



Full wwPDB EM Validation Report ⓘ

Jun 7, 2025 – 03:56 pm BST

PDB ID : 9FKB / pdb_00009fkb
EMDB ID : EMD-50521
Title : Tail of empty Haloferax tailed virus 1
Authors : Zhang, D.; Daum, B.; Isupov, M.N.; McLaren, M.
Deposited on : 2024-06-03
Resolution : 2.96 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.dev118
MolProbity : 4-5-2 with Phenix2.0rc1
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) : 2.43.1

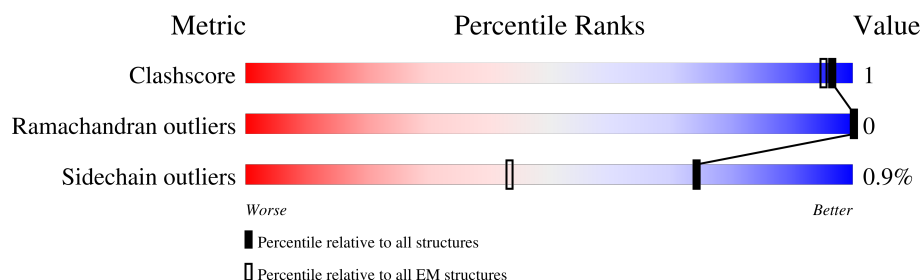
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.96 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.



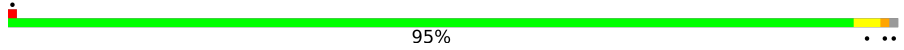
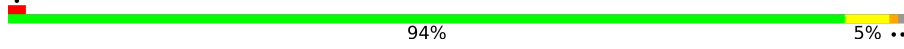
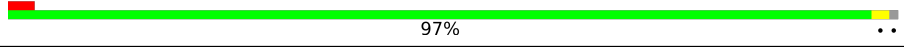
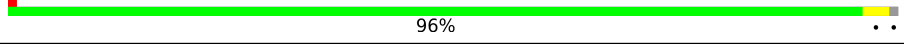
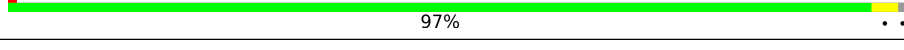
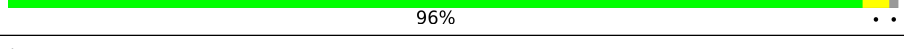
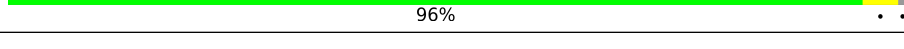
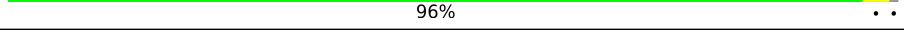
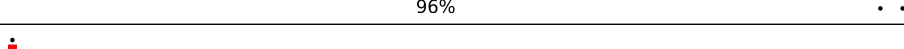
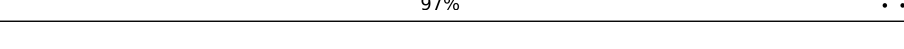
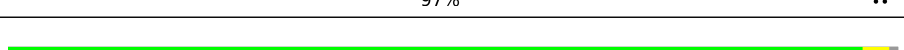
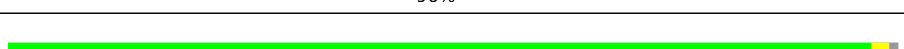
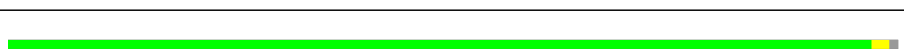
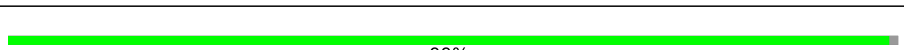
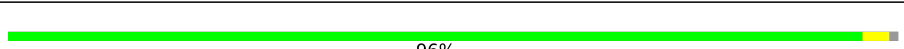
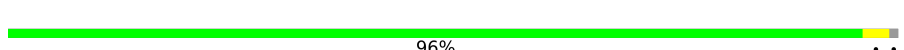
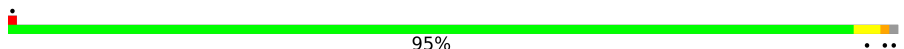
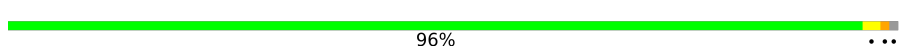
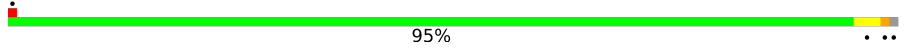
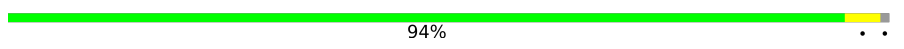
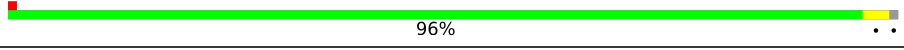
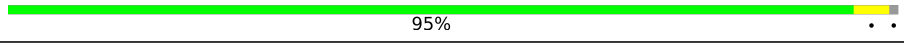
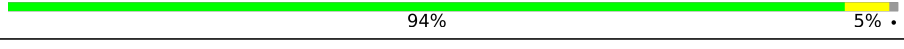
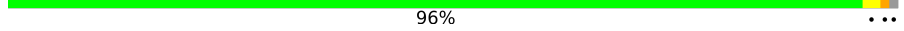

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	PM	141	95%
1	PN	141	94% 6%
1	PO	141	96%
1	PP	141	96%
1	PQ	141	96%
1	PR	141	96%
1	PS	141	96%
1	PT	141	96%

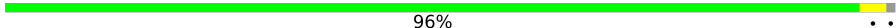
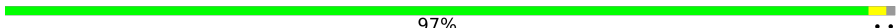
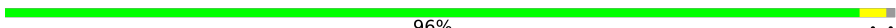
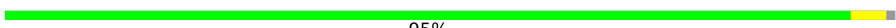
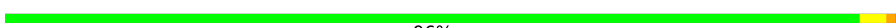








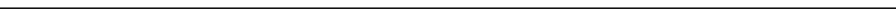

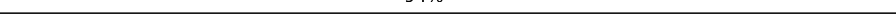
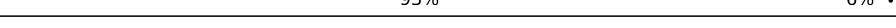
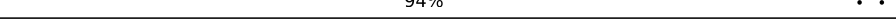
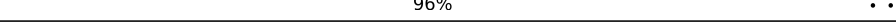
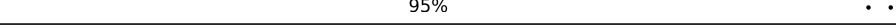
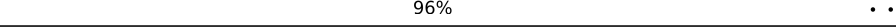
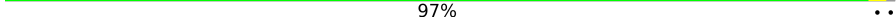
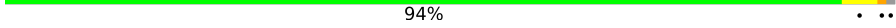
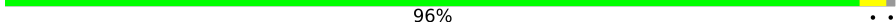
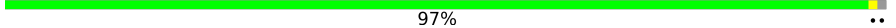
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Mol	Chain	Length	Quality of chain
1	PU	141	 95% ..
1	PV	141	 94% 5% ..
1	PW	141	 97% ..
1	PX	141	 96% ..
2	Pa	157	 97% ..
2	Pb	157	 96% ..
2	Pc	157	 96% ..
2	Pd	157	 96% ..
2	Pe	157	 96% ..
2	Pf	157	 97% ..
3	AM	158	 97% ..
3	AN	158	 96% ..
3	AO	158	 97% ..
3	AP	158	 97% ..
3	AQ	158	 99% .
3	AR	158	 96% ..
3	B1	158	 96% ..
3	B2	158	 95% ..
3	B3	158	 96% ...
3	B4	158	 95% ..
3	B5	158	 94% ..
3	B6	158	 96% ..
3	S1	158	 95% ..
3	S2	158	 94% 5% .
3	SA	158	 96% ...
















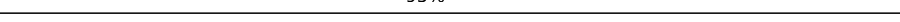
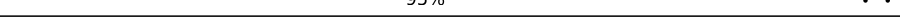


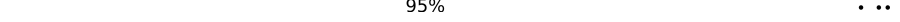
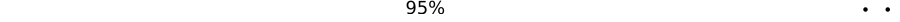

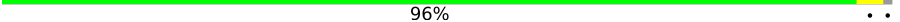
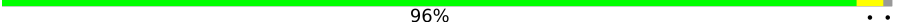
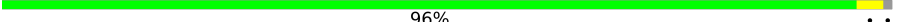
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Mol	Chain	Length	Quality of chain
3	SB	158	 96% ..
3	SC	158	 97% ..
3	SD	158	 96% ..
3	SE	158	 95% ..
3	SF	158	 96% ..
3	SG	158	 95% ..
3	SH	158	 97% ..
3	SI	158	 94% ..
3	SJ	158	 97% ..
3	SK	158	 97% ..
3	SL	158	 97% ..
3	SM	158	 95% ..
3	SN	158	 94% 5% ..
3	SO	158	 94% 5% ..
3	SP	158	 94% ..
3	SQ	158	 93% 6% ..
3	SR	158	 94% ..
3	SS	158	 96% ..
3	ST	158	 95% ..
3	SU	158	 96% ..
3	SV	158	 97% ..
3	SW	158	 94% ..
3	SX	158	 96% ..
3	SY	158	 97% ..
3	SZ	158	 96% ..

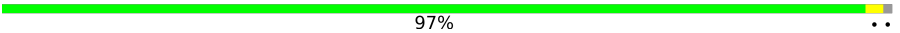
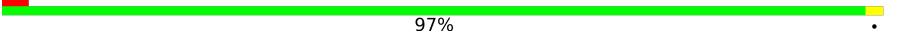
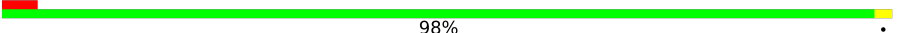
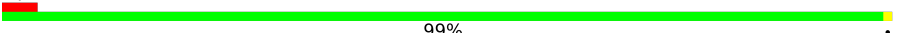
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Mol	Chain	Length	Quality of chain
3	Sa	158	 96% ..
3	Sb	158	 96% ..
3	Sc	158	 96% ..
3	Sd	158	 95% ..
3	Se	158	 95% ..
3	Sf	158	 92% 6% ..
3	Sg	158	 95% ..
3	Sh	158	 92% 7% ..
3	Si	158	 94% ..
3	Sj	158	 93% ..
3	Sk	158	 96% ..
3	Sl	158	 96% ..
3	Sm	158	 95% ..
3	Sn	158	 95% ..
3	So	158	 95% ..
3	Sp	158	 95% ..
3	Sq	158	 94% ..
3	Sr	158	 95% ..
3	Ss	158	 95% ..
3	St	158	 95% ..
3	Su	158	 94% ..
3	Sv	158	 96% ..
3	Sw	158	 96% ..
3	Sx	158	 96% ..
3	Sy	158	 97% ..

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Mol	Chain	Length	Quality of chain
3	Sz	158	 97% ..
4	BA	285	 97% .
4	BB	285	 98% .
4	BC	285	 99% .

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 105720 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 HK97 gp6-like/SPP1 gp15-like head-tail connector.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	PT	140	Total	C	N	O	S	0	0
			1087	666	184	235	2		
1	PM	140	Total	C	N	O	S	0	0
			1087	666	184	235	2		
1	PN	140	Total	C	N	O	S	0	0
			1087	666	184	235	2		
1	PO	140	Total	C	N	O	S	0	0
			1087	666	184	235	2		
1	PP	140	Total	C	N	O	S	0	0
			1087	666	184	235	2		
1	PQ	140	Total	C	N	O	S	0	0
			1087	666	184	235	2		
1	PR	140	Total	C	N	O	S	0	0
			1087	666	184	235	2		
1	PS	140	Total	C	N	O	S	0	0
			1087	666	184	235	2		
1	PU	140	Total	C	N	O	S	0	0
			1087	666	184	235	2		
1	PV	140	Total	C	N	O	S	0	0
			1087	666	184	235	2		
1	PW	140	Total	C	N	O	S	0	0
			1087	666	184	235	2		
1	PX	140	Total	C	N	O	S	0	0
			1087	666	184	235	2		

- Molecule 2 is a protein called SPP1 gp17-like tail completion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Pa	156	Total	C	N	O	S	0	0
			1220	753	200	264	3		
2	Pb	156	Total	C	N	O	S	0	0
			1220	753	200	264	3		
2	Pc	156	Total	C	N	O	S	0	0
			1220	753	200	264	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	Pd	156	Total	C	N	O	S	0	0
			1220	753	200	264	3		
2	Pe	156	Total	C	N	O	S	0	0
			1220	753	200	264	3		
2	Pf	156	Total	C	N	O	S	0	0
			1220	753	200	264	3		

- Molecule 3 is a protein called Tail tube protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B1	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
3	B2	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
3	B3	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
3	B4	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
3	B5	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
3	B6	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
3	AM	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
3	AN	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
3	AO	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
3	AP	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
3	AQ	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
3	AR	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
3	SB	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
3	SA	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
3	SC	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
3	SD	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	SE	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
3	SF	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
3	SG	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
3	SH	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
3	SI	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
3	SJ	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
3	SK	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
3	SL	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
3	SM	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
3	SN	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
3	SO	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
3	SP	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
3	SQ	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
3	SR	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
3	SS	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
3	ST	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
3	SU	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
3	SV	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
3	SW	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
3	SX	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
3	SY	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	SZ	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
3	Sa	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
3	Sb	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
3	Sc	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
3	Sd	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
3	Se	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
3	Sf	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
3	Sg	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
3	Sh	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
3	Si	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
3	Sj	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
3	Sk	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
3	Sl	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
3	Sm	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
3	Sn	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
3	So	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
3	Sp	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
3	Sq	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
3	Sr	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
3	Ss	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
3	St	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	Su	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
3	Sv	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
3	Sw	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
3	Sx	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
3	Sy	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
3	Sz	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
3	S1	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
3	S2	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		

- Molecule 4 is a protein called Baseplate to tube adapter protein gp41.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	BA	284	Total	C	N	O	0	0
			2136	1332	375	429		
4	BB	284	Total	C	N	O	0	0
			2136	1332	375	429		
4	BC	284	Total	C	N	O	0	0
			2136	1332	375	429		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
5	PT	1	Total	Mg	0
			1	1	
5	PM	1	Total	Mg	0
			1	1	
5	PN	1	Total	Mg	0
			1	1	
5	PO	1	Total	Mg	0
			1	1	
5	PP	1	Total	Mg	0
			1	1	
5	PQ	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
5	PR	1	Total 1	Mg 1	0
5	PS	1	Total 1	Mg 1	0
5	PU	1	Total 1	Mg 1	0
5	PV	1	Total 1	Mg 1	0
5	PW	1	Total 1	Mg 1	0
5	PX	1	Total 1	Mg 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: HK97 gp6-like/SPP1 gp15-like head-tail connector

Chain PT:  96%



- Molecule 1: HK97 gp6-like/SPP1 gp15-like head-tail connector

Chain PM:  95%



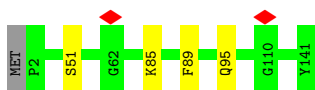
- Molecule 1: HK97 gp6-like/SPP1 gp15-like head-tail connector

Chain PN:  94% 6%



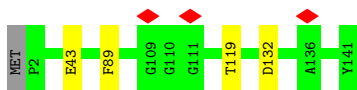
- Molecule 1: HK97 gp6-like/SPP1 gp15-like head-tail connector

Chain PO:  96%



- Molecule 1: HK97 gp6-like/SPP1 gp15-like head-tail connector

Chain PP:  96%



- Molecule 1: HK97 gp6-like/SPP1 gp15-like head-tail connector

Chain PQ:  96% ..



- Molecule 1: HK97 gp6-like/SPP1 gp15-like head-tail connector

Chain PR:  96% ..



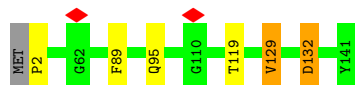
- Molecule 1: HK97 gp6-like/SPP1 gp15-like head-tail connector

Chain PS:  96% ..



- Molecule 1: HK97 gp6-like/SPP1 gp15-like head-tail connector

Chain PU:  95% ..



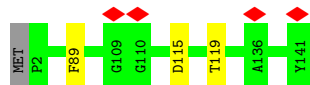
- Molecule 1: HK97 gp6-like/SPP1 gp15-like head-tail connector

Chain PV:  94% 5% ..



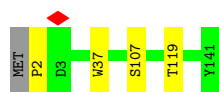
- Molecule 1: HK97 gp6-like/SPP1 gp15-like head-tail connector

Chain PW:  97% ..



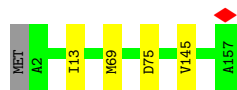
- Molecule 1: HK97 gp6-like/SPP1 gp15-like head-tail connector

Chain PX:  96% ..



- Molecule 2: SPP1 gp17-like tail completion protein

Chain Pa: 97%



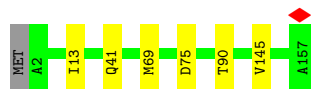
- Molecule 2: SPP1 gp17-like tail completion protein

Chain Pb: 96%



- Molecule 2: SPP1 gp17-like tail completion protein

Chain Pc: 96%



- Molecule 2: SPP1 gp17-like tail completion protein

Chain Pd: 96%



- Molecule 2: SPP1 gp17-like tail completion protein

Chain Pe: 96%



- Molecule 2: SPP1 gp17-like tail completion protein

Chain Pf: 97%



- Molecule 3: Tail tube protein

Chain B1:  96% ..



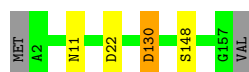
- Molecule 3: Tail tube protein

Chain B2:  95% ..



- Molecule 3: Tail tube protein

Chain B3:  96% ..



- Molecule 3: Tail tube protein

Chain B4:  95% ..



- Molecule 3: Tail tube protein

Chain B5:  94% ..



- Molecule 3: Tail tube protein

Chain B6:  96% ..



- Molecule 3: Tail tube protein

Chain AM:  97% ..



- Molecule 3: Tail tube protein

Chain AN:  96% ..



- Molecule 3: Tail tube protein

Chain AO:  97% ..



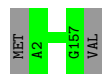
- Molecule 3: Tail tube protein

Chain AP:  97% ..



- Molecule 3: Tail tube protein

Chain AQ:  99% .



- Molecule 3: Tail tube protein

Chain AR:  96% ..



- Molecule 3: Tail tube protein

Chain SB:  96% ..



- Molecule 3: Tail tube protein

Chain SA:  96% ...



- Molecule 3: Tail tube protein

Chain SC:  97% ..



- Molecule 3: Tail tube protein

Chain SD:  96% ..



- Molecule 3: Tail tube protein

Chain SE:  95% ..



- Molecule 3: Tail tube protein

Chain SF:  96% ..



- Molecule 3: Tail tube protein

Chain SG:  95% ..



- Molecule 3: Tail tube protein

Chain SH:  97% ..



- Molecule 3: Tail tube protein

Chain SI:  94% ..



- Molecule 3: Tail tube protein

Chain SJ:  97% ..



- Molecule 3: Tail tube protein

Chain SK:  97% ..



- Molecule 3: Tail tube protein

Chain SL:  97% ..



- Molecule 3: Tail tube protein

Chain SM:  95% ..



- Molecule 3: Tail tube protein

Chain SN:  94% 5% ..



- Molecule 3: Tail tube protein

Chain SO:  94% 5% ..



- Molecule 3: Tail tube protein

Chain SP:  94% ..



- Molecule 3: Tail tube protein

Chain SQ:  93% 6% .



- Molecule 3: Tail tube protein

Chain SR:  94% . .



- Molecule 3: Tail tube protein

Chain SS:  96% . .



- Molecule 3: Tail tube protein

Chain ST:  95% . .



- Molecule 3: Tail tube protein

Chain SU:  96% . .



- Molecule 3: Tail tube protein

Chain SV:  97% . .

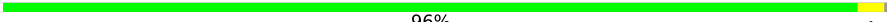


- Molecule 3: Tail tube protein

Chain SW:  94% . .



- Molecule 3: Tail tube protein

Chain SX:  96% ..



- Molecule 3: Tail tube protein

Chain SY:  97% ..



- Molecule 3: Tail tube protein

Chain SZ:  96% ..



- Molecule 3: Tail tube protein

Chain Sa:  96% ..



- Molecule 3: Tail tube protein

Chain Sb:  96% ..



- Molecule 3: Tail tube protein

Chain Sc:  96% ..

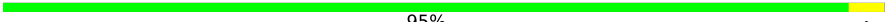


- Molecule 3: Tail tube protein

Chain Sd:  95% ..



- Molecule 3: Tail tube protein

Chain Se:  95% ..



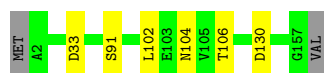
- Molecule 3: Tail tube protein

Chain Sf:  92% 6% ..



- Molecule 3: Tail tube protein

Chain Sg:  95% ..



- Molecule 3: Tail tube protein

Chain Sh:  92% 7% ..



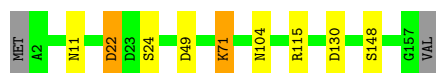
- Molecule 3: Tail tube protein

Chain Si:  94% ..



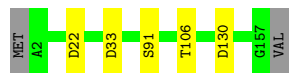
- Molecule 3: Tail tube protein

Chain Sj:  93% ..



- Molecule 3: Tail tube protein

Chain Sk:  96% ..



- Molecule 3: Tail tube protein

Chain Sl:  96% ..



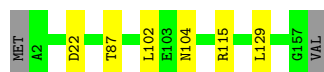
- Molecule 3: Tail tube protein

Chain Sm:  95% ..



- Molecule 3: Tail tube protein

Chain Sn:  95% ..



- Molecule 3: Tail tube protein

Chain So:  95% ..



- Molecule 3: Tail tube protein

Chain Sp:  95% ..



- Molecule 3: Tail tube protein

Chain Sq:  94% ..



- Molecule 3: Tail tube protein

Chain Sr:  95% ..



- Molecule 3: Tail tube protein

Chain Ss:  95% ..



- Molecule 3: Tail tube protein

Chain St:  95% ..



- Molecule 3: Tail tube protein

Chain Su:  94% ..



- Molecule 3: Tail tube protein

Chain Sv:  96% ..



- Molecule 3: Tail tube protein

Chain Sw:  96% ..



- Molecule 3: Tail tube protein

Chain Sx:  96% ..



- Molecule 3: Tail tube protein

Chain Sy:  97% ..



- Molecule 3: Tail tube protein

Chain Sz:  97% ..



- Molecule 3: Tail tube protein

Chain S1:  95% ..



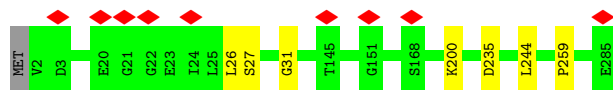
- Molecule 3: Tail tube protein

Chain S2:  94% 5% .



- Molecule 4: Baseplate to tube adapter protein gp41

Chain BA:  97% .



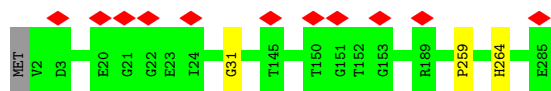
- Molecule 4: Baseplate to tube adapter protein gp41

Chain BB:  98% .



- Molecule 4: Baseplate to tube adapter protein gp41

Chain BC:  99% .



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	6580	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 ($e^-/\text{\AA}^2$)	50, 54.6	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k), GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.073	Depositor
Minimum map value	-0.031	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0062	Depositor
Map size (\AA)	899.328, 899.328, 899.328	wwPDB
Map dimensions	768, 768, 768	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.171, 1.171, 1.171	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	PM	0.60	0/1105	1.15	1/1492 (0.1%)
1	PN	0.60	0/1105	1.14	2/1492 (0.1%)
1	PO	0.61	0/1105	1.14	1/1492 (0.1%)
1	PP	0.61	0/1105	1.16	2/1492 (0.1%)
1	PQ	0.59	0/1105	1.15	1/1492 (0.1%)
1	PR	0.60	0/1105	1.14	1/1492 (0.1%)
1	PS	0.59	0/1105	1.14	0/1492
1	PT	0.60	0/1105	1.15	1/1492 (0.1%)
1	PU	0.60	0/1105	1.16	3/1492 (0.2%)
1	PV	0.61	0/1105	1.14	2/1492 (0.1%)
1	PW	0.60	0/1105	1.14	1/1492 (0.1%)
1	PX	0.60	0/1105	1.14	1/1492 (0.1%)
2	Pa	0.58	0/1248	1.03	1/1709 (0.1%)
2	Pb	0.60	0/1248	1.04	1/1709 (0.1%)
2	Pc	0.59	0/1248	1.03	1/1709 (0.1%)
2	Pd	0.61	0/1248	1.05	1/1709 (0.1%)
2	Pe	0.59	0/1248	1.05	1/1709 (0.1%)
2	Pf	0.59	0/1248	1.05	0/1709
3	AM	0.60	0/1224	0.96	0/1672
3	AN	0.59	0/1224	0.91	0/1672
3	AO	0.58	0/1224	0.95	0/1672
3	AP	0.59	0/1224	0.94	0/1672
3	AQ	0.59	0/1224	0.95	0/1672
3	AR	0.59	0/1224	0.90	0/1672
3	B1	0.58	0/1224	0.96	1/1672 (0.1%)
3	B2	0.60	0/1224	0.96	0/1672
3	B3	0.58	0/1224	0.96	2/1672 (0.1%)
3	B4	0.58	0/1224	0.93	1/1672 (0.1%)
3	B5	0.58	0/1224	0.94	1/1672 (0.1%)
3	B6	0.59	0/1224	0.94	1/1672 (0.1%)
3	S1	0.60	0/1224	0.95	2/1672 (0.1%)
3	S2	0.60	1/1224 (0.1%)	0.99	2/1672 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	SA	0.60	0/1224	0.99	2/1672 (0.1%)
3	SB	0.62	0/1224	0.96	1/1672 (0.1%)
3	SC	0.61	0/1224	0.98	1/1672 (0.1%)
3	SD	0.62	0/1224	0.96	0/1672
3	SE	0.61	0/1224	0.98	2/1672 (0.1%)
3	SF	0.63	0/1224	0.98	2/1672 (0.1%)
3	SG	0.63	0/1224	0.98	1/1672 (0.1%)
3	SH	0.64	0/1224	0.95	1/1672 (0.1%)
3	SI	0.65	0/1224	0.98	1/1672 (0.1%)
3	SJ	0.63	0/1224	0.92	0/1672
3	SK	0.64	0/1224	0.98	1/1672 (0.1%)
3	SL	0.63	0/1224	0.94	1/1672 (0.1%)
3	SM	0.63	0/1224	0.97	1/1672 (0.1%)
3	SN	0.63	0/1224	0.99	2/1672 (0.1%)
3	SO	0.63	0/1224	1.00	3/1672 (0.2%)
3	SP	0.63	0/1224	0.99	2/1672 (0.1%)
3	SQ	0.63	0/1224	0.99	3/1672 (0.2%)
3	SR	0.64	0/1224	1.01	1/1672 (0.1%)
3	SS	0.61	1/1224 (0.1%)	0.97	2/1672 (0.1%)
3	ST	0.62	0/1224	0.98	2/1672 (0.1%)
3	SU	0.61	1/1224 (0.1%)	0.97	2/1672 (0.1%)
3	SV	0.61	0/1224	0.98	1/1672 (0.1%)
3	SW	0.63	1/1224 (0.1%)	0.97	2/1672 (0.1%)
3	SX	0.62	0/1224	1.00	2/1672 (0.1%)
3	SY	0.63	0/1224	0.96	1/1672 (0.1%)
3	SZ	0.61	0/1224	0.99	1/1672 (0.1%)
3	Sa	0.64	0/1224	0.98	2/1672 (0.1%)
3	Sb	0.62	0/1224	0.97	1/1672 (0.1%)
3	Sc	0.64	0/1224	0.99	1/1672 (0.1%)
3	Sd	0.62	0/1224	0.97	0/1672
3	Se	0.62	0/1224	0.99	2/1672 (0.1%)
3	Sf	0.61	0/1224	0.99	1/1672 (0.1%)
3	Sg	0.62	0/1224	0.99	1/1672 (0.1%)
3	Sh	0.61	0/1224	0.98	2/1672 (0.1%)
3	Si	0.61	0/1224	1.00	2/1672 (0.1%)
3	Sj	0.65	1/1224 (0.1%)	0.98	2/1672 (0.1%)
3	Sk	0.61	0/1224	0.97	2/1672 (0.1%)
3	Sl	0.62	0/1224	0.96	1/1672 (0.1%)
3	Sm	0.64	0/1224	0.96	3/1672 (0.2%)
3	Sn	0.61	0/1224	0.97	1/1672 (0.1%)
3	So	0.62	0/1224	0.96	2/1672 (0.1%)
3	Sp	0.61	0/1224	0.96	2/1672 (0.1%)
3	Sq	0.59	0/1224	0.97	3/1672 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	Sr	0.59	0/1224	0.98	1/1672 (0.1%)
3	Ss	0.60	0/1224	1.00	4/1672 (0.2%)
3	St	0.60	0/1224	0.97	0/1672
3	Su	0.60	0/1224	0.99	2/1672 (0.1%)
3	Sv	0.60	0/1224	0.98	2/1672 (0.1%)
3	Sw	0.59	1/1224 (0.1%)	0.96	1/1672 (0.1%)
3	Sx	0.60	1/1224 (0.1%)	0.97	1/1672 (0.1%)
3	Sy	0.60	0/1224	0.94	1/1672 (0.1%)
3	Sz	0.60	1/1224 (0.1%)	0.97	0/1672
4	BA	0.64	0/2175	1.08	3/2970 (0.1%)
4	BB	0.64	0/2175	1.09	3/2970 (0.1%)
4	BC	0.64	0/2175	1.09	0/2970
All	All	0.61	8/108057 (0.0%)	1.01	115/147420 (0.1%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Sj	71	LYS	CE-NZ	6.70	1.69	1.49
3	Sx	42	HIS	CE1-NE2	5.62	1.38	1.32
3	S2	42	HIS	CE1-NE2	5.57	1.38	1.32
3	SU	42	HIS	CE1-NE2	5.49	1.38	1.32
3	Sz	42	HIS	CE1-NE2	5.43	1.38	1.32
3	Sw	42	HIS	CE1-NE2	5.10	1.37	1.32
3	SW	42	HIS	CE1-NE2	5.09	1.37	1.32
3	SS	42	HIS	CE1-NE2	5.01	1.37	1.32

All (115) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Si	33	ASP	CA-CB-CG	7.67	120.27	112.60
3	Sg	33	ASP	CA-CB-CG	7.60	120.20	112.60
3	SA	33	ASP	CA-CB-CG	7.01	119.61	112.60
3	Ss	33	ASP	CA-CB-CG	7.01	119.61	112.60
3	Sb	33	ASP	CA-CB-CG	6.84	119.44	112.60
3	Su	33	ASP	CA-CB-CG	6.75	119.35	112.60
3	Sm	33	ASP	CA-CB-CG	6.72	119.32	112.60
3	SZ	33	ASP	CA-CB-CG	6.68	119.28	112.60
3	Se	33	ASP	CA-CB-CG	6.68	119.28	112.60
3	SK	22	ASP	CA-CB-CG	6.56	119.16	112.60
3	SR	33	ASP	CA-CB-CG	6.42	119.02	112.60
3	Sa	22	ASP	CA-CB-CG	6.42	119.02	112.60
3	SF	22	ASP	CA-CB-CG	6.41	119.01	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	SU	22	ASP	CA-CB-CG	6.41	119.01	112.60
3	SW	22	ASP	CA-CB-CG	6.40	119.00	112.60
3	SX	33	ASP	CA-CB-CG	6.39	118.99	112.60
3	SI	22	ASP	CA-CB-CG	6.39	118.99	112.60
3	Sk	33	ASP	CA-CB-CG	6.32	118.92	112.60
3	SN	33	ASP	CA-CB-CG	6.30	118.90	112.60
3	SS	22	ASP	CA-CB-CG	6.25	118.85	112.60
3	Sq	33	ASP	CA-CB-CG	6.25	118.85	112.60
3	SU	33	ASP	CA-CB-CG	6.23	118.83	112.60
3	SG	22	ASP	CA-CB-CG	6.22	118.82	112.60
3	SS	33	ASP	CA-CB-CG	6.16	118.76	112.60
2	Pc	75	ASP	CA-CB-CG	6.14	118.74	112.60
3	SO	33	ASP	CA-CB-CG	6.13	118.73	112.60
3	Sc	22	ASP	CA-CB-CG	6.12	118.72	112.60
3	SW	33	ASP	CA-CB-CG	6.11	118.71	112.60
1	PO	89	PHE	CA-CB-CG	6.10	119.90	113.80
3	So	33	ASP	CA-CB-CG	6.05	118.65	112.60
3	SC	33	ASP	CA-CB-CG	6.02	118.62	112.60
3	SB	33	ASP	CA-CB-CG	5.98	118.58	112.60
3	B3	22	ASP	CA-CB-CG	5.96	118.56	112.60
3	Sj	22	ASP	CA-CB-CG	5.96	118.56	112.60
3	Sn	22	ASP	CA-CB-CG	5.94	118.54	112.60
3	Ss	115	ARG	NE-CZ-NH2	5.90	124.51	119.20
3	Sp	22	ASP	CA-CB-CG	5.89	118.49	112.60
3	S2	22	ASP	CA-CB-CG	5.89	118.49	112.60
3	B1	22	ASP	CA-CB-CG	5.88	118.48	112.60
3	SE	33	ASP	CA-CB-CG	5.87	118.47	112.60
3	Sq	22	ASP	CA-CB-CG	5.86	118.46	112.60
3	SX	25	GLU	CB-CG-CD	5.86	122.56	112.60
3	SQ	22	ASP	CA-CB-CG	5.83	118.43	112.60
3	SN	22	ASP	CA-CB-CG	5.82	118.42	112.60
3	Sl	22	ASP	CA-CB-CG	5.80	118.40	112.60
3	SH	33	ASP	CA-CB-CG	5.78	118.38	112.60
3	ST	33	ASP	CA-CB-CG	5.78	118.38	112.60
3	SQ	33	ASP	CA-CB-CG	5.77	118.37	112.60
3	Sx	22	ASP	CA-CB-CG	5.76	118.36	112.60
3	B5	22	ASP	CA-CB-CG	5.75	118.35	112.60
3	Sp	33	ASP	CA-CB-CG	5.71	118.31	112.60
1	PV	89	PHE	CA-CB-CG	5.69	119.49	113.80
3	SO	22	ASP	CA-CB-CG	5.66	118.25	112.60
3	SM	22	ASP	CA-CB-CG	5.65	118.25	112.60
2	Pe	75	ASP	CA-CB-CG	5.61	118.21	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Su	22	ASP	CA-CB-CG	5.60	118.20	112.60
1	PW	89	PHE	CA-CB-CG	5.57	119.37	113.80
3	SA	128	PRO	CB-CA-C	5.56	116.46	111.40
3	Sk	22	ASP	CA-CB-CG	5.54	118.14	112.60
2	Pd	118	ASP	CA-CB-CG	5.54	118.14	112.60
3	Sy	49	ASP	CA-CB-CG	5.54	118.14	112.60
1	PT	89	PHE	CA-CB-CG	5.53	119.33	113.80
1	PN	2	PRO	CA-N-CD	-5.52	104.27	112.00
3	SP	33	ASP	CA-CB-CG	5.50	118.11	112.60
3	Sh	49	ASP	CA-CB-CG	5.50	118.10	112.60
1	PU	89	PHE	CA-CB-CG	5.49	119.29	113.80
1	PU	2	PRO	CA-N-CD	-5.49	104.32	112.00
3	SQ	25	GLU	CB-CG-CD	5.47	121.90	112.60
3	Sw	49	ASP	CA-CB-CG	5.47	118.07	112.60
3	Sr	33	ASP	CA-CB-CG	5.45	118.05	112.60
3	Sa	33	ASP	CA-CB-CG	5.44	118.04	112.60
3	Sm	22	ASP	CA-CB-CG	5.44	118.04	112.60
3	SF	33	ASP	CA-CB-CG	5.42	118.02	112.60
3	Sh	22	ASP	CA-CB-CG	5.40	118.00	112.60
4	BA	235	ASP	CA-CB-CG	5.40	118.00	112.60
1	PR	89	PHE	CA-CB-CG	5.40	119.20	113.80
3	Sj	49	ASP	CA-CB-CG	5.39	117.99	112.60
3	Ss	49	ASP	CA-CB-CG	5.39	117.99	112.60
3	B3	130	ASP	CA-CB-CG	5.37	117.97	112.60
4	BA	200	LYS	CA-C-N	5.37	127.90	120.49
4	BA	200	LYS	C-N-CA	5.37	127.90	120.49
3	Sv	49	ASP	CA-CB-CG	5.37	117.97	112.60
3	SO	25	GLU	CB-CG-CD	5.35	121.70	112.60
3	Sf	22	ASP	CA-CB-CG	5.32	117.92	112.60
3	So	22	ASP	CA-CB-CG	5.29	117.89	112.60
1	PQ	133	ASN	CA-CB-CG	5.28	117.88	112.60
3	Si	115	ARG	NE-CZ-NH2	5.28	123.95	119.20
3	SL	33	ASP	CA-CB-CG	5.28	117.88	112.60
3	Se	115	ARG	NE-CZ-NH2	5.27	123.94	119.20
1	PU	132	ASP	CA-CB-CG	5.26	117.86	112.60
2	Pa	75	ASP	CA-CB-CG	5.23	117.83	112.60
3	SY	33	ASP	CA-CB-CG	5.23	117.83	112.60
3	SP	22	ASP	CA-CB-CG	5.20	117.80	112.60
3	SE	128	PRO	CB-CA-C	5.17	116.10	111.40
3	S1	49	ASP	CA-CB-CG	5.17	117.77	112.60
1	PN	89	PHE	CA-CB-CG	5.16	118.96	113.80
1	PX	2	PRO	CA-N-CD	-5.16	104.78	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	PP	132	ASP	CA-CB-CG	5.14	117.74	112.60
3	SV	25	GLU	CB-CG-CD	5.14	121.34	112.60
2	Pb	75	ASP	CA-CB-CG	5.13	117.73	112.60
3	Sv	33	ASP	CA-CB-CG	5.12	117.72	112.60
1	PP	89	PHE	CA-CB-CG	5.12	118.92	113.80
1	PV	3	ASP	CA-CB-CG	5.12	117.72	112.60
3	B4	52	PHE	CA-CB-CG	5.10	118.90	113.80
4	BB	200	LYS	CA-C-N	5.10	127.52	120.49
4	BB	200	LYS	C-N-CA	5.10	127.52	120.49
3	ST	25	GLU	CB-CG-CD	5.09	121.25	112.60
1	PM	132	ASP	CA-CB-CG	5.08	117.68	112.60
3	Ss	22	ASP	CA-CB-CG	5.05	117.65	112.60
3	B6	52	PHE	CA-CB-CG	5.05	118.85	113.80
3	S2	25	GLU	CB-CG-CD	5.05	121.18	112.60
4	BB	118	ARG	CG-CD-NE	5.04	123.08	112.00
3	Sm	115	ARG	NE-CZ-NH2	5.03	123.73	119.20
3	S1	130	ASP	CA-CB-CG	5.02	117.62	112.60
3	Sq	49	ASP	CA-CB-CG	5.01	117.61	112.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	PM	1087	0	1018	3	0
1	PN	1087	0	1018	5	0
1	PO	1087	0	1018	3	0
1	PP	1087	0	1018	1	0
1	PQ	1087	0	1018	2	0
1	PR	1087	0	1018	3	0
1	PS	1087	0	1018	3	0
1	PT	1087	0	1018	3	0
1	PU	1087	0	1018	3	0
1	PV	1087	0	1018	4	0
1	PW	1087	0	1018	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	PX	1087	0	1018	2	0
2	Pa	1220	0	1118	1	0
2	Pb	1220	0	1118	3	0
2	Pc	1220	0	1118	2	0
2	Pd	1220	0	1118	1	0
2	Pe	1220	0	1118	0	0
2	Pf	1220	0	1118	3	0
3	AM	1196	0	1094	2	0
3	AN	1196	0	1094	3	0
3	AO	1196	0	1094	3	0
3	AP	1196	0	1094	2	0
3	AQ	1196	0	1094	0	0
3	AR	1196	0	1094	6	0
3	B1	1196	0	1094	2	0
3	B2	1196	0	1094	4	0
3	B3	1196	0	1094	3	0
3	B4	1196	0	1094	4	0
3	B5	1196	0	1094	5	0
3	B6	1196	0	1094	2	0
3	S1	1196	0	1094	2	0
3	S2	1196	0	1094	3	0
3	SA	1196	0	1094	1	0
3	SB	1196	0	1094	3	0
3	SC	1196	0	1094	1	0
3	SD	1196	0	1094	3	0
3	SE	1196	0	1094	2	0
3	SF	1196	0	1094	3	0
3	SG	1196	0	1094	5	0
3	SH	1196	0	1094	1	0
3	SI	1196	0	1094	3	0
3	SJ	1196	0	1094	3	0
3	SK	1196	0	1094	1	0
3	SL	1196	0	1094	2	0
3	SM	1196	0	1094	3	0
3	SN	1196	0	1094	5	0
3	SO	1196	0	1094	4	0
3	SP	1196	0	1094	4	0
3	SQ	1196	0	1094	4	0
3	SR	1196	0	1094	4	0
3	SS	1196	0	1094	1	0
3	ST	1196	0	1094	2	0
3	SU	1196	0	1094	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	SV	1196	0	1094	0	0
3	SW	1196	0	1094	2	0
3	SX	1196	0	1094	2	0
3	SY	1196	0	1094	1	0
3	SZ	1196	0	1094	3	0
3	Sa	1196	0	1094	1	0
3	Sb	1196	0	1094	2	0
3	Sc	1196	0	1094	3	0
3	Sd	1196	0	1094	4	0
3	Se	1196	0	1094	3	0
3	Sf	1196	0	1094	6	0
3	Sg	1196	0	1094	4	0
3	Sh	1196	0	1094	7	0
3	Si	1196	0	1094	4	0
3	Sj	1196	0	1094	6	0
3	Sk	1196	0	1094	2	0
3	Sl	1196	0	1094	3	0
3	Sm	1196	0	1094	2	0
3	Sn	1196	0	1094	3	0
3	So	1196	0	1094	2	0
3	Sp	1196	0	1094	3	0
3	Sq	1196	0	1094	3	0
3	Sr	1196	0	1094	4	0
3	Ss	1196	0	1094	3	0
3	St	1196	0	1094	5	0
3	Su	1196	0	1094	4	0
3	Sv	1196	0	1094	2	0
3	Sw	1196	0	1094	2	0
3	Sx	1196	0	1094	2	0
3	Sy	1196	0	1094	1	0
3	Sz	1196	0	1094	1	0
4	BA	2136	0	2127	4	0
4	BB	2136	0	2127	4	0
4	BC	2136	0	2127	3	0
5	PM	1	0	0	0	0
5	PN	1	0	0	0	0
5	PO	1	0	0	0	0
5	PP	1	0	0	0	0
5	PQ	1	0	0	0	0
5	PR	1	0	0	0	0
5	PS	1	0	0	0	0
5	PT	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	PU	1	0	0	0	0
5	PV	1	0	0	0	0
5	PW	1	0	0	0	0
5	PX	1	0	0	0	0
All	All	105720	0	97509	143	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (143) 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:Sj:71:LYS:CE	3:Sj:71:LYS:NZ	1.69	1.50
1:PS:95:GLN:HB2	1:PV:107:SER:HB2	1.78	0.65
3:SA:48:ILE:HG12	3:SI:11:ASN:HA	1.79	0.65
2:Pc:69:MET:HG3	3:AR:134:TYR:HB3	1.85	0.59
3:SE:48:ILE:HG12	3:SG:11:ASN:HA	1.84	0.58
1:PM:95:GLN:HB2	1:PR:107:SER:HB2	1.86	0.57
3:Su:48:ILE:HG23	3:Sy:11:ASN:HA	1.86	0.57
4:BB:259:PRO:HD2	4:BC:31:GLY:HA2	1.87	0.56
4:BA:31:GLY:HA2	4:BC:259:PRO:HD2	1.88	0.56
3:SL:48:ILE:HG12	3:SP:11:ASN:HA	1.88	0.56
2:Pf:69:MET:HG3	3:AO:134:TYR:HB3	1.88	0.56
3:Sq:48:ILE:HG23	3:Sw:11:ASN:HA	1.89	0.55
1:PT:37:TRP:HA	2:Pb:136:THR:HG21	1.89	0.55
3:Sh:130:ASP:OD2	3:Si:104:ASN:ND2	2.35	0.54
3:Sf:130:ASP:OD2	3:Sg:104:ASN:ND2	2.36	0.54
3:SZ:48:ILE:HG12	3:Sh:11:ASN:HA	1.89	0.53
3:B5:11:ASN:HA	3:S2:48:ILE:HG23	1.90	0.53
3:SH:48:ILE:HG12	3:SR:11:ASN:HA	1.92	0.52
1:PU:95:GLN:HB2	1:PX:107:SER:HB2	1.92	0.52
3:Sd:48:ILE:HG12	3:Sf:11:ASN:HA	1.91	0.52
3:SQ:130:ASP:OD2	3:SR:104:ASN:ND2	2.43	0.52
1:PN:37:TRP:HA	2:Pd:136:THR:HG21	1.92	0.51
1:PQ:44:ARG:HH21	1:PQ:44:ARG:HG3	1.74	0.51
2:Pf:69:MET:HG3	3:AO:134:TYR:CB	2.41	0.50
3:AR:115:ARG:HH21	3:AR:115:ARG:HG3	1.76	0.50
3:SJ:48:ILE:HG12	3:SN:11:ASN:HA	1.93	0.50
4:BA:259:PRO:HD2	4:BB:31:GLY:HA2	1.95	0.49
3:SC:48:ILE:HG12	3:SK:11:ASN:HA	1.94	0.49
1:PX:37:TRP:HA	2:Pf:136:THR:HG21	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Sb:48:ILE:HG12	3:Sj:11:ASN:HA	1.96	0.48
3:Sq:27:LEU:HD23	3:Sr:5:PRO:HD3	1.96	0.48
3:AP:48:ILE:HG12	3:SD:11:ASN:HA	1.95	0.48
3:Sm:130:ASP:OD2	3:Sn:104:ASN:ND2	2.43	0.48
3:Si:130:ASP:OD2	3:Sj:104:ASN:ND2	2.38	0.48
3:B4:130:ASP:OD2	3:B5:104:ASN:ND2	2.45	0.47
2:Pa:69:MET:HG2	3:AO:11:ASN:HA	1.96	0.47
3:AR:48:ILE:HG12	3:SF:11:ASN:HA	1.97	0.47
2:Pb:69:MET:HB3	3:AM:134:TYR:CB	2.44	0.47
3:AN:48:ILE:HG12	3:SB:11:ASN:HA	1.97	0.47
3:AP:102:LEU:C	3:AP:102:LEU:HD23	2.40	0.47
3:SO:130:ASP:OD2	3:SP:104:ASN:ND2	2.46	0.47
1:PU:129:VAL:CG1	1:PU:129:VAL:O	2.63	0.46
1:PM:131:GLU:OE1	1:PN:114:LYS:HE3	2.14	0.46
3:Sk:130:ASP:OD2	3:Sl:104:ASN:ND2	2.47	0.46
3:B2:91:SER:HB2	3:B3:148:SER:HB2	1.98	0.46
3:SO:91:SER:HB2	3:SP:148:SER:HB2	1.98	0.46
3:Ss:48:ILE:HG23	3:S1:11:ASN:HA	1.97	0.46
3:SM:91:SER:HB2	3:SN:148:SER:HB2	1.98	0.46
1:PT:80:TYR:OH	1:PQ:85:LYS:HE3	2.16	0.46
3:B3:130:ASP:HA	3:B4:115:ARG:NH1	2.31	0.46
1:PM:44:ARG:HD3	1:PR:34:SER:HA	1.98	0.46
3:Sg:91:SER:HB2	3:Sh:148:SER:HB2	1.98	0.45
3:Sr:130:ASP:HA	3:Ss:115:ARG:NH1	2.32	0.45
1:PV:3:ASP:HB2	1:PV:4:PRO:CD	2.48	0.44
3:B4:91:SER:HB2	3:B5:148:SER:HB2	1.99	0.44
3:Se:104:ASN:ND2	3:Sj:130:ASP:OD2	2.41	0.44
3:AR:102:LEU:C	3:AR:102:LEU:HD23	2.43	0.44
3:SZ:129:LEU:HD23	3:SZ:129:LEU:HA	1.88	0.44
3:B1:148:SER:HB2	3:B6:91:SER:HB2	2.00	0.44
3:B3:11:ASN:HA	3:Sx:48:ILE:HG23	2.00	0.44
3:AR:45:LEU:HB2	3:SF:137:TYR:CE2	2.53	0.43
3:Se:130:ASP:OD2	3:Sf:104:ASN:ND2	2.38	0.43
3:Sk:91:SER:HB2	3:Sl:148:SER:HB2	2.00	0.43
3:Sf:13:GLY:HA2	3:Sf:106:THR:HG22	2.00	0.43
3:SQ:91:SER:HB2	3:SR:148:SER:HB2	2.00	0.43
3:Se:91:SER:HB2	3:Sf:148:SER:HB2	2.01	0.43
3:Sp:48:ILE:HG23	3:St:11:ASN:HA	2.00	0.43
3:St:48:ILE:HG12	3:S2:11:ASN:HA	2.00	0.43
3:SE:13:GLY:HA2	3:SE:106:THR:HG22	2.01	0.43
3:Sh:13:GLY:HA2	3:Sh:106:THR:HG22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Su:27:LEU:HD23	3:Sv:5:PRO:HD3	2.00	0.43
3:AR:115:ARG:HG3	3:AR:115:ARG:NH2	2.33	0.43
3:SI:17:PHE:CE1	3:SI:102:LEU:HD12	2.54	0.43
3:AN:102:LEU:HD23	3:AN:102:LEU:C	2.43	0.43
3:SS:22:ASP:HB2	3:SS:24:SER:H	1.84	0.43
3:SZ:102:LEU:C	3:SZ:102:LEU:HD23	2.43	0.43
3:Sg:130:ASP:OD2	3:Sh:104:ASN:ND2	2.37	0.43
2:Pb:69:MET:HB3	3:AM:134:TYR:HB2	2.00	0.43
1:PN:80:TYR:OH	1:PO:85:LYS:HE3	2.19	0.43
1:PP:43:GLU:CD	1:PP:43:GLU:H	2.26	0.43
1:PV:43:GLU:H	1:PV:43:GLU:CD	2.27	0.42
3:Sc:129:LEU:HD23	3:Sc:129:LEU:HA	1.85	0.42
1:PU:129:VAL:O	1:PU:129:VAL:HG12	2.19	0.42
3:Si:102:LEU:C	3:Si:102:LEU:HD23	2.45	0.42
3:SM:13:GLY:HA2	3:SM:106:THR:HG22	2.01	0.42
3:Sg:102:LEU:HD23	3:Sg:102:LEU:C	2.45	0.42
3:SR:129:LEU:HD23	3:SR:129:LEU:HA	1.88	0.42
3:SX:129:LEU:HD23	3:SX:129:LEU:HA	1.92	0.42
3:Sh:60:GLU:HG2	3:Sl:134:TYR:OH	2.20	0.42
3:SD:55:GLU:OE2	3:SG:110:SER:OG	2.38	0.42
3:SG:48:ILE:HG23	3:SQ:11:ASN:HA	2.02	0.42
3:Sn:129:LEU:HD23	3:Sn:129:LEU:HA	1.89	0.42
3:S2:17:PHE:CE1	3:S2:102:LEU:HD12	2.54	0.42
3:B2:11:ASN:HA	3:Sw:48:ILE:HB	2.01	0.42
3:SG:129:LEU:HD23	3:SG:129:LEU:HA	1.93	0.42
3:SP:59:TYR:O	3:SQ:51:THR:HB	2.19	0.42
3:SY:129:LEU:HD23	3:SY:129:LEU:HA	1.89	0.42
3:Sc:102:LEU:C	3:Sc:102:LEU:HD23	2.45	0.42
3:So:130:ASP:OD2	3:Sp:104:ASN:ND2	2.52	0.42
3:B1:130:ASP:HA	3:B2:115:ARG:NH1	2.35	0.42
3:SF:22:ASP:HB2	3:SF:24:SER:H	1.84	0.42
3:ST:48:ILE:HG12	3:Sd:11:ASN:HA	2.02	0.42
3:Si:91:SER:HB2	3:Sj:148:SER:HB2	2.01	0.42
3:Sm:48:ILE:HG23	3:Sq:11:ASN:HA	2.02	0.42
3:So:91:SER:HB2	3:Sp:148:SER:HB2	2.01	0.42
3:Ss:27:LEU:HD23	3:St:5:PRO:HD3	2.00	0.42
3:Sz:13:GLY:HA2	3:Sz:106:THR:HG22	2.02	0.42
1:PN:76:TYR:CE1	1:PO:51:SER:HB2	2.55	0.41
3:SB:48:ILE:HG12	3:SJ:11:ASN:HA	2.02	0.41
3:SI:91:SER:HB2	3:SJ:148:SER:HB2	2.02	0.41
3:Sh:129:LEU:HD23	3:Sh:129:LEU:HA	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:SN:130:ASP:OD2	3:SO:104:ASN:ND2	2.47	0.41
1:PT:59:LEU:HD11	1:PS:128:TYR:HA	2.02	0.41
3:SW:22:ASP:HB2	3:SW:24:SER:H	1.85	0.41
3:SM:130:ASP:OD2	3:SN:104:ASN:ND2	2.51	0.41
1:PN:107:SER:HB2	1:PO:95:GLN:HB2	2.02	0.41
3:B4:11:ASN:HA	3:S1:48:ILE:HB	2.02	0.41
3:ST:46:TYR:HB3	3:Sc:134:TYR:OH	2.21	0.41
3:SX:102:LEU:HD23	3:SX:102:LEU:C	2.45	0.41
3:St:102:LEU:C	3:St:102:LEU:HD23	2.46	0.41
4:BA:26:LEU:HD23	4:BA:27:SER:N	2.36	0.41
3:St:130:ASP:OD2	3:Su:104:ASN:ND2	2.42	0.41
3:B5:134:TYR:CE1	3:B6:11:ASN:ND2	2.86	0.41
3:Sr:48:ILE:HG12	3:Sx:11:ASN:HA	2.02	0.41
3:Sr:102:LEU:C	3:Sr:102:LEU:HD23	2.46	0.41
1:PS:44:ARG:HD3	1:PV:34:SER:HA	2.02	0.41
3:B2:48:ILE:HD11	4:BC:264:HIS:HB3	2.03	0.41
3:SD:102:LEU:C	3:SD:102:LEU:HD23	2.46	0.41
3:Sb:102:LEU:HD23	3:Sb:102:LEU:C	2.46	0.41
3:B5:48:ILE:HD11	4:BB:244:LEU:HD13	2.03	0.41
3:Sj:22:ASP:HB2	3:Sj:24:SER:H	1.86	0.41
3:AN:45:LEU:HB2	3:SB:137:TYR:CE2	2.56	0.40
3:SG:148:SER:HB2	3:SL:91:SER:HB2	2.03	0.40
3:Sa:129:LEU:HD23	3:Sa:129:LEU:HA	1.91	0.40
3:Sd:102:LEU:C	3:Sd:102:LEU:HD23	2.46	0.40
3:Sd:129:LEU:HD23	3:Sd:129:LEU:HA	1.85	0.40
4:BA:259:PRO:HD2	4:BB:31:GLY:CA	2.50	0.40
3:Su:130:ASP:OD2	3:Sv:104:ASN:ND2	2.52	0.40
3:SN:91:SER:HB2	3:SO:148:SER:HB2	2.03	0.40
1:PR:102:GLY:HA3	2:Pc:41:GLN:NE2	2.37	0.40
3:SW:13:GLY:HA2	3:SW:106:THR:HG22	2.04	0.40
3:Sn:102:LEU:C	3:Sn:102:LEU:HD23	2.46	0.40
3:Sf:129:LEU:HD23	3:Sf:129:LEU:HA	1.90	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	PM	138/141 (98%)	133 (96%)	5 (4%)	0	100	100
1	PN	138/141 (98%)	132 (96%)	6 (4%)	0	100	100
1	PO	138/141 (98%)	127 (92%)	11 (8%)	0	100	100
1	PP	138/141 (98%)	130 (94%)	8 (6%)	0	100	100
1	PQ	138/141 (98%)	132 (96%)	6 (4%)	0	100	100
1	PR	138/141 (98%)	134 (97%)	4 (3%)	0	100	100
1	PS	138/141 (98%)	129 (94%)	9 (6%)	0	100	100
1	PT	138/141 (98%)	135 (98%)	3 (2%)	0	100	100
1	PU	138/141 (98%)	131 (95%)	7 (5%)	0	100	100
1	PV	138/141 (98%)	132 (96%)	6 (4%)	0	100	100
1	PW	138/141 (98%)	132 (96%)	6 (4%)	0	100	100
1	PX	138/141 (98%)	135 (98%)	3 (2%)	0	100	100
2	Pa	154/157 (98%)	147 (96%)	7 (4%)	0	100	100
2	Pb	154/157 (98%)	149 (97%)	5 (3%)	0	100	100
2	Pc	154/157 (98%)	149 (97%)	5 (3%)	0	100	100
2	Pd	154/157 (98%)	148 (96%)	6 (4%)	0	100	100
2	Pe	154/157 (98%)	148 (96%)	6 (4%)	0	100	100
2	Pf	154/157 (98%)	147 (96%)	7 (4%)	0	100	100
3	AM	154/158 (98%)	153 (99%)	1 (1%)	0	100	100
3	AN	154/158 (98%)	151 (98%)	3 (2%)	0	100	100
3	AO	154/158 (98%)	152 (99%)	2 (1%)	0	100	100
3	AP	154/158 (98%)	151 (98%)	3 (2%)	0	100	100
3	AQ	154/158 (98%)	152 (99%)	2 (1%)	0	100	100
3	AR	154/158 (98%)	151 (98%)	3 (2%)	0	100	100
3	B1	154/158 (98%)	147 (96%)	7 (4%)	0	100	100
3	B2	154/158 (98%)	149 (97%)	5 (3%)	0	100	100
3	B3	154/158 (98%)	149 (97%)	5 (3%)	0	100	100
3	B4	154/158 (98%)	151 (98%)	3 (2%)	0	100	100
3	B5	154/158 (98%)	149 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	B6	154/158 (98%)	152 (99%)	2 (1%)	0	100	100
3	S1	154/158 (98%)	150 (97%)	4 (3%)	0	100	100
3	S2	154/158 (98%)	147 (96%)	7 (4%)	0	100	100
3	SA	154/158 (98%)	150 (97%)	4 (3%)	0	100	100
3	SB	154/158 (98%)	152 (99%)	2 (1%)	0	100	100
3	SC	154/158 (98%)	151 (98%)	3 (2%)	0	100	100
3	SD	154/158 (98%)	152 (99%)	2 (1%)	0	100	100
3	SE	154/158 (98%)	152 (99%)	2 (1%)	0	100	100
3	SF	154/158 (98%)	152 (99%)	2 (1%)	0	100	100
3	SG	154/158 (98%)	150 (97%)	4 (3%)	0	100	100
3	SH	154/158 (98%)	151 (98%)	3 (2%)	0	100	100
3	SI	154/158 (98%)	151 (98%)	3 (2%)	0	100	100
3	SJ	154/158 (98%)	152 (99%)	2 (1%)	0	100	100
3	SK	154/158 (98%)	149 (97%)	5 (3%)	0	100	100
3	SL	154/158 (98%)	151 (98%)	3 (2%)	0	100	100
3	SM	154/158 (98%)	151 (98%)	3 (2%)	0	100	100
3	SN	154/158 (98%)	150 (97%)	4 (3%)	0	100	100
3	SO	154/158 (98%)	152 (99%)	2 (1%)	0	100	100
3	SP	154/158 (98%)	149 (97%)	5 (3%)	0	100	100
3	SQ	154/158 (98%)	150 (97%)	4 (3%)	0	100	100
3	SR	154/158 (98%)	148 (96%)	6 (4%)	0	100	100
3	SS	154/158 (98%)	151 (98%)	3 (2%)	0	100	100
3	ST	154/158 (98%)	150 (97%)	4 (3%)	0	100	100
3	SU	154/158 (98%)	150 (97%)	4 (3%)	0	100	100
3	SV	154/158 (98%)	152 (99%)	2 (1%)	0	100	100
3	SW	154/158 (98%)	150 (97%)	4 (3%)	0	100	100
3	SX	154/158 (98%)	150 (97%)	4 (3%)	0	100	100
3	SY	154/158 (98%)	149 (97%)	5 (3%)	0	100	100
3	SZ	154/158 (98%)	148 (96%)	6 (4%)	0	100	100
3	Sa	154/158 (98%)	150 (97%)	4 (3%)	0	100	100
3	Sb	154/158 (98%)	150 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	Sc	154/158 (98%)	150 (97%)	4 (3%)	0	100	100
3	Sd	154/158 (98%)	149 (97%)	5 (3%)	0	100	100
3	Se	154/158 (98%)	150 (97%)	4 (3%)	0	100	100
3	Sf	154/158 (98%)	148 (96%)	6 (4%)	0	100	100
3	Sg	154/158 (98%)	151 (98%)	3 (2%)	0	100	100
3	Sh	154/158 (98%)	149 (97%)	5 (3%)	0	100	100
3	Si	154/158 (98%)	151 (98%)	3 (2%)	0	100	100
3	Sj	154/158 (98%)	148 (96%)	6 (4%)	0	100	100
3	Sk	154/158 (98%)	149 (97%)	5 (3%)	0	100	100
3	Sl	154/158 (98%)	150 (97%)	4 (3%)	0	100	100
3	Sm	154/158 (98%)	148 (96%)	6 (4%)	0	100	100
3	Sn	154/158 (98%)	152 (99%)	2 (1%)	0	100	100
3	So	154/158 (98%)	148 (96%)	6 (4%)	0	100	100
3	Sp	154/158 (98%)	152 (99%)	2 (1%)	0	100	100
3	Sq	154/158 (98%)	150 (97%)	4 (3%)	0	100	100
3	Sr	154/158 (98%)	149 (97%)	5 (3%)	0	100	100
3	Ss	154/158 (98%)	149 (97%)	5 (3%)	0	100	100
3	St	154/158 (98%)	149 (97%)	5 (3%)	0	100	100
3	Su	154/158 (98%)	149 (97%)	5 (3%)	0	100	100
3	Sv	154/158 (98%)	149 (97%)	5 (3%)	0	100	100
3	Sw	154/158 (98%)	151 (98%)	3 (2%)	0	100	100
3	Sx	154/158 (98%)	148 (96%)	6 (4%)	0	100	100
3	Sy	154/158 (98%)	150 (97%)	4 (3%)	0	100	100
3	Sz	154/158 (98%)	148 (96%)	6 (4%)	0	100	100
4	BA	282/285 (99%)	270 (96%)	12 (4%)	0	100	100
4	BB	282/285 (99%)	266 (94%)	16 (6%)	0	100	100
4	BC	282/285 (99%)	273 (97%)	9 (3%)	0	100	100
All	All	13590/13917 (98%)	13183 (97%)	407 (3%)	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	PM	116/117 (99%)	114 (98%)	2 (2%)	56	76
1	PN	116/117 (99%)	115 (99%)	1 (1%)	75	86
1	PO	116/117 (99%)	116 (100%)	0	100	100
1	PP	116/117 (99%)	115 (99%)	1 (1%)	75	86
1	PQ	116/117 (99%)	115 (99%)	1 (1%)	75	86
1	PR	116/117 (99%)	115 (99%)	1 (1%)	75	86
1	PS	116/117 (99%)	115 (99%)	1 (1%)	75	86
1	PT	116/117 (99%)	115 (99%)	1 (1%)	75	86
1	PU	116/117 (99%)	113 (97%)	3 (3%)	41	65
1	PV	116/117 (99%)	114 (98%)	2 (2%)	56	76
1	PW	116/117 (99%)	114 (98%)	2 (2%)	56	76
1	PX	116/117 (99%)	115 (99%)	1 (1%)	75	86
2	Pa	135/136 (99%)	133 (98%)	2 (2%)	60	78
2	Pb	135/136 (99%)	133 (98%)	2 (2%)	60	78
2	Pc	135/136 (99%)	132 (98%)	3 (2%)	47	69
2	Pd	135/136 (99%)	132 (98%)	3 (2%)	47	69
2	Pe	135/136 (99%)	130 (96%)	5 (4%)	29	54
2	Pf	135/136 (99%)	133 (98%)	2 (2%)	60	78
3	AM	129/131 (98%)	128 (99%)	1 (1%)	79	88
3	AN	129/131 (98%)	127 (98%)	2 (2%)	58	77
3	AO	129/131 (98%)	128 (99%)	1 (1%)	79	88
3	AP	129/131 (98%)	128 (99%)	1 (1%)	79	88
3	AQ	129/131 (98%)	129 (100%)	0	100	100
3	AR	129/131 (98%)	129 (100%)	0	100	100
3	B1	129/131 (98%)	127 (98%)	2 (2%)	58	77
3	B2	129/131 (98%)	126 (98%)	3 (2%)	45	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	B3	129/131 (98%)	129 (100%)	0	100	100
3	B4	129/131 (98%)	127 (98%)	2 (2%)	58	77
3	B5	129/131 (98%)	128 (99%)	1 (1%)	79	88
3	B6	129/131 (98%)	128 (99%)	1 (1%)	79	88
3	S1	129/131 (98%)	127 (98%)	2 (2%)	58	77
3	S2	129/131 (98%)	128 (99%)	1 (1%)	79	88
3	SA	129/131 (98%)	127 (98%)	2 (2%)	58	77
3	SB	129/131 (98%)	128 (99%)	1 (1%)	79	88
3	SC	129/131 (98%)	128 (99%)	1 (1%)	79	88
3	SD	129/131 (98%)	128 (99%)	1 (1%)	79	88
3	SE	129/131 (98%)	128 (99%)	1 (1%)	79	88
3	SF	129/131 (98%)	129 (100%)	0	100	100
3	SG	129/131 (98%)	129 (100%)	0	100	100
3	SH	129/131 (98%)	128 (99%)	1 (1%)	79	88
3	SI	129/131 (98%)	127 (98%)	2 (2%)	58	77
3	SJ	129/131 (98%)	129 (100%)	0	100	100
3	SK	129/131 (98%)	129 (100%)	0	100	100
3	SL	129/131 (98%)	129 (100%)	0	100	100
3	SM	129/131 (98%)	128 (99%)	1 (1%)	79	88
3	SN	129/131 (98%)	128 (99%)	1 (1%)	79	88
3	SO	129/131 (98%)	128 (99%)	1 (1%)	79	88
3	SP	129/131 (98%)	128 (99%)	1 (1%)	79	88
3	SQ	129/131 (98%)	127 (98%)	2 (2%)	58	77
3	SR	129/131 (98%)	127 (98%)	2 (2%)	58	77
3	SS	129/131 (98%)	128 (99%)	1 (1%)	79	88
3	ST	129/131 (98%)	127 (98%)	2 (2%)	58	77
3	SU	129/131 (98%)	128 (99%)	1 (1%)	79	88
3	SV	129/131 (98%)	127 (98%)	2 (2%)	58	77
3	SW	129/131 (98%)	128 (99%)	1 (1%)	79	88
3	SX	129/131 (98%)	128 (99%)	1 (1%)	79	88
3	SY	129/131 (98%)	129 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	SZ	129/131 (98%)	128 (99%)	1 (1%)	79	88
3	Sa	129/131 (98%)	128 (99%)	1 (1%)	79	88
3	Sb	129/131 (98%)	127 (98%)	2 (2%)	58	77
3	Sc	129/131 (98%)	128 (99%)	1 (1%)	79	88
3	Sd	129/131 (98%)	127 (98%)	2 (2%)	58	77
3	Se	129/131 (98%)	128 (99%)	1 (1%)	79	88
3	Sf	129/131 (98%)	127 (98%)	2 (2%)	58	77
3	Sg	129/131 (98%)	128 (99%)	1 (1%)	79	88
3	Sh	129/131 (98%)	128 (99%)	1 (1%)	79	88
3	Si	129/131 (98%)	128 (99%)	1 (1%)	79	88
3	Sj	129/131 (98%)	128 (99%)	1 (1%)	79	88
3	Sk	129/131 (98%)	128 (99%)	1 (1%)	79	88
3	Sl	129/131 (98%)	128 (99%)	1 (1%)	79	88
3	Sm	129/131 (98%)	128 (99%)	1 (1%)	79	88
3	Sn	129/131 (98%)	127 (98%)	2 (2%)	58	77
3	So	129/131 (98%)	127 (98%)	2 (2%)	58	77
3	Sp	129/131 (98%)	128 (99%)	1 (1%)	79	88
3	Sq	129/131 (98%)	128 (99%)	1 (1%)	79	88
3	Sr	129/131 (98%)	128 (99%)	1 (1%)	79	88
3	Ss	129/131 (98%)	129 (100%)	0	100	100
3	St	129/131 (98%)	128 (99%)	1 (1%)	79	88
3	Su	129/131 (98%)	128 (99%)	1 (1%)	79	88
3	Sv	129/131 (98%)	128 (99%)	1 (1%)	79	88
3	Sw	129/131 (98%)	128 (99%)	1 (1%)	79	88
3	Sx	129/131 (98%)	129 (100%)	0	100	100
3	Sy	129/131 (98%)	128 (99%)	1 (1%)	79	88
3	Sz	129/131 (98%)	129 (100%)	0	100	100
4	BA	238/239 (100%)	237 (100%)	1 (0%)	89	95
4	BB	238/239 (100%)	237 (100%)	1 (0%)	89	95
4	BC	238/239 (100%)	238 (100%)	0	100	100
All	All	11430/11583 (99%)	11324 (99%)	106 (1%)	74	86

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	PT	119	THR
1	PM	115	ASP
1	PM	119	THR
1	PN	119	THR
1	PP	119	THR
1	PQ	132	ASP
1	PR	119	THR
1	PS	119	THR
1	PU	119	THR
1	PU	129	VAL
1	PU	132	ASP
1	PV	40	THR
1	PV	119	THR
1	PW	115	ASP
1	PW	119	THR
1	PX	119	THR
2	Pa	13	ILE
2	Pa	145	VAL
2	Pb	7	SER
2	Pb	107	LEU
2	Pc	13	ILE
2	Pc	90	THR
2	Pc	145	VAL
2	Pd	69	MET
2	Pd	101	GLN
2	Pd	107	LEU
2	Pe	7	SER
2	Pe	13	ILE
2	Pe	43	GLU
2	Pe	73	VAL
2	Pe	90	THR
2	Pf	7	SER
2	Pf	101	GLN
3	B1	62	ASN
3	B1	115	ARG
3	B2	45	LEU
3	B2	62	ASN
3	B2	115	ARG
3	B4	62	ASN
3	B4	115	ARG
3	B5	127	LEU
3	B6	106	THR

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Mol	Chain	Res	Type
3	AM	155	THR
3	AN	31	VAL
3	AN	32	ARG
3	AO	49	ASP
3	AP	32	ARG
3	SB	115	ARG
3	SA	48	ILE
3	SA	115	ARG
3	SC	115	ARG
3	SD	115	ARG
3	SE	115	ARG
3	SH	106	THR
3	SI	79	GLU
3	SI	115	ARG
3	SM	115	ARG
3	SN	48	ILE
3	SO	115	ARG
3	SP	48	ILE
3	SQ	87	THR
3	SQ	115	ARG
3	SR	48	ILE
3	SR	115	ARG
3	SS	115	ARG
3	ST	87	THR
3	ST	115	ARG
3	SU	115	ARG
3	SV	62	ASN
3	SV	115	ARG
3	SW	125	PRO
3	SX	115	ARG
3	SZ	115	ARG
3	Sa	115	ARG
3	Sb	110	SER
3	Sb	115	ARG
3	Sc	115	ARG
3	Sd	87	THR
3	Sd	115	ARG
3	Se	106	THR
3	Sf	87	THR
3	Sf	115	ARG
3	Sg	106	THR
3	Sh	115	ARG

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Mol	Chain	Res	Type
3	Si	106	THR
3	Sj	115	ARG
3	Sk	106	THR
3	Sl	115	ARG
3	Sm	106	THR
3	Sn	87	THR
3	Sn	115	ARG
3	So	87	THR
3	So	106	THR
3	Sp	115	ARG
3	Sq	115	ARG
3	Sr	115	ARG
3	St	115	ARG
3	Su	115	ARG
3	Sv	115	ARG
3	Sw	115	ARG
3	Sy	79	GLU
3	S1	79	GLU
3	S1	115	ARG
3	S2	115	ARG
4	BA	244	LEU
4	BB	201	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (70) such sidechains are listed below:

Mol	Chain	Res	Type
1	PT	28	GLN
1	PT	95	GLN
1	PN	39	ASN
1	PN	95	GLN
1	PO	95	GLN
1	PS	28	GLN
1	PX	28	GLN
2	Pa	29	GLN
2	Pc	101	GLN
2	Pf	125	ASN
2	Pf	156	ASN
3	B1	61	HIS
3	B1	62	ASN
3	B1	64	ASN
3	B2	62	ASN
3	B2	64	ASN

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Continued from previous page...

Mol	Chain	Res	Type
3	B4	62	ASN
3	B4	64	ASN
3	B6	64	ASN
3	B6	104	ASN
3	AN	104	ASN
3	AO	104	ASN
3	AQ	104	ASN
3	AR	64	ASN
3	SC	104	ASN
3	SF	104	ASN
3	SG	104	ASN
3	SH	62	ASN
3	SH	104	ASN
3	SJ	104	ASN
3	SL	104	ASN
3	SM	42	HIS
3	SQ	42	HIS
3	SQ	151	ASN
3	SS	62	ASN
3	ST	104	ASN
3	SU	64	ASN
3	SV	104	ASN
3	SX	104	ASN
3	SY	104	ASN
3	Sa	104	ASN
3	Se	61	HIS
3	Se	62	ASN
3	Se	64	ASN
3	Sf	42	HIS
3	Sg	62	ASN
3	Sg	64	ASN
3	Si	62	ASN
3	Si	64	ASN
3	Sj	42	HIS
3	Sk	62	ASN
3	Sk	104	ASN
3	Sm	62	ASN
3	Sn	42	HIS
3	Sq	62	ASN
3	Sw	62	ASN
3	Sw	64	ASN
3	Sw	104	ASN

Continued on next page...

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Mol	Chain	Res	Type
3	Sy	104	ASN
3	S1	62	ASN
3	S1	64	ASN
3	S1	104	ASN
4	BA	72	GLN
4	BA	262	GLN
4	BA	264	HIS
4	BB	203	ASN
4	BB	262	GLN
4	BC	59	GLN
4	BC	72	GLN
4	BC	262	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](#)

Of 12 ligands modelled in this entry, 12 are 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

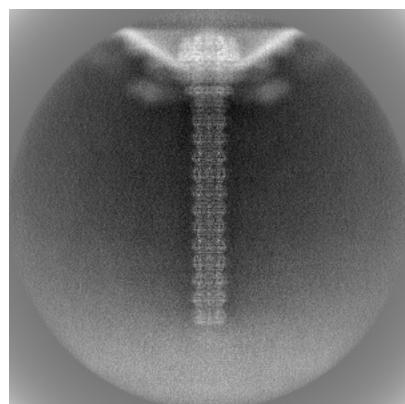
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50521. These allow visual inspection of the internal detail of the map and identification of artifacts.

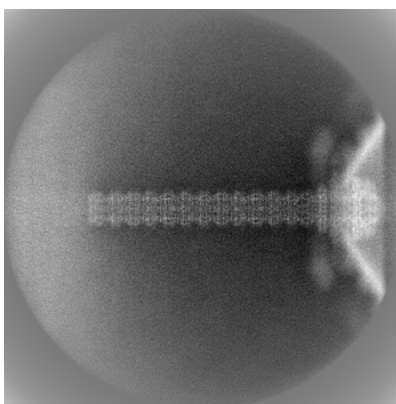
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

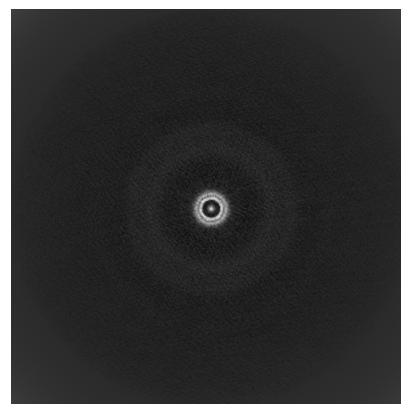
6.1.1 Primary map



X

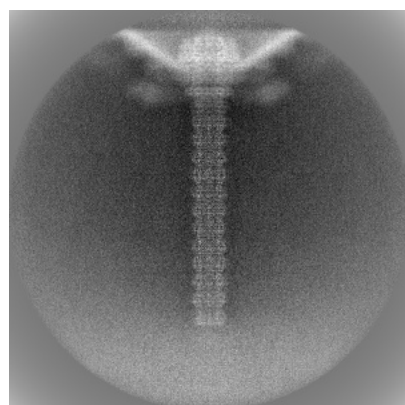


Y

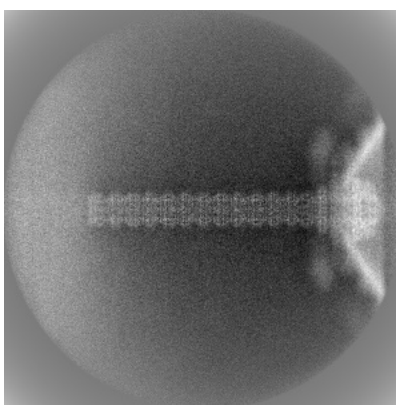


Z

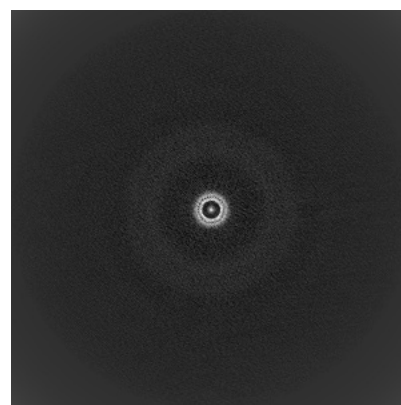
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices [i](#)

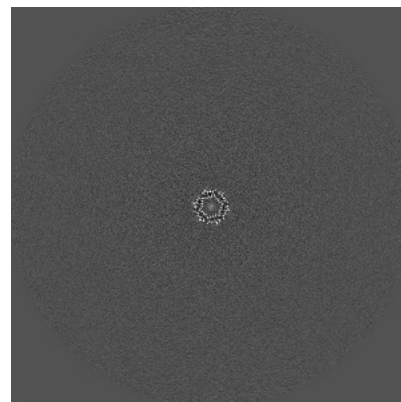
6.2.1 Primary map



X Index: 384

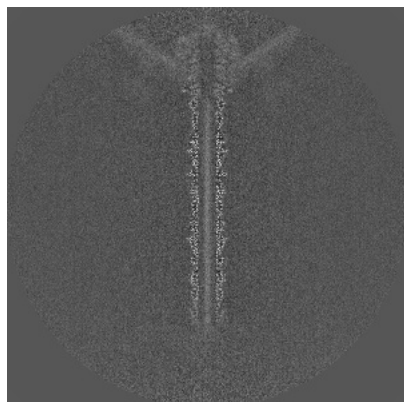


Y Index: 384

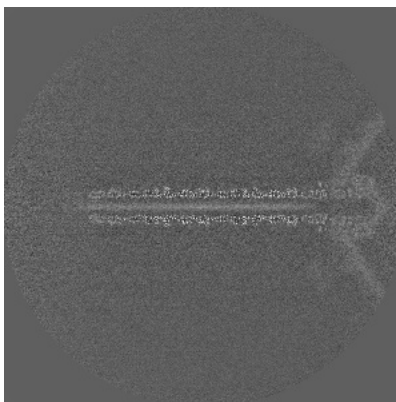


Z Index: 384

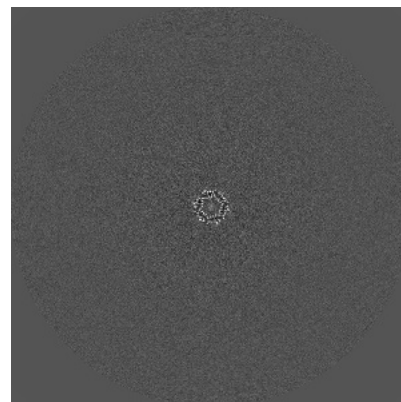
6.2.2 Raw map



X Index: 384



Y Index: 384

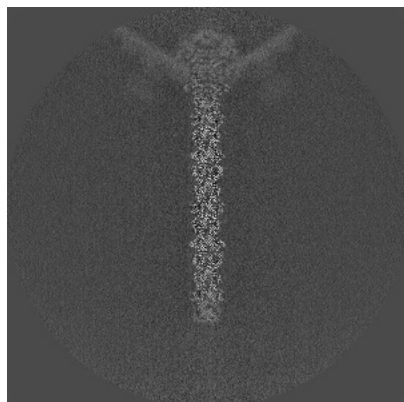


Z Index: 384

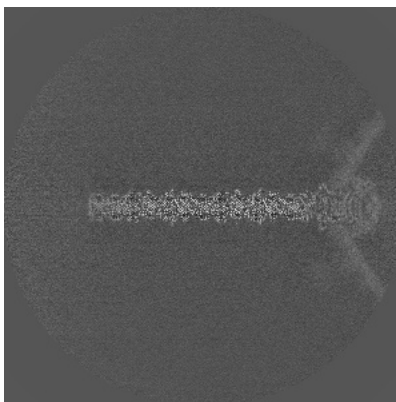
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

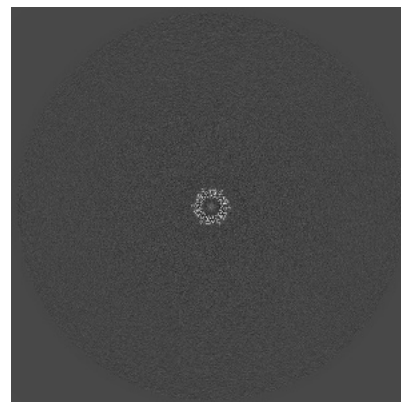
6.3.1 Primary map



X Index: 366

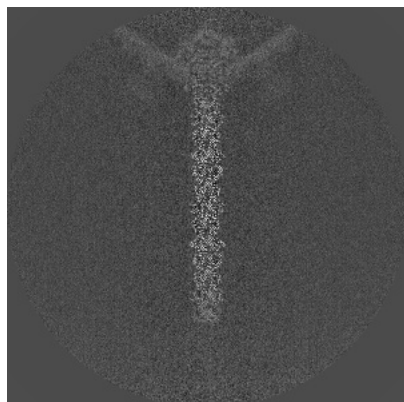


Y Index: 403

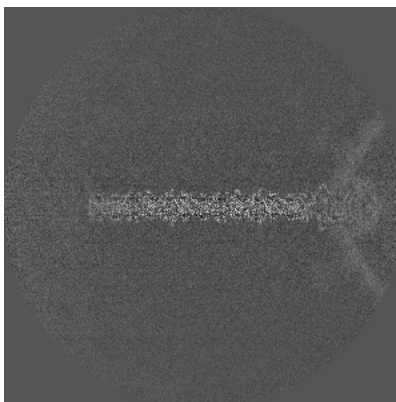


Z Index: 479

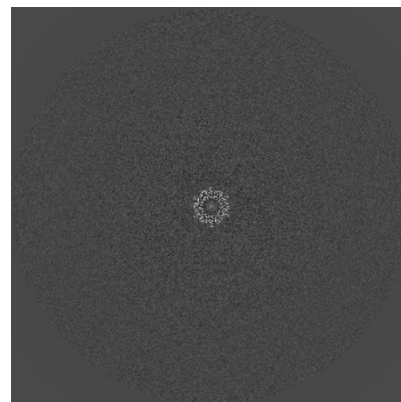
6.3.2 Raw map



X Index: 366



Y Index: 403

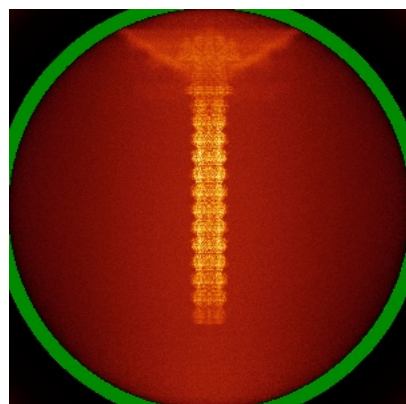


Z Index: 446

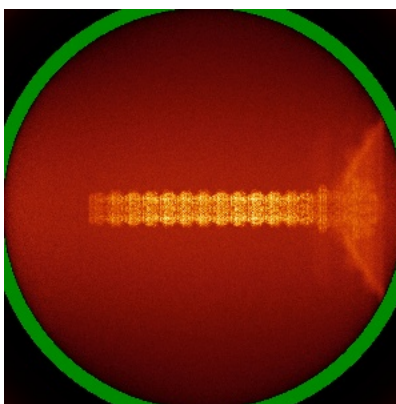
The images above show the largest variance slices of the map in three orthogonal directions.

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

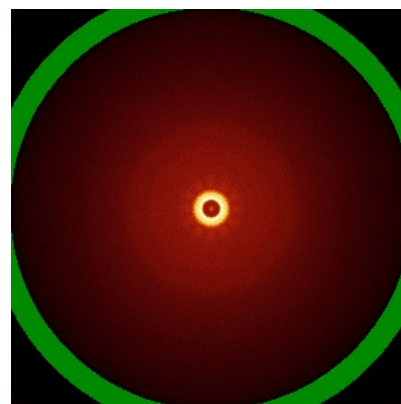
6.4.1 Primary map



X

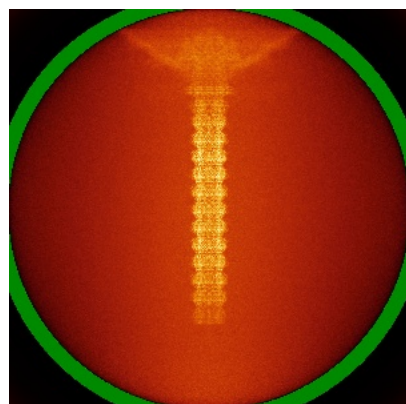


Y

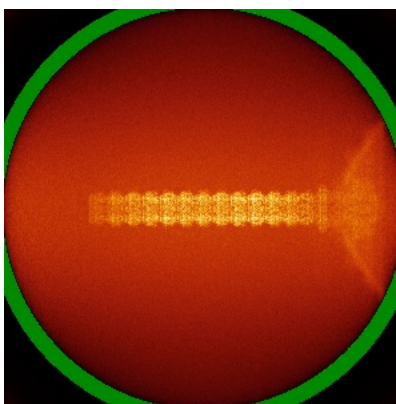


Z

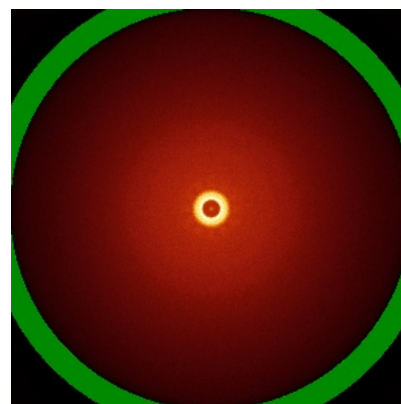
6.4.2 Raw map



X



Y

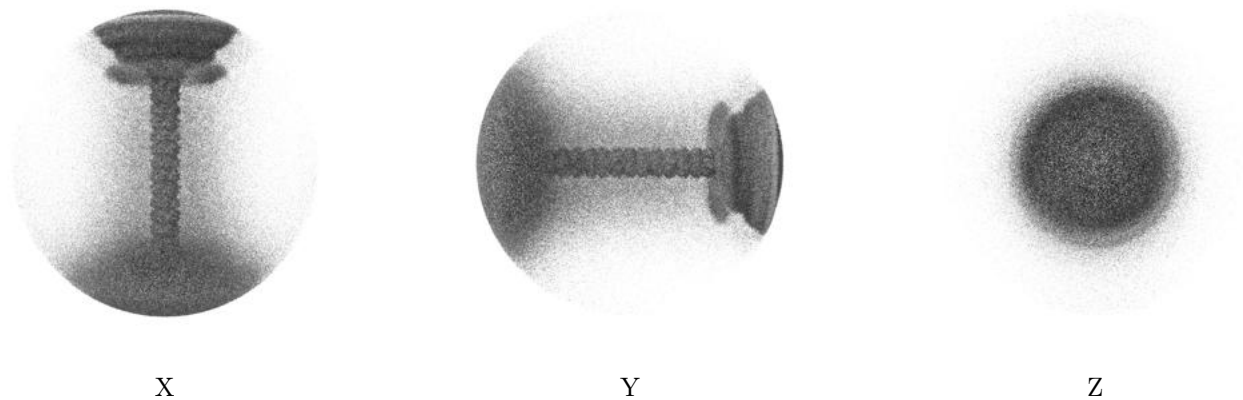


Z

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.

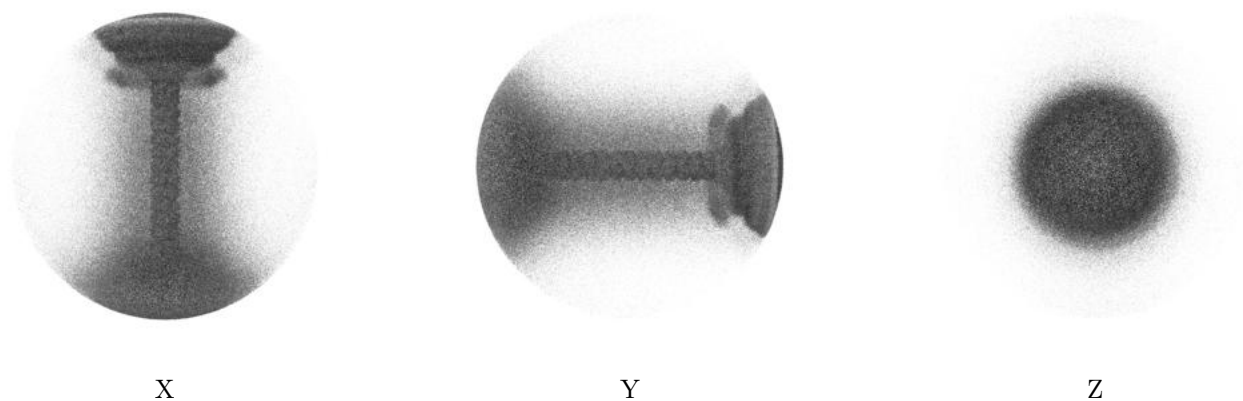
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0062. 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.

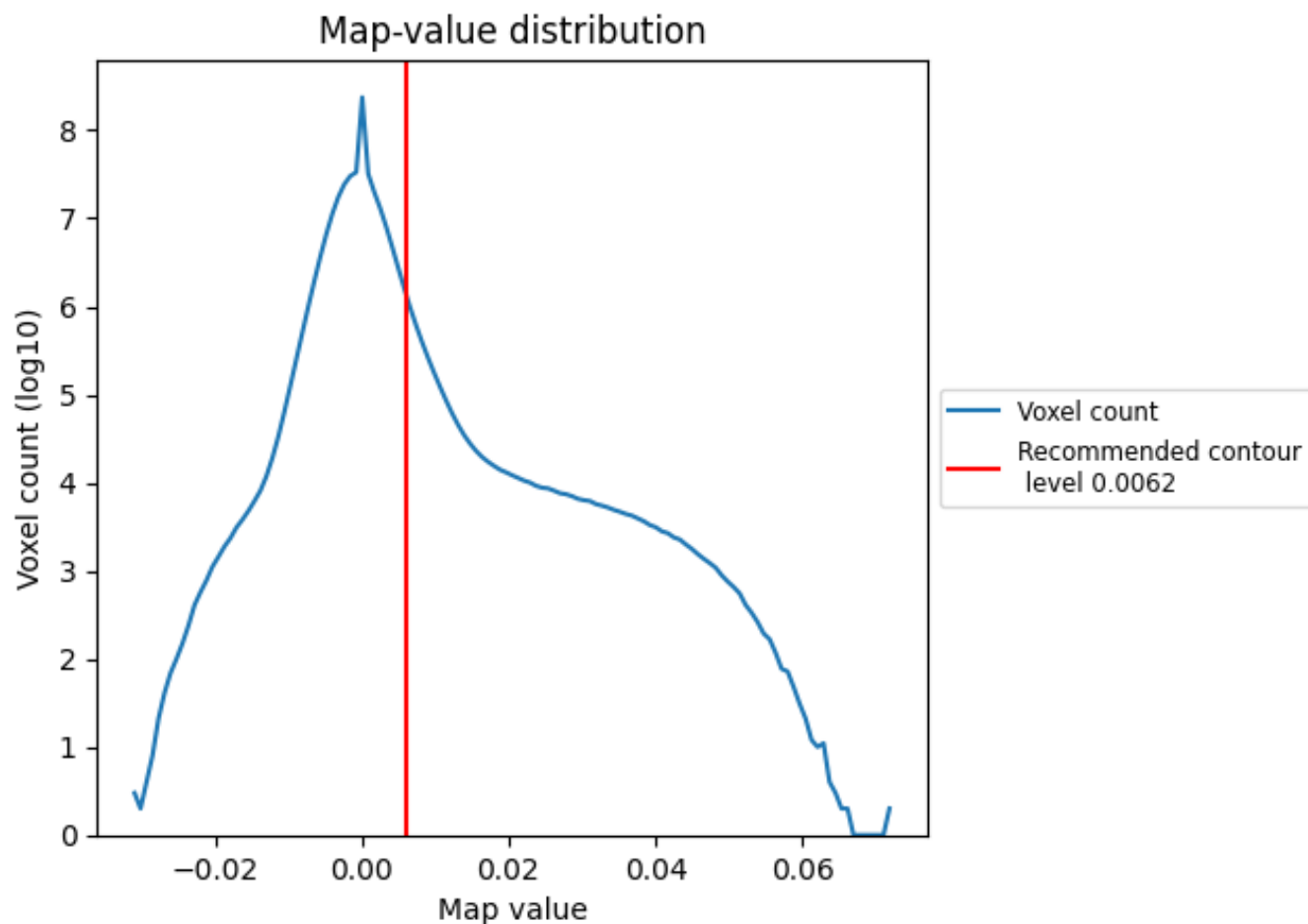
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

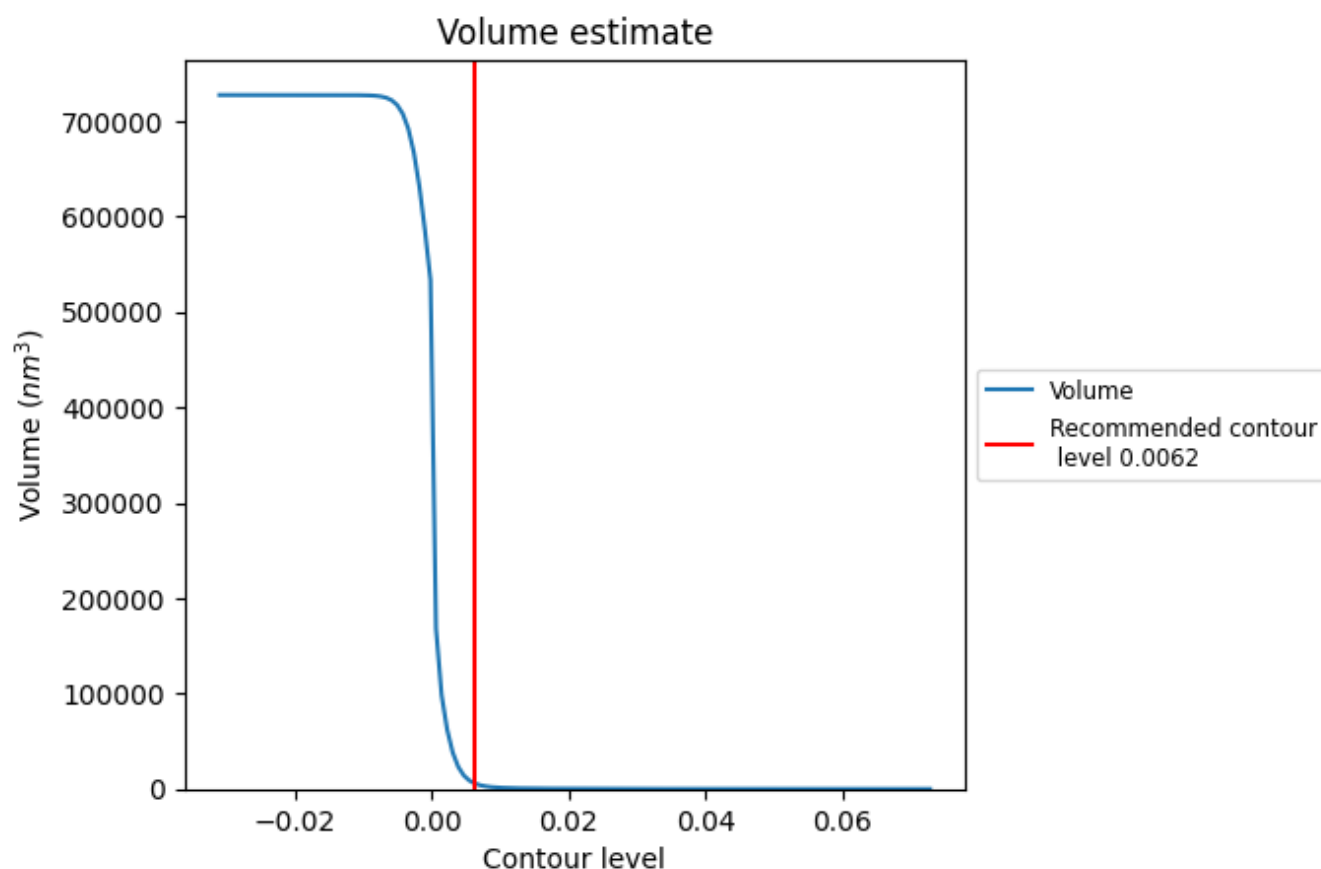
This section contains the results of statistical analysis of the map.

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.

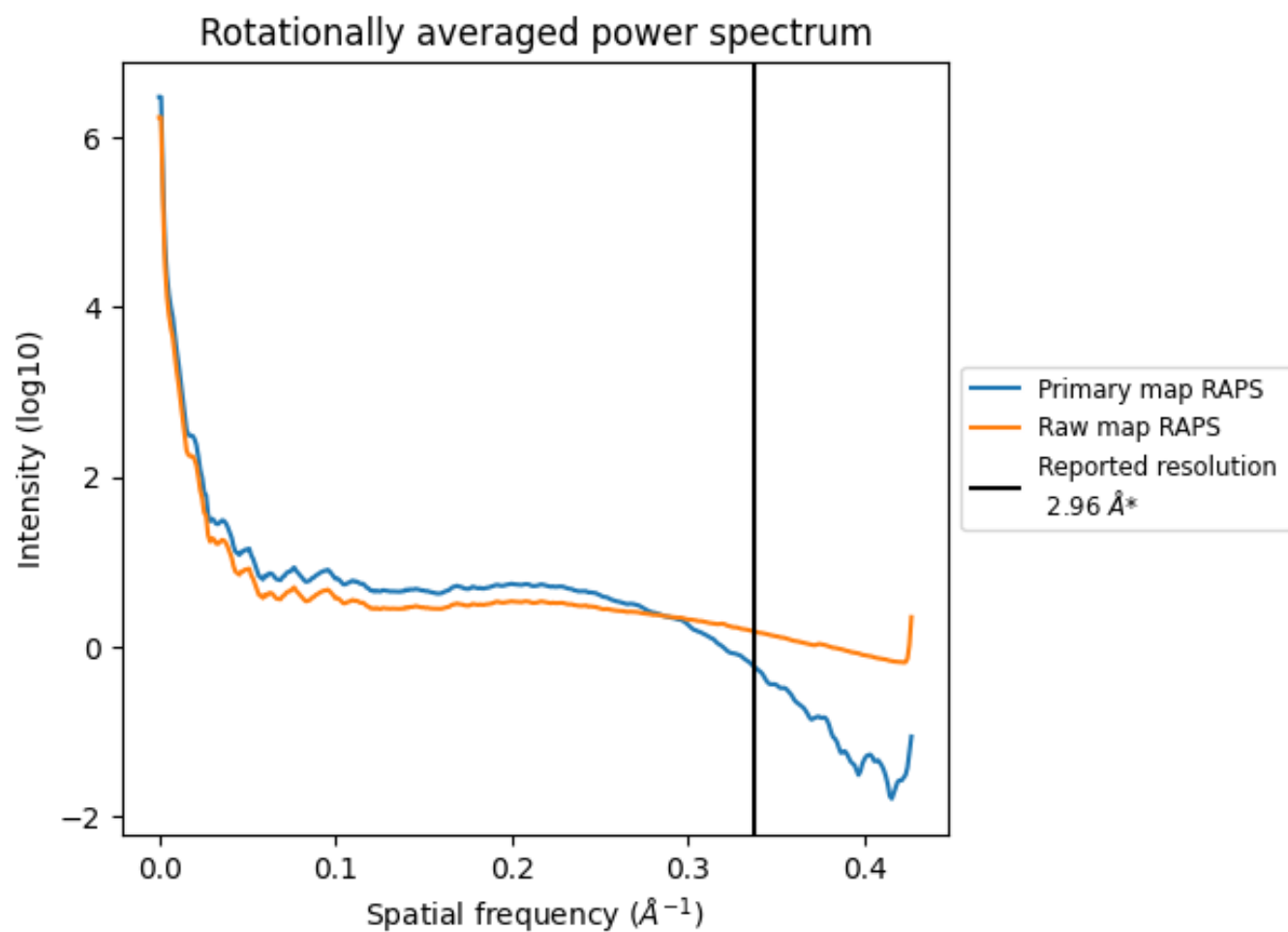
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 6151 nm^3 ; this corresponds to an approximate mass of 5556 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 ⓘ

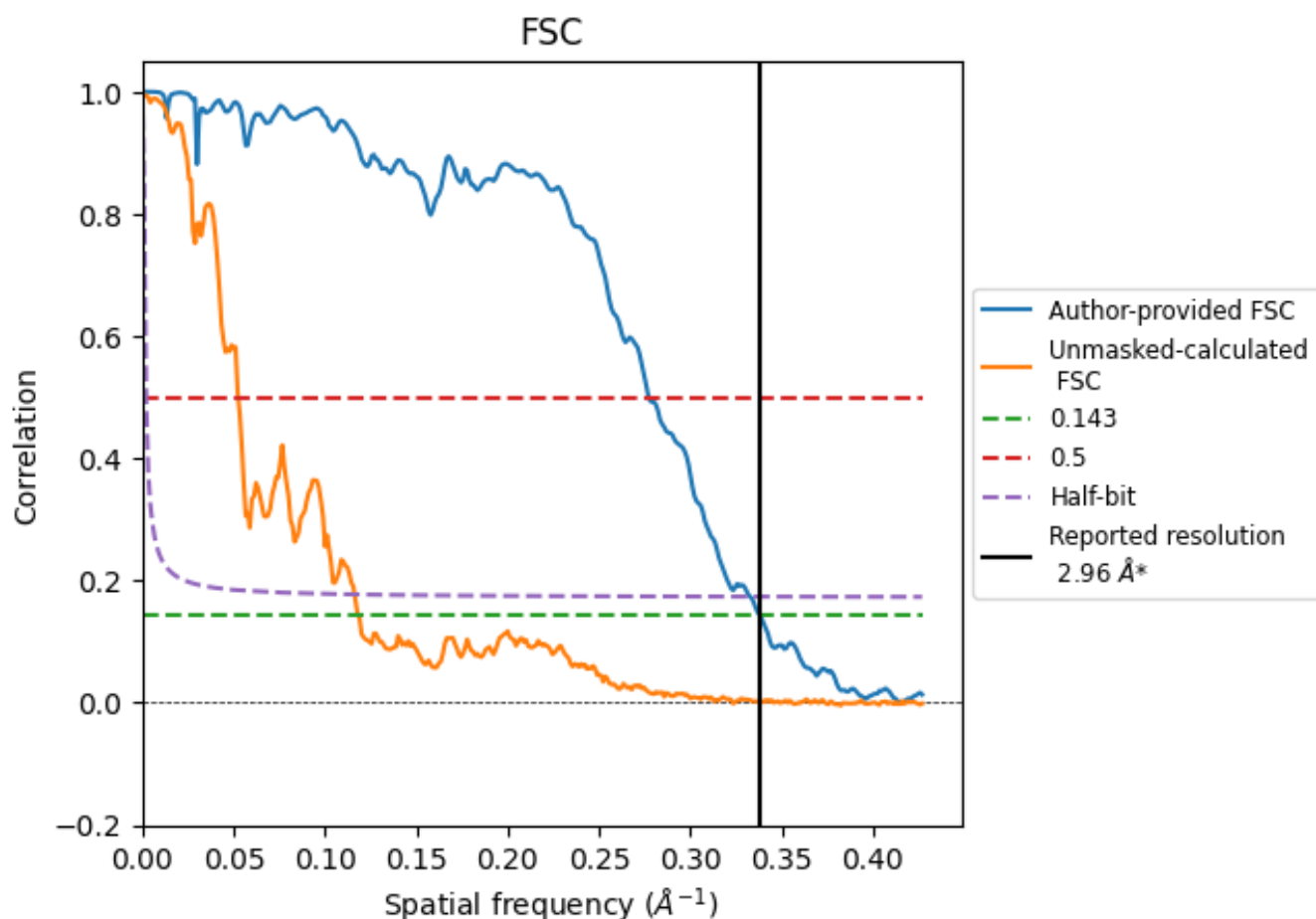


*Reported resolution corresponds to spatial frequency of 0.338 Å⁻¹

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 0.338 Å⁻¹

8.2 Resolution estimates [i](#)

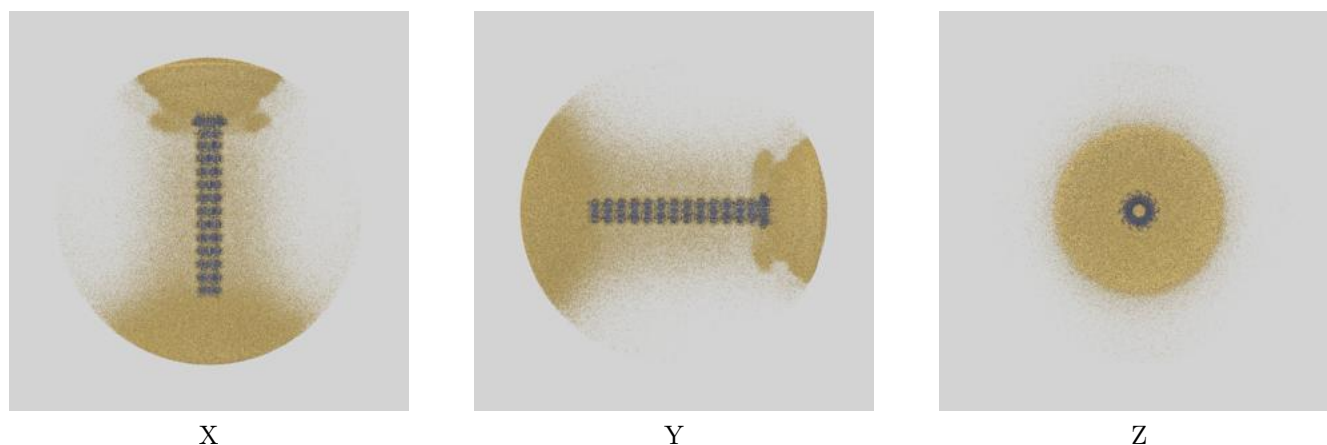
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.96	-	-
Author-provided FSC curve	2.96	3.60	3.01
Unmasked-calculated*	8.46	19.05	8.61

*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 8.46 differs from the reported value 2.96 by more than 10 %

9 Map-model fit [i](#)

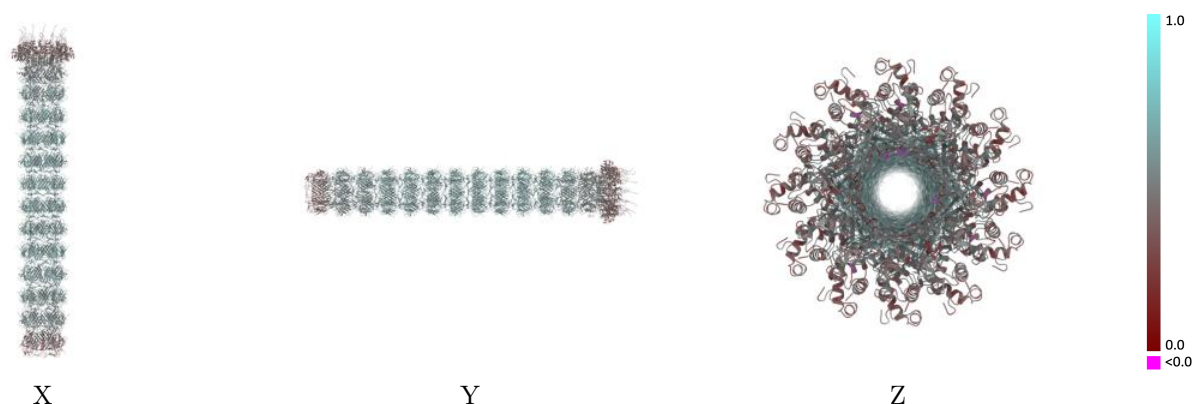
This section contains information regarding the fit between EMDB map EMD-50521 and PDB model 9FKB. Per-residue inclusion information can be found in section 3 on page 13.

9.1 Map-model overlay [i](#)



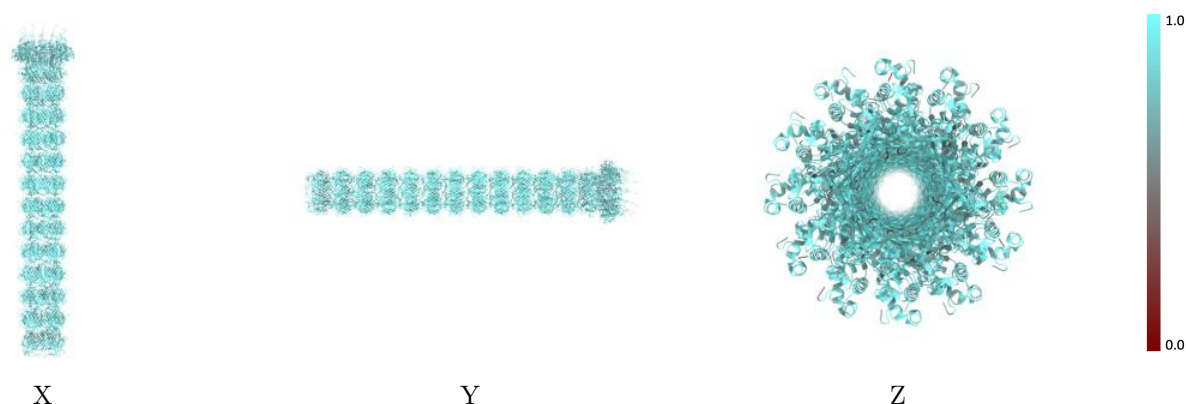
The images above show the 3D surface view of the map at the recommended contour level 0.0062 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



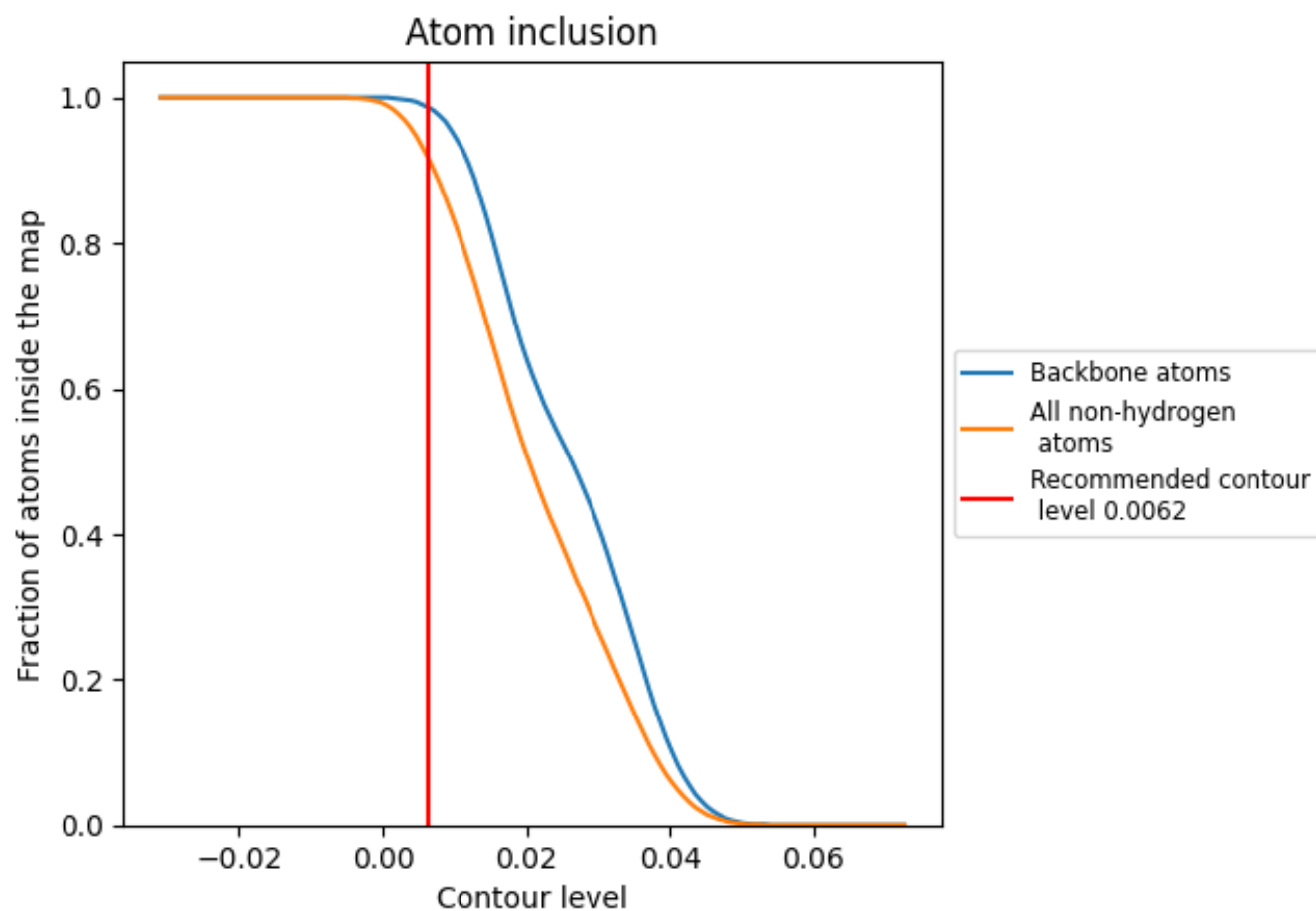
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0062).







































































9.4 Atom inclusion ⓘ



At the recommended contour level, 99% of all backbone atoms, 92% 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 (0.0062) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9200	 0.5290
AM	 0.9390	 0.5520
AN	 0.9370	 0.5520
AO	 0.9380	 0.5520
AP	 0.9380	 0.5530
AQ	 0.9390	 0.5520
AR	 0.9340	 0.5490
B1	 0.9230	 0.5160
B2	 0.9120	 0.5090
B3	 0.9190	 0.5180
B4	 0.9130	 0.5100
B5	 0.9180	 0.5150
B6	 0.9080	 0.5080
BA	 0.8100	 0.3830
BB	 0.8090	 0.3830
BC	 0.8150	 0.3840
PM	 0.8170	 0.4010
PN	 0.8020	 0.4000
PO	 0.8250	 0.4010
PP	 0.8240	 0.3940
PQ	 0.8250	 0.3990
PR	 0.8280	 0.3950
PS	 0.8220	 0.4010
PT	 0.7990	 0.4060
PU	 0.8260	 0.4000
PV	 0.8160	 0.3900
PW	 0.8160	 0.3980
PX	 0.7990	 0.4040
Pa	 0.8980	 0.4970
Pb	 0.9020	 0.4960
Pc	 0.9020	 0.4950
Pd	 0.8960	 0.5040
Pe	 0.8970	 0.4950
Pf	 0.8970	 0.4980
S1	 0.9410	 0.5470

























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Chain	Atom inclusion	Q-score
S2	 0.9370	 0.5440
SA	 0.9540	 0.5720
SB	 0.9470	 0.5720
SC	 0.9540	 0.5740
SD	 0.9520	 0.5720
SE	 0.9520	 0.5710
SF	 0.9520	 0.5760
SG	 0.9620	 0.5850
SH	 0.9570	 0.5830
SI	 0.9620	 0.5830
SJ	 0.9580	 0.5860
SK	 0.9630	 0.5830
SL	 0.9590	 0.5840
SM	 0.9590	 0.5810
SN	 0.9590	 0.5790
SO	 0.9570	 0.5840
SP	 0.9620	 0.5790
SQ	 0.9600	 0.5830
SR	 0.9610	 0.5820
SS	 0.9540	 0.5790
ST	 0.9560	 0.5800
SU	 0.9530	 0.5780
SV	 0.9570	 0.5790
SW	 0.9540	 0.5800
SX	 0.9570	 0.5780
SY	 0.9550	 0.5770
SZ	 0.9530	 0.5740
Sa	 0.9570	 0.5800
Sb	 0.9550	 0.5740
Sc	 0.9580	 0.5790
Sd	 0.9490	 0.5760
Se	 0.9520	 0.5730
Sf	 0.9510	 0.5720
Sg	 0.9490	 0.5740
Sh	 0.9520	 0.5720
Si	 0.9460	 0.5720
Sj	 0.9510	 0.5720
Sk	 0.9530	 0.5720
Sl	 0.9550	 0.5750
Sm	 0.9480	 0.5720
Sn	 0.9520	 0.5730
So	 0.9520	 0.5730

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Chain	Atom inclusion	Q-score
Sp	 0.9580	 0.5750
Sq	 0.9520	 0.5670
Sr	 0.9470	 0.5680
Ss	 0.9490	 0.5650
St	 0.9480	 0.5640
Su	 0.9540	 0.5690
Sv	 0.9480	 0.5660
Sw	 0.9370	 0.5480
Sx	 0.9340	 0.5450
Sy	 0.9360	 0.5480
Sz	 0.9350	 0.5460