



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 09:24 PM GMT

PDB ID : 4V4R
Title : Crystal structure of the whole ribosomal complex.
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 : 2005-09-30
Resolution : 5.90 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

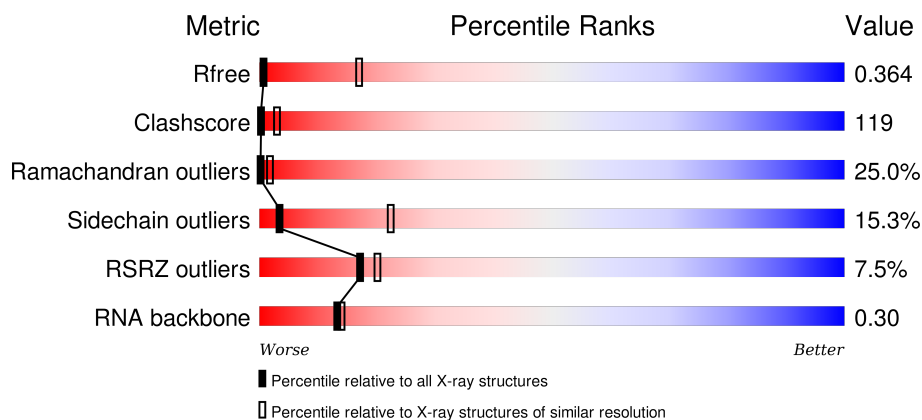
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 5.90 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}	91344	1000 (8.00-3.66)
Clashscore	102246	1048 (8.00-3.70)
Ramachandran outliers	100387	1021 (8.00-3.66)
Sidechain outliers	100360	1010 (8.00-3.64)
RSRZ outliers	91569	1015 (8.00-3.64)
RNA backbone	2183	1103 (8.70-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AA	1522	<div> <div>9%</div> <div>25% 42% 24% 9%</div> </div>
2	AV	76	<div> <div>7%</div> <div>17% 57% 22%</div> </div>
3	AW	76	<div> <div>18%</div> <div>30% 43% 18% 8%</div> </div>
4	AX	18	<div> <div>67%</div> <div>61% 33% 6%</div> </div>

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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	AY	354	
26	BB	123	
27	BA	2916	
28	BD	173	
29	BE	338	

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Mol	Chain	Length	Quality of chain
30	BF	246	
31	BG	176	
32	BH	177	
33	BI	149	
34	BN	145	
35	BO	122	
36	BP	164	
37	BQ	138	
38	BS	186	
39	BT	66	
40	BW	113	
41	BX	84	
42	BY	119	
43	BZ	253	
44	BR	118	
45	BU	118	
46	BV	100	
47	B2	70	
48	B3	60	
49	B0	91	
50	B4	73	
51	B5	60	
52	B6	82	
53	B7	47	
54	B8	64	

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Mol	Chain	Length	Quality of chain
55	B9	36	
56	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 56 unique types of molecules in this entry. The entry contains 142780 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			

- 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'-R(*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		0	0	0
			1011	639	198	174				

- 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	0	0	0
			794	499	156	138	1			

- 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	0	0	0
			885	549	168	165	3			

- 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	0	0	0
			970	611	195	163	1			

- 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	0	0	0
			997	617	207	171	2			

- 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	0	0	0
			492	312	104	72	4			

- 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	0	0	0
			734	459	147	126	2			

- 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 protein called Peptide chain release factor 1.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
25	AY	333	Total	C	0	0	333
			333	333			

- Molecule 26 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	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 27 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	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 28 is a protein called 50S ribosomal protein L2.

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

- Molecule 29 is a protein called 50S ribosomal protein L3.

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

- Molecule 30 is a protein called 50S ribosomal protein L4.

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

- Molecule 31 is a protein called 50S ribosomal protein L5.

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

- Molecule 32 is a protein called 50S ribosomal protein L6.

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

- Molecule 33 is a protein called 50S ribosomal protein L9.

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

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

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

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

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

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

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

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

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

- Molecule 38 is a protein called 50S ribosomal protein L18.

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

- Molecule 39 is a protein called 50S ribosomal protein L19.

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

- Molecule 40 is a protein called 50S ribosomal protein L22.

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

- Molecule 41 is a protein called 50S ribosomal protein L23.

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

- Molecule 42 is a protein called 50S ribosomal protein 24.

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

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

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

- Molecule 44 is a protein called 50S ribosomal protein L17.

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

- Molecule 45 is a protein called 50S ribosomal protein L20.

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

- Molecule 46 is a protein called 50S ribosomal protein L21.

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

- Molecule 47 is a protein called 50S ribosomal protein L29.

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

- Molecule 48 is a protein called 50S ribosomal protein L30.

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

- Molecule 49 is a protein called 50S ribosomal protein L27.

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

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

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

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

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

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

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

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

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

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

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

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

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

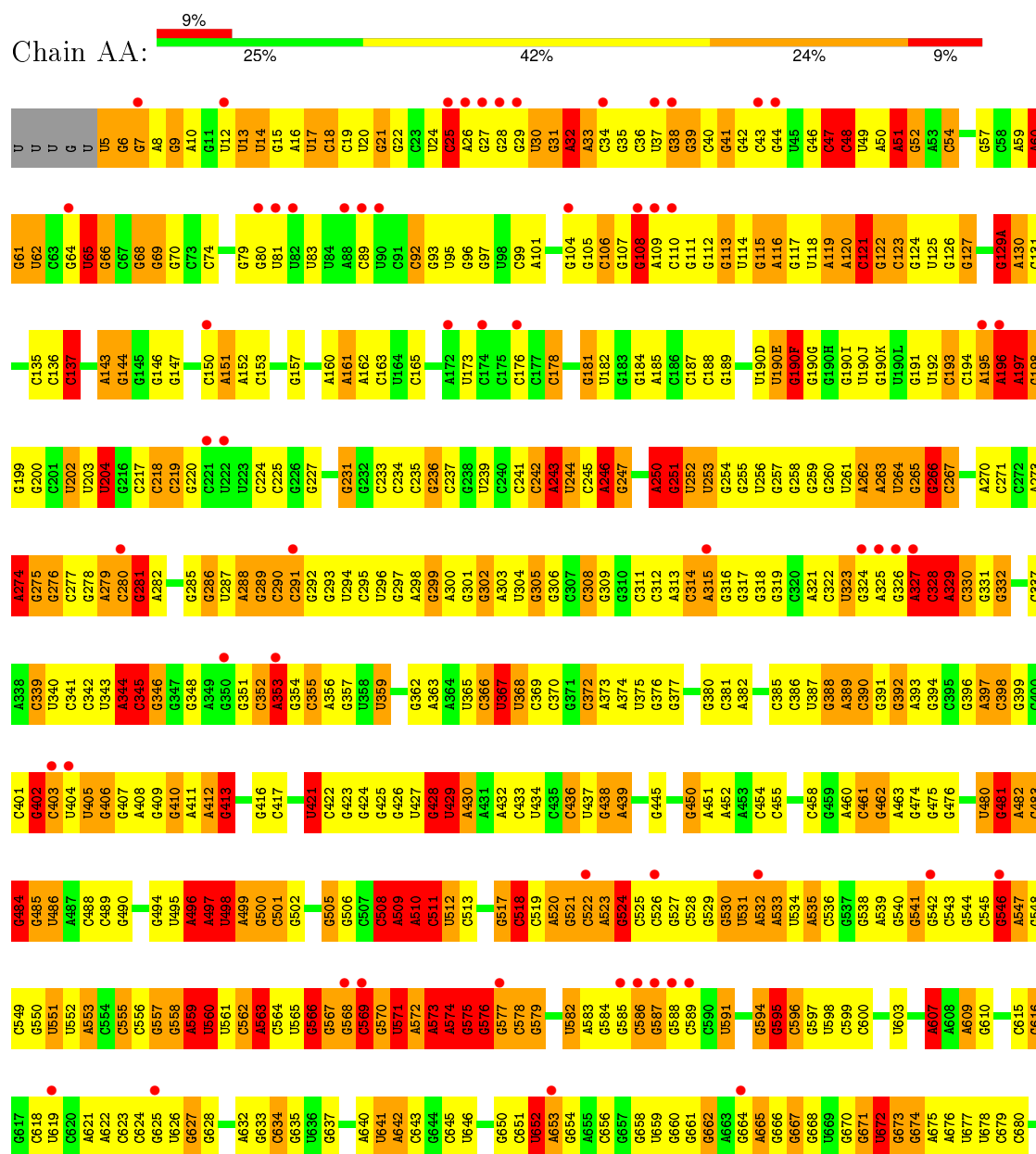
- Molecule 56 is a protein called 50S ribosomal protein L11.

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

3 Residue-property plots

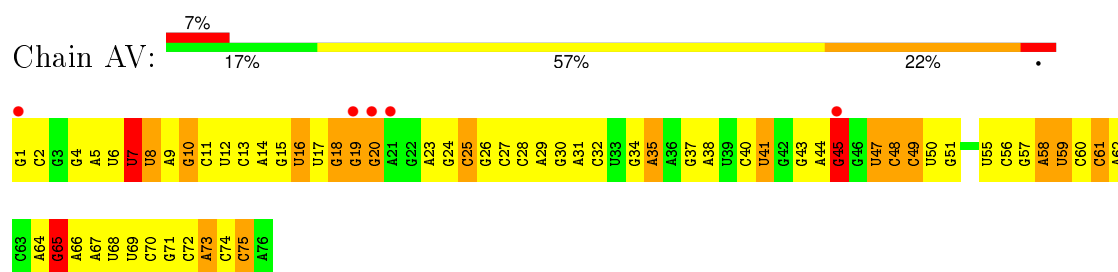
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($\text{RSRZ} > 2$). 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

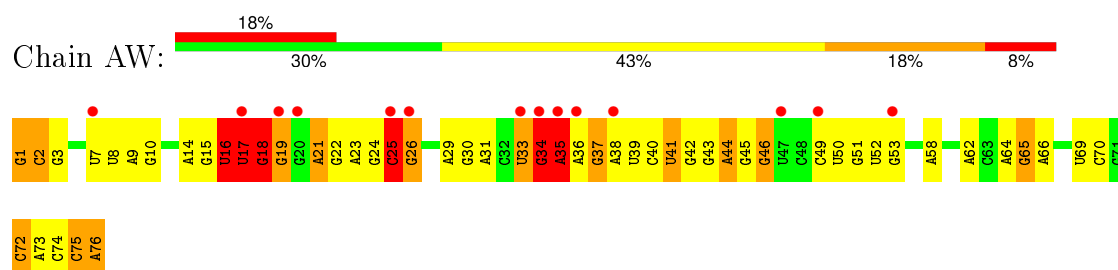


U1542	G1481	A1339	G1277	G1142	G1079	A1015	G947	G886	A814	U751	G685
C	G1401	A1340	U1278	G1143	A1080	A1016	C948	G887	A815	G752	U686
U	G1482	C1341	A1279	G1144	G1081	G1017	A949	G888	A816	A887	A687
	C1403	C1342	A1280	G1145	G1082	G1018	U950	A889	C817	G754	G688
	G1404	G1343	U1281	A1146	G1083	G1019	G951	G890	G818	G755	C689
	G1405	C1344	U1282	C1147	G1084	G1020	U952	G891	A819	G756	G690
	U1406	U1345	G1283	U1148	G1085	G1021	G953	A892	U820	U757	G691
	A1407	A1346	A1285	C1149	U1086	G1022	U956	C893	G821	G758	U692
	A1408	A1347	A1286	C1150	U1087	G1023	U957	C894	G822	G759	G693
	C1409	A1348	A1287	A1151	G1088	U1024	A958	G898	C826	G760	A694
	G1410	A1349	A1288	A1152	G1089	U1025	A959	G899	U827	G761	A695
	A1411	A1350	A1289	G1153	U1090	G1026	U960	C899	A828	G762	A696
	C1412	U1351	G1290	G1154	U1091	G1027	U961	A900	G829	G763	U697
	A1413	C1352	G1291	G1155	A1092	C1028	G962	A901	G830	G764	
	G1414	G1353	U1292	G1156	A1093	C1029	G963	A902	G831	G765	C701
	G1415	C1354	G1293	A1157	G1094	C1030	U964	G903	U832	A766	A702
	G1416	G1355	G1294	C1158	U1095	G30A	A965	G904	G833	A767	G703
	G1417	G1356	C1295	U1159	C1096	G30B	G966	U905	U834	A768	A704
	A1418	A1357	A1296	G1160	C1097	G30C	G967	G906	U835	G769	U705
	G1419	U1358	C1297	C1161	C1098	A30D	C968	A907	U836	G770	A706
	G1420	C1359	G1298	G1162	C1099	G1031	A968	A908	G837	G771	C707
	G1421	A1360	C1299	G1163	C1100	G1032	C970	A909	U839	G774	C708
	G1422	G1361	U1300	G1164	C1101	G1033	G971	A910	C840	G775	G709
	G1423	C361A	U1301	A1167	A1102	A1034	G972	C910	U841	G776	G713
	U1424	A1362	C1302	A1168	C1103	A1035	G973	C911	C846	A777	G714
	A1425	A1363	G1303	A1169	G1104	G1036	A974	A912	C849	G778	A715
	C1426	U1364	G1304	A1170	A1105	C1037	A975	A913	U850	C779	A716
	A1427	C1365	C1305	G1171	G1106	C1038	A976	A914	G851	A780	A717
	G1428	G1366	U1306	C1172	C1107	G1042	A977	A915	G852	A781	G718
	C1429	C1367	U1307	G1173	G1108	G1043	A978	A916	G853	A782	G719
	A1430	G1368	C1308	G1177	C1109	C1044	C979	A918	G854	G720	C720
	G1431	A1369	G1309	G1178	C1110	A1045	C980	A919	G855	G721	G721
	G1432	G1370	U1310	G1179	C1111	A1046	U981	A920	G856	A722	A722
	U1433	C1371	U1311	A1180	C1112	G1047	U982	A921	G857	U723	U723
	A1434	U1312	U1312	G1181	G1113	U1048	A983	A922	A859	U724	G724
	G1435	C1313	C1242	G1182	C1114	G1050	C984	A923	A860	U725	G725
	G1436	U1314	C1243	A1183	C1115	G1051	C985	A924	G861	C726	C726
	G1437	C1315	A1248	G1184	C1116	G1052	A986	A925	U863	G727	G727
	A1438	U1316	C1249	G1185	U1121	C1053	A987	A926	A864	A728	A728
	C1439	C1317	A1250	G1186	C1117	A1054	G988	A927	A865	U729	A729
	G1440	U1318	U1251	G1187	C1118	U1055	C989	A928	C866	G730	G730
	G1441	C1319	A1252	G1188	C1119	G1056	U990	A929	G867	G731	G731
	A1442	U1320	G1253	G1189	U1122	G1057	U991	C930	G869	C732	C732
	G1443	C1321	C1254	G1190	C1123	G1058	U992	C931	U870	A733	A733
	A1444	G1322	G1255	A1191	U1124	C1059	A993	C932	U871	G734	G734
	C1445	C1323	A1256	G1192	C1124	G1060	A994	A933	A872	G735	C735
	G1446	U1324	U1257	G1193	C1125	U1061	C995	A934	A873	G736	G736
	A1447	C1325	G1258	G1194	C1126	U1062	A996	A935	G874	A737	A737
	C1448	C1326	C1259	U1195	A1130	C1063	G997	A936	C875	G738	C738
	G1449	U1327	C1260	G1196	C1131	G1064	G1002	A937	G876	C739	C739
	U1450	C1328	C1261	U1197	C1132	U1065	G1003	A938	C877	U740	U740
	A1451	U1329	C1262	G1198	G1133	C1066	G1004	A939	G878	G741	G741
	C1452	C1330	A1263	G1199	U1134	A1067	A1005	A940	C879	C806	C806
	G1453	U1331	U1268	U1199	U1135	U1068	A1006	A941	G880	A807	A807
	A1454	A1332	A1269	U1200	U1136	C1069	C1007	A942	C881	G742	G742
	G1455	C1333	C1270	A1201	C1137	G1074	G1013	A944	C882	C745	C745
	C1456	U1334	G1271	G1202	G1138	C1075	G1014	G945	C883	C748	C748
	A1457	C1335	G1272	C1203	C1139	G1076	G1015	G946	C884	C749	C749
	U1458	U1336	G1273	U1204	C1140	C1077	G1016	G947	C885	U813	U813
	G1459	C1337	G1274	U1205	C1141	U1078					

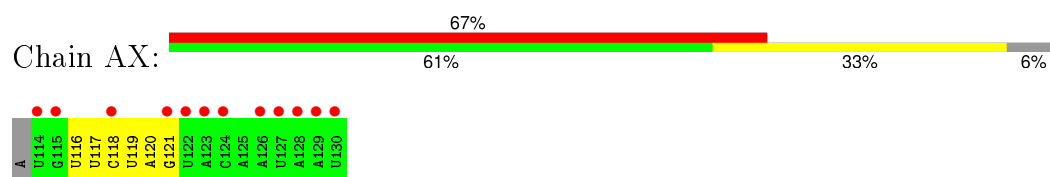
• Molecule 2: P-site tRNA (Phe)



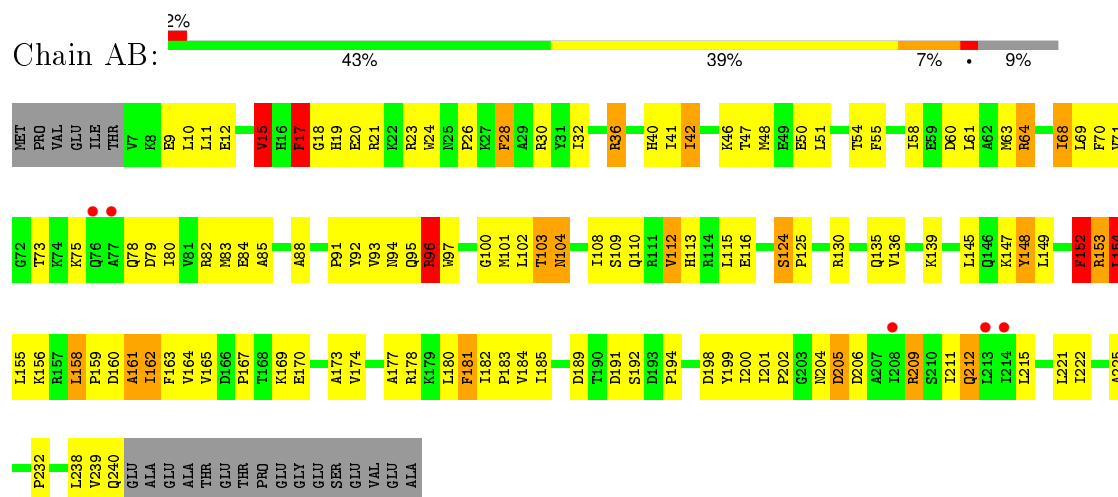
- Molecule 3: E-site tRNA (Phe)



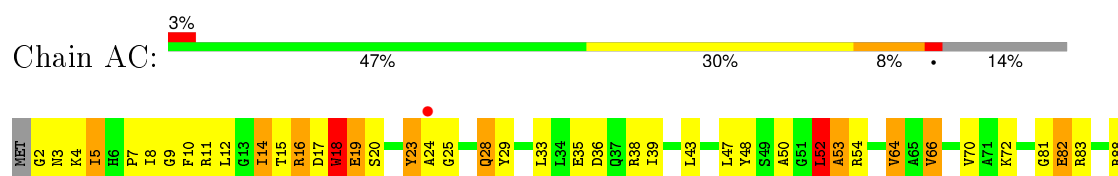
- Molecule 4: 5'-R(*AP*UP*GP*UP*UP*CP*UP*AP*GP*UP*AP*CP*AP*AP*UP*AP*AP*U)-3'

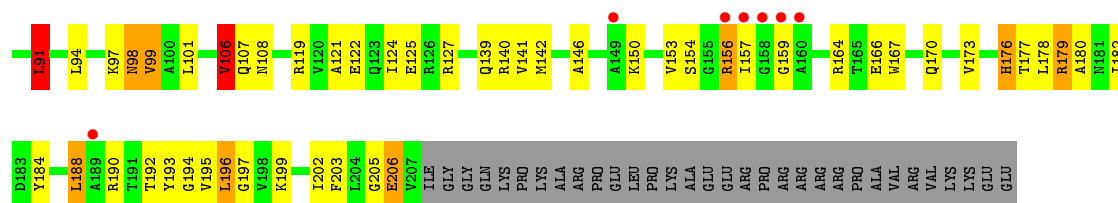


- Molecule 5: 30S ribosomal protein S2

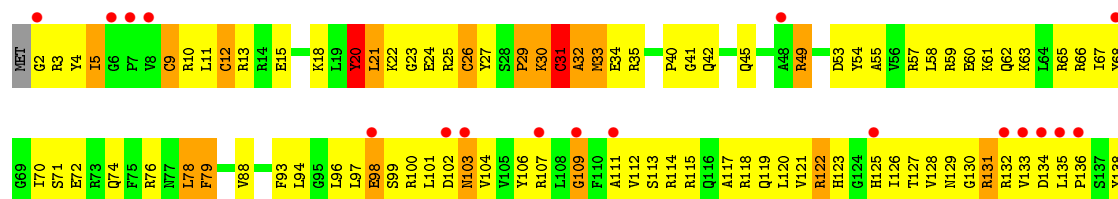


- Molecule 6: 30S ribosomal protein S3

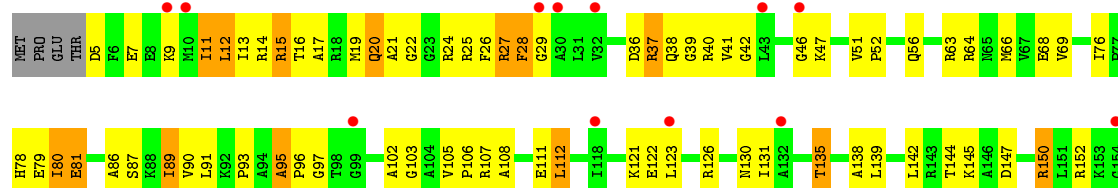




• Molecule 7: 30S ribosomal protein S4



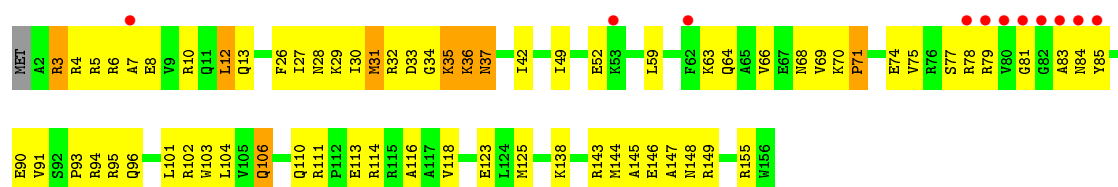
• Molecule 8: 30S ribosomal protein S5



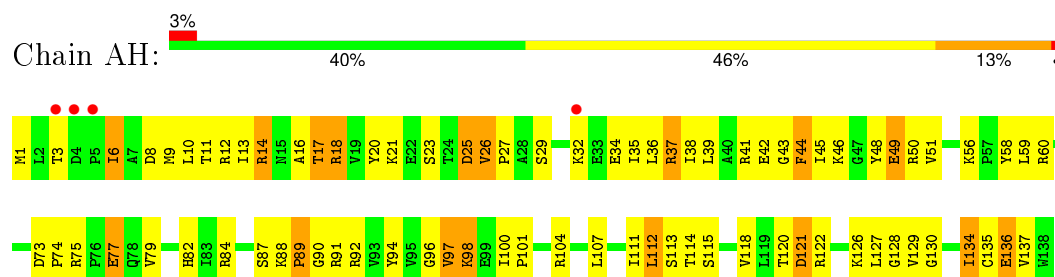
• Molecule 9: 30S ribosomal protein S6



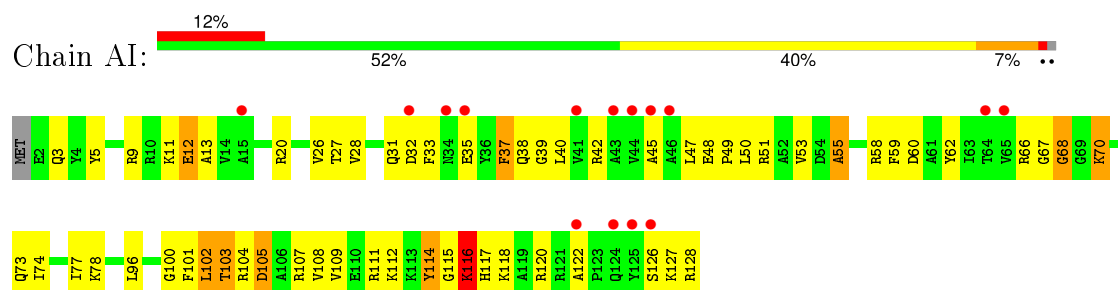
• Molecule 10: 30S ribosomal protein S7



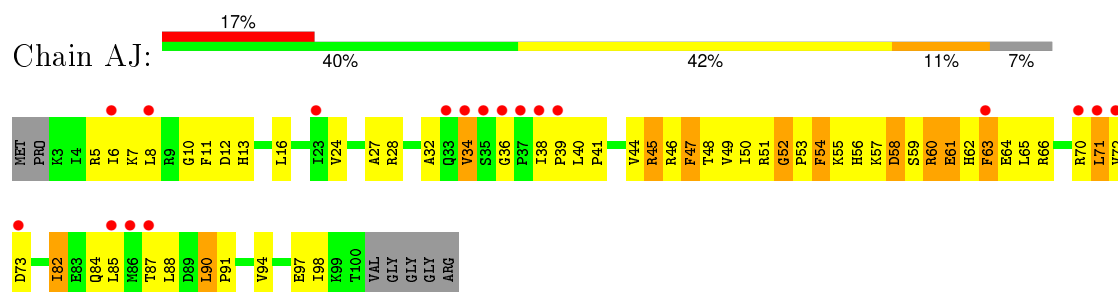
- Molecule 11: 30S ribosomal protein S8



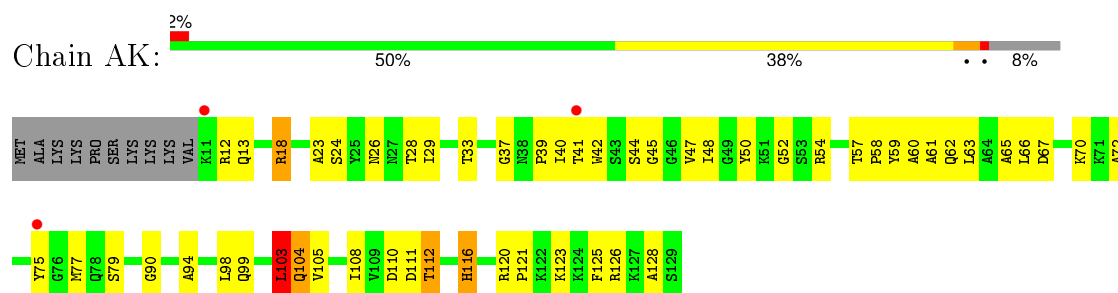
- Molecule 12: 30S ribosomal protein S9



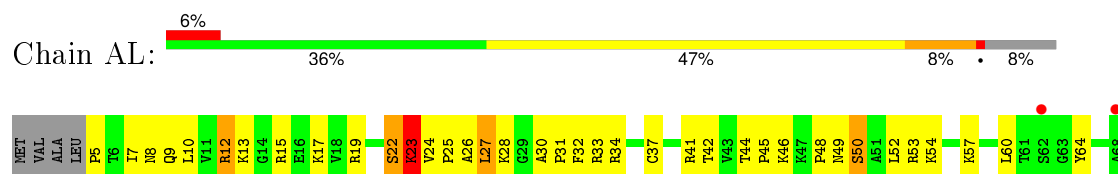
- Molecule 13: 30S ribosomal protein S10

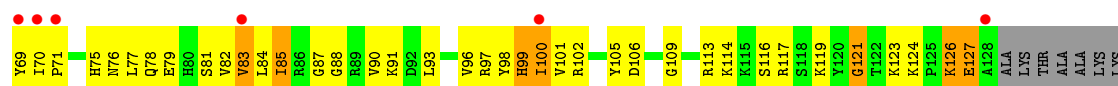


- Molecule 14: 30S ribosomal protein S11

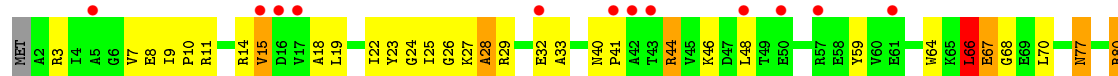


- Molecule 15: 30S ribosomal protein S12





• Molecule 16: 30S ribosomal protein S13



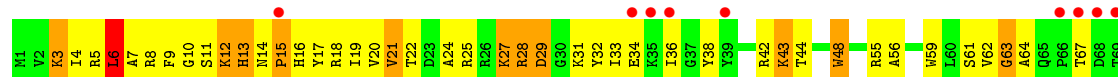
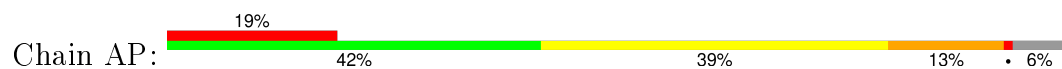
• Molecule 17: 30S ribosomal protein S14



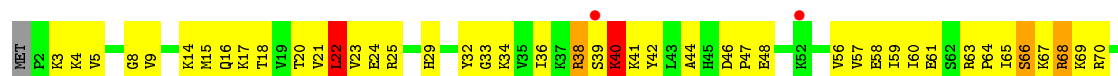
• Molecule 18: 30S ribosomal protein S15



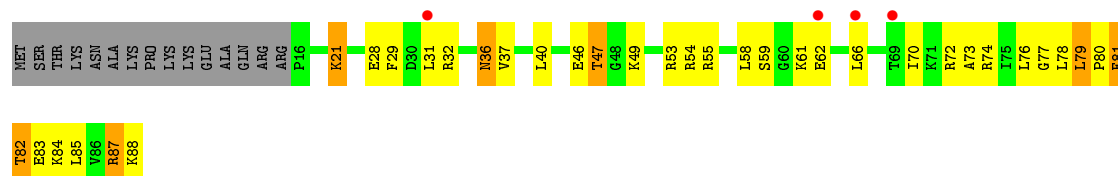
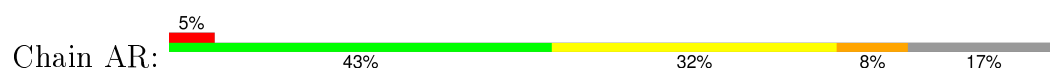
• Molecule 19: 30S ribosomal protein S16



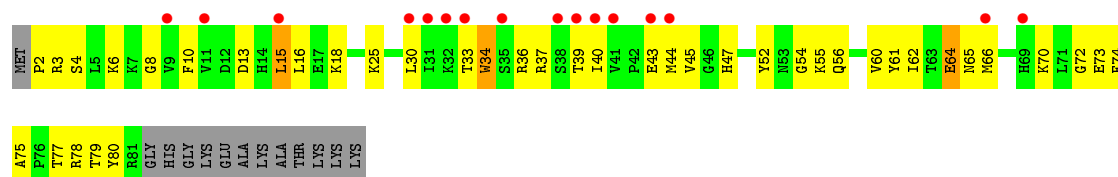
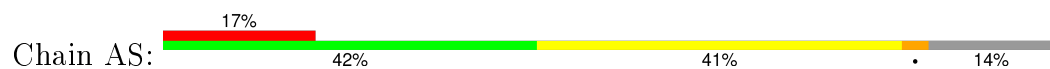
• Molecule 20: 30S ribosomal protein S17



• Molecule 21: 30S ribosomal protein S18



- Molecule 22: 30S ribosomal protein S19



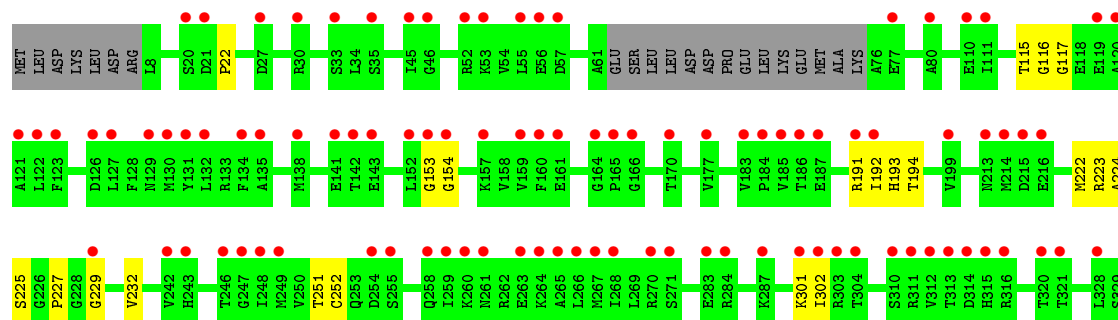
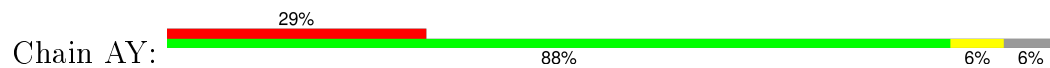
- Molecule 23: 30S ribosomal protein S20

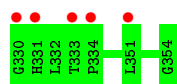


- Molecule 24: 30S ribosomal protein Thx



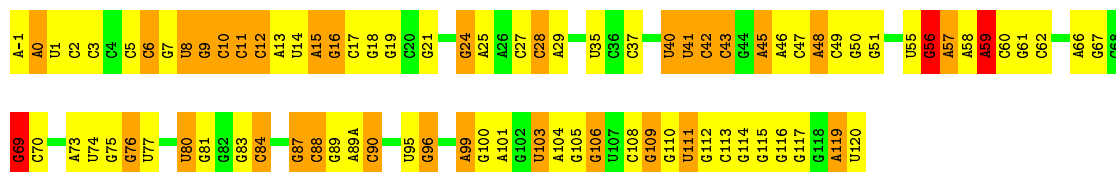
- Molecule 25: Peptide chain release factor 1





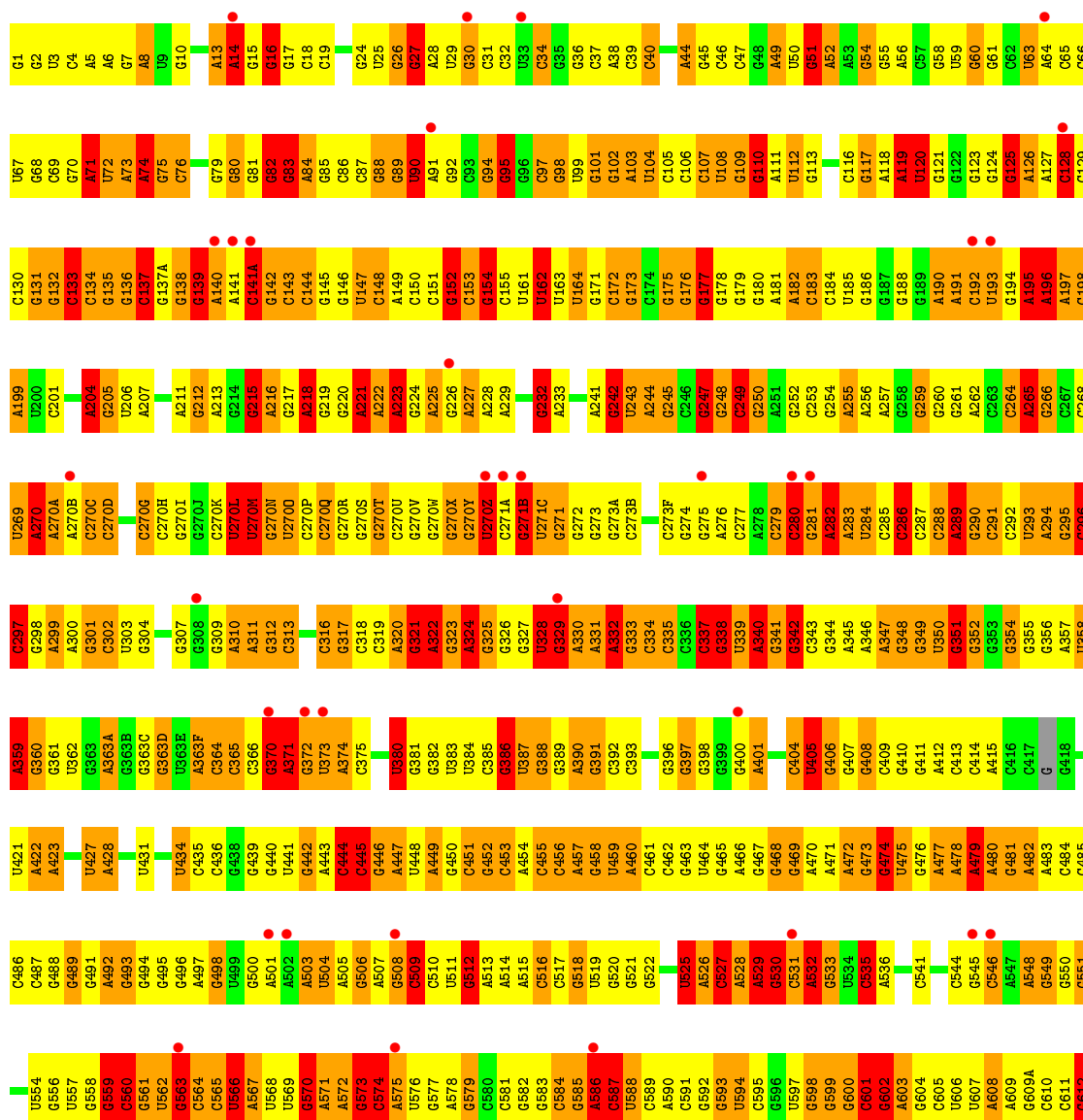
• Molecule 26: 5S ribosomal RNA

Chain BB: 30% 42% 25% .



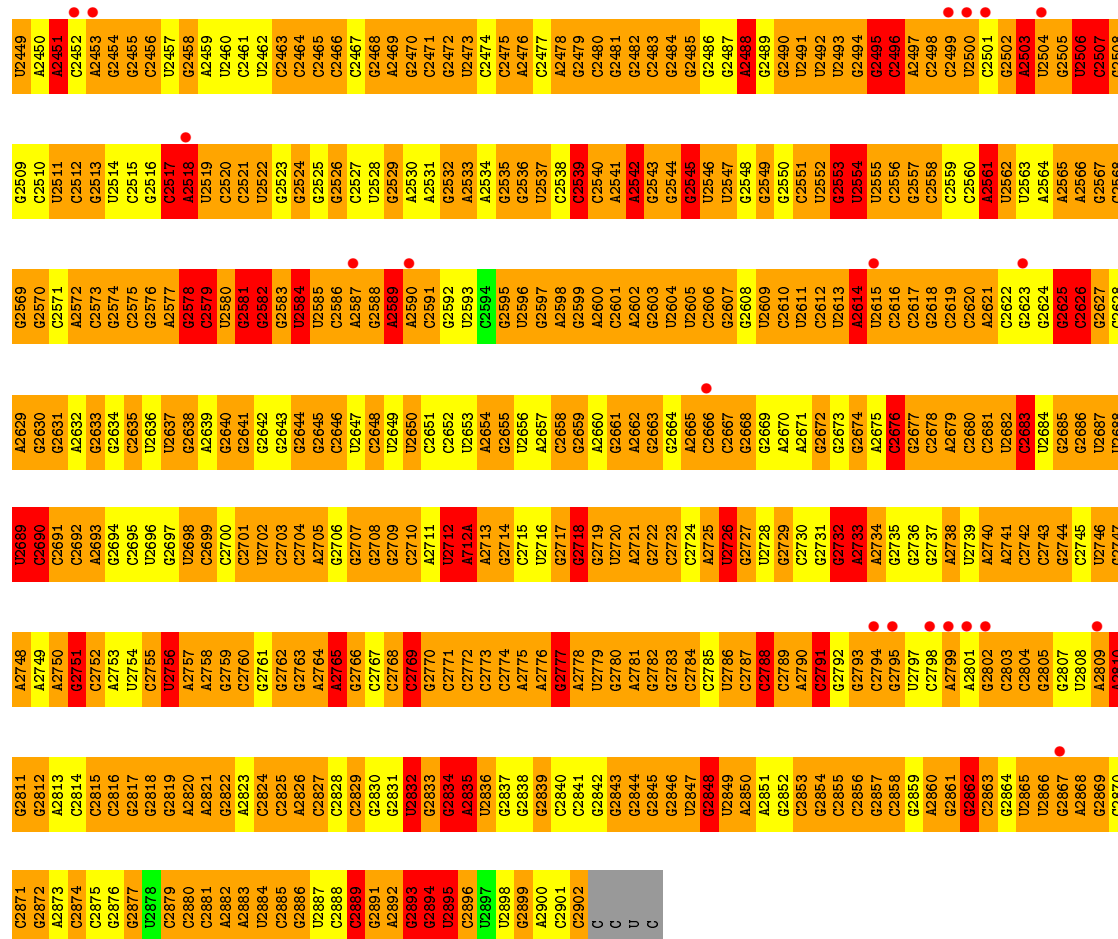
• Molecule 27: 23S ribosomal RNA

Chain BA: 6% 11% 34% 38% 13% .



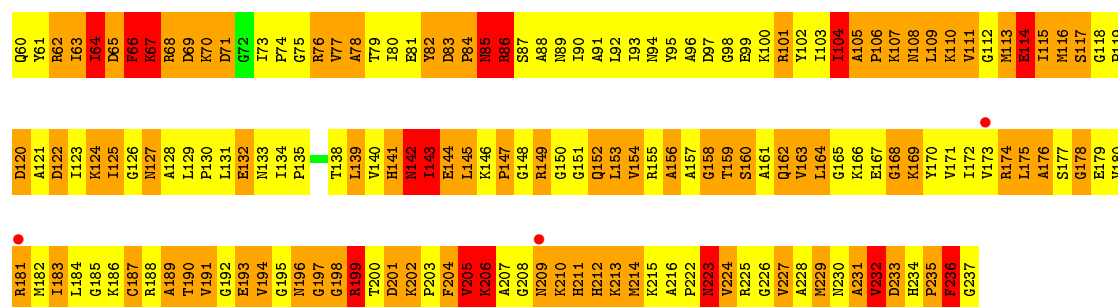






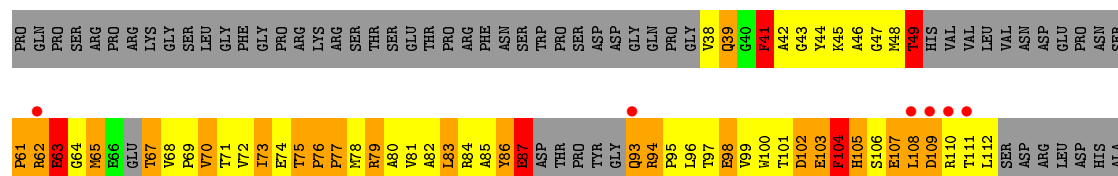
• Molecule 28: 50S ribosomal protein L2

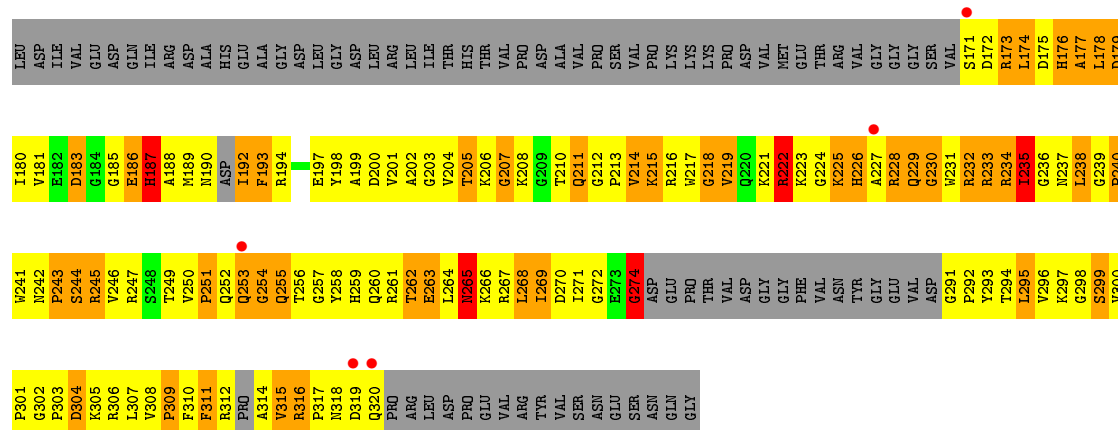
Chain BD: 2% 44% 46% 9%



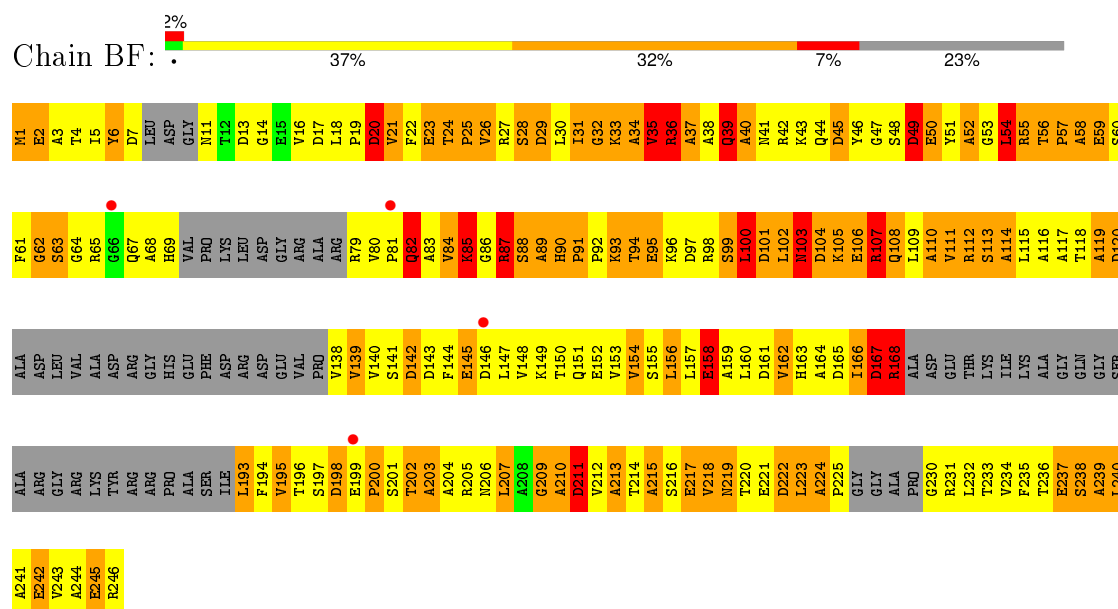
• Molecule 29: 50S ribosomal protein L3

Chain BE: 3% 31% 20% 43%

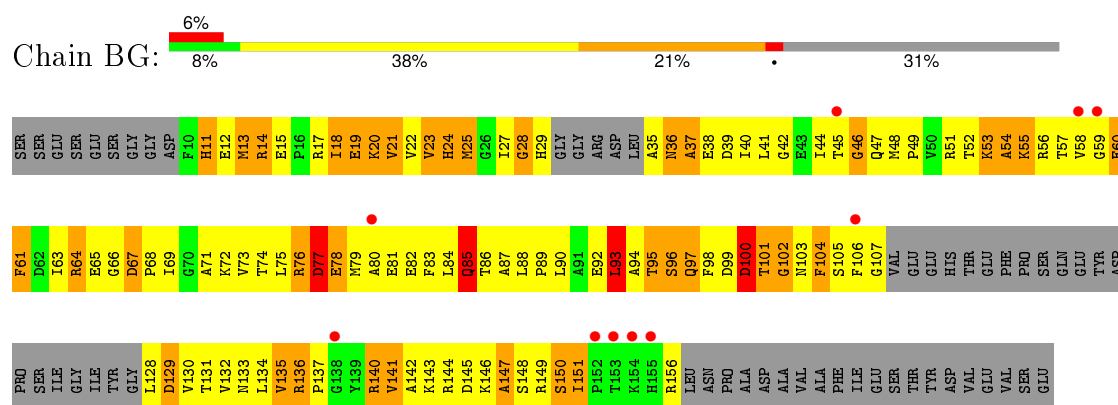




• Molecule 30: 50S ribosomal protein L4

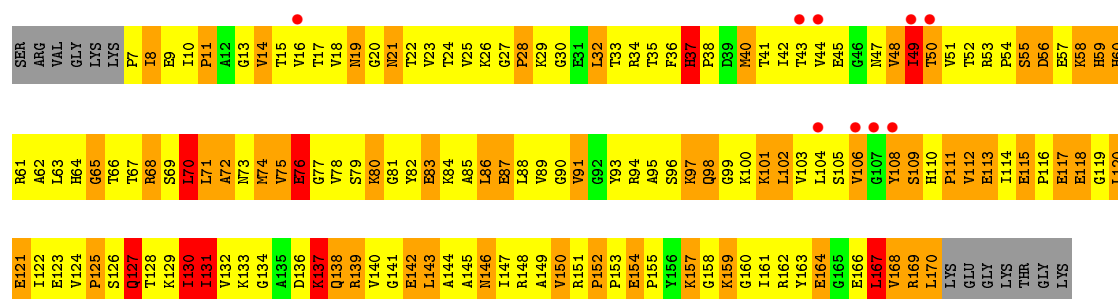


• Molecule 31: 50S ribosomal protein L5

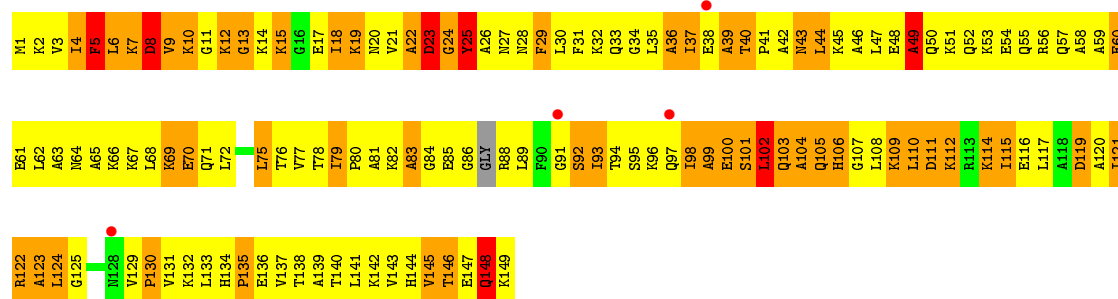


• Molecule 32: 50S ribosomal protein L6

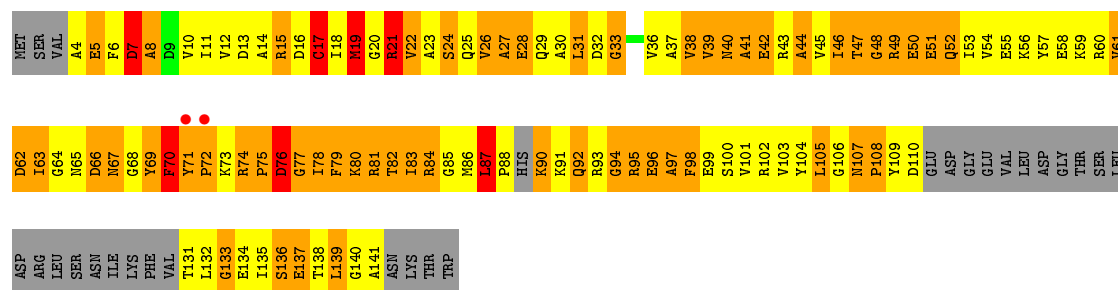




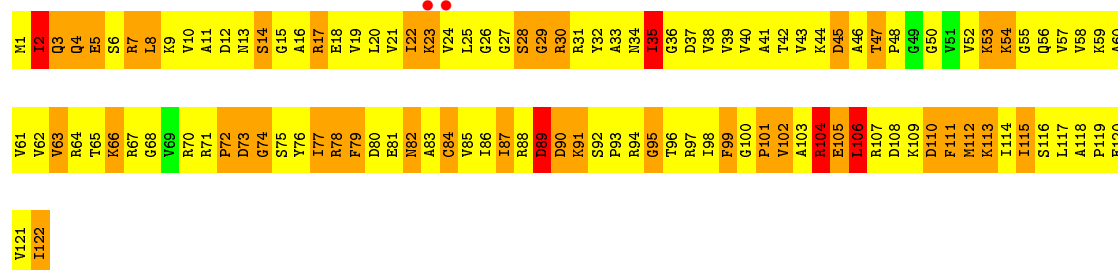
• Molecule 33: 50S ribosomal protein L9



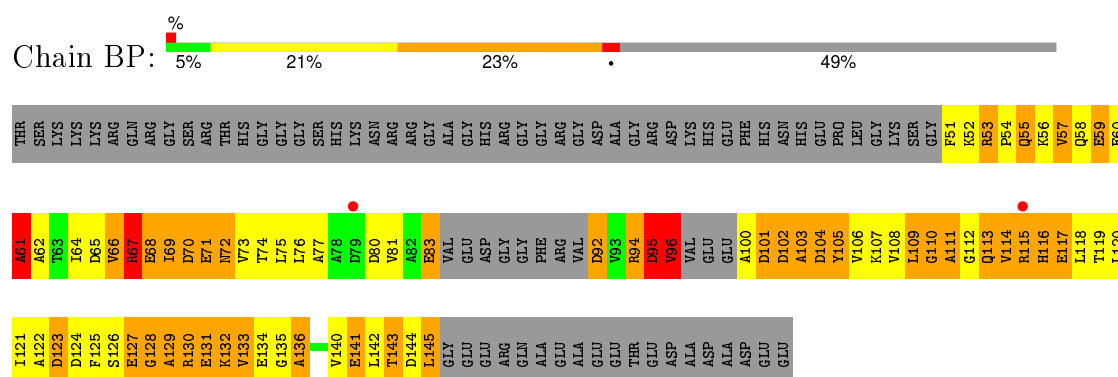
• Molecule 34: 50S ribosomal protein L13



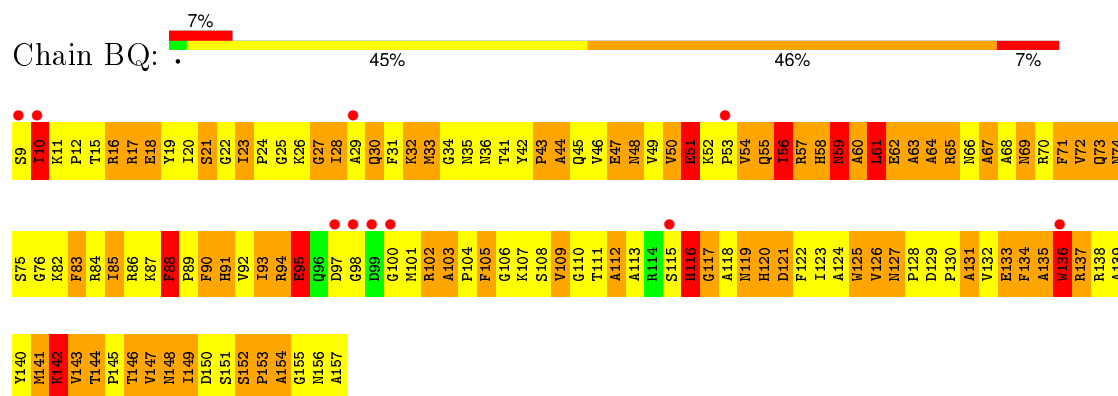
• Molecule 35: 50S ribosomal protein L14



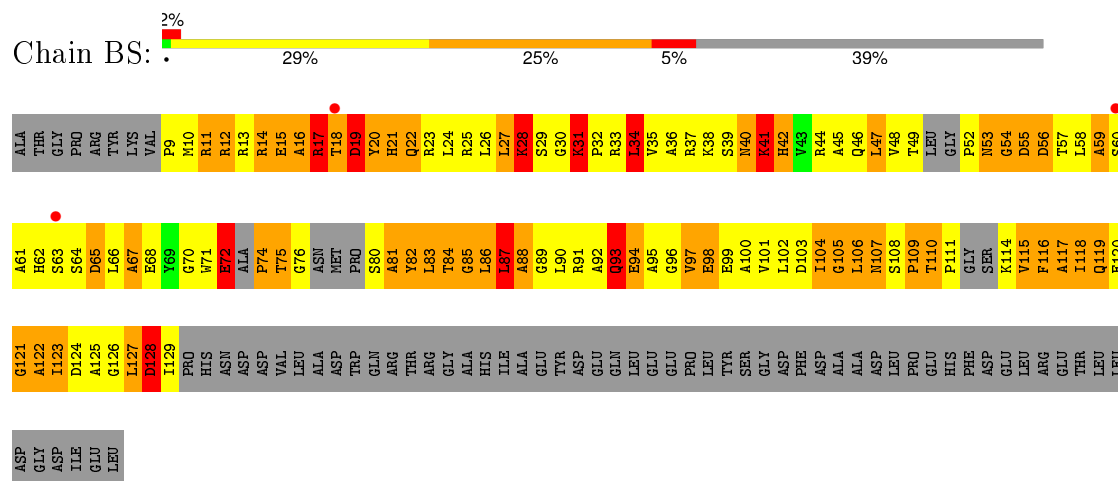
• Molecule 36: 50S ribosomal protein L15



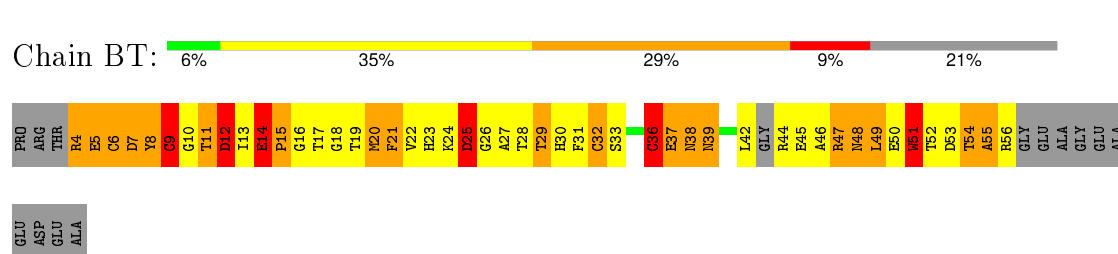
- Molecule 37: 50S ribosomal protein L16



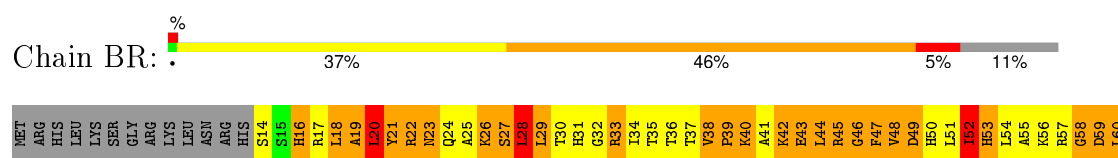
- Molecule 38: 50S ribosomal protein L18



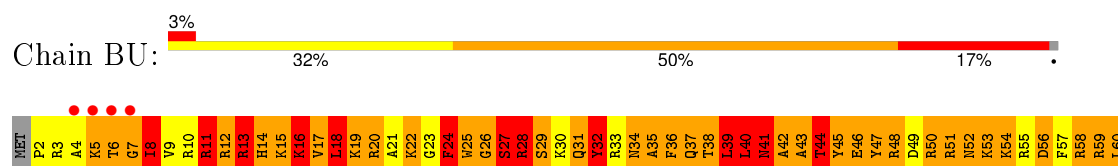
- Molecule 39: 50S ribosomal protein L19



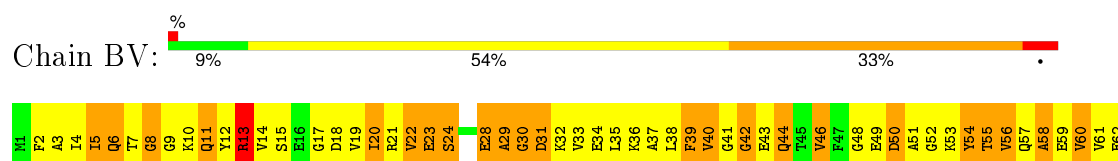
- Molecule 44: 50S ribosomal protein L17



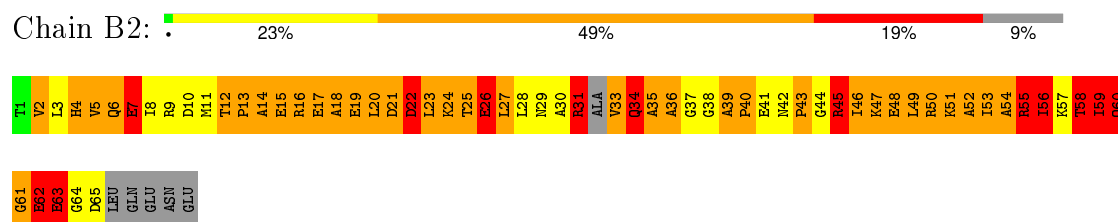
- Molecule 45: 50S ribosomal protein L20



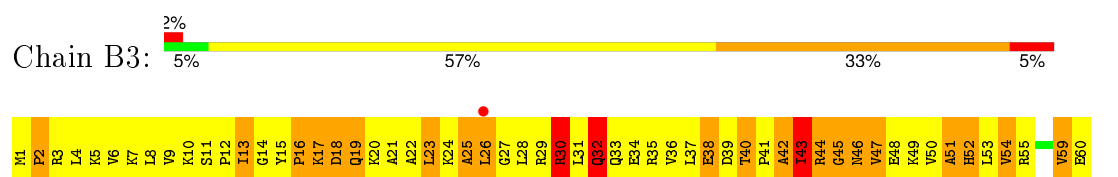
- Molecule 46: 50S ribosomal protein L21



- Molecule 47: 50S ribosomal protein L29

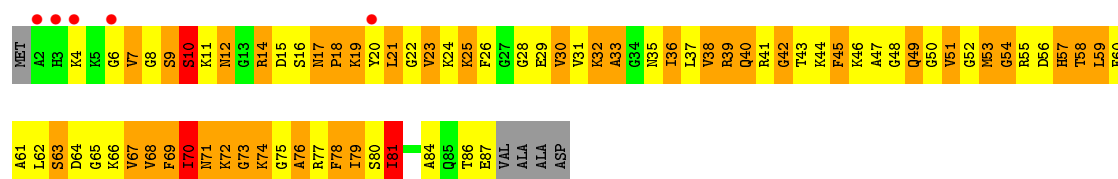


- Molecule 48: 50S ribosomal protein L30



- Molecule 49: 50S ribosomal protein L27





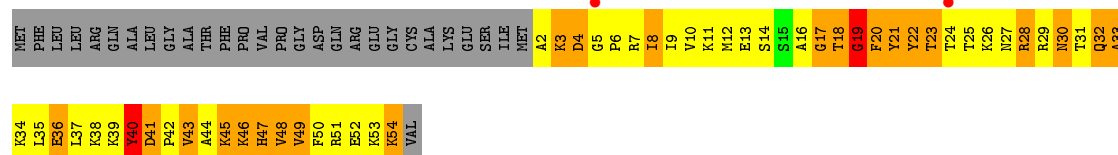
- Molecule 50: 50S ribosomal protein L31



- Molecule 51: 50S ribosomal protein L32



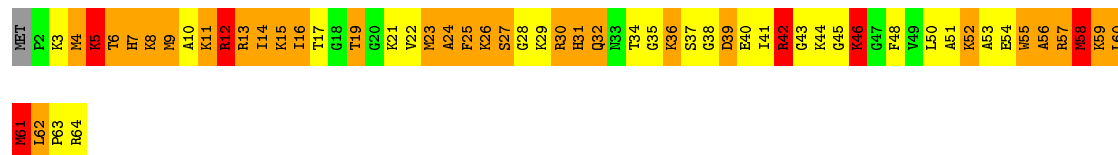
- Molecule 52: 50S ribosomal protein L33



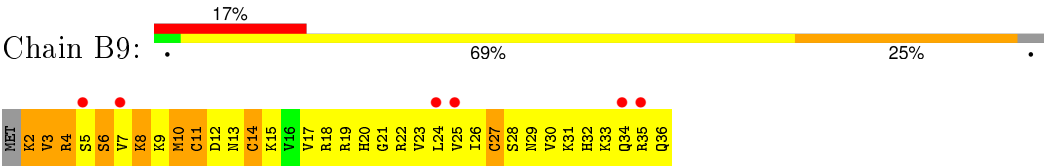
- Molecule 53: 50S ribosomal protein L34



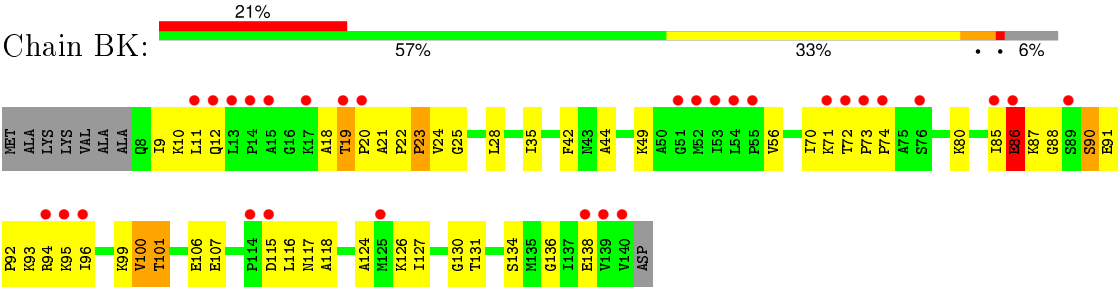
- Molecule 54: 50S ribosomal protein L35



- Molecule 55: 50S ribosomal protein L36



• Molecule 56: 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	518.99Å 518.99Å 365.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 5.90 49.92 – 5.54	Depositor EDS
% Data completeness (in resolution range)	97.4 (40.00-5.90) 94.5 (49.92-5.54)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.41 (at 5.39Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.351 , 0.371 0.344 , 0.364	Depositor DCC
R_{free} test set	6319 reflections (5.25%)	DCC
Wilson B-factor (Å ²)	223.1	Xtriage
Anisotropy	0.185	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.11 , 78.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 148368 reflections	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	142780	wwPDB-VP
Average B, all atoms (Å ²)	236.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.88% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	1.25	68/36411 (0.2%)	1.47	415/56769 (0.7%)
2	AV	2.34	3/1813 (0.2%)	1.16	11/2823 (0.4%)
3	AW	1.82	17/1739 (1.0%)	1.97	36/2698 (1.3%)
4	AX	0.18	0/139	0.66	0/213
5	AB	0.63	1/1935 (0.1%)	0.66	4/2609 (0.2%)
6	AC	0.60	2/1636 (0.1%)	1.10	6/2205 (0.3%)
7	AD	0.65	4/1733 (0.2%)	0.97	9/2318 (0.4%)
8	AE	0.46	0/1161	0.61	1/1561 (0.1%)
9	AF	0.35	0/856	0.54	0/1154
10	AG	0.60	1/1276 (0.1%)	0.59	2/1709 (0.1%)
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	0.87	1/900 (0.1%)	0.56	0/1213
15	AL	0.49	1/986 (0.1%)	0.70	1/1320 (0.1%)
16	AM	1.15	2/1008 (0.2%)	1.16	3/1347 (0.2%)
17	AN	0.49	1/501 (0.2%)	0.64	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	1.15	2/870 (0.2%)	1.38	5/1159 (0.4%)
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	0.48	0/277
26	BB	1.11	5/2950 (0.2%)	1.43	23/4602 (0.5%)
27	BA	1.21	152/67844 (0.2%)	1.45	897/105838 (0.8%)
28	BD	0.37	0/1328	0.61	0/1783
29	BE	0.64	3/1540 (0.2%)	1.07	7/2078 (0.3%)
30	BF	0.69	3/1444 (0.2%)	0.82	1/1954 (0.1%)
31	BG	0.25	0/971	0.46	0/1304
32	BH	0.58	1/1272 (0.1%)	0.48	0/1721
33	BI	0.39	1/1156 (0.1%)	0.64	3/1544 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
34	BN	0.35	0/927	0.55	0/1245
35	BO	0.32	0/946	0.57	0/1269
36	BP	1.55	3/643 (0.5%)	1.32	5/870 (0.6%)
37	BQ	0.32	0/1106	0.53	0/1490
38	BS	0.79	2/877 (0.2%)	0.87	5/1179 (0.4%)
39	BT	0.39	0/412	0.70	0/554
40	BW	0.37	0/869	0.59	0/1166
41	BX	0.49	1/608 (0.2%)	1.04	3/820 (0.4%)
42	BY	0.25	0/887	0.83	3/1195 (0.3%)
43	BZ	0.32	1/1385 (0.1%)	0.55	3/1883 (0.2%)
44	BR	0.31	0/867	0.49	0/1162
45	BU	0.70	1/994 (0.1%)	0.65	3/1323 (0.2%)
46	BV	0.75	1/796 (0.1%)	0.89	3/1058 (0.3%)
47	B2	0.37	0/497	1.00	2/668 (0.3%)
48	B3	0.31	0/482	0.50	0/646
49	B0	0.29	0/649	1.15	3/860 (0.3%)
50	B4	0.77	2/620 (0.3%)	0.57	0/831
51	B5	0.36	0/469	0.79	3/629 (0.5%)
52	B6	0.32	0/438	0.55	1/583 (0.2%)
53	B7	0.38	0/387	0.64	0/509
54	B8	0.73	2/503 (0.4%)	1.23	5/657 (0.8%)
55	B9	0.33	0/286	0.59	0/375
56	BK	0.30	0/1010	0.60	3/1349 (0.2%)
All	All	1.11	281/154800 (0.2%)	1.32	1469/231824 (0.6%)

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	2
7	AD	0	1
15	AL	0	1
16	AM	0	1
20	AQ	0	2
28	BD	0	1
29	BE	0	3
30	BF	0	3
32	BH	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
33	BI	0	1
36	BP	0	1
38	BS	0	1
41	BX	0	1
42	BY	0	1
47	B2	0	1
54	B8	0	1
56	BK	0	1
All	All	1	29

The worst 5 of 281 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	BA	2199	A	O3'-P	-71.12	0.75	1.61
2	AV	45	G	O3'-P	-70.03	0.77	1.61
2	AV	65	G	O3'-P	-62.91	0.85	1.61
27	BA	2196	C	O3'-P	-59.20	0.90	1.61
1	AA	1211	U	O3'-P	-53.33	0.97	1.61

The worst 5 of 1469 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	BA	712(A)	A	P-O3'-C3'	-48.47	61.54	119.70
1	AA	196	A	P-O3'-C3'	44.40	172.99	119.70
3	AW	25	C	O3'-P-O5'	-43.47	21.42	104.00
27	BA	2199	A	O3'-P-O5'	-43.09	22.13	104.00
26	BB	24	G	P-O3'-C3'	29.89	155.56	119.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	AW	37	YYG	C15

5 of 29 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	16464	1922	4
2	AV	1622	0	823	187	0
3	AW	1638	0	835	231	0
4	AX	136	0	63	35	0
5	AB	1900	0	1950	97	0
6	AC	1612	0	1675	104	0
7	AD	1703	0	1762	190	0
8	AE	1146	0	1206	57	0
9	AF	843	0	857	27	0
10	AG	1257	0	1294	138	0
11	AH	1116	0	1177	79	0
12	AI	1011	0	1041	80	0
13	AJ	794	0	840	118	0
14	AK	885	0	904	50	0
15	AL	970	0	1056	79	0
16	AM	997	0	1071	129	0
17	AN	492	0	529	111	0
18	AO	734	0	771	31	0
19	AP	700	0	720	68	0
20	AQ	857	0	929	96	0
21	AR	597	0	668	31	0
22	AS	647	0	672	146	0
23	AT	762	0	859	43	0
24	AU	208	0	221	22	0
25	AY	333	0	0	47	0
26	BB	2637	0	1338	198	0
27	BA	60600	0	30513	10823	139
28	BD	1308	0	1345	1087	0
29	BE	1507	0	1474	1127	3
30	BF	1430	0	1359	1069	0
31	BG	957	0	950	685	0
32	BH	1251	0	1289	743	0
33	BI	1145	0	1225	635	4
34	BN	917	0	896	775	1
35	BO	937	0	993	614	0
36	BP	639	0	605	490	0
37	BQ	1081	0	1048	916	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	BS	866	0	867	686	0
39	BT	406	0	360	166	0
40	BW	860	0	911	559	0
41	BX	602	0	558	457	0
42	BY	879	0	860	748	0
43	BZ	1360	0	1377	887	0
44	BR	855	0	904	580	0
45	BU	978	0	995	924	0
46	BV	787	0	783	652	0
47	B2	494	0	504	385	0
48	B3	477	0	528	446	0
49	B0	641	0	657	501	0
50	B4	604	0	587	493	0
51	B5	457	0	457	293	0
52	B6	431	0	454	288	0
53	B7	383	0	409	396	0
54	B8	496	0	541	358	0
55	B9	285	0	312	203	0
56	BK	999	0	1068	144	0
All	All	142780	0	94554	28108	146

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 119.

The worst 5 of 28108 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)
51:B5:33:CYS:SG	51:B5:36:CYS:HB2	1.24	1.69
27:BA:2470:G:C2	27:BA:2471:C:C5	1.81	1.68
27:BA:994:C:C2	45:BU:53:LYS:HD3	1.16	1.68
53:B7:30:ILE:HA	53:B7:33:ARG:CD	1.21	1.67
27:BA:2580:U:C6	27:BA:2581:G:C8	1.82	1.66

The worst 5 of 146 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)
27:BA:6:A:C4'	27:BA:2902:C:O2'[8_554]	0.49	1.71
1:AA:359:U:OP1	33:BI:82:LYS:NZ[3_454]	0.68	1.52
27:BA:6:A:N9	27:BA:2902:C:C6[8_554]	0.88	1.32

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:BA:1:G:O6	27:BA:2898:U:C2[8_554]	0.92	1.28
27:BA:6:A:O4'	27:BA:2902:C:C2'[8_554]	0.97	1.23

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%)	34 (15%)	15 (6%)	1	25
6	AC	204/239 (85%)	165 (81%)	23 (11%)	16 (8%)	1	20
7	AD	206/209 (99%)	156 (76%)	34 (16%)	16 (8%)	1	20
8	AE	146/162 (90%)	114 (78%)	29 (20%)	3 (2%)	9	50
9	AF	99/101 (98%)	85 (86%)	10 (10%)	4 (4%)	4	35
10	AG	153/156 (98%)	131 (86%)	18 (12%)	4 (3%)	7	45
11	AH	136/138 (99%)	101 (74%)	25 (18%)	10 (7%)	1	21
12	AI	125/128 (98%)	87 (70%)	30 (24%)	8 (6%)	2	25
13	AJ	96/105 (91%)	73 (76%)	14 (15%)	9 (9%)	1	16
14	AK	117/129 (91%)	89 (76%)	23 (20%)	5 (4%)	3	34
15	AL	122/135 (90%)	91 (75%)	14 (12%)	17 (14%)	0	6
16	AM	123/126 (98%)	96 (78%)	21 (17%)	6 (5%)	3	31
17	AN	58/61 (95%)	42 (72%)	12 (21%)	4 (7%)	1	22
18	AO	86/89 (97%)	76 (88%)	9 (10%)	1 (1%)	16	61
19	AP	81/88 (92%)	64 (79%)	10 (12%)	7 (9%)	1	17
20	AQ	102/105 (97%)	78 (76%)	17 (17%)	7 (7%)	1	22
21	AR	71/88 (81%)	54 (76%)	11 (16%)	6 (8%)	1	17
22	AS	78/93 (84%)	60 (77%)	15 (19%)	3 (4%)	4	37
23	AT	97/106 (92%)	79 (81%)	12 (12%)	6 (6%)	2	25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	AU	22/27 (82%)	17 (77%)	3 (14%)	2 (9%)	1	17
28	BD	169/173 (98%)	60 (36%)	34 (20%)	75 (44%)	0	0
29	BE	183/338 (54%)	89 (49%)	35 (19%)	59 (32%)	0	0
30	BF	179/246 (73%)	51 (28%)	47 (26%)	81 (45%)	0	0
31	BG	116/176 (66%)	46 (40%)	31 (27%)	39 (34%)	0	0
32	BH	162/177 (92%)	74 (46%)	39 (24%)	49 (30%)	0	0
33	BI	144/149 (97%)	71 (49%)	29 (20%)	44 (31%)	0	0
34	BN	111/145 (77%)	34 (31%)	21 (19%)	56 (50%)	0	0
35	BO	120/122 (98%)	61 (51%)	27 (22%)	32 (27%)	0	1
36	BP	82/164 (50%)	28 (34%)	21 (26%)	33 (40%)	0	0
37	BQ	130/138 (94%)	38 (29%)	35 (27%)	57 (44%)	0	0
38	BS	105/186 (56%)	36 (34%)	20 (19%)	49 (47%)	0	0
39	BT	48/66 (73%)	17 (35%)	13 (27%)	18 (38%)	0	0
40	BW	104/113 (92%)	42 (40%)	15 (14%)	47 (45%)	0	0
41	BX	72/84 (86%)	26 (36%)	18 (25%)	28 (39%)	0	0
42	BY	108/119 (91%)	49 (45%)	20 (18%)	39 (36%)	0	0
43	BZ	175/253 (69%)	52 (30%)	53 (30%)	70 (40%)	0	0
44	BR	103/118 (87%)	35 (34%)	20 (19%)	48 (47%)	0	0
45	BU	115/118 (98%)	22 (19%)	23 (20%)	70 (61%)	0	0
46	BV	96/100 (96%)	39 (41%)	25 (26%)	32 (33%)	0	0
47	B2	62/70 (89%)	8 (13%)	9 (14%)	45 (73%)	0	0
48	B3	58/60 (97%)	24 (41%)	13 (22%)	21 (36%)	0	0
49	B0	84/91 (92%)	33 (39%)	16 (19%)	35 (42%)	0	0
50	B4	71/73 (97%)	21 (30%)	16 (22%)	34 (48%)	0	0
51	B5	56/60 (93%)	16 (29%)	17 (30%)	23 (41%)	0	0
52	B6	51/82 (62%)	21 (41%)	9 (18%)	21 (41%)	0	0
53	B7	44/47 (94%)	4 (9%)	7 (16%)	33 (75%)	0	0
54	B8	61/64 (95%)	23 (38%)	9 (15%)	29 (48%)	0	0
55	B9	33/36 (92%)	14 (42%)	9 (27%)	10 (30%)	0	0
56	BK	124/141 (88%)	93 (75%)	26 (21%)	5 (4%)	4	35
All	All	5320/6250 (85%)	2968 (56%)	1021 (19%)	1331 (25%)	0	2

5 of 1331 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	25
6	AC	160/188 (85%)	146 (91%)	14 (9%)	12	45
7	AD	180/181 (99%)	162 (90%)	18 (10%)	9	38
8	AE	115/123 (94%)	94 (82%)	21 (18%)	2	15
9	AF	90/90 (100%)	83 (92%)	7 (8%)	16	52
10	AG	126/127 (99%)	116 (92%)	10 (8%)	15	51
11	AH	119/119 (100%)	91 (76%)	28 (24%)	1	7
12	AI	98/99 (99%)	90 (92%)	8 (8%)	14	49
13	AJ	88/92 (96%)	77 (88%)	11 (12%)	6	30
14	AK	90/99 (91%)	85 (94%)	5 (6%)	26	63
15	AL	104/111 (94%)	93 (89%)	11 (11%)	8	36
16	AM	100/101 (99%)	87 (87%)	13 (13%)	5	29
17	AN	49/50 (98%)	43 (88%)	6 (12%)	6	31
18	AO	79/80 (99%)	70 (89%)	9 (11%)	7	33
19	AP	72/74 (97%)	62 (86%)	10 (14%)	4	27
20	AQ	96/97 (99%)	87 (91%)	9 (9%)	11	42
21	AR	64/77 (83%)	57 (89%)	7 (11%)	8	35
22	AS	71/80 (89%)	64 (90%)	7 (10%)	10	39
23	AT	76/82 (93%)	68 (90%)	8 (10%)	8	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	AU	19/22 (86%)	19 (100%)	0	100	100
28	BD	135/135 (100%)	99 (73%)	36 (27%)	0	5
29	BE	156/284 (55%)	128 (82%)	28 (18%)	2	15
30	BF	152/193 (79%)	124 (82%)	28 (18%)	2	14
31	BG	102/147 (69%)	93 (91%)	9 (9%)	12	45
32	BH	137/147 (93%)	111 (81%)	26 (19%)	2	13
33	BI	119/119 (100%)	98 (82%)	21 (18%)	2	16
34	BN	95/121 (78%)	80 (84%)	15 (16%)	3	21
35	BO	101/101 (100%)	81 (80%)	20 (20%)	1	12
36	BP	67/126 (53%)	56 (84%)	11 (16%)	3	20
37	BQ	110/110 (100%)	83 (76%)	27 (24%)	1	6
38	BS	89/149 (60%)	73 (82%)	16 (18%)	2	15
39	BT	44/52 (85%)	30 (68%)	14 (32%)	0	2
40	BW	88/92 (96%)	74 (84%)	14 (16%)	3	21
41	BX	67/73 (92%)	44 (66%)	23 (34%)	0	2
42	BY	97/105 (92%)	80 (82%)	17 (18%)	2	17
43	BZ	151/203 (74%)	129 (85%)	22 (15%)	4	24
44	BR	89/101 (88%)	71 (80%)	18 (20%)	1	11
45	BU	96/97 (99%)	68 (71%)	28 (29%)	0	3
46	BV	79/79 (100%)	69 (87%)	10 (13%)	5	29
47	B2	51/56 (91%)	37 (72%)	14 (28%)	0	4
48	B3	52/52 (100%)	47 (90%)	5 (10%)	10	41
49	B0	64/67 (96%)	57 (89%)	7 (11%)	8	35
50	B4	66/66 (100%)	54 (82%)	12 (18%)	2	15
51	B5	51/53 (96%)	43 (84%)	8 (16%)	3	22
52	B6	46/69 (67%)	39 (85%)	7 (15%)	3	23
53	B7	39/40 (98%)	31 (80%)	8 (20%)	1	10
54	B8	50/51 (98%)	39 (78%)	11 (22%)	1	9
55	B9	34/35 (97%)	30 (88%)	4 (12%)	6	32
56	BK	108/113 (96%)	105 (97%)	3 (3%)	51	78
All	All	4533/5148 (88%)	3840 (85%)	693 (15%)	3	22

5 of 693 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
30	BF	107	ARG
34	BN	79	PHE
50	B4	5	LEU
30	BF	245	GLU
32	BH	131	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 124 such sidechains are listed below:

Mol	Chain	Res	Type
29	BE	260	GLN
33	BI	64	ASN
49	B0	71	ASN
29	BE	318	ASN
30	BF	219	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1498/1522 (98%)	518 (34%)	166 (11%)
2	AV	74/76 (97%)	16 (21%)	4 (5%)
26	BB	122/123 (99%)	44 (36%)	3 (2%)
27	BA	2785/2916 (95%)	1488 (53%)	360 (12%)
3	AW	70/76 (92%)	14 (20%)	4 (5%)
4	AX	5/18 (27%)	0	0
All	All	4554/4731 (96%)	2080 (45%)	537 (11%)

5 of 2080 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 537 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
27	BA	579	G

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Mol	Chain	Res	Type
27	BA	1069	A
27	BA	2610	C
27	BA	670	A
27	BA	801	G

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	YYG	AW	37	10,3	27,42,43	1.04	2 (7%)	29,62,65	2.22	8 (27%)
3	PSU	AW	39	3	13,21,22	1.34	2 (15%)	18,30,33	6.15	4 (22%)
3	PSU	AW	55	3	13,21,22	1.52	2 (15%)	18,30,33	6.01	6 (33%)

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	-3.35	1.33	1.38
3	AW	55	PSU	C6-C5	-2.83	1.34	1.38
3	AW	37	YYG	C2-N2	2.01	1.38	1.35
3	AW	37	YYG	C6-N1	2.90	1.43	1.37
3	AW	39	PSU	C4-N3	3.01	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	-22.02	114.28	128.33
3	AW	55	PSU	N1-C2-N3	-21.73	114.47	128.33
3	AW	37	YYG	C13-C12-C11	-4.16	123.50	130.59
3	AW	37	YYG	O23-C21-O22	-3.83	119.71	124.70
3	AW	55	PSU	C4-C5-C1'	-2.41	116.83	121.23

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	37	0
3	AW	39	PSU	5	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
27	BA	53

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Mol	Chain	Number of breaks
1	AA	40
3	AW	6
56	BK	5
2	AV	4
37	BQ	3
46	BV	2
45	BU	1
20	AQ	1
14	AK	1
8	AE	1
5	AB	1
6	AC	1
28	BD	1
36	BP	1
7	AD	1
26	BB	1
32	BH	1
16	AM	1

The worst 5 of 125 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	BK	70:ILE	C	71:LYS	N	5.81
1	BK	73:PRO	C	74:PRO	N	5.30
1	BK	72:THR	C	73:PRO	N	5.11
1	AA	30(D):A	O3'	1031:G	P	4.82
1	BA	142(A):A	O3'	1143:A	P	4.82

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%)	0.64	139 (9%) 11 15	236, 236, 236, 236	0
2	AV	76/76 (100%)	0.47	5 (6%) 22 23	236, 236, 236, 236	0
3	AW	73/76 (96%)	1.14	14 (19%) 2 6	236, 236, 236, 236	0
4	AX	17/18 (94%)	4.29	12 (70%) 0 2	236, 236, 236, 236	0
5	AB	234/256 (91%)	-0.02	5 (2%) 67 62	236, 236, 236, 236	0
6	AC	206/239 (86%)	0.02	8 (3%) 43 40	236, 236, 236, 236	0
7	AD	208/209 (99%)	0.32	21 (10%) 9 13	236, 236, 236, 236	0
8	AE	150/162 (92%)	0.21	12 (8%) 15 18	236, 236, 236, 236	0
9	AF	101/101 (100%)	0.09	7 (6%) 20 22	236, 236, 236, 236	0
10	AG	155/156 (99%)	0.19	11 (7%) 19 21	236, 236, 236, 236	0
11	AH	138/138 (100%)	-0.16	4 (2%) 55 50	236, 236, 236, 236	0
12	AI	127/128 (99%)	0.33	15 (11%) 6 11	236, 236, 236, 236	0
13	AJ	98/105 (93%)	0.98	18 (18%) 2 7	236, 236, 236, 236	0
14	AK	119/129 (92%)	-0.06	3 (2%) 61 56	236, 236, 236, 236	0
15	AL	124/135 (91%)	0.16	8 (6%) 22 23	236, 236, 236, 236	0
16	AM	125/126 (99%)	0.70	22 (17%) 2 7	236, 236, 236, 236	0
17	AN	60/61 (98%)	0.38	6 (10%) 9 13	236, 236, 236, 236	0
18	AO	88/89 (98%)	0.20	1 (1%) 82 78	236, 236, 236, 236	0
19	AP	83/88 (94%)	0.93	17 (20%) 1 6	236, 236, 236, 236	0
20	AQ	104/105 (99%)	-0.01	2 (1%) 70 65	236, 236, 236, 236	0
21	AR	73/88 (82%)	0.14	4 (5%) 29 29	236, 236, 236, 236	0
22	AS	80/93 (86%)	0.91	16 (20%) 1 6	236, 236, 236, 236	0
23	AT	99/106 (93%)	-0.02	5 (5%) 32 31	236, 236, 236, 236	0
24	AU	24/27 (88%)	1.13	6 (25%) 1 5	236, 236, 236, 236	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	AY	333/354 (94%)	1.48	101 (30%) 1 5	236, 236, 236, 236	0
26	BB	123/123 (100%)	0.33	0 100 100	236, 236, 236, 236	0
27	BA	2814/2916 (96%)	0.47	171 (6%) 25 25	236, 236, 236, 236	0
28	BD	173/173 (100%)	-0.28	3 (1%) 73 67	236, 236, 236, 236	0
29	BE	191/338 (56%)	0.22	11 (5%) 26 27	236, 236, 236, 236	0
30	BF	189/246 (76%)	-0.11	4 (2%) 67 62	236, 236, 236, 236	0
31	BG	122/176 (69%)	0.53	10 (8%) 14 17	236, 236, 236, 236	0
32	BH	164/177 (92%)	-0.01	9 (5%) 29 29	236, 236, 236, 236	0
33	BI	148/149 (99%)	0.10	4 (2%) 58 53	236, 236, 236, 236	0
34	BN	117/145 (80%)	-0.24	2 (1%) 73 67	236, 236, 236, 236	0
35	BO	122/122 (100%)	-0.05	2 (1%) 74 68	236, 236, 236, 236	0
36	BP	84/164 (51%)	0.16	2 (2%) 62 57	236, 236, 236, 236	0
37	BQ	138/138 (100%)	0.25	10 (7%) 18 21	236, 236, 236, 236	0
38	BS	113/186 (60%)	-0.05	3 (2%) 58 53	236, 236, 236, 236	0
39	BT	52/66 (78%)	0.33	0 100 100	236, 236, 236, 236	0
40	BW	108/113 (95%)	-0.10	1 (0%) 85 81	236, 236, 236, 236	0
41	BX	76/84 (90%)	-0.09	1 (1%) 79 73	236, 236, 236, 236	0
42	BY	110/119 (92%)	0.58	13 (11%) 6 11	236, 236, 236, 236	0
43	BZ	177/253 (69%)	0.16	12 (6%) 20 22	236, 236, 236, 236	0
44	BR	105/118 (88%)	-0.28	1 (0%) 84 79	236, 236, 236, 236	0
45	BU	117/118 (99%)	-0.31	4 (3%) 49 45	236, 236, 236, 236	0
46	BV	100/100 (100%)	-0.15	1 (1%) 84 79	236, 236, 236, 236	0
47	B2	64/70 (91%)	-0.62	0 100 100	236, 236, 236, 236	0
48	B3	60/60 (100%)	-0.35	1 (1%) 73 67	236, 236, 236, 236	0
49	B0	86/91 (94%)	0.14	5 (5%) 26 27	236, 236, 236, 236	0
50	B4	73/73 (100%)	0.01	2 (2%) 58 53	236, 236, 236, 236	0
51	B5	58/60 (96%)	0.14	5 (8%) 13 17	236, 236, 236, 236	0
52	B6	53/82 (64%)	-0.27	2 (3%) 44 41	236, 236, 236, 236	0
53	B7	46/47 (97%)	0.02	2 (4%) 39 36	236, 236, 236, 236	0
54	B8	63/64 (98%)	-0.25	0 100 100	236, 236, 236, 236	0
55	B9	35/36 (97%)	0.95	6 (17%) 2 7	236, 236, 236, 236	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
56	BK	133/141 (94%)	1.31	30 (22%)	1 5	236, 236, 236, 236	0
All	All	10424/11335 (91%)	0.36	779 (7%)	17 20	236, 236, 236, 236	0

The worst 5 of 779 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
25	AY	260	LYS	13.1
4	AX	123	A	12.7
56	BK	52	MET	10.5
27	BA	1532	C	9.5
4	AX	122	U	9.4

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	YYG	AW	37	39/40	0.52	0.68	-	236,236,236,236	0
3	PSU	AW	55	20/21	0.85	0.18	-	236,236,236,236	0
3	PSU	AW	39	20/21	0.72	0.44	-	236,236,236,236	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.