



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 01:50 PM UTC

PDB ID : 7Y1C / pdb_00007y1c
EMDB ID : EMD-33560
Title : CryoEM structure of Klebsiella phage Kp9 tail complex applied with C6 symmetry
Authors : Huang, L.; Xiang, Y.
Deposited on : 2022-06-08
Resolution : 3.13 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:

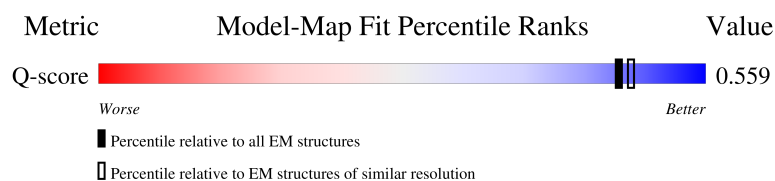
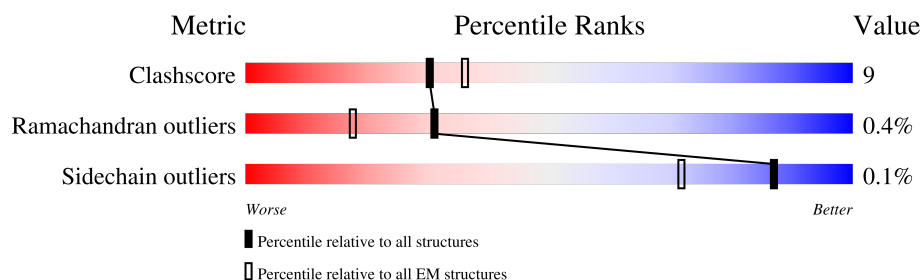
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 3.13 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	14478 (2.63 - 3.63)

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	535	16% 78% 16% 5%
1	L	535	16% 77% 18% 5%
2	W	192	83% 17%
2	X	192	7% 81% 19%

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Mol	Chain	Length	Quality of chain
3	Y	791	 74%25%
4	e	777	 16%80%
4	f	777	 16%80%
4	g	777	 15%5%80%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 20697 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 phage connector protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	506	Total	C	N	O	S	0	0
			3887	2442	646	778	21		
1	L	506	Total	C	N	O	S	0	0
			3887	2442	646	778	21		

- Molecule 2 is a protein called phage tail tubular protein A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	W	192	Total	C	N	O	S	0	0
			1498	933	253	302	10		
2	X	192	Total	C	N	O	S	0	0
			1498	933	253	302	10		

- Molecule 3 is a protein called phage tail tubular protein B.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	Y	790	Total	C	N	O	S	0	0
			6281	3972	1077	1215	17		

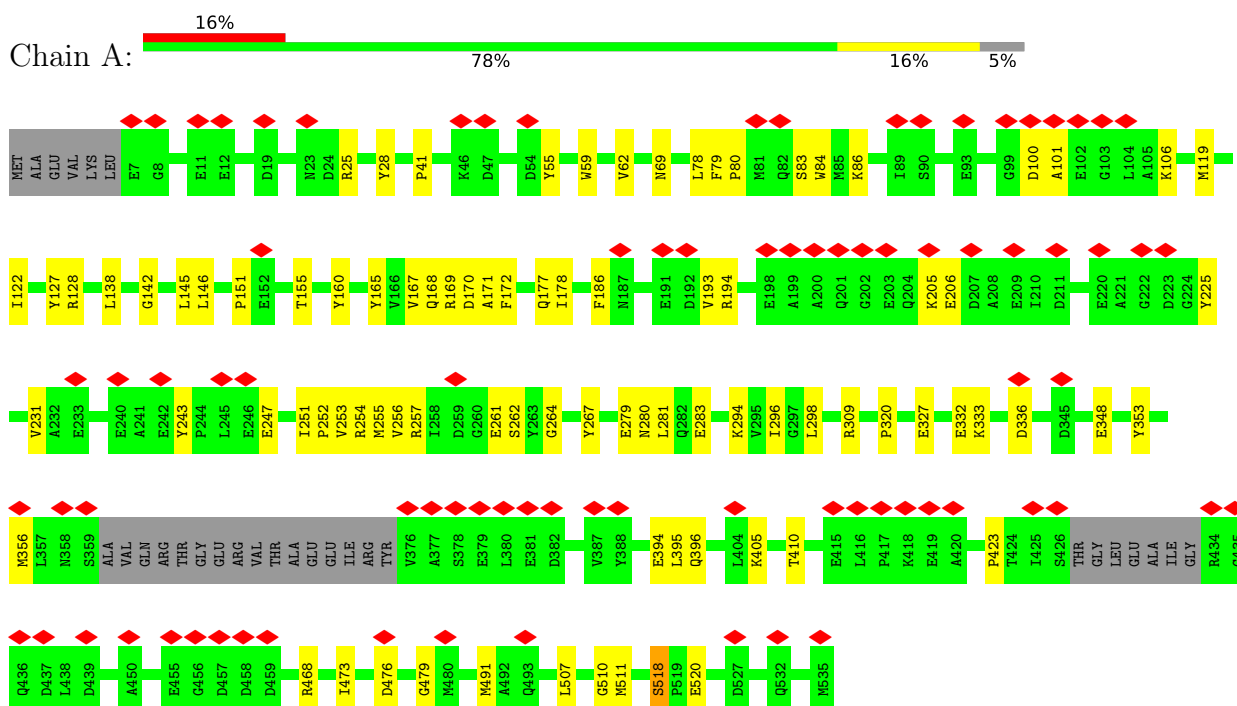
- Molecule 4 is a protein called phage type I tail fiber.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	e	153	Total	C	N	O	S	0	0
			1208	748	219	240	1		
4	f	156	Total	C	N	O	S	0	0
			1229	760	222	245	2		
4	g	155	Total	C	N	O	S	0	0
			1209	749	220	239	1		

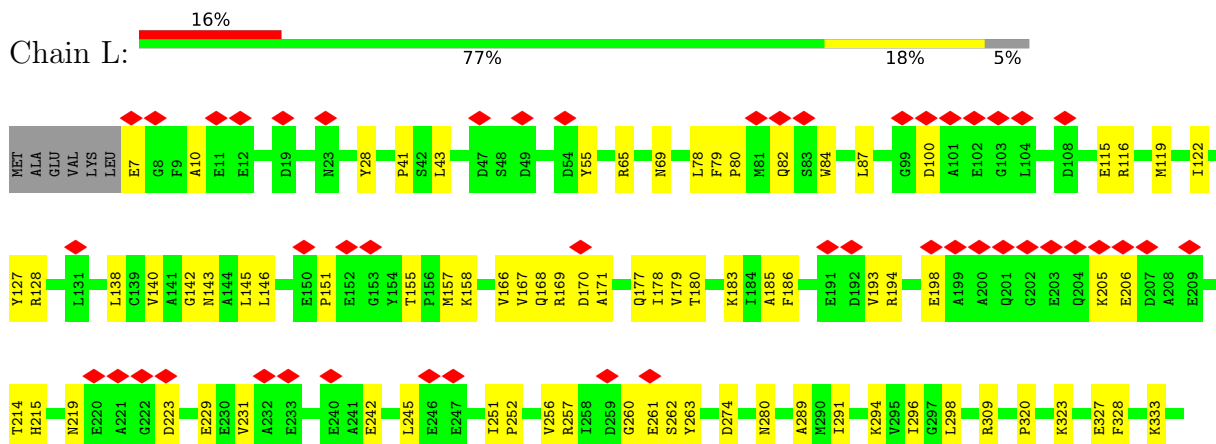
3 Residue-property plots

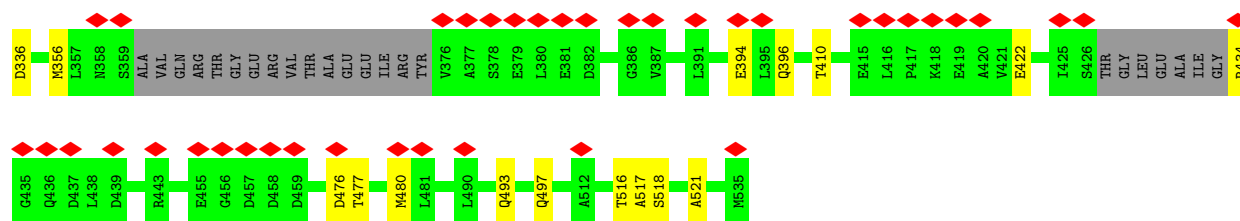
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: phage connector protein

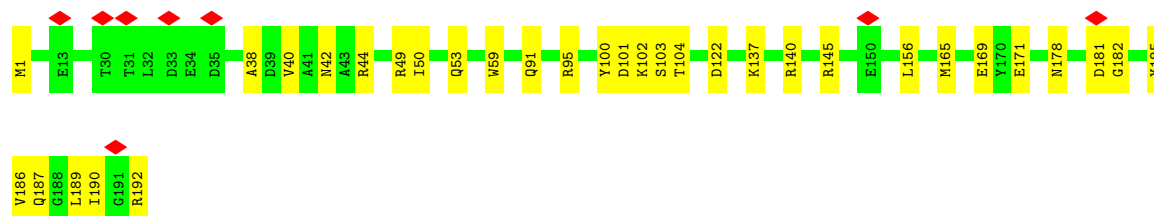
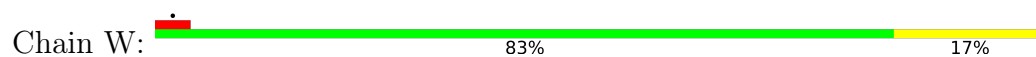


- Molecule 1: phage connector protein

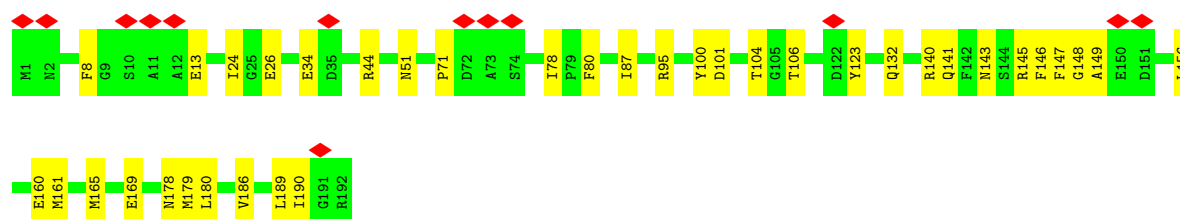
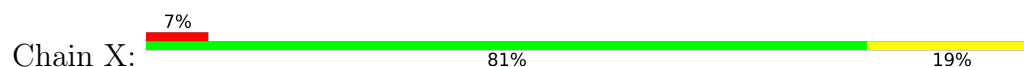




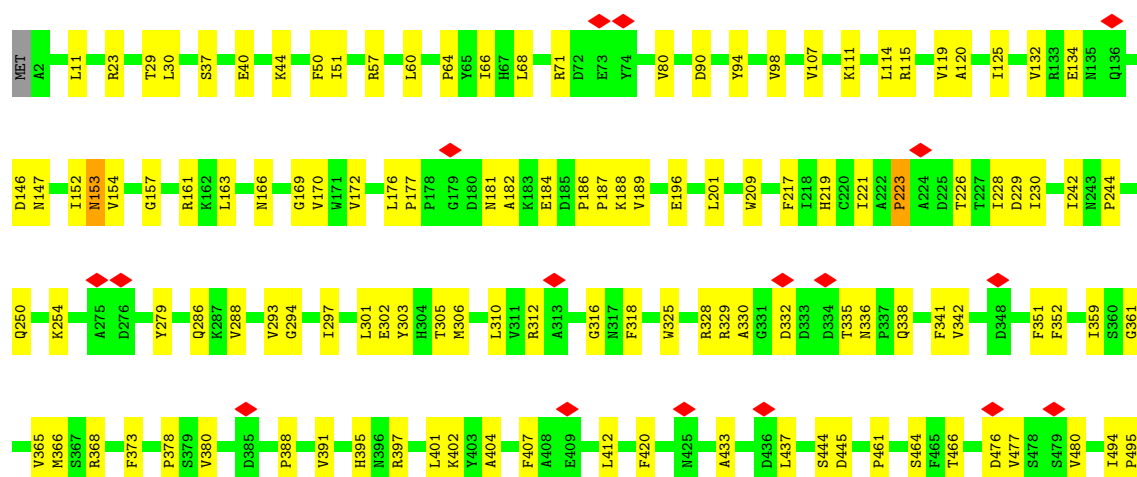
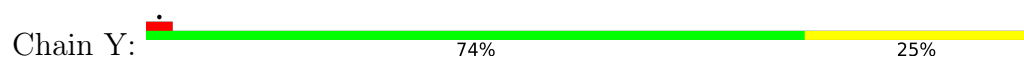
• Molecule 2: phage tail tubular protein A



• Molecule 2: phage tail tubular protein A



• Molecule 3: phage tail tubular protein B





M1	D2	Q3	D4	D23	R27	D37	D38	R39	R40	S44	M45	I46	T47	E48	V52	R56	E70	R73	E79	D83	E107	R110	L114	L115	D121	R128	M129	R130	K131	R134	L135	A136	P137	G138	E139	D143	A144	I145	N146	K147	N148	Q149						
L150	D151	T152	T153	L154	G155	E156	ALA	GLY	GLY	ILE	GLY	ASN	ILE	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY		
GLY	PRO	VAL	LEU	ALA	VAL	PRO	ILE	GLY	THR	ILE	GLY	THR	ALA	VAL	GLN	TYR	GLY	LEU	THR	ASP	ALA	LYS	THR	ILE	GLY	ASP	LEU	THR	VAL	THR	VAL	THR	VAL	THR	VAL	THR	VAL	THR	VAL	THR	VAL	THR	VAL	THR	VAL	THR	VAL	
PRO	THR	GLY	ALA	SER	GLN	ILE	ALA	VAL	PRO	ILE	GLY	THR	GLY	THR	VAL	ASN	GLY	LEU	THR	ASP	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
SER	ARG	GLN	ILE	VAL	PRO	PRO	GLY	THR	GLY	THR	ARG	THR	THR	THR	VAL	VAL	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
ASN	THR	ALA	CYS	ASN	ALA	GLY	GLY	THR	THR	THR	MET	PHE	ASP	GLY	ARG	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
PHE	ASN	GLN	ASN	ASN	ILE	GLY	THR	THR	THR	THR	ASN	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
ILE	GLN	VAL	ILE	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
SER	VAL	GLY	GLY	ASP	THR	GLY	THR	THR	THR	THR	SER	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
THR	TRP	GLU	ASP	THR	THR	GLY	VAL	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
ASN	ASN	ASN	GLY	THR	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
ASN	ASP	ALA	SER	THR	PHE	ASN	LEU	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR

● Molecule 4: phage type I tail fiber



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

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C6	Depositor
Number of particles used	41926	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)	1000	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.069	Depositor
Minimum map value	-0.031	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.018	Depositor
Map size (Å)	1074.2001, 1074.2001, 1074.2001	wwPDB
Map dimensions	1000, 1000, 1000	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0742, 1.0742, 1.0742	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	0.15	0/3944	0.27	0/5341
1	L	0.14	0/3944	0.27	0/5341
2	W	0.15	0/1526	0.27	0/2067
2	X	0.16	0/1526	0.30	0/2067
3	Y	0.15	0/6436	0.33	0/8752
4	e	0.14	0/1222	0.28	0/1654
4	f	0.15	0/1243	0.33	0/1681
4	g	0.14	0/1223	0.34	0/1654
All	All	0.15	0/21064	0.30	0/28557

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	3887	0	3858	61	0
1	L	3887	0	3858	60	0
2	W	1498	0	1417	23	0
2	X	1498	0	1417	23	0
3	Y	6281	0	6022	138	0
4	e	1208	0	1207	43	0
4	f	1229	0	1228	29	0
4	g	1209	0	1211	48	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	20697	0	20218	367	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 9.

All (367) 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)
4:e:147:LYS:CG	4:g:141:GLY:HA2	1.49	1.41
4:e:147:LYS:HG3	4:g:141:GLY:CA	1.90	1.02
4:e:147:LYS:HG3	4:g:141:GLY:HA2	1.02	1.00
1:A:146:LEU:HD11	1:A:251:ILE:HD11	1.43	1.00
4:e:147:LYS:CG	4:g:141:GLY:CA	2.45	0.89
3:Y:565:ASN:HD21	3:Y:624:PHE:HA	1.46	0.81
3:Y:711:THR:HA	3:Y:773:VAL:HA	1.62	0.80
1:A:146:LEU:HD11	1:A:251:ILE:CD1	2.13	0.78
4:e:147:LYS:CD	4:g:141:GLY:HA2	2.12	0.78
4:e:147:LYS:HG2	4:g:141:GLY:HA2	1.63	0.78
4:e:146:ASN:HB2	4:g:141:GLY:O	1.86	0.76
1:L:138:LEU:O	1:L:142:GLY:HA2	1.84	0.75
1:A:138:LEU:O	1:A:142:GLY:HA2	1.87	0.74
4:e:131:LYS:HE2	4:g:139:GLU:HG2	1.70	0.74
3:Y:306:MET:HE1	3:Y:341:PHE:HE1	1.53	0.73
3:Y:301:LEU:HD13	3:Y:306:MET:HE3	1.71	0.71
3:Y:338:GLN:HG3	3:Y:342:VAL:HG21	1.73	0.69
1:A:78:LEU:O	1:A:396:GLN:NE2	2.25	0.69
3:Y:98:VAL:HG12	3:Y:318:PHE:HB2	1.73	0.69
3:Y:565:ASN:HB2	3:Y:570:TRP:HZ3	1.56	0.69
2:W:181:ASP:O	2:W:187:GLN:NE2	2.26	0.69
3:Y:177:PRO:HG3	3:Y:188:LYS:HE2	1.75	0.68
4:e:147:LYS:HE3	4:g:140:ALA:O	1.93	0.68
1:A:294:LYS:HE2	1:A:296:ILE:HD11	1.75	0.67
4:f:52:VAL:HB	4:f:56:ARG:HG2	1.77	0.67
3:Y:444:SER:HB2	3:Y:461:PRO:HD3	1.74	0.67
1:L:78:LEU:O	1:L:396:GLN:NE2	2.28	0.67
3:Y:656:ILE:HG22	3:Y:657:SER:H	1.59	0.66
3:Y:701:LEU:HA	3:Y:782:GLY:HA3	1.78	0.66
1:A:80:PRO:HD2	1:A:84:TRP:HB3	1.77	0.66
3:Y:153:ASN:HA	3:Y:217:PHE:HA	1.79	0.65
1:L:151:PRO:HA	1:L:155:THR:HG21	1.79	0.65
3:Y:391:VAL:HG11	3:Y:433:ALA:HB3	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:170:ASP:OD1	1:L:171:ALA:N	2.30	0.64
1:A:170:ASP:OD2	1:L:185:ALA:N	2.28	0.64
4:e:147:LYS:HA	4:e:150:LEU:HB3	1.78	0.64
1:A:83:SER:H	1:A:119:MET:HE2	1.62	0.64
4:f:40:ARG:NH2	4:f:70:GLU:OE2	2.31	0.64
4:g:8:VAL:HG22	4:g:72:ARG:HG3	1.80	0.64
2:W:91:GLN:HB3	2:W:102:LYS:HB3	1.79	0.64
1:A:205:LYS:HE3	1:A:206:GLU:H	1.63	0.63
1:A:146:LEU:HD11	1:A:251:ILE:CG1	2.28	0.63
1:L:69:ASN:ND2	1:L:356:MET:O	2.31	0.63
3:Y:134:GLU:OE2	3:Y:338:GLN:NE2	2.32	0.63
2:W:95:ARG:HB2	2:W:100:TYR:HB2	1.79	0.63
1:A:167:VAL:HG23	1:A:178:ILE:HG12	1.81	0.62
3:Y:71:ARG:HE	3:Y:120:ALA:HA	1.65	0.62
1:A:280:ASN:HB3	2:X:189:LEU:HD22	1.81	0.62
4:e:147:LYS:HZ1	4:g:140:ALA:N	1.97	0.62
4:g:28:LYS:NZ	4:g:79:GLU:OE2	2.33	0.62
3:Y:250:GLN:HB3	3:Y:254:LYS:HD3	1.82	0.62
3:Y:500:SER:HB3	3:Y:513:LEU:HB2	1.81	0.61
4:f:130:ARG:NH1	4:g:119:GLU:OE1	2.28	0.61
1:A:146:LEU:HD12	1:A:146:LEU:O	1.99	0.61
2:W:50:ILE:HD12	2:W:137:LYS:HD3	1.82	0.61
1:L:122:ILE:HG23	1:L:127:TYR:HB2	1.80	0.61
1:A:79:PHE:O	1:A:128:ARG:NH2	2.34	0.61
4:e:52:VAL:HB	4:e:56:ARG:HG2	1.83	0.60
4:f:115:LEU:HB3	4:g:119:GLU:HG3	1.84	0.60
1:L:80:PRO:HD2	1:L:84:TRP:HB3	1.84	0.60
3:Y:209:TRP:CD1	3:Y:223:PRO:HD3	2.37	0.60
1:L:41:PRO:HB2	1:L:55:TYR:HB3	1.84	0.60
1:A:69:ASN:ND2	1:A:356:MET:O	2.34	0.59
3:Y:328:ARG:NH2	3:Y:336:ASN:O	2.35	0.59
3:Y:60:LEU:HG	3:Y:80:VAL:HG11	1.83	0.59
1:L:151:PRO:HG2	1:L:410:THR:HG21	1.83	0.59
3:Y:657:SER:OG	3:Y:658:GLY:N	2.35	0.59
3:Y:362:GLU:HA	3:Y:401:LEU:HG	1.85	0.59
1:L:143:ASN:ND2	1:L:263:TYR:HB3	2.17	0.59
4:e:153:THR:HG23	4:f:154:LEU:HD22	1.84	0.59
3:Y:44:LYS:HB2	3:Y:773:VAL:HG22	1.85	0.58
3:Y:71:ARG:NH2	3:Y:119:VAL:O	2.29	0.58
4:g:139:GLU:HA	4:g:139:GLU:OE1	2.03	0.58
3:Y:368:ARG:HD2	3:Y:378:PRO:HD3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:PRO:HA	1:A:155:THR:HG21	1.86	0.58
2:W:101:ASP:O	2:W:103:SER:N	2.35	0.58
2:X:143:ASN:O	2:X:148:GLY:N	2.34	0.57
4:e:134:ARG:HB3	4:f:129:ASN:H	1.69	0.57
1:A:145:LEU:HB3	1:A:160:TYR:HB2	1.87	0.57
1:L:223:ASP:HB3	1:L:245:LEU:HD13	1.85	0.57
3:Y:786:ARG:NE	3:Y:788:ALA:O	2.38	0.57
1:L:167:VAL:HG23	1:L:178:ILE:HG12	1.86	0.57
4:f:138:GLY:H	4:f:149:GLN:HE22	1.53	0.57
4:e:126:ASP:OD2	4:g:134:ARG:NH2	2.37	0.56
2:W:53:GLN:OE1	2:X:132:GLN:NE2	2.37	0.56
3:Y:64:PRO:HG2	3:Y:66:ILE:HD11	1.86	0.56
1:A:257:ARG:NH1	1:A:394:GLU:OE1	2.38	0.56
1:L:274:ASP:OD1	2:W:192:ARG:NH2	2.38	0.56
2:X:71:PRO:HA	2:X:78:ILE:HG12	1.86	0.56
3:Y:476:ASP:HB3	3:Y:480:VAL:HG21	1.88	0.56
3:Y:711:THR:HG22	3:Y:774:SER:H	1.70	0.56
3:Y:132:VAL:HA	3:Y:305:THR:HB	1.88	0.56
3:Y:466:THR:HG23	3:Y:496:ASN:HA	1.86	0.56
3:Y:599:HIS:ND1	3:Y:664:ASN:OD1	2.36	0.56
3:Y:153:ASN:C	3:Y:153:ASN:HD22	2.12	0.56
3:Y:297:ILE:HD13	3:Y:332:ASP:HA	1.86	0.56
1:A:332:GLU:HB2	1:L:328:PHE:HB2	1.88	0.56
3:Y:407:PHE:HB3	3:Y:412:LEU:HD13	1.88	0.56
2:X:101:ASP:OD2	2:X:104:THR:OG1	2.24	0.56
3:Y:107:VAL:HG11	3:Y:114:LEU:HD13	1.87	0.56
1:A:41:PRO:HB2	1:A:55:TYR:HB3	1.86	0.55
4:e:45:ASN:HB3	4:e:46:ILE:HD12	1.87	0.55
1:A:25:ARG:NH1	1:A:165:TYR:O	2.39	0.55
4:e:147:LYS:CE	4:g:140:ALA:O	2.54	0.55
3:Y:229:ASP:HB2	3:Y:230:ILE:HD12	1.88	0.55
4:f:44:SER:H	4:f:48:GLU:HG3	1.70	0.55
1:A:59:TRP:CE3	1:A:283:GLU:HA	2.41	0.55
1:A:473:ILE:O	1:L:434:ARG:NE	2.40	0.55
1:A:169:ARG:HB2	1:A:262:SER:HA	1.89	0.55
3:Y:341:PHE:HD2	3:Y:365:VAL:HG21	1.71	0.55
1:L:43:LEU:HD23	1:L:140:VAL:HG21	1.89	0.55
1:A:518:SER:OG	1:A:520:GLU:OE1	2.23	0.55
1:A:151:PRO:HG2	1:A:410:THR:HG21	1.88	0.55
2:X:140:ARG:NH1	2:X:160:GLU:OE1	2.40	0.55
3:Y:402:LYS:HD3	3:Y:445:ASP:HB3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:24:ILE:HG13	2:X:26:GLU:HG2	1.88	0.54
3:Y:279:TYR:CD2	3:Y:294:GLY:HA2	2.43	0.54
4:e:147:LYS:HZ1	4:g:139:GLU:C	2.14	0.54
3:Y:11:LEU:HD13	3:Y:777:GLY:HA2	1.88	0.54
2:W:178:ASN:HB3	2:W:182:GLY:H	1.73	0.54
3:Y:352:PHE:HB3	3:Y:366:MET:HE1	1.89	0.54
1:A:510:GLY:HA3	1:L:516:THR:HG21	1.90	0.54
1:A:333:LYS:HB3	1:A:336:ASP:HB2	1.90	0.53
1:A:146:LEU:CD1	1:A:251:ILE:CG1	2.86	0.53
3:Y:696:SER:OG	3:Y:786:ARG:NH1	2.41	0.53
3:Y:642:GLU:HG3	3:Y:643:PRO:HD2	1.90	0.53
3:Y:525:LYS:HB3	3:Y:537:SER:HB3	1.90	0.53
3:Y:368:ARG:HG3	3:Y:388:PRO:HD3	1.90	0.53
3:Y:502:ASN:O	3:Y:511:CYS:N	2.38	0.53
2:W:165:MET:O	2:W:169:GLU:HG3	2.09	0.53
3:Y:184:GLU:O	3:Y:188:LYS:NZ	2.32	0.53
3:Y:702:ARG:HG2	3:Y:782:GLY:HA2	1.91	0.53
1:L:7:GLU:HB3	1:L:10:ALA:HB3	1.91	0.53
3:Y:23:ARG:NH1	3:Y:29:THR:OG1	2.42	0.53
4:e:44:SER:H	4:e:48:GLU:HG3	1.73	0.53
1:L:168:GLN:OE1	1:L:177:GLN:NE2	2.34	0.52
2:X:141:GLN:O	2:X:145:ARG:HG2	2.09	0.52
4:f:137:PRO:HB3	4:f:149:GLN:HE21	1.74	0.52
1:L:171:ALA:HA	1:L:260:GLY:HA2	1.91	0.52
2:W:1:MET:HE2	4:f:27:ARG:NH2	2.25	0.52
3:Y:476:ASP:OD1	3:Y:477:VAL:N	2.42	0.52
1:A:171:ALA:HB3	1:L:183:LYS:HB2	1.91	0.52
1:A:225:TYR:N	1:A:243:TYR:O	2.42	0.52
2:X:161:MET:O	2:X:165:MET:HG3	2.10	0.52
3:Y:619:ILE:HD12	3:Y:667:ILE:HG21	1.91	0.52
4:e:128:ARG:HA	4:g:134:ARG:HE	1.75	0.51
3:Y:50:PHE:HD1	3:Y:596:ARG:HH11	1.57	0.51
3:Y:495:PRO:HB2	3:Y:516:GLY:HA3	1.91	0.51
4:f:131:LYS:NZ	4:g:124:ASN:OD1	2.43	0.51
1:A:507:LEU:HG	1:A:511:MET:HE2	1.92	0.51
2:W:140:ARG:HA	2:W:156:LEU:HD13	1.92	0.51
4:g:114:LEU:O	4:g:128:ARG:NH2	2.44	0.51
3:Y:146:ASP:OD1	3:Y:146:ASP:N	2.44	0.51
1:L:257:ARG:NH1	1:L:394:GLU:OE1	2.42	0.51
3:Y:37:SER:OG	3:Y:40:GLU:O	2.26	0.51
3:Y:157:GLY:O	3:Y:189:VAL:HG13	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:359:ILE:HD11	3:Y:404:ALA:HB2	1.92	0.51
3:Y:606:ASP:HB3	3:Y:609:THR:HG22	1.92	0.51
1:A:138:LEU:O	1:A:142:GLY:CA	2.57	0.51
1:L:179:VAL:HG22	1:L:215:HIS:CD2	2.46	0.51
2:W:59:TRP:HE3	2:W:171:GLU:HG3	1.75	0.51
3:Y:751:ARG:NH2	3:Y:781:GLU:OE2	2.43	0.51
4:e:28:LYS:NZ	4:e:79:GLU:OE1	2.33	0.51
3:Y:161:ARG:HB2	3:Y:176:LEU:HD12	1.92	0.51
1:L:214:THR:HG22	1:L:229:GLU:HG2	1.93	0.50
4:f:73:ARG:NH2	4:f:107:GLU:OE1	2.39	0.50
1:L:28:TYR:OH	1:L:261:GLU:OE1	2.28	0.50
2:W:101:ASP:OD2	2:W:104:THR:OG1	2.28	0.50
3:Y:705:TRP:CD1	3:Y:749:GLN:HE21	2.29	0.50
1:L:309:ARG:HD3	1:L:320:PRO:HD2	1.94	0.50
3:Y:565:ASN:ND2	3:Y:623:SER:O	2.45	0.50
4:e:147:LYS:HD2	4:g:141:GLY:HA2	1.94	0.50
1:L:298:LEU:N	1:L:327:GLU:O	2.46	0.49
2:X:8:PHE:HA	4:f:23:ASP:HB2	1.92	0.49
3:Y:565:ASN:HB2	3:Y:570:TRP:CZ3	2.41	0.49
4:e:45:ASN:O	4:e:47:THR:N	2.45	0.49
3:Y:461:PRO:HA	3:Y:466:THR:HA	1.94	0.49
3:Y:731:ALA:HB2	3:Y:744:ALA:HB1	1.93	0.49
1:A:327:GLU:HB3	1:L:323:LYS:HG3	1.94	0.49
4:g:24:TYR:OH	4:g:54:LYS:O	2.29	0.49
1:L:251:ILE:O	1:L:251:ILE:HG13	2.13	0.49
1:L:146:LEU:HD12	1:L:157:MET:SD	2.53	0.48
3:Y:223:PRO:HD2	3:Y:226:THR:OG1	2.13	0.48
3:Y:784:TYR:CE2	3:Y:786:ARG:HB2	2.47	0.48
2:X:34:GLU:OE1	2:X:44:ARG:HD3	2.13	0.48
3:Y:293:VAL:HB	3:Y:329:ARG:HA	1.94	0.48
1:L:291:ILE:HD11	2:X:180:LEU:HG	1.96	0.48
4:e:147:LYS:NZ	4:g:138:GLY:O	2.45	0.48
4:g:25:LEU:HD21	4:g:100:LEU:HD23	1.95	0.48
3:Y:153:ASN:O	3:Y:153:ASN:ND2	2.42	0.48
3:Y:293:VAL:HG22	3:Y:297:ILE:HD11	1.95	0.48
1:L:179:VAL:HG22	1:L:215:HIS:HD2	1.79	0.48
3:Y:44:LYS:NZ	3:Y:769:ASN:O	2.46	0.48
3:Y:57:ARG:HE	3:Y:566:GLY:HA2	1.79	0.48
2:X:165:MET:O	2:X:169:GLU:HG3	2.13	0.48
4:g:19:ASP:OD1	4:g:56:ARG:NE	2.38	0.48
1:A:28:TYR:OH	1:A:261:GLU:OE1	2.23	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:169:ARG:HB2	1:L:262:SER:HA	1.96	0.48
3:Y:229:ASP:OD1	3:Y:229:ASP:N	2.42	0.48
1:A:476:ASP:HA	1:L:116:ARG:NH2	2.29	0.48
1:L:186:PHE:CZ	1:L:194:ARG:HG2	2.49	0.48
4:e:147:LYS:NZ	4:g:139:GLU:C	2.72	0.48
4:f:45:ASN:O	4:f:47:THR:N	2.46	0.48
1:A:106:LYS:HD3	1:A:106:LYS:C	2.39	0.48
1:A:298:LEU:N	1:A:327:GLU:O	2.46	0.48
1:L:82:GLN:HB3	1:L:434:ARG:HH12	1.79	0.48
4:e:145:ILE:HD12	4:f:150:LEU:HD22	1.95	0.48
1:L:280:ASN:HB3	2:W:189:LEU:HD22	1.95	0.47
1:L:82:GLN:HG2	1:L:434:ARG:HH22	1.78	0.47
3:Y:743:LYS:HG2	3:Y:744:ALA:N	2.29	0.47
1:A:59:TRP:N	1:A:279:GLU:OE2	2.38	0.47
3:Y:219:HIS:CD2	3:Y:221:ILE:HD11	2.49	0.47
3:Y:66:ILE:HD13	3:Y:551:ALA:HB2	1.95	0.47
1:L:219:ASN:ND2	1:L:242:GLU:OE2	2.48	0.47
4:g:44:SER:H	4:g:48:GLU:HG3	1.79	0.47
1:A:491:MET:HE3	1:L:497:GLN:HA	1.96	0.47
3:Y:564:ARG:HG2	3:Y:569:VAL:HG22	1.97	0.47
4:e:147:LYS:O	4:e:151:ASP:N	2.32	0.47
3:Y:713:ALA:HA	3:Y:729:VAL:O	2.15	0.46
1:L:333:LYS:HB3	1:L:336:ASP:HB2	1.96	0.46
3:Y:733:VAL:HG22	4:e:90:LEU:HD12	1.97	0.46
3:Y:688:ASP:OD1	3:Y:690:THR:HG22	2.14	0.46
4:f:4:ASP:HB3	4:f:114:LEU:HD13	1.96	0.46
1:L:193:VAL:HG13	1:L:231:VAL:HG21	1.97	0.46
3:Y:619:ILE:HD11	3:Y:667:ILE:HD13	1.98	0.46
3:Y:51:ILE:HG13	3:Y:51:ILE:O	2.16	0.46
4:e:131:LYS:HD3	4:g:143:ASP:OD2	2.16	0.46
1:A:468:ARG:NH2	1:L:476:ASP:OD1	2.48	0.46
4:g:127:ALA:O	4:g:129:ASN:N	2.48	0.46
1:A:247:GLU:HB2	1:A:405:LYS:NZ	2.31	0.45
3:Y:552:ALA:HB1	3:Y:559:MET:HE2	1.98	0.45
1:L:186:PHE:HZ	1:L:198:GLU:HG2	1.81	0.45
1:L:477:THR:HA	1:L:480:MET:SD	2.56	0.45
3:Y:656:ILE:HG22	3:Y:657:SER:N	2.28	0.45
4:f:145:ILE:HD13	4:g:150:LEU:HB2	1.97	0.45
1:L:180:THR:HG1	1:L:214:THR:HG1	1.47	0.45
1:L:517:ALA:O	1:L:521:ALA:HB3	2.17	0.45
3:Y:68:LEU:HD21	3:Y:555:ILE:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:111:LYS:O	3:Y:115:ARG:NH1	2.47	0.45
3:Y:464:SER:O	3:Y:496:ASN:HB2	2.17	0.45
3:Y:676:VAL:HA	3:Y:764:SER:HA	1.97	0.45
3:Y:757:ASN:O	3:Y:761:GLN:HG2	2.17	0.45
4:g:17:GLU:OE2	4:g:56:ARG:HD3	2.17	0.45
2:X:95:ARG:HB2	2:X:100:TYR:HB2	1.99	0.45
1:L:205:LYS:HD2	1:L:206:GLU:H	1.82	0.45
3:Y:196:GLU:OE1	3:Y:196:GLU:N	2.49	0.45
1:A:251:ILE:HG13	1:A:251:ILE:O	2.17	0.45
2:W:178:ASN:HB3	2:W:182:GLY:N	2.32	0.45
2:X:146:PHE:O	3:Y:702:ARG:NH1	2.38	0.45
3:Y:312:ARG:NH2	3:Y:316:GLY:HA2	2.32	0.45
2:W:38:ALA:O	2:W:42:ASN:ND2	2.50	0.44
3:Y:561:MET:HE3	3:Y:563:MET:CE	2.48	0.44
3:Y:119:VAL:HG21	3:Y:351:PHE:CE2	2.52	0.44
4:g:23:ASP:O	4:g:73:ARG:NH1	2.47	0.44
2:W:101:ASP:HB3	2:W:104:THR:O	2.16	0.44
2:W:186:VAL:O	2:W:190:ILE:HG12	2.17	0.44
3:Y:29:THR:HB	3:Y:676:VAL:HG23	1.99	0.44
3:Y:594:ALA:O	3:Y:620:TYR:OH	2.21	0.44
4:e:22:PHE:CE1	4:e:73:ARG:HB2	2.52	0.44
1:A:62:VAL:HG21	1:A:348:GLU:HG3	2.00	0.44
1:A:193:VAL:HG13	1:A:231:VAL:HG21	1.98	0.44
3:Y:718:VAL:HG11	3:Y:754:VAL:HG23	2.00	0.44
1:L:145:LEU:HD12	1:L:252:PRO:HA	1.99	0.44
3:Y:125:ILE:HD11	3:Y:310:LEU:HD22	1.98	0.44
3:Y:495:PRO:HG2	3:Y:517:ALA:HB2	2.00	0.44
4:e:131:LYS:O	4:e:131:LYS:HG3	2.16	0.44
3:Y:219:HIS:HD2	3:Y:221:ILE:HD11	1.82	0.44
4:g:22:PHE:CE1	4:g:73:ARG:HB2	2.53	0.44
3:Y:279:TYR:CE2	3:Y:294:GLY:HA2	2.53	0.43
4:e:75:THR:HB	4:e:105:ILE:HG12	2.00	0.43
1:A:122:ILE:HG23	1:A:127:TYR:HB2	1.99	0.43
1:L:422:GLU:O	1:L:422:GLU:HG2	2.17	0.43
3:Y:172:VAL:HG11	3:Y:201:LEU:HB3	2.01	0.43
3:Y:740:LEU:HD23	3:Y:740:LEU:HA	1.79	0.43
4:e:38:ASP:OD1	4:e:39:ASN:N	2.52	0.43
1:L:166:VAL:HG12	1:L:179:VAL:HB	2.00	0.43
3:Y:600:ILE:HB	3:Y:661:SER:O	2.19	0.43
1:A:101:ALA:HA	1:A:479:GLY:HA3	2.01	0.43
1:A:353:TYR:CE1	1:L:65:ARG:HG3	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:e:44:SER:N	4:e:48:GLU:HG3	2.34	0.43
1:A:145:LEU:HD12	1:A:252:PRO:HA	2.00	0.43
2:X:186:VAL:O	2:X:190:ILE:HG12	2.18	0.43
3:Y:163:LEU:HD13	3:Y:242:ILE:HD13	2.01	0.43
2:X:80:PHE:CE2	2:X:87:ILE:HD12	2.53	0.43
4:e:139:GLU:O	4:f:147:LYS:NZ	2.49	0.43
1:A:255:MET:HE2	1:A:267:TYR:HB2	2.01	0.43
3:Y:554:CYS:HA	3:Y:559:MET:HA	2.00	0.43
1:A:281:LEU:HD21	1:L:289:ALA:HB1	2.01	0.42
3:Y:154:VAL:HG12	3:Y:242:ILE:HG22	2.00	0.42
3:Y:302:GLU:O	3:Y:303:TYR:HB2	2.19	0.42
3:Y:543:PHE:CZ	3:Y:561:MET:HE1	2.53	0.42
1:L:87:LEU:HD23	1:L:422:GLU:HB3	2.01	0.42
1:L:100:ASP:OD1	1:L:100:ASP:N	2.52	0.42
2:W:40:VAL:O	2:W:44:ARG:HG3	2.19	0.42
3:Y:325:TRP:CE3	3:Y:373:PHE:HA	2.54	0.42
3:Y:681:LEU:HD11	3:Y:759:LEU:HD23	2.02	0.42
1:A:86:LYS:O	1:A:423:PRO:HD2	2.19	0.42
3:Y:44:LYS:HG3	3:Y:673:PHE:HB2	2.02	0.42
3:Y:590:PHE:O	3:Y:592:VAL:N	2.51	0.42
3:Y:593:ASP:HB2	3:Y:671:TYR:CD1	2.55	0.42
4:e:147:LYS:HD2	4:g:141:GLY:N	2.34	0.42
4:g:35:VAL:HG12	4:g:68:ARG:HH21	1.84	0.42
4:g:155:GLY:O	4:g:159:GLY:N	2.43	0.42
1:A:186:PHE:CZ	1:A:194:ARG:HG2	2.54	0.42
1:L:115:GLU:O	1:L:119:MET:HG2	2.19	0.42
3:Y:57:ARG:NE	3:Y:566:GLY:HA2	2.33	0.42
4:f:134:ARG:O	4:f:135:LEU:HB3	2.18	0.42
4:f:153:THR:HG21	4:g:150:LEU:HD11	2.02	0.42
3:Y:186:PRO:N	3:Y:187:PRO:HD2	2.34	0.42
3:Y:502:ASN:OD1	3:Y:503:GLY:N	2.50	0.42
2:X:13:GLU:HG2	2:X:44:ARG:HH12	1.84	0.41
2:X:51:ASN:HD21	2:X:123:TYR:HA	1.85	0.41
2:W:49:ARG:NH2	2:W:145:ARG:HH12	2.18	0.41
2:X:140:ARG:HA	2:X:156:LEU:HD13	2.01	0.41
3:Y:610:ASN:HB2	4:g:27:ARG:CZ	2.50	0.41
2:W:185:TYR:CZ	2:W:189:LEU:HD11	2.55	0.41
3:Y:153:ASN:C	3:Y:153:ASN:ND2	2.76	0.41
3:Y:395:HIS:NE2	3:Y:397:ARG:HB2	2.35	0.41
3:Y:420:PHE:HA	3:Y:437:LEU:HA	2.02	0.41
1:A:100:ASP:N	1:A:100:ASP:OD1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:VAL:HG21	1:A:395:LEU:HB2	2.02	0.41
1:L:294:LYS:HE2	1:L:296:ILE:HD11	2.03	0.41
2:X:178:ASN:OD1	2:X:179:MET:N	2.53	0.41
1:L:79:PHE:O	1:L:128:ARG:NH2	2.48	0.41
3:Y:209:TRP:CD1	3:Y:209:TRP:N	2.88	0.41
3:Y:335:THR:HB	3:Y:380:VAL:HG21	2.02	0.41
1:A:84:TRP:NE1	1:A:119:MET:HE1	2.36	0.41
1:A:172:PHE:CE1	1:L:158:LYS:HE2	2.55	0.41
1:A:309:ARG:HD3	1:A:320:PRO:HD2	2.03	0.41
3:Y:166:ASN:HB2	3:Y:169:GLY:O	2.20	0.41
4:f:135:LEU:HA	4:g:127:ALA:HB3	2.03	0.41
3:Y:181:ASN:OD1	3:Y:182:ALA:N	2.53	0.41
4:g:34:LEU:HD23	4:g:69:VAL:HG22	2.03	0.41
1:A:168:GLN:OE1	1:A:177:GLN:NE2	2.40	0.41
4:f:149:GLN:O	4:f:153:THR:HG22	2.21	0.41
1:A:146:LEU:HD21	1:A:395:LEU:CD1	2.51	0.41
2:X:147:PHE:CE2	2:X:149:ALA:HB2	2.55	0.41
3:Y:30:LEU:HB3	3:Y:676:VAL:HG22	2.02	0.41
3:Y:147:ASN:O	3:Y:228:ILE:HG13	2.20	0.41
4:e:17:GLU:OE1	4:e:56:ARG:HD3	2.20	0.41
4:e:77:ALA:HB3	4:f:107:GLU:OE2	2.20	0.41
4:e:134:ARG:HD3	4:f:128:ARG:HA	2.03	0.41
4:f:23:ASP:O	4:f:73:ARG:NH1	2.48	0.41
4:f:138:GLY:N	4:f:149:GLN:HE22	2.16	0.41
4:g:137:PRO:HB3	4:g:149:GLN:HE21	1.86	0.41
3:Y:286:GLN:O	3:Y:288:VAL:N	2.51	0.41
3:Y:494:ILE:HA	3:Y:495:PRO:HD3	1.85	0.41
2:W:1:MET:N	2:W:122:ASP:OD2	2.41	0.40
3:Y:361:GLY:O	3:Y:362:GLU:HG2	2.21	0.40
4:e:40:ARG:NH2	4:e:70:GLU:OE2	2.54	0.40
4:e:108:GLU:OE2	4:f:110:ARG:NH1	2.54	0.40
3:Y:152:ILE:HG22	3:Y:244:PRO:HB3	2.03	0.40
3:Y:624:PHE:O	3:Y:648:TRP:HB2	2.21	0.40
4:e:147:LYS:CD	4:g:141:GLY:CA	2.93	0.40
4:f:143:ASP:O	4:g:147:LYS:N	2.53	0.40
4:g:134:ARG:O	4:g:135:LEU:HB3	2.22	0.40
3:Y:279:TYR:HD2	3:Y:294:GLY:HA2	1.85	0.40
3:Y:330:ALA:HB1	3:Y:380:VAL:HB	2.04	0.40
3:Y:607:ILE:O	4:g:27:ARG:NH1	2.39	0.40
4:g:114:LEU:HD23	4:g:118:PRO:HG3	2.03	0.40
3:Y:617:LYS:HE2	3:Y:652:PRO:HG3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:f:147:LYS:HE2	4:f:147:LYS:HB3	1.77	0.40
1:A:254:ARG:HB2	1:A:264:GLY:HA3	2.03	0.40
2:W:50:ILE:HD13	2:W:50:ILE:HA	1.92	0.40
2:X:104:THR:O	2:X:106:THR:N	2.54	0.40
3:Y:90:ASP:OD1	3:Y:94:TYR:N	2.55	0.40
4:e:147:LYS:HD2	4:g:141:GLY:CA	2.51	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	500/535 (94%)	476 (95%)	22 (4%)	2 (0%)	30	59
1	L	500/535 (94%)	475 (95%)	23 (5%)	2 (0%)	30	59
2	W	190/192 (99%)	181 (95%)	9 (5%)	0	100	100
2	X	190/192 (99%)	183 (96%)	7 (4%)	0	100	100
3	Y	788/791 (100%)	713 (90%)	70 (9%)	5 (1%)	21	50
4	e	151/777 (19%)	145 (96%)	5 (3%)	1 (1%)	18	47
4	f	154/777 (20%)	148 (96%)	5 (3%)	1 (1%)	21	50
4	g	153/777 (20%)	144 (94%)	9 (6%)	0	100	100
All	All	2626/4576 (57%)	2465 (94%)	150 (6%)	11 (0%)	31	59

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	Y	656	ILE
4	f	2	ASP
1	A	518	SER
1	L	518	SER

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Mol	Chain	Res	Type
3	Y	657	SER
3	Y	711	THR
1	A	256	VAL
4	e	46	ILE
1	L	256	VAL
3	Y	170	VAL
3	Y	223	PRO

5.3.2 Protein sidechains [i](#)

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	413/435 (95%)	413 (100%)	0	100	100
1	L	413/435 (95%)	412 (100%)	1 (0%)	87	87
2	W	157/157 (100%)	157 (100%)	0	100	100
2	X	157/157 (100%)	157 (100%)	0	100	100
3	Y	680/681 (100%)	679 (100%)	1 (0%)	88	89
4	e	133/636 (21%)	133 (100%)	0	100	100
4	f	135/636 (21%)	135 (100%)	0	100	100
4	g	131/636 (21%)	131 (100%)	0	100	100
All	All	2219/3773 (59%)	2217 (100%)	2 (0%)	87	89

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	493	GLN
3	Y	153	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	342	ASN

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Mol	Chain	Res	Type
1	A	484	GLN
1	L	82	GLN
1	L	204	GLN
1	L	493	GLN
1	L	501	GLN
3	Y	153	ASN
3	Y	492	ASN
3	Y	535	GLN
3	Y	553	ASN
3	Y	565	ASN
3	Y	684	GLN
3	Y	761	GLN
3	Y	783	ASN
4	f	10	GLN
4	f	93	ASN
4	f	149	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 ⓘ

There are no chain breaks in this entry.

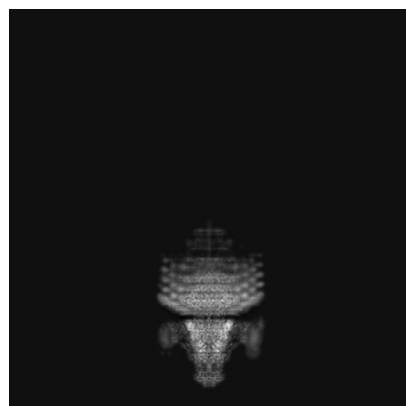
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33560. These allow visual inspection of the internal detail of the map and identification of artifacts.

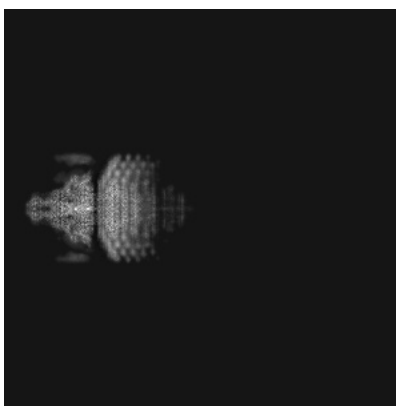
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

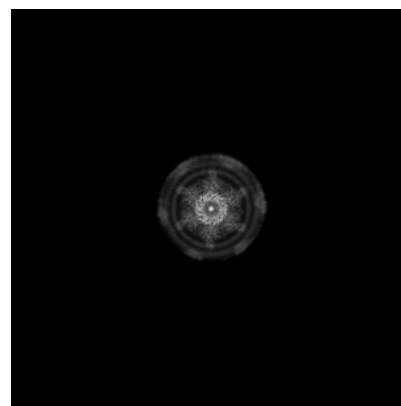
6.1.1 Primary map



X

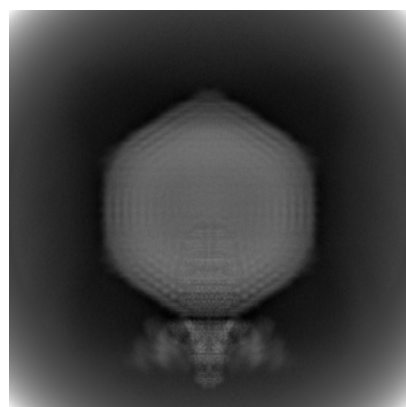


Y

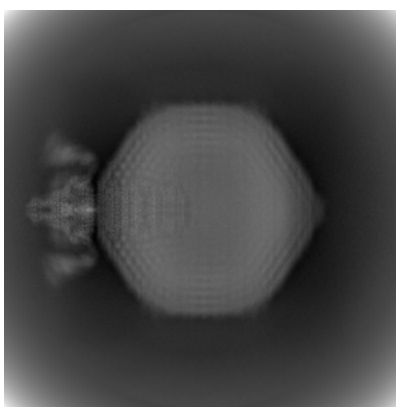


Z

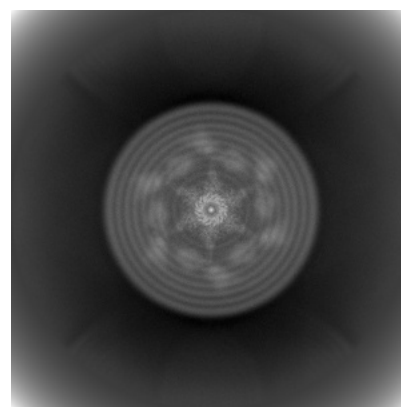
6.1.2 Raw map



X



Y

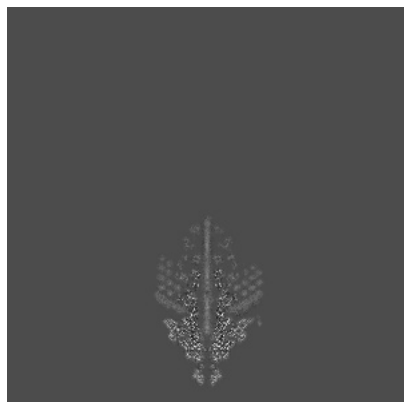


Z

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

6.2 Central slices [i](#)

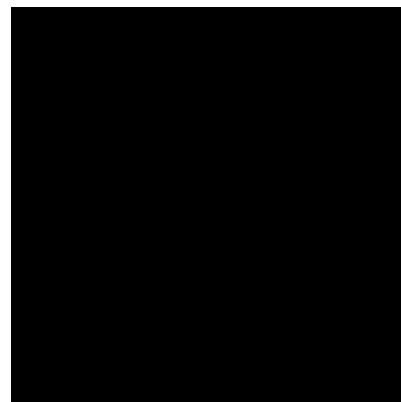
6.2.1 Primary map



X Index: 500

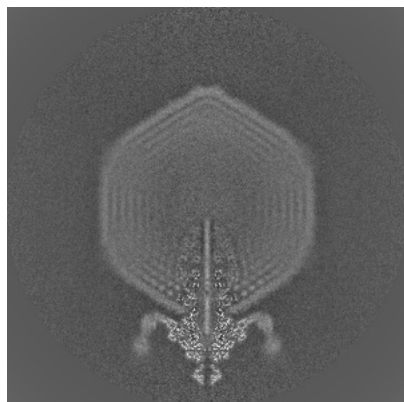


Y Index: 500

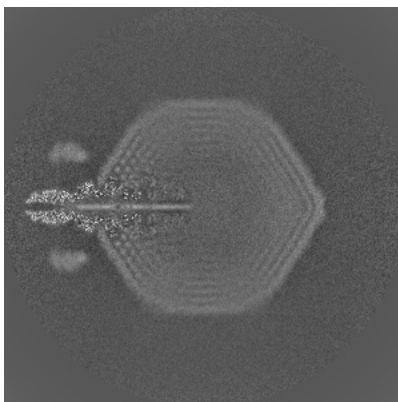


Z Index: 500

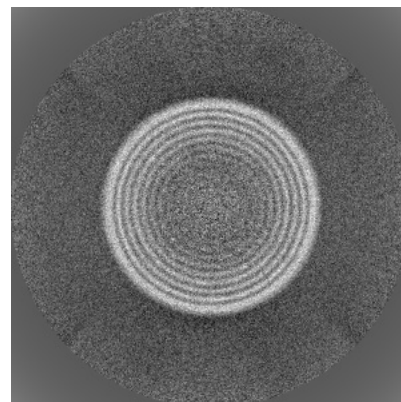
6.2.2 Raw map



X Index: 500



Y Index: 500

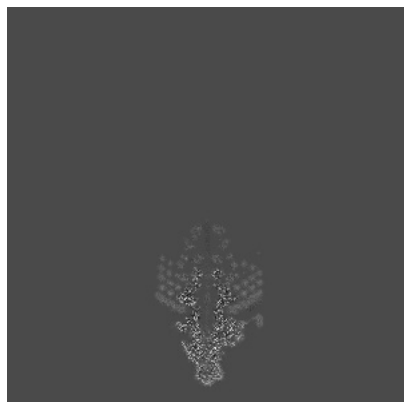


Z Index: 500

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

6.3 Largest variance slices [i](#)

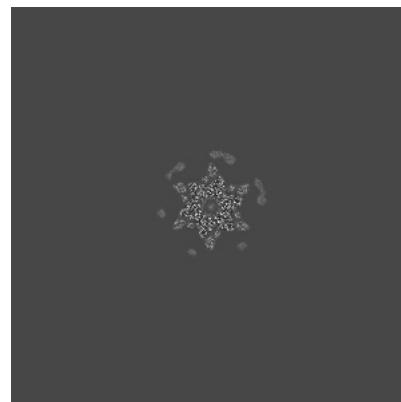
6.3.1 Primary map



X Index: 512

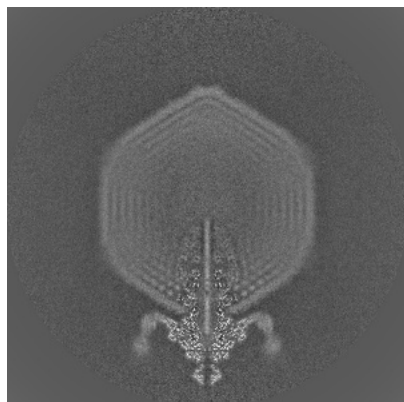


Y Index: 524

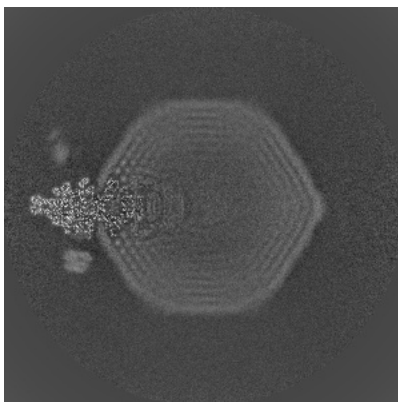


Z Index: 209

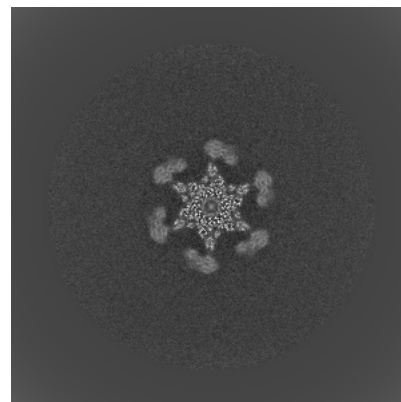
6.3.2 Raw map



X Index: 500



Y Index: 476

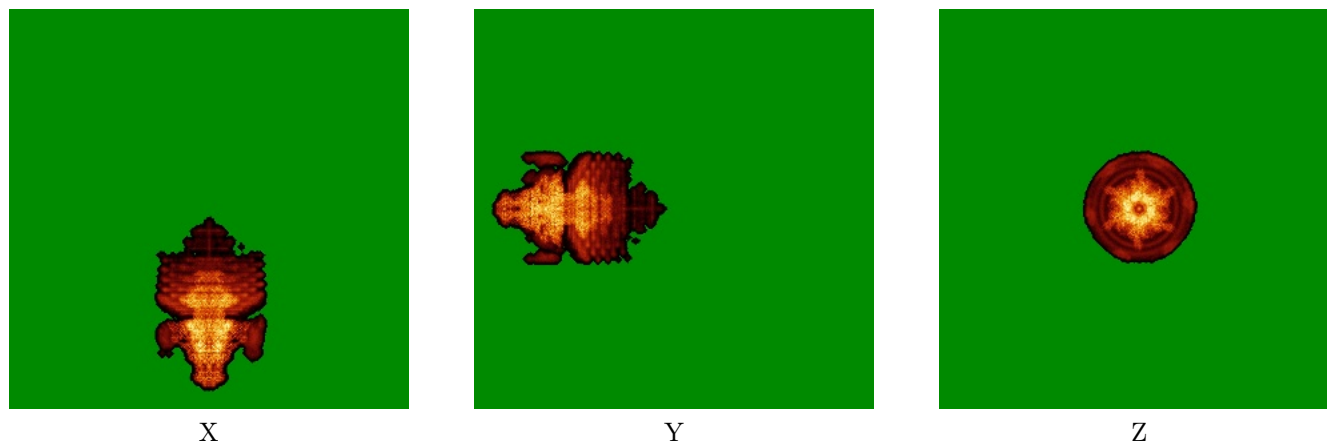


Z Index: 209

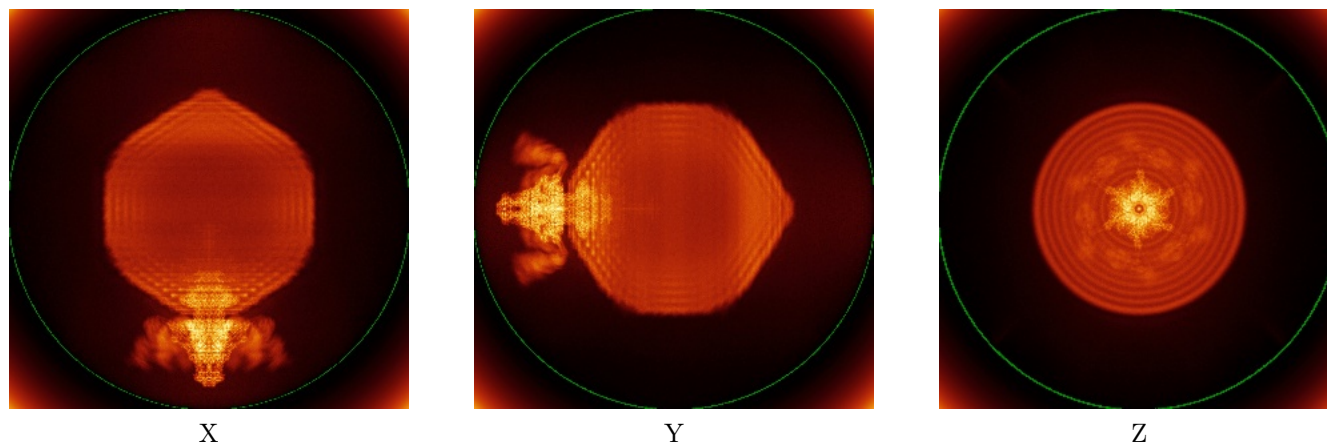
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



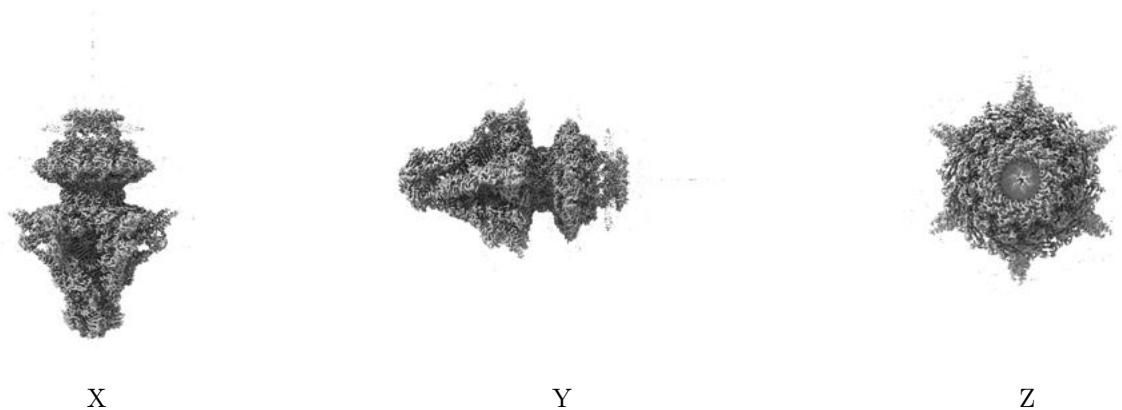
6.4.2 Raw map



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.

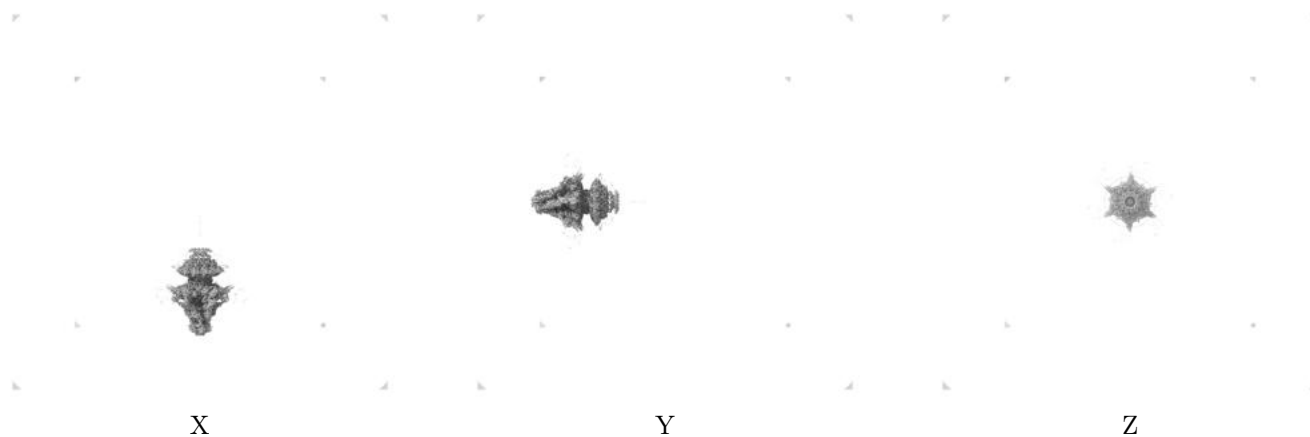
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.018. 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.

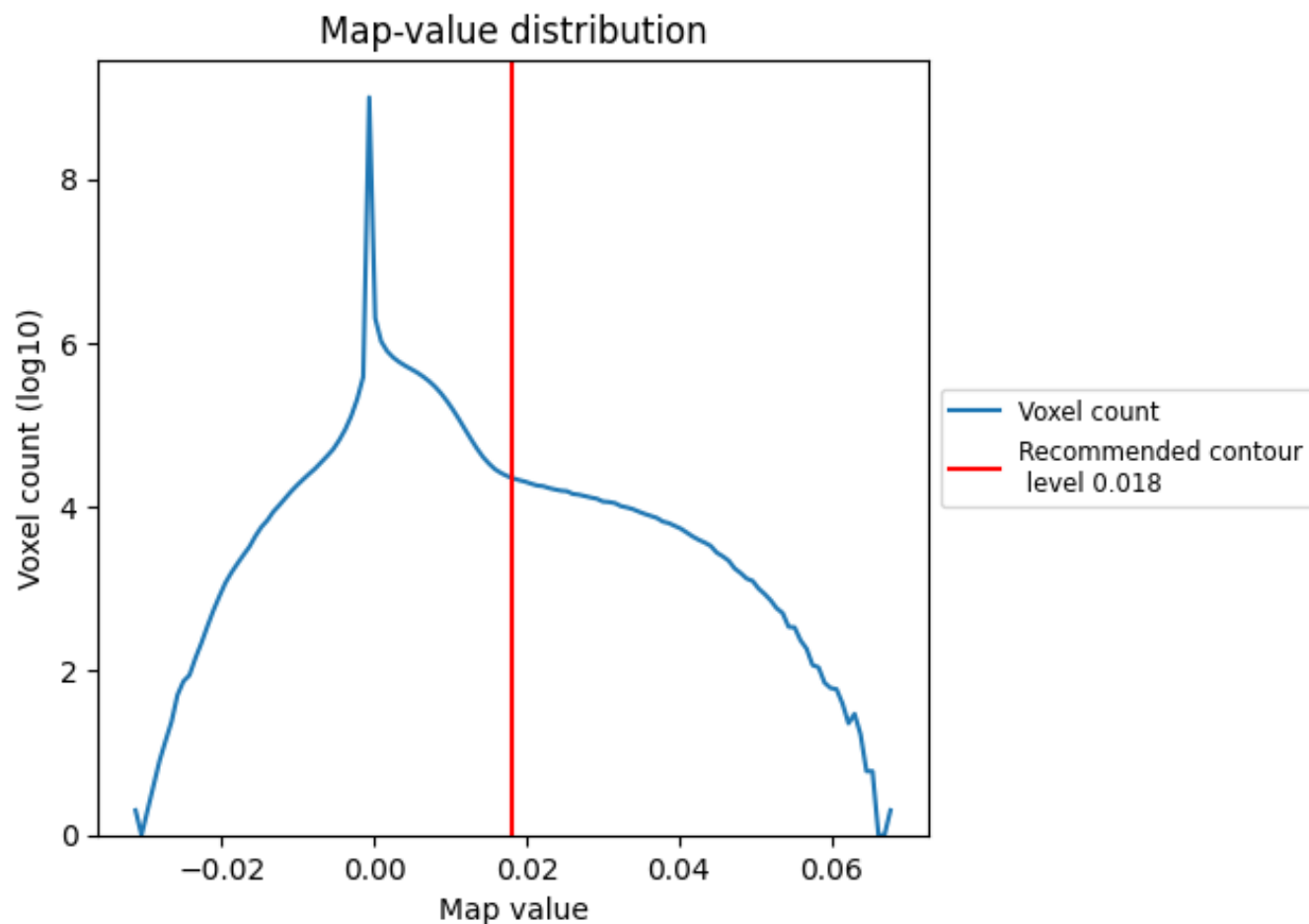
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

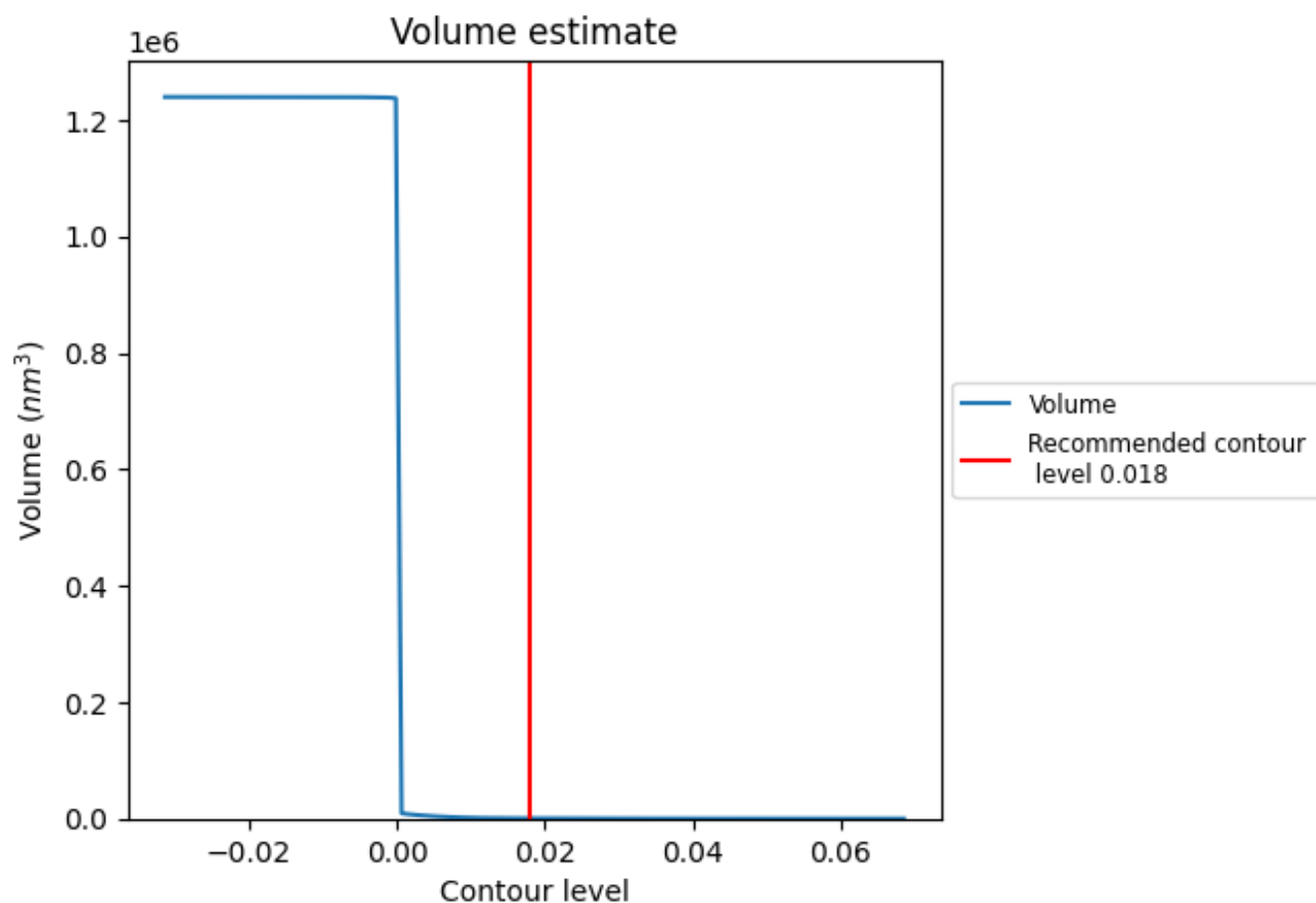
This section contains the results of statistical analysis of the map.

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.

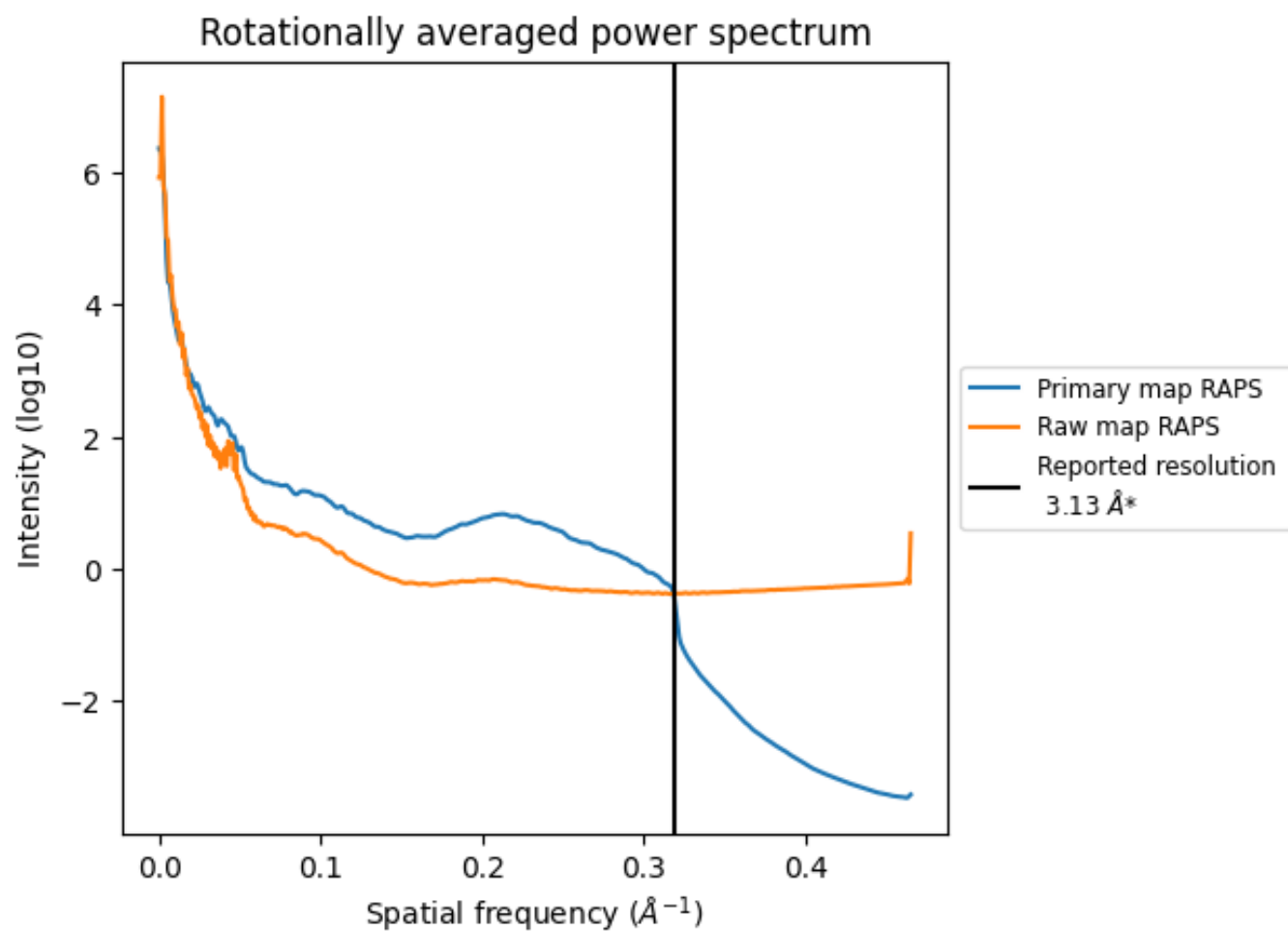
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 518 nm^3 ; this corresponds to an approximate mass of 468 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 ⓘ

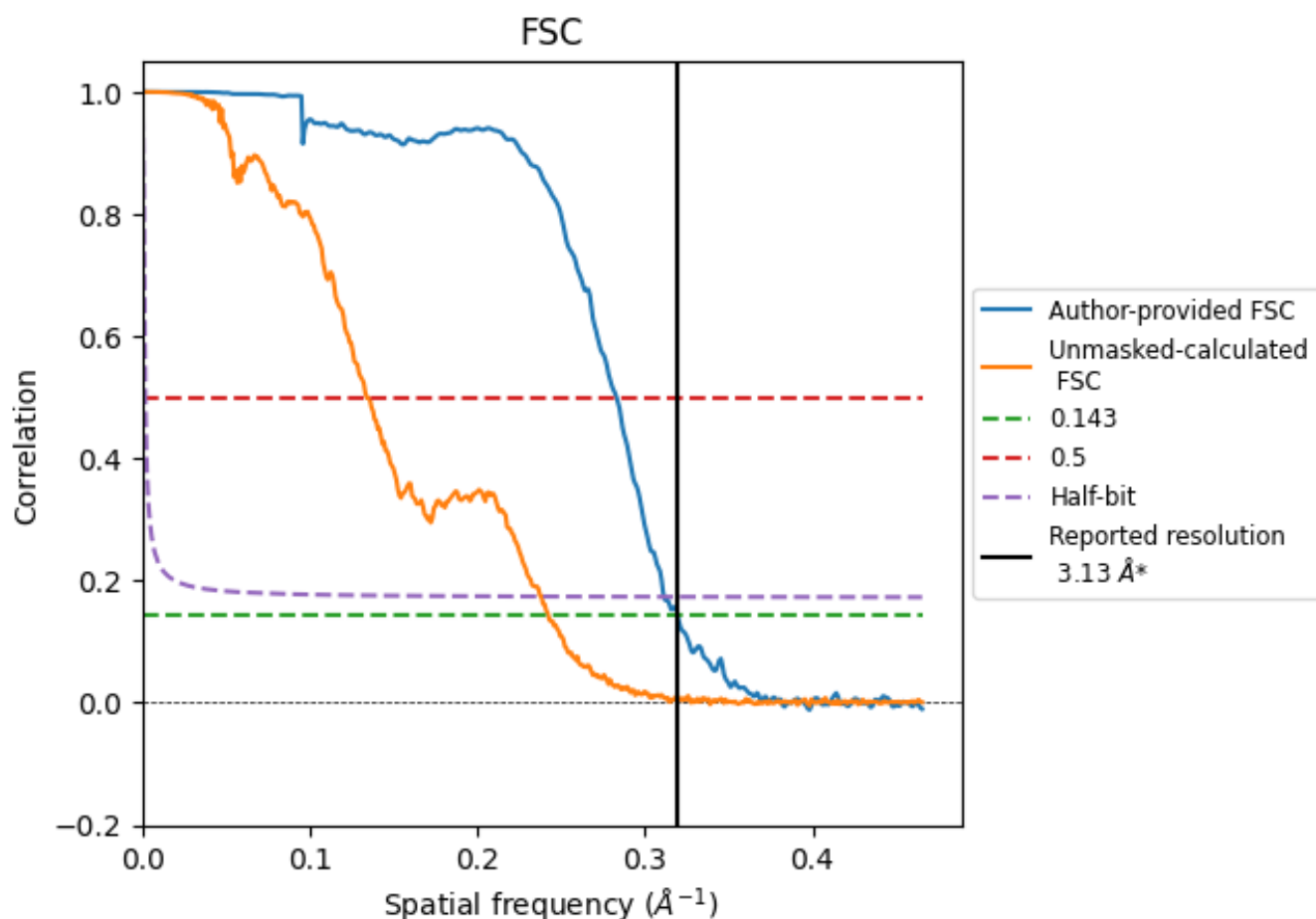


*Reported resolution corresponds to spatial frequency of 0.319 Å⁻¹

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 0.319 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.13	-	-
Author-provided FSC curve	3.13	3.53	3.21
Unmasked-calculated*	4.13	7.47	4.20

*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 4.13 differs from the reported value 3.13 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-33560 and PDB model 7Y1C. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay [i](#)

This section was not generated.

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

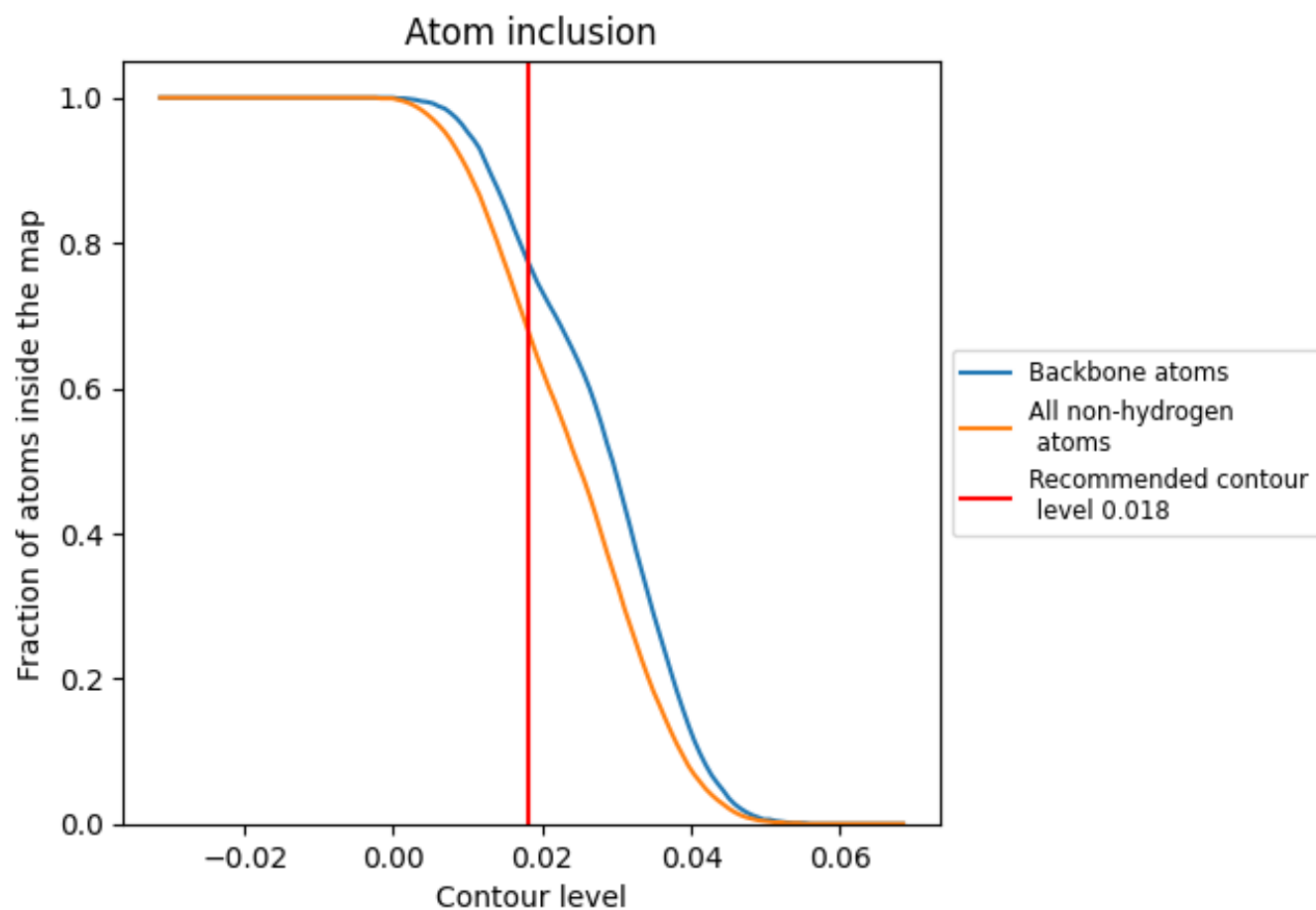


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 68% 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 (0.018) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6830	0.5590
A	0.5980	0.5620
L	0.5940	0.5590
W	0.7370	0.5710
X	0.7330	0.5700
Y	0.7680	0.5550
e	0.6860	0.5640
f	0.6900	0.5650
g	0.6600	0.5390

1.0

0.0

<0.0