



Full wwPDB EM Validation Report ⓘ

Jun 16, 2026 – 12:35 pm BST

PDB ID : 9RCE / pdb_00009rce
EMDB ID : EMD-53919
Title : Cryo-EM structure of a contractile injection system in *Salmonella enterica* subspecies *Salamae*, the baseplate portion in extended state.
Authors : Ejaz, R.N.; Tillmann, H.P.; Sofos, N.H.; Siborova, M.; Taylor, N.M.I.
Deposited on : 2025-05-28
Resolution : 2.86 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

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:

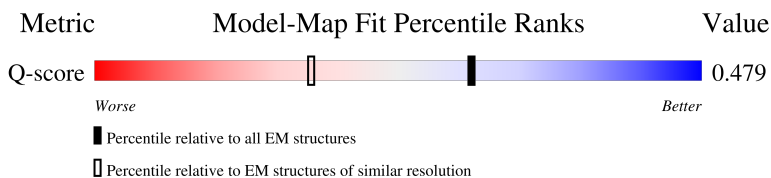
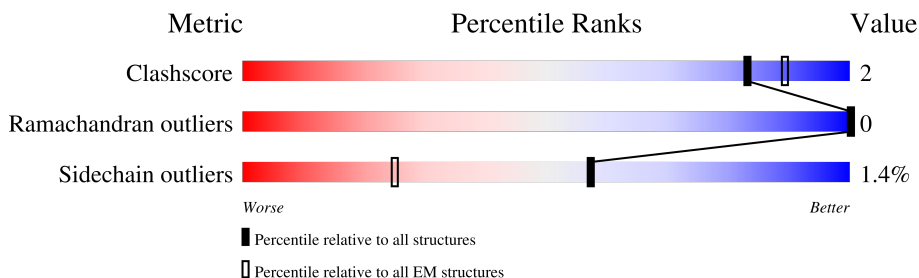
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 2.86 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.



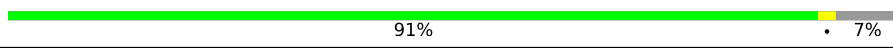
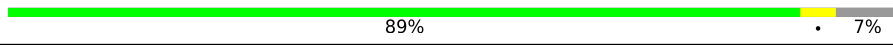
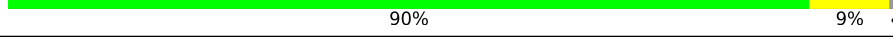
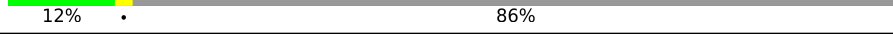
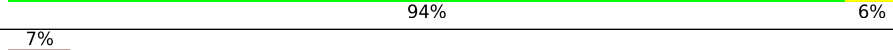
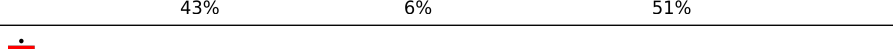
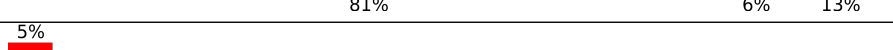
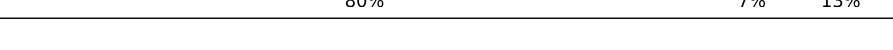
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12017 (2.36 - 3.36)

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	H	217	
1	M	217	
2	I	158	
2	N	158	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	B	804	
3	J	804	
4	C	149	
4	K	149	
5	D	519	
5	L	519	
6	E	56	
7	F	597	
8	c	99	
9	A	1323	
9	G	1323	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 100103 atoms, of which 49752 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 Peptidoglycan-binding protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	H	194	Total	C	H	N	O	S	0	0
			3033	963	1520	252	295	3		
1	M	194	Total	C	H	N	O	S	0	0
			3033	963	1520	252	295	3		

- Molecule 2 is a protein called Conserved hypothetical phage tail region protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	I	143	Total	C	H	N	O	S	0	0
			2235	709	1112	189	220	5		
2	N	143	Total	C	H	N	O	S	0	0
			2235	709	1112	189	220	5		

- Molecule 3 is a protein called SalCis12.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	B	697	Total	C	H	N	O	S	0	0
			11303	3669	5575	993	1052	14		
3	J	697	Total	C	H	N	O	S	0	0
			11303	3669	5575	993	1052	14		

- Molecule 4 is a protein called GPW/gp25 family protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	C	138	Total	C	H	N	O	S	0	0
			2192	710	1091	177	209	5		
4	K	138	Total	C	H	N	O	S	0	0
			2192	710	1091	177	209	5		

- Molecule 5 is a protein called Phage tail sheath family protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	D	514	Total	C	H	N	O	S	0	0
			7936	2525	3949	668	771	23		
5	L	514	Total	C	H	N	O	S	0	0
			7936	2525	3949	668	771	23		

- Molecule 6 is a protein called SalCis6.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	E	8	Total	C	H	N	O		0	0
			132	39	63	14	16			

- Molecule 7 is a protein called Type VI secretion system tip protein VgrG.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	F	595	Total	C	H	N	O	S	0	0
			8833	2751	4418	746	901	17		

- Molecule 8 is a protein called SalCis10.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	c	49	Total	C	H	N	O	S	0	0
			672	206	347	56	60	3		

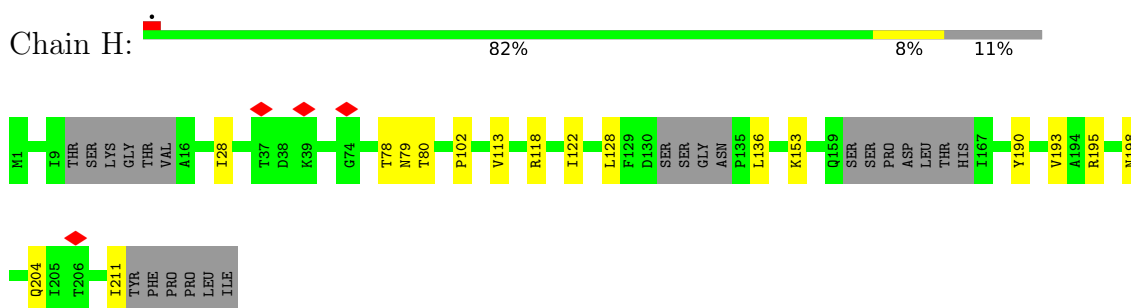
- Molecule 9 is a protein called Baseplate protein J-like domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	A	1149	Total	C	H	N	O	S	0	0
			18534	6003	9215	1601	1687	28		
9	G	1149	Total	C	H	N	O	S	0	0
			18534	6003	9215	1601	1687	28		

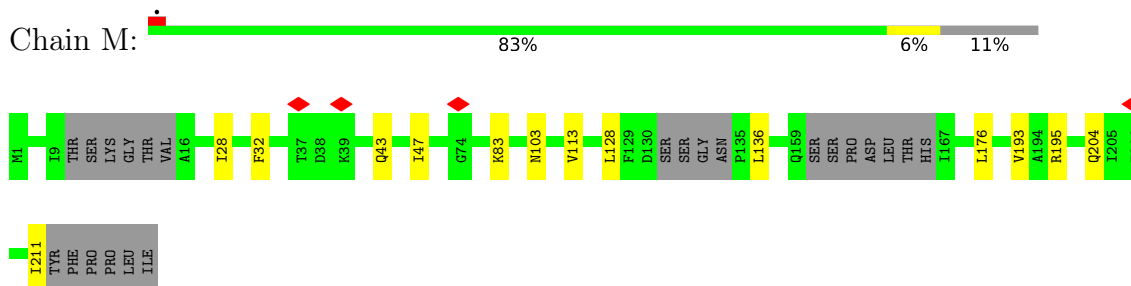
3 Residue-property plots [i](#)

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.

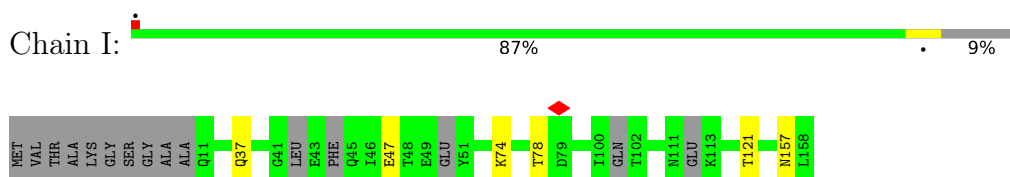
- Molecule 1: Peptidoglycan-binding protein



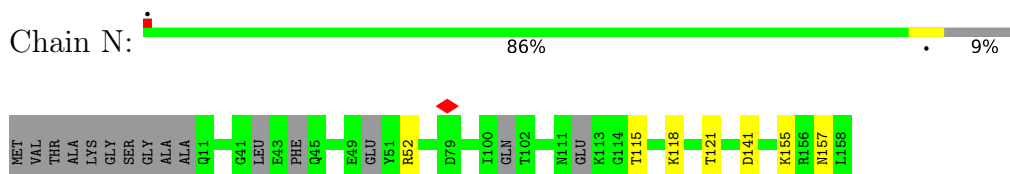
- Molecule 1: Peptidoglycan-binding protein



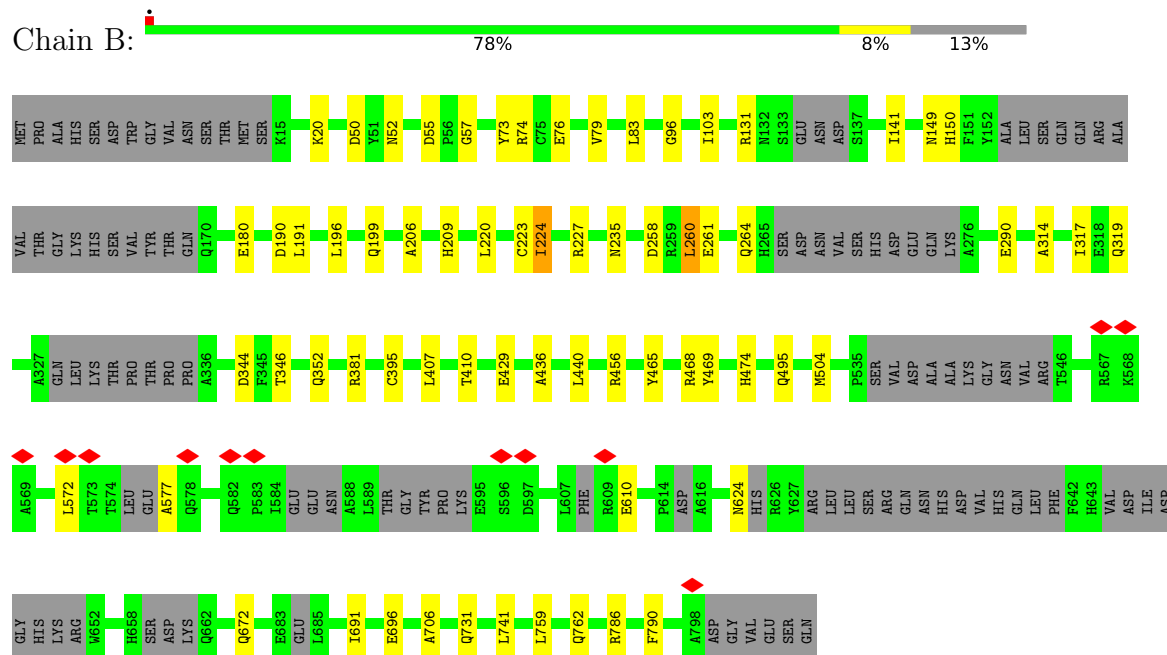
- Molecule 2: Conserved hypothetical phage tail region protein



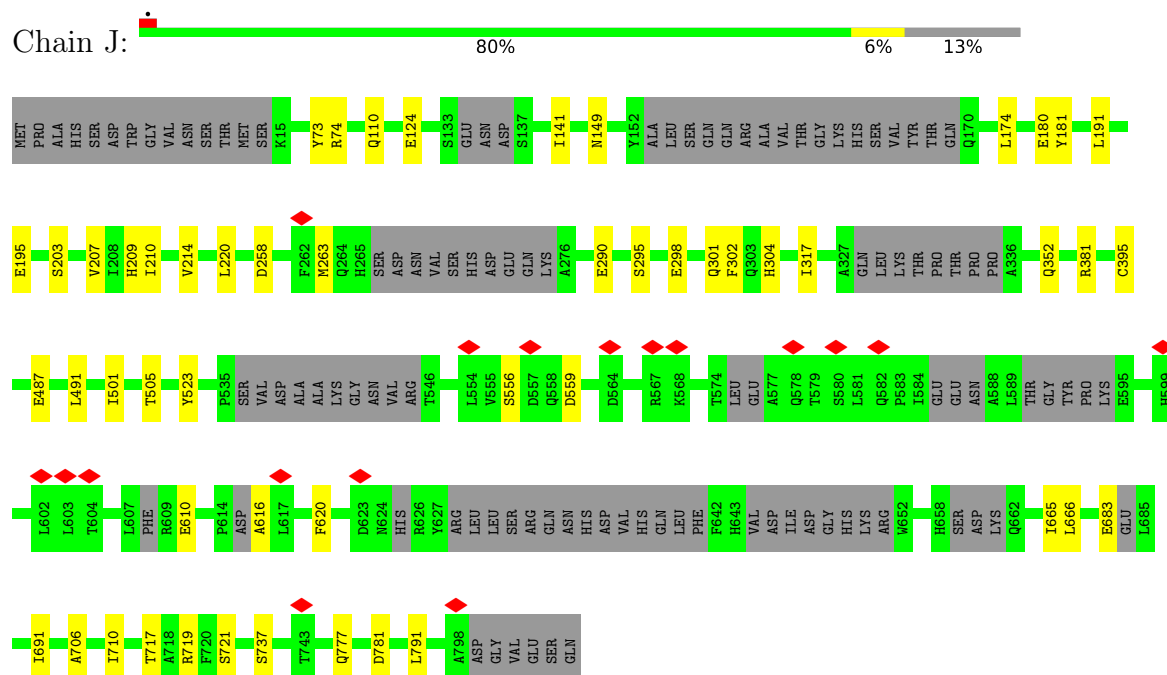
- Molecule 2: Conserved hypothetical phage tail region protein



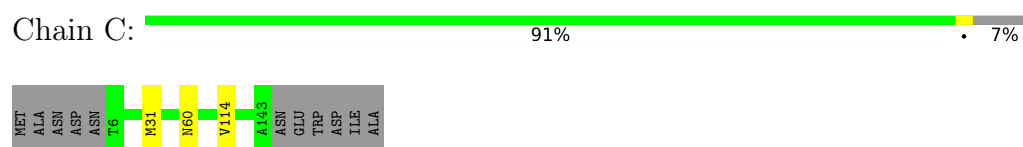
- Molecule 3: SalCis12



- Molecule 3: SalCis12



- Molecule 4: GPW/gp25 family protein



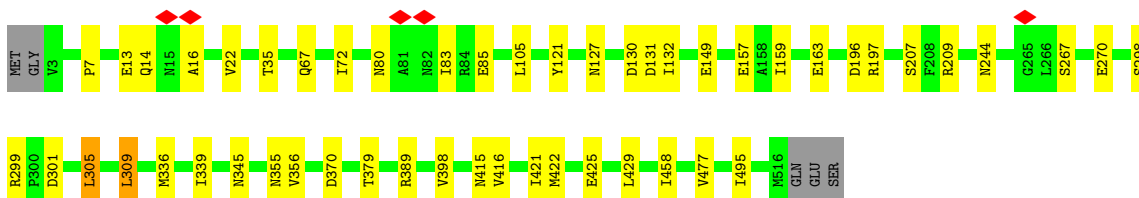
- Molecule 4: GPW/gp25 family protein

Chain K:  89% 7%



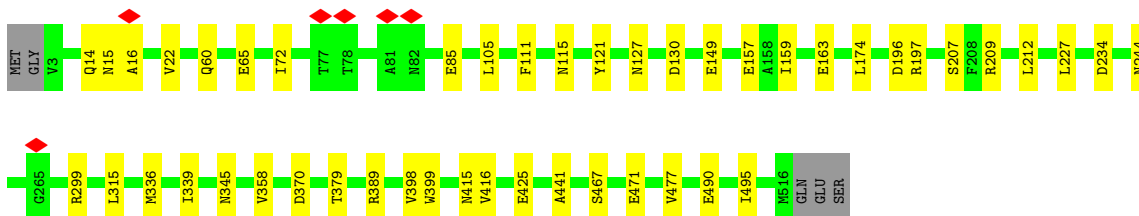
- Molecule 5: Phage tail sheath family protein

Chain D:  89% 9%



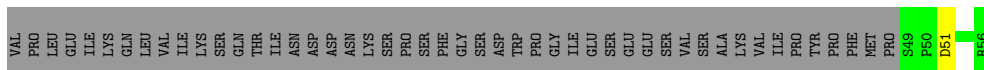
- Molecule 5: Phage tail sheath family protein

Chain L:  90% 9%

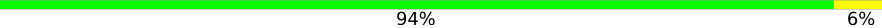


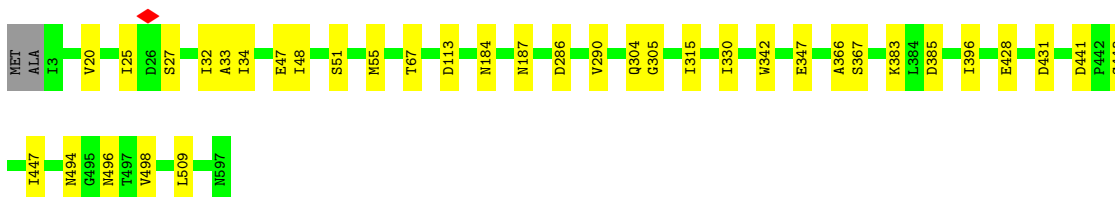
- Molecule 6: SalCis6

Chain E:  12% 86%

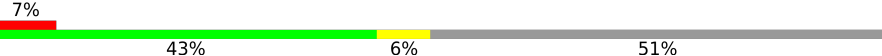


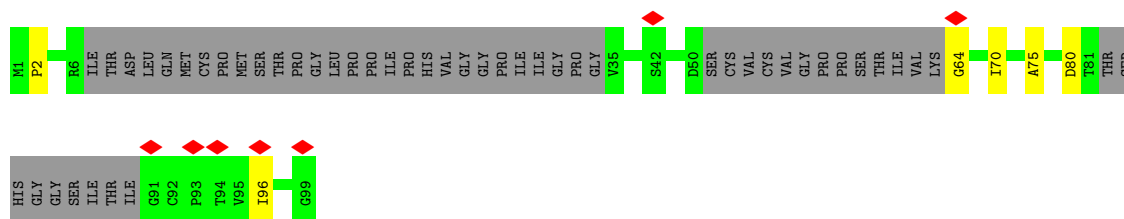
- Molecule 7: Type VI secretion system tip protein VgrG

Chain F:  94% 6%



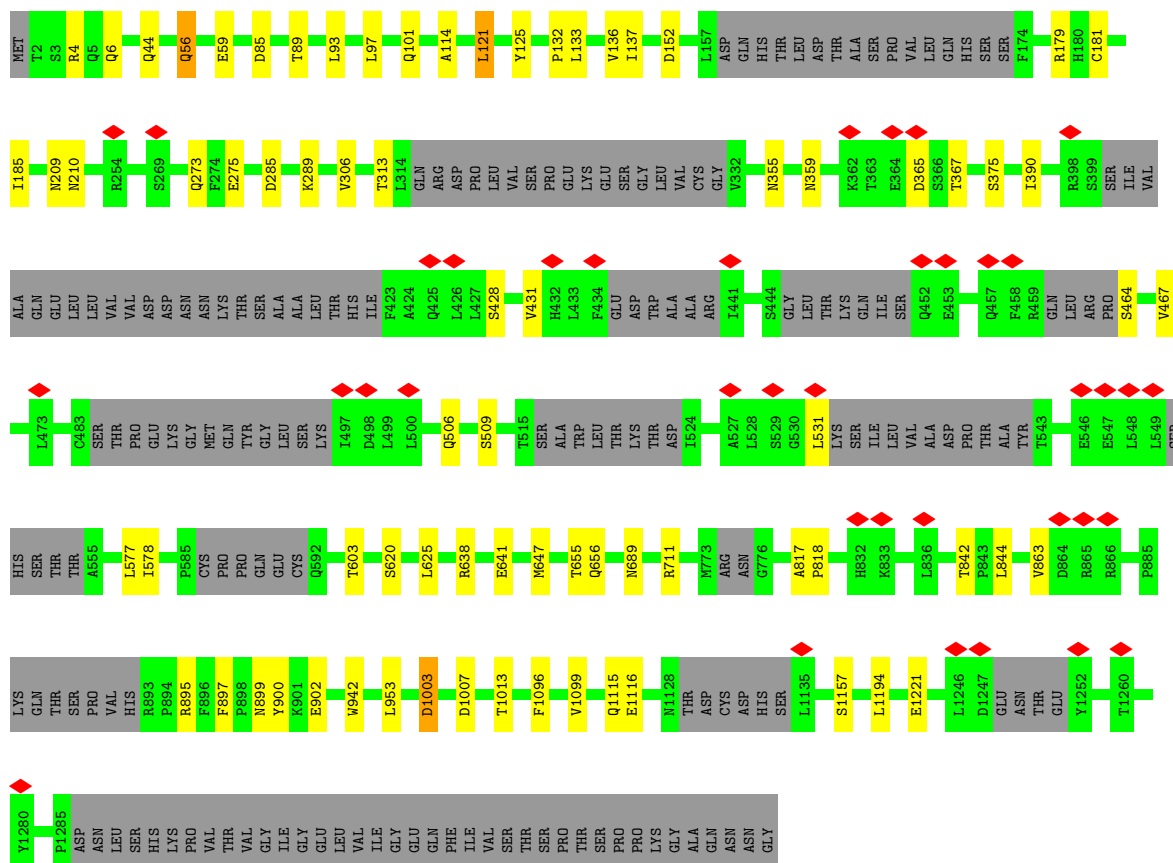
- Molecule 8: SalCis10

Chain c:  7% 43% 6% 51%



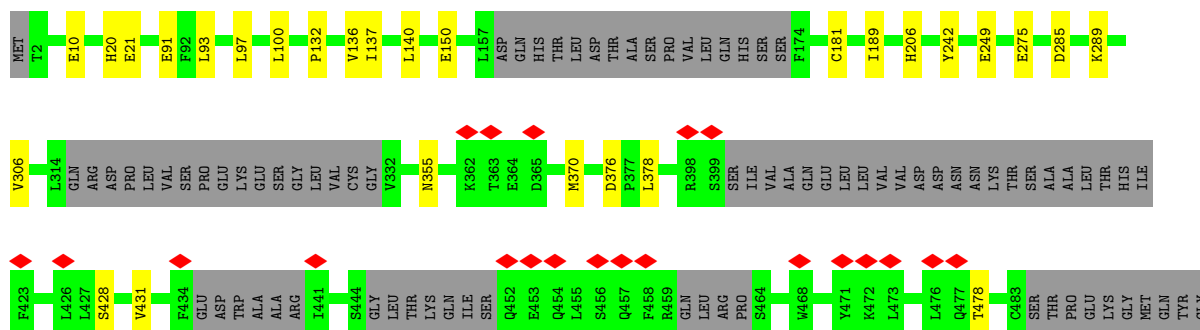
• Molecule 9: Baseplate protein J-like domain-containing protein

Chain A: 81% 6% 13%



• Molecule 9: Baseplate protein J-like domain-containing protein

Chain G: 5% 80% 7% 13%





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	20065	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 ($e^-/\text{\AA}^2$)	41	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.656	Depositor
Minimum map value	-0.431	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.027	Depositor
Recommended contour level	0.0678	Depositor
Map size ($\text{\AA}$)	456.75, 456.75, 456.75	wwPDB
Map dimensions	630, 630, 630	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.725, 0.725, 0.725	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	H	0.13	0/1540	0.33	0/2081
1	M	0.14	0/1540	0.35	0/2081
2	I	0.13	0/1141	0.32	0/1538
2	N	0.13	0/1141	0.33	0/1538
3	B	0.15	0/5865	0.30	0/7966
3	J	0.13	0/5865	0.29	0/7966
4	C	0.12	0/1128	0.28	0/1539
4	K	0.13	0/1128	0.29	0/1539
5	D	0.13	0/4066	0.30	0/5514
5	L	0.13	0/4066	0.29	0/5514
6	E	0.12	0/69	0.37	0/90
7	F	0.13	0/4483	0.31	0/6093
8	c	0.14	0/327	0.33	0/440
9	A	0.14	0/9562	0.33	0/12975
9	G	0.15	0/9562	0.34	0/12975
All	All	0.14	0/51483	0.31	0/69849

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	1513	1520	1518	9	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	M	1513	1520	1518	7	0
2	I	1123	1112	1105	4	0
2	N	1123	1112	1105	5	0
3	B	5728	5575	5552	39	0
3	J	5728	5575	5552	30	0
4	C	1101	1091	1090	2	0
4	K	1101	1091	1090	2	0
5	D	3987	3949	3947	27	0
5	L	3987	3949	3947	24	0
6	E	69	63	62	0	0
7	F	4415	4418	4414	19	0
8	c	325	347	344	3	0
9	A	9319	9215	9197	43	0
9	G	9319	9215	9197	41	0
All	All	50351	49752	49638	238	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 2.

All (238) 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)
2:I:47:GLU:OE1	2:N:52:ARG:NH2	2.19	0.76
9:G:634:TYR:OH	9:G:898:PRO:O	2.03	0.75
7:F:494:ASN:OD1	7:F:496:ASN:ND2	2.21	0.73
2:I:78:THR:O	2:N:118:LYS:NZ	2.21	0.73
9:G:722:GLU:OE2	9:G:835:THR:OG1	2.04	0.73
3:J:74:ARG:NH1	3:J:395:CYS:SG	2.63	0.72
3:B:74:ARG:NH1	3:B:395:CYS:SG	2.63	0.71
3:B:762:GLN:OE1	3:B:786:ARG:NH2	2.24	0.71
9:A:306:VAL:HG23	9:A:1013:THR:HG23	1.71	0.70
9:G:306:VAL:HG23	9:G:1013:THR:HG23	1.73	0.70
5:D:7:PRO:O	5:L:399:TRP:NE1	2.26	0.69
5:L:14:GLN:OE1	5:L:16:ALA:N	2.25	0.69
5:D:163:GLU:OE2	5:D:207:SER:OG	2.08	0.69
5:L:121:TYR:OH	5:L:149:GLU:OE1	2.10	0.69
9:A:655:THR:O	9:G:791:ASN:ND2	2.25	0.69
9:G:100:LEU:HD21	9:G:189:ILE:HD11	1.74	0.68
9:A:506:GLN:O	9:A:509:SER:OG	2.12	0.67
9:A:375:SER:HG	9:A:620:SER:HG	1.24	0.67
9:G:376:ASP:OD1	9:G:869:SER:OG	2.13	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:14:GLN:OE1	5:D:16:ALA:N	2.28	0.66
9:G:242:TYR:HH	9:G:1073:SER:HG	1.44	0.66
5:L:209:ARG:NH2	5:L:379:THR:OG1	2.29	0.65
9:G:150:GLU:OE2	9:G:150:GLU:N	2.29	0.65
5:D:298:SER:OG	5:D:301:ASP:OD1	2.14	0.65
9:A:101:GLN:OE1	9:A:152:ASP:N	2.29	0.65
5:D:267:SER:OG	5:D:270:GLU:OE1	2.16	0.64
2:I:121:THR:OG1	2:I:157:ASN:OD1	2.09	0.64
5:D:121:TYR:OH	5:D:149:GLU:OE1	2.11	0.64
2:N:121:THR:OG1	2:N:157:ASN:OD1	2.15	0.64
5:L:163:GLU:OE2	5:L:207:SER:OG	2.10	0.64
3:B:572:LEU:HD22	3:B:577:ALA:HB1	1.81	0.63
9:G:734:MET:SD	9:G:754:LEU:HD13	2.39	0.63
9:G:572:GLU:OE1	9:G:572:GLU:N	2.32	0.62
3:J:556:SER:OG	3:J:559:ASP:OD2	2.18	0.62
7:F:32:ILE:HG22	7:F:33:ALA:H	1.65	0.61
9:A:97:LEU:HD11	9:A:133:LEU:HD11	1.81	0.61
3:J:124:GLU:O	3:J:149:ASN:ND2	2.34	0.61
9:G:132:PRO:O	9:G:136:VAL:HG23	1.99	0.61
3:B:264:GLN:N	3:B:264:GLN:OE1	2.34	0.61
3:B:209:HIS:NE2	3:B:258:ASP:OD2	2.34	0.60
9:G:765:ASP:OD1	9:G:767:HIS:NE2	2.34	0.60
7:F:428:GLU:N	7:F:431:ASP:OD2	2.35	0.60
3:B:290:GLU:N	3:B:290:GLU:OE1	2.35	0.59
9:G:1109:SER:OG	9:G:1116:GLU:OE1	2.12	0.59
3:J:290:GLU:N	3:J:290:GLU:OE1	2.36	0.58
9:A:285:ASP:OD1	9:A:289:LYS:N	2.35	0.58
3:B:456:ARG:NH2	9:G:21:GLU:OE2	2.36	0.58
3:B:314:ALA:HB3	9:A:179:ARG:HH21	1.68	0.58
9:A:359:ASN:ND2	9:A:1003:ASP:OD2	2.36	0.58
7:F:305:GLY:N	7:F:342:TRP:O	2.37	0.57
5:L:336:MET:HE1	5:L:398:VAL:HG21	1.85	0.57
9:A:6:GLN:N	9:A:6:GLN:OE1	2.37	0.57
1:M:195:ARG:NH2	3:J:73:TYR:O	2.38	0.57
7:F:113:ASP:OD1	7:F:187:ASN:ND2	2.38	0.57
9:G:249:GLU:OE2	9:G:249:GLU:N	2.37	0.57
7:F:32:ILE:HD11	7:F:51:SER:HB2	1.87	0.57
9:G:355:ASN:ND2	9:G:1007:ASP:OD1	2.38	0.57
9:A:656:GLN:O	9:A:689:ASN:ND2	2.36	0.56
9:G:285:ASP:OD1	9:G:289:LYS:N	2.38	0.56
3:B:759:LEU:HD12	3:B:790:PHE:HD2	1.69	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:1115:GLN:N	9:G:1115:GLN:OE1	2.39	0.56
3:J:209:HIS:NE2	3:J:258:ASP:OD2	2.38	0.56
1:H:153:LYS:HA	1:M:47:ILE:HD11	1.88	0.56
3:B:196:LEU:O	3:B:199:GLN:NE2	2.39	0.56
4:K:31:MET:SD	4:K:114:VAL:HG21	2.46	0.56
3:B:103:ILE:O	9:G:1079:LYS:NZ	2.38	0.55
7:F:315:ILE:HB	7:F:330:ILE:HD11	1.88	0.55
4:C:31:MET:SD	4:C:114:VAL:HG21	2.46	0.55
3:B:141:ILE:HD11	3:B:691:ILE:HD11	1.87	0.55
5:D:305:LEU:HD13	5:D:309:LEU:HD23	1.88	0.55
3:B:96:GLY:O	3:B:465:TYR:OH	2.22	0.55
9:G:582:GLU:OE2	9:G:583:ILE:N	2.39	0.55
9:G:100:LEU:HD21	9:G:189:ILE:CD1	2.38	0.54
9:G:137:ILE:HA	9:G:140:LEU:HD13	1.89	0.54
3:J:203:SER:HG	3:J:295:SER:HG	1.55	0.54
1:M:128:LEU:O	1:M:136:LEU:N	2.40	0.54
9:A:895:ARG:NH1	9:A:899:ASN:OD1	2.41	0.54
9:A:355:ASN:ND2	9:A:1007:ASP:OD1	2.41	0.54
3:B:696:GLU:OE1	3:B:696:GLU:N	2.40	0.53
5:D:80:ASN:O	5:D:83:ILE:HG22	2.07	0.53
3:J:616:ALA:O	3:J:620:PHE:N	2.40	0.53
5:D:13:GLU:N	5:D:13:GLU:OE1	2.42	0.53
9:A:603:THR:OG1	9:G:741:ASN:O	2.17	0.53
9:G:700:LEU:HD23	9:G:701:SER:N	2.24	0.53
9:A:577:LEU:HD23	9:A:578:ILE:N	2.24	0.53
5:D:336:MET:HE1	5:D:398:VAL:HG21	1.90	0.52
5:D:72:ILE:O	5:D:244:ASN:ND2	2.43	0.52
3:J:523:TYR:OH	3:J:737:SER:OG	2.26	0.52
7:F:498:VAL:HG13	7:F:509:LEU:HD23	1.92	0.52
3:J:302:PHE:O	3:J:304:HIS:ND1	2.41	0.52
5:D:85:GLU:OE1	5:D:85:GLU:N	2.42	0.52
1:H:195:ARG:NH2	3:B:73:TYR:O	2.42	0.52
3:B:352:GLN:OE1	3:B:381:ARG:NE	2.42	0.52
5:L:65:GLU:OE1	5:L:65:GLU:N	2.41	0.52
9:A:132:PRO:O	9:A:136:VAL:HG23	2.10	0.52
5:L:85:GLU:N	5:L:85:GLU:OE1	2.42	0.51
3:J:352:GLN:OE1	3:J:381:ARG:NE	2.42	0.51
3:B:691:ILE:HD13	3:B:706:ALA:HA	1.93	0.51
9:A:1116:GLU:OE2	9:A:1116:GLU:N	2.43	0.51
3:B:407:LEU:HD23	3:B:495:GLN:OE1	2.11	0.51
5:L:370:ASP:OD1	5:L:389:ARG:NH2	2.41	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:942:TRP:HB3	9:G:953:LEU:HD12	1.93	0.51
7:F:383:LYS:NZ	7:F:385:ASP:O	2.39	0.51
7:F:396:ILE:HG21	7:F:447:ILE:HD11	1.93	0.51
3:B:223:CYS:SG	3:B:227:ARG:NH1	2.84	0.51
3:B:55:ASP:OD1	3:B:57:GLY:N	2.42	0.51
1:H:204:GLN:N	1:H:204:GLN:OE1	2.45	0.50
7:F:286:ASP:O	7:F:290:VAL:HG23	2.11	0.50
3:J:691:ILE:HD13	3:J:706:ALA:HA	1.94	0.50
9:G:1187:HIS:O	9:G:1191:LEU:HD23	2.11	0.50
3:B:131:ARG:NH1	3:B:235:ASN:O	2.42	0.50
5:D:127:ASN:ND2	5:D:130:ASP:OD2	2.45	0.50
7:F:498:VAL:HG13	7:F:509:LEU:CD2	2.41	0.50
3:B:149:ASN:OD1	3:B:150:HIS:N	2.45	0.50
1:M:204:GLN:N	1:M:204:GLN:OE1	2.45	0.49
3:J:141:ILE:HD11	3:J:691:ILE:HD11	1.93	0.49
9:A:1115:GLN:N	9:A:1115:GLN:OE1	2.44	0.49
5:L:127:ASN:ND2	5:L:130:ASP:OD2	2.45	0.49
5:D:370:ASP:OD1	5:D:389:ARG:NH2	2.43	0.49
5:L:15:ASN:ND2	5:L:60:GLN:OE1	2.43	0.49
9:G:378:LEU:HD21	9:G:649:THR:HB	1.94	0.49
5:D:477:VAL:HG22	5:D:495:ILE:HG23	1.95	0.49
9:G:1218:LEU:HD23	9:G:1219:SER:N	2.28	0.49
3:J:610:GLU:N	3:J:610:GLU:OE1	2.45	0.49
3:J:210:ILE:HD12	3:J:214:VAL:HG21	1.95	0.48
9:A:942:TRP:HB3	9:A:953:LEU:HD12	1.96	0.48
9:G:903:ASP:N	9:G:999:ASN:OD1	2.46	0.48
5:L:196:ASP:OD1	5:L:197:ARG:N	2.46	0.48
9:A:625:LEU:HD21	9:A:897:PHE:HE2	1.78	0.48
8:c:64:GLY:N	8:c:80:ASP:OD2	2.47	0.48
5:D:339:ILE:HG23	5:D:356:VAL:HG11	1.95	0.48
9:A:428:SER:HA	9:A:431:VAL:HG23	1.95	0.48
7:F:113:ASP:OD2	7:F:184:ASN:ND2	2.46	0.47
3:J:710:ILE:HG21	3:J:791:LEU:HD12	1.96	0.47
7:F:20:VAL:HG11	7:F:67:THR:O	2.14	0.47
9:G:275:GLU:OE1	9:G:275:GLU:N	2.45	0.47
9:A:365:ASP:OD1	9:A:367:THR:HG22	2.14	0.47
5:D:196:ASP:OD1	5:D:197:ARG:N	2.47	0.47
1:H:102:PRO:O	1:H:118:ARG:NH2	2.46	0.47
3:B:314:ALA:HB3	9:A:179:ARG:NH2	2.29	0.47
5:L:111:PHE:O	5:L:115:ASN:ND2	2.46	0.47
5:L:477:VAL:HG22	5:L:495:ILE:HG23	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:209:ARG:NH2	5:D:379:THR:OG1	2.47	0.47
5:L:72:ILE:O	5:L:244:ASN:ND2	2.47	0.47
9:G:93:LEU:O	9:G:97:LEU:HD23	2.15	0.47
1:M:28:ILE:HD13	1:M:113:VAL:HG21	1.97	0.46
5:L:415:ASN:OD1	5:L:416:VAL:N	2.49	0.46
5:D:270:GLU:OE1	5:D:270:GLU:N	2.49	0.46
9:G:1228:LEU:HD13	9:G:1228:LEU:O	2.14	0.46
8:c:2:PRO:HB2	8:c:96:ILE:HG23	1.98	0.46
3:J:665:ILE:HG23	3:J:666:LEU:HD23	1.98	0.46
3:B:469:TYR:HH	3:B:474:HIS:HE2	1.60	0.46
1:M:193:VAL:HG13	1:M:211:ILE:CG2	2.46	0.46
9:G:633:PRO:O	9:G:636:ILE:HG22	2.16	0.45
9:G:979:GLU:N	9:G:979:GLU:OE1	2.48	0.45
3:B:624:ASN:OD1	3:B:672:GLN:NE2	2.47	0.45
3:J:207:VAL:HG22	3:J:298:GLU:HB3	1.98	0.45
3:J:181:TYR:CE2	3:J:191:LEU:HD22	2.52	0.45
9:A:902:GLU:OE1	9:A:902:GLU:N	2.50	0.45
3:J:683:GLU:OE1	3:J:719:ARG:NH2	2.45	0.45
9:A:390:ILE:HG23	9:A:647:MET:HG2	1.98	0.45
3:B:468:ARG:NH2	9:G:10:GLU:O	2.50	0.45
3:J:263:MET:SD	3:J:263:MET:N	2.90	0.45
1:H:193:VAL:HG13	1:H:211:ILE:CG2	2.48	0.44
3:J:110:GLN:NE2	9:A:1157:SER:O	2.50	0.44
3:J:195:GLU:N	3:J:195:GLU:OE1	2.50	0.44
9:G:370:MET:HE3	9:G:876:PRO:HD3	1.99	0.44
3:B:206:ALA:CB	3:B:260:LEU:HD12	2.48	0.44
9:G:842:THR:O	9:G:844:LEU:N	2.51	0.44
1:H:128:LEU:O	1:H:136:LEU:N	2.50	0.44
3:J:691:ILE:HD13	3:J:706:ALA:CA	2.48	0.44
3:B:190:ASP:OD1	3:B:191:LEU:N	2.48	0.44
4:C:60:ASN:O	5:D:355:ASN:ND2	2.50	0.44
4:K:35:GLU:OE1	4:K:112:TYR:OH	2.28	0.44
3:B:220:LEU:O	3:B:224:ILE:HD12	2.18	0.43
5:D:22:VAL:HG11	5:D:345:ASN:ND2	2.33	0.43
3:B:206:ALA:HB1	3:B:260:LEU:HD12	2.00	0.43
5:D:415:ASN:OD1	5:D:416:VAL:N	2.51	0.43
5:L:174:LEU:HD11	5:L:212:LEU:HD11	1.98	0.43
3:B:261:GLU:OE2	3:B:261:GLU:N	2.51	0.43
3:J:191:LEU:HD23	3:J:191:LEU:H	1.82	0.43
2:I:37:GLN:N	2:I:74:LYS:O	2.49	0.43
5:D:105:LEU:N	5:D:157:GLU:OE2	2.52	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:141:ASP:N	2:N:141:ASP:OD1	2.51	0.43
9:G:1281:ILE:N	9:G:1281:ILE:HD12	2.34	0.43
1:H:28:ILE:HD13	1:H:113:VAL:HG21	2.00	0.43
3:J:180:GLU:N	3:J:180:GLU:OE2	2.52	0.43
9:A:4:ARG:NE	9:A:1099:VAL:O	2.44	0.43
9:A:1221:GLU:OE1	9:A:1221:GLU:N	2.45	0.43
3:B:429:GLU:OE1	3:B:429:GLU:N	2.47	0.43
9:G:1239:LEU:HD23	9:G:1240:SER:N	2.33	0.43
5:D:157:GLU:N	5:D:157:GLU:OE1	2.51	0.43
3:B:691:ILE:HD13	3:B:706:ALA:CA	2.48	0.43
5:L:157:GLU:OE1	5:L:157:GLU:N	2.51	0.43
9:A:817:ALA:HB3	9:A:818:PRO:HD3	2.01	0.43
9:A:209:ASN:OD1	9:A:210:ASN:N	2.52	0.42
9:A:638:ARG:NH2	9:A:900:TYR:O	2.52	0.42
9:G:428:SER:HA	9:G:431:VAL:HG23	2.01	0.42
3:B:50:ASP:OD1	3:B:52:ASN:ND2	2.50	0.42
3:J:501:ILE:O	3:J:505:THR:OG1	2.26	0.42
3:J:777:GLN:NE2	3:J:781:ASP:OD1	2.52	0.42
1:H:78:THR:OG1	1:H:79:ASN:N	2.43	0.42
9:A:121:LEU:HD22	9:A:125:TYR:CZ	2.55	0.42
3:B:79:VAL:HG12	3:B:83:LEU:HD23	2.01	0.42
5:L:467:SER:OG	5:L:471:GLU:OE2	2.37	0.42
9:A:85:ASP:O	9:A:89:THR:OG1	2.35	0.42
5:D:67:GLN:N	5:D:67:GLN:OE1	2.53	0.42
7:F:366:ALA:O	7:F:367:SER:OG	2.30	0.42
3:J:717:THR:O	3:J:721:SER:OG	2.24	0.42
9:G:817:ALA:HB3	9:G:818:PRO:HD3	2.02	0.42
3:J:487:GLU:O	3:J:491:LEU:HD13	2.20	0.42
9:A:44:GLN:OE1	9:A:44:GLN:N	2.52	0.42
9:A:275:GLU:OE2	9:A:275:GLU:N	2.50	0.42
5:L:339:ILE:HD11	5:L:358:VAL:HG13	2.02	0.41
5:D:131:ASP:OD1	5:D:132:ILE:N	2.53	0.41
5:L:105:LEU:N	5:L:157:GLU:OE2	2.53	0.41
8:c:70:ILE:HD11	8:c:75:ALA:HB2	2.03	0.41
9:A:313:THR:HG21	9:A:359:ASN:HA	2.01	0.41
1:H:78:THR:HG23	1:H:80:THR:HG23	2.02	0.41
9:A:842:THR:O	9:A:844:LEU:N	2.54	0.41
1:M:43:GLN:NE2	7:F:304:GLN:OE1	2.50	0.41
9:A:4:ARG:NH2	9:A:1096:PHE:O	2.54	0.41
5:D:422:MET:HE1	5:D:458:ILE:HD12	2.03	0.41
3:B:759:LEU:HD12	3:B:790:PHE:CD2	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:34:ILE:HG12	7:F:48:ILE:HG22	2.02	0.41
5:L:339:ILE:HD11	5:L:358:VAL:CG1	2.51	0.41
9:A:59:GLU:HG2	9:A:114:ALA:HB2	2.01	0.41
2:N:115:THR:HG23	5:L:441:ALA:CB	2.50	0.41
9:A:464:SER:O	9:A:467:VAL:HG22	2.21	0.41
9:A:711:ARG:HE	9:A:711:ARG:H	1.69	0.41
3:B:344:ASP:OD1	3:B:346:THR:OG1	2.35	0.40
3:B:610:GLU:OE1	3:B:610:GLU:N	2.50	0.40
7:F:441:ASP:OD1	7:F:443:SER:OG	2.30	0.40
5:L:22:VAL:HG11	5:L:345:ASN:ND2	2.36	0.40
7:F:25:ILE:O	7:F:27:SER:N	2.54	0.40
3:B:436:ALA:O	3:B:440:LEU:HD23	2.22	0.40
9:A:56:GLN:OE1	9:A:56:GLN:N	2.54	0.40
9:A:93:LEU:O	9:A:97:LEU:HD23	2.22	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	H	186/217 (86%)	177 (95%)	9 (5%)	0	100	100
1	M	186/217 (86%)	175 (94%)	11 (6%)	0	100	100
2	I	132/158 (84%)	127 (96%)	5 (4%)	0	100	100
2	N	132/158 (84%)	127 (96%)	5 (4%)	0	100	100
3	B	665/804 (83%)	654 (98%)	11 (2%)	0	100	100
3	J	665/804 (83%)	650 (98%)	15 (2%)	0	100	100
4	C	136/149 (91%)	132 (97%)	4 (3%)	0	100	100
4	K	136/149 (91%)	130 (96%)	6 (4%)	0	100	100
5	D	512/519 (99%)	503 (98%)	9 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	L	512/519 (99%)	503 (98%)	9 (2%)	0	100	100
6	E	6/56 (11%)	6 (100%)	0	0	100	100
7	F	593/597 (99%)	579 (98%)	14 (2%)	0	100	100
8	c	41/99 (41%)	39 (95%)	2 (5%)	0	100	100
9	A	1117/1323 (84%)	1103 (99%)	14 (1%)	0	100	100
9	G	1117/1323 (84%)	1102 (99%)	15 (1%)	0	100	100
All	All	6136/7092 (86%)	6007 (98%)	129 (2%)	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	H	169/190 (89%)	166 (98%)	3 (2%)	51	73
1	M	169/190 (89%)	165 (98%)	4 (2%)	43	67
2	I	127/137 (93%)	127 (100%)	0	100	100
2	N	127/137 (93%)	126 (99%)	1 (1%)	73	86
3	B	614/710 (86%)	603 (98%)	11 (2%)	51	73
3	J	614/710 (86%)	610 (99%)	4 (1%)	76	87
4	C	128/137 (93%)	128 (100%)	0	100	100
4	K	128/137 (93%)	126 (98%)	2 (2%)	55	76
5	D	436/440 (99%)	428 (98%)	8 (2%)	51	73
5	L	436/440 (99%)	429 (98%)	7 (2%)	55	76
6	E	8/53 (15%)	7 (88%)	1 (12%)	4	8
7	F	497/498 (100%)	494 (99%)	3 (1%)	78	89
8	c	33/75 (44%)	33 (100%)	0	100	100
9	A	1027/1181 (87%)	1016 (99%)	11 (1%)	65	81
9	G	1027/1181 (87%)	1006 (98%)	21 (2%)	48	71

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	5540/6216 (89%)	5464 (99%)	76 (1%)	57 78

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	122	ILE
1	H	190	TYR
1	H	198	ASN
3	B	20	LYS
3	B	76	GLU
3	B	180	GLU
3	B	224	ILE
3	B	260	LEU
3	B	317	ILE
3	B	319	GLN
3	B	410	THR
3	B	504	MET
3	B	731	GLN
3	B	741	LEU
5	D	35	THR
5	D	159	ILE
5	D	299	ARG
5	D	305	LEU
5	D	309	LEU
5	D	421	ILE
5	D	425	GLU
5	D	429	LEU
6	E	51	ASP
1	M	32	PHE
1	M	83	LYS
1	M	103	ASN
1	M	176	LEU
7	F	47	GLU
7	F	55	MET
7	F	347	GLU
2	N	155	LYS
3	J	174	LEU
3	J	220	LEU
3	J	301	GLN
3	J	317	ILE
4	K	75	LEU
4	K	138	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	L	159	ILE
5	L	227	LEU
5	L	234	ASP
5	L	299	ARG
5	L	315	LEU
5	L	425	GLU
5	L	490	GLU
9	A	56	GLN
9	A	121	LEU
9	A	137	ILE
9	A	181	CYS
9	A	185	ILE
9	A	273	GLN
9	A	531	LEU
9	A	641	GLU
9	A	863	VAL
9	A	1003	ASP
9	A	1194	LEU
9	G	20	HIS
9	G	91	GLU
9	G	181	CYS
9	G	206	HIS
9	G	478	THR
9	G	507	MET
9	G	531	LEU
9	G	582	GLU
9	G	602	ASP
9	G	609	ILE
9	G	682	ASP
9	G	699	GLN
9	G	733	GLN
9	G	863	VAL
9	G	874	LEU
9	G	879	GLU
9	G	913	ARG
9	G	949	GLU
9	G	1150	ARG
9	G	1206	GLU
9	G	1274	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
3	B	109	GLN
3	B	553	ASN
3	B	654	HIS
5	D	327	GLN
5	D	345	ASN
1	M	31	ASN
1	M	103	ASN
7	F	423	ASN
7	F	494	ASN
7	F	496	ASN
2	N	45	GLN
2	N	70	ASN
2	N	152	HIS
2	N	153	HIS
3	J	138	HIS
3	J	229	HIS
3	J	654	HIS
3	J	785	GLN
9	A	32	HIS
9	A	206	HIS
9	A	355	ASN
9	A	425	GLN
9	A	658	GLN
9	A	708	ASN
9	A	1090	HIS
9	A	1174	GLN
9	G	32	HIS
9	G	80	GLN
9	G	227	GLN
9	G	311	ASN
9	G	425	GLN
9	G	703	HIS
9	G	957	GLN
9	G	1232	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

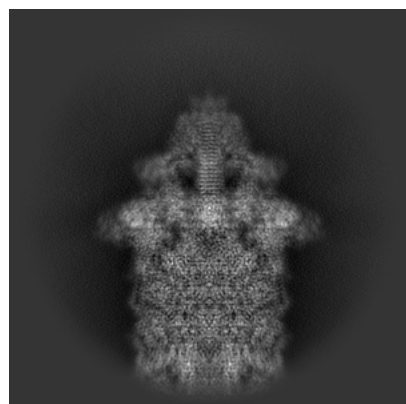
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53919. These allow visual inspection of the internal detail of the map and identification of artifacts.

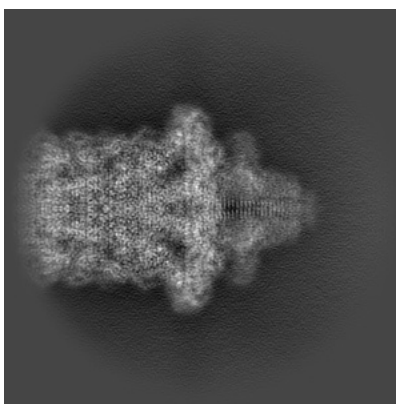
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

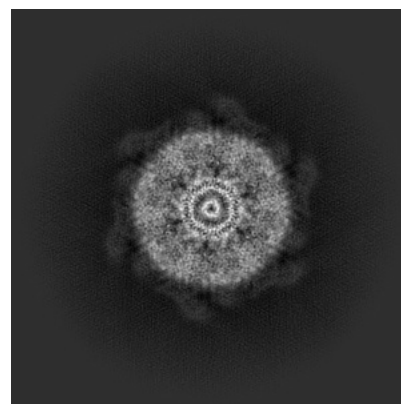
6.1.1 Primary map



X

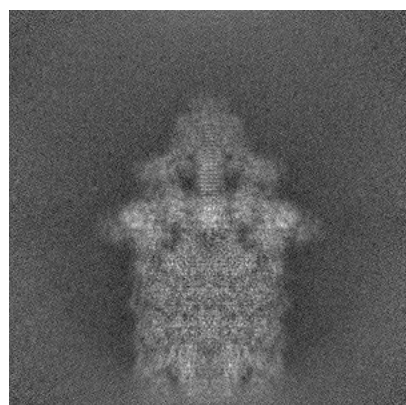


Y

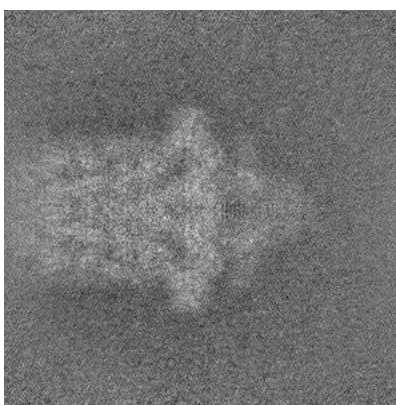


Z

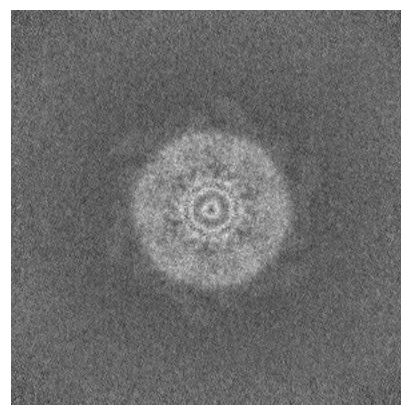
6.1.2 Raw map



X



Y

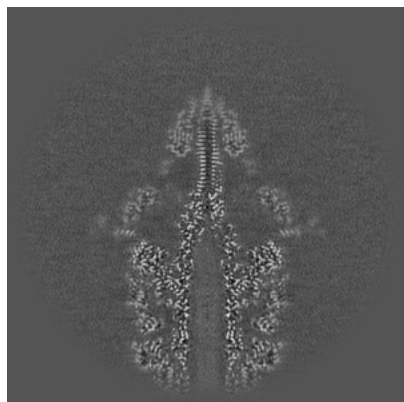


Z

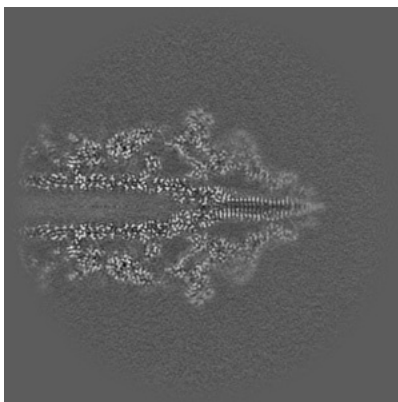
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

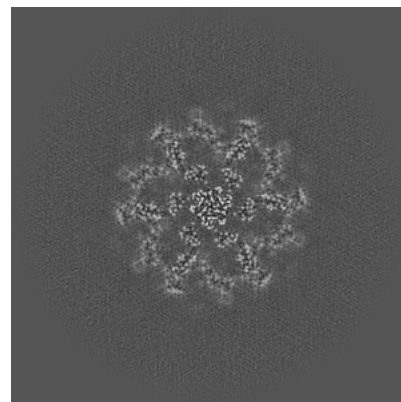
6.2.1 Primary map



X Index: 315

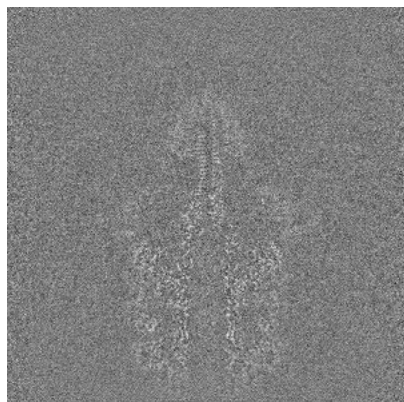


Y Index: 315

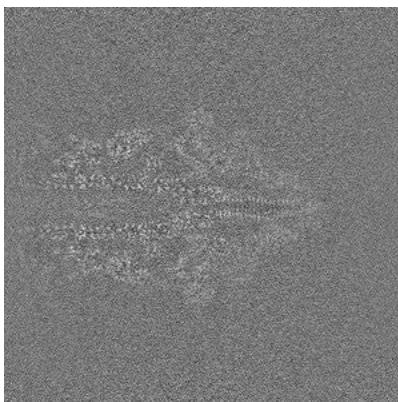


Z Index: 315

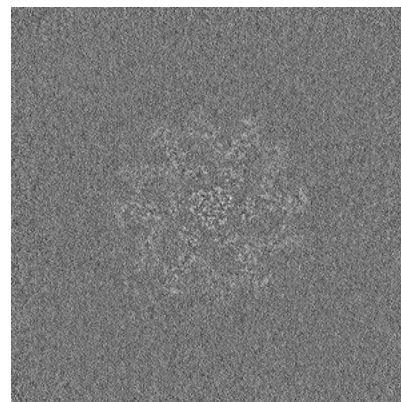
6.2.2 Raw map



X Index: 315



Y Index: 315

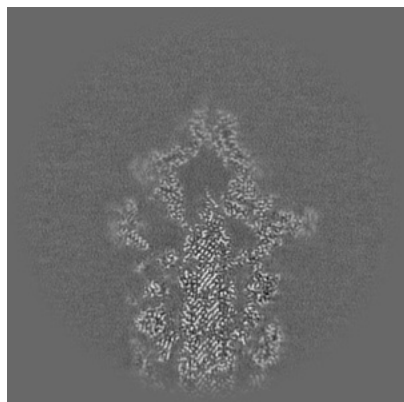


Z Index: 315

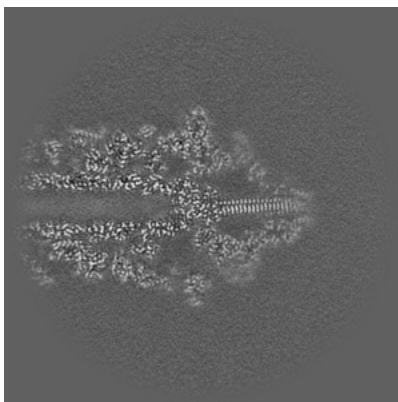
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

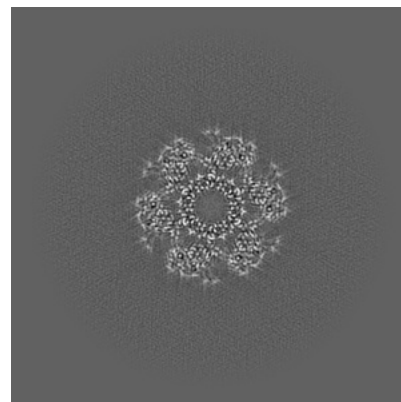
6.3.1 Primary map



X Index: 346

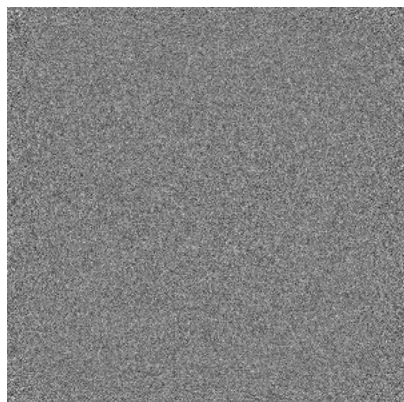


Y Index: 325

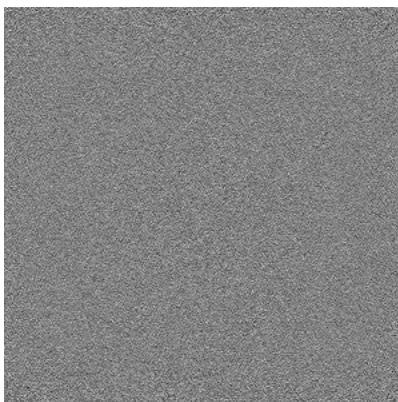


Z Index: 189

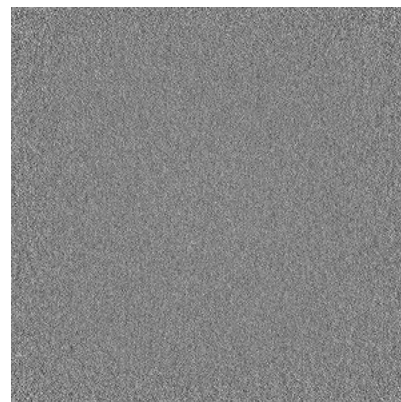
6.3.2 Raw map



X Index: 0



Y Index: 0

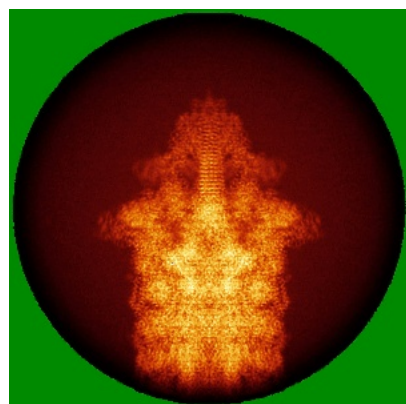


Z Index: 0

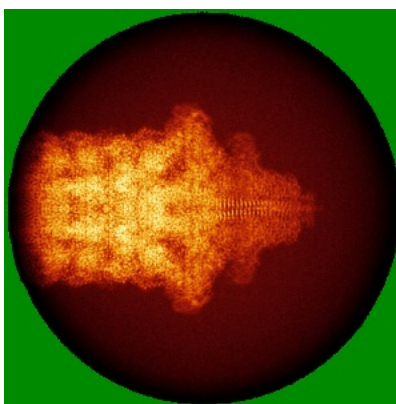
The images above show the largest variance slices of the map in three orthogonal directions.

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

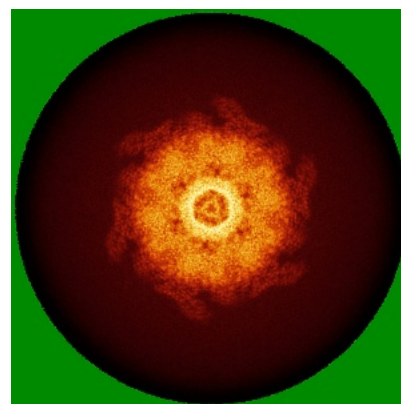
6.4.1 Primary map



X

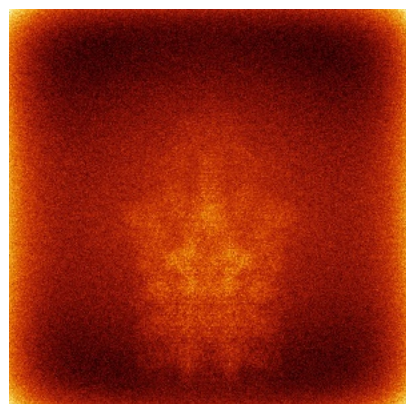


Y

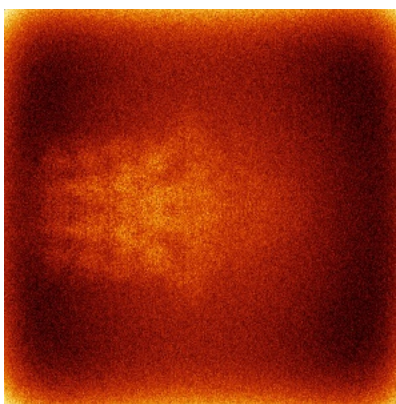


Z

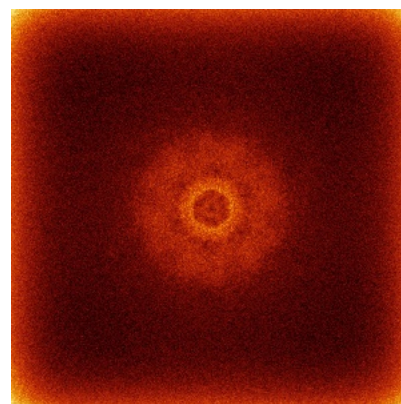
6.4.2 Raw map



X



Y

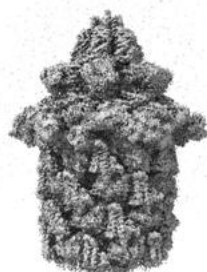


Z

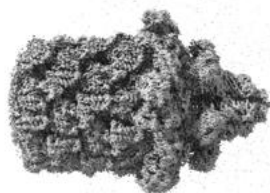
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



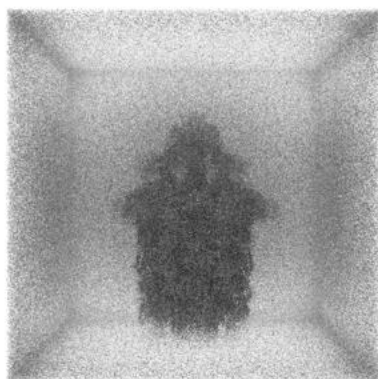
Y



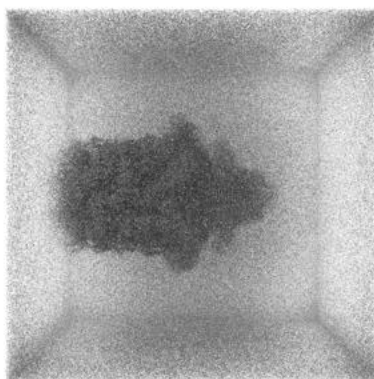
Z

The images above show the 3D surface view of the map at the recommended contour level 0.0678. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

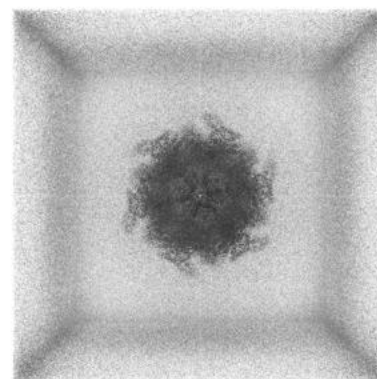
6.5.2 Raw map



X



Y



Z

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.

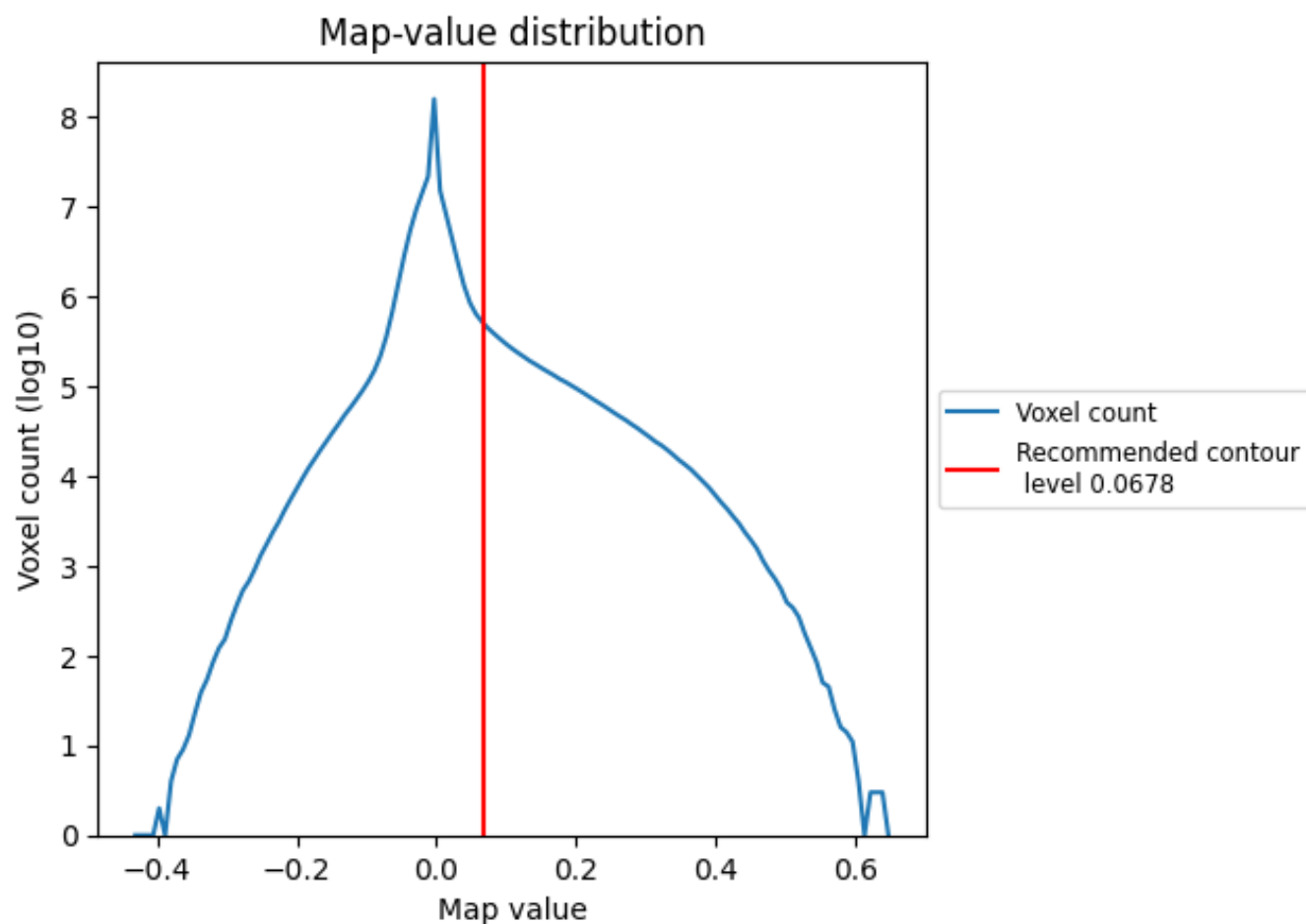
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

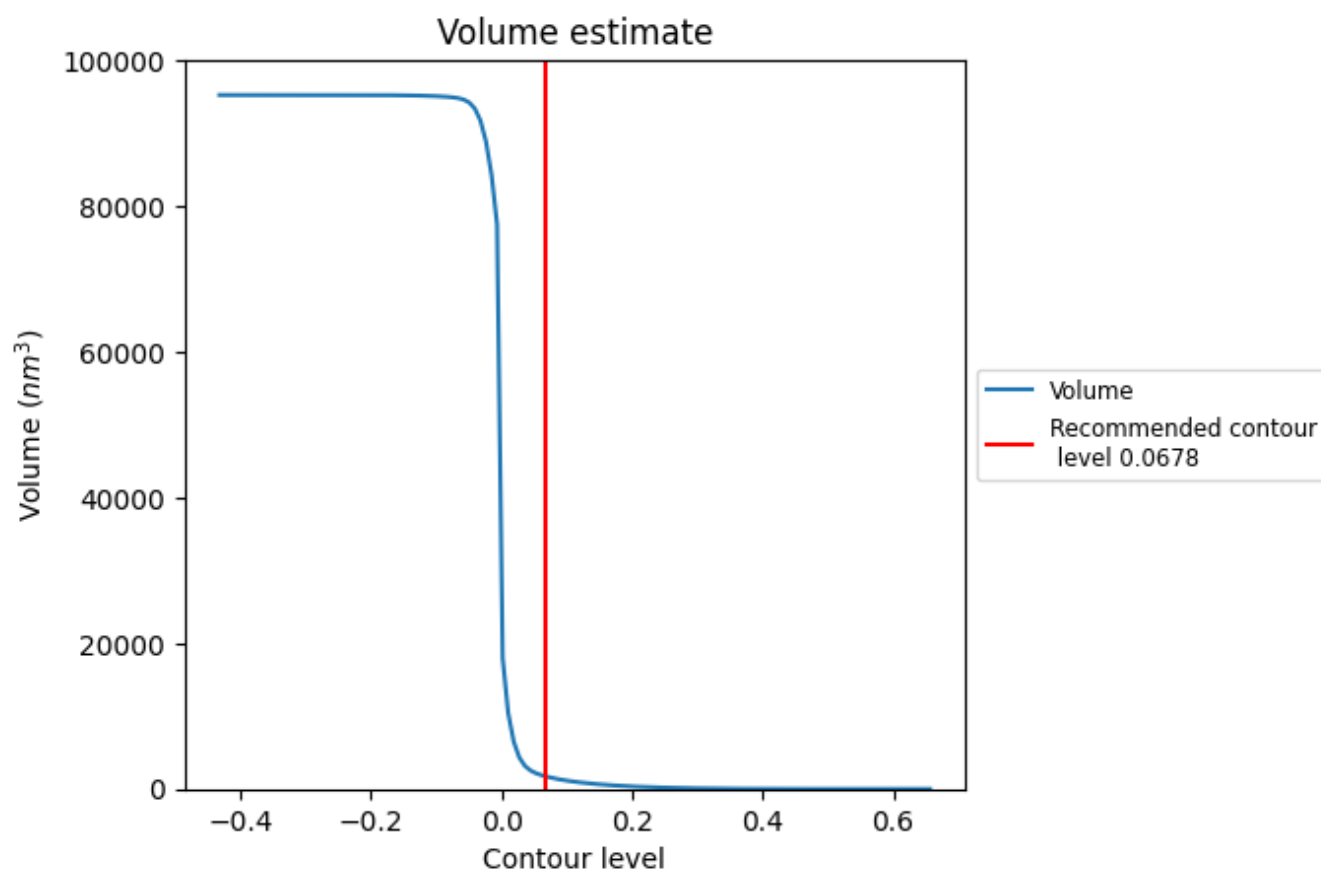
This section contains the results of statistical analysis of the map.

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.

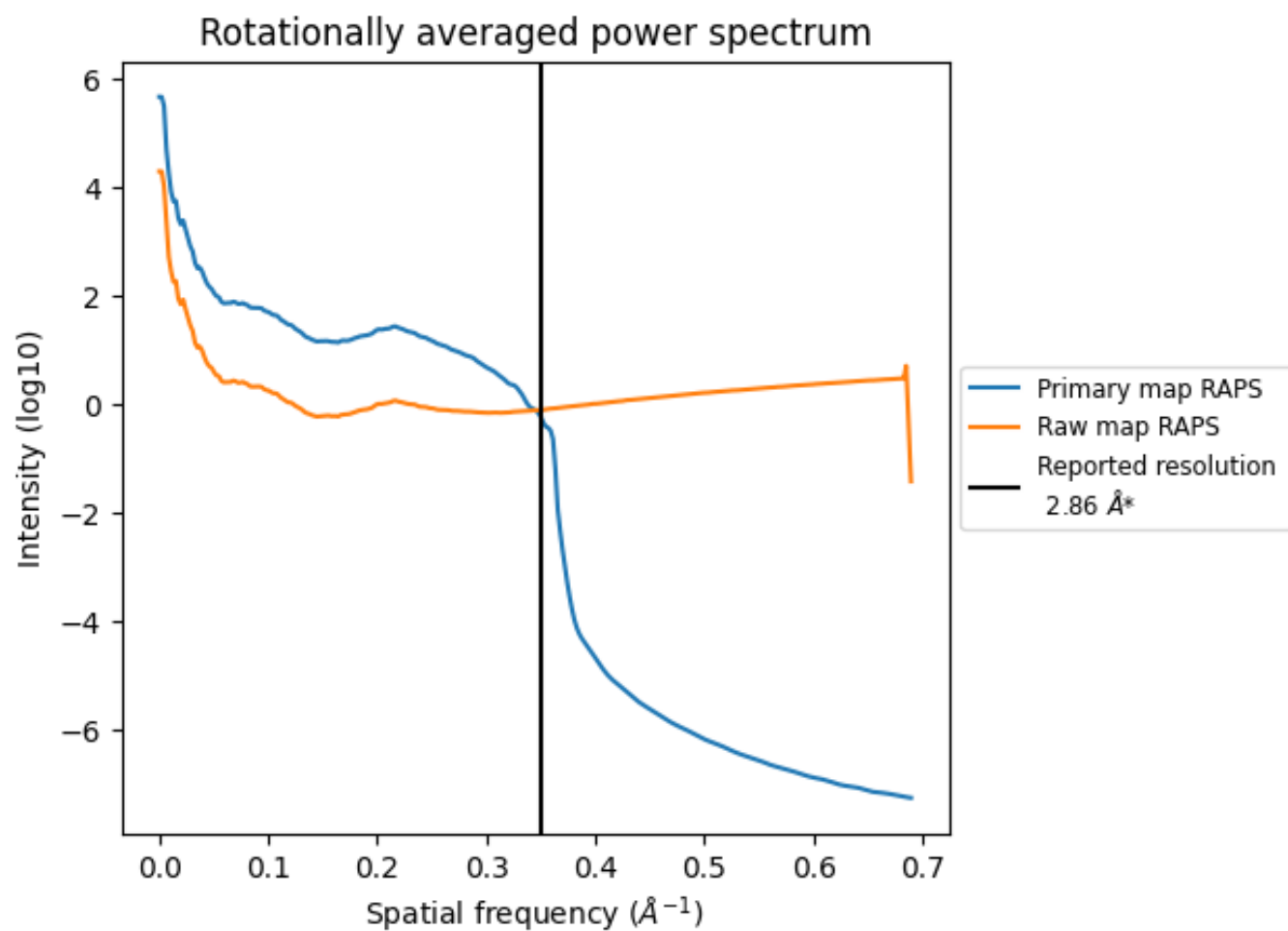
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1734 nm³; this corresponds to an approximate mass of 1566 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 ⓘ

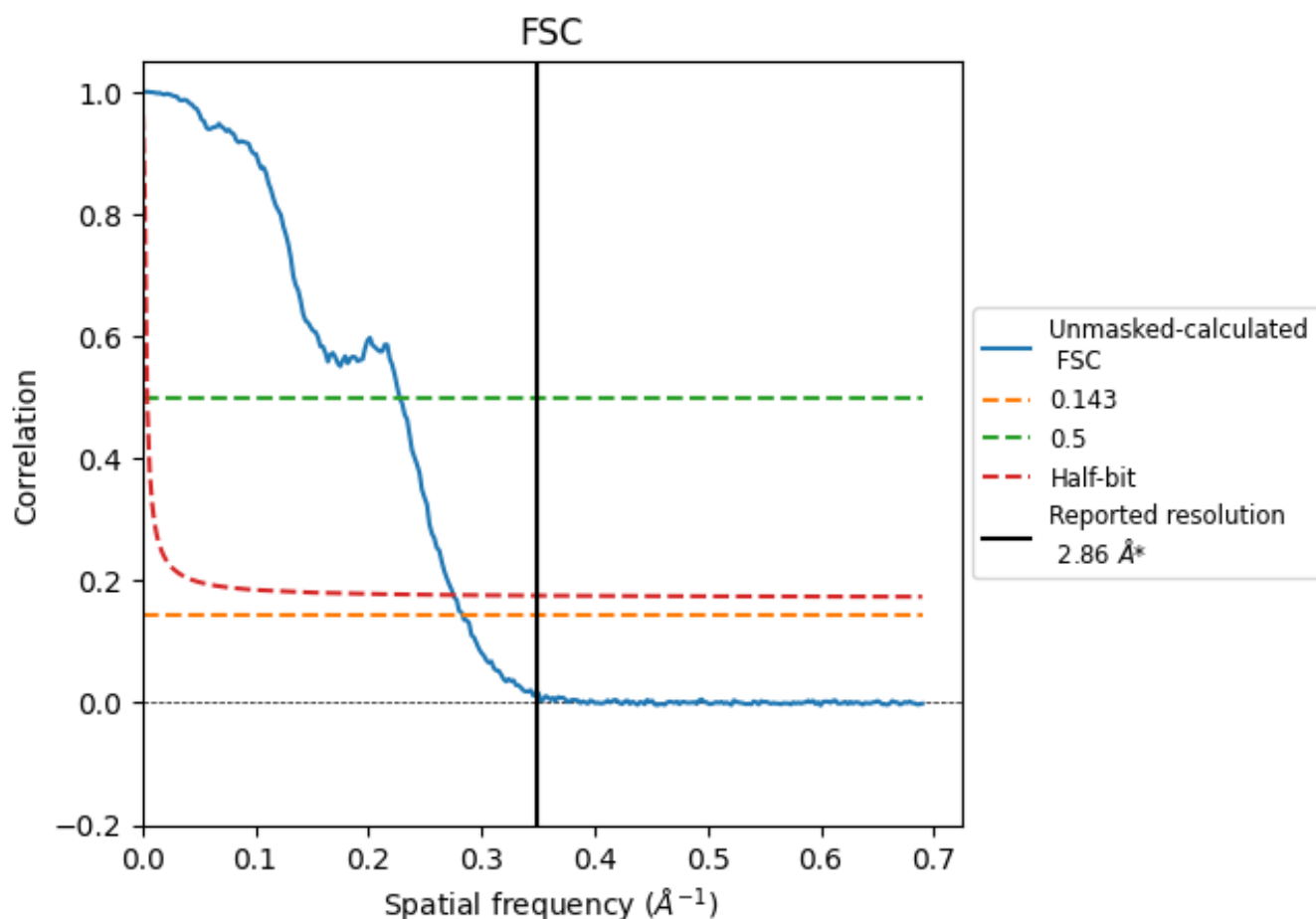


*Reported resolution corresponds to spatial frequency of $0.350 \text{ \AA}^{-1}$

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 0.350 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.86	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.53	4.39	3.63

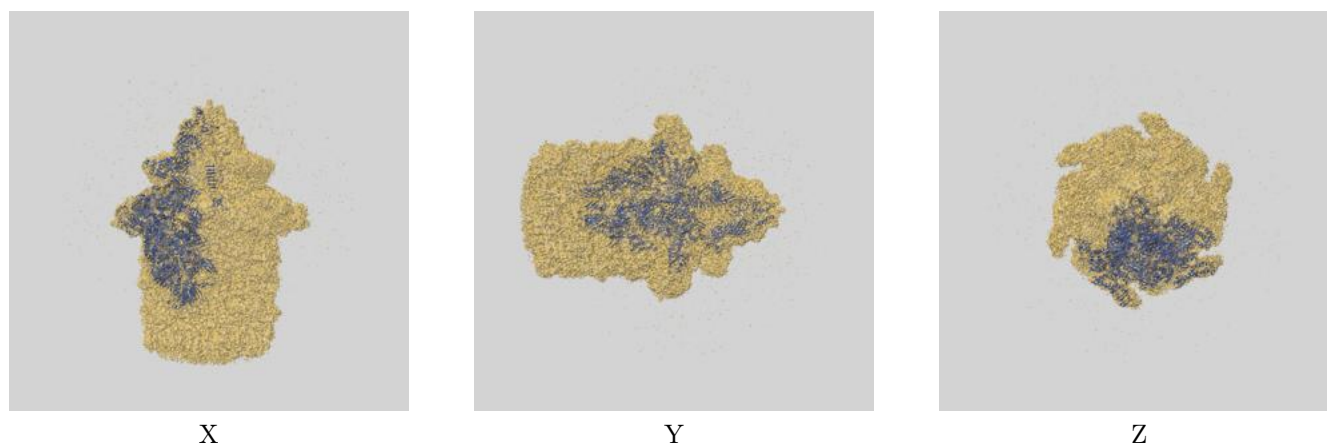
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.53 differs from the reported value 2.86 by more than 10 %

9 Map-model fit [i](#)

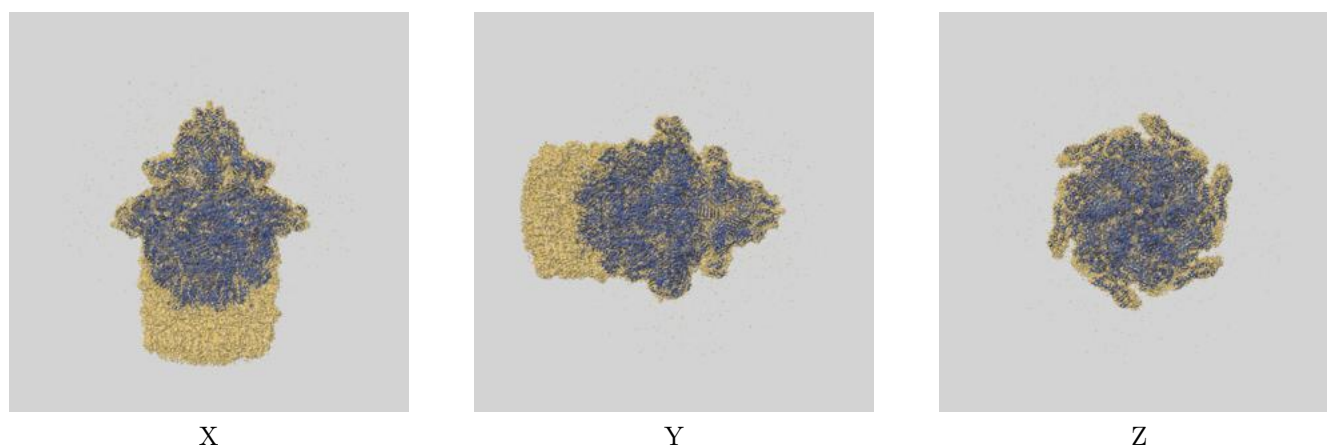
This section contains information regarding the fit between EMDB map EMD-53919 and PDB model 9RCE. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

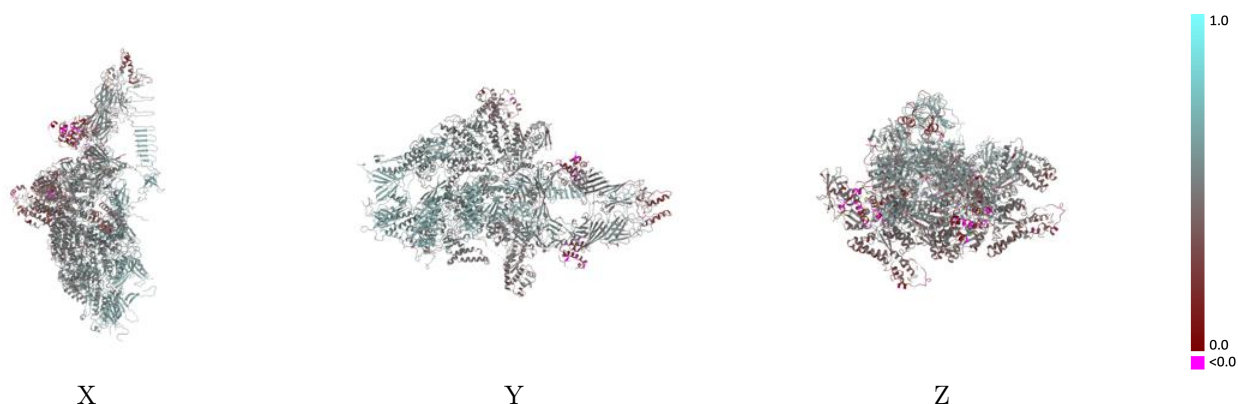


9.1.2 Map-model assembly overlay [i](#)



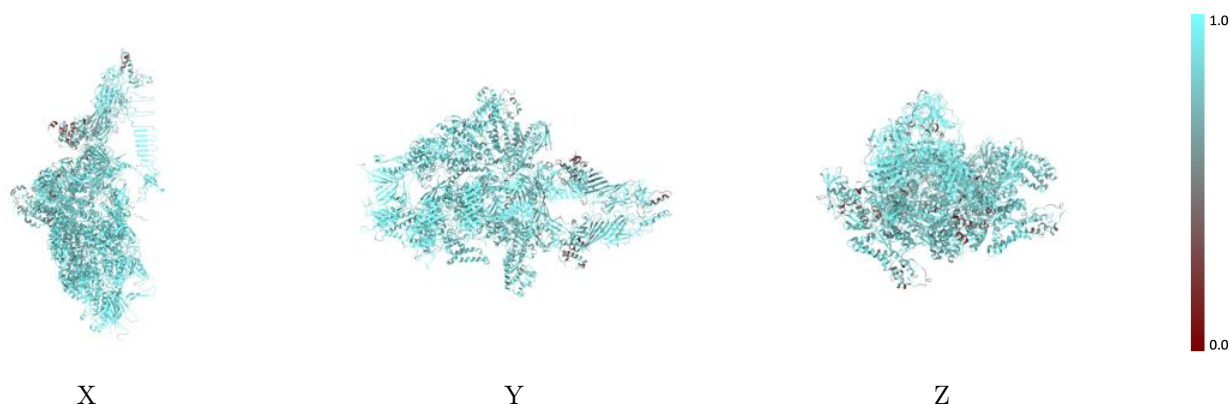
The images above show the 3D surface view of the map at the recommended contour level 0.0678 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



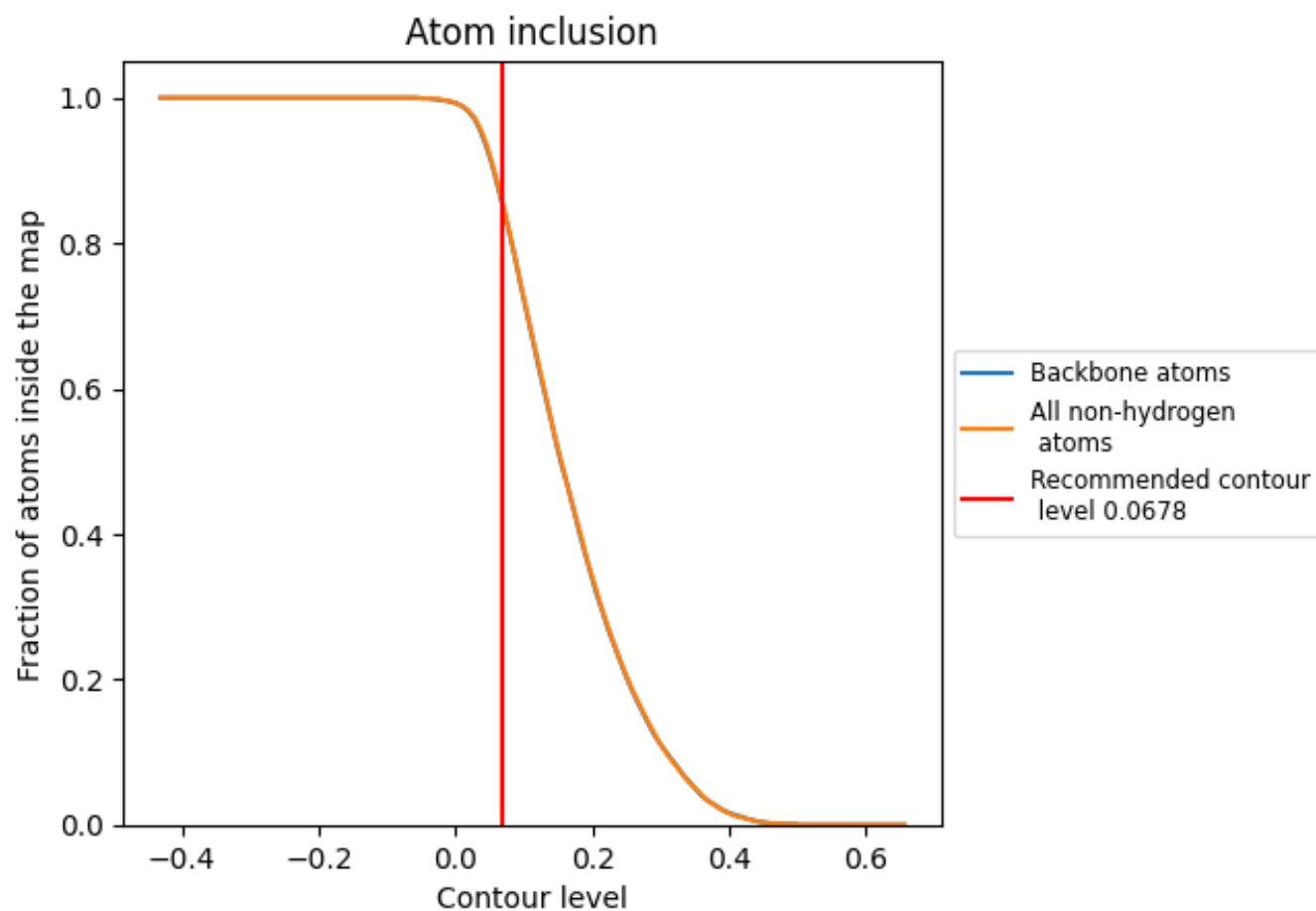
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0678).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% 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 (0.0678) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8590	0.4790
A	0.8250	0.4520
B	0.8530	0.4350
C	0.9140	0.5490
D	0.8900	0.5070
E	0.8000	0.5780
F	0.9290	0.5760
G	0.8160	0.4390
H	0.9110	0.5460
I	0.9130	0.5730
J	0.8510	0.4300
K	0.9260	0.5480
L	0.8950	0.5080
M	0.9100	0.5470
N	0.9240	0.5690
c	0.7130	0.3110

1.0

0.0

<0.0