



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 06:05 AM UTC

PDB ID : 9CWO / pdb_00009cwo
EMDB ID : EMD-45968
Title : Cryo EM structure of Nipah virus L-P polymerase complex
Authors : Deniston, C.; Buffalo, C.; Rohaim, A.
Deposited on : 2024-07-29
Resolution : 3.43 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

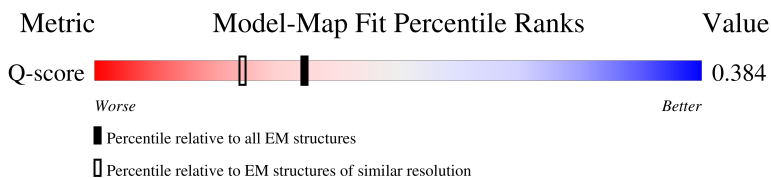
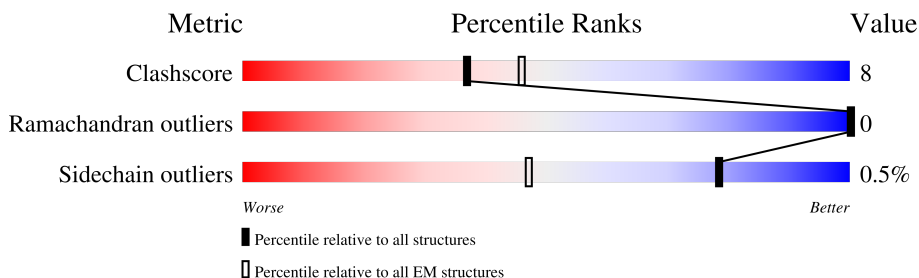
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.43 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	13927 (2.93 - 3.93)

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	1619	
2	C	717	
2	E	717	
2	F	717	

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Mol	Chain	Length	Quality of chain
2	G	717	<div><div><div></div><div></div><div></div></div><div>7%12% .86%</div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12722 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 RNA-directed RNA polymerase L.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1193	Total	C	N	O	S	0	0
			9180	5890	1559	1670	61		

There are 157 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-155	MET	-	initiating methionine	UNP Q4VCP4
A	-154	ALA	-	expression tag	UNP Q4VCP4
A	-153	SER	-	expression tag	UNP Q4VCP4
A	-152	HIS	-	expression tag	UNP Q4VCP4
A	-151	HIS	-	expression tag	UNP Q4VCP4
A	-150	HIS	-	expression tag	UNP Q4VCP4
A	-149	HIS	-	expression tag	UNP Q4VCP4
A	-148	HIS	-	expression tag	UNP Q4VCP4
A	-147	HIS	-	expression tag	UNP Q4VCP4
A	-146	HIS	-	expression tag	UNP Q4VCP4
A	-145	HIS	-	expression tag	UNP Q4VCP4
A	-144	HIS	-	expression tag	UNP Q4VCP4
A	-143	HIS	-	expression tag	UNP Q4VCP4
A	-142	ALA	-	expression tag	UNP Q4VCP4
A	-141	GLN	-	expression tag	UNP Q4VCP4
A	-140	HIS	-	expression tag	UNP Q4VCP4
A	-139	ASP	-	expression tag	UNP Q4VCP4
A	-138	GLU	-	expression tag	UNP Q4VCP4
A	-137	ALA	-	expression tag	UNP Q4VCP4
A	-136	VAL	-	expression tag	UNP Q4VCP4
A	-135	ASP	-	expression tag	UNP Q4VCP4
A	-134	ASN	-	expression tag	UNP Q4VCP4
A	-133	LYS	-	expression tag	UNP Q4VCP4
A	-132	PHE	-	expression tag	UNP Q4VCP4
A	-131	ASN	-	expression tag	UNP Q4VCP4
A	-130	LYS	-	expression tag	UNP Q4VCP4
A	-129	GLU	-	expression tag	UNP Q4VCP4
A	-128	GLN	-	expression tag	UNP Q4VCP4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-127	GLN	-	expression tag	UNP Q4VCP4
A	-126	ASN	-	expression tag	UNP Q4VCP4
A	-125	ALA	-	expression tag	UNP Q4VCP4
A	-124	PHE	-	expression tag	UNP Q4VCP4
A	-123	TYR	-	expression tag	UNP Q4VCP4
A	-122	GLU	-	expression tag	UNP Q4VCP4
A	-121	ILE	-	expression tag	UNP Q4VCP4
A	-120	LEU	-	expression tag	UNP Q4VCP4
A	-119	HIS	-	expression tag	UNP Q4VCP4
A	-118	LEU	-	expression tag	UNP Q4VCP4
A	-117	PRO	-	expression tag	UNP Q4VCP4
A	-116	ASN	-	expression tag	UNP Q4VCP4
A	-115	LEU	-	expression tag	UNP Q4VCP4
A	-114	ASN	-	expression tag	UNP Q4VCP4
A	-113	GLU	-	expression tag	UNP Q4VCP4
A	-112	GLU	-	expression tag	UNP Q4VCP4
A	-111	GLN	-	expression tag	UNP Q4VCP4
A	-110	ARG	-	expression tag	UNP Q4VCP4
A	-109	ASN	-	expression tag	UNP Q4VCP4
A	-108	ALA	-	expression tag	UNP Q4VCP4
A	-107	PHE	-	expression tag	UNP Q4VCP4
A	-106	ILE	-	expression tag	UNP Q4VCP4
A	-105	GLN	-	expression tag	UNP Q4VCP4
A	-104	SER	-	expression tag	UNP Q4VCP4
A	-103	LEU	-	expression tag	UNP Q4VCP4
A	-102	LYS	-	expression tag	UNP Q4VCP4
A	-101	ASP	-	expression tag	UNP Q4VCP4
A	-100	ASP	-	expression tag	UNP Q4VCP4
A	-99	PRO	-	expression tag	UNP Q4VCP4
A	-98	SER	-	expression tag	UNP Q4VCP4
A	-97	GLN	-	expression tag	UNP Q4VCP4
A	-96	SER	-	expression tag	UNP Q4VCP4
A	-95	ALA	-	expression tag	UNP Q4VCP4
A	-94	ASN	-	expression tag	UNP Q4VCP4
A	-93	ARG	-	expression tag	UNP Q4VCP4
A	-92	ARG	-	expression tag	UNP Q4VCP4
A	-91	ALA	-	expression tag	UNP Q4VCP4
A	-90	GLU	-	expression tag	UNP Q4VCP4
A	-89	ALA	-	expression tag	UNP Q4VCP4
A	-88	LYS	-	expression tag	UNP Q4VCP4
A	-87	LYS	-	expression tag	UNP Q4VCP4
A	-86	LEU	-	expression tag	UNP Q4VCP4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-85	ASN	-	expression tag	UNP Q4VCP4
A	-84	ASP	-	expression tag	UNP Q4VCP4
A	-83	ALA	-	expression tag	UNP Q4VCP4
A	-82	GLN	-	expression tag	UNP Q4VCP4
A	-81	ALA	-	expression tag	UNP Q4VCP4
A	-80	PRO	-	expression tag	UNP Q4VCP4
A	-79	LYS	-	expression tag	UNP Q4VCP4
A	-78	VAL	-	expression tag	UNP Q4VCP4
A	-77	ASP	-	expression tag	UNP Q4VCP4
A	-76	ASN	-	expression tag	UNP Q4VCP4
A	-75	LYS	-	expression tag	UNP Q4VCP4
A	-74	PHE	-	expression tag	UNP Q4VCP4
A	-73	ASN	-	expression tag	UNP Q4VCP4
A	-72	LYS	-	expression tag	UNP Q4VCP4
A	-71	GLU	-	expression tag	UNP Q4VCP4
A	-70	GLN	-	expression tag	UNP Q4VCP4
A	-69	GLN	-	expression tag	UNP Q4VCP4
A	-68	ASN	-	expression tag	UNP Q4VCP4
A	-67	ALA	-	expression tag	UNP Q4VCP4
A	-66	PHE	-	expression tag	UNP Q4VCP4
A	-65	TYR	-	expression tag	UNP Q4VCP4
A	-64	GLU	-	expression tag	UNP Q4VCP4
A	-63	ILE	-	expression tag	UNP Q4VCP4
A	-62	LEU	-	expression tag	UNP Q4VCP4
A	-61	HIS	-	expression tag	UNP Q4VCP4
A	-60	LEU	-	expression tag	UNP Q4VCP4
A	-59	PRO	-	expression tag	UNP Q4VCP4
A	-58	ASN	-	expression tag	UNP Q4VCP4
A	-57	LEU	-	expression tag	UNP Q4VCP4
A	-56	ASN	-	expression tag	UNP Q4VCP4
A	-55	GLU	-	expression tag	UNP Q4VCP4
A	-54	GLU	-	expression tag	UNP Q4VCP4
A	-53	GLN	-	expression tag	UNP Q4VCP4
A	-52	ARG	-	expression tag	UNP Q4VCP4
A	-51	ASN	-	expression tag	UNP Q4VCP4
A	-50	ALA	-	expression tag	UNP Q4VCP4
A	-49	PHE	-	expression tag	UNP Q4VCP4
A	-48	ILE	-	expression tag	UNP Q4VCP4
A	-47	GLN	-	expression tag	UNP Q4VCP4
A	-46	SER	-	expression tag	UNP Q4VCP4
A	-45	LEU	-	expression tag	UNP Q4VCP4
A	-44	LYS	-	expression tag	UNP Q4VCP4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-43	ASP	-	expression tag	UNP Q4VCP4
A	-42	ASP	-	expression tag	UNP Q4VCP4
A	-41	PRO	-	expression tag	UNP Q4VCP4
A	-40	SER	-	expression tag	UNP Q4VCP4
A	-39	GLN	-	expression tag	UNP Q4VCP4
A	-38	SER	-	expression tag	UNP Q4VCP4
A	-37	ALA	-	expression tag	UNP Q4VCP4
A	-36	ASN	-	expression tag	UNP Q4VCP4
A	-35	LEU	-	expression tag	UNP Q4VCP4
A	-34	LEU	-	expression tag	UNP Q4VCP4
A	-33	ALA	-	expression tag	UNP Q4VCP4
A	-32	GLU	-	expression tag	UNP Q4VCP4
A	-31	ALA	-	expression tag	UNP Q4VCP4
A	-30	LYS	-	expression tag	UNP Q4VCP4
A	-29	LYS	-	expression tag	UNP Q4VCP4
A	-28	LEU	-	expression tag	UNP Q4VCP4
A	-27	ASN	-	expression tag	UNP Q4VCP4
A	-26	ASP	-	expression tag	UNP Q4VCP4
A	-25	ALA	-	expression tag	UNP Q4VCP4
A	-24	GLN	-	expression tag	UNP Q4VCP4
A	-23	ALA	-	expression tag	UNP Q4VCP4
A	-22	PRO	-	expression tag	UNP Q4VCP4
A	-21	LYS	-	expression tag	UNP Q4VCP4
A	-20	VAL	-	expression tag	UNP Q4VCP4
A	-19	ASP	-	expression tag	UNP Q4VCP4
A	-18	ALA	-	expression tag	UNP Q4VCP4
A	-17	ASN	-	expression tag	UNP Q4VCP4
A	-16	GLY	-	expression tag	UNP Q4VCP4
A	-15	GLY	-	expression tag	UNP Q4VCP4
A	-14	GLY	-	expression tag	UNP Q4VCP4
A	-13	GLY	-	expression tag	UNP Q4VCP4
A	-12	SER	-	expression tag	UNP Q4VCP4
A	-11	GLY	-	expression tag	UNP Q4VCP4
A	-10	GLY	-	expression tag	UNP Q4VCP4
A	-9	GLY	-	expression tag	UNP Q4VCP4
A	-8	GLY	-	expression tag	UNP Q4VCP4
A	-7	SER	-	expression tag	UNP Q4VCP4
A	-6	LEU	-	expression tag	UNP Q4VCP4
A	-5	GLU	-	expression tag	UNP Q4VCP4
A	-4	VAL	-	expression tag	UNP Q4VCP4
A	-3	LEU	-	expression tag	UNP Q4VCP4
A	-2	PHE	-	expression tag	UNP Q4VCP4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLN	-	expression tag	UNP Q4VCP4
A	0	GLY	-	expression tag	UNP Q4VCP4
A	1	PRO	-	expression tag	UNP Q4VCP4

- Molecule 2 is a protein called Phosphoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	104	Total	C	N	O	S	0	0
			711	439	126	142	4		
2	C	103	Total	C	N	O	S	0	0
			706	442	125	135	4		
2	G	102	Total	C	N	O	S	0	0
			709	445	122	136	6		
2	E	197	Total	C	N	O	S	0	0
			1416	881	247	282	6		

There are 32 discrepancies between the modelled and reference sequences:

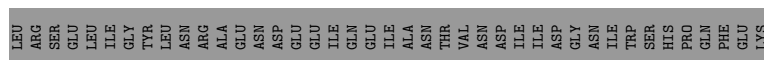
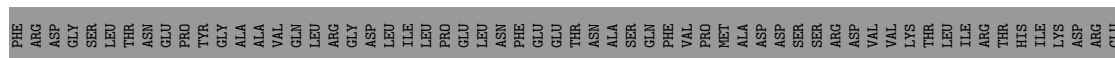
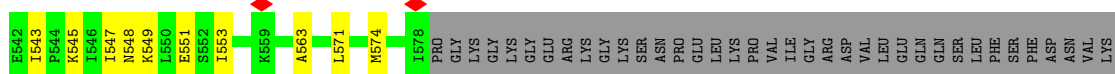
Chain	Residue	Modelled	Actual	Comment	Reference
F	710	TRP	-	expression tag	UNP Q4VCQ1
F	711	SER	-	expression tag	UNP Q4VCQ1
F	712	HIS	-	expression tag	UNP Q4VCQ1
F	713	PRO	-	expression tag	UNP Q4VCQ1
F	714	GLN	-	expression tag	UNP Q4VCQ1
F	715	PHE	-	expression tag	UNP Q4VCQ1
F	716	GLU	-	expression tag	UNP Q4VCQ1
F	717	LYS	-	expression tag	UNP Q4VCQ1
C	710	TRP	-	expression tag	UNP Q4VCQ1
C	711	SER	-	expression tag	UNP Q4VCQ1
C	712	HIS	-	expression tag	UNP Q4VCQ1
C	713	PRO	-	expression tag	UNP Q4VCQ1
C	714	GLN	-	expression tag	UNP Q4VCQ1
C	715	PHE	-	expression tag	UNP Q4VCQ1
C	716	GLU	-	expression tag	UNP Q4VCQ1
C	717	LYS	-	expression tag	UNP Q4VCQ1
G	710	TRP	-	expression tag	UNP Q4VCQ1
G	711	SER	-	expression tag	UNP Q4VCQ1
G	712	HIS	-	expression tag	UNP Q4VCQ1
G	713	PRO	-	expression tag	UNP Q4VCQ1
G	714	GLN	-	expression tag	UNP Q4VCQ1
G	715	PHE	-	expression tag	UNP Q4VCQ1
G	716	GLU	-	expression tag	UNP Q4VCQ1

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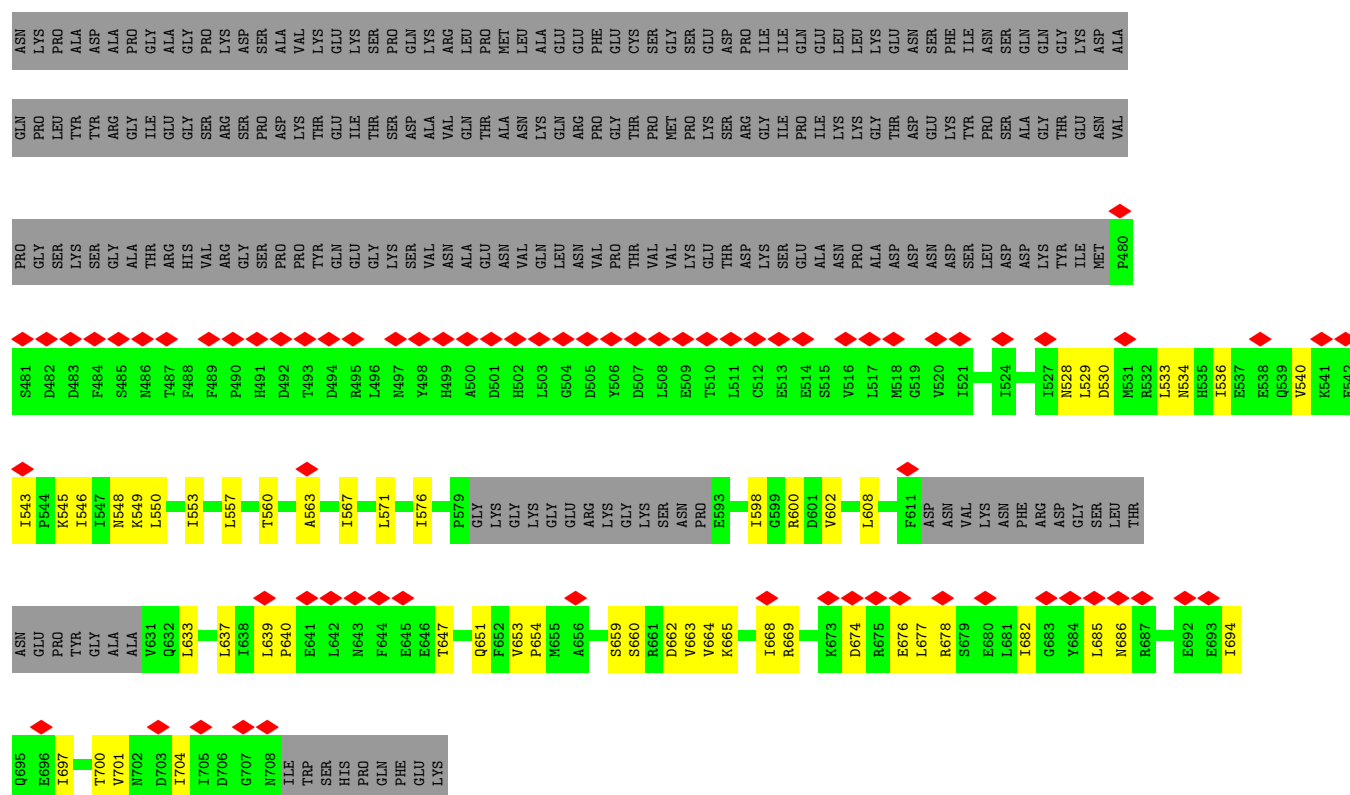
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Chain	Residue	Modelled	Actual	Comment	Reference
G	717	LYS	-	expression tag	UNP Q4VCQ1
E	710	TRP	-	expression tag	UNP Q4VCQ1
E	711	SER	-	expression tag	UNP Q4VCQ1
E	712	HIS	-	expression tag	UNP Q4VCQ1
E	713	PRO	-	expression tag	UNP Q4VCQ1
E	714	GLN	-	expression tag	UNP Q4VCQ1
E	715	PHE	-	expression tag	UNP Q4VCQ1
E	716	GLU	-	expression tag	UNP Q4VCQ1
E	717	LYS	-	expression tag	UNP Q4VCQ1



[illegible]

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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	335177	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.2	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	6.164	Depositor
Minimum map value	-4.608	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.085	Depositor
Recommended contour level	0.7	Depositor
Map size (Å)	357.76, 357.76, 357.76	wwPDB
Map dimensions	416, 416, 416	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.86, 0.86, 0.86	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.11	0/9365	0.26	0/12713
2	C	0.12	0/713	0.28	0/970
2	E	0.14	0/1429	0.34	0/1945
2	F	0.12	0/718	0.30	0/979
2	G	0.15	0/716	0.33	0/976
All	All	0.12	0/12941	0.28	0/17583

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	9180	0	8919	121	0
2	C	706	0	648	18	0
2	E	1416	0	1297	46	0
2	F	711	0	634	16	0
2	G	709	0	647	19	0
All	All	12722	0	12145	189	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 8.

The worst 5 of 189 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)
2:C:526:LEU:HD21	2:G:526:LEU:HD13	1.69	0.73
1:A:876:ASN:HA	2:E:639:LEU:HD11	1.71	0.72
2:E:682:ILE:O	2:E:686:ASN:ND2	2.23	0.72
1:A:301:LYS:O	1:A:1259:GLN:NE2	2.22	0.71
1:A:506:VAL:HG11	1:A:1138:LEU:HD13	1.73	0.69

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	1161/1619 (72%)	1124 (97%)	37 (3%)	0	100	100
2	C	101/717 (14%)	101 (100%)	0	0	100	100
2	E	191/717 (27%)	187 (98%)	4 (2%)	0	100	100
2	F	102/717 (14%)	96 (94%)	6 (6%)	0	100	100
2	G	100/717 (14%)	96 (96%)	4 (4%)	0	100	100
All	All	1655/4487 (37%)	1604 (97%)	51 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	960/1446 (66%)	956 (100%)	4 (0%)	84	82

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	66/629 (10%)	64 (97%)	2 (3%)	36	60
2	E	140/629 (22%)	139 (99%)	1 (1%)	76	78
2	F	67/629 (11%)	67 (100%)	0	100	100
2	G	67/629 (11%)	67 (100%)	0	100	100
All	All	1300/3962 (33%)	1293 (100%)	7 (0%)	78	81

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1185	LEU
2	C	488	PHE
2	E	576	ILE
2	C	543	ILE
1	A	1138	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
2	E	686	ASN
2	F	534	ASN
1	A	1083	ASN
1	A	1042	ASN
1	A	1237	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry [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.

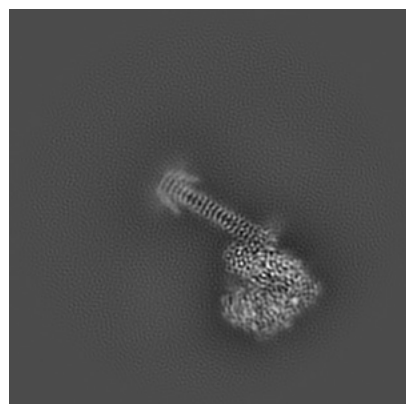
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45968. These allow visual inspection of the internal detail of the map and identification of artifacts.

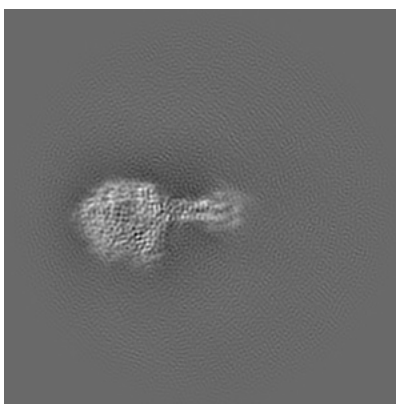
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

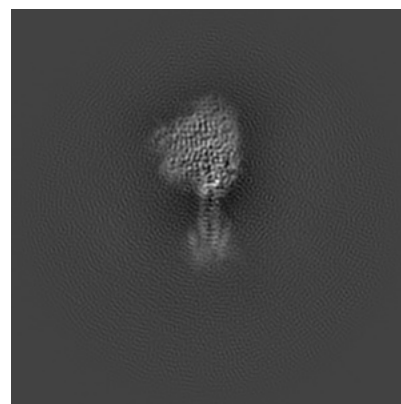
6.1.1 Primary map



X

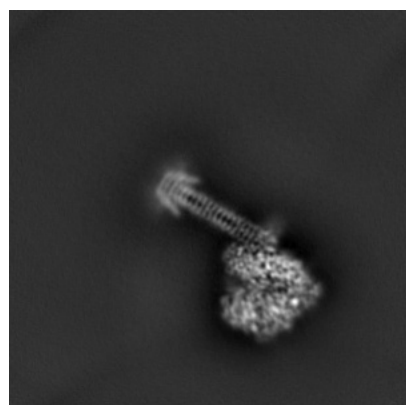


Y

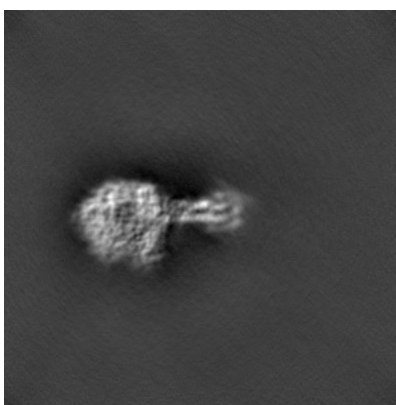


Z

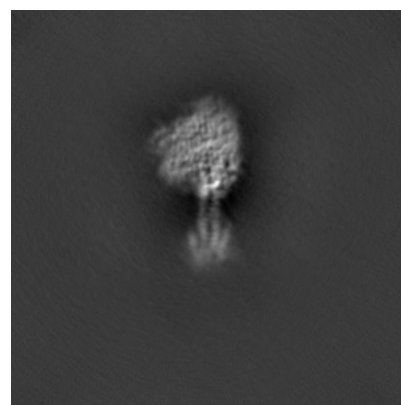
6.1.2 Raw map



X



Y

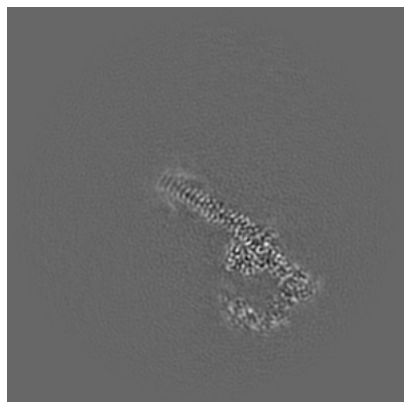


Z

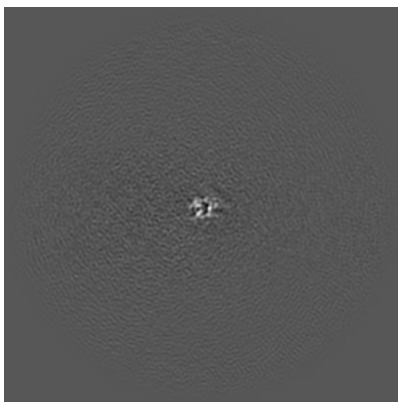
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 208

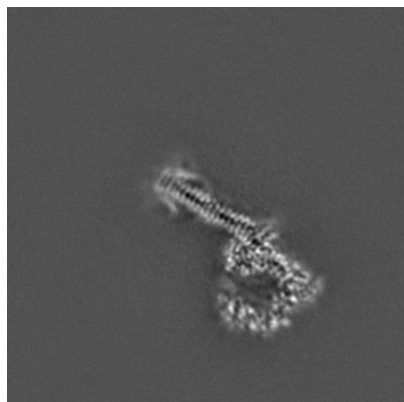


Y Index: 208

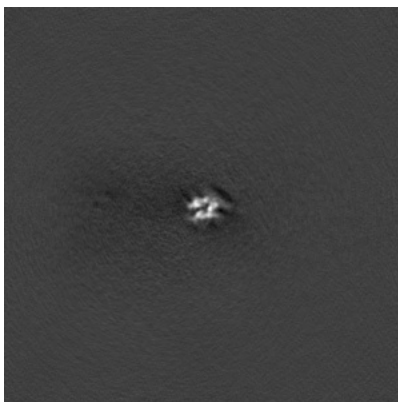


Z Index: 208

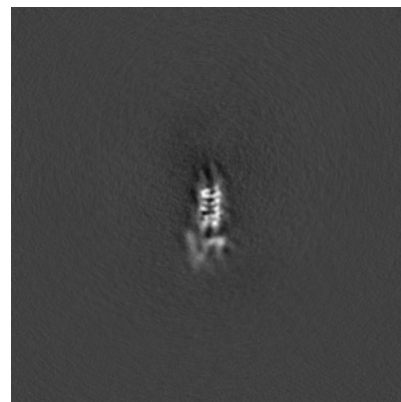
6.2.2 Raw map



X Index: 208



Y Index: 208

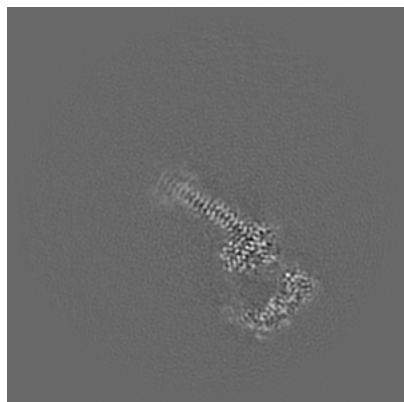


Z Index: 208

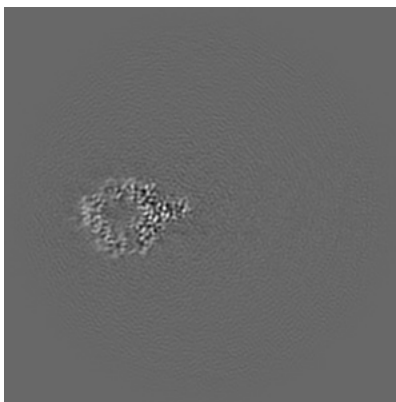
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

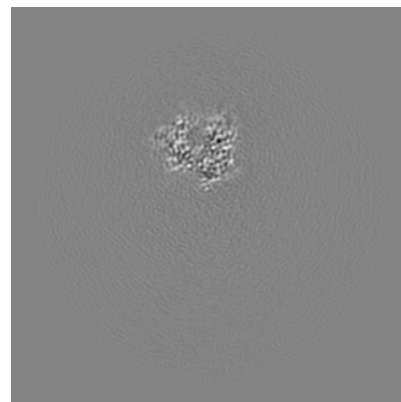
6.3.1 Primary map



X Index: 200

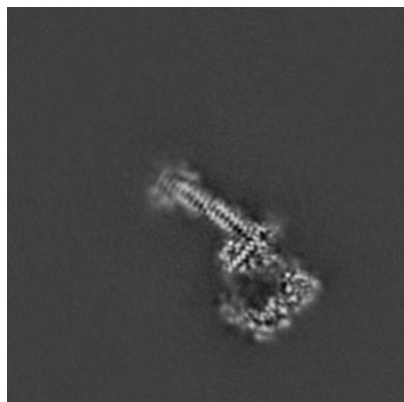


Y Index: 255

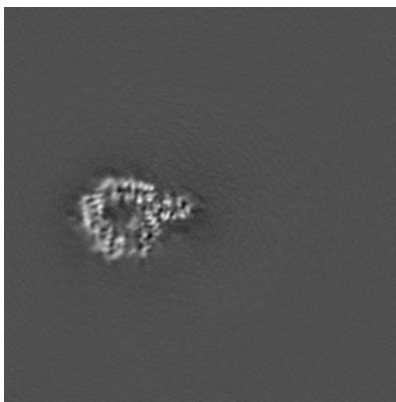


Z Index: 148

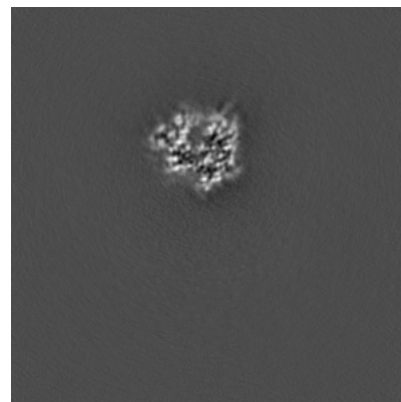
6.3.2 Raw map



X Index: 200



Y Index: 253

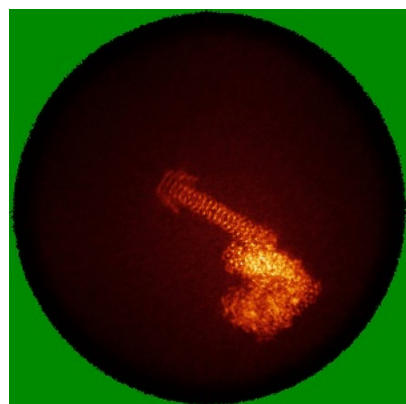


Z Index: 149

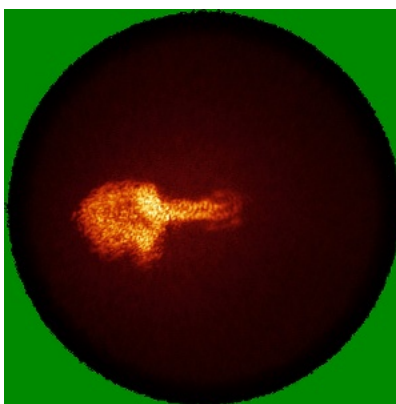
The images above show the largest variance slices of the map in three orthogonal directions.

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

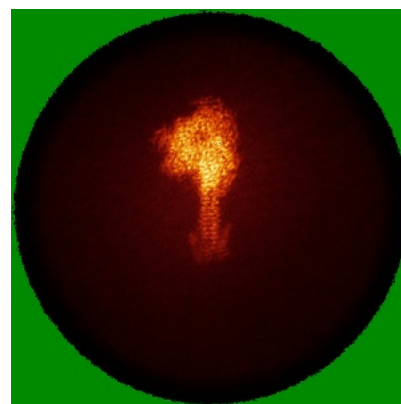
6.4.1 Primary map



X

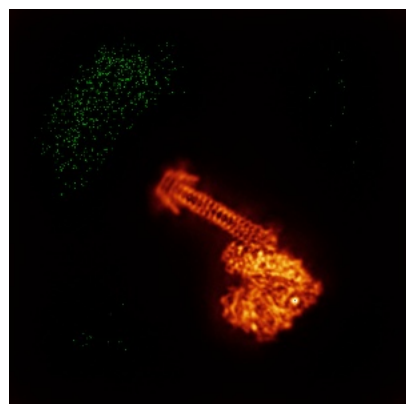


Y

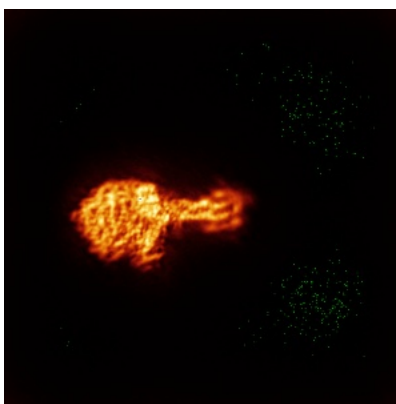


Z

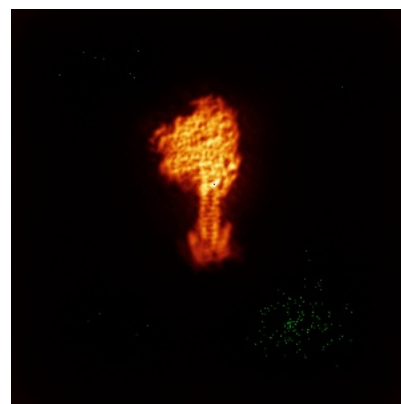
6.4.2 Raw map



X



Y

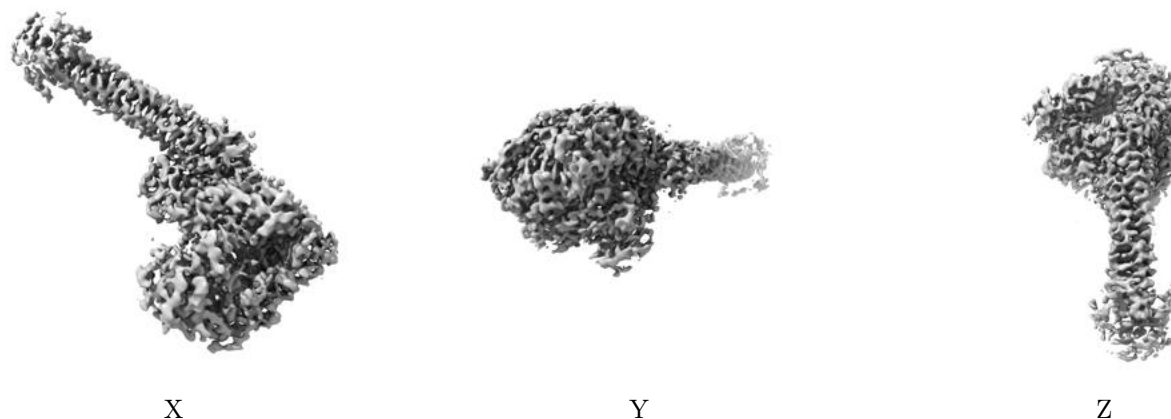


Z

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 0.7. 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.

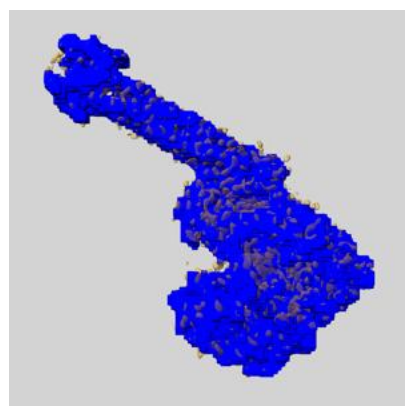
6.6 Mask visualisation [i](#)

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

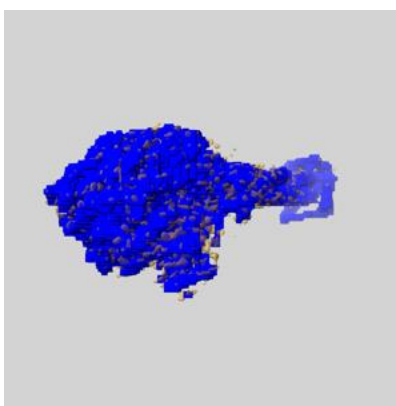
A mask typically either:

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

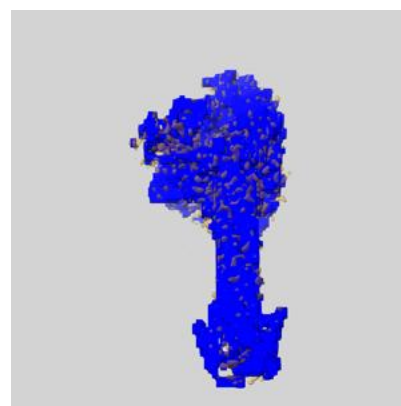
6.6.1 emd_45968_msk_1.map [i](#)



X



Y

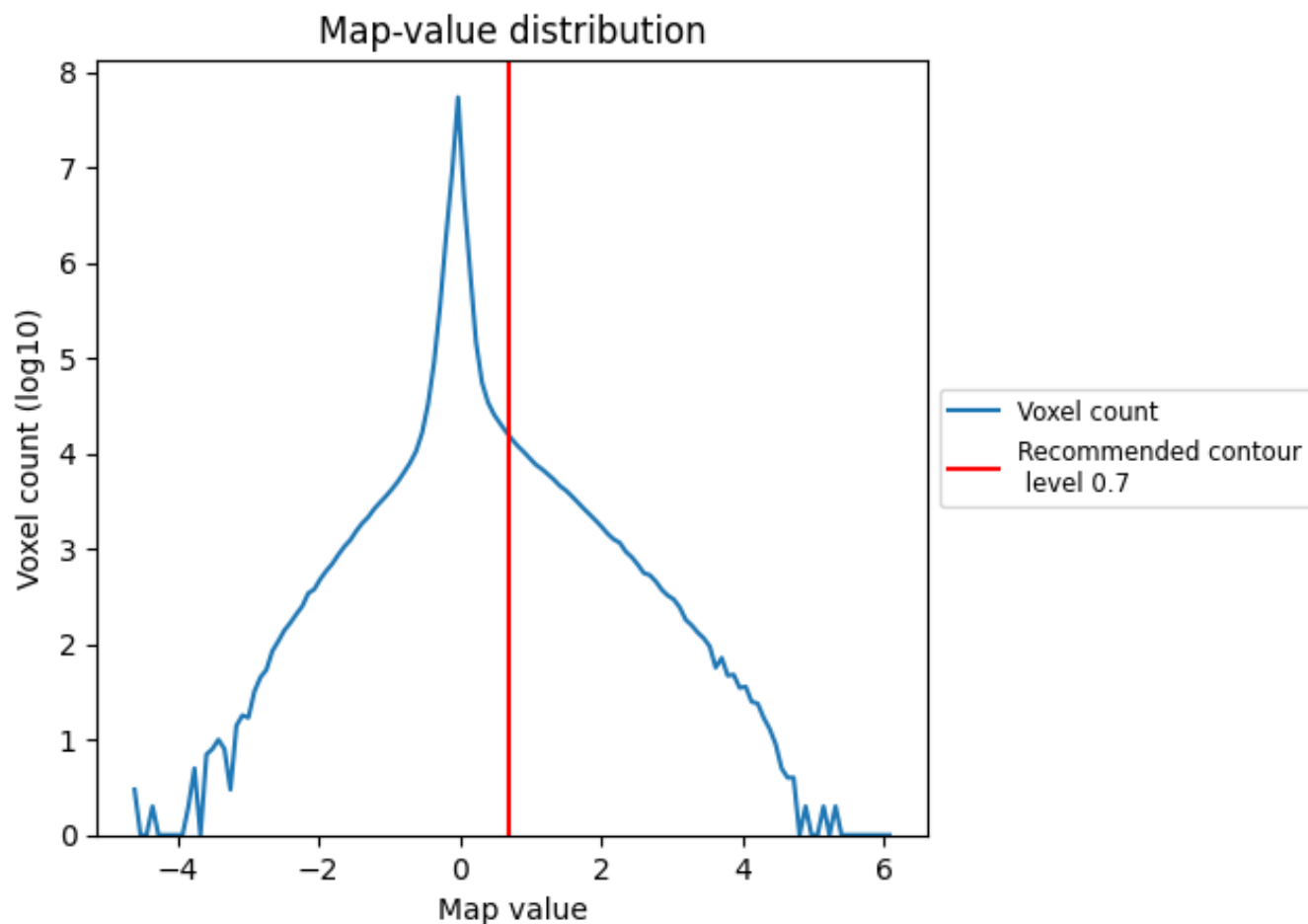


Z

7 Map analysis [i](#)

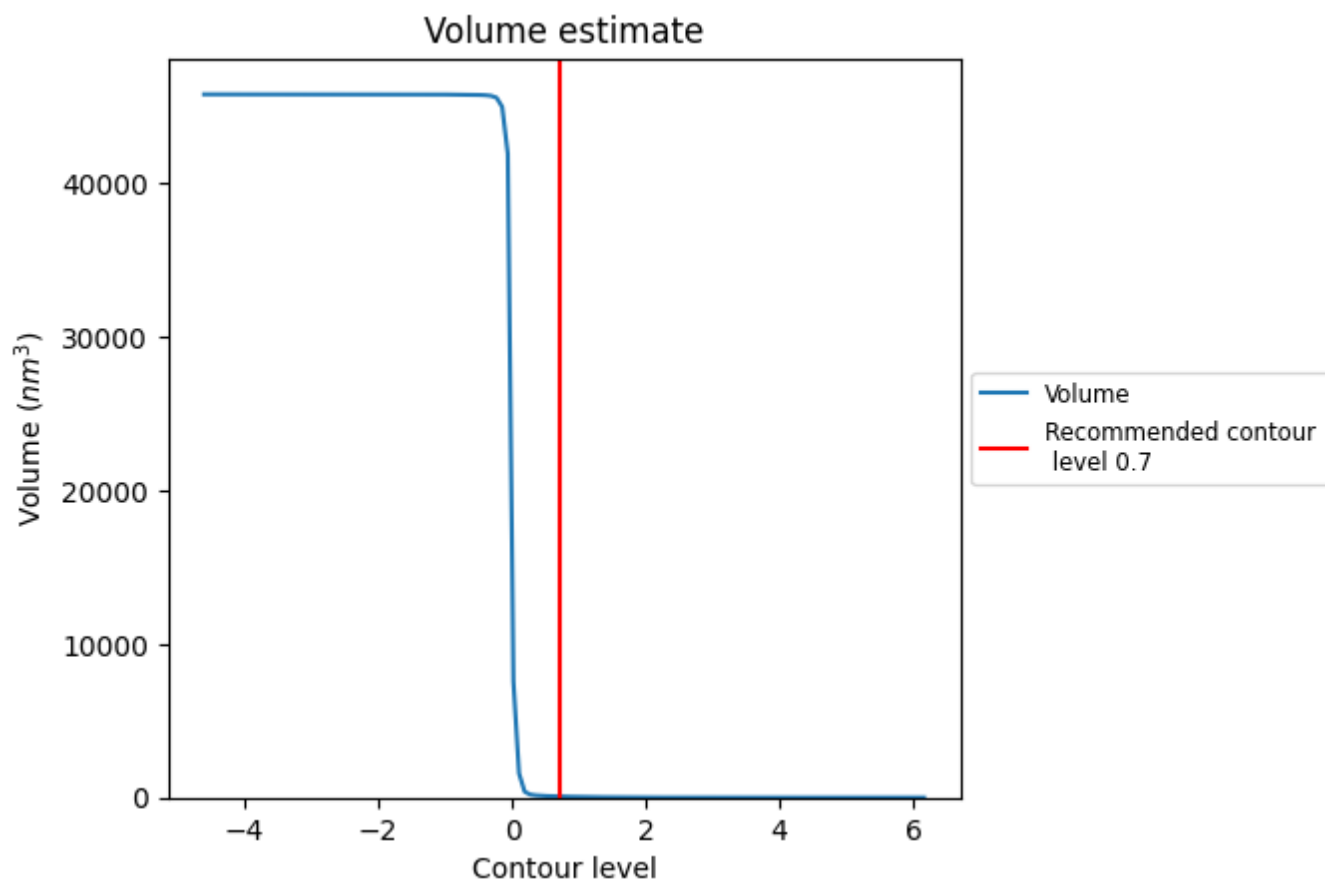
This section contains the results of statistical analysis of the map.

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.

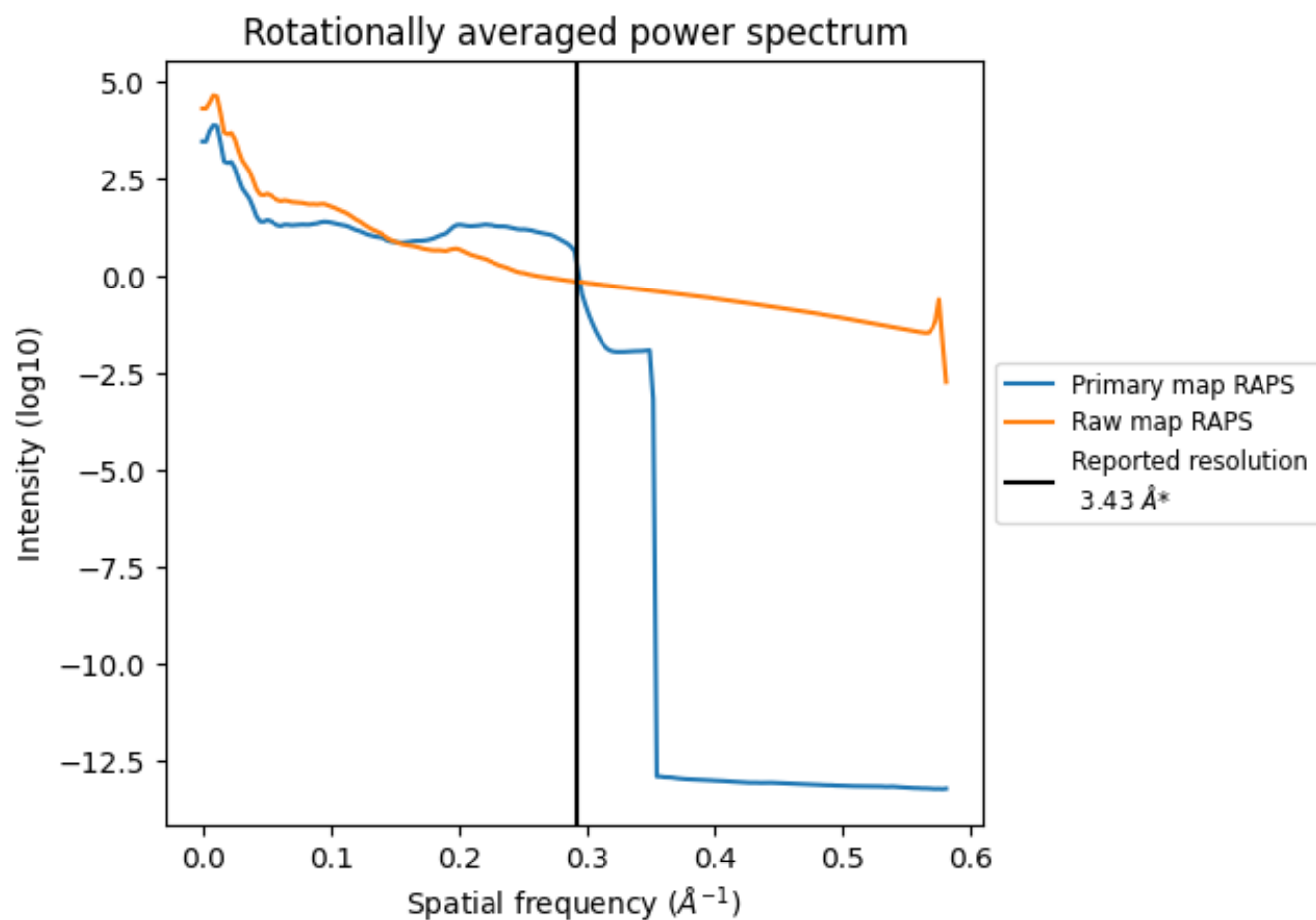
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 71 nm³; this corresponds to an approximate mass of 64 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 ⓘ

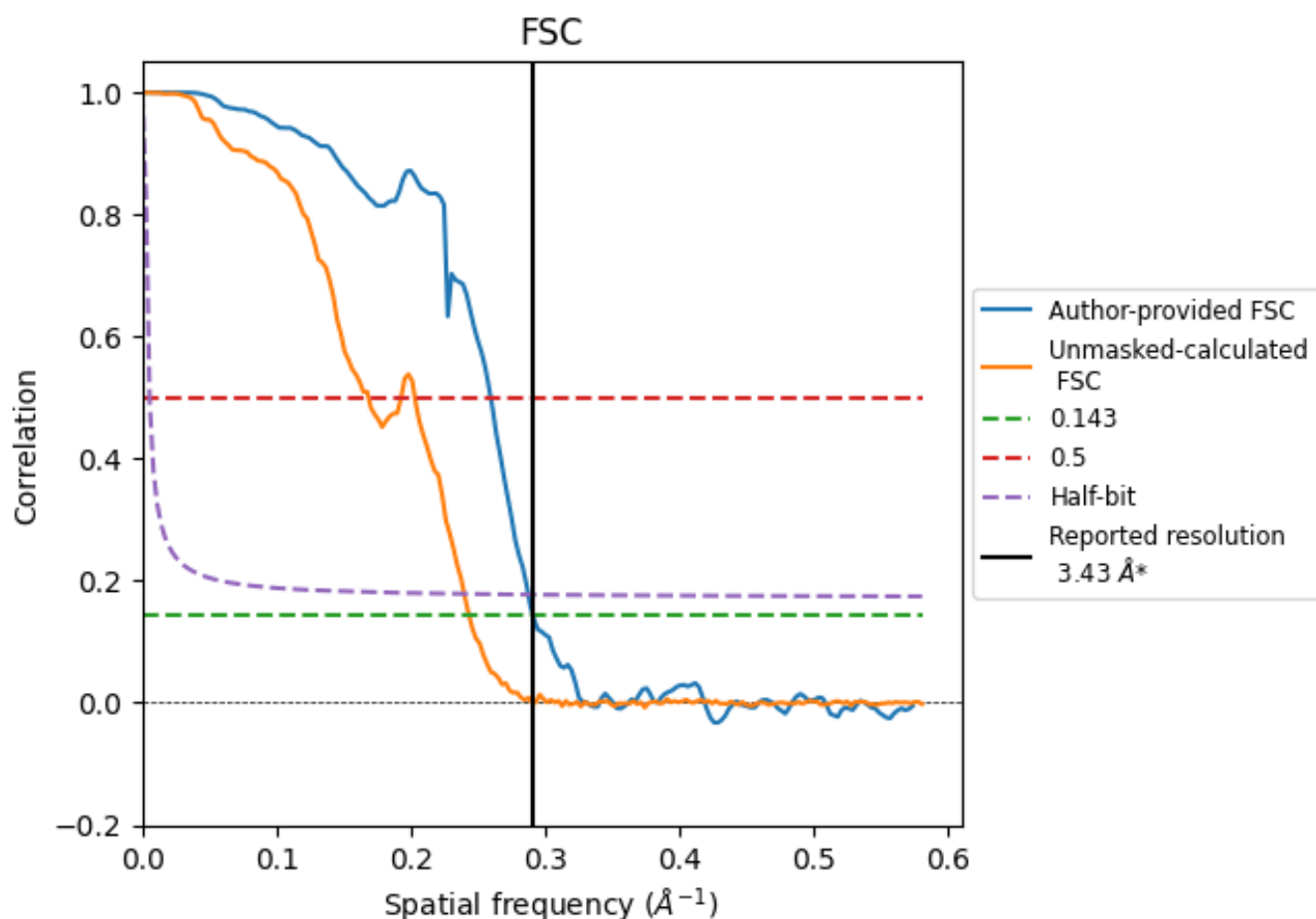


*Reported resolution corresponds to spatial frequency of 0.292 Å⁻¹

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 0.292 \AA^{-1}

8.2 Resolution estimates [i](#)

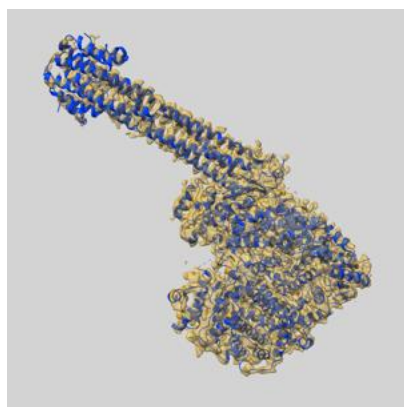
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.43	-	-
Author-provided FSC curve	3.43	3.85	3.47
Unmasked-calculated*	4.11	5.93	4.17

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.11 differs from the reported value 3.43 by more than 10 %

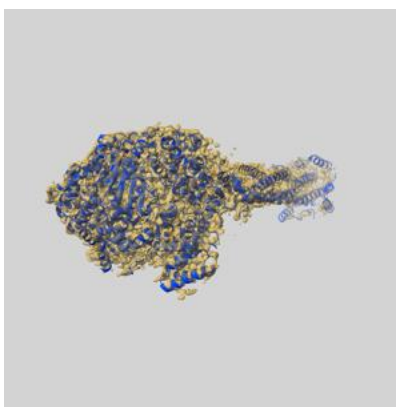
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-45968 and PDB model 9CWO. Per-residue inclusion information can be found in section [3](#) on page [10](#).

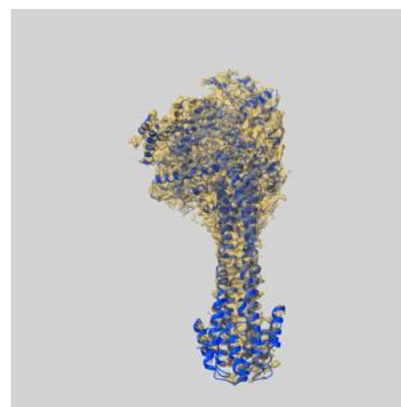
9.1 Map-model overlay [i](#)



X



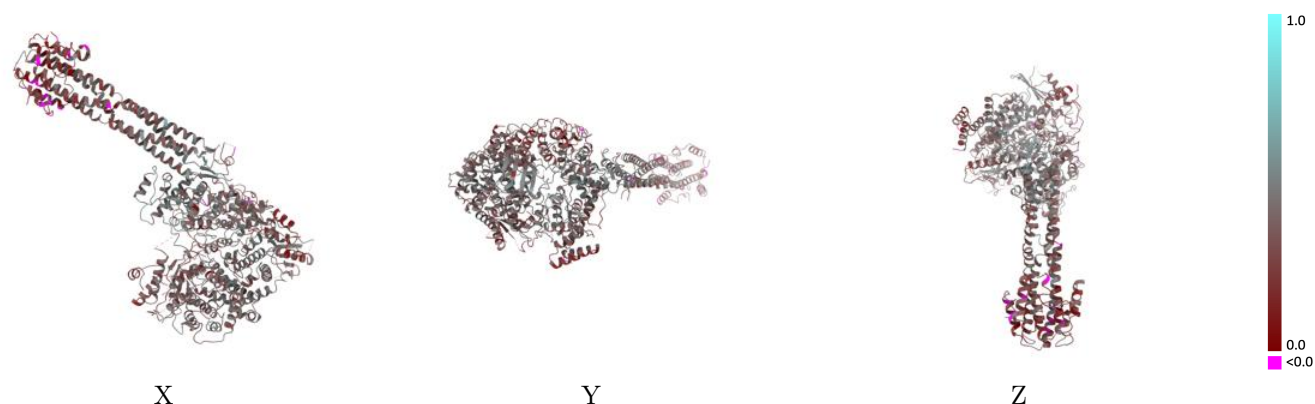
Y



Z

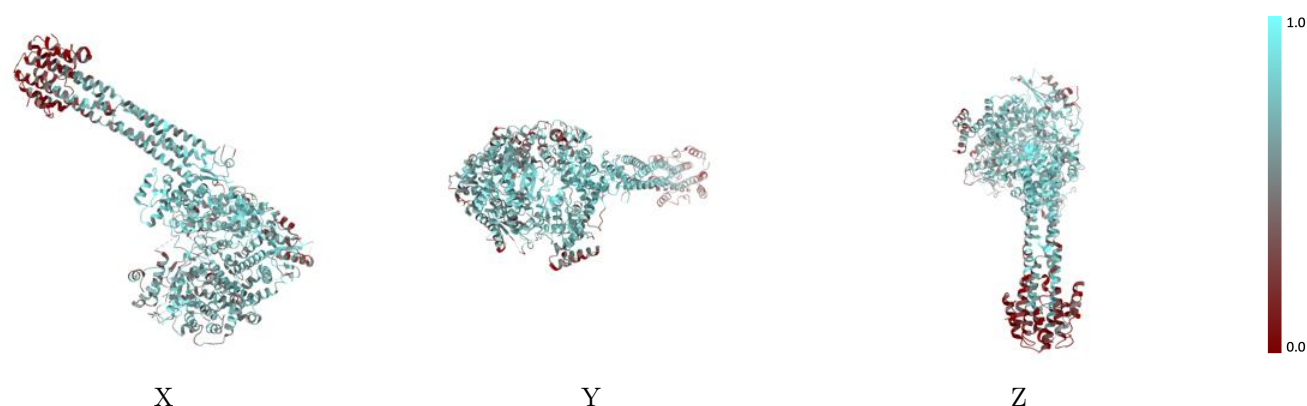
The images above show the 3D surface view of the map at the recommended contour level 0.7 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



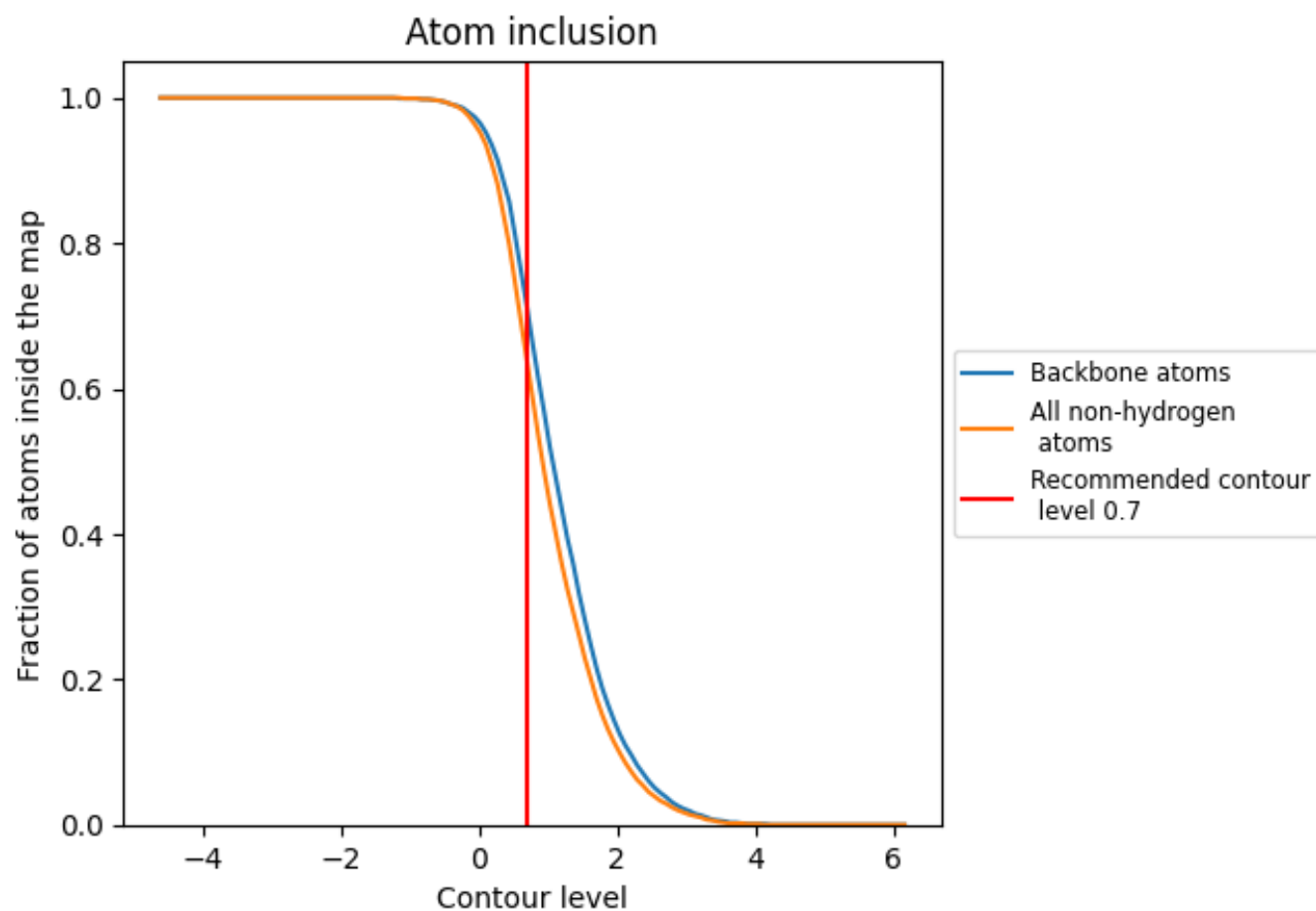
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.7).

9.4 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 64% 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 (0.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6350	<div></div> 0.3840
A	<div></div> 0.6840	<div></div> 0.4010
C	<div></div> 0.5310	<div></div> 0.3670
E	<div></div> 0.5120	<div></div> 0.3270
F	<div></div> 0.5250	<div></div> 0.3420
G	<div></div> 0.4600	<div></div> 0.3410

