



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 01:47 AM UTC

PDB ID : 1W2B / pdb_00001w2b
Title : Trigger Factor ribosome binding domain in complex with 50S
Authors : Ferbitz, L.; Maier, T.; Patzelt, H.; Bukau, B.; Deuerling, E.; Ban, N.
Deposited on : 2004-07-01
Resolution : 3.50 Å(reported)

This is a wwPDB X-ray Structure 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/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

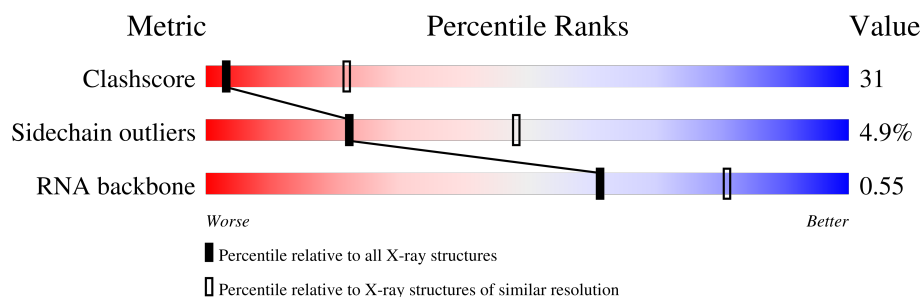
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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))
Clashscore	190562	1140 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RNA backbone	3983	1010 (3.98-3.02)

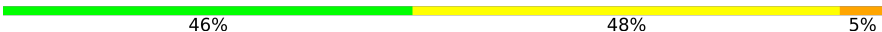
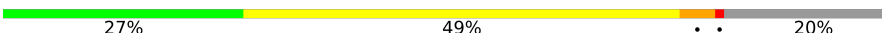
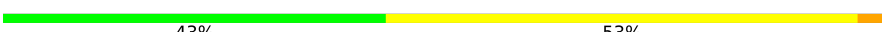
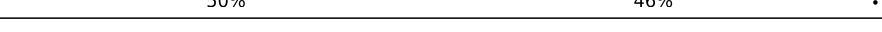
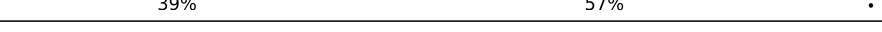
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively.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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	0	2922	32% 44% 13% 5% 6%
2	1	48	40% 54% . .
3	2	92	39% 52% 8% .
4	5	144	8% 11% 6% 76%
5	9	122	29% 50% 14% 7%
6	A	239	36% 59% .
7	B	337	38% 55% 7%

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Mol	Chain	Length	Quality of chain
8	C	246	
9	D	176	
10	E	177	
11	F	119	
12	G	348	
13	H	167	
14	I	145	
15	J	132	
16	K	164	
17	L	194	
18	M	186	
19	N	115	
20	O	148	
21	P	95	
22	Q	154	
23	R	84	
24	S	119	
25	T	66	
26	U	70	
27	V	154	
28	W	91	
29	X	240	
30	Y	73	
31	Z	56	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
35	CL	I	202	-	-	X	-
35	CL	L	202	-	-	X	-
35	CL	P	102	-	-	X	-
35	CL	X	301	-	-	X	-

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 98859 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 RNA chain called 23S RRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	0	2754	Total	C	N	O	P	0	0	0
			59017	26346	10878	19048	2745			

- Molecule 2 is a protein called 50S RIBOSOMAL PROTEIN L39E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1	46	Total	C	N	O	S	0	0	0
			394	238	86	69	1			

- Molecule 3 is a protein called 50S RIBOSOMAL PROTEIN L44E LA, HLA, RIBOSOMAL PROTEIN L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	2	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 4 is a protein called TRIGGER FACTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	5	35	Total	C	N	O	S	0	0	0
			273	173	52	47	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	9	122	Total	C	N	O	P	0	0	0
			2600	1160	472	847	121			

- Molecule 6 is a protein called 50S RIBOSOMAL PROTEIN L2P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	A	238	Total	C	N	O	S	0	0	1
			1755	1072	353	325	5			

- Molecule 7 is a protein called 50S RIBOSOMAL PROTEIN L3P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	B	337	Total	C	N	O	S	0	0	0
			2625	1616	493	511	5			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	310	ARG	PHE	conflict	UNP P20279

- Molecule 8 is a protein called 50S RIBOSOMAL PROTEIN L4P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	C	246	Total	C	N	O	S	0	0	0
			1859	1131	344	383	1			

- Molecule 9 is a protein called 50S RIBOSOMAL PROTEIN L5P HMAL5, HL13, RIBOSOMAL PROTEIN L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	D	141	Total	C	N	O	S	0	0	1
			1095	685	196	210	4			

- Molecule 10 is a protein called 50S RIBOSOMAL PROTEIN L6P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	E	173	Total	C	N	O	S	0	0	1
			1358	840	225	289	4			

- Molecule 11 is a protein called 50S RIBOSOMAL PROTEIN L7AE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	F	119	Total	C	N	O	S	0	0	0
			886	552	141	192	1			

- Molecule 12 is a protein called 50S RIBOSOMAL PROTEIN L10E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	G	30	Total	C	N	O	S	0	0	1
			241	149	40	51	1			

- Molecule 13 is a protein called 50S RIBOSOMAL PROTEIN L10E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	H	156	Total	C	N	O	S	0	0	0
			1216	766	233	213	4			

- Molecule 14 is a protein called 50S RIBOSOMAL PROTEIN L13P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	I	142	Total	C	N	O	S	0	0	0
			1120	696	199	222	3			

- Molecule 15 is a protein called 50S RIBOSOMAL PROTEIN L14P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	J	132	Total	C	N	O	S	0	0	0
			994	609	189	192	4			

- Molecule 16 is a protein called 50S RIBOSOMAL PROTEIN L15P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	K	146	Total	C	N	O	S	0	0	1
			1115	668	223	224				

- Molecule 17 is a protein called 50S RIBOSOMAL PROTEIN L15E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	L	194	Total	C	N	O	S	0	0	0
			1606	988	346	267	5			

- Molecule 18 is a protein called 50S RIBOSOMAL PROTEIN L18P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	M	186	Total	C	N	O	S	0	0	0
			1445	895	262	286	2			

- Molecule 19 is a protein called 50S RIBOSOMAL PROTEIN L18E.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
19	N	115	Total	C	N	O	0	0	0
			865	529	161	175			

- Molecule 20 is a protein called 50S RIBOSOMAL PROTEIN L19E.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	O	144	Total	C	N	O	0	0	1
			1134	680	231	223			

- Molecule 21 is a protein called 50S RIBOSOMAL PROTEIN L21E.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	P	95	Total	C	N	O	0	0	0
			735	450	141	144			

- Molecule 22 is a protein called 50S RIBOSOMAL PROTEIN L22P HMAL22, HL23, RIBOSOMAL PROTEIN L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	Q	151	Total	C	N	O	S	0	0	1
			1150	713	210	223	4			

- Molecule 23 is a protein called 50S RIBOSOMAL PROTEIN L23P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	R	84	Total	C	N	O	S	0	0	0
			664	405	114	142	3			

- Molecule 24 is a protein called RIBOSOMAL PROTEIN L24.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
24	S	119	Total	C	N	O	0	0	0
			950	568	180	202			

- Molecule 25 is a protein called 50S RIBOSOMAL PROTEIN L24P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	T	54	Total	C	N	O	S	0	0	1
			411	244	76	86	5			

- Molecule 26 is a protein called 50S RIBOSOMAL PROTEIN L24E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	U	66	Total	C	N	O	S	0	0	1
			500	304	95	100	1			

- Molecule 27 is a protein called 50S RIBOSOMAL PROTEIN L30P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	V	154	Total	C	N	O	S	0	0	0
			1196	737	209	244	6			

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L31E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	W	83	Total	C	N	O	S	0	0	1
			655	402	130	122	1			

- Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L32E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	X	143	Total	C	N	O	S	0	0	1
			1131	686	229	216				

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L37AE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	Y	73	Total	C	N	O	S	0	0	0
			564	359	111	87	7			

- Molecule 31 is a protein called RIBOSOMAL PROTEIN L37E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	Z	56	Total	C	N	O	S	0	0	0
			431	258	86	83	4			

- Molecule 32 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	0	105	Total	Mg	0	0
			105	105		
32	2	1	Total	Mg	0	0
			1	1		
32	9	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	A	3	Total 3	Mg 3	0	0
32	B	3	Total 3	Mg 3	0	0
32	J	1	Total 1	Mg 1	0	0
32	S	1	Total 1	Mg 1	0	0
32	X	1	Total 1	Mg 1	0	0

- Molecule 33 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	0	2	Total 2	K 2	0	0

- Molecule 34 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	0	74	Total 74	Na 74	0	0
34	9	2	Total 2	Na 2	0	0
34	A	1	Total 1	Na 1	0	0
34	C	1	Total 1	Na 1	0	0
34	I	1	Total 1	Na 1	0	0
34	K	1	Total 1	Na 1	0	0
34	L	1	Total 1	Na 1	0	0
34	P	1	Total 1	Na 1	0	0
34	Q	2	Total 2	Na 2	0	0
34	R	1	Total 1	Na 1	0	0
34	S	1	Total 1	Na 1	0	0

- Molecule 35 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	0	7	Total 7	Cl 7	0	0
35	2	1	Total 1	Cl 1	0	0
35	A	1	Total 1	Cl 1	0	0
35	B	1	Total 1	Cl 1	0	0
35	I	3	Total 3	Cl 3	0	0
35	J	1	Total 1	Cl 1	0	0
35	K	2	Total 2	Cl 2	0	0
35	L	1	Total 1	Cl 1	0	0
35	M	1	Total 1	Cl 1	0	0
35	N	1	Total 1	Cl 1	0	0
35	P	1	Total 1	Cl 1	0	0
35	Q	1	Total 1	Cl 1	0	0
35	X	1	Total 1	Cl 1	0	0

- Molecule 36 is CADMIUM ION (CCD ID: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	2	1	Total 1	Cd 1	0	0
36	N	1	Total 1	Cd 1	0	0
36	T	1	Total 1	Cd 1	0	0
36	Y	1	Total 1	Cd 1	0	0
36	Z	1	Total 1	Cd 1	0	0

- Molecule 37 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	0	5875	Total 5875	O 5875	0	0
37	1	49	Total 49	O 49	0	0
37	2	69	Total 69	O 69	0	0
37	9	153	Total 153	O 153	0	0
37	A	135	Total 135	O 135	0	0
37	B	156	Total 156	O 156	0	0
37	C	169	Total 169	O 169	0	0
37	D	52	Total 52	O 52	0	0
37	E	41	Total 41	O 41	0	0
37	F	30	Total 30	O 30	0	0
37	G	20	Total 20	O 20	0	0
37	H	80	Total 80	O 80	0	0
37	I	52	Total 52	O 52	0	0
37	J	61	Total 61	O 61	0	0
37	K	98	Total 98	O 98	0	0
37	L	155	Total 155	O 155	0	0
37	M	60	Total 60	O 60	0	0
37	N	38	Total 38	O 38	0	0
37	O	67	Total 67	O 67	0	0
37	P	53	Total 53	O 53	0	0
37	Q	83	Total 83	O 83	0	0
37	R	32	Total 32	O 32	0	0

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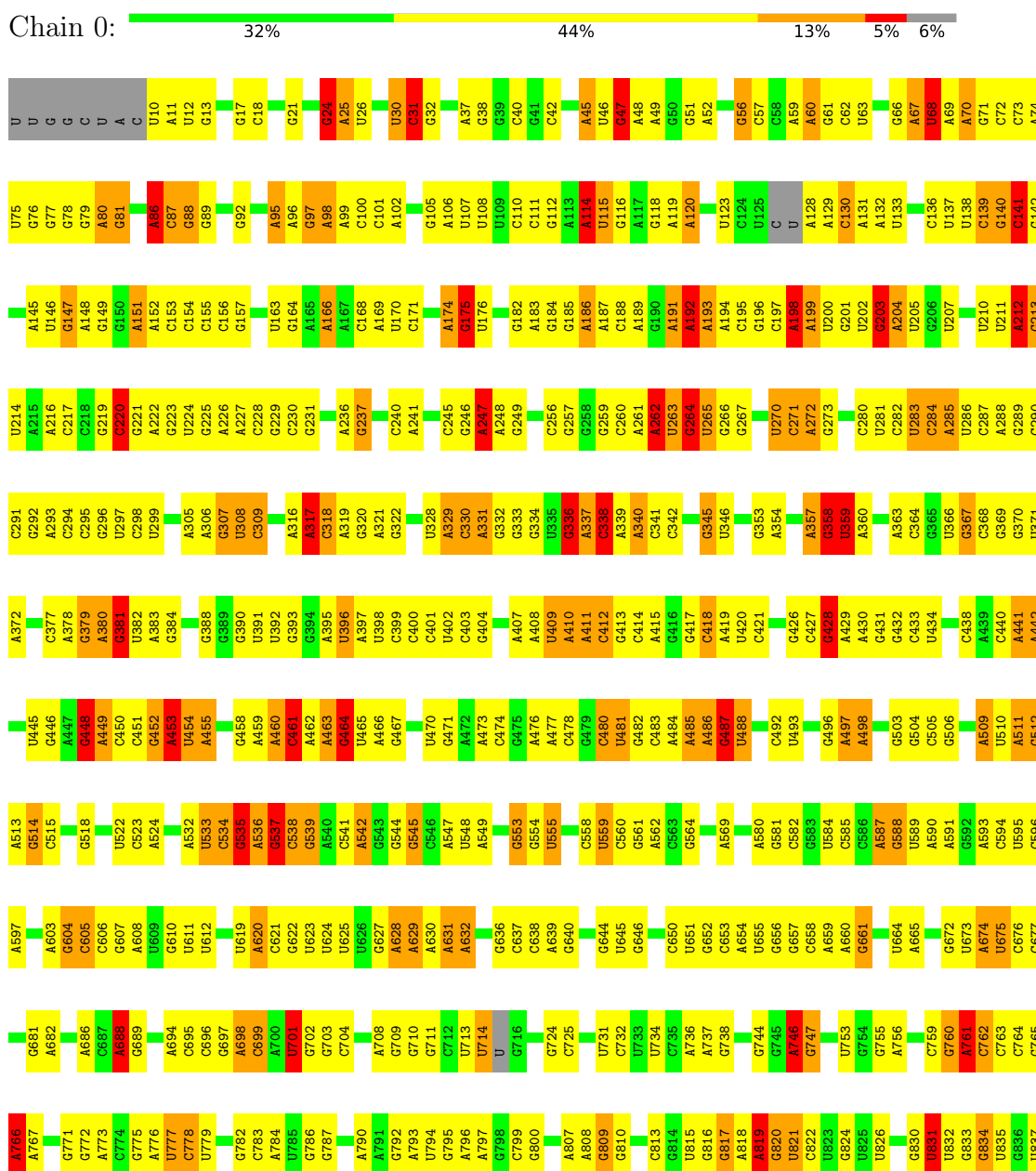
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	S	36	Total 36	O 36	0	0
37	T	25	Total 25	O 25	0	0
37	U	11	Total 11	O 11	0	0
37	V	69	Total 69	O 69	0	0
37	W	26	Total 26	O 26	0	0
37	X	107	Total 107	O 107	0	0
37	Y	35	Total 35	O 35	0	0
37	Z	50	Total 50	O 50	0	0

3 Residue-property plots

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

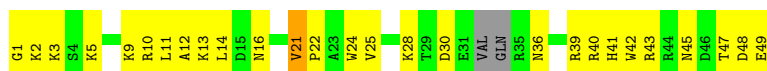
Note EDS was not executed.

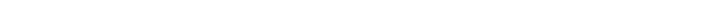
• Molecule 1: 23S rRNA

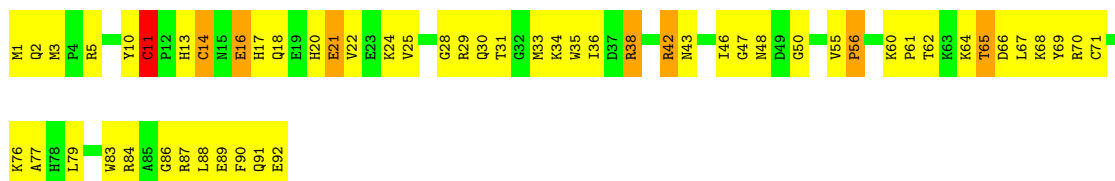


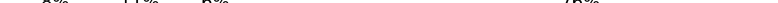


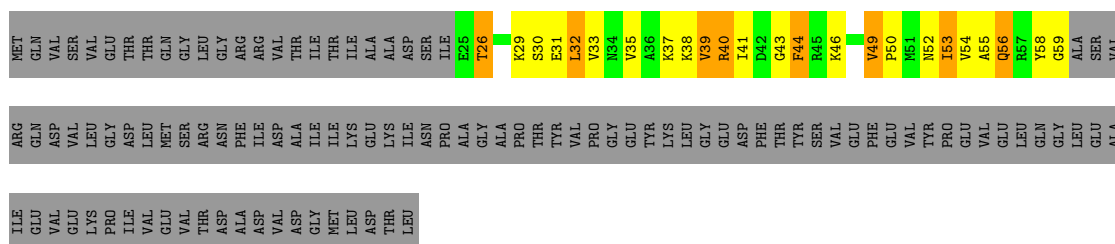
• Molecule 2: 50S RIBOSOMAL PROTEIN L39E



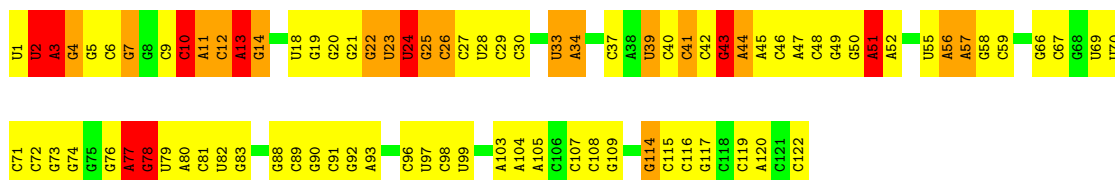
- Chain 2:  39% 52% 8%

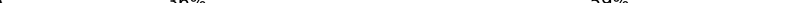


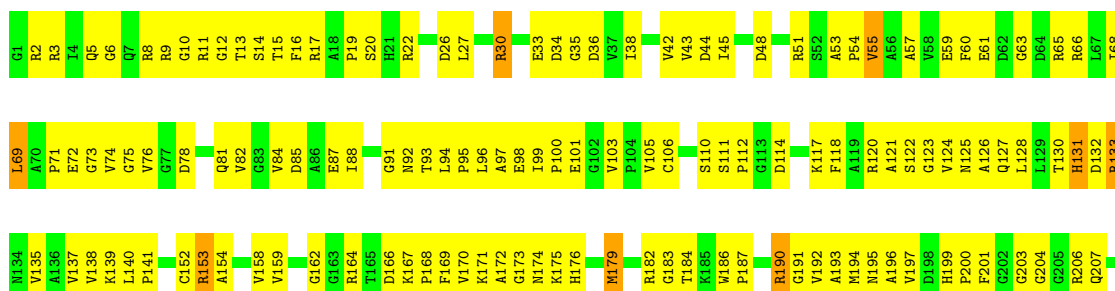
- Chain 5:  8% 11% 6% 76%



- Chain 9: 29% 50% 14% 7%



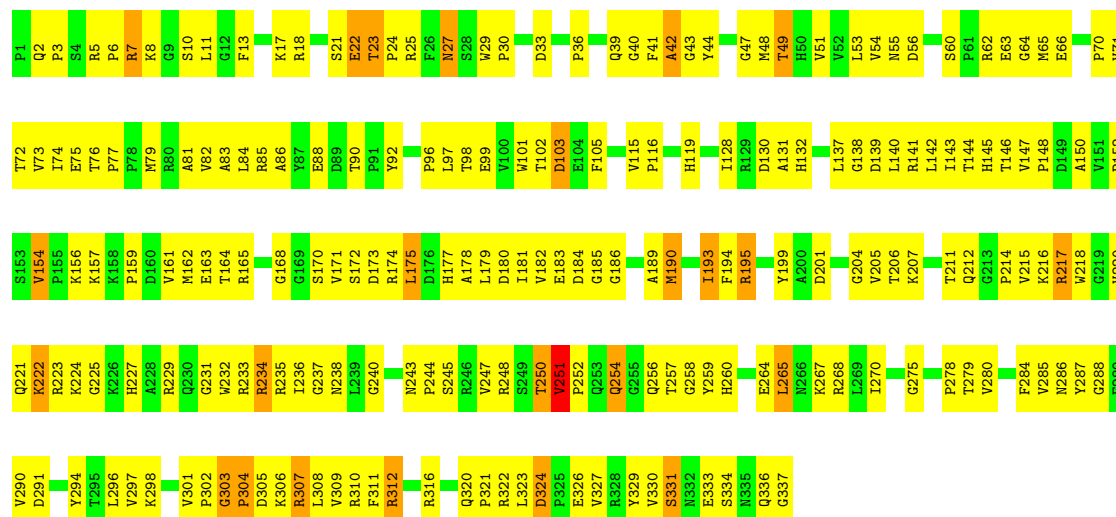
- Chain A:  36% 59% 5%





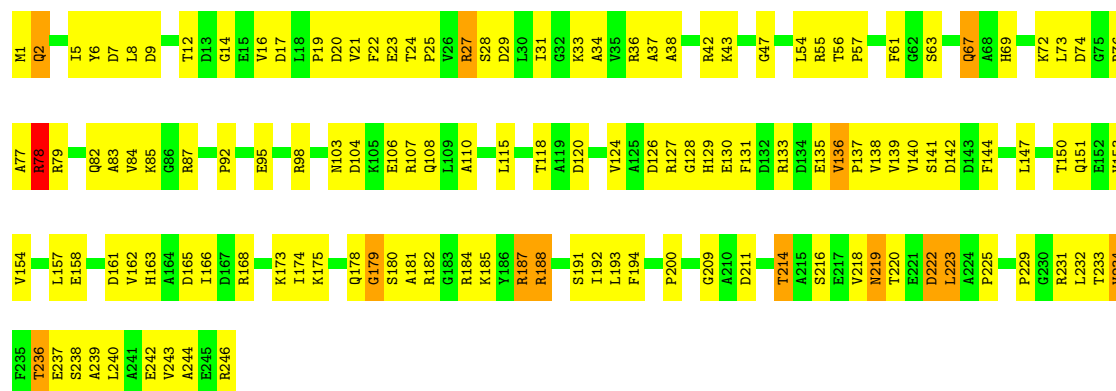
• Molecule 7: 50S RIBOSOMAL PROTEIN L3P

Chain B: 38% 55% 7%



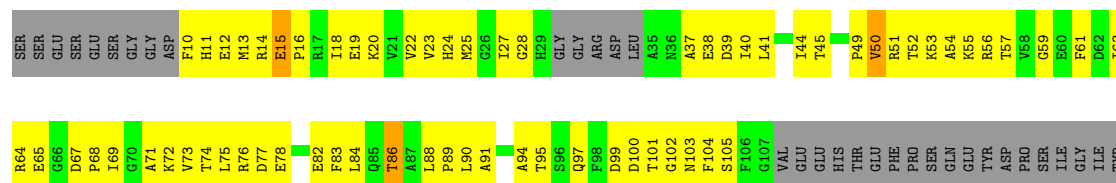
• Molecule 8: 50S RIBOSOMAL PROTEIN L4P

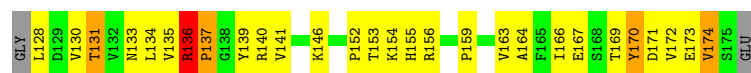
Chain C: 46% 48% 5%



• Molecule 9: 50S RIBOSOMAL PROTEIN L5P HMA15, HL13, RIBOSOMAL PROTEIN L5

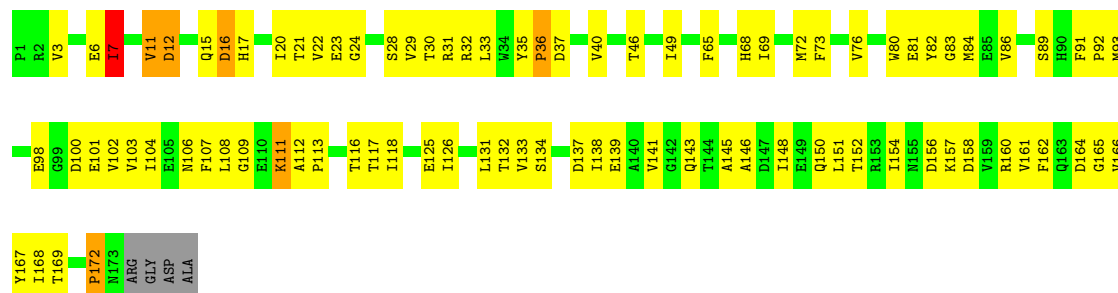
Chain D: 27% 49% 20%





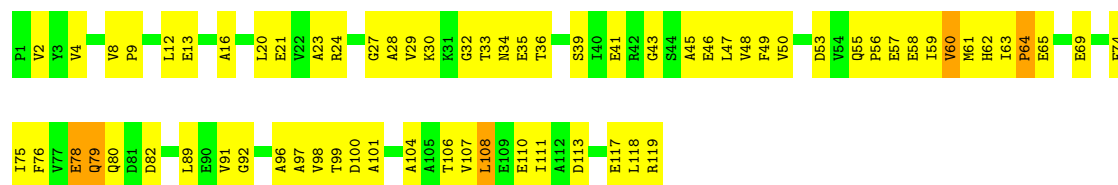
• Molecule 10: 50S RIBOSOMAL PROTEIN L6P

Chain E: 48% 46%



• Molecule 11: 50S RIBOSOMAL PROTEIN L7AE

Chain F: 43% 53%



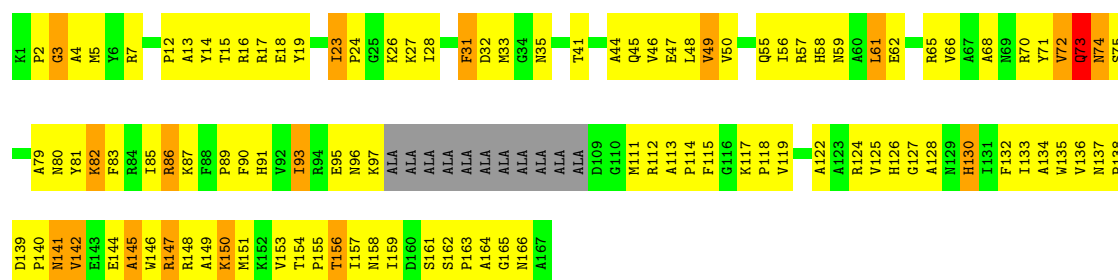
• Molecule 12: 50S RIBOSOMAL PROTEIN L10E

Chain G: 5% 91%



• Molecule 13: 50S RIBOSOMAL PROTEIN L10E

Chain H: 29% 54% 10% 7%



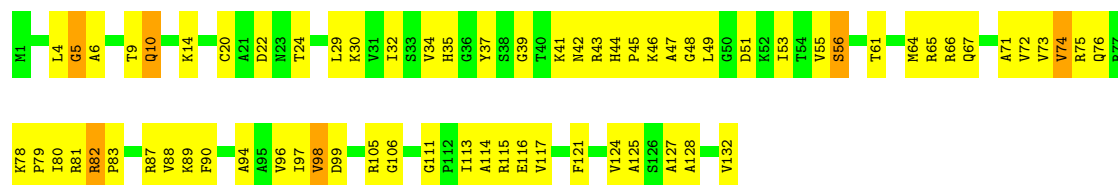
• Molecule 14: 50S RIBOSOMAL PROTEIN L13P

Chain I: 39% 53% 6%



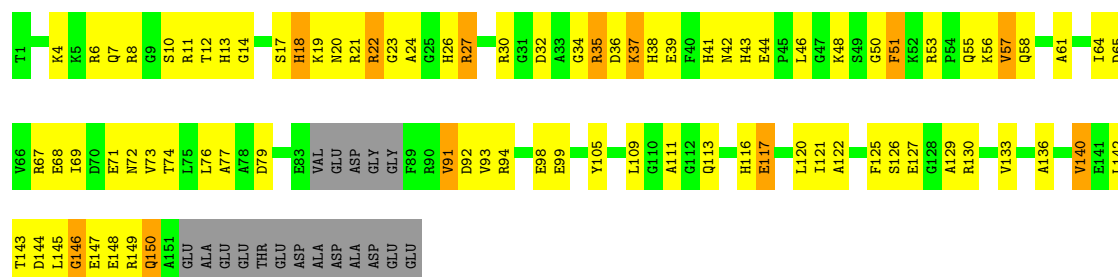
• Molecule 15: 50S RIBOSOMAL PROTEIN L14P

Chain J: 48% 48% 5%



• Molecule 16: 50S RIBOSOMAL PROTEIN L15P

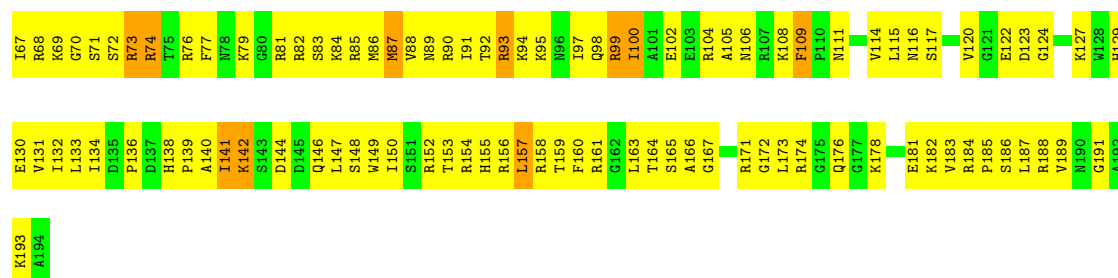
Chain K: 37% 45% 7% 11%



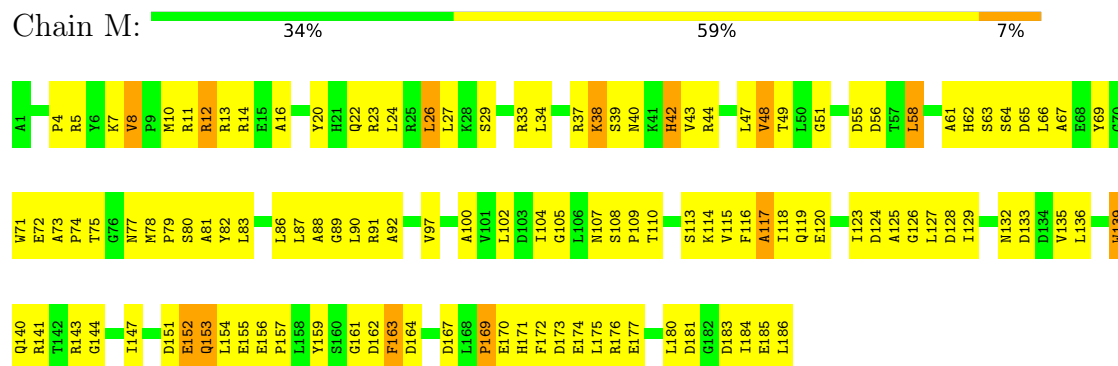
• Molecule 17: 50S RIBOSOMAL PROTEIN L15E

Chain L: 25% 68% 7%

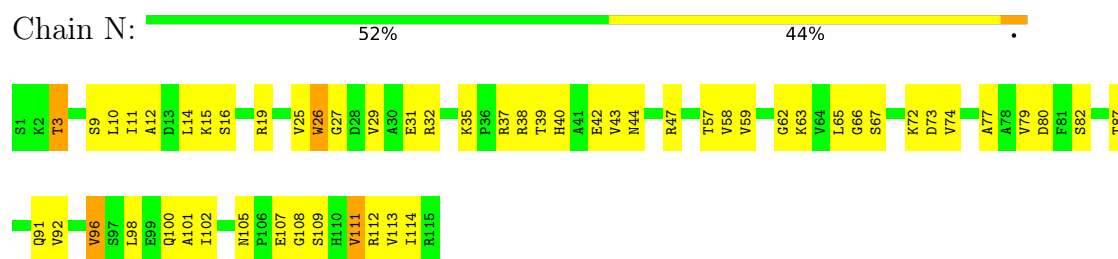




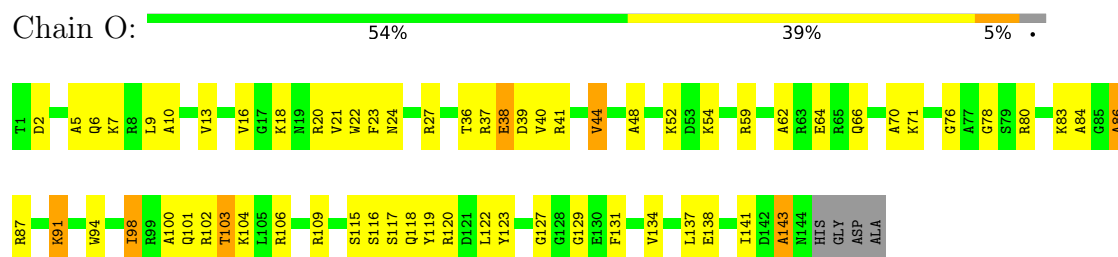
• Molecule 18: 50S RIBOSOMAL PROTEIN L18P



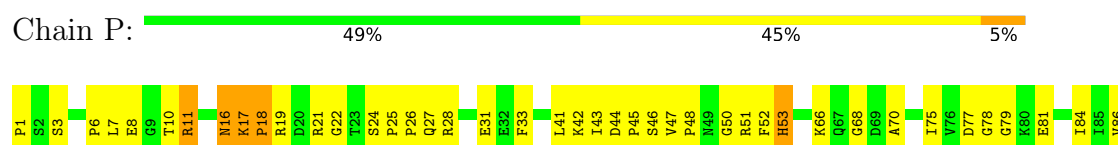
• Molecule 19: 50S RIBOSOMAL PROTEIN L18E



• Molecule 20: 50S RIBOSOMAL PROTEIN L19E



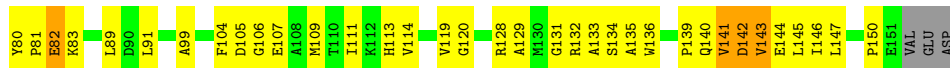
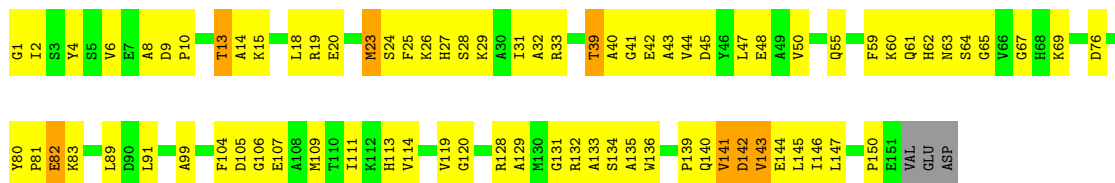
• Molecule 21: 50S RIBOSOMAL PROTEIN L21E





- Molecule 22: 50S RIBOSOMAL PROTEIN L22P HMAL22, HL23, RIBOSOMAL PROTEIN L22

Chain Q: 47% 47% 5% .



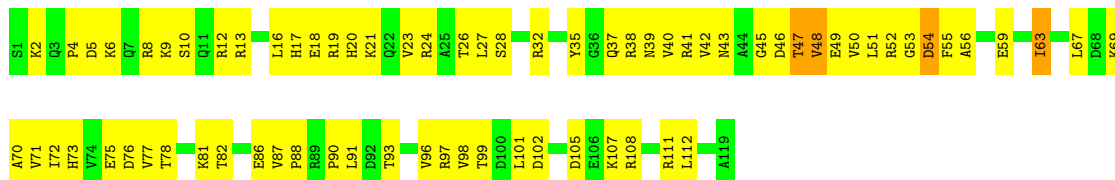
- Molecule 23: 50S RIBOSOMAL PROTEIN L23P

Chain R: 50% 46% .



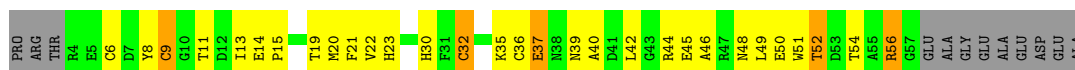
- Molecule 24: RIBOSOMAL PROTEIN L24

Chain S: 39% 57% .



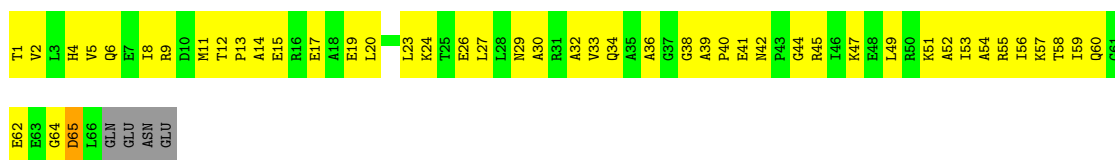
- Molecule 25: 50S RIBOSOMAL PROTEIN L24P

Chain T: 36% 38% 8% 18%

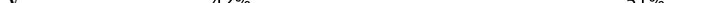


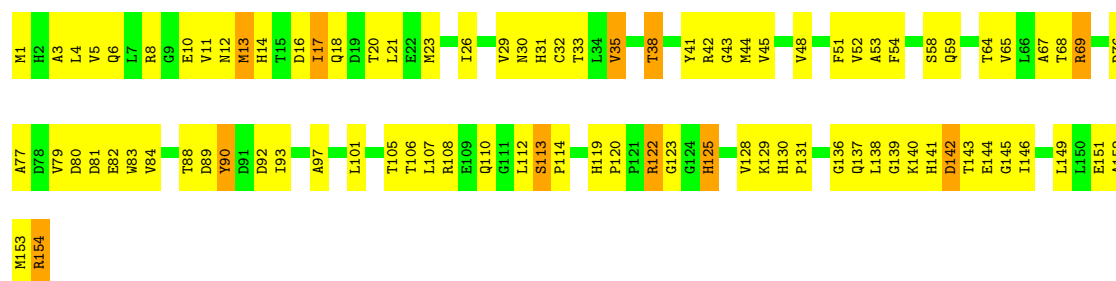
- Molecule 26: 50S RIBOSOMAL PROTEIN L24E

Chain U: 27% 66% 6%

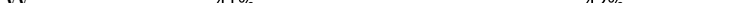


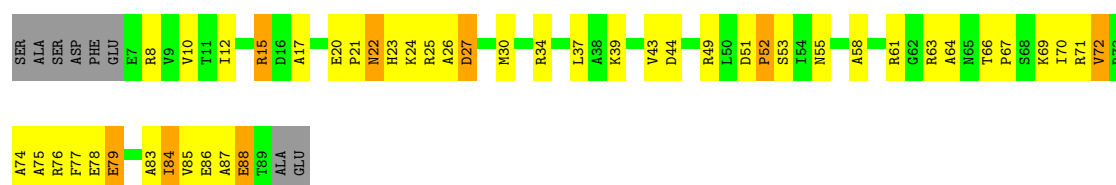
- Molecule 27: 50S RIBOSOMAL PROTEIN L30P

Chain V:  42% 51% 7%



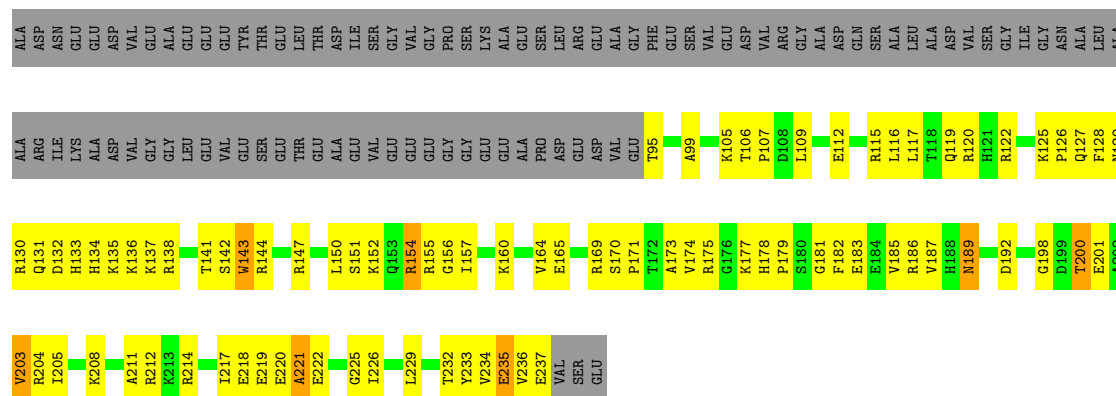
• Molecule 28: 50S RIBOSOMAL PROTEIN L31E

Chain W:  41% 42% 9% 9%



• Molecule 29: 50S RIBOSOMAL PROTEIN L32E

Chain X: 25% 32% . 40%



- Molecule 30: 50S RIBOSOMAL PROTEIN L37AE

Chain Y: 33% 62% 5%



- Molecule 31: RIBOSOMAL PROTEIN L37E

Chain Z: 34% 64%

T1	G2
T5	P6
S7	Q8
G9	K10
K11	M12
T13	T14
H15	H16
T17	K18
C19	R20
R21	C22
G23	E24
K25	S26
Y27	H28
T29	K30
K31	K32
S35	S36
C37	G38
F39	G40
K41	S42
R45	W50
R46	Q51
	S52
	K53
A54	F55
G56	T57

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	210.75Å 298.87Å 574.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.50	Depositor
% Data completeness (in resolution range)	80.3 (30.00-3.50)	Depositor
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.192 , 0.268	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	98859	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, CL, CD, NA, K

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	0.39	0/66076	0.85	233/103052 (0.2%)
2	1	0.39	0/399	0.88	2/527 (0.4%)
3	2	0.40	0/771	0.91	4/1024 (0.4%)
4	5	0.45	0/275	1.29	5/366 (1.4%)
5	9	0.37	0/2905	0.84	12/4528 (0.3%)
6	A	0.49	1/1788 (0.1%)	1.03	9/2411 (0.4%)
7	B	0.47	0/2690	1.07	20/3652 (0.5%)
8	C	0.47	0/1884	0.98	4/2551 (0.2%)
9	D	0.42	1/1112 (0.1%)	0.96	7/1500 (0.5%)
10	E	0.45	1/1383 (0.1%)	0.95	6/1882 (0.3%)
11	F	0.41	0/897	0.96	4/1219 (0.3%)
12	G	0.54	1/242 (0.4%)	0.90	0/326
13	H	0.48	0/1247	1.17	11/1686 (0.7%)
14	I	0.47	0/1136	0.97	6/1530 (0.4%)
15	J	0.50	0/1004	1.09	7/1351 (0.5%)
16	K	0.43	1/1127 (0.1%)	1.03	6/1506 (0.4%)
17	L	0.51	0/1634	1.03	9/2180 (0.4%)
18	M	0.42	0/1474	1.11	12/1999 (0.6%)
19	N	0.45	0/874	1.02	6/1181 (0.5%)
20	O	0.47	1/1144 (0.1%)	0.92	6/1523 (0.4%)
21	P	0.45	0/749	1.00	3/1005 (0.3%)
22	Q	0.53	1/1173 (0.1%)	0.94	2/1580 (0.1%)
23	R	0.61	0/672	1.06	5/906 (0.6%)
24	S	0.41	0/958	1.03	3/1289 (0.2%)
25	T	0.47	1/418 (0.2%)	0.88	1/564 (0.2%)
26	U	0.49	1/503 (0.2%)	0.97	1/677 (0.1%)
27	V	0.49	0/1219	1.03	8/1655 (0.5%)
28	W	0.51	1/665 (0.2%)	0.99	4/897 (0.4%)
29	X	0.50	1/1147 (0.1%)	0.98	6/1538 (0.4%)
30	Y	0.39	0/576	0.96	1/763 (0.1%)
31	Z	0.44	0/438	1.02	3/578 (0.5%)
All	All	0.41	11/98580 (0.0%)	0.89	406/147446 (0.3%)

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
1	0	0	65
5	9	0	4
27	V	0	1
All	All	0	70

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	G	73	ASP	C-N	-5.89	1.25	1.33
20	O	143	ALA	C-N	-5.87	1.25	1.33
26	U	65	ASP	C-N	-5.74	1.25	1.33
9	D	174	VAL	C-N	-5.64	1.25	1.33
28	W	88	GLU	C-N	-5.49	1.25	1.33

The worst 5 of 406 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	H	141	ASN	N-CA-C	-10.95	100.04	113.50
13	H	74	ASN	N-CA-C	-10.48	100.49	113.38
17	L	141	ILE	N-CA-C	-10.29	102.67	112.96
8	C	179	GLY	N-CA-C	-8.90	102.59	113.99
1	0	535	G	N9-C1'-C2'	8.71	127.07	114.00

There are no chirality outliers.

5 of 70 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	203	G	Sidechain
1	0	224	U	Sidechain
1	0	30	U	Sidechain
1	0	68	U	Sidechain
1	0	86	A	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	59017	0	29808	2089	0
2	1	394	0	406	39	0
3	2	755	0	732	83	0
4	5	273	0	296	27	0
5	9	2600	0	1326	120	0
6	A	1755	0	1763	194	0
7	B	2625	0	2533	255	0
8	C	1859	0	1816	169	0
9	D	1095	0	1085	130	0
10	E	1358	0	1266	100	0
11	F	886	0	854	81	0
12	G	241	0	231	20	0
13	H	1216	0	1215	174	0
14	I	1120	0	1098	100	0
15	J	994	0	1027	89	0
16	K	1115	0	1072	97	0
17	L	1606	0	1676	250	0
18	M	1445	0	1401	154	0
19	N	865	0	873	59	0
20	O	1134	0	1127	69	0
21	P	735	0	729	51	0
22	Q	1150	0	1122	87	0
23	R	664	0	626	55	0
24	S	950	0	924	82	0
25	T	411	0	368	34	0
26	U	500	0	511	53	0
27	V	1196	0	1137	129	0
28	W	655	0	653	57	0
29	X	1131	0	1133	104	0
30	Y	564	0	601	90	0
31	Z	431	0	426	47	0
32	0	105	0	0	0	0
32	2	1	0	0	0	0
32	9	2	0	0	0	0
32	A	3	0	0	0	0
32	B	3	0	0	0	0
32	J	1	0	0	0	0
32	S	1	0	0	0	0
32	X	1	0	0	0	0
33	0	2	0	0	0	0
34	0	74	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	9	2	0	0	0	0
34	A	1	0	0	0	0
34	C	1	0	0	0	0
34	I	1	0	0	0	0
34	K	1	0	0	0	0
34	L	1	0	0	0	0
34	P	1	0	0	0	0
34	Q	2	0	0	0	0
34	R	1	0	0	0	0
34	S	1	0	0	0	0
35	0	7	0	0	2	0
35	2	1	0	0	0	0
35	A	1	0	0	0	0
35	B	1	0	0	0	0
35	I	3	0	0	3	0
35	J	1	0	0	0	0
35	K	2	0	0	0	0
35	L	1	0	0	2	0
35	M	1	0	0	1	0
35	N	1	0	0	0	0
35	P	1	0	0	2	0
35	Q	1	0	0	0	0
35	X	1	0	0	2	0
36	2	1	0	0	0	0
36	N	1	0	0	0	0
36	T	1	0	0	0	0
36	Y	1	0	0	0	0
36	Z	1	0	0	0	0
37	0	5875	0	0	346	0
37	1	49	0	0	8	0
37	2	69	0	0	7	0
37	9	153	0	0	16	0
37	A	135	0	0	30	0
37	B	156	0	0	32	0
37	C	169	0	0	43	0
37	D	52	0	0	16	0
37	E	41	0	0	9	0
37	F	30	0	0	6	0
37	G	20	0	0	3	0
37	H	80	0	0	19	0
37	I	52	0	0	4	0
37	J	61	0	0	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	K	98	0	0	23	0
37	L	155	0	0	33	0
37	M	60	0	0	18	0
37	N	38	0	0	5	0
37	O	67	0	0	7	0
37	P	53	0	0	6	0
37	Q	83	0	0	8	0
37	R	32	0	0	6	0
37	S	36	0	0	4	0
37	T	25	0	0	6	0
37	U	11	0	0	2	0
37	V	69	0	0	10	0
37	W	26	0	0	6	0
37	X	107	0	0	13	0
37	Y	35	0	0	10	0
37	Z	50	0	0	2	0
All	All	98859	0	59835	4683	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 31.

The worst 5 of 4683 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)
1:O:156:C:H5''	17:L:171:ARG:HD3	1.28	1.14
3:2:46:ILE:HG21	17:L:87:MET:HG2	1.24	1.14
26:U:12:THR:HG22	26:U:15:GLU:HG3	1.28	1.14
11:F:91:VAL:HG12	11:F:92:GLY:H	1.09	1.13
5:9:6:C:H5''	18:M:37:ARG:HH12	1.08	1.11

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

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	
2	1	42/44 (96%)	42 (100%)	0	100	100
3	2	79/79 (100%)	73 (92%)	6 (8%)	12	37
4	5	29/122 (24%)	24 (83%)	5 (17%)	2	12
6	A	179/181 (99%)	170 (95%)	9 (5%)	22	48
7	B	282/282 (100%)	266 (94%)	16 (6%)	18	45
8	C	193/193 (100%)	180 (93%)	13 (7%)	15	41
9	D	117/147 (80%)	111 (95%)	6 (5%)	21	48
10	E	152/155 (98%)	146 (96%)	6 (4%)	28	54
11	F	92/92 (100%)	89 (97%)	3 (3%)	33	58
12	G	27/283 (10%)	27 (100%)	0	100	100
13	H	122/122 (100%)	111 (91%)	11 (9%)	9	32
14	I	118/121 (98%)	112 (95%)	6 (5%)	21	48
15	J	106/106 (100%)	102 (96%)	4 (4%)	29	55
16	K	112/126 (89%)	107 (96%)	5 (4%)	24	50
17	L	166/166 (100%)	160 (96%)	6 (4%)	31	57
18	M	149/149 (100%)	141 (95%)	8 (5%)	20	46
19	N	93/93 (100%)	89 (96%)	4 (4%)	26	51
20	O	113/116 (97%)	109 (96%)	4 (4%)	32	57
21	P	79/79 (100%)	75 (95%)	4 (5%)	21	48
22	Q	117/121 (97%)	112 (96%)	5 (4%)	26	51
23	R	73/73 (100%)	72 (99%)	1 (1%)	59	71
24	S	105/105 (100%)	99 (94%)	6 (6%)	18	45
25	T	44/52 (85%)	41 (93%)	3 (7%)	14	40
26	U	51/56 (91%)	51 (100%)	0	100	100
27	V	130/130 (100%)	124 (95%)	6 (5%)	24	50
28	W	66/73 (90%)	61 (92%)	5 (8%)	12	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	X	120/195 (62%)	115 (96%)	5 (4%)	26	52
30	Y	56/56 (100%)	53 (95%)	3 (5%)	20	46
31	Z	46/46 (100%)	46 (100%)	0	100	100
All	All	3058/3563 (86%)	2908 (95%)	150 (5%)	22	48

5 of 150 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
21	P	81	GLU
29	X	189	ASN
22	Q	82	GLU
25	T	52	THR
8	C	240	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 107 such sidechains are listed below:

Mol	Chain	Res	Type
16	K	58	GLN
20	O	66	GLN
29	X	129	ASN
17	L	58	GLN
18	M	22	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2745/2922 (93%)	565 (20%)	20 (0%)
5	9	121/122 (99%)	28 (23%)	0
All	All	2866/3044 (94%)	593 (20%)	20 (0%)

5 of 593 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	24	G
1	0	25	A
1	0	31	C
1	0	32	G
1	0	46	U

5 of 20 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	1996	U
1	0	2011	A
1	0	2037	C
1	0	2033	G
1	0	1977	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 232 ligands modelled in this entry, 232 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.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.