wwPDB X-ray Structure Validation Summary Report (i)

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)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

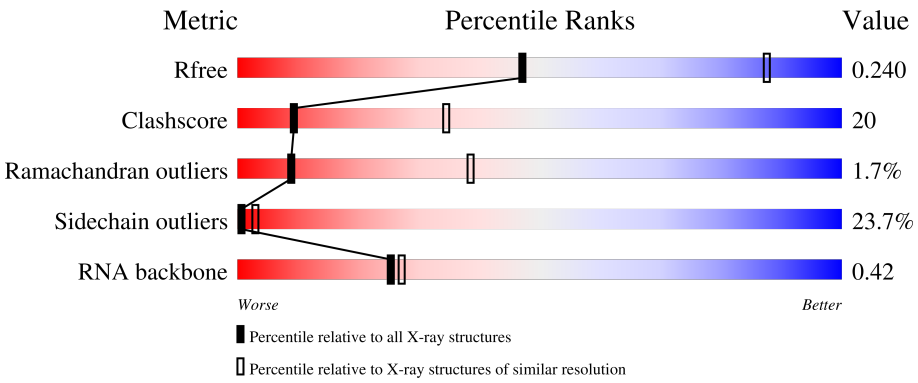
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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	42% 44% 14%
4	3E	209	50% 41% 9% •
5	42	162	41% 38% 14% 7%
5	4E	162	49% 34% 9% 8%
6	52	101	58% 33% 8% •
6	5E	101	57% 37% 6%
7	62	156	38% 41% 8% • 12%
7	6E	156	52% 41% 6% •
8	72	138	51% 39% 9%
8	7E	138	37% 53% 10%
9	82	128	37% 52% 7% • •
9	8E	128	42% 41% 14% • •
10	1A	105	28% 48% 19% 6%
10	1I	105	36% 44% 13% • 6%
11	2A	129	45% 33% 9% 12%
11	2I	129	40% 37% 9% 14%
12	3A	132	43% 36% 11% • 8%
12	3I	132	39% 42% 11% 8%
13	4A	126	31% 41% 14% • 12%
13	4I	126	44% 40% 10% 6%
14	5A	61	38% 44% 10% • 7%
14	5I	61	39% 46% 15%
15	6A	89	49% 46% • •
15	6I	89	47% 46% • •
16	7A	88	50% 41% 5% 5%

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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	44% 47% 9%
43	65	112	30% 46% 18%
43	A8	112	39% 45% 13%
44	75	146	34% 47% 11% 8%
44	B8	146	32% 49% 13% 7%
45	85	118	47% 42% 9%
45	C8	118	49% 38% 7%
46	95	101	37% 49% 10%
46	D8	101	49% 34% 16%
47	A5	113	49% 40% 10%
47	E8	113	63% 29% 7%
48	B5	96	46% 45% 7%
48	F8	96	53% 34% 11%
49	C5	110	35% 40% 17% 5%
49	G8	110	43% 41% 10% 5%
50	D5	206	38% 41% 16%
50	H8	206	31% 35% 12% 20%
51	E5	85	54% 28% 9% 8%
51	I8	85	53% 31% 9% 5%
52	F5	98	43% 36% 15%
52	J8	98	55% 31% 9% 5%
53	G5	72	38% 39% 14% 8%
53	K8	72	36% 42% 15%
54	H5	60	65% 28%
54	L8	60	48% 37% 12%

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Mol	Chain	Length	Quality of chain
55	M8	71	21% 28% 18% 32%
56	J5	60	47% 37% 10% 7%
56	N8	60	42% 30% 12% 17%
57	O8	54	13% 50% 19% • 17%
58	L5	49	49% 43% • •
58	P8	49	49% 43% • •
59	M5	65	38% 43% 12% 5% •
59	Q8	65	49% 35% 11% • •

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 (i)

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
			Total	C	N	O	P			
1	13	1512	32497	14464	6017	10504	1512	0	0	0
1	1G	1509	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
			Total	C	N	O	S			
2	1E	231	1874	1199	334	336	5	0	0	0
2	12	237	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
			Total	C	N	O	S			
3	2E	205	1605	1011	313	280	1	0	0	0
3	22	195	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
			Total	C	N	O	S			
4	3E	207	1690	1058	336	289	7	0	0	0
4	32	208	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
			Total	C	N	O	S			
5	4E	149	1142	722	216	200	4	0	0	0
5	42	151	1155	729	218	204	4	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
15	6I	87	729	457	146	124	2	0	0	0
			Total	C	N	O	S			
15	6A	87	729	457	146	124	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
			Total	C	N	O			
21	1F	24	208	128	50	30	0	0	0
21	1B	24	208	128	50	30	0	0	0

- Molecule 22 is a RNA chain called tRNAArg.

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

- Molecule 23 is a RNA chain called tRNAfMet.

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

- Molecule 24 is a RNA chain called tRNAArg.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
24	3K	73	1561	696	285	507	73	0	0	0
24	3L	74	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
			Total	C	N	O	P			
25	4K	21	462	207	97	137	21	0	0	0
25	4L	17	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
			Total	C	N	O	P			
26	1H	2895	62351	27751	11658	20047	2895	0	0	0
26	14	2895	62347	27751	11660	20042	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
			Total	C	N	O	P			
27	16	122	2617	1166	486	844	121	0	0	0
27	1J	122	2617	1166	486	844	121	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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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
			Total	C	N	O	S			
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
			Total	C	N	O	S			
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
			Total	C	N	O	S			
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
			Total	C	N	O	S			
40	78	147	1122	698	229	192	3	0	0	0
40	35	148	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
			Total	C	N	O	S			
41	88	141	1113	709	210	187	7	0	0	0
41	45	138	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
			Total	C	N	O	S			
42	98	118	967	604	203	159	1	0	0	0
42	55	118	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
			Total	C	N	O			
43	A8	111	881	556	176	149	0	0	0
43	65	110	876	553	175	148	0	0	0

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

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

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

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
45	85	117	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
			Total	C	N	O	S			
46	D8	101	778	501	142	134	1	0	0	0
46	95	100	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
			Total	C	N	O	S			
47	E8	112	890	560	175	153	2	0	0	0
47	A5	111	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
			Total	C	N	O	S			
48	F8	95	743	482	134	126	1	0	0	0
48	B5	94	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
			Total	C	N	O	S			
49	G8	105	784	504	147	128	5	0	0	0
49	C5	106	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
			Total	C	N	O	S			
50	H8	165	1330	851	241	236	2	0	0	0
50	D5	200	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
			Total	C	N	O	S			
51	I8	81	630	389	133	107	1	0	0	0
51	E5	78	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
			Total	C	N	O	S			
52	J8	93	729	457	145	126	1	0	0	0
52	F5	94	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
			Total	C	N	O	S			
53	K8	69	576	358	116	101	1	0	0	0
53	G5	66	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
			Total	C	N	O			
54	L8	58	459	293	89	77	0	0	0
54	H5	58	459	293	89	77	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
55	M8	48	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
			Total	C	N	O	S			
56	N8	50	386	241	77	63	5	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
56	J5	56	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
			Total	C	N	O	S			
57	O8	45	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
			Total	C	N	O	S			
58	P8	47	401	246	99	54	2	0	0	0
58	L5	47	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
			Total	C	N	O	S			
59	Q8	64	516	331	102	81	2	0	0	0
59	M5	64	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
			Total	Mg		
60	13	227	227	227	0	0
60	3E	2	2	2	0	0
60	5E	2	2	2	0	0
60	6I	1	1	1	0	0
60	1K	2	2	2	0	0
60	2K	7	7	7	0	0
60	4K	1	1	1	0	0

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

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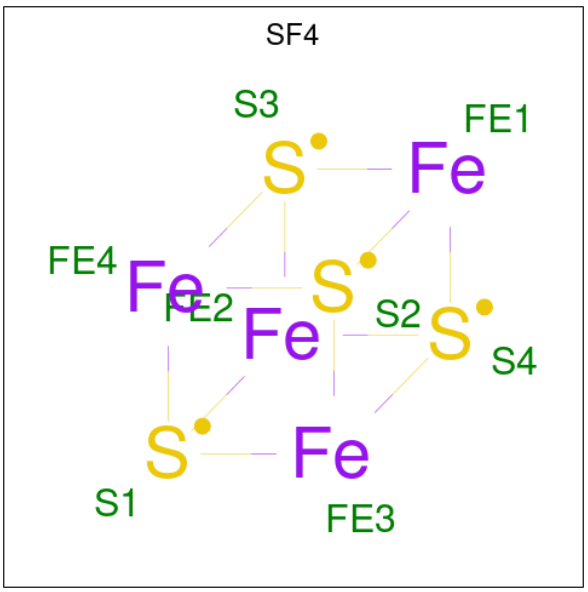
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
60	1J	8	8	8	0	0
60	29	5	5	5	0	0
60	39	2	2	2	0	0
60	25	2	2	2	0	0
60	35	1	1	1	0	0
60	45	2	2	2	0	0
60	55	2	2	2	0	0
60	75	1	1	1	0	0
60	C5	1	1	1	0	0
60	E5	1	1	1	0	0
60	F5	1	1	1	0	0
60	M5	1	1	1	0	0

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



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

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

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

- Molecule 63 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
63	13	544	544	544	0	0
			Total	O		
63	1E	1	1	1	0	0
			Total	O		
63	3E	1	1	1	0	0
			Total	O		
63	4E	2	2	2	0	0
			Total	O		
63	8E	1	1	1	0	0
			Total	O		
63	1I	1	1	1	0	0
			Total	O		
63	3I	5	5	5	0	0
			Total	O		
63	5I	3	3	3	0	0
			Total	O		
63	6I	4	4	4	0	0
			Total	O		
63	BI	1	1	1	0	0
			Total	O		
63	1F	1	1	1	0	0
			Total	O		
63	1K	1	1	1	0	0
			Total	O		
63	2K	16	16	16	0	0
			Total	O		
63	4K	13	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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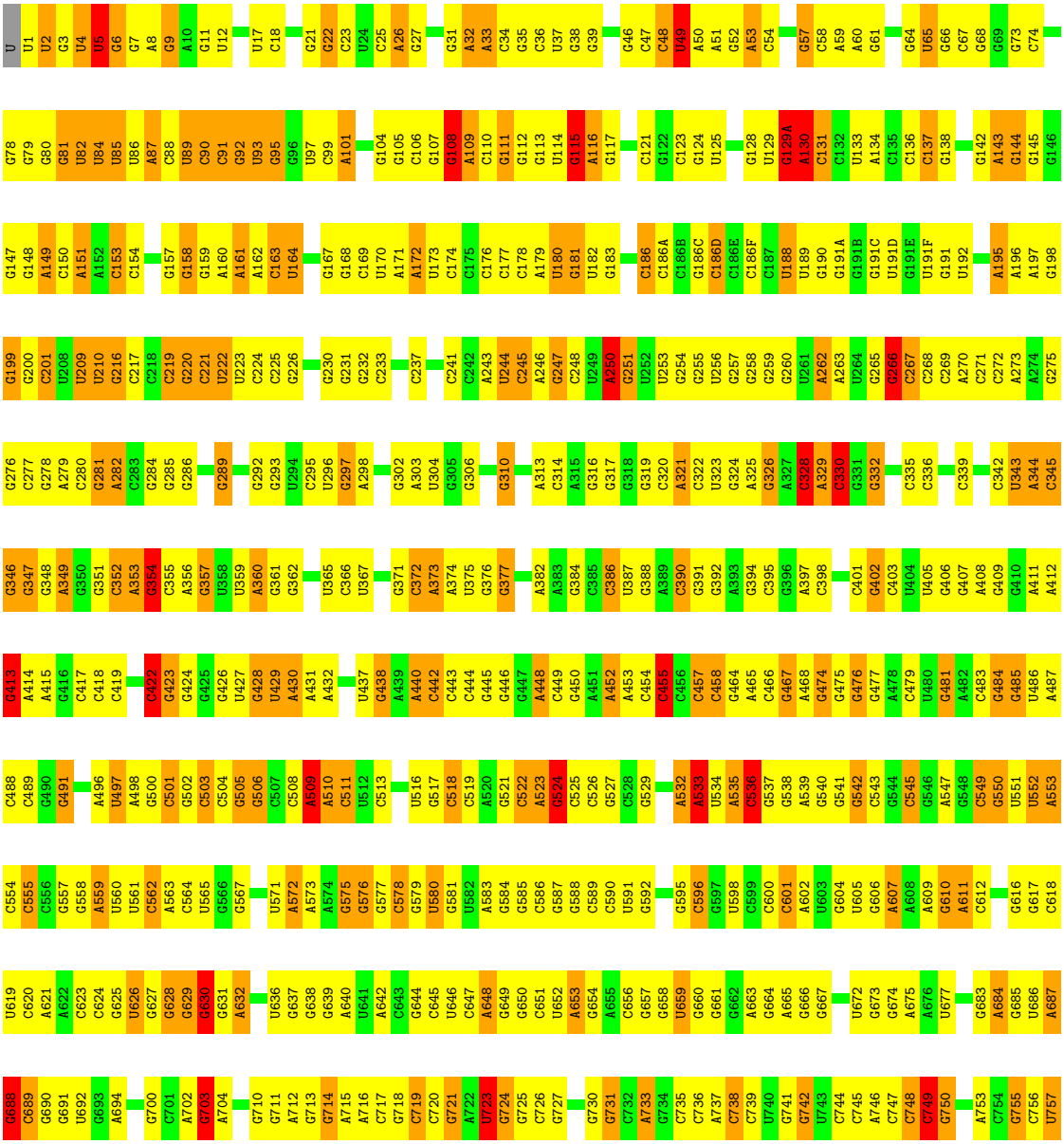
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
63	A5	1	1	1	0	0
			Total	O		
63	B5	1	1	1	0	0
			Total	O		
63	C5	1	1	1	0	0
			Total	O		
63	E5	3	3	3	0	0
			Total	O		
63	F5	6	6	6	0	0
			Total	O		
63	L5	2	2	2	0	0
			Total	O		
63	M5	9	9	9	0	0

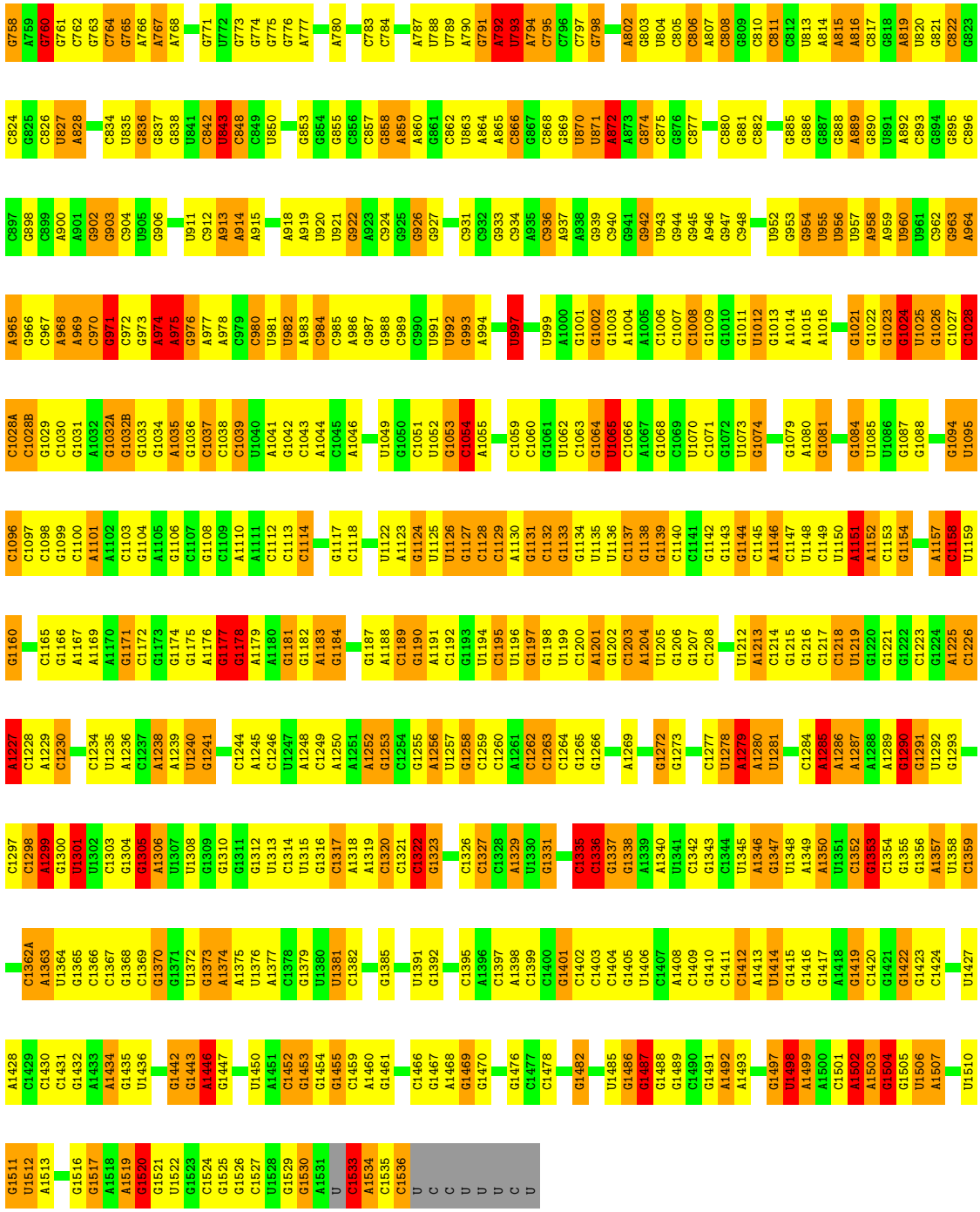
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 16S ribosomal RNA

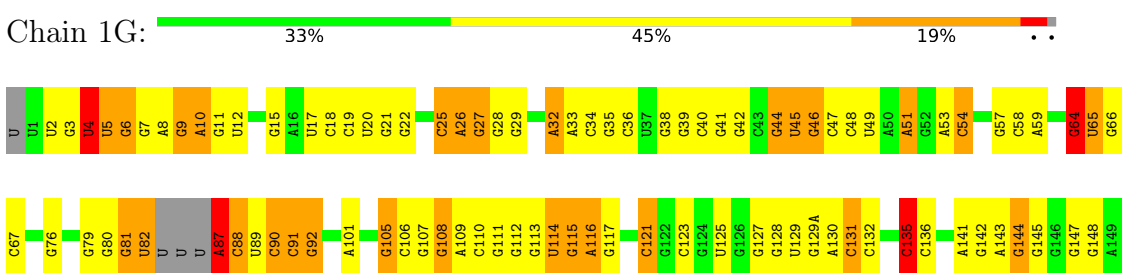
Chain 13: 28% 45% 22%

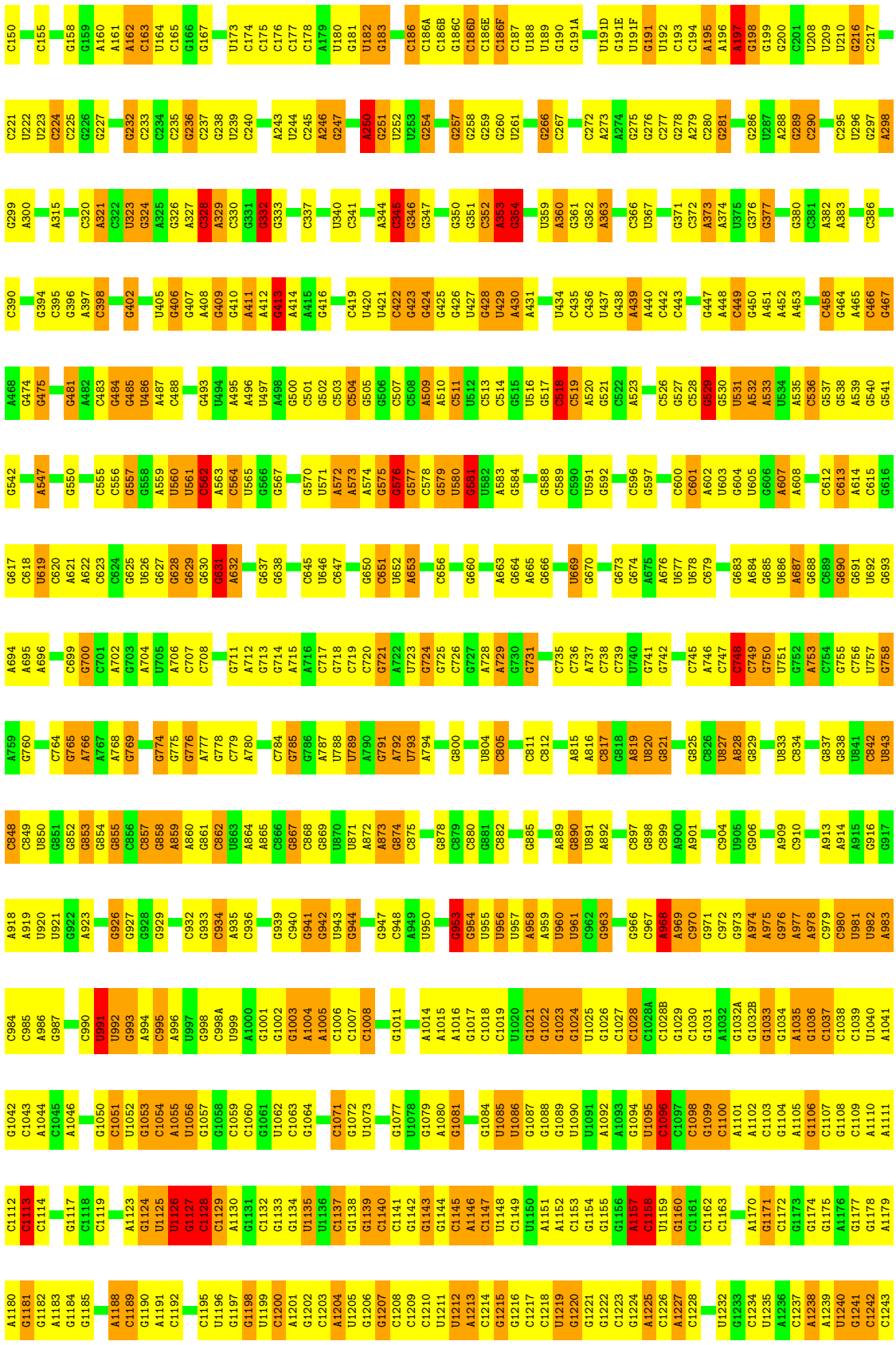


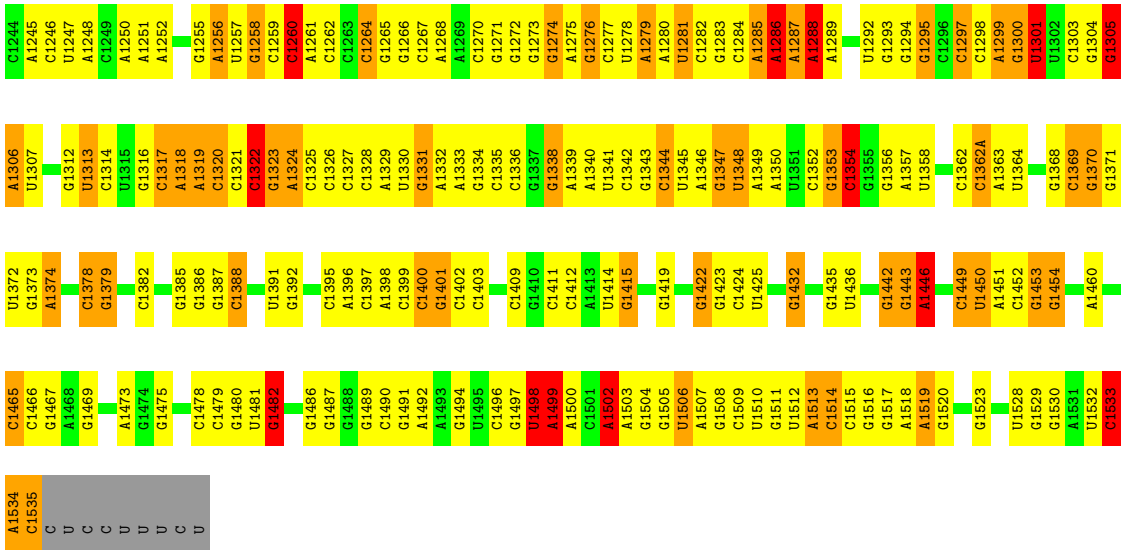


• Molecule 1: 16S ribosomal RNA

Chain 1G:

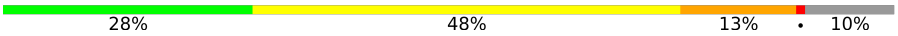


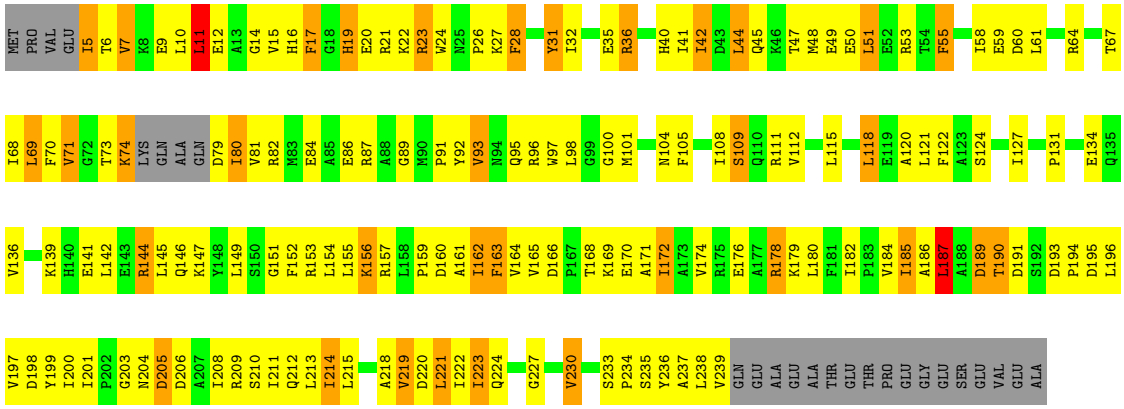

C150 C155 G158 G159 A160 A161 A162 C163 U164 C165 G166 G167 U173 C174 C175 C176 C177 C178 A179 U180 G181 U182 G183 C186 C186A C186B G186C C186D C186E C186F C187 U188 U189 G190 G191A U191D G191E U191F G191 U192 C193 C194 A195 A196 A197 G198 G199 G200 C201 U208 U209 U210 G216 C217
C221 U222 U223 C224 C225 G226 G227 G232 C233 C234 C235 G236 C237 C238 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 G328 A329 C330 G331 G332 G333 C337 U340 C341 A344 G345 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 G509 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 G685 U686 A687 G688 C689 G690 G691 U692 G693
A694 A695 A696 C699 G700 C701 A702 G703 A704 U705 A706 C707 C708 G711 A712 G713 G714 A715 A716 C717 G718 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 A819 U820 G821 G825 C826 U827 A828 G829 U833 C834 G837 G838 U841 C842 U843
C848 C849 U850 G851 G852 G853 G854 G855 C856 C857 G858 A859 A860 G861 C862 U863 A864 A865 C866 G867 C868 G869 U870 U871 A872 A873 G874 C875 G878 C879 C880 G881 C882 G885 A889 G890 U891 A892 C897 G898 C899 A900 A901 C904 U905 G906 A909 C910 A913 A914 A915 G916 G917
A918 A919 U920 U921 G922 A923 G926 G927 G928 G929 C932 G933 C934 A935 C936 G939 U940 G941 G942 U943 G944 G947 C948 A949 U950 G953 G954 U955 U956 U957 A958 A959 U960 U961 C962 G963 G966 C967 A968 A969 C970 G971 C972 G973 A974 A975 G976 A977 A978 C979 C980 U981 U982 A983
C984 C985 A986 G987 C990 U991 U992 G993 A994 C995 A996 U997 G998 C998A U999 A1000 G1001 G1002 G1003 A1004 A1005 C1006 C1007 C1008 G1011 A1014 A1015 A1016 G1017 C1018 C1019 U1020 G1021 G1022 G1023 G1024 U1025 G1026 C1027 C1028 C1028A C1028B G1029 C1030 G1031 A1032 G1032A G1032B G1033 G1034 A1035 G1036 C1037 C1038 C1039 U1040 A1041
G1042 C1043 A1044 C1045 A1046 G1050 C1051 U1052 G1053 C1054 A1055 U1056 G1057 G1058 C1059 C1060 G1061 U1062 C1063 G1064 C1071 C1072 U1073 G1077 U1078 G1079 A1080 G1081 G1084 U1085 U1086 G1087 G1088 G1089 U1090 U1091 A1092 A1093 G1094 U1095 C1096 C1097 C1098 G1099 C1100 A1101 A1102 C1103 G1104 A1105 G1106 C1107 G1108 C1109 A1110 A1111
C1112 C1113 C1114 G1117 C1118 C1119 A1123 G1124 U1125 U1126 G1127 C1128 C1129 A1130 G1131 C1132 G1133 A1134 U1135 U1136 C1137 G1138 G1139 G1140 C1141 G1142 G1143 G1144 C1145 A1146 C1147 U1148 C1149 U1150 A1151 A1152 C1153 G1154 G1155 G1156 A1157 C1158 U1159 C1160 C1161 C1162 C1163 A1170 G1171 C1172 G1173 G1174 G1175 A1176 G1177 G1178 A1179
A1180 G1181 G1182 A1183 G1184 G1185 A1188 C1189 G1190 A1191 C1192 C1195 U1196 G1197 G1198 U1199 C1200 A1201 G1202 C1203 A1204 U1205 G1206 G1207 C1208 C1209 C1210 U1211 U1212 A1213 C1214 G1215 G1216 C1217 C1218 U1219 G1220 G1221 G1222 C1223 G1224 A1225 C1226 A1227 C1228 U1232 G1233 C1234 U1235 A1236 C1237 A1238 A1239 U1240 G1241 C1242 C1243



- Molecule 2: 30S ribosomal protein S2

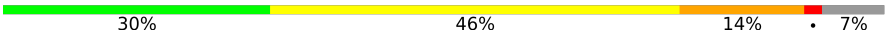
Chain 1E:

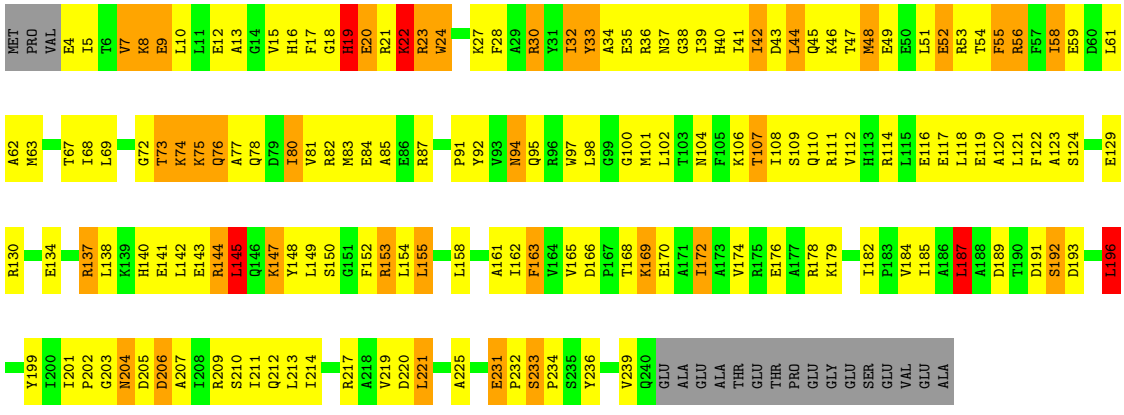




- Molecule 2: 30S ribosomal protein S2

Chain 12:





- Molecule 3: 30S ribosomal protein S3

Chain 2E: 48% 32% 6% 14%

MET G2 N3 K4 I5 H6 P7 I8 R11 L12 G13 I14 T15 R16 D17 W18 E19 S20 R21 W22 Y23 K26 R30 H31 L32 E35 D36 Q37 R38 I39 R40 E44 L47 Y48 S49 L52 A53 R54 E58 R59 N63 V64 A65 K72 P73 G74 V75 V76 I77 G78

R79 R83 L91 T95 G96 K97 N98 V99 Q104 E105 L111 V116 R119 Q123 I124 E125 R126 R127 F128 A129 V130 R131 R132 A133 I134 K135 Q136 A137 V138 Q139 R140 S144 V153 S154 Q162 E166 Q170 G171 R172 L175 H176 R179 A180 N181 I182

D183 Y184 L188 A189 R190 T191 T192 V195 Y201 I202 E206 VAL ILE GLY GLY GLN LYS PRO LYS ALA ARG PRO GLU LEU PRO LYS ALA GLU GLU ARG PRO ARG ARG ARG ARG PRO ALA VAL ARG VAL LYS LYS GLU GLU

- Molecule 3: 30S ribosomal protein S3

Chain 22: 38% 34% 9% 18%

MET G2 N3 K4 I5 H6 P7 I8 G9 F10 R11 I14 T15 R16 D17 W18 E19 S20 R21 W22 K27 Q28 Y29 L32 L33 L34 E35 D36 Q37 R40 G41 L42 L43 E44 K45 E46 L47 Y48 S49 A50 G51 L52 A53 R54 V55 D56 I57 E58 R59 D62 N63 V64 V68 H69

V70 A71 K72 P73 G74 V75 V76 ILE GLY ARG GLY GLY GLU ARG I84 R85 V86 L87 R88 E89 E90 L91 L94 T95 G96 K97 N98 V99 A100 L101 N102 V103 N108 P109 N110 L111 S112 A113 P114 L115 V116 A117 Q118 R119 V120 A121 E125 A129 V130 R131 R132 A133 I134 A137 V138

Q139 R140 V141 M142 E143 S144 G148 A149 K150 V151 I152 V153 S154 G155 R156 G159 W167 A168 A169 R172 L175 H176 T177 L178 R179 A180 N181 A189 R190 T191 T192 Y193 G194 V195 L196 G197 V198 K199 A200 Y201 I202 F203 LEU GLY GLU VAL ILE GLY GLY GLN LYS PRO LYS ALA

ARG PRO GLU LEU PRO LYS ALA GLU GLU ARG PRO ARG ARG ARG ARG PRO ALA VAL ARG VAL LYS LYS GLU GLU

- Molecule 4: 30S ribosomal protein S4

Chain 3E: 50% 41% 9%

MET GLY R3 P7 V8 C9 R10 L11 C12 R13 R14 E15 G16 V17 K18 L19 Y20 L21 K22 R25 C26 P29 K30 C31 A32 M33 E34 R35 R36 P37 Y38 G41 Q42 H43 K46 R50 Y54 A55 V56 R57 L58 R59 E60 L64 R65 R66 I67 I70 Q74 F75

R76 N77 L78 A82 K85 V88 T89 G90 S91 V92 F93 L96 L97 E98 S99 D102 N103 V104 R107 L108 G109 F110 A111 V112 S113 R114 R115 Q116 R122 H123 I126 T127 R132 L135 P136 S137 Y138 R139 V140 R141 V148 A149 E150 K151 S152 R153 N154 L155 E156

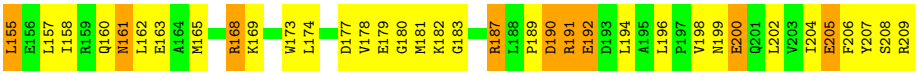
L157 I158 R159 Q160 N161 L162 E163 A164 M165 K166 G167 R168 W173 L174 S175 L176 M181 K184 R187 L188 P189 D190 R191 E192 D193 L194 A195 L196 P197 V198 N199 E200 Q201 L202 Y207 S208 R209

- Molecule 4: 30S ribosomal protein S4

Chain 32: 42% 44% 14%

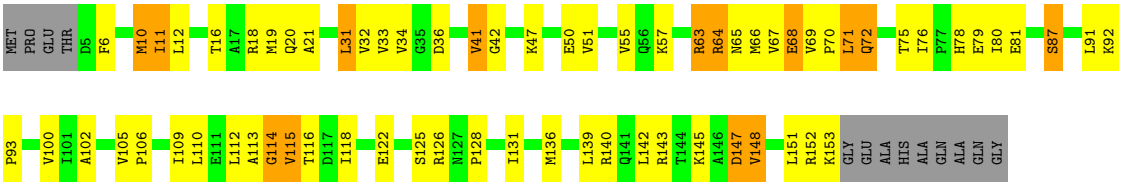
MET G2 R3 Y4 P7 V8 C9 R10 L11 C12 R13 R14 E15 G16 V17 K18 L19 Y20 L21 K22 G23 E24 R25 C26 Y27 S28 P29 K30 C31 A32 M33 E34 R35 R36 P37 Y38 P39 H43 G44 Q45 R49 R50 P51 S52 D53 R57 L58 R59 E60 K61 Q62 K63 L64 S71 E72

R73 Q74 F75 R76 N77 L78 F79 A82 S83 V88 T89 G90 L94 G95 L96 L97 E98 L101 D102 N103 V104 V105 L108 G109 F110 A111 V112 R115 Q116 A117 R118 Q119 L120 V121 R122 H123 T127 D134 L135 P136 S137 Y138 R139 V140 V148 A149 E150 K151 S152 R153 N154



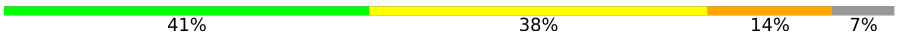
- Molecule 5: 30S ribosomal protein S5

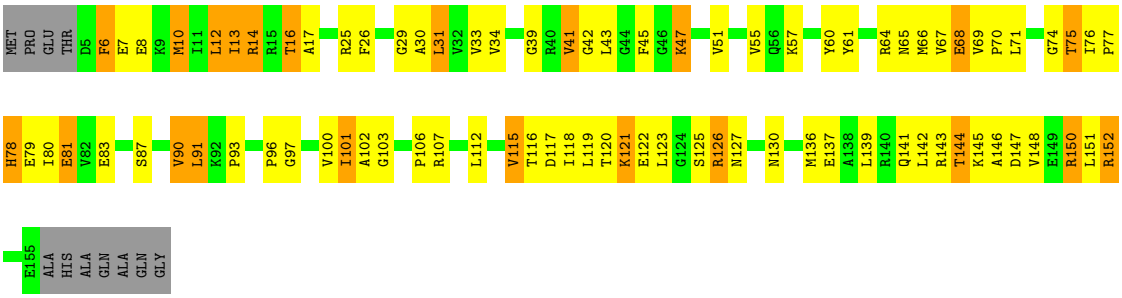
Chain 4E:



- Molecule 5: 30S ribosomal protein S5

Chain 42:



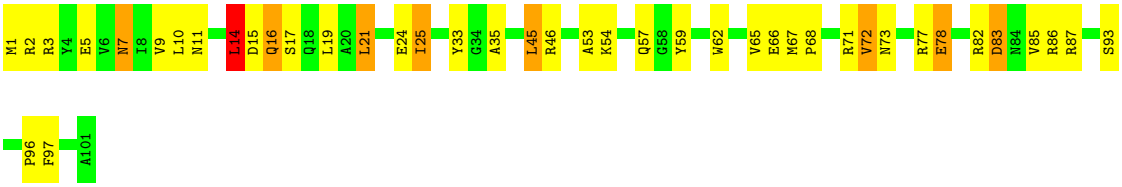


- Molecule 6: 30S ribosomal protein S6

Chain 5E:

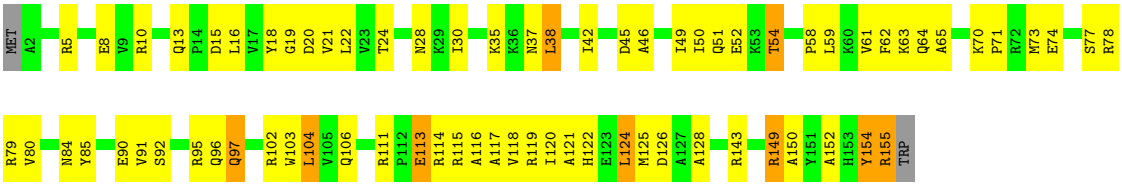
- Molecule 6: 30S ribosomal protein S6

Chain 52:



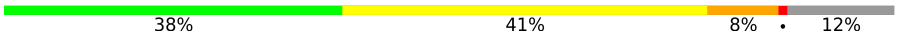
- Molecule 7: 30S ribosomal protein S7

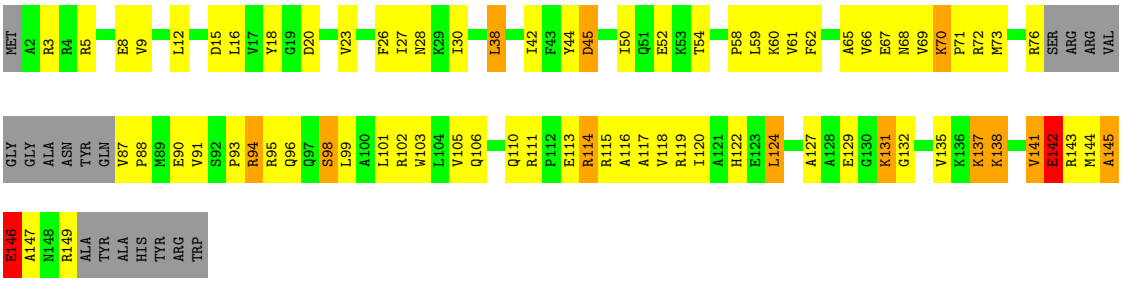
Chain 6E:



• Molecule 7: 30S ribosomal protein S7

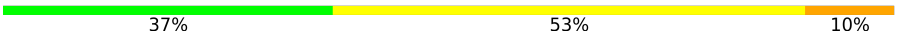
Chain 62:

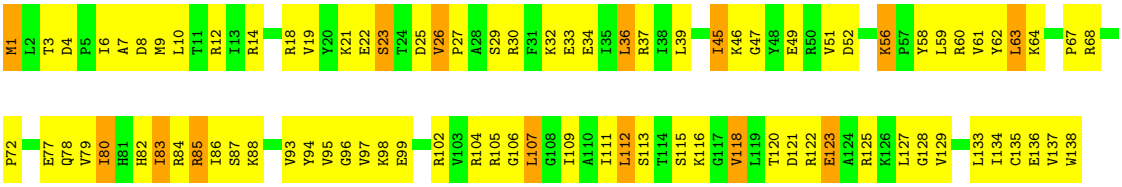




• Molecule 8: 30S ribosomal protein S8

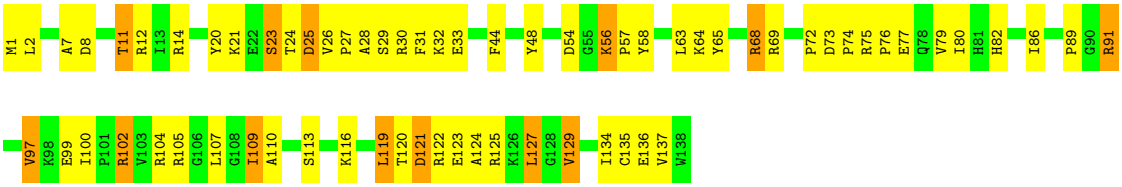
Chain 7E:





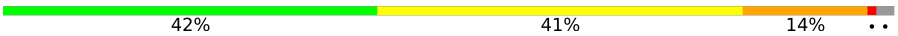
• Molecule 8: 30S ribosomal protein S8

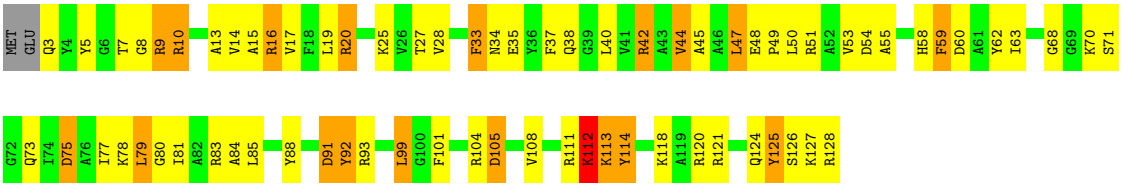
Chain 72:



• Molecule 9: 30S ribosomal protein S9

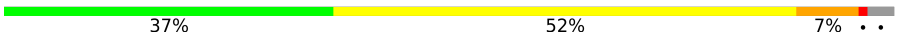
Chain 8E:

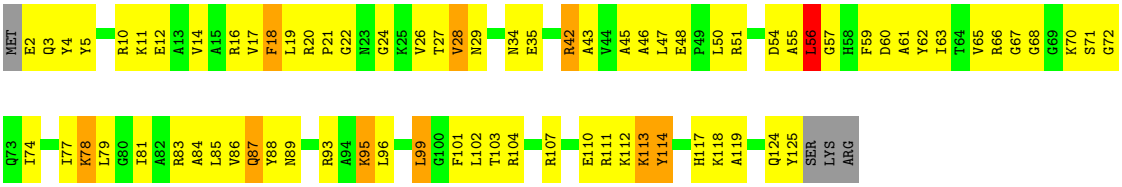




- Molecule 9: 30S ribosomal protein S9

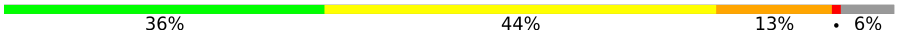
Chain 82:

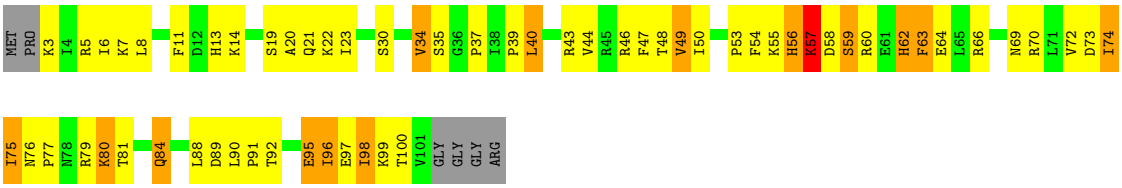




- Molecule 10: 30S ribosomal protein S10

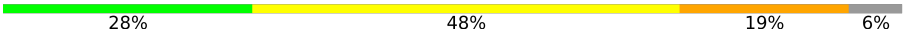
Chain 1I:

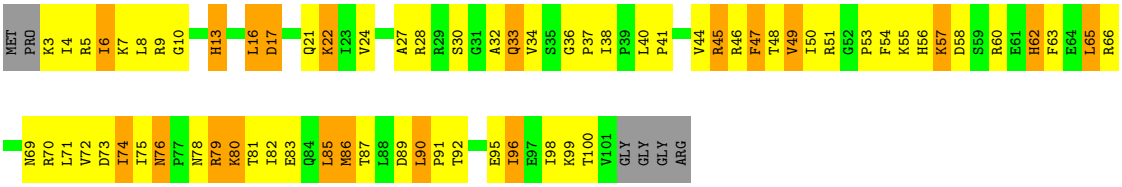




- Molecule 10: 30S ribosomal protein S10

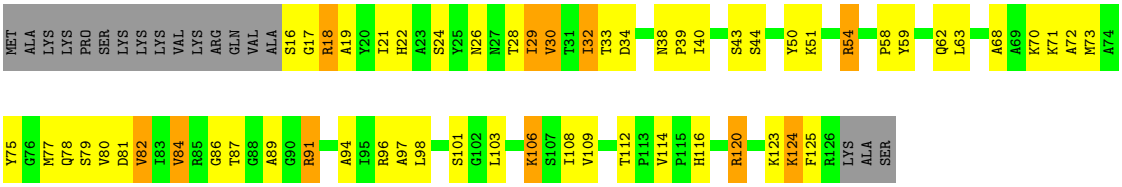
Chain 1A:





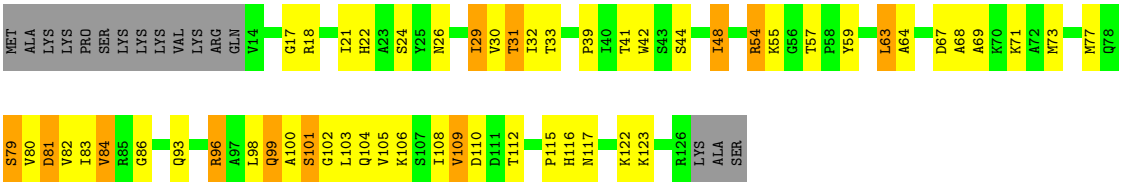
- Molecule 11: 30S ribosomal protein S11

Chain 2I:



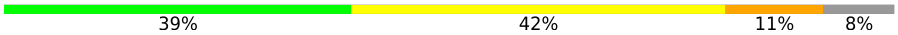
- Molecule 11: 30S ribosomal protein S11

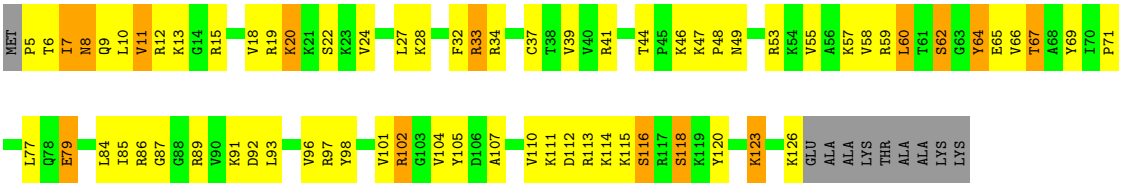
Chain 2A:



- Molecule 12: 30S ribosomal protein S12

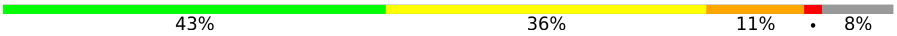
Chain 3I:

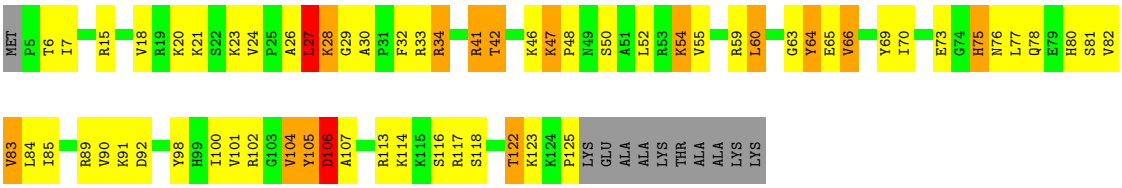




- Molecule 12: 30S ribosomal protein S12

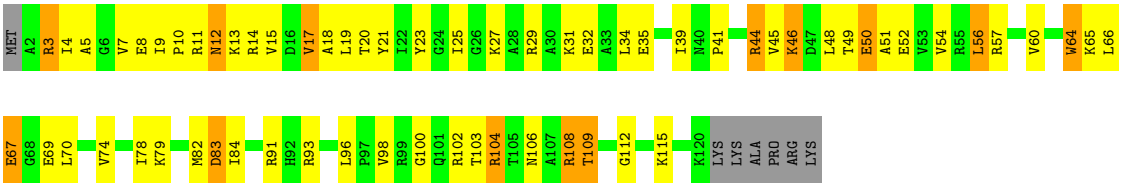
Chain 3A:





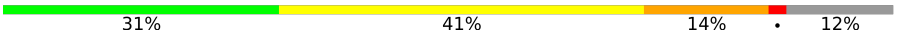
- Molecule 13: 30S ribosomal protein S13

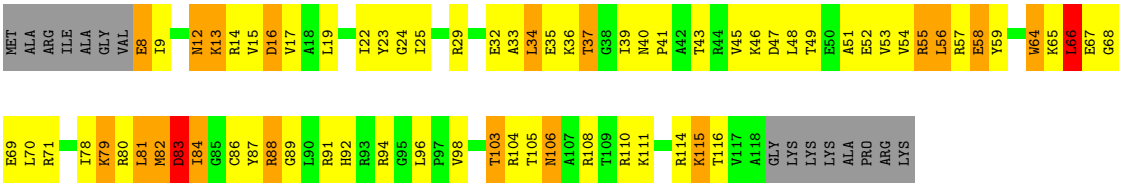
Chain 4I:



- Molecule 13: 30S ribosomal protein S13

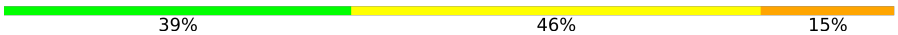
Chain 4A:

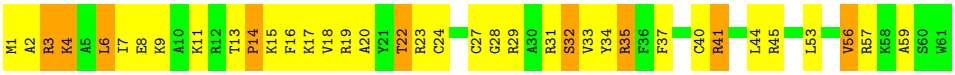




- Molecule 14: 30S ribosomal protein S14 type Z

Chain 5I:





- Molecule 14: 30S ribosomal protein S14 type Z

Chain 5A: 38% 44% 10% • 7%

MET ALA ARG LYS A5 L6 I7 E8 K9 A10 K11 R12 T13 P14 K17 V18 R19 A20 Y21 T22 R23 C24 Y25 R26 C27 G28 R29 A30 V33 F36 F37 C40 R41 I42 C43 L44 R45 H49 K50 L53 P54 G55 V56 R57 K58 A59 S60 W61

• Molecule 15: 30S ribosomal protein S15

Chain 6I: 47% 46% • •

MET P2 I3 T4 K5 E6 Q9 K10 V11 I12 Q13 E14 F15 A16 R17 F18 D21 T22 G23 S24 T25 E26 L31 L34 E41 H42 L43 K47 H51 L56 L57 M58 Q62 R63 R64 R65 L66 L67 R68 Y69 L70 Q71 R72 E73 E76 R77 Y78 R79 I82

E83 K84 L85 G86 I87 R88 GLY

• Molecule 15: 30S ribosomal protein S15

Chain 6A: 49% 46% • •

MET P2 I3 T4 K5 E6 E7 K8 Q9 I12 A16 R17 D21 T22 G23 S24 T25 E26 V27 Q28 L32 T33 L34 R35 L39 S40 E41 H42 L43 K44 V45 L56 G61 Q62 L66 Y69 L70 E73 D74 P75 E76 R77 Y78 R79 A80 L81 I82 E83 K84 L85

G86 I87 R88 GLY

• Molecule 16: 30S ribosomal protein S16

Chain 7I: 38% 45% 11% 6%

M1 V2 K3 I4 R5 L6 A7 R8 F9 G10 S11 K12 H13 N14 P15 H16 Y17 R18 I19 V20 V21 T22 D23 A24 R25 R26 K27 R28 D29 G30 K31 Y32 I33 I36 R42 K43 T44 T45 P46 D47 W48 L49 K50 V51 D52 V53 R57 Y58 S61 V62 P66 R71 R72 L73

L74 R75 Q76 A77 G78 V79 F80 R81 Q82 E83 ALA ARG GLU GLY ALA

• Molecule 16: 30S ribosomal protein S16

Chain 7A: 50% 41% 5% 5%

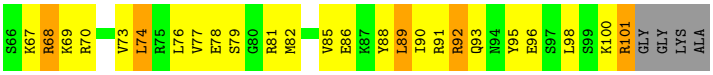
M1 V2 R5 L6 F9 G10 S11 N14 P15 H16 Y17 R18 I19 V20 V21 T22 K27 I33 E34 K35 I36 R42 K43 T44 T45 P46 D47 W48 L49 K50 V53 E54 R55 A56 R57 Y58 W59 L60 S61 V62 Q65 P66 T67 R72 L73 L74 R75 V79 F80

A84 ARG GLU GLY ALA

• Molecule 17: 30S ribosomal protein S17

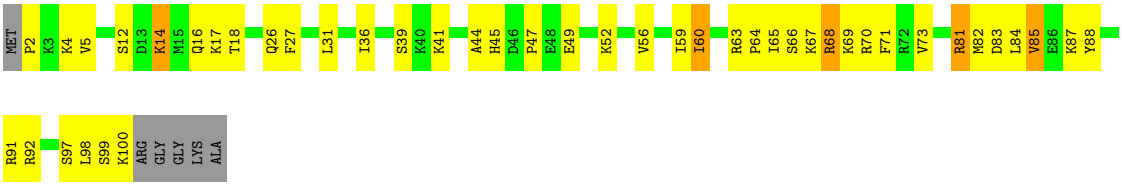
Chain 8I: 34% 53% 8% 5%

MET P2 K3 K4 T7 G8 V9 V10 V11 S12 D13 K14 M15 Q16 K17 T18 V19 T20 V21 L22 V23 E24 R25 P28 H29 P30 L31 Y32 G33 K34 V35 R38 S39 K40 K41 Y42 L43 A44 H45 E48 F49 K50 Y51 K52 D55 V56 V57 E58 I59 I60 E61 S62 R63 P64 I65



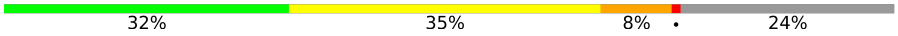
- Molecule 17: 30S ribosomal protein S17

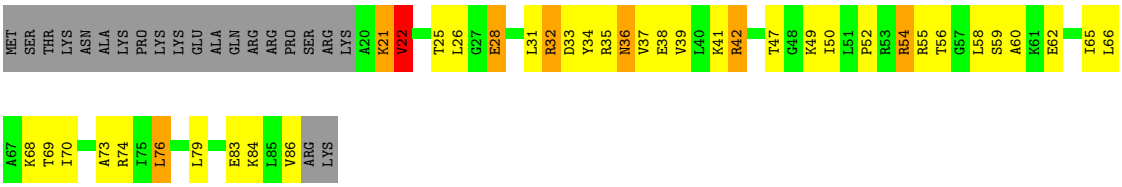
Chain 8A:



- Molecule 18: 30S ribosomal protein S18

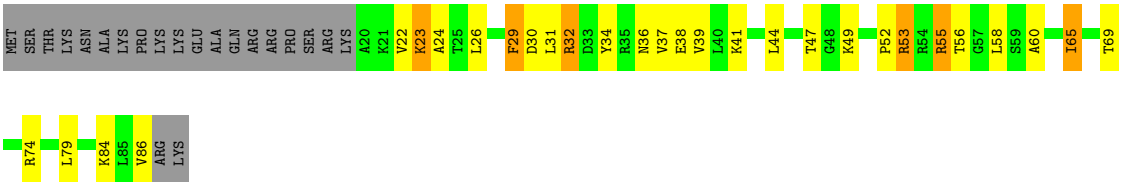
Chain 9I:





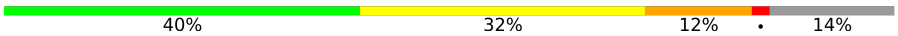
- Molecule 18: 30S ribosomal protein S18

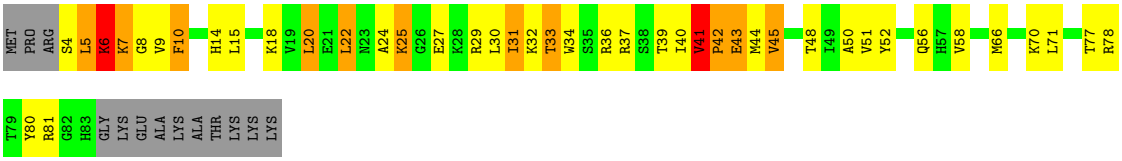
Chain 9A:



- Molecule 19: 30S ribosomal protein S19

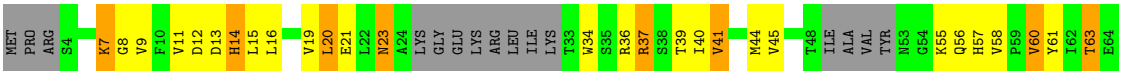
Chain AI:





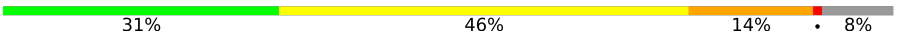
- Molecule 19: 30S ribosomal protein S19

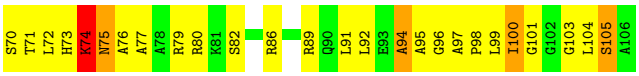
Chain AA:



• Molecule 20: 30S ribosomal protein S20

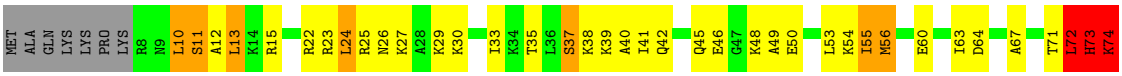
Chain BI:





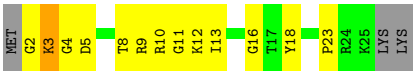
• Molecule 20: 30S ribosomal protein S20

Chain BA:



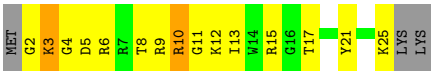
• Molecule 21: 30S ribosomal protein Thx

Chain 1F:



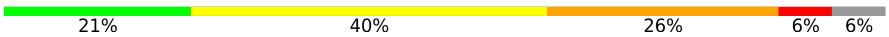
• Molecule 21: 30S ribosomal protein Thx

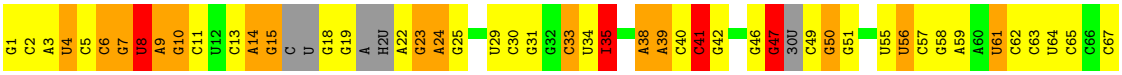
Chain 1B:

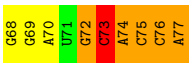


• Molecule 22: tRNAArg

Chain 1K:

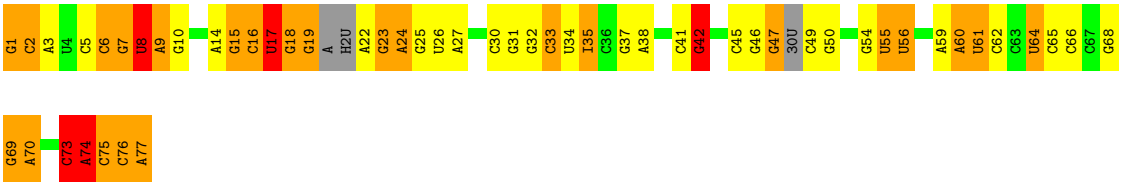






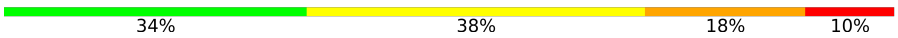
• Molecule 22: tRNAArg

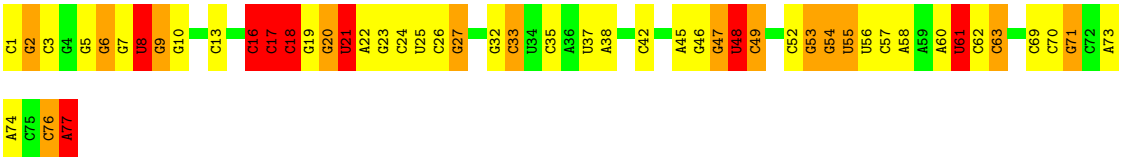
Chain 1L:



• Molecule 23: tRNAfMet

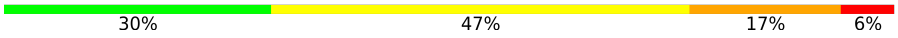
Chain 2K:

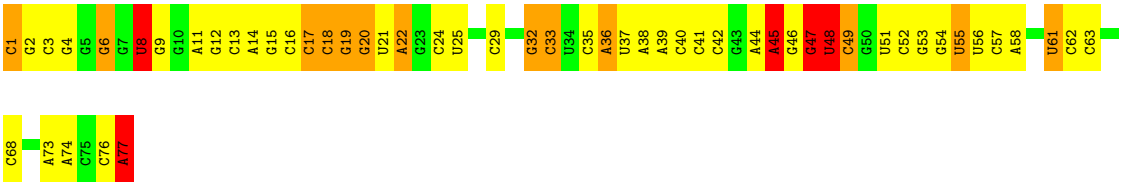




• Molecule 23: tRNAfMet

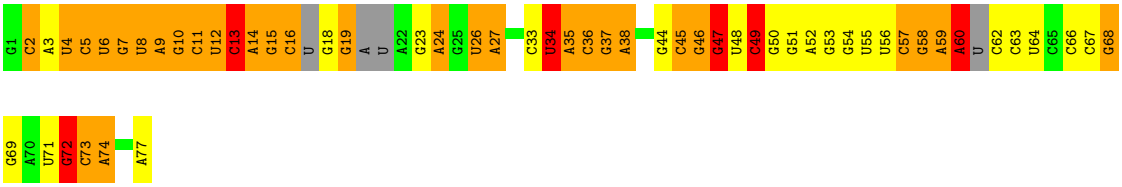
Chain 2L:





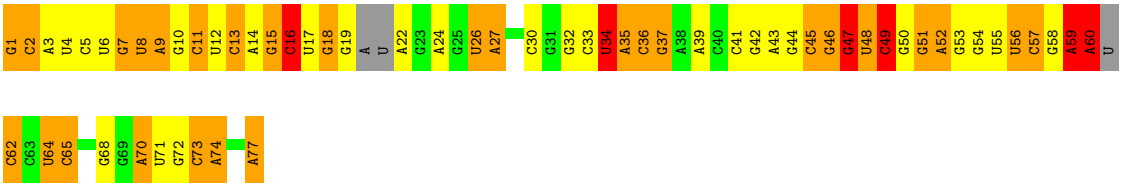
• Molecule 24: tRNAArg

Chain 3K:



• Molecule 24: tRNAArg

Chain 3L:

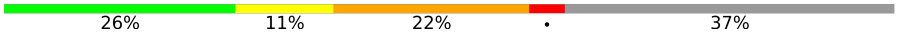


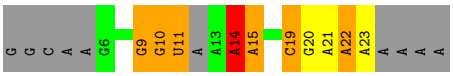
• Molecule 25: mRNA

Chain 4K:

• Molecule 25: mRNA

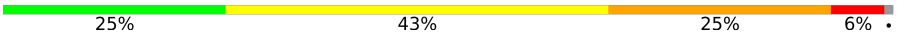
Chain 4L:

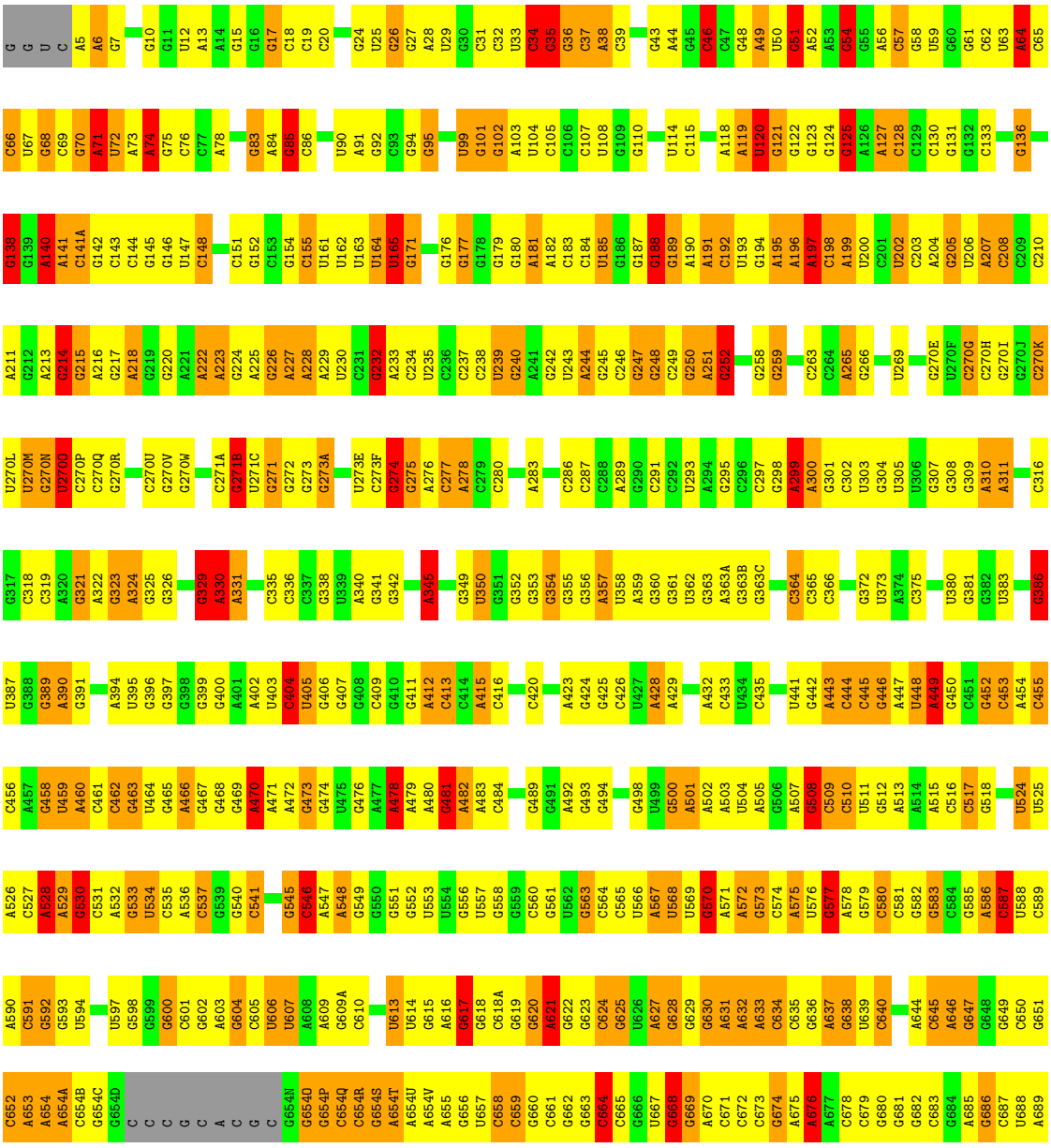


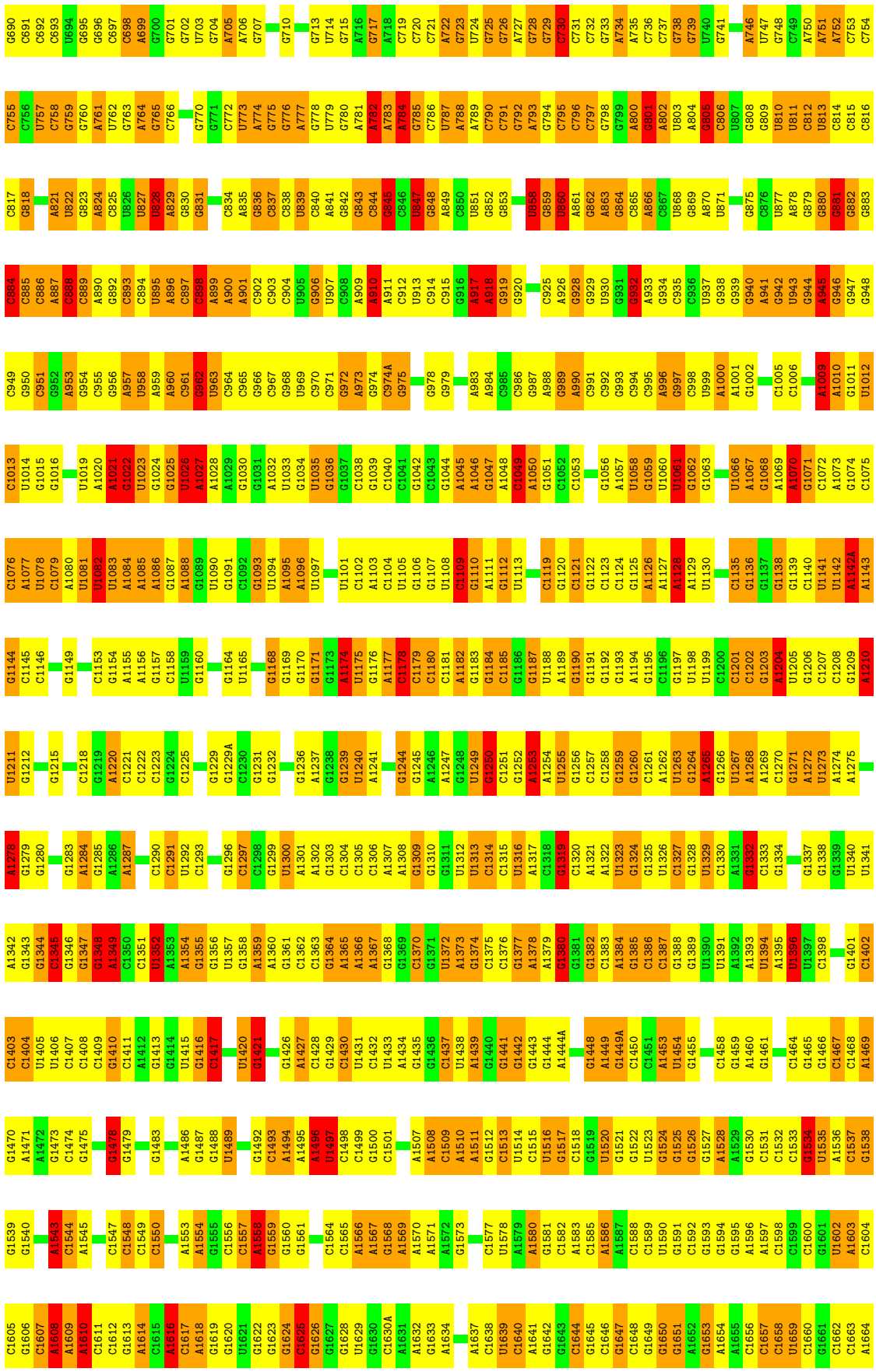


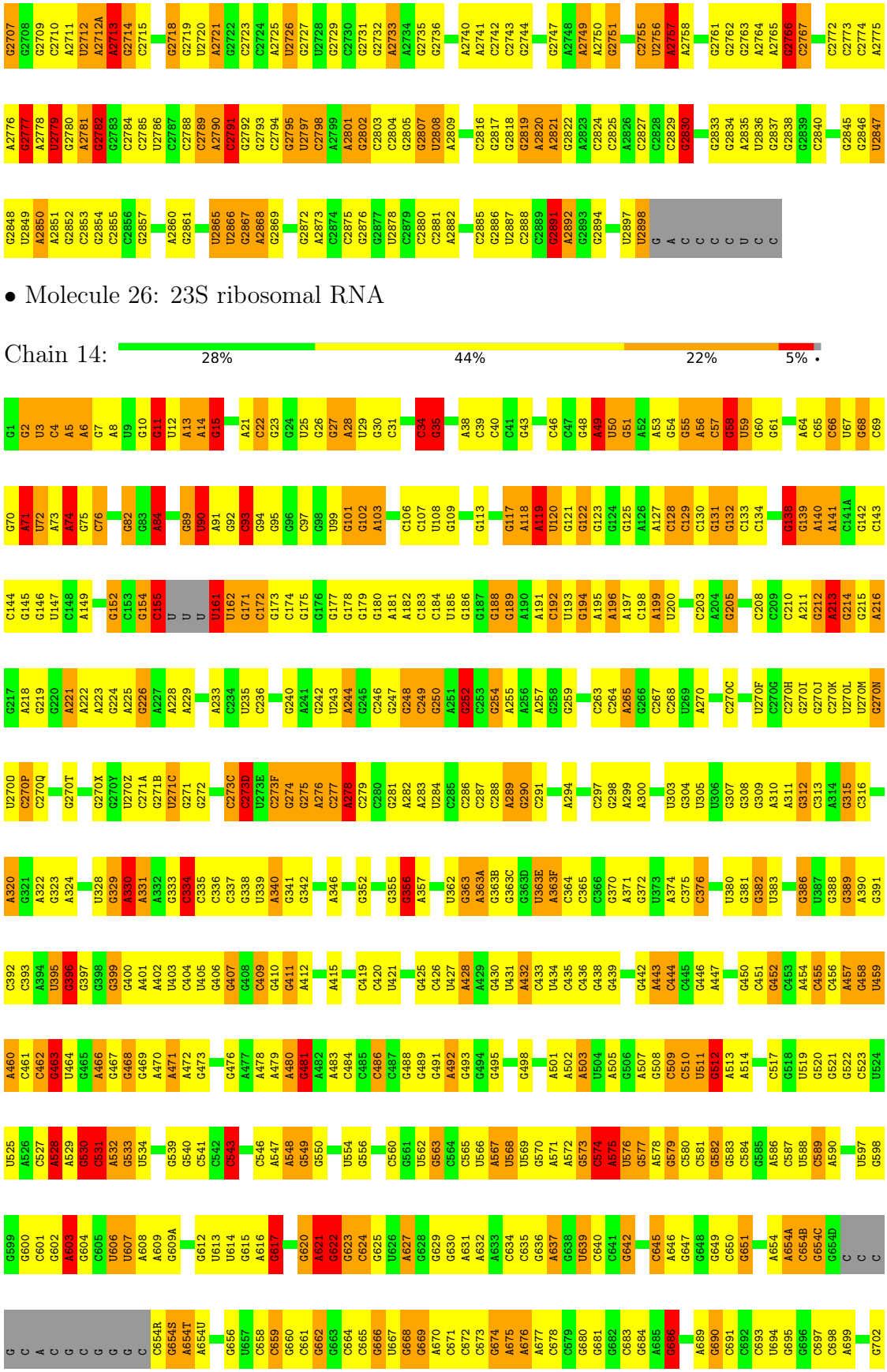
• Molecule 26: 23S ribosomal RNA

Chain 1H:



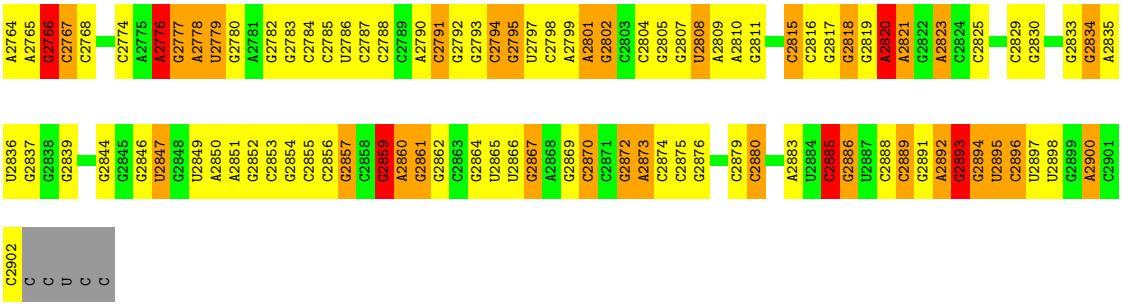






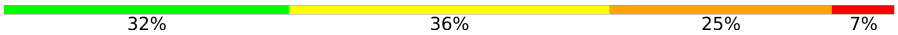
• Molecule 26: 23S ribosomal RNA

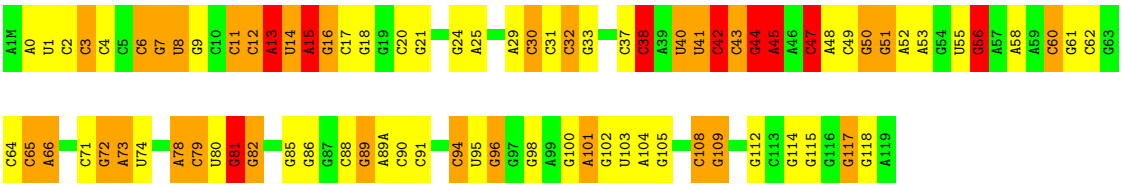
Chain 14: 28% 44% 22% 5% •



- Molecule 27: 5S ribosomal RNA

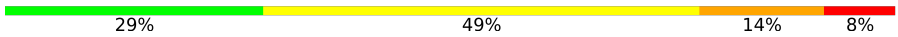
Chain 16:

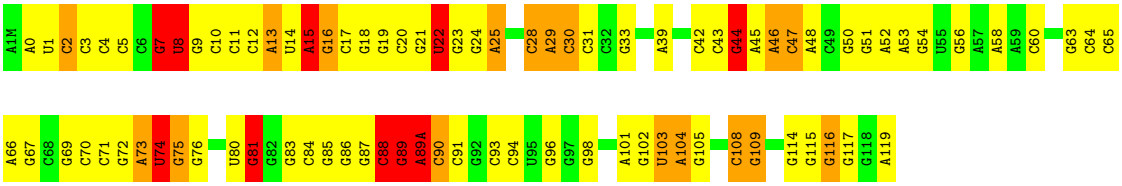




- Molecule 27: 5S ribosomal RNA

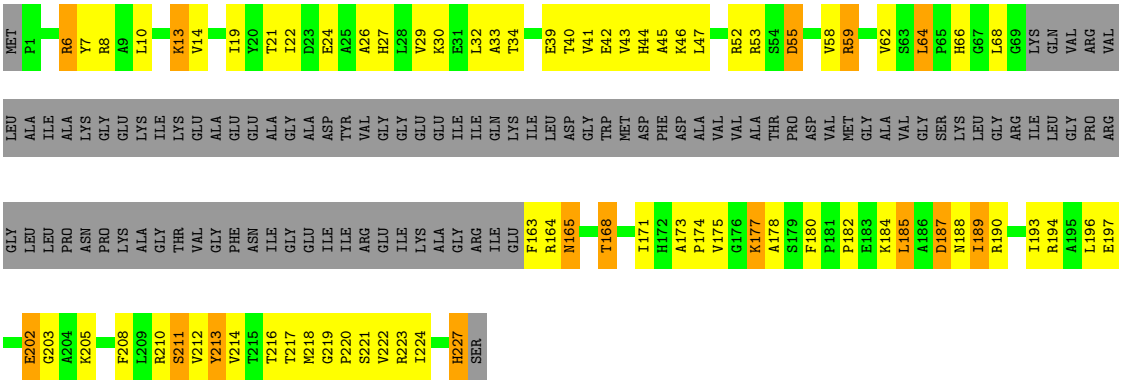
Chain 1J:





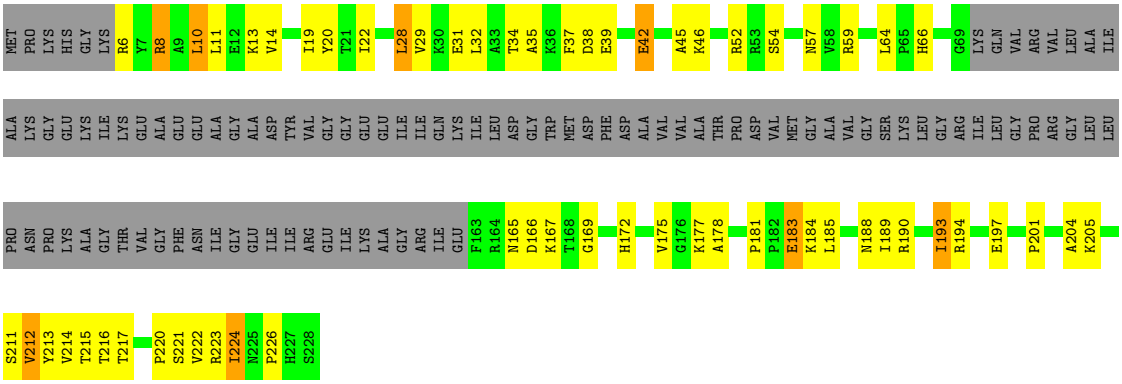
- Molecule 28: 50S ribosomal protein L1

Chain 71:



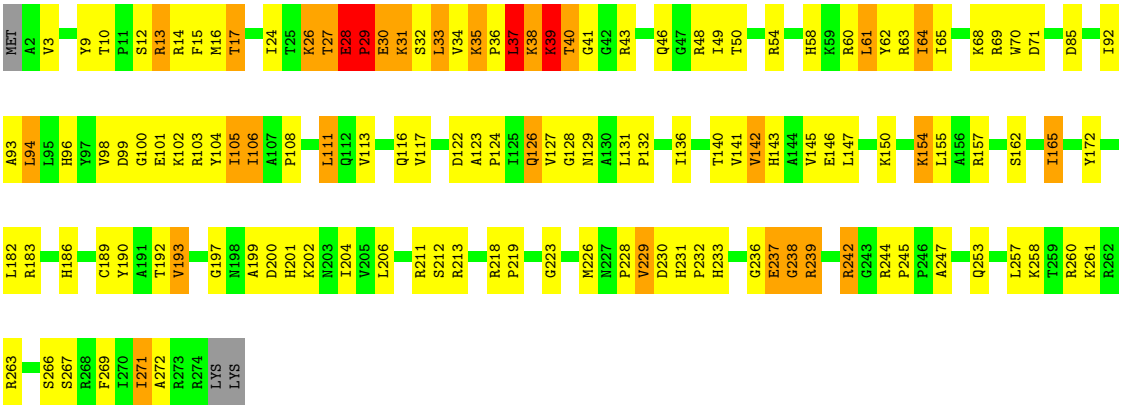
- Molecule 28: 50S ribosomal protein L1

Chain 79:



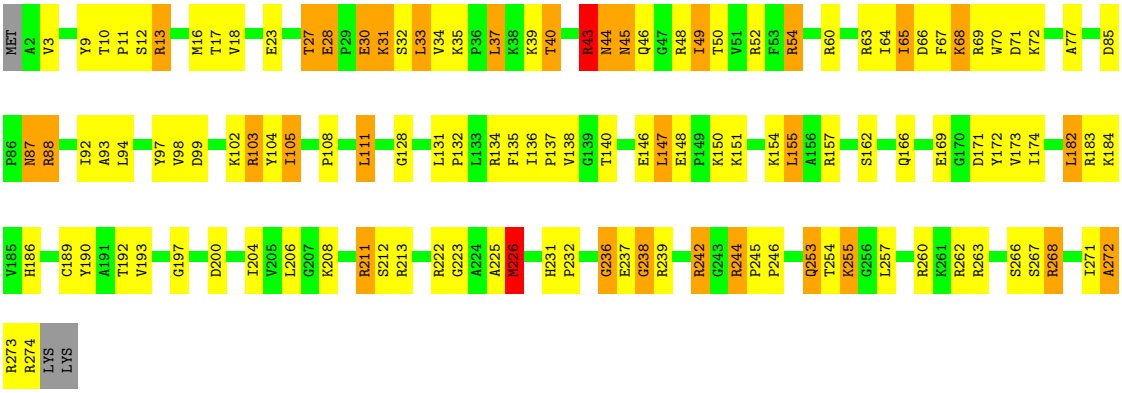
- Molecule 29: 50S ribosomal protein L2

Chain 11:



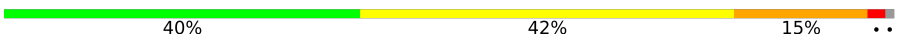
- Molecule 29: 50S ribosomal protein L2

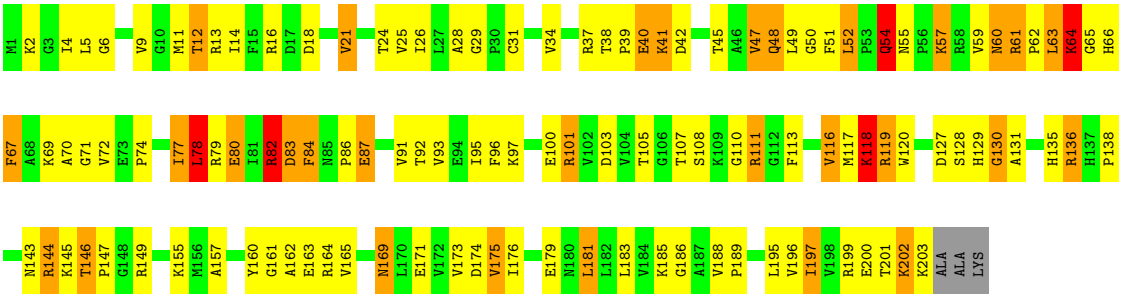
Chain 19:



- Molecule 30: 50S ribosomal protein L3

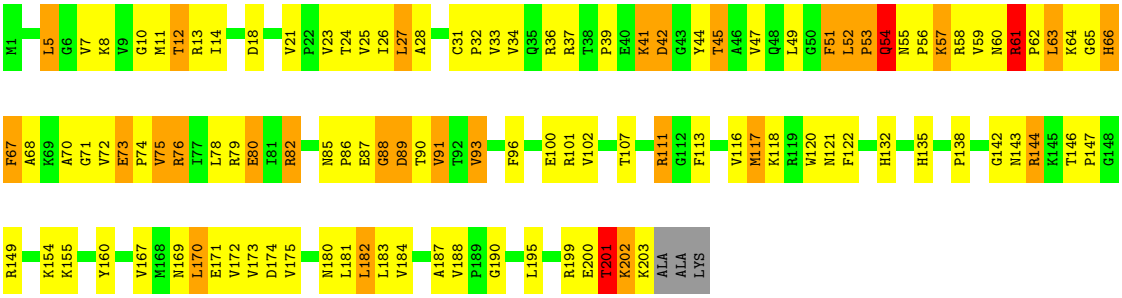
Chain 21:





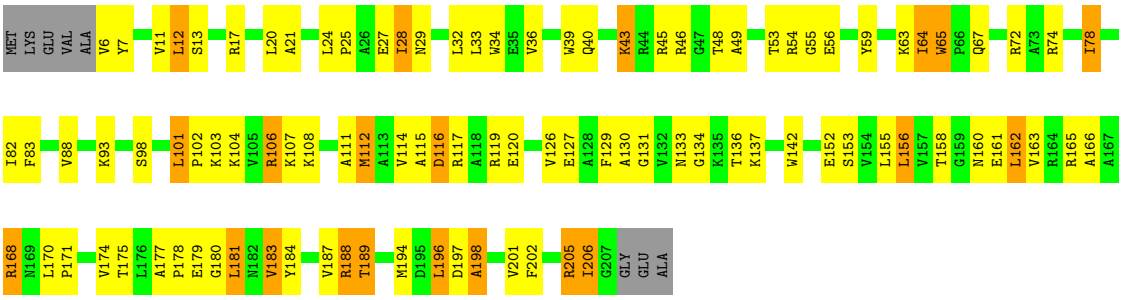
- Molecule 30: 50S ribosomal protein L3

Chain 29:



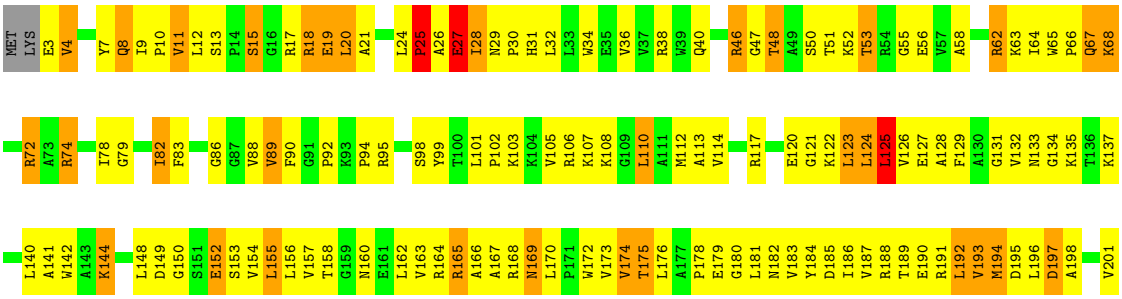
- Molecule 31: 50S ribosomal protein L4

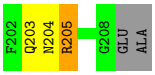
Chain 31:



- Molecule 31: 50S ribosomal protein L4

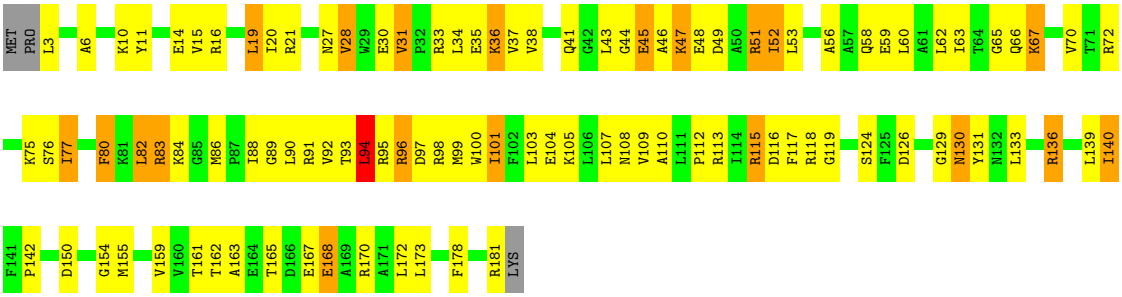
Chain 39:





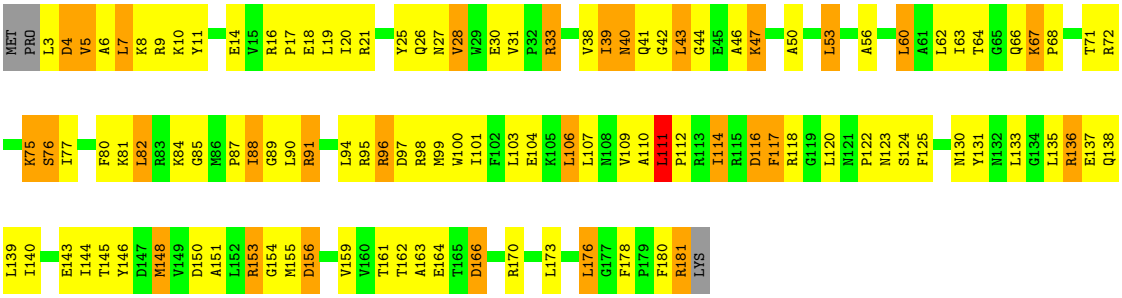
• Molecule 32: 50S ribosomal protein L5

Chain 41:



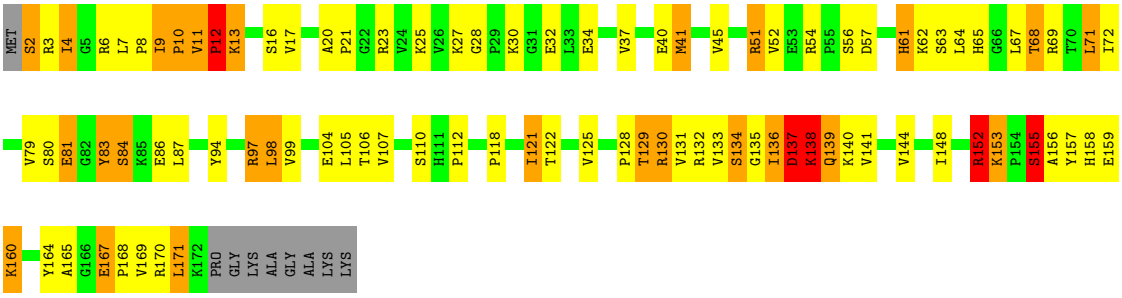
• Molecule 32: 50S ribosomal protein L5

Chain 49:



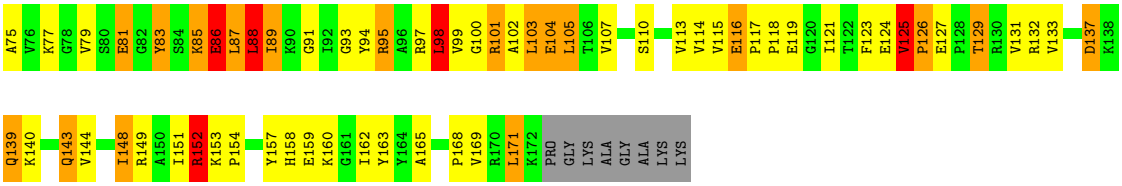
• Molecule 33: 50S ribosomal protein L6

Chain 51:



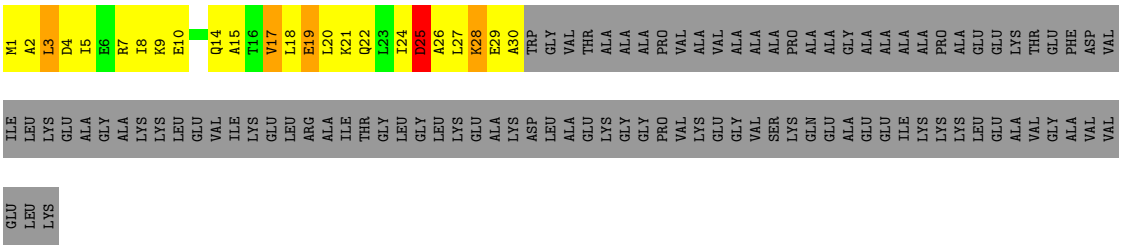
• Molecule 33: 50S ribosomal protein L6

Chain 59:



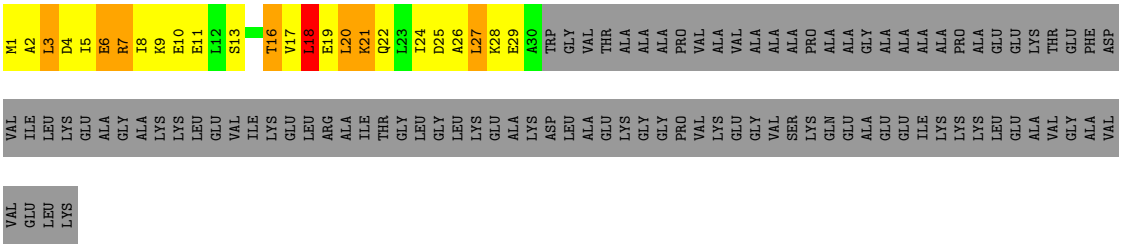
• Molecule 34: 50S ribosomal protein L7/L12

Chain 18:



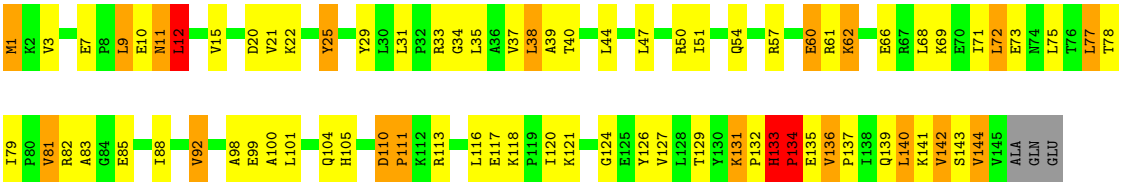
• Molecule 34: 50S ribosomal protein L7/L12

Chain 28:



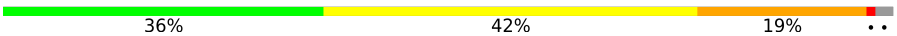
• Molecule 35: 50S ribosomal protein L9

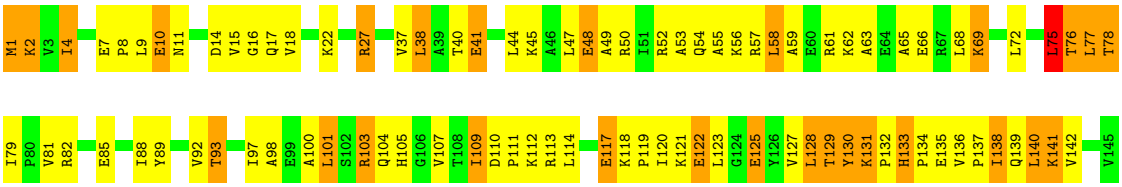
Chain 61:



• Molecule 35: 50S ribosomal protein L9

Chain 69:





ALA GLN GLU

- Molecule 36: 50S ribosomal protein L10

Chain 38: 18% 28% 21% 15% 17%

M1 P2 N3 K4 R5 N6 V7 E8 L9 L10 A11 T12 L13 K14 E15 N16 L17 E18 R19 A20 Q21 G22 S23 F24 F25 L26 V27 N28 Y29 Q30 G31 L32 P33 A34 K35 E36 T37 H38 A39 L40 R41 Q42 A43 L44 K45 Q46 N47 G48 A49 R50 L51 F52 V53 A54 K55 N56 T57 L58 I59 R60

L61 A62 L63 K64 E65 L66 G67 L68 P69 E70 L71 D72 G73 L74 V80 VAL PHE Y83 E84 D85 P86 V87 A88 A89 A90 K91 T92 L93 V94 Q95 F96 A97 K98 S99 N100 P101 K102 G103 I104 P105 Q106 V107 K108 S109 G110 L111 L112 L117 T118 A119 K120 D121 V122 L125 A126 E127 L128

P129 T130 M131 L134 E137 L138 V139 G140 V141 L142 Q143 A144 P145 MET ALA GLU LEU VAL GLY VAL LEU GLY GLY GLY VAL ALA ARG GLU LEU VAL GLY ILE LEU GLU ALA TYR ALA GLU LYS LYS ALA ALA

- Molecule 37: 50S ribosomal protein L11

Chain 48: 29% 46% 20%

MET LYS LYS VAL VAL A6 K9 L10 Q11 L12 P13 A14 G15 K16 A17 A20 P21 P22 V23 G24 P25 A26 L27 G28 Q29 I34 F37 V38 N42 A46 N47 M48 G49 D50 A51 I52 V53 P54 V55 E56 I57 T58 I59 Y60 A61 D62 R63 S64 F65 T66 F67 V68 T69 K70

T71 P72 P73 A74 S75 Y76 L77 I78 R79 K80 A81 A82 G83 L84 E85 K86 H89 K90 P91 G92 K95 V96 G97 R98 I99 T100 W101 E102 L105 E106 I107 A108 K109 Q110 K111 M112 P113 D114 L115 N116 T117 T118 D119 L120 E121 A122 A123 A124 R125 M126 I127 A128 G129 S130 A131 R132 S133

V136 E137 V138 V139 E143 V144 K145 D146 A147

- Molecule 38: 50S ribosomal protein L13

Chain 58: 42% 42% 13%

M1 V5 P6 K7 Q8 V9 E10 P11 R12 W13 V14 L15 I16 T22 L23 G24 R25 L26 I30 A31 T32 L33 L34 R35 G36 K37 H38 R39 P40 D41 W42 T43 P44 N45 V46 A47 M48 G49 D50 V55 N56 A57 D58 K59 I60 R61 V62 T63 G64 K65 K66 L67 E68 Q69 K70 I71

Y72 Y78 P86 L87 E88 K89 M90 T93 H94 P95 E96 R97 V98 L99 E100 V103 M106 L107 P108 P111 L112 G113 R114 R115 K118 R119 L120 G125 P126 D127 H128 P129 H130 Q131 A132 Q133 R134 P135 E136 K137 LEU GLU VAL

- Molecule 38: 50S ribosomal protein L13

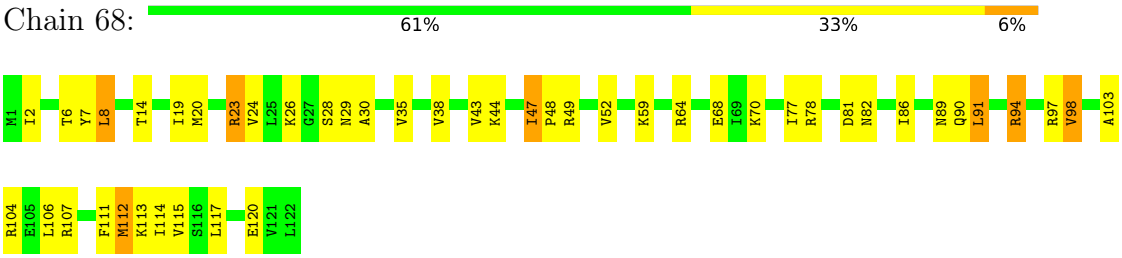
Chain 15: 51% 40% 6%

MET K2 T3 Y4 V5 P6 K7 Q8 V9 R12 W13 V14 L15 A18 E19 G20 K21 R25 T28 K29 I30 A31 T32 L33 L34 R35 G36 K37 H38 R39 P40 D41 W42 T43 A47 M48 G49 V52 V55 D58 K59 I60 R61 V62 K66 L67 E68 Q69 Y72

K84 I85 L91 A92 T93 H94 P95 E96 R97 V98 L99 E100 V103 M106 P111 L112 G113 R114 R115 L116 R119 A124 G125 P126 D127 H128 Q133 R134 P135 E136 K137 L138 GLU VAL

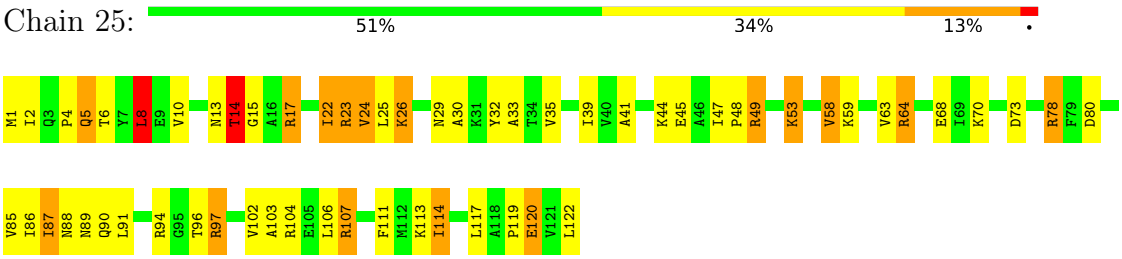
- Molecule 39: 50S ribosomal protein L14

Chain 68:



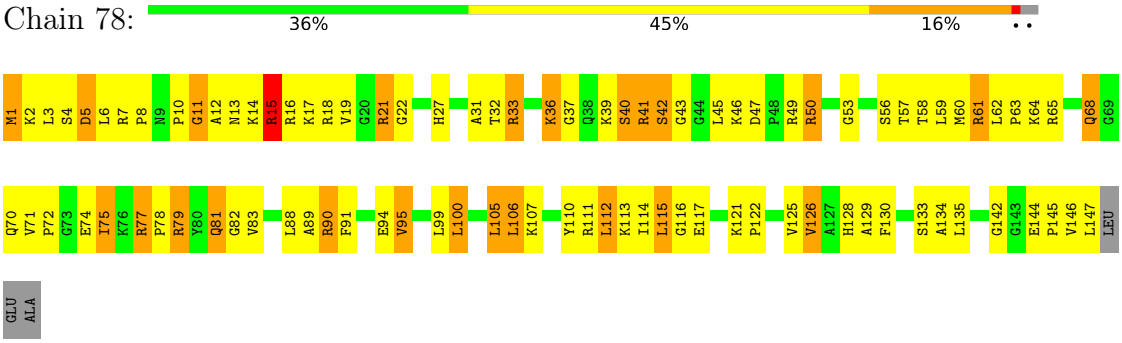
- Molecule 39: 50S ribosomal protein L14

Chain 25:



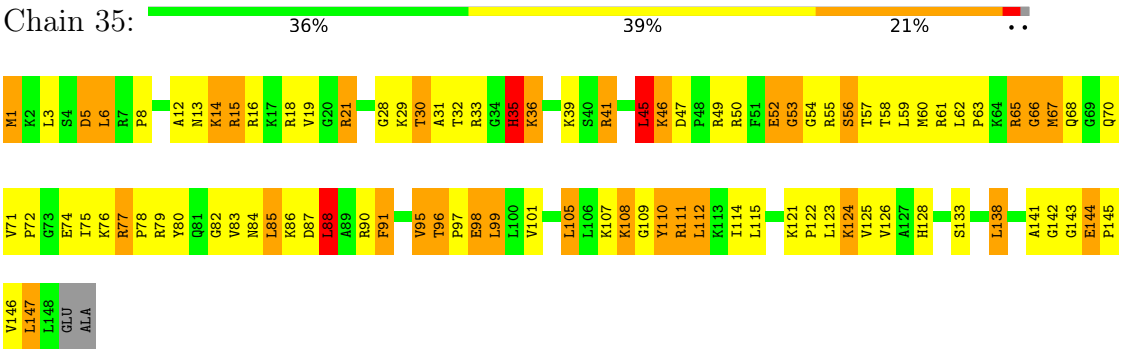
- Molecule 40: 50S ribosomal protein L15

Chain 78:



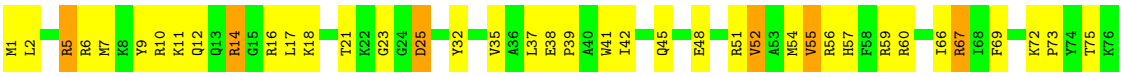
- Molecule 40: 50S ribosomal protein L15

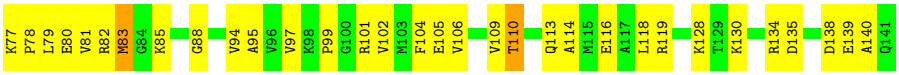
Chain 35:



- Molecule 41: 50S ribosomal protein L16

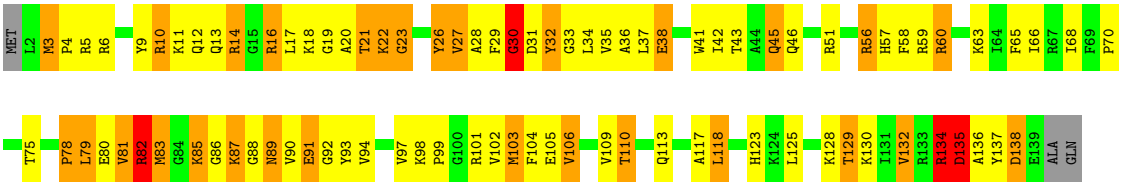
Chain 88:





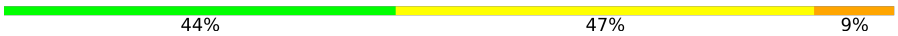
• Molecule 41: 50S ribosomal protein L16

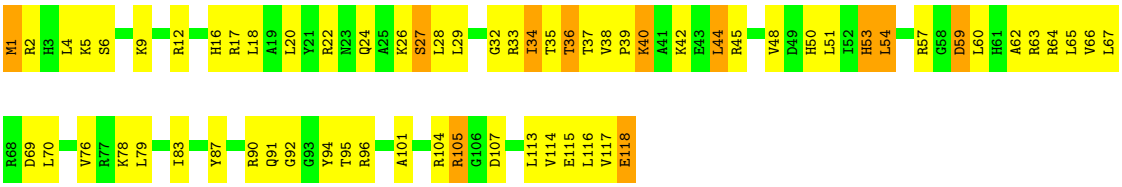
Chain 45:



• Molecule 42: 50S ribosomal protein L17

Chain 98:



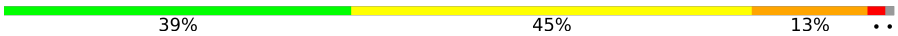


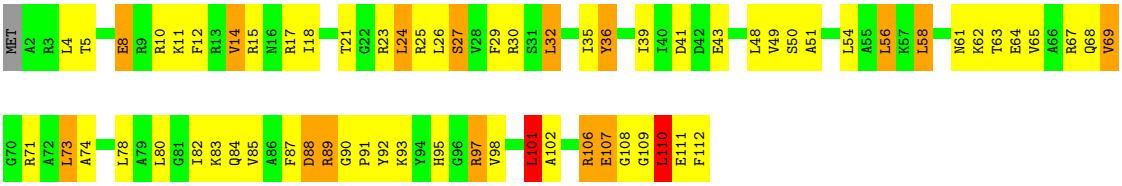
• Molecule 42: 50S ribosomal protein L17

Chain 55:

• Molecule 43: 50S ribosomal protein L18

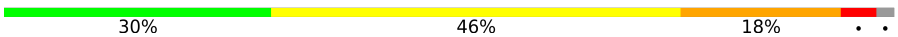
Chain A8:





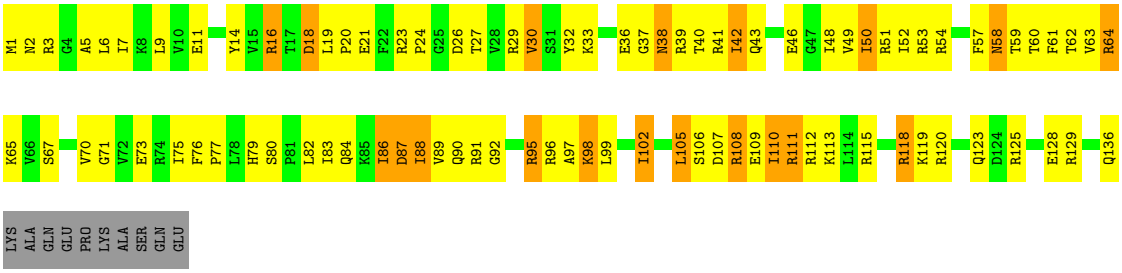
• Molecule 43: 50S ribosomal protein L18

Chain 65:



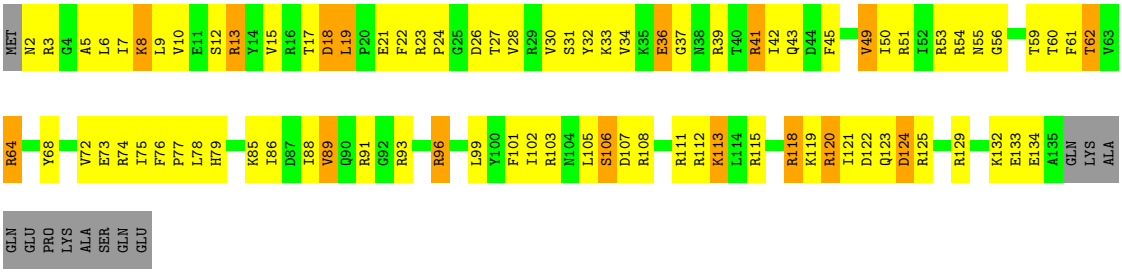
• Molecule 44: 50S ribosomal protein L19

Chain B8:



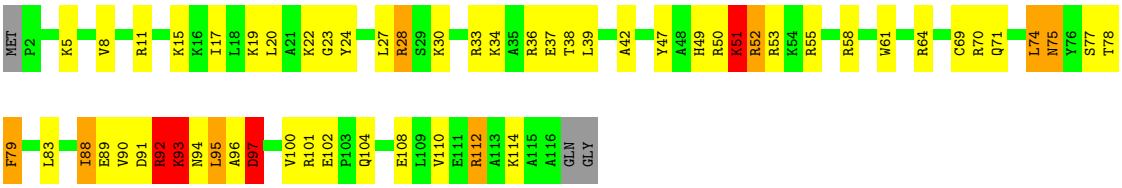
• Molecule 44: 50S ribosomal protein L19

Chain 75:



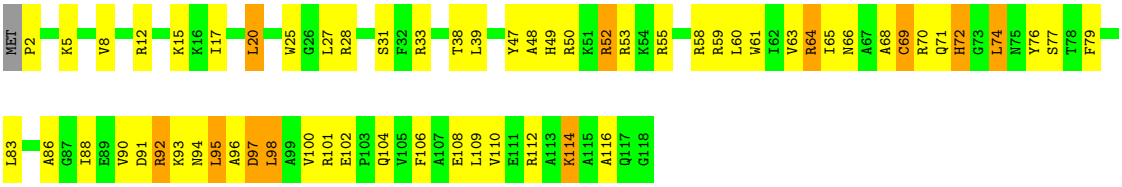
• Molecule 45: 50S ribosomal protein L20

Chain C8:



• Molecule 45: 50S ribosomal protein L20

Chain 85:



• Molecule 46: 50S ribosomal protein L21

Chain D8: 49% 34% 16%

M1 F2 K6 T7 G8 G9 K10 Q11 Y12 R13 V14 E15 P16 G17 L18 K19 L20 R21 K24 L25 G30 A31 T32 L35 P36 V37 L38 L39 L40 E43 K44 T45 V46 V47 G48 T49 P50 V51 V52 A55 S56 V57 V61 L62 G65 V72 K78 V79 R82

K85 Q89 P90 Y91 T92 E93 L94 L95 I96 I99 R100 G101

- Molecule 46: 50S ribosomal protein L21

Chain 95: 37% 49% 10%

M1 F2 A3 I4 V5 K6 T7 K10 Q11 Y12 R13 V14 L18 K19 L20 R21 V22 E23 A27 V33 E34 L35 P36 V37 L38 L39 L40 G41 G42 E43 K44 T45 V46 V47 G48 T49 P50 V51 V52 E53 G54 A55 S56 V57 V61 L62 G63 H64 G65 R66 G67 K68 K69 I70 L71

F75 K76 A77 K78 V79 Q80 Y81 R82 R83 K84 K85 R88 Q89 P90 Y91 T92 E93 L94 L95 I96 K97 E98 I99 R100 GLY

- Molecule 47: 50S ribosomal protein L22

Chain E8: 63% 29% 7%

M1 Y9 V10 R11 I12 S13 P14 R15 K16 V17 R18 L19 V20 L23 L29 I35 T39 R42 K49 V50 L51 V59 N60 M64 L65 E66 Y70 V71 K72 A73 V76 D77 E78 L82 L86 P87 R88 A89 R92 A93 D94 I95 I96 H102

V105 I106 L107 G108 E109 G112 LYS

- Molecule 47: 50S ribosomal protein L22

Chain A5: 49% 40% 10%

M1 K4 A5 I6 R11 I12 S13 P14 R15 K16 V17 R18 L23 S28 L29 E30 E31 A32 R33 T39 R42 G43 A44 Y45 F46 V47 A48 K49 V50 L51 E52 A58 V59 N60 N61 H62 D63 M64 L65 E66 D67 R68 L69 Y70 V71 K72 A73 V76 D77 E78 G79 P80

R84 V85 L86 P87 R88 A89 R90 D94 I95 I96 R99 T100 I103 I106 L107 G108 E109 K110 H111 GLY LYS

- Molecule 48: 50S ribosomal protein L23

Chain F8: 53% 34% 11%

M1 K2 T3 A4 Y5 I8 L9 A10 P11 V12 L13 S14 E15 K16 A17 Y18 A19 G20 E23 Y26 T27 F28 W29 V30 H31 A34 T35 K36 T37 E38 I39 K40 V43 E44 V49 K50 K53 V54 N55 T56 L57 R65 L66 G67 R68 Y69 L70 G71 K72 R76

I80 V81 Q82 V83 I89 L95 ILE

- Molecule 48: 50S ribosomal protein L23

Chain B5: 46% 45% 7% •

M1 Y5 I8 L9 V12 L13 S14 E15 K16 A17 Y18 A19 G20 F21 G24 K25 Y26 T27 F28 W29 V30 H31 P32 T35 K36 T37 E38 I39 K40 N41 A42 V43 E44 K48 V49 K50 V51 V52 K53 V54 N55 T56 L57 K63 R68 Y69 L70 G71 K72 D75 R76

K77 K78 A79 I80 V81 Q82 V83 Q87 K88 I89 G94 LEU ILE

• Molecule 49: 50S ribosomal protein L24

Chain G8: 43% 41% 10% • 5%

MET R2 V3 K4 M5 H6 V7 K8 K9 T12 V13 L14 K19 K28 E29 V30 L31 P32 K33 K34 V37 I38 V39 E40 G41 V42 N43 I44 V45 K46 V49 R50 V51 S52 P53 K54 Y55 P56 Q57 G58 G59 F60 I61 E62 K63 E64 L67 H68 K71 P74 I75 C76

P77 A78 P82 T83 R84 V85 R86 K87 K88 F89 L90 E91 I96 R97 V98 C99 A100 K101 L106 ASP THR GLU GLU

• Molecule 49: 50S ribosomal protein L24

Chain C5: 35% 40% 17% 5% •

MET R2 V3 K8 T12 V15 A16 S17 G18 K19 Y20 K21 G22 R23 V24 K28 E29 V30 L31 K34 Y35 A36 V37 I38 V39 E40 G41 V42 N43 K46 K47 A48 V49 R50 V51 S52 P53 K54 Y55 P56 Q57 G58 G59 F60 I61 E62 K63 E64 A65 P66 L67 H68 K71

V72 I75 C76 P77 A78 P82 T83 R84 V85 R86 F89 L90 E91 N92 I96 R97 V98 C99 A100 K101 C102 G103 G104 A105 L106 D107 THR GLU GLU

• Molecule 50: 50S ribosomal protein L25

Chain H8: 31% 35% 12% • 20%

MET E2 L5 K6 A7 Y8 Y9 R10 E11 G12 E13 K14 P15 S16 R19 M28 Y29 N34 R35 K36 V37 D40 L41 V42 E43 F44 D45 K46 V47 F48 R49 Q50 A51 S52 I53 H54 I57 V58 L59 E60 L61 P62 D63 G64 Q65 S66 L67 P68 T69 L70 V71 R72 L76

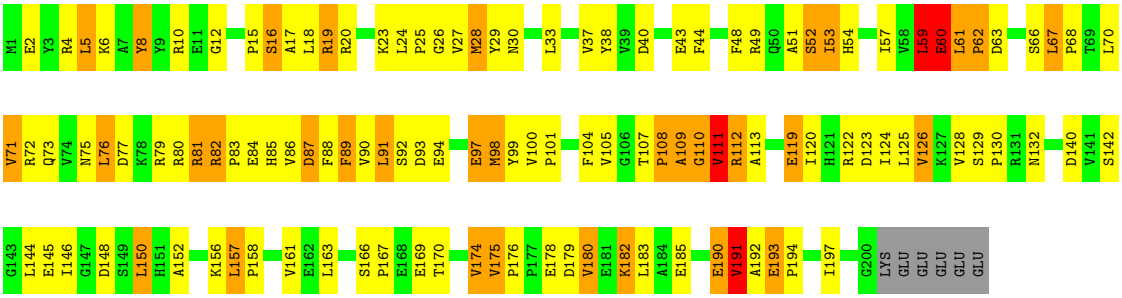
D77 K78 R79 R80 R81 R82 P83 E84 H85 V86 D87 V90 L91 S92 D93 E94 P95 V96 E97 M98 P101 L102 R103 F104 V105 P108 A109 G110 V111 R112 A113 G114 G115 V116 L117 Q118 E119 I120 H121 R122 D123 I124 L125 V126 K127 V128 S129 P130 R131 N132 V139 D140 V141 S142 G143 L144

GLU ILE GLY ASP SER L150 H151 A152 S153 D154 L155 K156 L157 P158 V161 E162 L163 A164 V165 S166 P167 E168 E169 T170 I171 ALA ALA VAL VAL PRO PRO GLU ASP VAL GLU LYS LEU ALA GLU GLU ALA ALA ALA GLU VAL ALA GLU PRO GLU VAL ILE LYS LYS GLY LYS GLU GLU GLU

GLU

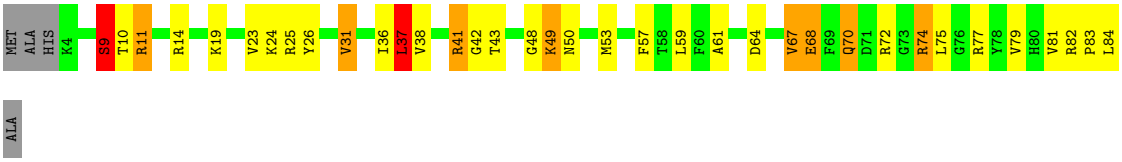
• Molecule 50: 50S ribosomal protein L25

Chain D5: 38% 41% 16% • •



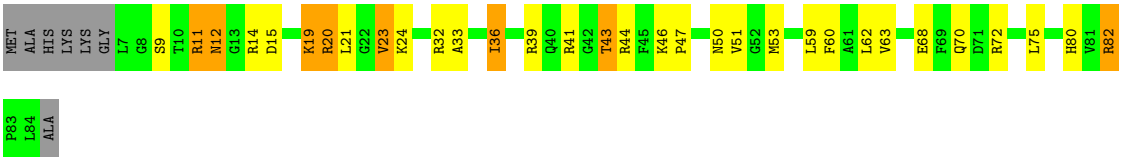
• Molecule 51: 50S ribosomal protein L27

Chain I8:



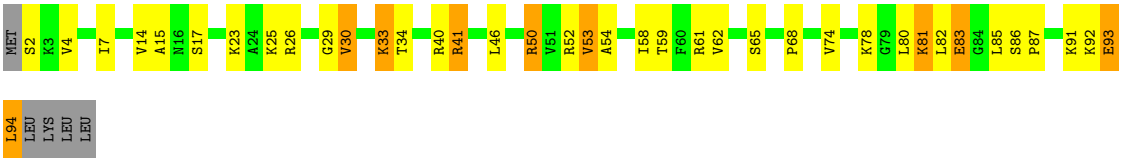
• Molecule 51: 50S ribosomal protein L27

Chain E5:



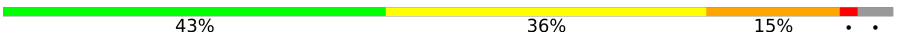
• Molecule 52: 50S ribosomal protein L28

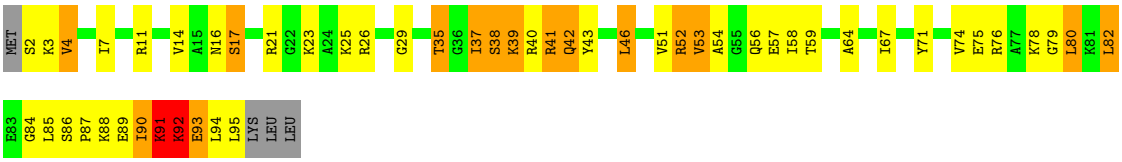
Chain J8:



• Molecule 52: 50S ribosomal protein L28

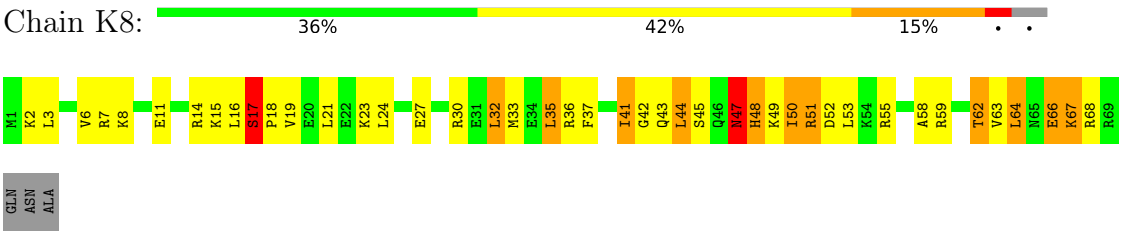
Chain F5:





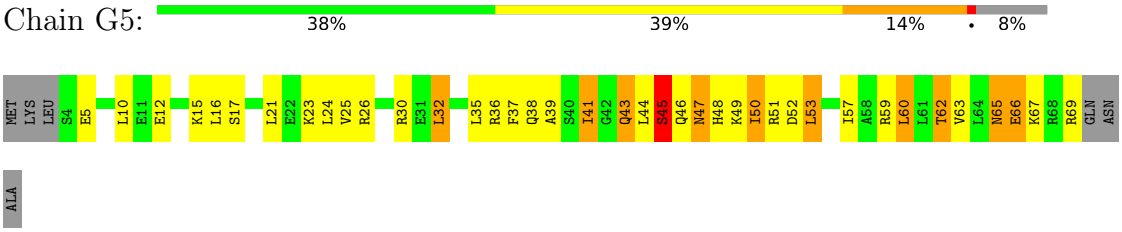
• Molecule 53: 50S ribosomal protein L29

Chain K8:



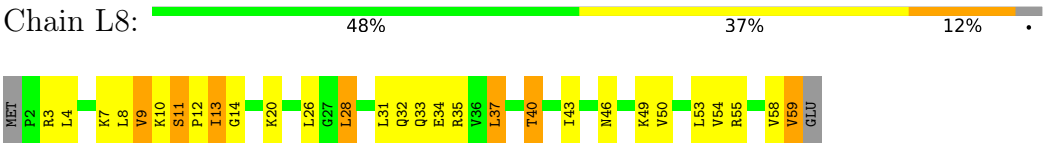
• Molecule 53: 50S ribosomal protein L29

Chain G5:



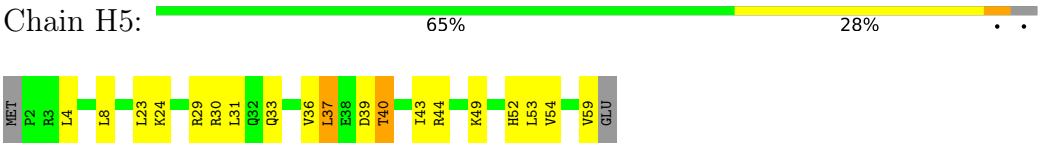
• Molecule 54: 50S ribosomal protein L30

Chain L8:



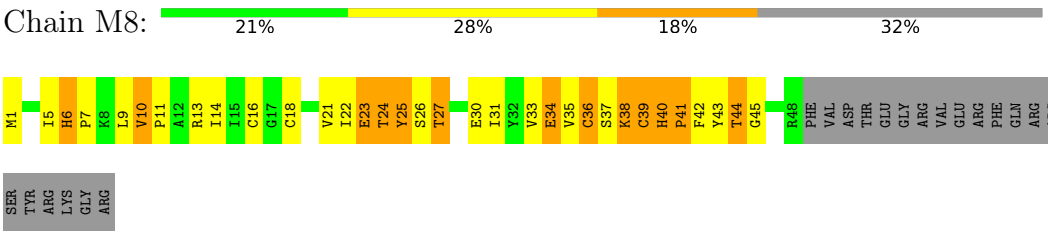
• Molecule 54: 50S ribosomal protein L30

Chain H5:



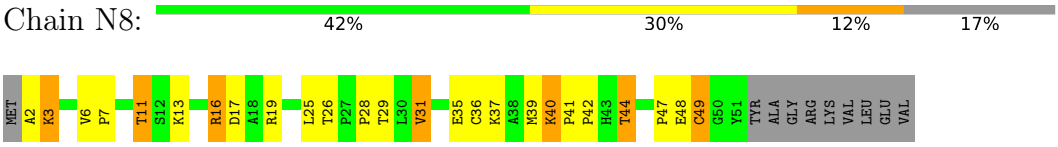
• Molecule 55: 50S ribosomal protein L31

Chain M8:



• Molecule 56: 50S ribosomal protein L32

Chain N8:



• Molecule 56: 50S ribosomal protein L32

Chain J5: 47% 37% 10% 7%

MET A2 K3 V6 P7 K8 K9 K10 K13 R16 D17 R20 H23 A24 L25 T26 T29 L30 V31 P32 C33 P34 E35 C36 K40 P41 P42 H43 T44 V45 C46 P47 E48 Y51 Y52 A53 G54 R55 K56 V57 LEU GLU VAL

- Molecule 57: 50S ribosomal protein L33

Chain O8: 13% 50% 19% • 17%

MET ALA SER GLU VAL ARG ILE LYS L9 L10 L11 E12 C13 T14 E15 C16 K17 R18 R19 N20 Y21 A22 T23 E24 K25 N26 K27 R28 N29 T30 P31 N32 K33 L34 E35 L36 R37 K38 Y39 C40 P41 W42 C43 R44 K45 H46 T47 V48 H49 R50 E51 V52 K53 ILE

- Molecule 58: 50S ribosomal protein L34

Chain P8: 49% 43% • •

M1 W5 Q6 P7 N8 R9 R10 K11 R12 T15 H16 G17 F18 M22 R23 T24 P25 G26 G27 V30 L31 K32 R33 R34 R39 W40 T43 P44 R47 LYS ARG

- Molecule 58: 50S ribosomal protein L34

Chain L5: 49% 43% • •

M1 K2 R3 T4 N8 R9 R10 K11 R12 A13 K14 T15 H16 R19 G26 K29 V30 L31 K32 R33 R34 R39 W40 R41 L42 T43 P44 R47 LYS ARG

- Molecule 59: 50S ribosomal protein L35

Chain Q8: 49% 35% 11% • •

MET P2 K3 M4 K5 T6 H7 K8 G9 A10 K11 K12 R13 V14 K15 I16 S19 V23 K29 R30 H31 L32 N33 W34 Q35 K36 S37 E40 I41 R46 K47 K52 P53 E54 I58 K59 L60 L61 L62 P63 Y64 E65

- Molecule 59: 50S ribosomal protein L35

Chain M5: 38% 43% 12% 5% •

MET P2 K3 M4 K5 T6 H7 K8 G9 A10 K11 K12 R13 V14 A18 V22 V23 A24 M25 K29 R30 H31 L32 N33 W34 Q35 K36 S37 G38 K39 E40 Q43 R46 K47 F48 V49 L50 A51 K52 P53 E54 A55 E56 R57 I58 K59 L60 L61 L62 E65

4 Data and refinement statistics (i)

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.*

[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 (i)

5.1 Standard geometry (i)

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	#|Z| >5	RMSZ	#|Z| >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%)
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 (i)

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 (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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 (i)

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 (i)

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 (i)

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 (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
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 (i)

6.1 Protein, DNA and RNA chains (i)

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

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

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

6.3 Carbohydrates (i)

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

6.4 Ligands (i)

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

6.5 Other polymers (i)

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