



## wwPDB EM Map/Model Validation Report ⓘ

Sep 20, 2016 – 06:32 PM EDT

PDB ID : 5KPS  
EMDB ID: : EMD-8279  
Title : Structure of RelA bound to ribosome in absence of A/R tRNA (Structure I)  
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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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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

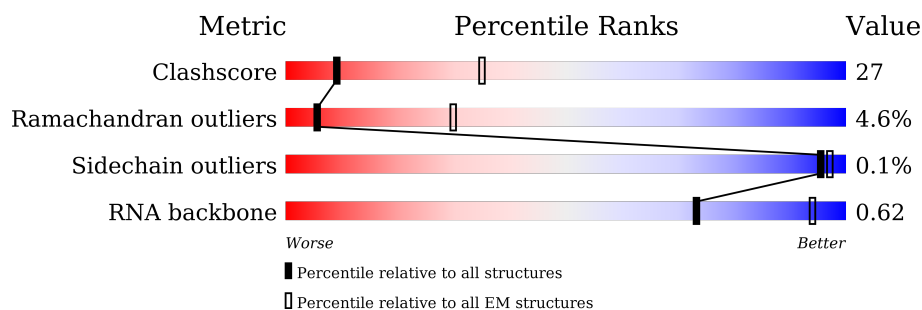
# 1 Overall quality at a glance

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.










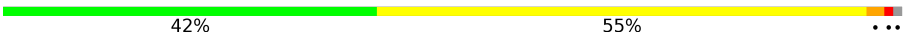

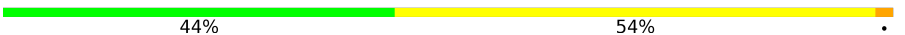
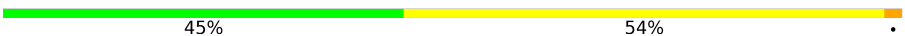
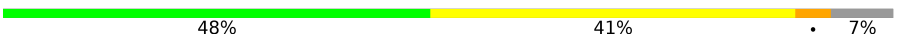
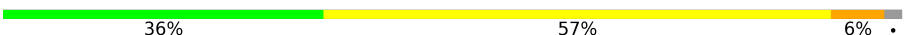












Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

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  $\geq 3$ , 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	750	7% 11% . 81%
2	B	273	47% 51% ..
3	C	209	54% 43% .
4	D	201	43% 52% .
5	E	179	40% 56% ..
6	F	177	41% 58% ..
7	G	149	38% 58% .
8	H	165	30% 42% 7% 21%




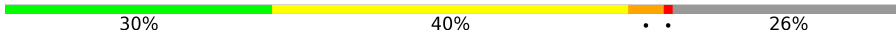
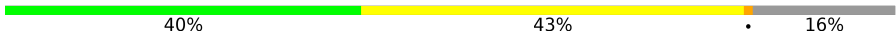

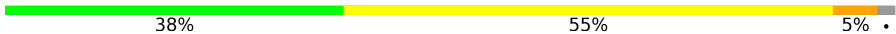
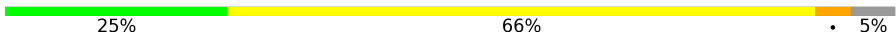
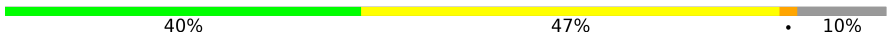
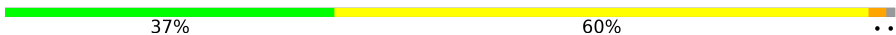
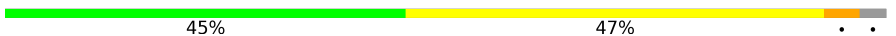
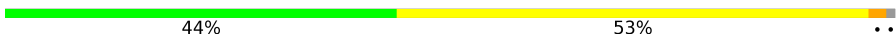
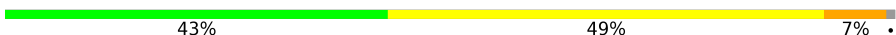
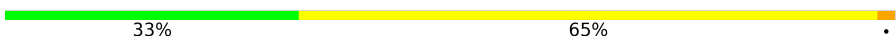










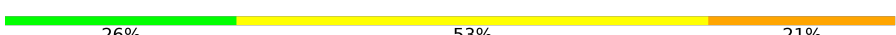
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Mol	Chain	Length	Quality of chain
9	I	142	
10	J	142	
11	K	123	
12	L	144	
13	M	136	
14	N	127	
15	O	117	
16	P	115	
17	Q	118	
18	R	103	
19	S	110	
20	T	100	
21	U	104	
22	V	94	
23	W	85	
24	X	78	
25	Y	63	
26	Z	59	
27	1	70	
28	2	57	
29	3	55	
30	4	46	
31	5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

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Mol	Chain	Length	Quality of chain
34	8	233	
35	9	206	
36	10	167	
37	11	135	
38	12	179	
39	13	130	
40	14	130	
41	15	103	
42	16	129	
43	17	124	
44	18	118	
45	19	101	
46	20	89	
47	21	82	
48	22	84	
49	23	75	
50	24	92	
51	25	87	
52	26	71	
53	27	1539	
54	28	2903	
55	29	120	
56	30	18	
57	31	77	
58	32	77	

## 2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 149128 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 GTP pyrophosphokinase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	143	Total	C	N	O	S	0	0
			1103	685	209	204	5		

There are 7 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is a protein called 50S ribosomal protein L2.

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

- Molecule 3 is a protein called 50S ribosomal protein L3.

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

- Molecule 4 is a protein called 50S ribosomal protein L4.

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

- Molecule 5 is a protein called 50S ribosomal protein L5.

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

- Molecule 6 is a protein called 50S ribosomal protein L6.

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

- Molecule 7 is a protein called 50S ribosomal protein L9.

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

- Molecule 8 is a protein called 50S ribosomal protein L10.

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

- Molecule 9 is a protein called 50S ribosomal protein L11.

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

- Molecule 10 is a protein called 50S ribosomal protein L13.

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

- Molecule 11 is a protein called 50S ribosomal protein L14.

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

- Molecule 12 is a protein called 50S ribosomal protein L15.

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

- Molecule 13 is a protein called 50S ribosomal protein L16.

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

- Molecule 14 is a protein called 50S ribosomal protein L17.

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

- Molecule 15 is a protein called 50S ribosomal protein L18.

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

- Molecule 16 is a protein called 50S ribosomal protein L19.

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

- Molecule 17 is a protein called 50S ribosomal protein L20.

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

- Molecule 18 is a protein called 50S ribosomal protein L21.

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

- Molecule 19 is a protein called 50S ribosomal protein L22.

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

- Molecule 20 is a protein called 50S ribosomal protein L23.

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

- Molecule 21 is a protein called 50S ribosomal protein L24.

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

- Molecule 22 is a protein called 50S ribosomal protein L25.

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

- Molecule 23 is a protein called 50S ribosomal protein L27.

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

- Molecule 24 is a protein called 50S ribosomal protein L28.

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

- Molecule 25 is a protein called 50S ribosomal protein L29.

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

- Molecule 26 is a protein called 50S ribosomal protein L30.



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

- Molecule 27 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	1	66	Total	C	N	O	S	0	0
			522	323	99	94	6		

- Molecule 28 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	2	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 29 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	3	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 30 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	4	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 31 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	5	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 32 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	6	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 33 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	7	218	Total	C	N	O	S	0	0
			1704	1081	305	311	7		

- Molecule 34 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	8	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 35 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	9	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 36 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	10	157	Total	C	N	O	S	0	0
			1156	719	218	213	6		

- Molecule 37 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	11	100	Total	C	N	O	S	0	0
			817	515	148	148	6		

- Molecule 38 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	12	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

- Molecule 39 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	13	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 40 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	14	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 41 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	15	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

- Molecule 42 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	16	116	Total	C	N	O	S	0	0
			869	535	173	158	3		

- Molecule 43 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	17	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 44 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	18	114	Total	C	N	O	S	0	0
			883	546	178	156	3		

- Molecule 45 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	19	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

- Molecule 46 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	20	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 47 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	21	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 48 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	22	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 49 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	23	65	Total	C	N	O	S	0	0
			535	339	100	95	1		

- Molecule 50 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	24	79	Total	C	N	O	S	0	0
			637	408	120	107	2		

- Molecule 51 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	25	85	Total	C	N	O	S	0	0
			665	411	137	114	3		

- Molecule 52 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	26	65	Total	C	N	O	S	0	0
			544	335	117	91	1		

- Molecule 53 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	27	1539	Total	C	N	O	P	0	0
			33016	14725	6052	10700	1539		

- Molecule 54 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	28	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
28	747	C	U	conflict	GB 802133627
28	1847	G	A	conflict	GB 802133627

- Molecule 55 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	29	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
29	120	A	-	conflict	GB 1028475309

- Molecule 56 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	30	18	Total	C	N	O	P	0	0
			388	175	76	120	17		

- Molecule 57 is a RNA chain called P site tRNA<sup>f</sup>met.

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 tRNA<sup>f</sup>Met.

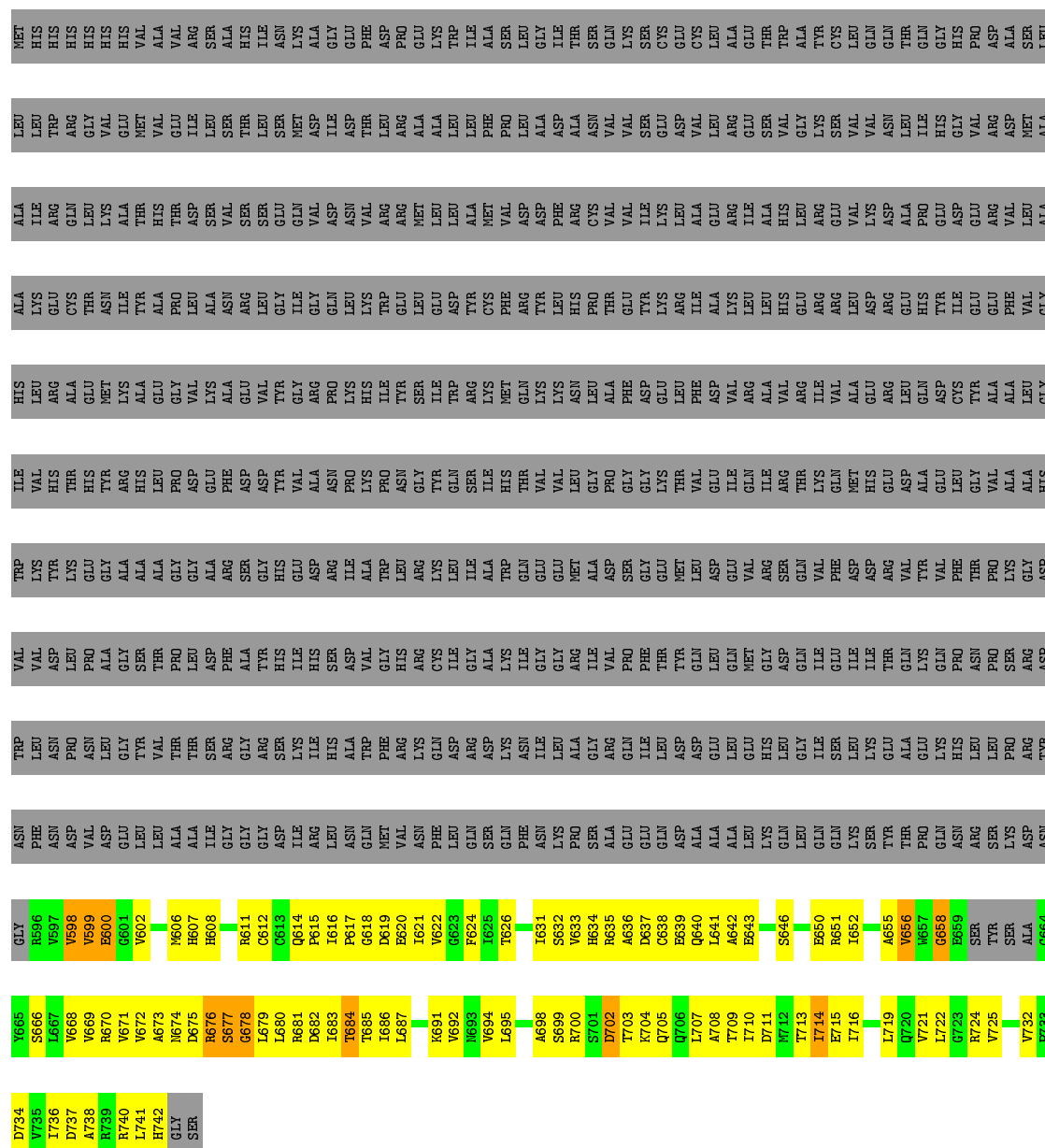
Mol	Chain	Residues	Atoms					AltConf	Trace
58	32	77	Total	C	N	O	P	0	0
			1643	732	297	537	77		

### 3 Residue-property plots

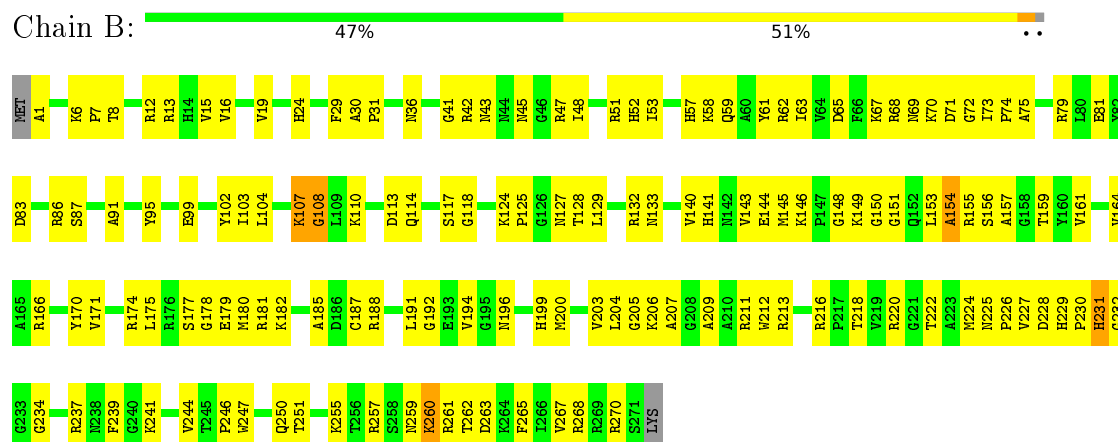
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric 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: GTP pyrophosphokinase

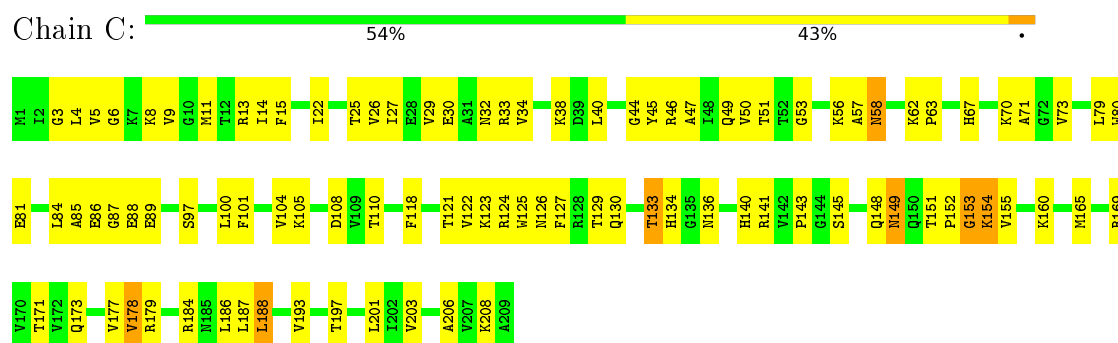
Chain A:  7% 11% . 81%



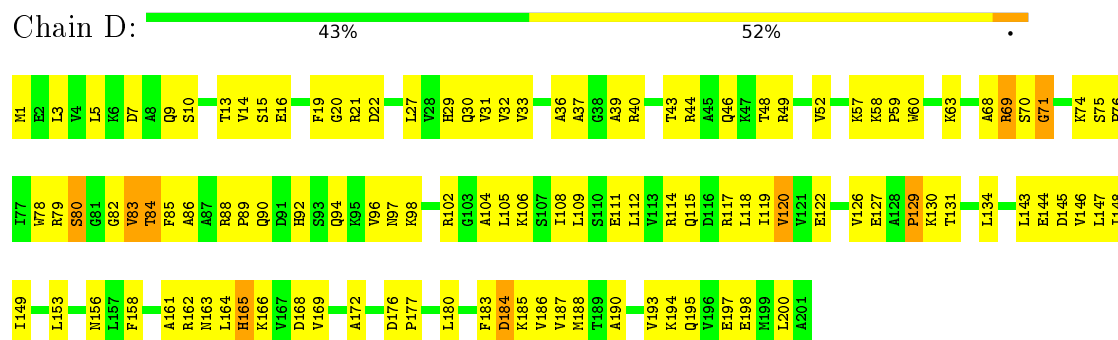
- Molecule 2: 50S ribosomal protein L2



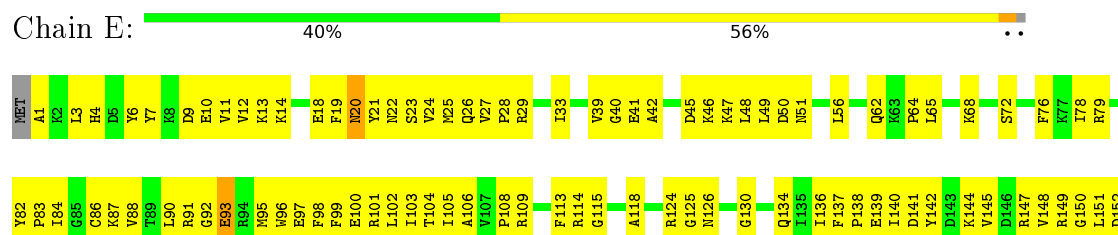
- Molecule 3: 50S ribosomal protein L3



- Molecule 4: 50S ribosomal protein L4



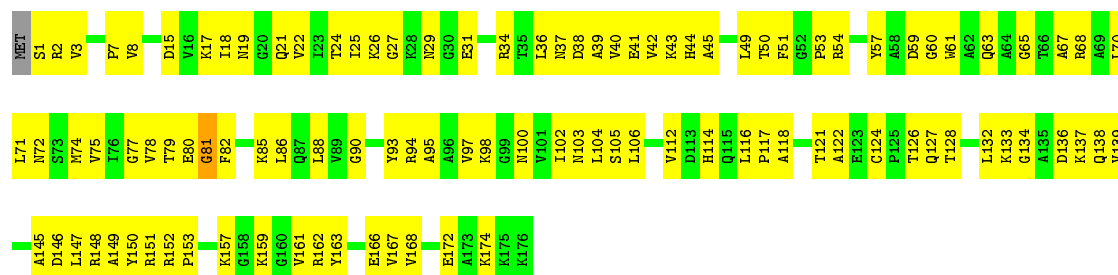
- Molecule 5: 50S ribosomal protein L5





• Molecule 6: 50S ribosomal protein L6

Chain F: 41% 58%



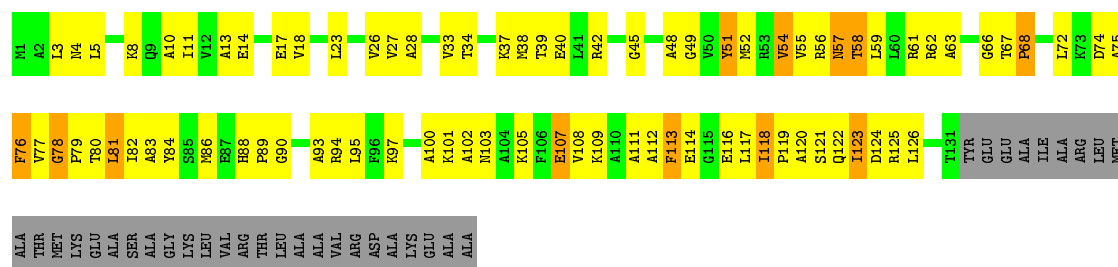
• Molecule 7: 50S ribosomal protein L9

Chain G: 38% 58%



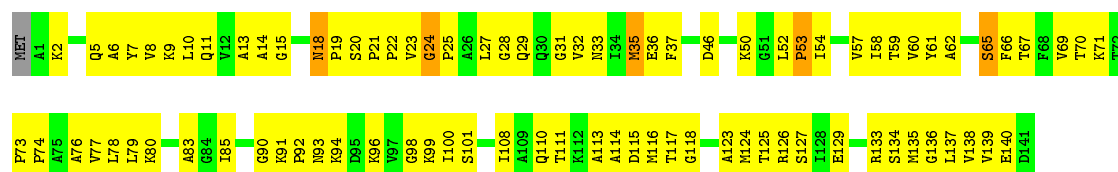
• Molecule 8: 50S ribosomal protein L10

Chain H: 30% 42% 7% 21%



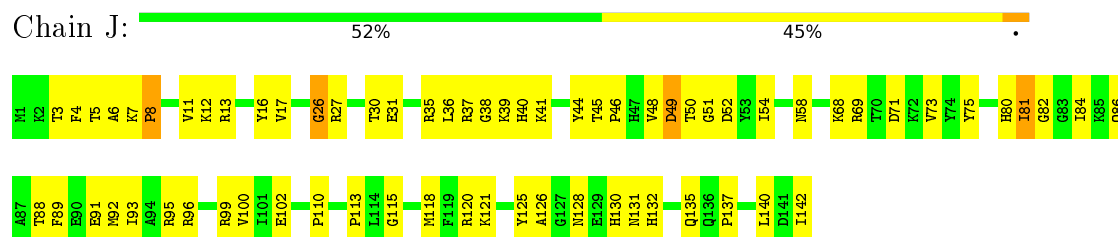
• Molecule 9: 50S ribosomal protein L11

Chain I: 38% 58%

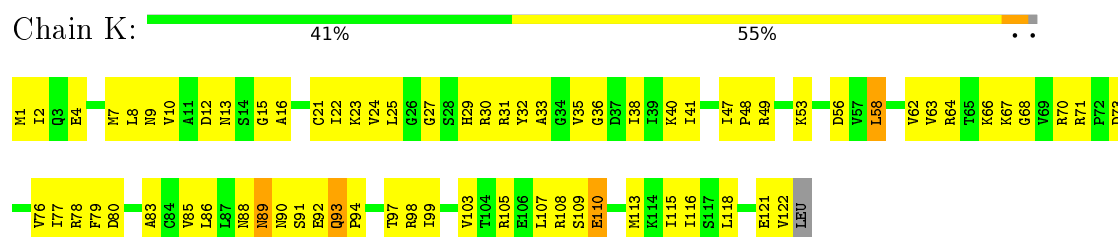




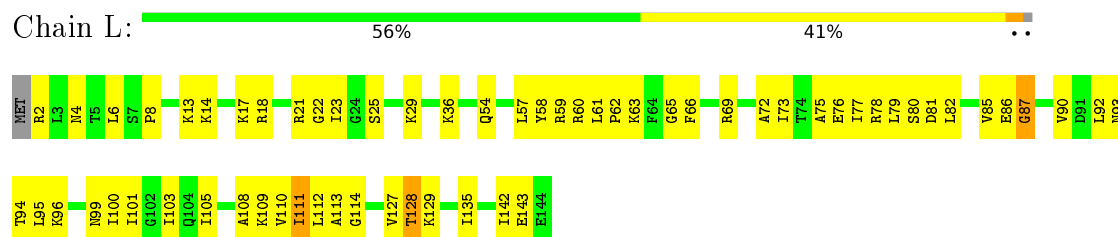
- Molecule 10: 50S ribosomal protein L13



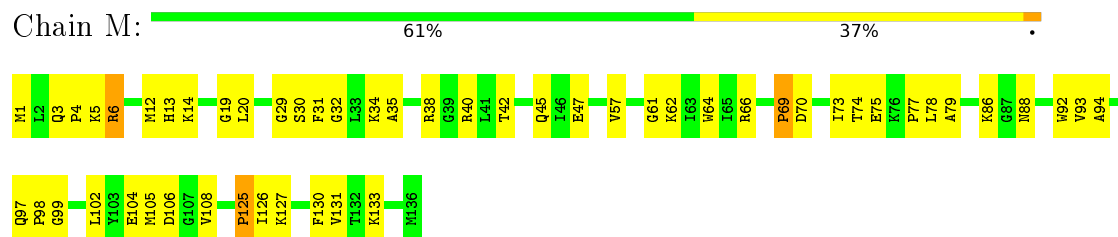
- Molecule 11: 50S ribosomal protein L14



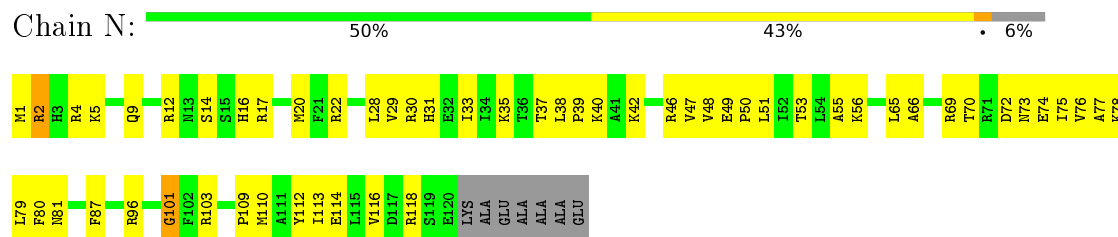
- Molecule 12: 50S ribosomal protein L15



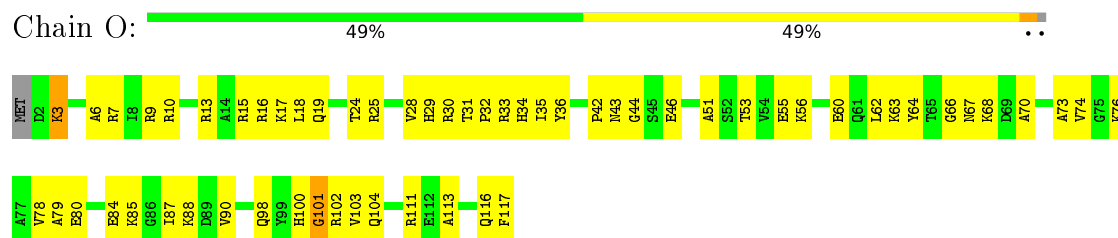
- Molecule 13: 50S ribosomal protein L16



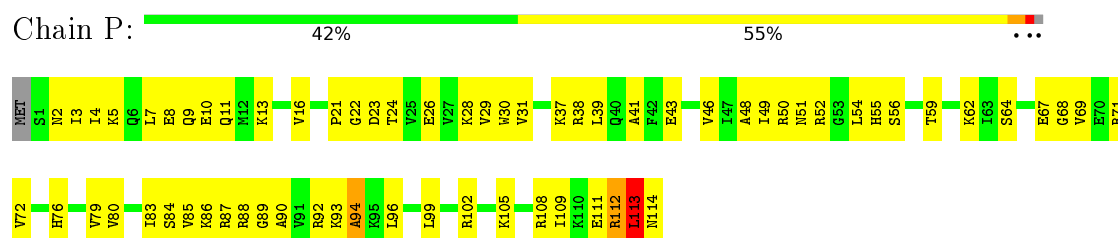
- Molecule 14: 50S ribosomal protein L17



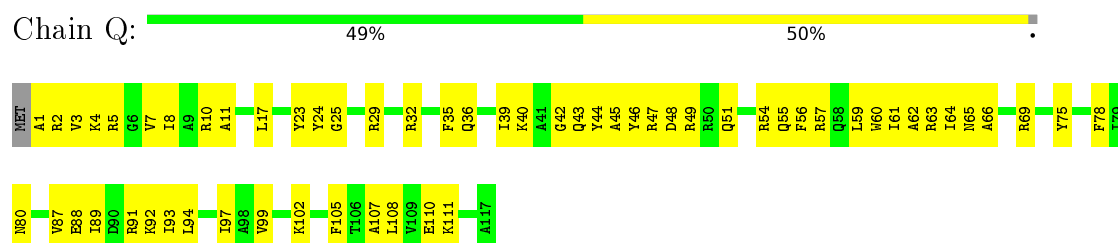
- Molecule 15: 50S ribosomal protein L18



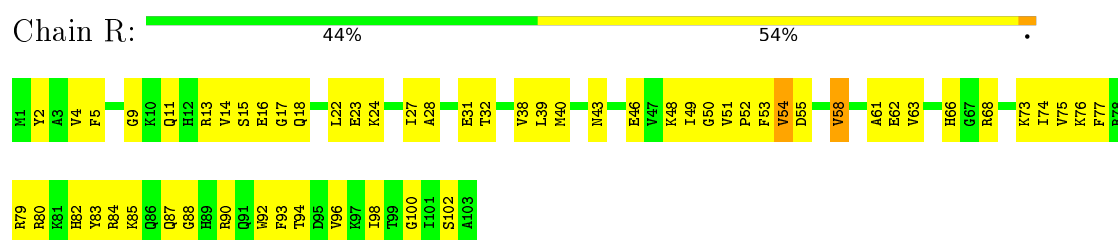
- Molecule 16: 50S ribosomal protein L19



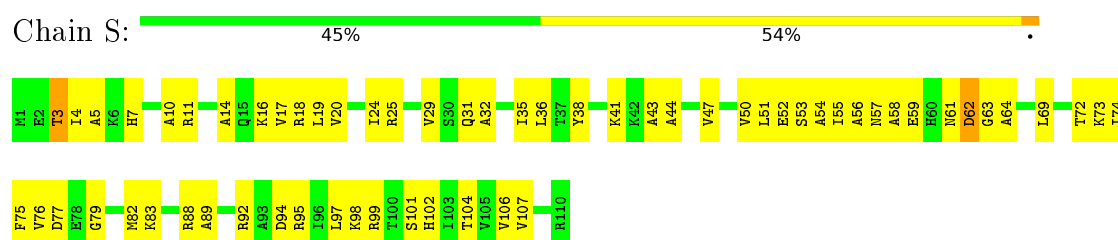
- Molecule 17: 50S ribosomal protein L20



- Molecule 18: 50S ribosomal protein L21

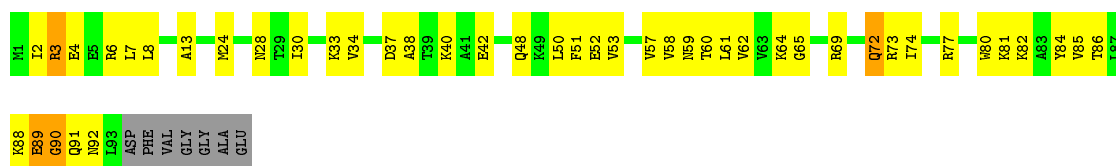


- Molecule 19: 50S ribosomal protein L22



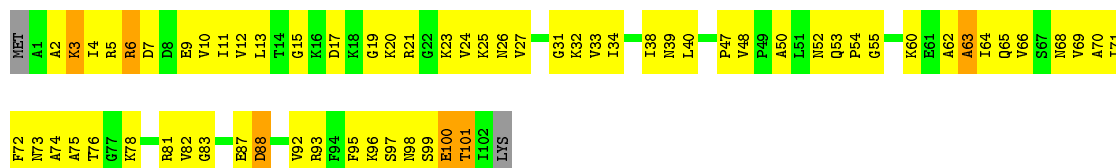
- Molecule 20: 50S ribosomal protein L23





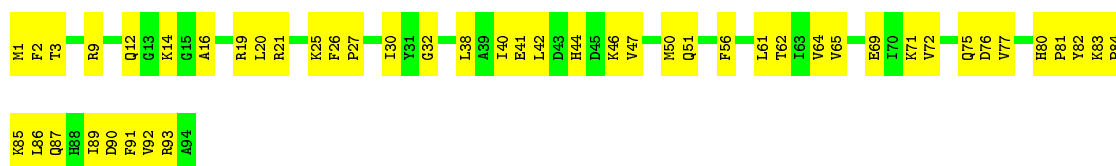
- Molecule 21: 50S ribosomal protein L24

Chain U: 36% 57% 6% .



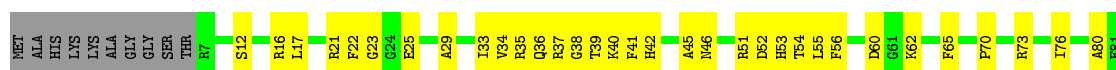
- Molecule 22: 50S ribosomal protein L25

Chain V: 49% 51%



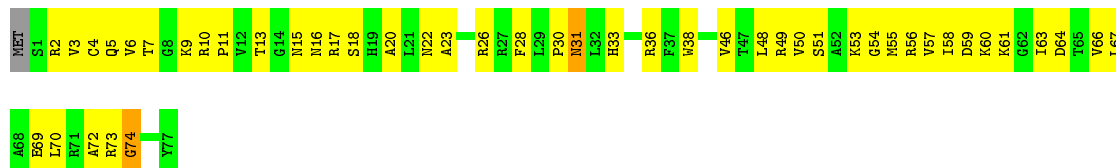
- Molecule 23: 50S ribosomal protein L27

Chain W: 49% 39% 12%



- Molecule 24: 50S ribosomal protein L28

Chain X: 38% 58% . .



- Molecule 25: 50S ribosomal protein L29

Chain Y: 43% 54% .



- Molecule 26: 50S ribosomal protein L30

Chain Z:  53% 44%



- Molecule 27: 50S ribosomal protein L31

Chain 1:  34% 51% 9% 6%



- Molecule 28: 50S ribosomal protein L32

Chain 2:  42% 56%



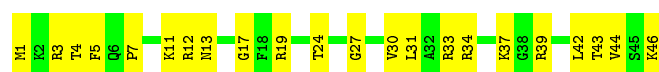
- Molecule 29: 50S ribosomal protein L33

Chain 3:  53% 38% 9%



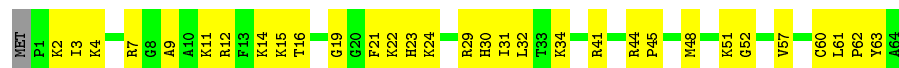
- Molecule 30: 50S ribosomal protein L34

Chain 4:  52% 48%



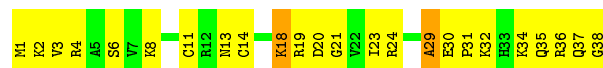
- Molecule 31: 50S ribosomal protein L35

Chain 5:  51% 48%



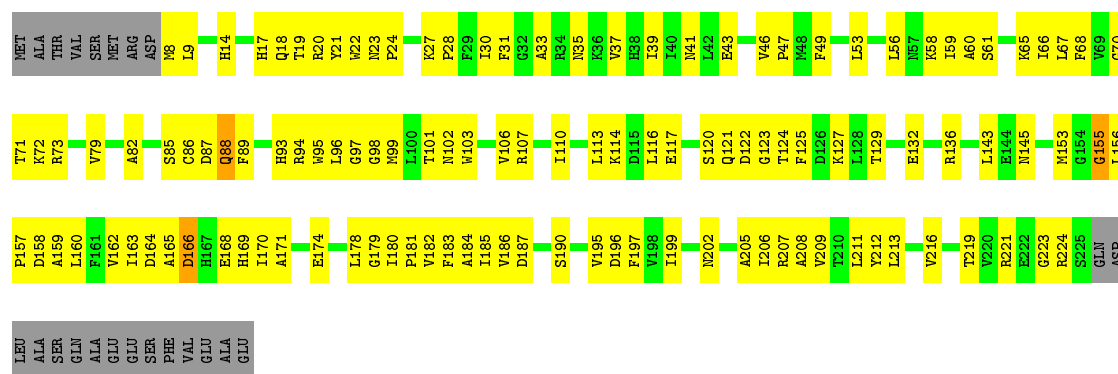
- Molecule 32: 50S ribosomal protein L36

Chain 6:  37% 58% 5%



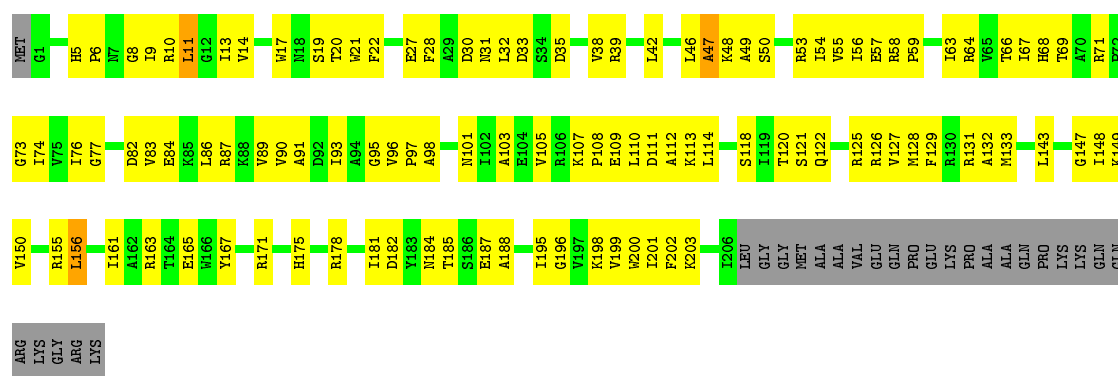
- Molecule 33: 30S ribosomal protein S2

Chain 7:  41% 49% 10%



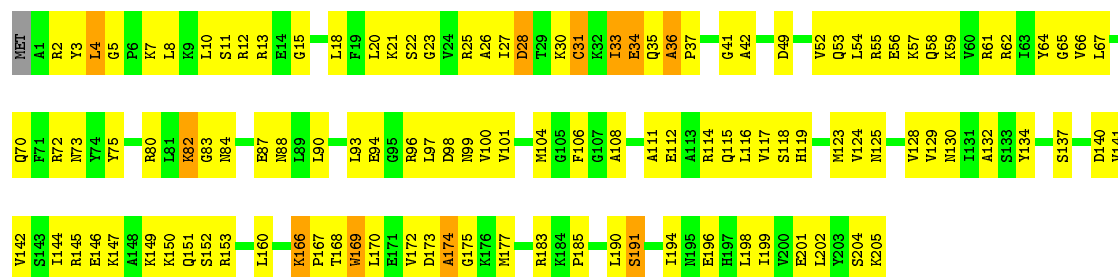
• Molecule 34: 30S ribosomal protein S3

Chain 8: 41% 46% 12%



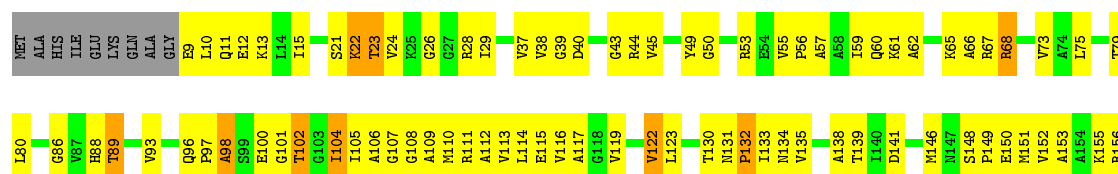
• Molecule 35: 30S ribosomal protein S4

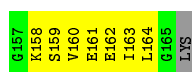
Chain 9: 42% 52% 5%



• Molecule 36: 30S ribosomal protein S5

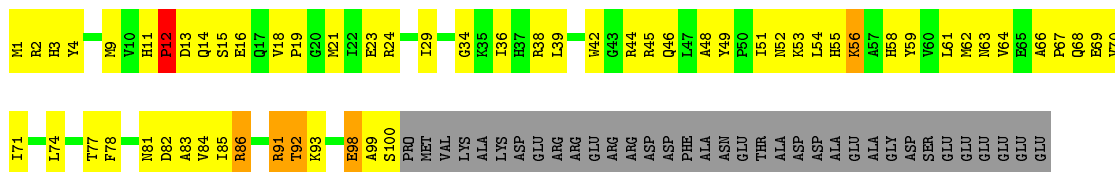
Chain 10: 40% 49% 5% 6%





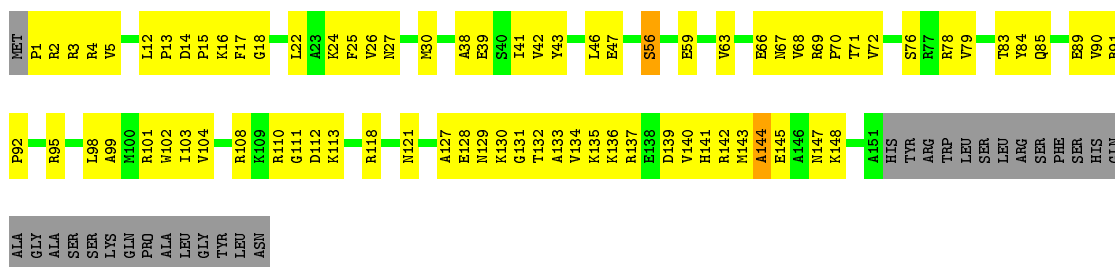
• Molecule 37: 30S ribosomal protein S6

Chain 11: 30% 40% 26%



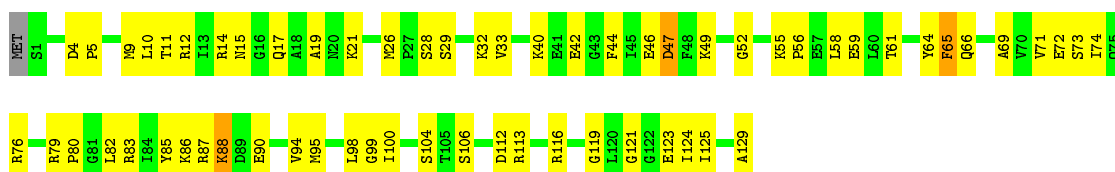
• Molecule 38: 30S ribosomal protein S7

Chain 12: 40% 43% 16%



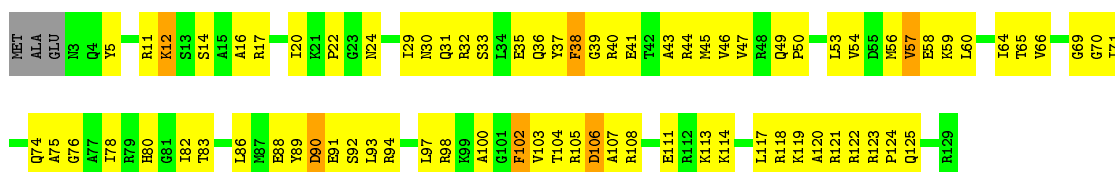
• Molecule 39: 30S ribosomal protein S8

Chain 13: 52% 45%



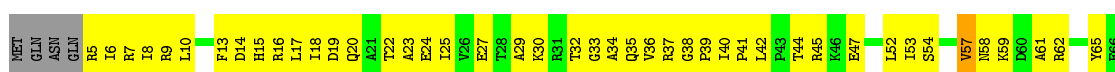
• Molecule 40: 30S ribosomal protein S9

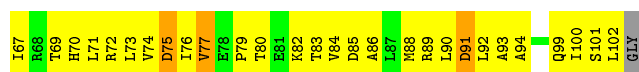
Chain 14: 38% 55% 5%



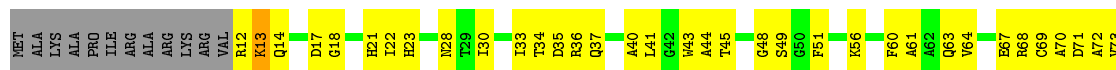
• Molecule 41: 30S ribosomal protein S10

Chain 15: 25% 66% 5%

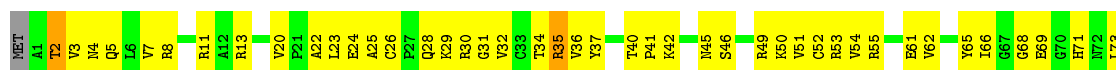




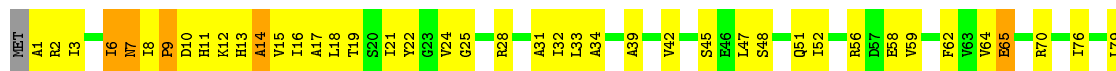
- Molecule 42: 30S ribosomal protein S11



- Molecule 43: 30S ribosomal protein S12



- Molecule 44: 30S ribosomal protein S13



- Molecule 45: 30S ribosomal protein S14



- Molecule 46: 30S ribosomal protein S15





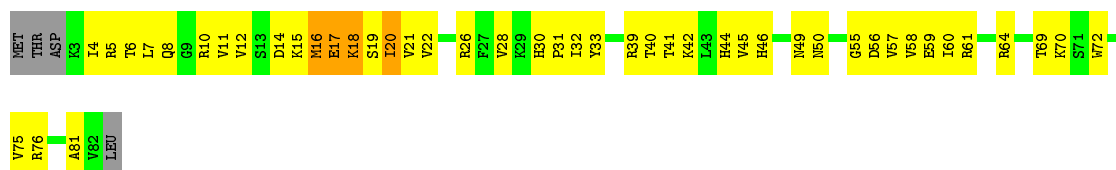
- Molecule 47: 30S ribosomal protein S16

Chain 21: 33% 65%



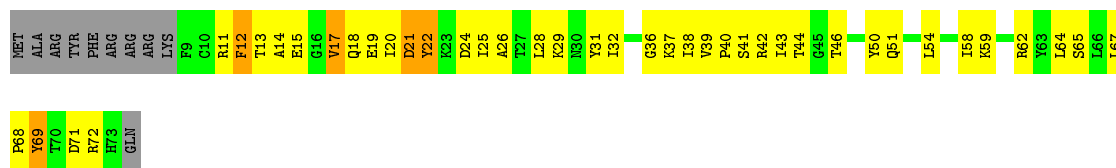
- Molecule 48: 30S ribosomal protein S17

Chain 22: 40% 50% 5% 5%



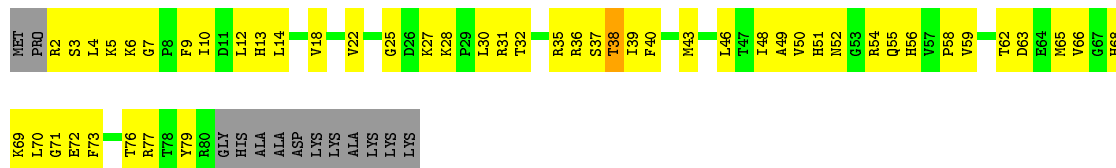
- Molecule 49: 30S ribosomal protein S18

Chain 23: 32% 48% 7% 13%



- Molecule 50: 30S ribosomal protein S19

Chain 24: 32% 53% 14%



- Molecule 51: 30S ribosomal protein S20

Chain 25: 47% 51%



- Molecule 52: 30S ribosomal protein S21

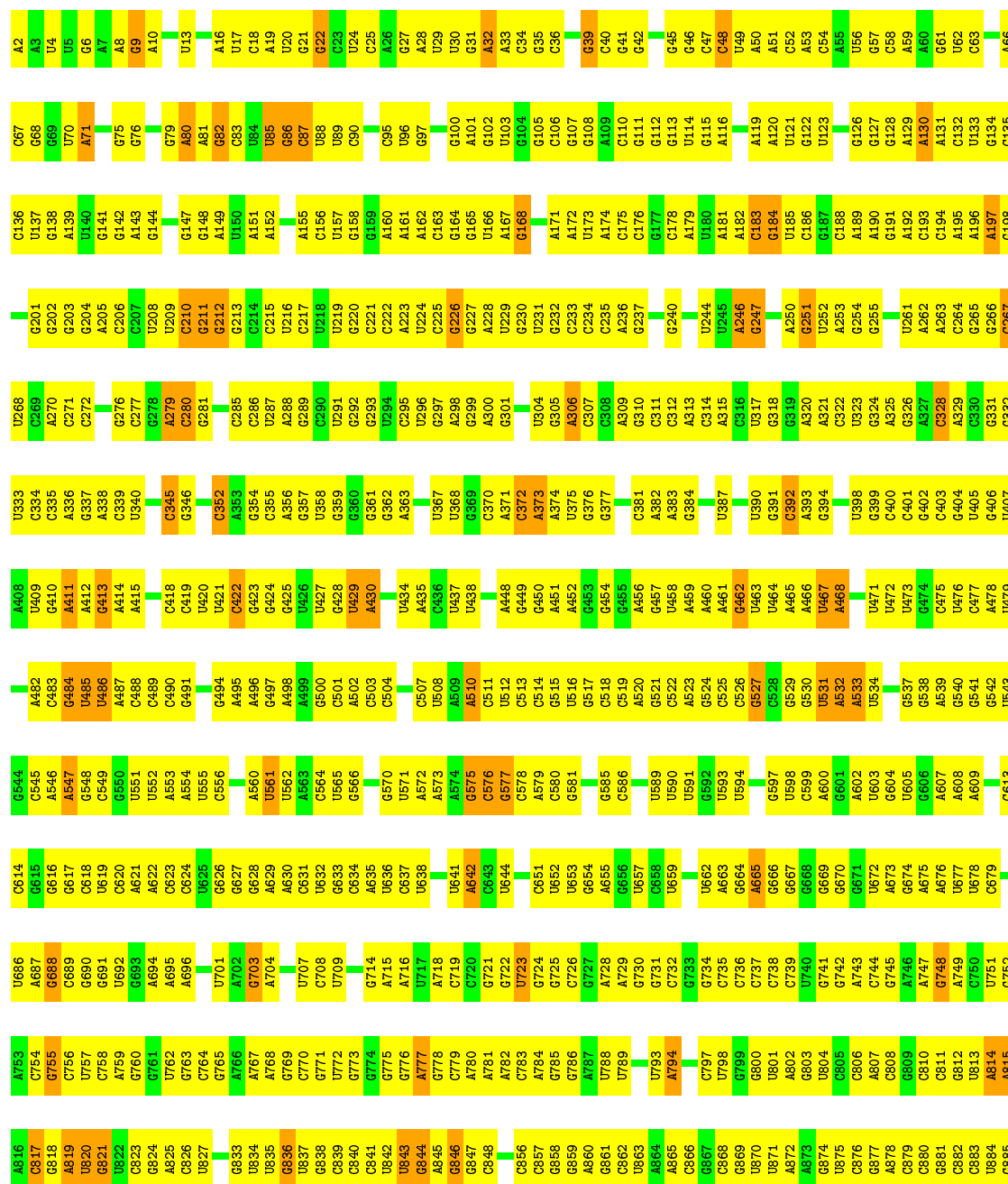


Chain 26:  27% 56% 8% 8%



- Molecule 53: 16S ribosomal RNA

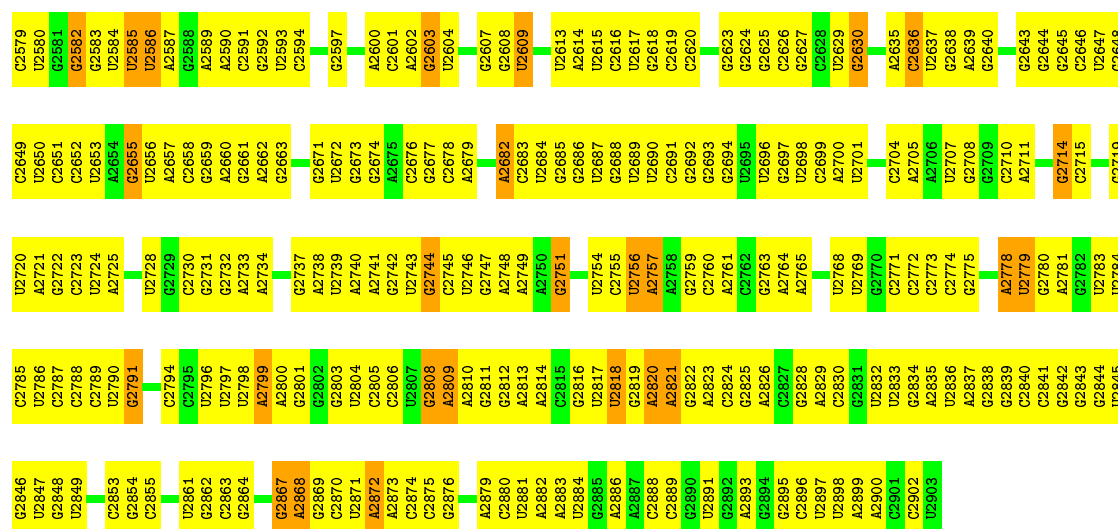
Chain 27:  27% 65% 8%



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U133	U134	U135	U136	U137	U138	U139	U140	U141	U142	U143	U144	U145	U146	U147	U148	U149	U150	U151	U152	U153	U154	U155	U156	U157	U158	U159	U160	U161	U162	U163	U164	U165	U166	U167	U168	U169	U170	U171	U172	U173	U174	U175	U176	U177	U178	U179	U180	U181	U182	U183	U184	U185	U186	U187	U188	U189	U190	U191	U192	U193	U194	U195	U196	U197	U198	U199	U200	U201	U202	U203	U204	U205	U206	U207	U208	U209	U210	U211	U212	U213	U214	U215	U216	U217	U218	U219	U220	U221	U222	U223	U224	U225	U226	U227	U228	U229	U230	U231	U232	U233	U234	U235	U236	U237	U238	U239	U240	U241	U242	U243	U244	U245	U246	U247	U248	U249	U250	U251	U252	U253	U254	U255	U256	U257	U258	U259	U260	U261	U262	U263	U264	U265	U266	U267	U268	U269	U270	U271	U272	U273	U274	U275	U276	U277	U278	U279	U280	U281	U282	U283	U284	U285	U286	U287	U288	U289	U290	U291	U292	U293	U294	U295	U296	U297	U298	U299	U300	U301	U302	U303	U304	U305	U306	U307	U308	U309	U310	U311	U312	U313	U314	U315	U316	U317	U318	U319	U320	U321	U322	U323	U324	U325	U326	U327	U328	U329	U330	U331	U332	U333	U334	U335	U336	U337	U338	U339	U340	U341	U342	U343	U344	U345	U346	U347	U348	U349	U350	U351	U352	U353	U354	U355	U356	U357	U358	U359	U360	U361	U362	U363	U364	U365	U366	U367	U368	U369	U370	U371	U372	U373	U374	U375	U376	U377	U378	U379	U380	U381	U382	U383	U384	U385	U386	U387	U388	U389	U390	U391	U392	U393	U394	U395	U396	U397	U398	U399	U400	U401	U402	U403	U404	U405	U406	U407	U408	U409	U410	U411	U412	U413	U414	U415	U416	U417	U418	U419	U420	U421	U422	U423	U424	U425	U426	U427	U428	U429	U430	U431	U432	U433	U434	U435	U436	U437	U438	U439	U440	U441	U442	U443	U444	U445	U446	U447	U448	U449	U450	U451	U452	U453	U454	U455	U456	U457	U458	U459	U460	U461	U462	U463	U464	U465	U466	U467	U468	U469	U470	U471	U472	U473	U474	U475	U476	U477	U478	U479	U480	U481	U482	U483	U484	U485	U486	U487	U488	U489	U490	U491	U492	U493	U494	U495	U496	U497	U498	U499	U500	U501	U502	U503	U504	U505	U506	U507	U508	U509	U510	U511	U512	U513	U514	U515	U516	U517	U518	U519	U520	U521	U522	U523	U524	U525	U526	U527	U528	U529	U530	U531	U532	U533	U534	U535	U536	U537	U538	U539	U540	U541	U542	U543	U544	U545	U546	U547	U548	U549	U550	U551	U552	U553	U554	U555	U556	U557	U558	U559	U560	U561	U562	U563	U564	U565	U566	U567	U568	U569	U570	U571	U572	U573	U574	U575	U576	U577	U578	U579	U580	U581	U582	U583	U584	U585	U586	U587	U588	U589	U590	U591	U592	U593	U594	U595	U596	U597	U598	U599	U600	U601	U602	U603	U604	U605	U606	U607	U608	U609	U610	U611	U612	U613	U614	U615	U616	U617	U618	U619	U620	U621	U622	U623	U624	U625	U626	U627	U628	U629	U630	U631	U632	U633	U634	U635	U636	U637	U638	U639	U640	U641	U642	U643	U644	U645	U646	U647	U648	U649	U650	U651	U652	U653	U654	U655	U656	U657	U658	U659	U660	U661	U662	U663	U664	U665	U666	U667	U668	U669	U670	U671	U672	U673	U674	U675	U676	U677	U678	U679	U680	U681	U682	U683	U684	U685	U686	U687	U688	U689	U690	U691	U692	U693	U694	U695	U696	U697	U698	U699	U700	U701	U702	U703	U704	U705	U706	U707	U708	U709	U710	U711	U712	U713	U714	U715	U716	U717	U718	U719	U720	U721	U722	U723	U724	U725	U726	U727	U728	U729	U730	U731	U732	U733	U734	U735	U736	U737	U738	U739	U740	U741	U742	U743	U744	U745	U746	U747	U748	U749	U750	U751	U752	U753	U754	U755	U756	U757	U758	U759	U760	U761	U762	U763	U764	U765	U766	U767	U768	U769	U770	U771	U772	U773	U774	U775	U776	U777	U778	U779	U780	U781	U782	U783	U784	U785	U786	U787	U788	U789	U790	U791	U792	U793	U794	U795	U796	U797	U798	U799	U800	U801	U802	U803	U804	U805	U806	U807	U808	U809	U810	U811	U812	U813	U814	U815	U816	U817	U818	U819	U820	U821	U822	U823	U824	U825	U826	U827	U828	U829	U830	U831	U832	U833	U834	U835	U836	U837	U838	U839	U840	U841	U842	U843	U844	U845	U846	U847	U848	U849	U850	U851	U852	U853	U854	U855	U856	U857	U858	U859	U860	U861	U862	U863	U864	U865	U866	U867	U868	U869	U870	U871	U872	U873	U874	U875	U876	U877	U878	U879	U880	U881	U882	U883	U884	U885	U886	U887	U888	U889	U890	U891	U892	U893	U894	U895	U896	U897	U898	U899	U900	U901	U902	U903	U904	U905	U906	U907	U908	U909	U910	U911	U912	U913	U914	U915	U916	U917	U918	U919	U920	U921	U922	U923	U924	U925	U926	U927	U928	U929	U930	U931	U932	U933	U934	U935	U936	U937	U938	U939	U940	U941	U942	U943	U944	U945	U946	U947	U948	U949	U950	U951	U952	U953	U954	U955	U956	U957	U958	U959	U960	U961	U962	U963	U964	U965	U966	U967	U968	U969	U970	U971	U972	U973	U974	U975	U976	U977	U978	U979	U980	U981	U982	U983	U984	U985	U986	U987	U988	U989	U990	U991	U992	U993	U994	U995	U996	U997	U998	U999	U1000	U1001	U1002	U1003	U1004	U1005	U1006	U1007	U1008	U1009	U1010	U1011	U1012	U1013	U1014	U1015	U1016	U1017	U1018	U1019	U1020	U1021	U1022	U1023	U1024	U1025	U1026	U1027	U1028	U1029	U1030	U1031	U1032	U1033	U1034	U1035	U1036	U1037	U1038	U1039	U1040	U1041	U1042	U1043	U1044	U1045	U1046	U1047	U1048	U1049	U1050	U1051	U1052	U1053	U1054	U1055	U1056	U1057	U1058	U1059	U1060	U1061	U1062	U1063	U1064	U1065	U1066	U1067	U1068	U1069	U1070	U1071	U1072	U1073	U1074	U1075	U1076	U1077	U1078	U1079	U1080	U1081	U1082	U1083	U1084	U1085	U1086	U1087	U1088	U1089	U1090	U1091	U1092	U1093	U1094	U1095	U1096	U1097	U1098	U1099	U1100	U1101	U1102	U1103	U1104	U1105	U1106	U1107	U1108	U1109	U1110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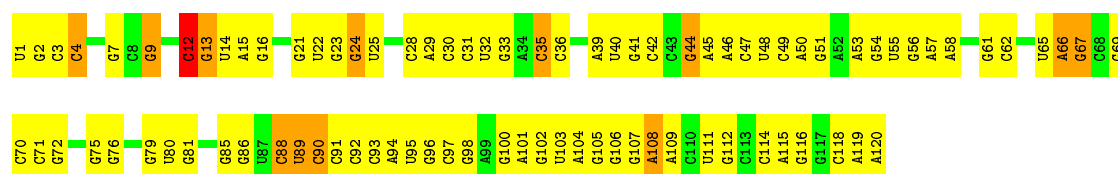



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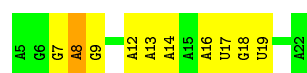
• Molecule 55: 5S ribosomal RNA

Chain 29: 28% 62% 10%



• Molecule 56: mRNA

Chain 30: 44% 50% 6%



• Molecule 57: P site tRNA<sup>fmet</sup>

Chain 31: 45% 53% 2%



• Molecule 58: E-site tRNA<sup>fMet</sup>

Chain 32: 26% 53% 21%



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	76158	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	0.63	1/1115 (0.1%)	0.83	1/1510 (0.1%)
10	J	0.40	0/1152	0.64	0/1551
11	K	0.35	0/947	0.63	0/1268
12	L	0.36	0/1054	0.68	0/1403
13	M	0.39	0/1093	0.64	0/1460
14	N	0.37	0/973	0.62	0/1301
15	O	0.36	0/902	0.59	0/1209
16	P	0.37	0/929	0.67	1/1242 (0.1%)
17	Q	0.42	0/960	0.57	0/1278
18	R	0.41	0/829	0.70	1/1107 (0.1%)
19	S	0.34	0/864	0.60	0/1156
2	B	0.38	0/2121	0.71	0/2852
20	T	0.36	0/744	0.63	0/994
21	U	0.37	0/787	0.69	0/1051
22	V	0.40	0/766	0.61	0/1025
23	W	0.40	0/582	0.65	0/769
24	X	0.38	0/635	0.62	0/848
25	Y	0.40	0/510	0.60	0/677
26	Z	0.35	0/453	0.61	0/605
27	1	0.55	0/531	0.81	0/709
28	2	0.34	0/450	0.66	0/599
29	3	0.41	0/416	0.65	0/554
3	C	0.39	0/1586	0.69	1/2134 (0.0%)
30	4	0.42	0/380	0.67	0/498
31	5	0.38	0/513	0.62	0/676
32	6	0.53	0/303	0.91	2/397 (0.5%)
33	7	0.46	0/1735	0.64	0/2338
34	8	0.39	0/1651	0.62	0/2225
35	9	0.37	0/1665	0.63	0/2227
36	10	0.36	0/1169	0.67	1/1573 (0.1%)
37	11	0.39	0/835	0.70	0/1128
38	12	0.35	0/1195	0.59	0/1602
39	13	0.35	0/989	0.66	0/1326
4	D	0.44	0/1571	0.71	1/2113 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
40	14	0.37	0/1034	0.64	0/1375
41	15	0.38	0/796	0.67	0/1077
42	16	0.38	0/885	0.71	0/1195
43	17	0.38	0/969	0.66	1/1300 (0.1%)
44	18	0.39	0/892	0.66	0/1193
45	19	0.38	0/817	0.57	0/1088
46	20	0.34	0/722	0.61	0/964
47	21	0.39	0/659	0.62	0/884
48	22	0.36	0/657	0.67	0/881
49	23	0.42	0/544	0.66	0/731
5	E	0.40	0/1434	0.64	0/1926
50	24	0.48	0/652	0.70	0/877
51	25	0.37	0/671	0.52	0/888
52	26	0.45	0/550	0.64	0/728
53	27	0.46	1/36967 (0.0%)	0.67	1/57666 (0.0%)
54	28	0.49	1/69801 (0.0%)	0.67	5/108894 (0.0%)
55	29	0.40	1/2876 (0.0%)	0.66	0/4483
56	30	0.62	0/436	0.69	0/679
57	31	0.45	1/1836 (0.1%)	0.66	0/2859
58	32	0.71	1/1835 (0.1%)	0.68	0/2857
6	F	0.38	0/1343	0.67	1/1816 (0.1%)
7	G	0.49	0/1122	0.73	0/1515
8	H	0.60	0/1001	0.75	0/1350
9	I	0.60	0/1046	0.86	2/1410 (0.1%)
All	All	0.46	6/161950 (0.0%)	0.67	18/242041 (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
53	27	0	6
54	28	0	9
55	29	0	1
All	All	0	16

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	29	1	U	OP3-P	-6.99	1.52	1.61
53	27	2	A	OP3-P	-6.92	1.52	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	31	1	C	OP3-P	-6.89	1.52	1.61
54	28	1	G	OP3-P	-6.88	1.52	1.61
58	32	1	C	OP3-P	-6.86	1.52	1.61

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	28	2504	U	N1-C1'-C2'	7.12	123.26	114.00
32	6	19	ARG	NE-CZ-NH1	-6.43	117.09	120.30
43	17	115	LYS	N-CA-C	-5.96	94.89	111.00
1	A	678	GLY	N-CA-C	5.72	127.41	113.10
16	P	113	LEU	CA-CB-CG	5.67	128.34	115.30

There are no chirality outliers.

5 of 16 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
53	27	80	A	Sidechain
53	27	82	G	Sidechain
53	27	820	U	Sidechain
53	27	898	G	Sidechain
53	27	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	1103	0	1130	102	0
2	B	2082	0	2157	138	0
3	C	1565	0	1616	96	0
4	D	1552	0	1619	118	0
5	E	1410	0	1447	121	0
6	F	1323	0	1374	92	0
7	G	1111	0	1148	84	0
8	H	988	0	1025	127	0
9	I	1032	0	1088	128	0
10	J	1129	0	1162	70	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	K	938	0	1012	68	0
12	L	1045	0	1117	73	0
13	M	1074	0	1157	47	0
14	N	960	0	1000	52	0
15	O	892	0	923	57	0
16	P	917	0	965	80	0
17	Q	947	0	1022	71	0
18	R	816	0	839	60	0
19	S	857	0	922	53	0
20	T	738	0	807	39	0
21	U	779	0	834	64	0
22	V	753	0	780	37	0
23	W	575	0	592	33	0
24	X	625	0	655	44	0
25	Y	509	0	543	38	0
26	Z	449	0	491	25	0
27	1	522	0	521	47	0
28	2	444	0	461	40	0
29	3	409	0	440	14	0
30	4	377	0	418	29	0
31	5	504	0	574	27	0
32	6	302	0	343	26	0
33	7	1704	0	1732	104	0
34	8	1624	0	1699	99	0
35	9	1643	0	1710	121	0
36	10	1156	0	1199	90	0
37	11	817	0	808	71	0
38	12	1181	0	1240	79	0
39	13	979	0	1034	64	0
40	14	1022	0	1070	98	0
41	15	786	0	828	81	0
42	16	869	0	878	67	0
43	17	955	0	1019	100	0
44	18	883	0	944	73	0
45	19	805	0	847	58	0
46	20	714	0	737	46	0
47	21	649	0	666	59	0
48	22	648	0	691	55	0
49	23	535	0	552	44	0
50	24	637	0	665	72	0
51	25	665	0	714	46	0
52	26	544	0	579	59	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
53	27	33016	0	16617	1316	0
54	28	62322	0	31345	2457	0
55	29	2572	0	1302	116	0
56	30	388	0	196	10	0
57	31	1644	0	836	31	0
58	32	1643	0	836	66	0
All	All	149128	0	100926	6677	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 27.

The worst 5 of 6677 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)
9:I:7:TYR:HA	9:I:58:ILE:O	1.26	1.26
22:V:75:GLN:HB3	22:V:90:ASP:O	1.47	1.13
9:I:90:GLY:HA2	54:28:1064:C:H1'	1.26	1.13
9:I:133:ARG:NH1	54:28:1079:C:H4'	1.63	1.12
53:27:1259:C:H3'	53:27:1260:G:H5''	1.31	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	139/750 (18%)	106 (76%)	21 (15%)	12 (9%)	1	17
2	B	269/273 (98%)	227 (84%)	31 (12%)	11 (4%)	3	36
3	C	207/209 (99%)	183 (88%)	17 (8%)	7 (3%)	5	42
4	D	199/201 (99%)	162 (81%)	28 (14%)	9 (4%)	3	33
5	E	175/179 (98%)	140 (80%)	31 (18%)	4 (2%)	8	50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	174/177 (98%)	145 (83%)	27 (16%)	2 (1%)	17	63
7	G	147/149 (99%)	115 (78%)	23 (16%)	9 (6%)	2	27
8	H	129/165 (78%)	85 (66%)	29 (22%)	15 (12%)	0	9
9	I	139/142 (98%)	112 (81%)	21 (15%)	6 (4%)	3	35
10	J	140/142 (99%)	123 (88%)	13 (9%)	4 (3%)	6	45
11	K	120/123 (98%)	102 (85%)	12 (10%)	6 (5%)	3	31
12	L	141/144 (98%)	110 (78%)	25 (18%)	6 (4%)	3	35
13	M	134/136 (98%)	115 (86%)	16 (12%)	3 (2%)	8	50
14	N	118/127 (93%)	96 (81%)	18 (15%)	4 (3%)	5	42
15	O	114/117 (97%)	100 (88%)	10 (9%)	4 (4%)	4	41
16	P	112/115 (97%)	99 (88%)	11 (10%)	2 (2%)	11	54
17	Q	115/118 (98%)	105 (91%)	10 (9%)	0	100	100
18	R	101/103 (98%)	84 (83%)	13 (13%)	4 (4%)	4	37
19	S	108/110 (98%)	95 (88%)	8 (7%)	5 (5%)	3	33
20	T	91/100 (91%)	77 (85%)	8 (9%)	6 (7%)	1	25
21	U	100/104 (96%)	83 (83%)	8 (8%)	9 (9%)	1	16
22	V	92/94 (98%)	79 (86%)	12 (13%)	1 (1%)	17	63
23	W	73/85 (86%)	66 (90%)	6 (8%)	1 (1%)	14	58
24	X	75/78 (96%)	67 (89%)	5 (7%)	3 (4%)	4	37
25	Y	61/63 (97%)	53 (87%)	5 (8%)	3 (5%)	3	32
26	Z	56/59 (95%)	52 (93%)	3 (5%)	1 (2%)	11	54
27	1	64/70 (91%)	48 (75%)	10 (16%)	6 (9%)	1	15
28	2	54/57 (95%)	46 (85%)	7 (13%)	1 (2%)	10	53
29	3	48/55 (87%)	45 (94%)	2 (4%)	1 (2%)	9	51
30	4	44/46 (96%)	40 (91%)	4 (9%)	0	100	100
31	5	62/65 (95%)	54 (87%)	6 (10%)	2 (3%)	5	43
32	6	36/38 (95%)	29 (81%)	6 (17%)	1 (3%)	6	46
33	7	216/241 (90%)	170 (79%)	36 (17%)	10 (5%)	3	33
34	8	204/233 (88%)	179 (88%)	20 (10%)	5 (2%)	7	48
35	9	203/206 (98%)	167 (82%)	22 (11%)	14 (7%)	1	23
36	10	155/167 (93%)	117 (76%)	26 (17%)	12 (8%)	1	20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	11	98/135 (73%)	77 (79%)	13 (13%)	8 (8%)	1	18
38	12	149/179 (83%)	127 (85%)	18 (12%)	4 (3%)	6	46
39	13	127/130 (98%)	116 (91%)	8 (6%)	3 (2%)	7	49
40	14	125/130 (96%)	105 (84%)	10 (8%)	10 (8%)	1	19
41	15	96/103 (93%)	75 (78%)	16 (17%)	5 (5%)	2	31
42	16	114/129 (88%)	95 (83%)	13 (11%)	6 (5%)	2	30
43	17	121/124 (98%)	91 (75%)	24 (20%)	6 (5%)	3	31
44	18	112/118 (95%)	98 (88%)	8 (7%)	6 (5%)	2	30
45	19	98/101 (97%)	80 (82%)	13 (13%)	5 (5%)	2	31
46	20	86/89 (97%)	62 (72%)	14 (16%)	10 (12%)	0	9
47	21	80/82 (98%)	64 (80%)	11 (14%)	5 (6%)	2	26
48	22	78/84 (93%)	60 (77%)	13 (17%)	5 (6%)	2	26
49	23	63/75 (84%)	52 (82%)	6 (10%)	5 (8%)	1	19
50	24	77/92 (84%)	64 (83%)	11 (14%)	2 (3%)	7	47
51	25	83/87 (95%)	77 (93%)	6 (7%)	0	100	100
52	26	63/71 (89%)	39 (62%)	15 (24%)	9 (14%)	0	5
All	All	5985/6970 (86%)	4958 (83%)	749 (12%)	278 (5%)	5	33

5 of 278 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	599	VAL
1	A	666	SER
1	A	677	SER
1	A	702	ASP
2	B	107	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	121/635 (19%)	121 (100%)	0	100	100
2	B	216/218 (99%)	216 (100%)	0	100	100
3	C	164/164 (100%)	164 (100%)	0	100	100
4	D	165/165 (100%)	165 (100%)	0	100	100
5	E	148/150 (99%)	147 (99%)	1 (1%)	88	94
6	F	137/138 (99%)	136 (99%)	1 (1%)	88	94
7	G	114/114 (100%)	114 (100%)	0	100	100
8	H	100/123 (81%)	100 (100%)	0	100	100
9	I	109/110 (99%)	109 (100%)	0	100	100
10	J	116/116 (100%)	116 (100%)	0	100	100
11	K	103/104 (99%)	102 (99%)	1 (1%)	82	91
12	L	102/103 (99%)	102 (100%)	0	100	100
13	M	109/109 (100%)	109 (100%)	0	100	100
14	N	100/103 (97%)	100 (100%)	0	100	100
15	O	86/87 (99%)	86 (100%)	0	100	100
16	P	99/100 (99%)	98 (99%)	1 (1%)	82	91
17	Q	89/90 (99%)	89 (100%)	0	100	100
18	R	84/84 (100%)	84 (100%)	0	100	100
19	S	93/93 (100%)	93 (100%)	0	100	100
20	T	80/84 (95%)	80 (100%)	0	100	100
21	U	83/85 (98%)	83 (100%)	0	100	100
22	V	78/78 (100%)	78 (100%)	0	100	100
23	W	57/63 (90%)	57 (100%)	0	100	100
24	X	67/68 (98%)	67 (100%)	0	100	100
25	Y	55/55 (100%)	55 (100%)	0	100	100
26	Z	48/49 (98%)	48 (100%)	0	100	100
27	1	59/62 (95%)	58 (98%)	1 (2%)	68	88
28	2	47/48 (98%)	47 (100%)	0	100	100
29	3	45/49 (92%)	45 (100%)	0	100	100
30	4	38/38 (100%)	38 (100%)	0	100	100
31	5	51/52 (98%)	51 (100%)	0	100	100
32	6	34/34 (100%)	34 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	7	180/199 (90%)	180 (100%)	0	100	100
34	8	170/190 (90%)	170 (100%)	0	100	100
35	9	172/173 (99%)	172 (100%)	0	100	100
36	10	119/126 (94%)	119 (100%)	0	100	100
37	11	87/116 (75%)	86 (99%)	1 (1%)	80	90
38	12	124/147 (84%)	124 (100%)	0	100	100
39	13	104/105 (99%)	104 (100%)	0	100	100
40	14	105/107 (98%)	105 (100%)	0	100	100
41	15	86/90 (96%)	86 (100%)	0	100	100
42	16	89/99 (90%)	89 (100%)	0	100	100
43	17	103/104 (99%)	103 (100%)	0	100	100
44	18	92/96 (96%)	92 (100%)	0	100	100
45	19	83/84 (99%)	83 (100%)	0	100	100
46	20	76/77 (99%)	76 (100%)	0	100	100
47	21	65/65 (100%)	65 (100%)	0	100	100
48	22	74/78 (95%)	74 (100%)	0	100	100
49	23	56/65 (86%)	56 (100%)	0	100	100
50	24	70/79 (89%)	70 (100%)	0	100	100
51	25	65/66 (98%)	65 (100%)	0	100	100
52	26	55/61 (90%)	55 (100%)	0	100	100
All	All	4972/5698 (87%)	4966 (100%)	6 (0%)	95	97

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	K	58	LEU
37	11	12	PRO
16	P	113	LEU
6	F	117	PRO
27	1	37	CYS

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

Mol	Chain	Res	Type
21	U	68	ASN
30	4	29	GLN
46	20	36	ASN
21	U	73	ASN
25	Y	39	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
53	27	1538/1539 (99%)	171 (11%)	7 (0%)
54	28	2902/2903 (99%)	386 (13%)	20 (0%)
55	29	119/120 (99%)	12 (10%)	3 (2%)
56	30	17/18 (94%)	3 (17%)	0
57	31	76/77 (98%)	5 (6%)	0
58	32	76/77 (98%)	17 (22%)	0
All	All	4728/4734 (99%)	594 (12%)	30 (0%)

5 of 594 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
53	27	4	U
53	27	6	G
53	27	9	G
53	27	13	U
53	27	22	G

5 of 30 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
54	28	1130	U
54	28	1626	A
55	29	44	G
54	28	1490	A
54	28	1730	C

## 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.