



wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 04:59 pm BST

PDB ID : 4V4A
Title : Crystal Structure of the Wild Type Ribosome from E. Coli 70S Ribosome.
Authors : Vila-Sanjurjo, A.; Ridgeway, W.K.; Seymaner, V.; Zhang, W.; Santoso, S.; Yu, K.; Cate, J.H.D.
Deposited on : 2003-06-13
Resolution : 9.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

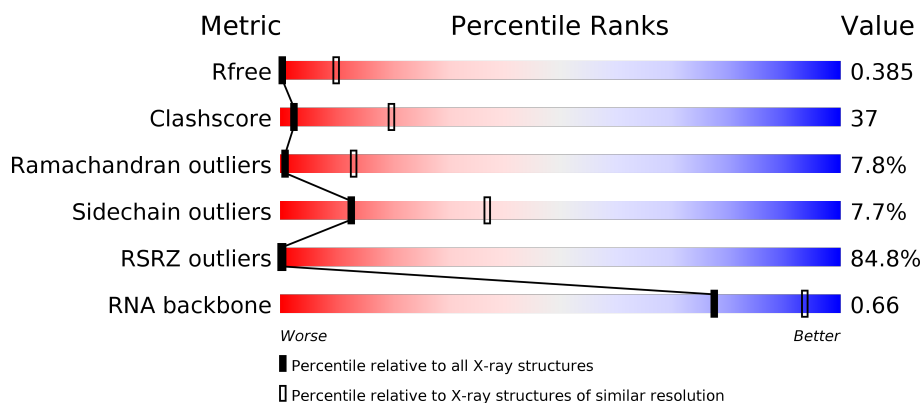
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 9.50 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}	130704	1005 (11.50-3.90)
Clashscore	141614	1071 (15.00-3.90)
Ramachandran outliers	138981	1003 (11.50-3.90)
Sidechain outliers	138945	1003 (11.50-3.86)
RSRZ outliers	127900	1004 (9.50-3.80)
RNA backbone	3102	1079 (11.50-3.00)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AA	1537	<div> <div>100%</div> <div>23% 58% 15% .</div> </div>
2	AB	234	<div> <div>31%</div> <div>29% 56% 13% .</div> </div>
3	AC	206	<div> <div>82%</div> <div>30% 51% 17% .</div> </div>
4	AD	208	<div> <div>97%</div> <div>39% 55% 5%</div> </div>

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Mol	Chain	Length	Quality of chain
5	AE	150	
6	AF	101	
7	AG	155	
8	AH	138	
9	AI	127	
10	AJ	98	
11	AK	119	
12	AL	124	
13	AM	125	
14	AN	60	
15	AO	88	
16	AP	83	
17	AQ	104	
18	AR	73	
19	AS	80	
20	AT	99	
21	B0	2887	
22	B9	118	
23	BA	270	
24	BB	205	
25	BC	197	
26	BD	178	
27	BE	177	
28	BF	52	
29	BG	143	

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Mol	Chain	Length	Quality of chain
30	BH	143	71% 100%
31	BI	132	42% 99%
32	BJ	141	82% 99%
33	BK	124	39% 100%
34	BL	114	89% 99%
35	BM	111	33% 100%
36	BN	125	42% 100%
37	BO	117	84% 100%
38	BP	100	83% 100%
39	BQ	130	84% 100%
40	BR	93	77% 100%
41	BS	113	99% 100%
42	BT	173	61% 100%
43	BU	86	69% 100%
44	BV	16	100%
45	BW	65	83% 100%
46	BX	55	82% 100%
47	BY	73	63% 100%
48	BZ	58	78% 100%
49	B1	53	49% 100%
50	B2	46	100%
51	B3	63	98% 100%
52	B4	35	74% 100%
53	B5	217	48% 96%

2 Entry composition

There are 53 unique types of molecules in this entry. The entry contains 118711 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	1533	Total	C	N	O	P	0	0	0
			32939	14664	6099	10643	1533			

- Molecule 2 is a protein called 30S ribosomal protein S2.

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

- Molecule 3 is a protein called 30S ribosomal protein S3.

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

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AD	208	Total	C	N	O	S	0	0	0
			1702	1066	339	290	7			

- Molecule 5 is a protein called 30S ribosomal protein S5.

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

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AF	101	Total	C	N	O	S	0	0	0
			842	531	155	153	3			

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AG	155	Total	C	N	O	S	0	0	0
			1256	781	252	217	6			

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AH	138	Total	C	N	O	S	0	0	0
			1115	705	215	192	3			

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	AI	127	Total	C	N	O	0	0	0
			1010	639	198	173			

- Molecule 10 is a protein called 30S ribosomal protein S10.

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

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AK	119	Total	C	N	O	S	0	0	0
			884	549	168	164	3			

- Molecule 12 is a protein called 30S ribosomal protein S12.

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

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	125	Total	C	N	O	S	0	0	0
			996	617	207	170	2			

- Molecule 14 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AN	60	Total	C	N	O	S	0	0	0
			491	312	104	71	4			

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AO	88	Total	C	N	O	S	0	0	0
			733	459	147	125	2			

- Molecule 16 is a protein called 30S ribosomal protein S16.

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

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AQ	104	Total	C	N	O	S	0	0	0
			856	547	161	146	2			

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	AR	73	Total	C	N	O	0	0	0
			596	380	118	98			

- Molecule 19 is a protein called 30S ribosomal protein S19.

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

- Molecule 20 is a protein called 30S ribosomal protein S20.

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

- Molecule 21 is a RNA chain called 23S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	B0	2825	Total	C	N	O	P	0	0	0
			60636	27047	11191	19573	2825			

- Molecule 22 is a RNA chain called 5S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	B9	118	Total	C	N	O	P	0	0	0
			2519	1124	464	813	118			

- Molecule 23 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
23	BA	270	Total	C	0	0	270
			270	270			

- Molecule 24 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
24	BB	205	Total	C	0	0	205
			205	205			

- Molecule 25 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
25	BC	197	Total	C	0	0	197
			197	197			

- Molecule 26 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
26	BD	178	Total	C	0	0	178
			178	178			

- Molecule 27 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
27	BE	177	Total	C	0	0	177
			177	177			

- Molecule 28 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
28	BF	52	Total C 52 52	0	0	52

- Molecule 29 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
29	BG	143	Total C 143 143	0	0	143

- Molecule 30 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
30	BH	143	Total C 143 143	0	0	143

- Molecule 31 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
31	BI	132	Total C 132 132	0	0	132

- Molecule 32 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
32	BJ	141	Total C 141 141	0	0	141

- Molecule 33 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
33	BK	124	Total C 124 124	0	0	124

- Molecule 34 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
34	BL	114	Total C 114 114	0	0	114

- Molecule 35 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
35	BM	111	Total C 111 111	0	0	111

- Molecule 36 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
36	BN	125	Total C 125 125	0	0	125

- Molecule 37 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
37	BO	117	Total C 117 117	0	0	117

- Molecule 38 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
38	BP	100	Total C 100 100	0	0	100

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
39	BQ	130	Total C 130 130	0	0	130

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
40	BR	93	Total C 93 93	0	0	93

- Molecule 41 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
41	BS	113	Total C 113 113	0	0	113

- Molecule 42 is a protein called general stress protein Ctc.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
42	BT	173	Total C 173 173	0	0	173

- Molecule 43 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
43	BU	86	Total C 86 86	0	0	86

- Molecule 44 is a protein called 50S RIBOSOMAL PROTEIN L28.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
44	BV	16	Total C 16 16	0	0	16

- Molecule 45 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
45	BW	65	Total C 65 65	0	0	65

- Molecule 46 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
46	BX	55	Total C 55 55	0	0	55

- Molecule 47 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
47	BY	73	Total C 73 73	0	0	73

- Molecule 48 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
48	BZ	58	Total C 58 58	0	0	58

- Molecule 49 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
49	B1	53	Total C 53 53	0	0	53

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
50	B2	46	Total C 46 46	0	0	46

- Molecule 51 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
51	B3	63	Total C 63 63	0	0	63

- Molecule 52 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
52	B4	35	Total C 35 35	0	0	35

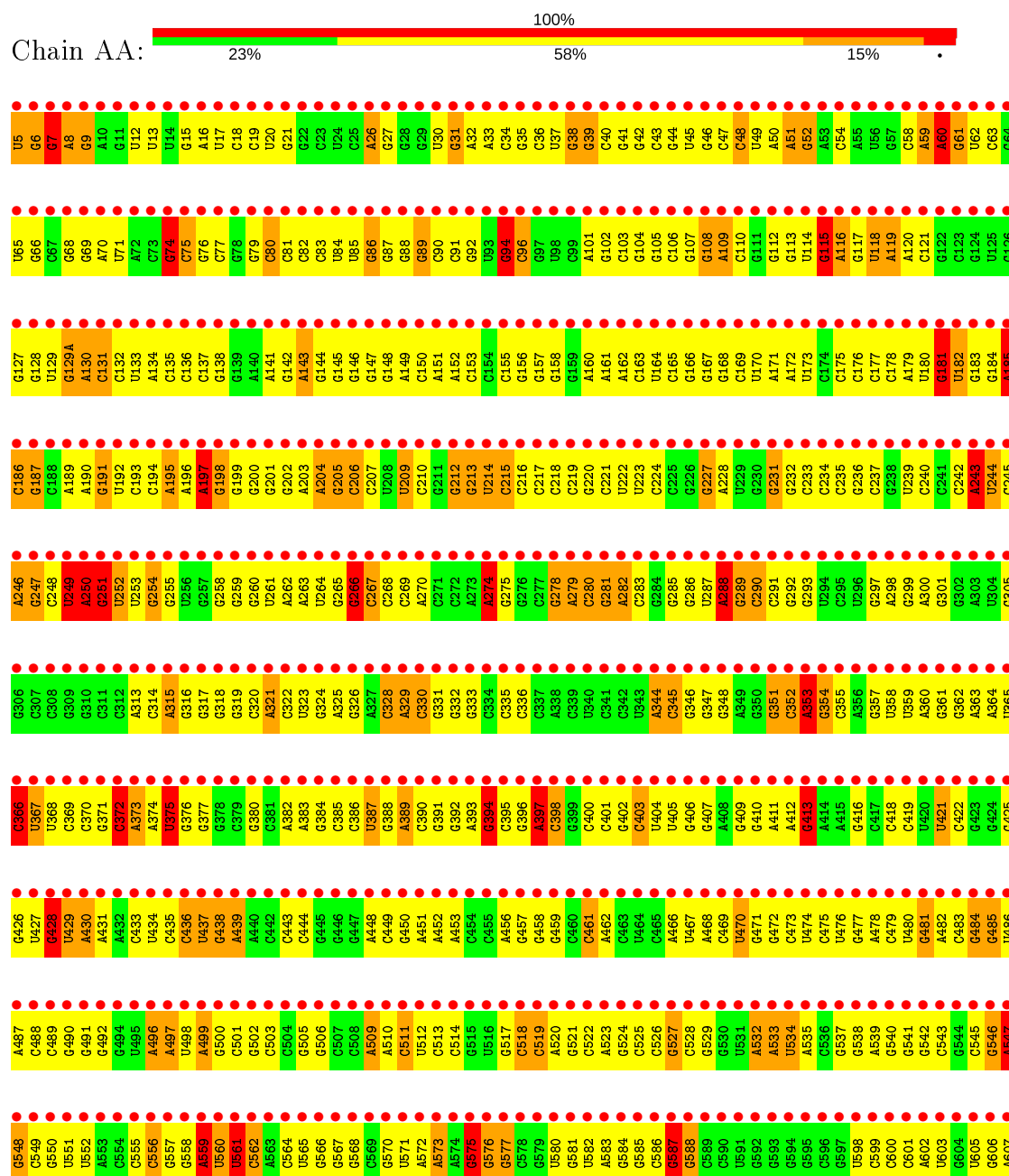
- Molecule 53 is a protein called 50S ribosomal protein L1P.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
53	B5	217	Total C 217 217	0	0	217

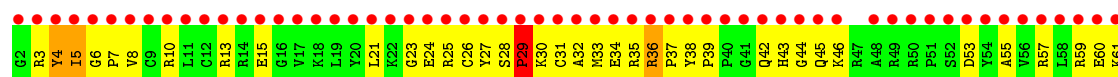
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: 16S RIBOSOMAL RNA

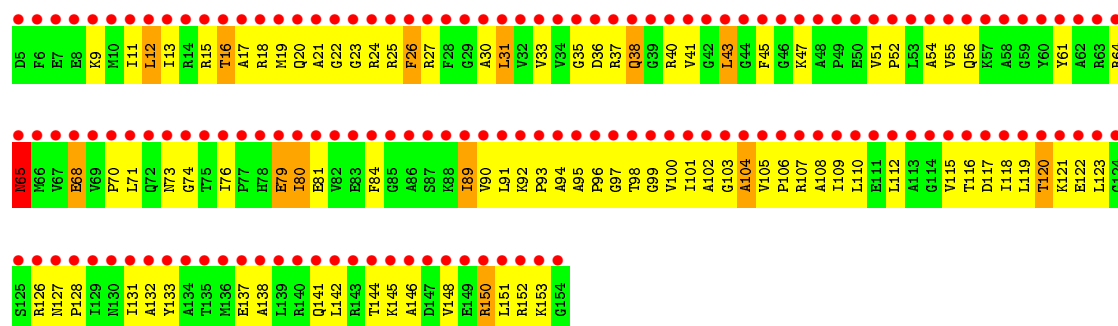


G1387	C1328	A1268	C1208	G1087	C1027	A968	G848	U788	A728	G688	A608
G1388	A1329	A1269	C1209	G1088	C1028	A969	C849	U789	A729	G689	A609
C1389	G1330	C1270	C1210	G1089	U1029	C970	U850	A790	G730	G690	G610
U1390	G1331	G1271	U1211	U1090	U1030	G971	G851	G791	G731	G671	A611
U1391	A1332	G1272	U1212	U1091	C1031	C972	G852	A792	C732	G672	G612
G1392	A1333	G1273	A1213	A1092	G1032	G973	G853	G793	A733	G673	C613
U1393	G1334	G1274	C1214	A1093	G1033	A974	G854	A794	G734	G674	A614
A1394	C1335	A1275	G1215	G1094	G1034	A975	G855	C795	C735	A675	G615
C1395	G1336	G1276	G1216	U1095	A1035	G976	C856	C796	C736	A676	G616
A1396	G1337	C1277	C1217	C1096	G1036	A977	C857	C797	A737	G677	G617
C1397	G1338	U1278	C1218	C1097	G1037	A978	G858	G798	C738	G678	C618
A1398	A1339	U1279	C1219	C1098	C1038	C979	A859	G799	G739	G679	U619
C1399	A1340	A1280	U1220	G1099	C1039	C980	A860	G800	U740	C680	C620
U1341	G1221	U1281	G1221	C1100	U1040	U861	G861	U801	G741	C681	A621
G1401	C1282	C1282	G1222	A1101	A1041	U862	C862	A802	G742	G682	A622
C1402	G1283	G1283	C1223	A1102	G1042	A983	U863	G803	U743	G683	C623
C1403	C1284	G1284	C1224	C1103	A1043	C984	A864	U804	C744	A684	C624
A1404	U1285	A1285	G1225	G1104	A1044	C985	A865	C905	C745	G685	G625
G1405	A1286	A1286	C1226	A1105	C1045	A986	C866	C806	A746	U686	U626
U1406	A1287	A1287	A1227	G1106	A1046	G987	C867	A807	C747	A687	G627
C1407	U1288	U1288	C1228	C1107	G1047	G988	C868	C808	C748	G688	G628
A1408	A1289	A1289	A1229	G1108	U1048	C989	G869	G809	C749	C689	G629
C1409	G1290	A1169	C1230	C1109	U1049	C990	U870	C810	G750	G690	G630
G1410	G1291	G1171	G1231	U991	G1050	U991	U871	C811	U751	G691	G631
C1411	U1292	G1172	U1232	A1111	C1051	U992	A872	C812	U752	G692	A632
C1412	G1293	G1173	C1233	C1112	U1052	G993	A873	U813	A753	G693	G633
C1354	G1294	G1174	G1234	C1113	G1053	C994	C874	A814	C754	A694	C634
G1355	U1295	G1175	U1235	C1114	C1054	A995	G875	A815	C755	A695	G635
G1356	A1296	C1176	A1236	C1115	A1055	A996	G876	A816	C756	A696	U636
G1357	C1297	G1177	C1237	C1116	U1056	A997	C877	C817	U757	G697	G637
C1358	C1298	G1178	A1238	G1117	G1057	G998	G878	G818	G758	G698	G638
A1418	U1299	A1179	A1239	C1118	G1058	C999	C879	A819	A759	C699	G639
A1360	G1300	A1800	U1240	C1119	C1059	U1000	C880	U820	G760	G700	A640
U1361	U1301	G1181	G1241	G1120	C1060	A1001	G881	G821	G761	C701	U641
C2361	G1302	G1182	C1242	U1121	G1061	C942	C882	C822	C762	A702	A642
C1362	C1303	A1183	U1222	U1122	U1062	U943	C883	G823	G763	G703	C643
A1363	G1304	G1184	G1243	C1123	C1063	G944	U884	C824	C764	A704	G644
U1364	U1305	G1185	A1244	G1124	G1064	A1004	G885	G825	G765	U705	C645
G1365	A1306	G1186	C1246	U1125	U1065	A1005	G886	G826	A766	G706	U646
C1426	U1307	U1187	U1247	U1126	C1066	G947	G887	U827	A767	C707	G647
U1427	U1308	A1188	A1248	C1127	A1067	C948	G888	A828	A768	G708	A648
A1428	G1309	C1189	C1249	C1128	G1068	A949	A889	G829	G769	G709	G649
C1369	G1310	G1190	A1250	C1129	C1069	U950	G890	G830	C770	G710	G650
U1370	G1311	A1191	A1251	A1130	U1070	G951	U891	U831	G771	G711	G651
G1371	G1312	C1192	A1252	G1131	C1071	U952	A892	C832	U772	A712	U652
G1372	U1313	G1193	G1253	C1132	U1072	G953	C893	U833	G773	G713	A653
A1433	C1314	U1194	C1254	G1133	G1073	G954	G894	C834	G774	G714	G654
A1434	A1374	C1195	G1255	G1134	G1074	U955	G895	U835	G775	A715	A655
G1435	G1316	U1196	A1256	U1135	C1075	U956	C896	G836	G776	A716	C656
U1436	C1317	G1197	U1257	U1136	C1076	U957	C897	G837	A777	G717	G657
C1437	A1318	G1198	G1258	C1137	G1077	A958	G898	C838	G778	G718	G658
G1438	A1319	U1199	C1259	G1138	U1078	A959	G899	G839	C779	G719	U659
C1379	C1320	G1200	C1260	C1139	G1079	U960	A900	G840	A780	G720	G660
C1440	A1281	A1201	A1261	C1140	A1080	U961	A901	C841	A781	G721	G661
G1441	C1322	G1202	C1262	C1141	G1081	C962	G902	U842	A782	G722	G662
G1442	G1323	C1203	G1263	G1082	G1082	G963	G903	C843	G783	U723	A663
C1443	A1324	A1204	C1264	G1143	U1083	A964	G904	A844	C784	G724	G664
U1444	C1325	G1205	G1265	G1144	U1084	A965	U905	C846	G785	G725	A665
G1385	G1326	G1206	C1266	C1145	U1085	U966	G906	G847	G786	C726	G666
G1386	C1327	G1207	C1267	A1146	U1086	C967	A907	C947	A787	G727	G667

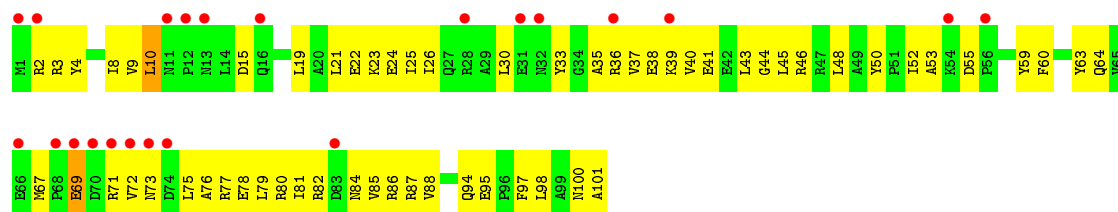
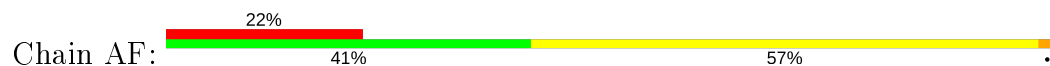




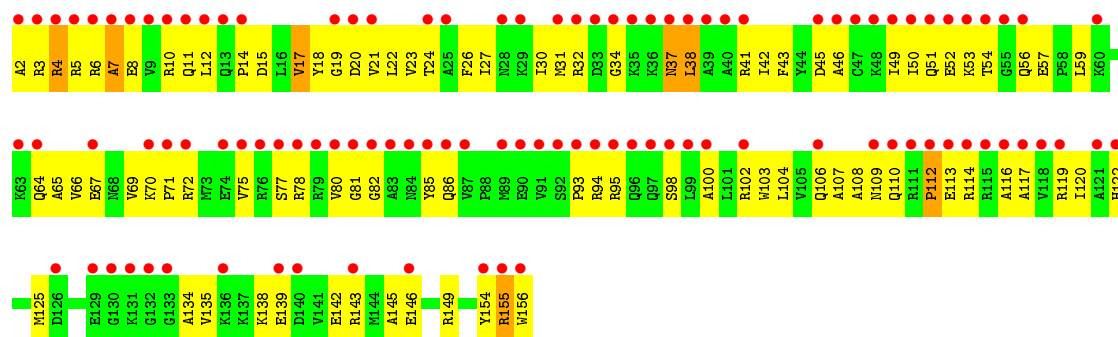
• Molecule 5: 30S ribosomal protein S5



• Molecule 6: 30S ribosomal protein S6



• Molecule 7: 30S ribosomal protein S7



Chain AH:

93% 40% 51% 8%

M1, L2, T3, D4, P5, I6, A7, D8, N9, L10, T11, I12, I13, I14, M15, A16, T17, R18, V19, Y20, K21, E22, S23, T24, D25, V26, P27, A28, S29, K30, F31, K32, E33, E34, I35, L36, K37, I38, L39, A40, R41, E42, G43, F44, T45, K46, G47, Y48, E49, R50, V51, D52, V53, D54, G55, K56, P57, V58, L59, R60, V61, Y62, L63, K64, Y65, G66, P67, R68, G69, Q70, D73, P74, R75, P76, E77, Q78, V79, R80, H81, H82, I83, R84, R85, L86, S87, K88, P89, G90, K91, R92, V93, Y94, V95, G96, G97, K98, E99, I100, P101, R102, V103, R104, R105, G106, L107, G108, I109, A110, I111, L112, T113, T114, S115, K116, G117, V118, L119, T120, R121, R122, E123, A124, R125, K126, L127, G128, V129, G130, G131, F132, L133, I134, G135, E136, V137, W138

Chain AI:

Category	Value
E2	61%
Q3	29%
Y4	61%
Y5	8%
G6	0%
T7	0%
G8	0%
R9	0%
R10	0%
K11	0%
E12	0%
A13	0%
V14	0%
A15	0%
R16	0%
V17	0%
F18	0%
L19	0%
R20	0%
P21	0%
G22	0%
N23	0%
G24	0%
K25	0%
V26	0%
T27	0%
V28	0%
N29	0%
G30	0%
Q31	0%
P32	0%
F33	0%
N34	0%
E35	0%
Y36	0%
F37	0%
Q38	0%
G39	0%
L40	0%
V41	0%
R42	0%
A43	0%
V44	0%
A45	0%
A46	0%
L47	0%
F48	0%
P49	0%
L50	0%
R51	0%
A52	0%
V53	0%
P54	0%
L55	0%
L56	0%
G57	0%
E58	0%
F59	0%
D60	0%
L61	0%
Y62	0%
V65	0%
R66	0%
G67	0%
G68	0%
G69	0%
K70	0%
S71	0%
G72	0%
O73	0%
T74	0%
D75	0%
A76	0%
I77	0%
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I81	0%
A84	0%
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V86	0%
Q87	0%
Y88	0%
N89	0%
P90	0%
D91	0%
Y92	0%
R93	0%
A94	0%
R95	0%
L96	0%
N97	0%
P98	0%
L99	0%
G100	0%
F101	0%
L102	0%
T103	0%
R104	0%
D105	0%
A106	0%
R107	0%
V108	0%
V109	0%
E110	0%
R111	0%
K112	0%
K113	0%
Y114	0%
G115	0%
K116	0%
H117	0%
K118	0%
A119	0%
R120	0%
R121	0%
A122	0%
F123	0%
Q124	0%
Y125	0%
S126	0%
K127	0%
R128	0%

Chain AJ:

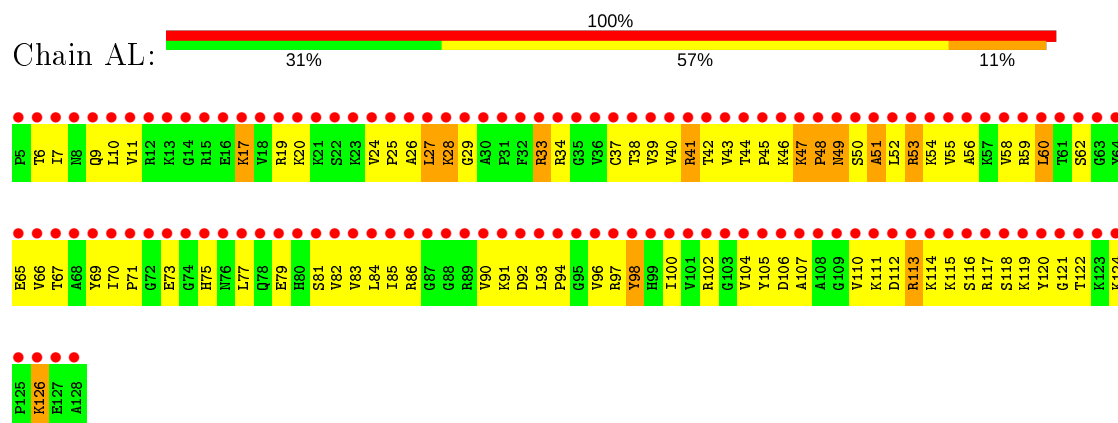
Category	Percentage
Green	12%
Red	67%
Orange	19%

Below the chart, there are two rows of 20 items each, represented by colored dots and labels. The top row labels are: K3, I4, R5, I6, K7, L8, R9, G10, F11, D12, H13, K14, T15, I16, D17, A18, S19, A20, Q21, R22, I23, V24, P25, A26, R27, R28, R29, S30, G31, A32, G33, V34, G35, G36, P37, I38, P39, L40, P41, T42, A43, V44, R45, F47, T48, V49, I50, H51, G52, P53, F54, K55, H56, K57, D58, S59, R60, R61, R62. The bottom row labels are: F63, B64, L65, R66, T67, H68, R69, R70, L71, W72, D73, T74, I75, M76, F77, D78, N78, R79, K80, T81, I82, B83, Q84, L85, R86, T87, L88, D89, L90, P91, T92, G93, V94, R95, I96, E97, I98, R99, T100.

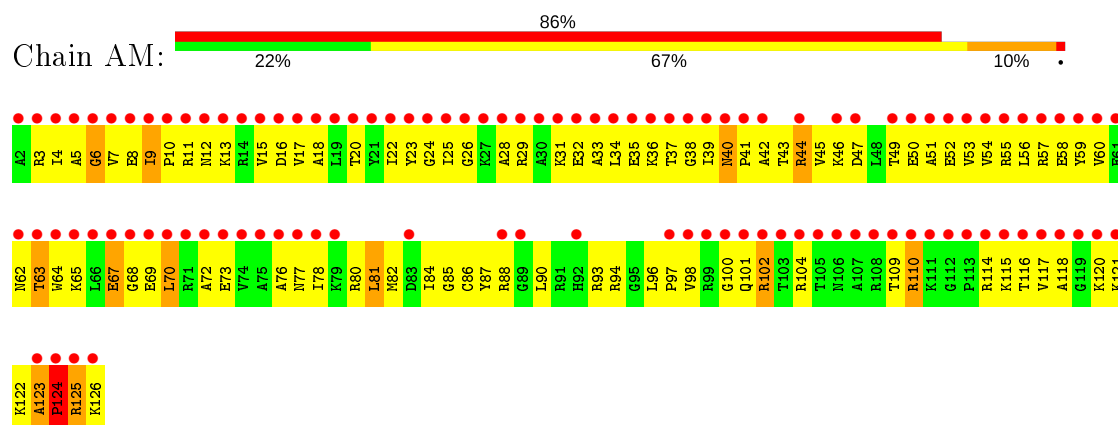
Chain AK:

Category	Percentage
Red	46%
Green	29%
Yellow	62%
Orange	8%

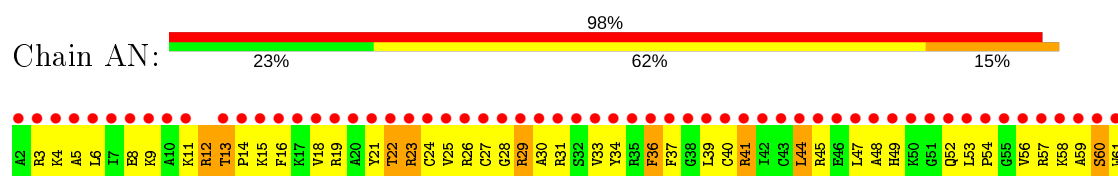
- Molecule 12: 30S ribosomal protein S12



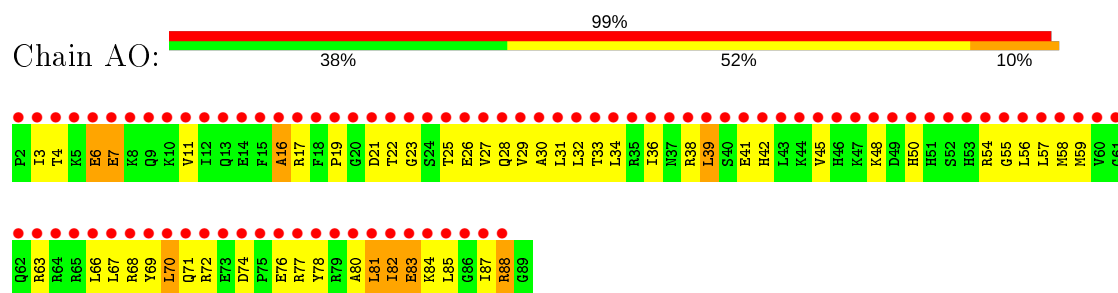
- Molecule 13: 30S ribosomal protein S13



- Molecule 14: 30S ribosomal protein S14

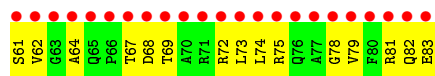
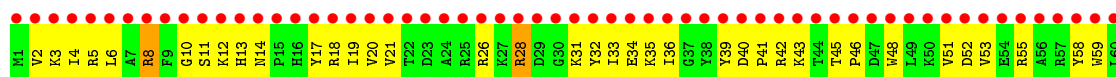


- Molecule 15: 30S ribosomal protein S15

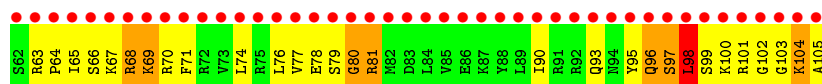
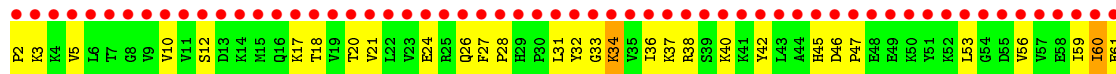
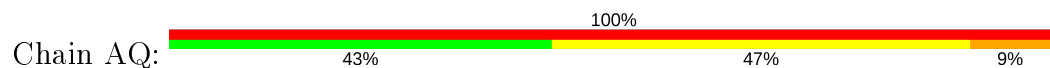


- Molecule 16: 30S ribosomal protein S16

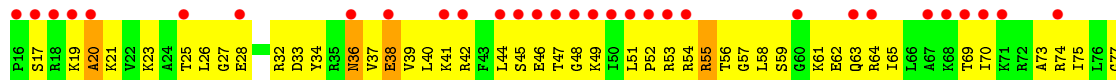




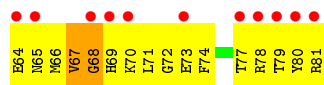
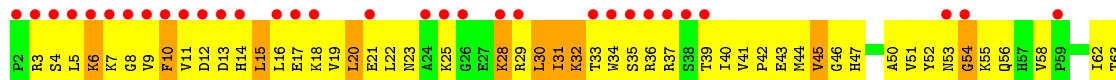
• Molecule 17: 30S ribosomal protein S17



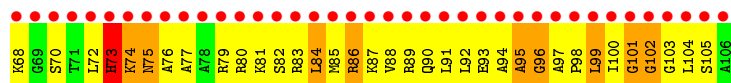
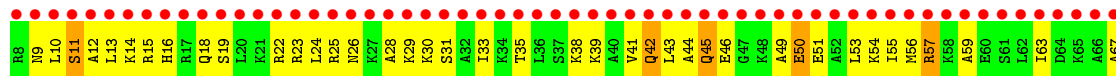
• Molecule 18: 30S ribosomal protein S18



• Molecule 19: 30S ribosomal protein S19



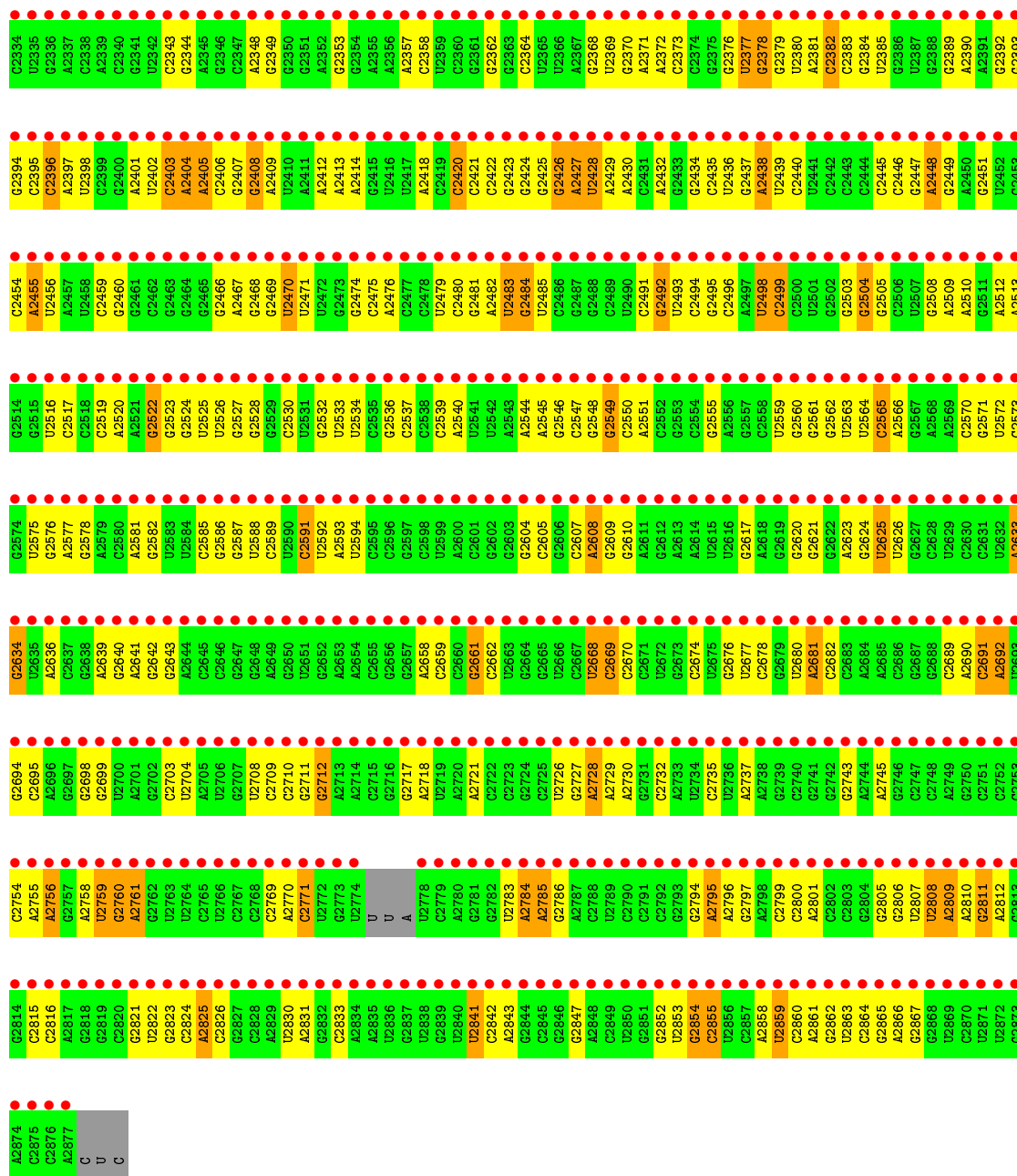
• Molecule 20: 30S ribosomal protein S20



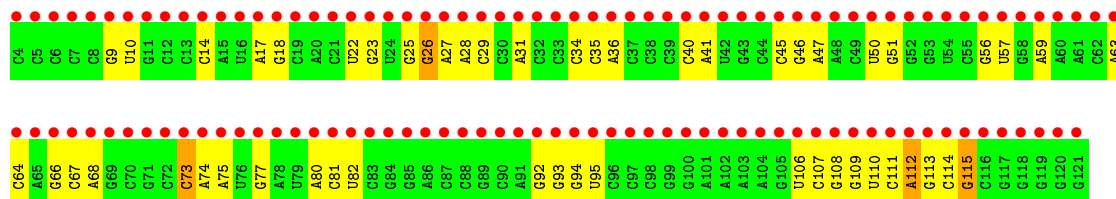
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G1503	G1443	G1383	G1323	C1263	A1203	A1143	C1083	A1023	G963	G902	A843	G783
G1504	G1444	G1384	G1324	C1264	A1204	U1144	A1084	G1204	A964	G903	G844	U784
G1505	A1445	C1385	U1325	G1265	G1205	G1145	C1085	A1025	G965	U904	U845	U785
G1506	U1446	A1386	U1326	G1266	G1206	G1146	C1086	U1026	A966	G905	A846	U786
G1507	U1447	G1387	C1327	U1267	G1207	G1147	C1087	C1027	G967	U906	C847	U787
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A1516	C1336	U1276	G1276	G1216	A1216	U1156	A1096	G1036	A976	U916	A856	A796
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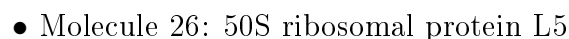
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C2303	C2183	C3138	C2061	U2001	U1941	U1881	C1830	U1770	U1710	A1650	G1590
G2304	C2184	U3139	U2062	A2002	G1942	G1882	G1831	A1771	C1711	U1651	U1591
C2305	U2185	G3140	A2063	A2003	A1943	A1883	G1832	C1772	U1592	G1652	U1592
A2306	U2186	C3141	U2064	U2004	G1944	A1884	U1833	C1773	C1593	G1653	C1593
A2307	A2187	C3142	A2065	U2005	C1945	C1885	G1834	A1774	A1714	A1654	U1594
A2308	A2188	U3143	G2066	G2006	U1946	G1886	C1835	A1775	C1655	C1655	A1595
G2309	A2189	A3146	U2067	G2007	G1947	G1887	C1836	A1776	U1656	U1656	A1596
G2310	A2190	C3147	C2068	C2008	C1948	C1888	G1837	A1777	A1657	A1657	A1597
U2311	A2191	G3148	U2069	U2009	A1949	C1889	G1838	U1778	A1718	A1658	C1598
A2312	U2192	C3149	G2070	G2010	C1950	G1890	A1839	C1779	G1719	G1659	G1599
G2313	C2193	C3150	G2071	U2011	G1951	C1891	A1840	A1780	G1720	G1660	U1600
A2314	A2194	U3151	A2072	A2012	A1952	C1892	G1841	C1781	G1721	C1661	U1601
C2315	C2195	G3152	C2073	A2013	A1953	G1893	U1842	A1782	G1722	G1662	G1602
G2316	U2196	G3153	U2074	A2014	A1954	U1894	U1843	G1783	U1723	C1663	A1603
G2317	U2197	C3154	U2075	G2015	G1955	A1895	C1844	G1784	G1724	G1664	A1604
U2318	U2198	G3155	C3093	A2016	G1956	A1896	U1845	A1785	C1725	C1665	A1605
A2319	C2199	G3156	A3095	U2017	C1957	C1897	A1846	C1786	G1726	G1666	C1606
G2320	G2200	C3157	G2018	G1958	G1958	U1898	U1847	U1787	A1607	A1667	A1607
C2321	G2201	A3158	C2019	C2019	A1899	U1899	U1848	U1789	U1608	G1668	U1608
U2322	G2202	G3159	G3097	A1900	U1900	U1900	G1849	G1790	G1609	A1669	G1609
G2323	G2203	C3160	C3098	G2020	A1901	A1901	G1850	C1791	A1610	G1670	A1610
A2324	A2204	C3161	U3099	G2021	A1981	A1902	A1851	C1792	U1611	A1671	U1611
C2325	C2205	G3162	G3100	C2022	G1962	C1903	G1852	C1793	U1732	A1672	U1612
C2326	C2206	C3163	G3101	U2024	A1964	G1904	G1853	A1794	U1733	G1673	G1613
U2327	G2207	C3164	G3102	A2025	U1965	G1905	G1854	A1795	C1674	C1674	G1614
G2328	U2208	G3165	A3103	C2026	G1966	U1906	G1855	G1795	G1735	C1675	C1615
C2329	G2209	C3166	C3104	C2027	U1967	C1907	U1856	A1796	C1736	U1676	C1616
G2330	G2210	U3167	G3105	C2028	G1968	C1908	A3865	C1797	G1737	G1677	G1617
A2331	U2211	G3168	U3106	G2029	G1969	U1909	A3866	G1798	U1738	G1678	U1618
C2332	U2212	C3169	G3107	U2030	A1970	A1910	G3867	A1799	U1739	U1679	A1619
A2333	G2213	A3170	G3108	A2031	C1971	A1911	U3868	A1800	G1740	U1680	C1620

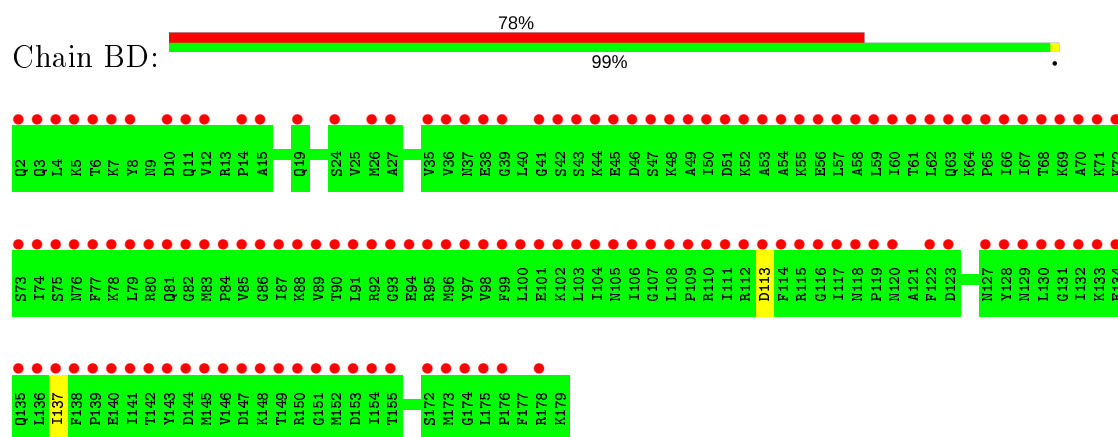


• Molecule 22: 5S RIBOSOMAL RNA

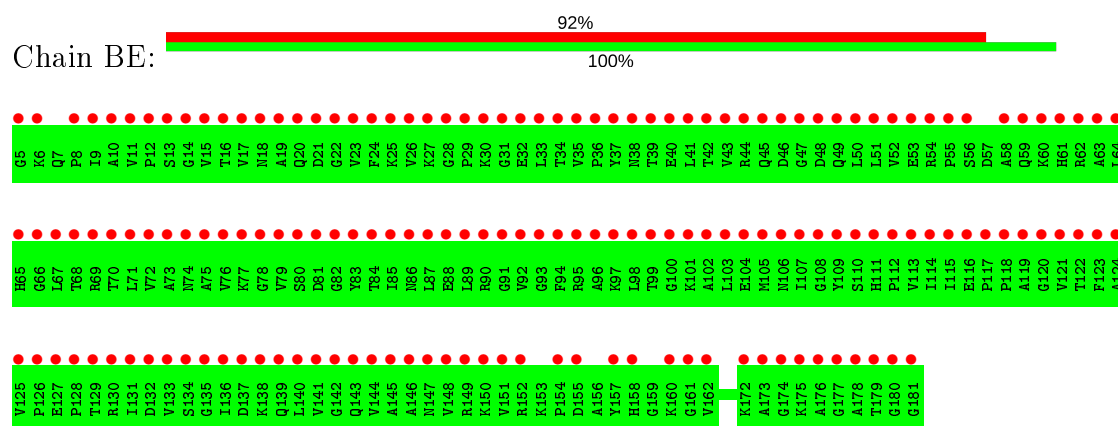


• Molecule 23: 50S ribosomal protein L2

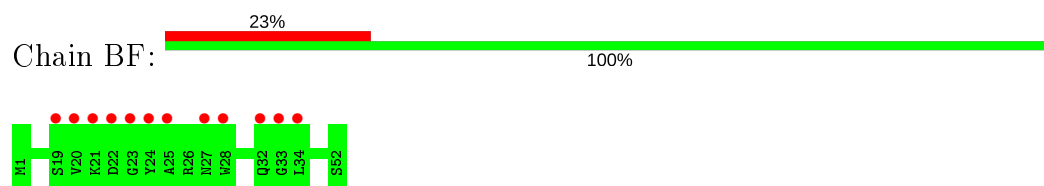




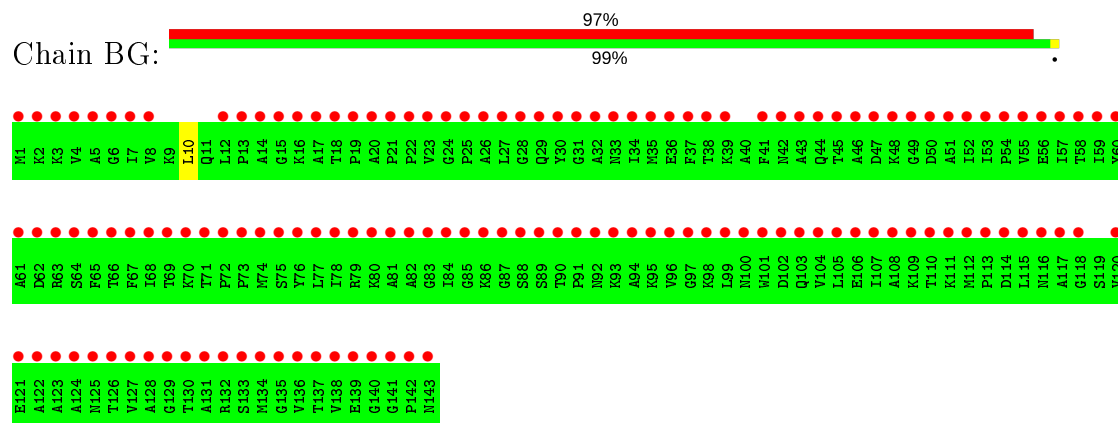
• Molecule 27: 50S ribosomal protein L6



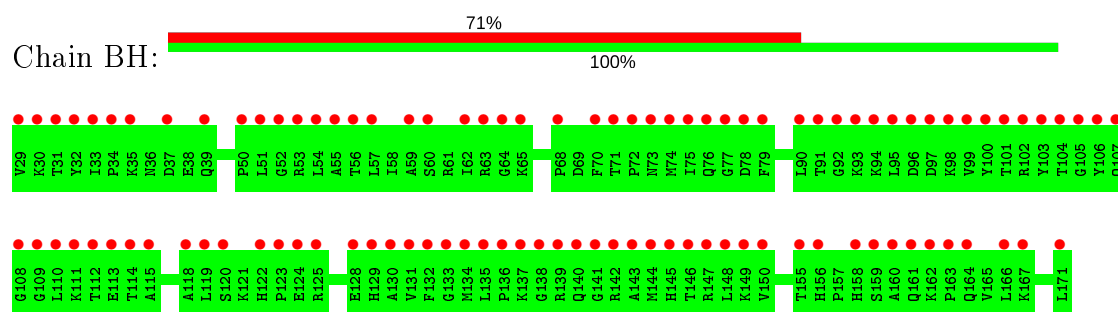
• Molecule 28: 50S ribosomal protein L9



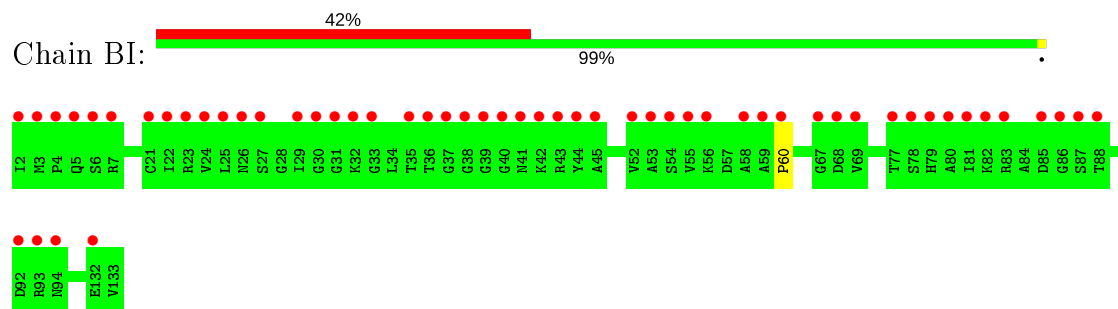
• Molecule 29: 50S ribosomal protein L11



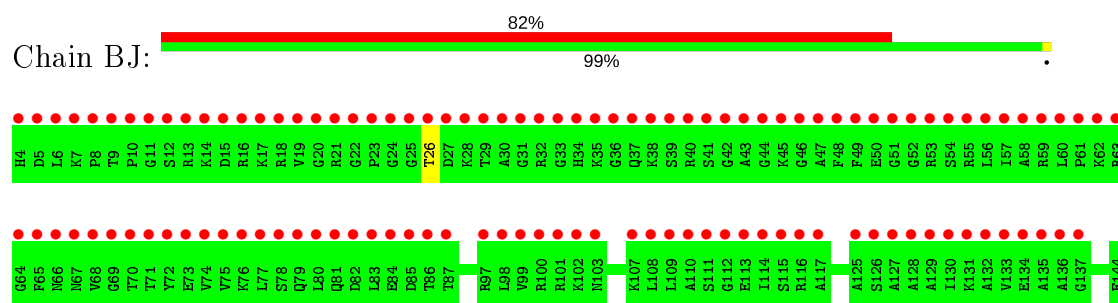
• Molecule 30: 50S ribosomal protein L13



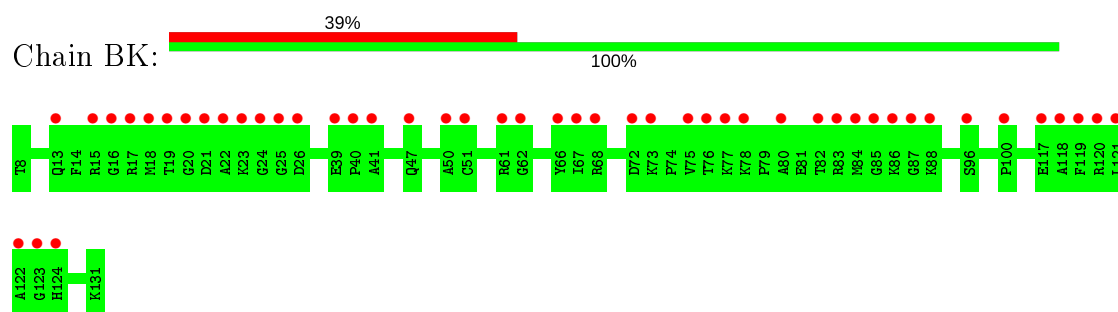
- Molecule 31: 50S ribosomal protein L14



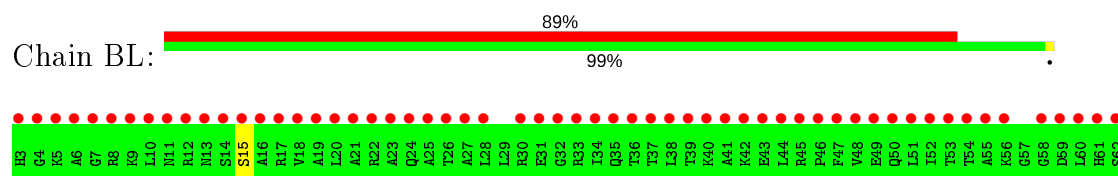
- Molecule 32: 50S ribosomal protein L15

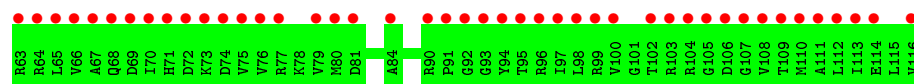


- Molecule 33: 50S ribosomal protein L16

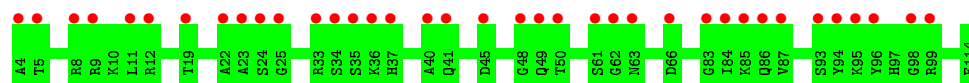


- Molecule 34: 50S ribosomal protein L17

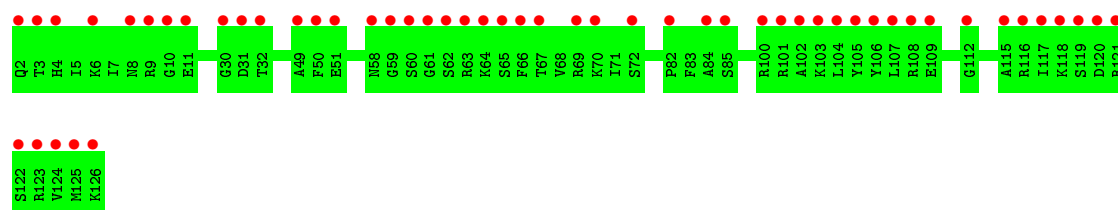
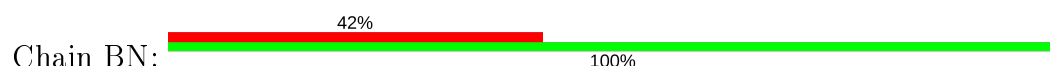




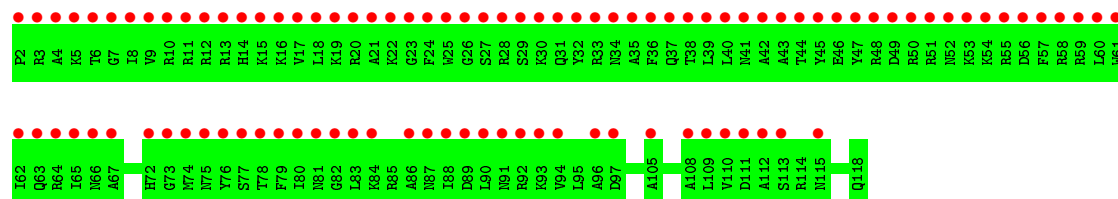
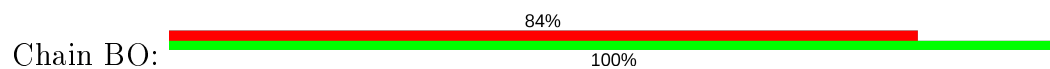
- Molecule 35: 50S ribosomal protein L18



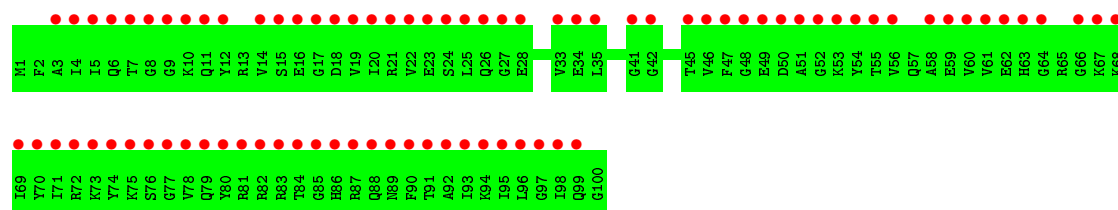
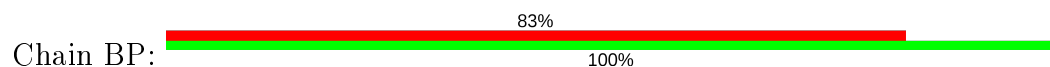
- Molecule 36: 50S ribosomal protein L19



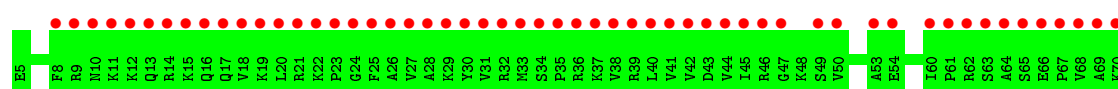
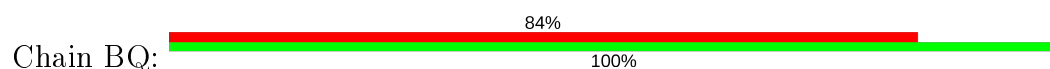
- Molecule 37: 50S ribosomal protein L20

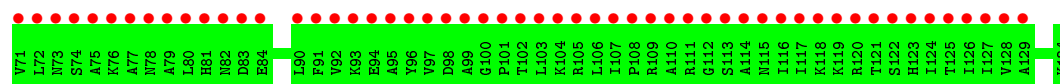


- Molecule 38: 50S ribosomal protein L21

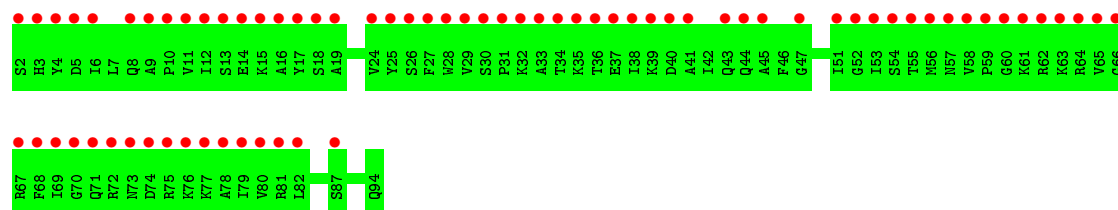
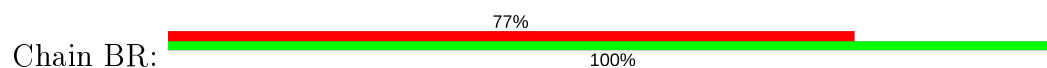


- Molecule 39: 50S ribosomal protein L22

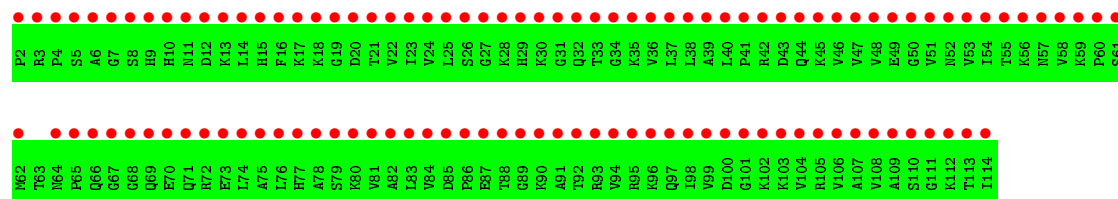




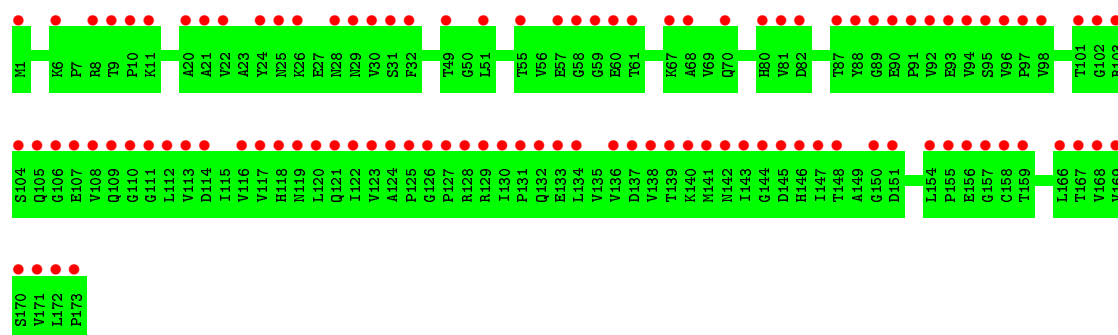
- Molecule 40: 50S ribosomal protein L23



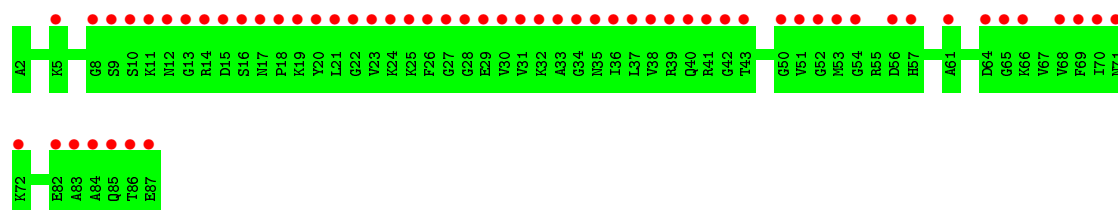
- Molecule 41: 50S ribosomal protein L24



- Molecule 42: general stress protein Ctc



- Molecule 43: 50S ribosomal protein L27




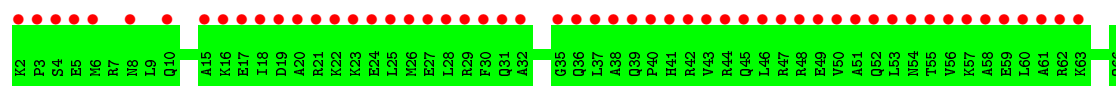
- Molecule 44: 50S RIBOSOMAL PROTEIN L28

Chain BV:  100%


There are no outlier residues recorded for this chain.

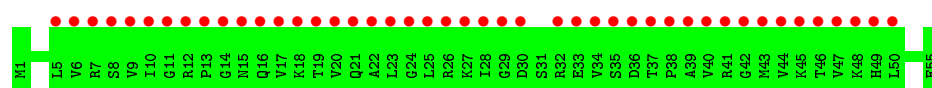
- Molecule 45: 50S ribosomal protein L29

Chain BW:  83%
100%



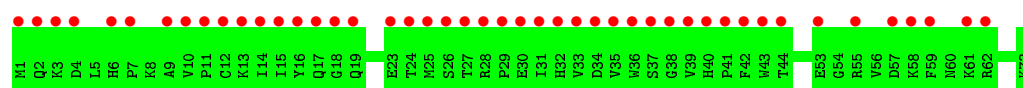
- Molecule 46: 50S ribosomal protein L30

Chain BX:  82%
100%




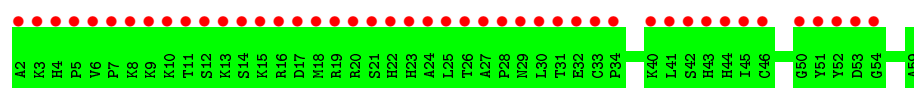
- Molecule 47: 50S ribosomal protein L31

Chain BY:  63%
100%



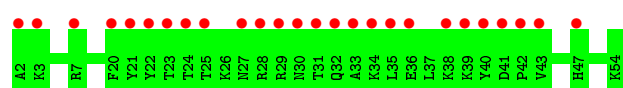
- Molecule 48: 50S ribosomal protein L32

Chain BZ:  78%
100%



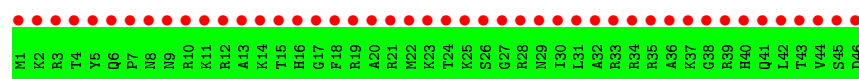
- Molecule 49: 50S ribosomal protein L33

Chain B1:  49%
100%

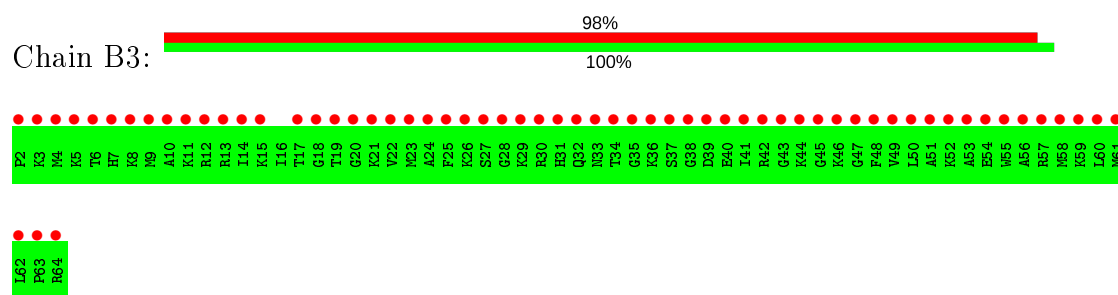


- Molecule 50: 50S ribosomal protein L34

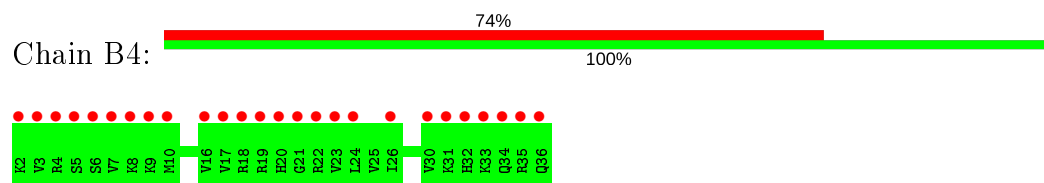
Chain B2:  100%
100%



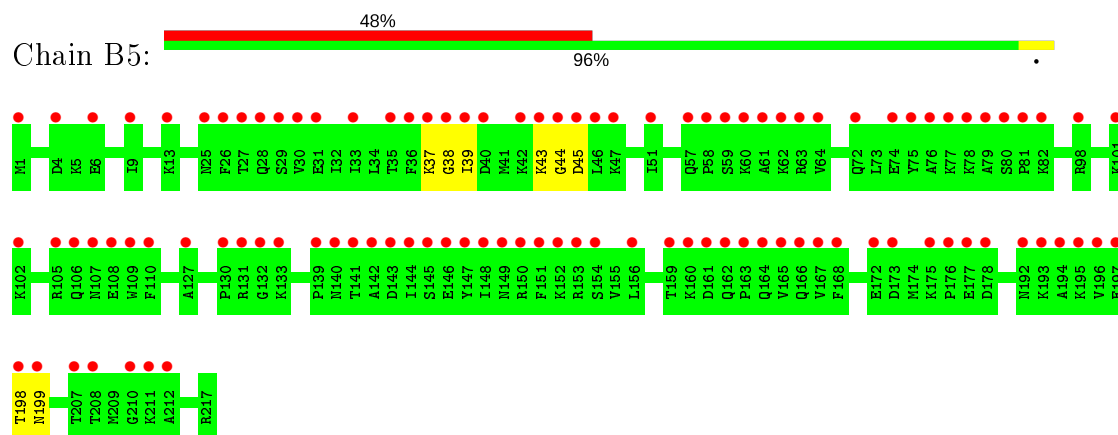
- Molecule 51: 50S ribosomal protein L35



- Molecule 52: 50S ribosomal protein L36



- Molecule 53: 50S ribosomal protein L1P



4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	683.89Å 683.89Å 386.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	70.00 – 9.50 241.79 – 9.50	Depositor EDS
% Data completeness (in resolution range)	92.1 (70.00-9.50) 87.2 (241.79-9.50)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	9.49 (at 9.99Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.389 , 0.407 0.369 , 0.385	Depositor DCC
R_{free} test set	1282 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å ²)	437.2	Xtriage
Anisotropy	0.460	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	1.31 , -10.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	118711	wwPDB-VP
Average B, all atoms (Å ²)	680.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.90% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	AA	1.68	75/36823 (0.2%)	1.26	270/57351 (0.5%)
2	AB	0.37	0/1935	0.68	1/2609 (0.0%)
3	AC	0.38	0/1636	0.66	0/2205
4	AD	0.37	0/1732	0.63	0/2318
5	AE	0.49	0/1162	0.79	0/1564
6	AF	0.33	0/855	0.62	0/1154
7	AG	0.34	0/1275	0.62	0/1709
8	AH	0.44	0/1135	0.74	0/1527
9	AI	0.36	0/1028	0.62	0/1378
10	AJ	0.36	0/807	0.71	0/1085
11	AK	0.39	0/899	0.70	0/1213
12	AL	0.43	0/985	0.73	0/1317
13	AM	0.36	0/1006	0.67	0/1344
14	AN	0.40	0/500	0.78	0/664
15	AO	0.36	0/744	0.63	1/992 (0.1%)
16	AP	0.43	0/716	0.76	0/963
17	AQ	0.44	0/869	0.75	0/1159
18	AR	0.36	0/602	0.63	0/799
19	AS	0.35	0/661	0.72	1/890 (0.1%)
20	AT	0.39	0/764	0.73	0/1006
21	B0	0.50	17/67885 (0.0%)	0.75	48/105852 (0.0%)
22	B9	0.68	1/2815 (0.0%)	0.76	3/4384 (0.1%)
All	All	0.99	93/126834 (0.1%)	0.93	324/193483 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AA	2	40
21	B0	0	5
All	All	2	45

The worst 5 of 93 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	59	A	O3'-P	-120.85	0.16	1.61
1	AA	1398	A	O3'-P	-86.38	0.57	1.61
1	AA	214	U	O3'-P	-73.42	0.73	1.61
1	AA	394	G	O3'-P	-71.42	0.75	1.61
1	AA	1505	G	O3'-P	-71.04	0.76	1.61

The worst 5 of 324 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	59	A	P-O3'-C3'	-58.31	49.73	119.70
21	B0	1856	U	O3'-P-O5'	-48.57	11.72	104.00
21	B0	3098	U	P-O3'-C3'	42.71	170.95	119.70
1	AA	1490	C	P-O3'-C3'	40.44	168.23	119.70
1	AA	651	C	P-O3'-C3'	-39.22	72.64	119.70

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	AA	181	G	C3'
1	AA	1528	U	C3'

5 of 45 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	12	U	Sidechain
1	AA	187	G	Sidechain
1	AA	191	G	Sidechain
1	AA	197	A	Sidechain
1	AA	231	G	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32939	0	16652	3455	1
2	AB	1900	0	1951	209	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	AC	1612	0	1675	286	0
4	AD	1702	0	1767	217	2
5	AE	1146	0	1207	255	0
6	AF	842	0	855	75	2
7	AG	1256	0	1296	138	2
8	AH	1115	0	1177	126	0
9	AI	1010	0	1043	183	0
10	AJ	794	0	839	206	2
11	AK	884	0	904	81	0
12	AL	970	0	1056	151	0
13	AM	996	0	1068	184	0
14	AN	491	0	529	153	0
15	AO	733	0	770	57	0
16	AP	700	0	720	78	0
17	AQ	856	0	925	239	0
18	AR	596	0	668	77	0
19	AS	647	0	673	156	0
20	AT	762	0	853	286	0
21	B0	60636	0	30557	1717	1
22	B9	2519	0	1287	43	0
23	BA	270	0	0	0	0
24	BB	205	0	0	0	0
25	BC	197	0	0	0	0
26	BD	178	0	0	4	0
27	BE	177	0	0	0	0
28	BF	52	0	0	0	0
29	BG	143	0	0	1	0
30	BH	143	0	0	0	0
31	BI	132	0	0	2	0
32	BJ	141	0	0	1	0
33	BK	124	0	0	0	0
34	BL	114	0	0	1	0
35	BM	111	0	0	0	0
36	BN	125	0	0	0	0
37	BO	117	0	0	0	0
38	BP	100	0	0	0	0
39	BQ	130	0	0	0	0
40	BR	93	0	0	0	0
41	BS	113	0	0	0	0
42	BT	173	0	0	0	0
43	BU	86	0	0	0	0
44	BV	16	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	BW	65	0	0	0	0
46	BX	55	0	0	0	0
47	BY	73	0	0	0	0
48	BZ	58	0	0	0	0
49	B1	53	0	0	0	0
50	B2	46	0	0	0	0
51	B3	63	0	0	0	0
52	B4	35	0	0	0	0
53	B5	217	0	0	22	0
All	All	118711	0	68472	6990	5

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 37.

The worst 5 of 6990 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)
1:AA:1278:U:H5''	1:AA:1279:A:P	1.31	1.68
1:AA:1458:G:C8	1:AA:1459:C:H2'	1.27	1.63
1:AA:191:G:C6	1:AA:192:U:C2	1.90	1.60
1:AA:1475:G:H5''	21:B0:1706:A:C4'	1.13	1.60
1:AA:1475:G:C5'	21:B0:1706:A:H4'	1.32	1.59

All (5) 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)
4:AD:172:PRO:O	6:AF:15:ASP:CB[3_555]	1.83	0.37
1:AA:416:G:OP1	21:B0:3140:G:O2'[3_555]	1.99	0.21
7:AG:51:GLN:NE2	10:AJ:87:THR:OG1[4_555]	2.08	0.12
7:AG:57:GLU:OE2	10:AJ:89:ASP:OD1[4_555]	2.14	0.06
4:AD:186:LEU:CD1	6:AF:15:ASP:OD2[3_555]	2.14	0.06

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	232/234 (99%)	174 (75%)	34 (15%)	24 (10%)	0	8
3	AC	204/206 (99%)	135 (66%)	40 (20%)	29 (14%)	0	4
4	AD	206/208 (99%)	166 (81%)	31 (15%)	9 (4%)	2	22
5	AE	148/150 (99%)	130 (88%)	13 (9%)	5 (3%)	3	26
6	AF	99/101 (98%)	79 (80%)	19 (19%)	1 (1%)	15	55
7	AG	153/155 (99%)	127 (83%)	16 (10%)	10 (6%)	1	16
8	AH	136/138 (99%)	125 (92%)	7 (5%)	4 (3%)	4	29
9	AI	125/127 (98%)	88 (70%)	27 (22%)	10 (8%)	1	12
10	AJ	96/98 (98%)	59 (62%)	20 (21%)	17 (18%)	0	3
11	AK	117/119 (98%)	88 (75%)	20 (17%)	9 (8%)	1	13
12	AL	120/124 (97%)	96 (80%)	15 (12%)	9 (8%)	1	13
13	AM	121/125 (97%)	87 (72%)	26 (22%)	8 (7%)	1	16
14	AN	58/60 (97%)	40 (69%)	11 (19%)	7 (12%)	0	6
15	AO	86/88 (98%)	70 (81%)	11 (13%)	5 (6%)	1	18
16	AP	81/83 (98%)	65 (80%)	15 (18%)	1 (1%)	13	50
17	AQ	102/104 (98%)	84 (82%)	10 (10%)	8 (8%)	1	13
18	AR	71/73 (97%)	62 (87%)	7 (10%)	2 (3%)	5	30
19	AS	78/80 (98%)	48 (62%)	19 (24%)	11 (14%)	0	4
20	AT	97/99 (98%)	65 (67%)	20 (21%)	12 (12%)	0	5
All	All	2330/2372 (98%)	1788 (77%)	361 (16%)	181 (8%)	1	13

5 of 181 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	8	LYS
2	AB	9	GLU
2	AB	15	VAL
2	AB	16	HIS
2	AB	17	PHE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	202/202 (100%)	180 (89%)	22 (11%)	6	23
3	AC	160/160 (100%)	142 (89%)	18 (11%)	6	21
4	AD	180/180 (100%)	172 (96%)	8 (4%)	28	53
5	AE	115/115 (100%)	100 (87%)	15 (13%)	4	18
6	AF	90/90 (100%)	88 (98%)	2 (2%)	52	71
7	AG	126/126 (100%)	122 (97%)	4 (3%)	39	61
8	AH	119/119 (100%)	109 (92%)	10 (8%)	11	33
9	AI	98/98 (100%)	90 (92%)	8 (8%)	11	34
10	AJ	88/88 (100%)	79 (90%)	9 (10%)	7	25
11	AK	90/90 (100%)	84 (93%)	6 (7%)	16	41
12	AL	104/104 (100%)	96 (92%)	8 (8%)	13	37
13	AM	100/100 (100%)	90 (90%)	10 (10%)	7	26
14	AN	49/49 (100%)	47 (96%)	2 (4%)	30	55
15	AO	79/79 (100%)	72 (91%)	7 (9%)	9	30
16	AP	72/72 (100%)	67 (93%)	5 (7%)	15	40
17	AQ	96/96 (100%)	90 (94%)	6 (6%)	18	43
18	AR	64/64 (100%)	61 (95%)	3 (5%)	26	51
19	AS	71/71 (100%)	68 (96%)	3 (4%)	30	54
20	AT	76/76 (100%)	69 (91%)	7 (9%)	9	29
All	All	1979/1979 (100%)	1826 (92%)	153 (8%)	13	37

5 of 153 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	AH	2	LEU
9	AI	111	ARG
18	AR	38	GLU
8	AH	52	ASP

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Mol	Chain	Res	Type
8	AH	105	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 57 such sidechains are listed below:

Mol	Chain	Res	Type
6	AF	64	GLN
9	AI	23	ASN
18	AR	36	ASN
6	AF	94	GLN
7	AG	37	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1487/1537 (96%)	218 (14%)	89 (5%)
21	B0	2802/2887 (97%)	430 (15%)	55 (1%)
22	B9	116/118 (98%)	10 (8%)	0
All	All	4405/4542 (96%)	658 (14%)	144 (3%)

5 of 658 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	6	G
1	AA	8	A
1	AA	9	G
1	AA	31	G
1	AA	32	A

5 of 144 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	AA	1196	U
1	AA	1380	U
21	B0	3171	A
1	AA	1214	C
1	AA	1300	G

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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
1	AA	106
21	B0	31
22	B9	2
12	AL	1
13	AM	1

The worst 5 of 141 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	AA	1443:G	O3'	1445:U	P	9.14
1	AA	1458:G	O3'	1459:C	P	8.01
1	B0	1888:C	O3'	1889:G	P	6.96
1	AA	1459:C	O3'	1460:A	P	6.03
1	B0	3180:U	O3'	3181:C	P	5.42

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	1533/1537 (99%)	34.46	1533 (100%) 0 0	207, 548, 819, 940	0
2	AB	234/234 (100%)	1.45	72 (30%) 0 2	754, 754, 754, 754	0
3	AC	206/206 (100%)	5.43	168 (81%) 0 0	378, 378, 378, 378	0
4	AD	208/208 (100%)	14.38	201 (96%) 0 0	709, 709, 709, 709	0
5	AE	150/150 (100%)	14.31	150 (100%) 0 0	756, 756, 756, 756	0
6	AF	101/101 (100%)	1.29	22 (21%) 0 3	748, 748, 748, 748	0
7	AG	155/155 (100%)	4.22	105 (67%) 0 0	374, 374, 374, 374	0
8	AH	138/138 (100%)	7.10	129 (93%) 0 0	856, 856, 856, 856	0
9	AI	127/127 (100%)	7.06	77 (60%) 0 0	439, 439, 439, 439	0
10	AJ	98/98 (100%)	7.10	78 (79%) 0 0	430, 430, 430, 430	0
11	AK	119/119 (100%)	3.04	55 (46%) 0 1	652, 652, 652, 652	0
12	AL	124/124 (100%)	10.88	124 (100%) 0 0	423, 541, 541, 541	0
13	AM	125/125 (100%)	5.97	108 (86%) 0 0	378, 572, 572, 572	0
14	AN	60/60 (100%)	10.29	59 (98%) 0 0	378, 378, 378, 378	0
15	AO	88/88 (100%)	11.20	87 (98%) 0 0	740, 740, 740, 740	0
16	AP	83/83 (100%)	19.81	83 (100%) 0 0	781, 781, 781, 781	0
17	AQ	104/104 (100%)	11.89	104 (100%) 0 0	857, 857, 857, 857	0
18	AR	73/73 (100%)	3.48	39 (53%) 0 1	748, 748, 748, 748	0
19	AS	80/80 (100%)	3.00	43 (53%) 0 1	633, 633, 633, 633	0
20	AT	99/99 (100%)	13.05	99 (100%) 0 0	940, 940, 940, 940	0
21	B0	2825/2887 (97%)	55.87	2825 (100%) 0 0	462, 737, 737, 940	0
22	B9	118/118 (100%)	44.84	118 (100%) 0 0	772, 938, 938, 938	0
23	BA	270/270 (100%)	6.09	179 (66%) 0 0	737, 737, 737, 737	0
24	BB	205/205 (100%)	5.86	143 (69%) 0 0	737, 737, 737, 737	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	BC	197/197 (100%)	8.25	186 (94%) 0 0	737, 737, 737, 737	0
26	BD	178/178 (100%)	17.24	138 (77%) 0 0	938, 938, 938, 938	0
27	BE	177/177 (100%)	13.08	163 (92%) 0 0	737, 737, 737, 737	0
28	BF	52/52 (100%)	1.36	12 (23%) 0 2	737, 737, 737, 737	0
29	BG	143/143 (100%)	17.89	138 (96%) 0 0	907, 907, 907, 907	0
30	BH	143/143 (100%)	5.92	102 (71%) 0 0	737, 737, 737, 737	0
31	BI	132/132 (100%)	3.04	55 (41%) 0 1	737, 737, 737, 737	0
32	BJ	141/141 (100%)	10.40	115 (81%) 0 0	737, 737, 737, 737	0
33	BK	124/124 (100%)	2.41	48 (38%) 0 1	737, 737, 737, 737	0
34	BL	114/114 (100%)	6.99	102 (89%) 0 0	737, 737, 737, 737	0
35	BM	111/111 (100%)	1.78	37 (33%) 0 2	938, 938, 938, 938	0
36	BN	125/125 (100%)	2.62	53 (42%) 0 1	737, 737, 737, 737	0
37	BO	117/117 (100%)	12.38	98 (83%) 0 0	737, 737, 737, 737	0
38	BP	100/100 (100%)	5.91	83 (83%) 0 0	737, 737, 737, 737	0
39	BQ	130/130 (100%)	7.52	109 (83%) 0 0	737, 737, 737, 737	0
40	BR	93/93 (100%)	4.86	72 (77%) 0 0	737, 737, 737, 737	0
41	BS	113/113 (100%)	11.17	112 (99%) 0 0	737, 737, 737, 737	0
42	BT	173/173 (100%)	8.24	105 (60%) 0 0	737, 772, 772, 772	0
43	BU	86/86 (100%)	6.53	59 (68%) 0 0	737, 737, 737, 737	0
44	BV	0/16	-	-	-	-
45	BW	65/65 (100%)	5.83	54 (83%) 0 0	737, 737, 737, 737	0
46	BX	55/55 (100%)	7.60	45 (81%) 0 0	737, 737, 737, 737	0
47	BY	73/73 (100%)	4.25	46 (63%) 0 0	737, 737, 737, 737	0
48	BZ	58/58 (100%)	11.78	45 (77%) 0 0	737, 737, 737, 737	0
49	B1	53/53 (100%)	5.78	26 (49%) 0 1	737, 737, 737, 737	0
50	B2	46/46 (100%)	9.41	46 (100%) 0 0	737, 737, 737, 737	0
51	B3	63/63 (100%)	7.36	62 (98%) 0 0	737, 737, 737, 737	0
52	B4	35/35 (100%)	6.72	26 (74%) 0 0	737, 737, 737, 737	0
53	B5	213/217 (98%)	4.43	104 (48%) 0 1	940, 940, 940, 940	0
All	All	10433/10519 (99%)	25.15	8842 (84%) 0 0	207, 737, 938, 940	0

The worst 5 of 8842 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
21	B0	1989	C	280.5
21	B0	2624	G	227.9
21	B0	1988	A	201.4
21	B0	2480	C	196.7
21	B0	2425	G	192.2

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

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

6.3 Carbohydrates [i](#)

There are no 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.