



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 04:36 PM GMT

PDB ID : 2B9N
Title : 50S ribosomal subunit from a crystal structure of release factor RF2, tRNAs and mRNA bound to the ribosome. This file contains the 50S subunit from a crystal structure of release factor RF1, tRNAs and mRNA bound to the ribosome and is described in remark 400.
Authors : Petry, S.; Brodersen, D.E.; Murphy IV, F.V.; Dunham, C.M.; Selmer, M.; Tarry, M.J.; Kelley, A.C.; Ramakrishnan, V.
Deposited on : 2005-10-12
Resolution : 6.76 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>

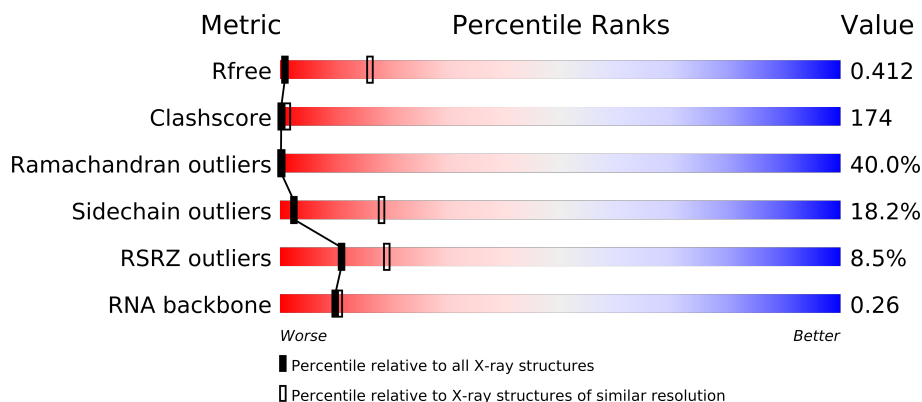
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
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)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 6.76 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	1098 (10.00-3.50)
Clashscore	79885	1039 (10.00-3.52)
Ramachandran outliers	78287	1291 (9.50-3.50)
Sidechain outliers	78261	1265 (9.50-3.50)
RSRZ outliers	66119	1097 (10.00-3.50)
RNA backbone	1838	1045 (10.00-2.80)

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	B	123	
2	A	2916	
3	D	173	
4	E	338	
5	F	246	
6	G	176	
7	H	177	
8	I	149	
9	N	145	
10	O	122	
11	P	164	
12	Q	138	

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Mol	Chain	Length	Quality of chain
13	S	186	
14	T	66	
15	W	113	
16	X	84	
17	Y	119	
18	Z	253	
19	R	118	
20	U	118	
21	V	100	
22	2	70	
23	3	60	
24	0	91	
25	4	73	
26	5	60	
27	6	82	
28	7	47	
29	8	64	
30	9	36	
31	K	141	

2 Entry composition

There are 31 unique types of molecules in this entry. The entry contains 87268 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 RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	123	Total	C	N	O	P	0	0	0
			2637	1175	488	852	122			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	A	-	INSERTION	GB 48271

- Molecule 2 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	2814	Total	C	N	O	P	0	0	0
			60599	26974	11331	19482	2812			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	493	G	-	INSERTION	GB 48268

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	173	Total	C	N	O	S	0	0	0
			1308	820	246	236	6			

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	191	Total	C	N	O	S	0	0	0
			1507	940	290	273	4			

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	189	Total	C	N	O	S	0	0	0
			1430	872	255	302	1			

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	122	Total	C	N	O	S	0	0	0
			957	597	176	180	4			

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	164	Total	C	N	O	S	0	0	0
			1251	787	225	237	2			

- Molecule 8 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	148	Total	C	N	O	S	0	0	0
			1145	727	205	212	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	N	117	Total	C	N	O	S	0	0	0
			917	570	164	180	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	O	122	Total	C	N	O	S	0	0	0
			937	585	180	169	3			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	P	84	Total	C	N	O	0	0	0
			639	391	109	139			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	Q	138	Total	C	N	O	S	0	0	0
			1081	678	208	192	3			

- Molecule 13 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	S	113	Total	C	N	O	S	0	0	0
			866	536	165	164	1			

- Molecule 14 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	52	Total	C	N	O	S	0	0	0
			406	242	74	85	5			

- Molecule 15 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	W	108	Total	C	N	O		0	0	0
			860	542	169	149				

- Molecule 16 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	X	76	Total	C	N	O	S	0	0	0
			602	366	102	131	3			

- Molecule 17 is a protein called 50S ribosomal protein 24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Y	110	Total	C	N	O		0	0	0
			879	531	166	182				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	Z	177	Total	C	N	O	S	0	0	0
			1360	859	238	257	6			

- Molecule 19 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
19	R	105	Total	C	N	O			
			855	536	174	145	0	0	0

- Molecule 20 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	U	117	Total	C	N	O	S		
			978	608	210	159	1	0	0

- Molecule 21 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	V	100	Total	C	N	O	S		
			787	495	146	145	1	0	0

- Molecule 22 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
22	2	64	Total	C	N	O	S		
			494	301	93	99	1	0	0

- Molecule 23 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
23	3	60	Total	C	N	O	S		
			477	303	91	82	1	0	0

- Molecule 24 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
24	0	86	Total	C	N	O	S		
			641	402	124	114	1	0	0

- Molecule 25 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
25	4	73	Total	C	N	O	S		
			604	382	110	108	4	0	0

- Molecule 26 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	5	58	Total	C	N	O	S	0	0	0
			457	281	94	77	5			

- Molecule 27 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	6	53	Total	C	N	O	S	0	0	0
			431	274	80	76	1			

- Molecule 28 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	7	46	Total	C	N	O	S	0	0	0
			383	230	91	60	2			

- Molecule 29 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	8	63	Total	C	N	O	S	0	0	0
			496	312	101	78	5			

- Molecule 30 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	9	35	Total	C	N	O	S	0	0	0
			285	172	64	45	4			

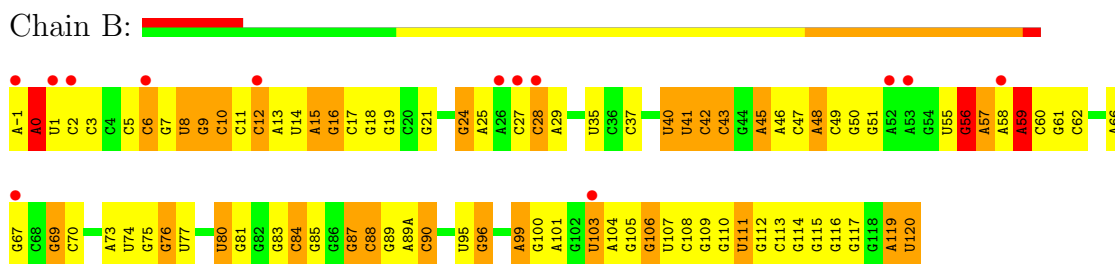
- Molecule 31 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	K	133	Total	C	N	O	S	0	0	0
			999	642	169	182	6			

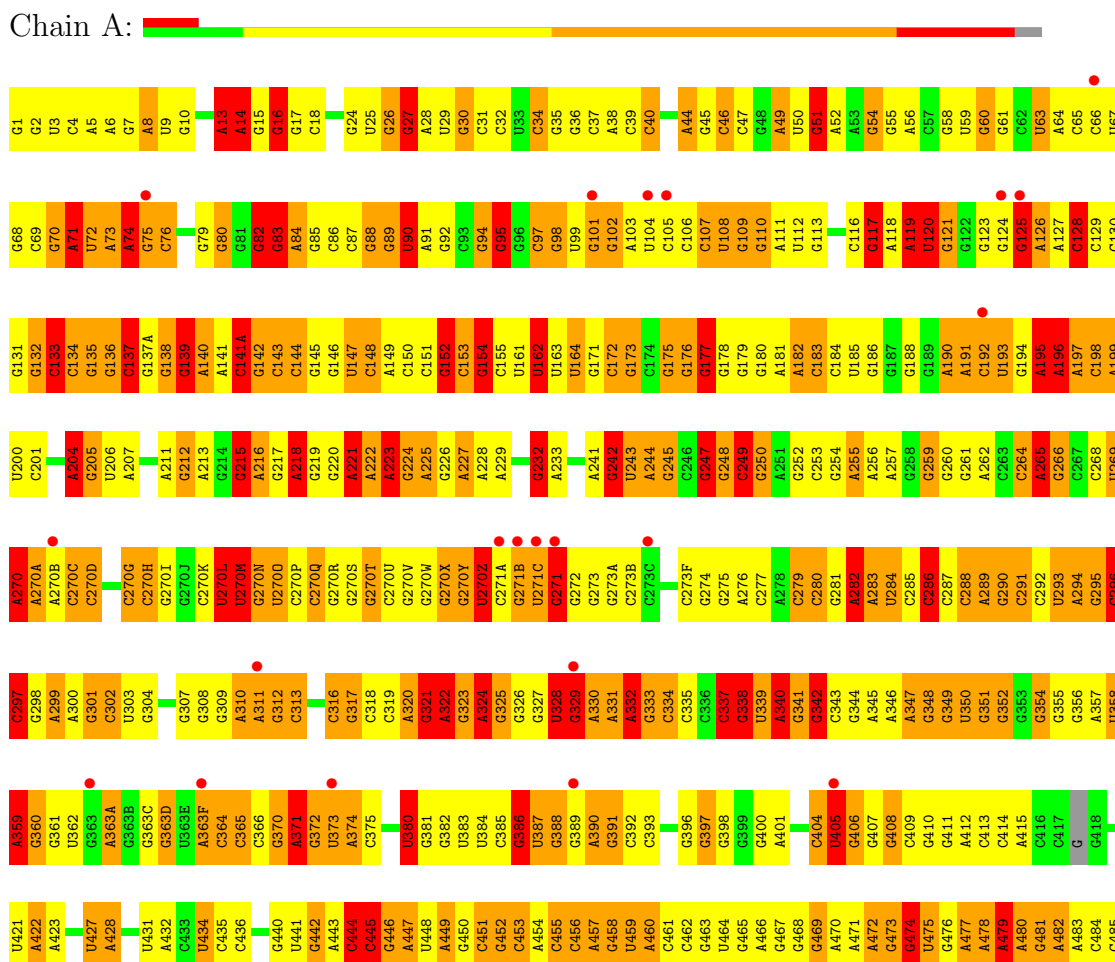
3 Residue-property plots

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: 5S ribosomal RNA

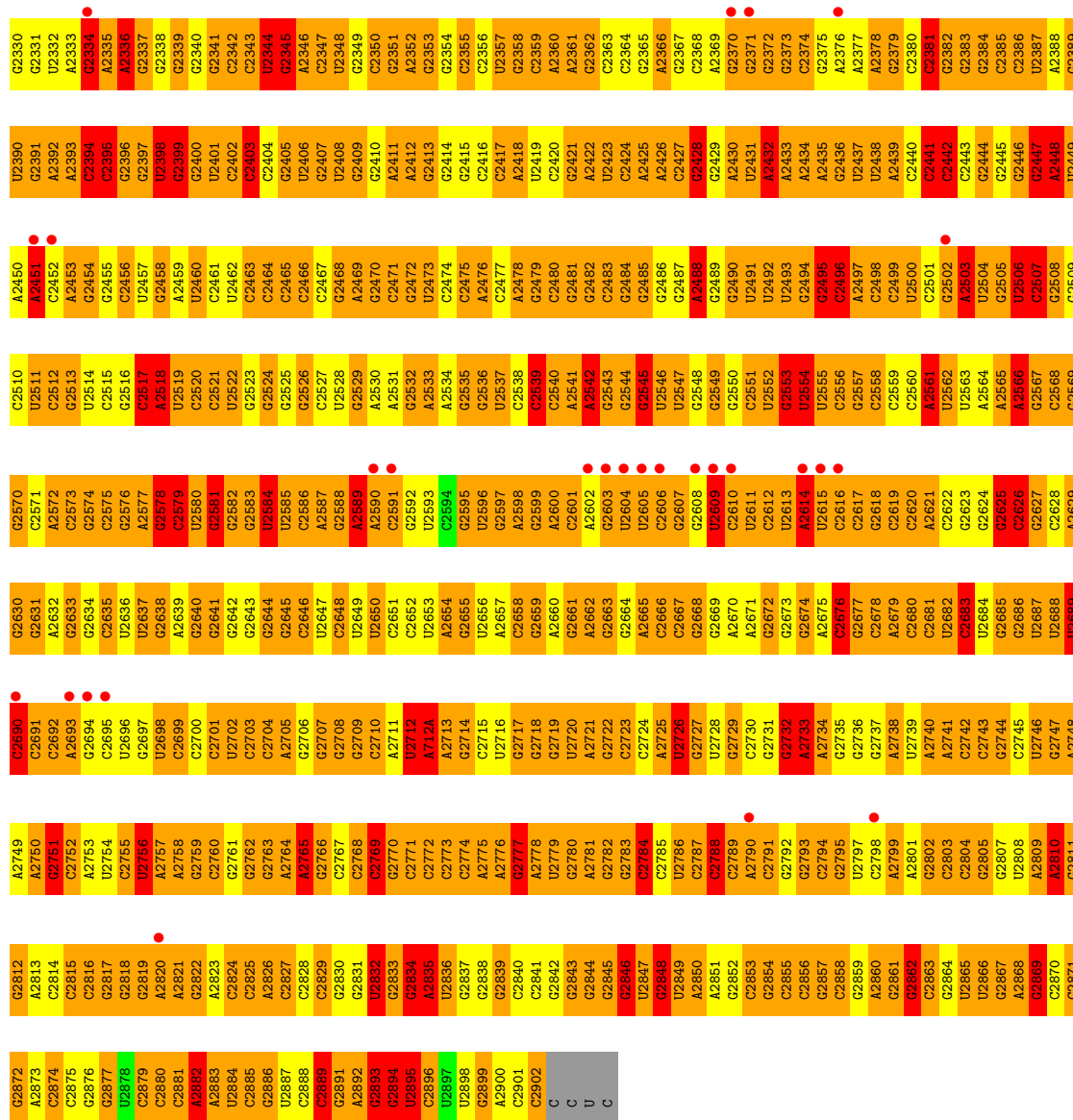


• Molecule 2: 23S ribosomal RNA



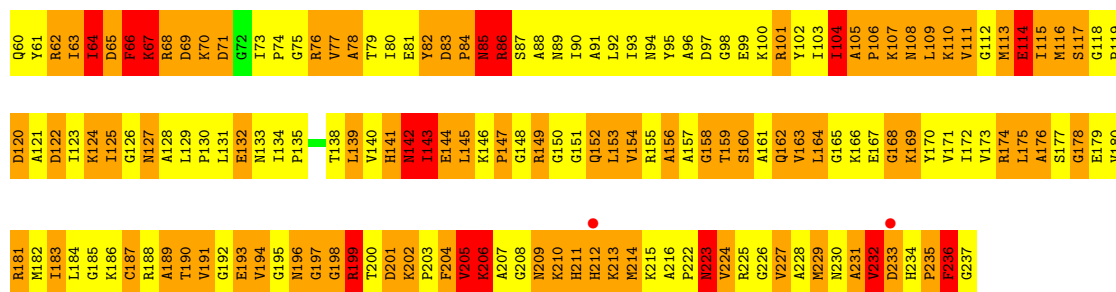
G1358	G1359	A1360	G1361	G1362	G1363	G1364	A1365	G1366	G1367	G1368	G1369	G1370	G1371	G1372	A1373	G1374	G1375	G1376	G1377	A1378	G1379	G1380	G1381	G1382	G1383	A1384	G1385	G1386
G1228	G1229	C1230	U1234	G1235	G1236	A1237	G1238	G1239	G1240	G1241	A1242	G1243	G1244	G1245	A1246	G1247	G1248	G1249	G1250	G1251	G1252	G1253	A1254	G1255	G1256	G1257	G1258	G1259
G1295	G1296	C1297	G1298	G1299	G1300	A1301	A1302	G1303	G1304	G1305	G1306	A1307	A1308	G1309	G1310	G1311	G1312	G1313	G1314	G1315	G1316	G1317	G1318	G1319	G1320	A1321	G1324	G1325
G1389	U1390	U1391	A1392	A1393	U1394	A1395	U1396	U1397	G1398	G1399	G1400	G1401	G1402	G1403	G1404	U1405	A1406	U1407	G1408	G1409	G1410	C1411	A1412	U1415	G1416	G1417	G1418	A1419
U1165	C1166	U1167	G1168	G1169	G1170	G1171	G1172	G1173	U1174	G1175	G1176	A1177	G1178	C1179	G1180	A1181	G1182	G1183	G1184	G1185	G1186	U1187	G1188	A1189	G1190	G1191	G1192	G1195
U1101	C1102	A1103	C1104	U1105	G1106	G1107	U1108	C1109	G1110	A1111	G1112	U1113	G1114	G1115	C1116	G1117	G1118	C1119	G1120	C1123	C1124	U1125	A1126	A1127	A1128	A1129	U1130	U1131
U1033	G1034	G1039	C1040	C1041	G1044	A1045	A1046	C1049	A1050	G1051	A1054	G1055	G1056	A1057	G1058	G1059	U1060	U1061	G1062	G1063	C1064	U1065	U1066	G1067	G1068	A1069	A1070	G1071
C971	G972	A973	C974	G975	C976	G977	G978	G979	A980	U981	A982	A983	A984	C985	G986	G987	A988	G989	A990	C991	G992	G993	C994	C995	A996	G997	C1000	G1003
U905	G906	U907	C908	A909	A910	A911	C912	U913	C914	U915	G916	G917	G918	G919	A920	A921	A922	A923	A924	A925	A926	A927	A928	A929	A930	A931	A932	A933
C838	U839	C840	G845	C846	U847	G848	A849	C850	U851	G852	G853	G854	G855	C856	U857	G858	U859	U860	A861	G862	A863	G864	C865	A866	C867	U868	G869	A870
A777	G778	U779	A780	A781	A782	A783	A784	G785	G786	U787	A788	A789	G790	G791	G792	A793	G794	C795	G796	G797	G798	A799	C800	G801	A802	U803	A804	G805
G713	U714	G715	A716	G717	A718	G719	C720	G721	A722	G723	U724	G725	G726	A727	G728	G729	C730	C731	G732	G733	A734	A735	C736	G737	G738	G739	U740	G741
C850	G851	C852	A853	A854	A855	G856	U857	C858	G859	G860	C861	G862	G863	C864	C865	G866	U867	G868	G869	A870	C871	C872	C873	G874	A875	G876	A877	G878
U613	U614	A615	A616	G617	G618	C618A	G619	G620	G621	G622	G623	G624	G625	U626	A627	G628	G629	G630	A631	A632	A633	C634	C635	G636	A637	U638	G639	A640
C486	C487	G488	G489	G491	A492	G493	G494	G495	G496	A497	G498	U499	G500	A501	A502	A503	U504	A505	G506	A507	C508	G509	C510	U511	G512	U513	A514	A515
U554	G555	U557	G558	G559	C560	G561	U562	G563	C564	G565	U566	A567	U568	U569	A570	A571	A572	G573	C574	A575	U576	G577	A578	G579	C580	A581	G582	A583
U525	A526	C527	A528	A529	G530	C531	A532	G533	U534	C535	A536	C541	C544	C545	C546	A547	A548	G549	C550	G551	G552	U553	A554	A555	A556	A557	A558	A559
C	G	C	A	A	G	C	C	G	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C

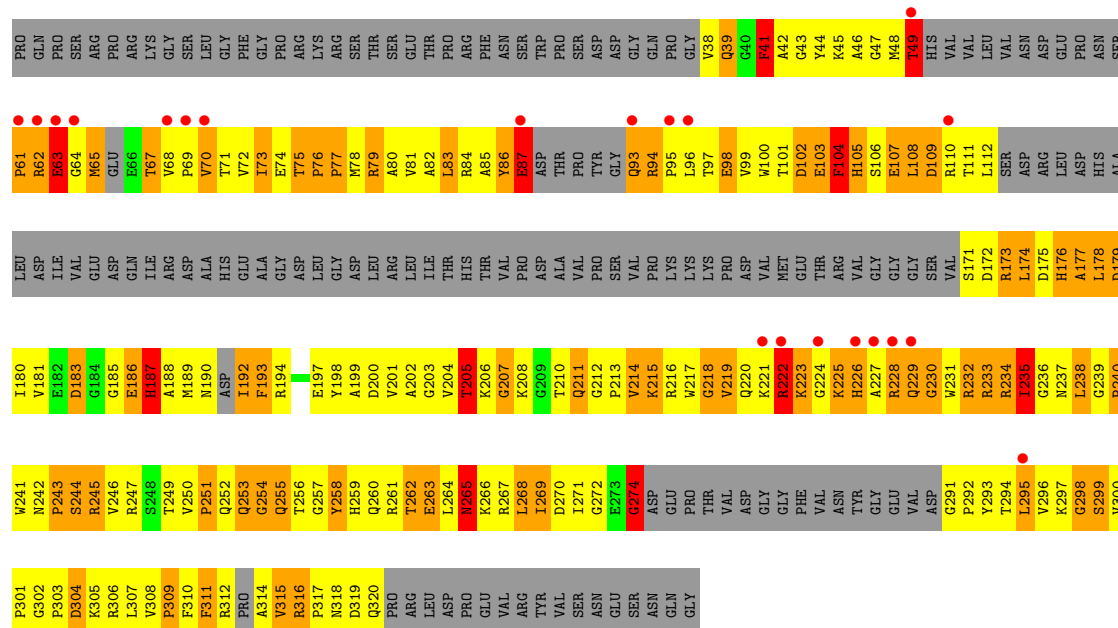




• Molecule 3: 50S ribosomal protein L2

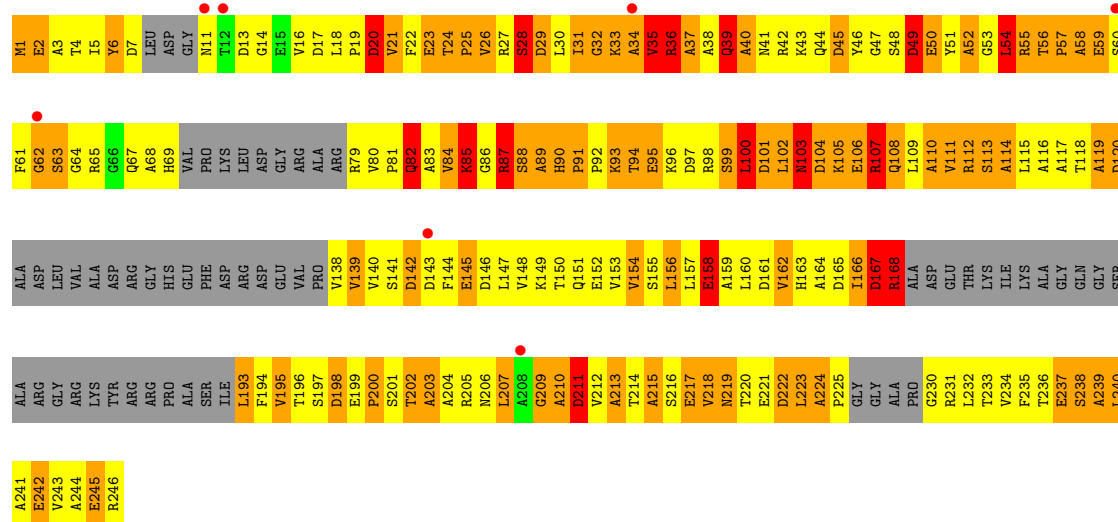
Chain D:





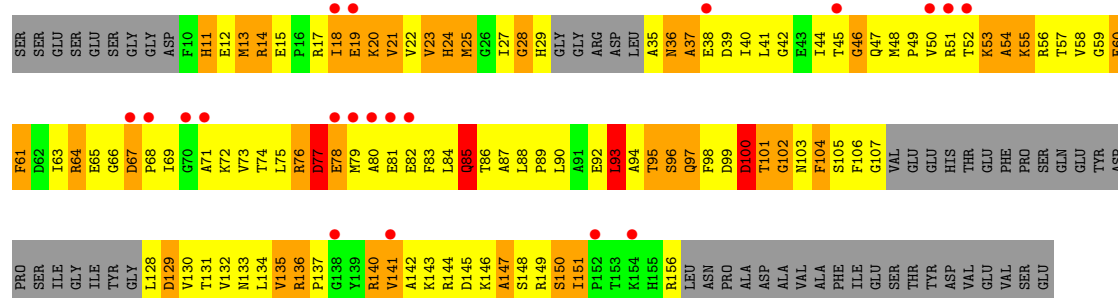
• Molecule 5: 50S ribosomal protein L4

Chain F:



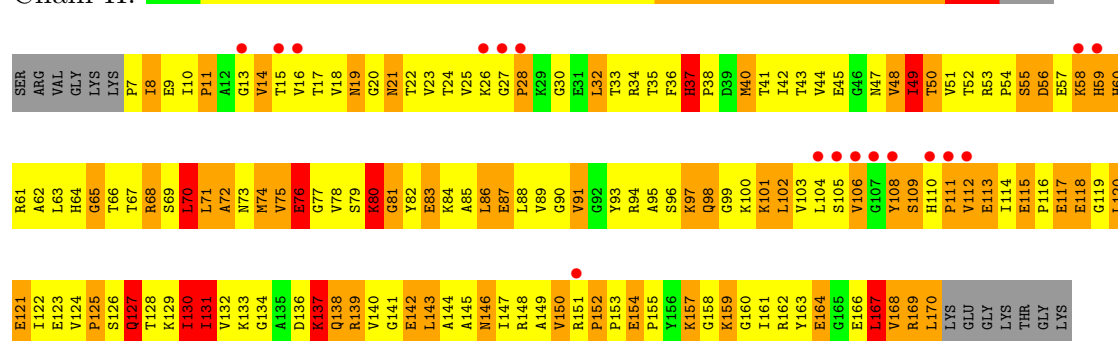
• Molecule 6: 50S ribosomal protein L5

Chain G:



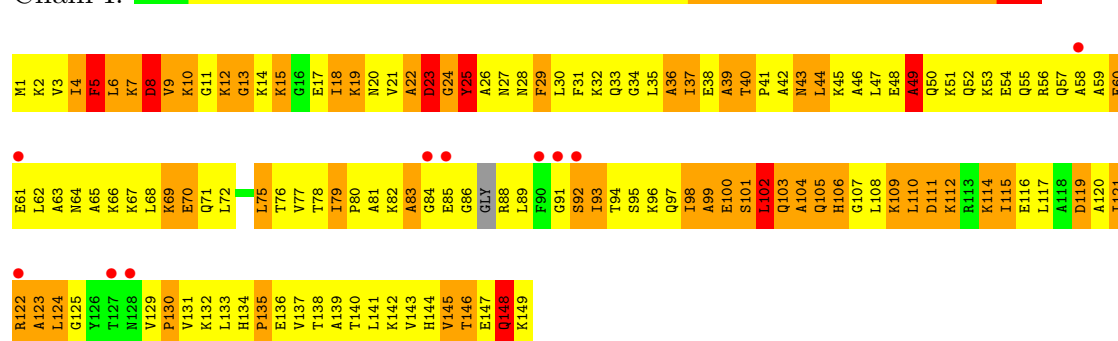
- Molecule 7: 50S ribosomal protein L6

Chain H:



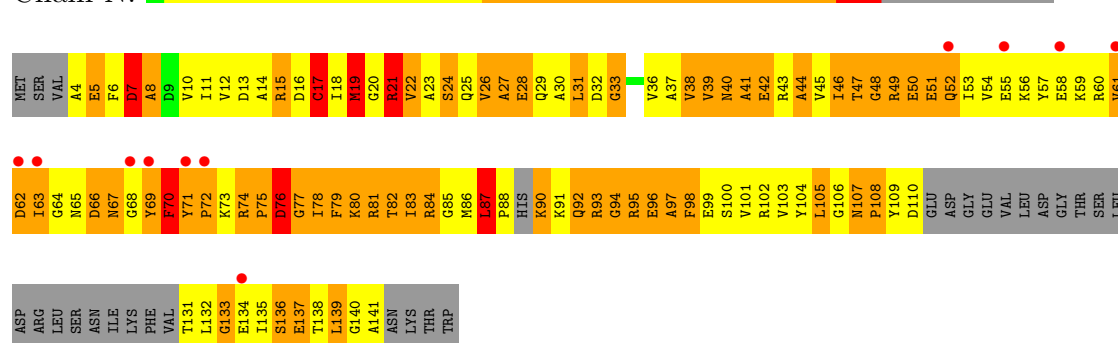
- Molecule 8: 50S ribosomal protein L9

Chain I:



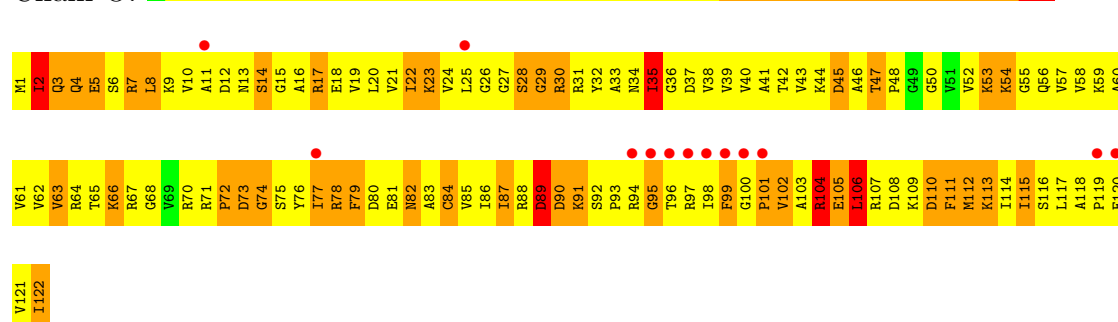
- Molecule 9: 50S ribosomal protein L13

Chain N:



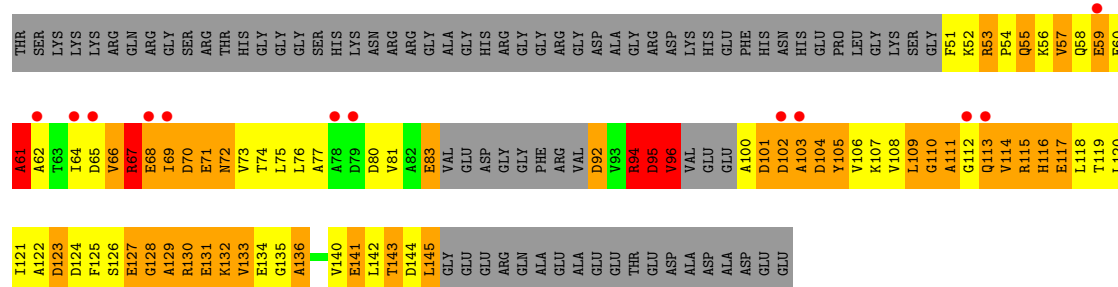
- Molecule 10: 50S ribosomal protein L14

Chain O:



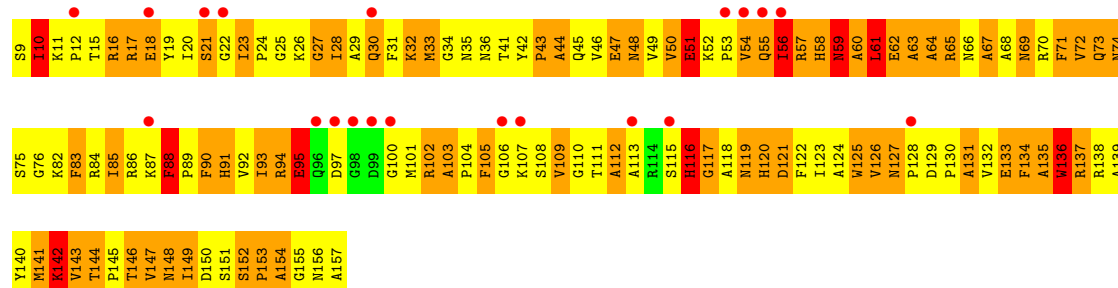
- Molecule 11: 50S ribosomal protein L15

Chain P:



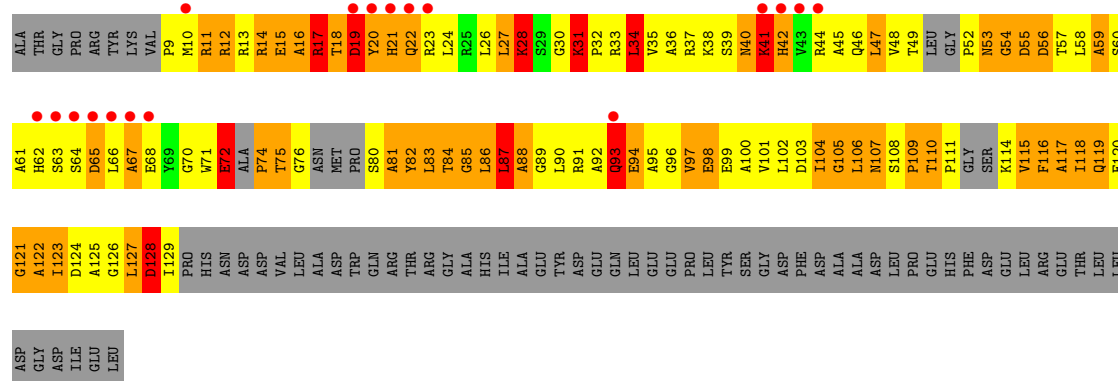
- Molecule 12: 50S ribosomal protein L16

Chain Q:



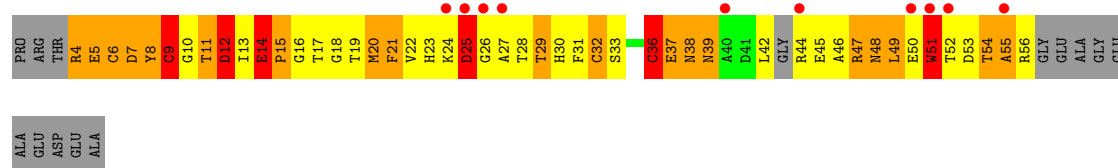
- Molecule 13: 50S ribosomal protein L18

Chain S:



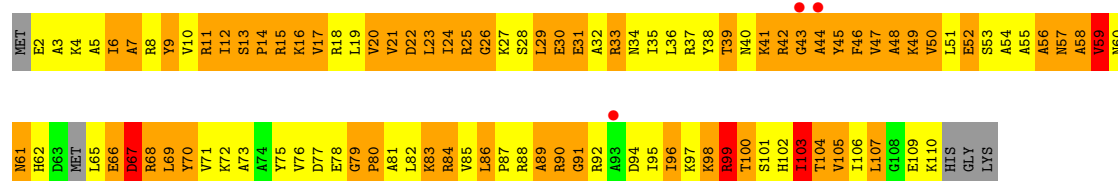
- Molecule 14: 50S ribosomal protein L19

Chain T:



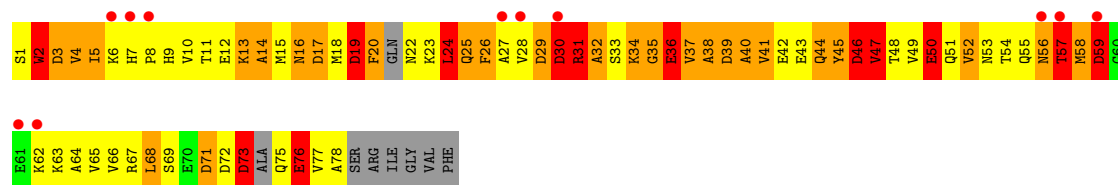
- Molecule 15: 50S ribosomal protein L22

Chain W:



- Molecule 16: 50S ribosomal protein L23

Chain X:



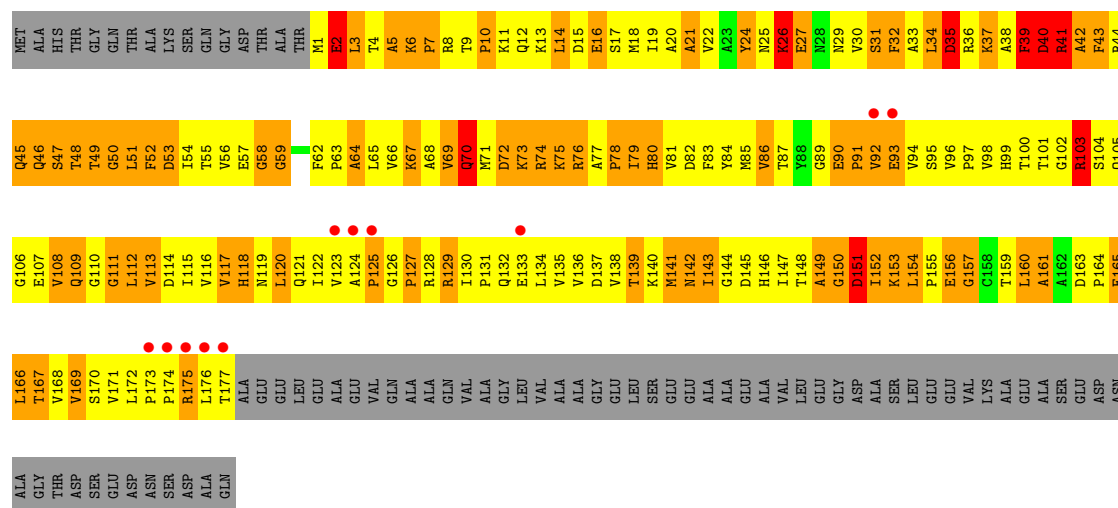
- Molecule 17: 50S ribosomal protein 24

Chain Y:



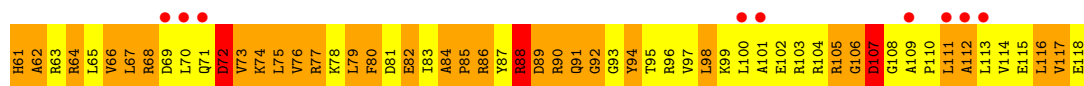
- Molecule 18: 50S ribosomal protein CTC

Chain Z:



- Molecule 19: 50S ribosomal protein L17

Chain R:



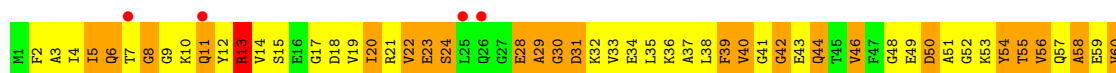
• Molecule 20: 50S ribosomal protein L20

Chain U:



• Molecule 21: 50S ribosomal protein L21

Chain V:



• Molecule 22: 50S ribosomal protein L29

Chain 2:



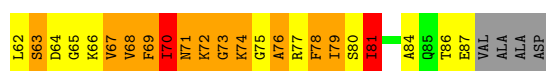
• Molecule 23: 50S ribosomal protein L30

Chain 3:

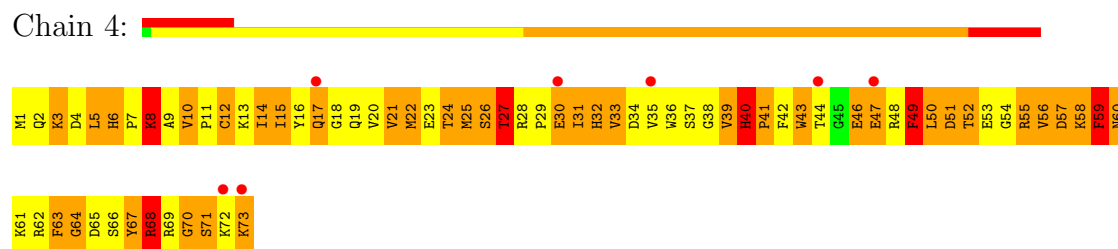


• Molecule 24: 50S ribosomal protein L27

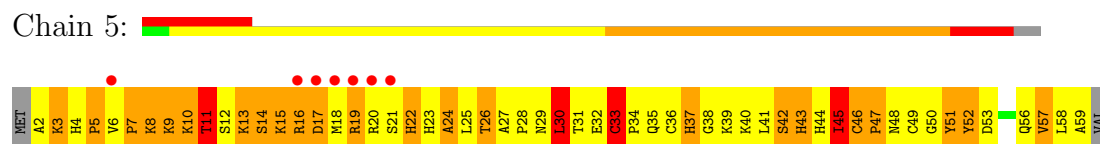
Chain 0:



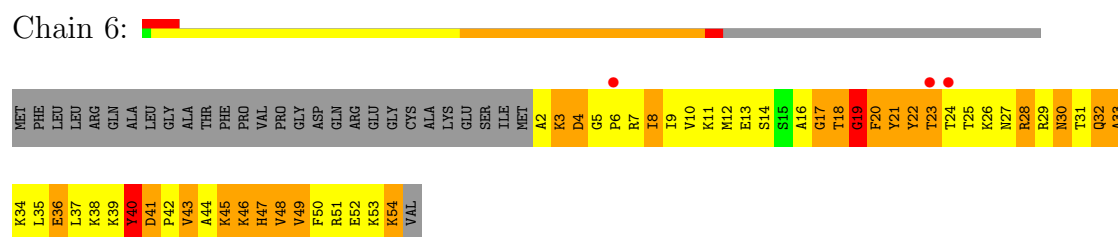
- Molecule 25: 50S ribosomal protein L31



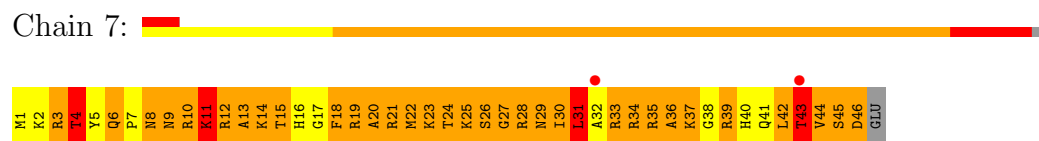
- Molecule 26: 50S ribosomal protein L32



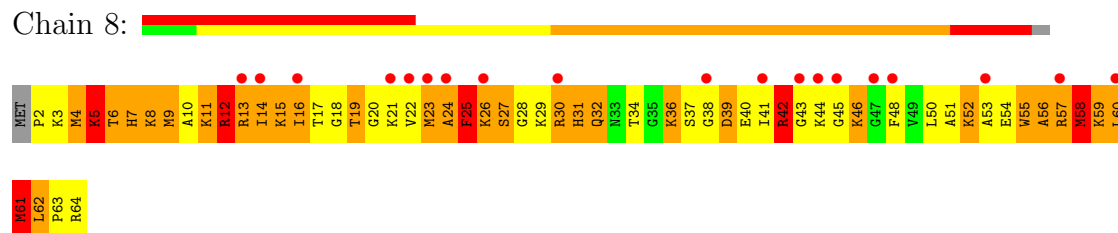
- Molecule 27: 50S ribosomal protein L33



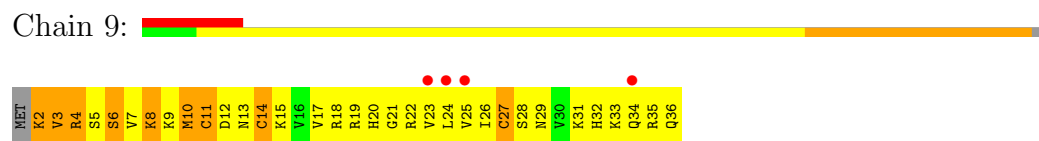
- Molecule 28: 50S ribosomal protein L34



- Molecule 29: 50S ribosomal protein L35

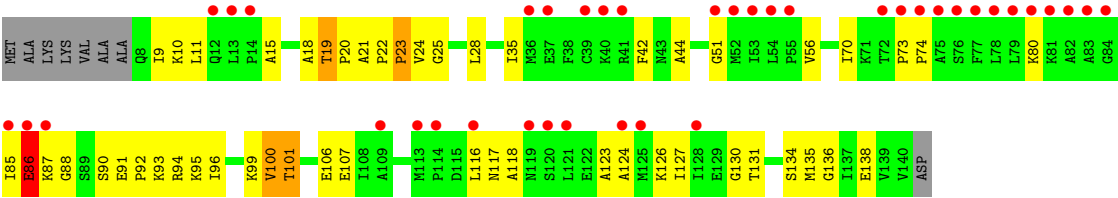


- Molecule 30: 50S ribosomal protein L36



- Molecule 31: 50S ribosomal protein L11





4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	520.21 Å 520.21 Å 365.90 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.35 – 6.76 43.35 – 6.02	Depositor EDS
% Data completeness (in resolution range)	96.2 (43.35-6.76) 91.3 (43.35-6.02)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.19	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.11 (at 6.14 Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.341 , 0.356 0.400 , 0.412	Depositor DCC
R_{free} test set	5634 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	233.6	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.07 , 25.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.20$	Xtriage
Outliers	0 of 112763 reflections	Xtriage
F_o, F_c correlation	0.80	EDS
Total number of atoms	87268	wwPDB-VP
Average B, all atoms (Å ²)	276.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.50% 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	B	0.79	2/2950 (0.1%)	1.32	17/4602 (0.4%)
2	A	1.31	147/67834 (0.2%)	1.47	923/105806 (0.9%)
3	D	0.41	1/1328 (0.1%)	0.65	2/1783 (0.1%)
4	E	0.67	4/1540 (0.3%)	1.08	8/2078 (0.4%)
5	F	0.72	3/1444 (0.2%)	0.84	2/1954 (0.1%)
6	G	0.25	0/971	0.46	0/1304
7	H	0.45	1/1272 (0.1%)	0.60	3/1721 (0.2%)
8	I	0.40	1/1156 (0.1%)	0.52	0/1544
9	N	0.35	0/927	0.55	0/1245
10	O	0.32	0/946	0.57	0/1269
11	P	1.44	3/643 (0.5%)	1.31	5/870 (0.6%)
12	Q	0.32	0/1106	0.52	0/1490
13	S	1.20	3/877 (0.3%)	0.70	2/1179 (0.2%)
14	T	0.39	0/412	0.70	0/554
15	W	0.95	3/869 (0.3%)	0.96	6/1166 (0.5%)
16	X	0.48	1/608 (0.2%)	1.04	3/820 (0.4%)
17	Y	0.25	0/887	0.83	3/1195 (0.3%)
18	Z	0.31	1/1385 (0.1%)	0.46	0/1883
19	R	0.30	0/867	0.49	0/1162
20	U	0.56	1/994 (0.1%)	0.69	3/1323 (0.2%)
21	V	0.69	1/796 (0.1%)	0.92	3/1058 (0.3%)
22	2	0.37	0/497	1.00	2/668 (0.3%)
23	3	0.31	0/482	0.50	0/646
24	0	0.40	1/649 (0.2%)	0.82	3/860 (0.3%)
25	4	1.31	2/620 (0.3%)	0.61	0/831
26	5	0.38	0/469	1.08	3/629 (0.5%)
27	6	0.32	0/438	0.55	1/583 (0.2%)
28	7	0.38	0/387	0.64	0/509
29	8	0.87	1/503 (0.2%)	0.95	6/657 (0.9%)
30	9	0.33	0/286	0.59	0/375
31	K	0.94	1/1010 (0.1%)	0.70	3/1349 (0.2%)
All	All	1.16	177/95153 (0.2%)	1.34	998/143113 (0.7%)

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
3	D	0	1
4	E	0	3
5	F	0	4
7	H	0	1
8	I	0	1
11	P	0	1
16	X	0	1
17	Y	0	1
22	2	0	1
24	0	0	1
26	5	0	1
All	All	0	16

The worst 5 of 177 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2199	A	O3'-P	-71.10	0.75	1.61
2	A	14	A	O3'-P	-50.73	1.00	1.61
2	A	1924	C	O3'-P	-48.85	1.02	1.61
2	A	176	G	O3'-P	-48.34	1.03	1.61
2	A	2454	G	O3'-P	-48.01	1.03	1.61

The worst 5 of 998 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	712(A)	A	P-O3'-C3'	-43.34	67.69	119.70
2	A	2199	A	O3'-P-O5'	-43.06	22.18	104.00
2	A	2454	G	P-O3'-C3'	-28.75	85.20	119.70
4	E	49	THR	O-C-N	-27.49	68.88	121.10
11	P	83	GLU	O-C-N	-27.09	79.36	122.70

There are no chirality outliers.

5 of 16 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	213	LYS	Peptide
4	E	274	GLY	Mainchain,Peptide
4	E	49	THR	Mainchain
5	F	103	ASN	Mainchain

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Mol	Chain	Res	Type	Group
5	F	28	SER	Mainchain

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	B	2637	0	1338	187	1
2	A	60599	0	30533	10726	127
3	D	1308	0	1346	1071	0
4	E	1507	0	1475	1137	4
5	F	1430	0	1357	1068	0
6	G	957	0	950	650	0
7	H	1251	0	1291	750	0
8	I	1145	0	1224	627	0
9	N	917	0	896	761	0
10	O	937	0	993	620	0
11	P	639	0	606	487	0
12	Q	1081	0	1047	928	0
13	S	866	0	868	691	0
14	T	406	0	359	160	0
15	W	860	0	909	568	0
16	X	602	0	559	447	0
17	Y	879	0	859	751	0
18	Z	1360	0	1377	897	0
19	R	855	0	904	561	0
20	U	978	0	1001	880	0
21	V	787	0	784	643	0
22	2	494	0	504	396	0
23	3	477	0	528	441	0
24	0	641	0	658	517	0
25	4	604	0	586	470	0
26	5	457	0	455	288	0
27	6	431	0	454	288	0
28	7	383	0	411	393	0
29	8	496	0	539	357	0
30	9	285	0	312	150	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	K	999	0	1065	116	0
All	All	87268	0	56188	24875	132

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 174.

The worst 5 of 24875 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
26:5:33:CYS:SG	26:5:36:CYS:HB2	1.24	1.69
2:A:2470:G:C2	2:A:2471:C:C5	1.81	1.69
2:A:2712:U:C6	2:A:712(A):A:C8	1.76	1.68
28:7:30:ILE:HA	28:7:33:ARG:CD	1.21	1.67
2:A:2580:U:C6	2:A:2581:G:C8	1.82	1.66

The worst 5 of 132 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:6:A:O4'	2:A:2902:C:C1'[8_554]	0.64	1.56
2:A:6:A:C4'	2:A:2902:C:O2'[8_554]	0.74	1.46
2:A:6:A:C4'	2:A:2902:C:C2'[8_554]	0.77	1.43
2:A:5:A:N7	2:A:2901:C:N1[8_554]	0.83	1.37
2:A:6:A:O4'	2:A:2902:C:C2'[8_554]	0.90	1.30

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	
3	D	169/173 (98%)	60 (36%)	34 (20%)	75 (44%)	0	0
4	E	183/338 (54%)	90 (49%)	34 (19%)	59 (32%)	0	1
5	F	179/246 (73%)	51 (28%)	47 (26%)	81 (45%)	0	0
6	G	116/176 (66%)	46 (40%)	31 (27%)	39 (34%)	0	0
7	H	162/177 (92%)	74 (46%)	39 (24%)	49 (30%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	I	144/149 (97%)	71 (49%)	29 (20%)	44 (31%)	0	1
9	N	111/145 (77%)	34 (31%)	20 (18%)	57 (51%)	0	0
10	O	120/122 (98%)	61 (51%)	27 (22%)	32 (27%)	0	2
11	P	82/164 (50%)	29 (35%)	19 (23%)	34 (42%)	0	0
12	Q	130/138 (94%)	38 (29%)	35 (27%)	57 (44%)	0	0
13	S	105/186 (56%)	36 (34%)	20 (19%)	49 (47%)	0	0
14	T	48/66 (73%)	17 (35%)	13 (27%)	18 (38%)	0	0
15	W	104/113 (92%)	41 (39%)	16 (15%)	47 (45%)	0	0
16	X	72/84 (86%)	26 (36%)	18 (25%)	28 (39%)	0	0
17	Y	108/119 (91%)	49 (45%)	20 (18%)	39 (36%)	0	0
18	Z	175/253 (69%)	53 (30%)	52 (30%)	70 (40%)	0	0
19	R	103/118 (87%)	35 (34%)	20 (19%)	48 (47%)	0	0
20	U	115/118 (98%)	22 (19%)	23 (20%)	70 (61%)	0	0
21	V	96/100 (96%)	39 (41%)	25 (26%)	32 (33%)	0	0
22	2	62/70 (89%)	8 (13%)	9 (14%)	45 (73%)	0	0
23	3	58/60 (97%)	24 (41%)	13 (22%)	21 (36%)	0	0
24	0	84/91 (92%)	33 (39%)	17 (20%)	34 (40%)	0	0
25	4	71/73 (97%)	21 (30%)	16 (22%)	34 (48%)	0	0
26	5	56/60 (93%)	16 (29%)	17 (30%)	23 (41%)	0	0
27	6	51/82 (62%)	21 (41%)	9 (18%)	21 (41%)	0	0
28	7	44/47 (94%)	4 (9%)	7 (16%)	33 (75%)	0	0
29	8	61/64 (95%)	22 (36%)	9 (15%)	30 (49%)	0	0
30	9	33/36 (92%)	14 (42%)	9 (27%)	10 (30%)	0	1
31	K	124/141 (88%)	92 (74%)	26 (21%)	6 (5%)	4	44
All	All	2966/3709 (80%)	1127 (38%)	654 (22%)	1185 (40%)	0	0

5 of 1185 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	64	ILE
3	D	66	PHE
3	D	67	LYS
3	D	82	TYR
3	D	85	ASN

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	
3	D	135/135 (100%)	99 (73%)	36 (27%)	1	6
4	E	156/284 (55%)	128 (82%)	28 (18%)	2	19
5	F	152/193 (79%)	124 (82%)	28 (18%)	2	17
6	G	102/147 (69%)	93 (91%)	9 (9%)	14	57
7	H	137/147 (93%)	111 (81%)	26 (19%)	2	16
8	I	119/119 (100%)	98 (82%)	21 (18%)	3	20
9	N	95/121 (78%)	80 (84%)	15 (16%)	4	27
10	O	101/101 (100%)	81 (80%)	20 (20%)	2	14
11	P	67/126 (53%)	56 (84%)	11 (16%)	3	24
12	Q	110/110 (100%)	83 (76%)	27 (24%)	1	8
13	S	89/149 (60%)	73 (82%)	16 (18%)	2	18
14	T	44/52 (85%)	30 (68%)	14 (32%)	0	4
15	W	88/92 (96%)	74 (84%)	14 (16%)	4	26
16	X	67/73 (92%)	44 (66%)	23 (34%)	0	3
17	Y	97/105 (92%)	80 (82%)	17 (18%)	3	20
18	Z	151/203 (74%)	130 (86%)	21 (14%)	5	33
19	R	89/101 (88%)	71 (80%)	18 (20%)	2	14
20	U	96/97 (99%)	68 (71%)	28 (29%)	0	5
21	V	79/79 (100%)	69 (87%)	10 (13%)	6	37
22	2	51/56 (91%)	37 (72%)	14 (28%)	0	6
23	3	52/52 (100%)	47 (90%)	5 (10%)	12	52
24	0	64/67 (96%)	57 (89%)	7 (11%)	9	46
25	4	66/66 (100%)	54 (82%)	12 (18%)	2	18
26	5	51/53 (96%)	43 (84%)	8 (16%)	4	27
27	6	46/69 (67%)	39 (85%)	7 (15%)	4	28
28	7	39/40 (98%)	31 (80%)	8 (20%)	2	13
29	8	50/51 (98%)	39 (78%)	11 (22%)	1	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
30	9	34/35 (97%)	30 (88%)	4 (12%)	8 41
31	K	108/113 (96%)	105 (97%)	3 (3%)	56 88
All	All	2535/3036 (84%)	2074 (82%)	461 (18%)	2 18

5 of 461 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	Q	85	ILE
15	W	84	ARG
26	5	33	CYS
12	Q	133	GLU
13	S	94	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 82 such sidechains are listed below:

Mol	Chain	Res	Type
13	S	21	HIS
17	Y	7	GLN
26	5	29	ASN
13	S	46	GLN
15	W	61	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	B	122/123 (99%)	44 (36%)	3 (2%)
2	A	2779/2916 (95%)	1485 (53%)	361 (12%)
All	All	2901/3039 (95%)	1529 (52%)	364 (12%)

5 of 1529 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	B	0	A
1	B	1	U
1	B	2	C
1	B	3	C
1	B	6	C

5 of 364 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	A	1325	G
2	A	1653	G
2	A	2717	G
2	A	1378	A
2	A	1535	U

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	B	123/123 (100%)	0.66	13 (10%) 7 15	242, 265, 342, 342	0
2	A	2814/2916 (96%)	0.43	180 (6%) 19 25	67, 222, 387, 400	0
3	D	173/173 (100%)	0.02	2 (1%) 75 64	398, 398, 400, 400	0
4	E	191/338 (56%)	0.61	21 (10%) 6 14	388, 400, 400, 400	0
5	F	189/246 (76%)	0.44	7 (3%) 39 37	398, 398, 399, 399	0
6	G	122/176 (69%)	0.81	20 (16%) 2 8	400, 400, 400, 400	0
7	H	164/177 (92%)	0.39	17 (10%) 7 15	399, 399, 400, 400	0
8	I	148/149 (99%)	0.51	10 (6%) 17 24	400, 400, 400, 400	0
9	N	117/145 (80%)	0.33	11 (9%) 9 17	388, 388, 388, 388	0
10	O	122/122 (100%)	0.71	13 (10%) 6 14	400, 400, 400, 400	0
11	P	84/164 (51%)	0.57	12 (14%) 3 9	400, 400, 400, 400	0
12	Q	138/138 (100%)	0.85	20 (14%) 3 9	391, 391, 391, 391	0
13	S	113/186 (60%)	0.83	18 (15%) 3 8	275, 370, 400, 400	0
14	T	52/66 (78%)	1.05	10 (19%) 2 6	400, 400, 400, 400	0
15	W	108/113 (95%)	0.11	3 (2%) 50 44	275, 277, 400, 400	0
16	X	76/84 (90%)	0.40	11 (14%) 3 9	400, 400, 400, 400	0
17	Y	110/119 (92%)	0.49	11 (10%) 8 16	400, 400, 400, 400	0
18	Z	177/253 (69%)	0.28	11 (6%) 20 26	376, 376, 379, 379	0
19	R	105/118 (88%)	0.45	12 (11%) 6 13	345, 345, 345, 345	0
20	U	117/118 (99%)	0.26	8 (6%) 17 24	356, 356, 392, 392	0
21	V	100/100 (100%)	0.34	7 (7%) 16 23	385, 385, 400, 400	0
22	2	64/70 (91%)	-0.05	0 100 100	287, 287, 287, 287	0
23	3	60/60 (100%)	-0.05	1 (1%) 67 57	343, 343, 343, 343	0
24	0	86/91 (94%)	0.64	10 (11%) 5 13	400, 400, 400, 400	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	4	73/73 (100%)	0.91	7 (9%) 8 16	400, 400, 400, 400	0
26	5	58/60 (96%)	0.60	7 (12%) 5 12	400, 400, 400, 400	0
27	6	53/82 (64%)	0.29	3 (5%) 23 27	400, 400, 400, 400	0
28	7	46/47 (97%)	0.61	2 (4%) 34 34	400, 400, 400, 400	0
29	8	63/64 (98%)	1.44	19 (30%) 1 4	400, 400, 400, 400	0
30	9	35/36 (97%)	1.03	4 (11%) 6 13	400, 400, 400, 400	0
31	K	133/141 (94%)	1.17	39 (29%) 1 4	397, 400, 400, 400	0
All	All	6014/6748 (89%)	0.48	509 (8%) 11 19	67, 356, 400, 400	0

The worst 5 of 509 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	546	C	11.4
13	S	42	HIS	8.7
12	Q	98	GLY	8.4
2	A	545	G	8.2
2	A	1467	C	8.1

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.