



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 08:41 PM UTC

PDB ID : 8CK1 / pdb_00008ck1
EMDB ID : EMD-16689
Title : Carin 1 bacteriophage tail, connector and tail fibers assembly
Authors : d'Acapito, A.; Neumann, E.; Schoehn, G.
Deposited on : 2023-02-14
Resolution : 3.90 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

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:

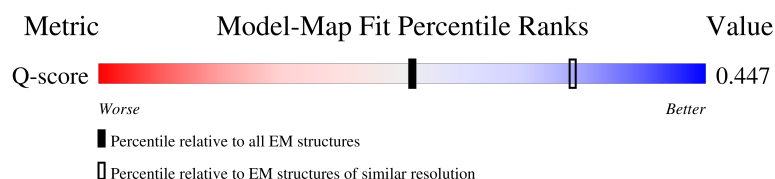
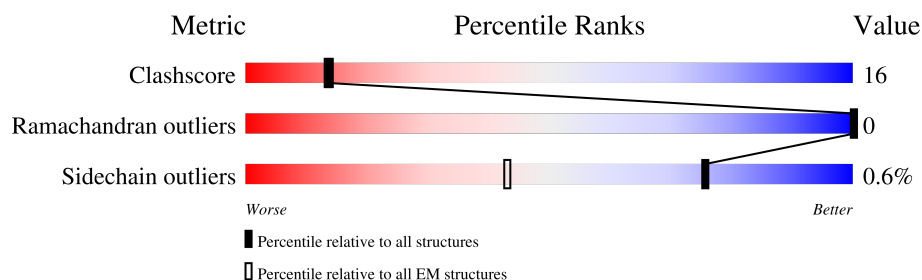
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

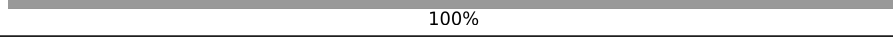
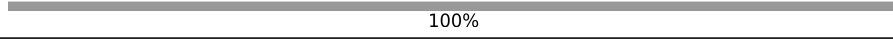
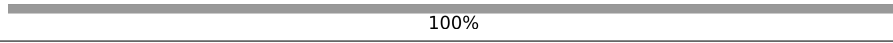
The reported resolution of this entry is 3.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8855 (3.40 - 4.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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	820	 72% 27%
2	B	523	 100%
2	C	523	 100%
2	D	523	 100%

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Mol	Chain	Length	Quality of chain
3	E	222	9% 63% 30% 7%
3	F	222	7% 57% 36% 7%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12580 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 Tail Nozzle.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	826	Total	C	N	O	S	0	0
			6419	4040	1100	1269	10		

- Molecule 2 is a protein called Tail fibers Dpo36.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	126	Total	C	N	O	S	0	0
			989	608	158	222	1		
2	B	126	Total	C	N	O	S	0	0
			989	608	158	222	1		
2	C	126	Total	C	N	O	S	0	0
			989	608	158	222	1		

- Molecule 3 is a protein called Connector Protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	206	Total	C	N	O	S	0	0
			1597	997	279	310	11		
3	F	206	Total	C	N	O	S	0	0
			1597	997	279	310	11		

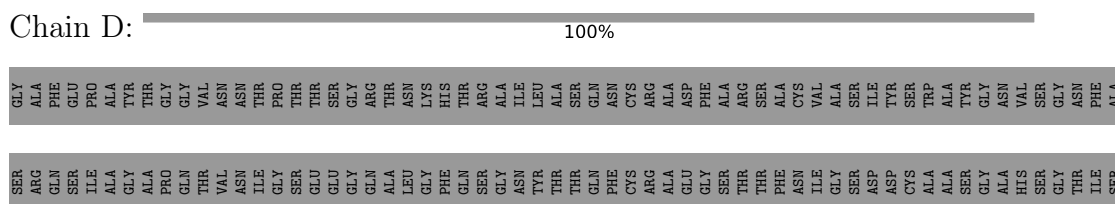
3 Residue-property plots

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: Tail Nozzle



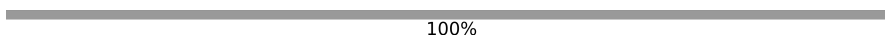
• Molecule 2: Tail fibers Dpo36



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

- Molecule 2: Tail fibers Dpo36

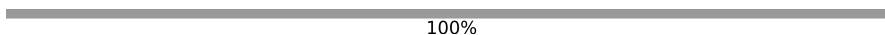
Chain B:



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

- Molecule 2: Tail fibers Dpo36

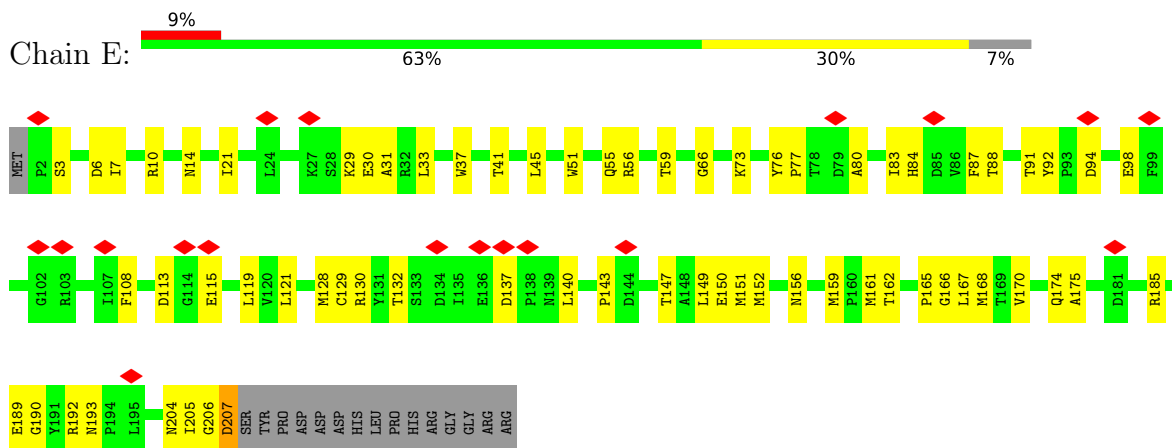
Chain C:



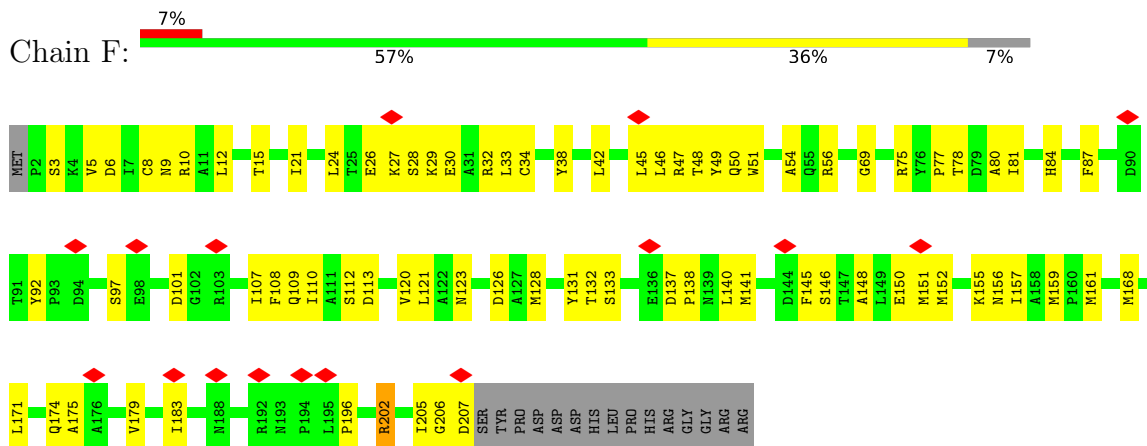
GLY	ALA	PHE	GLU	PRO	ALA	TYR	THR	GLY	VAL	ASN	ASN	THR	PRO	THR	THR	THR	SER	GLY	ARG	ALA	THR	ASN	ASN	LYS	HIS	THR	ALA	ARG	ALA	ILE	LEU	ALA	ALA	SER	GLN	ASN	CYS	ARG	ALA	ASP	PHE	ALA	ALA	ARG	SER	ALA	ALA	CYS	VAL	ALA	ALA	TYR	THR	ILE	TYR	SER	THR	TRP	ALA	ALA	ALA	GLY	ASN	ASN	PHE	ALA
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ALA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

- Molecule 3: Connector Protein



- Molecule 3: Connector Protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C6	Depositor
Number of particles used	11395	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 ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.043	Depositor
Minimum map value	-0.022	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0105	Depositor
Map size (Å)	405.0, 405.0, 405.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.35, 1.35, 1.35	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	0.21	1/6562 (0.0%)	0.41	0/8933
2	B	0.19	0/1004	0.41	0/1366
2	C	0.23	0/1004	0.58	0/1366
2	D	0.32	0/1004	0.53	0/1366
3	E	0.28	0/1631	0.49	0/2219
3	F	0.30	0/1631	0.54	0/2219
All	All	0.24	1/12836 (0.0%)	0.46	0/17469

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	47	VAL	C-N	5.06	1.40	1.33

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	6419	0	6184	169	0
2	B	989	0	902	38	0
2	C	989	0	902	47	0
2	D	989	0	902	47	0
3	E	1597	0	1548	52	0
3	F	1597	0	1548	71	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	12580	0	11986	387	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 16.

All (387) 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)
3:F:151:MET:HE2	3:F:174:GLN:HB3	1.34	1.09
2:D:21:PHE:CD2	2:D:81:LEU:HD22	2.01	0.95
3:E:98:GLU:OE1	3:F:107:ILE:HD13	1.72	0.89
2:D:21:PHE:CE2	2:D:81:LEU:HD22	2.07	0.89
3:E:152:MET:SD	3:E:175:ALA:HB1	2.13	0.89
3:F:152:MET:SD	3:F:175:ALA:HB1	2.16	0.85
1:A:629:THR:HB	1:A:659:LEU:HD13	1.58	0.84
3:F:205:ILE:O	3:F:205:ILE:HG22	1.76	0.83
2:D:87:ILE:HG13	2:D:115:MET:HB3	1.59	0.83
1:A:352:PRO:HG2	1:A:353:GLN:OE1	1.81	0.80
2:D:86:VAL:HA	2:D:119:GLN:HG2	1.64	0.78
3:F:151:MET:HE2	3:F:174:GLN:CB	2.11	0.77
1:A:47:VAL:HG21	1:A:519:ALA:HB1	1.66	0.76
2:D:21:PHE:CD2	2:D:81:LEU:CD2	2.68	0.76
2:B:10:GLU:HB2	2:B:83:ILE:HB	1.66	0.76
1:A:596:GLY:N	1:A:608:THR:O	2.20	0.74
3:F:151:MET:CE	3:F:174:GLN:HB3	2.14	0.74
2:C:49:GLU:HG2	2:C:50:GLY:N	2.03	0.73
1:A:485:LYS:HB3	1:A:500:VAL:HG23	1.69	0.73
3:F:34:CYS:O	3:F:38:TYR:HB3	1.88	0.72
2:C:112:ARG:O	2:C:116:ILE:HG13	1.90	0.71
2:D:103:PRO:HB3	2:C:101:TYR:HE1	1.53	0.71
1:A:780:TRP:HB3	2:C:103:PRO:HG3	1.73	0.70
3:F:151:MET:CE	3:F:174:GLN:CB	2.69	0.70
2:D:109:GLU:HG3	2:B:110:PHE:CE1	2.26	0.69
3:F:10:ARG:HB3	3:F:150:GLU:OE2	1.92	0.69
3:E:41:THR:HG22	3:E:156:ASN:HD22	1.57	0.69
2:B:112:ARG:O	2:B:116:ILE:HG13	1.91	0.69
1:A:488:ALA:HB1	1:A:535:VAL:HG13	1.74	0.69
1:A:55:ASN:OD1	1:A:566:ARG:NH2	2.28	0.67
3:E:98:GLU:O	3:E:193:ASN:ND2	2.26	0.67
3:F:3:SER:HA	3:F:138:PRO:HG2	1.76	0.66
1:A:231:ASP:OD1	1:A:232:GLU:HG3	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:91:GLN:NE2	2:C:93:THR:O	2.28	0.66
1:A:384:SER:OG	1:A:385:ARG:N	2.26	0.66
3:F:56:ARG:NH2	3:F:133:SER:OG	2.29	0.66
2:D:20:VAL:HG12	2:D:22:PRO:HD3	1.78	0.65
3:F:137:ASP:HB3	3:F:140:LEU:HD23	1.79	0.65
2:C:49:GLU:HG2	2:C:50:GLY:H	1.61	0.64
2:B:113:SER:OG	2:C:114:ARG:NH2	2.30	0.64
3:F:179:VAL:O	3:F:183:ILE:HG13	1.98	0.64
1:A:430:ARG:O	1:A:448:GLN:NE2	2.31	0.64
1:A:393:LEU:HB3	1:A:399:LEU:HD11	1.79	0.63
3:F:155:LYS:HD3	3:F:156:ASN:OD1	1.98	0.63
2:D:8:ASN:HD22	2:D:118:GLN:HB3	1.63	0.63
3:F:15:THR:HG21	3:F:157:ILE:HD11	1.81	0.63
1:A:239:SER:HB2	1:A:279:LYS:HG3	1.80	0.63
1:A:23:ALA:HB3	1:A:26:LEU:HD23	1.80	0.63
2:D:89:ILE:HA	2:D:116:ILE:HD11	1.82	0.62
2:B:6:ASN:HA	2:B:118:GLN:HE22	1.64	0.62
1:A:440:ILE:HD13	1:A:445:LEU:HD12	1.82	0.62
2:B:15:ASN:ND2	3:F:126:ASP:OD1	2.32	0.62
3:F:50:GLN:O	3:F:50:GLN:HG3	2.00	0.62
1:A:741:ALA:HA	1:A:759:ARG:HH22	1.64	0.62
2:D:21:PHE:HD2	2:D:81:LEU:CD2	2.12	0.62
1:A:751:LYS:H	1:A:788:THR:HG22	1.64	0.61
3:E:206:GLY:O	3:E:207:ASP:C	2.44	0.61
2:C:68:PHE:CD1	2:C:69:PRO:HA	2.36	0.61
3:F:110:ILE:CD1	3:F:120:VAL:HG22	2.31	0.61
2:D:89:ILE:HA	2:D:116:ILE:CD1	2.30	0.61
1:A:820:ILE:HG22	1:A:822:PRO:HD3	1.83	0.60
1:A:658:GLU:OE2	1:A:658:GLU:N	2.32	0.60
2:B:6:ASN:HA	2:B:118:GLN:NE2	2.16	0.60
1:A:603:THR:HG23	2:B:97:ASN:HD21	1.66	0.60
3:F:5:VAL:O	3:F:9:ASN:ND2	2.34	0.60
1:A:65:CYS:O	1:A:95:ARG:NH1	2.36	0.59
2:B:68:PHE:HE2	2:B:75:LEU:HB2	1.67	0.59
2:C:104:GLU:CD	2:C:104:GLU:H	2.10	0.59
2:D:109:GLU:OE1	2:D:112:ARG:NE	2.33	0.59
1:A:65:CYS:SG	1:A:66:LYS:N	2.76	0.59
2:C:23:TYR:CD2	2:C:64:GLY:O	2.56	0.59
1:A:346:ALA:HB1	1:A:390:ILE:HG21	1.84	0.58
1:A:357:MET:HE1	1:A:417:LEU:HD21	1.85	0.58
3:E:161:MET:HG2	3:E:162:THR:HG23	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:26:ARG:HG3	2:D:61:GLU:HA	1.83	0.58
2:B:109:GLU:OE1	2:B:112:ARG:NH1	2.37	0.58
1:A:60:ARG:NH1	1:A:582:THR:OG1	2.36	0.58
1:A:65:CYS:HB3	1:A:560:ILE:HD11	1.84	0.58
2:B:22:PRO:HB3	3:F:78:THR:HG23	1.85	0.58
1:A:40:LYS:HB3	1:A:724:GLU:OE1	2.03	0.58
3:F:205:ILE:O	3:F:205:ILE:CG2	2.46	0.58
3:E:152:MET:SD	3:E:175:ALA:CB	2.90	0.57
2:B:4:PRO:HG3	3:E:3:SER:OG	2.05	0.57
1:A:752:SER:OG	1:A:816:THR:N	2.37	0.57
1:A:19:GLY:HA2	1:A:34:ARG:HH21	1.70	0.57
3:E:45:LEU:HD23	3:E:149:LEU:HD13	1.87	0.57
1:A:629:THR:HB	1:A:659:LEU:CD1	2.34	0.56
2:C:69:PRO:HG2	2:C:73:ASP:HA	1.87	0.56
3:E:37:TRP:O	3:E:41:THR:HG23	2.05	0.56
3:E:56:ARG:NH1	3:F:112:SER:OG	2.39	0.56
2:D:103:PRO:HB3	2:C:101:TYR:CE1	2.38	0.56
1:A:119:ASP:N	1:A:119:ASP:OD1	2.38	0.56
2:D:88:ASP:O	2:D:116:ILE:HD11	2.06	0.56
3:E:113:ASP:OD2	3:E:115:GLU:N	2.39	0.56
2:D:85:ARG:CZ	2:D:115:MET:HG2	2.35	0.56
2:D:28:PHE:CE1	2:D:115:MET:HE1	2.41	0.56
2:C:12:TYR:CE2	2:C:21:PHE:HB3	2.40	0.56
3:F:159:MET:HB2	3:F:168:MET:HE2	1.88	0.56
2:C:47:LEU:C	2:C:48:ILE:HD13	2.32	0.55
1:A:123:GLU:OE1	1:A:123:GLU:N	2.39	0.55
3:F:207:ASP:OD1	3:F:207:ASP:O	2.24	0.55
1:A:534:ALA:O	1:A:545:TYR:N	2.34	0.55
2:B:8:ASN:ND2	2:B:85:ARG:O	2.40	0.55
2:C:91:GLN:HG2	2:C:109:GLU:OE2	2.06	0.55
2:C:10:GLU:HG3	2:C:12:TYR:CE2	2.42	0.55
2:C:102:TYR:HB3	2:C:104:GLU:OE2	2.07	0.55
3:F:87:PHE:O	3:F:128:MET:N	2.39	0.55
2:C:15:ASN:H	2:C:75:LEU:HD12	1.71	0.55
3:E:21:ILE:HD11	3:E:31:ALA:HB2	1.88	0.54
1:A:91:HIS:HB2	1:A:118:ARG:HB3	1.89	0.54
1:A:313:ILE:HD12	1:A:313:ILE:H	1.72	0.54
2:D:91:GLN:HB2	2:B:3:VAL:HG22	1.89	0.54
2:C:108:ASP:O	2:C:112:ARG:HG2	2.07	0.54
2:B:27:ILE:HG21	2:B:33:LEU:HD21	1.90	0.54
1:A:469:ASP:OD1	1:A:470:ASP:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:748:GLN:HA	1:A:790:LEU:HA	1.90	0.54
1:A:169:ASN:ND2	1:A:171:ASP:O	2.41	0.53
1:A:83:GLN:OE1	1:A:98:ARG:NE	2.41	0.53
3:F:26:GLU:HG2	3:F:27:LYS:HD3	1.90	0.53
1:A:407:GLU:N	1:A:407:GLU:OE1	2.41	0.53
1:A:753:ARG:NH2	2:C:98:GLN:O	2.42	0.53
3:E:98:GLU:OE1	3:F:107:ILE:CD1	2.49	0.53
1:A:753:ARG:NH1	1:A:784:THR:O	2.41	0.53
1:A:68:LYS:O	1:A:558:ARG:NH1	2.41	0.53
1:A:724:GLU:HG2	1:A:805:LEU:O	2.09	0.53
3:E:185:ARG:HH21	3:F:49:TYR:HA	1.73	0.53
3:E:159:MET:HE1	3:E:165:PRO:HD3	1.91	0.53
3:F:155:LYS:HB2	3:F:171:LEU:HB3	1.91	0.53
1:A:240:LEU:HD23	1:A:247:THR:HB	1.92	0.53
2:D:94:ASP:OD1	2:D:95:LEU:N	2.41	0.53
3:E:51:TRP:O	3:E:55:GLN:NE2	2.42	0.52
3:E:84:HIS:NE2	3:E:132:THR:HG23	2.25	0.52
3:E:147:THR:HA	3:E:150:GLU:HG2	1.91	0.52
3:E:59:THR:HA	3:E:128:MET:HA	1.91	0.52
3:E:94:ASP:HA	3:F:69:GLY:HA2	1.89	0.52
1:A:342:ARG:HH22	1:A:375:ASP:HA	1.75	0.52
1:A:590:GLY:O	1:A:612:SER:OG	2.27	0.52
1:A:614:SER:H	1:A:645:THR:HG22	1.75	0.52
1:A:659:LEU:HG	1:A:659:LEU:O	2.10	0.52
2:D:25:PHE:HB2	2:D:85:ARG:NH1	2.25	0.52
1:A:409:MET:O	1:A:409:MET:HG3	2.09	0.52
1:A:290:VAL:HG22	1:A:305:VAL:HG22	1.91	0.52
1:A:636:VAL:HG12	1:A:651:ALA:HA	1.91	0.52
1:A:401:ALA:HB3	1:A:408:TRP:HB2	1.92	0.52
1:A:723:ILE:HD13	1:A:817:ILE:HD12	1.91	0.52
1:A:291:ARG:N	1:A:304:ARG:O	2.40	0.51
1:A:401:ALA:O	1:A:408:TRP:N	2.43	0.51
2:D:21:PHE:HD2	2:D:81:LEU:HD22	1.65	0.51
1:A:494:ASP:O	1:A:496:VAL:N	2.43	0.51
2:D:102:TYR:O	2:D:105:VAL:HG22	2.11	0.51
1:A:498:TRP:HB3	1:A:506:LEU:HD11	1.91	0.51
2:C:49:GLU:HA	2:C:53:TYR:CZ	2.46	0.51
3:E:87:PHE:O	3:E:128:MET:N	2.44	0.51
1:A:472:THR:HG22	1:A:476:ASN:HA	1.93	0.51
3:F:33:LEU:HD12	3:F:161:MET:HE2	1.93	0.51
1:A:626:ARG:NH1	1:A:690:ASP:OD2	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:94:ASP:OD1	2:B:96:LYS:N	2.44	0.50
1:A:754:GLY:O	1:A:809:GLN:NE2	2.45	0.50
3:F:155:LYS:CD	3:F:156:ASN:OD1	2.59	0.50
1:A:535:VAL:HG12	1:A:544:PRO:HA	1.93	0.50
2:C:13:ALA:HA	2:C:80:THR:HG22	1.92	0.50
3:F:3:SER:H	3:F:6:ASP:HB3	1.77	0.50
2:B:94:ASP:OD1	2:B:95:LEU:N	2.45	0.49
1:A:13:ILE:HD11	1:A:819:SER:HB2	1.94	0.49
2:D:91:GLN:HB2	2:B:3:VAL:CG2	2.42	0.49
2:D:53:TYR:HB3	2:D:68:PHE:HB2	1.93	0.49
3:F:151:MET:CE	3:F:174:GLN:HB2	2.40	0.49
1:A:759:ARG:NE	1:A:800:ASP:OD2	2.46	0.49
1:A:499:LEU:HD21	1:A:520:TRP:HZ3	1.77	0.49
1:A:573:ASP:OD1	1:A:586:ARG:NH1	2.46	0.49
2:B:104:GLU:CD	2:B:104:GLU:H	2.19	0.49
1:A:470:ASP:OD1	1:A:471:LEU:N	2.46	0.49
1:A:653:ARG:NH1	2:C:104:GLU:OE1	2.46	0.49
3:F:146:SER:O	3:F:150:GLU:HG3	2.13	0.49
3:F:202:ARG:HA	3:F:206:GLY:O	2.13	0.49
1:A:601:TRP:HA	1:A:601:TRP:CE3	2.48	0.48
3:E:14:ASN:ND2	3:E:151:MET:SD	2.87	0.48
1:A:47:VAL:HG12	1:A:48:GLN:H	1.77	0.48
1:A:256:HIS:HB3	1:A:261:GLN:NE2	2.28	0.48
2:D:91:GLN:H	2:B:3:VAL:HG23	1.77	0.48
1:A:729:SER:HB3	1:A:736:ARG:HB2	1.94	0.48
3:F:8:CYS:O	3:F:12:LEU:HG	2.14	0.48
3:F:101:ASP:HB2	3:F:196:PRO:HG3	1.96	0.48
2:B:36:TYR:HB2	2:B:82:THR:OG1	2.14	0.48
1:A:6:TYR:H	3:E:166:GLY:HA3	1.79	0.48
1:A:312:GLU:N	1:A:312:GLU:OE1	2.46	0.48
1:A:478:LEU:O	1:A:501:ARG:HD2	2.12	0.48
1:A:499:LEU:HD21	1:A:520:TRP:CZ3	2.48	0.48
2:D:47:LEU:HD22	2:D:52:ASP:OD2	2.14	0.48
2:C:19:THR:HA	2:C:68:PHE:O	2.14	0.48
1:A:312:GLU:O	1:A:316:GLU:N	2.46	0.48
1:A:415:GLN:N	1:A:415:GLN:OE1	2.47	0.48
3:E:88:THR:HG23	3:E:91:THR:H	1.79	0.48
1:A:771:GLU:O	2:D:102:TYR:OH	2.31	0.48
3:F:141:MET:SD	3:F:145:PHE:HD1	2.37	0.48
1:A:48:GLN:O	1:A:49:PRO:C	2.55	0.48
2:B:7:ASP:OD2	2:B:10:GLU:OE2	2.32	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:87:ILE:N	2:B:119:GLN:OE1	2.46	0.48
2:B:87:ILE:HG23	2:B:116:ILE:HG12	1.96	0.47
1:A:433:SER:OG	1:A:434:ASP:N	2.46	0.47
1:A:452:THR:HG22	1:A:482:TYR:O	2.15	0.47
1:A:739:HIS:CD2	1:A:801:LYS:HE3	2.48	0.47
3:E:83:ILE:HG23	3:E:129:CYS:SG	2.54	0.47
1:A:162:PHE:HD2	1:A:367:LYS:HB2	1.79	0.47
1:A:477:HIS:CE1	1:A:478:LEU:HG	2.49	0.47
3:E:77:PRO:HB2	3:E:80:ALA:HB2	1.96	0.47
2:D:121:GLN:NE2	2:D:125:ASP:OD2	2.47	0.47
1:A:49:PRO:HD3	1:A:494:ASP:OD1	2.14	0.47
2:C:35:VAL:HB	2:C:53:TYR:CZ	2.50	0.47
3:E:137:ASP:HB3	3:E:140:LEU:HD23	1.96	0.47
1:A:352:PRO:HG2	1:A:353:GLN:CD	2.38	0.47
1:A:327:ASP:OD1	1:A:330:ARG:N	2.39	0.47
2:B:66:ILE:CD1	2:B:83:ILE:HD11	2.45	0.47
2:B:89:ILE:HD13	2:B:116:ILE:HG21	1.97	0.47
1:A:563:LEU:HD23	1:A:564:ASP:O	2.15	0.46
3:F:42:LEU:O	3:F:46:LEU:HD23	2.16	0.46
1:A:601:TRP:CD1	1:A:605:GLU:HG2	2.50	0.46
2:C:40:GLU:N	2:C:79:GLU:HG2	2.30	0.46
1:A:258:GLU:N	1:A:258:GLU:OE1	2.48	0.46
2:C:87:ILE:HD13	2:C:115:MET:HE2	1.98	0.46
3:F:49:TYR:HD2	3:F:51:TRP:CD2	2.33	0.46
3:F:131:TYR:HE1	3:F:133:SER:HB3	1.81	0.46
3:F:148:ALA:HB1	3:F:179:VAL:HG12	1.98	0.46
1:A:600:ASN:H	1:A:660:ARG:CZ	2.29	0.46
1:A:206:GLN:HG3	1:A:287:PHE:HB3	1.98	0.46
1:A:344:VAL:HG13	1:A:357:MET:HG2	1.97	0.46
1:A:409:MET:SD	1:A:427:GLN:OE1	2.74	0.46
2:C:52:ASP:OD2	2:C:53:TYR:HD1	1.99	0.46
3:E:150:GLU:HG3	3:E:151:MET:N	2.30	0.46
1:A:687:ILE:HB	1:A:694:HIS:HB3	1.98	0.45
2:C:23:TYR:CE1	2:C:25:PHE:O	2.69	0.45
1:A:393:LEU:HA	1:A:400:LEU:O	2.16	0.45
1:A:409:MET:HG2	1:A:427:GLN:OE1	2.16	0.45
3:F:49:TYR:HB3	3:F:51:TRP:CE2	2.50	0.45
3:F:175:ALA:O	3:F:179:VAL:HG13	2.16	0.45
1:A:737:ASP:O	1:A:801:LYS:HE2	2.17	0.45
1:A:584:ASP:OD1	1:A:585:GLY:N	2.50	0.45
1:A:492:GLU:HB3	1:A:493:PRO:HD3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:141:MET:SD	3:F:145:PHE:CD1	3.10	0.45
1:A:479:LEU:HD11	1:A:520:TRP:CH2	2.52	0.45
2:C:113:SER:HA	2:C:116:ILE:HD12	1.97	0.45
1:A:526:VAL:O	1:A:550:ARG:NH1	2.50	0.45
1:A:352:PRO:HB2	1:A:389:GLU:HB2	1.99	0.45
1:A:392:HIS:NE2	1:A:435:VAL:O	2.50	0.45
2:B:84:LEU:HG	2:B:86:VAL:HG23	1.98	0.45
3:E:192:ARG:O	3:F:107:ILE:HG13	2.16	0.45
1:A:39:LEU:HD13	1:A:723:ILE:HG23	1.99	0.44
1:A:750:GLU:HA	1:A:788:THR:HA	1.99	0.44
2:B:27:ILE:HG22	2:B:85:ARG:HG3	1.98	0.44
1:A:531:GLU:HB2	1:A:547:ILE:HB	1.98	0.44
1:A:779:ASP:OD1	2:B:100:ALA:HA	2.17	0.44
1:A:391:ARG:O	1:A:392:HIS:ND1	2.51	0.44
1:A:653:ARG:HH11	2:C:103:PRO:HD2	1.82	0.44
2:B:23:TYR:HB2	2:B:25:PHE:CZ	2.52	0.44
3:F:29:LYS:HG3	3:F:30:GLU:OE2	2.17	0.44
2:D:124:LEU:HD11	2:C:124:LEU:HB2	2.00	0.44
3:E:108:PHE:HA	3:E:121:LEU:O	2.17	0.44
1:A:90:GLY:HA3	1:A:93:TYR:CE2	2.53	0.44
1:A:272:VAL:O	1:A:273:THR:HG22	2.17	0.44
1:A:457:LEU:HD12	1:A:457:LEU:HA	1.87	0.44
1:A:592:LEU:HB3	1:A:663:GLN:HG2	1.99	0.44
3:E:76:TYR:CE1	3:E:80:ALA:HB3	2.53	0.44
3:F:21:ILE:HA	3:F:24:LEU:HB2	1.99	0.44
1:A:67:TYR:HB3	1:A:70:TYR:HB2	1.99	0.44
1:A:753:ARG:HA	1:A:774:GLN:HE22	1.83	0.44
1:A:602:THR:HB	2:B:97:ASN:HB3	1.99	0.44
3:E:73:LYS:HB2	3:E:119:LEU:HD23	2.00	0.44
3:E:189:GLU:OE2	3:F:47:ARG:NH2	2.51	0.44
2:D:55:VAL:HA	2:D:66:ILE:HA	2.00	0.44
3:F:101:ASP:OD1	3:F:101:ASP:C	2.61	0.44
1:A:461:PHE:HD1	1:A:461:PHE:O	2.01	0.43
1:A:574:PHE:CE2	1:A:576:CYS:HB2	2.53	0.43
2:B:21:PHE:HB2	2:B:66:ILE:HG13	2.00	0.43
3:E:55:GLN:OE1	3:E:55:GLN:HA	2.18	0.43
3:E:143:PRO:HD2	3:F:47:ARG:HD2	2.00	0.43
3:F:34:CYS:O	3:F:38:TYR:CB	2.63	0.43
1:A:54:SER:HB3	1:A:566:ARG:NH2	2.33	0.43
1:A:162:PHE:HE1	1:A:306:ILE:HG21	1.83	0.43
2:D:109:GLU:OE1	2:D:109:GLU:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:509:MET:HG2	1:A:511:TYR:HB2	1.99	0.43
1:A:656:PRO:HD2	1:A:659:LEU:HD23	1.99	0.43
3:F:161:MET:HE2	3:F:161:MET:HB2	1.85	0.43
1:A:216:TRP:CZ2	1:A:254:PRO:HD3	2.53	0.43
1:A:233:ARG:NH1	1:A:235:TYR:OH	2.45	0.43
1:A:117:HIS:ND1	1:A:119:ASP:OD1	2.51	0.43
1:A:497:VAL:HB	1:A:509:MET:HB3	1.99	0.43
1:A:746:GLY:O	1:A:821:ILE:N	2.40	0.43
3:F:46:LEU:HD22	3:F:145:PHE:HZ	1.83	0.43
1:A:773:LYS:HB2	2:D:100:ALA:HB1	1.99	0.43
2:C:26:ARG:HD3	2:C:61:GLU:HA	2.00	0.43
2:C:34:GLU:HG2	2:C:86:VAL:HB	2.00	0.43
1:A:706:LEU:HD23	1:A:706:LEU:HA	1.80	0.43
1:A:725:THR:O	1:A:804:SER:OG	2.31	0.43
1:A:27:GLN:OE1	1:A:40:LYS:HD2	2.18	0.43
1:A:742:ILE:HG13	1:A:824:VAL:HG22	2.01	0.43
2:C:53:TYR:HB3	2:C:68:PHE:CG	2.54	0.43
3:F:81:ILE:HD12	3:F:132:THR:O	2.18	0.43
3:F:84:HIS:NE2	3:F:132:THR:HG23	2.34	0.43
1:A:46:VAL:C	1:A:47:VAL:O	2.60	0.42
3:F:113:ASP:C	3:F:113:ASP:OD1	2.62	0.42
1:A:799:TRP:HZ3	1:A:827:GLY:HA3	1.83	0.42
3:F:33:LEU:HD13	3:F:157:ILE:HB	2.00	0.42
1:A:13:ILE:HD12	1:A:14:GLN:N	2.34	0.42
1:A:45:PHE:CG	1:A:723:ILE:HD11	2.55	0.42
1:A:761:ARG:HG3	1:A:763:ASP:N	2.35	0.42
3:E:167:LEU:HA	3:E:170:VAL:HG12	2.01	0.42
1:A:744:GLY:HA2	1:A:794:GLY:HA2	2.02	0.42
1:A:116:TRP:HH2	1:A:135:LEU:HD13	1.85	0.42
2:D:49:GLU:OE1	2:D:55:VAL:HG13	2.19	0.42
2:D:6:ASN:HA	2:D:118:GLN:NE2	2.35	0.42
2:D:94:ASP:OD1	2:D:94:ASP:C	2.62	0.42
3:E:159:MET:HB2	3:E:168:MET:HE2	2.02	0.42
1:A:149:SER:HB2	1:A:152:ASP:HB3	2.02	0.42
1:A:240:LEU:HB3	1:A:247:THR:HG21	2.02	0.42
1:A:269:ILE:O	1:A:272:VAL:HG22	2.20	0.42
3:F:148:ALA:O	3:F:152:MET:HG2	2.19	0.42
1:A:230:VAL:HG13	1:A:231:ASP:H	1.84	0.42
2:D:103:PRO:HG2	2:C:97:ASN:HA	2.01	0.42
3:E:6:ASP:O	3:E:10:ARG:HG3	2.20	0.42
2:D:96:LYS:HE2	2:D:96:LYS:HB2	1.79	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:98:GLU:CD	3:F:107:ILE:HD13	2.42	0.42
1:A:162:PHE:CE2	1:A:367:LYS:HD3	2.55	0.41
2:D:67:THR:HG22	2:D:67:THR:O	2.20	0.41
2:B:114:ARG:NE	2:B:114:ARG:HA	2.34	0.41
1:A:456:ASP:O	1:A:468:GLY:HA3	2.20	0.41
1:A:603:THR:HG22	1:A:651:ALA:HB3	2.02	0.41
1:A:753:ARG:CZ	1:A:784:THR:HB	2.51	0.41
1:A:753:ARG:HH21	2:C:98:GLN:HB3	1.85	0.41
1:A:761:ARG:HG3	1:A:763:ASP:H	1.85	0.41
2:D:52:ASP:O	2:D:69:PRO:HA	2.20	0.41
1:A:327:ASP:CG	1:A:329:ASP:H	2.28	0.41
1:A:742:ILE:H	1:A:759:ARG:HH12	1.69	0.41
2:D:47:LEU:C	2:D:48:ILE:HD13	2.45	0.41
2:D:121:GLN:NE2	2:D:121:GLN:O	2.52	0.41
2:B:28:PHE:CD1	2:B:28:PHE:N	2.89	0.41
3:E:98:GLU:OE2	3:F:123:ASN:ND2	2.48	0.41
3:E:205:ILE:O	3:E:205:ILE:HG23	2.20	0.41
3:F:109:GLN:O	3:F:121:LEU:N	2.46	0.41
1:A:162:PHE:CE1	1:A:306:ILE:HG21	2.55	0.41
1:A:773:LYS:HB3	2:D:102:TYR:CZ	2.54	0.41
2:D:89:ILE:HA	2:D:116:ILE:HD13	2.02	0.41
2:B:91:GLN:HE22	2:B:109:GLU:HG2	1.85	0.41
3:E:129:CYS:SG	3:E:130:ARG:N	2.93	0.41
1:A:45:PHE:CD2	1:A:723:ILE:HD11	2.56	0.41
1:A:794:GLY:HA3	3:E:29:LYS:HE2	2.01	0.41
2:D:26:ARG:HH21	2:D:28:PHE:HE1	1.67	0.41
1:A:21:GLU:HA	1:A:39:LEU:O	2.21	0.41
1:A:117:HIS:O	1:A:121:ILE:HG23	2.20	0.41
2:D:9:ARG:HG2	2:D:83:ILE:O	2.20	0.41
2:C:116:ILE:HG13	2:C:116:ILE:H	1.73	0.41
1:A:272:VAL:O	1:A:274:GLU:HG2	2.21	0.41
2:C:21:PHE:HD2	2:C:66:ILE:HG13	1.85	0.41
3:E:113:ASP:HB3	3:E:119:LEU:HD11	2.03	0.41
1:A:454:ILE:HD12	1:A:487:TRP:HZ2	1.86	0.41
2:D:37:LEU:HD12	2:D:47:LEU:HD11	2.03	0.41
2:B:36:TYR:HE1	2:B:46:LEU:HD13	1.85	0.41
2:C:23:TYR:CE2	2:C:64:GLY:O	2.73	0.41
2:C:37:LEU:N	2:C:45:ALA:O	2.54	0.41
3:E:33:LEU:HD23	3:E:33:LEU:HA	1.88	0.41
1:A:284:HIS:CD2	1:A:310:PRO:HA	2.56	0.41
3:F:45:LEU:O	3:F:48:THR:HG22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:ILE:HD13	1:A:821:ILE:CG1	2.50	0.40
2:B:5:THR:HG22	2:B:7:ASP:H	1.86	0.40
2:C:27:ILE:HG22	2:C:85:ARG:HG3	2.01	0.40
2:C:76:ASP:HB2	2:C:79:GLU:HG3	2.03	0.40
2:C:102:TYR:HB2	2:C:105:VAL:HG22	2.04	0.40
3:E:66:GLY:HA2	3:E:73:LYS:NZ	2.36	0.40
3:E:170:VAL:O	3:E:174:GLN:HG2	2.20	0.40
3:E:185:ARG:HH21	3:F:49:TYR:CA	2.34	0.40
3:F:54:ALA:O	3:F:132:THR:HA	2.21	0.40
1:A:531:GLU:OE2	1:A:558:ARG:NE	2.42	0.40
2:B:12:TYR:HD2	2:B:21:PHE:HD1	1.69	0.40
3:E:190:GLY:HA2	3:F:108:PHE:CZ	2.57	0.40
3:F:77:PRO:HB2	3:F:80:ALA:HB2	2.03	0.40
1:A:588:SER:O	1:A:588:SER:OG	2.33	0.40
1:A:660:ARG:HE	1:A:660:ARG:HB3	1.61	0.40
2:C:37:LEU:HD12	2:C:47:LEU:HD21	2.03	0.40
2:C:39:ASP:N	2:C:42:GLY:O	2.54	0.40
2:C:91:GLN:CG	2:C:109:GLU:OE2	2.68	0.40
3:E:21:ILE:HD13	3:E:30:GLU:HB2	2.03	0.40
3:F:28:SER:O	3:F:32:ARG:HG3	2.22	0.40
3:F:92:TYR:OH	3:F:97:SER:HB3	2.21	0.40
1:A:541:ARG:HB2	1:A:567:ARG:NH2	2.36	0.40
1:A:687:ILE:HD12	1:A:694:HIS:HD1	1.86	0.40
3:E:7:ILE:HD13	3:E:7:ILE:HA	1.84	0.40
1:A:771:GLU:OE1	1:A:771:GLU:N	2.50	0.40
3:F:5:VAL:HG22	3:F:9:ASN:ND2	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	824/820 (100%)	743 (90%)	81 (10%)	0	100	100
2	B	124/523 (24%)	120 (97%)	4 (3%)	0	100	100
2	C	124/523 (24%)	106 (86%)	18 (14%)	0	100	100
2	D	124/523 (24%)	115 (93%)	9 (7%)	0	100	100
3	E	204/222 (92%)	193 (95%)	11 (5%)	0	100	100
3	F	204/222 (92%)	192 (94%)	12 (6%)	0	100	100
All	All	1604/2833 (57%)	1469 (92%)	135 (8%)	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	687/683 (101%)	685 (100%)	2 (0%)	86	85
2	B	108/383 (28%)	108 (100%)	0	100	100
2	C	108/383 (28%)	108 (100%)	0	100	100
2	D	108/383 (28%)	107 (99%)	1 (1%)	70	75
3	E	168/182 (92%)	165 (98%)	3 (2%)	51	67
3	F	168/182 (92%)	166 (99%)	2 (1%)	63	72
All	All	1347/2196 (61%)	1339 (99%)	8 (1%)	76	80

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	PHE
1	A	660	ARG
2	D	90	THR
3	E	92	TYR
3	E	204	ASN
3	E	207	ASP
3	F	75	ARG

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Mol	Chain	Res	Type
3	F	202	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	ASN
1	A	252	ASN
1	A	261	GLN
1	A	347	ASN
1	A	477	HIS
1	A	512	GLN
1	A	663	GLN
2	D	8	ASN
2	D	98	GLN
2	B	97	ASN
3	E	109	GLN
3	E	204	ASN
3	F	106	GLN
3	F	109	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.

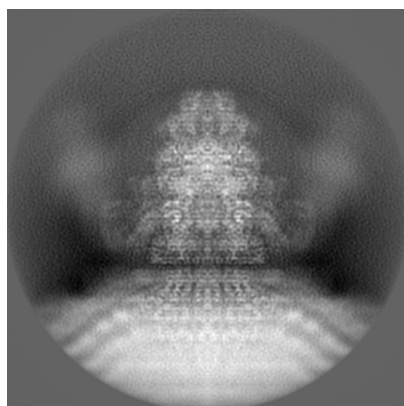
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16689. These allow visual inspection of the internal detail of the map and identification of artifacts.

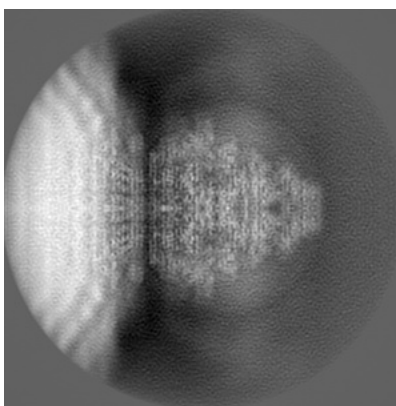
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

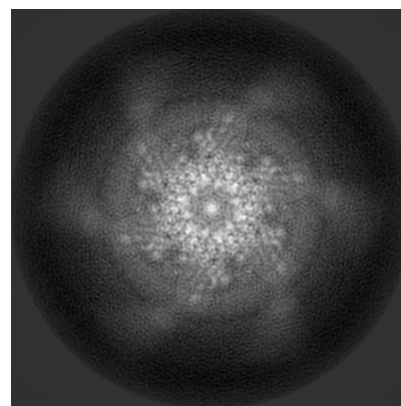
6.1.1 Primary map



X

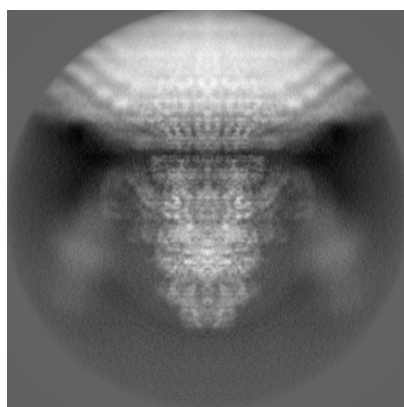


Y

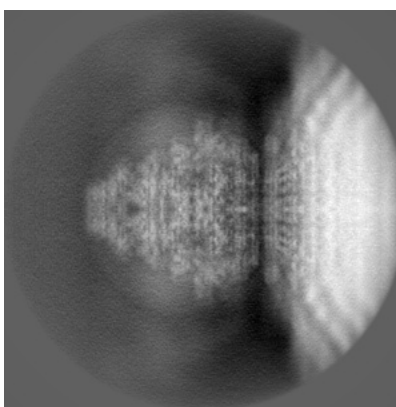


Z

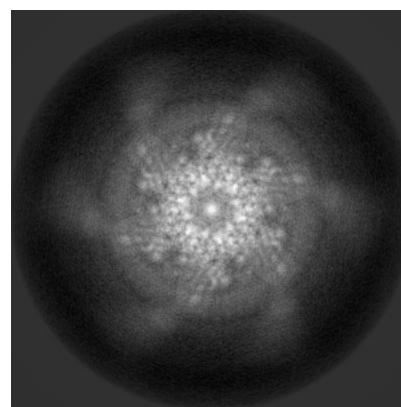
6.1.2 Raw map



X



Y

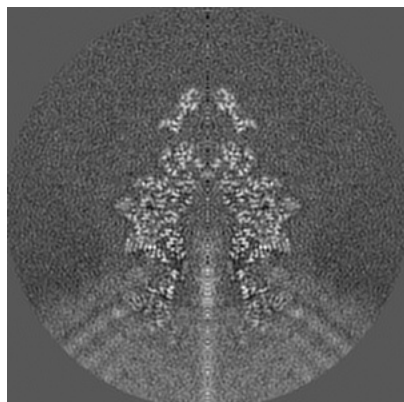


Z

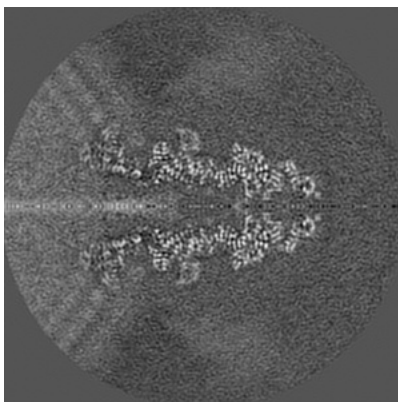
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

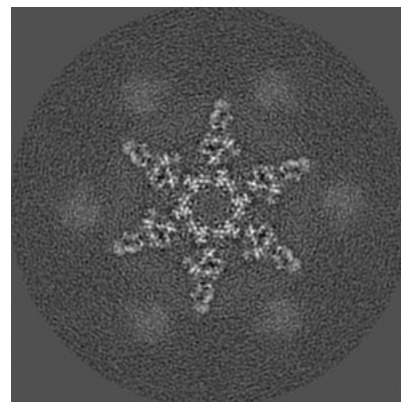
6.2.1 Primary map



X Index: 150

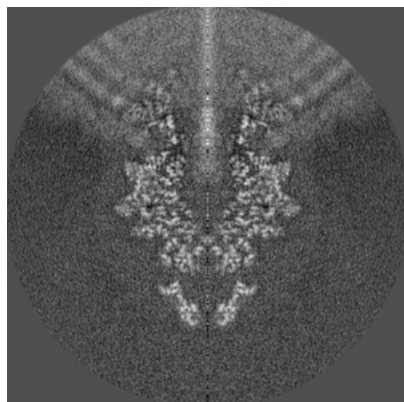


Y Index: 150

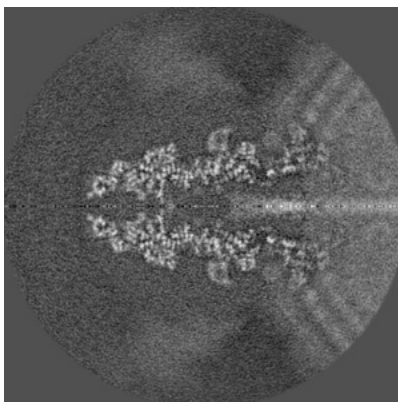


Z Index: 150

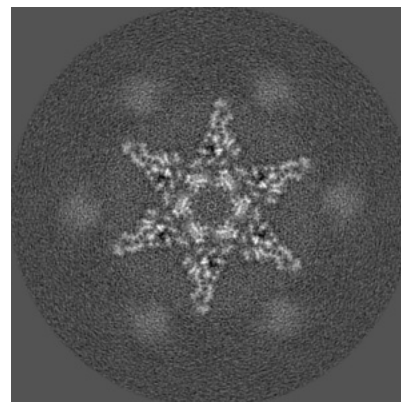
6.2.2 Raw map



X Index: 150



Y Index: 150

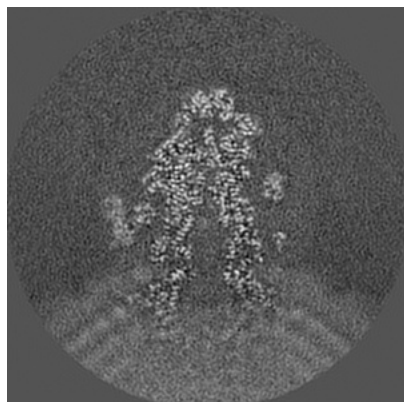


Z Index: 150

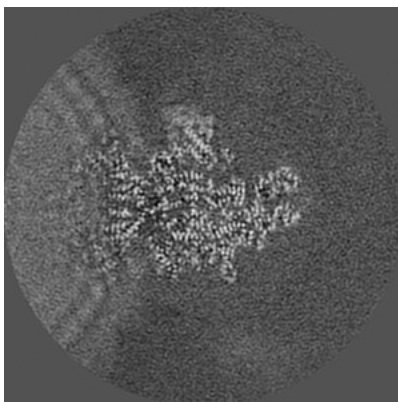
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

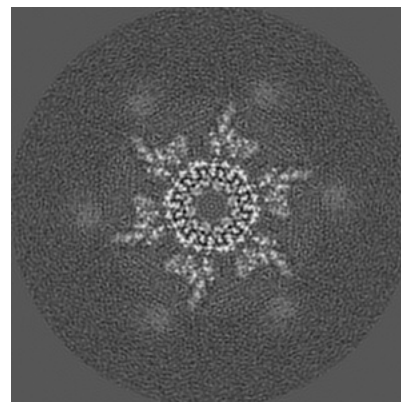
6.3.1 Primary map



X Index: 138

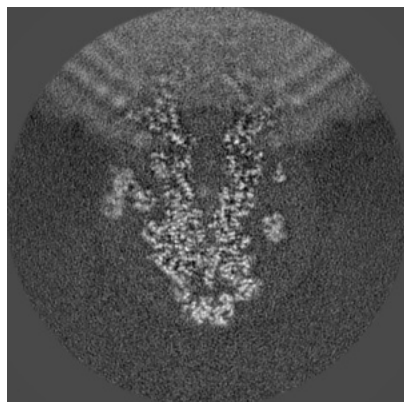


Y Index: 173

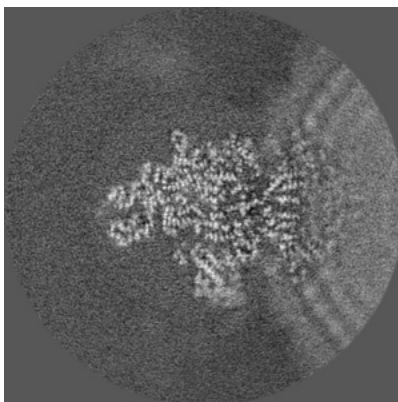


Z Index: 140

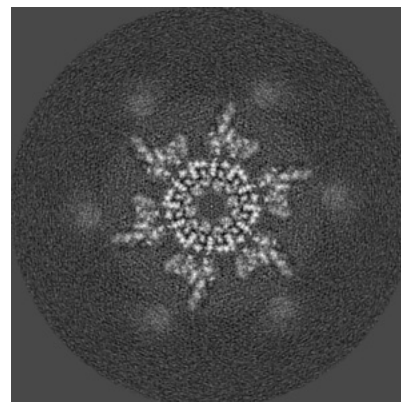
6.3.2 Raw map



X Index: 138



Y Index: 127

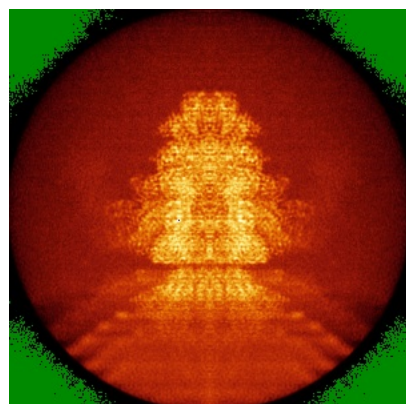


Z Index: 159

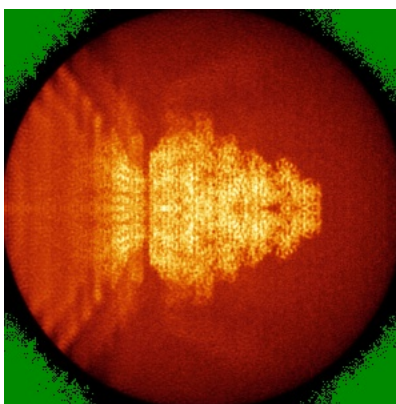
The images above show the largest variance slices of the map in three orthogonal directions.

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

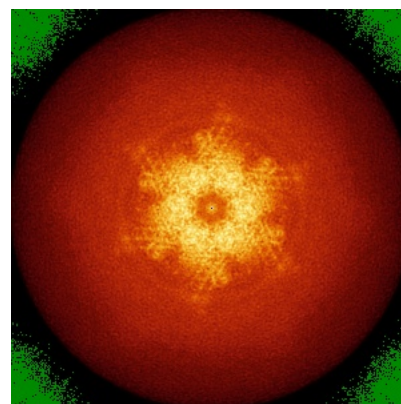
6.4.1 Primary map



X

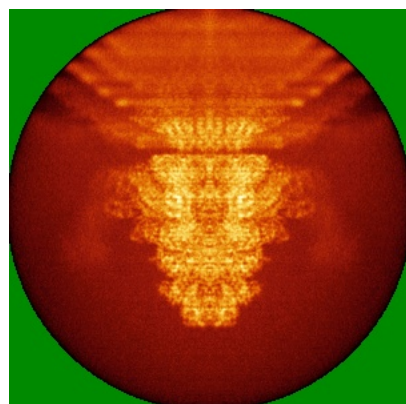


Y

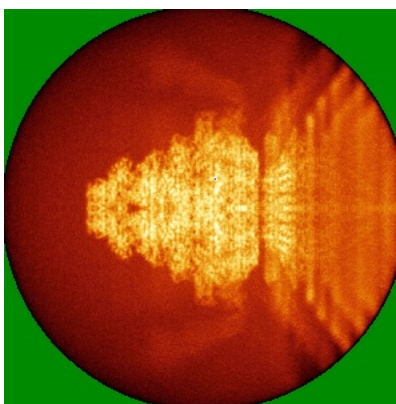


Z

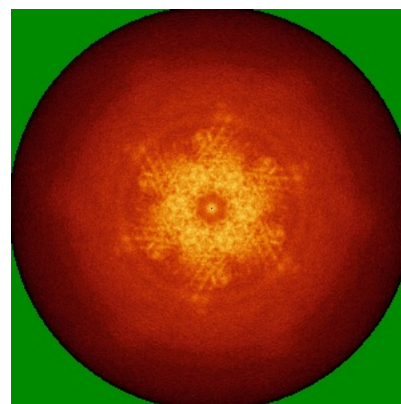
6.4.2 Raw map



X



Y

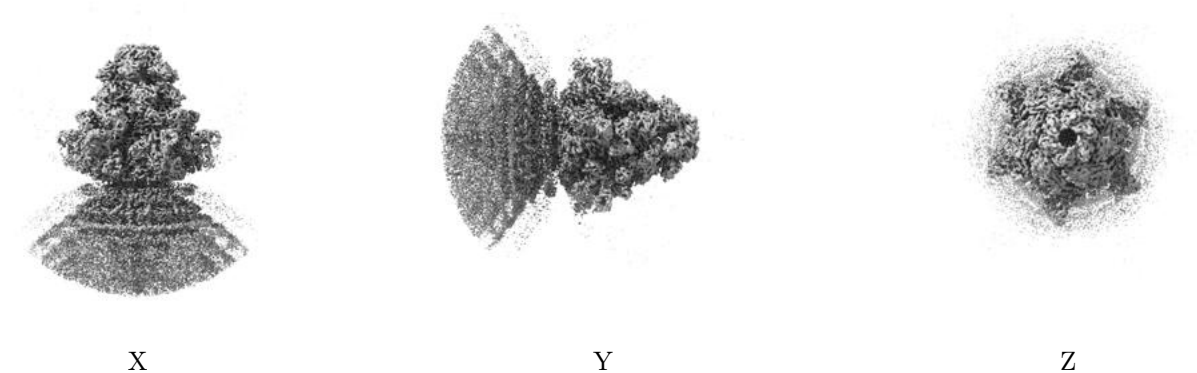


Z

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.

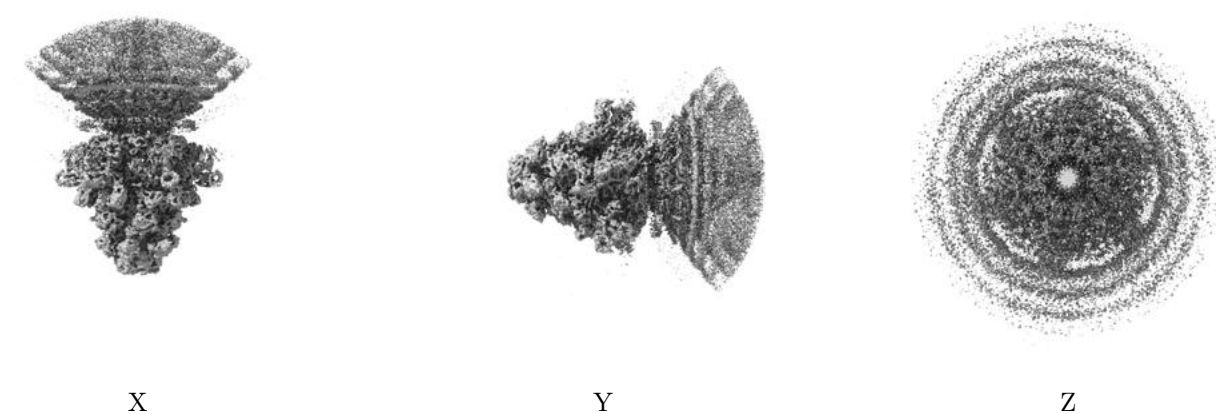
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0105. 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.

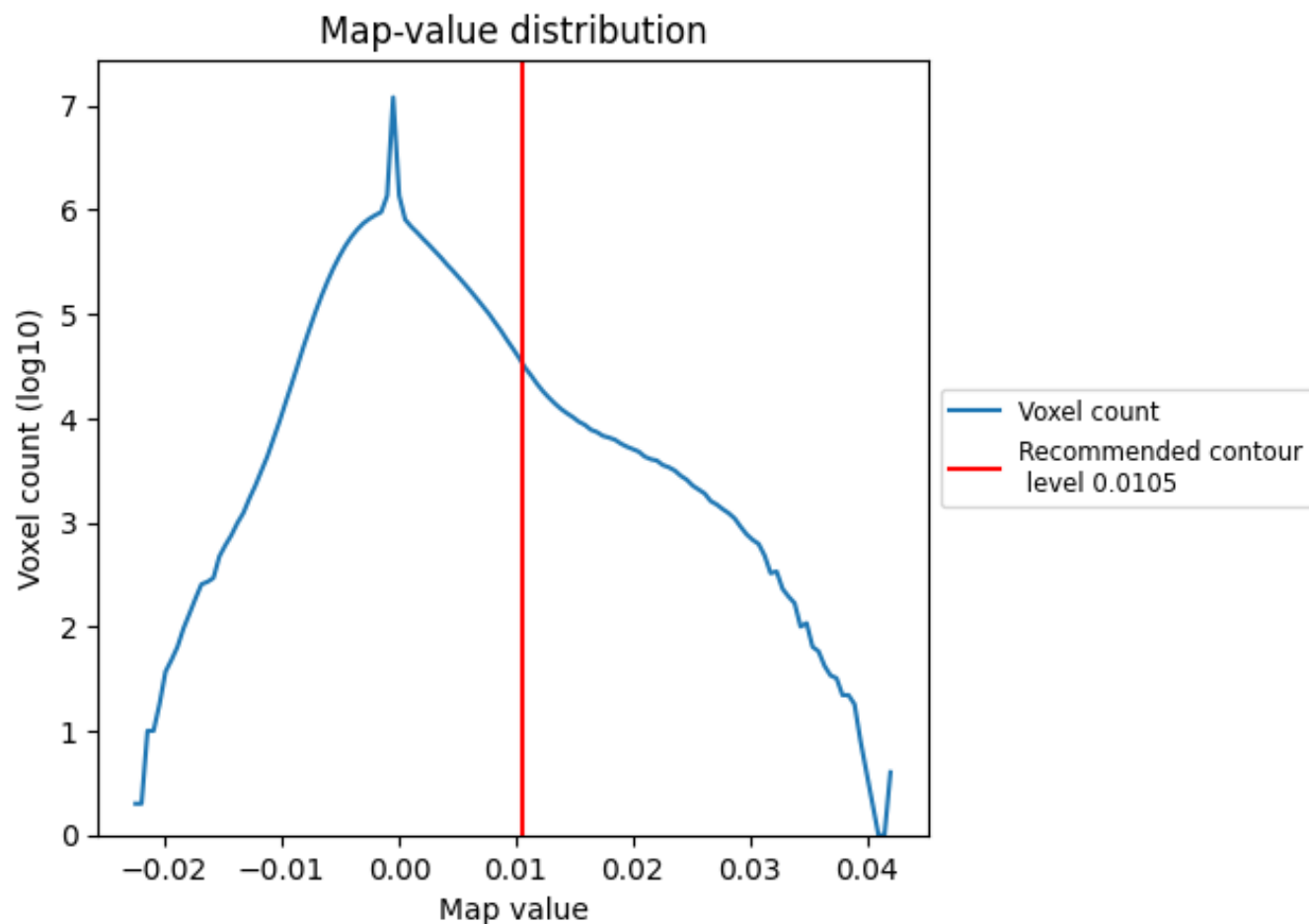
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

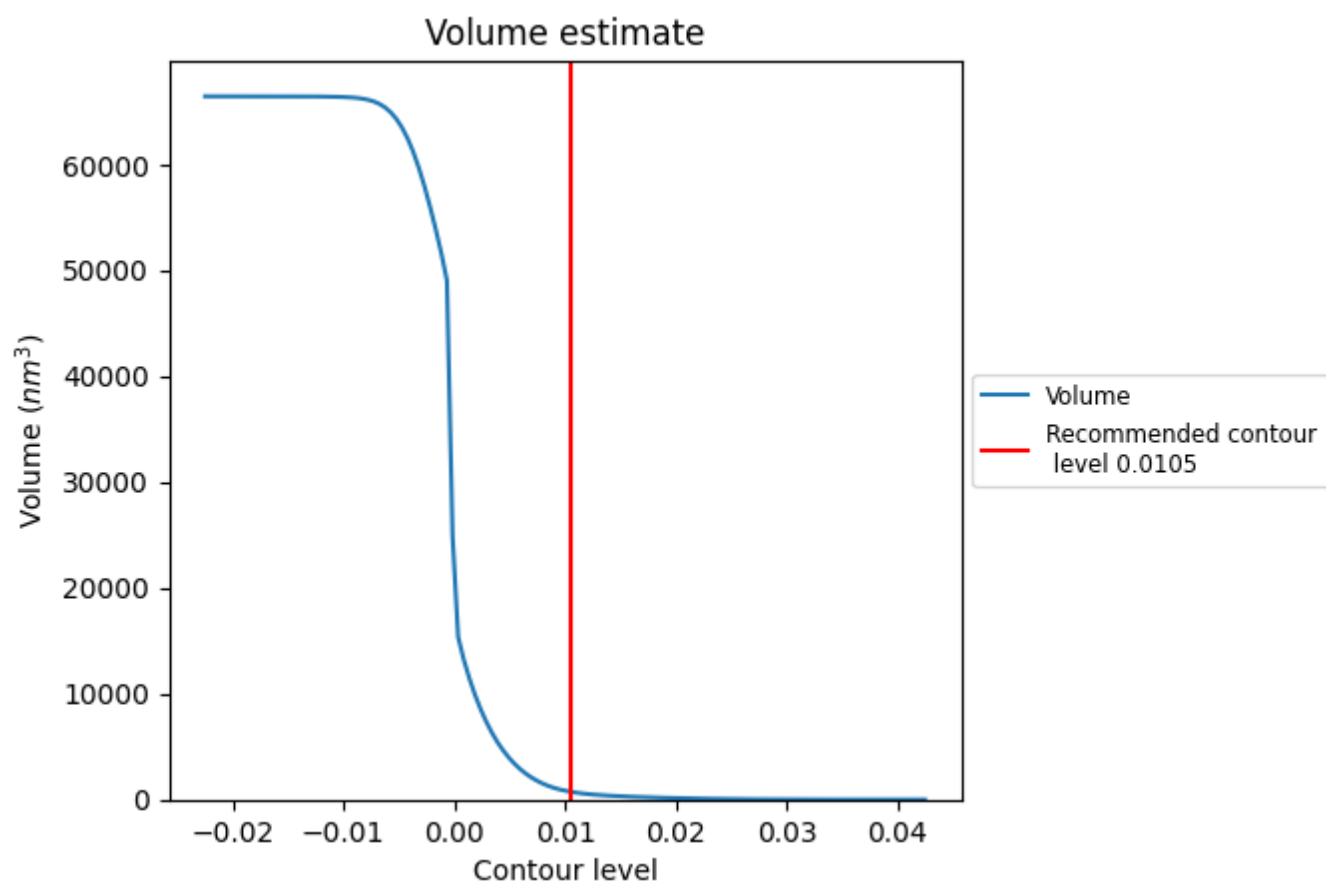
This section contains the results of statistical analysis of the map.

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.

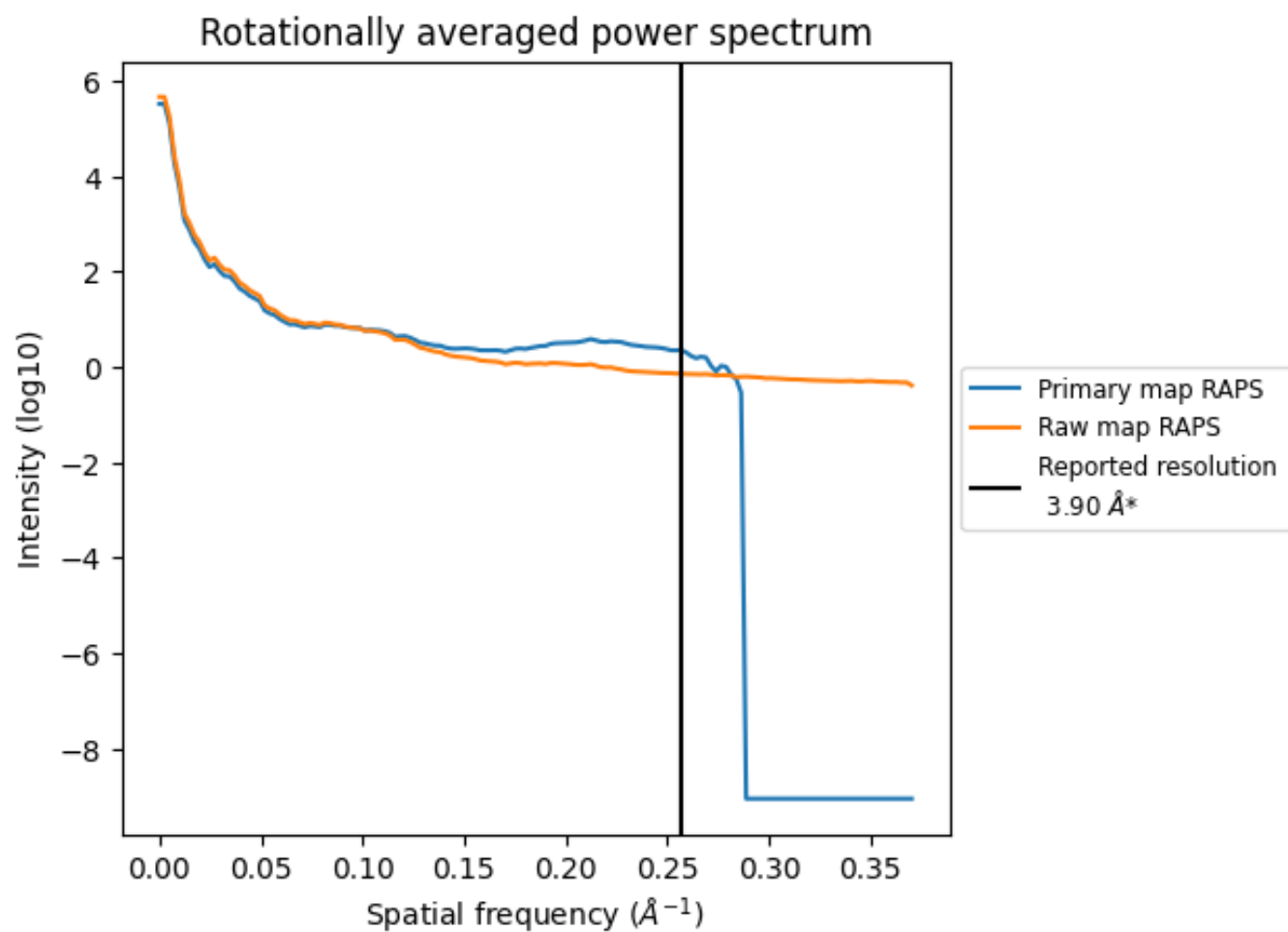
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 734 nm³; this corresponds to an approximate mass of 663 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 ⓘ

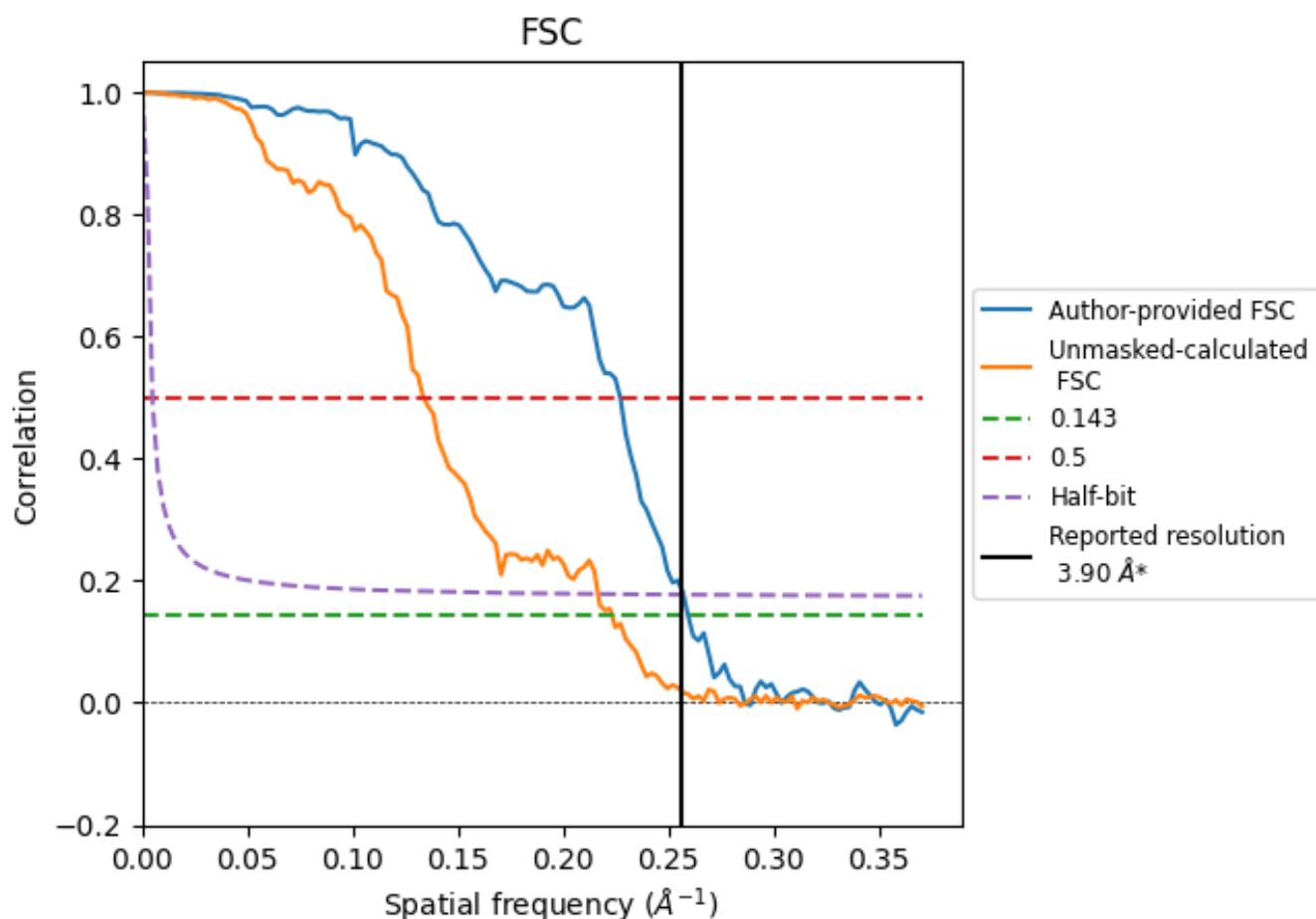


*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

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 0.256 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

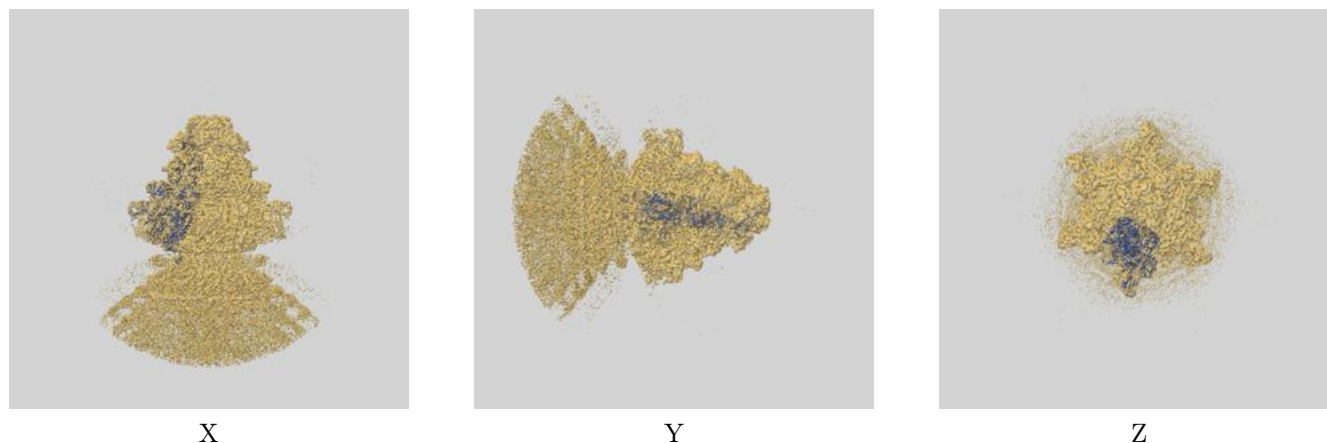
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.86	4.41	3.89
Unmasked-calculated*	4.48	7.48	4.62

*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 4.48 differs from the reported value 3.9 by more than 10 %

9 Map-model fit [i](#)

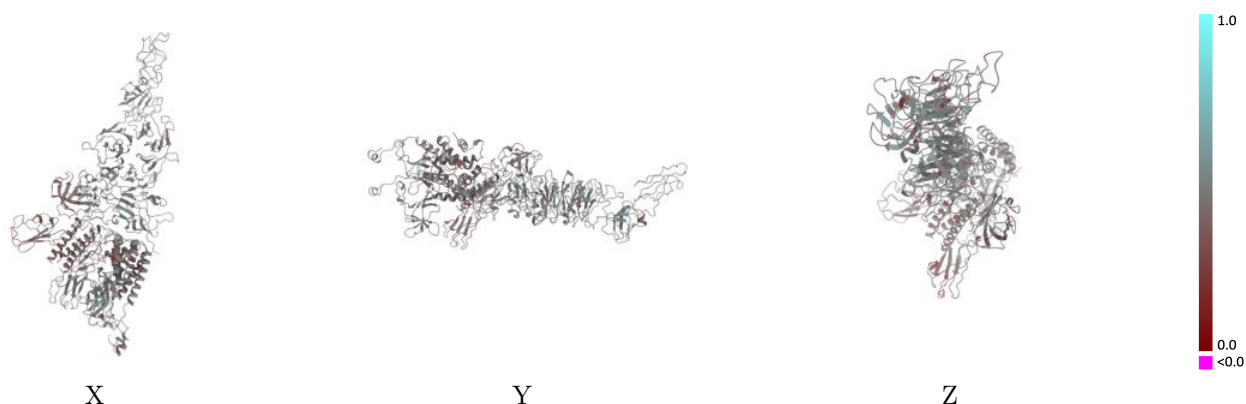
This section contains information regarding the fit between EMDB map EMD-16689 and PDB model 8CK1. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



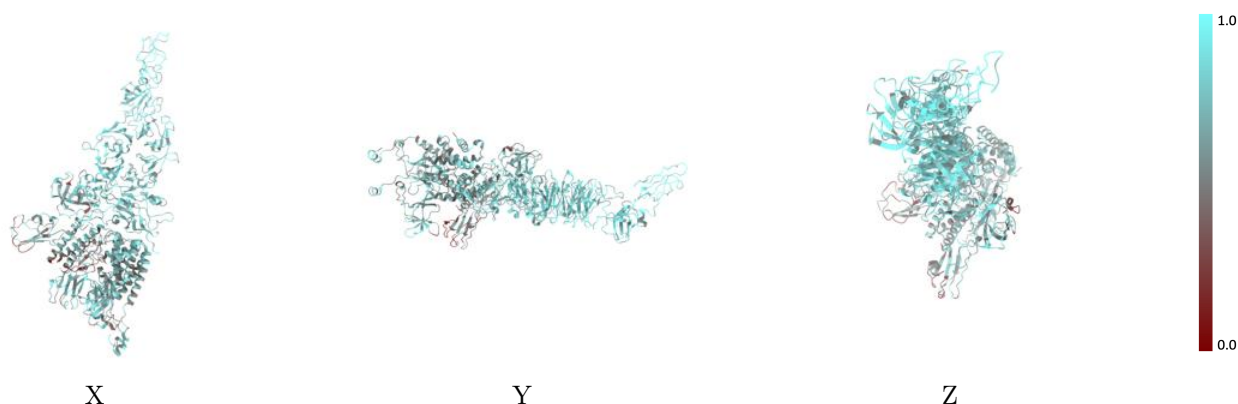
The images above show the 3D surface view of the map at the recommended contour level 0.0105 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



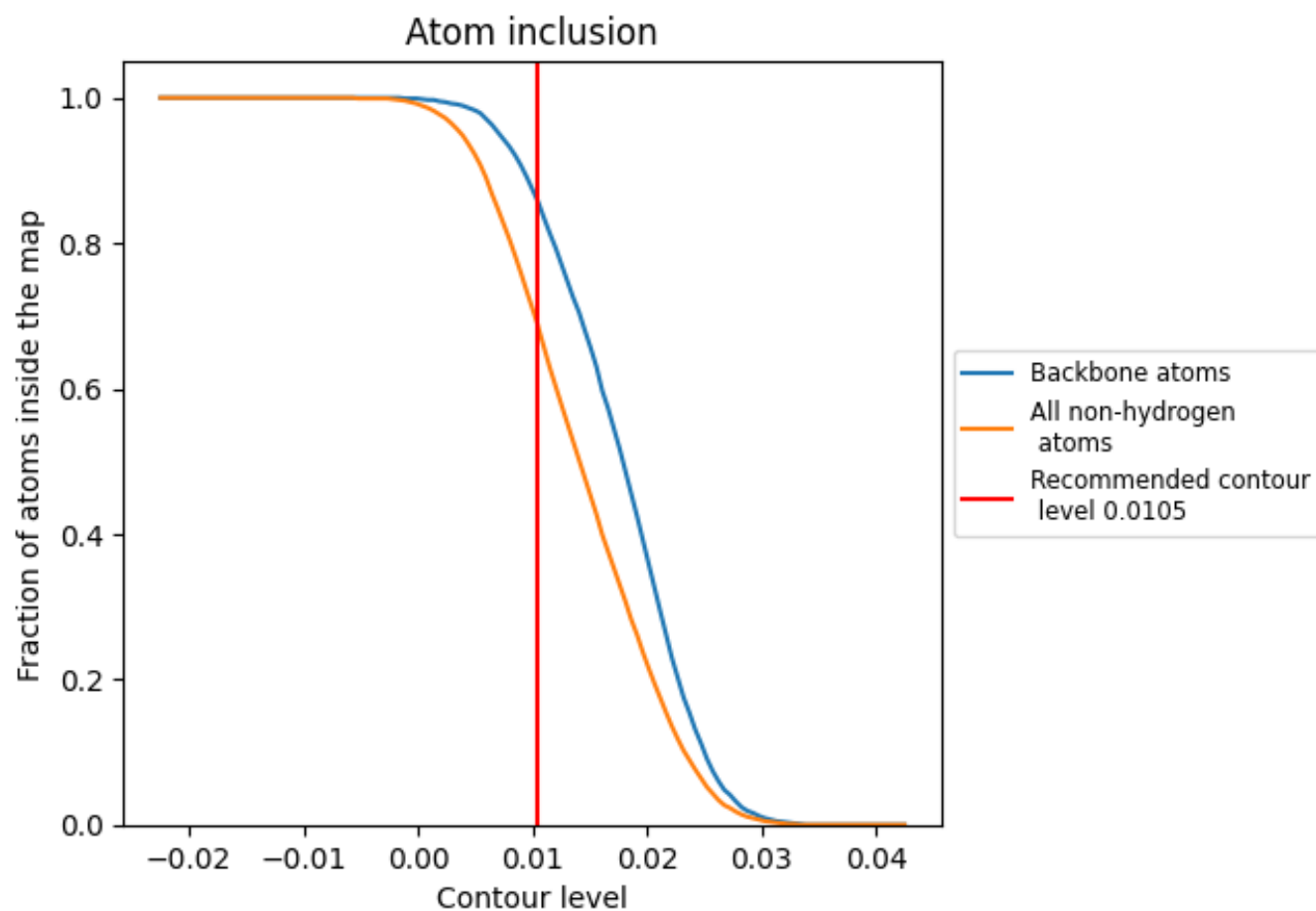
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0105).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 69% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0105) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6860	0.4470
A	0.7610	0.4670
B	0.6370	0.4350
C	0.5690	0.3840
D	0.4980	0.3850
E	0.6370	0.4570
F	0.6530	0.4440

1.0

0.0

<0.0