



## Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 02:51 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 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>.

---

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

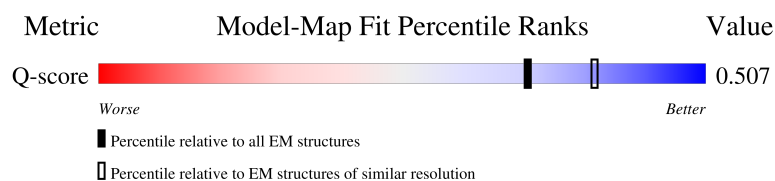
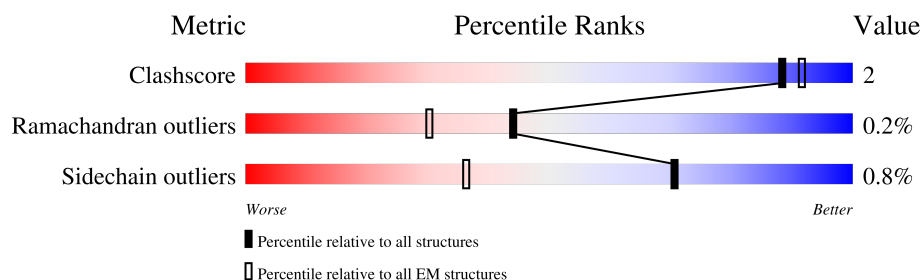
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : 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	

*Continued on next page...*

*Continued from previous page...*

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 [i](#)

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			

*Continued on next page...*

*Continued from previous page...*

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		



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

[illegible]

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

Chain b:  14% • 84%

[illegible]







[illegible]

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



ILE	LVS	ILE	TTR	ASP	GLU	LEU	LEU	GLY	ALA	THR	ILE	MET
LEU	THR	ILE	VAL	PRO	GLU	GLU	GLY	LEU	ILE	LEU	ASP	LEU
GLU	THR	MET	HIS	LVS	ILE	ILE	ARG	ASP	ALA	ASP	GLY	GLY
ASN	LVS	THR	ASP	PRO	ALA	GLU	GLN	TYR	ASN	ARG	THR	LEU
LEU	LEU	ASN	GLY	GLY	VAL	ILE	GLU	GLU	ILE	VAL	LEU	GLU
LEU	LEU	VAL	GLN	PHE	TRP	VAL	VAL	ARG	ALA	ASP	LEU	GLU
LEU	GLU	GLY	GLN	PHE	GLY	VAL	LVS	ILE	LEU	MET	GLY	GLY
GLY	THR	GLY	GLU	GLY	THR	GLY	ASN	ASN	ALA	GLY	ARG	THR
ASN	MET	LEU	LVS	GLY	GLY	ASN	ASN	ASN	ALA	GLY	THR	GLY
GLN	MET	GLN	VAL	PRO	ILE	GLY	LVS	ILE	GLY	THR	ASP	GLY
ILE	VAL	ILE	ARG	THR	PRO	LVS	GLY	SER	ARG	THR	LEU	HIS
GLU	ASN	GLN	ARG	VAL	LEU	ASP	ASP	ASP	GLU	VAL	LEU	GLY
GLY	LVS	ARG	LVS	GLY	ALA	ALA	ALA	ALA	GLN	ALA	ILE	GLN
LEU	LEU	PHE	TTR	GLY	LVS	ALA	ALA	ALA	CYS	THR	ARG	ASN
LVS	THR	ALA	TTR	LVS	ILE	VAL	ILE	ILE	ILE	THR	ARG	HIS
VAL	ASN	GLY	SER	THR	ASN	VAL	GLU	GLU	ILE	LVS	VAL	V75
THR	ARG	PHE	VAL	GLU	THR	ALA	ALA	ALA	GLY	TTR	ILE	K97
VAL	LEU	GLY	ILE	LEU	THR	GLN	GLU	VAL	THR	GLY	VAL	GLY
ASP	SER	GLY	LEU	ALA	SER	PHE	GLY	LVS	THR	GLU	LEU	H100
HIS	GLU	SER	ASP	ARG	GLU	GLY	GLU	LEU	LEU	PHE	SER	GLY
ASN	ASN	ASP	GLU	LEU	LVS	LEU	ALA	ASN	ASP	GLU	ARG	E106
LVS	ILE	GLY	ILE	ALA	LEU	LEU	ALA	ARG	TTR	ARG	THR	H107
ASN	GLN	GLN	GLU	GLU	LEU	SER	ASN	TYR	ARG	LEU	LVS	I113
ILE	ILE	TYR	ALA	MET	LEU	LEU	LEU	VAL	LVS	LVS	ASN	ASN
VAL	VAL	GLU	HIS	PHE	GLU	GLU	ARG	SER	ASN	LVS	ASN	R122
THR	THR	THR	PRO	GLY	ASP	ASP	ASP	ASP	ILE	VAL	PRO	PRO
ILE	ASP	ILE	ASP	THR	THR	THR	LVS	ARG	GLU	MET	VAL	VAL
ALA	LVS	ALA	VAL	ALA	GLN	GLY	GLN	PHE	LVS	GLU	LEU	LEU
GLU	ALA	GLU	VAL	ASP	GLY	HIS	THR	LEU	ASP	GLU	ILE	ILE
LVS	LVS	THR	ASN	ALA	GLU	GLY	LVS	PRO	ALA	ILE	GLY	SER
THR	ASP	MET	ILE	MET	ARG	ASP	ASP	ASP	ALA	GLN	GLY	ASN
PRO	GLY	ASN	ASP	SER	ILE	ILE	GLU	ILE	ALA	GLN	LVS	GLY
THR	TTR	SER	ASP	GLU	ALA	ALA	GLU	ILE	PRO	LEU	THR	THR
GLN	ASP	PHE	GLY	PHE	VAL	VAL	LVS	GLU	PRO	LEU	ALA	ALA
ALA	PRO	ARG	HIS	GLY	VAL	VAL	ASN	ALA	GLN	ILE	ALA	ASP
ASN	GLU	PRO	LEU	GLY	SER	THR	GLY	SER	VAL	ASP	GLY	ASN
TYR	TTR	GLY	ASP	LVS	SER	LVS	TRP	SER	ASP	GLU	GLY	THR
GLY	GLY	PHE	ASP	HIS	SER	LVS	LVS	LVS	GLU	LEU	LEU	PRO
ALA	ALA	LEU	THR	ALA	LVS	ALA	ASN	VAL	PRO	HIS	ALA	THR
PRO	ARG	ASN	LVS	VAL	ALA	ALA	ASN	ARG	SER	THR	GLN	LEU
LEU	PRO	VAL	GLY	SER	ARG	VAL	ASN	LVS	VAL	VAL	ALA	ASP
ILE	ILE	ASP	THR	LEU	ARG	GLY	GLY	SER	ASP	GLY	ILE	SER
ARG	ARG	ASP	VAL	VAL	ALA	ALA	MET	HIS	THR	ALA	ASN	ALA
ALA	ALA	ILE	ASP	GLY	ARG	ARG	SER	THR	VAL	GLY	ASN	ARG
ILE	ILE	ILE	PHE	ALA	ALA	ALA	THR	THR	ALA	GLY	VAL	ASP
GLN	GLN	VAL	ARG	PRO	GLY	GLY	SER	PRO	ILE	ALA	VAL	GLY
LVS	LVS	THR	THR	GLY	LEU	LVS	SER	ASN	LEU	GLY	PRO	THR

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

[illegible]



[illegible]

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

Chain i:  6% 94%

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

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

94%

[illegible]

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

94%

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

[illegible]

- 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.

All (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
2:c:13:VAL:HA	2:c:16:HIS:CE1	2.43	0.54
2:c:106:GLU:OE1	2:c:106:GLU:N	2.37	0.52
2:n:418:GLN:H	2:n:418:GLN:CD	2.18	0.52
2:a:16:HIS:CG	2:a:40:LYS:HD3	2.44	0.52
2:a:113:ILE:HG23	2:a:131:ILE:HG23	1.91	0.52
2:d:113:ILE:HG23	2:d:131:ILE:HG23	1.91	0.52
2:a:96:ARG:C	2:a:98:LEU:H	2.18	0.51
2:i:418:GLN:H	2:i:418:GLN:CD	2.18	0.51
2:e:106:GLU:OE1	2:e:106:GLU:N	2.36	0.51
2:f:106:GLU:OE1	2:f:106:GLU:N	2.36	0.49
2:b:106:GLU:OE1	2:b:106:GLU:N	2.33	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:ARG:NH1	1:A:188:VAL:O	2.46	0.49
2:b:9:ARG:NH2	2:b:101:ASN:OD1	2.45	0.48
2:b:96:ARG:C	2:b:98:LEU:H	2.22	0.47
2:a:32:GLU:OE2	2:a:33:HIS:ND1	2.31	0.47
2:c:94:GLU:CD	2:c:114:ARG:HH21	2.23	0.47
2:d:113:ILE:HD12	2:d:131:ILE:HG23	1.96	0.47
2:a:113:ILE:HD12	2:a:131:ILE:HG23	1.98	0.46
2:b:83:ARG:NH1	2:b:115:GLU:OE2	2.46	0.46
2:d:32:GLU:OE1	2:d:32:GLU:N	2.43	0.46
2:a:9:ARG:NH2	2:a:101:ASN:OD1	2.49	0.45
2:f:106:GLU:HG2	2:f:107:HIS:N	2.31	0.45
2:b:99:HIS:C	2:b:100:HIS:CG	2.94	0.45
2:d:106:GLU:HG2	2:d:107:HIS:N	2.32	0.45
1:A:195:ASP:OD1	2:f:122:ARG:NH1	2.47	0.45
2:l:460:TRP:CD1	2:l:464:GLN:HE21	2.35	0.44
2:b:16:HIS:CE1	2:b:37:GLY:CA	3.01	0.44
2:b:14:LEU:C	2:b:16:HIS:H	2.26	0.43
2:e:113:ILE:HG23	2:e:131:ILE:HG23	2.01	0.43
2:l:417:GLU:H	2:l:417:GLU:CD	2.26	0.43
2:a:106:GLU:HG2	2:a:107:HIS:N	2.34	0.43
2:a:100:HIS:C	2:a:102:PHE:H	2.27	0.42
1:C:158:TYR:CZ	1:C:236:GLU:HA	2.55	0.42
2:c:106:GLU:HG2	2:c:107:HIS:N	2.34	0.42
2:f:113:ILE:HG23	2:f:131:ILE:HG23	2.00	0.42
2:a:106:GLU:OE1	2:a:106:GLU:N	2.34	0.41
2:e:93:ASP:OD2	2:e:97:LYS:NZ	2.46	0.41
2:e:106:GLU:HG2	2:e:107:HIS:N	2.34	0.41
2:b:106:GLU:HG2	2:b:107:HIS:N	2.35	0.41
1:A:197:TYR:CE1	1:A:201:LEU:HD21	2.56	0.41
2:b:40:LYS:HE3	2:b:40:LYS:HB3	1.96	0.41
2:f:97:LYS:HE3	2:f:97:LYS:HB3	1.96	0.40
2:c:9:ARG:O	2:c:12:ARG:NH1	2.50	0.40
2:e:99:HIS:C	2:e:101:ASN:H	2.29	0.40
2:c:32:GLU:OE1	2:c:32:GLU:N	2.47	0.40
2:h:418:GLN:H	2:h:418:GLN:CD	2.26	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	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

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	a	18	GLN
2	a	32	GLU
2	a	56	THR
2	a	126	ASN
1	D	232	ARG
2	b	32	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	c	96	ARG
2	c	99	HIS
2	e	32	GLU
2	f	32	GLU
2	f	122	ARG
2	m	424	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	215	ASN
1	F	215	ASN
2	c	16	HIS
2	c	99	HIS
2	d	16	HIS
2	l	462	ASN
2	m	446	GLN
2	n	458	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

### 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.



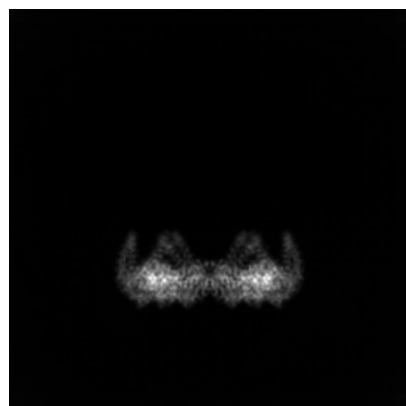
## 6 Map visualisation [i](#)

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

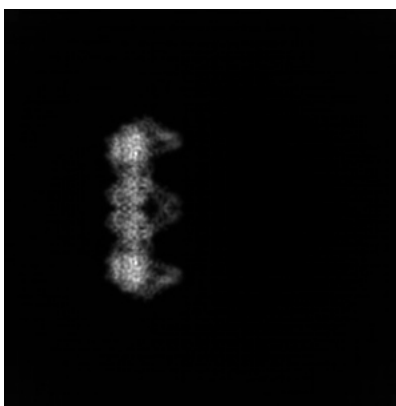
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

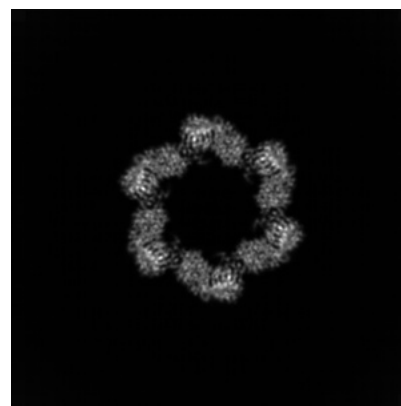
#### 6.1.1 Primary map



X

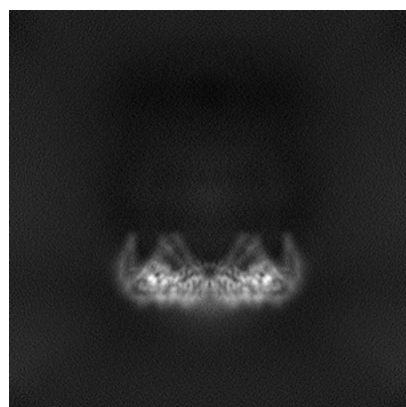


Y

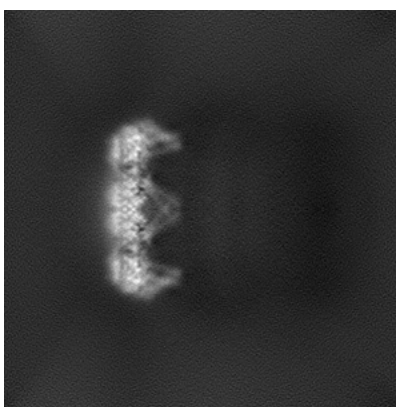


Z

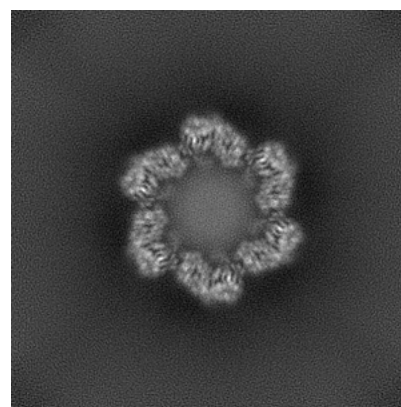
#### 6.1.2 Raw map



X



Y

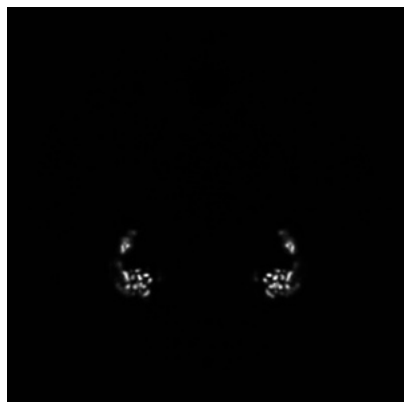


Z

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

## 6.2 Central slices [i](#)

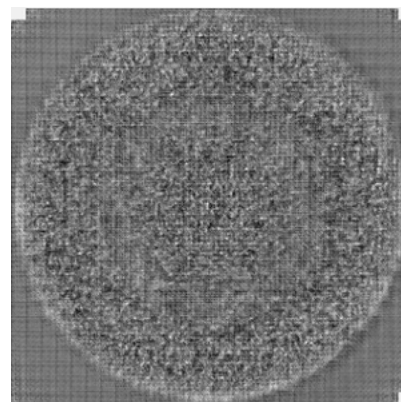
### 6.2.1 Primary map



X Index: 152

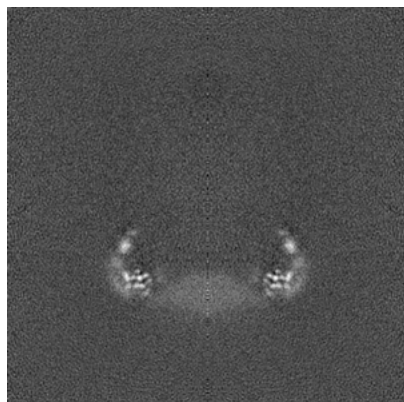


Y Index: 152

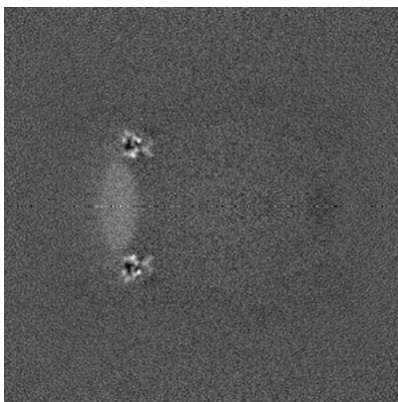


Z Index: 152

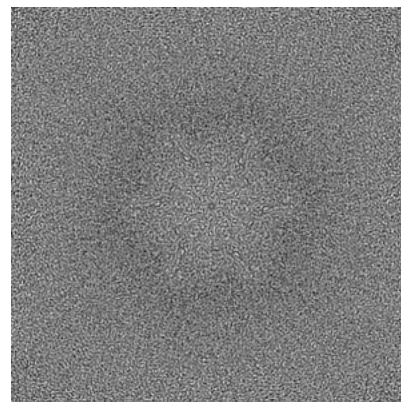
### 6.2.2 Raw map



X Index: 152



Y Index: 152



Z Index: 152

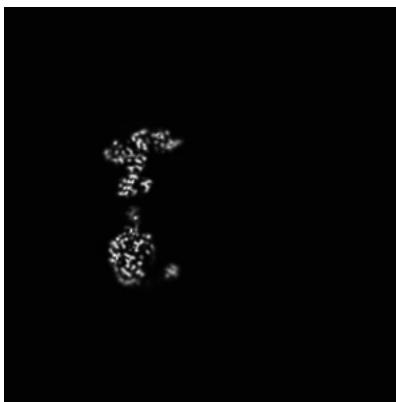
The images above show central slices of the map in three orthogonal directions.

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

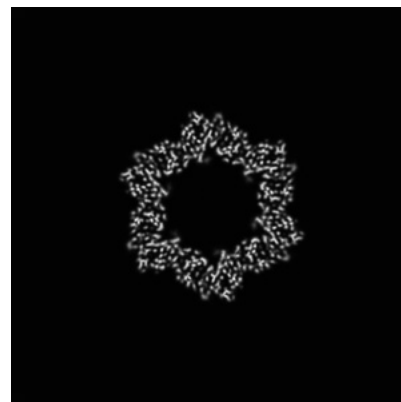
### 6.3.1 Primary map



X Index: 99

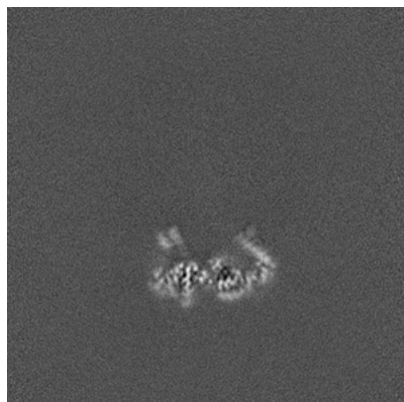


Y Index: 188

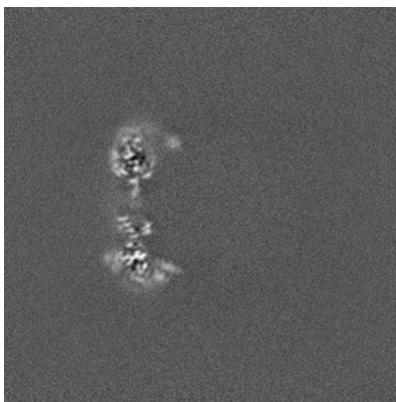


Z Index: 99

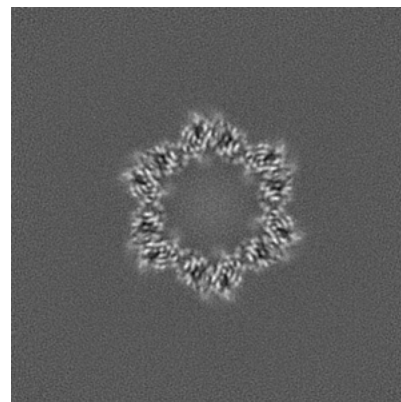
### 6.3.2 Raw map



X Index: 204



Y Index: 115

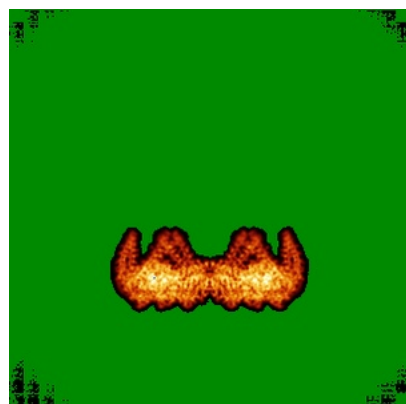


Z Index: 99

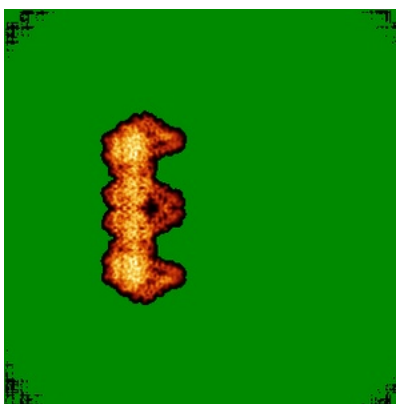
The images above show the largest variance slices of the map in three orthogonal directions.

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

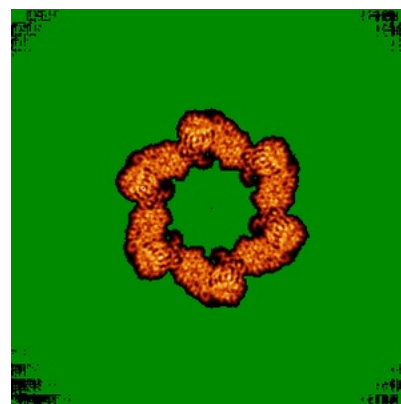
### 6.4.1 Primary map



X

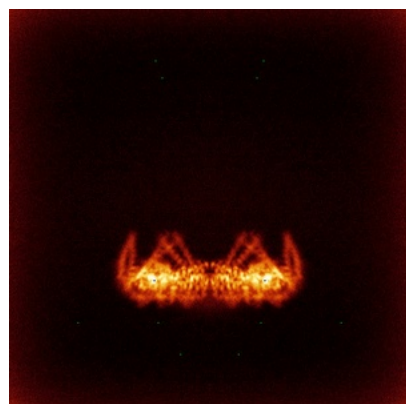


Y

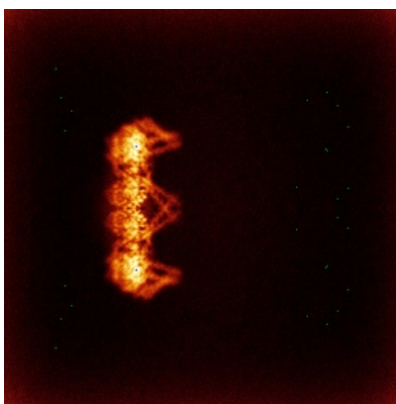


Z

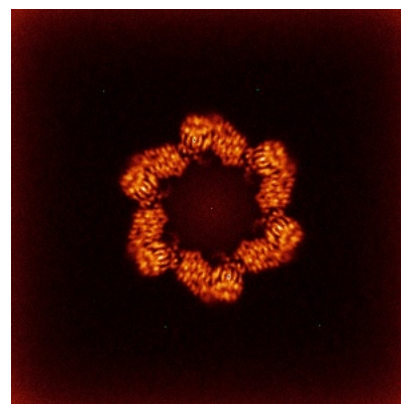
### 6.4.2 Raw map



X



Y

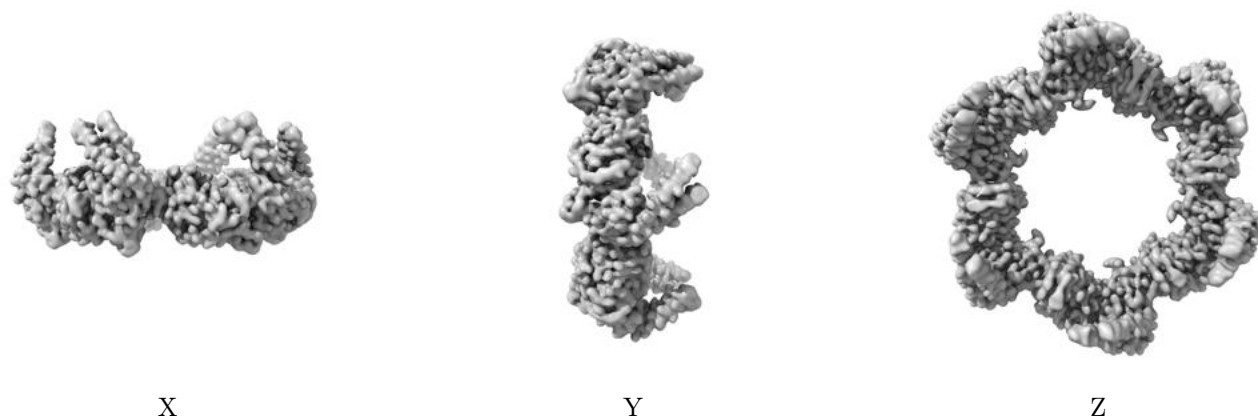


Z

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.

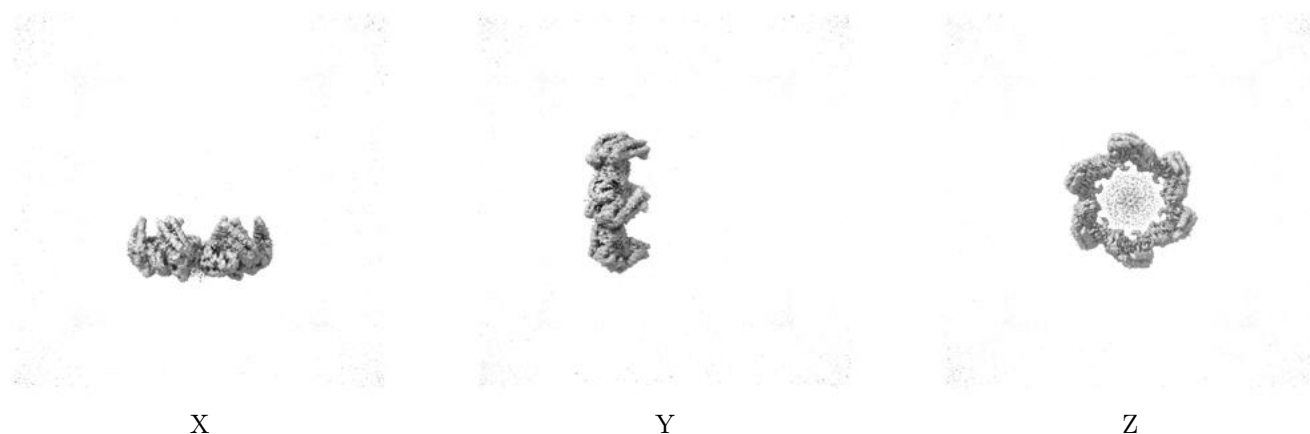
## 6.5 Orthogonal surface views [i](#)

### 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.

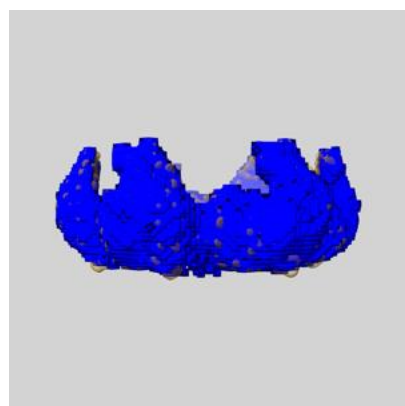
## 6.6 Mask visualisation [i](#)

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

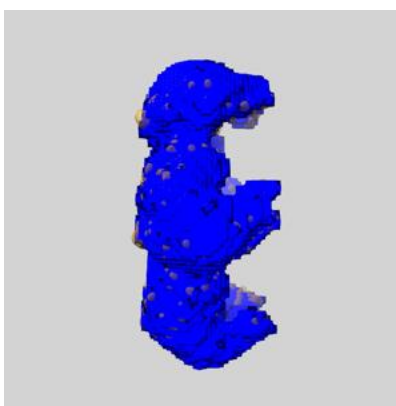
A mask typically either:

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

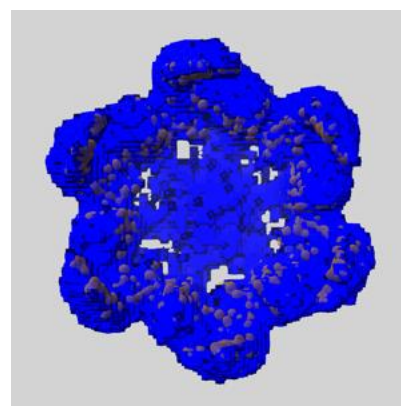
### 6.6.1 emd\_51498\_msk\_1.map [i](#)



X



Y



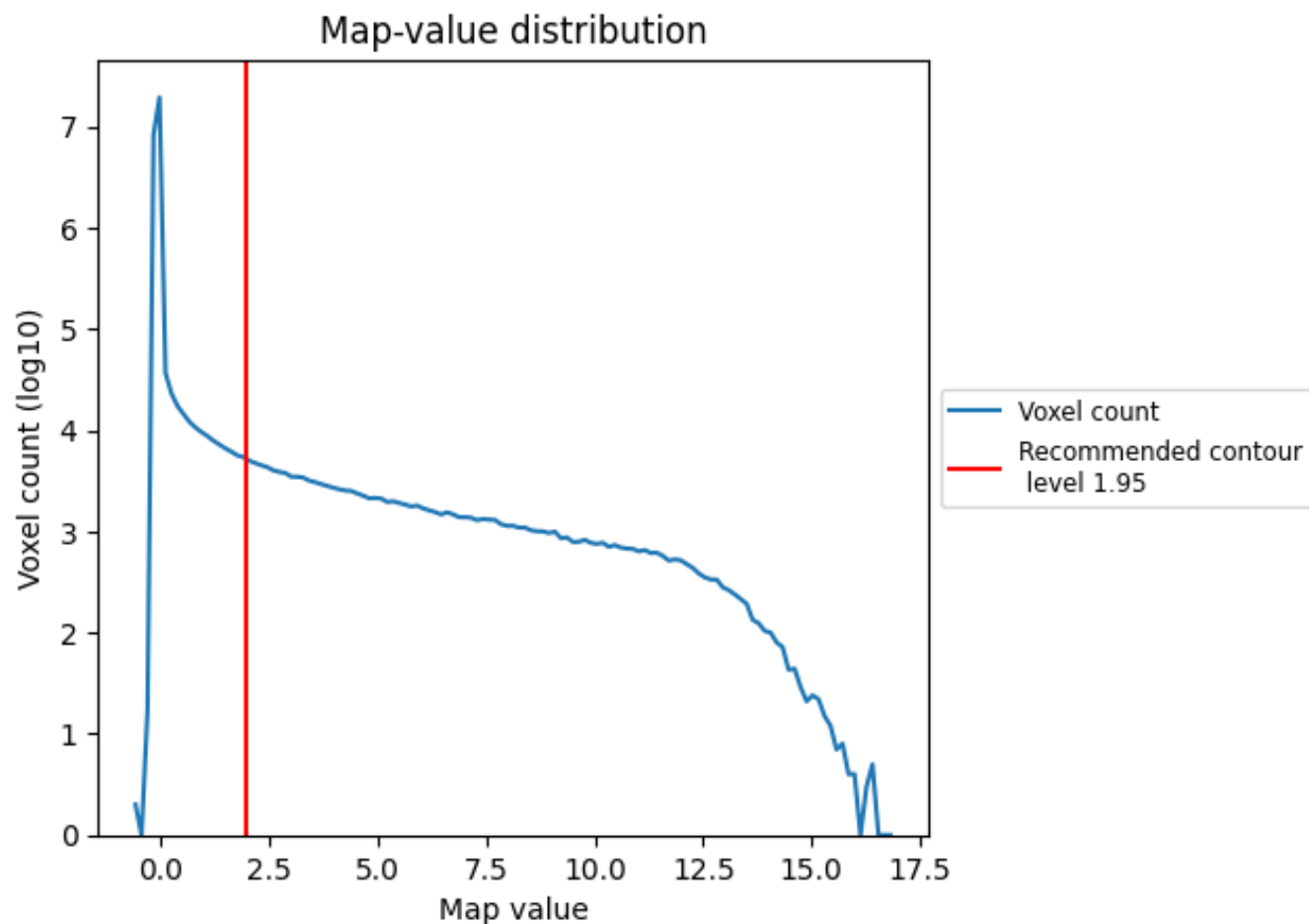
Z



## 7 Map analysis [i](#)

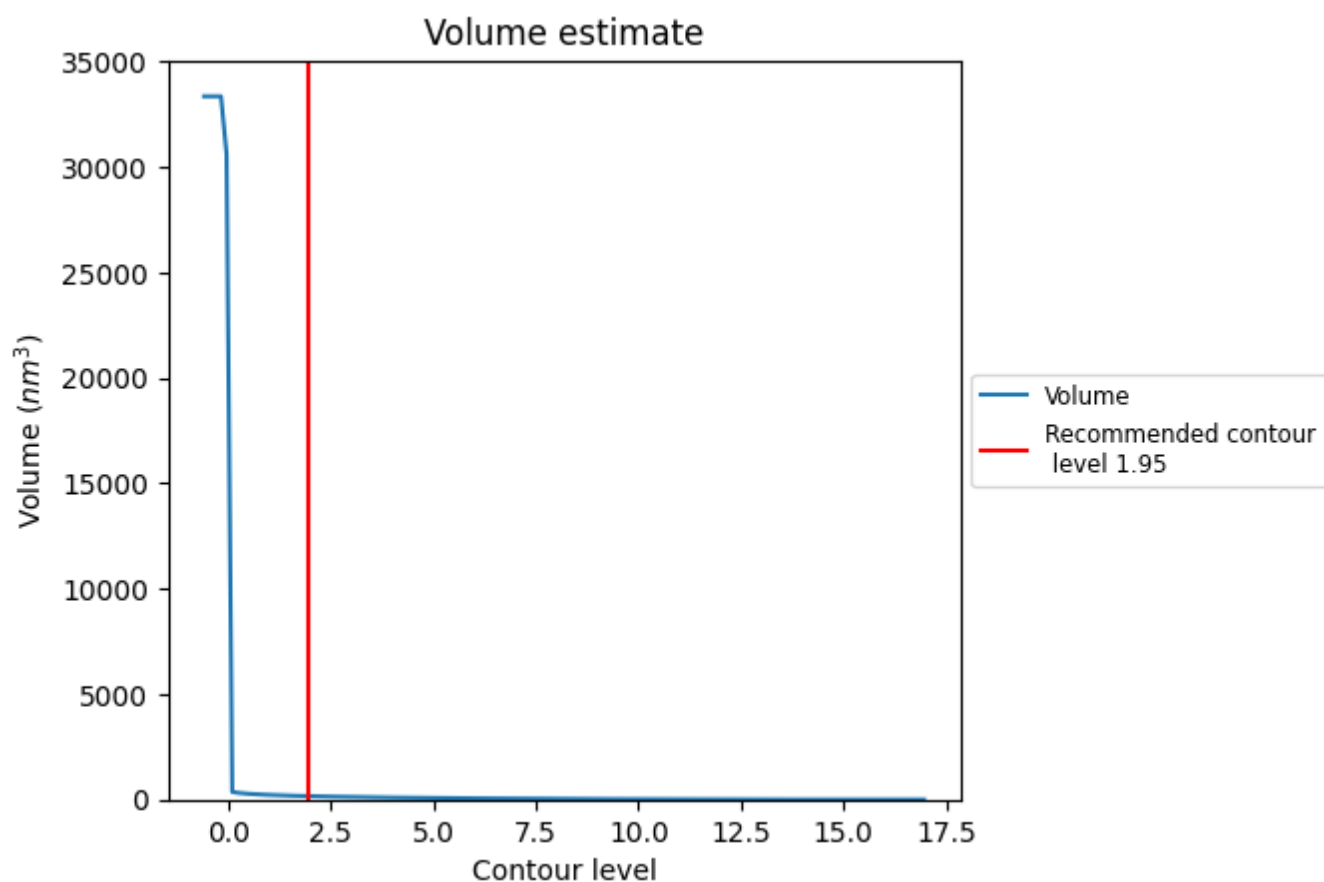
This section contains the results of statistical analysis of the map.

### 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](#)

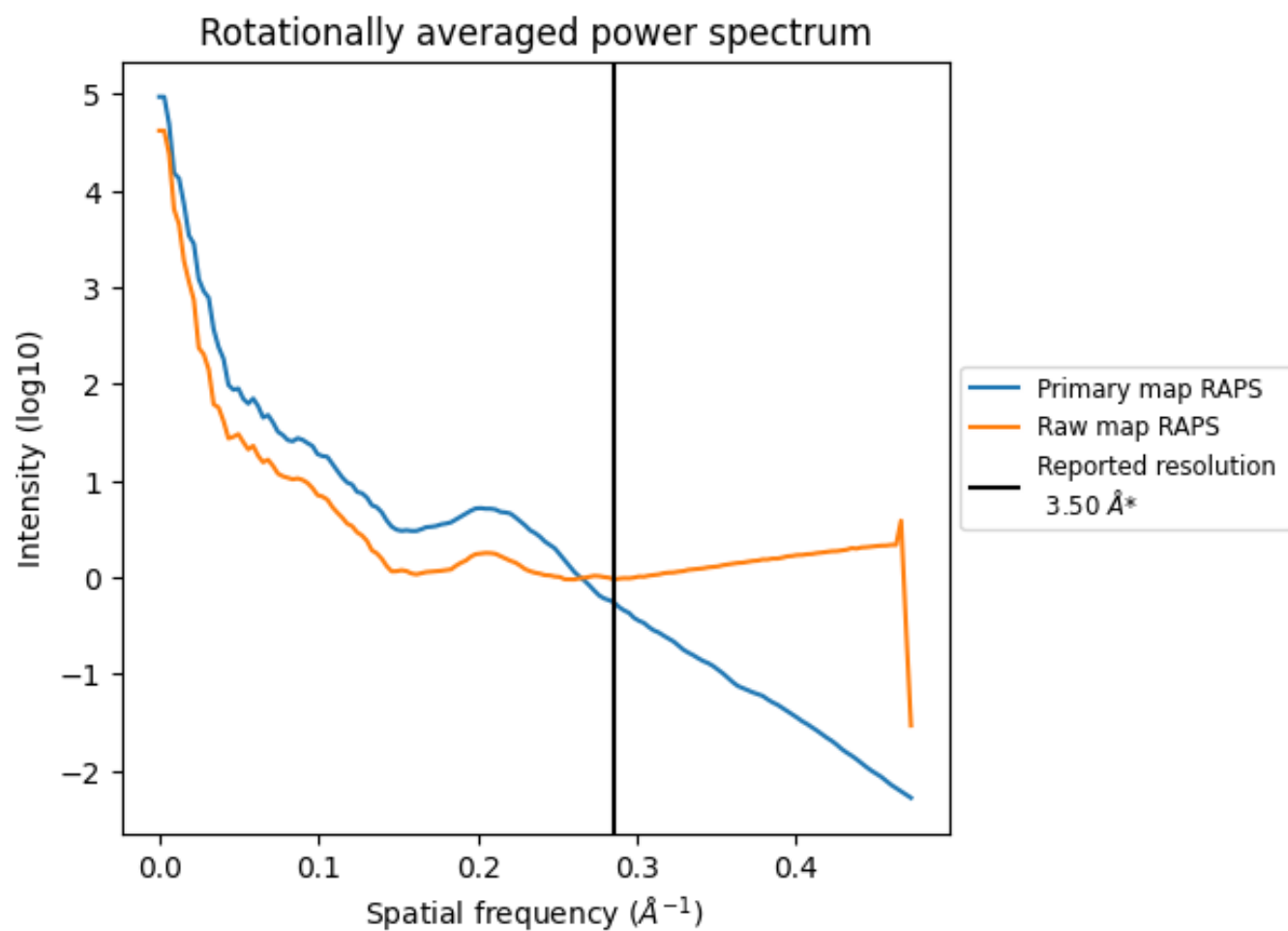


The volume at the recommended contour level is 163 nm<sup>3</sup>; this corresponds to an approximate mass of 147 kDa.

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 ⓘ

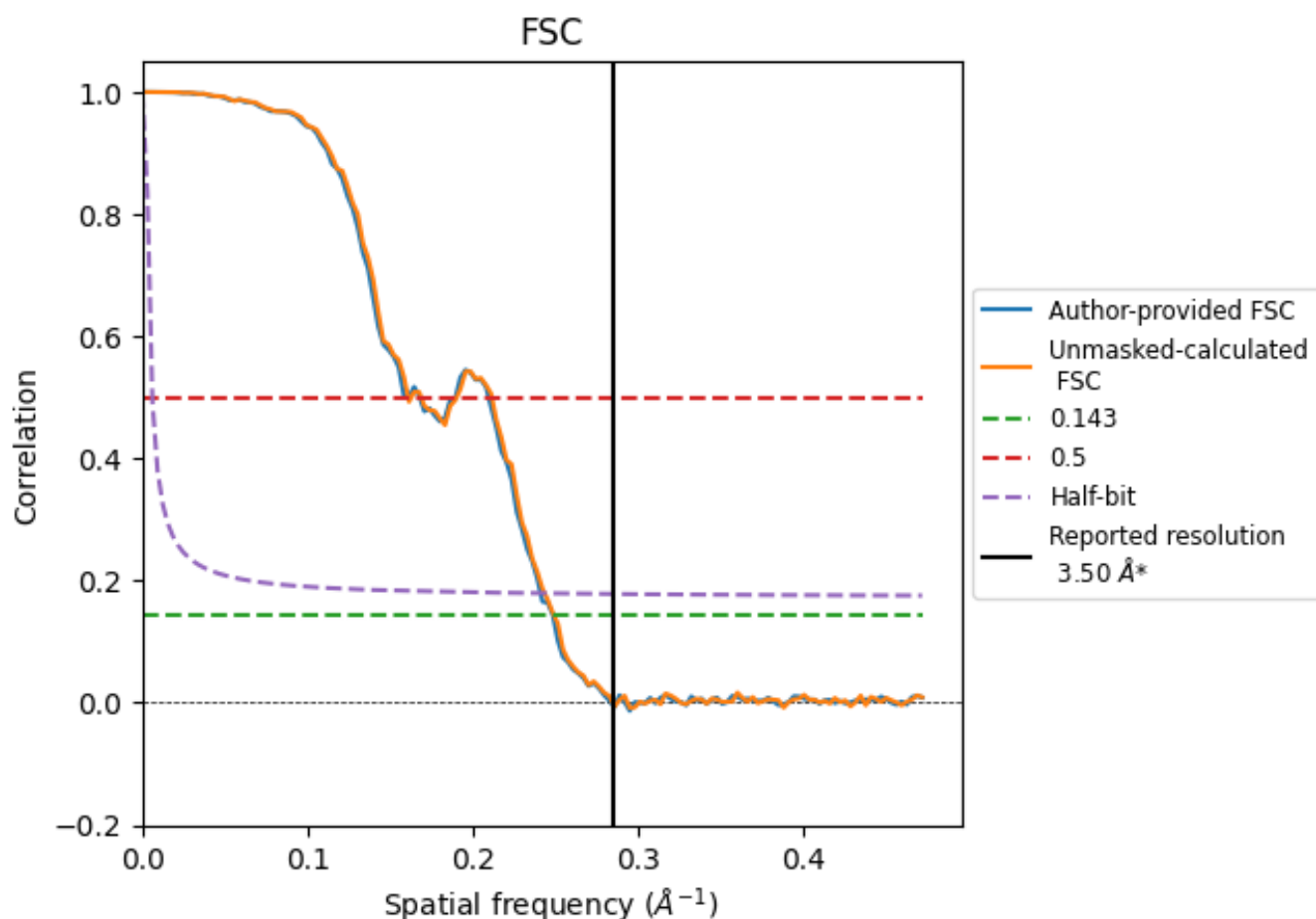


\*Reported resolution corresponds to spatial frequency of  $0.286 \text{ \AA}^{-1}$

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

## 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

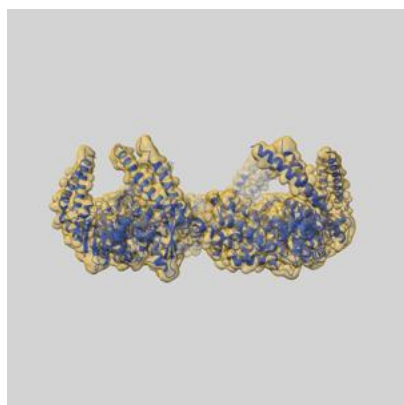
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 4.02 differs from the reported value 3.5 by more than 10 %

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 %

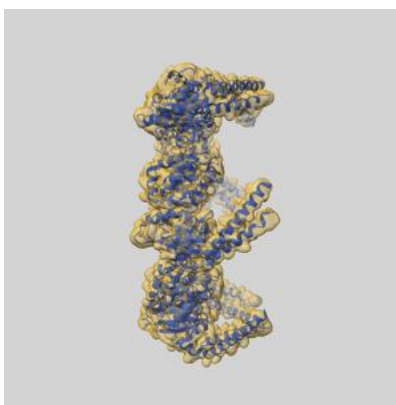
## 9 Map-model fit [i](#)

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](#).

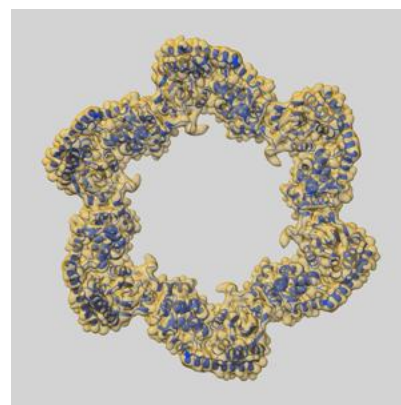
### 9.1 Map-model overlay [i](#)



X



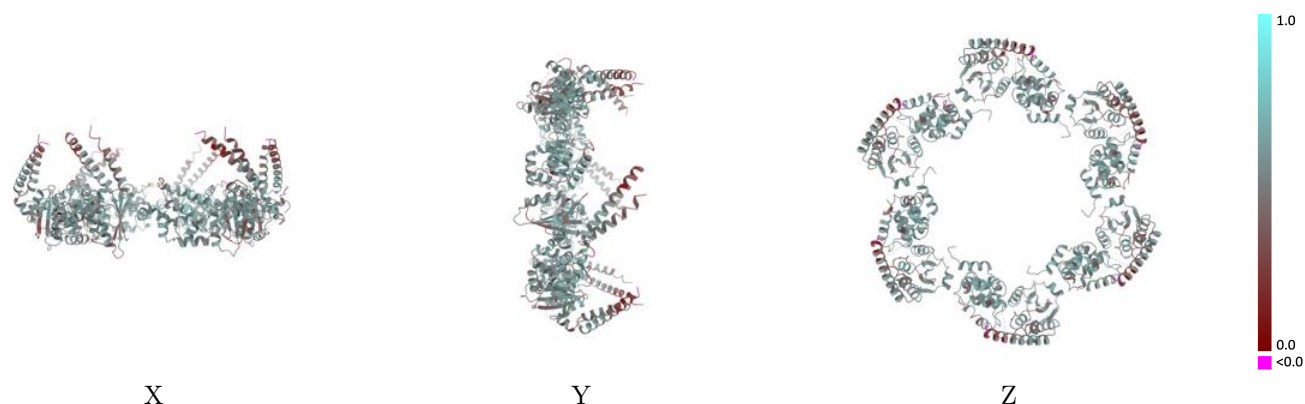
Y



Z

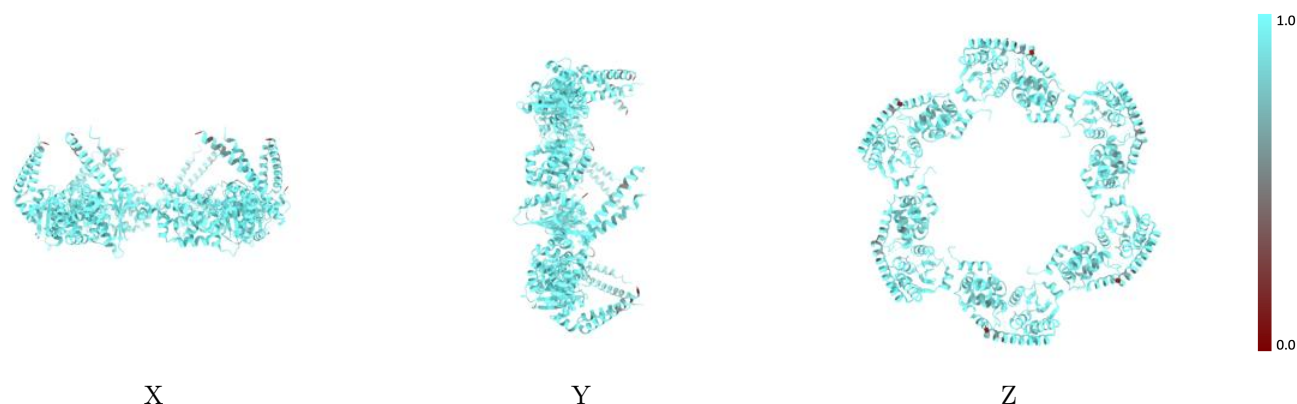
The images above show the 3D surface view of the map at the recommended contour level 1.95 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



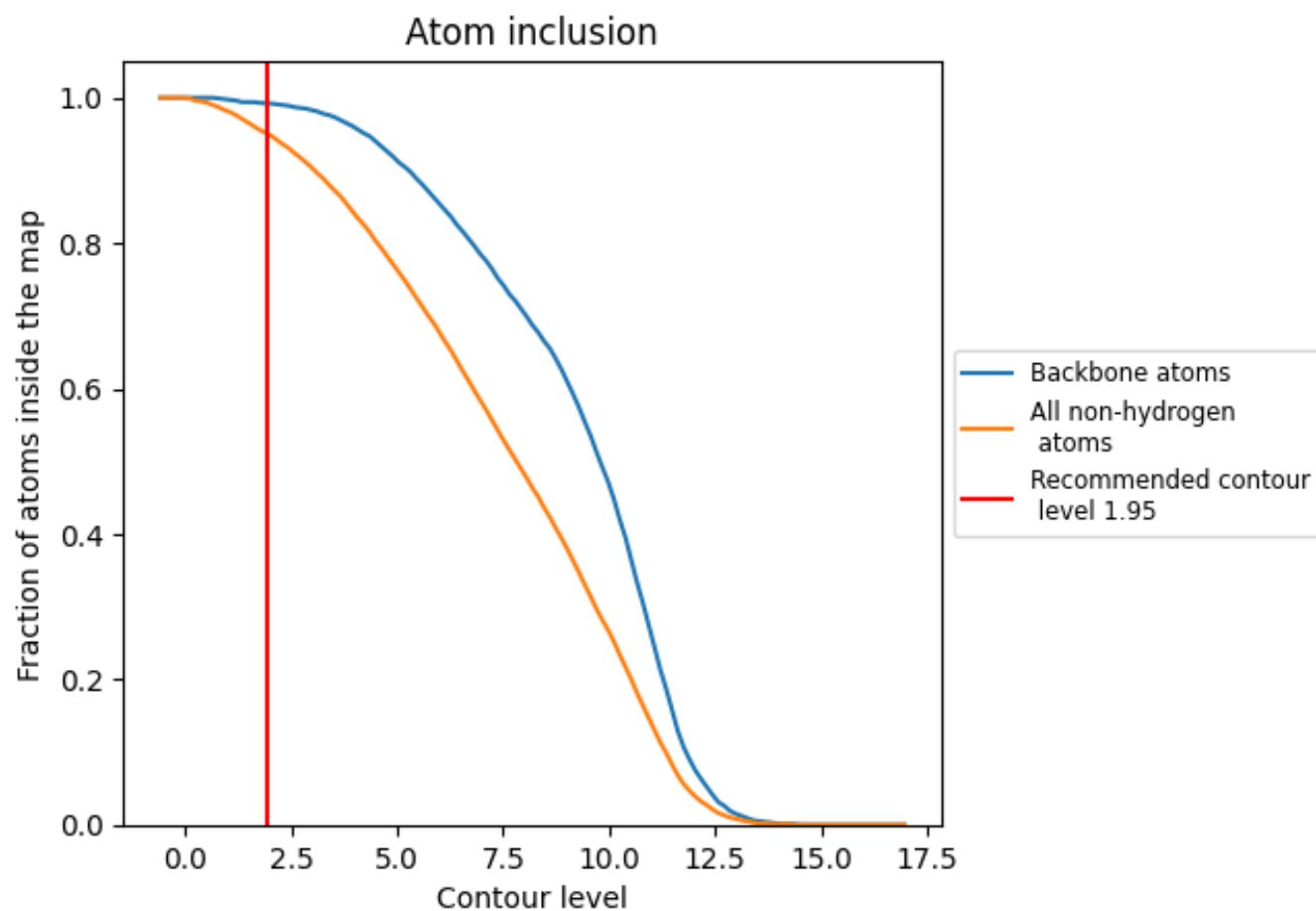
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	 0.9500	 0.5070
A	 0.9600	 0.5080
B	 0.9640	 0.5150
C	 0.9680	 0.5150
D	 0.9630	 0.5100
E	 0.9600	 0.5060
F	 0.9550	 0.5120
a	 0.9750	 0.5340
b	 0.9720	 0.5380
c	 0.9670	 0.5370
d	 0.9750	 0.5370
e	 0.9670	 0.5420
f	 0.9770	 0.5460
g	 0.8930	 0.4240
h	 0.8840	 0.4320
i	 0.8720	 0.4290
l	 0.8770	 0.4170
m	 0.8810	 0.4250
n	 0.8610	 0.4010

