



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 03:54 PM UTC

PDB ID : 9H7V / pdb_00009h7v
EMDB ID : EMD-51915
Title : The baseplate assembly of Haloferax tailed virus 1.
Authors : Zhang, D.; Daum, B.; Isupov, M.N.; McLaren, M.
Deposited on : 2024-10-28
Resolution : 2.60 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

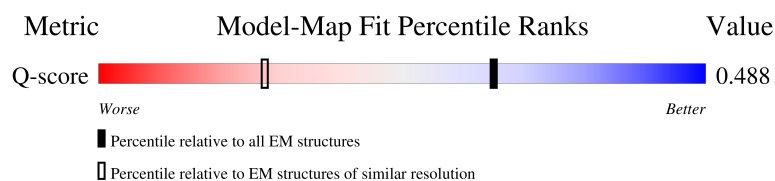
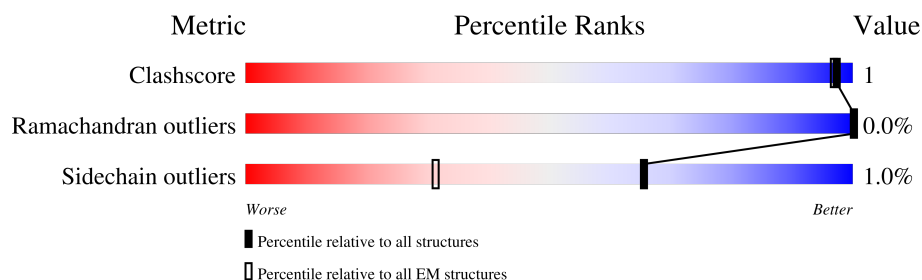
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

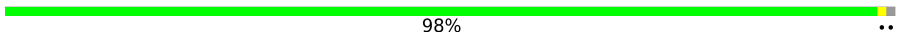
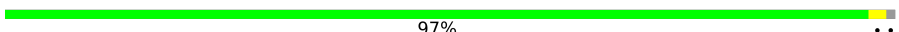
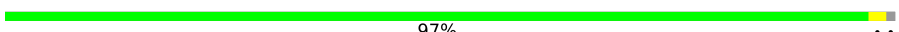
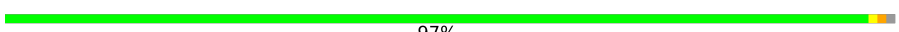
The reported resolution of this entry is 2.60 Å.

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



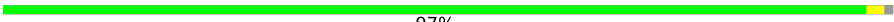
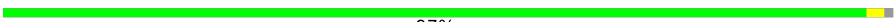





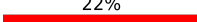

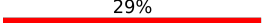



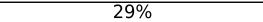

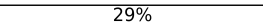
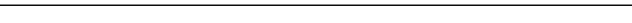
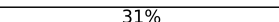

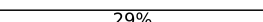

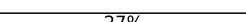

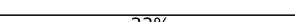






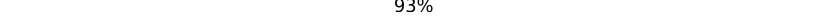

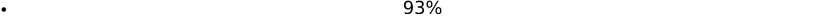
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8728 (2.10 - 3.10)

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	B1	158	 98% ..
1	B2	158	 97% ..
1	B3	158	 97% ..
1	B4	158	 97% ...

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Mol	Chain	Length	Quality of chain
1	B5	158	 97% ..
1	B6	158	 97% ..
2	BA	285	 98% .
2	BB	285	 96% .
2	BC	285	 98% .
3	BD	954	 97% .
3	BE	954	 97% .
3	BF	954	 22%  98% .
4	BG	285	 29%  97% .
4	BH	285	 32%  96% .
4	BI	285	 29%  96% .
4	BJ	285	 29%  97% .
4	BK	285	 31%  97% .
4	BL	285	 29%  96% .
4	BM	285	 27%  97% .
4	BN	285	 33%  97% .
4	BO	285	 29%  98% .
5	QE	341	 7% 93%
5	QF	341	 7% . 93%
5	QG	341	 7% 93%
5	QH	341	 7% . 93%
5	QI	341	 6% 93%
5	QJ	341	 7% 93%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 54689 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Tail tube protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B1	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
1	B2	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
1	B3	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
1	B4	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
1	B5	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		
1	B6	156	Total	C	N	O	S	0	0
			1196	747	189	259	1		

- Molecule 2 is a protein called Baseplate to tube adapter protein gp41.

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

- Molecule 3 is a protein called Baseplate hub.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	BD	953	Total	C	N	O	S	0	0
			7212	4427	1207	1573	5		
3	BE	953	Total	C	N	O	S	0	0
			7212	4427	1207	1573	5		
3	BF	953	Total	C	N	O	S	0	0
			7212	4427	1207	1573	5		

- Molecule 4 is a protein called Tail fiber protein gp42.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	BG	284	Total 2029	C 1221	N 334	O 473	S 1	0	0
4	BH	284	Total 2029	C 1221	N 334	O 473	S 1	0	0
4	BI	284	Total 2029	C 1221	N 334	O 473	S 1	0	0
4	BJ	284	Total 2029	C 1221	N 334	O 473	S 1	0	0
4	BK	284	Total 2029	C 1221	N 334	O 473	S 1	0	0
4	BL	284	Total 2029	C 1221	N 334	O 473	S 1	0	0
4	BM	284	Total 2029	C 1221	N 334	O 473	S 1	0	0
4	BN	284	Total 2029	C 1221	N 334	O 473	S 1	0	0
4	BO	284	Total 2029	C 1221	N 334	O 473	S 1	0	0

- Molecule 5 is a protein called Phate tail tape measure protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	QE	23	Total 183	C 105	N 40	O 38	0	0
5	QF	25	Total 199	C 115	N 44	O 40	0	0
5	QG	23	Total 183	C 105	N 40	O 38	0	0
5	QH	25	Total 199	C 115	N 44	O 40	0	0
5	QI	23	Total 183	C 105	N 40	O 38	0	0
5	QJ	25	Total 199	C 115	N 44	O 40	0	0

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
6	BD	7	Total 7	Mg 7	0
6	BE	8	Total 8	Mg 8	0

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Mol	Chain	Residues	Atoms		AltConf
6	BF	5	Total 5	Mg 5	0
6	BG	3	Total 3	Mg 3	0
6	BH	3	Total 3	Mg 3	0
6	BI	3	Total 3	Mg 3	0
6	BJ	3	Total 3	Mg 3	0
6	BK	3	Total 3	Mg 3	0
6	BL	4	Total 4	Mg 4	0
6	BM	3	Total 3	Mg 3	0
6	BN	3	Total 3	Mg 3	0
6	BO	3	Total 3	Mg 3	0

- Molecule 7 is POTASSIUM ION (CCD ID: K) (formula: K) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
7	BD	3	Total 3	K 3	0
7	BE	4	Total 4	K 4	0
7	BF	1	Total 1	K 1	0

- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
8	BG	1	Total 1	Zn 1	0
8	BH	1	Total 1	Zn 1	0
8	BJ	1	Total 1	Zn 1	0

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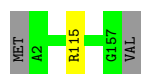
Mol	Chain	Residues	Atoms		AltConf
8	BK	1	Total 1	Zn 1	0
8	BM	1	Total 1	Zn 1	0
8	BN	1	Total 1	Zn 1	0

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: Tail tube protein

Chain B1:  98% ..



- Molecule 1: Tail tube protein

Chain B2:  97% ..



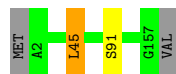
- Molecule 1: Tail tube protein

Chain B3:  97% ..



- Molecule 1: Tail tube protein

Chain B4:  97% ...



- Molecule 1: Tail tube protein

Chain B5:  97% ..



- Molecule 1: Tail tube protein

Chain B6:  97% ..



- Molecule 2: Baseplate to tube adapter protein gp41

Chain BA:  98% .



- Molecule 2: Baseplate to tube adapter protein gp41

Chain BB:  96% .



- Molecule 2: Baseplate to tube adapter protein gp41

Chain BC:  98% .



- Molecule 3: Baseplate hub

Chain BD:  97% .



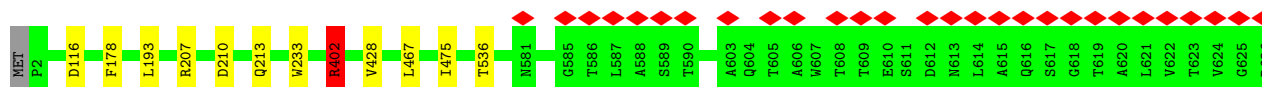
- Molecule 3: Baseplate hub

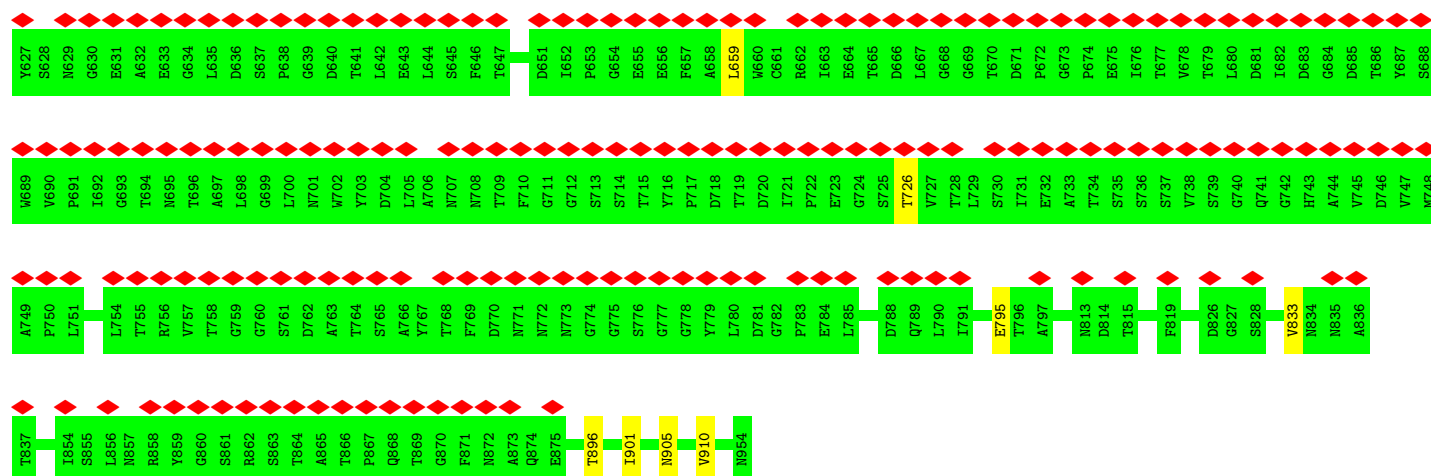
Chain BE:  97% .



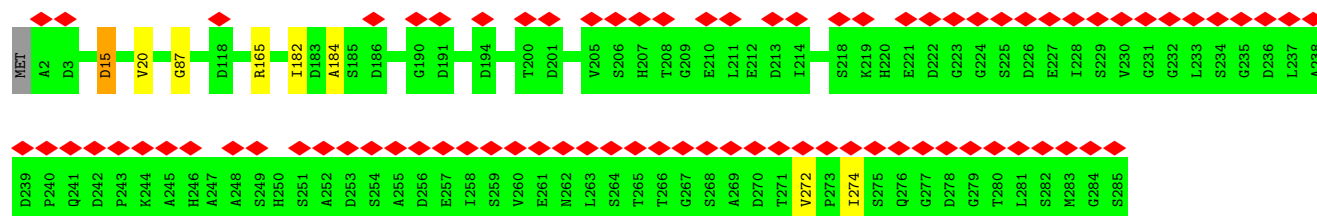
- Molecule 3: Baseplate hub

Chain BF:  22% 98% .

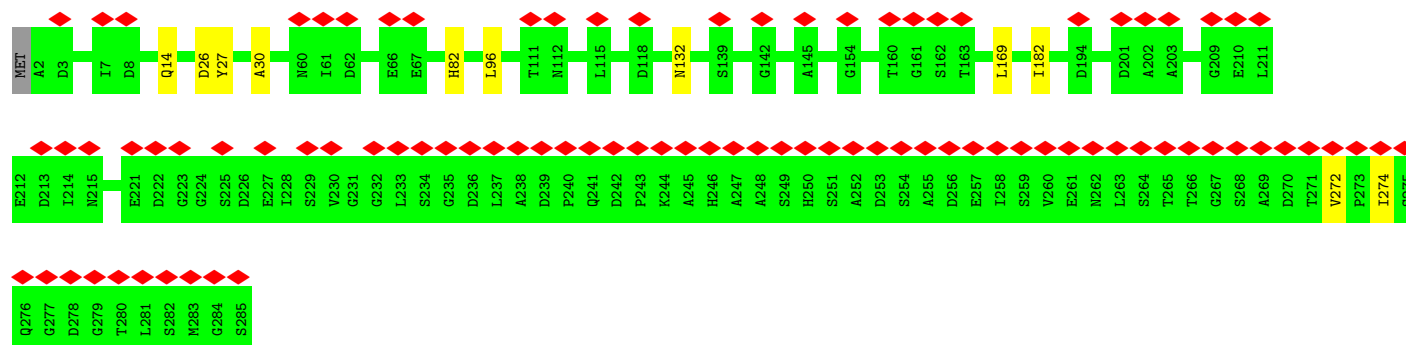




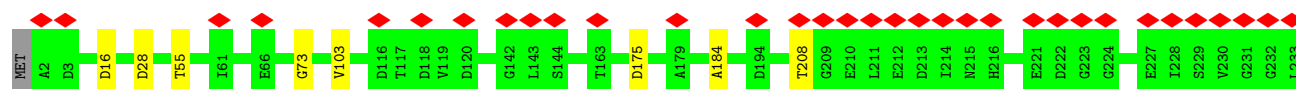
• Molecule 4: Tail fiber protein gp42

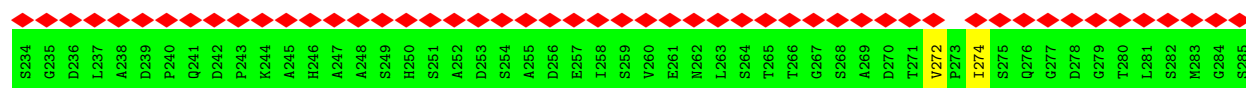


• Molecule 4: Tail fiber protein gp42

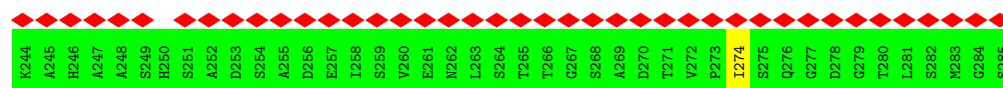
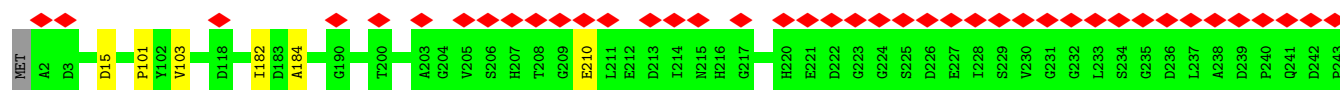


• Molecule 4: Tail fiber protein gp42

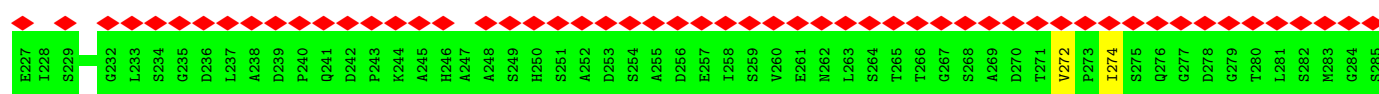
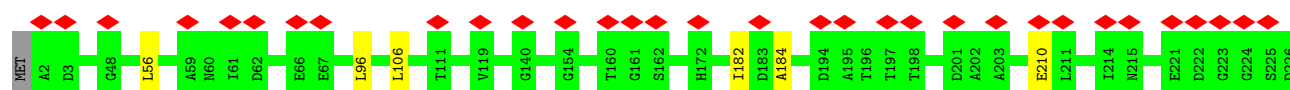




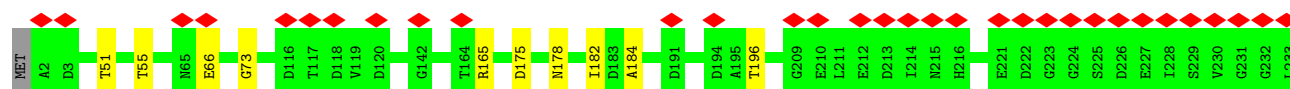
• Molecule 4: Tail fiber protein gp42



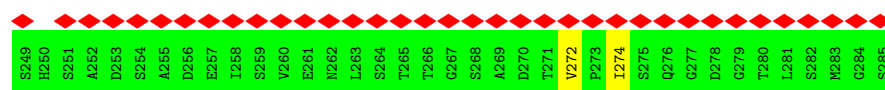
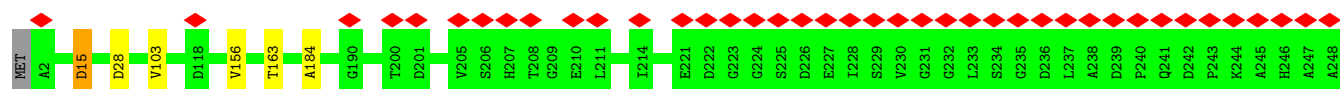
• Molecule 4: Tail fiber protein gp42



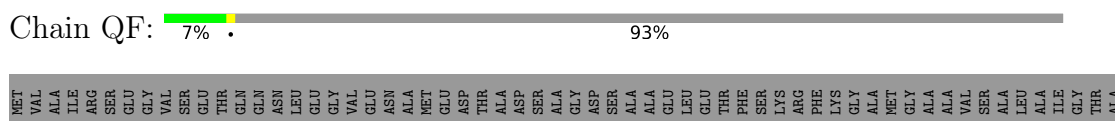
• Molecule 4: Tail fiber protein gp42



• Molecule 4: Tail fiber protein gp42



• Molecule 4: Tail fiber protein gp42





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	135152	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	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	0.066	Depositor
Minimum map value	-0.025	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.008	Depositor
Map size (Å)	374.72, 374.72, 374.72	wwPDB
Map dimensions	320, 320, 320	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: K, 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	B1	0.48	0/1224	0.90	0/1672
1	B2	0.48	0/1224	0.92	0/1672
1	B3	0.48	0/1224	0.89	0/1672
1	B4	0.47	0/1224	0.90	0/1672
1	B5	0.48	0/1224	0.92	0/1672
1	B6	0.48	0/1224	0.91	0/1672
2	BA	0.49	0/2175	0.94	0/2970
2	BB	0.48	0/2175	0.96	2/2970 (0.1%)
2	BC	0.49	0/2175	0.95	3/2970 (0.1%)
3	BD	0.47	0/7332	1.02	0/10023
3	BE	0.47	0/7332	1.01	5/10023 (0.0%)
3	BF	0.50	0/7332	1.03	4/10023 (0.0%)
4	BG	0.54	0/2062	1.07	2/2830 (0.1%)
4	BH	0.55	0/2062	1.06	0/2830
4	BI	0.55	0/2062	1.08	2/2830 (0.1%)
4	BJ	0.54	0/2062	1.06	2/2830 (0.1%)
4	BK	0.55	0/2062	1.07	0/2830
4	BL	0.54	0/2062	1.06	1/2830 (0.0%)
4	BM	0.55	0/2062	1.08	3/2830 (0.1%)
4	BN	0.55	0/2062	1.04	0/2830
4	BO	0.54	0/2062	1.08	1/2830 (0.0%)
5	QE	0.50	0/184	1.10	0/245
5	QF	0.48	0/200	1.20	0/264
5	QG	0.50	0/184	1.07	0/245
5	QH	0.47	0/200	1.16	0/264
5	QI	0.50	0/184	1.09	0/245
5	QJ	0.48	0/200	1.09	0/264
All	All	0.50	0/55575	1.02	25/76008 (0.0%)

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
2	BA	0	1
2	BB	0	1
3	BD	0	1
3	BE	0	2
3	BF	0	1
4	BL	0	1
4	BO	0	1
All	All	0	8

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	BI	28	ASP	CA-CB-CG	6.31	118.91	112.60
3	BF	116	ASP	CA-CB-CG	6.11	118.71	112.60
4	BG	15	ASP	CA-CB-CG	6.02	118.62	112.60
2	BB	16	PRO	N-CA-C	5.71	122.08	113.81
3	BF	536	THR	CB-CA-C	5.70	121.26	111.68
4	BO	28	ASP	CA-CB-CG	5.70	118.30	112.60
2	BC	215	ASN	CA-C-N	5.49	124.72	120.33
2	BC	215	ASN	C-N-CA	5.49	124.72	120.33
4	BM	15	ASP	CA-CB-CG	5.49	118.09	112.60
4	BM	28	ASP	CA-CB-CG	5.49	118.08	112.60
4	BG	15	ASP	CB-CA-C	-5.47	98.48	110.67
3	BE	178	PHE	CA-CB-CG	5.37	119.17	113.80
4	BJ	15	ASP	CB-CA-C	-5.34	99.89	111.11
4	BM	15	ASP	CB-CA-C	-5.34	98.83	111.65
2	BC	16	PRO	N-CA-C	5.32	123.42	112.47
2	BB	66	ASP	CA-CB-CG	5.30	117.90	112.60
4	BL	175	ASP	CB-CA-C	5.28	120.92	110.42
3	BF	178	PHE	CA-CB-CG	5.23	119.03	113.80
3	BF	402	ARG	CG-CD-NE	5.16	123.36	112.00
3	BE	654	GLY	CA-C-N	5.13	127.67	120.28
3	BE	654	GLY	C-N-CA	5.13	127.67	120.28
3	BE	350	VAL	CA-C-N	5.11	127.13	120.28
3	BE	350	VAL	C-N-CA	5.11	127.13	120.28
4	BI	175	ASP	CA-CB-CG	5.04	117.64	112.60
4	BJ	101	PRO	N-CA-C	5.04	118.76	110.55

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	BA	283	SER	Peptide
2	BB	103	ALA	Peptide
3	BD	199	PRO	Peptide
3	BE	220	PRO	Peptide
3	BE	47	ALA	Peptide
3	BF	795	GLU	Peptide
4	BL	66	GLU	Peptide
4	BO	66	GLU	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B1	1196	0	1094	0	0
1	B2	1196	0	1094	1	0
1	B3	1196	0	1094	2	0
1	B4	1196	0	1094	2	0
1	B5	1196	0	1094	3	0
1	B6	1196	0	1094	2	0
2	BA	2136	0	2127	1	0
2	BB	2136	0	2127	3	0
2	BC	2136	0	2127	1	0
3	BD	7212	0	6783	7	0
3	BE	7212	0	6781	10	0
3	BF	7212	0	6783	6	0
4	BG	2029	0	1856	8	0
4	BH	2029	0	1856	9	0
4	BI	2029	0	1856	4	0
4	BJ	2029	0	1856	3	0
4	BK	2029	0	1856	5	0
4	BL	2029	0	1856	4	0
4	BM	2029	0	1856	5	0
4	BN	2029	0	1856	5	0
4	BO	2029	0	1856	3	0
5	QE	183	0	175	0	0
5	QF	199	0	196	0	0
5	QG	183	0	175	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	QH	199	0	196	2	0
5	QI	183	0	175	2	0
5	QJ	199	0	196	0	0
6	BD	7	0	0	0	0
6	BE	8	0	0	0	0
6	BF	5	0	0	0	0
6	BG	3	0	0	0	0
6	BH	3	0	0	0	0
6	BI	3	0	0	0	0
6	BJ	3	0	0	0	0
6	BK	3	0	0	0	0
6	BL	4	0	0	0	0
6	BM	3	0	0	0	0
6	BN	3	0	0	0	0
6	BO	3	0	0	0	0
7	BD	3	0	0	0	0
7	BE	4	0	0	0	0
7	BF	1	0	0	0	0
8	BG	1	0	0	0	0
8	BH	1	0	0	0	0
8	BJ	1	0	0	0	0
8	BK	1	0	0	0	0
8	BM	1	0	0	0	0
8	BN	1	0	0	0	0
All	All	54689	0	51109	59	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 (59) 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:BE:8:LYS:HA	4:BH:27:TYR:HA	1.72	0.71
4:BM:184:ALA:HB2	4:BN:182:ILE:HD12	1.76	0.68
3:BD:428:VAL:HG12	3:BD:475:ILE:HG12	1.76	0.67
3:BF:402:ARG:HG3	3:BF:402:ARG:HH21	1.63	0.62
3:BF:428:VAL:HG12	3:BF:475:ILE:HD13	1.86	0.57
5:QH:330:ARG:NH1	5:QI:320:ASP:OD2	2.39	0.55
4:BJ:182:ILE:HD12	4:BL:184:ALA:HB2	1.89	0.54
4:BN:274:ILE:HG22	4:BO:272:VAL:HG22	1.92	0.52
4:BG:87:GLY:CA	4:BH:132:ASN:HD21	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BJ:184:ALA:HB2	4:BK:182:ILE:HD12	1.93	0.50
3:BF:402:ARG:HH21	3:BF:402:ARG:CG	2.25	0.50
2:BA:113:GLU:HB2	2:BA:123:ASP:HB2	1.94	0.50
5:QH:330:ARG:NH1	5:QI:320:ASP:CG	2.70	0.49
4:BG:87:GLY:HA3	4:BH:132:ASN:HD21	1.78	0.49
1:B5:48:ILE:HD11	2:BB:245:LEU:HD11	1.95	0.48
3:BE:3:GLN:HB2	3:BE:6:ASP:OD2	2.14	0.47
4:BN:184:ALA:HB2	4:BO:182:ILE:HD12	1.96	0.47
4:BG:184:ALA:HB2	4:BH:182:ILE:HD12	1.97	0.47
1:B4:45:LEU:HB3	2:BB:18:VAL:HB	1.98	0.46
3:BE:385:ALA:HB2	3:BE:518:MET:HE2	1.98	0.46
3:BE:898:SER:HB2	3:BE:946:GLU:HB3	1.98	0.46
4:BG:274:ILE:HG22	4:BH:272:VAL:HG22	1.98	0.46
4:BM:274:ILE:HG22	4:BN:272:VAL:HG22	1.98	0.46
2:BC:113:GLU:HB2	2:BC:123:ASP:HB2	1.99	0.45
4:BM:272:VAL:HG22	4:BO:274:ILE:HG22	1.98	0.45
1:B6:44:GLU:HG3	1:B6:53:ARG:HD2	1.97	0.45
4:BH:82:HIS:HB2	4:BH:96:LEU:HD12	1.98	0.45
4:BK:56:LEU:HD22	4:BK:106:LEU:HD12	1.97	0.45
4:BK:184:ALA:HB2	4:BL:182:ILE:HD12	1.98	0.45
1:B3:47:THR:HG23	1:B3:54:ASP:HB2	1.99	0.45
3:BE:297:THR:HG23	3:BE:340:ILE:HG23	1.99	0.44
4:BM:156:VAL:HG22	4:BM:163:THR:HG22	1.99	0.44
4:BG:272:VAL:HG22	4:BI:274:ILE:HG22	1.99	0.44
3:BF:905:ASN:HA	3:BF:910:VAL:HG11	2.00	0.44
4:BH:274:ILE:HG22	4:BI:272:VAL:HG22	2.00	0.43
3:BE:660:TRP:CD1	3:BE:751:LEU:HD21	2.53	0.43
1:B2:91:SER:HB2	1:B3:148:SER:HB2	1.99	0.43
3:BF:210:ASP:HB3	3:BF:213:GLN:HE21	1.84	0.43
4:BG:15:ASP:CG	4:BH:30:ALA:H	2.25	0.43
3:BD:898:SER:HB2	3:BD:946:GLU:HB3	2.00	0.42
1:B4:91:SER:HB2	1:B5:148:SER:HB2	2.01	0.42
3:BE:583:ILE:HD12	3:BE:794:LEU:HD13	2.01	0.42
1:B5:91:SER:HB2	1:B6:148:SER:HB2	2.02	0.42
4:BI:55:THR:HB	4:BI:73:GLY:HA3	2.02	0.42
4:BL:55:THR:HB	4:BL:73:GLY:HA3	2.02	0.42
3:BD:752:ASP:CG	3:BD:756:ARG:HH12	2.27	0.41
4:BG:15:ASP:O	4:BG:20:VAL:HG22	2.19	0.41
3:BD:366:MET:HE1	3:BF:233:TRP:CE3	2.55	0.41
4:BJ:274:ILE:HG22	4:BK:272:VAL:HG22	2.01	0.41
4:BM:15:ASP:CG	4:BN:30:ALA:H	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BD:716:TYR:CD1	3:BD:717:PRO:HD2	2.55	0.41
3:BD:458:ALA:O	3:BD:459:LYS:HB2	2.21	0.41
3:BE:428:VAL:HG12	3:BE:475:ILE:HD13	2.02	0.41
4:BH:14:GLN:HB2	4:BH:26:ASP:OD2	2.20	0.41
2:BB:137:ARG:HB3	3:BD:61:ARG:HD3	2.03	0.41
3:BE:6:ASP:N	3:BE:6:ASP:OD1	2.52	0.41
4:BK:274:ILE:HG22	4:BL:272:VAL:HG22	2.02	0.41
3:BE:407:GLY:HA2	3:BE:485:LEU:HD22	2.04	0.40
4:BG:182:ILE:HD12	4:BI:184:ALA:HB2	2.04	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	B1	154/158 (98%)	151 (98%)	3 (2%)	0	100	100
1	B2	154/158 (98%)	149 (97%)	5 (3%)	0	100	100
1	B3	154/158 (98%)	151 (98%)	3 (2%)	0	100	100
1	B4	154/158 (98%)	150 (97%)	4 (3%)	0	100	100
1	B5	154/158 (98%)	151 (98%)	3 (2%)	0	100	100
1	B6	154/158 (98%)	152 (99%)	2 (1%)	0	100	100
2	BA	282/285 (99%)	272 (96%)	10 (4%)	0	100	100
2	BB	282/285 (99%)	277 (98%)	4 (1%)	1 (0%)	30	51
2	BC	282/285 (99%)	274 (97%)	8 (3%)	0	100	100
3	BD	951/954 (100%)	906 (95%)	45 (5%)	0	100	100
3	BE	951/954 (100%)	908 (96%)	41 (4%)	2 (0%)	43	66
3	BF	951/954 (100%)	907 (95%)	44 (5%)	0	100	100
4	BG	282/285 (99%)	262 (93%)	20 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	BH	282/285 (99%)	264 (94%)	18 (6%)	0	100	100
4	BI	282/285 (99%)	265 (94%)	17 (6%)	0	100	100
4	BJ	282/285 (99%)	266 (94%)	16 (6%)	0	100	100
4	BK	282/285 (99%)	265 (94%)	17 (6%)	0	100	100
4	BL	282/285 (99%)	263 (93%)	19 (7%)	0	100	100
4	BM	282/285 (99%)	266 (94%)	16 (6%)	0	100	100
4	BN	282/285 (99%)	266 (94%)	16 (6%)	0	100	100
4	BO	282/285 (99%)	264 (94%)	18 (6%)	0	100	100
5	QE	21/341 (6%)	21 (100%)	0	0	100	100
5	QF	23/341 (7%)	22 (96%)	1 (4%)	0	100	100
5	QG	21/341 (6%)	21 (100%)	0	0	100	100
5	QH	23/341 (7%)	22 (96%)	1 (4%)	0	100	100
5	QI	21/341 (6%)	21 (100%)	0	0	100	100
5	QJ	23/341 (7%)	22 (96%)	1 (4%)	0	100	100
All	All	7293/9276 (79%)	6958 (95%)	332 (5%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	BE	8	LYS
2	BB	283	SER
3	BE	718	ASP

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	B1	129/131 (98%)	128 (99%)	1 (1%)	73	88
1	B2	129/131 (98%)	127 (98%)	2 (2%)	55	79
1	B3	129/131 (98%)	129 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B4	129/131 (98%)	128 (99%)	1 (1%)	73	88
1	B5	129/131 (98%)	129 (100%)	0	100	100
1	B6	129/131 (98%)	129 (100%)	0	100	100
2	BA	238/239 (100%)	236 (99%)	2 (1%)	73	88
2	BB	238/239 (100%)	234 (98%)	4 (2%)	53	78
2	BC	238/239 (100%)	236 (99%)	2 (1%)	73	88
3	BD	799/800 (100%)	788 (99%)	11 (1%)	59	81
3	BE	799/800 (100%)	792 (99%)	7 (1%)	70	87
3	BF	799/800 (100%)	790 (99%)	9 (1%)	65	84
4	BG	230/231 (100%)	229 (100%)	1 (0%)	84	93
4	BH	230/231 (100%)	229 (100%)	1 (0%)	84	93
4	BI	230/231 (100%)	227 (99%)	3 (1%)	61	82
4	BJ	230/231 (100%)	228 (99%)	2 (1%)	70	87
4	BK	230/231 (100%)	228 (99%)	2 (1%)	70	87
4	BL	230/231 (100%)	226 (98%)	4 (2%)	53	78
4	BM	230/231 (100%)	229 (100%)	1 (0%)	84	93
4	BN	230/231 (100%)	228 (99%)	2 (1%)	70	87
4	BO	230/231 (100%)	229 (100%)	1 (0%)	84	93
5	QE	20/262 (8%)	20 (100%)	0	100	100
5	QF	21/262 (8%)	19 (90%)	2 (10%)	8	18
5	QG	20/262 (8%)	20 (100%)	0	100	100
5	QH	21/262 (8%)	20 (95%)	1 (5%)	23	47
5	QI	20/262 (8%)	20 (100%)	0	100	100
5	QJ	21/262 (8%)	20 (95%)	1 (5%)	23	47
All	All	6078/7554 (80%)	6018 (99%)	60 (1%)	65	86

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B1	115	ARG
1	B2	87	THR
1	B2	106	THR
1	B4	45	LEU
2	BA	26	LEU

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Mol	Chain	Res	Type
2	BA	187	VAL
2	BB	26	LEU
2	BB	55	LEU
2	BB	237	VAL
2	BB	284	ASN
2	BC	68	SER
2	BC	187	VAL
3	BD	14	LEU
3	BD	30	VAL
3	BD	156	VAL
3	BD	207	ARG
3	BD	290	ARG
3	BD	387	VAL
3	BD	532	ASP
3	BD	613	ASN
3	BD	660	TRP
3	BD	748	MET
3	BD	799	THR
3	BE	6	ASP
3	BE	97	ARG
3	BE	156	VAL
3	BE	297	THR
3	BE	345	GLU
3	BE	564	THR
3	BE	629	ASN
3	BF	193	LEU
3	BF	207	ARG
3	BF	402	ARG
3	BF	467	LEU
3	BF	659	LEU
3	BF	726	THR
3	BF	833	VAL
3	BF	896	THR
3	BF	901	ILE
4	BG	165	ARG
4	BH	169	LEU
4	BI	16	ASP
4	BI	103	VAL
4	BI	208	THR
4	BJ	103	VAL
4	BJ	210	GLU
4	BK	96	LEU

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Mol	Chain	Res	Type
4	BK	210	GLU
4	BL	51	THR
4	BL	165	ARG
4	BL	178	ASN
4	BL	196	THR
4	BM	103	VAL
4	BN	165	ARG
4	BN	169	LEU
4	BO	169	LEU
5	QF	324	ILE
5	QF	336	SER
5	QH	324	ILE
5	QJ	324	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (77) such sidechains are listed below:

Mol	Chain	Res	Type
1	B5	104	ASN
1	B6	104	ASN
2	BA	36	ASN
2	BA	142	GLN
2	BA	203	ASN
2	BA	221	ASN
2	BA	262	GLN
2	BB	36	ASN
2	BB	181	ASN
2	BB	190	GLN
2	BB	262	GLN
2	BC	36	ASN
2	BC	142	GLN
2	BC	203	ASN
2	BC	231	GLN
2	BC	262	GLN
3	BD	103	GLN
3	BD	122	ASN
3	BD	131	ASN
3	BD	198	GLN
3	BD	269	GLN
3	BD	367	GLN
3	BD	695	ASN
3	BD	853	ASN
3	BD	868	GLN

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Mol	Chain	Res	Type
3	BE	22	GLN
3	BE	103	GLN
3	BE	122	ASN
3	BE	131	ASN
3	BE	198	GLN
3	BE	420	ASN
3	BE	425	ASN
3	BE	789	GLN
3	BE	834	ASN
3	BE	868	GLN
3	BF	88	ASN
3	BF	131	ASN
3	BF	150	ASN
3	BF	198	GLN
3	BF	213	GLN
3	BF	269	GLN
3	BF	420	ASN
3	BF	425	ASN
3	BF	445	GLN
3	BF	533	ASN
3	BF	613	ASN
3	BF	741	GLN
3	BF	802	ASN
3	BF	818	ASN
4	BG	71	GLN
4	BG	112	ASN
4	BG	172	HIS
4	BH	172	HIS
4	BH	215	ASN
4	BI	60	ASN
4	BI	167	ASN
4	BI	172	HIS
4	BJ	71	GLN
4	BJ	112	ASN
4	BJ	167	ASN
4	BK	85	GLN
4	BL	71	GLN
4	BL	167	ASN
4	BM	22	ASN
4	BM	71	GLN
4	BM	112	ASN
4	BM	167	ASN

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Mol	Chain	Res	Type
4	BM	172	HIS
4	BM	250	HIS
4	BN	85	GLN
4	BN	178	ASN
4	BN	250	HIS
4	BO	60	ASN
4	BO	85	GLN
4	BO	167	ASN
4	BO	250	HIS
5	QE	316	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 62 ligands modelled in this entry, 62 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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

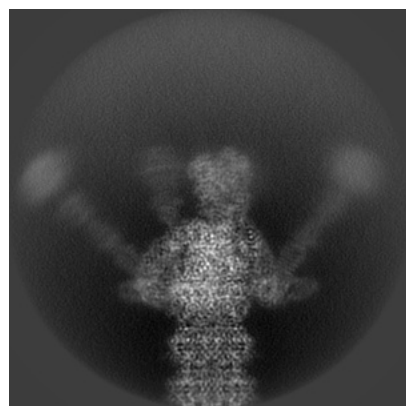
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51915. These allow visual inspection of the internal detail of the map and identification of artifacts.

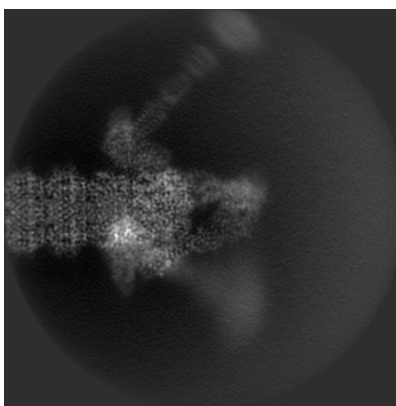
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

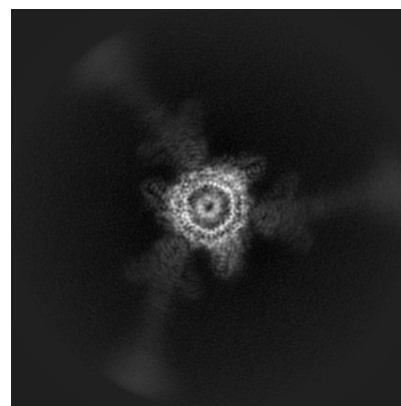
6.1.1 Primary map



X

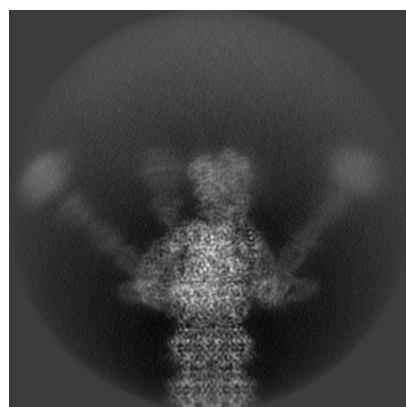


Y

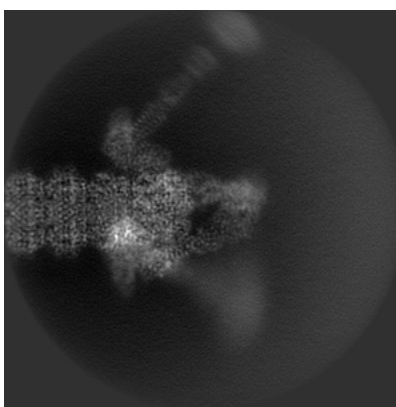


Z

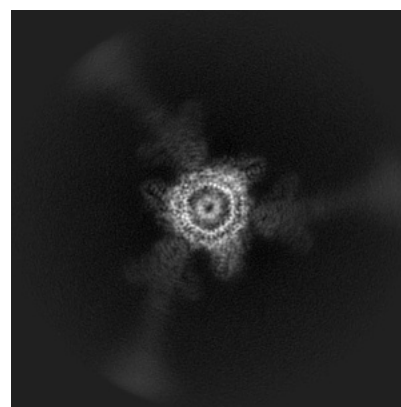
6.1.2 Raw map



X



Y

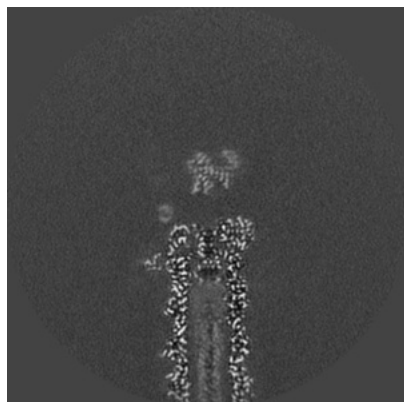


Z

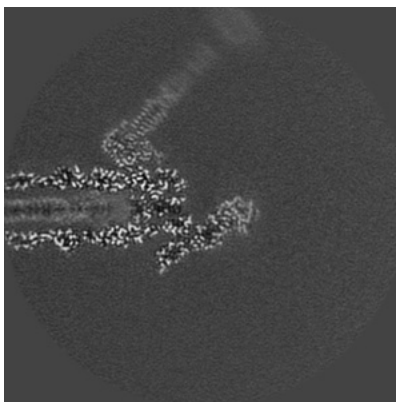
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

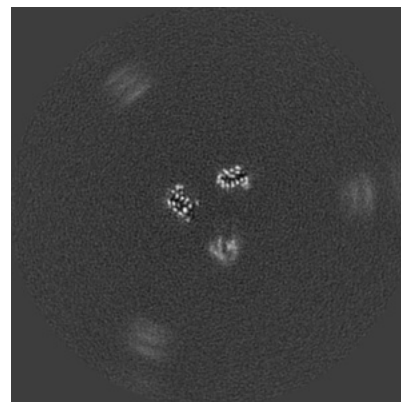
6.2.1 Primary map



X Index: 160

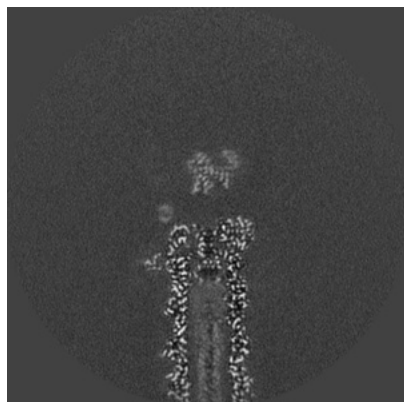


Y Index: 160

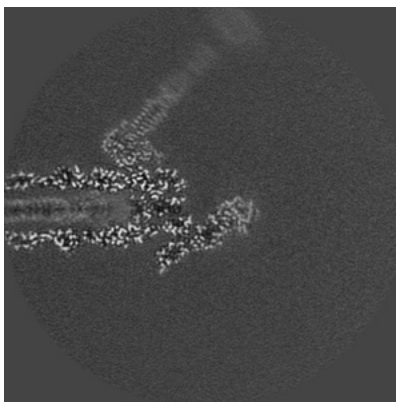


Z Index: 160

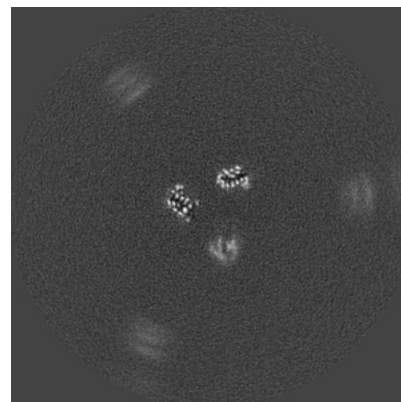
6.2.2 Raw map



X Index: 160



Y Index: 160

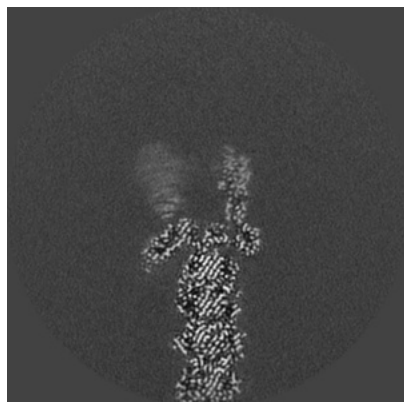


Z Index: 160

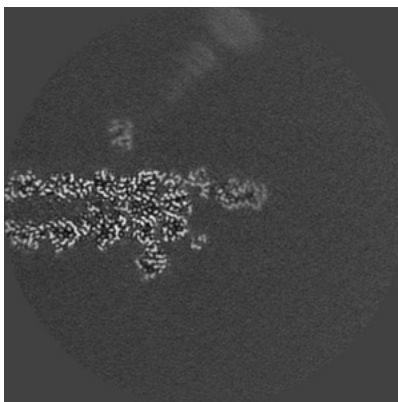
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

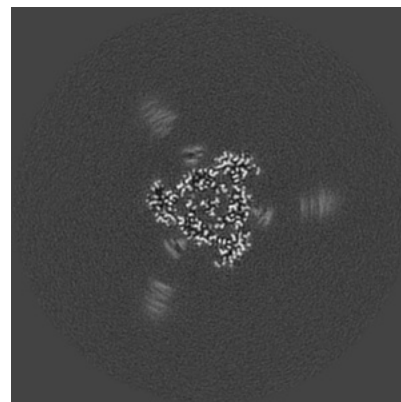
6.3.1 Primary map



X Index: 177

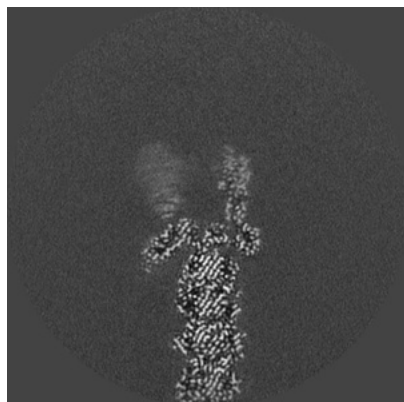


Y Index: 176

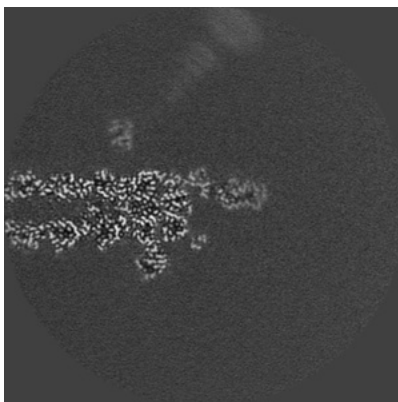


Z Index: 129

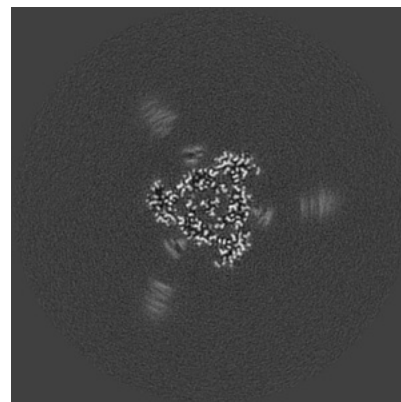
6.3.2 Raw map



X Index: 177



Y Index: 176



Z Index: 129

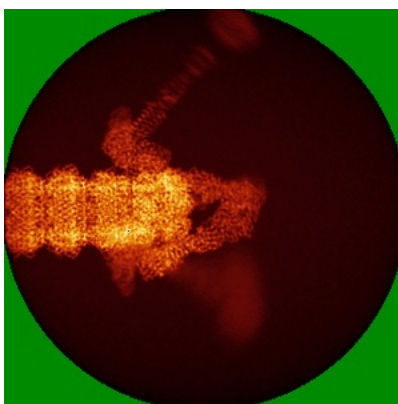
The images above show the largest variance slices of the map in three orthogonal directions.

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

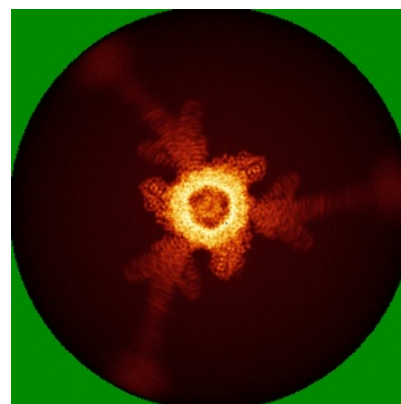
6.4.1 Primary map



X



Y

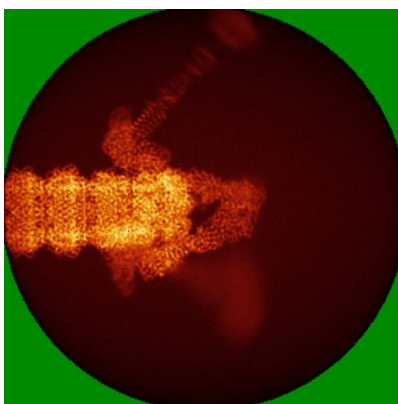


Z

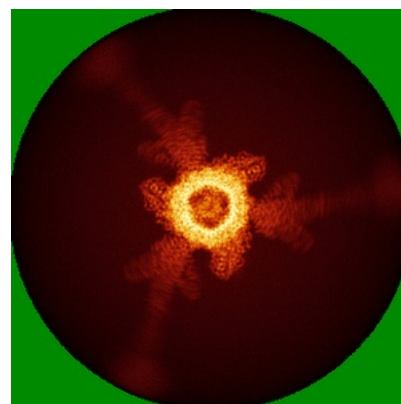
6.4.2 Raw map



X



Y

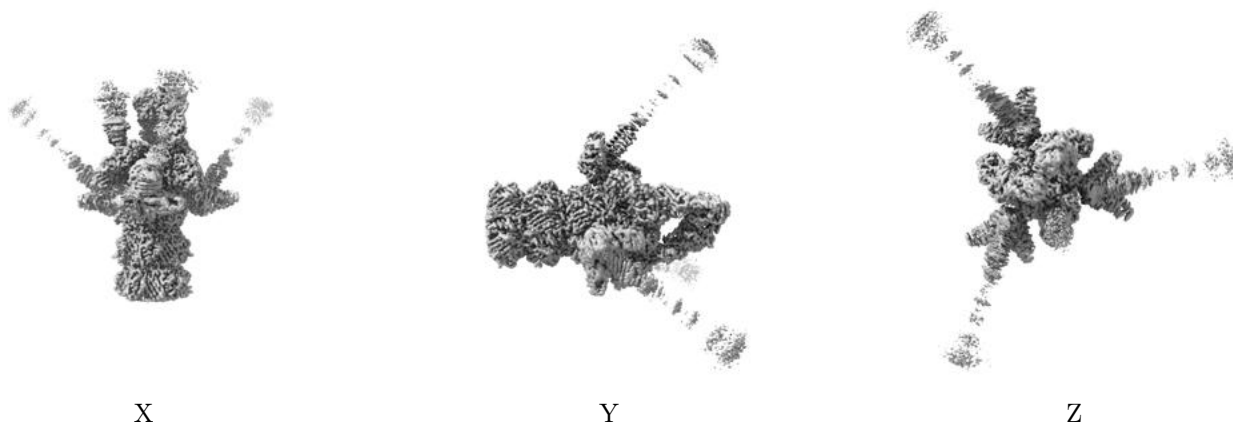


Z

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.

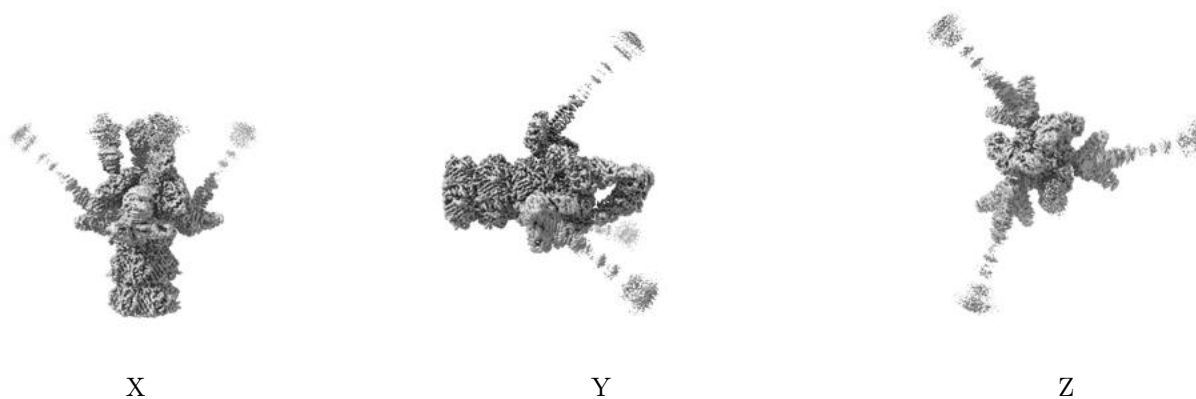
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.008. 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.

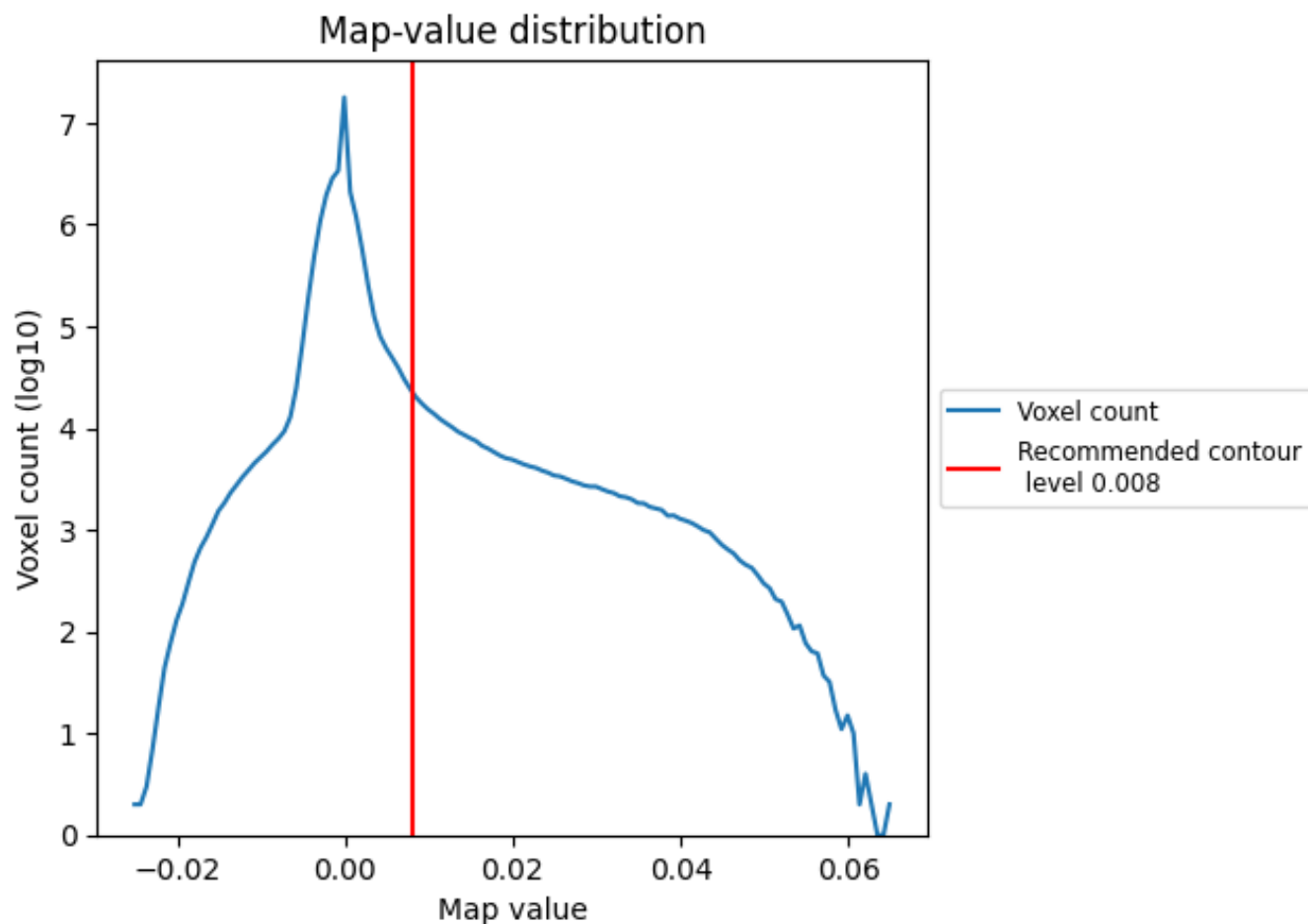
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

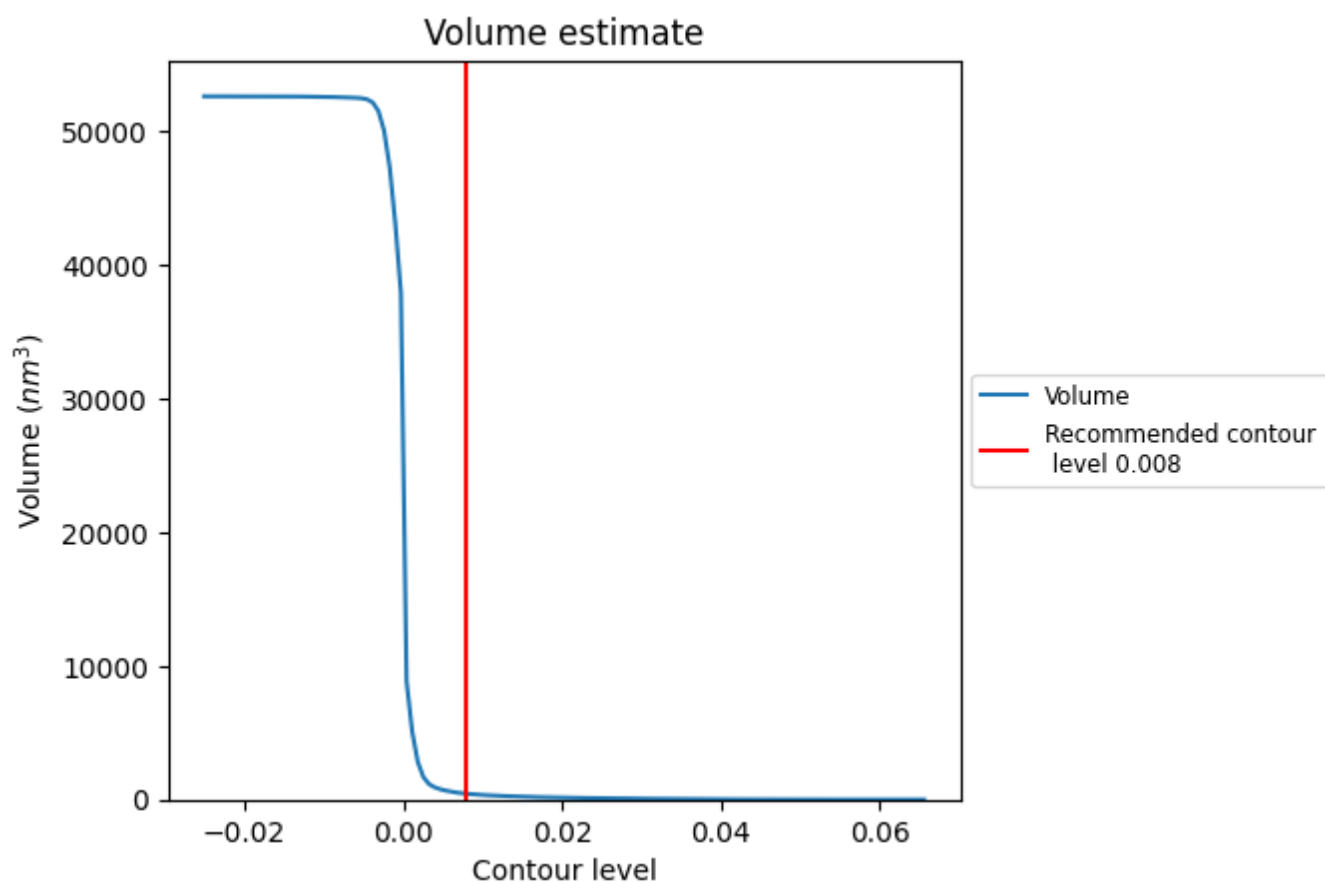
This section contains the results of statistical analysis of the map.

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.

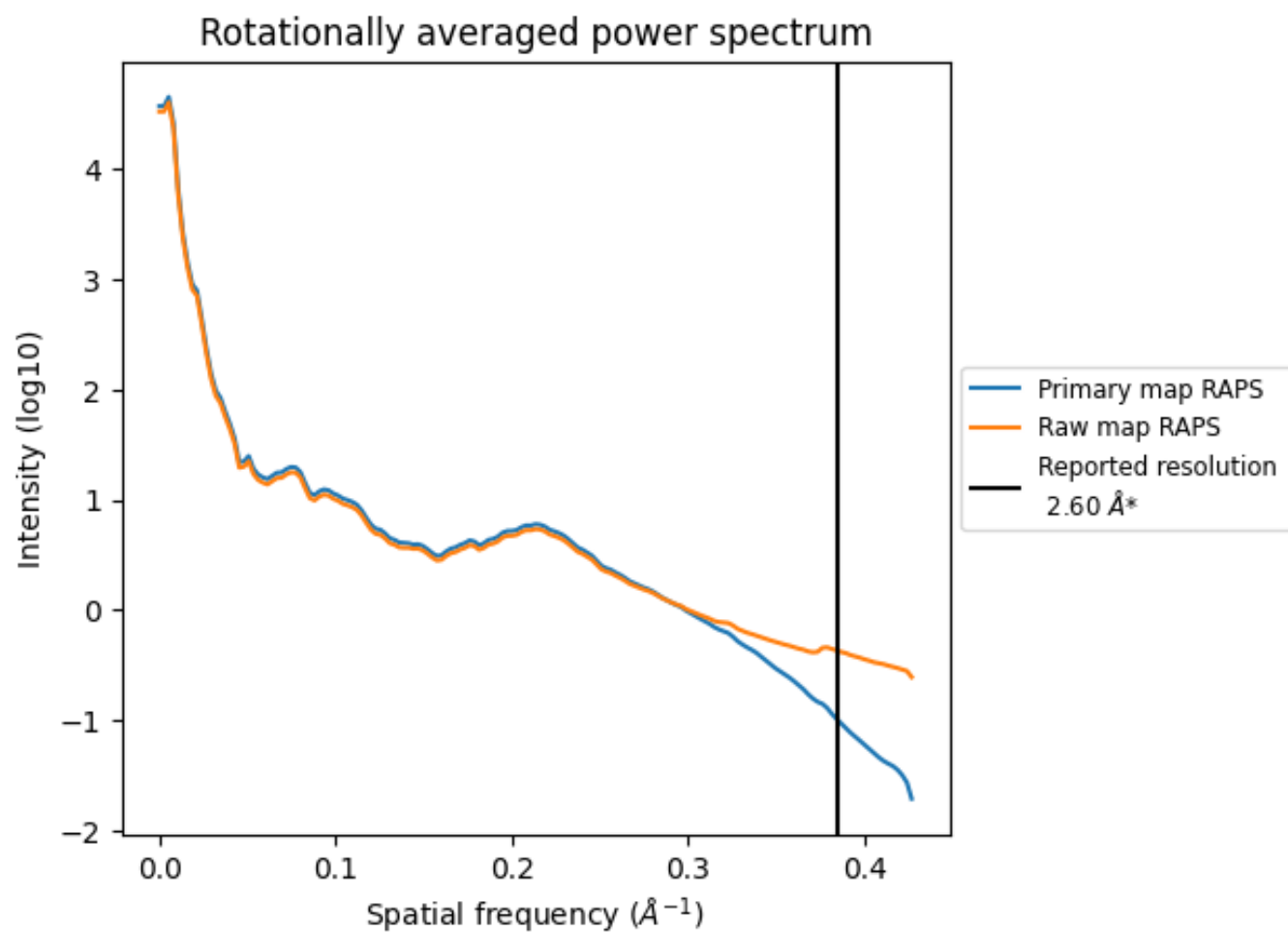
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 434 nm^3 ; this corresponds to an approximate mass of 392 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 ⓘ

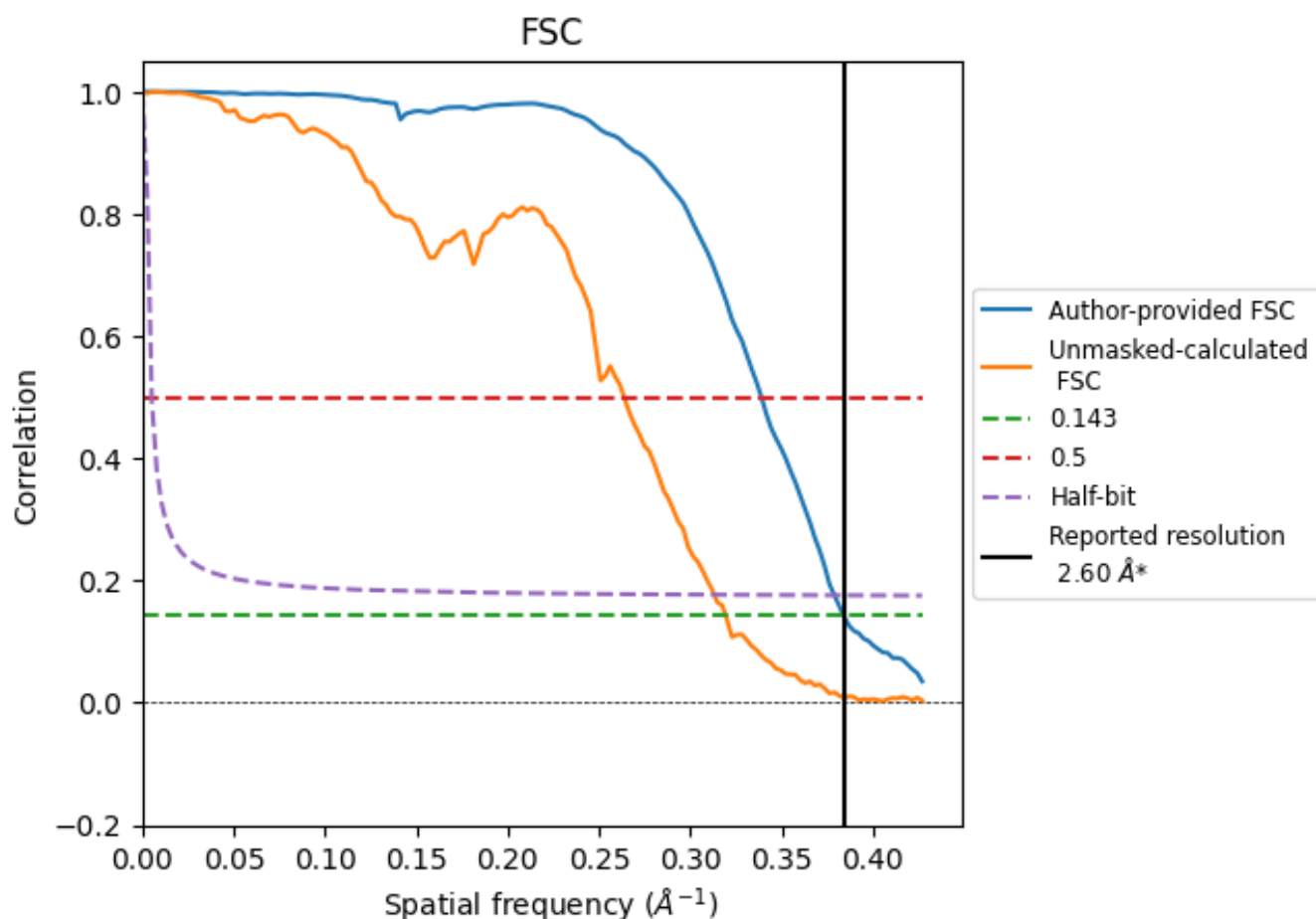


*Reported resolution corresponds to spatial frequency of 0.385 Å⁻¹

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 0.385 \AA^{-1}

8.2 Resolution estimates [i](#)

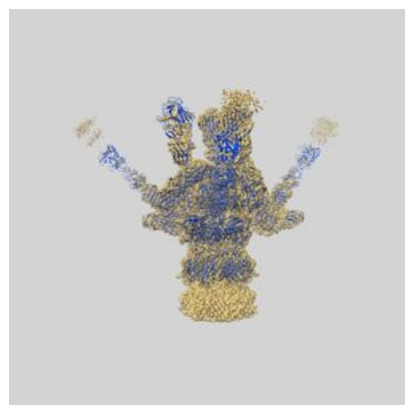
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	2.60	2.95	2.64
Unmasked-calculated*	3.13	3.79	3.19

*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 3.13 differs from the reported value 2.6 by more than 10 %

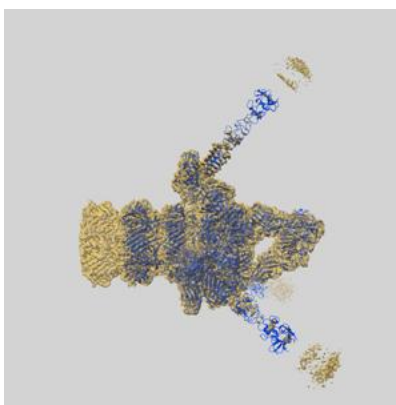
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-51915 and PDB model 9H7V. Per-residue inclusion information can be found in section [3](#) on page [8](#).

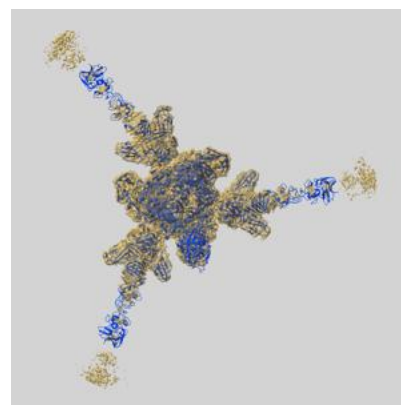
9.1 Map-model overlay [i](#)



X



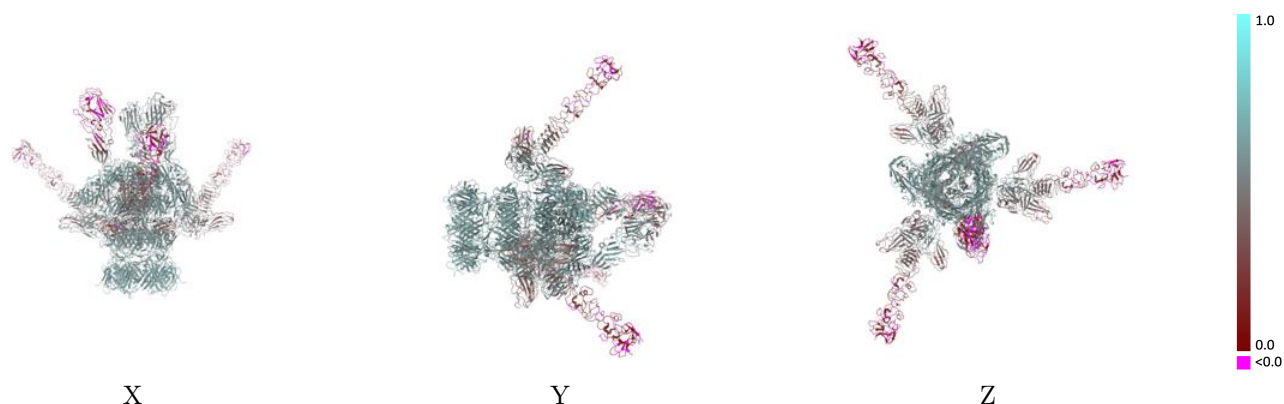
Y



Z

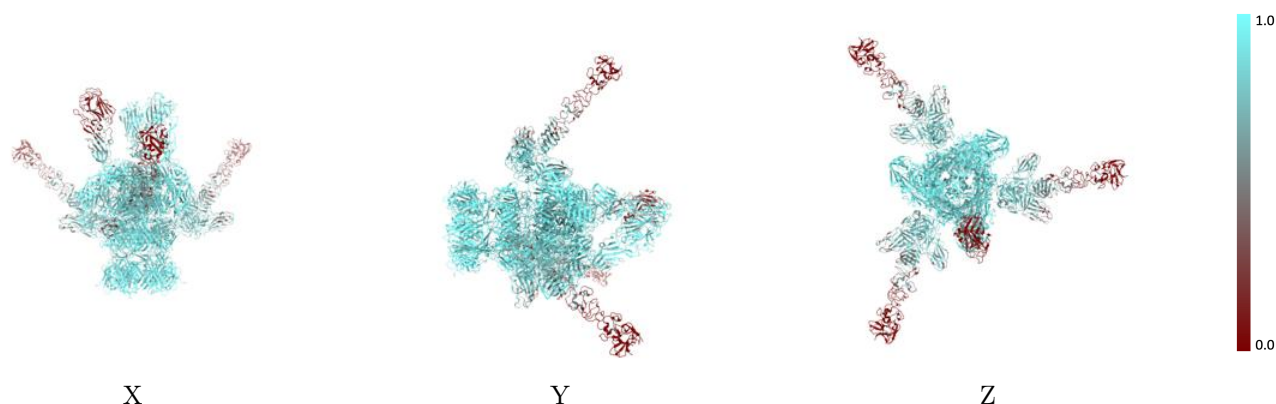
The images above show the 3D surface view of the map at the recommended contour level 0.008 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



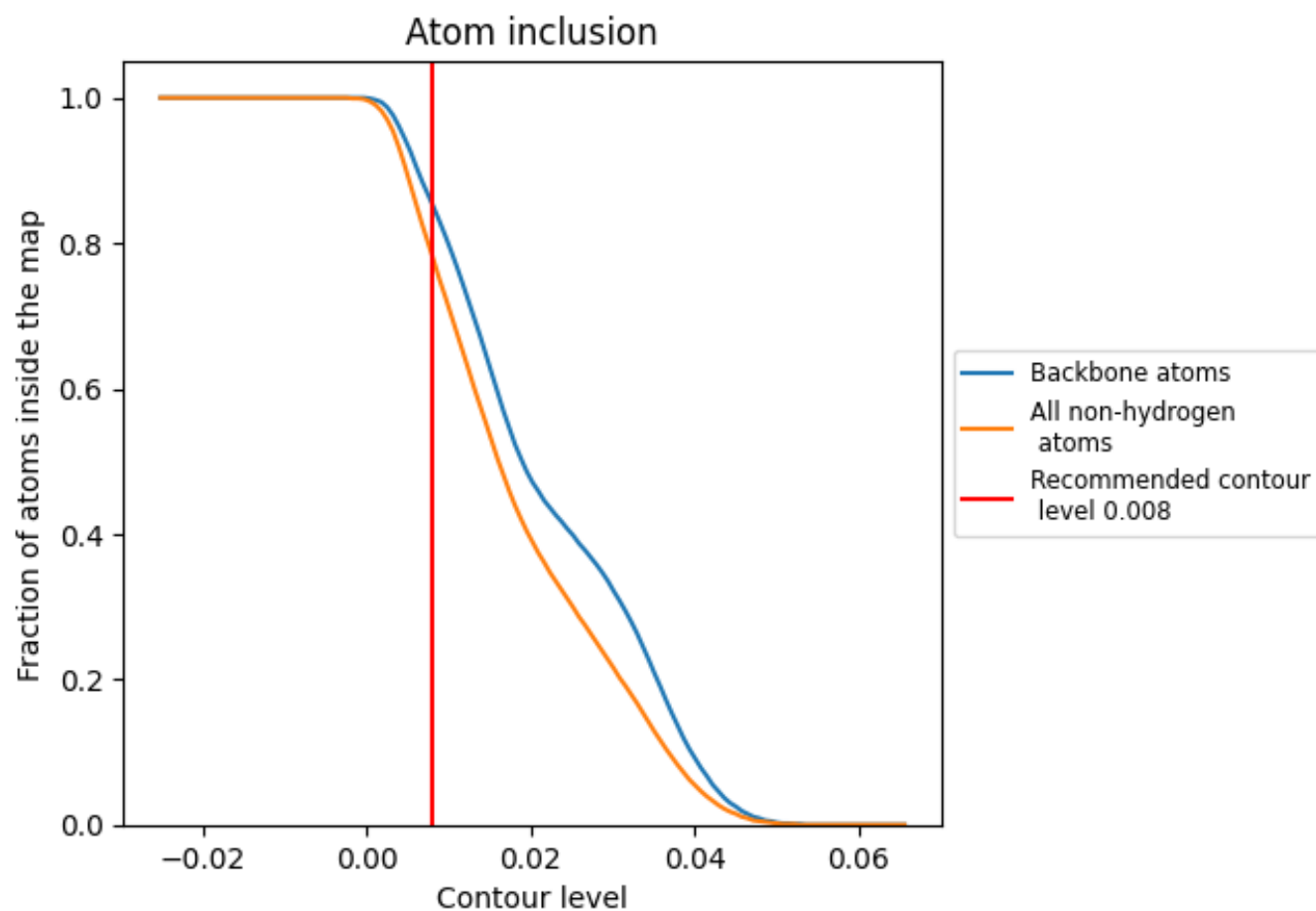
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.008).

























































9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 78% 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 (0.008) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7840	 0.4880
B1	 0.9400	 0.6010
B2	 0.9360	 0.5970
B3	 0.9360	 0.5990
B4	 0.9390	 0.5990
B5	 0.9350	 0.6010
B6	 0.9410	 0.5950
BA	 0.9430	 0.6010
BB	 0.9440	 0.5970
BC	 0.9450	 0.6010
BD	 0.9160	 0.5620
BE	 0.9270	 0.5710
BF	 0.7260	 0.4410
BG	 0.5990	 0.3640
BH	 0.5590	 0.3450
BI	 0.6040	 0.3690
BJ	 0.5920	 0.3660
BK	 0.5530	 0.3500
BL	 0.5870	 0.3620
BM	 0.5990	 0.3690
BN	 0.5360	 0.3280
BO	 0.6010	 0.3650
QE	 0.8020	 0.5230
QF	 0.8980	 0.5630
QG	 0.8310	 0.5040
QH	 0.9090	 0.5480
QI	 0.8370	 0.5010
QJ	 0.8920	 0.5690

