



wwPDB EM Validation Summary Report ⓘ

Oct 14, 2024 – 12:59 AM EDT

PDB ID : 8FQC
EMDB ID : EMD-29383
Title : Structure of baseplate with receptor binding complex of Agrobacterium phage Milano
Authors : Sonani, R.R.; Leiman, P.G.; Wang, F.; Kreutzberger, M.A.B.; Sebastian, A.; Esteves, N.C.; Kelly, R.J.; Scharf, B.; Egelman, E.H.
Deposited on : 2023-01-05
Resolution : 3.20 Å(reported)

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

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

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:

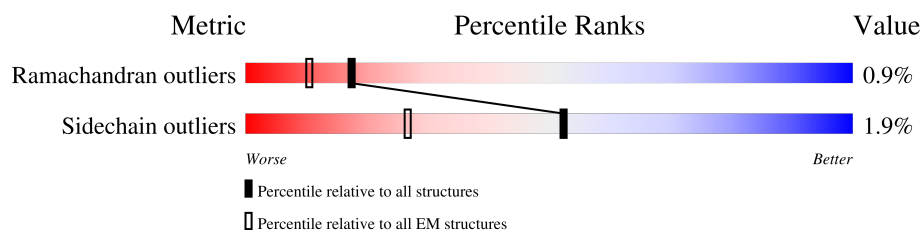
EMDB validation analysis : 0.0.1.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

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 3.20 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.



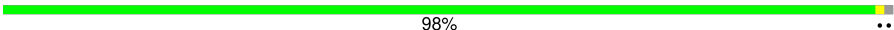
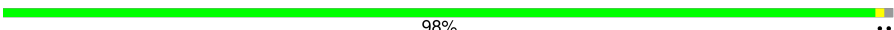
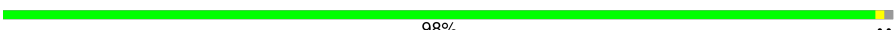
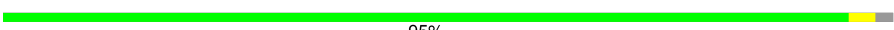






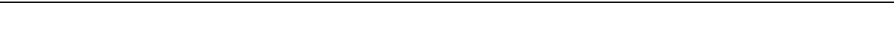

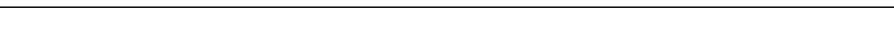
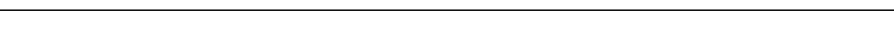











Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	C1	457	
2	E1	136	
2	a1	136	
2	f1	136	
2	g1	136	
3	F1	396	
3	G1	396	
3	h1	396	
3	i1	396	


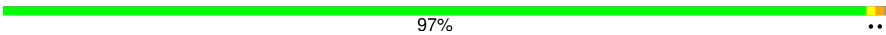
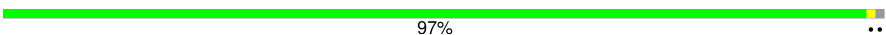

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Mol	Chain	Length	Quality of chain
4	H1	178	 98% ..
4	j1	178	 98% ..
5	I1	503	 98% ..
5	K1	503	 95% ..
5	k1	503	 96% ..
5	m1	503	 96% ..
6	J1	286	 93% 6%
6	l1	286	 97% .
7	P1	587	 27% 72%
7	Q1	587	 28% 71%
7	R1	587	 29% 71%
7	r1	587	 27% 72%
7	s1	587	 29% 71%
7	t1	587	 29% 71%
8	S1	300	 39% 60%
8	T1	300	 39% 60%
8	V1	300	 39% 60%
8	W1	300	 40% 60%
8	X1	300	 40% 60%
8	Y1	300	 40% 60%
8	u1	300	 39% 60%
8	v1	300	 39% 60%
8	w1	300	 40% 60%
8	x1	300	 39% 60%
8	y1	300	 40% 60%

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Mol	Chain	Length	Quality of chain
8	z1	300	 38% • 60%
9	U1	398	 97% ...
9	e1	398	 97% ..
10	A	188	 78% 10% • 11%

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 66089 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 Baseplate hub protein, gp26.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C1	326	Total	C	N	O	S	0	0
			2551	1610	434	500	7		

- Molecule 2 is a protein called Tail-tube, gp21.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E1	131	Total	C	N	O	S	0	0
			995	617	165	206	7		
2	a1	131	Total	C	N	O	S	0	0
			995	617	165	206	7		
2	f1	131	Total	C	N	O	S	0	0
			995	617	165	206	7		
2	g1	131	Total	C	N	O	S	0	0
			995	617	165	206	7		

- Molecule 3 is a protein called Baseplate Wedge 2 protein, gp29.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	F1	393	Total	C	N	O	S	0	0
			3016	1900	515	580	21		
3	G1	393	Total	C	N	O	S	0	0
			3016	1900	515	580	21		
3	h1	393	Total	C	N	O	S	0	0
			3016	1900	515	580	21		
3	i1	393	Total	C	N	O	S	0	0
			3016	1900	515	580	21		

- Molecule 4 is a protein called Baseplate wedge 1, gp28.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H1	176	Total	C	N	O	S	0	0
			1334	817	244	264	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	j1	176	Total	C	N	O	S	0	0
			1334	817	244	264	9		

- Molecule 5 is a protein called Tail sheath protein, gp20.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I1	498	Total	C	N	O	S	0	0
			3739	2342	633	742	22		
5	K1	494	Total	C	N	O	S	0	0
			3706	2322	628	735	21		
5	k1	498	Total	C	N	O	S	0	0
			3739	2342	633	742	22		
5	m1	494	Total	C	N	O	S	0	0
			3706	2322	628	735	21		

- Molecule 6 is a protein called Baseplate Wedge 3 protein, gp30.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J1	285	Total	C	N	O	S	0	0
			2185	1390	355	420	20		
6	l1	285	Total	C	N	O	S	0	0
			2185	1390	355	420	20		

- Molecule 7 is a protein called Tail Spike protein, gp124.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	P1	162	Total	C	N	O	S	0	0
			1227	782	194	248	3		
7	Q1	173	Total	C	N	O	S	0	0
			1308	835	210	260	3		
7	R1	173	Total	C	N	O	S	0	0
			1308	835	210	260	3		
7	r1	162	Total	C	N	O	S	0	0
			1227	782	194	248	3		
7	s1	173	Total	C	N	O	S	0	0
			1308	835	210	260	3		
7	t1	173	Total	C	N	O	S	0	0
			1308	835	210	260	3		

- Molecule 8 is a protein called Short Tail Fibers, gp31.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	S1	119	Total	C	N	O	S	0	0
			878	545	150	174	9		
8	T1	119	Total	C	N	O	S	0	0
			878	545	150	174	9		
8	V1	119	Total	C	N	O	S	0	0
			878	545	150	174	9		
8	W1	119	Total	C	N	O	S	0	0
			878	545	150	174	9		
8	X1	119	Total	C	N	O	S	0	0
			878	545	150	174	9		
8	Y1	119	Total	C	N	O	S	0	0
			878	545	150	174	9		
8	v1	119	Total	C	N	O	S	0	0
			878	545	150	174	9		
8	w1	119	Total	C	N	O	S	0	0
			878	545	150	174	9		
8	x1	119	Total	C	N	O	S	0	0
			878	545	150	174	9		
8	y1	119	Total	C	N	O	S	0	0
			878	545	150	174	9		
8	u1	119	Total	C	N	O	S	0	0
			878	545	150	174	9		
8	z1	119	Total	C	N	O	S	0	0
			878	545	150	174	9		

- Molecule 9 is a protein called Baseplate Centerpiece, gp25.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	U1	394	Total	C	N	O	S	0	0
			3027	1910	522	590	5		
9	e1	394	Total	C	N	O	S	0	0
			3027	1910	522	590	5		

- Molecule 10 is a protein called Baseplate Central Spike, gp27.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	A	168	Total	C	N	O	S	0	0
			1289	799	223	264	3		

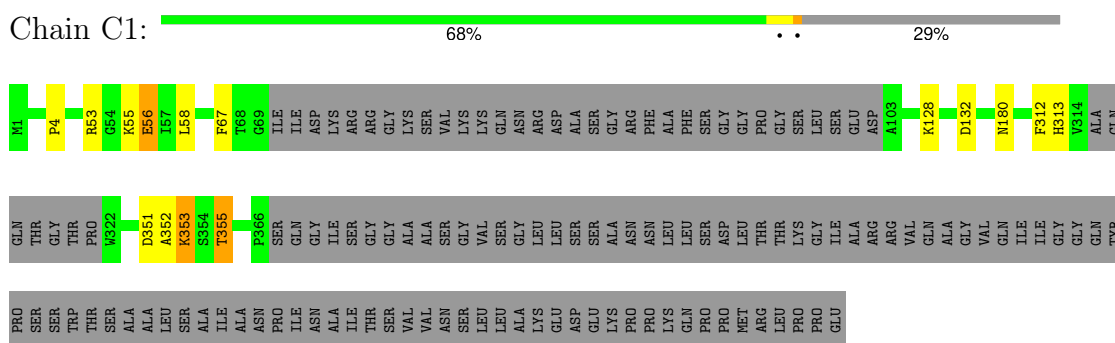
- Molecule 11 is FE (III) ION (three-letter code: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
11	A	1	Total 1	Fe 1	0

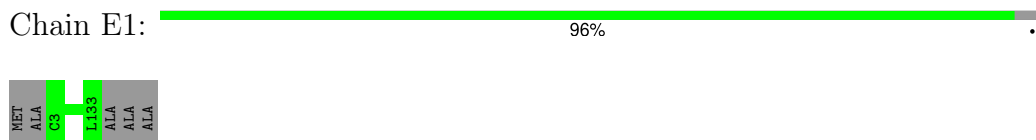
3 Residue-property plots [i](#)

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.

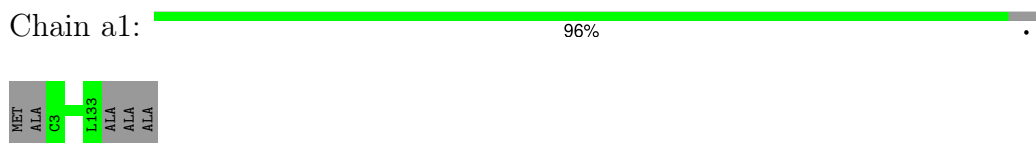
- Molecule 1: Baseplate hub protein, gp26



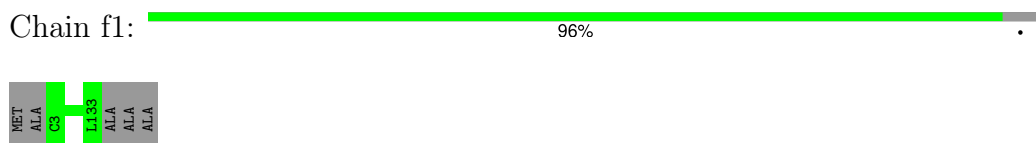
- Molecule 2: Tail-tube, gp21



- Molecule 2: Tail-tube, gp21



- Molecule 2: Tail-tube, gp21



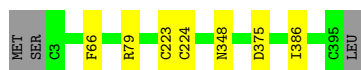
- Molecule 2: Tail-tube, gp21





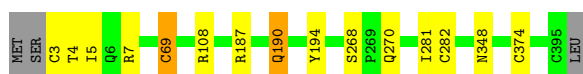
- Molecule 3: Baseplate Wedge 2 protein, gp29

Chain F1: 97%



- Molecule 3: Baseplate Wedge 2 protein, gp29

Chain G1: 95%



- Molecule 3: Baseplate Wedge 2 protein, gp29

Chain h1: 97%



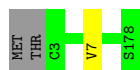
- Molecule 3: Baseplate Wedge 2 protein, gp29

Chain i1: 97%



- Molecule 4: Baseplate wedge 1, gp28

Chain H1: 98%



- Molecule 4: Baseplate wedge 1, gp28

Chain j1: 98%



- Molecule 5: Tail sheath protein, gp20

Chain I1: 98%

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

- Molecule 7: Tail Spike protein, gp124

[illegible]

- Molecule 7: Tail Spike protein, gp124

[illegible]

[illegible]

- Molecule 7: Tail Spike protein, gp124

Chain r1: 27% . 72%

LEU	THR	PHE	TYR	ASN	ALA	MET
VAL	ASP	ALA	GLY	GLY	THR	ALA
GLY	ASP	GLY	THR	ASN	THR	THR
HIS	SER	ILE	ILE	ASN	GLY	GLY
ARG	THR	ASP	SER	PRO	ASP	ARG
GLU	LEU	ALA	LYS	GLY	THR	PRO
VAL	ASP	ALA	THR	THR	VAL	LEU
VAL	GLY	LEU	GLY	THR	GLU	GLN
TYR	VAL	GLU	LEU	PHE	TYR	VAL
VAL	LEU	THR	CYS	ARG	GLY	GLY
ASN	ASN	THR	PRO	ASN	PRO	GLY
ILE	ILE	LEU	PHE	ASN	GLY	VAL
VAL	GLU	GLU	VAL	ARG	THR	PRO
VAL	GLY	TYR	PHE	ASN	ILE	G14
GLY	GLY	SER	GLN	VAL	THR	D23
VAL	PRO	PRO	ASP	GLU	GLY	C24
SER	SER	LEU	PHE	LYS	ASN	
VAL	VAL	ASP	GLY	VAL	PHE	
VAL	GLY	ARG	ASP	LEU	ALA	D175
THR	THR	LEU	ASP	ALA	PRO	PRO
GLY	ASP	GLY	ASN	THR	LYS	SER
THR	VAL	VAL	THR	GLY	SER	GLN
ILE	ILE	SER	THR	ASN	ASP	ILE
ALA	ALA	PHE	ASN	ARG	LEU	VAL
THR	THR	THR	PRO	PHE	GLU	THR
PHE	PHE	GLY	LYS	GLY	GLY	ARG
ALA	ALA	GLY	PHE	ASN	VAL	VAL
SER	SER	TRP	ILE	CYS	VAL	VAL
SER	SER	THR	VAL	ASP	ILE	ASP
SER	SER	ASP	SER	ILE	ASP	TYR
PHE	PHE	GLY	ASN	GLU	GLY	VAL
ASN	ASN	GLU	GLY	THR	ASP	THR
LEU	LEU	THR	ASP	ALA	VAL	GLY
PRO	ASP	ILE	ASP	ALA	THR	ASP
PRO	PRO	GLY	VAL	ILE	ILE	ASP
GLN	GLN	HIS	HIS	PRO	ALA	ALA
THR	THR	VAL	GLY	ASN	ALA	THR
VAL	VAL	VAL	ASN	GLY	GLY	ALA
VAL	VAL	VAL	TYR	THR	VAL	THR
ARG	ARG	SER	ASP	GLY	VAL	ASP
VAL	VAL	ARG	PRO	LEU	GLY	GLY
THR	THR	SER	ALA	ALA	ALA	LEU
THR	THR	THR	PHE	VAL	LEU	ALA
THR	THR	ILE	TYR	MET	VAL	LYS
ASP	SER	VAL	ALA	SER	ASP	PRO
ASP	ASP	PRO	LEU	PHE	GLY	PHE
GLY	GLY	GLU	PRO	SER	LEU	ALA
THR	THR	ASN	ASN	GLY	PHE	THR
PHE	PHE	MET	GLY	THR	VAL	VAL
ASP	ASP	ALA	GLN	VAL	ASP	SER
TYR	TYR	GLY	THR	PRO	GLY	ALA
ALA	ALA	SER	LEU	LEU	SER	ALA
ALA	ALA	VAL	ASN	THR	VAL	ILE
LEU	LEU	PHE	SER	ASP	THR	GLY

- Molecule 7: Tail Spike protein, gp124

Chain s1: 29% . 71%

[illegible]

[illegible]

- Molecule 8: Short Tail Fibers, gp31

Chain V1:  39% 60%

[illegible]

- Molecule 8: Short Tail Fibers, gp31

Chain W1:  40% 60%

GLY	VAL	GLN	VAL	TTR	VAL	TTR	LEU
VAL				VAL	GLY	GLY	ASP
				GLY	GLY	ARG	ALA
				THR	THR	ALA	VAL
				ALA	ALA	ILE	GLY
				ASP	ASP	THR	THR
				GLY	GLY	ASP	CYS
				GLY	GLY	THR	GLN
				ARG	ARG	VAL	LEU
				ILE	ILE	GLN	PRO
				GLN	GLN	SER	GLN
				ALA	ALA	THR	ILE
				VAL	VAL	ALA	GLY
				ILE	ILE	GLY	ALA
				ALA	ALA	ARG	ILE
				PHE	PHE	ALA	ASP
				LYS	LYS	VAL	ASP
				GLY	GLY	PHE	TTR
				ASN	ASN	ARG	LEU
				GLN	GLN	SER	ALA
				TTR	TTR	ARG	CYS
				THR	THR	LYS	ILE
				ALA	ALA	GLY	ASP
				LYS	LYS	ILE	GLY
				ALA	ALA	ILE	ALA
				GLY	GLY	ILE	ARG
				ASP	ASP	THR	ILE
				ILE	ILE	VAL	VAL
				LEU	LEU	SER	ARG
				PRO	PRO	THR	SER
				GLY	GLY	GLY	ALA
				GLY	GLY	ALA	GLY
				ASP	ASP	ILE	GLY
				ASP	ASP	THR	GLY
				VAL	VAL	GLY	ALA
				ILE	ILE	GLY	LEU
				ARG	ARG	ALA	GLY
				VAL	VAL	TTR	GLY
				ARG	ARG	GLN	GLY
				THR	THR	ILE	VAL
				PRO	PRO	SER	GLY
				GLY	GLY	SER	ILE
				THR	THR	GLY	GLY
				GLN	GLN	TTR	GLY
				ARG	ARG	GLY	VAL
				LEU	LEU	PRO	ILE
				GLN	GLN	SER	PRO
				ILE	ILE	THR	GLN
				TTR	TTR	PHE	ASN
				ASP	ASP	ALA	CYS

- Molecule 8: Short Tail Fibers, gp31

Chain X1: 

[illegible]

[illegible]

- Molecule 8: Short Tail Fibers, gp31

Chain y1:  40% 60%

[illegible]

- Molecule 8: Short Tail Fibers, gp31

Chain u1:  39% 60%

ILE	THR	GLN	MET
TRP	PHE	ASN	ALA
ASP	ALA	GLN	G3
GLY	VAL	LEU	D94
VAL	THR	PHE	D95
GLN	PRO	ASP	D96
VAL	PRO	SER	G121
	GLY	TRP	GLN
	THR	ALA	VAL
	ALA	GLY	GLY
	ILE	PHE	THR
	ASP	TRP	LEU
	GLY	ASP	CYS
	GLY	VAL	GLN
	ARG	SER	LEU
	ILE	GLN	PRO
	GLN	SER	GLN
	ALA	THR	ILE
	VAL	ALA	GLY
	ALA	GLY	ILE
	ILE	ARG	GLN
	ALA	THR	ASP
	PHE	ALA	ASP
	LYS	PHE	ASP
	LYS	VAL	TRP
	GLY	PHE	LEU
	ASN	ARG	ALA
	GLN	SER	GLY
	TRP	ARG	CYS
	TYR	LYS	ILE
	ALA	GLU	ASP
	LYS	GLY	GLY
	ALA	ILE	ALA
	GLY	GLY	ALA
	ASP	ILE	ARG
	ILE	THR	ILE
	ILE	VAL	VAL
	LEU	SER	PRO
	PRO	GLU	PHE
	LEU	LEU	ALA
	GLY	PHE	ALA
	GLY	ILE	VAL
	ASP	ALA	ARG
	ASP	THR	SER
	VAL	GLY	ALA
	ILE	GLY	LEU
	VAL	GLY	GLY
	ARG	ALA	GLY
	VAL	TYR	GLY
	ARG	GLN	GLY
	THR	SER	GLY
	PRO	ILE	VAL
	GLY	SER	ILE
	TYR	GLU	GLY
	GLN	TRP	GLY
	ARG	GLU	VAL
	LEU	PRO	ILE
	GLN	SER	PRO

- Molecule 8: Short Tail Fibers, gp31

Chain z1:  38% . 60%

[illegible]

Sequence logo for the 10th position. The y-axis represents information content in bits, ranging from 0 to 1.5. The x-axis shows the amino acid sequence: MET, ALA, G3, I53, F97, L129, S130, L138, K198, V396, ARG, ALA. The G3 position shows the highest information content, with a peak around 1.4 bits.

Sequence logo for the 10th position. The y-axis represents information content in bits, ranging from 0 to 1.5. The x-axis shows the amino acid sequence: MET, ALA, G3, R93, F97, L138, W199, H319, R395, V396, ARG, ALA. The 'G3' position shows a strong preference for Glycine (G), while 'H319' shows a strong preference for Histidine (H).

MET	THR	SER	LYS	THR	TYR	ASP	GLU	ARG	ASN	ARG	ASP	ILE	GLN	ASP	GLY	F18	E19	R20	H21	V22	I26	S36	V37	K38	G39	S40	G41	T42	Q43	V47	P48	V49	I50	G72	S73	D74	A75	S76	N77	K78	D114	S115	I116	D181	P185	ARG
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	-----

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	14856	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.478	Depositor
Minimum map value	-0.780	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.045	Depositor
Recommended contour level	0.1	Depositor
Map size (\AA)	624.24005, 624.24005, 624.24005	wwPDB
Map dimensions	578, 578, 578	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.08, 1.08, 1.08	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FE

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	C1	0.38	0/2598	0.57	0/3525
2	E1	0.46	0/1011	0.52	0/1382
2	a1	0.40	0/1011	0.52	0/1382
2	f1	0.38	0/1011	0.51	0/1382
2	g1	0.41	0/1011	0.52	0/1382
3	F1	0.42	0/3085	0.49	0/4207
3	G1	0.47	0/3085	0.55	0/4207
3	h1	0.42	0/3085	0.48	0/4207
3	i1	0.46	0/3085	0.54	0/4207
4	H1	0.37	0/1353	0.51	0/1831
4	j1	0.37	0/1353	0.51	0/1831
5	I1	0.41	0/3815	0.53	0/5211
5	K1	0.38	0/3781	0.51	0/5165
5	k1	0.42	0/3815	0.52	0/5211
5	m1	0.37	0/3781	0.50	0/5165
6	J1	0.44	0/2237	0.53	0/3063
6	l1	0.41	0/2237	0.50	0/3063
7	P1	0.33	0/1269	0.45	0/1755
7	Q1	0.35	0/1352	0.50	0/1868
7	R1	0.30	0/1352	0.47	0/1868
7	r1	0.33	0/1269	0.45	0/1755
7	s1	0.36	0/1352	0.46	0/1868
7	t1	0.32	0/1352	0.47	0/1868
8	S1	0.29	0/892	0.46	0/1217
8	T1	0.28	0/892	0.46	0/1217
8	V1	0.28	0/892	0.49	0/1217
8	W1	0.32	0/892	0.44	0/1217
8	X1	0.30	0/892	0.46	0/1217
8	Y1	0.29	0/892	0.45	0/1217
8	u1	0.31	0/892	0.48	0/1217
8	v1	0.30	0/892	0.47	0/1217
8	w1	0.28	0/892	0.45	0/1217

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
8	x1	0.28	0/892	0.49	0/1217
8	y1	0.31	0/892	0.45	0/1217
8	z1	0.31	0/892	0.44	0/1217
9	U1	0.44	0/3093	0.49	0/4214
9	e1	0.44	0/3093	0.50	1/4214 (0.0%)
10	A	0.62	0/1320	0.91	3/1791 (0.2%)
All	All	0.40	0/67510	0.51	4/92226 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	e1	138	LEU	CA-CB-CG	5.73	128.49	115.30
10	A	116	ILE	N-CA-C	-5.73	95.53	111.00
10	A	181	ASP	CB-CG-OD2	5.18	122.96	118.30
10	A	72	GLY	N-CA-C	-5.14	100.25	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	C1	320/457 (70%)	247 (77%)	65 (20%)	8 (2%)	4	28
2	E1	129/136 (95%)	117 (91%)	12 (9%)	0	100	100
2	a1	129/136 (95%)	117 (91%)	12 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	f1	129/136 (95%)	118 (92%)	11 (8%)	0	100	100
2	g1	129/136 (95%)	118 (92%)	10 (8%)	1 (1%)	16	51
3	F1	391/396 (99%)	371 (95%)	19 (5%)	1 (0%)	37	69
3	G1	391/396 (99%)	366 (94%)	21 (5%)	4 (1%)	13	47
3	h1	391/396 (99%)	378 (97%)	10 (3%)	3 (1%)	16	51
3	i1	391/396 (99%)	363 (93%)	26 (7%)	2 (0%)	25	60
4	H1	174/178 (98%)	149 (86%)	24 (14%)	1 (1%)	22	57
4	j1	174/178 (98%)	145 (83%)	27 (16%)	2 (1%)	12	44
5	I1	496/503 (99%)	439 (88%)	56 (11%)	1 (0%)	44	75
5	K1	492/503 (98%)	421 (86%)	64 (13%)	7 (1%)	9	40
5	k1	496/503 (99%)	441 (89%)	53 (11%)	2 (0%)	30	64
5	m1	492/503 (98%)	404 (82%)	80 (16%)	8 (2%)	8	37
6	J1	283/286 (99%)	258 (91%)	20 (7%)	5 (2%)	7	35
6	l1	283/286 (99%)	253 (89%)	27 (10%)	3 (1%)	12	44
7	P1	160/587 (27%)	146 (91%)	13 (8%)	1 (1%)	22	57
7	Q1	171/587 (29%)	155 (91%)	12 (7%)	4 (2%)	5	29
7	R1	171/587 (29%)	158 (92%)	12 (7%)	1 (1%)	22	57
7	r1	160/587 (27%)	147 (92%)	12 (8%)	1 (1%)	22	57
7	s1	171/587 (29%)	158 (92%)	10 (6%)	3 (2%)	7	35
7	t1	171/587 (29%)	156 (91%)	15 (9%)	0	100	100
8	S1	117/300 (39%)	109 (93%)	8 (7%)	0	100	100
8	T1	117/300 (39%)	112 (96%)	4 (3%)	1 (1%)	14	49
8	V1	117/300 (39%)	109 (93%)	8 (7%)	0	100	100
8	W1	117/300 (39%)	109 (93%)	8 (7%)	0	100	100
8	X1	117/300 (39%)	107 (92%)	10 (8%)	0	100	100
8	Y1	117/300 (39%)	111 (95%)	6 (5%)	0	100	100
8	u1	117/300 (39%)	110 (94%)	6 (5%)	1 (1%)	14	49
8	v1	117/300 (39%)	107 (92%)	10 (8%)	0	100	100
8	w1	117/300 (39%)	114 (97%)	3 (3%)	0	100	100
8	x1	117/300 (39%)	105 (90%)	12 (10%)	0	100	100
8	y1	117/300 (39%)	110 (94%)	7 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	z1	117/300 (39%)	108 (92%)	7 (6%)	2 (2%)	7	36
9	U1	392/398 (98%)	368 (94%)	21 (5%)	3 (1%)	16	51
9	e1	392/398 (98%)	361 (92%)	30 (8%)	1 (0%)	37	69
10	A	166/188 (88%)	142 (86%)	13 (8%)	11 (7%)	1	7
All	All	8648/13631 (63%)	7807 (90%)	764 (9%)	77 (1%)	17	49

5 of 77 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	F1	375	ASP
6	J1	2	ASN
5	K1	378	PRO
7	Q1	117	ILE
7	Q1	119	VAL

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	C1	281/383 (73%)	271 (96%)	10 (4%)	30	62
2	E1	115/116 (99%)	115 (100%)	0	100	100
2	a1	115/116 (99%)	115 (100%)	0	100	100
2	f1	115/116 (99%)	115 (100%)	0	100	100
2	g1	115/116 (99%)	115 (100%)	0	100	100
3	F1	330/333 (99%)	324 (98%)	6 (2%)	54	77
3	G1	330/333 (99%)	317 (96%)	13 (4%)	27	60
3	h1	330/333 (99%)	324 (98%)	6 (2%)	54	77
3	i1	330/333 (99%)	321 (97%)	9 (3%)	40	69
4	H1	145/147 (99%)	145 (100%)	0	100	100
4	j1	145/147 (99%)	145 (100%)	0	100	100
5	I1	404/408 (99%)	399 (99%)	5 (1%)	67	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	K1	400/408 (98%)	392 (98%)	8 (2%)	50	75
5	k1	404/408 (99%)	393 (97%)	11 (3%)	40	69
5	m1	400/408 (98%)	394 (98%)	6 (2%)	60	81
6	J1	245/247 (99%)	231 (94%)	14 (6%)	17	50
6	l1	245/247 (99%)	239 (98%)	6 (2%)	44	71
7	P1	129/473 (27%)	129 (100%)	0	100	100
7	Q1	138/473 (29%)	135 (98%)	3 (2%)	47	73
7	R1	138/473 (29%)	135 (98%)	3 (2%)	47	73
7	r1	129/473 (27%)	127 (98%)	2 (2%)	58	79
7	s1	138/473 (29%)	135 (98%)	3 (2%)	47	73
7	t1	138/473 (29%)	137 (99%)	1 (1%)	81	92
8	S1	97/229 (42%)	96 (99%)	1 (1%)	73	87
8	T1	97/229 (42%)	97 (100%)	0	100	100
8	V1	97/229 (42%)	95 (98%)	2 (2%)	48	74
8	W1	97/229 (42%)	97 (100%)	0	100	100
8	X1	97/229 (42%)	97 (100%)	0	100	100
8	Y1	97/229 (42%)	97 (100%)	0	100	100
8	u1	97/229 (42%)	95 (98%)	2 (2%)	48	74
8	v1	97/229 (42%)	95 (98%)	2 (2%)	48	74
8	w1	97/229 (42%)	97 (100%)	0	100	100
8	x1	97/229 (42%)	96 (99%)	1 (1%)	73	87
8	y1	97/229 (42%)	97 (100%)	0	100	100
8	z1	97/229 (42%)	94 (97%)	3 (3%)	35	66
9	U1	314/316 (99%)	308 (98%)	6 (2%)	52	76
9	e1	314/316 (99%)	309 (98%)	5 (2%)	58	79
10	A	143/162 (88%)	134 (94%)	9 (6%)	15	46
All	All	7194/10979 (66%)	7057 (98%)	137 (2%)	52	76

5 of 137 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	r1	175	ASP
7	t1	175	ASP

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Mol	Chain	Res	Type
10	A	38	LYS
5	K1	12	ARG
6	J1	277	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 112 such sidechains are listed below:

Mol	Chain	Res	Type
2	a1	84	GLN
10	A	28	HIS
3	i1	355	ASN
8	z1	117	ASN
8	x1	17	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

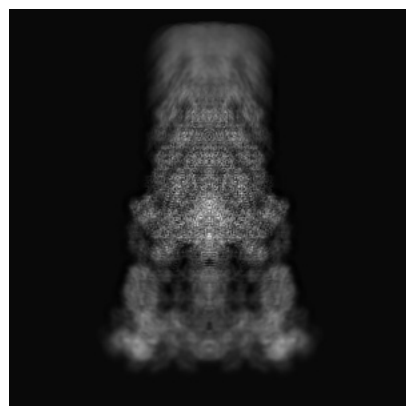
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29383. These allow visual inspection of the internal detail of the map and identification of artifacts.

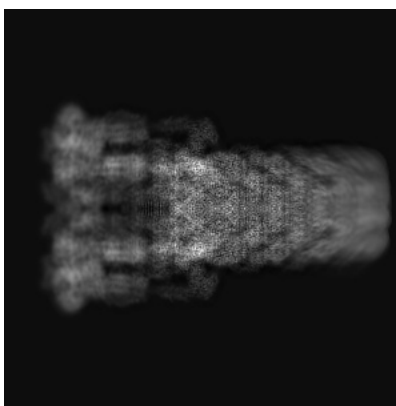
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

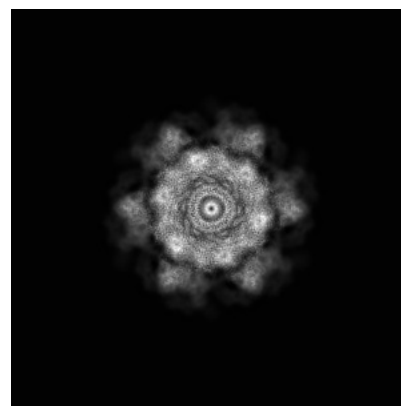
6.1.1 Primary map



X

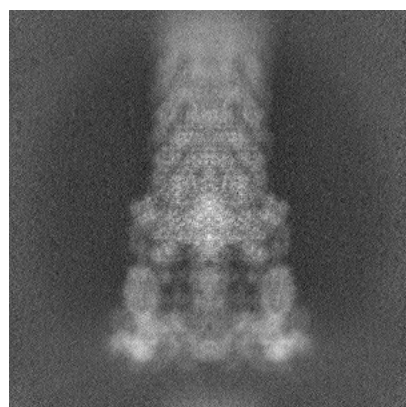


Y

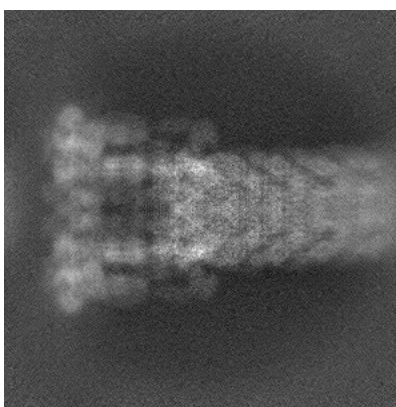


Z

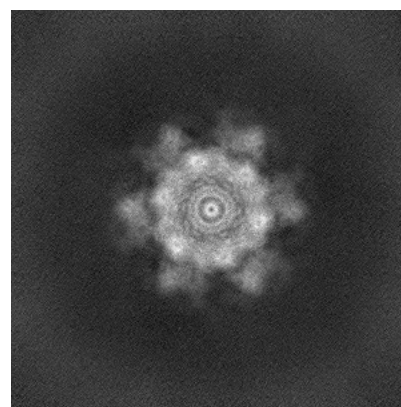
6.1.2 Raw map



X



Y

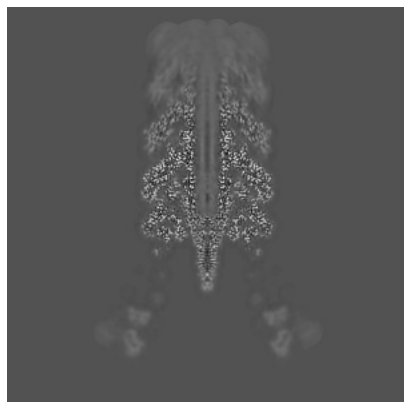


Z

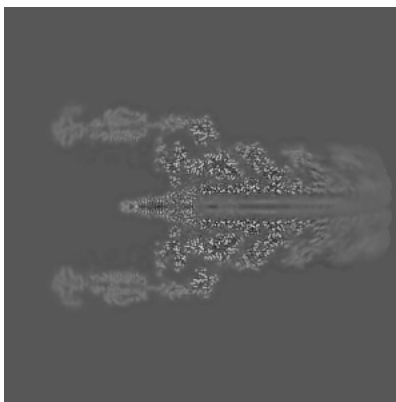
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

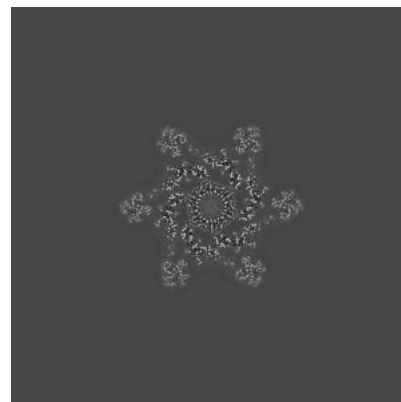
6.2.1 Primary map



X Index: 289

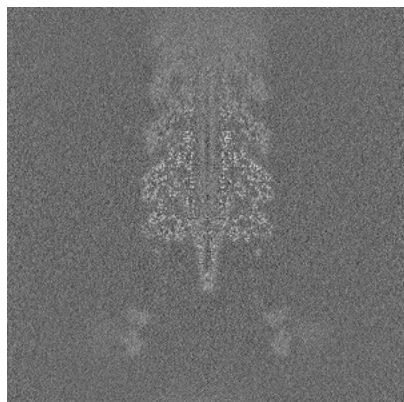


Y Index: 289

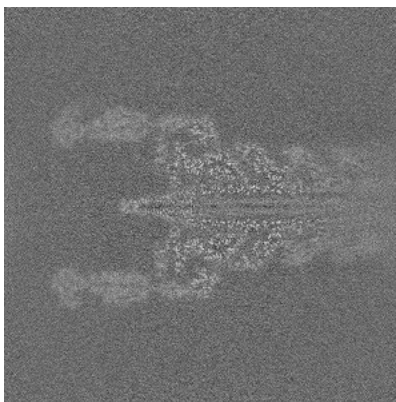


Z Index: 289

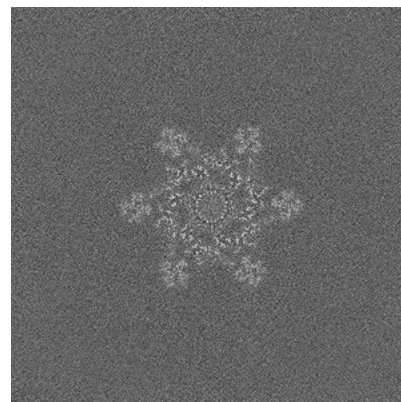
6.2.2 Raw map



X Index: 289



Y Index: 289

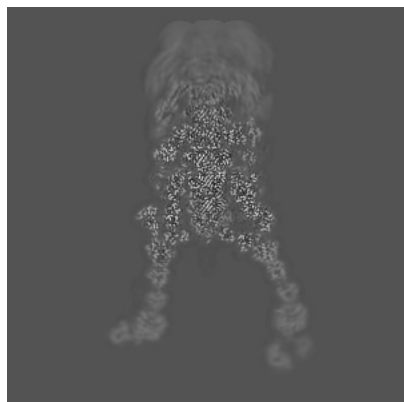


Z Index: 289

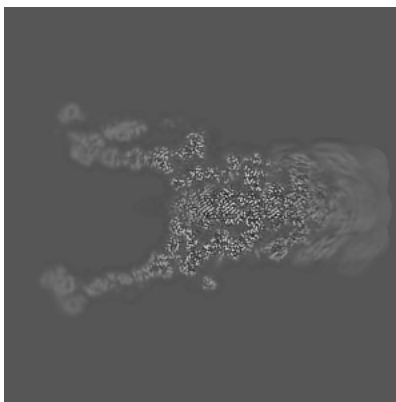
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

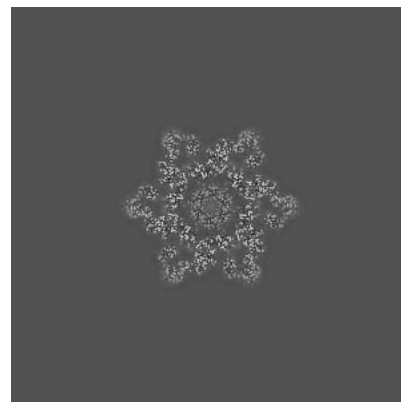
6.3.1 Primary map



X Index: 310

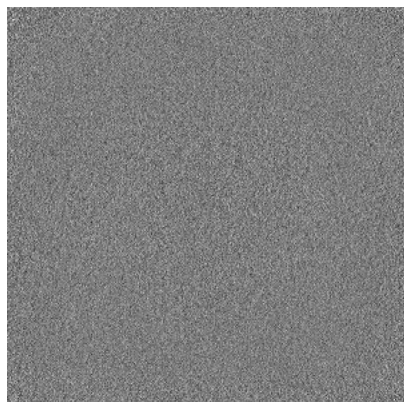


Y Index: 268

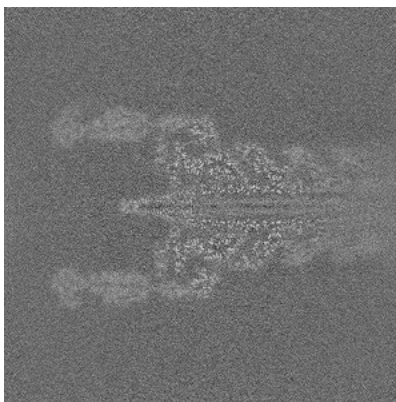


Z Index: 276

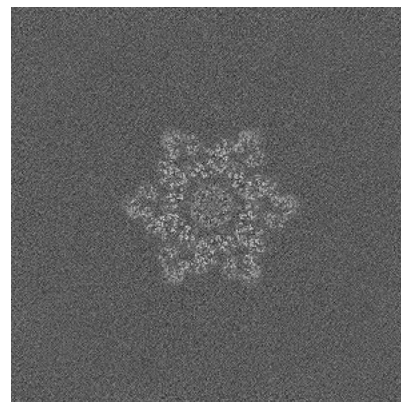
6.3.2 Raw map



X Index: 0



Y Index: 289

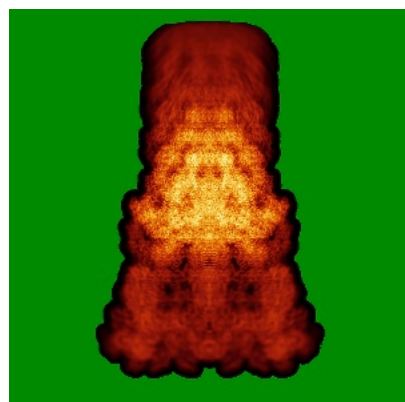


Z Index: 276

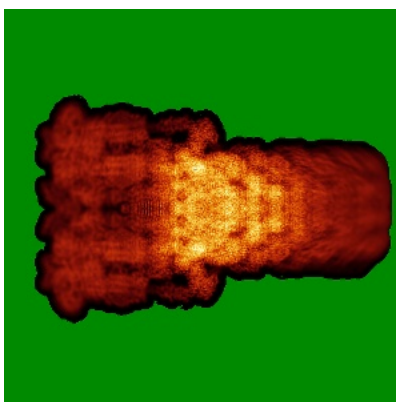
The images above show the largest variance slices of the map in three orthogonal directions.

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

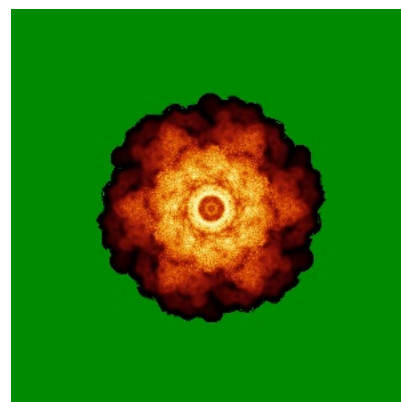
6.4.1 Primary map



X

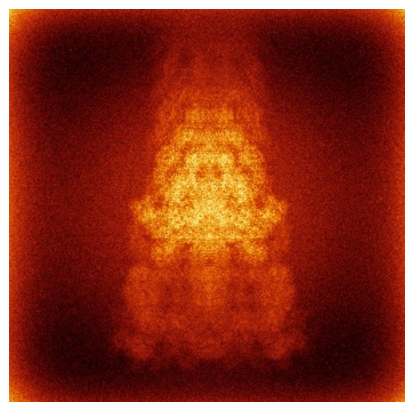


Y

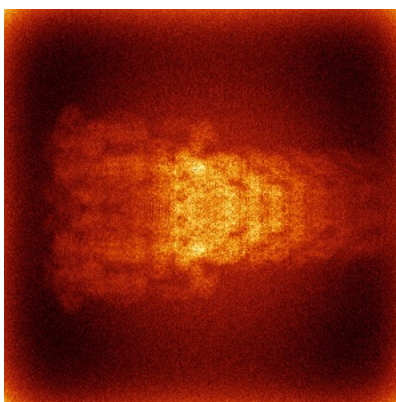


Z

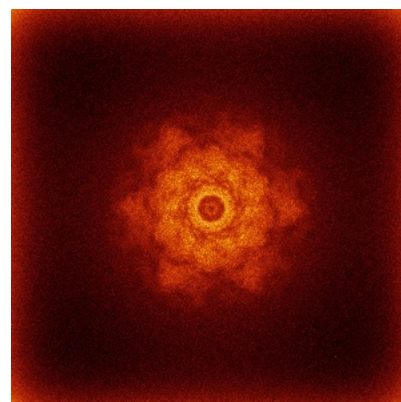
6.4.2 Raw map



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.

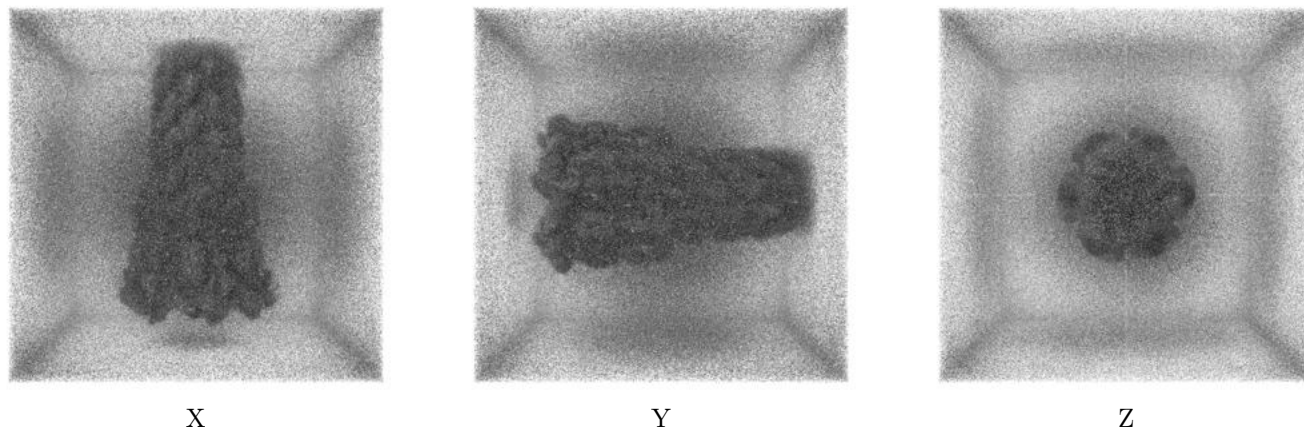
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. 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.

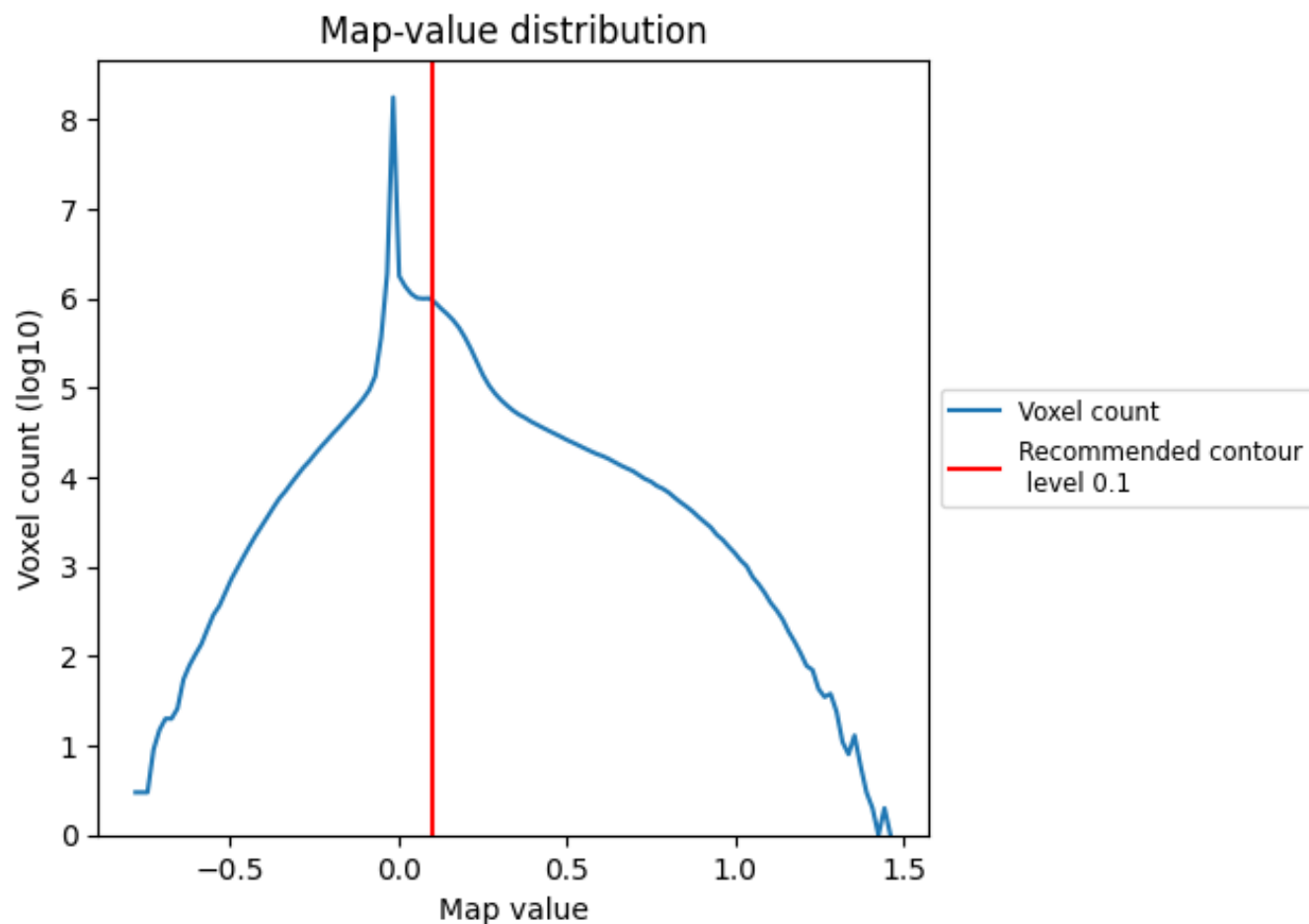
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

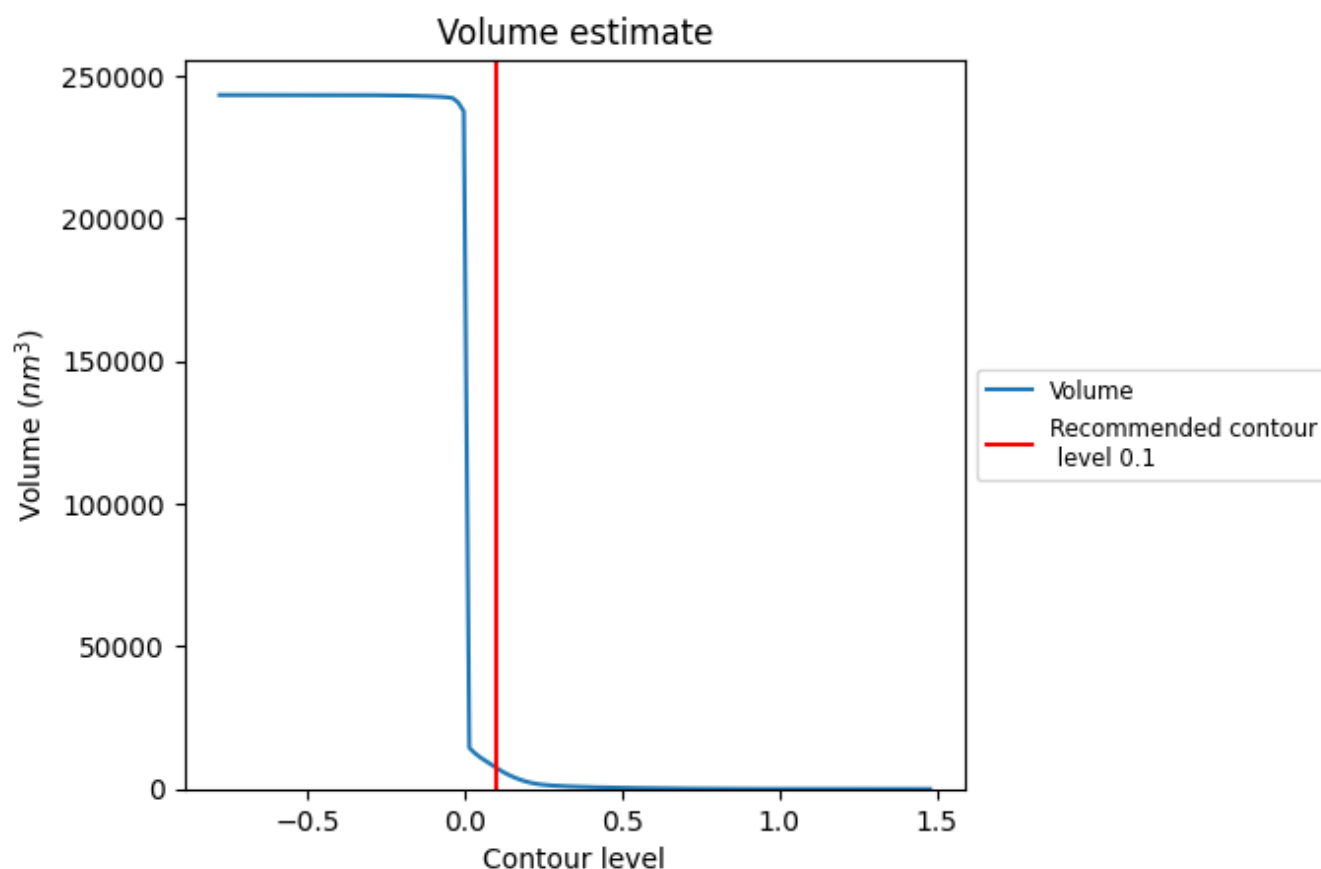
This section contains the results of statistical analysis of the map.

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.

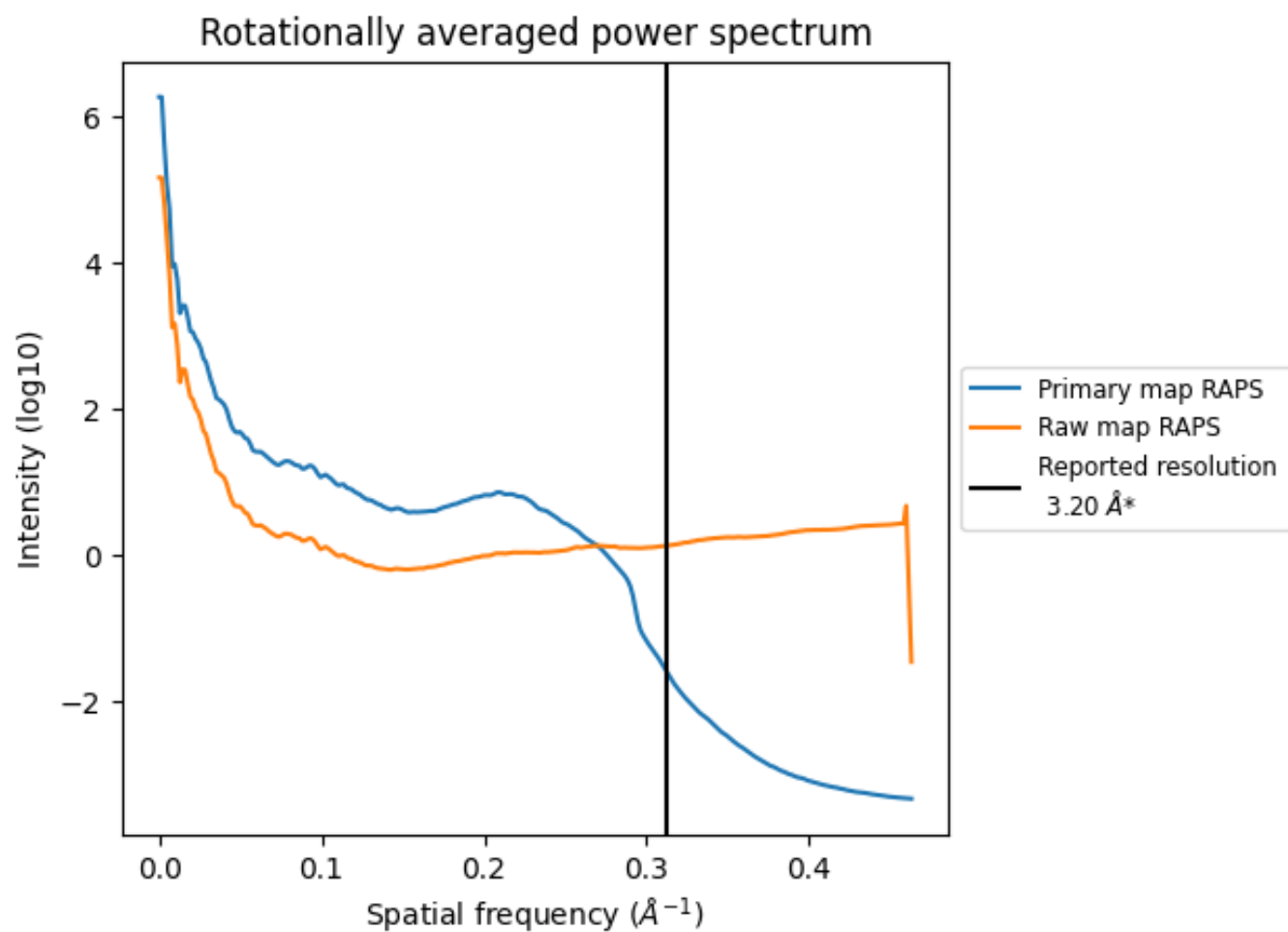
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 7391 nm³; this corresponds to an approximate mass of 6676 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 ⓘ

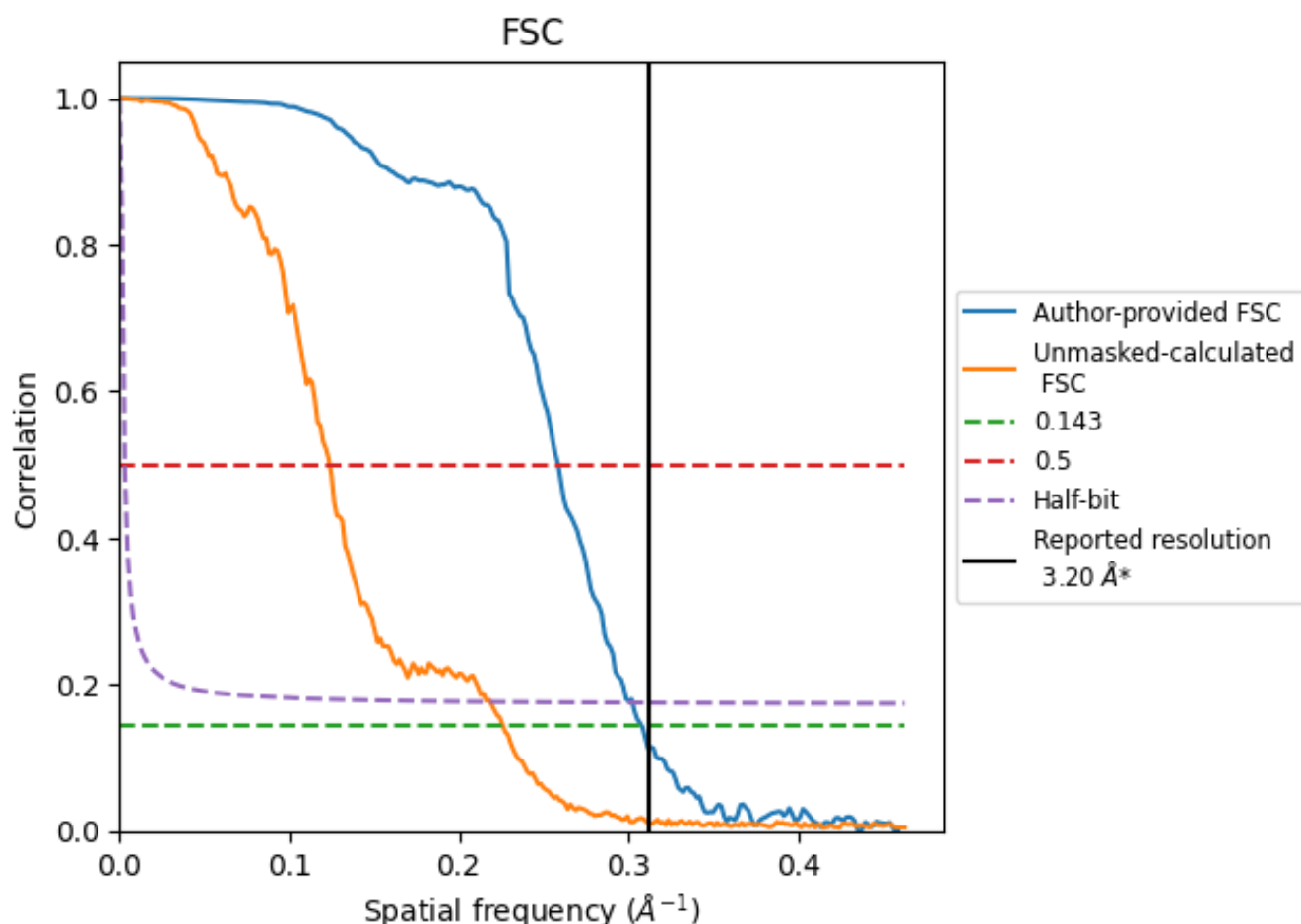


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

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 0.312 \AA^{-1}

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.25	3.87	3.31
Unmasked-calculated*	4.42	8.07	4.58

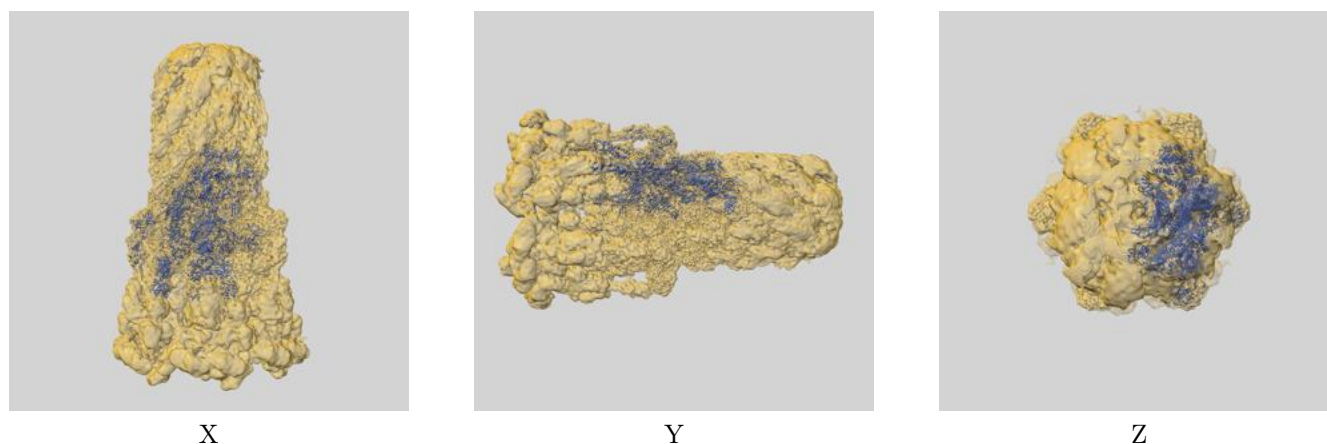
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.42 differs from the reported value 3.2 by more than 10 %

9 Map-model fit [i](#)

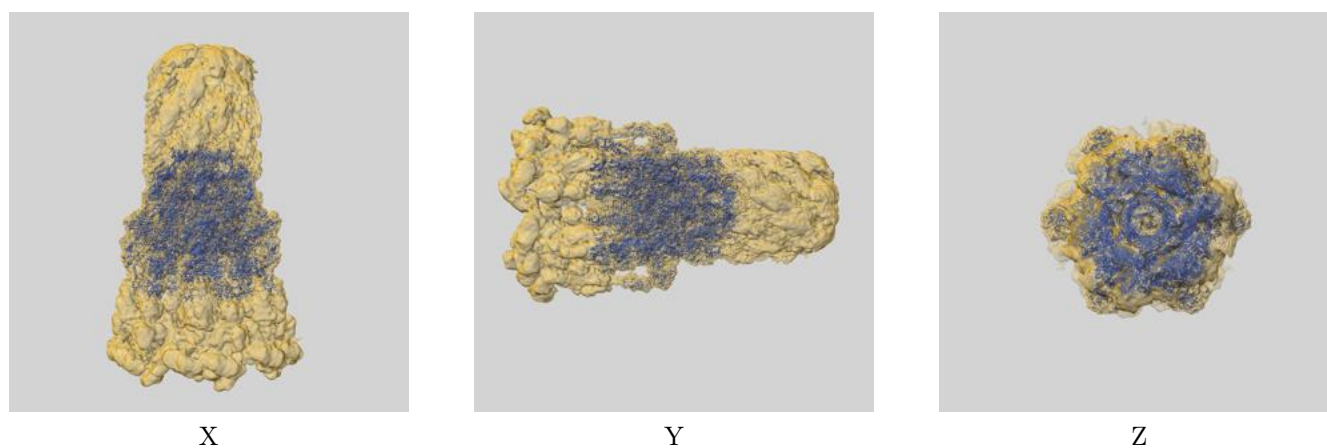
This section contains information regarding the fit between EMDB map EMD-29383 and PDB model 8FQC. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

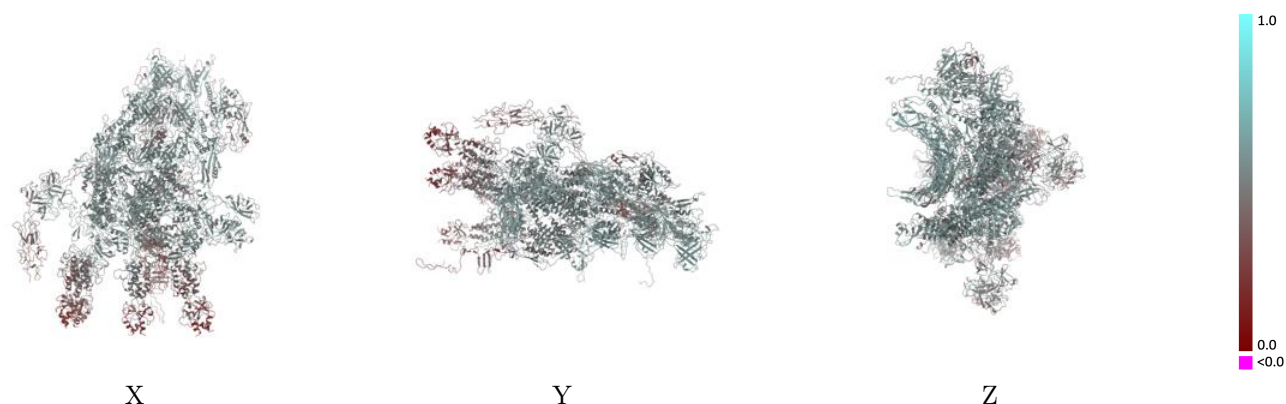


9.1.2 Map-model assembly overlay [i](#)



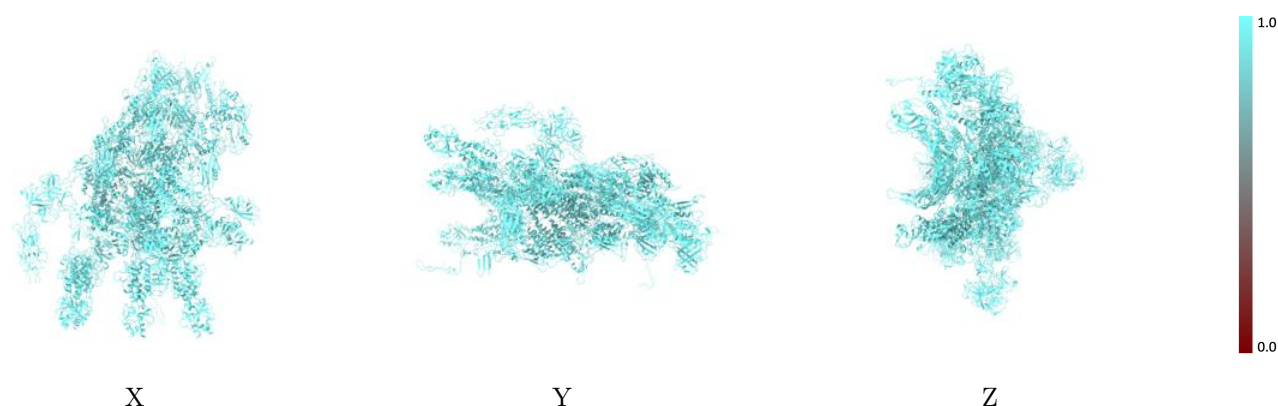
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



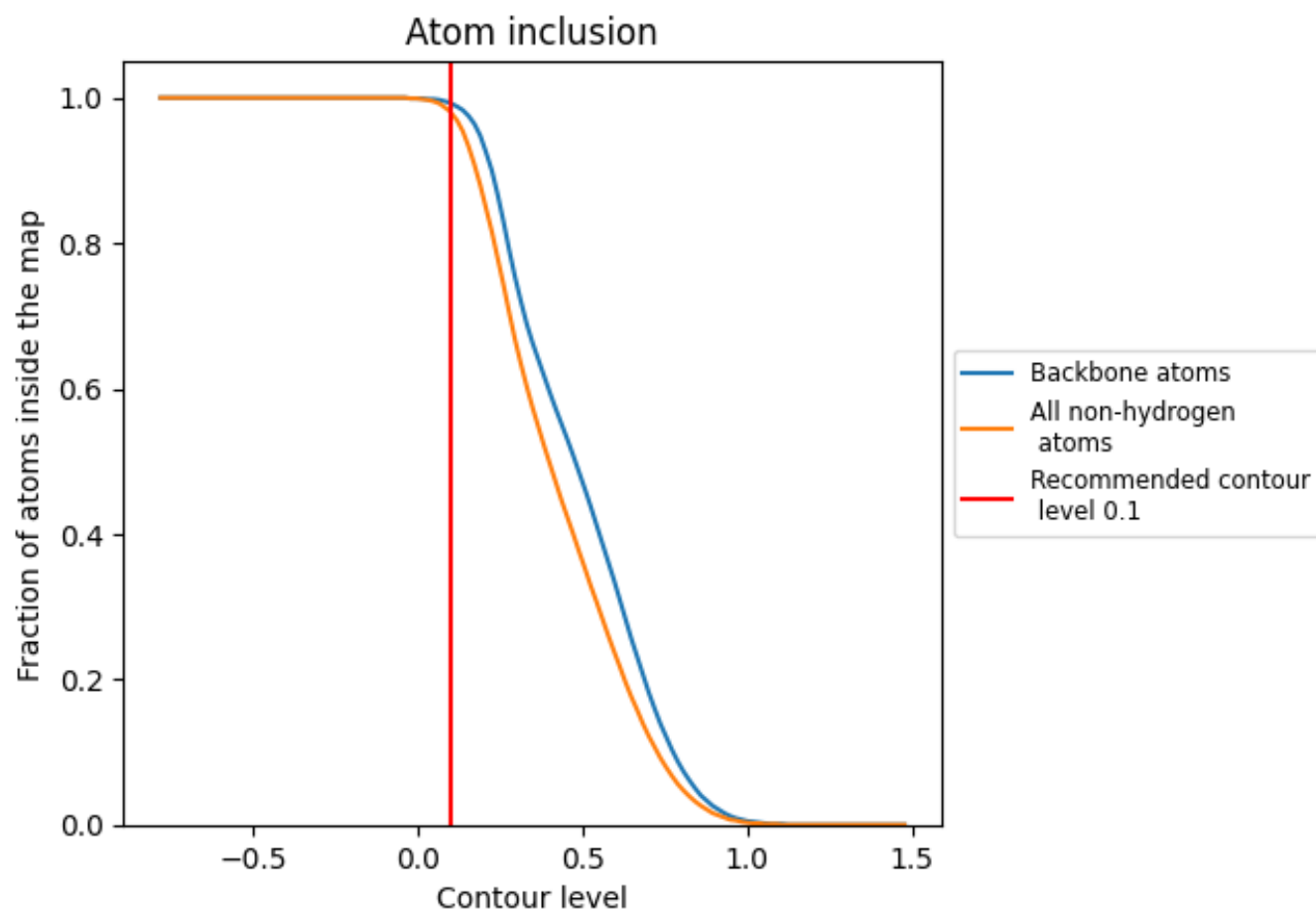
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 98% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9810	 0.4980
A	 0.9070	 0.3820
C1	 0.9400	 0.4770
E1	 0.9870	 0.5640
F1	 0.9840	 0.5370
G1	 0.9880	 0.5390
H1	 0.9770	 0.5290
I1	 0.9860	 0.5410
J1	 0.9880	 0.5400
K1	 0.9790	 0.4980
P1	 0.9880	 0.4520
Q1	 0.9890	 0.4560
R1	 0.9820	 0.4260
S1	 0.9780	 0.3790
T1	 0.9900	 0.3780
U1	 0.9780	 0.5470
V1	 0.9820	 0.3670
W1	 0.9910	 0.4300
X1	 0.9860	 0.4260
Y1	 0.9900	 0.4110
a1	 0.9840	 0.5560
e1	 0.9790	 0.5530
f1	 0.9910	 0.5590
g1	 0.9820	 0.5630
h1	 0.9840	 0.5390
i1	 0.9860	 0.5380
j1	 0.9780	 0.5300
k1	 0.9890	 0.5440
l1	 0.9840	 0.5380
m1	 0.9800	 0.5010
r1	 0.9860	 0.4470
s1	 0.9890	 0.4560
t1	 0.9870	 0.4320
u1	 0.9830	 0.4140
v1	 0.9760	 0.3780



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Chain	Atom inclusion	Q-score
w1	 0.9820	 0.3860
x1	 0.9680	 0.3610
y1	 0.9850	 0.4160
z1	 0.9780	 0.4070