wwPDB EM Validation Summary Report (i)

May 13, 2024 – 11:37 pm BST

PDB ID	:	6RXT
EMDB ID	:	EMD-10051
Title	:	Cryo-EM structure of the 90S pre-ribosome (Kre33-Noc4) from Chaetomium thermophilum, state A
Authors	:	Cheng, J.; Kellner, N.; Griesel, S.; Berninghausen, O.; Beckmann, R.; Hurt, E.
Deposited on	:	2019-06-10
Resolution	:	7.00 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 (i) 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 (i)) were used in the production of this report:

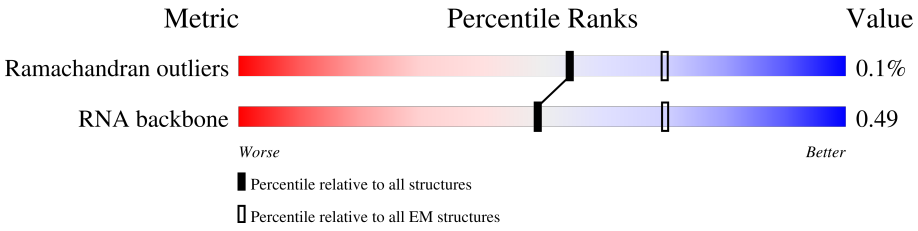
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 7.00 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)
Ramachandran outliers	154571	4023
RNA backbone	4643	859

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 <=5%

Mol	Chain	Length	Quality of chain
1	UA	904	92% · 7%
2	UB	907	56% 44%
3	UC	648	11% 89%
4	UD	884	87% 13%
5	UF	414	79% 20%
6	UG	558	85% · 14%
7	UJ	1802	25% 75%
8	UK	270	80% 20%
9	UL	962	81% · 18%
10	UM	912	79% · 20%

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Mol	Chain	Length	Quality of chain
11	UN	938	16% 84%
12	UO	557	90% 10%
13	UQ	960	81% 18%
14	UR	618	72% 28%
15	UU	1049	85% 14%
16	UX	193	98%
17	UZ	391	59% 40%
18	CA	313	77% 23%
18	CB	313	75% 24%
19	CC	523	74% 26%
20	CD	582	72% 28%
21	CE	127	94% 5%
21	CF	127	92% 6%
22	CG	630	60% 40%
23	CH	411	94% 5%
24	CI	1163	70% 29%
25	CJ	183	98%
26	CK	297	99%
27	CL	785	29% 71%
28	CM	446	100%
29	CN	252	89% 10%
29	CO	252	84% 15%
30	CP	322	62% 38%
31	CQ	259	67% 32%
32	CR	1073	69% 29%

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Mol	Chain	Length	Quality of chain
32	CS	1073	69% 29%
33	CT	203	65% 35%
34	Ca	255	88% 12%
35	Cc	212	90% 9%
36	Ce	203	77% 22%
37	Cg	190	84% 16%
38	Ch	151	44% 56%
39	Ci	150	77% 23%
40	Cj	143	88% 12%
41	Cm	130	97%
42	Cn	145	66% 34%
43	Cp	68	88% 10%
44	CU	311	57% 43%
45	C1	2352	31% 16% 51%
46	C2	230	63% 31% 7%
47	UH	930	39% 61%
48	UE	410	30% 70%
48	UI	410	30% 70%
49	US	549	82% 18%
50	Cl	156	51% 49%
51	CX	480	55% 44%
52	UP	364	15% 85%

2 Entry composition (i)

There are 55 unique types of molecules in this entry. The entry contains 169690 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
			Total	C	N	O	S		
1	UA	839	6366	4101	1136	1105	24	0	0

- Molecule 2 is a protein called Utp2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	UB	512	4079	2576	781	711	11	0	0

- Molecule 3 is a protein called Utp3.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	UC	74	588	371	120	97	0	0

- Molecule 4 is a protein called Utp4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	UD	772	6071	3851	1093	1103	24	0	0

- Molecule 5 is a protein called Utp6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	UF	331	2591	1674	504	399	14	0	0

- Molecule 6 is a protein called Utp7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	UG	479	3717	2369	700	636	12	0	0

- Molecule 7 is a protein called UTP10.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	UJ	445	Total	C	N	O	S	0	0
			3377	2169	604	590	14		

- 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
			1687	1062	351	269	5		

- Molecule 9 is a protein called Utp12.

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 Utp13".

Mol	Chain	Residues	Atoms					AltConf	Trace
10	UM	729	Total	C	N	O	S	0	0
			5643	3590	995	1045	13		

- Molecule 11 is a protein called Utp14.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	UN	154	Total	C	N	O	S	0	0
			1209	770	228	206	5		

- Molecule 12 is a protein called Utp15.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	UO	504	Total	C	N	O	S	0	0
			3819	2422	699	684	14		

- 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	S	0	0
			3491	2209	656	616	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	UU	902	Total	C	N	O	S	0	0
			6734	4336	1236	1136	26		

- Molecule 16 is a protein called Utp24.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	UX	190	Total	C	N	O	S	0	0
			1470	932	282	246	10		

- Molecule 17 is a protein called Utp30.

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

- Molecule 18 is a protein called Nop1.

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

- Molecule 19 is a protein called Putative nucleolar protein.

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

- Molecule 20 is a protein called Nop58.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	CD	420	Total	C	N	O	S	0	0
			3150	2023	560	557	10		

- Molecule 21 is a protein called snu13.

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 Rrp9.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	CG	378	Total	C	N	O	S	0	0
			2922	1865	527	517	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.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	CI	822	Total	C	N	O	S	0	0
			6486	4169	1213	1077	27		

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

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 Putative U3 small nucleolar ribonucleoprotein protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	CL	231	Total	C	N	O	S	0	0
			1786	1114	339	327	6		

- Molecule 28 is a protein called Sof1.

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 Emg1.

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	201	Total	C	N	O	S	0	0
			1625	1047	286	283	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	CQ	175	Total	C	N	O	S	0	0
			1361	862	250	242	7		

- Molecule 32 is a protein called Kre33.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	CR	760	Total	C	N	O	S	0	0
			5989	3851	1024	1087	27		
32	CS	760	Total	C	N	O	S	0	0
			5989	3851	1024	1087	27		

- Molecule 33 is a protein called Fcf2.

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 40S ribosomal protein S1.

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 s5-like protein.

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

- Molecule 36 is a protein called 40S ribosomal protein S7.

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

- Molecule 37 is a protein called 40S ribosomal protein s9-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Cg	159	Total	C	N	O	S	0	0
			1242	801	255	184	2		

- Molecule 38 is a protein called 40S ribosomal protein S13-like protein.

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

- Molecule 39 is a protein called 40S ribosomal protein S14-like protein.

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

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

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

- Molecule 41 is a protein called 40S ribosomal protein S22-like protein.

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

- Molecule 42 is a protein called 40S ribosomal protein s23-like protein.

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

- Molecule 43 is a protein called 40S ribosomal protein S28-like protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	Cp	61	Total 455	C 284	N 97	O 74	0	0

- Molecule 44 is a protein called Faf1.

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

- Molecule 45 is a RNA chain called 35S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	C1	1152	Total 24590	C 10964	N 4415	O 8059	P 1152	0	0

- Molecule 46 is a RNA chain called U3 snoRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	C2	230	Total 4891	C 2182	N 856	O 1623	P 230	0	0

- Molecule 47 is a protein called Utp8.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	UH	359	Total 2809	C 1773	N 496	O 527	S 13	0	0

- Molecule 48 is a protein called Utp5".

Mol	Chain	Residues	Atoms					AltConf	Trace
48	UE	125	Total 972	C 608	N 183	O 175	S 6	0	0
48	UI	125	Total 972	C 608	N 183	O 175	S 6	0	0

- Molecule 49 is a protein called Noc4.

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

- Molecule 50 is a protein called Putative ribosomal protein.

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

- Molecule 51 is a protein called Enp1.

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

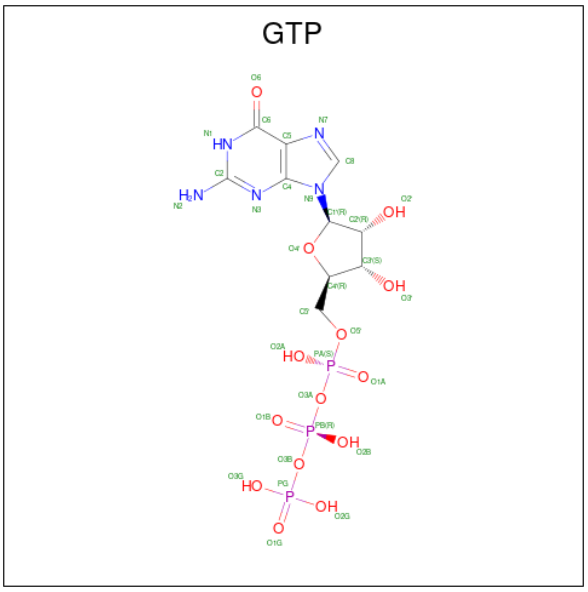
- Molecule 52 is a protein called Utp16.

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

- Molecule 53 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 54 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

- Molecule 55 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

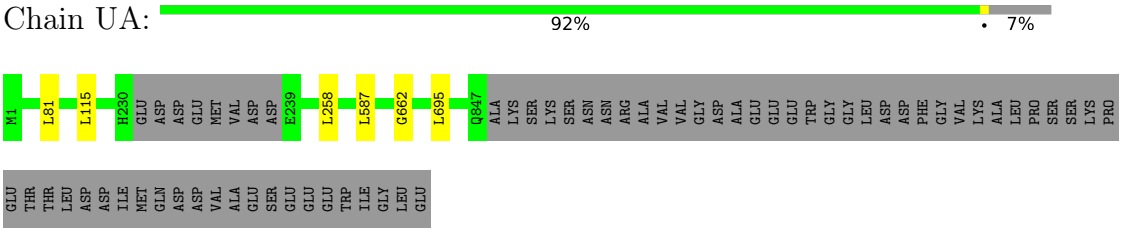
Mol	Chain	Residues	Atoms		AltConf
55	CI	1	Total	Mg	0
			1	1	

3 Residue-property plots (i)

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

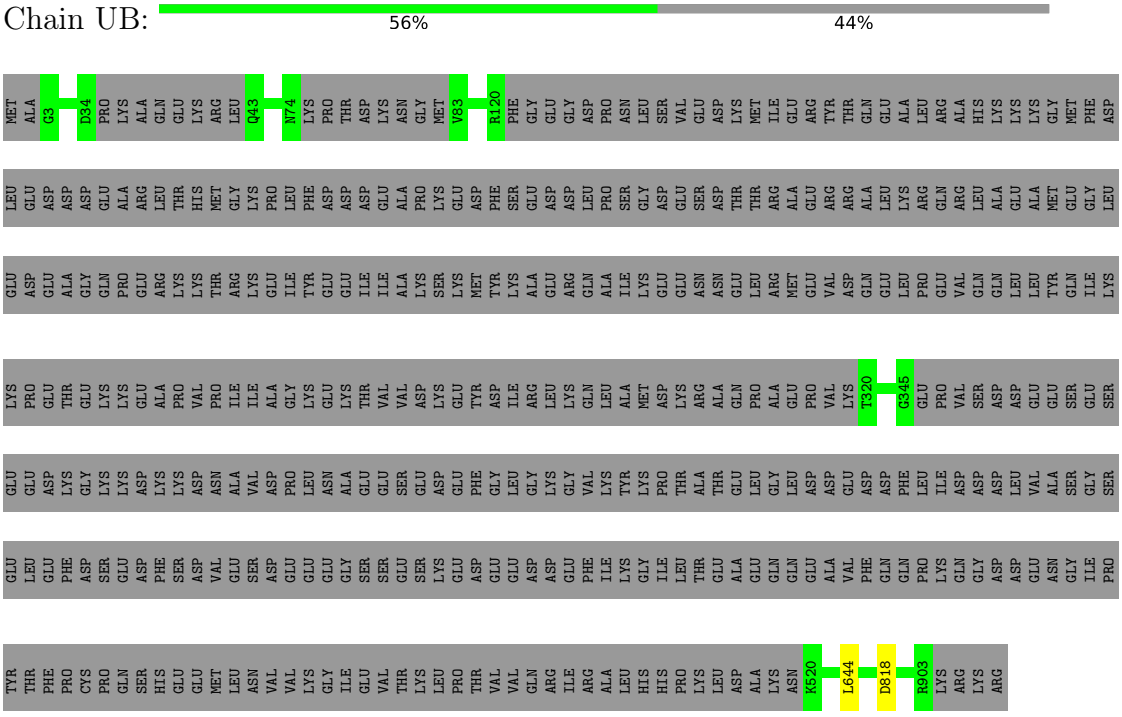
- Molecule 1: Periodic tryptophan protein 2-like protein

Chain UA:



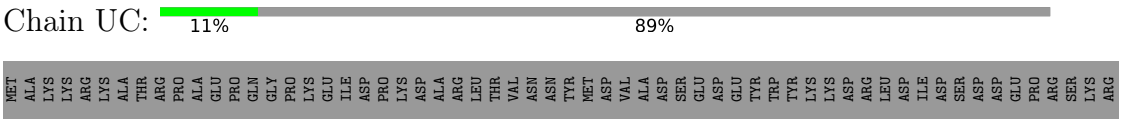
- Molecule 2: Utp2

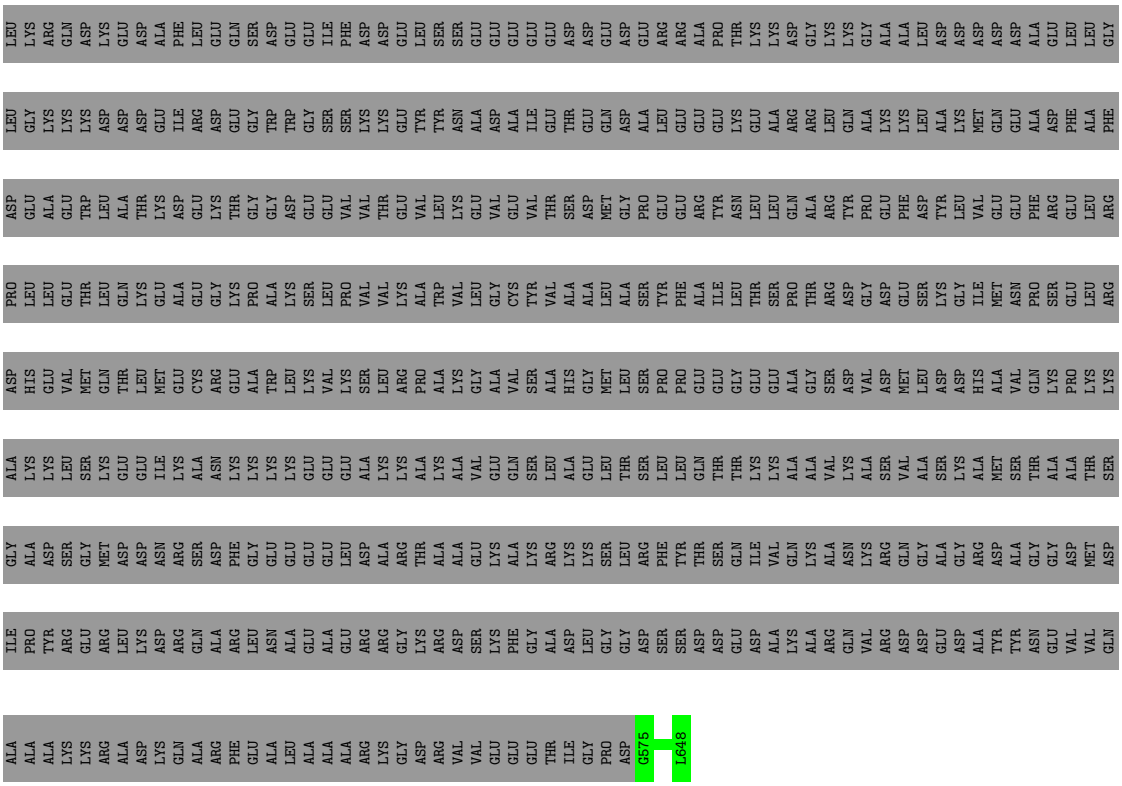
Chain UB:



- Molecule 3: Utp3

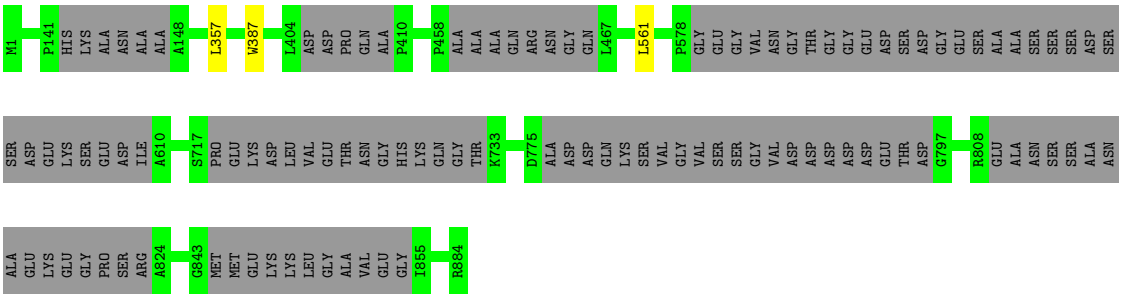
Chain UC:





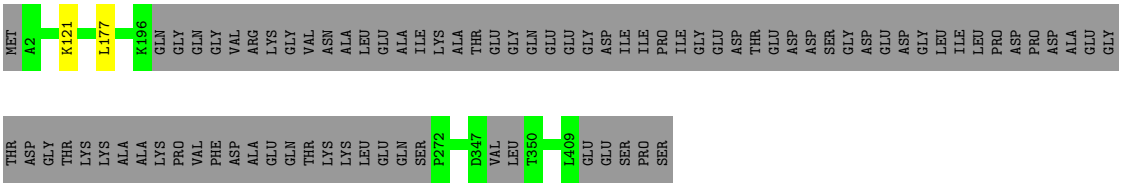
• Molecule 4: Utp4

Chain UD:



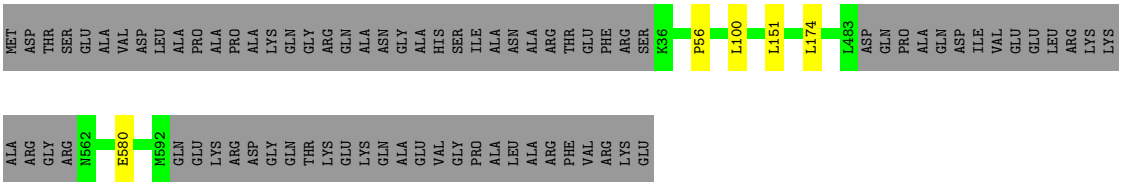
• Molecule 5: Utp6

Chain UF:



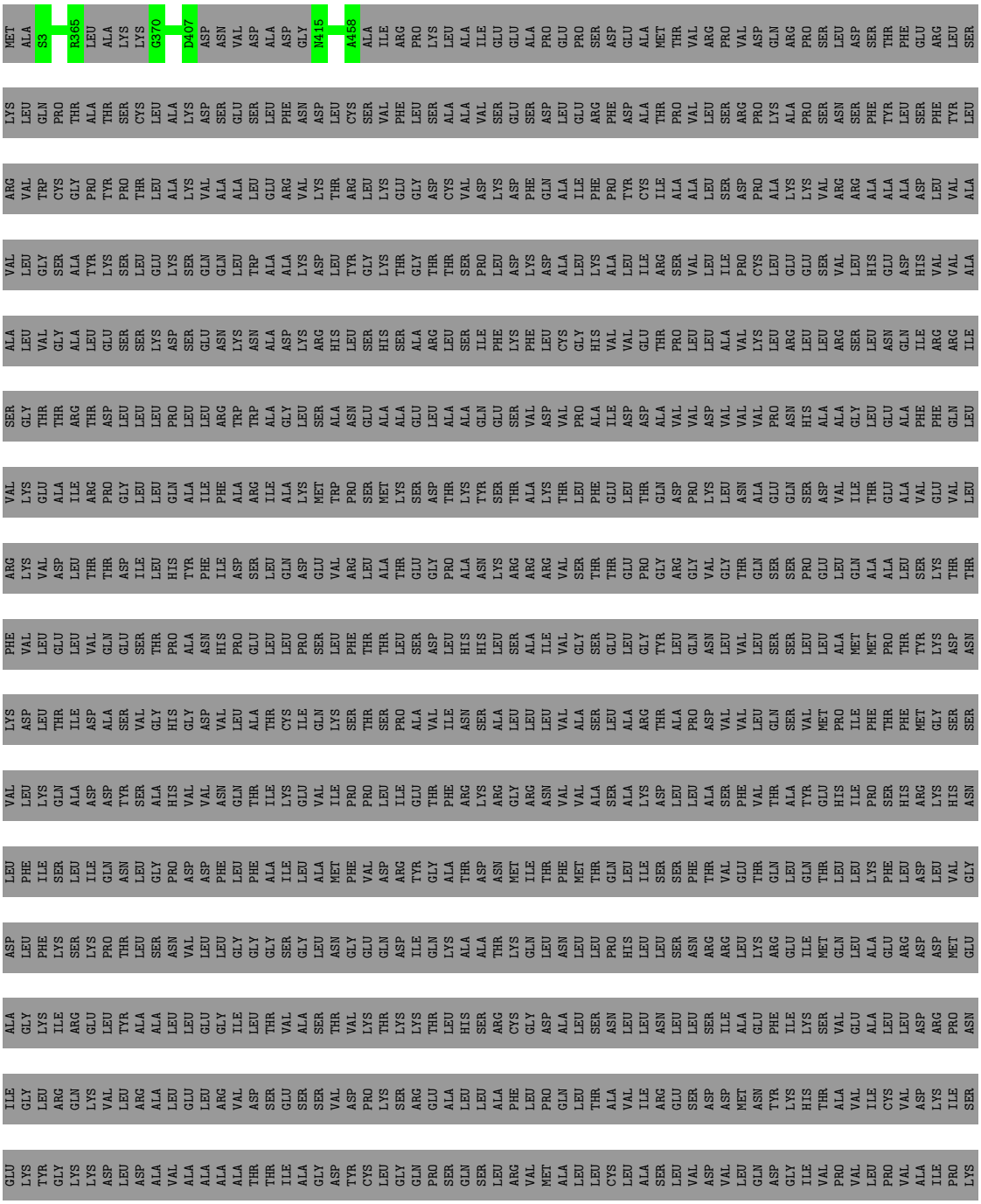
• Molecule 6: Utp7

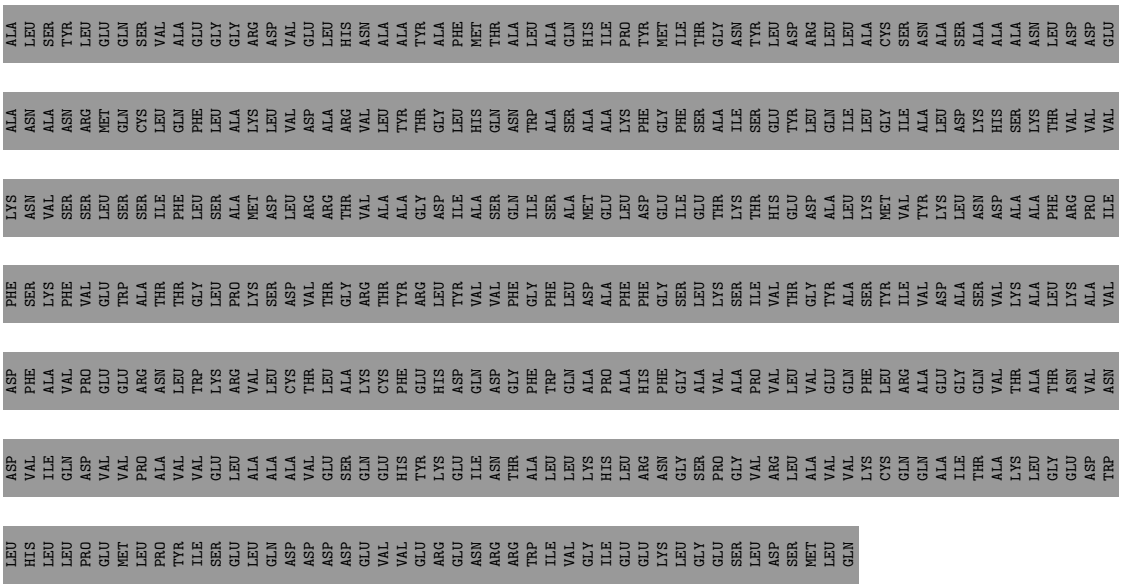
Chain UG:



• Molecule 7: UTP10

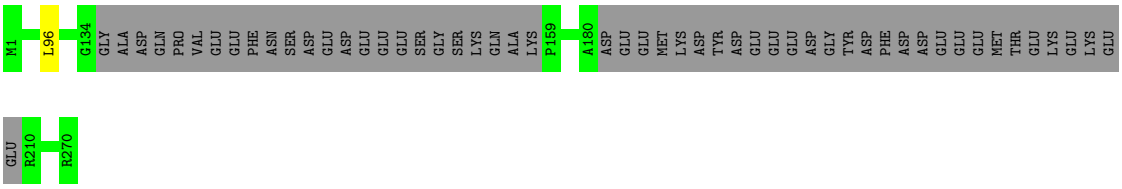
Chain UJ: 25% 75%





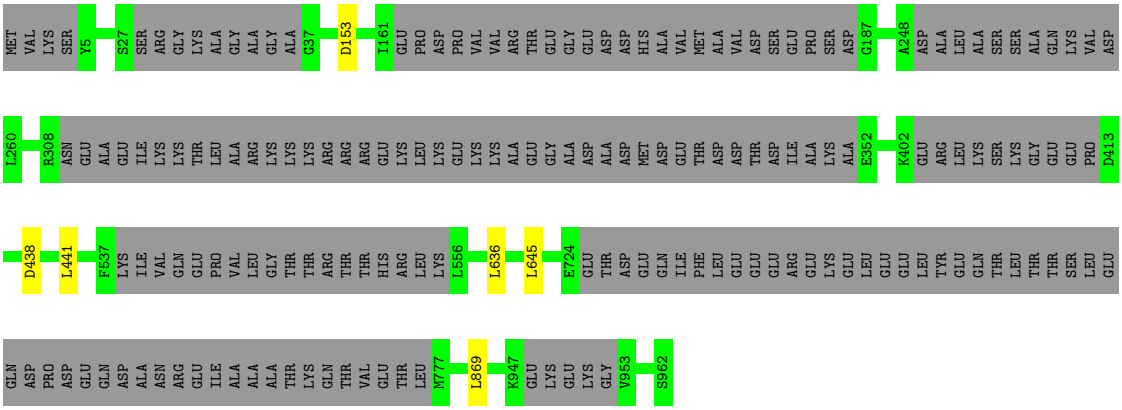
• Molecule 8: U3 small nucleolar RNA-associated protein 11

Chain UK:



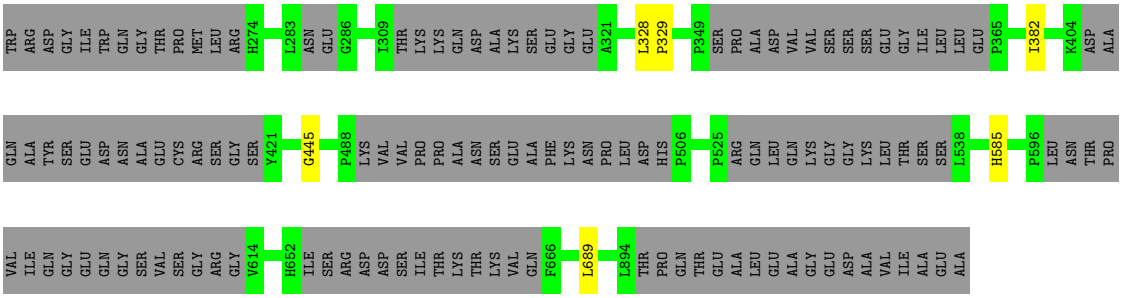
• Molecule 9: Utp12

Chain UL:



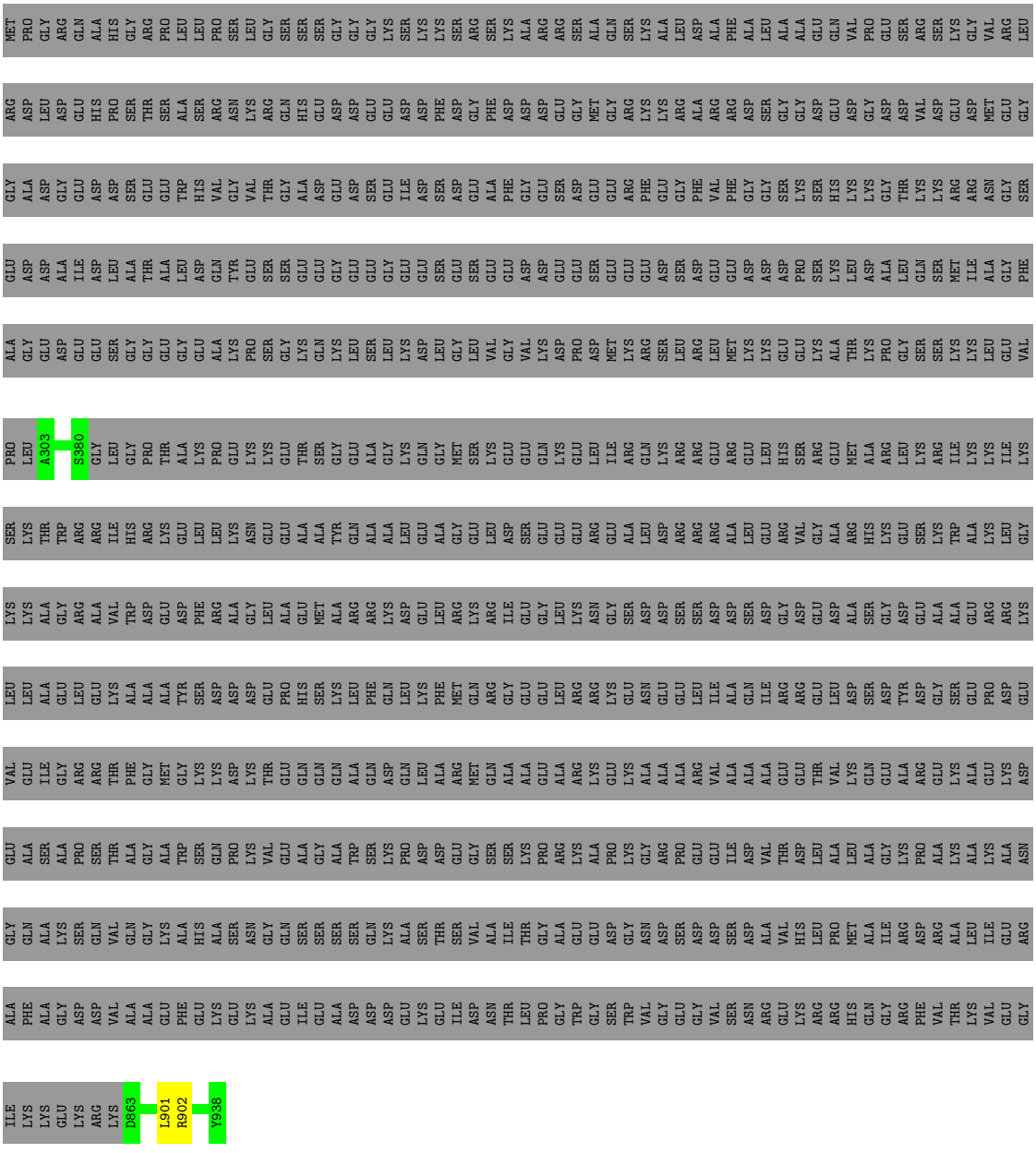
• Molecule 10: Utp13"

Chain UM:



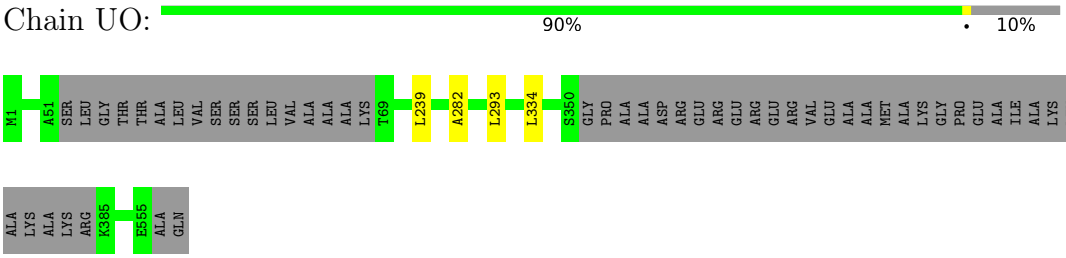
• Molecule 11: Utp14

Chain UN: 16% 84%



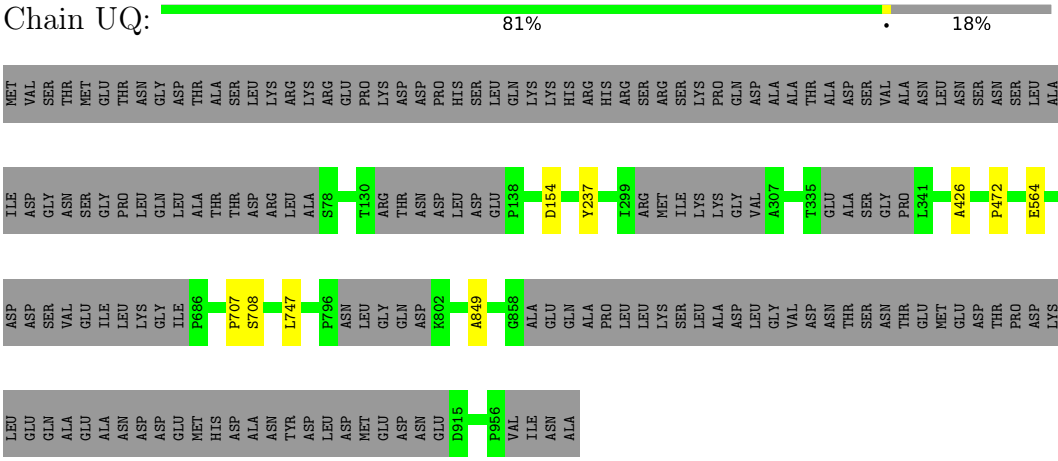
• Molecule 12: Utp15

Chain UO:



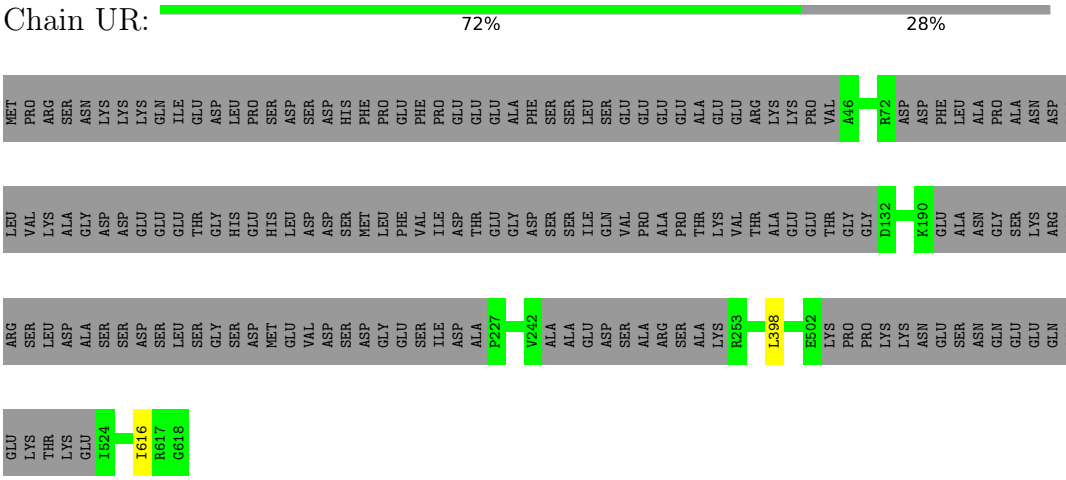
• Molecule 13: Utp17

Chain UQ:



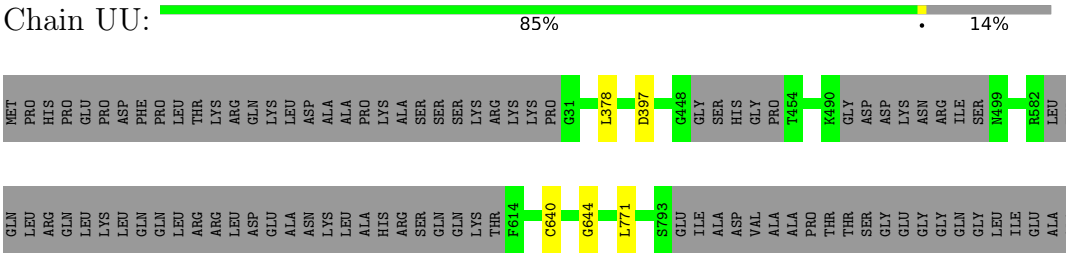
• Molecule 14: Utp18

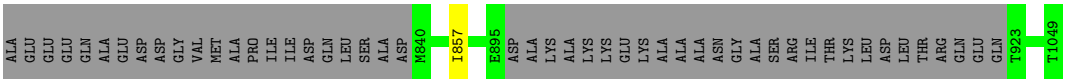
Chain UR:



• Molecule 15: Putative U3 snoRNP protein

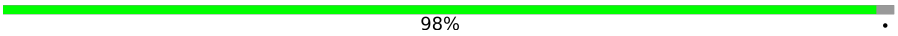
Chain UU:

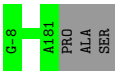




• Molecule 16: Utp24

Chain UX:



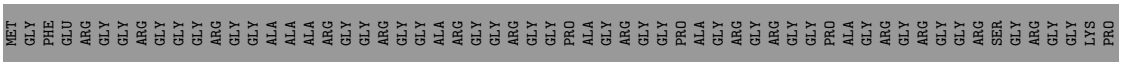


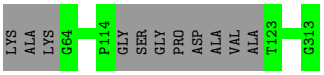
• Molecule 17: Utp30

Chain UZ:

• Molecule 18: Nop1

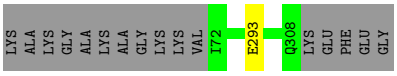
Chain CA:





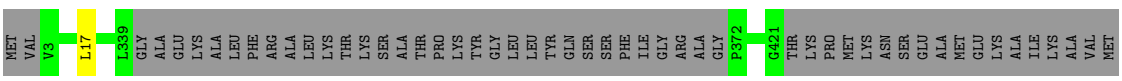
• Molecule 18: Nop1

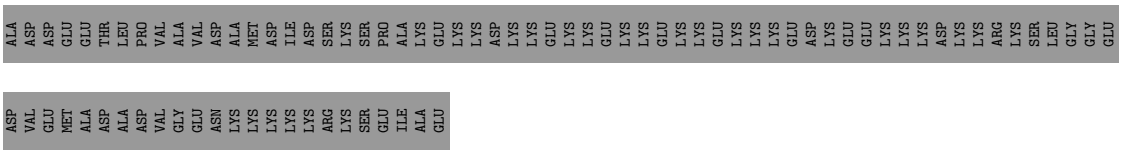
Chain CB:



• Molecule 19: Putative nucleolar protein

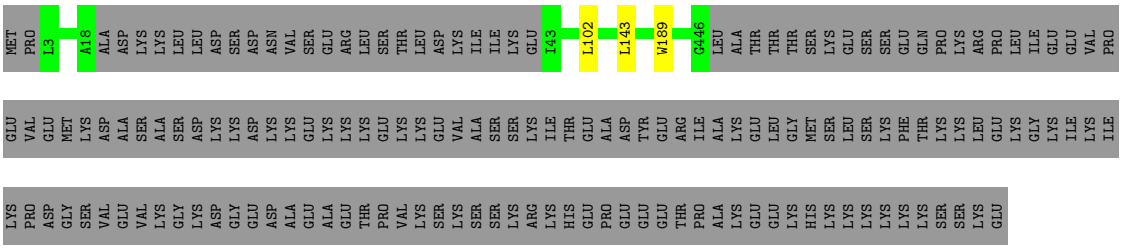
Chain CC:





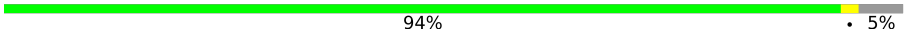
• Molecule 20: Nop58

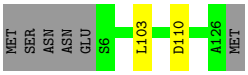
Chain CD:



• Molecule 21: snu13

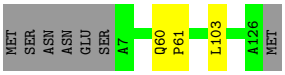
Chain CE:





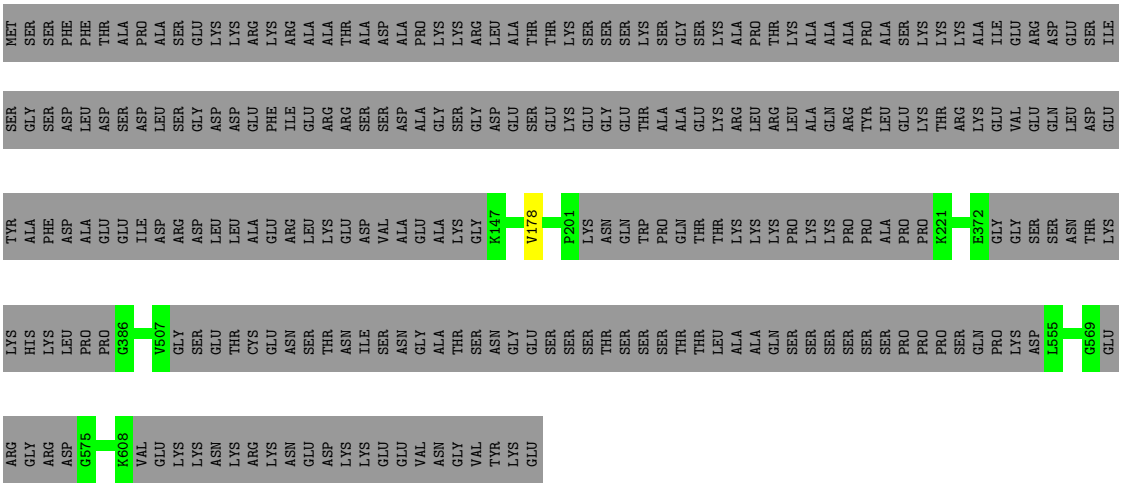
• Molecule 21: snu13

Chain CF:



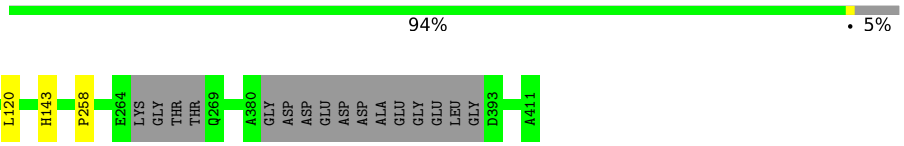
• Molecule 22: Rrp9

Chain CG:



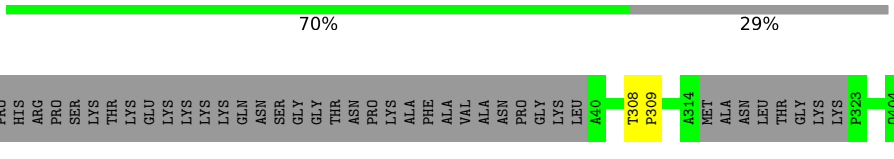
• Molecule 23: RNA 3'-terminal phosphate cyclase-like protein

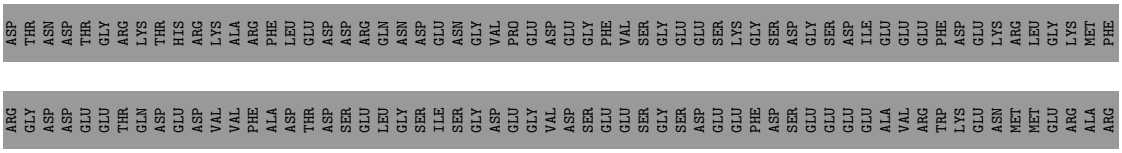
Chain CH:

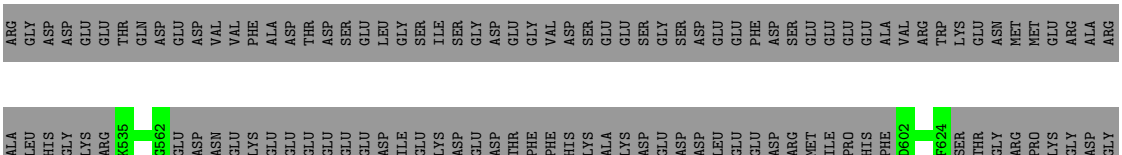


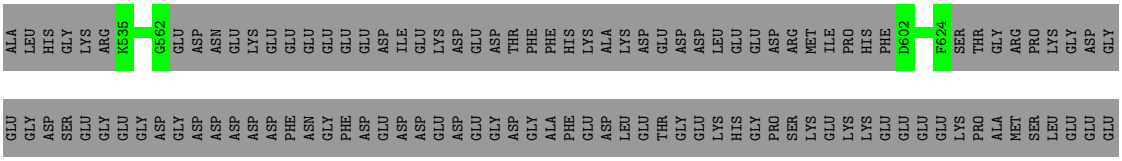
• Molecule 24: Bms1

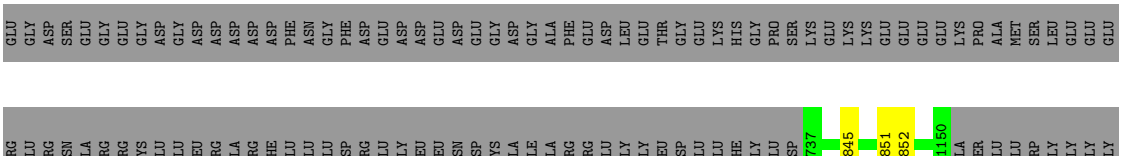
Chain CI:

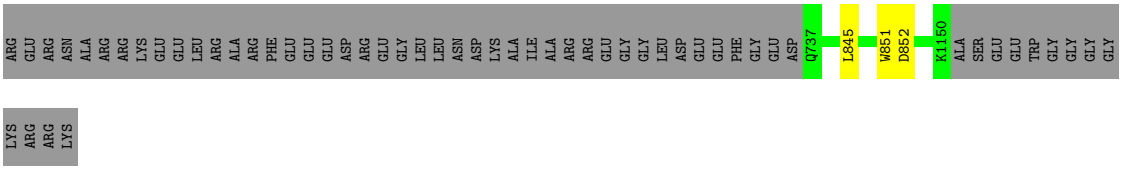






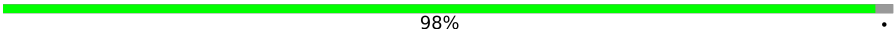


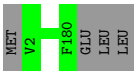




• Molecule 25: Imp3

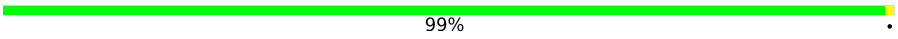
Chain CJ:

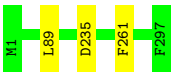




• Molecule 26: Putative U3 small nucleolar ribonucleoprotein

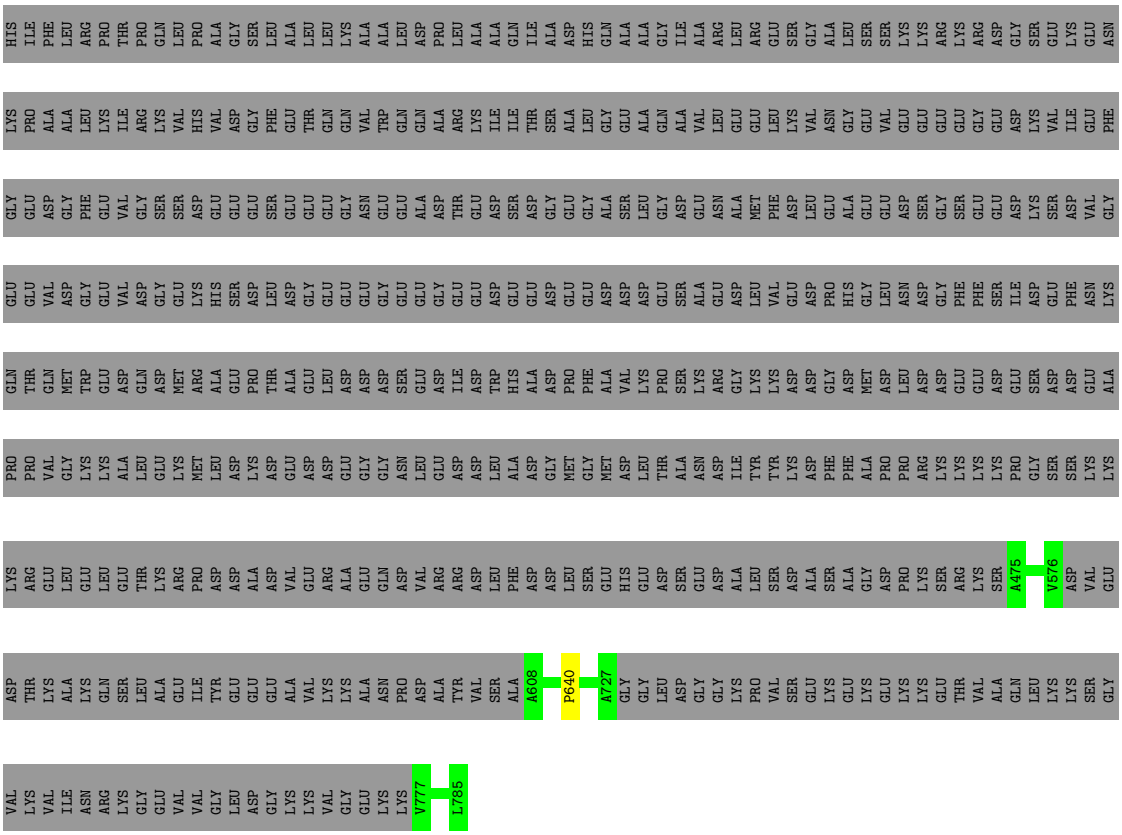
Chain CK:





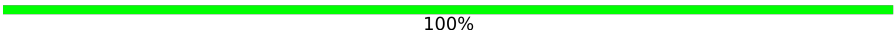
• Molecule 27: Putative U3 small nucleolar ribonucleoprotein protein

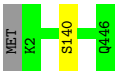
Chain CL:



• Molecule 28: Sof1

Chain CM:



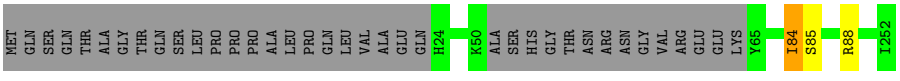


• Molecule 29: Emg1

Chain CN:

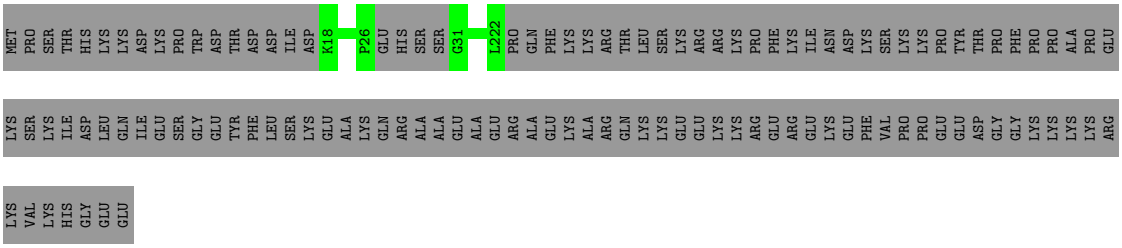
• Molecule 29: Emg1

Chain CO:



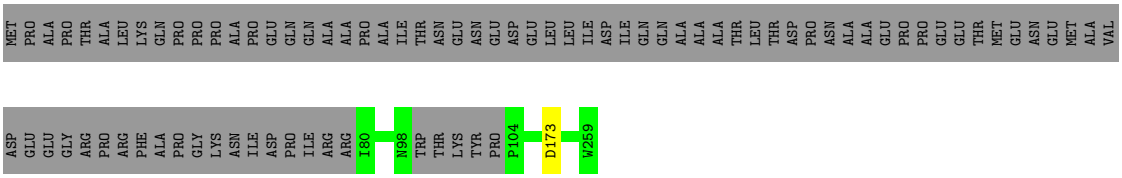
• Molecule 30: KRR1 small subunit processome component

Chain CP:



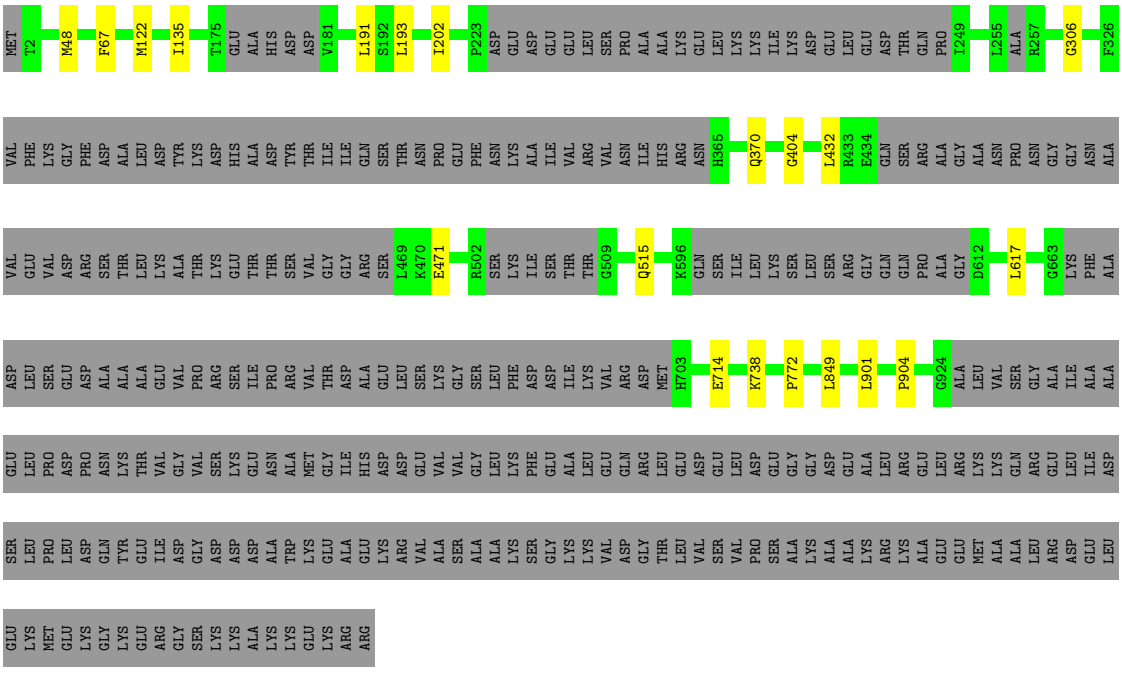
• Molecule 31: Pre-rRNA-processing protein PNO1

Chain CQ:



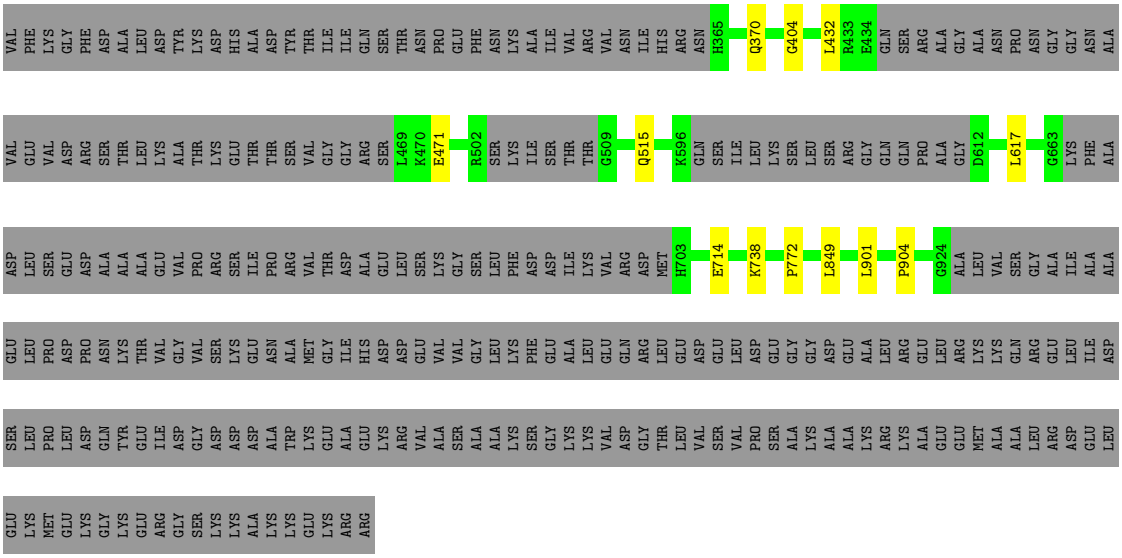
• Molecule 32: Kre33

Chain CR:



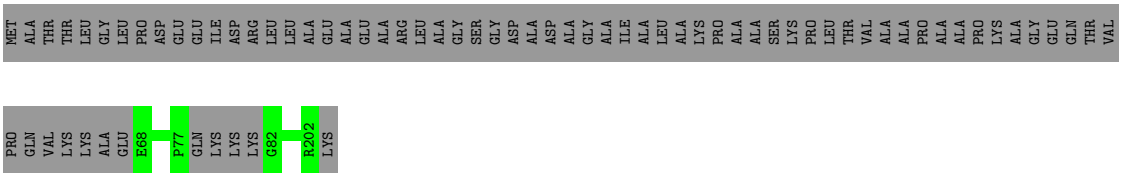
• Molecule 32: Kre33

Chain CS:



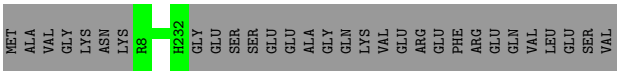
• Molecule 33: Fcf2

Chain CT:



• Molecule 34: 40S ribosomal protein S1

Chain Ca:



• Molecule 35: 40S ribosomal protein s5-like protein

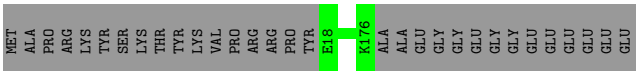
Chain Cc:

• Molecule 36: 40S ribosomal protein S7

Chain Ce:

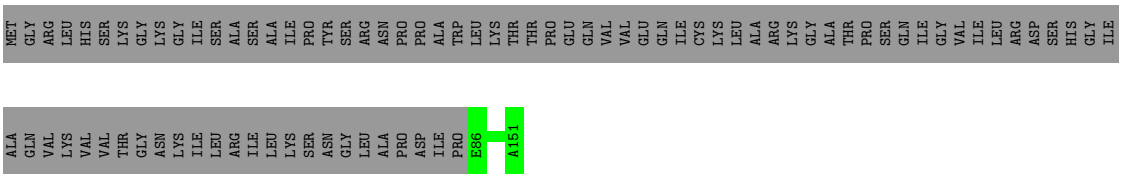
• Molecule 37: 40S ribosomal protein s9-like protein

Chain Cg:



• Molecule 38: 40S ribosomal protein S13-like protein

Chain Ch:



• Molecule 39: 40S ribosomal protein S14-like protein

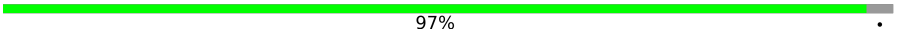
Chain Ci:

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

Chain Cj:

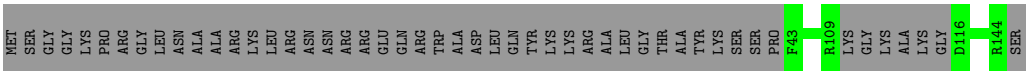
• Molecule 41: 40S ribosomal protein S22-like protein

Chain Cm:



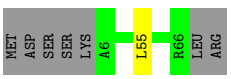
• Molecule 42: 40S ribosomal protein s23-like protein

Chain Cn:



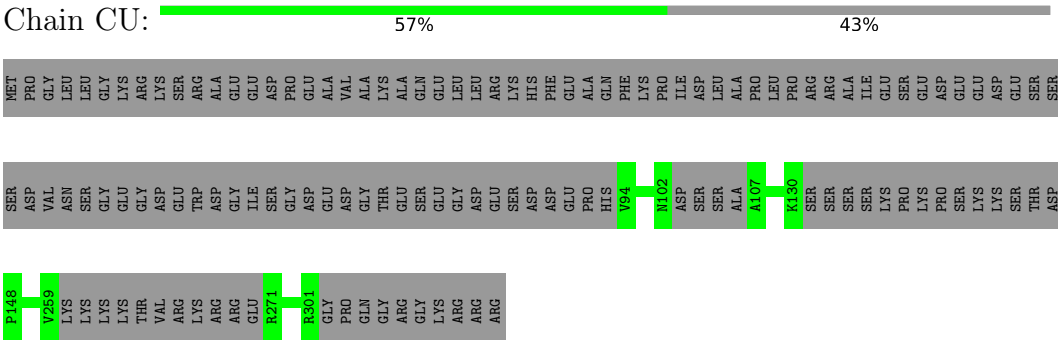
• Molecule 43: 40S ribosomal protein S28-like protein

Chain Cp:



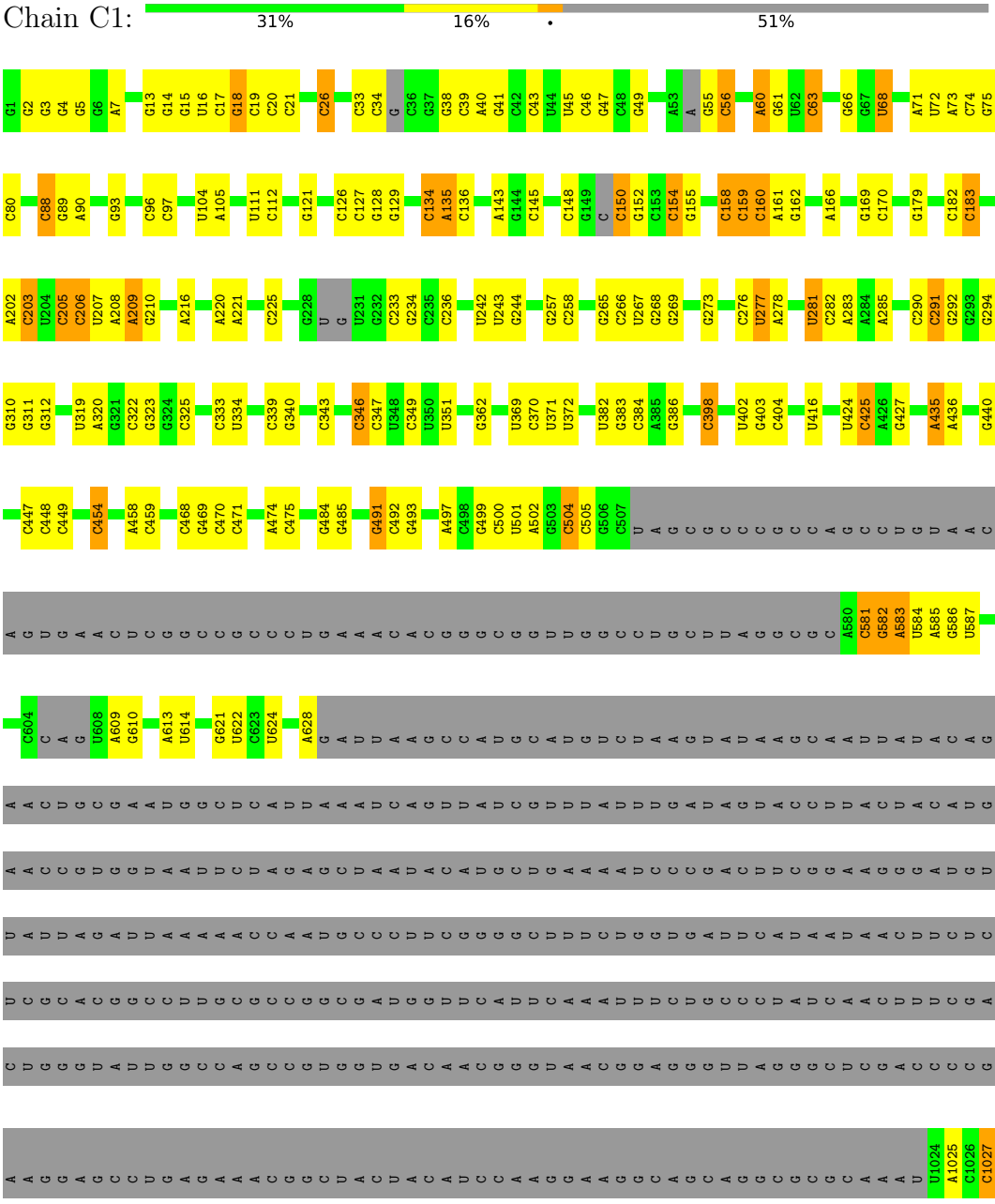
• Molecule 44: Faf1

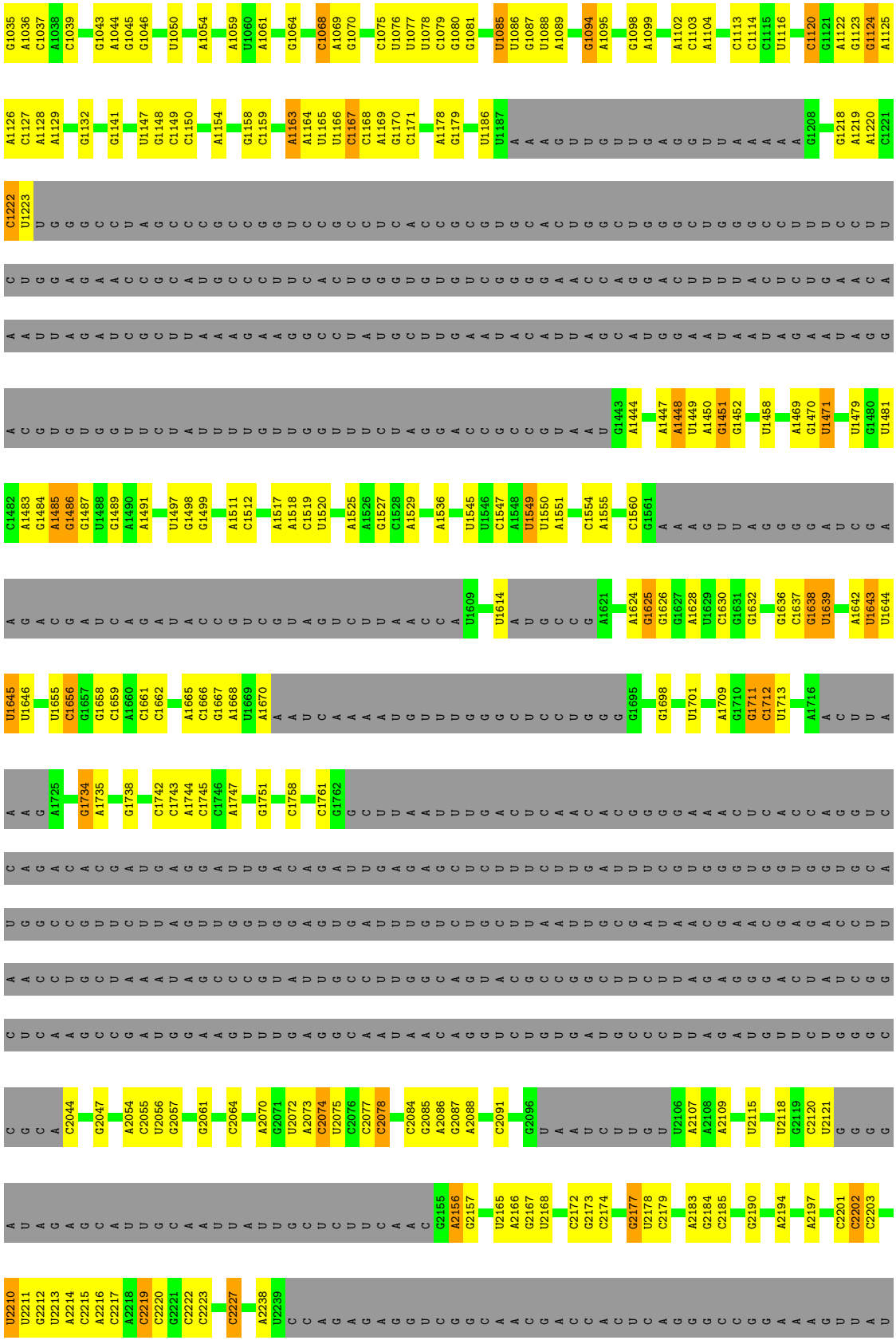
Chain CU:



• Molecule 45: 35S ribosomal RNA

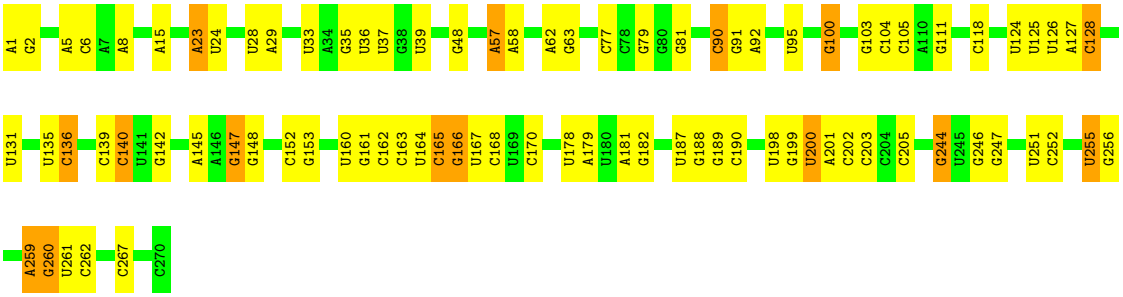
Chain C1:





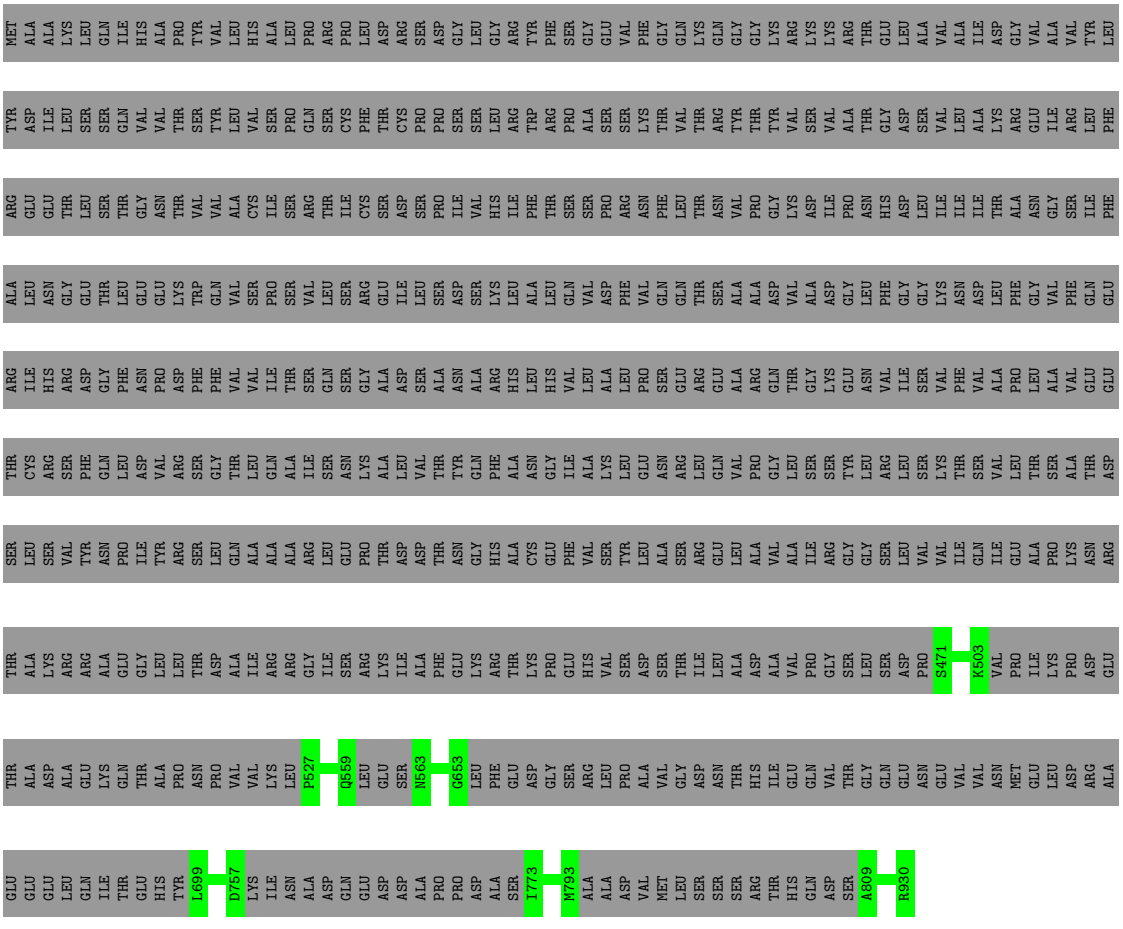
• Molecule 46: U3 snoRNA

Chain C2:



• Molecule 47: Utp8

Chain UH:

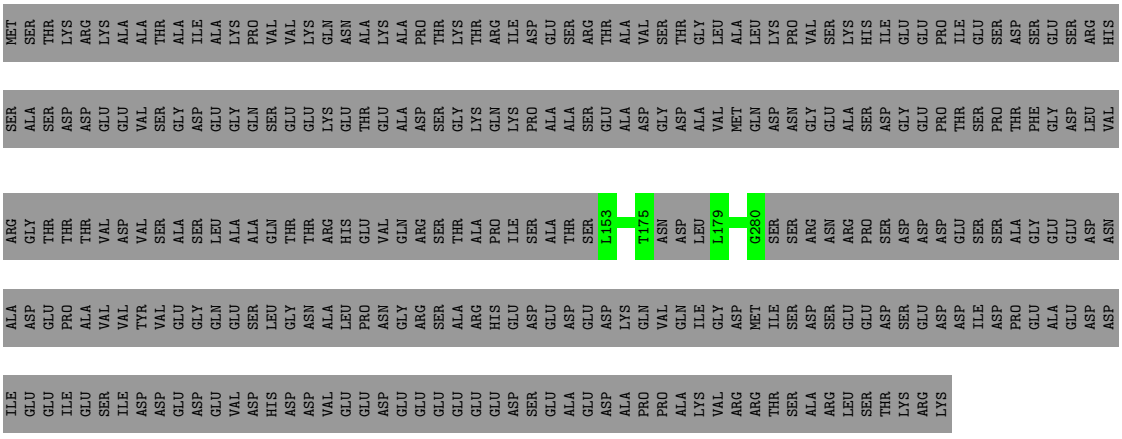


• Molecule 48: Utp5"

Chain UE:

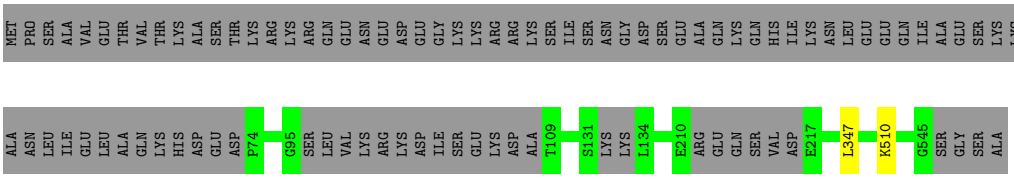
• Molecule 48: Utp5"

Chain UI:



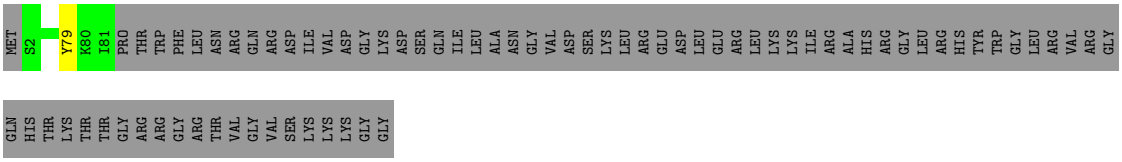
• Molecule 49: Noc4

Chain US:



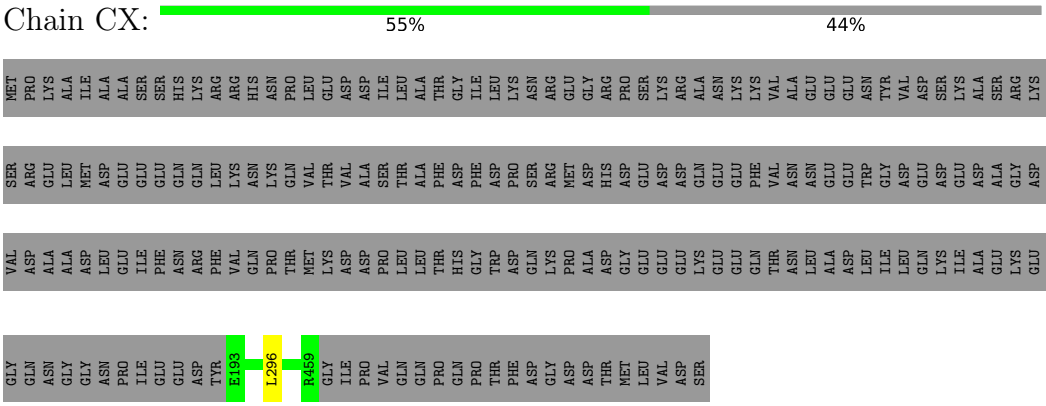
• Molecule 50: Putative ribosomal protein

Chain Cl:



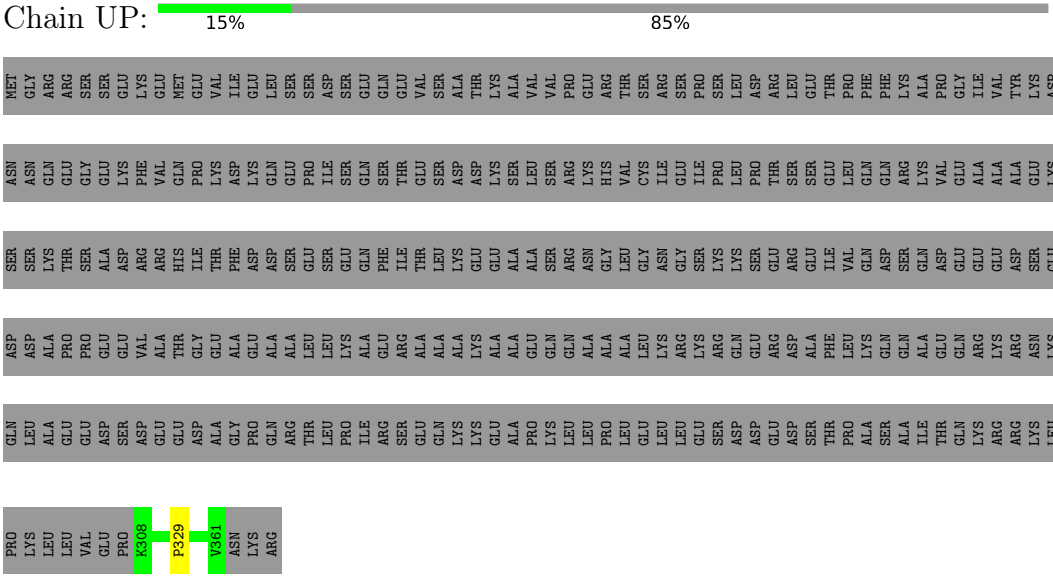
• Molecule 51: Enp1

Chain CX:



• Molecule 52: Utp16

Chain UP:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	8415	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	28	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.47	0/6521	0.65	5/8867 (0.1%)
2	UB	0.33	0/4154	0.54	2/5583 (0.0%)
3	UC	0.40	0/595	0.52	0/786
4	UD	0.38	0/6211	0.56	2/8408 (0.0%)
5	UF	0.35	0/2657	0.54	1/3596 (0.0%)
6	UG	0.47	0/3790	0.62	3/5120 (0.1%)
7	UJ	0.37	0/3435	0.57	0/4661
8	UK	0.41	0/1701	0.52	1/2251 (0.0%)
9	UL	0.37	0/6299	0.63	4/8531 (0.0%)
10	UM	0.33	0/5755	0.61	2/7827 (0.0%)
11	UN	0.41	0/1232	0.56	1/1662 (0.1%)
12	UO	0.42	0/3903	0.61	3/5312 (0.1%)
13	UQ	0.40	0/6136	0.63	4/8348 (0.0%)
14	UR	0.43	0/3564	0.59	1/4816 (0.0%)
15	UU	0.45	1/6903 (0.0%)	0.60	2/9392 (0.0%)
16	UX	0.42	0/1493	0.59	0/2011
17	UZ	0.34	0/1857	0.61	1/2526 (0.0%)
18	CA	0.46	0/1814	0.60	0/2456
18	CB	0.34	0/1853	0.54	0/2511
19	CC	0.37	0/2911	0.58	1/3937 (0.0%)
20	CD	0.36	0/3205	0.60	3/4338 (0.1%)
21	CE	0.45	0/891	0.66	2/1214 (0.2%)
21	CF	0.41	0/876	0.64	1/1195 (0.1%)
22	CG	0.37	0/2983	0.60	0/4032
23	CH	0.38	0/2939	0.58	1/3988 (0.0%)
24	CI	0.42	0/6631	0.58	1/8943 (0.0%)
25	CJ	0.48	0/1462	0.56	0/1967
26	CK	0.45	0/2376	0.64	2/3214 (0.1%)
27	CL	0.37	0/1812	0.51	0/2437
28	CM	0.48	0/3573	0.60	0/4829
29	CN	0.36	0/1797	0.56	1/2443 (0.0%)
29	CO	0.31	0/1714	0.55	0/2325

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
30	CP	0.35	0/1655	0.58	0/2229
31	CQ	0.30	0/1379	0.57	0/1850
32	CR	0.40	0/6108	0.80	14/8266 (0.2%)
32	CS	0.40	0/6108	0.80	14/8266 (0.2%)
33	CT	0.43	0/1053	0.58	0/1413
34	Ca	0.35	0/1850	0.61	0/2486
35	Cc	0.40	0/1485	0.54	0/2008
36	Ce	0.34	0/1298	0.66	3/1750 (0.2%)
37	Cg	0.39	0/1259	0.55	0/1687
38	Ch	0.32	0/557	0.52	0/749
39	Ci	0.35	0/819	0.54	0/1107
40	Cj	0.48	0/958	0.60	0/1293
41	Cm	0.41	0/1001	0.57	0/1345
42	Cn	0.44	0/712	0.56	0/954
43	Cp	0.44	0/458	0.61	1/617 (0.2%)
44	CU	0.32	0/1350	0.53	0/1810
45	C1	0.64	1/27472 (0.0%)	1.25	306/42792 (0.7%)
46	C2	0.64	0/5459	1.40	71/8498 (0.8%)
47	UH	0.33	0/2852	0.56	0/3846
48	UE	0.31	0/980	0.58	0/1316
48	UI	0.26	0/980	0.52	0/1316
49	US	0.33	0/3765	0.57	1/5100 (0.0%)
50	Cl	0.30	0/638	0.60	0/857
51	CX	0.29	0/2180	0.55	1/2956 (0.0%)
52	UP	0.34	0/428	0.60	0/570
All	All	0.45	2/175847 (0.0%)	0.80	455/244607 (0.2%)

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	UA	0	1
4	UD	0	1
9	UL	0	2
10	UM	0	4
12	UO	0	1
13	UQ	0	4
14	UR	0	1
15	UU	0	3
17	UZ	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
18	CB	0	1
21	CF	0	1
22	CG	0	1
23	CH	0	1
24	CI	0	2
26	CK	0	1
28	CM	0	1
29	CO	0	2
31	CQ	0	1
32	CR	0	3
32	CS	0	3
35	Cc	0	1
36	Ce	0	1
48	UE	0	1
49	US	0	1
50	Cl	0	1
All	All	0	42

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	C1	1081	G	C2-N3	-5.42	1.28	1.32
15	UU	640	CYS	CB-SG	-5.29	1.73	1.81

The worst 5 of 455 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
46	C2	2	G	O5'-P-OP1	-30.48	74.13	110.70
46	C2	2	G	OP1-P-OP2	-27.29	78.67	119.60
46	C2	2	G	O5'-P-OP2	18.11	132.43	110.70
46	C2	1	A	OP1-P-O3'	13.80	135.56	105.20
46	C2	1	A	OP2-P-O3'	-13.14	76.28	105.20

There are no chirality outliers.

5 of 42 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	UA	115	LEU	Peptide
4	UD	387	TRP	Peptide
9	UL	153	ASP	Peptide
9	UL	636	LEU	Peptide

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Mol	Chain	Res	Type	Group
10	UM	328	LEU	Peptide

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	UA	835/904 (92%)	768 (92%)	67 (8%)	0	100	100
2	UB	502/907 (55%)	470 (94%)	32 (6%)	0	100	100
3	UC	72/648 (11%)	64 (89%)	8 (11%)	0	100	100
4	UD	754/884 (85%)	722 (96%)	32 (4%)	0	100	100
5	UF	325/414 (78%)	310 (95%)	14 (4%)	1 (0%)	41	77
6	UG	475/558 (85%)	441 (93%)	32 (7%)	2 (0%)	34	72
7	UJ	439/1802 (24%)	422 (96%)	17 (4%)	0	100	100
8	UK	211/270 (78%)	210 (100%)	1 (0%)	0	100	100
9	UL	767/962 (80%)	711 (93%)	56 (7%)	0	100	100
10	UM	705/912 (77%)	656 (93%)	48 (7%)	1 (0%)	51	86
11	UN	150/938 (16%)	146 (97%)	3 (2%)	1 (1%)	22	63
12	UO	498/557 (89%)	474 (95%)	24 (5%)	0	100	100
13	UQ	775/960 (81%)	712 (92%)	61 (8%)	2 (0%)	41	77
14	UR	437/618 (71%)	416 (95%)	21 (5%)	0	100	100
15	UU	890/1049 (85%)	832 (94%)	58 (6%)	0	100	100
16	UX	188/193 (97%)	176 (94%)	12 (6%)	0	100	100
17	UZ	229/391 (59%)	215 (94%)	14 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	CA	238/313 (76%)	225 (94%)	13 (6%)	0	100	100
18	CB	235/313 (75%)	220 (94%)	15 (6%)	0	100	100
19	CC	383/523 (73%)	367 (96%)	16 (4%)	0	100	100
20	CD	416/582 (72%)	393 (94%)	23 (6%)	0	100	100
21	CE	119/127 (94%)	111 (93%)	8 (7%)	0	100	100
21	CF	118/127 (93%)	110 (93%)	7 (6%)	1 (1%)	19	60
22	CG	368/630 (58%)	343 (93%)	25 (7%)	0	100	100
23	CH	383/411 (93%)	346 (90%)	36 (9%)	1 (0%)	41	77
24	CI	812/1163 (70%)	760 (94%)	50 (6%)	2 (0%)	47	81
25	CJ	177/183 (97%)	166 (94%)	11 (6%)	0	100	100
26	CK	295/297 (99%)	284 (96%)	11 (4%)	0	100	100
27	CL	225/785 (29%)	212 (94%)	12 (5%)	1 (0%)	34	72
28	CM	443/446 (99%)	417 (94%)	26 (6%)	0	100	100
29	CN	222/252 (88%)	210 (95%)	12 (5%)	0	100	100
29	CO	211/252 (84%)	197 (93%)	12 (6%)	2 (1%)	17	57
30	CP	197/322 (61%)	191 (97%)	6 (3%)	0	100	100
31	CQ	171/259 (66%)	164 (96%)	7 (4%)	0	100	100
32	CR	746/1073 (70%)	682 (91%)	60 (8%)	4 (0%)	29	69
32	CS	746/1073 (70%)	682 (91%)	60 (8%)	4 (0%)	29	69
33	CT	127/203 (63%)	119 (94%)	8 (6%)	0	100	100
34	Ca	223/255 (88%)	212 (95%)	11 (5%)	0	100	100
35	Cc	188/212 (89%)	179 (95%)	9 (5%)	0	100	100
36	Ce	155/203 (76%)	139 (90%)	16 (10%)	0	100	100
37	Cg	157/190 (83%)	152 (97%)	5 (3%)	0	100	100
38	Ch	64/151 (42%)	61 (95%)	3 (5%)	0	100	100
39	Ci	113/150 (75%)	106 (94%)	7 (6%)	0	100	100
40	Cj	124/143 (87%)	116 (94%)	8 (6%)	0	100	100
41	Cm	122/130 (94%)	117 (96%)	5 (4%)	0	100	100
42	Cn	92/145 (63%)	89 (97%)	3 (3%)	0	100	100
43	Cp	59/68 (87%)	55 (93%)	4 (7%)	0	100	100
44	CU	168/311 (54%)	156 (93%)	12 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
47	UH	349/930 (38%)	340 (97%)	9 (3%)	0	100 100
48	UE	121/410 (30%)	117 (97%)	4 (3%)	0	100 100
48	UI	121/410 (30%)	121 (100%)	0	0	100 100
49	US	443/549 (81%)	415 (94%)	28 (6%)	0	100 100
50	Cl	78/156 (50%)	73 (94%)	5 (6%)	0	100 100
51	CX	265/480 (55%)	255 (96%)	10 (4%)	0	100 100
52	UP	52/364 (14%)	46 (88%)	5 (10%)	1 (2%)	8 38
All	All	17778/27558 (64%)	16693 (94%)	1062 (6%)	23 (0%)	54 86

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
29	CO	85	SER
6	UG	580	GLU
13	UQ	708	SER
6	UG	56	PRO
32	CR	48	MET

5.3.2 Protein sidechains (i)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
45	C1	1134/2352 (48%)	347 (30%)	26 (2%)
46	C2	226/230 (98%)	68 (30%)	4 (1%)
All	All	1360/2582 (52%)	415 (30%)	30 (2%)

5 of 415 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
45	C1	4	G
45	C1	5	G
45	C1	7	A
45	C1	13	G
45	C1	14	G

5 of 30 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
45	C1	1085	U
46	C2	35	G
45	C1	1485	A
46	C2	255	U
45	C1	2177	G

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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	$\#\|Z\| > 2$
54	GTP	CI	1201	-	26,34,34	0.97	1 (3%)	32,54,54	1.79	5 (15%)

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
54	GTP	CI	1201	-	-	2/18/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	CI	1201	GTP	C6-N1	-2.83	1.33	1.37

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	CI	1201	GTP	PA-O3A-PB	-5.40	114.28	132.83
54	CI	1201	GTP	PB-O3B-PG	-4.84	116.23	132.83
54	CI	1201	GTP	C3'-C2'-C1'	2.86	105.29	100.98
54	CI	1201	GTP	C5-C6-N1	2.75	118.81	113.95
54	CI	1201	GTP	C8-N7-C5	2.49	107.74	102.99

There are no chirality outliers.

All (2) torsion outliers are listed below:

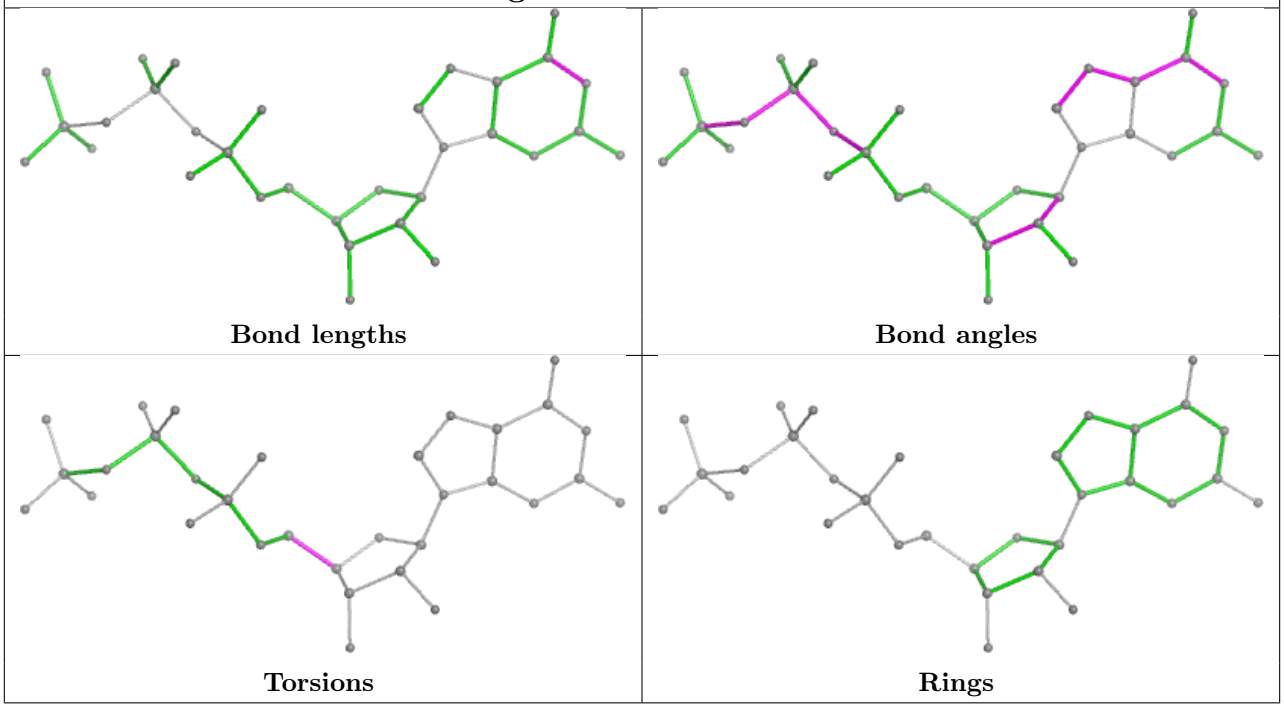
Mol	Chain	Res	Type	Atoms
54	CI	1201	GTP	O4'-C4'-C5'-O5'
54	CI	1201	GTP	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

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 then 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.

Ligand GTP CI 1201



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
46	C2	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C2	206:G	O3'	240:C	P	18.77
1	C2	105:C	O3'	110:A	P	16.05
1	C2	119:C	O3'	123:A	P	11.95

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-10051. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

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

7 Map analysis

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

7.1 Map-value distribution

This section was not generated.

7.2 Volume estimate versus contour level

This section was not generated.

7.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.