



Full wwPDB EM Validation Report ⓘ

Mar 19, 2026 – 09:31 PM UTC

PDB ID : 6SWE / pdb_00006swe
EMDB ID : EMD-10324
Title : IC2 head of cryo-EM structure of a full archaeal ribosomal translation initiation complex devoid of aIF1 in *P. abyssi*
Authors : Coureux, P.-D.; Mechulam, Y.; Schmitt, E.
Deposited on : 2019-09-20
Resolution : 3.10 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:

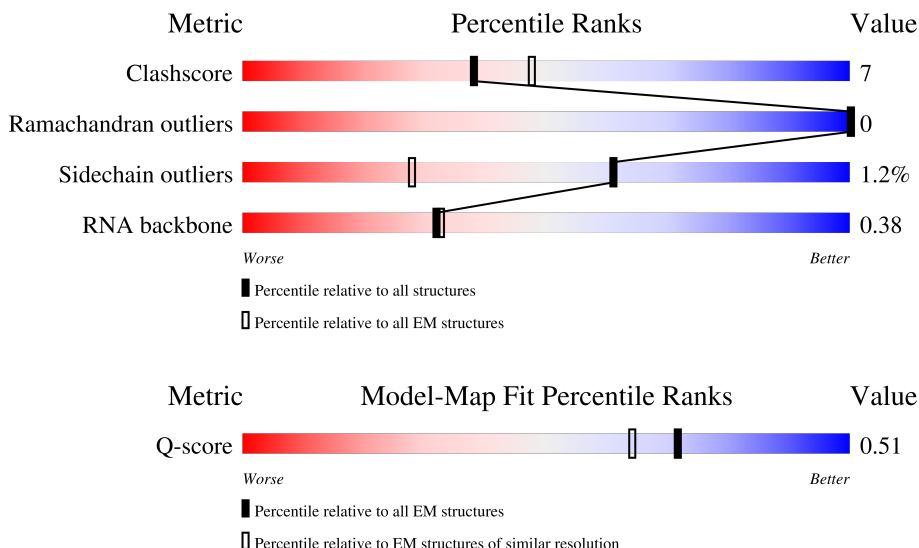
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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 3.10 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.



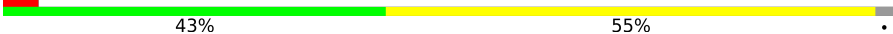
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14724 (2.60 - 3.60)

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	2	468	
2	H	215	
3	K	135	

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Mol	Chain	Length	Quality of chain
4	L	102	 78%21%.
5	O	148	 78%18%. .
6	P	56	 84%14%. .
7	S	67	 70%24%. . .
8	T	132	 82%17%. .
9	U	150	 87%13%. .
10	X	71	 68%25%. . 6%.
11	Y	51	 43%55%. .
12	Z	210	 78%16%6%.
13	3	123	 54%46%. .
14	4	18	 11%61%33%6%.
15	6	113	 25%54%29%. 16%.

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 22737 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 RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	468	Total	C	N	O	P	0	0
			10068	4487	1852	3261	468		

- Molecule 2 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	213	Total	C	N	O	S	0	0
			1720	1092	322	299	7		

- Molecule 3 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	K	134	Total	C	N	O	S	0	0
			1065	668	206	188	3		

- Molecule 4 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	101	Total	C	N	O	S	0	0
			817	507	158	148	4		

- Molecule 5 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	O	143	Total	C	N	O	S	0	0
			1151	721	229	196	5		

- Molecule 6 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	P	55	Total	C	N	O	S	0	0
			455	288	95	67	5		

- Molecule 7 is a protein called 30S ribosomal protein S17e.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	S	66	Total	C	N	O	S	0	0
			558	355	106	96	1		

- Molecule 8 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	T	130	Total	C	N	O	S	0	0
			1057	675	201	174	7		

- Molecule 9 is a protein called 30S ribosomal protein S19e.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	U	149	Total	C	N	O	0	0
			1223	790	221	212		

- Molecule 10 is a protein called 30S ribosomal protein S28e.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	X	67	Total	C	N	O	0	0
			536	327	111	98		

- Molecule 11 is a protein called 30S ribosomal protein S27ae.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Y	50	Total	C	N	O	S	0	0
			408	262	77	63	6		

- Molecule 12 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Z	197	Total	C	N	O	S	0	0
			1550	989	286	271	4		

- Molecule 13 is a protein called 50S ribosomal protein L7Ae.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	3	123	Total	C	N	O	S	0	0
			941	599	157	181	4		

- Molecule 14 is a RNA chain called initiator Met-tRNA fMet from E. coli (A1U72 variant).

Mol	Chain	Residues	Atoms					AltConf	Trace
14	4	18	Total	C	N	O	P	0	0
			384	172	69	125	18		

- Molecule 15 is a protein called Translation initiation factor 1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	6	95	Total	C	N	O	S	0	0
			777	496	148	130	3		

- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
16	2	7	Total	Mg	0
			7	7	
16	4	1	Total	Mg	0
			1	1	

- Molecule 17 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
17	P	1	Total	Zn	0
			1	1	

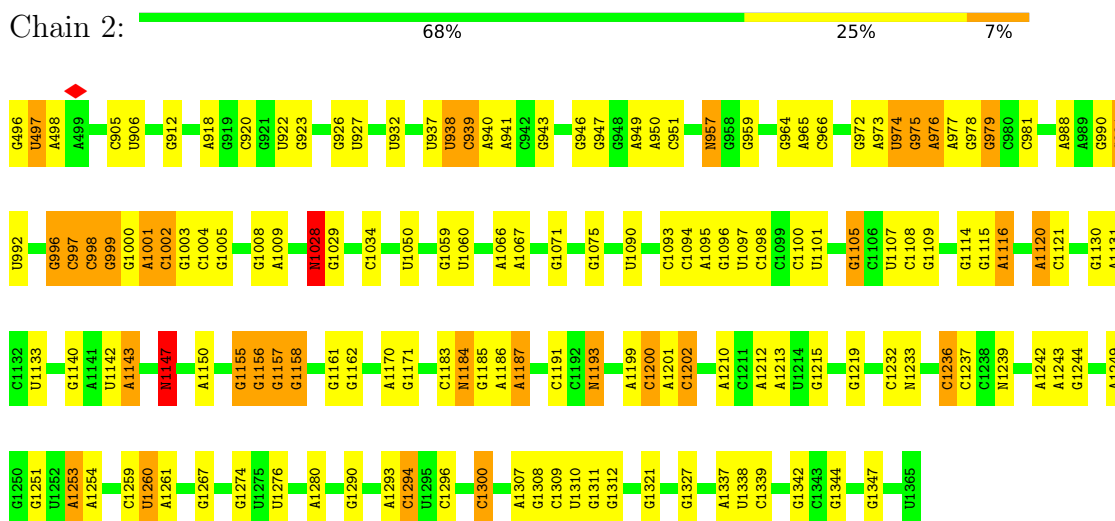
- Molecule 18 is water.

Mol	Chain	Residues	Atoms		AltConf
18	2	16	Total	O	0
			16	16	
18	K	1	Total	O	0
			1	1	
18	U	1	Total	O	0
			1	1	

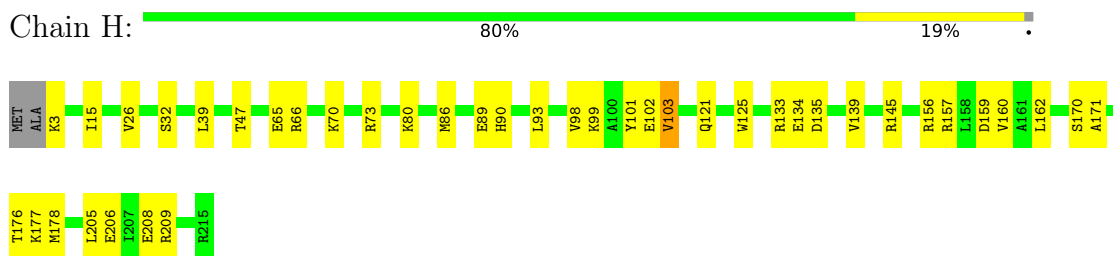
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

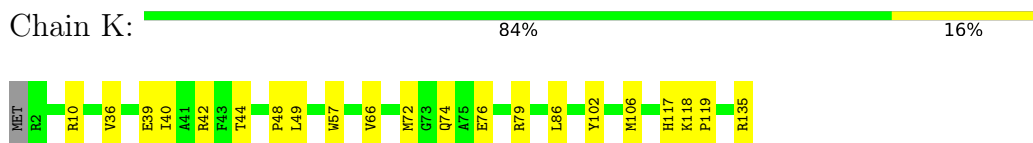
• Molecule 1: 16S ribosomal RNA



• Molecule 2: 30S ribosomal protein S7



• Molecule 3: 30S ribosomal protein S9



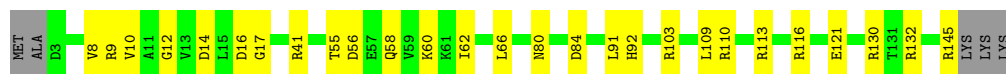
• Molecule 4: 30S ribosomal protein S10

Chain L:  78% 21%



- Molecule 5: 30S ribosomal protein S13

Chain O:  78% 18%



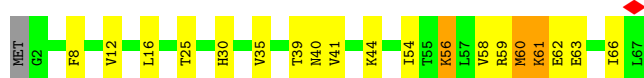
- Molecule 6: 30S ribosomal protein S14 type Z

Chain P:  84% 14%



- Molecule 7: 30S ribosomal protein S17e

Chain S:  70% 24%



- Molecule 8: 30S ribosomal protein S19

Chain T:  82% 17%



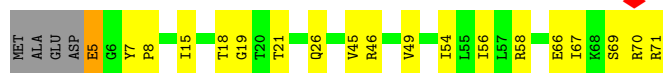
- Molecule 9: 30S ribosomal protein S19e

Chain U:  87% 13%



- Molecule 10: 30S ribosomal protein S28e

Chain X:  68% 25% 6%



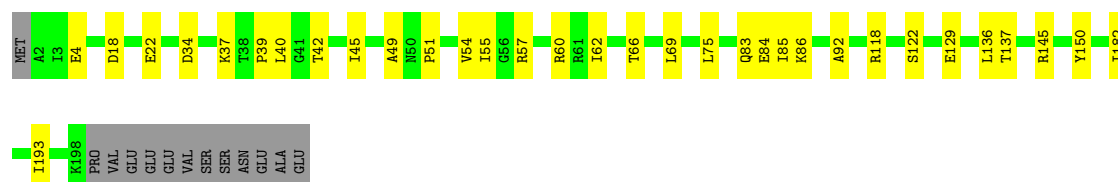
- Molecule 11: 30S ribosomal protein S27ae

Chain Y: 



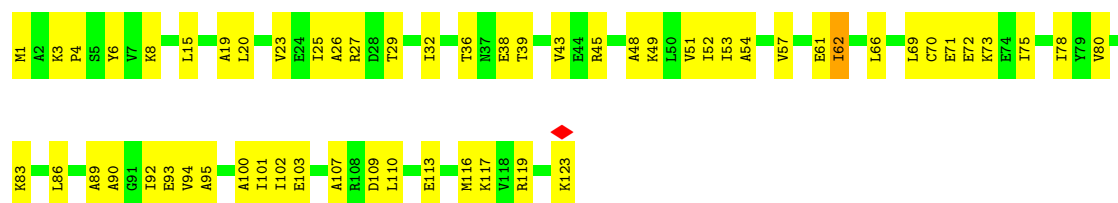
- Molecule 12: 30S ribosomal protein S3

Chain Z: 



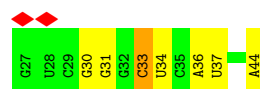
- Molecule 13: 50S ribosomal protein L7Ae

Chain 3: 



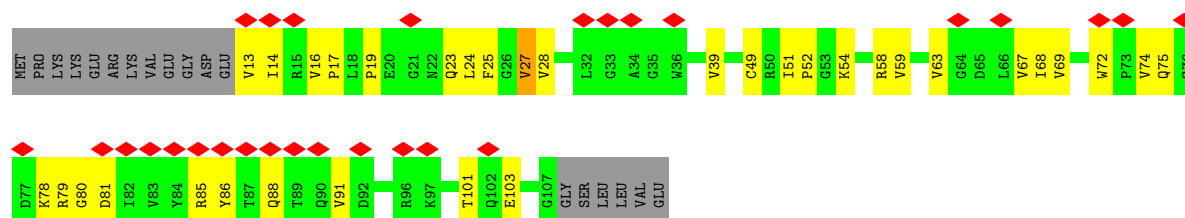
- Molecule 14: initiator Met-tRNA fMet from E. coli (A1U72 variant)

Chain 4: 



- Molecule 15: Translation initiation factor 1A

Chain 6: 



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	142000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	2	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	0.053	Depositor
Minimum map value	-0.021	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.004	Depositor
Map size (Å)	379.32, 379.32, 379.32	wwPDB
Map dimensions	348, 348, 348	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.09, 1.09, 1.09	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: B8H, ZN, OMC, 5MC, MG, 4AC

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	2	0.50	0/11008	0.46	0/17158
2	H	0.48	0/1757	0.57	0/2359
3	K	0.45	0/1081	0.62	0/1449
4	L	0.40	0/825	0.53	0/1107
5	O	0.45	0/1170	0.57	0/1573
6	P	0.48	0/465	0.55	0/613
7	S	0.38	0/565	0.56	0/747
8	T	0.48	0/1077	0.60	0/1439
9	U	0.48	0/1253	0.54	0/1689
10	X	0.42	0/538	0.58	0/719
11	Y	0.25	0/420	0.57	0/559
12	Z	0.41	0/1572	0.56	0/2110
13	3	0.26	0/953	0.57	1/1284 (0.1%)
14	4	0.42	0/405	0.38	0/629
15	6	0.23	0/793	0.55	0/1072
All	All	0.46	0/23882	0.51	1/34507 (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
3	K	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	3	62	ILE	N-CA-C	-6.92	105.78	112.29

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	K	119	PRO	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	10068	0	5091	74	0
2	H	1720	0	1775	26	0
3	K	1065	0	1121	16	0
4	L	817	0	871	13	0
5	O	1151	0	1191	17	0
6	P	455	0	475	8	0
7	S	558	0	595	13	0
8	T	1057	0	1131	14	0
9	U	1223	0	1263	15	0
10	X	536	0	571	15	0
11	Y	408	0	413	35	0
12	Z	1550	0	1637	21	0
13	3	941	0	994	47	0
14	4	384	0	198	5	0
15	6	777	0	806	27	0
16	2	7	0	0	0	0
16	4	1	0	0	0	0
17	P	1	0	0	0	0
18	2	16	0	0	2	0
18	K	1	0	0	0	0
18	U	1	0	0	1	0
All	All	22737	0	18132	301	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 7.

All (301) 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)
11:Y:8:TYR:O	11:Y:9:ILE:HG22	1.70	0.90
11:Y:9:ILE:HG23	11:Y:16:ILE:O	1.70	0.90
13:3:1:MET:HB3	13:3:53:ILE:HD12	1.60	0.84
1:2:1115:G:HO2'	1:2:1116:A:H8	1.26	0.81
11:Y:9:ILE:HG22	11:Y:18:LYS:HB2	1.60	0.81
13:3:92:ILE:HG13	13:3:93:GLU:H	1.49	0.78
15:6:23:GLN:HE21	15:6:68:ILE:HB	1.51	0.75
15:6:72:TRP:HB2	15:6:79:ARG:HD2	1.70	0.74
11:Y:8:TYR:O	11:Y:9:ILE:CG2	2.35	0.73
7:S:59:ARG:O	7:S:59:ARG:HG2	1.88	0.73
1:2:991:G:OP1	6:P:2:ALA:N	2.23	0.72
15:6:74:VAL:HB	15:6:79:ARG:HE	1.55	0.71
13:3:66:LEU:O	13:3:70:CYS:N	2.19	0.70
3:K:135:ARG:NH1	14:4:34:U:OP2	2.24	0.70
2:H:134:GLU:OE1	10:X:58:ARG:NH1	2.25	0.70
1:2:988:A:OP1	8:T:50:LYS:NZ	2.25	0.69
1:2:1193:4AC:O7	1:2:1193:4AC:H5	1.91	0.69
5:O:113:ARG:NH1	5:O:121:GLU:OE2	2.26	0.69
11:Y:45:TYR:CE2	11:Y:47:GLU:HB3	2.27	0.68
15:6:24:LEU:HB3	15:6:69:VAL:HG23	1.76	0.68
11:Y:27:PRO:O	13:3:45:ARG:NE	2.27	0.67
1:2:1155:G:O2'	1:2:1156:G:O5'	2.13	0.67
8:T:87:LYS:HG3	8:T:88:GLU:HG2	1.78	0.65
11:Y:37:ARG:HA	11:Y:49:LYS:H	1.62	0.65
1:2:981:C:N3	11:Y:37:ARG:NH2	2.41	0.65
15:6:75:GLN:OE1	15:6:78:LYS:NZ	2.30	0.64
12:Z:57:ARG:O	12:Z:60:ARG:NE	2.30	0.64
1:2:1034:C:OP2	18:2:1501:HOH:O	2.15	0.63
10:X:45:VAL:HG21	10:X:49:VAL:HG11	1.79	0.63
13:3:83:LYS:HD2	13:3:95:ALA:HB1	1.81	0.63
11:Y:47:GLU:OE2	11:Y:50:LYS:NZ	2.28	0.63
1:2:1130:G:N7	7:S:44:LYS:NZ	2.42	0.63
11:Y:20:LYS:NZ	11:Y:21:PHE:O	2.31	0.63
12:Z:83:GLN:HG3	12:Z:84:GLU:H	1.64	0.63
7:S:56:LYS:O	7:S:56:LYS:HG3	1.98	0.63
4:L:86:MET:HE2	4:L:86:MET:HA	1.79	0.62
1:2:996:G:O2'	1:2:997:C:O5'	2.18	0.62
1:2:1115:G:O2'	1:2:1116:A:H8	1.81	0.62
2:H:89:GLU:O	2:H:90:HIS:ND1	2.33	0.62
4:L:17:GLU:OE2	4:L:71:ARG:NH2	2.33	0.62
13:3:20:LEU:HD11	13:3:80:VAL:HG13	1.81	0.61
1:2:1311:G:OP2	2:H:80:LYS:NZ	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:976:A:OP2	1:2:1000:G:N2	2.33	0.60
1:2:1157:G:O2'	1:2:1158:G:OP1	2.19	0.60
4:L:10:SER:HB3	4:L:16:LEU:HD13	1.82	0.60
11:Y:9:ILE:HG22	11:Y:18:LYS:CB	2.30	0.60
1:2:1140:G:N1	1:2:1143:A:OP2	2.29	0.60
8:T:81:ILE:HD11	8:T:103:LEU:HD21	1.83	0.60
5:O:110:ARG:NH1	5:O:121:GLU:HG2	2.17	0.59
13:3:23:VAL:O	13:3:27:ARG:N	2.35	0.59
1:2:1193:4AC:O5'	1:2:1193:4AC:H6	2.03	0.59
1:2:1219:G:OP2	9:U:41:LYS:NZ	2.25	0.59
11:Y:9:ILE:CG2	11:Y:18:LYS:HB2	2.33	0.59
2:H:86:MET:HE1	2:H:171:ALA:HA	1.84	0.58
11:Y:10:VAL:HG13	11:Y:15:VAL:HG12	1.85	0.58
15:6:28:VAL:HG13	15:6:63:VAL:HG13	1.86	0.58
2:H:101:TYR:OH	3:K:39:GLU:OE1	2.17	0.57
1:2:1071:G:H5''	12:Z:150:TYR:HE1	1.70	0.57
10:X:70:ARG:HB2	10:X:71:ARG:HH11	1.70	0.57
10:X:67:ILE:HG23	10:X:70:ARG:H	1.70	0.57
3:K:135:ARG:O	8:T:124:ARG:NH2	2.38	0.56
13:3:52:ILE:HG22	13:3:78:ILE:HG12	1.86	0.56
1:2:973:A:N1	13:3:92:ILE:HG12	2.20	0.56
3:K:48:PRO:HG3	3:K:106:MET:HE3	1.86	0.56
13:3:66:LEU:HD13	13:3:69:LEU:HD23	1.87	0.56
1:2:951:C:O2	6:P:12:ARG:NH1	2.39	0.56
9:U:88:GLU:OE1	18:U:201:HOH:O	2.18	0.56
12:Z:39:PRO:O	12:Z:40:LEU:HG	2.06	0.56
8:T:123:THR:OG1	14:4:31:G:OP1	2.24	0.55
15:6:51:ILE:HG22	15:6:52:PRO:O	2.06	0.55
1:2:976:A:N7	1:2:1002:C:O2'	2.30	0.55
6:P:21:CYS:HB2	6:P:39:CYS:SG	2.46	0.55
13:3:71:GLU:HG3	13:3:72:GLU:OE1	2.07	0.55
11:Y:8:TYR:C	11:Y:9:ILE:HG22	2.32	0.55
4:L:15:SER:O	4:L:15:SER:OG	2.16	0.54
2:H:157:ARG:HH12	10:X:56:ILE:HD12	1.71	0.54
1:2:998:C:H2'	1:2:999:G:C8	2.42	0.54
8:T:50:LYS:HD2	8:T:59:TYR:CZ	2.43	0.54
15:6:67:VAL:HG12	15:6:68:ILE:H	1.72	0.54
7:S:41:VAL:HG22	12:Z:193:ILE:HD13	1.90	0.54
9:U:147:LEU:HD22	9:U:150:TYR:OH	2.09	0.53
1:2:1191:C:OP1	6:P:9:ARG:NH2	2.40	0.53
12:Z:92:ALA:HB2	12:Z:182:ILE:HD12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:3:109:ASP:O	13:3:113:GLU:HG2	2.08	0.53
5:O:9:ARG:HA	5:O:14:ASP:HA	1.90	0.53
13:3:49:LYS:HG3	13:3:103:GLU:H	1.74	0.53
13:3:49:LYS:HG2	13:3:102:ILE:HA	1.91	0.53
5:O:16:ASP:OD1	5:O:17:GLY:N	2.38	0.52
12:Z:51:PRO:HA	12:Z:54:VAL:HG12	1.91	0.52
6:P:9:ARG:HG2	6:P:10:LYS:H	1.74	0.52
11:Y:9:ILE:HG22	11:Y:18:LYS:N	2.25	0.52
1:2:1095:A:H2'	1:2:1096:G:H8	1.75	0.52
5:O:9:ARG:NH1	5:O:12:GLY:O	2.43	0.52
13:3:39:THR:HG21	13:3:100:ALA:HB3	1.91	0.52
1:2:972:G:O2'	1:2:1001:A:N1	2.41	0.52
10:X:66:GLU:OE2	10:X:67:ILE:N	2.40	0.52
1:2:1142:U:O2'	1:2:1143:A:O5'	2.24	0.52
2:H:206:GLU:CD	2:H:209:ARG:HH21	2.18	0.52
12:Z:37:LYS:HA	12:Z:42:THR:HG22	1.92	0.52
2:H:135:ASP:OD2	10:X:46:ARG:NH1	2.43	0.51
5:O:80:ASN:HB2	5:O:92:HIS:ND1	2.25	0.51
8:T:82:TYR:HB3	8:T:89:PHE:HB3	1.91	0.51
12:Z:62:ILE:O	12:Z:66:THR:HG23	2.10	0.51
15:6:23:GLN:NE2	15:6:68:ILE:HD12	2.26	0.51
4:L:22:GLN:HB3	4:L:88:ILE:HD11	1.92	0.51
11:Y:9:ILE:HG22	11:Y:18:LYS:CA	2.40	0.51
1:2:998:C:H2'	1:2:999:G:H8	1.75	0.51
13:3:116:MET:HG3	13:3:119:ARG:HE	1.76	0.51
2:H:176:THR:HG22	2:H:178:MET:H	1.76	0.51
1:2:973:A:C6	13:3:92:ILE:HG21	2.46	0.50
2:H:99:LYS:O	2:H:103:VAL:HG13	2.11	0.50
7:S:8:PHE:O	7:S:12:VAL:HG12	2.11	0.50
7:S:16:LEU:HD21	7:S:54:ILE:HD11	1.92	0.50
8:T:70:MET:HB3	8:T:103:LEU:HD22	1.93	0.50
1:2:1294:C:N4	8:T:69:ASP:OD1	2.44	0.50
2:H:47:THR:HG22	2:H:65:GLU:OE2	2.12	0.50
13:3:92:ILE:HG23	13:3:94:VAL:HG22	1.94	0.50
1:2:923:G:OP2	5:O:130:ARG:NH1	2.44	0.50
11:Y:40:CYS:SG	11:Y:41:GLY:N	2.85	0.50
15:6:14:ILE:HG13	15:6:16:VAL:HG23	1.91	0.50
7:S:61:LYS:O	7:S:61:LYS:HG2	2.12	0.50
13:3:27:ARG:NE	13:3:90:ALA:HA	2.27	0.50
11:Y:9:ILE:HG23	11:Y:9:ILE:O	2.11	0.50
11:Y:27:PRO:HG2	13:3:45:ARG:HG2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:3:19:ALA:HB3	13:3:78:ILE:HD13	1.93	0.50
1:2:975:G:OP1	11:Y:3:GLN:HA	2.12	0.49
3:K:49:LEU:HD23	3:K:86:LEU:HD11	1.93	0.49
13:3:92:ILE:HG13	13:3:93:GLU:N	2.24	0.49
11:Y:32:ALA:HB3	11:Y:39:ALA:HB3	1.94	0.49
9:U:57:SER:O	9:U:61:ARG:HB2	2.12	0.49
1:2:975:G:O6	13:3:38:GLU:HB2	2.13	0.49
11:Y:8:TYR:CB	11:Y:10:VAL:HG23	2.43	0.49
1:2:918:A:O2'	1:2:1307:A:N3	2.41	0.49
11:Y:37:ARG:HG3	11:Y:46:THR:HG23	1.95	0.49
1:2:1260:U:OP2	9:U:72:ARG:NH1	2.41	0.49
1:2:937:U:OP1	18:2:1502:HOH:O	2.19	0.48
1:2:997:C:H2'	1:2:998:C:H6	1.79	0.48
2:H:66:ARG:NH2	2:H:159:ASP:OD1	2.46	0.48
7:S:60:MET:HE3	7:S:66:ILE:HD12	1.96	0.48
7:S:61:LYS:C	7:S:61:LYS:CD	2.85	0.48
5:O:55:THR:OG1	5:O:56:ASP:N	2.46	0.48
1:2:977:A:H62	1:2:999:G:H21	1.60	0.48
13:3:70:CYS:O	13:3:123:LYS:NZ	2.40	0.48
11:Y:9:ILE:CG2	11:Y:16:ILE:O	2.54	0.48
15:6:28:VAL:HA	15:6:39:VAL:HA	1.96	0.47
6:P:21:CYS:HB3	6:P:25:GLY:H	1.78	0.47
11:Y:45:TYR:CE2	11:Y:47:GLU:HG2	2.49	0.47
1:2:1290:G:N1	1:2:1293:A:OP2	2.47	0.47
13:3:107:ALA:HB1	13:3:110:LEU:HD21	1.97	0.47
1:2:1200:C:N4	5:O:132:ARG:HD2	2.30	0.47
3:K:44:THR:O	3:K:79:ARG:HD3	2.15	0.47
8:T:25:ALA:O	8:T:33:ARG:HD3	2.14	0.47
11:Y:47:GLU:OE1	11:Y:49:LYS:HA	2.14	0.47
12:Z:69:LEU:HG	12:Z:75:LEU:HD22	1.97	0.47
1:2:1071:G:H5''	12:Z:150:TYR:CE1	2.50	0.47
5:O:145:ARG:HB2	14:4:30:G:OP2	2.15	0.47
7:S:61:LYS:C	7:S:61:LYS:HD3	2.39	0.47
13:3:43:VAL:HG22	13:3:48:ALA:HB3	1.95	0.47
10:X:18:THR:HG22	10:X:19:GLY:H	1.80	0.47
10:X:21:THR:O	10:X:21:THR:OG1	2.30	0.46
1:2:976:A:H5'	11:Y:1:MET:SD	2.55	0.46
8:T:123:THR:HG23	8:T:125:SER:H	1.80	0.46
3:K:10:ARG:NE	3:K:76:GLU:OE2	2.47	0.46
7:S:35:VAL:O	7:S:39:THR:HG22	2.16	0.46
2:H:205:LEU:HD23	2:H:205:LEU:HA	1.76	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:6:67:VAL:HG13	15:6:85:ARG:HA	1.97	0.46
1:2:1105:G:N3	9:U:138:LYS:NZ	2.51	0.46
15:6:101:THR:HB	15:6:103:GLU:OE2	2.16	0.46
1:2:1242:A:N3	1:2:1300:C:O2'	2.46	0.46
5:O:84:ASP:HB2	5:O:91:LEU:HD13	1.98	0.46
1:2:912:G:OP1	2:H:73:ARG:NH2	2.43	0.46
1:2:975:G:H8	1:2:975:G:OP2	1.98	0.46
1:2:1300:C:OP1	9:U:39:ARG:NH2	2.45	0.46
13:3:51:VAL:HG12	13:3:100:ALA:HB1	1.98	0.46
7:S:25:THR:HG22	7:S:30:HIS:CD2	2.51	0.46
13:3:70:CYS:HA	13:3:73:LYS:NZ	2.30	0.46
2:H:98:VAL:O	2:H:102:GLU:HG2	2.15	0.45
4:L:45:ILE:HG12	4:L:66:LEU:HB3	1.99	0.45
15:6:49:CYS:SG	15:6:80:GLY:HA3	2.56	0.45
1:2:1114:G:O2'	1:2:1115:G:H5'	2.16	0.45
10:X:5:GLU:OE1	10:X:5:GLU:HA	2.15	0.45
2:H:70:LYS:HD2	2:H:162:LEU:HB3	1.98	0.45
3:K:117:HIS:N	3:K:117:HIS:CD2	2.84	0.45
13:3:61:GLU:HG2	13:3:62:ILE:N	2.30	0.45
3:K:57:TRP:HD1	3:K:57:TRP:O	2.00	0.45
7:S:39:THR:OG1	7:S:40:ASN:N	2.49	0.45
11:Y:6:LYS:HG3	11:Y:7:LEU:HD23	1.97	0.45
11:Y:45:TYR:HE2	11:Y:47:GLU:HG2	1.81	0.45
1:2:973:A:H2'	13:3:94:VAL:HG21	1.98	0.45
10:X:69:SER:C	10:X:71:ARG:H	2.25	0.45
13:3:23:VAL:HB	13:3:89:ALA:HB1	1.98	0.45
13:3:25:ILE:HD12	13:3:25:ILE:H	1.82	0.45
11:Y:8:TYR:HB2	11:Y:10:VAL:HG23	1.98	0.45
1:2:1185:G:H5'	1:2:1187:A:H1'	1.98	0.45
1:2:1095:A:H2'	1:2:1096:G:C8	2.52	0.44
4:L:81:ALA:O	4:L:85:ILE:HG13	2.17	0.44
10:X:70:ARG:HB2	10:X:71:ARG:NH1	2.32	0.44
13:3:3:LYS:HG3	13:3:4:PRO:HD2	1.99	0.44
1:2:1236:C:H2'	1:2:1237:C:C6	2.52	0.44
9:U:146:GLU:N	9:U:146:GLU:OE1	2.50	0.44
1:2:1008:G:H2'	1:2:1009:A:O4'	2.18	0.44
15:6:24:LEU:HG	15:6:25:PHE:H	1.83	0.44
1:2:973:A:N6	1:2:1001:A:H2'	2.33	0.44
1:2:957:4AC:O7	1:2:957:4AC:H5	2.18	0.44
6:P:34:HIS:CD2	12:Z:4:GLU:HG3	2.53	0.44
1:2:496:G:H3'	1:2:497:U:C5'	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1161:G:H4'	3:K:118:LYS:HE2	2.00	0.44
1:2:1267:G:OP1	2:H:3:LYS:HG3	2.18	0.44
1:2:1184:4AC:O2'	1:2:1187:A:O2'	2.36	0.43
12:Z:18:ASP:O	12:Z:22:GLU:HG3	2.18	0.43
13:3:15:LEU:HD13	13:3:117:LYS:NZ	2.33	0.43
15:6:27:VAL:H	15:6:39:VAL:HG13	1.83	0.43
1:2:979:G:N2	11:Y:41:GLY:O	2.51	0.43
4:L:30:THR:HG22	4:L:31:GLY:N	2.33	0.43
12:Z:57:ARG:HB3	12:Z:60:ARG:CZ	2.47	0.43
15:6:74:VAL:HB	15:6:79:ARG:NE	2.30	0.43
13:3:6:TYR:HD2	13:3:8:LYS:HG3	1.83	0.43
13:3:32:ILE:HG23	13:3:101:ILE:HG22	2.01	0.43
12:Z:55:ILE:HD13	12:Z:62:ILE:HG13	2.01	0.43
2:H:121:GLN:HE21	2:H:125:TRP:NE1	2.17	0.43
1:2:1321:G:O6	3:K:10:ARG:NH2	2.51	0.43
3:K:135:ARG:NH2	14:4:36:A:OP2	2.51	0.43
9:U:14:GLU:OE2	9:U:53:TYR:OH	2.28	0.43
9:U:37:THR:O	9:U:37:THR:OG1	2.36	0.43
13:3:93:GLU:O	13:3:93:GLU:HG2	2.18	0.43
15:6:52:PRO:HG3	15:6:81:ASP:OD1	2.17	0.43
15:6:58:ARG:HG3	15:6:59:VAL:HG13	2.00	0.43
13:3:39:THR:HG22	13:3:43:VAL:HG23	2.00	0.43
13:3:27:ARG:HA	13:3:32:ILE:HD11	1.99	0.43
1:2:1155:G:O2'	1:2:1156:G:O4'	2.37	0.43
4:L:3:LYS:HB3	4:L:101:ILE:HD11	2.00	0.43
4:L:85:ILE:HG22	4:L:85:ILE:O	2.19	0.43
8:T:73:LEU:H	8:T:76:MET:HE3	1.84	0.43
15:6:27:VAL:O	15:6:39:VAL:HG13	2.19	0.43
1:2:1093:C:O2'	1:2:1094:C:H5'	2.19	0.42
12:Z:49:ALA:HB2	12:Z:85:ILE:HD11	2.01	0.42
3:K:36:VAL:O	3:K:42:ARG:NH1	2.52	0.42
15:6:19:PRO:HA	15:6:23:GLN:HB3	2.00	0.42
9:U:143:ILE:HG13	9:U:144:ILE:HD12	2.01	0.42
15:6:72:TRP:H	15:6:79:ARG:HB3	1.84	0.42
1:2:1120:A:H5'	1:2:1121:C:OP2	2.19	0.42
2:H:32:SER:OG	10:X:54:ILE:O	2.27	0.42
5:O:109:LEU:HD11	5:O:116:ARG:NH2	2.33	0.42
6:P:21:CYS:CB	6:P:39:CYS:SG	3.06	0.42
1:2:998:C:O2'	1:2:999:G:P	2.78	0.42
1:2:1311:G:H5''	1:2:1312:G:OP1	2.20	0.42
2:H:156:ARG:O	2:H:160:VAL:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:45:TYR:HE2	11:Y:47:GLU:HB3	1.82	0.42
2:H:26:VAL:HG21	2:H:39:LEU:HD22	2.02	0.42
4:L:29:ARG:HH21	4:L:84:GLN:NE2	2.18	0.42
1:2:1147:4AC:O7	1:2:1147:4AC:H5	2.19	0.42
9:U:20:LEU:HD23	9:U:20:LEU:HA	1.86	0.42
12:Z:129:GLU:OE2	12:Z:145:ARG:NE	2.36	0.42
5:O:58:GLN:O	5:O:62:ILE:HG12	2.20	0.42
4:L:18:GLU:O	4:L:22:GLN:HG3	2.20	0.42
11:Y:31:MET:SD	11:Y:38:TRP:HB3	2.60	0.42
13:3:66:LEU:O	13:3:69:LEU:N	2.51	0.42
1:2:1100:C:H2'	1:2:1101:U:C6	2.54	0.41
1:2:1251:G:H2'	1:2:1253:A:H2	1.85	0.41
2:H:170:SER:O	2:H:170:SER:OG	2.37	0.41
12:Z:34:ASP:OD1	12:Z:45:ILE:HB	2.20	0.41
13:3:52:ILE:HD12	13:3:86:LEU:HD11	2.02	0.41
1:2:496:G:N2	15:6:54:LYS:HD2	2.35	0.41
5:O:103:ARG:HE	5:O:103:ARG:HB2	1.64	0.41
8:T:47:LEU:HD22	8:T:67:CYS:SG	2.60	0.41
9:U:148:LYS:HE2	9:U:148:LYS:HB3	1.90	0.41
14:4:33:OMC:HM22	14:4:34:U:H5'	2.01	0.41
10:X:15:ILE:HD12	10:X:26:GLN:HE21	1.85	0.41
1:2:1028:4AC:O7	1:2:1028:4AC:H5	2.19	0.41
11:Y:9:ILE:CG2	11:Y:18:LYS:CA	2.97	0.41
13:3:73:LYS:HE2	13:3:73:LYS:HB2	1.88	0.41
15:6:19:PRO:HG3	15:6:25:PHE:CZ	2.55	0.41
9:U:49:ASP:OD1	9:U:49:ASP:N	2.53	0.41
15:6:17:PRO:O	15:6:86:TYR:OH	2.34	0.41
3:K:40:ILE:HG23	3:K:72:MET:HE1	2.02	0.41
12:Z:86:LYS:HA	12:Z:86:LYS:HD2	1.80	0.41
12:Z:136:LEU:HD12	12:Z:137:THR:HG22	2.03	0.41
1:2:974:U:H5'	1:2:975:G:C8	2.56	0.41
3:K:66:VAL:HG11	3:K:74:GLN:HB3	2.03	0.41
5:O:56:ASP:O	5:O:60:LYS:HG2	2.20	0.41
10:X:7:TYR:HA	10:X:8:PRO:HD3	1.92	0.41
12:Z:118:ARG:O	12:Z:122:SER:OG	2.24	0.41
15:6:13:VAL:HG13	15:6:14:ILE:H	1.85	0.41
1:2:974:U:OP2	13:3:36:THR:HG22	2.20	0.41
1:2:977:A:H62	1:2:999:G:N2	2.19	0.41
2:H:15:ILE:HD11	3:K:102:TYR:HE1	1.85	0.40
4:L:72:LEU:HD12	4:L:73:ILE:H	1.86	0.40
2:H:176:THR:HG22	2:H:177:LYS:N	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:24:ARG:HD3	11:Y:43:CYS:HB3	2.01	0.40
13:3:26:ALA:HA	13:3:29:THR:HG22	2.04	0.40
15:6:88:GLN:O	15:6:91:VAL:HG12	2.21	0.40
1:2:1100:C:H2'	1:2:1101:U:H6	1.86	0.40
1:2:973:A:H4'	1:2:975:G:H1'	2.03	0.40
2:H:133:ARG:HG2	2:H:208:GLU:OE2	2.20	0.40
2:H:139:VAL:O	2:H:145:ARG:HA	2.21	0.40
5:O:41:ARG:NH2	9:U:45:PRO:O	2.49	0.40
5:O:66:LEU:HD23	5:O:66:LEU:HA	1.95	0.40
13:3:19:ALA:CB	13:3:78:ILE:HD13	2.51	0.40
8:T:96:PRO:O	8:T:97:GLU:HB2	2.22	0.40
13:3:1:MET:HB2	13:3:54:ALA:O	2.22	0.40
13:3:70:CYS:HB3	13:3:75:ILE:HG21	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	
2	H	211/215 (98%)	189 (90%)	22 (10%)	0	100	100
3	K	132/135 (98%)	115 (87%)	17 (13%)	0	100	100
4	L	99/102 (97%)	91 (92%)	8 (8%)	0	100	100
5	O	141/148 (95%)	130 (92%)	11 (8%)	0	100	100
6	P	53/56 (95%)	47 (89%)	6 (11%)	0	100	100
7	S	64/67 (96%)	63 (98%)	1 (2%)	0	100	100
8	T	128/132 (97%)	116 (91%)	12 (9%)	0	100	100
9	U	147/150 (98%)	137 (93%)	10 (7%)	0	100	100
10	X	65/71 (92%)	49 (75%)	16 (25%)	0	100	100
11	Y	48/51 (94%)	33 (69%)	15 (31%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	Z	195/210 (93%)	172 (88%)	23 (12%)	0	100	100
13	3	121/123 (98%)	96 (79%)	25 (21%)	0	100	100
15	6	93/113 (82%)	80 (86%)	13 (14%)	0	100	100
All	All	1497/1573 (95%)	1318 (88%)	179 (12%)	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	
2	H	183/184 (100%)	181 (99%)	2 (1%)	65	78
3	K	110/111 (99%)	110 (100%)	0	100	100
4	L	90/91 (99%)	90 (100%)	0	100	100
5	O	119/123 (97%)	117 (98%)	2 (2%)	53	74
6	P	45/46 (98%)	45 (100%)	0	100	100
7	S	60/61 (98%)	54 (90%)	6 (10%)	7	29
8	T	113/114 (99%)	112 (99%)	1 (1%)	70	80
9	U	126/127 (99%)	126 (100%)	0	100	100
10	X	57/60 (95%)	56 (98%)	1 (2%)	51	73
11	Y	41/42 (98%)	40 (98%)	1 (2%)	43	69
12	Z	156/168 (93%)	156 (100%)	0	100	100
13	3	99/99 (100%)	98 (99%)	1 (1%)	68	79
15	6	83/99 (84%)	82 (99%)	1 (1%)	63	78
All	All	1282/1325 (97%)	1267 (99%)	15 (1%)	61	78

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	93	LEU

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Mol	Chain	Res	Type
2	H	103	VAL
5	O	8	VAL
5	O	10	VAL
7	S	56	LYS
7	S	58	VAL
7	S	60	MET
7	S	61	LYS
7	S	62	GLU
7	S	63	GLU
8	T	113	VAL
10	X	5	GLU
11	Y	42	ARG
13	3	57	VAL
15	6	27	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	46	HIS
2	H	51	HIS
2	H	69	ASN
2	H	94	ASN
2	H	129	ASN
4	L	84	GLN
6	P	34	HIS
7	S	31	ASN
7	S	48	ASN
8	T	84	HIS
9	U	85	HIS
10	X	26	GLN
12	Z	72	GLN
12	Z	79	GLN
12	Z	87	ASN
12	Z	95	GLN
12	Z	101	GLN
12	Z	108	HIS
12	Z	123	ASN
12	Z	168	GLN
15	6	70	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	465/468 (99%)	102 (21%)	3 (0%)
14	4	17/18 (94%)	2 (11%)	0
All	All	482/486 (99%)	104 (21%)	3 (0%)

All (104) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	497	U
1	2	498	A
1	2	905	C
1	2	906	U
1	2	920	C
1	2	922	U
1	2	926	G
1	2	927	U
1	2	932	U
1	2	938	B8H
1	2	939	5MC
1	2	940	A
1	2	941	A
1	2	943	G
1	2	946	G
1	2	947	G
1	2	949	A
1	2	950	A
1	2	959	G
1	2	964	G
1	2	965	A
1	2	966	C
1	2	974	U
1	2	975	G
1	2	976	A
1	2	978	G
1	2	979	G
1	2	990	G
1	2	991	G
1	2	992	U
1	2	996	G
1	2	997	C
1	2	999	G
1	2	1001	A
1	2	1002	C
1	2	1003	G

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Mol	Chain	Res	Type
1	2	1004	C
1	2	1005	G
1	2	1028	4AC
1	2	1029	G
1	2	1050	U
1	2	1059	G
1	2	1060	U
1	2	1066	A
1	2	1067	A
1	2	1075	G
1	2	1090	U
1	2	1097	U
1	2	1098	C
1	2	1105	G
1	2	1107	U
1	2	1108	C
1	2	1109	G
1	2	1116	A
1	2	1120	A
1	2	1131	A
1	2	1133	U
1	2	1143	A
1	2	1147	4AC
1	2	1150	A
1	2	1156	G
1	2	1157	G
1	2	1158	G
1	2	1162	G
1	2	1170	A
1	2	1171	G
1	2	1183	C
1	2	1186	A
1	2	1187	A
1	2	1199	A
1	2	1200	C
1	2	1201	A
1	2	1202	5MC
1	2	1210	A
1	2	1212	A
1	2	1213	A
1	2	1215	G
1	2	1232	C

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Mol	Chain	Res	Type
1	2	1236	C
1	2	1243	A
1	2	1244	G
1	2	1249	A
1	2	1253	A
1	2	1254	A
1	2	1259	C
1	2	1260	U
1	2	1261	A
1	2	1274	G
1	2	1276	U
1	2	1280	A
1	2	1294	C
1	2	1296	C
1	2	1300	C
1	2	1308	G
1	2	1309	C
1	2	1310	U
1	2	1327	G
1	2	1338	U
1	2	1339	C
1	2	1342	G
1	2	1344	G
1	2	1347	G
14	4	37	U
14	4	44	A

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	998	C
1	2	1155	G
1	2	1337	A

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	B8H	2	938	1	19,22,23	0.95	2 (10%)	21,32,35	1.50	4 (19%)
1	5MC	2	939	1	19,22,23	1.26	3 (15%)	26,32,35	1.37	5 (19%)
1	4AC	2	1193	1	21,24,25	1.09	2 (9%)	28,34,37	2.42	7 (25%)
1	5MC	2	1202	1	19,22,23	1.27	2 (10%)	26,32,35	1.16	3 (11%)
1	4AC	2	1239	1	21,24,25	1.03	2 (9%)	28,34,37	1.28	4 (14%)
1	4AC	2	1147	1	21,24,25	1.01	2 (9%)	28,34,37	1.39	3 (10%)
1	4AC	2	1028	1	21,24,25	1.06	2 (9%)	28,34,37	1.54	4 (14%)
1	4AC	2	1233	1	21,24,25	1.02	2 (9%)	28,34,37	1.31	5 (17%)
1	4AC	2	1184	1	21,24,25	1.04	2 (9%)	28,34,37	1.31	5 (17%)
14	OMC	4	33	14	19,22,23	0.88	2 (10%)	25,31,34	1.14	2 (8%)
1	4AC	2	957	1	21,24,25	1.12	2 (9%)	28,34,37	1.56	4 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	B8H	2	938	1	-	2/7/25/26	0/2/2/2
1	5MC	2	939	1	-	2/7/25/26	0/2/2/2
1	4AC	2	1193	1	-	1/11/29/30	0/2/2/2
1	5MC	2	1202	1	-	2/7/25/26	0/2/2/2
1	4AC	2	1239	1	-	0/11/29/30	0/2/2/2
1	4AC	2	1147	1	-	2/11/29/30	0/2/2/2
1	4AC	2	1028	1	-	2/11/29/30	0/2/2/2
1	4AC	2	1233	1	-	0/11/29/30	0/2/2/2
1	4AC	2	1184	1	-	0/11/29/30	0/2/2/2
14	OMC	4	33	14	-	1/9/27/28	0/2/2/2
1	4AC	2	957	1	-	0/11/29/30	0/2/2/2

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	1202	5MC	C5-C4	3.81	1.47	1.44
1	2	939	5MC	C5-C4	3.79	1.47	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	1028	4AC	C4-N3	-3.21	1.27	1.32
1	2	957	4AC	C4-N3	-3.20	1.27	1.32
1	2	1239	4AC	C4-N3	-3.13	1.27	1.32
1	2	1233	4AC	C4-N3	-3.10	1.27	1.32
1	2	1184	4AC	C4-N3	-3.04	1.27	1.32
1	2	1202	5MC	C6-N1	-2.91	1.33	1.38
1	2	939	5MC	C6-C5	2.85	1.39	1.34
1	2	1147	4AC	C4-N3	-2.77	1.28	1.32
1	2	1193	4AC	C4-N3	-2.74	1.28	1.32
1	2	957	4AC	C4-N4	-2.60	1.36	1.39
1	2	938	B8H	C4-C5	-2.52	1.37	1.44
1	2	1147	4AC	C5-C4	2.43	1.46	1.41
1	2	938	B8H	O4'-C1'	-2.36	1.40	1.43
1	2	939	5MC	C6-N1	-2.35	1.34	1.38
1	2	1239	4AC	C5-C4	2.31	1.46	1.41
1	2	1233	4AC	C5-C4	2.29	1.46	1.41
1	2	1184	4AC	C5-C4	2.27	1.46	1.41
1	2	1193	4AC	C6-C5	-2.25	1.29	1.35
14	4	33	OMC	C6-N1	-2.25	1.32	1.38
1	2	1028	4AC	C4-N4	-2.22	1.36	1.39
14	4	33	OMC	C5-C4	-2.10	1.38	1.42

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1193	4AC	N4-C4-N3	6.70	124.74	113.87
1	2	1193	4AC	O7-C7-N4	6.34	131.88	121.90
1	2	1193	4AC	C5-C4-N4	-6.01	112.82	122.94
1	2	957	4AC	O7-C7-N4	5.20	130.08	121.90
1	2	1028	4AC	O7-C7-N4	4.91	129.62	121.90
1	2	938	B8H	C4-N3-C2	-4.82	121.03	127.34
1	2	1184	4AC	O7-C7-N4	4.27	128.62	121.90
1	2	1233	4AC	O7-C7-N4	4.13	128.39	121.90
1	2	939	5MC	C5-C6-N1	-3.97	119.00	123.31
1	2	1239	4AC	O7-C7-N4	3.96	128.13	121.90
1	2	1147	4AC	O7-C7-N4	3.87	127.99	121.90
1	2	957	4AC	CM7-C7-N4	-3.80	109.14	115.27
1	2	1147	4AC	N4-C4-N3	3.59	119.69	113.87
1	2	1028	4AC	C5-C4-N4	-3.55	116.95	122.94
1	2	1028	4AC	N4-C4-N3	3.42	119.42	113.87
1	2	1193	4AC	C1'-N1-C2	3.12	125.32	118.44
14	4	33	OMC	O2-C2-N3	-3.04	117.54	122.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1028	4AC	CM7-C7-N4	-2.97	110.48	115.27
1	2	939	5MC	C5-C4-N3	-2.92	118.76	121.75
1	2	1202	5MC	C5-C4-N3	-2.90	118.78	121.75
1	2	1147	4AC	C5-C4-N4	-2.89	118.08	122.94
1	2	1193	4AC	O7-C7-CM7	-2.81	117.06	122.05
1	2	1202	5MC	O2-C2-N3	-2.78	117.94	122.33
1	2	957	4AC	C5-C4-N4	-2.70	118.39	122.94
1	2	938	B8H	N3-C2-N1	2.64	117.78	115.22
1	2	1193	4AC	CM7-C7-N4	-2.61	111.06	115.27
1	2	938	B8H	O2-C2-N1	-2.59	120.16	122.78
1	2	1233	4AC	N4-C4-N3	2.48	117.90	113.87
1	2	1239	4AC	N4-C4-N3	2.46	117.86	113.87
1	2	1202	5MC	C5-C6-N1	-2.44	120.67	123.31
1	2	1184	4AC	N4-C4-N3	2.42	117.80	113.87
1	2	1233	4AC	CM7-C7-N4	-2.41	111.37	115.27
14	4	33	OMC	C1'-N1-C2	2.39	123.73	118.44
1	2	1233	4AC	O2-C2-N3	-2.29	118.72	122.33
1	2	1233	4AC	C5-C4-N4	-2.28	119.11	122.94
1	2	1184	4AC	C5-C4-N4	-2.25	119.14	122.94
1	2	1184	4AC	O2-C2-N3	-2.21	118.84	122.33
1	2	1239	4AC	C5-C4-N4	-2.20	119.24	122.94
1	2	939	5MC	N1-C2-N3	2.17	122.56	118.80
1	2	939	5MC	O2-C2-N3	-2.15	118.94	122.33
1	2	1193	4AC	C1'-N1-C6	-2.15	116.19	120.78
1	2	1184	4AC	CM7-C7-N4	-2.13	111.83	115.27
1	2	938	B8H	O4'-C1'-C2'	2.13	108.09	105.15
1	2	939	5MC	CM5-C5-C4	-2.11	117.04	120.51
1	2	1239	4AC	O2-C2-N3	-2.11	119.01	122.33
1	2	957	4AC	O2-C2-N3	-2.09	119.03	122.33

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	2	939	5MC	O4'-C4'-C5'-O5'
1	2	939	5MC	C3'-C4'-C5'-O5'
1	2	1028	4AC	O4'-C4'-C5'-O5'
1	2	1147	4AC	O4'-C4'-C5'-O5'
1	2	1147	4AC	C3'-C4'-C5'-O5'
1	2	1202	5MC	O4'-C4'-C5'-O5'
1	2	1028	4AC	C3'-C4'-C5'-O5'
1	2	938	B8H	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	2	1202	5MC	C3'-C4'-C5'-O5'
1	2	938	B8H	C3'-C4'-C5'-O5'
14	4	33	OMC	C2'-C1'-N1-C6
1	2	1193	4AC	O4'-C4'-C5'-O5'

There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	2	1193	4AC	2	0
1	2	1147	4AC	1	0
1	2	1028	4AC	1	0
1	2	1184	4AC	1	0
14	4	33	OMC	1	0
1	2	957	4AC	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 9 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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	2	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2	499:A	O3'	893:G	P	38.48
1	2	1037:G	O3'	1047:G	P	18.83

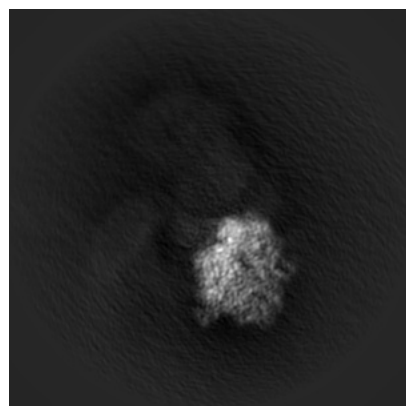
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10324. These allow visual inspection of the internal detail of the map and identification of artifacts.

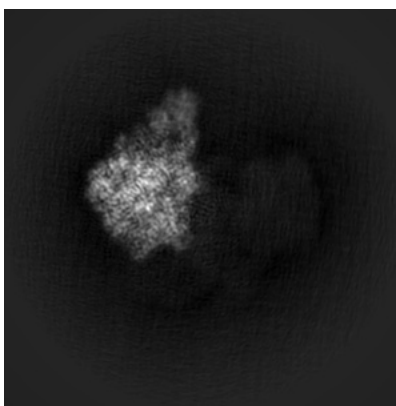
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

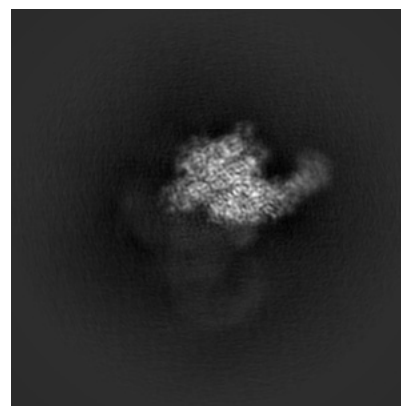
6.1.1 Primary map



X

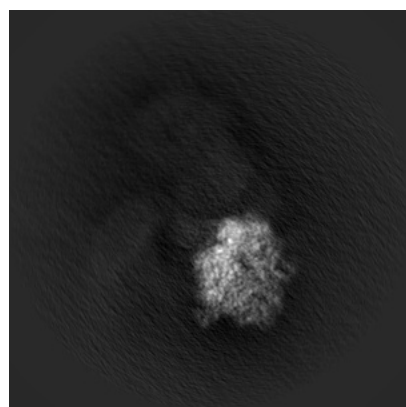


Y

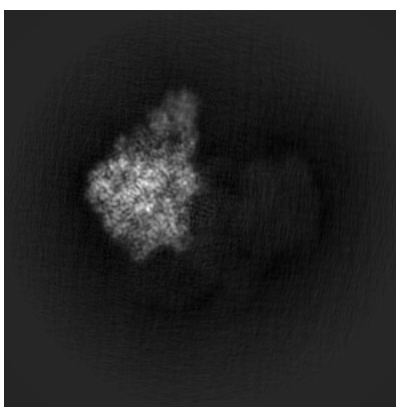


Z

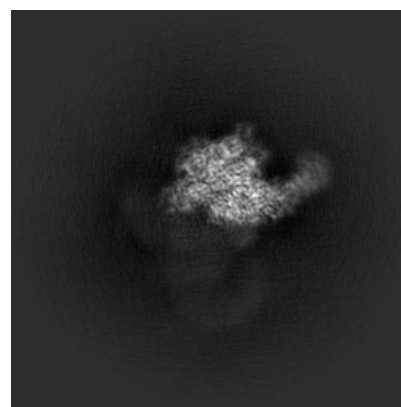
6.1.2 Raw map



X



Y

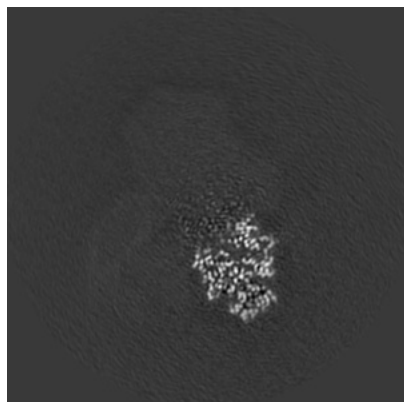


Z

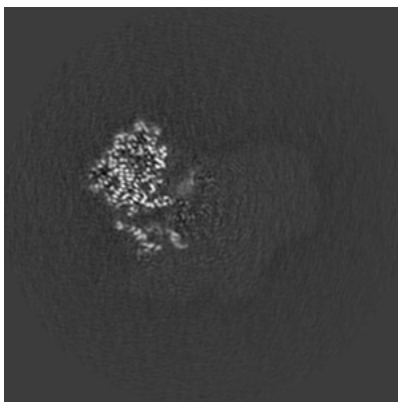
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

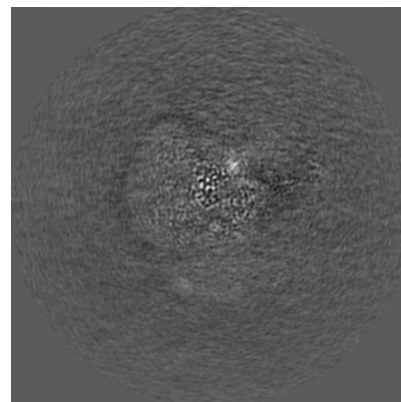
6.2.1 Primary map



X Index: 174

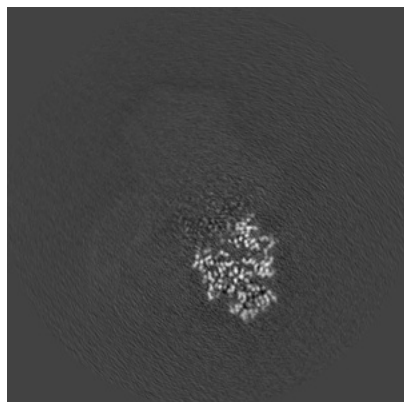


Y Index: 174

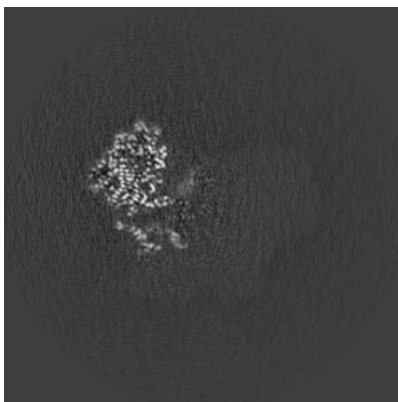


Z Index: 174

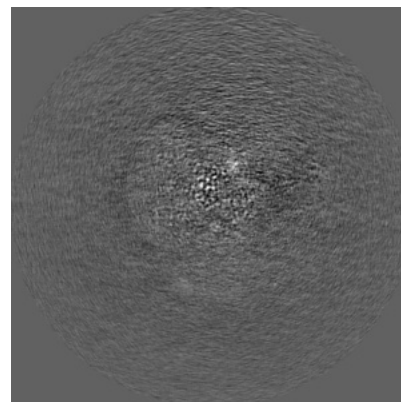
6.2.2 Raw map



X Index: 174



Y Index: 174

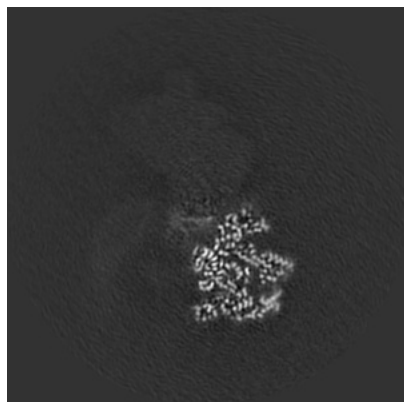


Z Index: 174

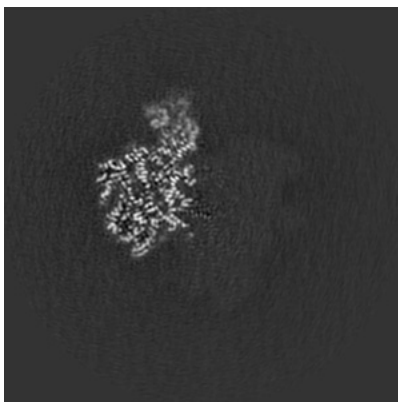
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

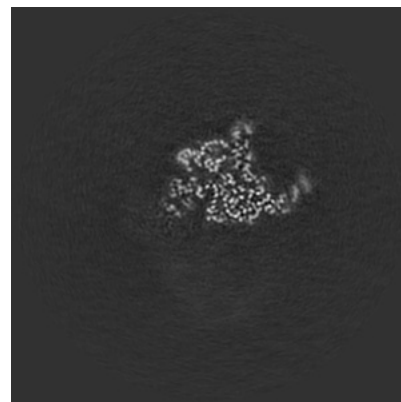
6.3.1 Primary map



X Index: 196

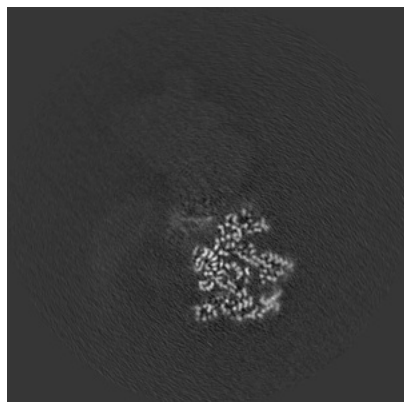


Y Index: 192

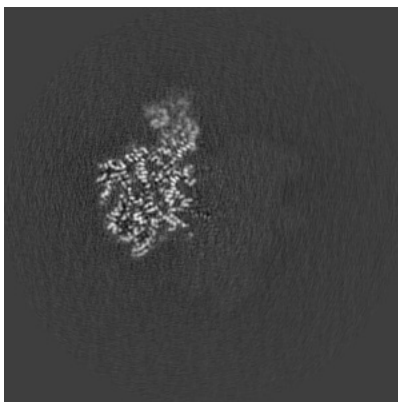


Z Index: 127

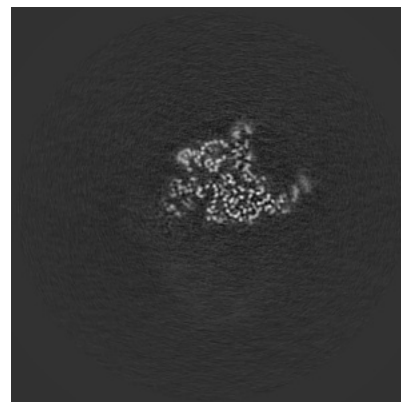
6.3.2 Raw map



X Index: 196



Y Index: 192



Z Index: 127

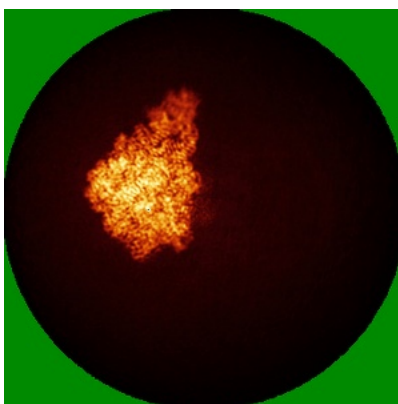
The images above show the largest variance slices of the map in three orthogonal directions.

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

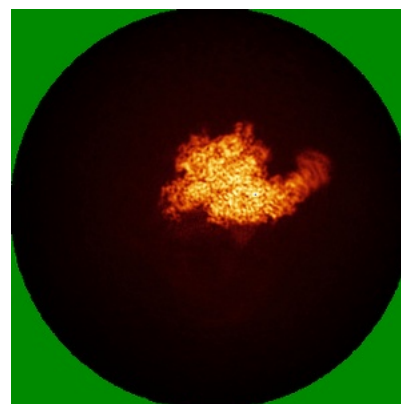
6.4.1 Primary map



X

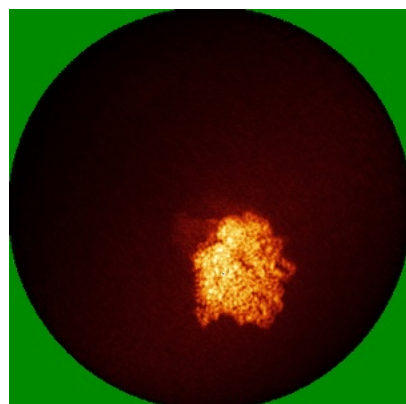


Y

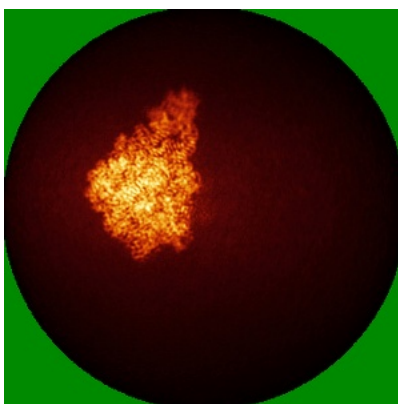


Z

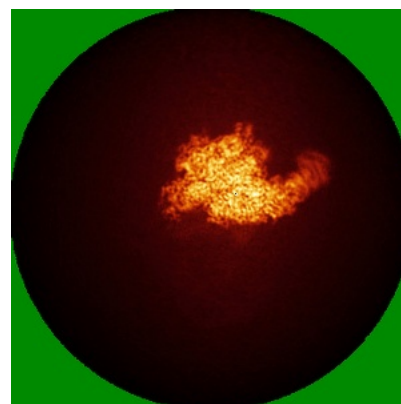
6.4.2 Raw map



X



Y

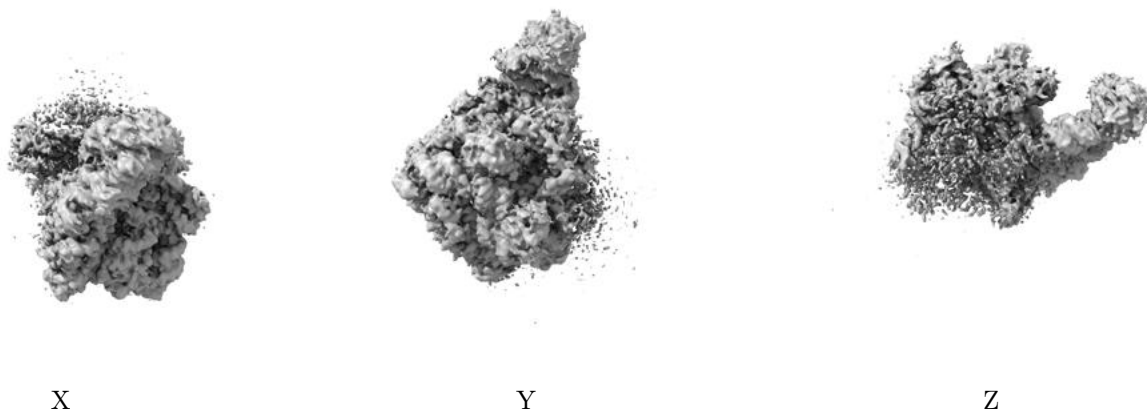


Z

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 0.004. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

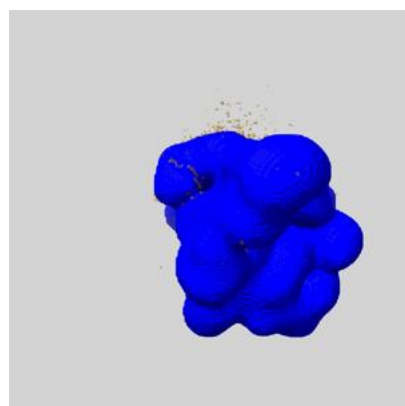
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

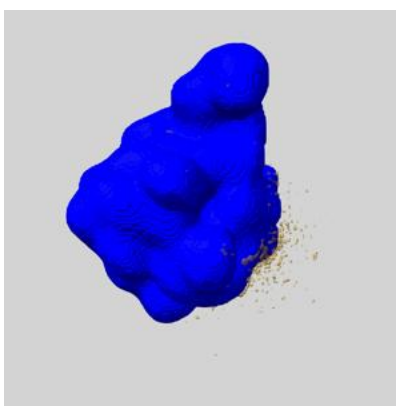
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

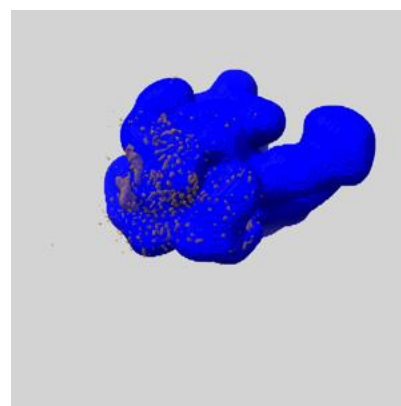
6.6.1 emd_10324_msk_1.map [i](#)



X



Y

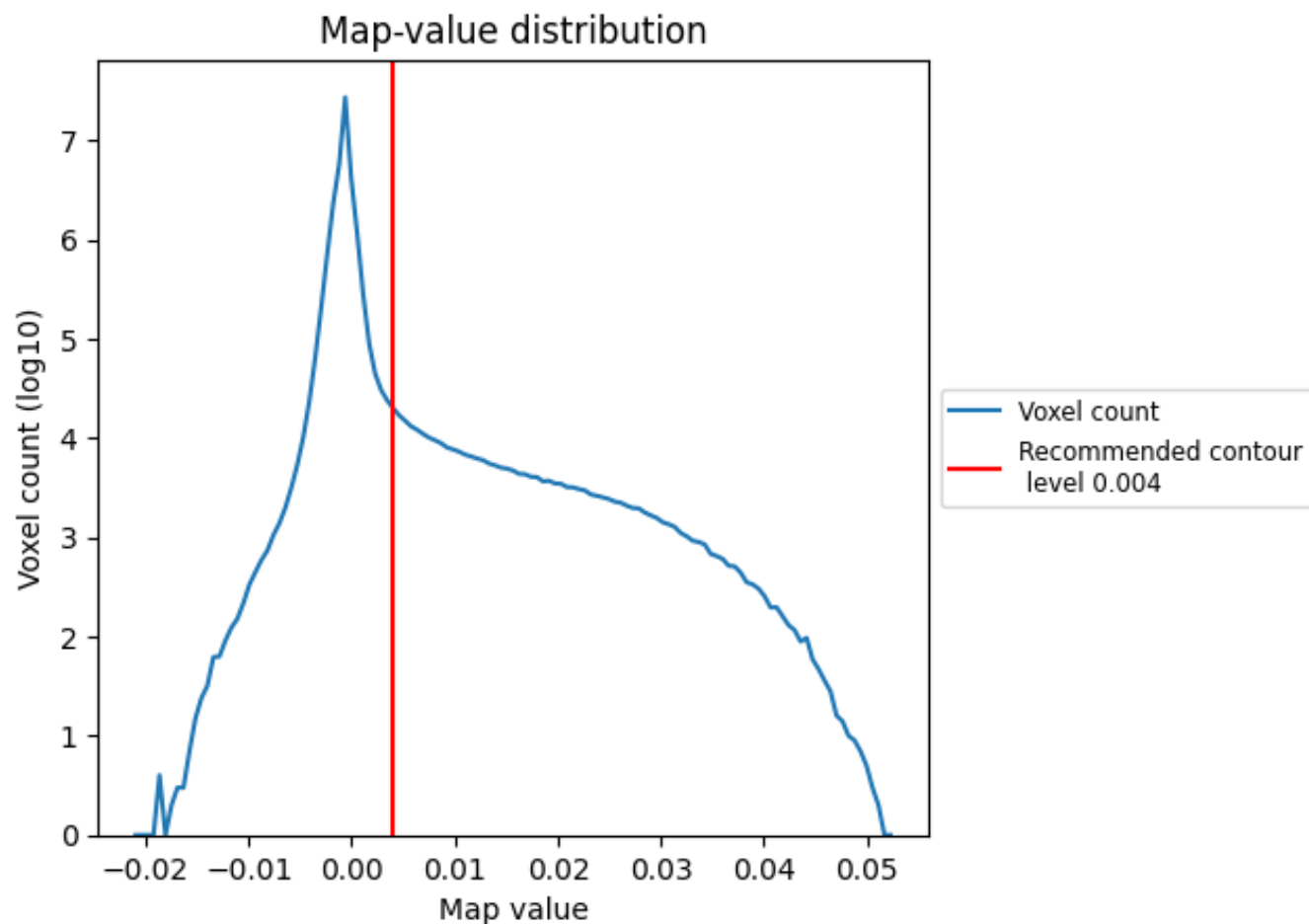


Z

7 Map analysis [i](#)

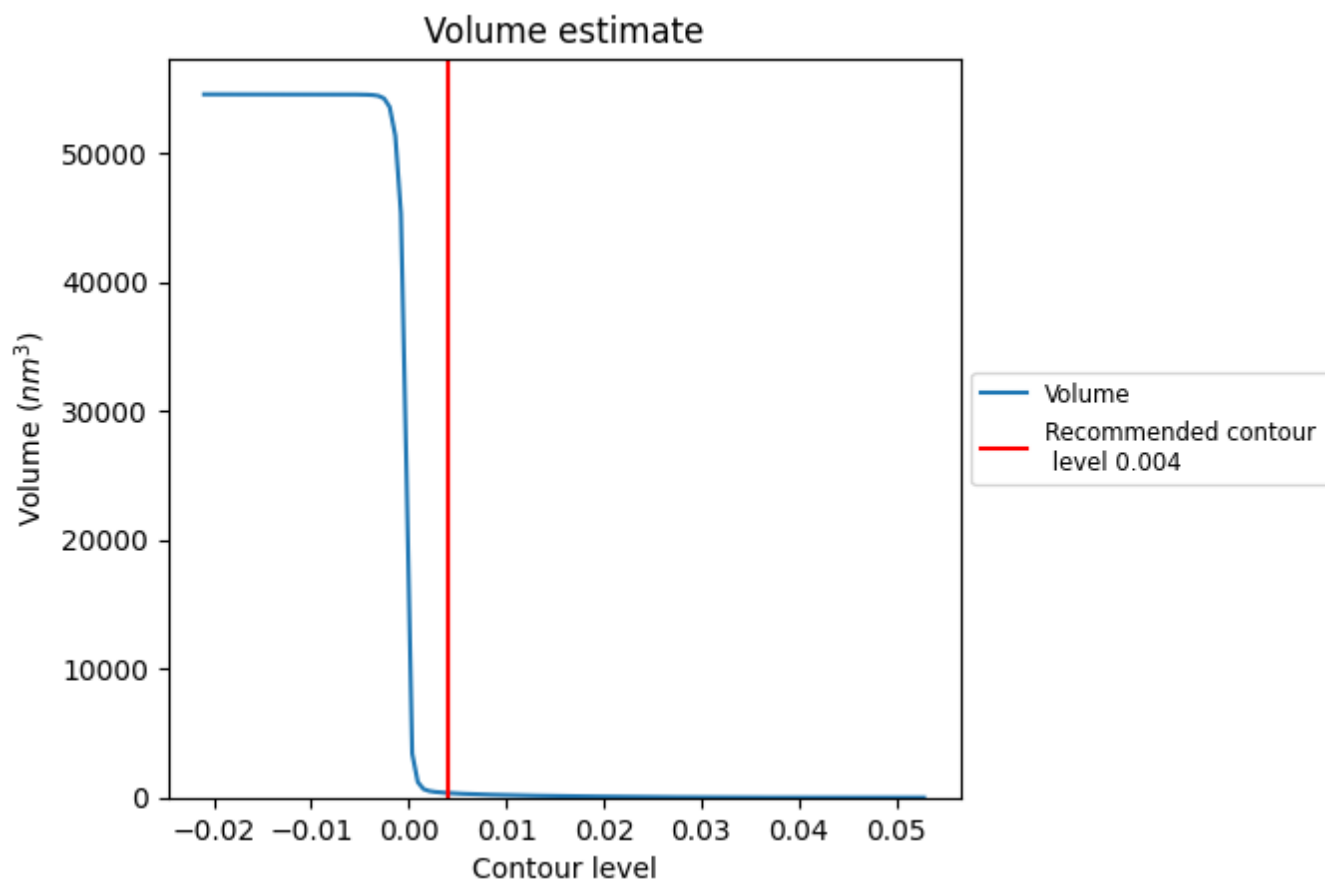
This section contains the results of statistical analysis of the map.

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.

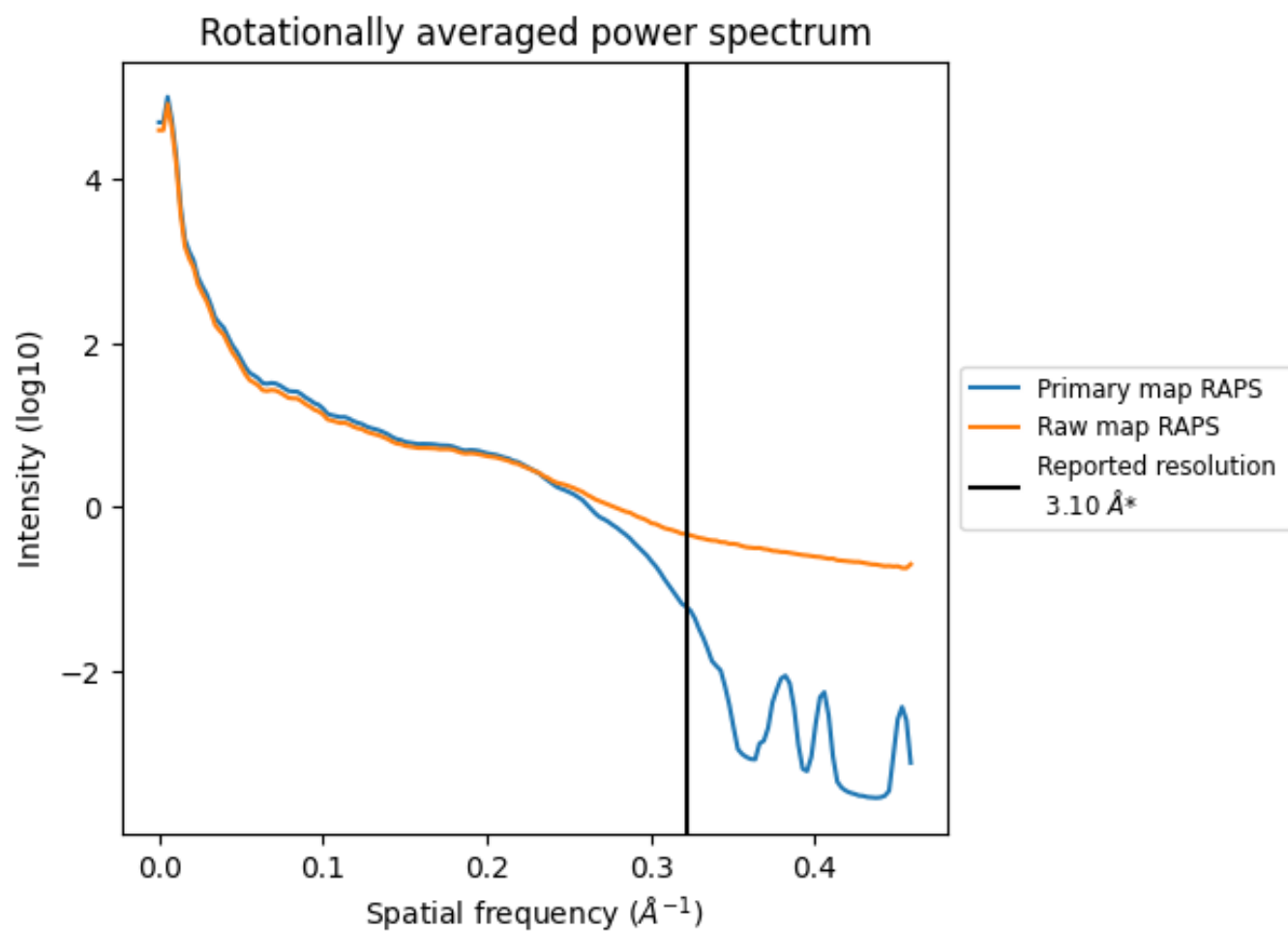
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 357 nm^3 ; this corresponds to an approximate mass of 322 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 ⓘ

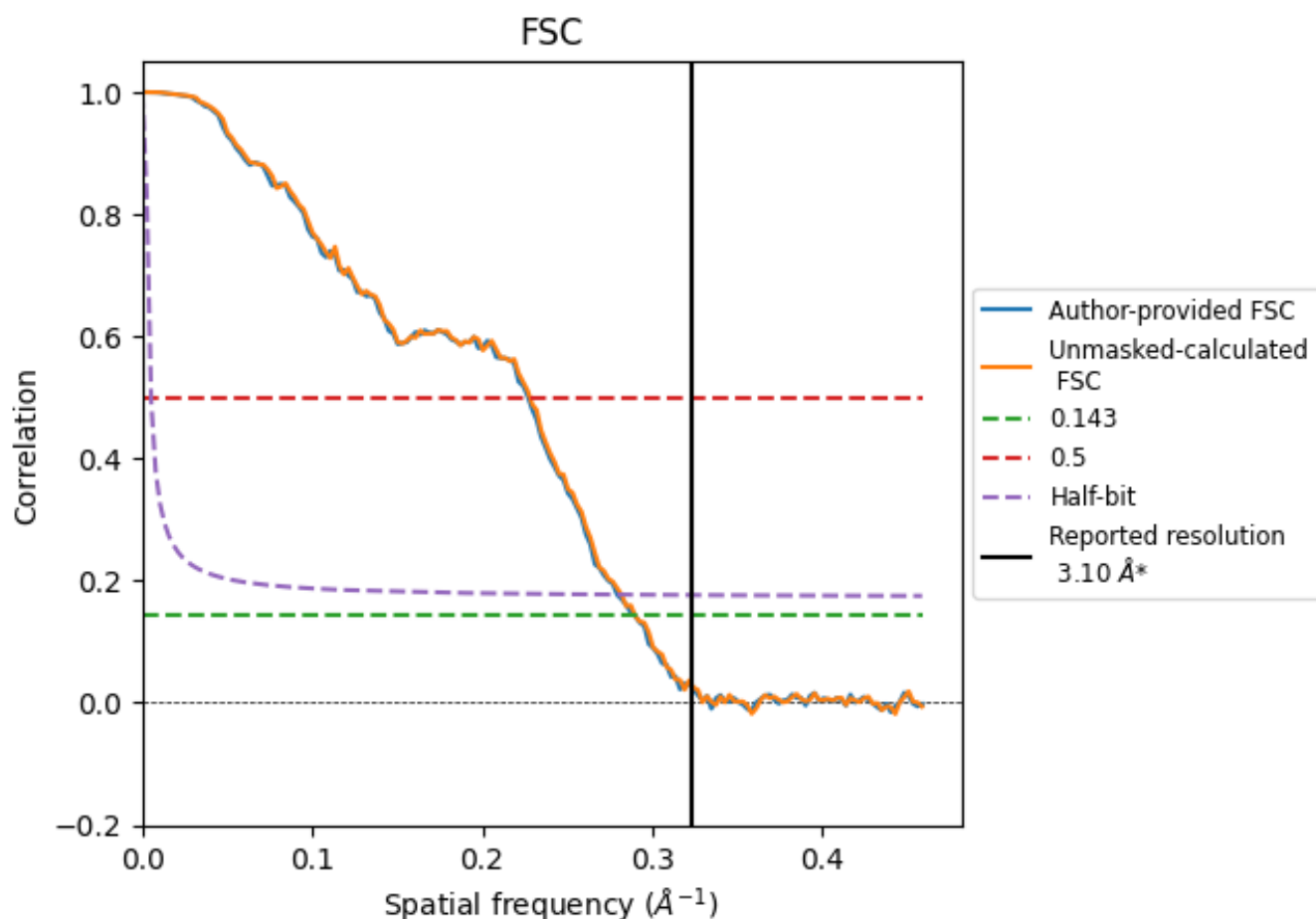


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

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 $0.323 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.46	4.41	3.58
Unmasked-calculated*	3.45	4.39	3.55

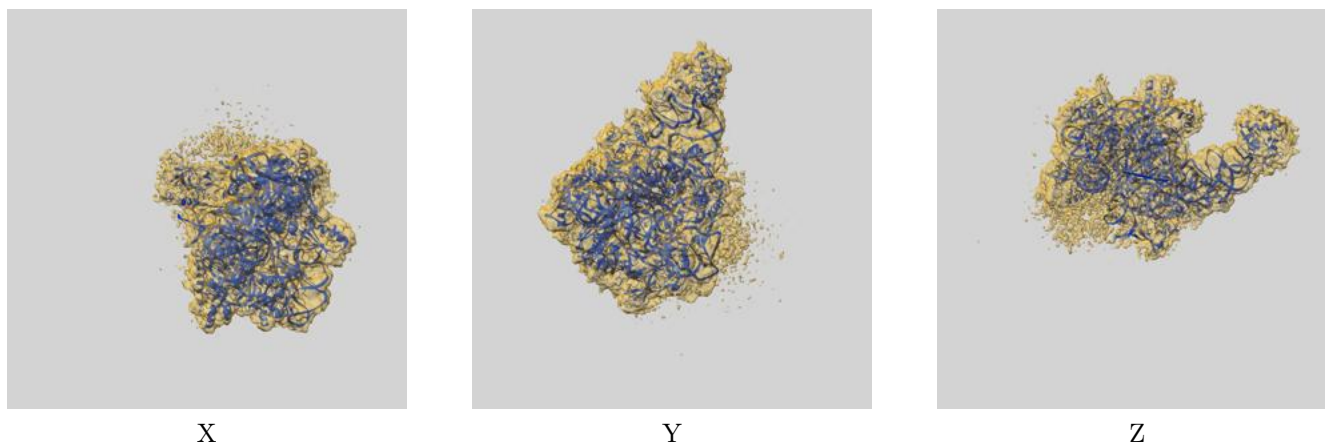
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 3.46 differs from the reported value 3.1 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.45 differs from the reported value 3.1 by more than 10 %

9 Map-model fit [i](#)

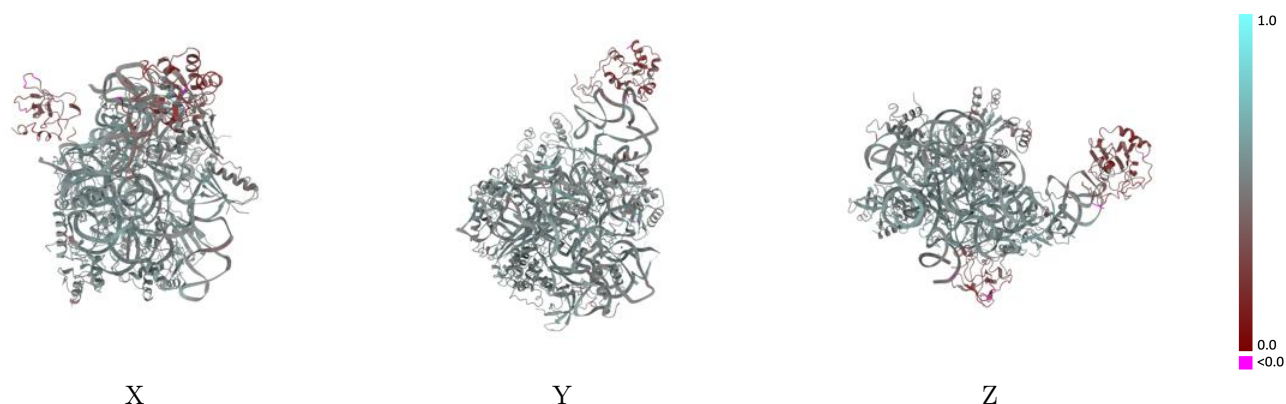
This section contains information regarding the fit between EMDB map EMD-10324 and PDB model 6SWE. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.004 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](#)

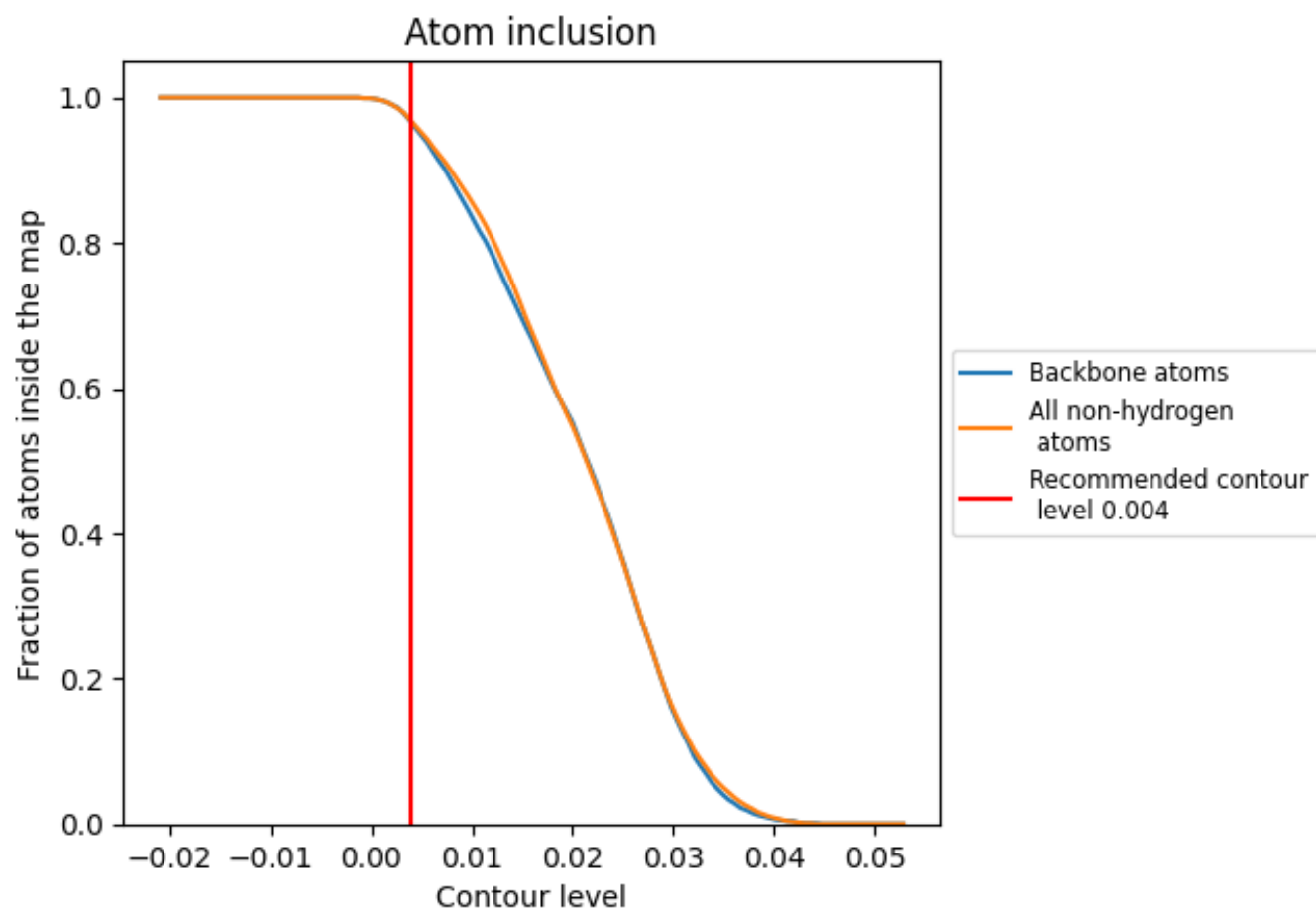


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 97% 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 (0.004) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9670	 0.5100
2	 0.9920	 0.5390
3	 0.9590	 0.3010
4	 0.8100	 0.4870
6	 0.5690	 0.3000
H	 0.9840	 0.5320
K	 0.9900	 0.5450
L	 0.9850	 0.5160
O	 0.9830	 0.5310
P	 0.9910	 0.5530
S	 0.9690	 0.4950
T	 0.9800	 0.5270
U	 0.9910	 0.5390
X	 0.9710	 0.5230
Y	 0.9160	 0.3100
Z	 0.9830	 0.5070

