



wwPDB EM Validation Summary Report ⓘ

Jul 14, 2026 – 01:48 PM JST

PDB ID : 9XAH / pdb_00009xah
EMDB ID : EMD-66687
Title : Cryo-EM structure of the 90S pre-ribosome (Enp1-Rrp12 Mut) from *Chaetomium thermophilum*, state B1*
Authors : Lau, B.; Li, Y.; Zhu, J.; Fischer, P.; Hong, X.; Yuan, R.; Beckmann, R.; Hurt, E.; Cheng, J.
Deposited on : 2025-10-22
Resolution : 3.10 Å (reported)
Based on initial model : 6RXU

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.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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) : 2.50

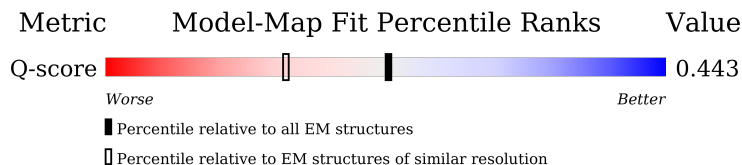
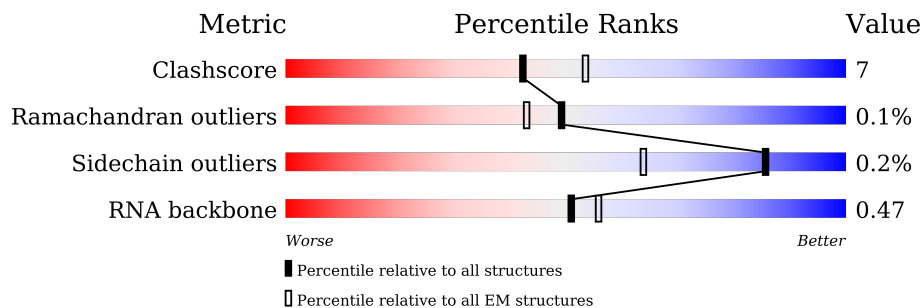
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



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

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

Mol	Chain	Length	Quality of chain
1	UA	904	
2	UB	907	

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Mol	Chain	Length	Quality of chain
3	UC	648	
4	UD	884	
5	UF	414	
6	UG	558	
7	UJ	1802	
8	UK	270	
9	UL	962	
10	UM	912	
11	UN	633	
12	UO	557	
13	UQ	960	
14	UR	618	
15	UU	1049	
16	UX	193	
17	UZ	391	
18	CA	313	
18	CB	313	
19	CC	523	
20	CD	582	
21	CE	127	
21	CF	127	
22	CG	630	
23	CH	411	
24	CI	1163	
25	CJ	183	

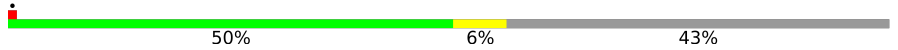
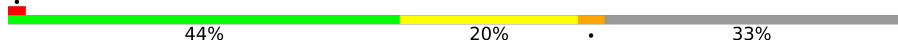
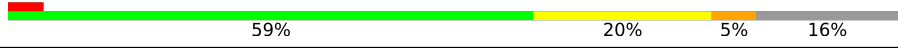
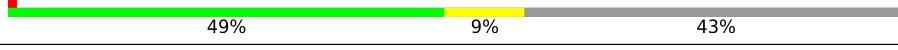
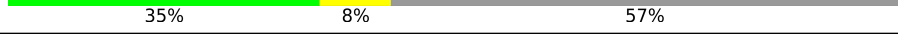
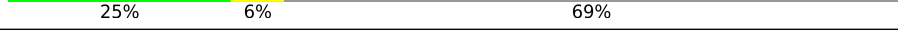
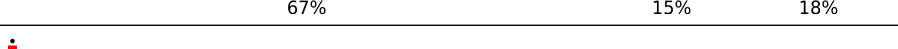
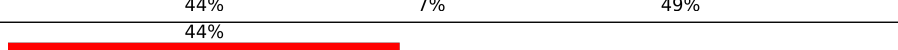
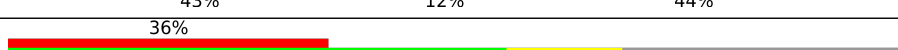
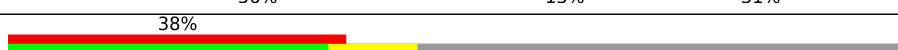
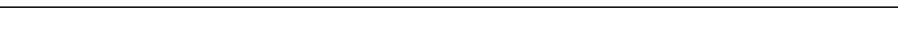
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Mol	Chain	Length	Quality of chain
26	CK	297	
27	CL	720	
28	CM	446	
29	CN	252	
29	CO	252	
30	CP	322	
31	CQ	259	
32	CR	1073	
32	CS	1073	
33	CT	203	
34	Ca	255	
35	Cb	264	
36	Cc	212	
37	Cd	239	
38	Ce	203	
39	Cf	202	
40	Cg	190	
41	Ch	151	
42	Ci	150	
43	Cj	143	
44	Ck	161	
45	Cm	130	
46	Cn	145	
47	Co	136	
48	Cp	68	

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Mol	Chain	Length	Quality of chain
49	CU	311	
50	C1	2344	
51	C2	274	
52	CW	668	
53	UT	2612	
54	UH	930	
55	UE	410	
55	UI	410	
56	US	549	
57	Cl	156	
58	CX	480	
59	CY	381	
60	CZ	609	
61	UP	364	

2 Entry composition [i](#)

There are 65 unique types of molecules in this entry. The entry contains 228132 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 protein called Periodic tryptophan protein 2-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	UA	839	Total	C	N	O	P	S	
			6411	4118	1136	1132	1	24	
								0	0

- Molecule 2 is a protein called Nucleolar complex protein 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	UB	566	Total	C	N	O	S		
			4506	2845	858	790	13		
								0	0

- Molecule 3 is a protein called Sas10 C-terminal domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	UC	248	Total	C	N	O	S		
			1970	1238	362	363	7		
								0	0

- Molecule 4 is a protein called UTP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	UD	777	Total	C	N	O	S		
			6108	3872	1099	1113	24		
								0	0

- Molecule 5 is a protein called U3 snoRNP protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	UF	331	Total	C	N	O	S		
			2599	1678	504	403	14		
								0	0

- Molecule 6 is a protein called U three protein 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	UG	479	Total	C	N	O	S		
			3765	2391	700	662	12		
								0	0

- Molecule 7 is a protein called U3 small nucleolar RNA-associated protein 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	UJ	1654	Total	C	N	O	S	0	0
			12725	8149	2177	2347	52		

- Molecule 8 is a protein called U3 small nucleolar RNA-associated protein 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	UK	217	Total	C	N	O	S	0	0
			1695	1066	351	273	5		

- Molecule 9 is a protein called Small-subunit processome Utp12 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	UL	785	Total	C	N	O	S	0	0
			6175	3940	1088	1130	17		

- Molecule 10 is a protein called U3 small nucleolar RNA-associated protein 13 C-terminal domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	UM	843	Total	C	N	O	S	0	0
			6545	4139	1151	1241	14		

- Molecule 11 is a protein called UTP14.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	UN	177	Total	C	N	O	S	0	0
			1401	892	263	239	7		

- Molecule 12 is a protein called U3 small nucleolar RNA-associated protein 15 C-terminal domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	UO	503	Total	C	N	O	S	0	0
			3811	2417	698	683	13		

- Molecule 13 is a protein called UTP17.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	UQ	789	Total	C	N	O	S	0	0
			6008	3831	1037	1119	21		

- Molecule 14 is a protein called UTP18.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	UR	447	Total	C	N	O	P	S	
			3495	2209	656	619	1	10	
								0	0

- Molecule 15 is a protein called Putative U3 snoRNP protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	UU	908	Total	C	N	O	S		
			6778	4361	1243	1148	26		
								0	0

- Molecule 16 is a protein called UTP24.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	UX	190	Total	C	N	O	S		
			1480	938	286	246	10		
								0	0

- Molecule 17 is a protein called Ribosome biogenesis protein C8F11.04.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	UZ	235	Total	C	N	O	S		
			1815	1184	330	298	3		
								0	0

- Molecule 18 is a protein called rRNA 2'-O-methyltransferase fibrillarin.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	CA	242	Total	C	N	O	S		
			1778	1149	327	293	9		
18	CB	237	Total	C	N	O	S		
			1816	1154	318	335	9		
								0	0

- Molecule 19 is a protein called Nucleolar protein 56.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	CC	387	Total	C	N	O	S		
			2866	1836	527	492	11		
								0	0

- Molecule 20 is a protein called Nucleolar protein 58.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	CD	446	Total	C	N	O	S		
			3355	2150	594	600	11		
								0	0

- Molecule 21 is a protein called H/ACA ribonucleoprotein complex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	CE	121	Total	C	N	O	S	0	0
			879	557	165	154	3		
21	CF	120	Total	C	N	O	S	0	0
			864	550	161	150	3		

- Molecule 22 is a protein called Ribosomal RNA-processing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	CG	416	Total	C	N	O	S	0	0
			3245	2065	587	580	13		

- Molecule 23 is a protein called RNA 3'-terminal phosphate cyclase-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	CH	389	Total	C	N	O	S	0	0
			2888	1827	526	525	10		

- Molecule 24 is a protein called Bms1-type G domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	CI	841	Total	C	N	O	S	0	0
			6666	4277	1246	1113	30		

- Molecule 25 is a protein called U3 small nucleolar ribonucleoprotein protein IMP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	CJ	179	Total	C	N	O	S	0	0
			1434	918	283	226	7		

- Molecule 26 is a protein called U3 small nucleolar ribonucleoprotein protein IMP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	CK	297	Total	C	N	O	S	0	0
			2329	1476	445	400	8		

- Molecule 27 is a protein called mpp10.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	CL	320	Total	C	N	O	S	0	0
			2466	1550	460	450	6		

- Molecule 28 is a protein called DDB1- and CUL4-associated factor 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	CM	445	Total	C	N	O	S	0	0
			3501	2195	672	619	15		

- Molecule 29 is a protein called Nucleolar essential protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	CN	226	Total	C	N	O	S	0	0
			1762	1119	306	327	10		
29	CO	215	Total	C	N	O	S	0	0
			1683	1067	293	313	10		

- Molecule 30 is a protein called KRR1 small subunit processome component.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	CP	233	Total	C	N	O	S	0	0
			1893	1209	340	335	9		

- Molecule 31 is a protein called Pre-rRNA-processing protein PNO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	CQ	180	Total	C	N	O	S	0	0
			1413	898	257	251	7		

- Molecule 32 is a protein called RNA cytidine acetyltransferase.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	CR	846	Total	C	N	O	S	0	0
			6677	4278	1137	1233	29		
32	CS	836	Total	C	N	O	S	0	0
			6591	4217	1118	1228	28		

- Molecule 33 is a protein called Fcf2 pre-rRNA processing C-terminal domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	CT	131	Total	C	N	O	S	0	0
			1035	656	197	178	4		

- Molecule 34 is a protein called Small ribosomal subunit protein eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Ca	225	Total	C	N	O	S	0	0
			1821	1160	341	315	5		

- Molecule 35 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Cb	232	Total	C	N	O	S	0	0
			1851	1179	340	325	7		

- Molecule 36 is a protein called 40S ribosomal protein s5-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Cc	192	Total	C	N	O	S	0	0
			1464	926	278	253	7		

- Molecule 37 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Cd	226	Total	C	N	O	S	0	0
			1819	1138	363	313	5		

- Molecule 38 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Ce	159	Total	C	N	O		0	0
			1279	810	237	232			

- Molecule 39 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Cf	174	Total	C	N	O	S	0	0
			1398	872	283	242	1		

- Molecule 40 is a protein called 40S ribosomal protein s9-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Cg	159	Total	C	N	O	S	0	0
			1248	804	258	184	2		

- Molecule 41 is a protein called 40S ribosomal protein S13-like protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	Ch	66	Total	C	N	O	0	0
			546	355	101	90		

- Molecule 42 is a protein called 40S ribosomal protein S14-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Ci	115	Total	C	N	O	S	0	0
			808	506	156	141	5		

- Molecule 43 is a protein called 40S ribosomal protein S16-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Cj	126	Total	C	N	O	S	0	0
			943	613	177	151	2		

- Molecule 44 is a protein called 40S ribosomal protein S11-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Ck	131	Total	C	N	O	S	0	0
			1082	695	210	172	5		

- Molecule 45 is a protein called 40S ribosomal protein S22-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Cm	126	Total	C	N	O	S	0	0
			985	632	184	164	5		

- Molecule 46 is a protein called 40S ribosomal protein s23-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Cn	96	Total	C	N	O	S	0	0
			702	456	134	110	2		

- Molecule 47 is a protein called Small ribosomal subunit protein eS24.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	Co	92	Total	C	N	O	S	0	0
			741	474	139	126	2		

- Molecule 48 is a protein called 40S ribosomal protein S28-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	Cp	61	Total	C	N	O	S	0	0
			458	286	97	74	1		

- Molecule 49 is a protein called Faf1.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	CU	176	Total	C	N	O	S	0	0
			1337	822	265	244	6		

- Molecule 50 is a RNA chain called 35s rna.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	C1	1574	Total	C	N	O	P	0	0
			33584	14984	6018	11008	1574		

- Molecule 51 is a RNA chain called u3 rna.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	C2	229	Total	C	N	O	P	0	0
			4869	2172	851	1617	229		

- Molecule 52 is a protein called Ribosome biogenesis protein ENP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	CW	383	Total	C	N	O	S	0	0
			2932	1862	531	525	14		

- Molecule 53 is a protein called UTP20.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	UT	2027	Total	C	N	O	S	0	0
			15998	10300	2811	2819	68		

- Molecule 54 is a protein called UTP8.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	UH	799	Total	C	N	O	S	0	0
			6198	3903	1105	1171	19		

- Molecule 55 is a protein called Small-subunit processome Utp12 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	UE	178	Total	C	N	O	S	0	0
			1362	851	251	254	6		
55	UI	128	Total	C	N	O	S	0	0
			996	622	187	181	6		

- Molecule 56 is a protein called CCAAT-binding factor domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	US	451	Total	C	N	O	S	0	0
			3672	2389	608	660	15		

- Molecule 57 is a protein called Putative ribosomal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	Cl	80	Total	C	N	O	S	0	0
			633	400	115	117	1		

- Molecule 58 is a protein called Bystin-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	CX	267	Total	C	N	O	S	0	0
			2130	1384	374	362	10		

- Molecule 59 is a protein called U3 small nucleolar ribonucleoprotein protein lcp5-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	CY	264	Total	C	N	O	S	0	0
			2095	1296	388	406	5		

- Molecule 60 is a protein called Protein BFR2.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	CZ	283	Total	C	N	O	S	0	0
			2270	1398	426	439	7		

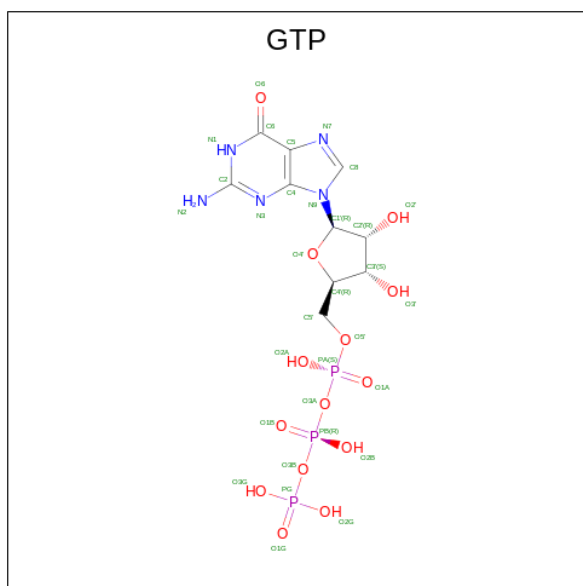
- Molecule 61 is a protein called UTP16.

Mol	Chain	Residues	Atoms				AltConf	Trace
61	UP	54	Total	C	N	O	0	0
			422	264	88	70		

- Molecule 62 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
62	UX	1	Total	Zn	0
			1	1	

- Molecule 63 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

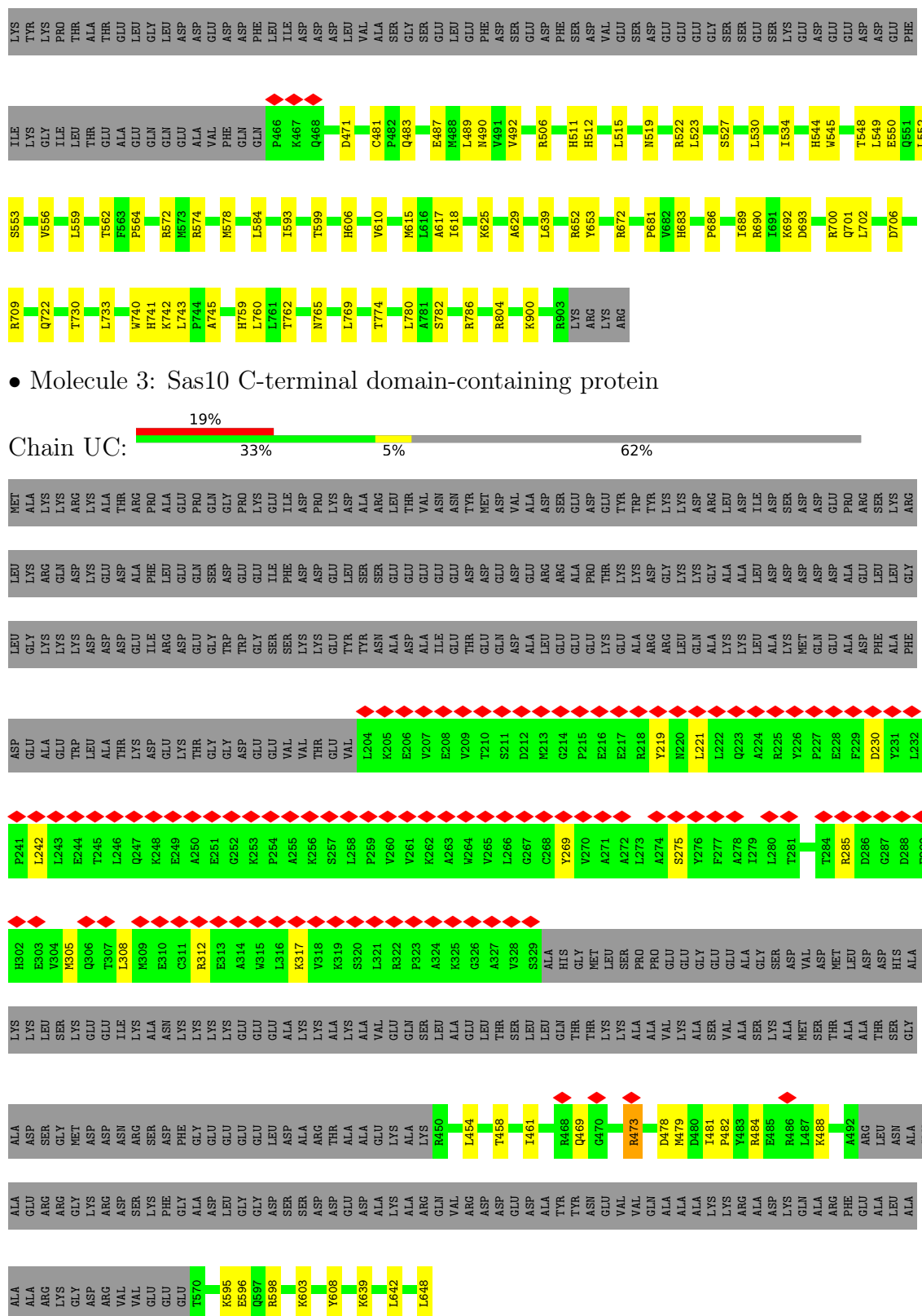


Mol	Chain	Residues	Atoms					AltConf
63	CI	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 64 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

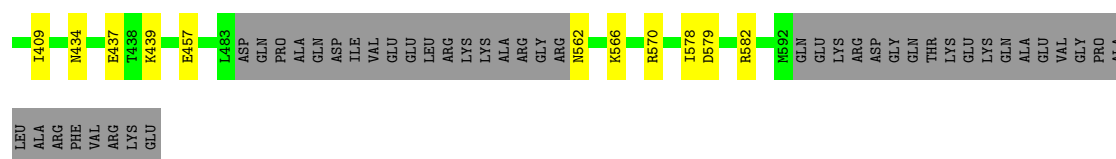
Mol	Chain	Residues	Atoms		AltConf
64	CI	1	Total	Mg	0
			1	1	

- Molecule 65 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

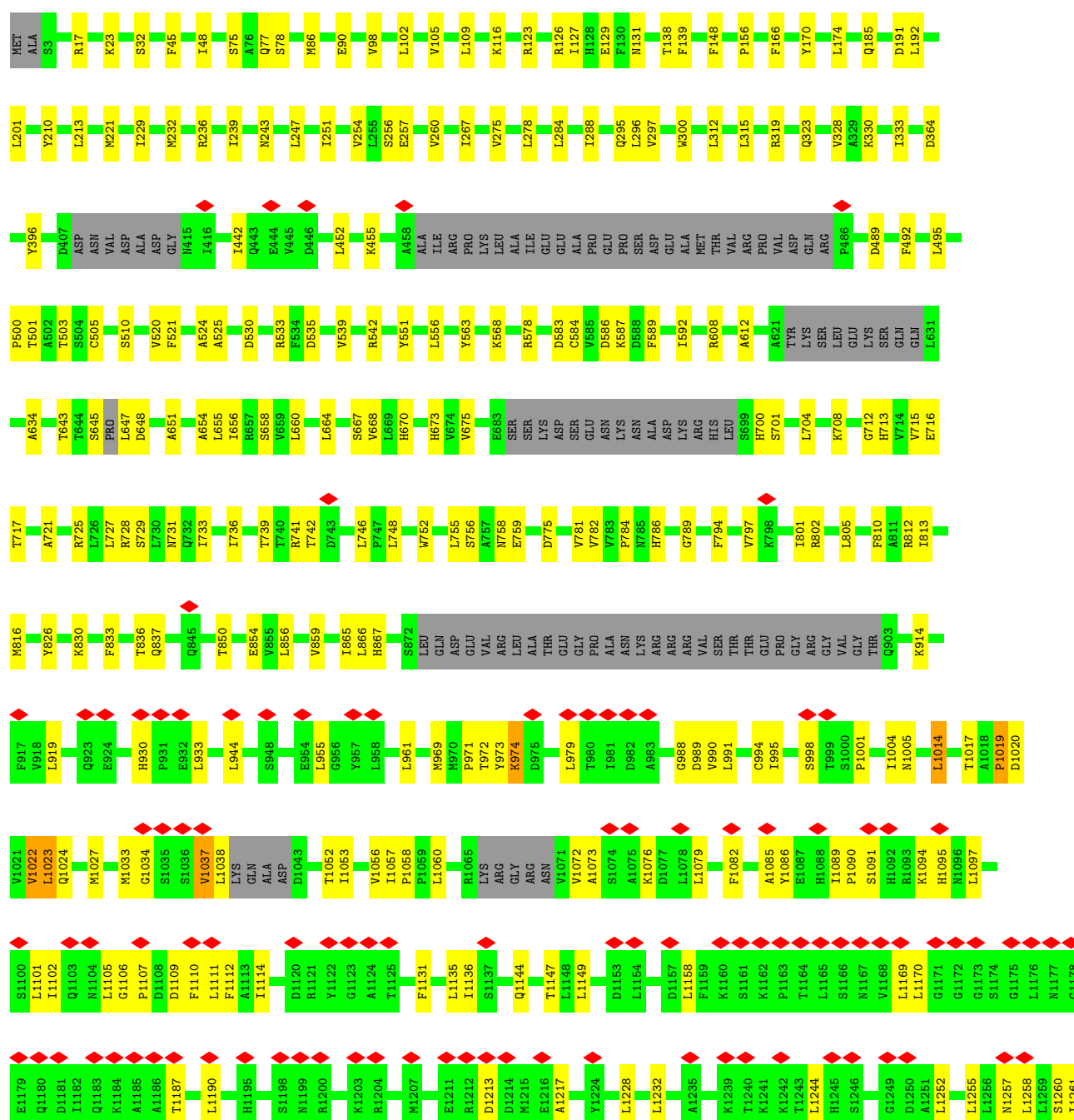


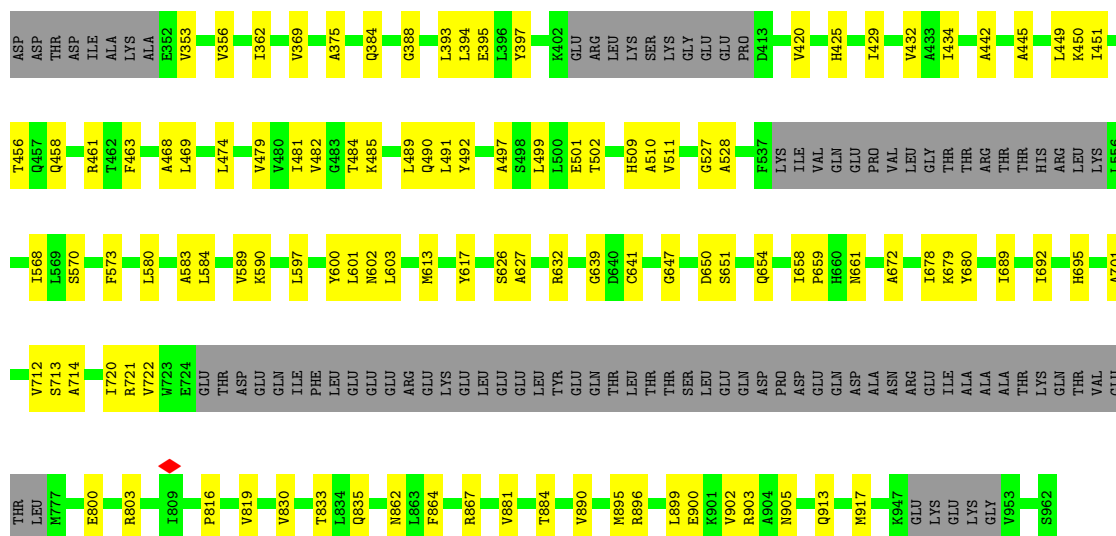
• Molecule 4: UTP4

Chain UD: 67% 21% 12%



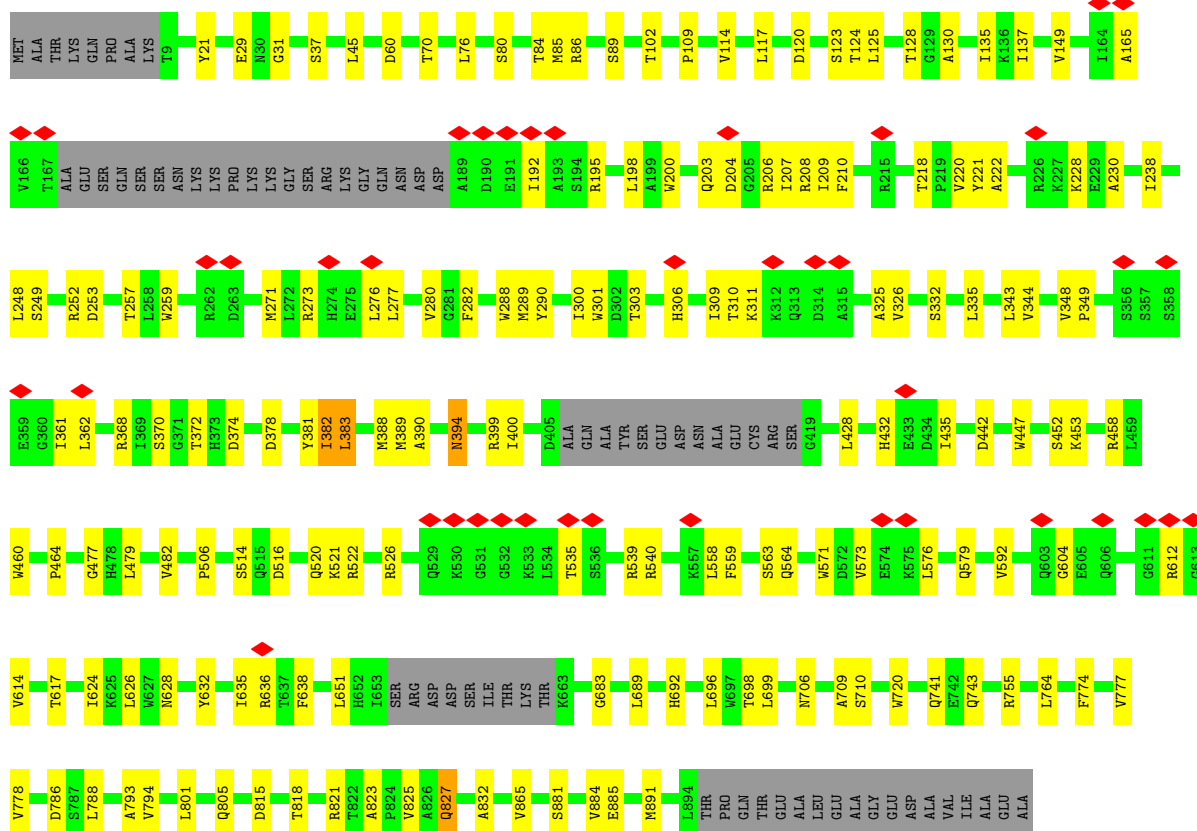
• Molecule 7: U3 small nucleolar RNA-associated protein 10





- Molecule 10: U3 small nucleolar RNA-associated protein 13 C-terminal domain-containing protein

Chain UM: 74% 18% 8%

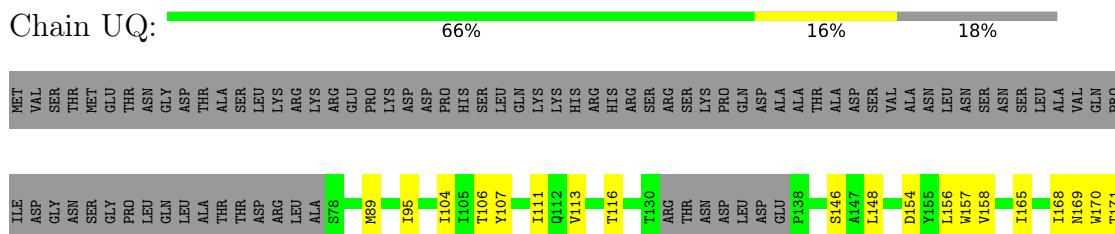


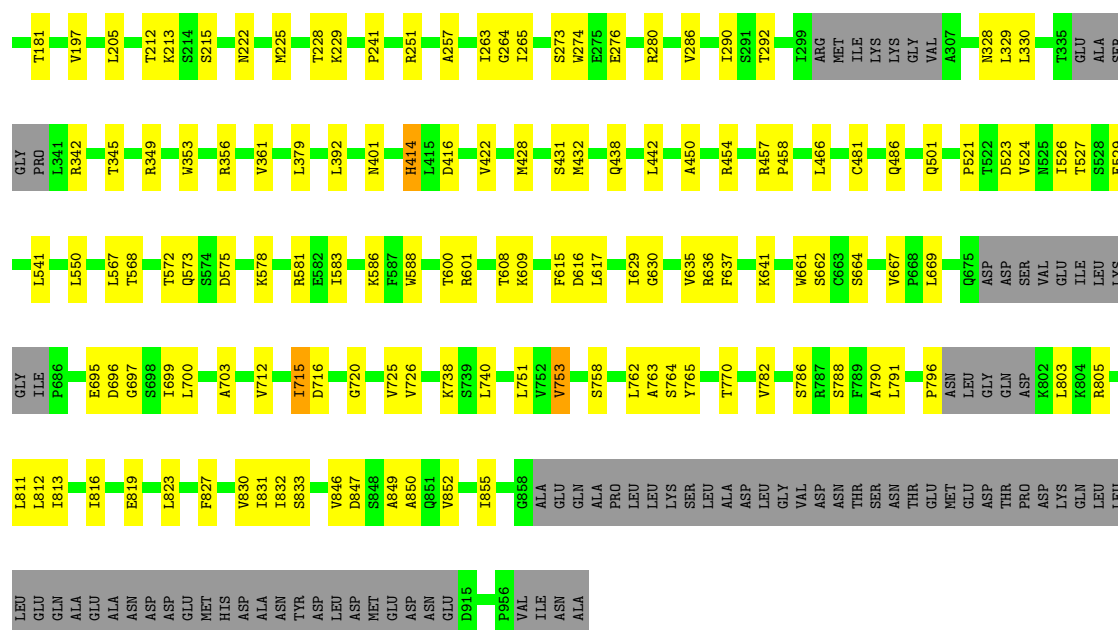
- Molecule 11: UTP14

Chain UN: 24% 72%

- Molecule 12: U3 small nucleolar RNA-associated protein 15 C-terminal domain-containing protein

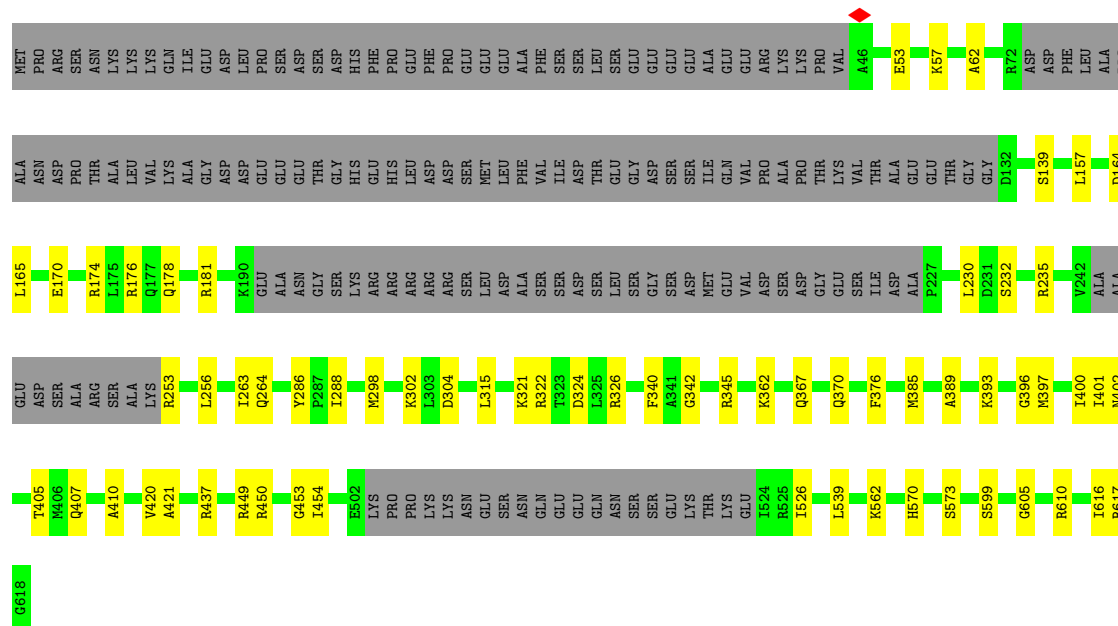
- Molecule 13: UTP17





• Molecule 14: UTP18

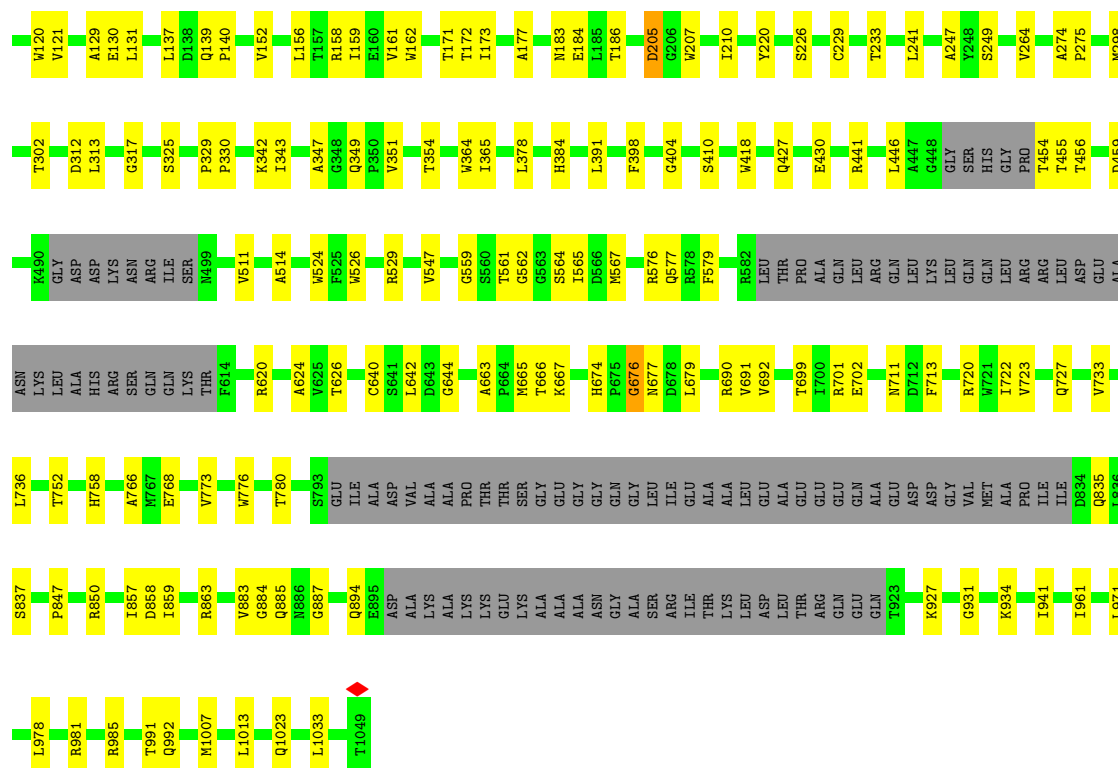
Chain UR: 62% 10% 28%



• Molecule 15: Putative U3 snoRNP protein

Chain UU: 71% 15% 13%





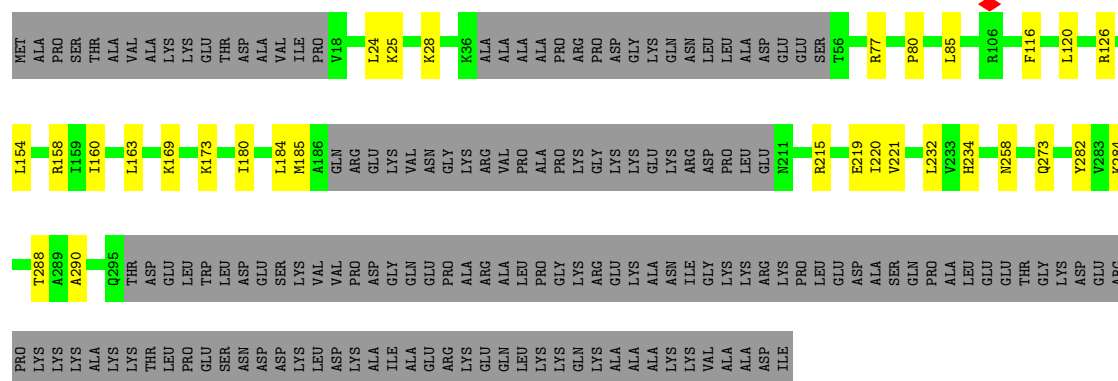
- Molecule 16: UTP24

Chain UX: 83% 16% .



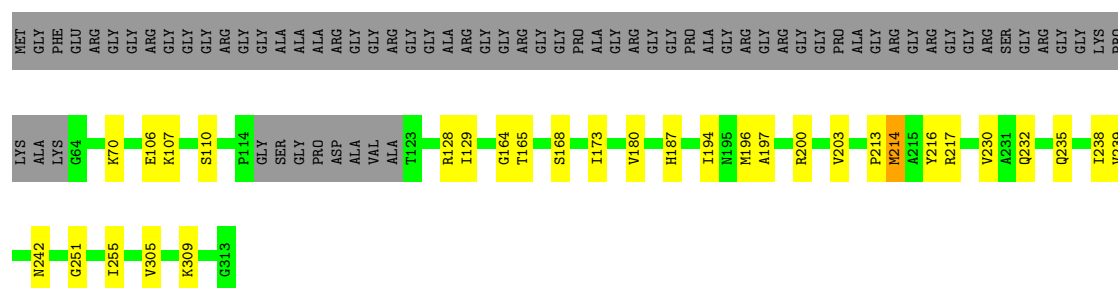
- Molecule 17: Ribosome biogenesis protein C8F11.04

Chain UZ: 52% 8% 40%

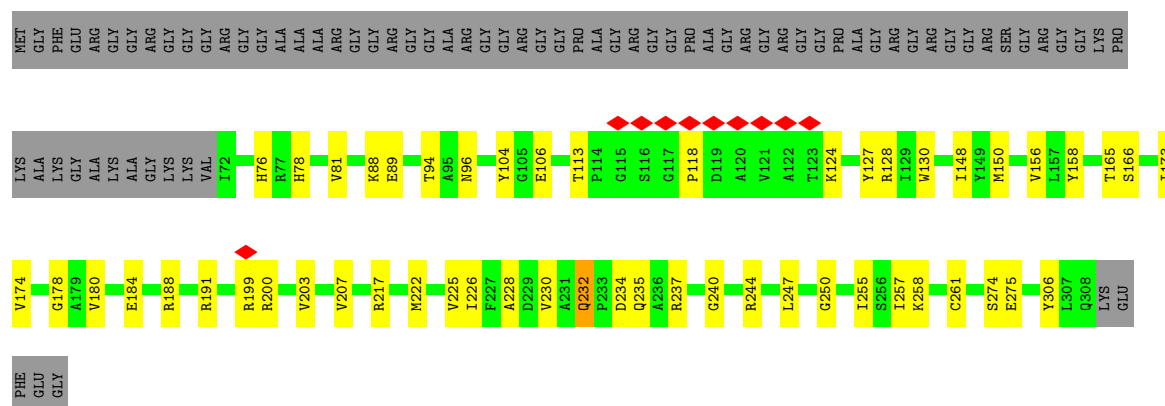


- Molecule 18: rRNA 2'-O-methyltransferase fibrillar

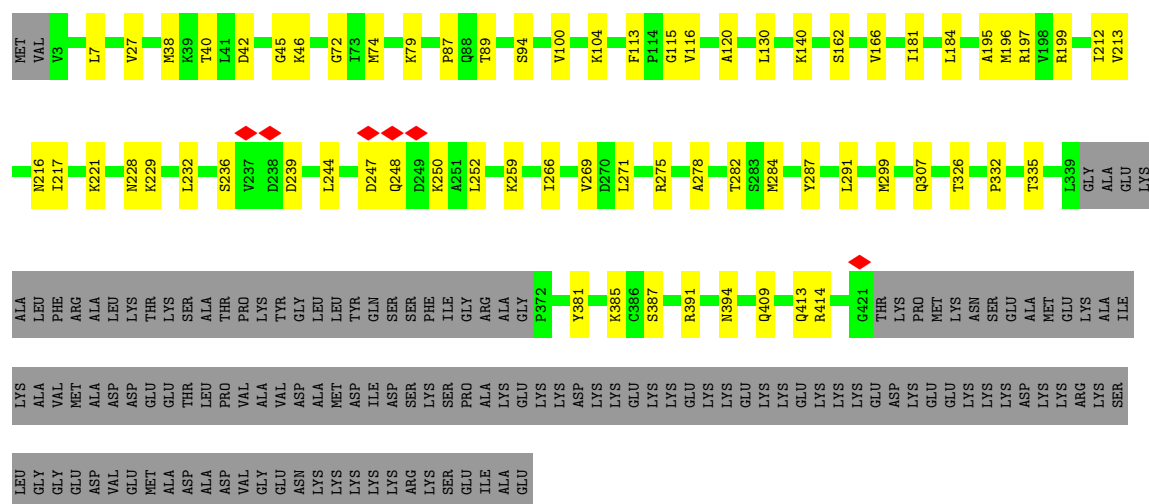
Chain CA: 67% 10% 23%



- Molecule 18: rRNA 2'-O-methyltransferase fibrillar

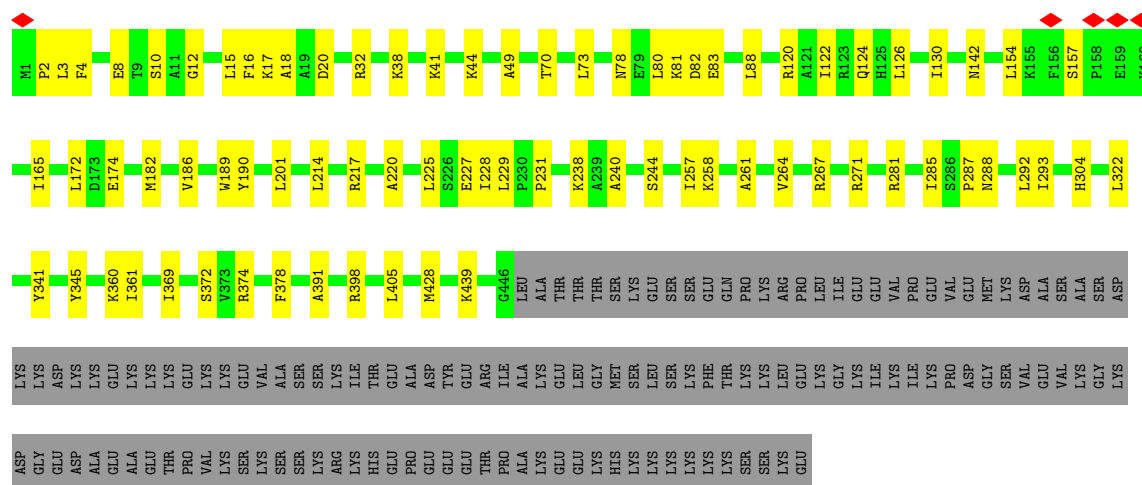


- Molecule 19: Nucleolar protein 56



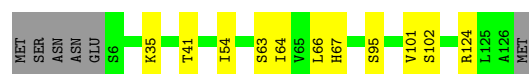
- Molecule 20: Nucleolar protein 58





- Molecule 21: H/ACA ribonucleoprotein complex subunit 2

Chain CE: 87% 9% 5%



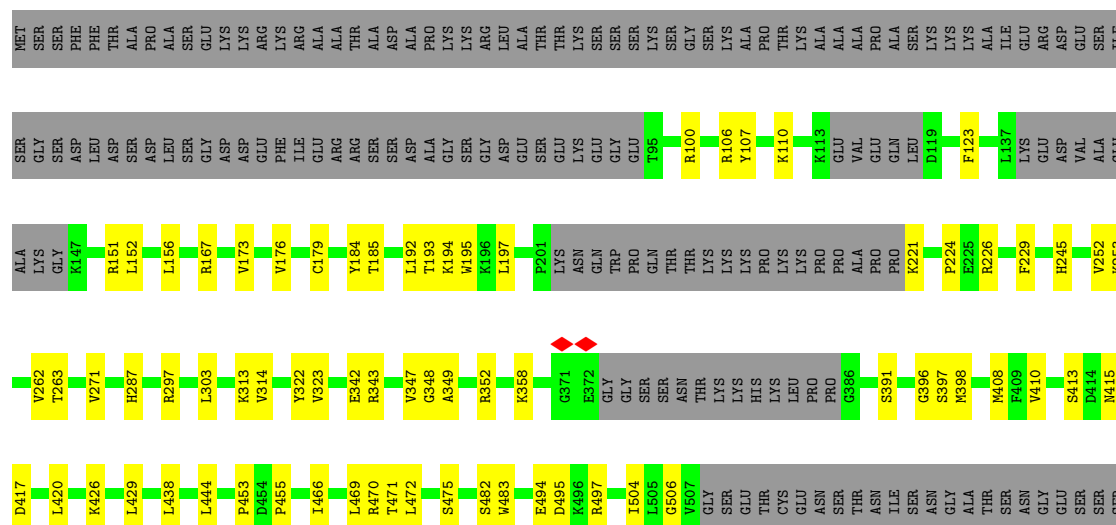
- Molecule 21: H/ACA ribonucleoprotein complex subunit 2

Chain CF: 83% 11% 6%



- Molecule 22: Ribosomal RNA-processing protein

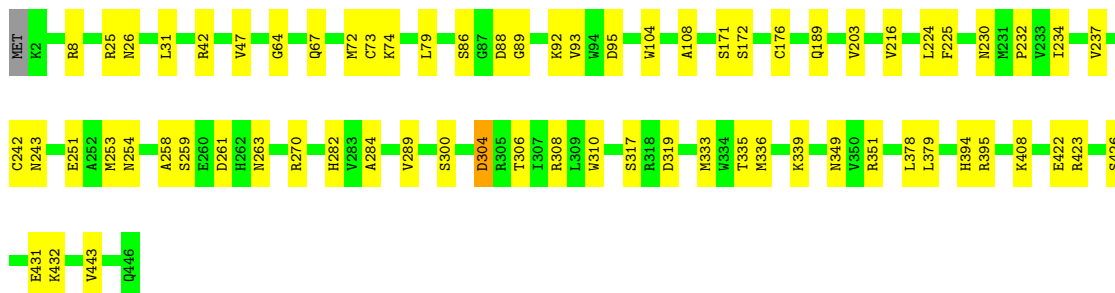
Chain CG: 53% 13% 34%





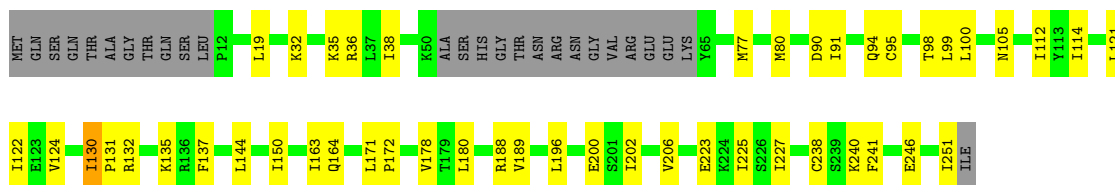
- Molecule 28: DDB1- and CUL4-associated factor 13

Chain CM:



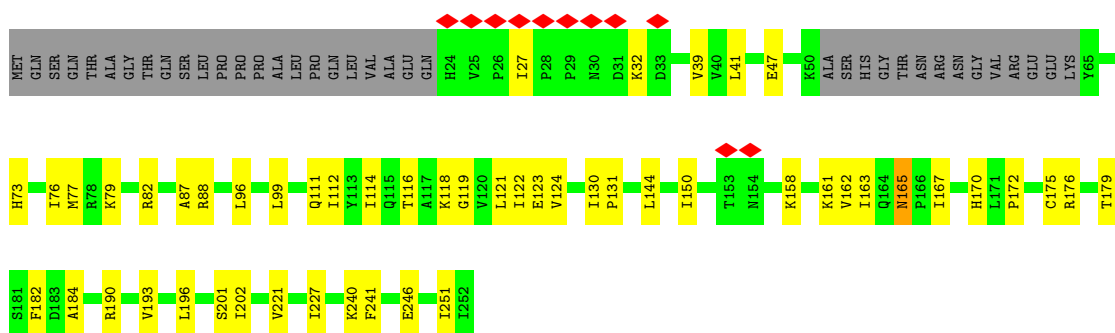
- Molecule 29: Nucleolar essential protein 1

Chain CN:



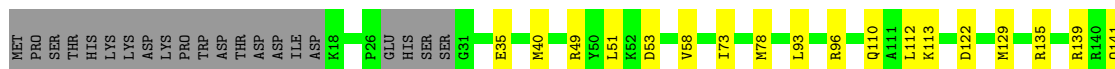
- Molecule 29: Nucleolar essential protein 1

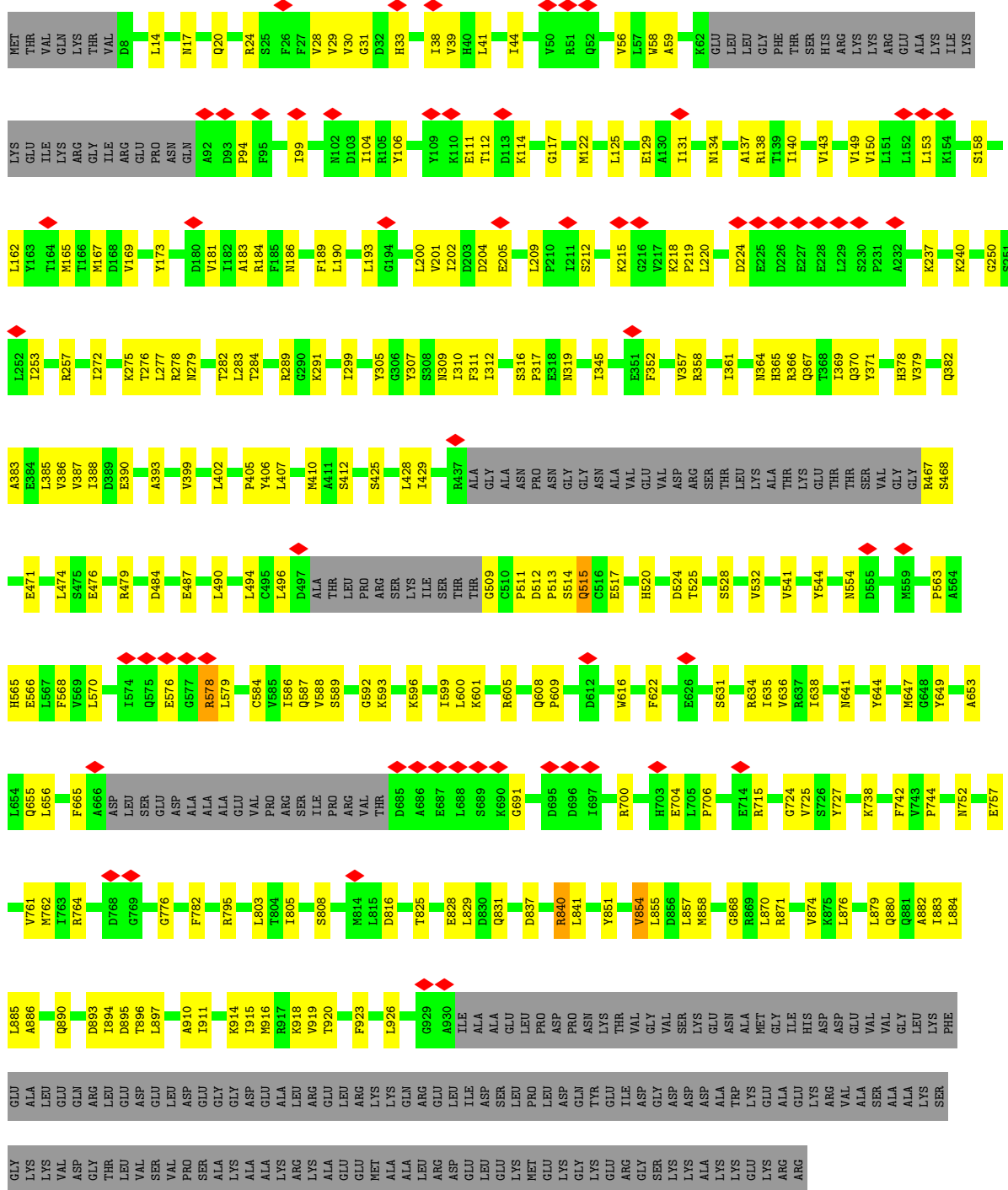
Chain CO:



- Molecule 30: KRR1 small subunit processome component

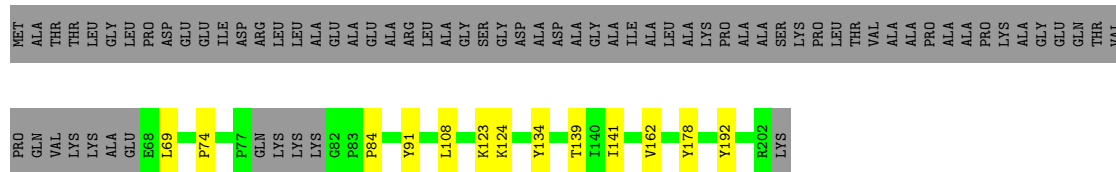
Chain CP:





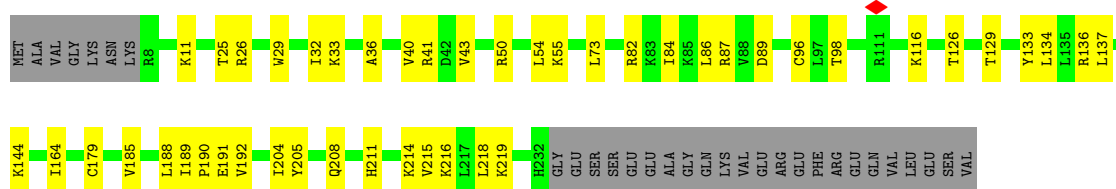
- Molecule 33: Fcf2 pre-rRNA processing C-terminal domain-containing protein

Chain CT: 



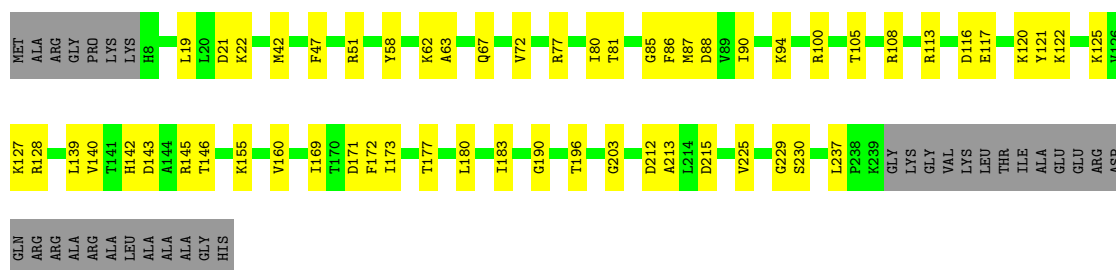
- Molecule 34: Small ribosomal subunit protein eS1

Chain Ca: 



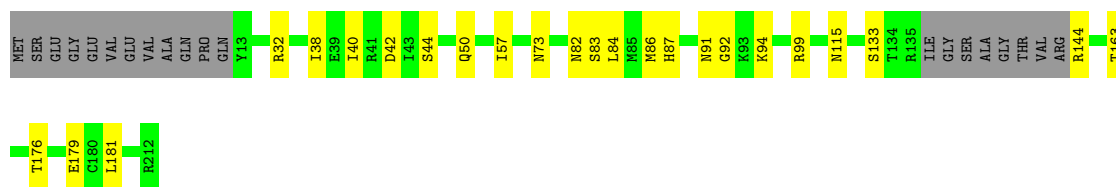
- Molecule 35: 40S ribosomal protein S4

Chain Cb: 



- Molecule 36: 40S ribosomal protein s5-like protein

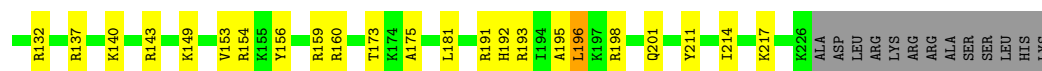
Chain Cc: 



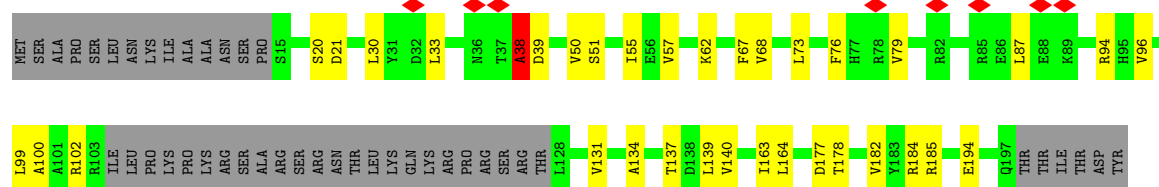
- Molecule 37: 40S ribosomal protein S6

Chain Cd: 

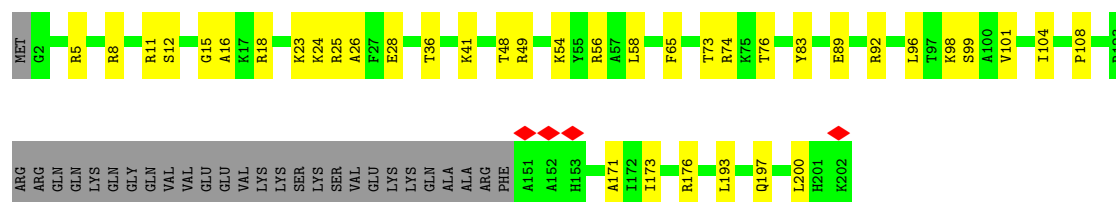




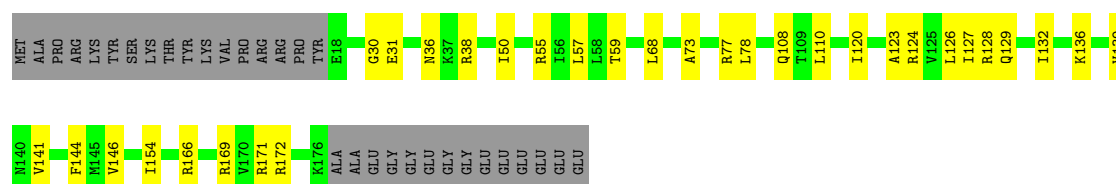
- Molecule 38: 40S ribosomal protein S7



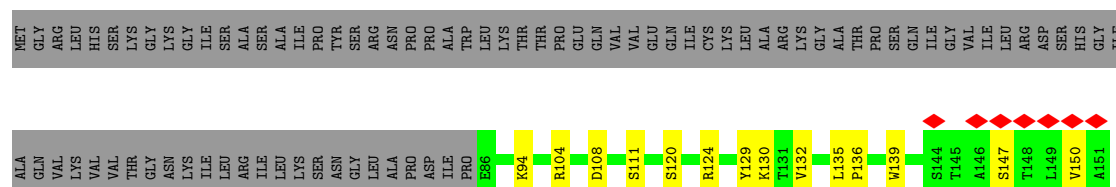
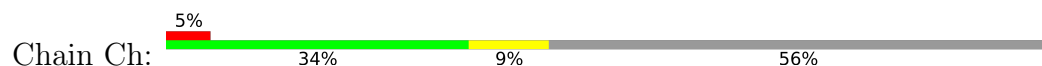
- Molecule 39: 40S ribosomal protein S8



- Molecule 40: 40S ribosomal protein s9-like protein

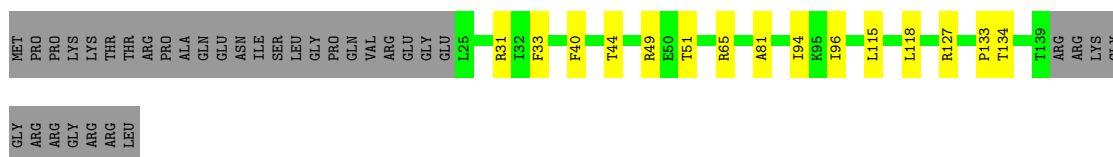


- Molecule 41: 40S ribosomal protein S13-like protein

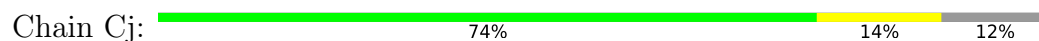


- Molecule 42: 40S ribosomal protein S14-like protein

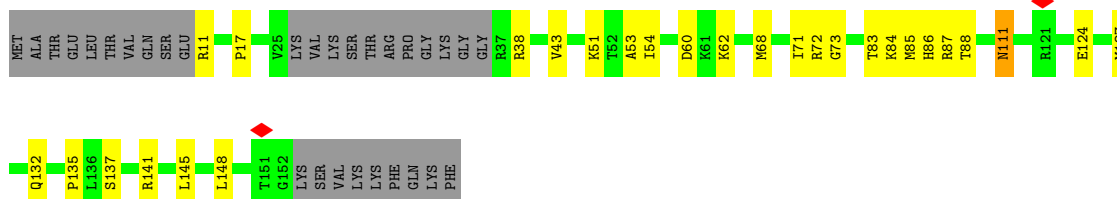




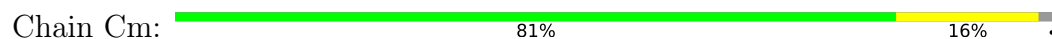
- Molecule 43: 40S ribosomal protein S16-like protein



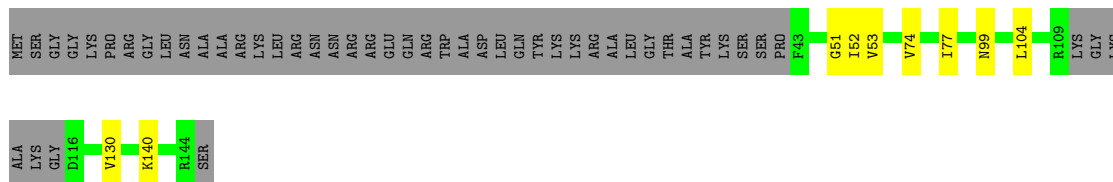
- Molecule 44: 40S ribosomal protein S11-like protein



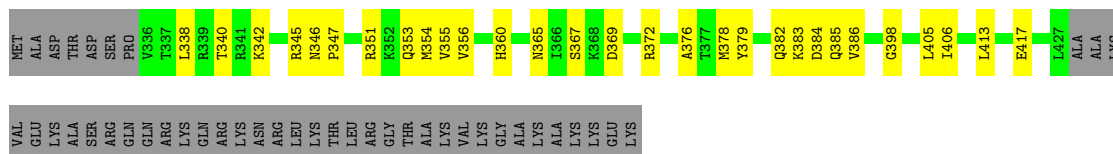
- Molecule 45: 40S ribosomal protein S22-like protein



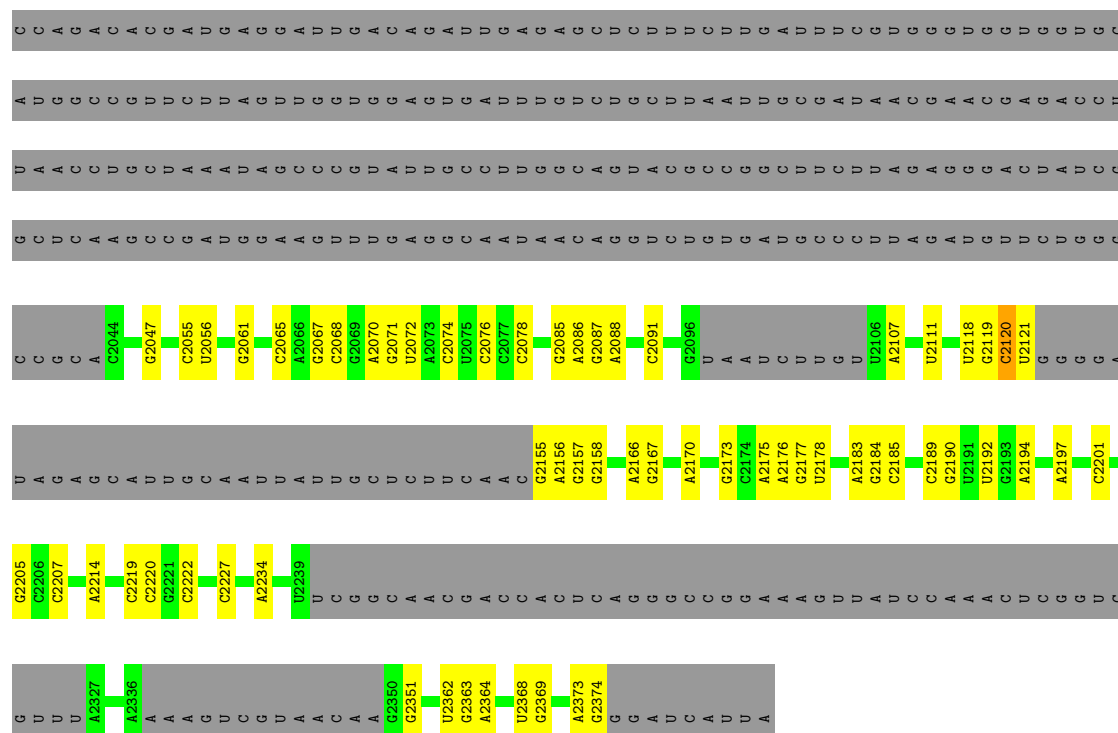
- Molecule 46: 40S ribosomal protein s23-like protein



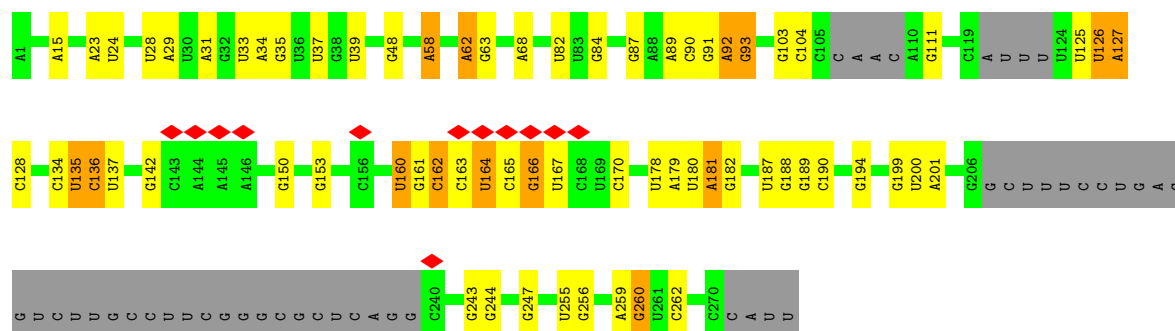
- Molecule 47: Small ribosomal subunit protein eS24



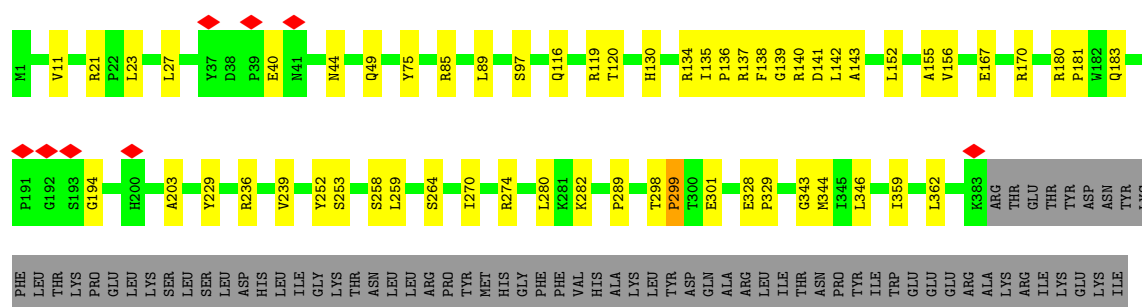




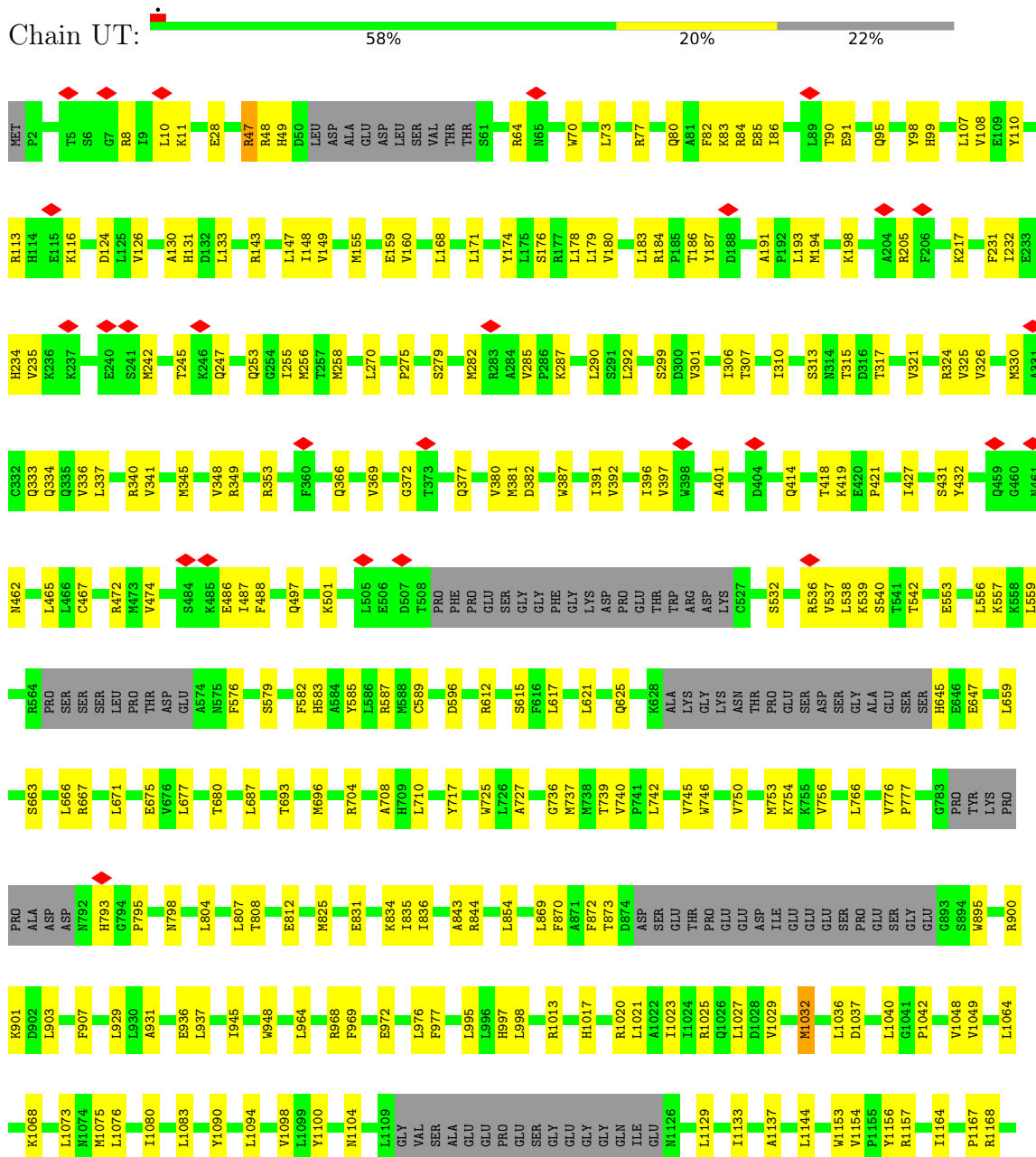
• Molecule 51: u3 rna



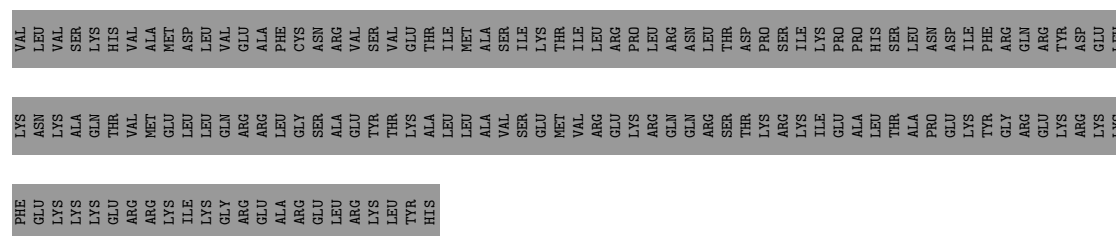
• Molecule 52: Ribosome biogenesis protein ENP2



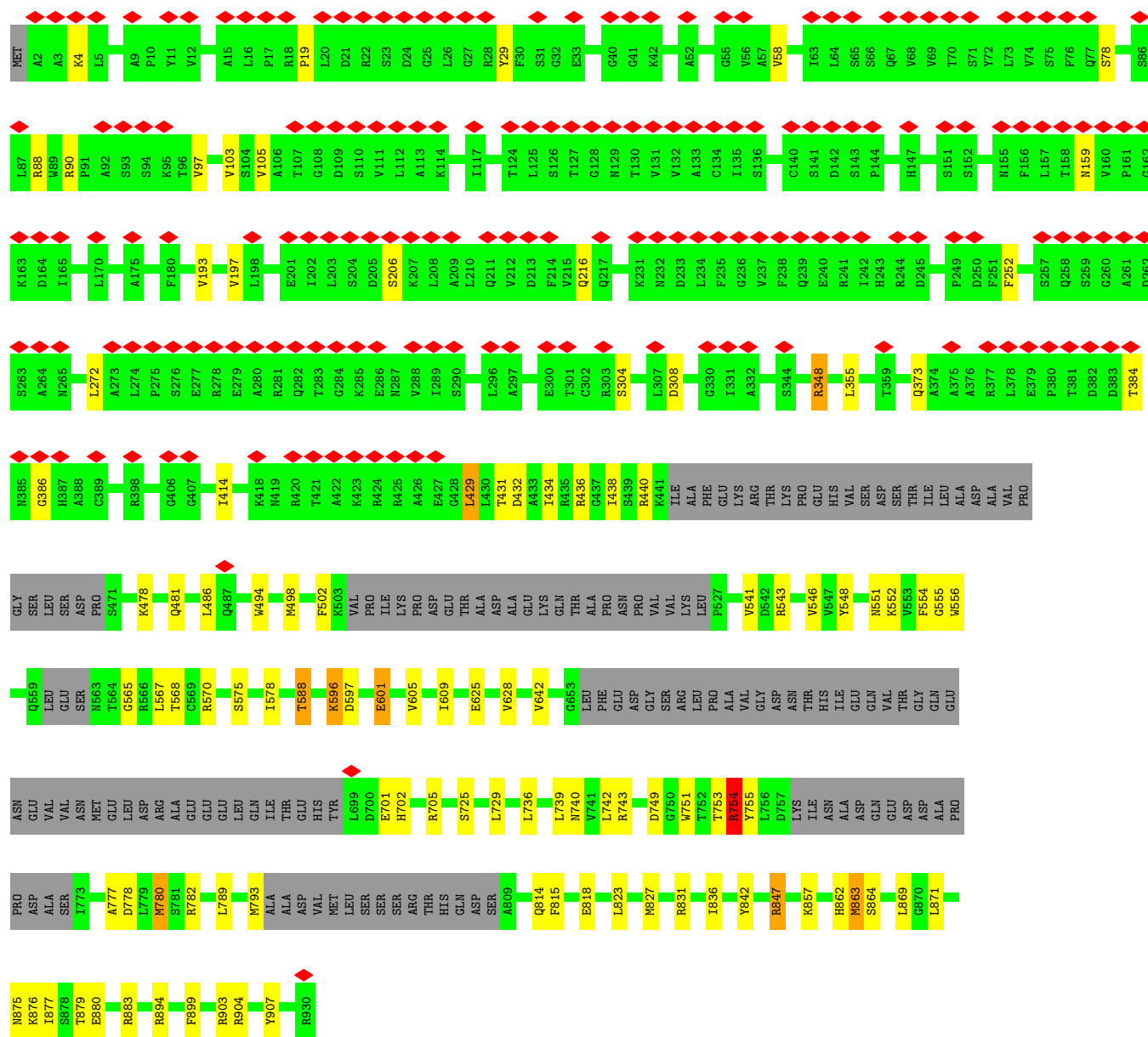
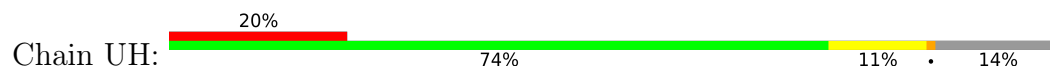
- Molecule 53: UTP20



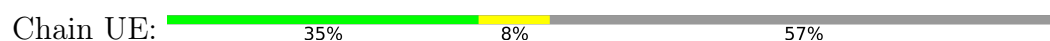


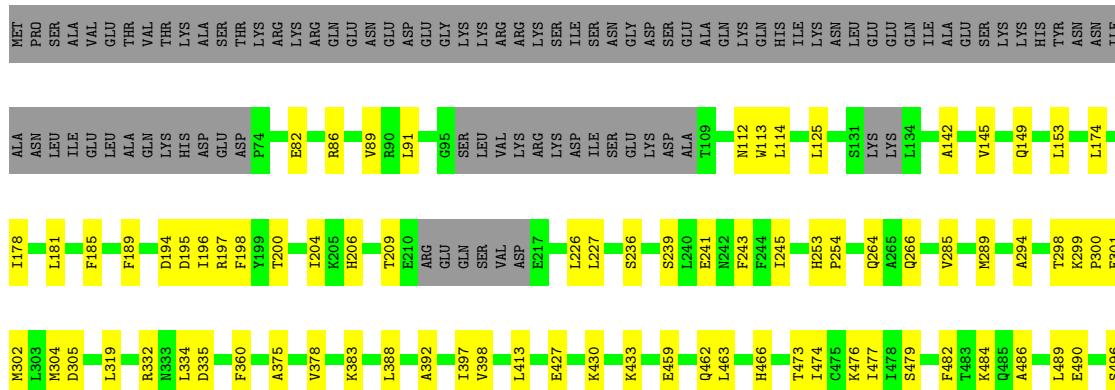


• Molecule 54: UTP8



• Molecule 55: Small-subunit processome Utp12 domain-containing protein





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	70904	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE; Relion	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	44	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.452	Depositor
Minimum map value	-0.240	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.017	Depositor
Map size ($\text{\AA}$)	501.59998, 501.59998, 501.59998	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.045, 1.045, 1.045	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, MG, GTP, ZN, SEP, A2M, OMC

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	UA	0.32	0/6555	0.60	3/8909 (0.0%)
2	UB	0.26	0/4592	0.60	1/6178 (0.0%)
3	UC	0.42	0/2001	0.70	0/2680
4	UD	0.30	0/6250	0.62	2/8465 (0.0%)
5	UF	0.27	0/2665	0.57	1/3606 (0.0%)
6	UG	0.29	0/3838	0.58	2/5181 (0.0%)
7	UJ	0.30	0/12938	0.68	6/17550 (0.0%)
8	UK	0.25	0/1709	0.47	0/2261
9	UL	0.28	0/6299	0.69	1/8531 (0.0%)
10	UM	0.23	0/6680	0.59	2/9090 (0.0%)
11	UN	0.28	0/1425	0.52	1/1913 (0.1%)
12	UO	0.29	0/3895	0.60	0/5302
13	UQ	0.33	0/6136	0.66	2/8348 (0.0%)
14	UR	0.29	0/3557	0.57	1/4805 (0.0%)
15	UU	0.29	0/6947	0.60	4/9452 (0.0%)
16	UX	0.29	0/1503	0.63	0/2022
17	UZ	0.22	0/1857	0.63	0/2526
18	CA	0.31	0/1814	0.57	1/2456 (0.0%)
18	CB	0.26	0/1853	0.62	0/2511
19	CC	0.24	0/2911	0.53	0/3937
20	CD	0.25	0/3412	0.60	2/4617 (0.0%)
21	CE	0.26	0/891	0.52	0/1214
21	CF	0.25	0/876	0.54	0/1195
22	CG	0.27	0/3307	0.65	0/4462
23	CH	0.29	0/2939	0.59	1/3988 (0.0%)
24	CI	0.28	0/6813	0.56	2/9182 (0.0%)
25	CJ	0.29	0/1462	0.49	0/1967
26	CK	0.28	0/2376	0.54	0/3214
27	CL	0.26	0/2504	0.53	1/3377 (0.0%)
28	CM	0.30	0/3573	0.59	0/4829
29	CN	0.34	0/1797	0.66	0/2443
29	CO	0.29	0/1714	0.66	0/2325

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
30	CP	0.25	0/1923	0.52	0/2577
31	CQ	0.22	0/1436	0.51	0/1932
32	CR	0.25	0/6809	0.66	3/9215 (0.0%)
32	CS	0.29	0/6722	0.70	6/9099 (0.1%)
33	CT	0.24	0/1053	0.49	0/1413
34	Ca	0.28	0/1850	0.68	6/2486 (0.2%)
35	Cb	0.30	0/1890	0.75	0/2548
36	Cc	0.26	0/1485	0.52	0/2008
37	Cd	0.29	0/1850	0.68	4/2474 (0.2%)
38	Ce	0.30	0/1298	0.74	2/1750 (0.1%)
39	Cf	0.25	0/1429	0.61	0/1915
40	Cg	0.28	0/1265	0.56	0/1694
41	Ch	0.23	0/557	0.62	0/749
42	Ci	0.24	0/819	0.52	0/1107
43	Cj	0.28	0/958	0.55	0/1293
44	Ck	0.21	0/1107	0.52	0/1486
45	Cm	0.27	0/1001	0.56	0/1345
46	Cn	0.30	0/712	0.61	0/954
47	Co	0.26	0/754	0.74	0/1011
48	Cp	0.28	0/461	0.52	0/620
49	CU	0.23	0/1350	0.49	0/1810
50	C1	0.24	0/37474	0.30	0/58363
51	C2	0.23	0/5434	0.29	0/8459
52	CW	0.25	0/3004	0.65	0/4085
53	UT	0.28	0/16312	0.71	6/22073 (0.0%)
54	UH	0.58	0/6301	0.99	5/8526 (0.1%)
55	UE	0.29	0/1374	0.69	2/1852 (0.1%)
55	UI	0.29	0/1005	0.75	0/1352
56	US	0.30	0/3765	0.68	2/5100 (0.0%)
57	Cl	0.20	0/638	0.67	2/857 (0.2%)
58	CX	0.23	0/2180	0.58	0/2956
59	CY	0.25	0/2111	0.60	1/2816 (0.0%)
60	CZ	0.26	0/2298	0.62	1/3080 (0.0%)
61	UP	0.26	0/428	0.56	0/570
All	All	0.29	0/236142	0.59	73/328111 (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
7	UJ	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
13	UQ	0	1
15	UU	0	1
17	UZ	0	1
18	CB	0	1
20	CD	0	2
22	CG	0	2
28	CM	0	1
29	CO	0	1
32	CS	0	2
38	Ce	0	1
52	CW	0	1
53	UT	0	2
54	UH	0	2
All	All	0	20

There are no bond length outliers.

The worst 5 of 73 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	UJ	1427	GLN	CA-C-N	9.54	139.76	121.54
7	UJ	1427	GLN	C-N-CA	9.54	139.76	121.54
53	UT	1032	MET	CA-CB-CG	8.23	130.57	114.10
32	CS	578	ARG	CA-C-N	8.18	131.78	120.65
32	CS	578	ARG	C-N-CA	8.18	131.78	120.65

There are no chirality outliers.

5 of 20 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	UJ	1427	GLN	Peptide
7	UJ	1768	SER	Peptide
13	UQ	849	ALA	Peptide
15	UU	205	ASP	Peptide
17	UZ	273	GLN	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	UA	6411	0	6306	66	0
2	UB	4506	0	4633	65	0
3	UC	1970	0	2023	24	0
4	UD	6108	0	6108	128	0
5	UF	2599	0	2650	27	0
6	UG	3765	0	3800	35	0
7	UJ	12725	0	13039	251	0
8	UK	1695	0	1828	22	0
9	UL	6175	0	6188	95	0
10	UM	6545	0	6547	110	0
11	UN	1401	0	1455	22	0
12	UO	3811	0	3861	50	0
13	UQ	6008	0	6033	92	0
14	UR	3495	0	3506	43	0
15	UU	6778	0	6782	93	0
16	UX	1480	0	1554	22	0
17	UZ	1815	0	1896	21	0
18	CA	1778	0	1830	21	0
18	CB	1816	0	1847	35	0
19	CC	2866	0	2960	43	0
20	CD	3355	0	3483	46	0
21	CE	879	0	918	10	0
21	CF	864	0	900	9	0
22	CG	3245	0	3262	57	0
23	CH	2888	0	2979	49	0
24	CI	6666	0	6825	84	0
25	CJ	1434	0	1482	20	0
26	CK	2329	0	2373	22	0
27	CL	2466	0	2532	36	0
28	CM	3501	0	3498	45	0
29	CN	1762	0	1807	30	0
29	CO	1683	0	1726	35	0
30	CP	1893	0	1993	26	0
31	CQ	1413	0	1479	12	0
32	CR	6677	0	6809	128	0
32	CS	6591	0	6674	154	0
33	CT	1035	0	1063	12	0
34	Ca	1821	0	1936	28	0
35	Cb	1851	0	1905	42	0
36	Cc	1464	0	1504	15	0
37	Cd	1819	0	1920	45	0
38	Ce	1279	0	1322	22	0
39	Cf	1398	0	1401	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	Cg	1248	0	1365	23	0
41	Ch	546	0	580	11	0
42	Ci	808	0	831	11	0
43	Cj	943	0	1002	15	0
44	Ck	1082	0	1138	20	0
45	Cm	985	0	1021	15	0
46	Cn	702	0	750	7	0
47	Co	741	0	785	25	0
48	Cp	458	0	489	7	0
49	CU	1337	0	1376	15	0
50	C1	33584	0	17007	212	0
51	C2	4869	0	2465	22	0
52	CW	2932	0	2866	42	0
53	UT	15998	0	16397	338	0
54	UH	6198	0	6272	69	0
55	UE	1362	0	1440	28	0
55	UI	996	0	1054	19	0
56	US	3672	0	3679	58	0
57	Cl	633	0	676	9	0
58	CX	2130	0	2219	36	0
59	CY	2095	0	2185	44	0
60	CZ	2270	0	2273	50	0
61	UP	422	0	457	7	0
62	UX	1	0	0	0	0
63	CI	32	0	12	0	0
64	CI	1	0	0	0	0
65	CS	27	0	11	3	0
All	All	228132	0	212987	2905	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 2905 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)
24:CI:286:VAL:O	24:CI:293:ASP:HA	1.31	1.30
4:UD:441:THR:HA	4:UD:456:LEU:O	1.43	1.17
54:UH:555:GLY:O	54:UH:567:LEU:HA	1.47	1.12
53:UT:1168:ARG:O	53:UT:1172:LEU:HB2	1.50	1.08
15:UU:159:ILE:O	15:UU:172:THR:HA	1.53	1.07

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	
1	UA	834/904 (92%)	800 (96%)	34 (4%)	0	100	100
2	UB	556/907 (61%)	531 (96%)	25 (4%)	0	100	100
3	UC	242/648 (37%)	232 (96%)	10 (4%)	0	100	100
4	UD	761/884 (86%)	731 (96%)	30 (4%)	0	100	100
5	UF	325/414 (78%)	315 (97%)	10 (3%)	0	100	100
6	UG	475/558 (85%)	452 (95%)	22 (5%)	1 (0%)	43	73
7	UJ	1620/1802 (90%)	1532 (95%)	81 (5%)	7 (0%)	30	61
8	UK	211/270 (78%)	207 (98%)	4 (2%)	0	100	100
9	UL	767/962 (80%)	714 (93%)	53 (7%)	0	100	100
10	UM	835/912 (92%)	789 (94%)	45 (5%)	1 (0%)	48	78
11	UN	171/633 (27%)	169 (99%)	2 (1%)	0	100	100
12	UO	497/557 (89%)	475 (96%)	21 (4%)	1 (0%)	43	73
13	UQ	775/960 (81%)	724 (93%)	49 (6%)	2 (0%)	36	67
14	UR	436/618 (71%)	423 (97%)	13 (3%)	0	100	100
15	UU	896/1049 (85%)	847 (94%)	47 (5%)	2 (0%)	43	73
16	UX	188/193 (97%)	177 (94%)	11 (6%)	0	100	100
17	UZ	229/391 (59%)	218 (95%)	11 (5%)	0	100	100
18	CA	238/313 (76%)	225 (94%)	13 (6%)	0	100	100
18	CB	235/313 (75%)	226 (96%)	9 (4%)	0	100	100
19	CC	383/523 (73%)	364 (95%)	18 (5%)	1 (0%)	36	67
20	CD	444/582 (76%)	430 (97%)	14 (3%)	0	100	100
21	CE	119/127 (94%)	116 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	CF	118/127 (93%)	112 (95%)	6 (5%)	0	100	100
22	CG	402/630 (64%)	390 (97%)	12 (3%)	0	100	100
23	CH	383/411 (93%)	375 (98%)	8 (2%)	0	100	100
24	CI	829/1163 (71%)	805 (97%)	23 (3%)	1 (0%)	48	78
25	CJ	177/183 (97%)	177 (100%)	0	0	100	100
26	CK	295/297 (99%)	285 (97%)	10 (3%)	0	100	100
27	CL	310/720 (43%)	294 (95%)	15 (5%)	1 (0%)	36	67
28	CM	443/446 (99%)	422 (95%)	21 (5%)	0	100	100
29	CN	222/252 (88%)	212 (96%)	10 (4%)	0	100	100
29	CO	211/252 (84%)	199 (94%)	11 (5%)	1 (0%)	24	57
30	CP	227/322 (70%)	220 (97%)	7 (3%)	0	100	100
31	CQ	178/259 (69%)	172 (97%)	6 (3%)	0	100	100
32	CR	836/1073 (78%)	793 (95%)	42 (5%)	1 (0%)	48	78
32	CS	826/1073 (77%)	784 (95%)	42 (5%)	0	100	100
33	CT	127/203 (63%)	120 (94%)	7 (6%)	0	100	100
34	Ca	223/255 (88%)	210 (94%)	12 (5%)	1 (0%)	30	61
35	Cb	230/264 (87%)	216 (94%)	14 (6%)	0	100	100
36	Cc	188/212 (89%)	180 (96%)	8 (4%)	0	100	100
37	Cd	224/239 (94%)	214 (96%)	10 (4%)	0	100	100
38	Ce	155/203 (76%)	139 (90%)	16 (10%)	0	100	100
39	Cf	170/202 (84%)	168 (99%)	2 (1%)	0	100	100
40	Cg	157/190 (83%)	155 (99%)	2 (1%)	0	100	100
41	Ch	64/151 (42%)	63 (98%)	1 (2%)	0	100	100
42	Ci	113/150 (75%)	109 (96%)	4 (4%)	0	100	100
43	Cj	124/143 (87%)	119 (96%)	5 (4%)	0	100	100
44	Ck	127/161 (79%)	121 (95%)	6 (5%)	0	100	100
45	Cm	122/130 (94%)	114 (93%)	8 (7%)	0	100	100
46	Cn	92/145 (63%)	90 (98%)	2 (2%)	0	100	100
47	Co	90/136 (66%)	83 (92%)	6 (7%)	1 (1%)	11	39
48	Cp	59/68 (87%)	56 (95%)	3 (5%)	0	100	100
49	CU	168/311 (54%)	161 (96%)	7 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	CW	381/668 (57%)	353 (93%)	28 (7%)	0	100	100
53	UT	1981/2612 (76%)	1873 (94%)	104 (5%)	4 (0%)	43	73
54	UH	787/930 (85%)	752 (96%)	29 (4%)	6 (1%)	16	47
55	UE	172/410 (42%)	156 (91%)	16 (9%)	0	100	100
55	UI	126/410 (31%)	120 (95%)	6 (5%)	0	100	100
56	US	443/549 (81%)	424 (96%)	18 (4%)	1 (0%)	43	73
57	Cl	78/156 (50%)	71 (91%)	7 (9%)	0	100	100
58	CX	265/480 (55%)	250 (94%)	15 (6%)	0	100	100
59	CY	258/381 (68%)	251 (97%)	7 (3%)	0	100	100
60	CZ	279/609 (46%)	268 (96%)	11 (4%)	0	100	100
61	UP	52/364 (14%)	50 (96%)	2 (4%)	0	100	100
All	All	23949/32460 (74%)	22823 (95%)	1094 (5%)	32 (0%)	49	78

5 of 32 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	UJ	1428	HIS
7	UJ	1430	PRO
32	CR	211	ILE
34	Ca	55	LYS
13	UQ	171	THR

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	UA	662/774 (86%)	662 (100%)	0	100	100
2	UB	474/788 (60%)	473 (100%)	1 (0%)	87	89
3	UC	208/536 (39%)	200 (96%)	8 (4%)	29	60
4	UD	657/738 (89%)	657 (100%)	0	100	100
5	UF	250/341 (73%)	250 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	UG	386/474 (81%)	386 (100%)	0	100	100
7	UJ	1379/1526 (90%)	1369 (99%)	10 (1%)	76	82
8	UK	161/227 (71%)	161 (100%)	0	100	100
9	UL	667/821 (81%)	667 (100%)	0	100	100
10	UM	712/770 (92%)	710 (100%)	2 (0%)	86	87
11	UN	146/522 (28%)	146 (100%)	0	100	100
12	UO	403/456 (88%)	402 (100%)	1 (0%)	87	89
13	UQ	650/817 (80%)	641 (99%)	9 (1%)	59	76
14	UR	359/523 (69%)	359 (100%)	0	100	100
15	UU	677/863 (78%)	677 (100%)	0	100	100
16	UX	152/167 (91%)	152 (100%)	0	100	100
17	UZ	186/329 (56%)	186 (100%)	0	100	100
18	CA	175/228 (77%)	175 (100%)	0	100	100
18	CB	195/228 (86%)	195 (100%)	0	100	100
19	CC	287/435 (66%)	287 (100%)	0	100	100
20	CD	344/489 (70%)	344 (100%)	0	100	100
21	CE	91/108 (84%)	91 (100%)	0	100	100
21	CF	88/108 (82%)	88 (100%)	0	100	100
22	CG	331/525 (63%)	331 (100%)	0	100	100
23	CH	303/320 (95%)	302 (100%)	1 (0%)	86	87
24	CI	681/1009 (68%)	680 (100%)	1 (0%)	88	90
25	CJ	147/169 (87%)	147 (100%)	0	100	100
26	CK	245/266 (92%)	245 (100%)	0	100	100
27	CL	251/588 (43%)	251 (100%)	0	100	100
28	CM	364/383 (95%)	364 (100%)	0	100	100
29	CN	202/223 (91%)	201 (100%)	1 (0%)	81	85
29	CO	193/223 (86%)	192 (100%)	1 (0%)	81	85
30	CP	202/287 (70%)	202 (100%)	0	100	100
31	CQ	151/215 (70%)	151 (100%)	0	100	100
32	CR	731/916 (80%)	731 (100%)	0	100	100
32	CS	722/916 (79%)	721 (100%)	1 (0%)	88	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	CT	108/167 (65%)	108 (100%)	0	100	100
34	Ca	198/223 (89%)	198 (100%)	0	100	100
35	Cb	199/221 (90%)	199 (100%)	0	100	100
36	Cc	149/178 (84%)	149 (100%)	0	100	100
37	Cd	192/204 (94%)	192 (100%)	0	100	100
38	Ce	137/177 (77%)	137 (100%)	0	100	100
39	Cf	139/164 (85%)	139 (100%)	0	100	100
40	Cg	123/162 (76%)	123 (100%)	0	100	100
41	Ch	58/130 (45%)	58 (100%)	0	100	100
42	Ci	78/117 (67%)	78 (100%)	0	100	100
43	Cj	92/115 (80%)	92 (100%)	0	100	100
44	Ck	117/143 (82%)	116 (99%)	1 (1%)	70	80
45	Cm	103/113 (91%)	103 (100%)	0	100	100
46	Cn	70/116 (60%)	70 (100%)	0	100	100
47	Co	79/115 (69%)	79 (100%)	0	100	100
48	Cp	47/61 (77%)	47 (100%)	0	100	100
49	CU	137/260 (53%)	137 (100%)	0	100	100
52	CW	310/587 (53%)	310 (100%)	0	100	100
53	UT	1725/2276 (76%)	1725 (100%)	0	100	100
54	UH	674/788 (86%)	664 (98%)	10 (2%)	57	75
55	UE	148/346 (43%)	148 (100%)	0	100	100
55	UI	108/346 (31%)	108 (100%)	0	100	100
56	US	404/493 (82%)	402 (100%)	2 (0%)	81	85
57	Cl	71/135 (53%)	71 (100%)	0	100	100
58	CX	227/411 (55%)	227 (100%)	0	100	100
59	CY	225/322 (70%)	225 (100%)	0	100	100
60	CZ	238/519 (46%)	238 (100%)	0	100	100
61	UP	44/314 (14%)	44 (100%)	0	100	100
All	All	20032/27511 (73%)	19983 (100%)	49 (0%)	85	89

5 of 49 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	UQ	726	VAL
32	CS	655	GLN
13	UQ	753	VAL
24	CI	612	ASN
54	UH	429	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 214 such sidechains are listed below:

Mol	Chain	Res	Type
28	CM	77	ASN
32	CS	741	GLN
54	UH	232	ASN
28	CM	421	ASN
32	CR	819	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
50	C1	1549/2344 (66%)	354 (22%)	23 (1%)
51	C2	225/274 (82%)	57 (25%)	2 (0%)
All	All	1774/2618 (67%)	411 (23%)	25 (1%)

5 of 411 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
50	C1	4	G
50	C1	5	G
50	C1	7	A
50	C1	14	G
50	C1	16	U

5 of 25 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
50	C1	1017	C
50	C1	1163	A
51	C2	255	U
50	C1	1087	G
50	C1	1712	C

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

4 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$
50	OMC	C1	998	50	19,22,23	2.92	8 (42%)	26,31,34	0.67	0
14	SEP	UR	139	14	8,9,10	1.51	1 (12%)	8,12,14	1.79	2 (25%)
50	A2M	C1	1004	50	22,25,26	3.44	9 (40%)	31,36,39	2.71	10 (32%)
1	SEP	UA	646	1	8,9,10	0.67	0	8,12,14	1.11	1 (12%)

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
50	OMC	C1	998	50	-	0/9/27/28	0/2/2/2
14	SEP	UR	139	14	-	0/5/8/10	-
50	A2M	C1	1004	50	-	0/9/27/28	0/3/3/3
1	SEP	UA	646	1	-	4/5/8/10	-

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	C1	1004	A2M	C2'-C1'	-8.57	1.31	1.53
50	C1	1004	A2M	O4'-C1'	8.40	1.61	1.42
50	C1	1004	A2M	O4'-C4'	-6.57	1.30	1.45
50	C1	998	OMC	C2-N3	6.18	1.48	1.36
50	C1	998	OMC	C6-C5	5.86	1.48	1.35

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	C1	1004	A2M	N6-C6-N1	-7.08	102.84	118.35
50	C1	1004	A2M	C5-C6-N6	6.22	136.96	123.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	C1	1004	A2M	N3-C2-N1	-5.51	119.98	128.60
50	C1	1004	A2M	C5-C4-N3	-5.42	119.68	126.75
50	C1	1004	A2M	N9-C8-N7	-4.28	108.06	113.91

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	UA	646	SEP	CB-OG-P-O1P
1	UA	646	SEP	CB-OG-P-O2P
1	UA	646	SEP	N-CA-CB-OG
1	UA	646	SEP	CB-OG-P-O3P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
50	C1	1004	A2M	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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$
63	GTP	CI	1201	64	30,34,34	0.90	2 (6%)	46,54,54	1.80	11 (23%)
65	ADP	CS	1101	-	27,29,29	2.96	9 (33%)	42,45,45	2.09	15 (35%)

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
63	GTP	CI	1201	64	-	3/22/38/38	0/3/3/3
65	ADP	CS	1101	-	-	0/16/32/32	0/3/3/3

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
65	CS	1101	ADP	O4'-C1'	8.38	1.61	1.42
65	CS	1101	ADP	C2'-C1'	-7.06	1.30	1.53
65	CS	1101	ADP	O4'-C4'	-6.46	1.30	1.45
65	CS	1101	ADP	C6-N6	4.70	1.45	1.34
65	CS	1101	ADP	O3'-C3'	-2.94	1.36	1.43

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
65	CS	1101	ADP	N3-C2-N1	-5.52	119.97	128.60
65	CS	1101	ADP	C5-C4-N3	-5.02	120.20	126.75
63	CI	1201	GTP	C5-C4-N3	-4.91	120.49	128.46
63	CI	1201	GTP	C2-N3-C4	4.47	120.27	112.30
65	CS	1101	ADP	N9-C8-N7	-4.11	108.29	113.91

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
63	CI	1201	GTP	PB-O3B-PG-O1G
63	CI	1201	GTP	PB-O3A-PA-O2A
63	CI	1201	GTP	O4'-C4'-C5'-O5'

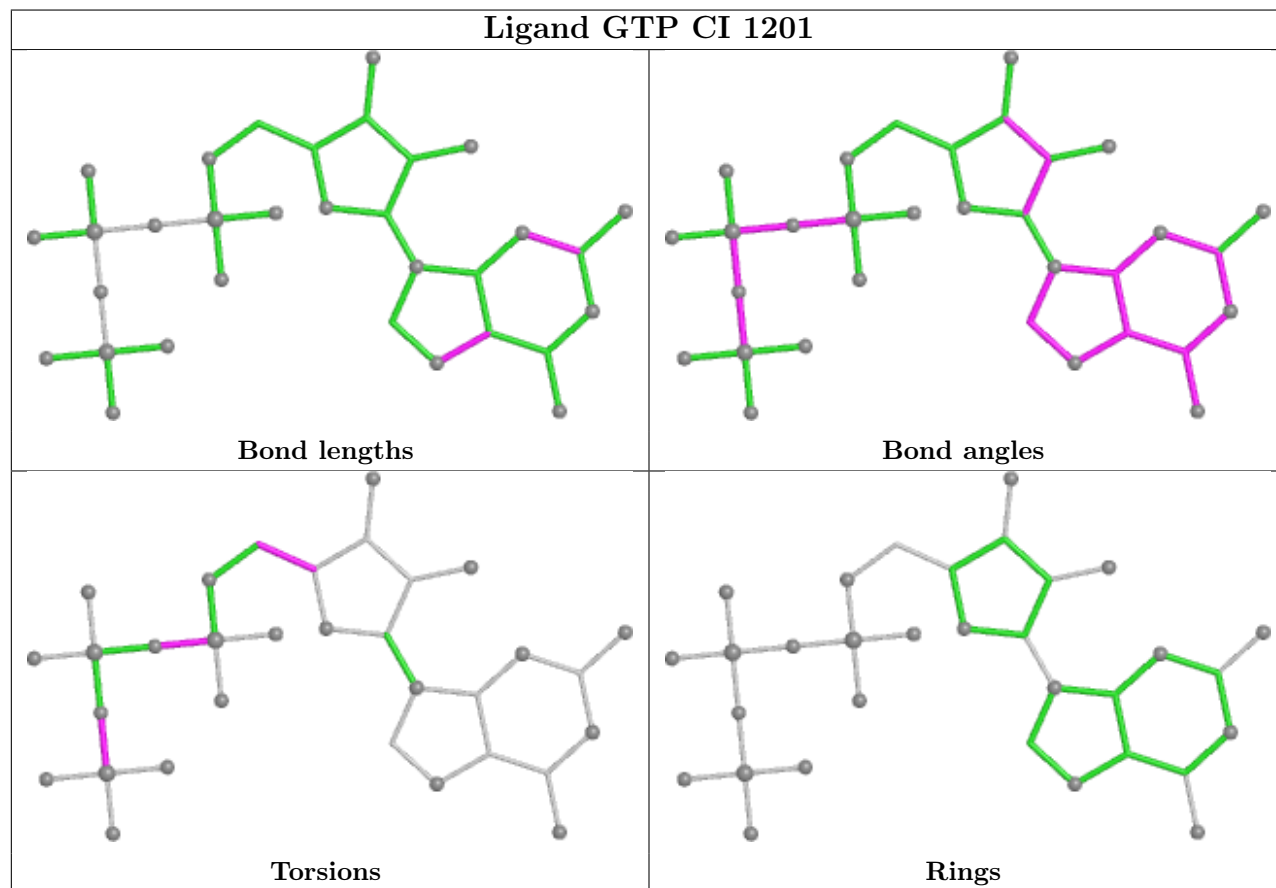
There are no ring outliers.

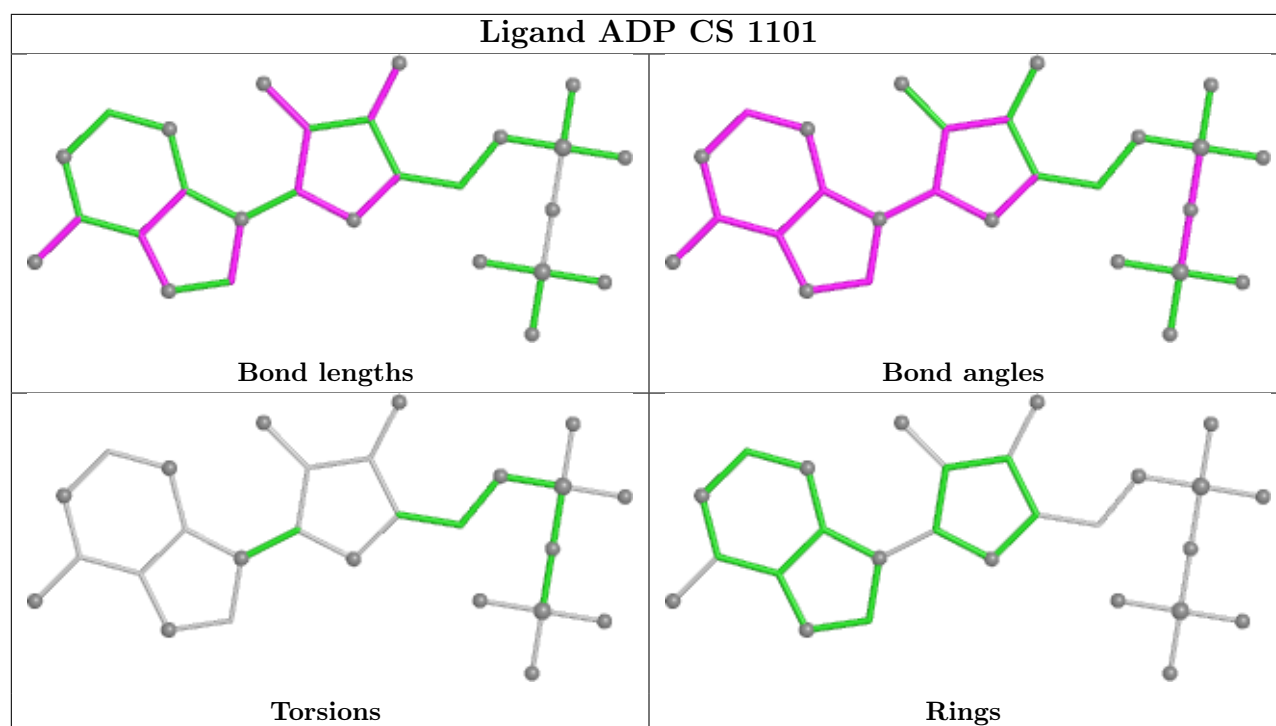
1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
65	CS	1101	ADP	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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.

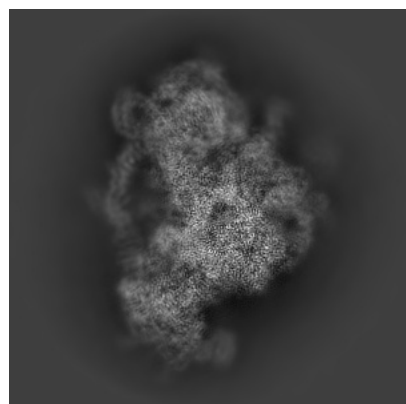
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-66687. These allow visual inspection of the internal detail of the map and identification of artifacts.

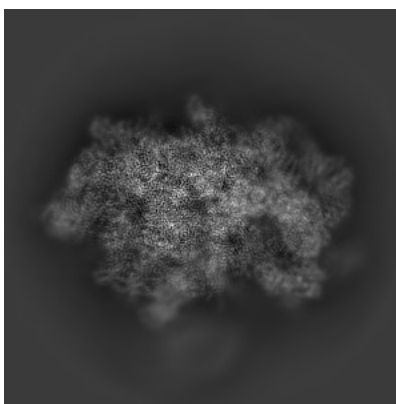
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

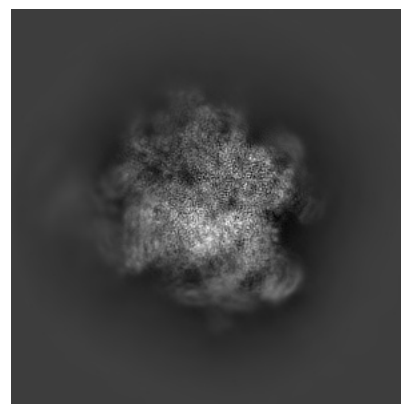
6.1.1 Primary map



X

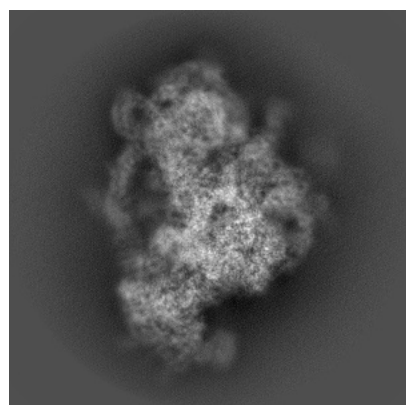


Y

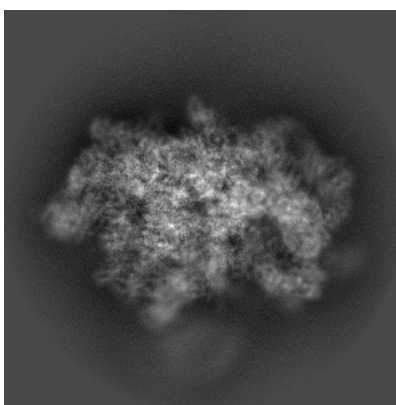


Z

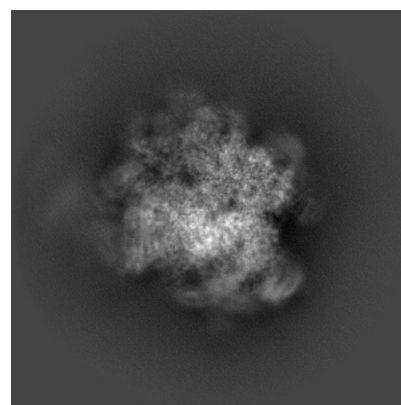
6.1.2 Raw map



X



Y

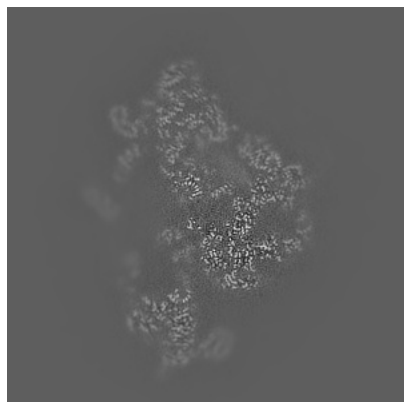


Z

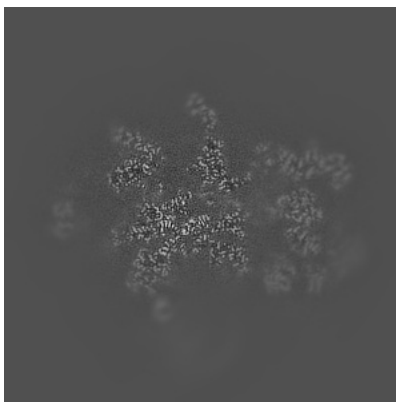
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

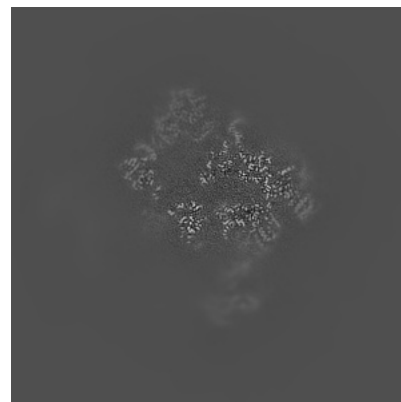
6.2.1 Primary map



X Index: 240

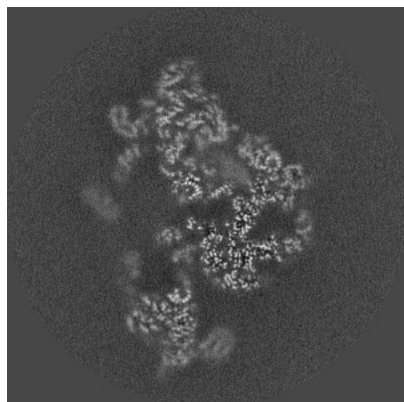


Y Index: 240

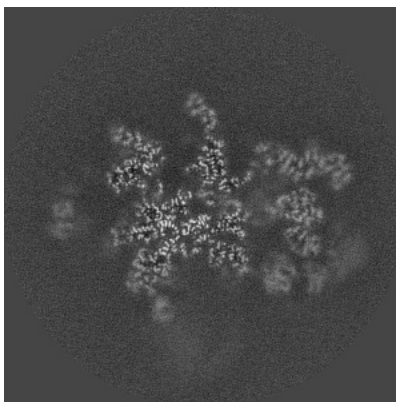


Z Index: 240

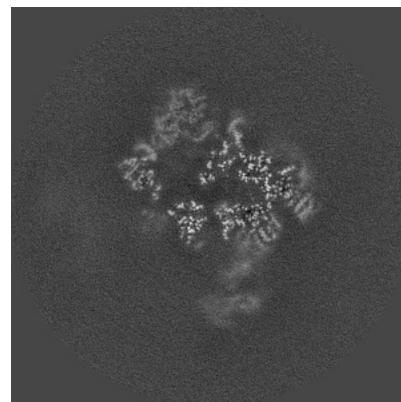
6.2.2 Raw map



X Index: 240



Y Index: 240

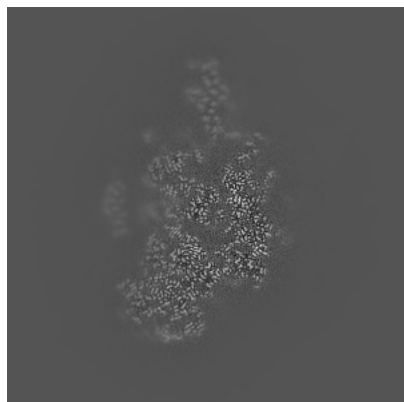


Z Index: 240

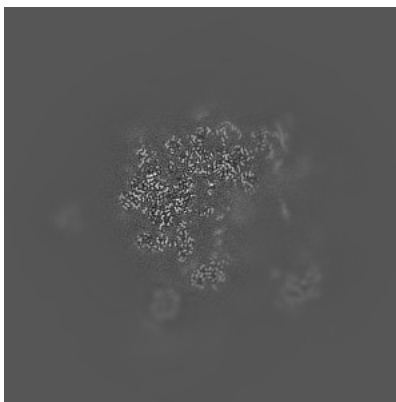
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

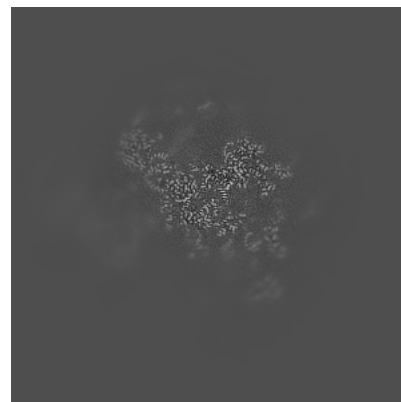
6.3.1 Primary map



X Index: 285

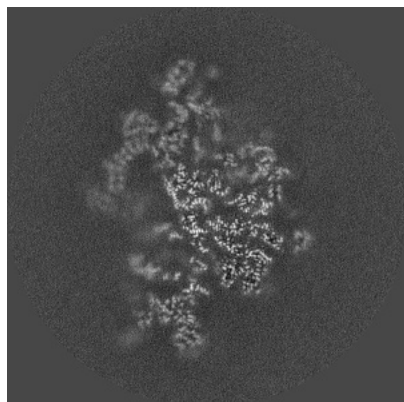


Y Index: 271

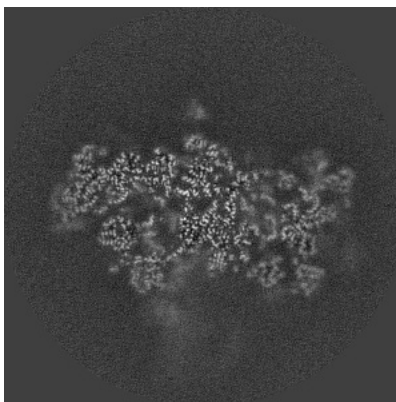


Z Index: 217

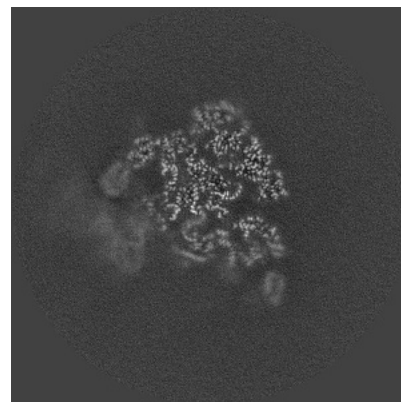
6.3.2 Raw map



X Index: 258



Y Index: 223

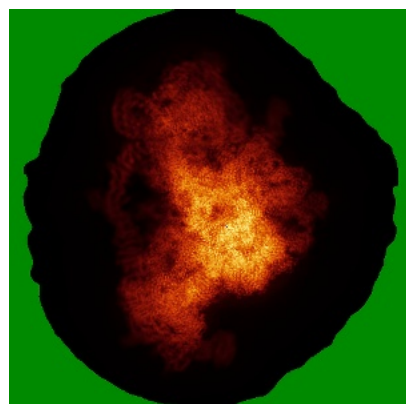


Z Index: 202

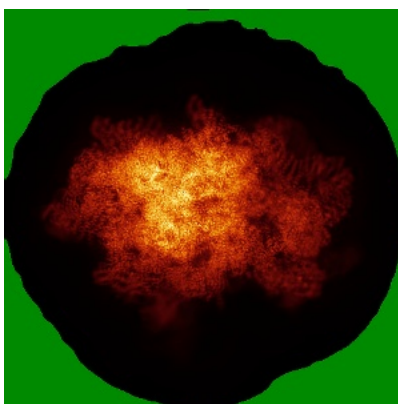
The images above show the largest variance slices of the map in three orthogonal directions.

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

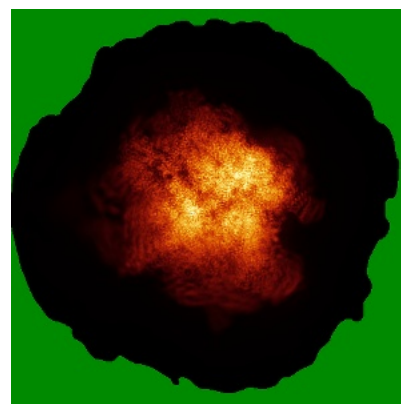
6.4.1 Primary map



X

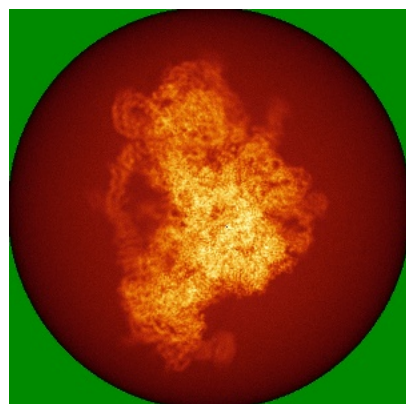


Y

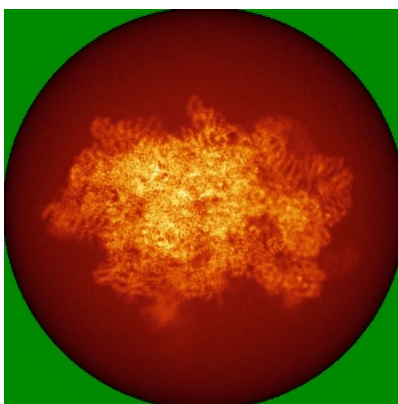


Z

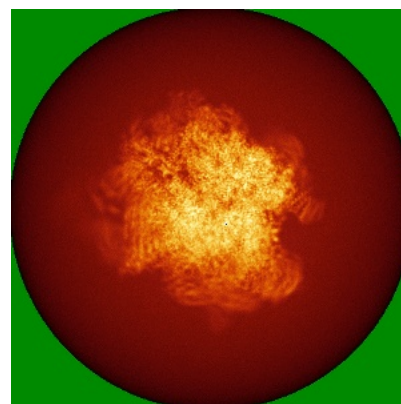
6.4.2 Raw map



X



Y

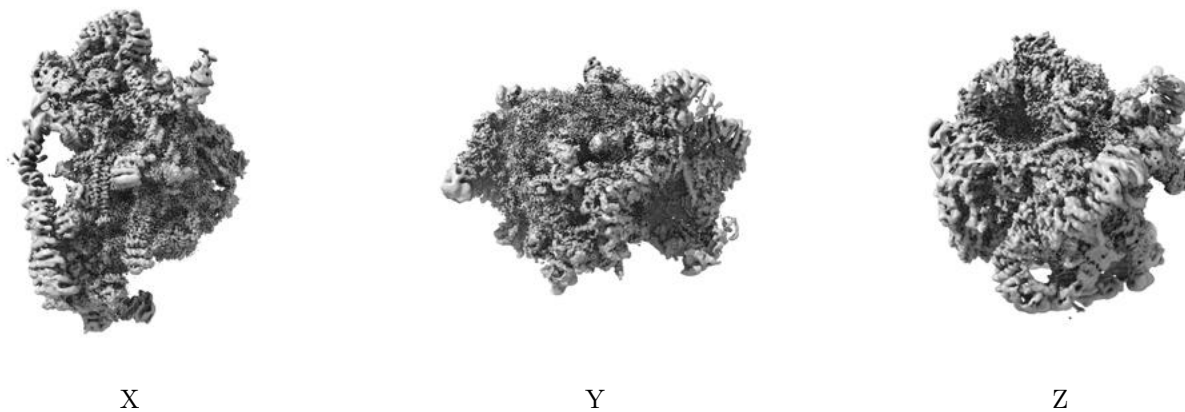


Z

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.

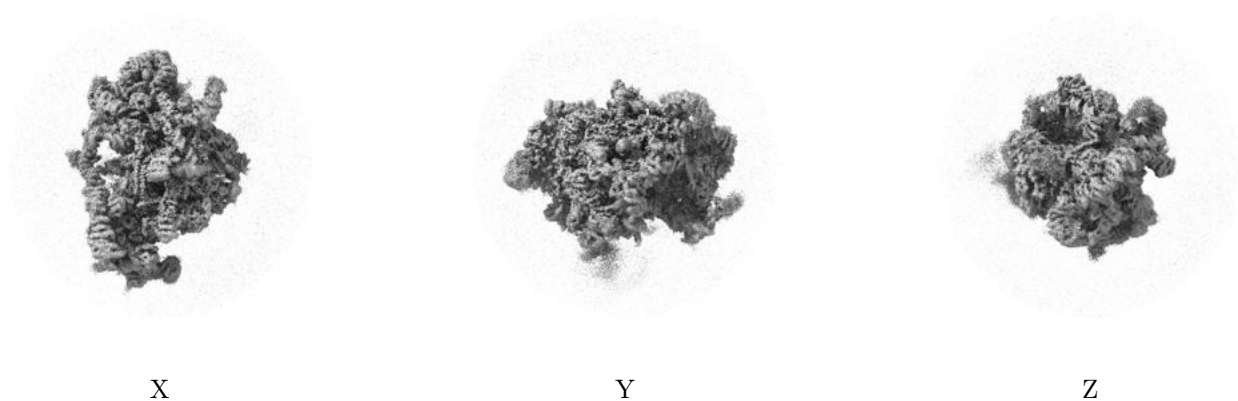
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.017. 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.

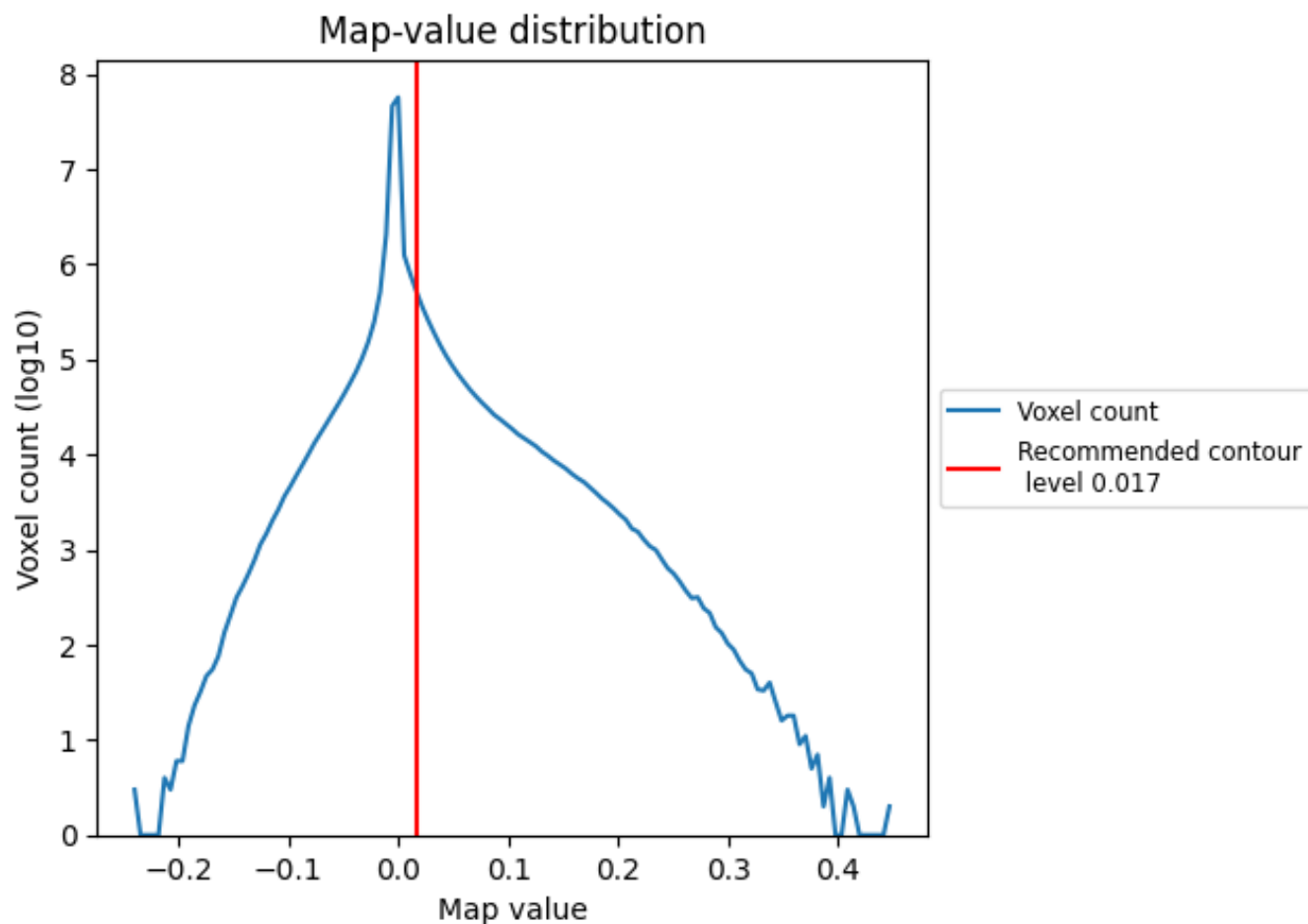
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

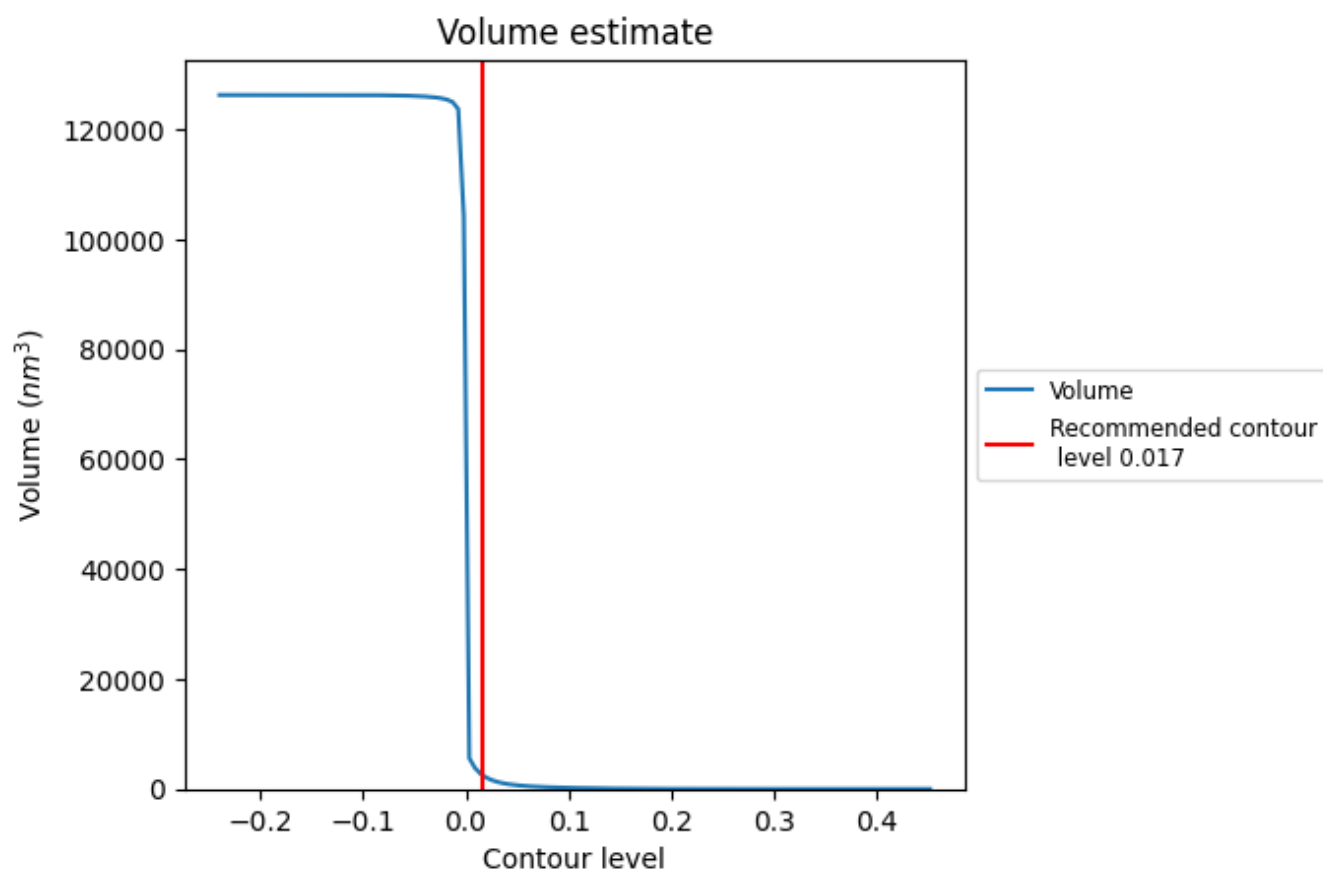
This section contains the results of statistical analysis of the map.

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.

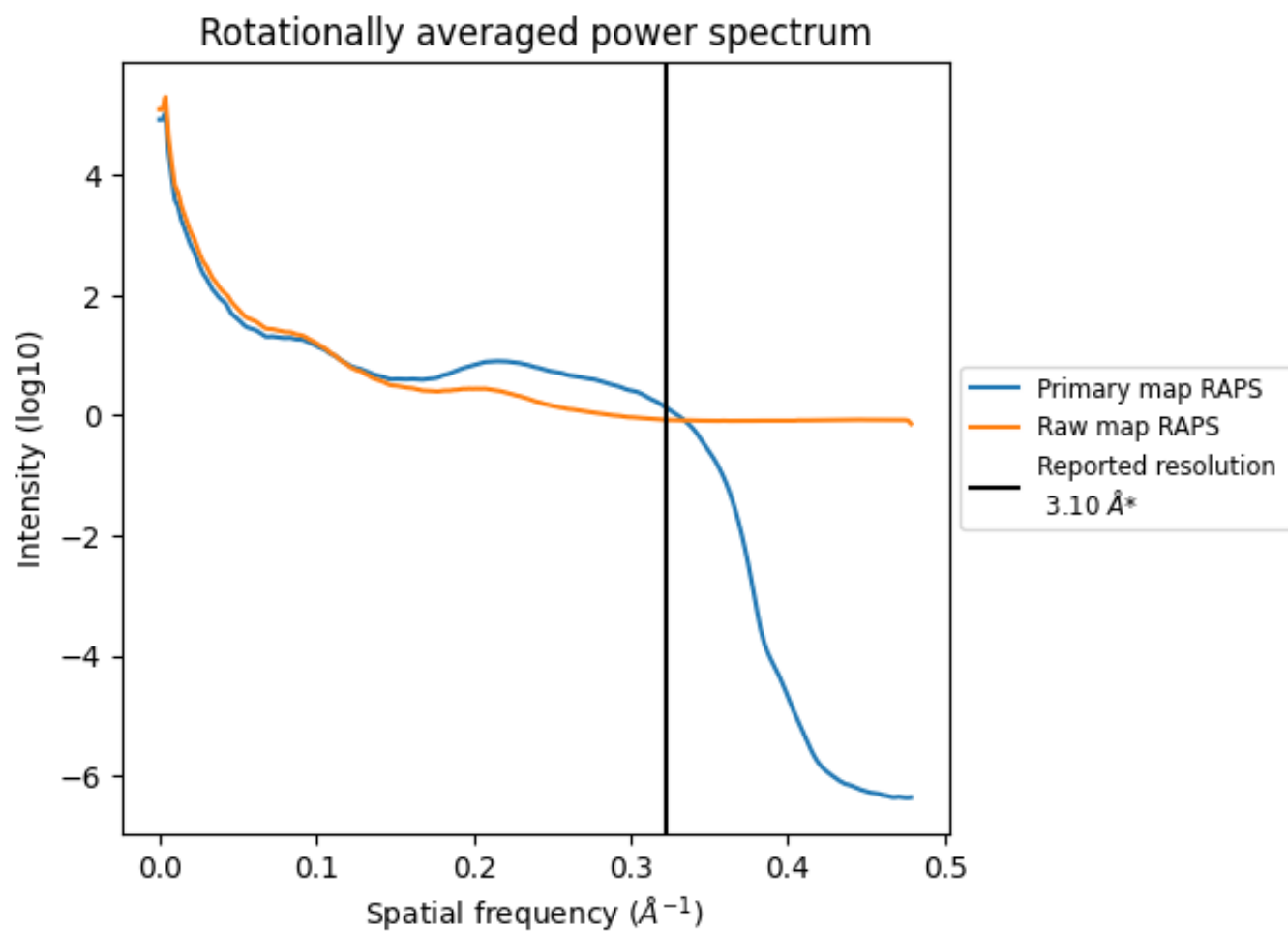
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2450 nm^3 ; this corresponds to an approximate mass of 2213 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

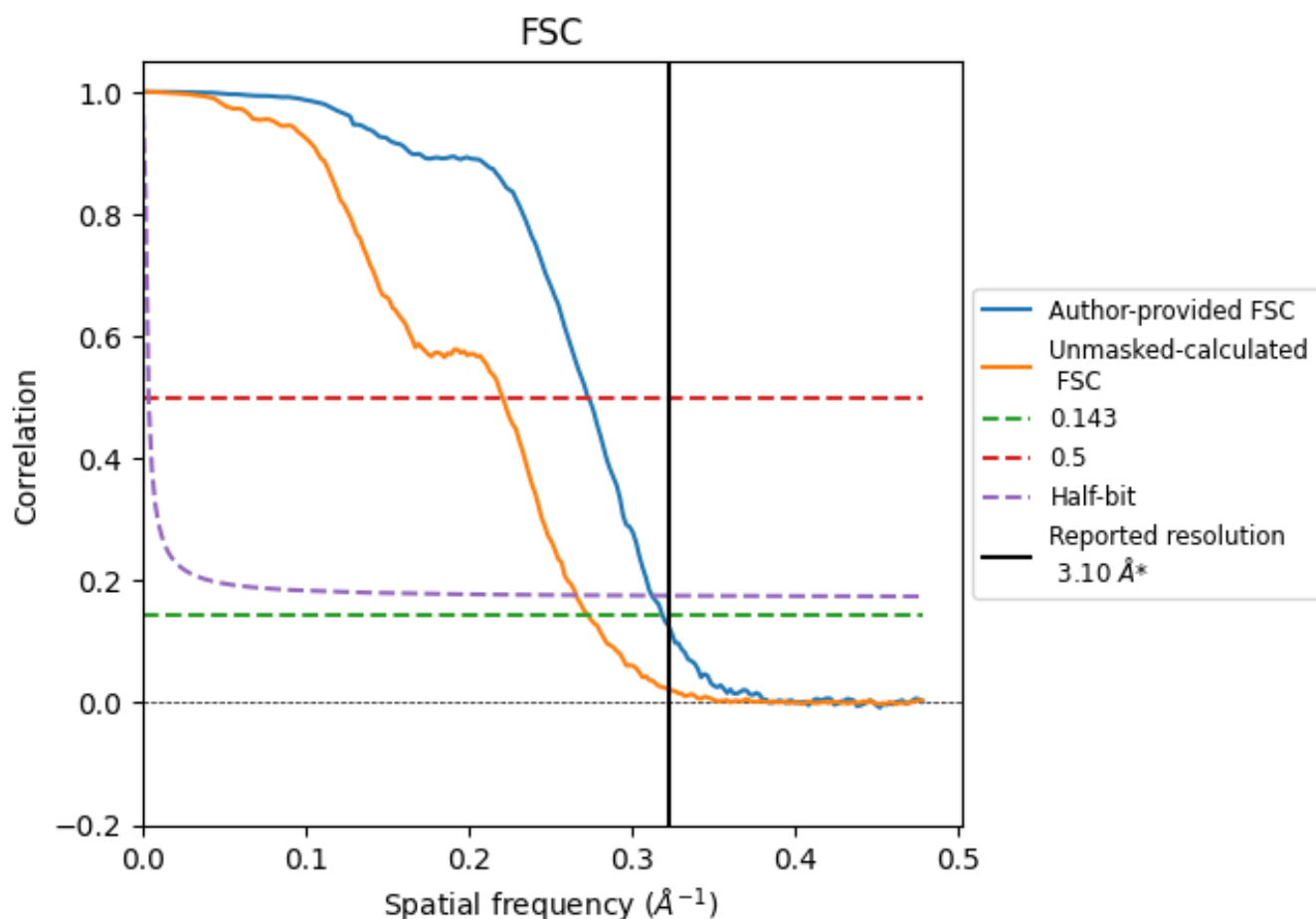


*Reported resolution corresponds to spatial frequency of $0.323 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.323 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

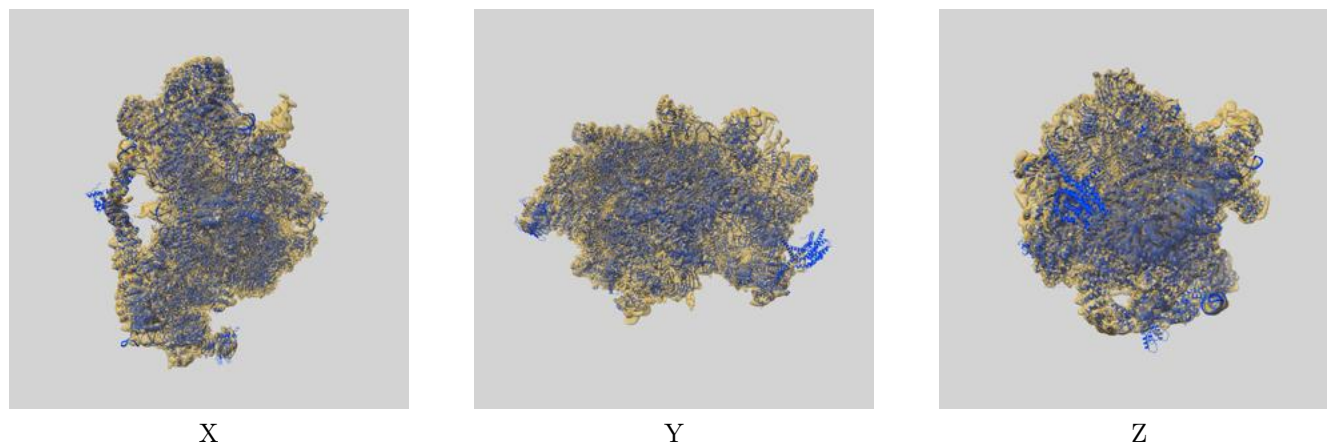
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.13	3.65	3.20
Unmasked-calculated*	3.65	4.52	3.76

*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 3.65 differs from the reported value 3.1 by more than 10 %

9 Map-model fit [i](#)

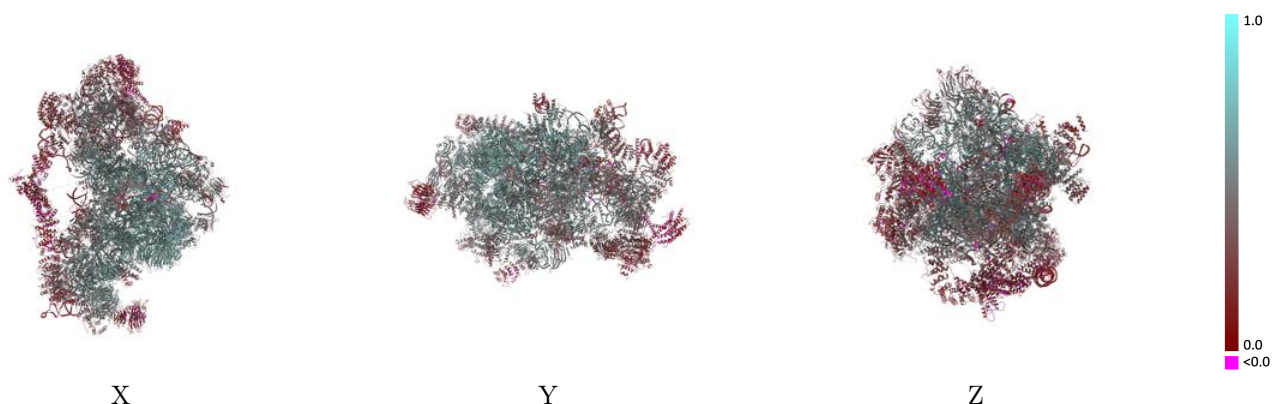
This section contains information regarding the fit between EMDB map EMD-66687 and PDB model 9XAH. Per-residue inclusion information can be found in section [3](#) on page [17](#).

9.1 Map-model overlay [i](#)



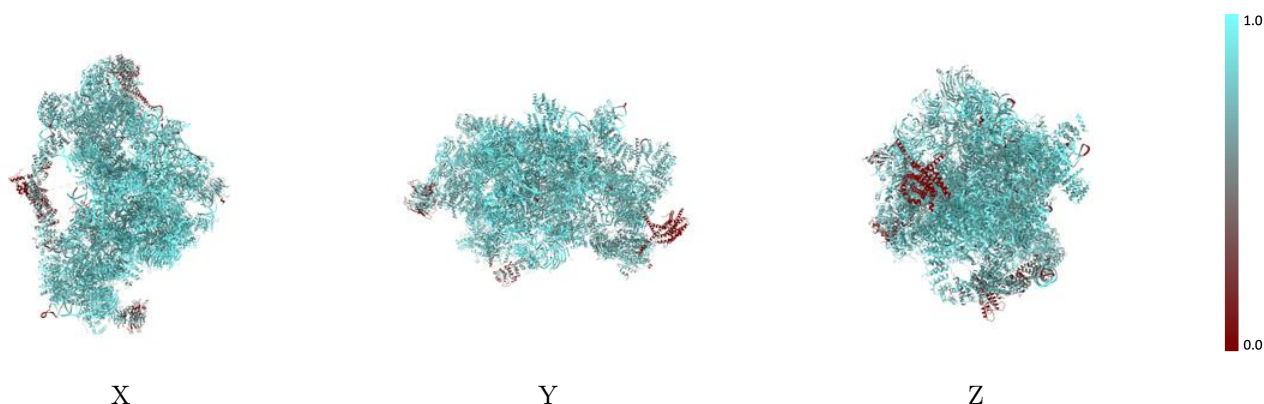
The images above show the 3D surface view of the map at the recommended contour level 0.017 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



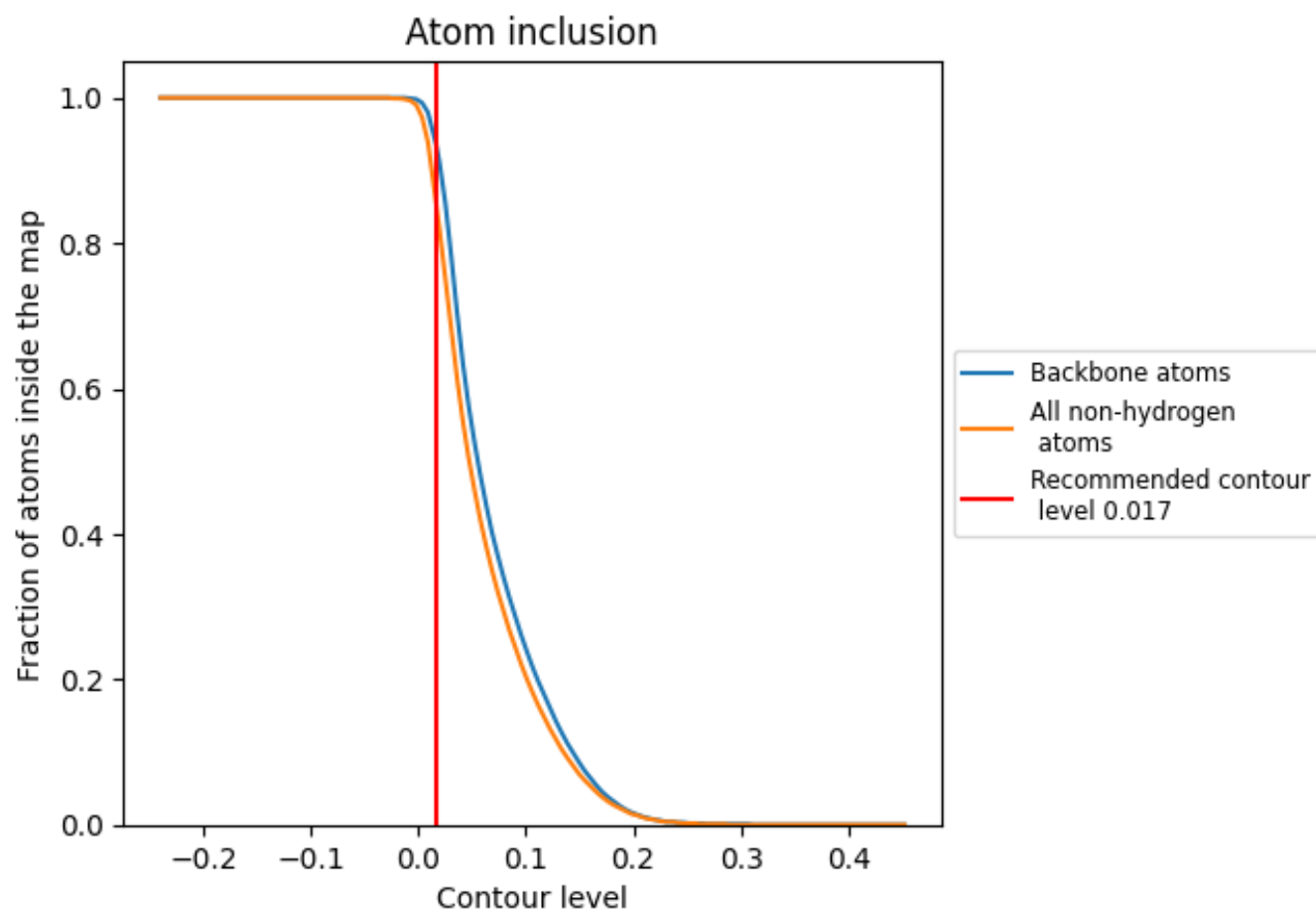
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.017).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 85% 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 (0.017) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8510	 0.4430
C1	 0.9370	 0.4800
C2	 0.9080	 0.4410
CA	 0.9680	 0.5950
CB	 0.8350	 0.4300
CC	 0.9110	 0.4860
CD	 0.8670	 0.4490
CE	 0.9520	 0.5650
CF	 0.9430	 0.5220
CG	 0.8950	 0.4700
CH	 0.9440	 0.5460
CI	 0.9370	 0.5420
CJ	 0.9770	 0.6290
CK	 0.9630	 0.5950
CL	 0.6970	 0.4320
CM	 0.9650	 0.6020
CN	 0.9050	 0.4970
CO	 0.8040	 0.3920
CP	 0.8700	 0.4690
CQ	 0.8750	 0.4330
CR	 0.7900	 0.3650
CS	 0.7150	 0.2660
CT	 0.9400	 0.5600
CU	 0.8810	 0.5050
CW	 0.8440	 0.4350
CX	 0.2060	 0.1360
CY	 0.4030	 0.2290
CZ	 0.1710	 0.1500
Ca	 0.8780	 0.4650
Cb	 0.8420	 0.4160
Cc	 0.9450	 0.5690
Cd	 0.8650	 0.4470
Ce	 0.8060	 0.3760
Cf	 0.8600	 0.4380
Cg	 0.9540	 0.5540



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Chain	Atom inclusion	Q-score
Ch	 0.7680	 0.3480
Ci	 0.9230	 0.5110
Cj	 0.9700	 0.5940
Ck	 0.8440	 0.3930
Cl	 0.7810	 0.3770
Cm	 0.9130	 0.5240
Cn	 0.9800	 0.6040
Co	 0.8350	 0.3880
Cp	 0.9590	 0.5680
UA	 0.9710	 0.6080
UB	 0.8640	 0.4170
UC	 0.4510	 0.3020
UD	 0.9120	 0.5010
UE	 0.8960	 0.4720
UF	 0.9200	 0.4740
UG	 0.9610	 0.5930
UH	 0.6320	 0.2580
UI	 0.8250	 0.3700
UJ	 0.7170	 0.2780
UK	 0.9390	 0.5600
UL	 0.9150	 0.4930
UM	 0.7870	 0.4050
UN	 0.9280	 0.5330
UO	 0.9460	 0.5410
UP	 0.8940	 0.4770
UQ	 0.9150	 0.5110
UR	 0.9560	 0.5790
US	 0.8630	 0.4150
UT	 0.7830	 0.3060
UU	 0.9670	 0.5880
UX	 0.9420	 0.5660
UZ	 0.8700	 0.4180