Full wwPDB EM Validation 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 Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (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 (1)) were used in the production of this report:

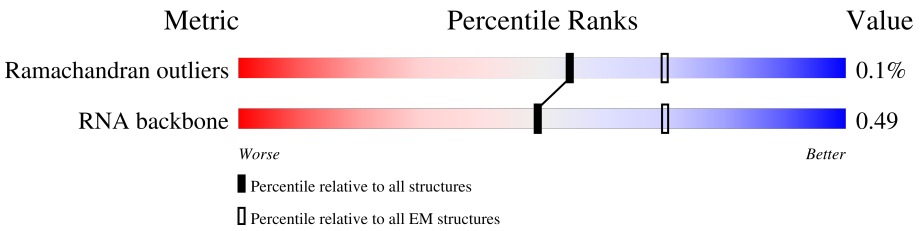
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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
			Total	C	N	O	S		
7	UJ	445	3377	2169	604	590	14	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	UK	217	1687	1062	351	269	5	0	0

- Molecule 9 is a protein called Utp12.

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

- Molecule 10 is a protein called Utp13".

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

- Molecule 11 is a protein called Utp14.

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

- Molecule 12 is a protein called Utp15.

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

- Molecule 13 is a protein called Utp17.

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

- Molecule 14 is a protein called Utp18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	UR	447	3491	2209	656	616	10	0	0

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

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

- Molecule 16 is a protein called Utp24.

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

- Molecule 17 is a protein called Utp30.

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

- Molecule 18 is a protein called Nop1.

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

- Molecule 19 is a protein called Putative nucleolar protein.

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

- Molecule 20 is a protein called Nop58.

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

- Molecule 21 is a protein called snu13.

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

- Molecule 22 is a protein called Rrp9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	CG	378	2922	1865	527	517	13	0	0

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

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

- Molecule 24 is a protein called Bms1.

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

- Molecule 25 is a protein called Imp3.

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

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

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

- Molecule 27 is a protein called Putative U3 small nucleolar ribonucleoprotein protein.

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

- Molecule 28 is a protein called Sof1.

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

- Molecule 29 is a protein called Emg1.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	CP	201	1625	1047	286	283	9	0	0

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

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

- Molecule 32 is a protein called Kre33.

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

- Molecule 33 is a protein called Fcf2.

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

- Molecule 34 is a protein called 40S ribosomal protein S1.

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

- Molecule 35 is a protein called 40S ribosomal protein s5-like protein.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 44 is a protein called Faf1.

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

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

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

- Molecule 46 is a RNA chain called U3 snoRNA.

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

- Molecule 47 is a protein called Utp8.

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

- Molecule 48 is a protein called Utp5".

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

- Molecule 49 is a protein called Noc4.

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

- Molecule 50 is a protein called Putative ribosomal protein.

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

- Molecule 51 is a protein called Enp1.

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

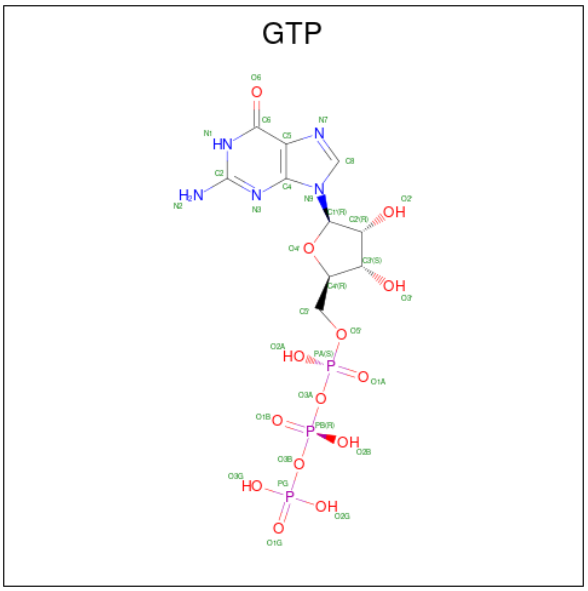
- Molecule 52 is a protein called Utp16.

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

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

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

- 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
			Total	C	N	O	P	
54	CI	1	32	10	5	14	3	0

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

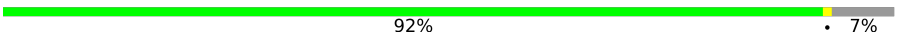
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
55	CI	1	1	1	0

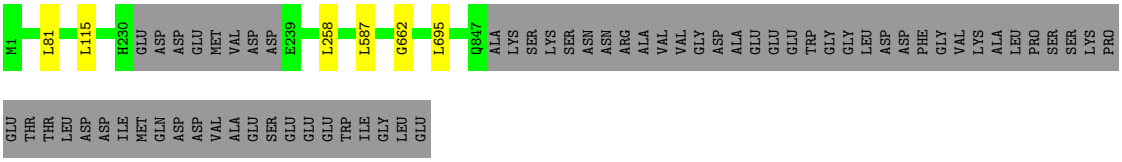
3 Residue-property plots (i)

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

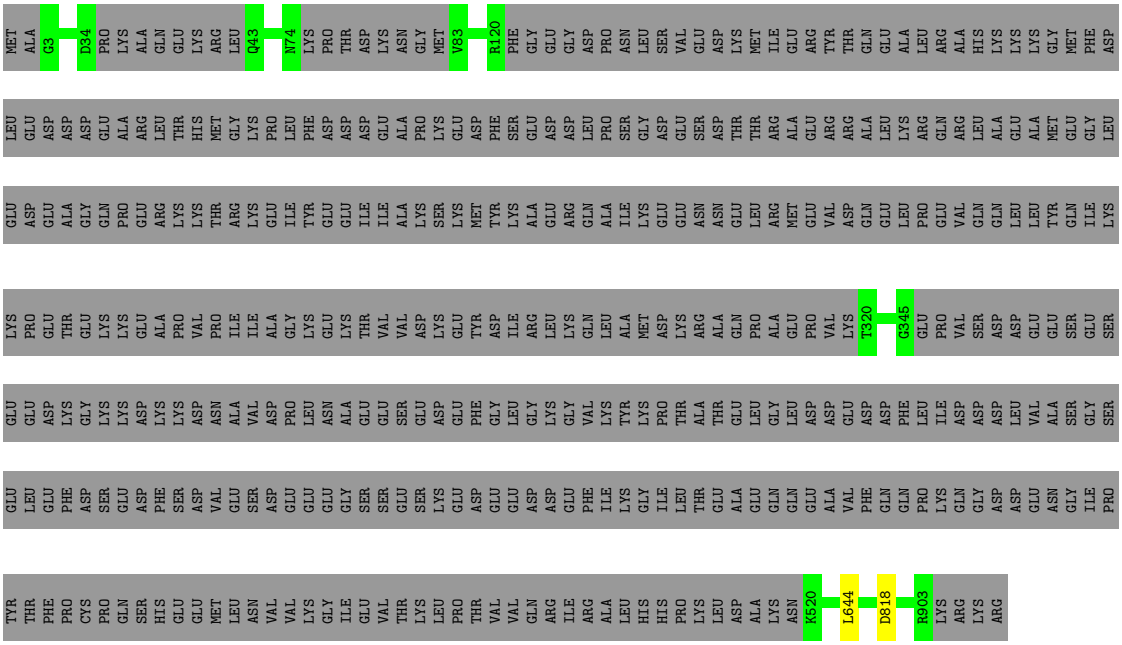
Chain UA:





- Molecule 2: Utp2

Chain UB:



- Molecule 3: Utp3

Chain UC:

LEU LYS ARG GLN ASP LYS GLU ASP ALA PHE LEU GLU GLN SER ASP GLU GLU ILE PHE ASP ASP GLU LEU SER SER GLU GLU GLU GLU GLU ASP ASP GLU ASP GLU ARG ARG ALA PRO THR LYS LYS ASP GLY LYS LYS GLY ALA ALA LEU ASP ASP ASP ASP ASP ALA GLU LEU LEU GLY

LEU GLY LYS LYS LYS ASP ASP ASP GLU ILE ILE ARG ASP GLU GLU GLY TRP TRP GLY SER SER LYS LYS GLU TYR TYR ASN ALA ASP ALA ILE GLU THR GLU GLN ASP ALA LEU GLU GLU GLU LYS GLU ALA ARG ARG LEU GLN ALA LYS LYS LEU ALA LYS MET GLN GLU ALA ASP PHE ALA PHE

ASP GLU ALA GLU TRP LEU ALA THR LYS ASP GLU LYS THR GLY GLY ASP GLU GLU VAL VAL THR GLU VAL LEU LYS GLU VAL GLU VAL THR SER ASP MET GLY PRO GLU GLU ARG TYR ASN LEU LEU GLN ALA ARG TYR PRO GLU PHE ASP TYR LEU VAL GLU GLU PHE ARG GLU LEU ARG

PRO LEU LEU GLU THR LEU GLN LYS GLU ALA ALA GLU GLY LYS PRO ALA LYS SER LEU PRO VAL VAL LYS ALA TRP VAL LEU GLY CYS TYR VAL ALA ALA SER TYR PHE ALA ILE LEU THR SER PRO GLY ASP GLU SER LYS GLY ILE MET ASN PRO SER GLU LEU ARG

ASP HIS GLU VAL MET GLN THR LEU MET GLU CYS ARG GLU ALA TRP LEU LYS VAL LYS SER LEU ARG PRO ALA LYS GLY VAL SER ALA HIS GLY MET LEU SER PRO PRO GLU GLU GLY GLU GLU ALA GLY SER ASP VAL ASP MET LEU ASP ASP HIS ALA VAL GLN LYS PRO LYS LYS

ALA LYS LYS LEU SER LYS GLU GLU ILE LYS ALA ASN LYS LYS LYS LYS GLU GLU ALA ALA LYS LYS ALA ALA LYS ALA VAL GLU GLN SER LEU ALA GLU LEU THR SER LEU LEU GLN THR THR LYS LYS ALA ALA VAL LYS ALA SER VAL ALA SER LYS ALA MET SER THR ALA ALA THR SER

GLY ALA ASP SER GLY MET ASP ASP ASN ARG SER ASP PHE GLY GLU GLU GLU GLU LEU ASP ALA ARG THR ALA ALA GLU LYS LYS ARG LYS ALA ARG PHE TYR THR SER GLN ILE VAL GLN LYS ALA ASN LYS ARG GLN GLY ALA GLY ARG ASP ASP GLY GLY ASP MET ASP

ILE PRO TYR ARG GLU ARG LEU LYS ASP ARG GLN ALA ARG LEU ASN ALA GLU ALA GLU ARG ARG GLY LYS ARG ASP SER LYS PHE GLY ALA ASP LEU GLY GLY ASP SER SER ASP ASP GLU ASP ALA LYS ALA ARG GLN VAL ARG ASP ASP GLU ASP ALA TYR TYR ASN GLU VAL VAL GLN

ALA ALA ALA LYS LYS ARG ALA ASP LYS GLN ALA ARG PHE GLU ALA LEU ALA ALA ALA ARG LYS GLY ASP ARG VAL VAL GLU GLU GLU THR ILE GLY PRO ASP G575 L648

- Molecule 4: Utp4

Chain UD: 87% 13%

M1 P141 HIS LYS ALA ASN ALA ALA A148 L357 W387 L404 ASP ASP PRO GLN ALA P410 P458 ALA ALA ALA GLN ARG ASN GLY GLN L467 L561 P578 GLY GLU GLY VAL ASN GLY THR GLY GLY GLU ASP SER ASP GLY GLU SER ALA ALA SER SER SER SER ASP SER

SER ASP GLU LYS SER GLU ASP ILE A610 S717 PRO GLU LYS ASP LEU VAL GLU THR ASN GLY HIS LYS GLN GLY THR K733 D775 ALA ASP ASP GLN LYS SER VAL GLY VAL SER SER GLY VAL ASP ASP ASP ASP GLU THR ASP G797 R808 GLU ALA ASN SER SER ALA ASN

ALA GLU LYS GLU GLY PRO SER ARG A824 G843 MET MET GLU LYS LYS LEU GLY ALA VAL GLU GLY I855 R884

- Molecule 5: Utp6

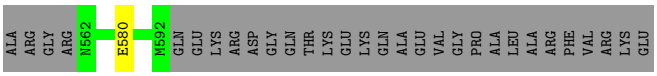
Chain UF: 79% 20%

MET A2 K121 L177 K196 GLN GLY GLN GLY VAL ARG LYS GLY VAL ASN ALA LEU GLU ALA ILE LYS ALA THR GLU GLY GLN GLU GLU GLY ASP ILE ILE PRO ILE GLY GLU ASP THR GLU ASP ASP SER GLY ASP GLU ASP GLY LEU ILE LEU PRO ASP PRO ASP ALA GLU GLY

THR ASP GLY THR LYS LYS ALA ALA LYS PRO VAL PHE ASP ALA GLU GLN THR LYS LYS LEU GLU GLN SER P272 D347 VAL LEU T350 L409 GLU GLU SER PRO SER

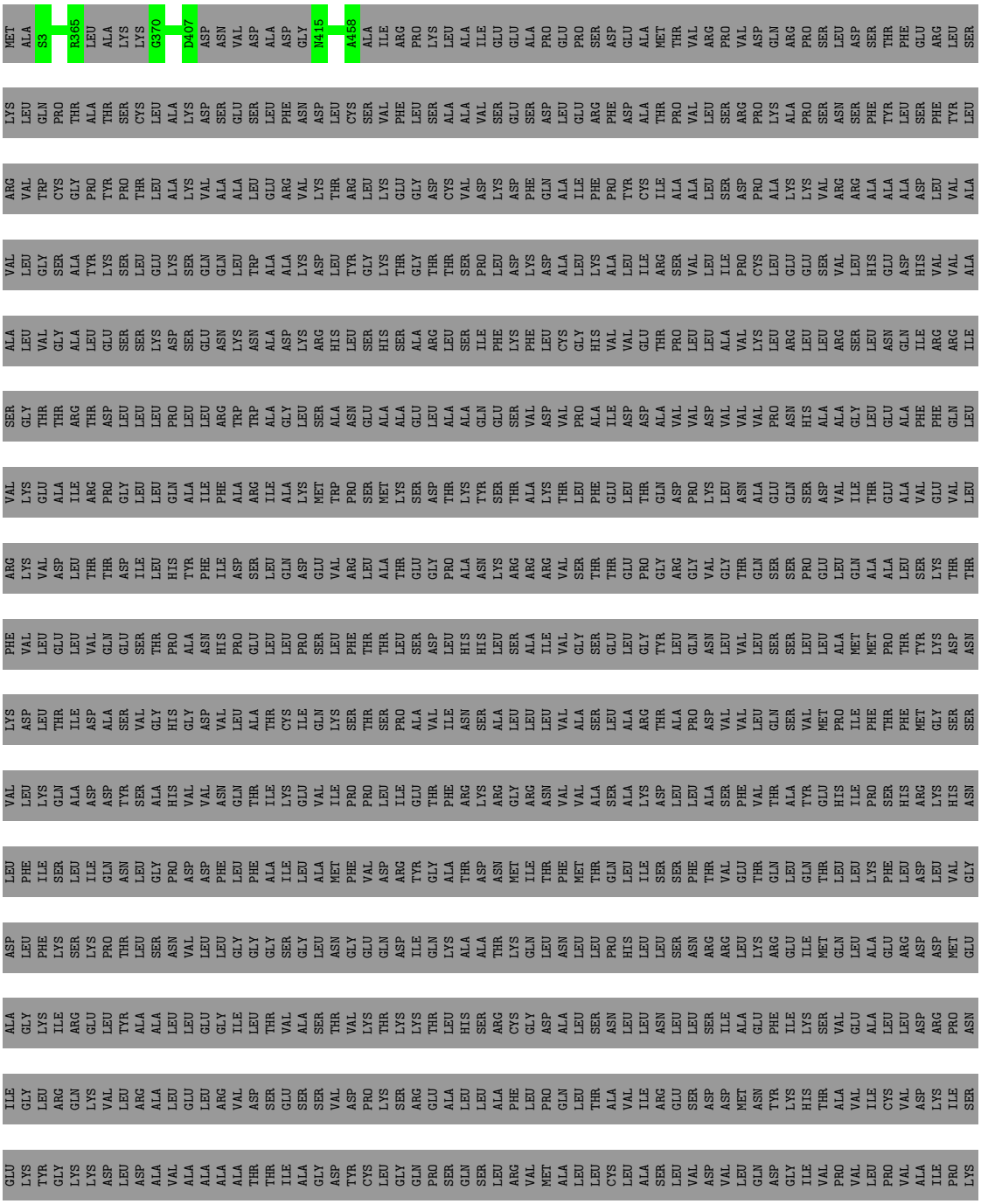
- Molecule 6: Utp7

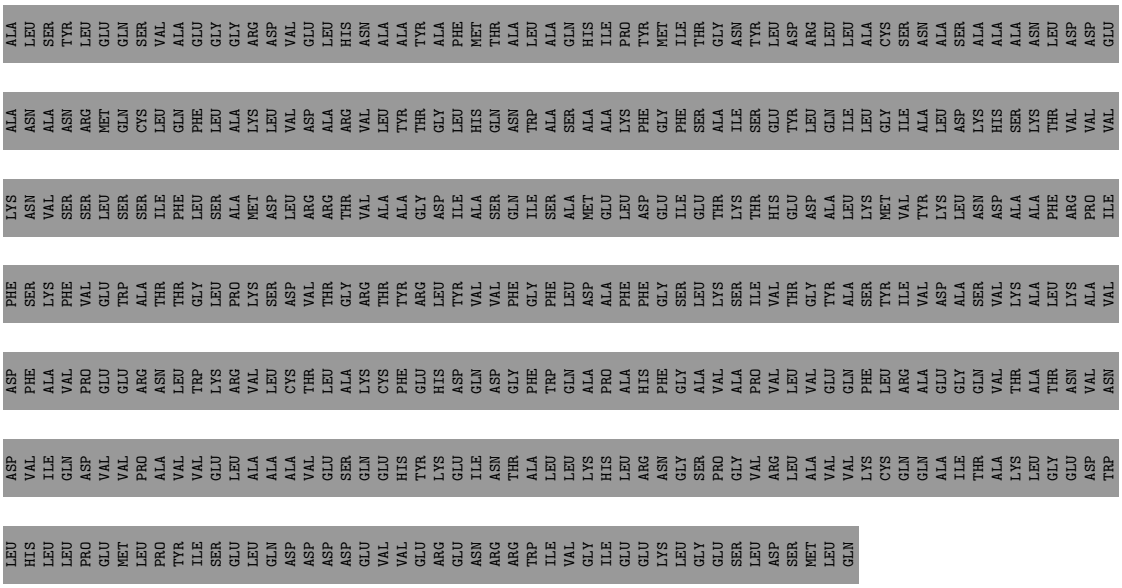
Chain UG: 85% 14%



- Molecule 7: UTP10

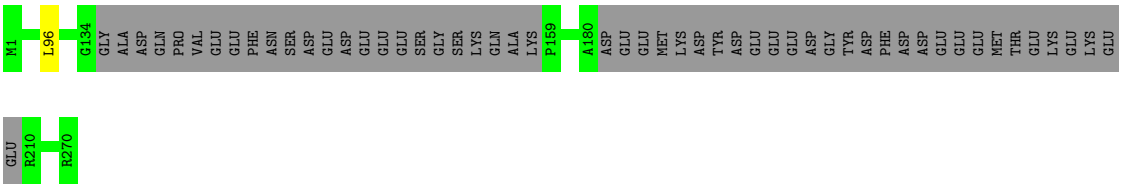
Chain UJ: 25% 75%





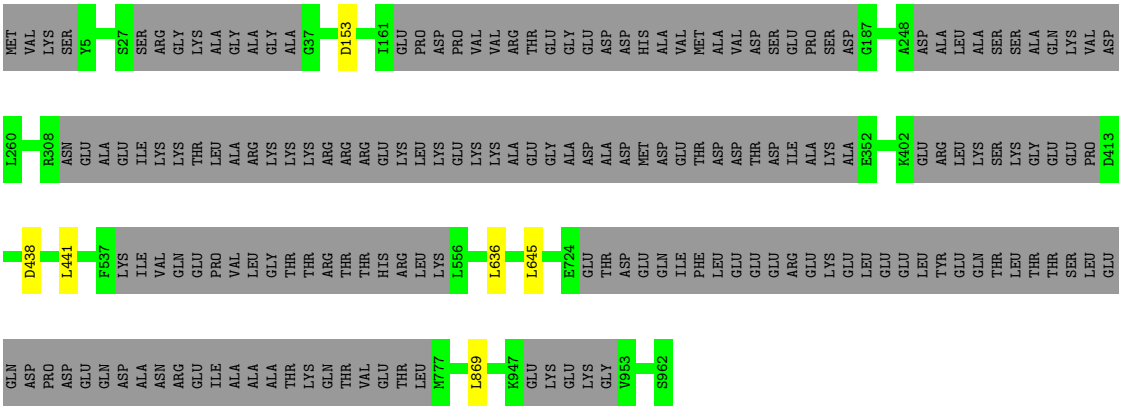
- Molecule 8: U3 small nucleolar RNA-associated protein 11

Chain UK:



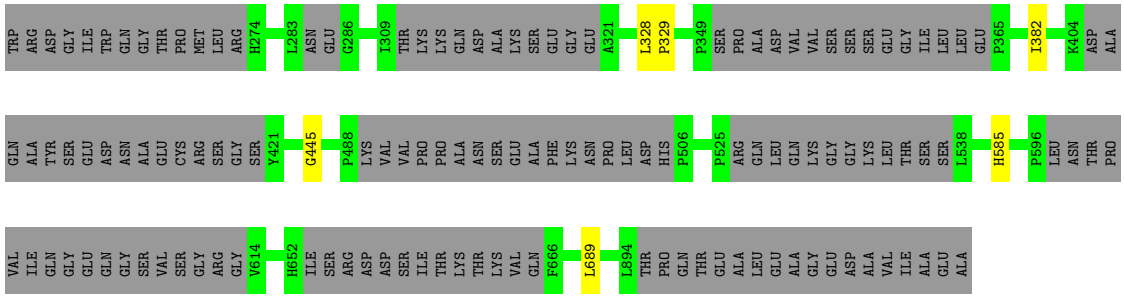
- Molecule 9: Utp12

Chain UL:



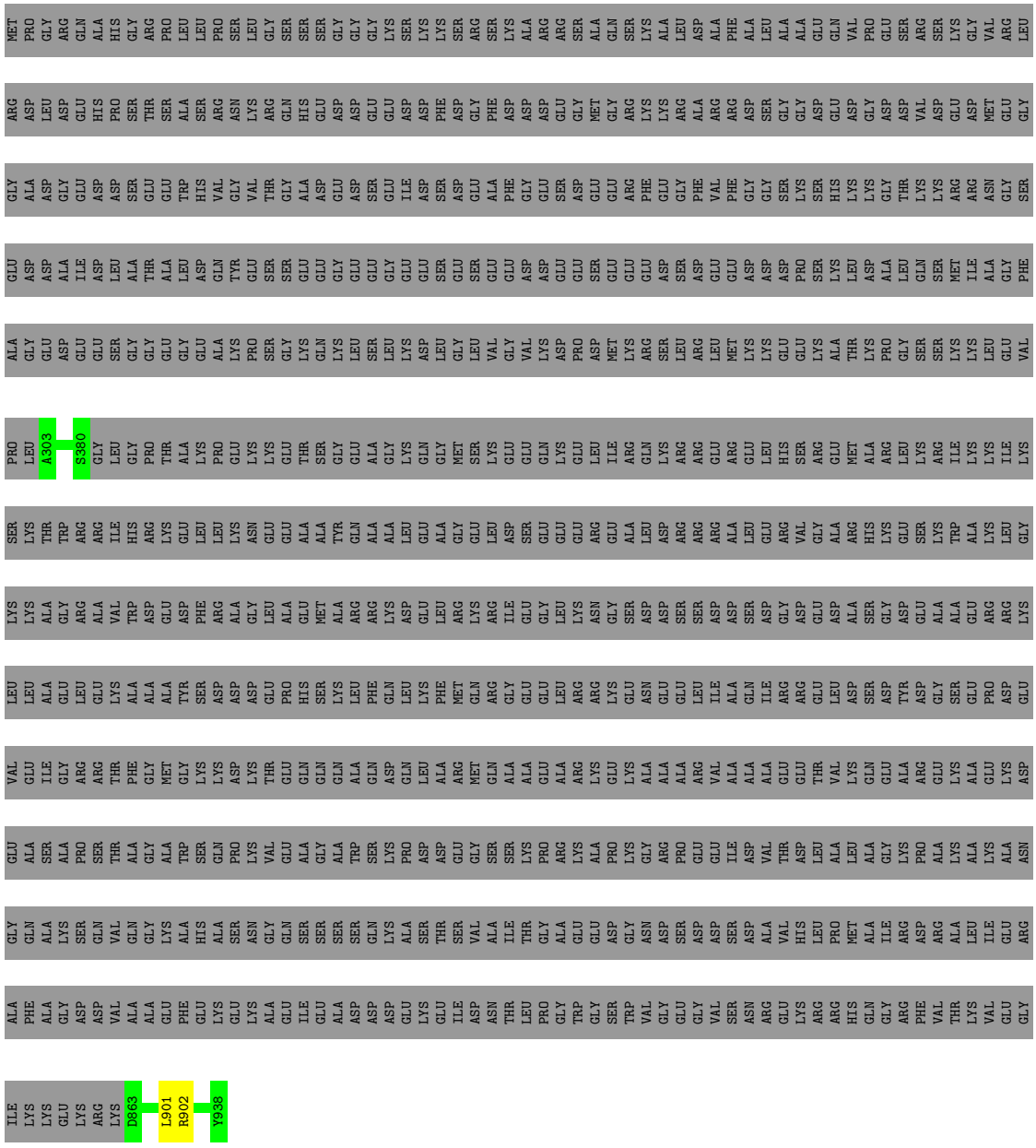
- Molecule 10: Utp13"

Chain UM:



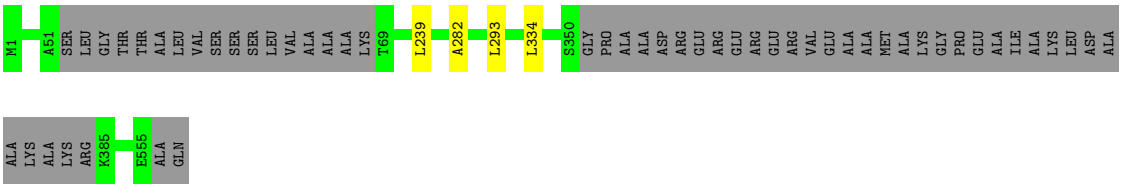
• Molecule 11: Utp14

Chain UN: 16% 84%



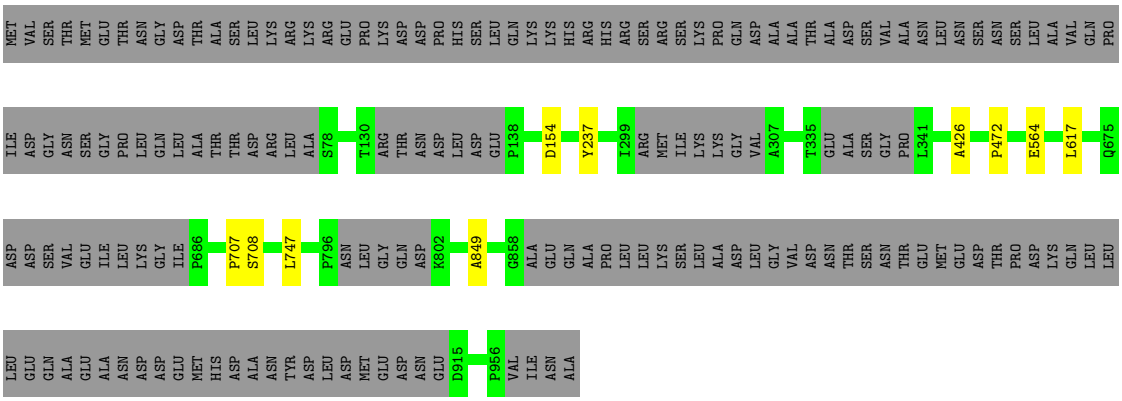
• Molecule 12: Utp15

Chain UO: 90% 10%



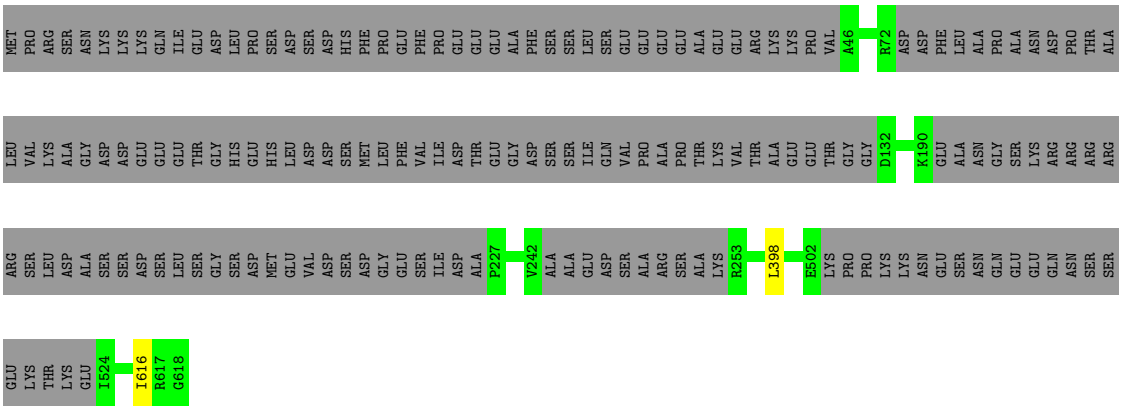
- Molecule 13: Utp17

Chain UQ: 81% 18%



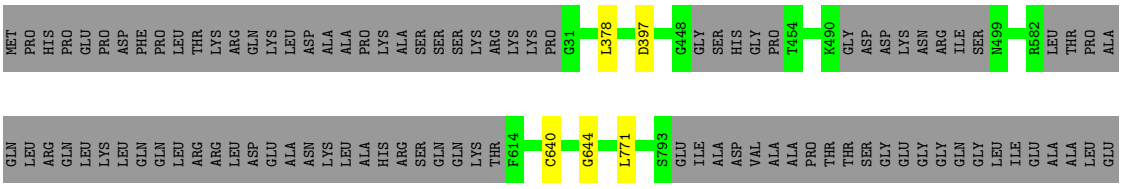
- Molecule 14: Utp18

Chain UR: 72% 28%



- Molecule 15: Putative U3 snoRNP protein

Chain UU: 85% 14%



ALA GLU GLU GLU GLN ALA GLU ASP ASP GLY VAL MET ALA PRO ILE ILE ASP GLN LEU SER ALA ASP M840 I857 E895 ASP ALA LYS ALA LYS LYS GLU LYS ALA ALA ALA ASN GLY ALA SER ARG ILE THR LYS LEU ASP LEU THR ARG GLN GLU GLN T923 T1049

• Molecule 16: Utp24

Chain UX: 98%

G-8 A181 PRO ALA SER

• Molecule 17: Utp30

Chain UZ: 59% 40%

MET ALA PRO SER THR ALA VAL ALA LYS LYS GLU THR ASP ALA VAL ILE PRO V18 K36 ALA ALA ALA ALA PRO ARG PRO ASP GLY LYS GLN ASN LEU LEU ALA ASP GLU GLU SER T56 L66 D103 D114 A186 GLN ARG GLU LYS VAL ASN GLY LYS ARG VAL PRO ALA

PRO LYS GLY LYS LYS GLU LYS ARG ASP PRO LEU GLU N211 Q273 Q295 THR ASP GLU LEU TRP LEU ASP GLU SER LYS VAL VAL PRO ASP GLY GLN GLU PRO ALA ARG ALA LEU PRO GLY LYS ARG GLU LYS ALA ASN ILE GLY LYS LYS ARG LYS PRO LEU GLU ASP ALA SER GLN

PRO ALA LEU GLU GLU THR GLY LYS ASP GLU ARG PRO LYS LYS LYS ALA LYS LYS THR LEU PRO GLU SER ASN ASP ASP LYS LEU ASP LYS ALA ILE ALA GLU ARG LYS GLU GLN LEU LYS LYS GLN LYS ALA ALA ALA LYS LYS VAL ALA ALA ASP ILE

• Molecule 18: Nop1

Chain CA: 77% 23%

MET GLY PHE GLU ARG GLY GLY ARG GLY GLY GLY ARG GLY GLY ALA ALA ALA ARG GLY GLY ARG GLY GLY ALA ARG GLY GLY ARG GLY GLY PRO ALA GLY ARG GLY GLY PRO ALA GLY ARG GLY GLY ARG GLY GLY PRO ALA GLY ARG GLY GLY ARG SER GLY ARG GLY GLY LYS PRO

LYS ALA LYS G64 P114 GLY SER GLY PRO ASP ALA VAL ALA T123 G313

• Molecule 18: Nop1

Chain CB: 75% 24%

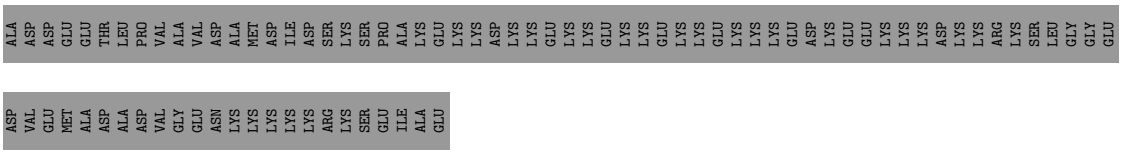
MET GLY PHE GLU ARG GLY GLY ARG GLY GLY GLY ARG GLY GLY ALA ALA ALA ARG GLY GLY ARG GLY GLY ALA ARG GLY GLY ARG GLY GLY PRO ALA GLY ARG GLY GLY PRO ALA GLY ARG GLY GLY ARG GLY GLY PRO ALA GLY ARG GLY GLY ARG SER GLY ARG GLY GLY LYS PRO

LYS ALA LYS GLY ALA LYS ALA GLY LYS LYS VAL I72 E293 Q308 LYS GLU PHE GLU GLY

• Molecule 19: Putative nucleolar protein

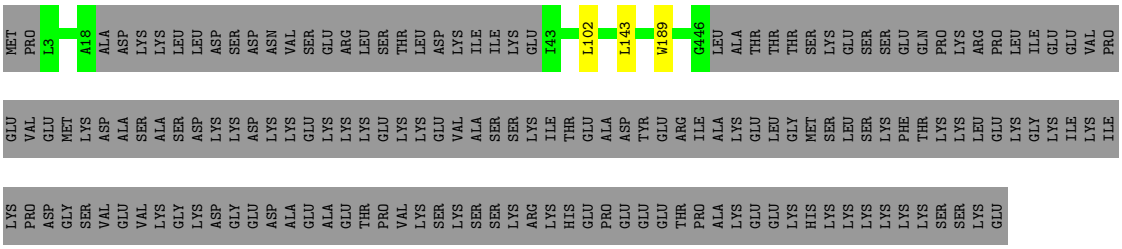
Chain CC: 74% 26%

MET VAL V3 L17 L339 GLY ALA GLU LYS ALA LEU PHE ARG ALA LEU LYS THR LYS SER ALA THR PRO LYS TYR GLY LEU LEU TYR GLN SER SER PHE ILE GLY ARG ALA GLY P372 G421 THR LYS PRO MET LYS ASN SER GLU ALA MET GLU LYS ALA ILE LYS ALA VAL MET



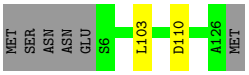
• Molecule 20: Nop58

Chain CD: 72% 28%



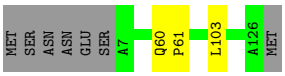
• Molecule 21: snu13

Chain CE: 94% 5%



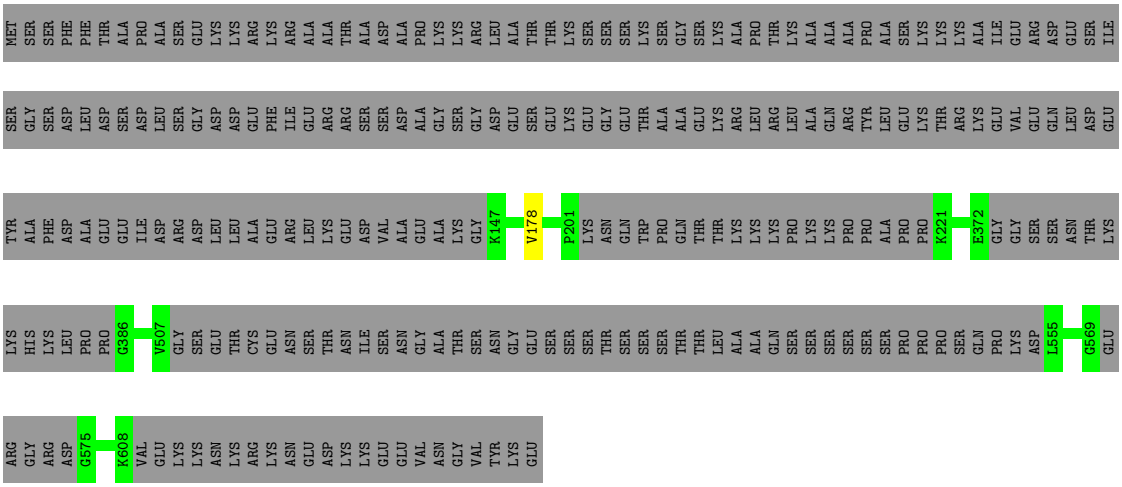
• Molecule 21: snu13

Chain CF: 92% 6%



• Molecule 22: Rrp9

Chain CG: 60% 40%



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

Chain CH: 94% 5%

MET ALA GLU PRO LYS PRO E7 L120 H143 P258 E264 LYS GLY THR THR Q269 A380 GLY ASP ASP GLU ASP ASP ALA GLU GLY GLU LEU GLY D393 A411

- Molecule 24: Bms1

Chain CI: 70% 29%

MET ASP SER GLN GLN HIS LYS PRO HIS ARG PRO SER LYS THR LYS GLU LYS LYS LYS LYS GLN ASN SER GLY GLY THR ASN PRO LYS ALA PHE ALA VAL ALA ASN PRO GLY LYS LEU A40 T308 P309 A314 MET ALA ASN LEU THR GLY LYS LYS P323 Q404 ILE PRO GLU GLU

ASP THR ASN ASP THR GLY ARG LYS THR HIS ARG PRO ARG LYS ALA ARG PHE LEU GLU ASP ASP ARG GLN ASN ASP GLU ASN GLY VAL PRO GLU ASP GLU GLY PHE VAL SER GLY GLU GLU SER LYS GLY SER ASP GLY SER ASP ILE GLU GLU PHE ASP GLU LYS ARG LEU GLY LYS MET PHE

ARG GLY ASP ASP GLU GLU THR GLN ASP GLU ASP VAL VAL PHE ALA ASP THR ASP SER GLU LEU GLY SER ILE SER GLY ASP GLU GLU GLY VAL ASP SER GLU SER GLY SER ASP GLU GLU PHE ASP SER GLU GLU GLU GLU ALA VAL ARG TRP LYS GLU ASN MET MET GLU ARG ALA ARG

ALA LEU HIS GLY LYS ARG K535 G562 GLU ASP ASN GLU LYS GLU GLU GLU GLU GLU GLU ASP ILE GLU LYS ASP GLU ASP THR PHE PHE HIS LYS ALA LYS ASP GLU ASP ASP LEU GLU GLU ASP ARG MET ILE PRO HIS PHE D602 F624 SER THR GLY ARG PRO LYS GLY ASP GLY

GLU GLY ASP SER GLU GLY GLU GLY ASP GLY ASP ASP ASP ASP PHE ASN GLY PHE ASP GLU ASP ASP GLU ASP GLU GLY ASP GLY ALA PHE GLU ASP LEU GLU THR GLY GLU LYS HIS GLY PRO SER LYS GLU LYS LYS GLU GLU GLU GLU LYS PRO ALA MET SER LEU GLU GLU GLU

ARG GLU ARG ASN ALA ARG ARG LYS GLU GLU LEU ARG ALA ARG PHE GLU GLU GLU ASP ARG GLU GLY LEU LEU ASN ASP LYS ALA ILE ALA ARG ARG GLU GLY GLY LEU ASP GLU GLU PHE GLY GLU ASP Q737 L845 W851 D852 K1150 ALA SER GLU GLU TRP GLY GLY GLY GLY

LYS ARG ARG LYS

- Molecule 25: Imp3

Chain CJ: 98%

MET V2 F180 GLU LEU LEU

- Molecule 26: Putative U3 small nucleolar ribonucleoprotein

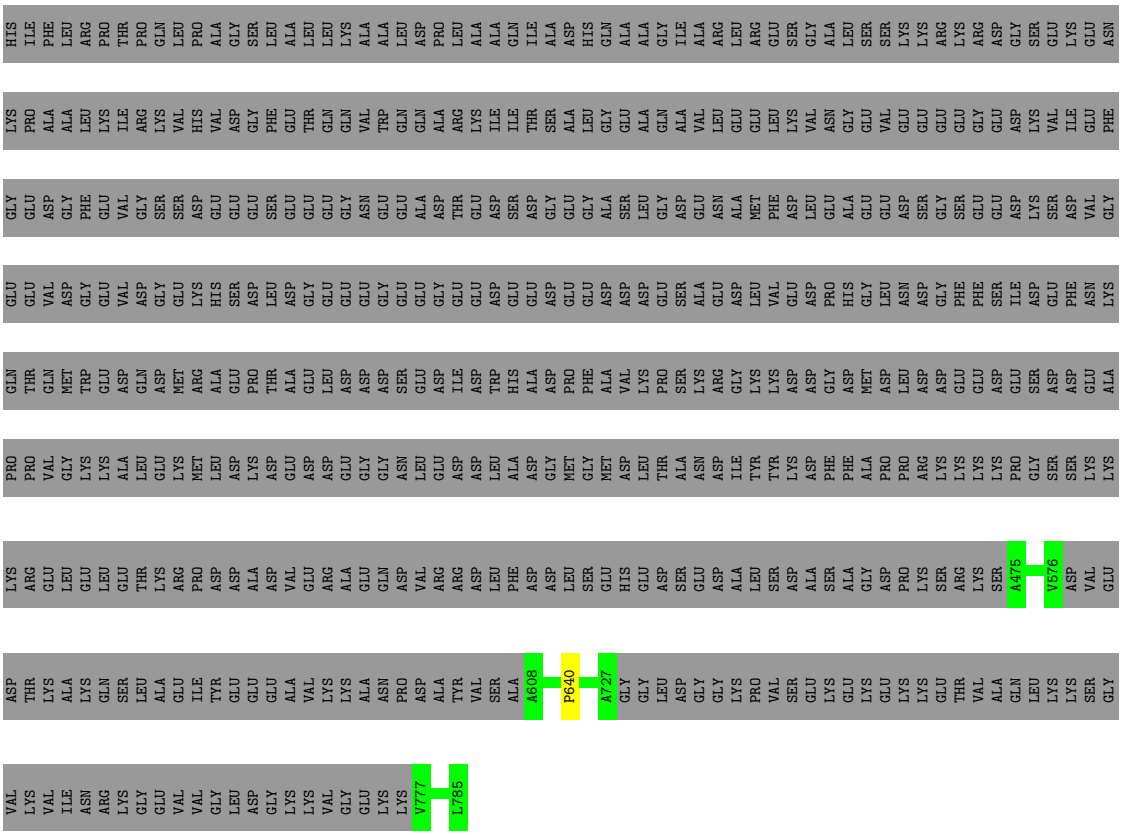
Chain CK: 99%

M1 L89 D235 F261 F297

- Molecule 27: Putative U3 small nucleolar ribonucleoprotein protein

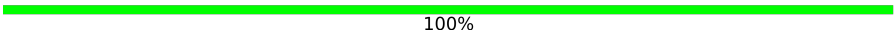
Chain CL: 29% 71%

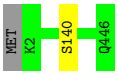
MET PRO GLY ALA PRO SER THR THR SER SER PHE THR SER THR SER HIS THR LEU SER ALA LEU PRO SER MET PRO GLN SER LEU SER ALA SER ALA ALA ASP GLY SER GLY SER GLY SER ASP GLY ALA ALA ALA ALA ALA ILE THR ALA PHE LEU ASP SER THR ALA PRO GLU ASN ARG



• Molecule 28: Sof1

Chain CM:



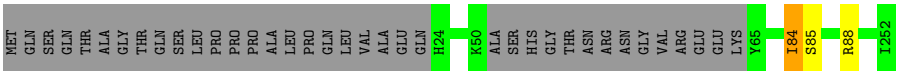


• Molecule 29: Emg1

Chain CN:

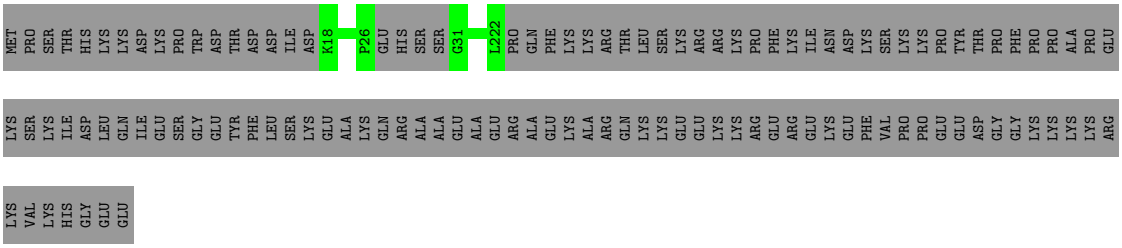
• Molecule 29: Emg1

Chain CO:



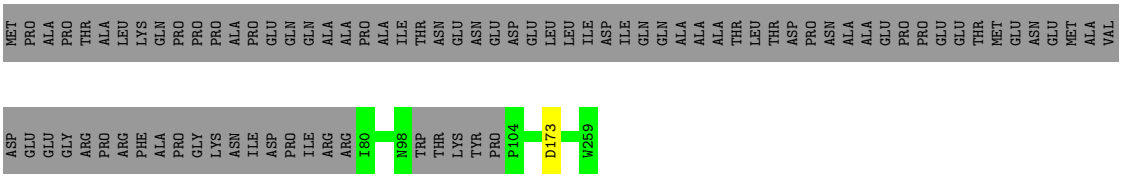
• Molecule 30: KRR1 small subunit processome component

Chain CP:



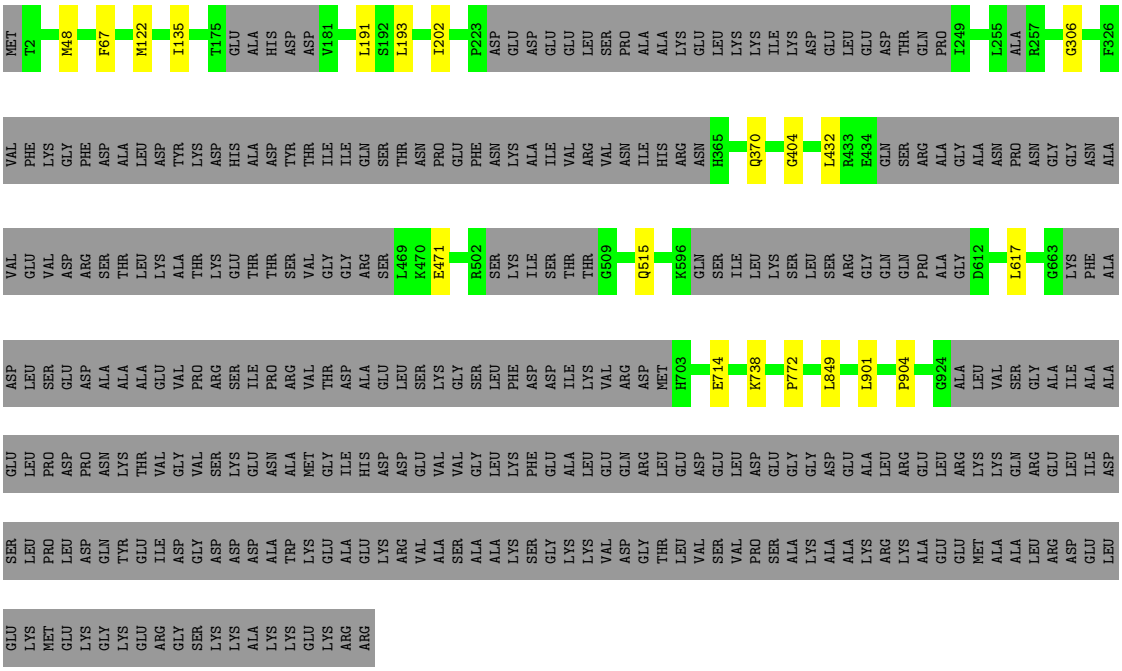
- Molecule 31: Pre-rRNA-processing protein PNO1

Chain CQ: 67% 32%



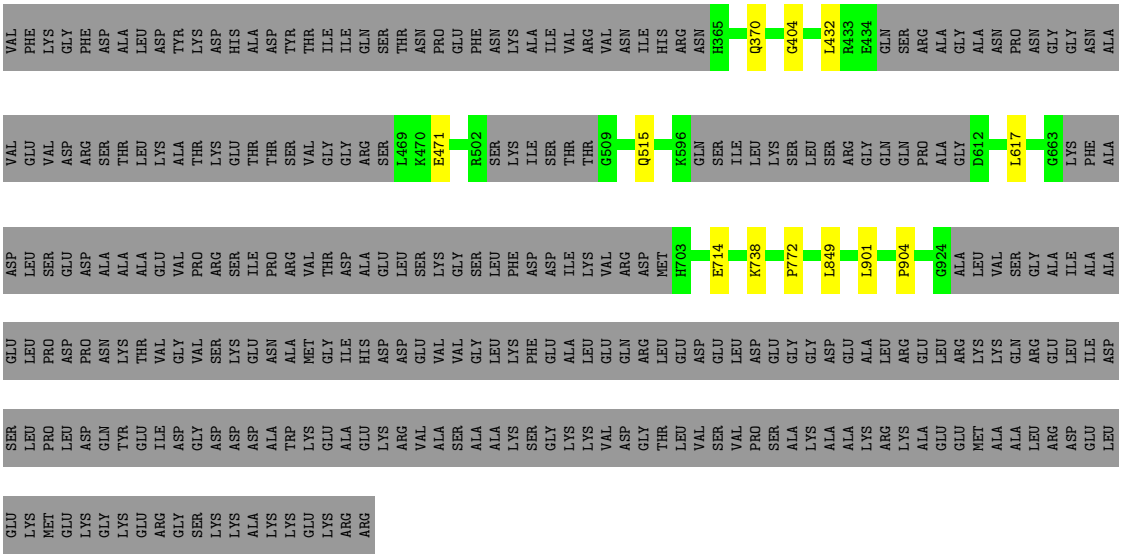
- Molecule 32: Kre33

Chain CR: 69% 29%



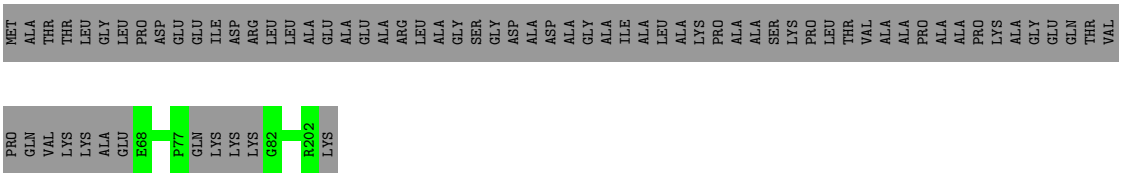
- Molecule 32: Kre33

Chain CS: 69% 29%



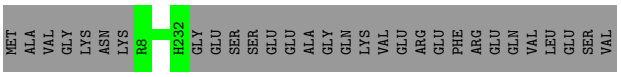
- Molecule 33: Fcf2

Chain CT: 65% 35%



- Molecule 34: 40S ribosomal protein S1

Chain Ca: 88% 12%



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

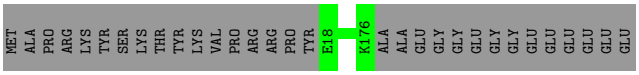
Chain Cc: 90% 9%

- Molecule 36: 40S ribosomal protein S7

Chain Ce: 77% 22%

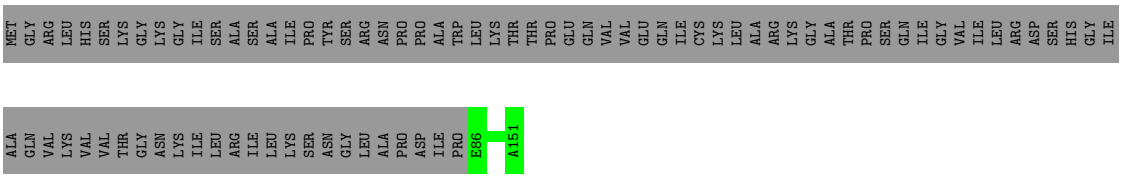
- Molecule 37: 40S ribosomal protein s9-like protein

Chain Cg: 84% 16%



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

Chain Ch: 44% 56%



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

Chain Ci: 77% 23%

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

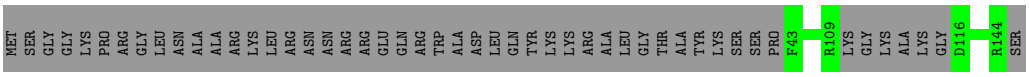
Chain Cj: 88% 12%

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

Chain Cm: 97%

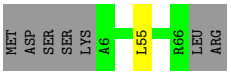
• Molecule 42: 40S ribosomal protein s23-like protein

Chain Cn: 66% 34%



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

Chain Cp: 88% 10%



• Molecule 44: Faf1

Chain CU: 57% 43%

MET PRO GLY LEU LEU GLY LYS ARG LYS SER ARG ALA GLU GLU ASP PRO GLU ALA VAL ALA LYS ALA GLN GLU LEU LEU ARG LYS HIS PHE GLU ALA GLN PHE LYS PRO ILE ASP LEU ALA PRO LEU PRO ARG ARG ALA ILE GLU SER GLU ASP GLU GLU ASP GLU SER SER GLU GLY

SER ASP VAL ASN SER GLY GLU GLY ASP GLU TRP ASP GLY ILE SER GLY ASP GLU ASP GLY THR GLU SER GLU GLY ASP GLU SER ASP ASP GLU PRO HIS V94 M102 ASP SER SER ALA A107 K130 SER SER SER SER LYS PRO LYS PRO SER LYS LYS SER THR ASP ASP SER PHE

P148 V259 LYS LYS LYS LYS THR VAL ARG LYS ARG ARG GLU R271 R301 GLY PRO GLN GLY ARG GLY LYS ARG ARG ARG

- Molecule 45: 35S ribosomal RNA

Chain C1: 31% 16% • 51%

G1 G2 G3 G4 G5 G6 A7 G13 G14 G15 U16 C17 G18 C19 C20 C21 C26 C33 C34 G C36 G37 G38 C39 A40 G41 C42 C43 U44 U45 C46 G47 C48 G49 A53 A G55 C56 A60 G61 U62 C63 G66 G67 U68 A71 U72 A73 C74 G75 U76 C77

C80 C88 G89 A90 G93 C96 C97 U104 A105 U111 C112 G121 C126 C127 G128 G129 C134 A135 C136 A143 G144 C145 C148 G149 C C150 G152 C153 C154 G155 C158 C159 C160 A161 G162 A166 G169 C170 G179 C182 C183 U193 G201

A202 C203 U204 C205 C206 U207 A208 A209 G210 A216 A220 A221 C225 G228 U G U231 G232 C233 G234 C235 C236 U242 U243 G244 G257 C258 G265 C266 U267 G268 G269 G273 C276 U277 A278 U281 C282 A283 A284 A285 C290 C291 G292 G293 G294 U308 G309

G310 G311 G312 U319 A320 G321 C322 G323 G324 C325 C333 U334 C339 G340 C343 C346 C347 U348 C349 U350 U351 G362 U369 C370 U371 U372 U382 G383 C384 A385 G386 C398 U402 G403 C404 U416 U424 C425 A426 G427 A435 A436 G440 A441 U442 G443

C447 C448 C449 C454 A458 C459 C468 G469 C470 C471 A474 C475 G484 G485 G491 C492 G493 A497 C498 G499 C500 U501 A502 G503 C504 C505 G506 C507 U A G C G C C C G C C A G C C U G U A A C

A G U G A A C U C G C C G C C C U G A A A C C A C G G G C U C G G U C A U G C U C U U A G G G C G C G

A580 C581 G582 A583 U584 A585 G586 U587 G593 G594 U595

C604 C A G U608 A609 G610 A613 U614 G621 U622 C623 U624 A628 G A U U A A G C C A U G C A U G U C U A U A A U A G G C C A A U U A C A A G G G A U U C U A A C A G C G C U C A U U U C U G U A G A

A A C U G G A A U A A U U G A A A U C U A G U A A U C G U U U A U C C U U A C U A A C A U G G G A A U

A A C C G G U U A A A A C C A G G A G C U A A U C A U G C U C G G A A A A U U C G U G A U U U

U A U U A A G A U U A A A A C C A A U G G C C U A U U C U U U C A A A C U U U C U G U C A U A U U

U C G C A C G G C C C C G G G C G A U G G C C C C U A U A U C A A A C U U C U C G A C G G

C U G G G U A U U G G C C A G U G G U A A C G G A G G G U U A G G G C G G G C U C G G A G

A A G G A G C C U G A A A C C A C U G A A A C A G G C A A G G C G C G C C A G G C C A A A A U G G G A A A G C C U U A A G C G C G C C A G G C C A A A A U

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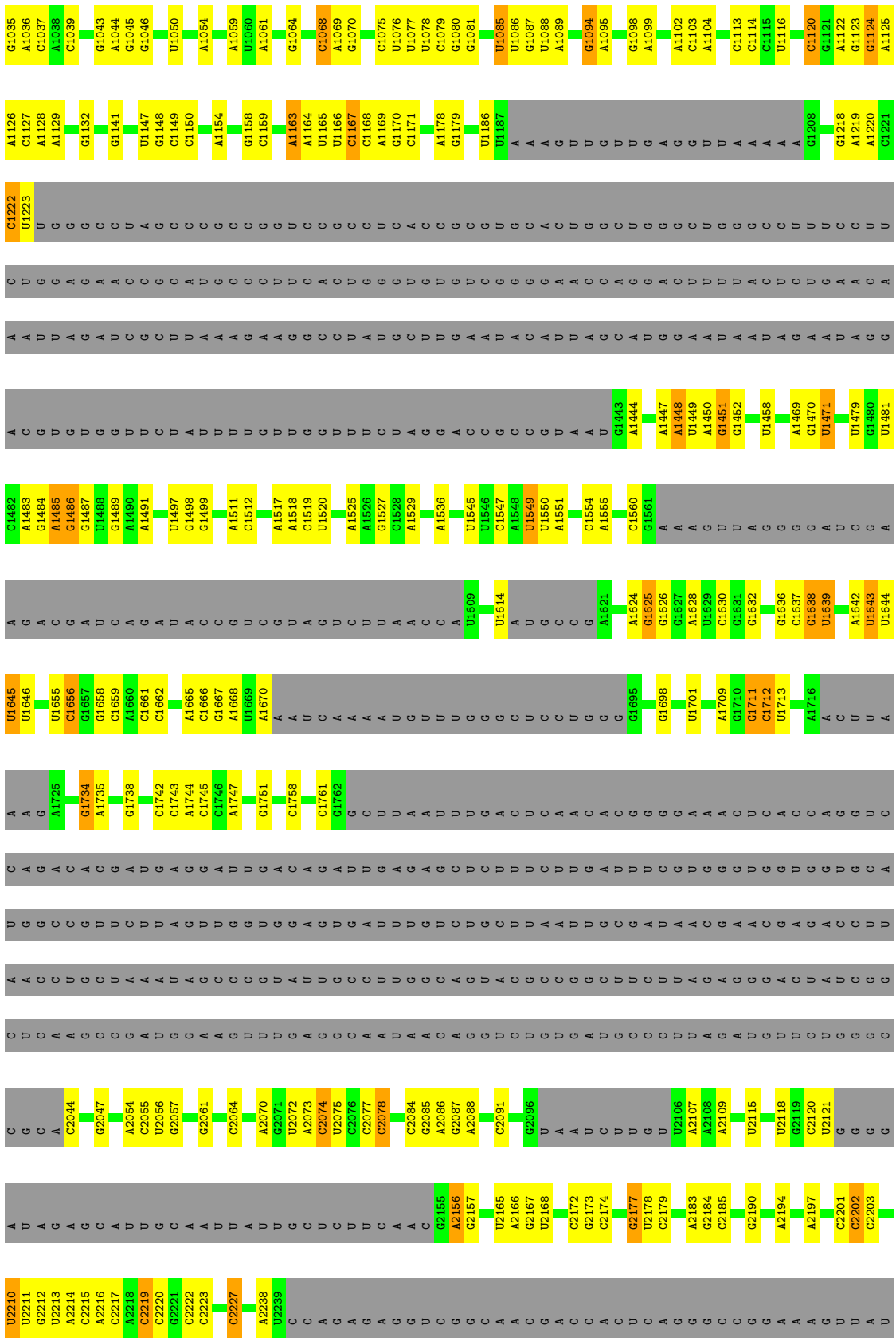
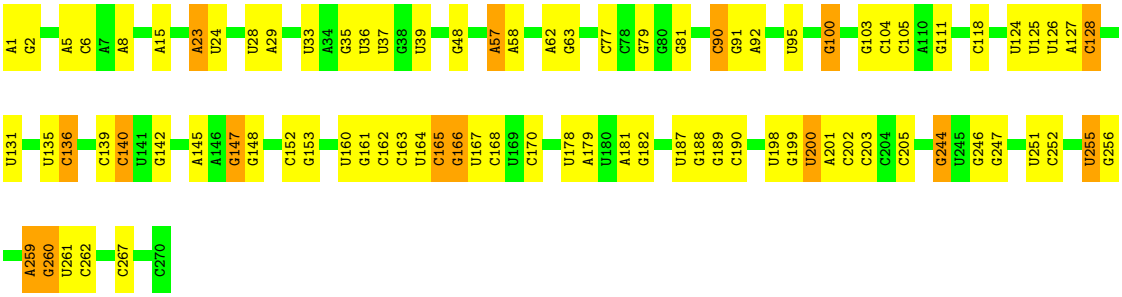

U2210 U2211 G2212 U2213 A2214 C2215 A2216 C2217 A2218 C2219 C2220 G2221 C2222 C2223 C2227 A2238 U2239
A U A G A G C A U U G A G A U A G G C A A U A G C C A U U A U U C G A C C A C U C G G C A G G U U C
C U C A A G C A U U G G A A U U G G A G U U C A A U A A C C U U G G C C U U C A G G U U C U U C A G
A A G A1725 G1734 A1735 G1738 C1742 C1743 A1744 C1745 C1746 A1747 G1751 C1758 C1761 G1762 G
U G G G C C U U C A U U G A A U U G G A A A U U U U G G G A A C C U U U G G G G G A A C C U U G G
A A C C A A U U C A A U U G A A A U U U U G G G A A C C U U U C C C C U U G G G G
U1645 U1646 U1655 C1656 G1657 G1658 C1659 A1660 C1661 C1662 A1665 C1666 G1667 A1668 U1669 A1670 A A A U C A A A A U G U U U U G G G A A C C U U U C C C C U U G G G G1695 G1698 U1701 A1709 G1710 G1711 C1712 U1713 A1716 A C U U A
A G A A U C G G A U G C A U U C C U U U A A C C C C G A1621 A1624 G1625 G1626 G1627 A1628 U1629 C1630 G1631 G1632 G1636 C1637 G1638 U1639 A1642 U1643 U1644
C1482 A1483 G1484 A1485 G1486 G1487 U1488 G1489 A1490 A1491 U1497 G1498 G1499 A1511 C1512 A1517 A1518 C1519 U1520 A1525 A1526 G1527 C1528 A1529 A1536 U1545 U1546 C1547 A1548 U1549 U1550 A1551 C1554 A1555 C1560 G1561 A A A G U U G1443 A1444 A1447 A1448 U1449 A1450 G1451 G1452 U1458 A1469 G1470 U1471 U1479 G1480 U1481
A U U G G A A U U C G G U U G G A A U U G G A A U U U U G G G A A C C U U U G G G G A A C C U U U G G G A A C C U U U G G G A A C C U U U

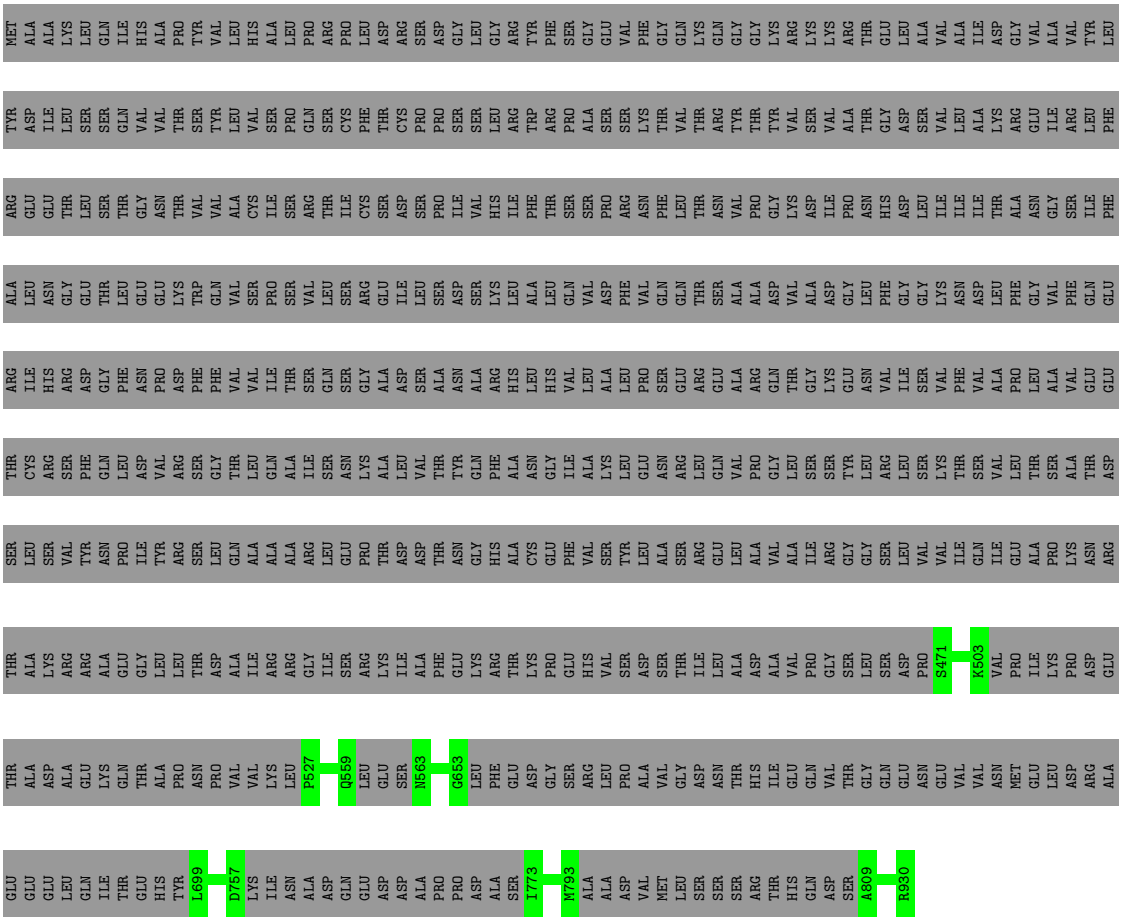
• Molecule 46: U3 snoRNA

Chain C2:



• Molecule 47: Utp8

Chain UH:

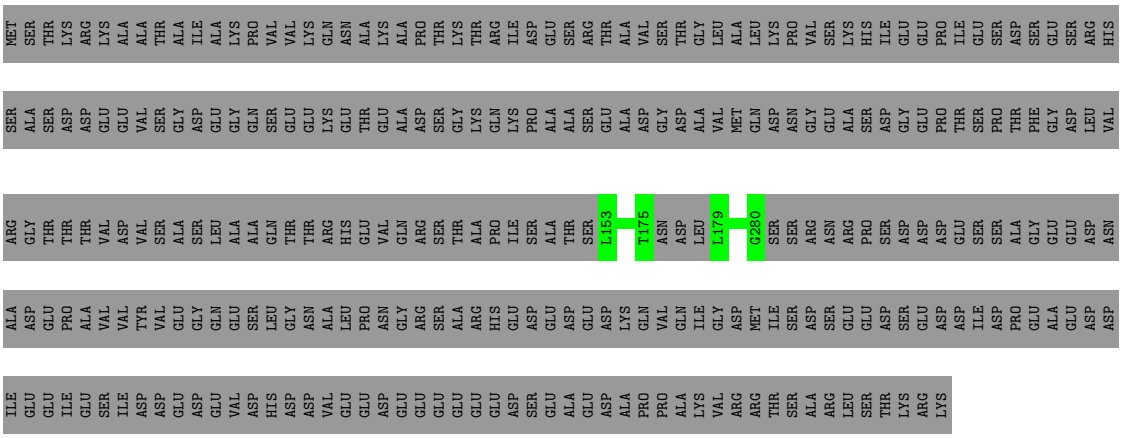


• Molecule 48: Utp5"

Chain UE:

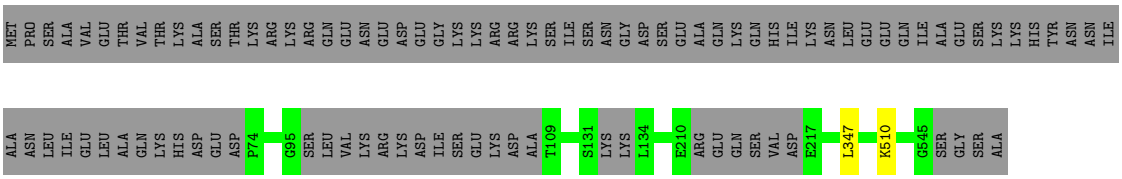
- Molecule 48: Utp5"

Chain UI:



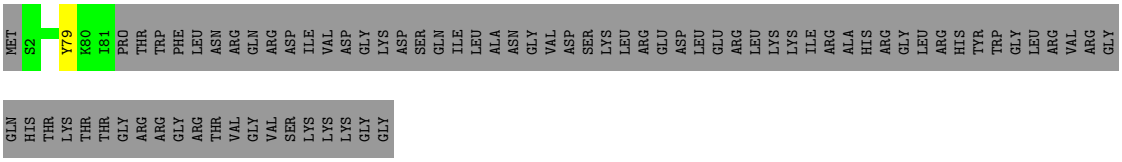
- Molecule 49: Noc4

Chain US:



- Molecule 50: Putative ribosomal protein

Chain Cl:



- Molecule 51: Enp1

Chain CX: 55% 44%

MET PRO LYS ALA ILE ALA ALA SER SER HIS LYS ARG ARG HIS ASN PRO LEU GLU ASP ASP ILE LEU ALA THR GLY ILE LEU LYS ASN ARG GLU GLY ARG PRO SER LYS ARG ALA ASN LYS LYS VAL ALA GLU GLU GLU ASN TYR VAL ASP SER LYS ALA SER ARG LYS ILE LEU ALA MET

SER ARG GLU LEU MET ASP GLU GLU GLU GLN GLN LEU LYS ASN LYS GLN VAL THR VAL ALA SER THR ALA PHE ASP PHE ASP PRO SER ARG MET ASP HIS ASP GLU ASP ASP GLN GLU GLU PHE VAL ASN ASN GLU GLU TRP GLY ASP GLU ASP GLU ASP ALA GLY ASP ASN ASP ASN GLU

VAL ASP ALA ALA ASP LEU GLU ILE PHE ASN ARG PHE VAL GLN PRO THR MET LYS ASP ASP PRO LEU LEU THR HIS GLY TRP ASP GLN LYS PRO ALA ASP GLY GLU GLU GLU LYS GLU GLU GLN THR ASN LEU ALA ASP LEU ILE LEU GLN LYS ILE ALA GLU LYS GLU ALA MET THR GLY

GLY GLN ASN GLY GLY ASN PRO ILE GLU GLU ASP TYR E193 L296 R459 GLY ILE PRO VAL GLN GLN PRO GLN PRO THR PHE ASP GLY ASP ASP THR MET LEU VAL ASP SER

- Molecule 52: Utp16

Chain UP: 15% 85%

MET GLY ARG ARG SER SER GLU LYS GLU MET GLU VAL ILE GLU LEU SER SER ASP SER GLU GLN GLU VAL SER ALA THR LYS ALA VAL VAL PRO GLU ARG THR SER ARG SER PRO SER LEU ASP ARG LEU GLU THR PRO PHE PHE LYS ALA PRO GLY ILE VAL TYR LYS ASP ASP ASP ALA

ASN ASN GLN GLU GLY GLU LYS PHE VAL GLN PRO LYS ASP LYS GLN GLU PRO ILE SER GLN SER THR GLU SER ASP ASP LYS SER LEU SER ARG LYS HIS VAL CYS ILE GLU ILE PRO LEU PRO THR SER SER GLU LEU GLN GLN ARG LYS VAL GLU ALA ALA ALA GLU LYS THR GLU GLU

SER SER LYS THR SER ALA ASP ARG ARG HIS ILE THR PHE ASP ASP SER GLU SER GLU GLN PHE ILE THR LEU LYS GLU GLU ALA ALA SER ARG ASN GLY LEU GLY ASN GLY SER LYS LYS SER GLU ARG GLU ILE VAL GLN ASP SER GLN ASP GLU GLU GLU ASP SER GLU GLU SER ASP

ASP ASP ALA PRO PRO GLU GLU VAL ALA THR GLY GLU ALA GLU ALA ALA LEU LEU LYS ALA GLU ARG ALA ALA ALA ALA ALA LYS ALA ALA ALA GLU GLN GLN GLN ALA ALA ALA ALA LEU GLU LYS ARG LYS ARG GLN GLU ARG ASP ALA PHE LEU LYS GLN GLN ALA GLU GLN ARG LYS ARG ARG ASN LYS LYS PRO ALA

GLN LEU ALA GLU GLU ASP SER ASP GLU GLU ASP ALA GLY PRO GLN ARG THR LEU PRO ILE ARG SER GLU GLN LYS LYS GLU ALA PRO LYS LEU LEU PRO LEU GLU LEU LEU GLU SER ASP GLU ASP SER THR PRO ALA SER ALA ILE THR GLN LYS ARG ARG LYS LEU ASP VAL ASP

PRO LYS LEU LEU VAL GLU PRO K308 P329 V361 ASN LYS ARG

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

All (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
45	C1	258	C	N1-C2-O2	12.91	126.64	118.90
45	C1	258	C	C2-N1-C1'	12.45	132.49	118.80
45	C1	55	G	OP1-P-O3'	-12.20	78.35	105.20
45	C1	160	C	N3-C2-O2	-11.72	113.69	121.90
45	C1	45	U	OP1-P-O3'	-11.39	80.14	105.20
45	C1	258	C	N3-C2-O2	-10.68	114.42	121.90
45	C1	206	C	N1-C2-O2	10.52	125.21	118.90
45	C1	206	C	C2-N1-C1'	10.48	130.33	118.80
45	C1	2168	U	N3-C2-O2	-10.41	114.92	122.20
45	C1	1222	C	N1-C2-O2	10.20	125.02	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
46	C2	140	C	N3-C2-O2	-9.71	115.10	121.90
45	C1	2168	U	N1-C2-O2	9.67	129.57	122.80
45	C1	1662	C	N3-C2-O2	-9.57	115.20	121.90
45	C1	2074	C	N1-C2-O2	9.57	124.64	118.90
46	C2	128	C	C6-N1-C2	-9.49	116.50	120.30
45	C1	1658	G	C5-C6-O6	9.40	134.24	128.60
46	C2	200	U	C2-N1-C1'	9.29	128.84	117.70
45	C1	1658	G	N3-C4-N9	-9.26	120.44	126.00
45	C1	160	C	C6-N1-C2	-9.18	116.63	120.30
45	C1	45	U	OP2-P-O3'	-9.16	85.05	105.20
46	C2	140	C	N1-C2-O2	9.11	124.37	118.90
46	C2	200	U	N1-C2-O2	9.07	129.15	122.80
45	C1	1550	U	C2-N1-C1'	9.06	128.58	117.70
45	C1	2217	C	N1-C2-O2	9.06	124.34	118.90
45	C1	160	C	N1-C2-O2	9.03	124.32	118.90
46	C2	128	C	C5-C6-N1	9.00	125.50	121.00
45	C1	258	C	C6-N1-C1'	-8.92	110.10	120.80
45	C1	1027	C	N3-C2-O2	-8.90	115.67	121.90
45	C1	1655	U	N3-C2-O2	-8.85	116.01	122.20
45	C1	206	C	N3-C2-O2	-8.83	115.72	121.90
45	C1	1658	G	N9-C4-C5	8.73	108.89	105.40
45	C1	291	C	N1-C2-O2	8.72	124.13	118.90
45	C1	2217	C	C2-N1-C1'	8.67	128.34	118.80
45	C1	158	C	N1-C2-O2	8.66	124.09	118.90
46	C2	200	U	N3-C2-O2	-8.62	116.17	122.20
45	C1	505	C	N3-C2-O2	-8.62	115.87	121.90
46	C2	136	C	N1-C2-O2	8.61	124.06	118.90
26	CK	235	ASP	CB-CG-OD1	8.56	126.01	118.30
26	CK	89	LEU	CA-CB-CG	8.43	134.70	115.30
45	C1	1486	G	C4-N9-C1'	8.40	137.43	126.50
45	C1	112	C	N1-C2-O2	8.35	123.91	118.90
1	UA	81	LEU	CA-CB-CG	8.35	134.50	115.30
32	CS	738	LYS	CD-CE-NZ	8.34	130.89	111.70
32	CR	738	LYS	CD-CE-NZ	8.34	130.89	111.70
45	C1	1547	C	N1-C2-O2	8.32	123.89	118.90
45	C1	471	C	N3-C2-O2	-8.29	116.10	121.90
45	C1	1222	C	C2-N1-C1'	8.22	127.84	118.80
45	C1	2202	C	N1-C2-O2	8.22	123.83	118.90
45	C1	159	C	N3-C2-O2	-8.16	116.19	121.90
45	C1	449	C	N3-C2-O2	-8.09	116.23	121.90
45	C1	68	U	N1-C2-O2	8.07	128.45	122.80
45	C1	2084	C	N3-C2-O2	-8.05	116.27	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	C1	1081	G	N3-C2-N2	-8.05	114.27	119.90
32	CS	191	LEU	CA-CB-CG	8.01	133.71	115.30
32	CR	191	LEU	CA-CB-CG	7.99	133.68	115.30
45	C1	1222	C	N3-C2-O2	-7.91	116.36	121.90
45	C1	80	C	N3-C2-O2	-7.90	116.37	121.90
45	C1	2210	U	N3-C2-O2	-7.89	116.67	122.20
45	C1	583	A	O5'-P-OP1	-7.88	98.61	105.70
46	C2	128	C	O4'-C1'-N1	7.86	114.48	108.20
46	C2	267	C	N3-C2-O2	-7.85	116.41	121.90
45	C1	1645	U	C2-N1-C1'	7.78	127.03	117.70
46	C2	103	G	N3-C4-C5	-7.77	124.72	128.60
45	C1	346	C	N3-C2-O2	-7.76	116.47	121.90
46	C2	203	C	N3-C2-O2	-7.72	116.50	121.90
9	UL	438	ASP	CB-CG-OD1	7.68	125.21	118.30
46	C2	6	C	C6-N1-C2	-7.61	117.25	120.30
45	C1	1645	U	N1-C2-O2	7.58	128.10	122.80
45	C1	1662	C	N1-C2-O2	7.58	123.45	118.90
32	CR	714	GLU	CA-CB-CG	7.58	130.07	113.40
32	CR	471	GLU	CA-CB-CG	7.58	130.06	113.40
45	C1	1658	G	N1-C6-O6	-7.58	115.36	119.90
32	CS	471	GLU	CA-CB-CG	7.57	130.06	113.40
45	C1	148	C	N3-C2-O2	-7.56	116.61	121.90
32	CS	714	GLU	CA-CB-CG	7.55	130.02	113.40
45	C1	2179	C	C2-N1-C1'	7.52	127.08	118.80
45	C1	2084	C	C6-N1-C2	-7.52	117.29	120.30
45	C1	470	C	N1-C2-O2	7.50	123.40	118.90
45	C1	1645	U	N3-C2-O2	-7.49	116.95	122.20
45	C1	1625	G	N3-C4-N9	7.46	130.47	126.00
45	C1	148	C	C6-N1-C2	-7.46	117.32	120.30
45	C1	291	C	N3-C2-O2	-7.45	116.68	121.90
45	C1	206	C	C6-N1-C2	-7.45	117.32	120.30
45	C1	1120	C	C2-N1-C1'	7.44	126.99	118.80
45	C1	2074	C	C2-N1-C1'	7.41	126.95	118.80
45	C1	291	C	C2-N1-C1'	7.37	126.90	118.80
46	C2	246	G	C4-N9-C1'	7.34	136.04	126.50
45	C1	491	G	C4-N9-C1'	7.33	136.03	126.50
45	C1	1711	G	C4-N9-C1'	7.31	136.01	126.50
45	C1	1745	C	C5-C6-N1	7.30	124.65	121.00
45	C1	56	C	OP1-P-OP2	7.27	130.50	119.60
45	C1	258	C	C6-N1-C2	-7.26	117.39	120.30
46	C2	136	C	C2-N1-C1'	7.25	126.77	118.80
12	UO	293	LEU	CA-CB-CG	7.23	131.92	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
46	C2	139	C	N3-C2-O2	-7.22	116.84	121.90
45	C1	1486	G	N3-C4-C5	-7.18	125.01	128.60
46	C2	139	C	N1-C2-O2	7.13	123.18	118.90
45	C1	2217	C	N3-C2-O2	-7.11	116.92	121.90
45	C1	1163	A	P-O3'-C3'	7.10	128.22	119.70
45	C1	46	C	OP1-P-OP2	7.08	130.22	119.60
45	C1	206	C	C6-N1-C1'	-7.08	112.30	120.80
45	C1	1512	C	C6-N1-C2	-7.07	117.47	120.30
32	CS	202	ILE	CG1-CB-CG2	-7.05	95.89	111.40
45	C1	1666	C	N1-C2-O2	7.05	123.13	118.90
32	CR	202	ILE	CG1-CB-CG2	-7.03	95.93	111.40
46	C2	252	C	N3-C2-O2	-7.02	116.98	121.90
45	C1	622	U	N3-C2-O2	-7.01	117.29	122.20
46	C2	255	U	P-O3'-C3'	7.00	128.10	119.70
45	C1	209	A	P-O3'-C3'	6.98	128.07	119.70
32	CS	515	GLN	CA-CB-CG	6.97	128.73	113.40
45	C1	1658	G	C4-C5-N7	-6.97	108.01	110.80
45	C1	56	C	C2-N1-C1'	6.96	126.46	118.80
32	CR	515	GLN	CA-CB-CG	6.96	128.70	113.40
45	C1	158	C	C2-N1-C1'	6.94	126.44	118.80
45	C1	454	C	C2-N1-C1'	6.94	126.43	118.80
45	C1	1549	U	N3-C4-C5	6.90	118.74	114.60
46	C2	260	G	C4-N9-C1'	6.89	135.46	126.50
21	CE	103	LEU	CA-CB-CG	6.88	131.12	115.30
45	C1	34	C	N1-C2-O2	6.88	123.03	118.90
45	C1	1113	C	N1-C2-O2	6.88	123.03	118.90
45	C1	34	C	N3-C2-O2	-6.88	117.08	121.90
45	C1	1114	C	N1-C2-O2	6.87	123.02	118.90
45	C1	504	C	N1-C2-O2	6.87	123.02	118.90
45	C1	1471	U	C2-N1-C1'	6.86	125.94	117.70
12	UO	239	LEU	CA-CB-CG	6.86	131.07	115.30
46	C2	57	A	O4'-C1'-N9	6.86	113.68	108.20
11	UN	901	LEU	CA-CB-CG	6.84	131.02	115.30
45	C1	2202	C	N3-C2-O2	-6.83	117.12	121.90
45	C1	159	C	C6-N1-C2	-6.82	117.57	120.30
45	C1	33	C	N3-C2-O2	-6.82	117.12	121.90
45	C1	68	U	N3-C2-O2	-6.81	117.43	122.20
45	C1	1487	G	O4'-C1'-N9	6.80	113.64	108.20
46	C2	161	G	C4-N9-C1'	6.79	135.33	126.50
46	C2	259	A	O4'-C1'-N9	6.79	113.64	108.20
46	C2	103	G	N3-C4-N9	6.79	130.07	126.00
46	C2	267	C	C6-N1-C2	-6.75	117.60	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	C1	447	C	N3-C2-O2	-6.75	117.18	121.90
45	C1	505	C	N1-C2-O2	6.75	122.95	118.90
45	C1	1666	C	C5-C6-N1	6.73	124.37	121.00
45	C1	112	C	N3-C2-O2	-6.72	117.19	121.90
46	C2	260	G	N3-C4-N9	6.71	130.03	126.00
45	C1	581	C	N3-C2-O2	-6.69	117.22	121.90
45	C1	203	C	N1-C2-O2	6.67	122.90	118.90
45	C1	1547	C	C5-C6-N1	6.67	124.33	121.00
9	UL	645	LEU	CA-CB-CG	6.61	130.50	115.30
45	C1	581	C	N1-C2-O2	6.60	122.86	118.90
45	C1	2179	C	N1-C2-O2	6.59	122.86	118.90
45	C1	1486	G	N7-C8-N9	6.59	116.39	113.10
45	C1	491	G	N3-C4-N9	6.59	129.95	126.00
45	C1	1486	G	C8-N9-C1'	-6.57	118.45	127.00
13	UQ	154	ASP	CB-CG-OD1	6.57	124.21	118.30
45	C1	1486	G	N3-C4-N9	6.57	129.94	126.00
45	C1	1711	G	N3-C4-N9	6.56	129.94	126.00
1	UA	587	LEU	CA-CB-CG	6.55	130.36	115.30
45	C1	281	U	P-O3'-C3'	6.55	127.56	119.70
45	C1	1625	G	N3-C4-C5	-6.54	125.33	128.60
46	C2	260	G	N3-C4-C5	-6.54	125.33	128.60
45	C1	454	C	C5-C6-N1	6.48	124.24	121.00
45	C1	1471	U	C5-C4-O4	-6.47	122.02	125.90
45	C1	1666	C	C2-N1-C1'	6.45	125.90	118.80
45	C1	277	U	P-O3'-C3'	6.45	127.44	119.70
45	C1	1068	C	C6-N1-C2	-6.45	117.72	120.30
45	C1	491	G	C8-N9-C1'	-6.45	118.62	127.00
1	UA	662	GLY	C-N-CA	6.44	137.79	121.70
45	C1	68	U	C5-C6-N1	6.43	125.92	122.70
45	C1	2074	C	N3-C2-O2	-6.42	117.41	121.90
46	C2	202	C	N1-C2-O2	6.42	122.75	118.90
45	C1	1448	A	C5-C6-N1	6.42	120.91	117.70
45	C1	1046	G	C5-C6-O6	6.41	132.44	128.60
46	C2	147	G	N3-C4-N9	6.40	129.84	126.00
32	CS	370	GLN	CA-CB-CG	6.38	127.44	113.40
45	C1	18	G	N3-C4-C5	-6.38	125.41	128.60
32	CR	370	GLN	CA-CB-CG	6.37	127.42	113.40
45	C1	454	C	C6-N1-C2	-6.37	117.75	120.30
46	C2	161	G	N3-C4-N9	6.36	129.81	126.00
45	C1	68	U	C2-N1-C1'	6.33	125.29	117.70
45	C1	581	C	C2-N1-C1'	6.32	125.75	118.80
45	C1	1547	C	C2-N1-C1'	6.32	125.75	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	C1	593	G	P-O3'-C3'	6.31	127.27	119.70
45	C1	1747	A	C6-N1-C2	-6.31	114.82	118.60
45	C1	1745	C	C6-N1-C2	-6.30	117.78	120.30
46	C2	161	G	C6-C5-N7	-6.30	126.62	130.40
45	C1	1114	C	N3-C2-O2	-6.28	117.51	121.90
45	C1	1550	U	C6-N1-C1'	-6.27	112.42	121.20
46	C2	246	G	C8-N9-C1'	-6.27	118.84	127.00
45	C1	1167	C	C6-N1-C2	-6.26	117.80	120.30
45	C1	205	C	P-O3'-C3'	6.26	127.21	119.70
45	C1	1711	G	N3-C4-C5	-6.25	125.48	128.60
2	UB	644	LEU	CA-CB-CG	6.24	129.66	115.30
10	UM	39	LEU	CA-CB-CG	6.24	129.66	115.30
45	C1	425	C	C6-N1-C2	-6.24	117.80	120.30
45	C1	1711	G	C8-N9-C1'	-6.22	118.92	127.00
45	C1	2156	A	P-O3'-C3'	6.21	127.15	119.70
45	C1	63	C	N1-C2-O2	6.19	122.61	118.90
45	C1	2194	A	C8-N9-C4	-6.18	103.33	105.80
45	C1	258	C	C5-C6-N1	6.17	124.09	121.00
45	C1	2210	U	C5-C4-O4	6.17	129.60	125.90
46	C2	23	A	P-O3'-C3'	6.16	127.10	119.70
12	UO	334	LEU	CA-CB-CG	6.15	129.44	115.30
45	C1	1638	G	P-O3'-C3'	6.14	127.07	119.70
45	C1	470	C	C2-N1-C1'	6.14	125.55	118.80
29	CN	86	ASP	CB-CG-OD1	6.11	123.80	118.30
9	UL	441	LEU	CA-CB-CG	6.10	129.34	115.30
45	C1	56	C	N1-C2-O2	6.10	122.56	118.90
45	C1	622	U	N1-C2-O2	6.09	127.06	122.80
45	C1	135	A	P-O3'-C3'	6.09	127.01	119.70
45	C1	1712	C	P-O3'-C3'	6.09	127.00	119.70
45	C1	1745	C	C2-N1-C1'	6.08	125.48	118.80
45	C1	21	C	N3-C2-O2	-6.07	117.65	121.90
45	C1	18	G	C4-N9-C1'	6.06	134.38	126.50
45	C1	1222	C	C6-N1-C2	-6.04	117.88	120.30
45	C1	1486	G	C8-N9-C4	-6.04	103.98	106.40
45	C1	183	C	C2-N1-C1'	6.03	125.44	118.80
45	C1	1549	U	N3-C4-O4	-6.03	115.18	119.40
45	C1	2217	C	C6-N1-C1'	-6.03	113.56	120.80
17	UZ	66	LEU	CA-CB-CG	6.03	129.16	115.30
45	C1	2078	C	N3-C2-O2	-6.03	117.68	121.90
45	C1	1451	G	N9-C4-C5	-6.02	102.99	105.40
45	C1	1485	A	P-O3'-C3'	6.02	126.93	119.70
19	CC	17	LEU	CA-CB-CG	6.02	129.15	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	C1	18	G	N3-C4-N9	6.02	129.61	126.00
45	C1	291	C	C6-N1-C2	-6.02	117.89	120.30
45	C1	369	U	N3-C2-O2	-6.00	118.00	122.20
32	CR	67	PHE	CB-CG-CD1	5.99	125.00	120.80
45	C1	1661	C	C2-N3-C4	-5.99	116.91	119.90
46	C2	105	C	C5-C6-N1	5.99	123.99	121.00
45	C1	1630	C	N3-C2-O2	-5.97	117.72	121.90
45	C1	1666	C	C6-N1-C2	-5.96	117.92	120.30
46	C2	6	C	C5-C6-N1	5.96	123.98	121.00
46	C2	161	G	C8-N9-C1'	-5.95	119.27	127.00
45	C1	1547	C	C6-N1-C2	-5.94	117.92	120.30
46	C2	103	G	C2-N3-C4	5.93	114.87	111.90
45	C1	55	G	OP2-P-O3'	-5.93	92.15	105.20
45	C1	1448	A	C6-N1-C2	-5.93	115.05	118.60
45	C1	1658	G	C6-C5-N7	5.92	133.95	130.40
45	C1	471	C	C6-N1-C2	-5.92	117.93	120.30
46	C2	136	C	C5-C6-N1	5.92	123.96	121.00
45	C1	1639	U	C2-N1-C1'	5.90	124.78	117.70
6	UG	174	LEU	CA-CB-CG	5.90	128.87	115.30
46	C2	200	U	C6-N1-C1'	-5.90	112.95	121.20
45	C1	1165	U	C2-N1-C1'	5.89	124.76	117.70
45	C1	398	C	N1-C2-O2	5.88	122.43	118.90
45	C1	1120	C	C6-N1-C2	-5.88	117.95	120.30
45	C1	1560	C	N1-C2-O2	5.87	122.42	118.90
45	C1	1458	U	C2-N1-C1'	5.87	124.74	117.70
45	C1	1113	C	N3-C2-O2	-5.87	117.79	121.90
46	C2	6	C	N1-C2-O2	5.87	122.42	118.90
32	CS	67	PHE	CB-CG-CD1	5.87	124.91	120.80
45	C1	2210	U	N1-C2-O2	5.87	126.91	122.80
46	C2	244	G	C5-C6-O6	5.85	132.11	128.60
46	C2	139	C	C6-N1-C2	-5.85	117.96	120.30
45	C1	2179	C	C6-N1-C1'	-5.84	113.79	120.80
45	C1	2358	U	N3-C2-O2	-5.84	118.11	122.20
45	C1	371	U	N1-C2-O2	5.80	126.86	122.80
46	C2	260	G	C8-N9-C1'	-5.80	119.46	127.00
45	C1	2217	C	C6-N1-C2	-5.79	117.98	120.30
45	C1	2177	G	P-O3'-C3'	5.78	126.63	119.70
45	C1	2217	C	C5-C6-N1	5.78	123.89	121.00
45	C1	2203	C	N1-C2-O2	5.77	122.36	118.90
45	C1	158	C	C6-N1-C1'	-5.76	113.88	120.80
45	C1	308	U	C5-C6-N1	5.75	125.58	122.70
45	C1	1511	A	C2-N3-C4	5.75	113.48	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	C1	1458	U	N1-C2-O2	5.75	126.83	122.80
1	UA	258	LEU	CA-CB-CG	5.75	128.52	115.30
21	CF	103	LEU	CA-CB-CG	5.75	128.52	115.30
45	C1	88	C	P-O3'-C3'	5.73	126.58	119.70
45	C1	1046	G	N1-C6-O6	-5.73	116.46	119.90
45	C1	1560	C	N3-C2-O2	-5.73	117.89	121.90
45	C1	1451	G	N3-C4-N9	5.72	129.43	126.00
45	C1	2165	U	C5-C6-N1	5.71	125.55	122.70
20	CD	189	TRP	CA-CB-CG	5.70	124.52	113.70
45	C1	493	G	N3-C4-N9	5.69	129.42	126.00
45	C1	134	C	N3-C2-O2	-5.69	117.92	121.90
45	C1	2358	U	C2-N1-C1'	5.69	124.53	117.70
15	UU	771	LEU	CA-CB-CG	5.68	128.37	115.30
45	C1	308	U	N1-C2-O2	5.68	126.78	122.80
15	UU	378	LEU	CA-CB-CG	5.67	128.35	115.30
46	C2	246	G	N3-C4-C5	-5.67	125.76	128.60
45	C1	56	C	C5-C6-N1	5.66	123.83	121.00
45	C1	183	C	C5-C6-N1	5.66	123.83	121.00
45	C1	3	G	N3-C4-N9	-5.65	122.61	126.00
6	UG	151	LEU	CA-CB-CG	5.65	128.30	115.30
13	UQ	747	LEU	C-N-CA	5.64	135.81	121.70
46	C2	6	C	N3-C2-O2	-5.63	117.96	121.90
10	UM	689	LEU	CA-CB-CG	5.62	128.23	115.30
45	C1	203	C	C2-N1-C1'	5.62	124.98	118.80
5	UF	177	LEU	CB-CG-CD2	-5.61	101.47	111.00
45	C1	1656	C	C6-N1-C2	-5.61	118.06	120.30
45	C1	370	C	N1-C2-O2	5.59	122.26	118.90
36	Ce	22	LEU	CA-CB-CG	5.59	128.16	115.30
45	C1	158	C	N3-C2-O2	-5.59	117.99	121.90
45	C1	206	C	C5-C6-N1	5.58	123.79	121.00
45	C1	371	U	C2-N1-C1'	5.58	124.40	117.70
45	C1	2202	C	C6-N1-C2	-5.58	118.07	120.30
45	C1	1639	U	N1-C2-O2	5.57	126.70	122.80
45	C1	1085	U	P-O3'-C3'	5.55	126.36	119.70
32	CR	193	LEU	CA-CB-CG	5.54	128.03	115.30
46	C2	246	G	N3-C4-N9	5.53	129.32	126.00
45	C1	491	G	N3-C4-C5	-5.53	125.83	128.60
45	C1	2179	C	N3-C2-O2	-5.53	118.03	121.90
46	C2	90	C	O4'-C1'-N1	5.53	112.62	108.20
45	C1	448	C	N3-C2-O2	-5.51	118.04	121.90
32	CS	193	LEU	CA-CB-CG	5.51	127.97	115.30
32	CR	849	LEU	CA-CB-CG	5.51	127.97	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
46	C2	152	C	C6-N1-C2	-5.51	118.10	120.30
32	CS	849	LEU	CA-CB-CG	5.50	127.95	115.30
45	C1	1165	U	N3-C2-O2	-5.50	118.35	122.20
45	C1	281	U	OP1-P-O3'	5.49	117.27	105.20
45	C1	1626	G	C6-N1-C2	-5.48	121.81	125.10
6	UG	100	LEU	CA-CB-CG	5.48	127.90	115.30
45	C1	2	G	N3-C4-N9	5.47	129.28	126.00
45	C1	369	U	C2-N1-C1'	5.47	124.26	117.70
46	C2	251	U	N3-C2-O2	-5.47	118.37	122.20
13	UQ	617	LEU	CA-CB-CG	5.47	127.87	115.30
45	C1	1625	G	N3-C2-N2	5.47	123.73	119.90
45	C1	1165	U	N1-C2-O2	5.46	126.62	122.80
45	C1	26	C	N3-C2-O2	-5.46	118.08	121.90
9	UL	869	LEU	CA-CB-CG	5.46	127.85	115.30
46	C2	105	C	C6-N1-C2	-5.45	118.12	120.30
45	C1	343	C	C6-N1-C2	-5.44	118.12	120.30
45	C1	1222	C	C6-N1-C1'	-5.44	114.27	120.80
45	C1	371	U	N3-C2-O2	-5.44	118.39	122.20
45	C1	60	A	C2-N3-C4	5.44	113.32	110.60
45	C1	308	U	C2-N1-C1'	5.44	124.23	117.70
45	C1	485	G	N3-C4-N9	-5.44	122.74	126.00
45	C1	2074	C	C6-N1-C1'	-5.43	114.28	120.80
45	C1	2194	A	N7-C8-N9	5.43	116.52	113.80
24	CI	845	LEU	CA-CB-CG	5.43	127.79	115.30
45	C1	294	G	N3-C4-N9	-5.42	122.75	126.00
45	C1	145	C	N1-C2-O2	5.42	122.15	118.90
46	C2	77	C	C5-C6-N1	5.42	123.71	121.00
46	C2	165	C	N1-C2-O2	5.42	122.15	118.90
45	C1	454	C	N1-C2-O2	5.42	122.15	118.90
45	C1	1068	C	C5-C6-N1	5.41	123.70	121.00
45	C1	470	C	N3-C2-O2	-5.41	118.11	121.90
45	C1	1549	U	C2-N3-C4	-5.41	123.76	127.00
46	C2	200	U	C5-C6-N1	5.40	125.40	122.70
32	CR	67	PHE	CB-CG-CD2	-5.39	117.03	120.80
45	C1	1027	C	C6-N1-C2	-5.38	118.15	120.30
45	C1	1758	C	C6-N1-C1'	5.38	127.25	120.80
45	C1	582	G	P-O3'-C3'	5.37	126.14	119.70
49	US	347	LEU	CA-CB-CG	5.37	127.64	115.30
51	CX	296	LEU	CA-CB-CG	5.36	127.64	115.30
45	C1	18	G	C2-N3-C4	5.36	114.58	111.90
45	C1	1643	U	C2-N1-C1'	5.36	124.13	117.70
45	C1	2219	C	P-O3'-C3'	5.36	126.13	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
46	C2	103	G	C4-N9-C1'	5.35	133.45	126.50
45	C1	203	C	N3-C2-O2	-5.35	118.16	121.90
32	CS	901	LEU	CA-CB-CG	5.34	127.58	115.30
43	Cp	55	LEU	CB-CG-CD2	-5.33	101.95	111.00
32	CR	901	LEU	CA-CB-CG	5.32	127.53	115.30
46	C2	136	C	N3-C2-O2	-5.32	118.18	121.90
45	C1	2177	G	OP2-P-O3'	5.31	116.89	105.20
45	C1	1451	G	C4-C5-N7	5.31	112.92	110.80
45	C1	1050	U	N3-C2-O2	-5.30	118.49	122.20
45	C1	1625	G	C6-C5-N7	-5.30	127.22	130.40
45	C1	2358	U	N1-C2-O2	5.30	126.51	122.80
45	C1	63	C	C2-N1-C1'	5.29	124.62	118.80
32	CS	67	PHE	CB-CG-CD2	-5.29	117.09	120.80
32	CR	135	ILE	CG1-CB-CG2	-5.29	99.77	111.40
32	CR	617	LEU	CA-CB-CG	5.29	127.45	115.30
32	CS	617	LEU	CA-CB-CG	5.29	127.46	115.30
45	C1	1120	C	N1-C2-O2	5.28	122.07	118.90
45	C1	1458	U	N3-C2-O2	-5.28	118.51	122.20
45	C1	1547	C	N3-C4-N4	5.28	121.69	118.00
45	C1	2091	C	C2-N1-C1'	5.28	124.61	118.80
46	C2	202	C	C6-N1-C2	-5.28	118.19	120.30
45	C1	2172	C	C6-N1-C2	-5.28	118.19	120.30
45	C1	2168	U	C2-N1-C1'	5.27	124.03	117.70
32	CS	135	ILE	CG1-CB-CG2	-5.27	99.81	111.40
46	C2	136	C	C6-N1-C2	-5.26	118.19	120.30
45	C1	1511	A	C5-C6-N1	5.26	120.33	117.70
45	C1	150	C	P-O3'-C3'	5.26	126.01	119.70
45	C1	1630	C	C6-N1-C1'	5.26	127.11	120.80
46	C2	79	G	N3-C4-N9	5.25	129.15	126.00
45	C1	1045	G	N3-C4-C5	-5.24	125.98	128.60
45	C1	1734	G	P-O3'-C3'	5.24	125.99	119.70
36	Ce	38	ALA	C-N-CA	5.23	134.77	121.70
45	C1	1625	G	C4-N9-C1'	5.22	133.29	126.50
45	C1	2227	C	C5-C6-N1	5.22	123.61	121.00
45	C1	281	U	N1-C2-O2	5.22	126.45	122.80
45	C1	1658	G	C8-N9-C1'	5.21	133.77	127.00
45	C1	1761	C	C5-C6-N1	5.21	123.60	121.00
45	C1	1511	A	N3-C4-N9	5.20	131.56	127.40
2	UB	818	ASP	CB-CG-OD2	5.19	122.97	118.30
45	C1	1045	G	N3-C4-N9	5.19	129.12	126.00
45	C1	2202	C	C2-N1-C1'	5.19	124.51	118.80
14	UR	398	LEU	CA-CB-CG	5.18	127.22	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	C1	1167	C	N1-C2-O2	5.18	122.01	118.90
45	C1	2203	C	N3-C2-O2	-5.18	118.28	121.90
45	C1	1451	G	C8-N9-C1'	-5.17	120.27	127.00
45	C1	154	C	N1-C2-O2	5.17	122.00	118.90
46	C2	202	C	C5-C6-N1	5.16	123.58	121.00
45	C1	111	U	N3-C2-O2	-5.16	118.59	122.20
45	C1	233	C	C6-N1-C2	-5.15	118.24	120.30
45	C1	1646	U	O4'-C1'-N1	5.15	112.32	108.20
45	C1	43	C	C2-N1-C1'	5.15	124.46	118.80
45	C1	63	C	N3-C2-O2	-5.15	118.30	121.90
45	C1	1560	C	C6-N1-C2	-5.13	118.25	120.30
1	UA	695	LEU	CA-CB-CG	5.13	127.11	115.30
45	C1	1471	U	N3-C4-O4	5.13	122.99	119.40
46	C2	147	G	N9-C4-C5	-5.13	103.35	105.40
20	CD	102	LEU	CA-CB-CG	5.12	127.08	115.30
45	C1	582	G	OP1-P-O3'	5.12	116.47	105.20
46	C2	161	G	N7-C8-N9	5.12	115.66	113.10
45	C1	2084	C	C6-N1-C1'	5.12	126.94	120.80
45	C1	2174	C	C5-C6-N1	5.12	123.56	121.00
45	C1	2	G	N3-C4-C5	-5.12	126.04	128.60
45	C1	1656	C	C5-C6-N1	5.11	123.56	121.00
45	C1	1149	C	N3-C2-O2	-5.11	118.32	121.90
8	UK	96	LEU	CA-CB-CG	5.11	127.05	115.30
45	C1	1068	C	P-O3'-C3'	5.11	125.83	119.70
45	C1	129	G	N1-C6-O6	-5.11	116.84	119.90
45	C1	1124	G	C4-N9-C1'	5.10	133.13	126.50
45	C1	1075	C	N3-C2-O2	-5.10	118.33	121.90
45	C1	1094	G	C6-C5-N7	-5.10	127.34	130.40
45	C1	2168	U	C5-C6-N1	5.10	125.25	122.70
45	C1	2064	C	C6-N1-C2	-5.09	118.26	120.30
45	C1	1222	C	C5-C6-N1	5.09	123.55	121.00
46	C2	166	G	N3-C4-C5	-5.08	126.06	128.60
21	CE	110	ASP	CB-CG-OD1	5.08	122.87	118.30
45	C1	370	C	C2-N1-C1'	5.08	124.39	118.80
45	C1	1114	C	C6-N1-C2	-5.08	118.27	120.30
46	C2	260	G	C2-N3-C4	5.07	114.44	111.90
45	C1	435	A	C6-N1-C2	5.07	121.64	118.60
4	UD	561	LEU	CA-CB-CG	5.06	126.95	115.30
45	C1	447	C	C6-N1-C2	-5.06	118.28	120.30
45	C1	203	C	C6-N1-C2	-5.06	118.28	120.30
45	C1	236	C	C6-N1-C2	-5.06	118.28	120.30
45	C1	80	C	C6-N1-C2	-5.05	118.28	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	UD	357	LEU	CB-CG-CD2	-5.05	102.41	111.00
46	C2	246	G	OP1-P-O3'	5.05	116.32	105.20
45	C1	179	G	N3-C2-N2	5.05	123.43	119.90
45	C1	160	C	C5-C6-N1	5.05	123.52	121.00
23	CH	120	LEU	CA-CB-CG	5.04	126.89	115.30
46	C2	100	G	N3-C4-N9	5.04	129.02	126.00
45	C1	129	G	C5-C6-O6	5.04	131.62	128.60
45	C1	1626	G	C8-N9-C4	-5.04	104.39	106.40
45	C1	1171	C	N3-C2-O2	-5.03	118.38	121.90
45	C1	2084	C	N1-C2-N3	5.03	122.72	119.20
45	C1	1081	G	N9-C4-C5	5.02	107.41	105.40
45	C1	2044	C	C2-N1-C1'	5.02	124.33	118.80
20	CD	143	LEU	CA-CB-CG	5.02	126.85	115.30
45	C1	1451	G	C6-C5-N7	-5.02	127.39	130.40
45	C1	112	C	C2-N1-C1'	5.02	124.32	118.80
13	UQ	472	PRO	C-N-CA	5.01	134.23	121.70
46	C2	131	U	N3-C2-O2	-5.01	118.69	122.20
36	Ce	40	LEU	CA-CB-CG	5.01	126.81	115.30
45	C1	56	C	C6-N1-C2	-5.01	118.30	120.30
45	C1	39	C	C2-N1-C1'	5.00	124.30	118.80

There are no chirality outliers.

All (42) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
18	CB	293	GLU	Peptide
21	CF	60	GLN	Peptide
22	CG	178	VAL	Peptide
23	CH	143	HIS	Peptide
24	CI	851	TRP	Peptide
24	CI	852	ASP	Peptide
26	CK	261	PHE	Peptide
28	CM	140	SER	Peptide
29	CO	84	ILE	Peptide
29	CO	88	ARG	Peptide
31	CQ	173	ASP	Peptide
32	CR	122	MET	Peptide
32	CR	306	GLY	Peptide
32	CR	432	LEU	Peptide
32	CS	122	MET	Peptide
32	CS	306	GLY	Peptide
32	CS	432	LEU	Peptide

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Mol	Chain	Res	Type	Group
35	Cc	86	MET	Peptide
36	Ce	38	ALA	Peptide
50	Cl	79	TYR	Peptide
1	UA	115	LEU	Peptide
4	UD	387	TRP	Peptide
48	UE	232	GLN	Peptide
9	UL	153	ASP	Peptide
9	UL	636	LEU	Peptide
10	UM	328	LEU	Peptide
10	UM	382	ILE	Peptide
10	UM	445	GLY	Peptide
10	UM	585	HIS	Peptide
12	UO	282	ALA	Peptide
13	UQ	237	TYR	Peptide
13	UQ	426	ALA	Peptide
13	UQ	707	PRO	Peptide
13	UQ	849	ALA	Peptide
14	UR	616	ILE	Peptide
49	US	510	LYS	Peptide
15	UU	397	ASP	Peptide
15	UU	644	GLY	Peptide
15	UU	857	ILE	Peptide
17	UZ	103	ASP	Peptide
17	UZ	114	ASP	Peptide
17	UZ	273	GLN	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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

All (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
32	CS	48	MET

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Mol	Chain	Res	Type
11	UN	902	ARG
27	CL	640	PRO
5	UF	121	LYS
10	UM	329	PRO
13	UQ	564	GLU
24	CI	309	PRO
52	UP	329	PRO
32	CR	772	PRO
32	CS	772	PRO
23	CH	258	PRO
32	CR	904	PRO
32	CS	904	PRO
21	CF	61	PRO
32	CR	404	GLY
32	CS	404	GLY
29	CO	84	ILE
24	CI	308	THR

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%)

All (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
45	C1	15	G
45	C1	16	U
45	C1	17	C
45	C1	18	G

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Mol	Chain	Res	Type
45	C1	19	C
45	C1	20	C
45	C1	26	C
45	C1	38	G
45	C1	40	A
45	C1	41	G
45	C1	47	G
45	C1	49	G
45	C1	56	C
45	C1	60	A
45	C1	61	G
45	C1	63	C
45	C1	66	G
45	C1	68	U
45	C1	71	A
45	C1	72	U
45	C1	73	A
45	C1	74	C
45	C1	75	G
45	C1	77	C
45	C1	89	G
45	C1	90	A
45	C1	93	G
45	C1	97	C
45	C1	104	U
45	C1	105	A
45	C1	121	G
45	C1	126	C
45	C1	127	C
45	C1	128	G
45	C1	134	C
45	C1	136	C
45	C1	143	A
45	C1	150	C
45	C1	152	G
45	C1	154	C
45	C1	155	G
45	C1	158	C
45	C1	159	C
45	C1	160	C
45	C1	161	A
45	C1	162	G

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Mol	Chain	Res	Type
45	C1	166	A
45	C1	169	G
45	C1	170	C
45	C1	182	C
45	C1	183	C
45	C1	193	U
45	C1	201	G
45	C1	202	A
45	C1	203	C
45	C1	205	C
45	C1	206	C
45	C1	207	U
45	C1	208	A
45	C1	209	A
45	C1	210	G
45	C1	216	A
45	C1	220	A
45	C1	221	A
45	C1	225	C
45	C1	234	G
45	C1	242	U
45	C1	243	U
45	C1	244	G
45	C1	257	G
45	C1	265	G
45	C1	266	C
45	C1	267	U
45	C1	268	G
45	C1	269	G
45	C1	273	G
45	C1	276	C
45	C1	277	U
45	C1	278	A
45	C1	281	U
45	C1	282	C
45	C1	283	A
45	C1	285	A
45	C1	290	C
45	C1	291	C
45	C1	292	G
45	C1	308	U
45	C1	310	G

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Mol	Chain	Res	Type
45	C1	311	G
45	C1	312	G
45	C1	319	U
45	C1	320	A
45	C1	322	C
45	C1	323	G
45	C1	325	C
45	C1	333	C
45	C1	334	U
45	C1	339	C
45	C1	340	G
45	C1	346	C
45	C1	347	C
45	C1	349	C
45	C1	351	U
45	C1	362	G
45	C1	372	U
45	C1	382	U
45	C1	383	G
45	C1	384	C
45	C1	386	G
45	C1	398	C
45	C1	402	U
45	C1	403	G
45	C1	404	C
45	C1	416	U
45	C1	425	C
45	C1	427	G
45	C1	435	A
45	C1	436	A
45	C1	440	G
45	C1	441	A
45	C1	442	U
45	C1	443	G
45	C1	454	C
45	C1	458	A
45	C1	459	C
45	C1	468	C
45	C1	469	G
45	C1	474	A
45	C1	475	C
45	C1	484	G

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Mol	Chain	Res	Type
45	C1	491	G
45	C1	492	C
45	C1	497	A
45	C1	499	G
45	C1	500	C
45	C1	501	U
45	C1	502	A
45	C1	504	C
45	C1	581	C
45	C1	582	G
45	C1	583	A
45	C1	584	U
45	C1	585	A
45	C1	586	G
45	C1	587	U
45	C1	594	G
45	C1	595	U
45	C1	609	A
45	C1	610	G
45	C1	613	A
45	C1	614	U
45	C1	621	G
45	C1	624	U
45	C1	628	A
45	C1	1025	A
45	C1	1027	C
45	C1	1028	C
45	C1	1029	A
45	C1	1035	G
45	C1	1036	A
45	C1	1037	C
45	C1	1039	C
45	C1	1043	G
45	C1	1044	A
45	C1	1054	A
45	C1	1059	A
45	C1	1061	A
45	C1	1064	G
45	C1	1069	A
45	C1	1070	G
45	C1	1076	U
45	C1	1077	U

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Mol	Chain	Res	Type
45	C1	1078	U
45	C1	1079	C
45	C1	1080	G
45	C1	1085	U
45	C1	1086	U
45	C1	1088	U
45	C1	1089	A
45	C1	1094	G
45	C1	1095	A
45	C1	1098	G
45	C1	1099	A
45	C1	1102	A
45	C1	1103	C
45	C1	1104	A
45	C1	1116	U
45	C1	1120	C
45	C1	1122	A
45	C1	1123	G
45	C1	1124	G
45	C1	1125	A
45	C1	1126	A
45	C1	1127	C
45	C1	1128	A
45	C1	1129	A
45	C1	1132	G
45	C1	1141	G
45	C1	1147	U
45	C1	1148	G
45	C1	1150	C
45	C1	1154	A
45	C1	1158	G
45	C1	1159	C
45	C1	1163	A
45	C1	1164	A
45	C1	1166	U
45	C1	1167	C
45	C1	1168	C
45	C1	1169	A
45	C1	1170	G
45	C1	1178	A
45	C1	1179	G
45	C1	1186	U

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Mol	Chain	Res	Type
45	C1	1218	G
45	C1	1219	A
45	C1	1220	A
45	C1	1222	C
45	C1	1223	U
45	C1	1444	A
45	C1	1447	A
45	C1	1448	A
45	C1	1449	U
45	C1	1450	A
45	C1	1451	G
45	C1	1452	G
45	C1	1469	A
45	C1	1470	G
45	C1	1471	U
45	C1	1479	U
45	C1	1481	U
45	C1	1483	A
45	C1	1484	G
45	C1	1486	G
45	C1	1489	G
45	C1	1491	A
45	C1	1497	U
45	C1	1498	G
45	C1	1499	G
45	C1	1517	A
45	C1	1518	A
45	C1	1519	C
45	C1	1520	U
45	C1	1525	A
45	C1	1527	G
45	C1	1529	A
45	C1	1536	A
45	C1	1545	U
45	C1	1549	U
45	C1	1551	A
45	C1	1554	C
45	C1	1555	A
45	C1	1614	U
45	C1	1624	A
45	C1	1625	G
45	C1	1628	A

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Mol	Chain	Res	Type
45	C1	1632	G
45	C1	1636	G
45	C1	1637	C
45	C1	1639	U
45	C1	1642	A
45	C1	1643	U
45	C1	1644	U
45	C1	1645	U
45	C1	1656	C
45	C1	1659	C
45	C1	1665	A
45	C1	1667	G
45	C1	1668	A
45	C1	1670	A
45	C1	1698	G
45	C1	1701	U
45	C1	1709	A
45	C1	1711	G
45	C1	1712	C
45	C1	1713	U
45	C1	1735	A
45	C1	1738	G
45	C1	1742	C
45	C1	1743	C
45	C1	1744	A
45	C1	1751	G
45	C1	2047	G
45	C1	2054	A
45	C1	2055	C
45	C1	2056	U
45	C1	2057	G
45	C1	2061	G
45	C1	2070	A
45	C1	2072	U
45	C1	2073	A
45	C1	2074	C
45	C1	2075	U
45	C1	2077	C
45	C1	2078	C
45	C1	2085	G
45	C1	2086	A
45	C1	2087	G

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Mol	Chain	Res	Type
45	C1	2088	A
45	C1	2107	A
45	C1	2109	A
45	C1	2115	U
45	C1	2118	U
45	C1	2120	C
45	C1	2121	U
45	C1	2156	A
45	C1	2157	G
45	C1	2166	A
45	C1	2167	G
45	C1	2173	G
45	C1	2177	G
45	C1	2178	U
45	C1	2183	A
45	C1	2184	G
45	C1	2185	C
45	C1	2190	G
45	C1	2197	A
45	C1	2201	C
45	C1	2202	C
45	C1	2210	U
45	C1	2211	U
45	C1	2212	G
45	C1	2213	U
45	C1	2214	A
45	C1	2215	C
45	C1	2216	A
45	C1	2220	C
45	C1	2222	C
45	C1	2223	C
45	C1	2227	C
45	C1	2238	A
45	C1	2328	G
45	C1	2329	A
45	C1	2330	G
45	C1	2351	G
45	C1	2362	U
45	C1	2363	G
45	C1	2364	A
45	C1	2365	A
45	C1	2366	C

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Mol	Chain	Res	Type
45	C1	2373	A
45	C1	2374	G
46	C2	5	A
46	C2	8	A
46	C2	15	A
46	C2	23	A
46	C2	24	U
46	C2	28	U
46	C2	29	A
46	C2	33	U
46	C2	36	U
46	C2	37	U
46	C2	39	U
46	C2	48	G
46	C2	57	A
46	C2	58	A
46	C2	62	A
46	C2	63	G
46	C2	81	G
46	C2	90	C
46	C2	91	G
46	C2	92	A
46	C2	95	U
46	C2	100	G
46	C2	104	C
46	C2	111	G
46	C2	118	C
46	C2	124	U
46	C2	125	U
46	C2	126	U
46	C2	127	A
46	C2	128	C
46	C2	135	U
46	C2	136	C
46	C2	140	C
46	C2	142	G
46	C2	145	A
46	C2	147	G
46	C2	148	G
46	C2	153	G
46	C2	160	U
46	C2	162	C

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Mol	Chain	Res	Type
46	C2	163	C
46	C2	164	U
46	C2	165	C
46	C2	166	G
46	C2	167	U
46	C2	168	C
46	C2	170	C
46	C2	178	U
46	C2	179	A
46	C2	181	A
46	C2	182	G
46	C2	187	U
46	C2	188	G
46	C2	189	G
46	C2	190	C
46	C2	198	U
46	C2	199	G
46	C2	200	U
46	C2	201	A
46	C2	205	C
46	C2	244	G
46	C2	247	G
46	C2	255	U
46	C2	256	G
46	C2	259	A
46	C2	260	G
46	C2	261	U
46	C2	262	C

All (30) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
45	C1	88	C
45	C1	89	G
45	C1	96	C
45	C1	135	A
45	C1	150	C
45	C1	205	C
45	C1	209	A
45	C1	277	U
45	C1	281	U
45	C1	424	U

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Mol	Chain	Res	Type
45	C1	582	G
45	C1	593	G
45	C1	1068	C
45	C1	1077	U
45	C1	1085	U
45	C1	1087	G
45	C1	1163	A
45	C1	1485	A
45	C1	1638	G
45	C1	1712	C
45	C1	1734	G
45	C1	2054	A
45	C1	2077	C
45	C1	2156	A
45	C1	2177	G
45	C1	2219	C
46	C2	23	A
46	C2	35	G
46	C2	91	G
46	C2	255	U

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'

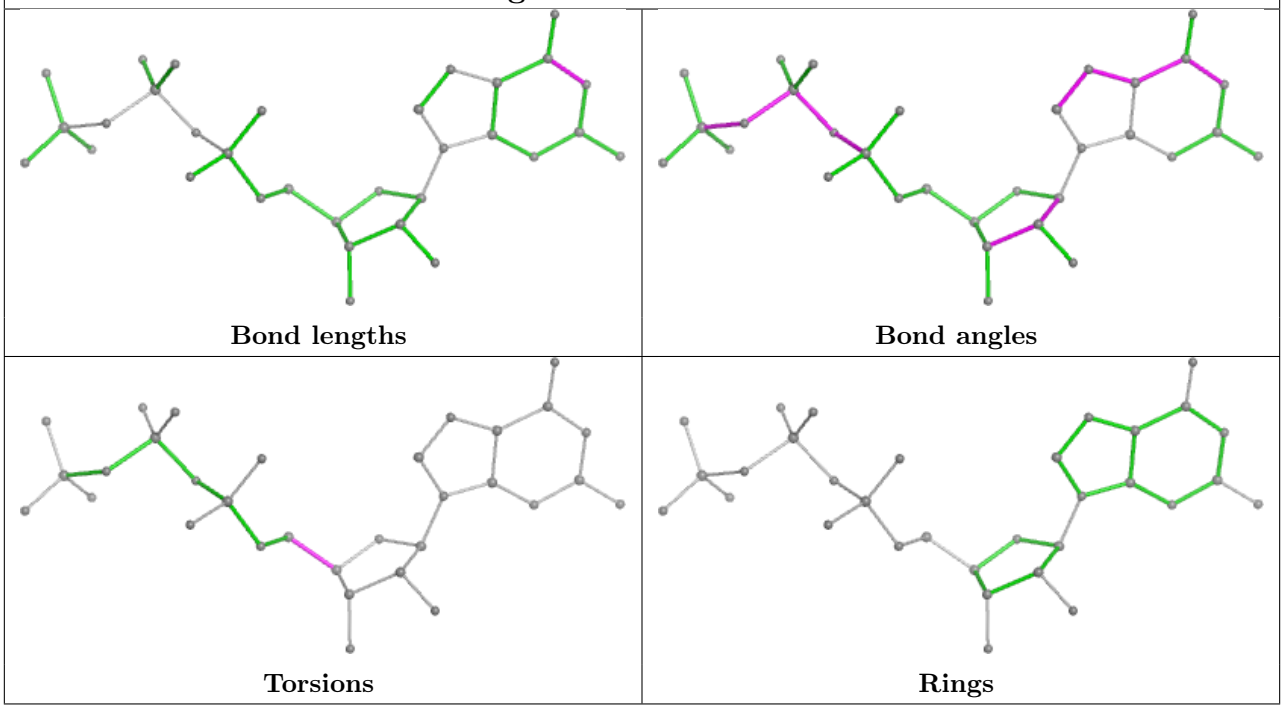
There are no ring outliers.

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 (i)

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 (i)

This section was not generated.

6.2 Central slices (i)

This section was not generated.

6.3 Largest variance slices (i)

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color) (i)

This section was not generated.

6.5 Orthogonal surface views (i)

This section was not generated.

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)

This section was not generated.

7.2 Volume estimate versus contour level (i)

This section was not generated.

7.3 Rotationally averaged power spectrum (i)

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 (i)

This section was not generated.