



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 28, 2026 – 07:39 PM UTC

PDB ID : 4V4T / pdb_00004v4t
Title : Crystal structure of the whole ribosomal complex with a stop codon in the A-site.
Authors : Petry, S.; Brodersen, D.E.; Murphy IV, F.V.; Dunham, C.M.; Selmer, M.; Tarry, M.J.; Kelley, A.C.; Ramakrishnan, V.
Deposited on : 2005-10-12
Resolution : 6.46 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

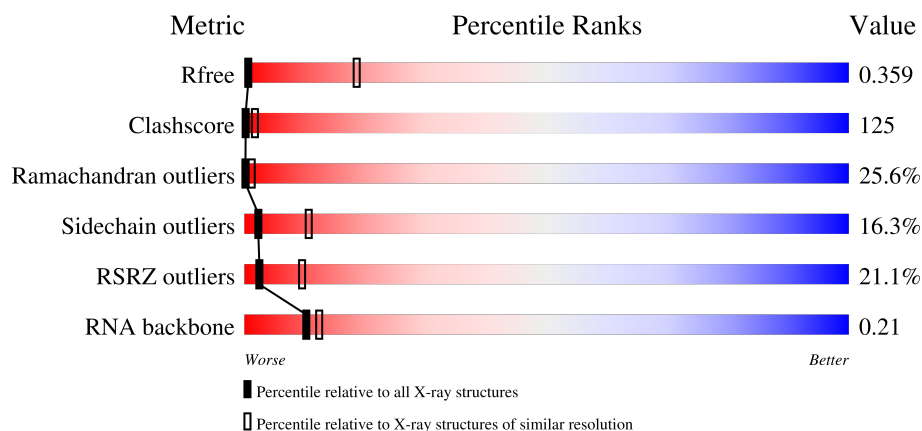
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 6.46 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	1157 (8.90-4.00)
Clashscore	190562	1019 (8.90-4.02)
Ramachandran outliers	187476	1045 (8.90-4.00)
Sidechain outliers	187428	1010 (8.90-4.00)
RSRZ outliers	180081	1150 (8.90-4.00)
RNA backbone	3983	1055 (9.50-3.10)

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	AV	76	
3	AW	76	
4	AX	18	

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Mol	Chain	Length	Quality of chain
5	AB	256	
6	AC	239	
7	AD	209	
8	AE	162	
9	AF	101	
10	AG	156	
11	AH	138	
12	AI	128	
13	AJ	105	
14	AK	129	
15	AL	135	
16	AM	126	
17	AN	61	
18	AO	89	
19	AP	88	
20	AQ	105	
21	AR	88	
22	AS	93	
23	AT	106	
24	AU	27	
25	BB	123	
26	BA	2916	
27	BD	173	
28	BE	338	
29	BF	246	

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Mol	Chain	Length	Quality of chain
30	BG	176	
31	BH	177	
32	BI	149	
33	BN	145	
34	BO	122	
35	BP	164	
36	BQ	138	
37	BS	186	
38	BT	66	
39	BW	113	
40	BX	84	
41	BY	119	
42	BZ	253	
43	BR	118	
44	BU	118	
45	BV	100	
46	B2	70	
47	B3	60	
48	B0	91	
49	B4	73	
50	B5	60	
51	B6	82	
52	B7	47	
53	B8	64	
54	B9	36	

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Mol	Chain	Length	Quality of chain
55	BK	141	

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
3	YYG	AW	37	X	-	X	-

2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 142447 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 ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1515	Total	C	N	O	P	0	0	0
			32551	14490	6022	10525	1514			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AA	416	G	-	insertion	GB 155076
AA	905	U	-	insertion	GB 155076
AA	1395	C	-	insertion	GB 155076

- Molecule 2 is a RNA chain called P-site tRNA (Phe).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AV	76	Total	C	N	O	P	0	0	0
			1622	725	293	529	75			

- Molecule 3 is a RNA chain called E-site tRNA (Phe).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AW	76	Total	C	N	O	P	0	0	0
			1638	736	294	533	75			

- Molecule 4 is a RNA chain called 5'-D(*AP*UP*GP*UP*UP*CP*UP*AP*GP*UP*AP*C
P*AP*AP*UP*AP*AP*U)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AX	17	Total	C	N	O	P	0	0	11
			136	56	19	44	17			

- Molecule 5 is a protein called 30S ribosomal protein S2.

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

- Molecule 6 is a protein called 30S ribosomal protein S3.

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

- Molecule 7 is a protein called 30S ribosomal protein S4.

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

- Molecule 8 is a protein called 30S ribosomal protein S5.

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

- Molecule 9 is a protein called 30S ribosomal protein S6.

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

- Molecule 10 is a protein called 30S ribosomal protein S7.

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

- Molecule 11 is a protein called 30S ribosomal protein S8.

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

- Molecule 12 is a protein called 30S ribosomal protein S9.

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

- Molecule 13 is a protein called 30S ribosomal protein S10.

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

- Molecule 14 is a protein called 30S ribosomal protein S11.

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

- Molecule 15 is a protein called 30S ribosomal protein S12.

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

- Molecule 16 is a protein called 30S ribosomal protein S13.

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

- Molecule 17 is a protein called 30S ribosomal protein S14.

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

- Molecule 18 is a protein called 30S ribosomal protein S15.

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

- Molecule 19 is a protein called 30S ribosomal protein S16.

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

- Molecule 20 is a protein called 30S ribosomal protein S17.

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

- Molecule 21 is a protein called 30S ribosomal protein S18.

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

- Molecule 22 is a protein called 30S ribosomal protein S19.

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

- Molecule 23 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AT	99	Total	C	N	O	S	0	0	0
			762	469	162	129	2			

- Molecule 24 is a protein called 30S ribosomal protein Thx.

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

- 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
			2637	1175	488	852	122			

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 26 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	BA	2814	Total	C	N	O	P	0	0	0
			60600	26974	11331	19482	2813			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BA	493	G	-	insertion	GB 48268

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 33 is a protein called 50S ribosomal protein L13.

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

- Molecule 34 is a protein called 50S ribosomal protein L14.

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

- Molecule 35 is a protein called 50S ribosomal protein L15.

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

- Molecule 36 is a protein called 50S ribosomal protein L16.

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

- Molecule 37 is a protein called 50S ribosomal protein L18.

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

- Molecule 38 is a protein called 50S ribosomal protein L19.

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

- Molecule 39 is a protein called 50S ribosomal protein L22.

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

- Molecule 40 is a protein called 50S ribosomal protein L23.

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

- Molecule 41 is a protein called 50S ribosomal protein 24.

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

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

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

- Molecule 43 is a protein called 50S ribosomal protein L17.

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

- Molecule 44 is a protein called 50S ribosomal protein L20.

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

- Molecule 45 is a protein called 50S ribosomal protein L21.

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

- Molecule 46 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	B2	64	Total	C	N	O	S	0	0	0
			494	301	93	99	1			

- Molecule 47 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	B3	60	Total	C	N	O	S	0	0	0
			477	303	91	82	1			

- Molecule 48 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	B0	86	Total	C	N	O	S	0	0	0
			641	402	124	114	1			

- Molecule 49 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	B4	73	Total	C	N	O	S	0	0	0
			604	382	110	108	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	B5	58	Total	C	N	O	S	0	0	0
			457	281	94	77	5			

- Molecule 51 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	B6	53	Total	C	N	O	S	0	0	0
			431	274	80	76	1			

- Molecule 52 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	B7	46	Total	C	N	O	S	0	0	0
			383	230	91	60	2			

- Molecule 53 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	B8	63	Total	C	N	O	S	0	0	0
			496	312	101	78	5			

- Molecule 54 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	B9	35	Total	C	N	O	S	0	0	0
			285	172	64	45	4			

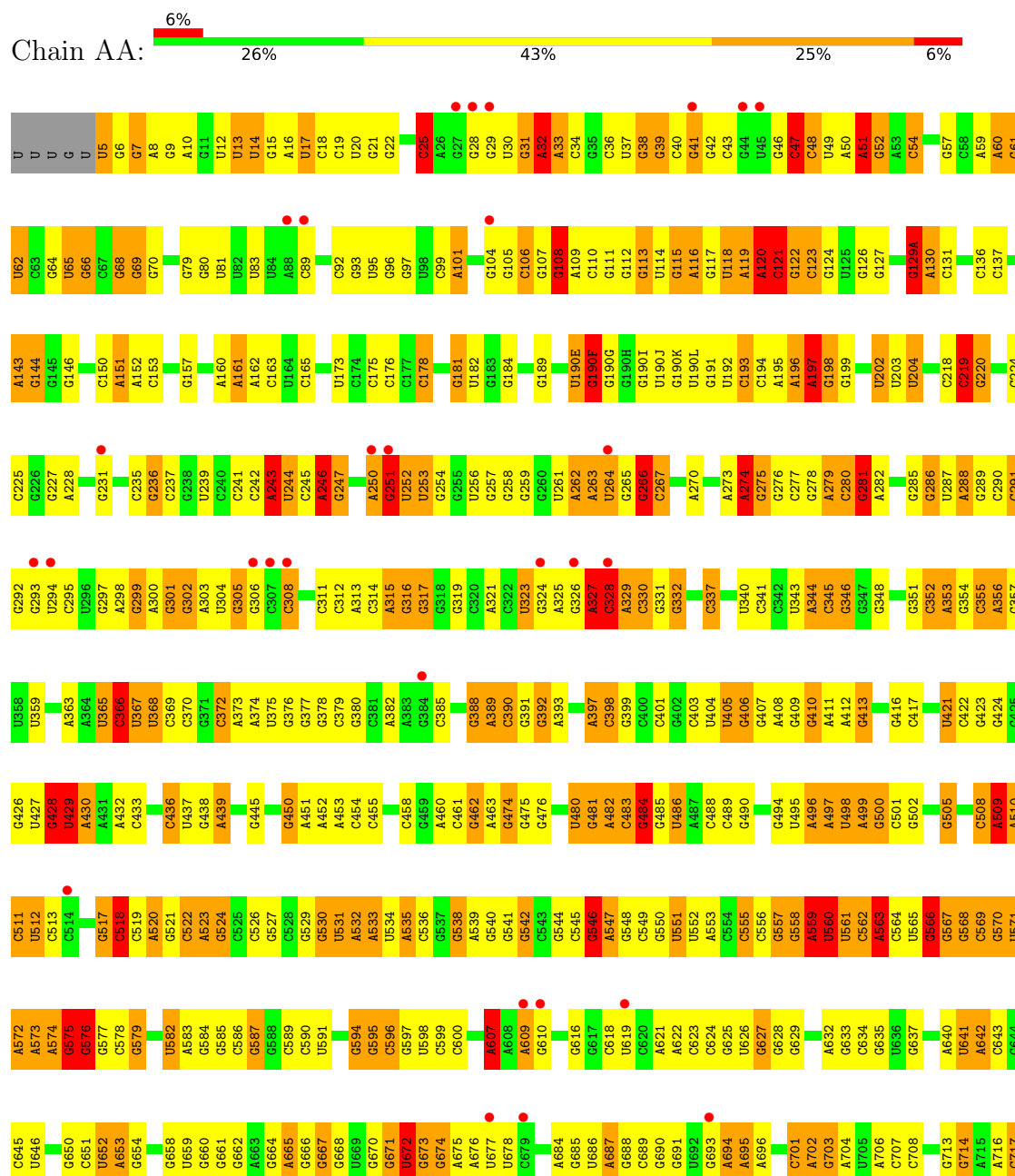
- Molecule 55 is a protein called 50S ribosomal protein L11.

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

3 Residue-property plots [i](#)

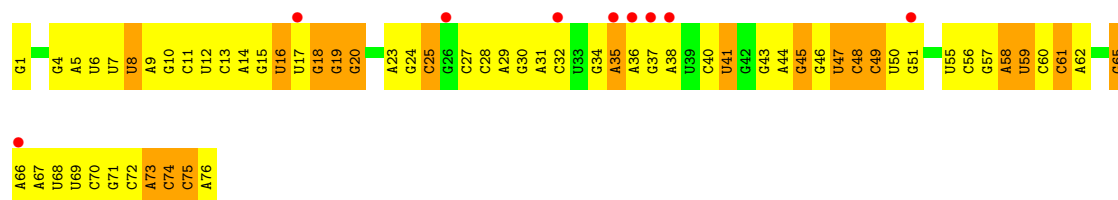
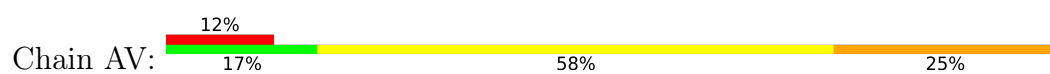
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 ribosomal RNA

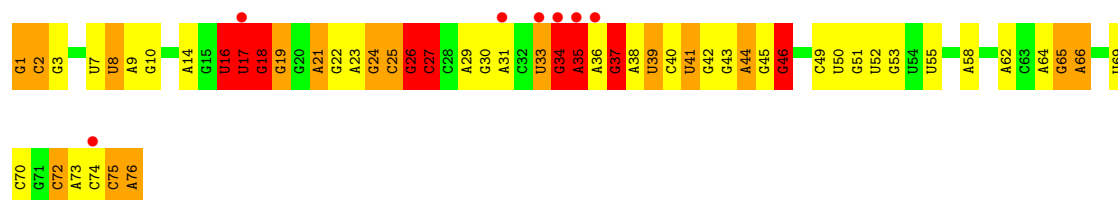


A1507	G1432	C1367	U1308	U1177	C1045	G976	A915	G853	A781	G718
G1508	U1436	G1368	G1309	G1178	A1046	A977	G916	G854	A782	C719
C1509	C1437	C1369	G1310	A1180	G1047	C978	G917	G855	C720	G721
G1510	G1438	G1370	G1311	A1179	G1048	C979	A918	G785	G786	G722
U1511	C1439	G1371	G1312	G1181	U1049	C980	A919	G858	A787	U723
A1512	C1440	U1372	U1313	G1182	U1050	U981	G922	A859	U724	G725
A1513	C1441	C1373	C1314	A1183	G1053	U982	A923	A860	G726	G727
C1514	G1442	A1374	U1315	G1184	C1054	A983	C924	G861	U789	G728
G1515	C1443	C1375	G1316	G1185	C1055	C984	G925	G862	A790	G729
G1516	C1444	U1376	A1317	G1186	U1056	A985	G926	A863	G791	G730
A1517	A1446	A1377	A1318	G1187	U1057	A986	G927	A865	U792	G731
A1518	C1447	C1378	A1319	A1188	G1058	G987	G928	A866	U793	G732
A1519	G1448	G1379	C1320	U1189	C1059	C988	G929	C867	A794	G733
G1520	C1449	U1380	C1321	G1190	U1060	C989	C930	C868	U795	G734
G1521	U1450	U1381	G1322	A1191	G1061	C990	C931	C869	A800	G735
U1522	A1451	C1382	G1323	C1192	U1062	U991	C932	U870	U801	G736
G1523	C1452	A1383	A1324	G1193	U1063	U992	G933	U871	A802	C737
C1524	G1453	C1325	C1325	U1194	C1064	A993	G934	A872	G803	A737
G1525	G1454	G1387	C1326	U1195	U1065	A994	A835	A873	U804	C738
G1526	G1455	A1388	C1327	C1196	U1066	C995	A936	A874	C805	C739
C1527	C1459	C1389	C1328	U1197	A1067	A996	A937	C875	A806	G741
U1528	A1460	U1390	G1329	G1198	U1068	G1002	A938	C876	A807	C744
G1529	C1461	U1391	U1330	U1199	C1069	G1003	G939	C877	C808	C745
G1530	G1462	G1392	G1331	U1199	U1070	G3A	C940	C878	C811	C748
A1531	C1463	U1393	A1332	A1201	C1136	A1004	G941	C879	C812	C749
U1532	A1464	A1394	A1333	G1202	U1137	C1006	G942	C880	U813	A814
C1533	C1465	C1395	G1334	C1203	G1138	C1007	U943	C881	A815	G749
A1534	G1466	C1396	C1335	U1204	C1140	G1073	U944	C882	A816	G750
G1535	C1467	C1397	G1336	A1205	C1141	C1074	G945	C883	C817	U751
C1536	A1468	A1398	G1337	U1206	C1142	C1075	G946	C884	C818	G752
U1539	G1469	C1399	G1338	G1207	U1078	G1013	A946	U884	C819	A753
U1540	C1474	G1401	A1339	C1210	C1079	A1014	C947	C885	C821	G755
U1541	G1475	U1402	A1340	U1211	G1081	A1015	C948	C886	C822	G756
U1542	C1476	C1403	C1342	U1212	U1082	A1016	U950	C887	C823	U757
C	U1481	C1404	G1343	A1213	U1083	G1017	G951	C888	C824	G758
U	G1482	G1405	C1344	C1214	U1084	C1018	U952	A889	G825	A759
	A1483	U1406	U1345	G1215	G1085	U1020	G953	C890	G826	G761
	C1484	C1407	A1346	A1151	U1086	G1021	G954	A892	U827	C762
	U1485	A1408	G1347	C1152	G1087	G1022	U955	C893	C828	G763
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	A1492	A1413	C1352	A1157	U1094	C1029	U960	A900	U831	A768
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	G1496	G1417	G1356	C1161	C1098	G1031	A965	C904	U835	G772
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	U1498	U1419	U1358	C1163	C1100	G1033	C967	G906	U839	G774
	A1499	G1420	A1299	A1228	A1101	U1034	A968	A907	C840	G775
	C1500	G1421	G1300	A1229	A1102	A1035	A969	A908	U841	G776
	G1501	U1426	U1301	G1231	G1103	G1036	C970	A909	C848	A777
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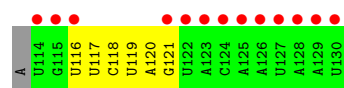
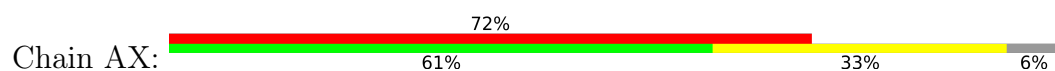
• Molecule 2: P-site tRNA (Phe)



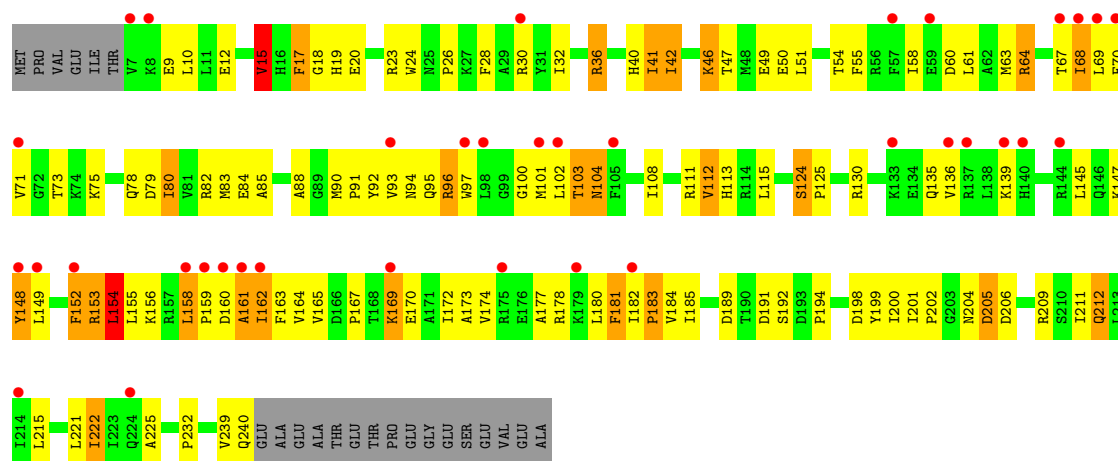
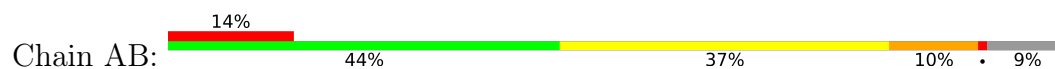
• Molecule 3: E-site tRNA (Phe)



• Molecule 4: 5'-D(*AP*UP*GP*UP*UP*CP*UP*AP*GP*UP*AP*CP*AP*AP*UP*AP*AP*U)-3'

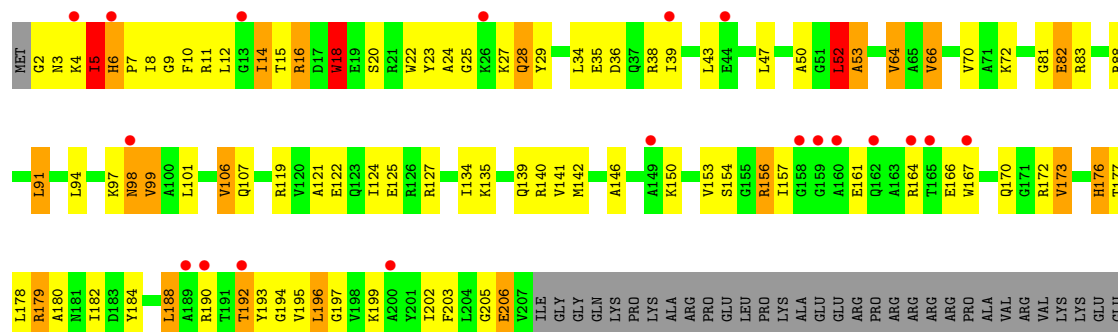


• Molecule 5: 30S ribosomal protein S2

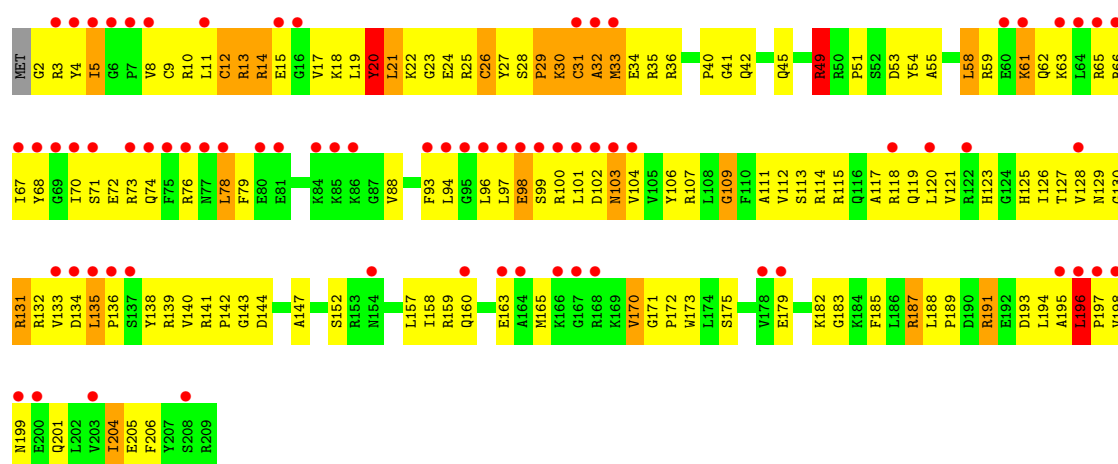


• Molecule 6: 30S ribosomal protein S3

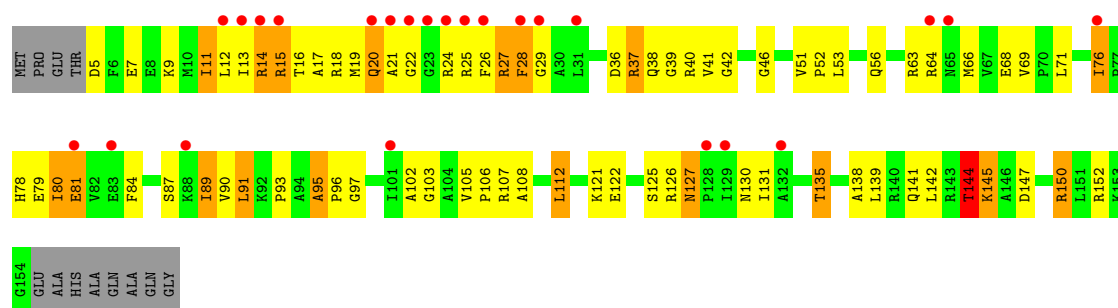




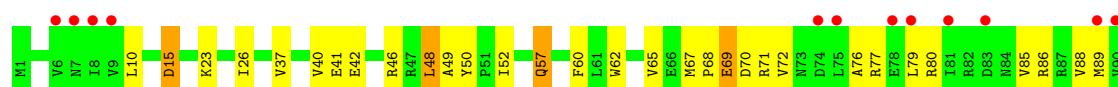
• Molecule 7: 30S ribosomal protein S4



• Molecule 8: 30S ribosomal protein S5

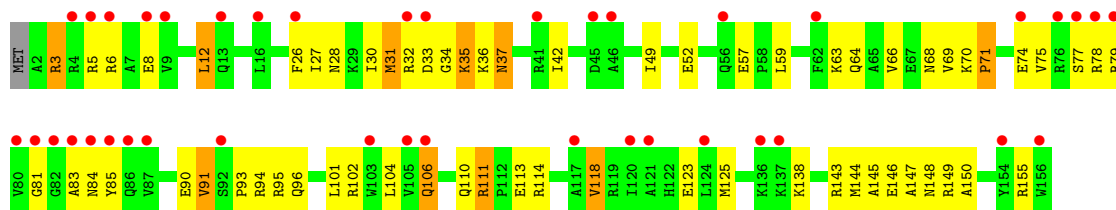


• Molecule 9: 30S ribosomal protein S6

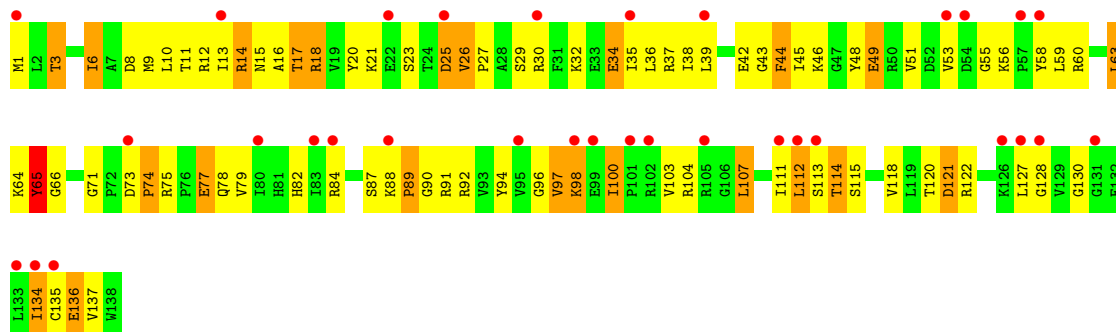




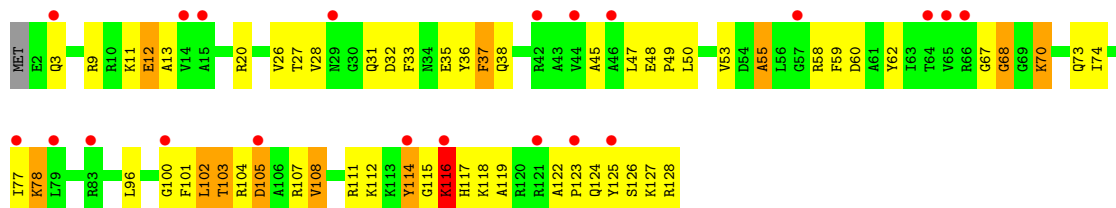
• Molecule 10: 30S ribosomal protein S7



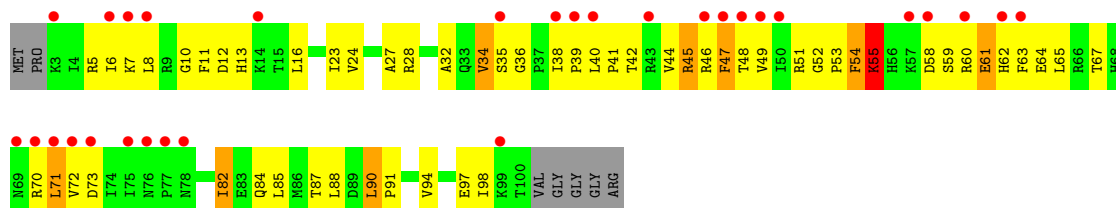
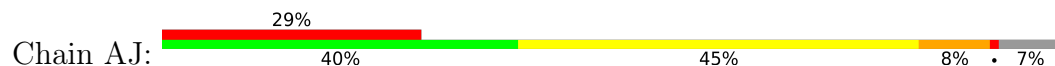
• Molecule 11: 30S ribosomal protein S8



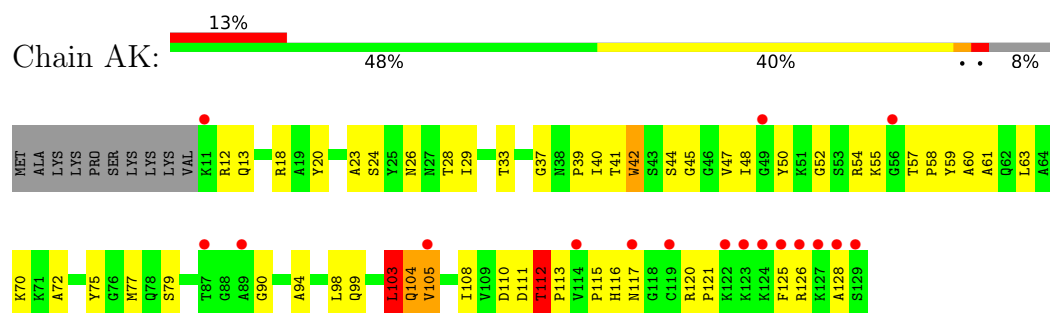
• Molecule 12: 30S ribosomal protein S9



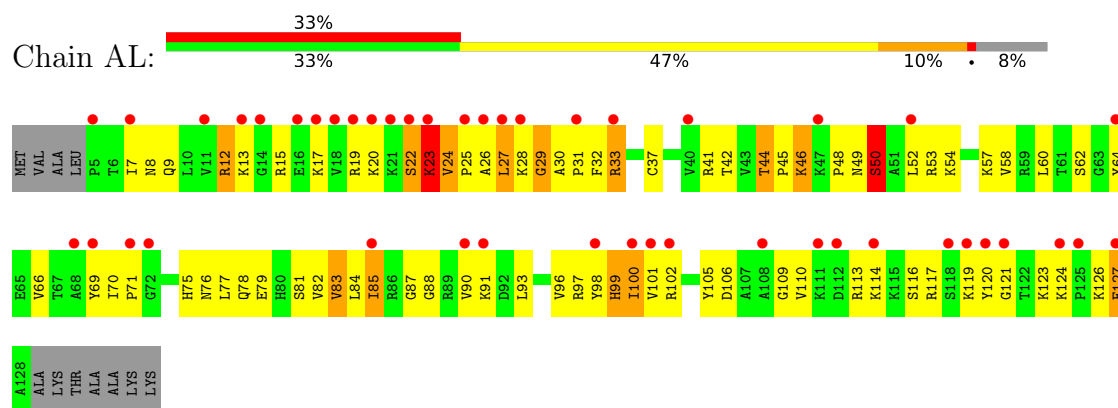
• Molecule 13: 30S ribosomal protein S10



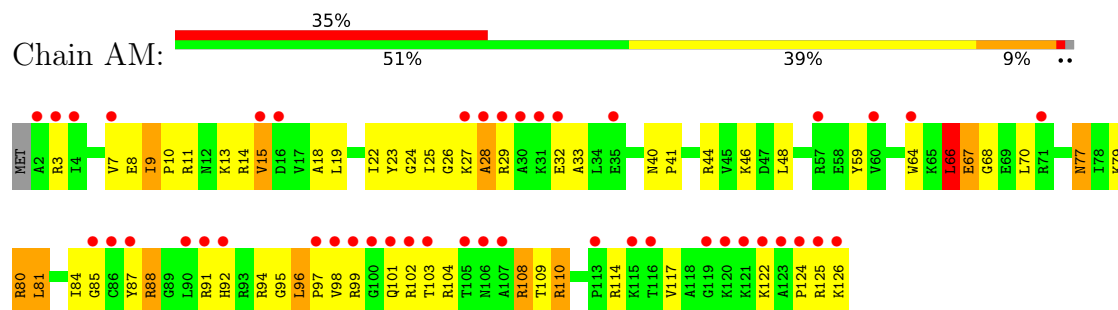
- Molecule 14: 30S ribosomal protein S11



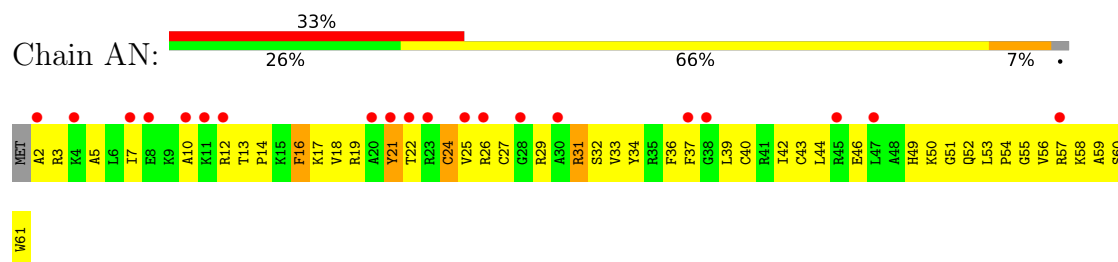
- Molecule 15: 30S ribosomal protein S12



- Molecule 16: 30S ribosomal protein S13

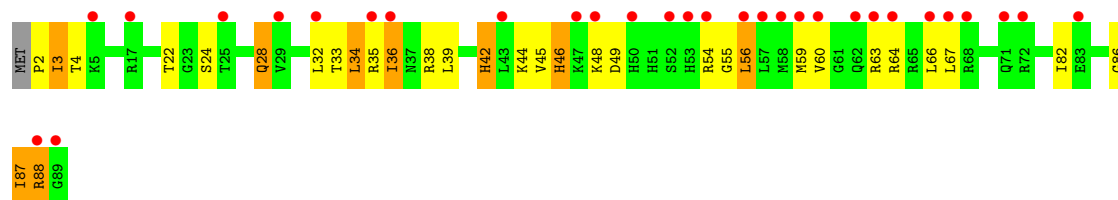


- Molecule 17: 30S ribosomal protein S14

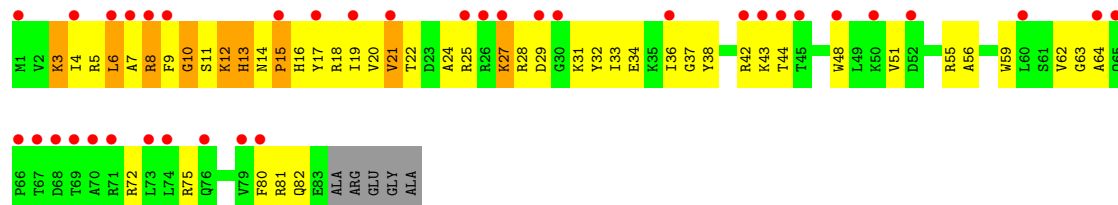


- Molecule 18: 30S ribosomal protein S15

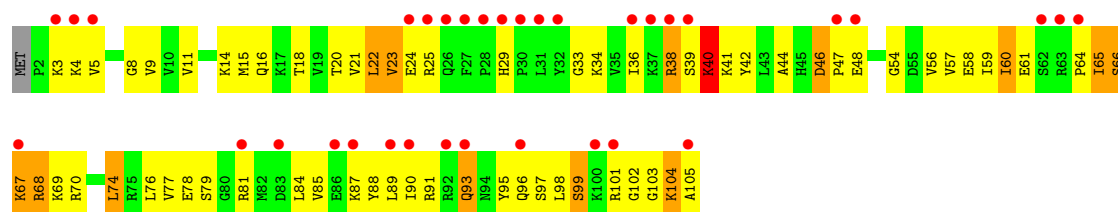




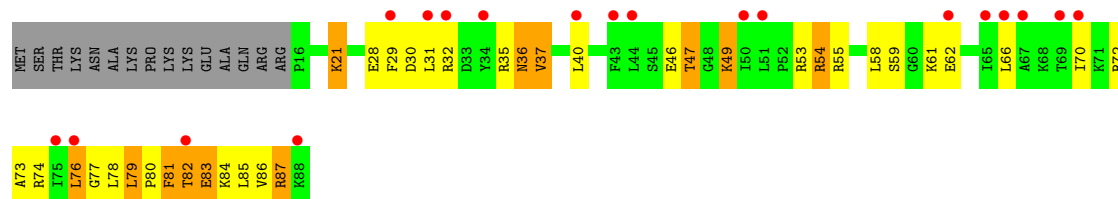
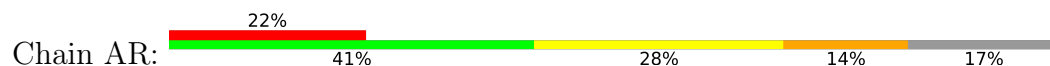
- Molecule 19: 30S ribosomal protein S16



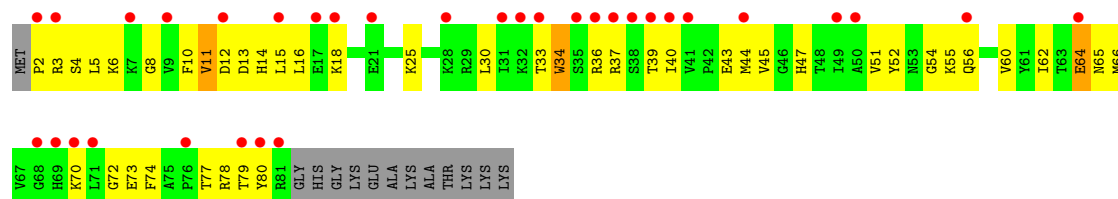
- Molecule 20: 30S ribosomal protein S17



- Molecule 21: 30S ribosomal protein S18

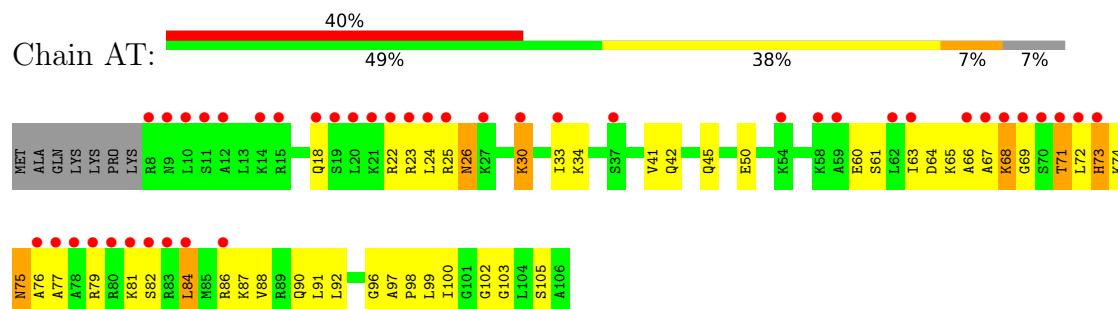


- Molecule 22: 30S ribosomal protein S19



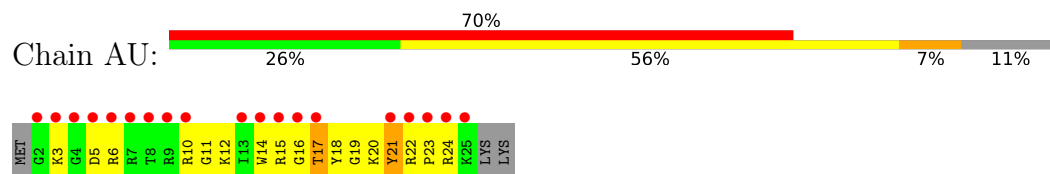
- Molecule 23: 30S ribosomal protein S20

Chain AT:



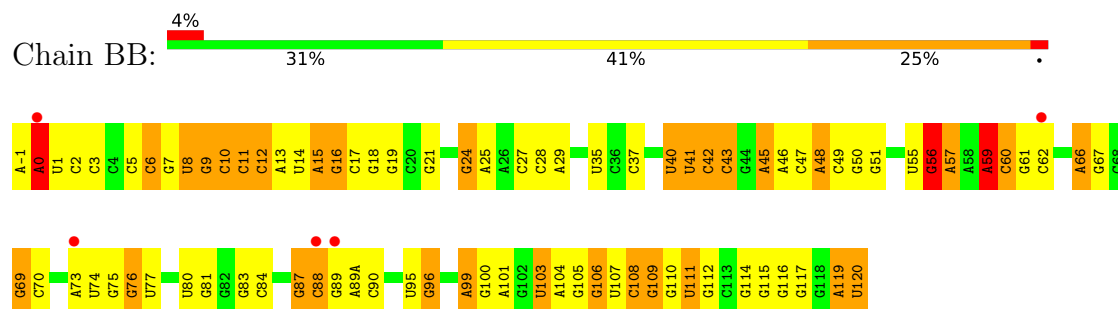
- Molecule 24: 30S ribosomal protein Thx

Chain AU:



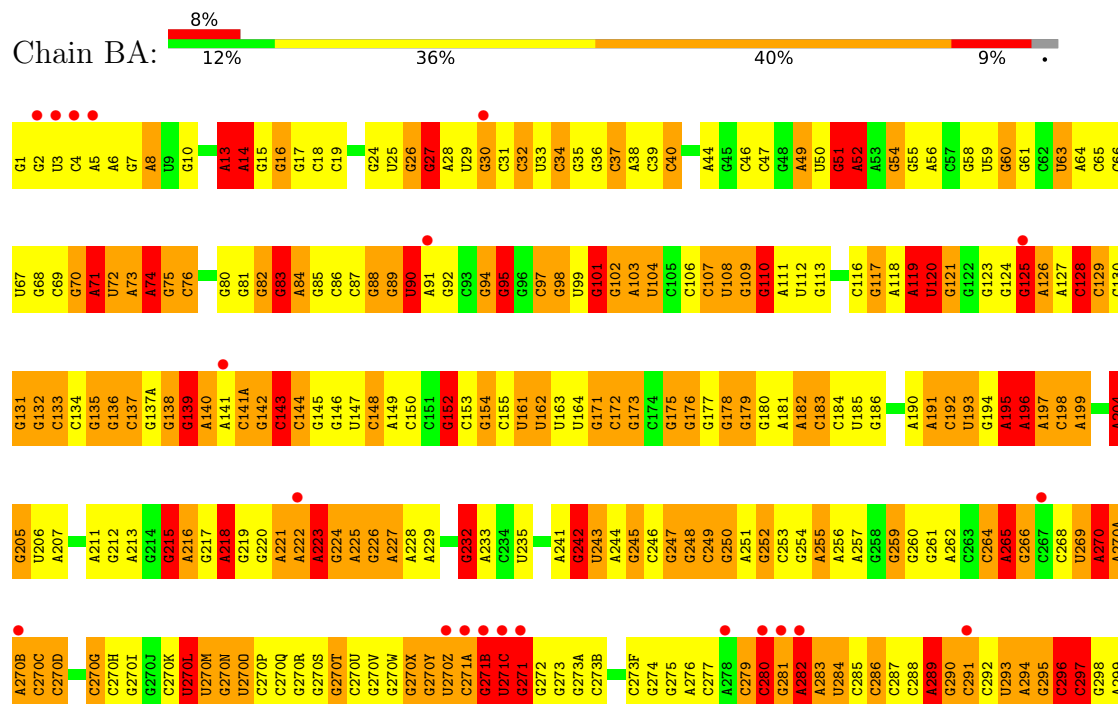
- Molecule 25: 5S ribosomal RNA

Chain BB:

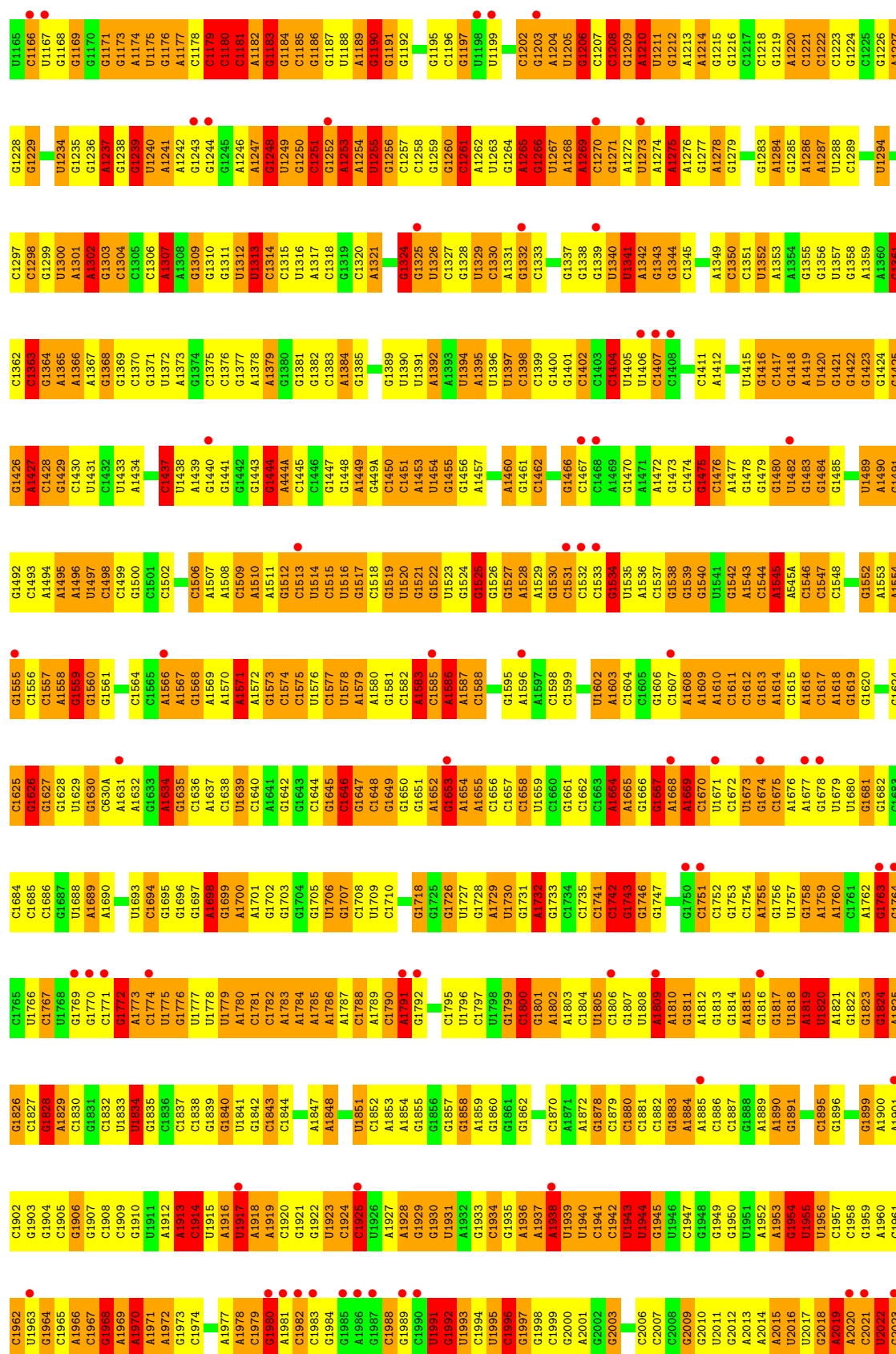


- Molecule 26: 23S ribosomal RNA

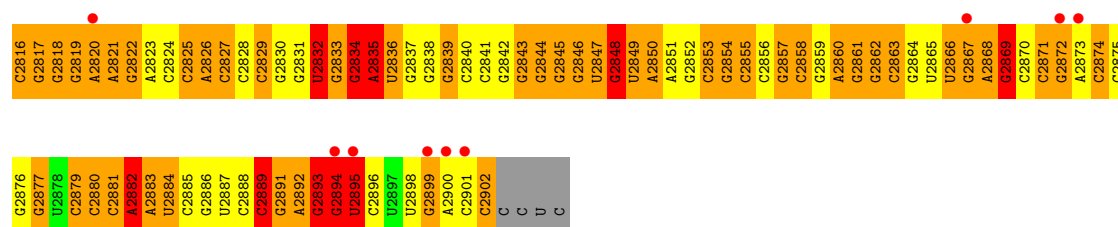
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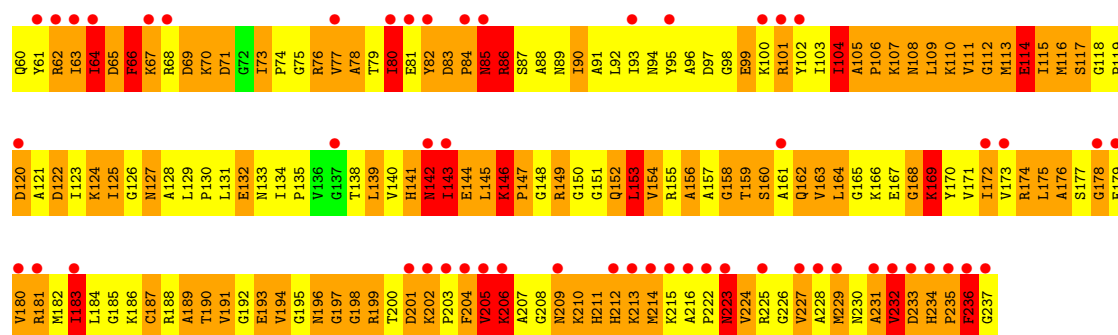
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C1104	C1041	G975	A911	U848	A784	C720	G656	G618	G558	C491	U429	G363C	U303
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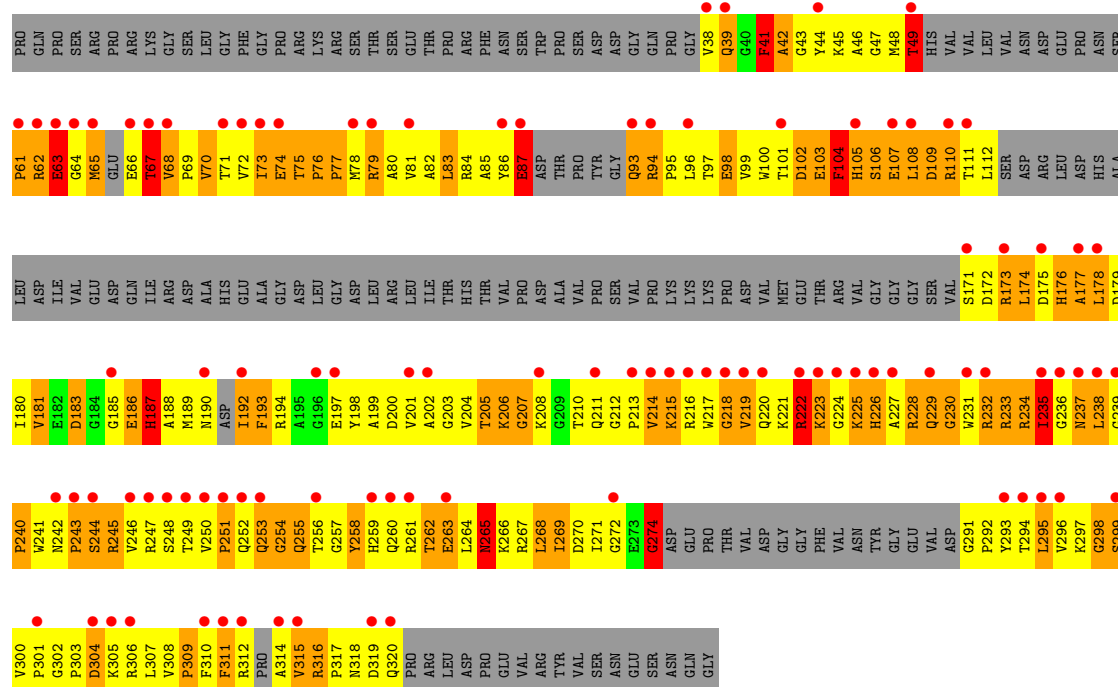
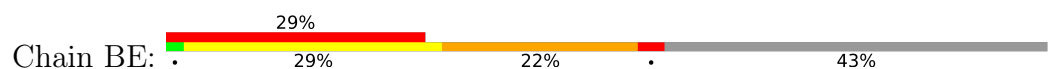
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G2780	U2720	G2661	C2601	A2541	G2481	A2421	A2361	C2301	C2241	A	C	A2051
A2781	A2721	A2662	A2602	A2542	G2482	A2422	G2362	G2302	G2242	U	G	G2052
G2782	G2722	G2663	G2603	G2543	C2483	G2423	C2363	G2303	U2243	A	U	G2053
G2783	C2723	G2664	U2604	G2544	G2484	G2424	C2364	G2304	U2244	C	A	A2054
G2784	C2724	A2665	U2605	G2545	G2485	A2425	G2365	A2305	U2245	C	G	C2055
C2785	A2725	C2666	C2606	U2546	G2486	A2426	A2366	C2306	G2246	A	G	C2056
U2786	U2726	G2667	G2607	U2547	G2487	C2427	G2367	G2307	A2247	C	A	A2057
G2787	G2727	G2668	G2608	G2548	A2488	G2428	A2368	G2308	C2248	C	U	A2058
G2788	U2728	G2669	U2609	U2549	G2489	G2429	A2369	A2309	U2249	C	A	A2059
C2789	G2729	A2670	C2610	G2550	G2490	A2430	G2370	G2250	G2250	U	G	A2060
A2790	C2730	A2671	U2611	U2551	U2491	U2431	G2371	G2251	G2251	G	G	G2061
C2791	G2731	G2672	C2612	U2552	U2492	A2432	G2372	G2252	G2252	U	U	A2062
G2792	G2732	G2673	U2613	G2553	U2493	A2433	G2373	C2253	G2253	G	G	C2063
G2793	A2733	G2674	A2614	U2554	G2494	A2434	C2374	C2314	C2254	G	G	C2064
C2794	G2734	A2675	U2615	U2555	G2495	A2435	G2375	G2315	G2255	G	G	C2065
G2795	G2735	C2676	C2616	C2556	G2496	G2436	A2376	G2256	G2256	A	A	C2066
U2797	G2736	G2677	C2617	G2557	A2497	U2437	A2377	U2257	G2257	G	G	G2067
G2797	G2737	C2678	G2618	C2558	C2498	U2438	A2378	C2258	C2258	C	C	U2068
A2799	A2738	A2679	C2619	C2559	C2499	A2439	G2379	G2259	G2259	U	G	G2069
A2801	U2739	C2680	C2620	U2560	U2500	C2440	C2380	C2260	C2260	U	U	G2070
G2802	C2681	A2681	A2621	A2561	C2501	C2441	G2381	G2321	C2261	G	G	A2071
C2803	A2741	U2682	C2622	U2562	G2502	C2442	G2382	A2322	U2262	U	U	G2072
G2804	C2742	C2683	G2623	U2563	A2503	G2443	G2383	G2323	C2263	G	G	C2073
G2805	C2743	U2684	G2624	A2564	U2504	G2444	G2384	C2324	C2264	A	A	U2074
G2807	G2744	G2685	G2625	A2565	U2505	G2445	C2385	G2325	U2265	A	A	U2075
U2808	C2745	G2686	C2626	A2566	U2506	G2446	C2386	C2326	A2266	C	C	U2076
A2809	U2746	U2687	G2627	G2567	G2507	G2447	U2387	A2267	A2267	C	C	A2077
G2747	G2747	U2688	C2628	G2568	A2448	A2448	G2388	A2268	A2268	C	C	C2078
A2748	U2689	A2629	G2629	G2569	G2509	U2449	G2389	C2269	A2269	C	C	U2079
A2749	C2890	G2630	G2630	C2570	C2510	A2450	U2390	G2330	G2270	C	C	G2080
A2813	G2750	C2691	C2631	C2571	U2511	A2451	G2391	G2331	G2271	G	G	C2081
C2814	A2751	C2692	A2632	C2572	C2452	A2452	A2392	U2332	U2272	C	C	A2082
C2815	C2752	A2693	G2633	C2573	G2513	A2453	A2393	A2333	A2273	U	C	G2083



• Molecule 27: 50S ribosomal protein L2

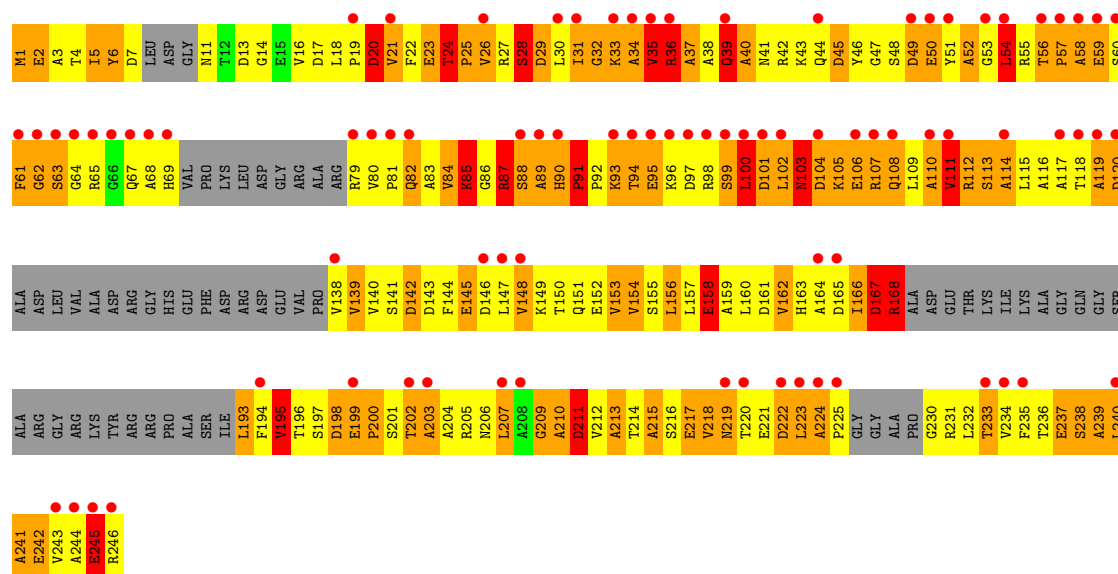


• Molecule 28: 50S ribosomal protein L3

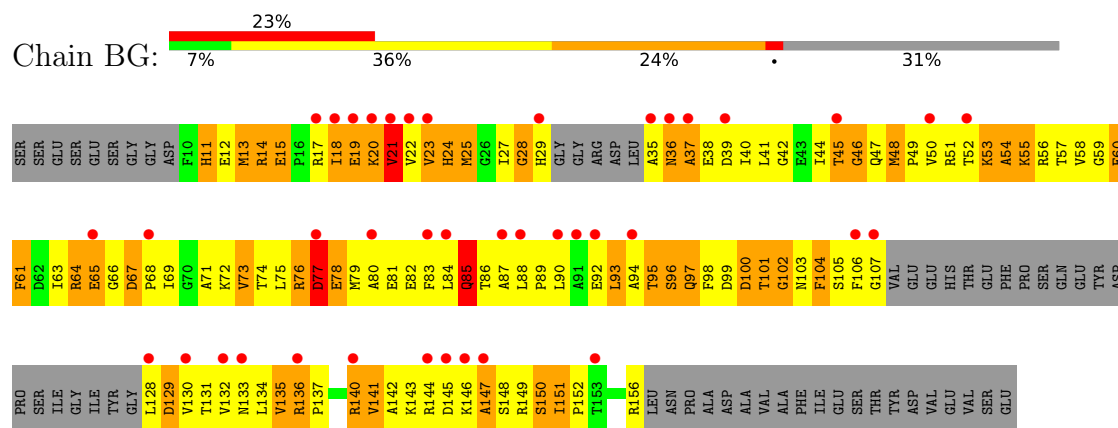


• Molecule 29: 50S ribosomal protein L4

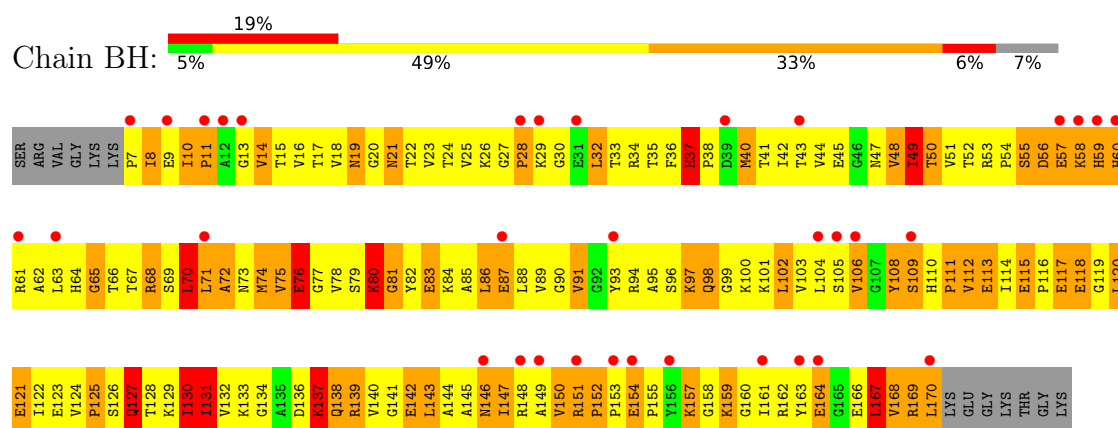




• Molecule 30: 50S ribosomal protein L5

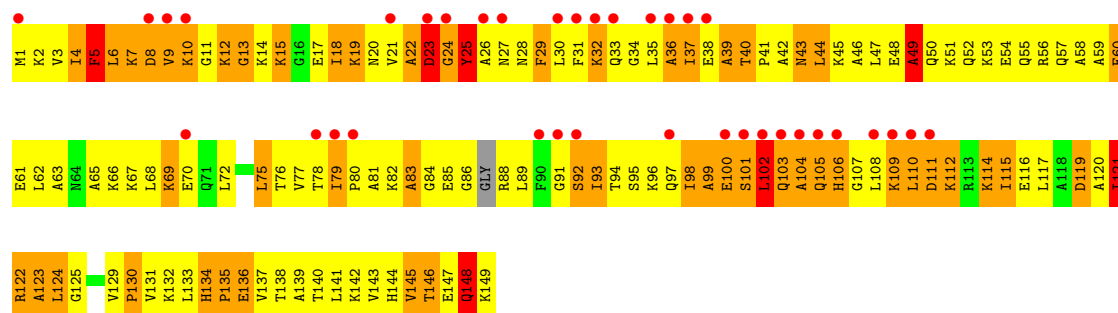


• Molecule 31: 50S ribosomal protein L6

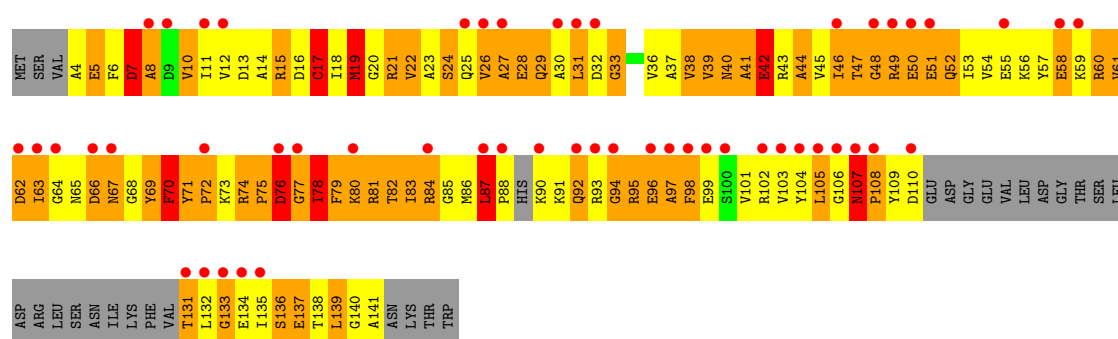


• Molecule 32: 50S ribosomal protein L9

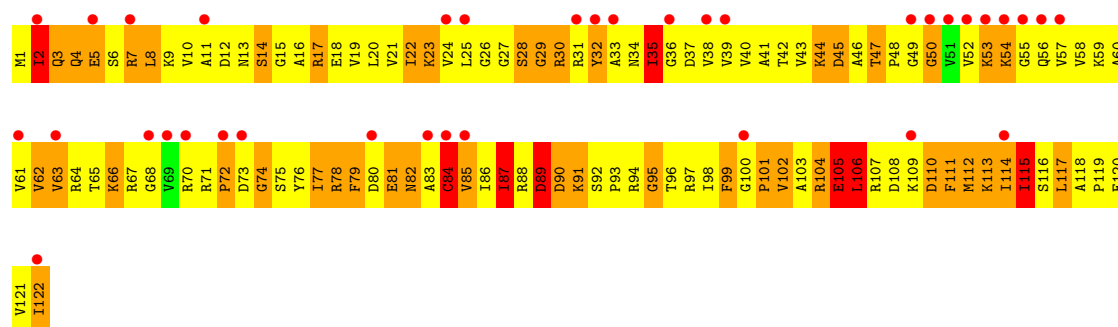




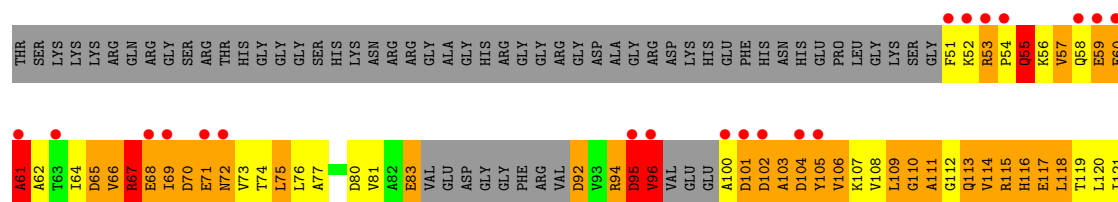
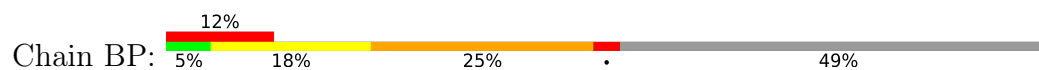
• Molecule 33: 50S ribosomal protein L13



• Molecule 34: 50S ribosomal protein L14

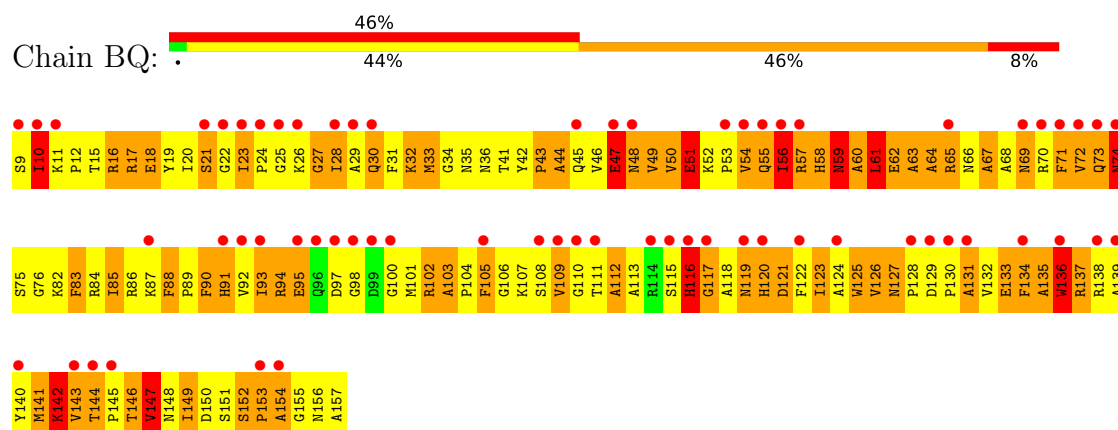


• Molecule 35: 50S ribosomal protein L15

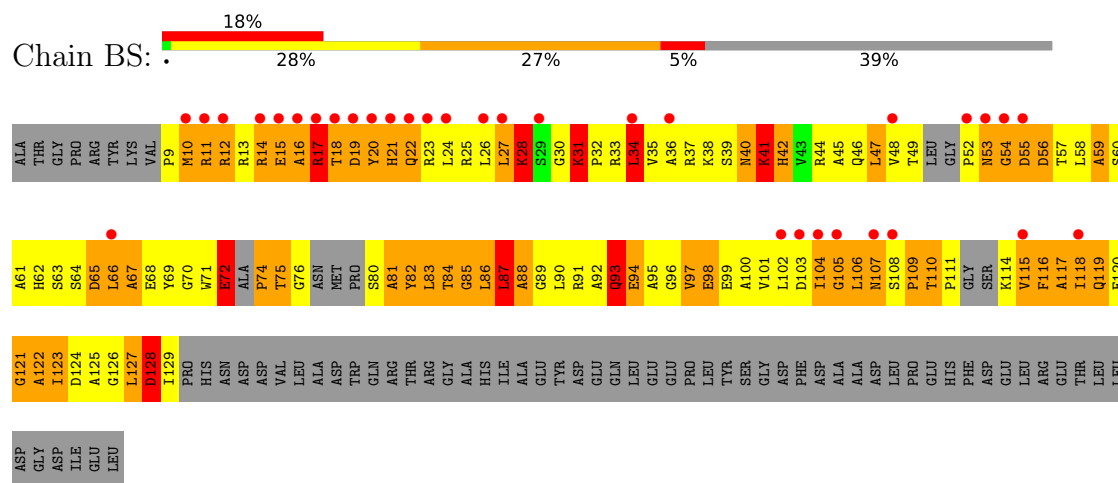




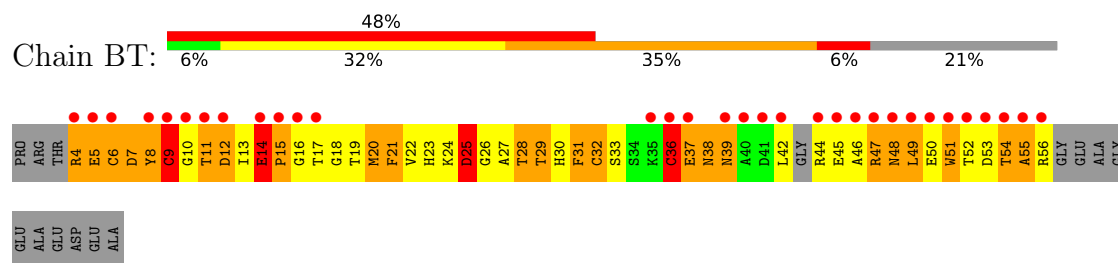
• Molecule 36: 50S ribosomal protein L16



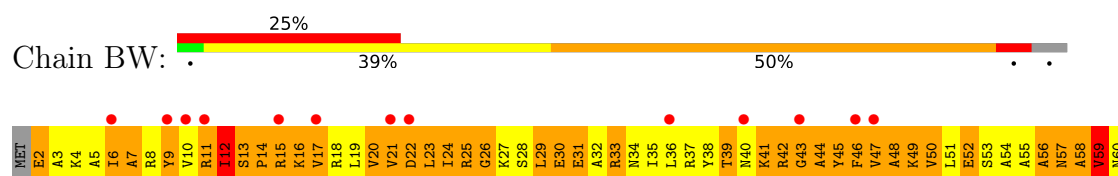
• Molecule 37: 50S ribosomal protein L18

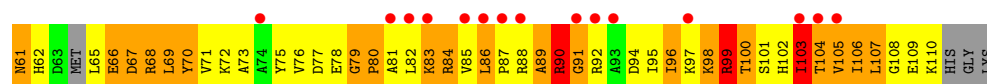


• Molecule 38: 50S ribosomal protein L19

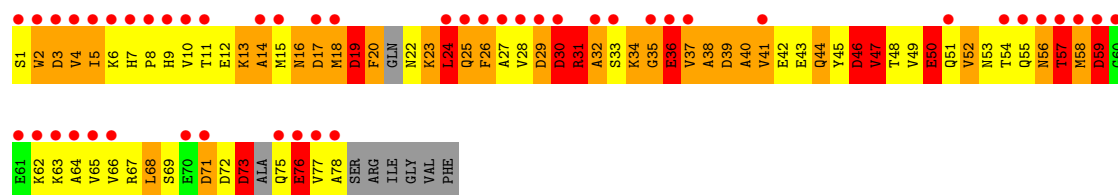


• Molecule 39: 50S ribosomal protein L22

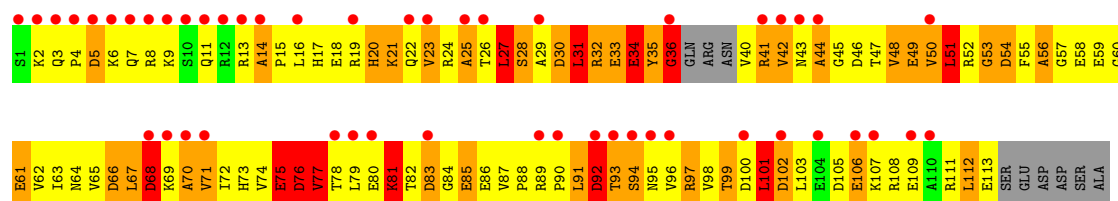




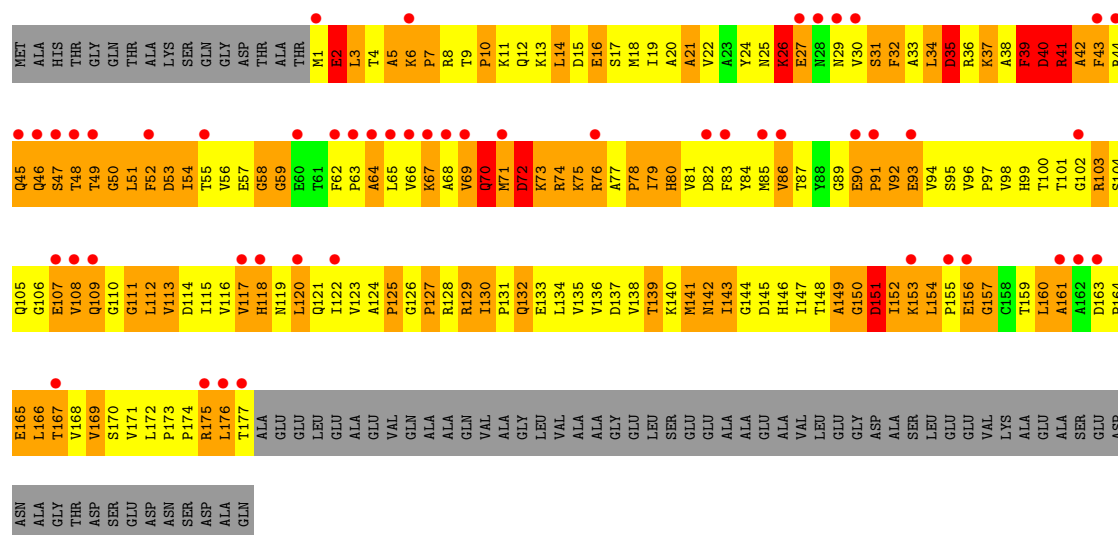
• Molecule 40: 50S ribosomal protein L23



• Molecule 41: 50S ribosomal protein 24

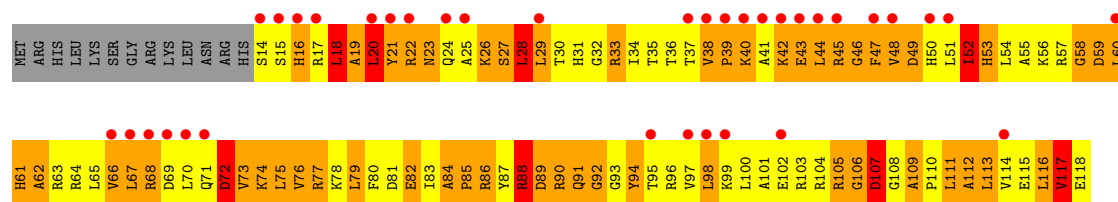


• Molecule 42: 50S ribosomal protein CTC

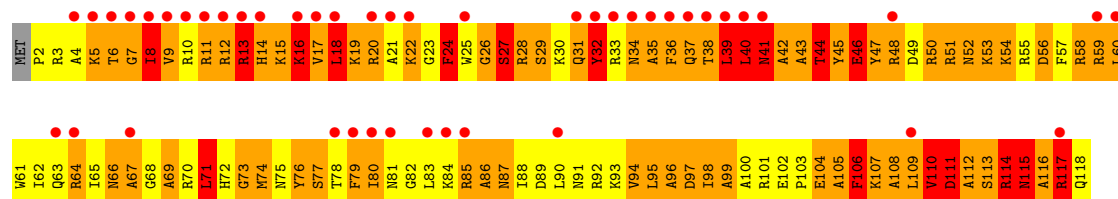


• Molecule 43: 50S ribosomal protein L17

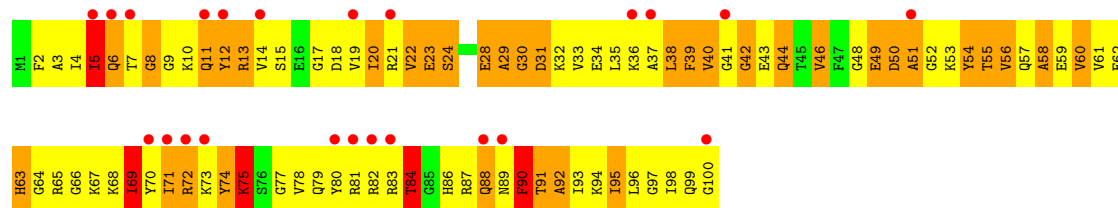




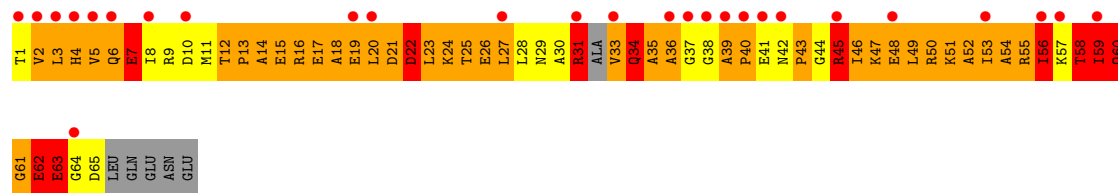
• Molecule 44: 50S ribosomal protein L20



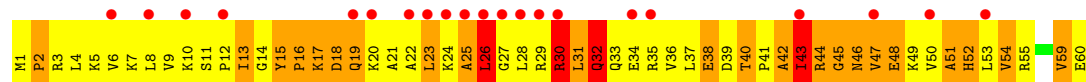
• Molecule 45: 50S ribosomal protein L21



• Molecule 46: 50S ribosomal protein L29

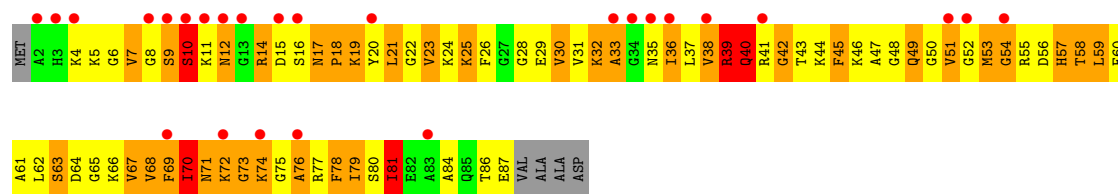


• Molecule 47: 50S ribosomal protein L30

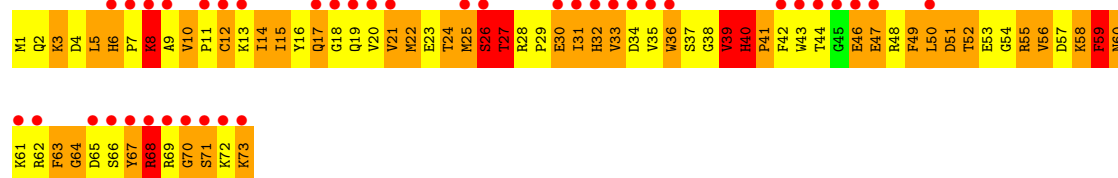
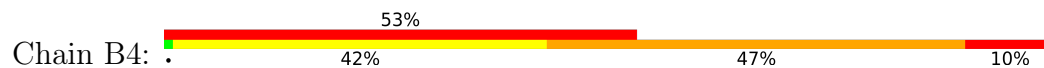


• Molecule 48: 50S ribosomal protein L27

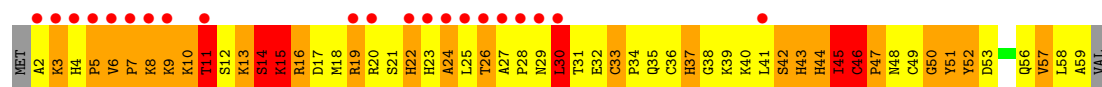




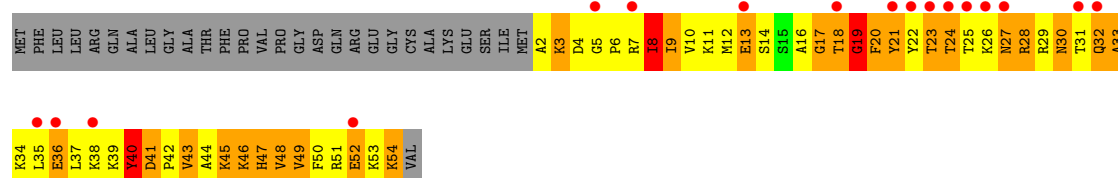
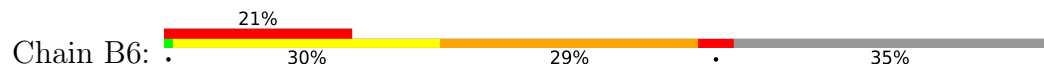
• Molecule 49: 50S ribosomal protein L31



• Molecule 50: 50S ribosomal protein L32



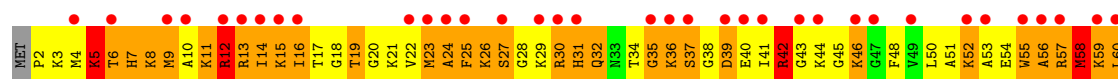
• Molecule 51: 50S ribosomal protein L33



• Molecule 52: 50S ribosomal protein L34

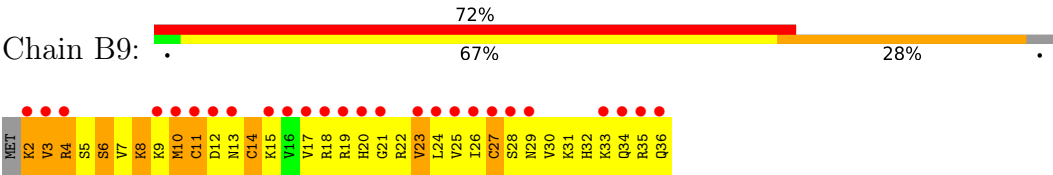


• Molecule 53: 50S ribosomal protein L35

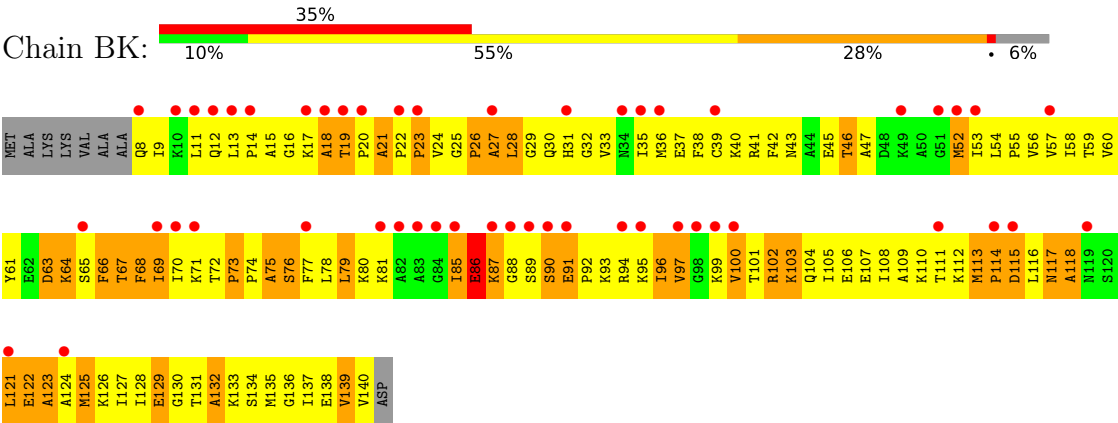




● Molecule 54: 50S ribosomal protein L36



● Molecule 55: 50S ribosomal protein L11



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	517.41Å 517.41Å 365.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 6.46 40.00 – 6.46	Depositor EDS
% Data completeness (in resolution range)	99.9 (40.00-6.46) 99.4 (40.00-6.46)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 6.19Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.354 , 0.361 0.346 , 0.359	Depositor DCC
R_{free} test set	6075 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	240.8	Xtriage
Anisotropy	0.222	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.17 , 103.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	142447	wwPDB-VP
Average B, all atoms (Å ²)	314.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.58% 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: YYG, PSU

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	1.06	64/36413 (0.2%)	1.18	256/56777 (0.5%)
2	AV	0.68	3/1812 (0.2%)	0.98	8/2819 (0.3%)
3	AW	1.17	10/1739 (0.6%)	1.73	35/2698 (1.3%)
4	AX	0.38	0/139	0.49	0/213
5	AB	0.96	2/1935 (0.1%)	0.92	4/2609 (0.2%)
6	AC	1.29	2/1636 (0.1%)	0.93	6/2205 (0.3%)
7	AD	1.00	2/1733 (0.1%)	1.34	14/2318 (0.6%)
8	AE	1.36	1/1162 (0.1%)	0.94	3/1564 (0.2%)
9	AF	0.47	0/856	0.81	0/1154
10	AG	0.48	0/1276	1.00	6/1709 (0.4%)
11	AH	0.60	0/1136	0.90	1/1527 (0.1%)
12	AI	0.47	0/1029	0.82	1/1378 (0.1%)
13	AJ	0.53	0/807	0.83	1/1085 (0.1%)
14	AK	0.64	1/900 (0.1%)	0.84	1/1213 (0.1%)
15	AL	2.60	1/986 (0.1%)	1.43	8/1320 (0.6%)
16	AM	1.50	1/1007 (0.1%)	0.83	0/1344
17	AN	0.56	0/501	0.89	0/664
18	AO	0.44	0/745	0.86	0/992
19	AP	0.56	0/716	0.84	2/963 (0.2%)
20	AQ	1.99	2/870 (0.2%)	2.15	10/1159 (0.9%)
21	AR	0.55	0/603	0.94	0/799
22	AS	0.49	0/661	0.79	0/890
23	AT	0.43	0/764	0.88	0/1006
24	AU	0.44	0/212	0.78	0/277
25	BB	1.00	5/2950 (0.2%)	1.14	18/4602 (0.4%)
26	BA	0.94	139/67839 (0.2%)	1.18	490/105818 (0.5%)
27	BD	0.50	0/1328	0.95	8/1783 (0.4%)
28	BE	0.93	4/1540 (0.3%)	1.66	16/2078 (0.8%)
29	BF	1.19	3/1444 (0.2%)	1.14	12/1954 (0.6%)
30	BG	0.32	0/971	0.82	5/1304 (0.4%)
31	BH	0.69	1/1272 (0.1%)	1.09	7/1721 (0.4%)
32	BI	0.40	1/1156 (0.1%)	1.06	6/1544 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	BN	0.41	0/927	0.83	5/1245 (0.4%)
34	BO	0.40	0/946	0.91	5/1269 (0.4%)
35	BP	3.05	3/643 (0.5%)	1.63	6/870 (0.7%)
36	BQ	0.43	1/1106 (0.1%)	0.80	2/1490 (0.1%)
37	BS	1.63	3/877 (0.3%)	1.08	2/1179 (0.2%)
38	BT	0.49	0/412	1.24	4/554 (0.7%)
39	BW	1.12	3/869 (0.3%)	1.26	5/1166 (0.4%)
40	BX	0.72	1/608 (0.2%)	1.49	4/820 (0.5%)
41	BY	0.32	0/887	1.25	4/1195 (0.3%)
42	BZ	0.46	1/1385 (0.1%)	0.88	4/1883 (0.2%)
43	BR	0.37	0/867	0.67	2/1162 (0.2%)
44	BU	0.96	1/994 (0.1%)	0.97	4/1323 (0.3%)
45	BV	1.33	1/796 (0.1%)	1.22	7/1058 (0.7%)
46	B2	0.49	0/497	1.24	3/668 (0.4%)
47	B3	0.38	0/482	0.77	2/646 (0.3%)
48	B0	0.53	1/649 (0.2%)	1.18	3/860 (0.3%)
49	B4	1.13	2/620 (0.3%)	0.82	2/831 (0.2%)
50	B5	0.44	0/469	1.27	7/629 (1.1%)
51	B6	0.40	0/438	0.76	3/583 (0.5%)
52	B7	0.47	0/387	0.77	0/509
53	B8	1.14	2/503 (0.4%)	1.26	5/657 (0.8%)
54	B9	0.45	0/286	0.92	1/375 (0.3%)
55	BK	0.39	1/1014 (0.1%)	0.75	2/1363 (0.1%)
All	All	0.99	262/154800 (0.2%)	1.16	1000/231822 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	AW	1	5
5	AB	0	1
6	AC	0	1
7	AD	0	1
14	AK	0	1
15	AL	0	1
20	AQ	0	1
27	BD	0	1
28	BE	0	3
29	BF	0	4
31	BH	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
32	BI	0	1
35	BP	0	1
37	BS	0	1
40	BX	0	1
41	BY	0	1
46	B2	0	1
50	B5	0	1
55	BK	0	1
All	All	1	28

The worst 5 of 262 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	AL	23	LYS	C-N	-79.20	0.43	1.33
26	BA	2199	A	O3'-P	-56.83	0.75	1.61
35	BP	61	ALA	C-N	55.46	1.85	1.33
20	AQ	22	LEU	C-N	-53.20	0.59	1.33
1	AA	1278	U	O3'-P	-45.22	0.93	1.61

The worst 5 of 1000 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BA	2199	A	O3'-P-O5'	-54.55	22.17	104.00
28	BE	49	THR	O-C-N	-45.66	68.81	121.32
3	AW	65	G	P-O3'-C3'	-40.88	58.88	120.20
26	BA	712(A)	A	P-O3'-C3'	-35.23	67.36	120.20
1	AA	1278	U	O3'-P-O5'	-33.60	53.59	104.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	AW	37	YYG	C15

5 of 28 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	AW	16	U	Sidechain
3	AW	17	U	Sidechain
3	AW	18	G	Sidechain
3	AW	19	G	Sidechain
3	AW	62	A	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32551	0	16459	2047	3
2	AV	1622	0	821	231	0
3	AW	1638	0	836	244	0
4	AX	136	0	63	26	0
5	AB	1900	0	1950	102	0
6	AC	1612	0	1675	101	0
7	AD	1703	0	1761	293	0
8	AE	1146	0	1206	70	0
9	AF	843	0	857	32	0
10	AG	1257	0	1295	106	0
11	AH	1116	0	1177	104	0
12	AI	1011	0	1040	83	0
13	AJ	794	0	840	81	0
14	AK	885	0	904	54	0
15	AL	970	0	1056	74	0
16	AM	997	0	1070	153	0
17	AN	492	0	529	87	0
18	AO	734	0	771	28	0
19	AP	700	0	720	72	0
20	AQ	857	0	928	81	0
21	AR	597	0	668	41	0
22	AS	647	0	673	157	0
23	AT	762	0	859	38	0
24	AU	208	0	221	85	0
25	BB	2637	0	1339	219	1
26	BA	60600	0	30514	11055	138
27	BD	1308	0	1346	1109	0
28	BE	1507	0	1478	1156	3
29	BF	1430	0	1357	1102	0
30	BG	957	0	952	719	0
31	BH	1251	0	1291	772	0
32	BI	1145	0	1225	638	3
33	BN	917	0	896	790	2
34	BO	937	0	992	626	0
35	BP	639	0	605	497	0
36	BQ	1081	0	1047	950	0
37	BS	866	0	866	693	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	BT	406	0	359	177	0
39	BW	860	0	909	568	0
40	BX	602	0	558	469	0
41	BY	879	0	860	758	0
42	BZ	1360	0	1378	915	0
43	BR	855	0	904	596	0
44	BU	978	0	996	914	0
45	BV	787	0	783	648	0
46	B2	494	0	504	398	0
47	B3	477	0	527	475	0
48	B0	641	0	661	546	0
49	B4	604	0	587	506	0
50	B5	457	0	456	288	0
51	B6	431	0	454	284	0
52	B7	383	0	409	391	0
53	B8	496	0	539	363	0
54	B9	285	0	312	197	0
55	BK	999	0	1065	586	0
All	All	142447	0	94548	29372	145

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 125.

The worst 5 of 29372 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)
50:B5:33:CYS:SG	50:B5:36:CYS:HB2	1.24	1.69
26:BA:2470:G:C2	26:BA:2471:C:C5	1.81	1.68
52:B7:30:ILE:HA	52:B7:33:ARG:CD	1.21	1.67
26:BA:2712:U:C6	26:BA:712(A):A:C8	1.77	1.67
26:BA:2580:U:C6	26:BA:2581:G:C8	1.82	1.66

The worst 5 of 145 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)
26:BA:6:A:O4'	26:BA:2902:C:C2'[8_554]	0.72	1.48
26:BA:2899:G:N1	26:BA:2901:C:C4[8_554]	0.79	1.41
26:BA:6:A:C4'	26:BA:2902:C:C2'[8_554]	0.97	1.23
26:BA:2900:A:N7	26:BA:2900:A:N6[8_554]	1.03	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:BA:3:U:O4	26:BA:2899:G:O2'[8_554]	1.09	1.11

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	
5	AB	232/256 (91%)	183 (79%)	33 (14%)	16 (7%)	1	11
6	AC	204/239 (85%)	166 (81%)	24 (12%)	14 (7%)	1	11
7	AD	206/209 (99%)	157 (76%)	33 (16%)	16 (8%)	1	9
8	AE	148/162 (91%)	116 (78%)	29 (20%)	3 (2%)	6	31
9	AF	99/101 (98%)	85 (86%)	10 (10%)	4 (4%)	2	18
10	AG	153/156 (98%)	131 (86%)	18 (12%)	4 (3%)	4	25
11	AH	136/138 (99%)	101 (74%)	25 (18%)	10 (7%)	1	10
12	AI	125/128 (98%)	86 (69%)	31 (25%)	8 (6%)	1	12
13	AJ	96/105 (91%)	73 (76%)	14 (15%)	9 (9%)	0	8
14	AK	117/129 (91%)	88 (75%)	22 (19%)	7 (6%)	1	13
15	AL	122/135 (90%)	90 (74%)	13 (11%)	19 (16%)	0	3
16	AM	121/126 (96%)	95 (78%)	20 (16%)	6 (5%)	1	15
17	AN	58/61 (95%)	42 (72%)	12 (21%)	4 (7%)	1	11
18	AO	86/89 (97%)	76 (88%)	9 (10%)	1 (1%)	10	44
19	AP	81/88 (92%)	64 (79%)	11 (14%)	6 (7%)	1	10
20	AQ	102/105 (97%)	78 (76%)	18 (18%)	6 (6%)	1	13
21	AR	71/88 (81%)	54 (76%)	11 (16%)	6 (8%)	0	9
22	AS	78/93 (84%)	60 (77%)	15 (19%)	3 (4%)	2	19
23	AT	97/106 (92%)	79 (81%)	12 (12%)	6 (6%)	1	12
24	AU	22/27 (82%)	17 (77%)	3 (14%)	2 (9%)	0	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	BD	169/173 (98%)	60 (36%)	34 (20%)	75 (44%)	0	0
28	BE	183/338 (54%)	89 (49%)	34 (19%)	60 (33%)	0	0
29	BF	179/246 (73%)	51 (28%)	47 (26%)	81 (45%)	0	0
30	BG	116/176 (66%)	46 (40%)	31 (27%)	39 (34%)	0	0
31	BH	162/177 (92%)	74 (46%)	39 (24%)	49 (30%)	0	0
32	BI	144/149 (97%)	71 (49%)	29 (20%)	44 (31%)	0	0
33	BN	111/145 (77%)	34 (31%)	21 (19%)	56 (50%)	0	0
34	BO	120/122 (98%)	61 (51%)	27 (22%)	32 (27%)	0	0
35	BP	82/164 (50%)	28 (34%)	21 (26%)	33 (40%)	0	0
36	BQ	130/138 (94%)	38 (29%)	35 (27%)	57 (44%)	0	0
37	BS	105/186 (56%)	36 (34%)	20 (19%)	49 (47%)	0	0
38	BT	48/66 (73%)	17 (35%)	13 (27%)	18 (38%)	0	0
39	BW	104/113 (92%)	41 (39%)	16 (15%)	47 (45%)	0	0
40	BX	72/84 (86%)	26 (36%)	18 (25%)	28 (39%)	0	0
41	BY	108/119 (91%)	49 (45%)	20 (18%)	39 (36%)	0	0
42	BZ	175/253 (69%)	52 (30%)	53 (30%)	70 (40%)	0	0
43	BR	103/118 (87%)	35 (34%)	20 (19%)	48 (47%)	0	0
44	BU	115/118 (98%)	22 (19%)	23 (20%)	70 (61%)	0	0
45	BV	96/100 (96%)	39 (41%)	25 (26%)	32 (33%)	0	0
46	B2	62/70 (89%)	8 (13%)	9 (14%)	45 (73%)	0	0
47	B3	58/60 (97%)	24 (41%)	13 (22%)	21 (36%)	0	0
48	B0	84/91 (92%)	32 (38%)	17 (20%)	35 (42%)	0	0
49	B4	71/73 (97%)	21 (30%)	16 (22%)	34 (48%)	0	0
50	B5	56/60 (93%)	16 (29%)	18 (32%)	22 (39%)	0	0
51	B6	51/82 (62%)	21 (41%)	9 (18%)	21 (41%)	0	0
52	B7	44/47 (94%)	4 (9%)	7 (16%)	33 (75%)	0	0
53	B8	61/64 (95%)	22 (36%)	10 (16%)	29 (48%)	0	0
54	B9	33/36 (92%)	14 (42%)	9 (27%)	10 (30%)	0	0
55	BK	129/141 (92%)	73 (57%)	18 (14%)	38 (30%)	0	0
All	All	5325/6250 (85%)	2945 (55%)	1015 (19%)	1365 (26%)	0	1

5 of 1365 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	AB	24	TRP
5	AB	104	ASN
5	AB	153	ARG
5	AB	154	LEU
5	AB	161	ALA

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	AB	202/220 (92%)	176 (87%)	26 (13%)	4	15
6	AC	160/188 (85%)	143 (89%)	17 (11%)	6	21
7	AD	180/181 (99%)	162 (90%)	18 (10%)	7	24
8	AE	115/123 (94%)	89 (77%)	26 (23%)	1	6
9	AF	90/90 (100%)	82 (91%)	8 (9%)	9	28
10	AG	126/127 (99%)	116 (92%)	10 (8%)	11	32
11	AH	119/119 (100%)	93 (78%)	26 (22%)	1	6
12	AI	98/99 (99%)	89 (91%)	9 (9%)	8	27
13	AJ	88/92 (96%)	78 (89%)	10 (11%)	5	18
14	AK	90/99 (91%)	87 (97%)	3 (3%)	33	55
15	AL	104/111 (94%)	92 (88%)	12 (12%)	5	18
16	AM	100/101 (99%)	86 (86%)	14 (14%)	3	13
17	AN	49/50 (98%)	42 (86%)	7 (14%)	3	13
18	AO	79/80 (99%)	67 (85%)	12 (15%)	3	12
19	AP	72/74 (97%)	64 (89%)	8 (11%)	6	20
20	AQ	96/97 (99%)	83 (86%)	13 (14%)	4	14
21	AR	64/77 (83%)	55 (86%)	9 (14%)	3	13
22	AS	71/80 (89%)	64 (90%)	7 (10%)	7	24
23	AT	76/82 (93%)	66 (87%)	10 (13%)	4	15
24	AU	19/22 (86%)	19 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	BD	135/135 (100%)	93 (69%)	42 (31%)	0	2
28	BE	156/284 (55%)	128 (82%)	28 (18%)	2	9
29	BF	152/193 (79%)	124 (82%)	28 (18%)	1	9
30	BG	102/147 (69%)	93 (91%)	9 (9%)	9	28
31	BH	137/147 (93%)	111 (81%)	26 (19%)	1	8
32	BI	119/119 (100%)	98 (82%)	21 (18%)	2	9
33	BN	95/121 (78%)	79 (83%)	16 (17%)	2	10
34	BO	101/101 (100%)	77 (76%)	24 (24%)	1	4
35	BP	67/126 (53%)	52 (78%)	15 (22%)	1	6
36	BQ	110/110 (100%)	83 (76%)	27 (24%)	1	4
37	BS	89/149 (60%)	72 (81%)	17 (19%)	1	8
38	BT	44/52 (85%)	32 (73%)	12 (27%)	0	3
39	BW	88/92 (96%)	73 (83%)	15 (17%)	2	10
40	BX	67/73 (92%)	45 (67%)	22 (33%)	0	2
41	BY	97/105 (92%)	79 (81%)	18 (19%)	1	8
42	BZ	151/203 (74%)	127 (84%)	24 (16%)	2	11
43	BR	89/101 (88%)	69 (78%)	20 (22%)	1	6
44	BU	96/97 (99%)	68 (71%)	28 (29%)	0	2
45	BV	79/79 (100%)	68 (86%)	11 (14%)	3	14
46	B2	51/56 (91%)	37 (72%)	14 (28%)	0	3
47	B3	52/52 (100%)	44 (85%)	8 (15%)	2	12
48	B0	64/67 (96%)	55 (86%)	9 (14%)	3	13
49	B4	66/66 (100%)	54 (82%)	12 (18%)	2	9
50	B5	51/53 (96%)	41 (80%)	10 (20%)	1	7
51	B6	46/69 (67%)	37 (80%)	9 (20%)	1	7
52	B7	39/40 (98%)	30 (77%)	9 (23%)	1	5
53	B8	50/51 (98%)	41 (82%)	9 (18%)	2	9
54	B9	34/35 (97%)	30 (88%)	4 (12%)	5	18
55	BK	108/113 (96%)	103 (95%)	5 (5%)	24	45
All	All	4533/5148 (88%)	3796 (84%)	737 (16%)	2	10

5 of 737 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
36	BQ	56	ILE
42	BZ	45	GLN
36	BQ	136	TRP
36	BQ	51	GLU
39	BW	96	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 137 such sidechains are listed below:

Mol	Chain	Res	Type
45	BV	44	GLN
47	B3	33	GLN
51	B6	27	ASN
19	AP	16	HIS
19	AP	14	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1509/1522 (99%)	540 (35%)	164 (10%)
2	AV	75/76 (98%)	18 (24%)	1 (1%)
25	BB	122/123 (99%)	45 (36%)	3 (2%)
26	BA	2808/2916 (96%)	1520 (54%)	359 (12%)
3	AW	73/76 (96%)	18 (24%)	4 (5%)
4	AX	5/18 (27%)	0	0
All	All	4592/4731 (97%)	2141 (46%)	531 (11%)

5 of 2141 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	6	G
1	AA	7	G
1	AA	8	A
1	AA	9	G
1	AA	12	U

5 of 531 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
26	BA	2454	G
26	BA	2532	G
26	BA	2451	A

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Mol	Chain	Res	Type
26	BA	2820	A
26	BA	241	A

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

3 non-standard protein/DNA/RNA residues are 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	$\# Z > 2$
3	PSU	AW	55	3	18,21,22	0.72	0	21,30,33	0.91	1 (4%)
3	PSU	AW	39	3	18,21,22	0.73	1 (5%)	21,30,33	0.71	0
3	YYG	AW	37	3	38,42,43	0.89	2 (5%)	45,62,65	2.33	10 (22%)

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
3	PSU	AW	55	3	-	0/7/25/26	0/2/2/2
3	PSU	AW	39	3	-	0/7/25/26	0/2/2/2
3	YYG	AW	37	3	1/1/8/9	7/24/42/43	0/4/4/4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	AW	37	YYG	C2-N2	3.12	1.38	1.33
3	AW	37	YYG	C3-N3	2.20	1.50	1.47
3	AW	39	PSU	C6-N1	-2.05	1.33	1.36

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

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	AW	37	YYG	C11-C12-N1	8.65	111.41	105.31
3	AW	37	YYG	C24-O23-C21	6.47	123.13	115.63
3	AW	37	YYG	C5-C4-N3	4.93	127.99	123.99
3	AW	37	YYG	O23-C21-N20	4.58	118.48	110.77
3	AW	37	YYG	C10-C11-N2	3.61	126.56	119.32

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	AW	37	YYG	C15

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	AW	37	YYG	C15-C16-O18-C19
3	AW	37	YYG	O17-C16-O18-C19
3	AW	37	YYG	C12-C13-C14-C15
3	AW	37	YYG	C13-C14-C15-C16
3	AW	37	YYG	C13-C14-C15-N20

There are no ring outliers.

2 monomers are involved in 43 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	AW	39	PSU	4	0
3	AW	37	YYG	39	0

5.5 Carbohydrates [i](#)

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 ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
26	BA	98
1	AA	68
3	AW	7
25	BB	4
36	BQ	3
2	AV	3
45	BV	2
16	AM	2
5	AB	2
49	B4	2
39	BW	2
20	AQ	2
6	AC	2
27	BD	1
55	BK	1
37	BS	1
8	AE	1
35	BP	1
53	B8	1
48	B0	1
14	AK	1
31	BH	1
29	BF	1
44	BU	1
7	AD	1
15	AL	1

The worst 5 of 210 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	AA	30(D):A	O3'	1031:G	P	5.01
1	BA	142(A):A	O3'	1143:A	P	4.98
1	AW	73:A	O3'	74:C	P	4.88
1	BA	1171:G	O3'	1173:G	P	4.41
1	AA	440:A	O3'	442:C	P	4.34

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%)	0.38	84 (5%) 30 33	188, 339, 400, 400	0
2	AV	76/76 (100%)	0.85	9 (11%) 9 17	242, 299, 394, 394	0
3	AW	73/76 (96%)	0.62	7 (9%) 13 21	253, 400, 400, 400	0
4	AX	17/18 (94%)	10.52	13 (76%) 0 1	400, 400, 400, 400	0
5	AB	234/256 (91%)	0.87	36 (15%) 5 13	395, 395, 400, 400	0
6	AC	206/239 (86%)	0.57	19 (9%) 14 21	393, 398, 398, 398	0
7	AD	208/209 (99%)	1.83	72 (34%) 1 6	257, 391, 400, 400	0
8	AE	150/162 (92%)	0.69	24 (16%) 5 12	371, 400, 400, 400	0
9	AF	101/101 (100%)	0.71	13 (12%) 7 15	400, 400, 400, 400	0
10	AG	155/156 (99%)	1.41	40 (25%) 1 8	358, 400, 400, 400	0
11	AH	138/138 (100%)	1.01	32 (23%) 2 9	396, 396, 396, 396	0
12	AI	127/128 (99%)	1.22	21 (16%) 4 12	395, 395, 395, 395	0
13	AJ	98/105 (93%)	1.75	30 (30%) 1 6	400, 400, 400, 400	0
14	AK	119/129 (92%)	0.69	17 (14%) 6 14	202, 202, 400, 400	0
15	AL	124/135 (91%)	1.79	45 (36%) 1 5	399, 399, 400, 400	0
16	AM	125/126 (99%)	2.13	44 (35%) 1 5	348, 400, 400, 400	0
17	AN	60/61 (98%)	1.95	20 (33%) 1 6	400, 400, 400, 400	0
18	AO	88/89 (98%)	2.29	30 (34%) 1 6	400, 400, 400, 400	0
19	AP	83/88 (94%)	2.49	37 (44%) 0 4	400, 400, 400, 400	0
20	AQ	104/105 (99%)	1.40	34 (32%) 1 6	400, 400, 400, 400	0
21	AR	73/88 (82%)	1.27	19 (26%) 1 7	400, 400, 400, 400	0
22	AS	80/93 (86%)	2.02	33 (41%) 0 4	400, 400, 400, 400	0
23	AT	99/106 (93%)	2.62	42 (42%) 0 4	400, 400, 400, 400	0
24	AU	24/27 (88%)	3.75	19 (79%) 0 1	400, 400, 400, 400	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)		Q<0.9
25	BB	123/123 (100%)	0.33	5 (4%) 41 40	267, 323, 388, 388		0
26	BA	2814/2916 (96%)	0.46	224 (7%) 18 25	65, 238, 393, 400		0
27	BD	173/173 (100%)	2.01	54 (31%) 1 6	392, 392, 400, 400		0
28	BE	191/338 (56%)	2.34	99 (51%) 0 3	400, 400, 400, 400		0
29	BF	189/246 (76%)	2.19	84 (44%) 0 4	393, 396, 396, 396		0
30	BG	122/176 (69%)	1.58	40 (32%) 1 6	400, 400, 400, 400		0
31	BH	164/177 (92%)	1.07	34 (20%) 2 9	400, 400, 400, 400		0
32	BI	148/149 (99%)	1.37	36 (24%) 2 8	400, 400, 400, 400		0
33	BN	117/145 (80%)	2.29	52 (44%) 0 4	400, 400, 400, 400		0
34	BO	122/122 (100%)	1.51	36 (29%) 1 7	400, 400, 400, 400		0
35	BP	84/164 (51%)	1.33	20 (23%) 2 8	395, 395, 400, 400		0
36	BQ	138/138 (100%)	2.34	64 (46%) 0 4	393, 393, 393, 393		0
37	BS	113/186 (60%)	1.43	33 (29%) 1 7	278, 400, 400, 400		0
38	BT	52/66 (78%)	3.23	32 (61%) 0 2	400, 400, 400, 400		0
39	BW	108/113 (95%)	1.49	28 (25%) 1 8	278, 395, 400, 400		0
40	BX	76/84 (90%)	3.54	48 (63%) 0 2	400, 400, 400, 400		0
41	BY	110/119 (92%)	3.01	49 (44%) 0 4	400, 400, 400, 400		0
42	BZ	177/253 (69%)	1.48	51 (28%) 1 7	396, 398, 398, 398		0
43	BR	105/118 (88%)	1.87	36 (34%) 1 6	400, 400, 400, 400		0
44	BU	117/118 (99%)	2.11	45 (38%) 1 5	391, 391, 400, 400		0
45	BV	100/100 (100%)	1.26	23 (23%) 2 9	400, 400, 400, 400		0
46	B2	64/70 (91%)	2.00	27 (42%) 0 4	400, 400, 400, 400		0
47	B3	60/60 (100%)	1.82	21 (35%) 1 5	398, 398, 398, 398		0
48	B0	86/91 (94%)	1.75	26 (30%) 1 6	396, 400, 400, 400		0
49	B4	73/73 (100%)	2.44	39 (53%) 0 3	396, 397, 397, 397		0
50	B5	58/60 (96%)	1.67	21 (36%) 1 5	400, 400, 400, 400		0
51	B6	53/82 (64%)	1.48	17 (32%) 1 6	400, 400, 400, 400		0
52	B7	46/47 (97%)	2.39	28 (60%) 0 2	396, 396, 396, 396		0
53	B8	63/64 (98%)	2.82	37 (58%) 0 3	400, 400, 400, 400		0
54	B9	35/36 (97%)	4.06	26 (74%) 0 1	400, 400, 400, 400		0
55	BK	133/141 (94%)	1.79	50 (37%) 1 5	392, 400, 400, 400		0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	10091/10981 (91%)	1.15	2125 (21%) 2 9	65, 395, 400, 400	0

The worst 5 of 2125 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	AX	126	A	38.6
4	AX	115	G	29.2
4	AX	124	C	26.8
16	AM	124	PRO	23.1
16	AM	123	ALA	22.7

6.2 Non-standard residues in protein, DNA, RNA chains [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. 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	B-factors(Å ²)	Q<0.9
3	PSU	AW	39	20/21	0.47	0.15	399,399,399,399	0
3	PSU	AW	55	20/21	0.52	0.08	400,400,400,400	0
3	YYG	AW	37	39/40	0.62	0.23	399,399,399,399	0

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.