wwPDB EM Validation Summary Report (i)

Dec 12, 2022 – 09:20 AM EST

PDB ID	:	6VYQ
EMDB ID	:	EMD-21468
Title	:	Escherichia coli transcription-translation complex A1 (TTC-A1) containing an 15 nt long mRNA spacer, NusG, and fMet-tRNAs at E-site and P-site
Authors	:	Molodtsov, V.; Wang, C.; Su, M.; Ebright, R.H.
Deposited on	:	2020-02-27
Resolution	:	3.70 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 (i) 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 (i)) were used in the production of this report:

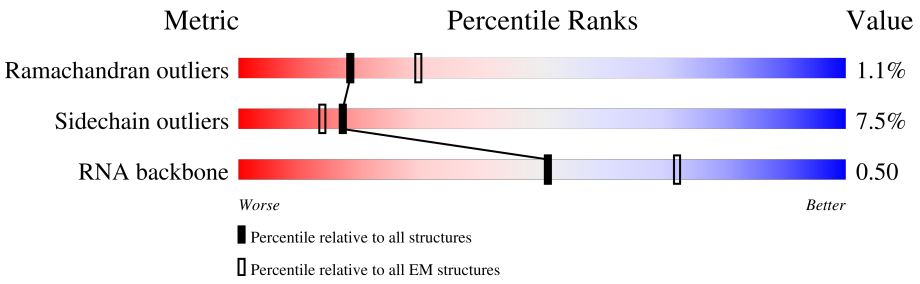
EMDB validation analysis	:	FAILED
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.70 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)
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 <=5%

Mol	Chain	Length	Quality of chain
1	0	103	93% 7%
2	1	110	92% 8%
3	2	100	89% 5% 6%
4	3	104	91% 8% •
5	4	94	96% •
6	5	36	47% 17% 36%
7	6	36	64% 11% 25%
8	7	32	25% 72% •
9	9	165	54% 33% • 10%

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Mol	Chain	Length	Quality of chain
10	A	76	58% 38% •
10	B	76	46% 49% 5%
11	AA	1341	89% 8% ••
12	AB	181	53% • 46%
13	AC	329	64% 5% 30%
13	AD	329	69% • 31%
14	AE	1407	89% 5% • 5%
15	C	75	85% • 12%
16	D	1542	78% 20% ••
17	E	87	93% 6% •
18	F	71	94% • •
19	G	241	90% • 7%
20	H	557	41% • • 54%
21	I	233	86% • 11%
22	J	206	96% •
23	K	167	89% 5% 7%
24	L	135	72% • • 23%
25	M	179	80% • • 16%
26	N	130	97% ••
27	O	130	93% 5% •
28	P	99	91% 9%
29	Q	129	87% • 9%
30	R	124	92% 6% •
31	S	101	95% • •
32	T	89	85% 13% •

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Mol	Chain	Length	Quality of chain
33	U	82	93% 7%
34	V	84	93% 5%
35	W	92	86% 10%
36	X	118	88% 10%
37	Y	142	68% 27%
38	Z	121	12% 12% 75%
39	a	2904	81% 18%
40	b	85	88% 11%
41	c	78	94% 5%
42	d	120	86% 14%
43	e	63	97%
44	f	59	95%
45	g	70	86% 9% 6%
46	h	273	93% 7%
47	i	57	88% 11%
48	j	209	97%
49	k	55	89% 5% 5%
50	l	201	93% 7%
51	m	46	93% 7%
52	n	179	89% 10%
53	o	65	91% 8%
54	p	177	97%
55	q	38	95% 5%
56	r	149	93% 7%
57	s	142	96%

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Mol	Chain	Length	Quality of chain
58	t	123	95% 5%
59	u	144	96%
60	v	136	96%
61	w	127	87% 6% 6%
62	x	117	94% 5%
63	y	115	95%
64	z	118	97%

2 Entry composition (i)

There are 66 unique types of molecules in this entry. The entry contains 300668 atoms, of which 124723 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 L21.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	0	103	1655	516	839	153	145	2	0	0

- Molecule 2 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	1	110	1779	532	922	166	156	3	0	0

- Molecule 3 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	2	94	1557	470	811	140	134	2	0	0

- Molecule 4 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
4	3	103	1632	498	844	148	142	0	0

- Molecule 5 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	4	94	1533	479	780	137	134	3	0	0

- Molecule 6 is a DNA chain called NT DNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
6	5	23	732	225	260	87	137	23	0	0

- Molecule 7 is a DNA chain called T DNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
7	6	27	847	259	305	89	167	27	0	0

- Molecule 8 is a RNA chain called mRNA with 15 nt long spacer.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
8	7	32	769	300	97	100	240	32	0	0

- Molecule 9 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	9	148	1117	705	196	209	7	0	0

- Molecule 10 is a RNA chain called E-site and P-site tRNA (fMet).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
10	A	76	2446	723	826	295	527	75	0	0
10	B	76	2433	723	813	295	527	75	0	0

- Molecule 11 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
11	AA	1322	20851	6539	10426	1817	2026	43	0	0

- Molecule 12 is a protein called Transcription termination/antitermination protein NusG.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
12	AB	98	1573	505	783	139	140	6	0	0

- Molecule 13 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
13	AC	230	3599	1112	1813	317	351	6	0	0

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Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
13	AD	228	3556	1100	1789	312	349	6	0	0

- Molecule 14 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
14	AE	1335	21000	6526	10612	1854	1958	50	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AE	1384	VAL	MET	variant	UNP A0A4S1NBU2

- Molecule 15 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
15	C	66	1103	344	559	102	97	1	0	0

- Molecule 16 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
16	D	1524	49126	14585	16423	6003	10591	1524	0	0

- Molecule 17 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
17	E	86	1388	414	719	138	114	3	0	0

- Molecule 18 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
18	F	70	1218	366	629	125	97	1	0	0

- Molecule 19 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
19	G	225	3545	1113	1785	316	323	8	0	0

- Molecule 20 is a protein called 30S ribosomal protein S1.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
20	H	259	3184	1073	1454	305	349	3	0	0

- Molecule 21 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
21	I	208	3346	1036	1710	307	290	3	0	0

- Molecule 22 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
22	J	205	3350	1026	1707	315	298	4	0	0

- Molecule 23 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
23	K	156	2348	717	1196	217	212	6	0	0

- Molecule 24 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
24	L	104	1694	536	846	153	152	7	0	0

- Molecule 25 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
25	M	151	2416	735	1235	227	215	4	0	0

- Molecule 26 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
26	N	129	2010	616	1031	173	184	6	0	0

- Molecule 27 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
27	O	127	2092	634	1070	206	179	3	0	0

- Molecule 28 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
28	P	99	1621	495	831	151	143	1	0	0

- Molecule 29 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
29	Q	117	1764	540	887	174	160	3	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
30	R	121	1940	580	1001	194	161	4	0	0

- Molecule 31 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
31	S	100	1649	499	844	164	139	3	0	0

- Molecule 32 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
32	T	88	1448	439	734	144	130	1	0	0

- Molecule 33 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
33	U	82	1315	406	666	128	114	1	0	0

- Molecule 34 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
34	V	80	1339	411	691	121	113	3	0	0

- Molecule 35 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
35	W	83	1351	424	688	126	111	2	0	0

- Molecule 36 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
36	X	116	1864	558	964	181	158	3	0	0

- Molecule 37 is a protein called 50S ribosomal protein L11.

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

- Molecule 38 is a protein called 50S ribosomal protein L7/L12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	Z	30	227	144	33	47	3	0	0

- Molecule 39 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
39	a	2880	92918	27587	31077	11398	19976	2880	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	887	A	U	variant	GB 937521852

- Molecule 40 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
40	b	76	1181	360	599	117	104	1	0	0

- Molecule 41 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
41	c	77	1277	388	652	129	106	2	0	0

- Molecule 42 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
42	d	120	3870	1144	1301	468	837	120	0	0

- Molecule 43 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
43	e	62	1032	308	531	98	94	1	0	0

- Molecule 44 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
44	f	58	936	281	488	87	78	2	0	0

- Molecule 45 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
45	g	66	1042	323	520	99	94	6	0	0

- Molecule 46 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
46	h	271	4236	1288	2154	423	364	7	0	0

- Molecule 47 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
47	i	56	903	269	459	94	80	1	0	0

- Molecule 48 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
48	j	209	3182	979	1617	288	294	4	0	0

- Molecule 49 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
49	k	52	890	275	464	78	73	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
50	l	201	3171	974	1619	283	290	5	0	0

- Molecule 51 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
51	m	46	795	228	418	90	57	2	0	0

- Molecule 52 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
52	n	177	2853	899	1443	249	256	6	0	0

- Molecule 53 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
53	o	64	1076	323	572	105	74	2	0	0

- Molecule 54 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
54	p	175	2671	826	1358	241	244	2	0	0

- Molecule 55 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
55	q	38	645	185	343	65	48	4	0	0

- Molecule 56 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
56	r	149	2259	699	1148	197	214	1	0	0

- Molecule 57 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
57	s	142	2291	714	1162	212	199	4	0	0

- Molecule 58 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
58	t	123	1969	593	1023	181	166	6	0	0

- Molecule 59 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
59	u	144	2182	654	1129	207	190	2	0	0

- Molecule 60 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
60	v	136	2231	686	1157	205	177	6	0	0

- Molecule 61 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
61	w	119	1945	588	994	195	163	5	0	0

- Molecule 62 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
62	x	116	1815	552	923	178	162	0	0

- Molecule 63 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
63	y	114	1879	574	962	179	163	1	0	0

- Molecule 64 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
64	z	117	1967	604	1020	192	151	0	0

- Molecule 65 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
65	AE	1	1	1	0

- Molecule 66 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
66	AE	2	2	2	0

3 Residue-property plots (i)

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 L21

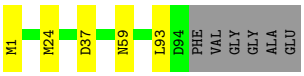
Chain 0: 93% 7%

• Molecule 2: 50S ribosomal protein L22

Chain 1: 92% 8%

• Molecule 3: 50S ribosomal protein L23

Chain 2: 89% 5% 6%

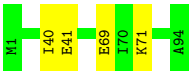


• Molecule 4: 50S ribosomal protein L24

Chain 3: 91% 8%

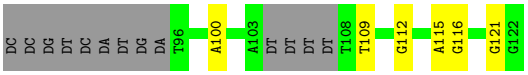
• Molecule 5: 50S ribosomal protein L25

Chain 4: 96%



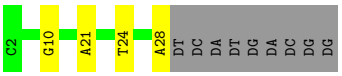
• Molecule 6: NT DNA

Chain 5: 47% 17% 36%



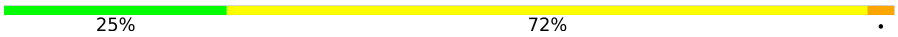
• Molecule 7: T DNA

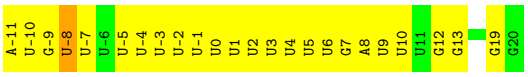
Chain 6:



• Molecule 8: mRNA with 15 nt long spacer

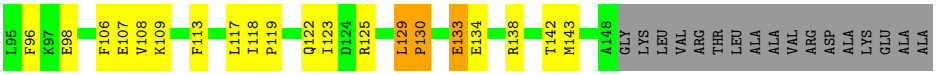
Chain 7:





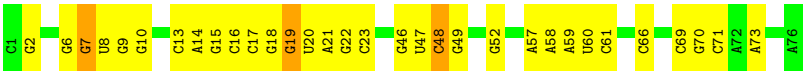
• Molecule 9: 50S ribosomal protein L10

Chain 9:



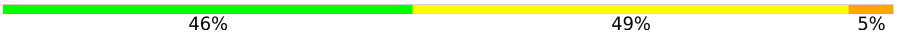
• Molecule 10: E-site and P-site tRNA (fMet)

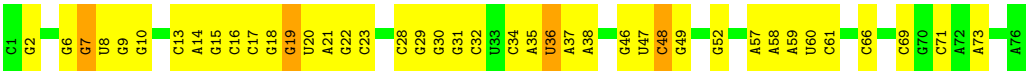
Chain A:



• Molecule 10: E-site and P-site tRNA (fMet)

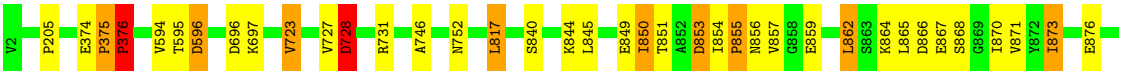
Chain B:

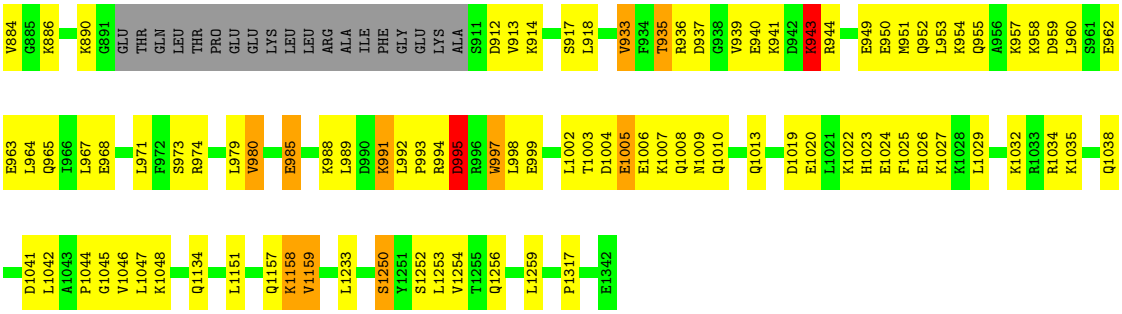




• Molecule 11: DNA-directed RNA polymerase subunit beta

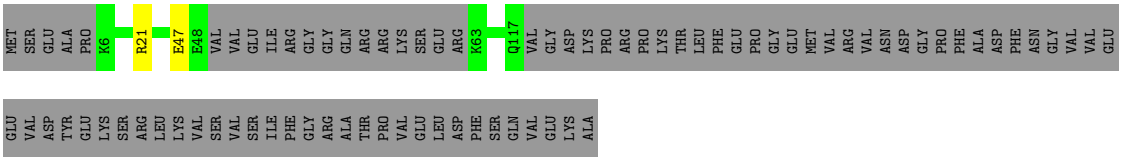
Chain AA:





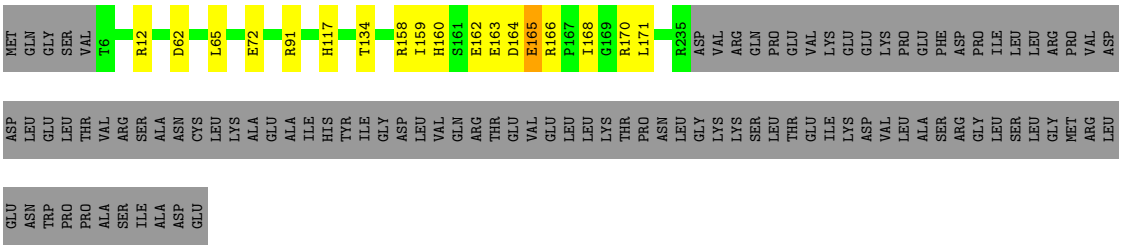
- Molecule 12: Transcription termination/antitermination protein NusG

Chain AB:



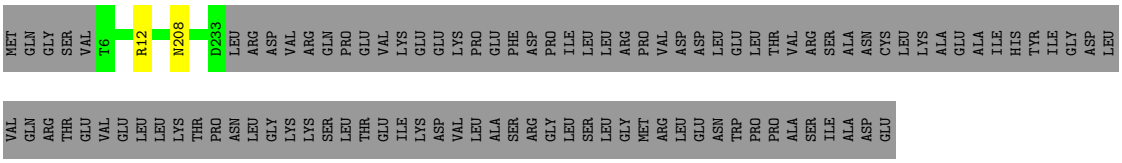
- Molecule 13: DNA-directed RNA polymerase subunit alpha

Chain AC:



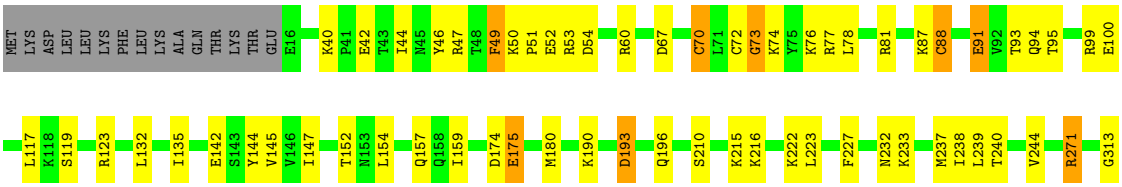
- Molecule 13: DNA-directed RNA polymerase subunit alpha

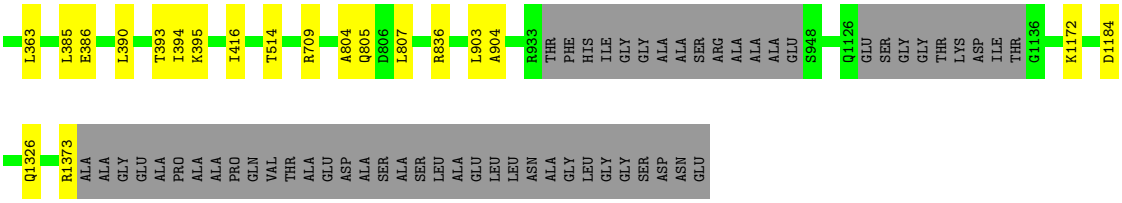
Chain AD:



- Molecule 14: DNA-directed RNA polymerase subunit beta'

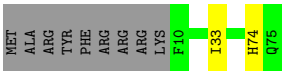
Chain AE:





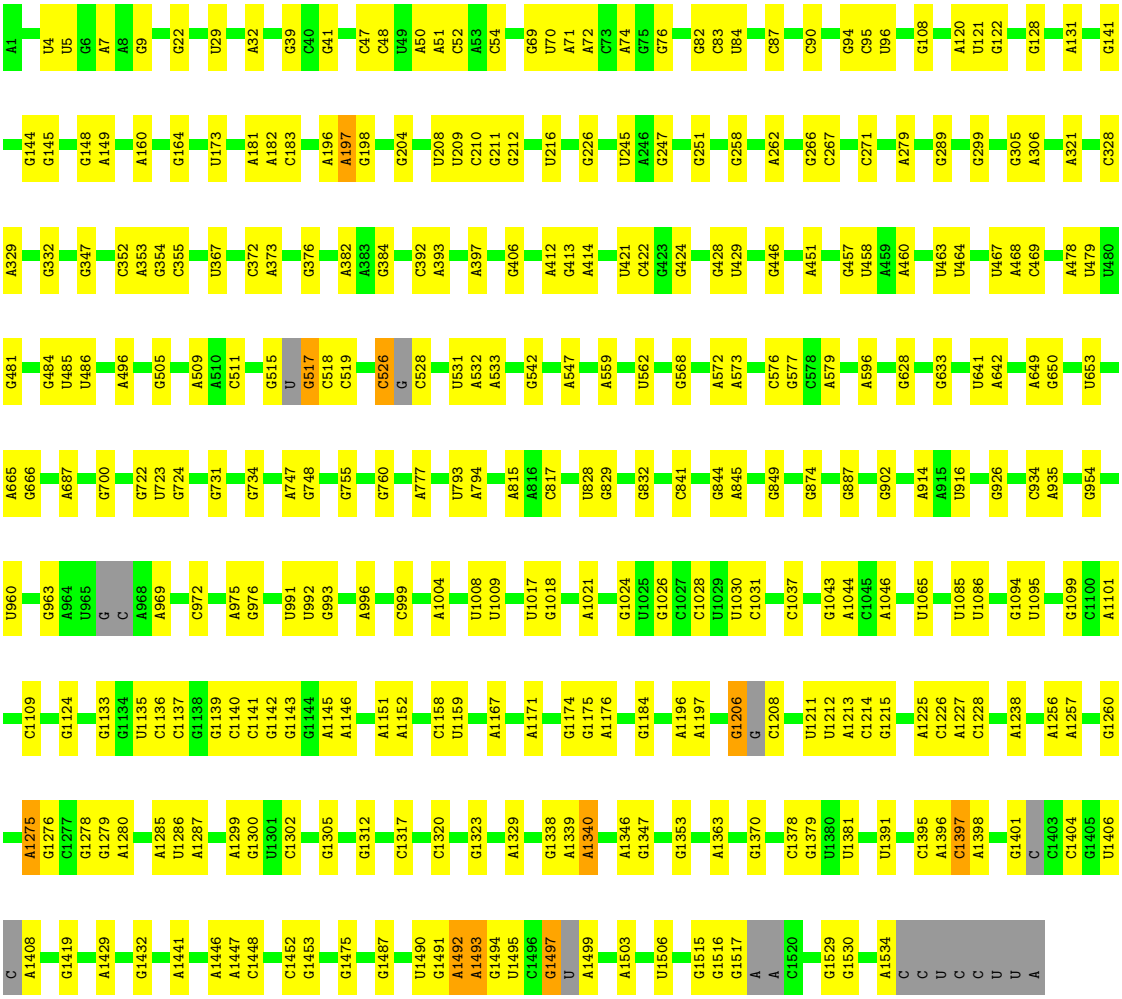
• Molecule 15: 30S ribosomal protein S18

Chain C:



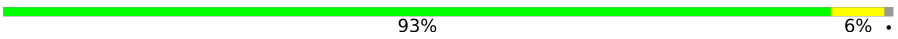
• Molecule 16: 16S rRNA

Chain D:



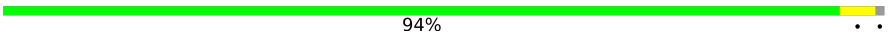
• Molecule 17: 30S ribosomal protein S20

Chain E:



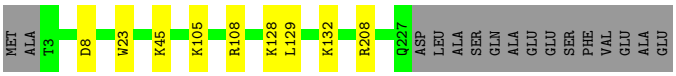
• Molecule 18: 30S ribosomal protein S21

Chain F:



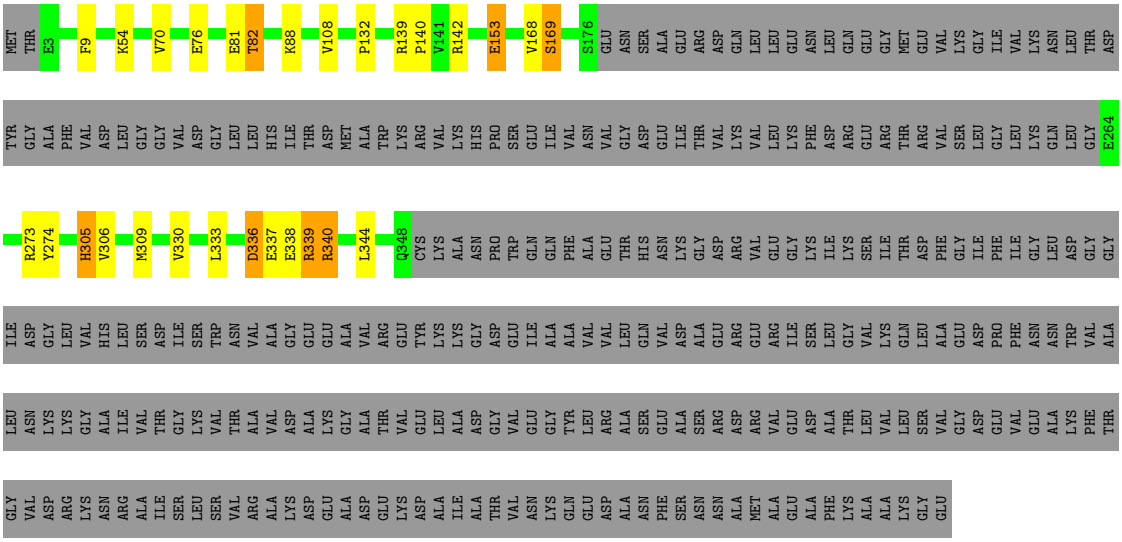
• Molecule 19: 30S ribosomal protein S2

Chain G:



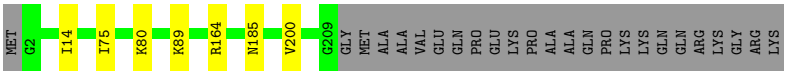
• Molecule 20: 30S ribosomal protein S1

Chain H:



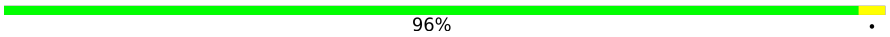
• Molecule 21: 30S ribosomal protein S3

Chain I:



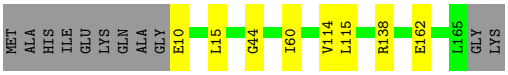
• Molecule 22: 30S ribosomal protein S4

Chain J:



• Molecule 23: 30S ribosomal protein S5

Chain K:

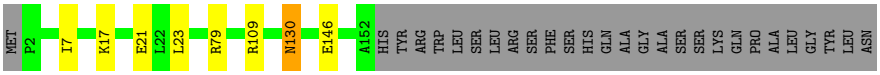


• Molecule 24: 30S ribosomal protein S6

Chain L:

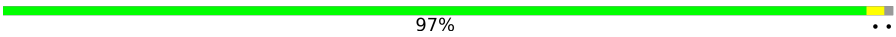
• Molecule 25: 30S ribosomal protein S7

Chain M:



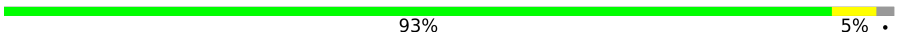
• Molecule 26: 30S ribosomal protein S8

Chain N:



• Molecule 27: 30S ribosomal protein S9

Chain O:



• Molecule 28: 30S ribosomal protein S10

Chain P:

• Molecule 29: 30S ribosomal protein S11

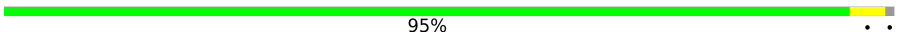
Chain Q:

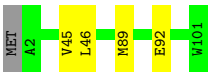
- Molecule 30: 30S ribosomal protein S12

Chain R:

- Molecule 31: 30S ribosomal protein S14

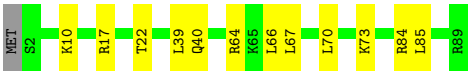
Chain S:





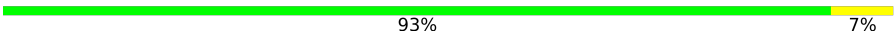
- Molecule 32: 30S ribosomal protein S15

Chain T:



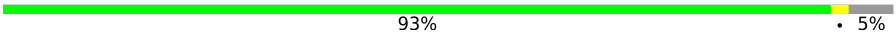
- Molecule 33: 30S ribosomal protein S16

Chain U:



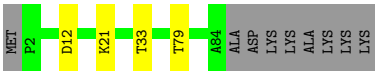
- Molecule 34: 30S ribosomal protein S17

Chain V:



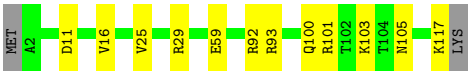
- Molecule 35: 30S ribosomal protein S19

Chain W:



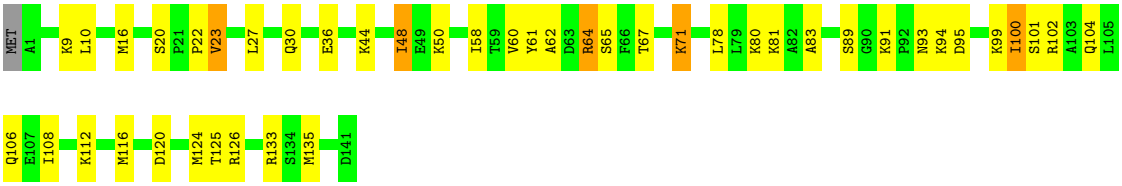
- Molecule 36: 30S ribosomal protein S13

Chain X:



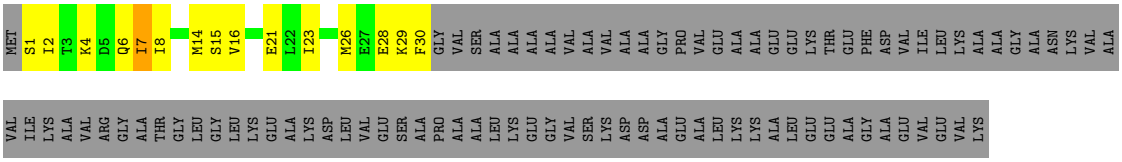
- Molecule 37: 50S ribosomal protein L11

Chain Y:



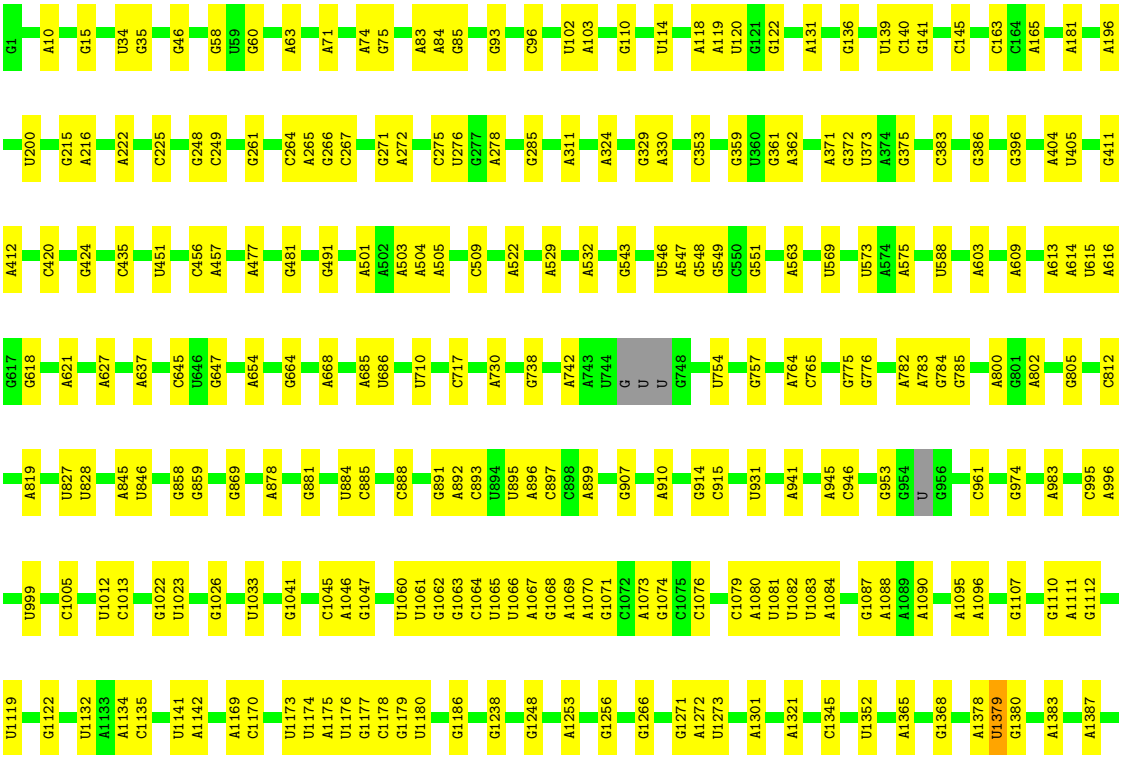
- Molecule 38: 50S ribosomal protein L7/L12

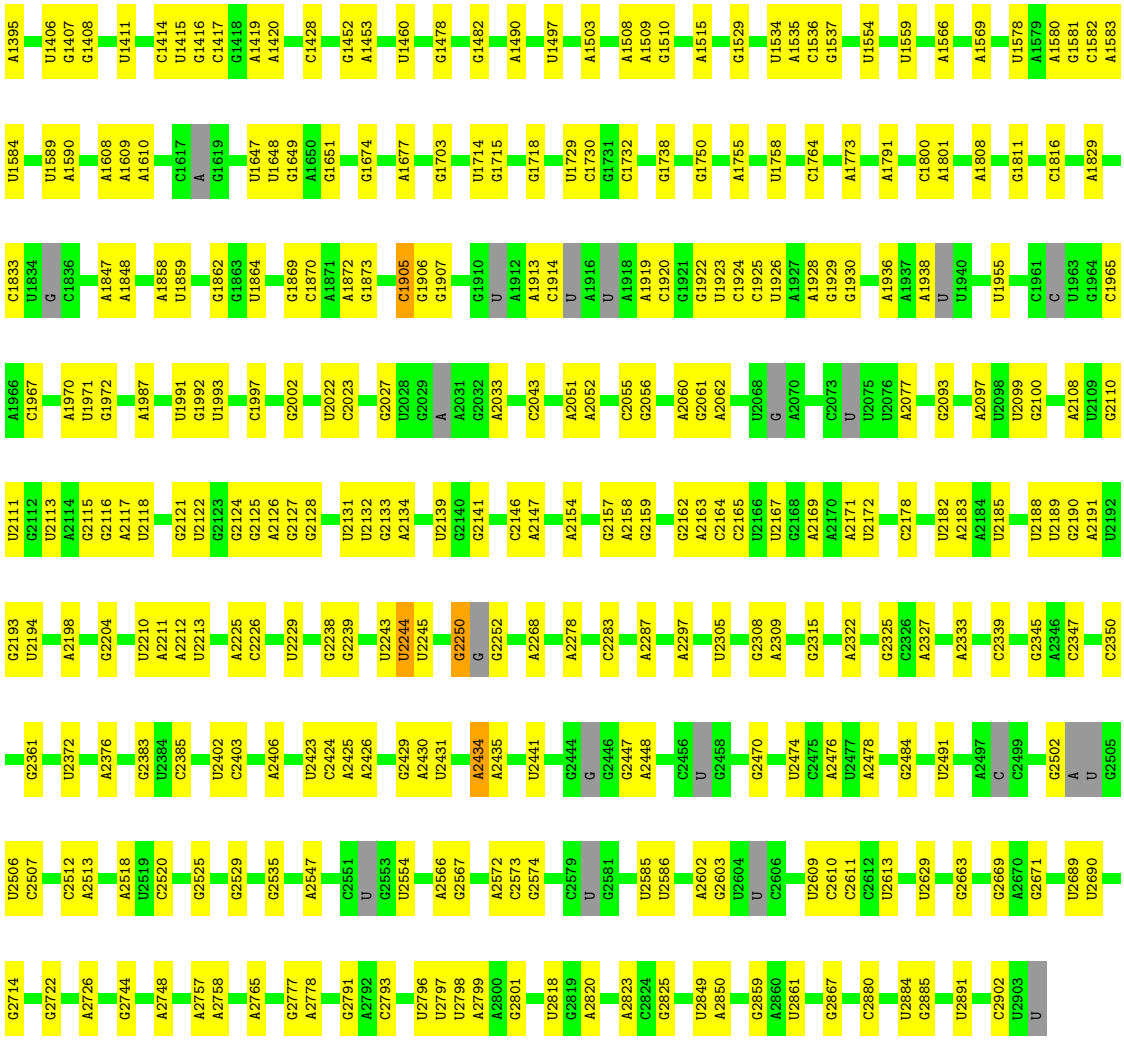
Chain Z:



- Molecule 39: 23S rRNA

Chain a:



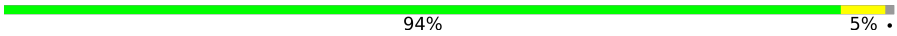


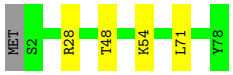
- Molecule 40: 50S ribosomal protein L27

Chain b:

- Molecule 41: 50S ribosomal protein L28

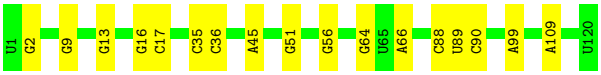
Chain c:





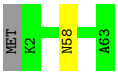
- Molecule 42: 5S rRNA

Chain d:



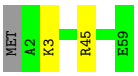
• Molecule 43: 50S ribosomal protein L29

Chain e: 97%



• Molecule 44: 50S ribosomal protein L30

Chain f: 95%

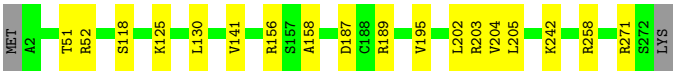


• Molecule 45: 50S ribosomal protein L31

Chain g: 86% 9% 6%

• Molecule 46: 50S ribosomal protein L2

Chain h: 93% 7%

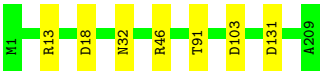


• Molecule 47: 50S ribosomal protein L32

Chain i: 88% 11%

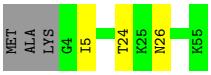
• Molecule 48: 50S ribosomal protein L3

Chain j: 97%



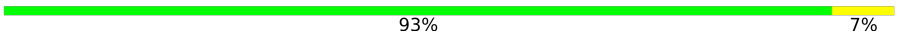
• Molecule 49: 50S ribosomal protein L33

Chain k: 89% 5% 5%



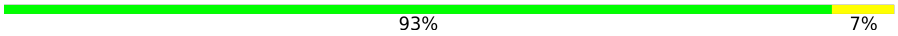
• Molecule 50: 50S ribosomal protein L4

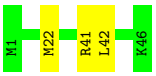
Chain l:



• Molecule 51: 50S ribosomal protein L34

Chain m:



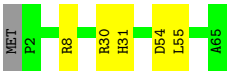


• Molecule 52: 50S ribosomal protein L5

Chain n:

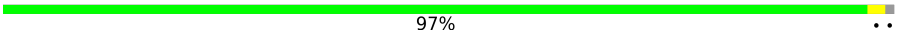
• Molecule 53: 50S ribosomal protein L35

Chain o:



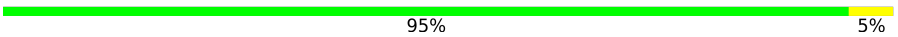
• Molecule 54: 50S ribosomal protein L6

Chain p:



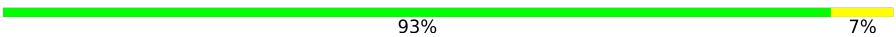
• Molecule 55: 50S ribosomal protein L36

Chain q:



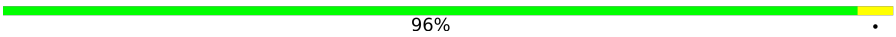
• Molecule 56: 50S ribosomal protein L9

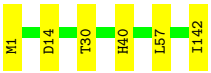
Chain r:



• Molecule 57: 50S ribosomal protein L13

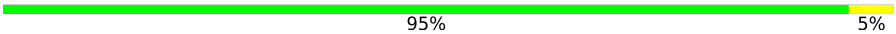
Chain s:





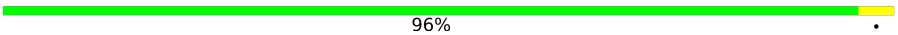
• Molecule 58: 50S ribosomal protein L14

Chain t:



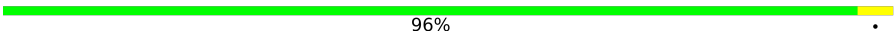
• Molecule 59: 50S ribosomal protein L15

Chain u:



• Molecule 60: 50S ribosomal protein L16

Chain v:

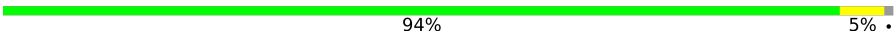


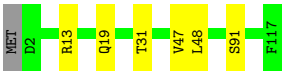
• Molecule 61: 50S ribosomal protein L17

Chain w:

• Molecule 62: 50S ribosomal protein L18

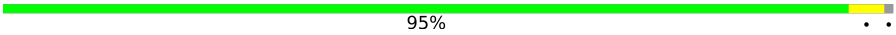
Chain x:





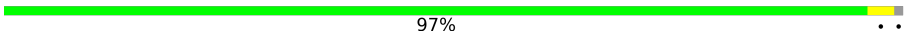
• Molecule 63: 50S ribosomal protein L19

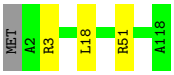
Chain y:



- Molecule 64: 50S ribosomal protein L20

Chain z:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	27378	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	45	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0	0.38	0/829	0.67	0/1107
2	1	0.48	0/864	0.82	0/1156
3	2	0.42	0/752	0.71	0/1005
4	3	0.35	0/796	0.66	2/1062 (0.2%)
5	4	0.40	0/766	0.68	0/1025
6	5	1.12	6/528 (1.1%)	0.97	1/810 (0.1%)
7	6	1.11	4/603 (0.7%)	0.97	0/926
8	7	0.57	2/747 (0.3%)	0.88	3/1160 (0.3%)
9	9	0.79	2/1131 (0.2%)	0.64	1/1524 (0.1%)
10	A	0.39	0/1810	0.75	1/2821 (0.0%)
10	B	0.46	1/1810 (0.1%)	0.86	7/2821 (0.2%)
11	AA	0.59	2/10591 (0.0%)	0.75	15/14289 (0.1%)
12	AB	0.43	0/808	0.60	0/1088
13	AC	0.48	0/1808	0.62	1/2450 (0.0%)
13	AD	0.40	0/1789	0.56	0/2425
14	AE	0.52	3/10545 (0.0%)	0.66	5/14236 (0.0%)
15	C	0.48	0/553	0.83	0/743
16	D	0.34	10/36610 (0.0%)	0.74	30/57091 (0.1%)
17	E	0.57	0/675	0.85	0/895
18	F	0.56	0/597	0.87	0/792
19	G	0.49	0/1791	0.71	0/2413
20	H	0.54	1/1746 (0.1%)	1.03	12/2382 (0.5%)
21	I	0.43	0/1663	0.71	0/2241
22	J	0.47	0/1665	0.73	0/2227
23	K	0.45	0/1165	0.75	0/1568
24	L	0.43	0/867	0.76	1/1171 (0.1%)
25	M	0.50	0/1195	0.81	0/1602
26	N	0.41	0/989	0.69	0/1326
27	O	0.43	0/1034	0.75	0/1375
28	P	0.43	0/800	0.75	0/1082
29	Q	0.40	0/893	0.70	0/1205
30	R	0.35	0/952	0.74	0/1274

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
31	S	0.49	0/817	0.79	0/1088
32	T	0.53	0/722	0.86	0/964
33	U	0.44	0/659	0.78	0/884
34	V	0.34	0/657	0.61	0/881
35	W	0.38	0/680	0.62	0/915
36	X	0.49	0/909	0.86	0/1215
37	Y	0.66	0/1046	0.59	0/1410
38	Z	0.69	0/227	0.57	0/304
39	a	0.38	3/69247 (0.0%)	0.72	17/107985 (0.0%)
40	b	0.39	0/589	0.70	0/779
41	c	0.48	0/635	0.81	1/848 (0.1%)
42	d	0.29	0/2872	0.70	0/4478
43	e	0.54	0/502	0.83	0/667
44	f	0.45	0/452	0.78	0/605
45	g	0.43	0/531	0.68	0/709
46	h	0.39	0/2121	0.78	0/2852
47	i	0.40	0/450	0.79	0/599
48	j	0.44	0/1586	0.69	0/2134
49	k	0.35	0/433	0.65	0/576
50	l	0.46	0/1571	0.77	0/2113
51	m	0.53	0/380	0.99	0/498
52	n	0.49	0/1434	0.88	3/1926 (0.2%)
53	o	0.45	0/513	0.83	0/676
54	p	0.39	0/1333	0.67	0/1805
55	q	0.37	0/303	0.77	0/397
56	r	0.44	0/1122	0.69	0/1515
57	s	0.50	0/1152	0.75	0/1551
58	t	0.41	0/955	0.78	0/1279
59	u	0.40	0/1062	0.76	0/1413
60	v	0.47	0/1093	0.81	0/1460
61	w	0.52	0/964	0.87	0/1289
62	x	0.46	0/902	0.81	0/1209
63	y	0.41	0/929	0.72	1/1242 (0.1%)
64	z	0.60	0/960	0.91	0/1278
All	All	0.43	34/189180 (0.0%)	0.74	101/278836 (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
10	A	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
10	B	0	2
11	AA	0	10
14	AE	0	5
20	H	0	3
36	X	0	1
All	All	0	23

The worst 5 of 34 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	9	130	PRO	N-CA	13.78	1.70	1.47
16	D	1516	G	O3'-P	-13.47	1.45	1.61
16	D	1339	A	O3'-P	10.63	1.74	1.61
11	AA	374	GLU	C-N	10.46	1.54	1.34
14	AE	88	CYS	CB-SG	-10.16	1.65	1.82

The worst 5 of 101 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	D	1516	G	P-O3'-C3'	-18.97	96.94	119.70
16	D	1516	G	O3'-P-O5'	13.79	130.20	104.00
11	AA	1250	SER	C-N-CA	11.14	149.56	121.70
39	a	2252	G	N9-C1'-C2'	-10.94	99.78	114.00
16	D	1401	G	N9-C1'-C2'	-10.67	100.13	114.00

There are no chirality outliers.

5 of 23 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	A	19	G	Sidechain
10	A	7	G	Sidechain
11	AA	205	PRO	Peptide
11	AA	594	VAL	Peptide
11	AA	595	THR	Peptide

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	0	101/103 (98%)	97 (96%)	3 (3%)	1 (1%)	15	51
2	1	108/110 (98%)	104 (96%)	4 (4%)	0	100	100
3	2	92/100 (92%)	90 (98%)	2 (2%)	0	100	100
4	3	101/104 (97%)	96 (95%)	4 (4%)	1 (1%)	15	51
5	4	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
9	9	146/165 (88%)	95 (65%)	37 (25%)	14 (10%)	0	8
11	AA	1318/1341 (98%)	1150 (87%)	136 (10%)	32 (2%)	6	35
12	AB	94/181 (52%)	88 (94%)	6 (6%)	0	100	100
13	AC	228/329 (69%)	215 (94%)	11 (5%)	2 (1%)	17	54
13	AD	226/329 (69%)	212 (94%)	14 (6%)	0	100	100
14	AE	1329/1407 (94%)	1200 (90%)	120 (9%)	9 (1%)	22	59
15	C	64/75 (85%)	63 (98%)	1 (2%)	0	100	100
17	E	84/87 (97%)	83 (99%)	1 (1%)	0	100	100
18	F	68/71 (96%)	68 (100%)	0	0	100	100
19	G	223/241 (92%)	210 (94%)	13 (6%)	0	100	100
20	H	255/557 (46%)	188 (74%)	55 (22%)	12 (5%)	2	23
21	I	206/233 (88%)	196 (95%)	9 (4%)	1 (0%)	29	66
22	J	203/206 (98%)	198 (98%)	5 (2%)	0	100	100
23	K	154/167 (92%)	146 (95%)	7 (4%)	1 (1%)	25	62
24	L	102/135 (76%)	97 (95%)	4 (4%)	1 (1%)	15	51
25	M	149/179 (83%)	144 (97%)	4 (3%)	1 (1%)	22	59
26	N	127/130 (98%)	121 (95%)	5 (4%)	1 (1%)	19	56
27	O	125/130 (96%)	115 (92%)	9 (7%)	1 (1%)	19	56
28	P	97/99 (98%)	88 (91%)	8 (8%)	1 (1%)	15	51
29	Q	115/129 (89%)	104 (90%)	9 (8%)	2 (2%)	9	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	R	117/124 (94%)	116 (99%)	1 (1%)	0	100	100
31	S	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
32	T	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
33	U	80/82 (98%)	76 (95%)	3 (4%)	1 (1%)	12	47
34	V	78/84 (93%)	74 (95%)	4 (5%)	0	100	100
35	W	81/92 (88%)	78 (96%)	3 (4%)	0	100	100
36	X	114/118 (97%)	107 (94%)	5 (4%)	2 (2%)	8	41
37	Y	139/142 (98%)	102 (73%)	25 (18%)	12 (9%)	1	10
38	Z	28/121 (23%)	19 (68%)	7 (25%)	2 (7%)	1	15
40	b	74/85 (87%)	69 (93%)	5 (7%)	0	100	100
41	c	75/78 (96%)	72 (96%)	3 (4%)	0	100	100
43	e	60/63 (95%)	57 (95%)	3 (5%)	0	100	100
44	f	56/59 (95%)	53 (95%)	3 (5%)	0	100	100
45	g	64/70 (91%)	63 (98%)	1 (2%)	0	100	100
46	h	269/273 (98%)	259 (96%)	9 (3%)	1 (0%)	34	69
47	i	54/57 (95%)	51 (94%)	3 (6%)	0	100	100
48	j	207/209 (99%)	198 (96%)	9 (4%)	0	100	100
49	k	50/55 (91%)	50 (100%)	0	0	100	100
50	l	199/201 (99%)	190 (96%)	8 (4%)	1 (0%)	29	66
51	m	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
52	n	175/179 (98%)	162 (93%)	11 (6%)	2 (1%)	14	50
53	o	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
54	p	173/177 (98%)	161 (93%)	12 (7%)	0	100	100
55	q	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
56	r	147/149 (99%)	136 (92%)	11 (8%)	0	100	100
57	s	140/142 (99%)	135 (96%)	5 (4%)	0	100	100
58	t	121/123 (98%)	111 (92%)	10 (8%)	0	100	100
59	u	142/144 (99%)	135 (95%)	7 (5%)	0	100	100
60	v	134/136 (98%)	129 (96%)	5 (4%)	0	100	100
61	w	117/127 (92%)	107 (92%)	10 (8%)	0	100	100
62	x	114/117 (97%)	108 (95%)	6 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
63	y	112/115 (97%)	105 (94%)	7 (6%)	0	100	100
64	z	115/118 (98%)	110 (96%)	4 (4%)	1 (1%)	17	54
All	All	9368/10481 (89%)	8607 (92%)	659 (7%)	102 (1%)	18	50

5 of 102 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	9	88	HIS
11	AA	596	ASP
11	AA	853	ASP
11	AA	859	GLU
11	AA	862	LEU

5.3.2 Protein sidechains (i)

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	0	84/84 (100%)	78 (93%)	6 (7%)	14	45
2	1	93/93 (100%)	84 (90%)	9 (10%)	8	33
3	2	81/84 (96%)	76 (94%)	5 (6%)	18	49
4	3	84/85 (99%)	78 (93%)	6 (7%)	14	45
5	4	78/78 (100%)	74 (95%)	4 (5%)	24	55
9	9	112/123 (91%)	65 (58%)	47 (42%)	0	0
11	AA	1140/1156 (99%)	1039 (91%)	101 (9%)	9	37
12	AB	86/158 (54%)	84 (98%)	2 (2%)	50	71
13	AC	198/286 (69%)	182 (92%)	16 (8%)	11	41
13	AD	196/286 (68%)	194 (99%)	2 (1%)	76	86
14	AE	1120/1168 (96%)	1051 (94%)	69 (6%)	18	49
15	C	57/65 (88%)	55 (96%)	2 (4%)	36	63
17	E	65/66 (98%)	60 (92%)	5 (8%)	13	43
18	F	60/61 (98%)	57 (95%)	3 (5%)	24	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	G	187/199 (94%)	178 (95%)	9 (5%)	25	56
20	H	137/461 (30%)	128 (93%)	9 (7%)	16	48
21	I	171/190 (90%)	165 (96%)	6 (4%)	36	63
22	J	172/173 (99%)	165 (96%)	7 (4%)	30	59
23	K	119/126 (94%)	112 (94%)	7 (6%)	19	51
24	L	91/116 (78%)	85 (93%)	6 (7%)	16	48
25	M	124/147 (84%)	116 (94%)	8 (6%)	17	48
26	N	104/105 (99%)	102 (98%)	2 (2%)	57	76
27	O	105/107 (98%)	100 (95%)	5 (5%)	25	56
28	P	86/86 (100%)	78 (91%)	8 (9%)	9	35
29	Q	90/99 (91%)	87 (97%)	3 (3%)	38	64
30	R	101/104 (97%)	94 (93%)	7 (7%)	15	46
31	S	83/84 (99%)	79 (95%)	4 (5%)	25	56
32	T	76/77 (99%)	64 (84%)	12 (16%)	2	16
33	U	65/65 (100%)	60 (92%)	5 (8%)	13	43
34	V	74/78 (95%)	72 (97%)	2 (3%)	44	68
35	W	72/79 (91%)	68 (94%)	4 (6%)	21	53
36	X	94/96 (98%)	85 (90%)	9 (10%)	8	34
37	Y	109/110 (99%)	72 (66%)	37 (34%)	0	1
38	Z	26/85 (31%)	12 (46%)	14 (54%)	0	0
40	b	58/63 (92%)	57 (98%)	1 (2%)	60	79
41	c	67/68 (98%)	64 (96%)	3 (4%)	27	57
43	e	54/55 (98%)	53 (98%)	1 (2%)	57	76
44	f	48/49 (98%)	46 (96%)	2 (4%)	30	59
45	g	59/62 (95%)	53 (90%)	6 (10%)	7	31
46	h	216/218 (99%)	199 (92%)	17 (8%)	12	42
47	i	47/48 (98%)	41 (87%)	6 (13%)	4	23
48	j	164/164 (100%)	157 (96%)	7 (4%)	29	58
49	k	47/49 (96%)	44 (94%)	3 (6%)	17	48
50	l	165/165 (100%)	151 (92%)	14 (8%)	10	40
51	m	38/38 (100%)	35 (92%)	3 (8%)	12	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
52	n	148/150 (99%)	134 (90%)	14 (10%)	8	34
53	o	51/52 (98%)	46 (90%)	5 (10%)	8	33
54	p	136/138 (99%)	132 (97%)	4 (3%)	42	66
55	q	34/34 (100%)	32 (94%)	2 (6%)	19	51
56	r	114/114 (100%)	104 (91%)	10 (9%)	10	38
57	s	116/116 (100%)	110 (95%)	6 (5%)	23	55
58	t	104/104 (100%)	98 (94%)	6 (6%)	20	52
59	u	103/103 (100%)	97 (94%)	6 (6%)	20	52
60	v	109/109 (100%)	103 (94%)	6 (6%)	21	53
61	w	99/103 (96%)	91 (92%)	8 (8%)	11	41
62	x	86/87 (99%)	80 (93%)	6 (7%)	15	45
63	y	99/100 (99%)	95 (96%)	4 (4%)	31	60
64	z	89/90 (99%)	87 (98%)	2 (2%)	52	72
All	All	7791/8659 (90%)	7208 (92%)	583 (8%)	17	43

5 of 583 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
46	h	195	VAL
62	x	31	THR
47	i	40	ARG
46	h	189	ARG
53	o	31	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
23	K	70	ASN
36	X	105	ASN
59	u	4	ASN
11	AA	1236	ASN
9	9	103	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	A	75/76 (98%)	29 (38%)	6 (8%)
10	B	75/76 (98%)	35 (46%)	6 (8%)
16	D	1515/1542 (98%)	288 (19%)	35 (2%)
39	a	2859/2904 (98%)	532 (18%)	0
42	d	119/120 (99%)	17 (14%)	0
8	7	31/32 (96%)	21 (67%)	3 (9%)
All	All	4674/4750 (98%)	922 (19%)	50 (1%)

5 of 922 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	7	-9	G
8	7	-8	U
8	7	-7	U
8	7	-5	U
8	7	-4	U

5 of 50 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
16	D	532	A
16	D	1109	C
16	D	1493	A
16	D	562	U
16	D	793	U

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)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.