



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 10:23 PM UTC

PDB ID : 7AGX / pdb_00007agx
EMDB ID : EMD-11780
Title : Apo-state type 3 secretion system export apparatus complex from *Salmonella enterica typhimurium*
Authors : Goessweiner-Mohr, N.; Fahrenkamp, D.; Miletic, S.; Wald, J.; Marlovits, T.
Deposited on : 2020-09-23
Resolution : 3.60 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

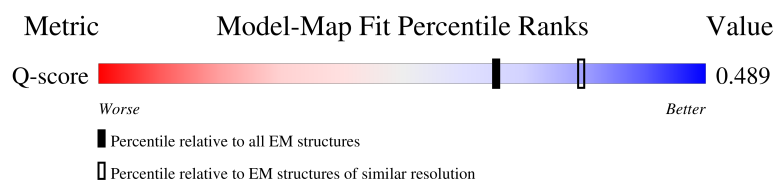
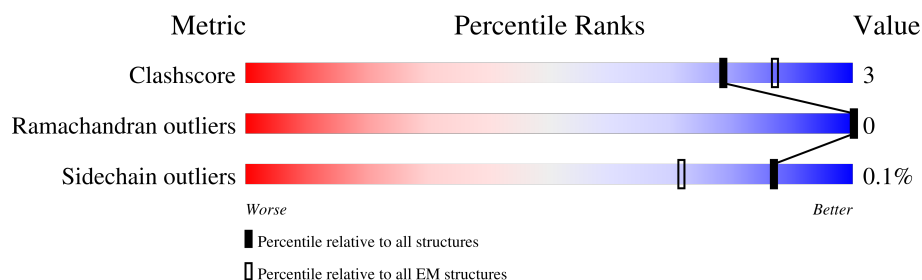
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 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.



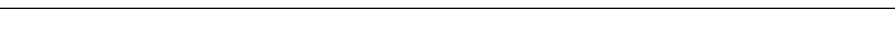
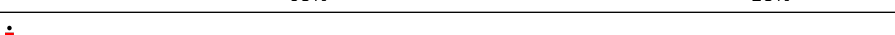
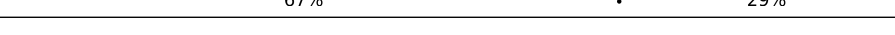
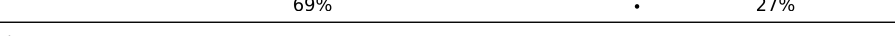
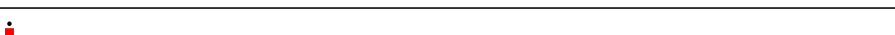
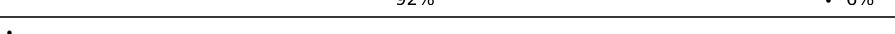
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12797 (3.10 - 4.10)

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	1A	224	
1	1B	224	
1	1C	224	
1	1D	224	

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Mol	Chain	Length	Quality of chain
1	1E	224	
2	1F	263	
3	1G	86	
3	1H	86	
3	1I	86	
3	1J	86	
4	1K	101	
4	1L	101	
4	1M	101	
4	1N	101	
4	1O	101	
4	1P	101	
5	2A	80	
5	2B	80	
5	2C	80	
5	2D	80	
5	2E	80	
5	2F	80	
5	2G	80	
5	2H	80	
5	2I	80	
5	2J	80	
5	2K	80	
5	2L	80	
5	2M	80	

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Mol	Chain	Length	Quality of chain
5	2N	80	65%6%29%
5	2O	80	54%9%38%
5	2P	80	45%10%45%
5	2Q	80	16%84%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 47749 atoms, of which 24089 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 Surface presentation of antigens protein SpaP.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	1A	200	Total	C	H	N	O	S	0	0
			3196	1050	1622	234	279	11		
1	1B	195	Total	C	H	N	O	S	0	0
			3120	1024	1587	228	270	11		
1	1C	194	Total	C	H	N	O	S	0	0
			3100	1021	1575	226	267	11		
1	1D	190	Total	C	H	N	O	S	0	0
			3055	1002	1558	221	263	11		
1	1E	199	Total	C	H	N	O	S	0	0
			3203	1051	1632	238	271	11		

- Molecule 2 is a protein called Surface presentation of antigens protein SpaR.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	1F	257	Total	C	H	N	O	S	0	0
			3968	1297	2008	311	338	14		

- Molecule 3 is a protein called Surface presentation of antigens protein SpaQ.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	1G	73	Total	C	H	N	O	S	0	0
			1160	385	602	82	89	2		
3	1H	83	Total	C	H	N	O	S	0	0
			1320	433	681	96	108	2		
3	1I	83	Total	C	H	N	O	S	0	0
			1320	433	681	96	108	2		
3	1J	83	Total	C	H	N	O	S	0	0
			1320	433	681	96	108	2		

- Molecule 4 is a protein called Protein PrgJ.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	1K	68	Total	C	H	N	O	S	
			1042	321	529	84	106	2	0
4	1L	73	Total	C	H	N	O	S	
			1129	347	571	94	115	2	0
4	1M	72	Total	C	H	N	O	S	
			1118	344	566	93	113	2	0
4	1N	74	Total	C	H	N	O	S	
			1140	350	576	95	117	2	0
4	1O	73	Total	C	H	N	O	S	
			1129	347	571	94	115	2	0
4	1P	73	Total	C	H	N	O	S	
			1129	347	571	94	115	2	0

- Molecule 5 is a protein called Protein PrgI.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	2A	59	Total	C	H	N	O		
			937	294	471	80	92	0	0
5	2B	61	Total	C	H	N	O		
			964	303	484	82	95	0	0
5	2C	59	Total	C	H	N	O		
			937	294	471	80	92	0	0
5	2D	60	Total	C	H	N	O		
			949	298	475	81	95	0	0
5	2E	60	Total	C	H	N	O		
			949	298	475	81	95	0	0
5	2F	72	Total	C	H	N	O		
			1120	353	558	94	115	0	0
5	2G	75	Total	C	H	N	O		
			1158	367	575	97	119	0	0
5	2H	75	Total	C	H	N	O		
			1159	367	575	97	120	0	0
5	2I	75	Total	C	H	N	O		
			1159	367	575	97	120	0	0
5	2J	75	Total	C	H	N	O		
			1159	367	575	97	120	0	0
5	2K	77	Total	C	H	N	O		
			1196	383	592	100	121	0	0
5	2L	66	Total	C	H	N	O		
			1033	333	506	87	107	0	0
5	2M	63	Total	C	H	N	O		
			992	320	486	84	102	0	0
5	2N	57	Total	C	H	N	O		
			901	289	442	77	93	0	0

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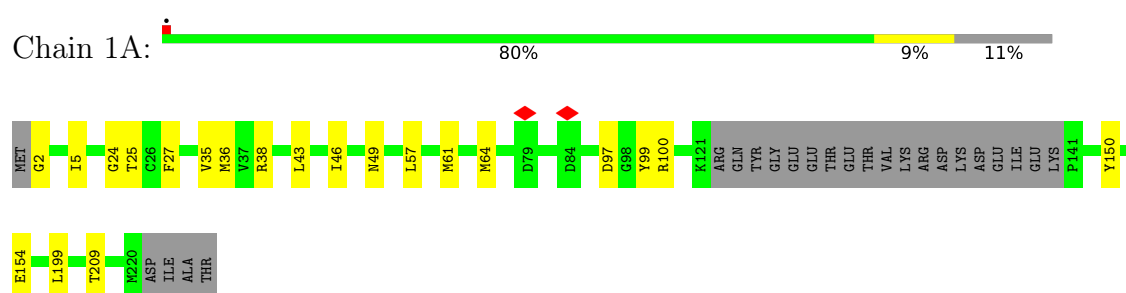
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Mol	Chain	Residues	Atoms					AltConf	Trace
5	2O	50	Total	C	H	N	O	0	0
			788	256	382	68	82		
5	2P	44	Total	C	H	N	O	0	0
			700	229	342	60	69		
5	2Q	13	Total	C	H	N	O	0	0
			199	70	94	15	20		

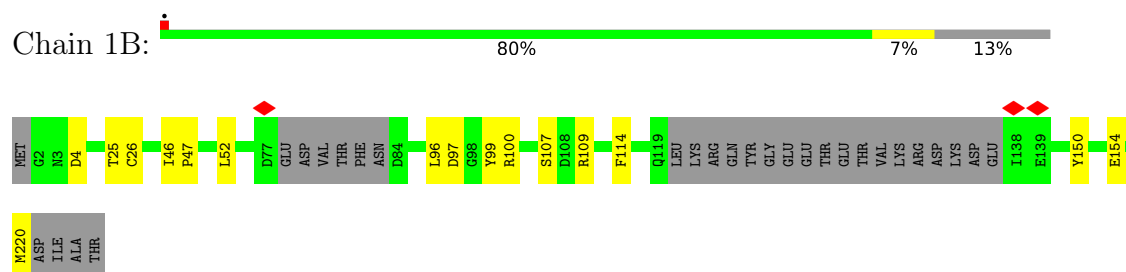
3 Residue-property plots [i](#)

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.

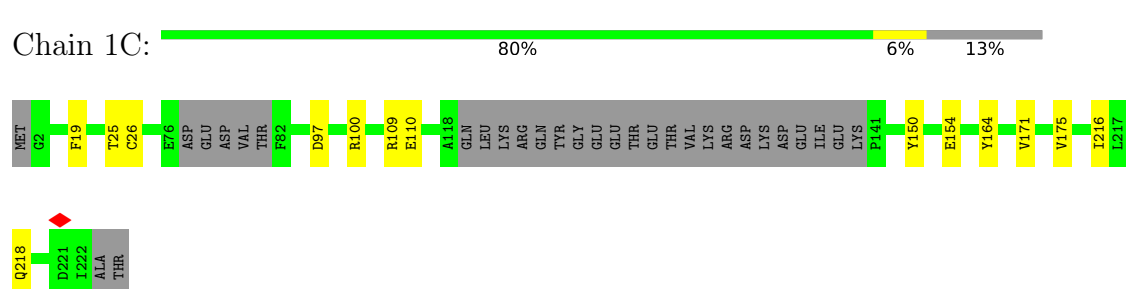
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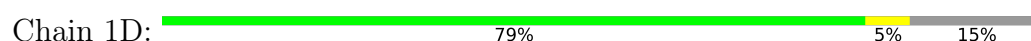
- Molecule 1: Surface presentation of antigens protein SpaP

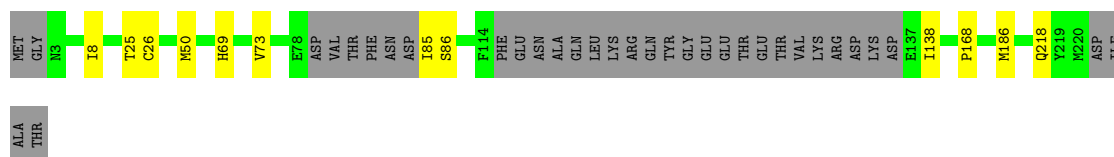


- Molecule 1: Surface presentation of antigens protein SpaP



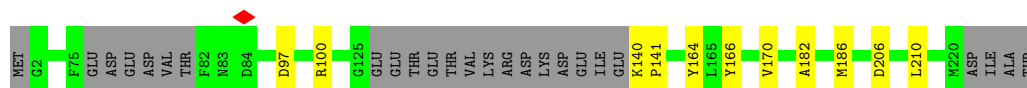
- Molecule 1: Surface presentation of antigens protein SpaP





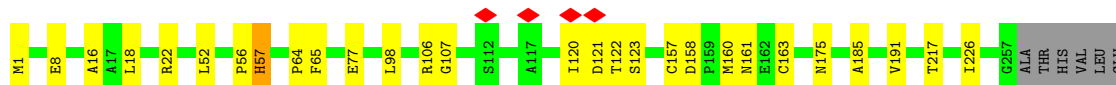
- Molecule 1: Surface presentation of antigens protein SpaP

Chain 1E: 84% 5% 11%



- Molecule 2: Surface presentation of antigens protein SpaR

Chain 1F: 87% 10% .



- Molecule 3: Surface presentation of antigens protein SpaQ

Chain 1G: 23% 85% 15%



- Molecule 3: Surface presentation of antigens protein SpaQ

Chain 1H: 8% 87% 9% .



- Molecule 3: Surface presentation of antigens protein SpaQ

Chain 1I: 90% 7% .

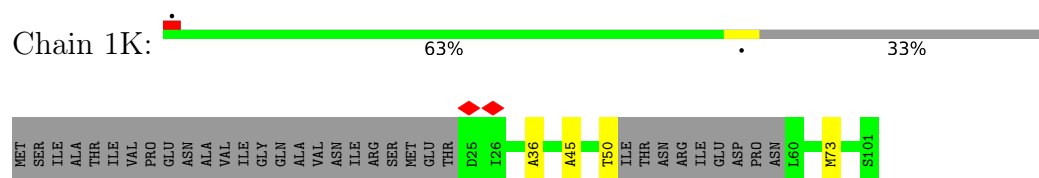


- Molecule 3: Surface presentation of antigens protein SpaQ

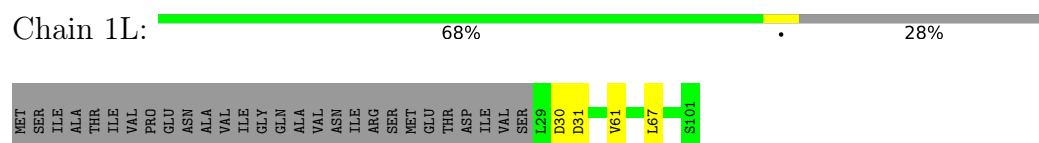
Chain 1J: 91% 6% .



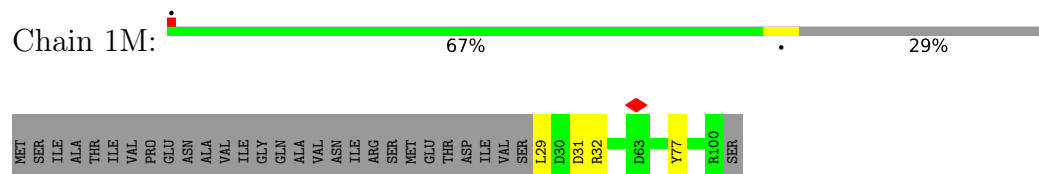
● Molecule 4: Protein PrgJ



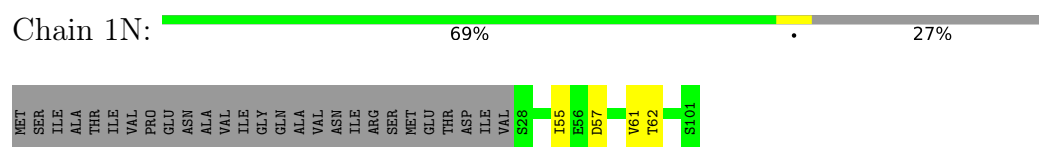
● Molecule 4: Protein PrgJ



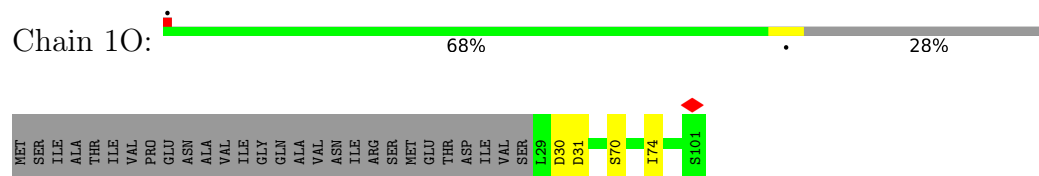
● Molecule 4: Protein PrgJ



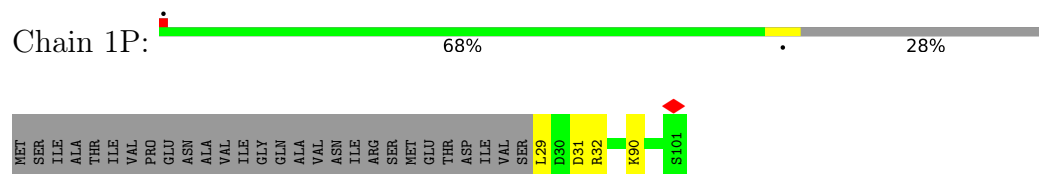
● Molecule 4: Protein PrgJ



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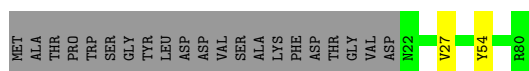


● Molecule 4: Protein PrgJ

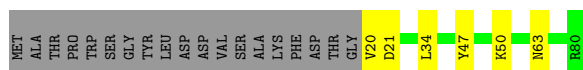


● Molecule 5: Protein PrgI

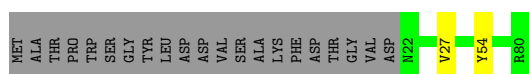




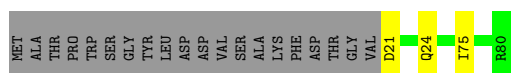
● Molecule 5: Protein PrgI



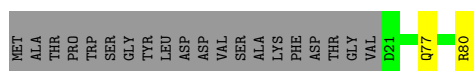
● Molecule 5: Protein PrgI



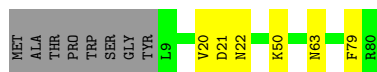
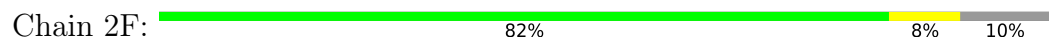
● Molecule 5: Protein PrgI



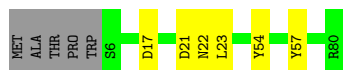
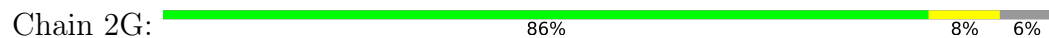
● Molecule 5: Protein PrgI



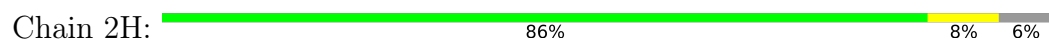
● Molecule 5: Protein PrgI



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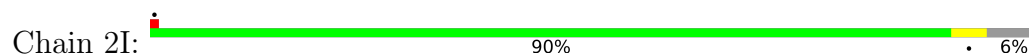


● Molecule 5: Protein PrgI

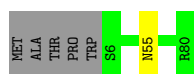




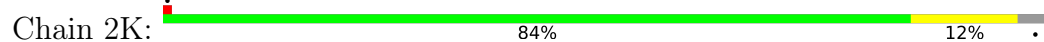
- Molecule 5: Protein PrgI



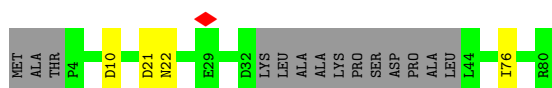
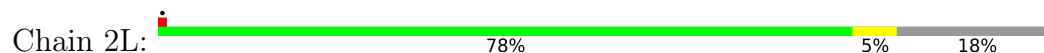
- Molecule 5: Protein PrgI



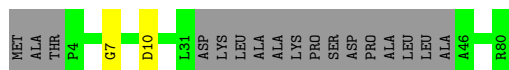
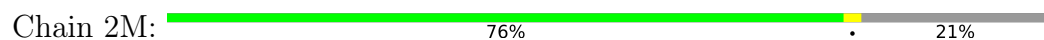
- Molecule 5: Protein PrgI



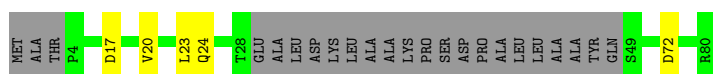
- Molecule 5: Protein PrgI



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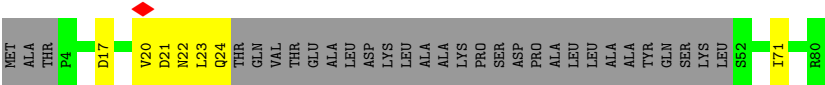


- Molecule 5: Protein PrgI

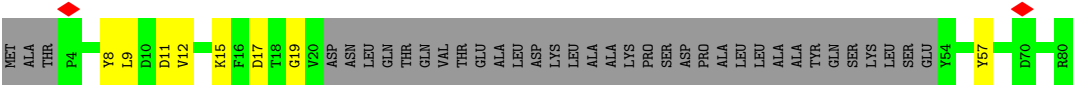


- Molecule 5: Protein PrgI

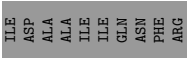




● Molecule 5: Protein PrgI



● Molecule 5: Protein PrgI



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	54491	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 ($e^-/\text{\AA}^2$)	31.5	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.087	Depositor
Minimum map value	-0.061	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.008	Depositor
Map size (Å)	470.88, 470.88, 470.88	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.09, 1.09, 1.09	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	1A	0.32	0/1610	0.52	0/2186
1	1B	0.31	0/1567	0.48	0/2126
1	1C	0.29	0/1560	0.48	0/2117
1	1D	0.30	0/1530	0.49	0/2076
1	1E	0.31	0/1607	0.51	0/2178
2	1F	0.32	0/2012	0.59	0/2754
3	1G	0.23	0/570	0.47	0/776
3	1H	0.24	0/652	0.55	0/890
3	1I	0.27	0/652	0.45	0/890
3	1J	0.28	0/652	0.48	0/890
4	1K	0.31	0/515	0.49	0/696
4	1L	0.34	0/562	0.48	0/762
4	1M	0.31	0/556	0.44	0/754
4	1N	0.29	0/568	0.52	0/770
4	1O	0.29	0/562	0.45	0/762
4	1P	0.32	0/562	0.44	0/762
5	2A	0.34	0/472	0.49	0/638
5	2B	0.36	0/486	0.44	0/659
5	2C	0.32	0/472	0.44	0/638
5	2D	0.32	0/480	0.48	0/649
5	2E	0.36	0/480	0.44	0/649
5	2F	0.33	0/569	0.51	0/770
5	2G	0.36	0/591	0.53	0/801
5	2H	0.32	0/592	0.43	0/801
5	2I	0.29	0/592	0.50	0/801
5	2J	0.30	0/592	0.45	0/801
5	2K	0.29	0/615	0.51	0/835
5	2L	0.31	0/535	0.45	0/724
5	2M	0.32	0/514	0.44	0/695
5	2N	0.30	0/466	0.49	0/628
5	2O	0.28	0/413	0.46	0/556
5	2P	0.31	0/365	0.47	0/491
5	2Q	0.30	0/109	0.41	0/147
All	All	0.31	0/24080	0.49	0/32672

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	1A	1574	1622	1621	15	0
1	1B	1533	1587	1584	13	0
1	1C	1525	1575	1573	10	0
1	1D	1497	1558	1555	10	0
1	1E	1571	1632	1629	9	0
2	1F	1960	2008	2008	20	0
3	1G	558	602	600	0	0
3	1H	639	681	680	5	0
3	1I	639	681	680	4	0
3	1J	639	681	680	3	0
4	1K	513	529	527	3	0
4	1L	558	571	570	2	0
4	1M	552	566	565	4	0
4	1N	564	576	575	3	0
4	1O	558	571	570	2	0
4	1P	558	571	570	3	0
5	2A	466	471	470	1	0
5	2B	480	484	483	4	0
5	2C	466	471	470	1	0
5	2D	474	475	474	2	0
5	2E	474	475	474	1	0
5	2F	562	558	557	5	0
5	2G	583	575	574	3	0
5	2H	584	575	574	4	0
5	2I	584	575	574	2	0
5	2J	584	575	574	2	0
5	2K	604	592	592	6	0
5	2L	527	506	505	3	0
5	2M	506	486	485	1	0
5	2N	459	442	441	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	2O	406	382	381	8	0
5	2P	358	342	341	4	0
5	2Q	105	94	94	0	0
All	All	23660	24089	24050	132	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 3.

All (132) 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)
5:2I:17:ASP:OD2	5:2I:57:TYR:OH	1.90	0.88
1:1E:97:ASP:OD1	1:1E:100:ARG:NH1	2.15	0.79
1:1B:107:SER:O	1:1B:109:ARG:NH2	2.18	0.77
2:1F:8:GLU:OE1	4:1P:32:ARG:NH1	2.18	0.76
2:1F:191:VAL:HG21	2:1F:226:ILE:CD1	2.17	0.75
5:2N:17:ASP:OD1	5:2N:24:GLN:NE2	2.21	0.73
5:2K:17:ASP:OD2	5:2K:57:TYR:OH	2.07	0.72
5:2P:17:ASP:OD1	5:2P:57:TYR:OH	2.06	0.72
1:1A:209:THR:HG23	2:1F:175:ASN:ND2	2.07	0.69
5:2H:17:ASP:OD1	5:2H:57:TYR:OH	2.11	0.68
5:2J:55:ASN:ND2	5:2O:71:ILE:HD11	2.09	0.68
1:1A:2:GLY:N	4:1K:36:ALA:O	2.27	0.68
2:1F:191:VAL:HG21	2:1F:226:ILE:HD13	1.76	0.66
2:1F:98:LEU:HD12	2:1F:185:ALA:HB2	1.78	0.65
1:1A:209:THR:HG23	2:1F:175:ASN:HD22	1.61	0.64
5:2E:77:GLN:OE1	5:2E:80:ARG:NH2	2.26	0.64
5:2G:17:ASP:OD1	5:2G:57:TYR:OH	2.15	0.63
1:1C:97:ASP:OD1	1:1C:100:ARG:NH1	2.32	0.62
3:1H:37:GLN:OE1	3:1H:43:GLN:NE2	2.31	0.62
2:1F:98:LEU:CD1	2:1F:185:ALA:HB2	2.30	0.62
5:2D:21:ASP:N	5:2D:24:GLN:OE1	2.33	0.61
4:1N:55:ILE:HG22	4:1N:55:ILE:O	2.01	0.61
5:2O:21:ASP:OD2	5:2O:22:ASN:N	2.37	0.58
1:1A:97:ASP:OD1	1:1A:100:ARG:NH1	2.38	0.57
1:1A:25:THR:HG23	1:1A:64:MET:HG3	1.86	0.56
1:1B:25:THR:HG22	1:1B:26:CYS:N	2.21	0.56
2:1F:1:MET:HE3	4:1K:50:THR:H	1.70	0.56
4:1O:30:ASP:OD1	4:1O:31:ASP:N	2.37	0.56
1:1D:25:THR:HG22	1:1D:26:CYS:N	2.21	0.55
5:2N:20:VAL:HG12	5:2N:20:VAL:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1D:218:GLN:NE2	3:1I:83:LEU:O	2.34	0.55
4:1N:61:VAL:HG23	4:1N:62:THR:HG23	1.88	0.54
5:2K:11:ASP:OD2	5:2K:15:LYS:NZ	2.37	0.54
5:2P:9:LEU:O	5:2P:12:VAL:HG22	2.07	0.54
1:1B:114:PHE:CE2	1:1C:216:ILE:HD11	2.42	0.54
5:2F:63:ASN:ND2	5:2L:76:ILE:O	2.41	0.54
5:2F:21:ASP:OD2	5:2F:22:ASN:N	2.41	0.53
5:2H:20:VAL:HB	5:2H:23:LEU:HD12	1.90	0.53
3:1I:13:TYR:CZ	3:1I:17:ILE:HD11	2.44	0.53
1:1E:140:LYS:N	1:1E:141:PRO:CD	2.72	0.53
1:1C:218:GLN:NE2	3:1H:83:LEU:O	2.43	0.52
3:1H:3:ASP:OD1	3:1H:4:LEU:N	2.43	0.51
3:1J:29:ILE:CG2	3:1J:51:ILE:HG22	2.41	0.51
1:1D:85:ILE:HG23	1:1D:86:SER:N	2.24	0.51
5:2K:65:VAL:O	5:2K:65:VAL:HG12	2.10	0.51
5:2B:20:VAL:HG13	5:2B:21:ASP:N	2.26	0.51
4:1L:30:ASP:OD1	4:1L:31:ASP:N	2.44	0.50
5:2J:55:ASN:HD21	5:2O:71:ILE:HD11	1.75	0.50
1:1B:220:MET:HA	1:1B:220:MET:HE2	1.94	0.50
5:2I:20:VAL:HG12	5:2I:20:VAL:O	2.11	0.50
5:2F:20:VAL:HG12	5:2F:20:VAL:O	2.12	0.50
5:2K:20:VAL:HG12	5:2K:23:LEU:HB3	1.94	0.49
1:1D:69:HIS:CE1	1:1D:73:VAL:HG11	2.48	0.49
5:2B:63:ASN:ND2	5:2H:76:ILE:O	2.46	0.48
5:2P:15:LYS:O	5:2P:19:GLY:N	2.46	0.48
1:1C:150:TYR:OH	1:1C:154:GLU:OE2	2.28	0.48
2:1F:157:CYS:HB3	2:1F:163:CYS:HB3	1.95	0.48
1:1A:38:ARG:NH1	1:1A:49:ASN:OD1	2.44	0.48
1:1B:150:TYR:CE2	1:1B:154:GLU:HG3	2.49	0.48
1:1B:47:PRO:HG2	1:1B:52:LEU:HD21	1.95	0.47
2:1F:158:ASP:OD1	2:1F:161:ASN:ND2	2.45	0.47
1:1A:24:GLY:O	1:1A:99:TYR:OH	2.29	0.47
5:2B:50:LYS:NZ	5:2H:10:ASP:OD2	2.37	0.47
1:1D:138:ILE:HG13	1:1D:138:ILE:O	2.15	0.47
1:1E:166:TYR:CZ	1:1E:170:VAL:HG22	2.49	0.47
2:1F:56:PRO:HG2	2:1F:57:HIS:ND1	2.30	0.46
5:2A:27:VAL:HG21	5:2A:54:TYR:HB2	1.96	0.46
4:1K:45:ALA:HB1	4:1K:73:MET:HE3	1.97	0.46
1:1E:140:LYS:N	1:1E:141:PRO:HD2	2.31	0.46
3:1H:13:TYR:CZ	3:1H:17:ILE:HD11	2.51	0.46
5:2C:27:VAL:HG21	5:2C:54:TYR:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:2N:20:VAL:HG12	5:2N:23:LEU:HB2	1.97	0.45
1:1E:182:ALA:HA	2:1F:217:THR:HG22	1.99	0.45
2:1F:18:LEU:HD12	2:1F:65:PHE:CE1	2.52	0.45
1:1E:206:ASP:HB2	1:1E:210:LEU:HG	1.99	0.45
1:1A:36:MET:HG3	1:1B:46:ILE:HD13	1.98	0.45
4:1P:29:LEU:HG	4:1P:31:ASP:H	1.81	0.45
2:1F:120:ILE:HG22	2:1F:121:ASP:N	2.32	0.45
1:1A:35:VAL:HB	1:1B:46:ILE:HD11	1.99	0.44
4:1N:57:ASP:OD2	4:1N:57:ASP:C	2.60	0.44
1:1A:43:LEU:HD12	1:1A:199:LEU:HD11	2.00	0.44
5:2O:20:VAL:O	5:2O:24:GLN:N	2.34	0.44
5:2G:23:LEU:HD21	5:2G:54:TYR:HA	1.98	0.44
5:2L:21:ASP:OD1	5:2L:22:ASN:N	2.51	0.44
1:1C:19:PHE:CD2	1:1D:50:MET:HE1	2.52	0.44
1:1B:25:THR:CG2	1:1B:26:CYS:N	2.81	0.44
1:1B:96:LEU:O	1:1B:99:TYR:N	2.48	0.43
5:2M:7:GLY:N	5:2M:10:ASP:OD2	2.50	0.43
5:2P:8:TYR:O	5:2P:11:ASP:HB3	2.18	0.43
5:2F:50:LYS:NZ	5:2L:10:ASP:OD2	2.43	0.43
1:1A:57:LEU:O	1:1A:61:MET:HG2	2.18	0.43
1:1E:164:TYR:CD1	3:1J:82:ALA:HB2	2.53	0.43
1:1A:150:TYR:CZ	1:1A:154:GLU:HG3	2.54	0.43
5:2K:17:ASP:OD2	5:2K:61:GLN:NE2	2.52	0.43
5:2O:20:VAL:HG22	5:2O:23:LEU:HB2	2.00	0.43
4:1M:31:ASP:OD1	4:1M:32:ARG:N	2.52	0.43
1:1A:5:ILE:HD12	1:1A:5:ILE:N	2.34	0.42
4:1O:70:SER:O	4:1O:74:ILE:HG22	2.19	0.42
5:2K:69:LYS:HD2	5:2K:69:LYS:O	2.20	0.42
1:1C:171:VAL:O	1:1C:175:VAL:HG23	2.19	0.42
2:1F:122:THR:O	2:1F:123:SER:C	2.62	0.42
1:1B:114:PHE:CZ	1:1C:216:ILE:HD11	2.54	0.42
4:1L:61:VAL:O	4:1L:67:LEU:HD21	2.20	0.42
5:2N:72:ASP:OD1	5:2N:72:ASP:C	2.62	0.42
1:1A:43:LEU:HB3	1:1A:46:ILE:HD12	2.02	0.42
2:1F:106:ARG:CG	2:1F:107:GLY:N	2.82	0.42
1:1C:164:TYR:CD1	3:1H:82:ALA:HB2	2.54	0.42
1:1D:8:ILE:HG13	5:2D:75:ILE:HD11	2.01	0.42
1:1B:4:ASP:OD2	4:1M:77:TYR:OH	2.26	0.42
3:1J:13:TYR:CZ	3:1J:17:ILE:HD11	2.55	0.42
1:1C:25:THR:HG22	1:1C:26:CYS:N	2.33	0.42
2:1F:191:VAL:HG21	2:1F:226:ILE:HD12	1.97	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:2O:17:ASP:O	5:2O:20:VAL:HG12	2.19	0.42
1:1B:97:ASP:OD1	1:1B:100:ARG:NH1	2.53	0.42
5:2B:34:LEU:HD22	5:2B:47:TYR:CD2	2.55	0.42
3:1I:37:GLN:NE2	3:1I:44:GLU:O	2.43	0.41
5:2O:20:VAL:CG2	5:2O:23:LEU:HB2	2.50	0.41
4:1M:29:LEU:HB2	4:1M:31:ASP:OD1	2.19	0.41
2:1F:64:PRO:HG2	2:1F:160:MET:HE3	2.02	0.41
5:2O:20:VAL:O	5:2O:23:LEU:N	2.51	0.41
4:1P:90:LYS:NZ	5:2F:79:PHE:O	2.42	0.41
1:1C:109:ARG:HG3	1:1C:110:GLU:N	2.36	0.41
5:2G:21:ASP:OD1	5:2G:22:ASN:ND2	2.54	0.41
1:1A:25:THR:HG22	1:1A:27:PHE:H	1.86	0.41
2:1F:22:ARG:HD2	2:1F:77:GLU:OE1	2.21	0.41
1:1D:186:MET:SD	1:1E:186:MET:HE3	2.61	0.41
4:1M:29:LEU:CB	4:1M:31:ASP:OD1	2.69	0.40
5:2N:23:LEU:O	5:2N:24:GLN:C	2.64	0.40
1:1E:166:TYR:CE2	1:1E:170:VAL:CG2	3.04	0.40
2:1F:16:ALA:HB2	2:1F:52:LEU:HD21	2.04	0.40
1:1D:25:THR:CG2	1:1D:26:CYS:N	2.83	0.40
1:1D:168:PRO:HG3	3:1I:78:VAL:HG21	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1A	196/224 (88%)	192 (98%)	4 (2%)	0	100	100
1	1B	189/224 (84%)	188 (100%)	1 (0%)	0	100	100
1	1C	188/224 (84%)	187 (100%)	1 (0%)	0	100	100
1	1D	184/224 (82%)	182 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1E	193/224 (86%)	190 (98%)	3 (2%)	0	100	100
2	1F	255/263 (97%)	251 (98%)	4 (2%)	0	100	100
3	1G	69/86 (80%)	69 (100%)	0	0	100	100
3	1H	81/86 (94%)	81 (100%)	0	0	100	100
3	1I	81/86 (94%)	81 (100%)	0	0	100	100
3	1J	81/86 (94%)	81 (100%)	0	0	100	100
4	1K	64/101 (63%)	63 (98%)	1 (2%)	0	100	100
4	1L	71/101 (70%)	70 (99%)	1 (1%)	0	100	100
4	1M	70/101 (69%)	70 (100%)	0	0	100	100
4	1N	72/101 (71%)	72 (100%)	0	0	100	100
4	1O	71/101 (70%)	71 (100%)	0	0	100	100
4	1P	71/101 (70%)	71 (100%)	0	0	100	100
5	2A	57/80 (71%)	57 (100%)	0	0	100	100
5	2B	59/80 (74%)	59 (100%)	0	0	100	100
5	2C	57/80 (71%)	57 (100%)	0	0	100	100
5	2D	58/80 (72%)	58 (100%)	0	0	100	100
5	2E	58/80 (72%)	58 (100%)	0	0	100	100
5	2F	70/80 (88%)	66 (94%)	4 (6%)	0	100	100
5	2G	73/80 (91%)	72 (99%)	1 (1%)	0	100	100
5	2H	73/80 (91%)	72 (99%)	1 (1%)	0	100	100
5	2I	73/80 (91%)	71 (97%)	2 (3%)	0	100	100
5	2J	73/80 (91%)	72 (99%)	1 (1%)	0	100	100
5	2K	75/80 (94%)	72 (96%)	3 (4%)	0	100	100
5	2L	62/80 (78%)	61 (98%)	1 (2%)	0	100	100
5	2M	59/80 (74%)	59 (100%)	0	0	100	100
5	2N	53/80 (66%)	52 (98%)	1 (2%)	0	100	100
5	2O	46/80 (58%)	46 (100%)	0	0	100	100
5	2P	40/80 (50%)	40 (100%)	0	0	100	100
5	2Q	11/80 (14%)	11 (100%)	0	0	100	100
All	All	2933/3693 (79%)	2902 (99%)	31 (1%)	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	1A	162/199 (81%)	162 (100%)	0	100	100
1	1B	120/199 (60%)	120 (100%)	0	100	100
1	1D	9/199 (4%)	9 (100%)	0	100	100
1	1E	171/199 (86%)	171 (100%)	0	100	100
2	1F	214/219 (98%)	213 (100%)	1 (0%)	81	80
3	1G	59/71 (83%)	59 (100%)	0	100	100
3	1H	69/71 (97%)	69 (100%)	0	100	100
3	1I	69/71 (97%)	69 (100%)	0	100	100
3	1J	69/71 (97%)	69 (100%)	0	100	100
4	1K	59/88 (67%)	59 (100%)	0	100	100
4	1L	64/88 (73%)	64 (100%)	0	100	100
4	1M	63/88 (72%)	63 (100%)	0	100	100
4	1N	65/88 (74%)	65 (100%)	0	100	100
4	1O	64/88 (73%)	64 (100%)	0	100	100
4	1P	64/88 (73%)	64 (100%)	0	100	100
5	2A	50/67 (75%)	50 (100%)	0	100	100
5	2B	52/67 (78%)	52 (100%)	0	100	100
5	2C	50/67 (75%)	50 (100%)	0	100	100
5	2D	51/67 (76%)	51 (100%)	0	100	100
5	2E	51/67 (76%)	51 (100%)	0	100	100
5	2F	61/67 (91%)	61 (100%)	0	100	100
5	2G	63/67 (94%)	63 (100%)	0	100	100
5	2H	63/67 (94%)	63 (100%)	0	100	100
5	2I	63/67 (94%)	63 (100%)	0	100	100
5	2J	63/67 (94%)	63 (100%)	0	100	100
5	2K	65/67 (97%)	64 (98%)	1 (2%)	57	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	2L	1/67 (2%)	1 (100%)	0	100	100
5	2P	35/67 (52%)	35 (100%)	0	100	100
5	2Q	11/67 (16%)	11 (100%)	0	100	100
All	All	2000/2765 (72%)	1998 (100%)	2 (0%)	87	87

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

Mol	Chain	Res	Type
2	1F	57	HIS
5	2K	22	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	1A	119	GLN
2	1F	130	ASN
4	1L	78	ASN
4	1P	59	ASN
5	2B	24	GLN
5	2C	59	ASN
5	2E	22	ASN
5	2G	22	ASN
5	2G	61	GLN
5	2J	22	ASN
5	2J	61	GLN
5	2K	22	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

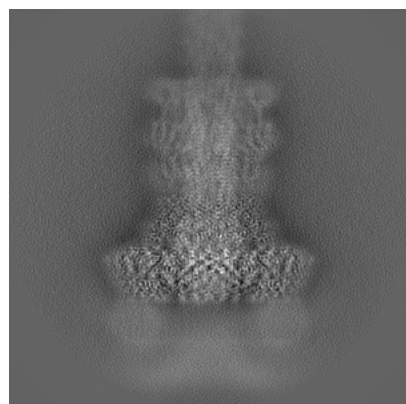
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11780. These allow visual inspection of the internal detail of the map and identification of artifacts.

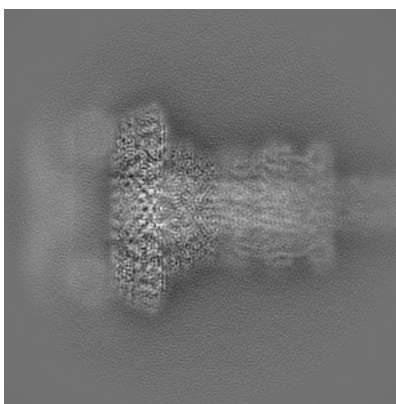
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

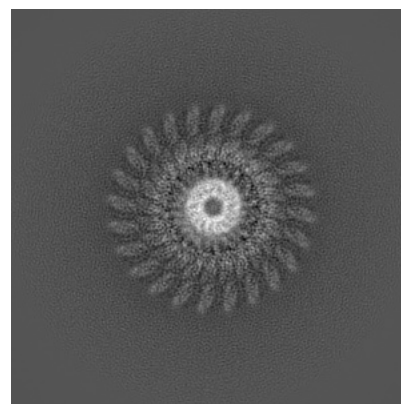
6.1.1 Primary map



X

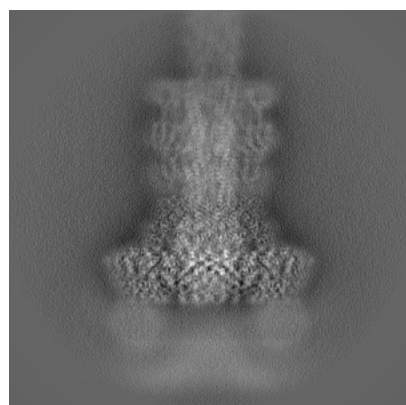


Y

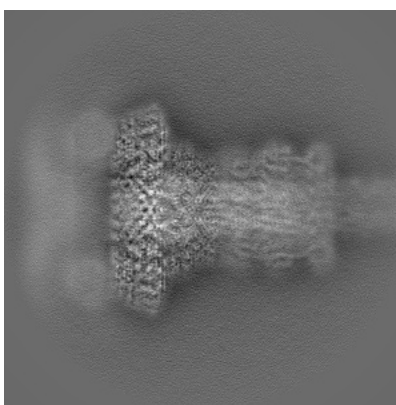


Z

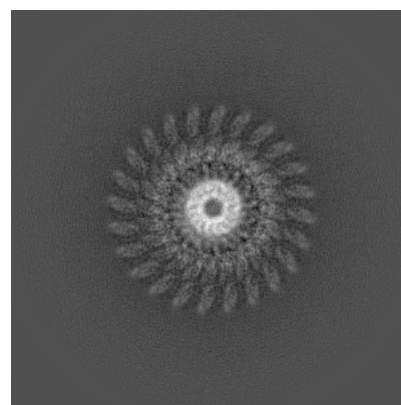
6.1.2 Raw map



X



Y

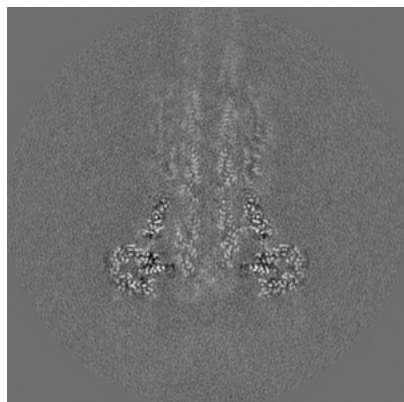


Z

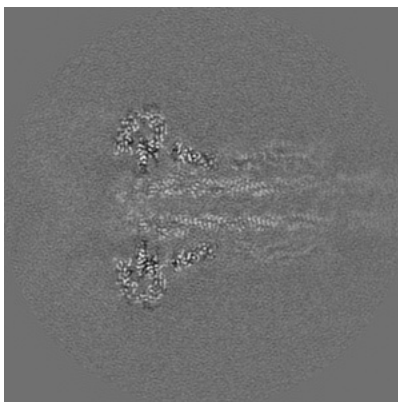
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

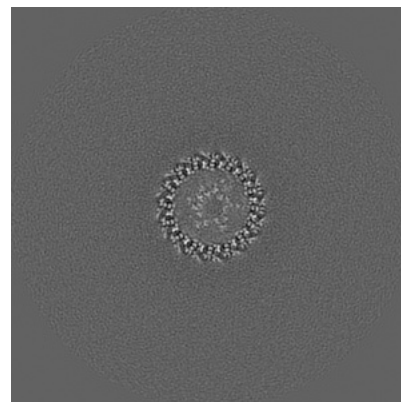
6.2.1 Primary map



X Index: 216

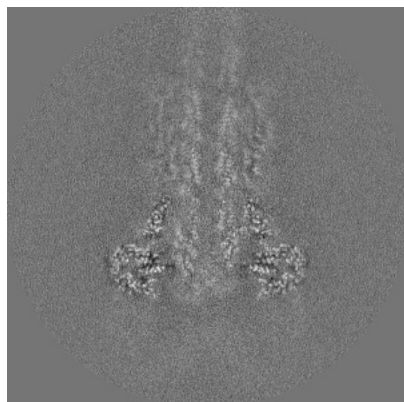


Y Index: 216

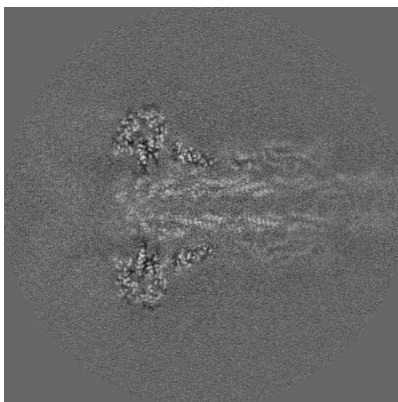


Z Index: 216

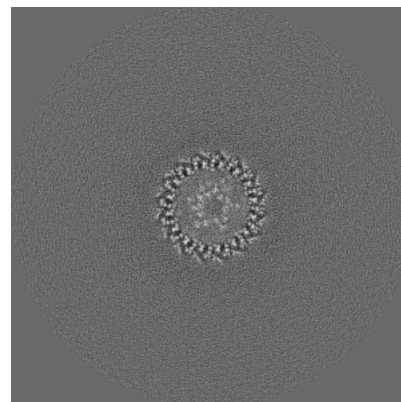
6.2.2 Raw map



X Index: 216



Y Index: 216

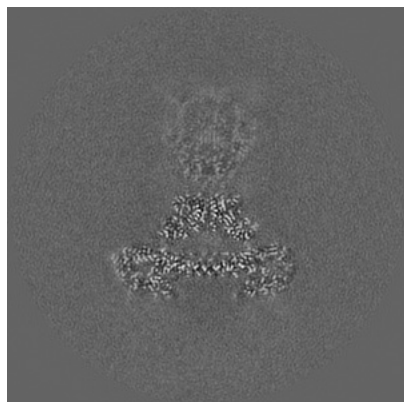


Z Index: 216

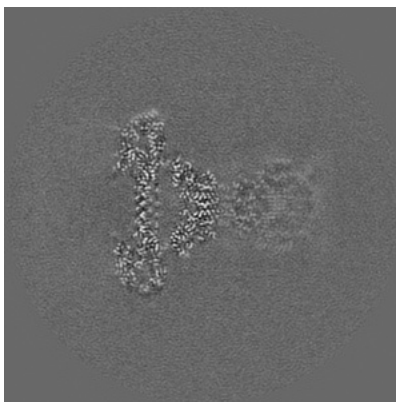
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

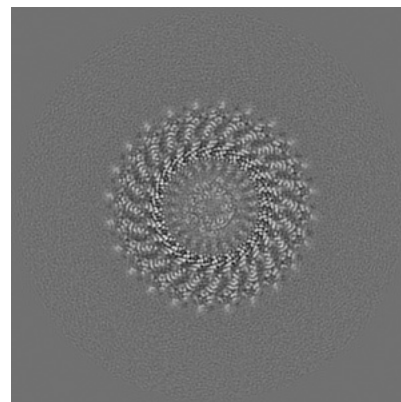
6.3.1 Primary map



X Index: 262

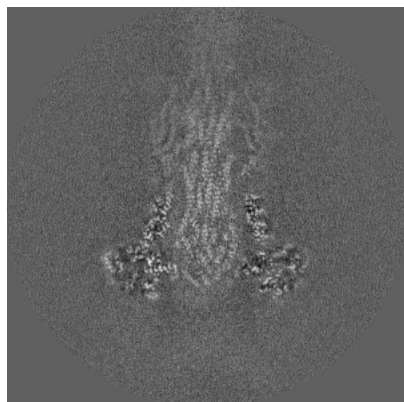


Y Index: 261

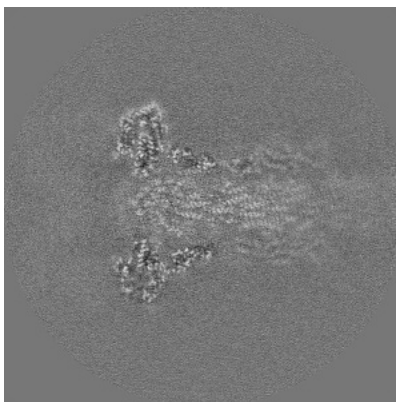


Z Index: 159

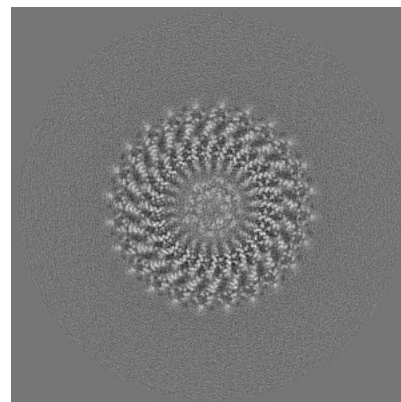
6.3.2 Raw map



X Index: 203



Y Index: 232

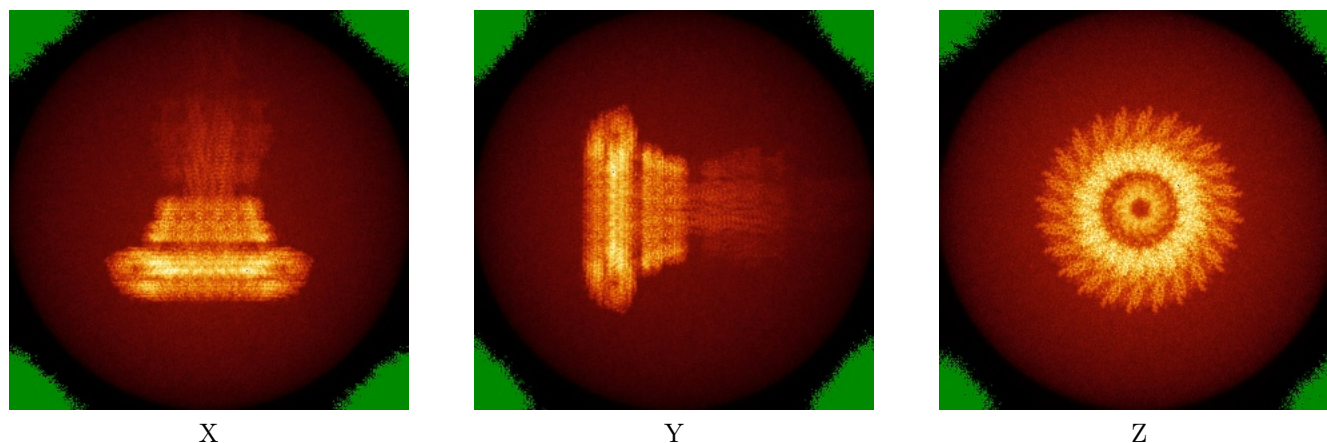


Z Index: 158

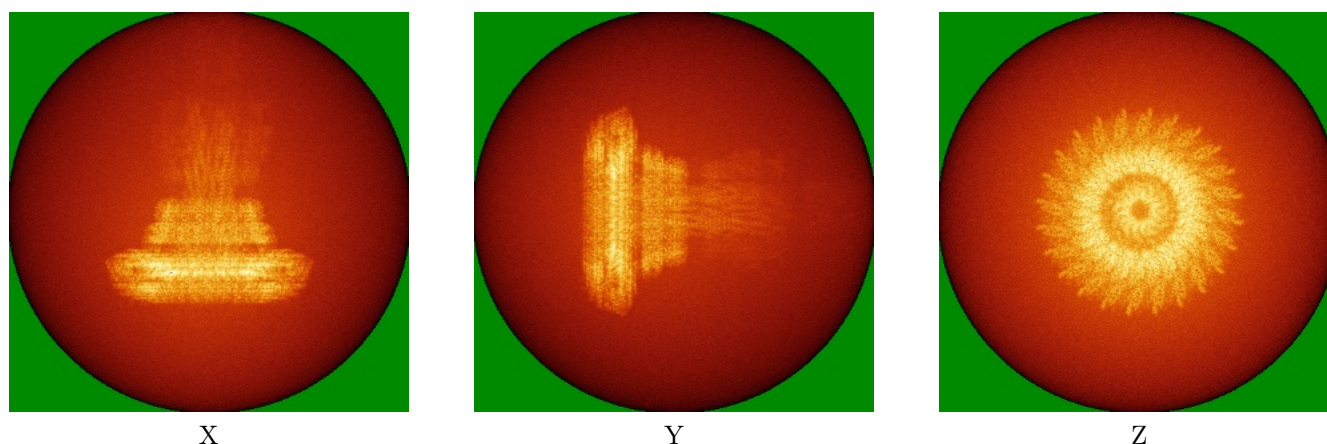
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

This section was not generated.

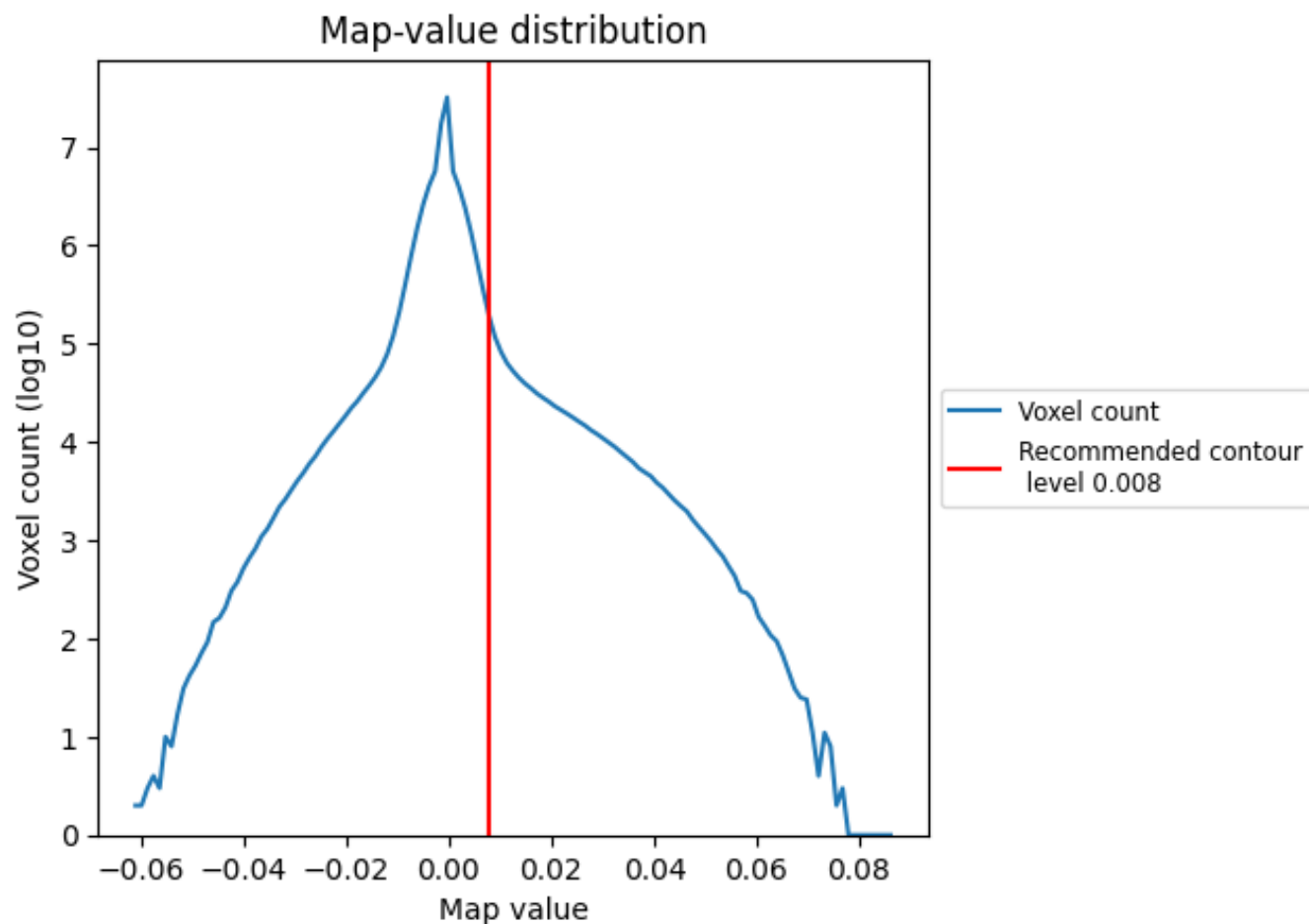
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

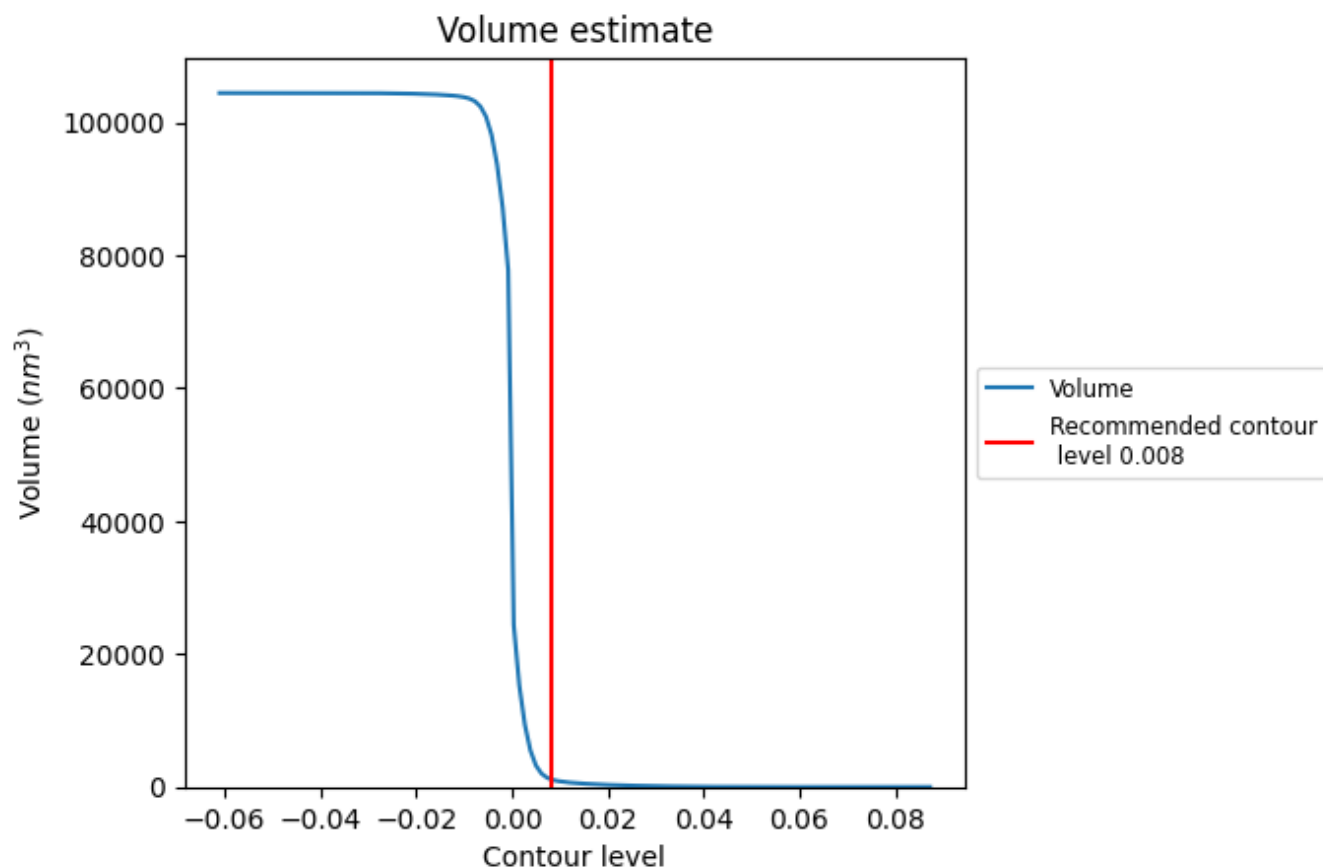
This section contains the results of statistical analysis of the map.

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.

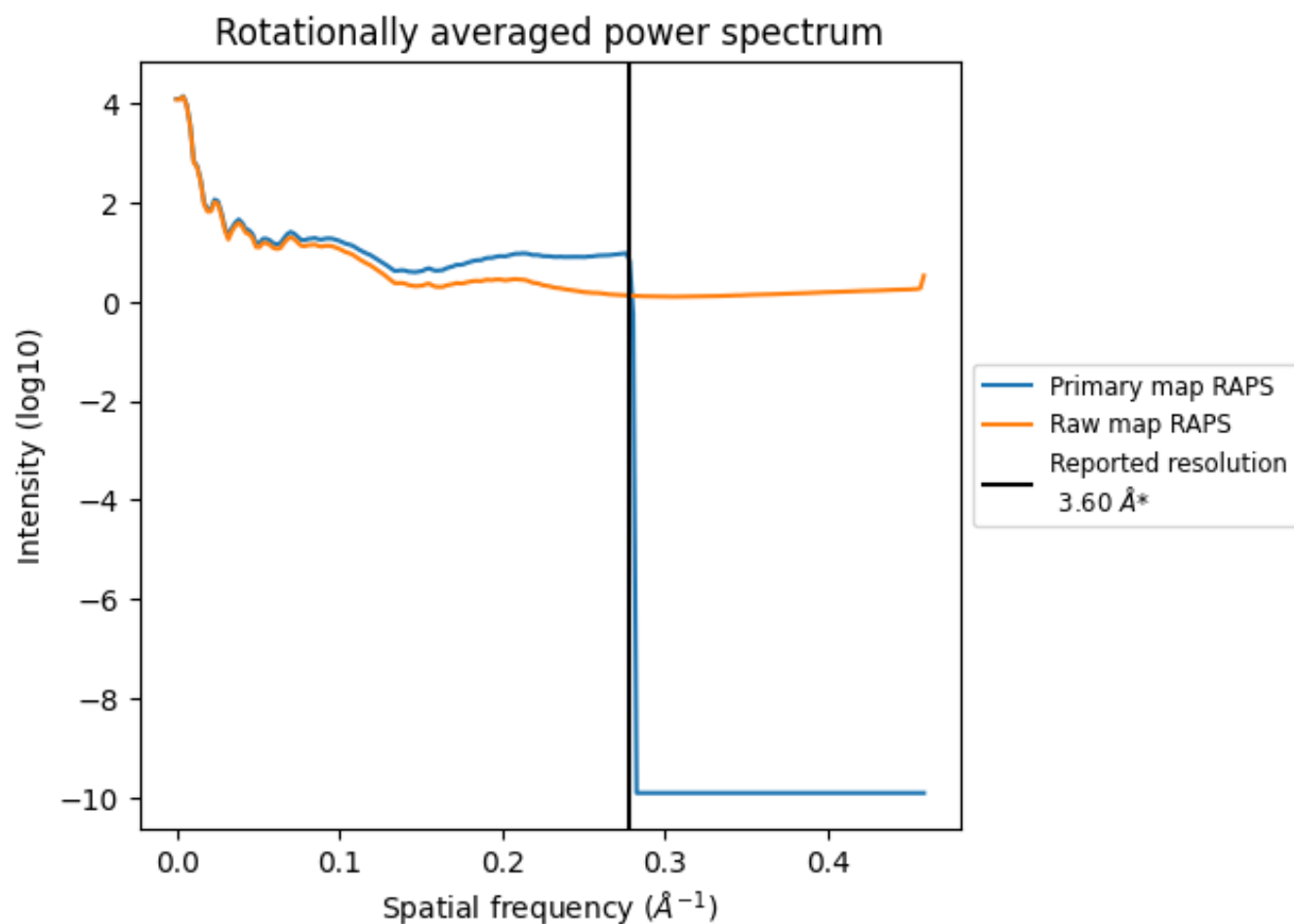
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1197 nm³; this corresponds to an approximate mass of 1081 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 ⓘ

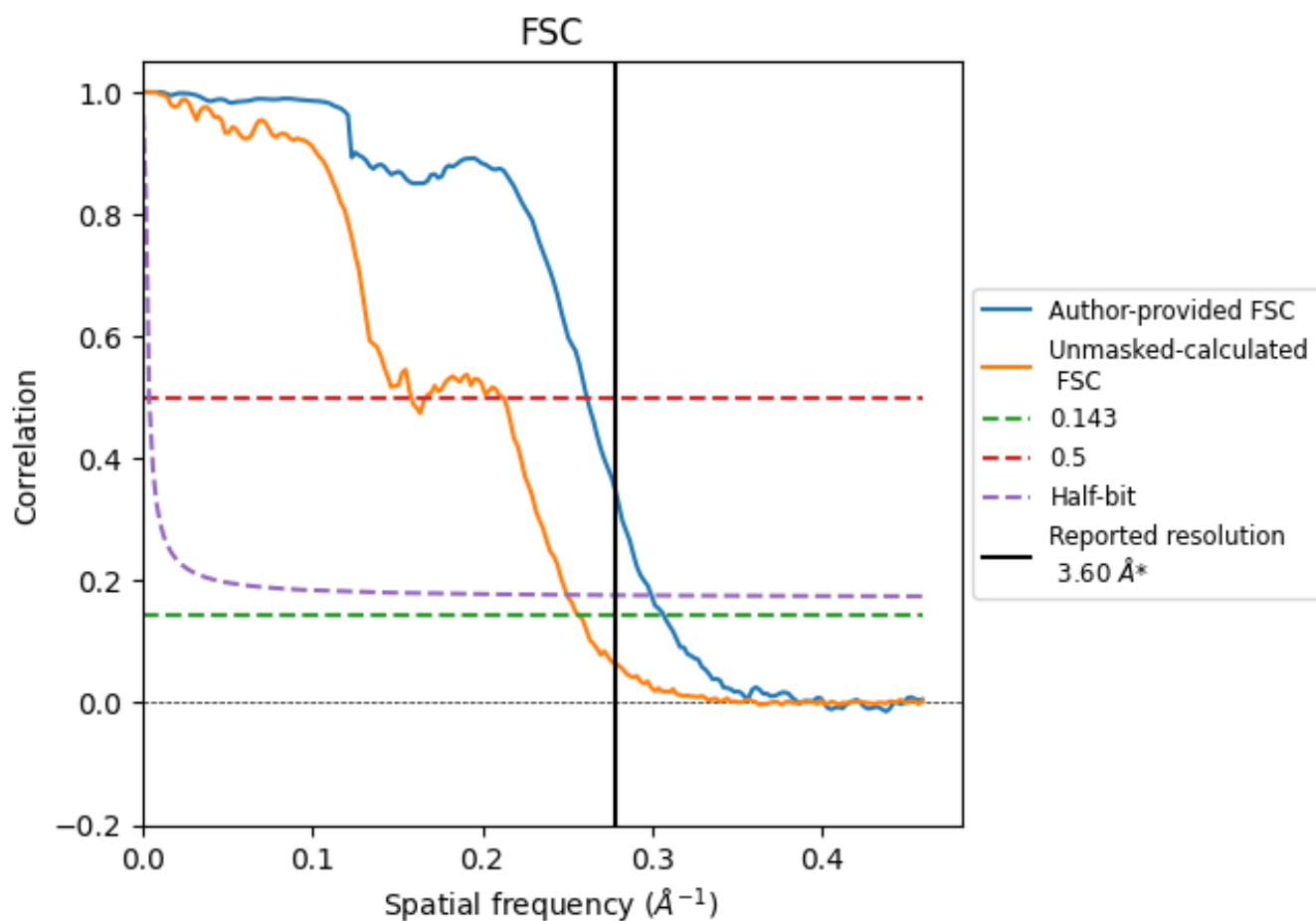


*Reported resolution corresponds to spatial frequency of 0.278 $\text{\AA}^{-1}$

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 0.278 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

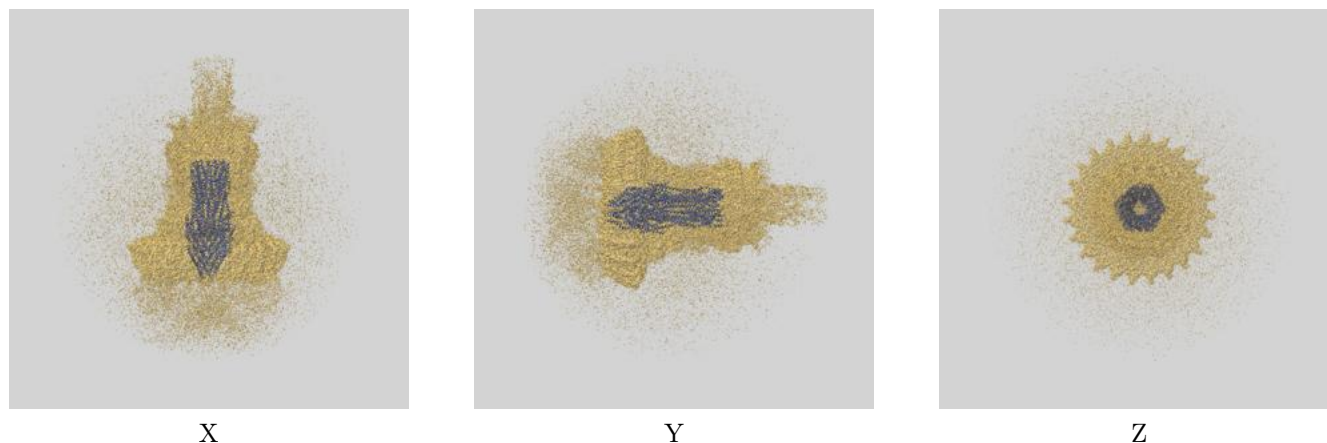
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.26	3.82	3.34
Unmasked-calculated*	3.89	6.32	4.00

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

9 Map-model fit [i](#)

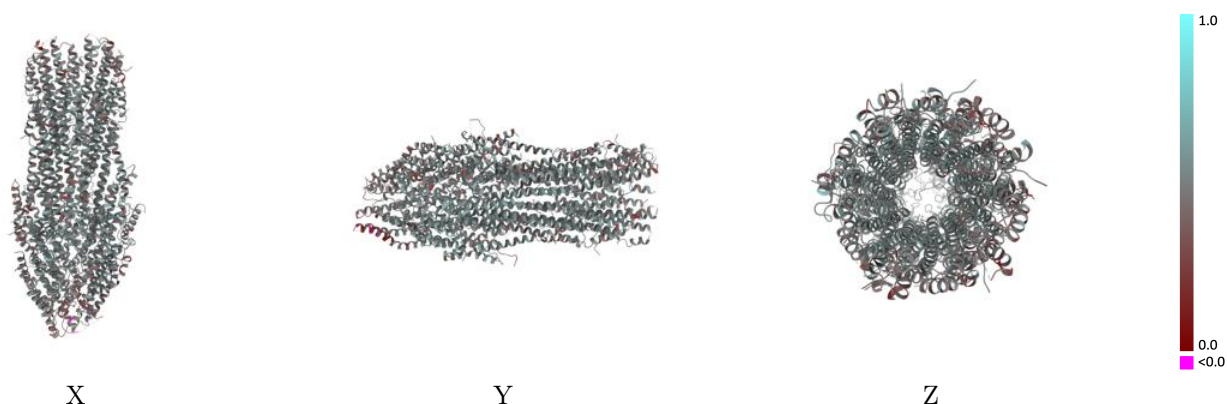
This section contains information regarding the fit between EMDB map EMD-11780 and PDB model 7AGX. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

9.1 Map-model overlay [i](#)



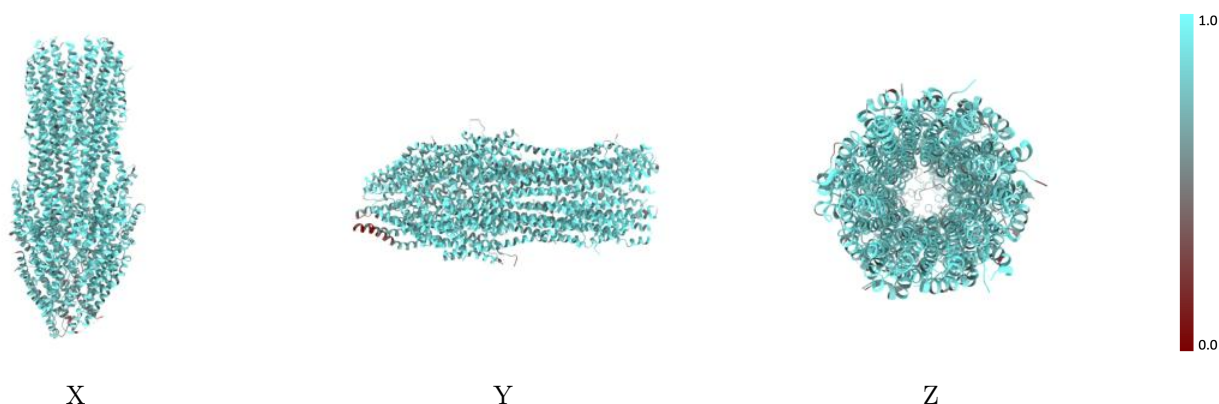
The images above show the 3D surface view of the map at the recommended contour level 0.008 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



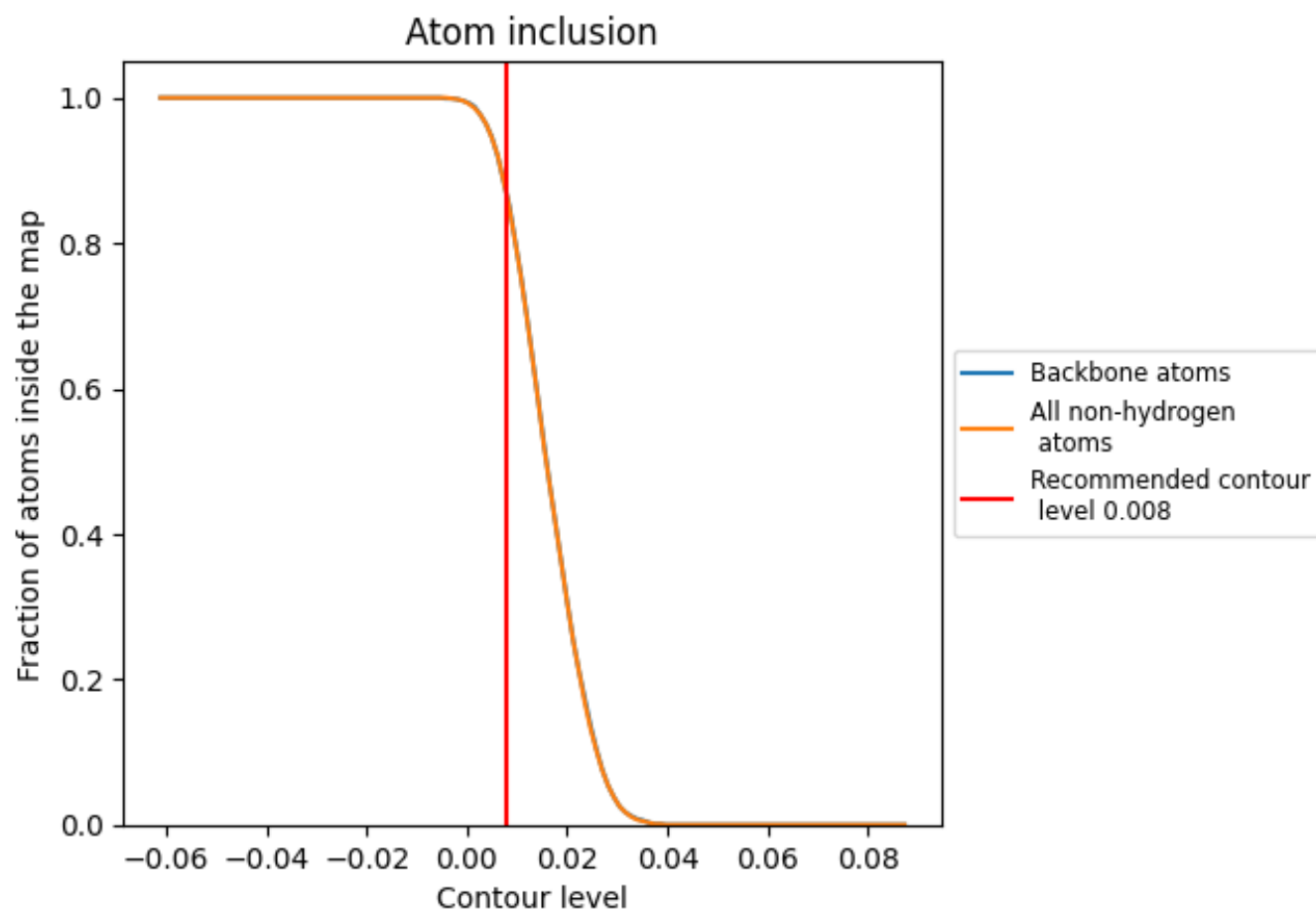
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 87% of all backbone atoms, 86% 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	 0.8650	 0.4890
1A	 0.8790	 0.5140
1B	 0.8800	 0.4960
1C	 0.8830	 0.4880
1D	 0.8790	 0.4930
1E	 0.8670	 0.4930
1F	 0.8730	 0.5020
1G	 0.6190	 0.3880
1H	 0.7330	 0.4240
1I	 0.7770	 0.4570
1J	 0.8130	 0.4430
1K	 0.8240	 0.4810
1L	 0.8890	 0.5160
1M	 0.8690	 0.4950
1N	 0.8540	 0.4850
1O	 0.8940	 0.5000
1P	 0.9090	 0.5160
2A	 0.9260	 0.5310
2B	 0.8820	 0.5010
2C	 0.9060	 0.4940
2D	 0.8840	 0.4870
2E	 0.8630	 0.4870
2F	 0.8970	 0.5070
2G	 0.9130	 0.5160
2H	 0.8750	 0.5030
2I	 0.8770	 0.4800
2J	 0.8610	 0.4810
2K	 0.8620	 0.4710
2L	 0.8760	 0.4990
2M	 0.8950	 0.5140
2N	 0.8630	 0.4750
2O	 0.8570	 0.4570
2P	 0.8630	 0.4890
2Q	 0.8640	 0.5080

