wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 8, 2023 – 02:12 PM EDT

PDB ID : 6GSL
Title : Structure of T. thermophilus 70S ribosome complex with mRNA, tRNAfMet and cognate tRNAArg in the A-site
Authors : Rozov, A.; Yusupov, M.; Yusupova, G.
Deposited on : 2018-06-14
Resolution : 3.16 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:

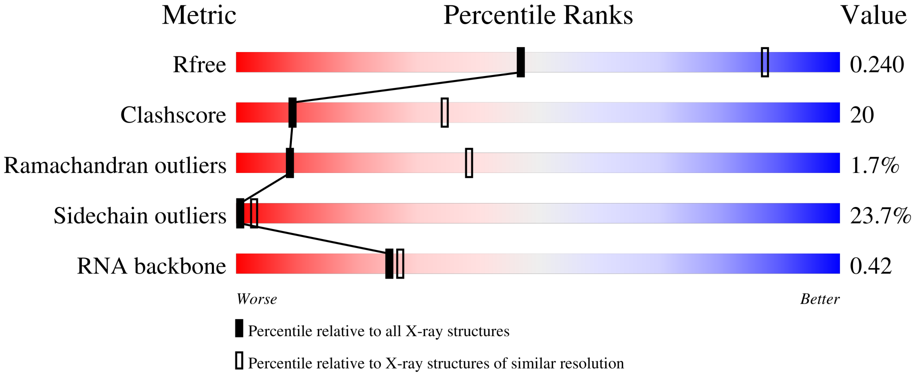
MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

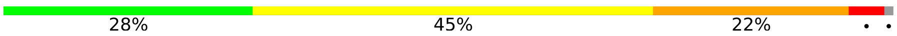
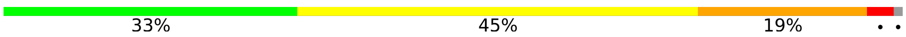
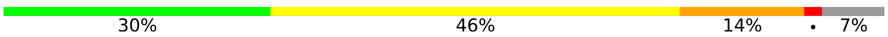
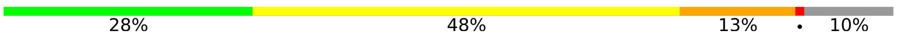
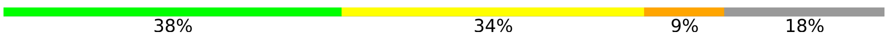
The reported resolution of this entry is 3.16 Å.

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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RNA backbone	3102	1073 (3.50-2.82)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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	13	1522	 28% 45% 22% • •
1	1G	1522	 33% 45% 19% • •
2	12	256	 30% 46% 14% • 7%
2	1E	256	 28% 48% 13% • 10%
3	22	239	 38% 34% 9% 18%
3	2E	239	 48% 32% 6% 14%

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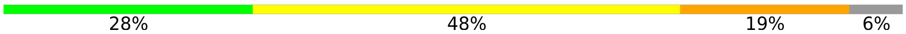
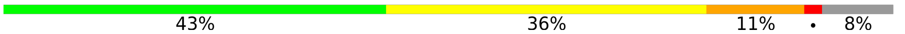
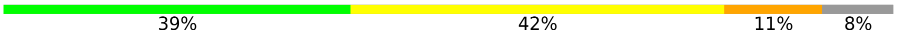
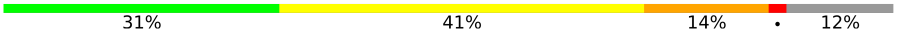
Mol	Chain	Length	Quality of chain
4	32	209	
4	3E	209	
5	42	162	
5	4E	162	
6	52	101	
6	5E	101	
7	62	156	
7	6E	156	
8	72	138	
8	7E	138	
9	82	128	
9	8E	128	
10	1A	105	
10	1I	105	
11	2A	129	
11	2I	129	
12	3A	132	
12	3I	132	
13	4A	126	
13	4I	126	
14	5A	61	
14	5I	61	
15	6A	89	
15	6I	89	
16	7A	88	

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Mol	Chain	Length	Quality of chain
16	7I	88	38% 45% 11% 6%
17	8A	105	51% 38% 5% 6%
17	8I	105	34% 53% 8% 5%
18	9A	88	43% 26% 7% 24%
18	9I	88	32% 35% 8% • 24%
19	AA	93	29% 28% 10% 33%
19	AI	93	40% 32% 12% • 14%
20	BA	106	39% 39% 12% • 8%
20	BI	106	31% 46% 14% • 8%
21	1B	27	33% 48% 7% 11%
21	1F	27	41% 44% • 11%
22	1K	77	21% 40% 26% 6% 6%
22	1L	77	26% 32% 31% 6% •
23	2K	77	34% 38% 18% 10%
23	2L	77	30% 47% 17% 6%
24	3K	77	22% 27% 38% 8% 5%
24	3L	77	17% 35% 36% 8% •
25	4K	27	15% 30% 30% • 22%
25	4L	27	26% 11% 22% • 37%
26	14	2917	28% 44% 22% 5% •
26	1H	2917	25% 43% 25% 6% •
27	16	122	32% 36% 25% 7%
27	1J	122	29% 49% 14% 8%
28	71	229	25% 27% 7% 41%
28	79	229	30% 23% • 43%

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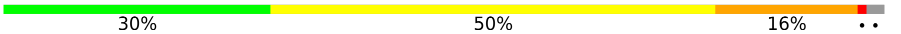
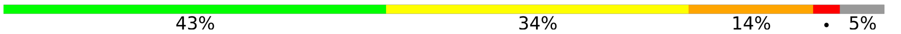
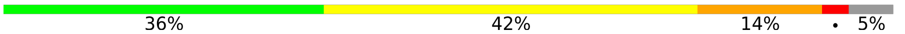
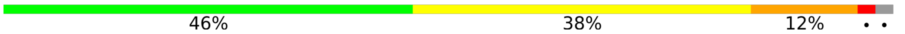
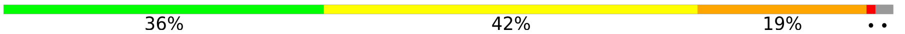
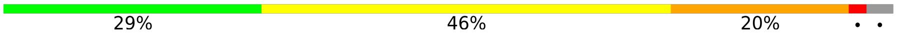
Mol	Chain	Length	Quality of chain
29	11	276	 51% 37% 10% • •
29	19	276	 54% 33% 11% • •
30	21	206	 40% 42% 15% • •
30	29	206	 44% 40% 14% • •
31	31	210	 49% 38% 10% •
31	39	210	 30% 50% 16% • •
32	41	182	 42% 45% 11% • •
32	49	182	 36% 46% 16% • •
33	51	180	 43% 34% 14% • 5%
33	59	180	 36% 42% 14% • 5%
34	18	125	 5% 15% • • 76%
34	28	125	 • 14% 6% • 76%
35	61	148	 46% 38% 12% • •
35	69	148	 36% 42% 19% • •
36	38	173	 18% 28% 21% 15% 17%
37	48	147	 29% 46% 20% • •
38	15	140	 51% 40% 6% • •
38	58	140	 42% 42% 13% • •
39	25	122	 51% 34% 13% •
39	68	122	 61% 33% 6%
40	35	150	 36% 39% 21% • •
40	78	150	 36% 45% 16% • •
41	45	141	 35% 40% 21% • •
41	88	141	 50% 45% 6%
42	55	118	 55% 39% 6%

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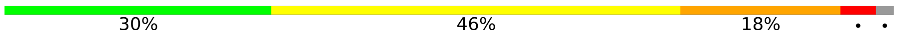
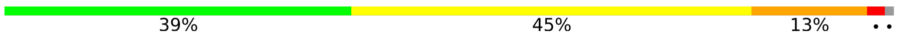
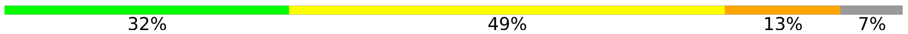
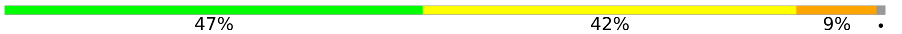
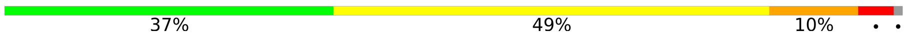
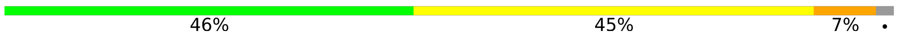
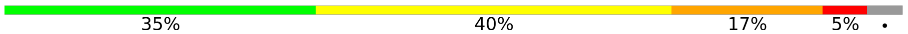
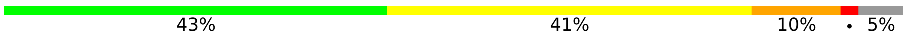
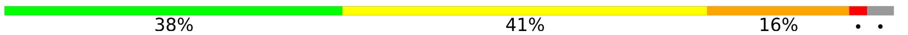
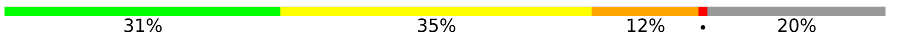
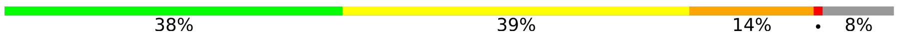
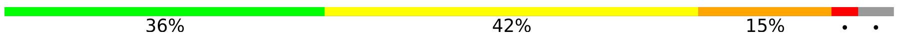
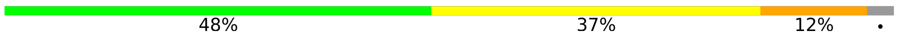
Mol	Chain	Length	Quality of chain
42	98	118	
43	65	112	
43	A8	112	
44	75	146	
44	B8	146	
45	85	118	
45	C8	118	
46	95	101	
46	D8	101	
47	A5	113	
47	E8	113	
48	B5	96	
48	F8	96	
49	C5	110	
49	G8	110	
50	D5	206	
50	H8	206	
51	E5	85	
51	I8	85	
52	F5	98	
52	J8	98	
53	G5	72	
53	K8	72	
54	H5	60	
54	L8	60	

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Mol	Chain	Length	Quality of chain
55	M8	71	
56	J5	60	
56	N8	60	
57	O8	54	
58	L5	49	
58	P8	49	
59	M5	65	
59	Q8	65	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
61	SF4	32	303	-	-	X	-
61	SF4	3E	303	-	-	X	-

2 Entry composition

There are 63 unique types of molecules in this entry. The entry contains 306138 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
1	13	1512	Total C N O P 32497 14464 6017 10504 1512	0	0	0
1	1G	1509	Total C N O P 32437 14437 6010 10481 1509	0	0	0

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	1E	231	Total C N O S 1874 1199 334 336 5	0	0	0
2	12	237	Total C N O S 1924 1228 344 347 5	0	0	0

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	2E	205	Total C N O S 1605 1011 313 280 1	0	0	0
3	22	195	Total C N O S 1533 969 297 266 1	0	0	0

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	3E	207	Total C N O S 1690 1058 336 289 7	0	0	0
4	32	208	Total C N O S 1702 1066 339 290 7	0	0	0

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	4E	149	Total 1142	C 722	N 216	O 200	S 4	0	0	0
5	42	151	Total 1155	C 729	N 218	O 204	S 4	0	0	0

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	5E	101	Total 842	C 531	N 155	O 153	S 3	0	0	0
6	52	101	Total 842	C 531	N 155	O 153	S 3	0	0	0

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	6E	154	Total 1242	C 770	N 250	O 216	S 6	0	0	0
7	62	138	Total 1110	C 689	N 221	O 194	S 6	0	0	0

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	7E	138	Total 1115	C 705	N 215	O 192	S 3	0	0	0
8	72	138	Total 1115	C 705	N 215	O 192	S 3	0	0	0

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	8E	126	Total 1000	C 634	N 196	O 170	0	0	0
9	82	124	Total 983	C 624	N 190	O 169	0	0	0

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	1I	99	Total 801	C 504	N 157	O 139	S 1	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	1A	99	Total 801	C 504	N 157	O 139	S 1	0	0	0

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	2I	111	Total 823	C 512	N 154	O 154	S 3	0	0	0
11	2A	113	Total 835	C 520	N 156	O 156	S 3	0	0	0

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	3I	122	Total 956	C 603	N 193	O 159	S 1	0	0	0
12	3A	121	Total 947	C 597	N 191	O 158	S 1	0	0	0

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	4I	119	Total 936	C 579	N 191	O 164	S 2	0	0	0
13	4A	111	Total 887	C 549	N 180	O 156	S 2	0	0	0

- Molecule 14 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	5I	61	Total 499	C 317	N 105	O 72	S 5	0	0	0
14	5A	57	Total 466	C 297	N 97	O 68	S 4	0	0	0

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	6I	87	Total 729	C 457	N 146	O 124	S 2	0	0	0
15	6A	87	Total 729	C 457	N 146	O 124	S 2	0	0	0

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
16	7I	83	700	443	139	117	1	0	0	0
16	7A	84	705	446	140	118	1	0	0	0

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
17	8I	100	834	534	155	143	2	0	0	0
17	8A	99	823	528	151	142	2	0	0	0

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
18	9I	67	544	349	104	91	0	0	0
18	9A	67	544	349	104	91	0	0	0

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
19	AI	80	643	411	118	112	2	0	0	0
19	AA	62	481	306	85	88	2	0	0	0

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
20	BI	98	751	464	158	127	2	0	0	0
20	BA	98	757	467	161	127	2	0	0	0

- Molecule 21 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
21	1F	24	Total C N O 208 128 50 30	0	0	0
21	1B	24	Total C N O 208 128 50 30	0	0	0

- Molecule 22 is a RNA chain called tRNAArg.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
22	1K	72	Total C N O P S 1544 690 282 498 72 2	0	0	0
22	1L	74	Total C N O P S 1584 708 287 513 74 2	0	0	0

- Molecule 23 is a RNA chain called tRNAfMet.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
23	2K	77	Total C N O P S 1646 735 298 535 77 1	0	0	0
23	2L	77	Total C N O P S 1646 735 298 535 77 1	0	0	0

- Molecule 24 is a RNA chain called tRNAArg.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
24	3K	73	Total C N O P 1561 696 285 507 73	0	0	0
24	3L	74	Total C N O P 1581 705 287 515 74	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3K	6	U	C	conflict	GB 1387059712
3L	6	U	C	conflict	GB 1387059712

- Molecule 25 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
25	4K	21	Total C N O P 462 207 97 137 21	0	0	0
25	4L	17	Total C N O P 374 167 77 113 17	0	0	0

- Molecule 26 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	1H	2895	Total 62351	C 27751	N 11658	O 20047	P 2895	0	0	0
26	14	2895	Total 62347	C 27751	N 11660	O 20042	P 2894	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1H	161	U	UNK	conflict	GB 55771382
1H	654A	A	G	conflict	GB 55771382
1H	654E	C	G	conflict	GB 55771382
1H	654P	G	C	conflict	GB 55771382
1H	654T	A	C	conflict	GB 55771382
1H	1058	U	G	conflict	GB 55771382
1H	1080	A	C	conflict	GB 55771382
14	158	U	UNK	conflict	GB 55771382
14	654A	A	G	conflict	GB 55771382
14	654E	C	G	conflict	GB 55771382
14	654P	G	C	conflict	GB 55771382
14	654T	A	C	conflict	GB 55771382
14	1058	U	G	conflict	GB 55771382
14	1080	A	C	conflict	GB 55771382

- Molecule 27 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	16	122	Total 2617	C 1166	N 486	O 844	P 121	0	0	0
27	1J	122	Total 2617	C 1166	N 486	O 844	P 121	0	0	0

- Molecule 28 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	71	134	Total 1043	C 659	N 196	O 187	S 1	0	0	0
28	79	130	Total 1010	C 637	N 188	O 184	S 1	0	0	0

- Molecule 29 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	11	273	Total	C	N	O	S	0	0	0
			2120	1338	421	358	3			
29	19	273	Total	C	N	O	S	0	0	0
			2120	1338	421	358	3			

- Molecule 30 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	21	203	Total	C	N	O	S	0	0	0
			1558	985	298	269	6			
30	29	203	Total	C	N	O	S	0	0	0
			1558	985	298	269	6			

- Molecule 31 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	31	202	Total	C	N	O	S	0	0	0
			1585	1011	297	275	2			
31	39	206	Total	C	N	O	S	0	0	0
			1610	1026	301	281	2			

- Molecule 32 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	41	179	Total	C	N	O	S	0	0	0
			1457	931	265	257	4			
32	49	179	Total	C	N	O	S	0	0	0
			1457	931	265	257	4			

- Molecule 33 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	51	171	Total	C	N	O	S	0	0	0
			1312	832	246	233	1			
33	59	171	Total	C	N	O	S	0	0	0
			1312	832	246	233	1			

- Molecule 34 is a protein called 50S ribosomal protein L7/L12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	18	30	Total	C	N	O	S	0	0	0
			237	150	38	48	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
34	28	30	237	150	38	48	1	0	0	0

- Molecule 35 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
35	61	145	1131	723	200	207	1	0	0	0
35	69	145	1131	723	200	207	1	0	0	0

- Molecule 36 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
36	38	143	1089	694	191	202	2	0	0	0

- Molecule 37 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
37	48	142	1047	665	184	193	5	0	0	0

- Molecule 38 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
38	58	137	1096	706	205	181	4	0	0	0
38	15	137	1096	707	205	181	3	0	0	0

- Molecule 39 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
39	68	122	932	588	171	169	4	0	0	0
39	25	122	932	588	171	169	4	0	0	0

- Molecule 40 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
40	78	147	Total C N O S 1122 698 229 192 3	0	0	0
40	35	148	Total C N O S 1130 704 230 193 3	0	0	0

- Molecule 41 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
41	88	141	Total C N O S 1113 709 210 187 7	0	0	0
41	45	138	Total C N O S 1099 702 208 183 6	0	0	0

- Molecule 42 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
42	98	118	Total C N O S 967 604 203 159 1	0	0	0
42	55	118	Total C N O S 967 604 203 159 1	0	0	0

- Molecule 43 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
43	A8	111	Total C N O 881 556 176 149	0	0	0
43	65	110	Total C N O 876 553 175 148	0	0	0

- Molecule 44 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
44	B8	136	Total C N O S 1132 704 232 195 1	0	0	0
44	75	134	Total C N O 1115 694 229 192	0	0	0

- Molecule 45 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
45	C8	115	Total C N O S 950 603 199 147 1	0	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
45	85	117	Total C N O S 963 610 202 150 1	0	0	0

- Molecule 46 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
46	D8	101	Total C N O S 778 501 142 134 1	0	0	0
46	95	100	Total C N O S 774 499 141 133 1	0	0	0

- Molecule 47 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
47	E8	112	Total C N O S 890 560 175 153 2	0	0	0
47	A5	111	Total C N O S 886 558 174 152 2	0	0	0

- Molecule 48 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
48	F8	95	Total C N O S 743 482 134 126 1	0	0	0
48	B5	94	Total C N O S 738 479 133 125 1	0	0	0

- Molecule 49 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
49	G8	105	Total C N O S 784 504 147 128 5	0	0	0
49	C5	106	Total C N O S 785 504 147 129 5	0	0	0

- Molecule 50 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
50	H8	165	Total C N O S 1330 851 241 236 2	0	0	0
50	D5	200	Total C N O S 1582 1008 279 292 3	0	0	0

- Molecule 51 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
51	I8	81	Total C N O S 630 389 133 107 1	0	0	0
51	E5	78	Total C N O S 616 381 130 104 1	0	0	0

- Molecule 52 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
52	J8	93	Total C N O S 729 457 145 126 1	0	0	0
52	F5	94	Total C N O S 737 463 146 127 1	0	0	0

- Molecule 53 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
53	K8	69	Total C N O S 576 358 116 101 1	0	0	0
53	G5	66	Total C N O S 558 346 113 98 1	0	0	0

- Molecule 54 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
54	L8	58	Total C N O 459 293 89 77	0	0	0
54	H5	58	Total C N O 459 293 89 77	0	0	0

- Molecule 55 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
55	M8	48	Total C N O S 371 237 62 67 5	0	0	0

- Molecule 56 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
56	N8	50	Total C N O S 386 241 77 63 5	0	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
56	J5	56	Total C N O S 434 272 87 70 5	0	0	0

- Molecule 57 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
57	O8	45	Total C N O S 389 241 79 65 4	0	0	0

- Molecule 58 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
58	P8	47	Total C N O S 401 246 99 54 2	0	0	0
58	L5	47	Total C N O S 409 251 102 54 2	0	0	0

- Molecule 59 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
59	Q8	64	Total C N O S 516 331 102 81 2	0	0	0
59	M5	64	Total C N O S 516 331 102 81 2	0	0	0

- Molecule 60 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	13	227	Total Mg 227 227	0	0
60	3E	2	Total Mg 2 2	0	0
60	5E	2	Total Mg 2 2	0	0
60	6I	1	Total Mg 1 1	0	0
60	1K	2	Total Mg 2 2	0	0
60	2K	7	Total Mg 7 7	0	0
60	4K	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	1H	669	Total Mg 669 669	0	0
60	16	20	Total Mg 20 20	0	0
60	11	6	Total Mg 6 6	0	0
60	21	2	Total Mg 2 2	0	0
60	31	2	Total Mg 2 2	0	0
60	41	1	Total Mg 1 1	0	0
60	78	1	Total Mg 1 1	0	0
60	88	4	Total Mg 4 4	0	0
60	98	2	Total Mg 2 2	0	0
60	I8	2	Total Mg 2 2	0	0
60	N8	1	Total Mg 1 1	0	0
60	P8	1	Total Mg 1 1	0	0
60	Q8	1	Total Mg 1 1	0	0
60	1G	167	Total Mg 167 167	0	0
60	32	2	Total Mg 2 2	0	0
60	52	1	Total Mg 1 1	0	0
60	2A	1	Total Mg 1 1	0	0
60	1L	1	Total Mg 1 1	0	0
60	2L	2	Total Mg 2 2	0	0
60	4L	2	Total Mg 2 2	0	0
60	14	607	Total Mg 607 607	0	0

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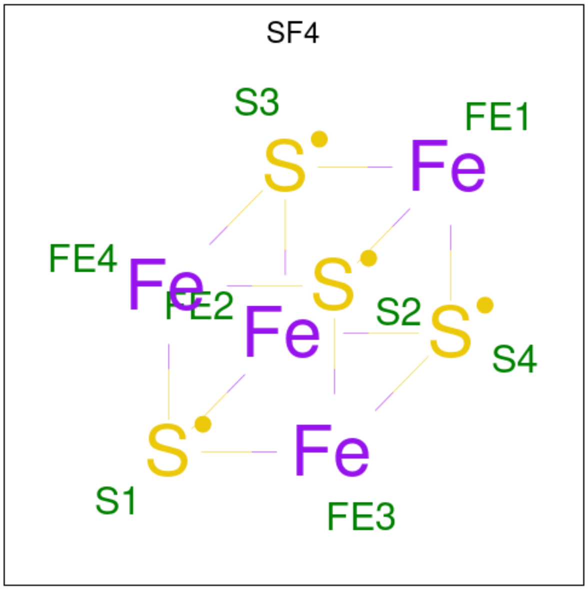
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	1J	8	Total Mg 8 8	0	0
60	29	5	Total Mg 5 5	0	0
60	39	2	Total Mg 2 2	0	0
60	25	2	Total Mg 2 2	0	0
60	35	1	Total Mg 1 1	0	0
60	45	2	Total Mg 2 2	0	0
60	55	2	Total Mg 2 2	0	0
60	75	1	Total Mg 1 1	0	0
60	C5	1	Total Mg 1 1	0	0
60	E5	1	Total Mg 1 1	0	0
60	F5	1	Total Mg 1 1	0	0
60	M5	1	Total Mg 1 1	0	0

- Molecule 61 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	3E	1	Total Fe S 8 4 4	0	0
61	32	1	Total Fe S 8 4 4	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	5I	1	Total Zn 1 1	0	0
62	5A	1	Total Zn 1 1	0	0

- Molecule 63 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
63	13	544	Total O 544 544	0	0
63	1E	1	Total O 1 1	0	0
63	3E	1	Total O 1 1	0	0
63	4E	2	Total O 2 2	0	0
63	8E	1	Total O 1 1	0	0
63	1I	1	Total O 1 1	0	0
63	3I	5	Total O 5 5	0	0
63	5I	3	Total O 3 3	0	0
63	6I	4	Total O 4 4	0	0
63	BI	1	Total O 1 1	0	0
63	1F	1	Total O 1 1	0	0
63	1K	1	Total O 1 1	0	0
63	2K	16	Total O 16 16	0	0
63	4K	13	Total O 13 13	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
63	1H	1966	Total O 1966 1966	0	0
63	16	42	Total O 42 42	0	0
63	11	12	Total O 12 12	0	0
63	21	9	Total O 9 9	0	0
63	31	8	Total O 8 8	0	0
63	58	3	Total O 3 3	0	0
63	78	10	Total O 10 10	0	0
63	88	7	Total O 7 7	0	0
63	98	1	Total O 1 1	0	0
63	A8	2	Total O 2 2	0	0
63	B8	3	Total O 3 3	0	0
63	C8	7	Total O 7 7	0	0
63	D8	1	Total O 1 1	0	0
63	F8	1	Total O 1 1	0	0
63	G8	3	Total O 3 3	0	0
63	I8	5	Total O 5 5	0	0
63	J8	10	Total O 10 10	0	0
63	L8	4	Total O 4 4	0	0
63	P8	1	Total O 1 1	0	0
63	Q8	7	Total O 7 7	0	0
63	1G	397	Total O 397 397	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
63	32	5	Total O 5 5	0	0
63	42	1	Total O 1 1	0	0
63	52	4	Total O 4 4	0	0
63	3A	2	Total O 2 2	0	0
63	5A	1	Total O 1 1	0	0
63	6A	1	Total O 1 1	0	0
63	7A	2	Total O 2 2	0	0
63	9A	2	Total O 2 2	0	0
63	BA	2	Total O 2 2	0	0
63	2L	7	Total O 7 7	0	0
63	4L	8	Total O 8 8	0	0
63	14	1520	Total O 1520 1520	0	0
63	1J	23	Total O 23 23	0	0
63	19	12	Total O 12 12	0	0
63	29	9	Total O 9 9	0	0
63	39	8	Total O 8 8	0	0
63	15	1	Total O 1 1	0	0
63	25	13	Total O 13 13	0	0
63	35	5	Total O 5 5	0	0
63	45	4	Total O 4 4	0	0
63	85	4	Total O 4 4	0	0

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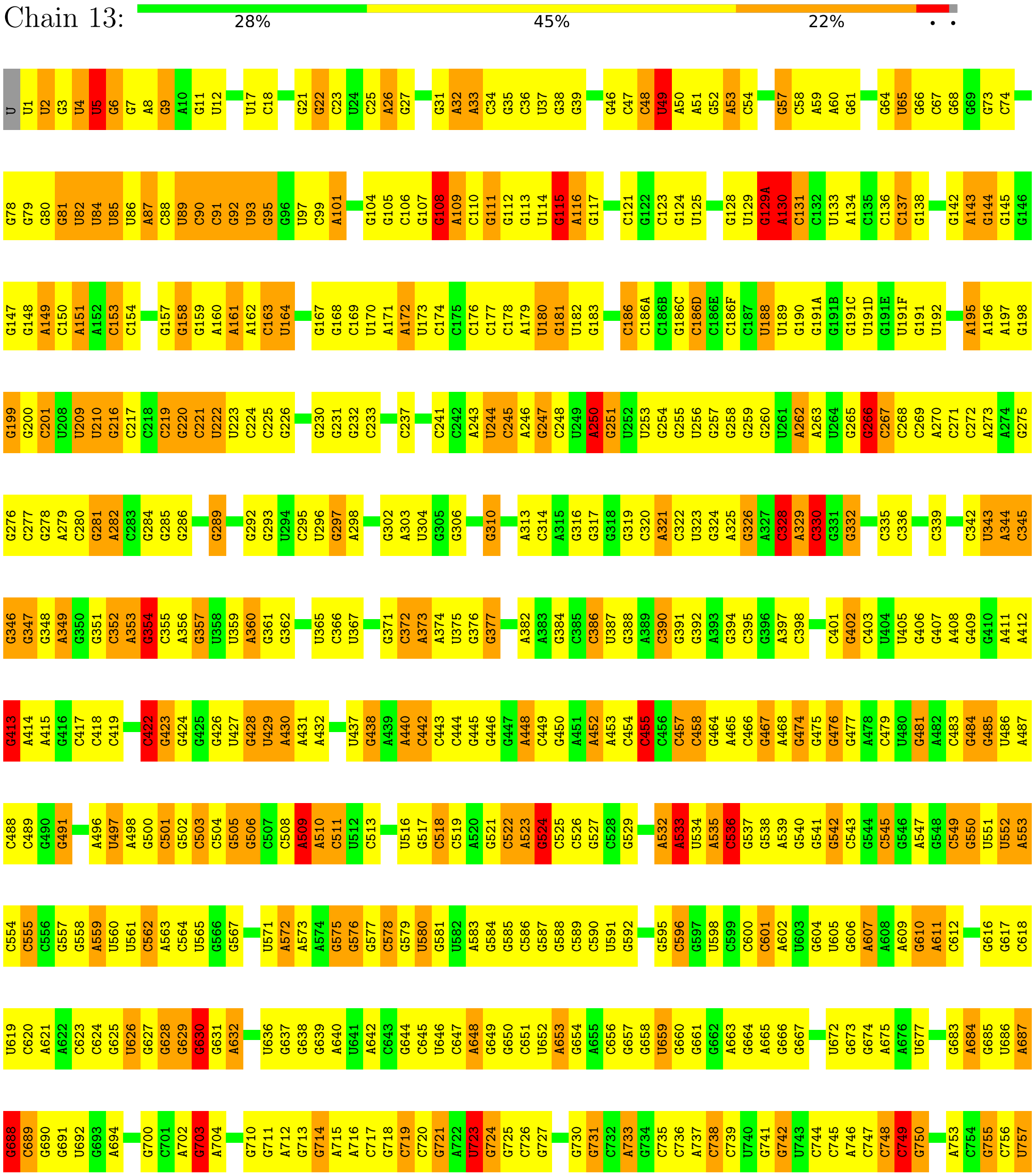
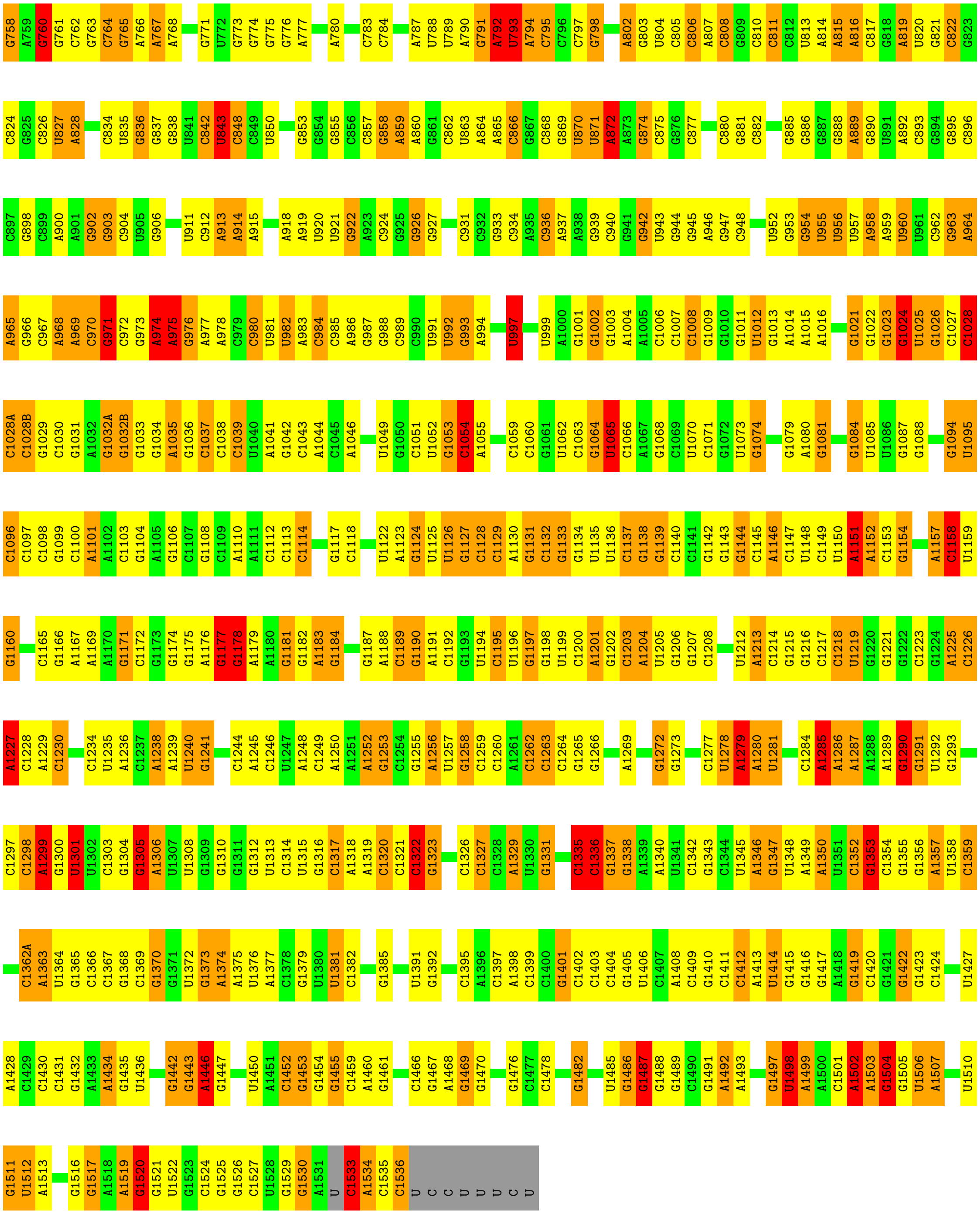
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
63	A5	1	Total O 1 1	0	0
63	B5	1	Total O 1 1	0	0
63	C5	1	Total O 1 1	0	0
63	E5	3	Total O 3 3	0	0
63	F5	6	Total O 6 6	0	0
63	L5	2	Total O 2 2	0	0
63	M5	9	Total O 9 9	0	0

3 Residue-property plots ⓘ

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

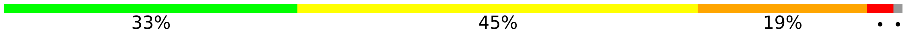
- Molecule 1: 16S ribosomal RNA

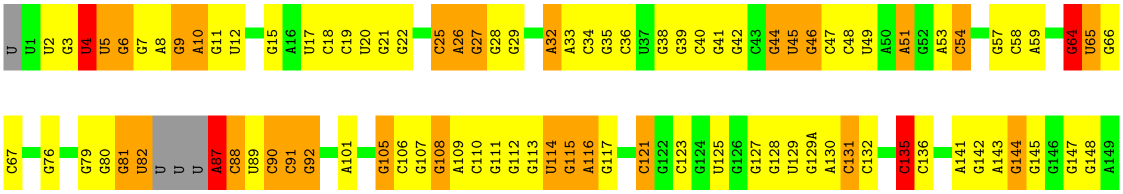


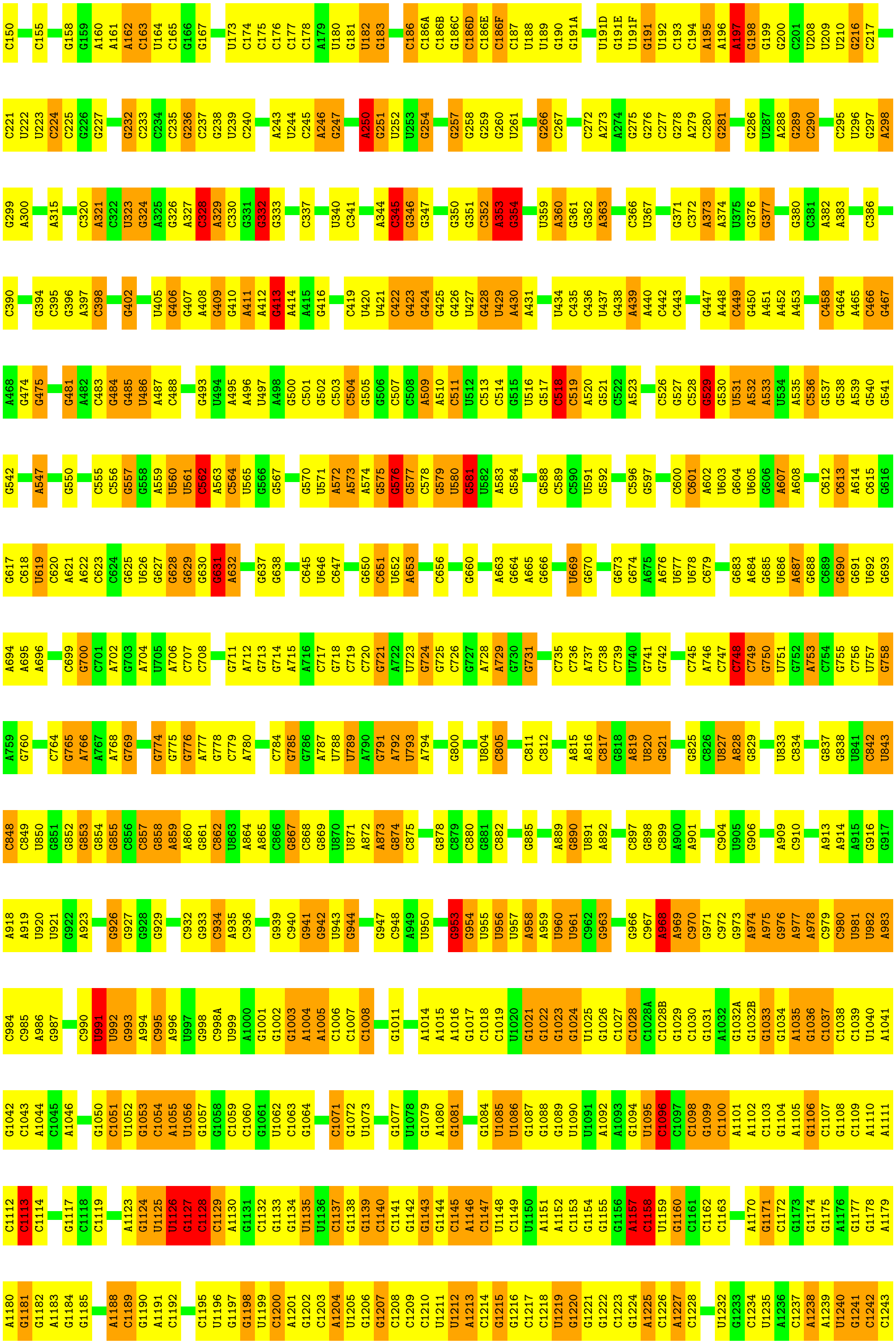


- Molecule 1: 16S ribosomal RNA

Chain 1G:






C150
C155
G158
G159
A160
A161
A162
C163
U164
C165
G166
G167
U173
C174
C175
C176
C177
C178
A179
U180
G181
U182
G183
C186
C186A
C186B
G186C
C186D
C186E
C186F
C187
U188
U189
G190
G191A
U191D
G191E
U191F
G191
U192
C193
C194
A195
A196
A197
G198
G199
G200
C201
U208
U209
U210
G216
C217
C221
U222
U223
C224
C225
G226
G227
G232
C233
C234
C235
G236
C237
G238
U239
C240
A243
U244
C245
A246
G247
A250
G251
U252
U253
G254
G257
G258
G259
G260
U261
G266
C267
C272
A273
A274
G275
G276
C277
G278
A279
C280
G281
G286
U287
A288
G289
C290
C295
U296
G297
A298
G299
A300
A315
C320
A321
C322
U323
G324
A325
G326
A327
C328
A329
C330
G331
G332
G333
C337
U340
C341
A344
C345
G346
G347
G350
G351
C352
A353
G354
U359
A360
G361
G362
A363
C366
U367
G371
C372
A373
A374
U375
G376
G377
G380
C381
A382
A383
C386
C390
G394
C395
G396
A397
C398
G402
U405
G406
G407
A408
G409
G410
A411
A412
G413
A414
A415
G416
C419
U420
U421
C422
G423
G424
G425
G426
U427
G428
U429
A430
A431
U434
C435
C436
U437
G438
A439
A440
C442
C443
G447
A448
C449
G450
A451
A452
A453
C458
G464
A465
C466
G467
A468
G474
G475
G481
A482
C483
G484
G485
U486
A487
C488
G493
U494
A495
A496
U497
A498
G500
C501
G502
C503
C504
G505
G506
C507
C508
A509
A510
C511
U512
C513
C514
G515
U516
G517
C518
C519
A520
G521
C522
A523
C526
G527
C528
G529
G530
U531
A532
A533
U534
A535
C536
G537
G538
A539
G540
G541
G542
A547
G550
C555
C556
G557
G558
A559
U560
U561
C562
A563
C564
U565
G566
G567
G570
U571
A572
A573
A574
G575
G576
G577
C578
G579
U580
G581
U582
A583
G584
G588
C589
C590
U591
G592
C596
G597
C600
C601
A602
U603
G604
U605
G606
A607
A608
C612
C613
A614
C615
G616
G617
C618
U619
C620
A621
A622
C623
C624
G625
U626
G627
G628
G629
G630
G631
A632
G637
G638
C645
U646
C647
G650
C651
U652
A653
C656
G660
A663
G664
A665
G666
U669
G670
G673
G674
A675
A676
U677
U678
C679
G683
A684
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G691
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G693
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A695
A696
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G703
A704
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C707
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G714
A715
A716
C717
C718
C719
C720
G721
A722
U723
G724
G725
C726
G727
A728
A729
G730
G731
C735
C736
A737
C738
C739
U740
G741
G742
C745
A746
C747
C748
C749
G750
U751
G752
A753
C754
G755
C756
U757
G758
A759
G760
C764
G765
A766
A767
A768
G769
G774
G775
G776
A777
G778
C779
A780
C784
G785
G786
A787
U788
U789
A790
G791
A792
U793
A794
G800
U804
C805
C811
C812
A815
A816
C817
G818
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U820
G821
G825
C826
U827
A828
G829
U833
C834
G837
G838
U841
C842
U843
C848
C849
U850
G851
G852
G853
G854
G855
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C857
G858
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G861
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U863
A864
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U871
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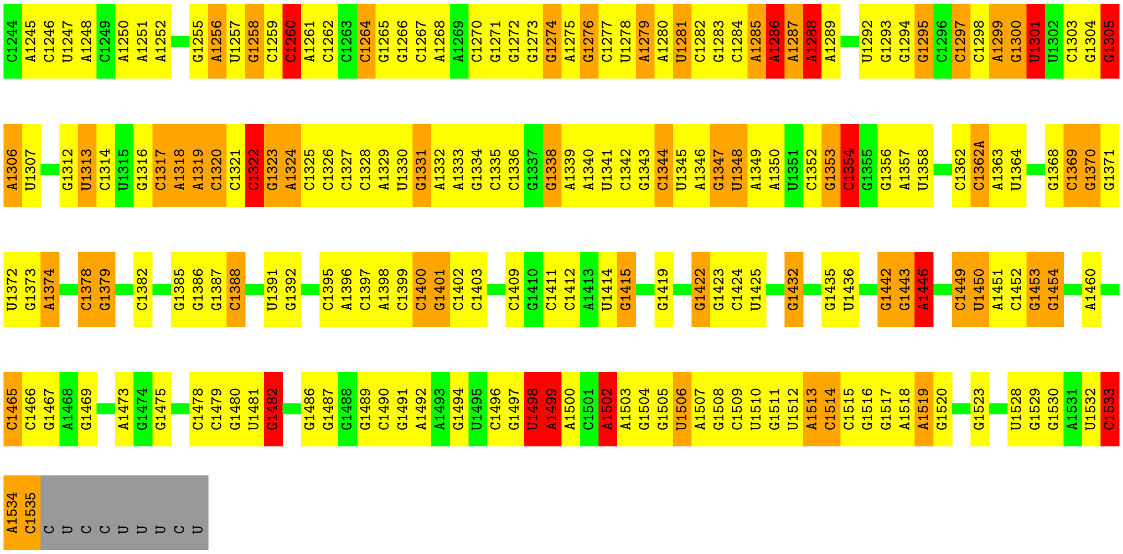
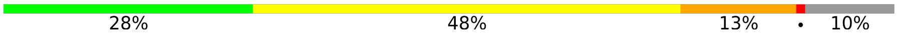
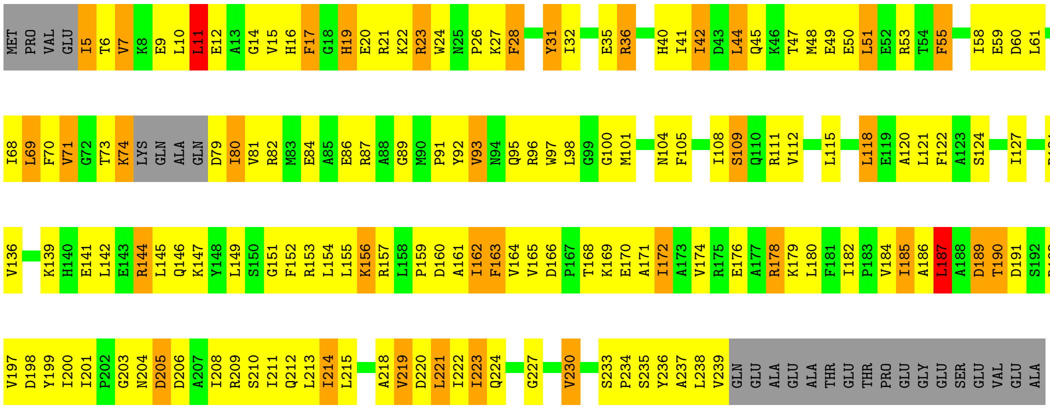


- Molecule 2: 30S ribosomal protein S2

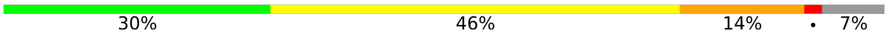
Chain 1E:

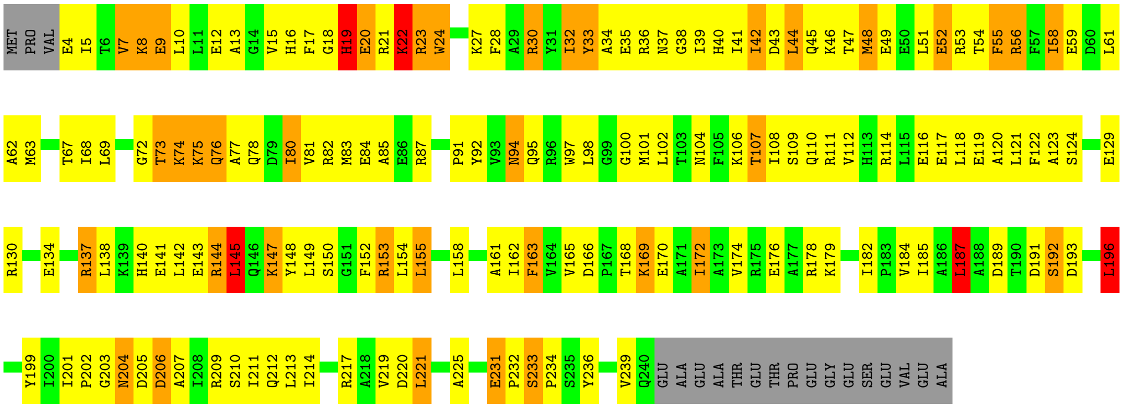




- Molecule 2: 30S ribosomal protein S2

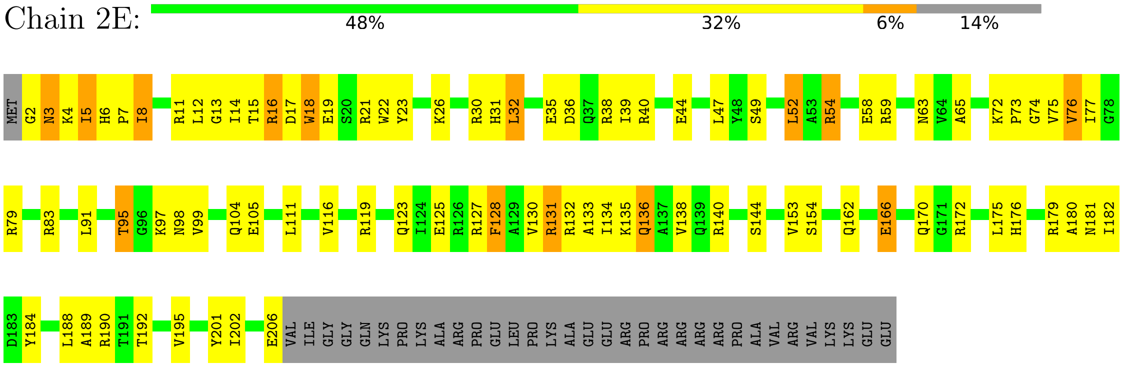
Chain 12:





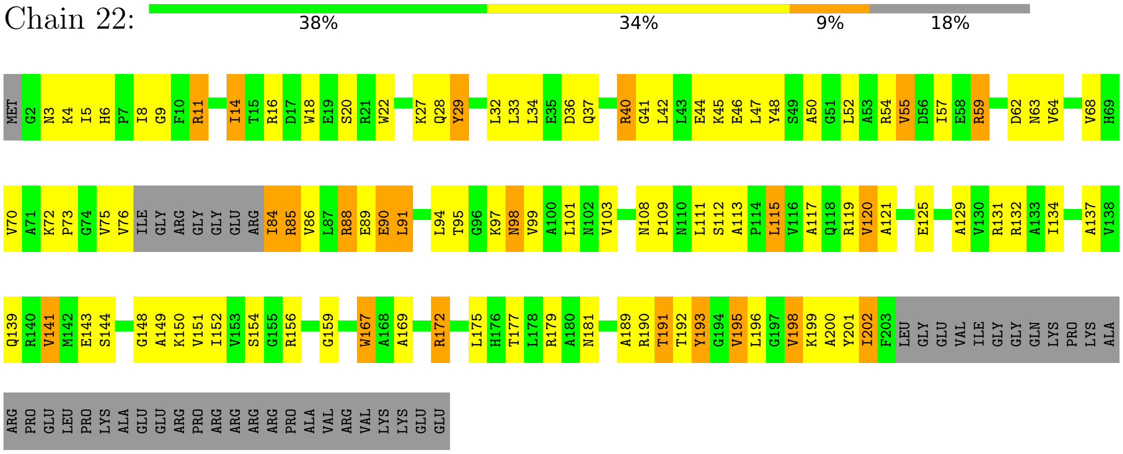
- Molecule 3: 30S ribosomal protein S3

Chain 2E:



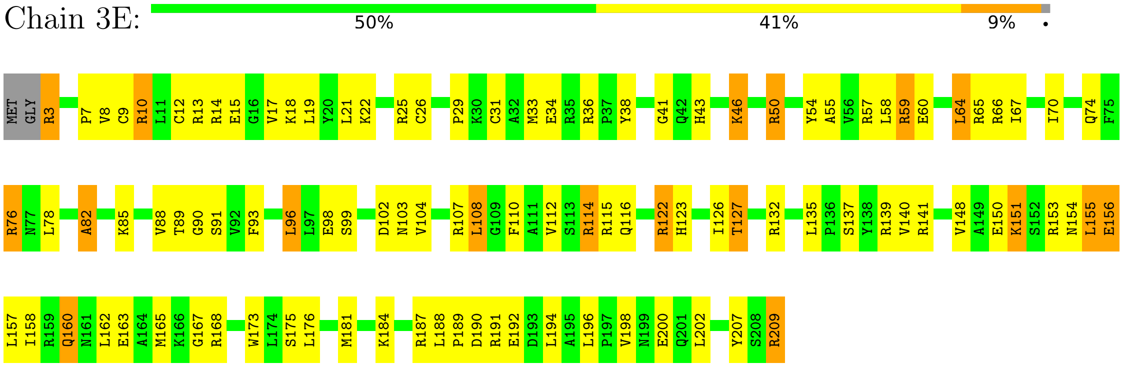
- Molecule 3: 30S ribosomal protein S3

Chain 22:



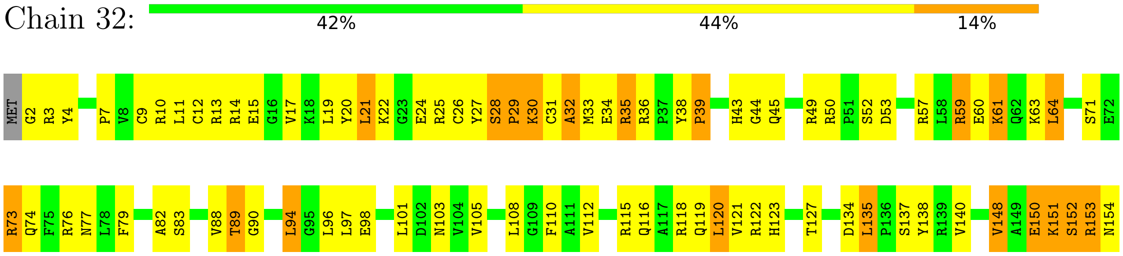
- Molecule 4: 30S ribosomal protein S4

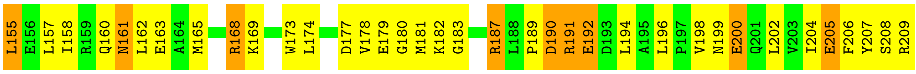
Chain 3E:



- Molecule 4: 30S ribosomal protein S4

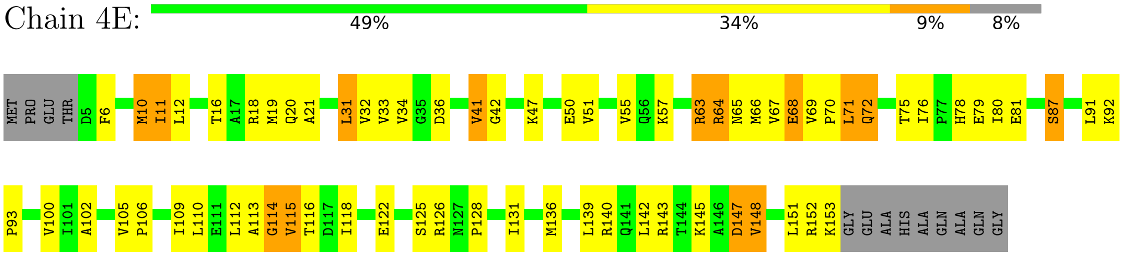
Chain 32:





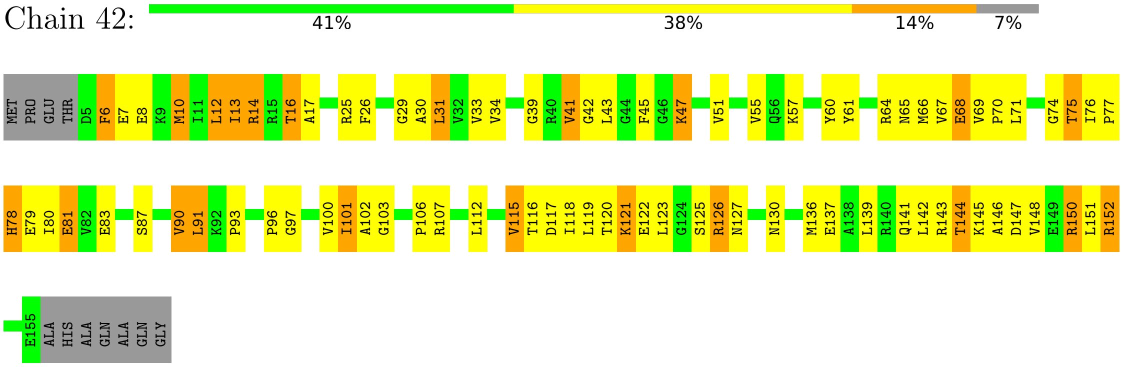
- Molecule 5: 30S ribosomal protein S5

Chain 4E:



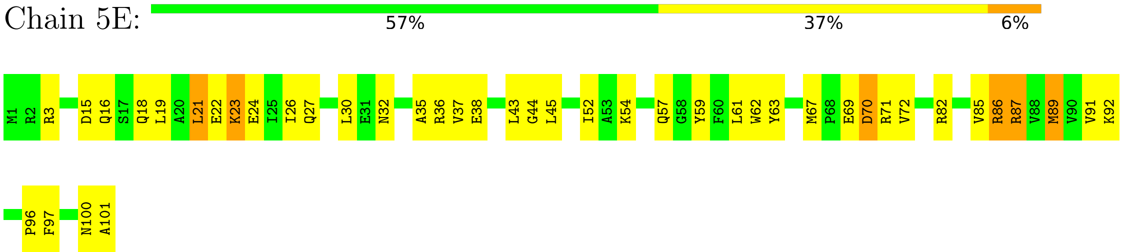
- Molecule 5: 30S ribosomal protein S5

Chain 42:



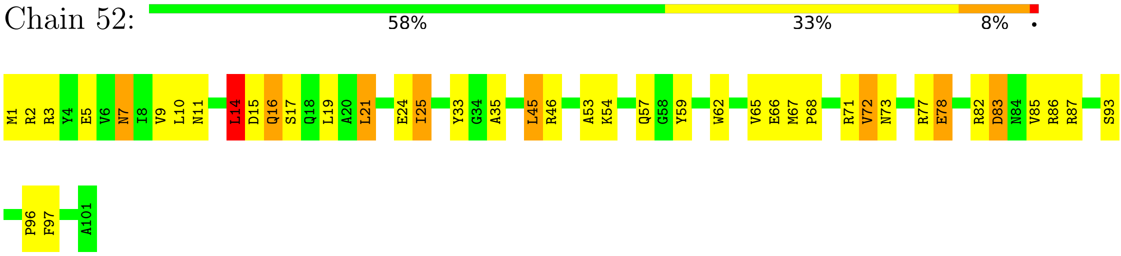
- Molecule 6: 30S ribosomal protein S6

Chain 5E:



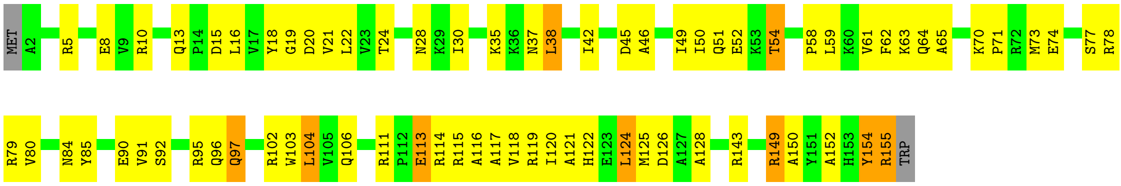
- Molecule 6: 30S ribosomal protein S6

Chain 52:



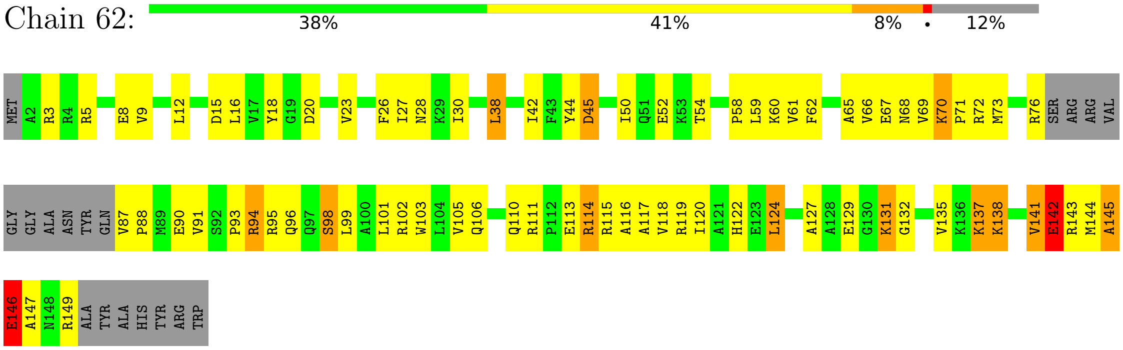
- Molecule 7: 30S ribosomal protein S7

Chain 6E:



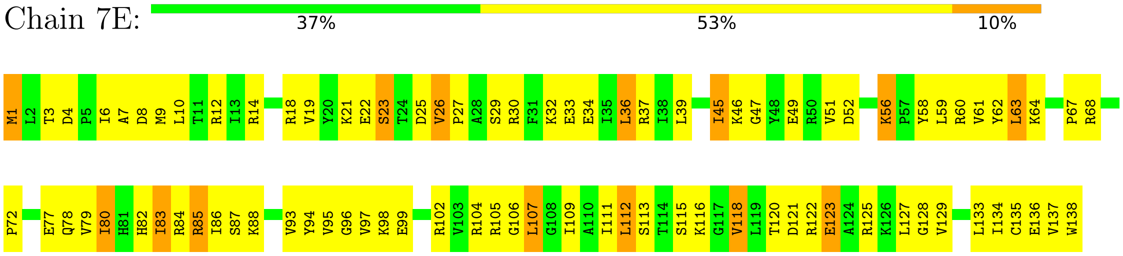
- Molecule 7: 30S ribosomal protein S7

Chain 62:



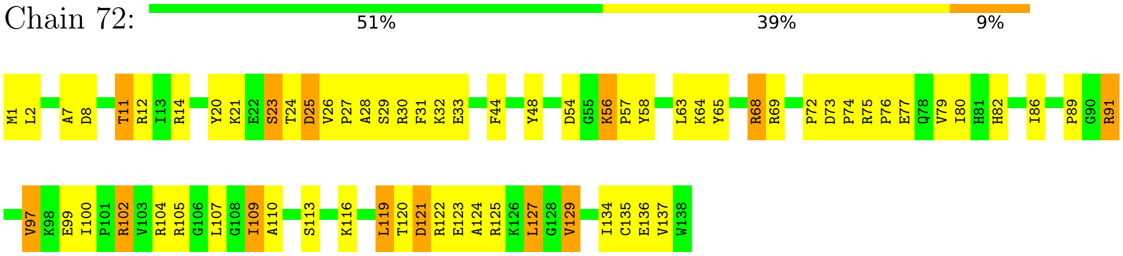
- Molecule 8: 30S ribosomal protein S8

Chain 7E:



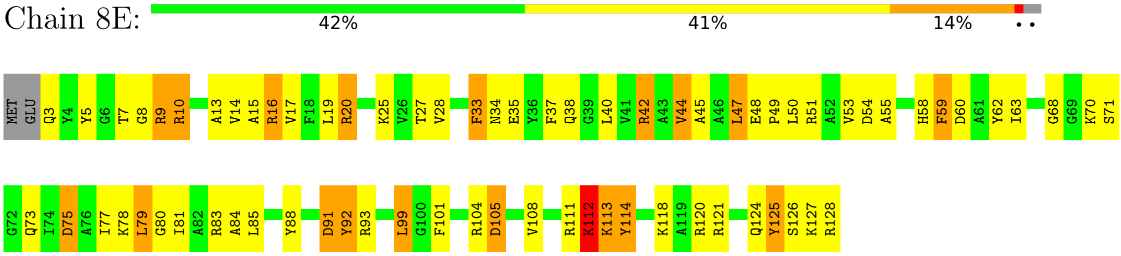
- Molecule 8: 30S ribosomal protein S8

Chain 72:



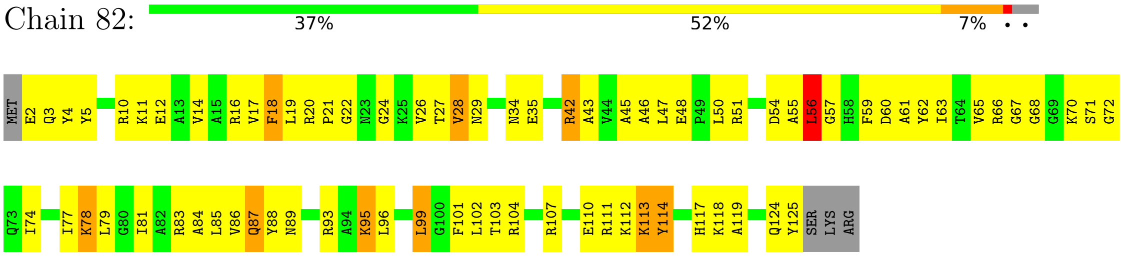
- Molecule 9: 30S ribosomal protein S9

Chain 8E:



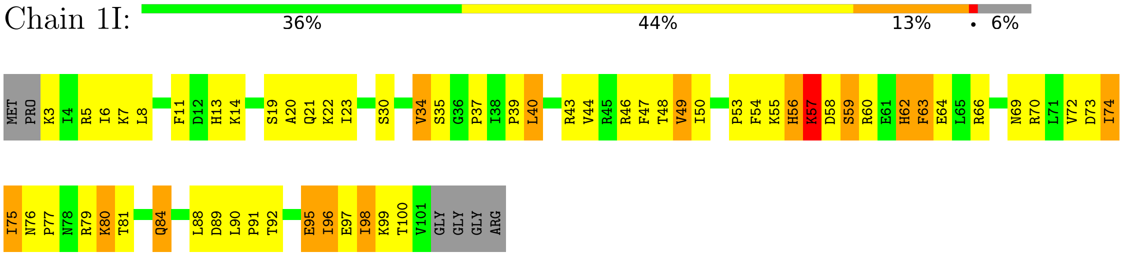
- Molecule 9: 30S ribosomal protein S9

Chain 82:



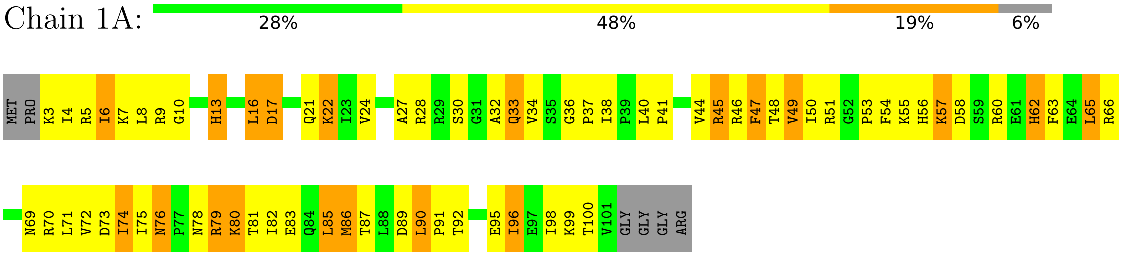
- Molecule 10: 30S ribosomal protein S10

Chain 1I:



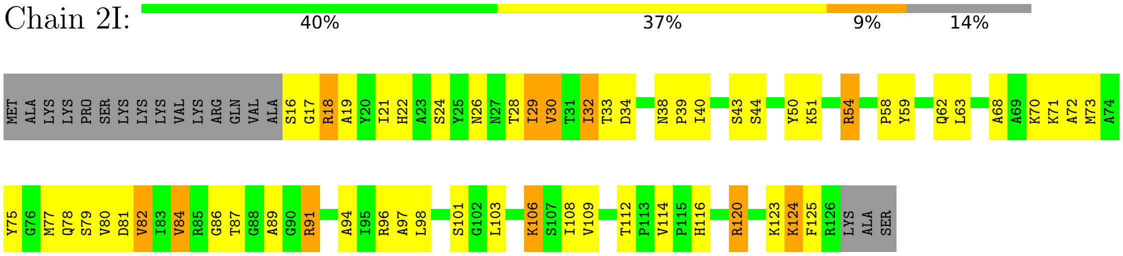
- Molecule 10: 30S ribosomal protein S10

Chain 1A:



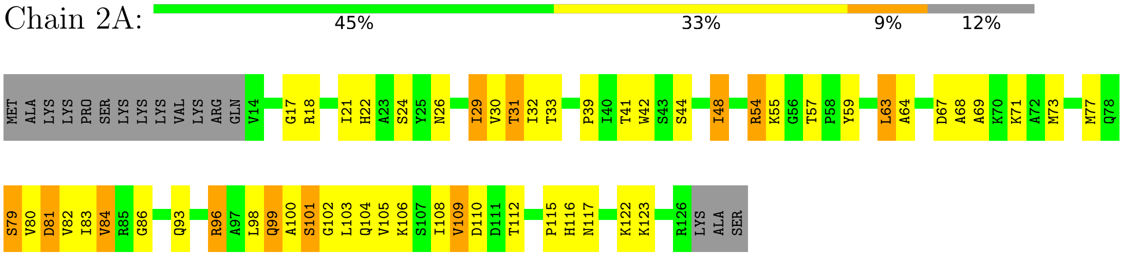
- Molecule 11: 30S ribosomal protein S11

Chain 2I:



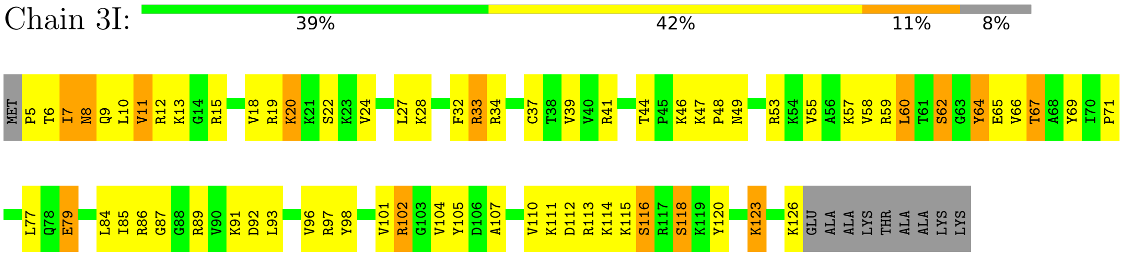
- Molecule 11: 30S ribosomal protein S11

Chain 2A:



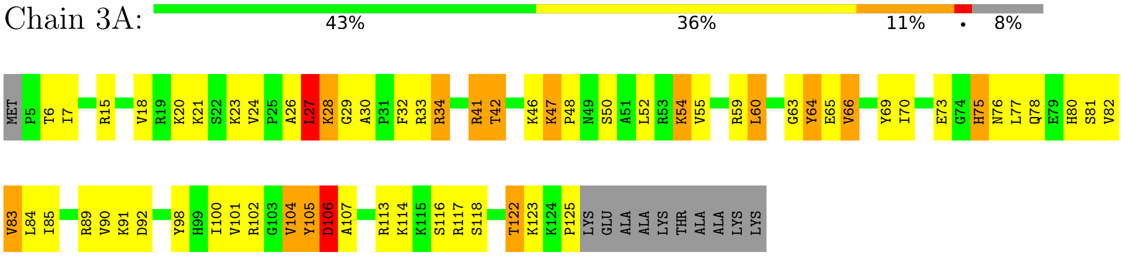
- Molecule 12: 30S ribosomal protein S12

Chain 3I:



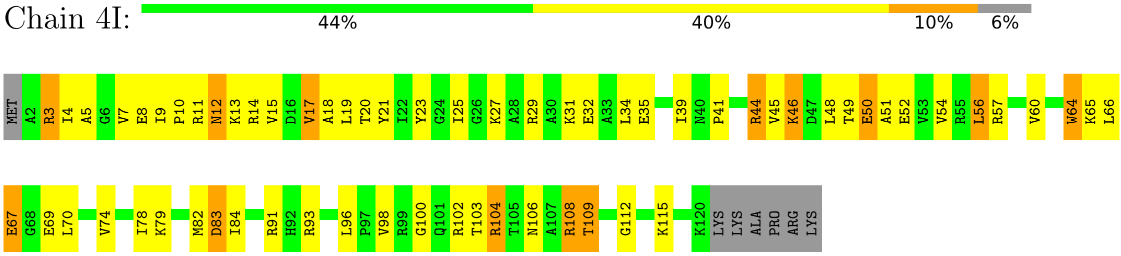
- Molecule 12: 30S ribosomal protein S12

Chain 3A:



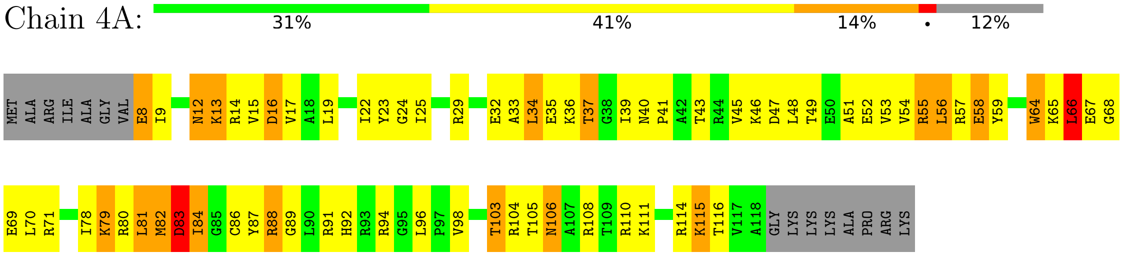
- Molecule 13: 30S ribosomal protein S13

Chain 4I:



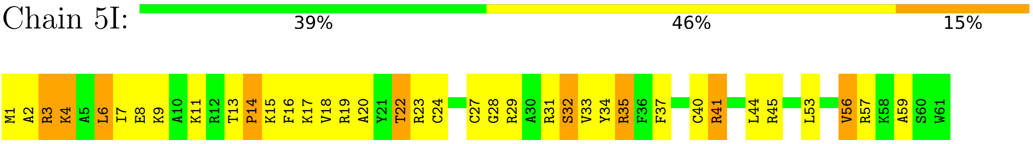
- Molecule 13: 30S ribosomal protein S13

Chain 4A:

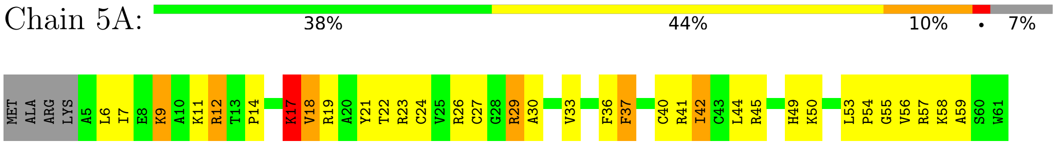


- Molecule 14: 30S ribosomal protein S14 type Z

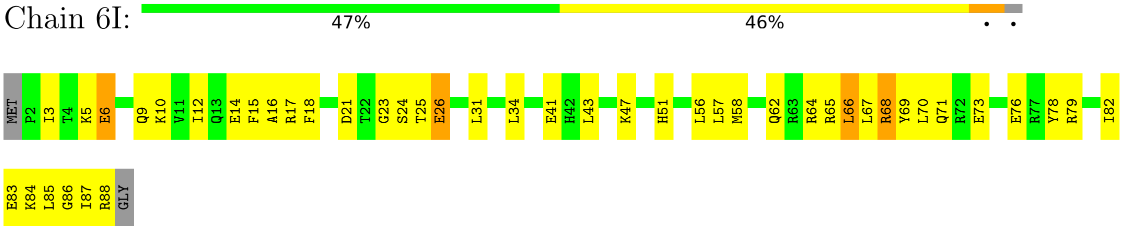
Chain 5I:



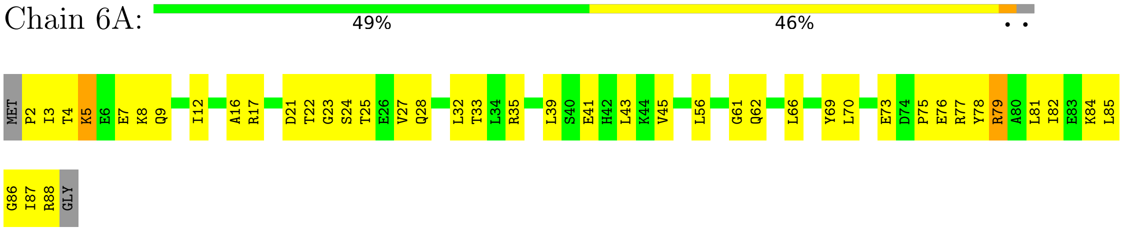
- Molecule 14: 30S ribosomal protein S14 type Z



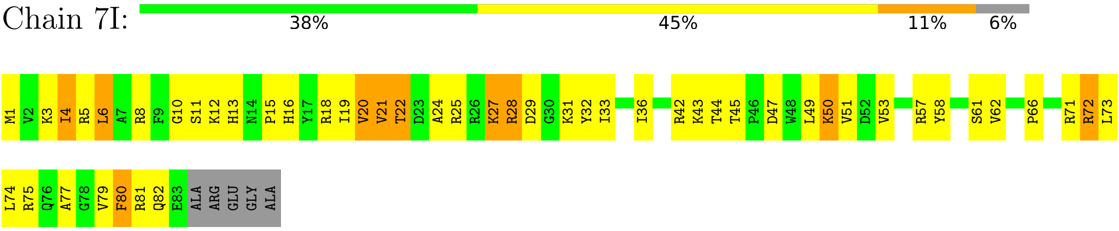
- Molecule 15: 30S ribosomal protein S15



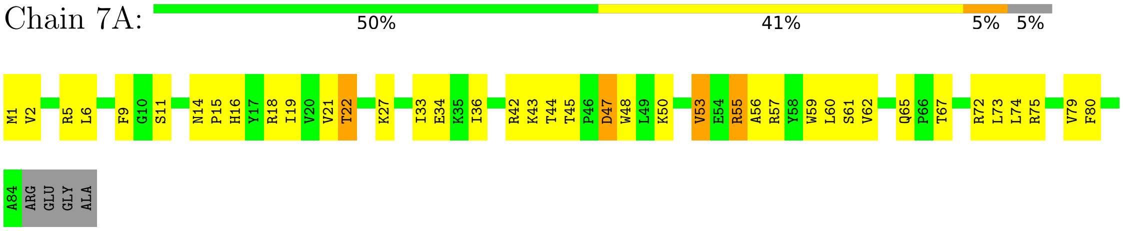
- Molecule 15: 30S ribosomal protein S15



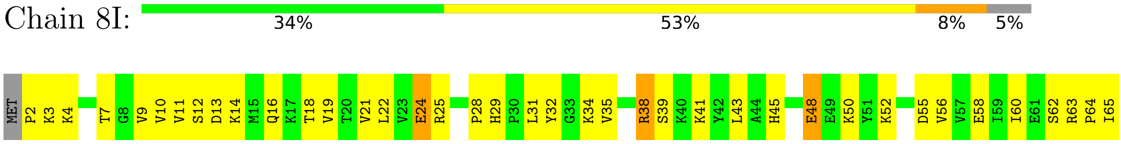
- Molecule 16: 30S ribosomal protein S16

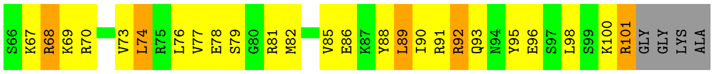


- Molecule 16: 30S ribosomal protein S16



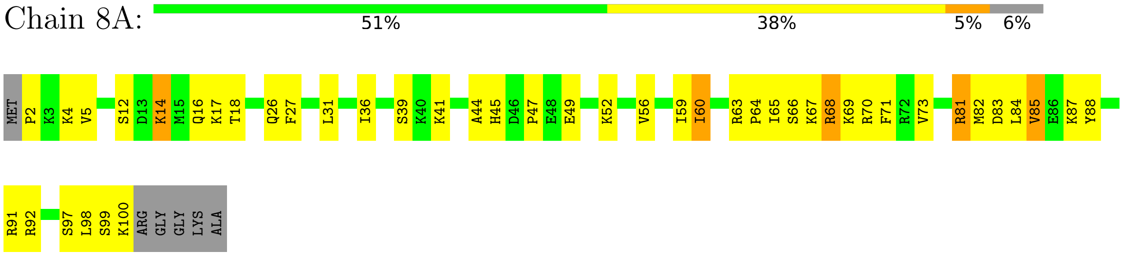
- Molecule 17: 30S ribosomal protein S17





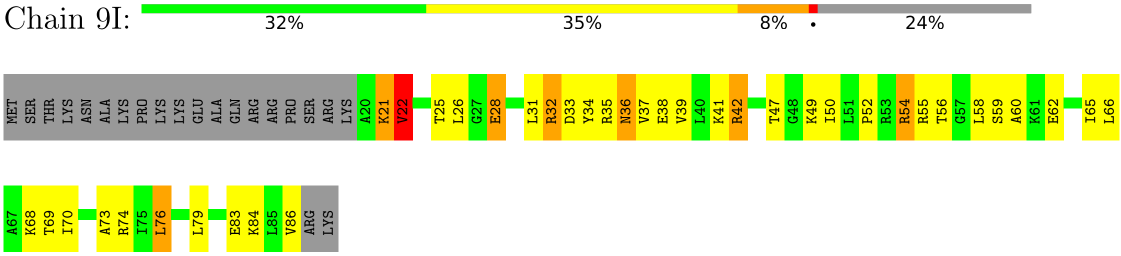
- Molecule 17: 30S ribosomal protein S17

Chain 8A:



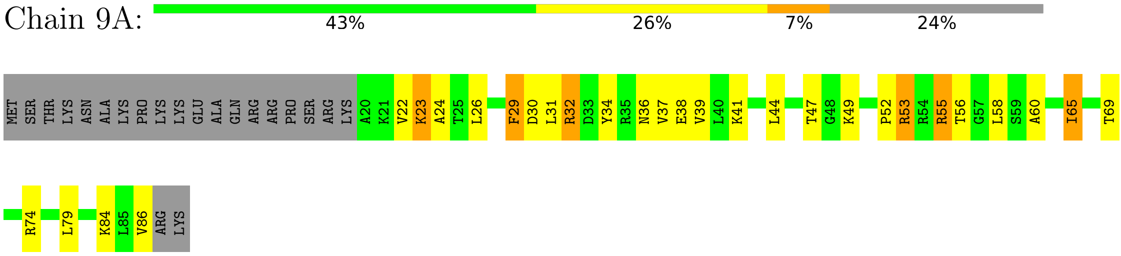
- Molecule 18: 30S ribosomal protein S18

Chain 9I:



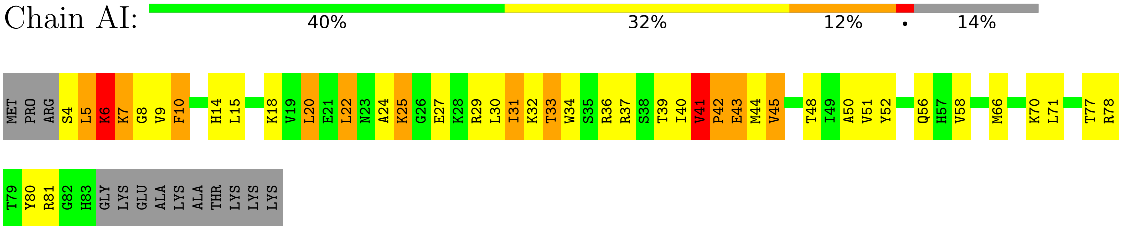
- Molecule 18: 30S ribosomal protein S18

Chain 9A:



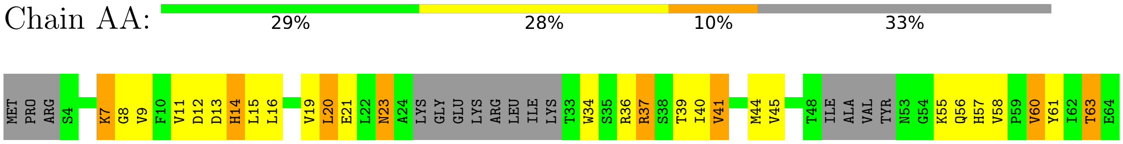
- Molecule 19: 30S ribosomal protein S19

Chain AI:



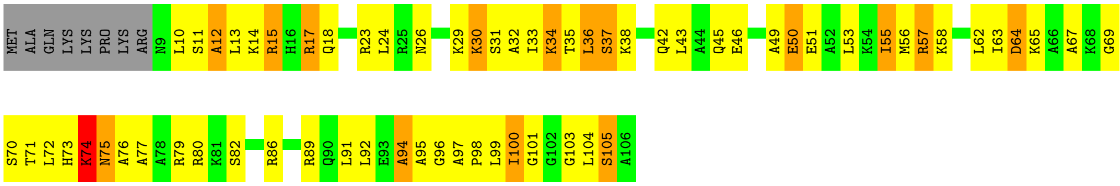
- Molecule 19: 30S ribosomal protein S19

Chain AA:



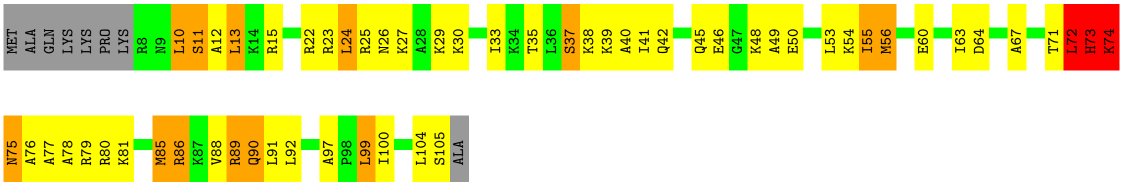
- Molecule 20: 30S ribosomal protein S20

Chain BI:



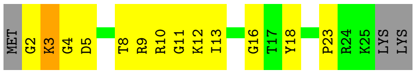
- Molecule 20: 30S ribosomal protein S20

Chain BA:



- Molecule 21: 30S ribosomal protein Thx

Chain 1F:

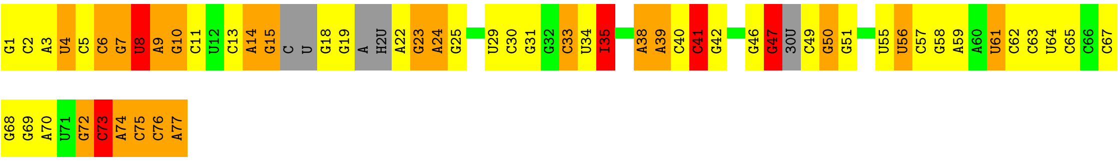


- Molecule 21: 30S ribosomal protein Thx

Chain 1B:

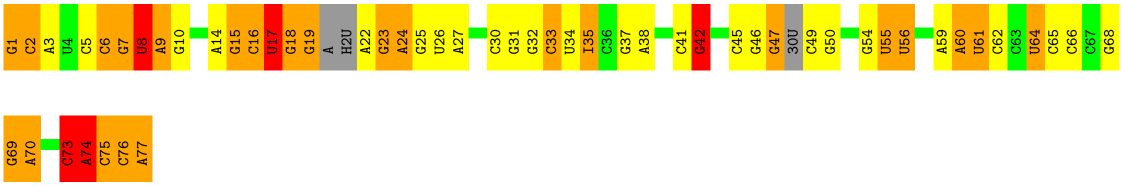
- Molecule 22: tRNAArg

Chain 1K:



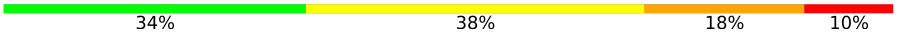
- Molecule 22: tRNAArg

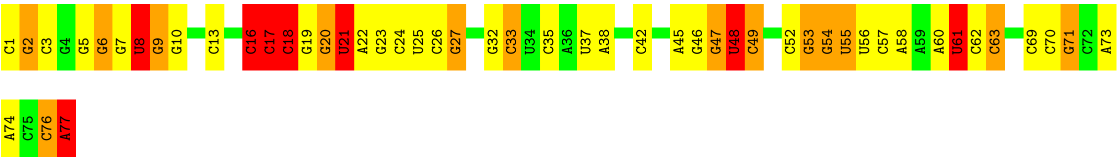
Chain 1L:



- Molecule 23: tRNAfMet

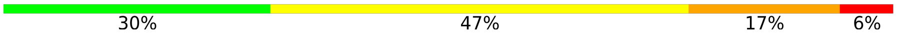
Chain 2K:

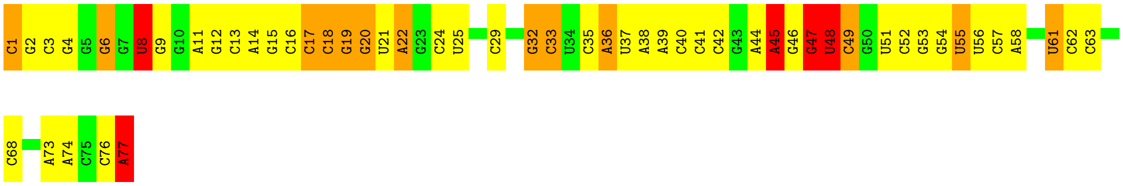




- Molecule 23: tRNAfMet

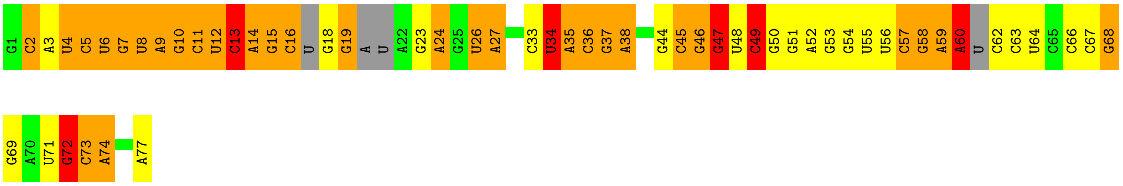
Chain 2L:





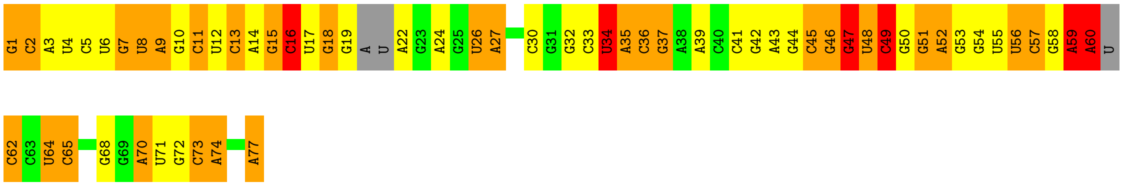
- Molecule 24: tRNAArg

Chain 3K:



- Molecule 24: tRNAArg

Chain 3L:



- Molecule 25: mRNA

Chain 4K:

- Molecule 25: mRNA

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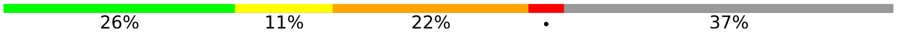

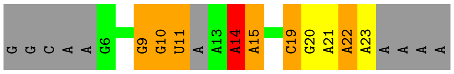

- Molecule 26: 23S ribosomal RNA

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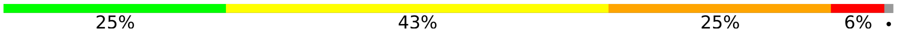

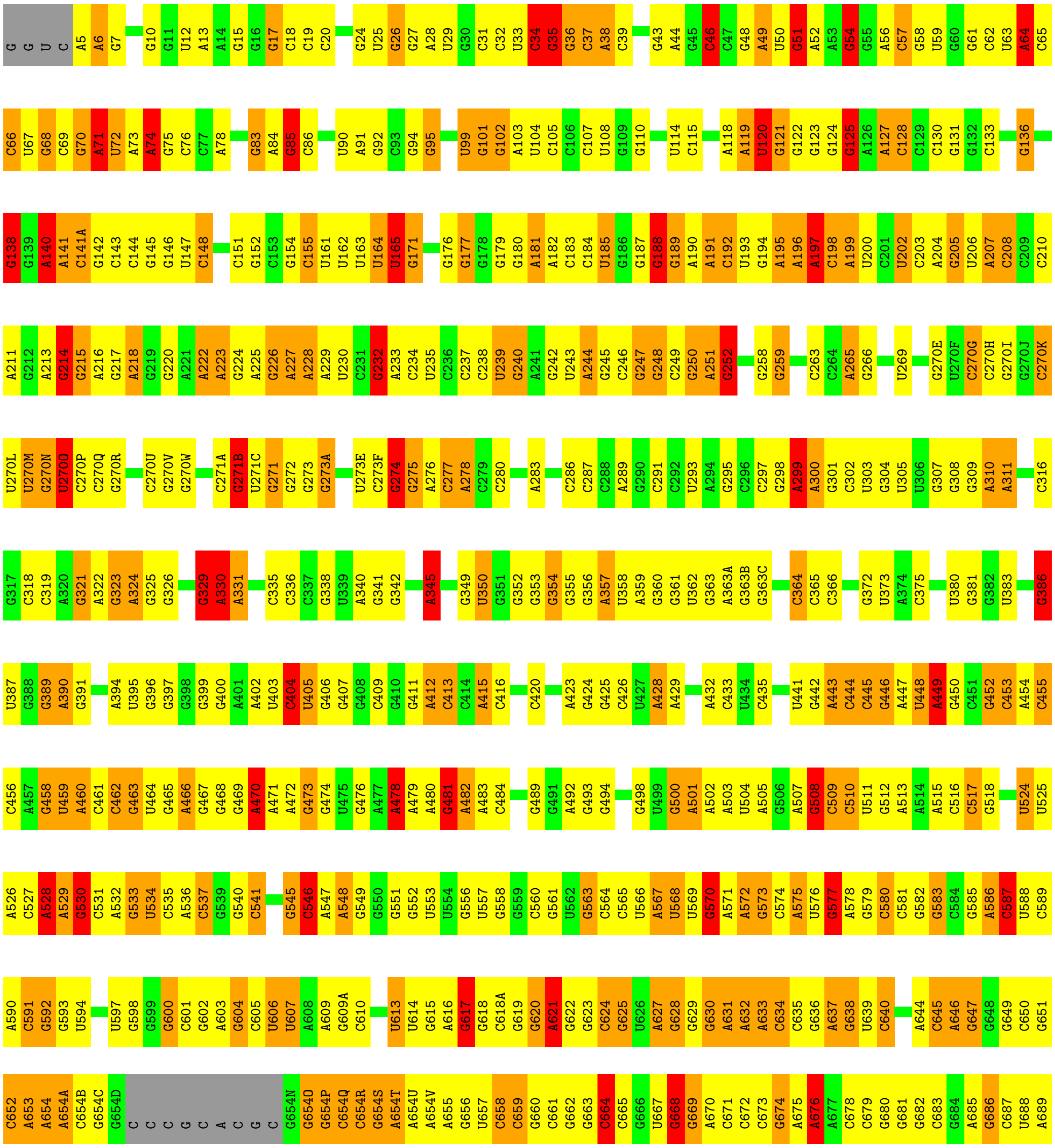

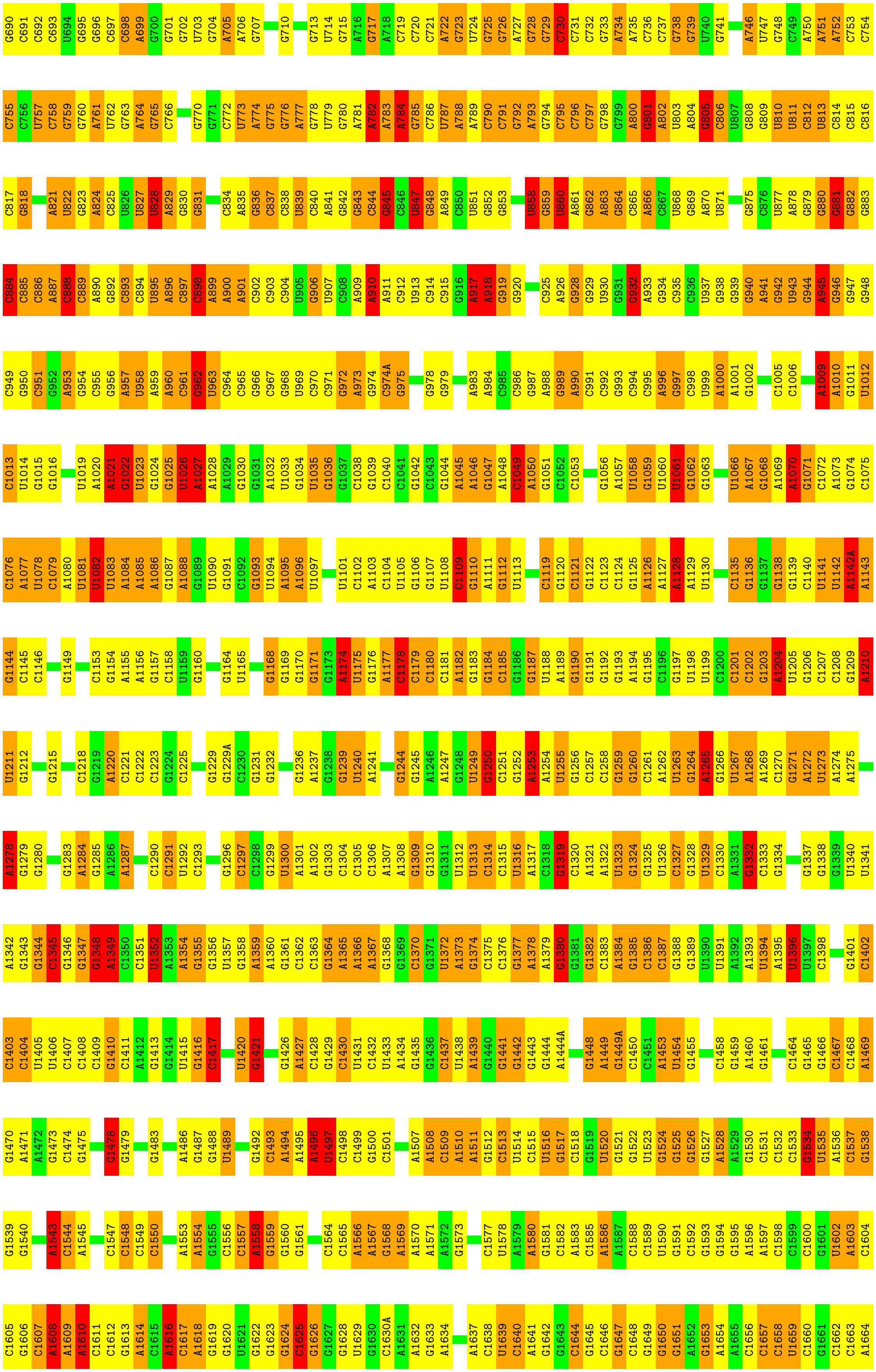
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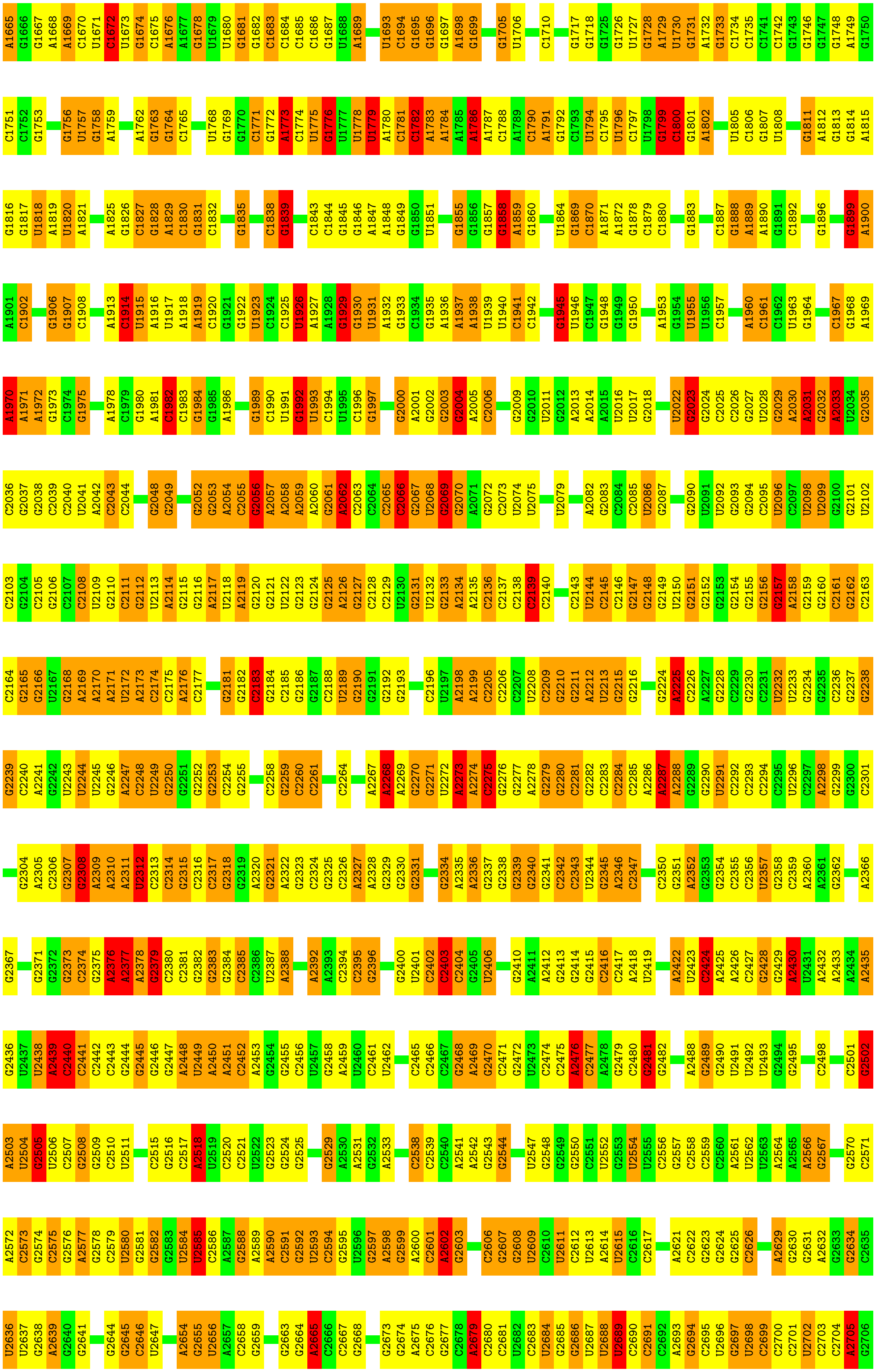
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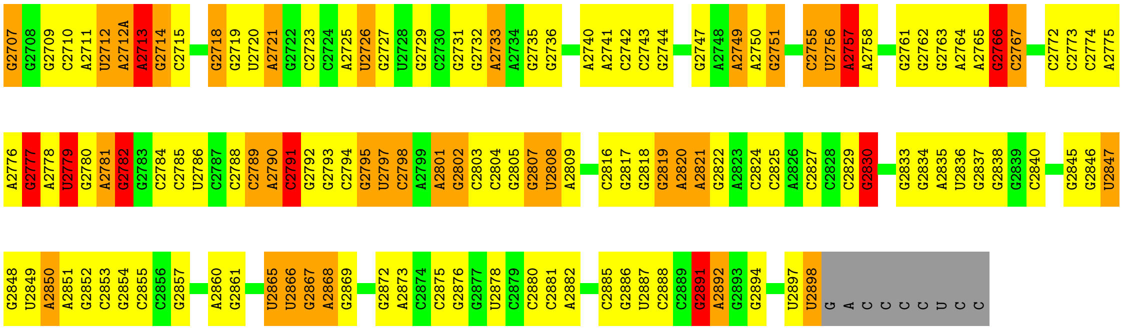
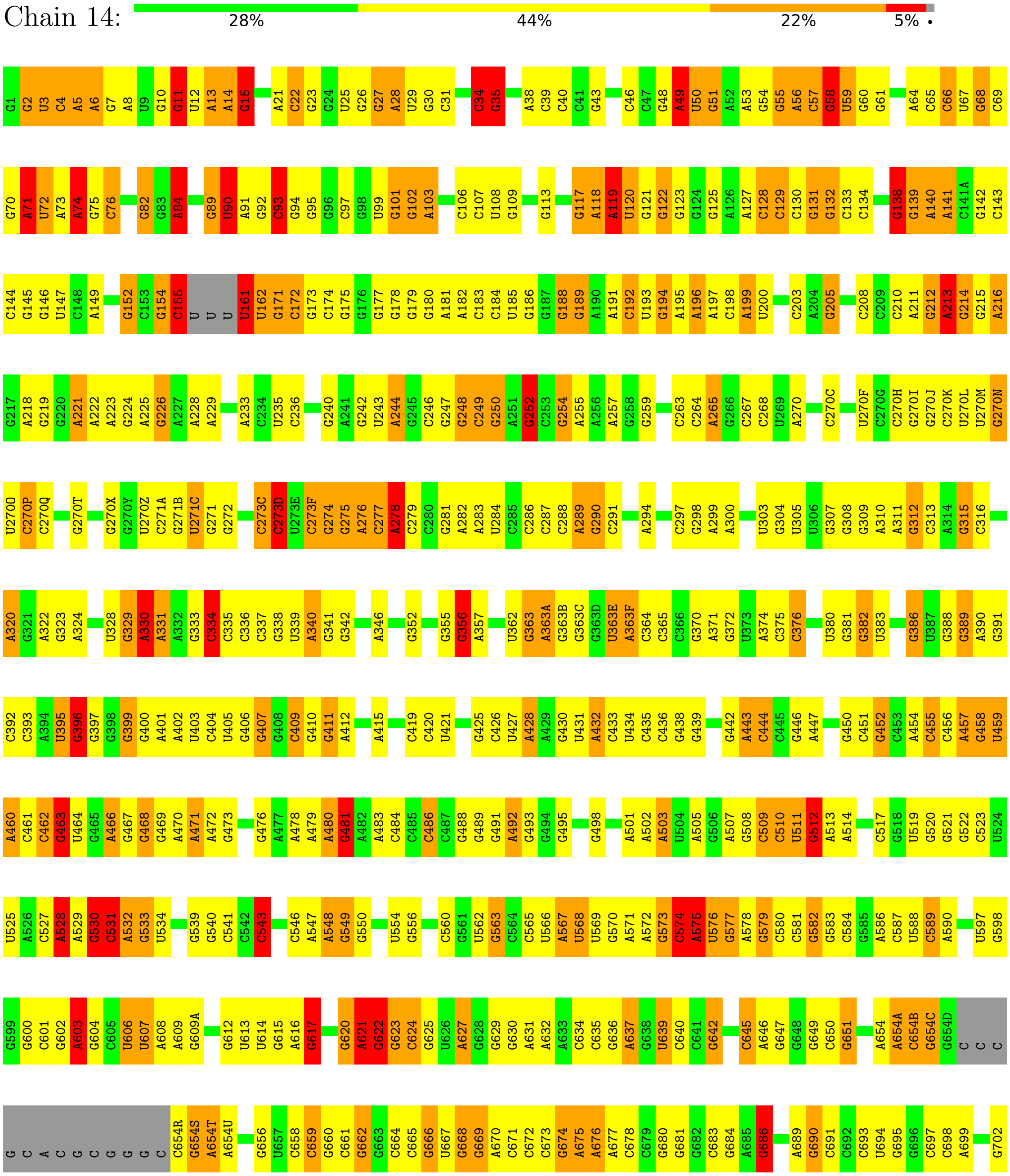
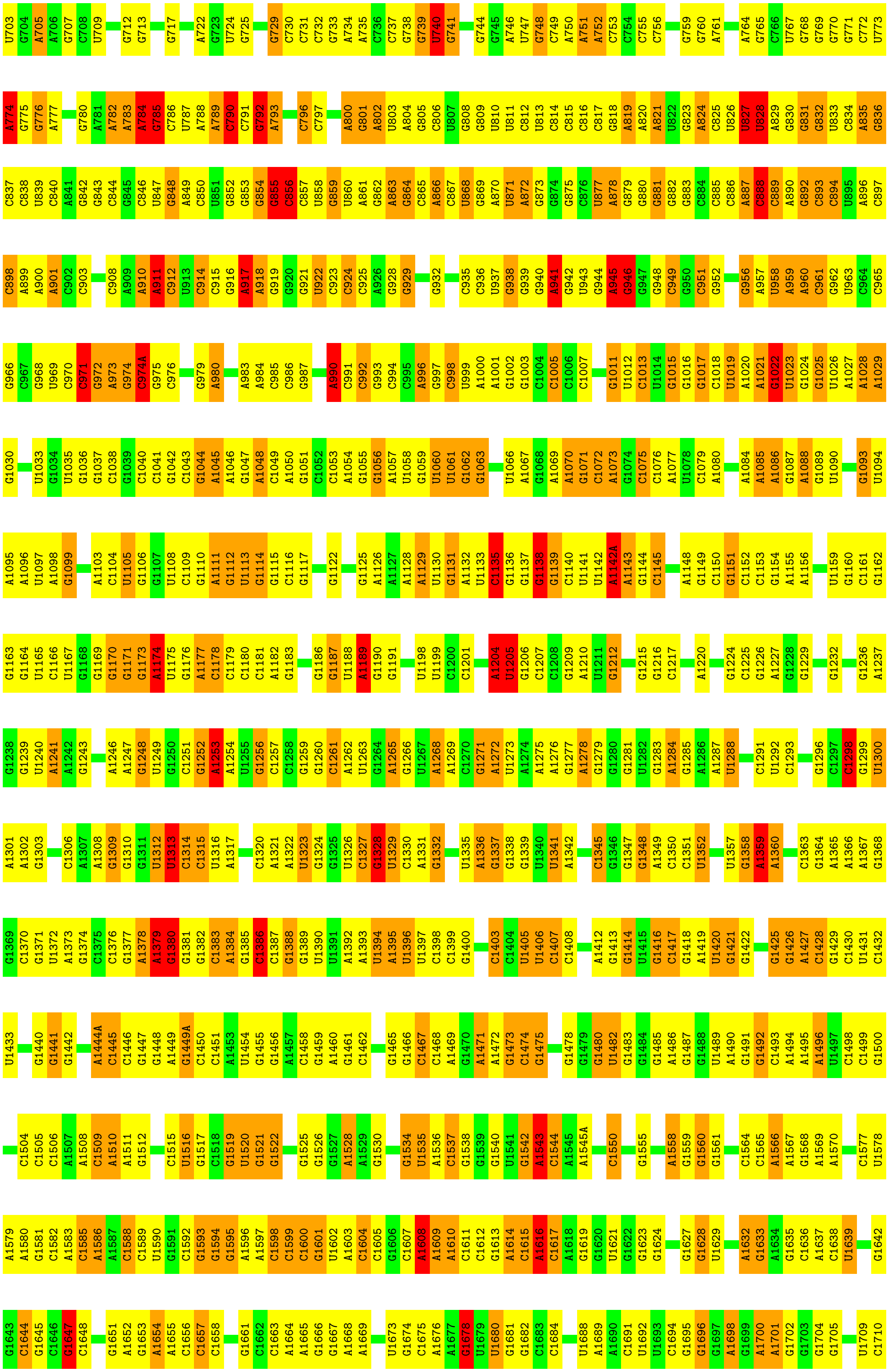


- Molecule 26: 23S ribosomal RNA

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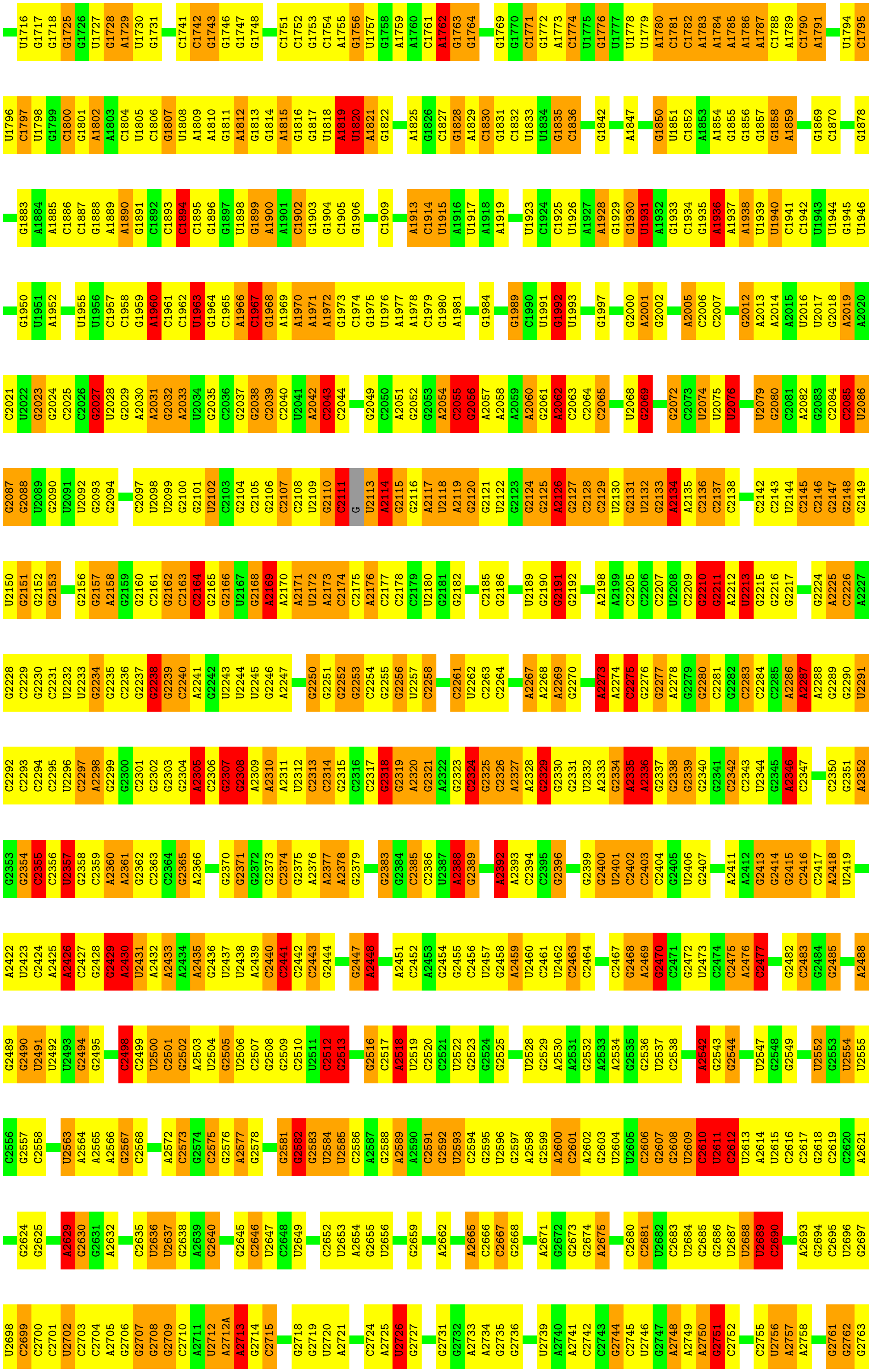
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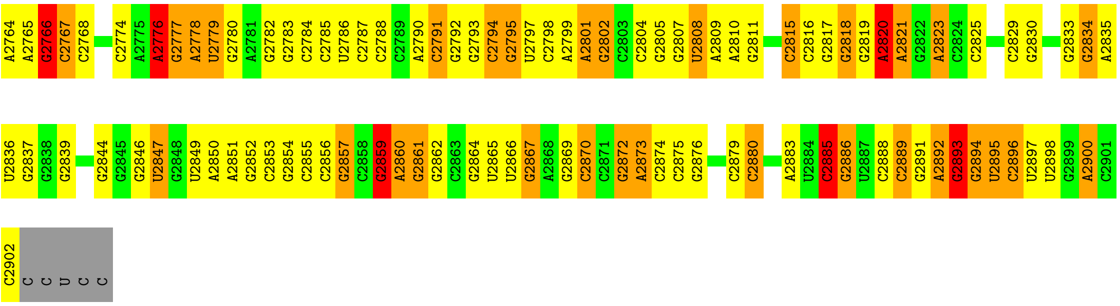

- Molecule 27: 5S ribosomal RNA

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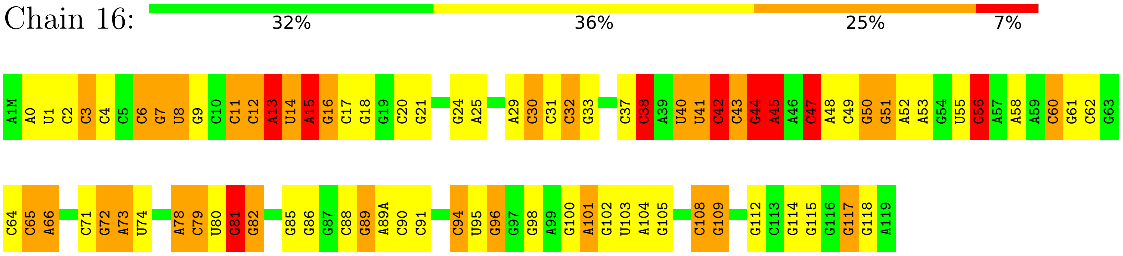

- Molecule 27: 5S ribosomal RNA

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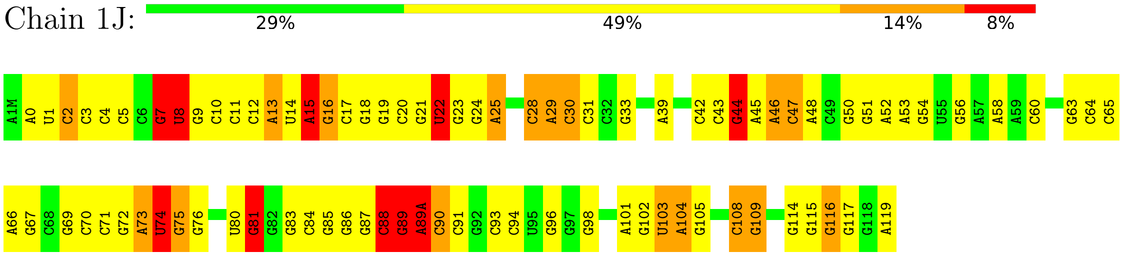

- Molecule 28: 50S ribosomal protein L1

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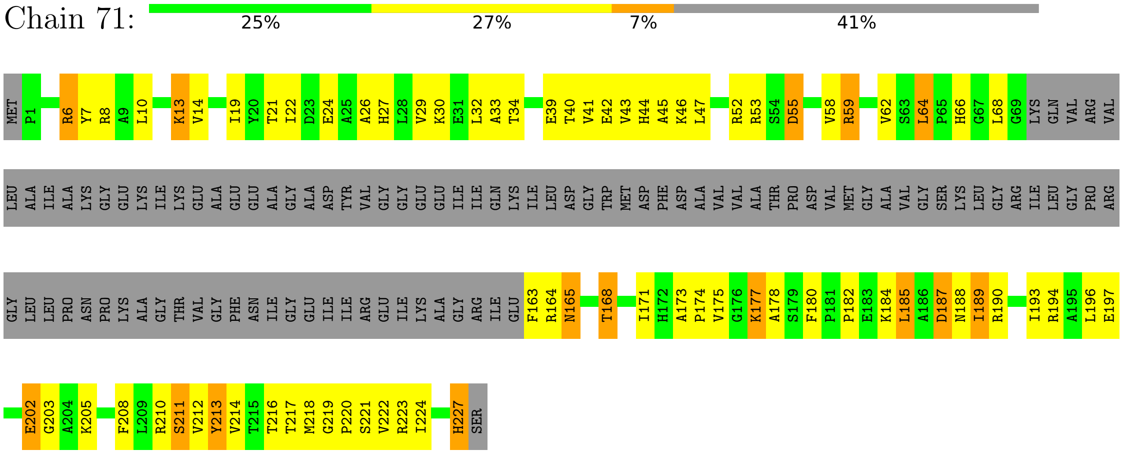

- Molecule 28: 50S ribosomal protein L1

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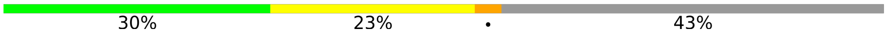
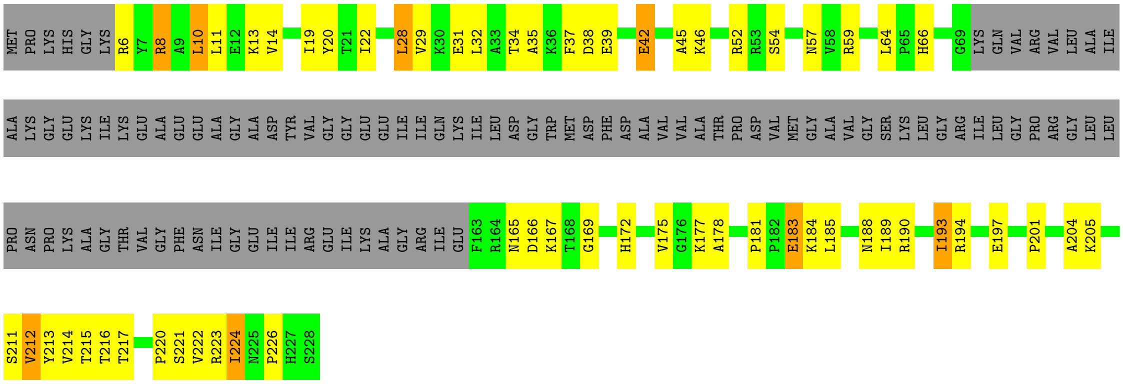
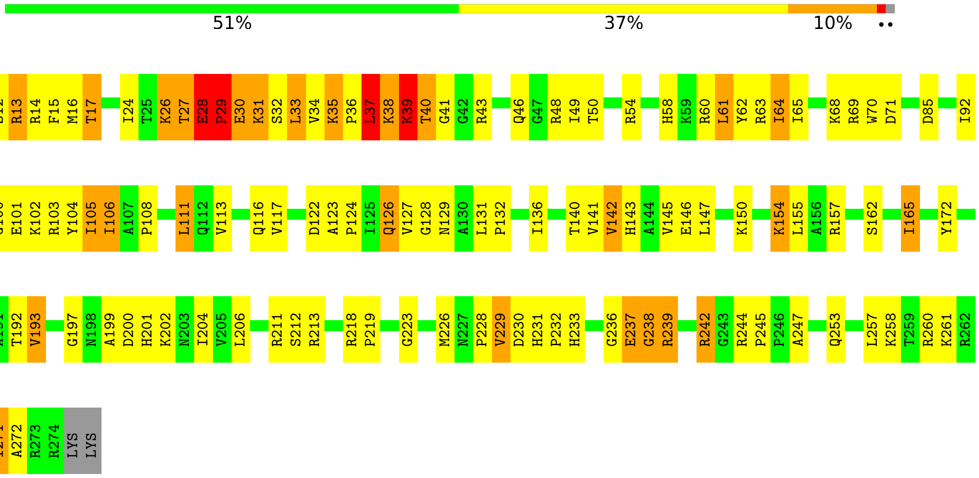




- Molecule 29: 50S ribosomal protein L2

Chain 11:



- Molecule 29: 50S ribosomal protein L2

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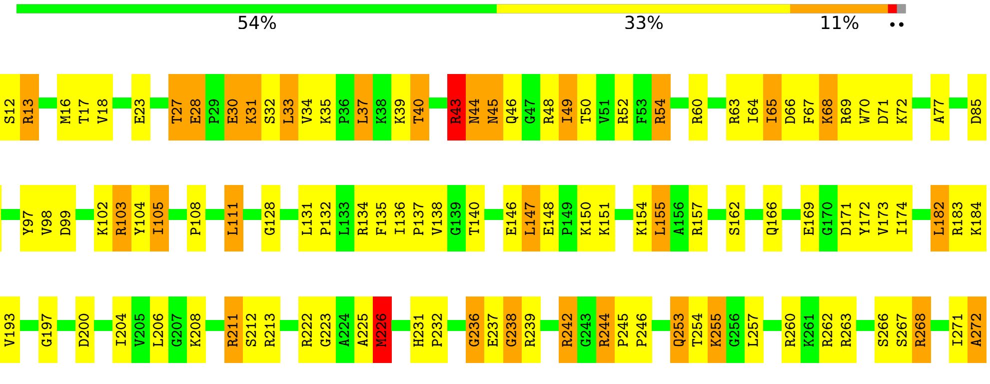

- Molecule 30: 50S ribosomal protein L3

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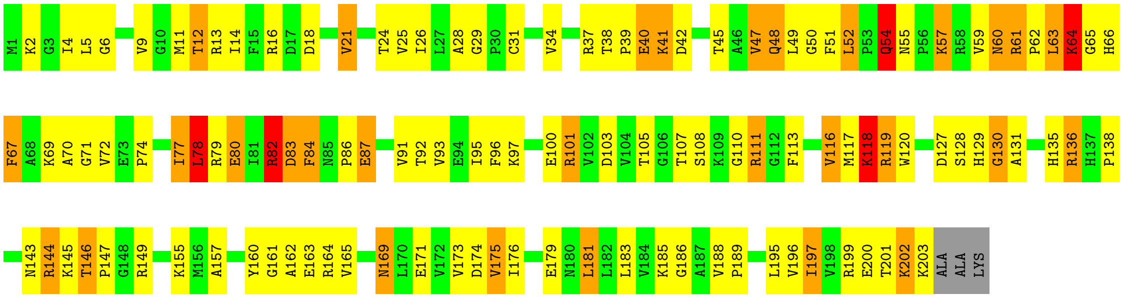

- Molecule 30: 50S ribosomal protein L3

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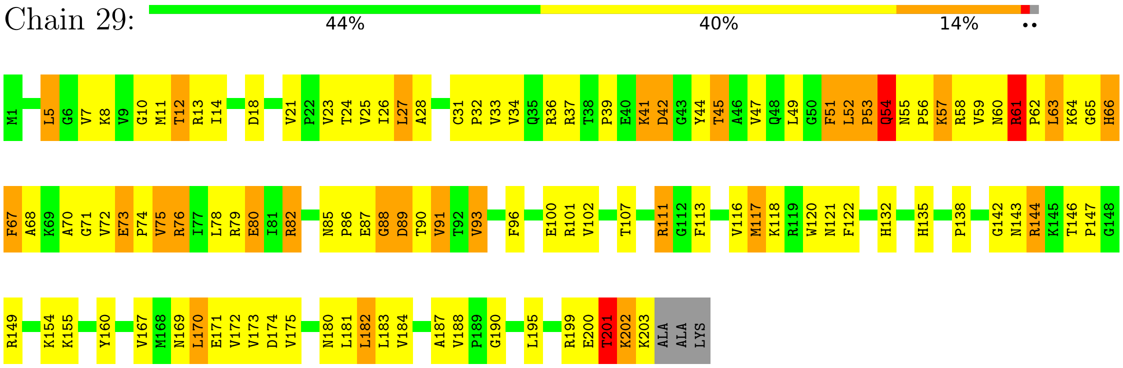
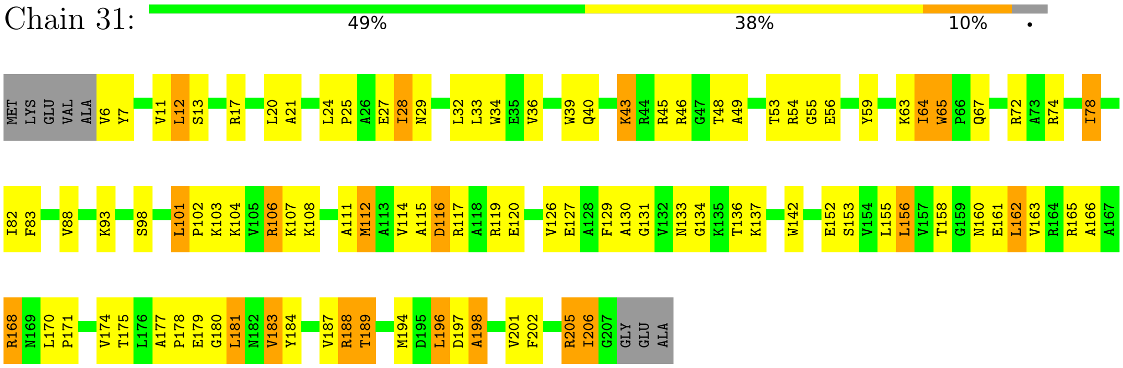


- Molecule 31: 50S ribosomal protein L4

Chain 31:



- Molecule 31: 50S ribosomal protein L4

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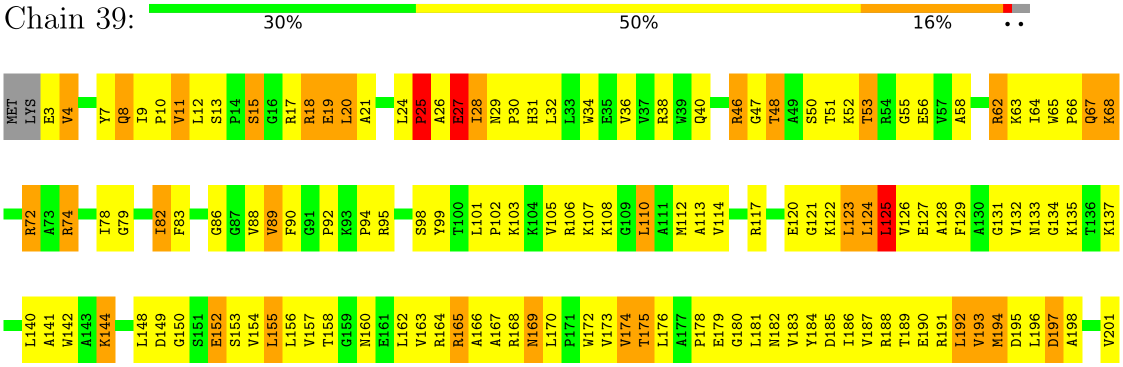
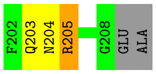
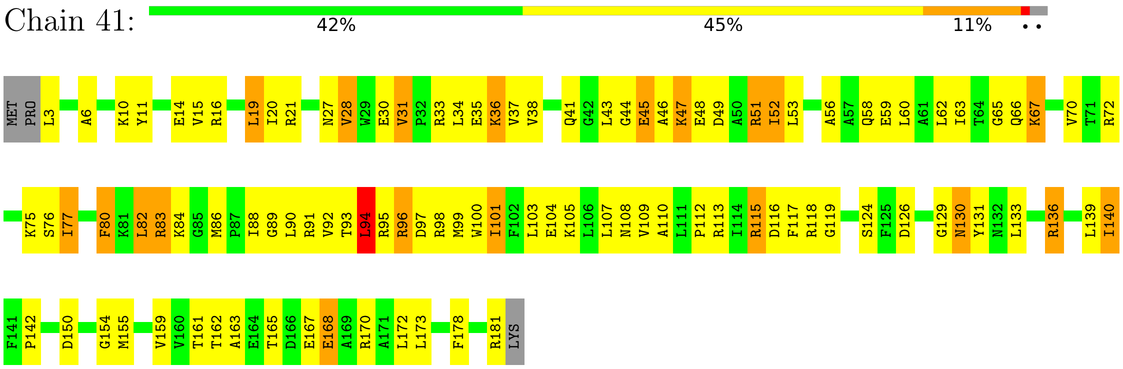
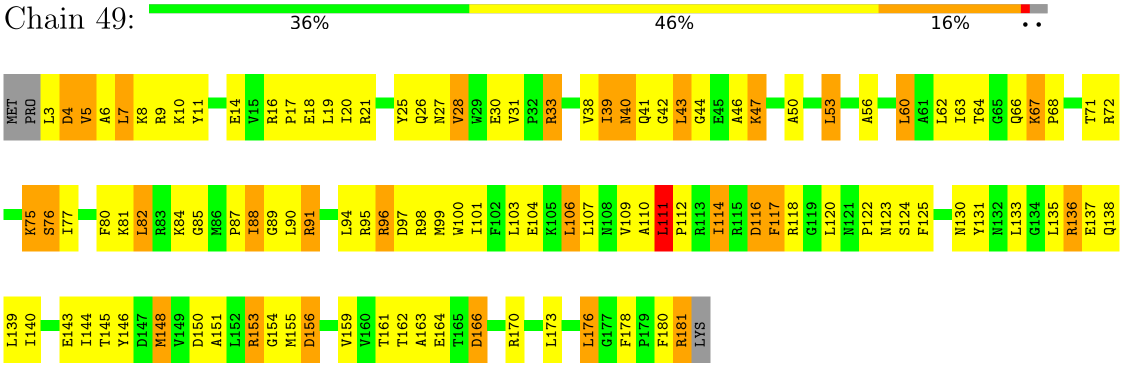




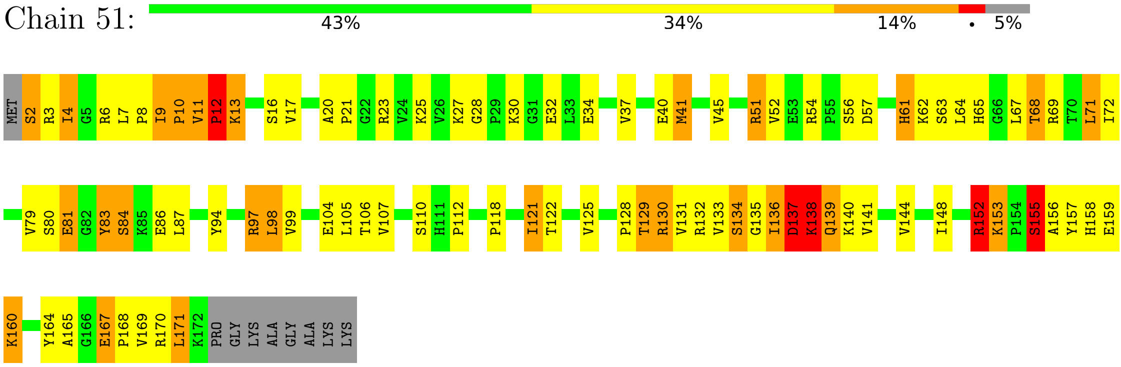
- Molecule 32: 50S ribosomal protein L5



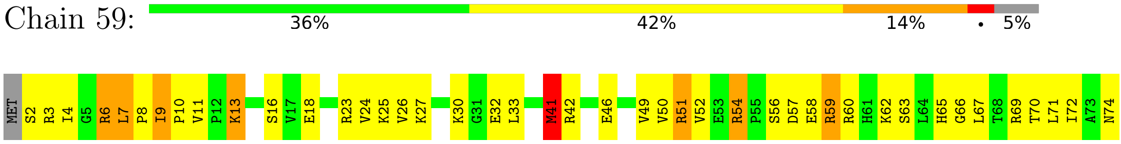
- Molecule 32: 50S ribosomal protein L5

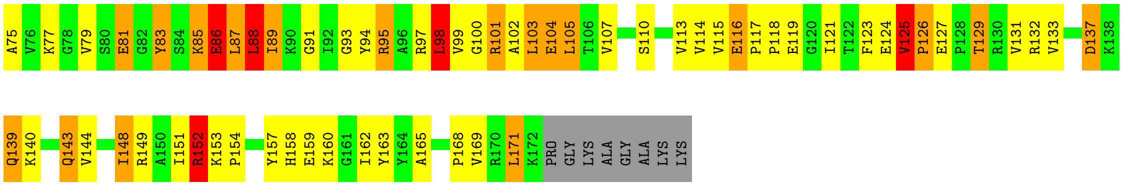


- Molecule 33: 50S ribosomal protein L6

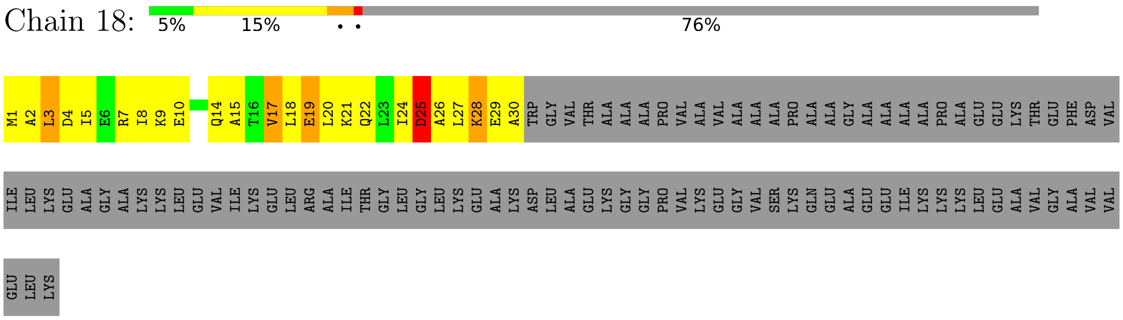


- Molecule 33: 50S ribosomal protein L6

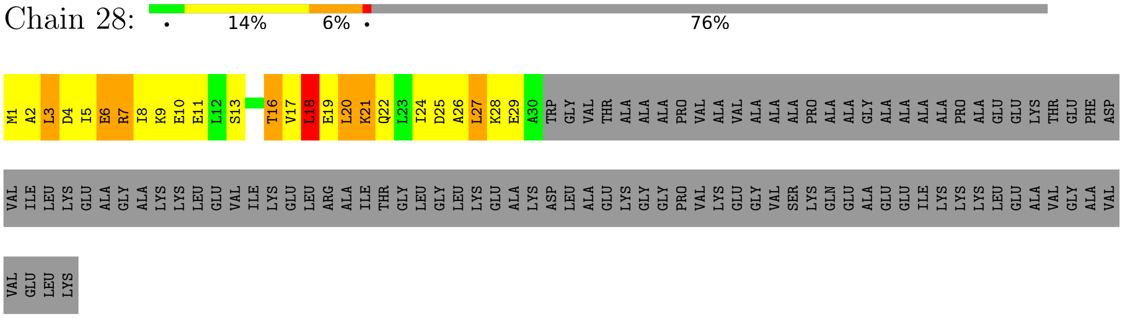




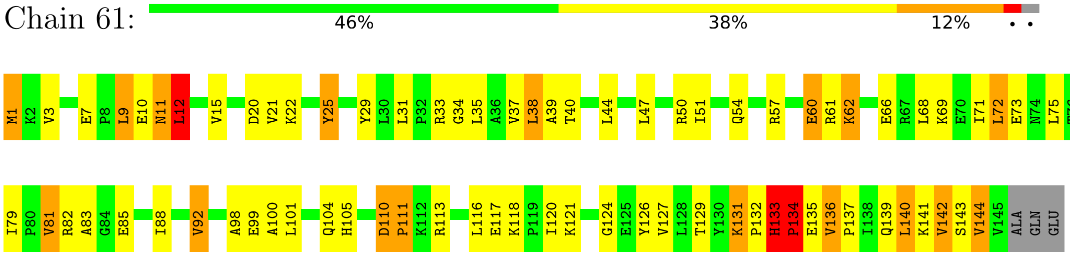
- Molecule 34: 50S ribosomal protein L7/L12



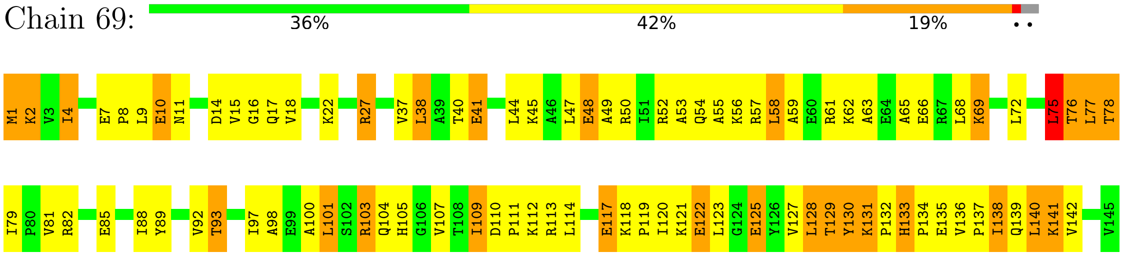
- Molecule 34: 50S ribosomal protein L7/L12



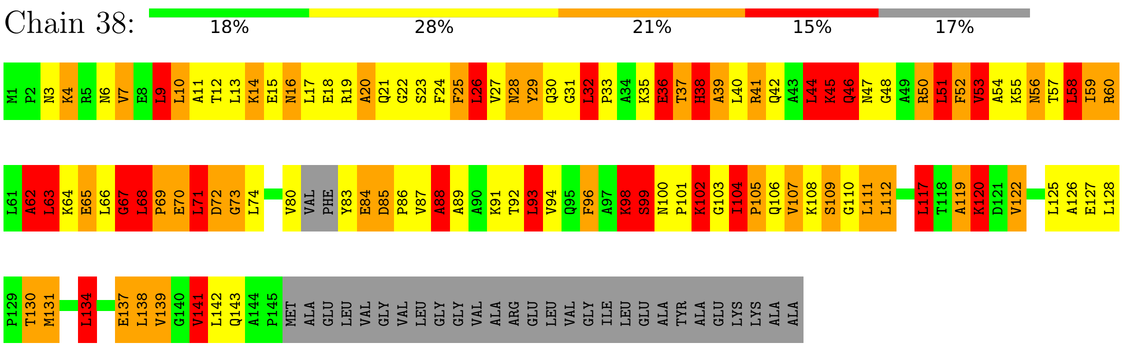
- Molecule 35: 50S ribosomal protein L9



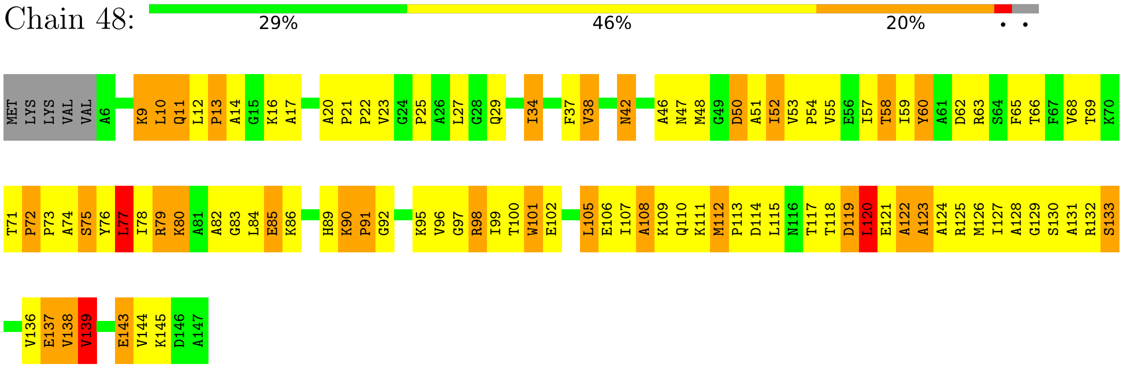
- Molecule 35: 50S ribosomal protein L9



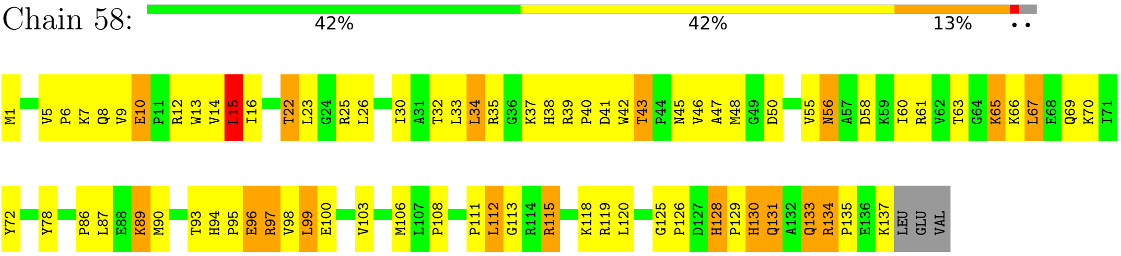
- Molecule 36: 50S ribosomal protein L10



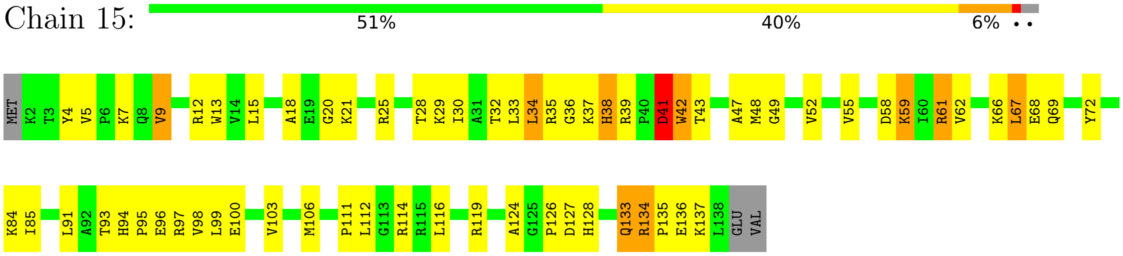
- Molecule 37: 50S ribosomal protein L11



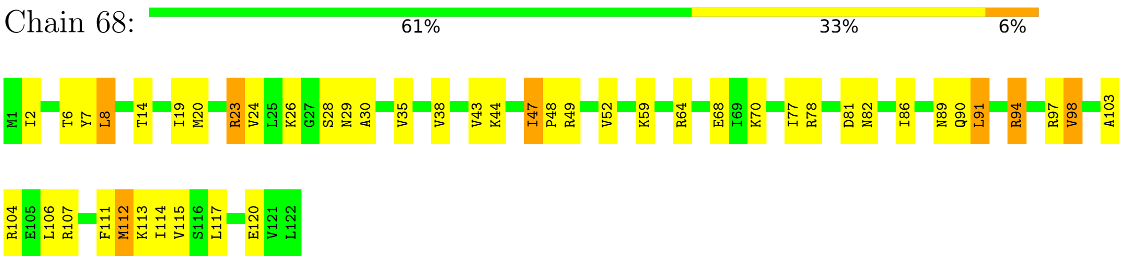
- Molecule 38: 50S ribosomal protein L13



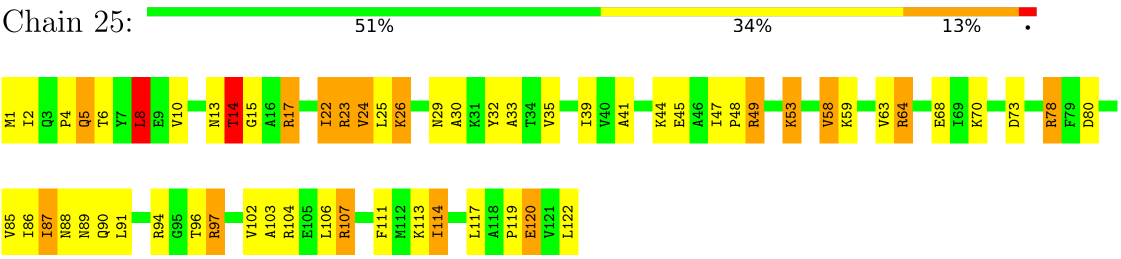
- Molecule 38: 50S ribosomal protein L13



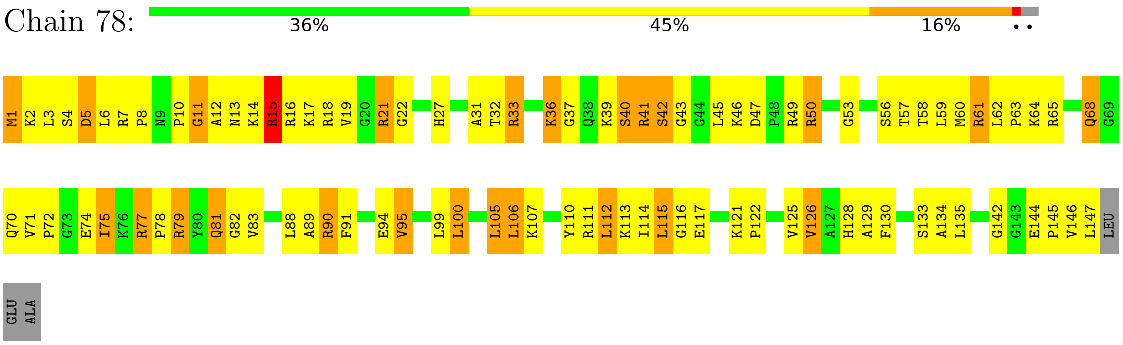
- Molecule 39: 50S ribosomal protein L14



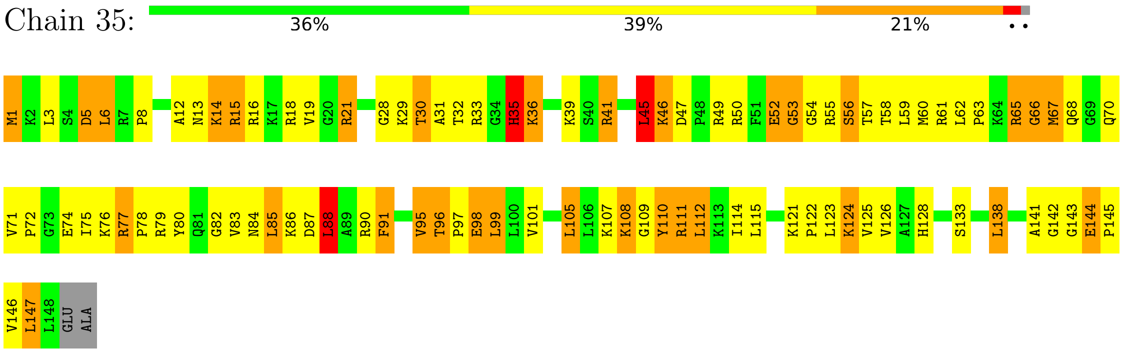
- Molecule 39: 50S ribosomal protein L14



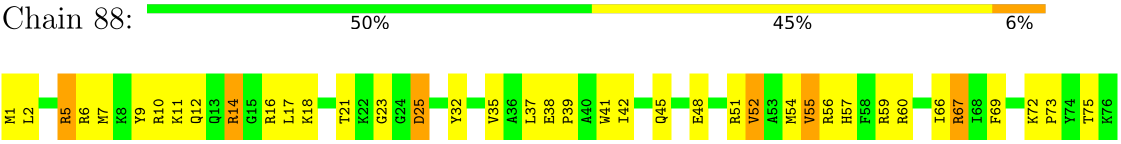
- Molecule 40: 50S ribosomal protein L15

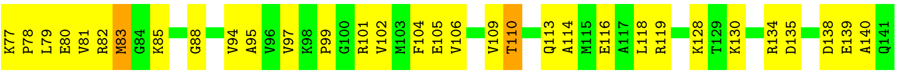


- Molecule 40: 50S ribosomal protein L15

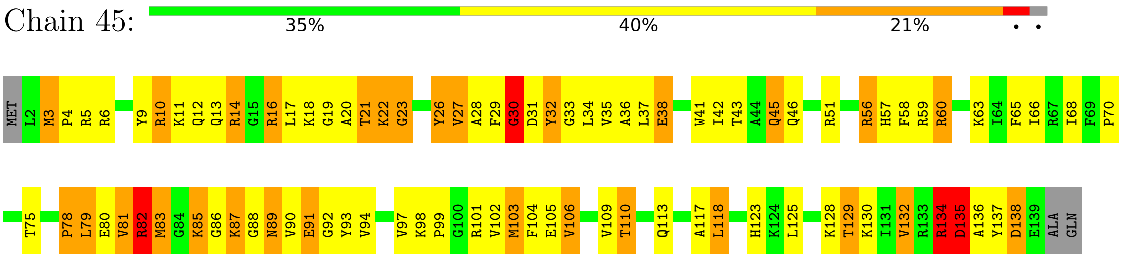


- Molecule 41: 50S ribosomal protein L16

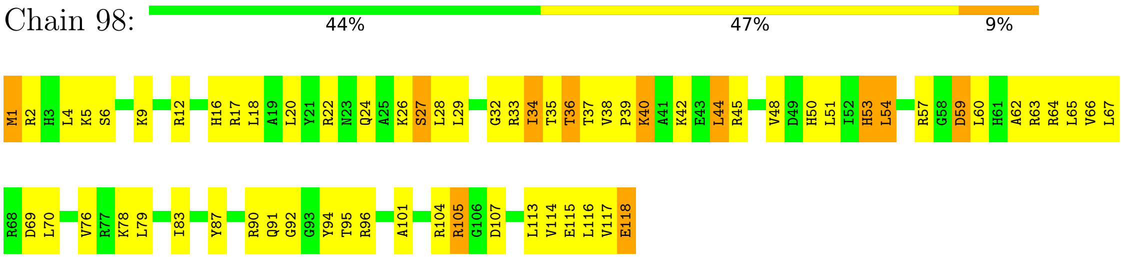




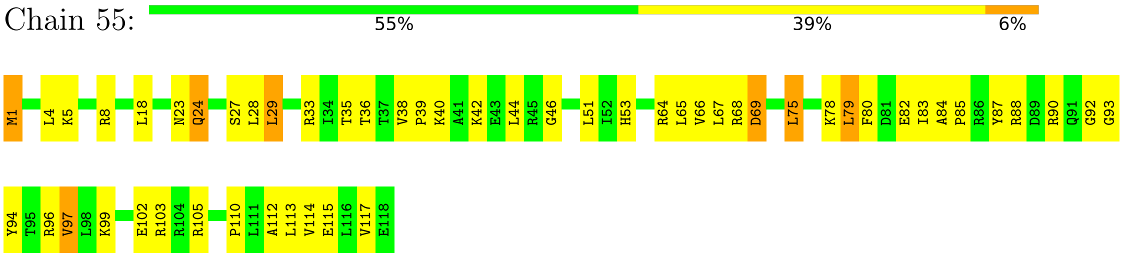
- Molecule 41: 50S ribosomal protein L16



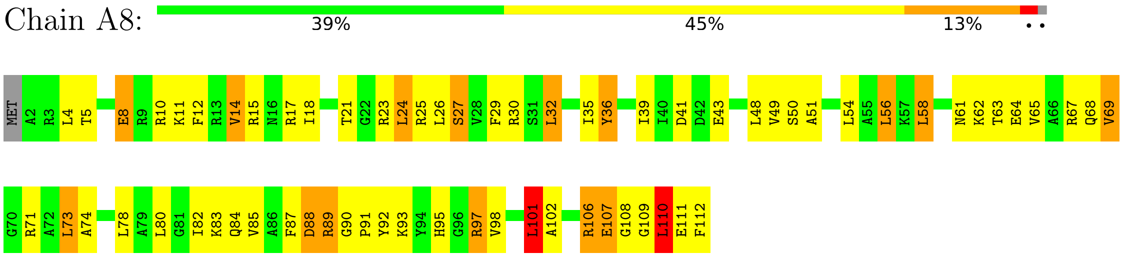
- Molecule 42: 50S ribosomal protein L17



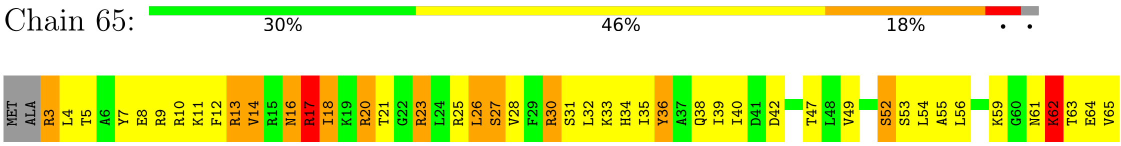
- Molecule 42: 50S ribosomal protein L17

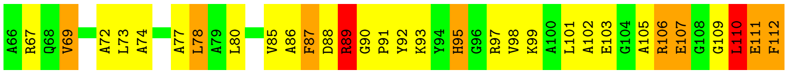


- Molecule 43: 50S ribosomal protein L18



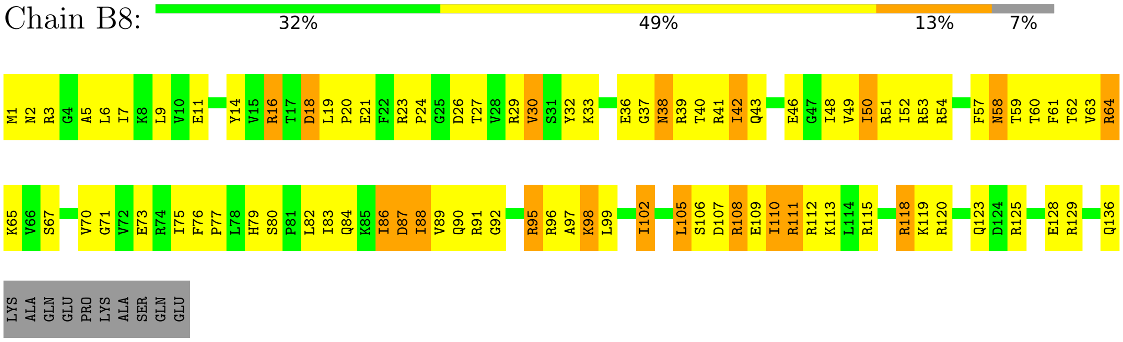
- Molecule 43: 50S ribosomal protein L18





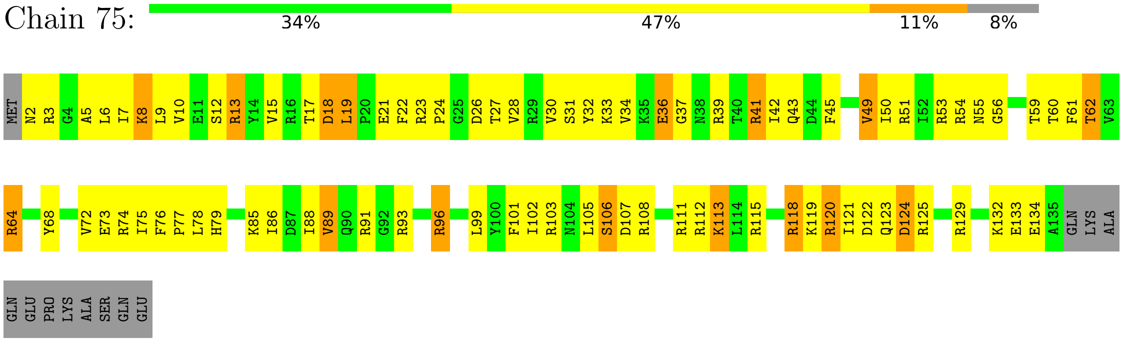
- Molecule 44: 50S ribosomal protein L19

Chain B8:



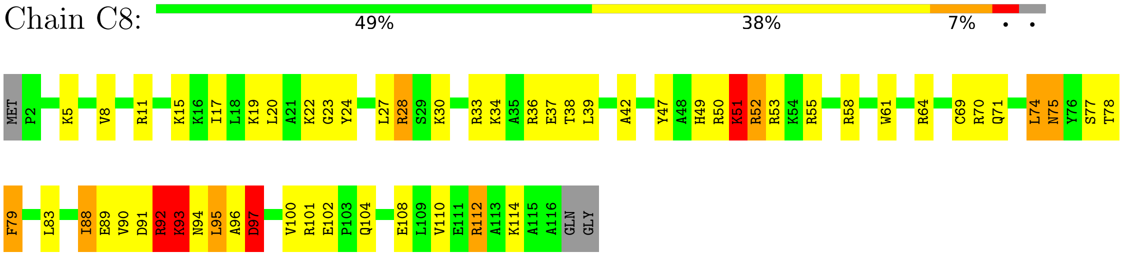
- Molecule 44: 50S ribosomal protein L19

Chain 75:



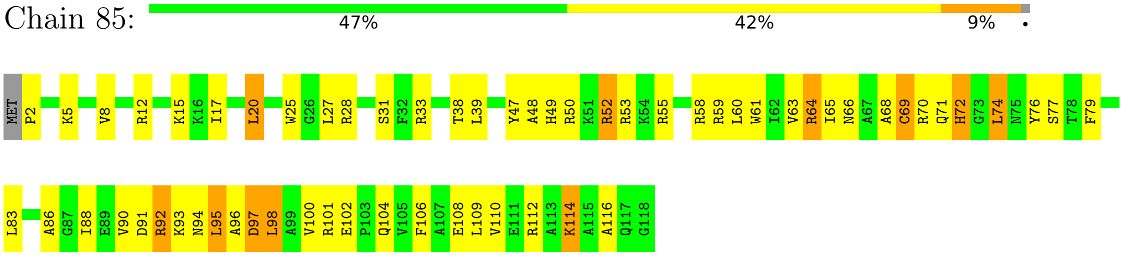
- Molecule 45: 50S ribosomal protein L20

Chain C8:



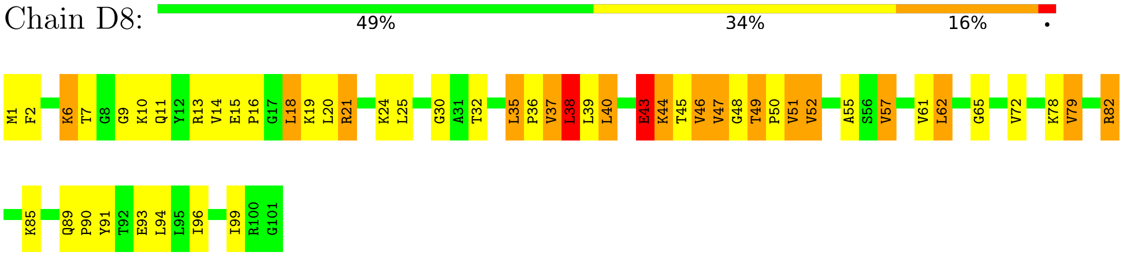
- Molecule 45: 50S ribosomal protein L20

Chain 85:



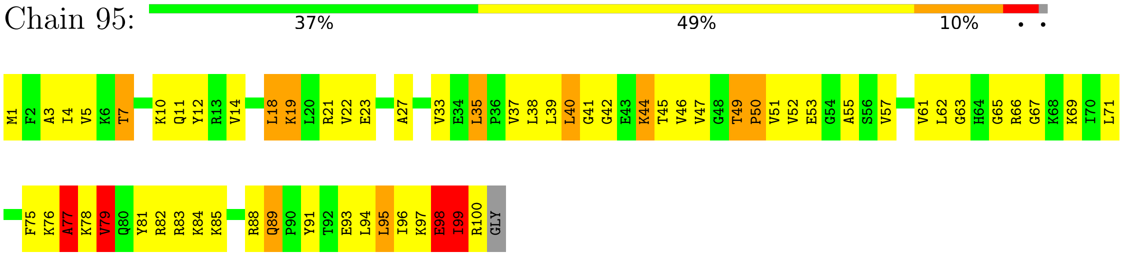
- Molecule 46: 50S ribosomal protein L21

Chain D8:



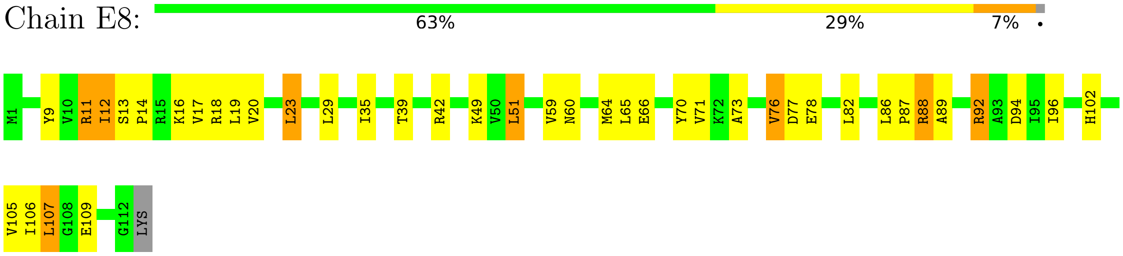
- Molecule 46: 50S ribosomal protein L21

Chain 95:



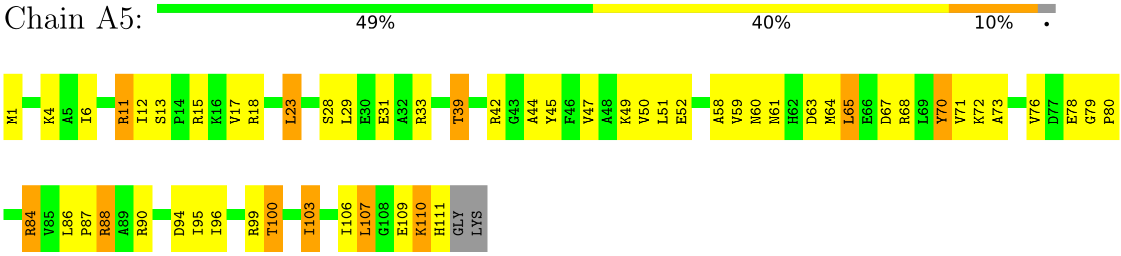
- Molecule 47: 50S ribosomal protein L22

Chain E8:



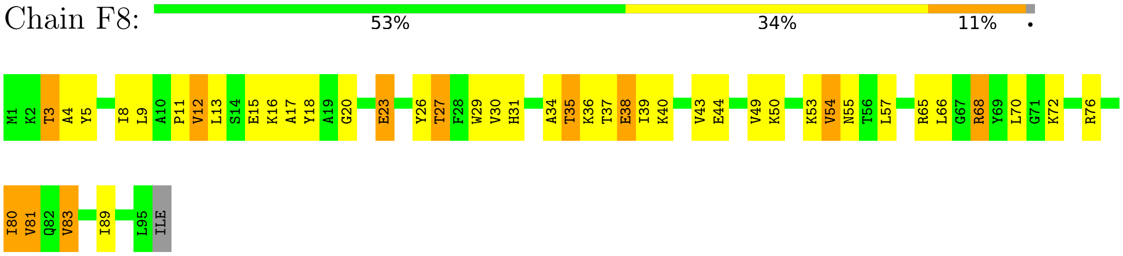
- Molecule 47: 50S ribosomal protein L22

Chain A5:



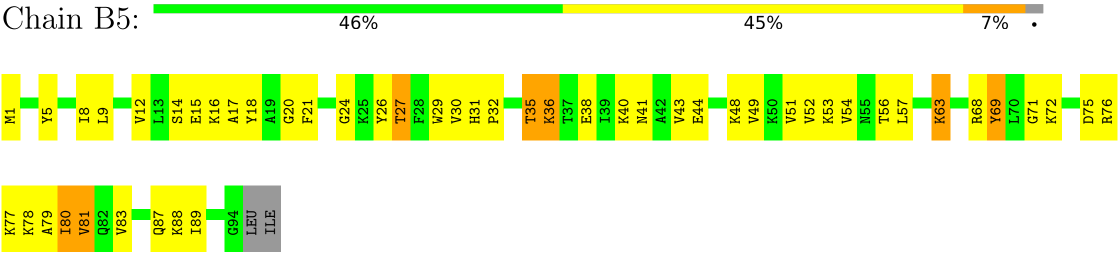
- Molecule 48: 50S ribosomal protein L23

Chain F8:



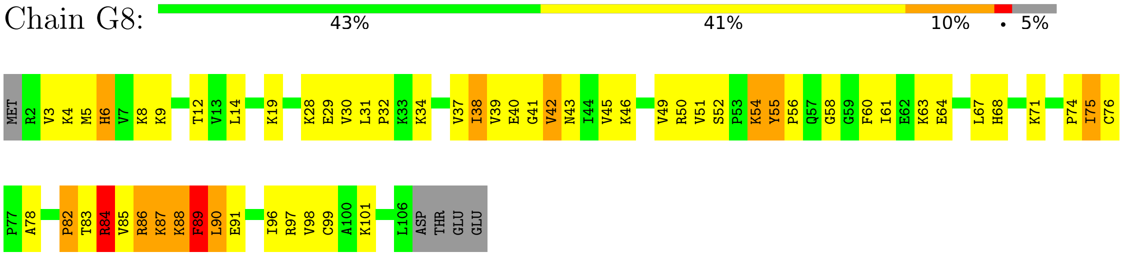
- Molecule 48: 50S ribosomal protein L23

Chain B5:



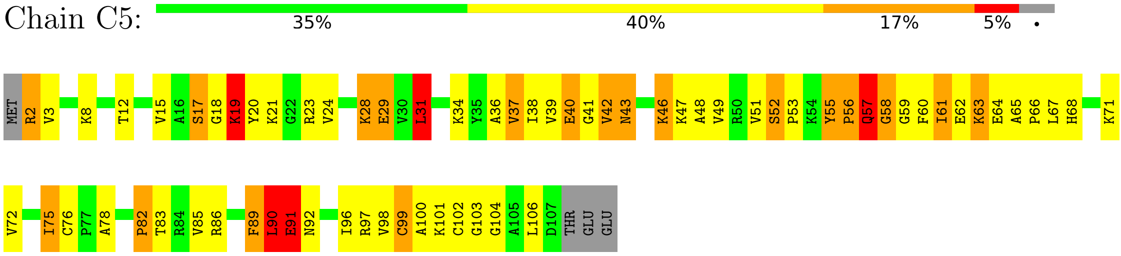
- Molecule 49: 50S ribosomal protein L24

Chain G8:



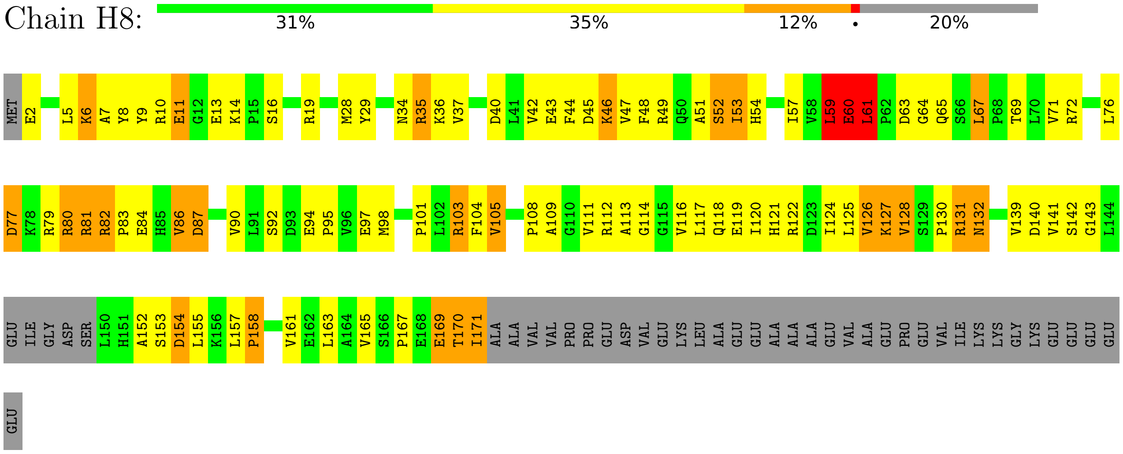
- Molecule 49: 50S ribosomal protein L24

Chain C5:



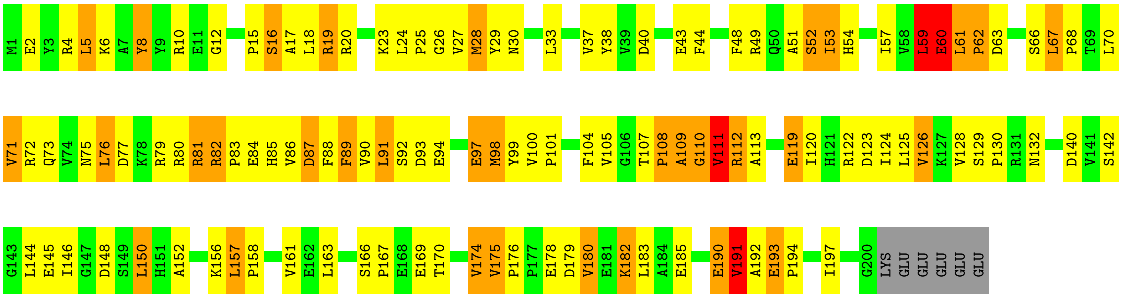
- Molecule 50: 50S ribosomal protein L25

Chain H8:



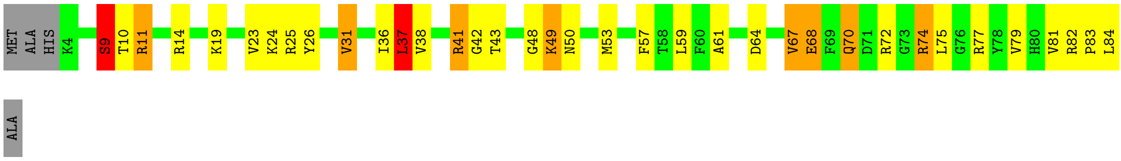
- Molecule 50: 50S ribosomal protein L25

Chain D5:



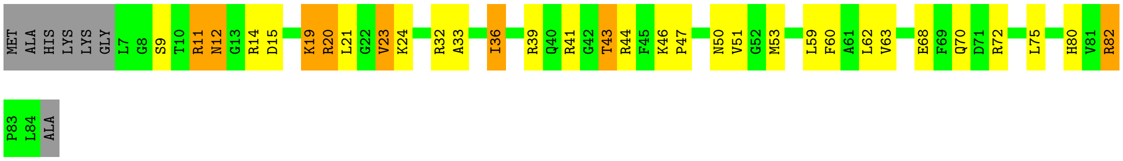
- Molecule 51: 50S ribosomal protein L27

Chain I8:



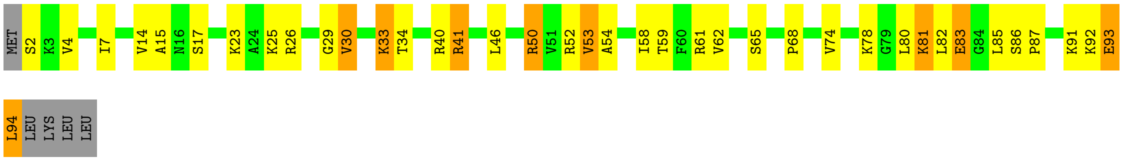
- Molecule 51: 50S ribosomal protein L27

Chain E5:



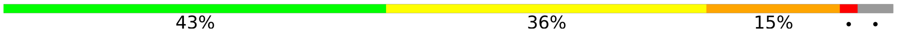
- Molecule 52: 50S ribosomal protein L28

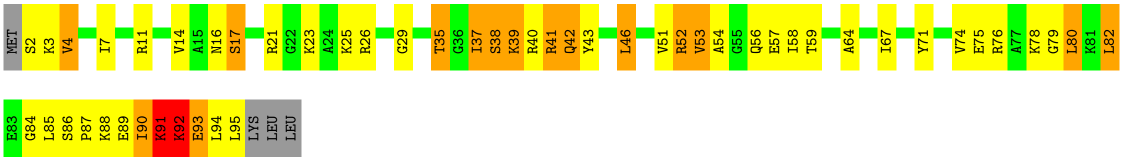
Chain J8:



- Molecule 52: 50S ribosomal protein L28

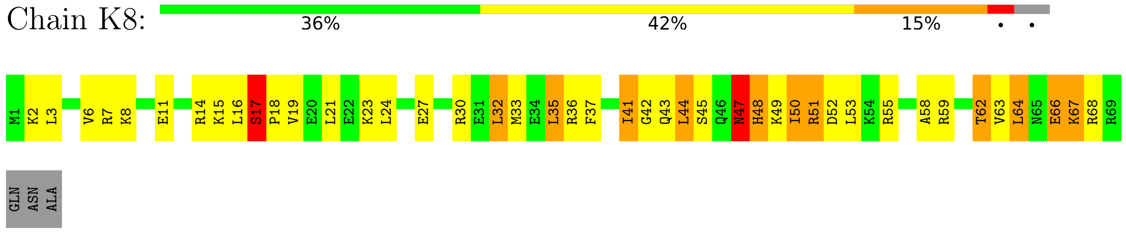
Chain F5:





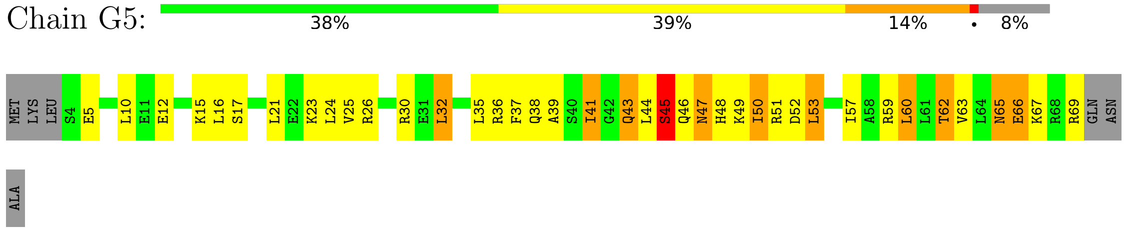
- Molecule 53: 50S ribosomal protein L29

Chain K8:



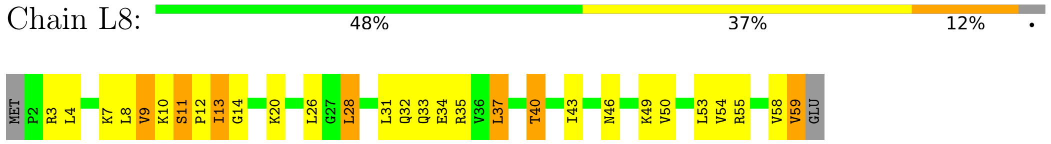
- Molecule 53: 50S ribosomal protein L29

Chain G5:



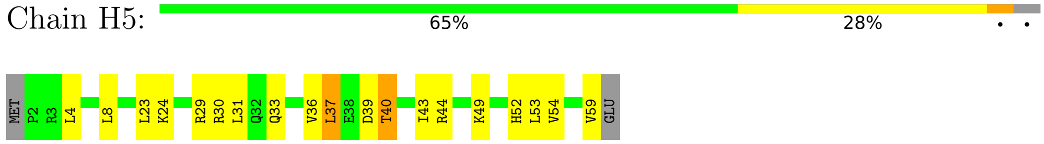
- Molecule 54: 50S ribosomal protein L30

Chain L8:



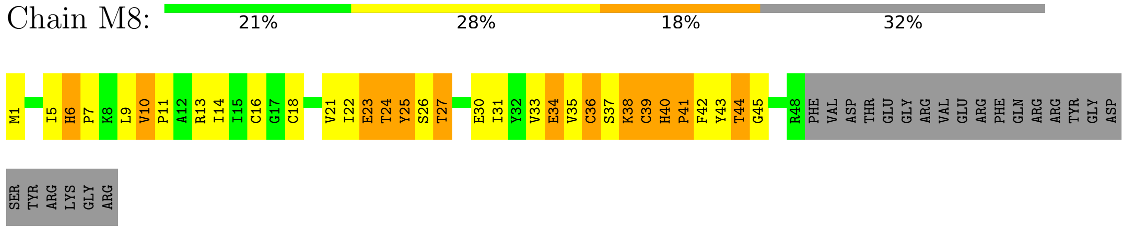
- Molecule 54: 50S ribosomal protein L30

Chain H5:



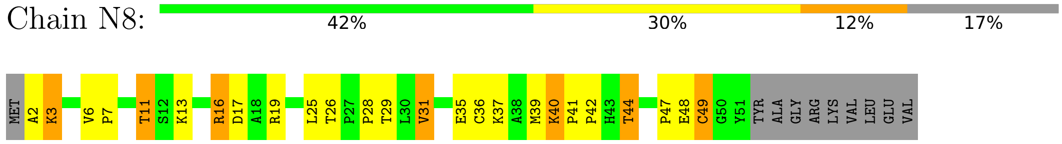
- Molecule 55: 50S ribosomal protein L31

Chain M8:



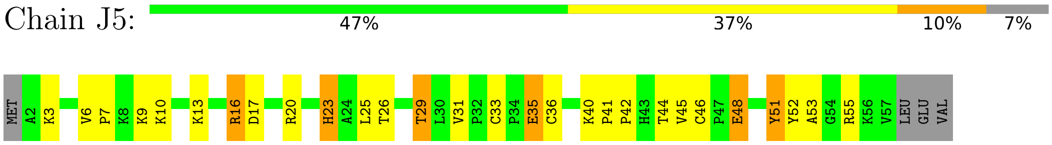
- Molecule 56: 50S ribosomal protein L32

Chain N8:



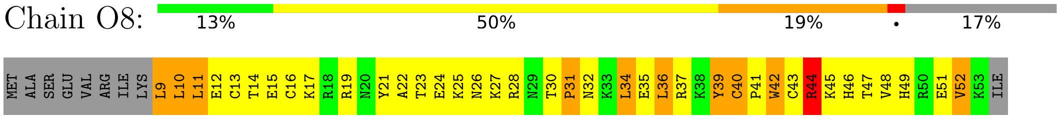
- Molecule 56: 50S ribosomal protein L32

Chain J5:



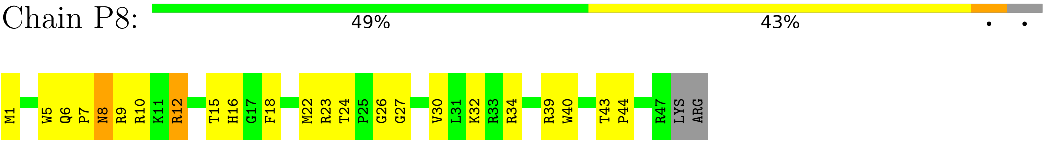
- Molecule 57: 50S ribosomal protein L33

Chain O8:



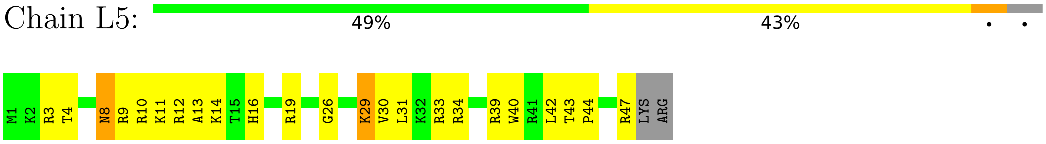
- Molecule 58: 50S ribosomal protein L34

Chain P8:



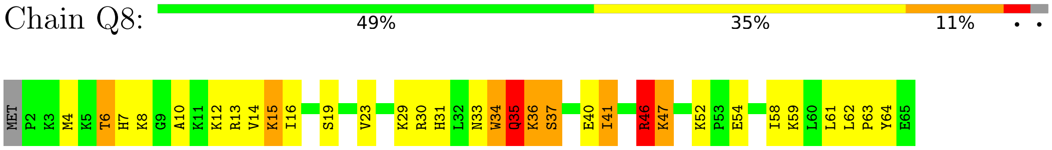
- Molecule 58: 50S ribosomal protein L34

Chain L5:



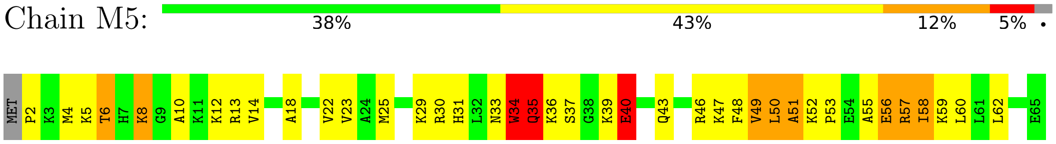
- Molecule 59: 50S ribosomal protein L35

Chain Q8:



- Molecule 59: 50S ribosomal protein L35

Chain M5:



4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	210.05Å 449.39Å 618.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	153.44 – 3.16 153.44 – 3.16	Depositor EDS
% Data completeness (in resolution range)	100.0 (153.44-3.16) 88.4 (153.44-3.16)	Depositor EDS
R_{merge}	0.38	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.57 (at 3.13Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	(Not available) , (Not available) 0.196 , 0.240	Depositor DCC
R_{free} test set	2000 reflections (0.20%)	wwPDB-VP
Wilson B-factor (Å^2)	90.7	Xtriage
Anisotropy	0.246	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.22 , 55.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	306138	wwPDB-VP
Average B, all atoms (Å^2)	112.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.45% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, RSP, PSU, 5MU, OMC, 4SU, ZN, 7MG, 2MA, 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	13	0.81	8/36375 (0.0%)	1.50	549/56770 (1.0%)
1	1G	0.71	1/36309 (0.0%)	1.36	301/56668 (0.5%)
2	12	0.49	0/1959	0.70	4/2642 (0.2%)
2	1E	0.46	0/1908	0.65	1/2573 (0.0%)
3	22	0.43	0/1556	0.63	1/2098 (0.0%)
3	2E	0.50	0/1629	0.66	0/2195
4	32	0.48	0/1732	0.67	1/2318 (0.0%)
4	3E	0.50	0/1720	0.68	0/2305
5	42	0.49	0/1171	0.66	1/1576 (0.1%)
5	4E	0.50	0/1158	0.67	0/1559
6	52	0.52	0/855	0.65	1/1154 (0.1%)
6	5E	0.55	0/855	0.67	0/1154
7	62	0.48	0/1122	0.65	2/1500 (0.1%)
7	6E	0.44	0/1259	0.59	0/1686
8	72	0.40	0/1135	0.61	0/1527
8	7E	0.47	0/1135	0.66	0/1527
9	82	0.39	0/1002	0.58	0/1346
9	8E	0.44	0/1019	0.65	0/1367
10	1A	0.44	0/814	0.71	1/1095 (0.1%)
10	1I	0.52	0/814	0.71	0/1095
11	2A	0.45	0/850	0.60	0/1150
11	2I	0.52	0/838	0.67	0/1133
12	3A	0.50	0/963	0.73	0/1290
12	3I	0.59	0/972	0.80	0/1301
13	4A	0.42	0/897	0.69	1/1204 (0.1%)
13	4I	0.48	0/946	0.66	0/1270
14	5A	0.47	0/475	0.75	0/632
14	5I	0.56	0/508	0.74	0/674
15	6A	0.44	0/740	0.61	0/987
15	6I	0.49	0/740	0.62	0/987
16	7A	0.45	0/721	0.64	0/970
16	7I	0.46	0/716	0.67	0/963

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\vert Z\vert >5$	RMSZ	$\#\vert Z\vert >5$
17	8A	0.51	0/836	0.64	0/1117
17	8I	0.58	1/847 (0.1%)	0.67	0/1131
18	9A	0.53	0/549	0.77	0/732
18	9I	0.51	0/549	0.75	0/732
19	AA	0.44	0/490	0.70	0/662
19	AI	0.54	0/657	0.82	0/885
20	BA	0.46	0/759	0.67	0/1000
20	BI	0.44	0/753	0.67	0/993
21	1B	0.38	0/212	0.66	0/277
21	1F	0.48	0/212	0.71	0/277
22	1K	0.78	3/1578 (0.2%)	1.35	12/2445 (0.5%)
22	1L	0.81	3/1623 (0.2%)	1.27	16/2517 (0.6%)
23	2K	0.90	1/1721 (0.1%)	1.64	42/2682 (1.6%)
23	2L	0.75	1/1721 (0.1%)	1.38	22/2682 (0.8%)
24	3K	0.82	0/1741	1.38	22/2703 (0.8%)
24	3L	0.84	0/1764	1.44	26/2741 (0.9%)
25	4K	0.92	0/521	1.37	1/812 (0.1%)
25	4L	0.79	1/420 (0.2%)	1.34	2/652 (0.3%)
26	14	0.94	72/69830 (0.1%)	1.65	1642/109010 (1.5%)
26	1H	1.08	153/69835 (0.2%)	1.82	2345/109020 (2.2%)
27	16	0.82	0/2928	1.65	67/4568 (1.5%)
27	1J	0.78	2/2928 (0.1%)	1.52	50/4568 (1.1%)
28	71	0.38	0/1066	0.59	0/1439
28	79	0.34	0/1031	0.58	1/1394 (0.1%)
29	11	0.76	3/2170 (0.1%)	0.94	6/2926 (0.2%)
29	19	0.65	1/2170 (0.0%)	0.87	4/2926 (0.1%)
30	21	0.62	0/1591	0.82	1/2146 (0.0%)
30	29	0.57	0/1591	0.79	0/2146
31	31	0.67	1/1620 (0.1%)	0.80	1/2194 (0.0%)
31	39	0.56	0/1645	0.78	1/2228 (0.0%)
32	41	0.53	1/1481 (0.1%)	0.74	2/1994 (0.1%)
32	49	0.44	0/1481	0.66	1/1994 (0.1%)
33	51	0.57	0/1337	0.87	2/1809 (0.1%)
33	59	0.45	0/1337	0.79	5/1809 (0.3%)
34	18	0.53	0/236	0.81	0/315
34	28	0.51	0/236	0.86	1/315 (0.3%)
35	61	0.48	0/1146	0.74	1/1551 (0.1%)
35	69	0.49	0/1146	0.73	1/1551 (0.1%)
36	38	0.62	1/1104 (0.1%)	1.25	16/1494 (1.1%)
37	48	0.42	0/1067	0.82	1/1448 (0.1%)
38	15	0.43	0/1123	0.64	0/1515
38	58	0.54	0/1123	0.74	1/1514 (0.1%)
39	25	0.58	0/942	0.78	2/1269 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
39	68	0.60	0/942	0.76	0/1269
40	35	0.60	0/1147	0.96	3/1525 (0.2%)
40	78	0.61	0/1139	0.95	2/1514 (0.1%)
41	45	0.59	0/1120	0.85	2/1498 (0.1%)
41	88	0.67	0/1134	0.83	0/1519
42	55	0.55	0/981	0.80	0/1312
42	98	0.54	0/981	0.78	0/1312
43	65	0.51	0/886	0.77	1/1180 (0.1%)
43	A8	0.57	0/891	0.90	3/1187 (0.3%)
44	75	0.68	1/1129 (0.1%)	0.71	0/1509
44	B8	0.58	0/1146	0.76	1/1531 (0.1%)
45	85	0.54	0/981	0.75	1/1306 (0.1%)
45	C8	0.64	0/968	0.87	4/1289 (0.3%)
46	95	0.55	0/785	0.78	0/1052
46	D8	0.66	0/789	0.86	5/1057 (0.5%)
47	A5	0.57	0/897	0.75	0/1204
47	E8	0.63	0/901	0.78	1/1209 (0.1%)
48	B5	0.63	0/752	0.74	0/1010
48	F8	0.67	0/757	0.79	0/1017
49	C5	0.53	0/798	0.83	2/1071 (0.2%)
49	G8	0.68	1/797 (0.1%)	0.79	1/1068 (0.1%)
50	D5	0.47	0/1615	0.77	2/2191 (0.1%)
50	H8	0.47	0/1359	0.78	2/1841 (0.1%)
51	E5	0.52	0/624	0.71	0/832
51	I8	0.74	2/638 (0.3%)	0.89	1/851 (0.1%)
52	F5	0.59	0/744	0.79	1/989 (0.1%)
52	J8	0.62	0/736	0.82	0/978
53	G5	0.61	0/560	0.71	0/741
53	K8	0.63	0/578	0.85	1/766 (0.1%)
54	H5	0.52	0/464	0.66	0/623
54	L8	0.58	0/464	0.72	0/623
55	M8	0.53	0/380	0.81	0/514
56	J5	0.61	0/448	0.74	0/606
56	N8	0.68	0/399	0.78	0/541
57	O8	0.69	0/396	1.08	3/529 (0.6%)
58	L5	0.65	0/417	0.84	1/550 (0.2%)
58	P8	0.73	0/409	0.95	2/540 (0.4%)
59	M5	0.83	3/524 (0.6%)	0.93	1/691 (0.1%)
59	Q8	0.67	0/524	0.91	2/691 (0.3%)
All	All	0.83	260/325210 (0.1%)	1.45	5199/486635 (1.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	12	0	3
2	1E	0	5
3	22	0	1
3	2E	0	1
4	32	0	4
4	3E	0	1
5	4E	0	1
9	8E	0	1
10	1I	0	1
12	3A	0	2
12	3I	0	3
13	4A	0	4
14	5I	0	1
18	9I	0	2
19	AA	0	2
19	AI	0	4
20	BA	0	4
20	BI	0	2
29	11	0	7
29	19	0	6
30	21	0	6
30	29	0	7
31	31	0	2
31	39	0	5
32	41	0	2
32	49	0	3
33	51	0	5
33	59	0	5
34	18	0	2
34	28	0	2
35	61	0	3
35	69	0	1
36	38	0	21
37	48	0	11
38	15	0	2
38	58	0	1
40	35	0	7
40	78	0	4
41	45	0	9
43	A8	0	1
44	75	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
45	85	0	2
45	C8	0	4
46	95	0	4
46	D8	0	2
48	F8	0	1
49	C5	0	8
49	G8	0	3
50	D5	0	10
50	H8	0	2
52	F5	0	2
52	J8	0	1
53	G5	0	3
53	K8	0	1
55	M8	0	3
57	O8	0	2
59	M5	0	4
59	Q8	0	1
All	All	0	208

The worst 5 of 260 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	14	783	A	N9-C4	-12.97	1.30	1.37
26	1H	774	A	N9-C4	-12.58	1.30	1.37
44	75	106	SER	CA-CB	11.37	1.70	1.52
29	11	239	ARG	C-N	-10.85	1.09	1.34
26	1H	2476	A	N9-C4	9.90	1.43	1.37

The worst 5 of 5199 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	14	945	A	N1-C6-N6	19.92	130.55	118.60
26	1H	676	A	C2-N3-C4	-19.33	100.94	110.60
26	1H	945	A	N1-C6-N6	17.89	129.34	118.60
26	14	783	A	C5-N7-C8	-17.43	95.19	103.90
26	14	783	A	C2-N3-C4	-17.33	101.93	110.60

There are no chirality outliers.

5 of 208 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1E	11	LEU	Peptide
2	1E	19	HIS	Peptide
2	1E	230	VAL	Peptide
2	1E	234	PRO	Peptide
2	1E	236	TYR	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	13	32497	0	16403	888	0
1	1G	32437	0	16372	860	0
2	12	1924	0	1975	127	0
2	1E	1874	0	1926	113	0
3	22	1533	0	1595	77	0
3	2E	1605	0	1668	55	0
4	32	1702	0	1765	94	0
4	3E	1690	0	1737	83	0
5	42	1155	0	1213	57	0
5	4E	1142	0	1204	50	0
6	52	842	0	857	33	0
6	5E	842	0	857	30	0
7	62	1110	0	1163	67	0
7	6E	1242	0	1286	50	0
8	72	1115	0	1177	54	0
8	7E	1115	0	1177	66	0
9	82	983	0	1006	68	0
9	8E	1000	0	1031	65	0
10	1A	801	0	849	85	0
10	1I	801	0	848	56	0
11	2A	835	0	847	36	0
11	2I	823	0	833	41	0
12	3A	947	0	1033	63	0
12	3I	956	0	1046	58	0
13	4A	887	0	935	66	0
13	4I	936	0	986	52	0
14	5A	466	0	499	29	0
14	5I	499	0	542	36	0
15	6A	729	0	768	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	6I	729	0	768	26	0
16	7A	705	0	725	26	0
16	7I	700	0	720	54	0
17	8A	823	0	891	34	0
17	8I	834	0	904	61	0
18	9A	544	0	605	21	0
18	9I	544	0	605	36	0
19	AA	481	0	468	28	0
19	AI	643	0	662	33	0
20	BA	757	0	856	47	0
20	BI	751	0	848	56	0
21	1B	208	0	221	21	0
21	1F	208	0	221	9	0
22	1K	1544	0	791	49	0
22	1L	1584	0	811	51	0
23	2K	1646	0	845	40	0
23	2L	1646	0	845	39	0
24	3K	1561	0	796	51	0
24	3L	1581	0	805	63	0
25	4K	462	0	229	11	0
25	4L	374	0	187	10	0
26	14	62347	0	31431	1547	0
26	1H	62351	0	31424	1621	0
27	16	2617	0	1328	74	0
27	1J	2617	0	1328	89	0
28	71	1043	0	1066	44	0
28	79	1010	0	1025	51	0
29	11	2120	0	2196	112	0
29	19	2120	0	2197	103	0
30	21	1558	0	1624	92	0
30	29	1558	0	1624	93	0
31	31	1585	0	1632	85	0
31	39	1610	0	1655	122	0
32	41	1457	0	1514	87	0
32	49	1457	0	1514	83	0
33	51	1312	0	1384	77	0
33	59	1312	0	1384	102	0
34	18	237	0	257	22	0
34	28	237	0	257	21	0
35	61	1131	0	1218	45	0
35	69	1131	0	1218	69	0
36	38	1089	0	1149	108	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	48	1047	0	1082	87	0
38	15	1096	0	1168	39	0
38	58	1096	0	1169	59	0
39	25	932	0	996	53	0
39	68	932	0	996	31	0
40	35	1130	0	1217	111	0
40	78	1122	0	1206	95	0
41	45	1099	0	1152	88	0
41	88	1113	0	1157	55	0
42	55	967	0	1033	37	0
42	98	967	0	1033	48	0
43	65	876	0	938	88	0
43	A8	881	0	943	45	0
44	75	1115	0	1169	66	0
44	B8	1132	0	1189	70	0
45	85	963	0	1022	68	0
45	C8	950	0	1011	49	0
46	95	774	0	849	63	0
46	D8	778	0	852	40	1
47	A5	886	0	948	34	0
47	E8	890	0	951	24	0
48	B5	738	0	792	44	0
48	F8	743	0	794	39	0
49	C5	785	0	844	62	0
49	G8	784	0	853	44	0
50	D5	1582	0	1613	79	0
50	H8	1330	0	1360	75	0
51	E5	616	0	633	38	0
51	I8	630	0	640	28	0
52	F5	737	0	813	48	0
52	J8	729	0	802	30	0
53	G5	558	0	610	27	0
53	K8	576	0	628	45	0
54	H5	459	0	512	12	0
54	L8	459	0	512	20	0
55	M8	371	0	372	35	0
56	J5	434	0	454	19	0
56	N8	386	0	402	31	0
57	O8	389	0	404	33	0
58	L5	409	0	454	17	0
58	P8	401	0	436	19	0
59	M5	516	0	582	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	Q8	516	0	582	36	0
60	11	6	0	0	0	0
60	13	227	0	0	0	0
60	14	607	0	0	0	0
60	16	20	0	0	0	0
60	1G	167	0	0	0	0
60	1H	669	0	0	0	0
60	1J	8	0	0	0	0
60	1K	2	0	0	0	0
60	1L	1	0	0	0	0
60	21	2	0	0	0	0
60	25	2	0	0	0	0
60	29	5	0	0	0	0
60	2A	1	0	0	0	0
60	2K	7	0	0	0	0
60	2L	2	0	0	0	0
60	31	2	0	0	0	0
60	32	2	0	0	0	0
60	35	1	0	0	0	0
60	39	2	0	0	0	0
60	3E	2	0	0	0	0
60	41	1	0	0	0	0
60	45	2	0	0	0	0
60	4K	1	0	0	0	0
60	4L	2	0	0	0	0
60	52	1	0	0	0	0
60	55	2	0	0	0	0
60	5E	2	0	0	0	0
60	6I	1	0	0	0	0
60	75	1	0	0	0	0
60	78	1	0	0	0	0
60	88	4	0	0	0	0
60	98	2	0	0	0	0
60	C5	1	0	0	0	0
60	E5	1	0	0	0	0
60	F5	1	0	0	0	0
60	I8	2	0	0	0	0
60	M5	1	0	0	0	0
60	N8	1	0	0	0	0
60	P8	1	0	0	0	0
60	Q8	1	0	0	0	0
61	32	8	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	3E	8	0	0	2	0
62	5A	1	0	0	0	0
62	5I	1	0	0	0	0
63	11	12	0	0	2	0
63	13	544	0	0	91	0
63	14	1520	0	0	275	0
63	15	1	0	0	0	0
63	16	42	0	0	7	0
63	19	12	0	0	4	0
63	1E	1	0	0	0	0
63	1F	1	0	0	0	0
63	1G	397	0	0	60	0
63	1H	1966	0	0	358	2
63	1I	1	0	0	0	0
63	1J	23	0	0	3	0
63	1K	1	0	0	0	0
63	21	9	0	0	2	0
63	25	13	0	0	1	0
63	29	9	0	0	1	0
63	2K	16	0	0	5	0
63	2L	7	0	0	0	0
63	31	8	0	0	0	0
63	32	5	0	0	0	0
63	35	5	0	0	1	0
63	39	8	0	0	1	0
63	3A	2	0	0	0	0
63	3E	1	0	0	0	0
63	3I	5	0	0	0	0
63	42	1	0	0	0	0
63	45	4	0	0	0	0
63	4E	2	0	0	0	0
63	4K	13	0	0	0	0
63	4L	8	0	0	1	0
63	52	4	0	0	1	0
63	58	3	0	0	0	0
63	5A	1	0	0	0	0
63	5I	3	0	0	2	0
63	6A	1	0	0	0	0
63	6I	4	0	0	0	0
63	78	10	0	0	4	0
63	7A	2	0	0	0	0
63	85	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
63	88	7	0	0	0	0
63	8E	1	0	0	0	0
63	98	1	0	0	0	0
63	9A	2	0	0	0	0
63	A5	1	0	0	0	0
63	A8	2	0	0	0	0
63	B5	1	0	0	0	0
63	B8	3	0	0	0	0
63	BA	2	0	0	0	0
63	BI	1	0	0	0	0
63	C5	1	0	0	0	0
63	C8	7	0	0	0	1
63	D8	1	0	0	0	0
63	E5	3	0	0	0	0
63	F5	6	0	0	1	0
63	F8	1	0	0	0	0
63	G8	3	0	0	0	0
63	I8	5	0	0	1	0
63	J8	10	0	0	2	0
63	L5	2	0	0	0	0
63	L8	4	0	0	2	0
63	M5	9	0	0	0	0
63	P8	1	0	0	0	0
63	Q8	7	0	0	0	0
All	All	306138	0	202999	9699	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

The worst 5 of 9699 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1H:1268:A:OP1	63:1H:3723:HOH:O	1.66	1.12
26:14:1604:C:OP2	63:14:3715:HOH:O	1.65	1.11
26:1H:2032:G:H21	30:21:146:THR:HG23	1.17	1.07
26:1H:2711:A:OP2	63:1H:3724:HOH:O	1.71	1.06
26:14:1603:A:OP1	63:14:3715:HOH:O	1.74	1.05

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:D8:45:THR:CG2	63:1H:4620:HOH:O[4_465]	1.38	0.82
63:1H:4955:HOH:O	63:C8:206:HOH:O[4_565]	2.19	0.01

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	
2	12	235/256 (92%)	183 (78%)	47 (20%)	5 (2%)	7	33
2	1E	227/256 (89%)	171 (75%)	54 (24%)	2 (1%)	17	53
3	22	191/239 (80%)	149 (78%)	41 (22%)	1 (0%)	29	65
3	2E	203/239 (85%)	169 (83%)	33 (16%)	1 (0%)	29	65
4	32	206/209 (99%)	168 (82%)	34 (16%)	4 (2%)	8	36
4	3E	205/209 (98%)	172 (84%)	31 (15%)	2 (1%)	15	51
5	42	149/162 (92%)	132 (89%)	17 (11%)	0	100	100
5	4E	147/162 (91%)	128 (87%)	18 (12%)	1 (1%)	22	59
6	52	99/101 (98%)	93 (94%)	6 (6%)	0	100	100
6	5E	99/101 (98%)	88 (89%)	11 (11%)	0	100	100
7	62	134/156 (86%)	108 (81%)	24 (18%)	2 (2%)	10	41
7	6E	152/156 (97%)	139 (91%)	13 (9%)	0	100	100
8	72	136/138 (99%)	120 (88%)	16 (12%)	0	100	100
8	7E	136/138 (99%)	116 (85%)	20 (15%)	0	100	100
9	82	122/128 (95%)	104 (85%)	17 (14%)	1 (1%)	19	55
9	8E	124/128 (97%)	100 (81%)	22 (18%)	2 (2%)	9	40
10	1A	97/105 (92%)	79 (81%)	18 (19%)	0	100	100
10	1I	97/105 (92%)	83 (86%)	13 (13%)	1 (1%)	15	51
11	2A	111/129 (86%)	94 (85%)	16 (14%)	1 (1%)	17	53
11	2I	109/129 (84%)	94 (86%)	15 (14%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	3A	119/132 (90%)	91 (76%)	23 (19%)	5 (4%)	3	17
12	3I	120/132 (91%)	101 (84%)	19 (16%)	0	100	100
13	4A	109/126 (86%)	84 (77%)	24 (22%)	1 (1%)	17	53
13	4I	117/126 (93%)	91 (78%)	25 (21%)	1 (1%)	17	53
14	5A	55/61 (90%)	38 (69%)	15 (27%)	2 (4%)	3	20
14	5I	59/61 (97%)	48 (81%)	9 (15%)	2 (3%)	3	21
15	6A	85/89 (96%)	77 (91%)	8 (9%)	0	100	100
15	6I	85/89 (96%)	72 (85%)	13 (15%)	0	100	100
16	7A	82/88 (93%)	71 (87%)	11 (13%)	0	100	100
16	7I	81/88 (92%)	73 (90%)	8 (10%)	0	100	100
17	8A	97/105 (92%)	87 (90%)	10 (10%)	0	100	100
17	8I	98/105 (93%)	88 (90%)	10 (10%)	0	100	100
18	9A	65/88 (74%)	56 (86%)	9 (14%)	0	100	100
18	9I	65/88 (74%)	57 (88%)	6 (9%)	2 (3%)	4	23
19	AA	56/93 (60%)	44 (79%)	12 (21%)	0	100	100
19	AI	78/93 (84%)	57 (73%)	15 (19%)	6 (8%)	1	5
20	BA	96/106 (91%)	79 (82%)	14 (15%)	3 (3%)	4	23
20	BI	96/106 (91%)	75 (78%)	17 (18%)	4 (4%)	3	17
21	1B	22/27 (82%)	16 (73%)	5 (23%)	1 (4%)	2	16
21	1F	22/27 (82%)	19 (86%)	2 (9%)	1 (4%)	2	16
28	71	130/229 (57%)	114 (88%)	16 (12%)	0	100	100
28	79	126/229 (55%)	107 (85%)	19 (15%)	0	100	100
29	11	271/276 (98%)	231 (85%)	37 (14%)	3 (1%)	14	48
29	19	271/276 (98%)	234 (86%)	37 (14%)	0	100	100
30	21	201/206 (98%)	149 (74%)	44 (22%)	8 (4%)	3	18
30	29	201/206 (98%)	145 (72%)	50 (25%)	6 (3%)	4	24
31	31	200/210 (95%)	169 (84%)	28 (14%)	3 (2%)	10	41
31	39	204/210 (97%)	152 (74%)	46 (22%)	6 (3%)	4	25
32	41	177/182 (97%)	150 (85%)	26 (15%)	1 (1%)	25	62
32	49	177/182 (97%)	142 (80%)	32 (18%)	3 (2%)	9	38
33	51	169/180 (94%)	125 (74%)	35 (21%)	9 (5%)	2	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	59	169/180 (94%)	108 (64%)	54 (32%)	7 (4%)	3	18
34	18	28/125 (22%)	20 (71%)	7 (25%)	1 (4%)	3	20
34	28	28/125 (22%)	23 (82%)	4 (14%)	1 (4%)	3	20
35	61	143/148 (97%)	104 (73%)	35 (24%)	4 (3%)	5	26
35	69	143/148 (97%)	109 (76%)	30 (21%)	4 (3%)	5	26
36	38	141/173 (82%)	65 (46%)	54 (38%)	22 (16%)	0	1
37	48	140/147 (95%)	75 (54%)	57 (41%)	8 (6%)	1	12
38	15	135/140 (96%)	115 (85%)	20 (15%)	0	100	100
38	58	135/140 (96%)	108 (80%)	25 (18%)	2 (2%)	10	41
39	25	120/122 (98%)	108 (90%)	11 (9%)	1 (1%)	19	55
39	68	120/122 (98%)	110 (92%)	10 (8%)	0	100	100
40	35	146/150 (97%)	95 (65%)	43 (30%)	8 (6%)	2	12
40	78	145/150 (97%)	112 (77%)	32 (22%)	1 (1%)	22	59
41	45	136/141 (96%)	98 (72%)	33 (24%)	5 (4%)	3	19
41	88	139/141 (99%)	116 (84%)	21 (15%)	2 (1%)	11	43
42	55	116/118 (98%)	103 (89%)	13 (11%)	0	100	100
42	98	116/118 (98%)	100 (86%)	16 (14%)	0	100	100
43	65	108/112 (96%)	82 (76%)	22 (20%)	4 (4%)	3	19
43	A8	109/112 (97%)	87 (80%)	22 (20%)	0	100	100
44	75	132/146 (90%)	110 (83%)	22 (17%)	0	100	100
44	B8	134/146 (92%)	105 (78%)	29 (22%)	0	100	100
45	85	115/118 (98%)	96 (84%)	19 (16%)	0	100	100
45	C8	113/118 (96%)	93 (82%)	18 (16%)	2 (2%)	8	37
46	95	98/101 (97%)	71 (72%)	21 (21%)	6 (6%)	1	10
46	D8	99/101 (98%)	84 (85%)	15 (15%)	0	100	100
47	A5	109/113 (96%)	97 (89%)	12 (11%)	0	100	100
47	E8	110/113 (97%)	95 (86%)	15 (14%)	0	100	100
48	B5	92/96 (96%)	79 (86%)	13 (14%)	0	100	100
48	F8	93/96 (97%)	81 (87%)	11 (12%)	1 (1%)	14	48
49	C5	104/110 (94%)	66 (64%)	31 (30%)	7 (7%)	1	8
49	G8	103/110 (94%)	73 (71%)	30 (29%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
50	D5	198/206 (96%)	136 (69%)	54 (27%)	8 (4%)	3	18
50	H8	161/206 (78%)	123 (76%)	32 (20%)	6 (4%)	3	19
51	E5	76/85 (89%)	65 (86%)	11 (14%)	0	100	100
51	I8	79/85 (93%)	63 (80%)	15 (19%)	1 (1%)	12	44
52	F5	92/98 (94%)	81 (88%)	9 (10%)	2 (2%)	6	32
52	J8	91/98 (93%)	79 (87%)	12 (13%)	0	100	100
53	G5	64/72 (89%)	58 (91%)	5 (8%)	1 (2%)	9	40
53	K8	67/72 (93%)	57 (85%)	8 (12%)	2 (3%)	4	24
54	H5	56/60 (93%)	52 (93%)	4 (7%)	0	100	100
54	L8	56/60 (93%)	54 (96%)	2 (4%)	0	100	100
55	M8	46/71 (65%)	24 (52%)	20 (44%)	2 (4%)	2	17
56	J5	54/60 (90%)	47 (87%)	7 (13%)	0	100	100
56	N8	48/60 (80%)	42 (88%)	6 (12%)	0	100	100
57	O8	43/54 (80%)	26 (60%)	16 (37%)	1 (2%)	6	31
58	L5	45/49 (92%)	42 (93%)	3 (7%)	0	100	100
58	P8	45/49 (92%)	43 (96%)	2 (4%)	0	100	100
59	M5	62/65 (95%)	49 (79%)	12 (19%)	1 (2%)	9	40
59	Q8	62/65 (95%)	47 (76%)	13 (21%)	2 (3%)	4	22
All	All	11677/12957 (90%)	9408 (81%)	2067 (18%)	202 (2%)	9	38

5 of 202 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	4I	12	ASN
30	21	78	LEU
30	21	83	ASP
33	51	10	PRO
34	18	25	ASP

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	
2	12	205/220 (93%)	155 (76%)	50 (24%)	0	2
2	1E	200/220 (91%)	146 (73%)	54 (27%)	0	1
3	22	153/188 (81%)	114 (74%)	39 (26%)	0	2
3	2E	159/188 (85%)	126 (79%)	33 (21%)	1	5
4	32	180/181 (99%)	143 (79%)	37 (21%)	1	5
4	3E	178/181 (98%)	145 (82%)	33 (18%)	1	8
5	42	116/123 (94%)	84 (72%)	32 (28%)	0	1
5	4E	115/123 (94%)	92 (80%)	23 (20%)	1	6
6	52	90/90 (100%)	77 (86%)	13 (14%)	3	14
6	5E	90/90 (100%)	74 (82%)	16 (18%)	2	8
7	62	114/127 (90%)	89 (78%)	25 (22%)	1	4
7	6E	125/127 (98%)	102 (82%)	23 (18%)	1	8
8	72	119/119 (100%)	101 (85%)	18 (15%)	3	13
8	7E	119/119 (100%)	94 (79%)	25 (21%)	1	5
9	82	95/99 (96%)	69 (73%)	26 (27%)	0	1
9	8E	97/99 (98%)	69 (71%)	28 (29%)	0	1
10	1A	89/92 (97%)	67 (75%)	22 (25%)	0	2
10	1I	89/92 (97%)	68 (76%)	21 (24%)	1	3
11	2A	85/99 (86%)	66 (78%)	19 (22%)	1	4
11	2I	84/99 (85%)	61 (73%)	23 (27%)	0	1
12	3A	102/109 (94%)	81 (79%)	21 (21%)	1	5
12	3I	103/109 (94%)	80 (78%)	23 (22%)	1	4
13	4A	90/101 (89%)	63 (70%)	27 (30%)	0	1
13	4I	93/101 (92%)	72 (77%)	21 (23%)	1	4
14	5A	47/50 (94%)	32 (68%)	15 (32%)	0	0
14	5I	50/50 (100%)	41 (82%)	9 (18%)	1	8
15	6A	79/80 (99%)	67 (85%)	12 (15%)	3	12
15	6I	79/80 (99%)	66 (84%)	13 (16%)	2	10
16	7A	72/74 (97%)	59 (82%)	13 (18%)	1	8
16	7I	72/74 (97%)	55 (76%)	17 (24%)	1	3
17	8A	94/97 (97%)	80 (85%)	14 (15%)	3	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	8I	95/97 (98%)	77 (81%)	18 (19%)	1	7
18	9A	58/77 (75%)	47 (81%)	11 (19%)	1	7
18	9I	58/77 (75%)	48 (83%)	10 (17%)	2	9
19	AA	52/80 (65%)	41 (79%)	11 (21%)	1	5
19	AI	70/80 (88%)	52 (74%)	18 (26%)	0	2
20	BA	76/82 (93%)	58 (76%)	18 (24%)	1	3
20	BI	75/82 (92%)	54 (72%)	21 (28%)	0	1
21	1B	19/22 (86%)	18 (95%)	1 (5%)	22	55
21	1F	19/22 (86%)	17 (90%)	2 (10%)	7	26
28	71	110/181 (61%)	82 (74%)	28 (26%)	0	2
28	79	107/181 (59%)	97 (91%)	10 (9%)	9	31
29	11	214/218 (98%)	170 (79%)	44 (21%)	1	5
29	19	214/218 (98%)	163 (76%)	51 (24%)	0	3
30	21	165/166 (99%)	119 (72%)	46 (28%)	0	1
30	29	165/166 (99%)	129 (78%)	36 (22%)	1	5
31	31	161/166 (97%)	122 (76%)	39 (24%)	0	2
31	39	163/166 (98%)	119 (73%)	44 (27%)	0	1
32	41	153/156 (98%)	117 (76%)	36 (24%)	1	3
32	49	153/156 (98%)	111 (72%)	42 (28%)	0	1
33	51	142/148 (96%)	100 (70%)	42 (30%)	0	1
33	59	142/148 (96%)	105 (74%)	37 (26%)	0	2
34	18	26/90 (29%)	18 (69%)	8 (31%)	0	1
34	28	26/90 (29%)	13 (50%)	13 (50%)	0	0
35	61	122/124 (98%)	90 (74%)	32 (26%)	0	2
35	69	122/124 (98%)	84 (69%)	38 (31%)	0	1
36	38	115/135 (85%)	64 (56%)	51 (44%)	0	0
37	48	106/111 (96%)	67 (63%)	39 (37%)	0	0
38	15	116/119 (98%)	89 (77%)	27 (23%)	1	3
38	58	116/119 (98%)	88 (76%)	28 (24%)	0	2
39	25	100/100 (100%)	78 (78%)	22 (22%)	1	4
39	68	100/100 (100%)	89 (89%)	11 (11%)	6	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	35	115/116 (99%)	82 (71%)	33 (29%)	0	1
40	78	114/116 (98%)	77 (68%)	37 (32%)	0	0
41	45	109/111 (98%)	79 (72%)	30 (28%)	0	1
41	88	109/111 (98%)	93 (85%)	16 (15%)	3	13
42	55	101/101 (100%)	82 (81%)	19 (19%)	1	7
42	98	101/101 (100%)	77 (76%)	24 (24%)	0	3
43	65	87/88 (99%)	59 (68%)	28 (32%)	0	0
43	A8	87/88 (99%)	57 (66%)	30 (34%)	0	0
44	75	117/127 (92%)	85 (73%)	32 (27%)	0	1
44	B8	119/127 (94%)	87 (73%)	32 (27%)	0	1
45	85	93/94 (99%)	77 (83%)	16 (17%)	2	9
45	C8	92/94 (98%)	73 (79%)	19 (21%)	1	5
46	95	82/82 (100%)	66 (80%)	16 (20%)	1	7
46	D8	82/82 (100%)	58 (71%)	24 (29%)	0	1
47	A5	91/92 (99%)	68 (75%)	23 (25%)	0	2
47	E8	91/92 (99%)	75 (82%)	16 (18%)	2	9
48	B5	75/78 (96%)	59 (79%)	16 (21%)	1	5
48	F8	75/78 (96%)	60 (80%)	15 (20%)	1	6
49	C5	81/91 (89%)	58 (72%)	23 (28%)	0	1
49	G8	82/91 (90%)	66 (80%)	16 (20%)	1	7
50	D5	173/179 (97%)	129 (75%)	44 (25%)	0	2
50	H8	147/179 (82%)	112 (76%)	35 (24%)	0	3
51	E5	62/67 (92%)	51 (82%)	11 (18%)	2	8
51	I8	62/67 (92%)	48 (77%)	14 (23%)	1	4
52	F5	79/83 (95%)	53 (67%)	26 (33%)	0	0
52	J8	78/83 (94%)	61 (78%)	17 (22%)	1	5
53	G5	62/67 (92%)	43 (69%)	19 (31%)	0	1
53	K8	63/67 (94%)	44 (70%)	19 (30%)	0	1
54	H5	50/52 (96%)	43 (86%)	7 (14%)	3	15
54	L8	50/52 (96%)	38 (76%)	12 (24%)	0	3
55	M8	42/63 (67%)	30 (71%)	12 (29%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
56	J5	48/52 (92%)	38 (79%)	10 (21%)	1	5
56	N8	44/52 (85%)	34 (77%)	10 (23%)	1	4
57	O8	44/52 (85%)	29 (66%)	15 (34%)	0	0
58	L5	40/42 (95%)	34 (85%)	6 (15%)	3	13
58	P8	38/42 (90%)	34 (90%)	4 (10%)	7	26
59	M5	54/55 (98%)	40 (74%)	14 (26%)	0	2
59	Q8	54/55 (98%)	41 (76%)	13 (24%)	0	2
All	All	9836/10671 (92%)	7504 (76%)	2332 (24%)	1	3

5 of 2332 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
33	59	89	ILE
53	G5	65	ASN
35	69	138	ILE
33	59	86	GLU
44	75	51	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
30	29	135	HIS
32	49	66	GLN
31	39	169	ASN
33	59	139	GLN
44	B8	58	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	13	1511/1522 (99%)	381 (25%)	36 (2%)
1	1G	1508/1522 (99%)	380 (25%)	37 (2%)
22	1K	67/77 (87%)	31 (46%)	5 (7%)
22	1L	70/77 (90%)	28 (40%)	6 (8%)
23	2K	76/77 (98%)	19 (25%)	2 (2%)
23	2L	76/77 (98%)	18 (23%)	1 (1%)
24	3K	68/77 (88%)	36 (52%)	4 (5%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
24	3L	70/77 (90%)	37 (52%)	3 (4%)
25	4K	20/27 (74%)	14 (70%)	1 (5%)
25	4L	15/27 (55%)	9 (60%)	0
26	14	2892/2917 (99%)	722 (24%)	51 (1%)
26	1H	2893/2917 (99%)	705 (24%)	67 (2%)
27	16	121/122 (99%)	28 (23%)	2 (1%)
27	1J	121/122 (99%)	32 (26%)	1 (0%)
All	All	9508/9638 (98%)	2440 (25%)	216 (2%)

5 of 2440 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	13	2	U
1	13	3	G
1	13	4	U
1	13	5	U
1	13	6	G

5 of 216 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
27	16	44	G
1	1G	1126	U
26	14	1819	A
1	1G	80	G
1	1G	485	G

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

22 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
23	OMC	2L	33	23	19,22,23	1.85	3 (15%)	26,31,34	1.06	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
22	2MA	1L	38	22	17,25,26	2.30	6 (35%)	17,37,40	1.31	3 (17%)
22	5MU	1K	55	22	19,22,23	3.97	5 (26%)	28,32,35	3.10	8 (28%)
22	4SU	1K	8	22	18,21,22	1.79	5 (27%)	26,30,33	2.70	8 (30%)
23	7MG	2L	47	23	22,26,27	3.02	5 (22%)	29,39,42	2.84	10 (34%)
22	4SU	1L	8	22	18,21,22	1.86	3 (16%)	26,30,33	2.23	6 (23%)
22	PSU	1L	56	22,41	18,21,22	1.13	1 (5%)	22,30,33	1.83	3 (13%)
23	4SU	2K	8	23	18,21,22	1.91	5 (27%)	26,30,33	2.71	8 (30%)
22	2MA	1K	38	22	17,25,26	2.07	5 (29%)	17,37,40	1.23	2 (11%)
22	RSP	1K	33	22	17,21,22	3.97	7 (41%)	22,30,33	0.92	1 (4%)
22	7MG	1L	47	22	22,26,27	3.09	6 (27%)	29,39,42	2.81	10 (34%)
23	5MU	2L	55	23	19,22,23	3.79	5 (26%)	28,32,35	3.33	9 (32%)
22	7MG	1K	47	22	22,26,27	3.08	6 (27%)	29,39,42	2.81	10 (34%)
23	4SU	2L	8	23	18,21,22	1.72	3 (16%)	26,30,33	2.46	4 (15%)
23	7MG	2K	47	23	22,26,27	3.01	7 (31%)	29,39,42	2.75	10 (34%)
22	PSU	1K	56	22	18,21,22	1.26	1 (5%)	22,30,33	1.56	4 (18%)
23	5MU	2K	55	23	19,22,23	3.88	5 (26%)	28,32,35	3.68	8 (28%)
23	PSU	2K	56	23	18,21,22	1.23	2 (11%)	22,30,33	2.04	4 (18%)
22	5MU	1L	55	22	19,22,23	3.82	5 (26%)	28,32,35	3.13	9 (32%)
23	PSU	2L	56	23	18,21,22	1.35	2 (11%)	22,30,33	1.46	2 (9%)
22	RSP	1L	33	22	17,21,22	4.02	7 (41%)	22,30,33	0.97	1 (4%)
23	OMC	2K	33	23	19,22,23	1.73	4 (21%)	26,31,34	0.92	0

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
23	OMC	2L	33	23	-	0/9/27/28	0/2/2/2
22	2MA	1L	38	22	-	0/3/25/26	0/3/3/3
22	5MU	1K	55	22	-	0/7/25/26	0/2/2/2
22	4SU	1K	8	22	-	2/7/25/26	0/2/2/2
23	7MG	2L	47	23	-	2/7/37/38	0/3/3/3
22	4SU	1L	8	22	-	3/7/25/26	0/2/2/2
22	PSU	1L	56	22,41	-	0/7/25/26	0/2/2/2
23	4SU	2K	8	23	-	0/7/25/26	0/2/2/2
22	2MA	1K	38	22	-	0/3/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	RSP	1K	33	22	-	3/7/25/26	0/2/2/2
22	7MG	1L	47	22	-	2/7/37/38	0/3/3/3
23	5MU	2L	55	23	-	0/7/25/26	0/2/2/2
22	7MG	1K	47	22	-	2/7/37/38	0/3/3/3
23	4SU	2L	8	23	-	0/7/25/26	0/2/2/2
23	7MG	2K	47	23	-	2/7/37/38	0/3/3/3
22	PSU	1K	56	22	-	0/7/25/26	0/2/2/2
23	5MU	2K	55	23	-	0/7/25/26	0/2/2/2
23	PSU	2K	56	23	-	0/7/25/26	0/2/2/2
22	5MU	1L	55	22	-	0/7/25/26	0/2/2/2
23	PSU	2L	56	23	-	0/7/25/26	0/2/2/2
22	RSP	1L	33	22	-	3/7/25/26	0/2/2/2
23	OMC	2K	33	23	-	1/9/27/28	0/2/2/2

The worst 5 of 98 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1K	55	5MU	C2-N1	12.82	1.59	1.38
23	2K	55	5MU	C2-N1	12.76	1.58	1.38
22	1L	33	RSP	C2-N3	12.50	1.49	1.36
22	1L	55	5MU	C2-N1	12.12	1.57	1.38
23	2L	55	5MU	C2-N1	11.90	1.57	1.38

The worst 5 of 122 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	2K	55	5MU	C5-C4-N3	12.77	126.21	115.31
23	2L	55	5MU	C5-C4-N3	10.91	124.63	115.31
22	1K	55	5MU	C5-C4-N3	9.76	123.64	115.31
22	1L	55	5MU	C5-C4-N3	9.67	123.57	115.31
23	2K	8	4SU	C4-N3-C2	-8.50	119.08	127.34

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	1K	33	RSP	C3'-C4'-C5'-O5'
23	2K	33	OMC	C1'-C2'-O2'-CM2
23	2K	47	7MG	C2'-C1'-N9-C8
22	1L	33	RSP	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
22	1K	8	4SU	O4'-C4'-C5'-O5'

There are no ring outliers.

17 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	2L	33	OMC	1	0
22	1K	8	4SU	4	0
23	2L	47	7MG	4	0
22	1L	8	4SU	1	0
22	1L	56	PSU	1	0
23	2K	8	4SU	1	0
22	1K	38	2MA	2	0
22	1K	33	RSP	3	0
23	2L	55	5MU	2	0
22	1K	47	7MG	3	0
23	2L	8	4SU	1	0
23	2K	47	7MG	1	0
22	1K	56	PSU	1	0
23	2K	55	5MU	3	0
22	1L	55	5MU	1	0
22	1L	33	RSP	4	0
23	2K	33	OMC	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 1768 ligands modelled in this entry, 1766 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
61	SF4	3E	303	4	0,12,12	-	-	-		
61	SF4	32	303	4	0,12,12	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
61	SF4	3E	303	4	-	-	0/6/5/5
61	SF4	32	303	4	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
61	3E	303	SF4	2	0
61	32	303	SF4	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
24	3L	1
24	3K	1
32	41	1
29	11	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	3L	49:C	O3’	50:G	P	6.50
1	3K	49:C	O3’	50:G	P	5.32
1	41	140:ILE	C	141:PHE	N	1.19
1	11	239:ARG	C	240:ALA	N	1.09

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.