



wwPDB/EMDatabank EM Map/Model Validation Summary Report ⓘ

Nov 14, 2019 – 03:00 AM EST

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/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

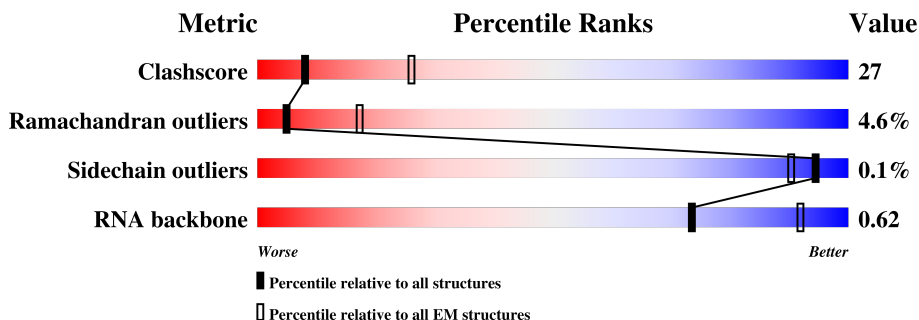
1 Overall quality at a glance

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.













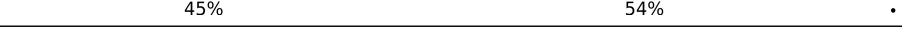
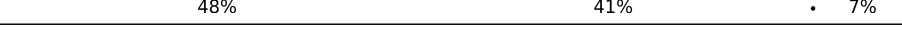

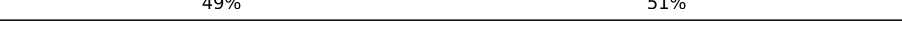


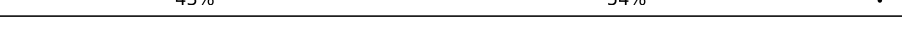

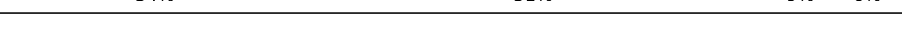




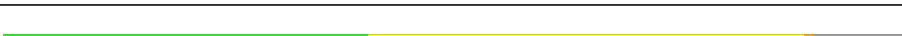

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531
RNA backbone	3747	458

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	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%

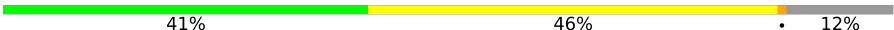


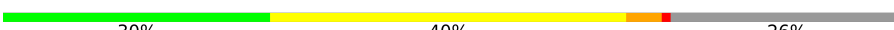
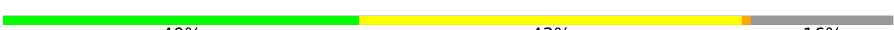





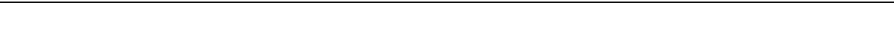

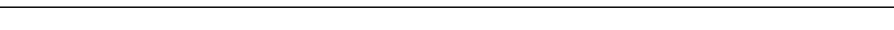
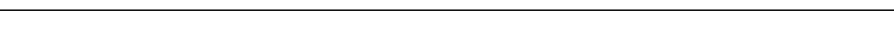










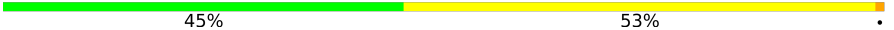
Continued on next page...

Continued from previous page...

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	

Continued on next page...

Continued from previous page...

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 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.

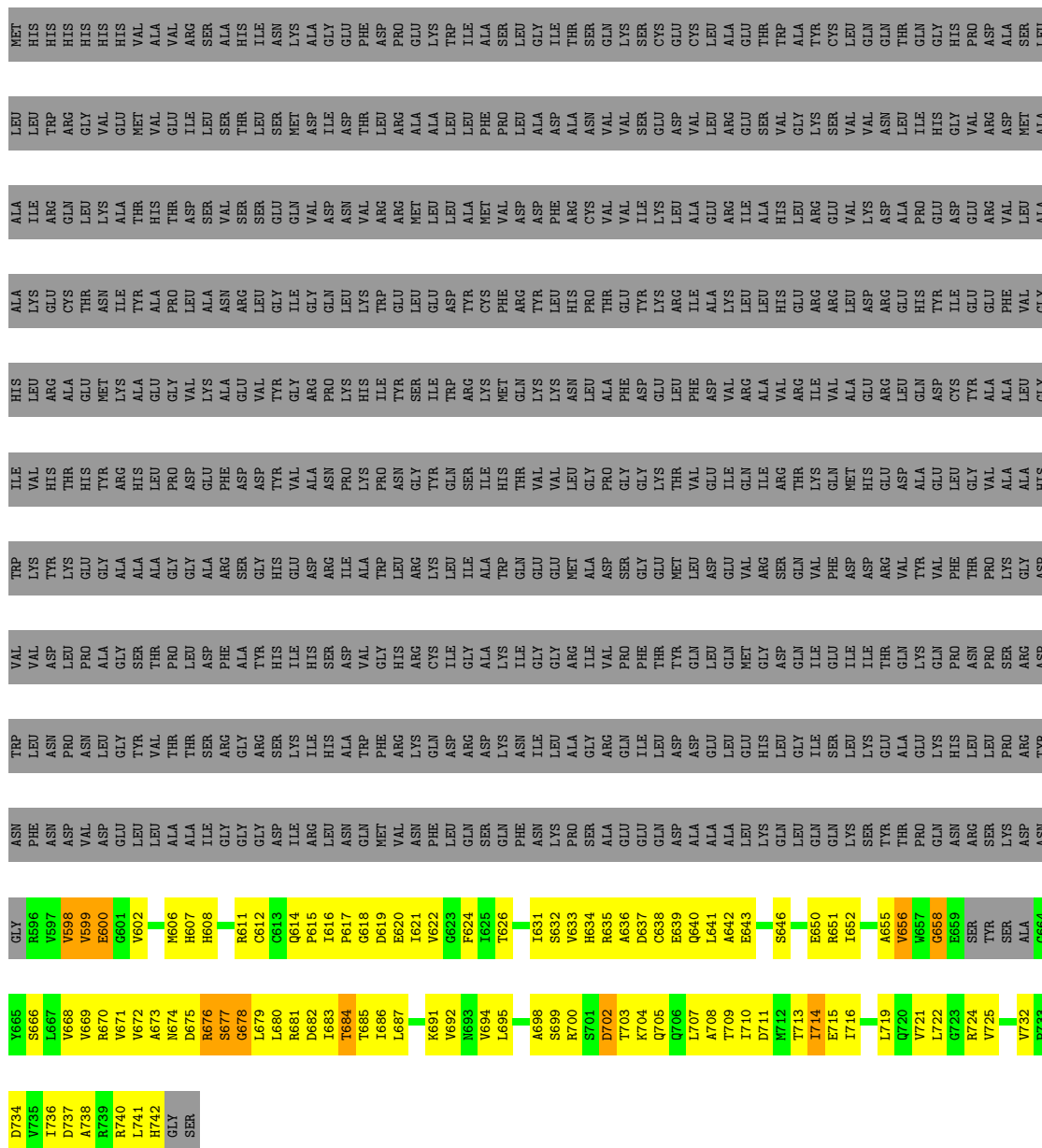
Mol	Chain	Residues	Atoms					AltConf	Trace
58	32	77	Total	C	N	O	P	0	0
			1643	732	297	537	77		

3 Residue-property plots

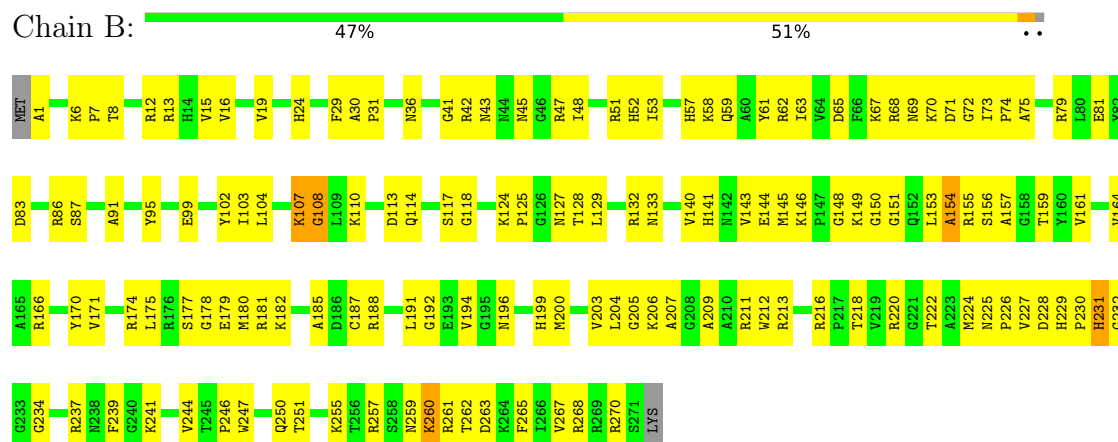
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

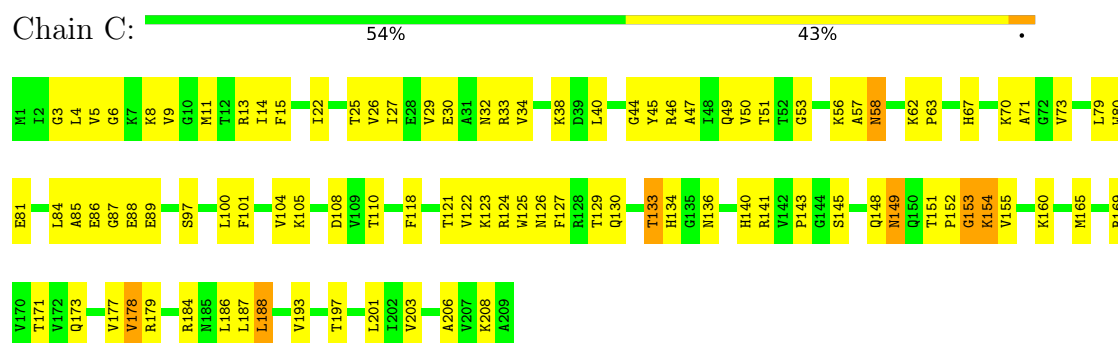
Chain A:  7% 11% . 81%



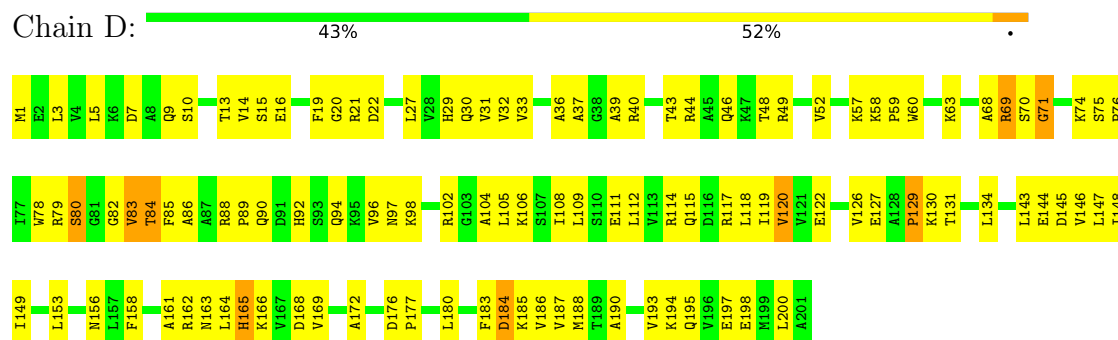
- Molecule 2: 50S ribosomal protein L2



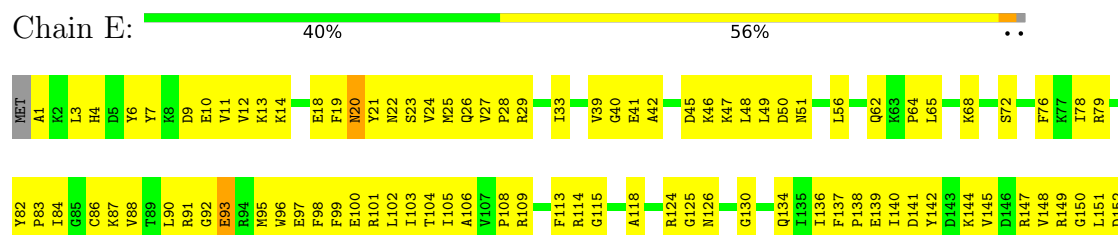
- Molecule 3: 50S ribosomal protein L3



- Molecule 4: 50S ribosomal protein L4



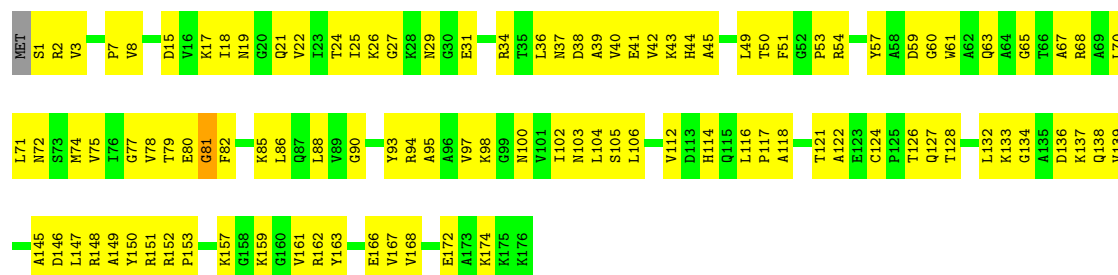
- Molecule 5: 50S ribosomal protein L5





• Molecule 6: 50S ribosomal protein L6

Chain F: 41% 58% ..



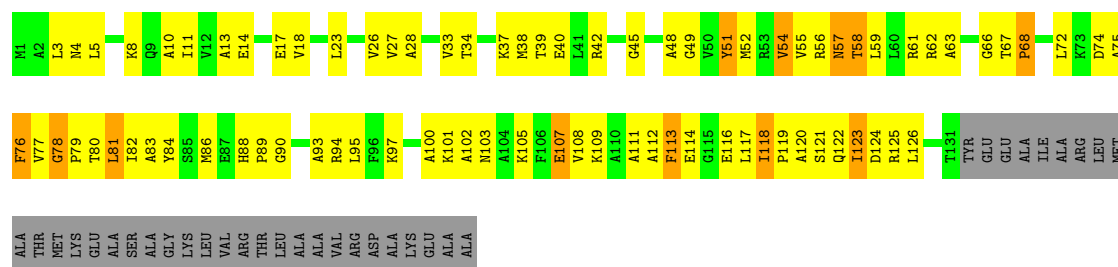
• Molecule 7: 50S ribosomal protein L9

Chain G: 38% 58% .



• Molecule 8: 50S ribosomal protein L10

Chain H: 30% 42% 7% 21%

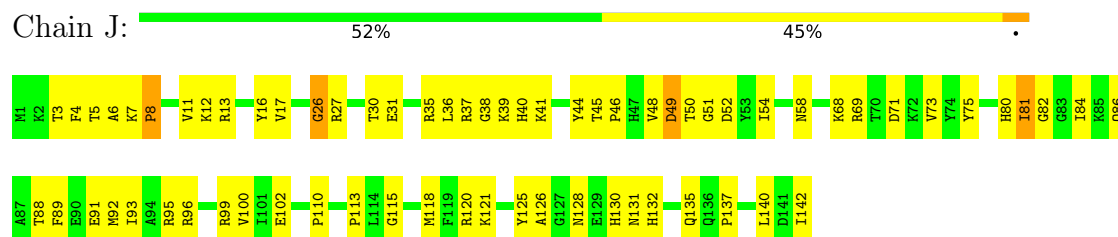


• Molecule 9: 50S ribosomal protein L11

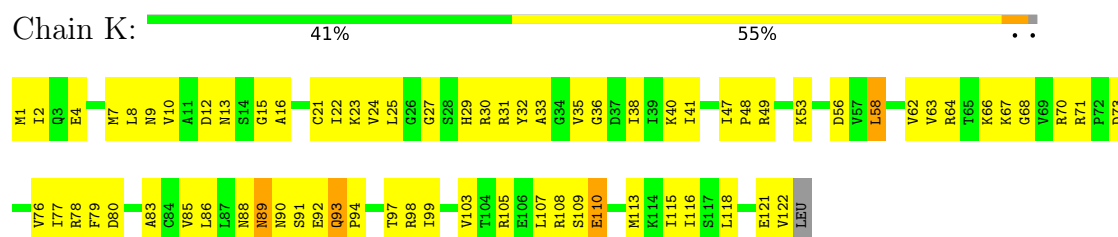
Chain I: 38% 58% ..



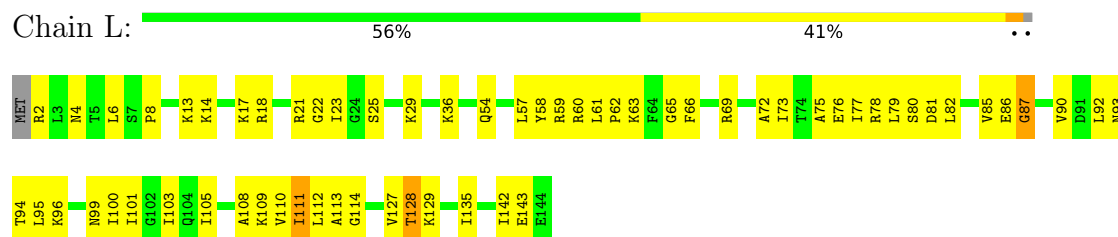
- Molecule 10: 50S ribosomal protein L13



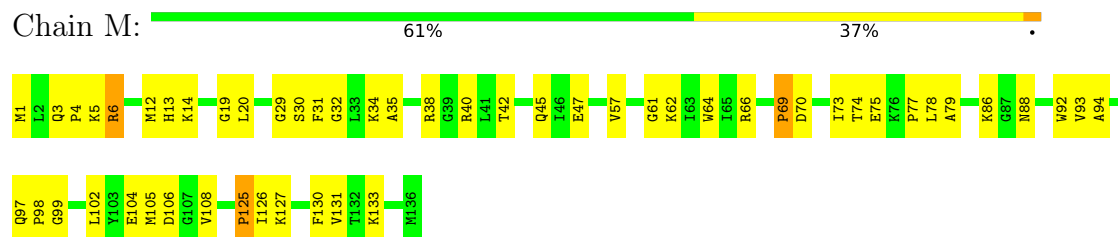
- Molecule 11: 50S ribosomal protein L14



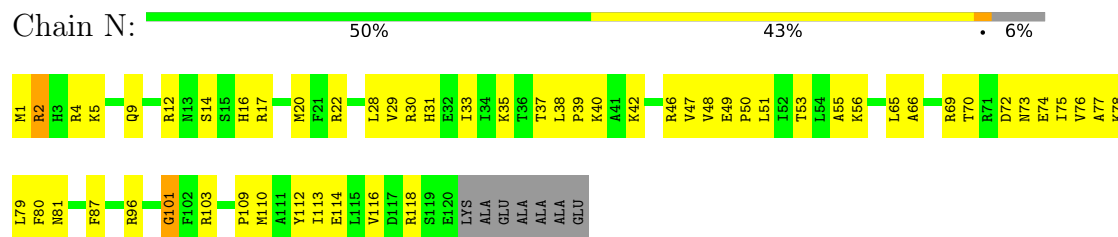
- Molecule 12: 50S ribosomal protein L15



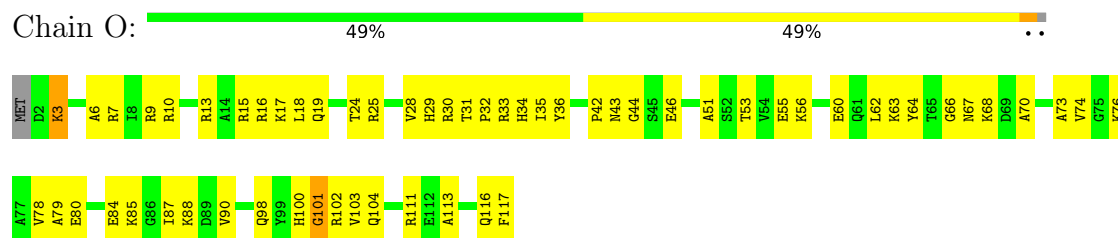
- Molecule 13: 50S ribosomal protein L16



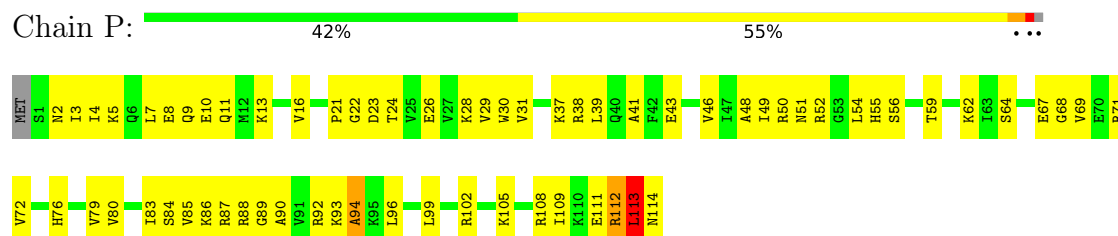
- Molecule 14: 50S ribosomal protein L17



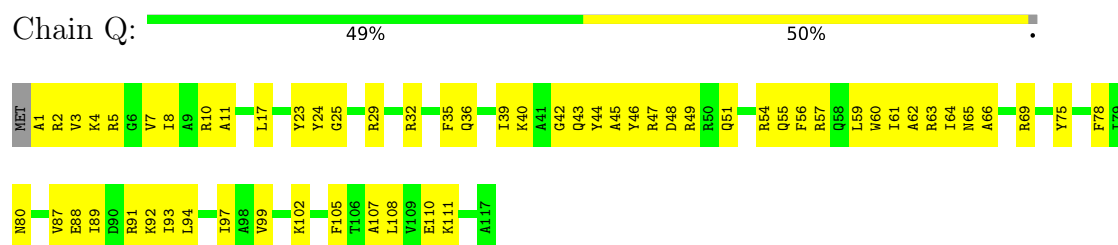
- Molecule 15: 50S ribosomal protein L18



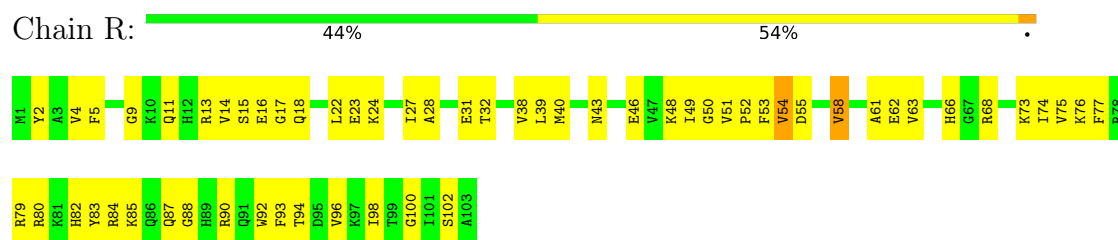
• Molecule 16: 50S ribosomal protein L19



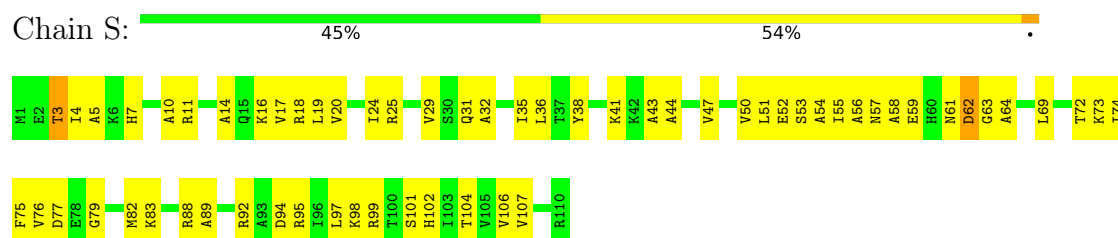
• Molecule 17: 50S ribosomal protein L20



• Molecule 18: 50S ribosomal protein L21

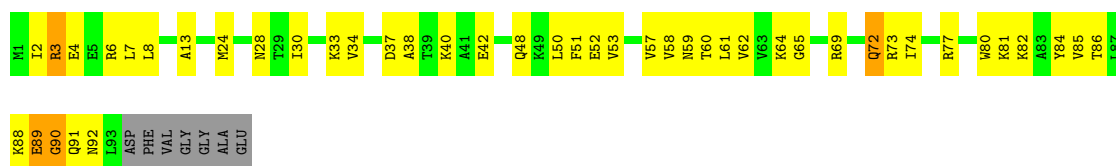


• Molecule 19: 50S ribosomal protein L22



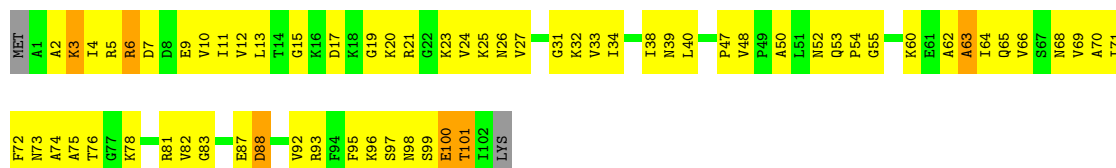
• Molecule 20: 50S ribosomal protein L23





- Molecule 21: 50S ribosomal protein L24

Chain U: 36% 57% 6%



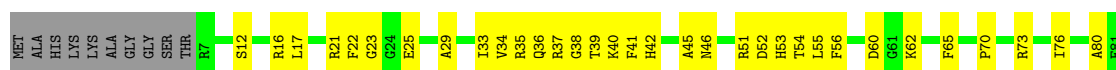
- Molecule 22: 50S ribosomal protein L25

Chain V: 49% 51%



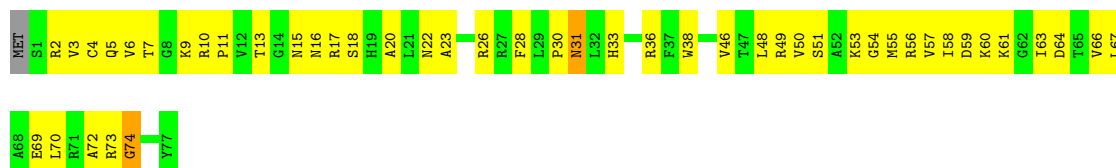
- Molecule 23: 50S ribosomal protein L27

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%



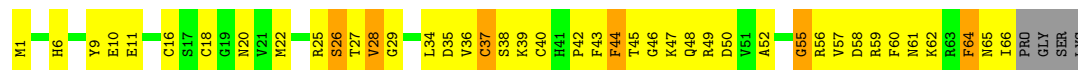
- Molecule 26: 50S ribosomal protein L30

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%



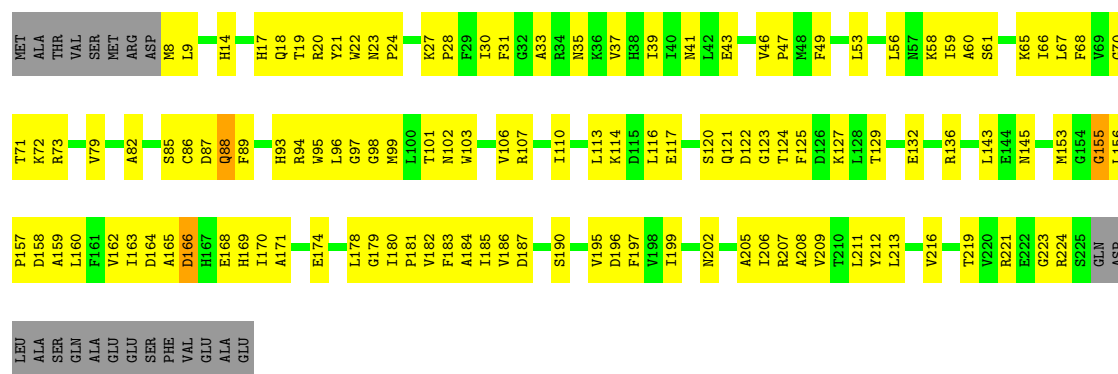
- Molecule 32: 50S ribosomal protein L36

Chain 6:  37% 58% 5%



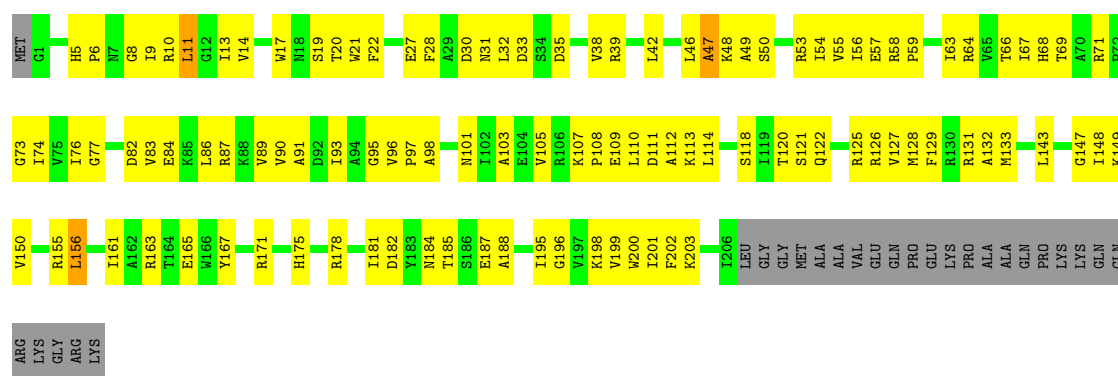
- Molecule 33: 30S ribosomal protein S2

Chain 7:  41% 49% 10%



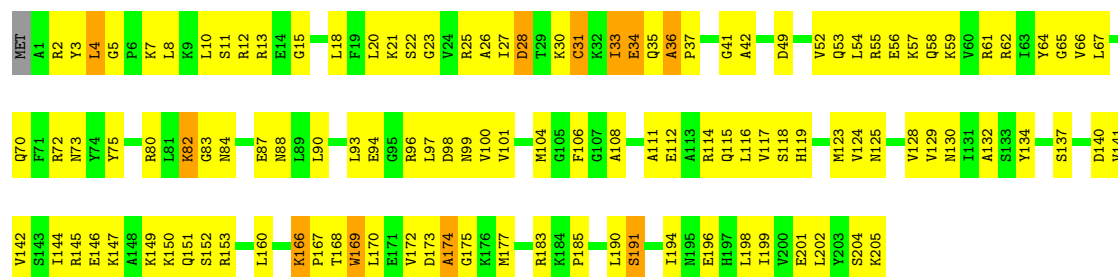
• Molecule 34: 30S ribosomal protein S3

Chain 8: 41% 46% 12%



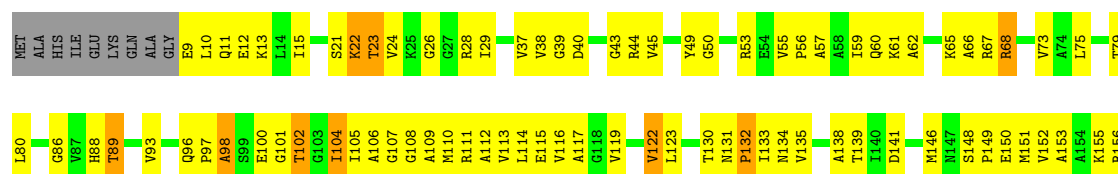
• Molecule 35: 30S ribosomal protein S4

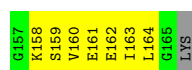
Chain 9: 42% 52% 5%



• Molecule 36: 30S ribosomal protein S5

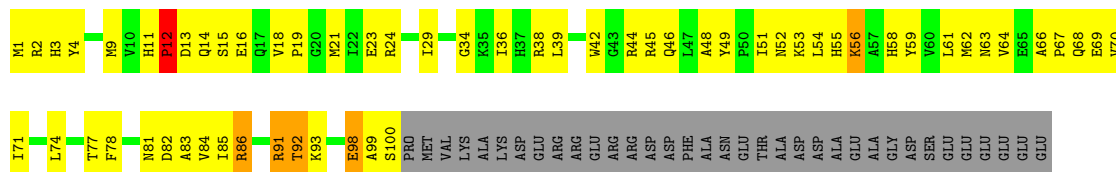
Chain 10: 40% 49% 5% 6%





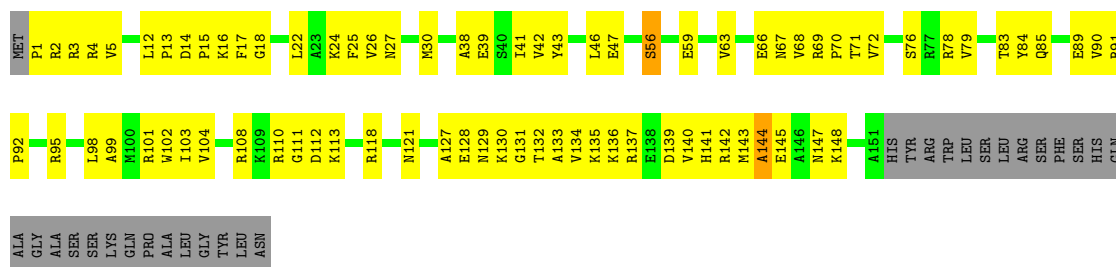
• Molecule 37: 30S ribosomal protein S6

Chain 11: 30% 40% 26%



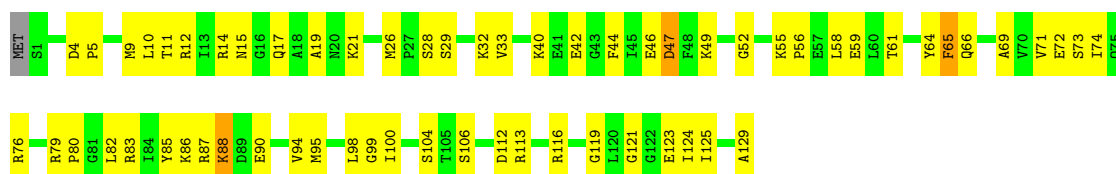
• Molecule 38: 30S ribosomal protein S7

Chain 12: 40% 43% 16%



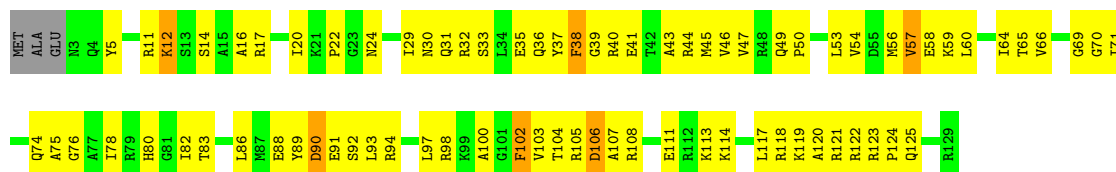
• Molecule 39: 30S ribosomal protein S8

Chain 13: 52% 45%



• Molecule 40: 30S ribosomal protein S9

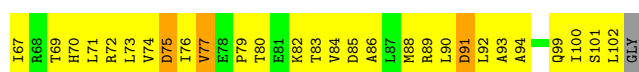
Chain 14: 38% 55% 5%



• Molecule 41: 30S ribosomal protein S10

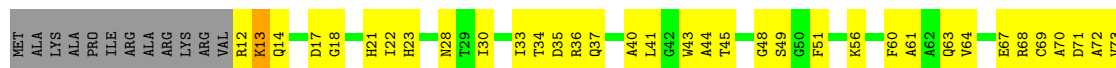
Chain 15: 25% 66% 5%





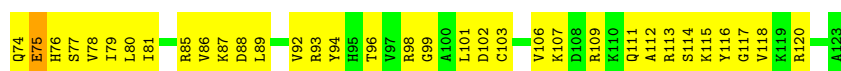
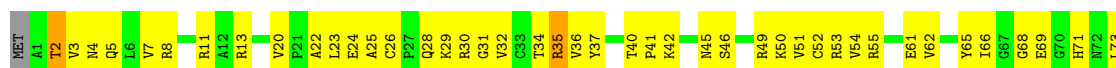
• Molecule 42: 30S ribosomal protein S11

Chain 16: 40% 47% 10%



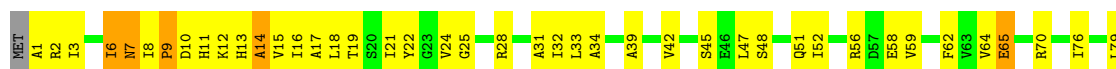
• Molecule 43: 30S ribosomal protein S12

Chain 17: 37% 60% ..



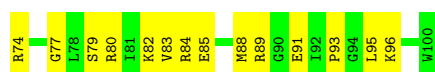
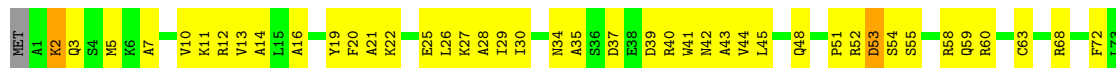
• Molecule 44: 30S ribosomal protein S13

Chain 18: 45% 47% ..



• Molecule 45: 30S ribosomal protein S14

Chain 19: 44% 53% ..



• Molecule 46: 30S ribosomal protein S15

Chain 20: 43% 49% 7%





- Molecule 47: 30S ribosomal protein S16

Chain 21: 33% 65%



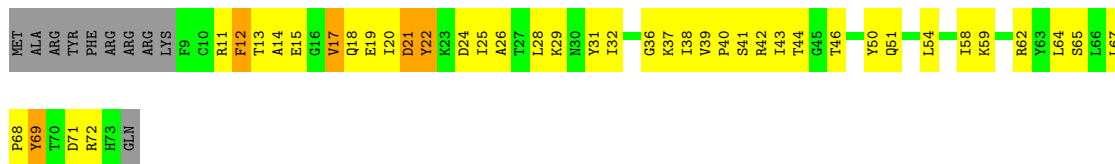
- Molecule 48: 30S ribosomal protein S17

Chain 22: 40% 50% 5% 5%



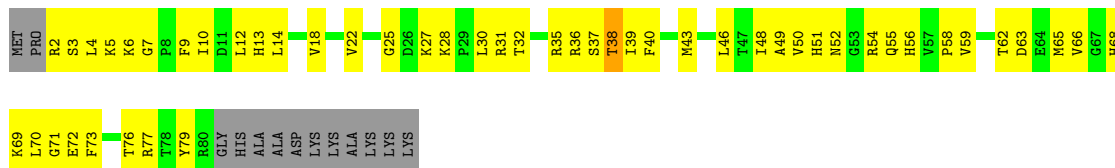
- Molecule 49: 30S ribosomal protein S18

Chain 23: 32% 48% 7% 13%



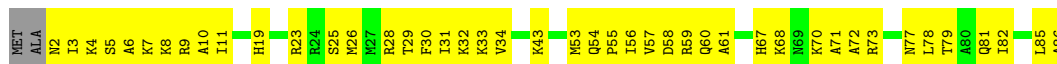
- Molecule 50: 30S ribosomal protein S19

Chain 24: 32% 53% 14%

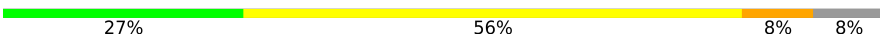


- Molecule 51: 30S ribosomal protein S20

Chain 25: 47% 51%



- Molecule 52: 30S ribosomal protein S21

Chain 26:  27% 56% 8% 8%

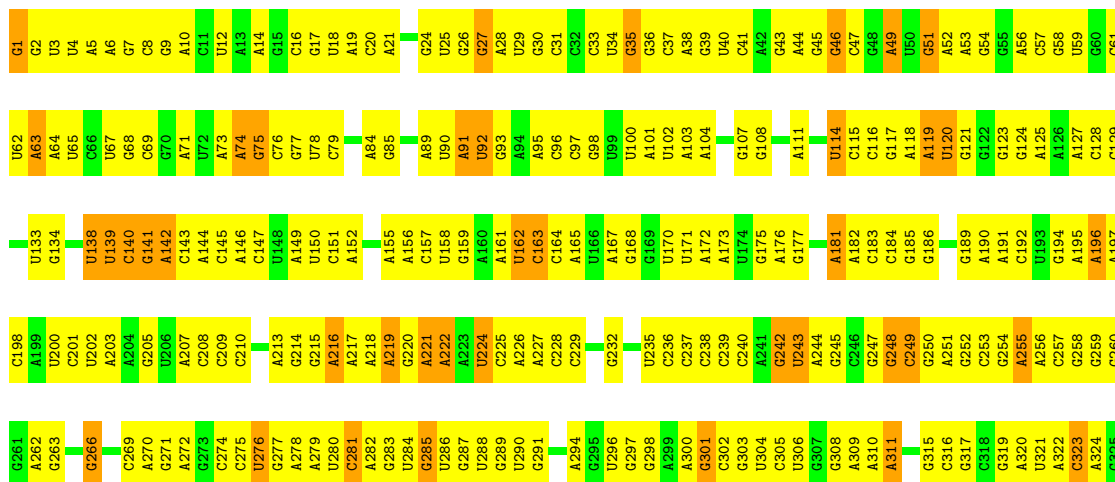
MET PRO VAL I3 K4 V5 R6 E9 P10 F11 D12 V13 A14 L15 R17 F18 K19 R20 S21 E22 E23 K24 A25 G26 V27 L28 A29 E30 V31 R32 R33 R34 E35 F36 Y37 E38 K39 P40 T41 T42 E43 R44 K45 K48 A49 S50 A51 V52 K53 E62 N63 A64 R65 R66 T67 ARG

LEU
TYR

• Molecule 53: 16S ribosomal RNA

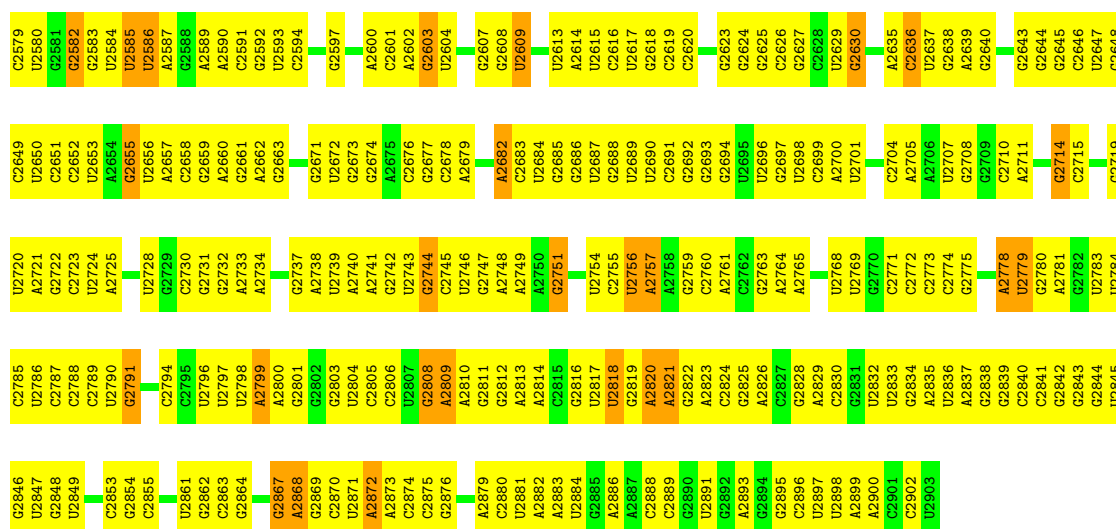
Chain 27:  27% 65% 8%

A2 A3 U4 U5 U6 A7 A8 A9 A10 U13 U16 U17 U18 U19 U20 U21 U22 U23 U24 U25 U26 U27 U28 U29 U30 U31 A32 A33 A34 A35 A36 A37 A38 A39 A40 A41 A42 A43 A44 G45 G46 G47 G48 A49 A50 A51 A52 A53 A54 A55 U56 U57 U58 U59 A60 A61 A62 A63 A64 A65 A66 A67 A68 A69 A70 A71 A72 A73 A74 A75 A76 A77 A78 A79 A80 A81 A82 A83 A84 A85 A86 A87 A88 A89 A90 A91 A92 A93 A94 A95 A96 A97 A98 A99 A100 A101 A102 A103 A104 A105 A106 A107 A108 A109 A110 A111 A112 A113 A114 A115 A116 A117 A118 A119 A120 A121 A122 A123 A124 A125 A126 A127 A128 A129 A130 A131 A132 A133 A134 A135 A136 A137 A138 A139 A140 A141 A142 A143 A144 G145 G146 G147 G148 G149 G150 G151 G152 G153 G154 G155 G156 G157 G158 G159 G160 G161 G162 G163 G164 G165 G166 G167 G168 A169 A170 A171 A172 A173 A174 A175 A176 A177 A178 A179 A180 A181 A182 A183 A184 A185 A186 A187 A188 A189 A190 A191 A192 A193 A194 A195 A196 A197 A198 A199 A200 A201 A202 A203 A204 A205 A206 A207 A208 A209 A210 A211 A212 A213 A214 A215 A216 A217 A218 A219 A220 A221 A222 A223 A224 A225 A226 A227 A228 A229 A230 A231 A232 A233 A234 A235 A236 A237 A238 A239 A240 A241 A242 A243 A244 A245 A246 A247 A248 A249 A250 A251 A252 A253 A254 A255 A256 A257 A258 A259 A260 A261 A262 A263 A264 A265 A266 A267 A268 A269 A270 A271 A272 A273 A274 A275 A276 A277 A278 A279 A280 A281 A282 A283 A284 A285 A286 A287 A288 A289 A290 A291 A292 A293 A294 A295 A296 A297 A298 A299 A300 A301 A302 A303 A304 A305 A306 A307 A308 A309 A310 A311 A312 A313 A314 A315 A316 A317 A318 A319 A320 A321 A322 A323 A324 A325 A326 A327 A328 A329 A330 A331 A332 A333 A334 A335 A336 A337 A338 A339 A340 A341 A342 A343 A344 A345 A346 A347 A348 A349 A350 A351 A352 A353 A354 A355 A356 A357 A358 A359 A360 A361 A362 A363 A364 A365 A366 A367 A368 A369 A370 A371 A372 A373 A374 A375 A376 A377 A378 A379 A380 A381 A382 A383 A384 A385 A386 A387 A388 A389 A390 A391 A392 A393 A394 A395 A396 A397 A398 A399 A400 A401 A402 A403 A404 A405 A406 A407 A408 A409 A410 A411 A412 A413 A414 A415 A416 A417 A418 A419 A420 A421 A422 A423 A424 A425 A426 A427 A428 A429 A430 A431 A432 A433 A434 A435 A436 A437 A438 A439 A440 A441 A442 A443 A444 A445 A446 A447 A448 A449 A450 A451 A452 A453 A454 A455 A456 A457 A458 A459 A460 A461 A462 A463 A464 A465 A466 A467 A468 A469 A470 A471 A472 A473 A474 A475 A476 A477 A478 A479 A480 A481 A482 A483 A484 A485 A486 A487 A488 A489 A490 A491 A492 A493 A494 A495 A496 A497 A498 A499 A500 A501 A502 A503 A504 A505 A506 A507 A508 A509 A510 A511 A512 A513 A514 A515 A516 A517 A518 A519 A520 A521 A522 A523 A524 A525 A526 A527 A528 A529 A530 A531 A532 A533 A534 A535 A536 A537 A538 A539 A540 A541 A542 A543 A544 A545 A546 A547 A548 A549 A550 A551 A552 A553 A554 A555 A556 A557 A558 A559 A560 A561 A562 A563 A564 A565 A566 A567 A568 A569 A570 A571 A572 A573 A574 A575 A576 A577 A578 A579 A580 A581 A582 A583 A584 A585 A586 A587 A588 A589 A590 A591 A592 A593 A594 A595 A596 A597 A598 A599 A600 A601 A602 A603 A604 A605 A606 A607 A608 A609 A610 A611 A612 A613 A614 A615 A616 A617 A618 A619 A620 A621 A622 A623 A624 A625 A626 A627 A628 A629 A630 A631 A632 A633 A634 A635 A636 A637 A638 A639 A640 A641 A642 A643 A644 A645 A646 A647 A648 A649 A650 A651 A652 A653 A654 A655 A656 A657 A658 A659 A660 A661 A662 A663 A664 A665 A666 A667 A668 A669 A670 A671 A672 A673 A674 A675 A676 A677 A678 A679 A680 A681 A682 A683 A684 A685 A686 A687 A688 A689 A690 A691 A692 A693 A694 A695 A696 A697 A698 A699 A700 A701 A702 A703 A704 A705 A706 A707 A708 A709 A710 A711 A712 A713 A714 A715 A716 A717 A718 A719 A720 A721 A722 A723 A724 A725 A726 A727 A728 A729 A730 A731 A732 A733 A734 A735 A736 A737 A738 A739 A740 A741 A742 A743 A744 A745 A746 A747 A748 A749 A750 A751 A752 A753 A754 A755 A756 A757 A758 A759 A760 A761 A762 A763 A764 A765 A766 A767 A768 A769 A770 A771 A772 A773 A774 A775 A776 A777 A778 A779 A780 A781 A782 A783 A784 A785 A786 A787 A788 A789 A790 A791 A792 A793 A794 A795 A796 A797 A798 A799 A800 A801 A802 A803 A804 A805 A806 A807 A808 A809 A810 A811 A812 A813 A814 A815 A816 A817 A818 A819 A820 A821 A822 A823 A824 A825 A826 A827 A828 A829 A830 A831 A832 A833 A834 A835 A836 A837 A838 A839 A840 A841 A842 A843 A844 A845 A846 A847 A848 A849 A850 A851 A852 A853 A854 A855 A856 A857 A858 A859 A860 A861 A862 A863 A864 A865 A866 A867 A868 A869 A870 A871 A872 A873 A874 A875 A876 A877 A878 A879 A880 A881 A882 A883 A884 A885 A886 A887 A888 A889 A890 A891 A892 A893 A894 A895 A896 A897 A898 A899 A900 A901 A902 A903 A904 A905 A906 A907 A908 A909 A910 A911 A912 A913 A914 A915 A916 A917 A918 A919 A920 A921 A922 A923 A924 A925 A926 A927 A928 A929 A930 A931 A932 A933 A934 A935 A936 A937 A938 A939 A940 A941 A942 A943 A944 A945 A946 A947 A948 A949 A950 A951 A952 A953 A954 A955 A956 A957 A958 A959 A960 A961 A962 A963 A964 A965 A966 A967 A968 A969 A970 A971 A972 A973 A974 A975 A976 A977 A978 A979 A980 A981 A982 A983 A984 A985 A986 A987 A988 A989 A990 A991 A992 A993 A994 A995 A996 A997 A998 A999



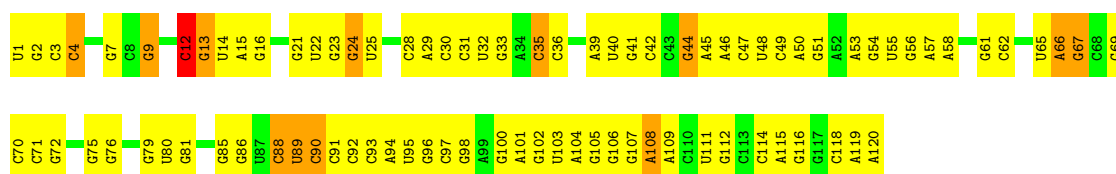



U1511	C2443	A2377	G2316	U2245	C2174	G2107	A2042	U1971	G1905	G1831	G1766	A1698	A1630	U1562	U1485
C2512	G2444	A2378	A2317	G2246	C2175	A2108	C2043	G1972	G1906	C1832	G1767	G1702	G1631	U1563	U1486
A2513	G2445	C2379	G2318	A2247	A2183	A2109	C2044	G1973	G1907	C1833	G1770	G1703	G1633	C1564	U1487
U2514	G2446	C2380	G2319	C2248	A2184	G2110	C2045	C1974	C1908	C1837	A1772	C1704	A1634	A1566	A1490
C2515	G2447	A2381	U2320	G2250	G2186	U2111	G2046	U1982	G1910	C1838	A1773	U1709	A1635	G1567	A1491
A2516	A2448	C2382	U2321	G2251	U2187	U2112	C2047	G1983	G1911	C1839	A1774	U1710	A1636	G1568	G1492
C2517	U2449	G2383	A2322	U2257	U2188	A2114	G2048	U1984	A1912	C1840	C1774	U1711	U1637	G1569	C1499
A2518	A2450	U2384	G2323	C2258	U2189	G2115	C2050	G1989	A1913	U1841	U1775	A1712	A1638	A1570	C1500
C2520	C2452	A2386	G2325	U2259	G2190	U2116	A2051	U1991	C1914	C1842	U1776	U1713	A1640	A1571	
C2521	G2456	U2387	G2326	C2260	A2191	G2117	A2052	G1992	A1915	C1843	U1777	U1714	A1641	A1572	
G2524	U2457	A2388	A2327	U2261	U2192	A2119	C2055	G1993	A1916	C1844	U1778	G1715	A1642	G1573	A1504
G2525	U2390	U2391	U2328	C2262	G2193	G2120	G2056	C1994	A1917	G1847	A1780	U1716	G1643	C1574	A1505
U2528	G2458	A2392	G2330	C2263	U2195	G2121	G2057	U1996	A1918	A1848		A1717	C1644	C1577	U1506
C2529	U2460	C2393	G2331	C2264	C2196	U2122	A2058	C1997	A1919	A1849	A1784	G1718	G1645	U1578	C1507
A2530	A2461	U2394	C2332	A2265	U2197	G2126	A2059	A1998	G1922	U1851	A1785	U1719	C1646	A1579	A1508
C2537	C2462	C2395	A2333	A2266	A2198	G2127	G2061	C1999	U1923	U1852	A1786	U1720	U1647	A1580	A1509
C2538	C2463	C2396	A2334	A2267	A2199	G2128	A2062	C2000	C1924	A1853	A1787	G1721	U1648	G1581	A1515
U2533	G2464	G2397	A2335	G2268	C2200	G2129	C2063	C2001	U1926	A1854	C1788	A1722	U1649	G1516	G1517
A2534	C2465	U2398	A2336	A2270	U2203	U2130	U2065	C2002	A1927	U1856	C1789	C1726	A1650	U1584	
G2535	C2466	C2399	G2337	G2271	G2204	U2131	C2064	G2003	A1928	C1857	A1791	C1727	G1651	C1585	U1520
U2544	C2467	U2402	A2340	U2272	A2205	U2132	C2065	G2004	U1929	A1858		C1728	G1652	G1521	
C2545	A2471	C2403	G2341	A2273	C2206	G2133	G2066	A2005	G1930	U1864	A1794	U1729	G1653	U1588	
U2546	U2472	U2404	C2342	A2274	C2207	A2134	U2067	C2006	U1931	U1865	C1795	C1730	A1654	A1590	G1524
C2547	G2473	G2405	U2343	G2277	C2208	A2135	U2068	C2007	A1932	U1866	C1796	G1731	A1655	C1525	A1525
U2548	A2478	A2406	G2344	A2278	G2209	U2137	A2070	C2008	G1933	C1867	U1797	C1732	U1656	C1526	C1527
G2549	C2475	U2407	A2345	G2279	U2210	G2138	A2071	C2009	C1934	U1798	U1798	G1733	C1658	A1528	U1529
U2552	U2476	G2408	G2346	G2280	A2211	G2139	C2072	G2010	G1935	C1867	U1799	U1736	C1659	G1530	G1531
C2553	U2477	G2409	C2347	A2281	A2212	G2140	C2073	U2011	A1936	A1871	C1800	U1737	G1660	A1535	A1536
U2554	A2478	G2410	U2348	G2282	U2213	C2141	C2074	C2012	A1937	A1872	A1801	G1738	G1661	C1537	G1538
G2555	C2482	A2411	G2349	C2283	U2214	C2142	U2075	A2013	U1938	A1873	A1802	A1739	A1662	U1602	U1603
U2556	G2485	U2412	C2350	A2284	G2216	C2143	C2078	A2014	C1947	C1874	A1803	A1745	A1663	C1604	C1605
C2557	G2486	G2413	A2351	C2285	G2217	C2144	U2079	A2015	G1948	C1881	C1804	U1746	A1664	C1606	G1540
U2558	U2487	G2414	A2352	G2286	G2218	A2146	A2080	U2016	U1943	A1877	A1805	U1747	A1665	U1541	U1542
C2559	U2491	G2421	G2353	A2287	U2219	G2147	U2081	U2017	U1951	G1878	C1806	C1748	G1674	U1543	A1544
U2560	U2492	G2422	G2360	A2288	U2220	U2149	U2082	G2018	A1952	U1883	G1807	A1749	C1675	A1608	A1609
U2561	U2493	U2423	G2361	U2291	G2221	C2150	A2082	A2019	A1953	A1884	A1808	G1750	A1676	A1610	A1545
U2562	G2494	C2424	C2362	U2292	G2222	U2151	U2086	C1947	G1954	A1889	A1816	U1751	A1677	C1611	
A2564	A2497	A2425	G2363	U2293	G2223	G2152	G2087	C1948	U1955	A1890	C1817	C1752	A1678	G1612	
C2565	C2498	A2426	A2364	G2294	G2224	C2153	U2092	U1956	U1956	C1891	U1818	G1753	A1679	G1613	A1548
U2566	C2499	G2428	G2365	C2295	A2226	C2161	G2093	C1957	C1957	C1892	U1820	A1755	U1680	A1614	A1549
C2567	U2500	G2429	A2366	U2306	U2232	G2162	A2096	C1958	G1959	A1896	A1821	G1756	G1682	C1615	C1550
U2568	A2501	A2430	C2367	C2307	A2097	C2165	C2097	U1962	C1962	G1897	C1822	U1757	U1683	A1616	A1551
U2569	C2502	U2431	A2368	U2308	U2098	U2166	U2034	C1963	U1963	G1898	G1823	U1758	G1684	C1617	G1555
C2572	A2503	A2432	G2370	A2309	A2101	U2167	G2035	G1964	U1964	A1899	G1824	U1759	C1685	A1618	G1556
U2573	U2504	C2433	G2371	G2310	A2168	G2239	C2036	U1967	U1967	A1900	G1825	C1761	C1686	G1619	C1557
C2574	G2505	A2435	U2372	A2311	A2169	U2240	A2037	G2038	C1967	A1901	U1826	U1762	U1688	A1626	C1558
U2577	U2506	C2440	G2373	U2312	A2241	A2170	C2103	U1968	G1968	C1902	U1827	A1763	U1689	G1627	U1559
C2578	G2507	U2441	C2374	C2313	G2242	A2171	C2104	U1969	U1969	C1903	A1828	G1764	A1690	G1560	C1561
	G2508	C2442	U2375	A2314	U2243	A2172	U2105	G2040	A1970	G1904	U1829	U1765	U1690	U1629	
			A2376	G2315	U2244	A2173	U2106	U2041							



• Molecule 55: 5S ribosomal RNA

Chain 29: 28% 62% 10%



• Molecule 56: mRNA

Chain 30: 44% 50% 6%



• Molecule 57: P site tRNA^{fmet}

Chain 31: 45% 53% 2%



• Molecule 58: E-site tRNA^{fMet}

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	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	0.63	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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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	14
2	B	269/273 (98%)	227 (84%)	31 (12%)	11 (4%)	3	30
3	C	207/209 (99%)	183 (88%)	17 (8%)	7 (3%)	4	35
4	D	199/201 (99%)	162 (81%)	28 (14%)	9 (4%)	3	28
5	E	175/179 (98%)	140 (80%)	31 (18%)	4 (2%)	7	43

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	174/177 (98%)	145 (83%)	27 (16%)	2 (1%)	16	56
7	G	147/149 (99%)	115 (78%)	23 (16%)	9 (6%)	1	22
8	H	129/165 (78%)	85 (66%)	29 (22%)	15 (12%)	0	7
9	I	139/142 (98%)	112 (81%)	21 (15%)	6 (4%)	3	29
10	J	140/142 (99%)	123 (88%)	13 (9%)	4 (3%)	5	38
11	K	120/123 (98%)	102 (85%)	12 (10%)	6 (5%)	2	26
12	L	141/144 (98%)	110 (78%)	25 (18%)	6 (4%)	3	29
13	M	134/136 (98%)	115 (86%)	16 (12%)	3 (2%)	7	43
14	N	118/127 (93%)	96 (81%)	18 (15%)	4 (3%)	4	35
15	O	114/117 (97%)	100 (88%)	10 (9%)	4 (4%)	4	35
16	P	112/115 (97%)	99 (88%)	11 (10%)	2 (2%)	9	47
17	Q	115/118 (98%)	105 (91%)	10 (9%)	0	100	100
18	R	101/103 (98%)	84 (83%)	13 (13%)	4 (4%)	3	31
19	S	108/110 (98%)	95 (88%)	8 (7%)	5 (5%)	2	28
20	T	91/100 (91%)	77 (85%)	8 (9%)	6 (7%)	1	21
21	U	100/104 (96%)	83 (83%)	8 (8%)	9 (9%)	1	14
22	V	92/94 (98%)	79 (86%)	12 (13%)	1 (1%)	16	56
23	W	73/85 (86%)	66 (90%)	6 (8%)	1 (1%)	12	51
24	X	75/78 (96%)	67 (89%)	5 (7%)	3 (4%)	3	31
25	Y	61/63 (97%)	53 (87%)	5 (8%)	3 (5%)	2	26
26	Z	56/59 (95%)	52 (93%)	3 (5%)	1 (2%)	9	47
27	1	64/70 (91%)	48 (75%)	10 (16%)	6 (9%)	1	13
28	2	54/57 (95%)	46 (85%)	7 (13%)	1 (2%)	9	46
29	3	48/55 (87%)	45 (94%)	2 (4%)	1 (2%)	8	44
30	4	44/46 (96%)	40 (91%)	4 (9%)	0	100	100
31	5	62/65 (95%)	54 (87%)	6 (10%)	2 (3%)	4	36
32	6	36/38 (95%)	29 (81%)	6 (17%)	1 (3%)	5	39
33	7	216/241 (90%)	170 (79%)	36 (17%)	10 (5%)	2	28
34	8	204/233 (88%)	179 (88%)	20 (10%)	5 (2%)	6	41
35	9	203/206 (98%)	167 (82%)	22 (11%)	14 (7%)	1	20
36	10	155/167 (93%)	117 (76%)	26 (17%)	12 (8%)	1	17

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	11	98/135 (73%)	77 (79%)	13 (13%)	8 (8%)	1	15
38	12	149/179 (83%)	127 (85%)	18 (12%)	4 (3%)	5	40
39	13	127/130 (98%)	116 (91%)	8 (6%)	3 (2%)	6	42
40	14	125/130 (96%)	105 (84%)	10 (8%)	10 (8%)	1	16
41	15	96/103 (93%)	75 (78%)	16 (17%)	5 (5%)	2	26
42	16	114/129 (88%)	95 (83%)	13 (11%)	6 (5%)	2	25
43	17	121/124 (98%)	91 (75%)	24 (20%)	6 (5%)	2	26
44	18	112/118 (95%)	98 (88%)	8 (7%)	6 (5%)	2	25
45	19	98/101 (97%)	80 (82%)	13 (13%)	5 (5%)	2	26
46	20	86/89 (97%)	62 (72%)	14 (16%)	10 (12%)	0	7
47	21	80/82 (98%)	64 (80%)	11 (14%)	5 (6%)	1	22
48	22	78/84 (93%)	60 (77%)	13 (17%)	5 (6%)	1	22
49	23	63/75 (84%)	52 (82%)	6 (10%)	5 (8%)	1	16
50	24	77/92 (84%)	64 (83%)	11 (14%)	2 (3%)	6	40
51	25	83/87 (95%)	77 (93%)	6 (7%)	0	100	100
52	26	63/71 (89%)	39 (62%)	15 (24%)	9 (14%)	0	4
All	All	5985/6970 (86%)	4958 (83%)	749 (12%)	278 (5%)	5	28

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%)	85	93
6	F	137/138 (99%)	136 (99%)	1 (1%)	85	93
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%)	78	89
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%)	78	89
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%)	63	83
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

Continued on next page...

Continued from previous page...

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%)	76	88
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%)	94	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.