



wwPDB EM Validation Summary Report ⓘ

Mar 6, 2026 – 10:13 AM UTC

PDB ID : 8P03 / pdb_00008p03
EMDB ID : EMD-17329
Title : 48S late-stage initiation complex with m6A mRNA
Authors : Guca, E.; Lima, L.H.F.; Boissier, F.; Hashem, Y.
Deposited on : 2023-05-09
Resolution : 3.04 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

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:

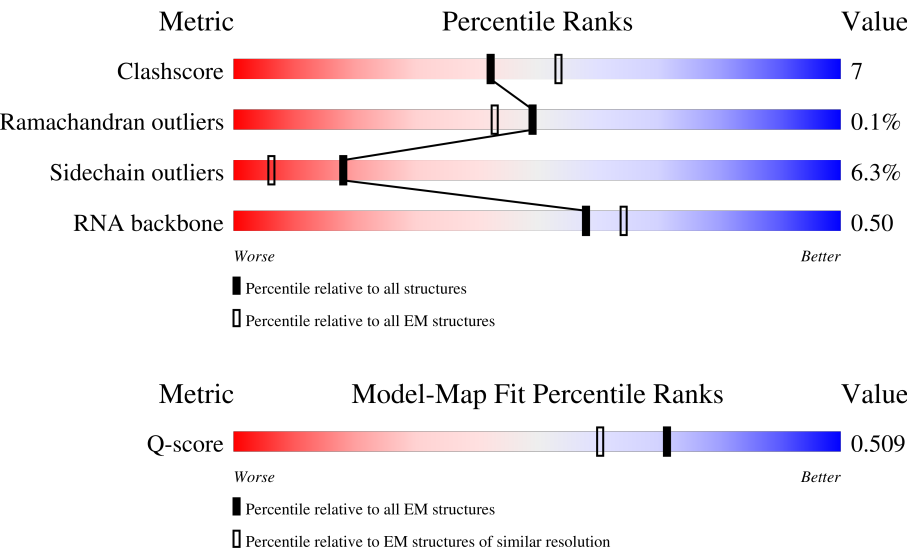
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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 3.04 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	13952 (2.54 - 3.54)

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	1	75	
2	2	1863	
3	3	9	

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Mol	Chain	Length	Quality of chain
4	A	284	
5	C	207	
6	D	215	
7	E	270	
8	F	227	
9	G	263	
10	H	191	
11	I	237	
12	J	190	
13	K	206	
14	L	194	
15	M	98	
16	N	158	
17	O	132	
18	P	150	
19	Q	151	
20	R	145	
21	S	141	
22	T	135	
23	U	152	
24	V	141	
25	W	119	
26	X	83	
27	Y	130	
28	Z	143	

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Mol	Chain	Length	Quality of chain
29	a	133	 5% 85% 8% • 5%
30	b	115	 68% 17% • 14%
31	c	84	 7% 83% 15% •
32	d	69	 62% 29% • 7%
33	e	56	 80% 14% 5%
34	f	71	 41% 69% 30% •
35	g	313	 79% 19% •
36	i	133	 8% 38% 5% • 56%
37	j	111	 28% 65% 28% 5% •
38	k	595	 98% 77% 21% •
39	l	25	 20% 64% 36%
40	n	124	 6% 45% 15% • 40%

2 Entry composition

There are 41 unique types of molecules in this entry. The entry contains 86276 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 initiator methionylated tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	75	Total	C	N	O	P	0	0
			1614	722	299	519	74		

- Molecule 2 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	1743	Total	C	N	O	P	0	0
			37193	16605	6660	12186	1742		

- Molecule 3 is a RNA chain called m6A-methylated mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	9	Total	C	N	O	P	0	0
			193	87	36	61	9		

- Molecule 4 is a protein called Eukaryotic translation initiation factor 2 subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	266	Total	C	N	O	S	0	0
			2146	1354	376	405	11		

- Molecule 5 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	207	Total	C	N	O	S	0	0
			1637	1042	288	299	8		

- Molecule 6 is a protein called ribosomal protein eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	D	215	Total	C	N	O	S	0	0
			1741	1107	309	310	15		

- Molecule 7 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	E	226	Total	C	N	O	S	0	0
			1754	1139	298	310	7		

- Molecule 8 is a protein called Ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	F	227	Total	C	N	O	S	0	0
			1764	1124	317	315	8		

- Molecule 9 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	G	263	Total	C	N	O	S	0	0
			2083	1329	385	359	10		

- Molecule 10 is a protein called Ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	H	187	Total	C	N	O	S	0	0
			1482	928	279	268	7		

- Molecule 11 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	I	237	Total	C	N	O	S	0	0
			1924	1199	387	331	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	130	THR	PRO	conflict	UNP A0A5K1UJS7

- Molecule 12 is a protein called ribosomal protein eS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	J	190	Total	C	N	O	S	0	0
			1530	975	281	273	1		

- Molecule 13 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	K	206	Total	C	N	O	S	0	0
			1680	1054	329	292	5		

- Molecule 14 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	L	188	Total	C	N	O	S	0	0
			1542	979	309	251	3		

- Molecule 15 is a protein called 40S ribosomal protein eS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	M	98	Total	C	N	O	S	0	0
			828	539	148	135	6		

- Molecule 16 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	N	158	Total	C	N	O	S	0	0
			1296	827	241	221	7		

- Molecule 17 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	O	124	Total	C	N	O	S	0	0
			958	600	170	179	9		

- Molecule 18 is a protein called ribosomal protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	P	150	Total	C	N	O	S	0	0
			1208	773	229	205	1		

- Molecule 19 is a protein called 40S ribosomal protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Q	136	Total	C	N	O	S	0	0
			1016	621	199	190	6		

- Molecule 20 is a protein called 40S ribosomal protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	R	140	Total	C	N	O	S	0	0
			1154	733	219	195	7		

- Molecule 21 is a protein called 40S ribosomal protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	S	141	Total	C	N	O	S	0	0
			1124	715	212	194	3		

- Molecule 22 is a protein called 40S ribosomal protein eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	T	126	Total	C	N	O	S	0	0
			1019	639	188	187	5		

- Molecule 23 is a protein called 40S ribosomal protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	U	145	Total	C	N	O	S	0	0
			1194	747	243	203	1		

- Molecule 24 is a protein called 40S ribosomal protein eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	V	141	Total	C	N	O	S	0	0
			1113	701	213	196	3		

- Molecule 25 is a protein called 40S ribosomal protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	W	104	Total	C	N	O	S	0	0
			822	514	156	148	4		

- Molecule 26 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	X	83	Total	C	N	O	S	0	0
			636	393	117	121	5		

- Molecule 27 is a protein called Ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Y	129	Total	C	N	O	S	0	0
			1034	659	193	176	6		

- Molecule 28 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Z	142	Total	C	N	O	S	0	0
			1106	698	220	184	4		

- Molecule 29 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	a	126	Total	C	N	O	S	0	0
			1021	645	198	173	5		

- Molecule 30 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	b	99	Total	C	N	O	S	0	0
			789	491	162	130	6		

- Molecule 31 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	c	84	Total	C	N	O	S	0	0
			659	413	122	116	8		

- Molecule 32 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	d	64	Total	C	N	O	S	0	0
			506	308	102	94	2		

- Molecule 33 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	e	53	Total	C	N	O	S	0	0
			444	278	90	71	5		

- Molecule 34 is a protein called ribosomal protein eS31.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	f	71	Total	C	N	O	S	0	0
			582	367	109	99	7		

- Molecule 35 is a protein called Ribosomal protein RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	g	313	Total	C	N	O	S	0	0
			2437	1535	424	466	12		

- Molecule 36 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	i	58	Total	C	N	O	S	0	0
			464	287	102	74	1		

- Molecule 37 is a protein called Eukaryotic translation initiation factor 4C.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	j	108	Total	C	N	O	S	0	0
			874	543	166	161	4		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
j	39	ILE	VAL	conflict	UNP G1SYS4
j	76	ILE	VAL	conflict	UNP G1SYS4

- Molecule 38 is a protein called ATP binding cassette subfamily E member 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	k	595	Total	C	N	O	S	0	0
			4693	2995	802	865	31		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
k	538	ILE	VAL	conflict	UNP G1SG72

- Molecule 39 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	1	25	Total	C	N	O	S	0	0
			240	145	64	28	3		

- Molecule 40 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	n	75	Total	C	N	O	S	0	0
			598	382	111	104	1		

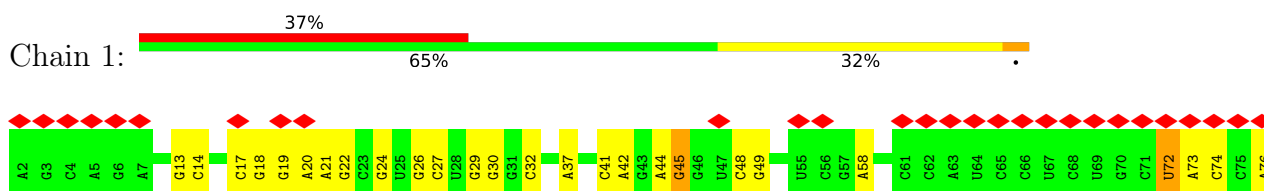
- Molecule 41 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
41	2	175	Total	Mg	0
			175	175	
41	3	1	Total	Mg	0
			1	1	
41	I	1	Total	Mg	0
			1	1	
41	Z	1	Total	Mg	0
			1	1	

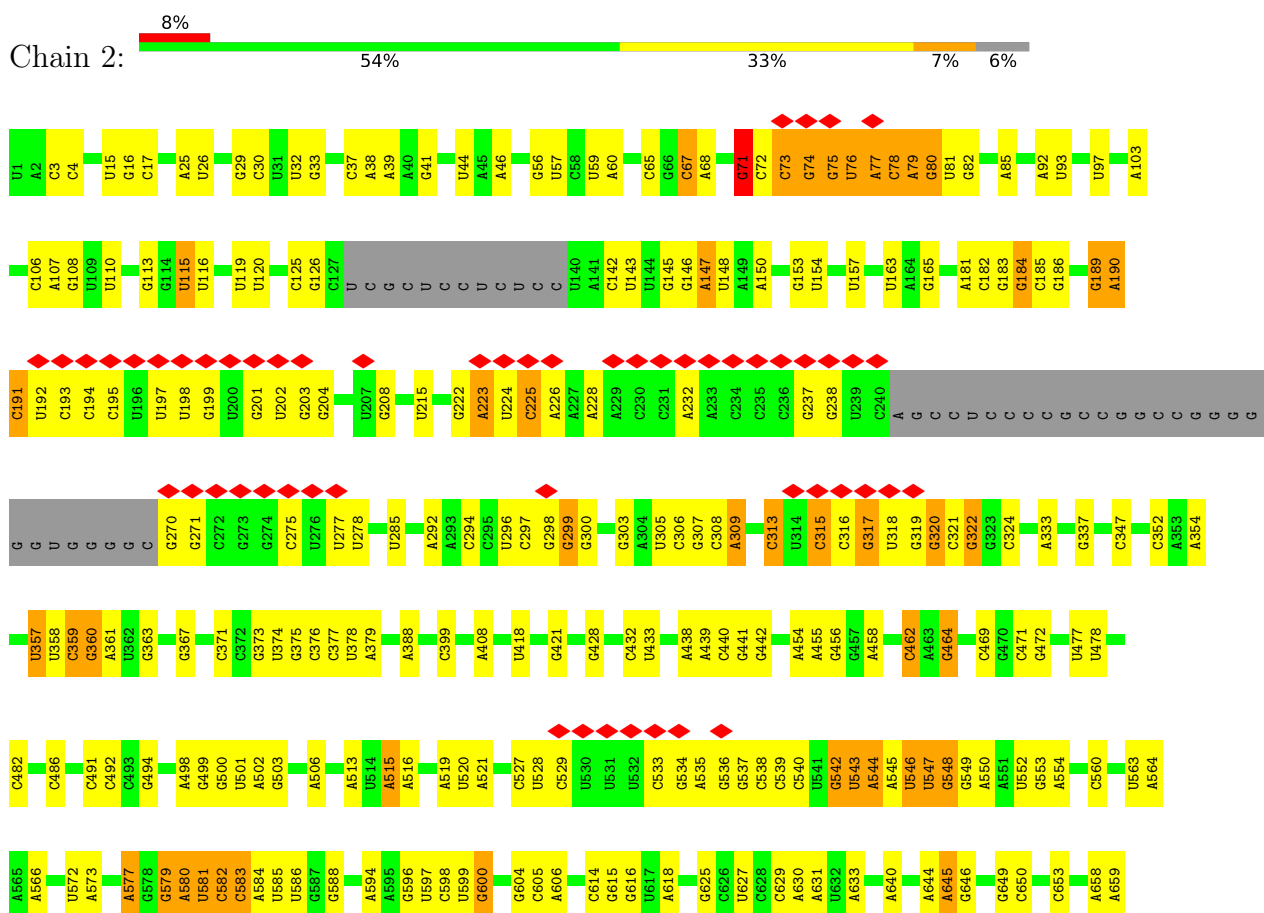
3 Residue-property plots

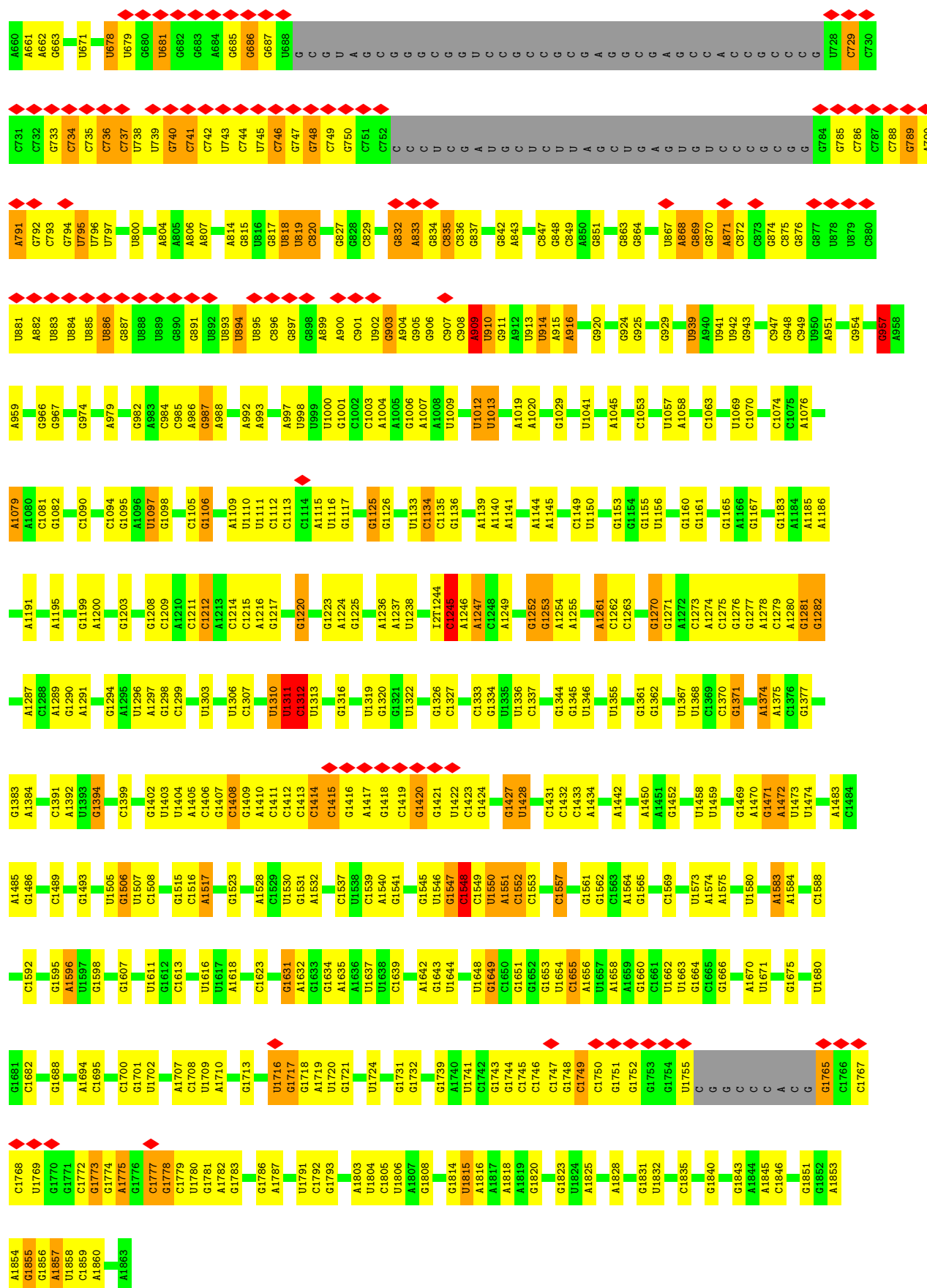
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: initiator methionylated tRNA

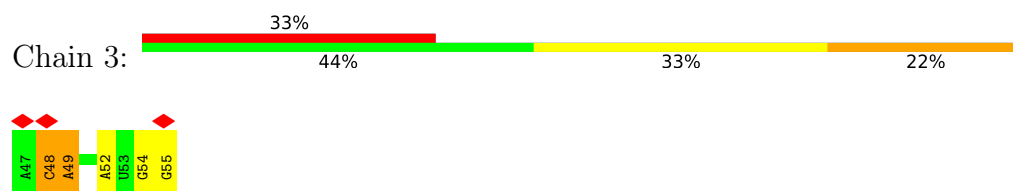


- Molecule 2: 18S ribosomal RNA

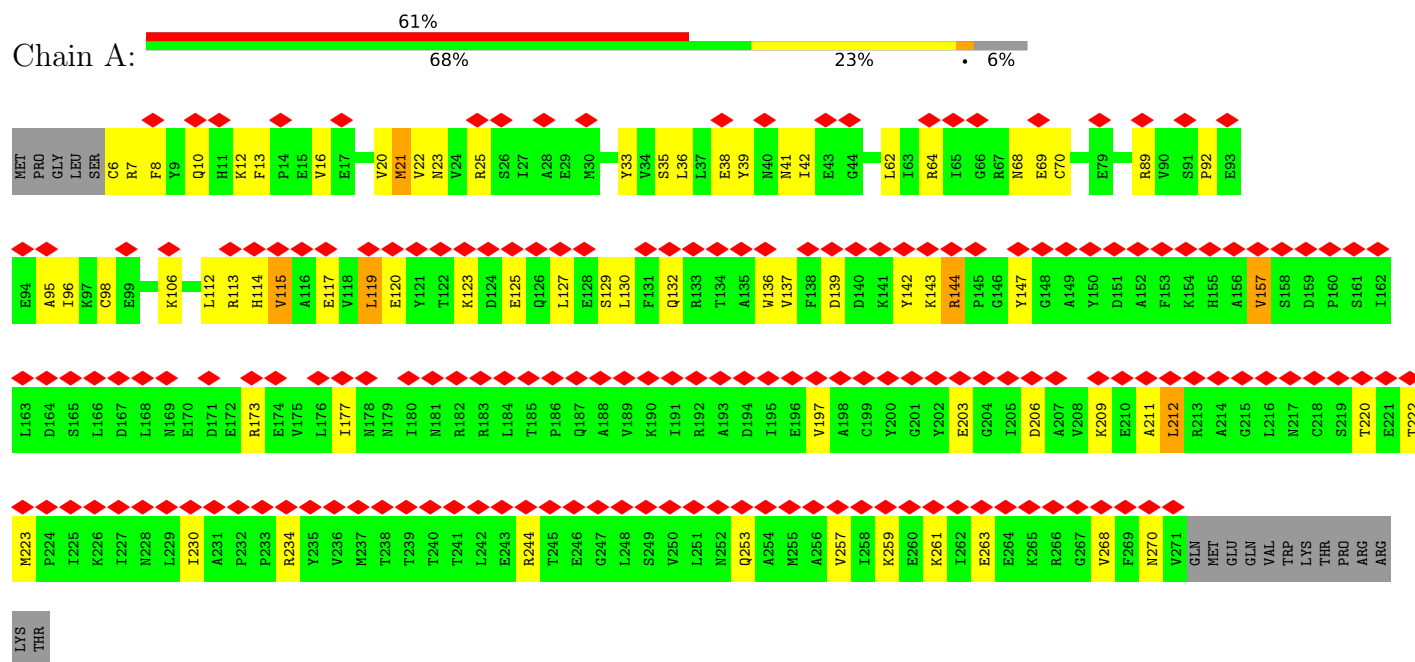




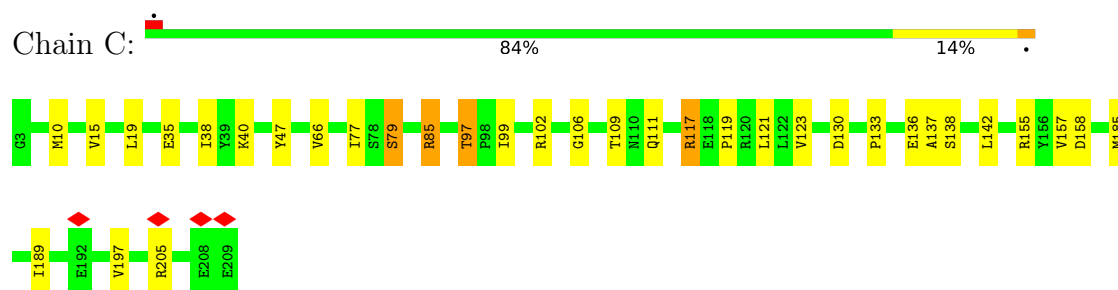
- Molecule 3: m6A-methylated mRNA



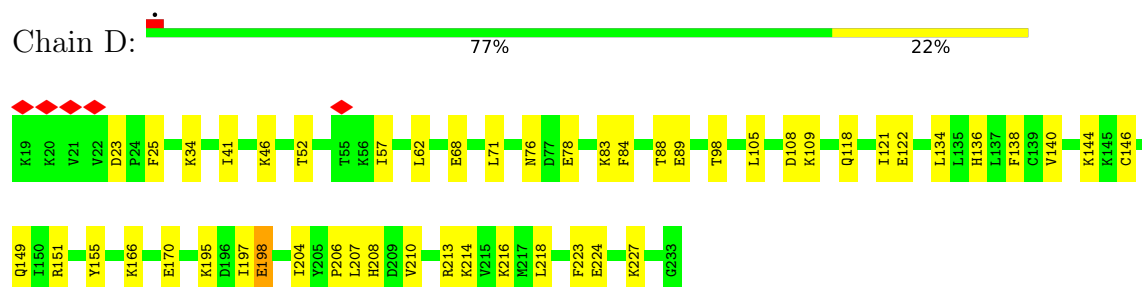
- Molecule 4: Eukaryotic translation initiation factor 2 subunit 1



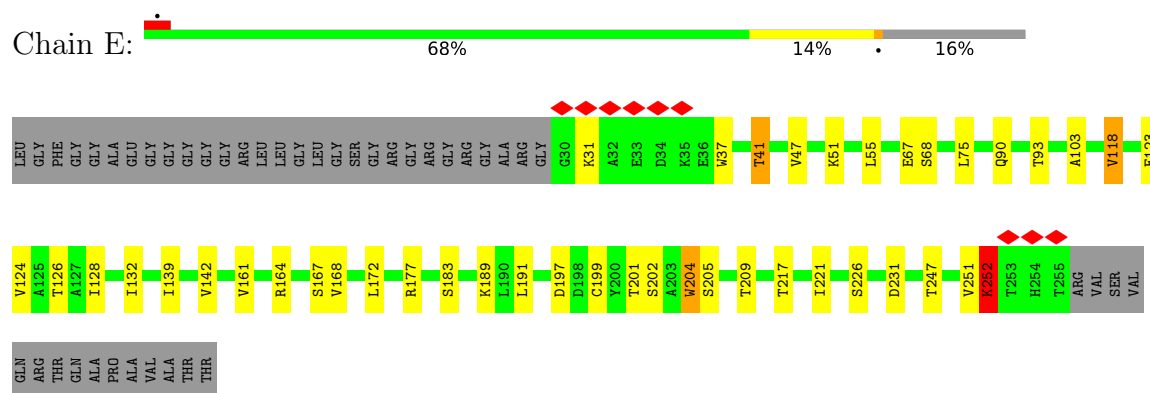
- Molecule 5: 40S ribosomal protein SA



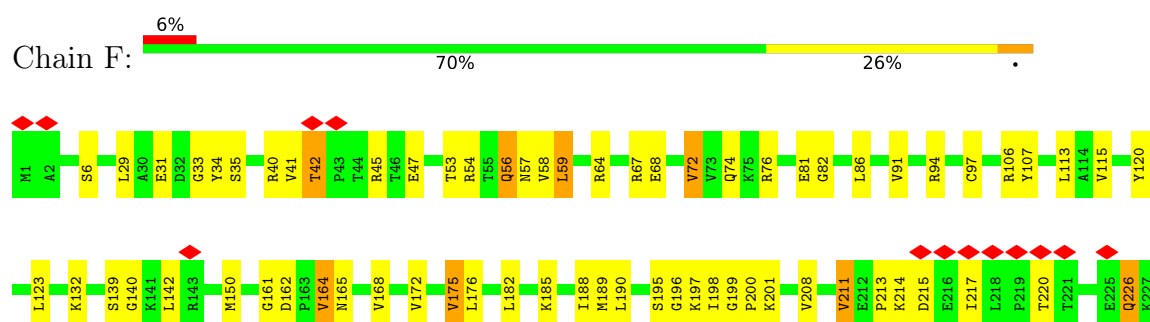
- Molecule 6: ribosomal protein eS1



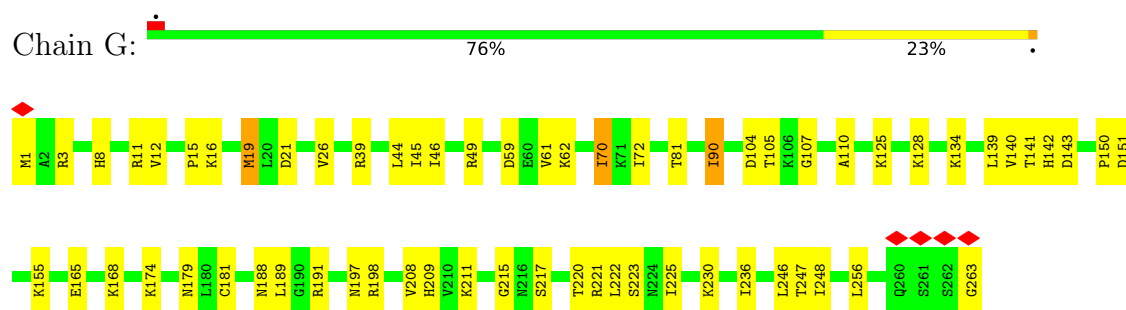
- Molecule 7: 40S ribosomal protein S2



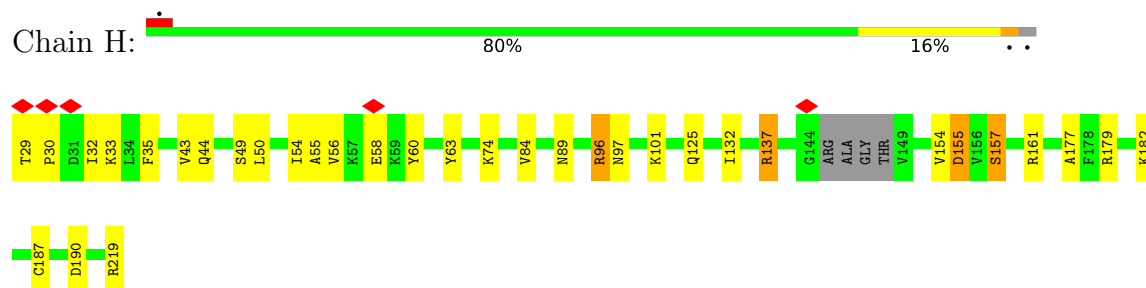
- Molecule 8: Ribosomal protein S3



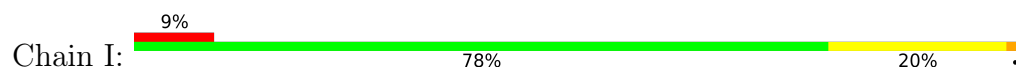
- Molecule 9: 40S ribosomal protein S4

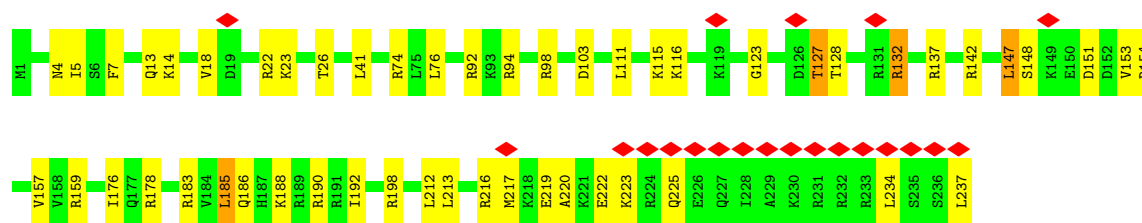


- Molecule 10: Ribosomal protein S5

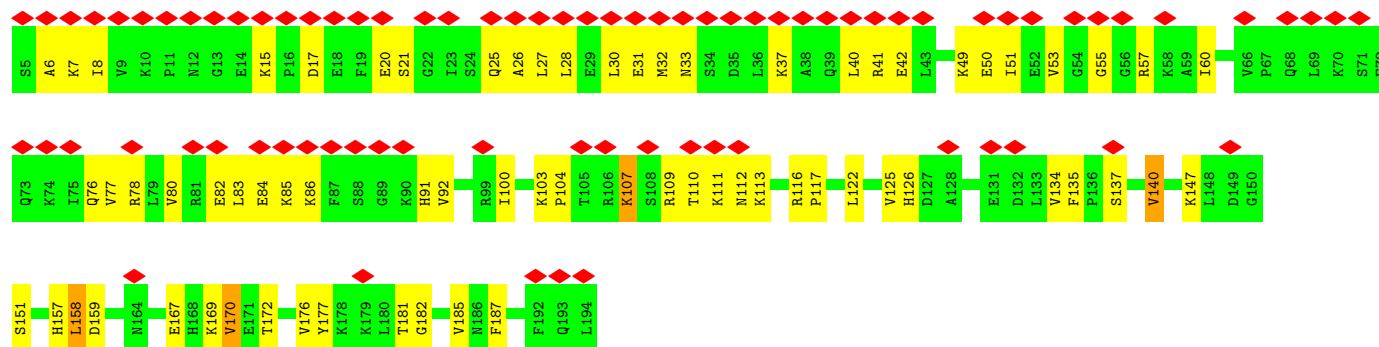
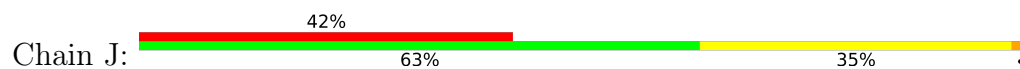


- Molecule 11: 40S ribosomal protein S6

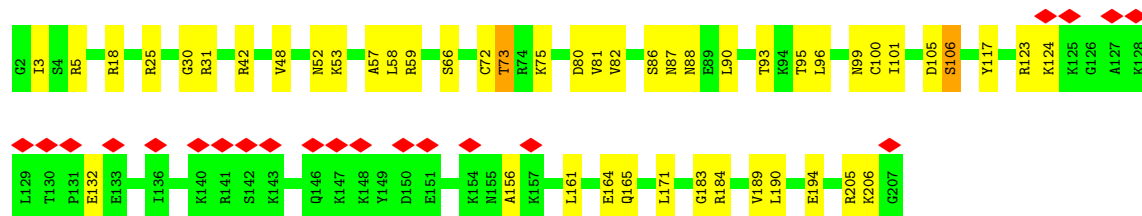
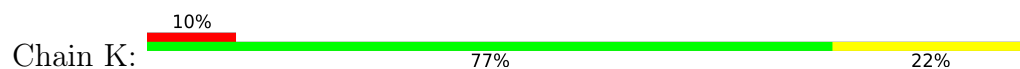




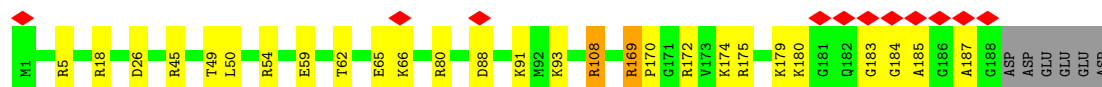
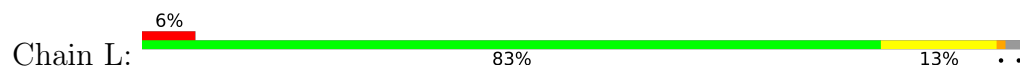
• Molecule 12: ribosomal protein eS7



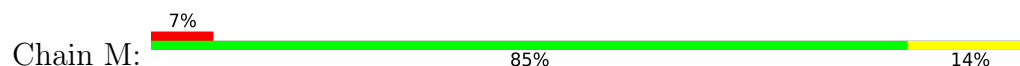
• Molecule 13: 40S ribosomal protein S8



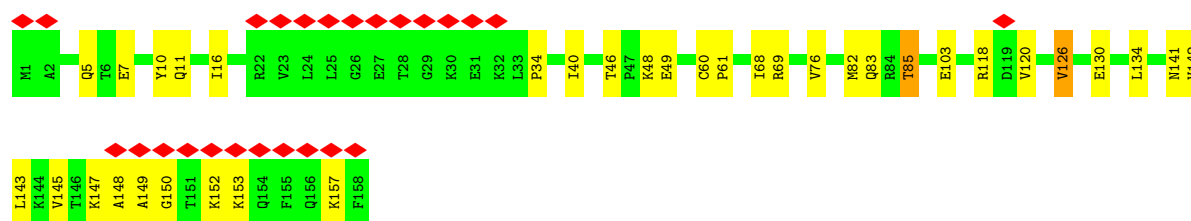
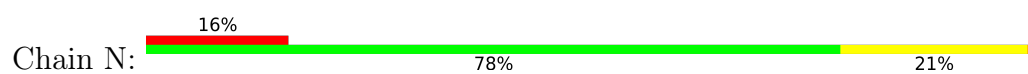
• Molecule 14: 40S ribosomal protein S9



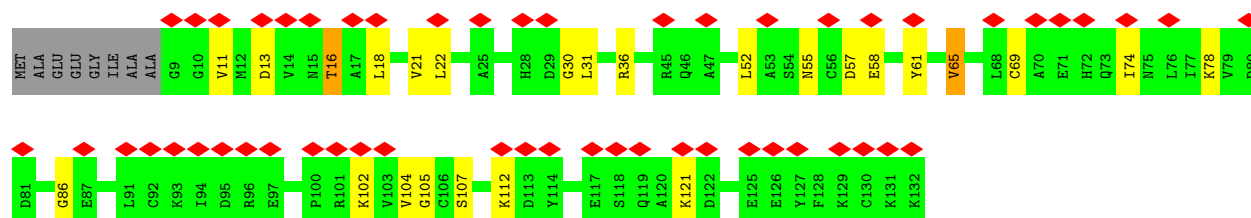
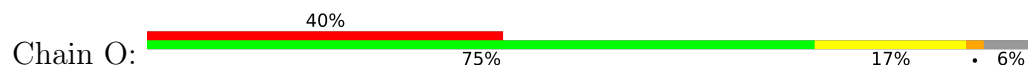
• Molecule 15: 40S ribosomal protein eS10



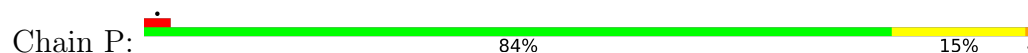
• Molecule 16: 40S ribosomal protein S11



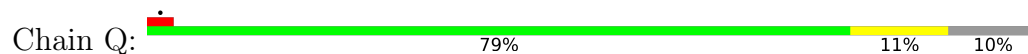
- Molecule 17: 40S ribosomal protein S12



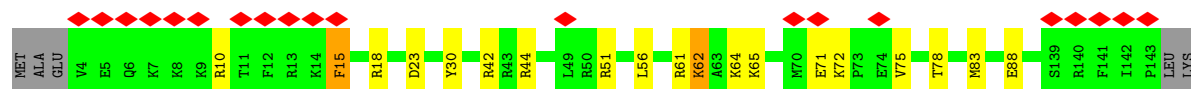
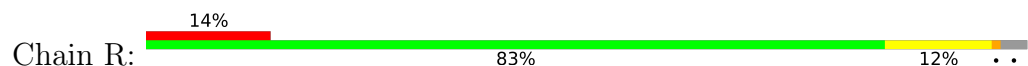
- Molecule 18: ribosomal protein uS15



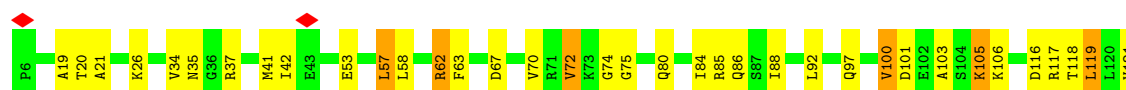
- Molecule 19: 40S ribosomal protein uS11



- Molecule 20: 40S ribosomal protein uS19

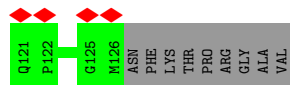
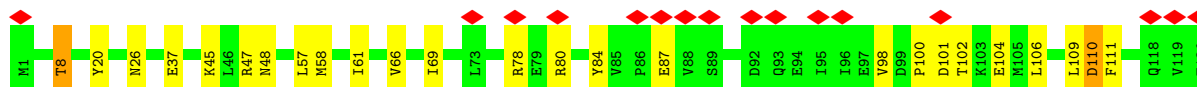
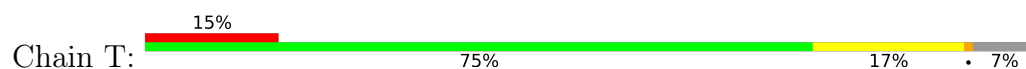


- Molecule 21: 40S ribosomal protein uS9

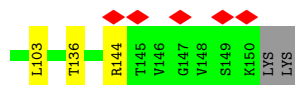
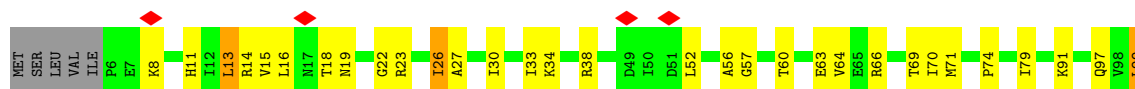
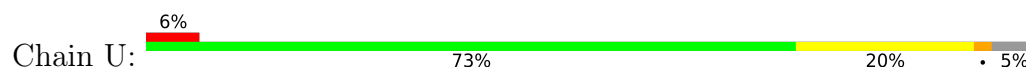




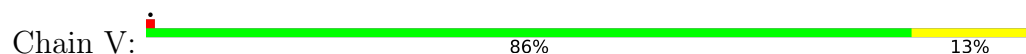
- Molecule 22: 40S ribosomal protein eS17



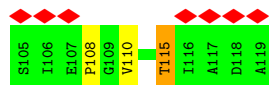
- Molecule 23: 40S ribosomal protein uS13



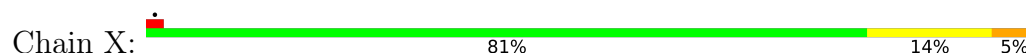
- Molecule 24: 40S ribosomal protein eS19



- Molecule 25: 40S ribosomal protein uS10

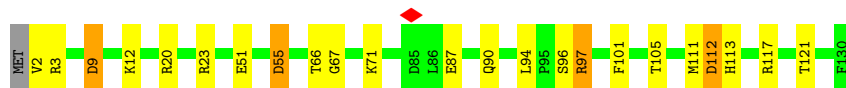
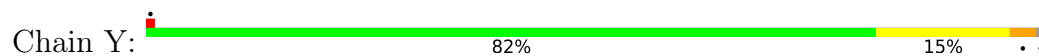


- Molecule 26: 40S ribosomal protein S21

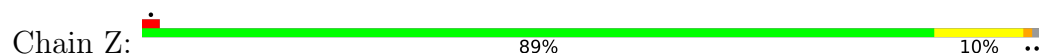




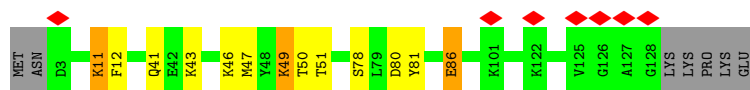
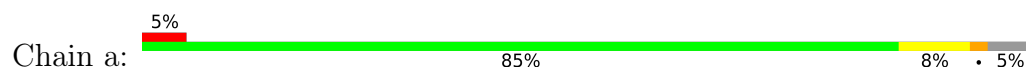
- Molecule 27: Ribosomal protein S15a



- Molecule 28: 40S ribosomal protein S23



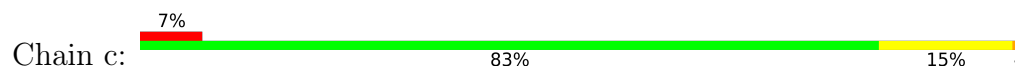
- Molecule 29: 40S ribosomal protein S24



- Molecule 30: 40S ribosomal protein S26



- Molecule 31: 40S ribosomal protein S27

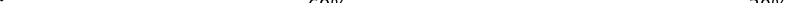


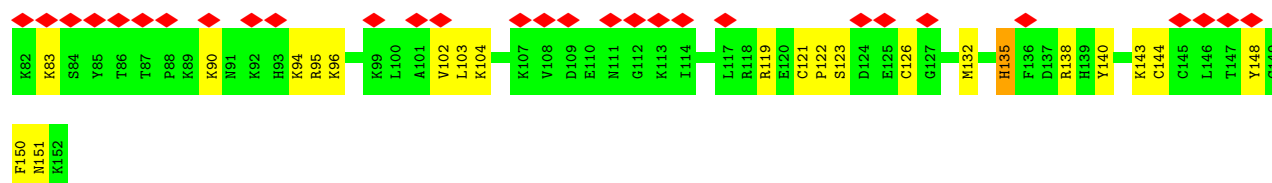
- Molecule 32: 40S ribosomal protein S28



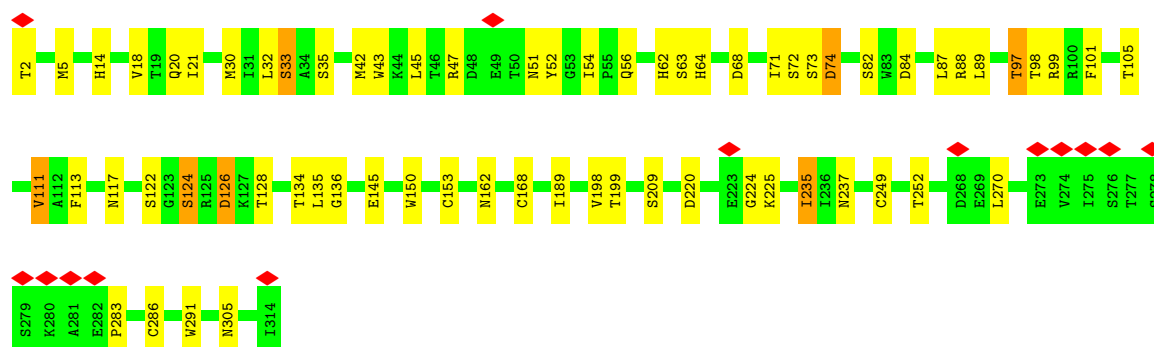
- Molecule 33: 40S ribosomal protein S29

Sequence logo for position 4. The y-axis represents information content in bits, ranging from 0 to 1.5. The x-axis shows amino acids: MET, GLY, HIS, Q4, H10, F14, R32, K33, Y34, F52, L55, D56. The Q4 position has a prominent red diamond above it, indicating a high information content.

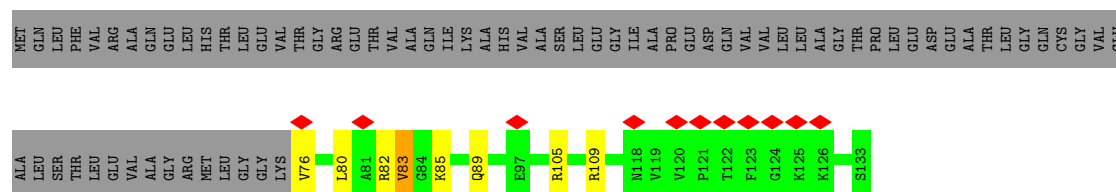
- Chain f:  41% 69% 30%

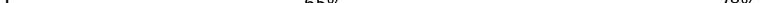


- Chain g:

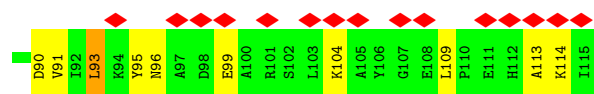


- Chain i: 

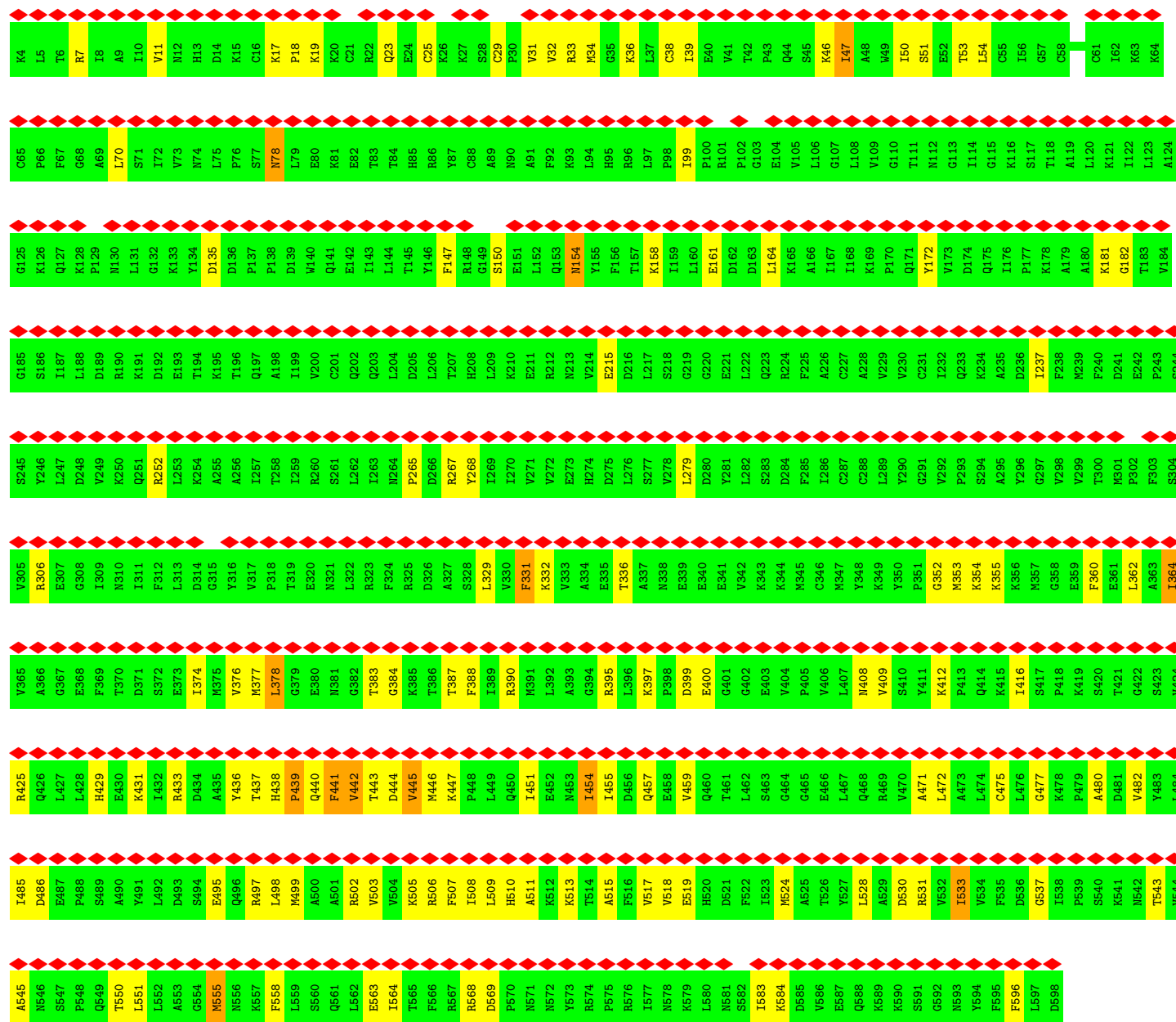
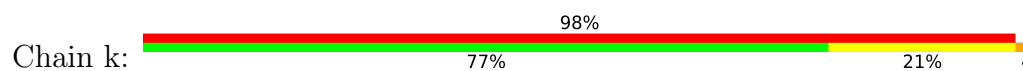


- Chain j: 



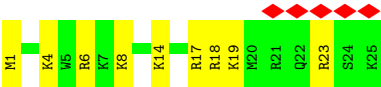


- Molecule 38: ATP binding cassette subfamily E member 1

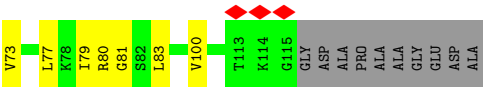
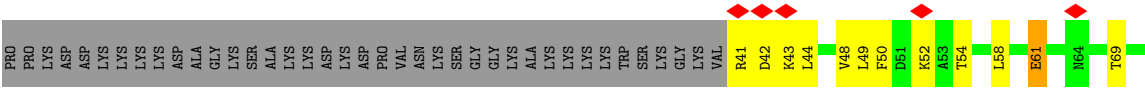


- Molecule 39: 60S ribosomal protein L41





• Molecule 40: 40S ribosomal protein S25



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	103050	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.161	Depositor
Minimum map value	-0.080	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	422.40002, 422.40002, 422.40002	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: I2T, MG, MA6, T6A

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	1	0.61	1/1770 (0.1%)	0.93	4/2759 (0.1%)
2	2	0.48	7/41554 (0.0%)	0.66	62/64761 (0.1%)
3	3	0.77	0/188	1.22	1/288 (0.3%)
4	A	0.53	0/2177	0.95	4/2935 (0.1%)
5	C	0.59	0/1674	1.00	2/2275 (0.1%)
6	D	0.35	0/1769	0.66	0/2367
7	E	0.38	0/1794	0.70	1/2430 (0.0%)
8	F	0.23	0/1792	0.46	1/2412 (0.0%)
9	G	0.22	0/2125	0.48	0/2856
10	H	0.44	0/1503	0.79	3/2020 (0.1%)
11	I	0.42	0/1946	0.79	2/2588 (0.1%)
12	J	0.33	0/1553	0.73	1/2079 (0.0%)
13	K	0.53	0/1709	0.95	2/2278 (0.1%)
14	L	0.50	0/1567	0.88	1/2092 (0.0%)
15	M	0.51	0/852	0.99	3/1147 (0.3%)
16	N	0.36	0/1319	0.65	0/1761
17	O	0.60	0/968	1.02	0/1296
18	P	0.45	0/1232	0.83	1/1656 (0.1%)
19	Q	0.63	0/1029	1.14	1/1380 (0.1%)
20	R	0.75	0/1177	1.27	5/1571 (0.3%)
21	S	0.32	0/1142	0.56	2/1528 (0.1%)
22	T	0.49	0/1031	0.90	2/1383 (0.1%)
23	U	0.36	0/1212	0.71	1/1621 (0.1%)
24	V	0.53	0/1133	0.93	1/1517 (0.1%)
25	W	0.23	0/832	0.48	0/1117
26	X	0.35	0/643	0.68	0/860
27	Y	0.54	0/1051	0.97	2/1406 (0.1%)
28	Z	0.35	0/1124	0.67	0/1500
29	a	0.69	0/1038	1.18	3/1380 (0.2%)
30	b	0.59	0/802	1.01	2/1076 (0.2%)
31	c	0.52	0/673	1.01	2/902 (0.2%)
32	d	0.29	0/508	0.67	0/680

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	e	0.61	0/454	1.12	0/603
34	f	0.36	0/594	0.68	0/786
35	g	0.37	0/2494	0.75	1/3394 (0.0%)
36	i	0.70	0/469	1.17	1/617 (0.2%)
37	j	0.40	0/884	0.77	1/1175 (0.1%)
38	k	0.59	0/4780	1.03	6/6452 (0.1%)
39	l	0.20	0/241	0.44	0/305
40	n	0.49	0/604	1.00	2/810 (0.2%)
All	All	0.48	8/91407 (0.0%)	0.77	120/132063 (0.1%)

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
1	1	0	9
2	2	0	94
3	3	0	1
4	A	0	1
5	C	0	1
10	H	0	1
11	I	0	2
13	K	0	2
14	L	0	1
18	P	0	1
19	Q	0	1
20	R	0	3
22	T	0	1
36	i	0	1
37	j	0	2
38	k	0	3
All	All	0	124

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	72	U	O3'-P	-12.68	1.42	1.61
2	2	1245	C	O3'-P	-8.61	1.48	1.61
2	2	270	G	P-OP1	6.27	1.61	1.49
2	2	1724	U	P-OP1	6.25	1.61	1.49
2	2	1765	G	P-OP1	6.24	1.61	1.49

The worst 5 of 120 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	72	U	OP2-P-O3'	-29.25	20.25	108.00
2	2	1515	G	C4'-C3'-O3'	-9.39	98.91	113.00
2	2	270	G	P-O5'-C5'	-9.37	106.84	120.90
2	2	1765	G	P-O5'-C5'	-9.37	106.85	120.90
1	1	72	U	OP1-P-O3'	8.18	132.54	108.00

There are no chirality outliers.

5 of 124 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	24	G	Sidechain
1	1	26	G	Sidechain
1	1	27	C	Sidechain
1	1	29	G	Sidechain
1	1	32	C	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1614	0	816	0	0
2	2	37193	0	18709	391	0
3	3	193	0	100	1	0
4	A	2146	0	2191	37	0
5	C	1637	0	1641	18	0
6	D	1741	0	1815	30	0
7	E	1754	0	1834	27	0
8	F	1764	0	1863	38	0
9	G	2083	0	2189	40	0
10	H	1482	0	1534	20	0
11	I	1924	0	2088	31	0
12	J	1530	0	1627	48	0
13	K	1680	0	1762	22	0
14	L	1542	0	1659	19	0
15	M	828	0	854	8	0
16	N	1296	0	1374	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	O	958	0	993	17	0
18	P	1208	0	1294	12	0
19	Q	1016	0	1039	9	0
20	R	1154	0	1213	6	0
21	S	1124	0	1193	24	0
22	T	1019	0	1075	15	0
23	U	1194	0	1253	24	0
24	V	1113	0	1149	10	0
25	W	822	0	887	13	0
26	X	636	0	637	10	0
27	Y	1034	0	1080	13	0
28	Z	1106	0	1179	11	0
29	a	1021	0	1085	6	0
30	b	789	0	837	10	0
31	c	659	0	683	8	0
32	d	506	0	536	10	0
33	e	444	0	442	5	0
34	f	582	0	599	18	0
35	g	2437	0	2393	33	0
36	i	464	0	511	4	0
37	j	874	0	893	18	0
38	k	4693	0	4826	81	0
39	l	240	0	289	5	0
40	n	598	0	656	15	0
41	2	175	0	0	0	0
41	3	1	0	0	0	0
41	I	1	0	0	0	0
41	Z	1	0	0	0	0
All	All	86276	0	68798	1010	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.

The worst 5 of 1010 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:874:G:N1	2:2:904:A:H2	1.35	1.23
2:2:874:G:N1	2:2:904:A:C2	2.09	1.13
7:E:247:THR:O	7:E:251:VAL:HG23	1.62	0.99
2:2:1098:G:H1	2:2:1126:G:H22	1.00	0.99
2:2:1416:G:N2	2:2:1423:C:O2	2.02	0.92

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	
4	A	264/284 (93%)	237 (90%)	27 (10%)	0	100	100
5	C	205/207 (99%)	184 (90%)	21 (10%)	0	100	100
6	D	213/215 (99%)	188 (88%)	25 (12%)	0	100	100
7	E	224/270 (83%)	209 (93%)	14 (6%)	1 (0%)	30	61
8	F	225/227 (99%)	206 (92%)	19 (8%)	0	100	100
9	G	261/263 (99%)	241 (92%)	20 (8%)	0	100	100
10	H	183/191 (96%)	169 (92%)	14 (8%)	0	100	100
11	I	235/237 (99%)	224 (95%)	11 (5%)	0	100	100
12	J	188/190 (99%)	162 (86%)	26 (14%)	0	100	100
13	K	204/206 (99%)	182 (89%)	22 (11%)	0	100	100
14	L	186/194 (96%)	174 (94%)	12 (6%)	0	100	100
15	M	96/98 (98%)	89 (93%)	7 (7%)	0	100	100
16	N	156/158 (99%)	150 (96%)	6 (4%)	0	100	100
17	O	122/132 (92%)	98 (80%)	24 (20%)	0	100	100
18	P	148/150 (99%)	143 (97%)	5 (3%)	0	100	100
19	Q	134/151 (89%)	118 (88%)	16 (12%)	0	100	100
20	R	138/145 (95%)	122 (88%)	16 (12%)	0	100	100
21	S	139/141 (99%)	130 (94%)	9 (6%)	0	100	100
22	T	124/135 (92%)	110 (89%)	14 (11%)	0	100	100
23	U	143/152 (94%)	131 (92%)	12 (8%)	0	100	100
24	V	139/141 (99%)	132 (95%)	7 (5%)	0	100	100
25	W	102/119 (86%)	97 (95%)	5 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	X	81/83 (98%)	74 (91%)	7 (9%)	0	100	100
27	Y	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
28	Z	140/143 (98%)	127 (91%)	13 (9%)	0	100	100
29	a	124/133 (93%)	107 (86%)	16 (13%)	1 (1%)	16	46
30	b	97/115 (84%)	91 (94%)	6 (6%)	0	100	100
31	c	82/84 (98%)	70 (85%)	11 (13%)	1 (1%)	10	37
32	d	62/69 (90%)	57 (92%)	5 (8%)	0	100	100
33	e	51/56 (91%)	48 (94%)	3 (6%)	0	100	100
34	f	69/71 (97%)	56 (81%)	13 (19%)	0	100	100
35	g	311/313 (99%)	284 (91%)	26 (8%)	1 (0%)	36	67
36	i	56/133 (42%)	49 (88%)	7 (12%)	0	100	100
37	j	106/111 (96%)	98 (92%)	8 (8%)	0	100	100
38	k	593/595 (100%)	516 (87%)	76 (13%)	1 (0%)	43	73
39	l	23/25 (92%)	23 (100%)	0	0	100	100
40	n	73/124 (59%)	68 (93%)	5 (7%)	0	100	100
All	All	5824/6191 (94%)	5286 (91%)	533 (9%)	5 (0%)	49	78

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	E	252	LYS
38	k	439	PRO
35	g	283	PRO
29	a	86	GLU
31	c	39	GLY

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	
4	A	238/255 (93%)	221 (93%)	17 (7%)	13	40
5	C	173/173 (100%)	162 (94%)	11 (6%)	16	44
6	D	196/196 (100%)	191 (97%)	5 (3%)	40	69
7	E	190/214 (89%)	173 (91%)	17 (9%)	9	32
8	F	190/190 (100%)	170 (90%)	20 (10%)	6	25
9	G	225/225 (100%)	210 (93%)	15 (7%)	15	43
10	H	159/161 (99%)	152 (96%)	7 (4%)	25	56
11	I	207/207 (100%)	199 (96%)	8 (4%)	28	59
12	J	170/170 (100%)	164 (96%)	6 (4%)	32	62
13	K	177/177 (100%)	163 (92%)	14 (8%)	11	36
14	L	162/168 (96%)	159 (98%)	3 (2%)	50	73
15	M	89/89 (100%)	84 (94%)	5 (6%)	19	49
16	N	142/142 (100%)	134 (94%)	8 (6%)	19	49
17	O	104/108 (96%)	98 (94%)	6 (6%)	18	48
18	P	130/130 (100%)	122 (94%)	8 (6%)	16	45
19	Q	106/119 (89%)	102 (96%)	4 (4%)	29	60
20	R	126/130 (97%)	120 (95%)	6 (5%)	23	54
21	S	117/117 (100%)	106 (91%)	11 (9%)	8	29
22	T	114/121 (94%)	108 (95%)	6 (5%)	20	51
23	U	125/132 (95%)	119 (95%)	6 (5%)	23	54
24	V	113/113 (100%)	107 (95%)	6 (5%)	20	51
25	W	94/107 (88%)	84 (89%)	10 (11%)	6	24
26	X	67/67 (100%)	60 (90%)	7 (10%)	7	25
27	Y	112/113 (99%)	103 (92%)	9 (8%)	11	36
28	Z	114/115 (99%)	109 (96%)	5 (4%)	25	56
29	a	108/115 (94%)	104 (96%)	4 (4%)	30	61
30	b	87/99 (88%)	79 (91%)	8 (9%)	8	30
31	c	76/76 (100%)	74 (97%)	2 (3%)	40	69
32	d	57/62 (92%)	50 (88%)	7 (12%)	4	18
33	e	47/49 (96%)	44 (94%)	3 (6%)	16	44
34	f	64/64 (100%)	60 (94%)	4 (6%)	16	45
35	g	272/272 (100%)	249 (92%)	23 (8%)	10	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
36	i	48/106 (45%)	46 (96%)	2 (4%)	26 58
37	j	91/93 (98%)	78 (86%)	13 (14%)	3 14
38	k	523/523 (100%)	496 (95%)	27 (5%)	21 51
39	l	24/24 (100%)	21 (88%)	3 (12%)	4 18
40	n	66/102 (65%)	63 (96%)	3 (4%)	24 56
All	All	5103/5324 (96%)	4784 (94%)	319 (6%)	18 45

5 of 319 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
30	b	88	SER
38	k	25	CYS
32	d	43	ILE
35	g	122	SER
38	k	437	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 102 such sidechains are listed below:

Mol	Chain	Res	Type
23	U	42	HIS
29	a	89	HIS
38	k	572	ASN
24	V	11	GLN
27	Y	24	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	74/75 (98%)	15 (20%)	1 (1%)
2	2	1736/1863 (93%)	321 (18%)	20 (1%)
3	3	8/9 (88%)	3 (37%)	0
All	All	1818/1947 (93%)	339 (18%)	21 (1%)

5 of 339 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	13	G
1	1	14	C

Continued on next page...

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Mol	Chain	Res	Type
1	1	17	C
1	1	18	G
1	1	19	G

5 of 21 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	2	1427	G
2	2	1472	A
2	2	1855	G
2	2	1548	C
2	2	1471	G

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

3 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	$\# Z > 2$
3	MA6	3	49	3	22,25,27	0.72	0	29,36,41	1.25	3 (10%)
1	T6A	1	37	1	31,34,35	1.21	3 (9%)	43,49,52	1.48	4 (9%)
2	I2T	2	1244	2	25,29,30	0.87	2 (8%)	28,42,45	1.15	3 (10%)

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
3	MA6	3	49	3	-	2/9/27/30	0/3/3/3
1	T6A	1	37	1	-	5/23/41/42	0/3/3/3
2	I2T	2	1244	2	-	0/16/34/35	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	37	T6A	ODA-C13	4.85	1.36	1.22
2	2	1244	I2T	O36-C34	-2.68	1.22	1.30
1	1	37	T6A	C6-N6	-2.42	1.34	1.39
1	1	37	T6A	ODB-C13	-2.39	1.23	1.30
2	2	1244	I2T	C4-N3	-2.04	1.36	1.40

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	37	T6A	C12-N11-C10	5.25	130.72	121.99
3	3	49	MA6	C10-N6-C6	3.87	126.44	122.85
2	2	1244	I2T	C3'-C2'-C1'	3.32	105.61	101.69
3	3	49	MA6	C4-C5-C6	-3.30	114.03	116.78
1	1	37	T6A	O10-C10-N6	-2.95	118.39	123.64

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1	37	T6A	C14-C12-N11-C10
3	3	49	MA6	O4'-C4'-C5'-O5'
3	3	49	MA6	C3'-C4'-C5'-O5'
1	1	37	T6A	N11-C10-N6-C6
1	1	37	T6A	O10-C10-N6-C6

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 178 ligands modelled in this entry, 178 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 [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	2	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2	730:C	O3'	731:C	P	9.48

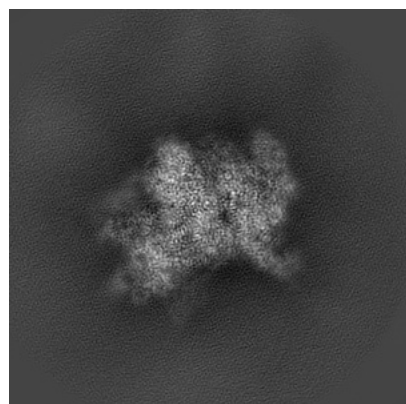
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17329. These allow visual inspection of the internal detail of the map and identification of artifacts.

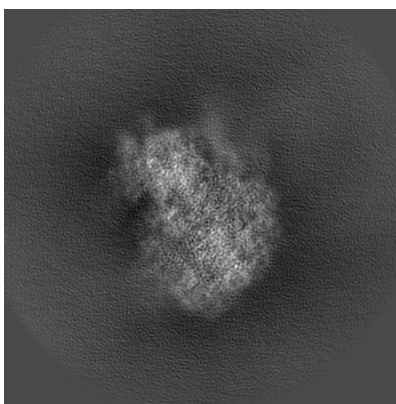
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

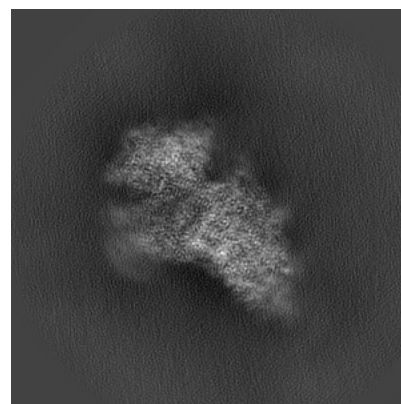
6.1.1 Primary map



X

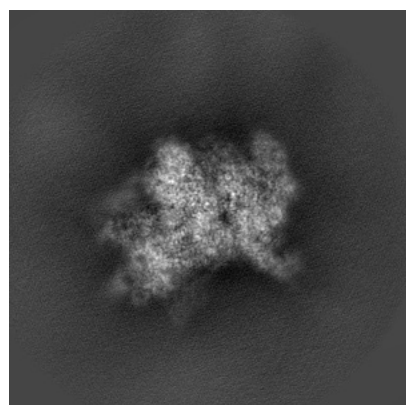


Y

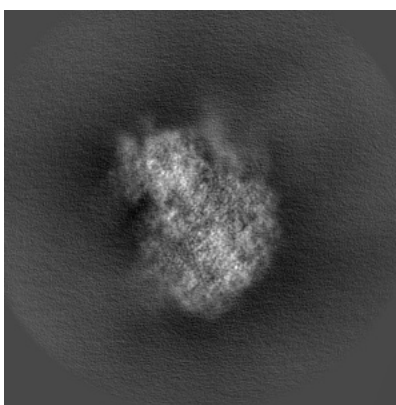


Z

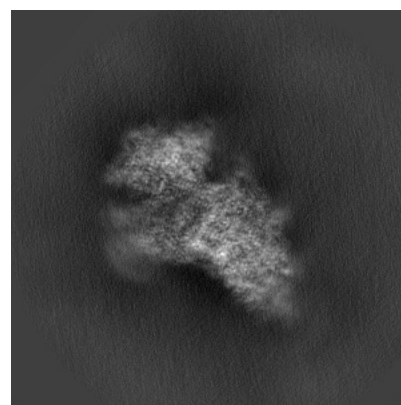
6.1.2 Raw map



X



Y

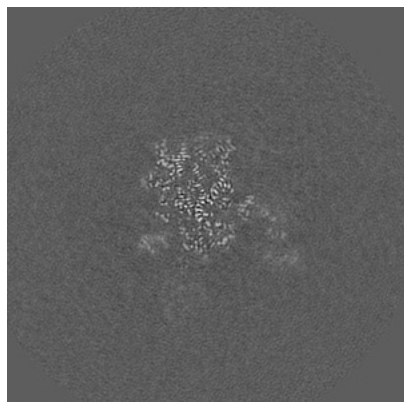


Z

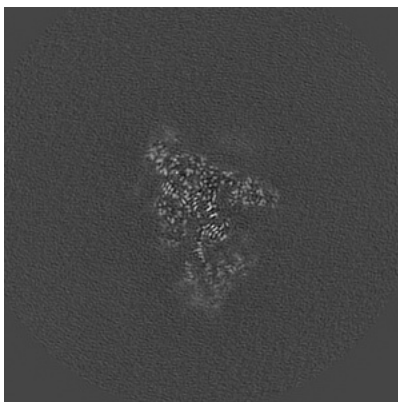
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

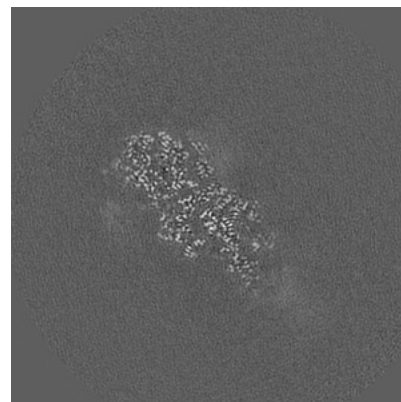
6.2.1 Primary map



X Index: 192

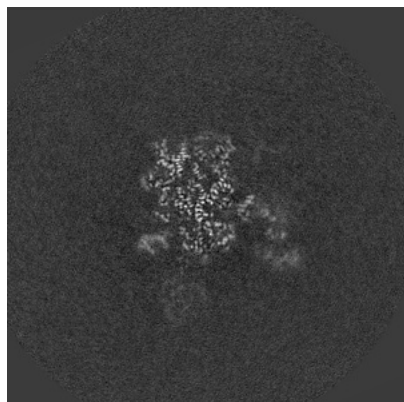


Y Index: 192

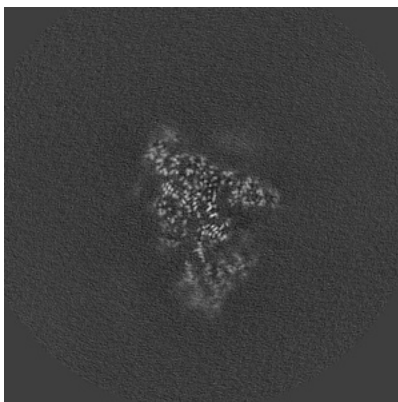


Z Index: 192

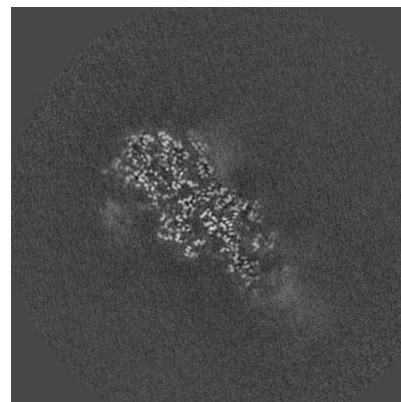
6.2.2 Raw map



X Index: 192



Y Index: 192

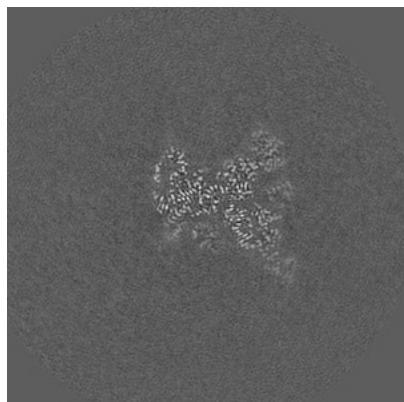


Z Index: 192

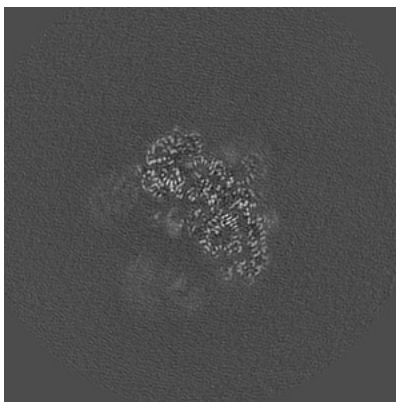
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

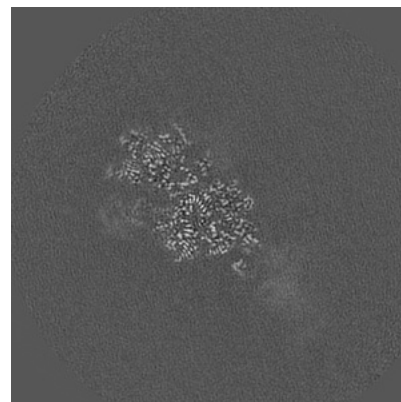
6.3.1 Primary map



X Index: 170

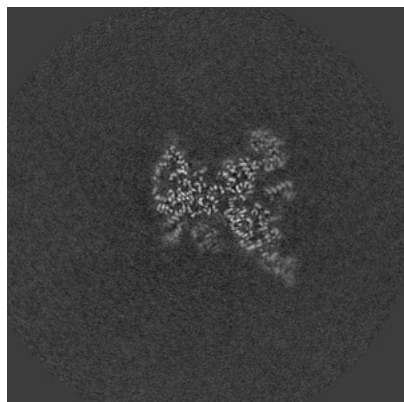


Y Index: 160

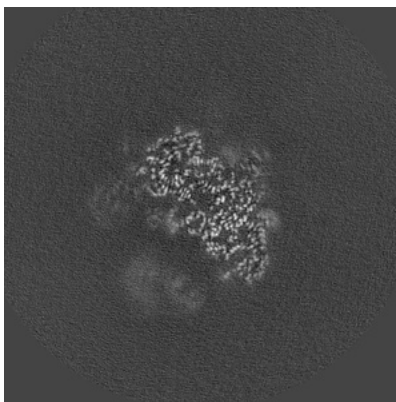


Z Index: 199

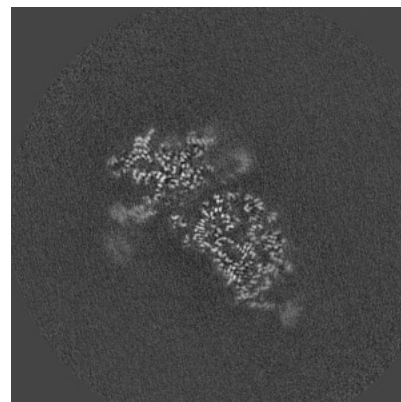
6.3.2 Raw map



X Index: 169



Y Index: 158

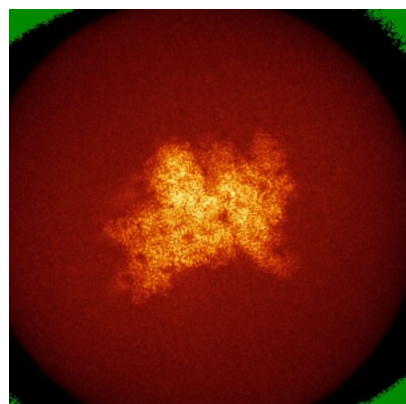


Z Index: 180

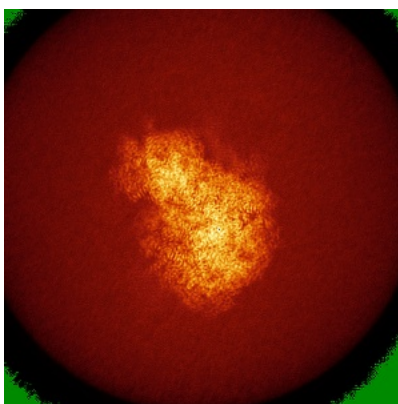
The images above show the largest variance slices of the map in three orthogonal directions.

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

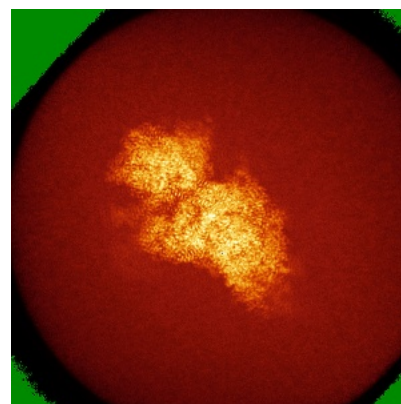
6.4.1 Primary map



X

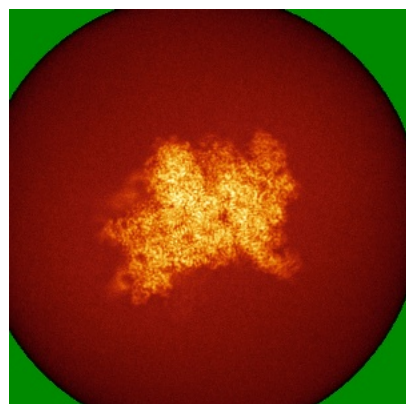


Y

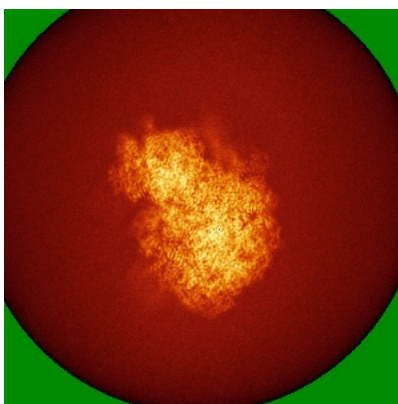


Z

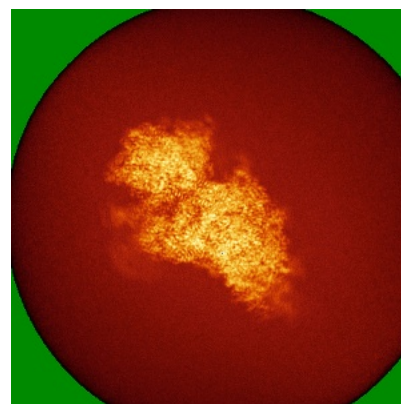
6.4.2 Raw map



X



Y

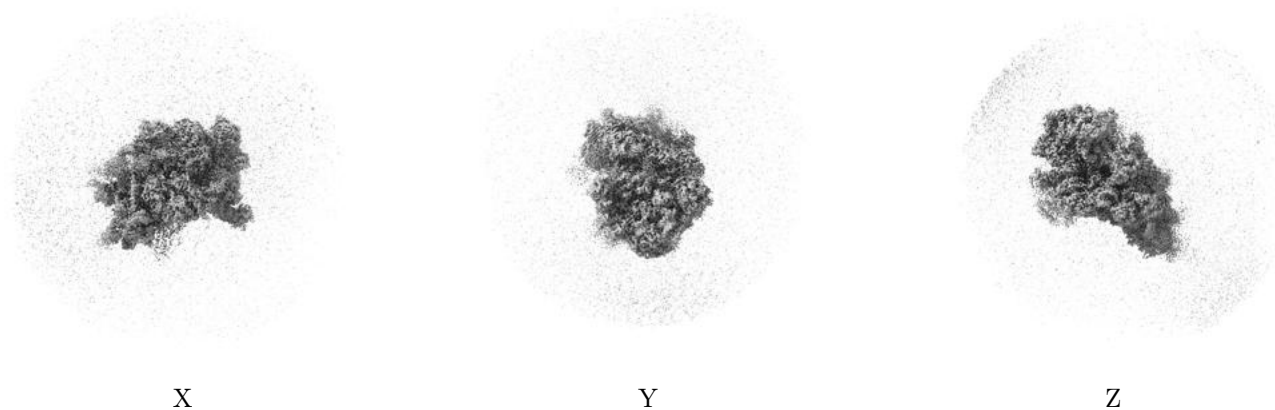


Z

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.

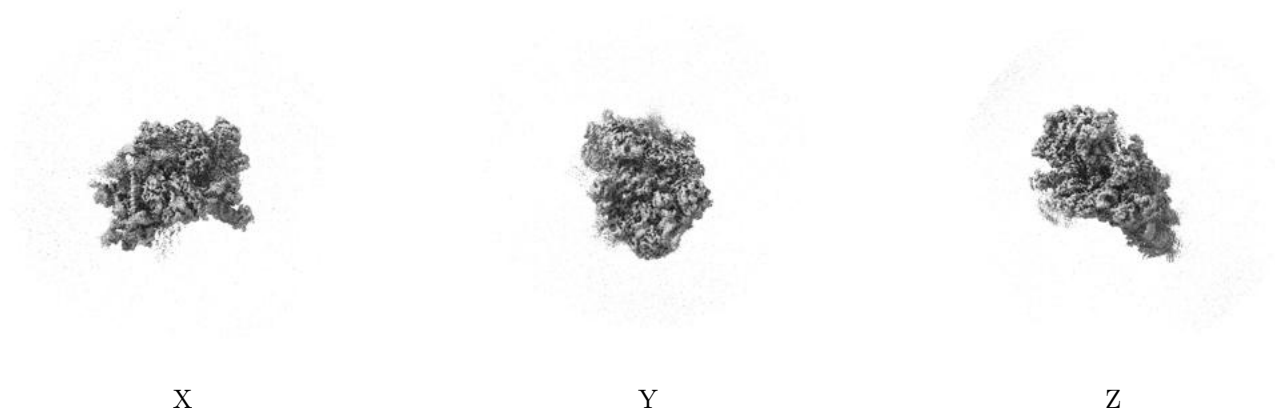
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

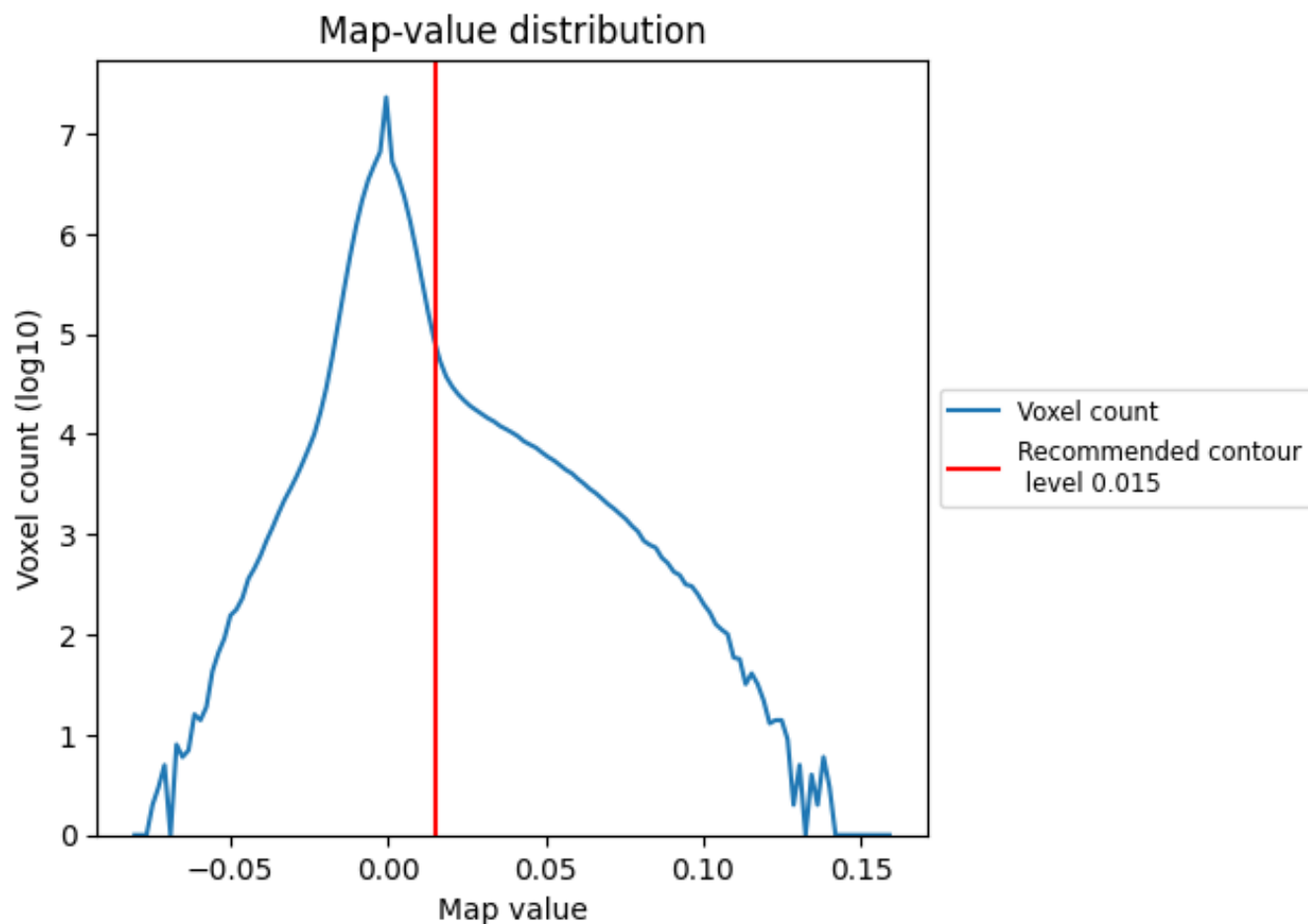
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

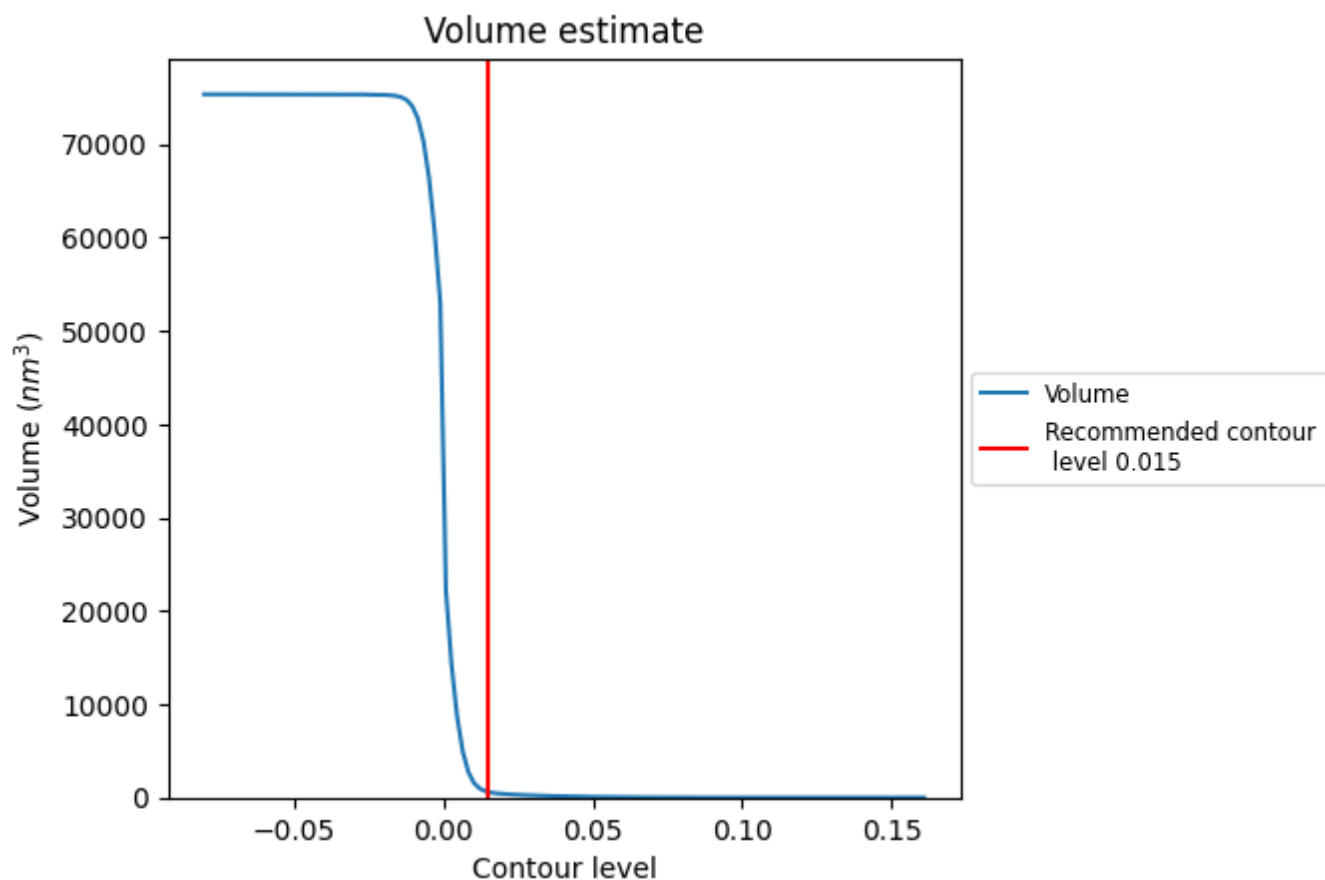
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

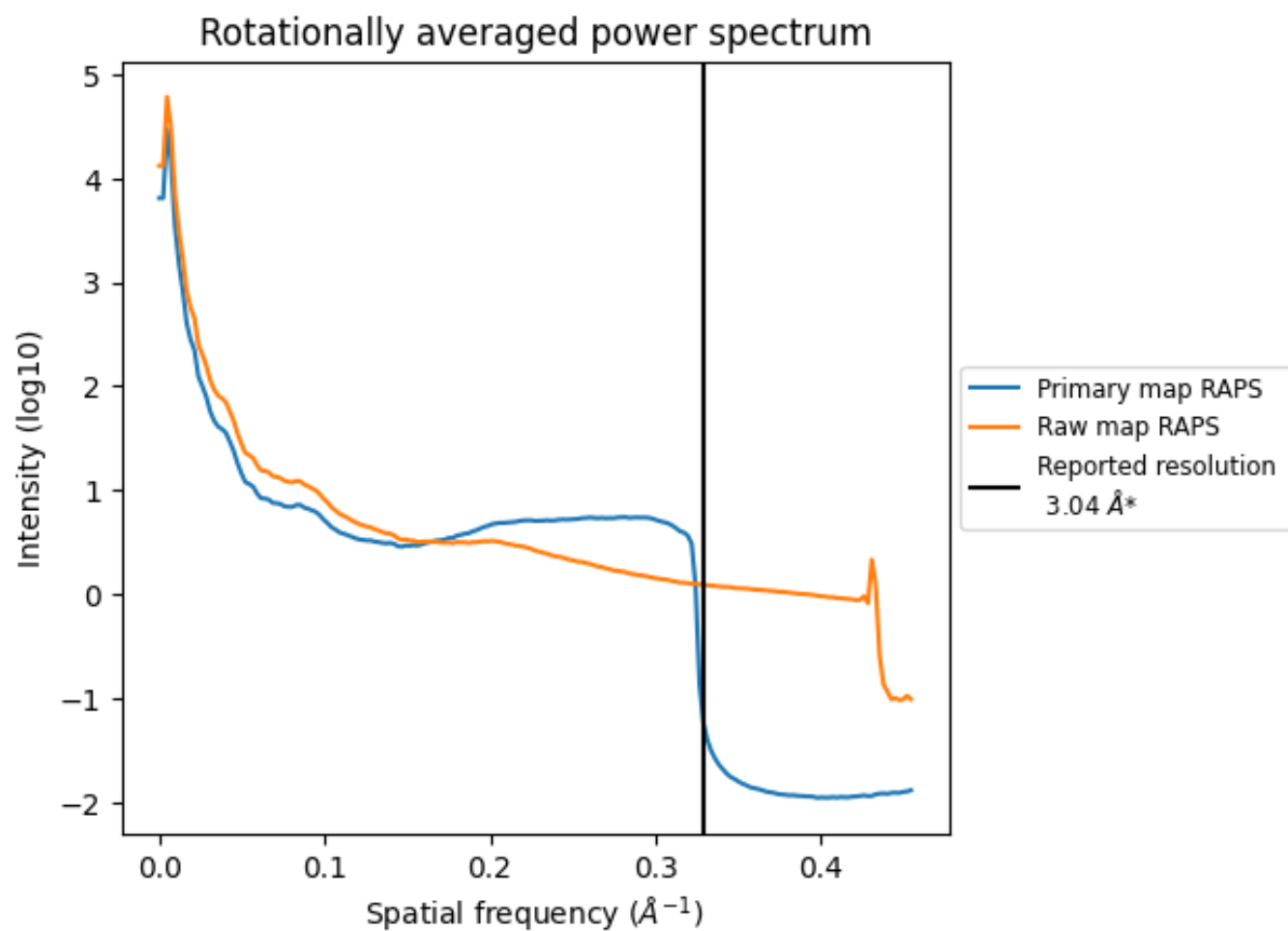
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 603 nm³; this corresponds to an approximate mass of 544 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 ⓘ

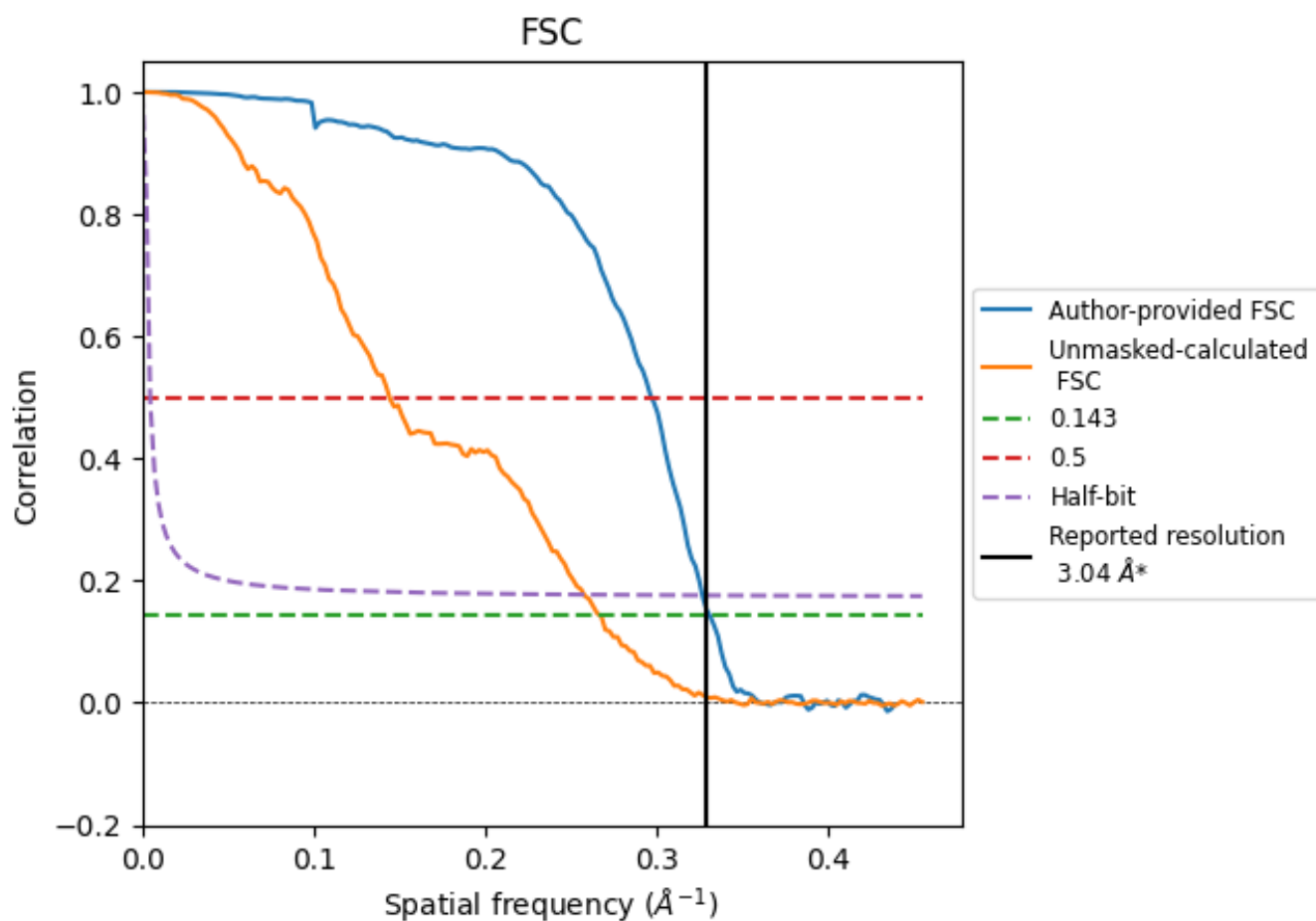


*Reported resolution corresponds to spatial frequency of 0.329 Å⁻¹

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 0.329 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

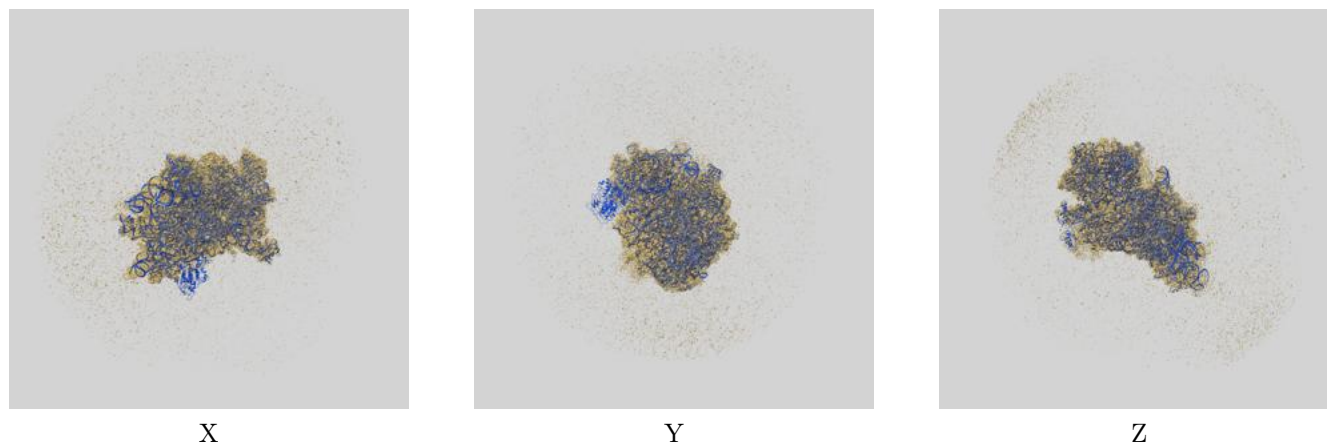
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.04	-	-
Author-provided FSC curve	3.02	3.37	3.06
Unmasked-calculated*	3.75	6.94	3.88

*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 3.75 differs from the reported value 3.04 by more than 10 %

9 Map-model fit [i](#)

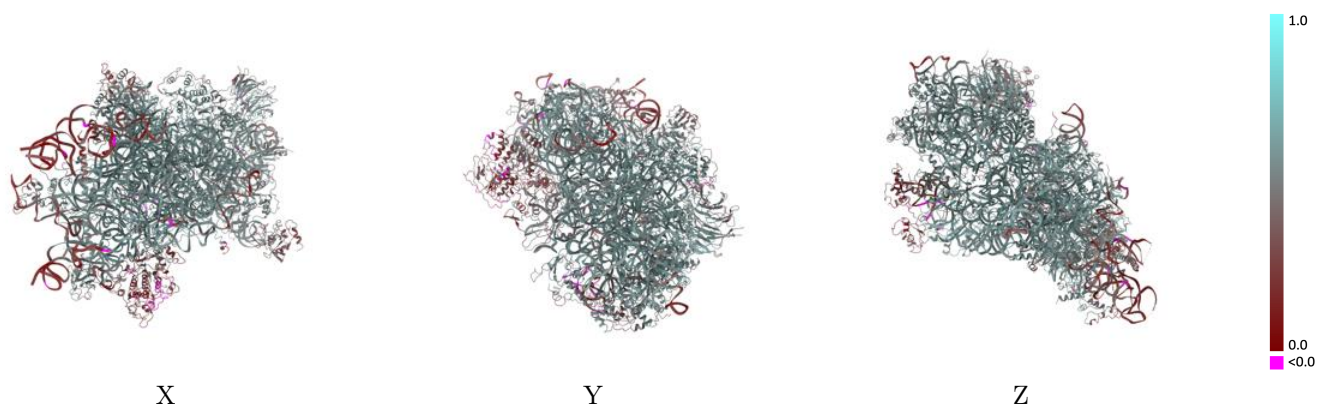
This section contains information regarding the fit between EMDB map EMD-17329 and PDB model 8P03. Per-residue inclusion information can be found in [section 3](#) on [page 12](#).

9.1 Map-model overlay [i](#)



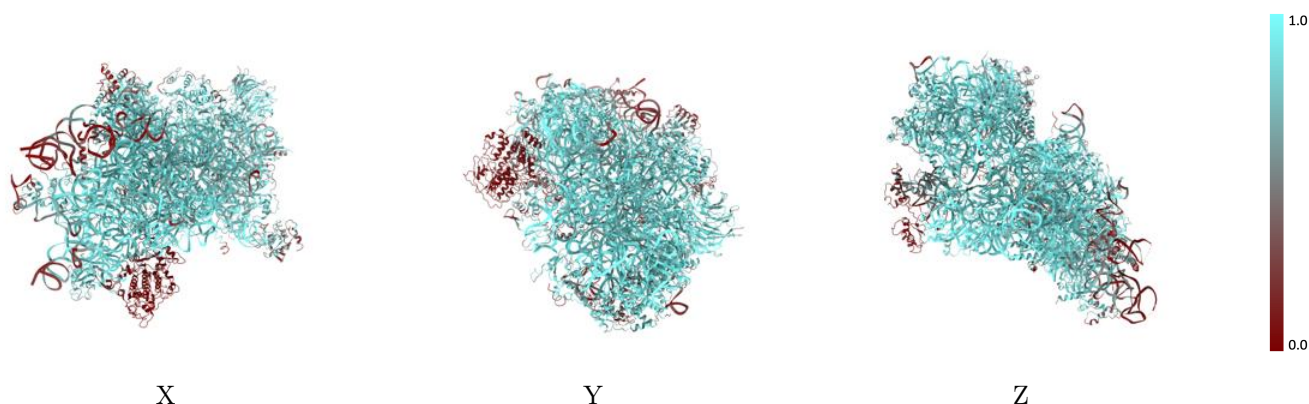
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



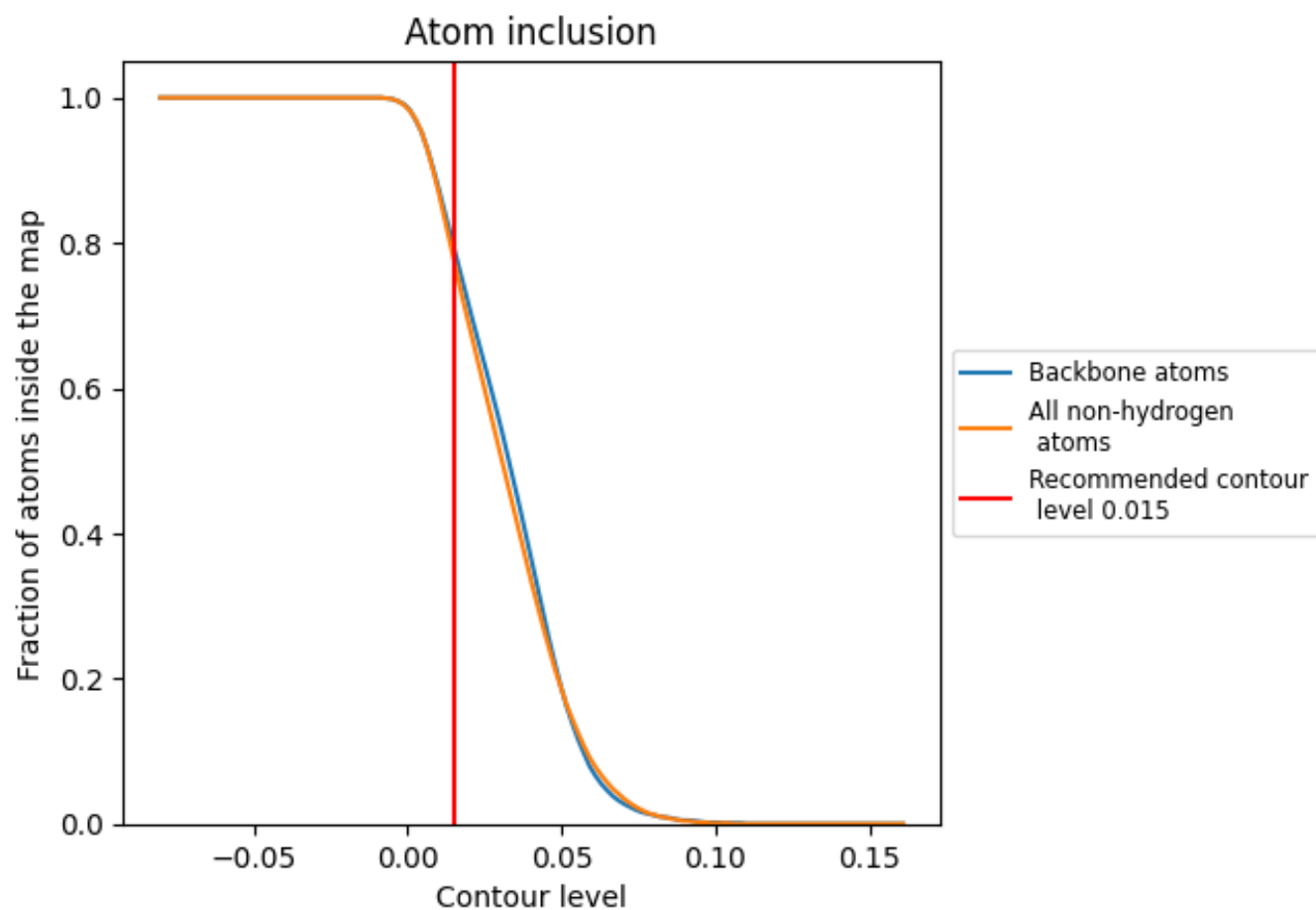
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.015).

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 78% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7770	 0.5090
1	 0.5590	 0.2840
2	 0.8780	 0.5300
3	 0.6750	 0.4840
A	 0.2870	 0.3460
C	 0.8770	 0.5660
D	 0.8720	 0.5610
E	 0.8640	 0.5720
F	 0.7900	 0.5310
G	 0.8780	 0.5760
H	 0.8550	 0.5580
I	 0.7760	 0.5120
J	 0.4800	 0.4390
K	 0.8050	 0.5290
L	 0.8560	 0.5610
M	 0.8420	 0.5300
N	 0.7750	 0.5430
O	 0.4710	 0.3690
P	 0.8740	 0.5650
Q	 0.8770	 0.5660
R	 0.7490	 0.5100
S	 0.9030	 0.5800
T	 0.7090	 0.4990
U	 0.8020	 0.5310
V	 0.8780	 0.5570
W	 0.7530	 0.5290
X	 0.8730	 0.5670
Y	 0.9100	 0.6000
Z	 0.8700	 0.5880
a	 0.8420	 0.5330
b	 0.8990	 0.5840
c	 0.8080	 0.5320
d	 0.8000	 0.5620
e	 0.9110	 0.5780
f	 0.5290	 0.3770



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Chain	Atom inclusion	Q-score
g	 0.8190	 0.5210
i	 0.7030	 0.5160
j	 0.5350	 0.4920
k	 0.0650	 0.2560
l	 0.7170	 0.5250
n	 0.7310	 0.5130