



# wwPDB EM Validation Summary Report ⓘ

Oct 6, 2025 – 10:24 AM EDT

PDB ID : 9MPV / pdb\_00009mpv  
EMDB ID : EMD-48506  
Title : Cryo-EM structure of three VCPIP1 VCPIDs bound to VCP  
Authors : Shah, B.; Hunkeler, M.; Buhrlage, S.J.; Fischer, E.F.  
Deposited on : 2024-12-31  
Resolution : 3.10 Å (reported)  
Based on initial model : 5FTK

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

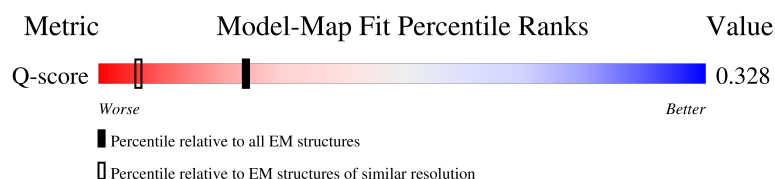
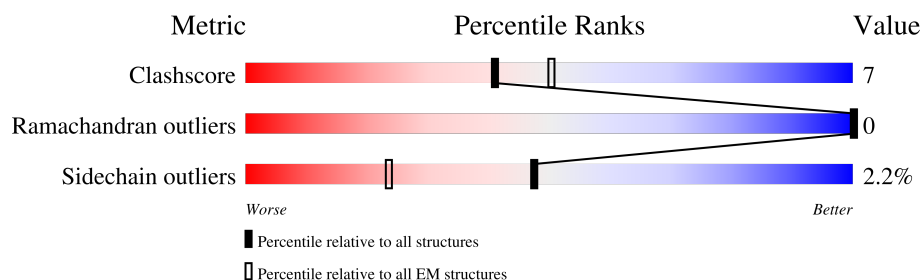
EMDB validation analysis : 0.0.1.dev129  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : 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 3.10 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	14724 ( 2.60 - 3.60 )

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	6% . 92%
1	H	1250	. . 95%
1	I	1250	5% . 92%
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>59%9%32%</div></div>
2	C	832	<div><div><div></div><div></div><div></div></div><div>56%11%33%</div></div>
2	D	832	<div><div><div></div><div></div><div></div></div><div>56%11%32%</div></div>
2	E	832	<div><div><div></div><div></div><div></div></div><div>58%10%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 56770 atoms, of which 28287 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	94	Total	C	H	N	O	S	0	0
			1484	487	723	130	141	3		
1	H	66	Total	C	H	N	O	S	0	0
			1054	351	514	88	100	1		
1	I	98	Total	C	H	N	O	S	0	0
			1525	503	736	134	149	3		

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	565	Total	C	H	N	O	S	0	0
			8808	2770	4400	785	831	22		
2	B	564	Total	C	H	N	O	S	0	0
			8782	2766	4382	783	829	22		
2	C	559	Total	C	H	N	O	S	0	0
			8699	2741	4338	778	821	21		
2	D	563	Total	C	H	N	O	S	0	0
			8779	2762	4387	781	827	22		
2	E	566	Total	C	H	N	O	S	0	0
			8813	2776	4397	786	832	22		
2	F	566	Total	C	H	N	O	S	0	0
			8826	2776	4410	786	832	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

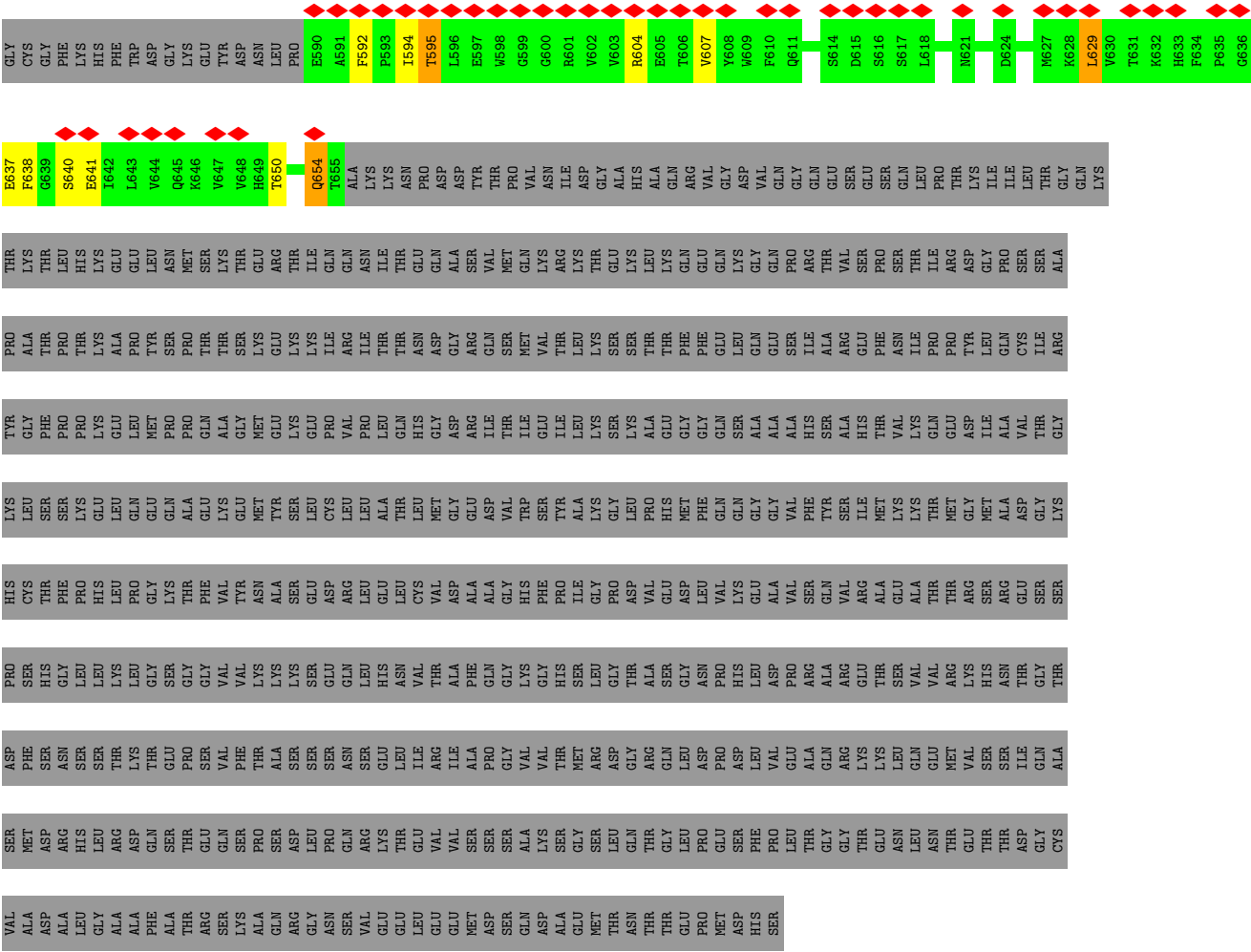


SER	GLN	ASN	ARG	LEU	VAL	ARG
VAL	ARG	SER	GLU	LEU	PRO	IIE
GLU	LYS	SER	HIS	LEU	LEU	THR
LEU	THR	ILE	ASN	THR	GLN	THR
GLU	GLU	ILE	CYS	LEU	HIS	ASP
GLU	VAL	ARG	VAL	MET	GLY	GLY
GLU	VAL	ILE	ASP	GLY	ASP	GLY
MET	SER	ALA	PHE	GLU	ARG	GLY
ASP	SER	PRO	GLN	ALA	ASP	ARG
SER	SER	GLY	GLY	ASP	IIE	GLN
GLN	ALA	VAL	HIS	TRP	ILE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

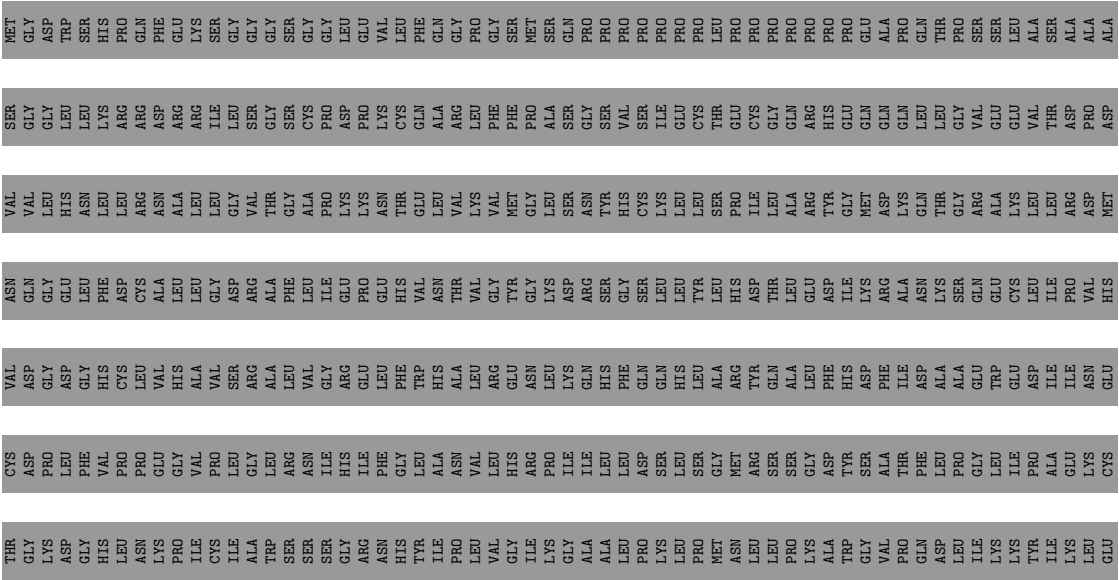
- Molecule 1: Deubiquitinating protein VCIPI1

Chain H:  95%

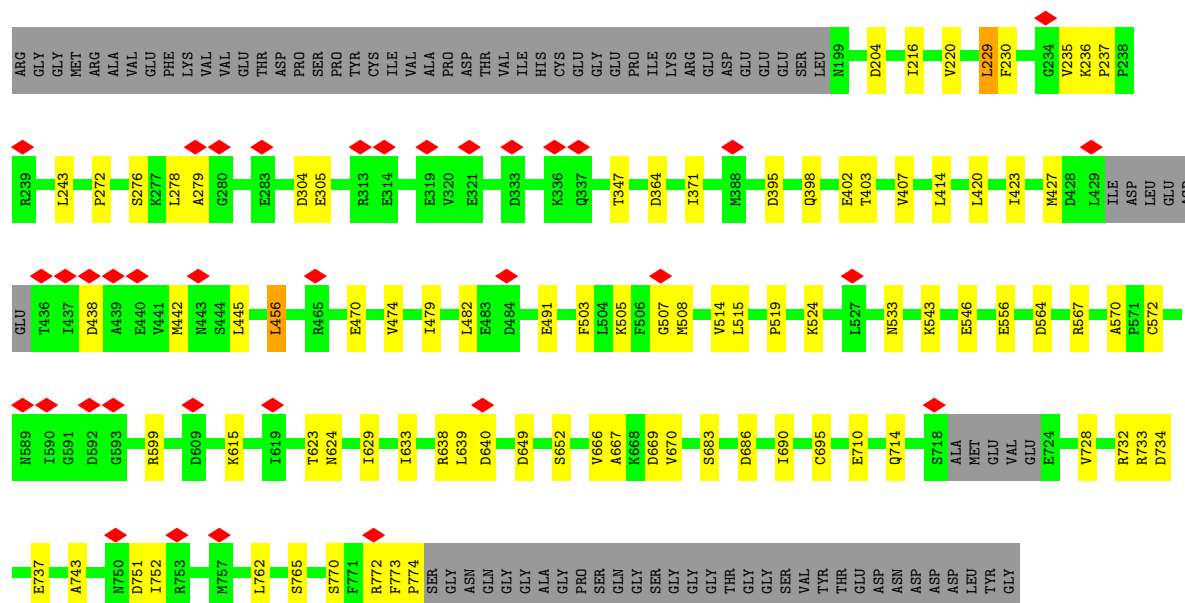
[illegible]



● Molecule 1: Deubiquitinating protein VCIPI1

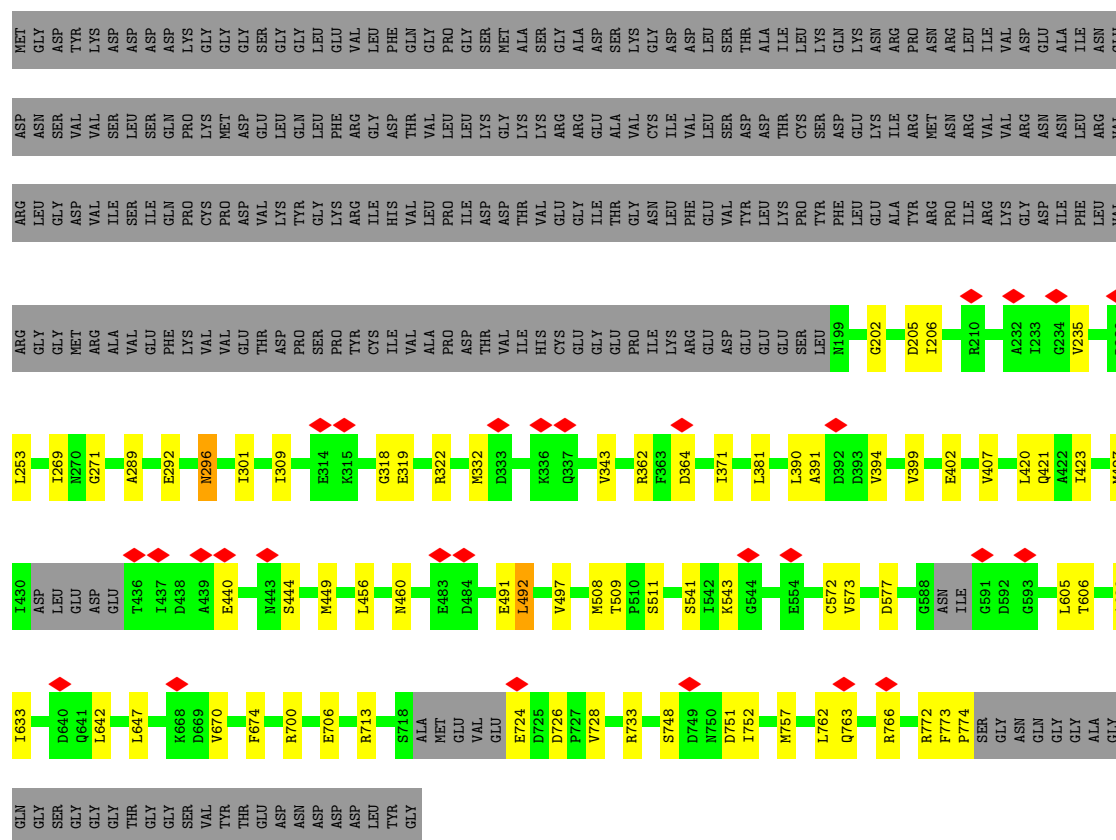






• Molecule 2: Transitional endoplasmic reticulum ATPase

Chain B:



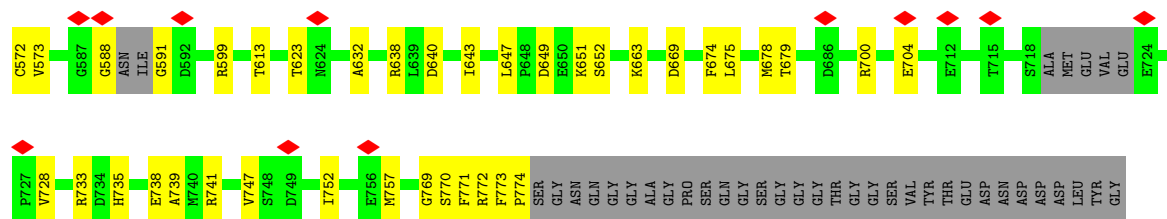
• Molecule 2: Transitional endoplasmic reticulum ATPase

Chain C:



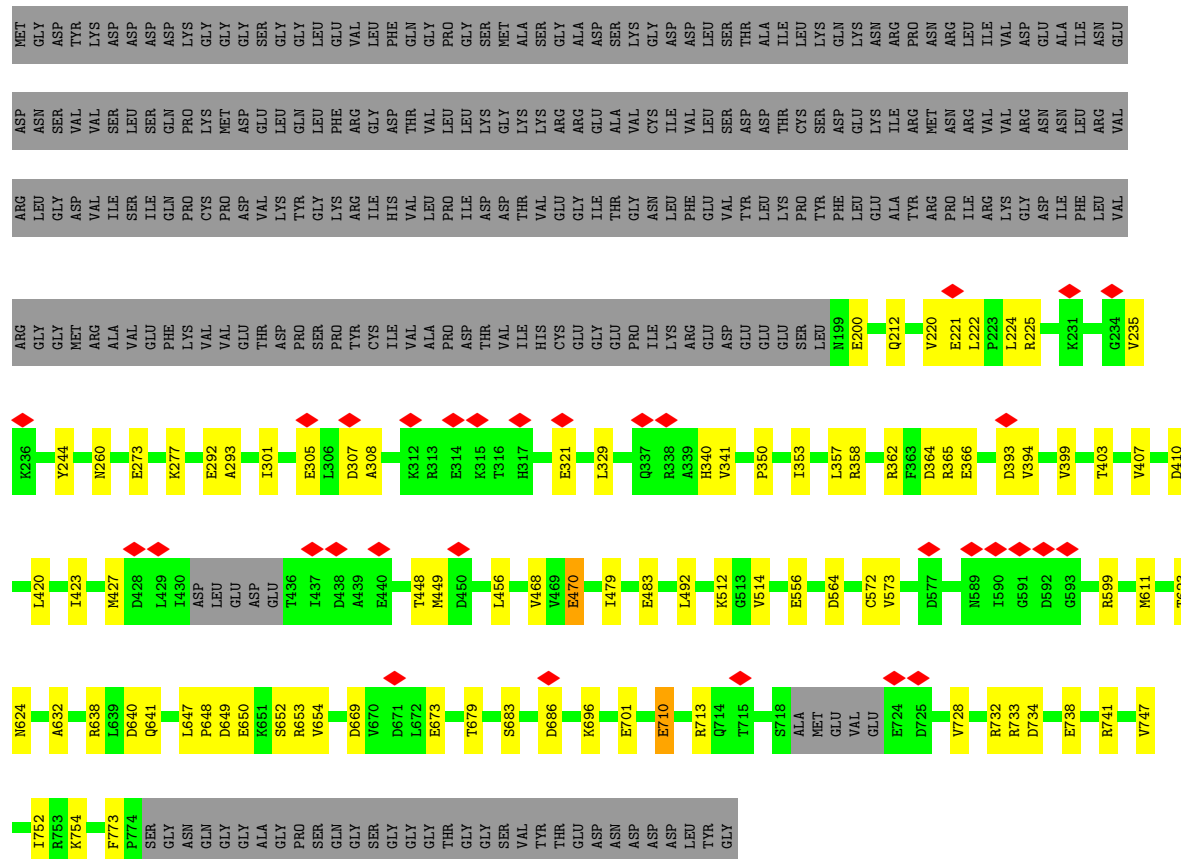






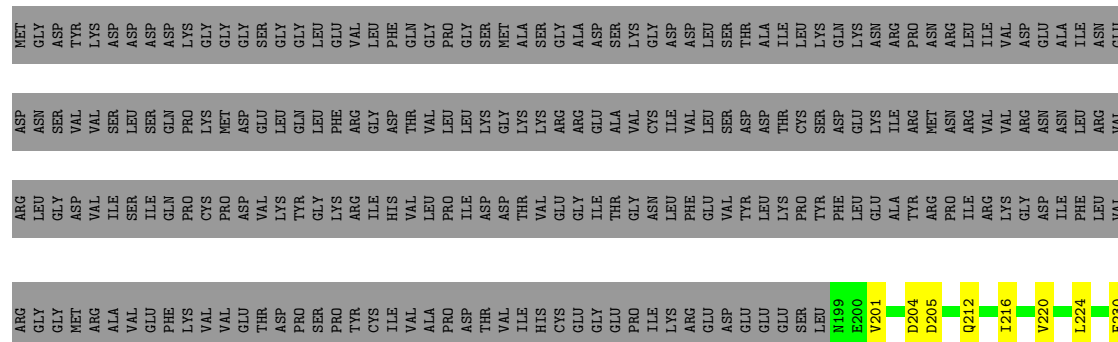
• Molecule 2: Transitional endoplasmic reticulum ATPase

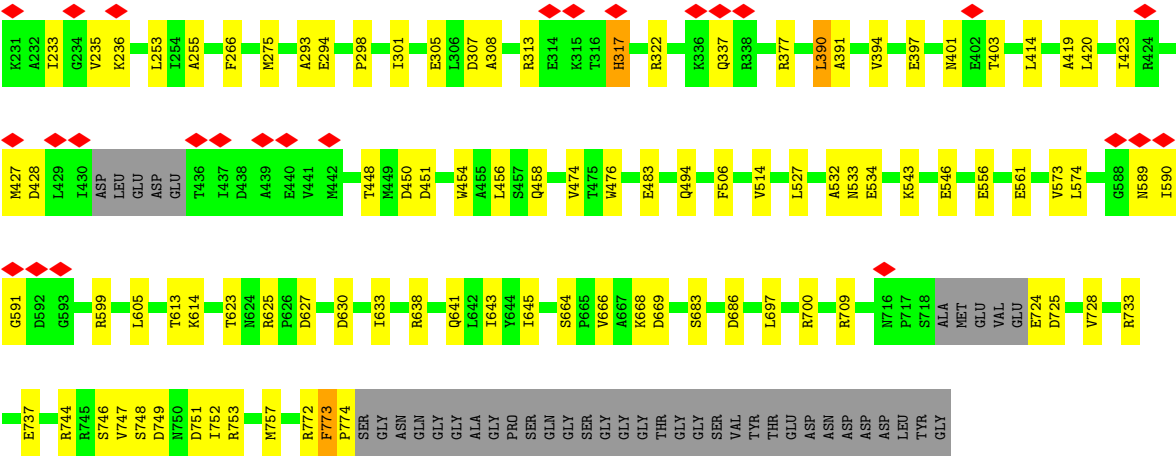
Chain E:



• Molecule 2: Transitional endoplasmic reticulum ATPase

Chain F:





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	77321	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 ( $e^-/\text{\AA}^2$ )	49.22	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	165000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.637	Depositor
Minimum map value	-0.309	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.0906	Depositor
Map size ( $\text{\AA}$ )	352.0, 352.0, 352.0	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.1, 1.1, 1.1	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	0.09	0/783	0.26	0/1060
1	H	0.08	0/555	0.23	0/755
1	I	0.10	0/811	0.25	0/1098
2	A	0.12	0/4482	0.24	0/6045
2	B	0.11	0/4473	0.24	0/6031
2	C	0.11	0/4434	0.28	2/5978 (0.0%)
2	D	0.12	0/4465	0.25	0/6020
2	E	0.11	0/4490	0.23	0/6056
2	F	0.11	0/4490	0.22	0/6056
All	All	0.11	0/28983	0.24	2/39099 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	C	739	ALA	CA-C-N	7.17	132.07	120.60
2	C	739	ALA	C-N-CA	7.17	132.07	120.60

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	761	723	722	14	0
1	H	540	514	522	9	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	789	736	744	22	0
2	A	4408	4400	4442	62	0
2	B	4400	4382	4435	56	0
2	C	4361	4338	4393	71	0
2	D	4392	4387	4429	72	0
2	E	4416	4397	4453	61	0
2	F	4416	4410	4453	74	0
All	All	28483	28287	28593	384	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.

The worst 5 of 384 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:A:414:LEU:HD11	2:A:456:LEU:HD22	1.55	0.89
2:C:235:VAL:HG11	2:D:420:LEU:HD23	1.59	0.84
1:H:638:PHE:HA	2:C:754:LYS:HE3	1.59	0.83
2:F:666:VAL:O	2:F:668:LYS:NZ	2.12	0.82
2:A:564:ASP:OD1	2:A:567:ARG:NH2	2.13	0.81

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	92/1250 (7%)	91 (99%)	1 (1%)	0	100	100
1	H	64/1250 (5%)	63 (98%)	1 (2%)	0	100	100
1	I	96/1250 (8%)	95 (99%)	1 (1%)	0	100	100
2	A	559/832 (67%)	539 (96%)	20 (4%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	556/832 (67%)	532 (96%)	24 (4%)	0	100	100
2	C	551/832 (66%)	536 (97%)	15 (3%)	0	100	100
2	D	555/832 (67%)	537 (97%)	18 (3%)	0	100	100
2	E	560/832 (67%)	539 (96%)	21 (4%)	0	100	100
2	F	560/832 (67%)	546 (98%)	14 (2%)	0	100	100
All	All	3593/8742 (41%)	3478 (97%)	115 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	83/1065 (8%)	80 (96%)	3 (4%)	30	60
1	H	60/1065 (6%)	56 (93%)	4 (7%)	13	40
1	I	86/1065 (8%)	84 (98%)	2 (2%)	45	70
2	A	470/696 (68%)	457 (97%)	13 (3%)	38	66
2	B	469/696 (67%)	462 (98%)	7 (2%)	60	80
2	C	464/696 (67%)	450 (97%)	14 (3%)	36	64
2	D	468/696 (67%)	458 (98%)	10 (2%)	48	72
2	E	471/696 (68%)	464 (98%)	7 (2%)	60	80
2	F	471/696 (68%)	464 (98%)	7 (2%)	60	80
All	All	3042/7371 (41%)	2975 (98%)	67 (2%)	47	71

5 of 67 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	623	THR
2	E	710	GLU
2	F	747	VAL
2	B	421	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	390	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	340	HIS
2	E	317	HIS
2	D	443	ASN
2	E	602	ASN
2	A	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 [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

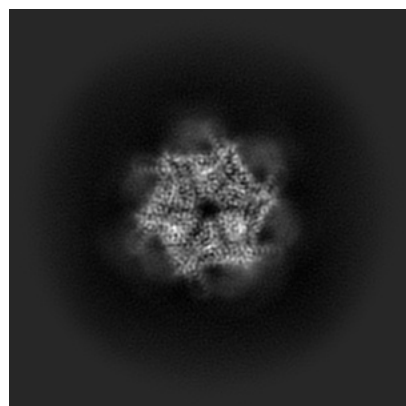
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-48506. These allow visual inspection of the internal detail of the map and identification of artifacts.

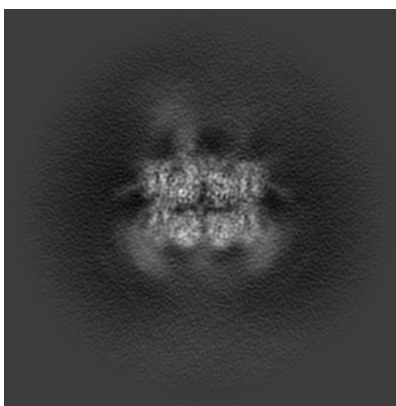
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

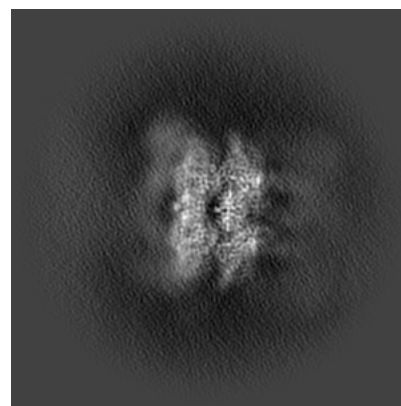
#### 6.1.1 Primary map



X

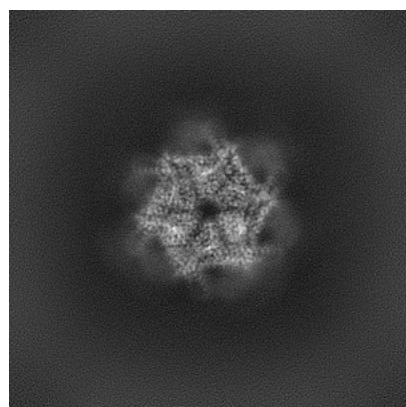


Y

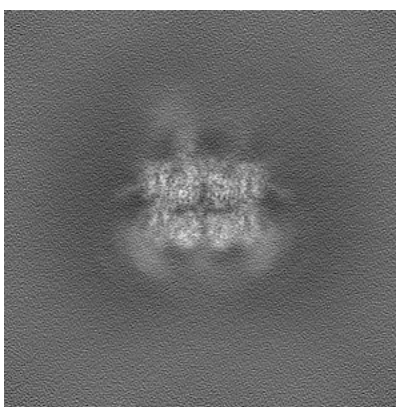


Z

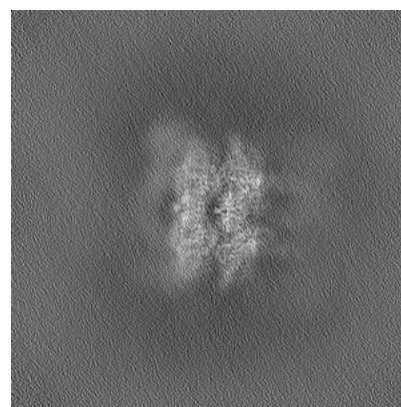
#### 6.1.2 Raw map



X



Y



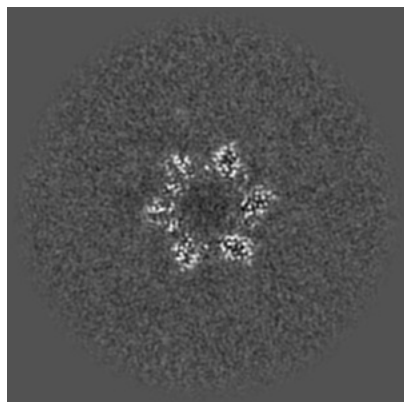
Z

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

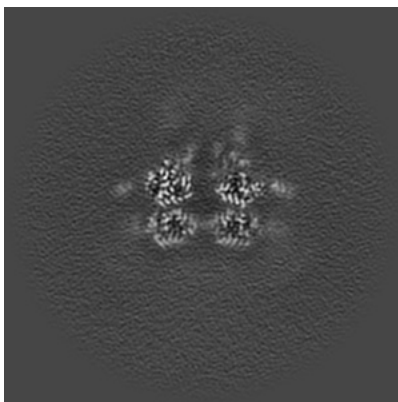


## 6.2 Central slices [i](#)

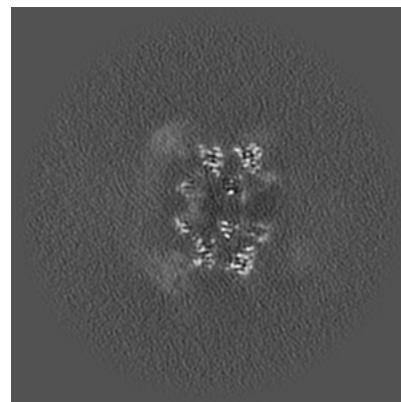
### 6.2.1 Primary map



X Index: 160

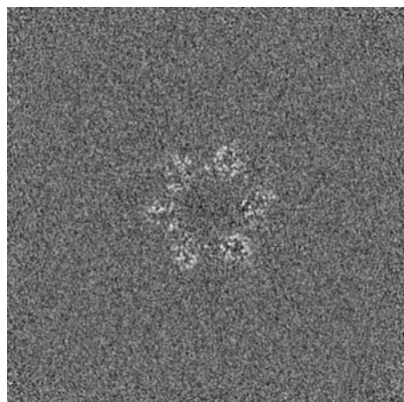


Y Index: 160

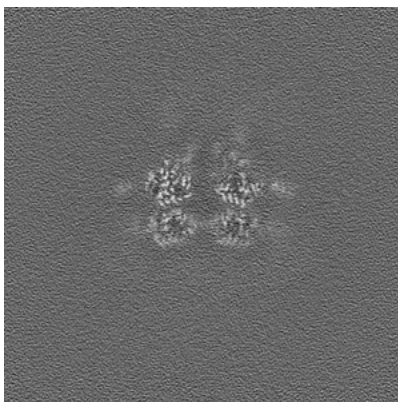


Z Index: 160

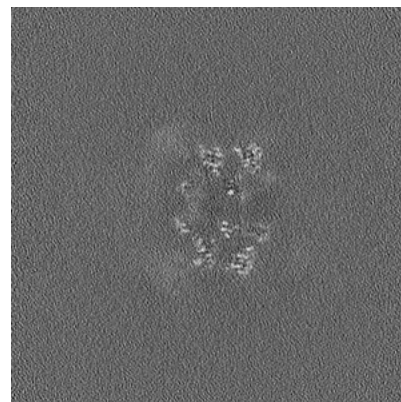
### 6.2.2 Raw map



X Index: 160



Y Index: 160

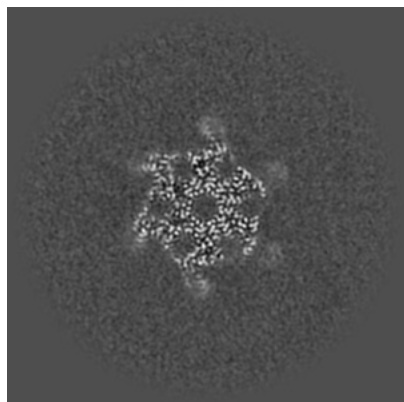


Z Index: 160

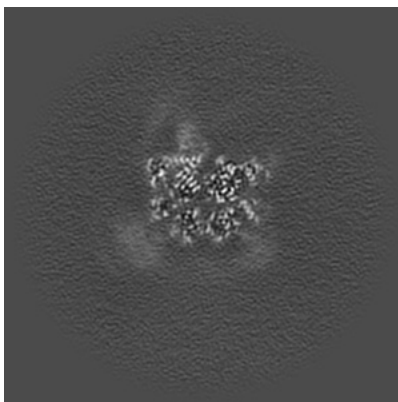
The images above show central slices of the map in three orthogonal directions.

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

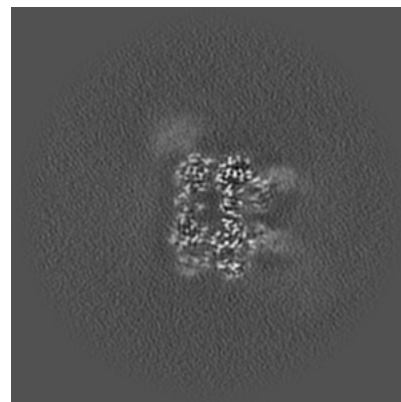
### 6.3.1 Primary map



X Index: 174

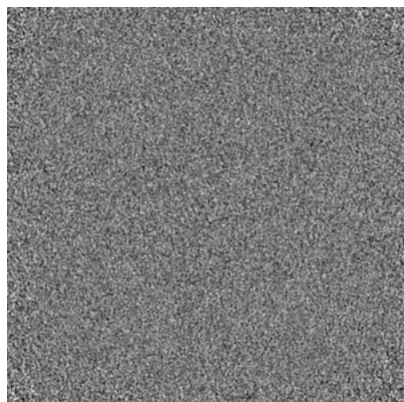


Y Index: 183

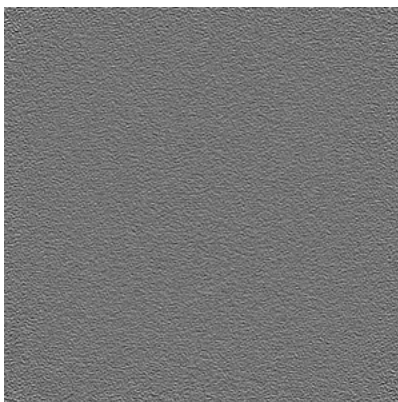


Z Index: 145

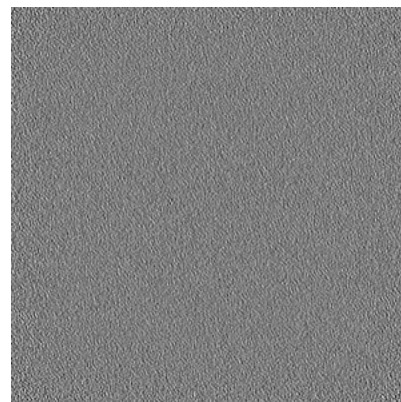
### 6.3.2 Raw map



X Index: 0



Y Index: 0

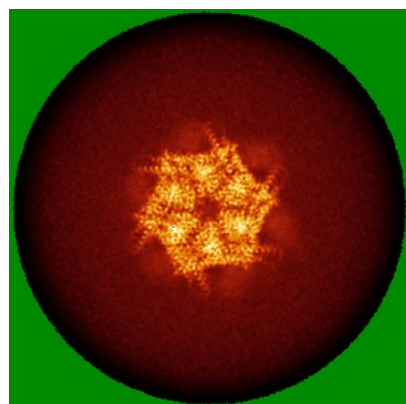


Z Index: 0

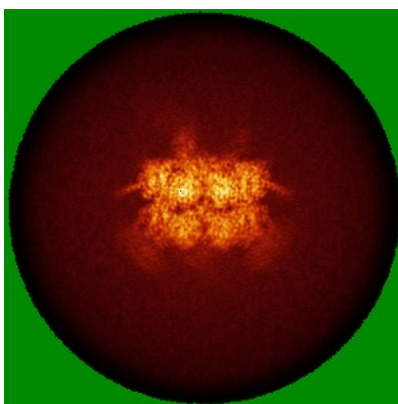
The images above show the largest variance slices of the map in three orthogonal directions.

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

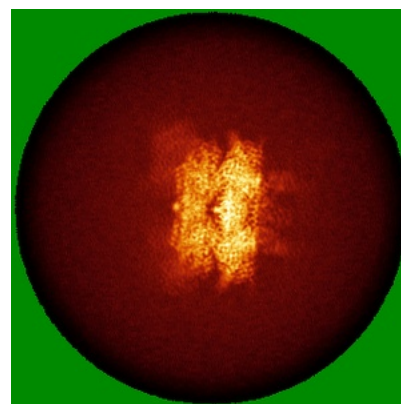
### 6.4.1 Primary map



X

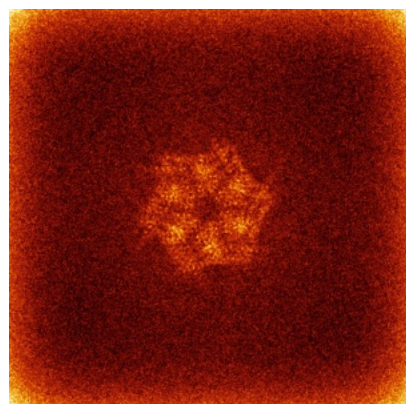


Y

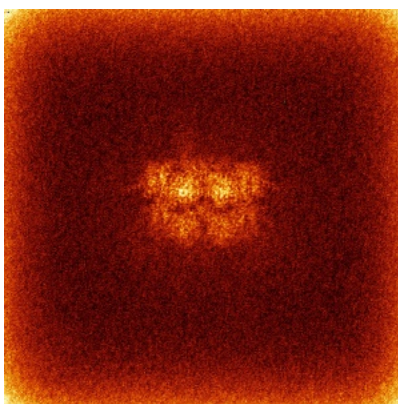


Z

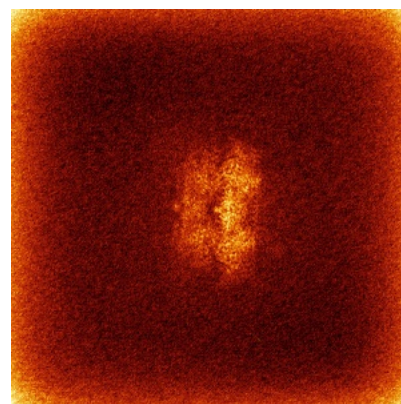
### 6.4.2 Raw map



X



Y



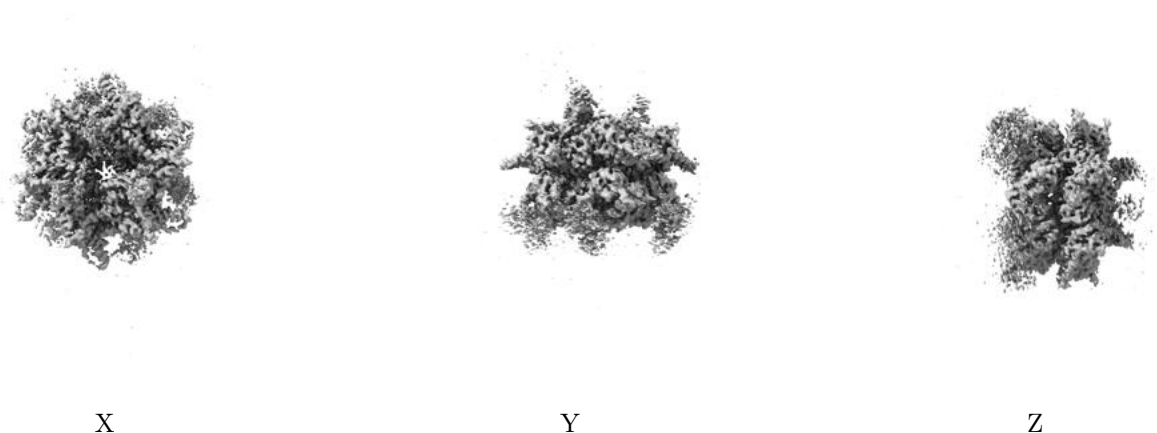
Z

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.



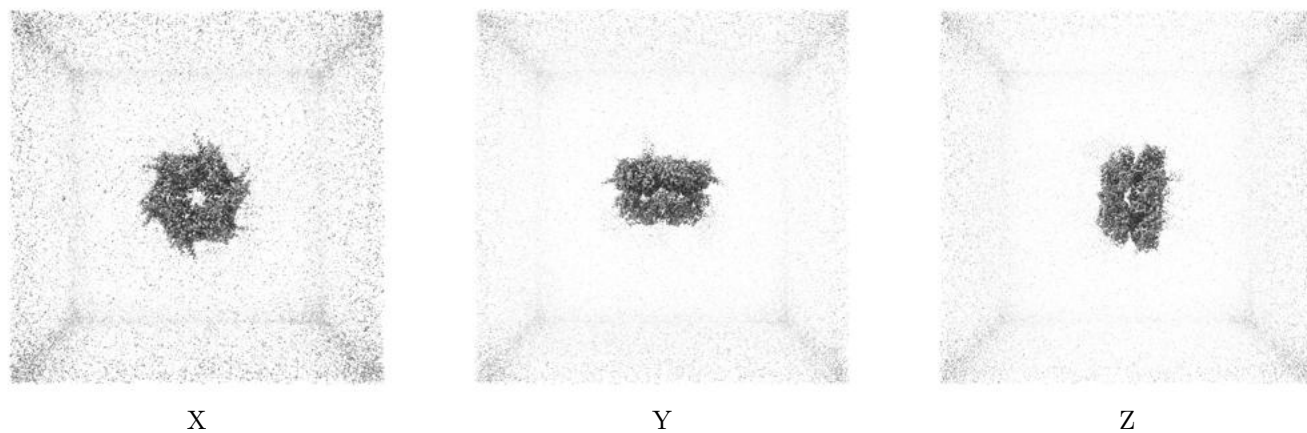
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0906. 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.

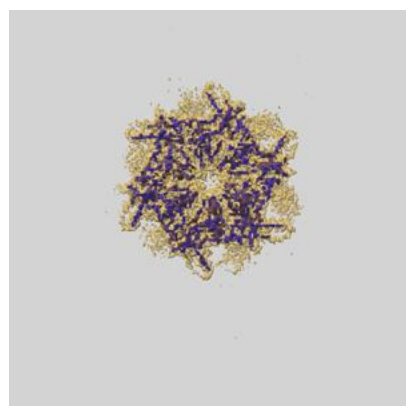
## 6.6 Mask visualisation [i](#)

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

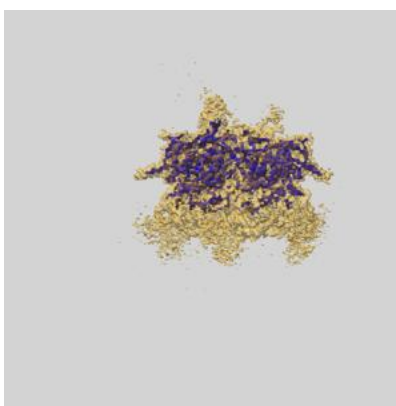
A mask typically either:

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

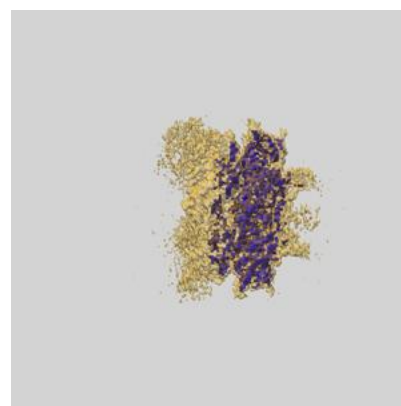
### 6.6.1 emd\_48506\_msk\_2.map [i](#)



X

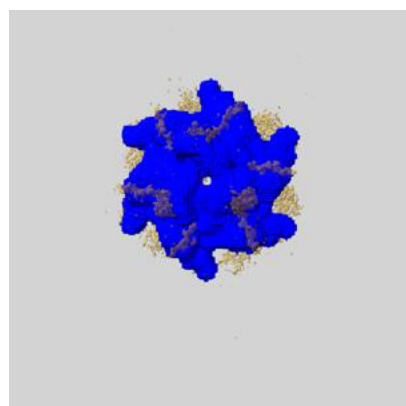


Y

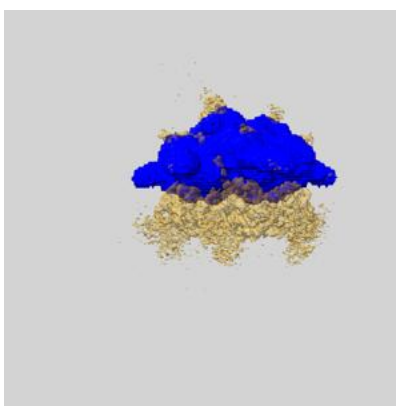


Z

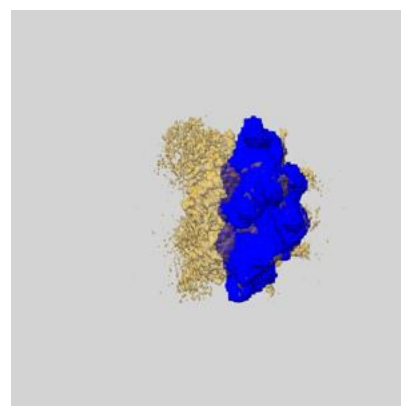
### 6.6.2 emd\_48506\_msk\_1.map [i](#)



X



Y

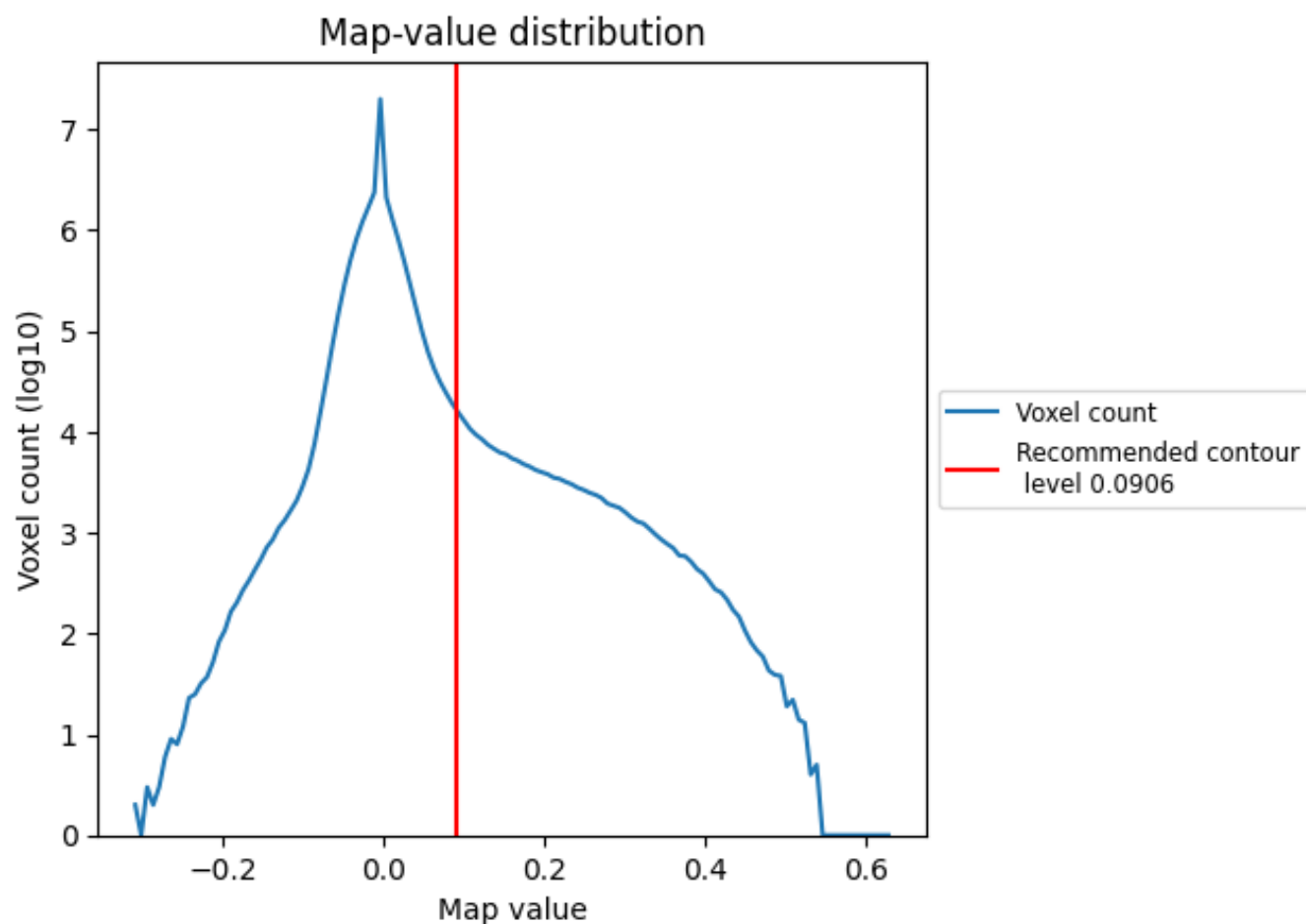


Z

## 7 Map analysis [i](#)

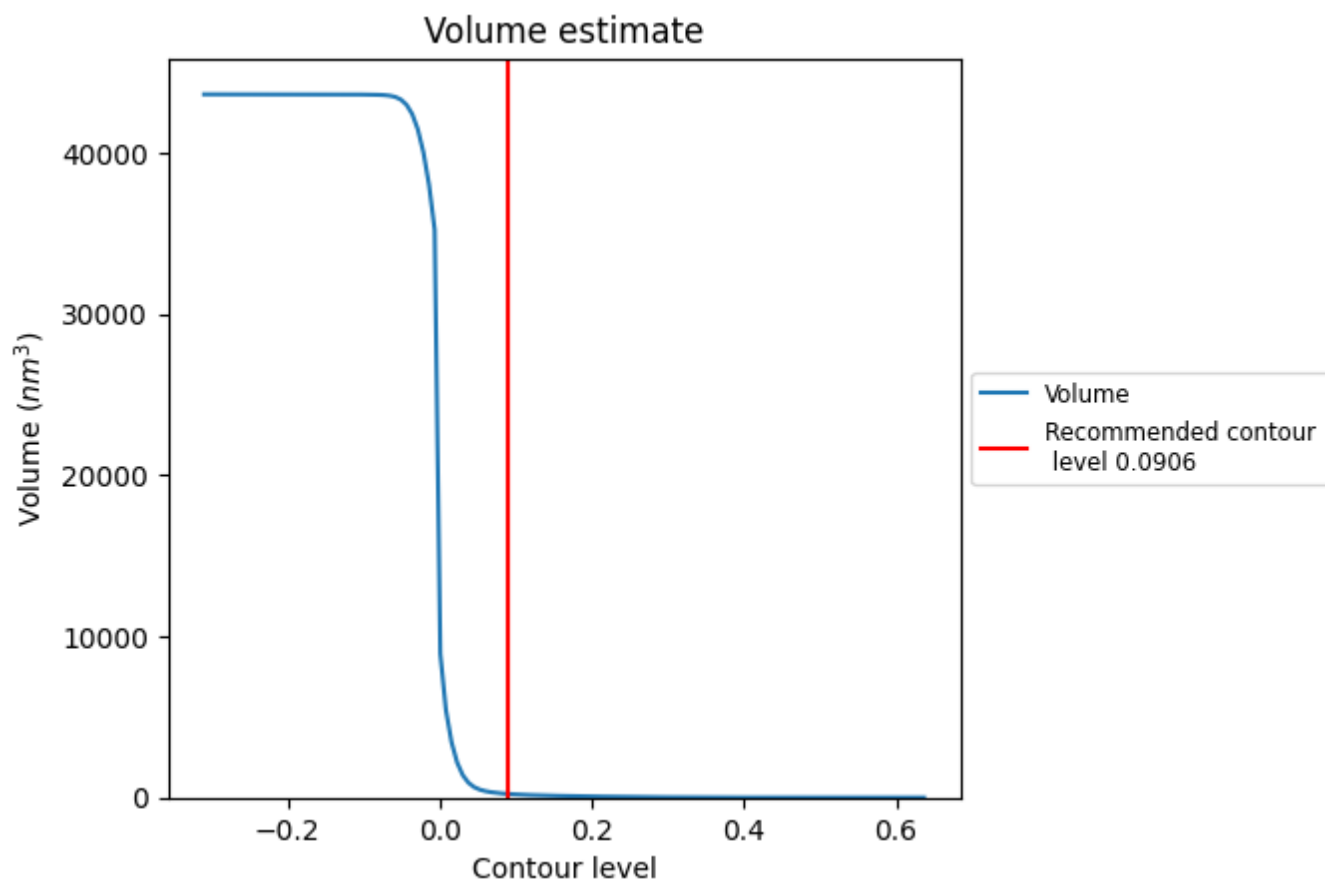
This section contains the results of statistical analysis of the map.

### 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.

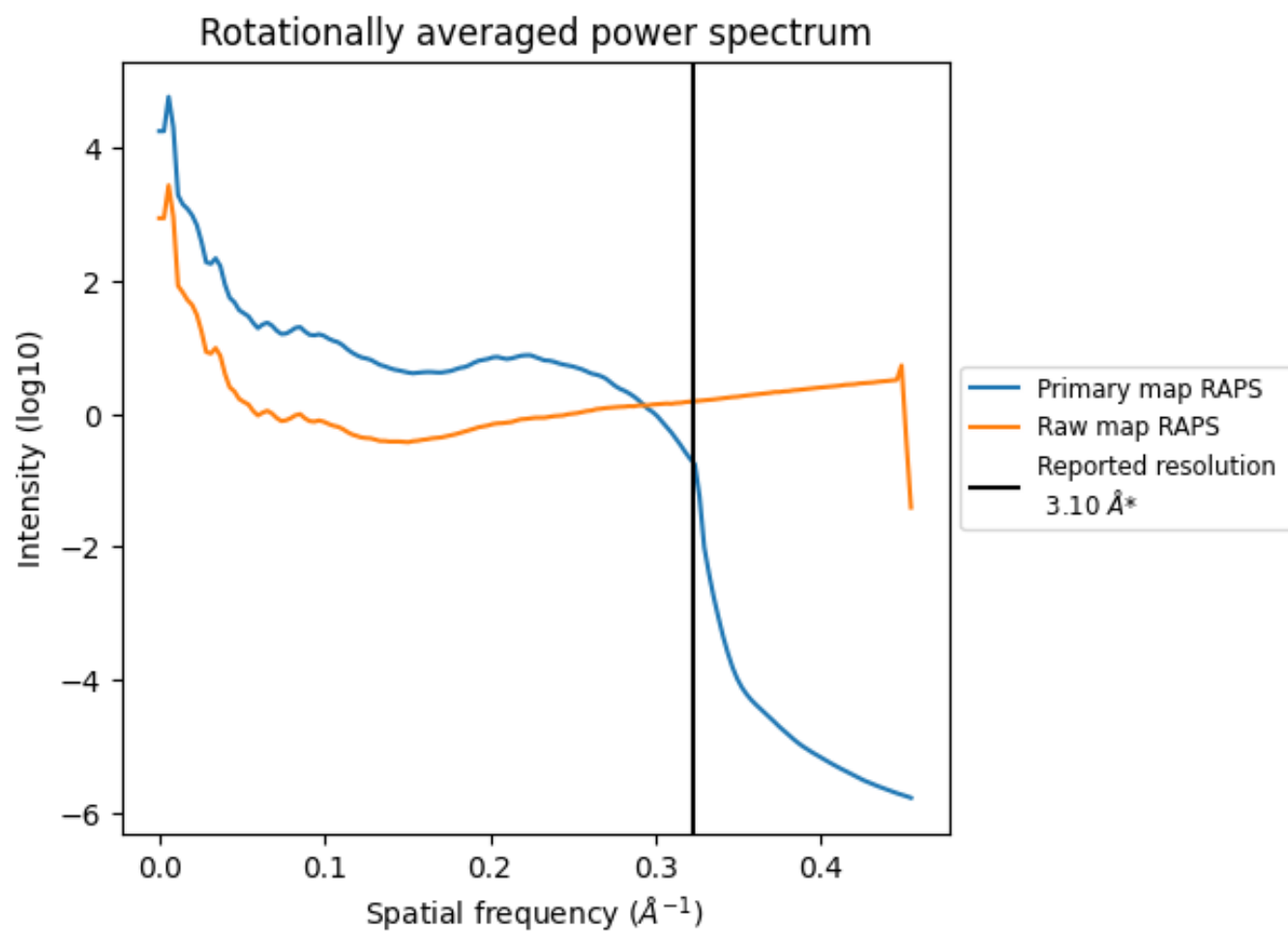
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 222 nm<sup>3</sup>; this corresponds to an approximate mass of 201 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 [i](#)



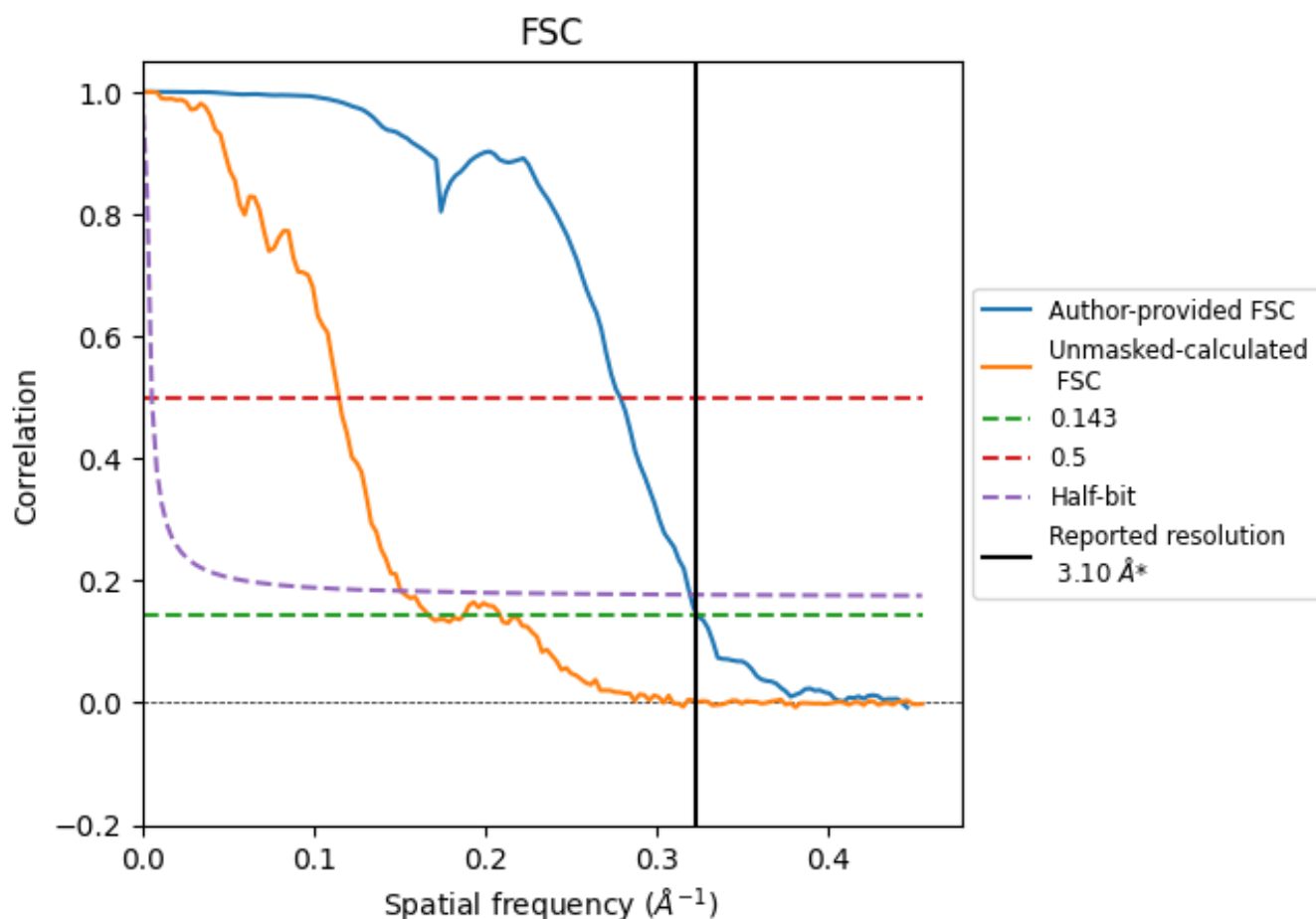
\*Reported resolution corresponds to spatial frequency of 0.323  $\text{\AA}^{-1}$



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

## 8.2 Resolution estimates [i](#)

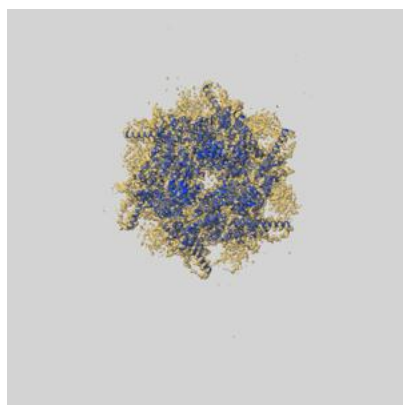
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.09	3.59	3.13
Unmasked-calculated*	5.99	8.73	6.64

\*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 5.99 differs from the reported value 3.1 by more than 10 %

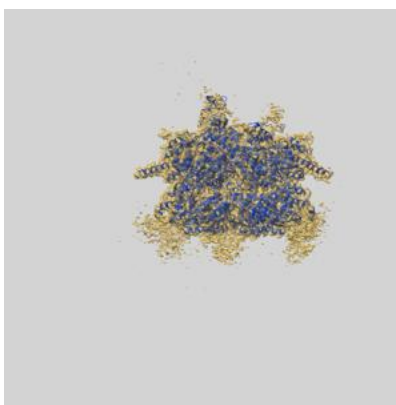
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-48506 and PDB model 9MPV. Per-residue inclusion information can be found in section [3](#) on page [11](#).

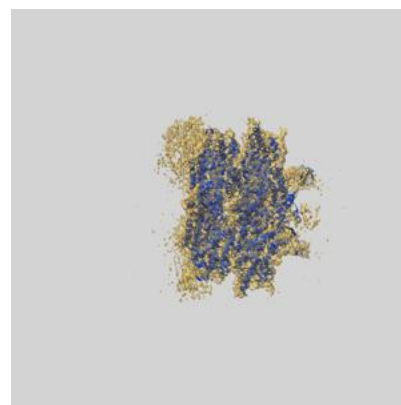
### 9.1 Map-model overlay [i](#)



X



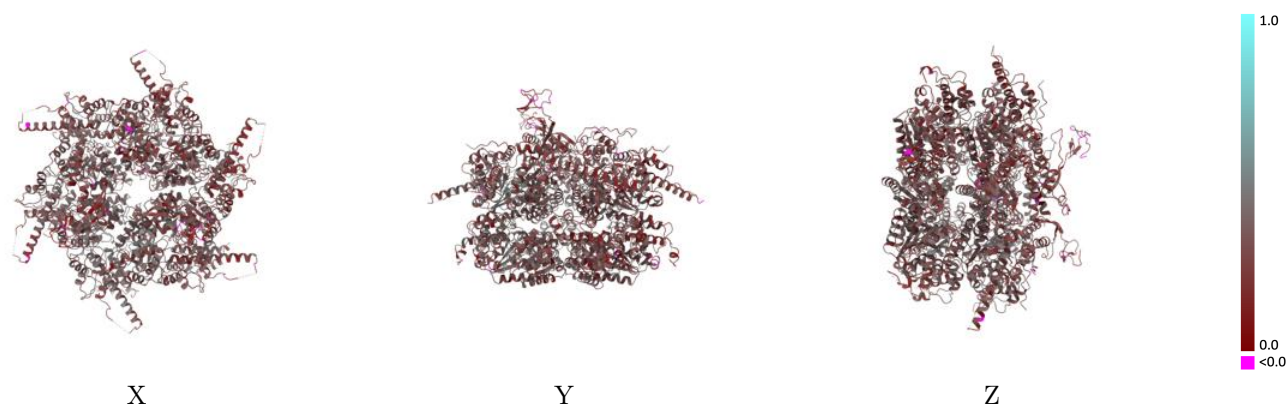
Y



Z

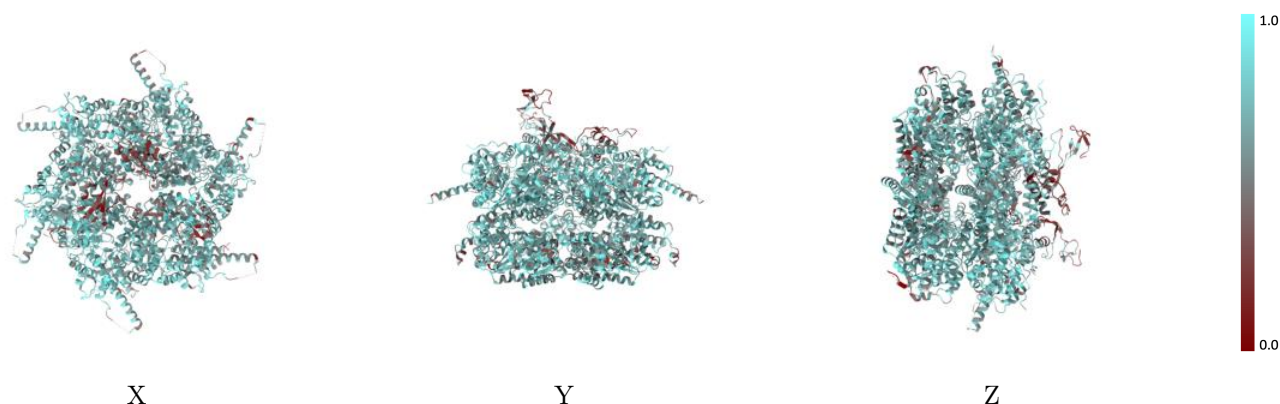
The images above show the 3D surface view of the map at the recommended contour level 0.0906 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



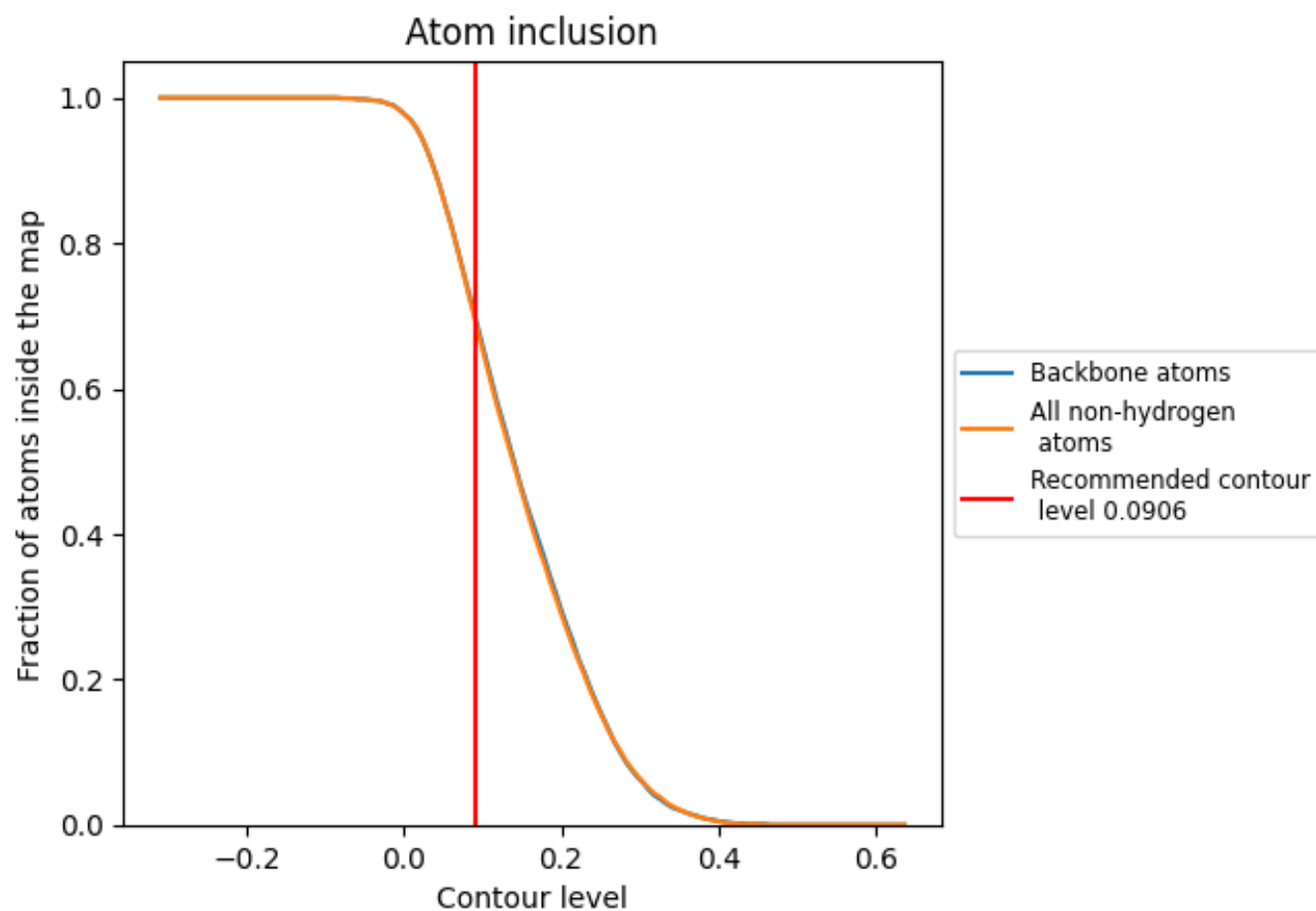
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0906).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 69% 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 (0.0906) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6940	<div></div> 0.3280
A	<div></div> 0.7240	<div></div> 0.3410
B	<div></div> 0.7140	<div></div> 0.3140
C	<div></div> 0.6960	<div></div> 0.3050
D	<div></div> 0.7180	<div></div> 0.3220
E	<div></div> 0.7320	<div></div> 0.3540
F	<div></div> 0.7590	<div></div> 0.3660
G	<div></div> 0.4850	<div></div> 0.2530
H	<div></div> 0.3320	<div></div> 0.2600
I	<div></div> 0.5440	<div></div> 0.2410

1.0

0.0

<0.0