



wwPDB EM Map/Model Validation Report ⓘ

Sep 20, 2016 – 07:04 PM EDT

PDB ID : 5KPW
EMDB ID: : EMD-8281
Title : Structure of RelA bound to ribosome in presence of A/R tRNA (Structure III)
Authors : Loveland, A.B.; Bah, E.; Madireddy, R.; Zhang, Y.; Brilot, A.F.; Grigorieff, N.; Korostelev, A.A.
Deposited on : 2016-07-05
Resolution : 3.90 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027939

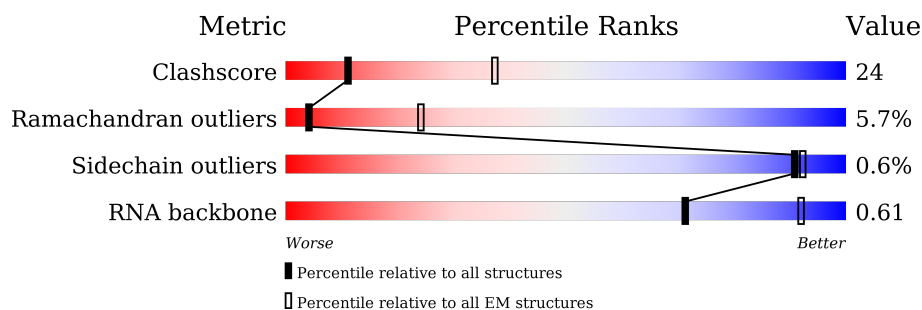
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.





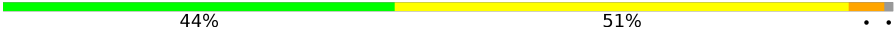








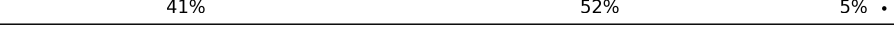







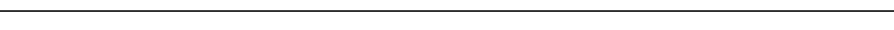

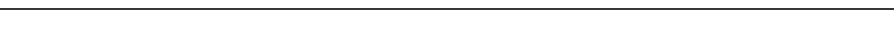
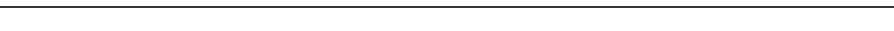


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	273	58% 40% ..
2	B	209	46% 50% .
3	C	201	48% 49% .
4	D	179	41% 54% ..
5	E	177	50% 48% ..
6	F	149	40% 54% 5% .
7	G	165	17% 52% 10% 21%
8	H	142	29% 67% ..



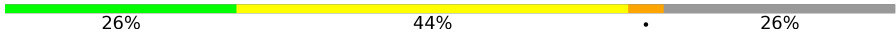
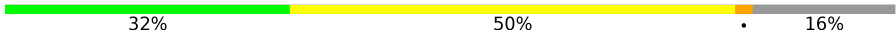

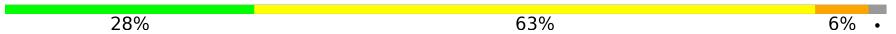
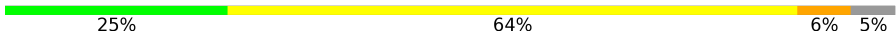
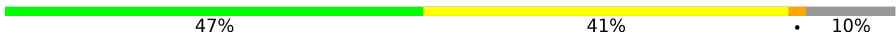
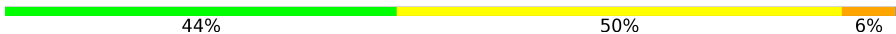
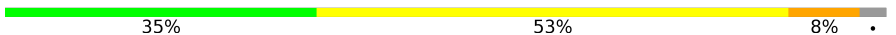
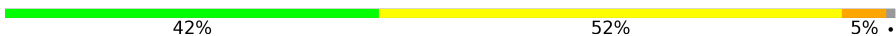

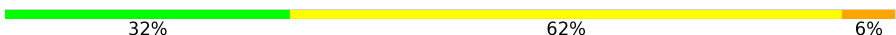
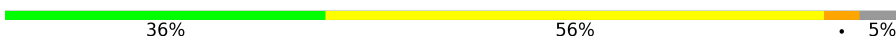








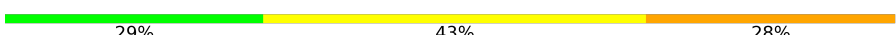

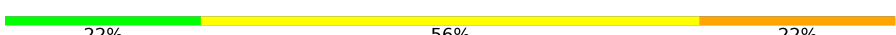
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Mol	Chain	Length	Quality of chain
9	I	142	
10	J	123	
11	K	144	
12	L	136	
13	M	127	
14	N	117	
15	O	115	
16	P	118	
17	Q	103	
18	R	110	
19	S	100	
20	T	104	
21	U	94	
22	V	85	
23	W	78	
24	X	63	
25	Y	59	
26	Z	70	
27	1	57	
28	2	55	
29	3	46	
30	4	65	
31	5	38	
32	6	241	
33	7	233	

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Mol	Chain	Length	Quality of chain
34	8	206	
35	9	167	
36	10	135	
37	11	179	
38	12	130	
39	13	130	
40	14	103	
41	15	129	
42	16	124	
43	17	118	
44	18	101	
45	19	89	
46	20	82	
47	21	84	
48	22	75	
49	23	92	
50	24	87	
51	25	71	
52	26	1539	
53	27	2903	
54	28	120	
55	29	20	
56	30	76	
57	31	77	
58	32	77	

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Mol	Chain	Length	Quality of chain
59	33	750	<div><div></div><div>38%</div><div>45%</div><div>6%</div><div>10%</div></div>

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 154603 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

- Molecule 2 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- Molecule 3 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 4 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

- Molecule 5 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 6 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 7 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	131	Total	C	N	O	S	0	0
			988	625	175	183	5		

- Molecule 8 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

- Molecule 9 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 10 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	122	Total	C	N	O	S	0	0
			938	587	180	165	6		

- Molecule 11 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	143	Total	C	N	O	S	0	0
			1045	649	206	189	1		

- Molecule 12 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 13 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

- Molecule 14 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	N	116	Total	C	N	O	0	0
			892	552	178	162		

- Molecule 15 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 16 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	P	117	Total	C	N	O	0	0
			947	604	192	151		

- Molecule 17 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 18 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 19 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

- Molecule 20 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	T	102	Total	C	N	O	0	0
			779	492	146	141		

- Molecule 21 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	75	Total	C	N	O	S	0	0
			575	356	116	102	1		

- Molecule 23 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 24 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

- Molecule 25 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 26 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	66	Total	C	N	O	S	0	0
			522	323	99	94	6		

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	1	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 28 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	2	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	3	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	4	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 31 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	5	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 32 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	6	218	Total	C	N	O	S	0	0
			1704	1081	305	311	7		

- Molecule 33 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	7	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 34 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	8	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 35 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	9	157	Total	C	N	O	S	0	0
			1156	719	218	213	6		

- Molecule 36 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	10	100	Total	C	N	O	S	0	0
			817	515	148	148	6		

- Molecule 37 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	11	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

- Molecule 38 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	12	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 39 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	13	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 40 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	14	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

- Molecule 41 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	15	116	Total	C	N	O	S	0	0
			869	535	173	158	3		

- Molecule 42 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	16	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 43 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	17	114	Total	C	N	O	S	0	0
			883	546	178	156	3		

- Molecule 44 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	18	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

- Molecule 45 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	19	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 46 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	20	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 47 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	21	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 48 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	22	65	Total	C	N	O	S	0	0
			535	339	100	95	1		

- Molecule 49 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	23	79	Total	C	N	O	S	0	0
			637	408	120	107	2		

- Molecule 50 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	24	85	Total	C	N	O	S	0	0
			665	411	137	114	3		

- Molecule 51 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	25	65	Total	C	N	O	S	0	0
			544	335	117	91	1		

- Molecule 52 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	26	1539	Total	C	N	O	P	0	0
			33016	14725	6052	10700	1539		

- Molecule 53 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	27	2903	Total	C	N	O	P	0	0
			62322	27801	11468	20150	2903		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
27	747	C	U	conflict	GB 802133627
27	1847	G	A	conflict	GB 802133627

- Molecule 54 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	28	120	Total	C	N	O	P	0	0
			2572	1145	471	836	120		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
28	120	A	-	conflict	GB 1028475309

- Molecule 55 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	29	20	Total	C	N	O	P	0	0
			432	195	86	132	19		

- Molecule 56 is a RNA chain called A-site tRNAPhe.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	30	76	Total	C	N	O	P	0	0
			1623	723	290	534	76		

- Molecule 57 is a RNA chain called P-site tRNAfMet.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	31	77	Total	C	N	O	P	0	0
			1644	732	297	538	77		

- Molecule 58 is a RNA chain called E-site tRNAfMet.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	32	77	Total	C	N	O	P	0	0
			1643	732	297	537	77		

- Molecule 59 is a protein called GTP pyrophosphokinase.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	33	675	Total	C	N	O	S	0	0
			4911	3070	904	915	22		

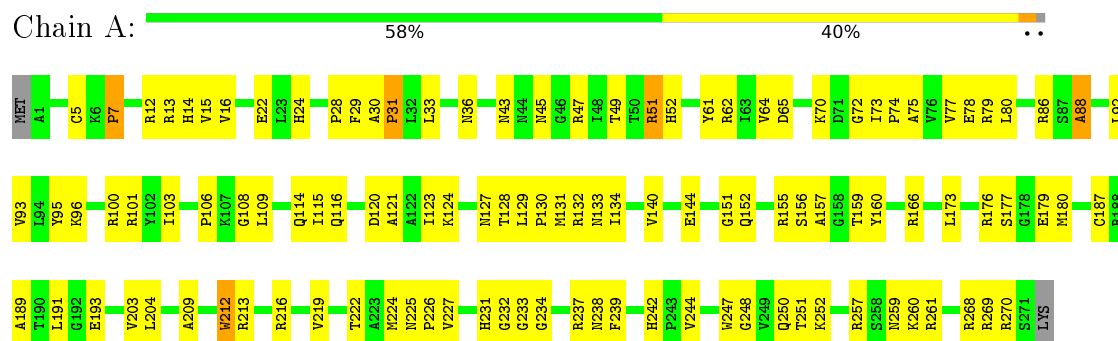
There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
33	-5	MET	-	expression tag	UNP P0AG20
33	-4	HIS	-	expression tag	UNP P0AG20
33	-3	HIS	-	expression tag	UNP P0AG20
33	-2	HIS	-	expression tag	UNP P0AG20
33	-1	HIS	-	expression tag	UNP P0AG20
33	0	HIS	-	expression tag	UNP P0AG20
33	1	HIS	-	expression tag	UNP P0AG20

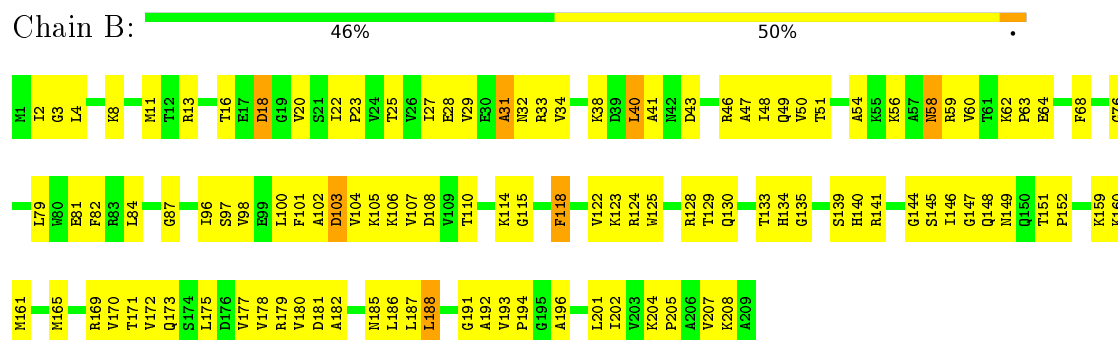
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

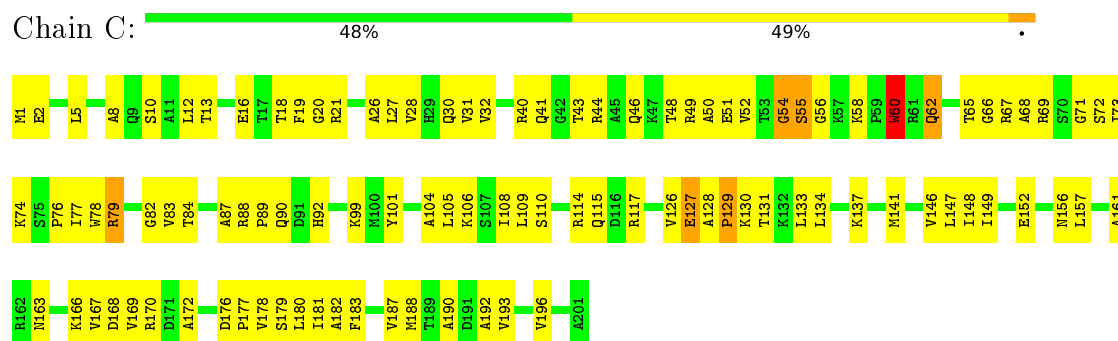
- Molecule 1: 50S ribosomal protein L2



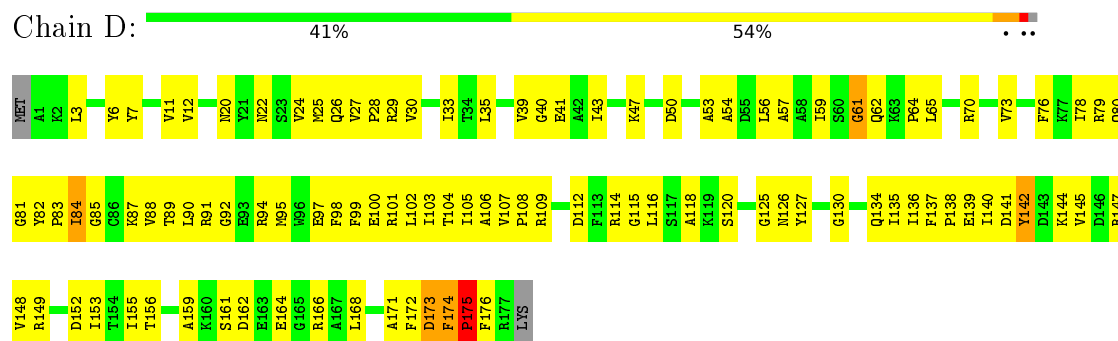
- Molecule 2: 50S ribosomal protein L3



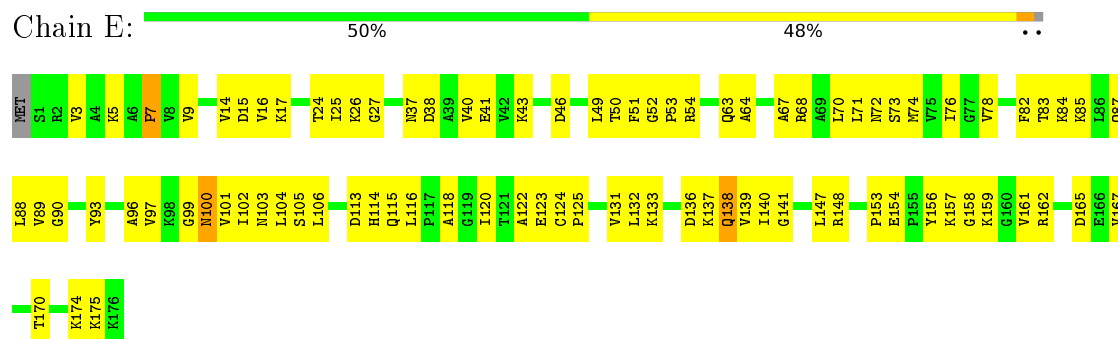
- Molecule 3: 50S ribosomal protein L4



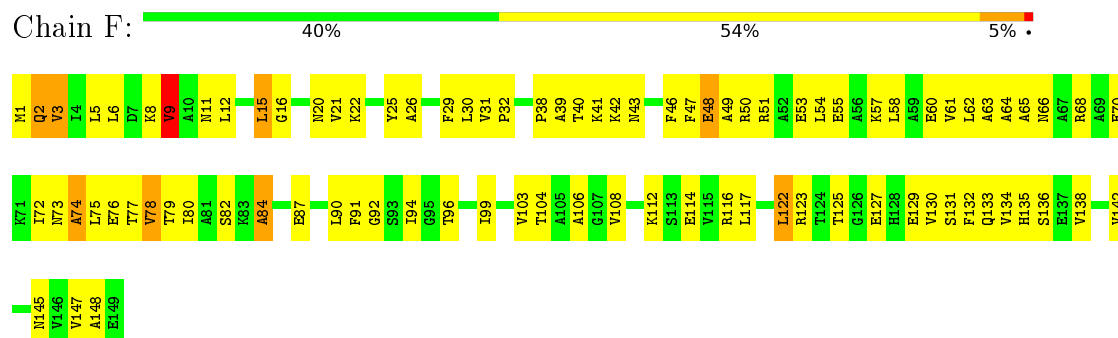
- Molecule 4: 50S ribosomal protein L5



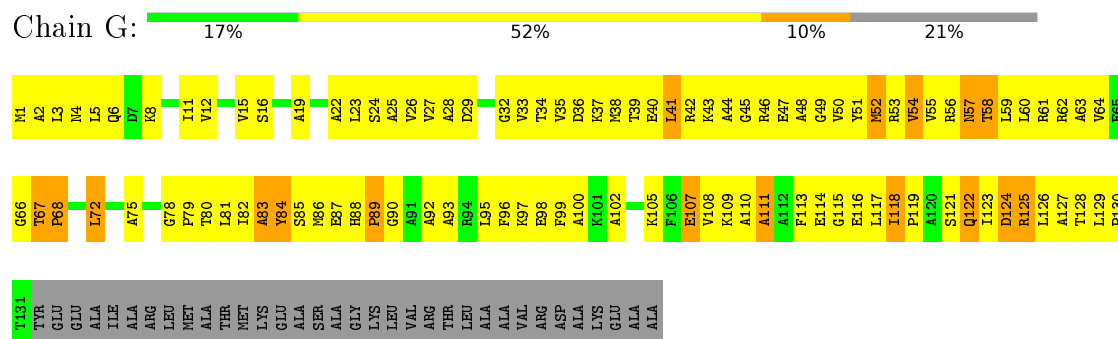
• Molecule 5: 50S ribosomal protein L6



• Molecule 6: 50S ribosomal protein L9

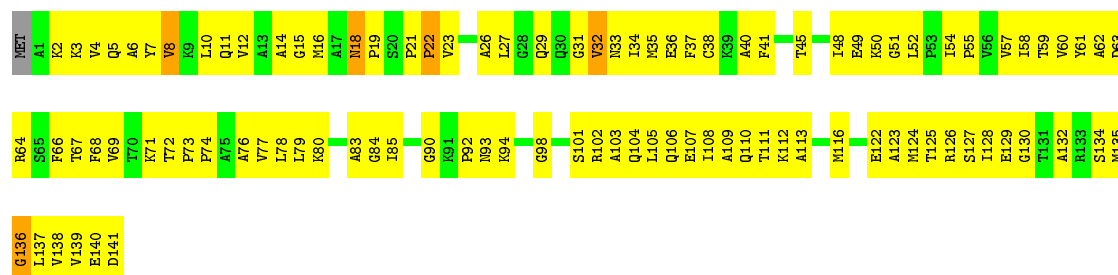


• Molecule 7: 50S ribosomal protein L10



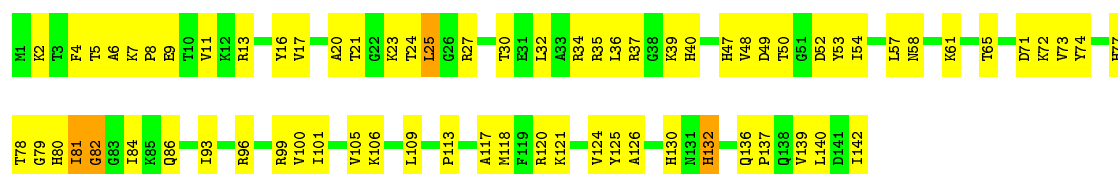
• Molecule 8: 50S ribosomal protein L11

Chain H:  29% 67%



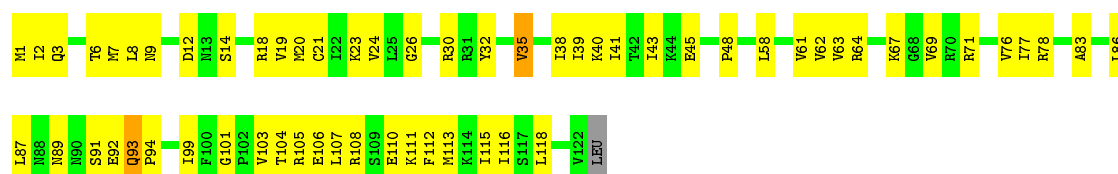
- Molecule 9: 50S ribosomal protein L13

Chain I:  50% 47%



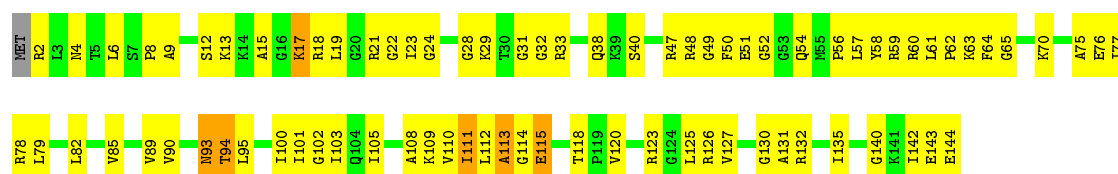
- Molecule 10: 50S ribosomal protein L14

Chain J:  50% 47%



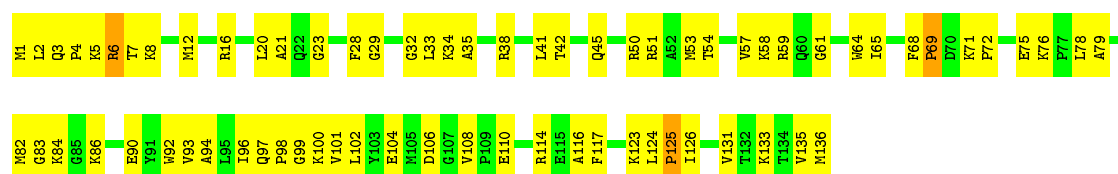
- Molecule 11: 50S ribosomal protein L15

Chain K:  44% 51%

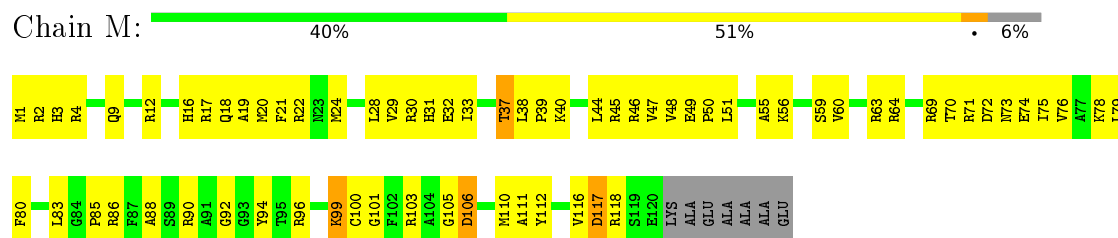


- Molecule 12: 50S ribosomal protein L16

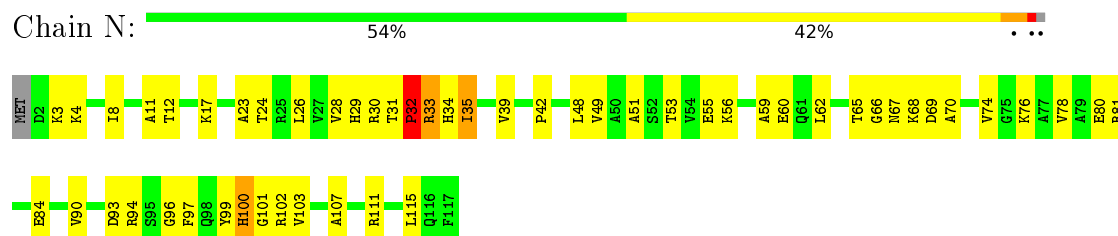
Chain L:  48% 50%



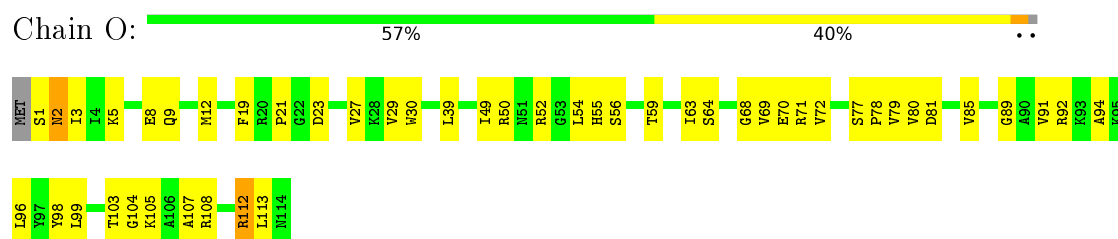
- Molecule 13: 50S ribosomal protein L17



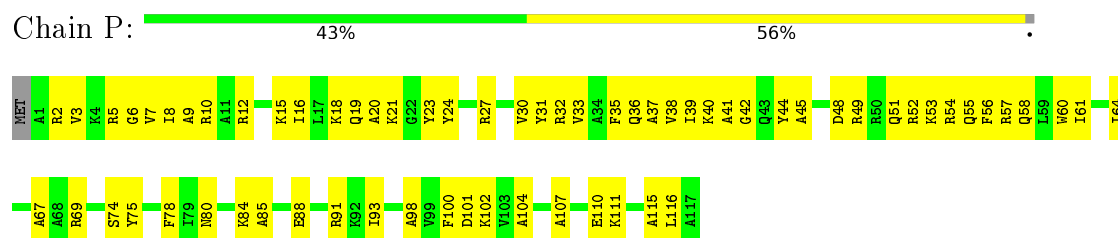
- Molecule 14: 50S ribosomal protein L18



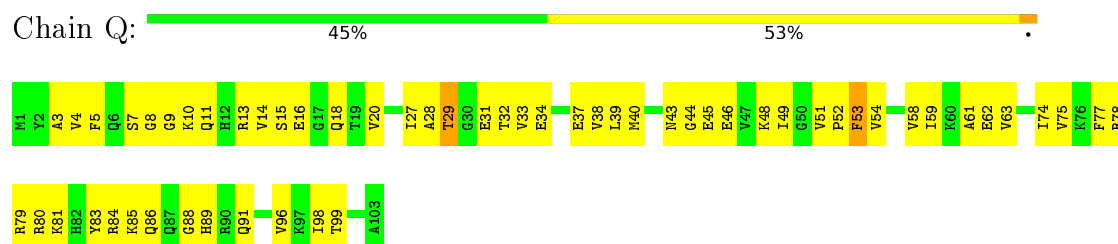
- Molecule 15: 50S ribosomal protein L19



- Molecule 16: 50S ribosomal protein L20

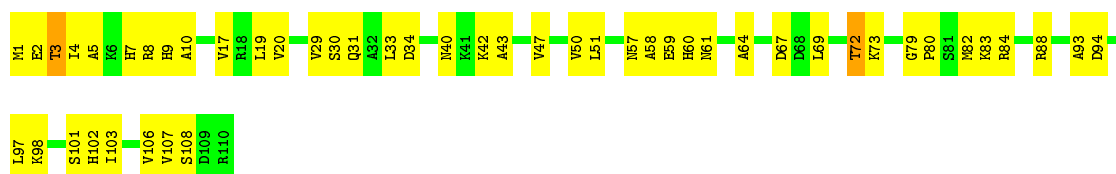


- Molecule 17: 50S ribosomal protein L21



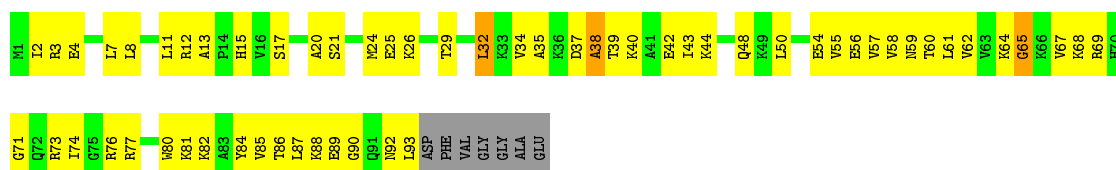
- Molecule 18: 50S ribosomal protein L22





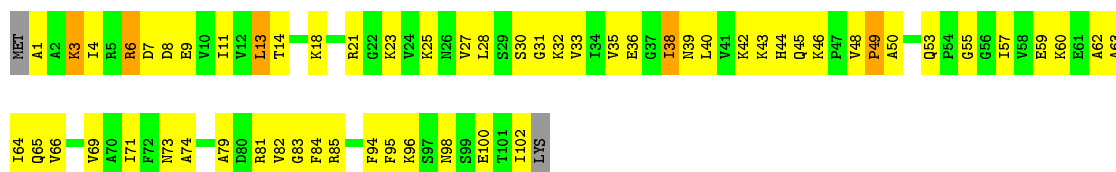
- Molecule 19: 50S ribosomal protein L23

Chain S: 34% 56% 7%



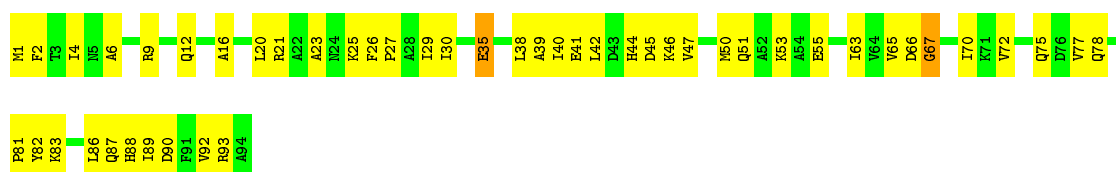
- Molecule 20: 50S ribosomal protein L24

Chain T: 41% 52% 5%



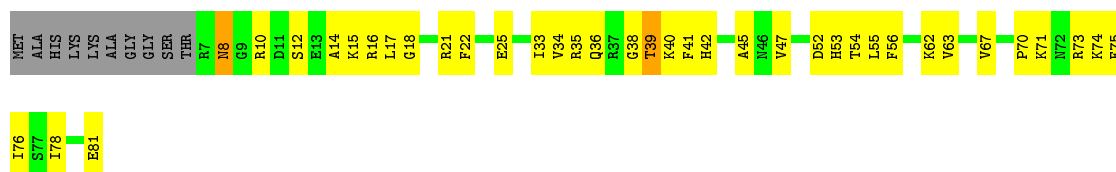
- Molecule 21: 50S ribosomal protein L25

Chain U: 49% 49% 2%



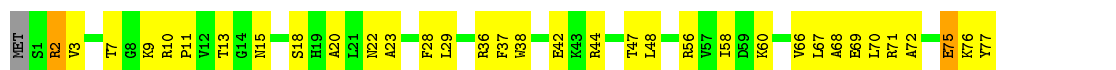
- Molecule 22: 50S ribosomal protein L27

Chain V: 44% 42% 12%

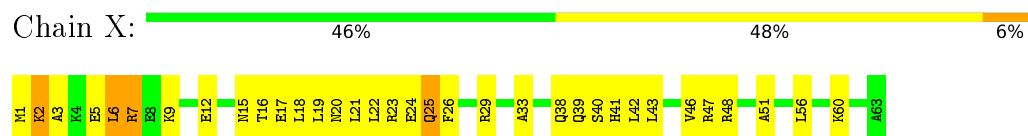


- Molecule 23: 50S ribosomal protein L28

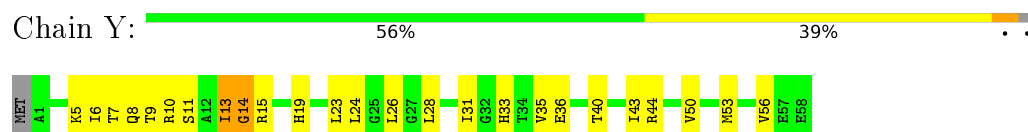
Chain W: 55% 41% 4%



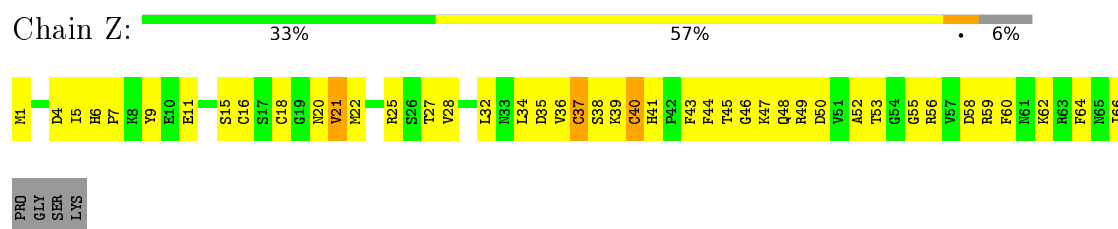
- Molecule 24: 50S ribosomal protein L29



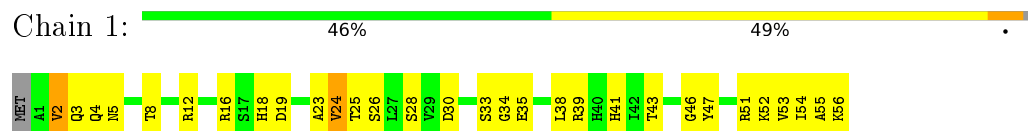
- Molecule 25: 50S ribosomal protein L30



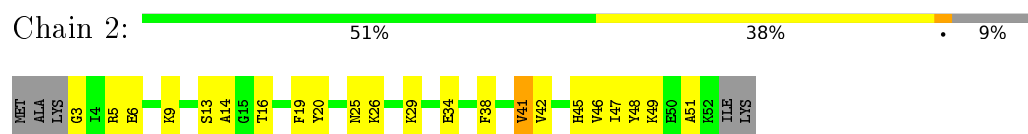
- Molecule 26: 50S ribosomal protein L31



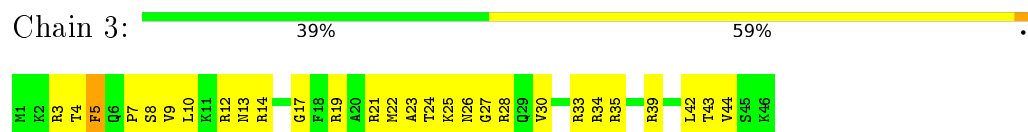
- Molecule 27: 50S ribosomal protein L32



- Molecule 28: 50S ribosomal protein L33



- Molecule 29: 50S ribosomal protein L34



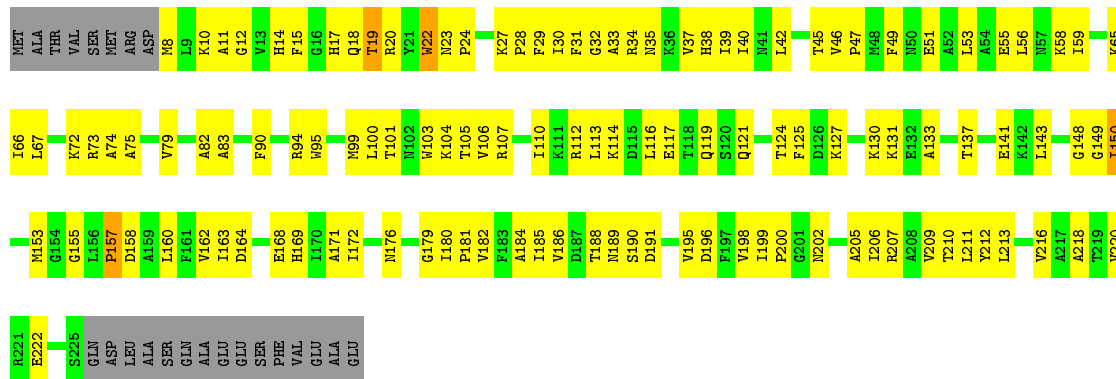
- Molecule 31: 50S ribosomal protein L36

Chain 5: 42% 47% 11%



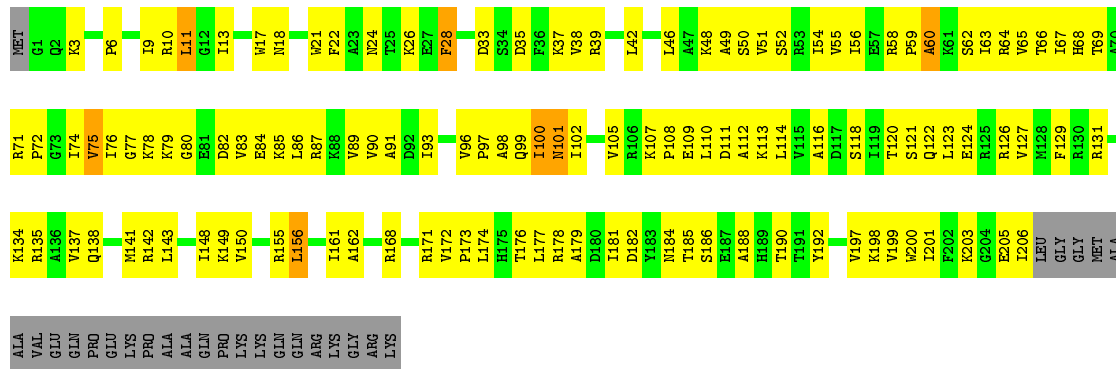
- Molecule 32: 30S ribosomal protein S2

Chain 6: 41% 48% 10%

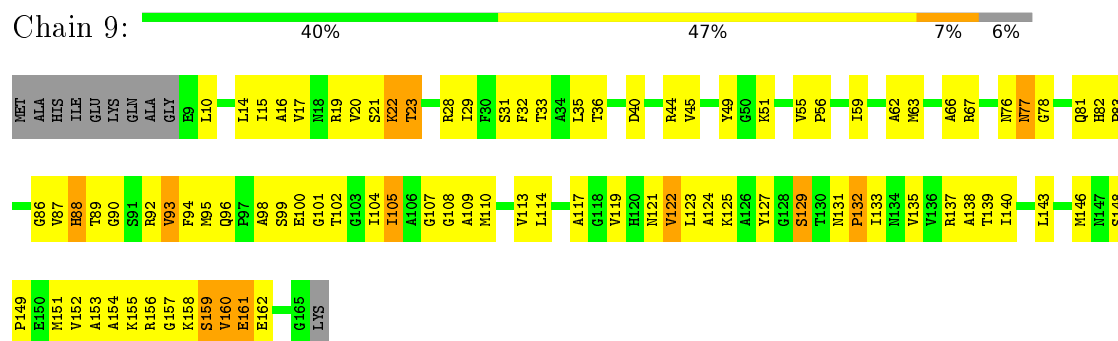


- Molecule 33: 30S ribosomal protein S3

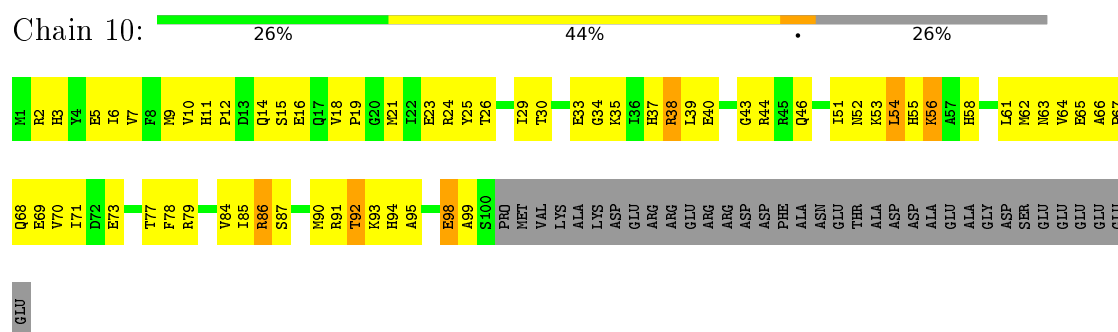
Chain 7: 35% 50% 12%



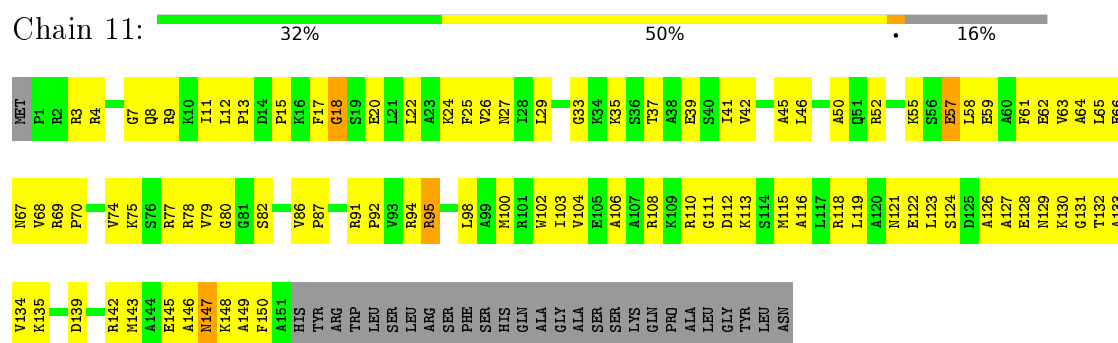
- Molecule 35: 30S ribosomal protein S5



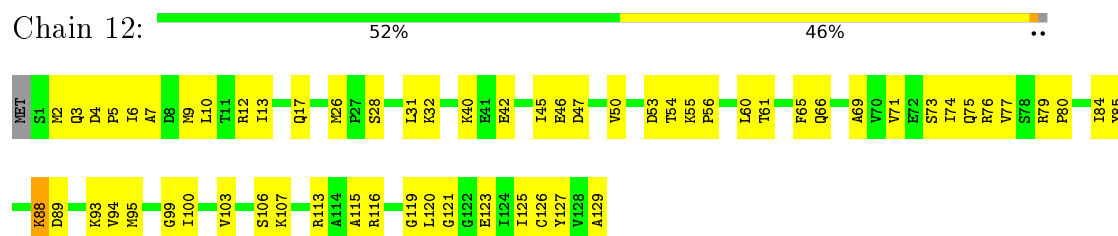
- Molecule 36: 30S ribosomal protein S6



- Molecule 37: 30S ribosomal protein S7

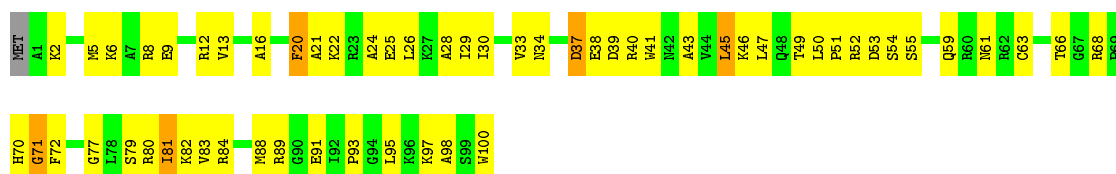


- Molecule 38: 30S ribosomal protein S8



- Molecule 39: 30S ribosomal protein S9

Chain 13:  28% 63% 6%



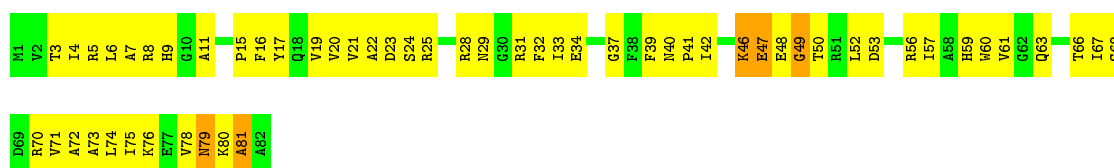
- Molecule 45: 30S ribosomal protein S15

Chain 19: 63% 34% ..



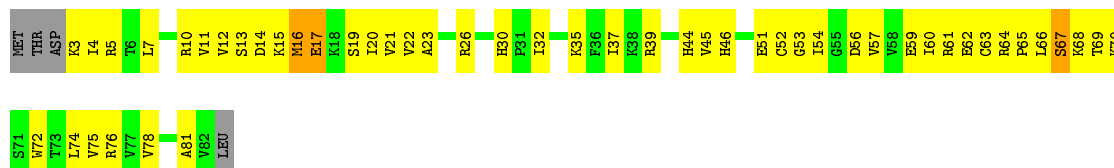
- Molecule 46: 30S ribosomal protein S16

Chain 20: 32% 62% 6%



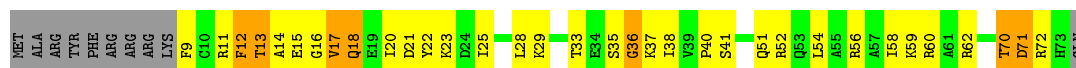
- Molecule 47: 30S ribosomal protein S17

Chain 21: 36% 56% 5%



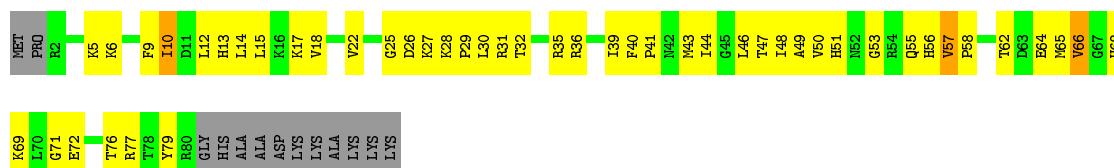
- Molecule 48: 30S ribosomal protein S18

Chain 22: 41% 36% 9% 13%



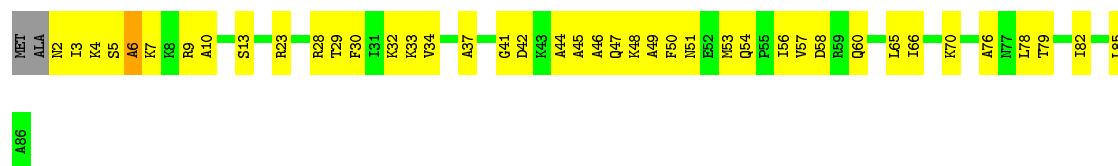
- Molecule 49: 30S ribosomal protein S19

Chain 23: 34% 49% 14%



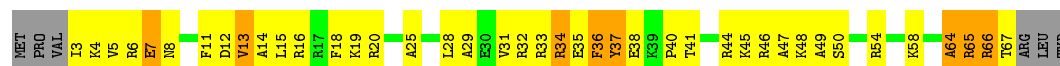
- Molecule 50: 30S ribosomal protein S20

Chain 24: 

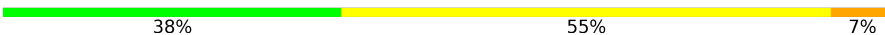


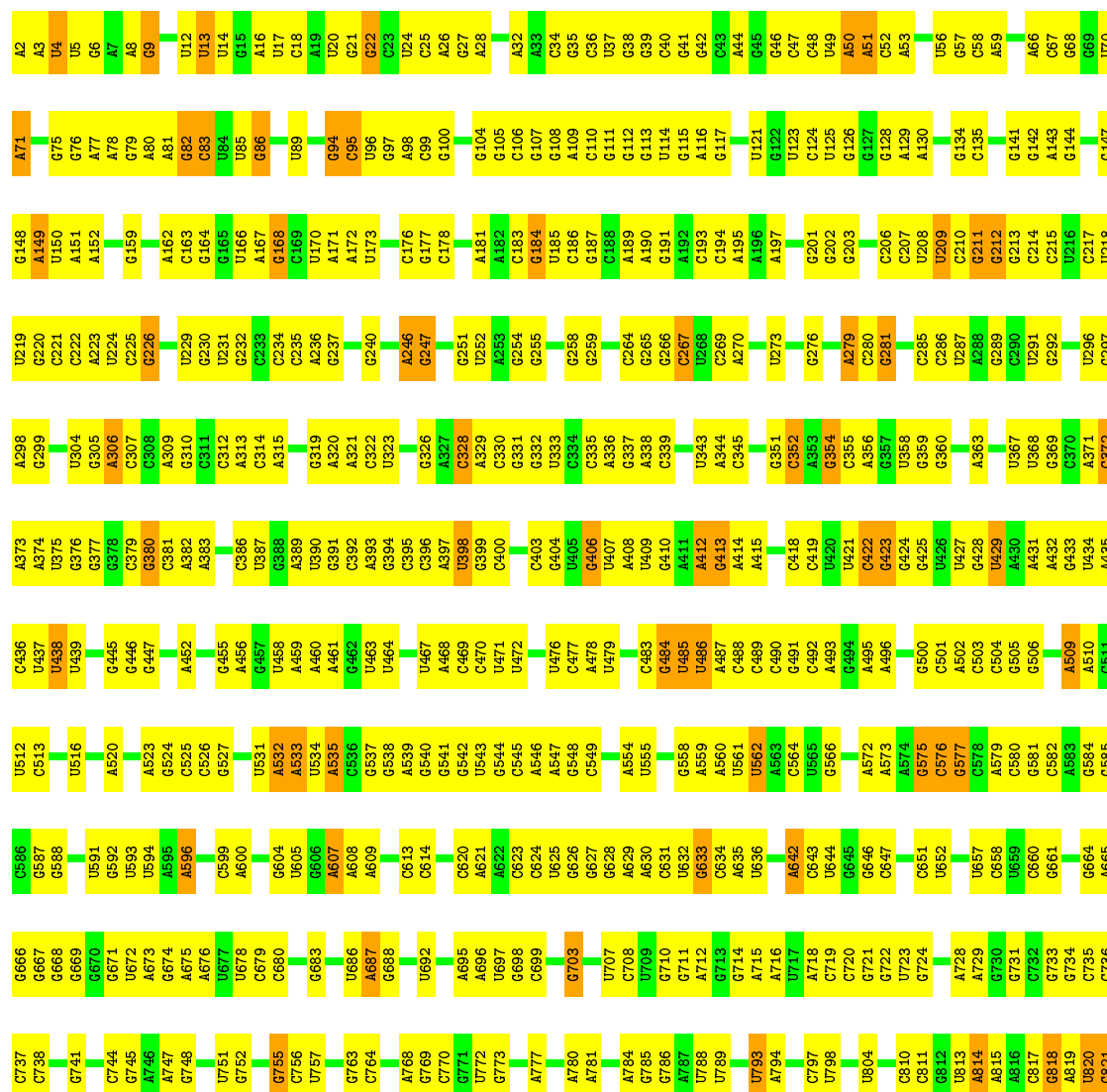
- Molecule 51: 30S ribosomal protein S21

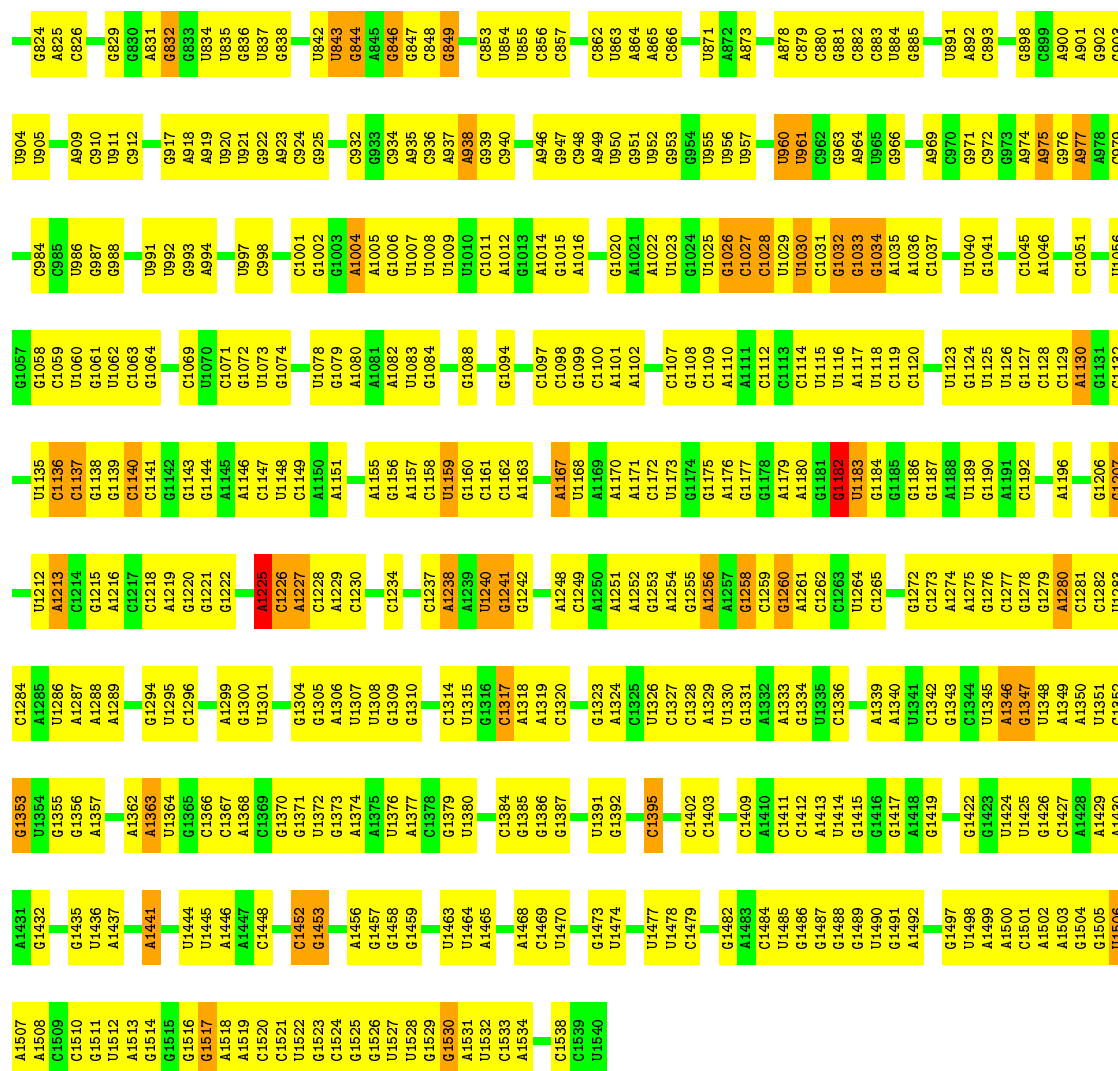
Chain 25: 



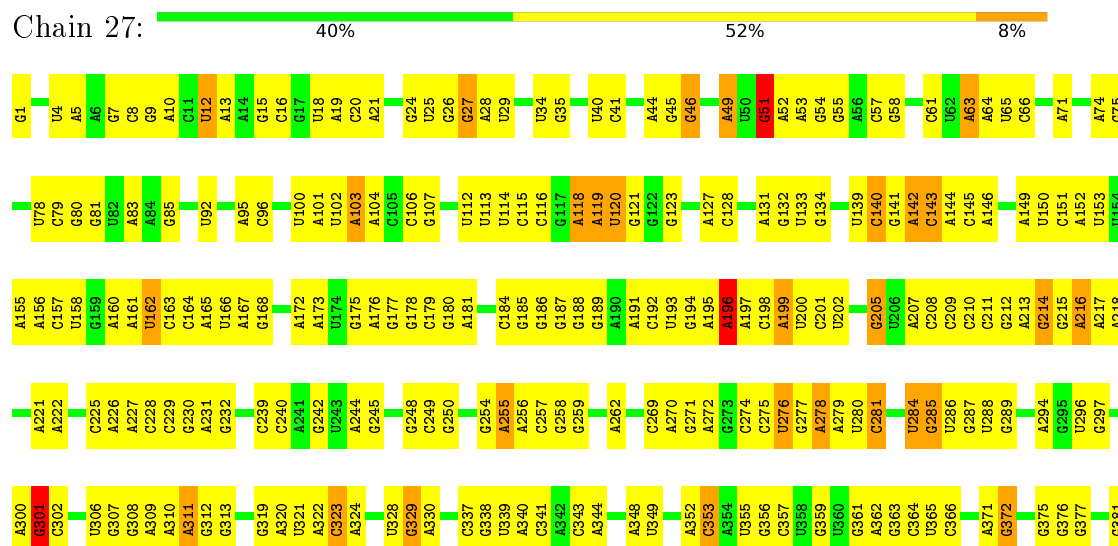
- Molecule 52: 16S ribosomal RNA

Chain 26: 



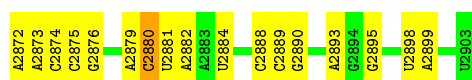


• Molecule 53: 23S ribosomal RNA



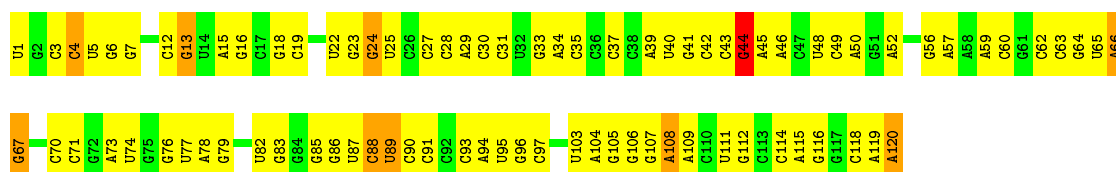


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G2863	G2796	A2720	U2639	U2562	U2488	U2419	U2350	U2263	U2191	U2128	G2058	U1987	C1896	G1824	G1747
C2864	U2797	G2721	G2640	G2563	U2489	U2420	U2351	U2264	U2192	U2129	C2059	U1988	C1897	G1825	G1748
U2865	A2798	U2722	U2641	U2564	U2490	U2421	U2352	U2265	U2193	U2130	G2060	U1989	C1898	G1826	G1749
G2866	C2799	A2723	G2642	U2565	U2491	U2422	U2353	U2266	U2194	U2131	C2061	U1990	C1899	G1827	G1750
C2867	U2800	U2724	G2643	U2566	U2492	U2423	U2354	U2267	U2195	U2132	G2062	U1991	C1900	G1828	G1751
U2868	G2801	G2725	G2644	U2567	U2493	U2424	U2355	U2268	U2196	U2133	C2063	U1992	C1901	G1829	G1752
G2869	U2802	A2726	G2645	U2568	U2494	U2425	U2356	U2269	U2197	U2134	G2064	U1993	C1902	G1830	G1753
C2870	C2803	U2727	G2646	U2569	U2495	U2426	U2357	U2270	U2198	U2135	C2065	U1994	C1903	G1831	G1754
U2871	A2804	G2728	G2647	G2570	U2496	U2427	U2358	U2271	U2199	U2136	G2066	U1995	C1904	G1832	G1755
G2872	U2805	U2729	G2648	U2571	U2497	U2428	U2359	U2272	U2200	U2137	C2067	U1996	C1905	G1833	G1756
C2873	C2806	G2730	G2649	U2572	U2498	U2429	U2360	U2273	U2201	U2138	G2068	U1997	C1906	G1834	G1757
U2874	U2807	A2731	G2650	U2573	U2499	U2430	U2361	U2274	U2202	U2139	U2069	U1998	C1907	G1835	G1758
G2875	G2808	U2732	G2651	G2574	U2500	U2431	U2362	U2275	U2203	U2140	G2070	U1999	C1908	G1836	G1759
C2876	A2809	U2733	U2652	U2575	U2501	U2432	U2363	U2276	U2204	U2141	C2071	U2000	C1909	G1837	G1760
U2877	C2810	G2734	G2653	U2576	U2502	U2433	U2364	U2277	U2205	U2142	G2072	U2001	G1910	U1765	U1671
G2878	U2811	A2735	U2654	U2577	U2503	U2434	U2365	U2278	U2206	U2143	C2073	U2002	G1911	G1766	A1672
C2879	C2812	U2736	G2655	U2578	U2504	U2435	U2366	U2279	U2207	U2144	G2074	U2003	G1912	G1767	A1673
U2880	A2813	G2737	G2656	U2579	U2505	U2436	U2367	U							



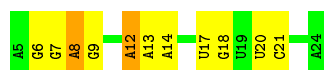
- Molecule 54: 5S ribosomal RNA

Chain 28: 30% 62% 8%



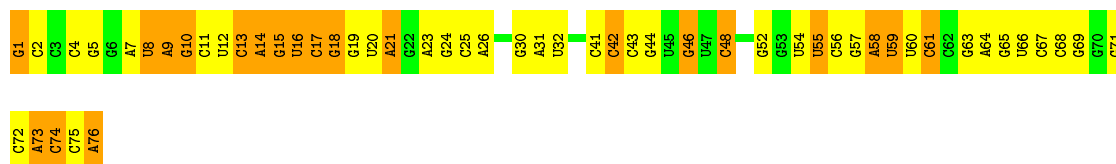
- Molecule 55: mRNA

Chain 29: 45% 45% 10%



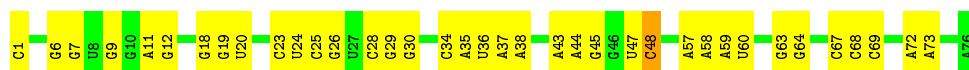
- Molecule 56: A-site tRNA^{Phe}

Chain 30: 29% 43% 28%



- Molecule 57: P-site tRNA^{fMet}

Chain 31: 52% 47% 1%



- Molecule 58: E-site tRNA^{fMet}

Chain 32: 22% 56% 22%



- Molecule 59: GTP pyrophosphokinase

Chain 33: 38% 45% 6% 10%




4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	77862	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	30488	Depositor
Image detector	Not provided	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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 >2	RMSZ	# Z >2
1	A	0.29	0/2121	0.64	0/2852
10	J	0.30	0/947	0.63	0/1268
11	K	0.30	0/1054	0.66	0/1403
12	L	0.33	0/1093	0.59	0/1460
13	M	0.32	0/973	0.63	0/1301
14	N	0.28	0/902	0.57	0/1209
15	O	0.32	0/929	0.61	0/1242
16	P	0.32	0/960	0.56	0/1278
17	Q	0.35	0/829	0.67	1/1107 (0.1%)
18	R	0.27	0/864	0.65	0/1156
19	S	0.30	0/744	0.61	0/994
2	B	0.33	0/1586	0.62	0/2134
20	T	0.35	0/787	0.69	0/1051
21	U	0.32	0/766	0.58	0/1025
22	V	0.34	0/582	0.60	0/769
23	W	0.34	0/635	0.63	0/848
24	X	0.31	0/510	0.59	0/677
25	Y	0.30	0/453	0.55	0/605
26	Z	0.37	0/531	0.91	3/709 (0.4%)
27	1	0.28	0/450	0.56	0/599
28	2	0.32	0/416	0.57	0/554
29	3	0.35	0/380	0.58	0/498
3	C	0.34	0/1571	0.62	0/2113
30	4	0.32	0/513	0.61	0/676
31	5	0.29	0/303	0.63	0/397
32	6	0.37	0/1735	0.60	0/2338
33	7	0.32	0/1651	0.60	0/2225
34	8	0.32	0/1665	0.60	0/2227
35	9	0.31	0/1169	0.70	1/1573 (0.1%)
36	10	0.34	0/835	0.64	0/1128
37	11	0.29	0/1195	0.60	0/1602
38	12	0.31	0/989	0.60	0/1326
39	13	0.33	0/1034	0.66	0/1375
4	D	0.34	0/1434	0.58	0/1926

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
40	14	0.31	0/796	0.62	0/1077
41	15	0.33	0/885	0.68	0/1195
42	16	0.33	0/969	0.73	0/1300
43	17	0.28	0/892	0.63	0/1193
44	18	0.40	0/817	0.58	0/1088
45	19	0.28	0/722	0.55	0/964
46	20	0.35	0/659	0.64	1/884 (0.1%)
47	21	0.33	0/657	0.66	0/881
48	22	0.34	0/544	0.67	0/731
49	23	0.33	0/652	0.62	0/877
5	E	0.30	0/1343	0.62	0/1816
50	24	0.29	0/671	0.55	0/888
51	25	0.38	0/550	0.73	0/728
52	26	0.38	1/36967 (0.0%)	0.70	5/57666 (0.0%)
53	27	0.39	1/69801 (0.0%)	0.70	5/108894 (0.0%)
54	28	0.36	1/2876 (0.0%)	0.70	1/4483 (0.0%)
55	29	0.84	0/486	0.70	0/757
56	30	0.50	1/1813 (0.1%)	0.74	0/2823
57	31	0.37	1/1836 (0.1%)	0.68	0/2859
58	32	0.80	2/1835 (0.1%)	0.74	1/2857 (0.0%)
59	33	0.66	6/4985 (0.1%)	1.08	38/6770 (0.6%)
6	F	0.36	0/1122	0.68	0/1515
7	G	0.41	0/1001	0.74	1/1350 (0.1%)
8	H	0.38	0/1046	0.72	1/1410 (0.1%)
9	I	0.30	0/1152	0.61	0/1551
All	All	0.39	13/167683 (0.0%)	0.70	58/250202 (0.0%)

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
52	26	0	9
53	27	0	22
56	30	0	1
59	33	0	2
All	All	0	34

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	33	156	ARG	CZ-NH2	-10.64	1.19	1.33
59	33	152	LYS	CD-CE	-7.75	1.31	1.51
59	33	17	PRO	CA-CB	-7.24	1.39	1.53
52	26	2	A	OP3-P	-7.10	1.52	1.61
58	32	1	C	OP3-P	-7.09	1.52	1.61

The worst 5 of 58 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	33	156	ARG	NE-CZ-NH1	19.60	130.10	120.30
59	33	156	ARG	NH1-CZ-NH2	-13.76	104.26	119.40
59	33	17	PRO	N-CA-CB	-11.19	89.87	103.30
59	33	17	PRO	CA-CB-CG	10.30	124.37	104.80
59	33	63	VAL	CG1-CB-CG2	-9.24	96.11	110.90

There are no chirality outliers.

5 of 34 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
52	26	159	G	Sidechain
52	26	380	G	Sidechain
52	26	820	U	Sidechain
52	26	898	G	Sidechain
52	26	938	A	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2082	0	2157	111	0
2	B	1565	0	1616	100	0
3	C	1552	0	1619	102	0
4	D	1410	0	1447	120	0
5	E	1323	0	1374	77	0
6	F	1111	0	1148	93	0
7	G	988	0	1025	135	0
8	H	1032	0	1088	109	0
9	I	1129	0	1162	65	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	J	938	0	1012	64	0
11	K	1045	0	1117	88	0
12	L	1074	0	1157	62	0
13	M	960	0	1000	65	0
14	N	892	0	923	51	0
15	O	917	0	965	61	0
16	P	947	0	1022	72	0
17	Q	816	0	839	54	0
18	R	857	0	922	45	0
19	S	738	0	807	51	0
20	T	779	0	834	55	0
21	U	753	0	780	37	0
22	V	575	0	592	31	0
23	W	625	0	655	32	0
24	X	509	0	543	40	0
25	Y	449	0	491	25	0
26	Z	522	0	521	41	0
27	1	444	0	461	36	0
28	2	409	0	440	17	0
29	3	377	0	418	35	0
30	4	504	0	574	32	0
31	5	302	0	343	28	0
32	6	1704	0	1732	100	0
33	7	1624	0	1699	126	0
34	8	1643	0	1710	136	0
35	9	1156	0	1199	80	0
36	10	817	0	808	68	0
37	11	1181	0	1240	65	0
38	12	979	0	1034	59	0
39	13	1022	0	1070	118	0
40	14	786	0	828	83	0
41	15	869	0	878	65	0
42	16	955	0	1019	65	0
43	17	883	0	944	85	0
44	18	805	0	847	62	0
45	19	714	0	737	26	0
46	20	649	0	666	62	0
47	21	648	0	691	50	0
48	22	535	0	552	40	0
49	23	637	0	665	52	0
50	24	665	0	714	42	0
51	25	544	0	579	72	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
52	26	33016	0	16617	892	0
53	27	62322	0	31345	1639	0
54	28	2572	0	1302	90	0
55	29	432	0	218	13	0
56	30	1623	0	821	66	0
57	31	1644	0	836	26	0
58	32	1643	0	836	76	0
59	33	4911	0	4550	616	0
All	All	154603	0	105189	6144	0

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 24.

The worst 5 of 6144 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)
59:33:17:PRO:HB3	59:33:39:TRP:NE1	1.57	1.18
52:26:484:G:H4'	52:26:485:U:H5'	1.23	1.18
51:25:20:ARG:HH22	52:26:1538:C:H1'	1.05	1.13
59:33:65:ILE:HG21	59:33:157:ILE:HD11	1.31	1.11
59:33:188:ARG:HH12	59:33:377:LEU:HA	1.08	1.11

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	269/273 (98%)	226 (84%)	34 (13%)	9 (3%)	5	42
2	B	207/209 (99%)	165 (80%)	29 (14%)	13 (6%)	2	26
3	C	199/201 (99%)	164 (82%)	23 (12%)	12 (6%)	2	27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	175/179 (98%)	140 (80%)	27 (15%)	8 (5%)	3	33
5	E	174/177 (98%)	145 (83%)	22 (13%)	7 (4%)	4	37
6	F	147/149 (99%)	119 (81%)	16 (11%)	12 (8%)	1	18
7	G	129/165 (78%)	92 (71%)	17 (13%)	20 (16%)	0	5
8	H	139/142 (98%)	106 (76%)	27 (19%)	6 (4%)	3	35
9	I	140/142 (99%)	127 (91%)	7 (5%)	6 (4%)	3	35
10	J	120/123 (98%)	101 (84%)	14 (12%)	5 (4%)	3	35
11	K	141/144 (98%)	116 (82%)	16 (11%)	9 (6%)	2	26
12	L	134/136 (98%)	110 (82%)	20 (15%)	4 (3%)	5	44
13	M	118/127 (93%)	99 (84%)	14 (12%)	5 (4%)	3	35
14	N	114/117 (97%)	92 (81%)	16 (14%)	6 (5%)	2	30
15	O	112/115 (97%)	88 (79%)	20 (18%)	4 (4%)	4	40
16	P	115/118 (98%)	108 (94%)	5 (4%)	2 (2%)	11	55
17	Q	101/103 (98%)	82 (81%)	16 (16%)	3 (3%)	5	44
18	R	108/110 (98%)	85 (79%)	19 (18%)	4 (4%)	4	39
19	S	91/100 (91%)	73 (80%)	13 (14%)	5 (6%)	2	30
20	T	100/104 (96%)	80 (80%)	13 (13%)	7 (7%)	1	23
21	U	92/94 (98%)	76 (83%)	13 (14%)	3 (3%)	5	42
22	V	73/85 (86%)	64 (88%)	7 (10%)	2 (3%)	6	46
23	W	75/78 (96%)	67 (89%)	6 (8%)	2 (3%)	6	46
24	X	61/63 (97%)	52 (85%)	5 (8%)	4 (7%)	1	25
25	Y	56/59 (95%)	50 (89%)	4 (7%)	2 (4%)	4	40
26	Z	64/70 (91%)	50 (78%)	9 (14%)	5 (8%)	1	20
27	1	54/57 (95%)	42 (78%)	6 (11%)	6 (11%)	0	10
28	2	48/55 (87%)	41 (85%)	6 (12%)	1 (2%)	9	51
29	3	44/46 (96%)	35 (80%)	7 (16%)	2 (4%)	3	33
30	4	62/65 (95%)	51 (82%)	6 (10%)	5 (8%)	1	18
31	5	36/38 (95%)	26 (72%)	6 (17%)	4 (11%)	0	10
32	6	216/241 (90%)	177 (82%)	31 (14%)	8 (4%)	4	39
33	7	204/233 (88%)	172 (84%)	26 (13%)	6 (3%)	6	45
34	8	203/206 (98%)	158 (78%)	30 (15%)	15 (7%)	1	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	9	155/167 (93%)	116 (75%)	25 (16%)	14 (9%)	1	16
36	10	98/135 (73%)	76 (78%)	15 (15%)	7 (7%)	1	23
37	11	149/179 (83%)	123 (83%)	17 (11%)	9 (6%)	2	27
38	12	127/130 (98%)	112 (88%)	13 (10%)	2 (2%)	12	56
39	13	125/130 (96%)	98 (78%)	17 (14%)	10 (8%)	1	19
40	14	96/103 (93%)	77 (80%)	11 (12%)	8 (8%)	1	18
41	15	114/129 (88%)	92 (81%)	18 (16%)	4 (4%)	4	41
42	16	121/124 (98%)	98 (81%)	11 (9%)	12 (10%)	1	14
43	17	112/118 (95%)	90 (80%)	11 (10%)	11 (10%)	1	14
44	18	98/101 (97%)	71 (72%)	20 (20%)	7 (7%)	1	23
45	19	86/89 (97%)	73 (85%)	8 (9%)	5 (6%)	2	28
46	20	80/82 (98%)	64 (80%)	12 (15%)	4 (5%)	3	31
47	21	78/84 (93%)	53 (68%)	19 (24%)	6 (8%)	1	20
48	22	63/75 (84%)	48 (76%)	9 (14%)	6 (10%)	1	15
49	23	77/92 (84%)	60 (78%)	13 (17%)	4 (5%)	2	31
50	24	83/87 (95%)	75 (90%)	5 (6%)	3 (4%)	4	40
51	25	63/71 (89%)	44 (70%)	9 (14%)	10 (16%)	0	5
59	33	663/750 (88%)	550 (83%)	78 (12%)	35 (5%)	2	30
All	All	6509/6970 (93%)	5299 (81%)	841 (13%)	369 (6%)	4	28

5 of 369 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	18	ASP
2	B	181	ASP
2	B	188	LEU
3	C	55	SER
3	C	127	GLU

5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	216/218 (99%)	215 (100%)	1 (0%)	92	96
2	B	164/164 (100%)	163 (99%)	1 (1%)	90	95
3	C	165/165 (100%)	164 (99%)	1 (1%)	90	95
4	D	148/150 (99%)	146 (99%)	2 (1%)	74	89
5	E	137/138 (99%)	136 (99%)	1 (1%)	88	94
6	F	114/114 (100%)	113 (99%)	1 (1%)	84	92
7	G	100/123 (81%)	99 (99%)	1 (1%)	82	91
8	H	109/110 (99%)	109 (100%)	0	100	100
9	I	116/116 (100%)	116 (100%)	0	100	100
10	J	103/104 (99%)	103 (100%)	0	100	100
11	K	102/103 (99%)	102 (100%)	0	100	100
12	L	109/109 (100%)	109 (100%)	0	100	100
13	M	100/103 (97%)	99 (99%)	1 (1%)	82	91
14	N	86/87 (99%)	84 (98%)	2 (2%)	58	83
15	O	99/100 (99%)	99 (100%)	0	100	100
16	P	89/90 (99%)	89 (100%)	0	100	100
17	Q	84/84 (100%)	84 (100%)	0	100	100
18	R	93/93 (100%)	93 (100%)	0	100	100
19	S	80/84 (95%)	79 (99%)	1 (1%)	76	89
20	T	83/85 (98%)	82 (99%)	1 (1%)	78	90
21	U	78/78 (100%)	78 (100%)	0	100	100
22	V	57/63 (90%)	57 (100%)	0	100	100
23	W	67/68 (98%)	67 (100%)	0	100	100
24	X	55/55 (100%)	55 (100%)	0	100	100
25	Y	48/49 (98%)	48 (100%)	0	100	100
26	Z	59/62 (95%)	58 (98%)	1 (2%)	68	88
27	1	47/48 (98%)	47 (100%)	0	100	100
28	2	45/49 (92%)	45 (100%)	0	100	100
29	3	38/38 (100%)	38 (100%)	0	100	100
30	4	51/52 (98%)	51 (100%)	0	100	100
31	5	34/34 (100%)	34 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	6	180/199 (90%)	179 (99%)	1 (1%)	90	95
33	7	170/190 (90%)	168 (99%)	2 (1%)	78	90
34	8	172/173 (99%)	171 (99%)	1 (1%)	90	95
35	9	119/126 (94%)	117 (98%)	2 (2%)	68	88
36	10	87/116 (75%)	86 (99%)	1 (1%)	80	90
37	11	124/147 (84%)	124 (100%)	0	100	100
38	12	104/105 (99%)	104 (100%)	0	100	100
39	13	105/107 (98%)	103 (98%)	2 (2%)	65	86
40	14	86/90 (96%)	86 (100%)	0	100	100
41	15	89/99 (90%)	89 (100%)	0	100	100
42	16	103/104 (99%)	103 (100%)	0	100	100
43	17	92/96 (96%)	91 (99%)	1 (1%)	80	90
44	18	83/84 (99%)	81 (98%)	2 (2%)	57	82
45	19	76/77 (99%)	76 (100%)	0	100	100
46	20	65/65 (100%)	65 (100%)	0	100	100
47	21	74/78 (95%)	74 (100%)	0	100	100
48	22	56/65 (86%)	55 (98%)	1 (2%)	66	87
49	23	70/79 (89%)	70 (100%)	0	100	100
50	24	65/66 (98%)	65 (100%)	0	100	100
51	25	55/61 (90%)	55 (100%)	0	100	100
59	33	452/635 (71%)	449 (99%)	3 (1%)	88	94
All	All	5303/5698 (93%)	5273 (99%)	30 (1%)	91	95

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
26	Z	37	CYS
33	7	101	ASN
59	33	267	ASN
33	7	100	ILE
34	8	170	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 94 such sidechains are listed below:

Mol	Chain	Res	Type
24	X	58	ASN
32	6	177	ASN
59	33	264	GLN
26	Z	61	ASN
31	5	37	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
52	26	1538/1539 (99%)	178 (11%)	5 (0%)
53	27	2902/2903 (99%)	379 (13%)	17 (0%)
54	28	119/120 (99%)	15 (12%)	1 (0%)
55	29	19/20 (95%)	3 (15%)	0
56	30	75/76 (98%)	22 (29%)	1 (1%)
57	31	76/77 (98%)	5 (6%)	0
58	32	76/77 (98%)	16 (21%)	0
All	All	4805/4812 (99%)	618 (12%)	24 (0%)

5 of 618 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
52	26	4	U
52	26	9	G
52	26	13	U
52	26	22	G
52	26	32	A

5 of 24 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
53	27	1020	A
53	27	1694	C
54	28	66	A
53	27	1130	U
53	27	1378	A

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.