



## Full wwPDB EM Validation Report ⓘ

Dec 31, 2024 – 10:45 PM EST

PDB ID : 8QPQ  
EMDB ID : EMD-18559  
Title : C1 turret to capsid interface of full Haloferax tailed virus 1 adjacent to the portal-capsid interface.  
Authors : Zhang, D.; Daum, B.; Isupov, M.N.; McLaren, M.  
Deposited on : 2023-10-02  
Resolution : 2.70 Å(reported)  
Based on initial model : .

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev113  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.40

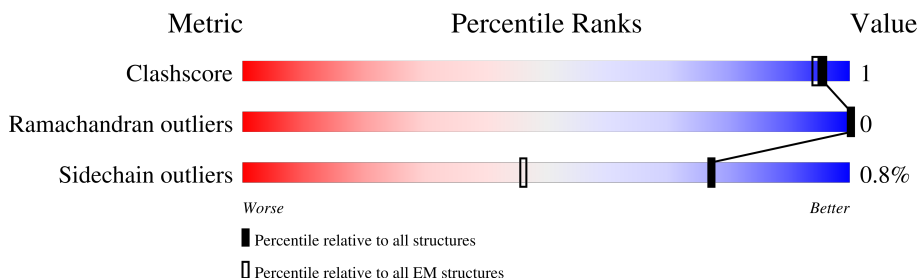
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.70 Å.

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



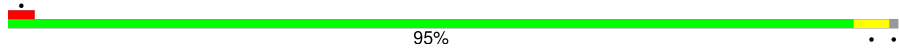

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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  $\geq 3$ , 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	TA	413	<div> <div>46%</div> <div>98%</div> </div>
1	TB	413	<div> <div>46%</div> <div>97%</div> </div>
1	TC	413	<div> <div>45%</div> <div>96%</div> </div>
2	TD	115	<div> <div>97%</div> </div>
2	TE	115	<div> <div>97%</div> </div>
2	TF	115	<div> <div>5%</div> <div>97%</div> </div>
2	TG	115	<div> <div>97%</div> </div>
2	TH	115	<div> <div>97%</div> </div>

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Mol	Chain	Length	Quality of chain
2	TI	115	 95%
3	LA	396	 71%25%
3	LB	396	 70%5%25%
3	LC	396	 71%25%
3	LD	396	 71%25%
3	LE	396	 72%25%
3	LF	396	 69%29%

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 28263 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 Prokaryotic polysaccharide deacetylase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	TC	412	Total	C	N	O	S	0	0
			3176	1959	545	664	8		
1	TA	412	Total	C	N	O	S	0	0
			3176	1959	545	664	8		
1	TB	412	Total	C	N	O	S	0	0
			3176	1959	545	664	8		

- Molecule 2 is a protein called gp30.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	TD	114	Total	C	N	O	P	0	0
			833	503	136	193	1		
2	TE	114	Total	C	N	O	P	0	0
			833	503	136	193	1		
2	TF	114	Total	C	N	O	P	0	0
			833	503	136	193	1		
2	TG	114	Total	C	N	O	P	0	0
			833	503	136	193	1		
2	TH	114	Total	C	N	O	P	0	0
			833	503	136	193	1		
2	TI	114	Total	C	N	O	P	0	0
			833	503	136	193	1		

- Molecule 3 is a protein called HK97 gp5-like major capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	LA	296	Total	C	N	O	S	0	0
			2298	1398	409	485	6		
3	LB	296	Total	C	N	O	S	0	0
			2298	1398	409	485	6		
3	LF	283	Total	C	N	O	S	0	0
			2194	1329	396	463	6		
3	LE	296	Total	C	N	O	S	0	0
			2298	1398	409	485	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	LD	296	Total	C	N	O	S	0	0
			2298	1398	409	485	6		
3	LC	296	Total	C	N	O	S	0	0
			2298	1398	409	485	6		

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
4	TC	1	Total	Zn	0
			1	1	
4	TA	1	Total	Zn	0
			1	1	
4	TB	1	Total	Zn	0
			1	1	

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

Mol	Chain	Residues	Atoms		AltConf
5	TC	1	Total	Mg	0
			1	1	
5	TD	2	Total	Mg	0
			2	2	
5	TE	2	Total	Mg	0
			2	2	
5	TF	2	Total	Mg	0
			2	2	
5	TG	2	Total	Mg	0
			2	2	
5	TH	2	Total	Mg	0
			2	2	
5	TI	2	Total	Mg	0
			2	2	
5	TA	1	Total	Mg	0
			1	1	
5	TB	1	Total	Mg	0
			1	1	
5	LA	7	Total	Mg	0
			7	7	
5	LB	6	Total	Mg	0
			6	6	

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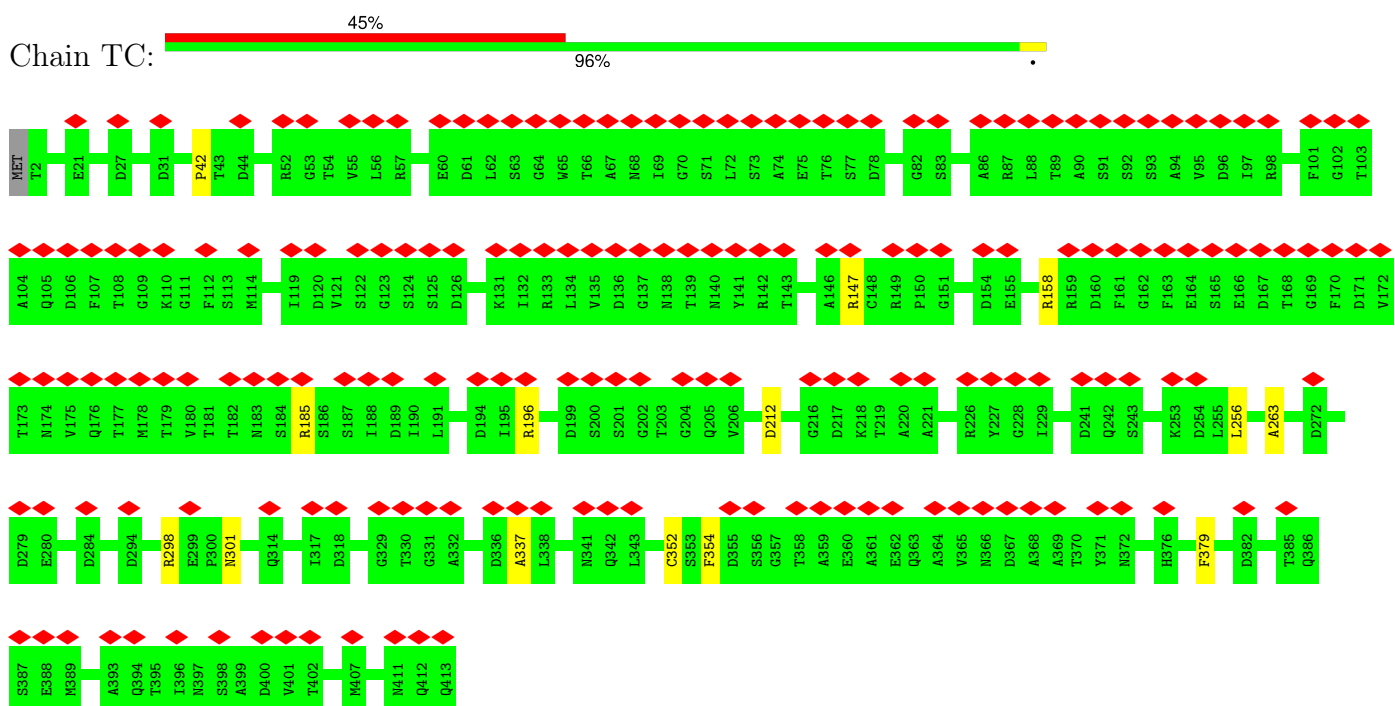
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Mol	Chain	Residues	Atoms		AltConf
5	LF	5	Total 5	Mg 5	0
5	LE	5	Total 5	Mg 5	0
5	LD	6	Total 6	Mg 6	0
5	LC	6	Total 6	Mg 6	0

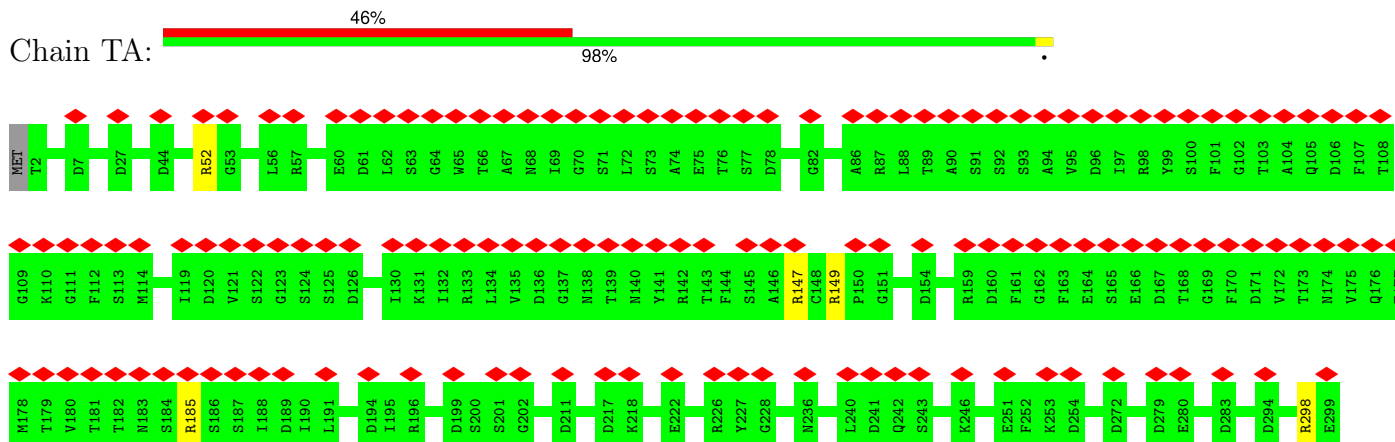
### 3 Residue-property plots

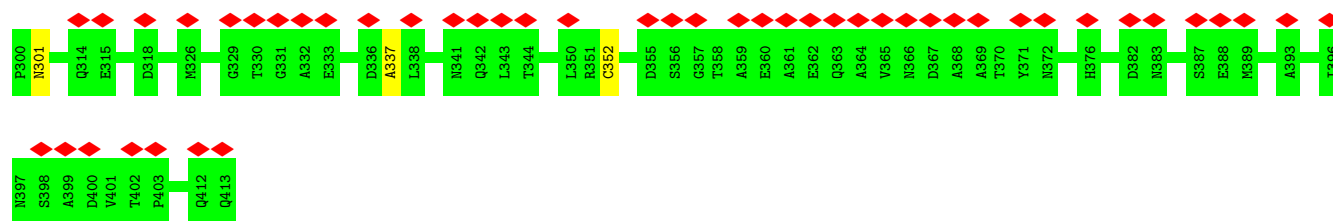
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

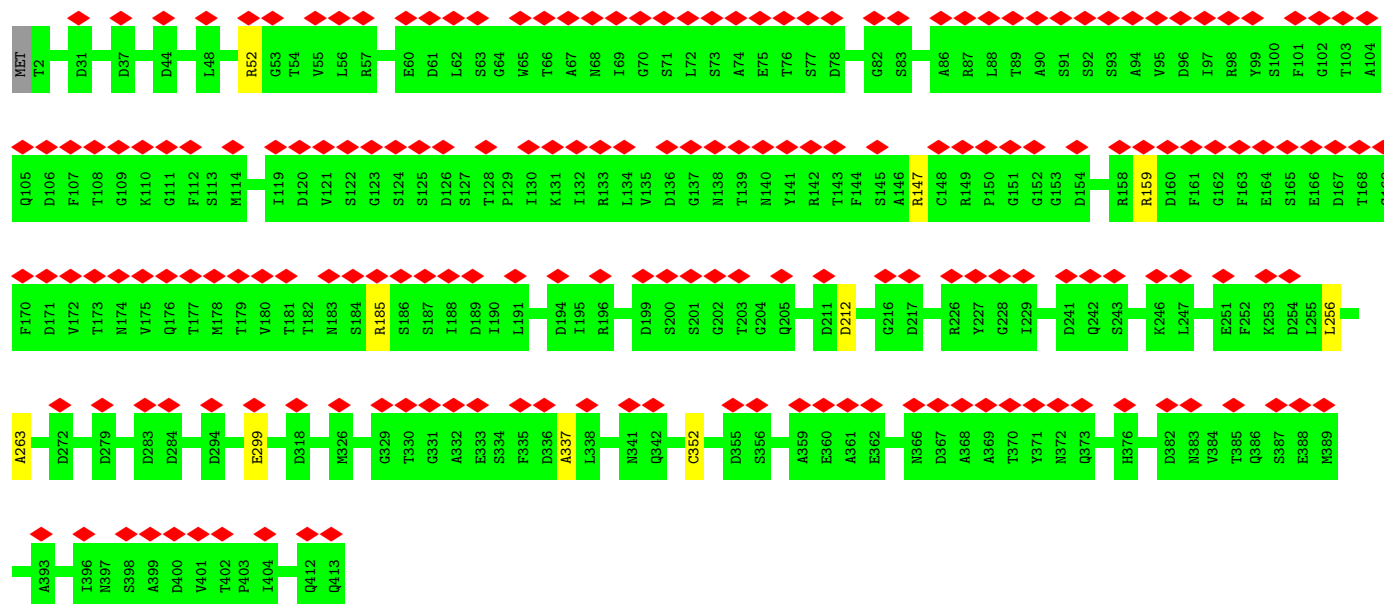


- Molecule 1: Prokaryotic polysaccharide deacetylase

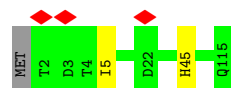




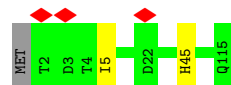
- Molecule 1: Prokaryotic polysaccharide deacetylase



- Molecule 2: gp30



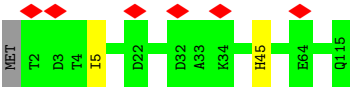
- Molecule 2: gp30



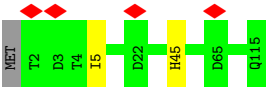
- Molecule 2: gp30



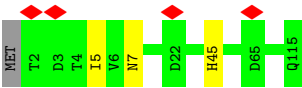




• Molecule 2: gp30



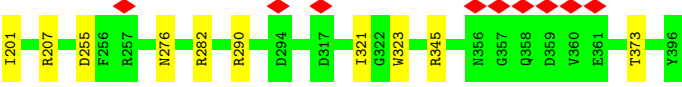
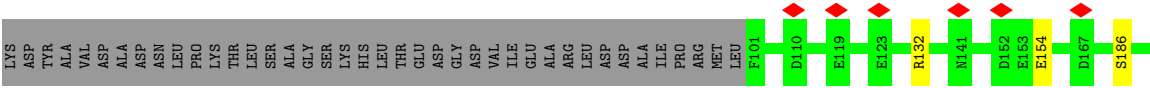
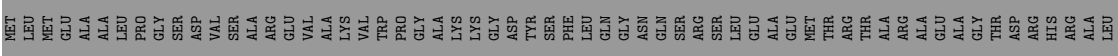
• Molecule 2: gp30



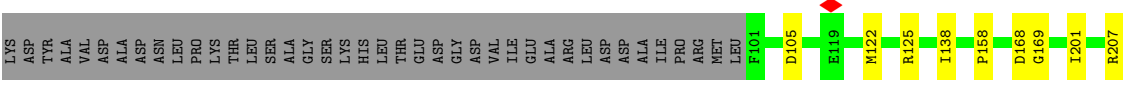
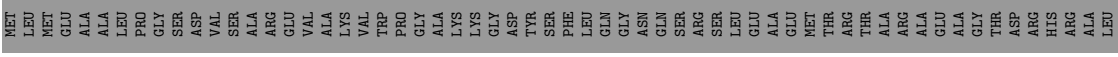
• Molecule 2: gp30



• Molecule 3: HK97 gp5-like major capsid protein



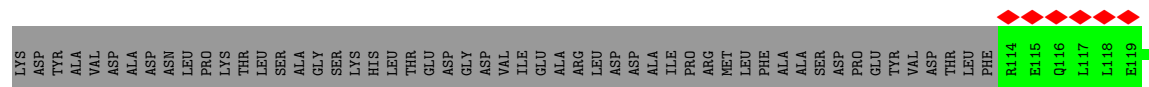
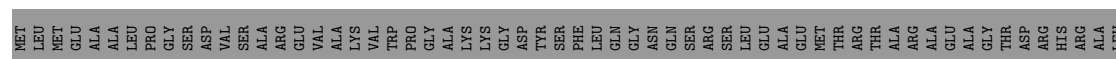
• Molecule 3: HK97 gp5-like major capsid protein





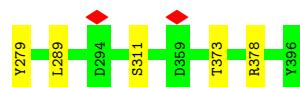
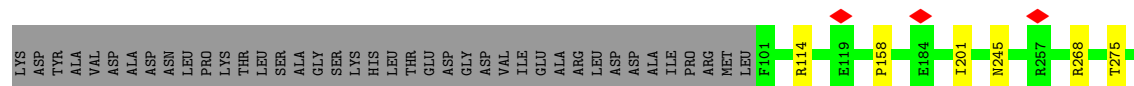
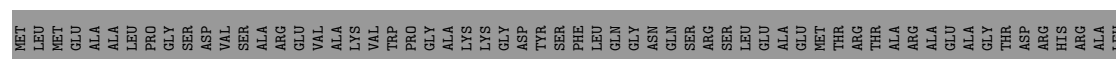
- Molecule 3: HK97 gp5-like major capsid protein

Chain LF: 69% 29%



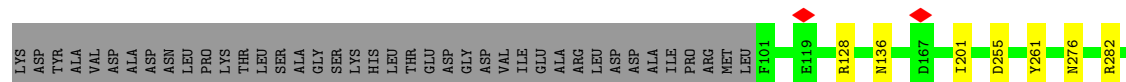
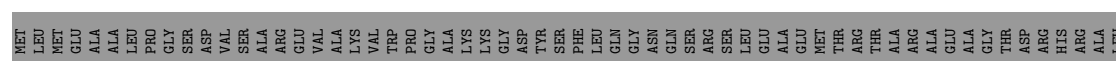
- Molecule 3: HK97 gp5-like major capsid protein

Chain LE: 72% 25%



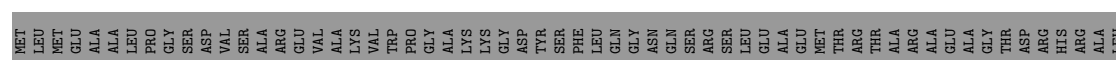
- Molecule 3: HK97 gp5-like major capsid protein

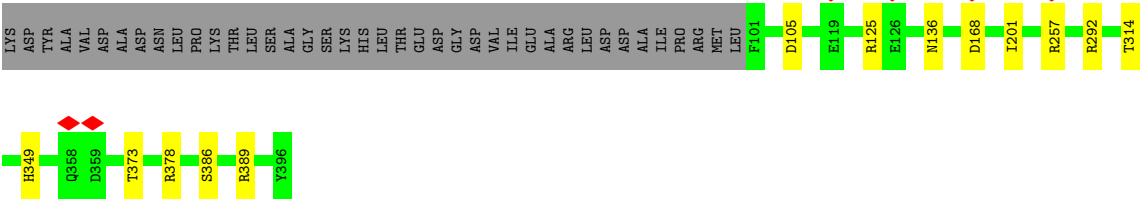
Chain LD: 71% 25%



- Molecule 3: HK97 gp5-like major capsid protein

Chain LC: 71% 25%





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	102012	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 ( $e^-/\text{\AA}^2$ )	54.6	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	0.087	Depositor
Minimum map value	-0.039	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.024	Depositor
Map size (Å)	299.776, 299.776, 299.776	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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: NEP, ZN, 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	TA	0.37	0/3238	0.78	4/4402 (0.1%)
1	TB	0.37	0/3238	0.78	5/4402 (0.1%)
1	TC	0.36	0/3238	0.78	4/4402 (0.1%)
2	TD	0.41	0/824	0.76	0/1119
2	TE	0.42	0/824	0.74	0/1119
2	TF	0.43	0/824	0.74	0/1119
2	TG	0.45	0/824	0.75	0/1119
2	TH	0.45	0/824	0.75	0/1119
2	TI	0.48	1/824 (0.1%)	0.84	2/1119 (0.2%)
3	LA	0.48	0/2335	0.89	4/3172 (0.1%)
3	LB	0.47	0/2335	0.89	0/3172
3	LC	0.44	0/2335	0.89	1/3172 (0.0%)
3	LD	0.46	0/2335	0.90	4/3172 (0.1%)
3	LE	0.43	0/2335	0.86	2/3172 (0.1%)
3	LF	0.45	0/2227	0.92	0/3023
All	All	0.42	1/28560 (0.0%)	0.83	26/38803 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	TA	0	1
1	TC	0	1
3	LF	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	TI	39	GLU	CD-OE1	-5.21	1.20	1.25

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	TI	93	TYR	CB-CG-CD1	-7.26	116.64	121.00
1	TC	158	ARG	NE-CZ-NH2	7.15	123.88	120.30
3	LC	389	ARG	NE-CZ-NH1	-7.13	116.73	120.30
2	TI	93	TYR	CB-CG-CD2	6.77	125.06	121.00
3	LA	282	ARG	CG-CD-NE	6.67	125.81	111.80
3	LE	114	ARG	CG-CD-NE	6.64	125.75	111.80
3	LA	132	ARG	NE-CZ-NH1	-6.33	117.14	120.30
1	TB	147	ARG	NE-CZ-NH2	6.08	123.34	120.30
3	LD	282	ARG	CG-CD-NE	6.08	124.56	111.80
1	TB	212	ASP	CB-CG-OD2	5.74	123.47	118.30
1	TC	212	ASP	CB-CG-OD2	5.71	123.44	118.30
1	TC	196	ARG	NE-CZ-NH1	-5.70	117.45	120.30
1	TB	52	ARG	NE-CZ-NH1	-5.67	117.47	120.30
1	TB	159	ARG	NE-CZ-NH2	5.62	123.11	120.30
1	TA	149	ARG	CG-CD-NE	5.46	123.26	111.80
1	TA	52	ARG	NE-CZ-NH1	-5.17	117.71	120.30
3	LA	345	ARG	NE-CZ-NH1	-5.15	117.72	120.30
1	TA	147	ARG	NE-CZ-NH1	-5.15	117.73	120.30
3	LD	378	ARG	NE-CZ-NH2	5.15	122.87	120.30
1	TA	147	ARG	NE-CZ-NH2	5.13	122.86	120.30
1	TB	147	ARG	NE-CZ-NH1	-5.10	117.75	120.30
3	LD	285	THR	CA-CB-CG2	5.09	119.53	112.40
3	LA	290	ARG	NE-CZ-NH1	-5.08	117.76	120.30
3	LD	128	ARG	NE-CZ-NH2	5.04	122.82	120.30
1	TC	147	ARG	NE-CZ-NH1	-5.02	117.79	120.30
3	LE	268	ARG	CG-CD-NE	5.02	122.35	111.80

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	LF	369	ILE	Peptide
1	TA	298	ARG	Peptide
1	TC	298	ARG	Peptide

## 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	TA	3176	0	2976	1	0
1	TB	3176	0	2976	4	0
1	TC	3176	0	2976	5	0
2	TD	833	0	777	2	0
2	TE	833	0	777	4	0
2	TF	833	0	777	2	0
2	TG	833	0	777	1	0
2	TH	833	0	777	3	0
2	TI	833	0	777	2	0
3	LA	2298	0	2139	8	0
3	LB	2298	0	2139	13	0
3	LC	2298	0	2139	6	0
3	LD	2298	0	2139	9	0
3	LE	2298	0	2139	4	0
3	LF	2194	0	2049	3	0
4	TA	1	0	0	0	0
4	TB	1	0	0	0	0
4	TC	1	0	0	0	0
5	LA	7	0	0	0	0
5	LB	6	0	0	0	0
5	LC	6	0	0	0	0
5	LD	6	0	0	0	0
5	LE	5	0	0	0	0
5	LF	5	0	0	0	0
5	TA	1	0	0	0	0
5	TB	1	0	0	0	0
5	TC	1	0	0	0	0
5	TD	2	0	0	0	0
5	TE	2	0	0	0	0
5	TF	2	0	0	0	0
5	TG	2	0	0	0	0
5	TH	2	0	0	0	0
5	TI	2	0	0	0	0
All	All	28263	0	26334	48	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 (48) 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:LB:285:THR:HG22	3:LB:297:ILE:HD12	1.61	0.81
3:LE:245:ASN:OD1	3:LD:292:ARG:NH2	2.18	0.77
3:LB:285:THR:CG2	3:LB:297:ILE:HD12	2.17	0.72
3:LB:122:MET:HE3	3:LC:386:SER:HB3	1.70	0.71
3:LE:275:THR:HG23	3:LE:279:TYR:CE2	2.42	0.54
3:LA:201:ILE:HD11	3:LA:373:THR:HG21	1.91	0.53
3:LD:136:ASN:HD22	3:LD:349:HIS:CD2	2.27	0.52
3:LD:261:TYR:CE1	3:LD:301:ILE:HD11	2.45	0.52
3:LD:287:GLU:HG2	3:LD:296:PRO:HD2	1.92	0.52
3:LB:138:ILE:N	3:LB:138:ILE:HD12	2.24	0.51
1:TC:337:ALA:HB2	1:TC:352:CYS:HB2	1.93	0.51
3:LD:255:ASP:HB2	3:LC:125:ARG:HG3	1.93	0.49
3:LD:255:ASP:HB2	3:LC:125:ARG:CG	2.43	0.49
3:LB:321:ILE:HD12	3:LB:321:ILE:H	1.78	0.48
3:LD:261:TYR:CZ	3:LD:301:ILE:HD11	2.49	0.47
3:LA:154:GLU:OE1	3:LF:207:ARG:NH1	2.48	0.47
1:TC:337:ALA:HB2	1:TC:352:CYS:CB	2.44	0.47
3:LB:207:ARG:NH2	3:LC:168:ASP:O	2.47	0.46
3:LE:158:PRO:HD3	3:LD:323:TRP:CE2	2.51	0.46
2:TH:7:ASN:ND2	2:TI:7:ASN:HD21	2.15	0.45
2:TE:5:ILE:HG21	2:TF:5:ILE:HD12	1.98	0.45
2:TE:5:ILE:HD13	2:TF:5:ILE:HD12	1.99	0.44
2:TG:5:ILE:HG21	2:TH:5:ILE:HD12	1.99	0.44
3:LA:207:ARG:NH2	3:LB:168:ASP:O	2.48	0.44
3:LA:323:TRP:CE2	3:LB:158:PRO:HD3	2.52	0.44
3:LE:201:ILE:HD11	3:LE:373:THR:HG21	2.00	0.44
3:LA:255:ASP:HB2	3:LF:125:ARG:HG3	2.00	0.43
1:TB:337:ALA:HB2	1:TB:352:CYS:HB2	1.99	0.43
3:LF:136:ASN:HD22	3:LF:349:HIS:CD2	2.37	0.43
3:LA:201:ILE:CD1	3:LA:373:THR:HG21	2.49	0.43
3:LC:136:ASN:HD22	3:LC:349:HIS:CD2	2.37	0.43
2:TD:5:ILE:HG21	2:TE:5:ILE:HD12	2.01	0.42
2:TH:5:ILE:HG21	2:TI:5:ILE:HD12	2.00	0.42
1:TC:256:LEU:HD21	1:TC:263:ALA:HB2	2.00	0.42
3:LB:285:THR:HG22	3:LB:297:ILE:CD1	2.41	0.42
1:TC:354:PHE:CZ	1:TC:379:PHE:CD1	3.08	0.41
1:TB:337:ALA:HB2	1:TB:352:CYS:CB	2.50	0.41
3:LB:201:ILE:HD11	3:LB:373:THR:HG21	2.02	0.41
3:LA:321:ILE:N	3:LA:321:ILE:HD12	2.36	0.41
1:TB:256:LEU:HD21	1:TB:263:ALA:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:TC:42:PRO:HB2	1:TB:299:GLU:HB2	2.03	0.41
2:TD:5:ILE:HD13	2:TE:5:ILE:HD12	2.02	0.41
1:TA:337:ALA:HB2	1:TA:352:CYS:HB2	2.02	0.41
3:LC:201:ILE:HD11	3:LC:373:THR:HG21	2.02	0.41
3:LA:186:SER:HB3	3:LB:169:GLY:HA2	2.02	0.40
3:LD:201:ILE:HD11	3:LD:373:THR:HG21	2.03	0.40
3:LB:262:VAL:HG13	3:LB:310:MET:HG3	2.03	0.40
3:LB:125:ARG:HH11	3:LB:313:ALA:CB	2.35	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	TA	410/413 (99%)	393 (96%)	17 (4%)	0	100	100
1	TB	410/413 (99%)	396 (97%)	14 (3%)	0	100	100
1	TC	410/413 (99%)	395 (96%)	15 (4%)	0	100	100
2	TD	111/115 (96%)	108 (97%)	3 (3%)	0	100	100
2	TE	111/115 (96%)	108 (97%)	3 (3%)	0	100	100
2	TF	111/115 (96%)	108 (97%)	3 (3%)	0	100	100
2	TG	111/115 (96%)	108 (97%)	3 (3%)	0	100	100
2	TH	111/115 (96%)	107 (96%)	4 (4%)	0	100	100
2	TI	111/115 (96%)	108 (97%)	3 (3%)	0	100	100
3	LA	294/396 (74%)	284 (97%)	10 (3%)	0	100	100
3	LB	294/396 (74%)	282 (96%)	12 (4%)	0	100	100
3	LC	294/396 (74%)	281 (96%)	13 (4%)	0	100	100
3	LD	294/396 (74%)	282 (96%)	12 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	LE	294/396 (74%)	283 (96%)	11 (4%)	0	100	100
3	LF	281/396 (71%)	270 (96%)	11 (4%)	0	100	100
All	All	3647/4305 (85%)	3513 (96%)	134 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	TA	348/349 (100%)	346 (99%)	2 (1%)	84	94
1	TB	348/349 (100%)	347 (100%)	1 (0%)	91	97
1	TC	348/349 (100%)	346 (99%)	2 (1%)	84	94
2	TD	91/92 (99%)	91 (100%)	0	100	100
2	TE	91/92 (99%)	91 (100%)	0	100	100
2	TF	91/92 (99%)	91 (100%)	0	100	100
2	TG	91/92 (99%)	91 (100%)	0	100	100
2	TH	91/92 (99%)	91 (100%)	0	100	100
2	TI	91/92 (99%)	91 (100%)	0	100	100
3	LA	244/322 (76%)	243 (100%)	1 (0%)	89	96
3	LB	244/322 (76%)	239 (98%)	5 (2%)	50	78
3	LC	244/322 (76%)	239 (98%)	5 (2%)	50	78
3	LD	244/322 (76%)	242 (99%)	2 (1%)	79	91
3	LE	244/322 (76%)	241 (99%)	3 (1%)	67	86
3	LF	233/322 (72%)	230 (99%)	3 (1%)	65	85
All	All	3043/3531 (86%)	3019 (99%)	24 (1%)	77	91

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	TC	185	ARG
1	TC	301	ASN
1	TA	185	ARG
1	TA	301	ASN
1	TB	185	ARG
3	LA	276	ASN
3	LB	105	ASP
3	LB	257	ARG
3	LB	275	THR
3	LB	293	GLU
3	LB	378	ARG
3	LF	144	VAL
3	LF	200	LEU
3	LF	378	ARG
3	LE	289	LEU
3	LE	311	SER
3	LE	378	ARG
3	LD	276	ASN
3	LD	378	ARG
3	LC	105	ASP
3	LC	257	ARG
3	LC	292	ARG
3	LC	314	THR
3	LC	378	ARG

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

Mol	Chain	Res	Type
1	TC	47	GLN
1	TC	183	ASN
1	TC	324	HIS
2	TD	7	ASN
2	TE	7	ASN
2	TF	7	ASN
2	TG	7	ASN
2	TH	7	ASN
1	TA	183	ASN
1	TA	324	HIS
1	TB	183	ASN
1	TB	301	ASN
1	TB	324	HIS
3	LA	380	HIS
3	LB	161	GLN

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Mol	Chain	Res	Type
3	LD	136	ASN
3	LD	349	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

6 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NEP	TE	45	2	11,14,15	1.24	2 (18%)	4,20,22	1.36	1 (25%)
2	NEP	TF	45	2	11,14,15	1.29	2 (18%)	4,20,22	1.10	0
2	NEP	TI	45	2	11,14,15	1.43	2 (18%)	4,20,22	1.19	0
2	NEP	TD	45	2	11,14,15	1.21	2 (18%)	4,20,22	0.90	0
2	NEP	TH	45	2	11,14,15	1.23	1 (9%)	4,20,22	0.82	0
2	NEP	TG	45	2	11,14,15	1.22	1 (9%)	4,20,22	1.04	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NEP	TE	45	2	-	1/5/12/14	0/1/1/1
2	NEP	TF	45	2	-	2/5/12/14	0/1/1/1
2	NEP	TI	45	2	-	1/5/12/14	0/1/1/1
2	NEP	TD	45	2	-	2/5/12/14	0/1/1/1
2	NEP	TH	45	2	-	2/5/12/14	0/1/1/1
2	NEP	TG	45	2	-	1/5/12/14	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	TI	45	NEP	P-O2P	-2.92	1.48	1.54
2	TI	45	NEP	P-O3P	2.84	1.49	1.47
2	TG	45	NEP	P-O2P	-2.81	1.48	1.54
2	TE	45	NEP	P-O2P	-2.80	1.48	1.54
2	TF	45	NEP	P-O2P	-2.52	1.49	1.54
2	TF	45	NEP	P-O1P	-2.52	1.49	1.54
2	TD	45	NEP	P-O1P	-2.37	1.49	1.54
2	TD	45	NEP	P-O2P	-2.27	1.50	1.54
2	TH	45	NEP	P-O2P	-2.20	1.50	1.54
2	TE	45	NEP	P-O3P	2.14	1.49	1.47

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	TE	45	NEP	O2P-P-O3P	2.07	118.11	113.76

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	TD	45	NEP	C-CA-CB-CG
2	TD	45	NEP	CA-CB-CG-ND1
2	TE	45	NEP	CA-CB-CG-ND1
2	TF	45	NEP	C-CA-CB-CG
2	TF	45	NEP	CA-CB-CG-ND1
2	TH	45	NEP	C-CA-CB-CG
2	TH	45	NEP	CA-CB-CG-ND1
2	TG	45	NEP	CA-CB-CG-ND1
2	TI	45	NEP	CA-CB-CG-ND1

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

Of 53 ligands modelled in this entry, 53 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.

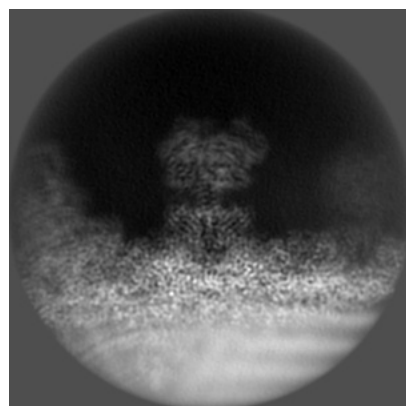
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18559. These allow visual inspection of the internal detail of the map and identification of artifacts.

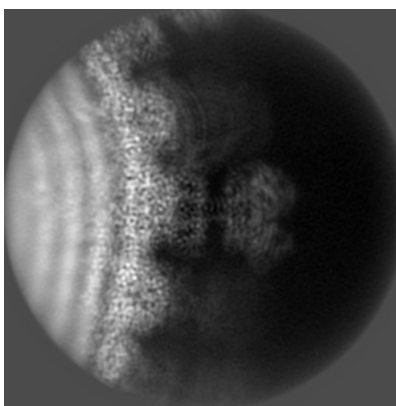
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

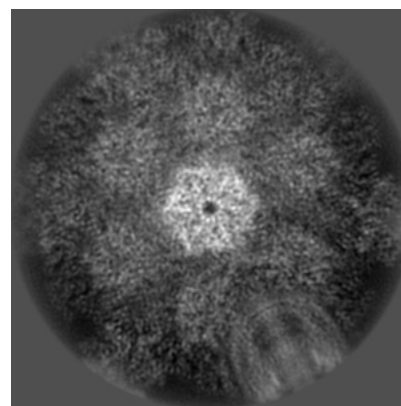
#### 6.1.1 Primary map



X

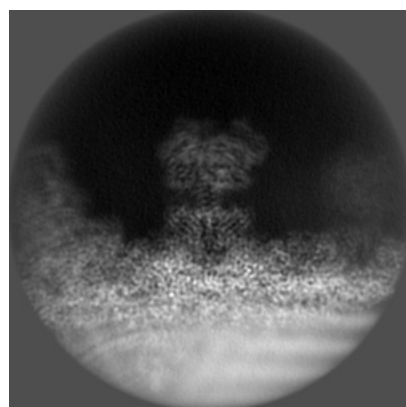


Y

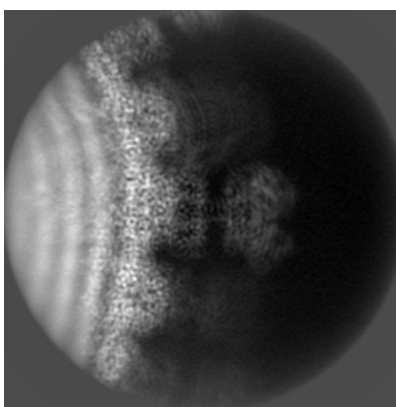


Z

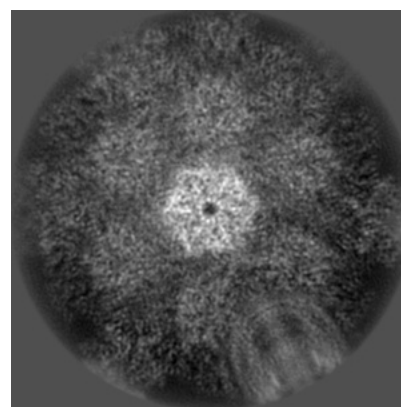
#### 6.1.2 Raw map



X



Y

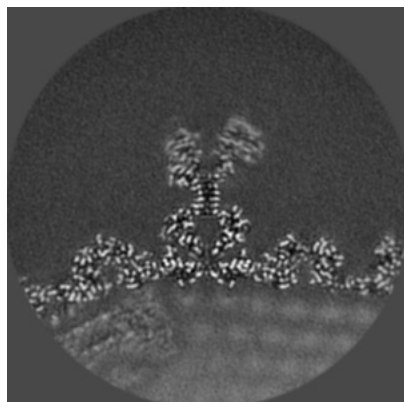


Z

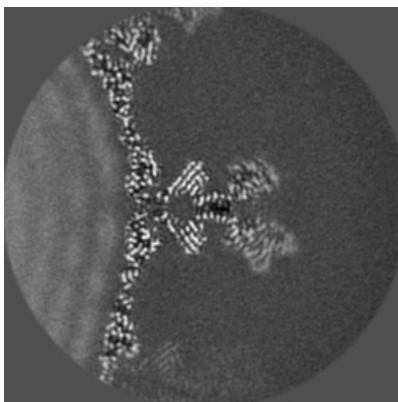
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

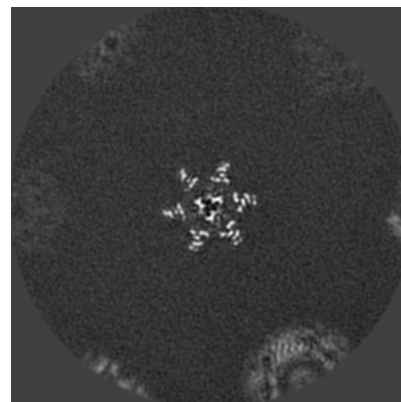
### 6.2.1 Primary map



X Index: 128

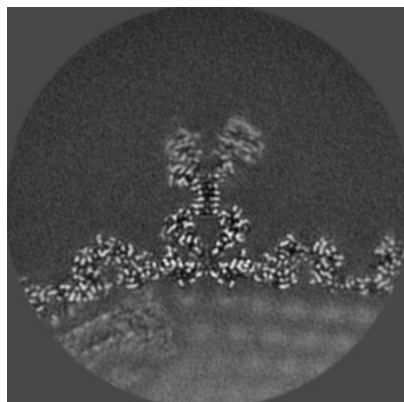


Y Index: 128

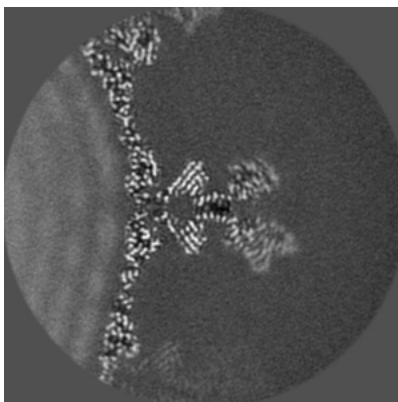


Z Index: 128

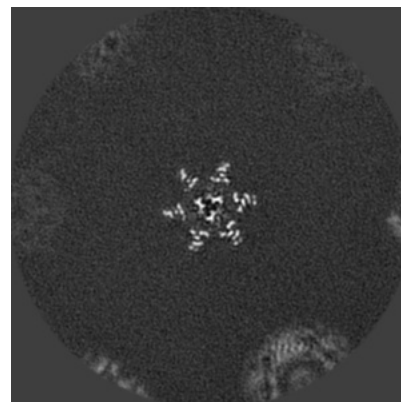
### 6.2.2 Raw map



X Index: 128



Y Index: 128



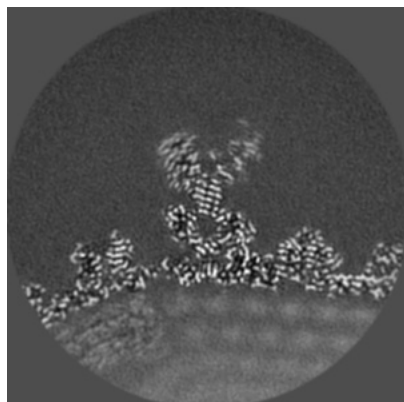
Z Index: 128

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

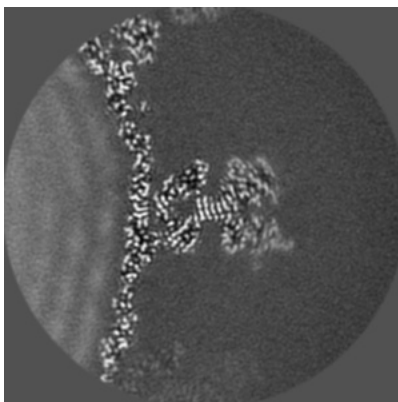


## 6.3 Largest variance slices [i](#)

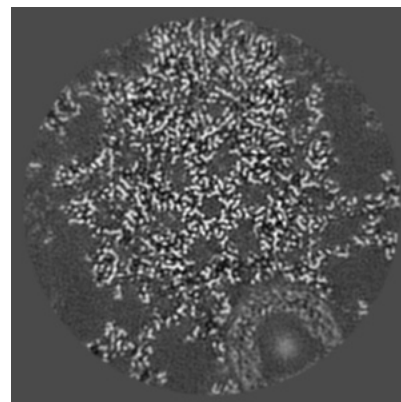
### 6.3.1 Primary map



X Index: 122

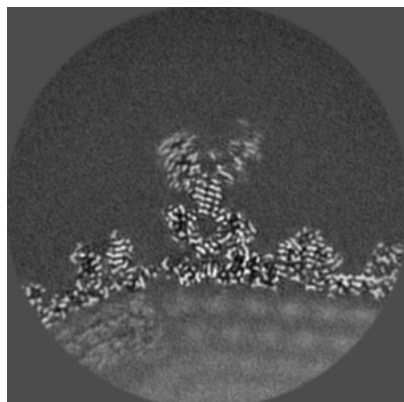


Y Index: 133

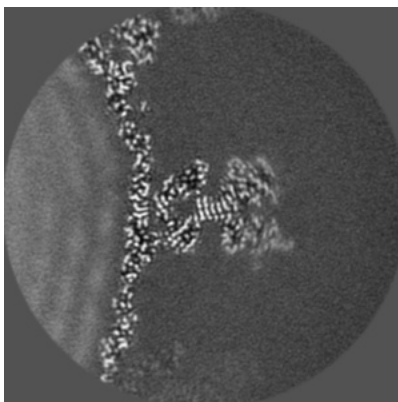


Z Index: 81

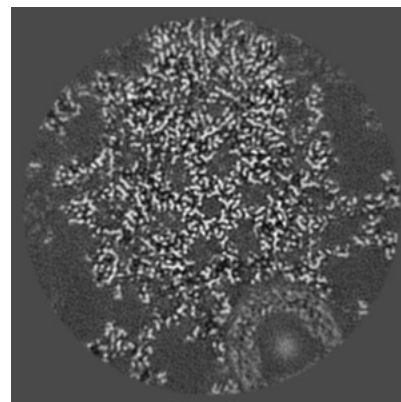
### 6.3.2 Raw map



X Index: 122



Y Index: 133

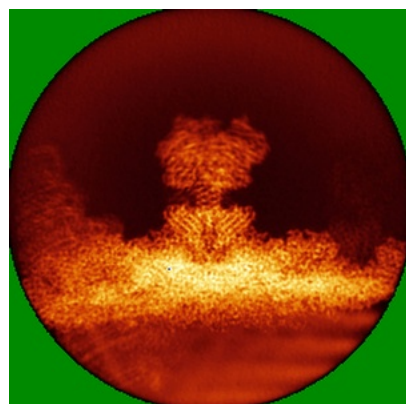


Z Index: 81

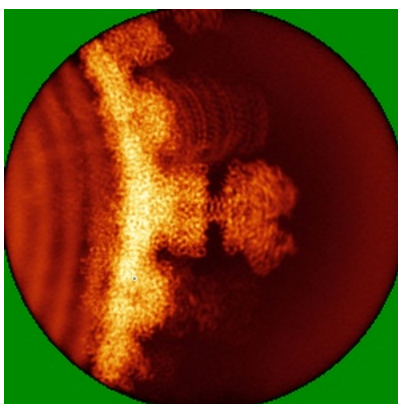
The images above show the largest variance slices of the map in three orthogonal directions.

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

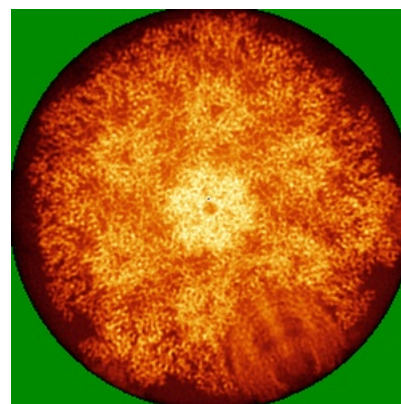
### 6.4.1 Primary map



X

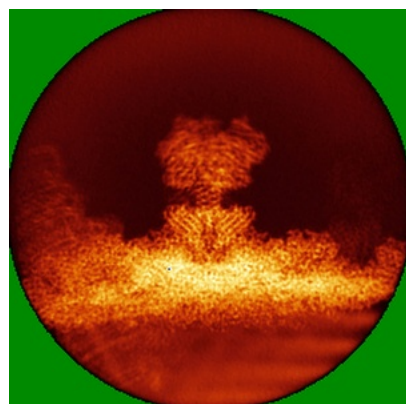


Y

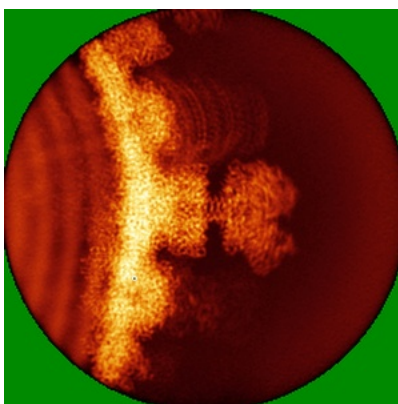


Z

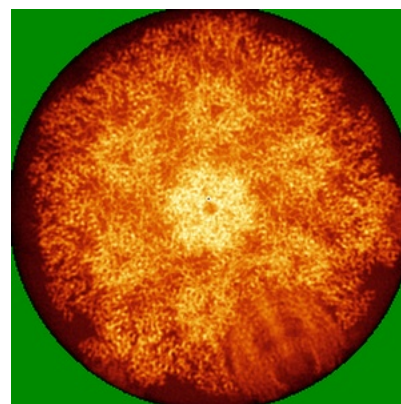
### 6.4.2 Raw map



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 0.024. 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.

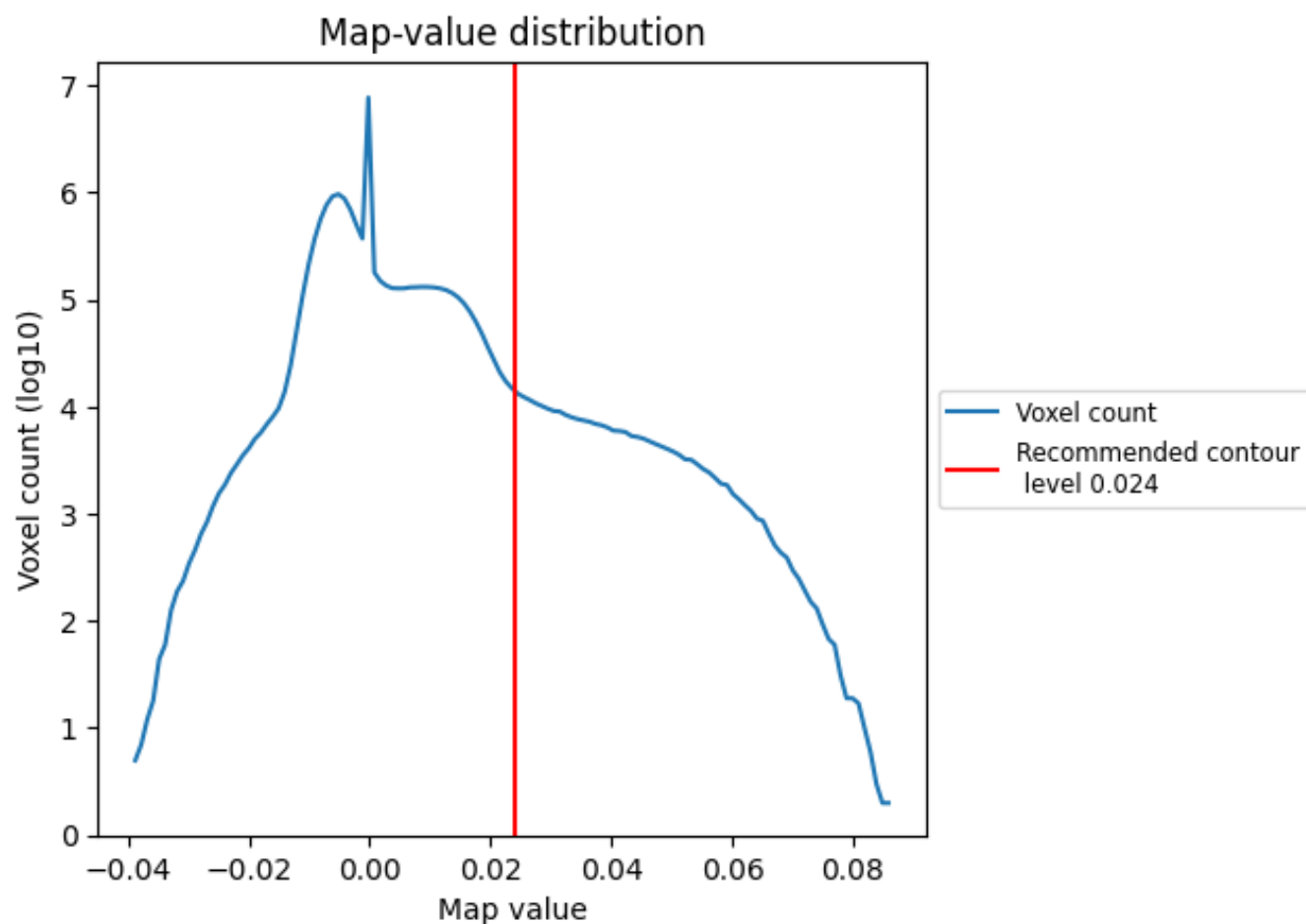
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

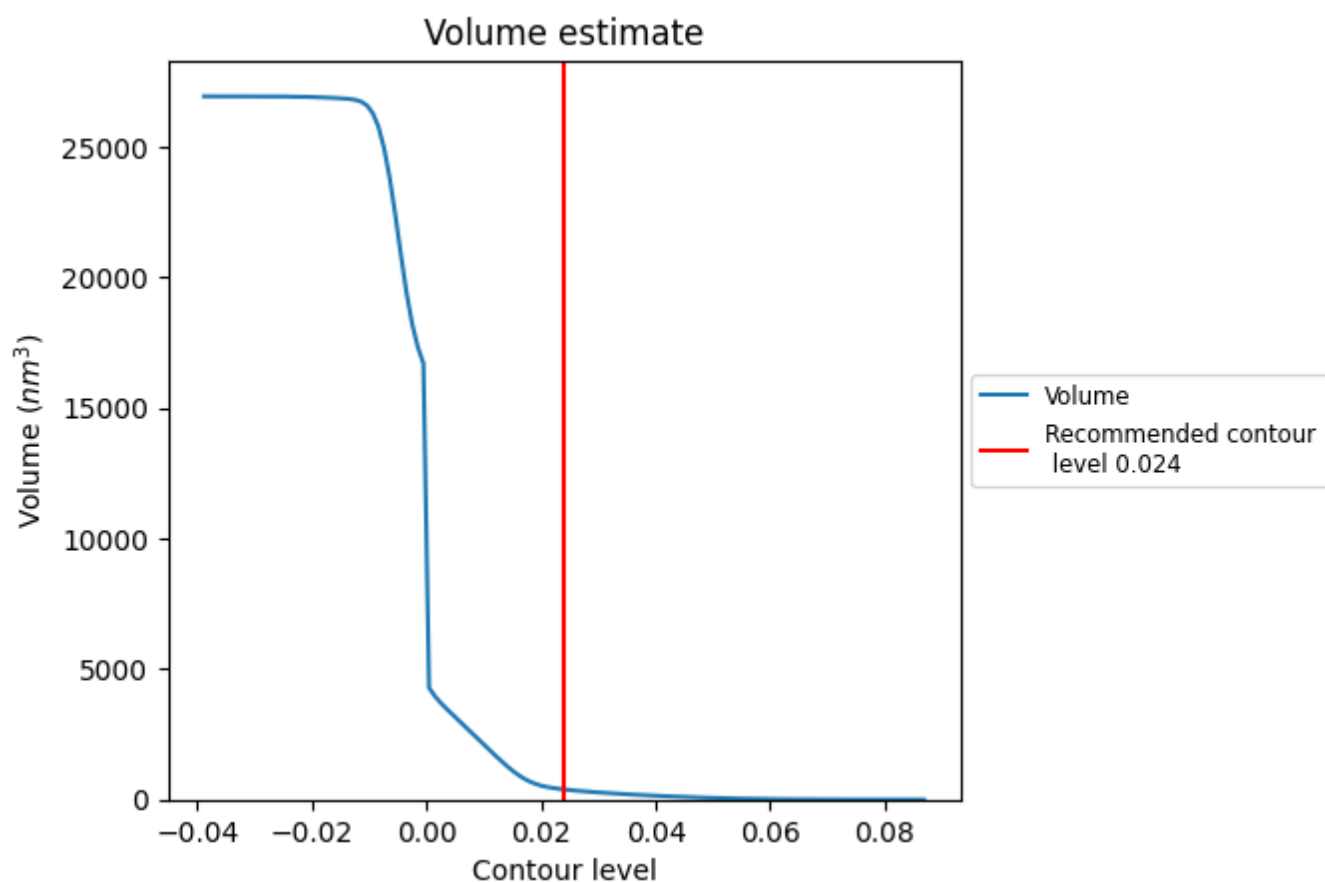
This section contains the results of statistical analysis of the map.

### 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.

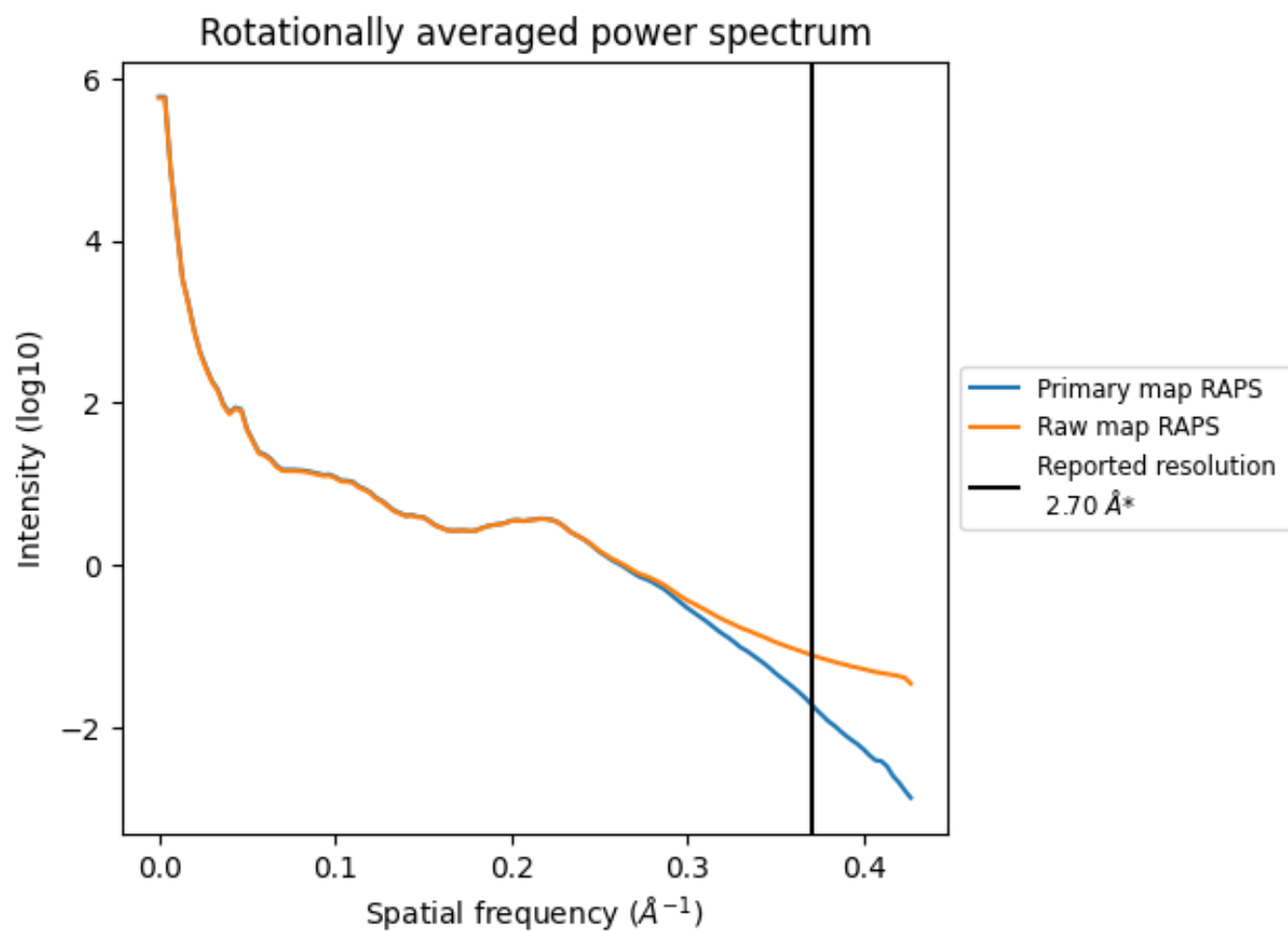
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 387  $\text{nm}^3$ ; this corresponds to an approximate mass of 350 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ

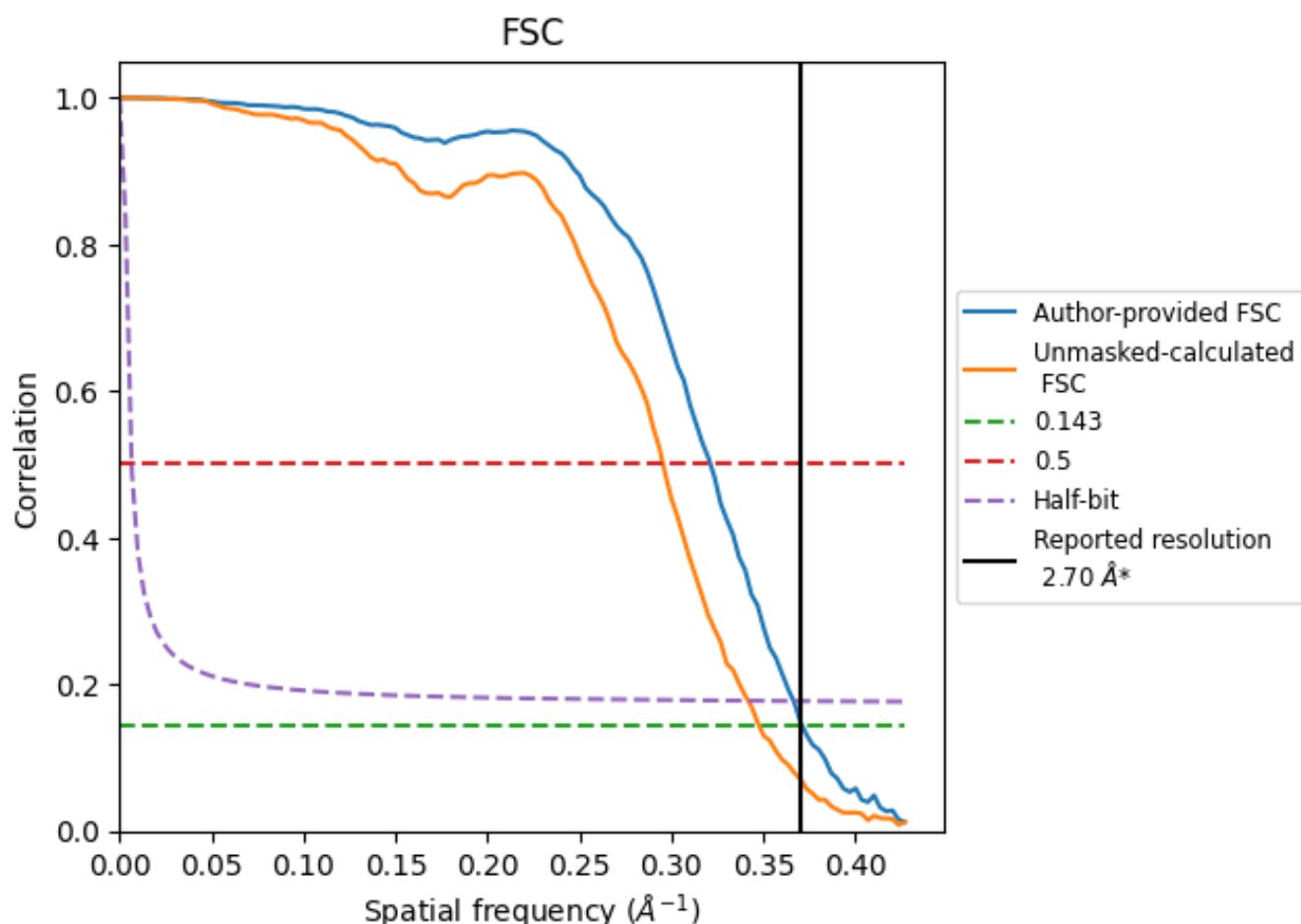


\*Reported resolution corresponds to spatial frequency of 0.370  $\text{\AA}^{-1}$

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.370 Å<sup>-1</sup>



## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.69	3.11	2.73
Unmasked-calculated*	2.87	3.38	2.93

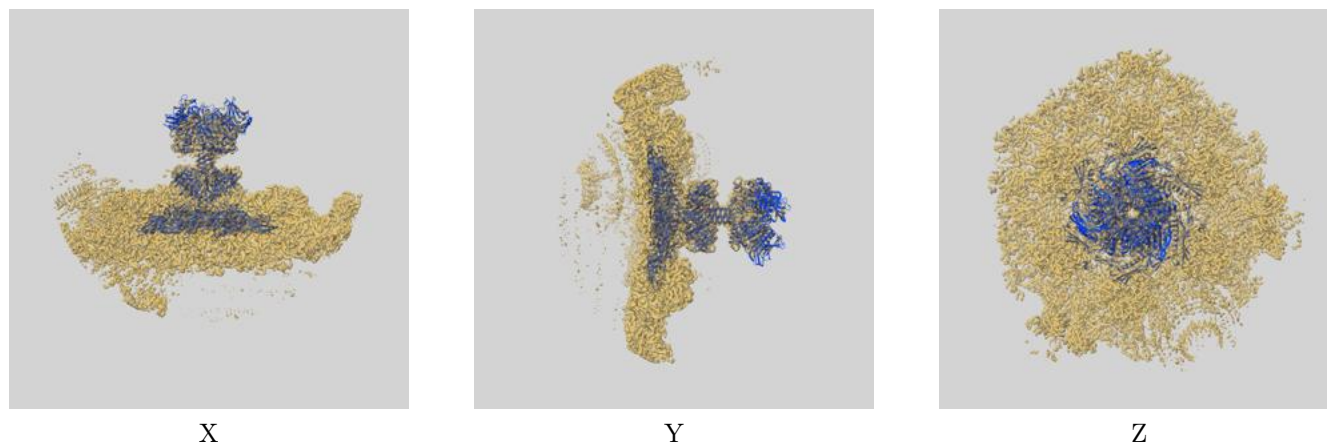
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.



## 9 Map-model fit [i](#)

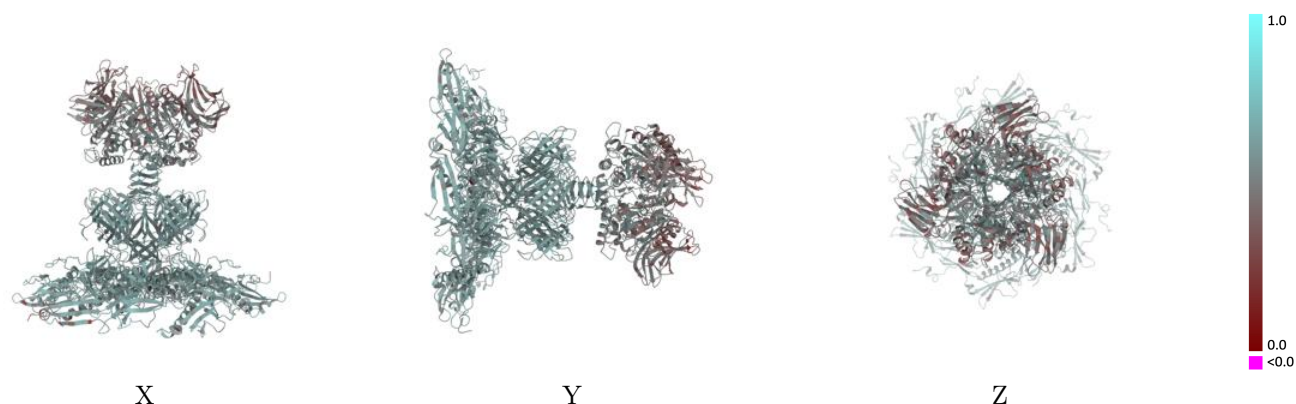
This section contains information regarding the fit between EMDB map EMD-18559 and PDB model 8QPQ. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

### 9.1 Map-model overlay [i](#)



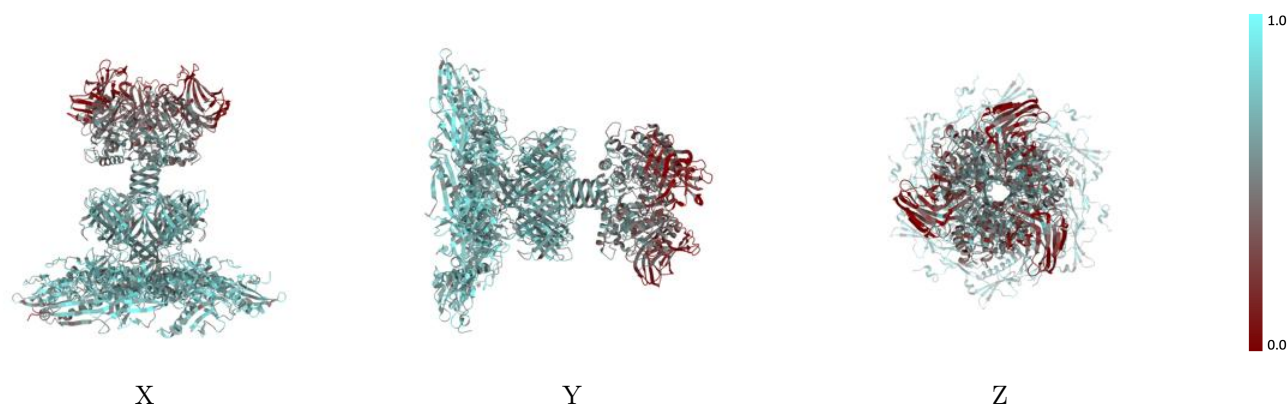
The images above show the 3D surface view of the map at the recommended contour level 0.024 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



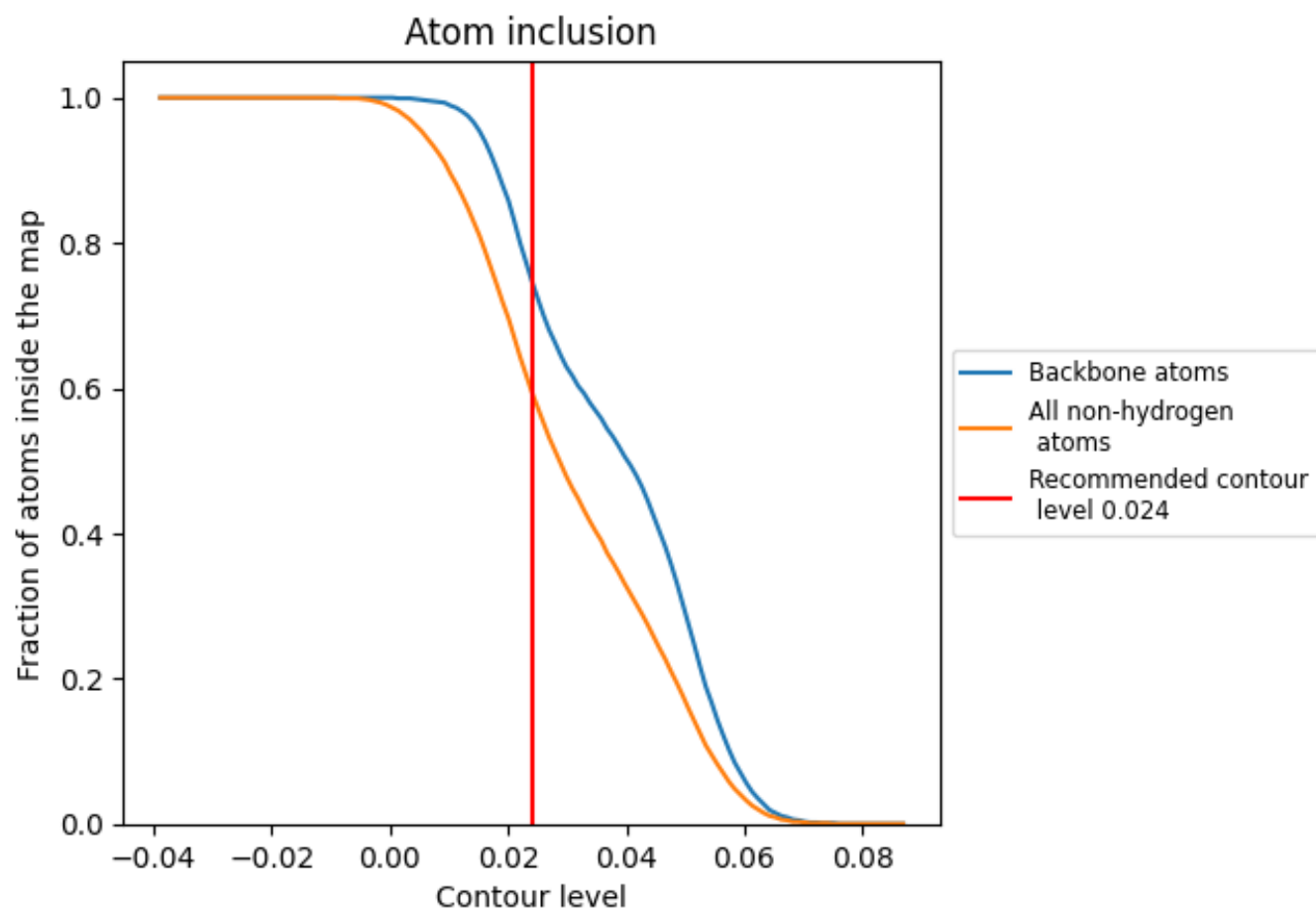
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.024).

































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 60% 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 (0.024) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5960	 0.5380
LA	 0.6780	 0.5660
LB	 0.6990	 0.5740
LC	 0.7100	 0.5690
LD	 0.7110	 0.5720
LE	 0.7070	 0.5690
LF	 0.6780	 0.5630
TA	 0.4120	 0.4710
TB	 0.4210	 0.4720
TC	 0.4200	 0.4790
TD	 0.6550	 0.5750
TE	 0.6570	 0.5760
TF	 0.6640	 0.5760
TG	 0.6570	 0.5750
TH	 0.6510	 0.5740
TI	 0.6570	 0.5730

