



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 08:56 am GMT

PDB ID : 4V4T  
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](mailto: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.

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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



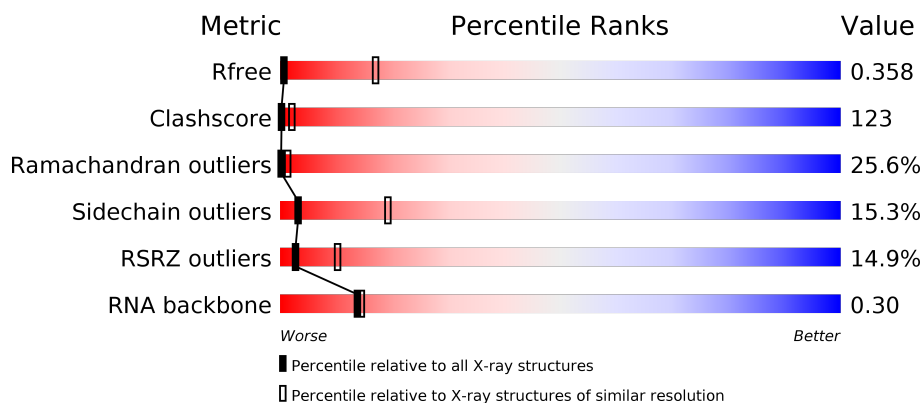
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	100719	1098 (9.00-3.70)
Clashscore	112137	1031 (9.00-3.80)
Ramachandran outliers	110173	1000 (9.00-3.76)
Sidechain outliers	110143	1096 (9.00-3.70)
RSRZ outliers	101464	1000 (9.00-3.72)
RNA backbone	2435	1053 (10.00-2.90)

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  $\geq 3$ , 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	
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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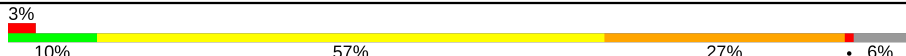
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Mol	Chain	Length	Quality of chain
30	BG	176	
31	BH	177	
32	BI	149	
33	BN	145	
34	BO	122	
35	BP	164	
36	BQ	138	
37	BS	186	
38	BT	66	
39	BW	113	
40	BX	84	
41	BY	119	
42	BZ	253	
43	BR	118	
44	BU	118	
45	BV	100	
46	B2	70	
47	B3	60	
48	B0	91	
49	B4	73	
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			

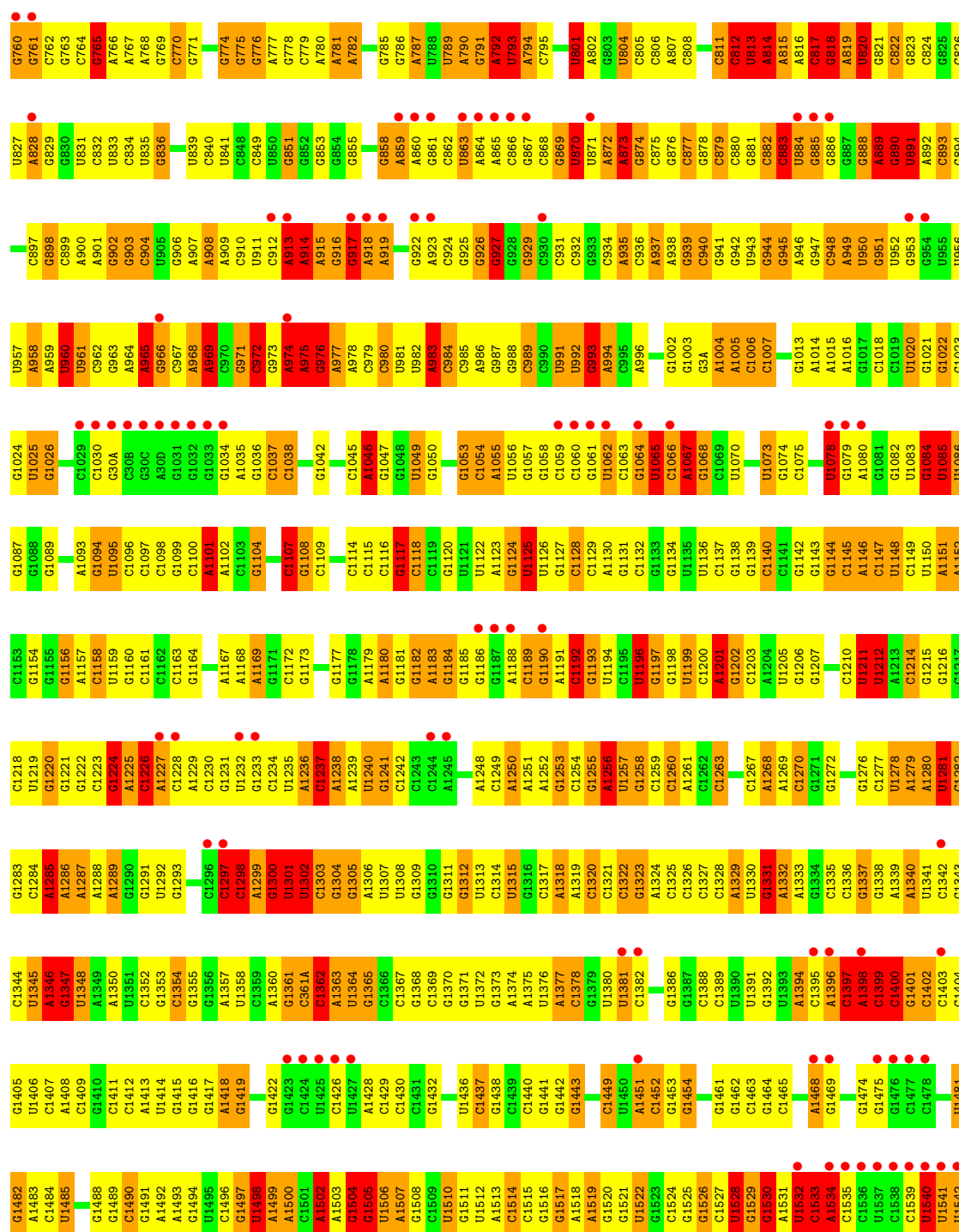
- Molecule 55 is a protein called 50S ribosomal protein L11.

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

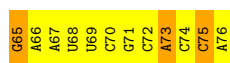




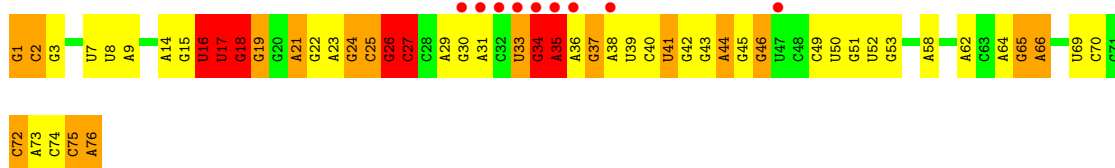








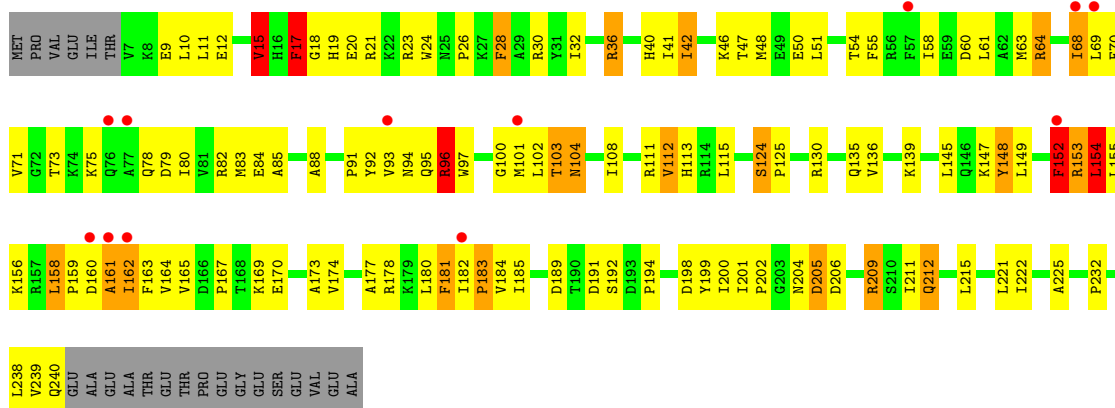
• Molecule 3: E-site tRNA (Phe)



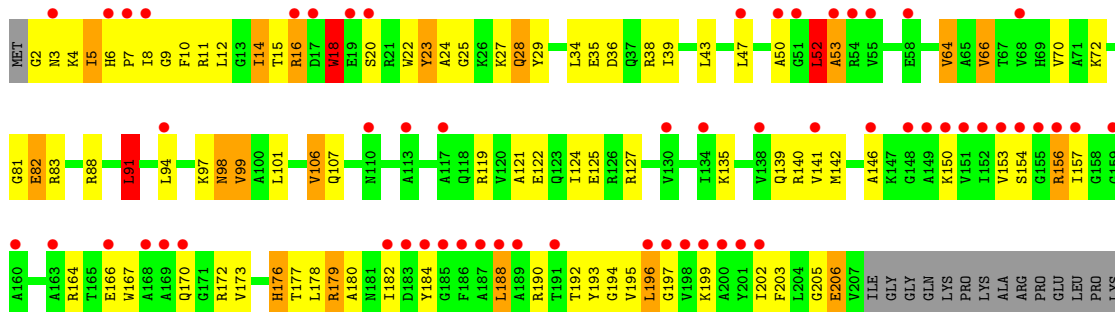
• Molecule 4: 5'-D(\*AP\*UP\*GP\*UP\*UP\*CP\*UP\*AP\*GP\*UP\*AP\*CP\*AP\*AP\*UP\*AP\*AP\*U)-3'



• Molecule 5: 30S ribosomal protein S2



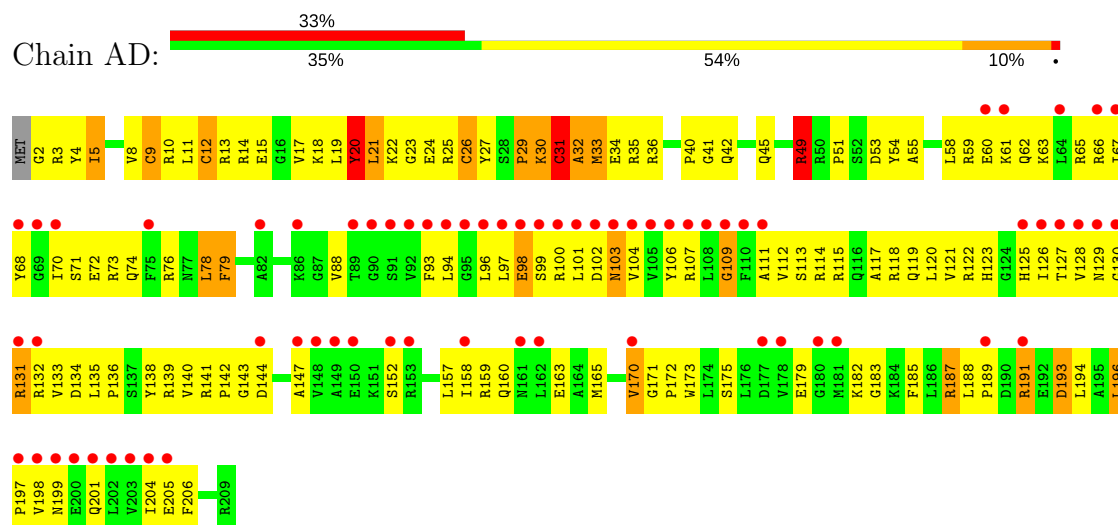
• Molecule 6: 30S ribosomal protein S3



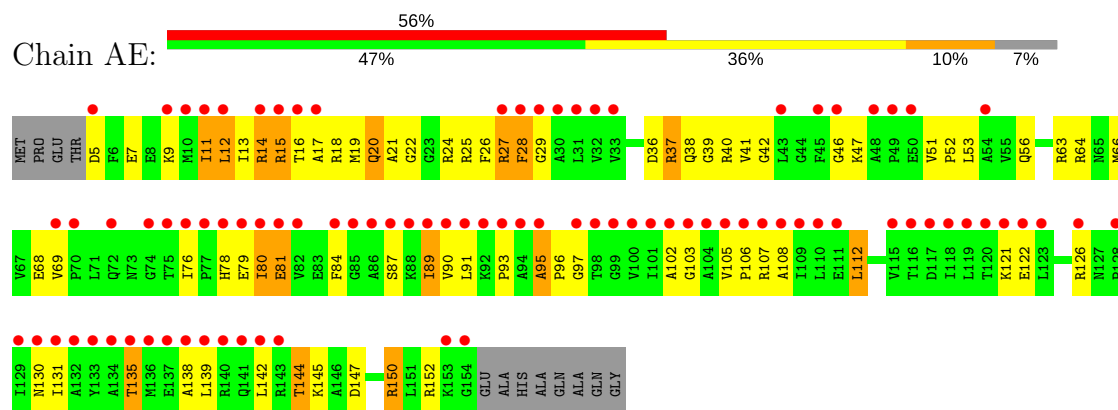


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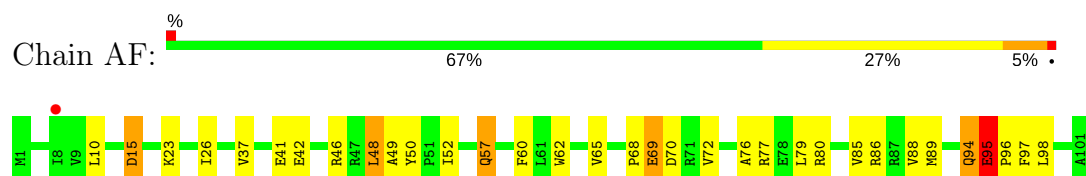
• Molecule 7: 30S ribosomal protein S4



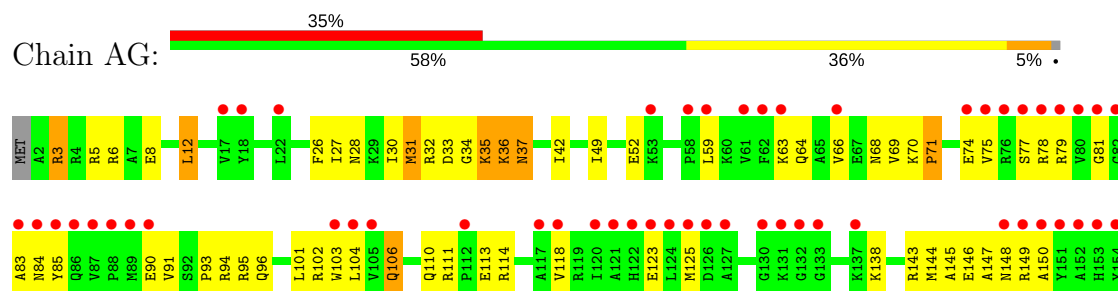
• Molecule 8: 30S ribosomal protein S5



• Molecule 9: 30S ribosomal protein S6



• Molecule 10: 30S ribosomal protein S7

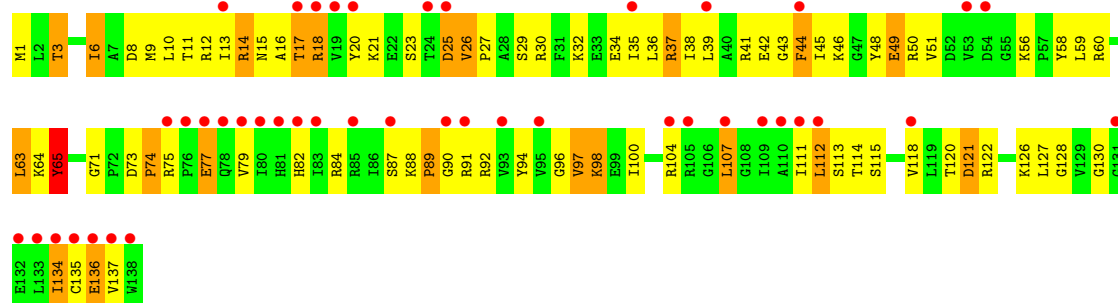






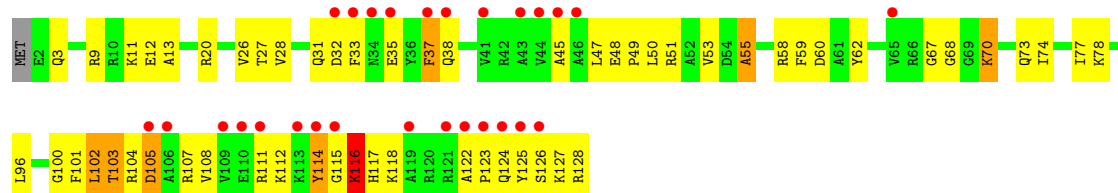
• Molecule 11: 30S ribosomal protein S8

Chain AH: 31% 39% 45% 15%



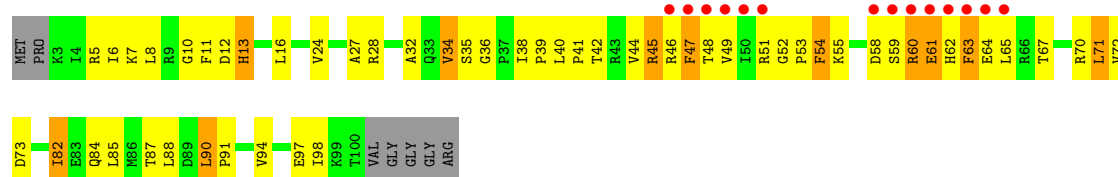
• Molecule 12: 30S ribosomal protein S9

Chain AI: 21% 55% 38% 5%



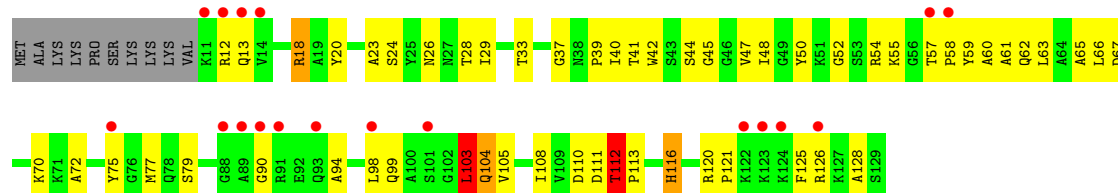
• Molecule 13: 30S ribosomal protein S10

Chain AJ: 13% 41% 42% 10% 7%



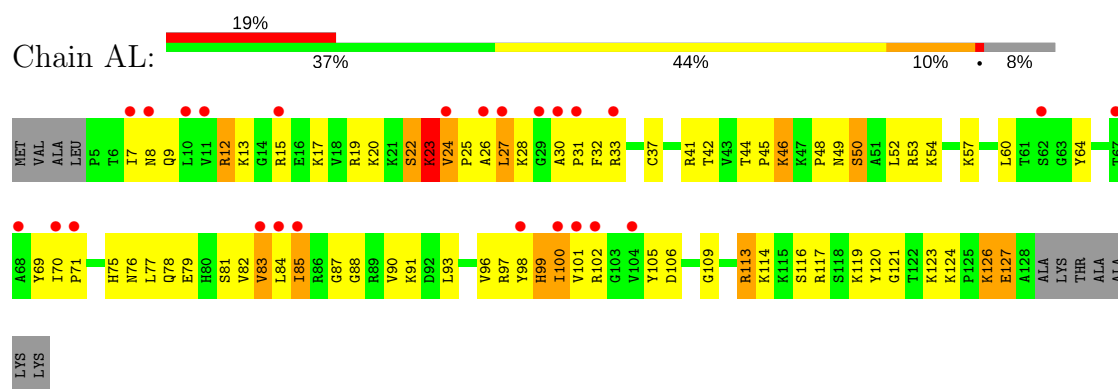
• Molecule 14: 30S ribosomal protein S11

Chain AK: 14% 49% 40% 8%

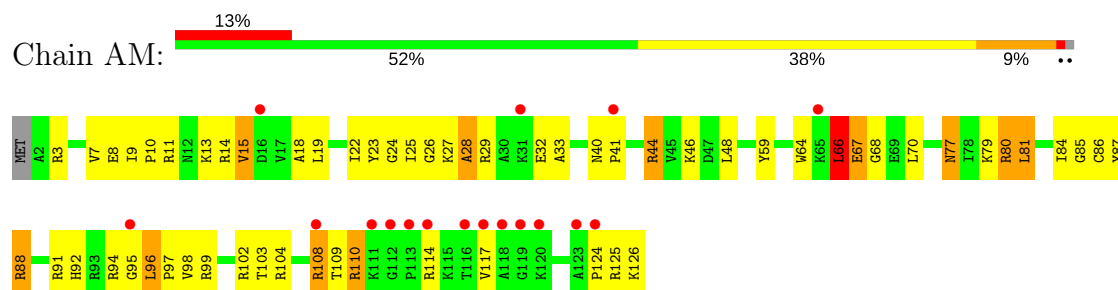


• Molecule 15: 30S ribosomal protein S12

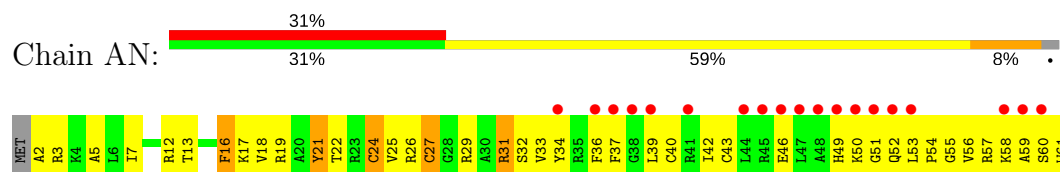




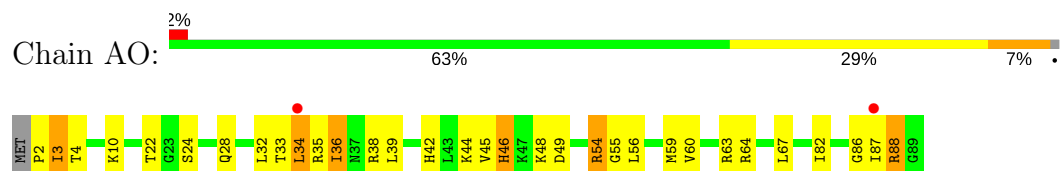
- Molecule 16: 30S ribosomal protein S13



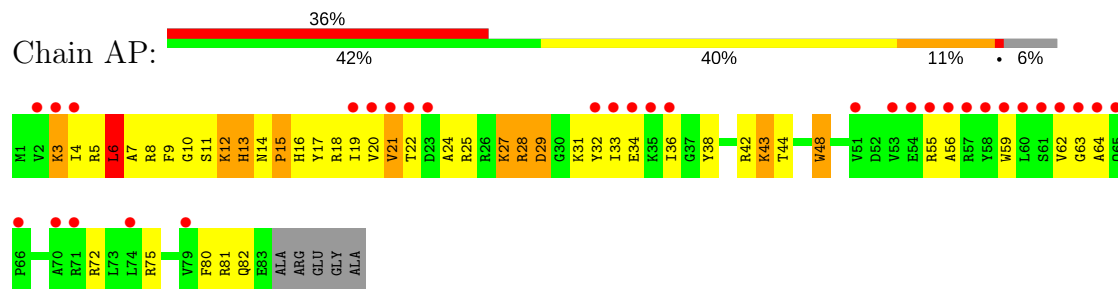
- Molecule 17: 30S ribosomal protein S14



- Molecule 18: 30S ribosomal protein S15



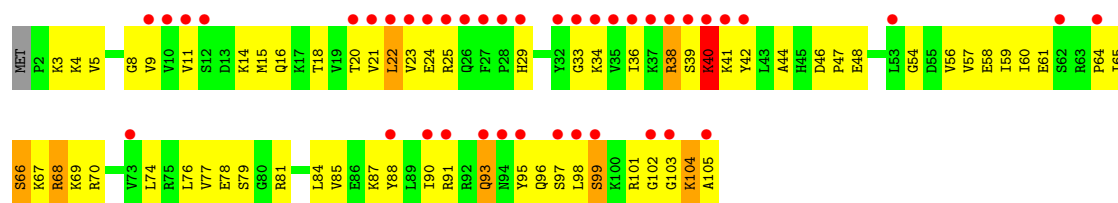
- Molecule 19: 30S ribosomal protein S16



- Molecule 20: 30S ribosomal protein S17

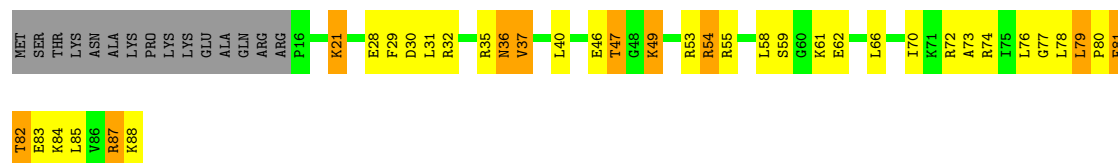






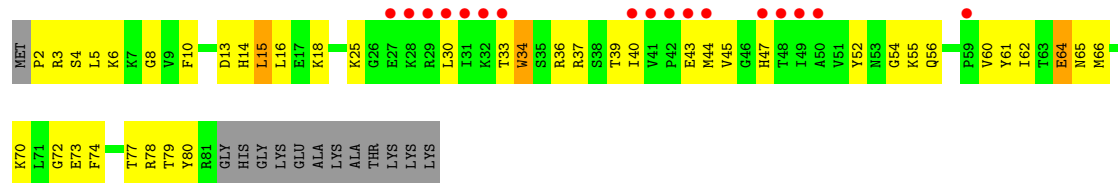
• Molecule 21: 30S ribosomal protein S18

Chain AR: 41% 31% 11% 17%



• Molecule 22: 30S ribosomal protein S19

Chain AS: 18% 41% 42% 14%



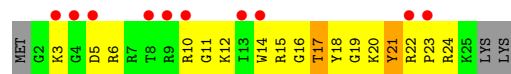
• Molecule 23: 30S ribosomal protein S20

Chain AT: 7% 50% 37% 7% 7%



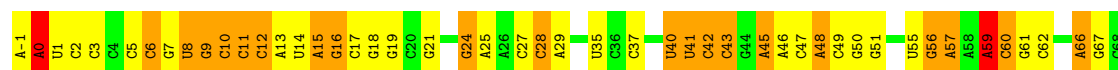
• Molecule 24: 30S ribosomal protein Thx

Chain AU: 37% 26% 56% 7% 11%

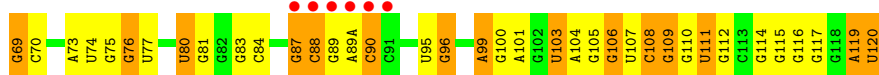


• Molecule 25: 5S ribosomal RNA

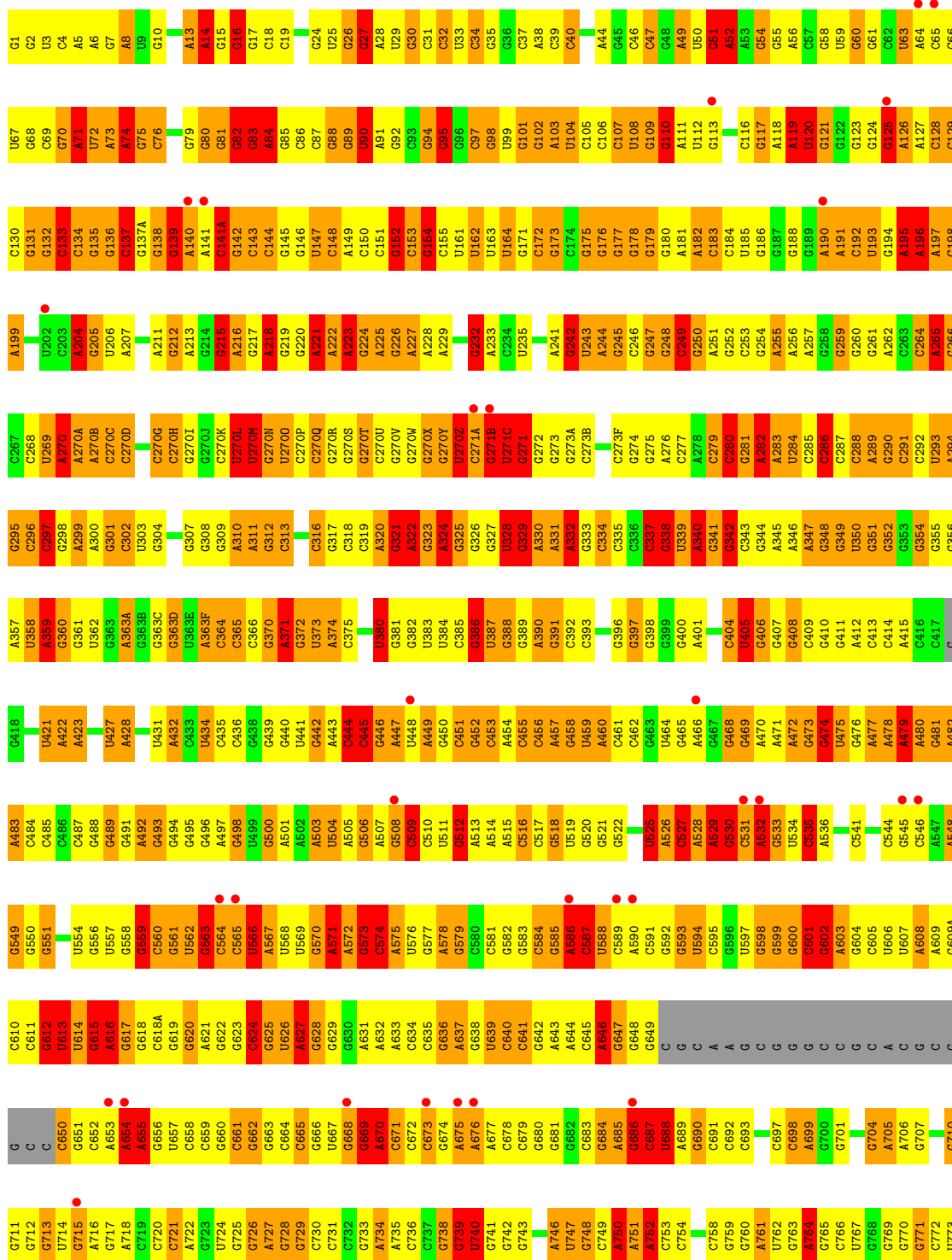
Chain BB: 5% 31% 39% 28%







• Molecule 26: 23S ribosomal RNA





A1610	G1542	A1477	C1351	A1284	A1220	G1157	C1092	A1027	C995	C834	A774
C1611	A1543	G1478	U1352	G1285	C1221	C1158	G1093	A1028	G966	A835	G775
C1612	C1544	G1479	A1353	A1286	C1222	U1159		A1029	G967	G776	A777
G1613	A1545	G1480	G1355	A1287	C1223	G1160	A1096	G1030	G968	C837	A778
A1614	A545A	G1482	G1356	U1288	G1224	C1161	U1097	G1031	U969	C838	G779
C1615	G1483	G1483	G1357	C1289	G1225	G1162	A1098	G1032	G970	U778	
A1616	C1547	G1484	U1357		G1226	G1163	A1099	U1033	C971	G840	G780
C1617	C1548	U1420	G1358	U1294	A1227	G1164	C1100	U1034	G972	A781	
A1618		G1421	A1359	C1297	G1228	U1165	U1101	U1035	C908	G845	A782
G1619	G1552	A1489	G1360	C1298	G1229	C1166	A1102	G1036	A910	C846	A783
G1620	A1553	A1490	A1361	G1299	C1230	U1167	A1103	G974A	A911	U847	A784
U1621	G1491	G1422	G1362	U1299	C1231	G1168	C1104	G975	G976	G848	G785
	G1492	G1425	G1363	U1300		G1169	U1105	C1040	C977	C850	G786
G1624	C1493	G1426	G1364	A1301	G1234	U1170	G1106	C1041		C914	U787
C1625	C1557	A1427	A1365	A1302	G1235	G1171	G1107	G1044	G978	C915	A788
G1626	C1558	C1428	A1366	G1303	A1236	G1172	G1108	A1045	G979	G916	A789
G1627	G1559	G1429	A1367	C1304	G1238	U1174	C1109	A1046	A980	A917	C790
G1628	U1497	C1430	G1368	C1305	G1239	U1175	G1110		A981	A918	G791
U1629	G1498	U1431	G1369	C1306	U1240	G1176	A1111	C1049	G982	G919	G792
G1630		U1432	C1370	A1307	A1241	A1177	G1112	A1050	A983	G920	A793
C630A	C1564	U1433	G1371	A1308	A1242	C1178	U1113	G1051	A984	G921	G794
A1631	C1565	A1434	U1372	G1309	G1243	C1180	G1114	A1054	C985	U922	C795
A1632	A1566	A1434	A1373	G1310	G1244	C1181	G1115	G1055	G986	C923	C796
G1633	G1567	C1437	G1374	U1312	G1245	C1182	G1116	G1056	G987	G1057	C797
A1634	A1568	U1438	C1375	U1313	A1246	A1183	G1117	A1057	A988	G928	G798
G1635	A1569	A1439	C1376	U1314	A1247	G1184	C1118	A1058	G989	G929	G799
C1636	C1570	G1440	G1377	C1315	U1248	G1185	C1119	G1059	A990	U930	A800
A1637	A1571	A1441	A1378	C1316	U1249	C1186	G1120	C991	G991	C931	A801
U1638	A1572	G1442	A1379	G1250	G1251	G1187	C1123	U1060	G992	G932	A802
G1639	G1573	G1443	G1380	C1317	C251	U1188	G1124	U1061	G993	A933	A803
C1640	C1574	G1444	G1381	U1318	G1252	A1189	G1125	G1062	C994	G934	A804
A1641	C1575	A444A	G1382	C1319	A1253	U1190	G1126	G1063	C995	C935	C805
	U1576		C1383	C1320	A1254	G1191	A1127	C1064	A996		C806
G1643	C1577	G1447	A1384	A1321	U1255	G1192	A1128	U1065	G997	G938	U807
C1644	U1578	G1448	G1385		G1256	C1193	A1129	A1067	C998	G939	A808
G1645	A1579	A1449	A1386	G1324	C1257	G1195	U1130	G1068	A872	G940	G809
G1646	A1580	G449A	G1389	G1325	C1258	C1196	G1131	A1069	G874	A941	U810
G1647	G1581	C1450	U1390	U1326	G1259	U1197	A1132	A1070	G875	U943	U811
C1648	C1582	C1451	U1391	G1327	G1260	G1198	U1133	G944		G944	C812
G1649	A1583	A1453	U1392	G1328	C1261	U1199	G1134	G1071	C885	G945	U813
G1650	C1585	U1454	A1392	U1329	A1262	U1199	G1135	A945	U877	A846	C814
G1651	A1586	G1455	A1393	C1330	U1263		C1136	A1073	U878	G946	C815
A1652	C1587	G1456	U1394	A1331	G1264	G1202	G1137	G1074	G879	G947	C816
G1653	C1588	A1457	A1395	G1332	A1265	G1203	G1138	C1075	C880	G948	C817
A1654	G1526		U1396	C1333	G1266	A1204	G1139	C1076	C881	C949	G818
	G1527	A1460	U1397	G1334	U1267	U1205	G1140	A1077	G882	G950	A819
C1655	A1528	G1461	C1398	U1335	A1268	G1206	C1141	U1078		C951	A820
C1656	C1529	C1462	C1399	A1336	A1269	C1207	U1141	G1079	C885	G952	A821
C1657	G1530	C1463	G1400	G1337	C1270	G1208	U1142	C1080	C886	A953	U822
C1658	C1531		G1401	U1338	G1271	G1209	A142A	U1081	A887	G954	G823
U1659	C1532	G1466	C1402	G1339	A1272	A1210	A1143	U1082	C888	C955	A824
C1660	G1533	C1467	G1403	U1340	U1273	G1211		U1083	G889	G956	C825
G1661	C1534		A1404	U1341	A1274	U1212	C1149	A1084	A890	A957	U826
C1662	U1535	G1470	U1405	A1342	A1275	A1213	C1150	A1085	U1019	U958	U827
A1664	A1536	A1471	U1406	G1343	A1276	A1214	C1151	A1086	A959	A894	U828
C1665	C1537	A1472	G1407	G1344	G1277	G1215	C1152	G1087	A960	U895	A829
G1666	G1538	G1473	C1408	C1345	A1278	G1216	G1153	A1088	C961	U1023	G830
	G1539	C1474	C1409		G1279	C1217	G1154	U1089	G962	U1024	G831
A1668	A1540	G1475	G1410	A1349	G1283	C1218	A1155	U1090	U963	G1025	G832
A1669	U1541	C1476	C1411	C1350		G1219	A1156	G1091	C964	U1026	U833

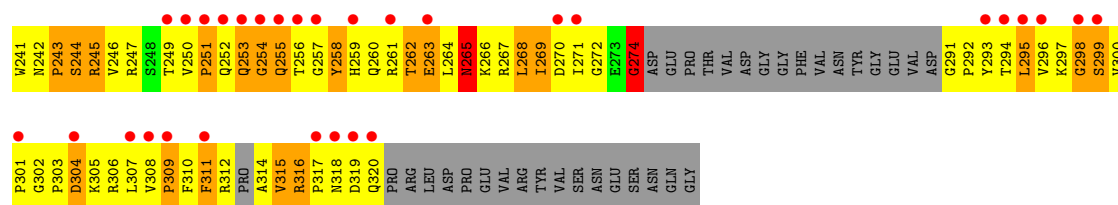




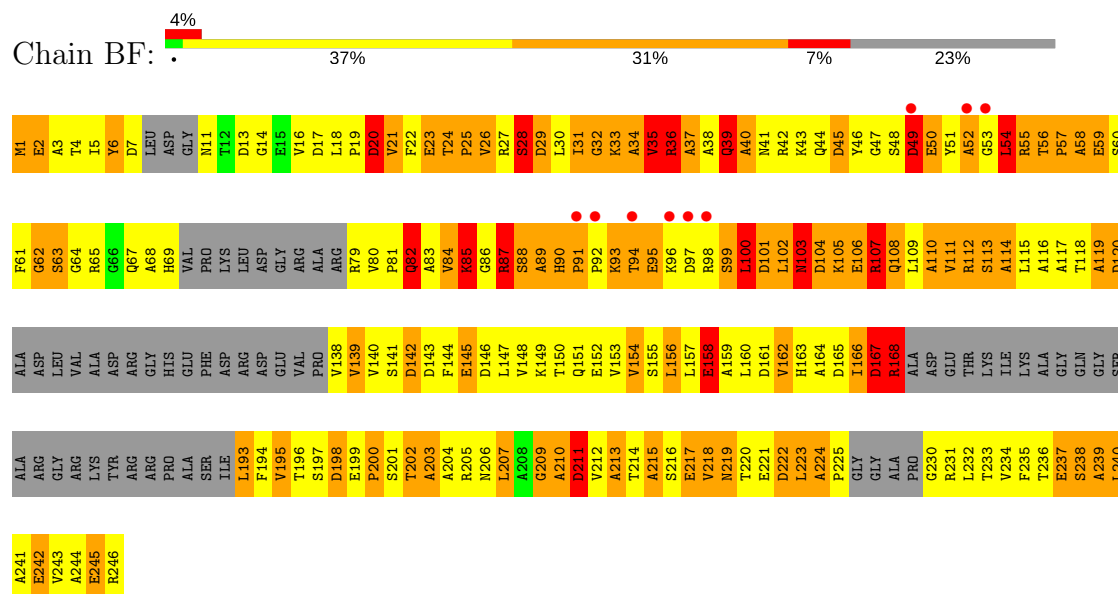




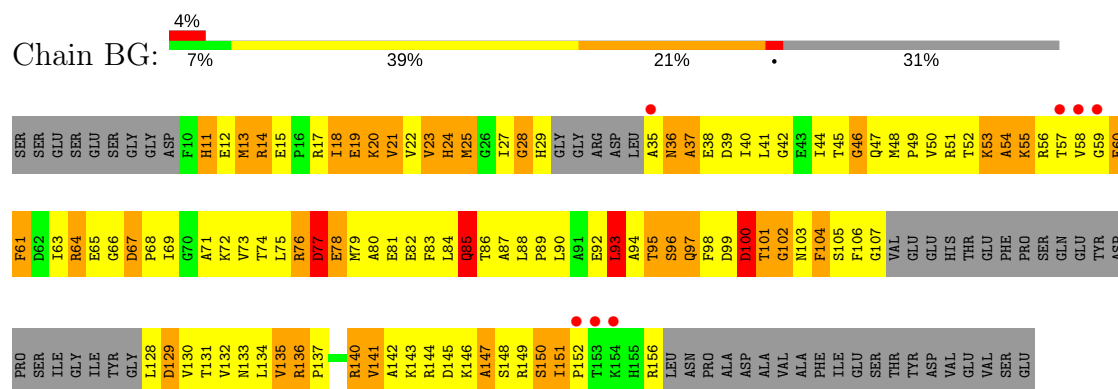




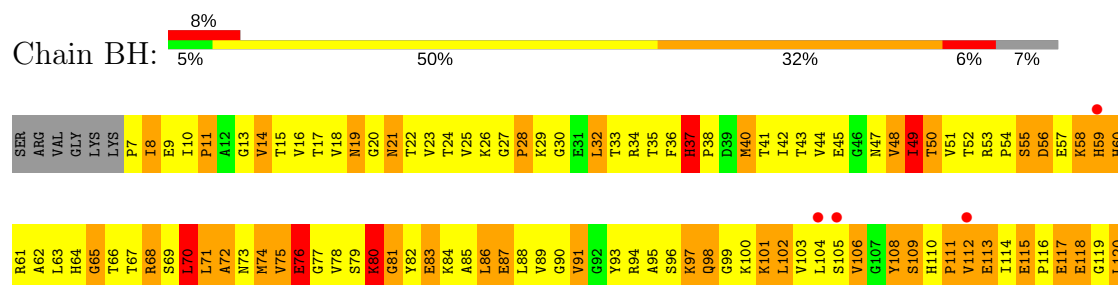
• Molecule 29: 50S ribosomal protein L4



• Molecule 30: 50S ribosomal protein L5



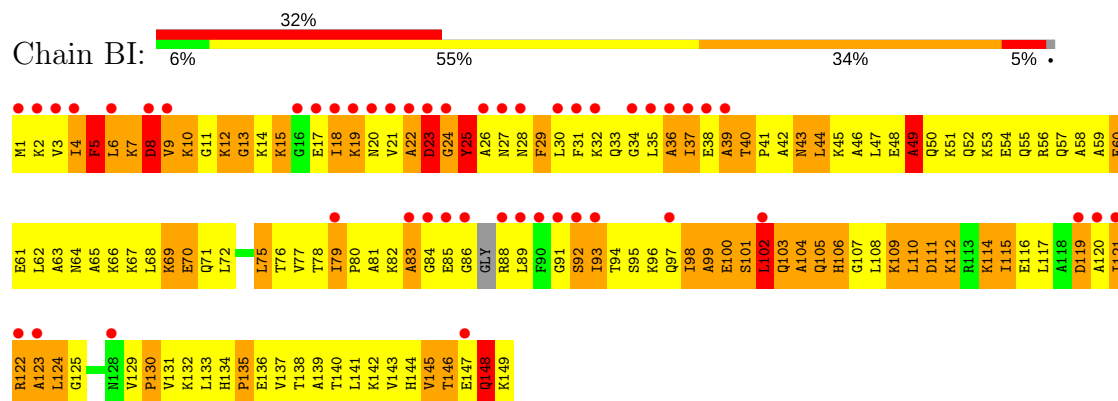
• Molecule 31: 50S ribosomal protein L6



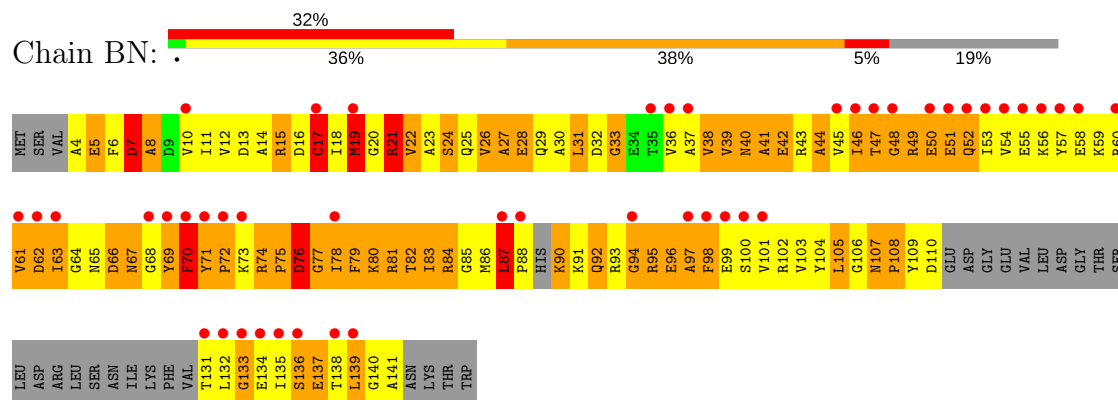




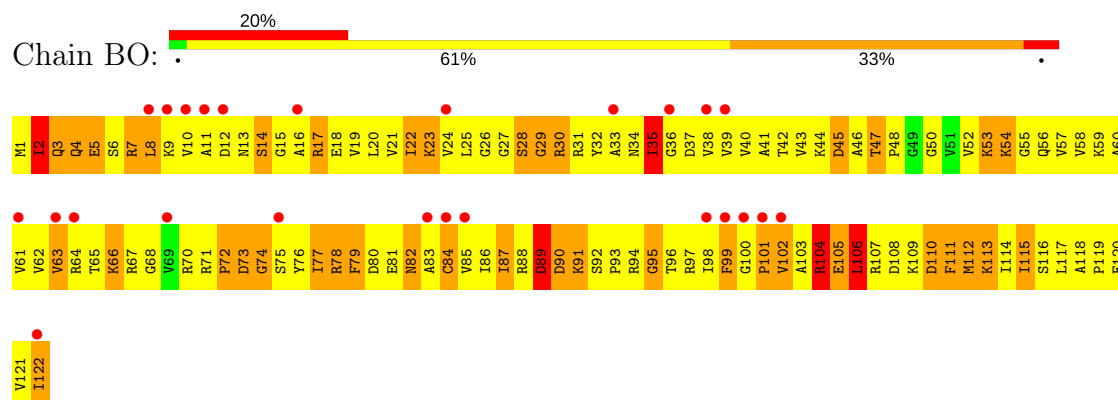
• Molecule 32: 50S ribosomal protein L9



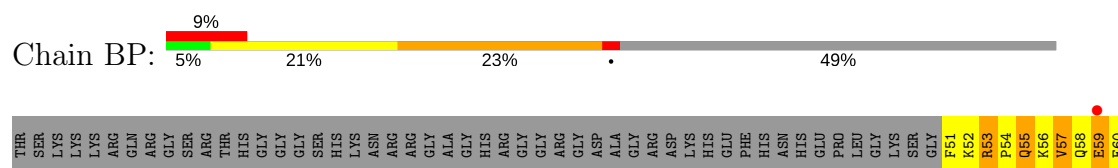
• Molecule 33: 50S ribosomal protein L13



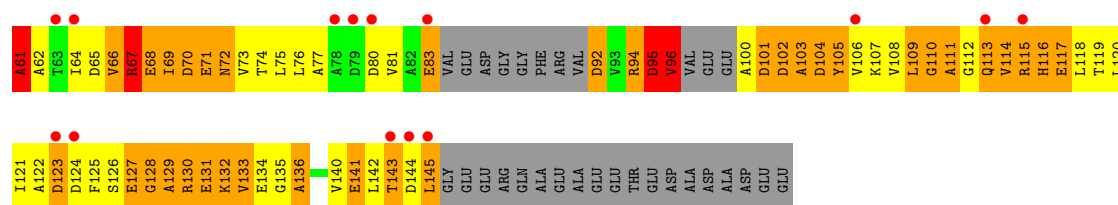
• Molecule 34: 50S ribosomal protein L14



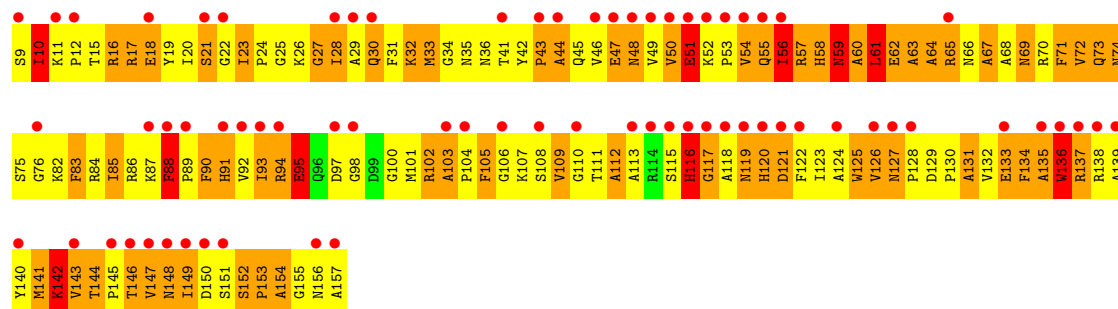
• Molecule 35: 50S ribosomal protein L15



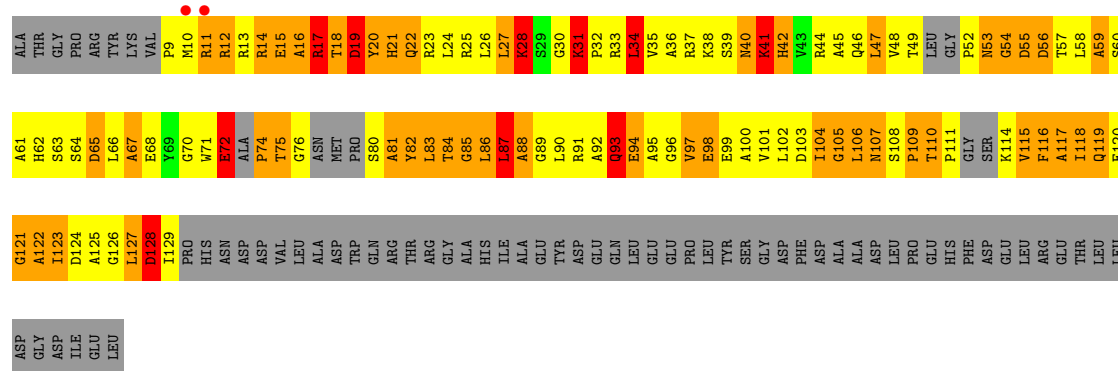
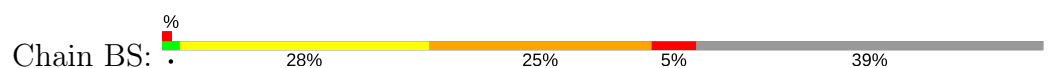




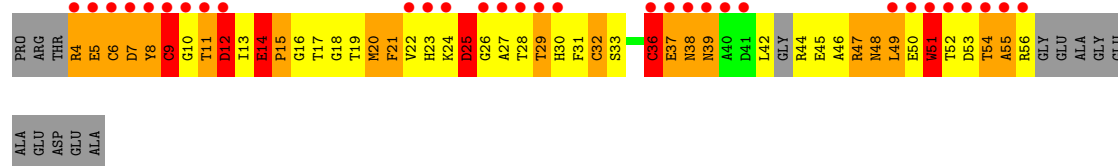
• Molecule 36: 50S ribosomal protein L16



• Molecule 37: 50S ribosomal protein L18



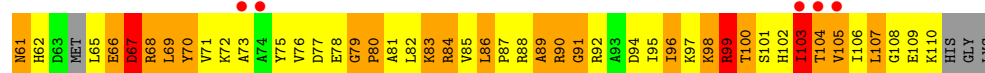
• Molecule 38: 50S ribosomal protein L19



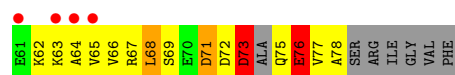
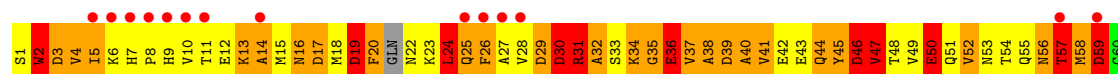
• Molecule 39: 50S ribosomal protein L22



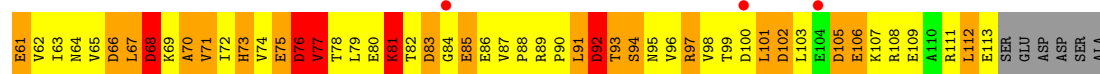
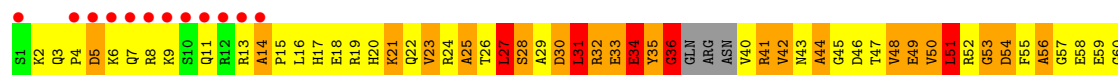




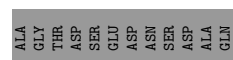
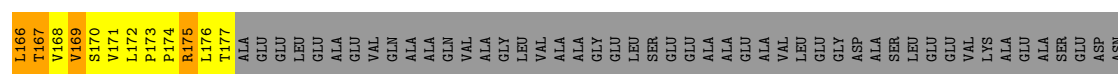
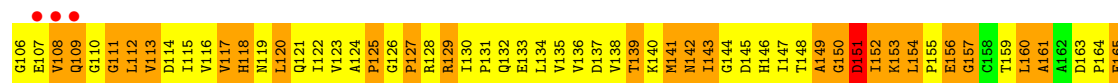
• Molecule 40: 50S ribosomal protein L23



• Molecule 41: 50S ribosomal protein 24



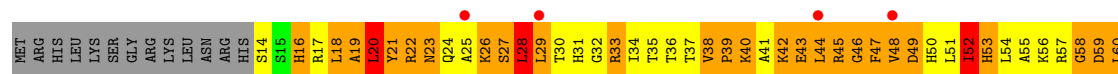
• Molecule 42: 50S ribosomal protein CTC



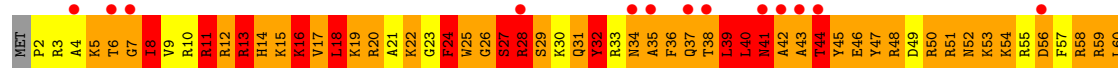
• Molecule 43: 50S ribosomal protein L17



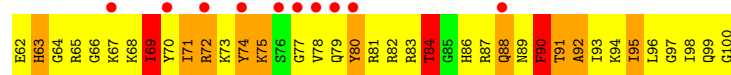
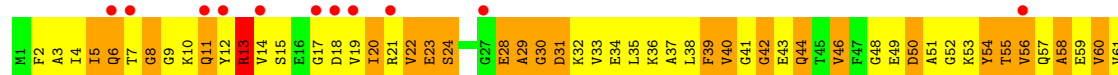
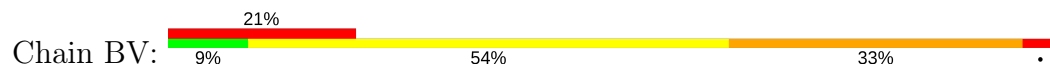




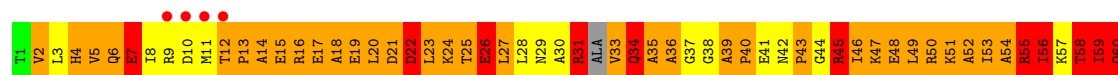
• Molecule 44: 50S ribosomal protein L20



• Molecule 45: 50S ribosomal protein L21



• Molecule 46: 50S ribosomal protein L29



• Molecule 47: 50S ribosomal protein L30



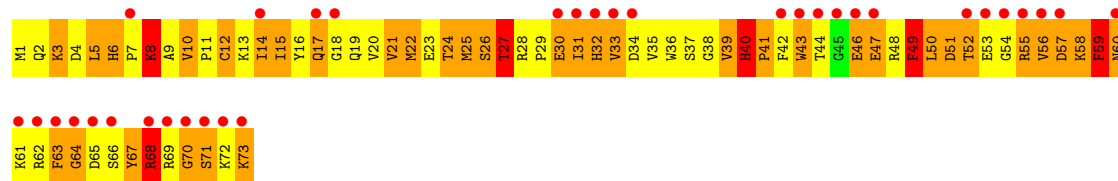
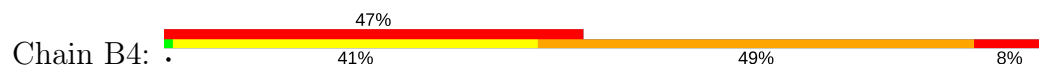
• Molecule 48: 50S ribosomal protein L27







• Molecule 49: 50S ribosomal protein L31



• Molecule 50: 50S ribosomal protein L32



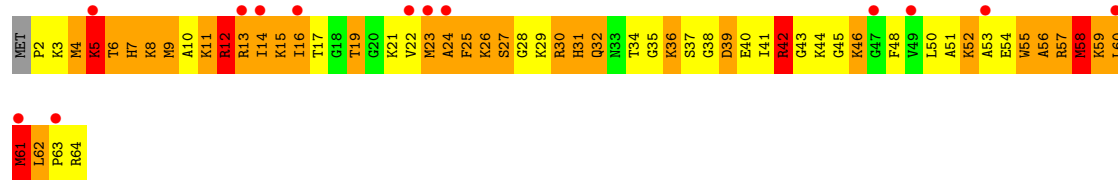
• Molecule 51: 50S ribosomal protein L33



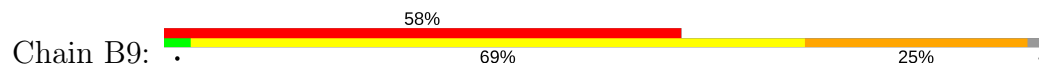
• Molecule 52: 50S ribosomal protein L34



• Molecule 53: 50S ribosomal protein L35



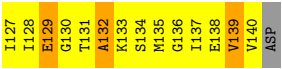
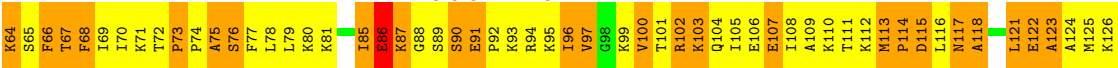
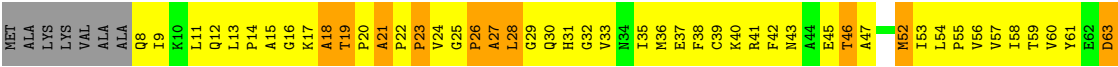
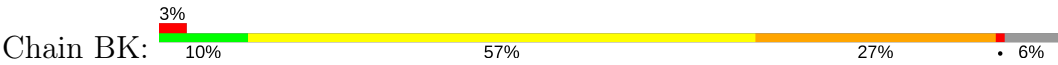
• Molecule 54: 50S ribosomal protein L36







● 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, $\alpha$ , $\beta$ , $\gamma$	517.41Å 517.41Å 365.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 6.46 99.57 – 6.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (40.00-6.46) 99.7 (99.57-6.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.13	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.87 (at 6.19Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.354 , 0.361 0.345 , 0.358	Depositor DCC
$R_{free}$ test set	4902 reflections (5.20%)	DCC
Wilson B-factor (Å <sup>2</sup> )	240.8	Xtriage
Anisotropy	0.222	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.10 , 90.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	142447	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	1.32	68/36413 (0.2%)	1.49	439/56777 (0.8%)
2	AV	0.74	3/1812 (0.2%)	1.20	8/2819 (0.3%)
3	AW	1.81	19/1739 (1.1%)	2.15	47/2698 (1.7%)
4	AX	0.18	0/139	0.67	0/213
5	AB	0.60	2/1935 (0.1%)	0.61	0/2609
6	AC	0.73	2/1636 (0.1%)	0.61	4/2205 (0.2%)
7	AD	0.70	4/1733 (0.2%)	1.03	11/2318 (0.5%)
8	AE	0.83	1/1162 (0.1%)	0.63	1/1564 (0.1%)
9	AF	0.35	0/856	0.54	0/1154
10	AG	0.34	0/1276	0.59	3/1709 (0.2%)
11	AH	0.41	0/1136	0.66	0/1527
12	AI	0.34	0/1029	0.54	0/1378
13	AJ	0.35	0/807	0.56	0/1085
14	AK	0.59	1/900 (0.1%)	0.54	0/1213
15	AL	1.33	1/986 (0.1%)	1.11	3/1320 (0.2%)
16	AM	0.92	1/1007 (0.1%)	0.59	1/1344 (0.1%)
17	AN	0.49	1/501 (0.2%)	0.65	1/664 (0.2%)
18	AO	0.32	0/745	0.54	0/992
19	AP	0.40	0/716	0.59	1/963 (0.1%)
20	AQ	1.23	2/870 (0.2%)	1.38	6/1159 (0.5%)
21	AR	0.40	0/603	0.70	0/799
22	AS	0.34	0/661	0.53	0/890
23	AT	0.32	0/764	0.57	1/1006 (0.1%)
24	AU	0.33	0/212	0.49	0/277
25	BB	1.25	6/2950 (0.2%)	1.44	25/4602 (0.5%)
26	BA	1.17	153/67839 (0.2%)	1.46	906/105818 (0.9%)
27	BD	0.38	0/1328	0.60	0/1783
28	BE	0.65	4/1540 (0.3%)	1.07	7/2078 (0.3%)
29	BF	0.76	3/1444 (0.2%)	0.83	1/1954 (0.1%)
30	BG	0.25	0/971	0.46	0/1304
31	BH	0.54	1/1272 (0.1%)	0.80	3/1721 (0.2%)
32	BI	0.32	0/1156	0.71	3/1544 (0.2%)



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	BN	0.35	0/927	0.55	0/1245
34	BO	0.32	0/946	0.57	0/1269
35	BP	1.59	3/643 (0.5%)	1.31	5/870 (0.6%)
36	BQ	0.32	0/1106	0.53	0/1490
37	BS	1.13	3/877 (0.3%)	0.69	1/1179 (0.1%)
38	BT	0.39	0/412	0.70	0/554
39	BW	0.75	3/869 (0.3%)	0.75	4/1166 (0.3%)
40	BX	0.49	1/608 (0.2%)	1.04	3/820 (0.4%)
41	BY	0.26	0/887	0.83	3/1195 (0.3%)
42	BZ	0.32	1/1385 (0.1%)	0.62	3/1883 (0.2%)
43	BR	0.30	0/867	0.50	0/1162
44	BU	0.64	1/994 (0.1%)	0.74	3/1323 (0.2%)
45	BV	0.82	1/796 (0.1%)	0.91	3/1058 (0.3%)
46	B2	0.37	0/497	1.00	2/668 (0.3%)
47	B3	0.31	0/482	0.50	0/646
48	B0	0.38	1/649 (0.2%)	0.87	3/860 (0.3%)
49	B4	0.89	2/620 (0.3%)	0.54	0/831
50	B5	0.36	0/469	0.90	3/629 (0.5%)
51	B6	0.32	0/438	0.55	1/583 (0.2%)
52	B7	0.38	0/387	0.64	0/509
53	B8	0.91	2/503 (0.4%)	0.92	3/657 (0.5%)
54	B9	0.33	0/286	0.59	0/375
55	BK	0.27	1/1014 (0.1%)	0.44	0/1363
All	All	1.09	291/154800 (0.2%)	1.33	1508/231822 (0.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	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 291 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BA	2199	A	O3'-P	-71.04	0.75	1.61
1	AA	1278	U	O3'-P	-56.53	0.93	1.61
1	AA	1337	G	O3'-P	-53.91	0.96	1.61
26	BA	1546	C	O3'-P	-51.62	0.99	1.61
1	AA	1004	A	O3'-P	48.18	2.19	1.61

The worst 5 of 1508 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AW	65	G	P-O3'-C3'	-50.68	58.88	119.70
26	BA	712(A)	A	P-O3'-C3'	-43.62	67.36	119.70
26	BA	2199	A	O3'-P-O5'	-43.07	22.17	104.00
2	AV	65	G	P-O3'-C3'	39.88	167.56	119.70
1	AA	1255	G	P-O3'-C3'	-38.36	73.67	119.70

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	2042	3
2	AV	1622	0	821	231	0
3	AW	1638	0	836	243	0
4	AX	136	0	63	26	0
5	AB	1900	0	1950	97	0
6	AC	1612	0	1675	99	0
7	AD	1703	0	1761	289	0
8	AE	1146	0	1206	68	0
9	AF	843	0	857	30	0
10	AG	1257	0	1295	102	0
11	AH	1116	0	1177	100	0
12	AI	1011	0	1040	80	0
13	AJ	794	0	840	81	0
14	AK	885	0	904	53	0
15	AL	970	0	1056	72	0
16	AM	997	0	1070	149	0
17	AN	492	0	529	82	0
18	AO	734	0	771	28	0
19	AP	700	0	720	70	0
20	AQ	857	0	928	80	0
21	AR	597	0	668	40	0
22	AS	647	0	673	155	0
23	AT	762	0	859	37	0
24	AU	208	0	221	84	0
25	BB	2637	0	1339	219	1
26	BA	60600	0	30514	11060	138
27	BD	1308	0	1346	1086	0
28	BE	1507	0	1478	1144	3
29	BF	1430	0	1357	1085	0
30	BG	957	0	952	692	0
31	BH	1251	0	1291	754	0
32	BI	1145	0	1225	625	3
33	BN	917	0	896	771	2
34	BO	937	0	992	613	0
35	BP	639	0	605	482	0
36	BQ	1081	0	1047	932	0
37	BS	866	0	866	677	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	BT	406	0	359	167	0
39	BW	860	0	909	557	0
40	BX	602	0	558	460	0
41	BY	879	0	860	755	0
42	BZ	1360	0	1378	902	0
43	BR	855	0	904	579	0
44	BU	978	0	996	895	0
45	BV	787	0	782	635	0
46	B2	494	0	504	393	0
47	B3	477	0	527	460	0
48	B0	641	0	661	531	0
49	B4	604	0	587	489	0
50	B5	457	0	456	279	0
51	B6	431	0	454	289	0
52	B7	383	0	409	382	0
53	B8	496	0	539	349	0
54	B9	285	0	312	195	0
55	BK	999	0	1064	573	0
All	All	142447	0	94546	28969	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 123.

The worst 5 of 28969 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	20
6	AC	204/239 (85%)	166 (81%)	24 (12%)	14 (7%)	1	20
7	AD	206/209 (99%)	157 (76%)	33 (16%)	16 (8%)	1	17
8	AE	148/162 (91%)	116 (78%)	29 (20%)	3 (2%)	9	46
9	AF	99/101 (98%)	85 (86%)	10 (10%)	4 (4%)	3	31
10	AG	153/156 (98%)	131 (86%)	18 (12%)	4 (3%)	6	40
11	AH	136/138 (99%)	101 (74%)	25 (18%)	10 (7%)	1	18
12	AI	125/128 (98%)	86 (69%)	31 (25%)	8 (6%)	1	22
13	AJ	96/105 (91%)	73 (76%)	14 (15%)	9 (9%)	1	14
14	AK	117/129 (91%)	88 (75%)	22 (19%)	7 (6%)	2	22
15	AL	122/135 (90%)	90 (74%)	13 (11%)	19 (16%)	0	4
16	AM	121/126 (96%)	95 (78%)	20 (16%)	6 (5%)	2	27
17	AN	58/61 (95%)	42 (72%)	12 (21%)	4 (7%)	1	20
18	AO	86/89 (97%)	76 (88%)	9 (10%)	1 (1%)	15	57
19	AP	81/88 (92%)	64 (79%)	11 (14%)	6 (7%)	1	18
20	AQ	102/105 (97%)	78 (76%)	18 (18%)	6 (6%)	2	23
21	AR	71/88 (81%)	54 (76%)	11 (16%)	6 (8%)	1	15
22	AS	78/93 (84%)	60 (77%)	15 (19%)	3 (4%)	4	32
23	AT	97/106 (92%)	79 (81%)	12 (12%)	6 (6%)	2	22
24	AU	22/27 (82%)	17 (77%)	3 (14%)	2 (9%)	1	15

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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	1
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%)	173 (86%)	29 (14%)	4	22
6	AC	160/188 (85%)	146 (91%)	14 (9%)	12	40
7	AD	180/181 (99%)	162 (90%)	18 (10%)	9	33
8	AE	115/123 (94%)	94 (82%)	21 (18%)	2	12
9	AF	90/90 (100%)	83 (92%)	7 (8%)	15	46
10	AG	126/127 (99%)	116 (92%)	10 (8%)	14	45
11	AH	119/119 (100%)	92 (77%)	27 (23%)	1	6
12	AI	98/99 (99%)	90 (92%)	8 (8%)	13	44
13	AJ	88/92 (96%)	77 (88%)	11 (12%)	5	26
14	AK	90/99 (91%)	85 (94%)	5 (6%)	25	57
15	AL	104/111 (94%)	93 (89%)	11 (11%)	8	31
16	AM	100/101 (99%)	87 (87%)	13 (13%)	5	25
17	AN	49/50 (98%)	43 (88%)	6 (12%)	6	26
18	AO	79/80 (99%)	70 (89%)	9 (11%)	7	28
19	AP	72/74 (97%)	62 (86%)	10 (14%)	4	23
20	AQ	96/97 (99%)	87 (91%)	9 (9%)	10	36
21	AR	64/77 (83%)	57 (89%)	7 (11%)	7	30
22	AS	71/80 (89%)	64 (90%)	7 (10%)	9	34
23	AT	76/82 (93%)	68 (90%)	8 (10%)	8	32
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%)	99 (73%)	36 (27%)	0	4
28	BE	156/284 (55%)	128 (82%)	28 (18%)	2	13
29	BF	152/193 (79%)	124 (82%)	28 (18%)	2	12
30	BG	102/147 (69%)	93 (91%)	9 (9%)	12	40
31	BH	137/147 (93%)	111 (81%)	26 (19%)	2	11
32	BI	119/119 (100%)	98 (82%)	21 (18%)	2	14
33	BN	95/121 (78%)	80 (84%)	15 (16%)	3	18
34	BO	101/101 (100%)	81 (80%)	20 (20%)	1	10
35	BP	67/126 (53%)	56 (84%)	11 (16%)	2	17
36	BQ	110/110 (100%)	83 (76%)	27 (24%)	1	5
37	BS	89/149 (60%)	73 (82%)	16 (18%)	2	13
38	BT	44/52 (85%)	30 (68%)	14 (32%)	0	2
39	BW	88/92 (96%)	74 (84%)	14 (16%)	3	18
40	BX	67/73 (92%)	44 (66%)	23 (34%)	0	1
41	BY	97/105 (92%)	80 (82%)	17 (18%)	2	14
42	BZ	151/203 (74%)	130 (86%)	21 (14%)	4	23
43	BR	89/101 (88%)	71 (80%)	18 (20%)	1	9
44	BU	96/97 (99%)	68 (71%)	28 (29%)	0	3
45	BV	79/79 (100%)	69 (87%)	10 (13%)	5	25
46	B2	51/56 (91%)	37 (72%)	14 (28%)	0	4
47	B3	52/52 (100%)	47 (90%)	5 (10%)	10	35
48	B0	64/67 (96%)	57 (89%)	7 (11%)	7	30
49	B4	66/66 (100%)	54 (82%)	12 (18%)	2	12
50	B5	51/53 (96%)	43 (84%)	8 (16%)	3	18
51	B6	46/69 (67%)	39 (85%)	7 (15%)	3	19
52	B7	39/40 (98%)	31 (80%)	8 (20%)	1	8
53	B8	50/51 (98%)	39 (78%)	11 (22%)	1	7
54	B9	34/35 (97%)	30 (88%)	4 (12%)	6	27
55	BK	108/113 (96%)	104 (96%)	4 (4%)	39	68
All	All	4533/5148 (88%)	3841 (85%)	692 (15%)	3	19

5 of 692 residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
29	BF	120	ASP
33	BN	87	LEU
49	B4	15	ILE
30	BG	13	MET
31	BH	137	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 129 such sidechains are listed below:

Mol	Chain	Res	Type
28	BE	242	ASN
32	BI	64	ASN
48	B0	71	ASN
28	BE	260	GLN
29	BF	219	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1492/1522 (98%)	520 (34%)	0
2	AV	73/76 (96%)	16 (21%)	0
25	BB	122/123 (99%)	45 (36%)	0
26	BA	2777/2916 (95%)	1487 (53%)	0
3	AW	70/76 (92%)	16 (22%)	0
4	AX	5/18 (27%)	0	0
All	All	4539/4731 (95%)	2084 (45%)	0

5 of 2084 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

There are no RNA pucker outliers to report.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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	YYG	AW	37	10,3	29,42,43	1.05	2 (6%)	29,62,65	2.24	8 (27%)
3	PSU	AW	39	3	16,21,22	1.28	2 (12%)	20,30,33	6.06	4 (20%)
3	PSU	AW	55	3	16,21,22	1.44	2 (12%)	20,30,33	5.93	6 (30%)

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	YYG	AW	37	10,3	1/1/8/9	0/20/42/43	0/4/4/4
3	PSU	AW	39	3	-	0/7/25/26	0/2/2/2
3	PSU	AW	55	3	-	0/7/25/26	0/2/2/2

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	AW	39	PSU	C6-C5	-3.43	1.33	1.38
3	AW	55	PSU	C6-C5	-2.97	1.34	1.38
3	AW	37	YYG	C2-N2	2.05	1.38	1.35
3	AW	37	YYG	C6-N1	2.86	1.42	1.37
3	AW	39	PSU	C4-N3	3.06	1.38	1.33

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AW	39	PSU	N1-C2-N3	-19.57	114.33	128.40
3	AW	55	PSU	N1-C2-N3	-19.32	114.51	128.40
3	AW	39	PSU	C5-C4-N3	-12.77	114.95	125.43
3	AW	55	PSU	C5-C4-N3	-12.33	115.32	125.43
3	AW	37	YYG	C13-C12-C11	-4.10	123.52	130.66

All (1) chirality outliers are listed below:



Mol	Chain	Res	Type	Atom
3	AW	37	YYG	C15

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 42 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	AW	37	YYG	38	0
3	AW	39	PSU	4	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
26	BA	58
1	AA	45
3	AW	6
36	BQ	3
25	BB	2
2	AV	2
6	AC	2
45	BV	2
16	AM	2
44	BU	1
20	AQ	1
5	AB	1

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Mol	Chain	Number of breaks
8	AE	1
29	BF	1
27	BD	1
37	BS	1
55	BK	1
35	BP	1
7	AD	1
31	BH	1
15	AL	1

The worst 5 of 134 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	AA	1515/1522 (99%)	0.48	151 (9%) 8 15	188, 339, 400, 400	0
2	AV	76/76 (100%)	0.90	8 (10%) 7 14	242, 299, 394, 394	0
3	AW	73/76 (96%)	0.44	9 (12%) 5 13	253, 400, 400, 400	0
4	AX	17/18 (94%)	1.31	5 (29%) 1 6	400, 400, 400, 400	0
5	AB	234/256 (91%)	0.10	12 (5%) 29 32	395, 395, 400, 400	0
6	AC	206/239 (86%)	1.60	58 (28%) 1 6	393, 398, 398, 398	0
7	AD	208/209 (99%)	1.61	68 (32%) 0 6	257, 391, 400, 400	0
8	AE	150/162 (92%)	3.17	90 (60%) 0 3	371, 400, 400, 400	0
9	AF	101/101 (100%)	-0.42	1 (0%) 82 78	400, 400, 400, 400	0
10	AG	155/156 (99%)	1.88	55 (35%) 0 5	358, 400, 400, 400	0
11	AH	138/138 (100%)	1.39	43 (31%) 0 6	396, 396, 396, 396	0
12	AI	127/128 (99%)	0.70	27 (21%) 1 7	395, 395, 395, 395	0
13	AJ	98/105 (93%)	1.24	14 (14%) 3 10	400, 400, 400, 400	0
14	AK	119/129 (92%)	0.82	18 (15%) 3 10	202, 202, 400, 400	0
15	AL	124/135 (91%)	0.96	25 (20%) 1 8	399, 399, 400, 400	0
16	AM	125/126 (99%)	0.47	17 (13%) 3 11	348, 400, 400, 400	0
17	AN	60/61 (98%)	1.49	19 (31%) 0 6	400, 400, 400, 400	0
18	AO	88/89 (98%)	-0.12	2 (2%) 61 59	400, 400, 400, 400	0
19	AP	83/88 (94%)	1.76	32 (38%) 0 5	400, 400, 400, 400	0
20	AQ	104/105 (99%)	1.84	41 (39%) 0 5	400, 400, 400, 400	0
21	AR	73/88 (82%)	-0.38	0 100 100	400, 400, 400, 400	0
22	AS	80/93 (86%)	0.67	17 (21%) 1 7	400, 400, 400, 400	0
23	AT	99/106 (93%)	-0.07	7 (7%) 17 21	400, 400, 400, 400	0
24	AU	24/27 (88%)	1.91	10 (41%) 0 5	400, 400, 400, 400	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
25	BB	123/123 (100%)	-0.16	6 (4%)	30 33	267, 323, 388, 388	0
26	BA	2814/2916 (96%)	0.34	155 (5%)	26 29	65, 238, 393, 400	0
27	BD	173/173 (100%)	1.55	60 (34%)	0 5	392, 392, 400, 400	0
28	BE	191/338 (56%)	2.04	89 (46%)	0 4	400, 400, 400, 400	0
29	BF	189/246 (76%)	-0.33	9 (4%)	31 34	393, 396, 396, 396	0
30	BG	122/176 (69%)	0.06	7 (5%)	24 28	400, 400, 400, 400	0
31	BH	164/177 (92%)	0.26	14 (8%)	11 18	400, 400, 400, 400	0
32	BI	148/149 (99%)	1.42	48 (32%)	0 6	400, 400, 400, 400	0
33	BN	117/145 (80%)	1.71	46 (39%)	0 5	400, 400, 400, 400	0
34	BO	122/122 (100%)	1.10	25 (20%)	1 7	400, 400, 400, 400	0
35	BP	84/164 (51%)	1.02	15 (17%)	2 9	395, 395, 400, 400	0
36	BQ	138/138 (100%)	2.38	70 (50%)	0 4	393, 393, 393, 393	0
37	BS	113/186 (60%)	-0.12	2 (1%)	69 65	278, 400, 400, 400	0
38	BT	52/66 (78%)	3.00	31 (59%)	0 3	400, 400, 400, 400	0
39	BW	108/113 (95%)	0.18	6 (5%)	25 29	278, 395, 400, 400	0
40	BX	76/84 (90%)	0.81	18 (23%)	1 7	400, 400, 400, 400	0
41	BY	110/119 (92%)	0.70	15 (13%)	3 11	400, 400, 400, 400	0
42	BZ	177/253 (69%)	0.28	10 (5%)	25 29	396, 398, 398, 398	0
43	BR	105/118 (88%)	0.35	8 (7%)	15 20	400, 400, 400, 400	0
44	BU	117/118 (99%)	0.44	14 (11%)	5 13	391, 391, 400, 400	0
45	BV	100/100 (100%)	1.10	21 (21%)	1 7	400, 400, 400, 400	0
46	B2	64/70 (91%)	0.03	4 (6%)	21 24	400, 400, 400, 400	0
47	B3	60/60 (100%)	0.28	4 (6%)	19 23	398, 398, 398, 398	0
48	B0	86/91 (94%)	1.44	23 (26%)	1 6	396, 400, 400, 400	0
49	B4	73/73 (100%)	1.92	34 (46%)	0 4	396, 397, 397, 397	0
50	B5	58/60 (96%)	-0.14	0	100 100	400, 400, 400, 400	0
51	B6	53/82 (64%)	-0.08	2 (3%)	41 40	400, 400, 400, 400	0
52	B7	46/47 (97%)	0.80	3 (6%)	20 24	396, 396, 396, 396	0
53	B8	63/64 (98%)	1.01	13 (20%)	1 7	400, 400, 400, 400	0
54	B9	35/36 (97%)	3.63	21 (60%)	0 3	400, 400, 400, 400	0
55	BK	133/141 (94%)	0.06	4 (3%)	51 49	392, 400, 400, 400	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
All	All	10091/10981 (91%)	0.70	1506 (14%) <b>3</b> <b>10</b>	65, 395, 400, 400	0

The worst 5 of 1506 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	AJ	61	GLU	17.3
13	AJ	62	HIS	15.9
13	AJ	48	THR	14.6
8	AE	134	ALA	13.8
54	B9	24	LEU	13.3

## 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. 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	PSU	AW	39	20/21	0.58	0.44	-	399,399,399,399	0
3	YYG	AW	37	39/40	0.17	0.79	-	399,399,399,399	0
3	PSU	AW	55	20/21	0.94	0.09	-	400,400,400,400	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates 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.