



## wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 11:23 AM UTC

PDB ID : 9FRL / pdb\_00009frl  
EMDB ID : EMD-50717  
Title : Cryo-EM structure of *Saccharolobus solfataricus* 30S initiation complex bound to SD mRNA with h44 in up position  
Authors : Bourgeois, G.; Coureux, P.D.; Mechulam, Y.; Schmitt, E.  
Deposited on : 2024-06-19  
Resolution : 2.97 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

---

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

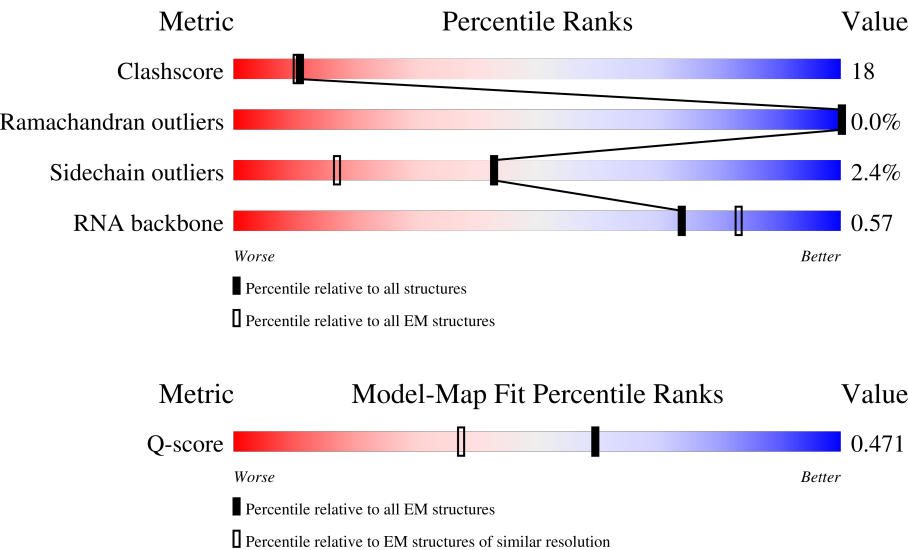


# 1 Overall quality at a glance i

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

The reported resolution of this entry is 2.97 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	13205 ( 2.47 - 3.47 )



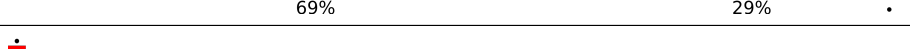
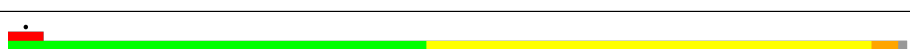


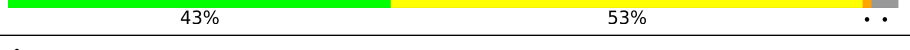
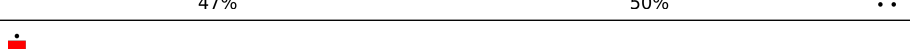



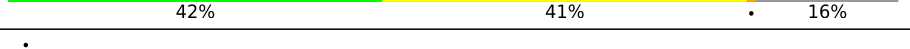

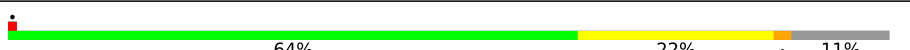


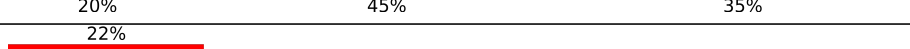
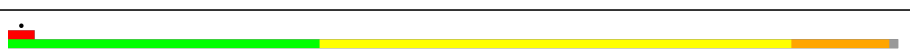






The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	2	1497	
2	A	208	
3	B	231	

Continued on next page...




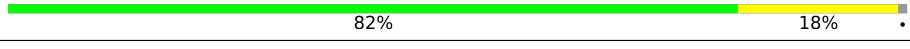
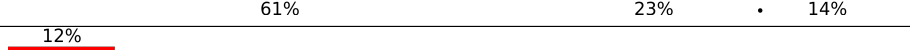
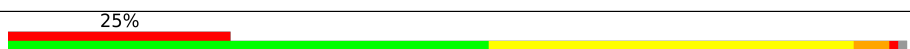


Continued from previous page...

Mol	Chain	Length	Quality of chain
4	C	65	
5	D	181	
6	F	214	
7	G	214	
8	H	193	
9	I	133	
10	J	133	
11	K	137	
12	L	102	
13	M	132	
14	N	147	
15	O	165	
16	Q	152	
17	S	79	
18	T	140	
19	U	158	
20	V	120	
21	W	66	
22	X	83	
23	Y	75	
24	3	127	
25	a	72	
26	e	52	
27	4	77	
28	5	28	

Continued on next page...



*Continued from previous page...*

Mol	Chain	Length	Quality of chain
29	P	54	
30	R	114	
31	Z	229	
32	d	72	
33	c	110	
34	E	239	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
36	SPM	2	1567	-	-	X	-
36	SPM	2	1576	-	-	X	-



## 2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 65224 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 rRNA 16S.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	1443	Total	C	N	O	P	0	0
			31042	13845	5740	10014	1443		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	843	4AC	C	conflict	GB AE006641.1
2	930	C4J	U	conflict	GB AE006641.1
2	1466	4AC	C	conflict	GB AE006641.1
2	1467	4AC	C	conflict	GB AE006641.1
2	1477	4AC	C	conflict	GB AE006641.1
2	1478	4AC	C	conflict	GB AE006641.1
2	1496	C	A	conflict	GB AE006641.1

- Molecule 2 is a protein called Small ribosomal subunit protein eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	186	Total	C	N	O	S	0	0
			1515	974	261	278	2		

- Molecule 3 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	215	Total	C	N	O	S	0	0
			1698	1092	291	312	3		

- Molecule 4 is a protein called Small zinc finger protein HVO-2753-like zinc-binding pocket domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	58	Total	C	N	O	S	0	0
			455	282	84	81	8		



- Molecule 5 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	166	Total	C	N	O	S	0	0
			1354	864	249	240	1		

- Molecule 6 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	210	Total	C	N	O	S	0	0
			1625	1041	275	303	6		

- Molecule 7 is a protein called Small ribosomal subunit protein eS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	213	Total	C	N	O	S	0	0
			1661	1052	292	315	2		

- Molecule 8 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	192	Total	C	N	O	S	0	0
			1543	983	283	274	3		

- Molecule 9 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	132	Total	C	N	O	S	0	0
			1050	675	187	182	6		

- Molecule 10 is a protein called Small ribosomal subunit protein eS8.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	J	127	Total	C	N	O	0	0
			982	617	186	179		

- Molecule 11 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	133	Total	C	N	O	S	0	0
			1068	675	201	185	7		

- Molecule 12 is a protein called Small ribosomal subunit protein uS10.



Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	101	Total	C	N	O	S	0	0
			840	536	157	142	5		

- Molecule 13 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	127	Total	C	N	O	S	0	0
			944	587	184	170	3		

- Molecule 14 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	146	Total	C	N	O	S	0	0
			1140	723	220	193	4		

- Molecule 15 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	140	Total	C	N	O	S	0	0
			1124	708	210	202	4		

- Molecule 16 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	145	Total	C	N	O	S	0	0
			1185	753	224	205	3		

- Molecule 17 is a protein called Small ribosomal subunit protein eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	S	66	Total	C	N	O	S	0	0
			571	364	101	105	1		

- Molecule 18 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	128	Total	C	N	O	S	0	0
			1064	684	192	184	4		

- Molecule 19 is a protein called Small ribosomal subunit protein eS19.



Mol	Chain	Residues	Atoms					AltConf	Trace
19	U	154	Total	C	N	O	S	0	0
			1247	805	223	217	2		

- Molecule 20 is a protein called Small ribosomal subunit protein eS24.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	V	107	Total	C	N	O	S	0	0
			836	524	154	156	2		

- Molecule 21 is a protein called Small ribosomal subunit protein eS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	65	Total	C	N	O	S	0	0
			503	319	93	84	7		

- Molecule 22 is a protein called Small ribosomal subunit protein eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	X	67	Total	C	N	O		0	0
			535	335	103	97			

- Molecule 23 is a protein called Small ribosomal subunit protein eS31.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Y	49	Total	C	N	O	S	0	0
			395	252	73	65	5		

- Molecule 24 is a protein called Large ribosomal subunit protein eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	3	117	Total	C	N	O	S	0	0
			893	567	149	175	2		

- Molecule 25 is a protein called aS34.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	a	71	Total	C	N	O	S	0	0
			562	361	98	96	7		

- Molecule 26 is a protein called LSU ribosomal protein S30E (Rps30E).



Mol	Chain	Residues	Atoms				AltConf	Trace
26	e	43	Total	C	N	O	0	0
			354	220	74	60		

- Molecule 27 is a RNA chain called tRNA Met initiator.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	4	77	Total	C	N	O	P	S	0	0
			1645	734	296	537	77	1		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	1	A	C	engineered mutation	GB 1334604293
4	72	U	A	engineered mutation	GB 1334604293

- Molecule 28 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	5	20	Total	C	N	O	P	0	0
			430	192	78	140	20		

- Molecule 29 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	P	53	Total	C	N	O	S	0	0
			440	282	80	74	4		

- Molecule 30 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	R	113	Total	C	N	O	S	0	0
			901	570	166	161	4		

- Molecule 31 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Z	196	Total	C	N	O	S	0	0
			1561	1009	274	272	6		

- Molecule 32 is a protein called aS33.



Mol	Chain	Residues	Atoms					AltConf	Trace
32	d	70	Total	C	N	O	S	0	0
			570	370	92	105	3		

- Molecule 33 is a protein called Small ribosomal subunit protein eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	c	109	Total	C	N	O	S	0	0
			856	539	152	164	1		

- Molecule 34 is a protein called Small ribosomal subunit protein eS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	E	238	Total	C	N	O	S	0	0
			1930	1238	342	344	6		

- Molecule 35 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
35	2	47	Total	Mg	0
			47	47	
35	F	2	Total	Mg	0
			2	2	
35	K	1	Total	Mg	0
			1	1	
35	5	1	Total	Mg	0
			1	1	
35	P	1	Total	Mg	0
			1	1	
35	R	1	Total	Mg	0
			1	1	

- Molecule 36 is SPERMINE (CCD ID: SPM) (formula: C<sub>10</sub>H<sub>26</sub>N<sub>4</sub>).





*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms			AltConf
36	2	1	Total	C	N	0
			14	10	4	
36	2	1	Total	C	N	0
			14	10	4	
36	2	1	Total	C	N	0
			14	10	4	
36	2	1	Total	C	N	0
			14	10	4	
36	2	1	Total	C	N	0
			14	10	4	
36	2	1	Total	C	N	0
			14	10	4	
36	2	1	Total	C	N	0
			14	10	4	
36	2	1	Total	C	N	0
			14	10	4	
36	2	1	Total	C	N	0
			14	10	4	
36	2	1	Total	C	N	0
			14	10	4	
36	2	1	Total	C	N	0
			14	10	4	
36	2	1	Total	C	N	0
			14	10	4	
36	2	1	Total	C	N	0
			14	10	4	
36	2	1	Total	C	N	0
			14	10	4	
36	2	1	Total	C	N	0
			14	10	4	

- Molecule 37 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
37	C	2	Total	Zn	0
			2	2	
37	F	1	Total	Zn	0
			1	1	

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms		AltConf
37	W	1	Total 1	Zn 1	0
37	a	2	Total 2	Zn 2	0
37	P	1	Total 1	Zn 1	0
37	R	1	Total 1	Zn 1	0

- Molecule 38 is water.

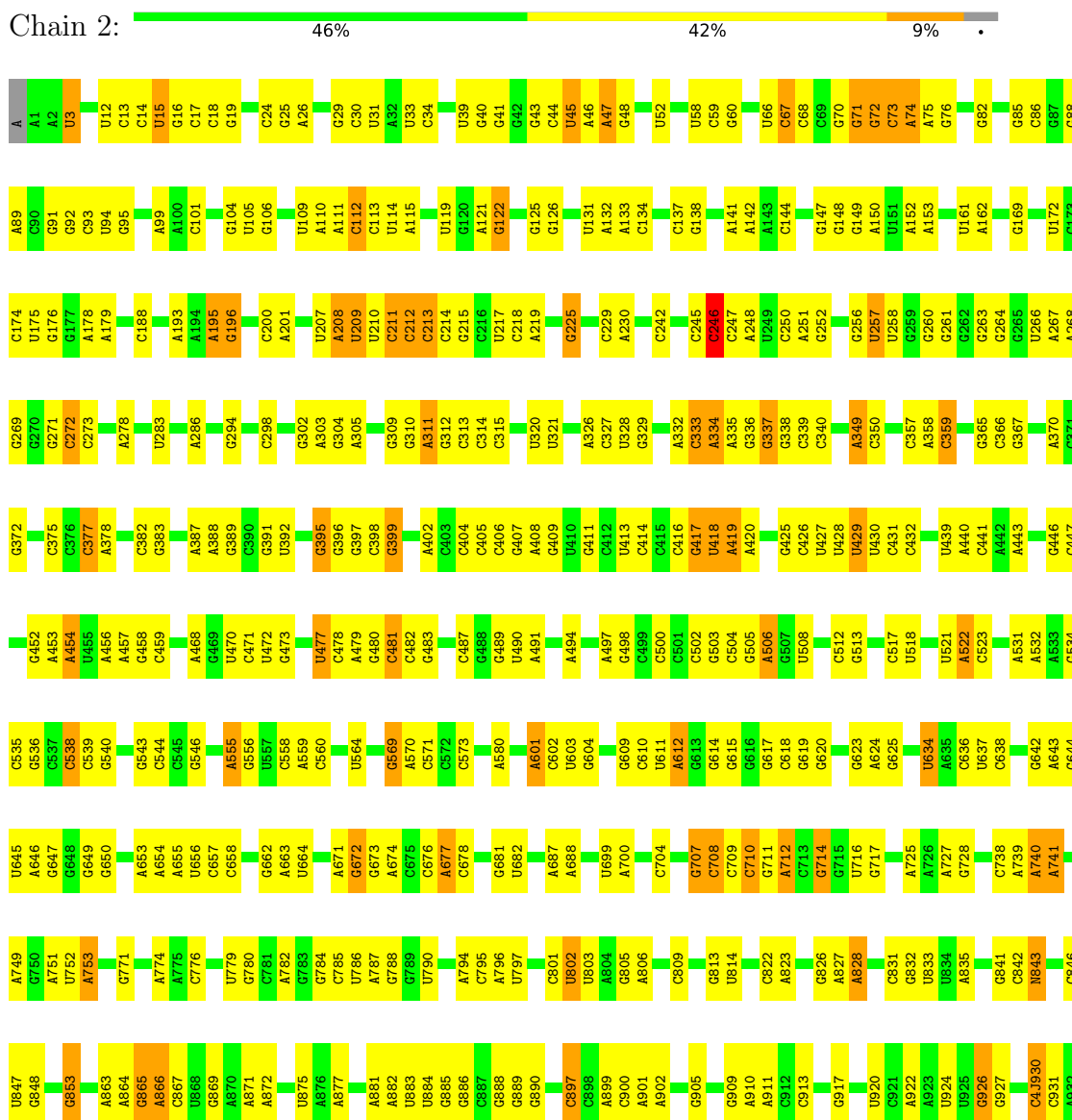
Mol	Chain	Residues	Atoms		AltConf
38	2	192	Total 192	O 192	0
38	D	1	Total 1	O 1	0
38	H	1	Total 1	O 1	0
38	I	2	Total 2	O 2	0
38	K	3	Total 3	O 3	0
38	4	3	Total 3	O 3	0
38	5	4	Total 4	O 4	0
38	P	1	Total 1	O 1	0
38	R	2	Total 2	O 2	0
38	E	1	Total 1	O 1	0



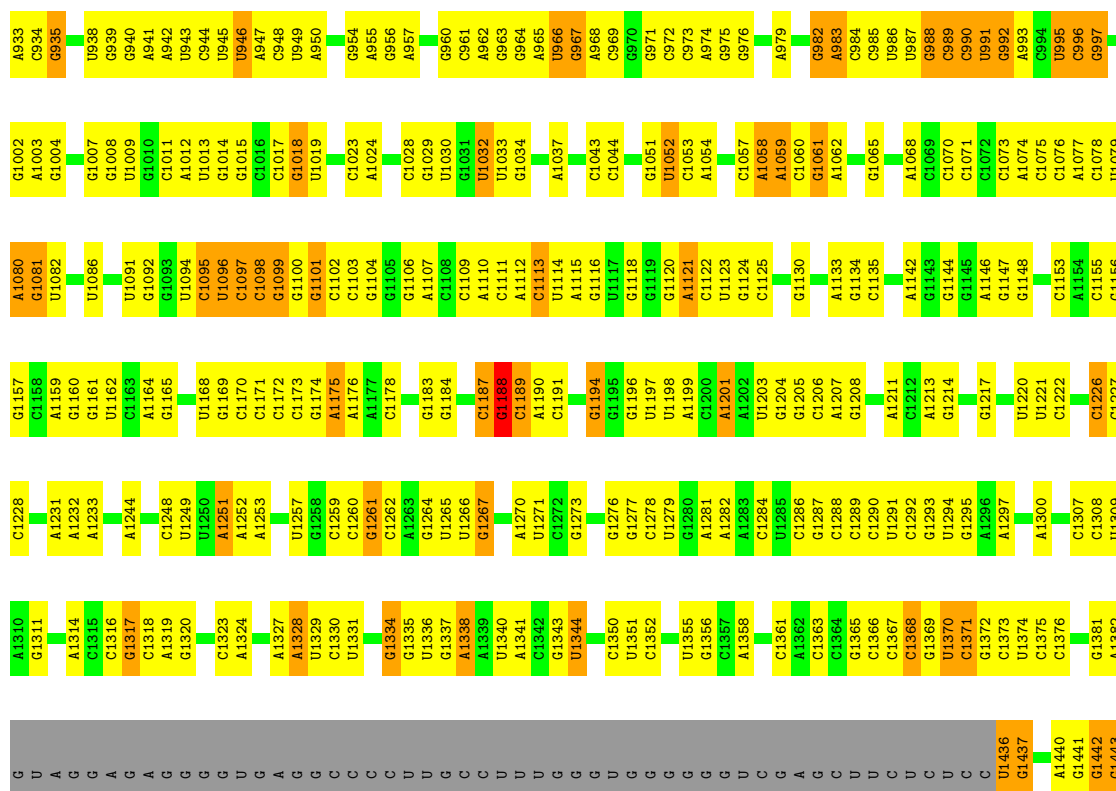
### 3 Residue-property plots

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

#### • Molecule 1: rRNA 16S





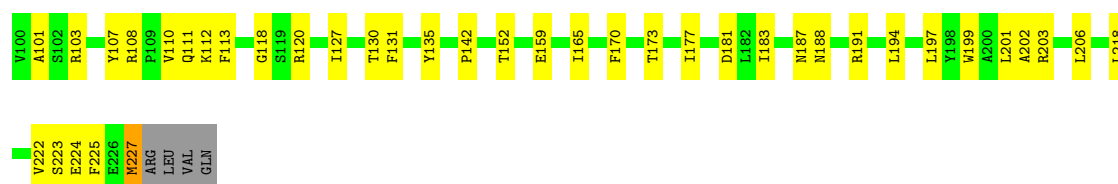


• Molecule 2: Small ribosomal subunit protein eS1

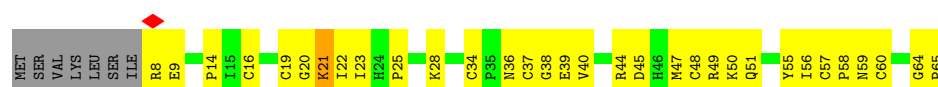
Chain A: 53% 34% 11%



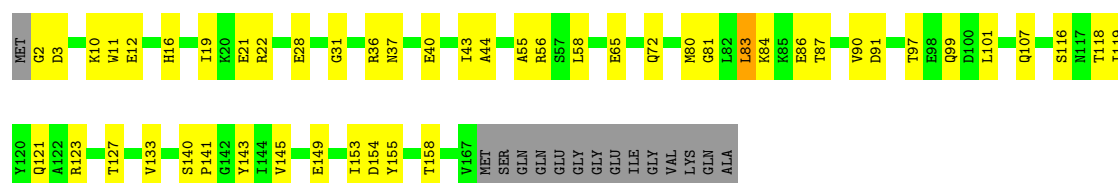




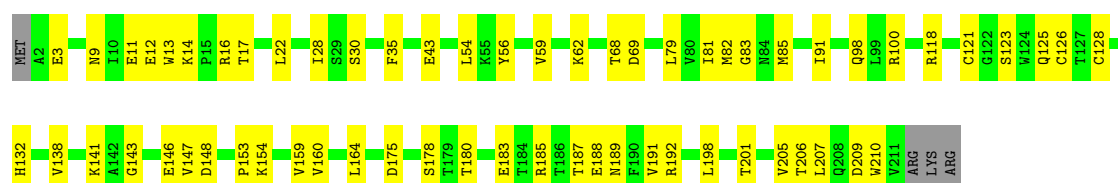
- Molecule 4: Small zinc finger protein HVO-2753-like zinc-binding pocket domain-containing protein



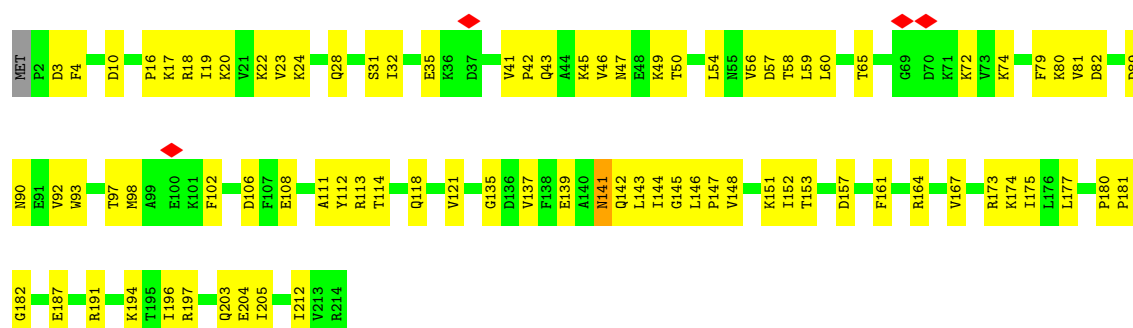
- Molecule 5: Small ribosomal subunit protein uS4



- Molecule 6: Small ribosomal subunit protein uS5

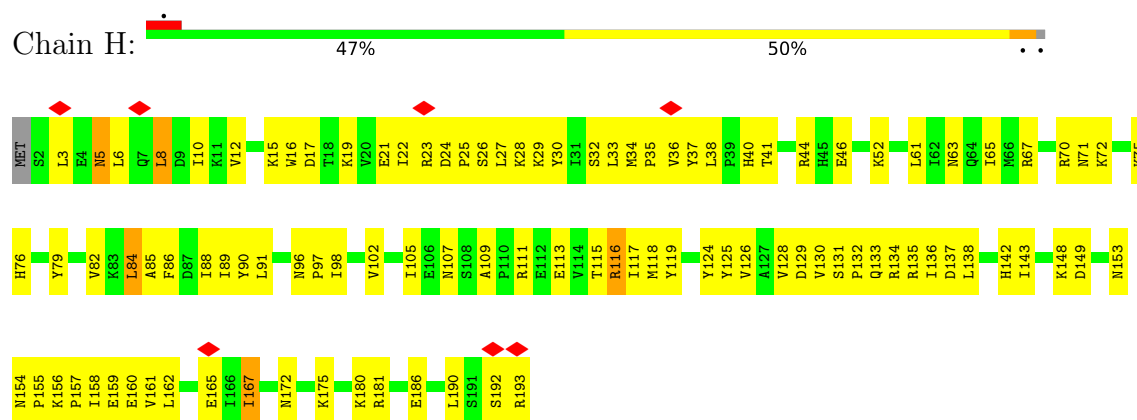


- Molecule 7: Small ribosomal subunit protein eS6

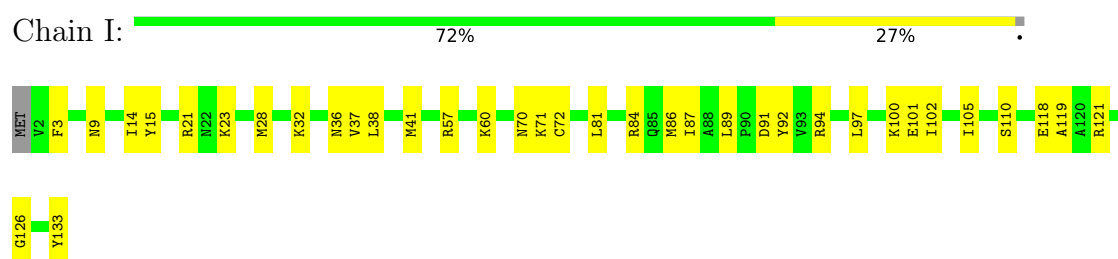


- Molecule 8: Small ribosomal subunit protein uS7

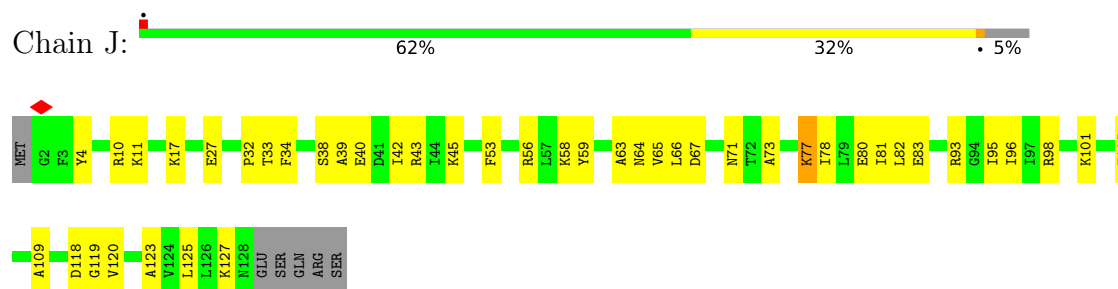




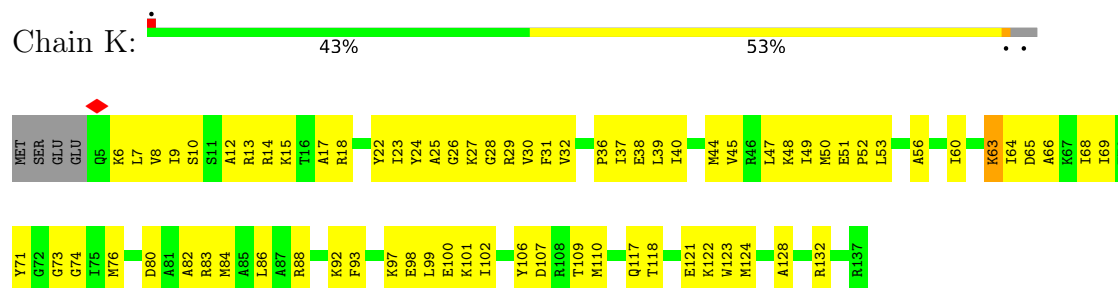
• Molecule 9: Small ribosomal subunit protein uS8



• Molecule 10: Small ribosomal subunit protein eS8



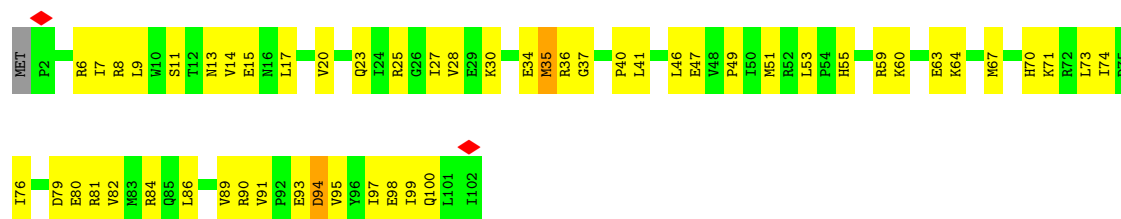
• Molecule 11: Small ribosomal subunit protein uS9



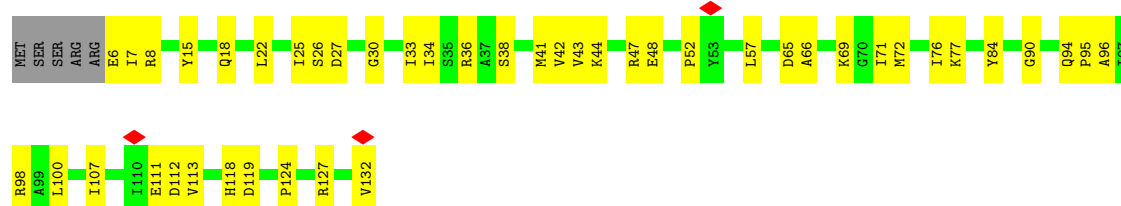
• Molecule 12: Small ribosomal subunit protein uS10



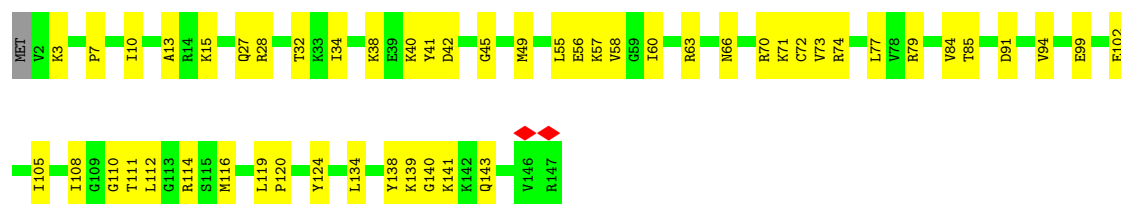




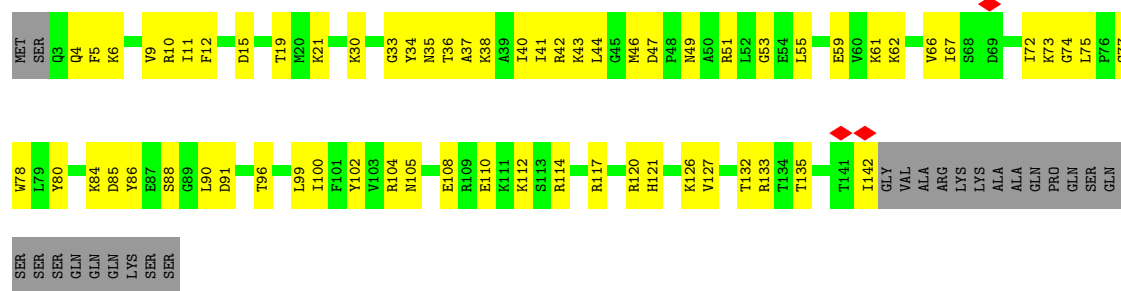
- Molecule 13: Small ribosomal subunit protein uS11



- Molecule 14: Small ribosomal subunit protein uS12



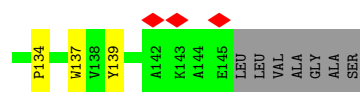
- Molecule 15: Small ribosomal subunit protein uS13



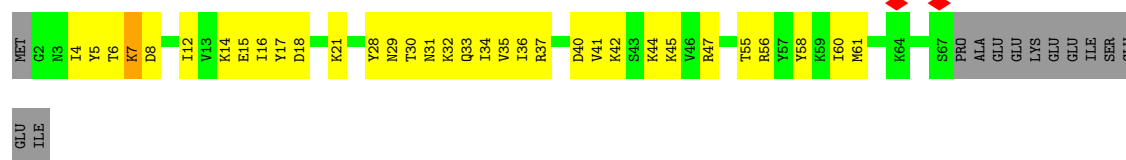
- Molecule 16: Small ribosomal subunit protein uS15



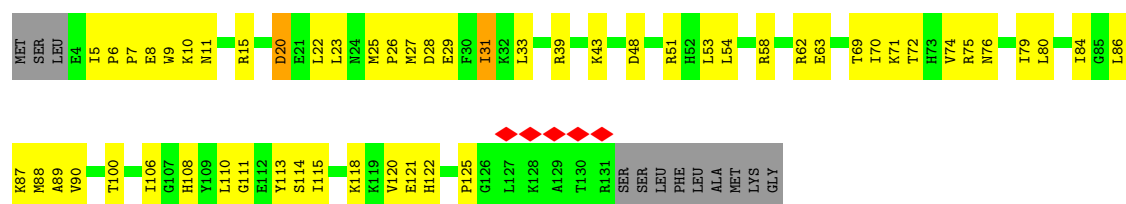




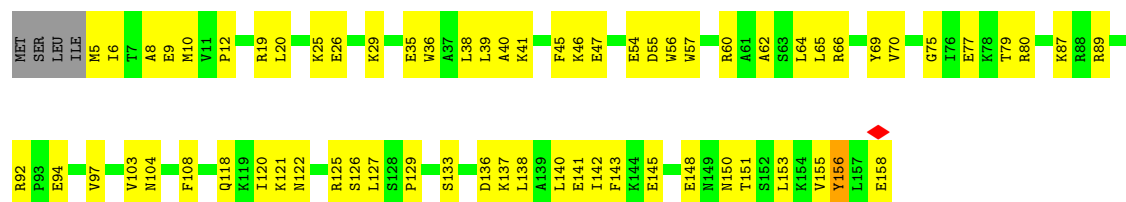
- Molecule 17: Small ribosomal subunit protein eS17



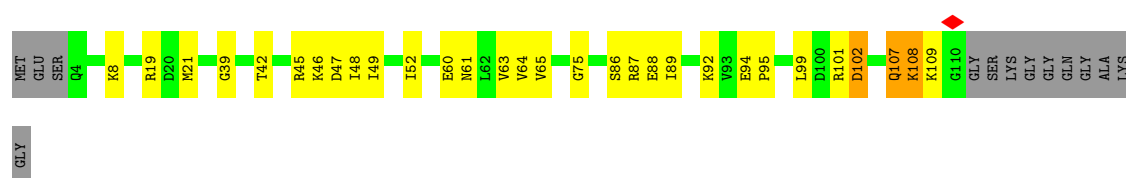
- Molecule 18: Small ribosomal subunit protein uS19



- Molecule 19: Small ribosomal subunit protein eS19



- Molecule 20: Small ribosomal subunit protein eS24



- Molecule 21: Small ribosomal subunit protein eS27



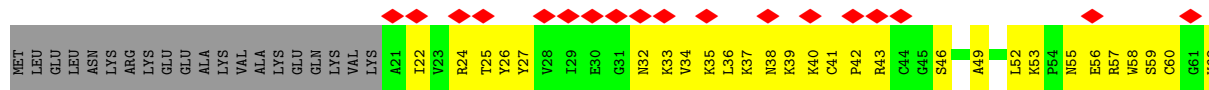
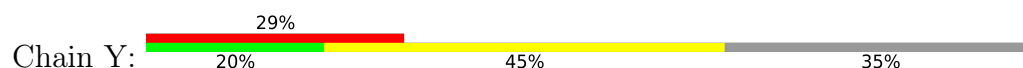




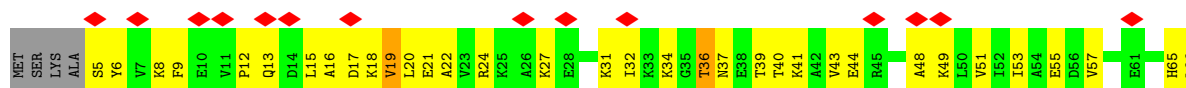
- Molecule 22: Small ribosomal subunit protein eS28



- Molecule 23: Small ribosomal subunit protein eS31



- Molecule 24: Large ribosomal subunit protein eL8



- Molecule 25: aS34



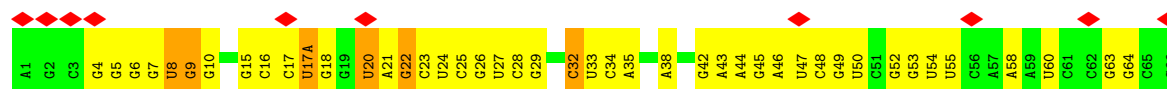
- Molecule 26: LSU ribosomal protein S30E (Rps30E)







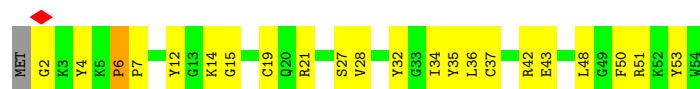
• Molecule 27: tRNA Met initiator



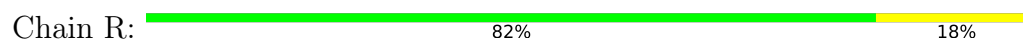
• Molecule 28: mRNA



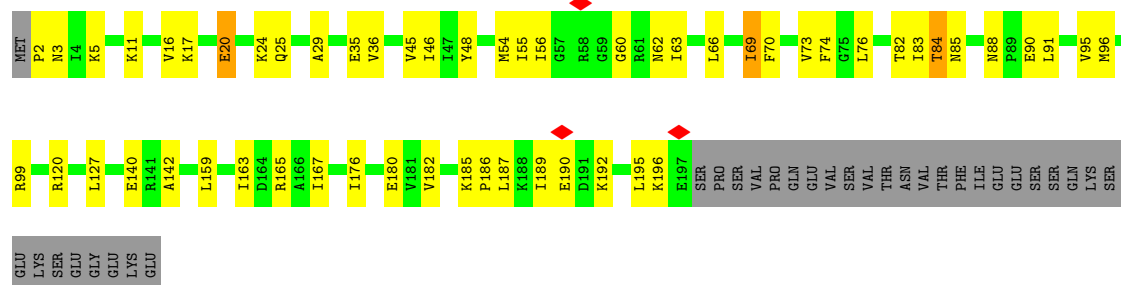
• Molecule 29: Small ribosomal subunit protein uS14



• Molecule 30: Small ribosomal subunit protein uS17

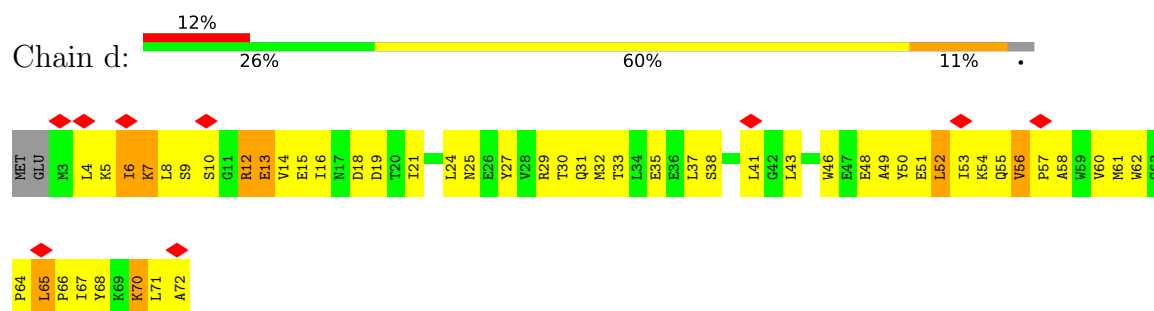


• Molecule 31: Small ribosomal subunit protein uS3

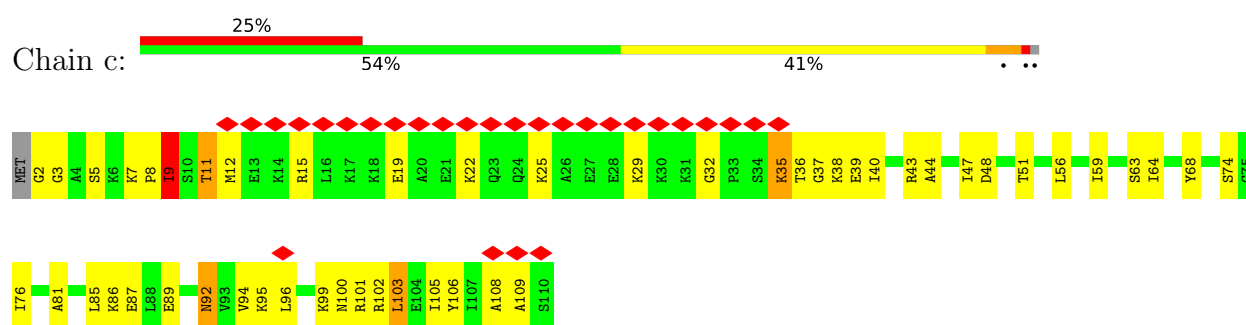




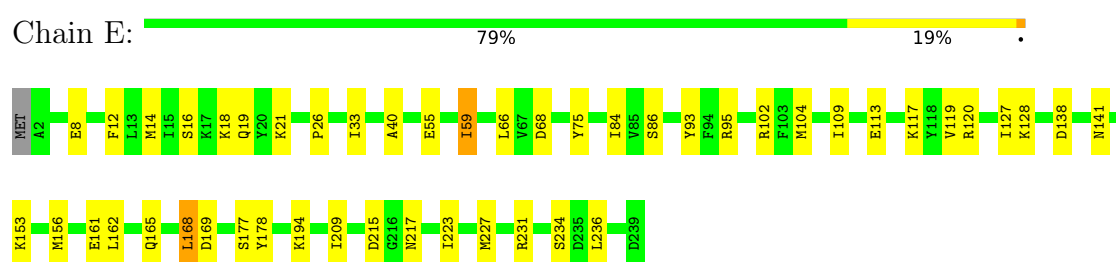
- Molecule 32: aS33



- Molecule 33: Small ribosomal subunit protein eS25



- Molecule 34: Small ribosomal subunit protein eS4





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	38561	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 ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.047	Depositor
Minimum map value	-0.018	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.007	Depositor
Map size (Å)	366.444, 366.444, 366.444	wwPDB
Map dimensions	348, 348, 348	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.053, 1.053, 1.053	Depositor



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: OMC, 5MU, 6MZ, SPM, 5MC, A2M, OMU, H2U, PSU, 4SU, C4J, ZN, OMG, 4AC, MG, MA6

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	0.20	0/33909	0.33	7/52900 (0.0%)
2	A	0.23	0/1543	0.52	0/2077
3	B	0.22	0/1731	0.47	0/2349
4	C	0.24	0/466	0.55	1/625 (0.2%)
5	D	0.20	0/1380	0.37	0/1859
6	F	0.21	0/1654	0.42	0/2240
7	G	0.19	0/1684	0.43	0/2265
8	H	0.24	0/1571	0.58	0/2116
9	I	0.22	0/1070	0.39	0/1444
10	J	0.20	0/994	0.40	0/1337
11	K	0.28	0/1084	0.67	1/1450 (0.1%)
12	L	0.26	0/856	0.61	0/1154
13	M	0.27	0/960	0.61	0/1294
14	N	0.21	0/1155	0.44	0/1540
15	O	0.26	0/1142	0.60	0/1532
16	Q	0.20	0/1206	0.42	0/1618
17	S	0.30	0/578	0.64	1/770 (0.1%)
18	T	0.21	0/1087	0.49	0/1456
19	U	0.22	0/1270	0.50	0/1710
20	V	0.23	0/843	0.50	1/1124 (0.1%)
21	W	0.26	0/511	0.68	0/684
22	X	0.29	0/538	0.72	0/722
23	Y	0.31	0/404	0.78	0/540
24	3	0.29	0/902	0.65	0/1216
25	a	0.45	0/574	1.17	2/770 (0.3%)
26	e	0.36	0/360	0.64	1/477 (0.2%)
27	4	0.16	1/1725 (0.1%)	0.21	0/2687
28	5	0.26	0/481	0.38	0/748
29	P	0.26	0/451	0.59	2/600 (0.3%)
30	R	0.32	0/918	0.44	0/1236
31	Z	0.25	0/1584	0.42	0/2124
32	d	0.24	0/581	0.59	0/786



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	c	0.36	1/861 (0.1%)	0.63	3/1143 (0.3%)
34	E	0.31	0/1965	0.48	0/2644
All	All	0.23	2/68038 (0.0%)	0.43	19/99237 (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
8	H	0	1
25	a	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	c	9	ILE	CA-C	-6.84	1.44	1.52
27	4	8	4SU	O3'-P	5.05	1.61	1.56

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1370	U	P-O3'-C3'	-27.41	79.09	120.20
1	2	1370	U	OP1-P-O3'	-14.58	64.27	108.00
1	2	1370	U	OP2-P-O3'	10.83	140.49	108.00
25	a	26	ARG	CA-C-N	-7.35	111.04	121.99
25	a	26	ARG	C-N-CA	-7.35	111.04	121.99

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	H	116	ARG	Sidechain
25	a	36	TYR	Sidechain

## 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	31042	0	15709	709	0
2	A	1515	0	1565	69	0
3	B	1698	0	1753	59	0
4	C	455	0	437	33	0
5	D	1354	0	1419	46	0
6	F	1625	0	1689	63	0
7	G	1661	0	1737	69	0
8	H	1543	0	1611	142	0
9	I	1050	0	1100	32	0
10	J	982	0	1046	35	0
11	K	1068	0	1125	98	0
12	L	840	0	893	61	0
13	M	944	0	978	42	0
14	N	1140	0	1244	47	0
15	O	1124	0	1162	66	0
16	Q	1185	0	1260	30	0
17	S	571	0	598	43	0
18	T	1064	0	1107	47	0
19	U	1247	0	1329	76	0
20	V	836	0	894	29	0
21	W	503	0	532	35	0
22	X	535	0	572	48	0
23	Y	395	0	405	40	0
24	3	893	0	940	77	0
25	a	562	0	575	83	0
26	e	354	0	386	22	0
27	4	1645	0	840	41	0
28	5	430	0	215	12	0
29	P	440	0	436	45	0
30	R	901	0	935	17	0
31	Z	1561	0	1667	62	0
32	d	570	0	590	98	0
33	c	856	0	941	75	0
34	E	1930	0	2013	32	0
35	2	47	0	0	0	0
35	5	1	0	0	0	0
35	F	2	0	0	0	0
35	K	1	0	0	0	0
35	P	1	0	0	0	0
35	R	1	0	0	0	0
36	2	434	0	805	74	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	C	2	0	0	0	0
37	F	1	0	0	0	0
37	P	1	0	0	0	0
37	R	1	0	0	0	0
37	W	1	0	0	0	0
37	a	2	0	0	0	0
38	2	192	0	0	9	0
38	4	3	0	0	0	0
38	5	4	0	0	0	0
38	D	1	0	0	0	0
38	E	1	0	0	0	0
38	H	1	0	0	1	0
38	I	2	0	0	0	0
38	K	3	0	0	0	0
38	P	1	0	0	0	0
38	R	2	0	0	0	0
All	All	65224	0	50508	2105	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 18.

The worst 5 of 2105 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)
8:H:3:LEU:HD21	32:d:70:LYS:CE	1.37	1.50
8:H:3:LEU:CD2	32:d:70:LYS:HE3	1.03	1.50
1:2:927:G:OP1	36:2:1576:SPM:C12	1.67	1.43
8:H:3:LEU:CD2	32:d:70:LYS:CE	1.89	1.40
25:a:51:GLU:OE2	25:a:54:LYS:HD3	1.30	1.29

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	
2	A	184/208 (88%)	179 (97%)	5 (3%)	0	100	100
3	B	213/231 (92%)	208 (98%)	5 (2%)	0	100	100
4	C	56/65 (86%)	54 (96%)	2 (4%)	0	100	100
5	D	164/181 (91%)	161 (98%)	3 (2%)	0	100	100
6	F	208/214 (97%)	201 (97%)	7 (3%)	0	100	100
7	G	211/214 (99%)	201 (95%)	10 (5%)	0	100	100
8	H	190/193 (98%)	183 (96%)	7 (4%)	0	100	100
9	I	130/133 (98%)	126 (97%)	4 (3%)	0	100	100
10	J	125/133 (94%)	123 (98%)	2 (2%)	0	100	100
11	K	131/137 (96%)	122 (93%)	9 (7%)	0	100	100
12	L	99/102 (97%)	92 (93%)	7 (7%)	0	100	100
13	M	125/132 (95%)	114 (91%)	11 (9%)	0	100	100
14	N	144/147 (98%)	137 (95%)	7 (5%)	0	100	100
15	O	138/165 (84%)	132 (96%)	6 (4%)	0	100	100
16	Q	143/152 (94%)	143 (100%)	0	0	100	100
17	S	64/79 (81%)	62 (97%)	2 (3%)	0	100	100
18	T	126/140 (90%)	126 (100%)	0	0	100	100
19	U	152/158 (96%)	147 (97%)	5 (3%)	0	100	100
20	V	105/120 (88%)	102 (97%)	3 (3%)	0	100	100
21	W	63/66 (96%)	60 (95%)	3 (5%)	0	100	100
22	X	65/83 (78%)	57 (88%)	8 (12%)	0	100	100
23	Y	47/75 (63%)	39 (83%)	8 (17%)	0	100	100
24	3	115/127 (91%)	99 (86%)	16 (14%)	0	100	100
25	a	69/72 (96%)	63 (91%)	5 (7%)	1 (1%)	9	34
26	e	41/52 (79%)	40 (98%)	1 (2%)	0	100	100
29	P	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
30	R	111/114 (97%)	108 (97%)	3 (3%)	0	100	100
31	Z	194/229 (85%)	189 (97%)	5 (3%)	0	100	100
32	d	68/72 (94%)	64 (94%)	4 (6%)	0	100	100
33	c	107/110 (97%)	99 (92%)	8 (8%)	0	100	100

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	E	236/239 (99%)	228 (97%)	8 (3%)	0	100	100
All	All	3875/4197 (92%)	3709 (96%)	165 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
25	a	58	LYS

### 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	A	168/184 (91%)	162 (96%)	6 (4%)	31	63
3	B	182/198 (92%)	180 (99%)	2 (1%)	65	82
4	C	51/58 (88%)	50 (98%)	1 (2%)	48	75
5	D	147/158 (93%)	146 (99%)	1 (1%)	76	87
6	F	180/184 (98%)	180 (100%)	0	100	100
7	G	186/187 (100%)	182 (98%)	4 (2%)	45	73
8	H	166/167 (99%)	162 (98%)	4 (2%)	43	72
9	I	113/114 (99%)	113 (100%)	0	100	100
10	J	104/110 (94%)	103 (99%)	1 (1%)	68	83
11	K	109/113 (96%)	106 (97%)	3 (3%)	38	69
12	L	93/94 (99%)	89 (96%)	4 (4%)	26	58
13	M	93/98 (95%)	90 (97%)	3 (3%)	34	65
14	N	122/123 (99%)	121 (99%)	1 (1%)	73	86
15	O	121/142 (85%)	120 (99%)	1 (1%)	73	86
16	Q	125/129 (97%)	125 (100%)	0	100	100
17	S	63/75 (84%)	63 (100%)	0	100	100
18	T	116/126 (92%)	112 (97%)	4 (3%)	32	64

*Continued on next page...*



Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	U	134/138 (97%)	131 (98%)	3 (2%)	45	73
20	V	92/99 (93%)	90 (98%)	2 (2%)	45	73
21	W	57/58 (98%)	56 (98%)	1 (2%)	51	76
22	X	58/73 (80%)	56 (97%)	2 (3%)	32	64
23	Y	43/65 (66%)	43 (100%)	0	100	100
24	3	97/105 (92%)	95 (98%)	2 (2%)	47	74
25	a	61/62 (98%)	56 (92%)	5 (8%)	10	35
26	e	40/46 (87%)	39 (98%)	1 (2%)	42	71
29	P	45/46 (98%)	45 (100%)	0	100	100
30	R	101/102 (99%)	100 (99%)	1 (1%)	68	83
31	Z	163/195 (84%)	159 (98%)	4 (2%)	42	71
32	d	63/65 (97%)	47 (75%)	16 (25%)	0	3
33	c	95/96 (99%)	89 (94%)	6 (6%)	16	46
34	E	214/215 (100%)	211 (99%)	3 (1%)	59	80
All	All	3402/3625 (94%)	3321 (98%)	81 (2%)	43	72

5 of 81 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
32	d	6	ILE
32	d	70	LYS
32	d	8	LEU
32	d	15	GLU
33	c	48	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
13	M	18	GLN
32	d	55	GLN
15	O	4	GLN
25	a	25	ASN
14	N	95	ASN

### 5.3.3 RNA



Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1442/1497 (96%)	226 (15%)	4 (0%)
27	4	76/77 (98%)	13 (17%)	1 (1%)
28	5	19/28 (67%)	10 (52%)	0
All	All	1537/1602 (95%)	249 (16%)	5 (0%)

5 of 249 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	3	U
1	2	33	U
1	2	34	C
1	2	43	G
1	2	45	U

All (5) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	256	G
1	2	1187	C
1	2	1188	G
1	2	1436	U
27	4	74	C

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

38 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	OMU	2	15	1	19,22,23	1.24	3 (15%)	25,31,34	1.82	4 (16%)
1	OMG	2	337	1	23,26,27	1.20	3 (13%)	32,38,41	2.01	5 (15%)
1	OMC	2	313	1	19,22,23	0.81	0	25,31,34	0.86	1 (4%)
1	6MZ	2	1457	35,1	22,25,26	1.52	5 (22%)	29,36,39	2.20	10 (34%)
1	OMG	2	1018	1	23,26,27	1.20	3 (13%)	32,38,41	1.98	6 (18%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	5MC	2	1368	1	19,22,23	1.47	3 (15%)	26,32,35	1.04	2 (7%)
1	OMG	2	905	1	23,26,27	1.19	3 (13%)	32,38,41	2.01	6 (18%)
27	5MU	4	54	27	19,22,23	1.36	5 (26%)	27,32,35	2.10	8 (29%)
1	OMC	2	481	1	19,22,23	0.85	1 (5%)	25,31,34	1.00	1 (4%)
27	OMC	4	32	27	19,22,23	0.83	0	25,31,34	1.07	2 (8%)
1	OMG	2	1061	1	23,26,27	1.20	3 (13%)	32,38,41	2.00	6 (18%)
1	A2M	2	494	1	22,25,26	1.48	4 (18%)	30,36,39	2.07	8 (26%)
1	OMG	2	865	1	23,26,27	1.22	3 (13%)	32,38,41	2.04	7 (21%)
1	4AC	2	843	1	21,24,25	1.03	2 (9%)	28,34,37	1.40	4 (14%)
1	4AC	2	1478	1	21,24,25	0.98	2 (9%)	28,34,37	1.47	4 (14%)
1	OMC	2	512	1	19,22,23	0.79	0	25,31,34	0.82	0
1	OMC	2	1060	1	19,22,23	0.78	0	25,31,34	0.72	0
1	OMG	2	1194	1	23,26,27	1.18	3 (13%)	32,38,41	2.01	6 (18%)
27	PSU	4	55	27	18,21,22	1.34	2 (11%)	21,30,33	2.02	3 (14%)
27	H2U	4	20	27	18,21,22	0.26	0	19,30,33	0.41	0
1	OMC	2	113	1	19,22,23	0.81	0	25,31,34	0.85	0
1	OMU	2	52	1	19,22,23	1.26	3 (15%)	25,31,34	1.82	4 (16%)
1	C4J	2	930	1	25,29,30	0.65	1 (4%)	28,42,45	0.87	1 (3%)
1	OMU	2	1344	1	19,22,23	1.24	3 (15%)	25,31,34	1.80	6 (24%)
1	4AC	2	1477	1	21,24,25	1.01	2 (9%)	28,34,37	1.59	6 (21%)
1	OMG	2	399	1	23,26,27	1.23	3 (13%)	32,38,41	1.96	6 (18%)
1	OMG	2	926	1	23,26,27	1.20	3 (13%)	32,38,41	1.99	6 (18%)
1	OMU	2	1032	1	19,22,23	1.27	3 (15%)	25,31,34	1.84	4 (16%)
1	OMC	2	710	1	19,22,23	0.82	0	25,31,34	0.92	1 (4%)
1	OMC	2	1366	1	19,22,23	0.79	0	25,31,34	0.78	0
27	4SU	4	8	27	18,21,22	0.20	0	25,30,33	0.32	0
1	OMC	2	538	1	19,22,23	0.79	0	25,31,34	0.89	1 (4%)
1	4AC	2	1466	1	21,24,25	0.98	2 (9%)	28,34,37	1.35	4 (14%)
1	MA6	2	1475	1	23,26,27	1.53	5 (21%)	33,38,41	2.06	10 (30%)
1	OMG	2	672	1	23,26,27	1.21	3 (13%)	32,38,41	1.99	6 (18%)
1	OMC	2	246	1	19,22,23	0.82	0	25,31,34	1.00	1 (4%)
1	OMG	2	546	1	23,26,27	1.18	3 (13%)	32,38,41	1.95	6 (18%)
1	4AC	2	1467	1	21,24,25	1.00	2 (9%)	28,34,37	1.44	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	OMU	2	15	1	-	0/9/27/28	0/2/2/2
1	OMG	2	337	1	-	1/9/27/28	0/3/3/3
1	OMC	2	313	1	-	0/9/27/28	0/2/2/2
1	6MZ	2	1457	35,1	-	0/9/27/28	0/3/3/3
1	OMG	2	1018	1	-	0/9/27/28	0/3/3/3
1	5MC	2	1368	1	-	0/7/25/26	0/2/2/2
1	OMG	2	905	1	-	0/9/27/28	0/3/3/3
27	5MU	4	54	27	-	0/7/25/26	0/2/2/2
1	OMC	2	481	1	-	0/9/27/28	0/2/2/2
27	OMC	4	32	27	-	2/9/27/28	0/2/2/2
1	OMG	2	1061	1	-	0/9/27/28	0/3/3/3
1	A2M	2	494	1	-	0/9/27/28	0/3/3/3
1	OMG	2	865	1	-	0/9/27/28	0/3/3/3
1	4AC	2	843	1	-	0/11/29/30	0/2/2/2
1	4AC	2	1478	1	-	0/11/29/30	0/2/2/2
1	OMC	2	512	1	-	0/9/27/28	0/2/2/2
1	OMC	2	1060	1	-	0/9/27/28	0/2/2/2
1	OMG	2	1194	1	-	0/9/27/28	0/3/3/3
27	PSU	4	55	27	-	2/7/25/26	0/2/2/2
27	H2U	4	20	27	-	3/7/38/39	0/2/2/2
1	OMC	2	113	1	-	0/9/27/28	0/2/2/2
1	OMU	2	52	1	-	0/9/27/28	0/2/2/2
1	C4J	2	930	1	-	2/16/34/35	0/2/2/2
1	OMU	2	1344	1	-	0/9/27/28	0/2/2/2
1	4AC	2	1477	1	-	0/11/29/30	0/2/2/2
1	OMG	2	399	1	-	0/9/27/28	0/3/3/3
1	OMG	2	926	1	-	0/9/27/28	0/3/3/3
1	OMU	2	1032	1	-	0/9/27/28	0/2/2/2
1	OMC	2	710	1	-	1/9/27/28	0/2/2/2
1	OMC	2	1366	1	-	0/9/27/28	0/2/2/2
27	4SU	4	8	27	-	0/7/25/26	0/2/2/2
1	OMC	2	538	1	-	0/9/27/28	0/2/2/2
1	4AC	2	1466	1	-	0/11/29/30	0/2/2/2
1	MA6	2	1475	1	-	0/11/29/30	0/3/3/3
1	OMG	2	672	1	-	0/9/27/28	0/3/3/3
1	OMC	2	246	1	-	3/9/27/28	0/2/2/2
1	OMG	2	546	1	-	0/9/27/28	0/3/3/3
1	4AC	2	1467	1	-	0/11/29/30	0/2/2/2

The worst 5 of 78 bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	1368	5MC	C5-C4	5.21	1.48	1.44
1	2	1475	MA6	C5-C4	4.74	1.47	1.39
1	2	1457	6MZ	C5-C4	4.66	1.47	1.39
1	2	494	A2M	C5-C4	4.46	1.47	1.39
27	4	55	PSU	C6-C5	3.42	1.39	1.35

The worst 5 of 149 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	672	OMG	C5-C4-N3	-6.36	118.27	128.39
1	2	399	OMG	C5-C4-N3	-6.21	118.50	128.39
1	2	1018	OMG	C5-C4-N3	-6.19	118.55	128.39
27	4	55	PSU	N1-C2-N3	6.18	121.68	115.17
1	2	1061	OMG	C5-C4-N3	-6.16	118.58	128.39

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
27	4	20	H2U	O4'-C1'-N1-C6
1	2	930	C4J	C4'-C5'-O5'-P
1	2	246	OMC	C3'-C4'-C5'-O5'
1	2	246	OMC	O4'-C4'-C5'-O5'
27	4	20	H2U	O4'-C1'-N1-C2

There are no ring outliers.

28 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	2	15	OMU	1	0
1	2	337	OMG	1	0
1	2	1018	OMG	1	0
1	2	1368	5MC	1	0
1	2	481	OMC	1	0
27	4	32	OMC	1	0
1	2	1061	OMG	1	0
1	2	865	OMG	1	0
1	2	843	4AC	2	0
1	2	1478	4AC	1	0
1	2	512	OMC	1	0
1	2	1060	OMC	2	0
1	2	1194	OMG	1	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	4	20	H2U	1	0
1	2	113	OMC	2	0
1	2	1344	OMU	2	0
1	2	1477	4AC	1	0
1	2	399	OMG	1	0
1	2	926	OMG	1	0
1	2	1032	OMU	1	0
1	2	710	OMC	1	0
1	2	1366	OMC	2	0
1	2	538	OMC	1	0
1	2	1466	4AC	2	0
1	2	1475	MA6	1	0
1	2	672	OMG	2	0
1	2	246	OMC	2	0
1	2	1467	4AC	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 92 ligands modelled in this entry, 61 are monoatomic - leaving 31 for Mogul analysis.

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	$\# Z  > 2$
36	SPM	2	1563	-	13,13,13	0.07	0	12,12,12	0.11	0
36	SPM	2	1572	-	13,13,13	0.10	0	12,12,12	0.07	0
36	SPM	2	1559	-	13,13,13	0.11	0	12,12,12	0.11	0
36	SPM	2	1578	-	13,13,13	0.10	0	12,12,12	0.06	0
36	SPM	2	1557	-	13,13,13	0.09	0	12,12,12	0.08	0
36	SPM	2	1554	-	13,13,13	0.07	0	12,12,12	0.14	0
36	SPM	2	1573	-	13,13,13	0.11	0	12,12,12	0.06	0
36	SPM	2	1558	-	13,13,13	0.07	0	12,12,12	0.12	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
36	SPM	2	1553	-	13,13,13	0.10	0	12,12,12	0.06	0
36	SPM	2	1576	-	13,13,13	0.11	0	12,12,12	0.06	0
36	SPM	2	1568	-	13,13,13	0.10	0	12,12,12	0.08	0
36	SPM	2	1550	-	13,13,13	0.09	0	12,12,12	0.11	0
36	SPM	2	1566	-	13,13,13	0.10	0	12,12,12	0.06	0
36	SPM	2	1569	-	13,13,13	0.11	0	12,12,12	0.06	0
36	SPM	2	1565	-	13,13,13	0.08	0	12,12,12	0.09	0
36	SPM	2	1551	-	13,13,13	0.10	0	12,12,12	0.06	0
36	SPM	2	1575	-	13,13,13	0.10	0	12,12,12	0.06	0
36	SPM	2	1564	-	13,13,13	0.08	0	12,12,12	0.09	0
36	SPM	2	1570	-	13,13,13	0.08	0	12,12,12	0.11	0
36	SPM	2	1577	-	13,13,13	0.13	0	12,12,12	0.10	0
36	SPM	2	1555	-	13,13,13	0.11	0	12,12,12	0.09	0
36	SPM	2	1567	-	13,13,13	0.11	0	12,12,12	0.06	0
36	SPM	2	1571	-	13,13,13	0.08	0	12,12,12	0.09	0
36	SPM	2	1574	-	13,13,13	0.11	0	12,12,12	0.06	0
36	SPM	2	1561	-	13,13,13	0.11	0	12,12,12	0.10	0
36	SPM	2	1552	-	13,13,13	0.06	0	12,12,12	0.10	0
36	SPM	2	1556	-	13,13,13	0.08	0	12,12,12	0.12	0
36	SPM	2	1562	-	13,13,13	0.10	0	12,12,12	0.06	0
36	SPM	2	1549	-	13,13,13	0.10	0	12,12,12	0.07	0
36	SPM	2	1560	-	13,13,13	0.10	0	12,12,12	0.11	0
36	SPM	2	1548	-	13,13,13	0.07	0	12,12,12	0.10	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	SPM	2	1563	-	-	1/11/11/11	-
36	SPM	2	1572	-	-	2/11/11/11	-
36	SPM	2	1559	-	-	4/11/11/11	-
36	SPM	2	1578	-	-	3/11/11/11	-
36	SPM	2	1557	-	-	2/11/11/11	-
36	SPM	2	1554	-	-	1/11/11/11	-
36	SPM	2	1573	-	-	3/11/11/11	-
36	SPM	2	1558	-	-	3/11/11/11	-
36	SPM	2	1553	-	-	4/11/11/11	-
36	SPM	2	1576	-	-	3/11/11/11	-
36	SPM	2	1568	-	-	2/11/11/11	-

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	SPM	2	1550	-	-	3/11/11/11	-
36	SPM	2	1566	-	-	3/11/11/11	-
36	SPM	2	1569	-	-	3/11/11/11	-
36	SPM	2	1565	-	-	3/11/11/11	-
36	SPM	2	1551	-	-	2/11/11/11	-
36	SPM	2	1575	-	-	2/11/11/11	-
36	SPM	2	1564	-	-	5/11/11/11	-
36	SPM	2	1570	-	-	3/11/11/11	-
36	SPM	2	1577	-	-	1/11/11/11	-
36	SPM	2	1555	-	-	2/11/11/11	-
36	SPM	2	1567	-	-	4/11/11/11	-
36	SPM	2	1571	-	-	2/11/11/11	-
36	SPM	2	1574	-	-	3/11/11/11	-
36	SPM	2	1561	-	-	2/11/11/11	-
36	SPM	2	1552	-	-	2/11/11/11	-
36	SPM	2	1556	-	-	2/11/11/11	-
36	SPM	2	1562	-	-	2/11/11/11	-
36	SPM	2	1549	-	-	1/11/11/11	-
36	SPM	2	1560	-	-	1/11/11/11	-
36	SPM	2	1548	-	-	2/11/11/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 76 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
36	2	1556	SPM	C12-C11-N10-C9
36	2	1565	SPM	C7-C6-N5-C4
36	2	1569	SPM	C3-C4-N5-C6
36	2	1573	SPM	C7-C6-N5-C4
36	2	1575	SPM	C3-C4-N5-C6

There are no ring outliers.

25 monomers are involved in 74 short contacts:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	2	1563	SPM	4	0
36	2	1559	SPM	2	0
36	2	1578	SPM	5	0
36	2	1554	SPM	1	0
36	2	1573	SPM	3	0
36	2	1558	SPM	2	0
36	2	1553	SPM	3	0
36	2	1576	SPM	9	0
36	2	1566	SPM	1	0
36	2	1565	SPM	1	0
36	2	1551	SPM	1	0
36	2	1575	SPM	7	0
36	2	1564	SPM	3	0
36	2	1570	SPM	1	0
36	2	1577	SPM	2	0
36	2	1555	SPM	1	0
36	2	1567	SPM	10	0
36	2	1574	SPM	2	0
36	2	1561	SPM	1	0
36	2	1552	SPM	1	0
36	2	1556	SPM	1	0
36	2	1562	SPM	3	0
36	2	1549	SPM	5	0
36	2	1560	SPM	3	0
36	2	1548	SPM	2	0

## 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.



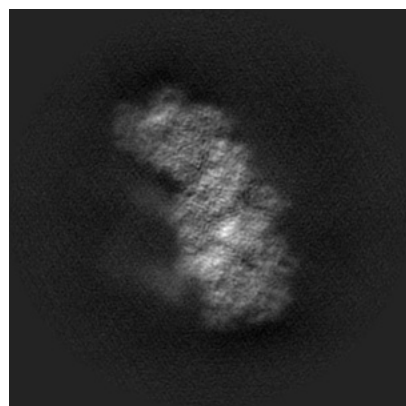
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50717. These allow visual inspection of the internal detail of the map and identification of artifacts.

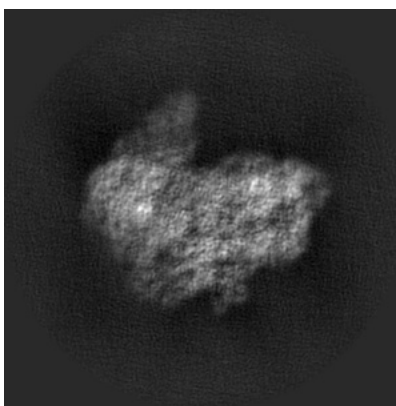
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

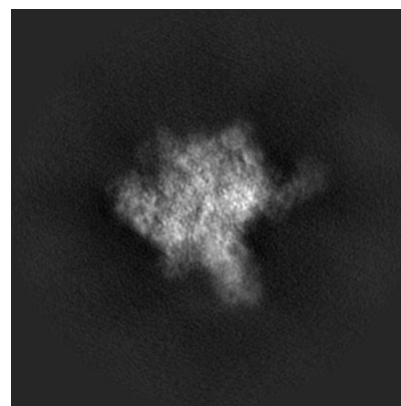
#### 6.1.1 Primary map



X

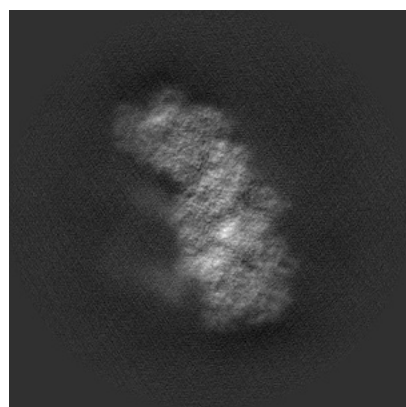


Y

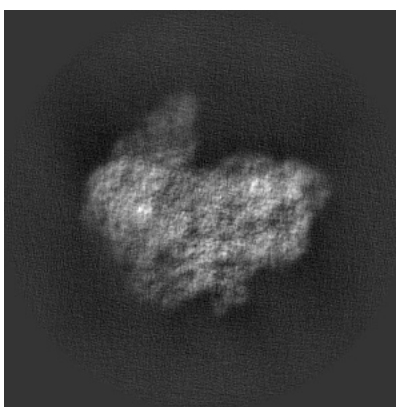


Z

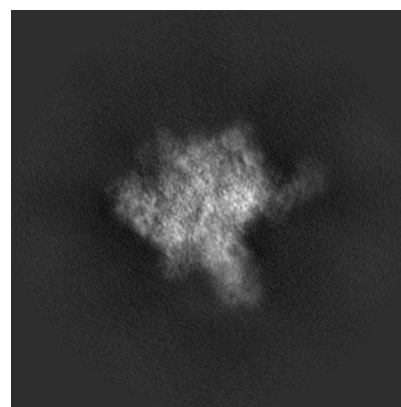
#### 6.1.2 Raw map



X



Y



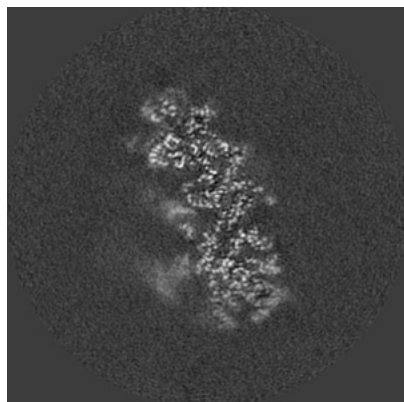
Z

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

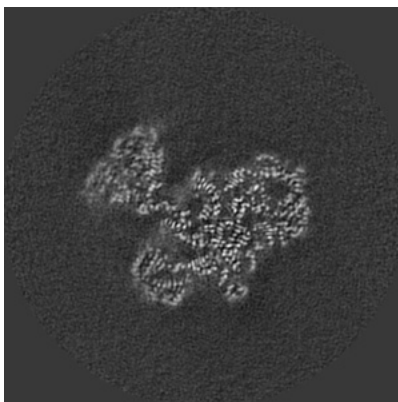


## 6.2 Central slices [i](#)

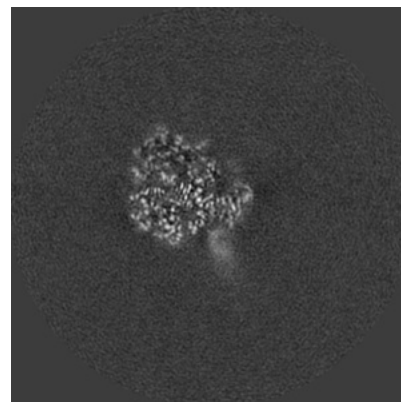
### 6.2.1 Primary map



X Index: 174

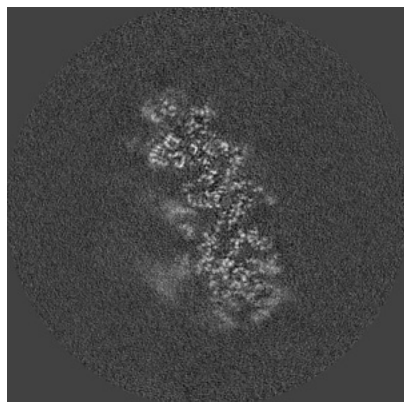


Y Index: 174

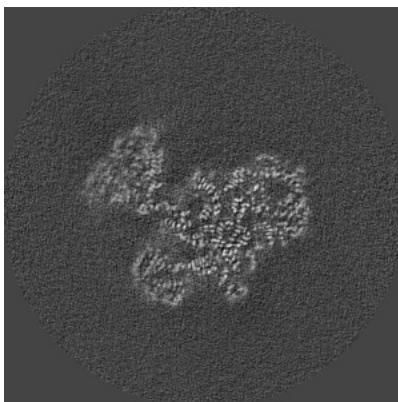


Z Index: 174

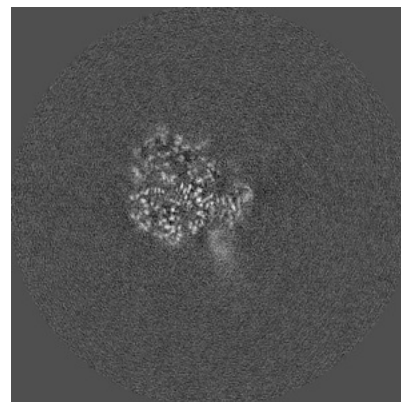
### 6.2.2 Raw map



X Index: 174



Y Index: 174



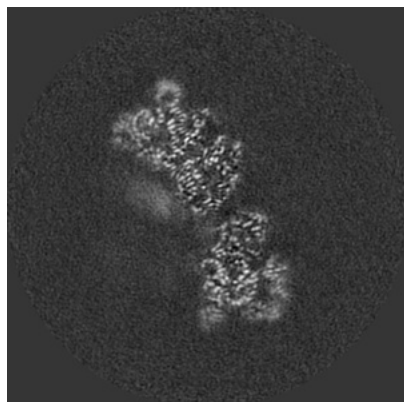
Z Index: 174

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

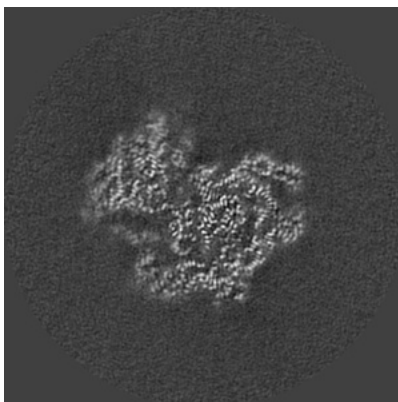


## 6.3 Largest variance slices [i](#)

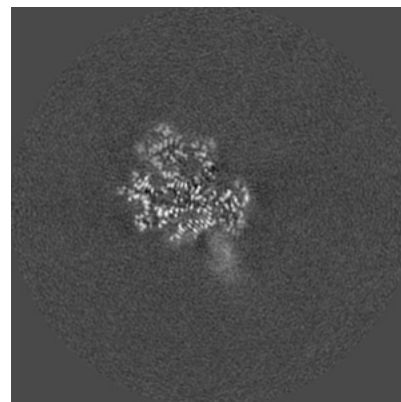
### 6.3.1 Primary map



X Index: 187

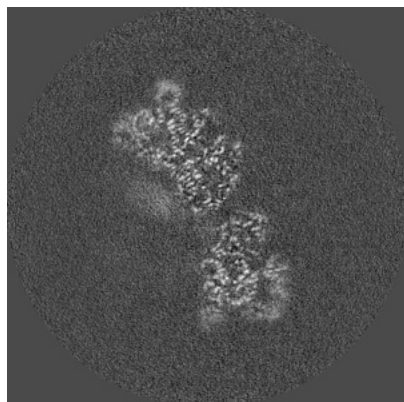


Y Index: 181

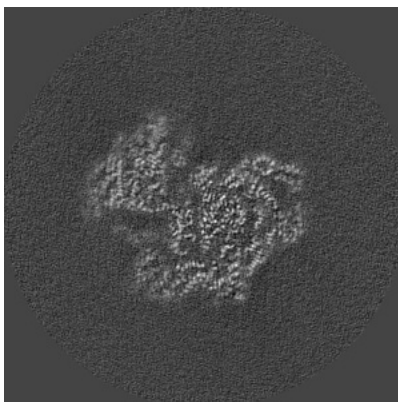


Z Index: 179

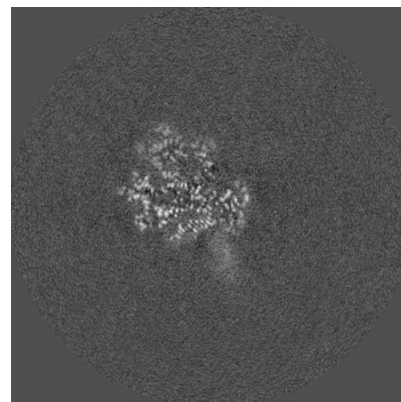
### 6.3.2 Raw map



X Index: 187



Y Index: 180



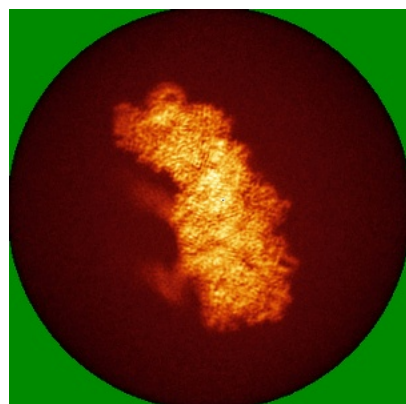
Z Index: 179

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

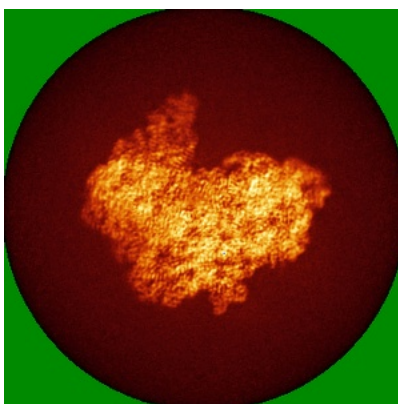


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

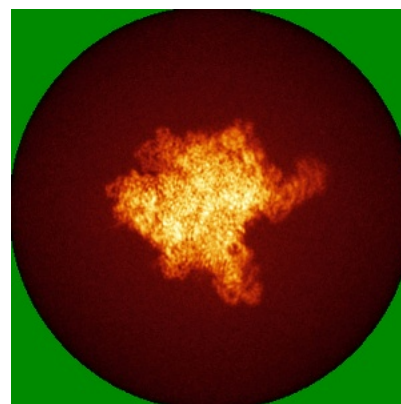
### 6.4.1 Primary map



X

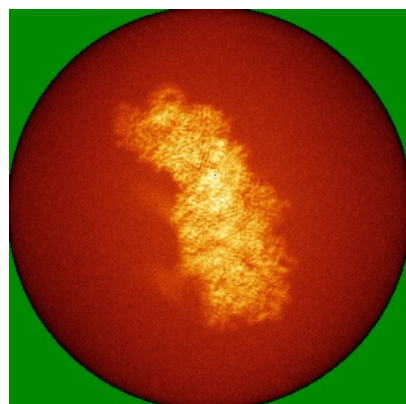


Y

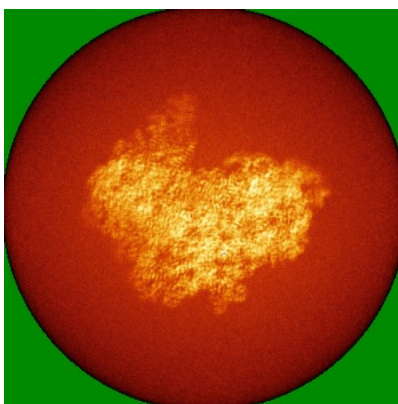


Z

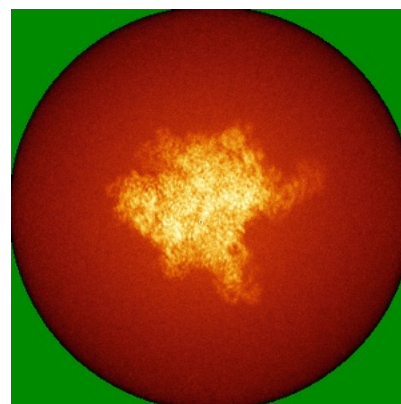
### 6.4.2 Raw map



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](#)

This section was not generated.



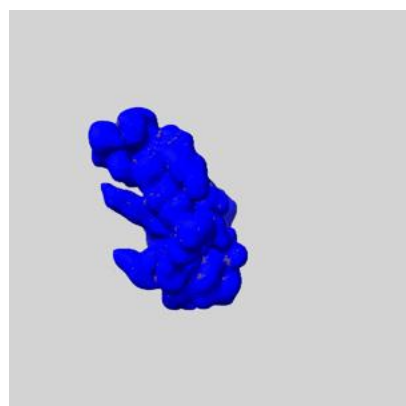
## 6.6 Mask visualisation [i](#)

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

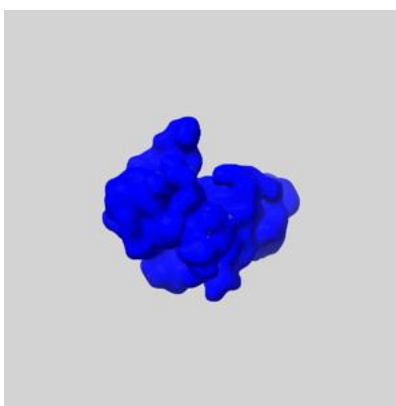
A mask typically either:

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

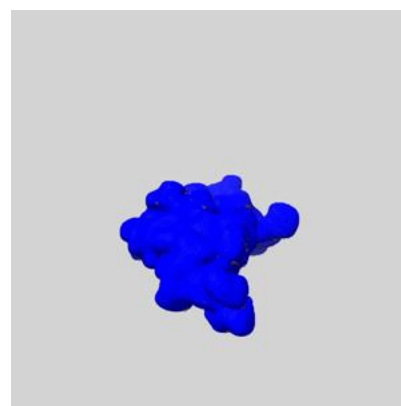
### 6.6.1 emd\_50717\_msk\_1.map [i](#)



X



Y



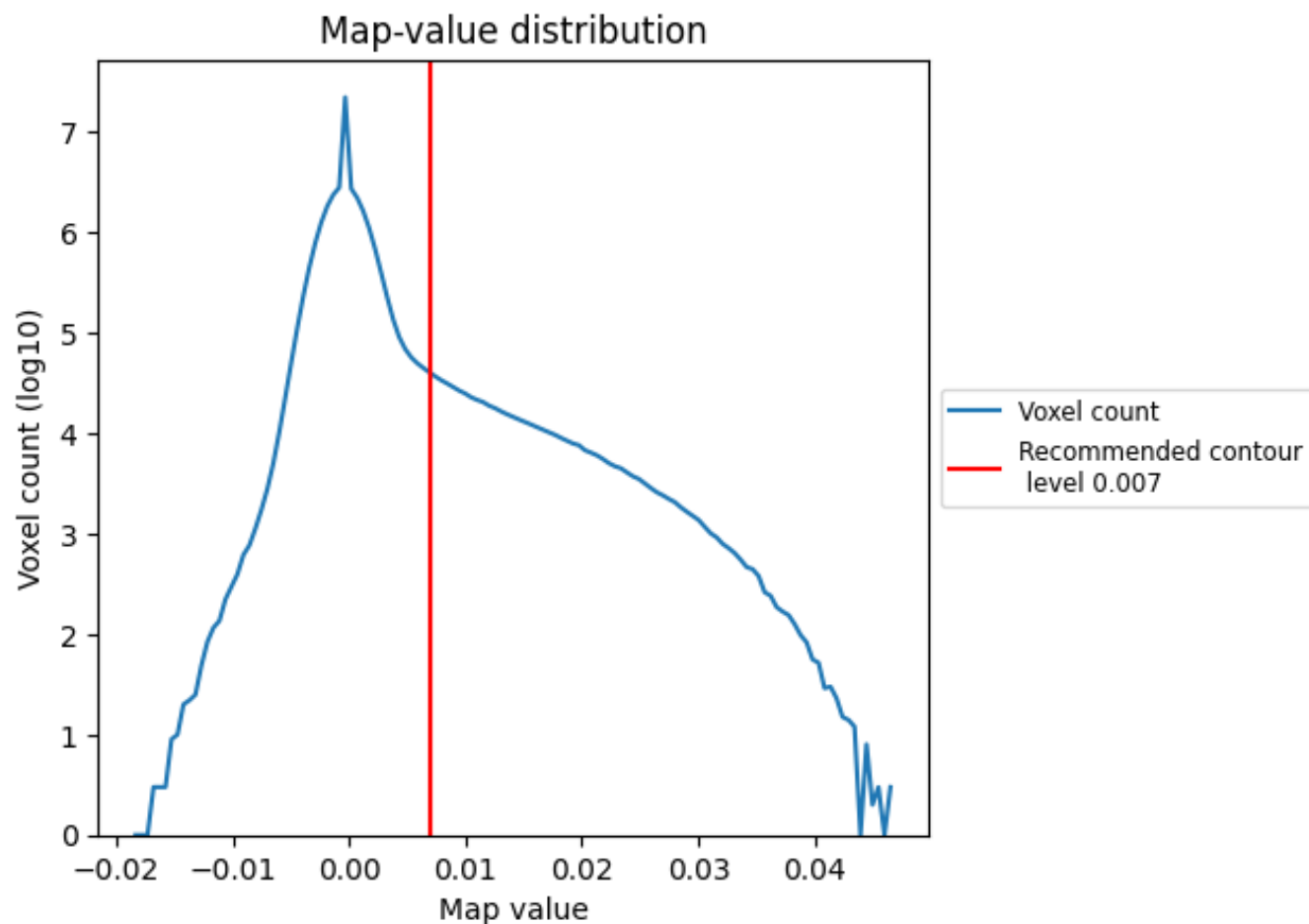
Z



## 7 Map analysis [i](#)

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

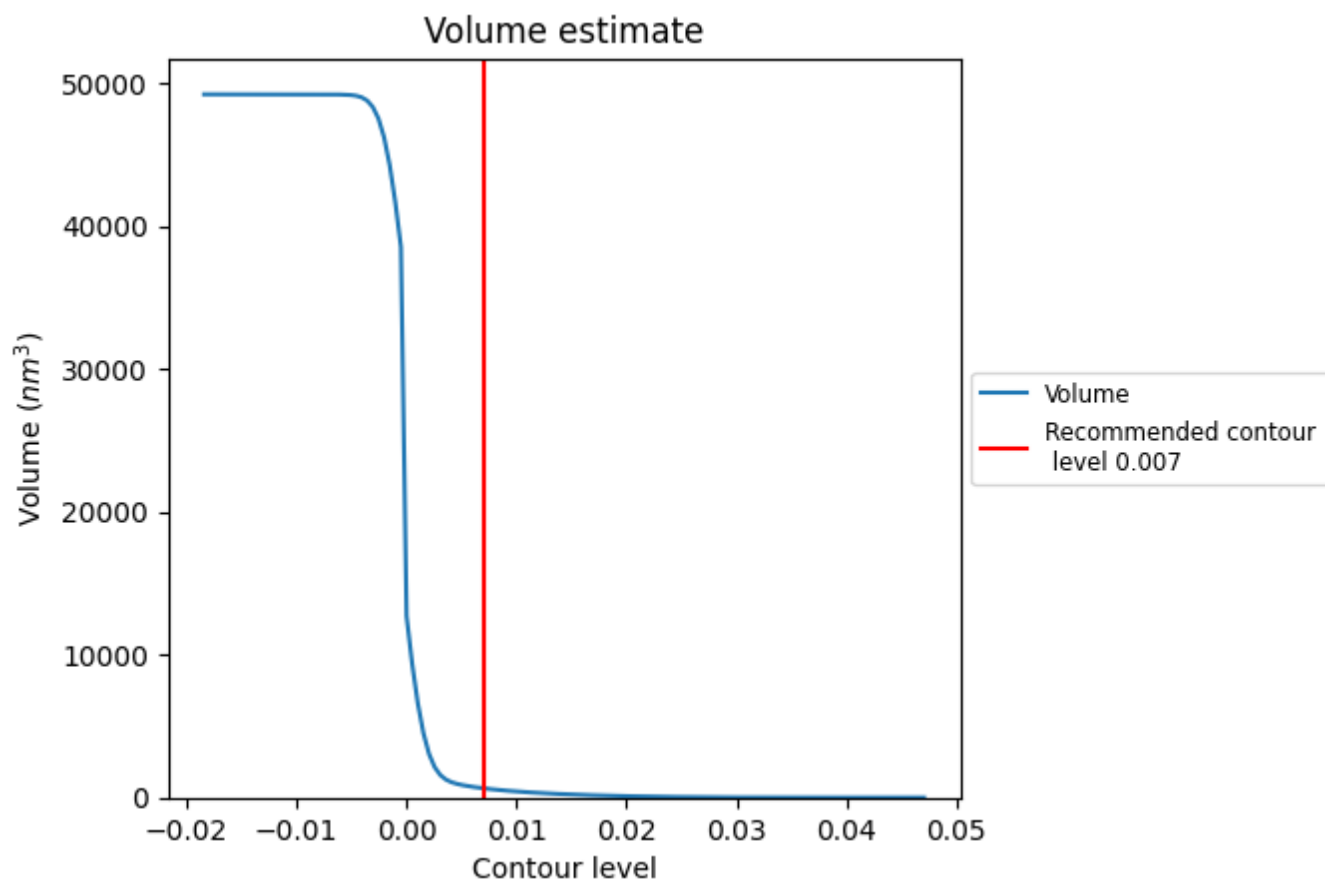
### 7.1 Map-value distribution [i](#)



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](#)

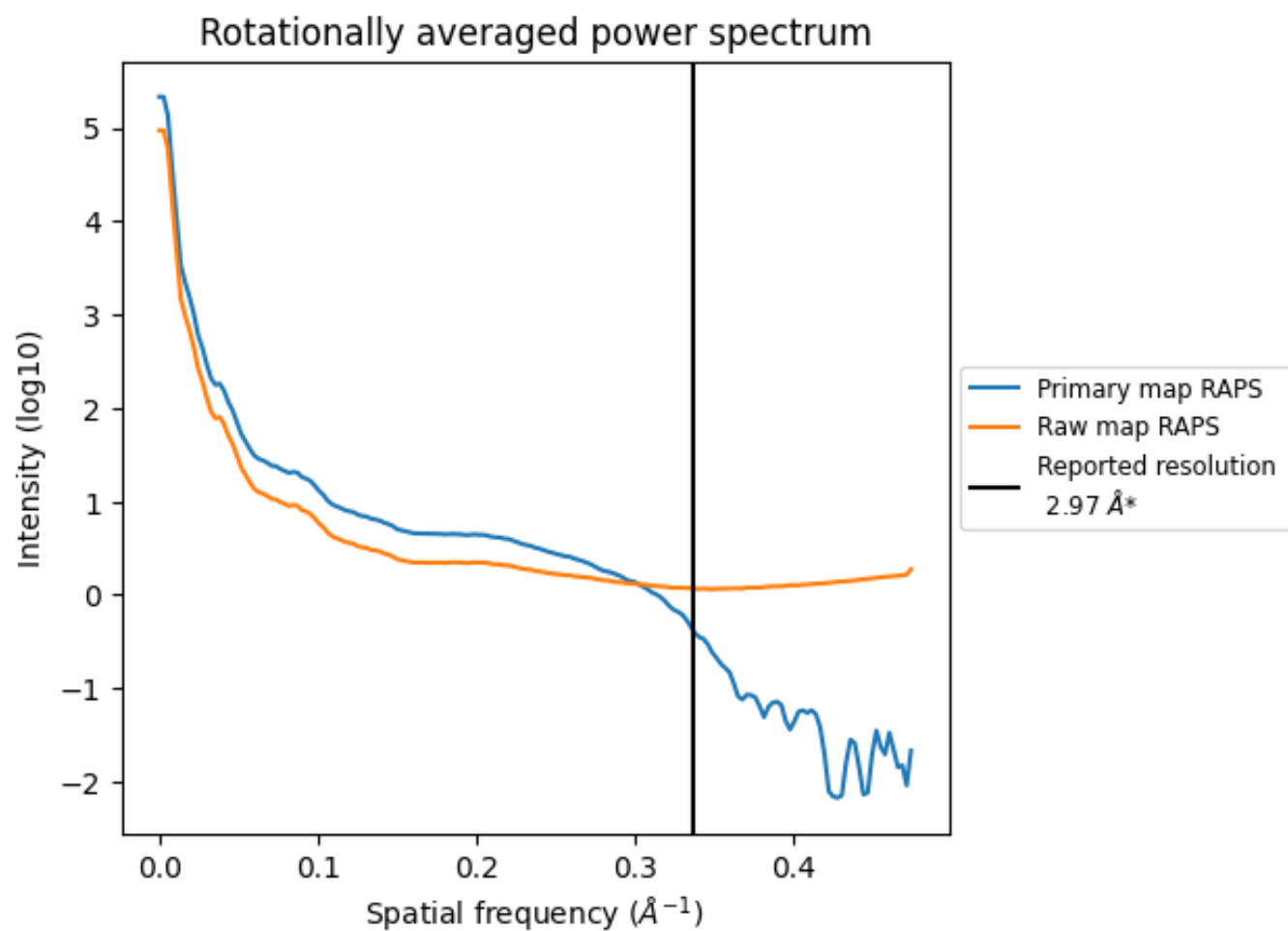


The volume at the recommended contour level is 651 nm<sup>3</sup>; this corresponds to an approximate mass of 588 kDa.

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 ⓘ



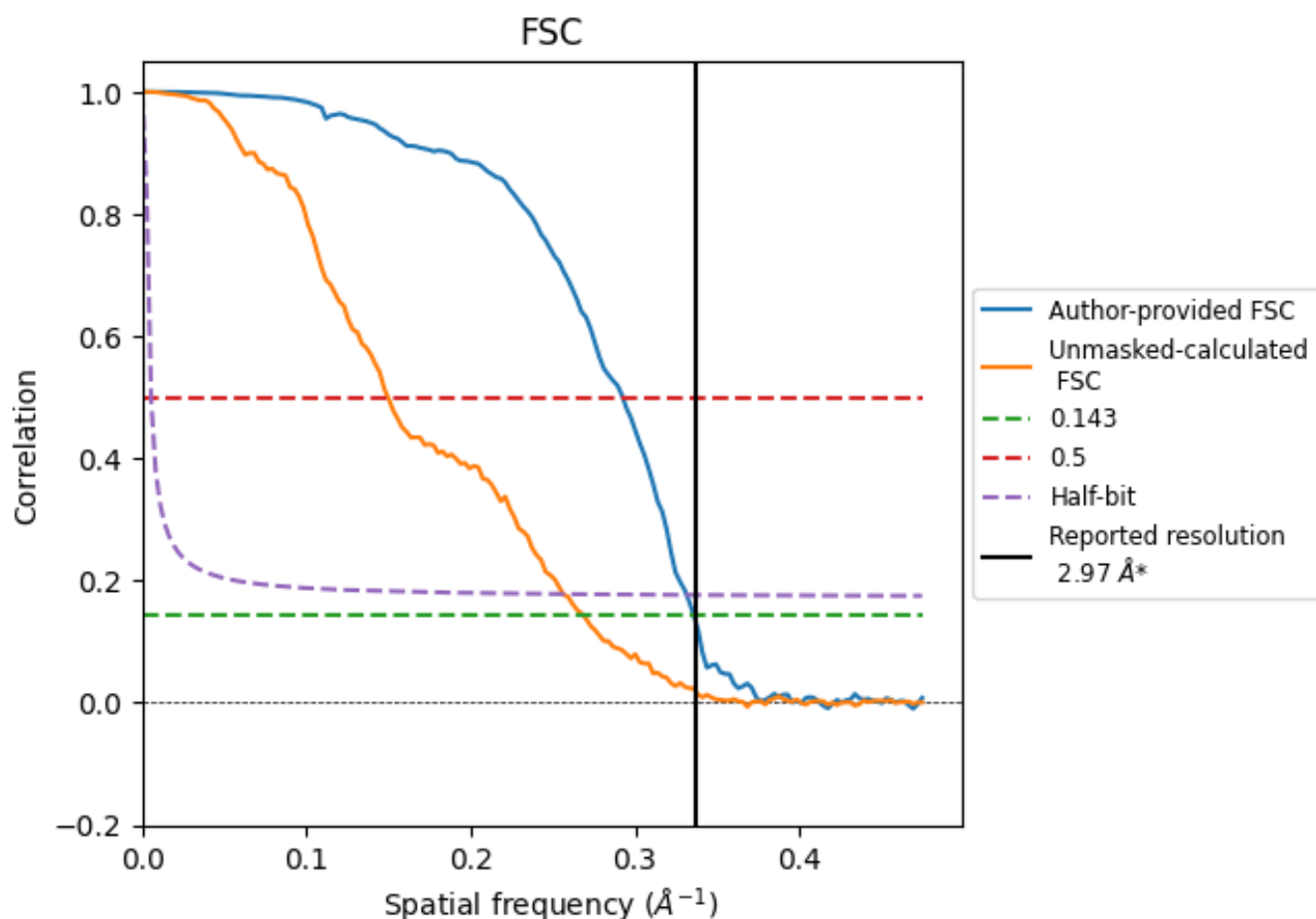
\*Reported resolution corresponds to spatial frequency of 0.337 Å<sup>-1</sup>



## 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 0.337  $\text{\AA}^{-1}$



## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.97	-	-
Author-provided FSC curve	2.98	3.42	3.02
Unmasked-calculated*	3.73	6.68	3.90

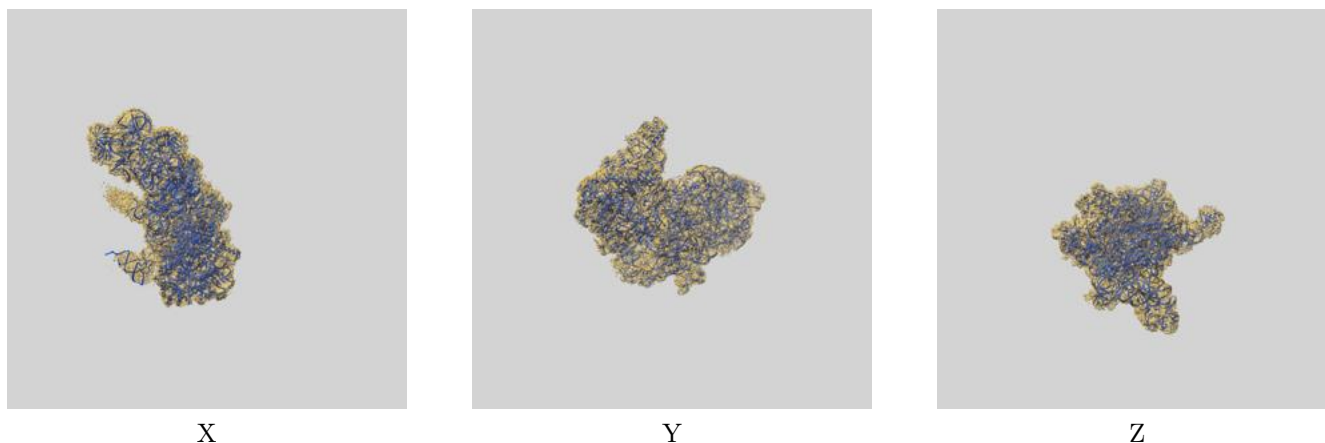
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.73 differs from the reported value 2.97 by more than 10 %



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

This section contains information regarding the fit between EMDB map EMD-50717 and PDB model 9FRL. Per-residue inclusion information can be found in [section 3](#) on [page 14](#).

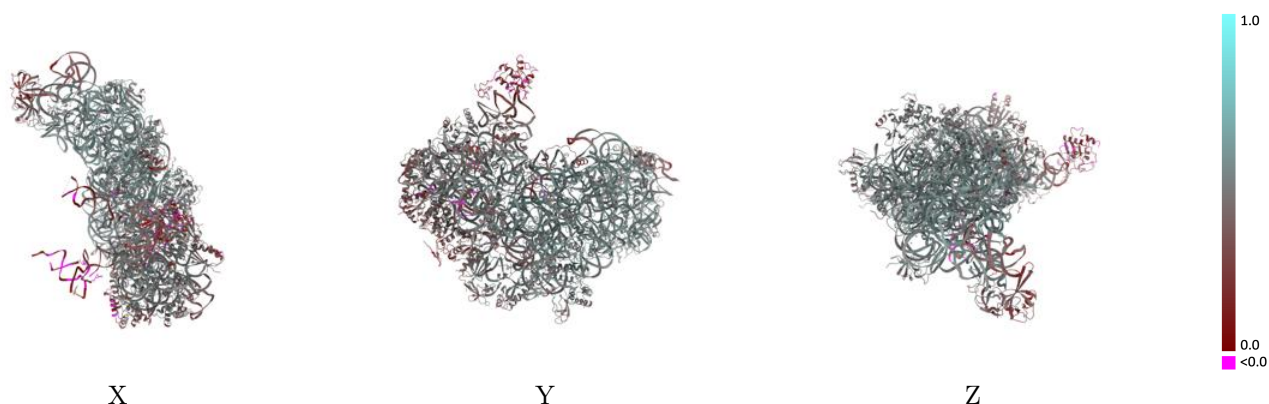
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.007 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.

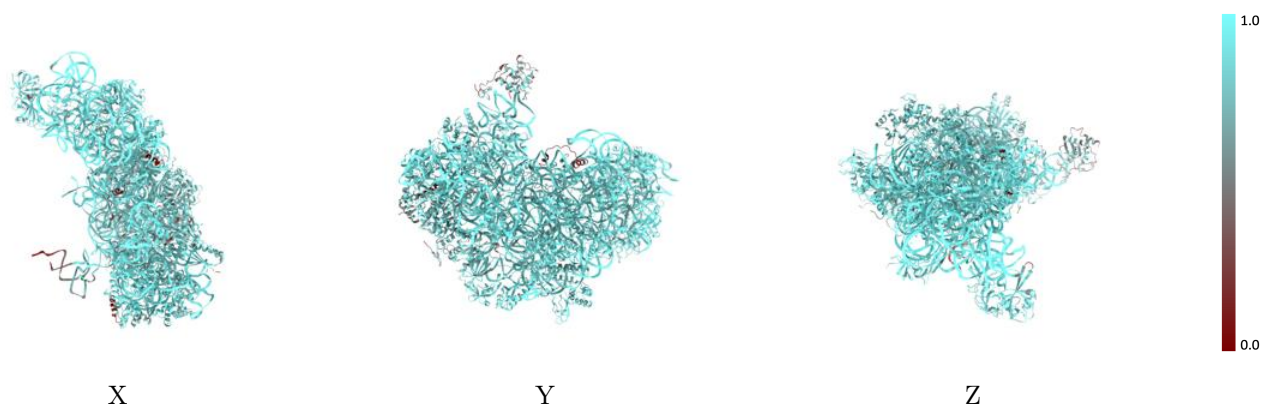


## 9.2 Q-score mapped to coordinate model [i](#)



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.

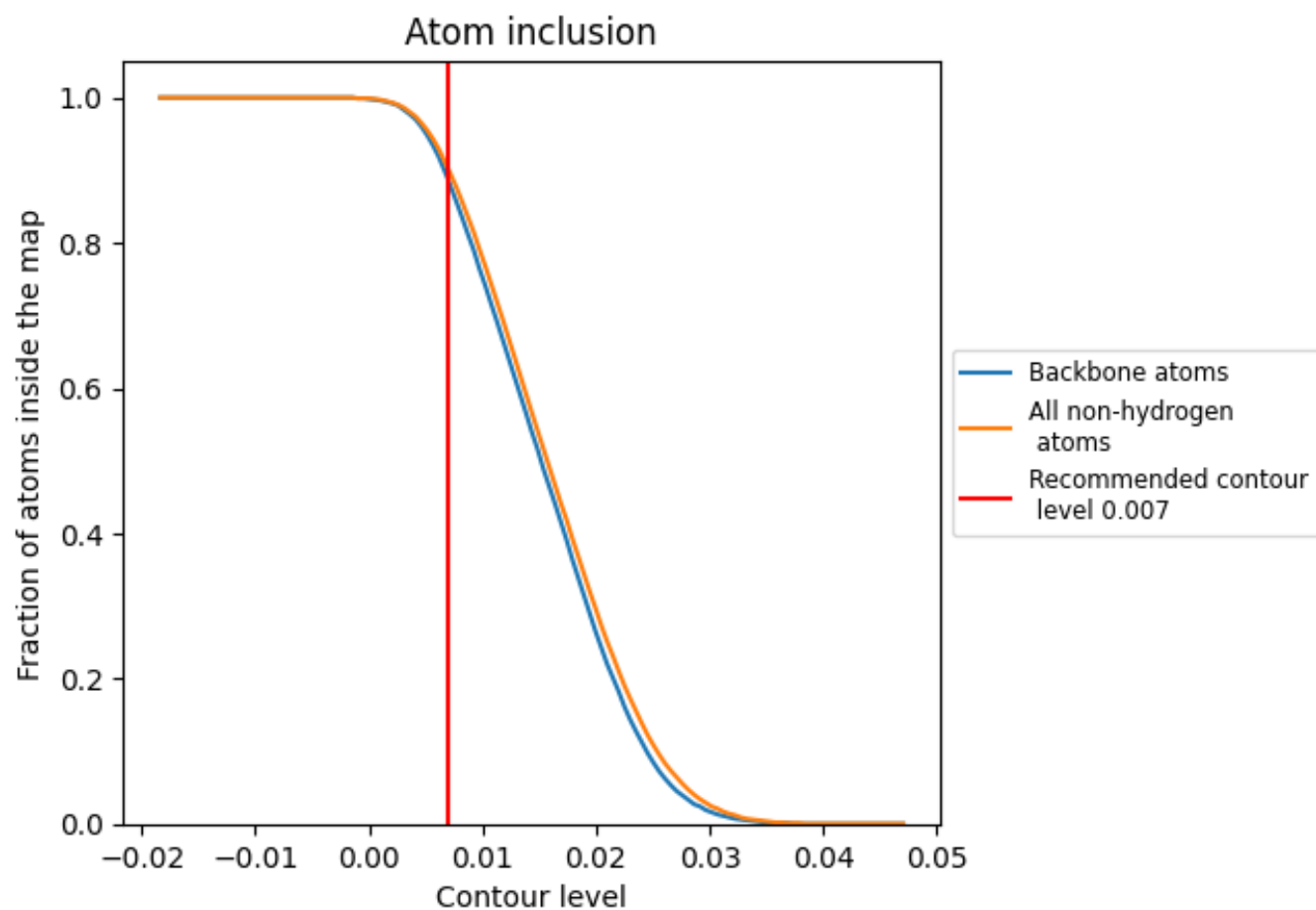
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.007).



## 9.4 Atom inclusion [i](#)









































































At the recommended contour level, 89% of all backbone atoms, 90% 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 (0.007) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9020	 0.4710
2	 0.9800	 0.5140
3	 0.5890	 0.1590
4	 0.6660	 0.1740
5	 0.8140	 0.3810
A	 0.8900	 0.4550
B	 0.8250	 0.4780
C	 0.8970	 0.5090
D	 0.9290	 0.5260
E	 0.9190	 0.5220
F	 0.8990	 0.5330
G	 0.8480	 0.3680
H	 0.8170	 0.3990
I	 0.9370	 0.5410
J	 0.9300	 0.5150
K	 0.8700	 0.4510
L	 0.8570	 0.4080
M	 0.8720	 0.4630
N	 0.8950	 0.5180
O	 0.8790	 0.4400
P	 0.8890	 0.4940
Q	 0.8730	 0.4980
R	 0.9140	 0.5320
S	 0.8530	 0.4450
T	 0.8430	 0.4270
U	 0.8880	 0.4560
V	 0.8960	 0.4890
W	 0.8620	 0.4450
X	 0.7770	 0.3680
Y	 0.4340	 0.1830
Z	 0.8610	 0.4540
a	 0.8620	 0.4140
c	 0.5430	 0.2660
d	 0.6940	 0.2830
e	 0.1140	 0.2440

