



## Full wwPDB EM Validation Report ⓘ

Oct 6, 2025 – 01:53 PM EDT

PDB ID : 9MPR / pdb\_00009mpr  
EMDB ID : EMD-48500  
Title : Cryo-EM structure of three VCPIP1 VCPIDs bound to VCP  
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](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.dev129  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
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) : 2.46

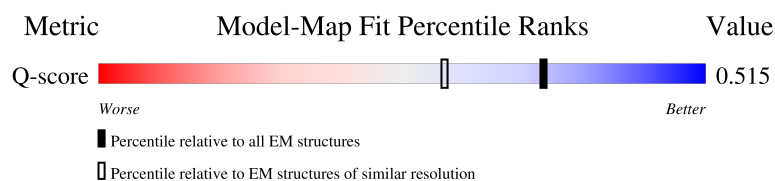
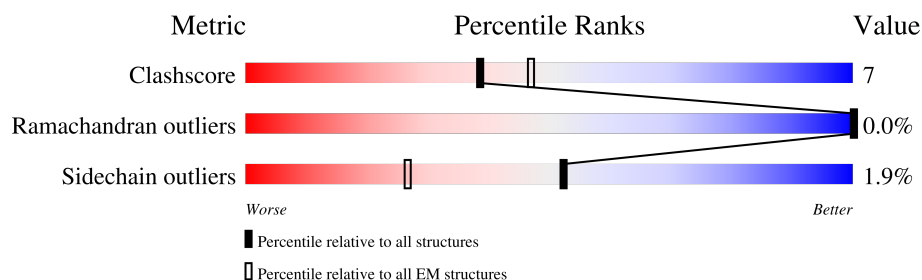
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

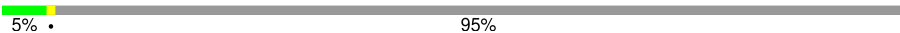
The reported resolution of this entry is 2.90 Å.

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	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
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  $\geq 3$ , 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	G	1250	 95%
1	H	1250	 95%
1	I	1250	 95%
2	A	832	 57% 10% 32%

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Mol	Chain	Length	Quality of chain
2	B	832	<div><div><div></div><div></div><div></div></div><div>57%10%32%</div></div>
2	C	832	<div><div><div></div><div></div><div></div></div><div>57%10%33%</div></div>
2	D	832	<div><div><div></div><div></div><div></div></div><div>55%11%33%</div></div>
2	E	832	<div><div><div></div><div></div><div></div></div><div>57%11%32%</div></div>
2	F	832	<div><div><div></div><div></div><div></div></div><div>56%12%32%</div></div>

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 55729 atoms, of which 27834 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 VCPIP1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	G	65	Total	C	H	N	O	S	0	0
			1048	347	519	87	94	1		
1	H	66	Total	C	H	N	O	S	0	0
			1070	353	532	89	95	1		
1	I	68	Total	C	H	N	O	S	0	0
			1087	359	535	90	102	1		

There are 84 discrepancies between the modelled and reference sequences:

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

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

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-17	LYS	-	expression tag	UNP Q96JH7
I	-16	SER	-	expression tag	UNP Q96JH7
I	-15	GLY	-	expression tag	UNP Q96JH7
I	-14	GLY	-	expression tag	UNP Q96JH7
I	-13	GLY	-	expression tag	UNP Q96JH7
I	-12	SER	-	expression tag	UNP Q96JH7
I	-11	GLY	-	expression tag	UNP Q96JH7
I	-10	GLY	-	expression tag	UNP Q96JH7
I	-9	LEU	-	expression tag	UNP Q96JH7
I	-8	GLU	-	expression tag	UNP Q96JH7
I	-7	VAL	-	expression tag	UNP Q96JH7
I	-6	LEU	-	expression tag	UNP Q96JH7
I	-5	PHE	-	expression tag	UNP Q96JH7
I	-4	GLN	-	expression tag	UNP Q96JH7
I	-3	GLY	-	expression tag	UNP Q96JH7
I	-2	PRO	-	expression tag	UNP Q96JH7
I	-1	GLY	-	expression tag	UNP Q96JH7
I	0	SER	-	expression tag	UNP Q96JH7

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

Mol	Chain	Residues	Atoms						AltConf	Trace
2	A	562	Total	C	H	N	O	S	0	0
			8782	2764	4390	781	825	22		
2	B	562	Total	C	H	N	O	S	0	0
			8770	2764	4378	781	825	22		
2	C	558	Total	C	H	N	O	S	0	0
			8708	2741	4351	777	818	21		
2	D	556	Total	C	H	N	O	S	0	0
			8686	2734	4343	774	813	22		
2	E	563	Total	C	H	N	O	S	0	0
			8789	2766	4393	782	826	22		
2	F	563	Total	C	H	N	O	S	0	0
			8789	2766	4393	782	826	22		

There are 156 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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
B	-25	MET	-	expression tag	UNP P55072
B	-24	GLY	-	expression tag	UNP P55072
B	-23	ASP	-	expression tag	UNP P55072
B	-22	TYR	-	expression tag	UNP P55072
B	-21	LYS	-	expression tag	UNP P55072
B	-20	ASP	-	expression tag	UNP P55072
B	-19	ASP	-	expression tag	UNP P55072
B	-18	ASP	-	expression tag	UNP P55072
B	-17	ASP	-	expression tag	UNP P55072
B	-16	LYS	-	expression tag	UNP P55072
B	-15	GLY	-	expression tag	UNP P55072
B	-14	GLY	-	expression tag	UNP P55072
B	-13	GLY	-	expression tag	UNP P55072
B	-12	SER	-	expression tag	UNP P55072
B	-11	GLY	-	expression tag	UNP P55072
B	-10	GLY	-	expression tag	UNP P55072
B	-9	LEU	-	expression tag	UNP P55072
B	-8	GLU	-	expression tag	UNP P55072
B	-7	VAL	-	expression tag	UNP P55072
B	-6	LEU	-	expression tag	UNP P55072

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

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-15	GLY	-	expression tag	UNP P55072
D	-14	GLY	-	expression tag	UNP P55072
D	-13	GLY	-	expression tag	UNP P55072
D	-12	SER	-	expression tag	UNP P55072
D	-11	GLY	-	expression tag	UNP P55072
D	-10	GLY	-	expression tag	UNP P55072
D	-9	LEU	-	expression tag	UNP P55072
D	-8	GLU	-	expression tag	UNP P55072
D	-7	VAL	-	expression tag	UNP P55072
D	-6	LEU	-	expression tag	UNP P55072
D	-5	PHE	-	expression tag	UNP P55072
D	-4	GLN	-	expression tag	UNP P55072
D	-3	GLY	-	expression tag	UNP P55072
D	-2	PRO	-	expression tag	UNP P55072
D	-1	GLY	-	expression tag	UNP P55072
D	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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

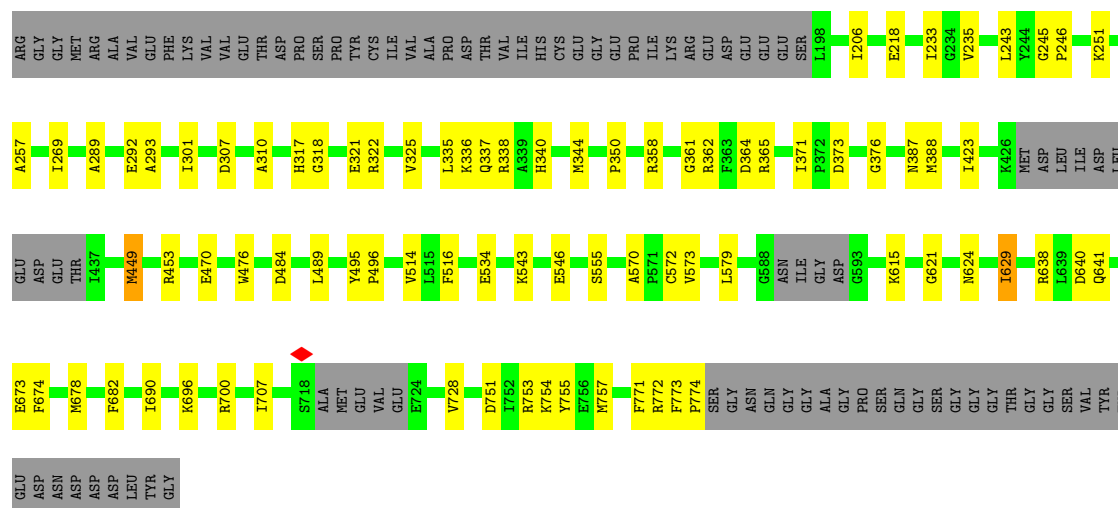






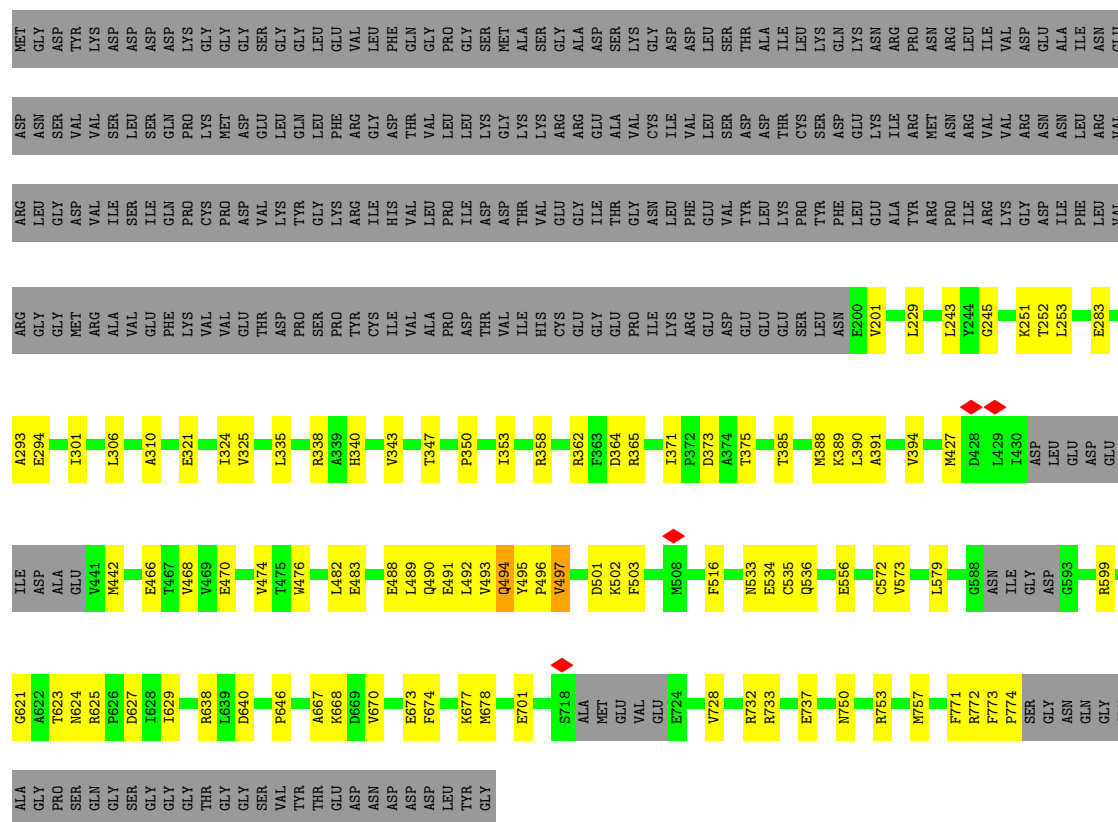






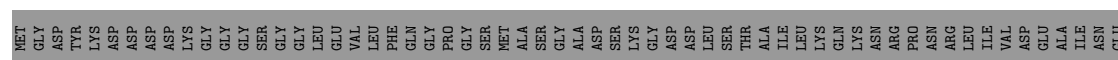
• Molecule 2: Transitional endoplasmic reticulum ATPase

Chain D: 55% 11% 33%



• Molecule 2: Transitional endoplasmic reticulum ATPase

Chain E: 57% 11% 32%







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	107859	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	0.190	Depositor
Minimum map value	-0.074	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0319	Depositor
Map size ( $\text{\AA}$ )	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 ( $\text{\AA}$ )	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	G	0.12	0/544	0.27	0/739
1	H	0.15	0/553	0.28	0/750
1	I	0.14	0/568	0.27	0/773
2	A	0.16	0/4465	0.25	0/6021
2	B	0.16	0/4465	0.25	0/6021
2	C	0.16	0/4430	0.25	0/5973
2	D	0.16	0/4416	0.26	0/5953
2	E	0.16	0/4469	0.25	0/6026
2	F	0.16	0/4469	0.25	0/6026
All	All	0.16	0/28379	0.25	0/38282

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	G	529	519	519	13	0
1	H	538	532	532	8	0
1	I	552	535	535	10	0
2	A	4392	4390	4436	65	0
2	B	4392	4378	4436	71	0
2	C	4357	4351	4397	57	0
2	D	4343	4343	4389	75	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	4396	4393	4439	71	0
2	F	4396	4393	4439	76	0
All	All	27895	27834	28122	395	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 7.

All (395) 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:B:634:LEU:HD22	2:B:642:LEU:HD11	1.33	1.06
2:B:233:ILE:HD13	2:C:423:ILE:HD11	1.56	0.87
2:B:491:GLU:OE2	2:C:700:ARG:NH1	2.07	0.87
2:A:512:LYS:NZ	2:A:611:MET:O	2.11	0.84
1:I:623:TYR:HB2	2:B:761:THR:HG21	1.60	0.84
2:B:371:ILE:HD11	2:B:466:GLU:HB2	1.61	0.81
2:A:350:PRO:O	2:A:358:ARG:NH1	2.16	0.79
2:A:470:GLU:OE1	2:A:470:GLU:N	2.16	0.78
2:D:389:LYS:NZ	2:D:442:MET:O	2.16	0.78
2:B:512:LYS:NZ	2:B:611:MET:O	2.16	0.78
2:C:470:GLU:OE1	2:C:470:GLU:N	2.18	0.76
1:H:603:VAL:HG12	1:H:605:GLU:OE1	1.83	0.76
2:E:700:ARG:NH1	2:E:704:GLU:OE2	2.17	0.76
2:D:294:GLU:OE2	2:D:338:ARG:NE	2.19	0.76
2:E:470:GLU:N	2:E:470:GLU:OE1	2.19	0.76
2:F:470:GLU:OE1	2:F:470:GLU:N	2.19	0.76
2:B:470:GLU:N	2:B:470:GLU:OE1	2.20	0.74
1:G:622:VAL:HG22	2:D:757:MET:HE3	1.67	0.74
2:D:470:GLU:N	2:D:470:GLU:OE1	2.21	0.74
2:A:469:VAL:HG13	2:A:540:ILE:HD11	1.68	0.74
2:E:224:LEU:HD12	2:E:264:ALA:HB2	1.70	0.73
2:F:350:PRO:O	2:F:358:ARG:NH1	2.20	0.73
1:G:647:VAL:O	1:G:651:ILE:HD12	1.89	0.73
2:A:230:PHE:HZ	2:B:420:LEU:HD11	1.52	0.73
2:F:425:LYS:NZ	2:F:450:ASP:OD2	2.21	0.72
2:B:350:PRO:O	2:B:358:ARG:NH1	2.23	0.72
2:E:570:ALA:HB1	2:E:571:PRO:HD2	1.71	0.72
2:E:221:GLU:N	2:E:221:GLU:OE1	2.23	0.71
2:D:750:ASN:OD1	2:D:753:ARG:NH2	2.23	0.71
2:A:726:ASP:OD2	2:F:505:LYS:NZ	2.22	0.71
2:E:414:LEU:HD11	2:E:456:LEU:HD22	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:622:VAL:HG22	2:F:757:MET:CE	2.23	0.69
2:B:770:SER:O	2:B:772:ARG:HD2	1.92	0.69
2:A:732:ARG:NH2	2:A:734:ASP:OD2	2.26	0.68
2:A:773:PHE:HB2	2:B:737:GLU:OE2	1.93	0.68
2:D:391:ALA:O	2:D:394:VAL:HG22	1.94	0.68
2:D:483:GLU:N	2:D:483:GLU:OE1	2.25	0.67
1:G:622:VAL:HG22	2:D:757:MET:CE	2.25	0.67
2:C:350:PRO:O	2:C:358:ARG:NH1	2.28	0.67
2:D:488:GLU:O	2:D:492:LEU:HD12	1.94	0.67
2:E:350:PRO:O	2:E:358:ARG:NH1	2.28	0.67
2:A:769:GLY:HA2	2:B:741:ARG:HA	1.76	0.67
2:E:647:LEU:HD21	2:E:747:VAL:HG21	1.77	0.67
2:B:716:ASN:OD1	2:B:718:SER:OG	2.13	0.66
2:B:292:GLU:O	2:B:296:ASN:ND2	2.28	0.66
2:B:427:MET:HA	2:B:427:MET:HE2	1.78	0.66
2:A:442:MET:N	2:A:442:MET:HE2	2.10	0.65
2:A:741:ARG:NH1	2:F:770:SER:H	1.95	0.65
2:F:397:GLU:O	2:F:401:ASN:ND2	2.29	0.65
2:B:514:VAL:HG23	2:B:641:GLN:HB3	1.79	0.64
2:E:570:ALA:HB1	2:E:571:PRO:CD	2.27	0.64
1:H:641:GLU:OE2	1:H:641:GLU:N	2.28	0.64
2:B:772:ARG:HA	2:B:772:ARG:NE	2.11	0.63
2:D:373:ASP:OD2	2:D:375:THR:OG1	2.16	0.63
2:F:649:ASP:N	2:F:652:SER:OG	2.31	0.63
2:B:522:CYS:SG	2:B:647:LEU:HD23	2.39	0.63
2:A:488:GLU:O	2:A:492:LEU:HD22	1.99	0.63
2:E:522:CYS:SG	2:E:647:LEU:HD23	2.39	0.63
2:E:457:SER:OG	2:E:458:GLN:NE2	2.32	0.62
2:B:673:GLU:N	2:B:673:GLU:OE1	2.32	0.62
2:E:774:PRO:HD3	2:F:674:PHE:CD2	2.34	0.62
2:E:669:ASP:OD2	2:E:733:ARG:NE	2.33	0.62
2:C:678:MET:HE3	2:C:678:MET:O	2.00	0.62
2:F:318:GLY:N	2:F:321:GLU:OE1	2.32	0.62
2:A:397:GLU:OE1	2:A:397:GLU:N	2.32	0.62
2:A:699:ILE:HD12	2:F:508:MET:HE3	1.82	0.62
2:B:428:ASP:N	2:B:428:ASP:OD1	2.32	0.61
2:A:489:LEU:HD21	2:A:516:PHE:HZ	1.66	0.61
2:F:202:GLY:N	2:F:205:ASP:OD2	2.32	0.61
2:F:391:ALA:O	2:F:394:VAL:HG22	2.00	0.61
2:D:773:PHE:HB2	2:E:733:ARG:HD2	1.81	0.61
2:E:701:GLU:OE2	2:E:732:ARG:NH1	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:615:ASP:OD1	1:I:616:SER:N	2.34	0.61
2:B:442:MET:SD	2:B:442:MET:N	2.74	0.61
2:E:224:LEU:HD13	2:E:298:PRO:HB2	1.82	0.60
1:G:605:GLU:OE2	1:G:606:THR:N	2.33	0.60
2:C:362:ARG:O	2:C:364:ASP:N	2.35	0.60
2:D:427:MET:HA	2:D:427:MET:HE2	1.83	0.60
2:F:653:ARG:HG2	2:F:687:LEU:HD11	1.83	0.60
2:A:484:ASP:OD1	2:A:484:ASP:N	2.35	0.60
2:D:673:GLU:OE1	2:D:673:GLU:N	2.35	0.60
2:B:757:MET:O	2:B:761:THR:HG23	2.02	0.60
2:D:347:THR:HG21	2:D:353:ILE:HG23	1.84	0.60
2:E:484:ASP:N	2:E:484:ASP:OD1	2.35	0.59
2:A:230:PHE:CZ	2:B:420:LEU:HD11	2.35	0.59
2:C:387:ASN:ND2	2:C:387:ASN:O	2.35	0.59
2:F:669:ASP:OD1	2:F:733:ARG:NH1	2.35	0.59
2:F:364:ASP:OD1	2:F:365:ARG:N	2.35	0.59
2:D:442:MET:SD	2:D:442:MET:N	2.75	0.59
2:C:514:VAL:HG23	2:C:641:GLN:HB3	1.83	0.59
2:D:773:PHE:HB3	2:D:774:PRO:HD2	1.84	0.59
2:D:350:PRO:O	2:D:358:ARG:NH1	2.36	0.58
2:E:728:VAL:O	2:E:728:VAL:HG13	2.03	0.58
2:F:514:VAL:HG21	2:F:643:ILE:CD1	2.33	0.58
2:B:362:ARG:O	2:B:364:ASP:N	2.37	0.58
2:D:501:ASP:OD1	2:D:502:LYS:N	2.37	0.58
2:B:543:LYS:N	2:B:546:GLU:OE1	2.37	0.58
2:E:745:ARG:NH2	2:E:749:ASP:OD1	2.35	0.57
2:D:474:VAL:O	2:D:533:ASN:ND2	2.34	0.57
2:F:362:ARG:O	2:F:364:ASP:N	2.37	0.57
2:F:272:PRO:O	2:F:276:SER:OG	2.22	0.57
2:A:420:LEU:HD11	2:F:230:PHE:CE2	2.40	0.57
2:D:625:ARG:NH2	2:D:627:ASP:OD2	2.38	0.57
2:C:484:ASP:OD1	2:C:484:ASP:N	2.35	0.57
2:F:286:LEU:HD12	2:F:324:ILE:HD11	1.85	0.57
2:D:772:ARG:HA	2:D:772:ARG:NH1	2.20	0.57
1:I:597:GLU:C	1:I:597:GLU:OE1	2.48	0.56
2:D:388:MET:O	2:D:390:LEU:HD12	2.05	0.56
2:D:533:ASN:O	2:D:536:GLN:NE2	2.38	0.56
2:B:390:LEU:HD22	2:B:394:VAL:HG21	1.87	0.56
2:D:491:GLU:OE2	2:E:700:ARG:NE	2.30	0.56
2:E:293:ALA:HB3	2:E:301:ILE:HD11	1.88	0.56
2:C:317:HIS:O	2:C:322:ARG:NH1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:385:THR:HB	2:D:390:LEU:HD11	1.88	0.56
2:C:728:VAL:O	2:C:728:VAL:HG23	2.06	0.56
2:B:772:ARG:HA	2:B:772:ARG:CZ	2.35	0.56
2:C:337:GLN:OE1	2:C:337:GLN:N	2.39	0.56
2:F:514:VAL:HG23	2:F:641:GLN:HB3	1.87	0.56
2:D:494:GLN:HA	2:D:497:VAL:HG22	1.86	0.55
2:D:773:PHE:CB	2:E:733:ARG:HD2	2.36	0.55
2:A:293:ALA:CB	2:A:301:ILE:HD11	2.36	0.55
2:D:489:LEU:HD21	2:D:516:PHE:HZ	1.71	0.55
2:B:634:LEU:CD2	2:B:642:LEU:HD11	2.24	0.55
2:C:682:PHE:CE2	2:C:690:ILE:HD11	2.42	0.55
1:G:616:SER:O	1:G:619:ASN:ND2	2.39	0.55
2:E:212:GLN:N	2:E:212:GLN:OE1	2.37	0.55
2:A:420:LEU:HD23	2:F:235:VAL:HG11	1.88	0.55
2:B:397:GLU:O	2:B:401:ASN:ND2	2.40	0.55
2:F:512:LYS:NZ	2:F:611:MET:O	2.40	0.54
2:A:330:THR:HG21	2:B:273:GLU:HA	1.89	0.54
2:C:245:GLY:O	2:C:251:LYS:NZ	2.36	0.54
2:C:449:MET:SD	2:C:453:ARG:NH1	2.81	0.54
2:B:640:ASP:OD1	2:B:641:GLN:N	2.41	0.54
2:A:737:GLU:OE2	2:F:772:ARG:HA	2.08	0.54
2:C:543:LYS:N	2:C:546:GLU:OE1	2.41	0.54
2:A:490:GLN:NE2	2:A:534:GLU:OE2	2.41	0.54
2:D:362:ARG:O	2:D:364:ASP:N	2.40	0.54
2:F:640:ASP:OD1	2:F:641:GLN:N	2.39	0.54
1:I:622:VAL:HG12	2:B:757:MET:HE3	1.90	0.54
2:A:292:GLU:O	2:A:296:ASN:ND2	2.40	0.54
2:A:771:PHE:C	2:A:772:ARG:HD2	2.32	0.54
2:D:502:LYS:NZ	2:E:702:SER:OG	2.19	0.54
2:C:638:ARG:O	2:C:640:ASP:N	2.41	0.53
2:E:653:ARG:HG2	2:E:687:LEU:HD11	1.90	0.53
2:E:280:GLY:O	2:E:284:SER:OG	2.20	0.53
2:A:332:MET:SD	2:A:343:VAL:HG11	2.49	0.53
2:C:233:ILE:HG23	2:C:235:VAL:HG22	1.90	0.53
2:D:572:CYS:SG	2:D:573:VAL:N	2.82	0.53
2:C:682:PHE:HE2	2:C:690:ILE:HD11	1.74	0.53
1:H:622:VAL:H	2:F:757:MET:HE3	1.74	0.53
2:A:293:ALA:HB3	2:A:301:ILE:HD11	1.90	0.53
2:E:516:PHE:N	2:E:621:GLY:O	2.41	0.53
2:E:489:LEU:HD21	2:E:516:PHE:HZ	1.74	0.53
2:D:579:LEU:HB3	2:D:629:ILE:HD11	1.89	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:225:ARG:HG2	2:F:262:THR:HG23	1.91	0.52
2:B:307:ASP:N	2:B:307:ASP:OD1	2.39	0.52
2:C:624:ASN:O	2:C:755:TYR:OH	2.14	0.52
2:C:773:PHE:HB3	2:D:733:ARG:NE	2.24	0.52
2:E:772:ARG:NE	2:F:737:GLU:OE2	2.41	0.52
2:A:469:VAL:HG22	2:A:540:ILE:HD12	1.90	0.52
2:E:640:ASP:OD1	2:E:641:GLN:N	2.43	0.52
2:A:748:SER:OG	2:A:751:ASP:OD2	2.28	0.52
2:E:321:GLU:O	2:E:324:ILE:HG22	2.10	0.52
2:E:235:VAL:HG11	2:F:420:LEU:HD21	1.91	0.52
2:F:638:ARG:O	2:F:640:ASP:N	2.43	0.52
2:E:602:ASN:HA	2:E:605:LEU:HD12	1.93	0.51
2:D:476:TRP:NE1	2:D:534:GLU:OE1	2.42	0.51
2:D:293:ALA:CB	2:D:301:ILE:HD11	2.41	0.51
2:F:335:LEU:HD11	2:F:343:VAL:CG2	2.40	0.51
2:D:390:LEU:HB3	2:D:394:VAL:HG21	1.93	0.51
2:D:640:ASP:OD1	2:D:640:ASP:N	2.43	0.51
2:F:319:GLU:OE2	2:F:323:ARG:NH2	2.43	0.51
2:B:300:ILE:HD13	2:B:344:MET:HE1	1.93	0.51
2:A:216:ILE:O	2:A:220:VAL:HG22	2.11	0.51
2:F:514:VAL:HG21	2:F:643:ILE:HD12	1.91	0.51
2:F:626:PRO:O	2:F:629:ILE:HG22	2.10	0.51
2:A:338:ARG:O	2:A:341:VAL:HG23	2.11	0.50
1:H:622:VAL:HA	1:H:625:VAL:HG22	1.93	0.50
2:D:773:PHE:CB	2:D:774:PRO:HD2	2.41	0.50
2:B:332:MET:HE2	2:B:363:PHE:CE2	2.46	0.50
2:D:503:PHE:CD1	2:E:699:ILE:HD13	2.46	0.50
2:F:224:LEU:CB	2:F:262:THR:HG21	2.42	0.50
2:D:728:VAL:HG13	2:D:728:VAL:O	2.12	0.50
2:B:765:SER:O	2:B:765:SER:OG	2.21	0.50
2:E:317:HIS:O	2:E:322:ARG:NH2	2.44	0.50
2:A:669:ASP:OD2	2:A:733:ARG:NE	2.44	0.50
2:B:750:ASN:OD1	2:B:753:ARG:NH1	2.45	0.50
2:E:293:ALA:CB	2:E:301:ILE:HD11	2.42	0.50
2:F:390:LEU:HB3	2:F:394:VAL:HG21	1.94	0.50
2:D:638:ARG:O	2:D:640:ASP:N	2.44	0.50
2:C:364:ASP:OD1	2:C:365:ARG:N	2.42	0.49
2:B:390:LEU:HD23	2:B:447:VAL:CG2	2.42	0.49
2:B:426:LYS:HZ3	2:B:430:ILE:HG21	1.78	0.49
2:B:515:LEU:HD22	2:B:634:LEU:HD21	1.95	0.49
2:A:638:ARG:O	2:A:640:ASP:N	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:469:VAL:HG22	2:A:540:ILE:CD1	2.43	0.49
2:C:673:GLU:OE1	2:C:673:GLU:N	2.43	0.49
2:E:748:SER:N	2:E:751:ASP:OD2	2.45	0.49
2:B:233:ILE:CD1	2:C:423:ILE:HD11	2.37	0.48
2:E:489:LEU:HD21	2:E:516:PHE:CZ	2.48	0.48
2:E:224:LEU:HD21	2:E:342:ILE:HD12	1.93	0.48
2:A:343:VAL:HG13	2:A:343:VAL:O	2.13	0.48
2:A:753:ARG:HG3	2:A:757:MET:HE2	1.96	0.48
2:F:474:VAL:O	2:F:533:ASN:ND2	2.47	0.48
2:B:676:ALA:HA	2:B:679:THR:HG22	1.96	0.48
2:D:489:LEU:HD21	2:D:516:PHE:CZ	2.49	0.48
2:B:629:ILE:HD13	2:B:630:ASP:H	1.79	0.48
2:D:772:ARG:HH12	2:E:737:GLU:CG	2.27	0.48
2:B:293:ALA:CB	2:B:301:ILE:HD11	2.44	0.48
2:B:484:ASP:N	2:B:484:ASP:OD1	2.45	0.48
2:B:774:PRO:HD2	2:C:674:PHE:CE2	2.49	0.48
2:F:243:LEU:HD11	2:F:344:MET:HE2	1.96	0.48
2:A:522:CYS:SG	2:A:647:LEU:HD23	2.54	0.48
2:A:772:ARG:HD2	2:A:772:ARG:N	2.29	0.48
2:C:771:PHE:O	2:C:772:ARG:HD2	2.14	0.48
2:F:262:THR:HG22	2:F:262:THR:O	2.12	0.48
2:E:216:ILE:HD11	2:E:367:VAL:HG21	1.96	0.48
2:E:428:ASP:OD1	2:E:429:LEU:N	2.46	0.48
2:A:733:ARG:HD2	2:F:773:PHE:HB3	1.95	0.47
2:F:243:LEU:HD11	2:F:344:MET:CE	2.44	0.47
2:F:335:LEU:HD11	2:F:343:VAL:HG23	1.96	0.47
2:F:602:ASN:HA	2:F:605:LEU:HD12	1.96	0.47
1:H:603:VAL:HG12	1:H:605:GLU:CD	2.38	0.47
2:A:728:VAL:HG13	2:A:728:VAL:O	2.14	0.47
2:B:364:ASP:OD1	2:B:365:ARG:N	2.44	0.47
2:B:627:ASP:OD1	2:B:627:ASP:N	2.47	0.47
2:D:482:LEU:HD21	2:D:646:PRO:HD2	1.95	0.47
2:D:503:PHE:CE1	2:E:699:ILE:HD13	2.50	0.47
2:E:216:ILE:CD1	2:E:367:VAL:HG21	2.44	0.47
2:B:416:SER:O	2:B:420:LEU:HD23	2.15	0.47
2:F:712:GLU:O	2:F:716:ASN:N	2.45	0.47
1:I:596:LEU:N	1:I:596:LEU:HD22	2.30	0.47
1:I:622:VAL:HG23	1:I:651:ILE:HG21	1.95	0.47
2:A:220:VAL:HG21	2:A:258:VAL:HG11	1.96	0.47
2:A:313:ARG:O	2:A:316:THR:OG1	2.32	0.47
2:A:476:TRP:NE1	2:A:534:GLU:OE1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:245:GLY:O	2:E:251:LYS:NZ	2.47	0.47
2:E:335:LEU:HD23	2:E:338:ARG:HG3	1.95	0.47
2:E:224:LEU:CD2	2:E:342:ILE:HD12	2.44	0.47
2:E:630:ASP:O	2:E:633:ILE:HG22	2.15	0.47
2:A:227:PRO:O	2:A:340:HIS:NE2	2.48	0.47
2:C:476:TRP:NE1	2:C:534:GLU:OE1	2.40	0.47
2:E:748:SER:OG	2:E:751:ASP:OD2	2.24	0.47
2:C:579:LEU:HB3	2:C:629:ILE:HD11	1.97	0.47
2:F:461:PRO:HG2	2:F:464:LEU:HD13	1.97	0.47
2:E:397:GLU:OE1	2:E:397:GLU:N	2.44	0.47
2:C:336:LYS:NZ	2:C:361:GLY:O	2.44	0.47
2:E:235:VAL:HG11	2:F:420:LEU:CD2	2.45	0.47
2:F:321:GLU:O	2:F:324:ILE:HG22	2.15	0.47
2:E:519:PRO:HB3	2:E:747:VAL:HG11	1.96	0.46
2:F:224:LEU:HB2	2:F:262:THR:HG21	1.98	0.46
2:B:647:LEU:HD21	2:B:747:VAL:HG21	1.97	0.46
2:C:678:MET:HE3	2:C:678:MET:CA	2.45	0.46
2:D:492:LEU:HD12	2:D:492:LEU:H	1.80	0.46
2:D:753:ARG:O	2:D:757:MET:HB2	2.15	0.46
2:E:673:GLU:N	2:E:673:GLU:OE1	2.47	0.46
1:G:595:THR:HG1	1:G:604:ARG:HH12	1.60	0.46
2:C:318:GLY:N	2:C:321:GLU:OE1	2.48	0.46
2:D:516:PHE:N	2:D:621:GLY:O	2.46	0.46
2:F:204:ASP:OD1	2:F:204:ASP:N	2.49	0.46
1:I:622:VAL:HG23	1:I:651:ILE:CG2	2.46	0.46
2:D:701:GLU:OE2	2:D:732:ARG:NH1	2.41	0.46
2:E:579:LEU:HB3	2:E:629:ILE:HD11	1.97	0.46
2:A:244:TYR:HA	2:A:347:THR:O	2.16	0.46
2:B:567:ARG:NH1	2:B:568:GLN:OE1	2.46	0.46
2:C:206:ILE:HD11	2:C:257:ALA:CB	2.46	0.46
2:B:245:GLY:O	2:B:251:LYS:NZ	2.48	0.46
2:A:326:SER:O	2:A:330:THR:HG23	2.15	0.46
2:C:678:MET:HE3	2:C:678:MET:HA	1.98	0.46
2:D:371:ILE:HD11	2:D:466:GLU:CB	2.45	0.46
1:H:622:VAL:HG22	2:F:757:MET:HE3	1.97	0.45
2:B:649:ASP:OD1	2:B:649:ASP:N	2.41	0.45
2:C:335:LEU:O	2:C:338:ARG:N	2.49	0.45
2:C:773:PHE:N	2:D:737:GLU:OE2	2.32	0.45
2:E:772:ARG:HA	2:E:772:ARG:HD3	1.63	0.45
2:B:224:LEU:HD11	2:B:300:ILE:HD11	1.99	0.45
2:C:774:PRO:HD3	2:D:674:PHE:CE2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:313:ARG:O	2:E:313:ARG:NH1	2.48	0.45
2:E:332:MET:HE2	2:E:363:PHE:CE2	2.52	0.45
2:F:479:ILE:HG23	2:F:479:ILE:O	2.17	0.45
2:A:772:ARG:HA	2:A:772:ARG:NE	2.31	0.45
2:D:772:ARG:NH1	2:E:737:GLU:OE2	2.50	0.45
2:F:216:ILE:O	2:F:220:VAL:HG22	2.16	0.45
2:F:282:SER:OG	2:F:324:ILE:HD13	2.16	0.45
2:A:489:LEU:HD21	2:A:516:PHE:CZ	2.50	0.45
2:D:335:LEU:HD11	2:D:343:VAL:HG23	1.97	0.45
2:B:426:LYS:NZ	2:B:430:ILE:HG21	2.31	0.45
2:B:771:PHE:HE1	2:C:678:MET:CB	2.29	0.45
2:F:216:ILE:HD11	2:F:367:VAL:HG21	1.99	0.45
2:A:696:LYS:HA	2:F:508:MET:HE1	1.99	0.45
2:D:245:GLY:O	2:D:251:LYS:NZ	2.50	0.44
2:D:310:ALA:HA	2:D:325:VAL:HG22	1.98	0.44
2:D:773:PHE:HD1	2:D:774:PRO:HD2	1.81	0.44
2:E:772:ARG:HD3	2:F:737:GLU:OE1	2.17	0.44
2:F:229:LEU:C	2:F:229:LEU:HD23	2.42	0.44
2:F:310:ALA:HA	2:F:325:VAL:HG22	1.99	0.44
2:F:317:HIS:N	2:F:321:GLU:OE1	2.48	0.44
2:B:605:LEU:HD21	2:B:633:ILE:HA	1.98	0.44
2:C:206:ILE:HD11	2:C:257:ALA:HB3	2.00	0.44
2:B:508:MET:HE1	2:C:696:LYS:HD3	1.99	0.44
2:F:293:ALA:HB3	2:F:301:ILE:HD11	1.99	0.44
2:F:582:ILE:HD13	2:F:600:VAL:HB	1.99	0.44
2:E:310:ALA:HA	2:E:325:VAL:HG22	1.99	0.44
2:A:262:THR:HG22	2:A:262:THR:O	2.18	0.44
2:C:310:ALA:HA	2:C:325:VAL:HG22	1.99	0.44
1:G:622:VAL:H	2:D:757:MET:HE3	1.82	0.44
2:D:677:LYS:HE3	2:D:678:MET:HE2	1.99	0.44
2:C:495:TYR:HB2	2:C:496:PRO:HD3	2.00	0.44
2:B:514:VAL:HG21	2:B:643:ILE:CD1	2.48	0.43
2:D:283:GLU:CD	2:D:324:ILE:HD12	2.43	0.43
2:F:627:ASP:N	2:F:627:ASP:OD1	2.51	0.43
2:E:438:ASP:OD1	2:E:440:GLU:N	2.50	0.43
2:A:627:ASP:OD1	2:A:627:ASP:N	2.51	0.43
2:F:725:ASP:OD1	2:F:726:ASP:N	2.51	0.43
1:G:621:ASN:CB	2:D:757:MET:HG2	2.48	0.43
2:B:483:GLU:OE1	2:B:483:GLU:N	2.45	0.43
2:B:771:PHE:HE2	2:B:773:PHE:CD2	2.36	0.43
2:C:307:ASP:OD1	2:C:307:ASP:N	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:667:ALA:O	2:D:670:VAL:HG12	2.19	0.43
1:G:594:ILE:HG13	1:G:650:THR:HG21	2.00	0.43
2:B:391:ALA:O	2:B:394:VAL:HG22	2.18	0.43
2:C:572:CYS:SG	2:C:573:VAL:N	2.91	0.43
2:A:246:PRO:O	2:A:249:THR:OG1	2.32	0.43
2:D:773:PHE:CD1	2:D:774:PRO:HD2	2.54	0.43
2:A:381:LEU:HD13	2:A:399:VAL:HG23	2.00	0.43
2:C:293:ALA:CB	2:C:301:ILE:HD11	2.49	0.43
2:D:495:TYR:HB2	2:D:496:PRO:HD3	2.01	0.43
2:F:385:THR:HB	2:F:390:LEU:HD11	2.01	0.43
2:A:222:LEU:H	2:A:222:LEU:HD22	1.83	0.43
2:E:439:ALA:O	2:E:443:ASN:ND2	2.47	0.43
2:F:407:VAL:HG12	2:F:408:GLY:H	1.84	0.43
2:B:669:ASP:O	2:B:733:ARG:NE	2.52	0.43
2:D:229:LEU:C	2:D:229:LEU:HD23	2.43	0.43
2:D:364:ASP:OD1	2:D:365:ARG:N	2.50	0.43
2:C:516:PHE:N	2:C:621:GLY:O	2.50	0.42
2:C:773:PHE:HB3	2:D:733:ARG:CZ	2.49	0.42
2:E:391:ALA:O	2:E:394:VAL:HG12	2.19	0.42
2:F:772:ARG:HA	2:F:772:ARG:HD3	1.65	0.42
1:I:595:THR:C	1:I:596:LEU:HD22	2.44	0.42
1:I:615:ASP:O	1:I:619:ASN:ND2	2.51	0.42
2:D:772:ARG:HH12	2:E:737:GLU:CD	2.27	0.42
2:A:423:ILE:HD13	2:F:233:ILE:HD13	2.01	0.42
1:I:622:VAL:H	2:B:757:MET:HE3	1.84	0.42
2:B:679:THR:O	2:B:679:THR:HG23	2.20	0.42
2:C:489:LEU:HD21	2:C:516:PHE:HZ	1.84	0.42
2:C:293:ALA:HB3	2:C:301:ILE:HD11	2.02	0.42
2:C:373:ASP:OD1	2:C:376:GLY:N	2.40	0.42
2:C:570:ALA:HB1	2:C:615:LYS:O	2.18	0.42
2:C:751:ASP:O	2:C:754:LYS:HG2	2.19	0.42
2:D:771:PHE:C	2:D:772:ARG:HD2	2.45	0.42
2:F:556:GLU:OE1	2:F:599:ARG:NE	2.33	0.42
2:C:243:LEU:HD11	2:C:344:MET:HE2	2.02	0.42
2:D:556:GLU:OE2	2:D:599:ARG:NE	2.52	0.42
1:G:621:ASN:OD1	1:G:621:ASN:N	2.53	0.42
2:F:438:ASP:OD1	2:F:441:VAL:HG12	2.20	0.42
2:F:678:MET:HE2	2:F:678:MET:O	2.20	0.42
2:D:321:GLU:O	2:D:324:ILE:HG22	2.19	0.41
1:G:636:GLY:HA2	2:E:754:LYS:HG2	2.02	0.41
2:F:608:MET:HE1	2:F:633:ILE:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:269:ILE:HD11	2:C:289:ALA:CB	2.50	0.41
2:D:306:LEU:HD23	2:D:353:ILE:HG21	2.01	0.41
2:D:490:GLN:O	2:D:493:VAL:O	2.38	0.41
2:B:335:LEU:HA	2:B:338:ARG:HG3	2.02	0.41
2:E:538:ASN:ND2	2:E:569:ALA:O	2.47	0.41
2:F:728:VAL:O	2:F:728:VAL:HG13	2.20	0.41
2:F:407:VAL:HG12	2:F:408:GLY:N	2.36	0.41
2:A:332:MET:HE2	2:A:363:PHE:CE2	2.55	0.41
2:E:514:VAL:HG23	2:E:641:GLN:HB3	2.03	0.41
2:F:633:ILE:HG23	2:F:634:LEU:HD23	2.03	0.41
1:H:609:TRP:CE2	1:H:655:THR:HG21	2.55	0.41
2:D:468:VAL:O	2:D:468:VAL:HG13	2.20	0.41
2:F:682:PHE:HE2	2:F:743:ALA:HB1	1.86	0.41
1:G:595:THR:HG23	1:G:604:ARG:HH22	1.86	0.41
2:A:224:LEU:CB	2:A:262:THR:HG21	2.51	0.41
2:A:395:ASP:OD1	2:A:395:ASP:N	2.53	0.41
2:A:514:VAL:HG22	2:A:515:LEU:N	2.36	0.41
2:A:751:ASP:O	2:A:754:LYS:HG2	2.21	0.41
2:B:747:VAL:HG23	2:B:747:VAL:O	2.20	0.41
2:E:570:ALA:CB	2:E:571:PRO:CD	2.96	0.41
1:G:603:VAL:O	1:G:604:ARG:NH2	2.54	0.41
2:A:246:PRO:HG3	2:A:371:ILE:HD11	2.02	0.41
2:A:582:ILE:CD1	2:A:600:VAL:HB	2.51	0.41
2:B:427:MET:HE2	2:B:430:ILE:HG23	2.03	0.41
2:C:772:ARG:HA	2:D:737:GLU:OE2	2.21	0.41
2:E:514:VAL:HG22	2:E:515:LEU:N	2.36	0.41
2:A:392:ASP:OD1	2:A:392:ASP:N	2.54	0.40
2:A:403:THR:HG22	2:A:456:LEU:HD21	2.03	0.40
2:E:442:MET:H	2:E:442:MET:HG2	1.75	0.40
2:B:774:PRO:HD2	2:C:674:PHE:CZ	2.56	0.40
2:C:753:ARG:NE	2:C:757:MET:HE3	2.36	0.40
2:E:307:ASP:OD1	2:E:307:ASP:N	2.53	0.40
2:B:712:GLU:OE1	2:B:713:ARG:NE	2.53	0.40
2:C:246:PRO:HG3	2:C:371:ILE:HD11	2.02	0.40
2:B:495:TYR:HB2	2:B:496:PRO:HD3	2.03	0.40
2:A:215:GLN:O	2:A:219:MET:HG3	2.21	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	G	61/1250 (5%)	60 (98%)	1 (2%)	0	100	100
1	H	62/1250 (5%)	61 (98%)	1 (2%)	0	100	100
1	I	66/1250 (5%)	65 (98%)	1 (2%)	0	100	100
2	A	554/832 (67%)	533 (96%)	21 (4%)	0	100	100
2	B	554/832 (67%)	534 (96%)	20 (4%)	0	100	100
2	C	550/832 (66%)	535 (97%)	15 (3%)	0	100	100
2	D	548/832 (66%)	527 (96%)	21 (4%)	0	100	100
2	E	555/832 (67%)	543 (98%)	11 (2%)	1 (0%)	44	73
2	F	555/832 (67%)	533 (96%)	22 (4%)	0	100	100
All	All	3505/8742 (40%)	3391 (97%)	113 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	570	ALA

### 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	G	58/1065 (5%)	56 (97%)	2 (3%)	32	67
1	H	59/1065 (6%)	59 (100%)	0	100	100
1	I	61/1065 (6%)	59 (97%)	2 (3%)	33	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	469/696 (67%)	460 (98%)	9 (2%)	52	81
2	B	469/696 (67%)	458 (98%)	11 (2%)	45	77
2	C	464/696 (67%)	456 (98%)	8 (2%)	56	83
2	D	463/696 (66%)	452 (98%)	11 (2%)	44	76
2	E	469/696 (67%)	462 (98%)	7 (2%)	60	85
2	F	469/696 (67%)	461 (98%)	8 (2%)	56	83
All	All	2981/7371 (40%)	2923 (98%)	58 (2%)	52	81

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	595	THR
1	G	629	LEU
1	I	624	ASP
1	I	653	HIS
2	A	199	ASN
2	A	222	LEU
2	A	249	THR
2	A	282	SER
2	A	340	HIS
2	A	479	ILE
2	A	492	LEU
2	A	515	LEU
2	A	624	ASN
2	B	352	SER
2	B	428	ASP
2	B	430	ILE
2	B	438	ASP
2	B	475	THR
2	B	515	LEU
2	B	613	THR
2	B	629	ILE
2	B	633	ILE
2	B	751	ASP
2	B	765	SER
2	C	218	GLU
2	C	292	GLU
2	C	340	HIS
2	C	388	MET
2	C	449	MET

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Mol	Chain	Res	Type
2	C	555	SER
2	C	629	ILE
2	C	707	ILE
2	D	201	VAL
2	D	243	LEU
2	D	252	THR
2	D	253	LEU
2	D	340	HIS
2	D	494	GLN
2	D	497	VAL
2	D	535	CYS
2	D	623	THR
2	D	624	ASN
2	D	668	LYS
2	E	317	HIS
2	E	375	THR
2	E	458	GLN
2	E	492	LEU
2	E	613	THR
2	E	623	THR
2	E	624	ASN
2	F	198	LEU
2	F	340	HIS
2	F	429	LEU
2	F	450	ASP
2	F	479	ILE
2	F	509	THR
2	F	695	CYS
2	F	773	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	649	HIS
2	A	421	GLN
2	A	473	GLN
2	B	443	ASN
2	C	327	GLN
2	C	421	GLN
2	C	568	GLN
2	C	624	ASN
2	D	317	HIS

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Mol	Chain	Res	Type
2	D	568	GLN
2	D	692	GLN
2	E	458	GLN
2	F	340	HIS
2	F	460	ASN
2	F	536	GLN

### 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.

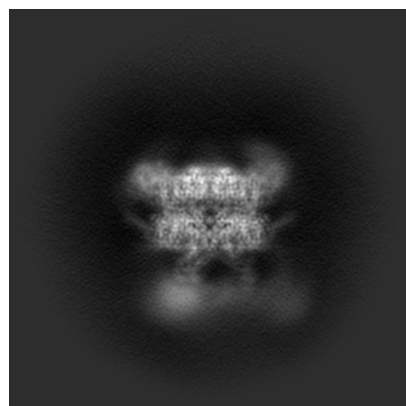
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-48500. These allow visual inspection of the internal detail of the map and identification of artifacts.

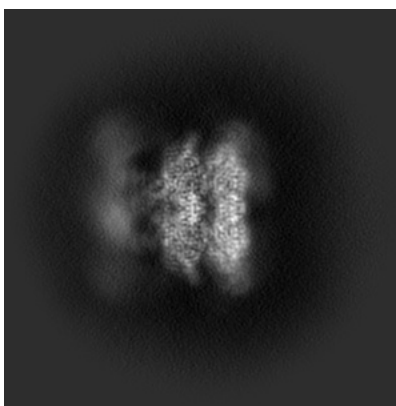
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

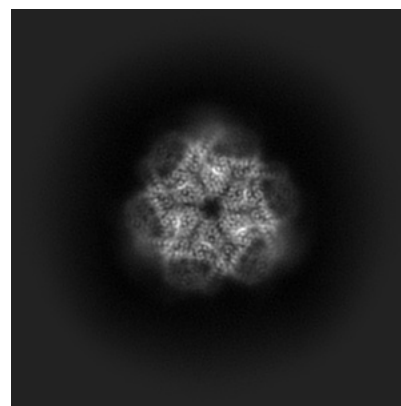
#### 6.1.1 Primary map



X

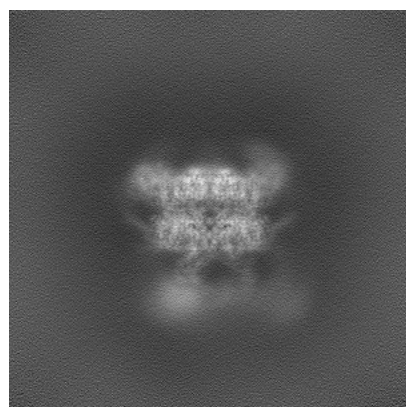


Y

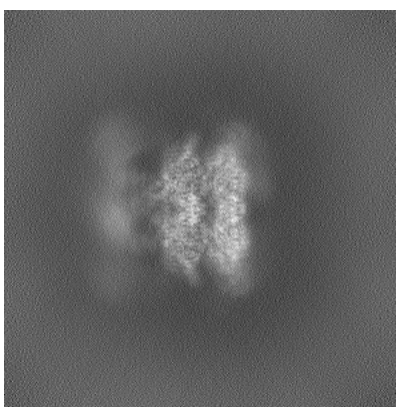


Z

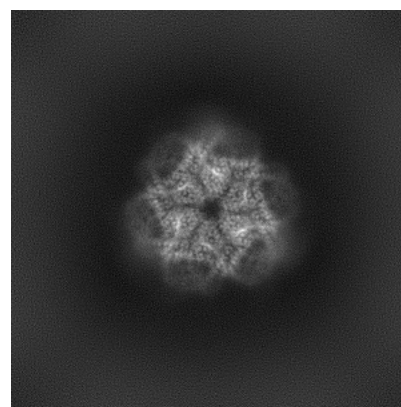
#### 6.1.2 Raw map



X



Y

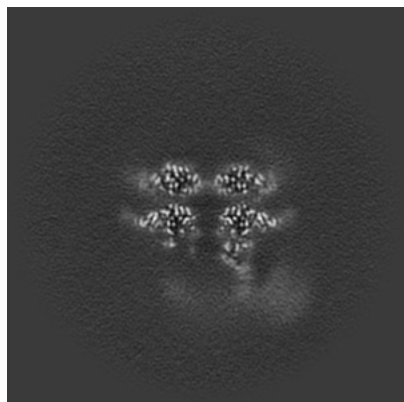


Z

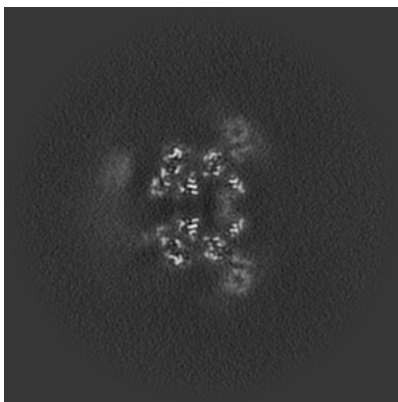
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

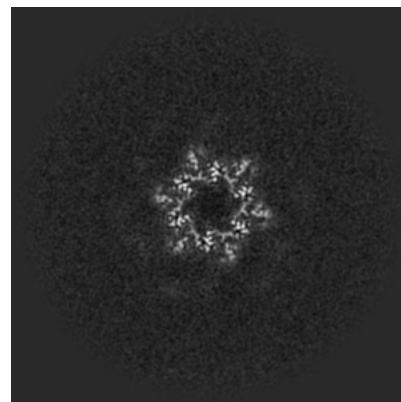
### 6.2.1 Primary map



X Index: 220

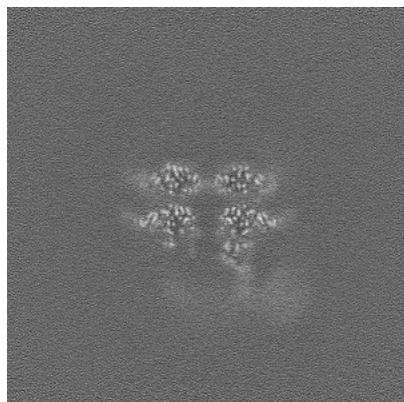


Y Index: 220

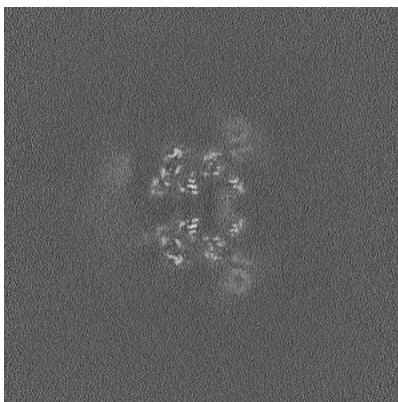


Z Index: 220

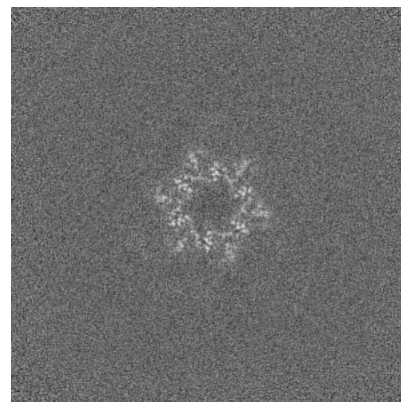
### 6.2.2 Raw map



X Index: 220



Y Index: 220

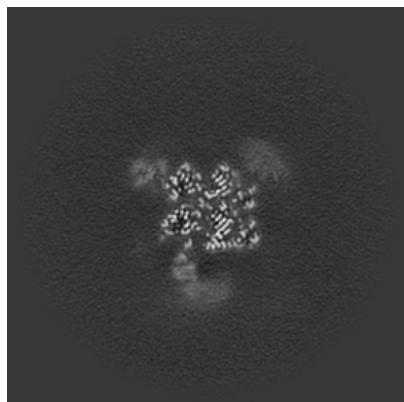


Z Index: 220

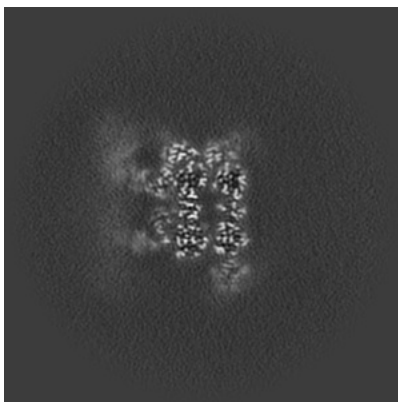
The images above show central slices of the map in three orthogonal directions.

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

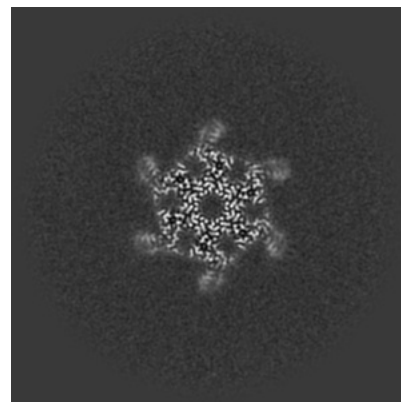
### 6.3.1 Primary map



X Index: 257

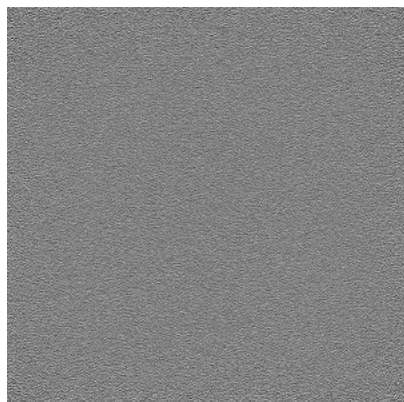


Y Index: 201

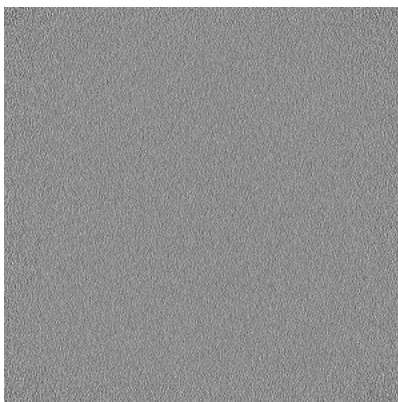


Z Index: 206

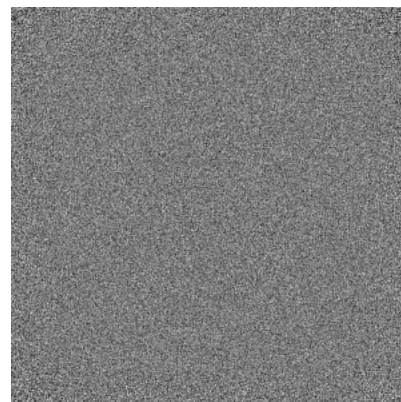
### 6.3.2 Raw map



X Index: 0



Y Index: 0



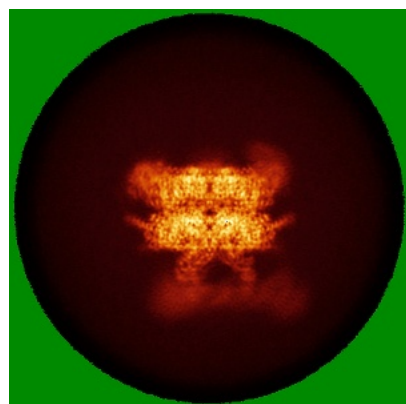
Z Index: 0

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

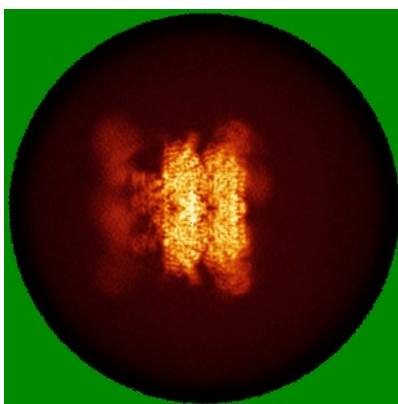


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

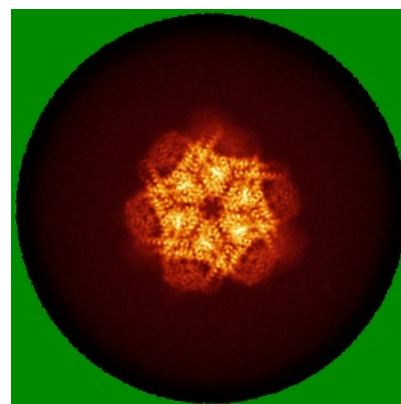
### 6.4.1 Primary map



X

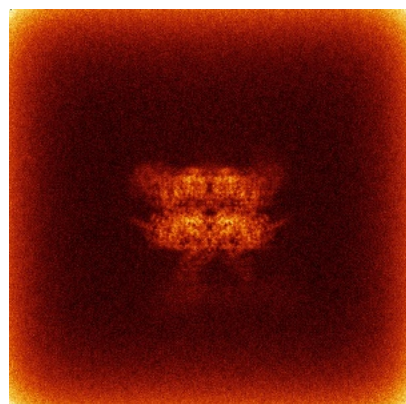


Y

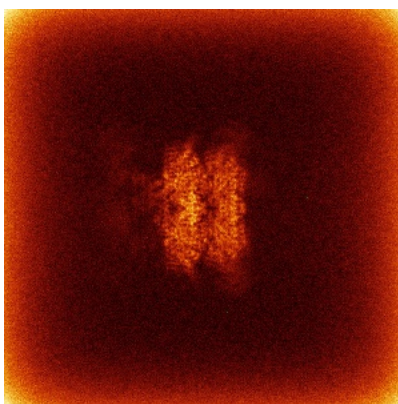


Z

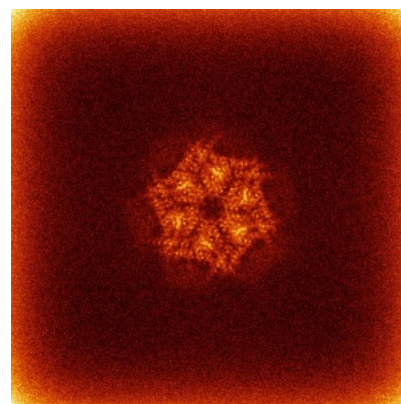
### 6.4.2 Raw map



X



Y



Z

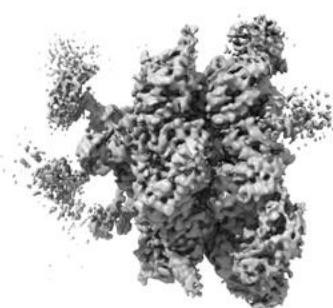
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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

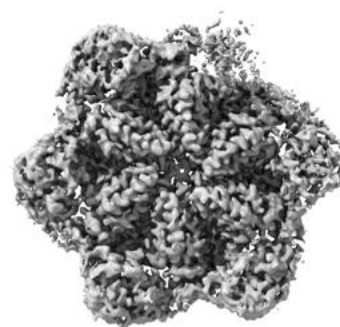
### 6.5.1 Primary map



X



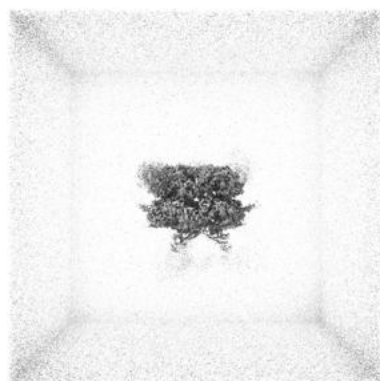
Y



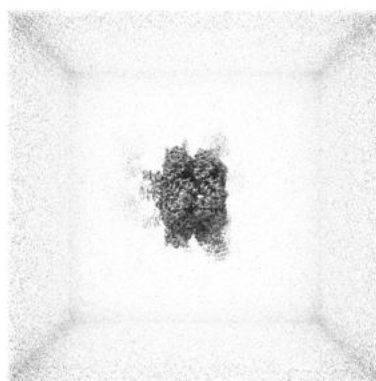
Z

The images above show the 3D surface view of the map at the recommended contour level 0.0319. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

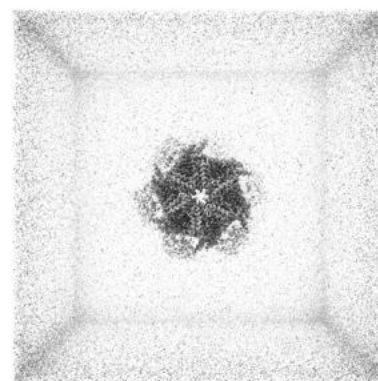
### 6.5.2 Raw map



X



Y



Z

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.

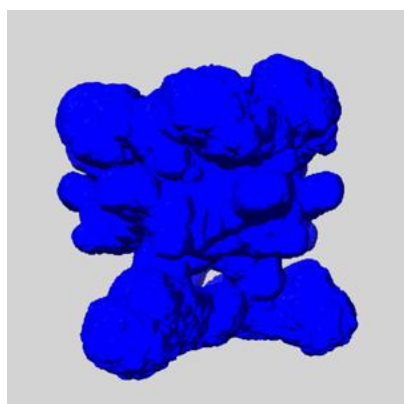
## 6.6 Mask visualisation [i](#)

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

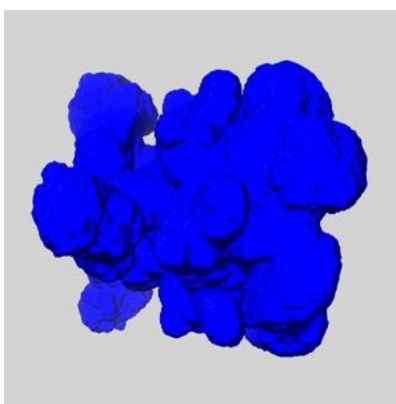
A mask typically either:

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

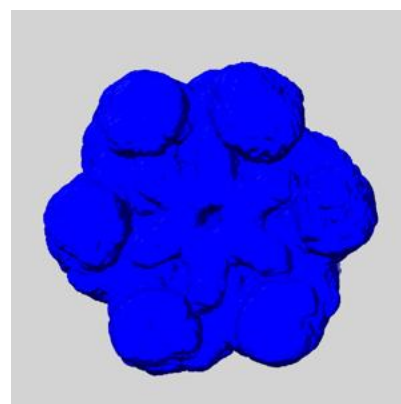
### 6.6.1 emd\_48500\_msk\_2.map [i](#)



X

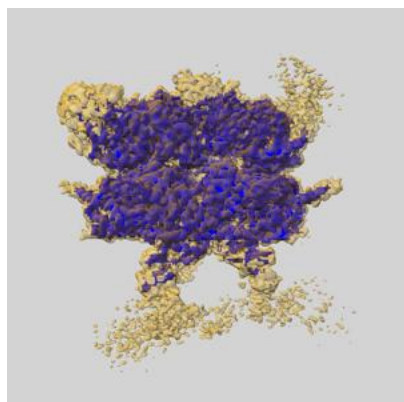


Y

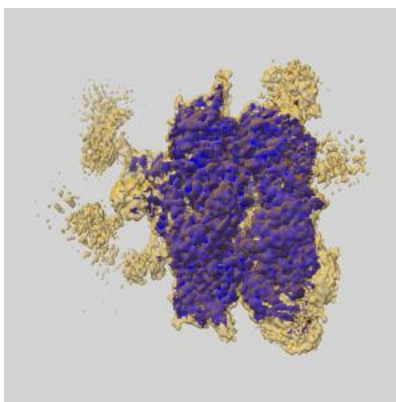


Z

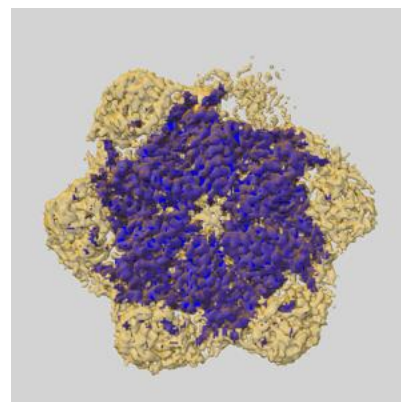
### 6.6.2 emd\_48500\_msk\_1.map [i](#)



X



Y

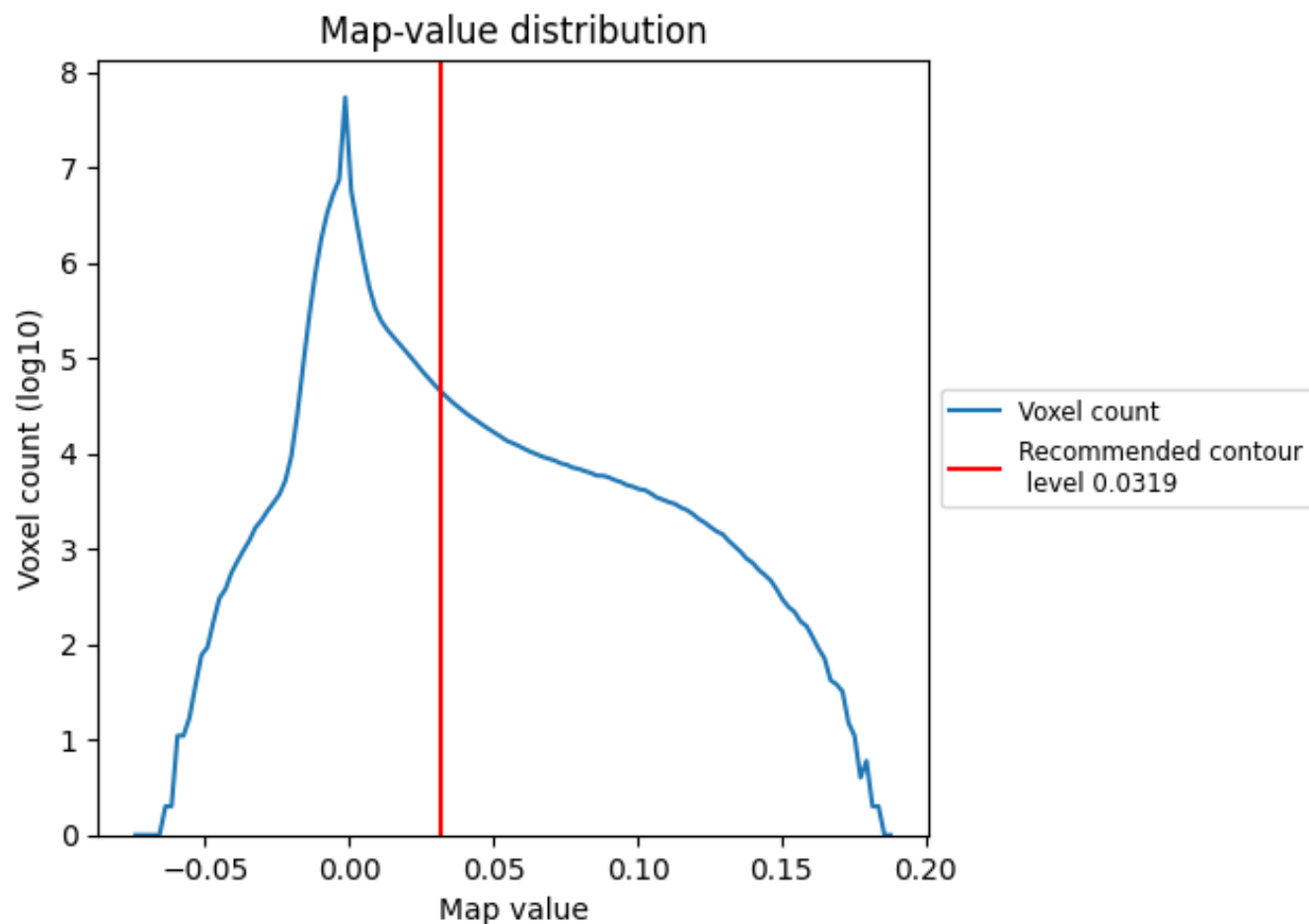


Z

## 7 Map analysis [i](#)

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

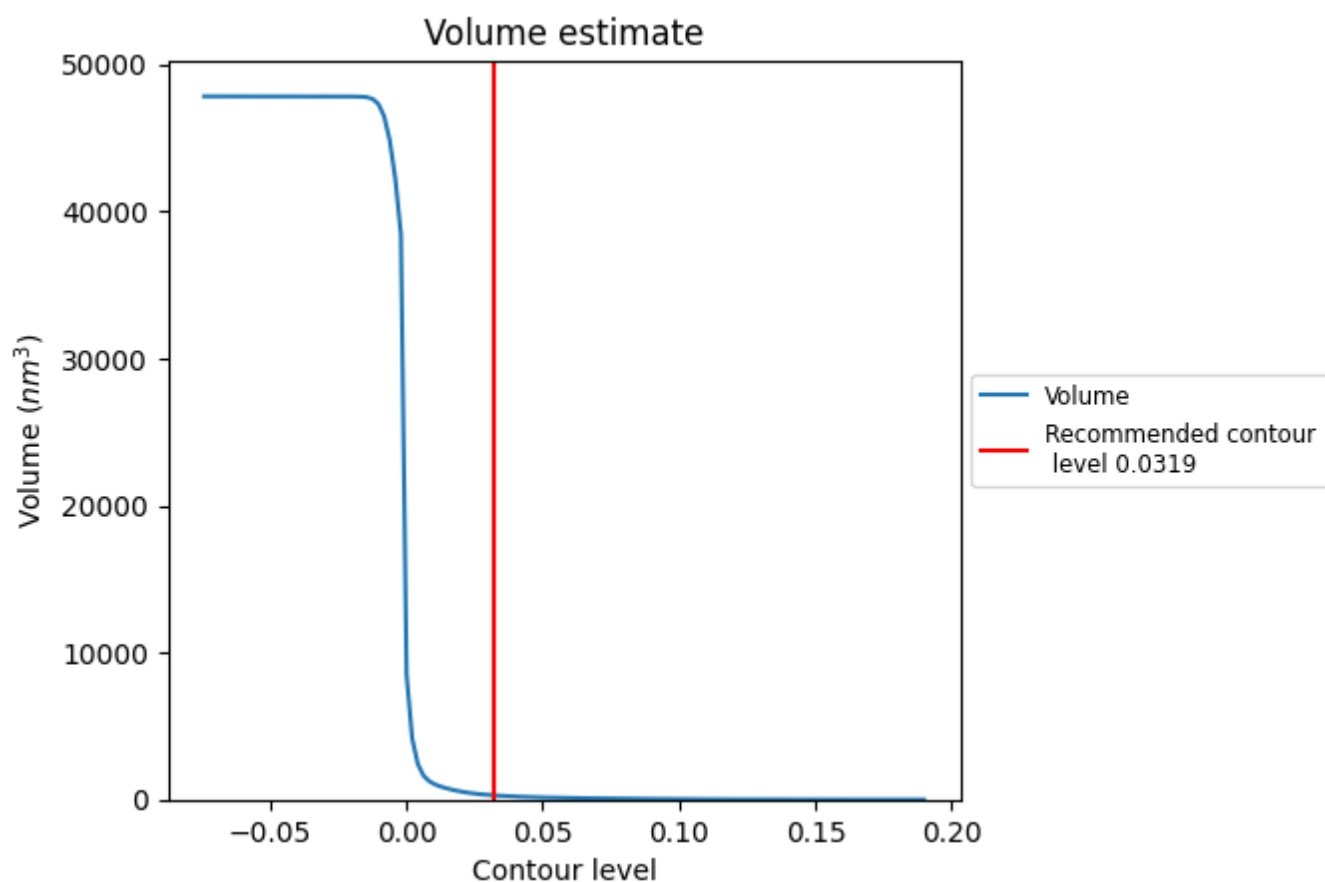
### 7.1 Map-value distribution [i](#)



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.



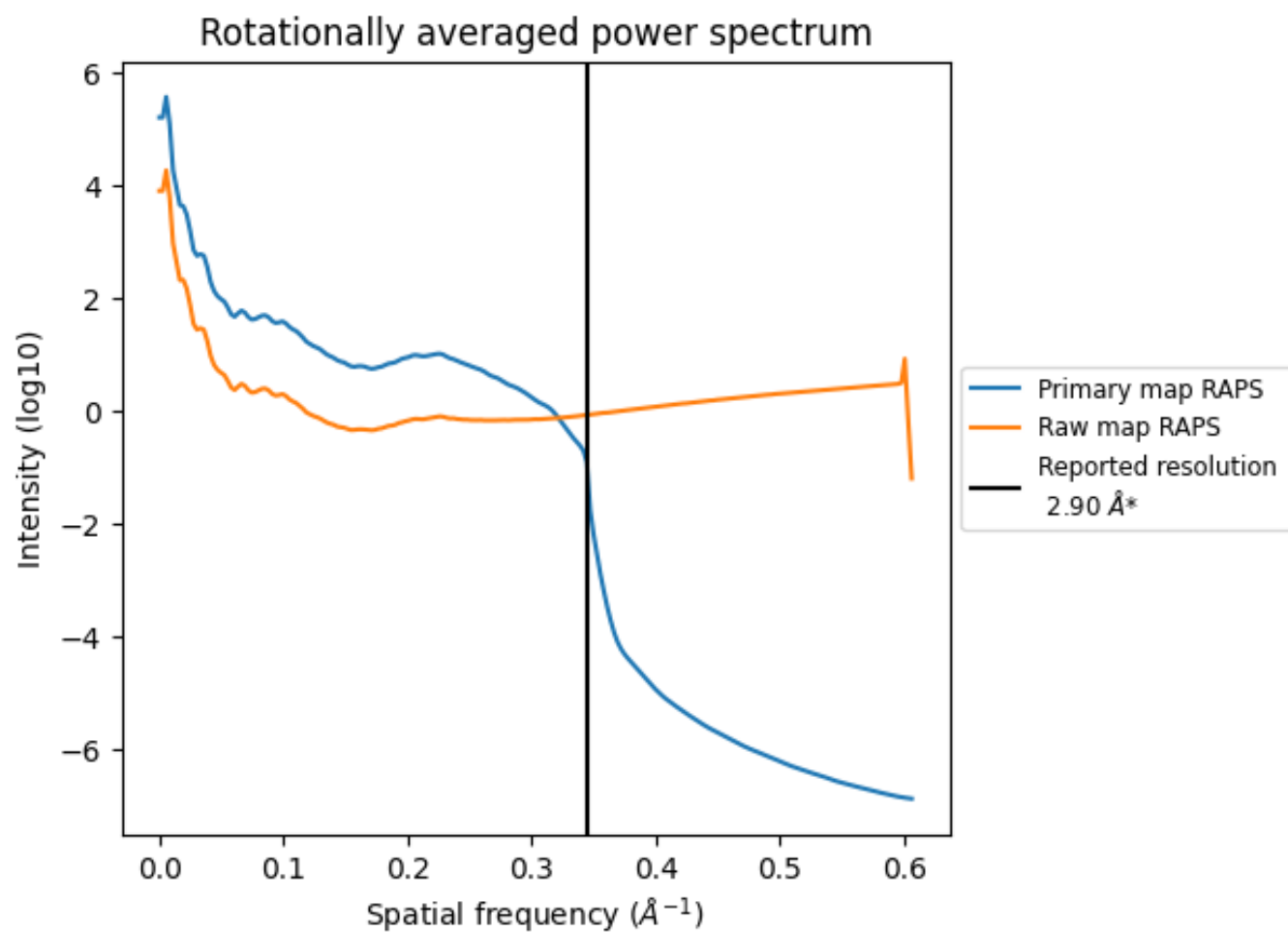
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 289 nm<sup>3</sup>; this corresponds to an approximate mass of 261 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 ⓘ

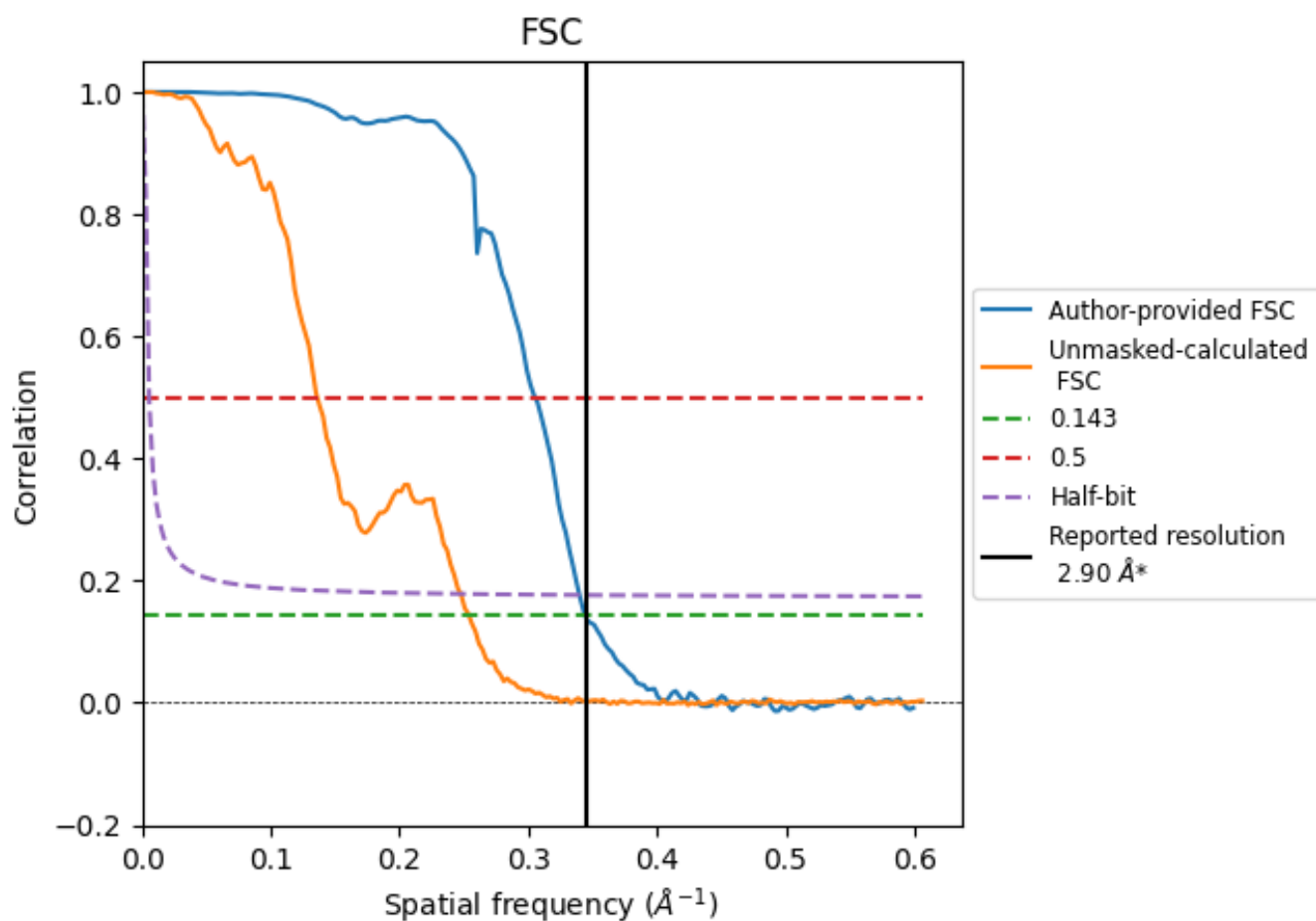


\*Reported resolution corresponds to spatial frequency of 0.345  $\text{\AA}^{-1}$

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

## 8.2 Resolution estimates [i](#)

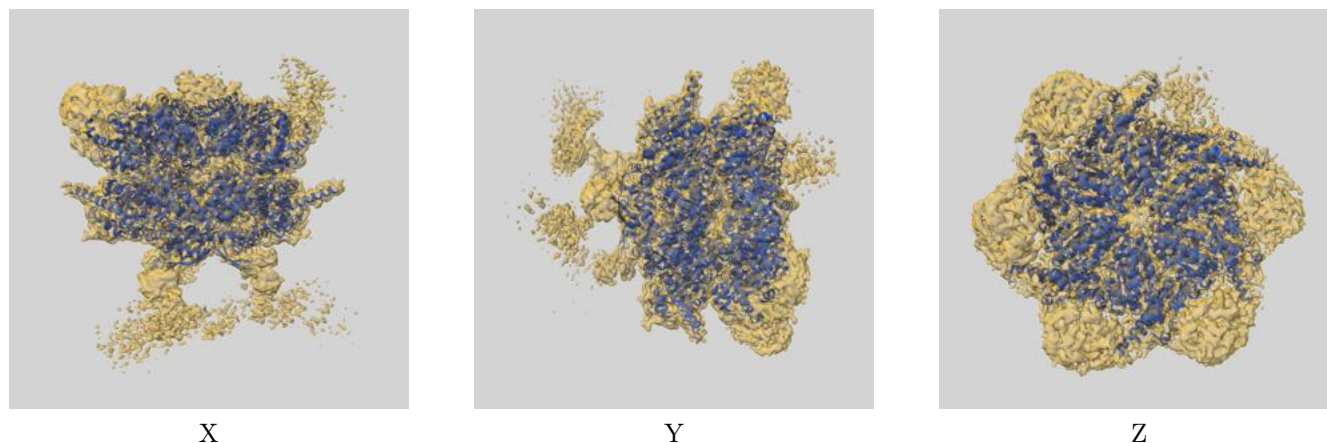
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.91	3.28	2.94
Unmasked-calculated*	3.94	7.35	4.04

\*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 3.94 differs from the reported value 2.9 by more than 10 %

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

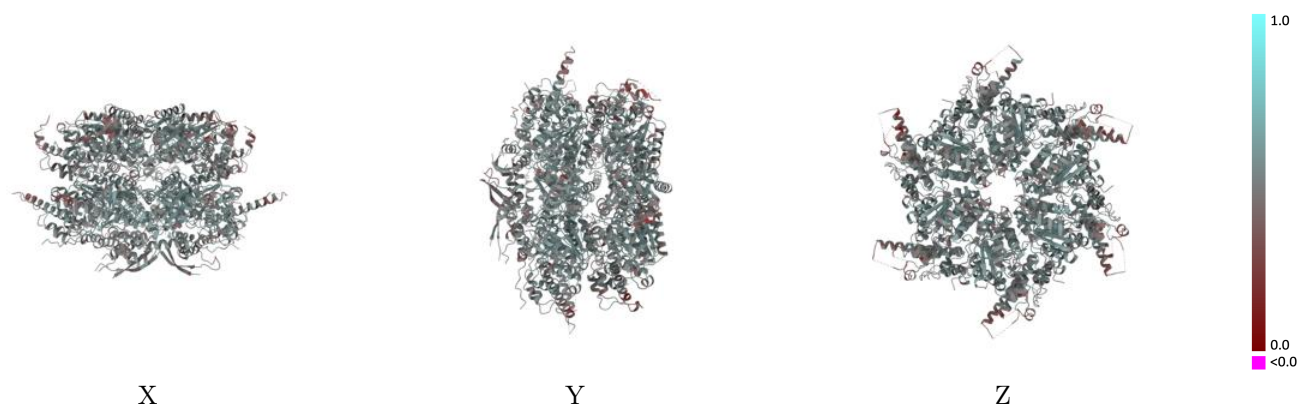
This section contains information regarding the fit between EMDB map EMD-48500 and PDB model 9MPR. Per-residue inclusion information can be found in section [3](#) on page [11](#).

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



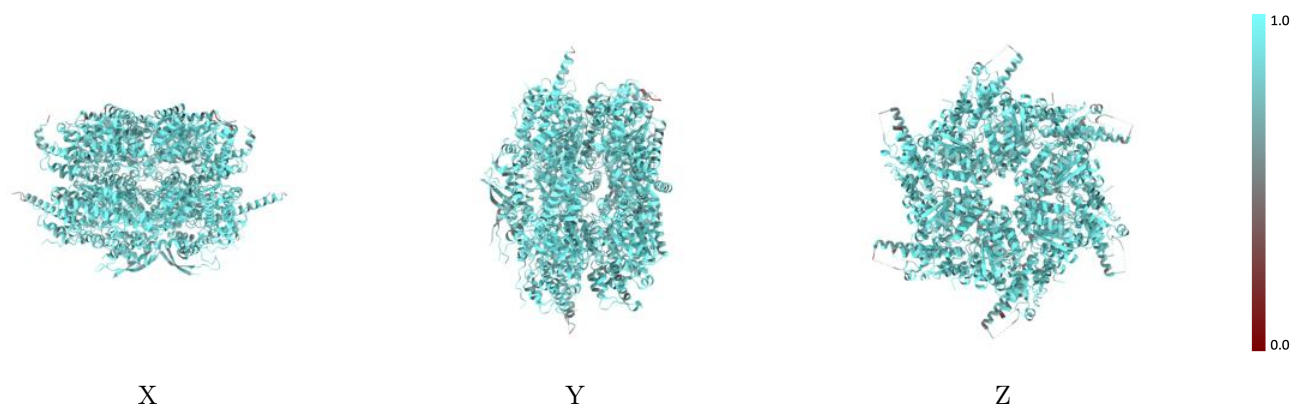
The images above show the 3D surface view of the map at the recommended contour level 0.0319 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



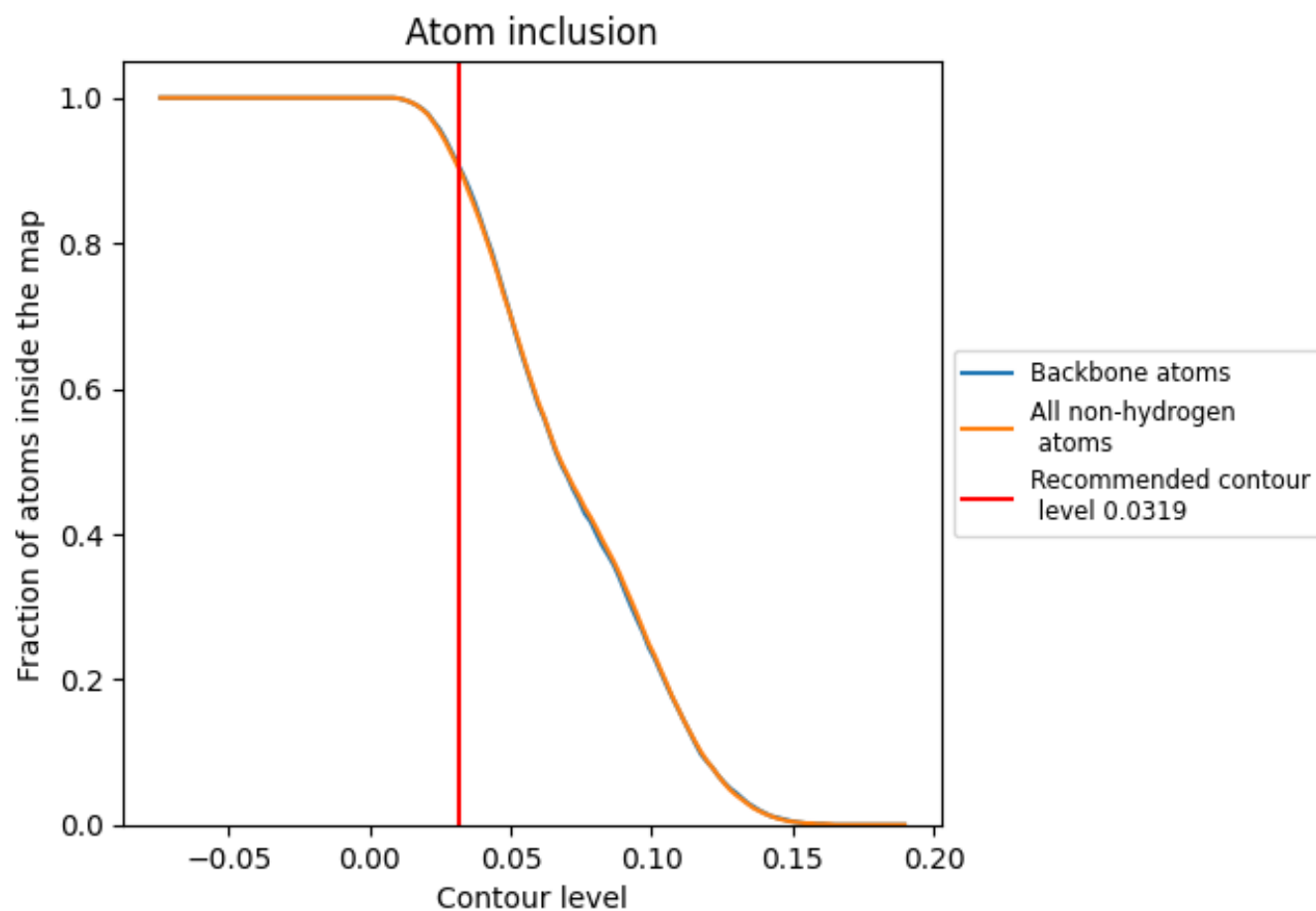
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0319).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 90% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0319) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.9020</div>	<div><div></div>0.5150</div>
A	<div><div></div>0.9130</div>	<div><div></div>0.5160</div>
B	<div><div></div>0.9110</div>	<div><div></div>0.5170</div>
C	<div><div></div>0.9200</div>	<div><div></div>0.5190</div>
D	<div><div></div>0.9060</div>	<div><div></div>0.5140</div>
E	<div><div></div>0.9090</div>	<div><div></div>0.5190</div>
F	<div><div></div>0.9060</div>	<div><div></div>0.5190</div>
G	<div><div></div>0.7250</div>	<div><div></div>0.4750</div>
H	<div><div></div>0.9000</div>	<div><div></div>0.5010</div>
I	<div><div></div>0.8510</div>	<div><div></div>0.4770</div>

1.0

0.0

<0.0