



Full wwPDB EM Validation Report ⓘ

May 27, 2026 – 01:25 PM EDT

PDB ID : 13HR / pdb_000013hr
EMDB ID : EMD-77072
Title : Cryo-EM structure of Pseudomonas aeruginosa outer-membrane lipoprotein PA3214 bound to MCE protein PA3213 C-terminal peptide
Authors : Giacometti, S.I.; Coudray, N.; Bhabha, G.; Ekiert, D.C.
Deposited on : 2026-05-06
Resolution : 2.70 Å(reported)
Based on initial model : .

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

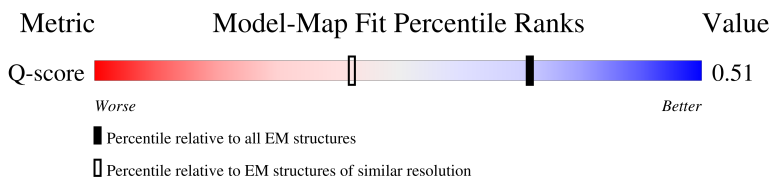
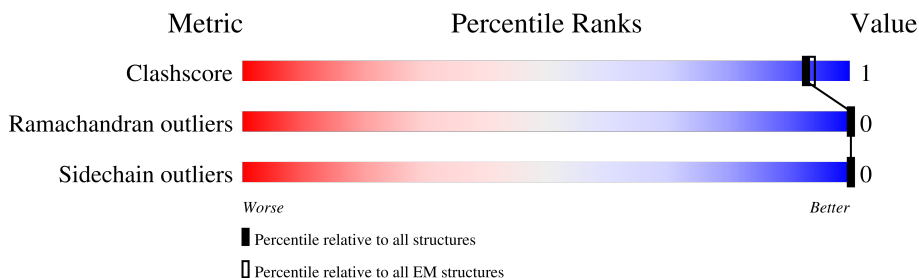
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.70 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.



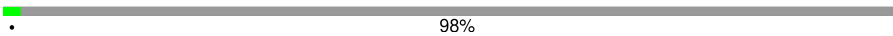
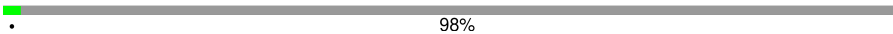
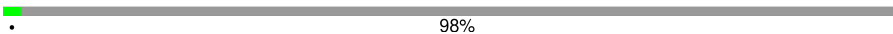
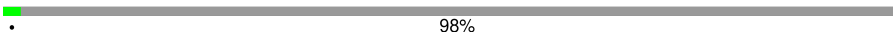
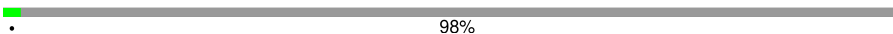
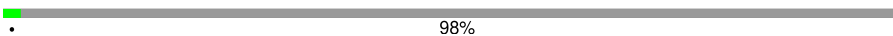
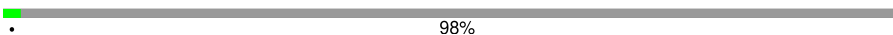
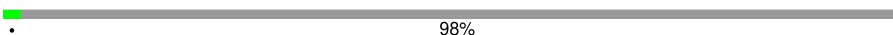
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10327 (2.20 - 3.20)

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

Mol	Chain	Length	Quality of chain
1	A	214	
1	B	214	
1	C	214	
1	D	214	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	E	214	 81%17%
1	F	214	 81%17%
1	G	214	 81%17%
1	H	214	 81%17%
2	I	312	 98%
2	J	312	 98%
2	K	312	 98%
2	L	312	 98%
2	M	312	 98%
2	N	312	 98%
2	O	312	 98%
2	P	312	 98%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 11520 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 ABC-type transport auxiliary lipoprotein component domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	178	Total	C	N	O	S	0	0
			1380	860	261	258	1		
1	B	178	Total	C	N	O	S	0	0
			1380	860	261	258	1		
1	C	178	Total	C	N	O	S	0	0
			1380	860	261	258	1		
1	D	178	Total	C	N	O	S	0	0
			1380	860	261	258	1		
1	E	178	Total	C	N	O	S	0	0
			1380	860	261	258	1		
1	F	178	Total	C	N	O	S	0	0
			1380	860	261	258	1		
1	G	178	Total	C	N	O	S	0	0
			1380	860	261	258	1		
1	H	178	Total	C	N	O	S	0	0
			1380	860	261	258	1		

- Molecule 2 is a protein called Mce/MlaD domain-containing protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	I	7	Total	C	N	O	0	0
			60	39	9	12		
2	J	7	Total	C	N	O	0	0
			60	39	9	12		
2	K	7	Total	C	N	O	0	0
			60	39	9	12		
2	L	7	Total	C	N	O	0	0
			60	39	9	12		
2	M	7	Total	C	N	O	0	0
			60	39	9	12		
2	N	7	Total	C	N	O	0	0
			60	39	9	12		

Continued on next page...

Continued from previous page...

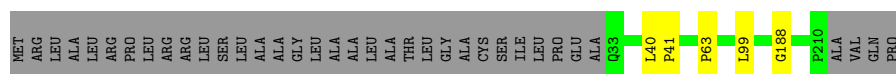
Mol	Chain	Residues	Atoms				AltConf	Trace
2	O	7	Total	C	N	O	0	0
			60	39	9	12		
2	P	7	Total	C	N	O	0	0
			60	39	9	12		

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.

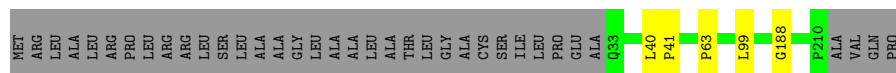
- Molecule 1: ABC-type transport auxiliary lipoprotein component domain-containing protein

Chain A: 



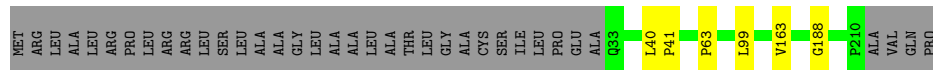
- Molecule 1: ABC-type transport auxiliary lipoprotein component domain-containing protein

Chain B: 



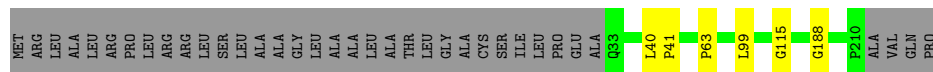
- Molecule 1: ABC-type transport auxiliary lipoprotein component domain-containing protein

Chain C: 



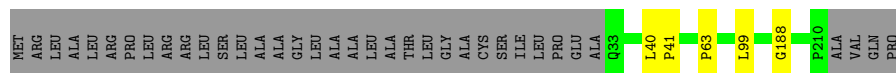
- Molecule 1: ABC-type transport auxiliary lipoprotein component domain-containing protein

Chain D: 



- Molecule 1: ABC-type transport auxiliary lipoprotein component domain-containing protein

Chain E: 



- Molecule 1: ABC-type transport auxiliary lipoprotein component domain-containing protein

MET	ARG	LEU	ALA	LEU	ARG	PRO	LEU	ARG	ARG	LEU	SER	LEU	ALA	GLY	LEU	ALA	ALA	ALA	ALA	THR	LEU	GLY	CYS	ILE	LEU	PRO	GLU	ALA	Q33	L40	P41	P63	L99	G188	P210	ALA	VAL	GLN	GLN
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	-----	-----	-----	-----

- | | | | | | |
|------|------|-----|-----|-----|-----|
| MET | ARG | LEU | ALA | LEU | ARG | PRO | LEU | ARG | ARG | SER | LEU | ALA | ALA | GLY | LEU | ALA | ALA | CYS | SER | ILE | LEU | PRO | GLU | ALA | 333 | L40 | P41 | P63 | G188 | P210 | ALA | VAL | GLN | PRO |
|------|------|-----|-----|-----|-----|

- | | | | | | |
|------|------|-----|-----|-----|-----|
| MET | ARG | LEU | ALA | LEU | ARG | PRO | LEU | ARG | ARG | LEU | SER | LEU | ALA | ALA | GLY | LEU | ALA | ALA | LEU | THR | LEU | GLY | ALA | ALA | Q93 | L40 | P41 | P63 | L99 | G188 | P210 | ALA | VAL | GLN | PRO |
|------|------|-----|-----|-----|-----|

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

GLY	ILE	LYS	VAL	GLY	ASP	VAL	ALA	ALA	LEU	ARG	ASP	PRO	LYS	ASP	ARG	VAL	TRP	ALA	ALA	ARG	ILE	ARG	ARG	VAL	VAL	ALA	ALA	ALA	SER	ASP	GLN	ASP	THR	THR	ALA	ALA	LYS	LEU	ALA	LEU	THR	GLY	ILE	ILE	ILE	GLN	LEU	SER	SER	GLY	THR	THR	PRO	ALA
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

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

ASP	GLN	ALA	THR	GLY	ALA	LEU	SER	GLU	ARG	GLU	ASN	VAL	SER	ALA	VAL	MET	GLN	GLN	LEU	ALA	GLN	ALA	ALA	SER	ARG	GLN	ASN	ALA	ALA	LEU	ALA	GLN	ALA	SER	GLU	LEU	MET	MET	ARG	SER	ALA	ASN	GLY	GLY	LEU	LEU	ASN	GLU	GLN	GLY	GLY	LYS	MET	LEU	MET	GLY	GLY	LYS	ASN	ASN	LYS
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

MET	ALA	SER	LEU	GLU	ARG	THR	SER	ALA	THR	THR	LEU	ASP	GLN	LEU	ILE	SER	GLU	ASN	ARG	HIS	SER	LEU	ASP	GLY	GLY	ILE	GLN	GLY	PRO	ALA	ALA	VAL	SER	GLU	LEU	ARG	ASP	THR	THR	LEU	ALA	ALA	LEU	LEU	ARG	GLY	ILE	SER	ARG	ARG	LEU	GLU	ASN	PRO	ALA	ALA	ASN
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

LEU	K306		
LEU	T307		
GLY	K308		
ARG			
GLU			P312

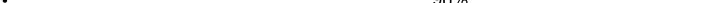
- | |
|-----|
| MET | GLU | THR | ARG | ALA | HIS | VAL | LEU | ILE | GLY | LEU | PHE | SER | VAL | ILE | ILE | VAL | ILE | GLY | ALA | ALA | LEU | LEU | PHE | GLY | THR | LEU | LEU | ALA | LYS | SER | GLY | SER | GLU | GLY | LYS | PHE | ASN | TYR | TYR | ASP | ILE | VAL | PHE | ASN | ASN | GLU | GLU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

GLY ILE LYS VAL GLY ASP VAL VAL VAL PHE LEU LEU ARG ARG ASP ASP PRO PRO LYS LYS ASP ASP PRO PRO ARG ARG LYS VAL TRP TRP ALA TRP ALA ARG ILE ILE ARG ARG VAL VAL VAL VAL ALA ALA ALA ALA ALA PRO PRO ILE ILE LYS LYS GLN LYS ASP ASP THR THR THR THR ALA ALA LYS LYS LEU LEU ALA ALA LEU LEU THR THR GLY GLY ILE ILE THR THR GLY GLY THR THR SER SER ILE ILE ILE ILE GLN GLN LEU LEU SER SER SER SER GLY GLY THR THR PRO PRO ALA ALA

[illegible]

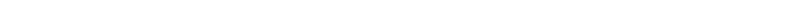
[illegible]

- Molecule 2: Mce/MlaD domain-containing protein

Chain K:  98%

LEU	GLY	GLN	ASP	PRO	GLY	MET
LEU	GLY	GLN	ASP	PRO	GLY	MET
GLY	SER	ALA	ALA	MET	LYS	THR
ARG	LEU	THR	GLY	GLU	VAL	ARG
GLU	GLY	GLY	ALA	LYS	ASP	ALA
K306	THR	LEU	LEU	LYS	VAL	HIS
T367	THR	ALA	ALA	GLY	ALA	HIS
K308	THR	ALA	ALA	LYS	PHE	LEU
P312	THR	LEU	LEU	PRO	ARG	GLY
	ASP	GLU	GLU	VAL	LEU	LEU
	GLN	ASN	ASN	ILE	ASP	PHE
	LEU	VAL	VAL	VAL	PRO	SER
	ILE	SER	ALA	THR	LYS	VAL
	SER	ALA	MET	THR	ASP	ILE
	GLY	GLN	GLN	PRO	ARG	GLY
	ARG	GLN	GLN	LEU	LYS	ALA
	HIS	LEU	ALA	LEU	VAL	ALA
	SER	LEU	ALA	GLN	TRP	ALA
	LEU	ALA	GLN	LEU	ALA	LEU
	ASP	GLY	GLN	LEU	ARG	LEU
	GLY	SER	ALA	LEU	ILE	PHE
	ILE	ARG	GLN	SER	ARG	GLY
	GLN	GLN	GLN	ASN	VAL	LEU
	GLY	ALA	ALA	GLU	TRP	LEU
	LEU	ASN	ASP	ASP	ALA	LEU
	ALA	ALA	LEU	LEU	ALA	ALA
	GLU	ALA	MET	LEU	PRO	LYS
	LEU	LEU	GLY	GLY	ILE	SER
	GLY	ALA	ASN	ASN	LYS	GLY
	PRO	GLN	ILE	ILE	GLN	GLU
	ALA	ALA	ASN	ASN	ASP	GLY
	VAL	SER	GLN	GLN	THR	LYS
	SER	GLU	GLU	THR	THR	PHE
	GLU	LEU	LEU	ILE	ALA	ASN
	LEU	MET	MET	ALA	LYS	TYR
	ARG	ARG	SER	ARG	LEU	TYR
	ASP	SER	ALA	PHE	ALA	ASP
	THR	ALA	SER	SER	LEU	ILE
	LEU	ASN	ASN	THR	THR	VAL
	ALA	GLY	GLY	LEU	GLY	PHE
	ALA	LEU	LEU	LEU	ILE	ASN
	LEU	LEU	LEU	SER	THR	GLU
	ARG	ASN	ASN	GLU	GLY	ALA
	GLY	GLU	GLU	GLU	THR	VAL
	ILE	ILE	GLN	ASN	SER	SER
	SER	GLY	GLY	THR	ILE	GLY
	ARG	LYS	LYS	ALA	ILE	LEU
	ARG	GLY	GLY	ARG	GLN	SER
	LEU	MET	ILE	ILE	LEU	GLN
	GLU	LEU	SER	SER	SER	GLY
	GLU	GLU	ARG	THR	SER	SER
	ASN	ASN	ASN	THR	GLY	SER
	PRO	ALA	ALA	LEU	THR	VAL
	ALA	ASN	ASN	ASP	PRO	GLN
	ASN	LYS	LYS	HIS	TYR	ALA
	THR	THR	THR	ILE	SER	SER

- Molecule 2: Mce/MlaD domain-containing protein

Chain L:  98%

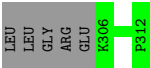
[illegible]

- Molecule 2: Mce/MlaD domain-containing protein

Chain M: 98%

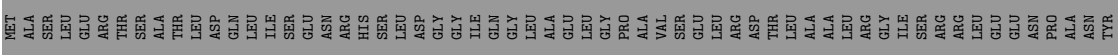
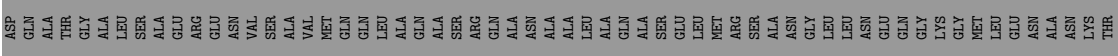
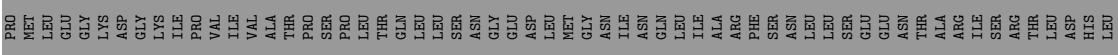
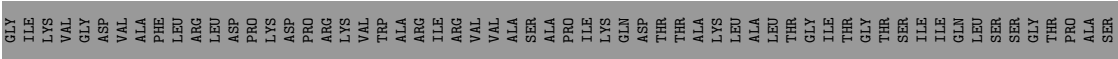
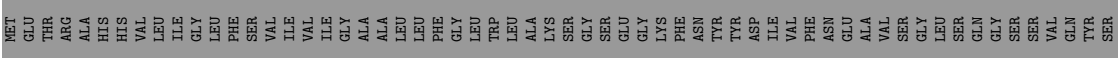


WORLD WIDE
PDB
PROTEIN DATA BANK



- Molecule 2: Mce/MlaD domain-containing protein

Chain P: 98%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C8	Depositor
Number of particles used	378252	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 ($e^-/\text{\AA}^2$)	51.51, 51.43	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k), GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.302	Depositor
Minimum map value	-0.409	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.050	Depositor
Recommended contour level	0.249	Depositor
Map size ($\text{\AA}$)	277.248, 277.248, 277.248	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.083, 1.083, 1.083	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	0.14	0/1408	0.32	0/1915
1	B	0.14	0/1408	0.32	0/1915
1	C	0.14	0/1408	0.32	0/1915
1	D	0.14	0/1408	0.32	0/1915
1	E	0.14	0/1408	0.32	0/1915
1	F	0.14	0/1408	0.32	0/1915
1	G	0.14	0/1408	0.32	0/1915
1	H	0.14	0/1408	0.32	0/1915
2	I	0.09	0/61	0.17	0/79
2	J	0.09	0/61	0.17	0/79
2	K	0.08	0/61	0.18	0/79
2	L	0.09	0/61	0.18	0/79
2	M	0.08	0/61	0.17	0/79
2	N	0.08	0/61	0.17	0/79
2	O	0.09	0/61	0.17	0/79
2	P	0.09	0/61	0.17	0/79
All	All	0.14	0/11752	0.32	0/15952

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	1380	0	1375	3	0
1	B	1380	0	1375	3	0
1	C	1380	0	1375	4	0
1	D	1380	0	1375	4	0
1	E	1380	0	1375	3	0
1	F	1380	0	1375	3	0
1	G	1380	0	1375	3	0
1	H	1380	0	1375	3	0
2	I	60	0	61	1	0
2	J	60	0	61	1	0
2	K	60	0	61	1	0
2	L	60	0	61	1	0
2	M	60	0	61	1	0
2	N	60	0	61	0	0
2	O	60	0	61	0	0
2	P	60	0	61	1	0
All	All	11520	0	11488	31	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 1.

All (31) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:163:VAL:HB	1:D:115:GLY:HA2	1.94	0.50
1:H:40:LEU:HD12	1:H:41:PRO:HD2	1.97	0.47
1:A:40:LEU:HD12	1:A:41:PRO:HD2	1.97	0.47
1:G:40:LEU:HD12	1:G:41:PRO:HD2	1.97	0.47
1:B:40:LEU:HD12	1:B:41:PRO:HD2	1.97	0.46
1:F:40:LEU:HD12	1:F:41:PRO:HD2	1.97	0.46
1:E:40:LEU:HD12	1:E:41:PRO:HD2	1.97	0.46
1:C:40:LEU:HD12	1:C:41:PRO:HD2	1.97	0.45
1:D:40:LEU:HD12	1:D:41:PRO:HD2	1.97	0.45
2:I:308:LYS:HE2	2:I:308:LYS:HB3	1.83	0.44
1:D:63:PRO:HG2	1:D:99:LEU:HD23	2.00	0.44
1:C:63:PRO:HG2	1:C:99:LEU:HD23	2.00	0.44
1:B:63:PRO:HG2	1:B:99:LEU:HD23	2.00	0.43
1:E:63:PRO:HG2	1:E:99:LEU:HD23	2.00	0.43
1:H:63:PRO:HG2	1:H:99:LEU:HD23	1.99	0.43
2:L:308:LYS:HE2	2:L:308:LYS:HB3	1.83	0.43
1:A:63:PRO:HG2	1:A:99:LEU:HD23	2.00	0.43
1:F:41:PRO:HG2	1:F:188:GLY:HA3	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:63:PRO:HG2	1:F:99:LEU:HD23	2.00	0.43
1:E:41:PRO:HG2	1:E:188:GLY:HA3	2.01	0.43
1:G:63:PRO:HG2	1:G:99:LEU:HD23	2.00	0.43
2:M:308:LYS:HB3	2:M:308:LYS:HE2	1.83	0.42
1:D:41:PRO:HG2	1:D:188:GLY:HA3	2.01	0.42
2:K:308:LYS:HE2	2:K:308:LYS:HB3	1.83	0.42
1:G:41:PRO:HG2	1:G:188:GLY:HA3	2.01	0.42
2:J:308:LYS:HE2	2:J:308:LYS:HB3	1.83	0.42
1:C:41:PRO:HG2	1:C:188:GLY:HA3	2.01	0.42
1:B:41:PRO:HG2	1:B:188:GLY:HA3	2.01	0.41
1:H:41:PRO:HG2	1:H:188:GLY:HA3	2.01	0.41
1:A:41:PRO:HG2	1:A:188:GLY:HA3	2.01	0.41
2:P:308:LYS:HE2	2:P:308:LYS:HB3	1.83	0.41

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	176/214 (82%)	172 (98%)	4 (2%)	0	100	100
1	B	176/214 (82%)	172 (98%)	4 (2%)	0	100	100
1	C	176/214 (82%)	172 (98%)	4 (2%)	0	100	100
1	D	176/214 (82%)	172 (98%)	4 (2%)	0	100	100
1	E	176/214 (82%)	172 (98%)	4 (2%)	0	100	100
1	F	176/214 (82%)	172 (98%)	4 (2%)	0	100	100
1	G	176/214 (82%)	172 (98%)	4 (2%)	0	100	100
1	H	176/214 (82%)	172 (98%)	4 (2%)	0	100	100
2	I	5/312 (2%)	5 (100%)	0	0	100	100
2	J	5/312 (2%)	5 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	K	5/312 (2%)	5 (100%)	0	0	100	100
2	L	5/312 (2%)	5 (100%)	0	0	100	100
2	M	5/312 (2%)	5 (100%)	0	0	100	100
2	N	5/312 (2%)	5 (100%)	0	0	100	100
2	O	5/312 (2%)	5 (100%)	0	0	100	100
2	P	5/312 (2%)	5 (100%)	0	0	100	100
All	All	1448/4208 (34%)	1416 (98%)	32 (2%)	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	A	145/170 (85%)	145 (100%)	0	100	100
1	B	145/170 (85%)	145 (100%)	0	100	100
1	C	145/170 (85%)	145 (100%)	0	100	100
1	D	145/170 (85%)	145 (100%)	0	100	100
1	E	145/170 (85%)	145 (100%)	0	100	100
1	F	145/170 (85%)	145 (100%)	0	100	100
1	G	145/170 (85%)	145 (100%)	0	100	100
1	H	145/170 (85%)	145 (100%)	0	100	100
2	I	7/251 (3%)	7 (100%)	0	100	100
2	J	7/251 (3%)	7 (100%)	0	100	100
2	K	7/251 (3%)	7 (100%)	0	100	100
2	L	7/251 (3%)	7 (100%)	0	100	100
2	M	7/251 (3%)	7 (100%)	0	100	100
2	N	7/251 (3%)	7 (100%)	0	100	100
2	O	7/251 (3%)	7 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	P	7/251 (3%)	7 (100%)	0	100	100
All	All	1216/3368 (36%)	1216 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	87	GLN
1	A	124	GLN
1	A	137	GLN
1	B	33	GLN
1	B	87	GLN
1	B	124	GLN
1	B	137	GLN
1	C	33	GLN
1	C	87	GLN
1	C	124	GLN
1	C	137	GLN
1	D	33	GLN
1	D	87	GLN
1	D	124	GLN
1	D	137	GLN
1	E	33	GLN
1	E	87	GLN
1	E	124	GLN
1	E	137	GLN
1	F	33	GLN
1	F	87	GLN
1	F	124	GLN
1	F	137	GLN
1	G	33	GLN
1	G	87	GLN
1	G	124	GLN
1	G	137	GLN
1	H	33	GLN
1	H	87	GLN
1	H	124	GLN
1	H	137	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

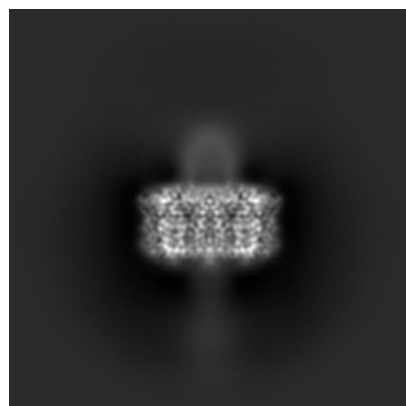
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-77072. These allow visual inspection of the internal detail of the map and identification of artifacts.

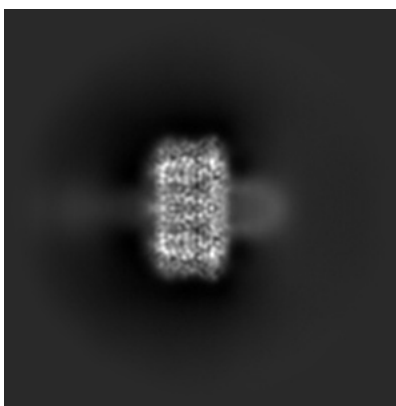
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

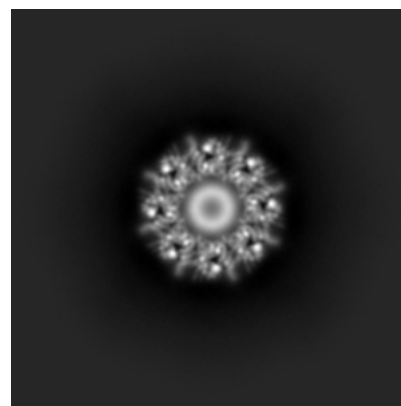
6.1.1 Primary map



X

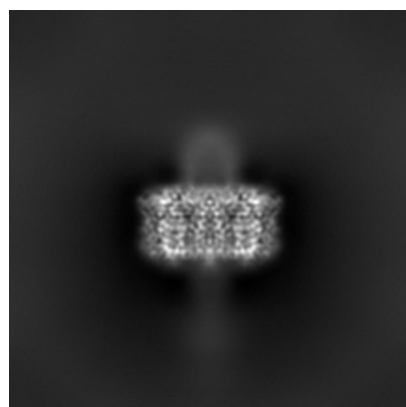


Y

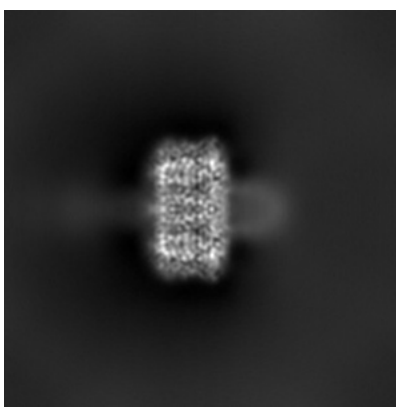


Z

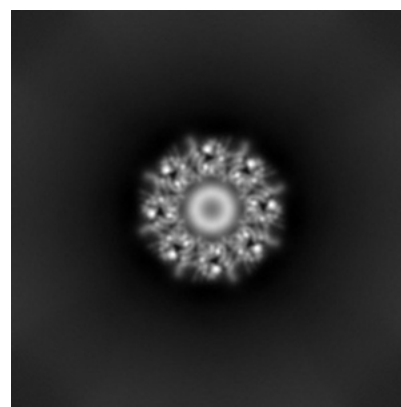
6.1.2 Raw map



X



Y

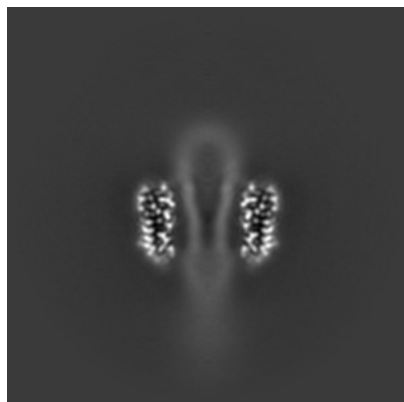


Z

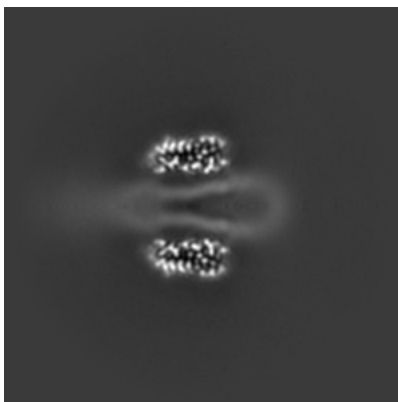
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

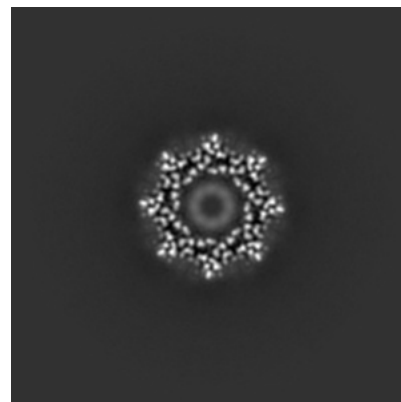
6.2.1 Primary map



X Index: 128

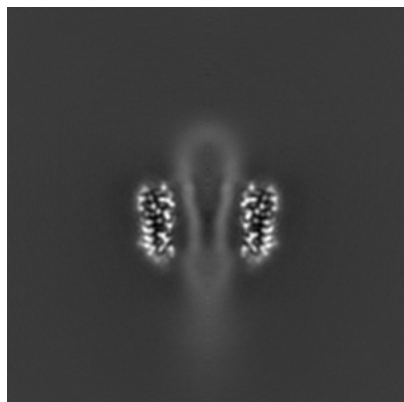


Y Index: 128

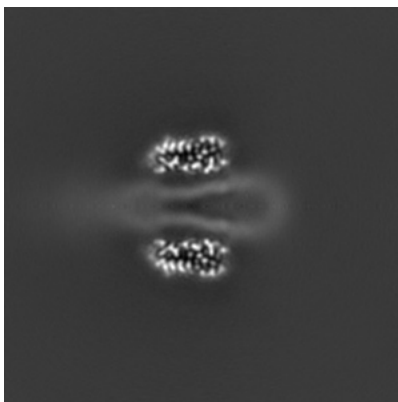


Z Index: 128

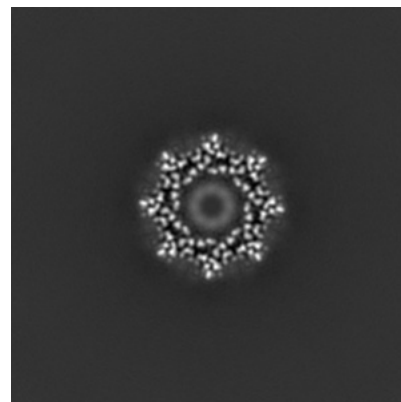
6.2.2 Raw map



X Index: 128



Y Index: 128

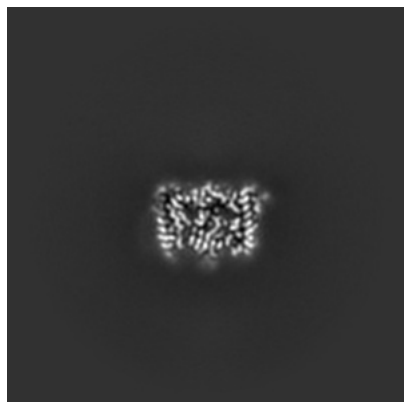


Z Index: 128

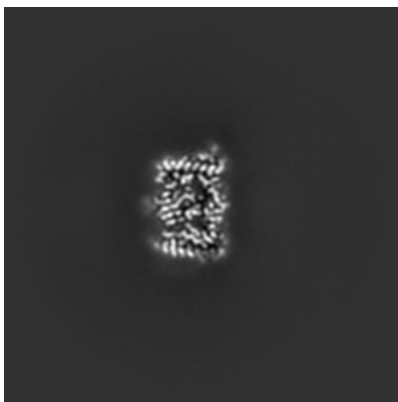
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

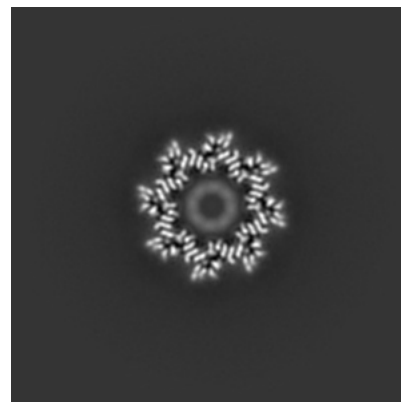
6.3.1 Primary map



X Index: 100

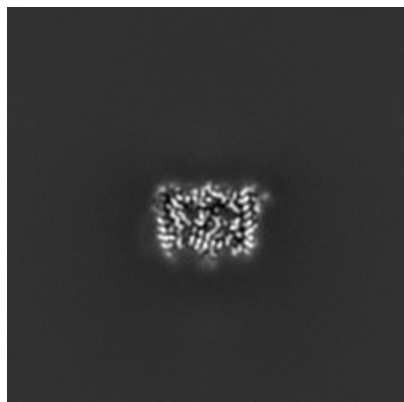


Y Index: 156

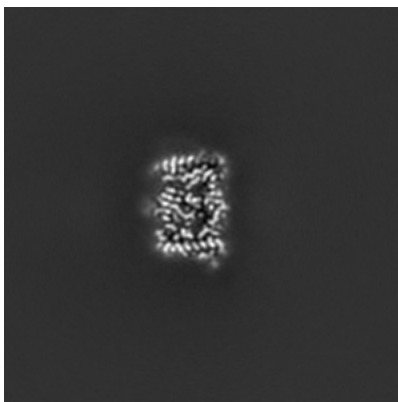


Z Index: 133

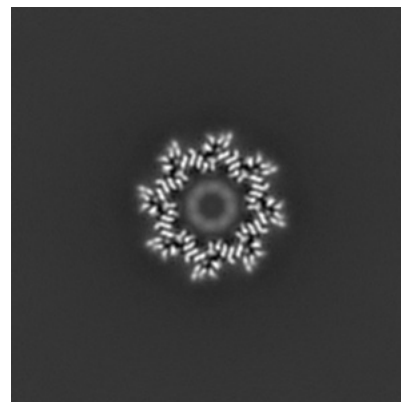
6.3.2 Raw map



X Index: 100



Y Index: 100

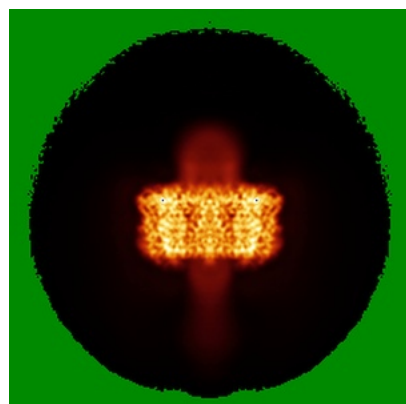


Z Index: 133

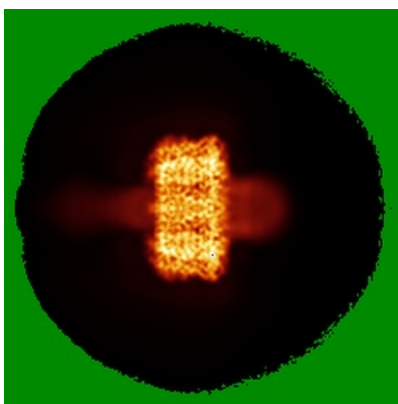
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X

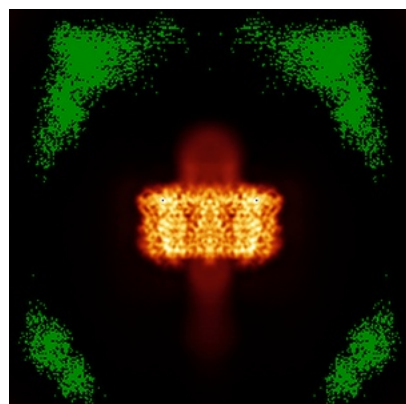


Y

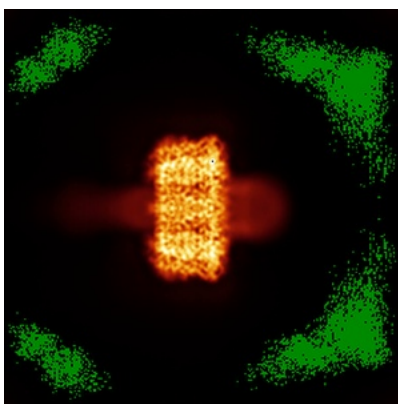


Z

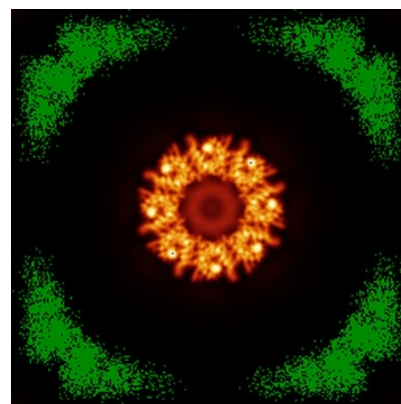
6.4.2 Raw map



X



Y

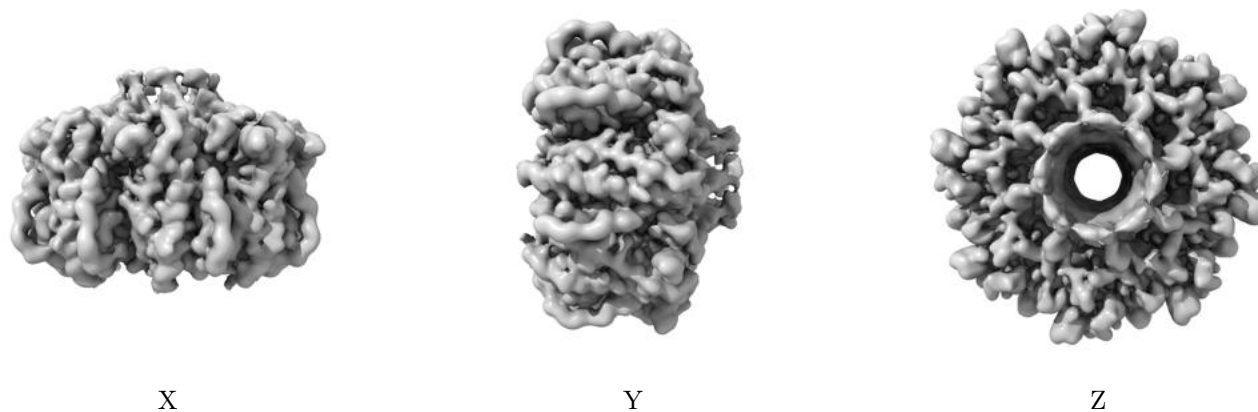


Z

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.

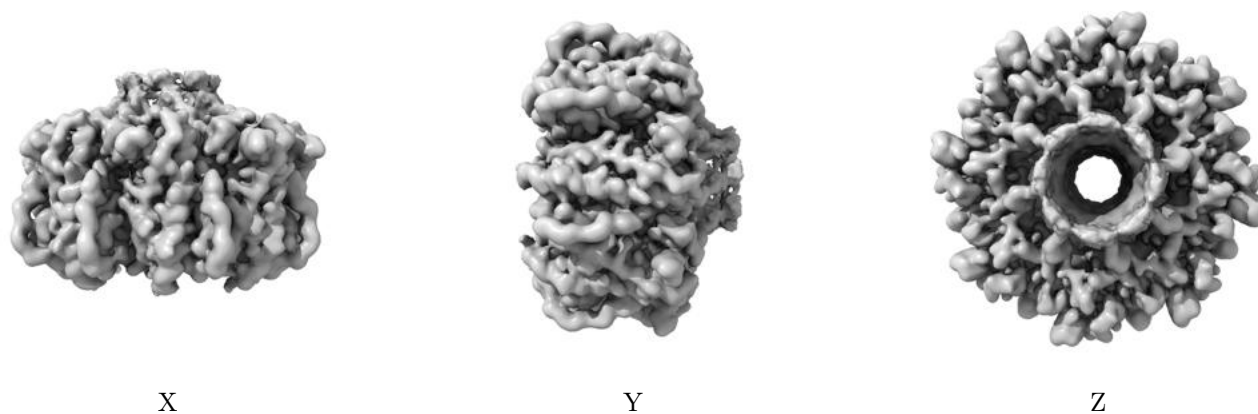
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.249. 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.

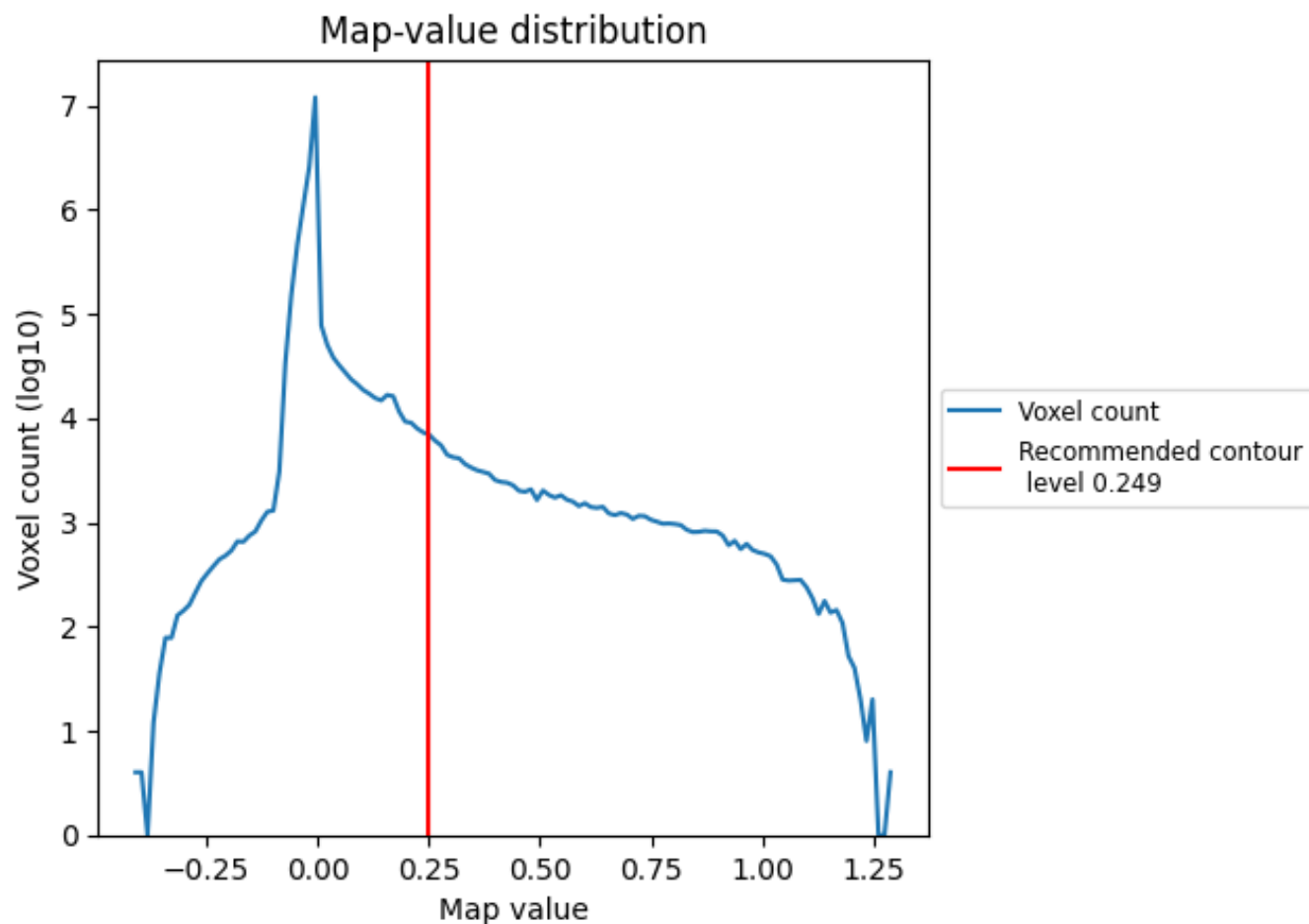
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

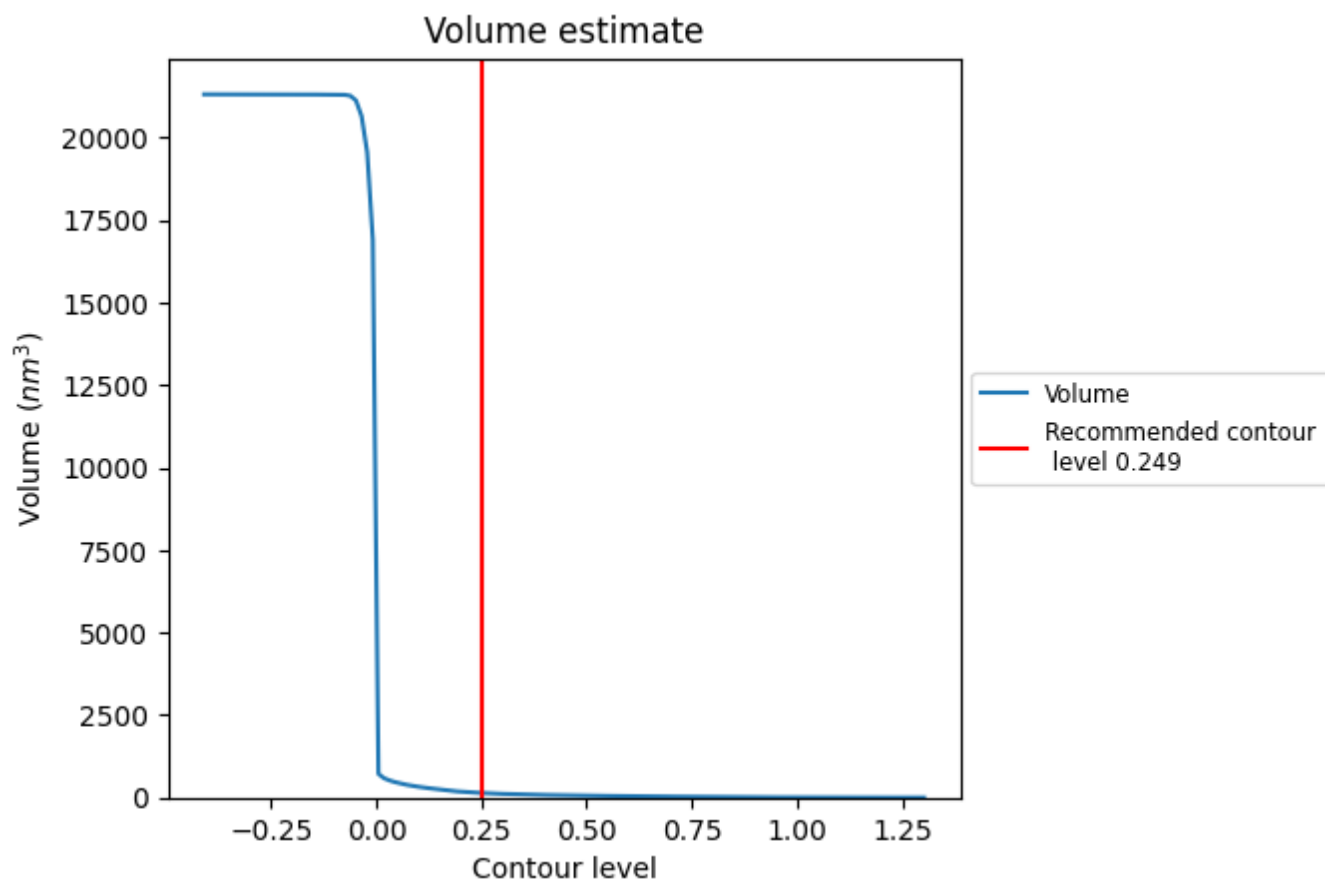
This section contains the results of statistical analysis of the map.

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.

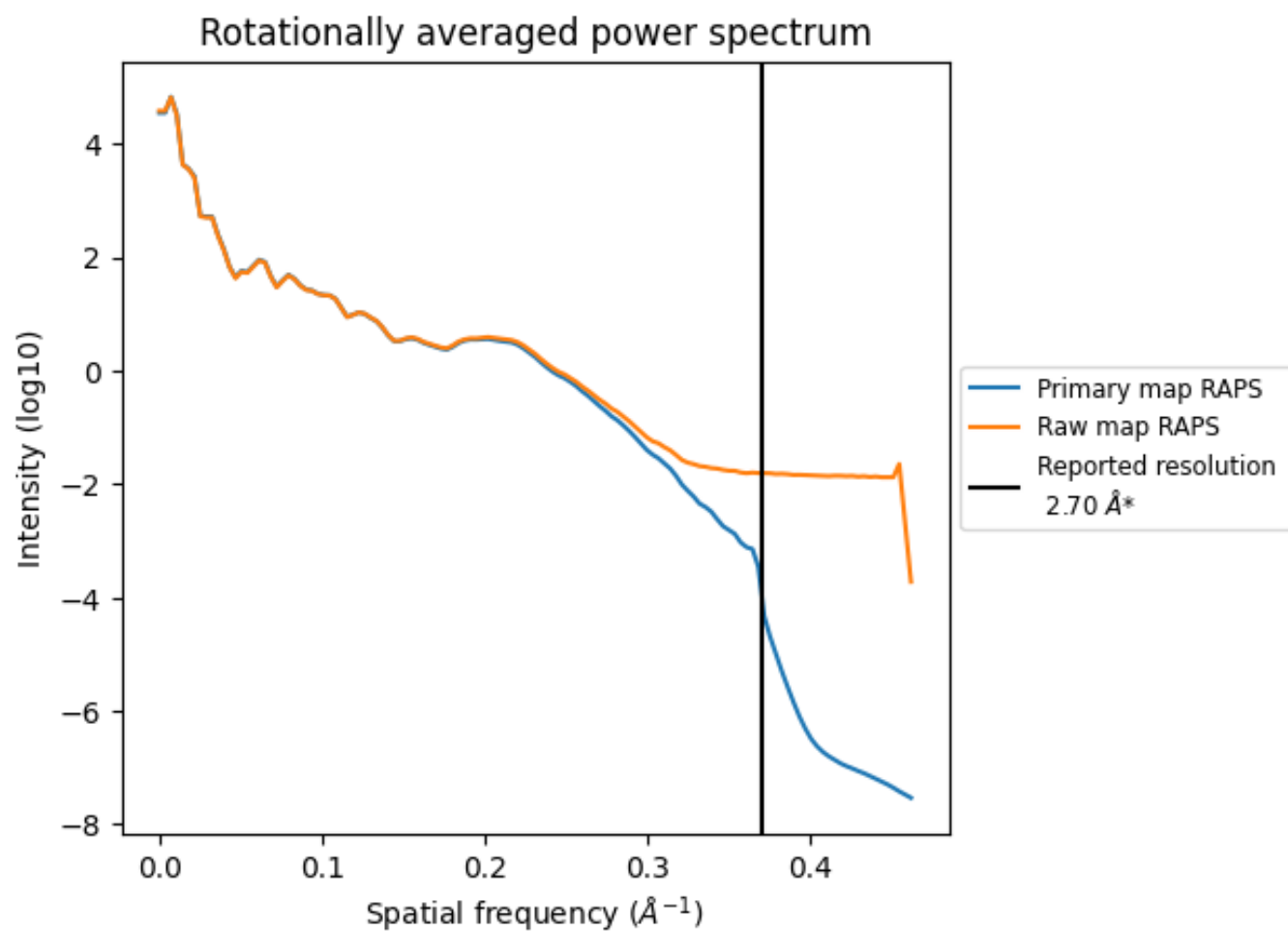
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 140 nm³; this corresponds to an approximate mass of 127 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 ⓘ

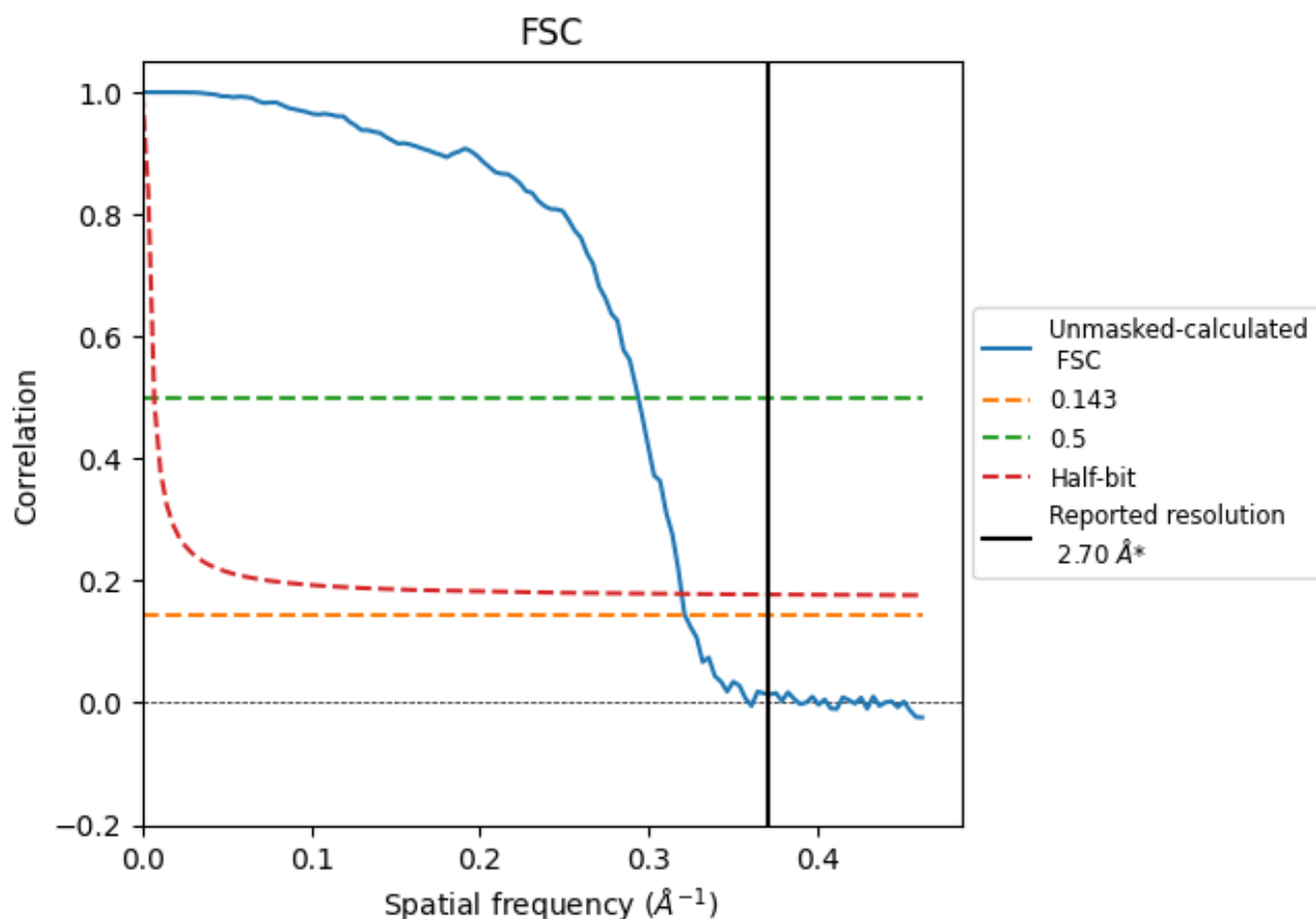


*Reported resolution corresponds to spatial frequency of 0.370 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.370 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

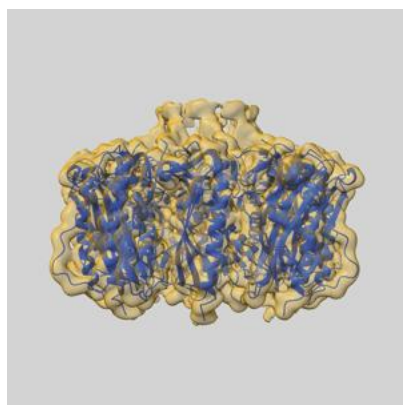
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.11	3.41	3.13

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.11 differs from the reported value 2.7 by more than 10 %

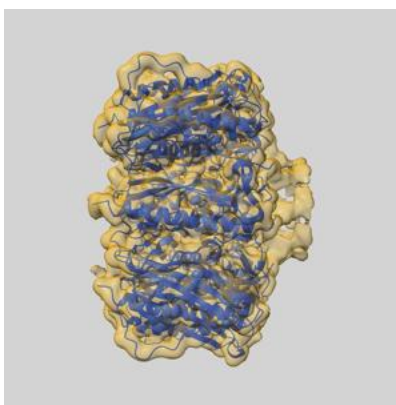
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-77072 and PDB model 13HR. Per-residue inclusion information can be found in section [3](#) on page [6](#).

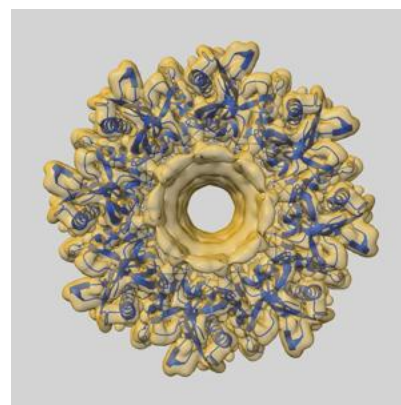
9.1 Map-model overlay [i](#)



X



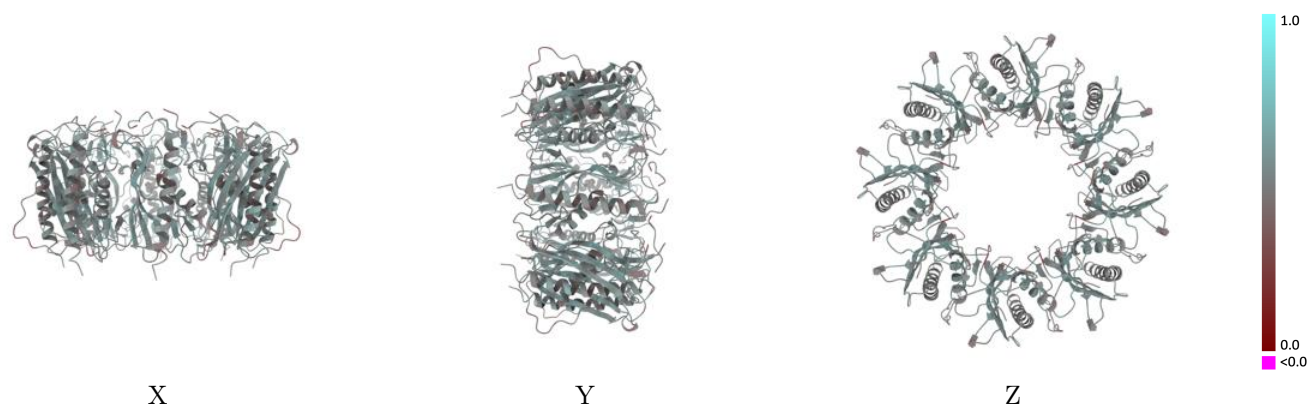
Y



Z

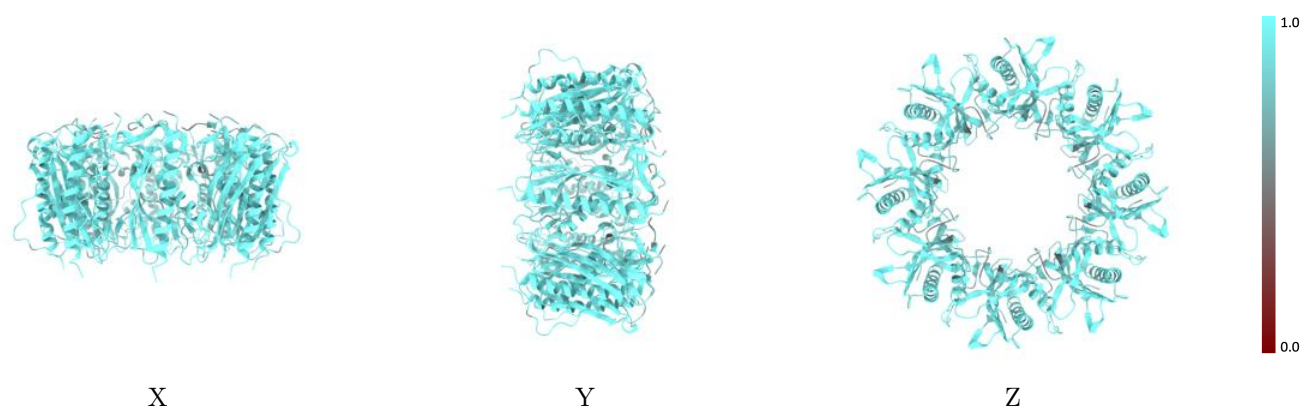
The images above show the 3D surface view of the map at the recommended contour level 0.249 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



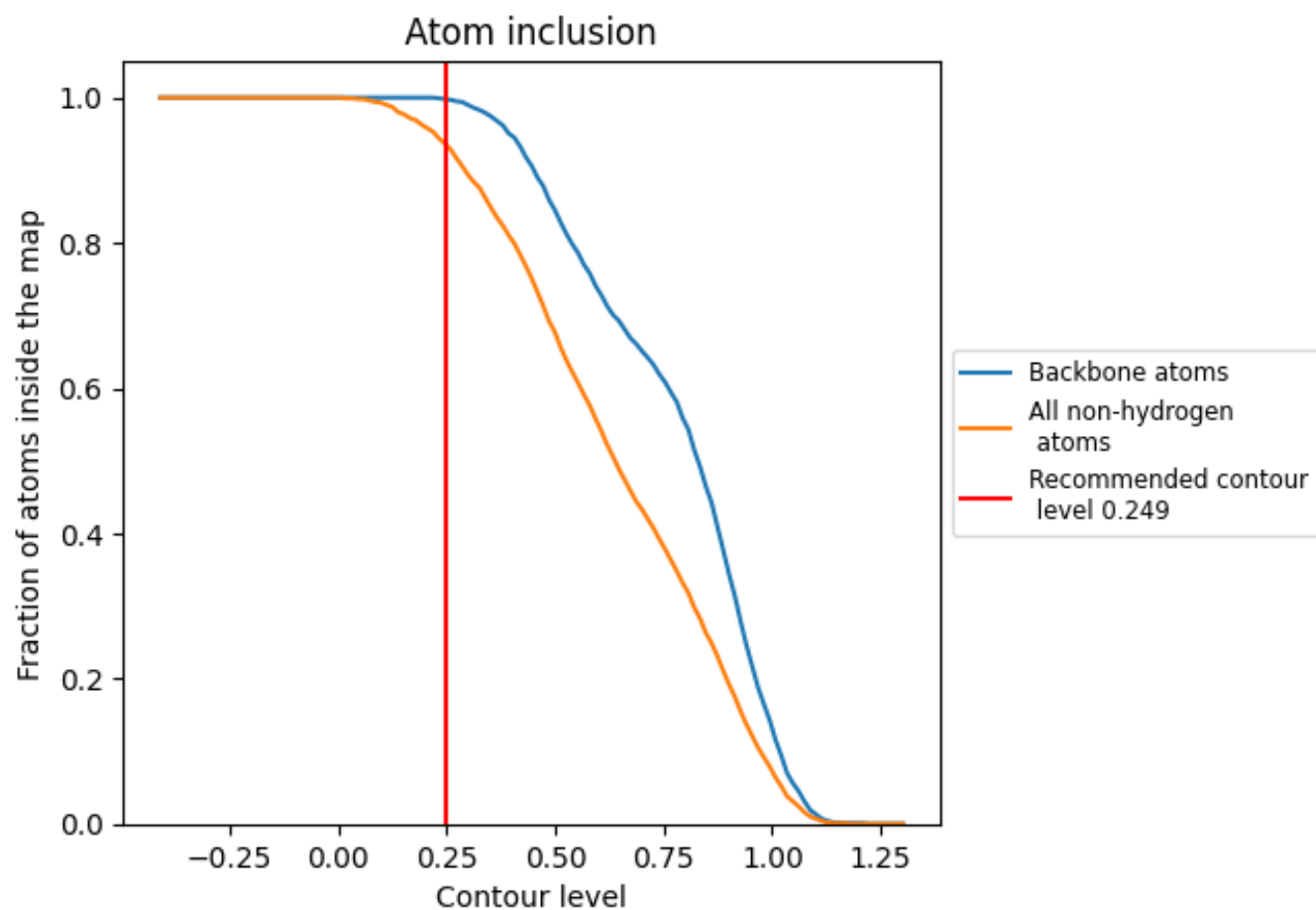
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.249).

9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 94% 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 (0.249) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9350	0.5100
A	0.9510	0.5150
B	0.9480	0.5160
C	0.9450	0.5080
D	0.9480	0.5160
E	0.9480	0.5100
F	0.9480	0.5140
G	0.9480	0.5100
H	0.9480	0.5140
I	0.6500	0.4500
J	0.6500	0.4540
K	0.6670	0.4570
L	0.6500	0.4530
M	0.6500	0.4520
N	0.6500	0.4500
O	0.6670	0.4530
P	0.6500	0.4550

1.0

0.0

<0.0