Full wwPDB EM Validation Report (i)

May 13, 2024 – 11:38 pm BST

PDB ID	:	6RXU
EMDB ID	:	EMD-10052
Title	:	Cryo-EM structure of the 90S pre-ribosome (Kre33-Noc4) from Chaetomium thermophilum, state B1
Authors	:	Cheng, J.; Kellner, N.; Griesel, S.; Berninghausen, O.; Beckmann, R.; Hurt, E.
Deposited on	:	2019-06-10
Resolution	:	3.50 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:

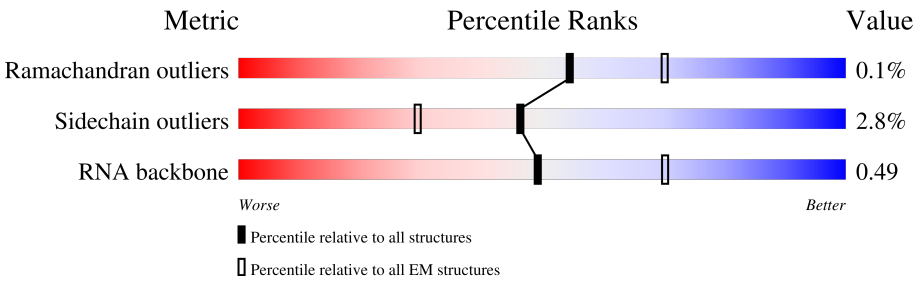
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.50 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
Sidechain outliers	154315	3826
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	84% • 14%
7	UJ	1802	60% • 40%
8	UK	270	80% 20%
9	UL	962	81% • 18%

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Mol	Chain	Length	Quality of chain
10	UM	912	79% 20%
11	UN	938	19% 81%
12	UO	557	89% 10%
13	UQ	960	81% 18%
14	UR	618	72% 28%
15	UU	1049	85% 14%
16	UX	193	98%
17	UZ	391	58% 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	91% 6%
22	CG	630	66% 34%
23	CH	411	93% 5%
24	CI	1163	70% 29%
25	CJ	183	98%
26	CK	297	97%
27	CL	785	29% 71%
28	CM	446	99%
29	CN	252	89% 10%
29	CO	252	83% 15%
30	CP	322	72% 28%
31	CQ	259	67% 32%

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Mol	Chain	Length	Quality of chain
32	CR	1073	51% 19% 29%
32	CS	1073	51% 19% 29%
33	CT	203	65% 35%
34	Ca	255	88% 12%
35	Cb	264	87% 12%
36	Cc	212	89% 9%
37	Cd	239	94% 5%
38	Ce	203	77% 22%
39	Cf	202	86% 14%
40	Cg	190	83% 16%
41	Ch	151	44% 56%
42	Ci	150	77% 23%
43	Cj	143	88% 12%
44	Ck	161	87% 13%
45	Cm	130	97%
46	Cn	145	66% 34%
47	Co	136	68% 32%
48	Cp	68	88% 10%
49	CU	311	56% 43%
50	C1	2352	42% 22% 33%
51	C2	230	63% 31% 7%
52	CW	668	56% 43%
53	UT	2612	77% 22%
54	UH	930	38% 61%
55	UE	410	30% 70%

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Mol	Chain	Length	Quality of chain
55	UI	410	30% 70%
56	US	549	82% 18%
57	Cl	156	50% 49%
58	CX	480	55% 44%
59	CY	381	30% 68%
60	CZ	609	7% 93%
61	UP	364	15% 85%

2 Entry composition (i)

There are 64 unique types of molecules in this entry. The entry contains 211834 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	1090	8416	5408	1452	1525	31	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	177	1401	892	263	239	7	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	1819	1186	331	299	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 Nop56.

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	416	3245	2065	587	580	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	233	1893	1209	340	335	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 S4.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	Ck	140	1163	750	224	184	5	0	0

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

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

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

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

- Molecule 47 is a protein called 40S ribosomal protein S24.

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

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

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

- Molecule 49 is a protein called Faf1.

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

- Molecule 50 is a RNA chain called 35S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
50	C1	1575	33604	14992	6023	11014	1575	0	0

- Molecule 51 is a RNA chain called U3 snoRNA.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
52	CW	382	2924	1857	530	524	13	0	0

- Molecule 53 is a protein called Utp20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
53	UT	2033	16053	10338	2819	2828	68	0	0

- Molecule 54 is a protein called Utp8.

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

- Molecule 55 is a protein called Utp5.

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

- Molecule 56 is a protein called Noc4.

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

- Molecule 57 is a protein called Putative ribosomal protein.

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

- Molecule 58 is a protein called Enp1.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
59	CY	123	979	592	195	189	3	0	0

- Molecule 60 is a protein called Bfr2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
60	CZ	44	376	235	76	64	1	0	0

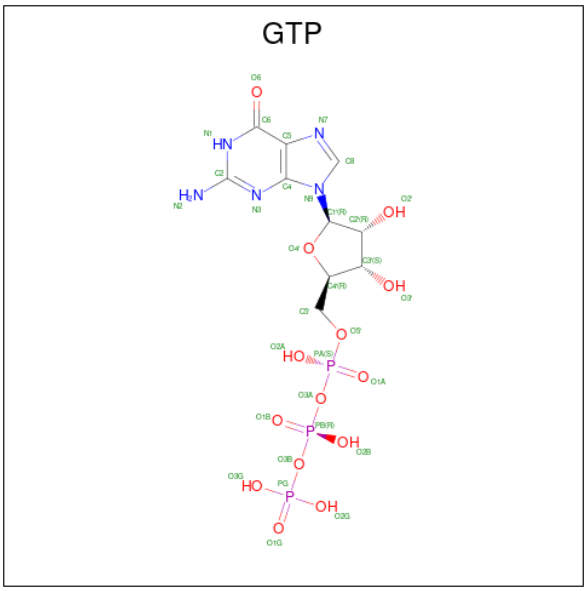
- Molecule 61 is a protein called Utp16.

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

- Molecule 62 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 63 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	
63	CI	1	32	10	5	14	3	0

- Molecule 64 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

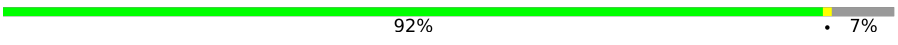
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
64	CI	1	1	1	0

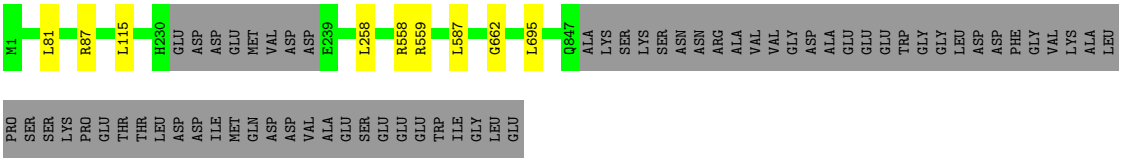
3 Residue-property plots (i)

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

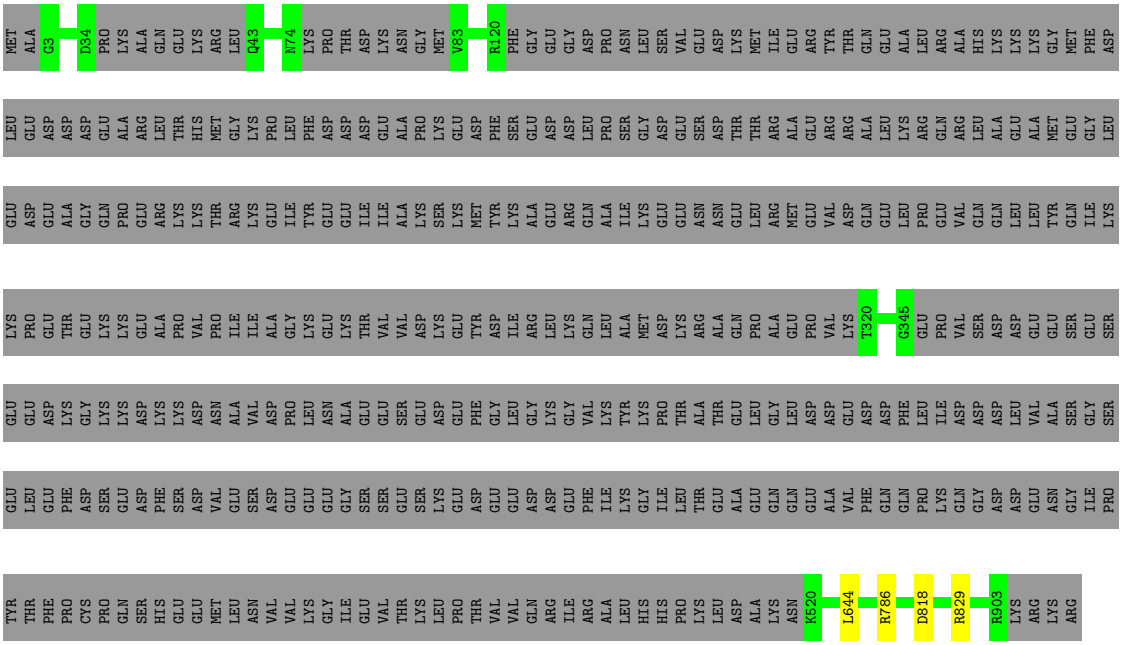
Chain UA:





- 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 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 GLY 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 VAL ALA GLY ALA 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 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 LYS SER LEU ARG PHE TYR THR SER GLN ILE VAL GLN LYS ALA ALA ASN LYS ARG GLN GLY ALA GLY ARG ASP ASP ASP ALA 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 T180 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

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

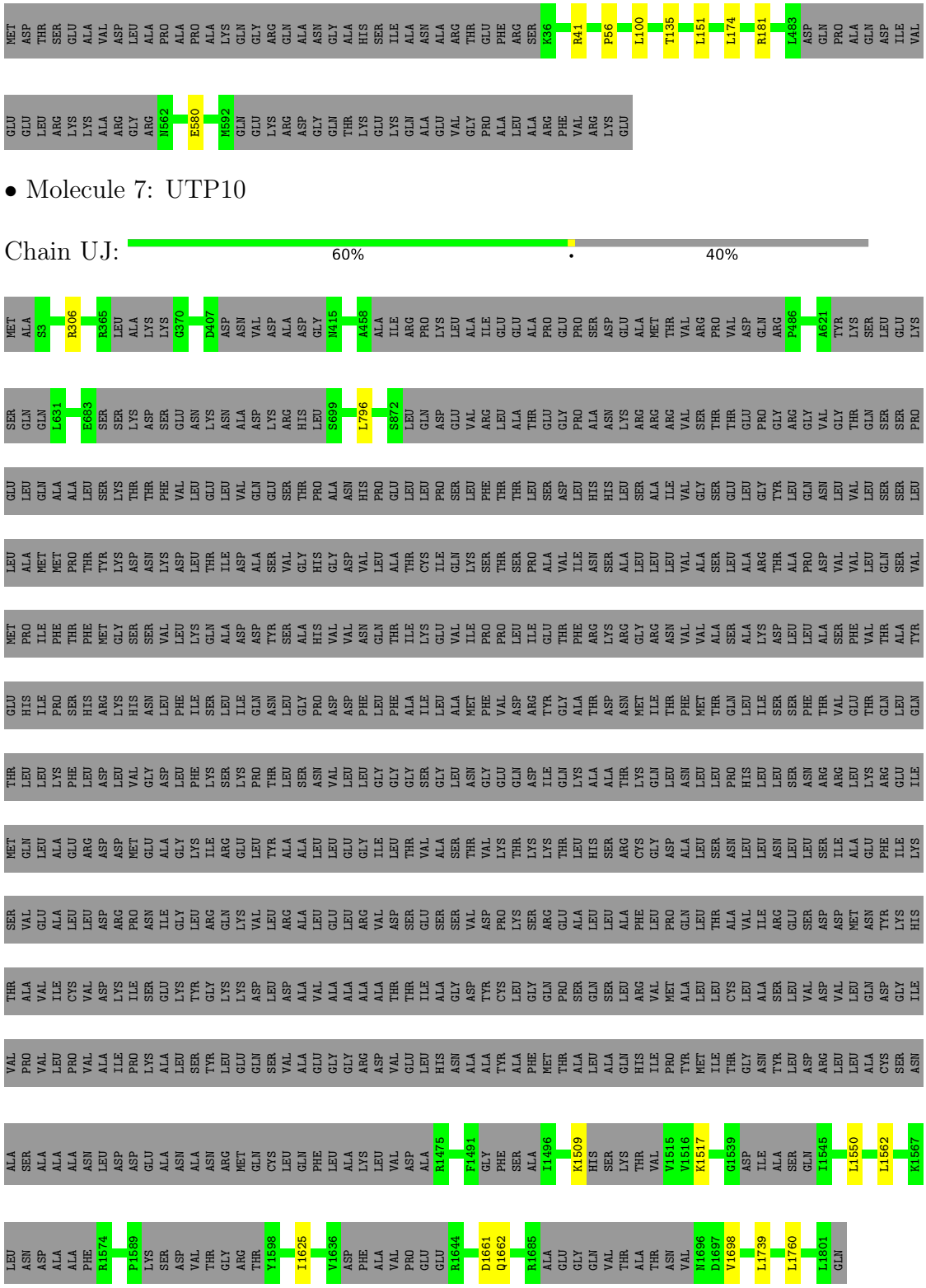
Chain UF: 79% 20%

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: 84% • 14%

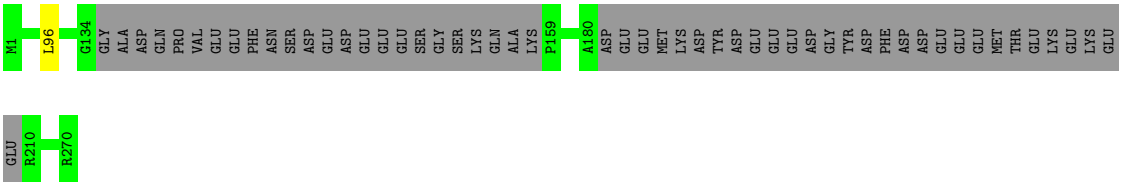


• Molecule 7: UTP10

Chain UJ: 60% 40%

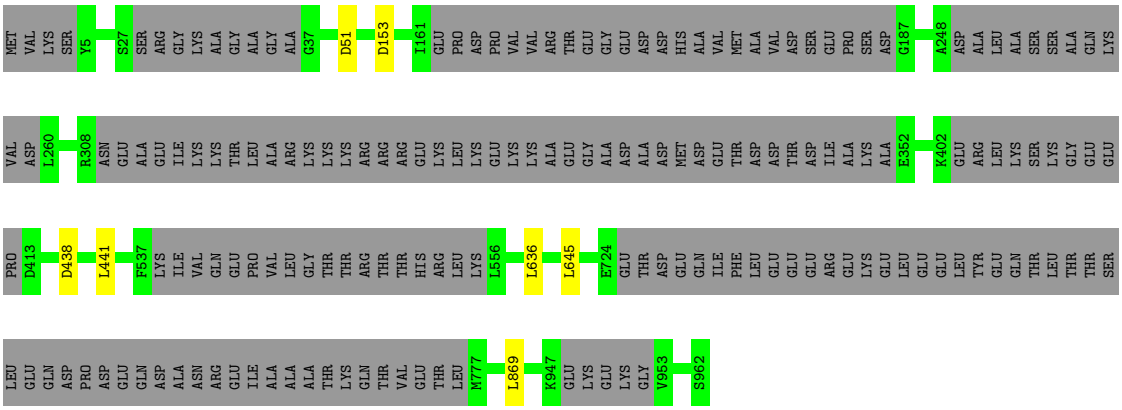
• Molecule 8: U3 small nucleolar RNA-associated protein 11

Chain UK: 80% 20%



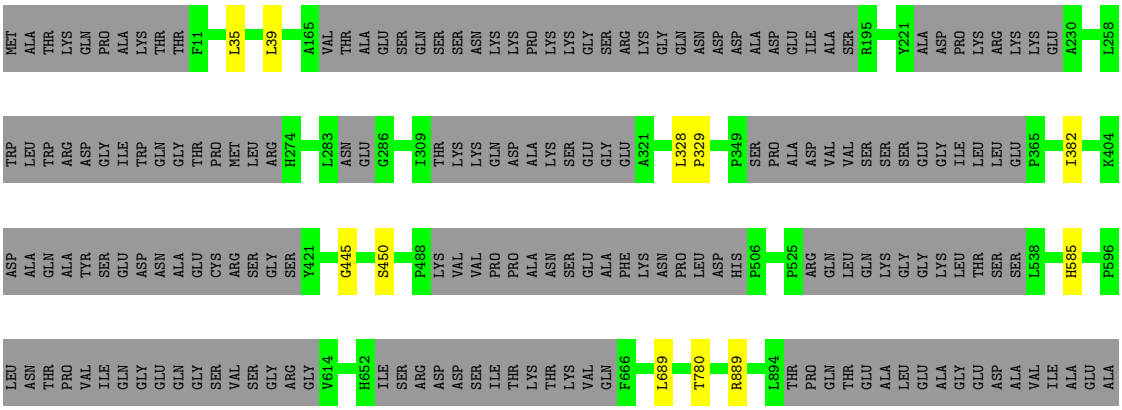
- Molecule 9: Utp12

Chain UL:



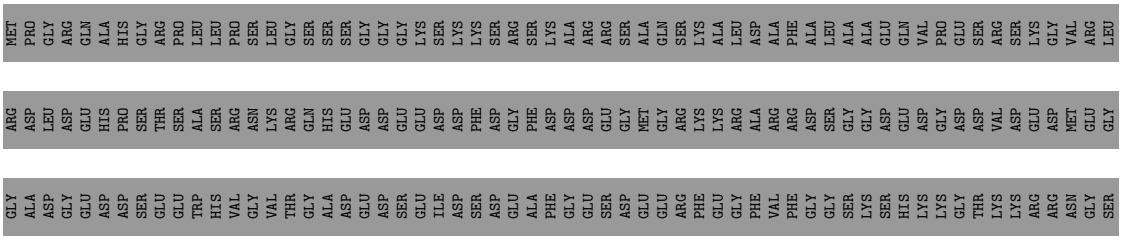
- Molecule 10: Utp13

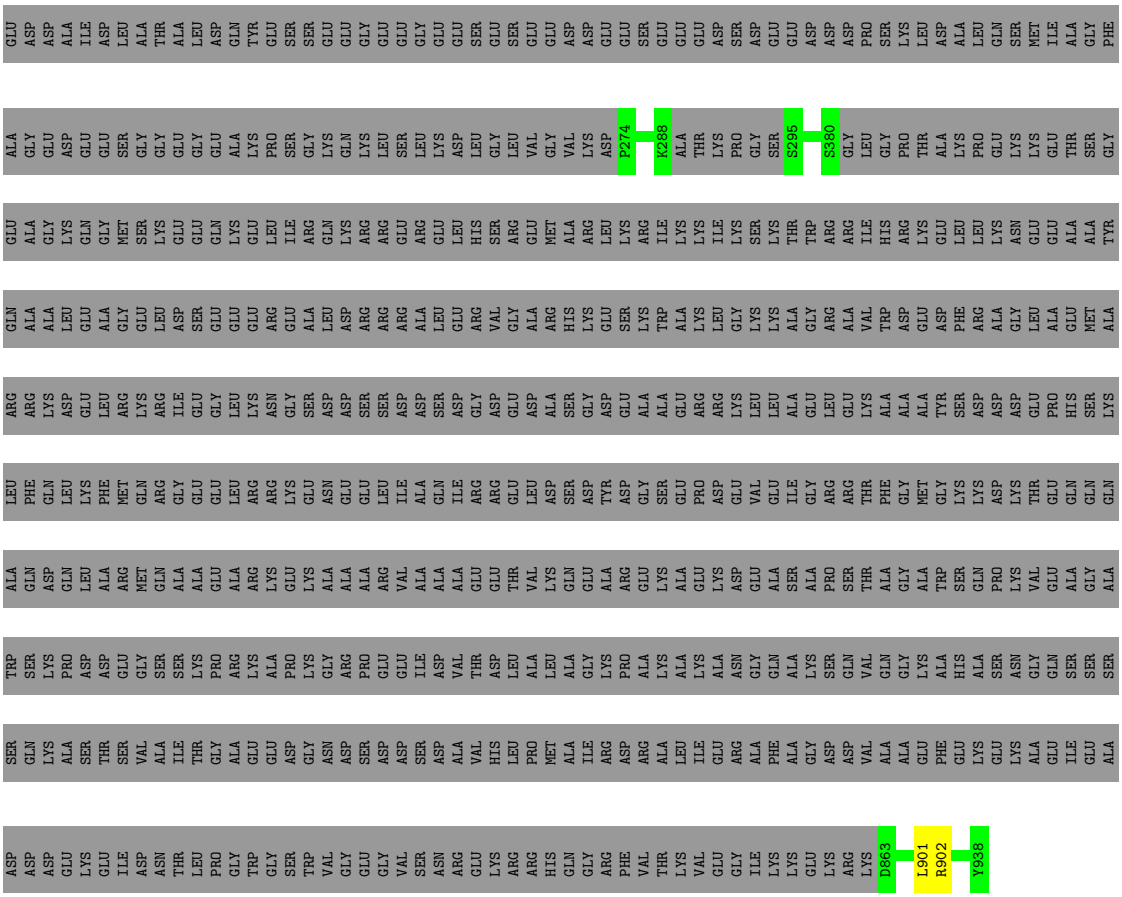
Chain UM:



- Molecule 11: Utp14

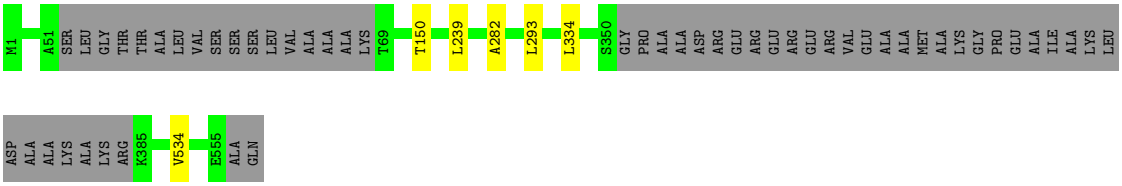
Chain UN:





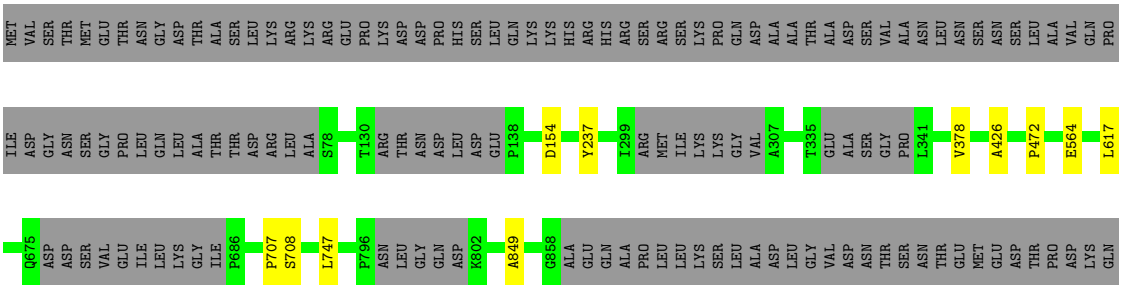
- Molecule 12: Utp15

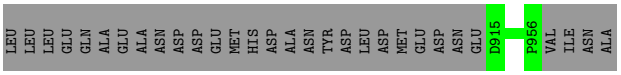
Chain UO:



- Molecule 13: Utp17

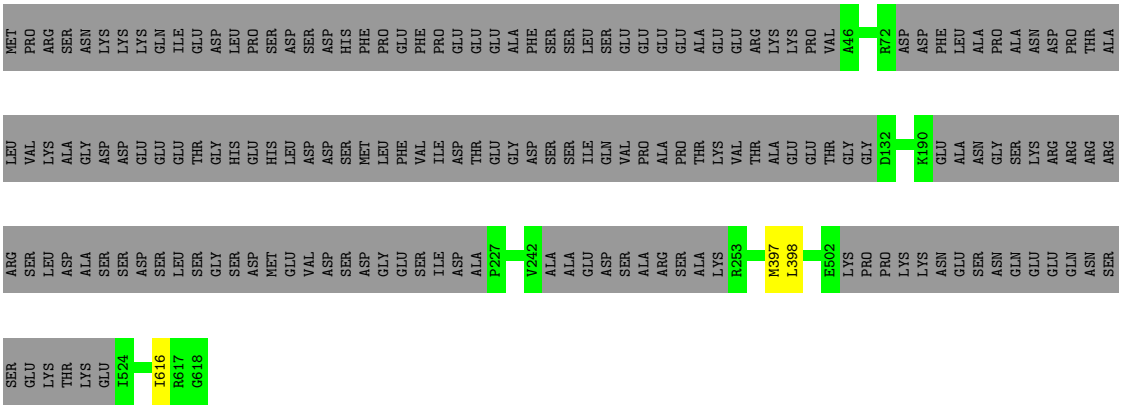
Chain UQ:





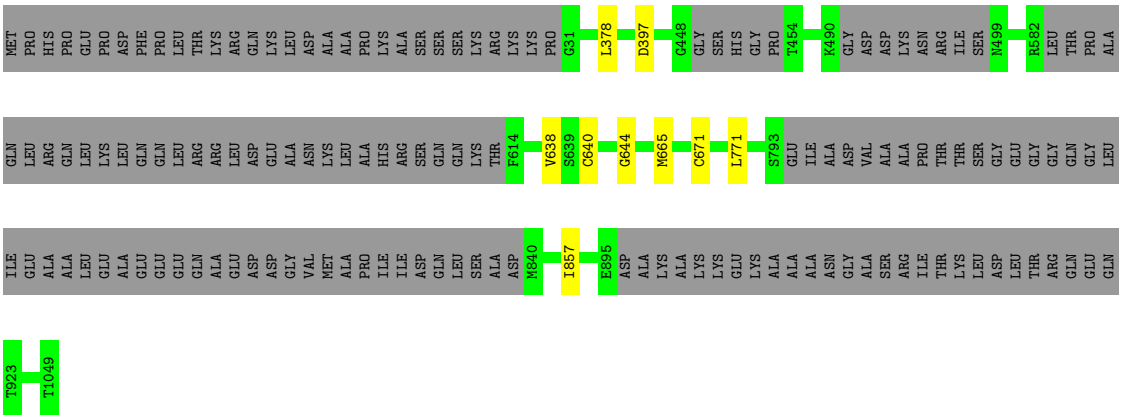
• Molecule 14: Utp18

Chain UR:



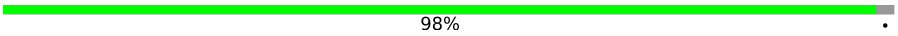
• Molecule 15: Putative U3 snoRNP protein

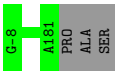
Chain UU:



• Molecule 16: Utp24

Chain UX:





• Molecule 17: Utp30

Chain UZ:

PRO ALA PRO LYS GLY LYS LYS GLU LYS ARG ASP PRO LEU GLU N211 Q273 N280 I293 Y294 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 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 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 L292 C304 G313

- Molecule 18: Nop1

Chain CB: 75% 24%

MET GLY PHE GLU ARG GLY GLY 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 T125 E293 Q308 LYS GLU PHE GLU GLY

- Molecule 19: Nop56

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 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

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

ASP VAL GLU MET ALA ASP ALA ASP VAL GLY GLU ASN LYS LYS LYS LYS LYS ARG LYS SER GLU ILE ALA GLU

- Molecule 20: Nop58

Chain CD: 72% 28%

MET PRO L3 A18 ALA ASP LYS LYS LEU LEU ASP SER ASP ASN VAL SER GLU ARG LEU SER THR LEU ASP LYS ILE ILE LYS GLU I43 L102 L143 W189 G446 LEU ALA THR THR THR SER LYS GLU SER SER GLU GLN PRO LYS ARG PRO LEU ILE GLU GLU VAL PRO

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

LYS PRO ASP GLY SER VAL GLU VAL LYS GLY LYS ASP GLY GLU ASP ALA GLU ALA GLU THR PRO VAL LYS SER LYS SER SER LYS ARG LYS HIS GLU PRO GLU GLU GLU THR PRO ALA LYS GLU GLU LYS HIS LYS LYS LYS LYS LYS SER SER LYS GLU

- Molecule 21: Snu13

Chain CE: 94% • 5%

MET SER ASN ASN GLU S6 L103 D110 A126 MET

- Molecule 21: Snu13

Chain CF: 91% • 6%

MET SER ASN ASN GLU SER A7 Q60 P61 H67 L103 A126 MET

- Molecule 22: Rrp9

Chain CG: 66% 34%

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

SER GLY SER ASP LEU ASP SER ASP LEU SER GLY ASP ASP GLU PHE ILE GLU ARG ARG SER SER ASP ALA GLY SER GLY ASP GLU SER GLU LYS GLU GLY GLU T95 K113 GLU VAL GLU GLN LEU D119 L137 LYS GLU ASP VAL ALA GLU ALA LYS GLY K147 V178 P201 LYS

ASN GLN TRP PRO GLN THR THR LYS LYS LYS PRO LYS LYS PRO PRO ALA PRO PRO K221 T263 E372 GLY GLY SER SER ASN THR LYS LYS HIS LYS LEU PRO PRO G386 V507 GLY SER GLU THR CYS GLU ASN SER THR ASN ILE SER ASN GLY ALA THR SER ASN GLY GLU SER

SER SER THR SER SER THR THR LEU ALA ALA GLN SER SER SER SER SER PRO PRO PRO SER GLN PRO LYS ASP L555 G569 GLU ARG GLY ARG ASP G575 K608 VAL GLU LYS LYS ASN LYS ARG LYS ASN GLU ASP LYS LYS GLU GLU VAL ASN GLY VAL TYR LYS GLU

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

Chain CH: 93% • 5%

MET ALA GLU PRO LYS PRO E7 T85 L120 H143 R210 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

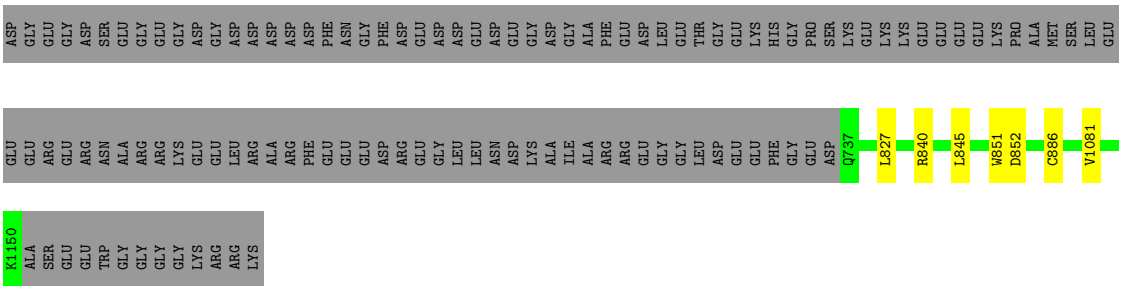
Chain CI: 70% • 29%

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 R91 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 LYS ALA ARG PHE LEU GLU ASP ASP ARG ASN ASP 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 GLU PHE ASP GLU LYS ARG LEU GLY LYS

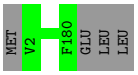
MET PHE ARG GLY ASP ASP GLU GLU THR GLN ASP GLU ASP VAL VAL PHE ALA ASP THR ASP ASP SER GLU LEU GLY SER ILE SER GLY ASP GLU GLY VAL ASP SER GLU GLU SER GLY GLU GLU SER ASP GLU GLU PHE ASP SER GLU GLU GLU GLU ALA VAL ARG TRP LYS GLU ASN MET MET GLU ARG

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



- Molecule 25: Imp3

Chain CJ: 98%

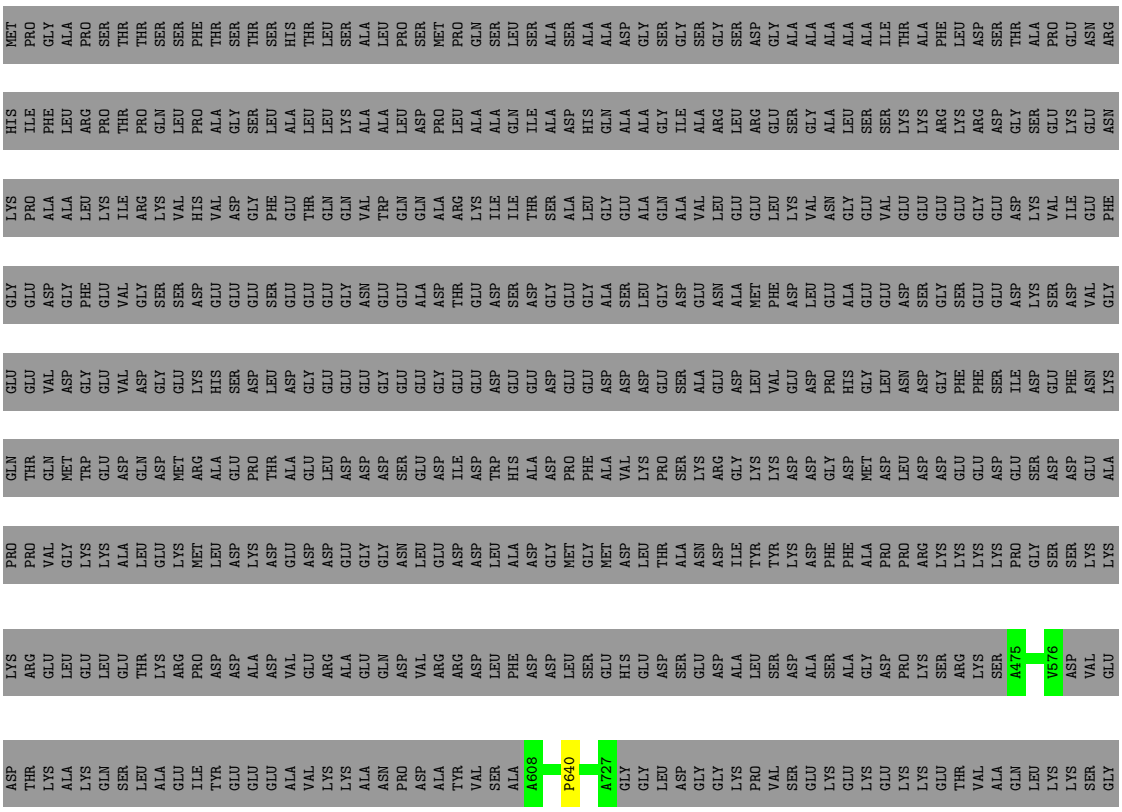


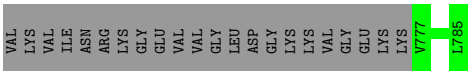
- Molecule 26: Putative U3 small nucleolar ribonucleoprotein

Chain CK: 97%

- Molecule 27: Putative U3 small nucleolar ribonucleoprotein protein

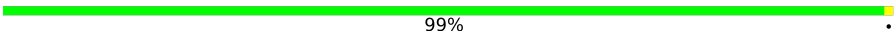
Chain CL: 29% 71%





• Molecule 28: Sof1

Chain CM:

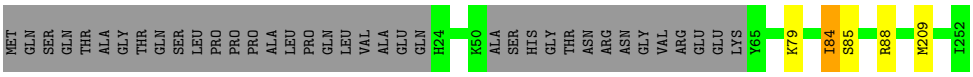


• Molecule 29: Emg1

Chain CN:

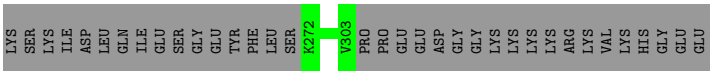
• Molecule 29: Emg1

Chain CO:



• Molecule 30: KRR1 small subunit processome component

Chain CP:

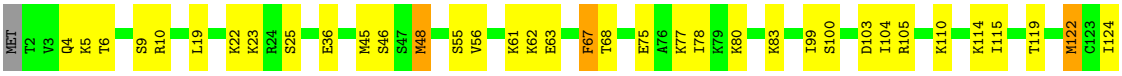


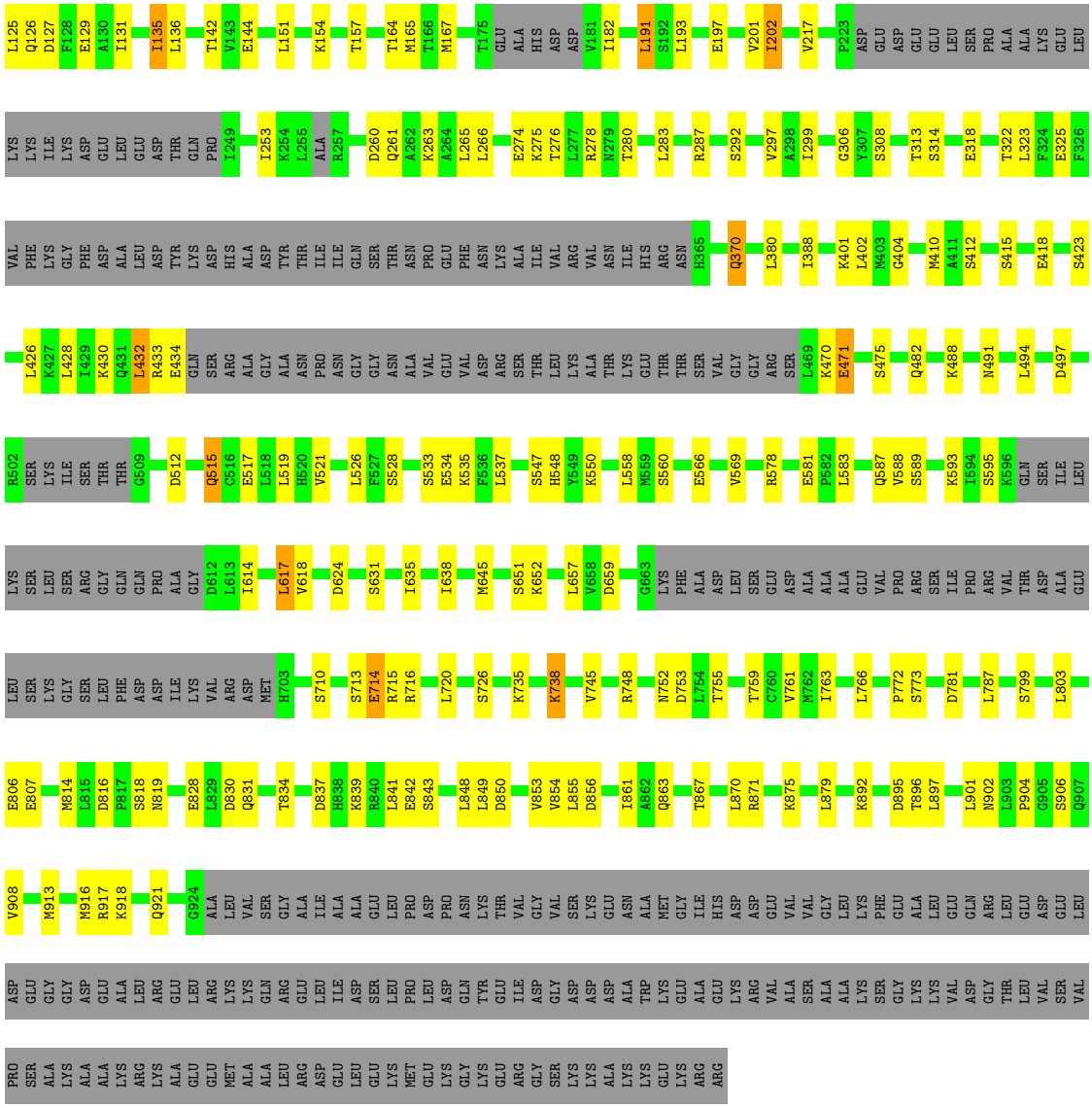
• Molecule 31: Pre-rRNA-processing protein PNO1

Chain CQ:

• Molecule 32: Kre33

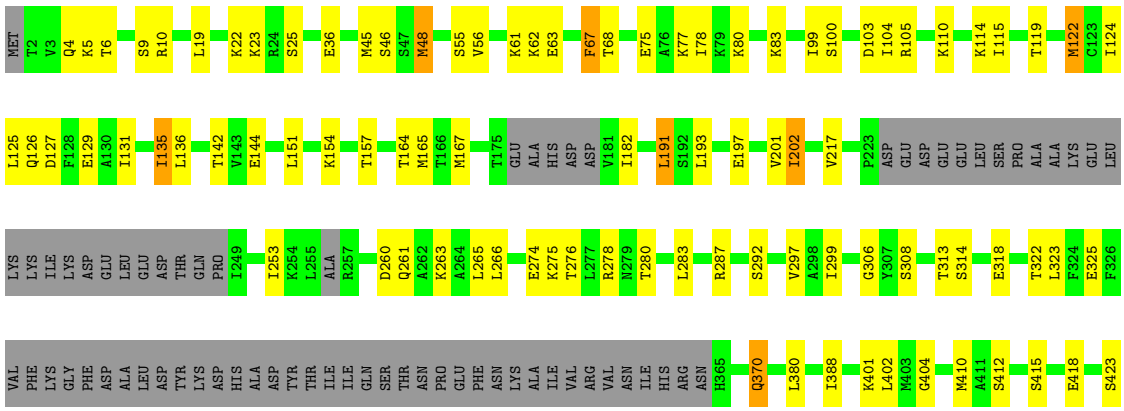
Chain CR:

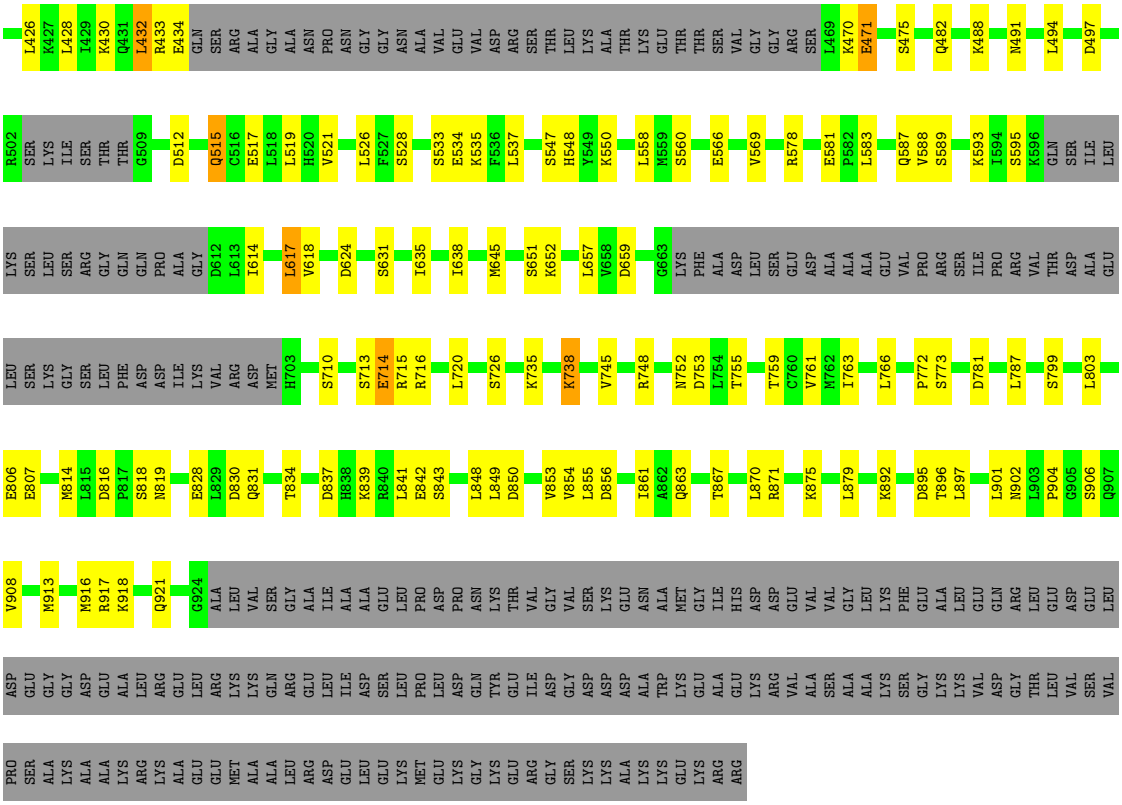




- Molecule 32: Kre33

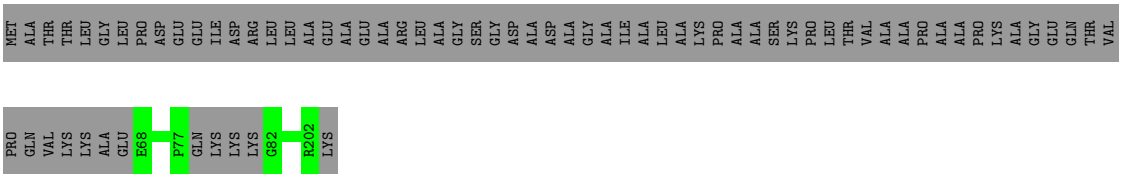
Chain CS:





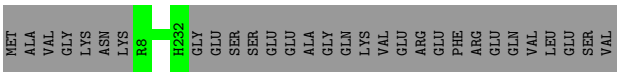
- Molecule 33: Fcf2

Chain CT: 65% 35%



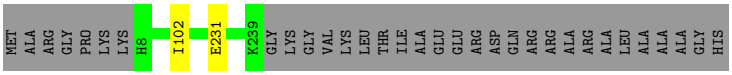
- Molecule 34: 40S ribosomal protein S1

Chain Ca: 88% 12%



- Molecule 35: 40S ribosomal protein S4

Chain Cb: 87% 12%



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

Chain Cc: 89% 9%

• Molecule 37: 40S ribosomal protein S6

Chain Cd: 94% 5%

• Molecule 38: 40S ribosomal protein S7

Chain Ce: 77% • 22%

• Molecule 39: 40S ribosomal protein S8

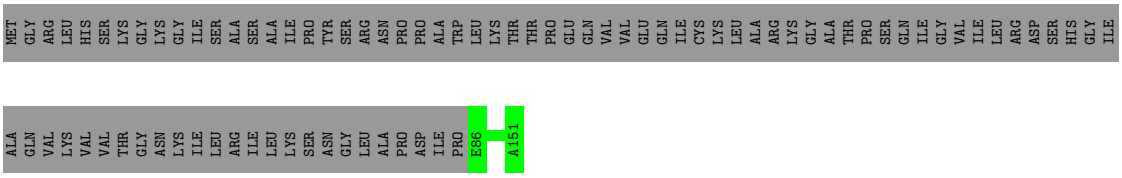
Chain Cf: 86% 14%

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

Chain Cg: 83% • 16%

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

Chain Ch: 44% 56%



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

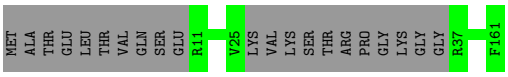
Chain Ci: 77% 23%

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

Chain Cj: 88% 12%

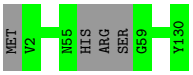
- Molecule 44: 40S ribosomal protein S11-like protein

Chain Ck: 87% 13%



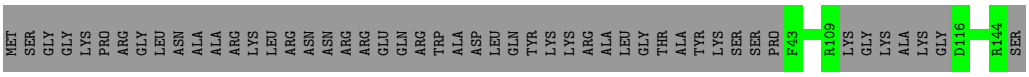
- Molecule 45: 40S ribosomal protein S22-like protein

Chain Cm: 97%



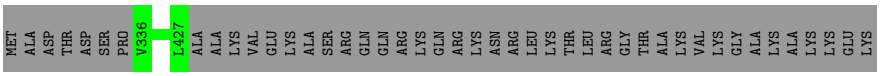
- Molecule 46: 40S ribosomal protein s23-like protein

Chain Cn: 66% 34%



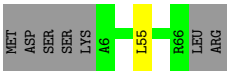
- Molecule 47: 40S ribosomal protein S24

Chain Co: 68% 32%



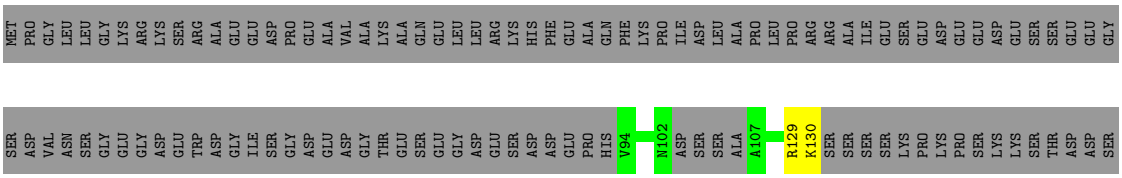
- Molecule 48: 40S ribosomal protein S28-like protein

Chain Cp: 88% 10%



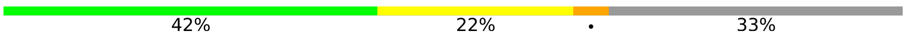
- Molecule 49: Faf1

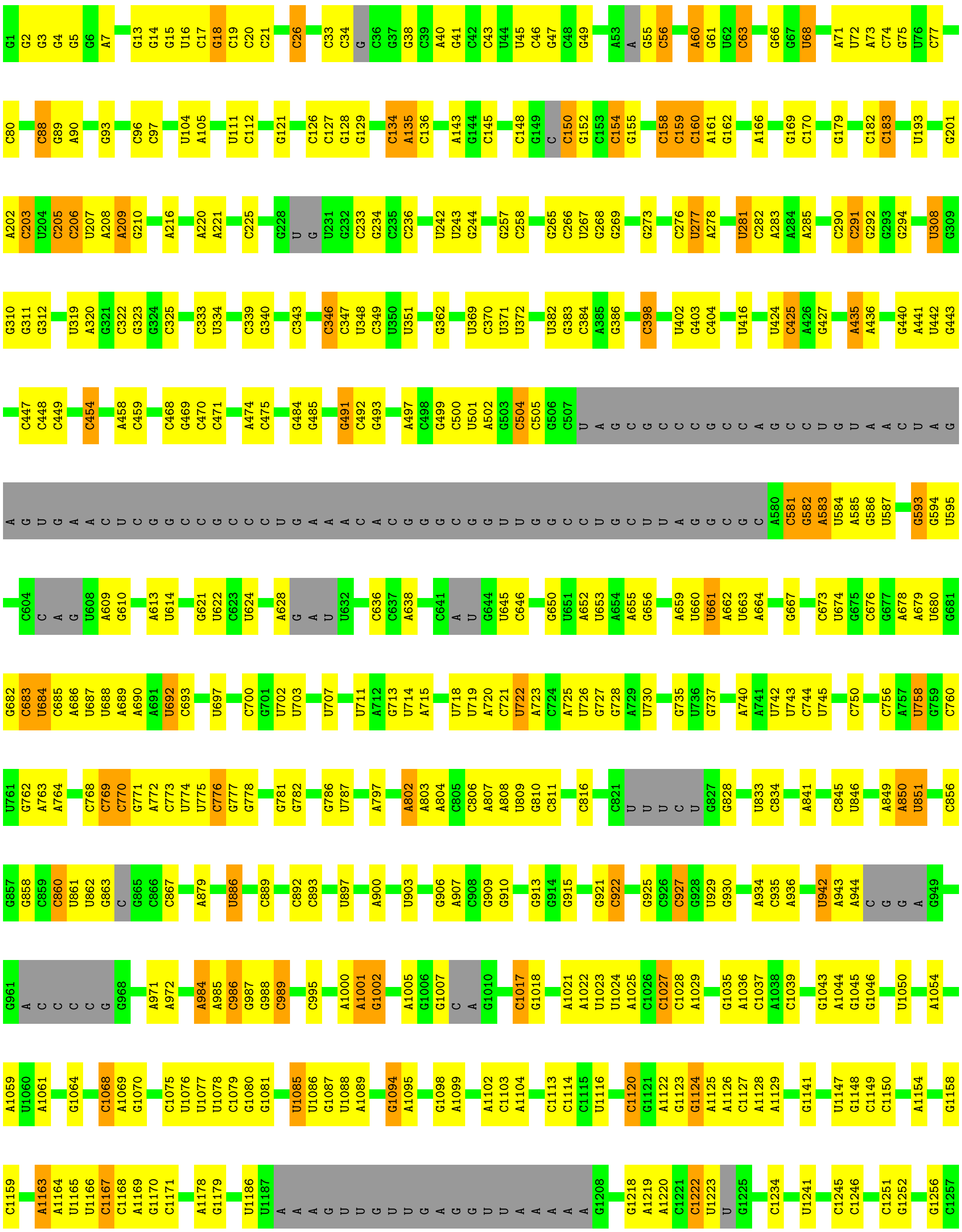
Chain CU: 56% 43%

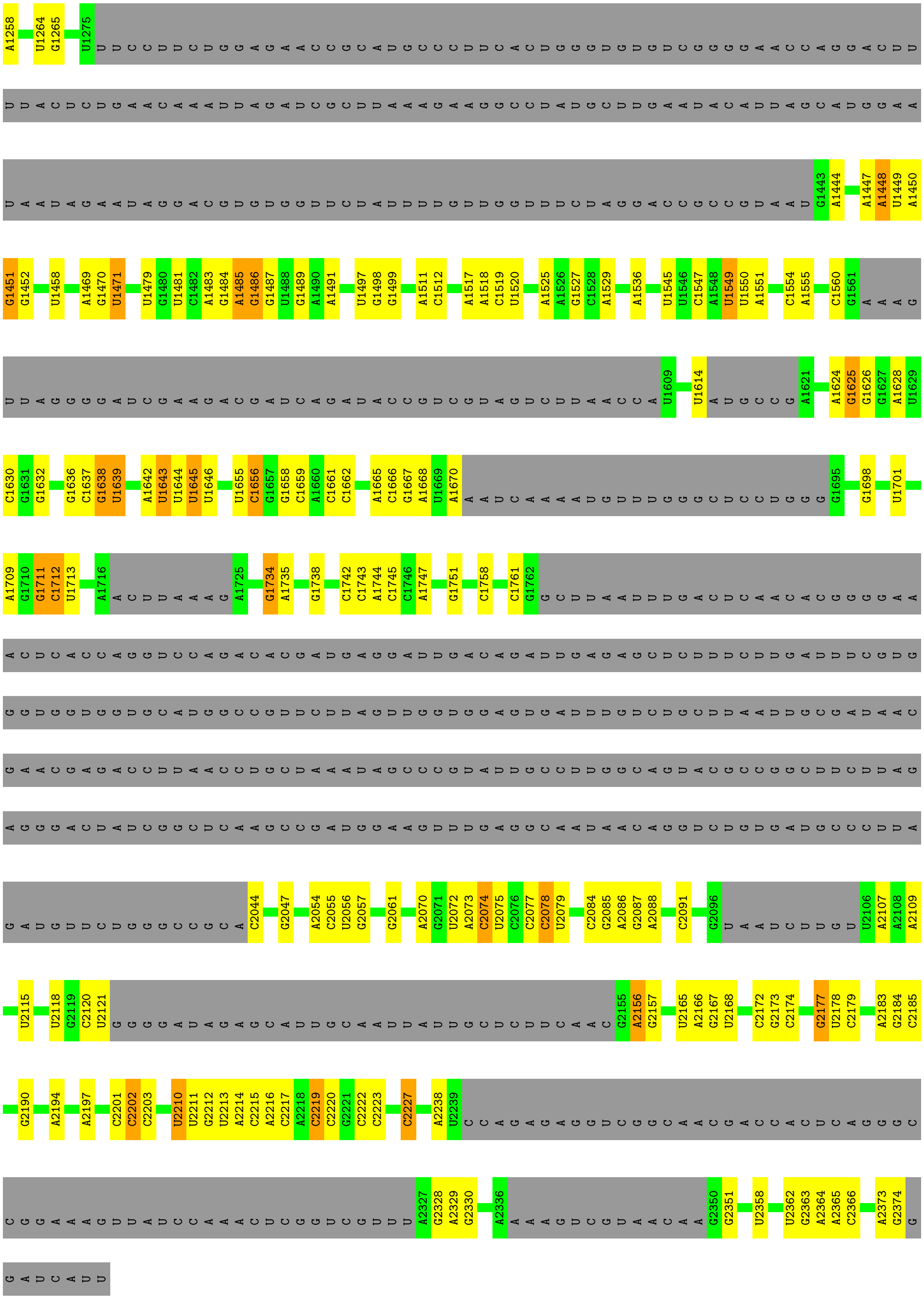


• Molecule 50: 35S rRNA

Chain C1:





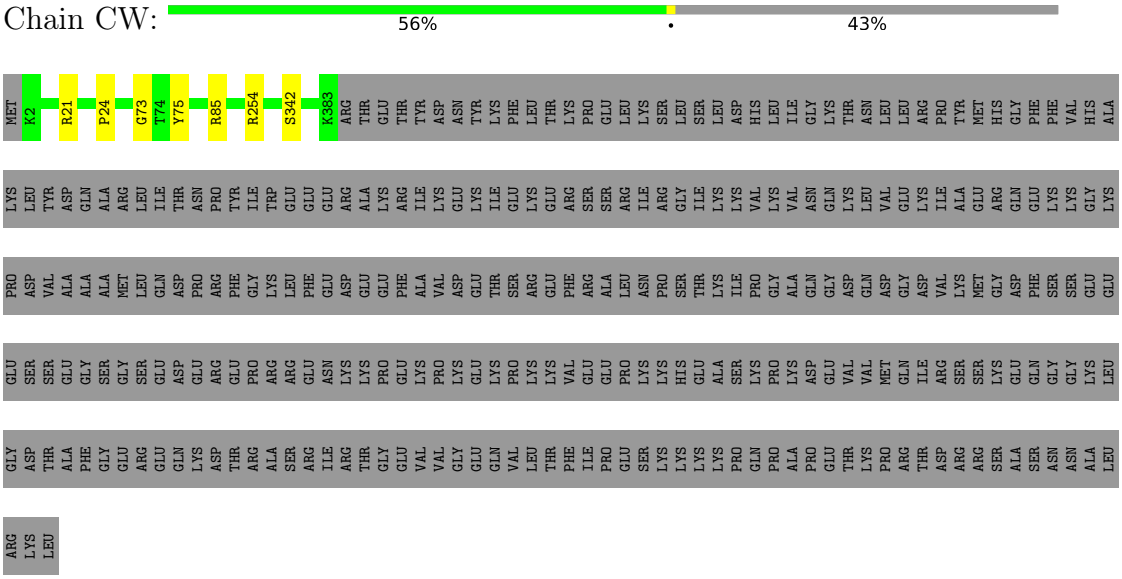


• Molecule 51: U3 snoRNA

Chain C2:

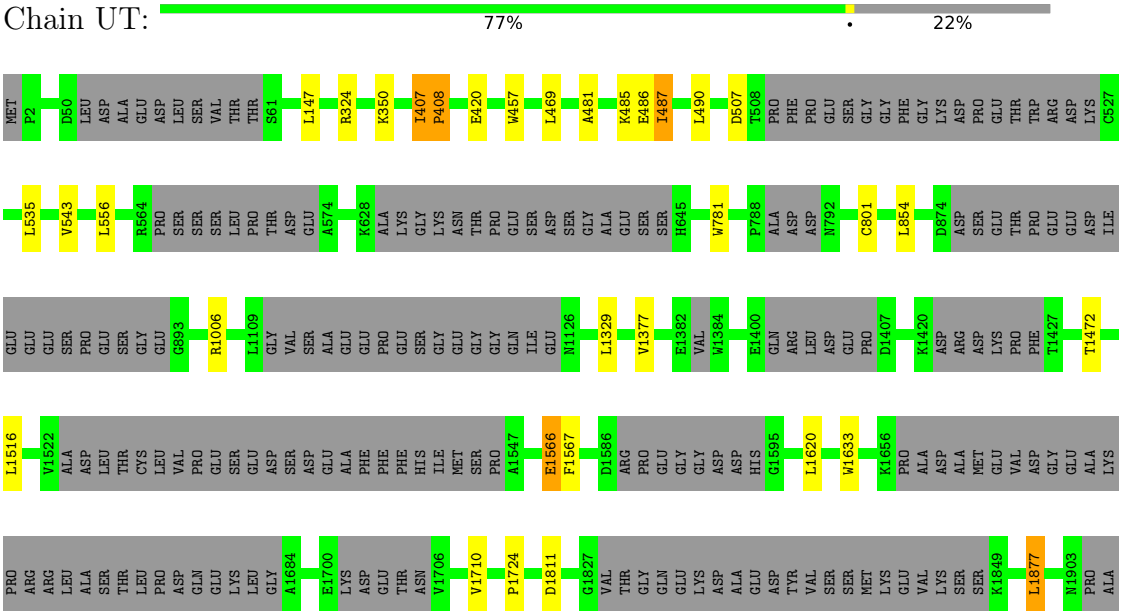
- Molecule 52: Ribosome biogenesis protein ENP2

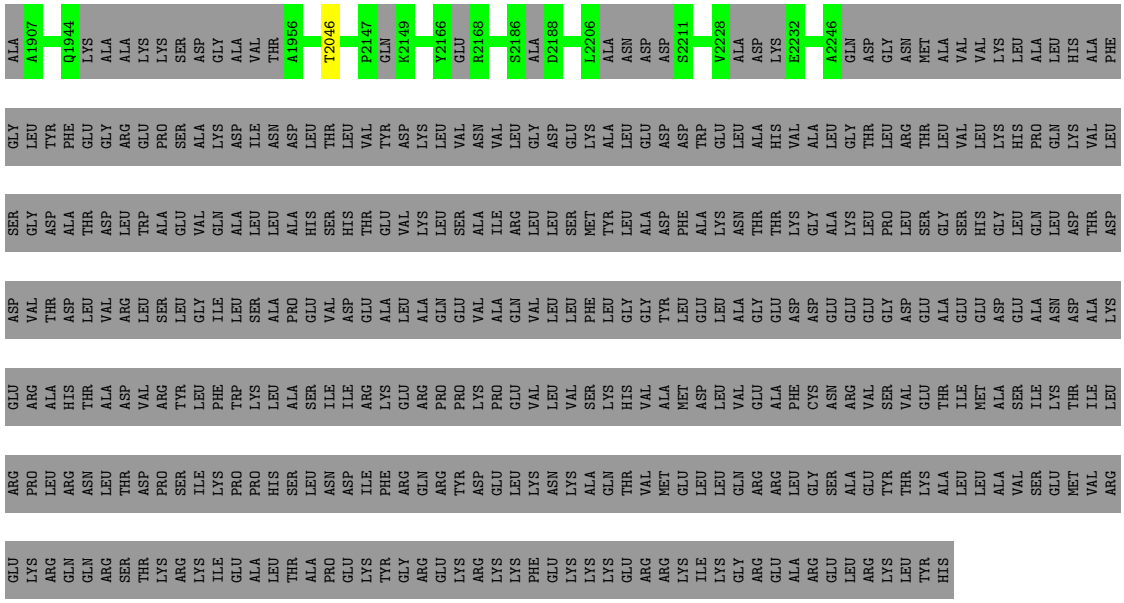
Chain CW:



- Molecule 53: Utp20

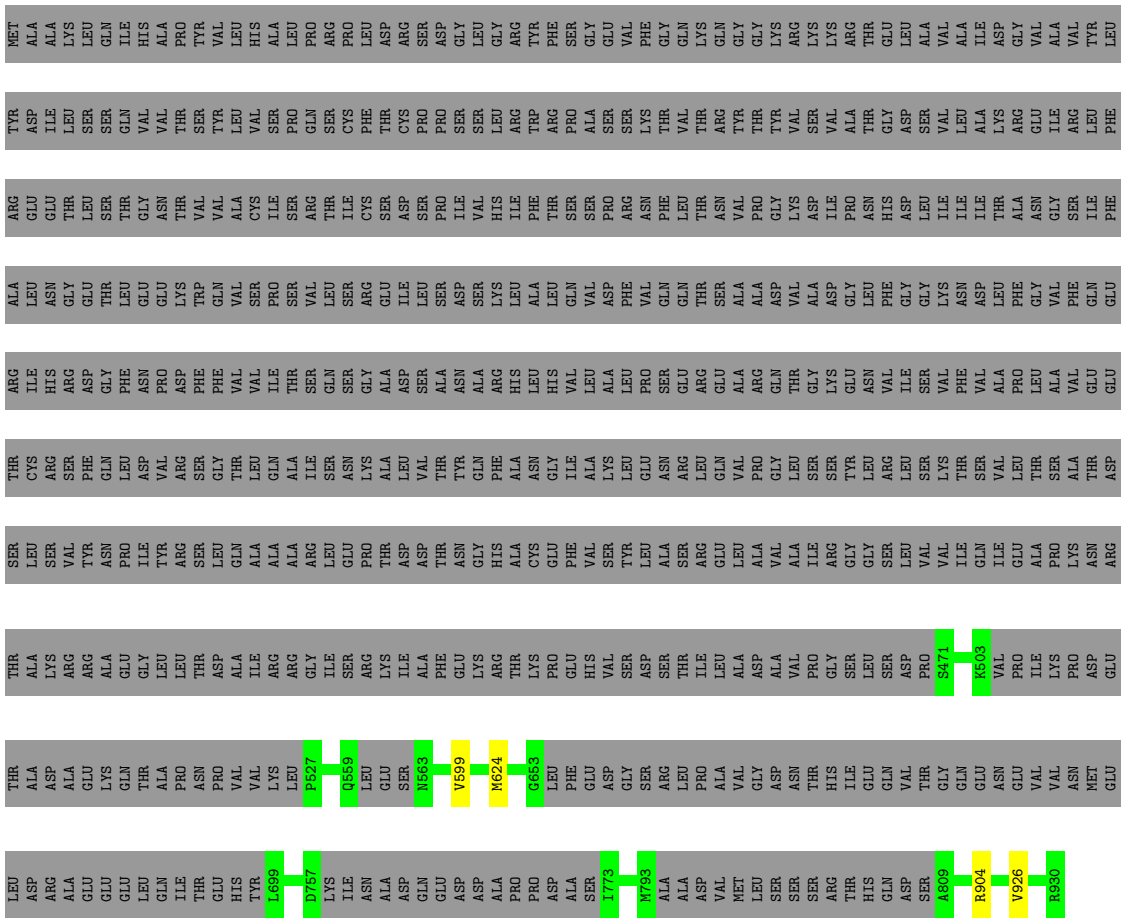
Chain UT:





- Molecule 54: Utp8

Chain UH: 38% 61%



- Molecule 55: Utp5

Chain UE: 30% 70%

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

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

ARG GLY THR THR THR VAL ASP VAL SER ALA SER LEU ALA ALA GLN THR THR ARG HIS GLU VAL GLN ARG SER THR ALA PRO ILE SER ALA THR SER L153 T175 ASN ASP LEU L179 Q232 G280 SER SER ARG ASN ARG PRO SER ASP ASP GLU SER SER ALA GLY GLU GLU

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

ASP ASP ILE GLU GLU ILE GLU SER ILE ASP ASP GLU ASP GLU VAL ASP HIS ASP ASP VAL GLU GLU ASP GLU GLU GLU GLU ASP SER GLU ALA GLU ASP ALA PRO PRO ALA LYS VAL ARG ARG THR SER ALA ARG LEU SER THR LYS ARG LYS

- Molecule 55: Utp5

Chain UI: 30% 70%

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

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

ARG GLY THR THR THR VAL ASP VAL SER ALA SER LEU ALA ALA GLN THR THR ARG HIS GLU VAL GLN ARG SER THR ALA PRO ILE SER ALA THR SER L153 T175 ASN ASP LEU L179 G280 SER SER ARG ASN ARG PRO SER ASP ASP ASP GLU SER SER ALA GLY GLU GLU ASP ASN

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

ILE GLU GLU ILE GLU SER ILE ASP ASP GLU ASP GLU VAL ASP HIS ASP ASP VAL GLU GLU ASP GLU GLU GLU GLU ASP SER GLU ALA GLU ASP ALA PRO PRO ALA LYS VAL ARG ARG THR SER ALA ARG LEU SER THR LYS ARG LYS

- Molecule 56: Noc4

Chain US: 82% • 18%

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

ALA ASN LEU ILE GLU LEU ALA GLN LYS HIS ASP GLU ASP P74 G95 SER LEU VAL LYS ARG LYS ASP ILE SER GLU LYS ASP ALA T109 S131 LYS LYS L134 E210 ARG GLU GLN SER VAL ASP E217 M302 L347 K510 G545 SER GLY SER ALA

- Molecule 57: Putative ribosomal protein

Chain Cl: 50% • 49%

MET S2 K25 Y79 K80 I81 PRO THR TRP PHE LEU ASN ARG GLN ARG ASP ILE VAL ASP GLY LYS ASP SER GLN ILE LEU ALA ASN GLY VAL ASP SER LYS LEU ARG GLU ASP LEU GLU ARG LEU LYS LYS ILE ARG ALA HIS ARG GLY LEU ARG HIS TYR TRP GLY LEU ARG VAL

ARG GLY GLN HIS THR LYS THR THR GLY ARG ARG GLY ARG THR VAL GLY VAL SER LYS LYS LYS GLY GLY

- Molecule 58: 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 ALA GLY ASP ASN ASP ASN GLU

VAL ASP ALA ALA ASP LEU GLU GLU ILE PHE ASN ARG PHE VAL GLN PRO THR MET LYS ASP ASP PRO LEU LEU LEU THR HIS GLY TRP ASP GLN LYS PRO ALA ASP GLY GLU GLU GLU LYS GLU 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 59: U3 small nucleolar ribonucleoprotein protein lcp5-like protein

Chain CY: 30% 68%

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

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

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

SER ASN PHE GLN ARG PRO ALA ALA ALA THR LYS VAL THR LYS GLU LYS ASP ASN SER GLY VAL TYR ARG PRO PRO ARG ILE ALA PRO ILE ALA MET PRO THR ASN ASP ARG ARG ASP LYS ALA GLU ARG ARG PRO LEU LYS S228 K328 S329 S330 GLY GLY GLY GLY THR LYS ALA LEU LEU

GLU LYS SER ARG LYS ARG THR ILE ASP THR VAL ASN GLY SER ARG GLY SER GLY VAL ALA MET G360 L367 K368 V369 L370 E371 S372 G373 R374 R377 G378 K379 GLY ARG

- Molecule 60: Bfr2

Chain CZ: 7% 93%

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

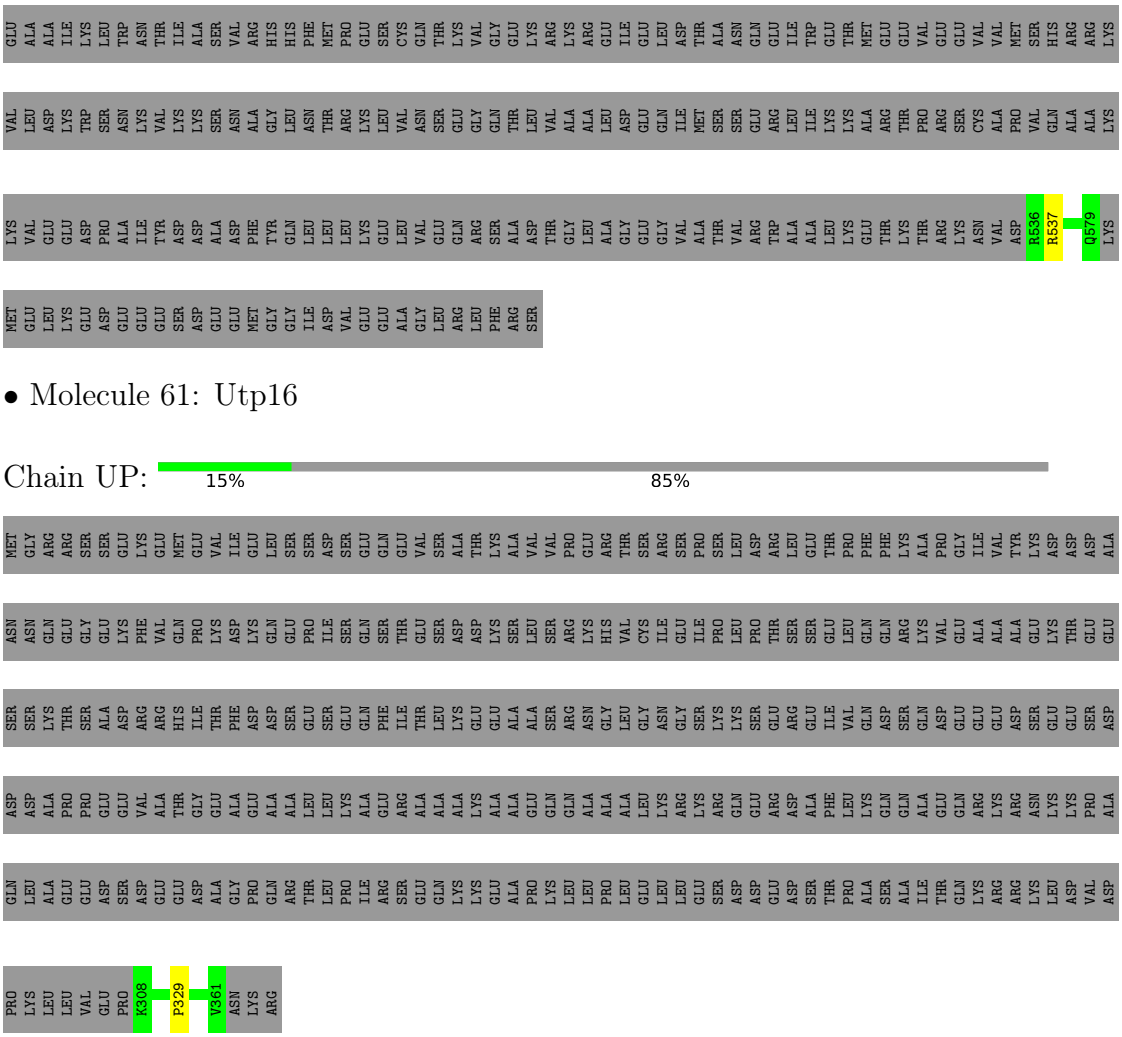
GLN LYS GLU PRO LEU ALA LEU GLY PRO GLU TYR ARG GLY THR ARG VAL SER ARG ALA GLN LEU GLU ALA SER SER GLU GLU GLU GLU ASP GLU GLU ASN ASP ASP GLU GLU GLU ASP ASP GLU ASP LYS GLU GLU GLY SER GLU ASP GLU SER GLY GLU GLU TYR ASP PRO

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

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

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

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



- Molecule 61: Utp16

Chain UP: 15% 85%

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	343726	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, ZN, MG

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	0.34	0/8567	0.61	5/11619 (0.0%)
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	0.39	0/1425	0.55	1/1913 (0.1%)
12	UO	0.41	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	0/1861	0.61	1/2531 (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	0.36	0/3307	0.59	0/4462
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	0.34	0/1923	0.56	0/2577
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	Cb	0.32	0/1890	0.61	1/2548 (0.0%)
36	Cc	0.40	0/1485	0.54	0/2008
37	Cd	0.34	0/1850	0.55	0/2474
38	Ce	0.34	0/1298	0.66	3/1750 (0.2%)
39	Cf	0.33	0/1429	0.54	0/1915
40	Cg	0.39	0/1259	0.55	0/1687
41	Ch	0.32	0/557	0.51	0/749
42	Ci	0.34	0/819	0.54	0/1107
43	Cj	0.49	0/958	0.60	0/1293
44	Ck	0.30	0/1190	0.54	0/1592
45	Cm	0.41	0/1001	0.57	0/1345
46	Cn	0.44	0/712	0.56	0/954
47	Co	0.32	0/754	0.59	0/1011
48	Cp	0.44	0/458	0.61	1/617 (0.2%)
49	CU	0.32	0/1350	0.53	0/1810
50	C1	0.61	1/37546 (0.0%)	1.24	401/58475 (0.7%)
51	C2	0.64	0/5459	1.40	72/8498 (0.8%)
52	CW	0.33	0/2996	0.67	2/4075 (0.0%)
53	UT	0.34	0/16371	0.63	10/22154 (0.0%)
54	UH	0.33	0/2852	0.56	0/3846
55	UE	0.31	0/980	0.58	0/1316
55	UI	0.26	0/980	0.52	0/1316
56	US	0.33	0/3765	0.57	1/5100 (0.0%)
57	Cl	0.30	0/638	0.60	0/857
58	CX	0.28	0/2180	0.55	1/2956 (0.0%)
59	CY	0.36	0/986	0.53	0/1303
60	CZ	0.39	0/384	0.68	0/511
61	UP	0.34	0/428	0.60	0/570
All	All	0.44	2/219692 (0.0%)	0.80	569/305865 (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

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Mol	Chain	#Chirality outliers	#Planarity outliers
4	UD	0	1
7	UJ	0	2
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
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	Cb	0	1
36	Cc	0	1
37	Cd	0	1
38	Ce	0	1
52	CW	0	2
53	UT	0	10
55	UE	0	1
56	US	0	1
57	Cl	0	1
59	CY	0	1
All	All	0	59

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	C1	1081	G	C2-N3	-5.49	1.28	1.32
15	UU	640	CYS	CB-SG	-5.31	1.73	1.81

All (569) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	C2	2	G	O5'-P-OP1	-30.49	74.11	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	C2	2	G	OP1-P-OP2	-27.27	78.70	119.60
51	C2	2	G	O5'-P-OP2	18.13	132.46	110.70
51	C2	1	A	OP1-P-O3'	13.81	135.58	105.20
51	C2	1	A	OP2-P-O3'	-13.14	76.29	105.20
50	C1	258	C	N1-C2-O2	12.92	126.65	118.90
50	C1	258	C	C2-N1-C1'	12.45	132.49	118.80
50	C1	55	G	OP1-P-O3'	-12.21	78.35	105.20
50	C1	160	C	N3-C2-O2	-11.66	113.74	121.90
50	C1	45	U	OP1-P-O3'	-11.39	80.14	105.20
50	C1	258	C	N3-C2-O2	-10.66	114.44	121.90
50	C1	206	C	N1-C2-O2	10.49	125.19	118.90
50	C1	206	C	C2-N1-C1'	10.46	130.30	118.80
50	C1	2168	U	N3-C2-O2	-10.36	114.95	122.20
50	C1	1222	C	N1-C2-O2	10.15	124.99	118.90
50	C1	758	U	N3-C2-O2	-9.86	115.30	122.20
51	C2	140	C	N3-C2-O2	-9.74	115.08	121.90
50	C1	2168	U	N1-C2-O2	9.61	129.53	122.80
50	C1	1662	C	N3-C2-O2	-9.58	115.19	121.90
50	C1	2074	C	N1-C2-O2	9.53	124.62	118.90
53	UT	556	LEU	CA-CB-CG	9.44	137.02	115.30
51	C2	128	C	C6-N1-C2	-9.41	116.54	120.30
50	C1	1658	G	C5-C6-O6	9.38	134.23	128.60
50	C1	1658	G	N3-C4-N9	-9.30	120.42	126.00
50	C1	160	C	C6-N1-C2	-9.30	116.58	120.30
51	C2	200	U	C2-N1-C1'	9.28	128.84	117.70
50	C1	661	U	C2-N1-C1'	9.24	128.79	117.70
50	C1	45	U	OP2-P-O3'	-9.16	85.05	105.20
51	C2	140	C	N1-C2-O2	9.15	124.39	118.90
51	C2	200	U	N1-C2-O2	9.15	129.20	122.80
50	C1	1550	U	C2-N1-C1'	9.09	128.60	117.70
50	C1	2217	C	N1-C2-O2	9.07	124.34	118.90
51	C2	128	C	C5-C6-N1	8.97	125.48	121.00
50	C1	160	C	N1-C2-O2	8.95	124.27	118.90
50	C1	258	C	C6-N1-C1'	-8.92	110.09	120.80
50	C1	692	U	N1-C2-O2	8.91	129.03	122.80
50	C1	1655	U	N3-C2-O2	-8.90	115.97	122.20
50	C1	1027	C	N3-C2-O2	-8.89	115.67	121.90
50	C1	1658	G	N9-C4-C5	8.87	108.95	105.40
50	C1	927	C	N3-C2-O2	-8.84	115.72	121.90
50	C1	206	C	N3-C2-O2	-8.80	115.74	121.90
50	C1	2217	C	C2-N1-C1'	8.68	128.35	118.80
51	C2	200	U	N3-C2-O2	-8.68	116.13	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	C1	291	C	N1-C2-O2	8.66	124.10	118.90
51	C2	136	C	N1-C2-O2	8.62	124.07	118.90
50	C1	158	C	N1-C2-O2	8.61	124.07	118.90
50	C1	505	C	N3-C2-O2	-8.61	115.88	121.90
50	C1	922	C	N3-C2-O2	-8.60	115.88	121.90
26	CK	235	ASP	CB-CG-OD1	8.58	126.02	118.30
50	C1	661	U	N1-C2-O2	8.52	128.76	122.80
50	C1	915	G	N3-C4-N9	-8.47	120.92	126.00
50	C1	692	U	N3-C2-O2	-8.46	116.28	122.20
50	C1	1486	G	C4-N9-C1'	8.45	137.49	126.50
50	C1	850	A	N1-C6-N6	-8.43	113.54	118.60
26	CK	89	LEU	CA-CB-CG	8.43	134.68	115.30
50	C1	683	C	C2-N1-C1'	8.37	128.01	118.80
1	UA	81	LEU	CA-CB-CG	8.36	134.53	115.30
50	C1	1547	C	N1-C2-O2	8.36	123.92	118.90
50	C1	471	C	N3-C2-O2	-8.36	116.05	121.90
32	CR	738	LYS	CD-CE-NZ	8.34	130.88	111.70
32	CS	738	LYS	CD-CE-NZ	8.33	130.86	111.70
50	C1	112	C	N1-C2-O2	8.29	123.88	118.90
50	C1	2202	C	N1-C2-O2	8.29	123.88	118.90
50	C1	758	U	C2-N1-C1'	8.28	127.64	117.70
50	C1	1222	C	C2-N1-C1'	8.25	127.88	118.80
50	C1	159	C	N3-C2-O2	-8.19	116.17	121.90
50	C1	661	U	N3-C2-O2	-8.18	116.48	122.20
52	CW	24	PRO	CA-N-CD	-8.14	100.10	111.50
50	C1	2084	C	N3-C2-O2	-8.11	116.22	121.90
50	C1	68	U	N1-C2-O2	8.06	128.44	122.80
50	C1	449	C	N3-C2-O2	-8.06	116.26	121.90
32	CS	191	LEU	CA-CB-CG	8.01	133.73	115.30
50	C1	1081	G	N3-C2-N2	-8.01	114.29	119.90
32	CR	191	LEU	CA-CB-CG	8.01	133.72	115.30
50	C1	2210	U	N3-C2-O2	-7.92	116.65	122.20
50	C1	583	A	O5'-P-OP1	-7.89	98.60	105.70
50	C1	1222	C	N3-C2-O2	-7.88	116.38	121.90
50	C1	80	C	N3-C2-O2	-7.87	116.39	121.90
50	C1	915	G	N9-C4-C5	7.84	108.54	105.40
51	C2	128	C	O4'-C1'-N1	7.84	114.47	108.20
50	C1	346	C	N3-C2-O2	-7.81	116.43	121.90
51	C2	267	C	N3-C2-O2	-7.80	116.44	121.90
53	UT	1877	LEU	CA-CB-CG	7.75	133.13	115.30
51	C2	203	C	N3-C2-O2	-7.73	116.49	121.90
50	C1	1645	U	C2-N1-C1'	7.73	126.97	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	C2	103	G	N3-C4-C5	-7.72	124.74	128.60
50	C1	1645	U	N1-C2-O2	7.66	128.16	122.80
9	UL	438	ASP	CB-CG-OD1	7.65	125.19	118.30
50	C1	915	G	N1-C6-O6	-7.64	115.32	119.90
32	CS	471	GLU	CA-CB-CG	7.59	130.09	113.40
32	CR	471	GLU	CA-CB-CG	7.58	130.09	113.40
32	CR	714	GLU	CA-CB-CG	7.57	130.06	113.40
50	C1	1662	C	N1-C2-O2	7.57	123.44	118.90
32	CS	714	GLU	CA-CB-CG	7.57	130.05	113.40
50	C1	1658	G	N1-C6-O6	-7.56	115.37	119.90
51	C2	6	C	C6-N1-C2	-7.56	117.28	120.30
50	C1	2179	C	C2-N1-C1'	7.56	127.11	118.80
50	C1	148	C	N3-C2-O2	-7.55	116.62	121.90
50	C1	707	U	C2-N1-C1'	7.53	126.74	117.70
50	C1	1645	U	N3-C2-O2	-7.52	116.94	122.20
50	C1	148	C	C6-N1-C2	-7.46	117.32	120.30
50	C1	1625	G	N3-C4-N9	7.45	130.47	126.00
50	C1	470	C	N1-C2-O2	7.45	123.37	118.90
50	C1	776	C	N1-C2-O2	7.43	123.36	118.90
50	C1	206	C	C6-N1-C2	-7.43	117.33	120.30
50	C1	768	C	C2-N1-C1'	7.42	126.97	118.80
50	C1	1120	C	C2-N1-C1'	7.42	126.96	118.80
50	C1	2084	C	C6-N1-C2	-7.42	117.33	120.30
50	C1	989	C	C2-N1-C1'	7.42	126.96	118.80
50	C1	291	C	N3-C2-O2	-7.40	116.72	121.90
50	C1	2074	C	C2-N1-C1'	7.40	126.94	118.80
50	C1	291	C	C2-N1-C1'	7.40	126.94	118.80
50	C1	1745	C	C5-C6-N1	7.37	124.68	121.00
51	C2	246	G	C4-N9-C1'	7.32	136.02	126.50
50	C1	1711	G	C4-N9-C1'	7.30	135.99	126.50
50	C1	491	G	C4-N9-C1'	7.29	135.98	126.50
50	C1	56	C	OP1-P-OP2	7.28	130.52	119.60
50	C1	258	C	C6-N1-C2	-7.25	117.40	120.30
51	C2	136	C	C2-N1-C1'	7.23	126.75	118.80
12	UO	293	LEU	CA-CB-CG	7.22	131.90	115.30
50	C1	915	G	C5-C6-O6	7.21	132.93	128.60
7	UJ	1625	ILE	CG1-CB-CG2	-7.18	95.60	111.40
51	C2	139	C	N3-C2-O2	-7.18	116.87	121.90
50	C1	1512	C	C6-N1-C2	-7.15	117.44	120.30
50	C1	1486	G	N3-C4-C5	-7.15	125.03	128.60
50	C1	942	U	N3-C2-O2	-7.14	117.20	122.20
51	C2	139	C	N1-C2-O2	7.13	123.18	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	C1	2217	C	N3-C2-O2	-7.13	116.91	121.90
50	C1	1163	A	P-O3'-C3'	7.12	128.24	119.70
50	C1	46	C	OP1-P-OP2	7.11	130.27	119.60
50	C1	1658	G	C4-C5-N7	-7.11	107.96	110.80
50	C1	206	C	C6-N1-C1'	-7.06	112.32	120.80
50	C1	989	C	C6-N1-C2	-7.06	117.48	120.30
32	CS	202	ILE	CG1-CB-CG2	-7.05	95.89	111.40
32	CR	202	ILE	CG1-CB-CG2	-7.03	95.93	111.40
51	C2	255	U	P-O3'-C3'	7.03	128.13	119.70
50	C1	622	U	N3-C2-O2	-7.00	117.30	122.20
50	C1	209	A	P-O3'-C3'	6.99	128.09	119.70
50	C1	1666	C	N1-C2-O2	6.99	123.10	118.90
50	C1	454	C	C2-N1-C1'	6.99	126.48	118.80
51	C2	252	C	N3-C2-O2	-6.98	117.02	121.90
50	C1	750	C	N1-C2-O2	6.98	123.09	118.90
32	CS	515	GLN	CA-CB-CG	6.96	128.71	113.40
50	C1	158	C	C2-N1-C1'	6.96	126.45	118.80
32	CR	515	GLN	CA-CB-CG	6.96	128.70	113.40
50	C1	56	C	C2-N1-C1'	6.96	126.45	118.80
50	C1	851	U	N3-C2-O2	-6.95	117.34	122.20
50	C1	34	C	N1-C2-O2	6.94	123.07	118.90
50	C1	1549	U	N3-C4-C5	6.93	118.76	114.60
51	C2	57	A	O4'-C1'-N9	6.89	113.72	108.20
51	C2	260	G	C4-N9-C1'	6.89	135.45	126.50
50	C1	1113	C	N1-C2-O2	6.88	123.03	118.90
21	CE	103	LEU	CA-CB-CG	6.87	131.11	115.30
12	UO	239	LEU	CA-CB-CG	6.87	131.10	115.30
50	C1	34	C	N3-C2-O2	-6.87	117.09	121.90
50	C1	159	C	C6-N1-C2	-6.87	117.55	120.30
50	C1	2202	C	N3-C2-O2	-6.86	117.10	121.90
50	C1	1471	U	C2-N1-C1'	6.85	125.92	117.70
11	UN	901	LEU	CA-CB-CG	6.84	131.04	115.30
51	C2	161	G	C4-N9-C1'	6.84	135.40	126.50
50	C1	1487	G	O4'-C1'-N9	6.84	113.67	108.20
50	C1	1114	C	N1-C2-O2	6.83	123.00	118.90
50	C1	504	C	N1-C2-O2	6.82	122.99	118.90
50	C1	33	C	N3-C2-O2	-6.81	117.13	121.90
51	C2	103	G	N3-C4-N9	6.78	130.07	126.00
50	C1	68	U	N3-C2-O2	-6.77	117.46	122.20
50	C1	505	C	N1-C2-O2	6.76	122.96	118.90
50	C1	447	C	N3-C2-O2	-6.76	117.17	121.90
51	C2	267	C	C6-N1-C2	-6.74	117.60	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	C2	259	A	O4'-C1'-N9	6.72	113.58	108.20
51	C2	260	G	N3-C4-N9	6.71	130.03	126.00
50	C1	581	C	N3-C2-O2	-6.67	117.23	121.90
50	C1	112	C	N3-C2-O2	-6.67	117.23	121.90
50	C1	203	C	N1-C2-O2	6.67	122.90	118.90
50	C1	1666	C	C5-C6-N1	6.65	124.33	121.00
50	C1	769	C	C2-N1-C1'	6.65	126.11	118.80
50	C1	491	G	N3-C4-N9	6.62	129.97	126.00
50	C1	1486	G	N7-C8-N9	6.61	116.40	113.10
50	C1	1547	C	C5-C6-N1	6.61	124.30	121.00
50	C1	581	C	N1-C2-O2	6.60	122.86	118.90
9	UL	645	LEU	CA-CB-CG	6.60	130.49	115.30
50	C1	1486	G	C8-N9-C1'	-6.59	118.44	127.00
13	UQ	154	ASP	CB-CG-OD1	6.58	124.22	118.30
53	UT	854	LEU	CA-CB-CG	6.58	130.42	115.30
50	C1	281	U	P-O3'-C3'	6.57	127.59	119.70
1	UA	587	LEU	CA-CB-CG	6.56	130.39	115.30
50	C1	1625	G	N3-C4-C5	-6.55	125.33	128.60
50	C1	2179	C	N1-C2-O2	6.54	122.83	118.90
50	C1	1711	G	N3-C4-N9	6.53	129.92	126.00
50	C1	1486	G	N3-C4-N9	6.49	129.90	126.00
50	C1	661	U	C5-C6-N1	6.49	125.95	122.70
51	C2	260	G	N3-C4-C5	-6.49	125.35	128.60
50	C1	454	C	C5-C6-N1	6.49	124.24	121.00
50	C1	1471	U	C5-C4-O4	-6.49	122.01	125.90
50	C1	915	G	C8-N9-C1'	6.47	135.42	127.00
50	C1	776	C	C2-N1-C1'	6.47	125.91	118.80
50	C1	1666	C	C2-N1-C1'	6.47	125.91	118.80
50	C1	1448	A	C5-C6-N1	6.44	120.92	117.70
50	C1	984	A	C2-N3-C4	6.44	113.82	110.60
50	C1	277	U	P-O3'-C3'	6.42	127.41	119.70
1	UA	662	GLY	C-N-CA	6.42	137.75	121.70
50	C1	2074	C	N3-C2-O2	-6.42	117.41	121.90
50	C1	454	C	C6-N1-C2	-6.42	117.73	120.30
51	C2	202	C	N1-C2-O2	6.42	122.75	118.90
50	C1	491	G	C8-N9-C1'	-6.42	118.66	127.00
50	C1	1046	G	C5-C6-O6	6.40	132.44	128.60
50	C1	989	C	C5-C6-N1	6.40	124.20	121.00
53	UT	407	ILE	CG1-CB-CG2	-6.40	97.32	111.40
50	C1	683	C	N1-C2-O2	6.38	122.73	118.90
50	C1	1068	C	C6-N1-C2	-6.38	117.75	120.30
32	CR	370	GLN	CA-CB-CG	6.37	127.42	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	C1	68	U	C5-C6-N1	6.37	125.89	122.70
32	CS	370	GLN	CA-CB-CG	6.37	127.42	113.40
50	C1	692	U	C2-N1-C1'	6.36	125.33	117.70
53	UT	1811	ASP	CB-CG-OD1	6.36	124.03	118.30
50	C1	1547	C	C2-N1-C1'	6.36	125.79	118.80
51	C2	147	G	N3-C4-N9	6.35	129.81	126.00
50	C1	1747	A	C6-N1-C2	-6.35	114.79	118.60
50	C1	1745	C	C6-N1-C2	-6.34	117.76	120.30
50	C1	860	C	C2-N1-C1'	-6.33	111.84	118.80
50	C1	581	C	C2-N1-C1'	6.32	125.75	118.80
50	C1	1114	C	N3-C2-O2	-6.31	117.48	121.90
50	C1	68	U	C2-N1-C1'	6.31	125.27	117.70
50	C1	915	G	C6-C5-N7	6.31	134.18	130.40
51	C2	161	G	N3-C4-N9	6.30	129.78	126.00
50	C1	18	G	N3-C4-C5	-6.30	125.45	128.60
50	C1	1550	U	C6-N1-C1'	-6.30	112.38	121.20
50	C1	593	G	P-O3'-C3'	6.28	127.24	119.70
51	C2	246	G	C8-N9-C1'	-6.26	118.86	127.00
51	C2	161	G	C6-C5-N7	-6.25	126.65	130.40
50	C1	63	C	N1-C2-O2	6.25	122.65	118.90
50	C1	205	C	P-O3'-C3'	6.25	127.20	119.70
10	UM	39	LEU	CA-CB-CG	6.24	129.66	115.30
2	UB	644	LEU	CA-CB-CG	6.24	129.66	115.30
7	UJ	1760	LEU	CA-CB-CG	6.23	129.62	115.30
50	C1	758	U	N1-C2-O2	6.21	127.15	122.80
50	C1	1711	G	C8-N9-C1'	-6.20	118.94	127.00
50	C1	1167	C	C6-N1-C2	-6.20	117.82	120.30
50	C1	2156	A	P-O3'-C3'	6.20	127.14	119.70
50	C1	258	C	C5-C6-N1	6.20	124.10	121.00
50	C1	683	C	C6-N1-C2	-6.18	117.83	120.30
51	C2	23	A	P-O3'-C3'	6.18	127.12	119.70
50	C1	56	C	N1-C2-O2	6.17	122.61	118.90
50	C1	850	A	C6-N1-C2	-6.17	114.89	118.60
50	C1	470	C	C2-N1-C1'	6.17	125.59	118.80
50	C1	1222	C	C6-N1-C2	-6.17	117.83	120.30
50	C1	1711	G	N3-C4-C5	-6.16	125.52	128.60
12	UO	334	LEU	CA-CB-CG	6.15	129.44	115.30
50	C1	622	U	N1-C2-O2	6.15	127.10	122.80
29	CN	86	ASP	CB-CG-OD1	6.14	123.83	118.30
50	C1	1017	C	P-O3'-C3'	6.14	127.07	119.70
50	C1	425	C	C6-N1-C2	-6.14	117.84	120.30
50	C1	1486	G	C8-N9-C4	-6.14	103.95	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	C1	910	G	C5-C6-O6	6.13	132.28	128.60
9	UL	441	LEU	CA-CB-CG	6.10	129.34	115.30
51	C2	105	C	C5-C6-N1	6.10	124.05	121.00
50	C1	1638	G	P-O3'-C3'	6.09	127.01	119.70
50	C1	2194	A	C8-N9-C4	-6.09	103.36	105.80
50	C1	135	A	P-O3'-C3'	6.08	126.99	119.70
50	C1	2210	U	C5-C4-O4	6.07	129.54	125.90
50	C1	18	G	C4-N9-C1'	6.07	134.38	126.50
50	C1	1745	C	C2-N1-C1'	6.06	125.47	118.80
50	C1	183	C	C2-N1-C1'	6.06	125.47	118.80
50	C1	1549	U	N3-C4-O4	-6.06	115.16	119.40
50	C1	886	U	N3-C2-O2	-6.06	117.96	122.20
50	C1	1485	A	P-O3'-C3'	6.05	126.97	119.70
50	C1	2217	C	C6-N1-C1'	-6.05	113.54	120.80
50	C1	850	A	C5-C6-N1	6.05	120.72	117.70
50	C1	2078	C	N3-C2-O2	-6.05	117.67	121.90
50	C1	1712	C	P-O3'-C3'	6.04	126.95	119.70
50	C1	1234	C	C2-N1-C1'	6.04	125.44	118.80
17	UZ	66	LEU	CA-CB-CG	6.04	129.18	115.30
50	C1	369	U	N3-C2-O2	-6.03	117.98	122.20
19	CC	17	LEU	CA-CB-CG	6.02	129.16	115.30
50	C1	291	C	C6-N1-C2	-6.02	117.89	120.30
50	C1	1245	C	N1-C2-O2	6.02	122.51	118.90
50	C1	18	G	N3-C4-N9	6.02	129.61	126.00
50	C1	21	C	N3-C2-O2	-6.02	117.69	121.90
50	C1	1451	G	N9-C4-C5	-6.01	102.99	105.40
50	C1	1630	C	N3-C2-O2	-6.01	117.69	121.90
50	C1	909	G	N3-C4-N9	6.01	129.60	126.00
50	C1	684	U	P-O3'-C3'	5.99	126.89	119.70
50	C1	1661	C	C2-N3-C4	-5.98	116.91	119.90
50	C1	1658	G	C6-C5-N7	5.98	133.99	130.40
51	C2	161	G	C8-N9-C1'	-5.97	119.23	127.00
52	CW	75	TYR	CA-CB-CG	-5.96	102.08	113.40
50	C1	1448	A	C6-N1-C2	-5.96	115.03	118.60
51	C2	6	C	C5-C6-N1	5.95	123.97	121.00
51	C2	136	C	C5-C6-N1	5.95	123.97	121.00
51	C2	103	G	C2-N3-C4	5.94	114.87	111.90
50	C1	55	G	OP2-P-O3'	-5.93	92.16	105.20
50	C1	1639	U	C2-N1-C1'	5.92	124.81	117.70
32	CR	67	PHE	CB-CG-CD1	5.91	124.94	120.80
51	C2	6	C	N1-C2-O2	5.91	122.44	118.90
50	C1	636	C	C2-N1-C1'	5.90	125.29	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	C1	1666	C	C6-N1-C2	-5.90	117.94	120.30
51	C2	200	U	C6-N1-C1'	-5.90	112.94	121.20
50	C1	471	C	C6-N1-C2	-5.90	117.94	120.30
6	UG	174	LEU	CA-CB-CG	5.89	128.85	115.30
50	C1	927	C	N1-C2-O2	5.89	122.43	118.90
50	C1	1113	C	N3-C2-O2	-5.88	117.78	121.90
32	CS	67	PHE	CB-CG-CD1	5.88	124.92	120.80
50	C1	922	C	C6-N1-C2	-5.88	117.95	120.30
50	C1	1547	C	C6-N1-C2	-5.88	117.95	120.30
50	C1	1560	C	N1-C2-O2	5.88	122.42	118.90
50	C1	1458	U	C2-N1-C1'	5.87	124.75	117.70
50	C1	2210	U	N1-C2-O2	5.86	126.90	122.80
50	C1	802	A	P-O3'-C3'	5.86	126.73	119.70
50	C1	886	U	C2-N1-C1'	5.86	124.73	117.70
50	C1	398	C	N1-C2-O2	5.85	122.41	118.90
50	C1	776	C	N3-C2-O2	-5.85	117.81	121.90
50	C1	2179	C	C6-N1-C1'	-5.85	113.78	120.80
50	C1	308	U	C5-C6-N1	5.85	125.62	122.70
50	C1	1165	U	C2-N1-C1'	5.84	124.71	117.70
51	C2	260	G	C8-N9-C1'	-5.83	119.42	127.00
50	C1	1120	C	C6-N1-C2	-5.83	117.97	120.30
53	UT	535	LEU	CA-CB-CG	5.82	128.69	115.30
51	C2	244	G	C5-C6-O6	5.82	132.09	128.60
50	C1	371	U	N1-C2-O2	5.81	126.87	122.80
50	C1	722	U	N1-C2-O2	5.81	126.87	122.80
50	C1	1560	C	N3-C2-O2	-5.79	117.84	121.90
50	C1	2358	U	N3-C2-O2	-5.79	118.15	122.20
7	UJ	1562	LEU	CA-CB-CG	5.77	128.57	115.30
50	C1	942	U	N1-C2-O2	5.77	126.84	122.80
50	C1	2177	G	P-O3'-C3'	5.77	126.62	119.70
50	C1	2217	C	C6-N1-C2	-5.77	117.99	120.30
50	C1	158	C	C6-N1-C1'	-5.75	113.90	120.80
21	CF	103	LEU	CA-CB-CG	5.75	128.52	115.30
50	C1	1451	G	N3-C4-N9	5.75	129.45	126.00
50	C1	770	C	C2-N1-C1'	5.75	125.12	118.80
51	C2	139	C	C6-N1-C2	-5.75	118.00	120.30
50	C1	886	U	N1-C2-O2	5.74	126.82	122.80
50	C1	1252	G	N1-C6-O6	-5.74	116.46	119.90
50	C1	2203	C	N1-C2-O2	5.74	122.34	118.90
1	UA	258	LEU	CA-CB-CG	5.73	128.48	115.30
50	C1	2358	U	C2-N1-C1'	5.73	124.57	117.70
50	C1	88	C	P-O3'-C3'	5.73	126.57	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	C1	1001	A	P-O3'-C3'	5.72	126.57	119.70
50	C1	1511	A	C2-N3-C4	5.72	113.46	110.60
50	C1	183	C	C5-C6-N1	5.72	123.86	121.00
50	C1	2217	C	C5-C6-N1	5.72	123.86	121.00
50	C1	1458	U	N1-C2-O2	5.71	126.80	122.80
50	C1	1002	G	O5'-P-OP2	-5.71	100.56	105.70
50	C1	2165	U	C5-C6-N1	5.70	125.55	122.70
20	CD	189	TRP	CA-CB-CG	5.70	124.52	113.70
50	C1	1046	G	N1-C6-O6	-5.69	116.49	119.90
50	C1	134	C	N3-C2-O2	-5.69	117.92	121.90
50	C1	370	C	N1-C2-O2	5.68	122.31	118.90
15	UU	378	LEU	CA-CB-CG	5.68	128.37	115.30
50	C1	308	U	N1-C2-O2	5.68	126.78	122.80
50	C1	3	G	N3-C4-N9	-5.67	122.59	126.00
53	UT	1329	LEU	CA-CB-CG	5.67	128.35	115.30
15	UU	771	LEU	CA-CB-CG	5.67	128.34	115.30
50	C1	56	C	C5-C6-N1	5.67	123.83	121.00
13	UQ	747	LEU	C-N-CA	5.65	135.83	121.70
50	C1	661	U	C6-N1-C1'	-5.65	113.29	121.20
6	UG	151	LEU	CA-CB-CG	5.65	128.29	115.30
50	C1	770	C	C5-C6-N1	5.64	123.82	121.00
50	C1	206	C	C5-C6-N1	5.64	123.82	121.00
50	C1	1656	C	C6-N1-C2	-5.63	118.05	120.30
50	C1	727	G	N3-C4-N9	5.63	129.38	126.00
10	UM	689	LEU	CA-CB-CG	5.63	128.24	115.30
50	C1	787	U	N3-C2-O2	-5.62	118.26	122.20
50	C1	493	G	N3-C4-N9	5.62	129.37	126.00
51	C2	6	C	N3-C2-O2	-5.61	117.97	121.90
50	C1	203	C	C2-N1-C1'	5.61	124.97	118.80
50	C1	371	U	C2-N1-C1'	5.60	124.42	117.70
38	Ce	22	LEU	CA-CB-CG	5.59	128.16	115.30
50	C1	158	C	N3-C2-O2	-5.59	117.99	121.90
5	UF	177	LEU	CB-CG-CD2	-5.59	101.50	111.00
50	C1	750	C	N3-C2-O2	-5.59	117.99	121.90
50	C1	2202	C	C6-N1-C2	-5.59	118.07	120.30
50	C1	1246	C	N3-C2-O2	-5.58	117.99	121.90
50	C1	1639	U	N1-C2-O2	5.58	126.71	122.80
51	C2	105	C	C6-N1-C2	-5.58	118.07	120.30
50	C1	683	C	C6-N1-C1'	-5.58	114.11	120.80
50	C1	448	C	N3-C2-O2	-5.57	118.00	121.90
51	C2	246	G	N3-C4-C5	-5.57	125.81	128.60
50	C1	1085	U	P-O3'-C3'	5.56	126.38	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	C2	90	C	O4'-C1'-N1	5.56	112.65	108.20
50	C1	1165	U	N1-C2-O2	5.55	126.69	122.80
51	C2	251	U	N3-C2-O2	-5.55	118.32	122.20
53	UT	490	LEU	CA-CB-CG	5.54	128.04	115.30
51	C2	152	C	C6-N1-C2	-5.54	118.08	120.30
7	UJ	1739	LEU	CA-CB-CG	5.54	128.03	115.30
50	C1	673	C	C6-N1-C2	-5.54	118.09	120.30
50	C1	26	C	N3-C2-O2	-5.53	118.03	121.90
32	CR	193	LEU	CA-CB-CG	5.53	128.01	115.30
51	C2	246	G	N3-C4-N9	5.53	129.31	126.00
50	C1	2	G	N3-C4-N9	5.52	129.31	126.00
32	CS	193	LEU	CA-CB-CG	5.51	127.98	115.30
50	C1	1165	U	N3-C2-O2	-5.51	118.34	122.20
32	CR	849	LEU	CA-CB-CG	5.51	127.97	115.30
50	C1	781	G	O4'-C1'-N9	5.51	112.61	108.20
50	C1	491	G	N3-C4-C5	-5.50	125.85	128.60
32	CS	849	LEU	CA-CB-CG	5.50	127.95	115.30
50	C1	2179	C	N3-C2-O2	-5.49	118.06	121.90
50	C1	60	A	C2-N3-C4	5.49	113.34	110.60
50	C1	369	U	C2-N1-C1'	5.48	124.28	117.70
6	UG	100	LEU	CA-CB-CG	5.48	127.90	115.30
50	C1	989	C	N1-C2-O2	5.48	122.19	118.90
50	C1	281	U	OP1-P-O3'	5.47	117.24	105.20
50	C1	308	U	C2-N1-C1'	5.47	124.26	117.70
13	UQ	617	LEU	CA-CB-CG	5.46	127.86	115.30
50	C1	343	C	C6-N1-C2	-5.46	118.12	120.30
51	C2	77	C	C5-C6-N1	5.45	123.73	121.00
9	UL	869	LEU	CA-CB-CG	5.45	127.84	115.30
50	C1	986	C	N1-C2-O2	5.44	122.17	118.90
24	CI	845	LEU	CA-CB-CG	5.44	127.81	115.30
50	C1	995	C	C2-N1-C1'	5.44	124.78	118.80
51	C2	200	U	C5-C6-N1	5.44	125.42	122.70
50	C1	371	U	N3-C2-O2	-5.43	118.40	122.20
50	C1	145	C	N1-C2-O2	5.43	122.16	118.90
50	C1	1549	U	C2-N3-C4	-5.43	123.74	127.00
50	C1	1027	C	C6-N1-C2	-5.42	118.13	120.30
50	C1	1222	C	C6-N1-C1'	-5.42	114.29	120.80
50	C1	915	G	C4-C5-N7	-5.42	108.63	110.80
50	C1	1626	G	C6-N1-C2	-5.42	121.85	125.10
50	C1	470	C	N3-C2-O2	-5.41	118.11	121.90
50	C1	1068	C	C5-C6-N1	5.41	123.70	121.00
50	C1	1625	G	N3-C2-N2	5.41	123.69	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	C1	2074	C	C6-N1-C1'	-5.41	114.31	120.80
50	C1	915	G	C4-N9-C1'	-5.41	119.47	126.50
50	C1	485	G	N3-C4-N9	-5.40	122.76	126.00
50	C1	676	C	N3-C2-O2	-5.40	118.12	121.90
50	C1	768	C	C6-N1-C1'	-5.40	114.32	120.80
50	C1	203	C	N3-C2-O2	-5.39	118.12	121.90
50	C1	661	U	C6-N1-C2	-5.39	117.76	121.00
50	C1	722	U	N3-C2-O2	-5.39	118.43	122.20
50	C1	2194	A	N7-C8-N9	5.38	116.49	113.80
53	UT	1620	LEU	CA-CB-CG	5.38	127.68	115.30
32	CR	67	PHE	CB-CG-CD2	-5.38	117.03	120.80
50	C1	582	G	P-O3'-C3'	5.38	126.15	119.70
51	C2	165	C	N1-C2-O2	5.38	122.13	118.90
50	C1	1643	U	C2-N1-C1'	5.38	124.15	117.70
50	C1	1758	C	C6-N1-C1'	5.37	127.25	120.80
50	C1	294	G	N3-C4-N9	-5.37	122.78	126.00
35	Cb	102	ILE	CG1-CB-CG2	-5.37	99.59	111.40
56	US	347	LEU	CA-CB-CG	5.36	127.64	115.30
58	CX	296	LEU	CA-CB-CG	5.36	127.63	115.30
32	CS	901	LEU	CA-CB-CG	5.34	127.59	115.30
50	C1	758	U	C2-N3-C4	-5.34	123.79	127.00
50	C1	1050	U	N3-C2-O2	-5.34	118.46	122.20
50	C1	2219	C	P-O3'-C3'	5.33	126.10	119.70
50	C1	454	C	N1-C2-O2	5.33	122.10	118.90
32	CR	901	LEU	CA-CB-CG	5.33	127.55	115.30
51	C2	202	C	C6-N1-C2	-5.33	118.17	120.30
51	C2	103	G	C4-N9-C1'	5.33	133.42	126.50
50	C1	1120	C	N1-C2-O2	5.32	122.09	118.90
32	CS	67	PHE	CB-CG-CD2	-5.32	117.08	120.80
48	Cp	55	LEU	CB-CG-CD2	-5.32	101.97	111.00
50	C1	683	C	C5-C6-N1	5.32	123.66	121.00
50	C1	1256	G	N3-C4-C5	-5.31	125.94	128.60
50	C1	18	G	C2-N3-C4	5.31	114.56	111.90
50	C1	2177	G	OP2-P-O3'	5.31	116.89	105.20
50	C1	2091	C	C2-N1-C1'	5.31	124.64	118.80
51	C2	136	C	N3-C2-O2	-5.30	118.19	121.90
50	C1	1241	U	N3-C2-O2	-5.30	118.49	122.20
50	C1	1547	C	N3-C4-N4	5.30	121.71	118.00
32	CR	135	ILE	CG1-CB-CG2	-5.29	99.75	111.40
50	C1	2168	U	C2-N1-C1'	5.29	124.05	117.70
51	C2	136	C	C6-N1-C2	-5.29	118.18	120.30
32	CS	617	LEU	CA-CB-CG	5.28	127.45	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	C1	851	U	N1-C2-O2	5.28	126.50	122.80
50	C1	1761	C	C5-C6-N1	5.28	123.64	121.00
32	CR	617	LEU	CA-CB-CG	5.28	127.45	115.30
32	CS	135	ILE	CG1-CB-CG2	-5.27	99.81	111.40
50	C1	1458	U	N3-C2-O2	-5.26	118.52	122.20
50	C1	1451	G	C4-C5-N7	5.26	112.90	110.80
50	C1	63	C	C2-N1-C1'	5.25	124.58	118.80
50	C1	150	C	P-O3'-C3'	5.25	126.00	119.70
50	C1	645	U	N3-C2-O2	-5.25	118.52	122.20
50	C1	1001	A	OP2-P-O3'	5.25	116.75	105.20
50	C1	281	U	N1-C2-O2	5.25	126.47	122.80
50	C1	768	C	N1-C2-O2	5.25	122.05	118.90
50	C1	879	A	C6-N1-C2	-5.25	115.45	118.60
50	C1	1734	G	P-O3'-C3'	5.25	126.00	119.70
51	C2	79	G	N3-C4-N9	5.25	129.15	126.00
38	Ce	38	ALA	C-N-CA	5.24	134.81	121.70
51	C2	202	C	C5-C6-N1	5.24	123.62	121.00
50	C1	1625	G	C6-C5-N7	-5.24	127.26	130.40
50	C1	1167	C	N1-C2-O2	5.24	122.04	118.90
50	C1	1511	A	C5-C6-N1	5.24	120.32	117.70
50	C1	1630	C	C6-N1-C1'	5.23	127.08	120.80
50	C1	867	C	N1-C2-O2	5.23	122.04	118.90
50	C1	2358	U	N1-C2-O2	5.23	126.46	122.80
50	C1	1625	G	C4-N9-C1'	5.23	133.29	126.50
50	C1	1045	G	N3-C4-C5	-5.21	125.99	128.60
50	C1	1451	G	C8-N9-C1'	-5.21	120.22	127.00
50	C1	1658	G	C8-N9-C1'	5.21	133.77	127.00
50	C1	1471	U	N3-C4-O4	5.20	123.04	119.40
2	UB	818	ASP	CB-CG-OD2	5.19	122.97	118.30
14	UR	398	LEU	CA-CB-CG	5.19	127.23	115.30
50	C1	2	G	N3-C4-C5	-5.18	126.01	128.60
50	C1	2172	C	C6-N1-C2	-5.18	118.23	120.30
51	C2	147	G	N9-C4-C5	-5.18	103.33	105.40
50	C1	2174	C	C5-C6-N1	5.18	123.59	121.00
7	UJ	796	LEU	CA-CB-CG	5.18	127.21	115.30
50	C1	684	U	N3-C2-O2	-5.17	118.58	122.20
50	C1	1222	C	C5-C6-N1	5.16	123.58	121.00
50	C1	2202	C	C2-N1-C1'	5.16	124.48	118.80
50	C1	111	U	N3-C2-O2	-5.16	118.59	122.20
50	C1	203	C	C6-N1-C2	-5.16	118.24	120.30
50	C1	1511	A	N3-C4-N9	5.15	131.52	127.40
50	C1	2168	U	C5-C6-N1	5.15	125.28	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	C1	80	C	C6-N1-C2	-5.15	118.24	120.30
50	C1	1068	C	P-O3'-C3'	5.15	125.88	119.70
50	C1	1124	G	C4-N9-C1'	5.15	133.19	126.50
50	C1	2227	C	C5-C6-N1	5.15	123.57	121.00
50	C1	447	C	C6-N1-C2	-5.14	118.24	120.30
50	C1	1114	C	C6-N1-C2	-5.14	118.24	120.30
50	C1	2203	C	N3-C2-O2	-5.14	118.30	121.90
50	C1	43	C	C2-N1-C1'	5.14	124.45	118.80
50	C1	1560	C	C6-N1-C2	-5.14	118.24	120.30
1	UA	695	LEU	CA-CB-CG	5.14	127.12	115.30
50	C1	63	C	N3-C2-O2	-5.13	118.31	121.90
50	C1	1246	C	C6-N1-C1'	5.13	126.96	120.80
53	UT	507	ASP	CB-CG-OD1	5.13	122.92	118.30
50	C1	435	A	C6-N1-C2	5.13	121.68	118.60
8	UK	96	LEU	CA-CB-CG	5.13	127.09	115.30
50	C1	154	C	N1-C2-O2	5.13	121.98	118.90
50	C1	1646	U	O4'-C1'-N1	5.13	112.30	108.20
20	CD	102	LEU	CA-CB-CG	5.12	127.08	115.30
50	C1	160	C	C5-C6-N1	5.12	123.56	121.00
50	C1	582	G	OP1-P-O3'	5.12	116.47	105.20
50	C1	770	C	N1-C2-O2	5.12	121.97	118.90
50	C1	1149	C	N3-C2-O2	-5.12	118.32	121.90
50	C1	1045	G	N3-C4-N9	5.12	129.07	126.00
50	C1	1075	C	N3-C2-O2	-5.12	118.32	121.90
50	C1	1256	G	C4-N9-C1'	5.12	133.15	126.50
50	C1	1656	C	C5-C6-N1	5.12	123.56	121.00
51	C2	166	G	N3-C4-C5	-5.11	126.04	128.60
50	C1	846	U	N1-C2-O2	5.11	126.38	122.80
51	C2	161	G	N7-C8-N9	5.11	115.66	113.10
50	C1	910	G	N3-C4-N9	-5.11	122.94	126.00
50	C1	1245	C	N3-C2-O2	-5.10	118.33	121.90
50	C1	1171	C	N3-C2-O2	-5.10	118.33	121.90
50	C1	2084	C	C6-N1-C1'	5.09	126.91	120.80
50	C1	1094	G	C6-C5-N7	-5.08	127.35	130.40
21	CE	110	ASP	CB-CG-OD1	5.08	122.87	118.30
51	C2	260	G	C2-N3-C4	5.07	114.44	111.90
51	C2	131	U	N3-C2-O2	-5.06	118.66	122.20
50	C1	236	C	C6-N1-C2	-5.06	118.28	120.30
4	UD	561	LEU	CA-CB-CG	5.06	126.93	115.30
50	C1	233	C	C6-N1-C2	-5.06	118.28	120.30
50	C1	2044	C	C6-N1-C2	-5.06	118.28	120.30
4	UD	357	LEU	CB-CG-CD2	-5.05	102.41	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	C2	246	G	OP1-P-O3'	5.05	116.31	105.20
50	C1	179	G	N3-C2-N2	5.05	123.43	119.90
50	C1	129	G	N1-C6-O6	-5.04	116.87	119.90
50	C1	860	C	C6-N1-C1'	5.04	126.85	120.80
50	C1	112	C	C2-N1-C1'	5.04	124.34	118.80
50	C1	769	C	C6-N1-C2	-5.04	118.28	120.30
50	C1	2044	C	C2-N1-C1'	5.04	124.34	118.80
50	C1	370	C	C2-N1-C1'	5.04	124.34	118.80
50	C1	1451	G	C6-C5-N7	-5.04	127.38	130.40
23	CH	120	LEU	CA-CB-CG	5.04	126.88	115.30
50	C1	750	C	C2-N1-C1'	5.03	124.34	118.80
51	C2	92	A	C2-N3-C4	5.03	113.12	110.60
50	C1	2084	C	N1-C2-N3	5.03	122.72	119.20
50	C1	684	U	N1-C2-O2	5.03	126.32	122.80
50	C1	1662	C	C6-N1-C2	-5.03	118.29	120.30
51	C2	202	C	N3-C2-O2	-5.02	118.39	121.90
50	C1	348	U	C5-C6-N1	5.01	125.21	122.70
50	C1	2079	U	N1-C2-O2	5.01	126.31	122.80
20	CD	143	LEU	CA-CB-CG	5.01	126.82	115.30
50	C1	674	U	N3-C2-O2	-5.00	118.70	122.20
38	Ce	40	LEU	CA-CB-CG	5.00	126.81	115.30
13	UQ	472	PRO	C-N-CA	5.00	134.20	121.70

There are no chirality outliers.

All (59) 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

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Mol	Chain	Res	Type	Group
32	CS	306	GLY	Peptide
32	CS	432	LEU	Peptide
52	CW	342	SER	Peptide
52	CW	73	GLY	Peptide
59	CY	377	ARG	Sidechain
35	Cb	231	GLU	Peptide
36	Cc	86	MET	Peptide
37	Cd	132	ARG	Sidechain
38	Ce	38	ALA	Peptide
57	Cl	79	TYR	Peptide
1	UA	115	LEU	Peptide
4	UD	387	TRP	Peptide
55	UE	232	GLN	Peptide
7	UJ	1661	ASP	Peptide
7	UJ	1662	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
56	US	510	LYS	Peptide
53	UT	1516	LEU	Peptide
53	UT	1566	GLU	Peptide
53	UT	1724	PRO	Peptide
53	UT	408	PRO	Peptide
53	UT	420	GLU	Peptide
53	UT	481	ALA	Peptide
53	UT	485	LYS	Peptide
53	UT	486	GLU	Peptide
53	UT	487	ILE	Peptide
53	UT	781	TRP	Peptide
15	UU	397	ASP	Peptide
15	UU	644	GLY	Peptide
15	UU	857	ILE	Peptide
17	UZ	103	ASP	Peptide

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Mol	Chain	Res	Type	Group
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	75
6	UG	475/558 (85%)	441 (93%)	32 (7%)	2 (0%)	34	72
7	UJ	1062/1802 (59%)	1010 (95%)	52 (5%)	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	84
11	UN	171/938 (18%)	167 (98%)	3 (2%)	1 (1%)	25	64
12	UO	498/557 (89%)	474 (95%)	24 (5%)	0	100	100
13	UQ	775/960 (81%)	712 (92%)	61 (8%)	2 (0%)	41	75
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%)	212 (93%)	16 (7%)	1 (0%)	34	72

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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	58
22	CG	402/630 (64%)	375 (93%)	27 (7%)	0	100	100
23	CH	383/411 (93%)	344 (90%)	38 (10%)	1 (0%)	41	75
24	CI	812/1163 (70%)	761 (94%)	49 (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	56
30	CP	227/322 (70%)	221 (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	68
32	CS	746/1073 (70%)	682 (91%)	60 (8%)	4 (0%)	29	68
33	CT	127/203 (63%)	119 (94%)	8 (6%)	0	100	100
34	Ca	223/255 (88%)	211 (95%)	12 (5%)	0	100	100
35	Cb	230/264 (87%)	204 (89%)	26 (11%)	0	100	100
36	Cc	188/212 (89%)	179 (95%)	9 (5%)	0	100	100
37	Cd	224/239 (94%)	211 (94%)	13 (6%)	0	100	100
38	Ce	155/203 (76%)	140 (90%)	15 (10%)	0	100	100
39	Cf	170/202 (84%)	164 (96%)	6 (4%)	0	100	100
40	Cg	157/190 (83%)	152 (97%)	5 (3%)	0	100	100
41	Ch	64/151 (42%)	61 (95%)	3 (5%)	0	100	100
42	Ci	113/150 (75%)	106 (94%)	7 (6%)	0	100	100
43	Cj	124/143 (87%)	116 (94%)	8 (6%)	0	100	100
44	Ck	136/161 (84%)	129 (95%)	7 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	Cm	122/130 (94%)	117 (96%)	5 (4%)	0	100	100
46	Cn	92/145 (63%)	89 (97%)	3 (3%)	0	100	100
47	Co	90/136 (66%)	82 (91%)	8 (9%)	0	100	100
48	Cp	59/68 (87%)	55 (93%)	4 (7%)	0	100	100
49	CU	168/311 (54%)	156 (93%)	12 (7%)	0	100	100
52	CW	380/668 (57%)	349 (92%)	31 (8%)	0	100	100
53	UT	1987/2612 (76%)	1871 (94%)	110 (6%)	6 (0%)	41	75
54	UH	349/930 (38%)	340 (97%)	9 (3%)	0	100	100
55	UE	121/410 (30%)	117 (97%)	4 (3%)	0	100	100
55	UI	121/410 (30%)	121 (100%)	0	0	100	100
56	US	443/549 (81%)	415 (94%)	28 (6%)	0	100	100
57	Cl	78/156 (50%)	73 (94%)	5 (6%)	0	100	100
58	CX	265/480 (55%)	255 (96%)	10 (4%)	0	100	100
59	CY	119/381 (31%)	109 (92%)	10 (8%)	0	100	100
60	CZ	42/609 (7%)	34 (81%)	8 (19%)	0	100	100
61	UP	52/364 (14%)	46 (88%)	5 (10%)	1 (2%)	8	40
All	All	21864/32830 (67%)	20513 (94%)	1321 (6%)	30 (0%)	54	84

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
29	CO	85	SER
53	UT	487	ILE
6	UG	580	GLU
13	UQ	708	SER
17	UZ	293	ILE
53	UT	1566	GLU
53	UT	1567	PHE
6	UG	56	PRO
32	CR	48	MET
32	CS	48	MET
53	UT	457	TRP
11	UN	902	ARG
27	CL	640	PRO
53	UT	407	ILE
53	UT	408	PRO

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Mol	Chain	Res	Type
5	UF	121	LYS
10	UM	329	PRO
13	UQ	564	GLU
24	CI	309	PRO
61	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)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	UA	651/775 (84%)	648 (100%)	3 (0%)	88	94
2	UB	425/788 (54%)	423 (100%)	2 (0%)	88	94
3	UC	61/536 (11%)	61 (100%)	0	100	100
4	UD	653/738 (88%)	652 (100%)	1 (0%)	93	98
5	UF	248/341 (73%)	248 (100%)	0	100	100
6	UG	373/474 (79%)	370 (99%)	3 (1%)	81	91
7	UJ	898/1526 (59%)	893 (99%)	5 (1%)	86	94
8	UK	159/227 (70%)	159 (100%)	0	100	100
9	UL	667/821 (81%)	666 (100%)	1 (0%)	93	98
10	UM	606/770 (79%)	602 (99%)	4 (1%)	84	93
11	UN	146/765 (19%)	146 (100%)	0	100	100
12	UO	404/456 (89%)	402 (100%)	2 (0%)	88	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	UQ	650/817 (80%)	649 (100%)	1 (0%)	93	98
14	UR	360/524 (69%)	359 (100%)	1 (0%)	92	97
15	UU	672/863 (78%)	669 (100%)	3 (0%)	91	96
16	UX	150/167 (90%)	150 (100%)	0	100	100
17	UZ	187/329 (57%)	183 (98%)	4 (2%)	53	79
18	CA	175/228 (77%)	173 (99%)	2 (1%)	73	88
18	CB	195/228 (86%)	194 (100%)	1 (0%)	88	94
19	CC	287/435 (66%)	287 (100%)	0	100	100
20	CD	319/489 (65%)	319 (100%)	0	100	100
21	CE	91/108 (84%)	91 (100%)	0	100	100
21	CF	88/108 (82%)	87 (99%)	1 (1%)	73	88
22	CG	331/525 (63%)	330 (100%)	1 (0%)	92	97
23	CH	303/320 (95%)	301 (99%)	2 (1%)	84	93
24	CI	661/1009 (66%)	656 (99%)	5 (1%)	81	91
25	CJ	147/169 (87%)	147 (100%)	0	100	100
26	CK	245/266 (92%)	239 (98%)	6 (2%)	49	76
27	CL	181/642 (28%)	181 (100%)	0	100	100
28	CM	364/383 (95%)	362 (100%)	2 (0%)	88	94
29	CN	202/223 (91%)	202 (100%)	0	100	100
29	CO	193/223 (86%)	191 (99%)	2 (1%)	76	88
30	CP	202/287 (70%)	202 (100%)	0	100	100
31	CQ	145/215 (67%)	144 (99%)	1 (1%)	84	93
32	CR	654/916 (71%)	449 (69%)	205 (31%)	0	2
32	CS	654/916 (71%)	449 (69%)	205 (31%)	0	2
33	CT	108/167 (65%)	108 (100%)	0	100	100
34	Ca	198/223 (89%)	198 (100%)	0	100	100
35	Cb	199/221 (90%)	199 (100%)	0	100	100
36	Cc	149/178 (84%)	147 (99%)	2 (1%)	69	86
37	Cd	192/204 (94%)	191 (100%)	1 (0%)	88	94
38	Ce	137/177 (77%)	137 (100%)	0	100	100
39	Cf	139/164 (85%)	139 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	Cg	122/162 (75%)	120 (98%)	2 (2%)	62	83
41	Ch	58/130 (45%)	58 (100%)	0	100	100
42	Ci	78/117 (67%)	78 (100%)	0	100	100
43	Cj	92/115 (80%)	92 (100%)	0	100	100
44	Ck	126/143 (88%)	126 (100%)	0	100	100
45	Cm	103/113 (91%)	103 (100%)	0	100	100
46	Cn	70/116 (60%)	70 (100%)	0	100	100
47	Co	79/115 (69%)	79 (100%)	0	100	100
48	Cp	46/61 (75%)	46 (100%)	0	100	100
49	CU	137/260 (53%)	135 (98%)	2 (2%)	65	84
52	CW	309/587 (53%)	306 (99%)	3 (1%)	76	88
53	UT	1732/2276 (76%)	1719 (99%)	13 (1%)	81	91
54	UH	301/788 (38%)	297 (99%)	4 (1%)	69	86
55	UE	105/346 (30%)	105 (100%)	0	100	100
55	UI	105/346 (30%)	105 (100%)	0	100	100
56	US	404/493 (82%)	403 (100%)	1 (0%)	93	98
57	Cl	71/135 (53%)	70 (99%)	1 (1%)	67	85
58	CX	227/411 (55%)	227 (100%)	0	100	100
59	CY	100/322 (31%)	92 (92%)	8 (8%)	12	41
60	CZ	38/519 (7%)	37 (97%)	1 (3%)	46	74
61	UP	44/314 (14%)	44 (100%)	0	100	100
All	All	18216/27810 (66%)	17715 (97%)	501 (3%)	46	72

All (501) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	UA	87	ARG
1	UA	558	ARG
1	UA	559	ARG
2	UB	786	ARG
2	UB	829	ARG
4	UD	180	THR
6	UG	41	ARG
6	UG	135	THR
6	UG	181	ARG

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Mol	Chain	Res	Type
7	UJ	306	ARG
7	UJ	1509	LYS
7	UJ	1517	LYS
7	UJ	1550	LEU
7	UJ	1698	VAL
9	UL	51	ASP
10	UM	35	LEU
10	UM	450	SER
10	UM	780	THR
10	UM	889	ARG
12	UO	150	THR
12	UO	534	VAL
13	UQ	378	VAL
14	UR	397	MET
15	UU	638	VAL
15	UU	665	MET
15	UU	671	CYS
17	UZ	175	THR
17	UZ	280	ASN
17	UZ	293	ILE
17	UZ	295	GLN
18	CA	292	LEU
18	CA	304	CYS
18	CB	125	THR
21	CF	67	HIS
22	CG	263	THR
23	CH	85	THR
23	CH	210	ARG
24	CI	91	ARG
24	CI	827	LEU
24	CI	840	ARG
24	CI	886	CYS
24	CI	1081	VAL
26	CK	91	THR
26	CK	146	ARG
26	CK	148	THR
26	CK	163	LEU
26	CK	218	THR
26	CK	262	THR
28	CM	287	MET
28	CM	305	ARG
29	CO	79	LYS

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Mol	Chain	Res	Type
29	CO	209	MET
31	CQ	254	ARG
32	CR	4	GLN
32	CR	5	LYS
32	CR	6	THR
32	CR	9	SER
32	CR	10	ARG
32	CR	19	LEU
32	CR	22	LYS
32	CR	23	LYS
32	CR	25	SER
32	CR	36	GLU
32	CR	45	MET
32	CR	46	SER
32	CR	48	MET
32	CR	55	SER
32	CR	56	VAL
32	CR	61	LYS
32	CR	62	LYS
32	CR	63	GLU
32	CR	67	PHE
32	CR	68	THR
32	CR	75	GLU
32	CR	77	LYS
32	CR	78	ILE
32	CR	80	LYS
32	CR	83	LYS
32	CR	99	ILE
32	CR	100	SER
32	CR	103	ASP
32	CR	104	ILE
32	CR	105	ARG
32	CR	110	LYS
32	CR	114	LYS
32	CR	115	ILE
32	CR	119	THR
32	CR	122	MET
32	CR	124	ILE
32	CR	125	LEU
32	CR	126	GLN
32	CR	127	ASP
32	CR	129	GLU

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Mol	Chain	Res	Type
32	CR	131	ILE
32	CR	135	ILE
32	CR	136	LEU
32	CR	142	THR
32	CR	144	GLU
32	CR	151	LEU
32	CR	154	LYS
32	CR	157	THR
32	CR	164	THR
32	CR	165	MET
32	CR	167	MET
32	CR	182	ILE
32	CR	191	LEU
32	CR	197	GLU
32	CR	201	VAL
32	CR	202	ILE
32	CR	217	VAL
32	CR	253	ILE
32	CR	260	ASP
32	CR	261	GLN
32	CR	263	LYS
32	CR	265	LEU
32	CR	266	LEU
32	CR	274	GLU
32	CR	275	LYS
32	CR	276	THR
32	CR	278	ARG
32	CR	280	THR
32	CR	283	LEU
32	CR	287	ARG
32	CR	292	SER
32	CR	297	VAL
32	CR	299	ILE
32	CR	308	SER
32	CR	313	THR
32	CR	314	SER
32	CR	318	GLU
32	CR	322	THR
32	CR	323	LEU
32	CR	325	GLU
32	CR	370	GLN
32	CR	380	LEU

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Mol	Chain	Res	Type
32	CR	388	ILE
32	CR	401	LYS
32	CR	402	LEU
32	CR	410	MET
32	CR	412	SER
32	CR	415	SER
32	CR	418	GLU
32	CR	423	SER
32	CR	426	LEU
32	CR	428	LEU
32	CR	430	LYS
32	CR	432	LEU
32	CR	433	ARG
32	CR	434	GLU
32	CR	470	LYS
32	CR	471	GLU
32	CR	475	SER
32	CR	482	GLN
32	CR	488	LYS
32	CR	491	ASN
32	CR	494	LEU
32	CR	497	ASP
32	CR	512	ASP
32	CR	515	GLN
32	CR	517	GLU
32	CR	519	LEU
32	CR	521	VAL
32	CR	526	LEU
32	CR	528	SER
32	CR	533	SER
32	CR	534	GLU
32	CR	535	LYS
32	CR	537	LEU
32	CR	547	SER
32	CR	548	HIS
32	CR	550	LYS
32	CR	558	LEU
32	CR	560	SER
32	CR	566	GLU
32	CR	569	VAL
32	CR	578	ARG
32	CR	581	GLU

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Mol	Chain	Res	Type
32	CR	583	LEU
32	CR	587	GLN
32	CR	588	VAL
32	CR	589	SER
32	CR	593	LYS
32	CR	595	SER
32	CR	614	ILE
32	CR	617	LEU
32	CR	618	VAL
32	CR	624	ASP
32	CR	631	SER
32	CR	635	ILE
32	CR	638	ILE
32	CR	645	MET
32	CR	651	SER
32	CR	652	LYS
32	CR	657	LEU
32	CR	659	ASP
32	CR	710	SER
32	CR	713	SER
32	CR	714	GLU
32	CR	715	ARG
32	CR	716	ARG
32	CR	720	LEU
32	CR	726	SER
32	CR	735	LYS
32	CR	738	LYS
32	CR	745	VAL
32	CR	748	ARG
32	CR	752	ASN
32	CR	753	ASP
32	CR	755	THR
32	CR	759	THR
32	CR	761	VAL
32	CR	763	ILE
32	CR	766	LEU
32	CR	773	SER
32	CR	781	ASP
32	CR	787	LEU
32	CR	799	SER
32	CR	803	LEU
32	CR	806	GLU

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Mol	Chain	Res	Type
32	CR	807	GLU
32	CR	814	MET
32	CR	816	ASP
32	CR	818	SER
32	CR	819	ASN
32	CR	828	GLU
32	CR	830	ASP
32	CR	831	GLN
32	CR	834	THR
32	CR	837	ASP
32	CR	839	LYS
32	CR	841	LEU
32	CR	842	GLU
32	CR	843	SER
32	CR	848	LEU
32	CR	850	ASP
32	CR	853	VAL
32	CR	854	VAL
32	CR	855	LEU
32	CR	856	ASP
32	CR	861	ILE
32	CR	863	GLN
32	CR	867	THR
32	CR	870	LEU
32	CR	871	ARG
32	CR	875	LYS
32	CR	879	LEU
32	CR	892	LYS
32	CR	895	ASP
32	CR	896	THR
32	CR	897	LEU
32	CR	902	ASN
32	CR	906	SER
32	CR	908	VAL
32	CR	913	MET
32	CR	916	MET
32	CR	917	ARG
32	CR	918	LYS
32	CR	921	GLN
32	CS	4	GLN
32	CS	5	LYS
32	CS	6	THR

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Mol	Chain	Res	Type
32	CS	9	SER
32	CS	10	ARG
32	CS	19	LEU
32	CS	22	LYS
32	CS	23	LYS
32	CS	25	SER
32	CS	36	GLU
32	CS	45	MET
32	CS	46	SER
32	CS	48	MET
32	CS	55	SER
32	CS	56	VAL
32	CS	61	LYS
32	CS	62	LYS
32	CS	63	GLU
32	CS	67	PHE
32	CS	68	THR
32	CS	75	GLU
32	CS	77	LYS
32	CS	78	ILE
32	CS	80	LYS
32	CS	83	LYS
32	CS	99	ILE
32	CS	100	SER
32	CS	103	ASP
32	CS	104	ILE
32	CS	105	ARG
32	CS	110	LYS
32	CS	114	LYS
32	CS	115	ILE
32	CS	119	THR
32	CS	122	MET
32	CS	124	ILE
32	CS	125	LEU
32	CS	126	GLN
32	CS	127	ASP
32	CS	129	GLU
32	CS	131	ILE
32	CS	135	ILE
32	CS	136	LEU
32	CS	142	THR
32	CS	144	GLU

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Mol	Chain	Res	Type
32	CS	151	LEU
32	CS	154	LYS
32	CS	157	THR
32	CS	164	THR
32	CS	165	MET
32	CS	167	MET
32	CS	182	ILE
32	CS	191	LEU
32	CS	197	GLU
32	CS	201	VAL
32	CS	202	ILE
32	CS	217	VAL
32	CS	253	ILE
32	CS	260	ASP
32	CS	261	GLN
32	CS	263	LYS
32	CS	265	LEU
32	CS	266	LEU
32	CS	274	GLU
32	CS	275	LYS
32	CS	276	THR
32	CS	278	ARG
32	CS	280	THR
32	CS	283	LEU
32	CS	287	ARG
32	CS	292	SER
32	CS	297	VAL
32	CS	299	ILE
32	CS	308	SER
32	CS	313	THR
32	CS	314	SER
32	CS	318	GLU
32	CS	322	THR
32	CS	323	LEU
32	CS	325	GLU
32	CS	370	GLN
32	CS	380	LEU
32	CS	388	ILE
32	CS	401	LYS
32	CS	402	LEU
32	CS	410	MET
32	CS	412	SER

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Mol	Chain	Res	Type
32	CS	415	SER
32	CS	418	GLU
32	CS	423	SER
32	CS	426	LEU
32	CS	428	LEU
32	CS	430	LYS
32	CS	432	LEU
32	CS	433	ARG
32	CS	434	GLU
32	CS	470	LYS
32	CS	471	GLU
32	CS	475	SER
32	CS	482	GLN
32	CS	488	LYS
32	CS	491	ASN
32	CS	494	LEU
32	CS	497	ASP
32	CS	512	ASP
32	CS	515	GLN
32	CS	517	GLU
32	CS	519	LEU
32	CS	521	VAL
32	CS	526	LEU
32	CS	528	SER
32	CS	533	SER
32	CS	534	GLU
32	CS	535	LYS
32	CS	537	LEU
32	CS	547	SER
32	CS	548	HIS
32	CS	550	LYS
32	CS	558	LEU
32	CS	560	SER
32	CS	566	GLU
32	CS	569	VAL
32	CS	578	ARG
32	CS	581	GLU
32	CS	583	LEU
32	CS	587	GLN
32	CS	588	VAL
32	CS	589	SER
32	CS	593	LYS

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Mol	Chain	Res	Type
32	CS	595	SER
32	CS	614	ILE
32	CS	617	LEU
32	CS	618	VAL
32	CS	624	ASP
32	CS	631	SER
32	CS	635	ILE
32	CS	638	ILE
32	CS	645	MET
32	CS	651	SER
32	CS	652	LYS
32	CS	657	LEU
32	CS	659	ASP
32	CS	710	SER
32	CS	713	SER
32	CS	714	GLU
32	CS	715	ARG
32	CS	716	ARG
32	CS	720	LEU
32	CS	726	SER
32	CS	735	LYS
32	CS	738	LYS
32	CS	745	VAL
32	CS	748	ARG
32	CS	752	ASN
32	CS	753	ASP
32	CS	755	THR
32	CS	759	THR
32	CS	761	VAL
32	CS	763	ILE
32	CS	766	LEU
32	CS	773	SER
32	CS	781	ASP
32	CS	787	LEU
32	CS	799	SER
32	CS	803	LEU
32	CS	806	GLU
32	CS	807	GLU
32	CS	814	MET
32	CS	816	ASP
32	CS	818	SER
32	CS	819	ASN

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Mol	Chain	Res	Type
32	CS	828	GLU
32	CS	830	ASP
32	CS	831	GLN
32	CS	834	THR
32	CS	837	ASP
32	CS	839	LYS
32	CS	841	LEU
32	CS	842	GLU
32	CS	843	SER
32	CS	848	LEU
32	CS	850	ASP
32	CS	853	VAL
32	CS	854	VAL
32	CS	855	LEU
32	CS	856	ASP
32	CS	861	ILE
32	CS	863	GLN
32	CS	867	THR
32	CS	870	LEU
32	CS	871	ARG
32	CS	875	LYS
32	CS	879	LEU
32	CS	892	LYS
32	CS	895	ASP
32	CS	896	THR
32	CS	897	LEU
32	CS	902	ASN
32	CS	906	SER
32	CS	908	VAL
32	CS	913	MET
32	CS	916	MET
32	CS	917	ARG
32	CS	918	LYS
32	CS	921	GLN
36	Cc	52	ARG
36	Cc	144	ARG
37	Cd	132	ARG
40	Cg	55	ARG
40	Cg	77	ARG
49	CU	129	ARG
49	CU	130	LYS
52	CW	21	ARG

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Mol	Chain	Res	Type
52	CW	85	ARG
52	CW	254	ARG
53	UT	147	LEU
53	UT	324	ARG
53	UT	350	LYS
53	UT	469	LEU
53	UT	543	VAL
53	UT	801	CYS
53	UT	1006	ARG
53	UT	1377	VAL
53	UT	1472	THR
53	UT	1633	TRP
53	UT	1710	VAL
53	UT	1877	LEU
53	UT	2046	THR
54	UH	599	VAL
54	UH	624	MET
54	UH	904	ARG
54	UH	926	VAL
56	US	302	MET
57	Cl	25	LYS
59	CY	328	LYS
59	CY	367	LEU
59	CY	368	LYS
59	CY	369	VAL
59	CY	370	LEU
59	CY	371	GLU
59	CY	372	SER
59	CY	374	ARG
60	CZ	537	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (208) such sidechains are listed below:

Mol	Chain	Res	Type
1	UA	291	HIS
1	UA	336	GLN
1	UA	381	HIS
1	UA	685	ASN
2	UB	525	ASN
2	UB	645	GLN
2	UB	759	HIS
3	UC	578	GLN

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Mol	Chain	Res	Type
4	UD	124	HIS
4	UD	206	ASN
4	UD	222	GLN
4	UD	257	GLN
4	UD	324	HIS
4	UD	416	ASN
4	UD	548	ASN
4	UD	697	GLN
5	UF	45	HIS
5	UF	59	ASN
5	UF	62	ASN
5	UF	319	HIS
6	UG	159	HIS
6	UG	175	GLN
6	UG	205	HIS
6	UG	206	ASN
6	UG	267	ASN
6	UG	270	ASN
6	UG	322	ASN
6	UG	378	GLN
7	UJ	15	ASN
7	UJ	51	GLN
7	UJ	77	GLN
7	UJ	158	GLN
7	UJ	184	GLN
7	UJ	349	HIS
7	UJ	670	HIS
7	UJ	731	ASN
7	UJ	842	ASN
7	UJ	1682	GLN
8	UK	13	HIS
9	UL	107	ASN
9	UL	207	HIS
9	UL	377	ASN
9	UL	384	GLN
9	UL	515	GLN
9	UL	517	HIS
9	UL	661	ASN
9	UL	823	ASN
9	UL	862	ASN
9	UL	905	ASN
9	UL	930	GLN

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Mol	Chain	Res	Type
10	UM	30	ASN
10	UM	386	GLN
10	UM	394	ASN
10	UM	548	ASN
10	UM	641	HIS
10	UM	750	HIS
10	UM	808	GLN
11	UN	879	ASN
11	UN	916	GLN
12	UO	339	GLN
12	UO	393	ASN
13	UQ	112	GLN
13	UQ	262	HIS
13	UQ	310	GLN
13	UQ	383	GLN
13	UQ	414	HIS
13	UQ	477	HIS
13	UQ	501	GLN
13	UQ	603	ASN
13	UQ	606	HIS
13	UQ	783	ASN
13	UQ	924	GLN
14	UR	364	GLN
14	UR	399	ASN
14	UR	411	GLN
14	UR	560	GLN
15	UU	197	ASN
15	UU	577	GLN
15	UU	621	HIS
16	UX	39	GLN
16	UX	49	ASN
16	UX	119	GLN
17	UZ	105	GLN
17	UZ	234	HIS
17	UZ	280	ASN
17	UZ	295	GLN
18	CB	289	GLN
19	CC	22	HIS
19	CC	171	HIS
19	CC	321	HIS
19	CC	410	GLN
19	CC	413	GLN

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Mol	Chain	Res	Type
20	CD	91	HIS
20	CD	128	ASN
20	CD	263	GLN
20	CD	273	GLN
20	CD	404	ASN
21	CE	67	HIS
22	CG	198	GLN
22	CG	243	GLN
22	CG	245	HIS
22	CG	430	HIS
22	CG	561	ASN
23	CH	43	ASN
23	CH	199	GLN
24	CI	155	ASN
24	CI	284	GLN
24	CI	930	ASN
24	CI	1029	GLN
24	CI	1030	ASN
25	CJ	135	HIS
26	CK	48	ASN
26	CK	121	ASN
26	CK	225	ASN
28	CM	14	GLN
28	CM	77	ASN
28	CM	120	ASN
28	CM	243	ASN
29	CN	111	GLN
29	CN	243	HIS
29	CO	111	GLN
32	CR	126	GLN
32	CR	207	ASN
32	CR	261	GLN
32	CR	365	HIS
32	CR	482	GLN
32	CR	485	ASN
32	CR	538	GLN
32	CR	565	HIS
32	CR	587	GLN
32	CR	655	GLN
32	CR	749	GLN
32	CR	819	ASN
32	CS	126	GLN

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Mol	Chain	Res	Type
32	CS	261	GLN
32	CS	365	HIS
32	CS	482	GLN
32	CS	485	ASN
32	CS	538	GLN
32	CS	565	HIS
32	CS	587	GLN
32	CS	655	GLN
32	CS	819	ASN
33	CT	107	GLN
34	Ca	149	GLN
34	Ca	183	GLN
35	Cb	98	ASN
35	Cb	224	ASN
36	Cc	87	HIS
37	Cd	81	HIS
38	Ce	17	GLN
38	Ce	36	ASN
38	Ce	95	HIS
38	Ce	132	HIS
39	Cf	52	ASN
39	Cf	94	ASN
40	Cg	121	HIS
40	Cg	129	GLN
42	Ci	93	HIS
43	Cj	15	ASN
43	Cj	83	GLN
44	Ck	22	ASN
44	Ck	103	ASN
45	Cm	113	HIS
46	Cn	63	GLN
46	Cn	94	ASN
47	Co	353	GLN
47	Co	382	GLN
47	Co	385	GLN
49	CU	169	HIS
52	CW	43	ASN
52	CW	177	GLN
52	CW	243	GLN
52	CW	361	ASN
53	UT	25	HIS
53	UT	65	ASN

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Mol	Chain	Res	Type
53	UT	247	GLN
53	UT	311	HIS
53	UT	335	GLN
53	UT	389	HIS
53	UT	492	GLN
53	UT	495	GLN
53	UT	618	GLN
53	UT	793	HIS
53	UT	803	ASN
53	UT	815	ASN
53	UT	924	GLN
53	UT	1096	ASN
53	UT	1272	HIS
53	UT	1315	GLN
53	UT	1348	GLN
53	UT	1436	HIS
53	UT	1909	GLN
53	UT	1985	ASN
53	UT	2163	ASN
54	UH	590	ASN
56	US	184	HIS
56	US	225	ASN
56	US	466	HIS
57	Cl	21	ASN
58	CX	263	GLN
58	CX	322	GLN
58	CX	364	ASN
58	CX	423	ASN
55	UI	174	GLN
55	UI	232	GLN
55	UI	237	ASN
61	UP	341	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
50	C1	1550/2352 (65%)	483 (31%)	33 (2%)
51	C2	226/230 (98%)	68 (30%)	4 (1%)
All	All	1776/2582 (68%)	551 (31%)	37 (2%)

All (551) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
50	C1	4	G
50	C1	5	G
50	C1	7	A
50	C1	13	G
50	C1	14	G
50	C1	15	G
50	C1	16	U
50	C1	17	C
50	C1	18	G
50	C1	19	C
50	C1	20	C
50	C1	26	C
50	C1	38	G
50	C1	40	A
50	C1	41	G
50	C1	47	G
50	C1	49	G
50	C1	56	C
50	C1	60	A
50	C1	61	G
50	C1	63	C
50	C1	66	G
50	C1	68	U
50	C1	71	A
50	C1	72	U
50	C1	73	A
50	C1	74	C
50	C1	75	G
50	C1	77	C
50	C1	89	G
50	C1	90	A
50	C1	93	G
50	C1	97	C
50	C1	104	U
50	C1	105	A
50	C1	121	G
50	C1	126	C
50	C1	127	C
50	C1	128	G
50	C1	134	C
50	C1	136	C
50	C1	143	A
50	C1	150	C

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Mol	Chain	Res	Type
50	C1	152	G
50	C1	154	C
50	C1	155	G
50	C1	158	C
50	C1	159	C
50	C1	160	C
50	C1	161	A
50	C1	162	G
50	C1	166	A
50	C1	169	G
50	C1	170	C
50	C1	182	C
50	C1	183	C
50	C1	193	U
50	C1	201	G
50	C1	202	A
50	C1	203	C
50	C1	205	C
50	C1	206	C
50	C1	207	U
50	C1	208	A
50	C1	209	A
50	C1	210	G
50	C1	216	A
50	C1	220	A
50	C1	221	A
50	C1	225	C
50	C1	234	G
50	C1	242	U
50	C1	243	U
50	C1	244	G
50	C1	257	G
50	C1	265	G
50	C1	266	C
50	C1	267	U
50	C1	268	G
50	C1	269	G
50	C1	273	G
50	C1	276	C
50	C1	277	U
50	C1	278	A
50	C1	281	U

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Mol	Chain	Res	Type
50	C1	282	C
50	C1	283	A
50	C1	285	A
50	C1	290	C
50	C1	291	C
50	C1	292	G
50	C1	308	U
50	C1	310	G
50	C1	311	G
50	C1	312	G
50	C1	319	U
50	C1	320	A
50	C1	322	C
50	C1	323	G
50	C1	325	C
50	C1	333	C
50	C1	334	U
50	C1	339	C
50	C1	340	G
50	C1	346	C
50	C1	347	C
50	C1	349	C
50	C1	351	U
50	C1	362	G
50	C1	372	U
50	C1	382	U
50	C1	383	G
50	C1	384	C
50	C1	386	G
50	C1	398	C
50	C1	402	U
50	C1	403	G
50	C1	404	C
50	C1	416	U
50	C1	425	C
50	C1	427	G
50	C1	435	A
50	C1	436	A
50	C1	440	G
50	C1	441	A
50	C1	442	U
50	C1	443	G

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Mol	Chain	Res	Type
50	C1	454	C
50	C1	458	A
50	C1	459	C
50	C1	468	C
50	C1	469	G
50	C1	474	A
50	C1	475	C
50	C1	484	G
50	C1	491	G
50	C1	492	C
50	C1	497	A
50	C1	499	G
50	C1	500	C
50	C1	501	U
50	C1	502	A
50	C1	504	C
50	C1	581	C
50	C1	582	G
50	C1	583	A
50	C1	584	U
50	C1	585	A
50	C1	586	G
50	C1	587	U
50	C1	594	G
50	C1	595	U
50	C1	609	A
50	C1	610	G
50	C1	613	A
50	C1	614	U
50	C1	621	G
50	C1	624	U
50	C1	628	A
50	C1	638	A
50	C1	646	C
50	C1	650	G
50	C1	652	A
50	C1	653	U
50	C1	655	A
50	C1	656	G
50	C1	659	A
50	C1	660	U
50	C1	661	U

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Mol	Chain	Res	Type
50	C1	662	A
50	C1	663	U
50	C1	664	A
50	C1	667	G
50	C1	678	A
50	C1	679	A
50	C1	680	U
50	C1	682	G
50	C1	683	C
50	C1	685	C
50	C1	686	A
50	C1	687	U
50	C1	688	U
50	C1	689	A
50	C1	690	A
50	C1	692	U
50	C1	693	C
50	C1	697	U
50	C1	700	C
50	C1	702	U
50	C1	703	U
50	C1	711	U
50	C1	713	G
50	C1	714	U
50	C1	715	A
50	C1	718	U
50	C1	719	U
50	C1	720	A
50	C1	721	C
50	C1	722	U
50	C1	723	A
50	C1	725	A
50	C1	726	U
50	C1	728	G
50	C1	730	U
50	C1	735	G
50	C1	737	G
50	C1	740	A
50	C1	742	U
50	C1	743	U
50	C1	744	C
50	C1	745	U

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Mol	Chain	Res	Type
50	C1	756	C
50	C1	758	U
50	C1	760	C
50	C1	762	G
50	C1	763	A
50	C1	764	A
50	C1	769	C
50	C1	770	C
50	C1	772	A
50	C1	773	C
50	C1	774	U
50	C1	775	U
50	C1	776	C
50	C1	777	G
50	C1	778	G
50	C1	782	G
50	C1	786	G
50	C1	797	A
50	C1	802	A
50	C1	803	A
50	C1	804	A
50	C1	806	C
50	C1	807	A
50	C1	808	A
50	C1	809	U
50	C1	810	G
50	C1	811	C
50	C1	816	C
50	C1	828	G
50	C1	833	U
50	C1	834	C
50	C1	841	A
50	C1	845	C
50	C1	849	A
50	C1	850	A
50	C1	851	U
50	C1	856	C
50	C1	858	G
50	C1	860	C
50	C1	861	U
50	C1	862	U
50	C1	863	G

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Mol	Chain	Res	Type
50	C1	886	U
50	C1	889	C
50	C1	892	C
50	C1	893	C
50	C1	897	U
50	C1	900	A
50	C1	903	U
50	C1	907	A
50	C1	913	G
50	C1	921	G
50	C1	922	C
50	C1	925	G
50	C1	927	C
50	C1	929	U
50	C1	930	G
50	C1	934	A
50	C1	935	C
50	C1	936	A
50	C1	942	U
50	C1	943	A
50	C1	944	A
50	C1	971	A
50	C1	972	A
50	C1	984	A
50	C1	985	A
50	C1	986	C
50	C1	987	G
50	C1	988	G
50	C1	989	C
50	C1	1000	A
50	C1	1001	A
50	C1	1002	G
50	C1	1005	A
50	C1	1007	G
50	C1	1017	C
50	C1	1018	G
50	C1	1021	A
50	C1	1022	A
50	C1	1023	U
50	C1	1024	U
50	C1	1025	A
50	C1	1027	C

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Mol	Chain	Res	Type
50	C1	1028	C
50	C1	1029	A
50	C1	1035	G
50	C1	1036	A
50	C1	1037	C
50	C1	1039	C
50	C1	1043	G
50	C1	1044	A
50	C1	1054	A
50	C1	1059	A
50	C1	1061	A
50	C1	1064	G
50	C1	1069	A
50	C1	1070	G
50	C1	1076	U
50	C1	1077	U
50	C1	1078	U
50	C1	1079	C
50	C1	1080	G
50	C1	1085	U
50	C1	1086	U
50	C1	1088	U
50	C1	1089	A
50	C1	1094	G
50	C1	1095	A
50	C1	1098	G
50	C1	1099	A
50	C1	1102	A
50	C1	1103	C
50	C1	1104	A
50	C1	1116	U
50	C1	1120	C
50	C1	1122	A
50	C1	1123	G
50	C1	1124	G
50	C1	1125	A
50	C1	1126	A
50	C1	1127	C
50	C1	1128	A
50	C1	1129	A
50	C1	1141	G
50	C1	1147	U

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Mol	Chain	Res	Type
50	C1	1148	G
50	C1	1150	C
50	C1	1154	A
50	C1	1158	G
50	C1	1159	C
50	C1	1163	A
50	C1	1164	A
50	C1	1166	U
50	C1	1167	C
50	C1	1168	C
50	C1	1169	A
50	C1	1170	G
50	C1	1178	A
50	C1	1179	G
50	C1	1186	U
50	C1	1218	G
50	C1	1219	A
50	C1	1220	A
50	C1	1222	C
50	C1	1223	U
50	C1	1251	C
50	C1	1258	A
50	C1	1265	G
50	C1	1444	A
50	C1	1447	A
50	C1	1448	A
50	C1	1449	U
50	C1	1450	A
50	C1	1451	G
50	C1	1452	G
50	C1	1469	A
50	C1	1470	G
50	C1	1471	U
50	C1	1479	U
50	C1	1481	U
50	C1	1483	A
50	C1	1484	G
50	C1	1486	G
50	C1	1489	G
50	C1	1491	A
50	C1	1497	U
50	C1	1498	G

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Mol	Chain	Res	Type
50	C1	1499	G
50	C1	1517	A
50	C1	1518	A
50	C1	1519	C
50	C1	1520	U
50	C1	1525	A
50	C1	1527	G
50	C1	1529	A
50	C1	1536	A
50	C1	1545	U
50	C1	1549	U
50	C1	1551	A
50	C1	1554	C
50	C1	1555	A
50	C1	1614	U
50	C1	1624	A
50	C1	1625	G
50	C1	1628	A
50	C1	1632	G
50	C1	1636	G
50	C1	1637	C
50	C1	1639	U
50	C1	1642	A
50	C1	1643	U
50	C1	1644	U
50	C1	1645	U
50	C1	1656	C
50	C1	1659	C
50	C1	1665	A
50	C1	1667	G
50	C1	1668	A
50	C1	1670	A
50	C1	1698	G
50	C1	1701	U
50	C1	1709	A
50	C1	1711	G
50	C1	1712	C
50	C1	1713	U
50	C1	1735	A
50	C1	1738	G
50	C1	1742	C
50	C1	1743	C

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Mol	Chain	Res	Type
50	C1	1744	A
50	C1	1751	G
50	C1	2047	G
50	C1	2054	A
50	C1	2055	C
50	C1	2056	U
50	C1	2057	G
50	C1	2061	G
50	C1	2070	A
50	C1	2072	U
50	C1	2073	A
50	C1	2074	C
50	C1	2075	U
50	C1	2077	C
50	C1	2078	C
50	C1	2085	G
50	C1	2086	A
50	C1	2087	G
50	C1	2088	A
50	C1	2107	A
50	C1	2109	A
50	C1	2115	U
50	C1	2118	U
50	C1	2120	C
50	C1	2121	U
50	C1	2156	A
50	C1	2157	G
50	C1	2166	A
50	C1	2167	G
50	C1	2173	G
50	C1	2177	G
50	C1	2178	U
50	C1	2183	A
50	C1	2184	G
50	C1	2185	C
50	C1	2190	G
50	C1	2197	A
50	C1	2201	C
50	C1	2202	C
50	C1	2210	U
50	C1	2211	U
50	C1	2212	G

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Mol	Chain	Res	Type
50	C1	2213	U
50	C1	2214	A
50	C1	2215	C
50	C1	2216	A
50	C1	2220	C
50	C1	2222	C
50	C1	2223	C
50	C1	2227	C
50	C1	2238	A
50	C1	2328	G
50	C1	2329	A
50	C1	2330	G
50	C1	2351	G
50	C1	2362	U
50	C1	2363	G
50	C1	2364	A
50	C1	2365	A
50	C1	2366	C
50	C1	2373	A
50	C1	2374	G
51	C2	5	A
51	C2	8	A
51	C2	15	A
51	C2	23	A
51	C2	24	U
51	C2	28	U
51	C2	29	A
51	C2	33	U
51	C2	36	U
51	C2	37	U
51	C2	39	U
51	C2	48	G
51	C2	57	A
51	C2	58	A
51	C2	62	A
51	C2	63	G
51	C2	81	G
51	C2	90	C
51	C2	91	G
51	C2	92	A
51	C2	95	U
51	C2	100	G

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Mol	Chain	Res	Type
51	C2	104	C
51	C2	111	G
51	C2	118	C
51	C2	124	U
51	C2	125	U
51	C2	126	U
51	C2	127	A
51	C2	128	C
51	C2	135	U
51	C2	136	C
51	C2	140	C
51	C2	142	G
51	C2	145	A
51	C2	147	G
51	C2	148	G
51	C2	153	G
51	C2	160	U
51	C2	162	C
51	C2	163	C
51	C2	164	U
51	C2	165	C
51	C2	166	G
51	C2	167	U
51	C2	168	C
51	C2	170	C
51	C2	178	U
51	C2	179	A
51	C2	181	A
51	C2	182	G
51	C2	187	U
51	C2	188	G
51	C2	189	G
51	C2	190	C
51	C2	198	U
51	C2	199	G
51	C2	200	U
51	C2	201	A
51	C2	205	C
51	C2	244	G
51	C2	247	G
51	C2	255	U
51	C2	256	G

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Mol	Chain	Res	Type
51	C2	259	A
51	C2	260	G
51	C2	261	U
51	C2	262	C

All (37) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
50	C1	88	C
50	C1	89	G
50	C1	96	C
50	C1	135	A
50	C1	150	C
50	C1	205	C
50	C1	209	A
50	C1	277	U
50	C1	281	U
50	C1	424	U
50	C1	582	G
50	C1	593	G
50	C1	684	U
50	C1	771	G
50	C1	802	A
50	C1	906	G
50	C1	1001	A
50	C1	1017	C
50	C1	1068	C
50	C1	1077	U
50	C1	1085	U
50	C1	1087	G
50	C1	1163	A
50	C1	1264	U
50	C1	1485	A
50	C1	1638	G
50	C1	1712	C
50	C1	1734	G
50	C1	2054	A
50	C1	2077	C
50	C1	2156	A
50	C1	2177	G
50	C1	2219	C
51	C2	23	A

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Mol	Chain	Res	Type
51	C2	35	G
51	C2	91	G
51	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	$\#\|Z\| > 2$
63	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
63	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)
63	CI	1201	GTP	C6-N1	-2.87	1.33	1.37

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
63	CI	1201	GTP	PA-O3A-PB	-5.41	114.27	132.83
63	CI	1201	GTP	PB-O3B-PG	-4.84	116.23	132.83
63	CI	1201	GTP	C3'-C2'-C1'	2.86	105.28	100.98
63	CI	1201	GTP	C5-C6-N1	2.76	118.83	113.95
63	CI	1201	GTP	C8-N7-C5	2.50	107.75	102.99

There are no chirality outliers.

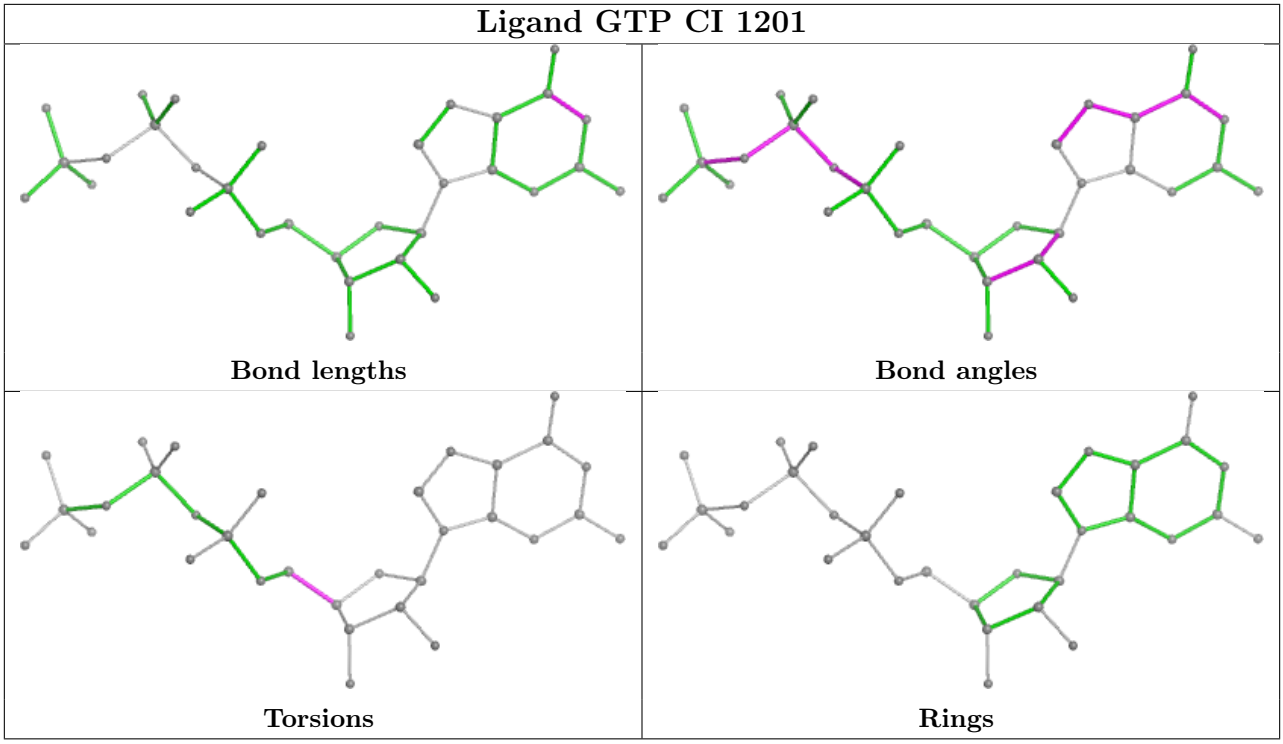
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
63	CI	1201	GTP	O4'-C4'-C5'-O5'
63	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.



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
51	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-10052. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections (i)

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.