



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 08:59 am GMT

PDB ID : 4V8O
Title : Crystal structure of the hybrid state of ribosome in complex with the guanosine triphosphatase release factor 3
Authors : Jin, H.; Kelley, A.C.; Ramakrishnan, V.
Deposited on : 2011-07-26
Resolution : 3.80 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28972

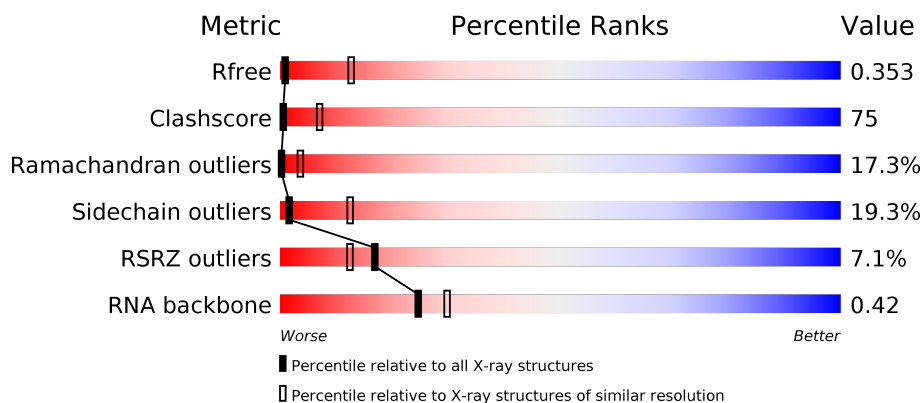
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1019 (4.08-3.52)
Clashscore	112137	1030 (4.04-3.56)
Ramachandran outliers	110173	1011 (4.06-3.54)
Sidechain outliers	110143	1005 (4.06-3.54)
RSRZ outliers	101464	1032 (4.08-3.52)
RNA backbone	2435	1016 (4.70-2.90)

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. 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	<div> <div>2%</div> <div>11% 65% 20% . .</div> </div>
2	AB	256	<div> <div>9% 46% 31% 5% 8%</div> </div>
3	AC	239	<div> <div>% 18% 46% 21% . 13%</div> </div>
4	AD	209	<div> <div>6% 20% 60% 19%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	AE	162	
6	AF	101	
7	AG	156	
8	AH	138	
9	AI	128	
10	AJ	105	
11	AK	129	
12	AL	135	
13	AM	126	
14	AN	61	
15	AO	89	
16	AP	88	
17	AQ	105	
18	AR	88	
19	AS	93	
20	AT	106	
21	AU	27	
22	AV	77	
23	AX	9	
24	AY	529	
25	B0	85	
26	B1	98	
27	B2	72	
28	B3	60	
29	B4	71	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
30	B5	60	
31	B6	54	
32	B7	49	
33	B8	65	
34	B9	37	
35	BA	2915	
36	BB	122	
37	BC	229	
38	BD	276	
39	BE	206	
40	BF	210	
41	BG	182	
42	BH	180	
43	BJ	173	
44	BK	147	
45	BN	140	
46	BO	122	
47	BP	150	
48	BQ	141	
49	BR	118	
50	BS	112	
51	BT	146	
52	BU	118	
53	BV	101	
54	BW	113	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
55	BX	96	
56	BY	110	
57	BZ	206	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
58	GCP	AY	1000	-	-	X	-

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 151017 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	1504	Total	C	N	O	P	0	0	0
			32329	14390	5992	10444	1503			

- Molecule 2 is a protein called 30S RIBOSOMAL PROTEIN S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	235	Total	C	N	O	S	0	0	1
			1901	1213	342	341	5			

- Molecule 3 is a protein called 30S RIBOSOMAL PROTEIN S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	207	Total	C	N	O	S	0	0	1
			1613	1016	315	281	1			

- Molecule 4 is a protein called 30S RIBOSOMAL PROTEIN S4.

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

- Molecule 5 is a protein called 30S RIBOSOMAL PROTEIN S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AE	151	Total	C	N	O	S	0	0	1
			1147	724	218	201	4			

- Molecule 6 is a protein called 30S RIBOSOMAL PROTEIN S6.

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

- Molecule 7 is a protein called 30S RIBOSOMAL PROTEIN S7.

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

- Molecule 8 is a protein called 30S RIBOSOMAL PROTEIN S8.

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

- Molecule 9 is a protein called 30S RIBOSOMAL PROTEIN S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AI	127	Total	C	N	O	S	0	0	0
			1011	639	198	174				

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AI	58	ARG	HIS	CONFLICT	UNP P80374

- Molecule 10 is a protein called 30S RIBOSOMAL PROTEIN S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AJ	99	Total	C	N	O	S	0	0	1
			795	499	157	138	1			

- Molecule 11 is a protein called 30S RIBOSOMAL PROTEIN S11.

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

- Molecule 12 is a protein called 30S RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AL	125	Total	C	N	O	S	0	0	1
			971	611	196	163	1			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AL	1	MET	-	EXPRESSION TAG	UNP P17293
AL	2	VAL	-	EXPRESSION TAG	UNP P17293
AL	3	ALA	-	EXPRESSION TAG	UNP P17293
AL	4	LEU	-	EXPRESSION TAG	UNP P17293

- Molecule 13 is a protein called 30S RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	125	Total	C	N	O	S	0	0	1
			988	611	206	169	2			

- Molecule 14 is a protein called 30S RIBOSOMAL PROTEIN S14 TYPE Z.

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

- Molecule 15 is a protein called 30S RIBOSOMAL PROTEIN S15.

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

- Molecule 16 is a protein called 30S RIBOSOMAL PROTEIN S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AP	84	Total	C	N	O	S	0	0	1
			701	443	140	117	1			

- Molecule 17 is a protein called 30S RIBOSOMAL PROTEIN S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AQ	100	Total	C	N	O	S	0	0	1
			824	528	152	142	2			

- Molecule 18 is a protein called 30S RIBOSOMAL PROTEIN S18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	AR	70	Total	C	N	O		0	0	0
			574	367	112	95				

- Molecule 19 is a protein called 30S RIBOSOMAL PROTEIN S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AS	79	Total	C	N	O	S	0	0	1
			630	403	115	110	2			

- Molecule 20 is a protein called 30S RIBOSOMAL PROTEIN S20.

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

- Molecule 21 is a protein called 30S RIBOSOMAL PROTEIN THX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	AU	25	Total	C	N	O	0	0	1
			209	128	51	30			

- Molecule 22 is a RNA chain called PE HYBRID STATE TRNA FMET.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			

- Molecule 23 is a RNA chain called MRNA 5'-R(*AP*AP*AP*AP*AP*AP*UP*GP*UP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AX	9	Total	C	N	O	P	0	0	0
			192	88	39	57	8			

- Molecule 24 is a protein called PEPTIDE CHAIN RELEASE FACTOR 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	AY	496	Total	C	N	O	S	0	0	0
			3934	2492	677	744	21			

- Molecule 25 is a protein called 50S RIBOSOMAL PROTEIN L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	B0	84	Total	C	N	O	S	0	0	0
			662	410	140	111	1			

- Molecule 26 is a protein called 50S RIBOSOMAL PROTEIN L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	B1	94	Total	C	N	O	S	0	0	1
			732	460	146	125	1			

- Molecule 27 is a protein called 50S RIBOSOMAL PROTEIN L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	B2	71	Total	C	N	O	S	0	0	0
			598	370	121	106	1			

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	B3	60	Total	C	N	O	S	0	0	1
			468	298	91	78	1			

- Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	B4	45	Total	C	N	O	S	0	0	1
			341	218	58	61	4			

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	B5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			

- Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	B6	50	Total	C	N	O	S	0	0	0
			433	270	88	71	4			

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	B7	49	Total	C	N	O	S	0	0	1
			419	257	105	55	2			

- Molecule 33 is a protein called 50S RIBOSOMAL PROTEIN L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	B8	64	Total	C	N	O	S	0	0	1
			508	326	102	78	2			

- Molecule 34 is a protein called 50S RIBOSOMAL PROTEIN L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	B9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

- Molecule 35 is a RNA chain called 23S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BA	2901	Total	C	N	O	P	0	0	0
			62477	27807	11683	20087	2900			

- Molecule 36 is a RNA chain called 5S RIBOSOMAL RNA.

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

- Molecule 37 is a protein called 50S RIBOSOMAL PROTEIN L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BC	228	Total	C	N	O	S	0	0	0
			1742	1101	318	319	4			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BC	19	ILE	VAL	CONFLICT	UNP Q5SLP7
BC	27	HIS	ARG	CONFLICT	UNP Q5SLP7
BC	127	MET	LEU	CONFLICT	UNP Q5SLP7

- Molecule 38 is a protein called 50S RIBOSOMAL PROTEIN L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BD	275	Total	C	N	O	S	0	0	0
			2145	1353	428	361	3			

- Molecule 39 is a protein called 50S RIBOSOMAL PROTEIN L3.

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

- Molecule 40 is a protein called 50S RIBOSOMAL PROTEIN L4.

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

- Molecule 41 is a protein called 50S RIBOSOMAL PROTEIN L5.

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

- Molecule 42 is a protein called 50S RIBOSOMAL PROTEIN L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BH	156	Total	C	N	O	S	0	0	1
			1189	752	222	214	1			

- Molecule 43 is a protein called 50S RIBOSOMAL PROTEIN L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BJ	131	Total	C	N	O		0	0	1
			654	393	131	130				

- Molecule 44 is a protein called 50S RIBOSOMAL PROTEIN L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BK	141	Total	C	N	O		0	0	1
			701	420	141	140				

- Molecule 45 is a protein called 50S RIBOSOMAL PROTEIN L13.

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

- Molecule 46 is a protein called 50S RIBOSOMAL PROTEIN L14.

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

- Molecule 47 is a protein called 50S RIBOSOMAL PROTEIN L15.

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

- Molecule 48 is a protein called 50S RIBOSOMAL PROTEIN L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	BQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

- Molecule 49 is a protein called 50S RIBOSOMAL PROTEIN L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	BR	117	Total	C	N	O	S	0	0	0
			960	599	202	159				

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

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

- Molecule 51 is a protein called 50S RIBOSOMAL PROTEIN L19.

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

- Molecule 52 is a protein called 50S RIBOSOMAL PROTEIN L20.

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

- Molecule 53 is a protein called 50S RIBOSOMAL PROTEIN L21.

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

- Molecule 54 is a protein called 50S RIBOSOMAL PROTEIN L22.

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

- Molecule 55 is a protein called 50S RIBOSOMAL PROTEIN L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	BX	93	Total	C	N	O	S	0	0	1
			726	471	132	123				

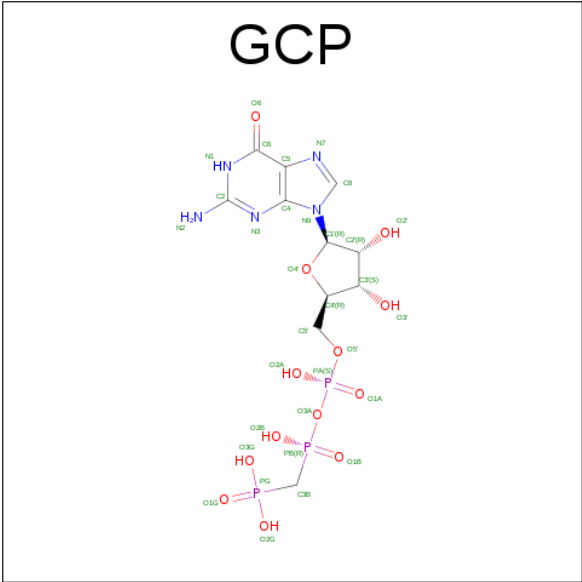
- Molecule 56 is a protein called 50S RIBOSOMAL PROTEIN L24.

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

- Molecule 57 is a protein called 50S RIBOSOMAL PROTEIN L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	BZ	176	Total	C	N	O	S	0	0	0
			1403	897	252	252	2			

- Molecule 58 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: GCP) (formula: $C_{11}H_{18}N_5O_{13}P_3$).



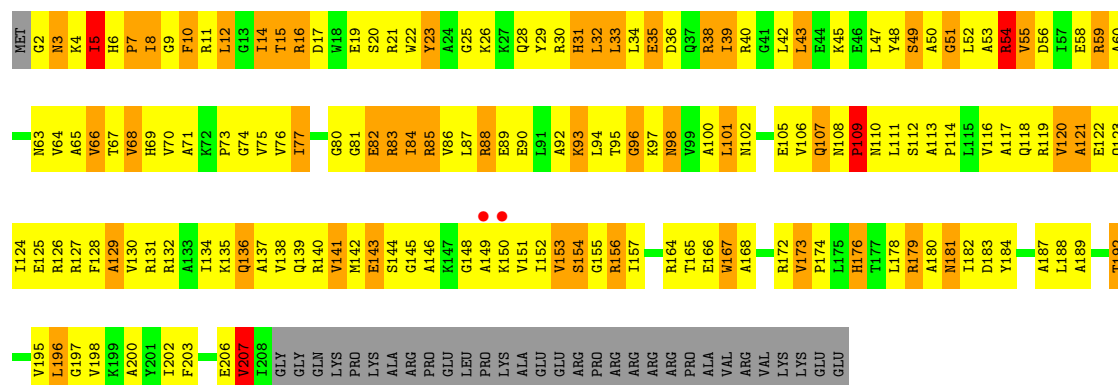
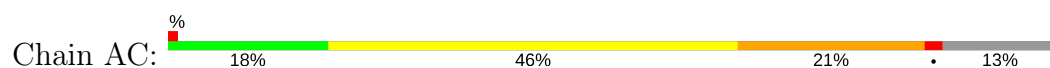
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
58	AY	1	Total	C	N	O	P	0	0
			32	11	5	13	3		

A1503	G1438	G1316	A1256	U1194	C1132	G1072	U1012	U952	A892	C826	A766	U705
G1504	C1439	C1317	U1257	C1195	G1133	U1073	G1013	G953	C893	U827	A767	A706
G1505	C1440	A1318	G1258	U1196	A1318	G1074	A1015	G954	C894	A828	A768	A707
U1506	G1441	A1319	G1259	U1197	U1135	C1075	A1016	U955	C895	G929	A769	C708
A1507	G1442	C1320	C1260	G1198	U1136	C1076	U1017	U956	C896	U830	C770	G709
G1508	U1380	C1321	U1199	U1199	C1137	G1077	C1018	U957	C897	G831	G771	G710
C1509	U1381	C1322	C1262	C1200	G1138	U1078	C1019	A958	C898	C832	U772	G711
U1510	G1443	G1323	C1263	A1201	G1139	G1079	U1020	A959	C899	U833	G773	A712
G1511	C1444	A1324	C1264	C1202	C1141	A1080	U1021	U960	A900	U834	G774	G713
U1512	C1445	C1325	G1265	C1203	C1142	G1082	G1021	U961	A901	U835	G775	G714
A1513	G1446	C1326	G1266	A1204	G1143	G1083	U1025	C962	G902	G836	G776	A715
C1514	G1386	C1327	C1267	U1205	G1143	U1084	G1026	G963	G903	G837	A777	A716
C1515	G1387	C1328	A1268	G1206	G1144	U1085	G1027	A964	C904	G838	G778	C717
G1516	C1388	A1329	A1269	G1207	C1145	U1085	C1028	A965	U965	U839	G779	G718
G1517	C1389	U1330	C1270	C1208	A1146	U1086	C1029	G966	G906	C840	C779	C719
A1518	U1390	G1331	G1271	C1209	U1147	G1087	G1030	G967	A907	U841	A781	C720
G1519	U1391	A1332	G1272	C1210	U1148	G1088	G1031	A968	A908	A782	A782	G721
U1520	G1392	A1333	G1273	C1211	C1149	G1089	G1032	A969	A909	C849	C783	A722
G1521	U1393	C1334	G1274	U1212	U1150	U1090	C1033	C970	C910	U850	C784	U723
U1522	A1394	C1335	A1275	A1213	U1151	U1091	G1030C	G971	U911	G851	G785	G724
G1523	C1463	C1336	G1276	C1214	A1152	U1092	A1030D	C972	C912	G852	G786	G725
G1526	G1464	G1337	C1277	G1215	G1153	A1093	G1031	A974	A914	G853	A787	C726
C1527	C1465	G1338	U1278	G1216	G1154	G1094	G1032	C980	U920	G854	U788	G727
U1528	C1466	A1339	A1279	C1217	G1155	U1095	G1033	U981	U921	G855	U789	A728
G1529	G1467	A1340	U1280	C1218	G1156	C1096	G1034	U982	G922	C856	A790	A729
U1530	A1468	U1341	U1281	U1219	A1157	C1097	A1035	A983	A923	U863	C797	G730
A1531	G1469	C1342	C1282	G1220	U1158	C1098	G1036	C984	C924	A964	G798	C737
U	G1470	G1343	G1283	G1221	C1159	G1099	C1037	C985	G925	A865	G799	C738
C	G1471	C1344	A1284	G1222	G1160	C1100	C1038	A986	G926	C866	G800	U740
C	U1472	U1345	C1285	C1223	C1161	A1101	C1039	G987	G927	G867	U801	G741
A	A1473	G1346	A1286	G1224	C1162	A1102	U1040	U988	C928	C868	A802	G742
C	G1474	C1347	A1287	A1225	U1165	C1103	A1041	A989	G929	G869	G803	U743
C	G1475	U1348	A1288	C1226	C1166	A1105	G1042	C990	C930	U870	U804	C744
U	A1476	A1349	A1289	C1227	G1166	A1106	A1046	C988	G931	C876	C810	G750
C	G1477	A1350	G1290	C1228	A1168	G1106	G1047	U991	A937	G877	C811	U751
C	C1478	U1351	U1291	A1229	A1169	C1107	G1048	U992	A938	C878	C812	U752
U	C1479	C1352	U1292	C1230	A1170	C1108	U1049	G993	G939	C879	U813	A753
U	G1480	G1353	G1293	G1231	G1171	C1109	G1050	A994	C934	C875	A814	C754
U	U1481	C1354	G1294	U1232	C1172	A1110	U1051	C995	A935	C874	A815	G755
C	G1482	G1355	G1295	G1233	G1173	A1111	C1052	A996	G936	G876	A816	C756
A1483	G1415	G1356	C1296	C1234	G1174	C1112	U1053	U997	A937	G877	C817	U757
C1484	G1416	A1357	C1297	U1235	G1175	C1113	G1054	U998	A938	C878	G818	G758
U1485	G1417	U1358	C1298	A1236	A1176	C1114	C1055	C999	G939	C879	U819	A759
G1486	A1418	C1359	U1299	C1237	G1177	C1115	U1056	A1001	C940	C880	U820	G760
G1487	G1419	A1360	G1300	A1238	G1178	C1116	U1057	U1000	G941	G881	G821	G761
G1488	U1420	G1361	U1301	A1239	A1179	G1117	U1058	G1001A	G942	C882	A817	C762
G1489	G1423	C1362	U1302	U1240	A1180	C1118	G1059	G1002	G943	C883	C817	U763
C1490	C1424	C1363	C1303	G1241	G1181	C1119	U1060	G1003	G944	C884	G818	G764
G1491	U1425	A1363A	G1304	U1242	G1182	C1120	U1061	A1004	G945	G885	A819	A769
A1492	C1426	U1364	G1305	C1243	A1183	U1121	U1062	A1005	A946	G886	U820	G760
A1493	U1427	G1365	A1306	C1244	G1184	U1122	U1063	C1006	G947	G887	G821	G761
G1494	U1430	C1366	U1307	A1248	G1185	A1123	U1064	G1009	G948	G888	C822	C762
U1495	C1431	C1367	U1308	C1249	U1186	G1124	U1065	G1010	G949	G889	G823	G763
C1496	G1432	G1368	G1309	U1250	G1187	U1125	U1066	U1070	U950	C890	C824	U764
G1497	A1433	C1369	G1310	A1251	A1188	U1126	C1067	G1009	G951	U891	G825	G765
U1498	G1434	G1370	G1311	A1252	A1189	U1127	U1068	G1010				
A1499	A1434	G1371	G1312	A1253	G1190	C1128	G1069	G1011				
U1500	G1435	U1372	U1313	G1254	A1191	C1129	U1071					
C1501	U1436	C1373	C1314	G1255	A1192	C1130	U1072					
A1502	C1437	A1374	U1315	G1256	G1193	G1131	C1071					

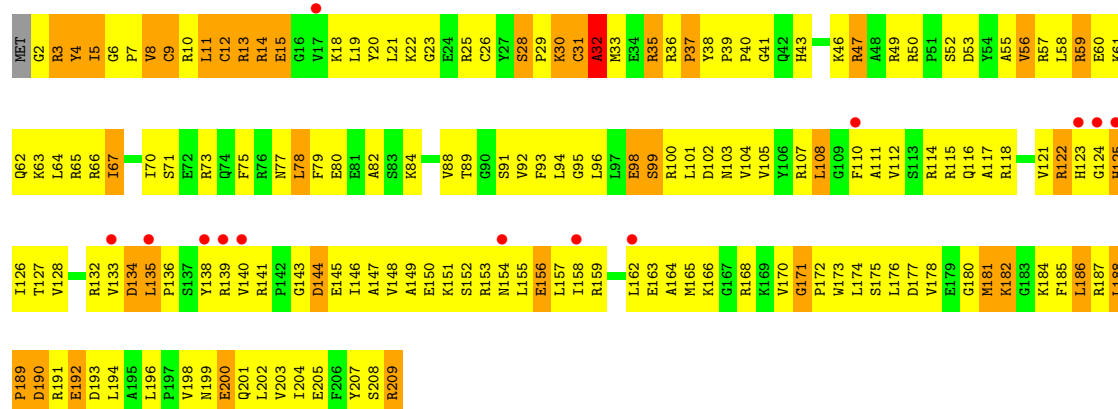
• Molecule 2: 30S RIBOSOMAL PROTEIN S2

Chain AB: 9% 46% 31% 5% 8%

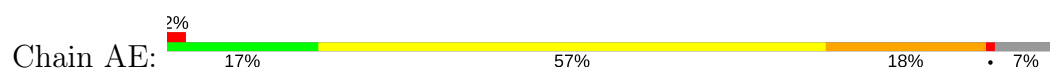
- Molecule 3: 30S RIBOSOMAL PROTEIN S3

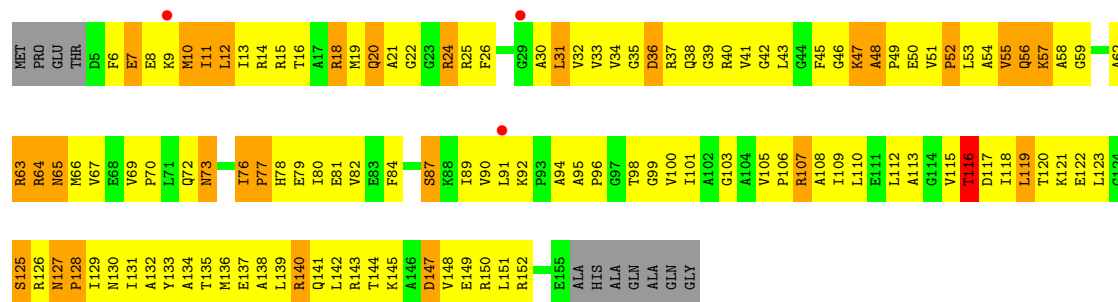


- Molecule 4: 30S RIBOSOMAL PROTEIN S4



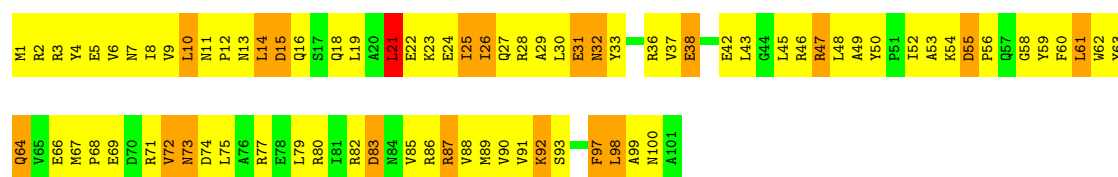
- Molecule 5: 30S RIBOSOMAL PROTEIN S5





• Molecule 6: 30S RIBOSOMAL PROTEIN S6

Chain AF: 20% 60% 19%



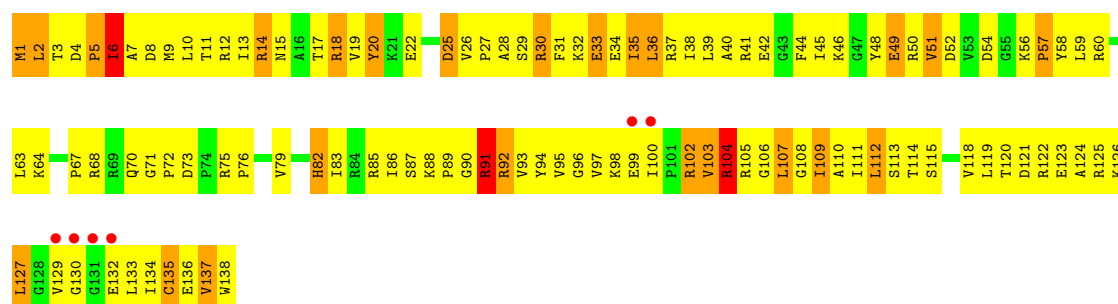
• Molecule 7: 30S RIBOSOMAL PROTEIN S7

Chain AG: 3% 18% 65% 15%



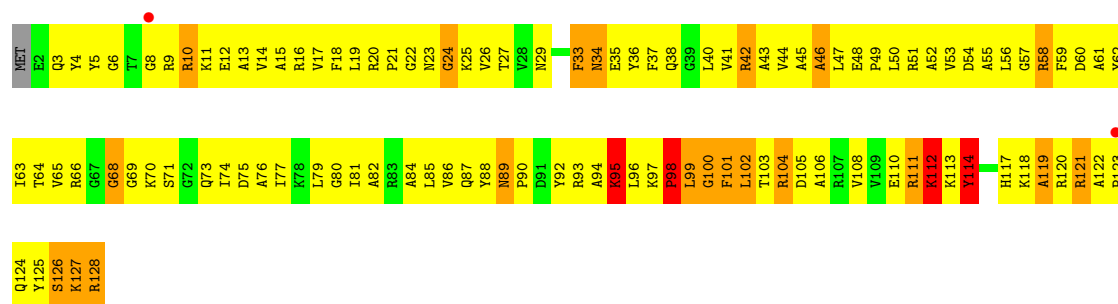
• Molecule 8: 30S RIBOSOMAL PROTEIN S8

Chain AH: 4% 17% 63% 17%

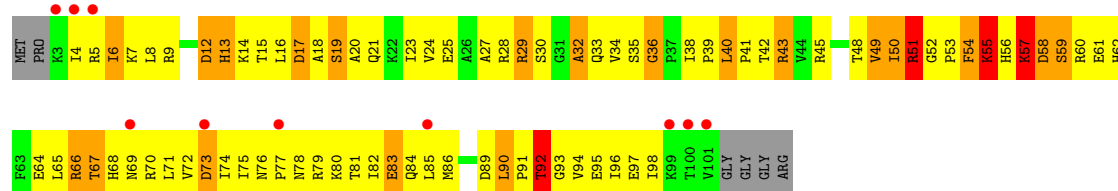
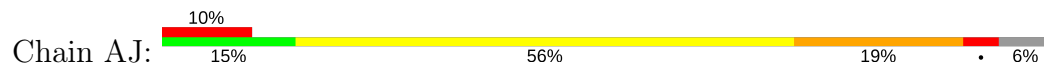


• Molecule 9: 30S RIBOSOMAL PROTEIN S9

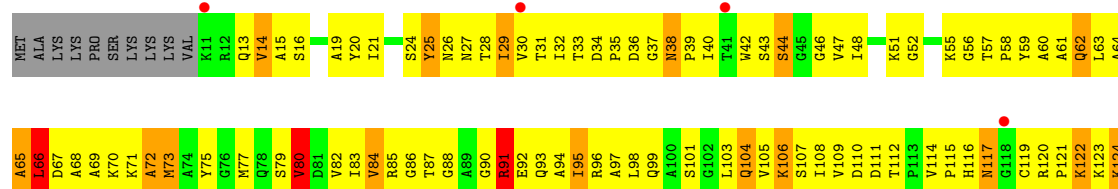
Chain AI: 2% 13% 68% 16%



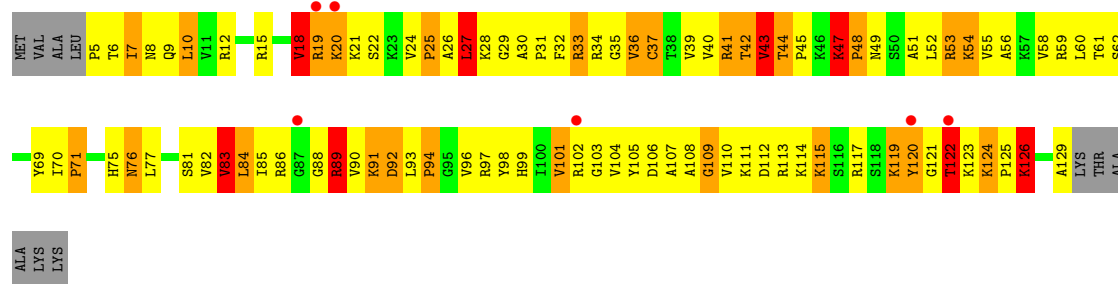
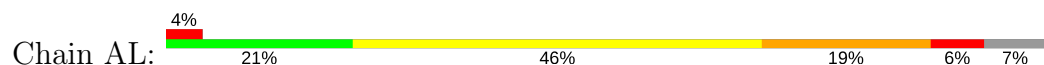
• Molecule 10: 30S RIBOSOMAL PROTEIN S10



• Molecule 11: 30S RIBOSOMAL PROTEIN S11

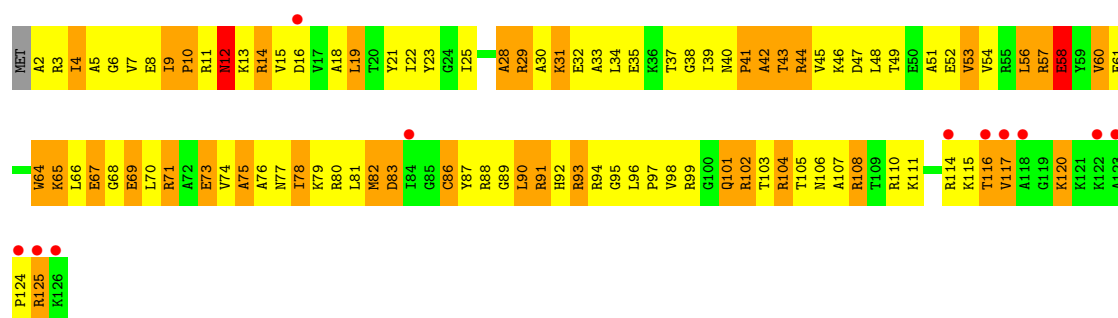


• Molecule 12: 30S RIBOSOMAL PROTEIN S12



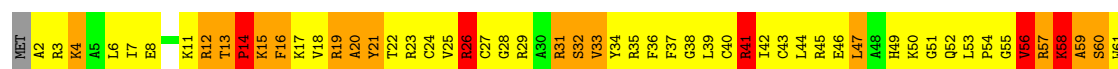
• Molecule 13: 30S RIBOSOMAL PROTEIN S13





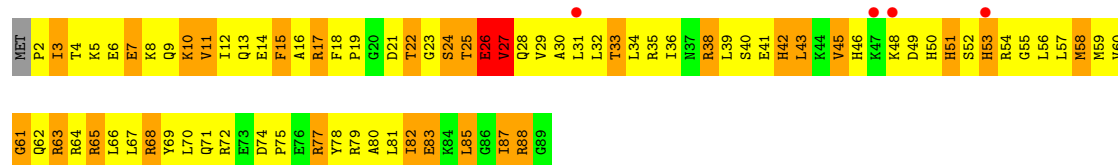
• Molecule 14: 30S RIBOSOMAL PROTEIN S14 TYPE Z

Chain AN: 8% 57% 25% 8%



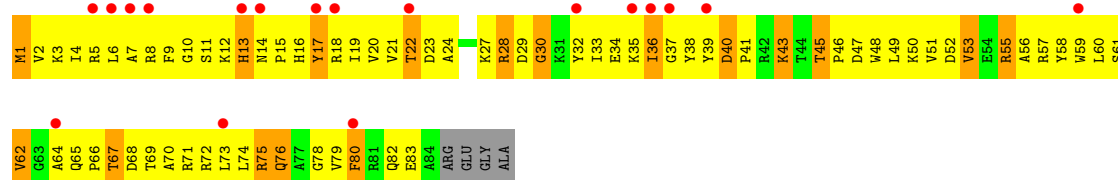
• Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain AO: 4% 10% 56% 30% 2%



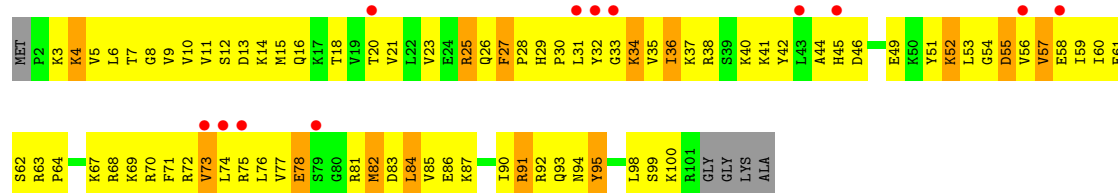
• Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain AP: 20% 11% 65% 19% 5%



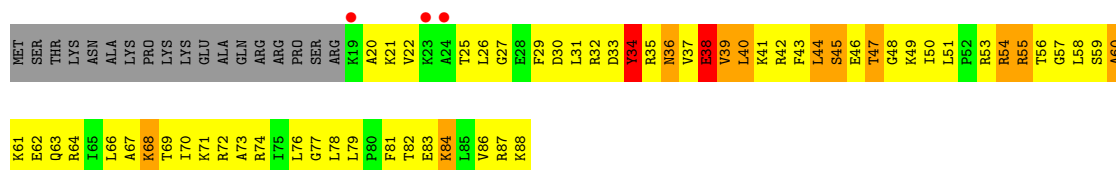
• Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain AQ: 11% 18% 64% 13% 5%

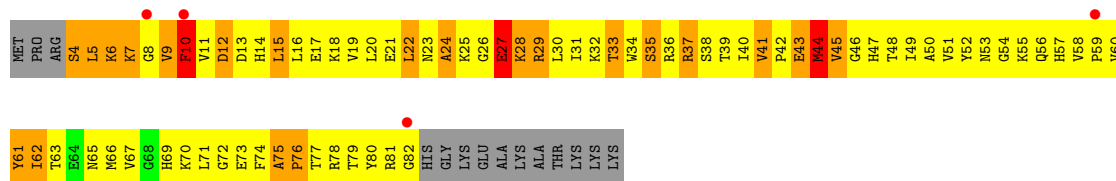


• Molecule 18: 30S RIBOSOMAL PROTEIN S18

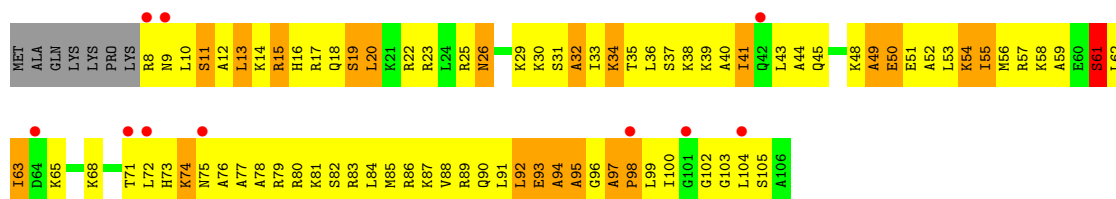
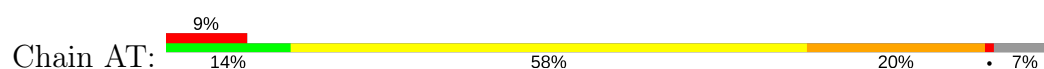
Chain AR: 3% 10% 55% 13% 20%



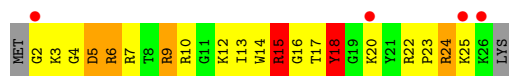
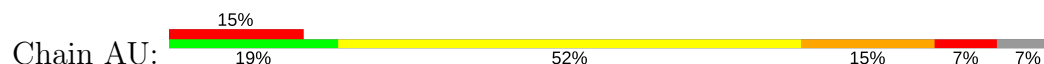
• Molecule 19: 30S RIBOSOMAL PROTEIN S19



• Molecule 20: 30S RIBOSOMAL PROTEIN S20



• Molecule 21: 30S RIBOSOMAL PROTEIN THX



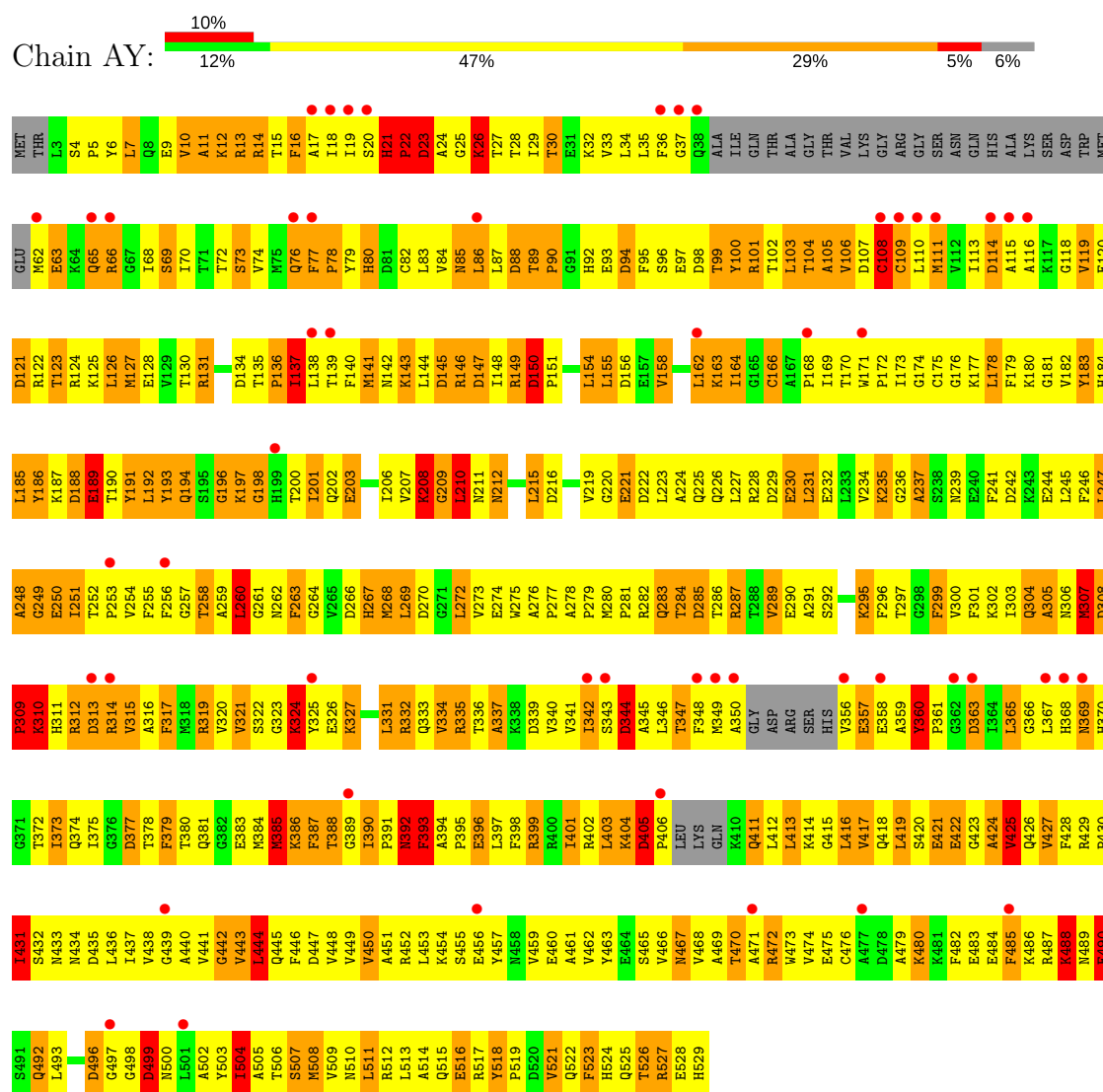
• Molecule 22: PE HYBRID STATE TRNA FMET



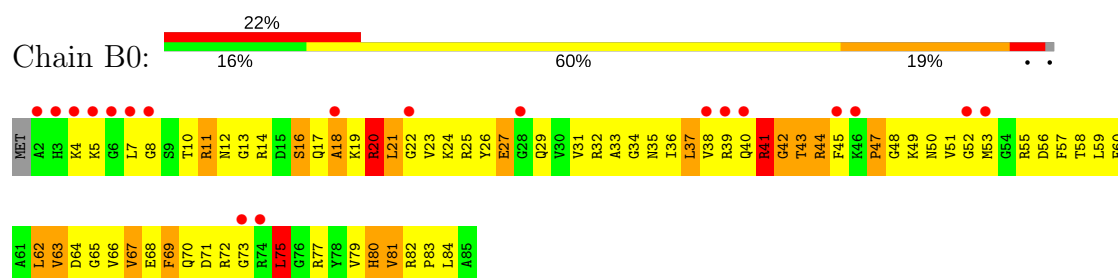
• Molecule 23: MRNA 5'-R(*AP*AP*AP*AP*AP*AP*UP*GP*UP)-3'



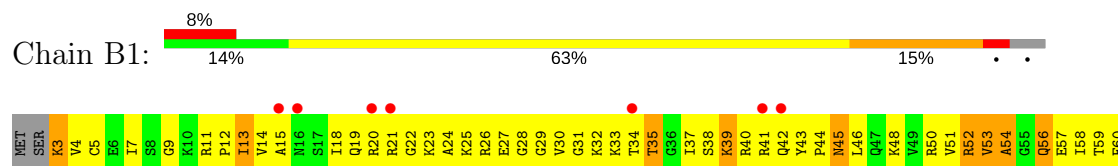
• Molecule 24: PEPTIDE CHAIN RELEASE FACTOR 3

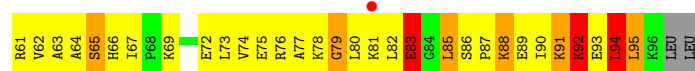


• Molecule 25: 50S RIBOSOMAL PROTEIN L27

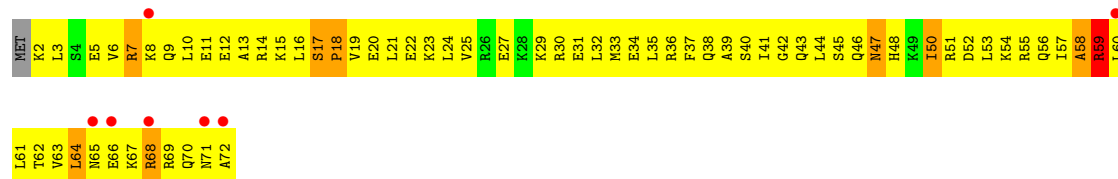


• Molecule 26: 50S RIBOSOMAL PROTEIN L28





• Molecule 27: 50S RIBOSOMAL PROTEIN L29



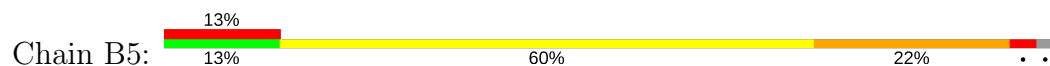
• Molecule 28: 50S RIBOSOMAL PROTEIN L30



• Molecule 29: 50S RIBOSOMAL PROTEIN L31



• Molecule 30: 50S RIBOSOMAL PROTEIN L32



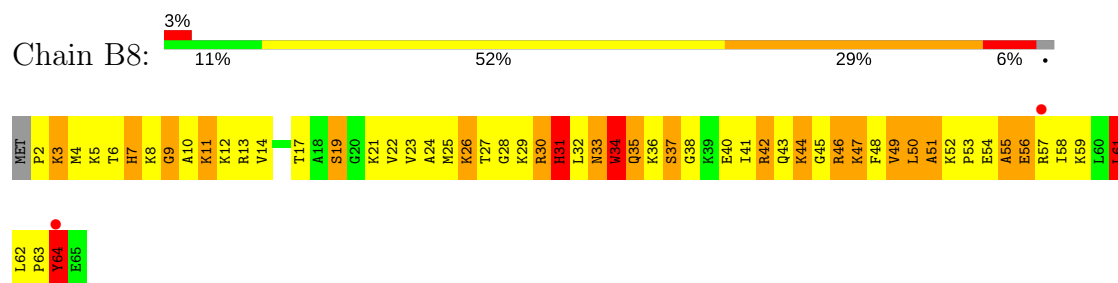
• Molecule 31: 50S RIBOSOMAL PROTEIN L33



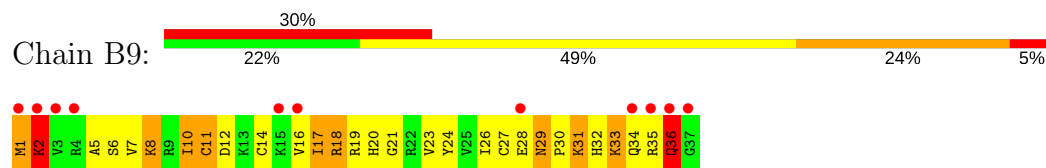
• Molecule 32: 50S RIBOSOMAL PROTEIN L34



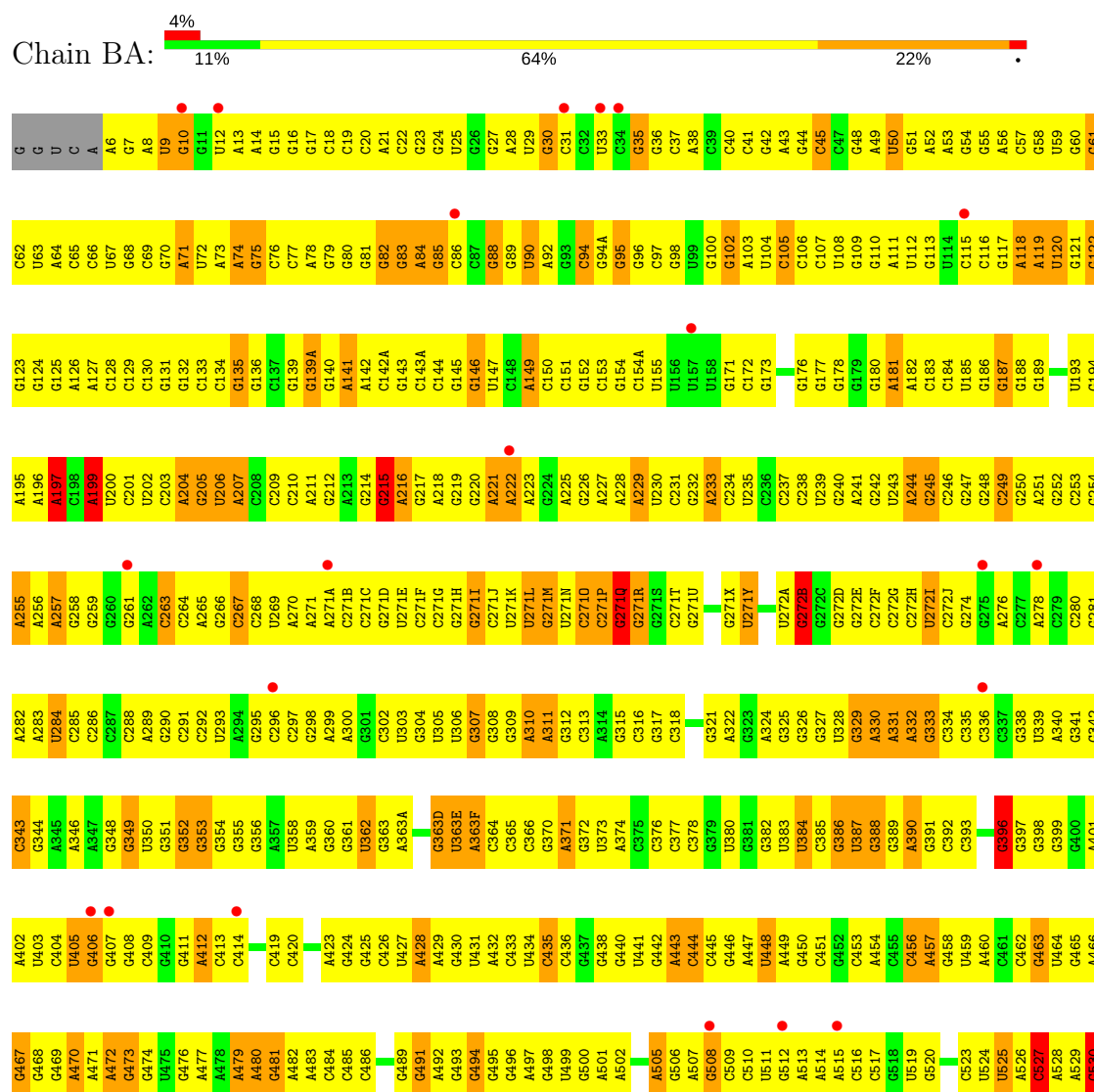
● Molecule 33: 50S RIBOSOMAL PROTEIN L35



● Molecule 34: 50S RIBOSOMAL PROTEIN L36

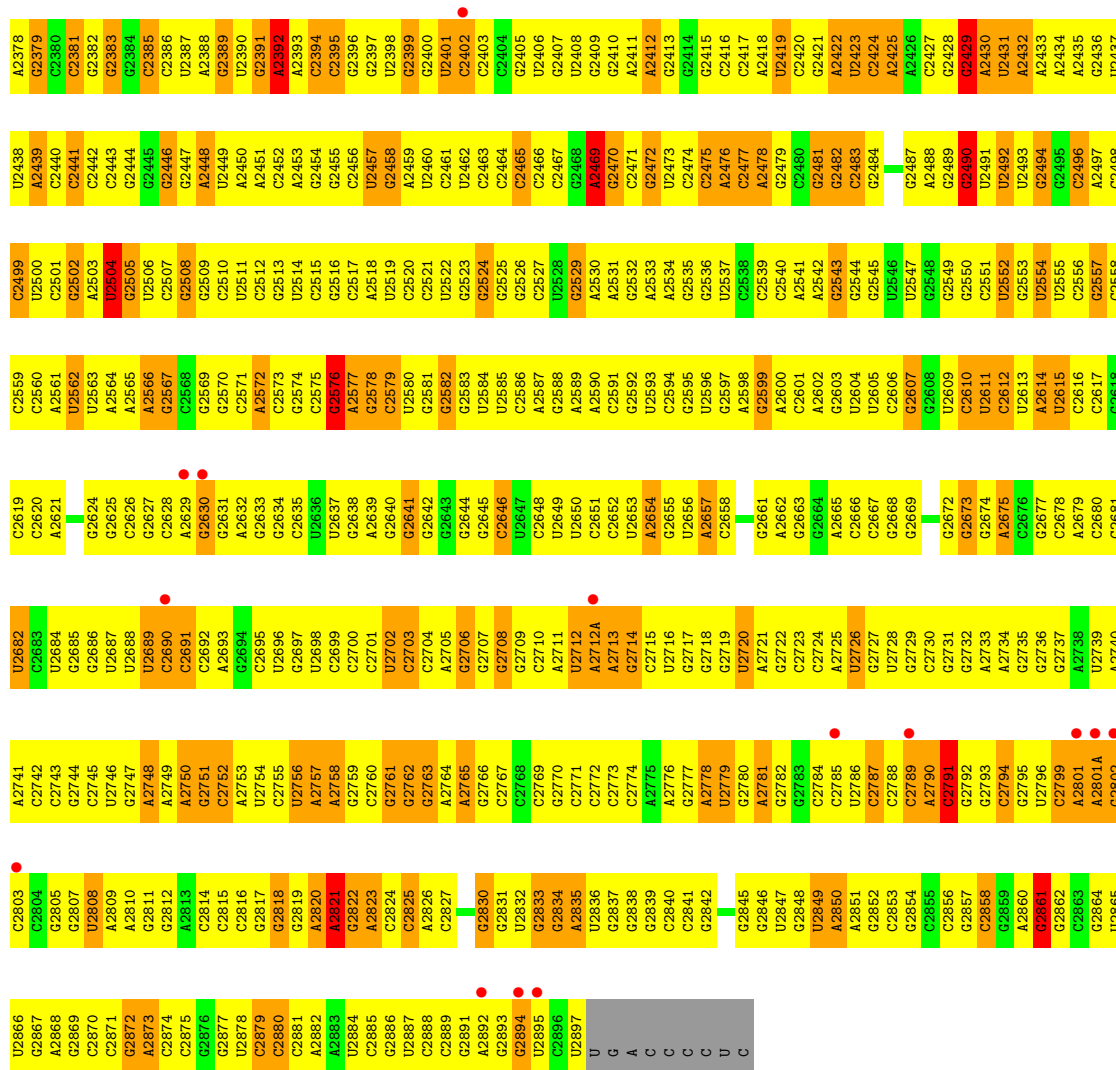


● Molecule 35: 23S RIBOSOMAL RNA



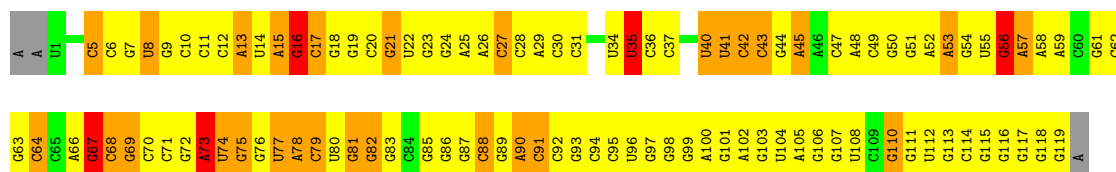
A1365	G1303	A1242	G1120	U1060	A1000	A941	A878	C817	A752	C692	A653	U594	C531
A1366	C1304	G1182	C1121	U1061	A1001	G942	G879	C818	C753	C693	A654	C895	A532
A1367	C1305	G1244	G1122	G1062	G1002	U943	G880	A819	C754	U694	G854C	C896	U533
A1368	C1306	C1185	C1123	G1063	G1003	G944	G881	A820	C755	C695	G854D	U597	C534
A1369	A1307	G1246	C1124	C1064	C1004	A945	G882	G823	C756	C696	G854E	G598	C535
C1370	A1308	G1187	G1125	U1065	C1005	G946	G883	C823		C697	G854F	G599	A536
G1371	G1309	U1188	A1126	U1066	C1006	G947	C884	A824	A761	C698	C854G	G600	C537
U1372	G1310	G1189		A1067	G1007	G948	C885	C825	U762	A699	C854H	C801	G538
A1373	G1311	G1190	A1129	U1068	C1008	C949	C886	C826	U763	G700	G854I	G602	G539
G1374	U1312	G1191	U1130	A1069	G1009	G950	A887	U827	A764	G701	C854J	A603	C540
C1375	U1313	G1192	G1131	A1070	A1010	C951	C888	U828	G765	G702	G854K	G604	C541
G1376	C1314	G1193	A1132	G1071	G1011	G952	C889	A829	C766	U703	C854L	C605	C542
G1377	C1315	A1194	U1133	C1072	U1012	A953	A890	C830	U767	G704	G854M	U606	C543
A1378	U1316		C1135	A1073	G1013	G954	C892	G831	G768	A705	C854N	U607	
A1379	G1317	G1197	G1136	G1074	U1014	G955	C893	G832	G769	A706	G854O	A608	A547
G1380	C1318	U1198	G1137	C1075	G1015	G956	C894	U833	G770	G707	G854P	A609	A548
G1381	U1319	U1199	G1138	A1076	G1016	A957	U895	C834	C771	C708	C854Q		G612
G1382	C1320	G1200	G1139	U1077	G1017	U958	A896	A835	C772	U709	G854R	G613	U614
C1383	A1321	G1201	C1140	U1078	C1018	A959	C897	C836	C773	G710	C854S	G614	G613
A1384	C1322	C1202	U1141	C1079	U1019	A960	C898	C837	A774	G711	C854T	U614	U614
G1385		G1203	U1142	C1080	A1020	G961	A899	C838	G775	G712	C854U	G614B	U554
C1386	U1263	A1204	A1142A	U1081	A1021	G962	A900	U839	G776	G713	A654V	A614C	U555
C1387	G1264	U1205	A1143	U1082	G1022	U963	A901	C840	A777	U714	A655	U557	G556
G1388	A1265	G1206	C1145	U1083	U1023	G964	C902	A841	G778	G715	G855	G615	U557
G1389	G1266	C1207	G1146	A1084	G1024	G965	C903	G842	U779	A716	G856	G616	G558
U1390	U1267	G1208	C1147	A1085	G1025	G966	C904	G843	G780	G717	U857	C618	G559
U1391	G1209	G1209	C1147	U1086	U1026	G967	U905	C844	A781	A718	C858	G619	C560
A1392	A1210	A1210	A1148	A1087	A1027	G968	G906	G845	A782	C719	C859	G620	U561
A1393	U1211	U1211	G1149	A1088	A1028	U969	U907	C846	A783	G720	G860	A621	U562
A1394	G1212	C1150	C1150	U1089	A1029	C970	C908	U847	A784	C721	C861	G622	G563
G1395	A1213	G1151	G1151	U1090	G1030	C971	A909	G848	G785	A722	G862	G623	C564
A1396	C1214	C1152	C1152	G1091	G1031	G972	A910	A849	C786	G723	G863	C624	C565
U1397	G1215	C1153	C1153	C1092	A1032	A973	A911	C850	U787	U724	C864	G625	U566
C1398	C1216	G1154	G1093	U1094	G1033	G974	C912	U851	A788	G725	C865	G626	A567
C1399	C1217	A1155	U1094	G1095	U1035	G975	C913	C852	A789	G726	G866	A627	U568
G1400	G1218	A1156	U1095	A1096	G1036	G976A	C914	C853	C790	A727	U867	G628	U569
A1401	C1219	G1157	C1157	A1097	U1037	C977	C915	G854	G791	G728	G868	G629	G570
C1402	A1220	C1158	C1158	U1097	G1037	G977	G916	C855	G792	G729	G669	G630	A571
C1403	C1221	U1159	U1159	A1098	C1038	G978	A917	C856	A793	C730	A670	A631	A572
C1404	C1221A	G1160	C1160	G1099	G1039	G979	A918	C857	C796	C731	C871	A632	G573
U1405	C1222	C1161	C1161	C1100	C1040	A980	G919	U858	C797	C732	C872	A633	C574
U1406	G1223	G1162	G1162	U1101	G1041	A981	G920	C859	G798	C733	C873	C634	A575
C1407	C1224	G1163	G1163	C1102	C1042	C982	G921	U860		A734	G674	G635	U576
C1408	G1225	U1164	U1164	A1103	C1043	A983	U922	A861	G801	C735	A675	G636	G577
C1409	A1226	U1165	U1165	C1104	G1044	A984	C923	G862	A676	C736	A676	A637	A578
G1410	G1227	C1166	C1166	U1105	A1045	C985	C924	A863	A802	G737	A677	G638	G579
C1411	U1228	U1167	U1167	G1106	A1046	C986	C925	C864	U803	G738	C878	U639	C580
A1412	G1229	G1168	G1168	G1107	G1047	G987	A926	C865	A804	G739	C879	C640	C581
G1413	C1230	G1169	G1169	U1108	A1048	A988	G927	A866	G805	U740	C880	C641	G582
U1414	G1231	G1170	C1170	C1109	G1049	G989	G928	C867	C806	G741	G681	G642	G583
G1415	C1232	G1171	G1171	G1110	A1050	A990	U930	U868	U807	G742	G682	A643	C584
C1416	U1233	G1173	U1173	A1111	G1051	A991	G931	U869	G808	G743	C683	A644	G585
C1417	U1234	A1174	G1174	C1112	C1052	C992	G932	A870	G809	G744	G684	C645	A586
G1418	G1235	U1175	U1175	G1113	C1053	G993	A933	U871	U810	G745	A685	A646	C587
U1419	A1236	G1176	G1176	G1114	A1054	C994	G934	A872	U811	A746	G886	G647	U588
A1420	G1237	A1177	C1177	G1115	G1055	C995	C935	G873	C812	U747	C687	G648	C589
G1421	G1238	C1178	C1178	C1116	G1056	A996		G874	U813	G748	U688	G649	A590
G1422	U1300	C1179	C1179	U1057	G1057	G997	G938	G875	C814	G749	A689	C650	C591
G1423	U1240	C1180	C1180	G1118	G1058	G998	G939	C876	A750		G690	G651	G592
G1424	A1241	C1181	C1181	C1119	G1059	U999	G940	U877	C816	A751	C691	G652	G593

G2318	G2319	G2320	G2321	G2322	G2323	G2324	G2325	G2326	G2327	G2328	G2329	G2330	G2331	G2332	G2333	G2334	G2335	G2336	G2337	G2338	G2339	G2340	G2341	G2342	G2343	G2344	G2345	G2346	G2347	G2348	G2349	G2350	G2351	G2352	G2353	G2354	G2355	G2356	G2357	G2358	G2359	G2360	G2361	G2362	G2363	G2364	G2365	G2366	G2367	G2368	G2369	G2370	G2371	G2372	G2373	G2374	G2375	G2376	G2377													
C2258	G2259	G2260	C2261	C2262	C2263	C2264	C2265	C2266	C2267	C2268	C2269	C2270	C2271	C2272	C2273	C2274	C2275	C2276	C2277	C2278	C2279	C2280	C2281	C2282	C2283	C2284	C2285	C2286	C2287	C2288	C2289	C2290	C2291	C2292	C2293	C2294	C2295	C2296	C2297	C2298	C2299	C2300	C2301	C2302	C2303	C2304	C2305	C2306	C2307	C2308	C2309	C2310	C2311	C2312	C2313	C2314	C2315	C2316	C2317													
U2122	G2123	G2124	G2125	G2126	G2127	G2128	G2129	G2130	G2131	G2132	G2133	G2134	G2135	G2136	G2137	G2138	G2139	G2140	G2141	G2142	G2143	G2144	G2145	G2146	G2147	G2148	G2149	G2150	G2151	G2152	G2153	G2154	G2155	G2156	G2157	G2158	G2159	G2160	G2161	G2162	G2163	G2164	G2165	G2166	G2167	G2168	G2169	G2170	G2171	G2172	G2173	G2174	G2175	G2176	G2177	G2178	G2179	G2180	G2181	G2182	G2183	G2184										
C2185	G2186	G2187	C2188	G2189	G2190	G2191	G2192	G2193	G2194	G2195	G2196	G2197	G2198	G2199	G2200	G2201	G2202	G2203	G2204	G2205	G2206	G2207	G2208	G2209	G2210	G2211	G2212	G2213	G2214	G2215	G2216	G2217	G2218	G2219	G2220	G2221	G2222	G2223	G2224	G2225	G2226	G2227	G2228	G2229	G2230	G2231	G2232	G2233	G2234	G2235	G2236	G2237	G2238	G2239	G2240	G2241	G2242	G2243	G2244	G2245	G2246	G2247	G2248	G2249	G2250	G2251	G2252	G2253	G2254	G2255	G2256	G2257
A2062	C2063	C2064	C2065	C2066	C2067	C2068	G2069	G2070	G2071	G2072	C2073	G2074	G2075	G2076	G2077	C2078	G2079	G2080	C2081	G2082	G2083	G2084	C2085	G2086	G2087	G2088	G2089	G2090	G2091	G2092	G2093	G2094	G2095	G2096	G2097	G2098	G2099	G2100	G2101	G2102	C2103	G2104	G2105	G2106	G2107	C2108	G2109	G2110	G2111	G2112	G2113	G2114	G2115	G2116	G2117	C2118	G2119	G2120	G2121	G2122												
G2000	A2001	G2002	C2003	C2004	C2005	C2006	C2007	C2008	G2009	G2010	G2011	G2012	C2013	G2014	G2015	G2016	G2017	G2018	G2019	G2020	G2021	G2022	G2023	G2024	G2025	G2026	G2027	G2028	G2029	G2030	G2031	G2032	G2033	G2034	G2035	G2036	G2037	G2038	G2039	G2040	G2041	G2042	C2043	G2044	G2045	G2046	G2047	G2048	G2049	G2050	G2051	G2052	G2053	G2054	G2055	G2056	G2057	G2058	G2059	G2060	G2061											
U1939	C1940	C1941	C1942	C1943	C1944	C1945	C1946	C1947	G1948	G1949	G1950	G1951	G1952	A1953	G1954	G1955	G1956	C1957	C1958	G1959	G1960	C1961	C1962	C1963	C1964	C1965	A1966	C1967	G1968	G1969	A1970	C1971	C1972	G1973	C1974	C1975	G1976	G1977	C1978	C1979	C1980	C1981	C1982	G1983	G1984	G1985	G1986	G1987	C1988	G1989	C1990	C1991	C1992	C1993	C1994	C1995	G1996	G1997	G1998	C1999												
C1879	C1880	C1881	C1882	G1883	C1884	C1885	C1886	C1887	C1888	G1889	A1890	C1891	C1892	C1893	G1894	C1895	G1896	C1897	C1898	C1899	C1900	C1901	C1902	C1903	G1904	C1905	C1906	C1907	G1908	C1909	C1910	C1911	C1912	C1913	C1914	C1915	C1916	C1917	C1918	C1919	C1920	C1921	C1922	C1923	C1924	C1925	G1926	C1927	C1928	C1929	C1930	C1931	C1932	C1933	C1934	C1935	C1936	C1937	C1938													
A1809	A1810	A1811	A1812	A1813	G1814	C1815	A1816	G1817	G1818	A1819	C1820	A1821	G1822	G1823	G1824	A1825	G1826	C1827	C1828	A1829	C1830	G1831	C1832	C1833	A1834	C1835	C1836	C1837	C1838	G1839	C1840	C1841	C1842	C1843	C1844	C1845	C1846	C1847	A1848	G1849	C1850	C1851	C1852	A1853	C1854	C1855	C1856	C1857	C1858	C1859	C1860	G1861	C1862	C1863	A1864	C1865	C1866	C1867														
A1749	G1750	C1751	C1752	G1753	C1754	A1755	C1756	C1757	C1758	A1759	A1760	C1761	A1762	G1763	G1764	C1765	A1766	C1767	C1768	C1769	G1770	C1771	C1772	A1773	C1774	C1775	C1776	C1777	C1778	C1779	A1780	C1781	C1782	A1783	A1784	C1785	A1786	C1787	C1788	A1789	C1790	C1791	G1792	C1793	C1794	C1795	C1796	C1797	C1798	C1799	C1800	C1801	A1802	C1803	C1804	C1805	C1806	C1807	C1808													
A1609	A1610	C1611	C1612	G1613	A1614	C1615	A1616	A1617	C1617	G1618	C1619	C1620	C1621	G1622	G1623	G1624	C1625	G1626	C1627	C1628	C1629	A1630	A1631	A1632	C1633	A1634	C1635	C1636	C1637	C1638	C1639	A1640	C1641	G1642	C1643	C1644	C1645	C1646	G1647	C1648	C1649	C1650	C1651	C1652	C1653	A1654	C1655	C1656	C1657	C1658	C1659	C1660	C1661	C1662	C1663	C1664	C1665	C1666	C1667	C1668												
C1547	C1548	C1549	C1550	C1551	G1552	C1553	A1554	C1555	C1556	C1557	C1558	C1559	A1560	C1561	G1562	C1563	C1564	C1565	C1566	C1567	A1568	C1569	C1570	C1571	C1572	C1573	C1574	C1575	C1576	C1577	C1578	C1579	A1580	C1581	C1582	C1583	C1584	C1585	C1586	C1587	C1588	C1589	C1590	C1591	C1592	C1593	C1594	C1595	C1596	C1597	C1598	C1599	C1600	C1601	C1602	C1603	C1604	C1605	C1606	C1607	C1608											
G1485	A1486	C1487	C1488	C1489	G1490	G1491	G1492	C1493	A1494	C1495	A1496	C1497	C1498	C1499	C1500	C1501	C1502	C1503	C1504	C1505	C1506	A1507	C1508	C1509	C1510	C1509B	A1499	C1511	C1512	C1513	C1514	C1515	C1516	C1517	C1518	C1519	C1520	C1521	C1522	C1523	C1524	C1525	C1526	C1527	C1528	A1528A	C1529	C1468	C1530	C1531	C1532	C1533	C1534	C1535	C1536	C1537	C1538	C1539	C1540	C1541	C1542	C1543	C1544	C1545	C1546	C1547						
G1425	G1426	A1427	C1428	G1429	C1430	C1431	C1432	C1433	A1434	C1435	C1436	C1437	C1438	C1439	C1440	C1441	C1442	C1443	C1444	C1445	C1446	C1447	C1448	C1449	C1450	C1451	C1452	C1453	C1454	C1455	C1456	C1457	C1458	C1459	C1460	C1461	C1462	C1463	C1464	C1465	C1466	C1467	C1468	C1469	G1470	C1471	C1472	C1473	C1474	C1475	C1476	C1477	C1478	C1479	C1480	C1481	C1482	C1483	C1484	C1485	C1486	C1487										



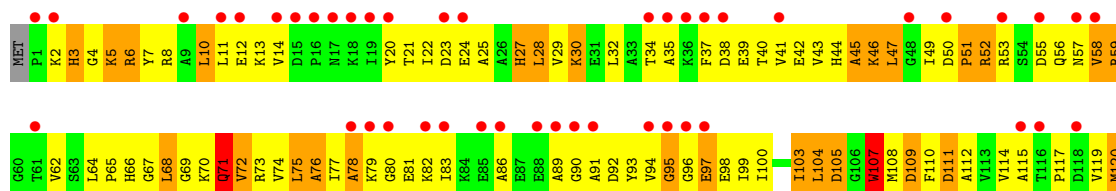
• Molecule 36: 5S RIBOSOMAL RNA

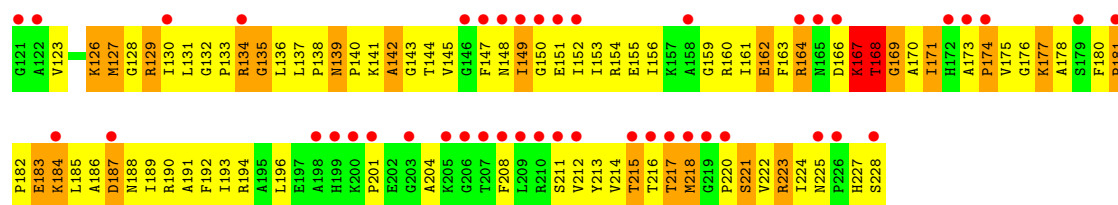
Chain BB: 11% 60% 23%



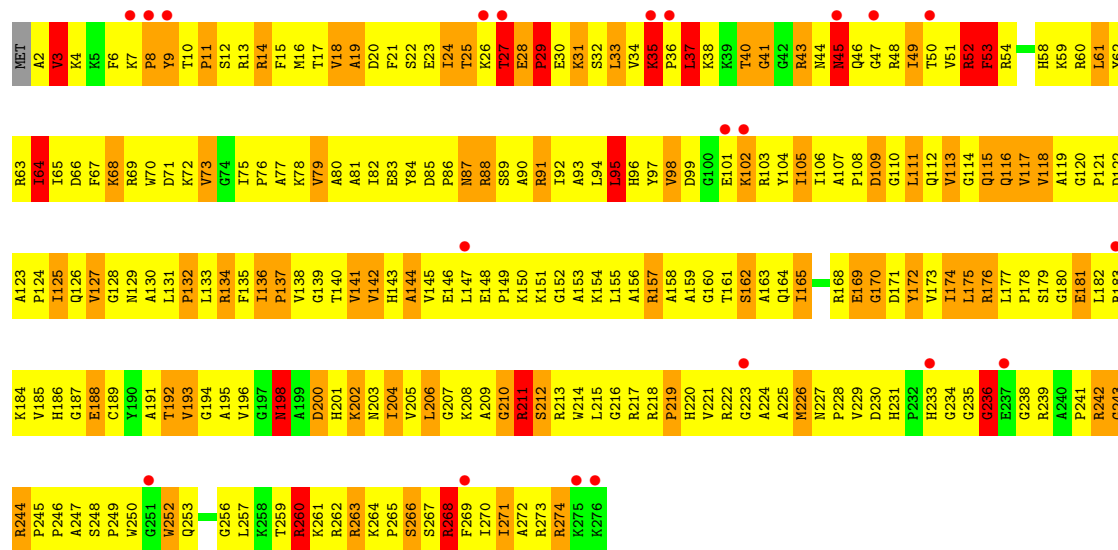
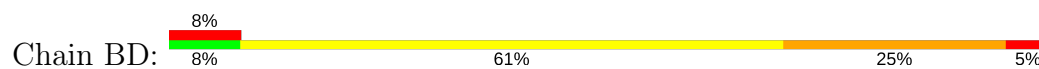
• Molecule 37: 50S RIBOSOMAL PROTEIN L1

Chain BC: 22% 39% 54% 22%

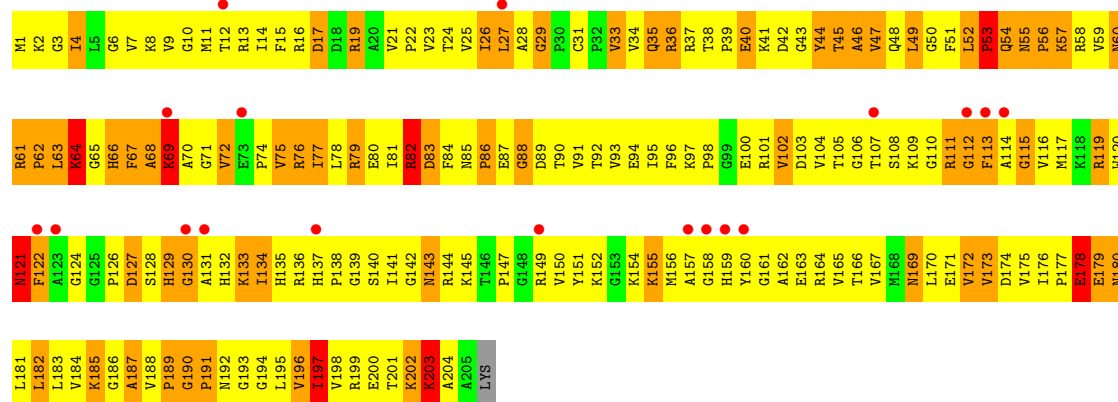
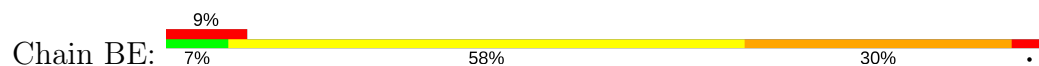




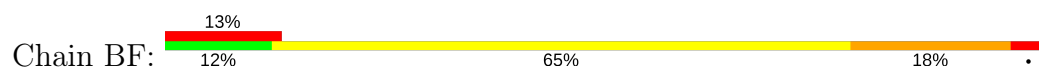
• Molecule 38: 50S RIBOSOMAL PROTEIN L2

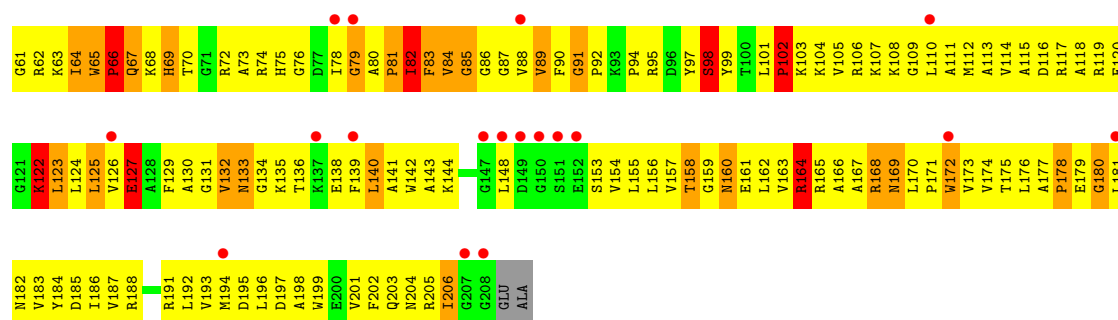


• Molecule 39: 50S RIBOSOMAL PROTEIN L3

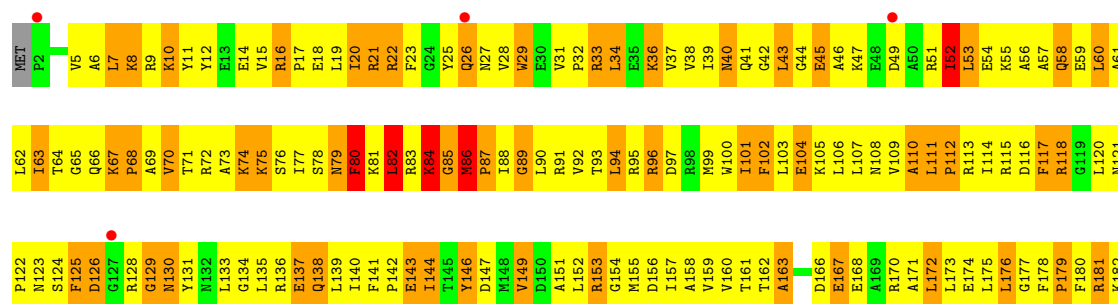
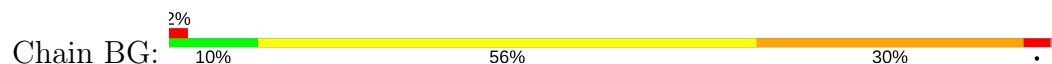


• Molecule 40: 50S RIBOSOMAL PROTEIN L4

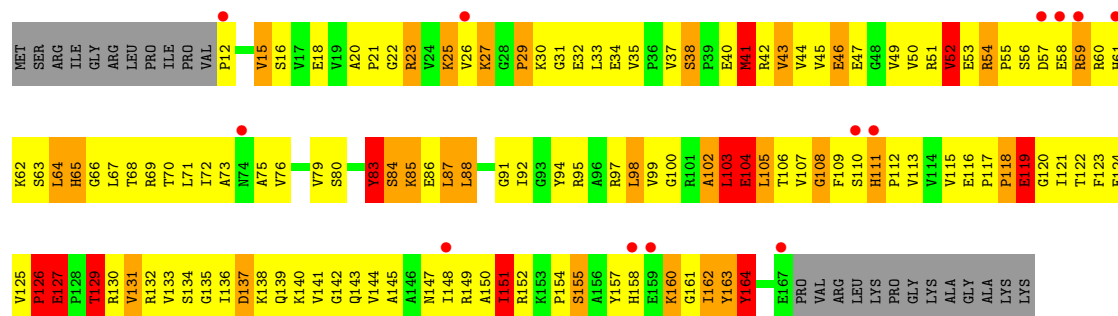
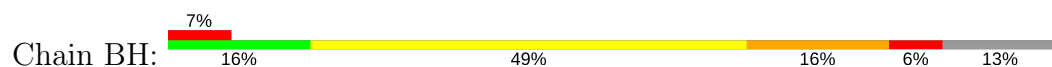




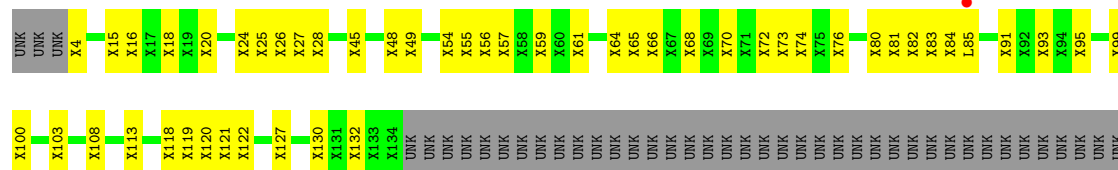
• Molecule 41: 50S RIBOSOMAL PROTEIN L5



• Molecule 42: 50S RIBOSOMAL PROTEIN L6

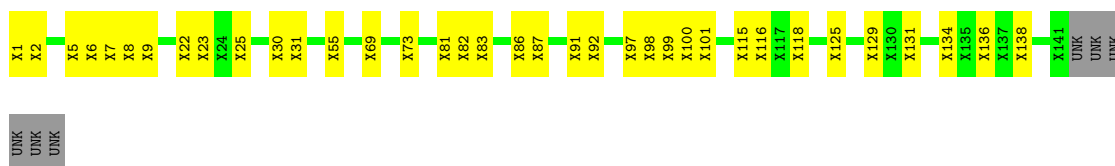


• Molecule 43: 50S RIBOSOMAL PROTEIN L10

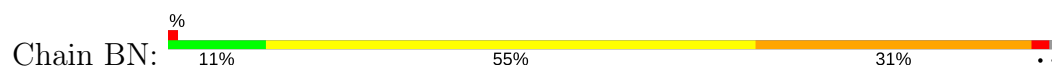


• Molecule 44: 50S RIBOSOMAL PROTEIN L11

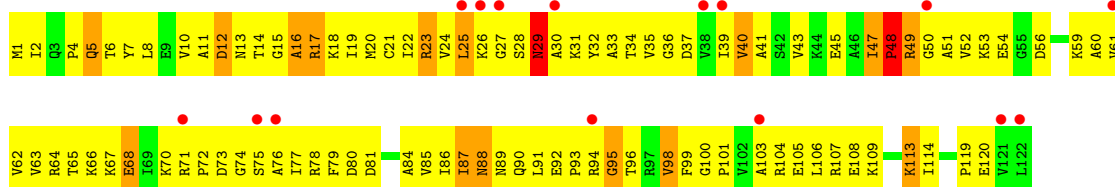




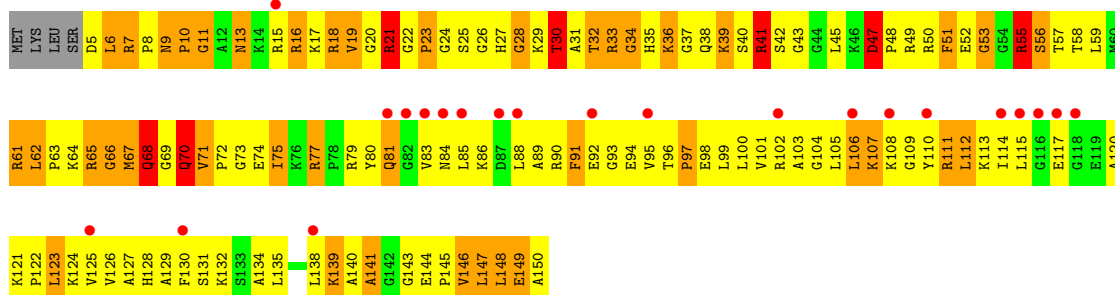
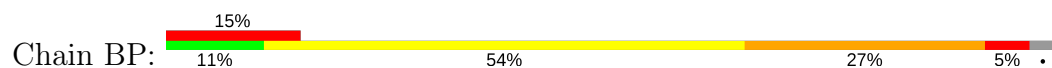
• Molecule 45: 50S RIBOSOMAL PROTEIN L13



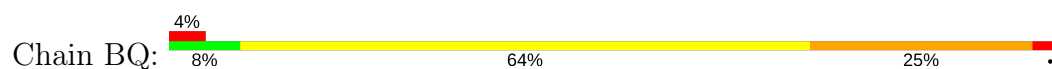
• Molecule 46: 50S RIBOSOMAL PROTEIN L14

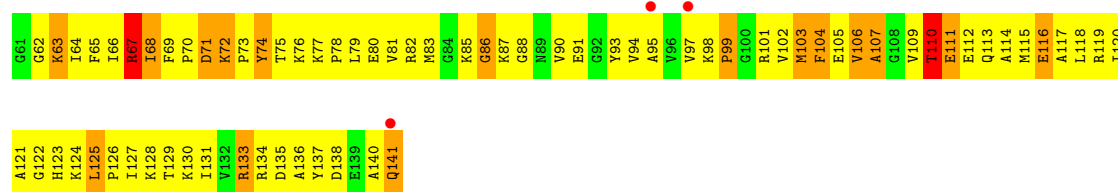


• Molecule 47: 50S RIBOSOMAL PROTEIN L15

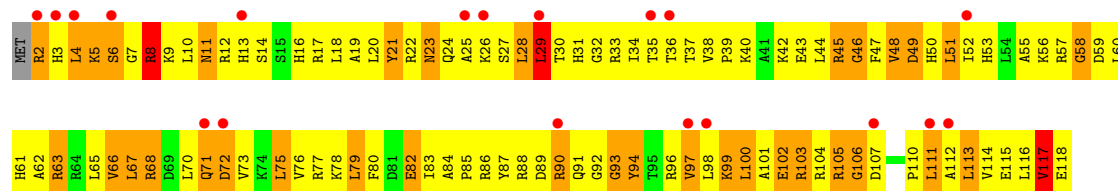
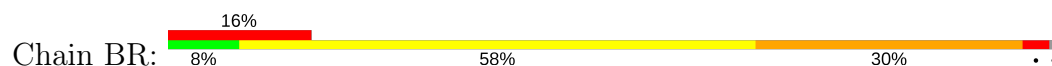


• Molecule 48: 50S RIBOSOMAL PROTEIN L16

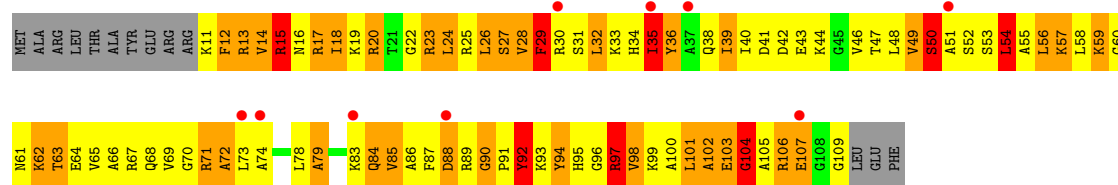




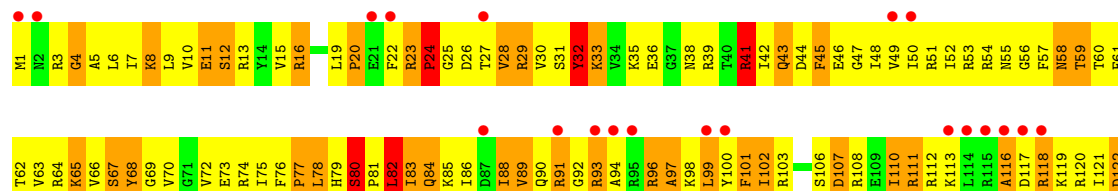
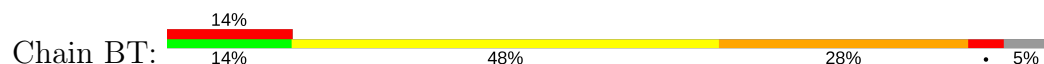
● Molecule 49: 50S RIBOSOMAL PROTEIN L17



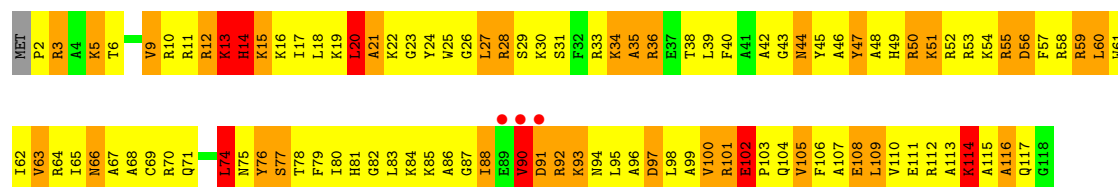
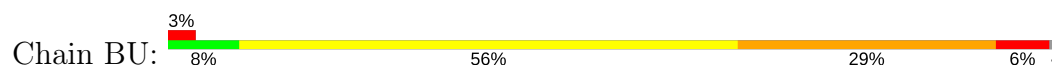
● Molecule 50: 50S RIBOSOMAL PROTEIN L18



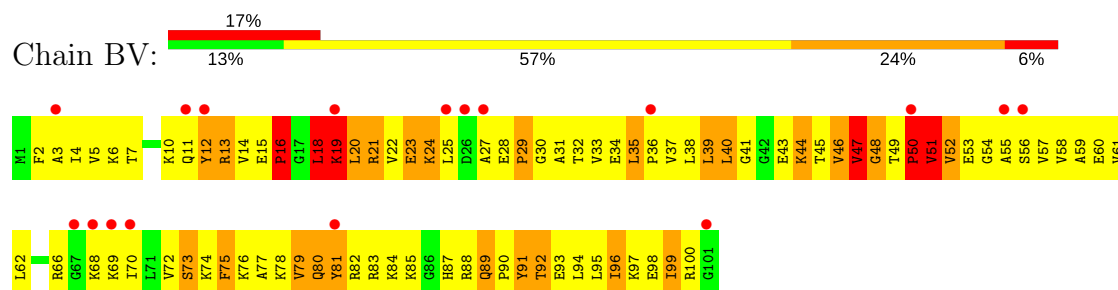
● Molecule 51: 50S RIBOSOMAL PROTEIN L19



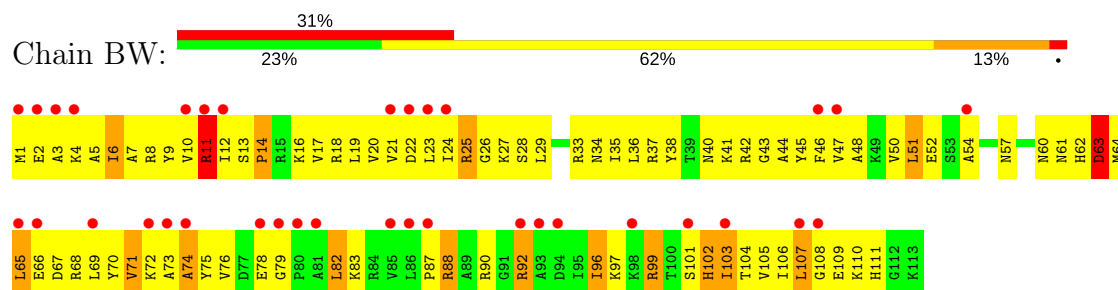
● Molecule 52: 50S RIBOSOMAL PROTEIN L20



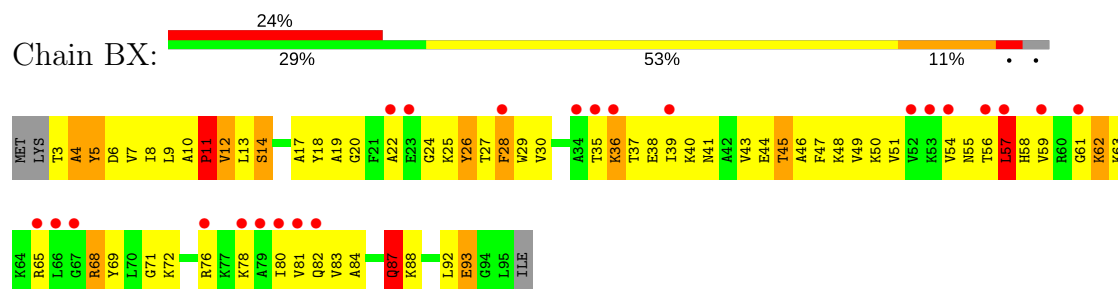
• Molecule 53: 50S RIBOSOMAL PROTEIN L21



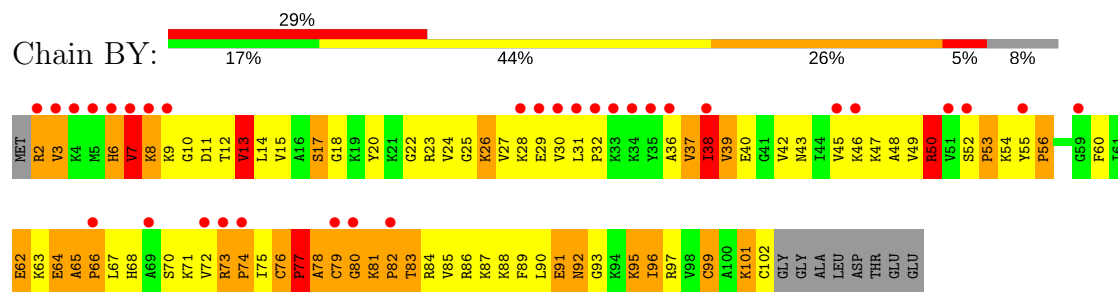
• Molecule 54: 50S RIBOSOMAL PROTEIN L22



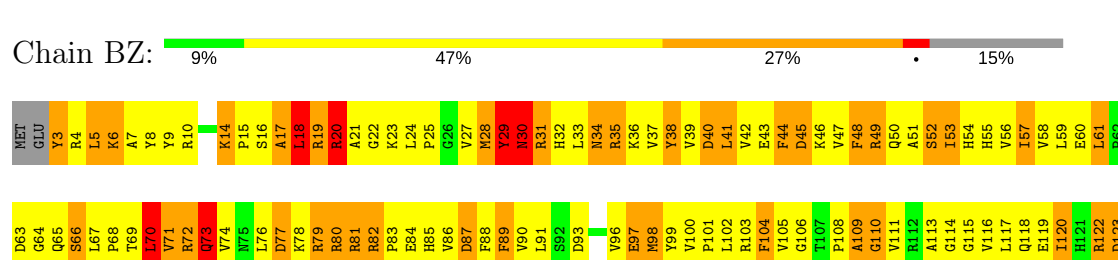
• Molecule 55: 50S RIBOSOMAL PROTEIN L23

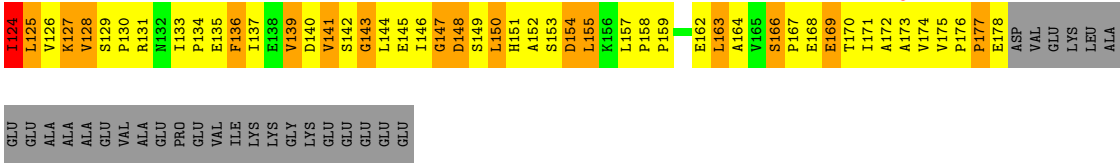


• Molecule 56: 50S RIBOSOMAL PROTEIN L24



• Molecule 57: 50S RIBOSOMAL PROTEIN L25





GLU
GLU
ALA
ALA
ALA
GLU
VAL
ALA
ALA
PRO
GLU
VAL
ILE
LYS
LYS
GLY
LYS
GLU
GLU
GLU
GLU

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	204.70Å 229.30Å 307.00Å 90.00° 90.17° 90.00°	Depositor
Resolution (Å)	44.90 – 3.80 44.91 – 3.60	Depositor EDS
% Data completeness (in resolution range)	98.7 (44.90-3.80) 96.6 (44.91-3.60)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 3.57Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.293 , 0.351 0.306 , 0.353	Depositor DCC
R_{free} test set	5623 reflections (2.09%)	DCC
Wilson B-factor (Å ²)	110.2	Xtriage
Anisotropy	0.390	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.17 , 38.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.31$, $\langle L^2 \rangle = 0.15$	Xtriage
Estimated twinning fraction	0.166 for h,-k,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	151017	wwPDB-VP
Average B, all atoms (Å ²)	147.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.32% 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 ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GCP

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	0.79	12/36190 (0.0%)	0.89	56/56486 (0.1%)
2	AB	0.62	0/1936	0.96	1/2611 (0.0%)
3	AC	0.60	0/1637	0.93	3/2207 (0.1%)
4	AD	0.50	0/1733	0.86	2/2318 (0.1%)
5	AE	0.63	0/1163	0.94	1/1566 (0.1%)
6	AF	0.56	0/856	0.88	0/1154
7	AG	0.59	0/1276	0.85	0/1709
8	AH	0.56	0/1136	0.91	1/1527 (0.1%)
9	AI	0.56	0/1029	0.83	0/1378
10	AJ	0.59	0/808	0.88	0/1087
11	AK	0.57	0/900	0.89	0/1213
12	AL	0.59	0/987	1.01	2/1322 (0.2%)
13	AM	0.59	0/999	0.95	0/1338
14	AN	0.71	0/501	1.03	1/664 (0.2%)
15	AO	0.65	0/745	0.86	0/992
16	AP	0.53	0/717	0.88	0/965
17	AQ	0.61	0/837	0.92	1/1119 (0.1%)
18	AR	0.60	0/579	0.89	1/768 (0.1%)
19	AS	0.68	0/643	0.91	1/867 (0.1%)
20	AT	0.54	0/765	0.80	0/1007
21	AU	0.70	0/213	0.95	1/279 (0.4%)
22	AV	0.65	0/1832	0.82	0/2855
23	AX	0.66	0/216	0.77	0/335
24	AY	1.05	19/4005 (0.5%)	1.16	32/5407 (0.6%)
25	B0	0.61	0/671	0.98	2/892 (0.2%)
26	B1	0.49	0/739	0.85	0/983
27	B2	0.51	0/600	0.82	0/793
28	B3	0.57	0/473	0.93	0/636
29	B4	0.69	0/350	0.80	0/476
30	B5	0.64	0/473	0.89	0/639
31	B6	0.79	0/440	1.09	2/586 (0.3%)
32	B7	0.53	0/427	0.79	0/563

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	B8	0.68	0/516	0.92	0/681
34	B9	0.53	0/310	0.85	0/407
35	BA	0.76	16/69976 (0.0%)	0.86	82/109244 (0.1%)
36	BB	0.76	1/2853 (0.0%)	0.89	5/4451 (0.1%)
37	BC	0.81	4/1775 (0.2%)	0.94	4/2392 (0.2%)
38	BD	0.69	0/2195	1.07	9/2955 (0.3%)
39	BE	0.59	0/1597	0.95	1/2155 (0.0%)
40	BF	0.61	0/1659	0.88	0/2246
41	BG	0.58	0/1499	0.92	3/2016 (0.1%)
42	BH	0.66	0/1211	0.88	0/1636
43	BJ	0.53	0/7	0.70	0/8
45	BN	0.57	0/1132	0.91	1/1527 (0.1%)
46	BO	0.60	0/943	0.90	0/1269
47	BP	0.57	0/1131	1.08	6/1504 (0.4%)
48	BQ	0.63	0/1143	1.00	3/1527 (0.2%)
49	BR	0.49	0/974	0.92	1/1302 (0.1%)
50	BS	0.66	0/779	1.12	6/1038 (0.6%)
51	BT	0.60	0/1156	0.92	3/1544 (0.2%)
52	BU	0.63	0/975	0.91	1/1297 (0.1%)
53	BV	0.54	0/790	0.97	2/1057 (0.2%)
54	BW	0.59	0/907	0.82	0/1216
55	BX	0.63	0/740	0.83	1/995 (0.1%)
56	BY	0.61	0/789	0.90	0/1053
57	BZ	0.62	0/1435	0.95	0/1949
All	All	0.73	52/162368 (0.0%)	0.89	235/242211 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AA	3	125
9	AI	0	1
11	AK	0	1
17	AQ	0	1
21	AU	0	1
22	AV	0	5
24	AY	0	5
30	B5	0	1
35	BA	3	160
36	BB	0	12

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
42	BH	0	1
45	BN	0	1
48	BQ	0	1
53	BV	0	1
All	All	6	316

The worst 5 of 52 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AY	191	TYR	CE2-CZ	11.85	1.53	1.38
24	AY	189	GLU	CG-CD	-10.57	1.36	1.51
24	AY	191	TYR	CD1-CE1	10.46	1.55	1.39
24	AY	504	ILE	C-N	-9.62	1.11	1.34
24	AY	444	LEU	C-N	-9.54	1.12	1.34

The worst 5 of 235 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AY	191	TYR	CB-CG-CD1	-18.01	110.19	121.00
24	AY	307	MET	CG-SD-CE	13.35	121.55	100.20
24	AY	319	ARG	NE-CZ-NH1	12.45	126.52	120.30
24	AY	504	ILE	C-N-CA	-12.18	91.26	121.70
1	AA	1498	U	C2'-C3'-O3'	11.78	135.42	109.50

5 of 6 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	AA	1049	U	C3'
1	AA	1399	C	C3'
1	AA	1498	U	C3'
35	BA	1300	U	C3'
35	BA	1799	G	C3'

5 of 316 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	12	U	Sidechain
1	AA	17	U	Sidechain
1	AA	19	C	Sidechain
1	AA	28	G	Sidechain
1	AA	96	U	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	32329	0	16318	2581	0
2	AB	1901	0	1951	513	1
3	AC	1613	0	1677	306	0
4	AD	1703	0	1767	335	0
5	AE	1147	0	1207	231	0
6	AF	843	0	857	144	0
7	AG	1257	0	1296	177	0
8	AH	1116	0	1177	205	0
9	AI	1011	0	1043	205	0
10	AJ	795	0	840	196	0
11	AK	885	0	904	152	0
12	AL	971	0	1057	217	0
13	AM	988	0	1059	192	0
14	AN	492	0	533	153	0
15	AO	734	0	771	229	0
16	AP	701	0	720	131	0
17	AQ	824	0	891	158	0
18	AR	574	0	644	122	0
19	AS	630	0	652	209	0
20	AT	763	0	861	150	0
21	AU	209	0	221	48	0
22	AV	1640	0	837	194	0
23	AX	192	0	99	22	0
24	AY	3934	0	3922	1256	0
25	B0	662	0	688	138	0
26	B1	732	0	808	131	0
27	B2	598	0	653	126	0
28	B3	468	0	523	108	0
29	B4	341	0	339	89	0
30	B5	459	0	480	131	0
31	B6	433	0	461	109	0
32	B7	419	0	467	110	0
33	B8	508	0	576	154	0
34	B9	307	0	338	70	0
35	BA	62477	0	31497	5291	0
36	BB	2551	0	1295	230	0
37	BC	1742	0	1794	377	1

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	BD	2145	0	2234	780	0
39	BE	1564	0	1629	448	0
40	BF	1624	0	1677	415	0
41	BG	1474	0	1535	340	0
42	BH	1189	0	1247	282	0
43	BJ	654	0	157	36	0
44	BK	701	0	168	41	0
45	BN	1105	0	1180	270	0
46	BO	933	0	996	182	0
47	BP	1114	0	1187	361	0
48	BQ	1122	0	1179	291	0
49	BR	960	0	1021	236	0
50	BS	771	0	832	206	0
51	BT	1142	0	1202	332	0
52	BU	958	0	1015	317	0
53	BV	779	0	852	219	0
54	BW	896	0	953	173	0
55	BX	726	0	778	114	0
56	BY	776	0	870	193	0
57	BZ	1403	0	1432	371	0
58	AY	32	0	14	11	0
All	All	151017	0	103381	18980	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 75.

The worst 5 of 18980 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)
24:AY:111:MET:CE	24:AY:139:THR:HG23	1.18	1.62
24:AY:331:LEU:CD2	24:AY:379:PHE:HD2	1.19	1.51
24:AY:331:LEU:HD22	24:AY:379:PHE:CD2	1.46	1.47
37:BC:127:MET:SD	37:BC:127:MET:CG	2.03	1.45
24:AY:135:THR:CG2	24:AY:136:PRO:HD2	1.44	1.45

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)
2:AB:62:ALA:O	37:BC:30:LYS:O[2_656]	2.18	0.02

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	
2	AB	233/256 (91%)	110 (47%)	62 (27%)	61 (26%)	0	1
3	AC	205/239 (86%)	134 (65%)	39 (19%)	32 (16%)	0	4
4	AD	206/209 (99%)	131 (64%)	51 (25%)	24 (12%)	0	8
5	AE	149/162 (92%)	108 (72%)	31 (21%)	10 (7%)	1	23
6	AF	99/101 (98%)	67 (68%)	24 (24%)	8 (8%)	1	17
7	AG	153/156 (98%)	85 (56%)	44 (29%)	24 (16%)	0	4
8	AH	136/138 (99%)	94 (69%)	26 (19%)	16 (12%)	0	8
9	AI	125/128 (98%)	78 (62%)	28 (22%)	19 (15%)	0	5
10	AJ	97/105 (92%)	60 (62%)	23 (24%)	14 (14%)	0	5
11	AK	117/129 (91%)	72 (62%)	32 (27%)	13 (11%)	0	9
12	AL	123/135 (91%)	66 (54%)	33 (27%)	24 (20%)	0	2
13	AM	123/126 (98%)	63 (51%)	31 (25%)	29 (24%)	0	1
14	AN	58/61 (95%)	33 (57%)	12 (21%)	13 (22%)	0	1
15	AO	86/89 (97%)	59 (69%)	21 (24%)	6 (7%)	1	22
16	AP	82/88 (93%)	55 (67%)	17 (21%)	10 (12%)	0	7
17	AQ	98/105 (93%)	82 (84%)	10 (10%)	6 (6%)	2	25
18	AR	68/88 (77%)	37 (54%)	18 (26%)	13 (19%)	0	2
19	AS	77/93 (83%)	42 (54%)	18 (23%)	17 (22%)	0	1
20	AT	97/106 (92%)	46 (47%)	32 (33%)	19 (20%)	0	2
21	AU	23/27 (85%)	11 (48%)	8 (35%)	4 (17%)	0	3
24	AY	488/529 (92%)	314 (64%)	88 (18%)	86 (18%)	0	3
25	B0	82/85 (96%)	64 (78%)	9 (11%)	9 (11%)	0	9
26	B1	92/98 (94%)	63 (68%)	16 (17%)	13 (14%)	0	5
27	B2	69/72 (96%)	38 (55%)	22 (32%)	9 (13%)	0	6
28	B3	58/60 (97%)	38 (66%)	15 (26%)	5 (9%)	1	16

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	B4	43/71 (61%)	26 (60%)	9 (21%)	8 (19%)	0	2
30	B5	57/60 (95%)	34 (60%)	11 (19%)	12 (21%)	0	2
31	B6	48/54 (89%)	18 (38%)	16 (33%)	14 (29%)	0	0
32	B7	47/49 (96%)	29 (62%)	10 (21%)	8 (17%)	0	4
33	B8	62/65 (95%)	30 (48%)	16 (26%)	16 (26%)	0	1
34	B9	35/37 (95%)	19 (54%)	10 (29%)	6 (17%)	0	4
37	BC	226/229 (99%)	158 (70%)	39 (17%)	29 (13%)	0	7
38	BD	273/276 (99%)	195 (71%)	46 (17%)	32 (12%)	0	8
39	BE	203/206 (98%)	99 (49%)	48 (24%)	56 (28%)	0	0
40	BF	206/210 (98%)	134 (65%)	35 (17%)	37 (18%)	0	3
41	BG	179/182 (98%)	95 (53%)	47 (26%)	37 (21%)	0	2
42	BH	154/180 (86%)	111 (72%)	23 (15%)	20 (13%)	0	6
43	BJ	1/173 (1%)	1 (100%)	0	0	100	100
45	BN	137/140 (98%)	78 (57%)	28 (20%)	31 (23%)	0	1
46	BO	120/122 (98%)	84 (70%)	23 (19%)	13 (11%)	0	10
47	BP	144/150 (96%)	70 (49%)	37 (26%)	37 (26%)	0	1
48	BQ	139/141 (99%)	79 (57%)	40 (29%)	20 (14%)	0	5
49	BR	115/118 (98%)	69 (60%)	27 (24%)	19 (16%)	0	4
50	BS	97/112 (87%)	41 (42%)	23 (24%)	33 (34%)	0	0
51	BT	136/146 (93%)	75 (55%)	31 (23%)	30 (22%)	0	1
52	BU	115/118 (98%)	59 (51%)	27 (24%)	29 (25%)	0	1
53	BV	99/101 (98%)	56 (57%)	21 (21%)	22 (22%)	0	1
54	BW	111/113 (98%)	72 (65%)	25 (22%)	14 (13%)	0	7
55	BX	91/96 (95%)	55 (60%)	27 (30%)	9 (10%)	1	12
56	BY	99/110 (90%)	33 (33%)	36 (36%)	30 (30%)	0	0
57	BZ	174/206 (84%)	88 (51%)	48 (28%)	38 (22%)	0	1
All	All	6255/6850 (91%)	3758 (60%)	1413 (23%)	1084 (17%)	0	3

5 of 1084 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	9	GLU
2	AB	15	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	AB	18	GLY
2	AB	19	HIS
2	AB	24	TRP

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	AB	202/220 (92%)	152 (75%)	50 (25%)	1	6
3	AC	160/188 (85%)	133 (83%)	27 (17%)	2	18
4	AD	180/181 (99%)	154 (86%)	26 (14%)	4	25
5	AE	115/123 (94%)	94 (82%)	21 (18%)	2	14
6	AF	90/90 (100%)	76 (84%)	14 (16%)	3	22
7	AG	126/127 (99%)	114 (90%)	12 (10%)	10	42
8	AH	119/119 (100%)	101 (85%)	18 (15%)	3	23
9	AI	98/99 (99%)	82 (84%)	16 (16%)	3	20
10	AJ	88/92 (96%)	71 (81%)	17 (19%)	1	12
11	AK	90/99 (91%)	73 (81%)	17 (19%)	2	13
12	AL	104/111 (94%)	86 (83%)	18 (17%)	2	17
13	AM	99/101 (98%)	79 (80%)	20 (20%)	1	11
14	AN	49/50 (98%)	36 (74%)	13 (26%)	0	4
15	AO	79/80 (99%)	52 (66%)	27 (34%)	0	1
16	AP	72/74 (97%)	64 (89%)	8 (11%)	7	35
17	AQ	94/97 (97%)	85 (90%)	9 (10%)	10	41
18	AR	61/77 (79%)	54 (88%)	7 (12%)	6	34
19	AS	69/80 (86%)	58 (84%)	11 (16%)	3	21
20	AT	76/82 (93%)	69 (91%)	7 (9%)	11	43
21	AU	19/22 (86%)	17 (90%)	2 (10%)	8	37
24	AY	427/453 (94%)	308 (72%)	119 (28%)	0	4

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	B0	66/67 (98%)	49 (74%)	17 (26%)	0	5
26	B1	78/83 (94%)	65 (83%)	13 (17%)	2	19
27	B2	66/67 (98%)	61 (92%)	5 (8%)	15	52
28	B3	51/52 (98%)	42 (82%)	9 (18%)	2	16
29	B4	39/63 (62%)	29 (74%)	10 (26%)	0	5
30	B5	51/52 (98%)	47 (92%)	4 (8%)	15	51
31	B6	49/52 (94%)	37 (76%)	12 (24%)	1	6
32	B7	41/42 (98%)	36 (88%)	5 (12%)	6	30
33	B8	53/55 (96%)	42 (79%)	11 (21%)	1	10
34	B9	34/34 (100%)	26 (76%)	8 (24%)	1	7
37	BC	180/181 (99%)	150 (83%)	30 (17%)	2	19
38	BD	217/218 (100%)	150 (69%)	67 (31%)	0	3
39	BE	165/166 (99%)	134 (81%)	31 (19%)	2	13
40	BF	165/166 (99%)	142 (86%)	23 (14%)	4	27
41	BG	155/156 (99%)	127 (82%)	28 (18%)	2	15
42	BH	128/148 (86%)	90 (70%)	38 (30%)	0	3
43	BJ	1/1 (100%)	1 (100%)	0	100	100
45	BN	117/119 (98%)	99 (85%)	18 (15%)	3	22
46	BO	100/100 (100%)	89 (89%)	11 (11%)	7	36
47	BP	112/116 (97%)	91 (81%)	21 (19%)	2	13
48	BQ	111/111 (100%)	87 (78%)	24 (22%)	1	9
49	BR	100/101 (99%)	78 (78%)	22 (22%)	1	8
50	BS	77/88 (88%)	60 (78%)	17 (22%)	1	8
51	BT	120/127 (94%)	96 (80%)	24 (20%)	1	11
52	BU	92/94 (98%)	74 (80%)	18 (20%)	1	12
53	BV	82/82 (100%)	65 (79%)	17 (21%)	1	10
54	BW	91/92 (99%)	81 (89%)	10 (11%)	7	36
55	BX	74/78 (95%)	63 (85%)	11 (15%)	3	23
56	BY	84/91 (92%)	69 (82%)	15 (18%)	2	15
57	BZ	155/179 (87%)	117 (76%)	38 (24%)	1	6
All	All	5271/5546 (95%)	4255 (81%)	1016 (19%)	1	12

5 of 1016 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
25	B0	5	LYS
37	BC	108	MET
53	BV	91	TYR
25	B0	80	HIS
30	B5	25	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 184 such sidechains are listed below:

Mol	Chain	Res	Type
25	B0	70	GLN
33	B8	35	GLN
53	BV	89	GLN
26	B1	45	ASN
28	B3	52	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1503/1522 (98%)	273 (18%)	0
22	AV	76/77 (98%)	36 (47%)	0
23	AX	8/9 (88%)	5 (62%)	0
35	BA	2900/2915 (99%)	654 (22%)	0
36	BB	118/122 (96%)	24 (20%)	0
All	All	4605/4645 (99%)	992 (21%)	0

5 of 992 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	7	G
1	AA	9	G
1	AA	31	G
1	AA	32	A
1	AA	39	G

There are no RNA pucker outliers to report.

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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
58	GCP	AY	1000	-	25,34,34	2.79	7 (28%)	28,54,54	1.43	7 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	GCP	AY	1000	-	-	0/18/38/38	0/3/3/3

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	AY	1000	GCP	C4-N9	-5.77	1.40	1.47
58	AY	1000	GCP	C5-C6	-5.04	1.43	1.53
58	AY	1000	GCP	PG-O2G	-2.72	1.48	1.54
58	AY	1000	GCP	PG-O3G	-2.02	1.50	1.54
58	AY	1000	GCP	PG-O1G	2.15	1.54	1.50

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	AY	1000	GCP	O3G-PG-O1G	-2.61	105.32	112.32
58	AY	1000	GCP	PA-O3A-PB	-2.37	124.74	132.39
58	AY	1000	GCP	O2G-PG-O1G	-2.32	106.11	112.32
58	AY	1000	GCP	O6-C6-N1	-2.27	119.68	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	AY	1000	GCP	O2'-C2'-C3'	2.01	118.27	111.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	AY	1000	GCP	11	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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	1504/1522 (98%)	-0.13	36 (2%) 59 49	52, 140, 199, 200	0
2	AB	235/256 (91%)	-0.44	1 (0%) 92 88	40, 110, 177, 200	0
3	AC	207/239 (86%)	-0.49	2 (0%) 82 75	37, 117, 174, 200	0
4	AD	208/209 (99%)	0.23	13 (6%) 21 15	48, 158, 200, 200	0
5	AE	151/162 (93%)	-0.17	3 (1%) 65 56	38, 112, 171, 200	0
6	AF	101/101 (100%)	-0.60	0 100 100	59, 135, 188, 200	0
7	AG	155/156 (99%)	-0.37	4 (2%) 56 46	46, 128, 189, 200	0
8	AH	138/138 (100%)	-0.10	6 (4%) 36 28	36, 114, 180, 200	0
9	AI	127/128 (99%)	-0.11	2 (1%) 72 63	32, 121, 172, 200	0
10	AJ	99/105 (94%)	0.40	10 (10%) 8 7	32, 125, 191, 200	0
11	AK	119/129 (92%)	-0.10	5 (4%) 37 29	40, 116, 179, 200	0
12	AL	125/135 (92%)	0.25	6 (4%) 31 25	45, 119, 192, 200	0
13	AM	125/126 (99%)	0.29	11 (8%) 11 9	64, 127, 200, 200	0
14	AN	60/61 (98%)	-0.28	0 100 100	28, 104, 172, 200	0
15	AO	88/89 (98%)	0.05	4 (4%) 34 27	59, 130, 188, 200	0
16	AP	84/88 (95%)	1.03	18 (21%) 1 1	79, 156, 200, 200	0
17	AQ	100/105 (95%)	0.70	12 (12%) 5 5	66, 141, 200, 200	0
18	AR	70/88 (79%)	-0.01	3 (4%) 36 28	59, 124, 176, 200	0
19	AS	79/93 (84%)	0.13	4 (5%) 29 23	57, 118, 197, 200	0
20	AT	99/106 (93%)	0.54	10 (10%) 8 7	87, 153, 200, 200	0
21	AU	25/27 (92%)	0.71	4 (16%) 2 3	46, 117, 175, 185	0
22	AV	77/77 (100%)	-0.67	1 (1%) 77 69	77, 151, 189, 199	0
23	AX	9/9 (100%)	0.17	0 100 100	79, 156, 192, 199	0
24	AY	496/529 (93%)	0.43	52 (10%) 7 6	71, 170, 202, 202	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	B0	84/85 (98%)	1.14	19 (22%) 1 1	37, 118, 194, 200	0
26	B1	94/98 (95%)	0.58	8 (8%) 11 10	65, 143, 197, 200	0
27	B2	71/72 (98%)	0.13	7 (9%) 8 7	101, 153, 200, 200	0
28	B3	60/60 (100%)	0.68	6 (10%) 8 7	54, 126, 198, 200	0
29	B4	45/71 (63%)	-0.05	3 (6%) 19 14	108, 174, 200, 200	0
30	B5	59/60 (98%)	0.39	8 (13%) 3 4	62, 150, 200, 200	0
31	B6	50/54 (92%)	0.79	11 (22%) 1 1	62, 139, 186, 200	0
32	B7	49/49 (100%)	0.56	5 (10%) 7 6	78, 153, 197, 200	0
33	B8	64/65 (98%)	0.13	2 (3%) 49 39	66, 129, 179, 200	0
34	B9	37/37 (100%)	1.40	11 (29%) 1 1	71, 142, 178, 194	0
35	BA	2901/2915 (99%)	0.10	113 (3%) 40 32	51, 159, 201, 202	0
36	BB	119/122 (97%)	-0.47	0 100 100	66, 123, 172, 190	0
37	BC	228/229 (99%)	2.01	89 (39%) 0 1	87, 182, 200, 200	0
38	BD	275/276 (99%)	0.15	21 (7%) 15 11	40, 117, 175, 200	0
39	BE	205/206 (99%)	0.20	18 (8%) 11 9	51, 143, 199, 200	0
40	BF	208/210 (99%)	0.51	27 (12%) 4 4	51, 156, 200, 200	0
41	BG	181/182 (99%)	-0.08	4 (2%) 62 53	47, 134, 194, 200	0
42	BH	156/180 (86%)	0.31	13 (8%) 12 10	78, 165, 200, 200	0
43	BJ	1/173 (0%)	3.30	1 (100%) 0 0	174, 174, 174, 174	0
44	BK	0/147	-	-	-	-
45	BN	139/140 (99%)	0.01	2 (1%) 75 67	69, 131, 190, 200	0
46	BO	122/122 (100%)	0.47	15 (12%) 5 5	59, 133, 198, 200	0
47	BP	146/150 (97%)	0.86	22 (15%) 3 3	65, 147, 200, 200	0
48	BQ	141/141 (100%)	0.04	6 (4%) 36 28	20, 107, 171, 200	0
49	BR	117/118 (99%)	0.80	19 (16%) 2 3	81, 169, 200, 200	0
50	BS	99/112 (88%)	0.05	9 (9%) 10 8	49, 123, 194, 200	0
51	BT	138/146 (94%)	0.51	20 (14%) 3 3	89, 162, 200, 200	0
52	BU	117/118 (99%)	-0.05	3 (2%) 56 46	47, 121, 179, 200	0
53	BV	101/101 (100%)	0.82	17 (16%) 2 2	42, 146, 200, 200	0
54	BW	113/113 (100%)	1.30	35 (30%) 0 1	78, 165, 200, 200	0
55	BX	93/96 (96%)	1.10	23 (24%) 1 1	38, 167, 200, 200	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
56	BY	101/110 (91%)	1.53	32 (31%) 0 1	86, 169, 200, 200	0
57	BZ	176/206 (85%)	-0.29	1 (0%) 89 85	43, 122, 195, 200	0
All	All	10971/11642 (94%)	0.18	777 (7%) 17 12	20, 146, 200, 202	0

The worst 5 of 777 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
37	BC	165	ASN	14.2
37	BC	173	ALA	12.1
37	BC	216	THR	11.9
28	B3	1	MET	11.1
24	AY	349	MET	10.9

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 carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
58	GCP	AY	1000	32/32	0.82	0.24	-0.50	95,109,121,122	0

6.5 Other polymers [i](#)

There are no such residues in this entry.