



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 09:59 PM UTC

PDB ID : 9MPS / pdb_00009mps
EMDB ID : EMD-48501
Title : Cryo-EM structure of VCPIP1 VCPID bound to VCP D2 domain dimer (with extra D2 domain)
Authors : Shah, B.; Hunkeler, M.; Buhrlage, S.J.; Fischer, E.S.
Deposited on : 2024-12-31
Resolution : 2.90 Å(reported)
Based on initial model : 5FTK

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
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

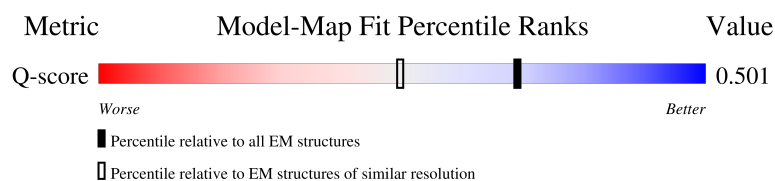
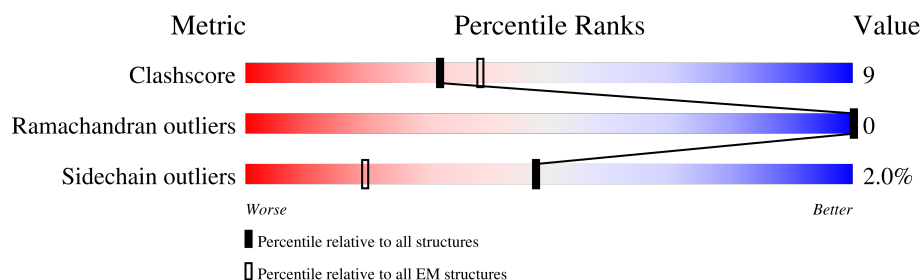
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 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	13054 (2.40 - 3.40)

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	D	1250	 8% 7% 90%
2	A	832	 7% 30% 66%
2	E	832	 6% 18% 5% 77%
2	F	832	 6% 24% 8% 68%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13626 atoms, of which 6754 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 Deubiquitinating protein VCP1P1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	D	126	Total	C	H	N	O	S	0	0
			1956	636	953	173	191	3		

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-27	MET	-	expression tag	UNP Q96JH7
D	-26	GLY	-	expression tag	UNP Q96JH7
D	-25	ASP	-	expression tag	UNP Q96JH7
D	-24	TRP	-	expression tag	UNP Q96JH7
D	-23	SER	-	expression tag	UNP Q96JH7
D	-22	HIS	-	expression tag	UNP Q96JH7
D	-21	PRO	-	expression tag	UNP Q96JH7
D	-20	GLN	-	expression tag	UNP Q96JH7
D	-19	PHE	-	expression tag	UNP Q96JH7
D	-18	GLU	-	expression tag	UNP Q96JH7
D	-17	LYS	-	expression tag	UNP Q96JH7
D	-16	SER	-	expression tag	UNP Q96JH7
D	-15	GLY	-	expression tag	UNP Q96JH7
D	-14	GLY	-	expression tag	UNP Q96JH7
D	-13	GLY	-	expression tag	UNP Q96JH7
D	-12	SER	-	expression tag	UNP Q96JH7
D	-11	GLY	-	expression tag	UNP Q96JH7
D	-10	GLY	-	expression tag	UNP Q96JH7
D	-9	LEU	-	expression tag	UNP Q96JH7
D	-8	GLU	-	expression tag	UNP Q96JH7
D	-7	VAL	-	expression tag	UNP Q96JH7
D	-6	LEU	-	expression tag	UNP Q96JH7
D	-5	PHE	-	expression tag	UNP Q96JH7
D	-4	GLN	-	expression tag	UNP Q96JH7
D	-3	GLY	-	expression tag	UNP Q96JH7
D	-2	PRO	-	expression tag	UNP Q96JH7
D	-1	GLY	-	expression tag	UNP Q96JH7
D	0	SER	-	expression tag	UNP Q96JH7

- Molecule 2 is a protein called Transitional endoplasmic reticulum ATPase.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	A	285	Total	C	H	N	O	S	0	0
			4503	1414	2255	397	425	12		
2	E	192	Total	C	H	N	O	S	0	0
			2958	963	1454	257	276	8		
2	F	269	Total	C	H	N	O	S	0	0
			4209	1345	2092	373	387	12		

There are 78 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-25	MET	-	expression tag	UNP P55072
A	-24	GLY	-	expression tag	UNP P55072
A	-23	ASP	-	expression tag	UNP P55072
A	-22	TYR	-	expression tag	UNP P55072
A	-21	LYS	-	expression tag	UNP P55072
A	-20	ASP	-	expression tag	UNP P55072
A	-19	ASP	-	expression tag	UNP P55072
A	-18	ASP	-	expression tag	UNP P55072
A	-17	ASP	-	expression tag	UNP P55072
A	-16	LYS	-	expression tag	UNP P55072
A	-15	GLY	-	expression tag	UNP P55072
A	-14	GLY	-	expression tag	UNP P55072
A	-13	GLY	-	expression tag	UNP P55072
A	-12	SER	-	expression tag	UNP P55072
A	-11	GLY	-	expression tag	UNP P55072
A	-10	GLY	-	expression tag	UNP P55072
A	-9	LEU	-	expression tag	UNP P55072
A	-8	GLU	-	expression tag	UNP P55072
A	-7	VAL	-	expression tag	UNP P55072
A	-6	LEU	-	expression tag	UNP P55072
A	-5	PHE	-	expression tag	UNP P55072
A	-4	GLN	-	expression tag	UNP P55072
A	-3	GLY	-	expression tag	UNP P55072
A	-2	PRO	-	expression tag	UNP P55072
A	-1	GLY	-	expression tag	UNP P55072
A	0	SER	-	expression tag	UNP P55072
E	-25	MET	-	expression tag	UNP P55072
E	-24	GLY	-	expression tag	UNP P55072
E	-23	ASP	-	expression tag	UNP P55072
E	-22	TYR	-	expression tag	UNP P55072
E	-21	LYS	-	expression tag	UNP P55072
E	-20	ASP	-	expression tag	UNP P55072

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-19	ASP	-	expression tag	UNP P55072
E	-18	ASP	-	expression tag	UNP P55072
E	-17	ASP	-	expression tag	UNP P55072
E	-16	LYS	-	expression tag	UNP P55072
E	-15	GLY	-	expression tag	UNP P55072
E	-14	GLY	-	expression tag	UNP P55072
E	-13	GLY	-	expression tag	UNP P55072
E	-12	SER	-	expression tag	UNP P55072
E	-11	GLY	-	expression tag	UNP P55072
E	-10	GLY	-	expression tag	UNP P55072
E	-9	LEU	-	expression tag	UNP P55072
E	-8	GLU	-	expression tag	UNP P55072
E	-7	VAL	-	expression tag	UNP P55072
E	-6	LEU	-	expression tag	UNP P55072
E	-5	PHE	-	expression tag	UNP P55072
E	-4	GLN	-	expression tag	UNP P55072
E	-3	GLY	-	expression tag	UNP P55072
E	-2	PRO	-	expression tag	UNP P55072
E	-1	GLY	-	expression tag	UNP P55072
E	0	SER	-	expression tag	UNP P55072
F	-25	MET	-	expression tag	UNP P55072
F	-24	GLY	-	expression tag	UNP P55072
F	-23	ASP	-	expression tag	UNP P55072
F	-22	TYR	-	expression tag	UNP P55072
F	-21	LYS	-	expression tag	UNP P55072
F	-20	ASP	-	expression tag	UNP P55072
F	-19	ASP	-	expression tag	UNP P55072
F	-18	ASP	-	expression tag	UNP P55072
F	-17	ASP	-	expression tag	UNP P55072
F	-16	LYS	-	expression tag	UNP P55072
F	-15	GLY	-	expression tag	UNP P55072
F	-14	GLY	-	expression tag	UNP P55072
F	-13	GLY	-	expression tag	UNP P55072
F	-12	SER	-	expression tag	UNP P55072
F	-11	GLY	-	expression tag	UNP P55072
F	-10	GLY	-	expression tag	UNP P55072
F	-9	LEU	-	expression tag	UNP P55072
F	-8	GLU	-	expression tag	UNP P55072
F	-7	VAL	-	expression tag	UNP P55072
F	-6	LEU	-	expression tag	UNP P55072
F	-5	PHE	-	expression tag	UNP P55072
F	-4	GLN	-	expression tag	UNP P55072

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-3	GLY	-	expression tag	UNP P55072
F	-2	PRO	-	expression tag	UNP P55072
F	-1	GLY	-	expression tag	UNP P55072
F	0	SER	-	expression tag	UNP P55072

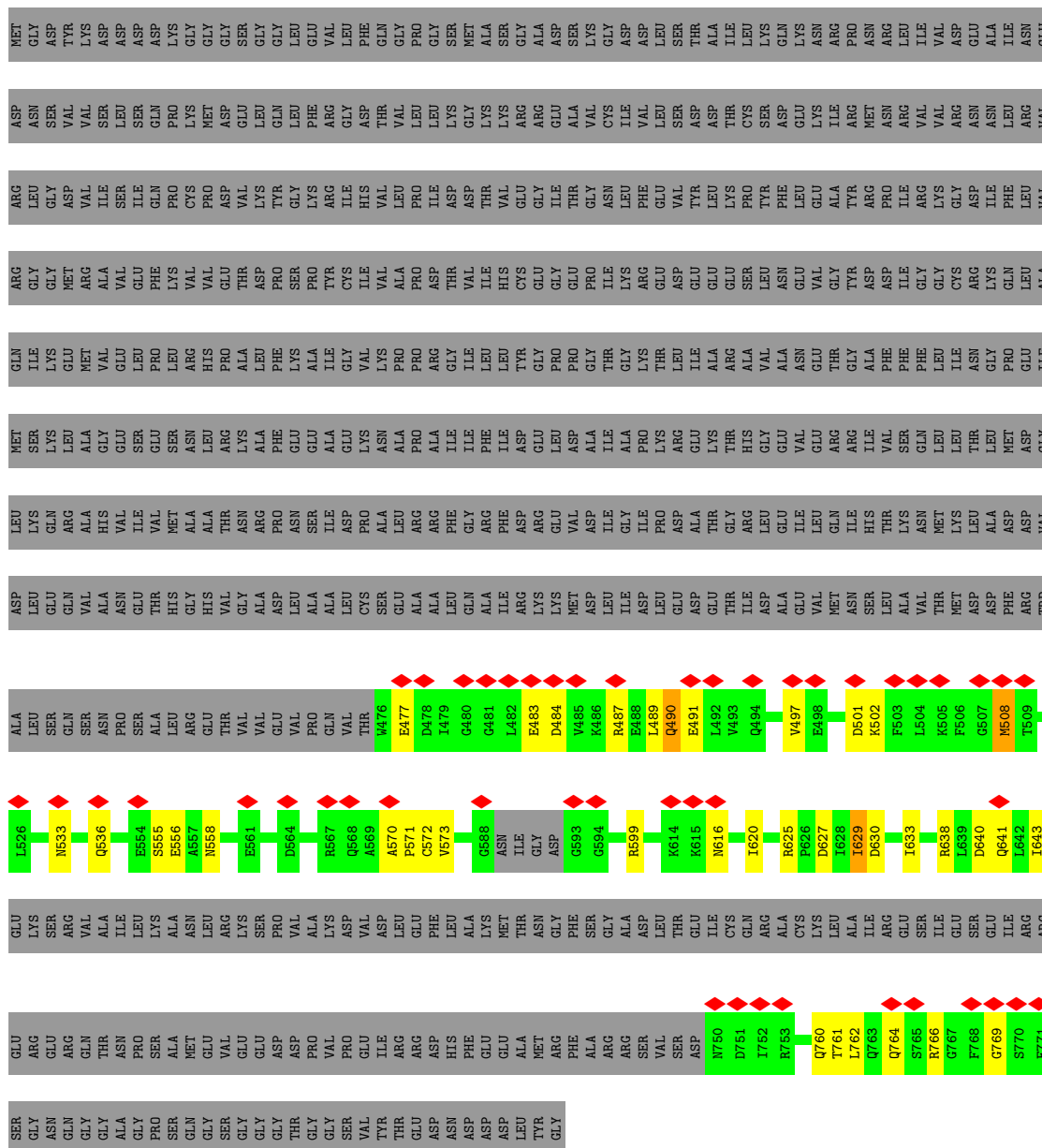
VAL	SER	ASP	PRO	ASP	PRO	HIS	HIS	LYS	TYR
ALA	MET	PHE	SER	SER	SER	HIS	CYS	LEU	GLY
ASP	ASP	ASP	ASN	GLY	GLY	LEU	THR	SER	PRO
ALA	HIS	LEU	SER	LEU	LYS	LEU	PRO	LYS	PRO
GLY	LEU	SER	SER	LEU	GLY	LEU	HIS	GLY	LYS
ALA	ARG	THR	THR	LYS	LEU	LYS	LEU	LEU	GLU
ALA	ARG	THR	THR	LYS	LEU	LYS	LEU	GLN	LEU
ALA	ARG	THR	THR	LYS	LEU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

- Molecule 2: Transitional endoplasmic reticulum ATPase



E546	ALA	ASP	LEU	LEU	MET	GLN	ARG	ARG	ASP	MET
E549	SER	GLU	GLN	LYS	SER	ILE	GLY	GLY	ASN	ASN
E556	GLN	ARG	ARG	LEU	LEU	GLU	MET	GLY	VAL	VAL
A557	SER	VAL	ALA	HIS	GLY	VAL	ALA	ALA	ILE	SER
V559	ASN	ASN	ASN	HIS	GLU	GLU	VAL	VAL	SER	LEU
	PRO	GLU	ILE	VAL	SER	ILE	GLU	GLU	ASP	ASP
	SER	GLU	ILE	ILE	GLU	ILE	GLU	GLU	GLN	ASP
R560	ALA	HIS	VAL	VAL	GLU	PRO	PHE	PRO	PRO	LYS
E561	ARG	GLY	ALA	ALA	ASN	ARG	VAL	CYS	GLY	GLY
E562	GLU	HIS	THR	THR	LEU	ARG	VAL	VAL	PRO	MET
F563	THR	VAL	GLY	ASN	LYS	GLU	THR	ASP	GLY	GLY
D564	VAL	ALA	ARG	ARG	ALA	LEU	ASP	LYS	LEU	SER
K565	ASP	LEU	PRO	ASN	PHE	LYS	PRO	TYR	GLN	GLY
G471	GLU	ASN	ASN	GLU	GLU	ALA	GLY	GLY	LEU	GLU
	P472	SER	ILE	ILE	GLU	PRO	PRO	ARG	PHE	VAL
	Q473	ALA	ALA	ALA	ALA	ILE	TYR	ARG	ARG	VAL
E477		CYS	CYS	LYS	LYS	VAL	ILE	CYS	ILE	GLY
	D478	SER	SER	ALA	ASN	VAL	VAL	VAL	THR	THR
		GLU	LEU	ALA	ALA	PRO	ALA	ALA	LEU	VAL
P571	ALA	ALA	ARG	ARG	PRO	PRO	PRO	PRO	LEU	PRO
	C572	ALA	ARG	ALA	ALA	ARG	ASP	ASP	LEU	GLY
		LEU	PHE	GLY	ILE	ARG	THR	GLY	LEU	SER
D577		GLN	GLN	ILE	ILE	ILE	VAL	ASP	LYS	MET
	G588	ILE	ALA	PHE	ILE	LEU	HIS	VAL	LYS	ALA
	L489	ARG	ASP	ASP	ASP	TYR	CYS	GLY	ARG	GLY
Q490	ASN	LYS	ARG	ARG	GLU	GLY	GLY	GLY	ARG	ALA
	E491	ILE	LYS	VAL	VAL	PRO	ILE	ILE	GLU	ALA
	L492	GLY	MET	ASP	ASP	GLY	PRO	GLY	VAL	LYS
G593	ASP	ASP	LEU	ILE	ILE	THR	ILE	ASN	CYS	GLY
	E496	ILE	ILE	GLY	ALA	GLY	LYS	LEU	ILE	ASP
	D501	ASP	ASP	PRO	PRO	LYS	ARG	PHE	VAL	ASP
D598	R599	LEU	LEU	PRO	LYS	THR	GLU	GLU	LEU	LEU
	K502	GLU	GLU	ASP	ARG	LEU	VAL	VAL	SER	SER
	F503	GLU	GLU	ASP	GLU	ILE	GLU	TYR	ASP	THR
D609	L504	ASP	GLU	THR	LYS	ALA	GLU	LEU	ASP	ALA
G610	K505	GLU	THR	ALA	GLY	ARG	GLY	LYS	THR	ILE
M611	F506	THR	GLY	GLY	HIS	ALA	SER	CYS	THR	LYS
S612	G507	ILE	ARG	GLY	GLY	VAL	TYR	TYR	GLY	LYS
T613	H508	ALA	ALA	GLU	GLU	ASN	ASN	PHE	ASP	LYS
K614	T509	GLU	ILE	VAL	VAL	GLU	VAL	GLU	LYS	ASN
K615	F510	VAL	LEU	LEU	GLU	THR	ALA	ILE	ILE	ARG
M616	P510	MET	GLN	GLN	ARG	THR	GLY	PRO	ARG	ASN
V617	S511	ASN	ILE	ILE	ARG	GLY	TYR	ASP	MET	ASN
F618	K512	SER	THR	THR	VAL	PHE	ASP	ARG	ASN	ASN
D630	C522	VAL	ALA	ASN	ALA	PHE	ILE	ILE	ARG	VAL
		VAL	THR	MET	LEU	LEU	GLY	GLY	VAL	VAL
	K529	THR	MET	LYS	MET	LEU	GLY	LYS	VAL	VAL
R635		ASP	ASP	THR	LEU	ILE	CYS	GLY	ARG	ARG
	E534	ASP	ASP	GLU	GLU	ASN	ASN	GLY	ASN	ASN
	C535	PHE	ASP	ALA	ALA	LEU	ILE	ILE	ASN	GLU
R638	L639	THR	ARG	ASN	ASP	PRO	GLN	PHE	LEU	ILE
L640	Q536	THR	VAL	VAL	GLY	GLU	LEU	LEU	ARG	ARG

- Molecule 2: Transitional endoplasmic reticulum ATPase



- Molecule 2: Transitional endoplasmic reticulum ATPase





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	592034	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 ($e^-/\text{\AA}^2$)	53.69	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.276	Depositor
Minimum map value	-0.108	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0471	Depositor
Map size (\AA)	363.0, 363.0, 363.0	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.825, 0.825, 0.825	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	D	0.13	0/1029	0.32	0/1394
2	A	0.13	0/2286	0.26	0/3079
2	E	0.13	0/1535	0.28	0/2067
2	F	0.12	0/2156	0.25	0/2901
All	All	0.13	0/7006	0.27	0/9441

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	D	1003	953	960	19	0
2	A	2248	2255	2255	27	0
2	E	1504	1454	1500	38	0
2	F	2117	2092	2138	49	0
All	All	6872	6754	6853	118	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (118) 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:D:588:LEU:O	1:D:663:TYR:OH	1.97	0.81
2:A:701:GLU:OE2	2:A:732:ARG:NH2	2.14	0.80
1:D:568:THR:OG1	1:D:614:SER:OG	1.97	0.77
2:E:764:GLN:OE1	2:E:764:GLN:N	2.17	0.76
2:E:556:GLU:OE1	2:E:599:ARG:NH1	2.22	0.72
2:F:555:SER:OG	2:F:558:ASN:OD1	2.06	0.72
2:E:533:ASN:O	2:E:536:GLN:NE2	2.23	0.71
2:E:487:ARG:O	2:E:490:GLN:NE2	2.24	0.70
1:D:568:THR:HG1	1:D:614:SER:HG	1.24	0.69
2:A:484:ASP:OD1	2:A:485:VAL:N	2.24	0.69
2:A:728:VAL:O	2:A:728:VAL:HG13	1.93	0.69
2:F:649:ASP:N	2:F:652:SER:OG	2.27	0.67
2:A:733:ARG:HH21	2:F:773:PHE:HB3	1.60	0.67
1:D:595:THR:OG1	1:D:604:ARG:NH2	2.30	0.65
2:F:493:VAL:HG22	2:F:618:PHE:CD2	2.33	0.64
2:F:678:MET:SD	2:F:678:MET:N	2.71	0.63
2:A:609:ASP:OD2	2:A:638:ARG:NH1	2.32	0.62
1:D:610:PHE:N	1:D:620:SER:OG	2.33	0.61
2:E:501:ASP:OD1	2:E:502:LYS:N	2.34	0.61
2:E:761:THR:O	2:F:744:ARG:NH2	2.33	0.61
2:A:700:ARG:NE	2:F:491:GLU:OE2	2.34	0.61
2:E:625:ARG:NH2	2:E:627:ASP:OD2	2.35	0.60
2:A:543:LYS:N	2:A:546:GLU:OE1	2.35	0.59
2:E:769:GLY:HA2	2:F:741:ARG:HA	1.84	0.59
2:F:489:LEU:HD21	2:F:516:PHE:HZ	1.68	0.59
1:D:662:ASP:OD1	1:D:663:TYR:N	2.36	0.58
1:D:566:ARG:NH2	1:D:575:GLY:O	2.36	0.58
1:D:662:ASP:OD1	1:D:664:THR:HG23	2.04	0.58
2:A:733:ARG:NH2	2:F:773:PHE:HB3	2.18	0.58
2:A:673:GLU:OE1	2:A:673:GLU:N	2.37	0.57
2:E:570:ALA:HB3	2:E:571:PRO:HD3	1.86	0.57
2:E:570:ALA:HB3	2:E:571:PRO:CD	2.34	0.57
1:D:641:GLU:OE2	1:D:641:GLU:N	2.30	0.57
2:F:602:ASN:O	2:F:606:THR:HG23	2.05	0.57
2:E:640:ASP:OD1	2:E:641:GLN:N	2.39	0.56
2:F:738:GLU:OE2	2:F:741:ARG:NH1	2.39	0.56
2:F:627:ASP:OD1	2:F:628:ILE:HG23	2.06	0.55
2:E:774:PRO:HD3	2:F:674:PHE:CD2	2.42	0.54
2:F:598:ASP:OD1	2:F:598:ASP:C	2.51	0.54
2:F:627:ASP:OD1	2:F:628:ILE:N	2.40	0.54
2:F:522:CYS:SG	2:F:647:LEU:HD23	2.48	0.54
2:F:514:VAL:HG23	2:F:641:GLN:HB3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:640:ASP:OD1	2:F:641:GLN:N	2.40	0.54
1:D:580:TRP:C	1:D:581:ASP:OD1	2.51	0.54
2:E:774:PRO:HD3	2:F:674:PHE:CE2	2.43	0.54
2:E:508:MET:HE1	2:F:695:CYS:SG	2.48	0.53
2:F:771:PHE:O	2:F:772:ARG:NH1	2.41	0.53
2:A:744:ARG:NE	2:F:765:SER:OG	2.41	0.53
2:F:611:MET:HE1	2:F:619:ILE:HD13	1.91	0.53
1:D:589:PRO:O	1:D:666:VAL:HG13	2.09	0.52
2:E:627:ASP:N	2:E:627:ASP:OD1	2.42	0.52
2:A:488:GLU:O	2:A:492:LEU:HG	2.09	0.52
2:E:638:ARG:O	2:E:640:ASP:N	2.43	0.52
2:A:598:ASP:OD1	2:A:598:ASP:C	2.52	0.51
2:E:514:VAL:HG23	2:E:641:GLN:HB2	1.93	0.51
2:E:773:PHE:HD1	2:E:774:PRO:HD2	1.75	0.51
2:E:502:LYS:C	2:F:699:ILE:HD11	2.36	0.51
2:E:497:VAL:HG12	2:E:616:ASN:HD22	1.76	0.51
2:E:760:GLN:O	2:E:764:GLN:N	2.43	0.51
1:D:566:ARG:O	1:D:577:LYS:NZ	2.44	0.50
2:F:555:SER:OG	2:F:555:SER:O	2.28	0.50
2:E:491:GLU:OE2	2:F:700:ARG:NH2	2.45	0.50
2:E:629:ILE:HD13	2:E:630:ASP:H	1.76	0.49
2:F:666:VAL:O	2:F:668:LYS:NZ	2.45	0.49
2:A:549:THR:HG23	2:F:602:ASN:ND2	2.28	0.49
2:E:760:GLN:HA	2:E:760:GLN:OE1	2.14	0.48
2:A:556:GLU:OE2	2:A:599:ARG:NH2	2.47	0.48
2:E:555:SER:O	2:E:555:SER:OG	2.20	0.48
2:E:572:CYS:SG	2:E:573:VAL:N	2.87	0.48
2:A:490:GLN:NE2	2:A:534:GLU:OE2	2.44	0.48
2:E:477:GLU:N	2:E:477:GLU:OE1	2.47	0.48
1:D:563:THR:OG1	1:D:584:GLU:OE1	2.32	0.47
2:F:638:ARG:O	2:F:640:ASP:N	2.44	0.47
2:F:626:PRO:O	2:F:629:ILE:HG22	2.15	0.47
2:F:669:ASP:O	2:F:733:ARG:NE	2.47	0.47
2:F:690:ILE:HD11	2:F:743:ALA:HB1	1.96	0.47
1:D:662:ASP:OD1	1:D:662:ASP:C	2.56	0.47
2:A:549:THR:HG22	2:F:603:GLN:OE1	2.15	0.47
2:A:713:ARG:O	2:A:714:GLN:HB3	2.15	0.47
2:E:508:MET:HA	2:E:508:MET:HE2	1.96	0.47
2:E:514:VAL:HG21	2:E:643:ILE:HD11	1.97	0.47
2:F:489:LEU:HD21	2:F:516:PHE:CZ	2.48	0.47
1:D:642:ILE:H	1:D:642:ILE:HD12	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:546:GLU:O	2:F:550:MET:HG3	2.16	0.46
2:A:546:GLU:O	2:A:549:THR:OG1	2.29	0.46
2:E:558:ASN:OD1	2:E:558:ASN:O	2.34	0.46
2:E:762:LEU:O	2:E:766:ARG:NH1	2.49	0.46
2:F:611:MET:HE1	2:F:619:ILE:CD1	2.45	0.46
2:F:550:MET:HE1	2:F:559:VAL:N	2.31	0.46
2:F:512:LYS:NZ	2:F:611:MET:O	2.44	0.45
2:F:547:LEU:HB3	2:F:582:ILE:HD11	1.98	0.45
2:A:751:ASP:N	2:A:751:ASP:OD1	2.48	0.45
1:D:550:ARG:NH2	1:D:556:VAL:O	2.49	0.45
2:A:728:VAL:O	2:A:728:VAL:CG1	2.62	0.45
2:A:653:ARG:HG2	2:A:687:LEU:HD11	1.99	0.44
2:E:483:GLU:OE1	2:E:483:GLU:N	2.47	0.44
2:E:772:ARG:HA	2:F:737:GLU:OE2	2.17	0.44
2:F:679:THR:O	2:F:679:THR:OG1	2.35	0.44
2:A:640:ASP:OD1	2:A:641:GLN:N	2.51	0.43
1:D:664:THR:O	1:D:664:THR:OG1	2.27	0.43
2:E:484:ASP:N	2:E:484:ASP:OD1	2.52	0.43
1:D:601:ARG:NH2	1:D:633:HIS:O	2.52	0.43
2:A:522:CYS:SG	2:A:647:LEU:HD23	2.58	0.42
2:E:508:MET:CE	2:F:695:CYS:SG	3.08	0.42
2:E:558:ASN:OD1	2:E:558:ASN:C	2.62	0.42
2:E:573:VAL:CG1	2:E:620:ILE:HD12	2.50	0.42
1:D:624:ASP:OD1	1:D:624:ASP:C	2.63	0.41
2:F:758:PHE:O	2:F:761:THR:HG22	2.20	0.41
2:F:653:ARG:HG2	2:F:687:LEU:HD11	2.03	0.41
2:A:713:ARG:C	2:A:715:THR:H	2.28	0.41
2:F:694:ALA:HA	2:F:739:ALA:HB2	2.02	0.41
2:A:558:ASN:O	2:A:559:VAL:C	2.64	0.41
2:E:772:ARG:HA	2:E:772:ARG:NE	2.36	0.40
2:F:748:SER:N	2:F:751:ASP:OD2	2.49	0.40
2:A:630:ASP:OD1	2:A:630:ASP:C	2.64	0.40
2:F:647:LEU:HD11	2:F:752:ILE:HD11	2.03	0.40
2:A:716:ASN:OD1	2:A:716:ASN:C	2.65	0.40
2:F:623:THR:HG22	2:F:625:ARG:H	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	124/1250 (10%)	115 (93%)	9 (7%)	0	100	100
2	A	279/832 (34%)	269 (96%)	10 (4%)	0	100	100
2	E	186/832 (22%)	180 (97%)	6 (3%)	0	100	100
2	F	263/832 (32%)	255 (97%)	8 (3%)	0	100	100
All	All	852/3746 (23%)	819 (96%)	33 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	109/1065 (10%)	109 (100%)	0	100	100
2	A	242/696 (35%)	239 (99%)	3 (1%)	63	86
2	E	158/696 (23%)	153 (97%)	5 (3%)	34	68
2	F	225/696 (32%)	218 (97%)	7 (3%)	35	69
All	All	734/3153 (23%)	719 (98%)	15 (2%)	48	78

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	661	LEU
2	A	714	GLN

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Mol	Chain	Res	Type
2	A	725	ASP
2	E	489	LEU
2	E	490	GLN
2	E	508	MET
2	E	629	ILE
2	E	633	ILE
2	F	484	ASP
2	F	504	LEU
2	F	514	VAL
2	F	691	CYS
2	F	699	ILE
2	F	751	ASP
2	F	762	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	692	GLN
2	E	536	GLN
2	F	680	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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

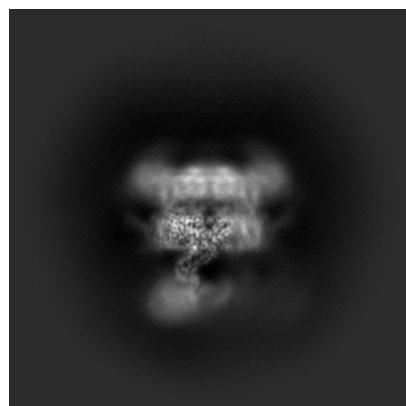
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-48501. These allow visual inspection of the internal detail of the map and identification of artifacts.

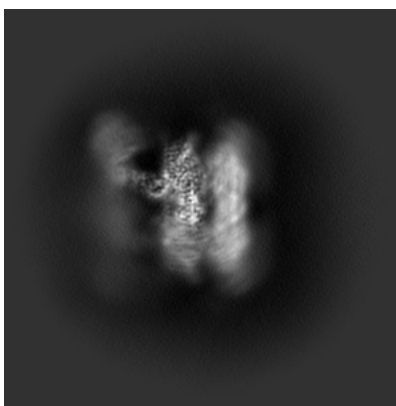
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

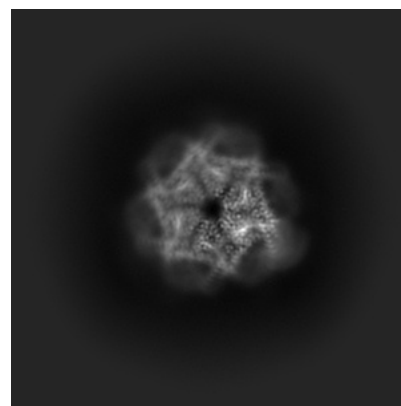
6.1.1 Primary map



X

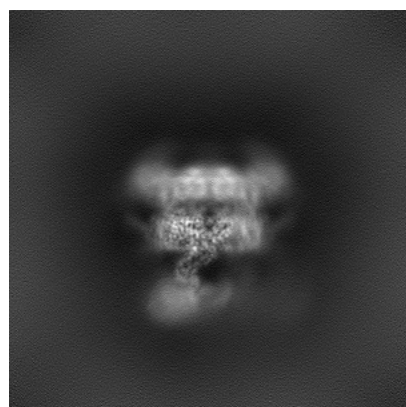


Y

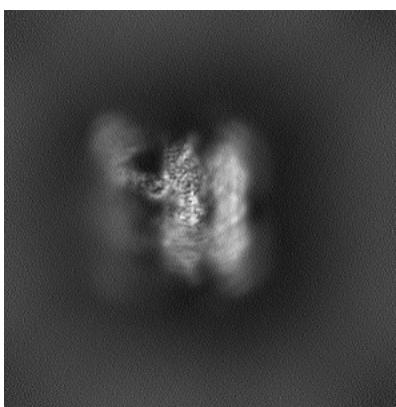


Z

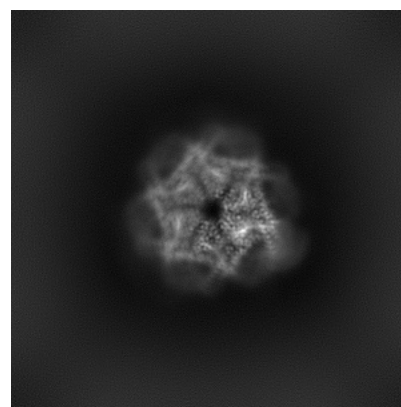
6.1.2 Raw map



X



Y

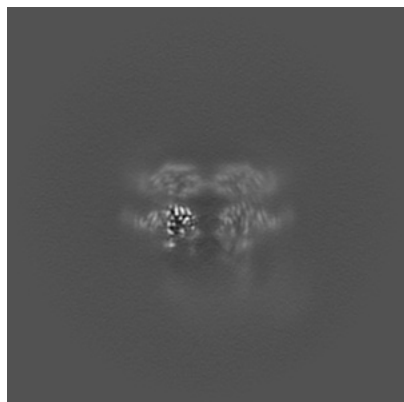


Z

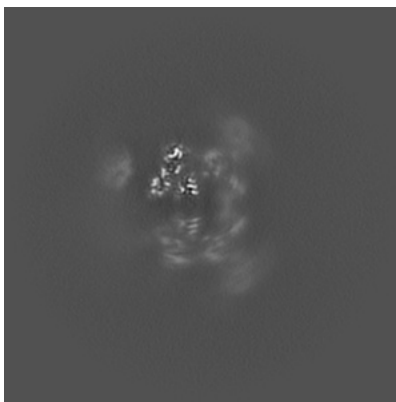
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

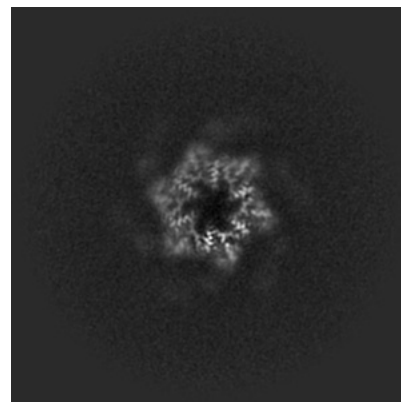
6.2.1 Primary map



X Index: 220

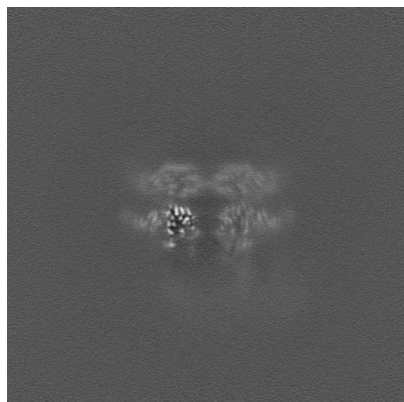


Y Index: 220

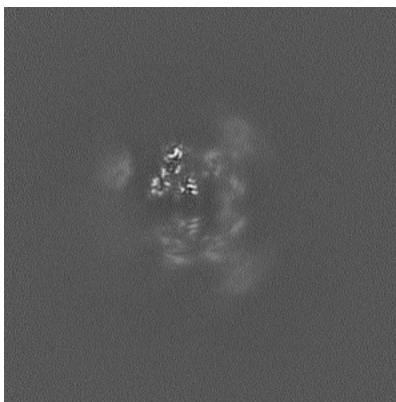


Z Index: 220

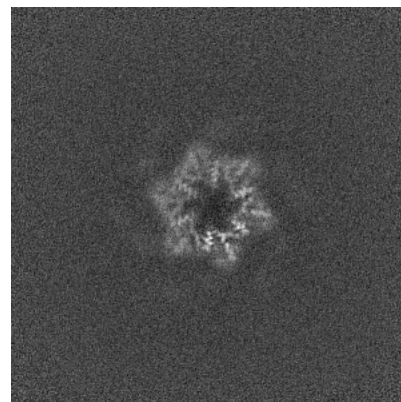
6.2.2 Raw map



X Index: 220



Y Index: 220

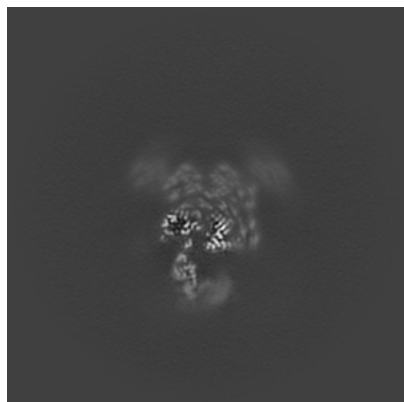


Z Index: 220

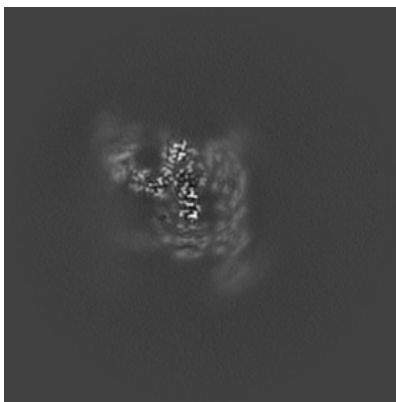
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

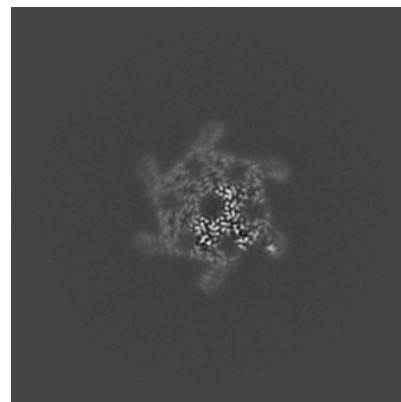
6.3.1 Primary map



X Index: 257

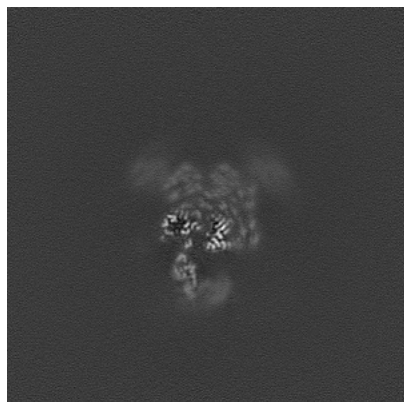


Y Index: 201

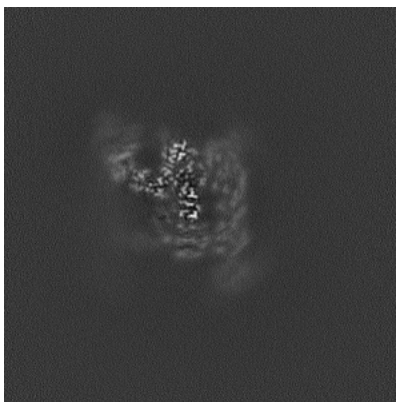


Z Index: 206

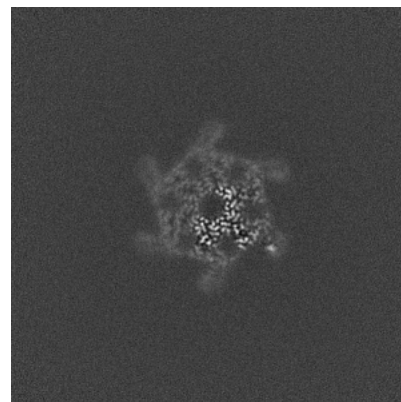
6.3.2 Raw map



X Index: 257



Y Index: 201

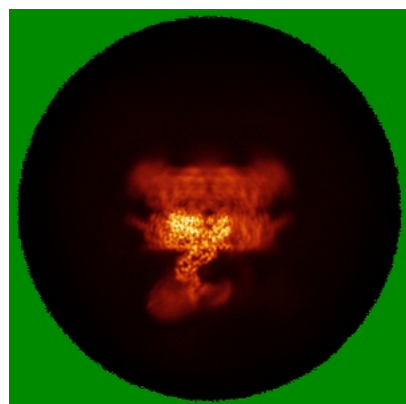


Z Index: 206

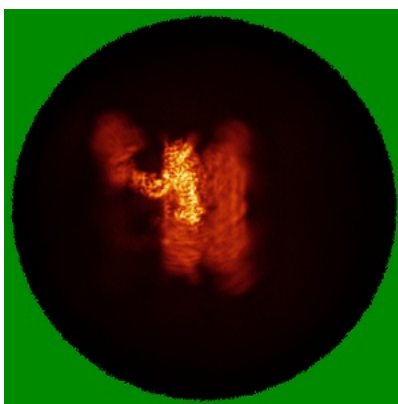
The images above show the largest variance slices of the map in three orthogonal directions.

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

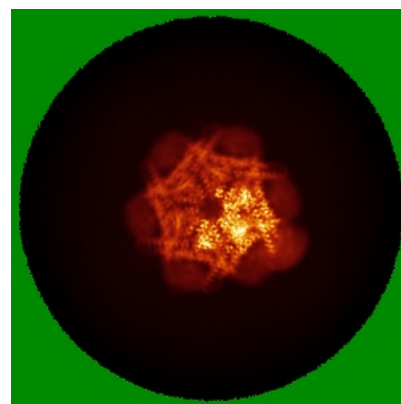
6.4.1 Primary map



X

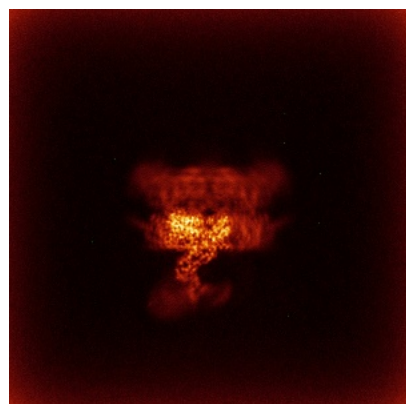


Y

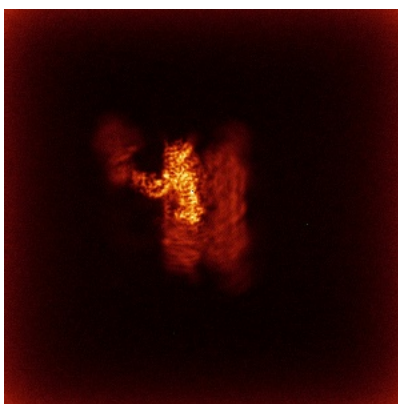


Z

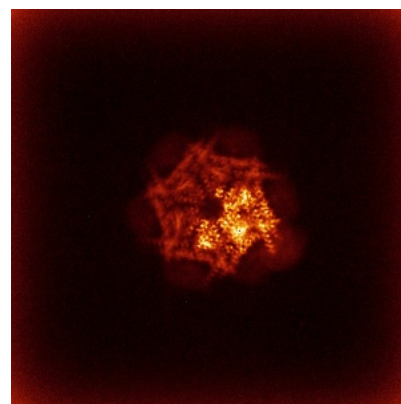
6.4.2 Raw map



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.

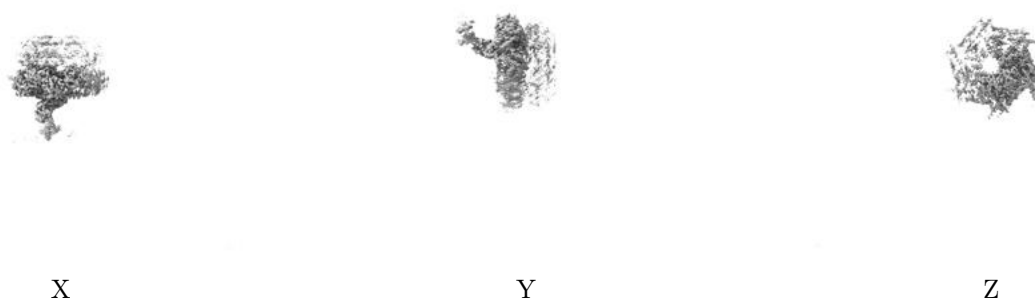
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0471. 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.

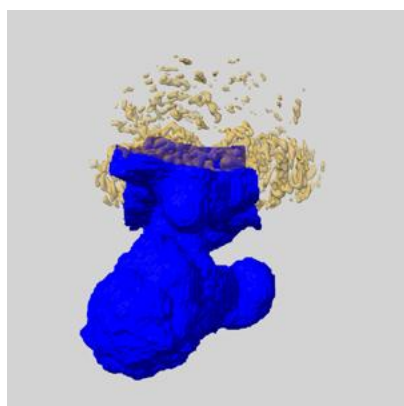
6.6 Mask visualisation [i](#)

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

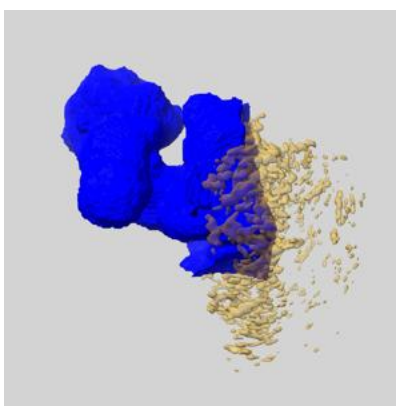
A mask typically either:

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

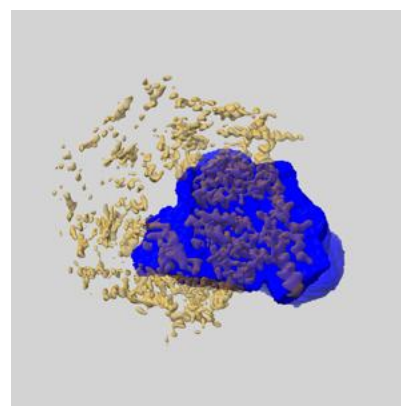
6.6.1 emd_48501_msk_1.map [i](#)



X

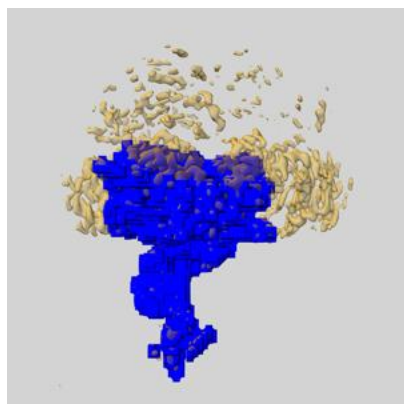


Y

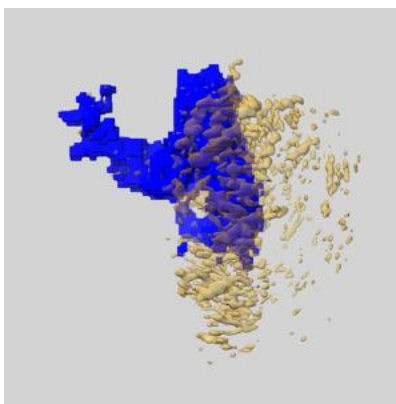


Z

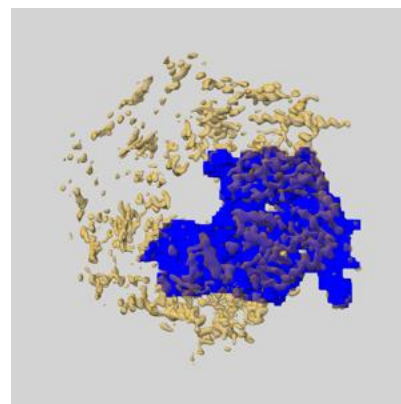
6.6.2 emd_48501_msk_2.map [i](#)



X



Y

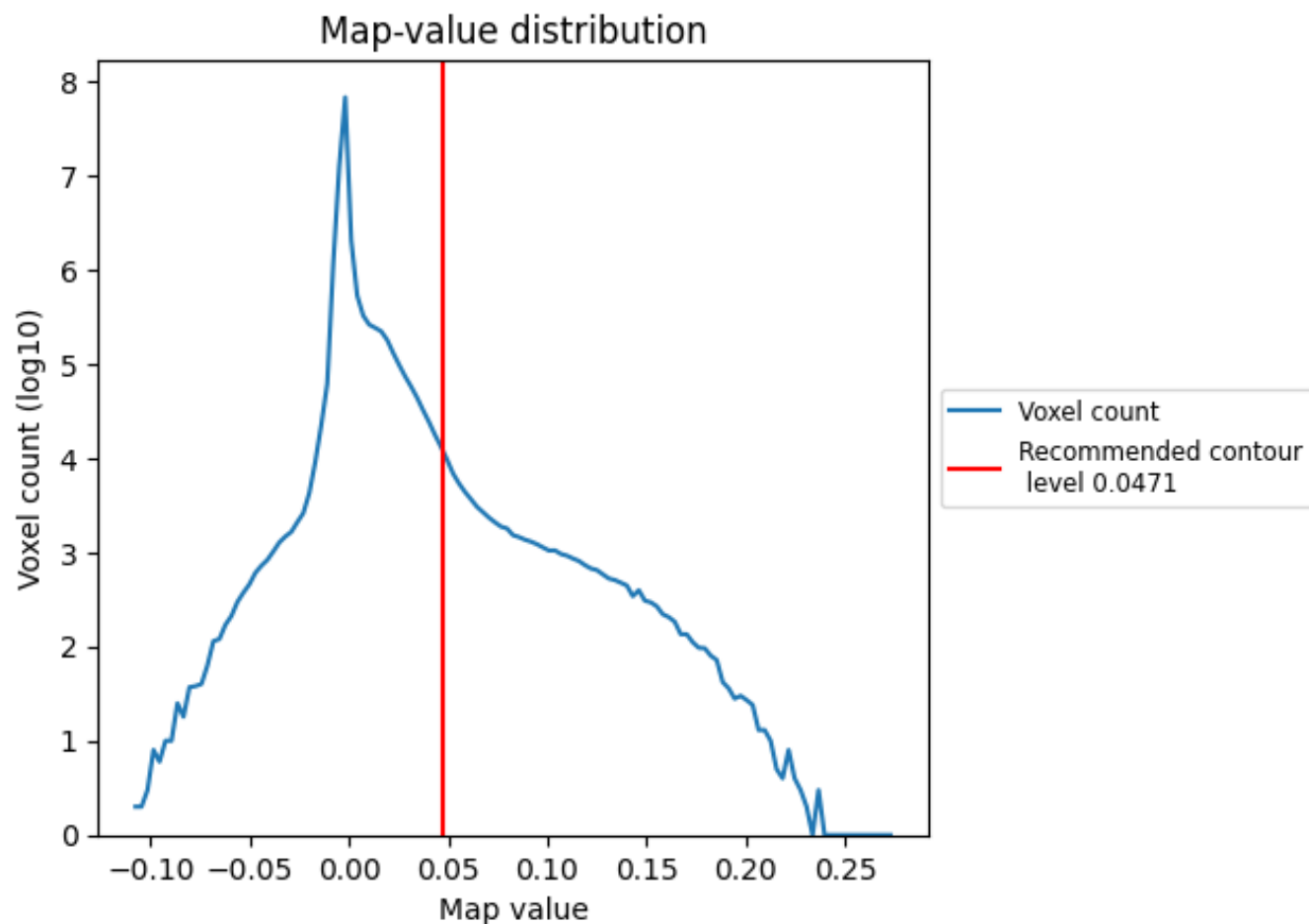


Z

7 Map analysis [i](#)

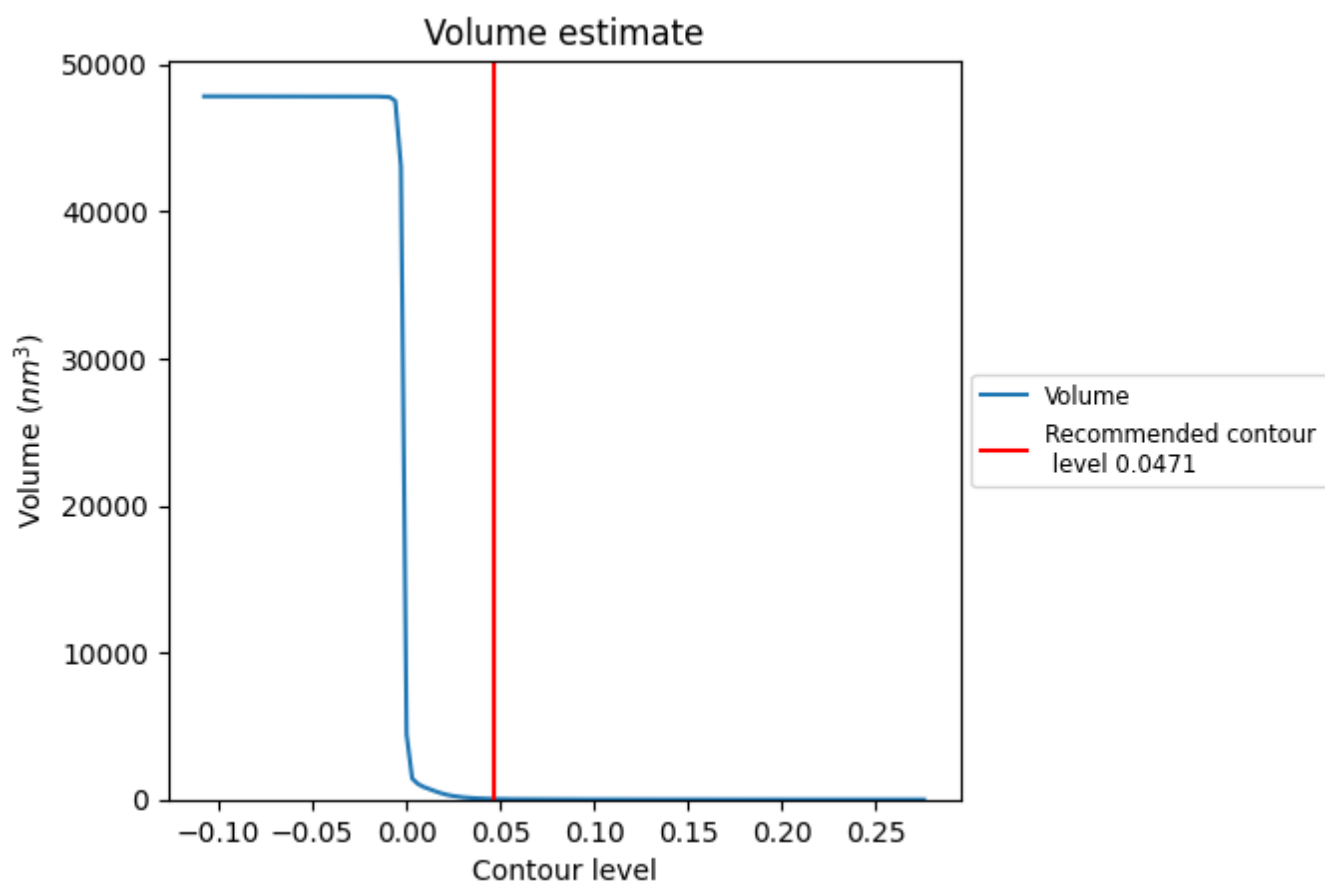
This section contains the results of statistical analysis of the map.

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.

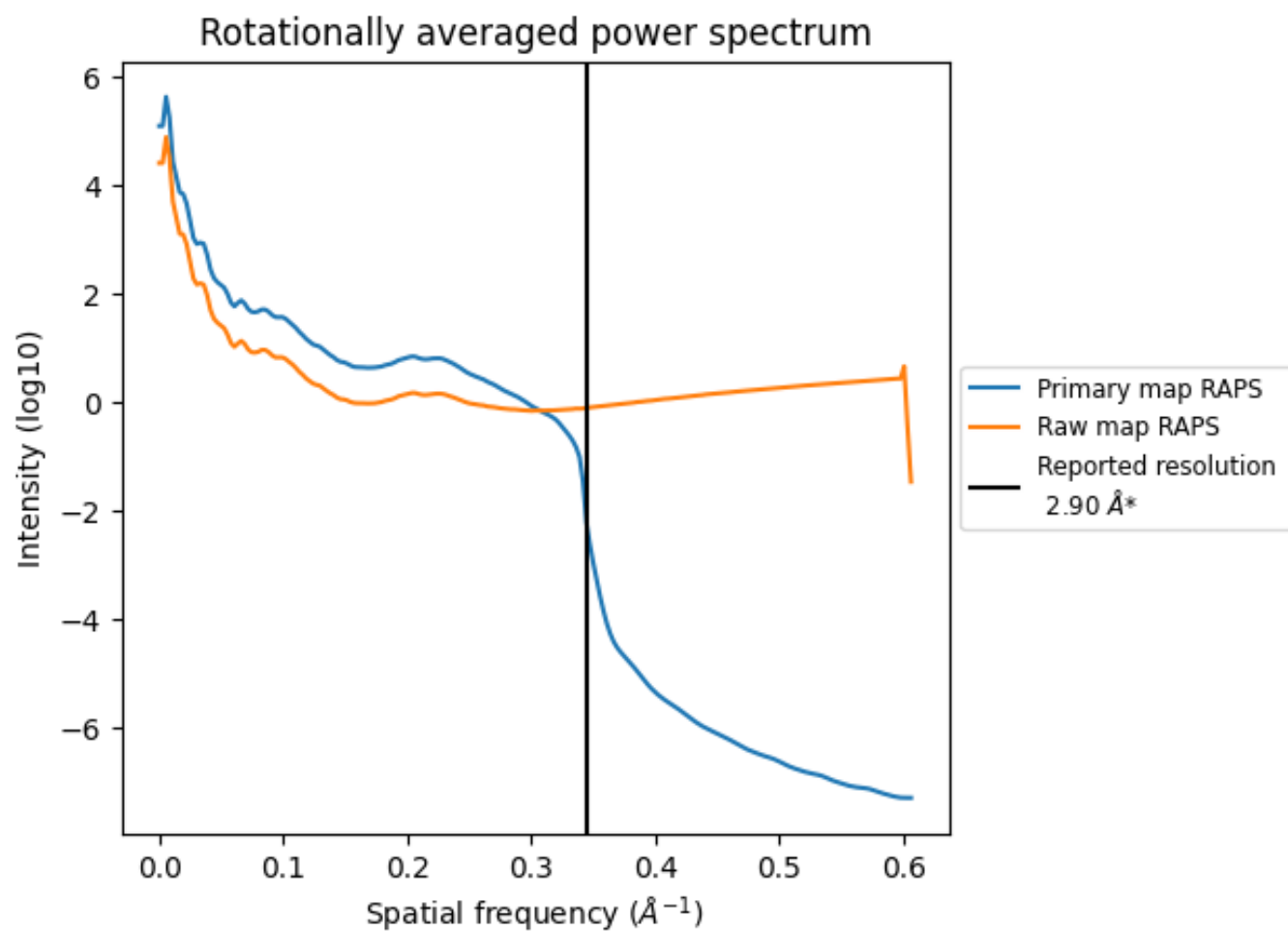
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 42 nm³; this corresponds to an approximate mass of 38 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 ⓘ

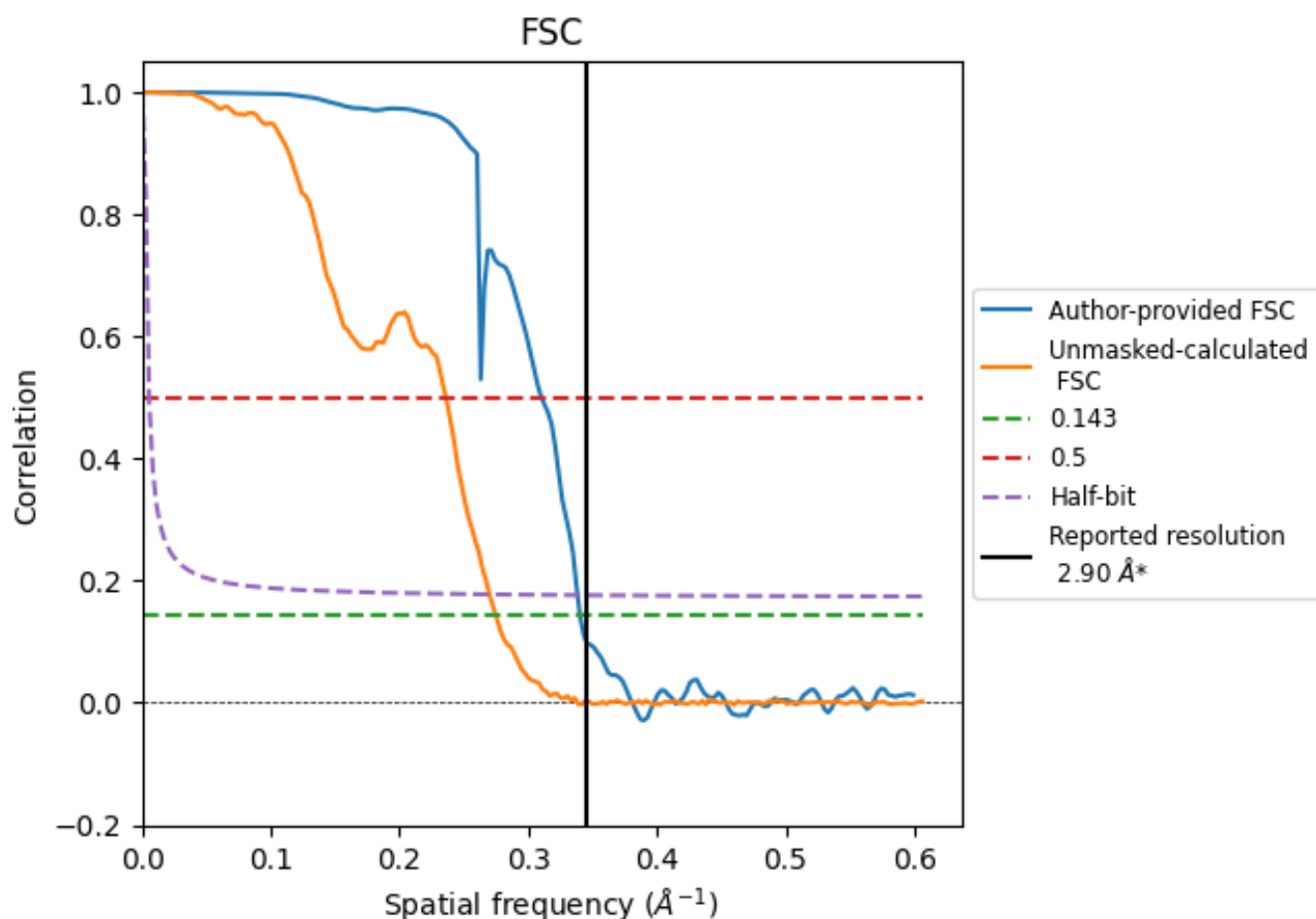


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

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 0.345 \AA^{-1}

8.2 Resolution estimates [i](#)

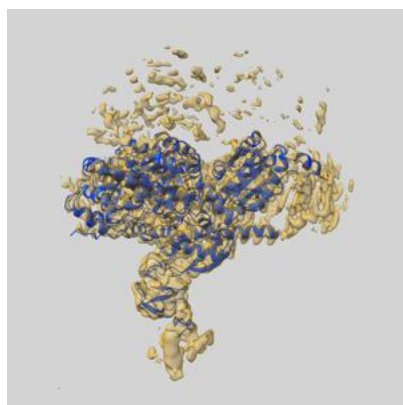
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.94	3.22	2.96
Unmasked-calculated*	3.64	4.24	3.71

*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 3.64 differs from the reported value 2.9 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-48501 and PDB model 9MPS. Per-residue inclusion information can be found in section [3](#) on page [7](#).

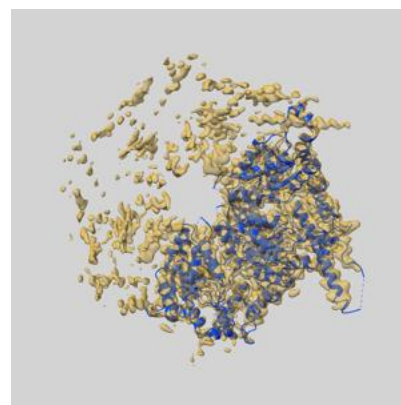
9.1 Map-model overlay [i](#)



X



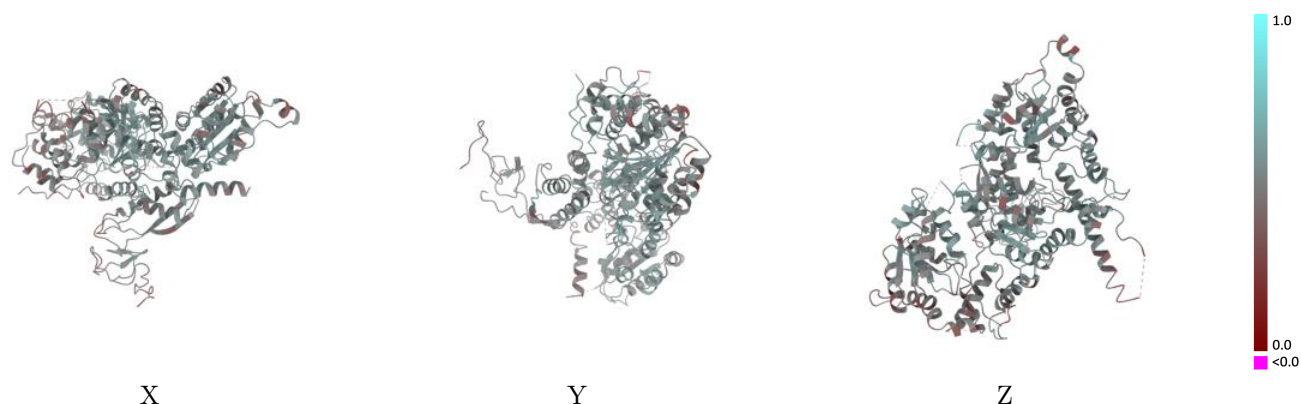
Y



Z

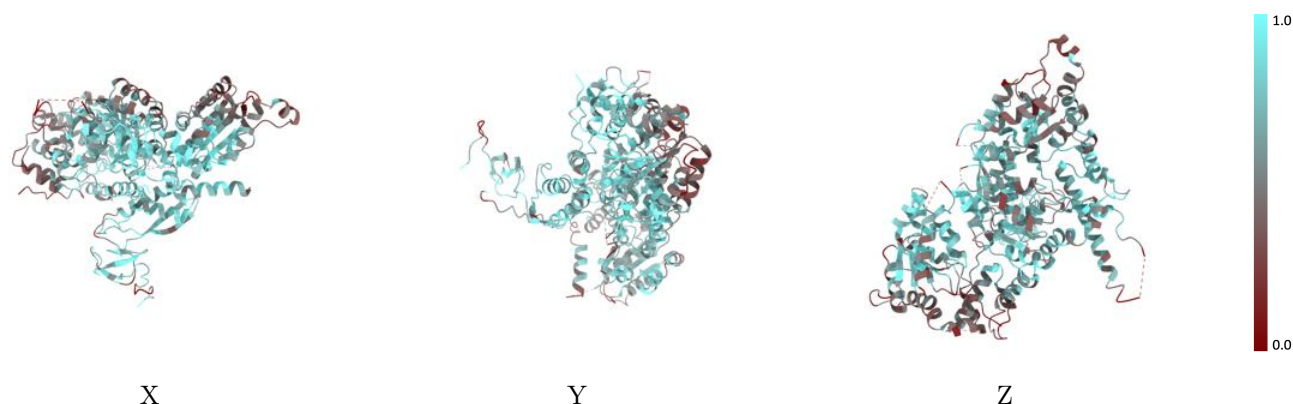
The images above show the 3D surface view of the map at the recommended contour level 0.0471 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



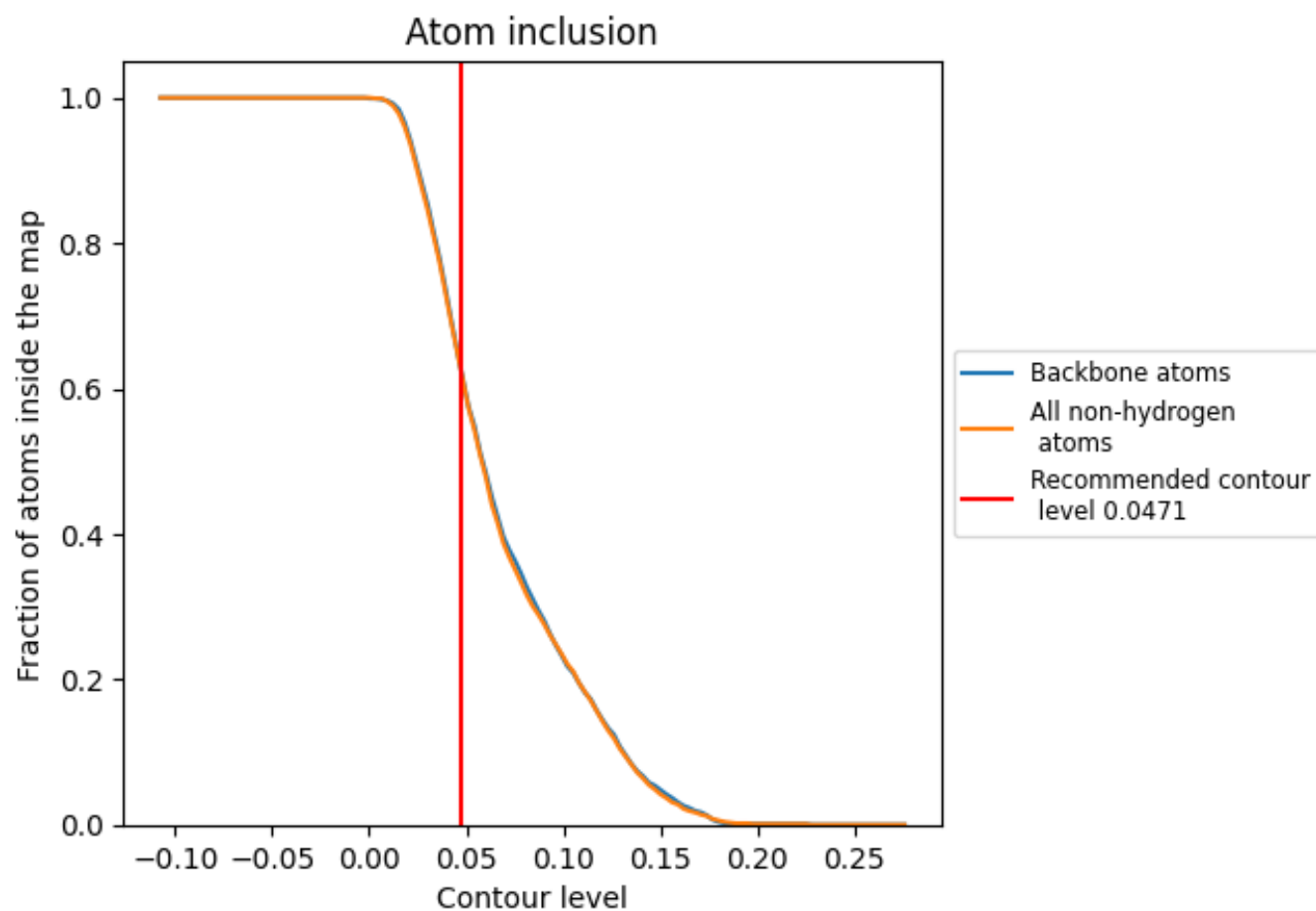
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0471).

9.4 Atom inclusion [i](#)



At the recommended contour level, 63% of all backbone atoms, 63% 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 (0.0471) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6280	<div></div> 0.5010
A	<div></div> 0.6510	<div></div> 0.5120
D	<div></div> 0.7160	<div></div> 0.4730
E	<div></div> 0.5780	<div></div> 0.4850
F	<div></div> 0.6540	<div></div> 0.5140

