



wwPDB X-ray Structure Validation Summary Report i

Mar 11, 2014 – 03:09 PM GMT

PDB ID : 2J01
Title : STRUCTURE OF THE THERMUS THERMOPHILUS 70S RIBOSOME COMPLEXED WITH MRNA, TRNA AND PAROMOMYCIN (PART 2 OF 4). THIS FILE CONTAINS THE 50S SUBUNIT FROM MOLECULE I.
Authors : Selmer, M.; Dunham, C.M.; Murphy, F.V.; Weixlbaumer, A.; Petry, S.; Weir, J.R.; Kelley, A.C.; Ramakrishnan, V.
Deposited on : 2006-07-31
Resolution : 2.80 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

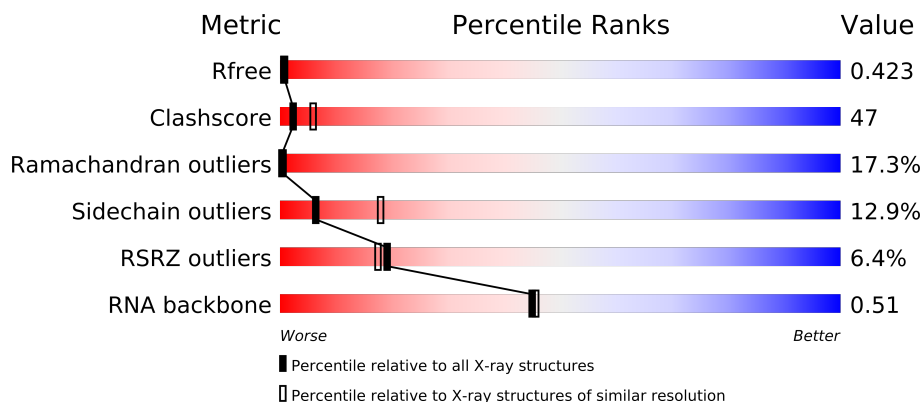
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1323
EDS : trunk22699
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk22699

1 Overall quality at a glance

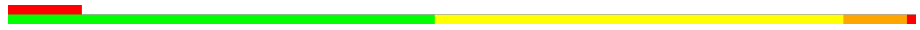
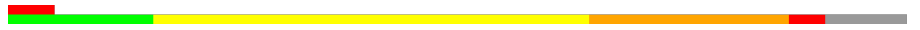

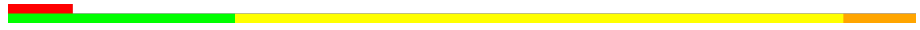
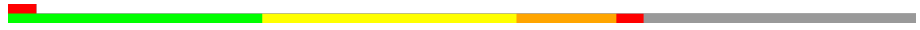
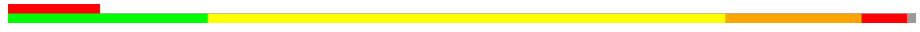
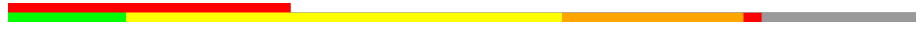





The reported resolution of this entry is 2.80 Å.

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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1799 (2.80-2.80)
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (2.80-2.80)
RNA backbone	1838	1076 (3.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	0	85	
2	1	98	
3	2	72	
4	3	60	
5	4	71	
6	5	60	
7	6	54	
8	7	49	
9	8	65	
10	A	2787	
11	B	122	
12	C	229	

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Mol	Chain	Length	Quality of chain
13	D	276	
14	E	206	
15	F	210	
16	G	182	
17	H	180	
18	I	148	
19	N	140	
20	O	122	
21	P	150	
22	Q	141	
23	R	118	
24	S	112	
25	T	146	
26	U	118	
27	V	101	
28	W	113	
29	X	96	
30	Y	110	
31	Z	206	

2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 89408 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	0	85	Total	C	N	O	S	0	0	0
			650	401	137	111	1			

- Molecule 2 is a protein called 50S RIBOSOMAL PROTEIN L28.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	1	89	Total	C	N	O	0	0	1
			693	435	140	118			

- Molecule 3 is a protein called 50S RIBOSOMAL PROTEIN L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	2	51	Total	C	N	O	S	0	0	1
			421	263	85	72	1			

- Molecule 4 is a protein called 50S RIBOSOMAL PROTEIN L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	3	60	Total	C	N	O	S	0	0	1
			468	298	91	78	1			

- Molecule 5 is a protein called 50S RIBOSOMAL PROTEIN L31.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	4	50	Total	C	N	O	0	0	1
			242	143	50	49			

- Molecule 6 is a protein called 50S RIBOSOMAL PROTEIN L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			

- Molecule 7 is a protein called 50S RIBOSOMAL PROTEIN L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	6	45	Total	C	N	O	S	0	0	1
			381	235	78	64	4			

- Molecule 8 is a protein called 50S RIBOSOMAL PROTEIN L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	7	49	Total	C	N	O	S	0	0	1
			419	257	105	55	2			

- Molecule 9 is a protein called 50S RIBOSOMAL PROTEIN L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	8	64	Total	C	N	O	S	0	0	1
			508	326	102	78	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	A	2772	Total	C	N	O	P	0	0	0
			59708	26573	11171	19193	2771			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	B	119	Total	C	N	O	P	0	0	0
			2551	1136	471	826	118			

- Molecule 12 is a protein called 50S RIBOSOMAL PROTEIN L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	C	191	Total	C	N	O		0	0	1
			1142	691	221	230				

- Molecule 13 is a protein called 50S RIBOSOMAL PROTEIN L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	D	272	Total	C	N	O	S	0	0	1
			2105	1329	417	356	3			

- Molecule 14 is a protein called 50S RIBOSOMAL PROTEIN L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	E	205	Total	C	N	O	S	0	0	1
			1564	988	300	270	6			

- Molecule 15 is a protein called 50S RIBOSOMAL PROTEIN L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	F	208	Total	C	N	O	S	0	0	1
			1624	1035	304	282	3			

- Molecule 16 is a protein called 50S RIBOSOMAL PROTEIN L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	G	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			

- Molecule 17 is a protein called 50S RIBOSOMAL PROTEIN L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	H	160	Total	C	N	O	S	0	0	1
			1223	773	229	220	1			

- Molecule 18 is a protein called 50S RIBOSOMAL PROTEIN L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	I	146	Total	C	N	O	S	0	0	1
			1132	723	201	207	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	N	139	Total	C	N	O	S	0	0	1
			1105	712	207	182	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	O	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	P	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	Q	136	Total	C	N	O	S	0	0	0
			1080	688	204	183	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	R	117	Total	C	N	O		0	0	0
			960	599	202	159				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	S	99	Total	C	N	O		0	0	1
			771	486	155	130				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	T	138	Total	C	N	O	S	0	0	1
			1142	710	235	196	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	U	117	Total	C	N	O	S	0	0	0
			958	604	202	151	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	V	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	W	113	Total	C	N	O	S	0	0	0
			896	563	176	155	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	X	93	Total	C	N	O		0	0	1
			726	471	132	123				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	Y	101	Total	C	N	O	S	0	0	1
			776	500	149	123	4			

- Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	Z	177	Total	C	N	O	S	0	0	1
			1404	897	253	252	2			

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L36.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
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- Molecule 33 is a protein called 50S RIBOSOMAL PROTEIN L10.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
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- Molecule 34 is a protein called 50S RIBOSOMAL PROTEIN L11.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
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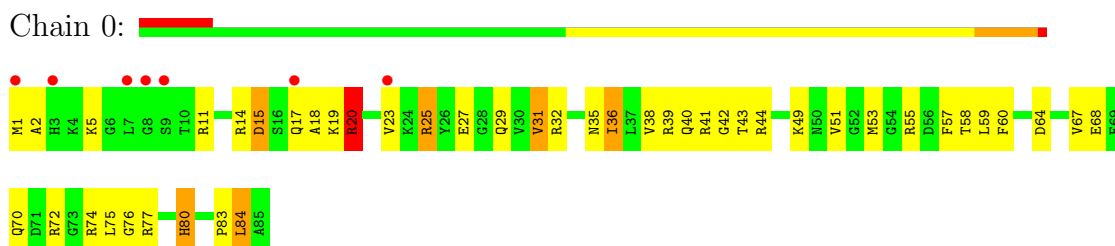
- Molecule 35 is a protein called 50S RIBOSOMAL PROTEIN L7.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
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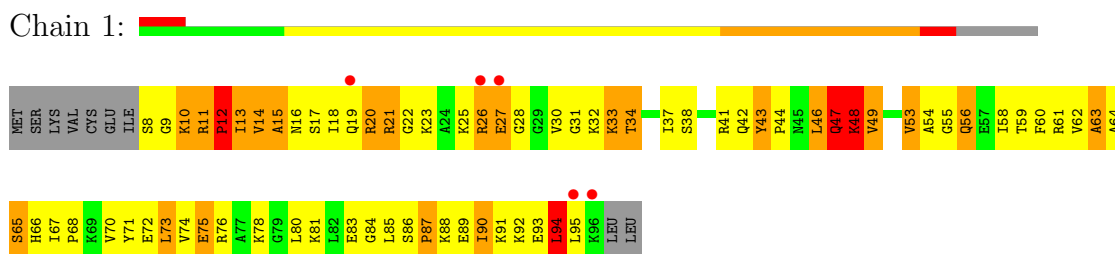
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

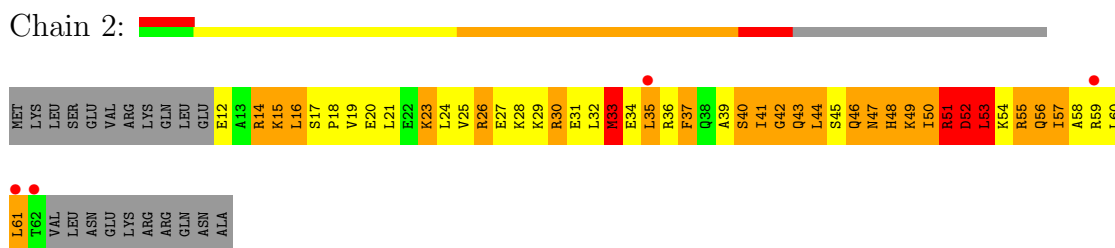
- Molecule 1: 50S RIBOSOMAL PROTEIN L27



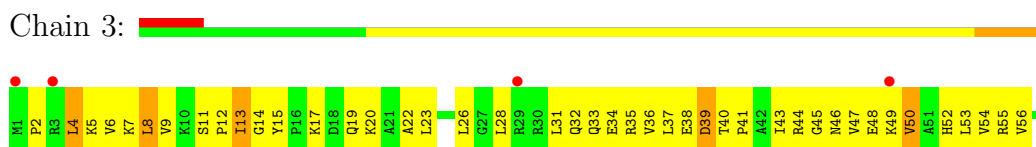
- Molecule 2: 50S RIBOSOMAL PROTEIN L28



- Molecule 3: 50S RIBOSOMAL PROTEIN L29

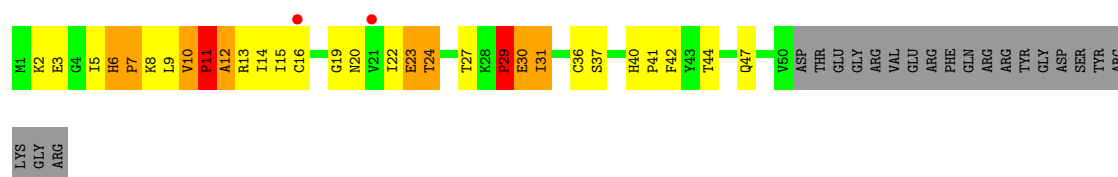


- Molecule 4: 50S RIBOSOMAL PROTEIN L30



- Molecule 5: 50S RIBOSOMAL PROTEIN L31





• Molecule 6: 50S RIBOSOMAL PROTEIN L32

Chain 5:

• Molecule 7: 50S RIBOSOMAL PROTEIN L33

Chain 6:

• Molecule 8: 50S RIBOSOMAL PROTEIN L34

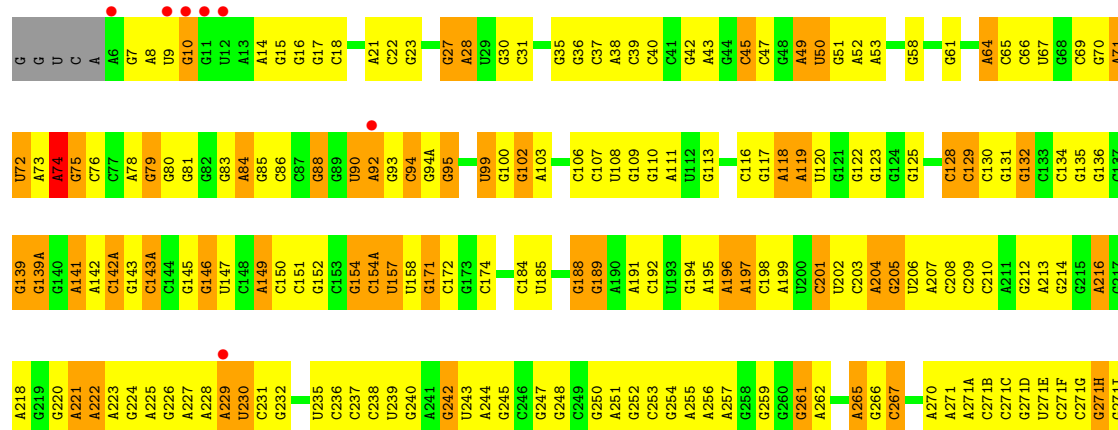
Chain 7:

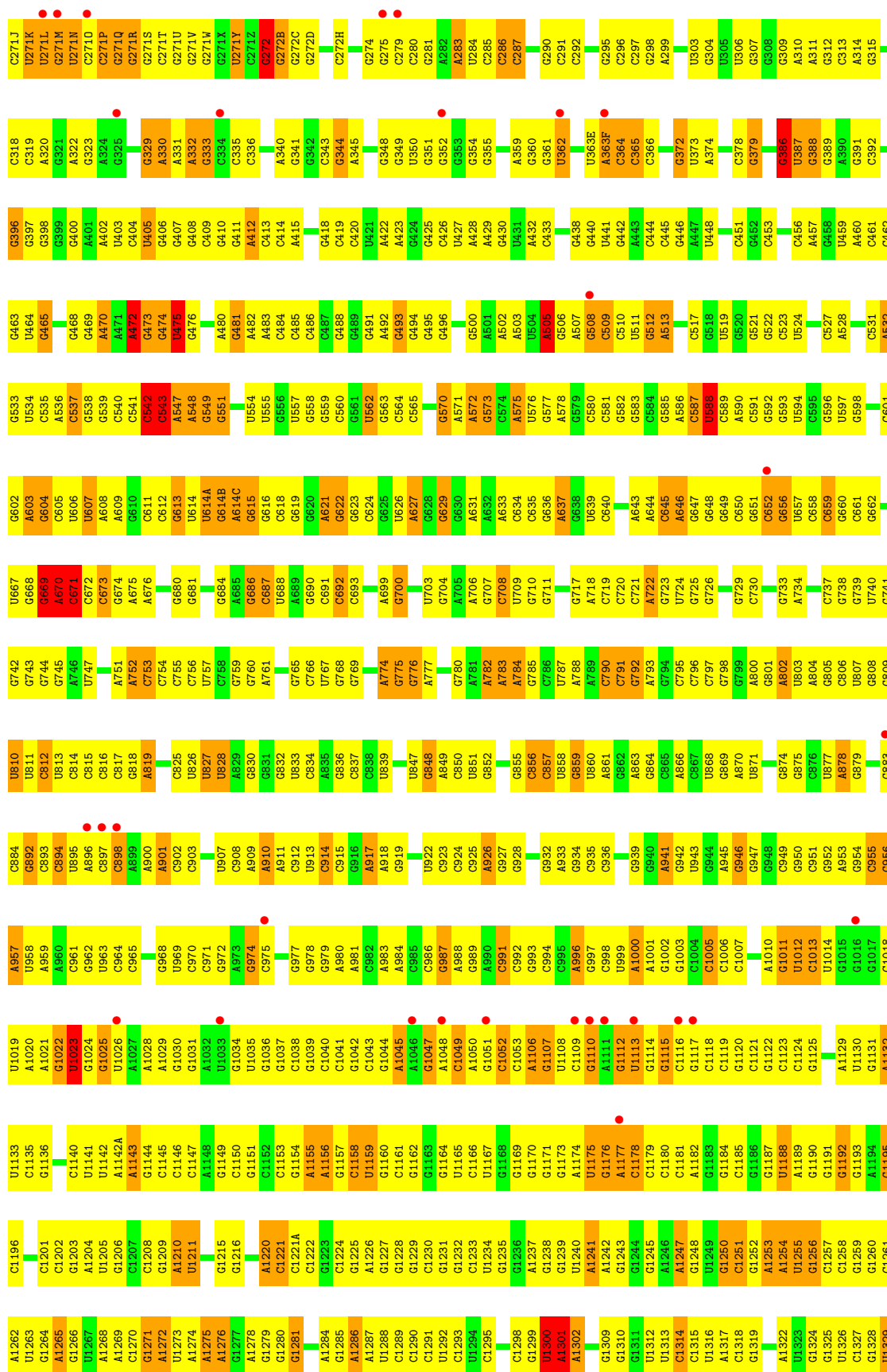
• Molecule 9: 50S RIBOSOMAL PROTEIN L35

Chain 8:

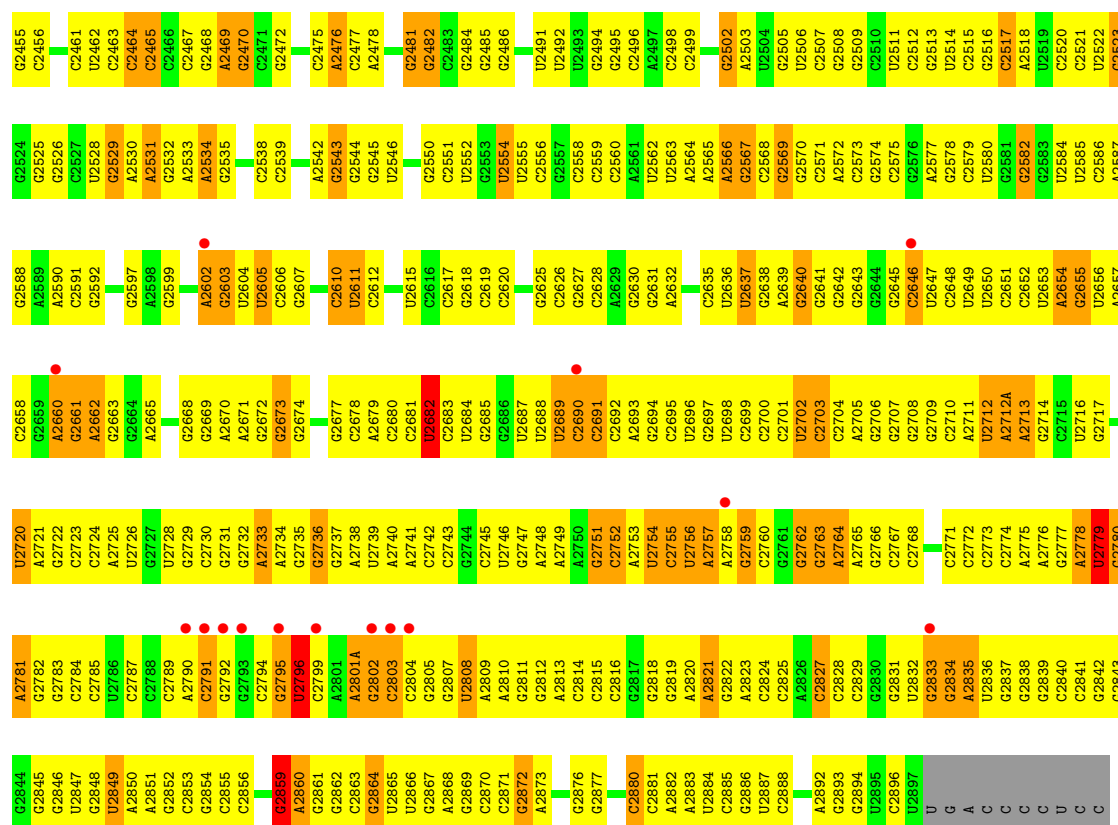
• Molecule 10: 23S RIBOSOMAL RNA

Chain A:



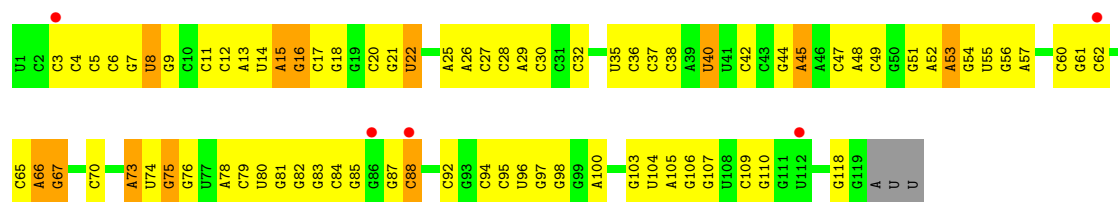






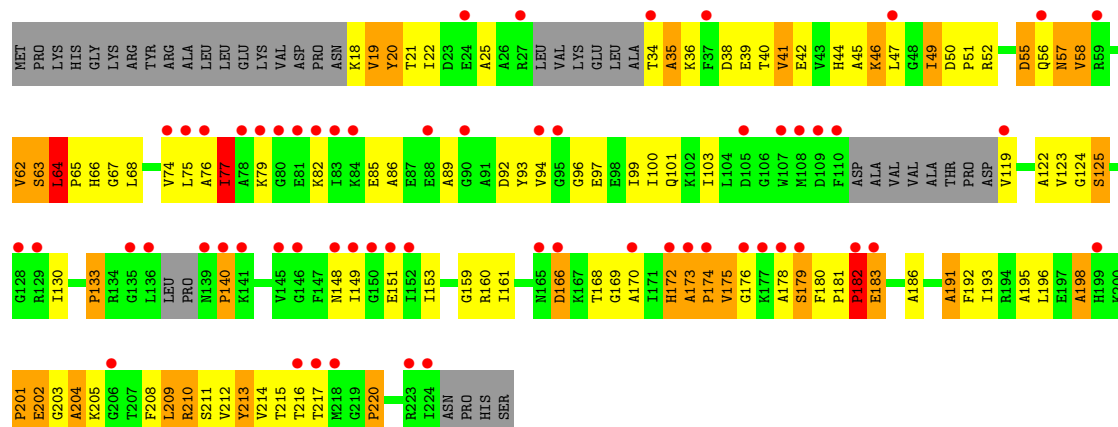
• Molecule 11: 5S RIBOSOMAL RNA

Chain B:



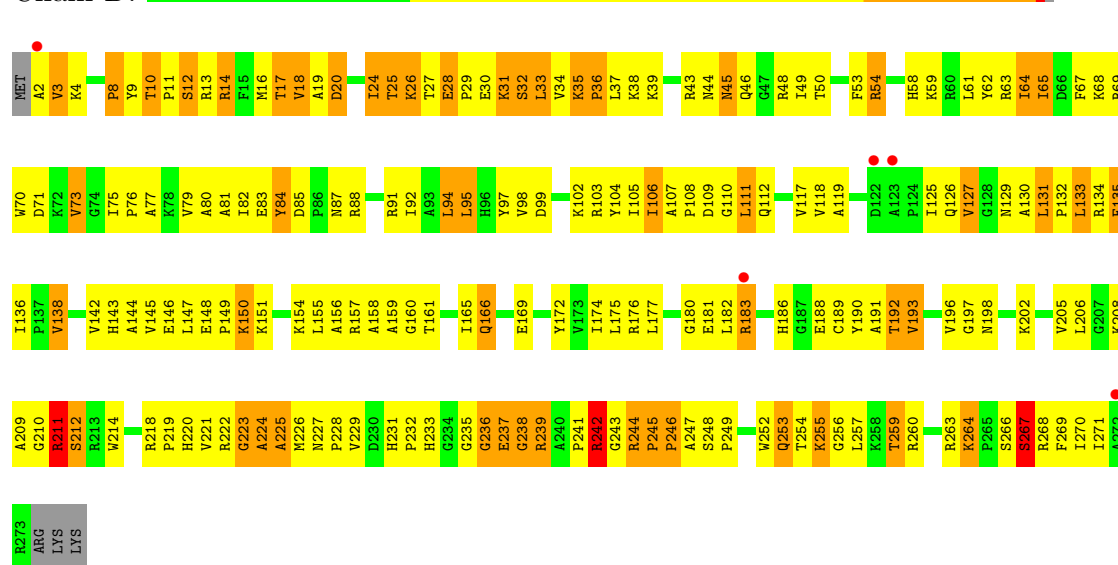
• Molecule 12: 50S RIBOSOMAL PROTEIN L1

Chain C:



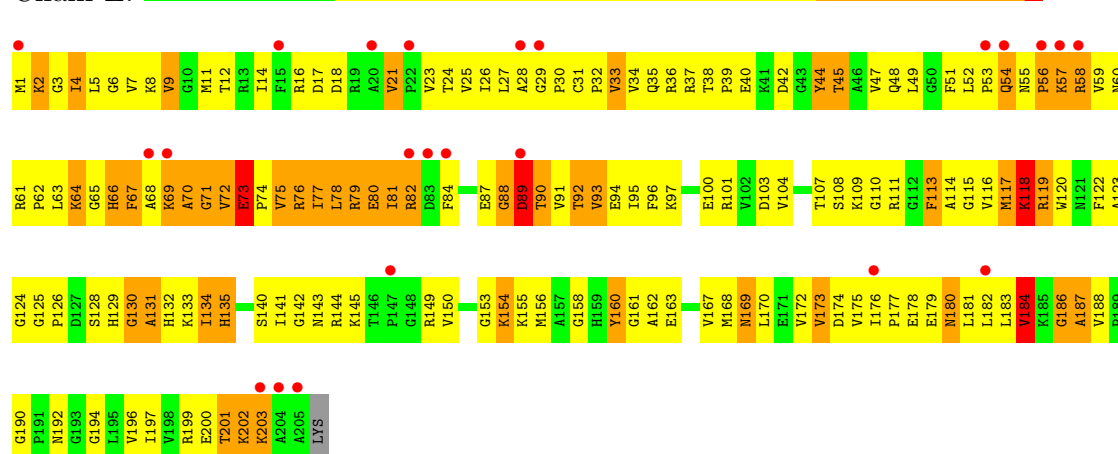
● Molecule 13: 50S RIBOSOMAL PROTEIN L2

Chain D:



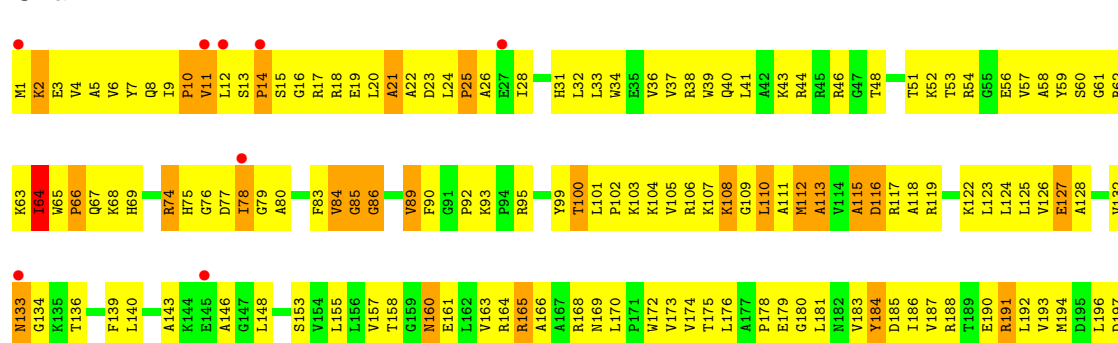
● Molecule 14: 50S RIBOSOMAL PROTEIN L3

Chain E:



● Molecule 15: 50S RIBOSOMAL PROTEIN L4

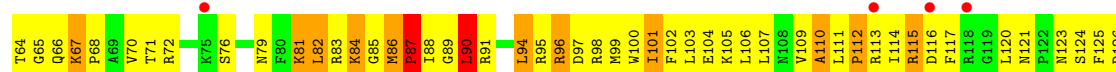
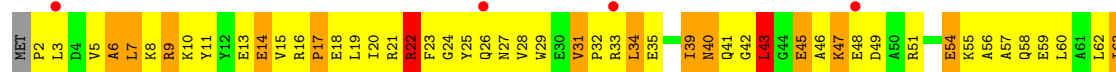
Chain F:





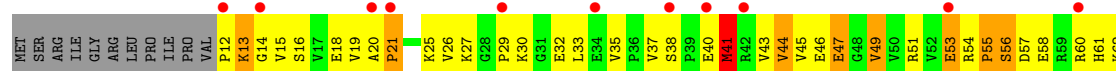
• Molecule 16: 50S RIBOSOMAL PROTEIN L5

Chain G:



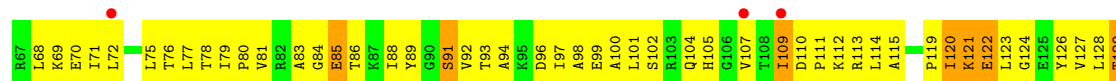
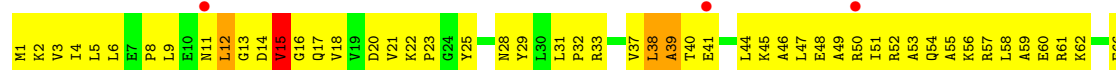
• Molecule 17: 50S RIBOSOMAL PROTEIN L6

Chain H:



• Molecule 18: 50S RIBOSOMAL PROTEIN L9

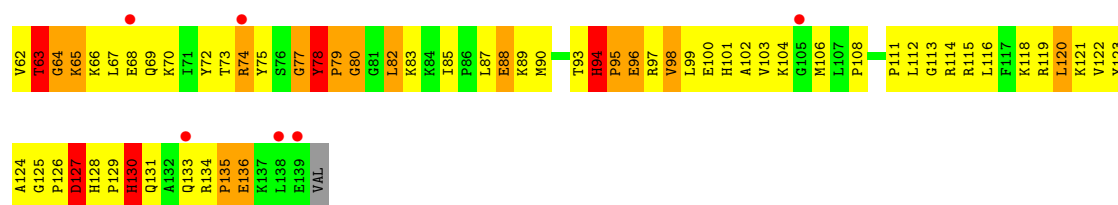
Chain I:



• Molecule 19: 50S RIBOSOMAL PROTEIN L13

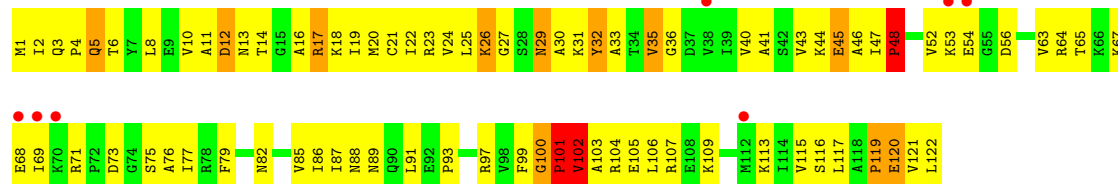
Chain N:





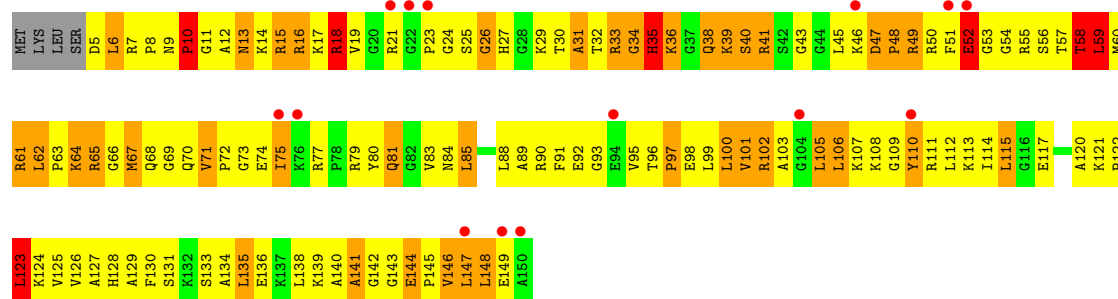
• Molecule 20: 50S RIBOSOMAL PROTEIN L14

Chain O:



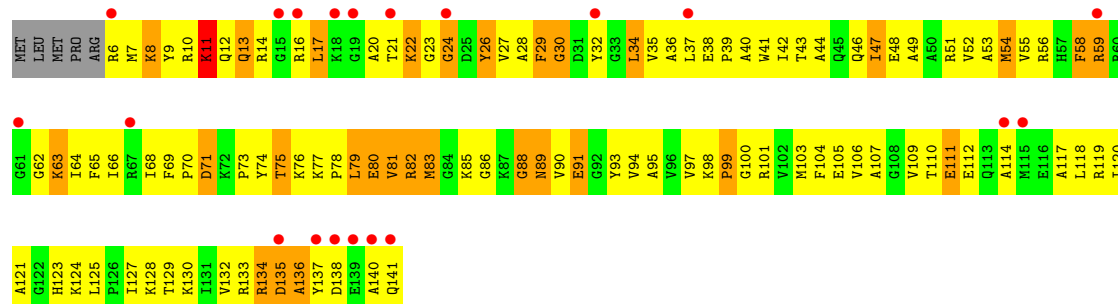
• Molecule 21: 50S RIBOSOMAL PROTEIN L15

Chain P:



• Molecule 22: 50S RIBOSOMAL PROTEIN L16

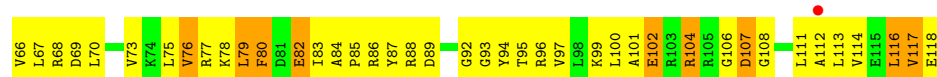
Chain Q:



• Molecule 23: 50S RIBOSOMAL PROTEIN L17

Chain R:





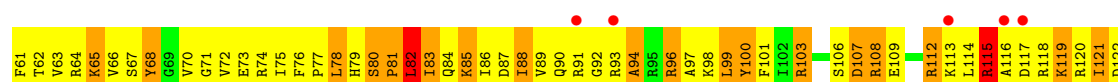
• Molecule 24: 50S RIBOSOMAL PROTEIN L18

Chain S:



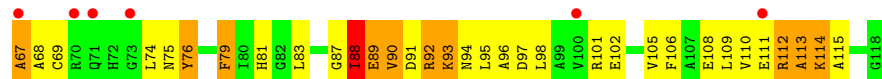
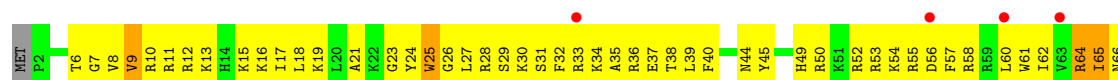
• Molecule 25: 50S RIBOSOMAL PROTEIN L19

Chain T:



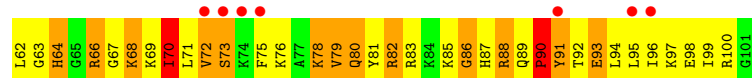
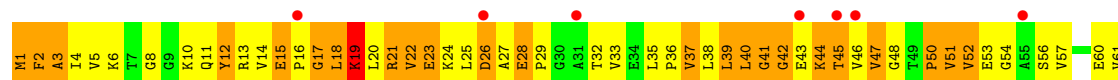
• Molecule 26: 50S RIBOSOMAL PROTEIN L20

Chain U:



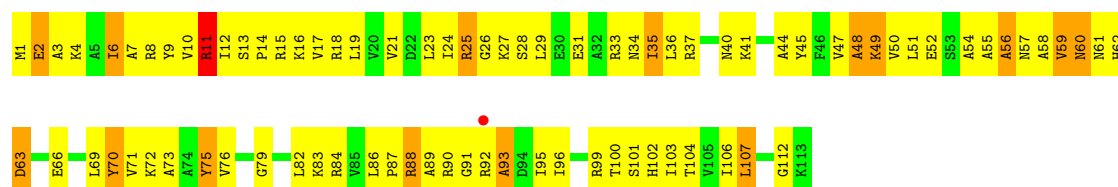
• Molecule 27: 50S RIBOSOMAL PROTEIN L21

Chain V:



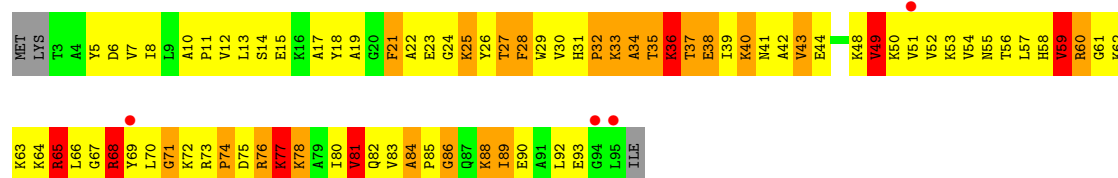
• Molecule 28: 50S RIBOSOMAL PROTEIN L22

Chain W:



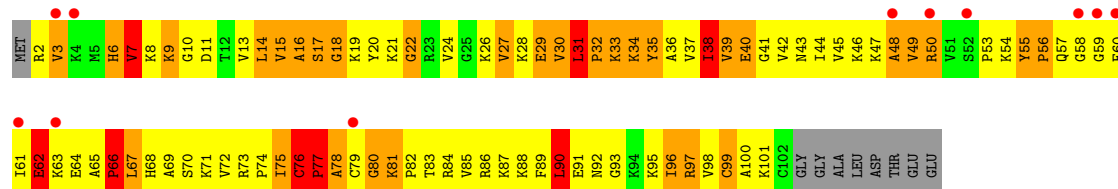
• Molecule 29: 50S RIBOSOMAL PROTEIN L23

Chain X:



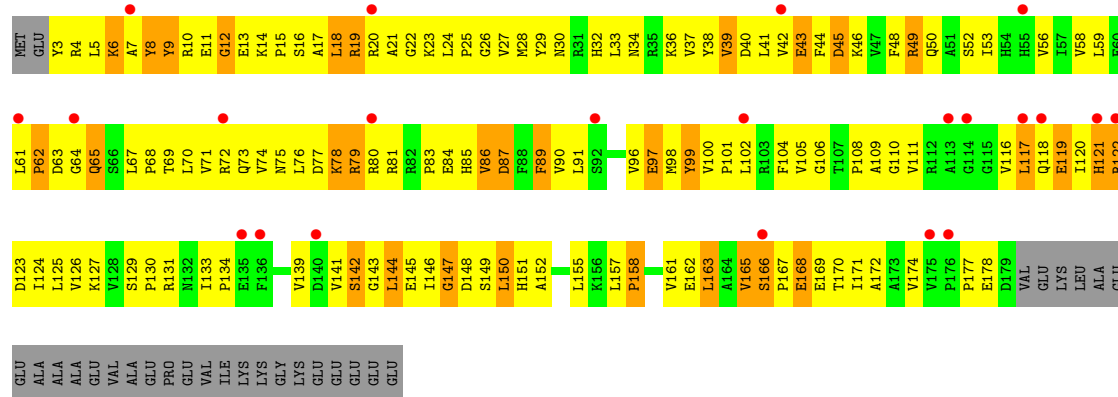
• Molecule 30: 50S RIBOSOMAL PROTEIN L24

Chain Y:



• Molecule 31: 50S RIBOSOMAL PROTEIN L25

Chain Z:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	213.32Å 452.95Å 631.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.80 49.96 – 2.80	Depositor EDS
% Data completeness (in resolution range)	90.7 (50.00-2.80) 90.7 (49.96-2.80)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 2.81Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.272 , 0.313 0.421 , 0.423	Depositor DCC
R_{free} test set	64102 reflections (5.01%)	DCC
Wilson B-factor (Å ²)	36.9	Xtriage
Anisotropy	0.160	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.15 , 39.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.35$, $\langle L^2 \rangle = 0.17$	Xtriage
Outliers	0 of 1342659 reflections	Xtriage
F_o, F_c correlation	0.55	EDS
Total number of atoms	89408	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.24% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	0	0.38	0/658	0.65	0/878
2	1	0.61	0/700	1.04	1/931 (0.1%)
3	2	0.45	0/423	0.99	3/560 (0.5%)
4	3	0.37	0/473	0.61	0/636
5	4	0.47	0/241	0.88	4/334 (1.2%)
6	5	0.42	0/473	0.74	0/639
7	6	0.39	0/387	0.62	0/517
8	7	0.51	0/427	0.73	0/563
9	8	0.50	0/516	0.81	0/681
10	A	0.62	4/66876 (0.0%)	0.77	56/104407 (0.1%)
11	B	0.39	0/2853	0.70	0/4451
12	C	0.38	0/1145	0.68	7/1556 (0.4%)
13	D	0.52	0/2155	0.87	3/2907 (0.1%)
14	E	0.43	0/1597	0.76	0/2155
15	F	0.45	0/1659	0.70	0/2246
16	G	0.39	0/1498	0.72	1/2013 (0.0%)
17	H	0.33	0/1246	0.69	0/1684
18	I	0.35	0/1147	0.66	0/1553
19	N	0.40	0/1132	0.78	0/1527
20	O	0.48	0/943	0.74	0/1269
21	P	0.42	0/1131	1.00	6/1504 (0.4%)
22	Q	0.37	0/1100	0.72	1/1470 (0.1%)
23	R	0.40	0/974	0.74	1/1302 (0.1%)
24	S	0.40	0/779	0.73	0/1038
25	T	0.42	0/1156	0.77	2/1544 (0.1%)
26	U	0.37	0/975	0.68	0/1297
27	V	0.38	0/789	0.73	0/1054
28	W	0.43	0/907	0.72	0/1216
29	X	0.53	0/740	0.89	3/995 (0.3%)
30	Y	0.41	0/789	0.78	0/1053
31	Z	0.35	0/1436	0.64	0/1951
All	All	0.56	4/97325 (0.0%)	0.76	88/145931 (0.1%)

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
2	1	0	1
10	A	30	81
All	All	30	82

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	783	A	C5-C6	-6.34	1.35	1.41
10	A	774	A	C5-C6	-6.20	1.35	1.41
10	A	652	C	C3'-O3'	5.41	1.49	1.42
10	A	656	G	O5'-C5'	5.32	1.52	1.44

The worst 5 of 88 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	1962	C	N1-C1'-C2'	10.48	127.62	114.00
10	A	669	G	N9-C1'-C2'	10.36	127.47	114.00
10	A	1722	A	N9-C1'-C2'	9.93	126.91	114.00
10	A	1397	U	C2'-C3'-O3'	9.86	131.19	109.50
10	A	1250	G	C2'-C3'-O3'	9.26	129.88	109.50

5 of 30 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
10	A	100	G	C1'
10	A	283	A	C3'
10	A	472	A	C3'
10	A	669	G	C4',C3',C1'
10	A	945	A	C1'

5 of 82 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1	43	TYR	Sidechain
10	A	188	G	Sidechain
10	A	189	G	Sidechain
10	A	74	A	Sidechain
10	A	79	G	Sidechain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	650	0	654	71	0
2	1	693	0	764	182	0
3	2	421	0	461	124	0
4	3	468	0	523	53	0
5	4	242	0	103	22	0
6	5	459	0	480	75	0
7	6	381	0	390	59	0
8	7	419	0	467	35	0
9	8	508	0	576	110	0
10	A	59708	0	30099	2489	0
11	B	2551	0	1295	106	0
12	C	1142	0	865	109	0
13	D	2105	0	2182	357	0
14	E	1564	0	1629	325	0
15	F	1624	0	1677	237	0
16	G	1474	0	1534	231	0
17	H	1223	0	1282	199	0
18	I	1132	0	1218	198	0
19	N	1105	0	1180	209	0
20	O	933	0	996	136	0
21	P	1114	0	1187	322	0
22	Q	1080	0	1127	224	0
23	R	960	0	1021	171	0
24	S	771	0	832	182	0
25	T	1142	0	1202	219	0
26	U	958	0	1015	183	0
27	V	779	0	851	212	0
28	W	896	0	953	111	0
29	X	726	0	778	203	0
30	Y	776	0	870	220	0
31	Z	1404	0	1432	219	0
All	All	89408	0	59643	6918	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 47.

The worst 5 of 6918 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
18:I:79:ILE:HG12	18:I:140:LEU:HD11	1.21	1.17
10:A:2128:C:H2'	10:A:2129:C:H5''	1.28	1.16
10:A:1590:U:H2'	10:A:1591:G:H5''	1.29	1.15
10:A:2701:C:H3'	10:A:2702:U:H5''	1.24	1.15
27:V:70:ILE:HB	27:V:90:PRO:HB2	1.20	1.15

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 X-ray entries followed by that with respect to entries of similar resolution. 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	83/85 (98%)	62 (75%)	16 (19%)	5 (6%)	2	6
2	1	87/98 (89%)	43 (49%)	25 (29%)	19 (22%)	0	0
3	2	49/72 (68%)	16 (33%)	16 (33%)	17 (35%)	0	0
4	3	58/60 (97%)	42 (72%)	12 (21%)	4 (7%)	2	4
5	4	48/71 (68%)	14 (29%)	11 (23%)	23 (48%)	0	0
6	5	57/60 (95%)	37 (65%)	13 (23%)	7 (12%)	1	1
7	6	41/54 (76%)	18 (44%)	16 (39%)	7 (17%)	0	0
8	7	47/49 (96%)	36 (77%)	10 (21%)	1 (2%)	11	33
9	8	62/65 (95%)	38 (61%)	13 (21%)	11 (18%)	0	0
12	C	183/229 (80%)	88 (48%)	52 (28%)	43 (24%)	0	0
13	D	270/276 (98%)	193 (72%)	51 (19%)	26 (10%)	1	2
14	E	203/206 (98%)	116 (57%)	49 (24%)	38 (19%)	0	0
15	F	206/210 (98%)	142 (69%)	40 (19%)	24 (12%)	1	1
16	G	177/182 (97%)	93 (52%)	56 (32%)	28 (16%)	0	1
17	H	158/180 (88%)	100 (63%)	31 (20%)	27 (17%)	0	0
18	I	144/148 (97%)	98 (68%)	36 (25%)	10 (7%)	2	4
19	N	137/140 (98%)	75 (55%)	35 (26%)	27 (20%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	O	120/122 (98%)	92 (77%)	17 (14%)	11 (9%)	1	2
21	P	144/150 (96%)	72 (50%)	37 (26%)	35 (24%)	0	0
22	Q	134/141 (95%)	81 (60%)	34 (25%)	19 (14%)	0	1
23	R	115/118 (98%)	74 (64%)	20 (17%)	21 (18%)	0	0
24	S	97/112 (87%)	49 (50%)	19 (20%)	29 (30%)	0	0
25	T	136/146 (93%)	77 (57%)	34 (25%)	25 (18%)	0	0
26	U	115/118 (98%)	61 (53%)	42 (36%)	12 (10%)	1	1
27	V	97/101 (96%)	47 (48%)	23 (24%)	27 (28%)	0	0
28	W	111/113 (98%)	74 (67%)	23 (21%)	14 (13%)	0	1
29	X	91/96 (95%)	45 (50%)	23 (25%)	23 (25%)	0	0
30	Y	99/110 (90%)	41 (41%)	24 (24%)	34 (34%)	0	0
31	Z	175/206 (85%)	99 (57%)	48 (27%)	28 (16%)	0	1
All	All	3444/3718 (93%)	2023 (59%)	826 (24%)	595 (17%)	0	0

5 of 595 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	1	10	LYS
2	1	12	PRO
2	1	13	ILE
2	1	14	VAL
2	1	15	ALA

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 X-ray entries followed by that with respect to entries of similar resolution. 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	61/67 (91%)	54 (88%)	7 (12%)	8	23
2	1	73/83 (88%)	62 (85%)	11 (15%)	4	12
3	2	46/67 (69%)	35 (76%)	11 (24%)	1	3
4	3	51/52 (98%)	49 (96%)	2 (4%)	43	80
6	5	51/52 (98%)	41 (80%)	10 (20%)	2	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	6	43/52 (83%)	36 (84%)	7 (16%)	3	10
8	7	41/42 (98%)	37 (90%)	4 (10%)	12	32
9	8	53/55 (96%)	45 (85%)	8 (15%)	4	12
12	C	61/181 (34%)	54 (88%)	7 (12%)	8	23
13	D	213/218 (98%)	179 (84%)	34 (16%)	3	10
14	E	165/166 (99%)	145 (88%)	20 (12%)	7	21
15	F	165/166 (99%)	153 (93%)	12 (7%)	20	49
16	G	155/156 (99%)	135 (87%)	20 (13%)	6	18
17	H	132/148 (89%)	117 (89%)	15 (11%)	8	24
18	I	122/124 (98%)	113 (93%)	9 (7%)	20	48
19	N	117/119 (98%)	98 (84%)	19 (16%)	3	10
20	O	100/100 (100%)	92 (92%)	8 (8%)	17	44
21	P	112/116 (97%)	92 (82%)	20 (18%)	2	7
22	Q	106/111 (96%)	93 (88%)	13 (12%)	7	20
23	R	100/101 (99%)	91 (91%)	9 (9%)	14	37
24	S	77/88 (88%)	65 (84%)	12 (16%)	4	11
25	T	120/127 (94%)	99 (82%)	21 (18%)	3	8
26	U	92/94 (98%)	85 (92%)	7 (8%)	19	46
27	V	82/82 (100%)	64 (78%)	18 (22%)	1	4
28	W	91/92 (99%)	85 (93%)	6 (7%)	24	56
29	X	74/78 (95%)	59 (80%)	15 (20%)	2	5
30	Y	84/91 (92%)	67 (80%)	17 (20%)	2	5
31	Z	155/179 (87%)	144 (93%)	11 (7%)	21	51
All	All	2742/3007 (91%)	2389 (87%)	353 (13%)	6	18

5 of 353 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
17	H	136	ILE
20	O	32	TYR
30	Y	7	VAL
17	H	157	TYR
19	N	22	THR

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

Mol	Chain	Res	Type
18	I	43	ASN
21	P	38	GLN
29	X	55	ASN
18	I	133	HIS
19	N	128	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	A	2771/2787 (99%)	563 (20%)	76 (2%)
11	B	118/122 (96%)	14 (11%)	1 (0%)
All	All	2889/2909 (99%)	577 (19%)	77 (2%)

5 of 577 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
10	A	10	G
10	A	28	A
10	A	35	G
10	A	45	C
10	A	49	A

5 of 77 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
10	A	1427	A
10	A	1653	G
10	A	2756	U
10	A	1458	C
10	A	1558	A

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	0	85/85 (100%)	0.15	7 (8%) 12 10	8, 43, 138, 196	0
2	1	89/98 (90%)	-0.07	5 (5%) 24 23	1, 35, 143, 157	0
3	2	51/72 (70%)	0.05	4 (7%) 13 11	5, 66, 145, 200	0
4	3	60/60 (100%)	0.16	4 (6%) 17 16	5, 57, 140, 190	0
5	4	50/71 (70%)	0.16	2 (4%) 36 37	38, 90, 158, 173	0
6	5	59/60 (98%)	0.65	6 (10%) 7 6	5, 51, 192, 200	0
7	6	45/54 (83%)	1.56	17 (37%) 1 0	54, 103, 171, 180	0
8	7	49/49 (100%)	-0.10	3 (6%) 21 20	1, 19, 115, 165	0
9	8	64/65 (98%)	0.34	7 (10%) 6 5	4, 44, 140, 195	0
10	A	2772/2787 (99%)	0.05	63 (2%) 57 58	1, 29, 145, 200	0
11	B	119/122 (97%)	0.34	5 (4%) 35 35	22, 64, 108, 197	0
12	C	191/229 (83%)	2.02	60 (31%) 1 1	51, 144, 186, 200	0
13	D	272/276 (98%)	-0.29	5 (1%) 65 66	1, 19, 89, 196	0
14	E	205/206 (99%)	0.38	23 (11%) 6 5	1, 46, 141, 193	0
15	F	208/210 (99%)	-0.03	10 (4%) 29 30	1, 44, 155, 200	0
16	G	181/182 (99%)	0.03	13 (7%) 15 14	8, 65, 142, 188	0
17	H	160/180 (88%)	1.13	32 (20%) 2 1	51, 124, 175, 200	0
18	I	146/148 (98%)	-0.02	6 (4%) 35 36	5, 78, 148, 187	0
19	N	139/140 (99%)	0.25	10 (7%) 15 14	10, 68, 144, 163	0
20	O	122/122 (100%)	-0.16	7 (5%) 23 23	3, 32, 103, 177	0
21	P	146/150 (97%)	0.38	14 (9%) 8 7	1, 61, 159, 193	0
22	Q	136/141 (96%)	0.54	20 (14%) 3 3	7, 58, 171, 200	0
23	R	117/118 (99%)	-0.01	2 (1%) 67 68	3, 32, 132, 146	0
24	S	99/112 (88%)	0.41	11 (11%) 6 5	21, 76, 134, 173	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	T	138/146 (94%)	0.15	11 (7%) 12 11	3, 67, 169, 190	0
26	U	117/118 (99%)	0.40	10 (8%) 11 9	5, 50, 142, 200	0
27	V	101/101 (100%)	0.51	14 (13%) 4 3	14, 96, 174, 192	0
28	W	113/113 (100%)	-0.14	1 (0%) 81 81	1, 26, 121, 161	0
29	X	93/96 (96%)	-0.08	4 (4%) 34 34	1, 46, 137, 168	0
30	Y	101/110 (91%)	0.63	11 (10%) 6 5	1, 79, 170, 195	0
31	Z	177/206 (85%)	0.53	22 (12%) 5 4	19, 96, 177, 200	0
All	All	6405/6627 (96%)	0.21	409 (6%) 19 17	1, 44, 159, 200	0

The worst 5 of 409 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
12	C	224	ILE	26.4
12	C	136	LEU	18.4
17	H	171	LEU	16.8
6	5	60	VAL	16.6
30	Y	60	PHE	14.3

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.