



## Full wwPDB EM Validation Report ⓘ

Aug 5, 2025 – 12:44 PM EDT

PDB ID : 9P00 / pdb\_00009p00  
EMDB ID : EMD-71062  
Title : Cryo-EM structure of apo S. Mansoni p97  
Authors : Stephens, D.R.; Han, Y.; Chen, Z.; Collins, J.J.; Fung, H.Y.J.  
Deposited on : 2025-06-06  
Resolution : 2.72 Å(reported)  
Based on initial model : 9OX9

This is a Full wwPDB EM Validation 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.dev126  
MolProbity : 4-5-2 with Phenix2.0rc1  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.45.1

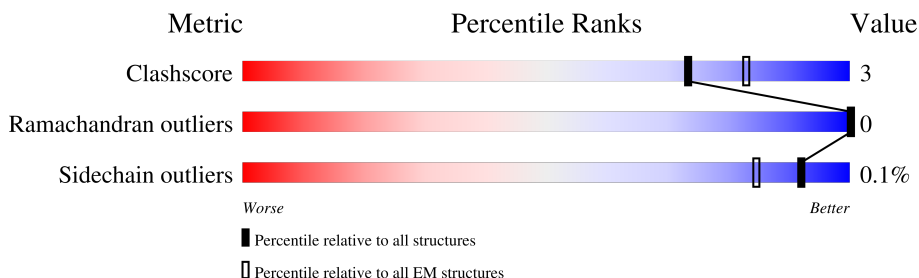
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.72 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	839	58% 5% 37%
1	B	839	57% 6% 37%
1	C	839	60% 5% 37%
1	D	839	59% 5% 37%
1	E	839	59% 5% 37%
1	F	839	59% 5% 37%

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 50287 atoms, of which 25357 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 vesicle-fusing ATPase.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	530	Total	C	H	N	O	S	3	0
			8377	2613	4224	742	779	19		
1	C	532	Total	C	H	N	O	S	5	0
			8432	2627	4254	751	782	18		
1	D	532	Total	C	H	N	O	S	4	0
			8409	2621	4241	747	782	18		
1	F	530	Total	C	H	N	O	S	1	0
			8349	2605	4205	741	780	18		
1	B	530	Total	C	H	N	O	S	2	0
			8374	2612	4224	742	777	19		
1	E	529	Total	C	H	N	O	S	0	0
			8346	2604	4209	740	775	18		

There are 216 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-35	MET	-	initiating methionine	UNP G4M0P7
A	-34	GLY	-	expression tag	UNP G4M0P7
A	-33	SER	-	expression tag	UNP G4M0P7
A	-32	SER	-	expression tag	UNP G4M0P7
A	-31	HIS	-	expression tag	UNP G4M0P7
A	-30	HIS	-	expression tag	UNP G4M0P7
A	-29	HIS	-	expression tag	UNP G4M0P7
A	-28	HIS	-	expression tag	UNP G4M0P7
A	-27	HIS	-	expression tag	UNP G4M0P7
A	-26	HIS	-	expression tag	UNP G4M0P7
A	-25	SER	-	expression tag	UNP G4M0P7
A	-24	SER	-	expression tag	UNP G4M0P7
A	-23	GLY	-	expression tag	UNP G4M0P7
A	-22	LEU	-	expression tag	UNP G4M0P7
A	-21	VAL	-	expression tag	UNP G4M0P7
A	-20	PRO	-	expression tag	UNP G4M0P7
A	-19	ARG	-	expression tag	UNP G4M0P7
A	-18	GLY	-	expression tag	UNP G4M0P7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	SER	-	expression tag	UNP G4M0P7
A	-16	HIS	-	expression tag	UNP G4M0P7
A	-15	MET	-	expression tag	UNP G4M0P7
A	-14	ALA	-	expression tag	UNP G4M0P7
A	-13	SER	-	expression tag	UNP G4M0P7
A	-12	MET	-	expression tag	UNP G4M0P7
A	-11	THR	-	expression tag	UNP G4M0P7
A	-10	GLY	-	expression tag	UNP G4M0P7
A	-9	GLY	-	expression tag	UNP G4M0P7
A	-8	GLN	-	expression tag	UNP G4M0P7
A	-7	GLN	-	expression tag	UNP G4M0P7
A	-6	MET	-	expression tag	UNP G4M0P7
A	-5	GLY	-	expression tag	UNP G4M0P7
A	-4	ARG	-	expression tag	UNP G4M0P7
A	-3	GLY	-	expression tag	UNP G4M0P7
A	-2	SER	-	expression tag	UNP G4M0P7
A	-1	GLU	-	expression tag	UNP G4M0P7
A	0	PHE	-	expression tag	UNP G4M0P7
C	-35	MET	-	initiating methionine	UNP G4M0P7
C	-34	GLY	-	expression tag	UNP G4M0P7
C	-33	SER	-	expression tag	UNP G4M0P7
C	-32	SER	-	expression tag	UNP G4M0P7
C	-31	HIS	-	expression tag	UNP G4M0P7
C	-30	HIS	-	expression tag	UNP G4M0P7
C	-29	HIS	-	expression tag	UNP G4M0P7
C	-28	HIS	-	expression tag	UNP G4M0P7
C	-27	HIS	-	expression tag	UNP G4M0P7
C	-26	HIS	-	expression tag	UNP G4M0P7
C	-25	SER	-	expression tag	UNP G4M0P7
C	-24	SER	-	expression tag	UNP G4M0P7
C	-23	GLY	-	expression tag	UNP G4M0P7
C	-22	LEU	-	expression tag	UNP G4M0P7
C	-21	VAL	-	expression tag	UNP G4M0P7
C	-20	PRO	-	expression tag	UNP G4M0P7
C	-19	ARG	-	expression tag	UNP G4M0P7
C	-18	GLY	-	expression tag	UNP G4M0P7
C	-17	SER	-	expression tag	UNP G4M0P7
C	-16	HIS	-	expression tag	UNP G4M0P7
C	-15	MET	-	expression tag	UNP G4M0P7
C	-14	ALA	-	expression tag	UNP G4M0P7
C	-13	SER	-	expression tag	UNP G4M0P7
C	-12	MET	-	expression tag	UNP G4M0P7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-11	THR	-	expression tag	UNP G4M0P7
C	-10	GLY	-	expression tag	UNP G4M0P7
C	-9	GLY	-	expression tag	UNP G4M0P7
C	-8	GLN	-	expression tag	UNP G4M0P7
C	-7	GLN	-	expression tag	UNP G4M0P7
C	-6	MET	-	expression tag	UNP G4M0P7
C	-5	GLY	-	expression tag	UNP G4M0P7
C	-4	ARG	-	expression tag	UNP G4M0P7
C	-3	GLY	-	expression tag	UNP G4M0P7
C	-2	SER	-	expression tag	UNP G4M0P7
C	-1	GLU	-	expression tag	UNP G4M0P7
C	0	PHE	-	expression tag	UNP G4M0P7
D	-35	MET	-	initiating methionine	UNP G4M0P7
D	-34	GLY	-	expression tag	UNP G4M0P7
D	-33	SER	-	expression tag	UNP G4M0P7
D	-32	SER	-	expression tag	UNP G4M0P7
D	-31	HIS	-	expression tag	UNP G4M0P7
D	-30	HIS	-	expression tag	UNP G4M0P7
D	-29	HIS	-	expression tag	UNP G4M0P7
D	-28	HIS	-	expression tag	UNP G4M0P7
D	-27	HIS	-	expression tag	UNP G4M0P7
D	-26	HIS	-	expression tag	UNP G4M0P7
D	-25	SER	-	expression tag	UNP G4M0P7
D	-24	SER	-	expression tag	UNP G4M0P7
D	-23	GLY	-	expression tag	UNP G4M0P7
D	-22	LEU	-	expression tag	UNP G4M0P7
D	-21	VAL	-	expression tag	UNP G4M0P7
D	-20	PRO	-	expression tag	UNP G4M0P7
D	-19	ARG	-	expression tag	UNP G4M0P7
D	-18	GLY	-	expression tag	UNP G4M0P7
D	-17	SER	-	expression tag	UNP G4M0P7
D	-16	HIS	-	expression tag	UNP G4M0P7
D	-15	MET	-	expression tag	UNP G4M0P7
D	-14	ALA	-	expression tag	UNP G4M0P7
D	-13	SER	-	expression tag	UNP G4M0P7
D	-12	MET	-	expression tag	UNP G4M0P7
D	-11	THR	-	expression tag	UNP G4M0P7
D	-10	GLY	-	expression tag	UNP G4M0P7
D	-9	GLY	-	expression tag	UNP G4M0P7
D	-8	GLN	-	expression tag	UNP G4M0P7
D	-7	GLN	-	expression tag	UNP G4M0P7
D	-6	MET	-	expression tag	UNP G4M0P7

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-5	GLY	-	expression tag	UNP G4M0P7
D	-4	ARG	-	expression tag	UNP G4M0P7
D	-3	GLY	-	expression tag	UNP G4M0P7
D	-2	SER	-	expression tag	UNP G4M0P7
D	-1	GLU	-	expression tag	UNP G4M0P7
D	0	PHE	-	expression tag	UNP G4M0P7
F	-35	MET	-	initiating methionine	UNP G4M0P7
F	-34	GLY	-	expression tag	UNP G4M0P7
F	-33	SER	-	expression tag	UNP G4M0P7
F	-32	SER	-	expression tag	UNP G4M0P7
F	-31	HIS	-	expression tag	UNP G4M0P7
F	-30	HIS	-	expression tag	UNP G4M0P7
F	-29	HIS	-	expression tag	UNP G4M0P7
F	-28	HIS	-	expression tag	UNP G4M0P7
F	-27	HIS	-	expression tag	UNP G4M0P7
F	-26	HIS	-	expression tag	UNP G4M0P7
F	-25	SER	-	expression tag	UNP G4M0P7
F	-24	SER	-	expression tag	UNP G4M0P7
F	-23	GLY	-	expression tag	UNP G4M0P7
F	-22	LEU	-	expression tag	UNP G4M0P7
F	-21	VAL	-	expression tag	UNP G4M0P7
F	-20	PRO	-	expression tag	UNP G4M0P7
F	-19	ARG	-	expression tag	UNP G4M0P7
F	-18	GLY	-	expression tag	UNP G4M0P7
F	-17	SER	-	expression tag	UNP G4M0P7
F	-16	HIS	-	expression tag	UNP G4M0P7
F	-15	MET	-	expression tag	UNP G4M0P7
F	-14	ALA	-	expression tag	UNP G4M0P7
F	-13	SER	-	expression tag	UNP G4M0P7
F	-12	MET	-	expression tag	UNP G4M0P7
F	-11	THR	-	expression tag	UNP G4M0P7
F	-10	GLY	-	expression tag	UNP G4M0P7
F	-9	GLY	-	expression tag	UNP G4M0P7
F	-8	GLN	-	expression tag	UNP G4M0P7
F	-7	GLN	-	expression tag	UNP G4M0P7
F	-6	MET	-	expression tag	UNP G4M0P7
F	-5	GLY	-	expression tag	UNP G4M0P7
F	-4	ARG	-	expression tag	UNP G4M0P7
F	-3	GLY	-	expression tag	UNP G4M0P7
F	-2	SER	-	expression tag	UNP G4M0P7
F	-1	GLU	-	expression tag	UNP G4M0P7
F	0	PHE	-	expression tag	UNP G4M0P7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-35	MET	-	initiating methionine	UNP G4M0P7
B	-34	GLY	-	expression tag	UNP G4M0P7
B	-33	SER	-	expression tag	UNP G4M0P7
B	-32	SER	-	expression tag	UNP G4M0P7
B	-31	HIS	-	expression tag	UNP G4M0P7
B	-30	HIS	-	expression tag	UNP G4M0P7
B	-29	HIS	-	expression tag	UNP G4M0P7
B	-28	HIS	-	expression tag	UNP G4M0P7
B	-27	HIS	-	expression tag	UNP G4M0P7
B	-26	HIS	-	expression tag	UNP G4M0P7
B	-25	SER	-	expression tag	UNP G4M0P7
B	-24	SER	-	expression tag	UNP G4M0P7
B	-23	GLY	-	expression tag	UNP G4M0P7
B	-22	LEU	-	expression tag	UNP G4M0P7
B	-21	VAL	-	expression tag	UNP G4M0P7
B	-20	PRO	-	expression tag	UNP G4M0P7
B	-19	ARG	-	expression tag	UNP G4M0P7
B	-18	GLY	-	expression tag	UNP G4M0P7
B	-17	SER	-	expression tag	UNP G4M0P7
B	-16	HIS	-	expression tag	UNP G4M0P7
B	-15	MET	-	expression tag	UNP G4M0P7
B	-14	ALA	-	expression tag	UNP G4M0P7
B	-13	SER	-	expression tag	UNP G4M0P7
B	-12	MET	-	expression tag	UNP G4M0P7
B	-11	THR	-	expression tag	UNP G4M0P7
B	-10	GLY	-	expression tag	UNP G4M0P7
B	-9	GLY	-	expression tag	UNP G4M0P7
B	-8	GLN	-	expression tag	UNP G4M0P7
B	-7	GLN	-	expression tag	UNP G4M0P7
B	-6	MET	-	expression tag	UNP G4M0P7
B	-5	GLY	-	expression tag	UNP G4M0P7
B	-4	ARG	-	expression tag	UNP G4M0P7
B	-3	GLY	-	expression tag	UNP G4M0P7
B	-2	SER	-	expression tag	UNP G4M0P7
B	-1	GLU	-	expression tag	UNP G4M0P7
B	0	PHE	-	expression tag	UNP G4M0P7
E	-35	MET	-	initiating methionine	UNP G4M0P7
E	-34	GLY	-	expression tag	UNP G4M0P7
E	-33	SER	-	expression tag	UNP G4M0P7
E	-32	SER	-	expression tag	UNP G4M0P7
E	-31	HIS	-	expression tag	UNP G4M0P7
E	-30	HIS	-	expression tag	UNP G4M0P7

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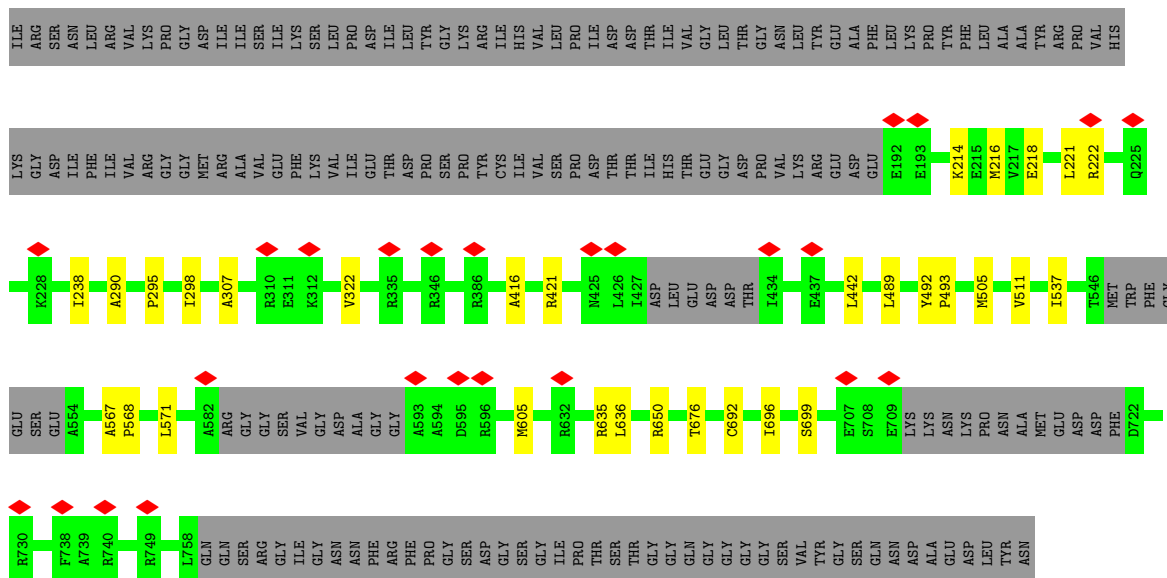


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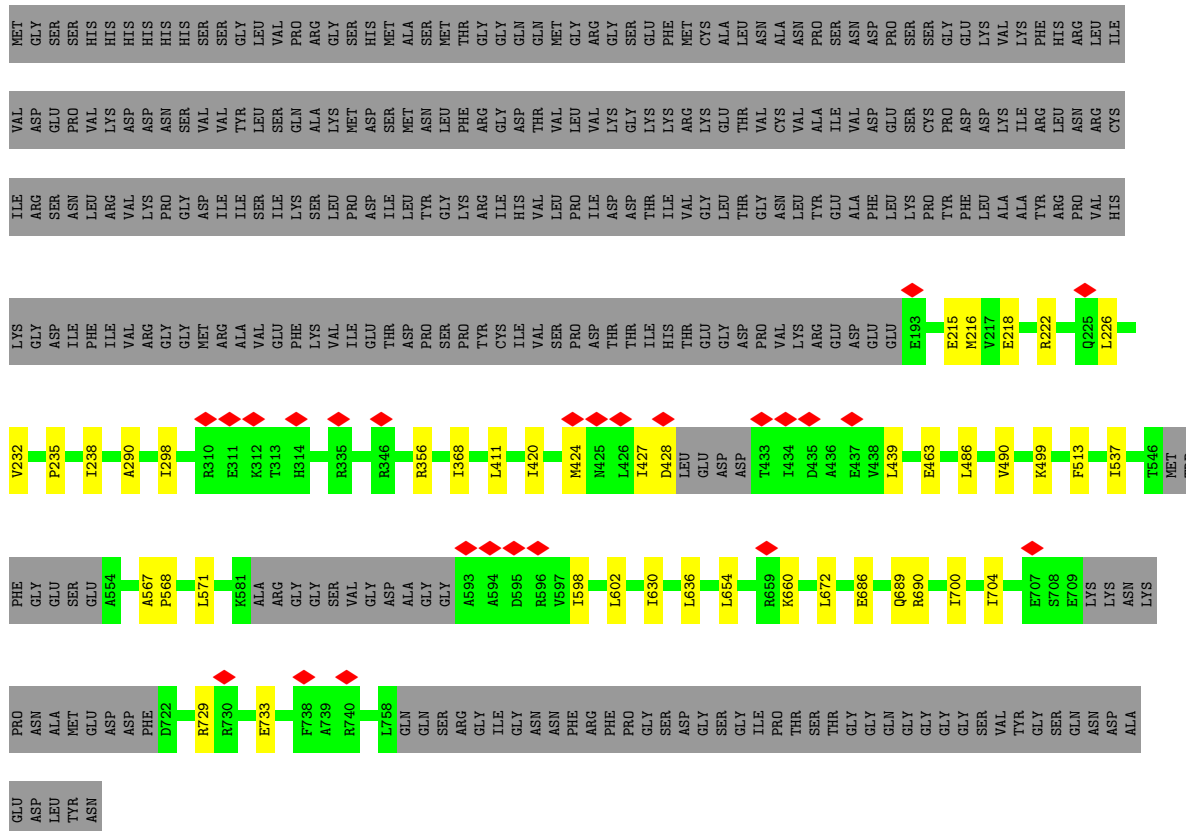
Chain	Residue	Modelled	Actual	Comment	Reference
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E	-28	HIS	-	expression tag	UNP G4M0P7
E	-27	HIS	-	expression tag	UNP G4M0P7
E	-26	HIS	-	expression tag	UNP G4M0P7
E	-25	SER	-	expression tag	UNP G4M0P7
E	-24	SER	-	expression tag	UNP G4M0P7
E	-23	GLY	-	expression tag	UNP G4M0P7
E	-22	LEU	-	expression tag	UNP G4M0P7
E	-21	VAL	-	expression tag	UNP G4M0P7
E	-20	PRO	-	expression tag	UNP G4M0P7
E	-19	ARG	-	expression tag	UNP G4M0P7
E	-18	GLY	-	expression tag	UNP G4M0P7
E	-17	SER	-	expression tag	UNP G4M0P7
E	-16	HIS	-	expression tag	UNP G4M0P7
E	-15	MET	-	expression tag	UNP G4M0P7
E	-14	ALA	-	expression tag	UNP G4M0P7
E	-13	SER	-	expression tag	UNP G4M0P7
E	-12	MET	-	expression tag	UNP G4M0P7
E	-11	THR	-	expression tag	UNP G4M0P7
E	-10	GLY	-	expression tag	UNP G4M0P7
E	-9	GLY	-	expression tag	UNP G4M0P7
E	-8	GLN	-	expression tag	UNP G4M0P7
E	-7	GLN	-	expression tag	UNP G4M0P7
E	-6	MET	-	expression tag	UNP G4M0P7
E	-5	GLY	-	expression tag	UNP G4M0P7
E	-4	ARG	-	expression tag	UNP G4M0P7
E	-3	GLY	-	expression tag	UNP G4M0P7
E	-2	SER	-	expression tag	UNP G4M0P7
E	-1	GLU	-	expression tag	UNP G4M0P7
E	0	PHE	-	expression tag	UNP G4M0P7





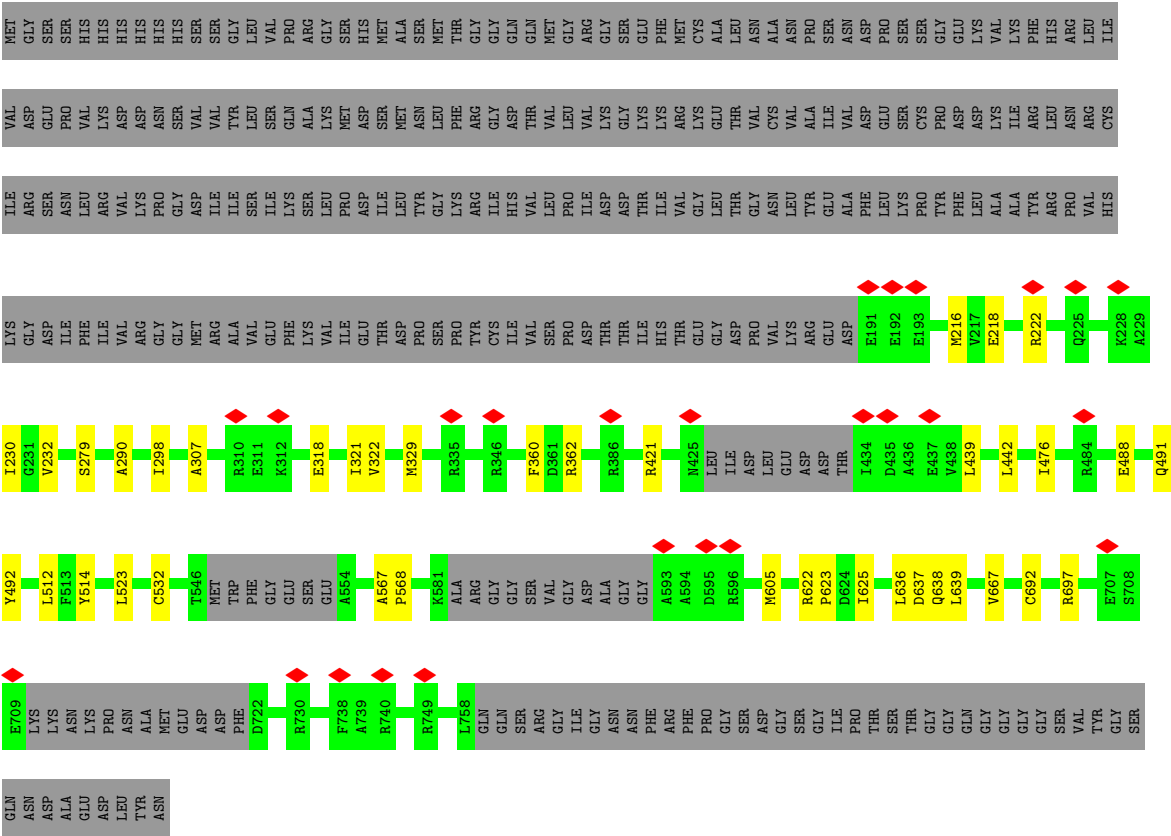


- Molecule 1: vesicle-fusing ATPase

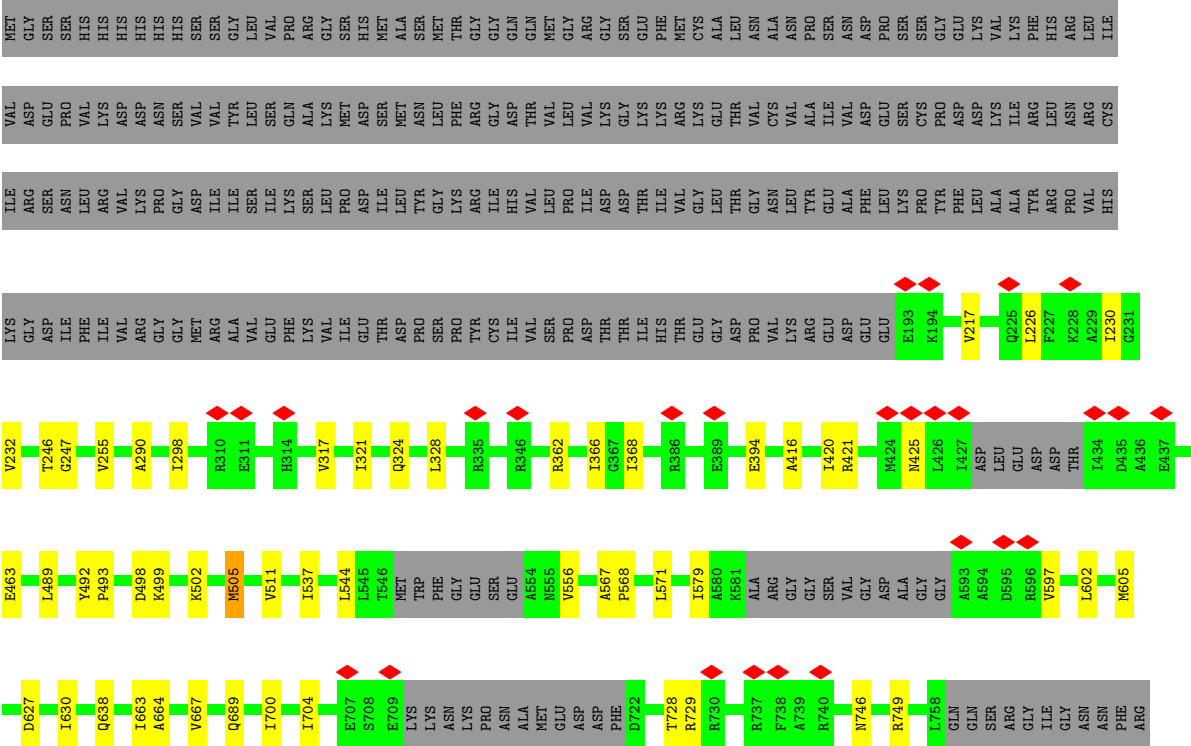


- Molecule 1: vesicle-fusing ATPase





• Molecule 1: vesicle-fusing ATPase



PHE  
PRO  
GLY  
SER  
SER  
ASP  
GLY  
GLY  
SER  
GLY  
ILE  
PRO  
THR  
SER  
THR  
GLY  
GLY  
GLN  
GLY  
GLY  
GLY  
GLY  
GLY  
SER  
SER  
VAL  
TYR  
GLY  
SER  
GLN  
ASN  
ASP  
ALA  
GLU  
ASP  
LEU  
TYR  
ASN

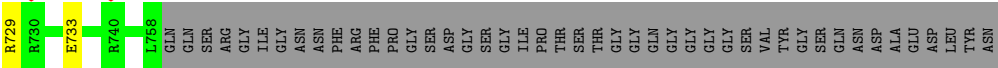
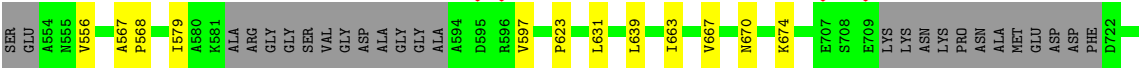
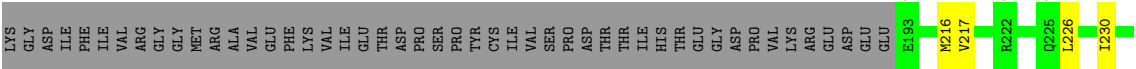
● Molecule 1: vesicle-fusing ATPase



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



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C6	Depositor
Number of particles used	478635	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 ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.881	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.028	Depositor
Recommended contour level	0.126	Depositor
Map size (Å)	336.0, 336.0, 336.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.84, 0.84, 0.84	Depositor

## 5 Model quality

### 5.1 Standard geometry

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	0.18	0/4232	0.29	0/5707
1	B	0.20	0/4220	0.29	0/5692
1	C	0.19	0/4261	0.28	0/5744
1	D	0.19	0/4257	0.31	0/5740
1	E	0.18	0/4200	0.27	0/5664
1	F	0.19	0/4216	0.30	0/5684
All	All	0.19	0/25386	0.29	0/34231

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2
1	D	0	1
1	E	0	1
1	F	0	1
All	All	0	5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	362	ARG	Sidechain
1	B	505[B]	MET	Mainchain
1	D	356	ARG	Sidechain
1	E	356	ARG	Sidechain
1	F	697	ARG	Sidechain

## 5.2 Too-close contacts ⓘ

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	4153	4224	4202	34	0
1	B	4150	4224	4216	37	0
1	C	4178	4254	4228	21	0
1	D	4168	4241	4208	31	0
1	E	4137	4209	4209	22	0
1	F	4144	4205	4191	27	0
All	All	24930	25357	25254	155	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.

All (155) 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:567:ALA:HB3	1:C:568:PRO:HD3	1.66	0.76
1:D:598:ILE:HD11	1:D:630:ILE:HD11	1.72	0.71
1:B:246:THR:HG21	1:B:366:ILE:HG22	1.72	0.71
1:A:567:ALA:HB3	1:A:568:PRO:HD3	1.71	0.71
1:B:663:ILE:HD11	1:B:667:VAL:HG11	1.74	0.70
1:F:218:GLU:OE2	1:F:222:ARG:NH2	2.27	0.68
1:B:579:ILE:HD12	1:B:597:VAL:HG11	1.76	0.67
1:A:577:ASP:OD2	1:A:622:ARG:NH1	2.30	0.65
1:B:324:GLN:HE22	1:B:328:LEU:HD11	1.61	0.65
1:E:579:ILE:HD12	1:E:597:VAL:HG11	1.79	0.64
1:F:605:MET:HE1	1:F:636:LEU:HG	1.79	0.64
1:F:216:MET:HE3	1:F:362:ARG:HE	1.62	0.63
1:C:505:MET:HE3	1:B:689:GLN:OE1	1.98	0.63
1:A:215:GLU:OE1	1:F:421:ARG:NH2	2.32	0.62
1:B:605:MET:HE1	1:B:630:ILE:CD1	2.29	0.62
1:A:420:ILE:HD11	1:B:230:ILE:HG21	1.82	0.61
1:F:567:ALA:HB3	1:F:568:PRO:CD	2.31	0.61
1:C:221:LEU:HD22	1:C:295:PRO:HB3	1.82	0.61
1:B:246:THR:HG22	1:B:247:GLY:H	1.66	0.60
1:B:567:ALA:HB3	1:B:568:PRO:HD3	1.83	0.60
1:F:230:ILE:HG21	1:E:420:ILE:HD11	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:324:GLN:NE2	1:B:328:LEU:HD11	2.17	0.59
1:B:567:ALA:HB3	1:B:568:PRO:CD	2.33	0.59
1:E:567:ALA:HB3	1:E:568:PRO:HD3	1.84	0.59
1:D:567:ALA:HB3	1:D:568:PRO:CD	2.32	0.59
1:D:567:ALA:HB3	1:D:568:PRO:HD3	1.84	0.58
1:D:602:LEU:HD21	1:D:630:ILE:HD13	1.86	0.57
1:F:567:ALA:HB3	1:F:568:PRO:HD3	1.87	0.57
1:A:216:MET:HE3	1:A:238:ILE:HD13	1.86	0.57
1:B:246:THR:HG22	1:B:247:GLY:N	2.20	0.57
1:F:514:TYR:HB2	1:F:623:PRO:HG3	1.90	0.54
1:A:424:MET:HA	1:A:427:ILE:HG22	1.90	0.54
1:A:226:LEU:HD11	1:F:442:LEU:HD11	1.90	0.53
1:D:216:MET:HE3	1:D:238:ILE:HD13	1.91	0.52
1:C:421:ARG:NH2	1:D:215:GLU:OE1	2.42	0.52
1:E:216:MET:HE3	1:E:362:ARG:HE	1.73	0.52
1:D:486:LEU:HD11	1:D:513:PHE:HZ	1.75	0.52
1:E:514:TYR:HB2	1:E:623:PRO:HG3	1.92	0.52
1:A:686:GLU:OE2	1:A:690:ARG:NH2	2.43	0.52
1:C:605:MET:HE1	1:C:636:LEU:HG	1.91	0.52
1:E:290:ALA:CB	1:E:298:ILE:HD11	2.40	0.51
1:A:579:ILE:O	1:A:598:ILE:HD11	2.10	0.51
1:B:663:ILE:CD1	1:B:667:VAL:HG11	2.40	0.51
1:C:218:GLU:HG2	1:C:222:ARG:NE	2.26	0.51
1:E:631:LEU:HD22	1:E:639:LEU:HD21	1.91	0.51
1:C:216:MET:HE3	1:C:238:ILE:HD13	1.91	0.51
1:C:692:CYS:O	1:C:696:ILE:HG12	2.11	0.51
1:A:424:MET:HE1	1:B:226:LEU:HD22	1.93	0.51
1:E:567:ALA:HB3	1:E:568:PRO:CD	2.41	0.50
1:F:279:SER:HB3	1:F:321:ILE:HD12	1.94	0.50
1:B:627:ASP:O	1:B:630:ILE:HG22	2.12	0.50
1:D:486:LEU:HD11	1:D:513:PHE:CZ	2.47	0.49
1:A:567:ALA:CB	1:A:568:PRO:HD3	2.39	0.49
1:E:567:ALA:CB	1:E:568:PRO:HD3	2.42	0.49
1:B:664:ALA:O	1:B:667:VAL:HG12	2.12	0.49
1:A:729:ARG:O	1:A:733:GLU:OE1	2.31	0.49
1:F:318:GLU:O	1:F:321:ILE:HG22	2.13	0.48
1:D:686:GLU:OE2	1:D:690:ARG:NH2	2.46	0.48
1:A:567:ALA:HB3	1:A:568:PRO:CD	2.41	0.48
1:B:489:LEU:HD21	1:B:638:GLN:OE1	2.14	0.48
1:B:290:ALA:CB	1:B:298:ILE:HD11	2.43	0.48
1:E:498:ASP:OD1	1:E:499:LYS:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:442:LEU:HD11	1:D:226:LEU:HD11	1.95	0.48
1:D:654:LEU:CD1	1:D:672:LEU:HD22	2.44	0.48
1:F:329:MET:HE1	1:F:360:PHE:CD2	2.49	0.48
1:D:729:ARG:O	1:D:733:GLU:OE1	2.32	0.47
1:A:368:ILE:HD11	1:A:463:GLU:HB2	1.95	0.47
1:A:216:MET:HE3	1:A:238:ILE:CD1	2.44	0.47
1:A:539:ILE:CD1	1:A:559:ILE:HG21	2.45	0.47
1:B:394:GLU:N	1:B:394:GLU:OE1	2.47	0.47
1:B:499:LYS:O	1:B:502:LYS:HG2	2.14	0.47
1:D:427:ILE:HG22	1:D:427:ILE:O	2.15	0.47
1:B:728:THR:HG22	1:B:729:ARG:N	2.28	0.46
1:C:216:MET:HE3	1:C:238:ILE:CD1	2.45	0.46
1:B:544:LEU:HD11	1:B:556:VAL:HG22	1.97	0.46
1:D:420:ILE:HD11	1:E:230:ILE:HG21	1.97	0.46
1:F:637:ASP:OD1	1:F:638:GLN:OE1	2.34	0.46
1:A:622:ARG:HD2	1:A:625:ILE:HD11	1.98	0.46
1:D:368:ILE:HD11	1:D:463:GLU:HB2	1.97	0.46
1:F:290:ALA:CB	1:F:298:ILE:HD11	2.46	0.46
1:F:512:LEU:HB3	1:F:639:LEU:HD23	1.98	0.46
1:E:499:LYS:HA	1:E:502:LYS:HG2	1.99	0.45
1:E:670:ASN:O	1:E:674:LYS:HG3	2.16	0.45
1:C:567:ALA:CB	1:C:568:PRO:HD3	2.42	0.45
1:D:218:GLU:HG2	1:D:222:ARG:HD3	1.98	0.45
1:B:498:ASP:OD1	1:B:499:LYS:N	2.49	0.45
1:E:499:LYS:O	1:E:502:LYS:HG2	2.16	0.45
1:C:650:ARG:NE	1:C:676:THR:O	2.49	0.45
1:D:630:ILE:CG2	1:D:636:LEU:HD12	2.46	0.45
1:D:490:VAL:HG12	1:D:490:VAL:O	2.17	0.44
1:E:544:LEU:HD11	1:E:556:VAL:HG22	1.98	0.44
1:F:488:GLU:HG2	1:F:492:TYR:CE2	2.52	0.44
1:E:663:ILE:HD11	1:E:667:VAL:HG11	1.99	0.44
1:D:439:LEU:CD2	1:E:226:LEU:HD13	2.48	0.44
1:A:427:ILE:O	1:A:427:ILE:HG23	2.16	0.44
1:F:232:VAL:HG22	1:E:416:ALA:HB3	1.99	0.44
1:A:512:LEU:HD22	1:A:631:LEU:HD21	2.00	0.43
1:A:416:ALA:HB3	1:B:232:VAL:HG22	2.00	0.43
1:A:322:VAL:O	1:A:326:LEU:HD13	2.19	0.43
1:C:635:ARG:O	1:C:636:LEU:HD23	2.18	0.43
1:F:476:ILE:HG21	1:F:523:LEU:HB3	2.00	0.43
1:B:602:LEU:HA	1:B:605:MET:HE3	1.99	0.43
1:A:492:TYR:HB2	1:A:493:PRO:HD3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:290:ALA:CB	1:D:298:ILE:HD11	2.49	0.43
1:B:421:ARG:O	1:B:425:ASN:OD1	2.37	0.43
1:A:226:LEU:HD12	1:F:439:LEU:HD23	2.01	0.43
1:D:216:MET:HG2	1:D:235:PRO:HG3	2.01	0.43
1:D:216:MET:HE3	1:D:238:ILE:CD1	2.49	0.43
1:F:667:VAL:O	1:F:667:VAL:HG23	2.18	0.43
1:A:511:VAL:N	1:A:636:LEU:HD23	2.34	0.42
1:C:290:ALA:CB	1:C:298:ILE:HD11	2.49	0.42
1:A:539:ILE:HD13	1:A:559:ILE:HD13	2.01	0.42
1:E:217:VAL:HG11	1:E:255:VAL:HG11	2.00	0.42
1:A:509:LYS:HG3	1:A:615:PHE:CD1	2.54	0.42
1:F:622:ARG:O	1:F:625:ILE:HG22	2.19	0.42
1:E:729:ARG:O	1:E:733:GLU:OE1	2.37	0.42
1:A:290:ALA:CB	1:A:298:ILE:HD11	2.49	0.42
1:D:700:ILE:O	1:D:704:ILE:HG12	2.19	0.42
1:D:689:GLN:OE1	1:E:505:MET:SD	2.78	0.42
1:A:700:ILE:O	1:A:704:ILE:HG12	2.20	0.42
1:C:489:LEU:HD23	1:C:511:VAL:CG2	2.50	0.42
1:B:492:TYR:HB2	1:B:493:PRO:HD3	2.02	0.42
1:A:577:ASP:OD2	1:A:622:ARG:HG2	2.20	0.42
1:D:660:LYS:O	1:D:660:LYS:HG2	2.20	0.42
1:D:424:MET:O	1:D:428:ASP:N	2.53	0.42
1:A:685:THR:O	1:A:689:GLN:HG2	2.20	0.41
1:A:622:ARG:HG3	1:A:622:ARG:O	2.21	0.41
1:D:411:LEU:HD23	1:D:411:LEU:C	2.45	0.41
1:C:492:TYR:HB2	1:C:493:PRO:HD3	2.02	0.41
1:D:654:LEU:HD13	1:D:672:LEU:HD22	2.02	0.41
1:F:567:ALA:CB	1:F:568:PRO:CD	2.98	0.41
1:B:368:ILE:HD11	1:B:463:GLU:HB2	2.03	0.41
1:B:489:LEU:HD23	1:B:511:VAL:CG2	2.51	0.41
1:C:416:ALA:HB3	1:D:232:VAL:HG22	2.03	0.41
1:F:329:MET:HE1	1:F:360:PHE:CE2	2.56	0.41
1:B:537:ILE:HB	1:B:571:LEU:HD12	2.03	0.41
1:B:700:ILE:O	1:B:704:ILE:HG12	2.21	0.41
1:C:214:LYS:HG3	1:C:218:GLU:OE1	2.20	0.41
1:B:368:ILE:CD1	1:B:463:GLU:HB2	2.51	0.41
1:B:746:ASN:OD1	1:B:749:ARG:NH2	2.54	0.41
1:C:307:ALA:HA	1:C:322:VAL:HG22	2.03	0.41
1:C:699:SER:OG	1:D:499:LYS:HE3	2.20	0.41
1:A:503:PHE:HB3	1:F:692:CYS:SG	2.62	0.40
1:A:666:ASP:OD1	1:A:666:ASP:O	2.40	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:317:VAL:O	1:B:321:ILE:HG13	2.22	0.40
1:C:537:ILE:HB	1:C:571:LEU:HD12	2.03	0.40
1:B:544:LEU:HD11	1:B:556:VAL:CG2	2.51	0.40
1:F:637:ASP:OD1	1:F:638:GLN:N	2.53	0.40
1:B:217:VAL:HG11	1:B:255:VAL:HG11	2.03	0.40
1:A:216:MET:HG2	1:A:235:PRO:HG3	2.03	0.40
1:D:537:ILE:HB	1:D:571:LEU:HD12	2.03	0.40
1:F:307:ALA:HA	1:F:322:VAL:HG22	2.03	0.40
1:F:491:GLN:HA	1:F:532:CYS:SG	2.62	0.40
1:B:416:ALA:O	1:B:420:ILE:HG12	2.22	0.40
1:E:492:TYR:HB2	1:E:493:PRO:HD3	2.03	0.40

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	523/839 (62%)	509 (97%)	14 (3%)	0	100	100
1	B	522/839 (62%)	506 (97%)	16 (3%)	0	100	100
1	C	527/839 (63%)	517 (98%)	10 (2%)	0	100	100
1	D	526/839 (63%)	507 (96%)	19 (4%)	0	100	100
1	E	519/839 (62%)	504 (97%)	15 (3%)	0	100	100
1	F	521/839 (62%)	505 (97%)	16 (3%)	0	100	100
All	All	3138/5034 (62%)	3048 (97%)	90 (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	448/704 (64%)	448 (100%)	0	100	100
1	B	446/704 (63%)	444 (100%)	2 (0%)	89	96
1	C	449/704 (64%)	449 (100%)	0	100	100
1	D	450/704 (64%)	450 (100%)	0	100	100
1	E	444/704 (63%)	443 (100%)	1 (0%)	92	98
1	F	445/704 (63%)	445 (100%)	0	100	100
All	All	2682/4224 (64%)	2679 (100%)	3 (0%)	92	98

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	505[A]	MET
1	B	505[B]	MET
1	E	356	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	223	HIS
1	A	418	GLN
1	A	440	ASN
1	A	621	ASN
1	C	314	HIS
1	C	496	HIS
1	C	599	ASN
1	C	613	ASN
1	C	670	ASN
1	C	731	HIS
1	D	533	GLN
1	D	670	ASN
1	F	223	HIS
1	F	314	HIS

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Mol	Chain	Res	Type
1	F	457	ASN
1	F	496	HIS
1	F	694	GLN
1	B	267	ASN
1	E	403	HIS
1	E	670	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

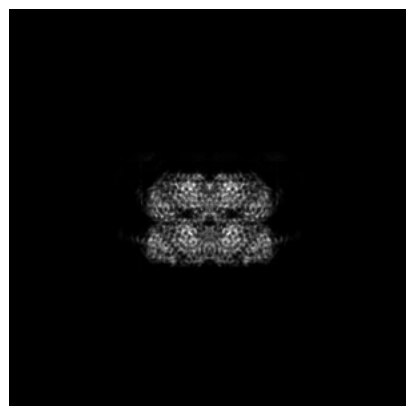
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71062. These allow visual inspection of the internal detail of the map and identification of artifacts.

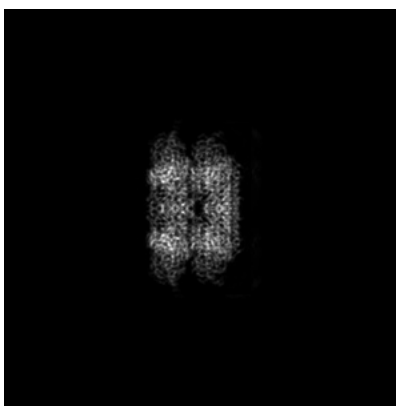
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

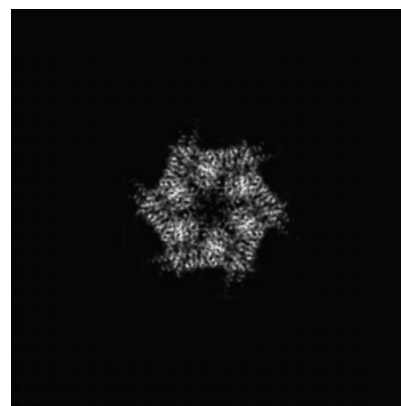
#### 6.1.1 Primary map



X

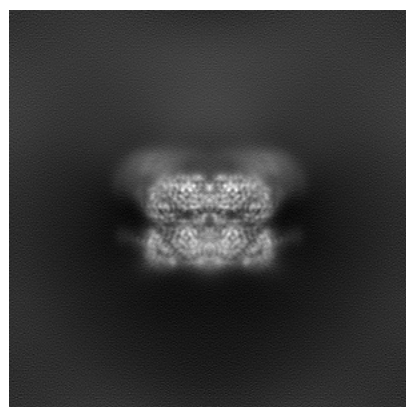


Y

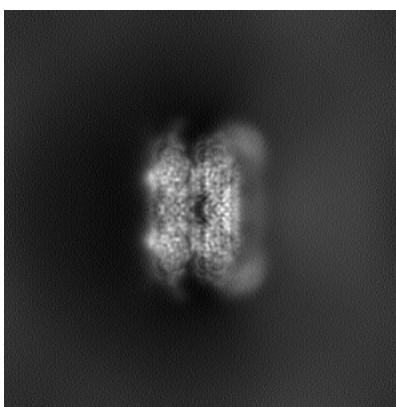


Z

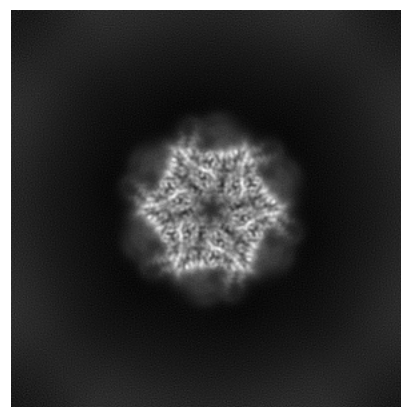
#### 6.1.2 Raw map



X



Y



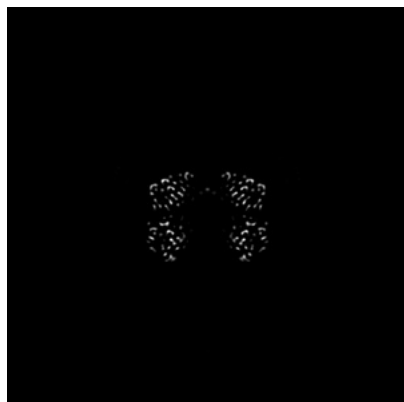
Z

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



## 6.2 Central slices [i](#)

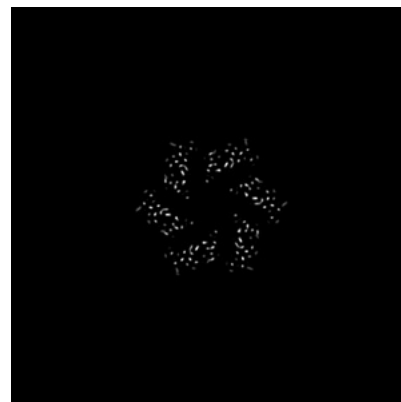
### 6.2.1 Primary map



X Index: 200

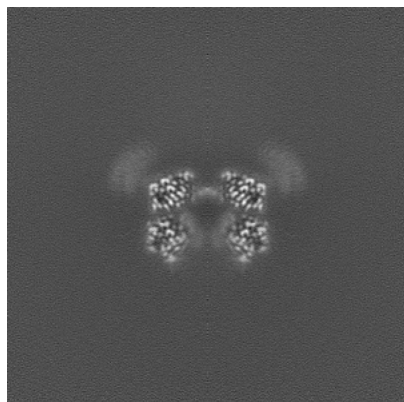


Y Index: 200

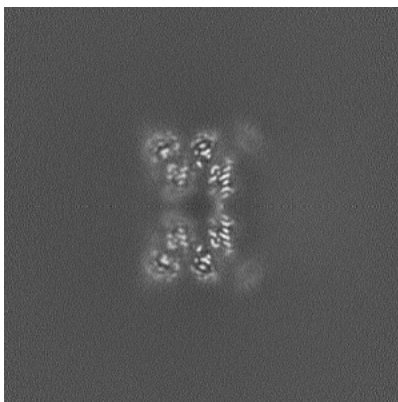


Z Index: 200

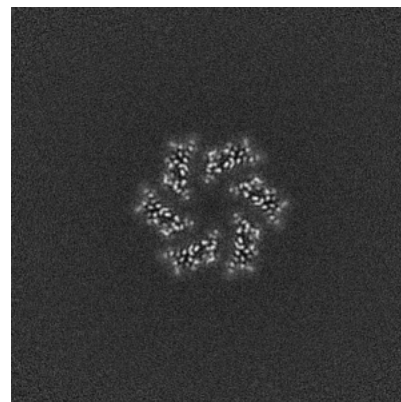
### 6.2.2 Raw map



X Index: 200



Y Index: 200



Z Index: 200

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: 169

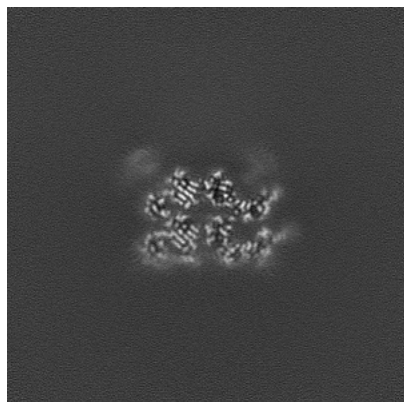


Y Index: 218

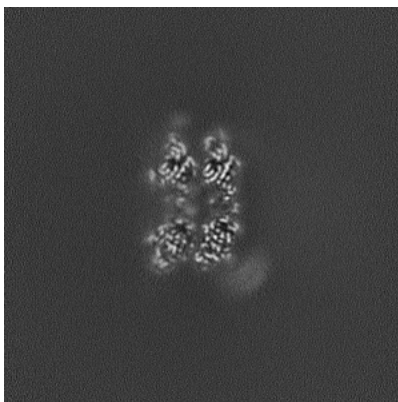


Z Index: 168

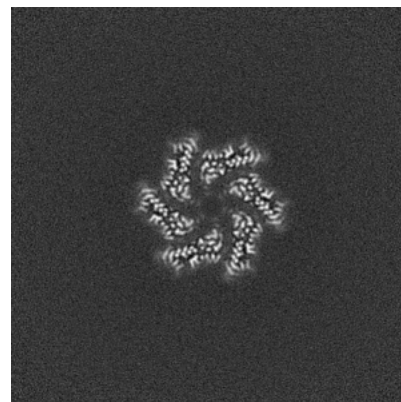
### 6.3.2 Raw map



X Index: 170



Y Index: 183

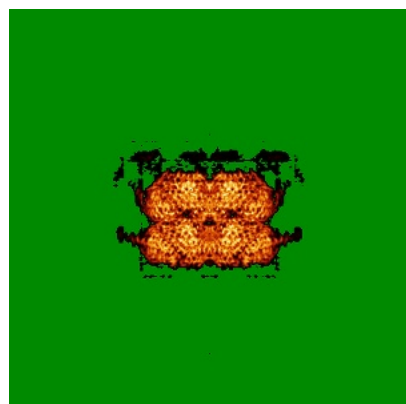


Z Index: 203

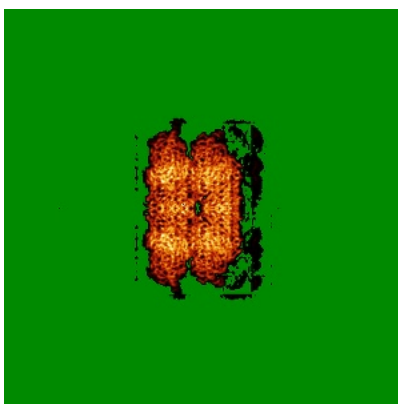
The images above show the largest variance slices of the map in three orthogonal directions.

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

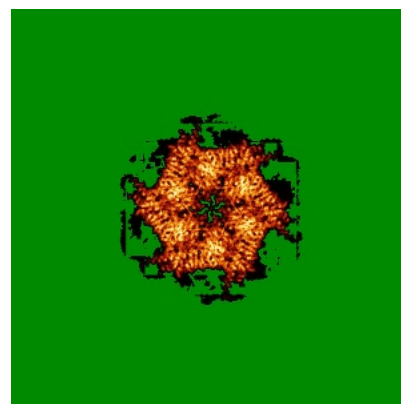
### 6.4.1 Primary map



X

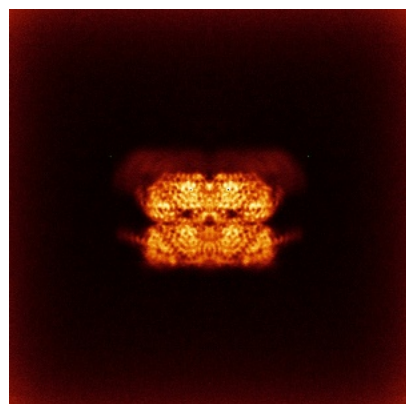


Y

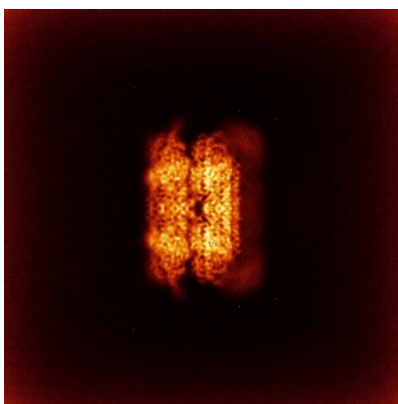


Z

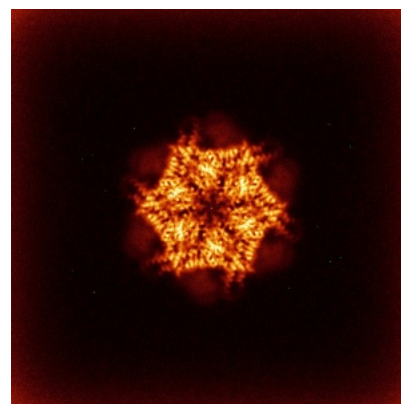
### 6.4.2 Raw map



X



Y

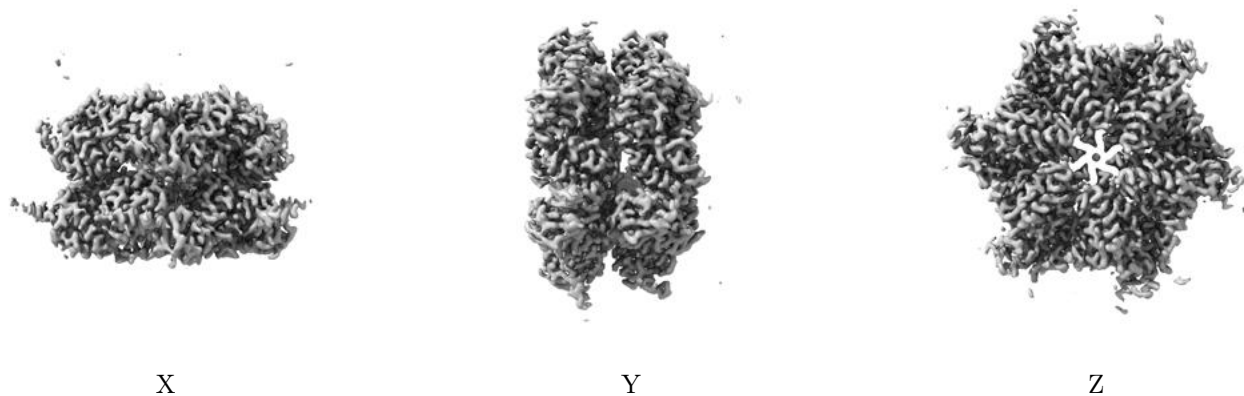


Z

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 0.126. 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.

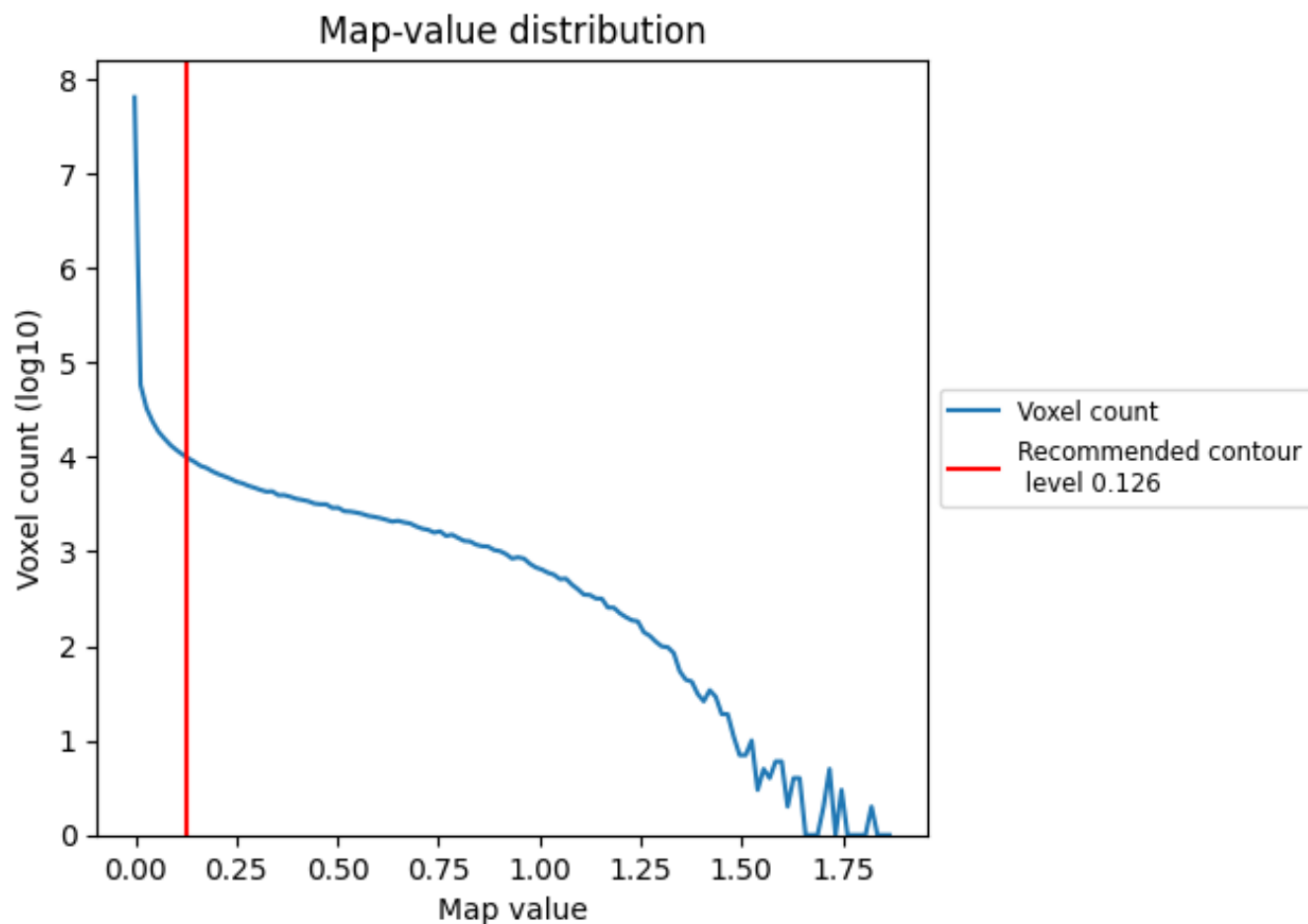
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

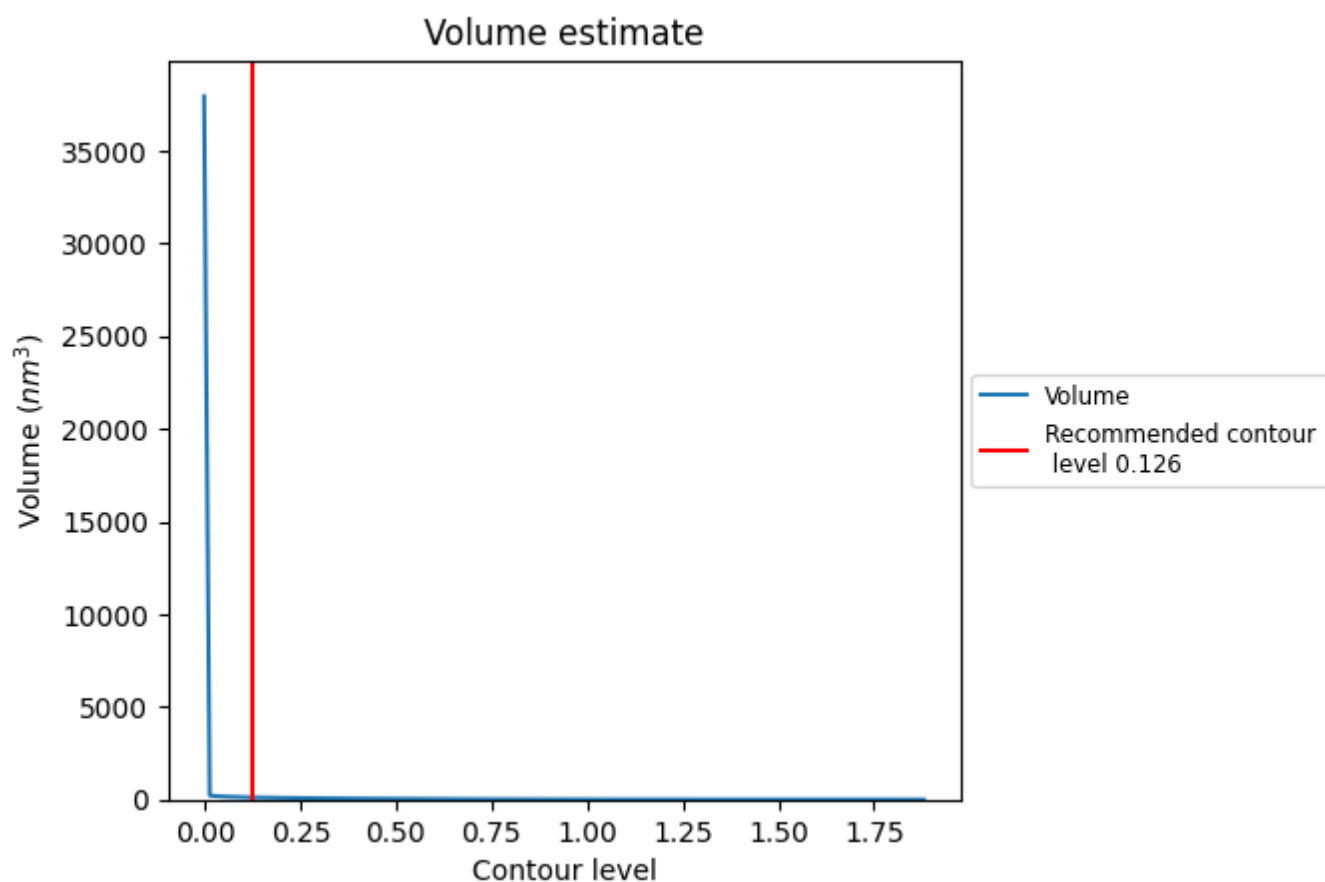
This section contains the results of statistical analysis of the map.

### 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.

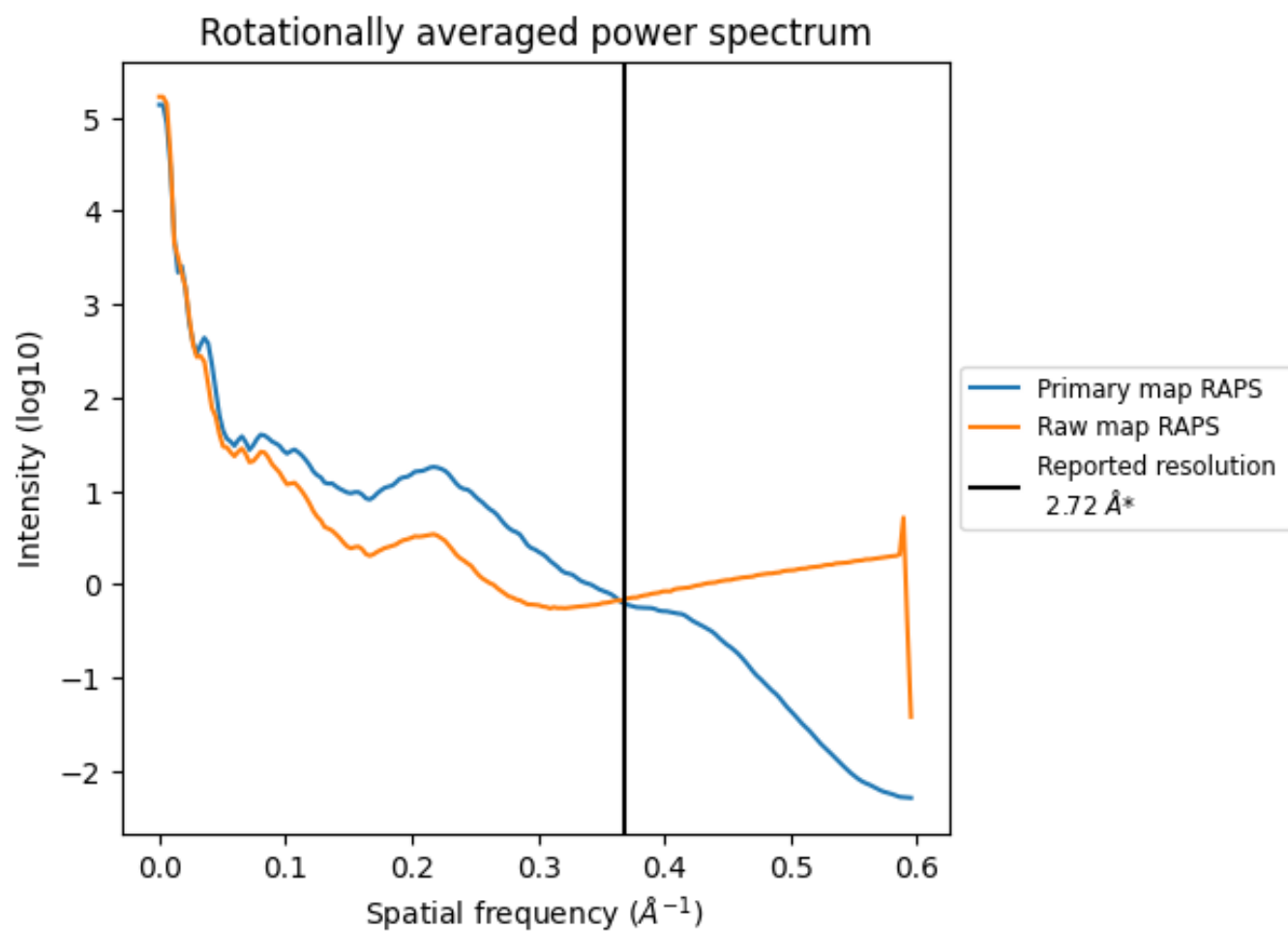
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 116  $\text{nm}^3$ ; this corresponds to an approximate mass of 105 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 ⓘ



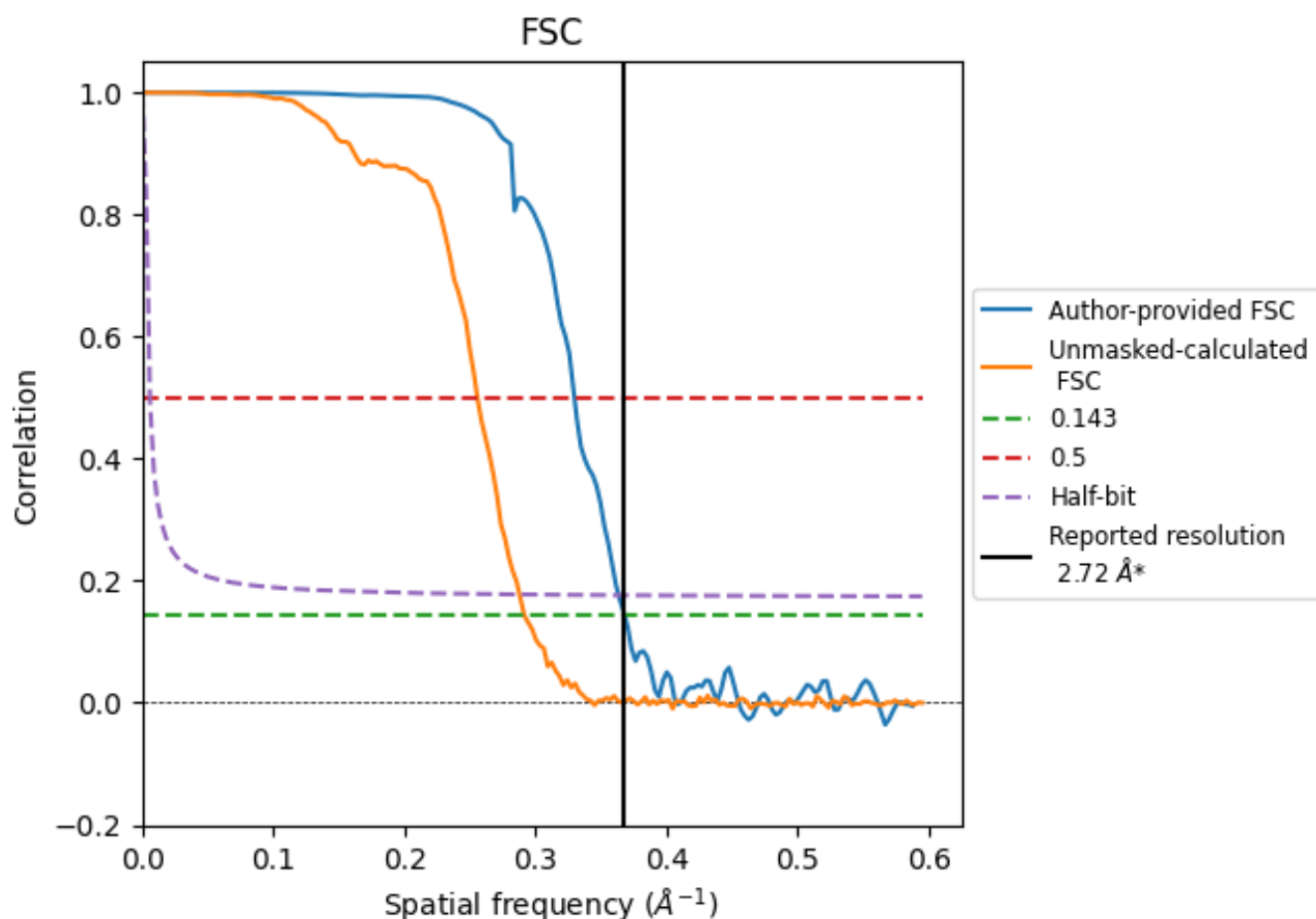
\*Reported resolution corresponds to spatial frequency of 0.368 Å<sup>-1</sup>



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

## 8.2 Resolution estimates

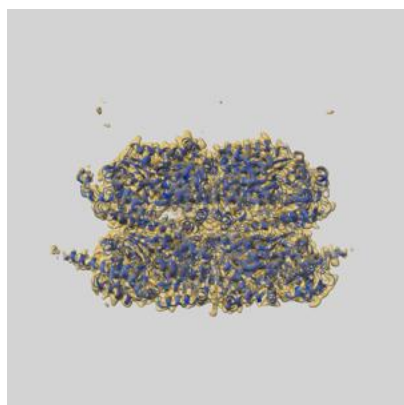
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.72	-	-
Author-provided FSC curve	2.72	3.03	2.75
Unmasked-calculated*	3.43	3.91	3.47

\*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 3.43 differs from the reported value 2.72 by more than 10 %

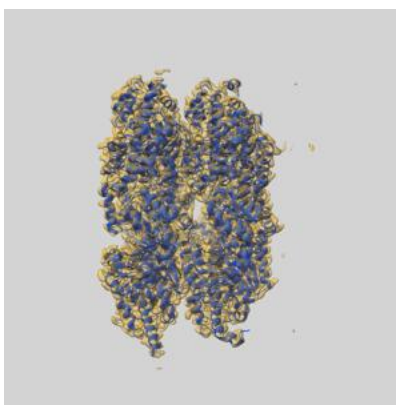
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-71062 and PDB model 9P00. Per-residue inclusion information can be found in section [3](#) on page [9](#).

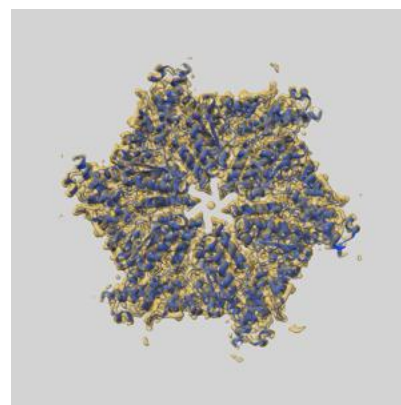
### 9.1 Map-model overlay [i](#)



X



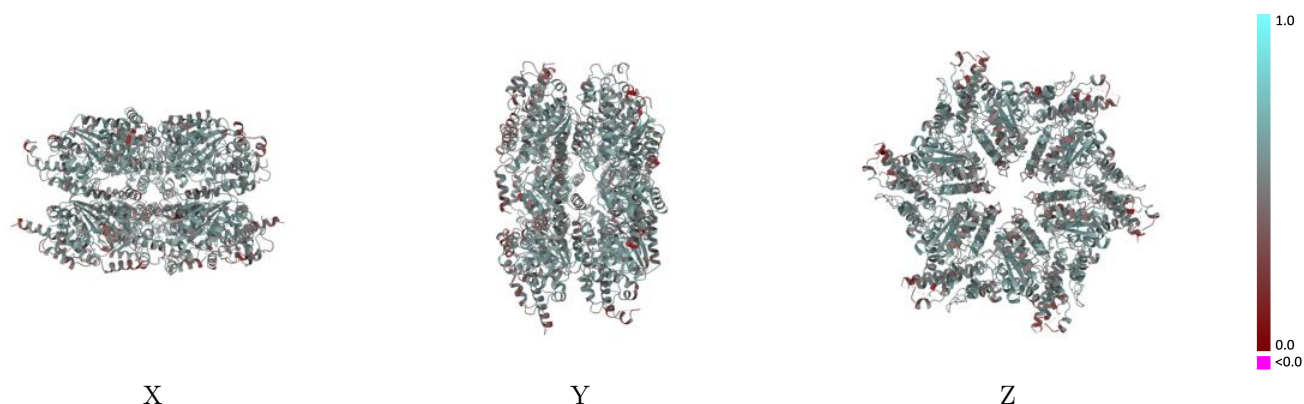
Y



Z

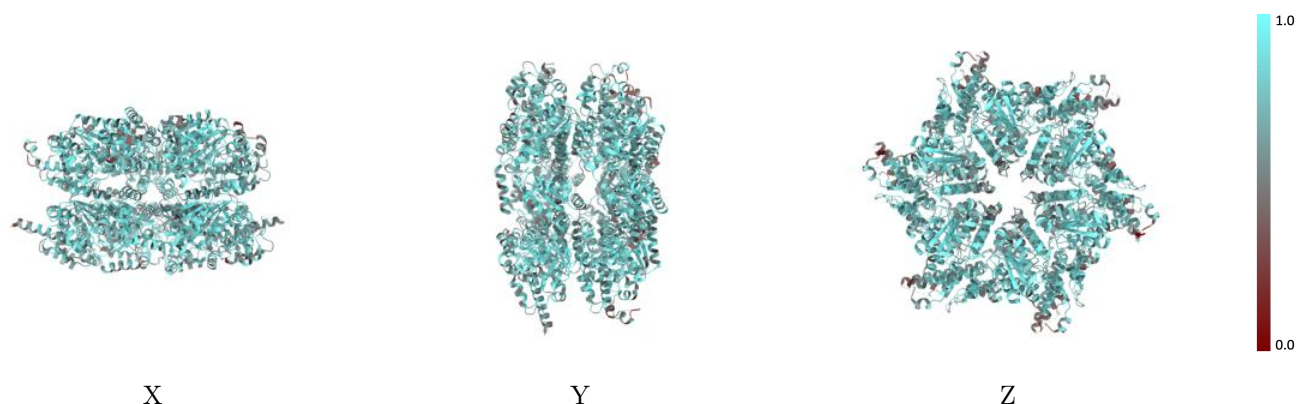
The images above show the 3D surface view of the map at the recommended contour level 0.126 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



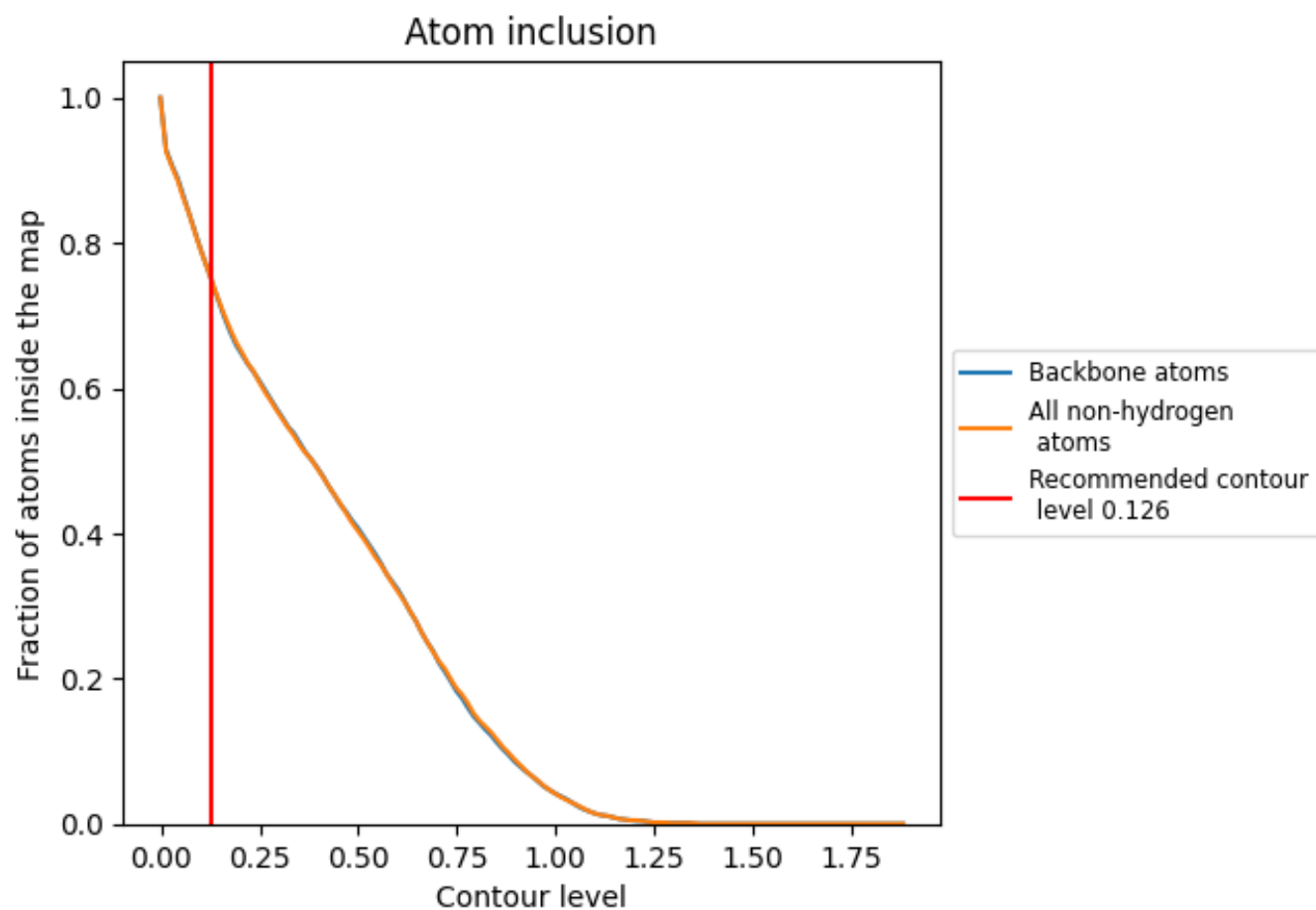
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.126).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 75% 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 (0.126) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.7520	<div><div></div></div> 0.5130
A	<div><div></div></div> 0.7610	<div><div></div></div> 0.5120
B	<div><div></div></div> 0.7610	<div><div></div></div> 0.5110
C	<div><div></div></div> 0.7640	<div><div></div></div> 0.5140
D	<div><div></div></div> 0.7700	<div><div></div></div> 0.5160
E	<div><div></div></div> 0.7660	<div><div></div></div> 0.5130
F	<div><div></div></div> 0.7590	<div><div></div></div> 0.5100

1.0

0.0

<0.0