wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 02:24 PM BST

PDB ID	:	4UY8
EMDB ID:	:	EMD-2773
Title	:	Molecular basis for the ribosome functioning as a L-tryptophan sensor - Cryo-EM structure of a TnaC stalled E.coli ribosome
Authors	:	Bischoff, L.; Berninghausen, O.; Beckmann, R.
Deposited on	:	2014-08-29
Resolution	:	3.80 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could
stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp

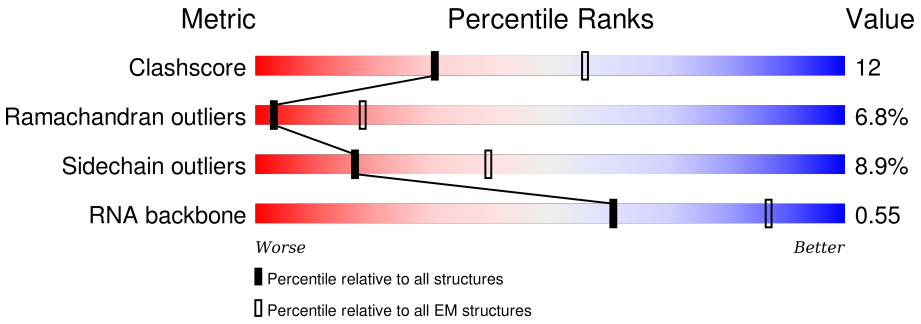
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

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 3.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



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

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

Mol	Chain	Length	Quality of chain
1	0	56	71% 25% • •
2	1	50	64% 28% 8%
3	2	46	76% 22% •
4	3	64	77% 19% 5%
5	4	38	55% 39% • •
6	5	148	29% 41% 20% 9%
7	6	30	60% 30% 10%
8	7	20	10% 25% 40% 25%

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Mol	Chain	Length	Quality of chain
9	8	94	77% 21%
10	A	2854	58% 32% 9%
11	B	118	66% 27% 7%
12	C	271	69% 27%
13	D	209	66% 28% 5%
14	E	201	69% 25% 5%
15	F	177	67% 29%
16	G	176	63% 29% 7%
17	H	50	58% 36% 6%
18	I	141	52% 42% 6%
19	J	142	61% 29% 9%
20	K	122	56% 34% 8%
21	L	143	70% 24%
22	M	136	63% 29% 7%
23	N	120	66% 31%
24	O	116	67% 30%
25	P	114	66% 25% 6%
26	Q	117	63% 31% 5%
27	R	103	63% 34%
28	S	110	61% 25% 11%
29	T	93	58% 35% 5%
30	U	102	63% 31% 5%
31	V	77	49% 36% 13%
32	W	79	37% 41% 20%
33	X	77	70% 23% 5%

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Mol	Chain	Length	Quality of chain
34	Y	63	60% 38%
35	Z	58	53% 36% 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
36	TRP	7	1001	-	-	X	-
36	TRP	7	1002	-	-	X	-

2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 92995 atoms, of which 8 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 L32.

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

- Molecule 2 is a protein called 50S RIBOSOMAL PROTEIN L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	1	50	409	263	75	71	0	0

- Molecule 3 is a protein called 50S RIBOSOMAL PROTEIN L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	2	46	377	228	90	57	2	0	0

- Molecule 4 is a protein called 50S RIBOSOMAL PROTEIN L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	3	64	504	323	105	74	2	0	0

- Molecule 5 is a protein called 50S RIBOSOMAL PROTEIN L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	4	38	302	185	65	48	4	0	0

- Molecule 6 is a protein called 50S RIBOSOMAL PROTEIN L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	5	148	1117	705	196	209	7	0	0

- Molecule 7 is a protein called RIBOSOMAL L7 PROTEIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	30	Total	C	N	O	S	0	0
			227	144	33	47	3		

- Molecule 8 is a protein called TRYPTOPHANASE.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7	20	Total	C	N	O	S	0	0
			170	109	32	28	1		

- Molecule 9 is a protein called 50S RIBOSOMAL PROTEIN L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	8	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 10 is a RNA chain called RRNA-23S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	A	2854	Total	C	N	O	P	0	0
			61274	27334	11279	19807	2854		

- Molecule 11 is a RNA chain called RRNA-5S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	B	118	Total	C	N	O	P	0	0
			2529	1126	464	821	118		

- Molecule 12 is a protein called 50S RIBOSOMAL PROTEIN L2.

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

- Molecule 13 is a protein called 50S RIBOSOMAL PROTEIN L3.

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

- Molecule 14 is a protein called 50S RIBOSOMAL PROTEIN L4.

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

- Molecule 15 is a protein called 50S RIBOSOMAL PROTEIN L5.

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

- Molecule 16 is a protein called 50S RIBOSOMAL PROTEIN L6.

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

- Molecule 17 is a protein called RIBOSOMAL PROTEIN L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	H	50	Total	C	N	O	S	0	0
			384	247	68	68	1		

- Molecule 18 is a protein called 50S RIBOSOMAL PROTEIN L11.

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

- Molecule 19 is a protein called 50S RIBOSOMAL PROTEIN L13.

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

- Molecule 20 is a protein called 50S RIBOSOMAL PROTEIN L14.

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

- Molecule 21 is a protein called 50S RIBOSOMAL PROTEIN L15.

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

- Molecule 22 is a protein called 50S RIBOSOMAL PROTEIN L16.

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

- Molecule 23 is a protein called 50S RIBOSOMAL PROTEIN L17.

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

- Molecule 24 is a protein called 50S RIBOSOMAL PROTEIN L18.

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

- Molecule 25 is a protein called 50S RIBOSOMAL PROTEIN L19.

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

- Molecule 26 is a protein called 50S RIBOSOMAL PROTEIN L20.

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

- Molecule 27 is a protein called 50S RIBOSOMAL PROTEIN L21.

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

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L22.

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

- Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L23.

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

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L24.

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

- Molecule 31 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	V	77	Total	C	N	O	P	0	0
			1649	733	297	542	77		

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	W	79	Total	C	N	O	S	0	0
			596	367	120	108	1		

- Molecule 33 is a protein called 50S RIBOSOMAL PROTEIN L28.

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

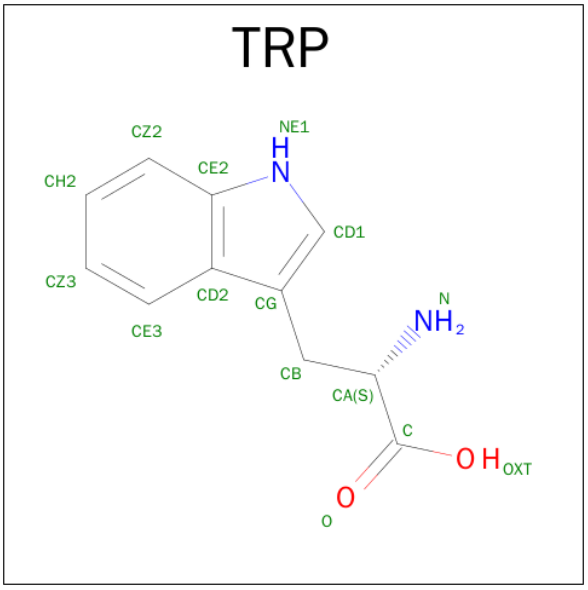
- Molecule 34 is a protein called 50S RIBOSOMAL PROTEIN L29.

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

- Molecule 35 is a protein called 50S RIBOSOMAL PROTEIN L30.

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

- Molecule 36 is TRYPTOPHAN (three-letter code: TRP) (formula: $C_{11}H_{12}N_2O_2$).



Mol	Chain	Residues	Atoms					AltConf
36	7	1	Total	C	H	N	O	0
			38	22	8	4	4	
36	7	1	Total	C	H	N	O	0
			38	22	8	4	4	

- Molecule 37 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
37	B	4	Total	Mg	0
			4	4	
37	A	135	Total	Mg	0
			135	135	
37	4	1	Total	Mg	0
			1	1	
37	C	2	Total	Mg	0
			2	2	
37	E	1	Total	Mg	0
			1	1	

- Molecule 38 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
38	4	1	Total Zn 1 1	0

- Molecule 39 is water.

Mol	Chain	Residues	Atoms	AltConf
39	A	416	Total O 416 416	0
39	B	14	Total O 14 14	0
39	C	2	Total O 2 2	0
39	D	3	Total O 3 3	0
39	E	2	Total O 2 2	0
39	L	2	Total O 2 2	0

3 Residue-property plots (i)

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

- Molecule 1: 50S RIBOSOMAL PROTEIN L32

Chain 0:

- Molecule 2: 50S RIBOSOMAL PROTEIN L33

Chain 1:

- Molecule 3: 50S RIBOSOMAL PROTEIN L34

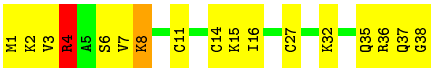
Chain 2:

- Molecule 4: 50S RIBOSOMAL PROTEIN L35

Chain 3:

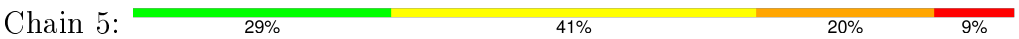
- Molecule 5: 50S RIBOSOMAL PROTEIN L36

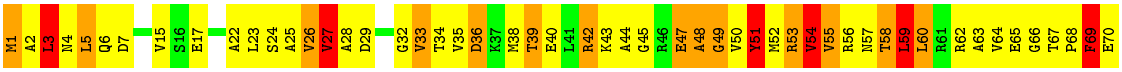
Chain 4:

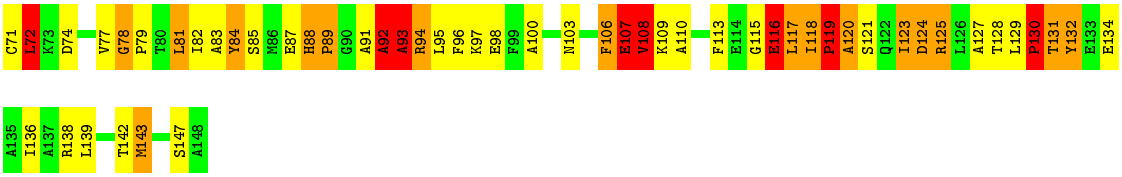


- Molecule 6: 50S RIBOSOMAL PROTEIN L10

Chain 5:







• Molecule 7: RIBOSOMAL L7 PROTEIN

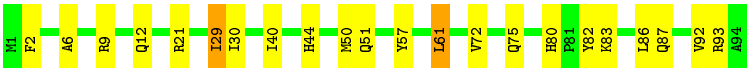
Chain 6:

• Molecule 8: TRYPTOPHANASE

Chain 7:

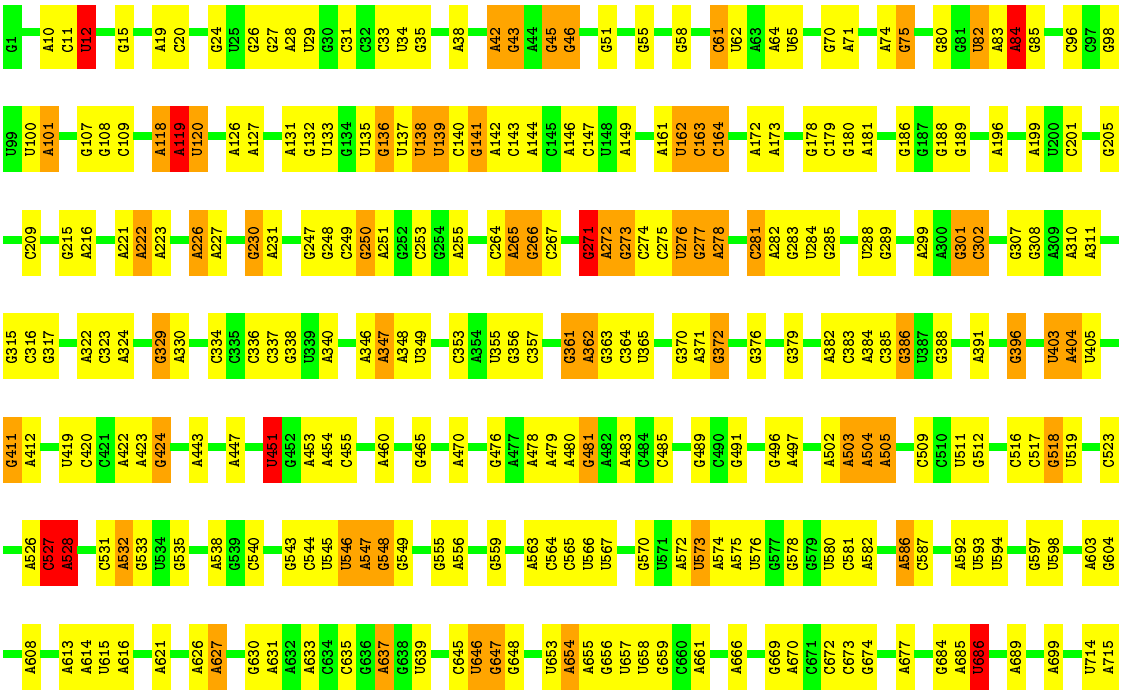
• Molecule 9: 50S RIBOSOMAL PROTEIN L25

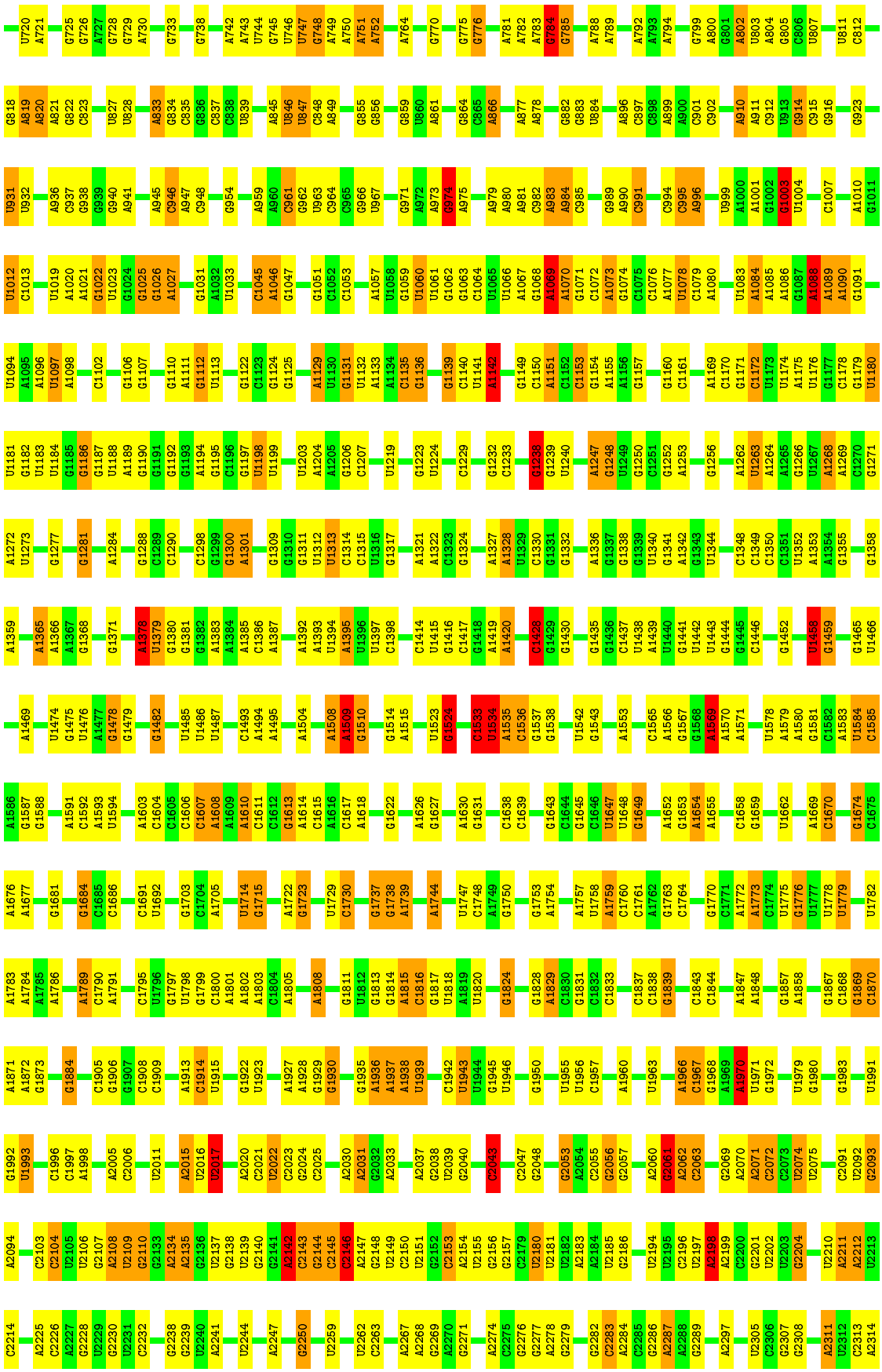
Chain 8:

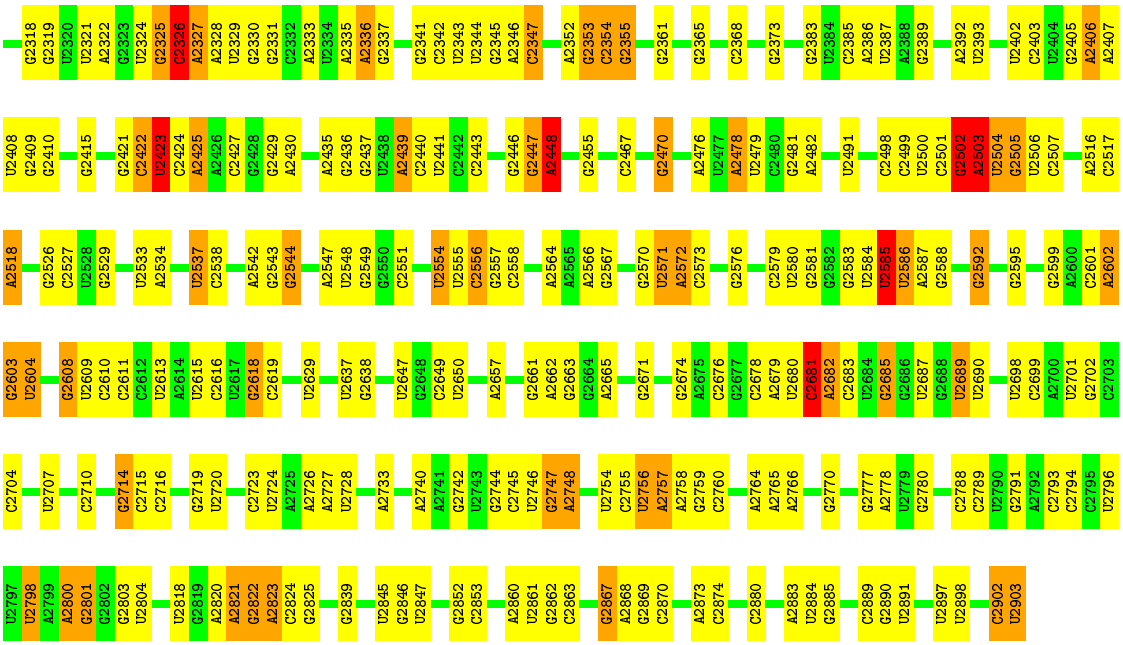


• Molecule 10: RRNA-23S RIBOSOMAL RNA

Chain A:

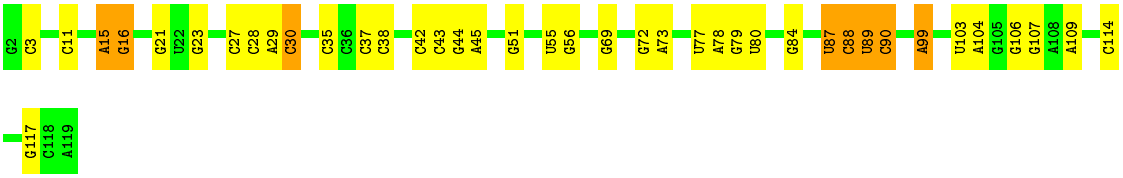






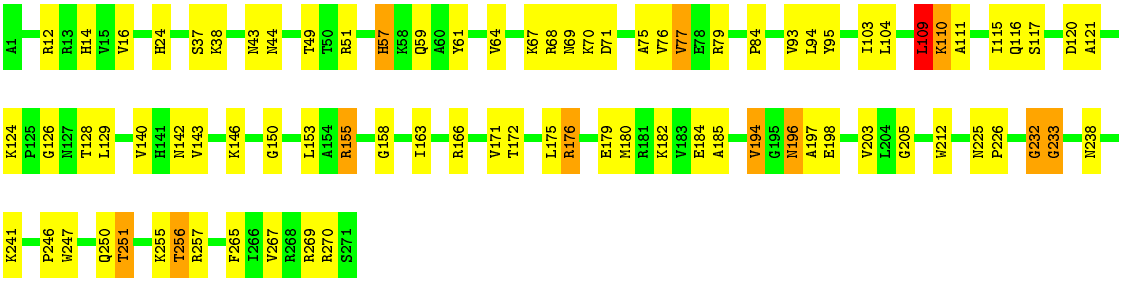
- Molecule 11: RRNA-5S RIBOSOMAL RNA

Chain B:



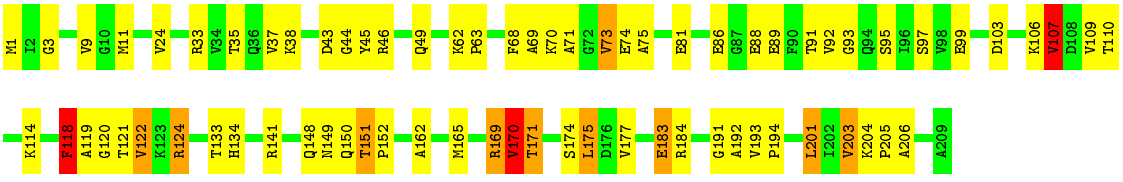
- Molecule 12: 50S RIBOSOMAL PROTEIN L2

Chain C:



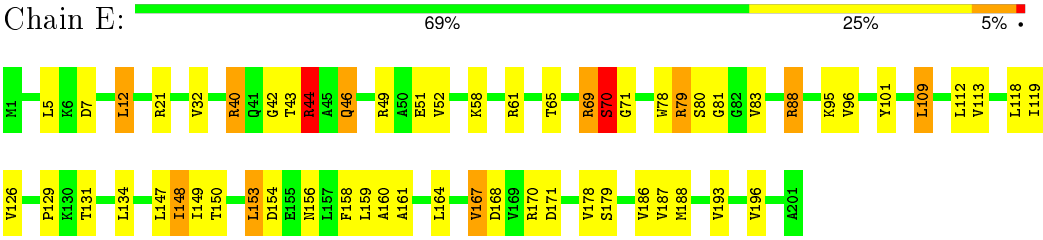
- Molecule 13: 50S RIBOSOMAL PROTEIN L3

Chain D:



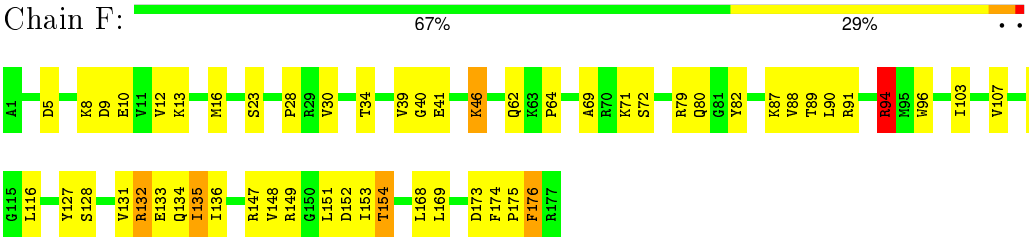
• Molecule 14: 50S RIBOSOMAL PROTEIN L4

Chain E:



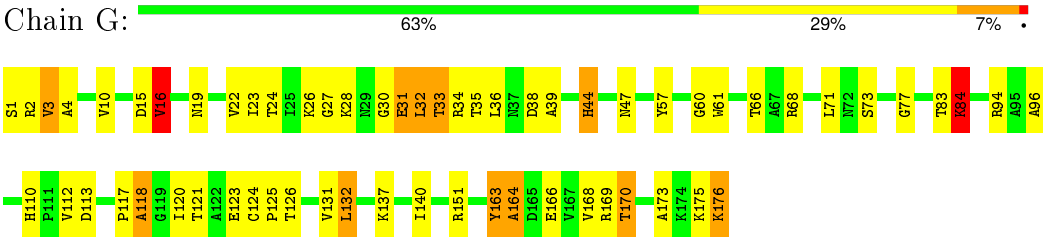
• Molecule 15: 50S RIBOSOMAL PROTEIN L5

Chain F:



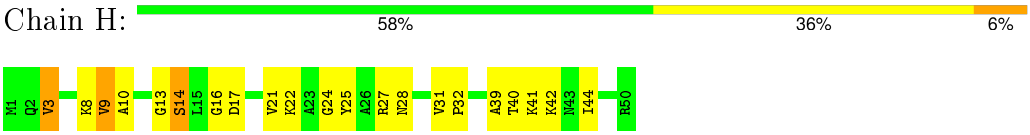
• Molecule 16: 50S RIBOSOMAL PROTEIN L6

Chain G:



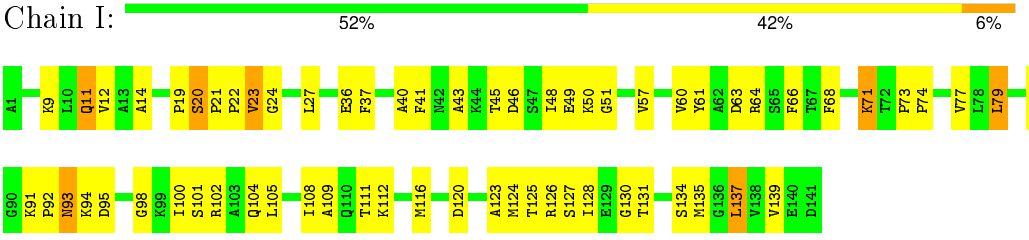
• Molecule 17: RIBOSOMAL PROTEIN L9

Chain H:



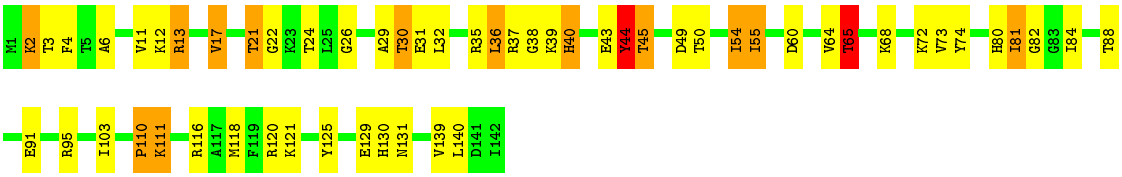
• Molecule 18: 50S RIBOSOMAL PROTEIN L11

Chain I:



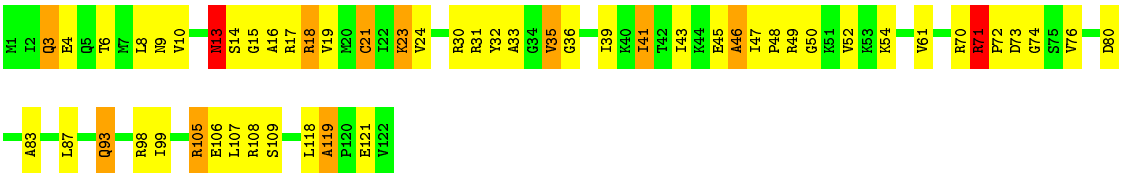
• Molecule 19: 50S RIBOSOMAL PROTEIN L13

Chain J:



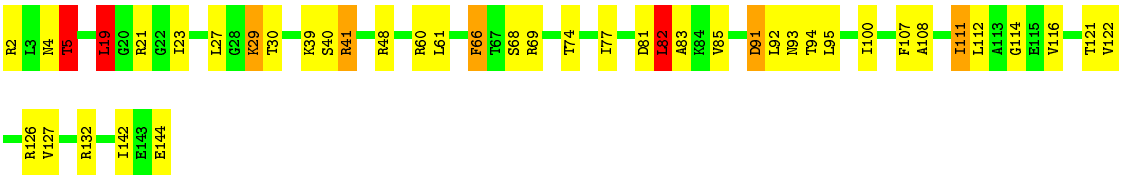
• Molecule 20: 50S RIBOSOMAL PROTEIN L14

Chain K:



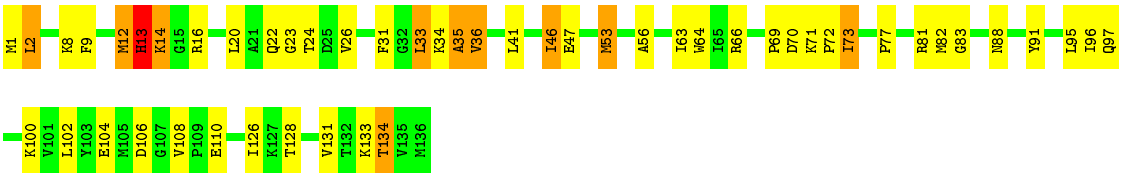
• Molecule 21: 50S RIBOSOMAL PROTEIN L15

Chain L:



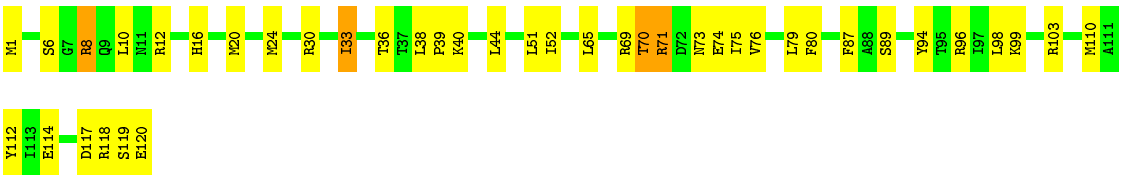
• Molecule 22: 50S RIBOSOMAL PROTEIN L16

Chain M:



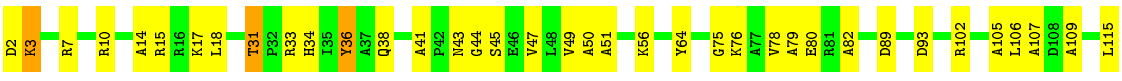
• Molecule 23: 50S RIBOSOMAL PROTEIN L17

Chain N:



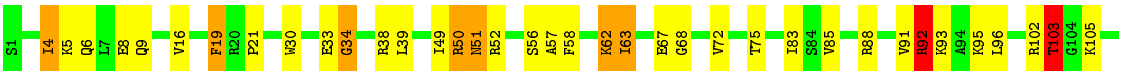
• Molecule 24: 50S RIBOSOMAL PROTEIN L18

Chain O:



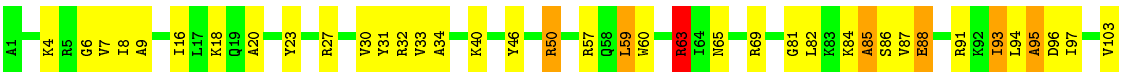
• Molecule 25: 50S RIBOSOMAL PROTEIN L19

Chain P:



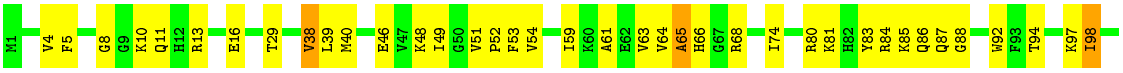
• Molecule 26: 50S RIBOSOMAL PROTEIN L20

Chain Q:



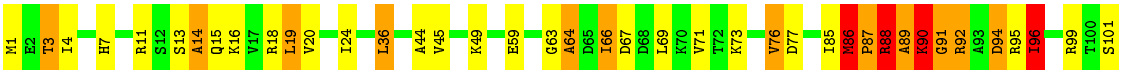
• Molecule 27: 50S RIBOSOMAL PROTEIN L21

Chain R:



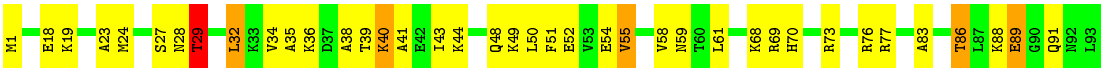
• Molecule 28: 50S RIBOSOMAL PROTEIN L22

Chain S:



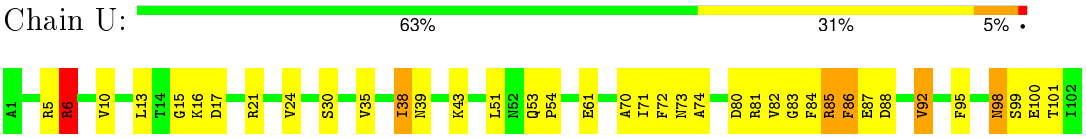
• Molecule 29: 50S RIBOSOMAL PROTEIN L23

Chain T:



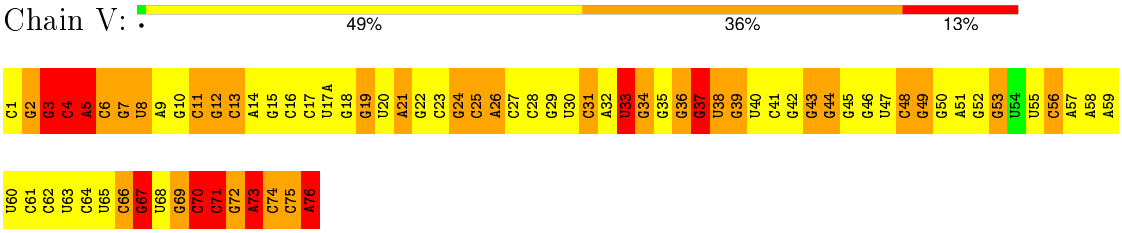
• Molecule 30: 50S RIBOSOMAL PROTEIN L24

Chain U:



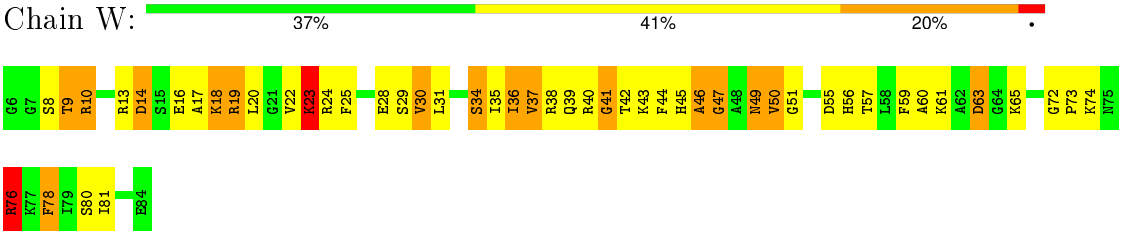
- Molecule 31: RNA

Chain V:



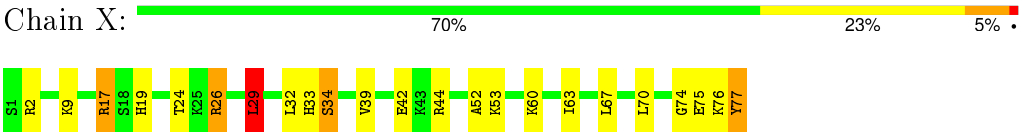
- Molecule 32: 50S RIBOSOMAL PROTEIN L27

Chain W:



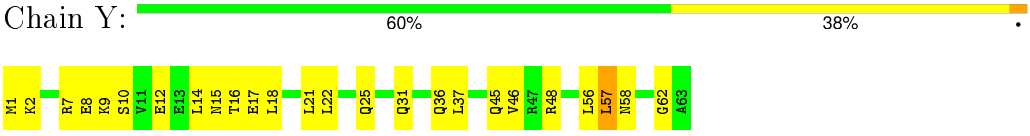
- Molecule 33: 50S RIBOSOMAL PROTEIN L28

Chain X:



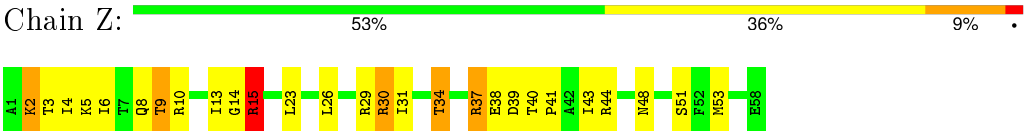
- Molecule 34: 50S RIBOSOMAL PROTEIN L29

Chain Y:



- Molecule 35: 50S RIBOSOMAL PROTEIN L30

Chain Z:



4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	MICROGRAPH	Depositor
Microscope	OTHER	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	FEI FALCON II (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: 5MU, 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	#$\|Z\|>2$	RMSZ	#$\|Z\|>2$
1	0	0.54	0/450	0.70	0/599
10	A	0.81	19/68626 (0.0%)	1.23	316/107056 (0.3%)
11	B	0.66	0/2828	1.10	2/4410 (0.0%)
12	C	0.54	0/2121	0.79	3/2852 (0.1%)
13	D	0.57	0/1586	0.77	1/2134 (0.0%)
14	E	0.53	0/1571	0.76	2/2113 (0.1%)
15	F	0.50	0/1434	0.71	1/1926 (0.1%)
16	G	0.55	0/1343	0.73	0/1816
17	H	0.53	0/389	0.73	0/523
18	I	0.62	0/1046	0.84	1/1410 (0.1%)
19	J	0.63	1/1152 (0.1%)	0.78	0/1551
2	1	0.53	0/416	0.74	0/554
20	K	0.65	1/947 (0.1%)	0.77	0/1268
21	L	0.56	0/1054	0.79	2/1403 (0.1%)
22	M	0.61	0/1093	0.77	0/1460
23	N	0.51	0/973	0.68	0/1301
24	O	0.46	0/902	0.70	0/1209
25	P	0.52	0/929	0.78	1/1242 (0.1%)
26	Q	0.62	0/960	0.71	1/1278 (0.1%)
27	R	0.61	1/829 (0.1%)	0.76	0/1107
28	S	0.88	3/864 (0.3%)	1.34	8/1156 (0.7%)
29	T	0.55	0/744	0.85	1/994 (0.1%)
3	2	0.53	0/380	0.70	0/498
30	U	0.56	0/787	0.78	0/1051
31	V	2.39	77/1820 (4.2%)	2.84	254/2836 (9.0%)
32	W	0.69	0/603	1.00	1/797 (0.1%)
33	X	0.50	0/635	0.79	1/848 (0.1%)
34	Y	0.46	0/510	0.75	0/677
35	Z	0.54	0/453	0.84	1/605 (0.2%)
4	3	0.53	0/513	0.75	0/676
5	4	0.59	0/303	0.84	0/397
6	5	0.74	0/1131	1.32	26/1524 (1.7%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >2	RMSZ	#|Z| >2
7	6	0.58	0/227	0.65	0/304
8	7	0.62	0/175	2.72	9/237 (3.8%)
9	8	0.48	0/766	0.67	1/1025 (0.1%)
All	All	0.81	102/100560 (0.1%)	1.20	632/150837 (0.4%)

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
12	C	0	1
13	D	0	1
19	J	0	1
20	K	0	1
28	S	0	3
31	V	0	13
6	5	0	1
8	7	0	4
All	All	0	25

The worst 5 of 102 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	V	39	G	N9-C4	15.38	1.50	1.38
31	V	69	G	C6-N1	13.21	1.48	1.39
31	V	5	A	C6-N1	12.91	1.44	1.35
31	V	39	G	C2-N3	12.19	1.42	1.32
31	V	39	G	N1-C2	11.42	1.46	1.37

The worst 5 of 632 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	S	86	MET	C-N-CD	-30.06	54.48	120.60
31	V	73	A	N1-C6-N6	22.84	132.30	118.60
10	A	1073	A	N1-C6-N6	-19.93	106.64	118.60
31	V	69	G	N1-C6-O6	19.71	131.73	119.90
31	V	69	G	C5-C6-O6	-19.59	116.85	128.60

There are no chirality outliers.

5 of 25 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	5	130	PRO	Peptide
8	7	15	ILE	Peptide
8	7	21	ASP	Peptide
8	7	23	ARG	Sidechain
8	7	6	ILE	Peptide

5.2 Too-close contacts (i)

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	0	444	0	461	19	0
2	1	409	0	440	15	0
3	2	377	0	418	9	0
4	3	504	0	574	10	0
5	4	302	0	340	16	0
6	5	1117	0	1155	121	0
7	6	227	0	237	7	0
8	7	170	0	166	94	0
9	8	753	0	780	14	0
10	A	61274	0	30816	829	0
11	B	2529	0	1281	21	0
12	C	2082	0	2157	54	0
13	D	1565	0	1616	47	0
14	E	1552	0	1619	41	0
15	F	1410	0	1445	45	0
16	G	1323	0	1374	38	0
17	H	384	0	405	13	0
18	I	1032	0	1088	51	0
19	J	1129	0	1162	53	0
20	K	938	0	1012	38	0
21	L	1045	0	1117	36	0
22	M	1074	0	1157	29	0
23	N	960	0	1000	30	0
24	O	892	0	923	20	0
25	P	917	0	965	40	0
26	Q	947	0	1022	51	0
27	R	816	0	839	35	0
28	S	857	0	922	53	0
29	T	738	0	807	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	U	779	0	834	26	0
31	V	1649	0	832	49	0
32	W	596	0	610	79	0
33	X	625	0	655	18	0
34	Y	509	0	543	13	0
35	Z	449	0	491	18	0
36	7	30	8	18	24	0
37	4	1	0	0	0	0
37	A	135	0	0	0	0
37	B	4	0	0	0	0
37	C	2	0	0	0	0
37	E	1	0	0	0	0
38	4	1	0	0	0	0
39	A	416	0	0	78	0
39	B	14	0	0	1	0
39	C	2	0	0	0	0
39	D	3	0	0	0	0
39	E	2	0	0	0	0
39	L	2	0	0	0	0
All	All	92987	8	61281	1783	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 12.

The worst 5 of 1783 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)
8:7:11:LYS:CE	28:S:91:GLY:HA3	1.51	1.40
8:7:7:CYS:SG	28:S:95:ARG:NH2	2.05	1.29
15:F:79:ARG:NH2	31:V:56:C:O2	1.62	1.27
8:7:14:ASN:O	8:7:15:ILE:HD13	1.35	1.25
10:A:1923:U:H5"	31:V:24:G:O2'	1.04	1.19

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	0	54/56 (96%)	43 (80%)	7 (13%)	4 (7%)	1 21
2	1	48/50 (96%)	42 (88%)	3 (6%)	3 (6%)	2 26
3	2	44/46 (96%)	41 (93%)	3 (7%)	0	100 100
4	3	62/64 (97%)	53 (86%)	7 (11%)	2 (3%)	5 44
5	4	36/38 (95%)	29 (81%)	4 (11%)	3 (8%)	1 18
6	5	146/148 (99%)	77 (53%)	41 (28%)	28 (19%)	0 3
7	6	28/30 (93%)	20 (71%)	7 (25%)	1 (4%)	4 41
8	7	18/20 (90%)	7 (39%)	1 (6%)	10 (56%)	0 0
9	8	92/94 (98%)	81 (88%)	11 (12%)	0	100 100
12	C	269/271 (99%)	211 (78%)	43 (16%)	15 (6%)	2 29
13	D	207/209 (99%)	163 (79%)	30 (14%)	14 (7%)	1 24
14	E	199/201 (99%)	162 (81%)	27 (14%)	10 (5%)	3 31
15	F	175/177 (99%)	141 (81%)	30 (17%)	4 (2%)	8 51
16	G	174/176 (99%)	127 (73%)	30 (17%)	17 (10%)	1 14
17	H	48/50 (96%)	29 (60%)	14 (29%)	5 (10%)	1 12
18	I	139/141 (99%)	97 (70%)	33 (24%)	9 (6%)	1 25
19	J	140/142 (99%)	113 (81%)	18 (13%)	9 (6%)	2 26
20	K	120/122 (98%)	95 (79%)	15 (12%)	10 (8%)	1 18
21	L	141/143 (99%)	104 (74%)	32 (23%)	5 (4%)	4 42
22	M	134/136 (98%)	107 (80%)	16 (12%)	11 (8%)	1 18
23	N	118/120 (98%)	101 (86%)	16 (14%)	1 (1%)	24 70
24	O	114/116 (98%)	95 (83%)	18 (16%)	1 (1%)	21 68
25	P	112/114 (98%)	86 (77%)	17 (15%)	9 (8%)	1 19
26	Q	115/117 (98%)	99 (86%)	12 (10%)	4 (4%)	4 42
27	R	101/103 (98%)	83 (82%)	15 (15%)	3 (3%)	5 46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
28	S	108/110 (98%)	90 (83%)	10 (9%)	8 (7%)	1 21
29	T	91/93 (98%)	57 (63%)	24 (26%)	10 (11%)	0 10
30	U	100/102 (98%)	74 (74%)	16 (16%)	10 (10%)	1 13
32	W	77/79 (98%)	39 (51%)	21 (27%)	17 (22%)	0 1
33	X	75/77 (97%)	64 (85%)	8 (11%)	3 (4%)	4 38
34	Y	61/63 (97%)	39 (64%)	18 (30%)	4 (7%)	1 25
35	Z	56/58 (97%)	46 (82%)	8 (14%)	2 (4%)	4 41
All	All	3402/3466 (98%)	2615 (77%)	555 (16%)	232 (7%)	3 24

5 of 232 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	0	23	ALA
4	3	22	LYS
5	4	8	LYS
6	5	27	VAL
6	5	48	ALA

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	47/47 (100%)	46 (98%)	1 (2%)	61 86
2	1	45/45 (100%)	42 (93%)	3 (7%)	20 62
3	2	38/38 (100%)	35 (92%)	3 (8%)	15 55
4	3	51/51 (100%)	46 (90%)	5 (10%)	10 44
5	4	34/34 (100%)	31 (91%)	3 (9%)	12 50
6	5	112/112 (100%)	93 (83%)	19 (17%)	2 19
7	6	26/26 (100%)	22 (85%)	4 (15%)	3 24
8	7	20/20 (100%)	15 (75%)	5 (25%)	1 6
9	8	78/78 (100%)	75 (96%)	3 (4%)	40 76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
12	C	216/216 (100%)	202 (94%)	14 (6%)	21 62
13	D	164/164 (100%)	151 (92%)	13 (8%)	15 55
14	E	165/165 (100%)	146 (88%)	19 (12%)	7 37
15	F	148/148 (100%)	138 (93%)	10 (7%)	20 61
16	G	137/137 (100%)	122 (89%)	15 (11%)	8 40
17	H	40/40 (100%)	39 (98%)	1 (2%)	55 83
18	I	109/109 (100%)	105 (96%)	4 (4%)	41 76
19	J	116/116 (100%)	100 (86%)	16 (14%)	4 30
20	K	103/103 (100%)	92 (89%)	11 (11%)	8 41
21	L	102/102 (100%)	95 (93%)	7 (7%)	19 60
22	M	109/109 (100%)	93 (85%)	16 (15%)	4 27
23	N	100/100 (100%)	93 (93%)	7 (7%)	19 60
24	O	86/86 (100%)	78 (91%)	8 (9%)	11 47
25	P	99/99 (100%)	91 (92%)	8 (8%)	15 54
26	Q	89/89 (100%)	81 (91%)	8 (9%)	12 49
27	R	84/84 (100%)	78 (93%)	6 (7%)	18 59
28	S	93/93 (100%)	83 (89%)	10 (11%)	8 41
29	T	80/80 (100%)	78 (98%)	2 (2%)	55 83
30	U	83/83 (100%)	77 (93%)	6 (7%)	18 58
32	W	59/59 (100%)	53 (90%)	6 (10%)	9 43
33	X	67/67 (100%)	61 (91%)	6 (9%)	12 49
34	Y	55/55 (100%)	52 (94%)	3 (6%)	27 68
35	Z	48/48 (100%)	40 (83%)	8 (17%)	3 20
All	All	2803/2803 (100%)	2553 (91%)	250 (9%)	17 50

5 of 250 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
16	G	132	LEU
20	K	8	LEU
32	W	49	ASN
16	G	176	LYS
19	J	36	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
9	8	80	HIS
34	Y	41	HIS
15	F	26	GLN
8	7	22	HIS
15	F	4	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	A	2850/2854 (99%)	453 (15%)	40 (1%)
11	B	117/118 (99%)	17 (14%)	0
31	V	76/77 (98%)	15 (19%)	0
All	All	3043/3049 (99%)	485 (15%)	40 (1%)

5 of 485 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
10	A	10	A
10	A	12	U
10	A	15	G
10	A	34	U
10	A	35	G

5 of 40 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
10	A	1088	A
10	A	1458	U
10	A	2423	U
10	A	1247	A
10	A	1509	A

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

1 non-standard protein/DNA/RNA residue 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	$\#\|Z\| > 2$
31	5MU	V	54	31	13,21,23	1.53	2 (15%)	17,30,35	3.31	3 (17%)

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
31	5MU	V	54	31	-	0/3/25/26	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	V	54	5MU	C6-N1	2.26	1.38	1.35
31	V	54	5MU	C4-N3	4.32	1.40	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	V	54	5MU	C5-C4-N3	-3.97	113.54	123.28
31	V	54	5MU	O4'-C1'-N1	3.06	113.91	108.10
31	V	54	5MU	C4-N3-C2	12.44	127.32	114.21

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 146 ligands modelled in this entry, 144 are monoatomic - leaving 2 for Mogul analysis.

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	$\#\|Z\| > 2$
36	TRP	7	1001	-	11,16,16	0.55	0	9,22,22	0.81	0
36	TRP	7	1002	-	11,16,16	0.54	0	9,22,22	0.86	0

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
36	TRP	7	1001	-	-	0/3/8/8	0/2/2/2
36	TRP	7	1002	-	-	0/3/8/8	0/2/2/2

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.

2 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	7	1001	TRP	8	0
36	7	1002	TRP	16	0

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.