



wwPDB EM Validation Summary Report ⓘ

Nov 3, 2022 – 01:43 AM EDT

PDB ID : 5UYK
EMDB ID : EMD-8615
Title : 70S ribosome bound with cognate ternary complex not base-paired to A site codon (Structure I)
Authors : Loveland, A.B.; Demo, G.; Grigorieff, N.; Korostelev, A.A.
Deposited on : 2017-02-24
Resolution : 3.90 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

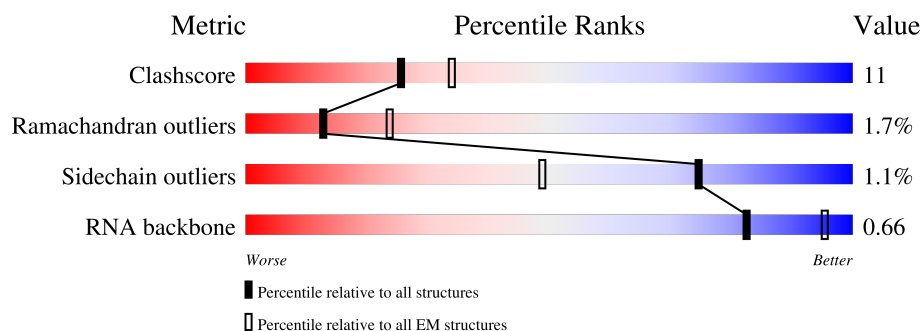
1 Overall quality at a glance

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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	04	271	64% 34% .
2	05	209	69% 30%
3	06	201	73% 26% .
4	07	177	66% 32% .
5	08	176	63% 36% .
6	09	149	59% 40% .
7	10	131	47% 47% 5%


























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Mol	Chain	Length	Quality of chain
8	11	141	 53% 46%
9	12	142	 70% 30%
10	13	122	 71% 27%
11	14	143	 76% 23%
12	15	136	 68% 31%
13	16	120	 69% 30%
14	17	116	 74% 26%
15	18	114	 68% 32%
16	19	117	 68% 32%
17	20	103	 74% 24%
18	21	110	 67% 32%
19	22	93	 70% 30%
20	23	102	 70% 29%
21	24	94	 65% 35%
22	25	75	 67% 33%
23	26	77	 69% 31%
24	27	63	 57% 40%
25	28	58	 76% 22%
26	29	66	 67% 33%
27	30	56	 50% 50%
28	31	50	 70% 30%
29	32	46	 76% 24%
30	33	64	 83% 16%
31	34	38	 58% 39%
32	B	218	 57% 41%

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Mol	Chain	Length	Quality of chain
33	C	206	
34	D	205	
35	E	157	
36	F	100	
37	G	151	
38	H	129	
39	I	127	
40	J	98	
41	K	116	
42	L	123	
43	M	114	
44	N	100	
45	O	88	
46	P	82	
47	Q	80	
48	R	65	
49	S	79	
50	T	85	
51	U	65	
52	03	223	
53	A	1539	
54	01	2903	
55	02	120	
56	W	77	
56	X	77	

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Mol	Chain	Length	Quality of chain
57	V	20	<div><div></div><div>75%</div><div>25%</div></div>
58	Y	76	<div><div></div><div>57%</div><div>34%</div><div>9%</div></div>
59	Z	392	<div><div></div><div>47%</div><div>52%</div><div>.</div></div>

2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 154412 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	04	271	Total	C	N	O	S	0	0
			2083	1288	423	365	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	05	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	06	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	07	177	Total	C	N	O	S	0	0
			1411	899	249	257	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	08	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	09	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	10	131	Total	C	N	O	S	0	0
			989	625	175	184	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	11	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	12	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	13	122	Total	C	N	O	S	0	0
			939	587	180	166	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	14	143	Total	C	N	O	S	0	0
			1045	649	206	189	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	15	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	16	120	Total	C	N	O	S	0	0
			961	593	196	167	5		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
14	17	116	Total	C	N	O	0	0
			892	552	178	162		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	18	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
16	19	117	Total	C	N	O	0	0
			947	604	192	151		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	20	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	21	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	22	93	Total	C	N	O	S	0	0
			739	466	139	132	2		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
20	23	102	Total	C	N	O	0	0
			780	492	146	142		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	24	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	25	75	Total	C	N	O	S	0	0
			575	356	116	102	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	26	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
24	27	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	28	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	29	66	Total	C	N	O	S	0	0
			523	323	99	95	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	30	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
28	31	50	Total	C	N	O	0	0
			410	263	75	72		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
29	32	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	33	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	34	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
32	B	218	Total	C	N	O	S	0	0
			1705	1081	305	312	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
33	C	206	Total	C	N	O	S	0	0
			1625	1028	305	289	3		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
35	E	157	Total	C	N	O	S	0	0
			1157	719	218	214	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
36	F	100	Total	C	N	O	S	0	0
			818	515	148	149	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
37	G	151	Total	C	N	O	S	0	0
			1182	735	227	216	4		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
40	J	98	Total	C	N	O	S	0	0
			787	493	150	143	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
41	K	116	Total	C	N	O	S	0	0
			870	535	173	159	3		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
43	M	114	Total	C	N	O	S	0	0
			884	546	178	157	3		

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
47	Q	80	Total	C	N	O	S	0	0
			649	411	121	114	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
48	R	65	Total	C	N	O	S	0	0
			536	339	100	96	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
49	S	79	Total	C	N	O	S	0	0
			638	408	120	108	2		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
51	U	65	Total	C	N	O	S	0	0
			545	335	117	92	1		

- Molecule 52 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	03	223	Total	C	N	O	S	0	0
			1662	1039	302	315	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
53	A	1539	Total	C	N	O	P	0	0
			33012	14725	6052	10697	1538		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
54	01	2903	Total	C	N	O	P	0	0
			62317	27801	11468	20146	2902		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
01	747	C	U	conflict	GB 802133627

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

Mol	Chain	Residues	Atoms					AltConf	Trace
55	02	120	Total	C	N	O	P	0	0
			2568	1145	471	833	119		

- Molecule 56 is a RNA chain called tRNAfMet.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	X	77	Total	C	N	O	P	0	0
			1640	732	297	535	76		
56	W	77	Total	C	N	O	P	0	0
			1640	732	297	535	76		

- Molecule 57 is a RNA chain called mRNA.

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

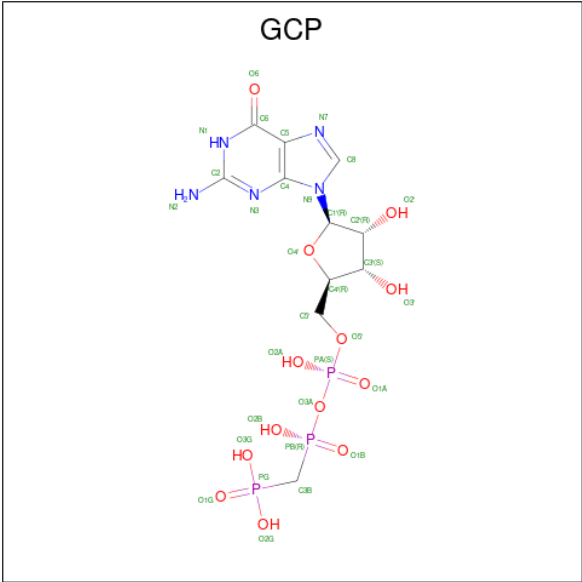
- Molecule 58 is a RNA chain called tRNAPhe.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	Y	76	Total	C	N	O	P	0	0
			1619	723	290	531	75		

- Molecule 59 is a protein called Elongation factor Tu 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	Z	392	Total	C	N	O	S	0	0
			3029	1915	521	580	13		

- Molecule 60 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: GCP) (formula: C₁₁H₁₈N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					AltConf
60	Z	1	Total	C	N	O	P	0
			32	11	5	13	3	

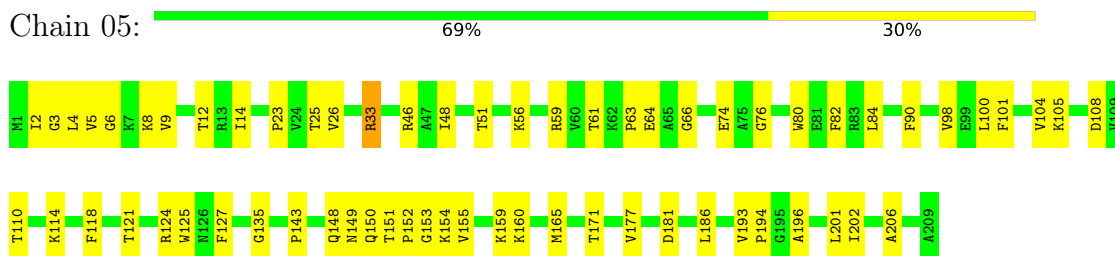
3 Residue-property plots

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

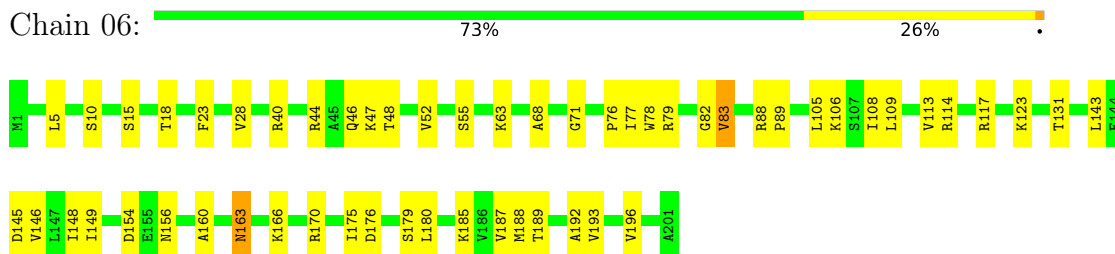
- Molecule 1: 50S ribosomal protein L2



- Molecule 2: 50S ribosomal protein L3

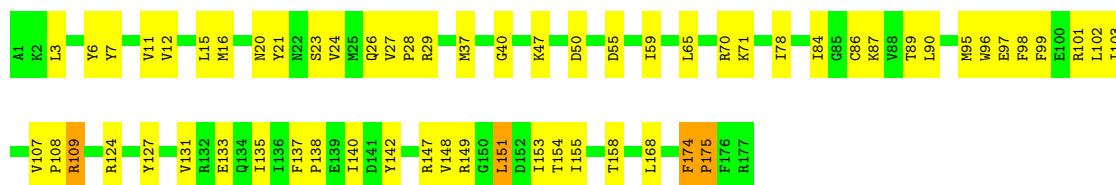


- Molecule 3: 50S ribosomal protein L4



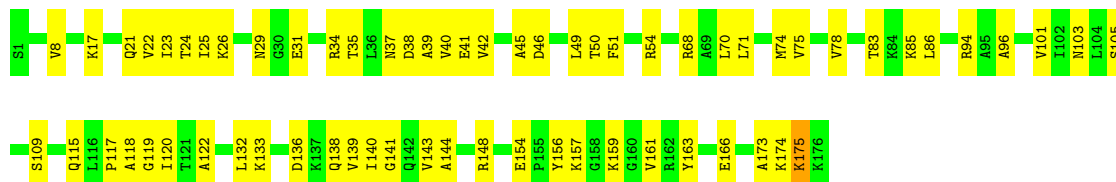
- Molecule 4: 50S ribosomal protein L5





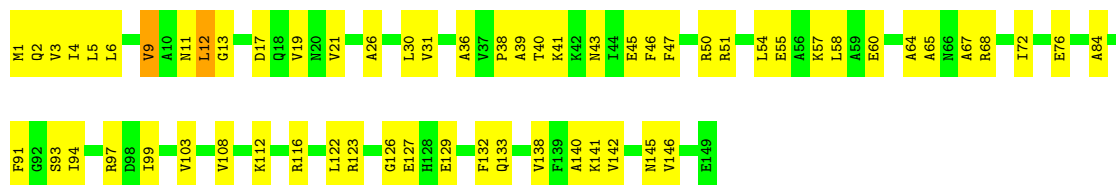
• Molecule 5: 50S ribosomal protein L6

Chain 08: 63% 36%



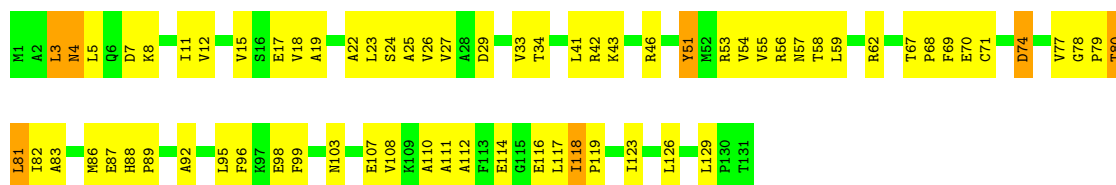
• Molecule 6: 50S ribosomal protein L9

Chain 09: 59% 40%



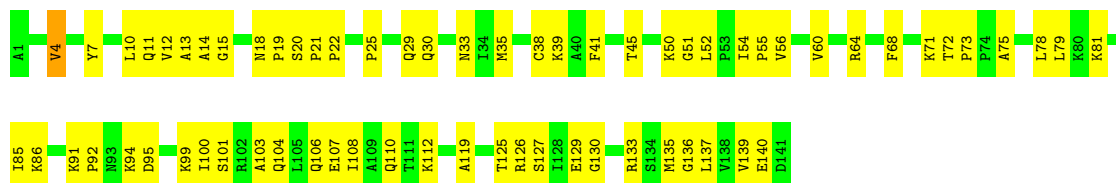
• Molecule 7: 50S ribosomal protein L10

Chain 10: 47% 47% 5%



• Molecule 8: 50S ribosomal protein L11

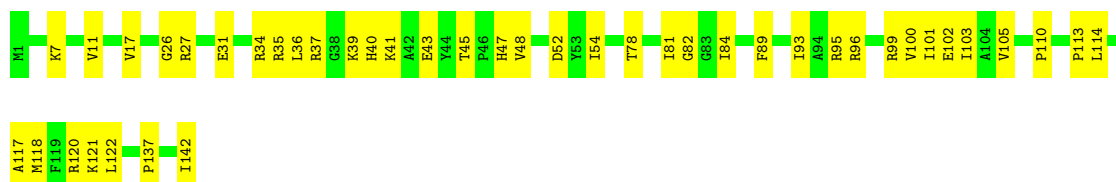
Chain 11: 53% 46%



• Molecule 9: 50S ribosomal protein L13

Chain 12: 70% 30%





- Molecule 10: 50S ribosomal protein L14

Chain 13: 71% 27% .



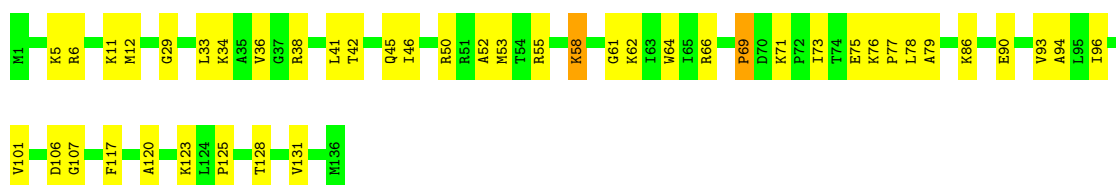
- Molecule 11: 50S ribosomal protein L15

Chain 14: 76% 23% .



- Molecule 12: 50S ribosomal protein L16

Chain 15: 68% 31% .



- Molecule 13: 50S ribosomal protein L17

Chain 16: 69% 30% .




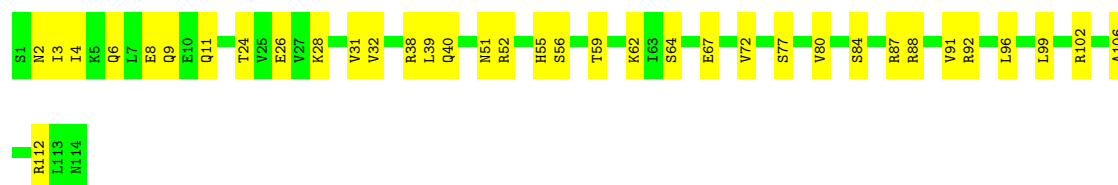
- Molecule 14: 50S ribosomal protein L18

Chain 17: 74% 26% .



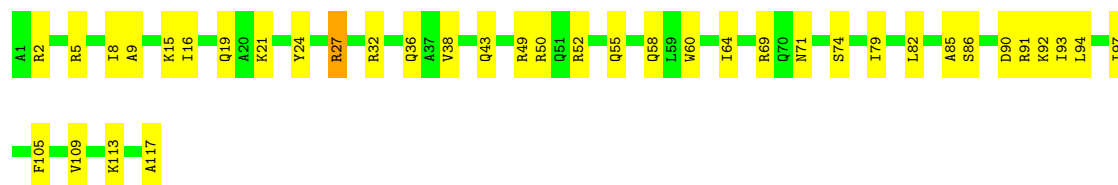
- Molecule 15: 50S ribosomal protein L19

Chain 18:  68% 32%



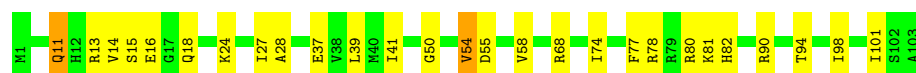
- Molecule 16: 50S ribosomal protein L20

Chain 19:  68% 32%



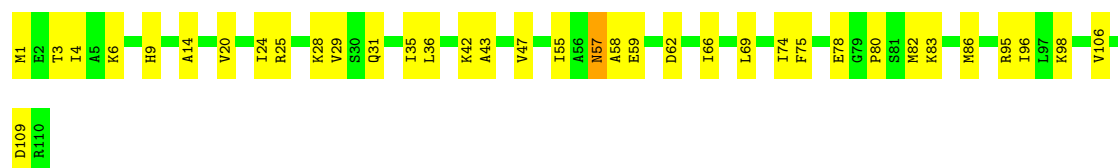
- Molecule 17: 50S ribosomal protein L21

Chain 20:  74% 24%



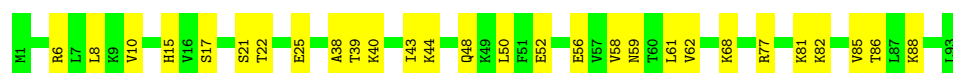
- Molecule 18: 50S ribosomal protein L22

Chain 21:  67% 32%



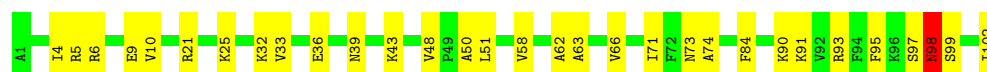
- Molecule 19: 50S ribosomal protein L23

Chain 22:  70% 30%



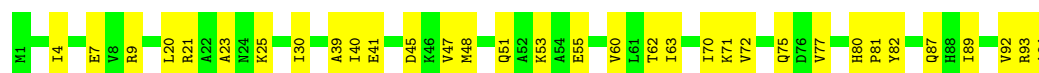
- Molecule 20: 50S ribosomal protein L24

Chain 23:  70% 29%



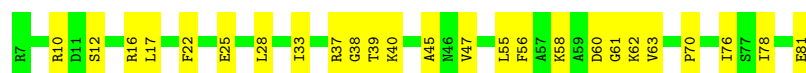
- Molecule 21: 50S ribosomal protein L25

Chain 24:  65% 35%



- Molecule 22: 50S ribosomal protein L27

Chain 25:  67% 33%



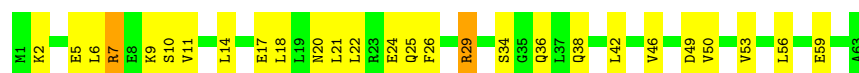
- Molecule 23: 50S ribosomal protein L28

Chain 26:  69% 31%




- Molecule 24: 50S ribosomal protein L29

Chain 27:  57% 40% .



- Molecule 25: 50S ribosomal protein L30

Chain 28:  76% 22% .



- Molecule 26: 50S ribosomal protein L31

Chain 29:  67% 33%



- Molecule 27: 50S ribosomal protein L32

Chain 30:  50% 50%




- Molecule 28: 50S ribosomal protein L33

Chain 31:  70% 30%




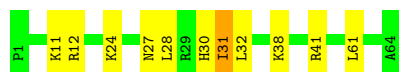
- Molecule 29: 50S ribosomal protein L34

Chain 32:  76% 24%



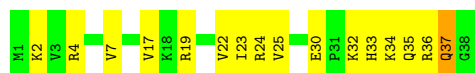
- Molecule 30: 50S ribosomal protein L35

Chain 33:  83% 16% .



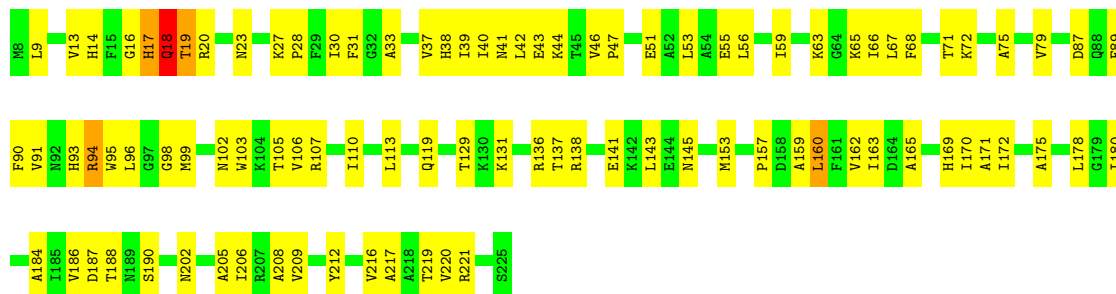
- Molecule 31: 50S ribosomal protein L36

Chain 34:  58% 39% .



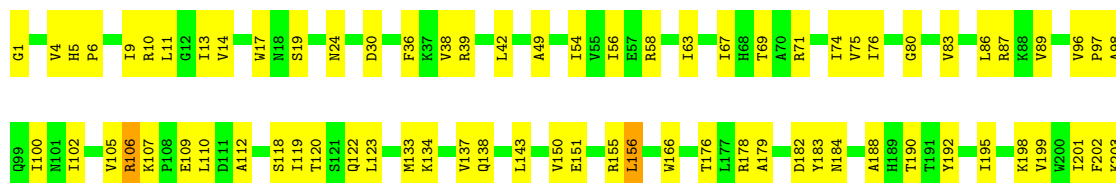
- Molecule 32: 30S ribosomal protein S2

Chain B:  57% 41% .



- Molecule 33: 30S ribosomal protein S3

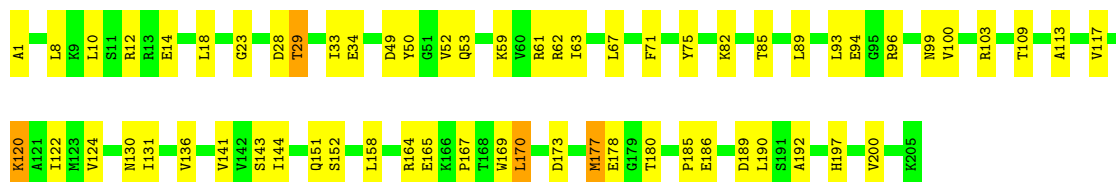
Chain C:  64% 35% .





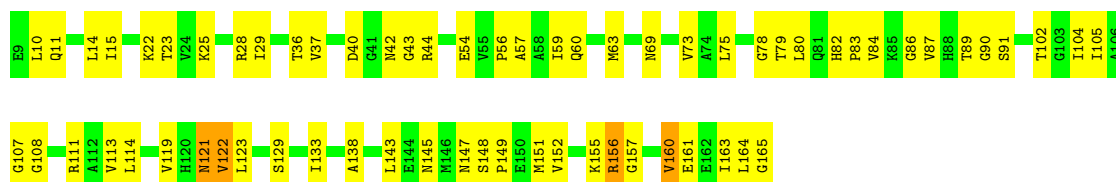
- Molecule 34: 30S ribosomal protein S4

Chain D: 70% 28%



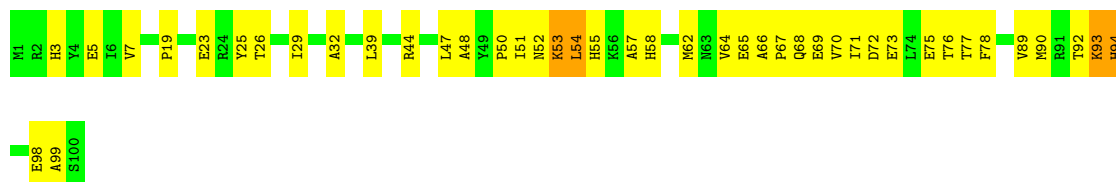
- Molecule 35: 30S ribosomal protein S5

Chain E: 59% 39%



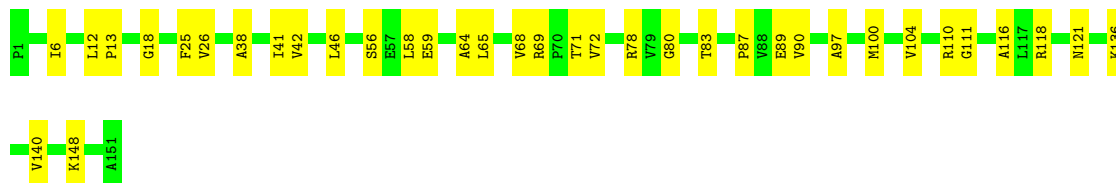
- Molecule 36: 30S ribosomal protein S6

Chain F: 57% 39%



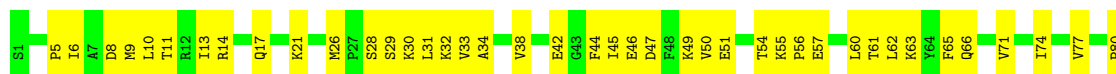
- Molecule 37: 30S ribosomal protein S7

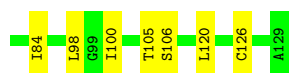
Chain G: 76% 24%



- Molecule 38: 30S ribosomal protein S8

Chain H: 63% 37%





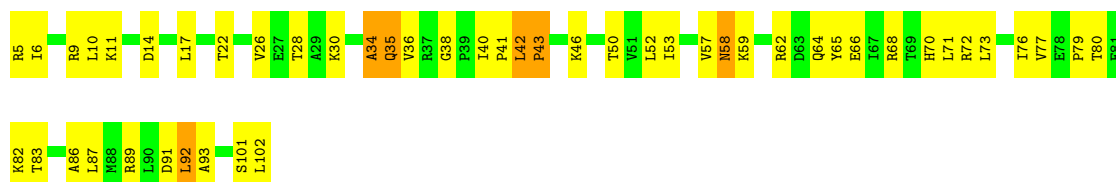
- Molecule 39: 30S ribosomal protein S9

Chain I: 59% 39% .



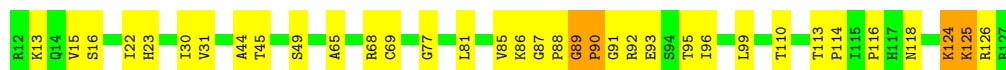
- Molecule 40: 30S ribosomal protein S10

Chain J: 50% 44% 6%



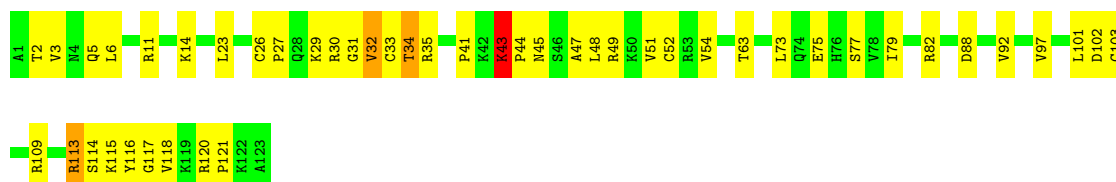
- Molecule 41: 30S ribosomal protein S11

Chain K: 70% 27%



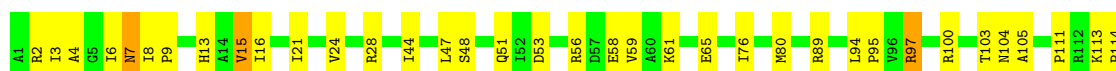
- Molecule 42: 30S ribosomal protein S12

Chain L: 62% 35%



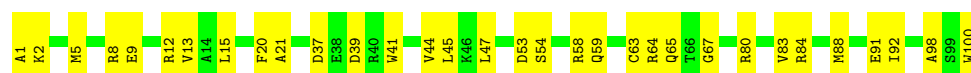
- Molecule 43: 30S ribosomal protein S13

Chain M: 68% 29%



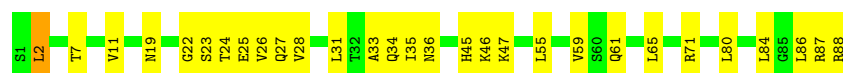
- Molecule 44: 30S ribosomal protein S14

Chain N:  68% 32%



- Molecule 45: 30S ribosomal protein S15

Chain O:  67% 32%



- Molecule 46: 30S ribosomal protein S16

Chain P:  60% 39%



- Molecule 47: 30S ribosomal protein S17

Chain Q:  59% 39%



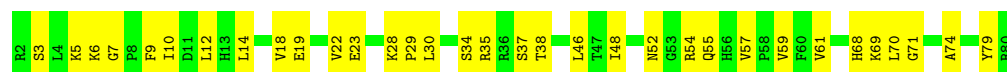
- Molecule 48: 30S ribosomal protein S18

Chain R:  71% 26%



- Molecule 49: 30S ribosomal protein S19

Chain S:  58% 42%



- Molecule 50: 30S ribosomal protein S20

Chain T:  68% 31%



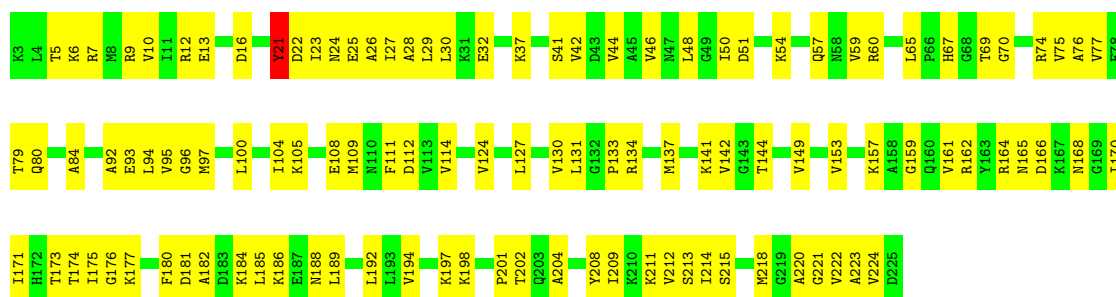
- Molecule 51: 30S ribosomal protein S21

Chain U:  48% 52%



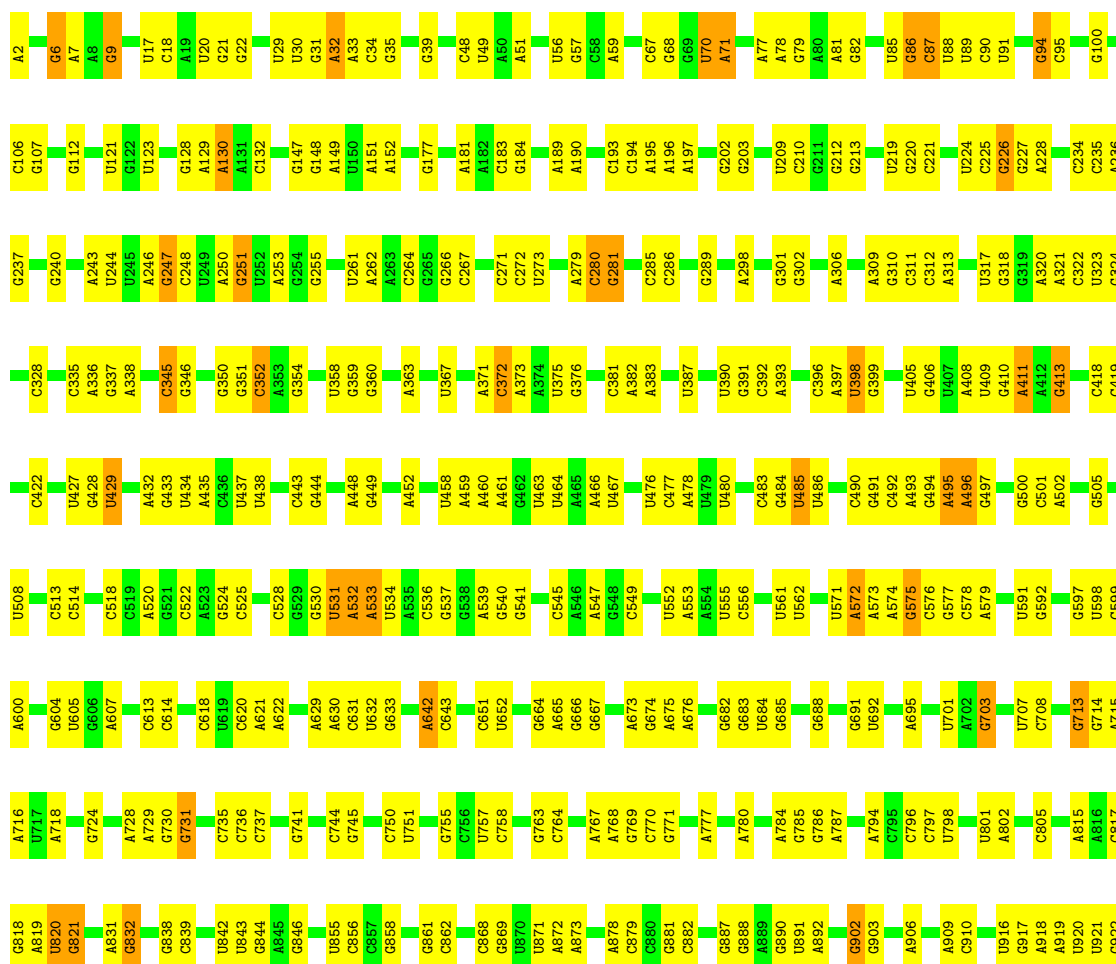
• Molecule 52: 50S ribosomal protein L1

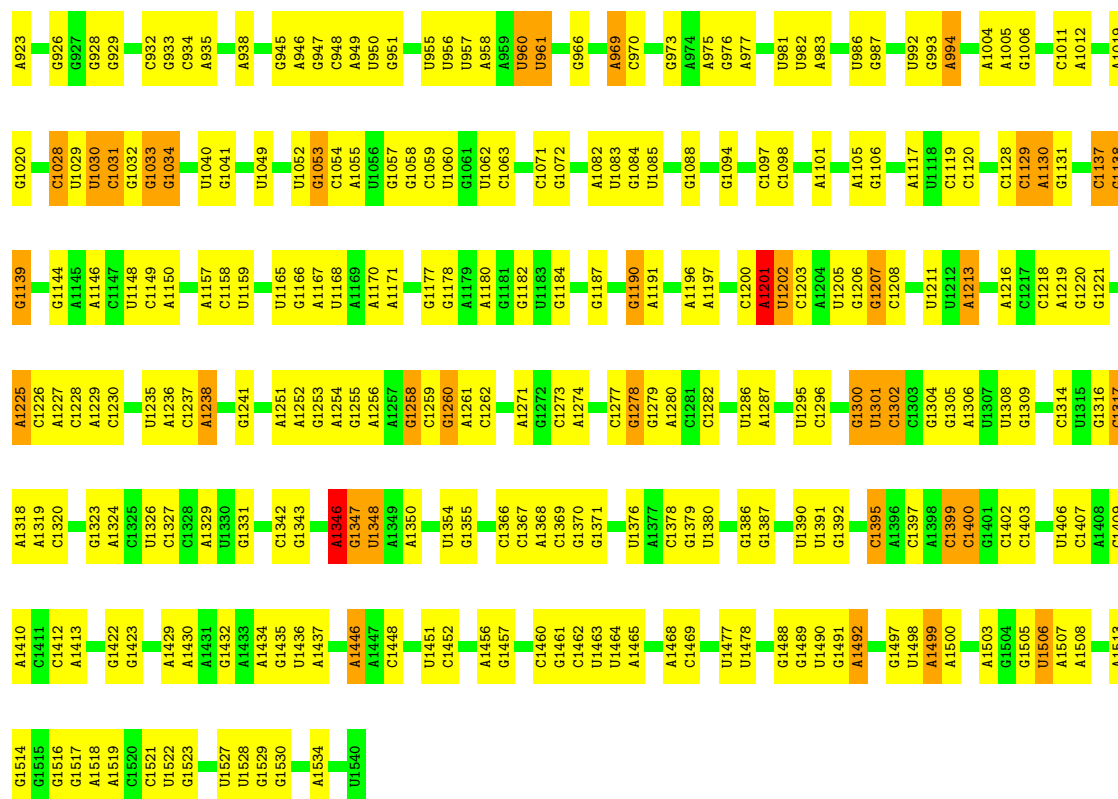
Chain 03:  50% 49%



• Molecule 53: 16S ribosomal RNA

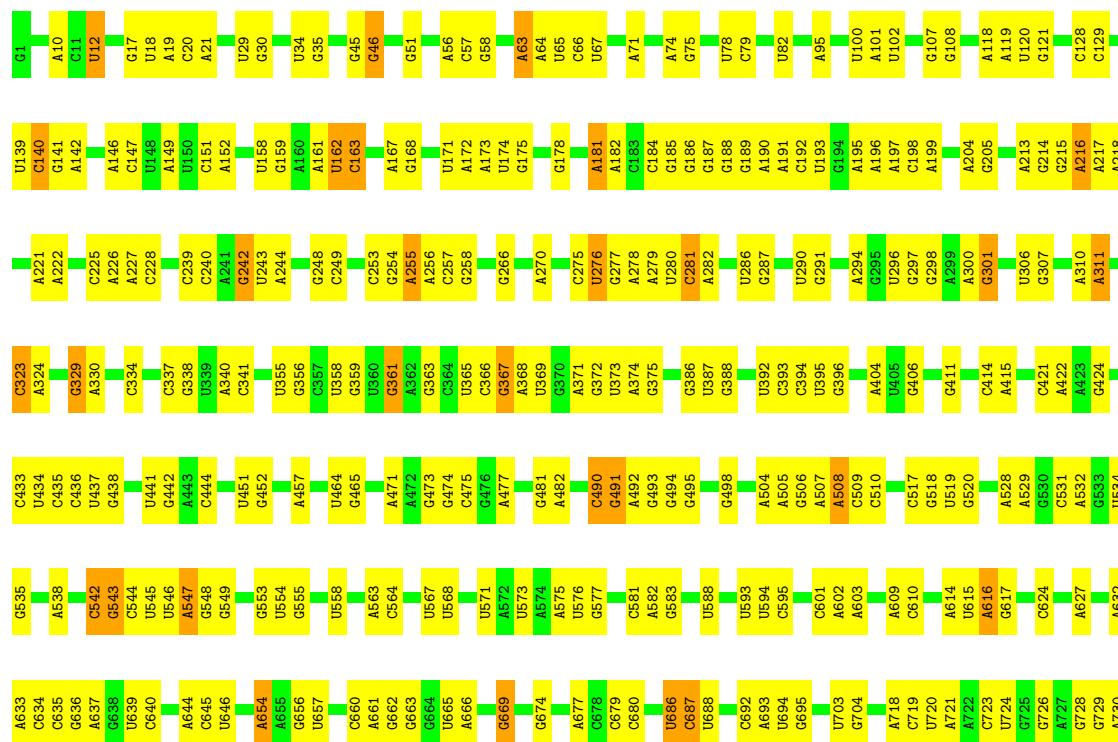
Chain A:  58% 37% 5%



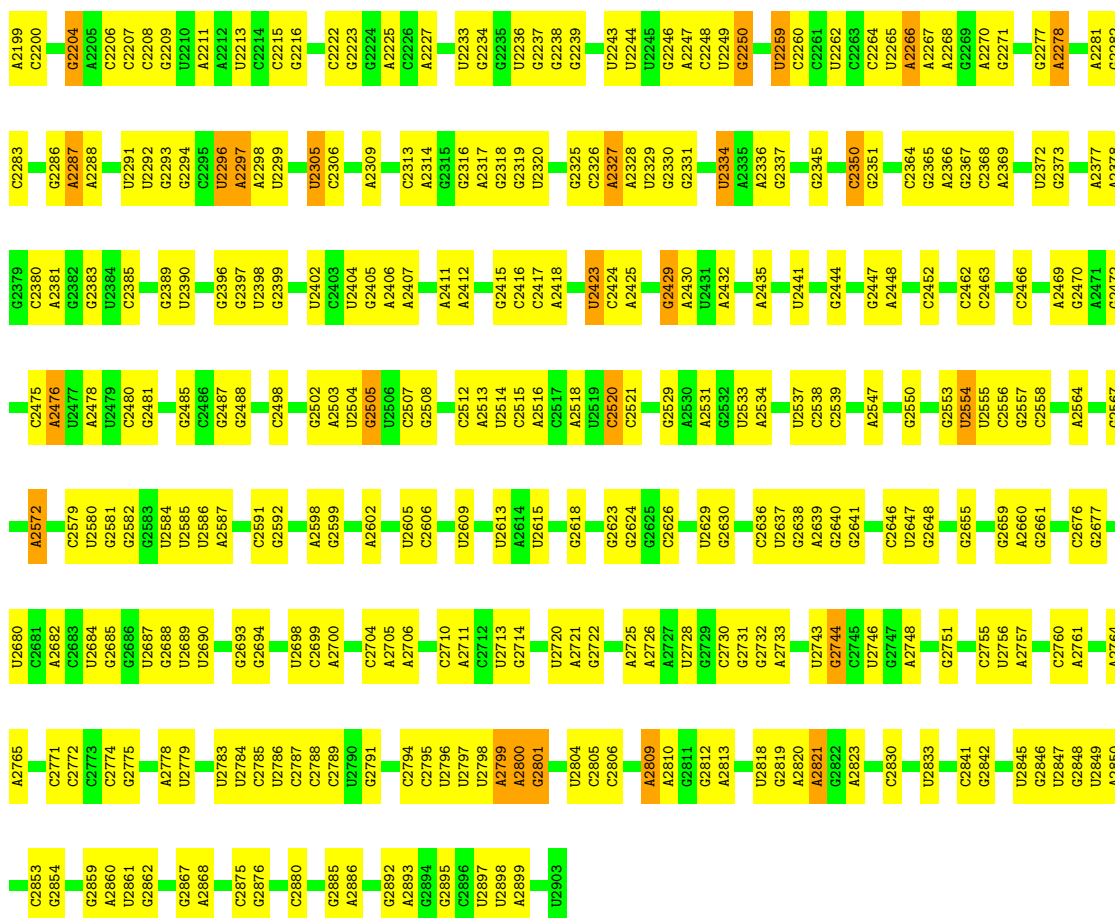


• Molecule 54: 23S ribosomal RNA

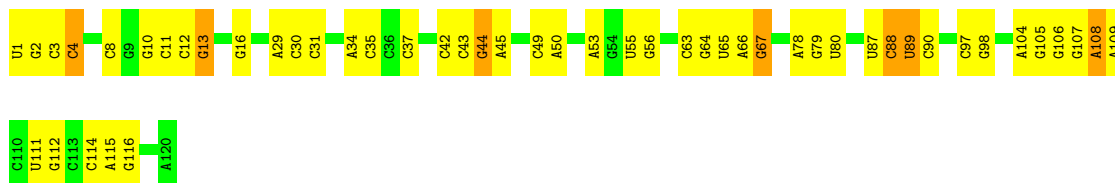
Chain 01: 57% 39%



U2137	C2065	C1967	G1845	C1760	A1564	G1555	G1441	U1329	G1212	C1102	A1001	A899	A819	C731
G2138	C2066	A1970	U1856	C1761	A1665	G1555	U1442	G1332	A1213	A1103	G1002	A905	A820	C732
U2139	G2067	G1857	G1862	A1763	G1666	U1559	G1443	G1332	G1236	C1104	G1011	U906	A821	G733
G2140	U2068	C1764	A1858	C1764	A1569	U1559	G1444	U1344	G1237	U1105	G1012	A910	A826	U741
G2141	G2069	U1765	U1859	G1766	A1569	U1563	C1447	G1346	G1238	U1106	C1013	A911	U826	U742
A2142	A2070	G1767	G1860	G1767	A1569	C1564	G1448	G1347	A1246	U1107	U1019	A911	U827	A743
C2143	A2071	A1772	G1869	G1767	A1569	U1563	C1449	G1348	A1247	G1110	A1020	C915	U828	U744
G2144	C2072	A1773	A1870	A1772	A1569	C1564	C1454	C1349	G1248	A1111	A1021	C916	U829	U745
C2145	C2073	A1773	A1871	A1773	A1569	C1564	C1454	C1349	G1248	A1111	A1021	C916	U830	U746
C2146	U2074	U1775	A1872	C1774	A1569	C1564	C1454	C1349	G1248	A1111	A1021	C916	U830	U746
A2147	U2075	G1776	C1874	G1776	A1569	C1564	C1454	C1349	G1248	A1111	A1021	C916	U830	C747
C2148	A2080	A1780	G1875	G1776	A1569	C1564	C1454	C1349	G1248	A1111	A1021	C916	U830	G748
U2149	A2081	A1780	G1875	G1776	A1569	C1564	C1454	C1349	G1248	A1111	A1021	C916	U830	A752
C2150	A2082	A1780	G1875	G1776	A1569	C1564	C1454	C1349	G1248	A1111	A1021	C916	U830	U755
U2151	G2083	A1780	G1875	G1776	A1569	C1564	C1454	C1349	G1248	A1111	A1021	C916	U830	A756
C2152	U2086	A1780	G1875	G1776	A1569	C1564	C1454	C1349	G1248	A1111	A1021	C916	U830	G760
U2155	G2087	A1780	G1875	G1776	A1569	C1564	C1454	C1349	G1248	A1111	A1021	C916	U830	U762
C2156	G2087	A1780	G1875	G1776	A1569	C1564	C1454	C1349	G1248	A1111	A1021	C916	U830	A764
G2157	C2091	A1780	G1875	G1776	A1569	C1564	C1454	C1349	G1248	A1111	A1021	C916	U830	U767
A2158	U2092	A1780	G1875	G1776	A1569	C1564	C1454	C1349	G1248	A1111	A1021	C916	U830	G768
G2159	C2093	A1780	G1875	G1776	A1569	C1564	C1454	C1349	G1248	A1111	A1021	C916	U830	G774
C2160	A2094	A1780	G1875	G1776	A1569	C1564	C1454	C1349	G1248	A1111	A1021	C916	U830	G775
C2161	U2095	A1780	G1875	G1776	A1569	C1564	C1454	C1349	G1248	A1111	A1021	C916	U830	G776
G2162	C2096	A1780	G1875	G1776	A1569	C1564	C1454	C1349	G1248	A1111	A1021	C916	U830	U779
A2163	U2097	A1780	G1875	G1776	A1569	C1564	C1454	C1349	G1248	A1111	A1021	C916	U830	G780
C2164	U2098	A1780	G1875	G1776	A1569	C1564	C1454	C1349	G1248	A1111	A1021	C916	U830	A781
U2167	C2102	A1780	G1875	G1776	A1569	C1564	C1454	C1349	G1248	A1111	A1021	C916	U830	A782
G2168	C2103	A1780	G1875	G1776	A1569	C1564	C1454	C1349	G1248	A1111	A1021	C916	U830	A783
A2169	C2104	A1780	G1875	G1776	A1569	C1564	C1454	C1349	G1248	A1111	A1021	C916	U830	G784
C2170	U2105	A1780	G1875	G1776	A1569	C1564	C1454	C1349	G1248	A1111	A1021	C916	U830	G785
U2171	G2028	A1780	G1875	G1776	A1569	C1564	C1454	C1349	G1248	A1111	A1021	C916	U830	C795
U2172	U2029	A1780	G1875	G1776	A1569	C1564	C1454	C1349	G1248	A1111	A1021	C916	U830	C796
A2173	C2107	A1780	G1875	G1776	A1569	C1564	C1454	C1349	G1248	A1111	A1021	C916	U830	C797
C2174	U2109	A1780	G1875	G1776	A1569	C1564	C1454	C1349	G1248	A1111	A1021	C916	U830	G798
C2175	G2110	A1780	G1875	G1776	A1569	C1564	C1454	C1349	G1248	A1111	A1021	C916	U830	G799
A2176	U2111	A1780	G1875	G1776	A1569	C1564	C1454	C1349	G1248	A1111	A1021	C916	U830	A800
C2177	C2112	A1780	G1875	G1776	A1569	C1564	C1454	C1349	G1248	A1111	A1021	C916	U830	A801
U2180	U2113	A1780	G1875	G1776	A1569	C1564	C1454	C1349	G1248	A1111	A1021	C916	U830	A802
U2181	C2114	A1780	G1875	G1776	A1569	C1564	C1454	C1349	G1248	A1111	A1021	C916	U830	U803
U2182	G2115	A1780	G1875	G1776	A1569	C1564	C1454	C1349	G1248	A1111	A1021	C916	U830	A804
A2183	C2116	A1780	G1875	G1776	A1569	C1564	C1454	C1349	G1248	A1111	A1021	C916	U830	G805
C2184	U2117	A1780	G1875	G1776	A1569	C1564	C1454	C1349	G1248	A1111	A1021	C916	U830	G806
U2185	U2118	A1780	G1875	G1776	A1569	C1564	C1454	C1349	G1248	A1111	A1021	C916	U830	U807
G2186	A2119	A1780	G1875	G1776	A1569	C1564	C1454	C1349	G1248	A1111	A1021	C916	U830	G808
U2187	C2120	A1780	G1875	G1776	A1569	C1564	C1454	C1349	G1248	A1111	A1021	C916	U830	C812
C2188	U2121	A1780	G1875	G1776	A1569	C1564	C1454	C1349	G1248	A1111	A1021	C916	U830	C815
U2189	U2122	A1780	G1875	G1776	A1569	C1564	C1454	C1349	G1248	A1111	A1021	C916	U830	C816
G2190	C2123	A1780	G1875	G1776	A1569	C1564	C1454	C1349	G1248	A1111	A1021	C916	U830	C817
A2191	A2054	A1780	G1875	G1776	A1569	C1564	C1454	C1349	G1248	A1111	A1021	C916	U830	G818
U2192	C2055	A1780	G1875	G1776	A1569	C1564	C1454	C1349	G1248	A1111	A1021	C916	U830	
C2193	G2056	A1780	G1875	G1776	A1569	C1564	C1454	C1349	G1248	A1111	A1021	C916	U830	
U2194	A2126	A1780	G1875	G1776	A1569	C1564	C1454	C1349	G1248	A1111	A1021	C916	U830	
U2195	C2127	A1780	G1875	G1776	A1569	C1564	C1454	C1349	G1248	A1111	A1021	C916	U830	
C2196	G2128	A1780	G1875	G1776	A1569	C1564	C1454	C1349	G1248	A1111	A1021	C916	U830	
U2197	U2132	A1780	G1875	G1776	A1569	C1564	C1454	C1349	G1248	A1111	A1021	C916	U830	
A2198	C2133	A1780	G1875	G1776	A1569	C1564	C1454	C1349	G1248	A1111	A1021	C916	U830	



• Molecule 55: 5S ribosomal RNA



• Molecule 56: tRNA^{fMet}



• Molecule 56: tRNA^{fMet}



- Molecule 57: mRNA

Chain V:  75% 25%



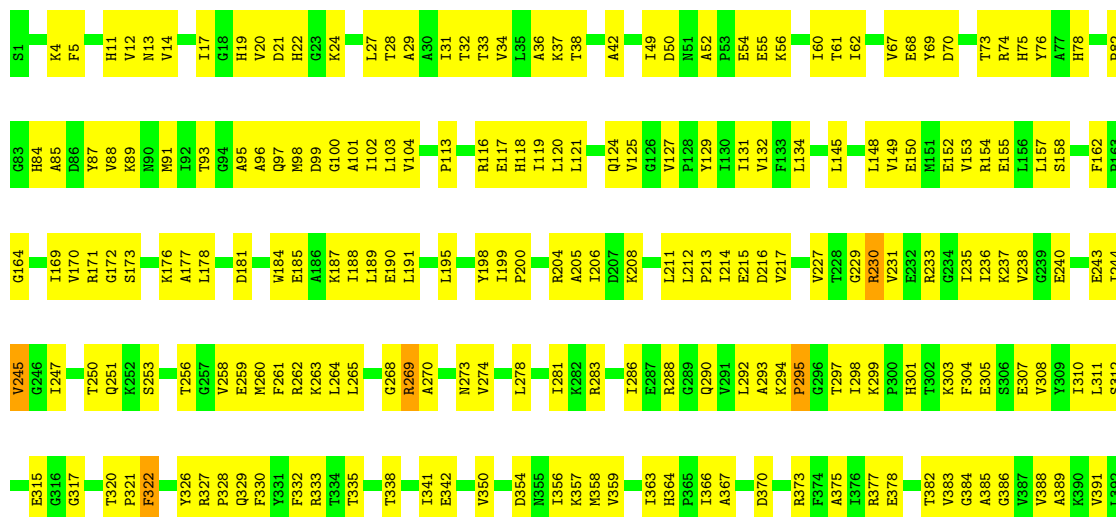
- Molecule 58: tRNAPhe

Chain Y:  57% 34% 9%



- Molecule 59: Elongation factor Tu 2

Chain Z:  47% 52%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	6726	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; CTFFIND3 was used to determine CTF values. FREALIGN applied CTF correction.	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.0	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	60976	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GCP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	04	0.32	0/2122	0.60	0/2852
2	05	0.34	0/1586	0.57	0/2134
3	06	0.33	0/1571	0.56	0/2113
4	07	0.37	0/1435	0.57	0/1926
5	08	0.31	0/1343	0.57	0/1816
6	09	0.37	0/1122	0.58	0/1515
7	10	0.41	0/1002	0.69	0/1350
8	11	0.38	0/1046	0.56	0/1410
9	12	0.33	0/1152	0.56	0/1551
10	13	0.32	0/948	0.59	0/1268
11	14	0.33	0/1054	0.61	0/1403
12	15	0.36	0/1093	0.57	0/1460
13	16	0.35	0/974	0.55	0/1301
14	17	0.32	0/902	0.52	0/1209
15	18	0.34	0/929	0.57	0/1242
16	19	0.36	0/960	0.49	0/1278
17	20	0.36	0/829	0.63	0/1107
18	21	0.30	0/864	0.60	0/1156
19	22	0.31	0/745	0.54	0/994
20	23	0.35	0/788	0.64	1/1051 (0.1%)
21	24	0.35	0/766	0.57	0/1025
22	25	0.37	0/582	0.51	0/769
23	26	0.35	0/635	0.53	0/848
24	27	0.32	0/510	0.55	0/677
25	28	0.31	0/453	0.54	0/605
26	29	0.40	0/532	0.58	0/709
27	30	0.31	0/450	0.57	0/599
28	31	0.37	0/417	0.59	0/554
29	32	0.37	0/380	0.54	0/498
30	33	0.34	0/513	0.61	0/676
31	34	0.29	0/303	0.54	0/397
32	B	0.36	0/1736	0.64	2/2338 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
33	C	0.33	0/1652	0.53	0/2225
34	D	0.33	0/1665	0.58	0/2227
35	E	0.34	0/1170	0.65	0/1573
36	F	0.34	0/836	0.63	0/1128
37	G	0.33	0/1196	0.57	0/1602
38	H	0.33	0/989	0.60	0/1326
39	I	0.35	0/1034	0.65	0/1375
40	J	0.33	0/797	0.64	0/1077
41	K	0.35	0/886	0.57	0/1195
42	L	0.33	0/969	0.73	2/1300 (0.2%)
43	M	0.30	0/893	0.58	0/1193
44	N	0.33	0/817	0.51	0/1088
45	O	0.33	0/722	0.54	0/964
46	P	0.36	0/659	0.60	0/884
47	Q	0.34	0/658	0.62	0/881
48	R	0.37	0/545	0.58	0/731
49	S	0.37	0/653	0.54	0/877
50	T	0.32	0/671	0.50	0/888
51	U	0.40	0/551	0.59	0/728
52	03	1.26	0/1677	0.68	0/2259
53	A	0.41	0/36963	0.68	6/57662 (0.0%)
54	01	0.41	0/69796	0.67	3/108888 (0.0%)
55	02	0.36	0/2872	0.67	0/4479
56	W	0.42	0/1832	0.66	0/2855
56	X	0.55	0/1832	0.68	0/2855
57	V	0.51	0/486	0.68	0/757
58	Y	0.51	0/1809	0.69	0/2819
59	Z	1.24	0/3085	0.69	0/4173
All	All	0.44	0/167457	0.65	14/249840 (0.0%)

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	B	160	LEU	O-C-N	-6.91	111.65	122.70
54	01	974	G	N9-C1'-C2'	6.48	122.42	114.00
53	A	1300	G	N9-C1'-C2'	6.31	122.21	114.00
53	A	1201	A	C2'-C3'-O3'	5.85	123.05	113.70
53	A	438	U	N1-C1'-C2'	5.84	121.59	114.00

There are no chirality outliers.

There are no planarity outliers.

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	04	2083	0	2157	85	0
2	05	1565	0	1616	53	0
3	06	1552	0	1619	44	0
4	07	1411	0	1447	48	0
5	08	1323	0	1374	47	0
6	09	1111	0	1148	42	0
7	10	989	0	1025	67	0
8	11	1032	0	1088	52	0
9	12	1129	0	1162	41	0
10	13	939	0	1012	26	0
11	14	1045	0	1117	30	0
12	15	1074	0	1157	38	0
13	16	961	0	1000	26	0
14	17	892	0	923	22	0
15	18	917	0	965	32	0
16	19	947	0	1022	34	0
17	20	816	0	839	25	0
18	21	857	0	922	28	0
19	22	739	0	807	18	0
20	23	780	0	834	22	0
21	24	753	0	780	21	0
22	25	575	0	592	21	0
23	26	625	0	655	16	0
24	27	509	0	543	27	0
25	28	449	0	491	9	0
26	29	523	0	524	16	0
27	30	444	0	461	22	0
28	31	410	0	440	10	0
29	32	377	0	418	9	0
30	33	504	0	574	8	0
31	34	302	0	343	15	0
32	B	1705	0	1732	79	0
33	C	1625	0	1699	63	0
34	D	1643	0	1710	45	0
35	E	1157	0	1199	56	0
36	F	818	0	808	36	0
37	G	1182	0	1240	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	H	979	0	1034	35	0
39	I	1022	0	1070	40	0
40	J	787	0	828	39	0
41	K	870	0	878	27	0
42	L	955	0	1019	39	0
43	M	884	0	944	31	0
44	N	805	0	847	31	0
45	O	714	0	737	17	0
46	P	649	0	666	27	0
47	Q	649	0	691	31	0
48	R	536	0	552	12	0
49	S	638	0	665	26	0
50	T	665	0	714	20	0
51	U	545	0	579	29	0
52	03	1662	0	1750	101	0
53	A	33012	0	16618	425	0
54	01	62317	0	31346	822	0
55	02	2568	0	1303	43	0
56	W	1640	0	837	10	0
56	X	1640	0	837	23	0
57	V	432	0	218	3	0
58	Y	1619	0	822	23	0
59	Z	3029	0	3043	167	0
60	Z	32	0	14	4	0
All	All	154412	0	105455	2964	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 11.

The worst 5 of 2964 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)
52:03:137:MET:SD	52:03:137:MET:CE	2.01	1.49
54:01:45:G:H5''	54:01:46:G:H5'	1.31	1.07
52:03:26:ALA:HB2	52:03:224:VAL:HG11	1.41	1.02
36:F:3:HIS:H	36:F:92:THR:HG22	1.30	0.97
37:G:12:LEU:HD11	39:I:49:GLN:HE22	1.30	0.95

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	04	269/271 (99%)	241 (90%)	26 (10%)	2 (1%)	22	60
2	05	207/209 (99%)	185 (89%)	21 (10%)	1 (0%)	29	67
3	06	199/201 (99%)	174 (87%)	24 (12%)	1 (0%)	29	67
4	07	175/177 (99%)	155 (89%)	16 (9%)	4 (2%)	6	38
5	08	174/176 (99%)	157 (90%)	12 (7%)	5 (3%)	4	33
6	09	147/149 (99%)	124 (84%)	21 (14%)	2 (1%)	11	46
7	10	129/131 (98%)	95 (74%)	27 (21%)	7 (5%)	2	22
8	11	139/141 (99%)	111 (80%)	27 (19%)	1 (1%)	22	60
9	12	140/142 (99%)	130 (93%)	10 (7%)	0	100	100
10	13	120/122 (98%)	100 (83%)	18 (15%)	2 (2%)	9	43
11	14	141/143 (99%)	116 (82%)	21 (15%)	4 (3%)	5	34
12	15	134/136 (98%)	122 (91%)	10 (8%)	2 (2%)	10	45
13	16	118/120 (98%)	103 (87%)	15 (13%)	0	100	100
14	17	114/116 (98%)	105 (92%)	9 (8%)	0	100	100
15	18	112/114 (98%)	97 (87%)	15 (13%)	0	100	100
16	19	115/117 (98%)	110 (96%)	5 (4%)	0	100	100
17	20	101/103 (98%)	82 (81%)	18 (18%)	1 (1%)	15	52
18	21	108/110 (98%)	99 (92%)	9 (8%)	0	100	100
19	22	91/93 (98%)	80 (88%)	10 (11%)	1 (1%)	14	51
20	23	100/102 (98%)	84 (84%)	13 (13%)	3 (3%)	4	33
21	24	92/94 (98%)	86 (94%)	6 (6%)	0	100	100
22	25	73/75 (97%)	65 (89%)	8 (11%)	0	100	100
23	26	75/77 (97%)	68 (91%)	7 (9%)	0	100	100
24	27	61/63 (97%)	57 (93%)	4 (7%)	0	100	100
25	28	56/58 (97%)	52 (93%)	4 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	29	64/66 (97%)	50 (78%)	14 (22%)	0	100	100
27	30	54/56 (96%)	51 (94%)	3 (6%)	0	100	100
28	31	48/50 (96%)	41 (85%)	7 (15%)	0	100	100
29	32	44/46 (96%)	40 (91%)	4 (9%)	0	100	100
30	33	62/64 (97%)	56 (90%)	4 (6%)	2 (3%)	4	32
31	34	36/38 (95%)	28 (78%)	6 (17%)	2 (6%)	2	21
32	B	216/218 (99%)	173 (80%)	40 (18%)	3 (1%)	11	46
33	C	204/206 (99%)	188 (92%)	16 (8%)	0	100	100
34	D	203/205 (99%)	174 (86%)	23 (11%)	6 (3%)	4	33
35	E	155/157 (99%)	119 (77%)	27 (17%)	9 (6%)	1	21
36	F	98/100 (98%)	73 (74%)	21 (21%)	4 (4%)	3	27
37	G	149/151 (99%)	127 (85%)	20 (13%)	2 (1%)	12	48
38	H	127/129 (98%)	117 (92%)	9 (7%)	1 (1%)	19	57
39	I	125/127 (98%)	103 (82%)	16 (13%)	6 (5%)	2	24
40	J	96/98 (98%)	78 (81%)	10 (10%)	8 (8%)	1	14
41	K	114/116 (98%)	95 (83%)	14 (12%)	5 (4%)	2	25
42	L	121/123 (98%)	93 (77%)	19 (16%)	9 (7%)	1	16
43	M	112/114 (98%)	95 (85%)	14 (12%)	3 (3%)	5	35
44	N	98/100 (98%)	83 (85%)	15 (15%)	0	100	100
45	O	86/88 (98%)	80 (93%)	4 (5%)	2 (2%)	6	38
46	P	80/82 (98%)	68 (85%)	11 (14%)	1 (1%)	12	48
47	Q	78/80 (98%)	66 (85%)	9 (12%)	3 (4%)	3	28
48	R	63/65 (97%)	56 (89%)	5 (8%)	2 (3%)	4	32
49	S	77/79 (98%)	65 (84%)	10 (13%)	2 (3%)	5	35
50	T	83/85 (98%)	79 (95%)	3 (4%)	1 (1%)	13	49
51	U	63/65 (97%)	43 (68%)	19 (30%)	1 (2%)	9	44
52	03	221/223 (99%)	193 (87%)	27 (12%)	1 (0%)	29	67
59	Z	390/392 (100%)	349 (90%)	39 (10%)	2 (0%)	29	67
All	All	6457/6563 (98%)	5581 (86%)	765 (12%)	111 (2%)	13	43

5 of 111 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	04	232	GLY
3	06	83	VAL
4	07	175	PRO
5	08	46	ASP
5	08	119	GLY

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	04	216/216 (100%)	210 (97%)	6 (3%)	43	66
2	05	164/164 (100%)	163 (99%)	1 (1%)	86	91
3	06	165/165 (100%)	164 (99%)	1 (1%)	86	91
4	07	148/148 (100%)	146 (99%)	2 (1%)	67	81
5	08	137/137 (100%)	136 (99%)	1 (1%)	84	90
6	09	114/114 (100%)	114 (100%)	0	100	100
7	10	100/100 (100%)	99 (99%)	1 (1%)	76	86
8	11	109/109 (100%)	107 (98%)	2 (2%)	59	77
9	12	116/116 (100%)	116 (100%)	0	100	100
10	13	103/103 (100%)	102 (99%)	1 (1%)	76	86
11	14	102/102 (100%)	102 (100%)	0	100	100
12	15	109/109 (100%)	109 (100%)	0	100	100
13	16	100/100 (100%)	99 (99%)	1 (1%)	76	86
14	17	86/86 (100%)	86 (100%)	0	100	100
15	18	99/99 (100%)	99 (100%)	0	100	100
16	19	89/89 (100%)	88 (99%)	1 (1%)	73	84
17	20	84/84 (100%)	83 (99%)	1 (1%)	71	83
18	21	93/93 (100%)	91 (98%)	2 (2%)	52	71
19	22	80/80 (100%)	78 (98%)	2 (2%)	47	69
20	23	83/83 (100%)	83 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	24	78/78 (100%)	78 (100%)	0	100	100
22	25	57/57 (100%)	57 (100%)	0	100	100
23	26	67/67 (100%)	67 (100%)	0	100	100
24	27	55/55 (100%)	53 (96%)	2 (4%)	35	61
25	28	48/48 (100%)	47 (98%)	1 (2%)	53	73
26	29	59/59 (100%)	59 (100%)	0	100	100
27	30	47/47 (100%)	47 (100%)	0	100	100
28	31	45/45 (100%)	45 (100%)	0	100	100
29	32	38/38 (100%)	37 (97%)	1 (3%)	46	68
30	33	51/51 (100%)	51 (100%)	0	100	100
31	34	34/34 (100%)	34 (100%)	0	100	100
32	B	180/180 (100%)	177 (98%)	3 (2%)	60	78
33	C	170/170 (100%)	167 (98%)	3 (2%)	59	77
34	D	172/172 (100%)	169 (98%)	3 (2%)	60	78
35	E	119/119 (100%)	116 (98%)	3 (2%)	47	69
36	F	87/87 (100%)	87 (100%)	0	100	100
37	G	124/124 (100%)	124 (100%)	0	100	100
38	H	104/104 (100%)	104 (100%)	0	100	100
39	I	105/105 (100%)	105 (100%)	0	100	100
40	J	86/86 (100%)	86 (100%)	0	100	100
41	K	89/89 (100%)	88 (99%)	1 (1%)	73	84
42	L	103/103 (100%)	101 (98%)	2 (2%)	57	75
43	M	92/92 (100%)	89 (97%)	3 (3%)	38	63
44	N	83/83 (100%)	83 (100%)	0	100	100
45	O	76/76 (100%)	76 (100%)	0	100	100
46	P	65/65 (100%)	62 (95%)	3 (5%)	27	55
47	Q	74/74 (100%)	74 (100%)	0	100	100
48	R	56/56 (100%)	55 (98%)	1 (2%)	59	77
49	S	70/70 (100%)	70 (100%)	0	100	100
50	T	65/65 (100%)	62 (95%)	3 (5%)	27	55
51	U	55/55 (100%)	54 (98%)	1 (2%)	59	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
52	03	174/174 (100%)	172 (99%)	2 (1%)	73	84
59	Z	324/325 (100%)	317 (98%)	7 (2%)	52	71
All	All	5349/5350 (100%)	5288 (99%)	61 (1%)	74	84

5 of 61 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
32	B	94	ARG
59	Z	237	LYS
35	E	69	ASN
59	Z	230	ARG
59	Z	357	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 86 such sidechains are listed below:

Mol	Chain	Res	Type
37	G	27	ASN
48	R	51	GLN
38	H	17	GLN
42	L	45	ASN
50	T	60	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
53	A	1538/1539 (99%)	161 (10%)	10 (0%)
54	01	2902/2903 (99%)	355 (12%)	12 (0%)
55	02	119/120 (99%)	9 (7%)	1 (0%)
56	W	76/77 (98%)	7 (9%)	0
56	X	76/77 (98%)	11 (14%)	0
57	V	19/20 (95%)	2 (10%)	0
58	Y	75/76 (98%)	12 (16%)	0
All	All	4805/4812 (99%)	557 (11%)	23 (0%)

5 of 557 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
53	A	6	G
53	A	7	A

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Mol	Chain	Res	Type
53	A	9	G
53	A	22	G
53	A	31	G

5 of 23 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
54	01	858	G
54	01	1130	U
54	01	1020	A
54	01	1378	A
53	A	1190	G

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
60	GCP	Z	401	-	27,34,34	2.03	8 (29%)	34,54,54	4.00	18 (52%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	GCP	Z	401	-	-	9/15/38/38	0/3/3/3

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	Z	401	GCP	O4'-C1'	4.68	1.47	1.41
60	Z	401	GCP	PB-O3A	-3.92	1.54	1.58
60	Z	401	GCP	C6-N1	3.84	1.39	1.33
60	Z	401	GCP	C5-C6	3.54	1.47	1.41
60	Z	401	GCP	C2'-C1'	2.97	1.58	1.53

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	Z	401	GCP	C1'-N9-C4	13.35	150.09	126.64
60	Z	401	GCP	C5-C6-N1	-9.07	111.03	123.43
60	Z	401	GCP	O1G-PG-C3B	-7.45	95.19	111.24
60	Z	401	GCP	C2-N1-C6	6.79	126.72	115.93
60	Z	401	GCP	O4'-C1'-C2'	-6.74	97.07	106.93

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
60	Z	401	GCP	PB-C3B-PG-O1G
60	Z	401	GCP	PB-C3B-PG-O2G
60	Z	401	GCP	PG-C3B-PB-O1B
60	Z	401	GCP	C5'-O5'-PA-O3A
60	Z	401	GCP	O4'-C4'-C5'-O5'

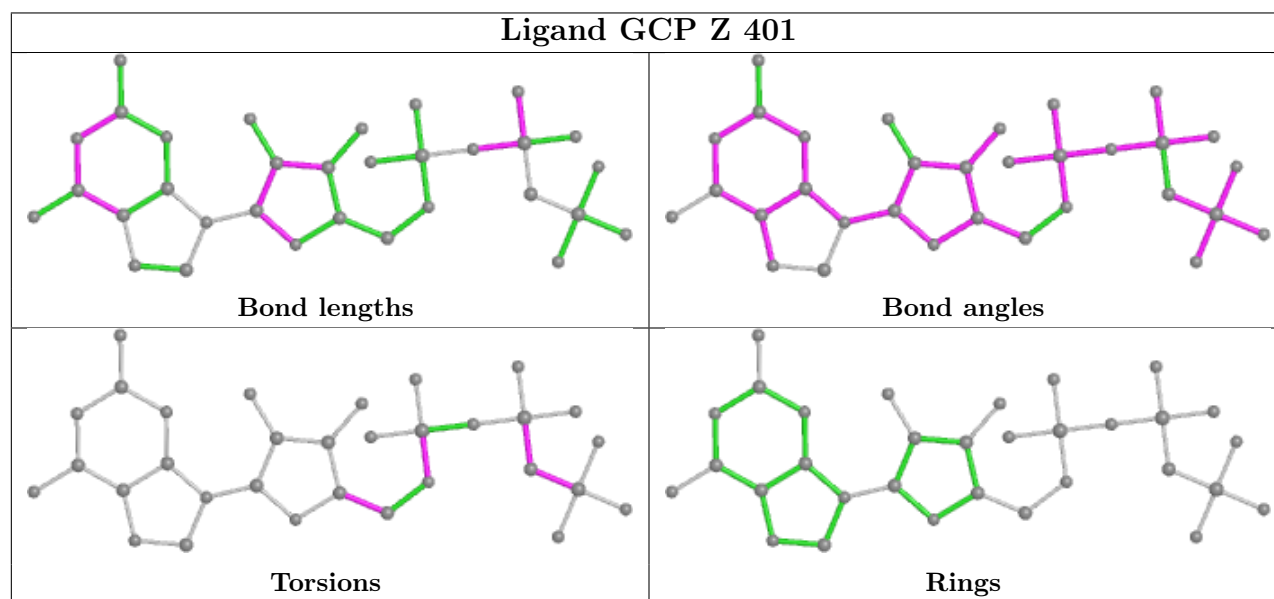
There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
60	Z	401	GCP	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-8615. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal surface views

This section was not generated.

6.5 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis ⓘ

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.