



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 28, 2026 – 01:30 PM UTC

PDB ID : 4V4X / pdb_00004v4x
Title : Crystal structure of the 70S *Thermus thermophilus* ribosome showing how the 16S 3'-end mimicks mRNA E and P codons.
Authors : Jenner, L.; Yusupova, G.; Rees, B.; Moras, D.; Yusupov, M.
Deposited on : 2006-06-27
Resolution : 5.00 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)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

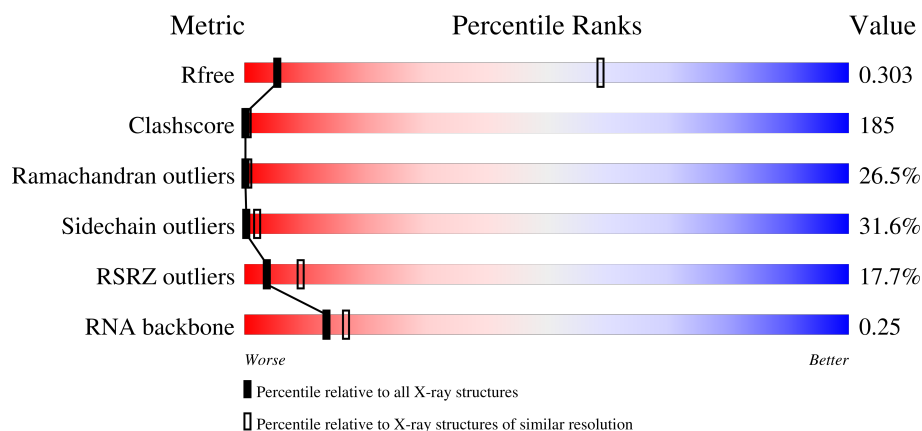
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 5.00 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}	180053	1009 (6.02-3.98)
Clashscore	190562	1040 (6.00-4.00)
Ramachandran outliers	187476	1015 (6.06-3.92)
Sidechain outliers	187428	1136 (6.10-3.90)
RSRZ outliers	180081	1004 (6.02-3.98)
RNA backbone	3983	1045 (6.76-3.10)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AA	1522	2% 56% 32% 9%
2	AC	77	9% 43% 43% 12%
3	AD	76	28% 54% 42%
4	AE	256	9% 40% 39% 11% 9%

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Mol	Chain	Length	Quality of chain
5	AF	239	
6	AG	209	
7	AH	162	
8	AI	101	
9	AJ	156	
10	AK	138	
11	AL	128	
12	AM	105	
13	AN	129	
14	AO	132	
15	AP	126	
16	AQ	61	
17	AR	89	
18	AS	88	
19	AT	105	
20	AU	88	
21	AV	93	
22	AW	106	
23	AX	27	
24	BA	2916	
25	BB	123	
26	BC	229	
27	BD	276	
28	BE	206	
29	BF	210	

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Mol	Chain	Length	Quality of chain
30	BG	182	
31	BH	180	
32	BK	148	
33	BL	147	
34	BM	140	
35	BN	122	
36	BO	150	
37	BP	141	
38	BQ	118	
39	BR	112	
40	BS	146	
41	BT	118	
42	BU	101	
43	BV	113	
44	BW	96	
45	BX	110	
46	BY	206	
47	BZ	85	
48	B1	67	
49	B2	60	
50	B3	71	
51	B4	60	
52	B5	54	
53	B6	49	
54	B7	65	

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Mol	Chain	Length	Quality of chain
55	B8	37	5%22%51%38%5%

2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 149044 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 16S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1515	Total	C	N	O	P	0	0	0
			32554	14490	6022	10527	1515			

- Molecule 2 is a RNA chain called tRNA fMET (unmodified bases).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AC	76	Total	C	N	O	P	0	0	0
			1624	723	295	530	76			

- Molecule 3 is a RNA chain called tRNA PHE (unmodified bases).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AD	76	Total	C	N	O	P	0	0	0
			1623	723	290	534	76			

- Molecule 4 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AE	234	Total	C	N	O	S	0	0	0
			1900	1213	341	341	5			

- Molecule 5 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AF	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	1			

- Molecule 6 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AG	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

- Molecule 7 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AH	150	Total	C	N	O	S	0	0	0
			1146	724	217	201	4			

- Molecule 8 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AI	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

- Molecule 9 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AJ	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

- Molecule 10 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AK	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

- Molecule 11 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AL	127	Total	C	N	O		0	0	0
			1010	639	197	174				

- Molecule 12 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AM	98	Total	C	N	O	S	0	0	0
			794	499	156	138	1			

- Molecule 13 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AN	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			

- Molecule 14 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AO	124	Total	C	N	O	S	0	0	0
			970	611	195	163	1			

- Molecule 15 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AP	125	Total	C	N	O	S	0	0	0
			997	617	207	171	2			

- Molecule 16 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AQ	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 17 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AR	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

- Molecule 18 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	AS	83	Total	C	N	O	S	0	0	0
			700	443	139	117	1			

- Molecule 19 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AT	104	Total	C	N	O	S	0	0	0
			857	547	161	147	2			

- Molecule 20 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	AU	73	Total	C	N	O	0	0	0
			597	380	118	99			

- Molecule 21 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	AV	80	Total	C	N	O	S	0	0	0
			647	414	119	112	2			

- Molecule 22 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AW	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
23	AX	24	Total	C	N	O	0	0	0
			208	128	50	30			

- Molecule 24 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	BA	2889	Total	C	N	O	P	0	0	0
			62218	27691	11629	20009	2889			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BA	496	G	-	insertion	GB 48268

- Molecule 25 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	BB	123	Total	C	N	O	P	0	0	0
			2641	1175	488	855	123			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BB	-1	A	-	insertion	GB 48271
BB	120	U	-	insertion	GB 48271

- Molecule 26 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	BC	228	Total	C	N	O	S	0	0	0
			1742	1102	318	319	3			

- Molecule 27 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	BD	272	Total	C	N	O	S	0	0	0
			2124	1339	424	358	3			

- Molecule 28 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	BE	206	Total	C	N	O	S	0	0	0
			1578	997	302	273	6			

- Molecule 29 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	BF	208	Total	C	N	O	S	0	0	0
			1625	1034	303	286	2			

- Molecule 30 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	BG	182	Total	C	N	O	S	0	0	0
			1482	947	269	261	5			

- Molecule 31 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	BH	174	Total	C	N	O	S	0	0	0
			1328	844	248	235	1			

- Molecule 32 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BK	148	Total	C	N	O	S	0	0	0
			1155	737	205	212	1			

- Molecule 33 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BL	138	Total	C	N	O	S	0	0	0
			1025	654	181	185	5			

- Molecule 34 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BM	139	Total	C	N	O	S	0	0	0
			1113	717	207	186	3			

- Molecule 35 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BN	122	Total	C	N	O	S	0	0	0
			932	587	171	170	4			

- Molecule 36 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BO	145	Total	C	N	O	S	0	0	0
			1106	688	226	190	2			

- Molecule 37 is a protein called 50S ribosomal protein L16.

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

- Molecule 38 is a protein called 50S ribosomal protein L17.

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

- Molecule 39 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
39	BR	110	Total	C	N	O	0	0	0
			877	553	175	149			

- Molecule 40 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BS	117	Total	C	N	O	S	0	0	0
			976	614	197	164	1			

- Molecule 41 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BT	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			

- Molecule 42 is a protein called 50S ribosomal protein L21.

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

- Molecule 43 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BV	110	Total	C	N	O	S	0	0	0
			876	552	171	151	2			

- Molecule 44 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
44	BW	94	Total	C	N	O	0	0	0
			742	483	133	126			

- Molecule 45 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BX	110	Total	C	N	O	S	0	0	0
			844	539	158	141	6			

- Molecule 46 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BY	180	Total	C	N	O	S	0	0	0
			1435	916	256	260	3			

- Molecule 47 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	BZ	85	Total	C	N	O	S	0	0	0
			670	415	141	112	2			

- Molecule 48 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	B1	67	Total	C	N	O	S	0	0	0
			567	350	116	99	2			

- Molecule 49 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	B2	59	Total	C	N	O	S	0	0	0
			469	298	90	81				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	B3	71	Total	C	N	O	S	0	0	0
			581	364	108	104	5			

- Molecule 51 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	B4	57	Total	C	N	O	S	0	0	0
			445	279	87	74	5			

- Molecule 52 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	B5	49	Total	C	N	O	S	0	0	0
			426	265	87	70	4			

- Molecule 53 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	B6	49	Total	C	N	O	S	0	0	0
			430	263	108	57	2			

- Molecule 54 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	B7	64	Total	C	N	O	S	0	0	0
			515	331	102	79	3			

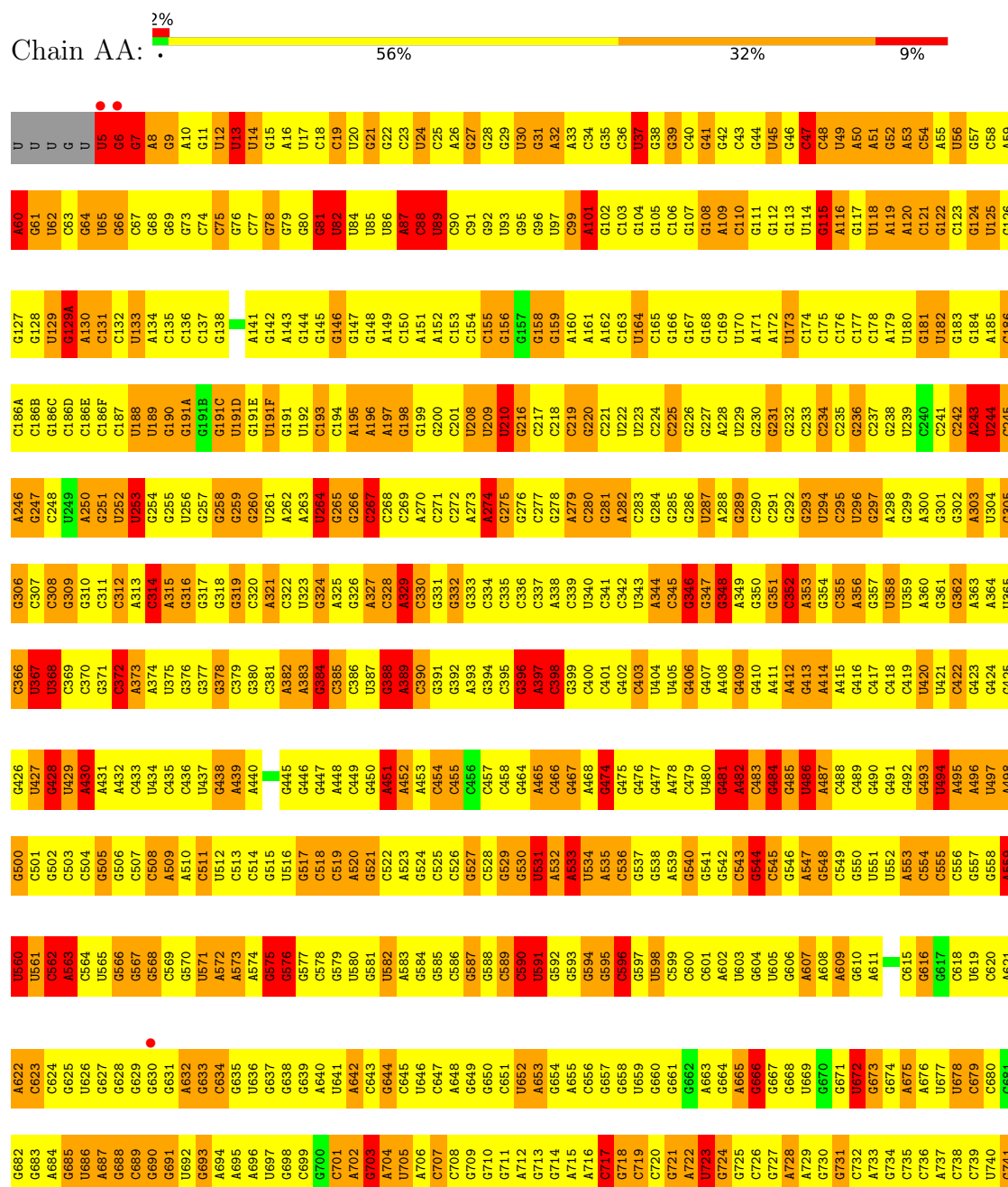
- Molecule 55 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	B8	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

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 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.

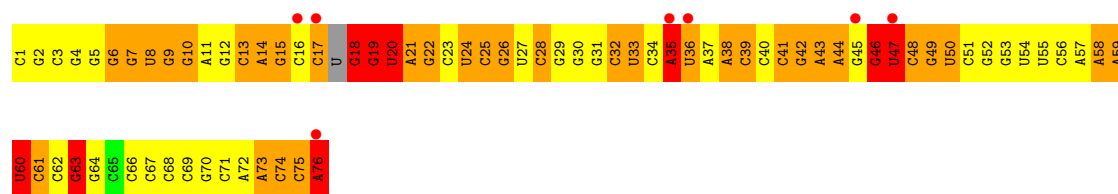
• Molecule 1: 16S rRNA



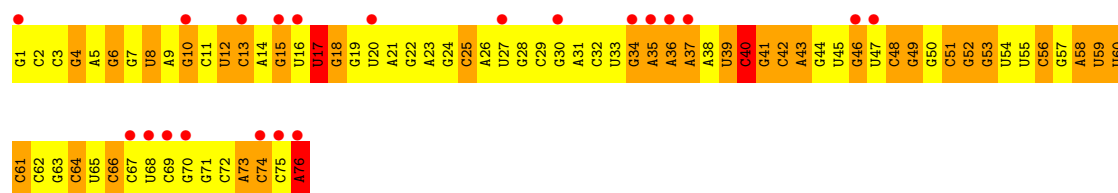
G1529	G1469	C1404	U1345	A1285	A1225	C1164	G1104	A1044	C989	G929	G869	A802	G742
G1530	G1470	G1405	A1346	A1286	C1226	C1165	A1105	C1045	C990	C930	U870	G803	U743
U1531	G1471	U1406	G1347	A1287	A1227	G1166	A1106	A1046	U991	C931	U871	U804	C744
C1533	U1472	U1407	U1348	A1288	C1228	A1167	C1107	G1047	U992	C932	A872		C745
A1534	A1473	A1408	A1349	A1289	A1229	A1169	G1108	U1048	G993	G933	A873	A807	A746
C1535	G1474	C1409	A1350	G1290	C1230	A1170	C1109	U1049	A994	C934	G874	G808	C747
C1536	G1475	G1410	U1351	G1291	G1231	G1171	A1110	G1050	C995	A935	C875	G809	C748
U1537	C1476	C1411	C1352	U1292	U1232	C1172	A1111	C1051	A996	C936	G876	C810	C749
C1477	C1477	C1412	G1353	G1293	U1233	C1173	A1112	U1052	U997	C937	C877	C811	G750
C1538	C1478	A1413	G1354	G1294	C1234	G1174	C1113	C1053	G998	A938	G878	C812	U751
C1539	C1479	G1414	G1355	G1295	U1235	G1175	C1114	C1054	C998A	G939	C879	U813	G752
U1540	G1480	G1415	G1356	U1296	U1236	A1176	C1115	A1055	U999	C940	G880	A814	A753
U1541	A1481	G1416	A1357	C1297	A1237	G1177	C1116	U1056	A1000	C941	G881	A815	C754
U1542	G1482	G1417	U1358	C1298	A1238	G1178	G1117	G1057	G1001	G942	C882	A816	G755
A1483	A1483	A1418	C1359	A1299	U1239	A1179	C1118	G1058	G1002	U943	C883	C817	G756
C1484	C1484	A1419	A1360	G1300	A1240	A1180	C1119	G1059	G1003	U944	U884	G818	U757
U1485	U1485	C1420	G1361	U1301	C1241	A1181	G1120	C1060	A1004	G945	G885	A819	G758
G1486	G1486	C1421	C1362	U1302	G1242	G1182	U1121	G1061	A1005	A946	G886	U820	A759
G1487	G1487	G1422	C1362A	C1303	C1243	A1183	U1122	U1062	G1006	G947	G887	G821	G760
G1488	G1488	C1423	A1363	G1304	C1244	G1184	A1123	G1063	C1007	C948	G888	C822	G761
G1489	G1489	C1424	U1364	G1305	A1245	G1185	G1124	G1064	C1008	A949	U889	C823	G762
C1490	C1490	U1425	G1365	A1306	C1246	G1186	U1125	U1065	G1009	U950	G890	C824	G763
A1491	G1491	C1426	C1366	U1307	U1247	G1187	U1126	C1066	G1010	G951	U891	G825	C764
A1492	A1492	U1427	G1367	U1308	A1248	A1188	G1127	A1067	G1011	U952	C892	C826	G765
A1493	A1493	A1428	G1368	G1309	C1249	C1189	C1128	G1068	U1012	G953	C893	U827	G766
G1494	G1494	C1429	C1369	G1310	A1250	G1190	C1129	C1069	G1013	G954	G894	A828	A767
U1495	U1495	C1430	G1370	G1311	A1251	A1191	A1130	U1070	A1014	U955	G895	G829	A768
U1496	C1496	C1431	G1371	G1312	A1252	C1192	A1131	C1071	A1015	U956	G896	G830	G769
U1497	G1497	G1432	C1372	U1313	C1253	G1193	C1132	U1072	A1016	U957	C897	U831	C770
U1498	U1498	A1433	G1373	C1314	C1254	U1194	G1133	U1073	G1017	A958	G898	C832	G771
A1499	A1499	A1434	A1374	U1315	G1255	C1195	G1134	G1074	C1018	A959	C899	U833	U772
A1500	A1500	G1435	A1375	U1316	A1256	U1196	U1135	C1075	C1019	U960	A900	C834	G773
U1501	U1501	U1436	U1376	C1317	U1257	G1197	U1136	C1076	U1020	U961	A901	U835	G774
A1502	A1502	C1437	A1377	A1318	G1258	U1198	C1137	G1077	G1021	C962	G902	G836	G775
A1503	A1503	G1438	C1378	A1319	C1259	U1199	G1138	U1078	G1022	G963	G903	G837	G776
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U1506	U1506	G1441	U1381	C1322	C1262	G1202	C1141	G1081	U1025	G966	G906	C842	C779
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U1512	U1512	G1449	G1387	C1328	A1268	C1208	C1147	U1087	G1029	C972	C912	G852	G785
A1513	A1513	U1450	C1388	A1329	A1269	C1209	U1148	G1088	C1030	G973	A913	G853	G786
C1514	C1514	A1451	C1389	U1330	C1270	C1210	U1149	G1089	G1031	A974	A914	G854	A787
C1515	C1515	G1452	U1390	G1331	G1271	U1211	U1150	U1090	A1032	A975	A915	G855	U788
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G1517	G1517	G1454	G1392	A1333	G1273	A1213	A1152	A1092	G1032B	A977	G917	C857	A790
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G1520	G1520	A1460	C1395	C1336	G1276	C1216	G1155	U1095	A1035	C980	U920	A860	U793
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U1528	U1528	A1468	C1403	C1344	C1284	G1224	C1163	C1103	C1043	G988	G928	C868	U801

• Molecule 2: tRNA fMET (unmodified bases)

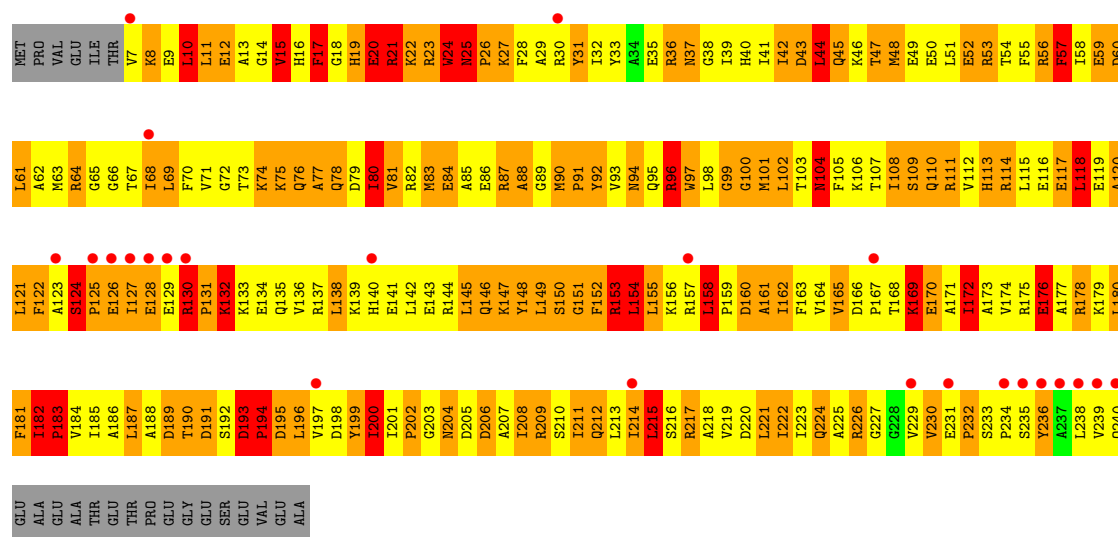




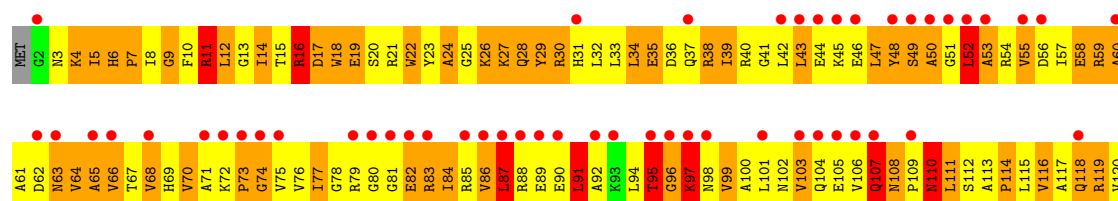
• Molecule 3: tRNA PHE (unmodified bases)

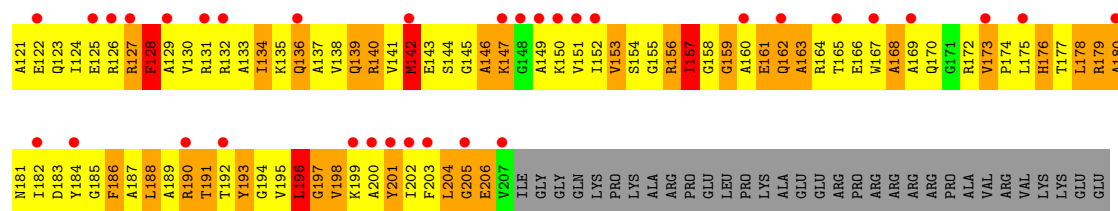


• Molecule 4: 30S ribosomal protein S2

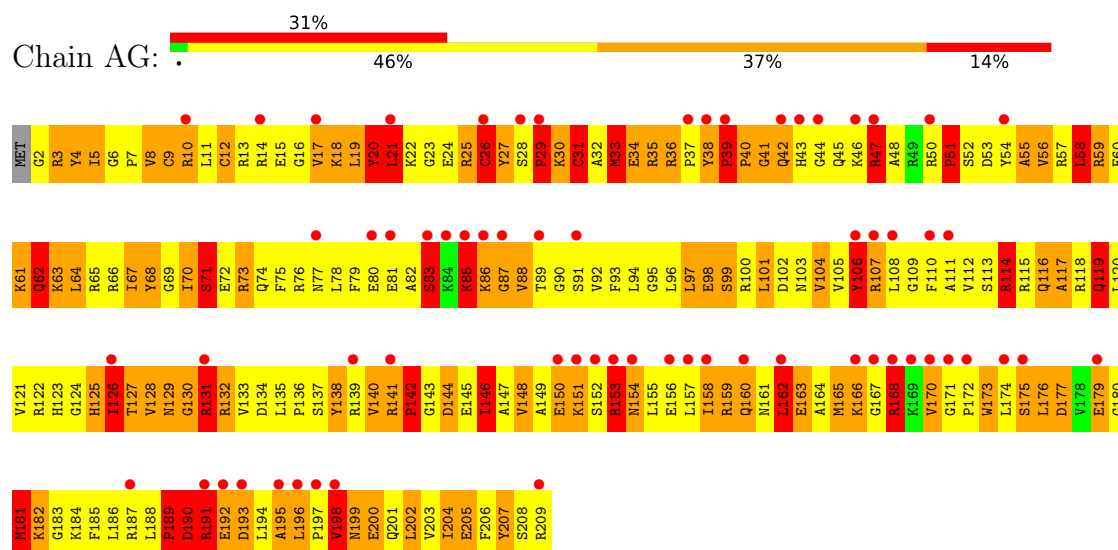


• Molecule 5: 30S ribosomal protein S3

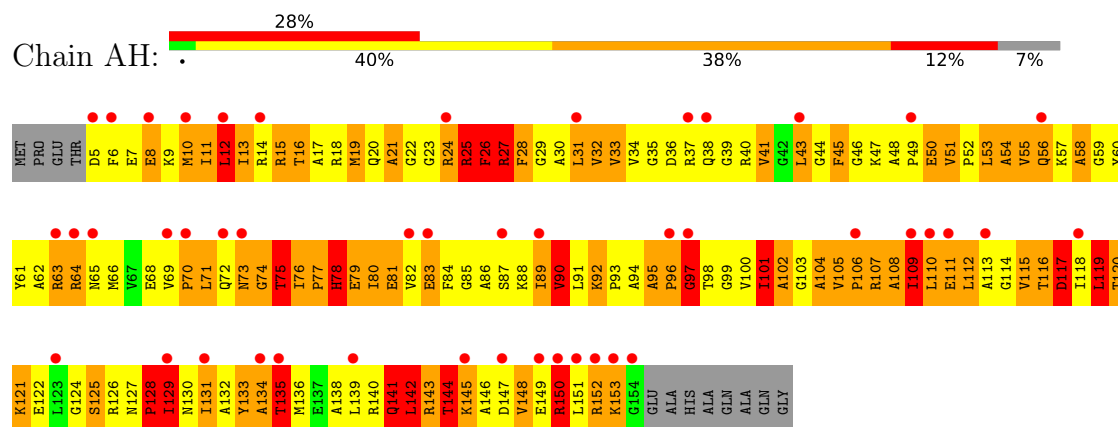




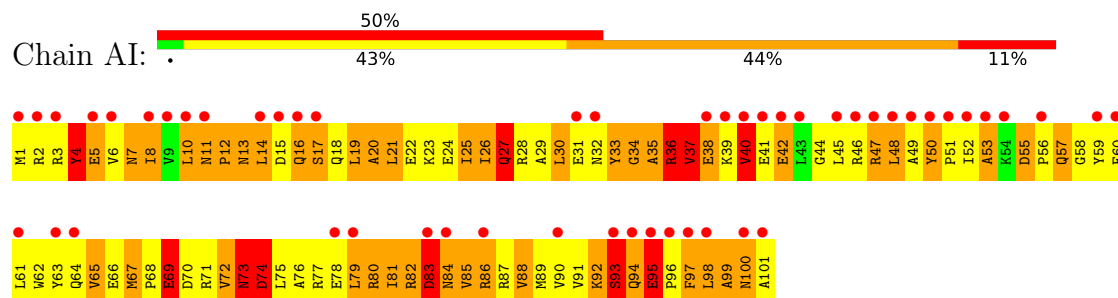
• Molecule 6: 30S ribosomal protein S4



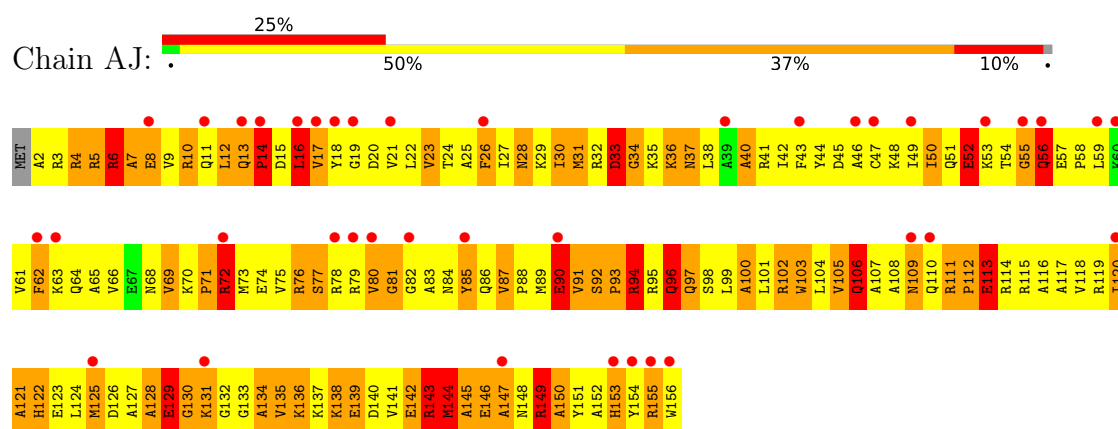
• Molecule 7: 30S ribosomal protein S5



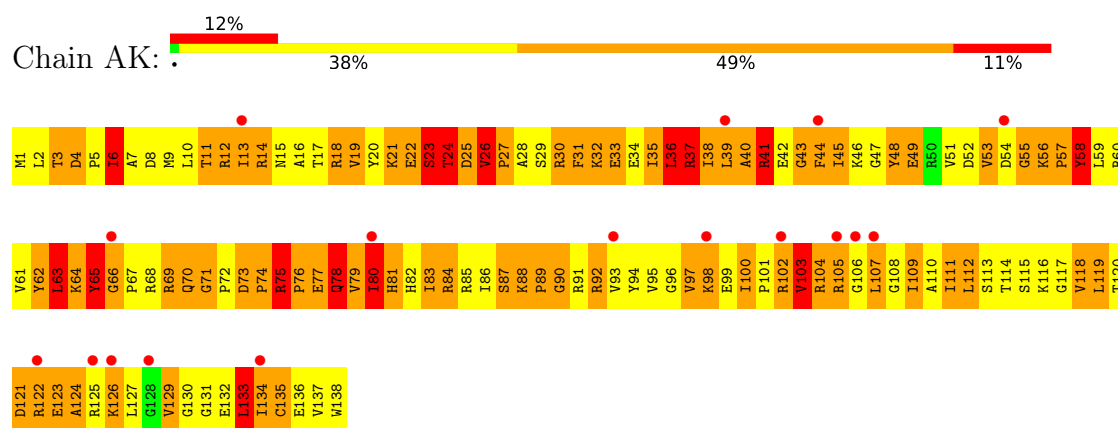
• Molecule 8: 30S ribosomal protein S6



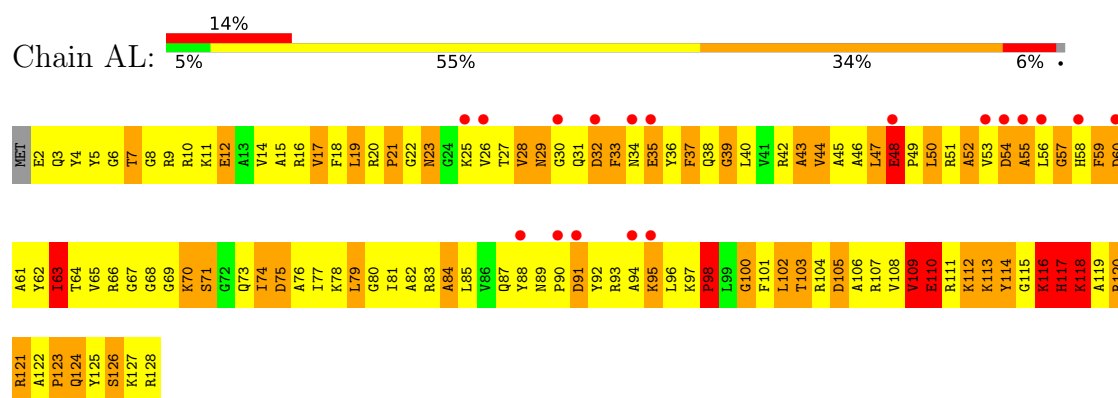
• Molecule 9: 30S ribosomal protein S7



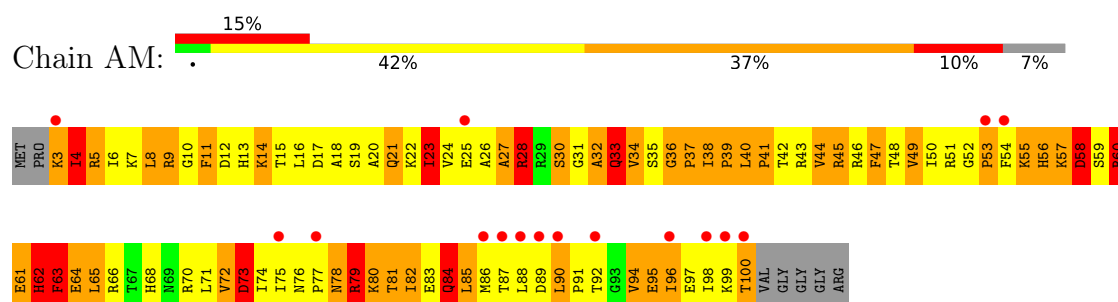
• Molecule 10: 30S ribosomal protein S8



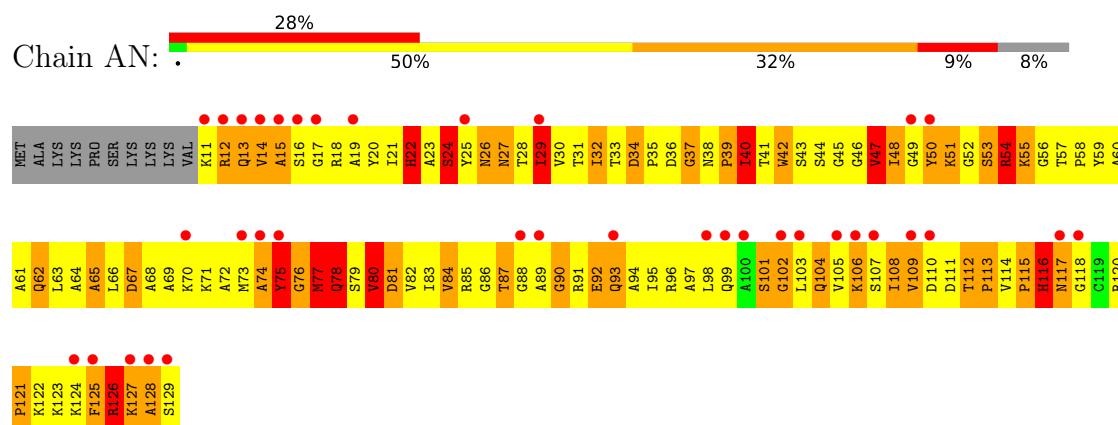
• Molecule 11: 30S ribosomal protein S9



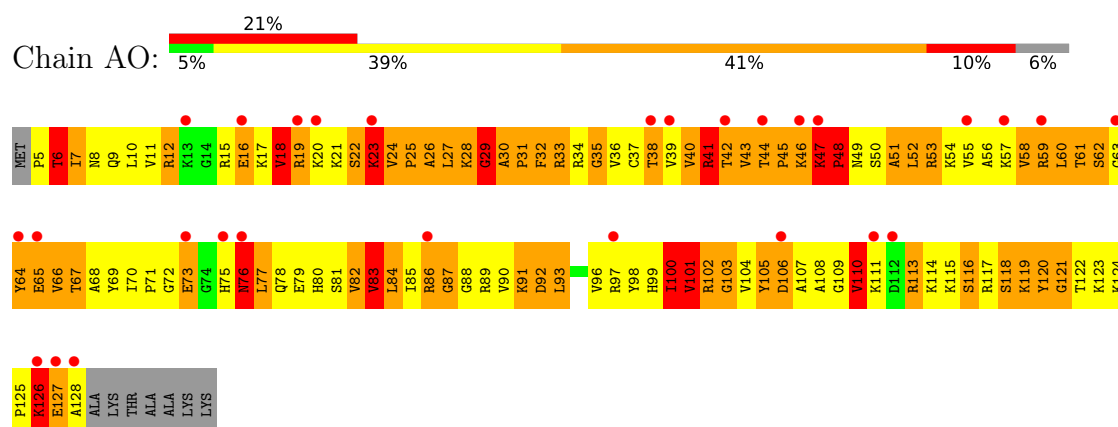
• Molecule 12: 30S ribosomal protein S10



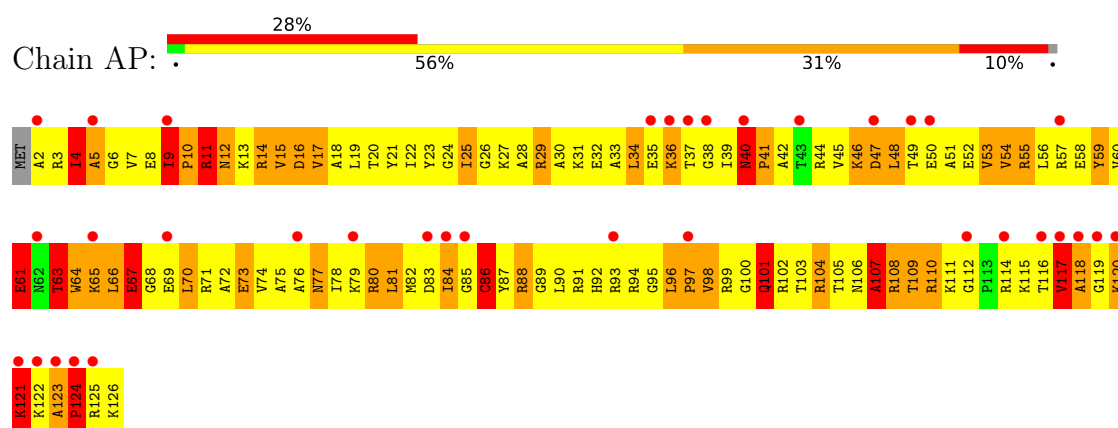
• Molecule 13: 30S ribosomal protein S11



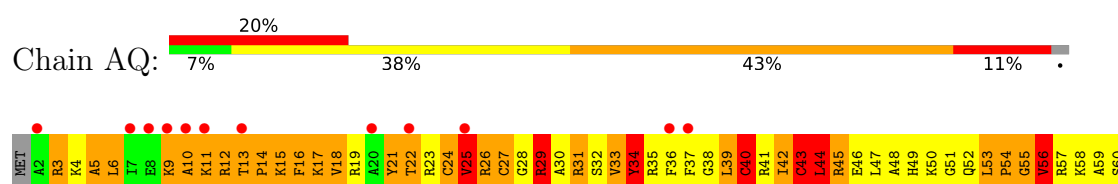
• Molecule 14: 30S ribosomal protein S12



• Molecule 15: 30S ribosomal protein S13

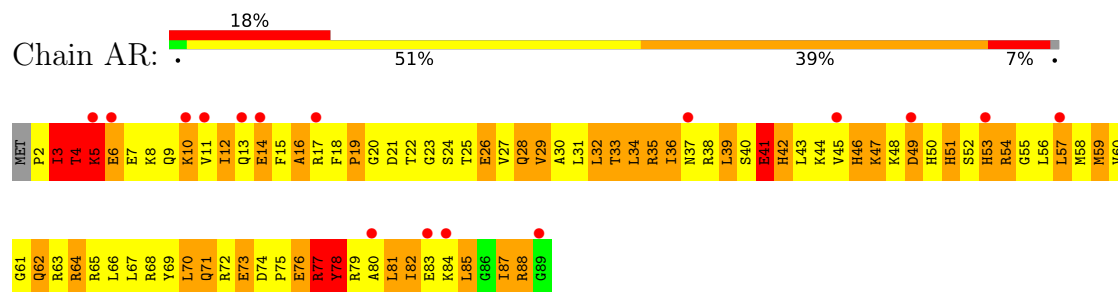


• Molecule 16: 30S ribosomal protein S14

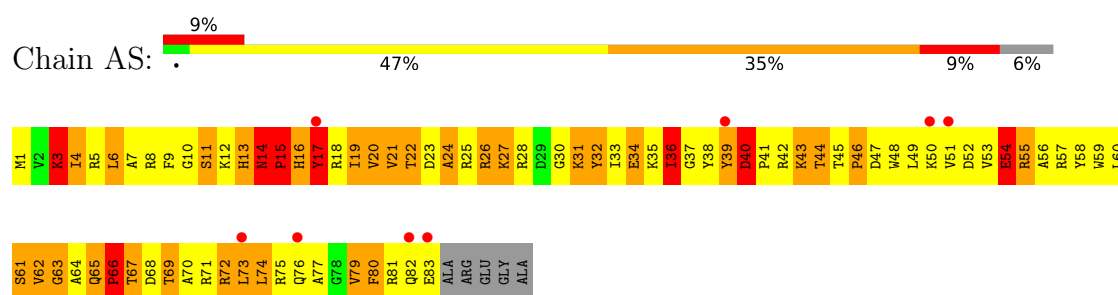


M61

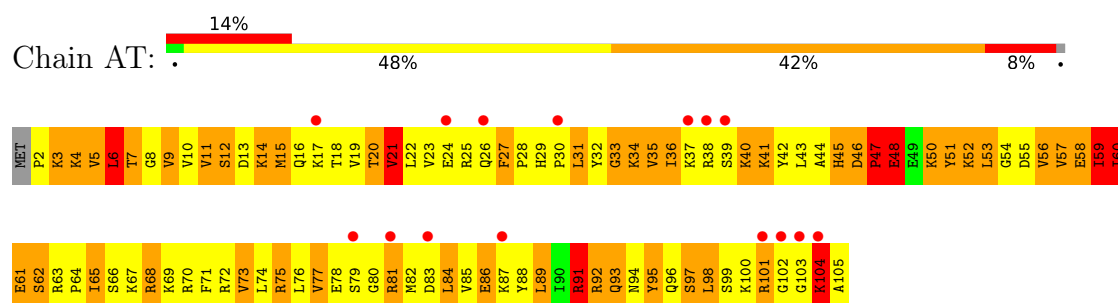
• Molecule 17: 30S ribosomal protein S15



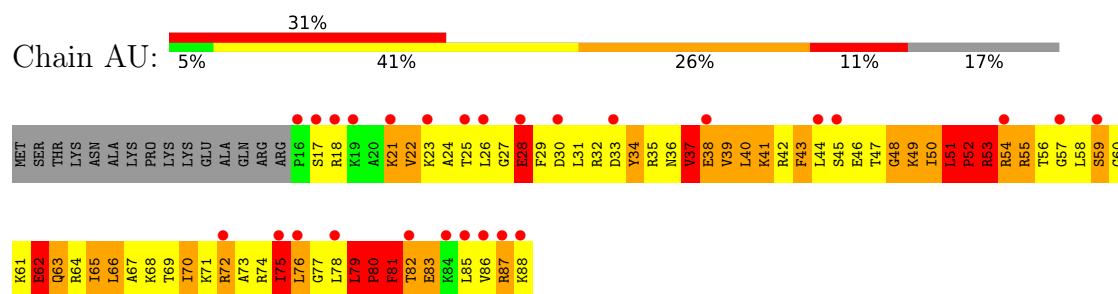
• Molecule 18: 30S ribosomal protein S16



• Molecule 19: 30S ribosomal protein S17

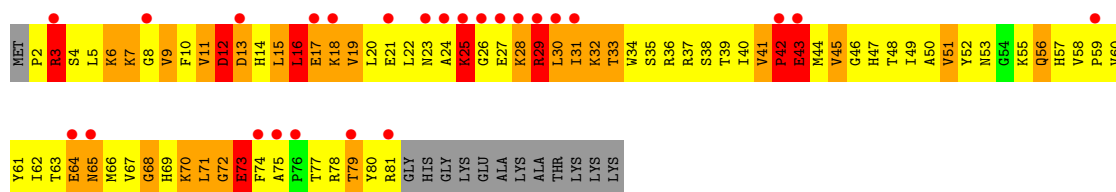


• Molecule 20: 30S ribosomal protein S18

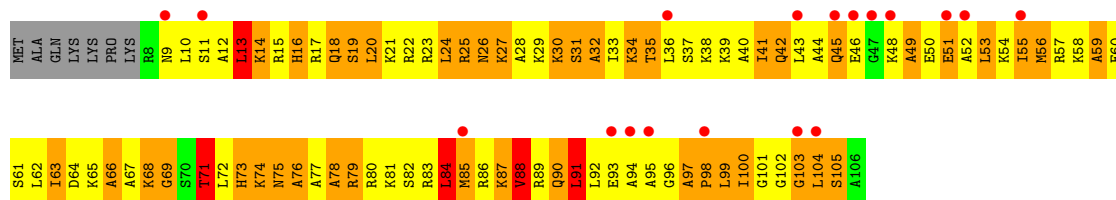
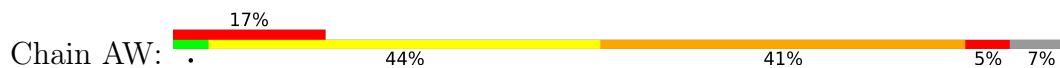


• Molecule 21: 30S ribosomal protein S19





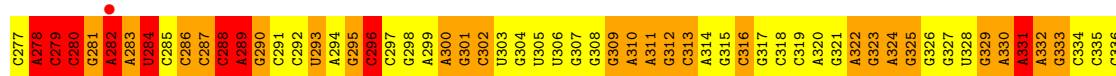
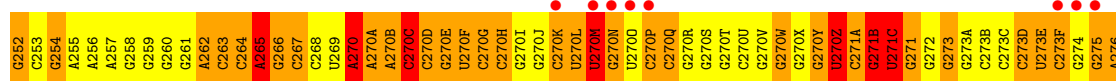
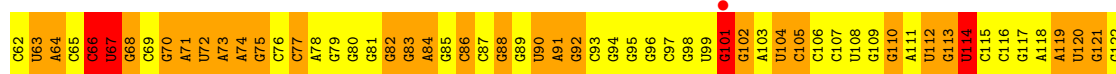
• Molecule 22: 30S ribosomal protein S20



• Molecule 23: 30S ribosomal protein Thx



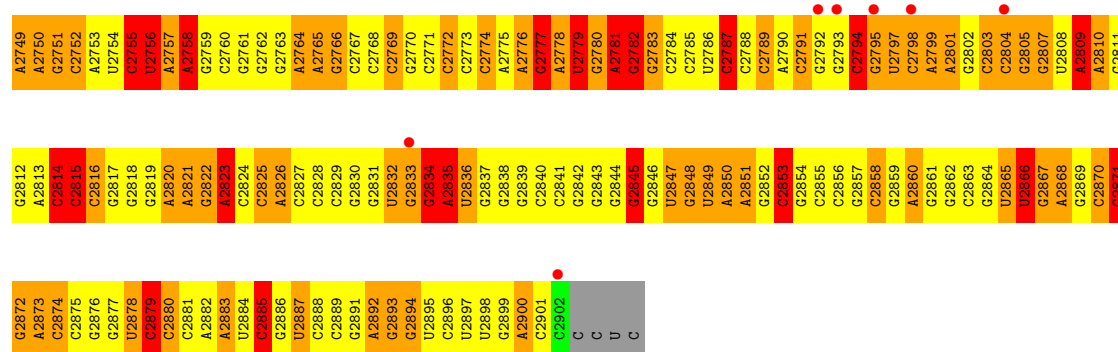
• Molecule 24: 23S ribosomal RNA



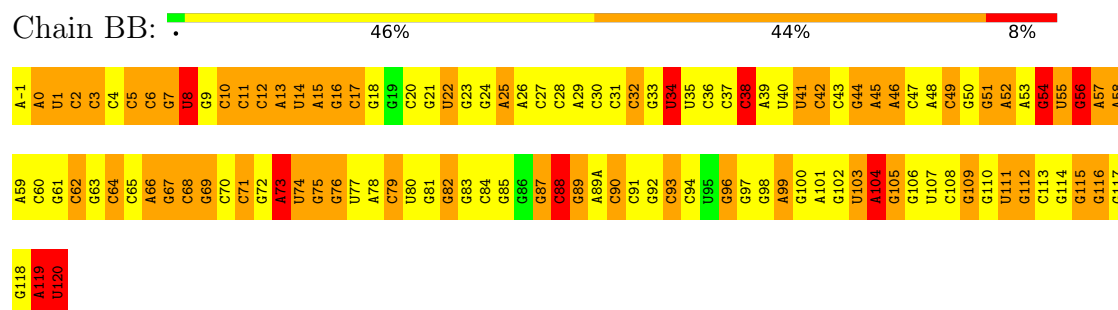
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A1096	G1036	G976	G855	G795	A735	G675	A637	G579	C517	C456	G396	U339
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G1099	G1039	G979	U858	G798	G738	C678	C640	G582	G520	U459	G399	G342
C1100	G1040	G980	G859	G799	G739	C679	C641	G583	C521	A460	G400	C343
U1101	G1041	G981	U860	A800	U740	G680	G642	G584	C522	C461	A401	C344
C1102	G1042	U922	A861	G801	G741	G681	A643	G585	C523	C462	A402	A345
A1103	C1043	C923	G862	A802	G742	G682	A644	G586	U524	U463	U403	A346
C1104	G1044	A984	A863	U803	G743	C683	C645	C587	U525	U464	C404	A347
U1105	A1045	C925	G864	A804	G744	G684	A646	U588	A526	G465	U405	G348
G1106	C986	A926	C865	G805	G745	A685	G647	C589	C527	A466	G406	G349
G1047	G887	G928	A866	C806	A746	G686	G648	A590	A528	C467	G407	U850
U1108	A988	G929	U867	U807	U747	C687	G649	C591	A529	G468	G408	G351
C1109	C1048	U930	U868	G808	G748	U688	C	C592	C530	C469	C409	G352
G1110	A990	G931	G869	G809	C749	A689	C	G593	C531	A470	G410	G353
A1111	A1050	G932	A870	U810	A750	G690	C	U594	A532	A471	G411	G354
G1112	C992	A933	U871	U811	A751	C691	A	C595	G533	A472	A412	G355
U1113	G993	G934	A872	C812	A752	C692	G	G596	U534	G473	C413	G356
G1114	C994	C935	G873	U813	C753	C693	G	U597	C535	G474	C414	A357
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G1117	G1056	G997	G876	C816	C756	G696	C	G600	C539	A477	C417	G360
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C1930	G1861	C1734	A1665	G1606	A1545A	A1486	G1426	A1366	C1306	A1246	G1186
U1931	G1862	C1735	G1666	C1607	C1546	G1487	A1427	A1367	A1307	A1247	G1187
A1932	G1863	G1741	G1667	A1608	C1547	G1488	C1428	G1368	A1308	G1248	U1188
G1933	U1864	C1742	A1668	A1609	C1548	U1489	G1429	G1369	G1309	U1249	A1189
C1934	G1869	G1743	A1669	A1610	U1549	A1490	C1430	C1370	G1310	G1250	G1190
G1935	C1870	G1746	C1670	C1611	C1550	G1491	U1431	G1371	G1311	C1251	G1191
A1936	A1871	G1747	U1671	C1612	C1551	G1492	C1432	U1372	U1312	G1252	G1192
U1937	A1872	G1748	C1672	G1613	G1552	C1493	U1433	A1373	U1313	A1253	G1193
A1938	G1878	A1749	U1673	A1614	A1553	A1494	A1434	G1374	C1314	A1254	A1194
U1939	C1879	G1750	G1674	C1615	A1554	A1495	G1435	C1375	C1315	U1255	G1195
U1940	C1880	C1751	C1675	A1616	G1555	A1496	G1436	C1376	U1316	G1256	C1196
C1941	C1881	G1752	A1676	C1617	C1556	U1497	C1437	G1377	A1317	G1257	G1197
C1942	C1882	G1753	A1677	A1618	C1557	C1498	U1438	A1378	C1318	C1258	U1198
U1943	G1883	C1754	G1678	G1619	A1558	C1499	A1439	A1379	G1319	G1259	U1199
U1944	A1884	A1755	U1679	G1620	G1559	G1500	G1440	G1380	C1320	G1260	C1200
G1945	G1885	G1756	U1680	G1621	G1560	C1501	G1441	G1381	C1321	C1261	C1201
U1946	C1886	U1757	G1681	G1622	U1561	C1502	G1442	G1382	A1322	A1262	C1202
C1947	C1887	G1758	G1682	G1623	A1562	U1503	G1443	C1383	C1323	U1263	G1203
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G1950	A1890	C1761	C1685	G1626	C1565	C1506	G1445	G1386	U1326	G1266	G1206
U1951	G1891	A1762	C1686	G1627	A1566	A1507	G1446	C1387	C1327	U1267	C1207
A1952	C1892	G1763	G1687	G1628	A1567	A1508	G1447	G1388	G1328	A1268	C1208
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U1954	G1894	C1765	A1689	G1630	A1569	A1510	A1449	U1390	U1330	C1270	A1210
U1955	C1895	U1766	A1690	C1630A	A1570	A1511	G1449A	U1391	A1331	G1271	U1211
U1956	G1896	G1767	C1691	A1631	A1572	C1512	C1450	A1392	G1332	A1272	G1212
C1957	U1897	U1768	U1692	C1513	A1573	C1513	C1451	A1393	C1333	U1273	A1213
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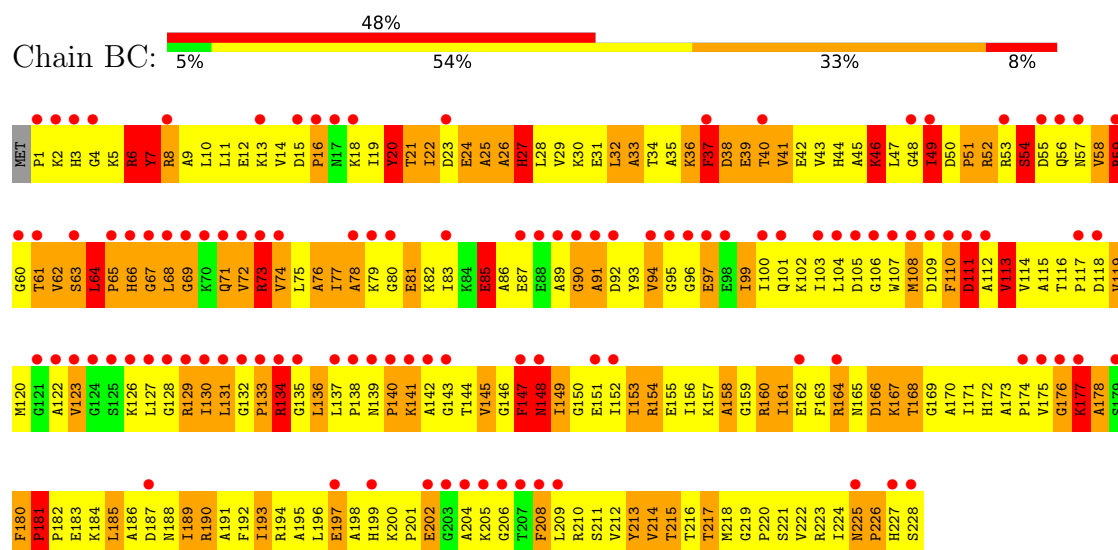
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C2691	G2570	U2611	A2451	G2331	G2271	C2141	G2081	C2021	C1961
C2692	A2571	C2512	G2452	U2332	G2272	C2142	A2082	U2022	C1962
A2693	G2513	G2513	G2453	G2333	U2208	C2143	G2083	G2023	U1963
C2694	G2514	G2454	G2454	G2334	A2274	U2144	G2084	G2024	G1964
C2695	C2515	C2395	G2455	A2335	G2275	C2145	C2085	C2025	C1965
C2696	C2516	G2396	G2456	A2336	G2276	C2146	U2086	C2026	A1966
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C2698	A2518	U2398	G2458	G2338	U2213	G2148	G2088	U2028	G1968
C2699	U2519	U2399	G2459	G2339	G2279	G2149	U2089	G2029	A1969
C2700	G2620	U2460	U2460	G2340	G2280	U2150	G2090	A2030	A1970
C2701	C2521	U2461	U2461	G2341	G2281	G2151	U2091	A2031	A1971
U2702	U2522	U2462	U2462	C2342	G2282	G2152	U2092	G2032	A1972
C2703	G2523	C2463	C2403	U2343	C2283	G2153	G2093	A2033	G1973
C2704	G2524	C2464	C2404	U2344	G2284	G2154	G2094	U2034	C1974
A2705	G2525	C2465	G2405	A2345	C2285	A2225	C2095	G2035	G1975
C2706	G2526	C2466	U2406	A2346	A2286	G2156	U2096	G2036	U1976
G2707	U2527	C2467	G2407	C2347	A2287	G2157	C2097	G2037	A1977
C2708	U2528	G2468	U2408	U2348	A2288	A2158	U2098	G2038	A1978
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C2710	A2530	G2470	G2410	C2350	G2290	G2160	G2100	G2040	G1980
C2711	A2531	C2471	A2411	G2351	U2291	C2161	G2101	U2041	A1981
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C2715	G2536	A2476	A2416	C2356	U2296	G2166	G2106	G2046	A1986
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C2717	C2538	A2478	A2418	G2358	G2298	G2168	C2108	G2048	C1988
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U2720	A2541	G2481	G2421	A2361	C2301	A2171	C2111	A2051	U1991
A2721	A2542	G2482	U2422	G2362	G2302	U2172	G2112	G2052	U1992
G2722	G2543	G2483	U2423	C2363	G2303	A2173	U2113	G2053	U1993
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C2724	G2545	G2485	A2425	G2365	A2305	C2175	G2115	G2055	U1995
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G2727	G2548	A2488	G2428	C2368	G2308	C2178	U2118	A2058	G1998
C2728	G2549	G2489	G2429	A2369	A2309	C2179	A2119	A2059	C1999
U2729	C2550	G2490	A2430	G2370	A2310	U2180	G2120	A2060	G2000
C2730	C2551	U2491	U2431	G2371	A2311	G2181	G2121	G2061	A2001
C2731	U2552	U2492	A2432	G2372	U2312	G2182	U2122	A2062	G2002
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A2734	U2555	G2495	A2435	G2375	G2315	C2185	G2125	C2065	A2005
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U2736	G2557	A2497	G2437	U2377	U2257	G2187	G2127	G2067	C2007
C2737	C2558	U2498	U2438	A2378	C2258	C2188	C2128	U2068	C2008
C2738	C2559	C2499	A2439	G2379	G2259	U2189	C2129	G2069	G2009
C2739	U2560	U2500	C2440	C2380	A2320	G2190	U2130	G2070	G2010
A2740	A2561	C2501	C2441	C2381	G2261	G2191	A2071	A2071	U2011
C2741	U2562	G2502	C2442	G2382	U2262	G2192	U2132	G2072	G2012
C2742	U2563	A2503	C2443	G2383	G2323	G2193	G2133	A2073	A2013
C2743	G2564	U2504	G2444	G2384	C2264	G2194	A2134	U2074	C2014
C2744	A2565	G2505	G2445	C2385	G2265	C2195	A2135	U2075	A2015
C2745	A2566	U2506	G2446	C2386	A2266	C2196	U2076	U2076	U2016
U2746	G2567	G2507	G2447	U2387	A2267	U2197	C2137	A2077	U2017
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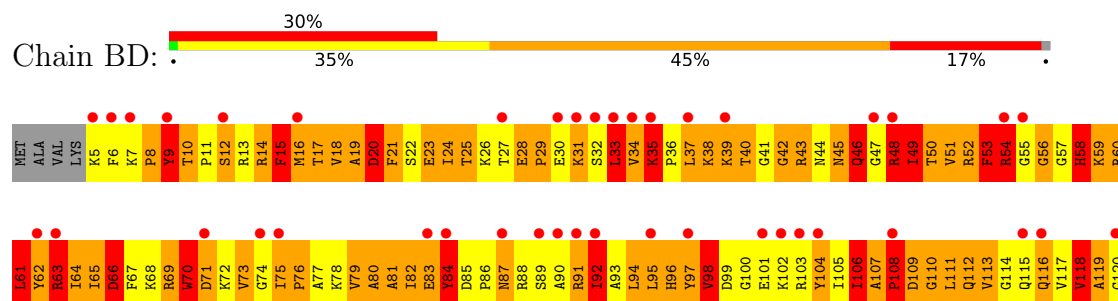
• Molecule 25: 5S ribosomal RNA

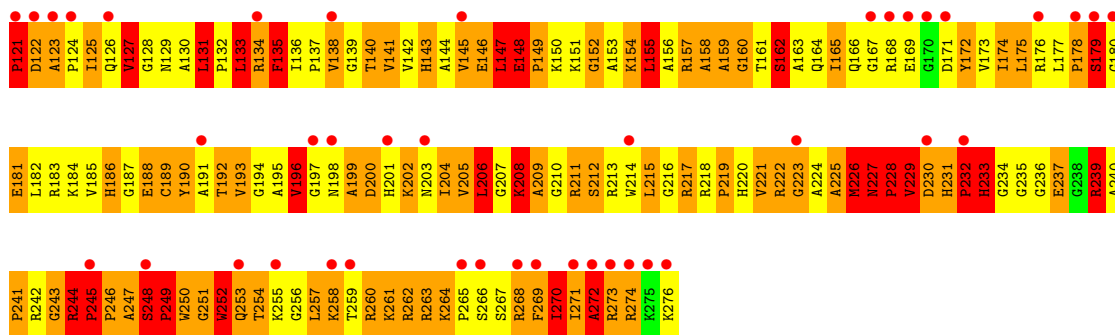


• Molecule 26: 50S ribosomal protein L1

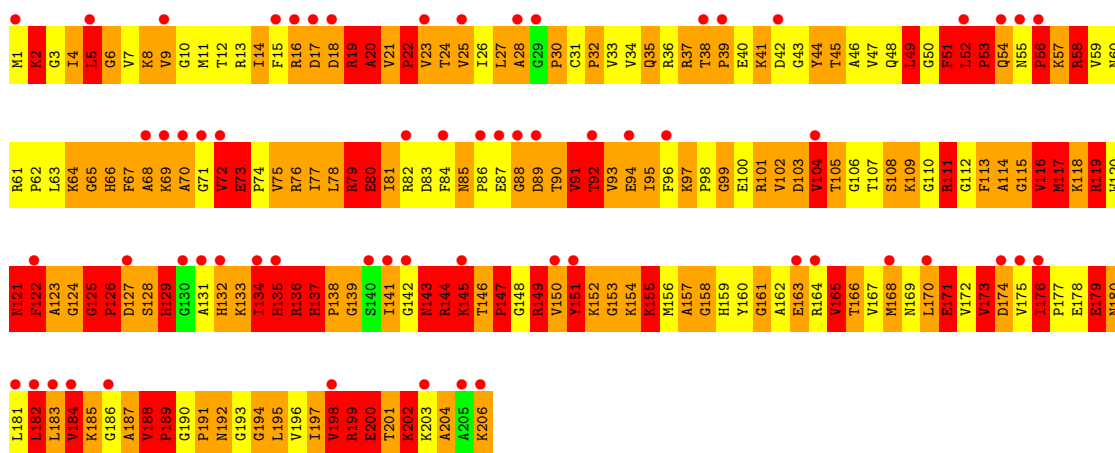


• Molecule 27: 50S ribosomal protein L2

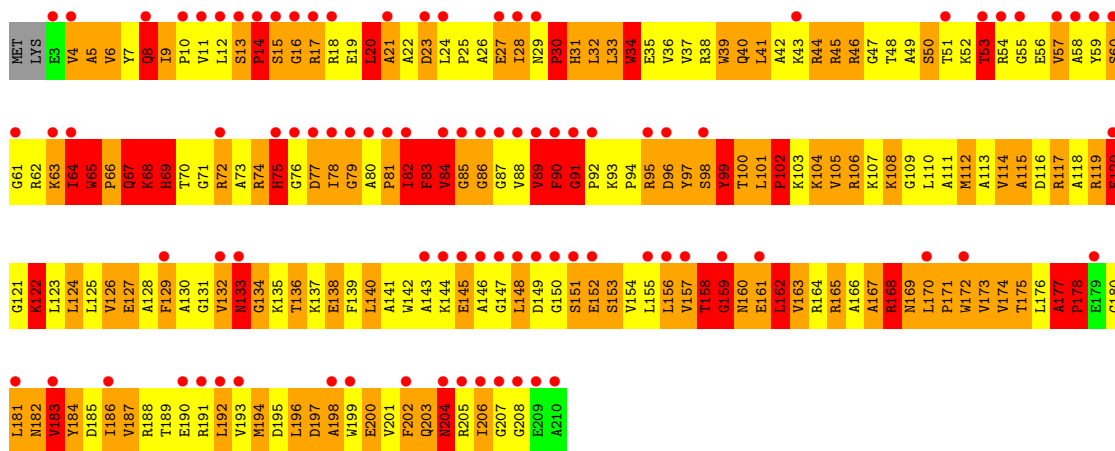
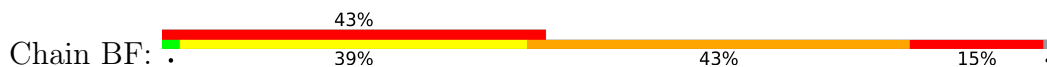




• Molecule 28: 50S ribosomal protein L3

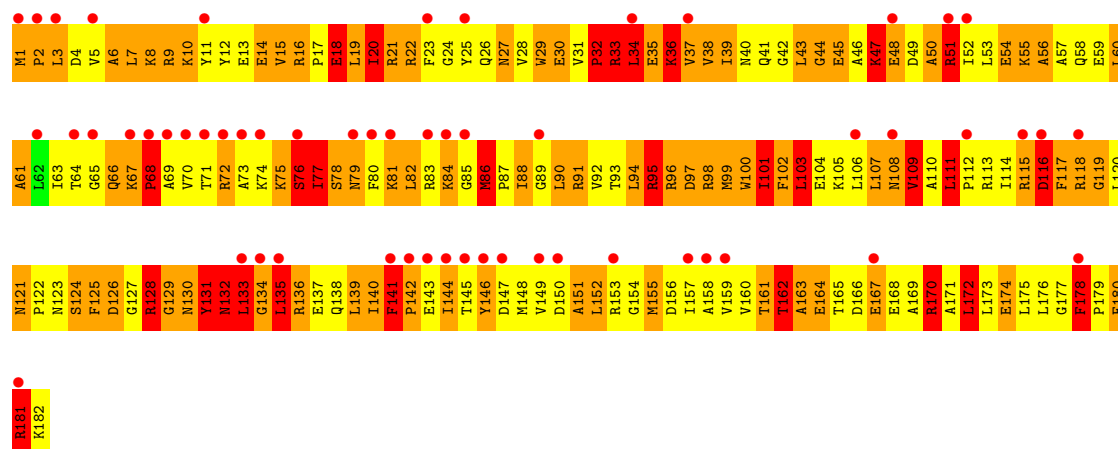


• Molecule 29: 50S ribosomal protein L4

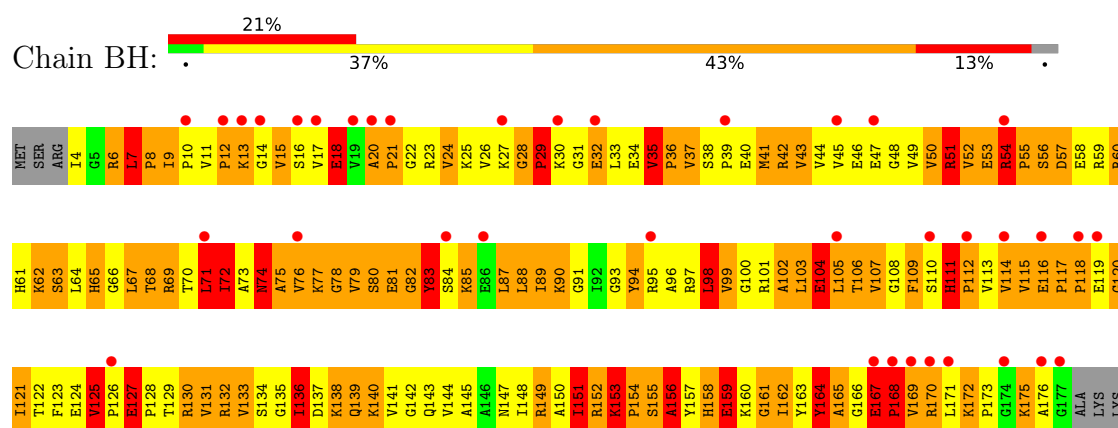


• Molecule 30: 50S ribosomal protein L5

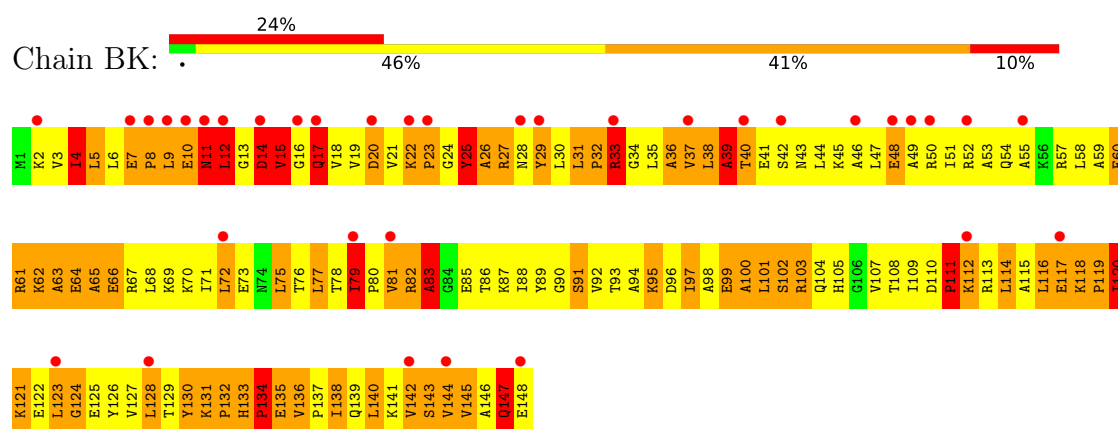




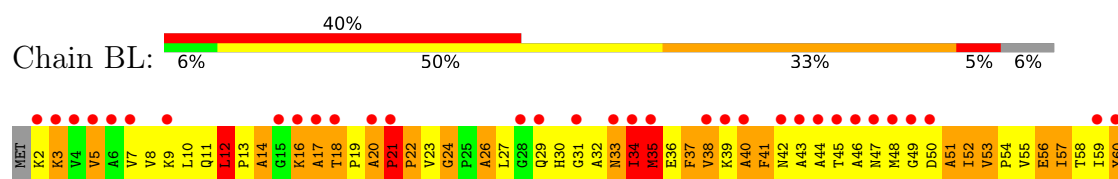
• Molecule 31: 50S ribosomal protein L6

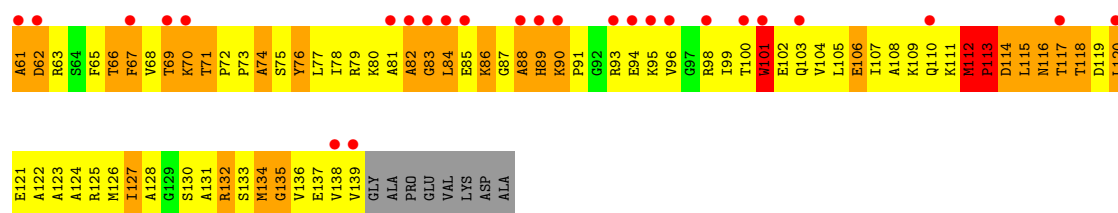


• Molecule 32: 50S ribosomal protein L9

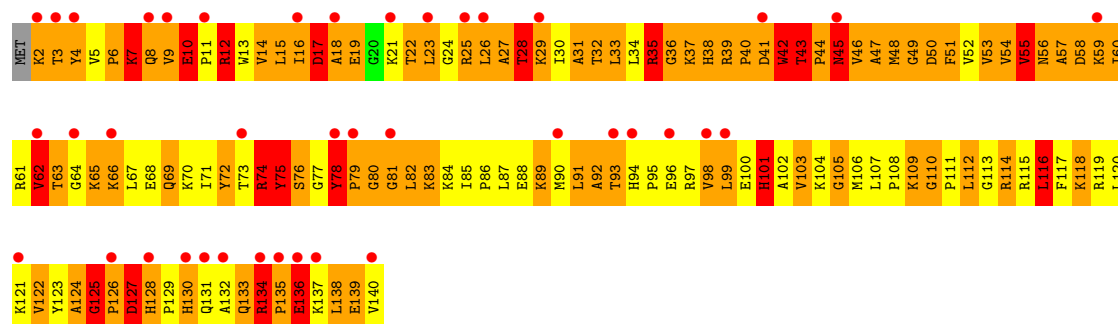


• Molecule 33: 50S ribosomal protein L11

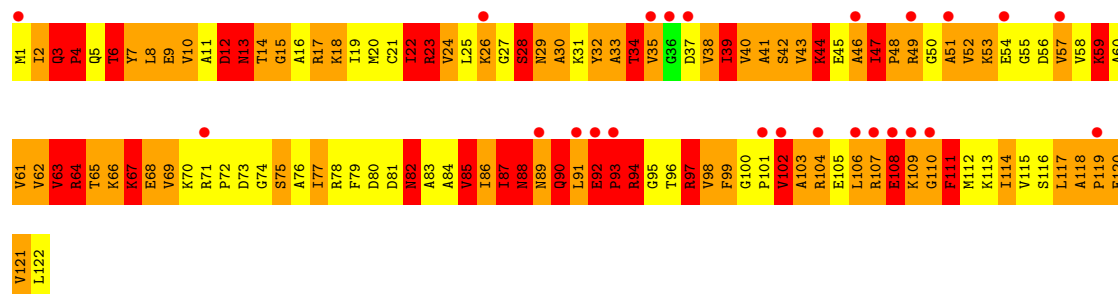




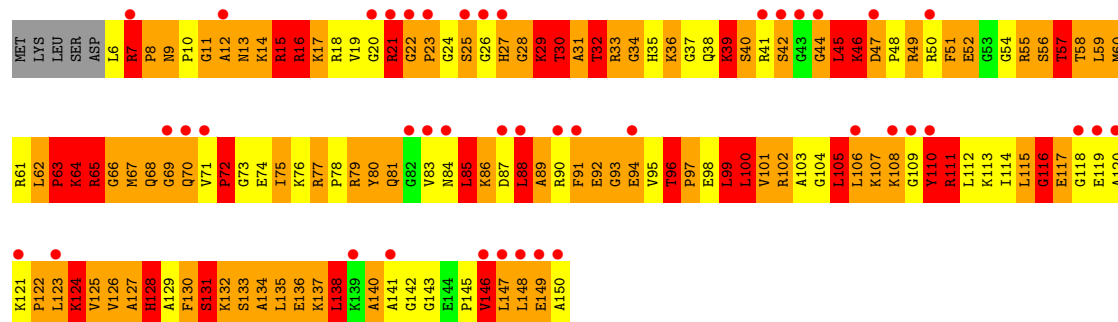
• Molecule 34: 50S ribosomal protein L13



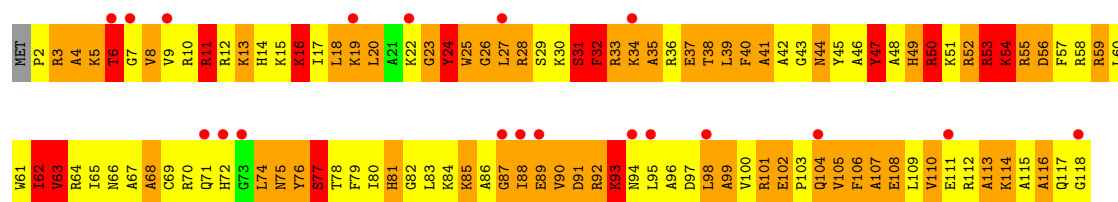
• Molecule 35: 50S ribosomal protein L14



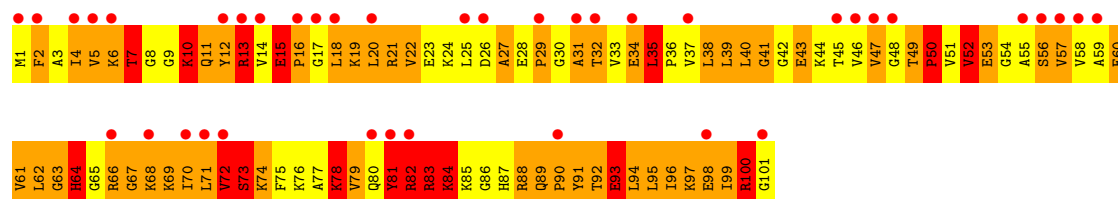
• Molecule 36: 50S ribosomal protein L15



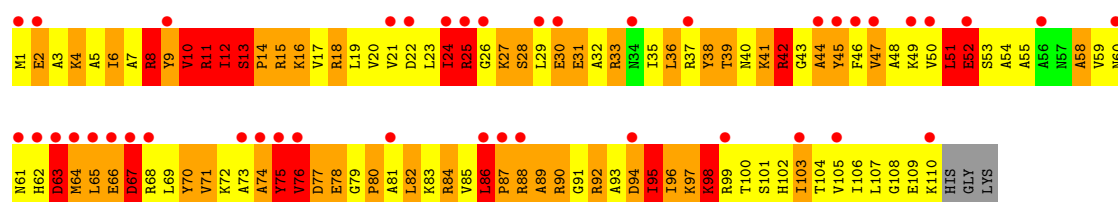
• Molecule 37: 50S ribosomal protein L16



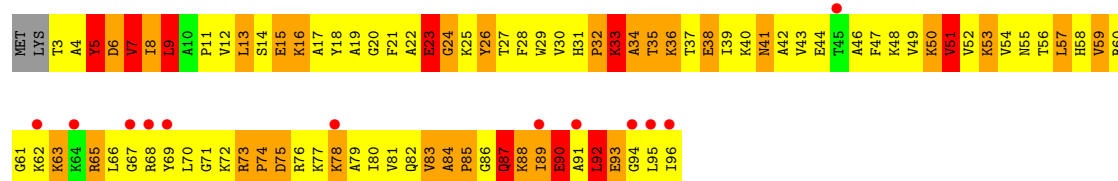
• Molecule 42: 50S ribosomal protein L21



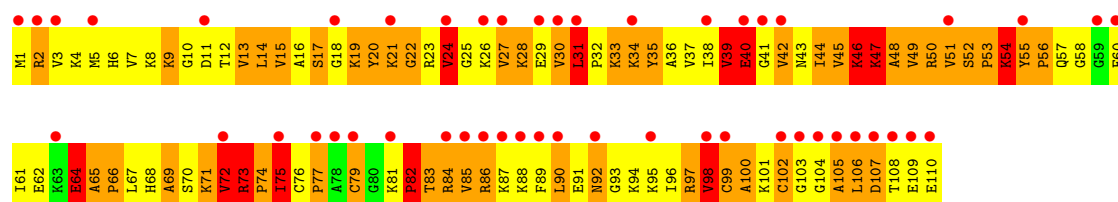
• Molecule 43: 50S ribosomal protein L22



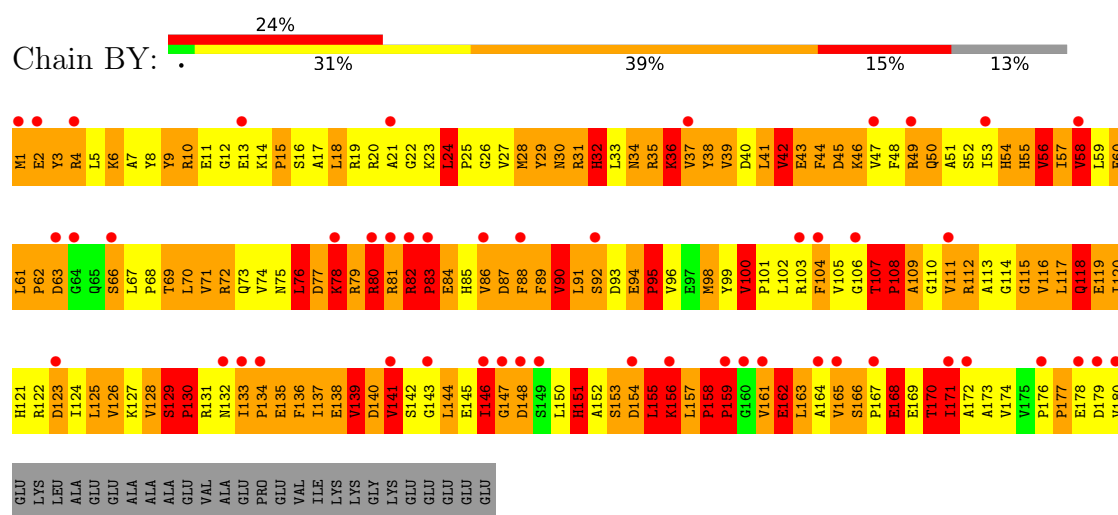
• Molecule 44: 50S ribosomal protein L23



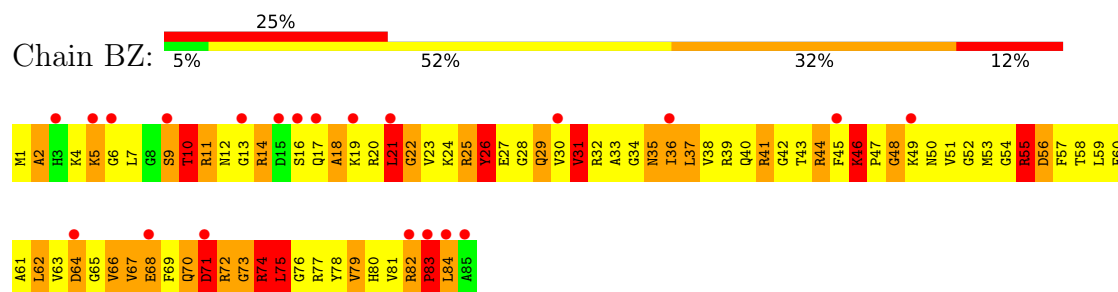
• Molecule 45: 50S ribosomal protein L24



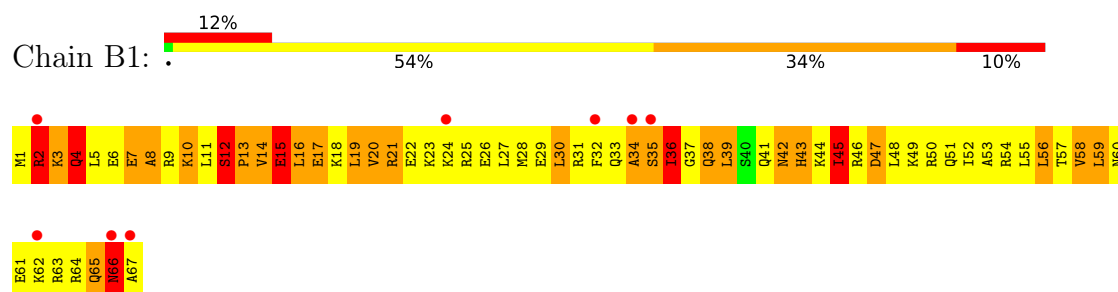
• Molecule 46: 50S ribosomal protein L25



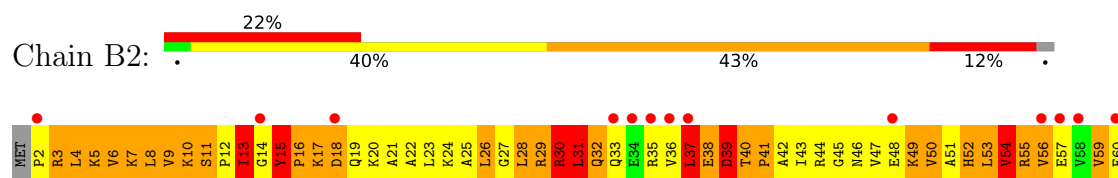
• Molecule 47: 50S ribosomal protein L27



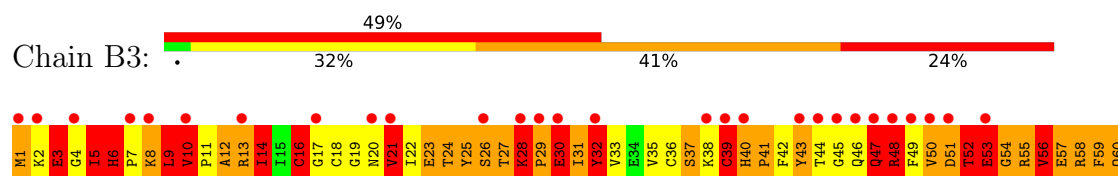
• Molecule 48: 50S ribosomal protein L29



• Molecule 49: 50S ribosomal protein L30



• Molecule 50: 50S ribosomal protein L31

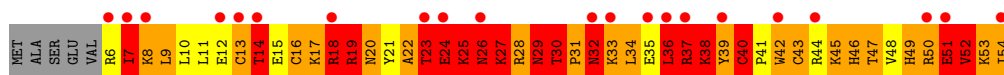
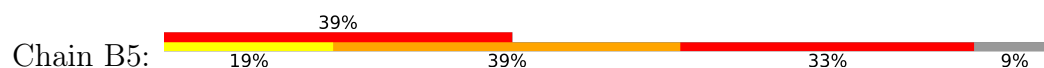




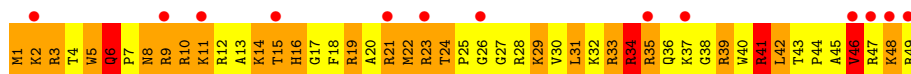
- Molecule 51: 50S ribosomal protein L32



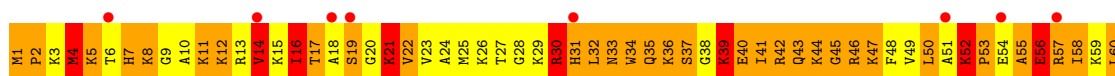
- Molecule 52: 50S ribosomal protein L33



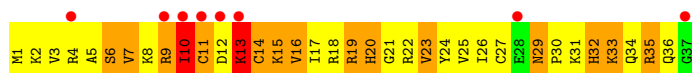
- Molecule 53: 50S ribosomal protein L34



- Molecule 54: 50S ribosomal protein L35



- Molecule 55: 50S ribosomal protein L36



4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	509.52Å 509.52Å 804.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	300.00 – 5.00 300.00 – 5.00	Depositor EDS
% Data completeness (in resolution range)	93.9 (300.00-5.00) 97.3 (300.00-5.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.09 (at 4.88Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.263 , 0.323 0.250 , 0.303	Depositor DCC
R_{free} test set	10840 reflections (4.30%)	wwPDB-VP
Wilson B-factor (Å ²)	99.7	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.08 , 0.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.55$, $\langle L^2 \rangle = 0.39$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	149044	wwPDB-VP
Average B, all atoms (Å ²)	167.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.30% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	AA	0.63	5/36438 (0.0%)	1.02	142/56869 (0.2%)
2	AC	0.67	0/1814	1.02	8/2825 (0.3%)
3	AD	0.55	0/1813	0.96	7/2823 (0.2%)
4	AE	0.87	0/1935	1.54	38/2609 (1.5%)
5	AF	0.74	1/1636 (0.1%)	1.43	29/2205 (1.3%)
6	AG	0.93	3/1733 (0.2%)	1.63	41/2318 (1.8%)
7	AH	0.96	1/1162 (0.1%)	1.55	25/1564 (1.6%)
8	AI	0.88	1/856 (0.1%)	1.36	12/1154 (1.0%)
9	AJ	0.82	0/1276	1.33	22/1709 (1.3%)
10	AK	0.90	1/1136 (0.1%)	1.47	23/1527 (1.5%)
11	AL	0.75	1/1029 (0.1%)	1.20	10/1379 (0.7%)
12	AM	0.69	0/807	1.34	13/1085 (1.2%)
13	AN	0.99	1/900 (0.1%)	1.61	16/1213 (1.3%)
14	AO	0.84	0/986	1.63	26/1320 (2.0%)
15	AP	0.74	0/1008	1.36	16/1347 (1.2%)
16	AQ	0.74	0/501	1.51	11/664 (1.7%)
17	AR	0.94	0/745	1.34	8/992 (0.8%)
18	AS	0.93	0/716	1.54	18/963 (1.9%)
19	AT	1.01	4/870 (0.5%)	1.46	18/1159 (1.6%)
20	AU	0.88	0/603	1.56	13/799 (1.6%)
21	AV	0.76	0/661	1.28	8/890 (0.9%)
22	AW	1.10	0/765	1.42	9/1007 (0.9%)
23	AX	0.66	0/212	1.36	2/277 (0.7%)
24	BA	0.71	24/69685 (0.0%)	1.11	483/108786 (0.4%)
25	BB	0.58	0/2954	1.01	12/4606 (0.3%)
26	BC	0.72	0/1775	1.34	34/2393 (1.4%)
27	BD	1.08	3/2174 (0.1%)	1.78	59/2927 (2.0%)
28	BE	1.19	9/1611 (0.6%)	1.88	73/2171 (3.4%)
29	BF	0.92	0/1660	1.67	45/2247 (2.0%)
30	BG	0.85	0/1507	1.55	45/2027 (2.2%)
31	BH	0.88	1/1354 (0.1%)	1.60	41/1831 (2.2%)
32	BK	0.97	1/1170 (0.1%)	1.61	38/1581 (2.4%)
33	BL	0.74	0/1044	1.44	21/1415 (1.5%)
34	BM	1.06	0/1140	1.73	45/1537 (2.9%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
35	BN	1.32	4/942 (0.4%)	2.22	48/1268 (3.8%)
36	BO	1.10	5/1123 (0.4%)	1.81	40/1493 (2.7%)
37	BP	1.14	3/1100 (0.3%)	1.84	42/1470 (2.9%)
38	BQ	0.95	0/974	1.56	11/1302 (0.8%)
39	BR	1.05	0/887	1.68	21/1180 (1.8%)
40	BS	1.27	4/990 (0.4%)	2.00	42/1325 (3.2%)
41	BT	1.07	1/982 (0.1%)	1.61	25/1306 (1.9%)
42	BU	1.18	1/790 (0.1%)	2.21	36/1057 (3.4%)
43	BV	0.97	0/886	1.58	20/1189 (1.7%)
44	BW	0.76	0/756	1.32	6/1015 (0.6%)
45	BX	0.76	0/857	1.60	22/1142 (1.9%)
46	BY	0.94	0/1467	1.81	54/1992 (2.7%)
47	BZ	0.97	0/679	1.61	14/902 (1.6%)
48	B1	0.88	0/569	1.27	8/751 (1.1%)
49	B2	0.88	1/474 (0.2%)	1.67	11/635 (1.7%)
50	B3	1.23	3/594 (0.5%)	1.86	20/795 (2.5%)
51	B4	1.06	1/459 (0.2%)	1.66	16/621 (2.6%)
52	B5	1.18	2/433 (0.5%)	2.21	30/576 (5.2%)
53	B6	1.09	0/438	1.30	4/575 (0.7%)
54	B7	0.98	1/523 (0.2%)	1.79	18/690 (2.6%)
55	B8	0.95	0/310	1.71	5/407 (1.2%)
All	All	0.77	82/161909 (0.1%)	1.25	1904/241910 (0.8%)

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	AA	0	217
2	AC	0	13
3	AD	0	7
5	AF	0	1
10	AK	0	1
13	AN	0	1
24	BA	0	546
25	BB	0	16
27	BD	0	2
28	BE	0	1
29	BF	0	1
31	BH	0	1
37	BP	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
40	BS	0	2
42	BU	0	2
43	BV	0	1
44	BW	0	1
50	B3	0	2
All	All	0	818

The worst 5 of 82 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	BA	1203	G	O3'-P	-27.76	1.19	1.61
24	BA	2501	C	O3'-P	19.68	1.90	1.61
1	AA	173	U	O3'-P	15.95	1.85	1.61
24	BA	2499	C	O3'-P	-15.17	1.38	1.61
24	BA	607	U	N3-C4	-14.22	1.10	1.38

The worst 5 of 1904 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	BU	49	THR	CA-C-N	23.79	149.58	119.84
42	BU	49	THR	C-N-CA	23.79	149.58	119.84
24	BA	1203	G	P-O3'-C3'	21.86	153.00	120.20
24	BA	2501	C	O3'-P-O5'	-21.82	71.28	104.00
1	AA	1064	G	N1-C2-N2	-21.21	52.57	116.20

There are no chirality outliers.

5 of 818 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	12	U	Sidechain
1	AA	21	G	Sidechain
1	AA	24	U	Sidechain
1	AA	6	G	Sidechain
1	AA	7	G	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	AA	32554	0	16429	6474	0
2	AC	1624	0	826	364	0
3	AD	1623	0	821	382	0
4	AE	1900	0	1951	984	0
5	AF	1612	0	1677	714	0
6	AG	1703	0	1763	827	0
7	AH	1146	0	1207	509	0
8	AI	843	0	857	387	0
9	AJ	1257	0	1296	579	0
10	AK	1116	0	1177	662	0
11	AL	1010	0	1037	468	0
12	AM	794	0	840	375	0
13	AN	885	0	904	423	0
14	AO	970	0	1057	451	0
15	AP	997	0	1072	521	0
16	AQ	492	0	529	260	0
17	AR	734	0	771	313	0
18	AS	700	0	720	316	0
19	AT	857	0	930	429	0
20	AU	597	0	668	346	0
21	AV	647	0	673	307	0
22	AW	763	0	861	368	0
23	AX	208	0	221	83	0
24	BA	62218	0	31353	15023	0
25	BB	2641	0	1337	587	1
26	BC	1742	0	1796	869	0
27	BD	2124	0	2207	1560	0
28	BE	1578	0	1647	1104	0
29	BF	1625	0	1666	916	0
30	BG	1482	0	1546	1001	0
31	BH	1328	0	1408	754	0
32	BK	1155	0	1244	565	0
33	BL	1025	0	1074	511	0
34	BM	1113	0	1183	795	0
35	BN	932	0	994	705	0
36	BO	1106	0	1183	846	0
37	BP	1080	0	1127	725	0
38	BQ	960	0	1021	520	0
39	BR	877	0	938	602	0
40	BS	976	0	1033	682	0
41	BT	964	0	1022	683	0
42	BU	779	0	852	590	0
43	BV	876	0	941	459	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	BW	742	0	800	388	0
45	BX	844	0	930	516	0
46	BY	1435	0	1463	749	0
47	BZ	670	0	700	380	0
48	B1	567	0	621	329	0
49	B2	469	0	518	308	0
50	B3	581	0	577	373	0
51	B4	445	0	459	303	0
52	B5	426	0	452	300	0
53	B6	430	0	480	273	0
54	B7	515	0	587	397	0
55	B8	307	0	335	150	0
All	All	149044	0	101781	46212	1

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 185.

The worst 5 of 46212 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)
46:BY:27:VAL:HG23	46:BY:85:HIS:CE1	1.45	1.50
46:BY:27:VAL:CG2	46:BY:85:HIS:CE1	1.95	1.45
35:BN:64:ARG:HH11	35:BN:68:GLU:N	1.15	1.44
24:BA:775:G:H2'	24:BA:794:G:C8	1.54	1.42
24:BA:1201:C:N4	24:BA:1241:A:H61	1.15	1.39

All (1) 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	Interatomic distance (Å)	Clash overlap (Å)
25:BB:-1:A:O2'	25:BB:-1:A:O2'[15_545]	2.14	0.06

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	
4	AE	232/256 (91%)	119 (51%)	48 (21%)	65 (28%)	0	0
5	AF	204/239 (85%)	117 (57%)	41 (20%)	46 (22%)	0	1
6	AG	206/209 (99%)	99 (48%)	52 (25%)	55 (27%)	0	0
7	AH	148/162 (91%)	89 (60%)	26 (18%)	33 (22%)	0	1
8	AI	99/101 (98%)	62 (63%)	14 (14%)	23 (23%)	0	1
9	AJ	153/156 (98%)	65 (42%)	45 (29%)	43 (28%)	0	0
10	AK	136/138 (99%)	71 (52%)	28 (21%)	37 (27%)	0	0
11	AL	125/128 (98%)	57 (46%)	38 (30%)	30 (24%)	0	1
12	AM	96/105 (91%)	53 (55%)	21 (22%)	22 (23%)	0	1
13	AN	117/129 (91%)	63 (54%)	28 (24%)	26 (22%)	0	1
14	AO	122/132 (92%)	60 (49%)	29 (24%)	33 (27%)	0	0
15	AP	123/126 (98%)	64 (52%)	33 (27%)	26 (21%)	0	1
16	AQ	58/61 (95%)	24 (41%)	16 (28%)	18 (31%)	0	0
17	AR	86/89 (97%)	43 (50%)	26 (30%)	17 (20%)	0	1
18	AS	81/88 (92%)	46 (57%)	22 (27%)	13 (16%)	0	3
19	AT	102/105 (97%)	63 (62%)	20 (20%)	19 (19%)	0	2
20	AU	71/88 (81%)	29 (41%)	23 (32%)	19 (27%)	0	0
21	AV	78/93 (84%)	32 (41%)	24 (31%)	22 (28%)	0	0
22	AW	97/106 (92%)	31 (32%)	43 (44%)	23 (24%)	0	1
23	AX	22/27 (82%)	11 (50%)	5 (23%)	6 (27%)	0	0
26	BC	226/229 (99%)	110 (49%)	62 (27%)	54 (24%)	0	1
27	BD	270/276 (98%)	110 (41%)	66 (24%)	94 (35%)	0	0
28	BE	204/206 (99%)	108 (53%)	40 (20%)	56 (28%)	0	0
29	BF	206/210 (98%)	106 (52%)	45 (22%)	55 (27%)	0	0
30	BG	180/182 (99%)	71 (39%)	52 (29%)	57 (32%)	0	0
31	BH	172/180 (96%)	75 (44%)	50 (29%)	47 (27%)	0	0
32	BK	146/148 (99%)	85 (58%)	36 (25%)	25 (17%)	0	2
33	BL	136/147 (92%)	68 (50%)	38 (28%)	30 (22%)	0	1
34	BM	137/140 (98%)	63 (46%)	28 (20%)	46 (34%)	0	0
35	BN	120/122 (98%)	60 (50%)	24 (20%)	36 (30%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	BO	143/150 (95%)	52 (36%)	40 (28%)	51 (36%)	0	0
37	BP	134/141 (95%)	53 (40%)	36 (27%)	45 (34%)	0	0
38	BQ	115/118 (98%)	60 (52%)	37 (32%)	18 (16%)	0	3
39	BR	108/112 (96%)	43 (40%)	35 (32%)	30 (28%)	0	0
40	BS	115/146 (79%)	55 (48%)	27 (24%)	33 (29%)	0	0
41	BT	115/118 (98%)	46 (40%)	40 (35%)	29 (25%)	0	1
42	BU	99/101 (98%)	53 (54%)	19 (19%)	27 (27%)	0	0
43	BV	108/113 (96%)	64 (59%)	20 (18%)	24 (22%)	0	1
44	BW	92/96 (96%)	53 (58%)	18 (20%)	21 (23%)	0	1
45	BX	108/110 (98%)	39 (36%)	34 (32%)	35 (32%)	0	0
46	BY	178/206 (86%)	85 (48%)	50 (28%)	43 (24%)	0	1
47	BZ	83/85 (98%)	48 (58%)	20 (24%)	15 (18%)	0	2
48	B1	65/67 (97%)	30 (46%)	20 (31%)	15 (23%)	0	1
49	B2	57/60 (95%)	33 (58%)	12 (21%)	12 (21%)	0	1
50	B3	69/71 (97%)	20 (29%)	23 (33%)	26 (38%)	0	0
51	B4	55/60 (92%)	14 (26%)	22 (40%)	19 (34%)	0	0
52	B5	47/54 (87%)	15 (32%)	8 (17%)	24 (51%)	0	0
53	B6	47/49 (96%)	18 (38%)	14 (30%)	15 (32%)	0	0
54	B7	62/65 (95%)	23 (37%)	18 (29%)	21 (34%)	0	0
55	B8	35/37 (95%)	21 (60%)	6 (17%)	8 (23%)	0	1
All	All	5988/6337 (94%)	2879 (48%)	1522 (25%)	1587 (26%)	0	0

5 of 1587 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	AE	13	ALA
4	AE	15	VAL
4	AE	17	PHE
4	AE	20	GLU
4	AE	42	ILE

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	
4	AE	202/220 (92%)	140 (69%)	62 (31%)	0	2
5	AF	160/188 (85%)	118 (74%)	42 (26%)	0	3
6	AG	180/181 (99%)	129 (72%)	51 (28%)	0	3
7	AH	115/123 (94%)	69 (60%)	46 (40%)	0	1
8	AI	90/90 (100%)	58 (64%)	32 (36%)	0	1
9	AJ	126/127 (99%)	95 (75%)	31 (25%)	1	4
10	AK	119/119 (100%)	73 (61%)	46 (39%)	0	1
11	AL	98/99 (99%)	75 (76%)	23 (24%)	1	5
12	AM	88/92 (96%)	60 (68%)	28 (32%)	0	2
13	AN	90/99 (91%)	66 (73%)	24 (27%)	0	3
14	AO	104/109 (95%)	75 (72%)	29 (28%)	0	3
15	AP	100/101 (99%)	72 (72%)	28 (28%)	0	3
16	AQ	49/50 (98%)	37 (76%)	12 (24%)	1	4
17	AR	79/80 (99%)	55 (70%)	24 (30%)	0	2
18	AS	72/74 (97%)	50 (69%)	22 (31%)	0	2
19	AT	96/97 (99%)	70 (73%)	26 (27%)	0	3
20	AU	64/77 (83%)	49 (77%)	15 (23%)	1	5
21	AV	71/80 (89%)	58 (82%)	13 (18%)	2	9
22	AW	76/82 (93%)	52 (68%)	24 (32%)	0	2
23	AX	19/22 (86%)	15 (79%)	4 (21%)	1	6
26	BC	180/181 (99%)	146 (81%)	34 (19%)	1	9
27	BD	215/218 (99%)	142 (66%)	73 (34%)	0	2
28	BE	166/166 (100%)	90 (54%)	76 (46%)	0	0
29	BF	164/166 (99%)	97 (59%)	67 (41%)	0	0
30	BG	156/156 (100%)	107 (69%)	49 (31%)	0	2
31	BH	143/148 (97%)	90 (63%)	53 (37%)	0	1
32	BK	124/124 (100%)	89 (72%)	35 (28%)	0	3
33	BL	105/111 (95%)	87 (83%)	18 (17%)	2	11
34	BM	118/119 (99%)	80 (68%)	38 (32%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	BN	100/100 (100%)	58 (58%)	42 (42%)	0	0
36	BO	111/116 (96%)	64 (58%)	47 (42%)	0	0
37	BP	106/111 (96%)	64 (60%)	42 (40%)	0	1
38	BQ	100/101 (99%)	69 (69%)	31 (31%)	0	2
39	BR	87/88 (99%)	59 (68%)	28 (32%)	0	2
40	BS	105/127 (83%)	69 (66%)	36 (34%)	0	2
41	BT	93/94 (99%)	64 (69%)	29 (31%)	0	2
42	BU	82/82 (100%)	56 (68%)	26 (32%)	0	2
43	BV	90/92 (98%)	52 (58%)	38 (42%)	0	0
44	BW	76/78 (97%)	56 (74%)	20 (26%)	0	3
45	BX	91/91 (100%)	70 (77%)	21 (23%)	1	5
46	BY	159/179 (89%)	99 (62%)	60 (38%)	0	1
47	BZ	67/67 (100%)	46 (69%)	21 (31%)	0	2
48	B1	62/62 (100%)	45 (73%)	17 (27%)	0	3
49	B2	51/52 (98%)	32 (63%)	19 (37%)	0	1
50	B3	63/63 (100%)	43 (68%)	20 (32%)	0	2
51	B4	50/52 (96%)	34 (68%)	16 (32%)	0	2
52	B5	48/52 (92%)	33 (69%)	15 (31%)	0	2
53	B6	42/42 (100%)	29 (69%)	13 (31%)	0	2
54	B7	54/55 (98%)	36 (67%)	18 (33%)	0	2
55	B8	34/34 (100%)	26 (76%)	8 (24%)	1	5
All	All	5040/5237 (96%)	3448 (68%)	1592 (32%)	0	2

5 of 1592 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
31	BH	152	ARG
37	BP	111	GLU
32	BK	91	SER
31	BH	151	ILE
35	BN	39	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 197 such sidechains are listed below:

Mol	Chain	Res	Type
32	BK	28	ASN
38	BQ	31	HIS
33	BL	11	GLN
35	BN	89	ASN
40	BS	104	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1515/1522 (99%)	431 (28%)	157 (10%)
2	AC	75/77 (97%)	29 (38%)	6 (8%)
24	BA	2888/2916 (99%)	1223 (42%)	266 (9%)
25	BB	122/123 (99%)	49 (40%)	4 (3%)
3	AD	75/76 (98%)	27 (36%)	4 (5%)
All	All	4675/4714 (99%)	1759 (37%)	437 (9%)

5 of 1759 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	6	G
1	AA	8	A
1	AA	9	G
1	AA	13	U
1	AA	14	U

5 of 437 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
24	BA	686	G
24	BA	1241	A
24	BA	2468	G
24	BA	745	G
24	BA	945	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
24	BA	4
1	AA	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	BA	2501:C	O3'	2502:G	P	1.90
1	AA	173:U	O3'	174:C	P	1.85
1	BA	2446:G	O3'	2447:G	P	1.40
1	BA	2499:C	O3'	2500:U	P	1.38
1	BA	1203:G	O3'	1204:A	P	1.19

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	AA	1515/1522 (99%)	0.11	28 (1%) 67 55	88, 158, 260, 350	0
2	AC	76/77 (98%)	0.88	7 (9%) 14 19	133, 166, 216, 249	0
3	AD	76/76 (100%)	1.68	21 (27%) 1 6	219, 265, 316, 334	0
4	AE	234/256 (91%)	0.76	24 (10%) 12 17	122, 163, 221, 265	0
5	AF	206/239 (86%)	2.08	86 (41%) 0 3	143, 182, 210, 228	0
6	AG	208/209 (99%)	1.53	65 (31%) 1 5	106, 148, 170, 187	0
7	AH	150/162 (92%)	1.48	46 (30%) 1 5	114, 139, 171, 200	0
8	AI	101/101 (100%)	2.49	51 (50%) 0 2	121, 150, 168, 203	0
9	AJ	155/156 (99%)	1.30	39 (25%) 1 6	155, 180, 208, 214	0
10	AK	138/138 (100%)	0.82	17 (12%) 8 13	113, 133, 153, 160	0
11	AL	127/128 (99%)	0.85	18 (14%) 6 12	161, 225, 247, 255	0
12	AM	98/105 (93%)	1.07	16 (16%) 4 10	146, 208, 237, 240	0
13	AN	119/129 (92%)	1.58	36 (30%) 1 5	114, 142, 176, 206	0
14	AO	124/132 (93%)	1.40	28 (22%) 2 7	96, 129, 162, 184	0
15	AP	125/126 (99%)	1.52	35 (28%) 1 5	167, 194, 223, 230	0
16	AQ	60/61 (98%)	1.07	12 (20%) 3 8	163, 188, 203, 206	0
17	AR	88/89 (98%)	1.07	16 (18%) 3 9	113, 131, 168, 183	0
18	AS	83/88 (94%)	0.74	8 (9%) 13 18	104, 128, 155, 185	0
19	AT	104/105 (99%)	0.97	15 (14%) 6 12	98, 126, 169, 214	0
20	AU	73/88 (82%)	1.80	27 (36%) 1 4	109, 136, 190, 224	0
21	AV	80/93 (86%)	1.43	25 (31%) 1 5	175, 198, 217, 222	0
22	AW	99/106 (93%)	1.19	18 (18%) 3 9	105, 134, 163, 166	0
23	AX	24/27 (88%)	0.17	0 100 100	168, 210, 224, 229	0
24	BA	2889/2916 (99%)	0.50	168 (5%) 29 30	63, 155, 266, 322	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	BB	123/123 (100%)	-0.06	0 100 100	146, 209, 257, 291	0
26	BC	228/229 (99%)	2.30	109 (47%) 0 2	220, 256, 308, 312	0
27	BD	272/276 (98%)	1.81	83 (30%) 1 5	80, 125, 153, 198	0
28	BE	206/206 (100%)	1.45	62 (30%) 1 5	69, 117, 172, 224	0
29	BF	208/210 (99%)	2.03	90 (43%) 0 3	111, 179, 215, 231	0
30	BG	182/182 (100%)	1.41	56 (30%) 1 5	160, 198, 226, 240	0
31	BH	174/180 (96%)	1.15	37 (21%) 2 7	146, 186, 216, 238	0
32	BK	148/148 (100%)	1.29	35 (23%) 2 6	135, 161, 188, 190	0
33	BL	138/147 (93%)	1.85	59 (42%) 0 3	277, 307, 330, 334	0
34	BM	139/140 (99%)	1.53	40 (28%) 1 5	107, 133, 167, 183	0
35	BN	122/122 (100%)	1.29	24 (19%) 3 8	78, 106, 140, 154	0
36	BO	145/150 (96%)	1.44	42 (28%) 1 5	106, 190, 227, 239	0
37	BP	136/141 (96%)	1.68	49 (36%) 1 4	109, 141, 173, 186	0
38	BQ	117/118 (99%)	0.75	8 (6%) 23 26	91, 124, 157, 173	0
39	BR	110/112 (98%)	0.57	11 (10%) 12 18	152, 183, 210, 248	0
40	BS	117/146 (80%)	1.42	32 (27%) 1 6	83, 127, 165, 184	0
41	BT	117/118 (99%)	1.01	19 (16%) 4 10	100, 138, 152, 158	0
42	BU	101/101 (100%)	1.74	39 (38%) 1 3	104, 160, 186, 197	0
43	BV	110/113 (97%)	1.91	42 (38%) 1 4	110, 143, 179, 195	0
44	BW	94/96 (97%)	1.02	12 (12%) 7 13	153, 170, 232, 237	0
45	BX	110/110 (100%)	1.93	49 (44%) 0 3	157, 199, 247, 273	0
46	BY	180/206 (87%)	1.33	49 (27%) 1 6	142, 190, 211, 226	0
47	BZ	85/85 (100%)	1.16	21 (24%) 2 6	139, 166, 181, 197	0
48	B1	67/67 (100%)	0.84	8 (11%) 9 14	172, 186, 199, 209	0
49	B2	59/60 (98%)	1.30	13 (22%) 2 7	127, 163, 188, 202	0
50	B3	71/71 (100%)	2.40	35 (49%) 0 2	127, 160, 176, 185	0
51	B4	57/60 (95%)	1.83	22 (38%) 1 3	96, 147, 217, 241	0
52	B5	49/54 (90%)	1.96	21 (42%) 0 3	141, 163, 183, 198	0
53	B6	49/49 (100%)	1.60	13 (26%) 1 6	87, 145, 164, 188	0
54	B7	64/65 (98%)	1.23	11 (17%) 4 10	113, 131, 153, 165	0
55	B8	37/37 (100%)	0.93	8 (21%) 2 7	146, 157, 169, 172	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	10767/11051 (97%)	0.98	1905 (17%) 4 9	63, 160, 260, 350	0

The worst 5 of 1905 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
15	AP	123	ALA	13.1
27	BD	275	LYS	12.7
26	BC	127	LEU	11.7
5	AF	201	TYR	11.7
26	BC	126	LYS	11.2

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.