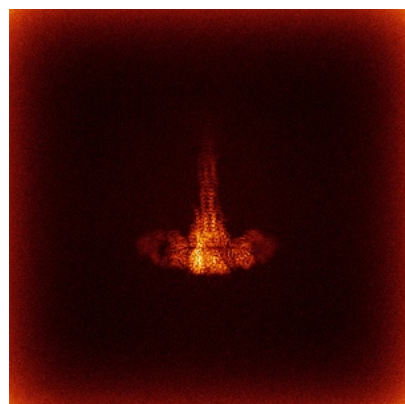


Y

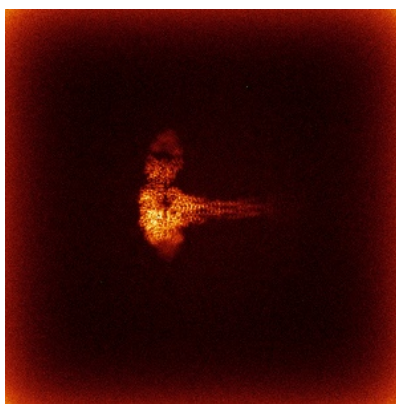


Z

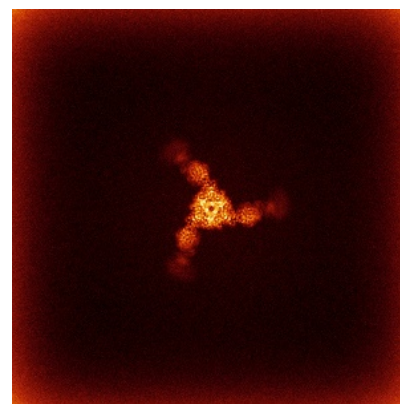
### 6.4.2 Raw map



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.

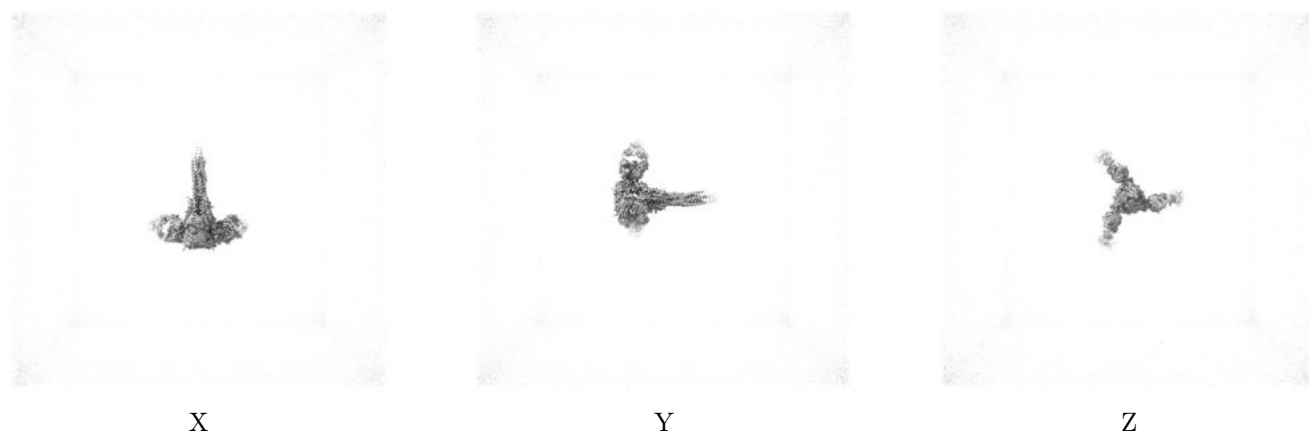
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0519. 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.

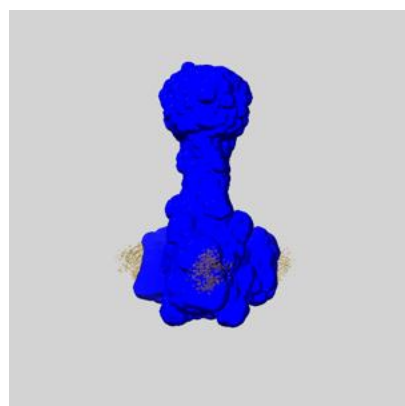
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

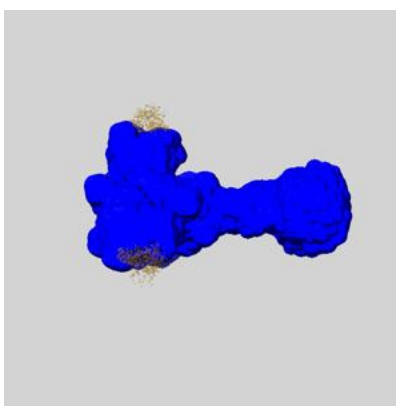
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

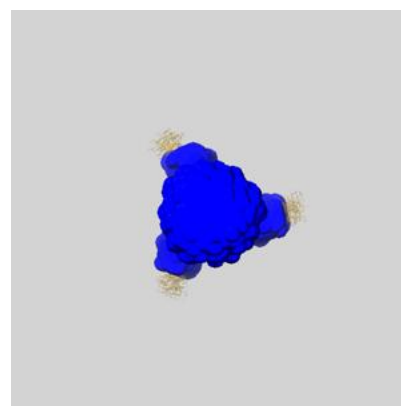
### 6.6.1 emd\_72283\_msk\_1.map [i](#)



X



Y



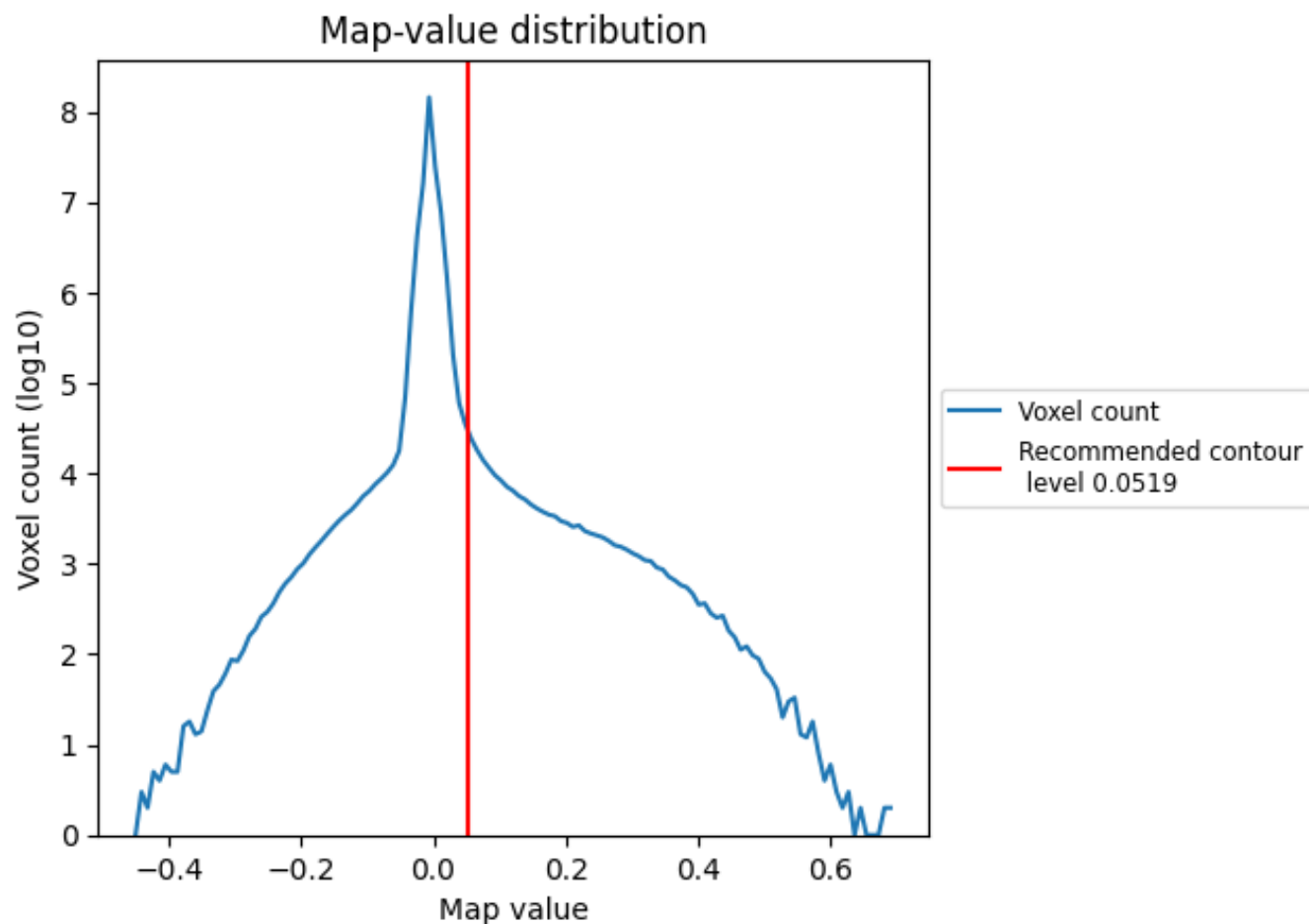
Z



## 7 Map analysis [i](#)

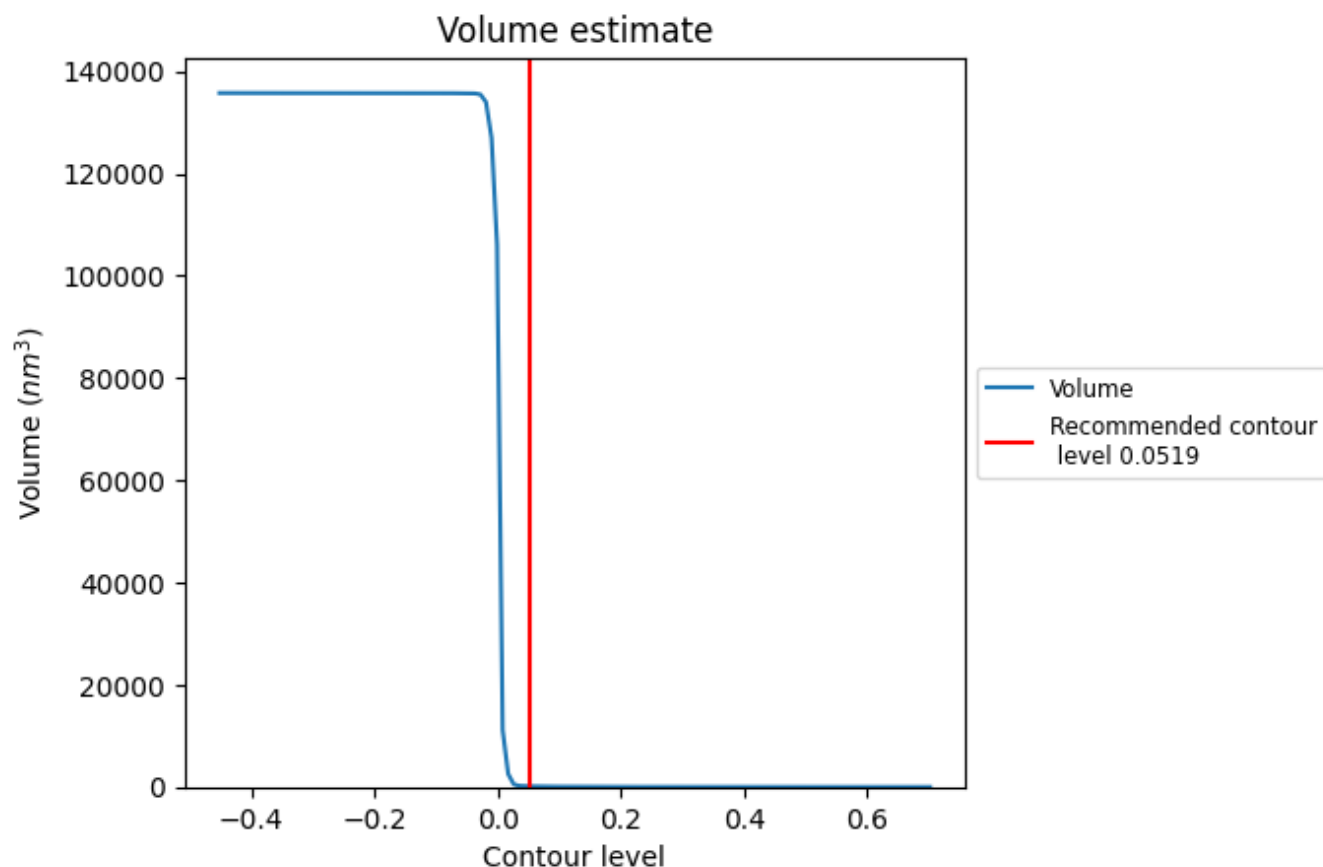
This section contains the results of statistical analysis of the map.

### 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.

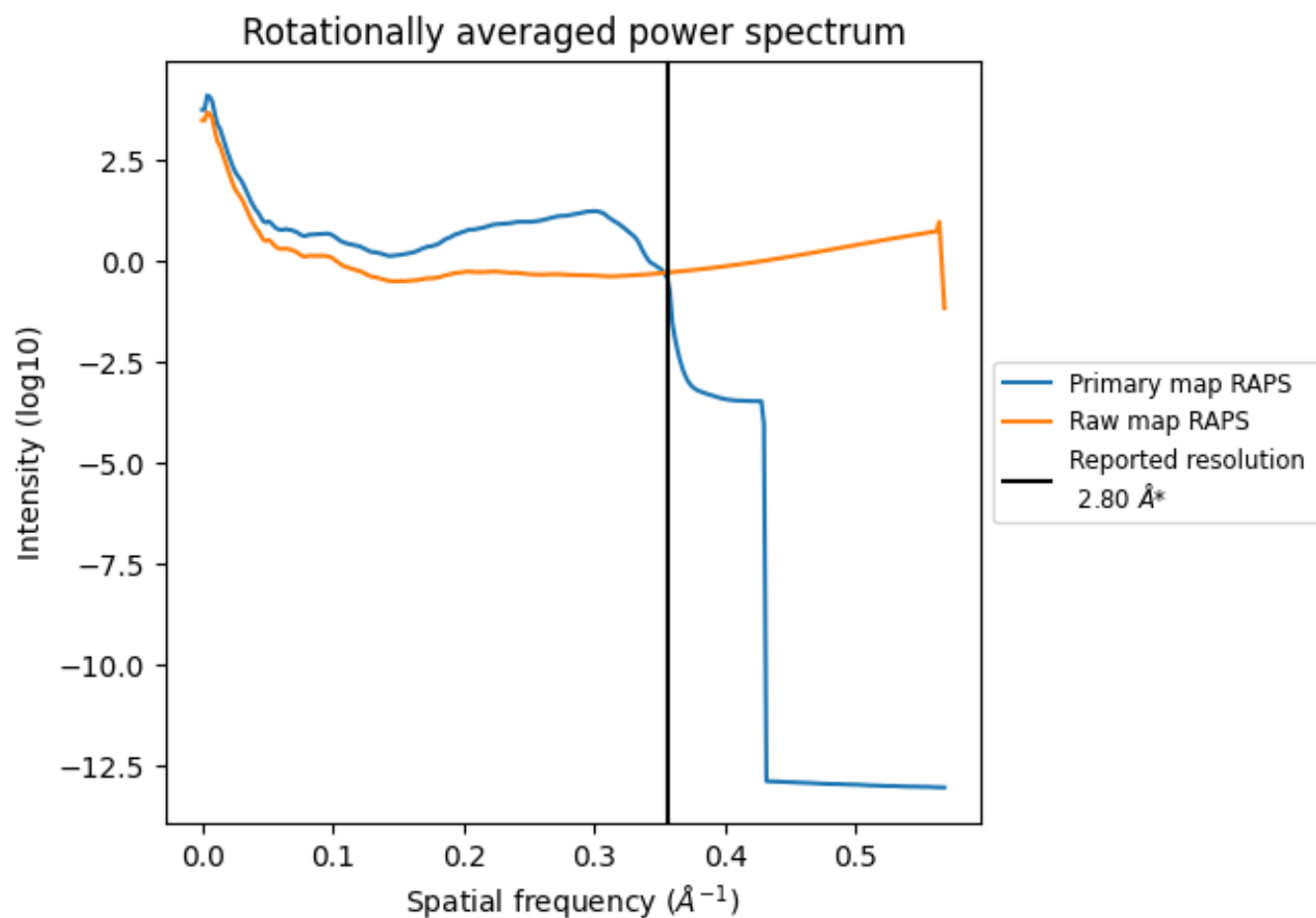
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 127  $\text{nm}^3$ ; this corresponds to an approximate mass of 115 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 ⓘ

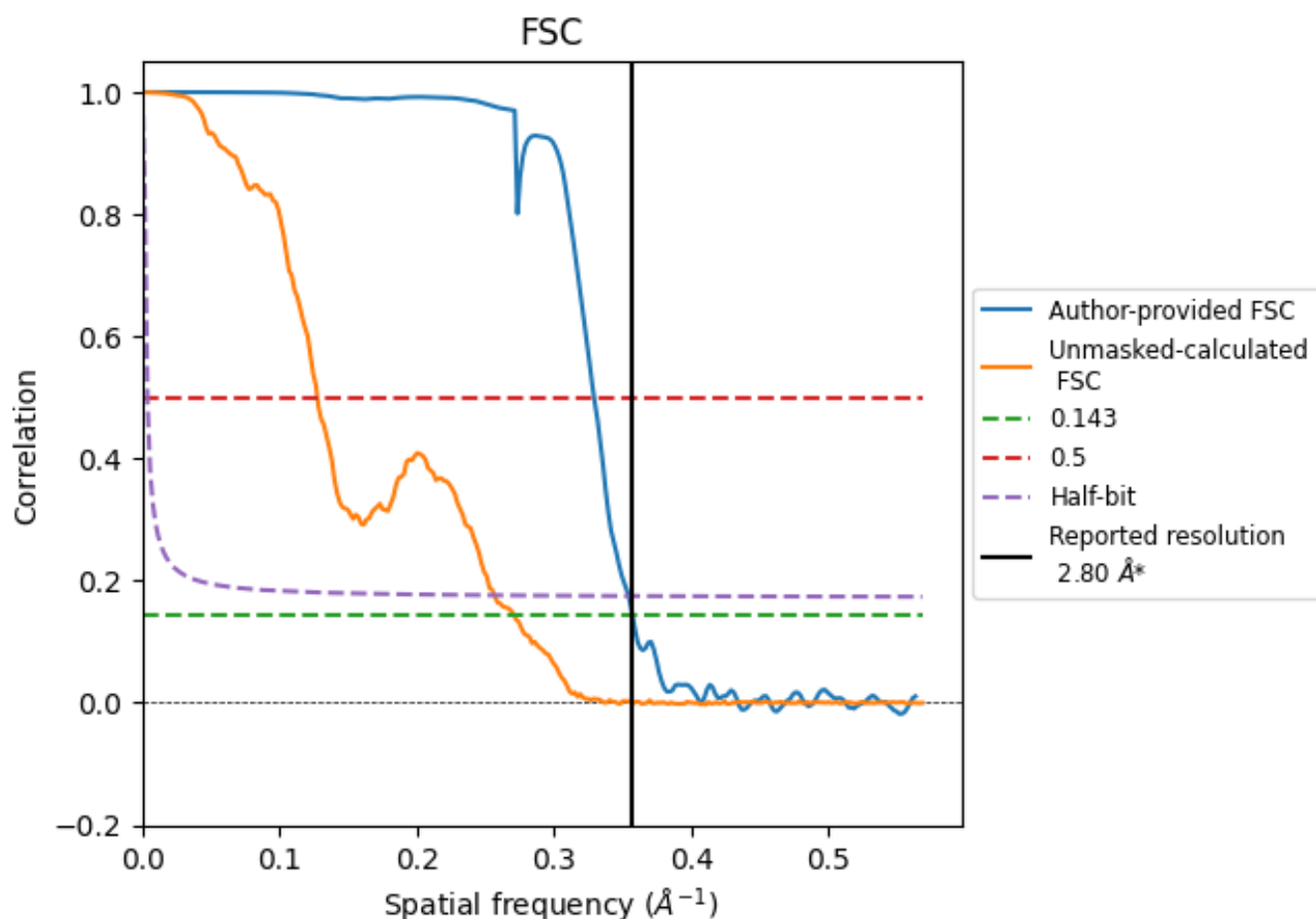


\*Reported resolution corresponds to spatial frequency of 0.357 Å<sup>-1</sup>

## 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  $0.357 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

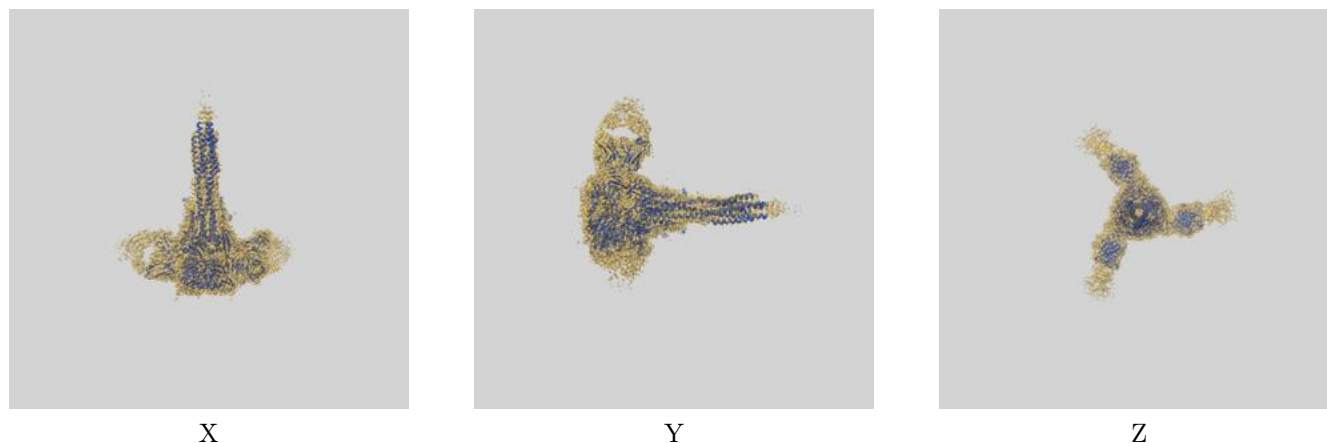
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.80	3.04	2.82
Unmasked-calculated*	3.69	7.84	3.90

\*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 3.69 differs from the reported value 2.8 by more than 10 %

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

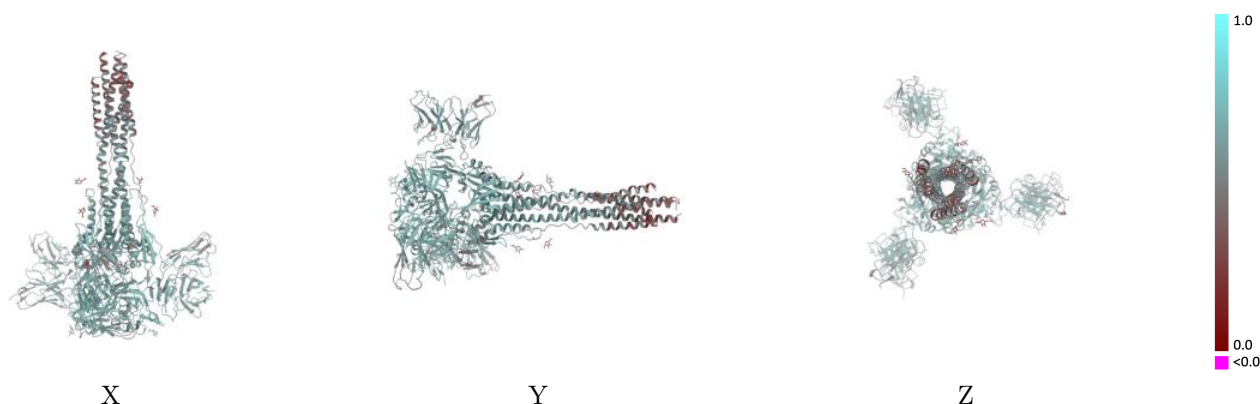
This section contains information regarding the fit between EMDB map EMD-72283 and PDB model 9Q71. Per-residue inclusion information can be found in [section 3](#) on [page 12](#).

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



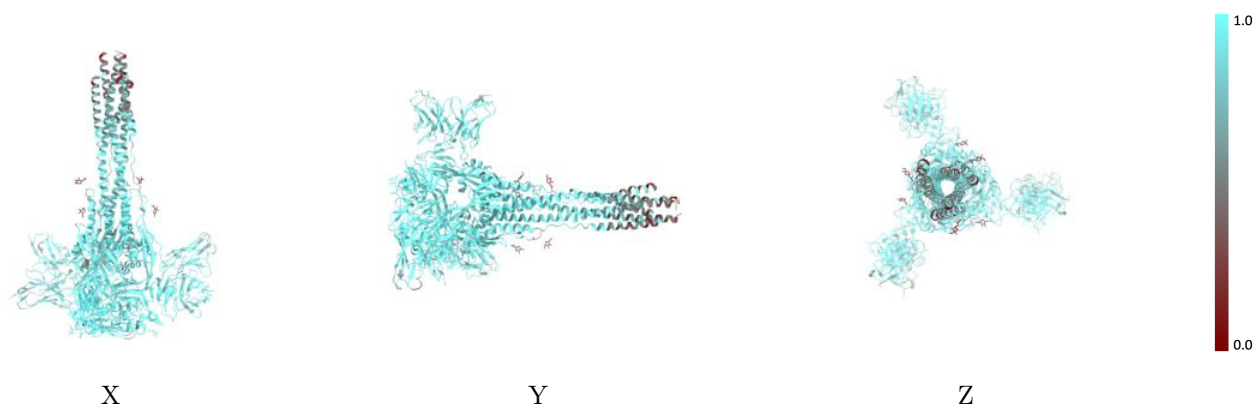
The images above show the 3D surface view of the map at the recommended contour level 0.0519 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



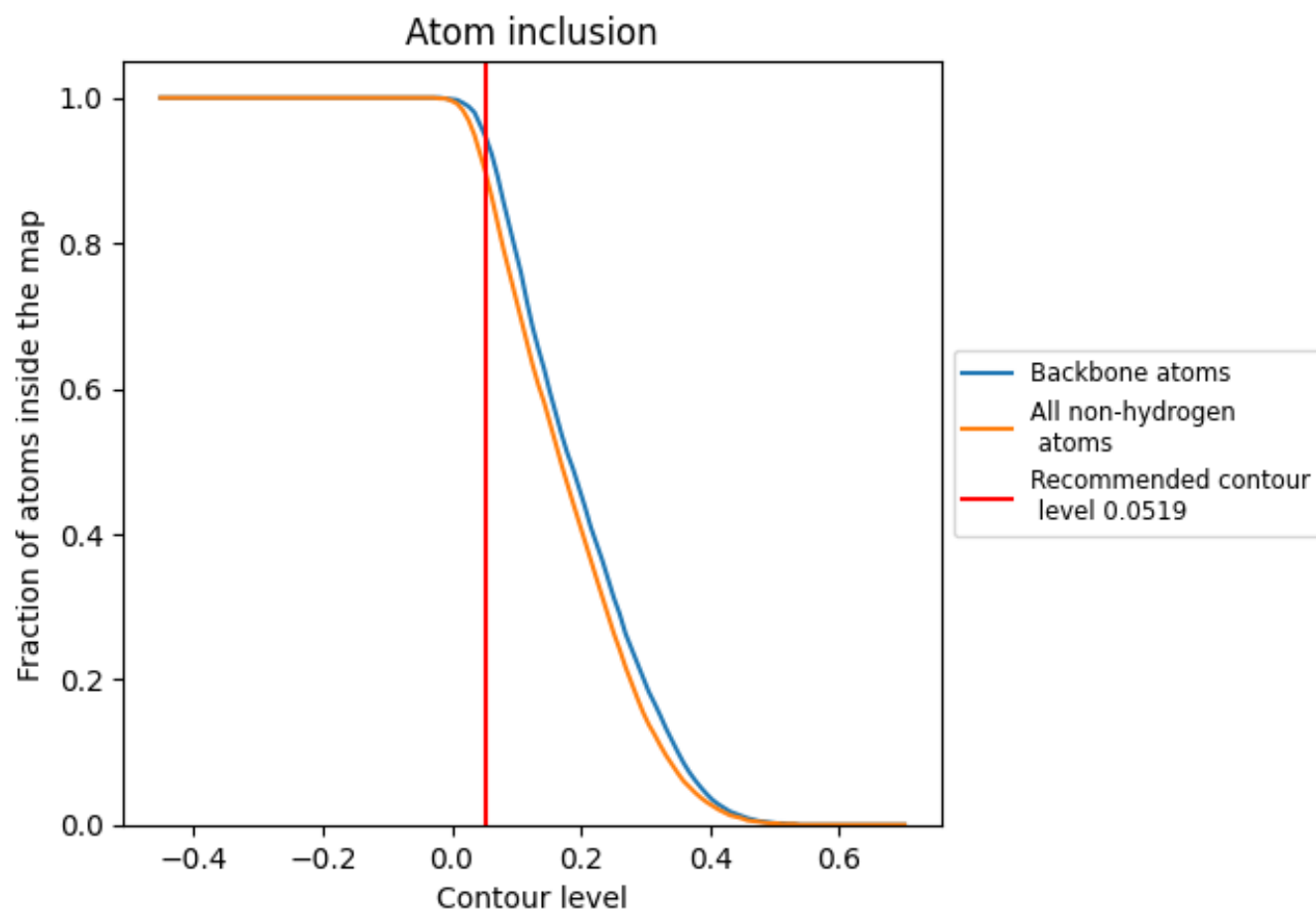
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0519).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 90% 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 (0.0519) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.8990</div>	<div><div></div>0.5730</div>
A	<div><div></div>0.9120</div>	<div><div></div>0.5900</div>
B	<div><div></div>0.8970</div>	<div><div></div>0.5770</div>
C	<div><div></div>0.9070</div>	<div><div></div>0.5860</div>
D	<div><div></div>0.9000</div>	<div><div></div>0.5750</div>
E	<div><div></div>0.9260</div>	<div><div></div>0.5900</div>
F	<div><div></div>0.8970</div>	<div><div></div>0.5760</div>
G	<div><div></div>0.9100</div>	<div><div></div>0.5770</div>
H	<div><div></div>0.8980</div>	<div><div></div>0.5560</div>
I	<div><div></div>0.8840</div>	<div><div></div>0.5580</div>
J	<div><div></div>0.8900</div>	<div><div></div>0.5560</div>
K	<div><div></div>0.8950</div>	<div><div></div>0.5660</div>
L	<div><div></div>0.8860</div>	<div><div></div>0.5570</div>

1.0

0.0

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