



wwPDB/EMDatabank EM Map/Model Validation Summary Report ⓘ

Nov 14, 2019 – 03:05 AM EST

PDB ID : 5KPV
EMDB ID: : EMD-8280
Title : Structure of RelA bound to ribosome in presence of A/R tRNA (Structure II)
Authors : Loveland, A.B.; Bah, E.; Madireddy, R.; Zhang, Y.; Brilot, A.F.; Grigorieff, N.; Korostelev, A.A.
Deposited on : 2016-07-05
Resolution : 4.10 Å(reported)

This is a wwPDB/EMDatabank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

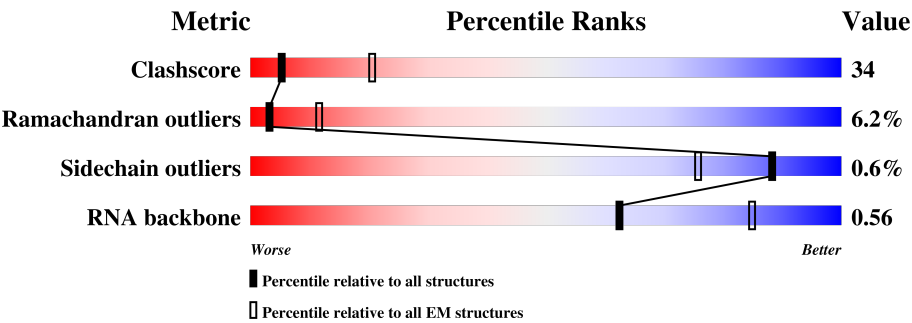
MolProbity : 4.02b-467
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.10 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.




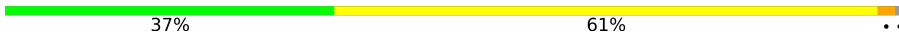
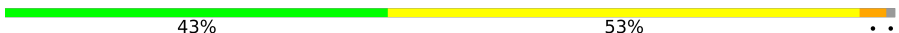


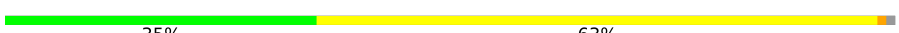
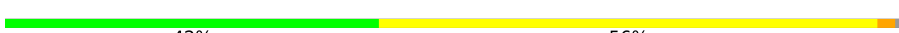




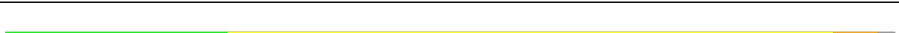













Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531
RNA backbone	3747	458

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	<div><div>43%</div><div>53%</div><div>..</div></div>
2	B	209	<div><div>45%</div><div>53%</div><div>.</div></div>
3	C	201	<div><div>39%</div><div>55%</div><div>6%</div></div>
4	D	179	<div><div>34%</div><div>62%</div><div>...</div></div>
5	E	177	<div><div>46%</div><div>52%</div><div>..</div></div>
6	F	149	<div><div>37%</div><div>54%</div><div>9%</div></div>
7	G	165	<div><div>21%</div><div>52%</div><div>6%</div><div>21%</div></div>
8	H	142	<div><div>27%</div><div>67%</div><div>5%</div><div>..</div></div>





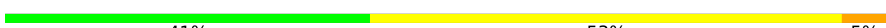
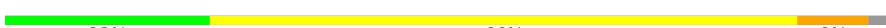







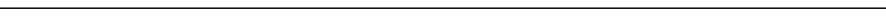

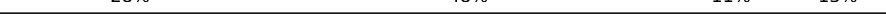









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Mol	Chain	Length	Quality of chain
9	I	142	
10	J	123	
11	K	144	
12	L	136	
13	M	127	
14	N	117	
15	O	115	
16	P	118	
17	Q	103	
18	R	110	
19	S	100	
20	T	104	
21	U	94	
22	V	85	
23	W	78	
24	X	63	
25	Y	59	
26	Z	70	
27	1	57	
28	2	55	
29	3	46	
30	4	65	
31	5	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>35%</div><div>48%</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		

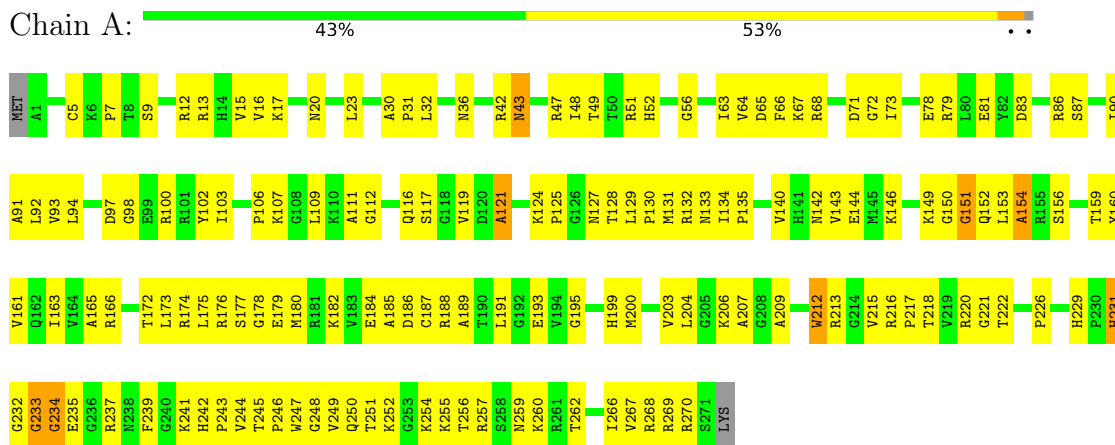
There are 7 discrepancies between the modelled and reference sequences:

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 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: 50S ribosomal protein L2



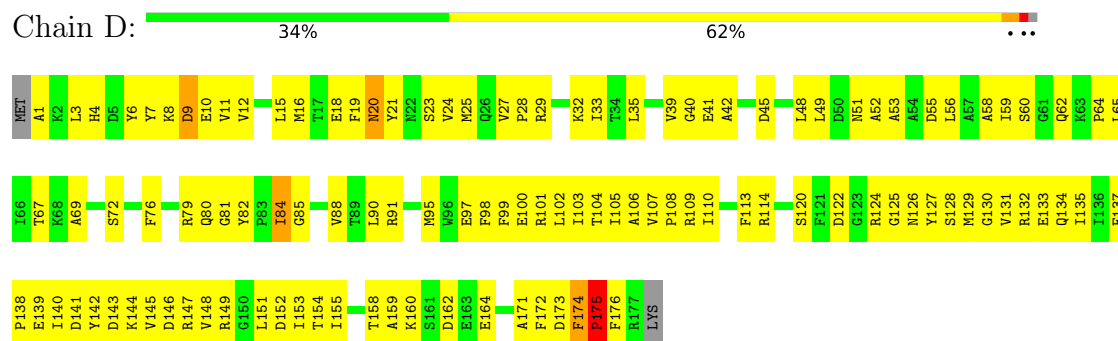
- Molecule 2: 50S ribosomal protein L3



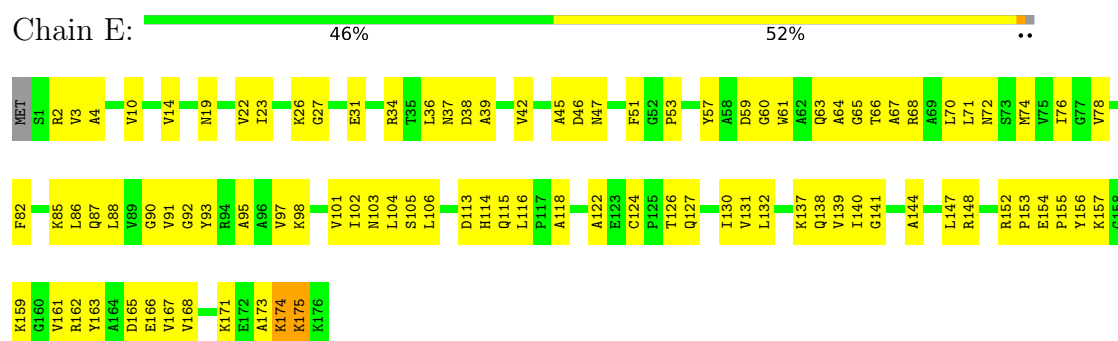
- Molecule 3: 50S ribosomal protein L4



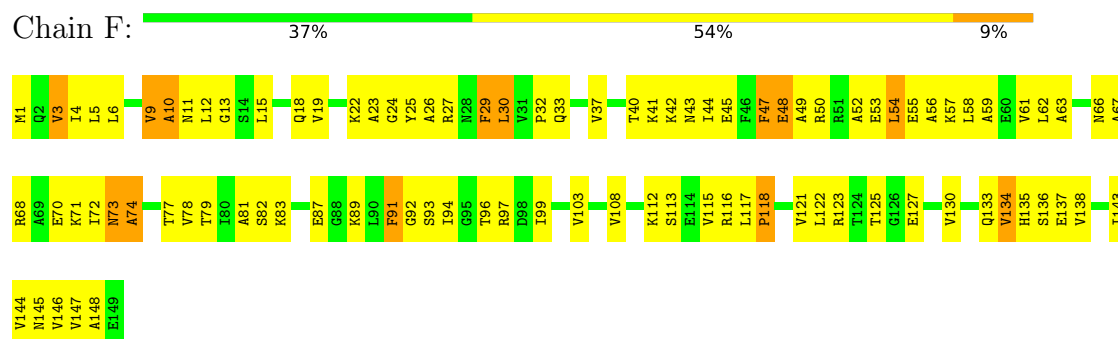
- Molecule 4: 50S ribosomal protein L5



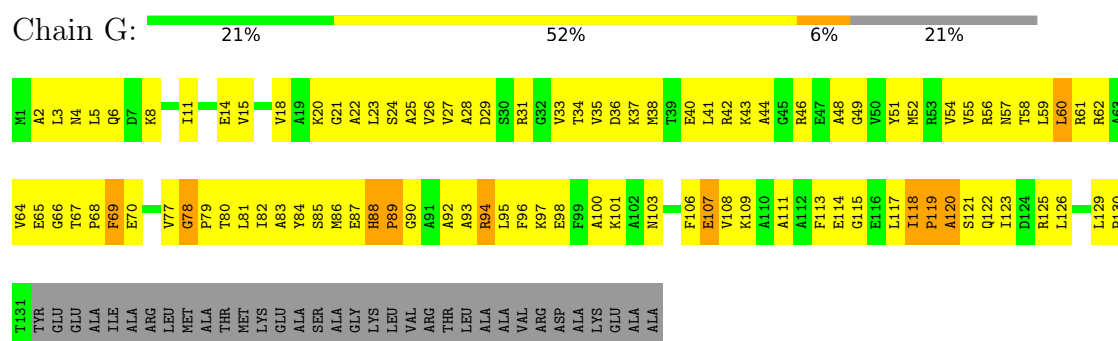
- Molecule 5: 50S ribosomal protein L6



- Molecule 6: 50S ribosomal protein L9

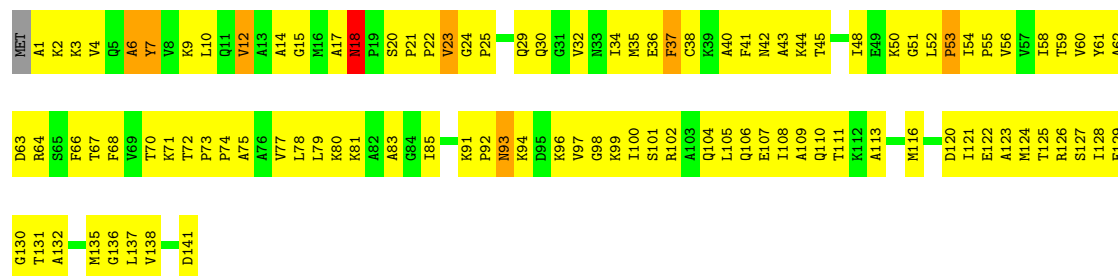


- Molecule 7: 50S ribosomal protein L10



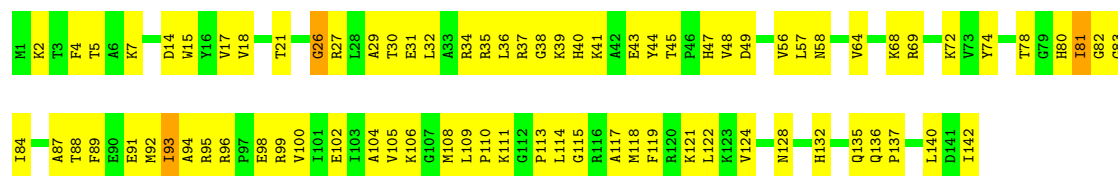
- Molecule 8: 50S ribosomal protein L11

Chain H:  27% 67% 5% ..



- Molecule 9: 50S ribosomal protein L13

Chain I:  44% 54% .



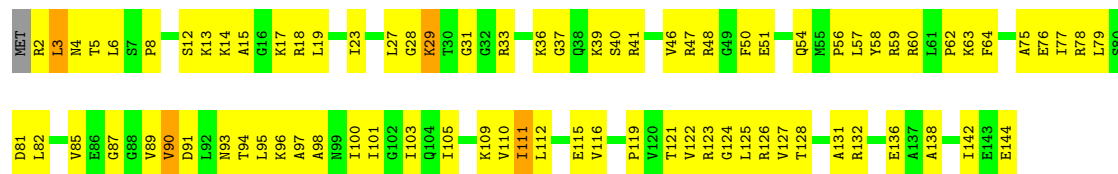
- Molecule 10: 50S ribosomal protein L14

Chain J:  37% 61% ..



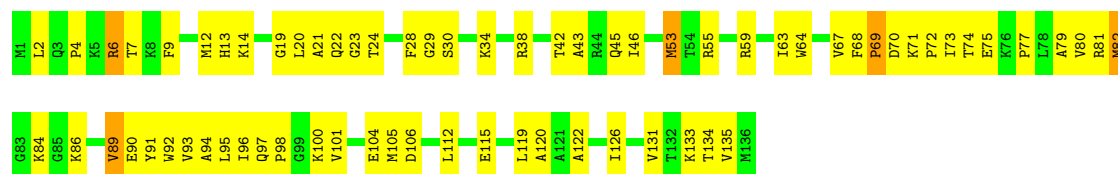
- Molecule 11: 50S ribosomal protein L15

Chain K:  43% 53% ..

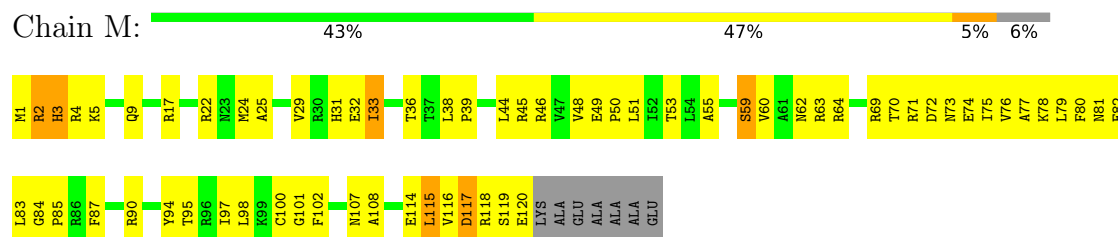


- Molecule 12: 50S ribosomal protein L16

Chain L:  49% 47% .



- Molecule 13: 50S ribosomal protein L17



- Molecule 14: 50S ribosomal protein L18



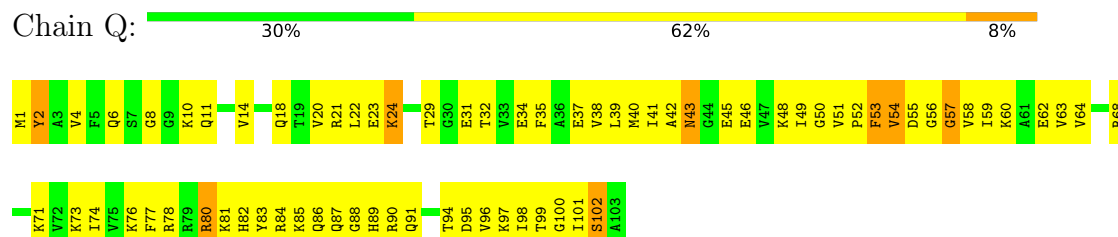
- Molecule 15: 50S ribosomal protein L19



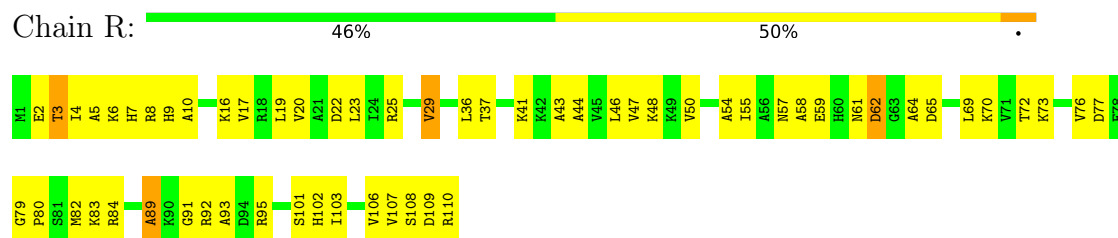
- Molecule 16: 50S ribosomal protein L20



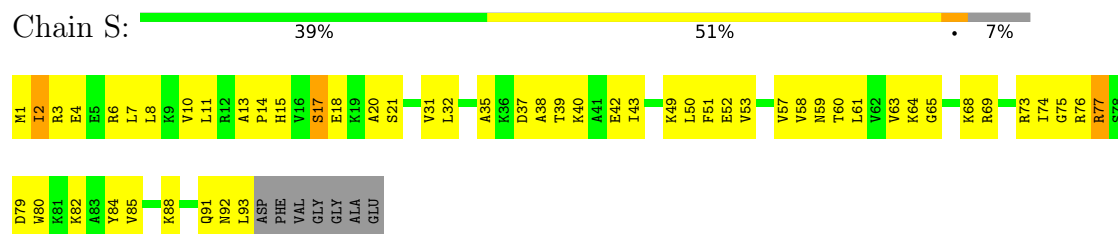
- Molecule 17: 50S ribosomal protein L21



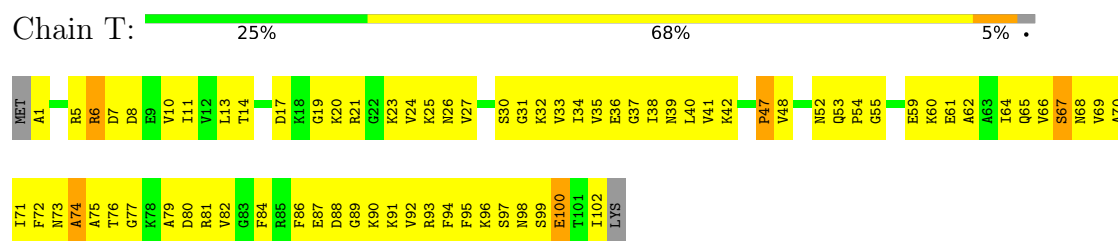
- Molecule 18: 50S ribosomal protein L22



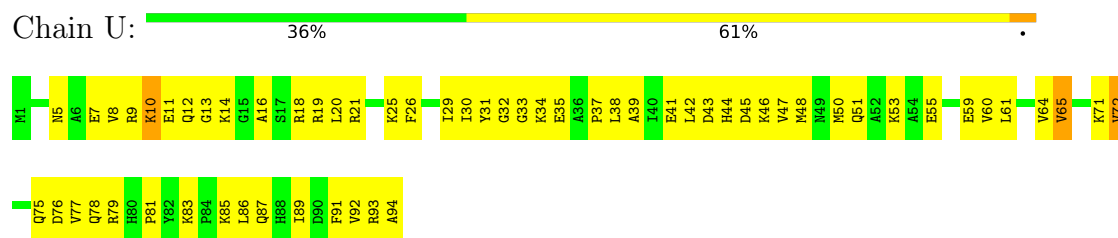
• Molecule 19: 50S ribosomal protein L23



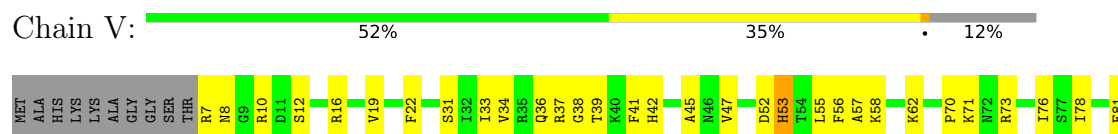
• Molecule 20: 50S ribosomal protein L24



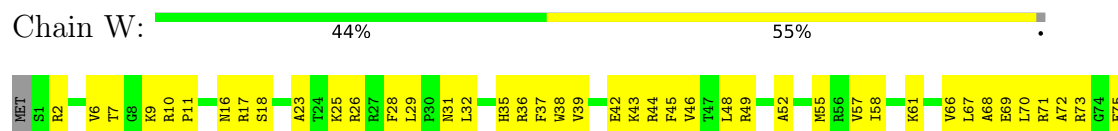
• Molecule 21: 50S ribosomal protein L25



• Molecule 22: 50S ribosomal protein L27



• Molecule 23: 50S ribosomal protein L28





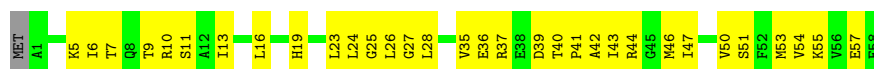
- Molecule 24: 50S ribosomal protein L29

Chain X: 29% 63% 8%



- Molecule 25: 50S ribosomal protein L30

Chain Y: 44% 54% 2%



- Molecule 26: 50S ribosomal protein L31

Chain Z: 37% 49% 9% 6%



- Molecule 27: 50S ribosomal protein L32

Chain 1: 32% 58% 9% 1%



- Molecule 28: 50S ribosomal protein L33

Chain 2: 47% 44% 9%



- Molecule 29: 50S ribosomal protein L34

Chain 3: 46% 52% 2%



- Molecule 30: 50S ribosomal protein L35

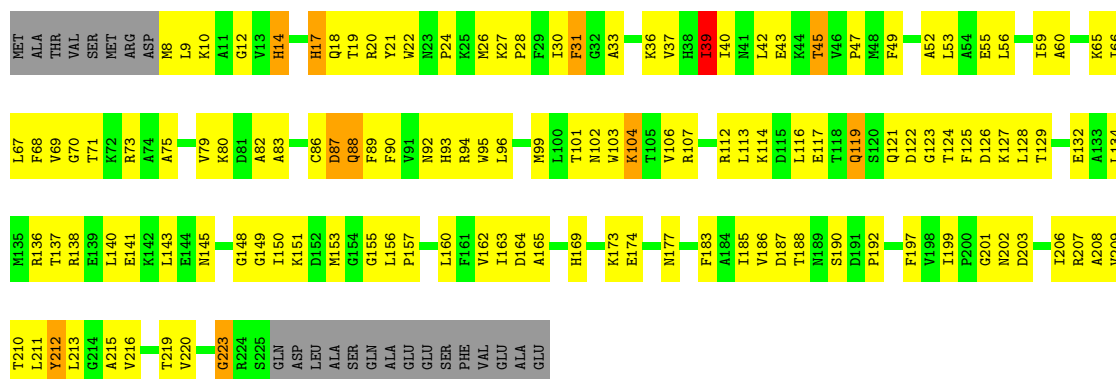
Chain 4: 46% 51% 3% 2%



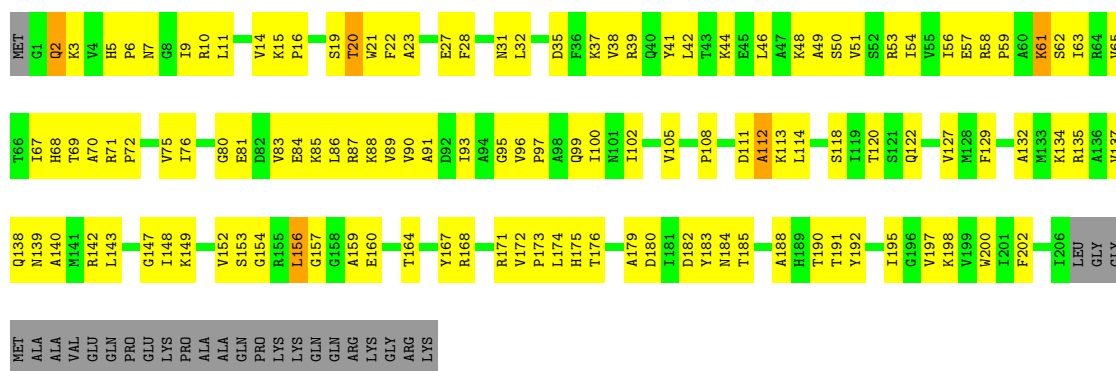
- Molecule 31: 50S ribosomal protein L36



- Molecule 32: 30S ribosomal protein S2



- Molecule 33: 30S ribosomal protein S3



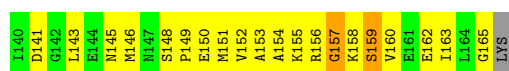
- Molecule 34: 30S ribosomal protein S4





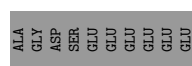
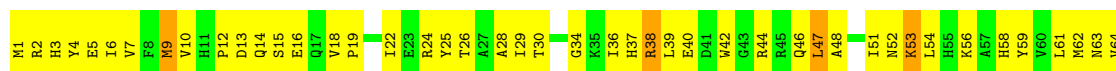
• Molecule 35: 30S ribosomal protein S5

Chain 9: 32% 54% 7% • 6%



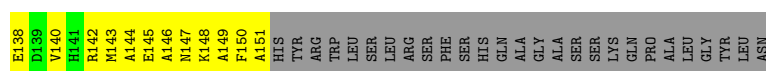
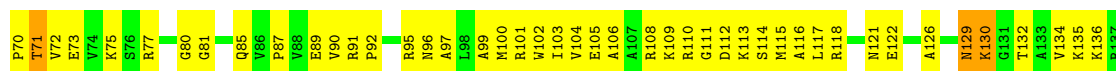
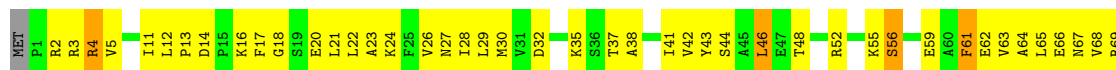
• Molecule 36: 30S ribosomal protein S6

Chain 10: 19% 50% 5% • 26%



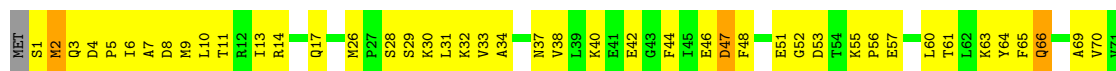
• Molecule 37: 30S ribosomal protein S7

Chain 11: 28% 53% • 16%

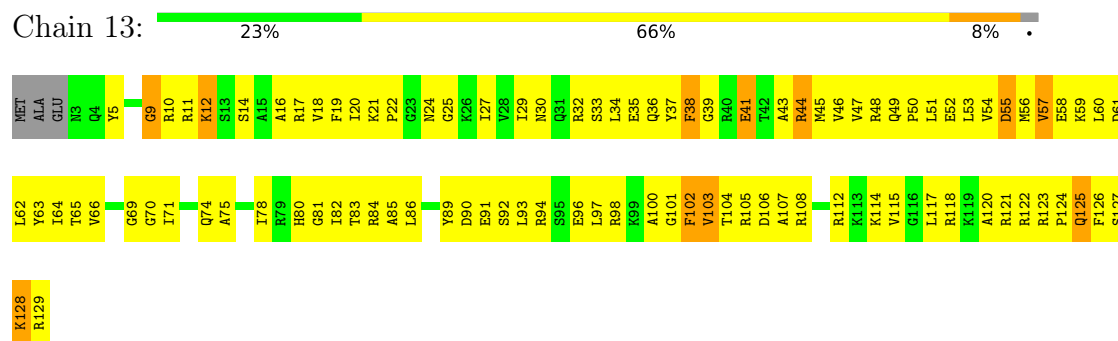


• Molecule 38: 30S ribosomal protein S8

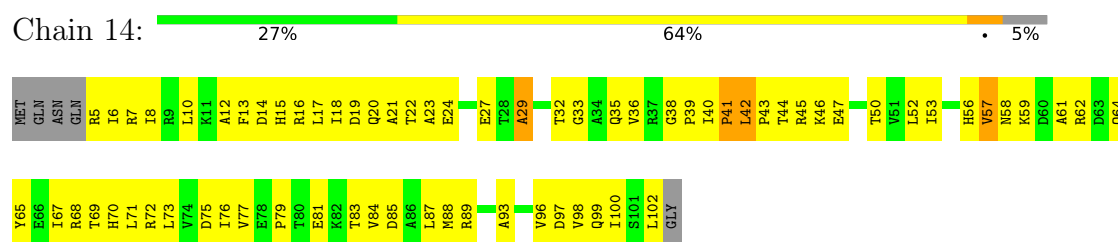
Chain 12: 41% 53% 5% •



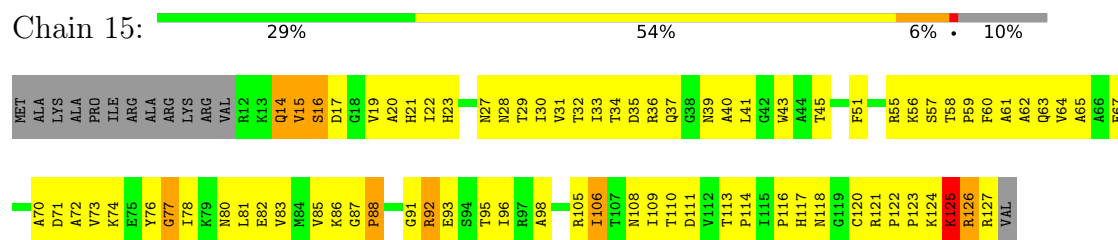
- Molecule 39: 30S ribosomal protein S9



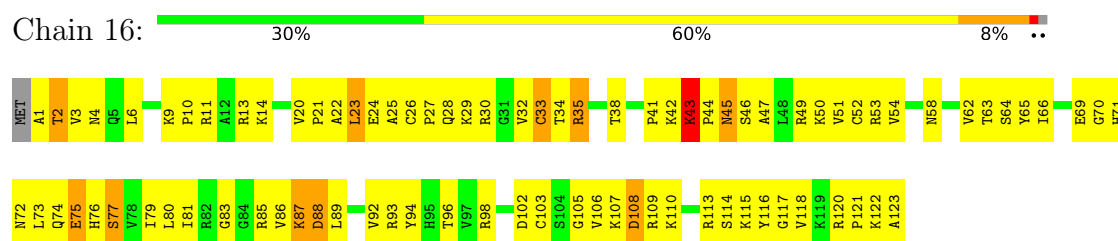
- Molecule 40: 30S ribosomal protein S10



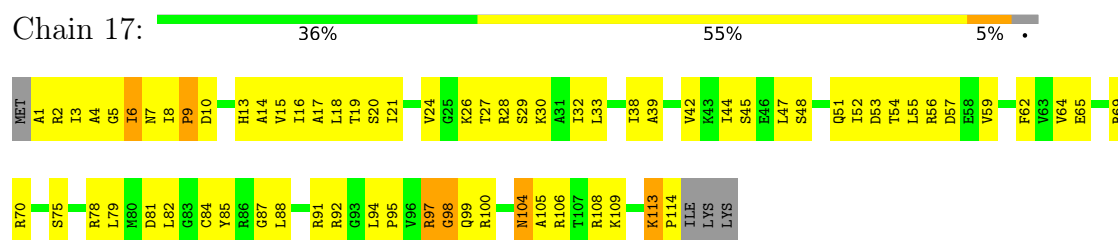
- Molecule 41: 30S ribosomal protein S11



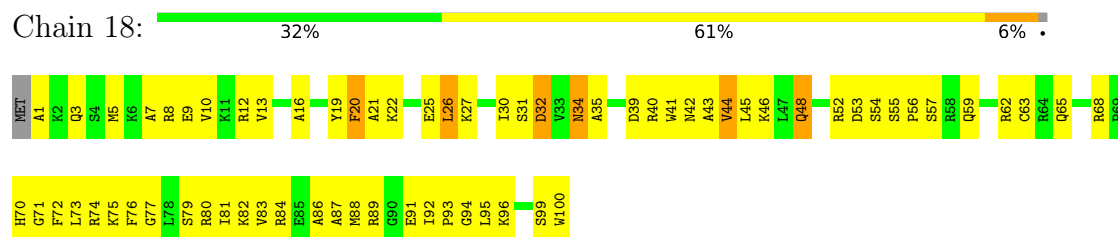
- Molecule 42: 30S ribosomal protein S12



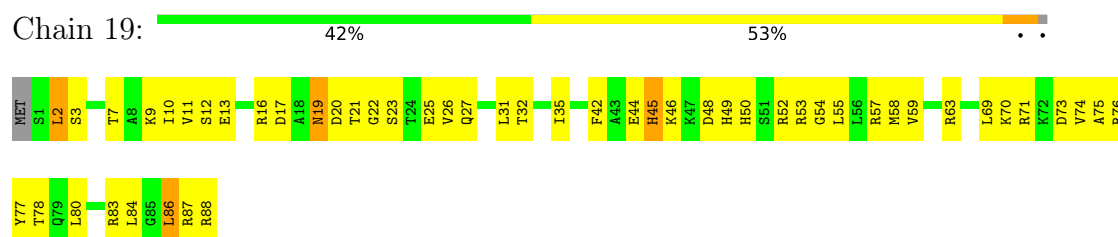
- Molecule 43: 30S ribosomal protein S13



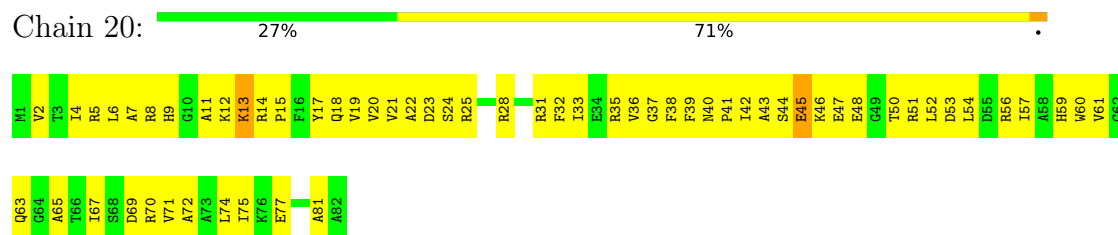
- Molecule 44: 30S ribosomal protein S14



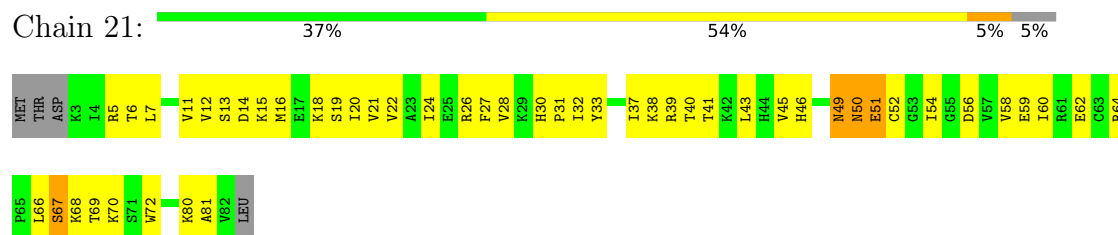
- Molecule 45: 30S ribosomal protein S15



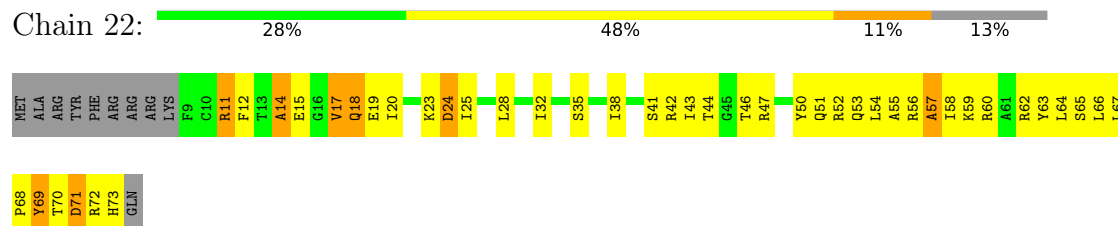
- Molecule 46: 30S ribosomal protein S16



- Molecule 47: 30S ribosomal protein S17

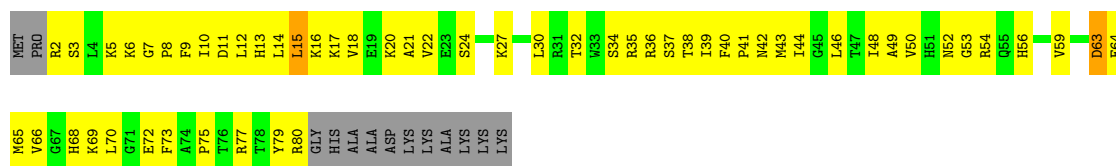


- Molecule 48: 30S ribosomal protein S18



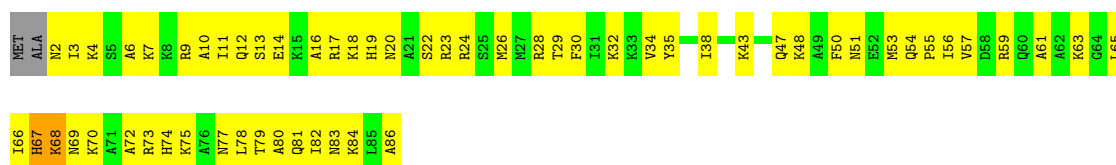
- Molecule 49: 30S ribosomal protein S19

Chain 23: 25% 59% 14%



• Molecule 50: 30S ribosomal protein S20

Chain 24: 30% 66%



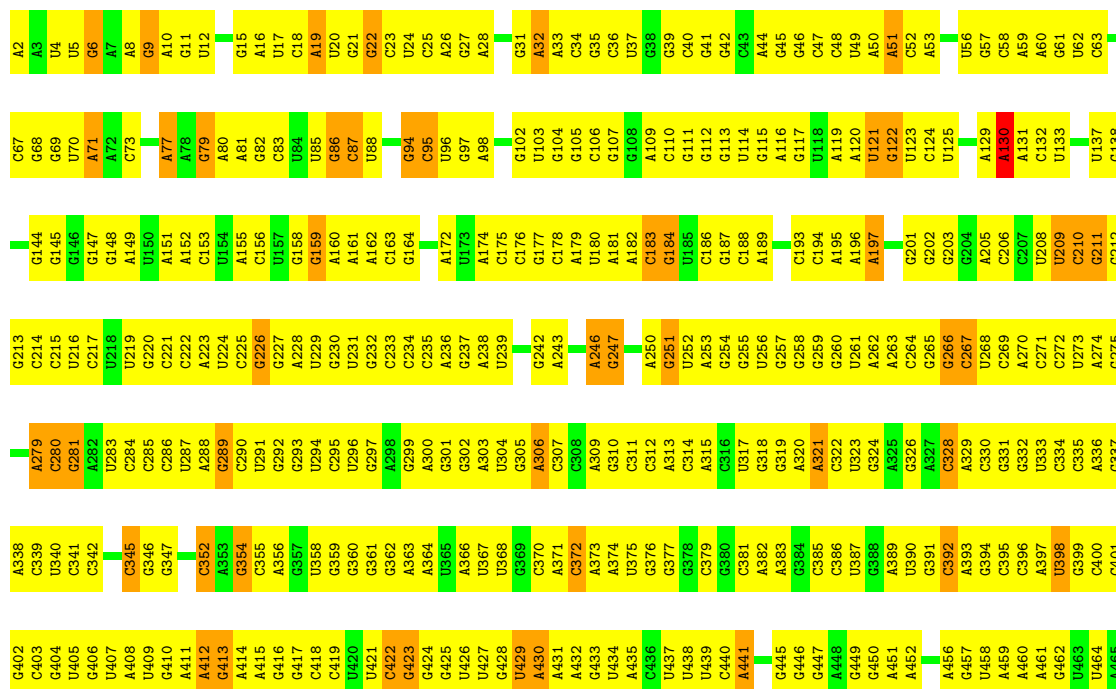
• Molecule 51: 30S ribosomal protein S21

Chain 25: 23% 62% 7% 8%

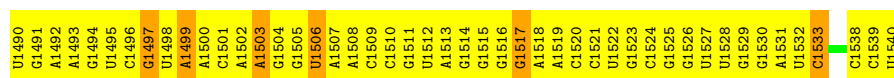


• Molecule 52: 16S ribosomal RNA

Chain 26: 20% 70% 10%

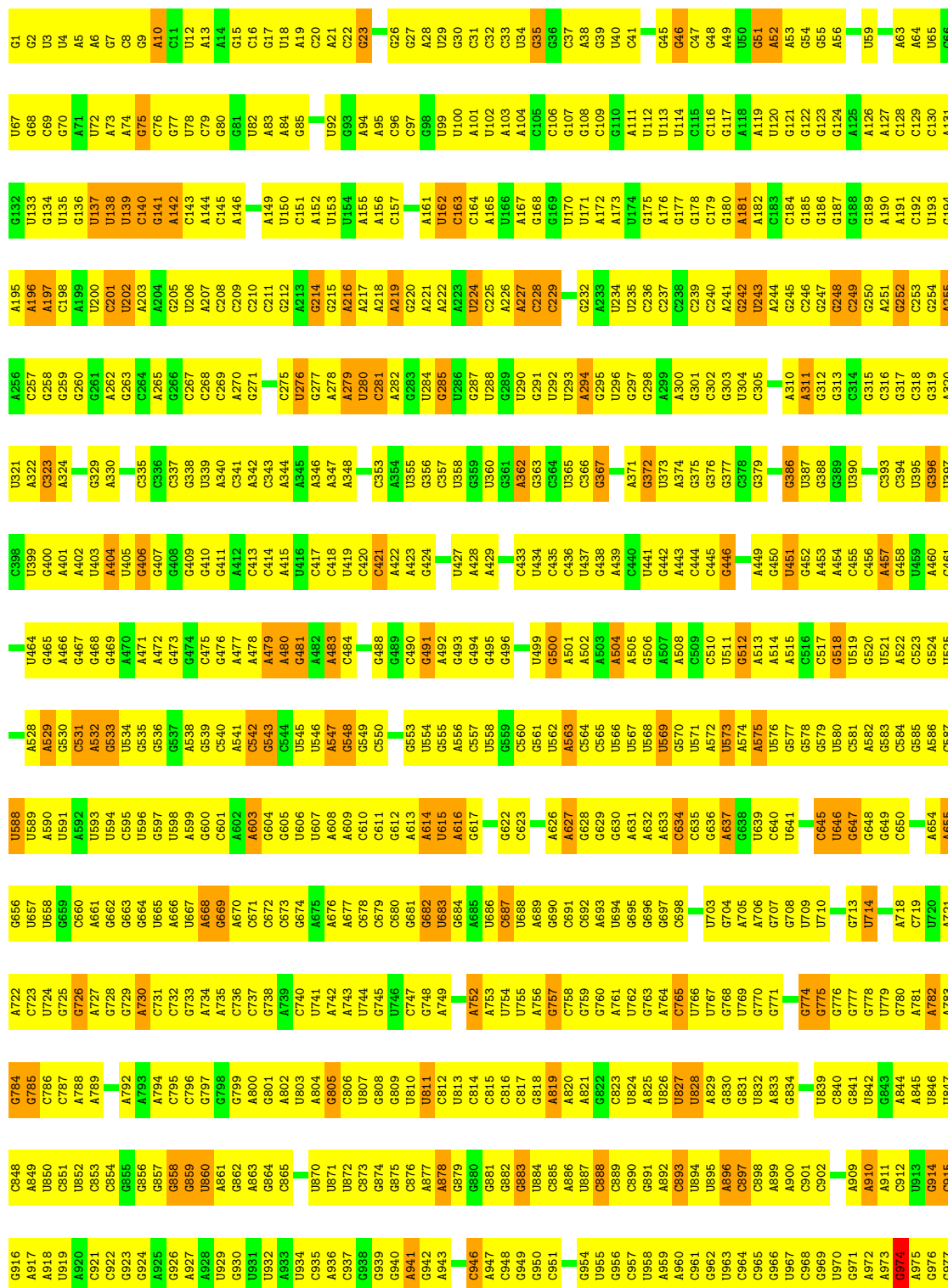




• Molecule 53: 23S ribosomal RNA

Chain 27: 19% 68% 12%

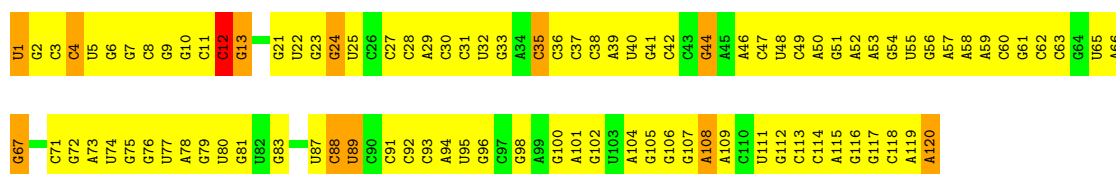


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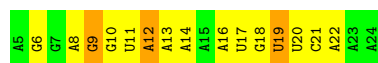
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G2641	G2642	G2643	G2644	G2645	G2646	U2647	G2648	G2649	U2650	C2651	A2654	G2655	U2656	G2659	A2660	G2661	A2662	G2663	G2664	A2665	G2671	U2672	G2673	G2674	A2675	G2676	G2677	G2678	G2679	G2680	C2681	A2682	G2683	U2684	G2685	G2686	U2687	G2688	U2689	U2690	C2691	G2692	G2693	G2694	U2695	U2696	G2697	U2698	G2699	A2700	U2701	G2702	C2703	A2704	A2705							
C2579	U2580	G2581	G2582	G2583	U2584	C2585	U2586	U2587	G2588	A2589	A2590	C2591	G2592	U2593	G2594	G2595	U2596	G2597	A2598	G2599	A2600	C2601	A2602	G2603	U2604	U2605	G2606	G2607	G2608	U2609	G2610	C2611	G2612	U2613	A2614	G2615	C2616	U2617	G2618	C2619	G2620		G2623	G2626	G2627	G2628	U2629	G2630	G2631	U2632	G2633	A2634	U2635	C2636	G2637	A2638	U2639	G2640				
A2516	C2517	A2518	U2519	G2520	C2521	U2522	G2523	G2524	G2525	G2526	C2527	U2528	G2529	A2534	G2535	G2536	U2537	C2538	G2539	A2540	C2541	A2542	G2543	G2544	U2545	G2546	U2547	A2548	G2549	G2550	C2551	U2552	G2553	U2554	G2555	C2556	G2557	G2558	C2559	A2560	U2561	U2562	U2563	A2564	U2565	A2566	U2567	U2568	G2569	U2570	U2571	A2572	C2573	G2574	C2575	U2576	A2577	G2578				
C2452	A2453	G2454	G2455	C2456	U2457	G2458	A2459	U2460	A2461	C2462	U2463	G2464	C2465	C2466	A2468	A2469	G2470	A2471	G2472		C2475	A2476	U2477	A2478	U2479	C2480	U2481	A2482		G2485	U2486	G2487	U2488	U2489	G2490	U2491	U2492	U2493	U2494	U2495		C2498	C2499	U2500	G2501	G2502	A2503	U2504	G2505	U2506	C2507	U2508	G2509		C2512	U2513	A2450	C2515				
U2329	G2330	C2331	U2332	A2333	U2334	A2335	G2336	C2337	C2338	C2339	U2340	C2341	C2342	U2343	U2344	G2345	C2346	C2347	U2348	G2349	C2350	G2351	A2352		G2355	U2356	C2357	A2358	C2359	G2360	G2361	C2362	U2363	G2364	C2365	A2366	G2367	C2368	U2369	G2370	U2371	U2372	C2373	C2374	G2375	U2376	A2377	U2378	G2379	C2380	A2381	U2382	G2383	U2384	C2385	A2386	U2387	G2388	C2389			
U2262	C2263	C2264	U2265	A2266	A2267	A2268		G2271	U2272	A2273		G2277	A2278		C2283	C2284	C2285	G2286	A2287	A2288	G2289	A2290	U2291	U2292	C2293	G2294	C2295	U2296	A2297	A2298	U2299	C2300	C2301	A2302	G2303	G2304	U2305		G2308	A2309	C2310		A2314	G2315	U2316	U2317	A2318	G2319	U2320	U2321	A2322	G2323	U2324	C2325	A2326	U2327	G2328	A2329	C2330			
A2199	C2200	G2201	U2202	A2203	G2204		C2208	G2209	U2210	C2211	A2212	U2213	C2214	C2215	U2216	G2217	U2218	U2219	U2220	G2221	C2222	G2223	G2224	A2225	C2226	A2227	C2228	U2229	G2230	U2231	C2232	U2233	U2234	U2235	U2236	U2237	U2238	U2239	U2240	A2241	G2242	U2243	U2244	U2245	G2246	A2247	C2248	U2249	G2250	G2251	G2252	U2253	C2254	A2255	U2256	C2257	U2258	C2259	U2260	C2261		
U2132	G2133	A2134	U2135	G2136	U2137		G2144	C2145	C2146	A2147	G2148	U2149		G2152	C2153	A2154	U2155	G2156	C2157	A2158	G2159	C2160	G2161	A2162	A2163	C2164	C2165	U2166	U2167	G2168	A2169	C2170	A2171	U2172	A2173	C2174	C2175	A2176	C2177	C2178	C2179		U2182	A2183	A2184	U2185	U2186	G2187	U2188	G2189	G2190	A2191	U2192	G2193	A2194	U2195	C2196	U2197	U2198	U2199	U2200	
A2009	G2010	U2011	G2012	A2013	A2014	A2015	U2016	U2017	G2018	A2019	A2020	C2021	U2022	C2023	G2024	G2025	U2026	G2027	U2028	G2029	A2030	A2031		U2034	G2035	C2036	A2037	G2038	U2039	G2040	U2041	A2042	C2043	C2044	C2045	G2046	G2047	G2048	G2049	C2050	A2051	A2052	G2053	A2054	C2055	G2056	G2057	A2058	A2059	A2060	G2061	A2062	C2063	G2064	G2065	C2066	U2067	U2068	G2069			

• Molecule 54: 5S ribosomal RNA

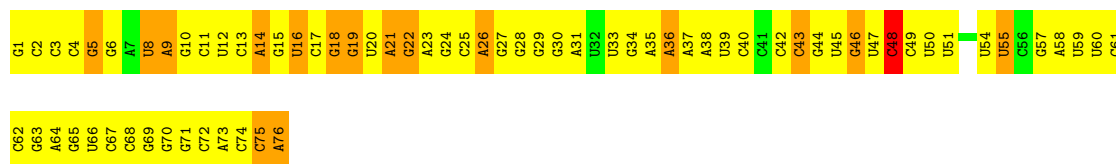
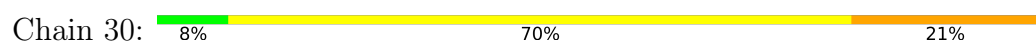
Chain 28:  20% 70% 90%



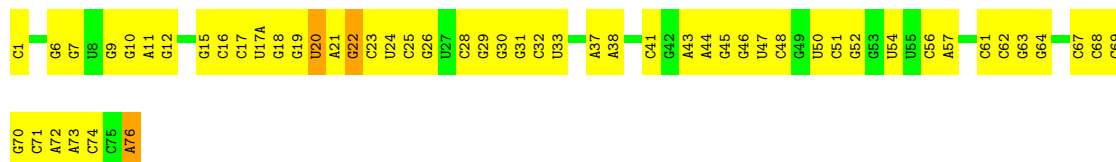
- Molecule 55: mRNA



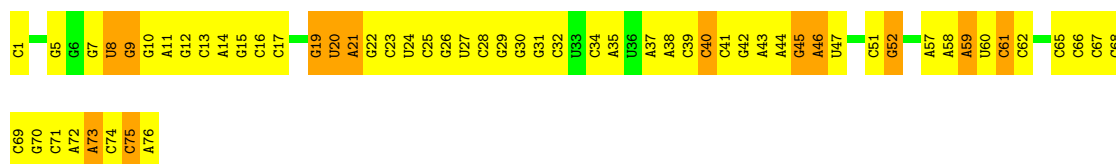
- Molecule 56: A-site tRNA^{Phe}



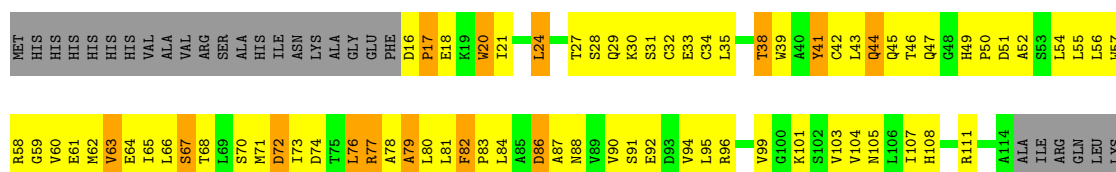
- Molecule 57: P-site tRNA^{fMet}



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



- Molecule 59: GTP pyrophosphokinase



G723	R724	V725	L726	G727	K728	L729	W730	Q731	V732	P733	D734	W735	I736	D737	A738	R739	R740	L741	H742	GLY	SER																																					
SER	ALA	G664	Y665	S666	L605	N606	V668	V669	R670	V671	A672	N673	D674	R675	S676	G677	G678	L680	R681	D682	I683	T684	T685	E686	L687	E688	N689	E690	K691	G694	L695	G696	V697	A698	S699	R700	S701	D702	T703	K704	Q705	Q706	L707	A708	T709	I710	D711	H712	T713	I714	E715	T716	Y717	N718	L719	Q720	V721	L722
E600	G601	N604	L605	N606	H607	H608	I609	A610	R611	C612	C613	Q614	P615	I616	P617	G618	D619	E620	I621	V633	H634	R635	A636	D637	C638	E639	Q640	L641	A642	E643	L644	R645	S646	H647	A648	P649	E650	R651	I652	V653	D654	A655	V656	H657	G658	E659	SER	TYR										
K491	A494	W495	F496	R497	R501	D514	I521	S522	E527	L531	P532	R533	D540	A544	I551	N554	N565	K566	A569	Q572	D573	A576	L577	L580	Q581	GLN	LYS	SER	Y585	T586	P587	R590	R596	V597	V598	V599																						
P419	A420	G421	S422	P424	F427	A428	Y429	H430	I431	H432	S433	D434	V435	G436	H437	R438	C439	A442	K443	I444	G445	G446	R447	I448	F451	T452	Y453	G458	D459	Q460	T461	E462	I463	T465	Q466	K467	Q468	P469	M470	S471	A472	R473	M477	P478	M479	Y482	V483	T484	T485	S486	R487							
E336	I336	Q337	I338	T340	K341	Q342	M343	V351	ALA	ALA	HIS	TRP	LYS	TYR	LYS	GLU	G360	S368	E371	I374	A382	TRP	GLN	H297	T298	H299	Y300	R301	L302	L303	P304	D305	E306	F307	LEU	ASP	GLU	VAL	ARG	SER	GLN	VAL	PHE	ASP	D404	R405	V406	Y407	V408	F409	T410	P411	D417	L418				
Q264	L194	K195	W196	E197	L198	E199	D200	Y201	C202	F203	R204	Y205	L206	E210	Y211	I214	A215	L218	H219	F146	E220	R221	D224	R225	E226	H227	L153	Y228	I229	E230	E231	F232	V233	G234	H235	L236	R237	A238	E239	M240	K241	A242	E243	G244	L173	V245	K246	A247	E248	V249	Y250	G251	R252	I259	W260	M263		
ALA	THR	HIS	THR	ASP	SER	VAL	SER	SER	GLU	Q131	V132	D133	N134	V135	R136	E137	M138	V143	D144	D145	F146	R147	C148	V149	V150	I151	K152	L153	A154	E155	R156	I157	A158	H159	L160	R161	E162	V163	K164	D169	E170	R171	V172	L173	A174	A175	K176	E177	C178	T179	N180	I181	Y182	A183	P184	I191		

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	46935	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.6	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	30488	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	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	0.34	0/2121	0.71	0/2852
10	J	0.32	0/947	0.68	0/1268
11	K	0.34	0/1054	0.71	1/1403 (0.1%)
12	L	0.36	0/1093	0.64	0/1460
13	M	0.35	0/973	0.65	1/1301 (0.1%)
14	N	0.33	0/902	0.63	0/1209
15	O	0.35	0/929	0.67	0/1242
16	P	0.38	0/960	0.60	0/1278
17	Q	0.36	0/829	0.79	1/1107 (0.1%)
18	R	0.32	0/864	0.67	0/1156
19	S	0.34	0/744	0.76	0/994
2	B	0.37	0/1586	0.70	0/2134
20	T	0.35	0/787	0.68	0/1051
21	U	0.35	0/766	0.66	1/1025 (0.1%)
22	V	0.39	0/582	0.68	0/769
23	W	0.34	0/635	0.65	0/848
24	X	0.32	0/510	0.62	0/677
25	Y	0.33	0/453	0.68	0/605
26	Z	0.40	0/531	0.76	0/709
27	1	0.31	0/450	0.71	0/599
28	2	0.38	0/416	0.68	0/554
29	3	0.39	0/380	0.67	0/498
3	C	0.39	0/1571	0.70	0/2113
30	4	0.35	0/513	0.62	0/676
31	5	0.33	0/303	0.74	0/397
32	6	0.40	0/1735	0.67	1/2338 (0.0%)
33	7	0.35	0/1651	0.64	0/2225
34	8	0.33	0/1665	0.68	2/2227 (0.1%)
35	9	0.33	0/1169	0.67	0/1573
36	10	0.35	0/835	0.75	1/1128 (0.1%)
37	11	0.32	0/1195	0.62	0/1602
38	12	0.35	0/989	0.70	0/1326
39	13	0.35	0/1034	0.71	0/1375
4	D	0.35	0/1434	0.62	0/1926

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
40	14	0.35	0/796	0.71	1/1077 (0.1%)
41	15	0.36	0/885	0.73	1/1195 (0.1%)
42	16	0.36	0/969	0.76	1/1300 (0.1%)
43	17	0.31	0/892	0.70	0/1193
44	18	0.46	0/817	0.61	0/1088
45	19	0.32	0/722	0.58	0/964
46	20	0.37	0/659	0.71	0/884
47	21	0.35	0/657	0.72	0/881
48	22	0.38	0/544	0.62	0/731
49	23	0.36	0/652	0.72	0/877
5	E	0.32	0/1343	0.65	0/1816
50	24	0.33	0/671	0.55	0/888
51	25	0.41	0/550	0.73	1/728 (0.1%)
52	26	0.51	1/36967 (0.0%)	0.72	4/57666 (0.0%)
53	27	0.54	3/69801 (0.0%)	0.72	7/108894 (0.0%)
54	28	0.41	1/2876 (0.0%)	0.71	1/4483 (0.0%)
55	29	0.97	0/486	0.74	0/757
56	30	0.65	1/1813 (0.1%)	0.77	0/2823
57	31	0.44	1/1836 (0.1%)	0.70	0/2859
58	32	0.89	2/1835 (0.1%)	0.77	1/2857 (0.0%)
59	33	0.65	6/4985 (0.1%)	1.09	37/6770 (0.5%)
6	F	0.40	0/1122	0.66	0/1515
7	G	0.45	0/1001	0.79	3/1350 (0.2%)
8	H	0.42	0/1046	0.79	1/1410 (0.1%)
9	I	0.33	0/1152	0.64	0/1551
All	All	0.50	15/167683 (0.0%)	0.72	66/250202 (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	13
53	27	0	34
56	30	0	1
59	33	0	3
All	All	0	51

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	33	156	ARG	CZ-NH2	-10.66	1.19	1.33
59	33	152	LYS	CD-CE	-7.76	1.31	1.51
53	27	1379	U	O3'-P	-7.76	1.51	1.61
59	33	17	PRO	CA-CB	-7.25	1.39	1.53
52	26	2	A	OP3-P	-7.00	1.52	1.61

The worst 5 of 66 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	33	156	ARG	NE-CZ-NH1	19.76	130.18	120.30
59	33	156	ARG	NH1-CZ-NH2	-13.83	104.19	119.40
59	33	17	PRO	N-CA-CB	-11.16	89.90	103.30
59	33	17	PRO	CA-CB-CG	10.28	124.33	104.80
59	33	63	VAL	CG1-CB-CG2	-9.25	96.11	110.90

There are no chirality outliers.

5 of 51 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
52	26	130	A	Sidechain
52	26	159	G	Sidechain
52	26	266	G	Sidechain
52	26	820	U	Sidechain
52	26	88	U	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	183	0
2	B	1565	0	1616	121	0
3	C	1552	0	1619	137	0
4	D	1410	0	1447	150	0
5	E	1323	0	1374	88	0
6	F	1111	0	1148	83	0
7	G	988	0	1025	124	0
8	H	1032	0	1088	136	0
9	I	1129	0	1162	89	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	J	938	0	1012	90	0
11	K	1045	0	1117	89	0
12	L	1074	0	1157	70	0
13	M	960	0	1000	75	0
14	N	892	0	923	73	0
15	O	917	0	965	78	0
16	P	947	0	1022	94	0
17	Q	816	0	839	90	0
18	R	857	0	922	52	0
19	S	738	0	807	55	0
20	T	779	0	834	79	0
21	U	753	0	780	71	0
22	V	575	0	592	29	0
23	W	625	0	655	45	0
24	X	509	0	543	60	0
25	Y	449	0	491	41	0
26	Z	522	0	521	52	0
27	1	444	0	461	52	0
28	2	409	0	440	20	0
29	3	377	0	418	33	0
30	4	504	0	574	33	0
31	5	302	0	343	30	0
32	6	1704	0	1732	124	0
33	7	1624	0	1699	111	0
34	8	1643	0	1710	168	0
35	9	1156	0	1199	110	0
36	10	817	0	808	98	0
37	11	1181	0	1240	97	0
38	12	979	0	1034	84	0
39	13	1022	0	1070	130	0
40	14	786	0	828	92	0
41	15	869	0	878	89	0
42	16	955	0	1019	118	0
43	17	883	0	944	97	0
44	18	805	0	847	95	0
45	19	714	0	737	54	0
46	20	649	0	666	87	0
47	21	648	0	691	52	0
48	22	535	0	552	54	0
49	23	637	0	665	71	0
50	24	665	0	714	67	0
51	25	544	0	579	80	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
52	26	33016	0	16617	1573	0
53	27	62322	0	31345	2882	0
54	28	2572	0	1302	116	0
55	29	432	0	218	14	0
56	30	1623	0	821	75	0
57	31	1644	0	836	46	0
58	32	1643	0	836	66	0
59	33	4911	0	4550	655	0
All	All	154603	0	105189	8829	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 34.

The worst 5 of 8829 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)
53:27:45:G:H5''	53:27:46:G:H5'	1.22	1.18
59:33:17:PRO:HB3	59:33:39:TRP:NE1	1.57	1.17
7:G:55:VAL:HA	53:27:1084:A:H5'	1.26	1.15
53:27:1702:G:H2'	53:27:1703:G:H5''	1.15	1.14
59:33:24:LEU:HD21	59:33:70:SER:HA	1.19	1.12

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%)	218 (81%)	41 (15%)	10 (4%)	4	32
2	B	207/209 (99%)	172 (83%)	28 (14%)	7 (3%)	4	34
3	C	199/201 (99%)	147 (74%)	32 (16%)	20 (10%)	0	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	175/179 (98%)	143 (82%)	27 (15%)	5 (3%)	5	37
5	E	174/177 (98%)	149 (86%)	20 (12%)	5 (3%)	5	37
6	F	147/149 (99%)	108 (74%)	20 (14%)	19 (13%)	0	5
7	G	129/165 (78%)	93 (72%)	25 (19%)	11 (8%)	1	14
8	H	139/142 (98%)	104 (75%)	25 (18%)	10 (7%)	1	18
9	I	140/142 (99%)	120 (86%)	14 (10%)	6 (4%)	3	29
10	J	120/123 (98%)	97 (81%)	16 (13%)	7 (6%)	2	23
11	K	141/144 (98%)	110 (78%)	20 (14%)	11 (8%)	1	17
12	L	134/136 (98%)	113 (84%)	15 (11%)	6 (4%)	3	28
13	M	118/127 (93%)	91 (77%)	22 (19%)	5 (4%)	3	29
14	N	114/117 (97%)	98 (86%)	15 (13%)	1 (1%)	19	60
15	O	112/115 (97%)	93 (83%)	15 (13%)	4 (4%)	4	33
16	P	115/118 (98%)	103 (90%)	7 (6%)	5 (4%)	3	29
17	Q	101/103 (98%)	77 (76%)	16 (16%)	8 (8%)	1	16
18	R	108/110 (98%)	87 (81%)	15 (14%)	6 (6%)	2	24
19	S	91/100 (91%)	71 (78%)	16 (18%)	4 (4%)	3	28
20	T	100/104 (96%)	79 (79%)	14 (14%)	7 (7%)	1	19
21	U	92/94 (98%)	76 (83%)	11 (12%)	5 (5%)	2	25
22	V	73/85 (86%)	65 (89%)	7 (10%)	1 (1%)	12	51
23	W	75/78 (96%)	67 (89%)	6 (8%)	2 (3%)	5	39
24	X	61/63 (97%)	49 (80%)	7 (12%)	5 (8%)	1	15
25	Y	56/59 (95%)	52 (93%)	4 (7%)	0	100	100
26	Z	64/70 (91%)	47 (73%)	7 (11%)	10 (16%)	0	3
27	1	54/57 (95%)	43 (80%)	6 (11%)	5 (9%)	1	13
28	2	48/55 (87%)	41 (85%)	7 (15%)	0	100	100
29	3	44/46 (96%)	32 (73%)	11 (25%)	1 (2%)	7	42
30	4	62/65 (95%)	51 (82%)	8 (13%)	3 (5%)	2	27
31	5	36/38 (95%)	26 (72%)	5 (14%)	5 (14%)	0	4
32	6	216/241 (90%)	170 (79%)	32 (15%)	14 (6%)	1	21
33	7	204/233 (88%)	175 (86%)	22 (11%)	7 (3%)	4	34
34	8	203/206 (98%)	157 (77%)	30 (15%)	16 (8%)	1	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	9	155/167 (93%)	109 (70%)	33 (21%)	13 (8%)	1	15
36	10	98/135 (73%)	77 (79%)	14 (14%)	7 (7%)	1	19
37	11	149/179 (83%)	123 (83%)	14 (9%)	12 (8%)	1	16
38	12	127/130 (98%)	110 (87%)	8 (6%)	9 (7%)	1	19
39	13	125/130 (96%)	93 (74%)	19 (15%)	13 (10%)	0	10
40	14	96/103 (93%)	76 (79%)	15 (16%)	5 (5%)	2	25
41	15	114/129 (88%)	90 (79%)	13 (11%)	11 (10%)	1	12
42	16	121/124 (98%)	95 (78%)	13 (11%)	13 (11%)	0	9
43	17	112/118 (95%)	88 (79%)	14 (12%)	10 (9%)	1	14
44	18	98/101 (97%)	72 (74%)	21 (21%)	5 (5%)	2	25
45	19	86/89 (97%)	70 (81%)	11 (13%)	5 (6%)	2	23
46	20	80/82 (98%)	59 (74%)	18 (22%)	3 (4%)	3	31
47	21	78/84 (93%)	54 (69%)	19 (24%)	5 (6%)	1	21
48	22	63/75 (84%)	50 (79%)	5 (8%)	8 (13%)	0	6
49	23	77/92 (84%)	64 (83%)	11 (14%)	2 (3%)	6	39
50	24	83/87 (95%)	75 (90%)	6 (7%)	2 (2%)	6	41
51	25	63/71 (89%)	40 (64%)	19 (30%)	4 (6%)	1	22
59	33	663/750 (88%)	557 (84%)	60 (9%)	46 (7%)	1	19
All	All	6509/6970 (93%)	5226 (80%)	879 (14%)	404 (6%)	3	22

5 of 404 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	86	GLU
2	B	102	ALA
3	C	6	LYS
3	C	11	ALA
3	C	57	LYS

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%)	90	95
2	B	164/164 (100%)	164 (100%)	0	100	100
3	C	165/165 (100%)	165 (100%)	0	100	100
4	D	148/150 (99%)	146 (99%)	2 (1%)	69	85
5	E	137/138 (99%)	137 (100%)	0	100	100
6	F	114/114 (100%)	114 (100%)	0	100	100
7	G	100/123 (81%)	100 (100%)	0	100	100
8	H	109/110 (99%)	107 (98%)	2 (2%)	62	82
9	I	116/116 (100%)	116 (100%)	0	100	100
10	J	103/104 (99%)	102 (99%)	1 (1%)	78	89
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%)	78	89
14	N	86/87 (99%)	86 (100%)	0	100	100
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%)	83 (99%)	1 (1%)	74	87
18	R	93/93 (100%)	93 (100%)	0	100	100
19	S	80/84 (95%)	80 (100%)	0	100	100
20	T	83/85 (98%)	82 (99%)	1 (1%)	74	87
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%)	63	83
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%)	50 (98%)	1 (2%)	58	79
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%)	178 (99%)	2 (1%)	76	87
33	7	170/190 (90%)	169 (99%)	1 (1%)	87	93
34	8	172/173 (99%)	172 (100%)	0	100	100
35	9	119/126 (94%)	117 (98%)	2 (2%)	63	83
36	10	87/116 (75%)	85 (98%)	2 (2%)	53	76
37	11	124/147 (84%)	123 (99%)	1 (1%)	83	91
38	12	104/105 (99%)	103 (99%)	1 (1%)	78	89
39	13	105/107 (98%)	104 (99%)	1 (1%)	78	89
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%)	92 (100%)	0	100	100
44	18	83/84 (99%)	80 (96%)	3 (4%)	38	67
45	19	76/77 (99%)	75 (99%)	1 (1%)	71	86
46	20	65/65 (100%)	65 (100%)	0	100	100
47	21	74/78 (95%)	73 (99%)	1 (1%)	69	85
48	22	56/65 (86%)	55 (98%)	1 (2%)	62	82
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%)	54 (98%)	1 (2%)	62	82
59	33	452/635 (71%)	449 (99%)	3 (1%)	85	92
All	All	5303/5698 (93%)	5272 (99%)	31 (1%)	88	93

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
35	9	80	LEU
36	10	47	LEU
59	33	267	ASN
35	9	87	VAL
37	11	61	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 128 such sidechains are listed below:

Mol	Chain	Res	Type
21	U	24	ASN
32	6	177	ASN
51	25	63	ASN
22	V	8	ASN
29	3	29	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
52	26	1538/1539 (99%)	205 (13%)	9 (0%)
53	27	2902/2903 (99%)	447 (15%)	24 (0%)
54	28	119/120 (99%)	14 (11%)	1 (0%)
55	29	19/20 (95%)	5 (26%)	1 (5%)
56	30	75/76 (98%)	19 (25%)	0
57	31	76/77 (98%)	8 (10%)	0
58	32	76/77 (98%)	19 (25%)	1 (1%)
All	All	4805/4812 (99%)	717 (14%)	36 (0%)

5 of 717 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
52	26	4	U
52	26	6	G
52	26	9	G
52	26	19	A
52	26	22	G

5 of 36 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
53	27	859	G
53	27	1801	A
54	28	88	C
53	27	1130	U
53	27	1818	U

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.