



## wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 02:48 PM UTC

PDB ID : 9GOQ / pdb\_00009goq  
EMDB ID : EMD-51498  
Title : Structure of the S.aureus MecA protein, in complex with ClpC  
Authors : Carroni, M.; Azinas, S.  
Deposited on : 2024-09-06  
Resolution : 3.50 Å(reported)

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

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

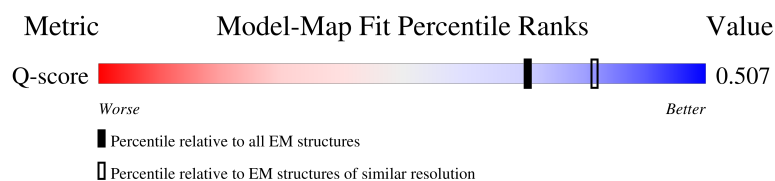
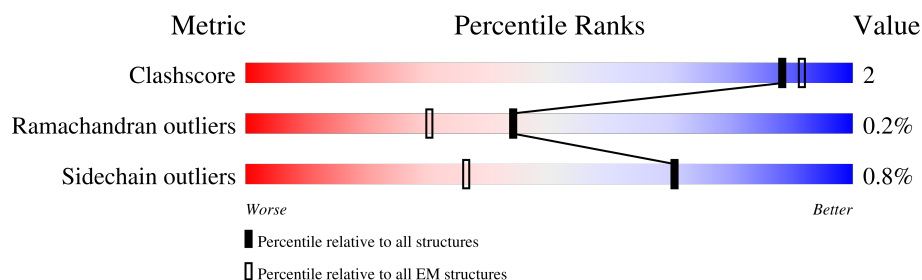
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13950 ( 3.00 - 4.00 )

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	239	
1	B	239	
1	C	239	
1	D	239	

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Mol	Chain	Length	Quality of chain
1	E	239	 41%59%
1	F	239	 41%59%
2	a	818	 14%84%
2	b	818	 14%84%
2	c	818	 15%84%
2	d	818	 15%84%
2	e	818	 15%84%
2	f	818	 15%84%
2	g	818	 6%94%
2	h	818	 6%94%
2	i	818	 6%94%
2	l	818	 6%94%
2	m	818	 6%94%
2	n	818	 6%94%

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13878 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Adapter protein MecA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	98	Total	C	N	O	S	0	0
			827	533	127	165	2		
1	B	98	Total	C	N	O	S	0	0
			827	533	127	165	2		
1	C	98	Total	C	N	O	S	0	0
			827	533	127	165	2		
1	D	98	Total	C	N	O	S	0	0
			827	533	127	165	2		
1	E	98	Total	C	N	O	S	0	0
			827	533	127	165	2		
1	F	98	Total	C	N	O	S	0	0
			827	533	127	165	2		

- Molecule 2 is a protein called ATP-dependent Clp protease ATP-binding subunit ClpC.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	a	133	Total	C	N	O	S	0	0
			1043	657	191	192	3		
2	b	133	Total	C	N	O	S	0	0
			1043	657	191	192	3		
2	c	133	Total	C	N	O	S	0	0
			1043	657	191	192	3		
2	d	133	Total	C	N	O	S	0	0
			1043	657	191	192	3		
2	e	133	Total	C	N	O	S	0	0
			1043	657	191	192	3		
2	f	133	Total	C	N	O	S	0	0
			1043	657	191	192	3		
2	g	53	Total	C	N	O		0	0
			443	272	79	92			
2	h	53	Total	C	N	O		0	0
			443	272	79	92			
2	i	53	Total	C	N	O		0	0
			443	272	79	92			

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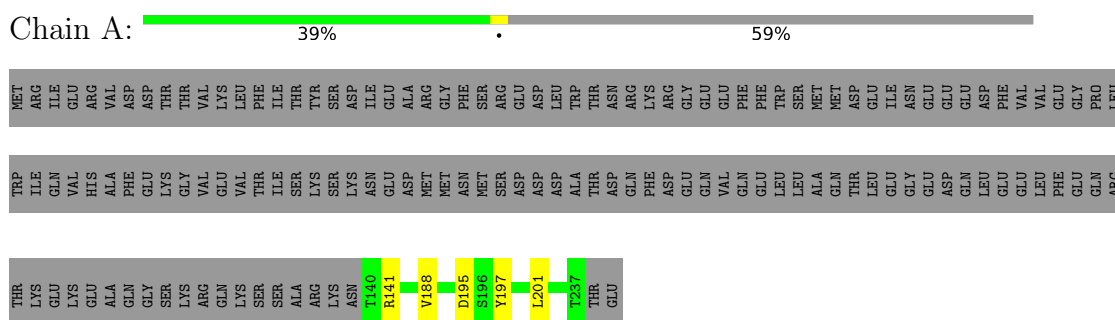
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Mol	Chain	Residues	Atoms				AltConf	Trace
2	l	53	Total	C	N	O	0	0
			443	272	79	92		
2	m	53	Total	C	N	O	0	0
			443	272	79	92		
2	n	53	Total	C	N	O	0	0
			443	272	79	92		

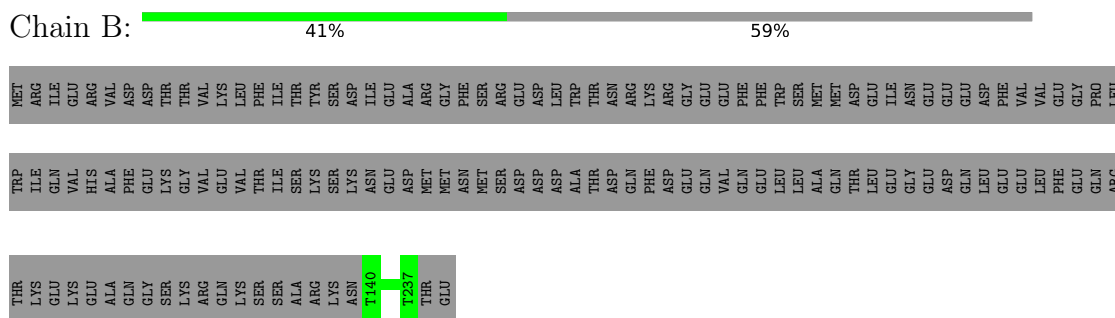
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

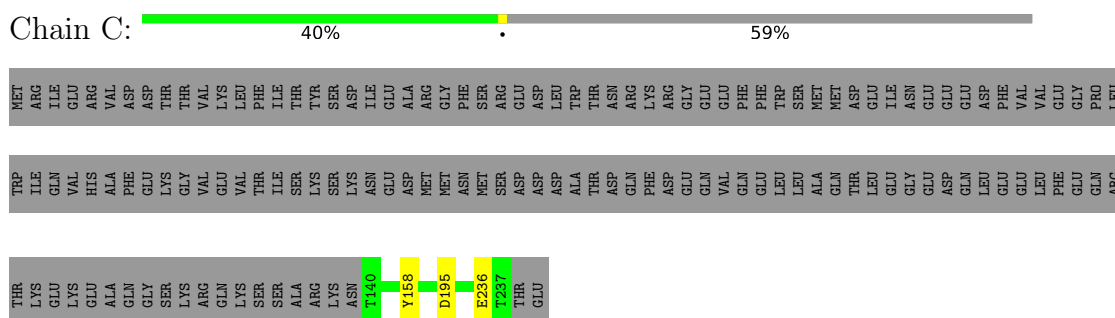
#### • Molecule 1: Adapter protein MecA



#### • Molecule 1: Adapter protein MecA



#### • Molecule 1: Adapter protein MecA



#### • Molecule 1: Adapter protein MecA

[illegible][illegible][illegible][illegible]

[illegible]

- Molecule 2: ATP-dependent Clp protease ATP-binding subunit ClpC

Chain b:  14% • 84%

[illegible]





- Molecule 2: ATP-dependent Clp protease ATP-binding subunit ClpC

Chain e:  15% 84%



PHE	HIS	LYS	LEU	THR	LYS	GLU	GLU	LEU	LYS	LEU	GLU	ILE	VAL	THR	ASN	ASN	LEU	THR	ARG	LEU	SER	GLN	ASN	ILE	ASN	ILE	VAL	THR	LYS	ASP	THR	LYS	LYS	ALA	GLU	GLU	GLY	THR	GLY	ARG	LEU	ALA	ALA	GLN	ILE	THR	GLN
LYS	THR	ILE	GLU	ASP	ASN	ASN	LEU	SER	GLU	GLU	ILE	ILE	ASP	GLY	ASN	GLN	GLY	LYS	LYS	VAL	THR	THR	THR	GLY	GLU	GLU	ILE	ILE	VAL	ASP	HIS	ASP	GLY	LYS	GLU	PHE	LYS	THR	THR	SER	GLY	THR	LYS	THR	ALA		

- Molecule 2: ATP-dependent Clp protease ATP-binding subunit ClpC

[illegible]

- Molecule 2: ATP-dependent Clp protease ATP-binding subunit ClpC

[illegible]

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

- Molecule 2: ATP-dependent Clp protease ATP-binding subunit ClpC

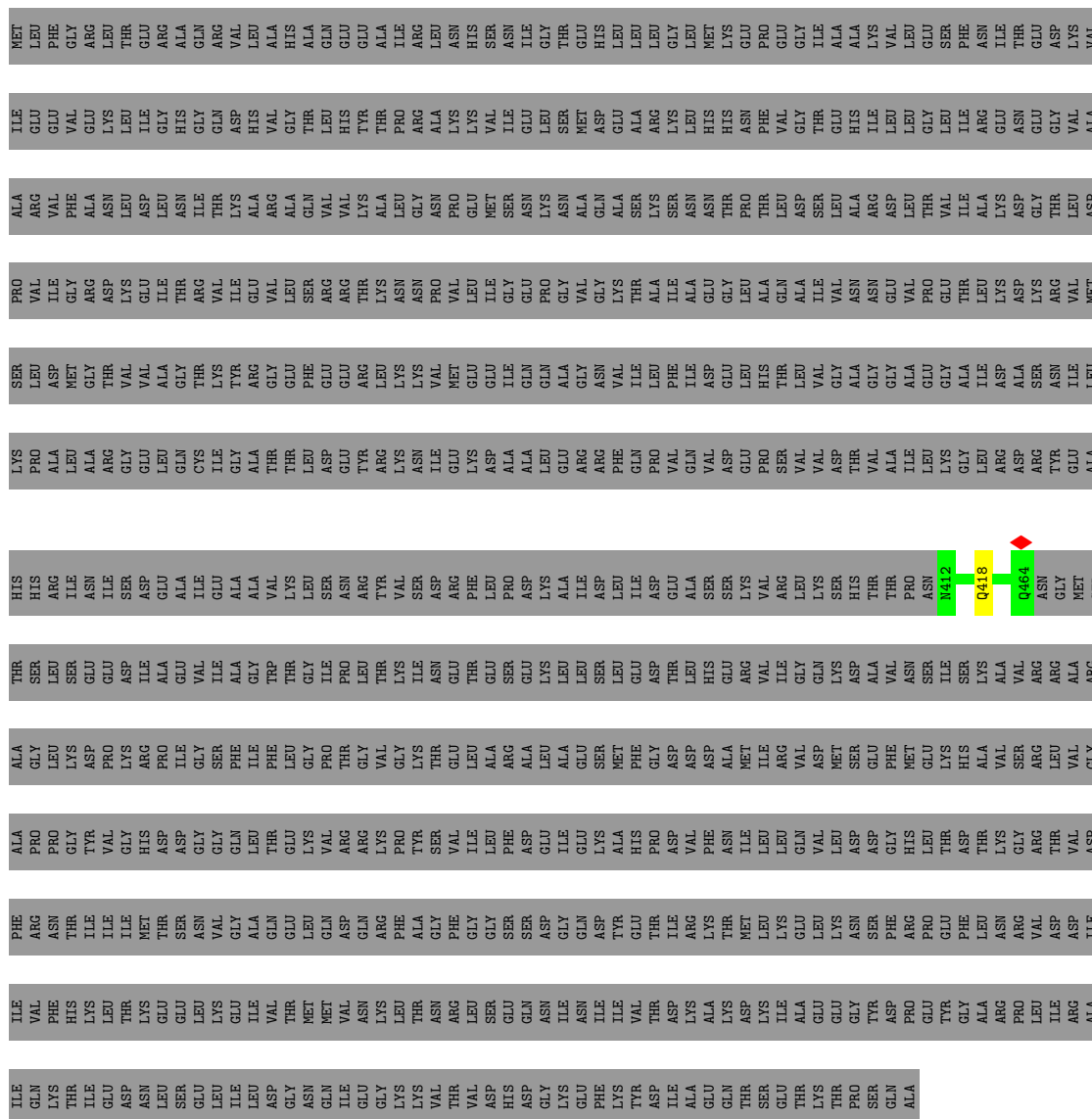
Chain h:  6% 94%

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



- Molecule 2: ATP-dependent Clp protease ATP-binding subunit ClpC

Chain i:  6% 94%



- Molecule 2: ATP-dependent Clp protease ATP-binding subunit ClpC

94%

- Molecule 2: ATP-dependent Clp protease ATP-binding subunit ClpC

94%



- Molecule 2: ATP-dependent Clp protease ATP-binding subunit ClpC

Chain n:  6% 94%

[illegible]

[illegible]



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	82800	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 ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	24000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	16.961	Depositor
Minimum map value	-0.582	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.442	Depositor
Recommended contour level	1.95	Depositor
Map size (Å)	321.936, 321.936, 321.936	wwPDB
Map dimensions	304, 304, 304	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.059, 1.059, 1.059	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.39	0/849	0.53	0/1160
1	B	0.39	0/849	0.51	0/1160
1	C	0.39	0/849	0.53	0/1160
1	D	0.39	0/849	0.54	0/1160
1	E	0.39	0/849	0.50	0/1160
1	F	0.39	0/849	0.53	0/1160
2	a	0.34	0/1055	0.54	0/1420
2	b	0.34	0/1055	0.54	0/1420
2	c	0.34	0/1055	0.54	0/1420
2	d	0.34	0/1055	0.52	0/1420
2	e	0.34	0/1055	0.51	0/1420
2	f	0.34	0/1055	0.51	0/1420
2	g	0.26	0/447	0.46	0/596
2	h	0.26	0/447	0.46	0/596
2	i	0.26	0/447	0.43	0/596
2	l	0.25	0/447	0.48	0/596
2	m	0.26	0/447	0.43	0/596
2	n	0.26	0/447	0.43	0/596
All	All	0.34	0/14106	0.51	0/19056

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	827	0	768	3	0
1	B	827	0	768	0	0
1	C	827	0	768	2	0
1	D	827	0	768	0	0
1	E	827	0	768	0	0
1	F	827	0	768	0	0
2	a	1043	0	1079	10	0
2	b	1043	0	1079	9	0
2	c	1043	0	1079	7	0
2	d	1043	0	1079	6	0
2	e	1043	0	1079	5	0
2	f	1043	0	1079	5	0
2	g	443	0	429	0	0
2	h	443	0	429	1	0
2	i	443	0	429	1	0
2	l	443	0	429	2	0
2	m	443	0	429	1	0
2	n	443	0	429	1	0
All	All	13878	0	13656	51	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 2.

The worst 5 of 51 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:d:9:ARG:NH1	2:d:101:ASN:O	2.33	0.61
2:a:16:HIS:CE1	2:a:40:LYS:HB3	2.38	0.58
2:d:106:GLU:OE1	2:d:106:GLU:N	2.32	0.57
1:C:195:ASP:OD1	2:c:122:ARG:NH1	2.38	0.57
2:m:418:GLN:H	2:m:418:GLN:CD	2.12	0.55

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	A	96/239 (40%)	91 (95%)	5 (5%)	0	100	100
1	B	96/239 (40%)	91 (95%)	5 (5%)	0	100	100
1	C	96/239 (40%)	91 (95%)	5 (5%)	0	100	100
1	D	96/239 (40%)	91 (95%)	5 (5%)	0	100	100
1	E	96/239 (40%)	91 (95%)	5 (5%)	0	100	100
1	F	96/239 (40%)	92 (96%)	4 (4%)	0	100	100
2	a	129/818 (16%)	122 (95%)	4 (3%)	3 (2%)	5	30
2	b	129/818 (16%)	121 (94%)	8 (6%)	0	100	100
2	c	129/818 (16%)	125 (97%)	4 (3%)	0	100	100
2	d	129/818 (16%)	124 (96%)	5 (4%)	0	100	100
2	e	129/818 (16%)	126 (98%)	3 (2%)	0	100	100
2	f	129/818 (16%)	122 (95%)	7 (5%)	0	100	100
2	g	51/818 (6%)	49 (96%)	2 (4%)	0	100	100
2	h	51/818 (6%)	50 (98%)	1 (2%)	0	100	100
2	i	51/818 (6%)	49 (96%)	2 (4%)	0	100	100
2	l	51/818 (6%)	50 (98%)	1 (2%)	0	100	100
2	m	51/818 (6%)	51 (100%)	0	0	100	100
2	n	51/818 (6%)	51 (100%)	0	0	100	100
All	All	1656/11250 (15%)	1587 (96%)	66 (4%)	3 (0%)	44	74

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	a	103	VAL
2	a	101	ASN
2	a	97	LYS

### 5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	92/221 (42%)	92 (100%)	0	100	100
1	B	92/221 (42%)	92 (100%)	0	100	100
1	C	92/221 (42%)	92 (100%)	0	100	100
1	D	92/221 (42%)	91 (99%)	1 (1%)	65	74
1	E	92/221 (42%)	92 (100%)	0	100	100
1	F	92/221 (42%)	92 (100%)	0	100	100
2	a	111/695 (16%)	107 (96%)	4 (4%)	31	57
2	b	111/695 (16%)	110 (99%)	1 (1%)	70	76
2	c	111/695 (16%)	109 (98%)	2 (2%)	51	69
2	d	111/695 (16%)	111 (100%)	0	100	100
2	e	111/695 (16%)	110 (99%)	1 (1%)	70	76
2	f	111/695 (16%)	109 (98%)	2 (2%)	51	69
2	g	46/695 (7%)	46 (100%)	0	100	100
2	h	46/695 (7%)	46 (100%)	0	100	100
2	i	46/695 (7%)	46 (100%)	0	100	100
2	l	46/695 (7%)	46 (100%)	0	100	100
2	m	46/695 (7%)	45 (98%)	1 (2%)	45	65
2	n	46/695 (7%)	46 (100%)	0	100	100
All	All	1494/9666 (16%)	1482 (99%)	12 (1%)	70	77

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	c	99	HIS
2	e	32	GLU
2	m	424	LYS
2	f	32	GLU
2	a	126	ASN

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

Mol	Chain	Res	Type
2	n	458	ASN
2	m	446	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	d	16	HIS
2	c	99	HIS
2	l	462	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.

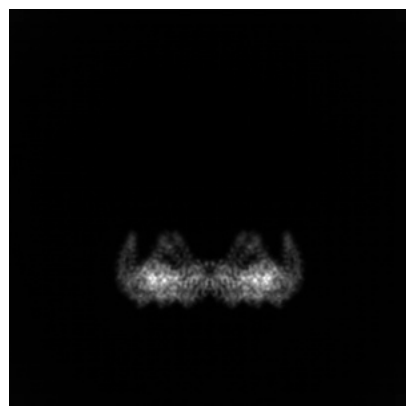
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51498. These allow visual inspection of the internal detail of the map and identification of artifacts.

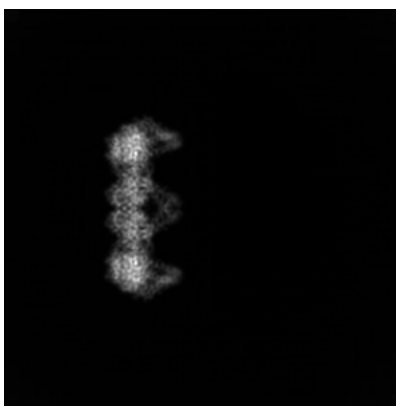
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

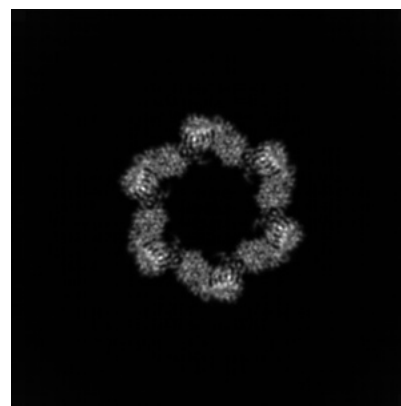
#### 6.1.1 Primary map



X

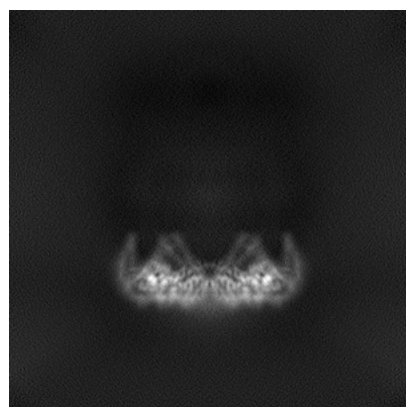


Y

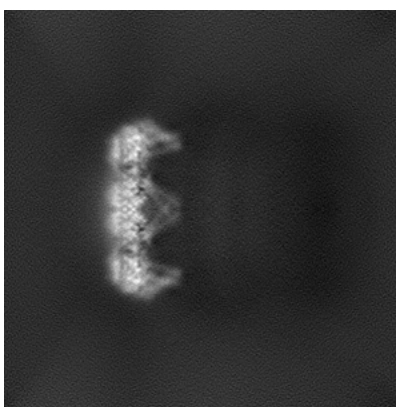


Z

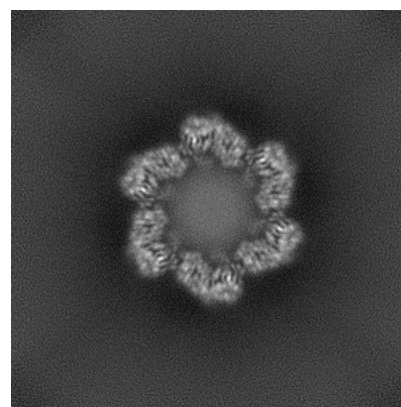
#### 6.1.2 Raw map



X



Y

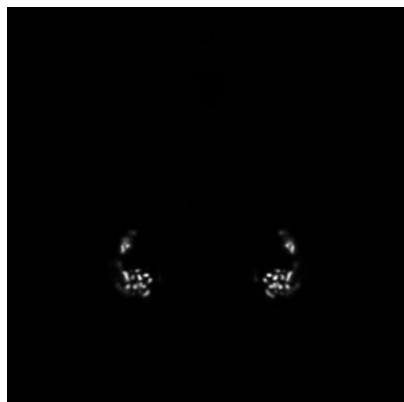


Z

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

## 6.2 Central slices [i](#)

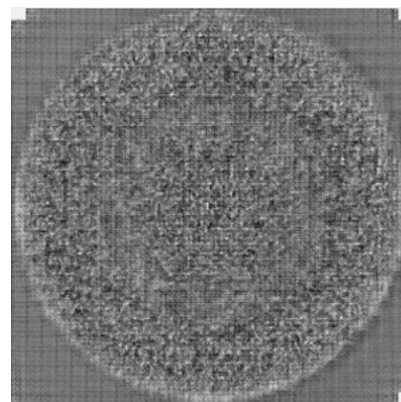
### 6.2.1 Primary map



X Index: 152

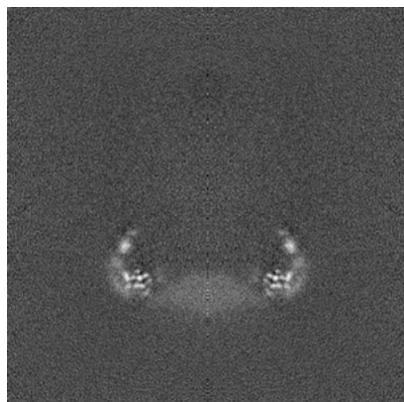


Y Index: 152

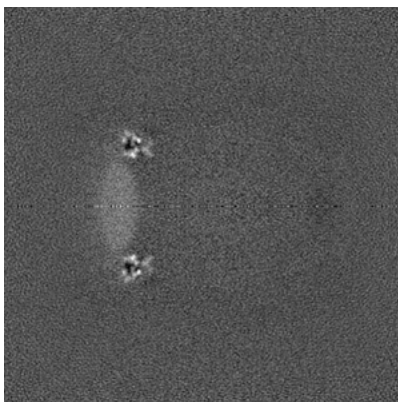


Z Index: 152

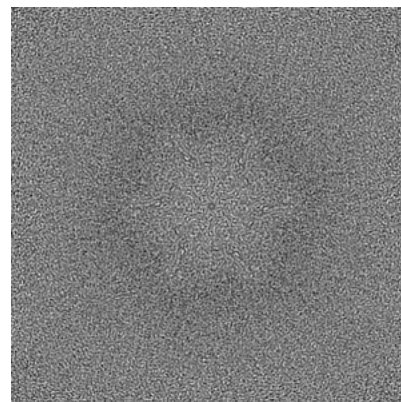
### 6.2.2 Raw map



X Index: 152



Y Index: 152



Z Index: 152

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

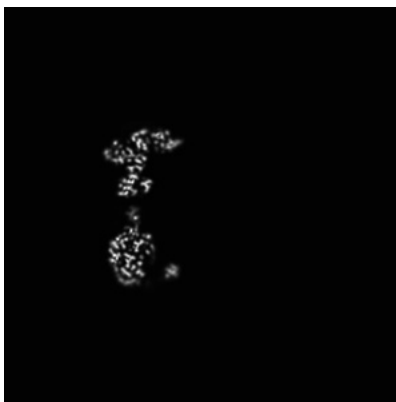


## 6.3 Largest variance slices [i](#)

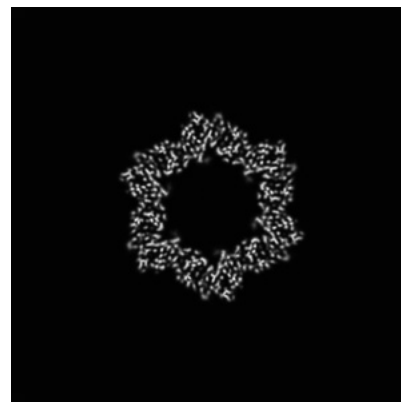
### 6.3.1 Primary map



X Index: 99

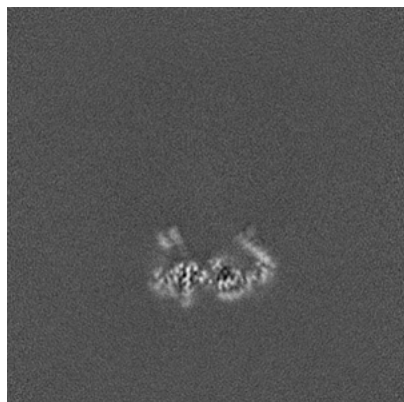


Y Index: 188

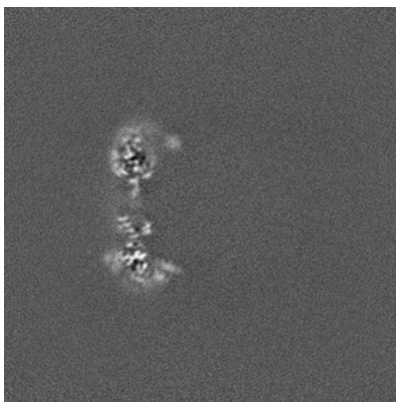


Z Index: 99

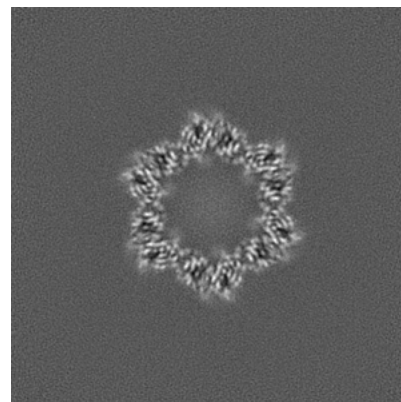
### 6.3.2 Raw map



X Index: 204



Y Index: 115

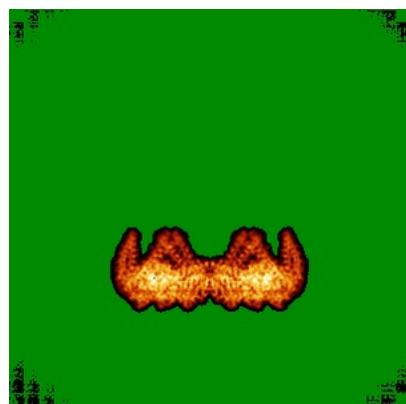


Z Index: 99

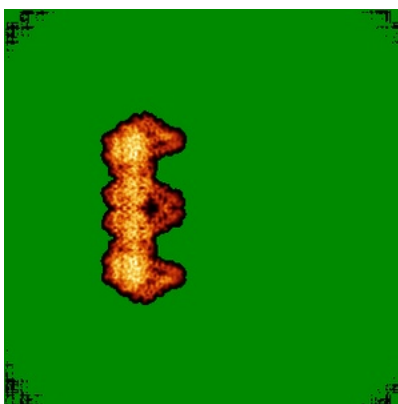
The images above show the largest variance slices of the map in three orthogonal directions.

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

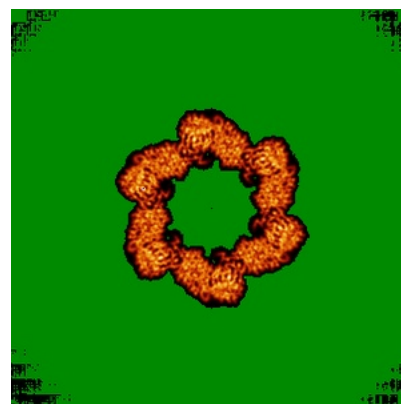
### 6.4.1 Primary map



X

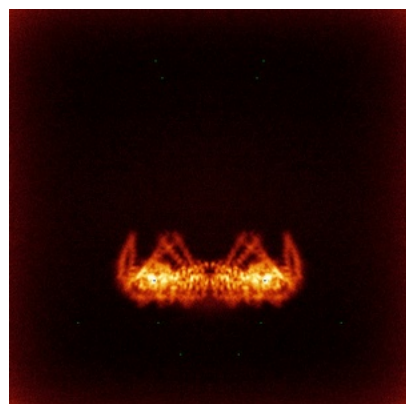


Y

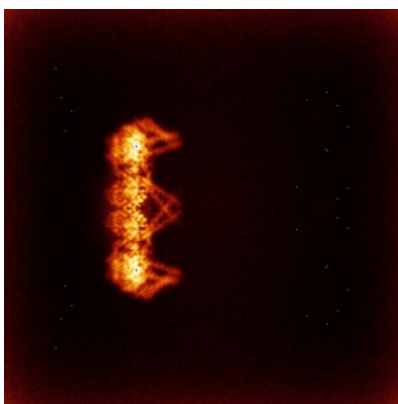


Z

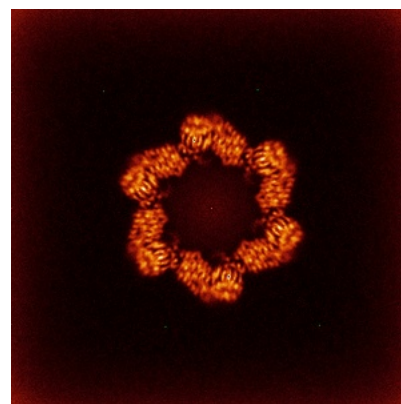
### 6.4.2 Raw map



X



Y

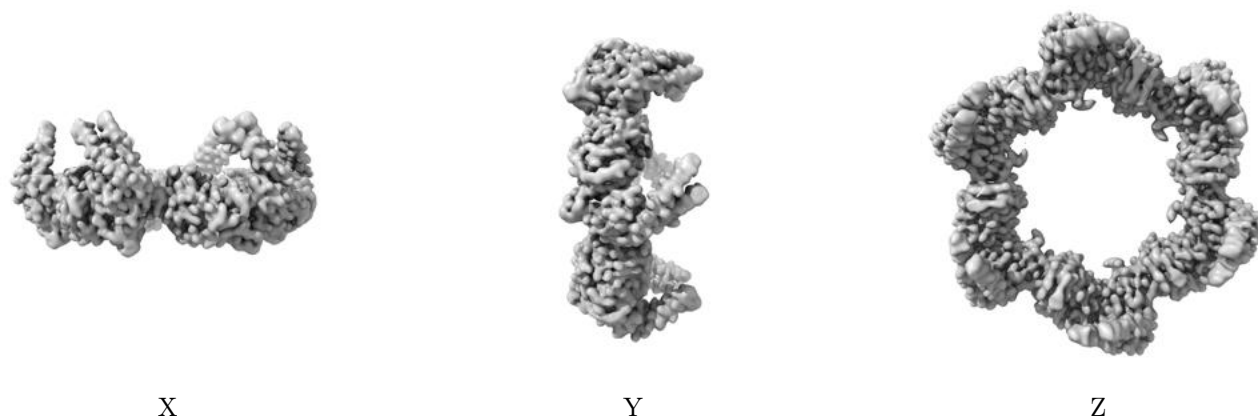


Z

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.

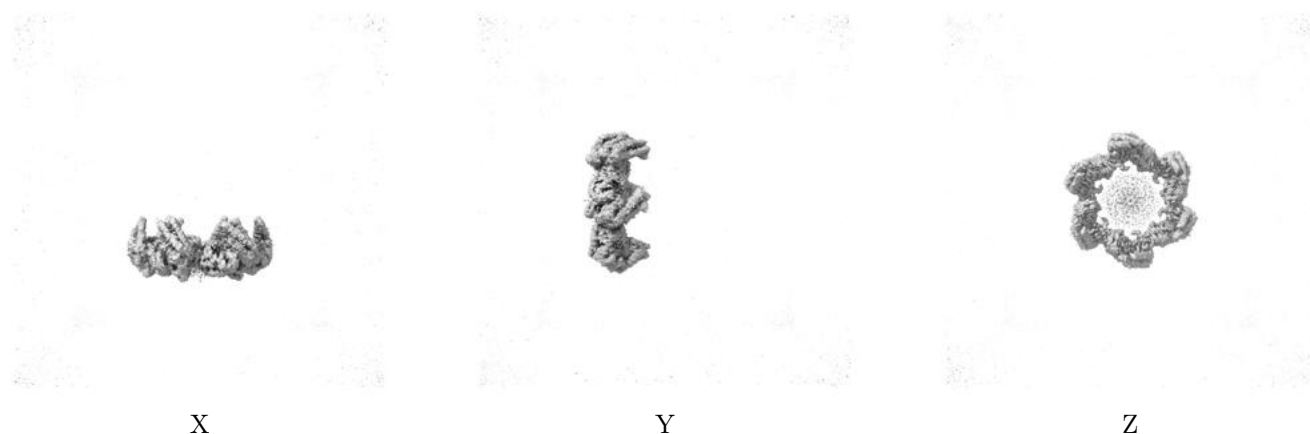
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 1.95. 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.

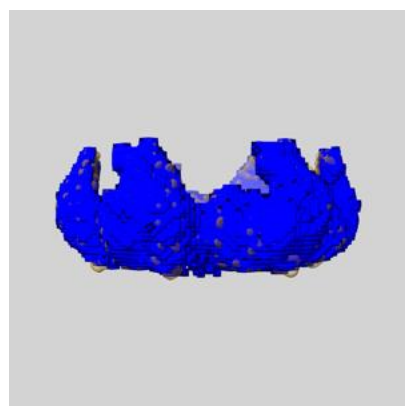
## 6.6 Mask visualisation [i](#)

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

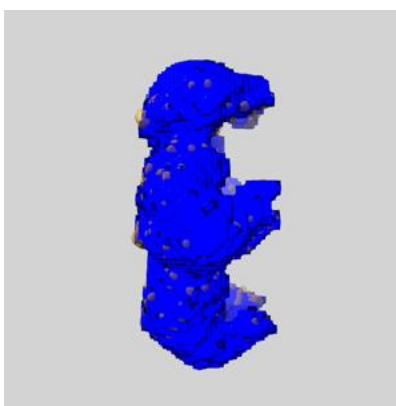
A mask typically either:

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

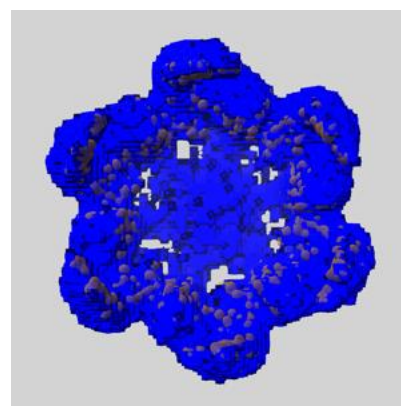
### 6.6.1 emd\_51498\_msk\_1.map [i](#)



X



Y

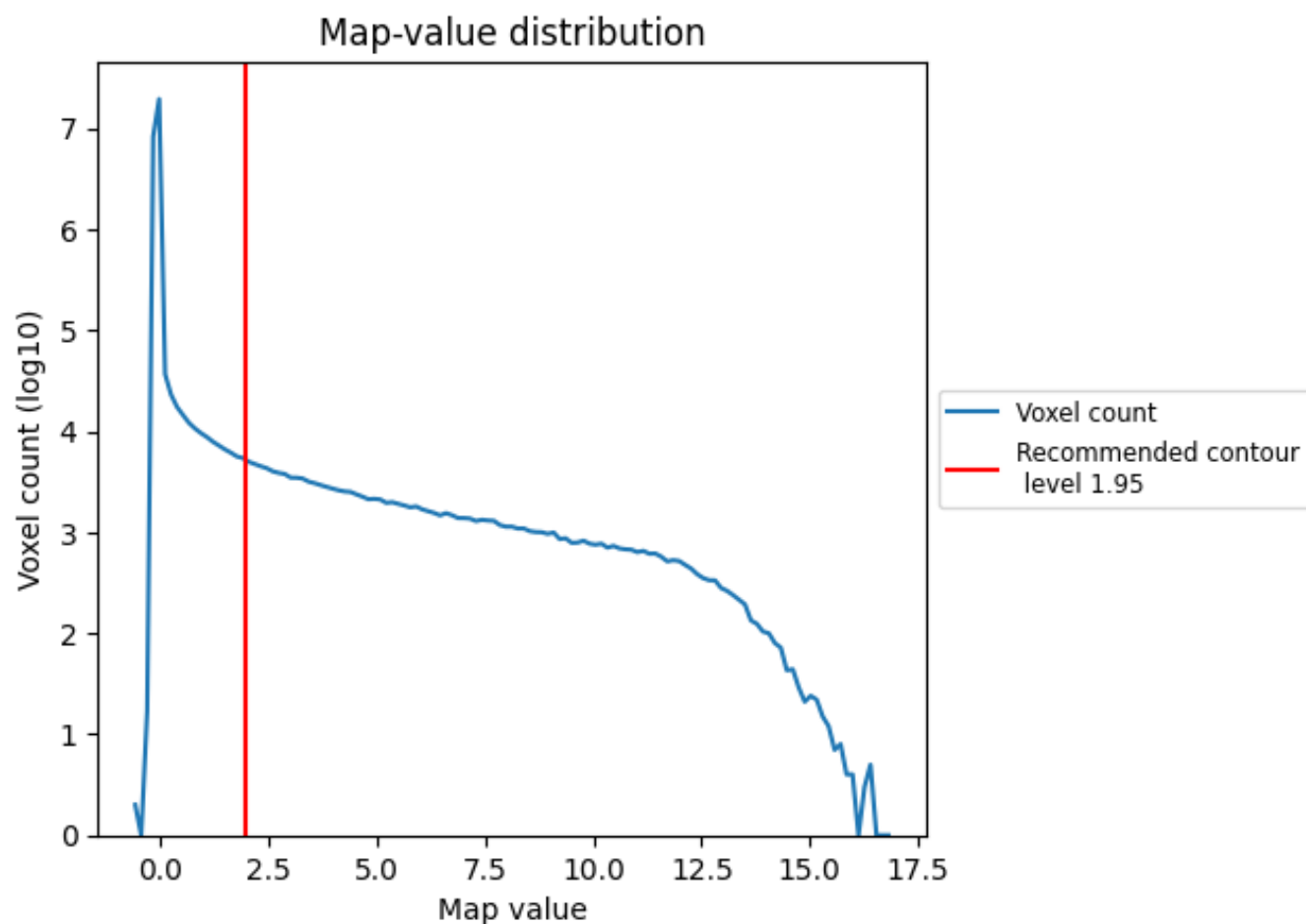


Z

## 7 Map analysis [i](#)

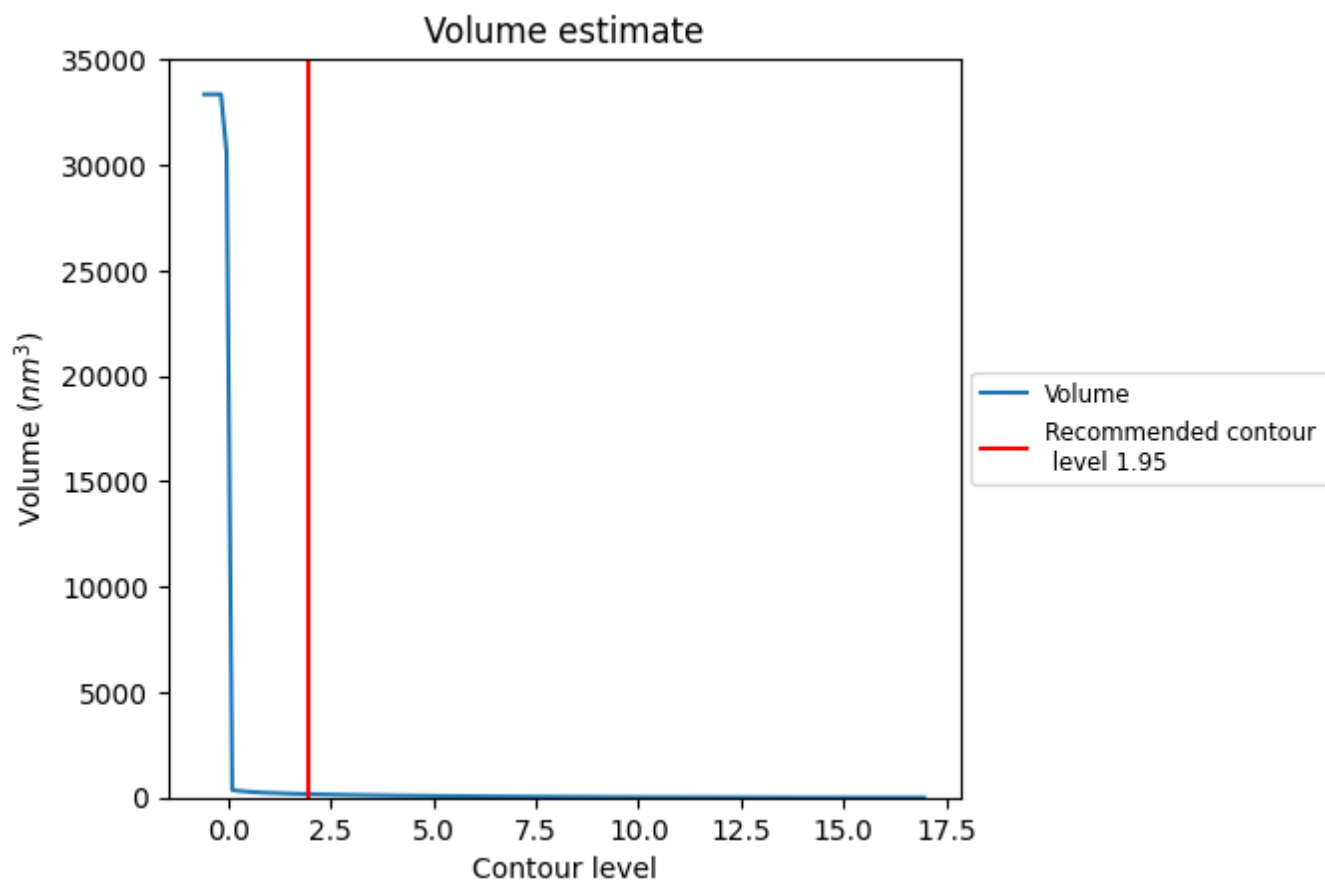
This section contains the results of statistical analysis of the map.

### 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.

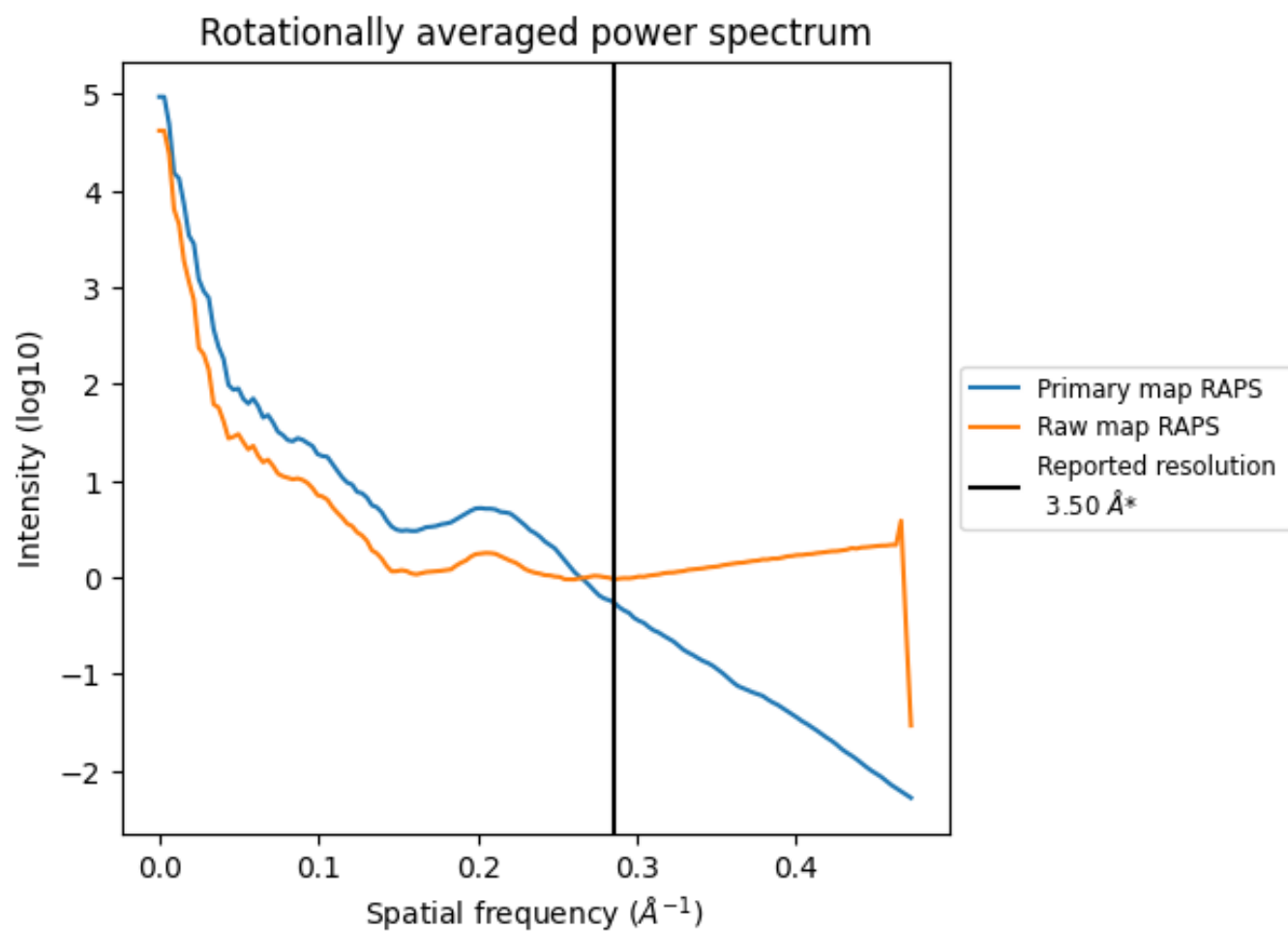
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 163 nm<sup>3</sup>; this corresponds to an approximate mass of 147 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 ⓘ

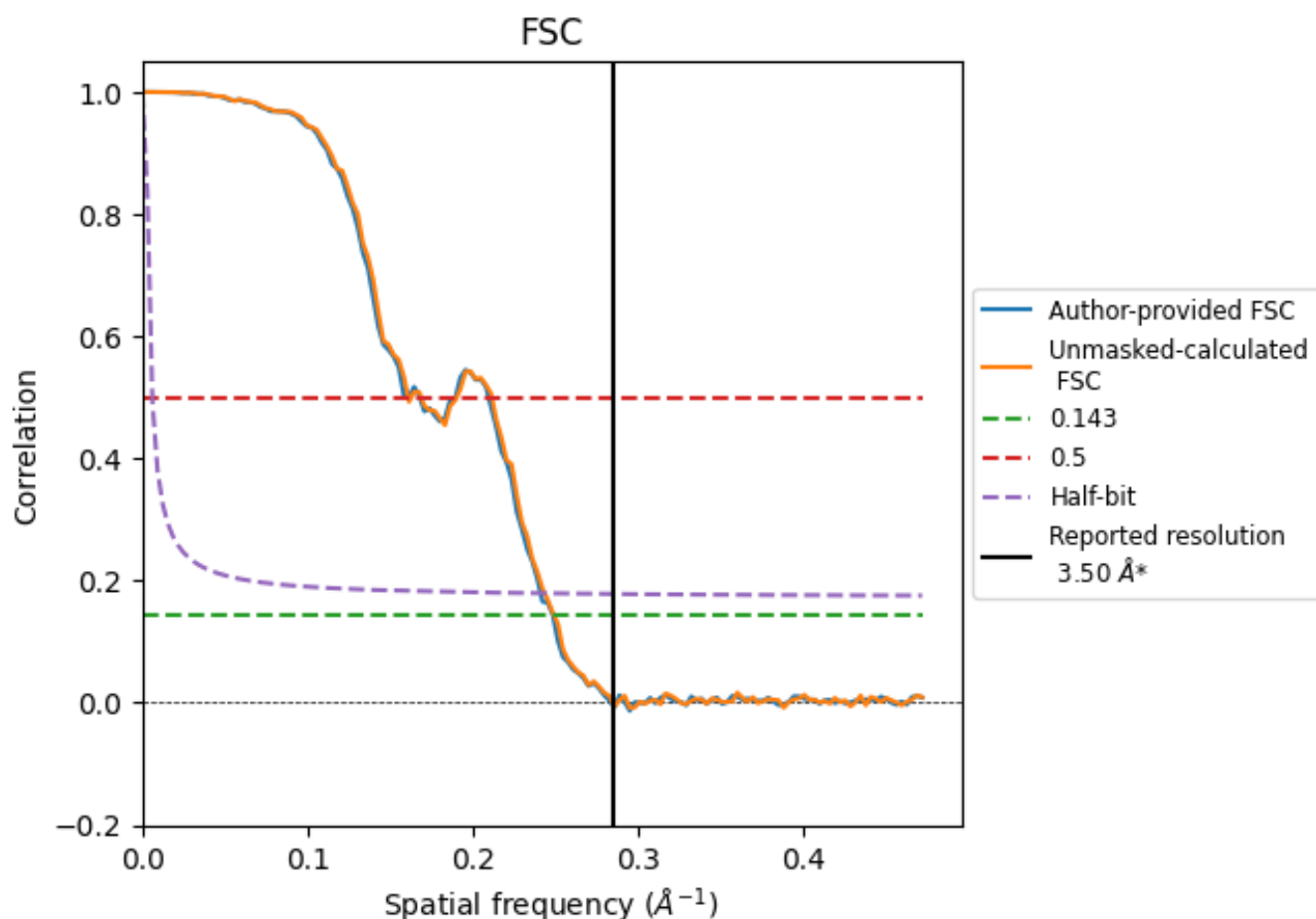


\*Reported resolution corresponds to spatial frequency of 0.286 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of  $0.286 \text{ \AA}^{-1}$



## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	4.02	5.95	4.15
Unmasked-calculated*	4.01	6.21	4.11

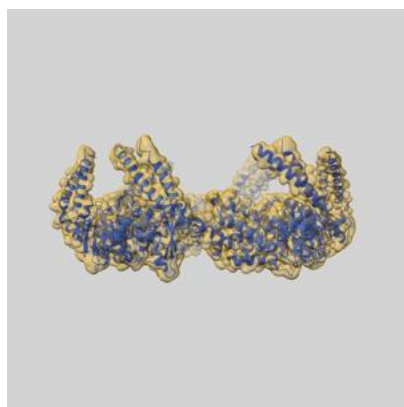
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 4.02 differs from the reported value 3.5 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.01 differs from the reported value 3.5 by more than 10 %

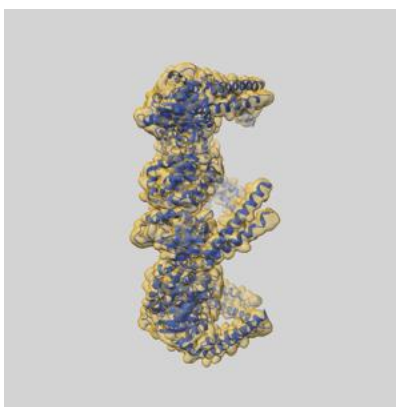
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-51498 and PDB model 9GOQ. Per-residue inclusion information can be found in section [3](#) on page [6](#).

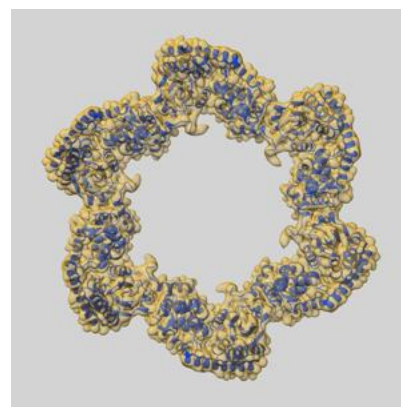
### 9.1 Map-model overlay [i](#)



X



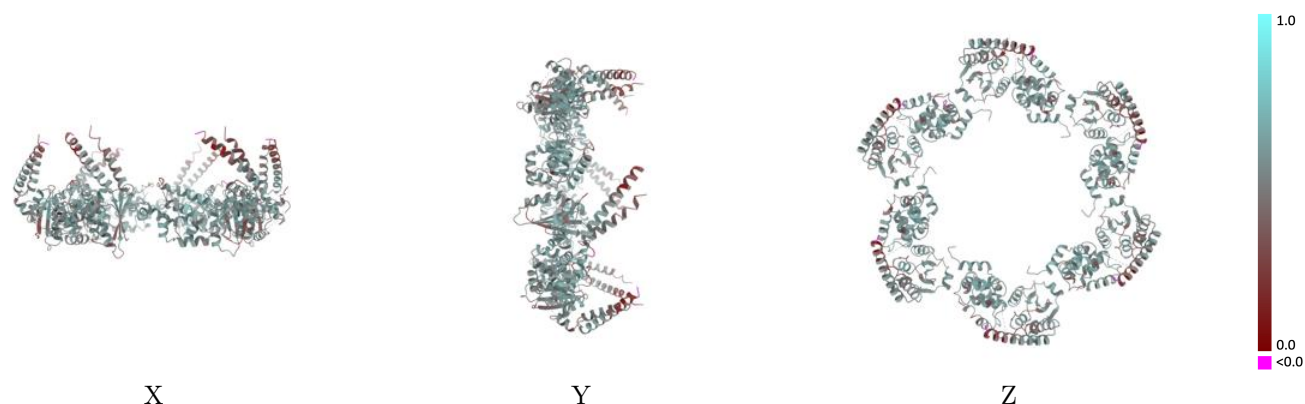
Y



Z

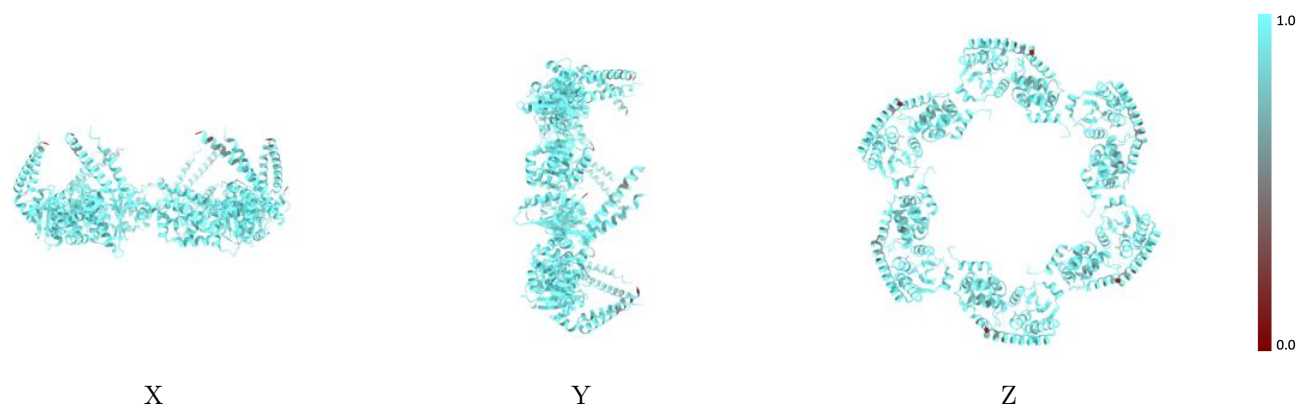
The images above show the 3D surface view of the map at the recommended contour level 1.95 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



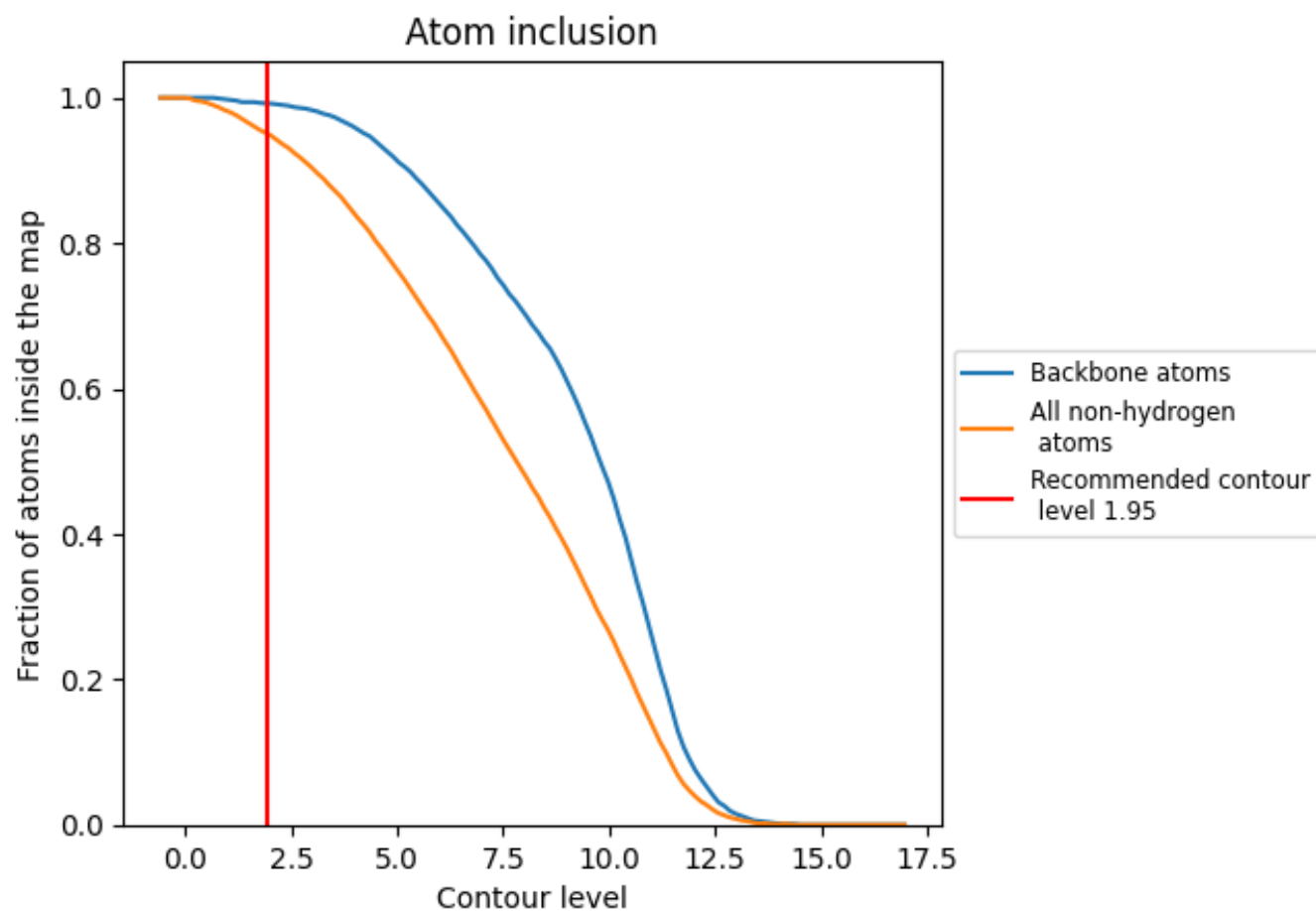
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.95).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 95% 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 (1.95) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.9500	<div><div></div></div> 0.5070
A	<div><div></div></div> 0.9600	<div><div></div></div> 0.5080
B	<div><div></div></div> 0.9640	<div><div></div></div> 0.5150
C	<div><div></div></div> 0.9680	<div><div></div></div> 0.5150
D	<div><div></div></div> 0.9630	<div><div></div></div> 0.5100
E	<div><div></div></div> 0.9600	<div><div></div></div> 0.5060
F	<div><div></div></div> 0.9550	<div><div></div></div> 0.5120
a	<div><div></div></div> 0.9750	<div><div></div></div> 0.5340
b	<div><div></div></div> 0.9720	<div><div></div></div> 0.5380
c	<div><div></div></div> 0.9670	<div><div></div></div> 0.5370
d	<div><div></div></div> 0.9750	<div><div></div></div> 0.5370
e	<div><div></div></div> 0.9670	<div><div></div></div> 0.5420
f	<div><div></div></div> 0.9770	<div><div></div></div> 0.5460
g	<div><div></div></div> 0.8930	<div><div></div></div> 0.4240
h	<div><div></div></div> 0.8840	<div><div></div></div> 0.4320
i	<div><div></div></div> 0.8720	<div><div></div></div> 0.4290
l	<div><div></div></div> 0.8770	<div><div></div></div> 0.4170
m	<div><div></div></div> 0.8810	<div><div></div></div> 0.4250
n	<div><div></div></div> 0.8610	<div><div></div></div> 0.4010

