



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 09:20 PM GMT

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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (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

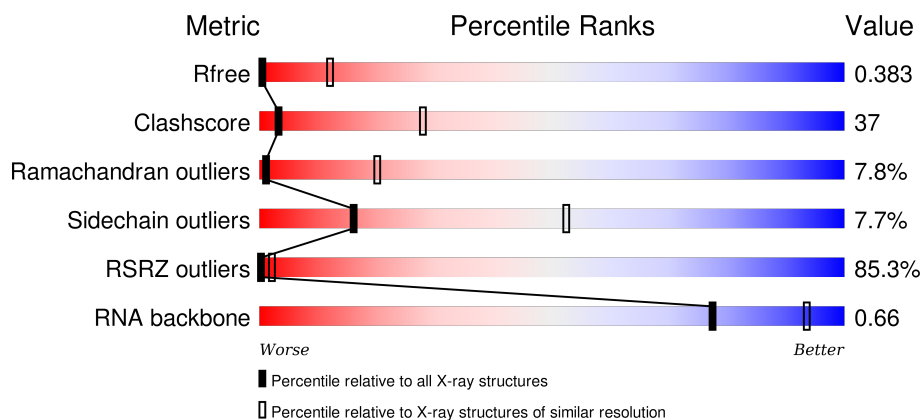
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	91344	1015 (11.50-3.66)
Clashscore	102246	1065 (15.00-3.70)
Ramachandran outliers	100387	1036 (11.50-3.66)
Sidechain outliers	100360	1006 (11.50-3.66)
RSRZ outliers	91569	1014 (11.50-3.66)
RNA backbone	2183	1106 (11.50-2.80)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AA	1537	<div> <div>100%</div> <div> <div>23%</div> <div>58%</div> <div>15%</div> <div>.</div> </div> </div>
2	AB	234	<div> <div>33%</div> <div>29%</div> <div>56%</div> <div>13%</div> <div>.</div> </div>
3	AC	206	<div> <div>82%</div> <div>30%</div> <div>51%</div> <div>17%</div> <div>.</div> </div>
4	AD	208	<div> <div>97%</div> <div>39%</div> <div>55%</div> <div>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	73% 100%
31	BI	132	43% 99%
32	BJ	141	82% 99%
33	BK	124	40% 100%
34	BL	114	92% 99%
35	BM	111	35% 100%
36	BN	125	44% 100%
37	BO	117	85% 100%
38	BP	100	87% 100%
39	BQ	130	85% 100%
40	BR	93	82% 100%
41	BS	113	99% 100%
42	BT	173	61% 100%
43	BU	86	71% 100%
44	BV	16	100%
45	BW	65	83% 100%
46	BX	55	82% 100%
47	BY	73	64% 100%
48	BZ	58	79% 100%
49	B1	53	51% 100%
50	B2	46	100%
51	B3	63	98% 100%
52	B4	35	77% 100%
53	B5	217	49% 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

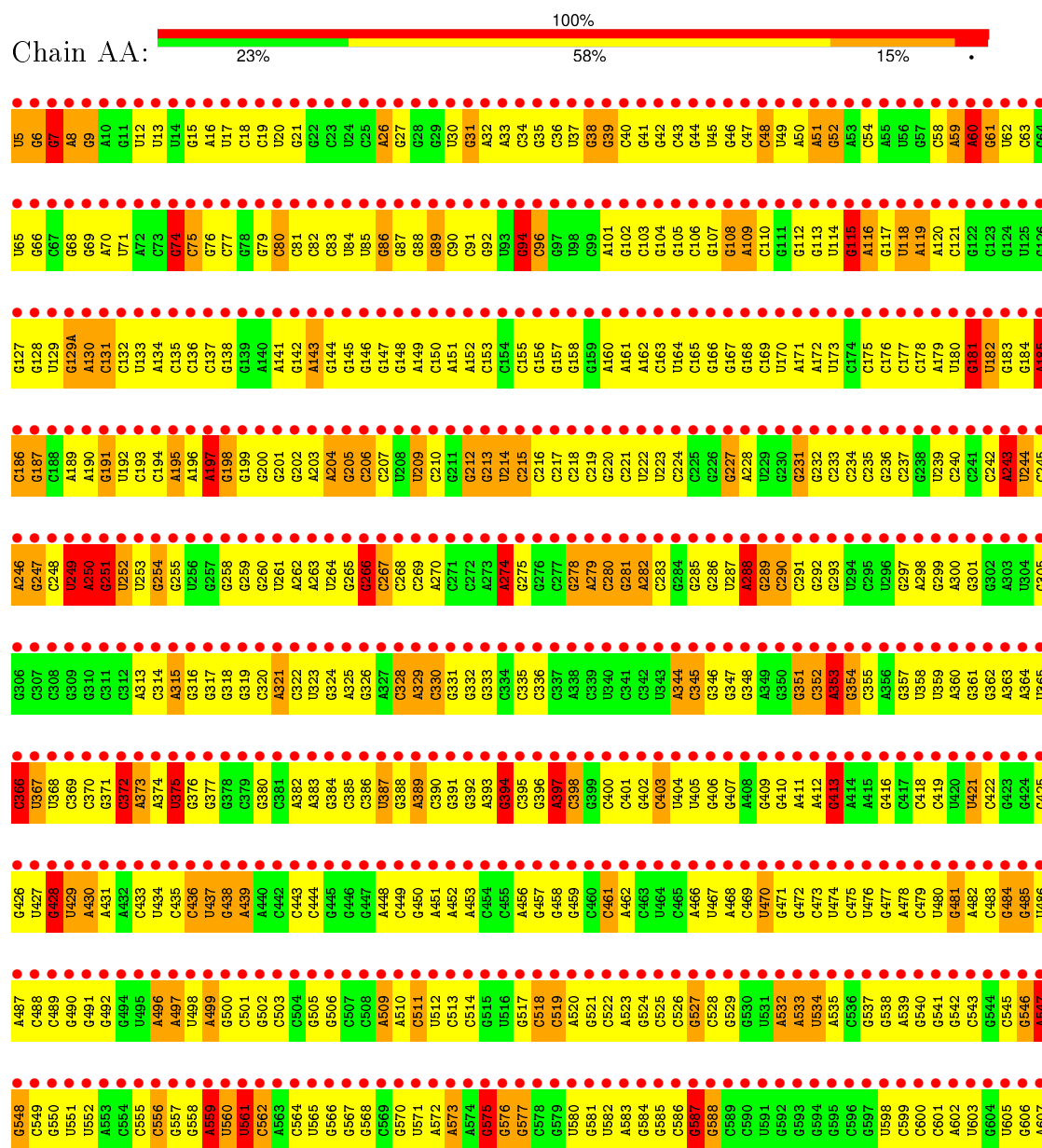
- Molecule 53 is a protein called 50S ribosomal protein L1P.

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

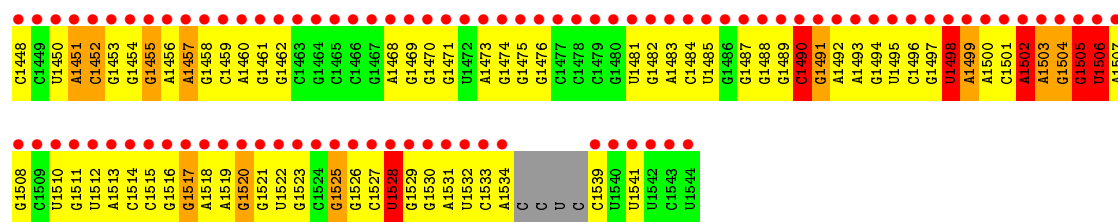
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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 ( $RSRZ > 2$ ). 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.

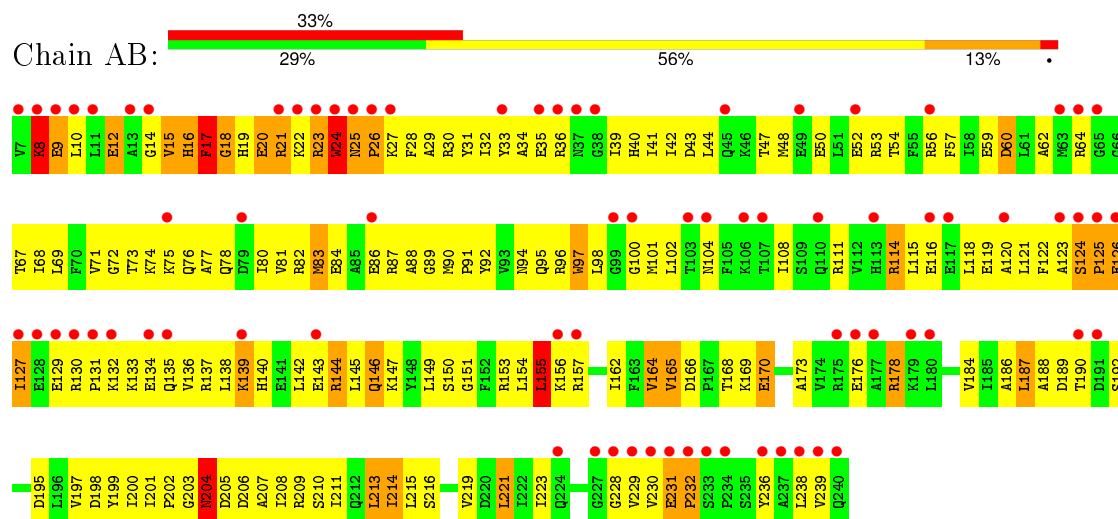
#### • Molecule 1: 16S RIBOSOMAL RNA



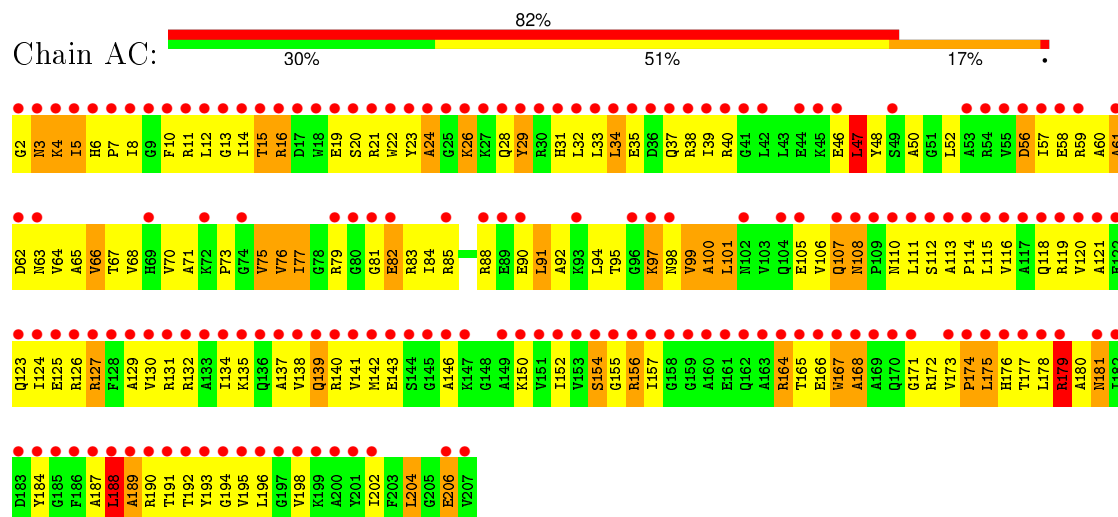
G1387	C1328	A1268	C1208	C1147	G1087	C1027	A968	A908	G948	U788	C728	G668	A608
C1388	A1329	A1269	C1209	U1148	G1088	C1028	A969	A909	C949	U789	A729	U669	A609
C1389	A1330	C1270	C1210	C1149	G1089	U1029	C970	C910	C950	A790	G729	G670	G610
G1390	A1331	G1271	U1211	U1150	U1030	U1030	G971	U911	G951	G791	C731	G671	A611
A1391	A1332	G1272	U1212	A1151	C1031	C1031	C972	C912	G952	U792	G732	U672	C612
C1392	A1333	G1273	A1213	A1152	A1092	G1032	G973	A913	G953	U793	A733	G673	C613
U1393	G1334	G1274	C1214	C1153	A1093	G1033	A974	A914	G954	A794	G734	G674	A614
A1394	C1335	A1275	G1215	G1154	G1094	G1034	A975	A915	G955	C795	G735	A675	C615
C1395	G1336	G1276	G1216	G1155	U1095	A1035	G976	G916	C956	G796	C736	A676	G616
A1396	G1337	G1277	C1217	G1156	U1096	G1036	A977	G917	C957	G797	A737	U677	G617
C1397	A1338	U1278	C1218	A1157	C1097	G1037	A978	A918	G958	G798	C738	U678	C618
U1398	G1339	A1279	U1219	C1158	C1098	C1038	C979	A919	A859	G799	C739	C679	U619
C1399	A1340	A1280	G1220	U1159	G1099	C1039	C980	U920	A860	G800	U740	C680	C620
G1400	U1341	U1281	G1221	G1160	A1100	U1040	U981	U921	G861	U801	G741	C681	A621
G1401	C1342	C1282	G1222	C1161	C1101	A1041	U982	G922	C962	A802	G742	C682	A622
C1402	G1343	G1283	C1223	C1162	A1102	G1042	A983	A923	U963	G803	U743	C683	C623
C1403	C1344	C1284	G1224	C1163	C1103	C1043	C984	C924	A864	U804	C744	A684	C624
C1404	U1345	A1285	A1225	G1164	G1104	A1044	C985	G925	A865	C805	G745	G685	G625
G1405	A1346	A1286	C1226	C1165	A1105	C1045	A986	G926	C966	C806	G746	U686	U626
U1406	G1347	A1287	A1227	G1166	C1106	A1046	G987	G927	G867	A807	C747	A687	G627
C1407	U1348	A1288	C1228	A1167	C1107	G1047	G988	G928	C968	C808	C748	G688	G628
A1408	A1349	A1289	A1229	A1168	G1108	G1048	C989	G929	G869	G809	C749	C689	G629
C1409	A1350	G1290	C1230	A1169	C1109	U1049	C990	C930	U870	C810	U750	G690	G630
G1410	U1351	G1291	G1231	G1171	A1110	G1050	U991	C931	U871	C811	U751	G691	G631
C1411	C1352	U1292	U1232	C1172	A1111	C1051	U992	C932	A872	C812	G752	U692	A632
G1412	G1353	G1293	G1233	G1173	C1112	U1052	G993	G933	A873	U813	A753	G693	G633
A1413	C1354	G1294	C1234	G1174	C1113	G1053	A994	C934	G874	A814	C754	A694	C634
G1414	G1355	G1295	U1235	G1175	C1114	C1054	C995	A935	C975	A815	G755	A695	G635
U1415	C1356	C1296	A1236	A1176	C1115	A1055	A996	C936	G876	A816	C756	G696	U636
A1357	G1357	C1297	C1237	G1177	C1116	U1056	U997	A937	C877	C817	U757	U697	G637
G1417	U1358	C1298	A1238	G1178	G1117	G1057	G998	A938	G878	G818	C758	G698	G638
C1418	C1359	A1299	A1239	A1179	C1118	G1058	C999	G939	C879	A819	A759	C699	G639
G1419	A1360	G1300	U1240	C1180	C1119	C1059	U1000	C940	C880	U820	G760	G700	A640
U1420	G1361	U1301	G1241	G1181	G1120	C1060	A1001	G941	G881	G821	G761	C701	U641
C1421	C2361	U1302	C1242	G1182	U1121	G1061	G1002	G942	C982	C822	C762	A702	A642
G1422	C1362	C1303	G1243	A1183	U1122	U1062	G1003	U943	C983	G823	G763	G703	C643
G1423	A1363	G1304	C1244	G1184	A1123	C1063	G2003	G944	U884	C824	C764	A704	G644
C1424	U1364	A1305	C1245	G1185	G1124	G1064	A1004	G945	G885	C825	G765	U705	C645
U1425	G1365	C1306	A1246	G1186	U1125	U1065	A1005	A946	G886	C826	A766	A706	U646
C1426	G1366	U1307	U1247	G1187	U1126	C1066	C1006	G947	G887	U827	A767	C707	C647
U1427	C1367	U1308	A1248	A1188	G1127	A1067	C1007	C948	G888	A828	C768	G708	A648
A1428	G1368	G1309	C1249	C1189	C1128	G1068	C1008	A949	A889	G829	C769	G709	G649
C1429	C1369	G1310	A1250	G1190	C1129	C1069	G1009	U950	G890	G830	U770	G710	G650
G1430	U1370	C1311	C1251	A1191	A1130	U1070	G1010	U951	U891	U831	G771	G711	C651
C1431	G1371	G1312	A1252	C1192	G1131	C1071	G1011	U952	A892	C832	U772	A712	U652
G1432	C1372	U1313	G1253	G1193	C1132	G1072	U1012	G953	C993	U833	G773	G713	A653
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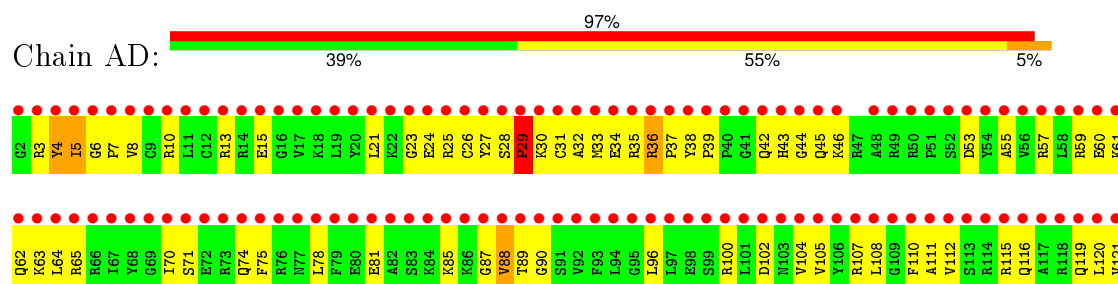
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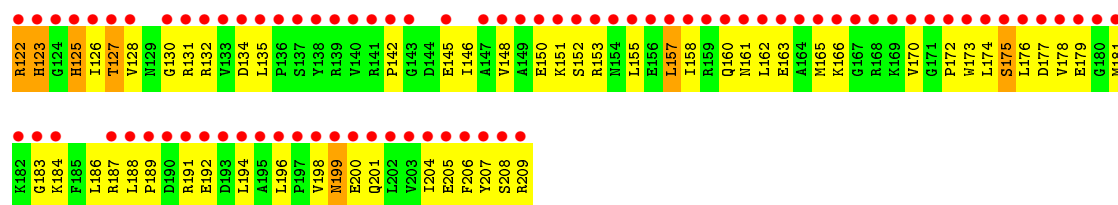


• Molecule 3: 30S ribosomal protein S3

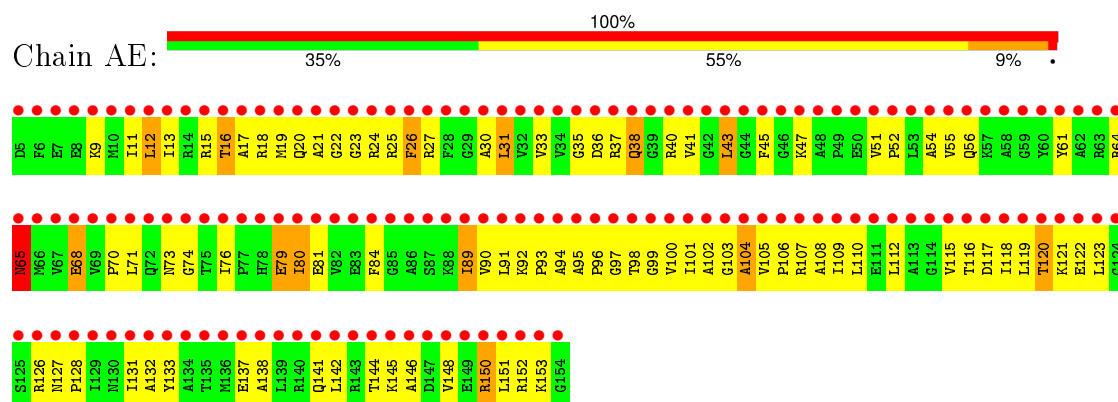


• Molecule 4: 30S ribosomal protein S4

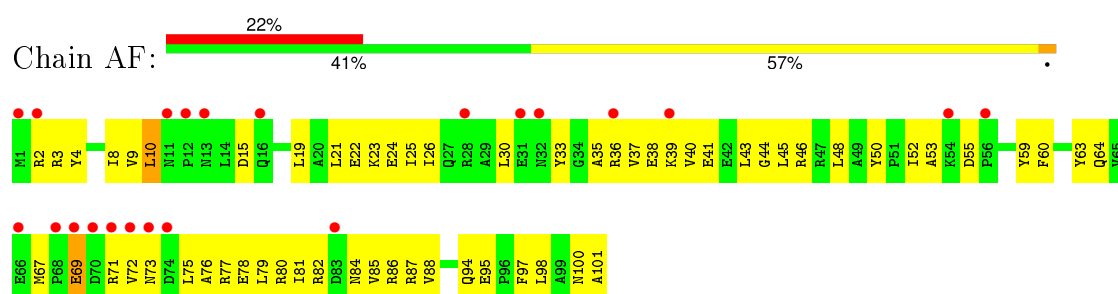




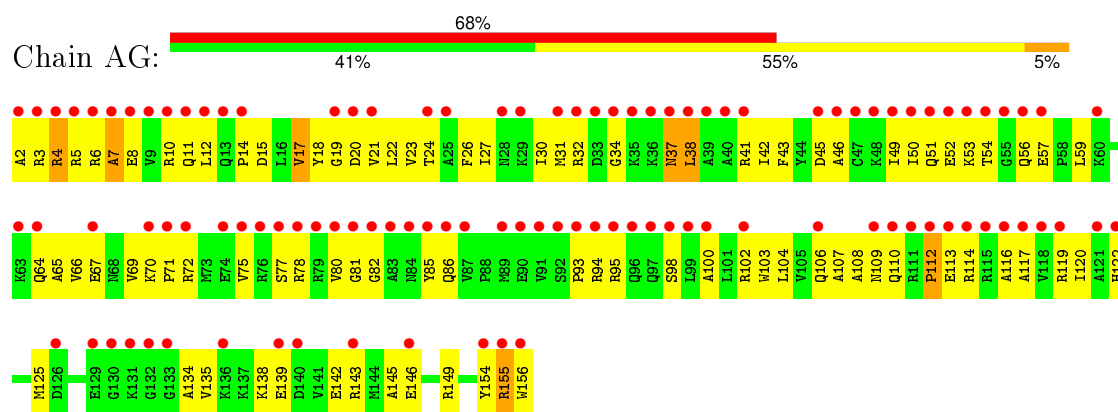
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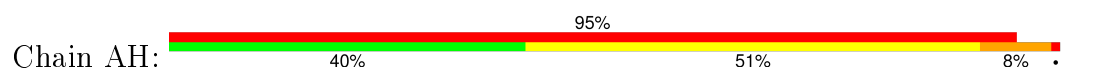
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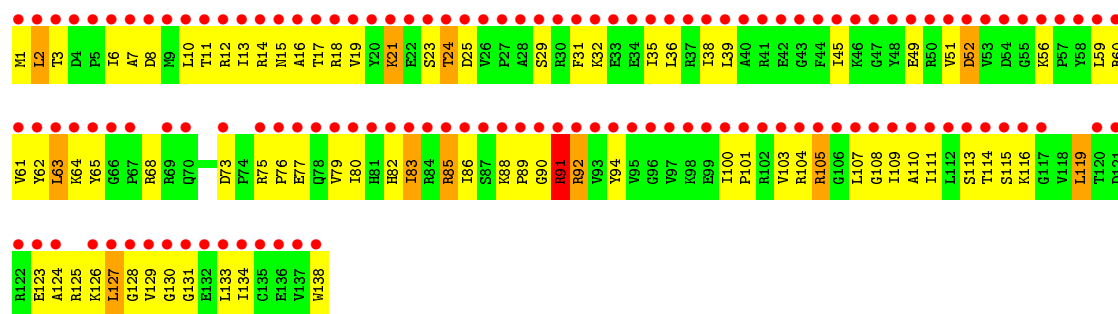
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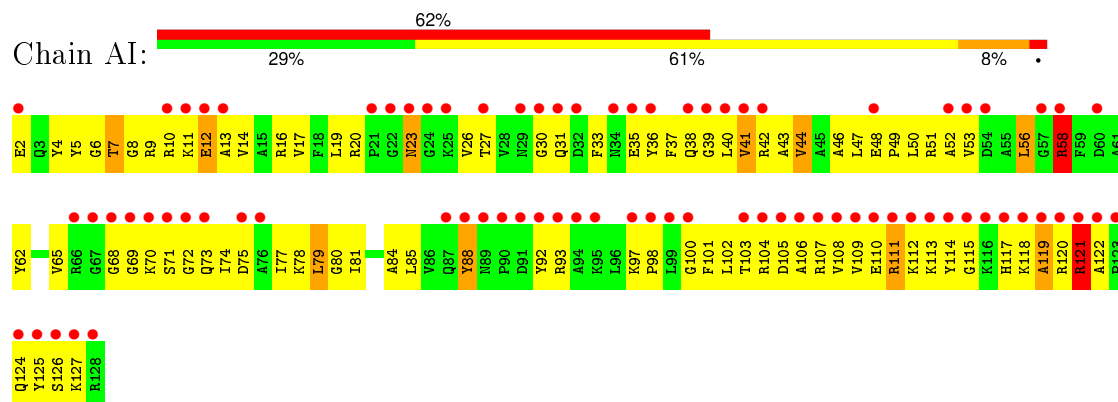
• Molecule 8: 30S ribosomal protein S8



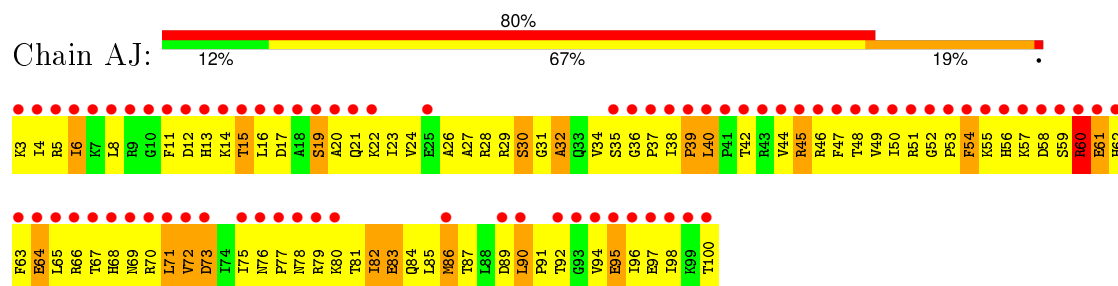




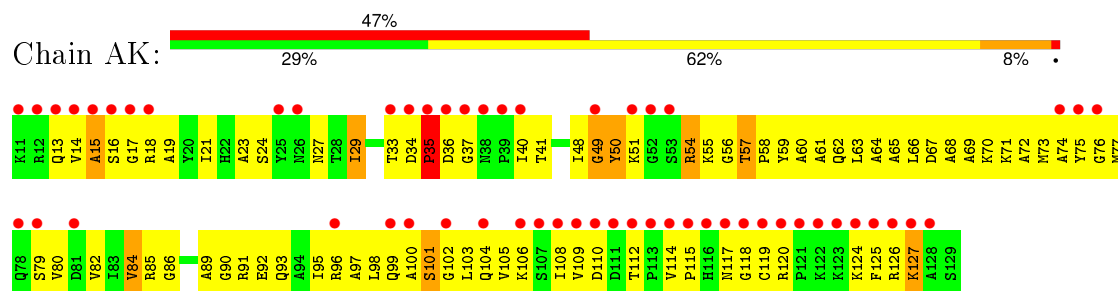
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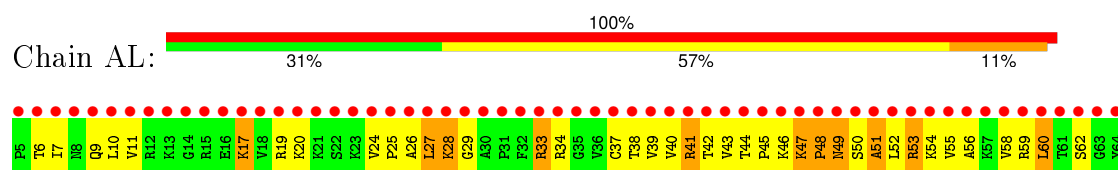
• Molecule 10: 30S ribosomal protein S10

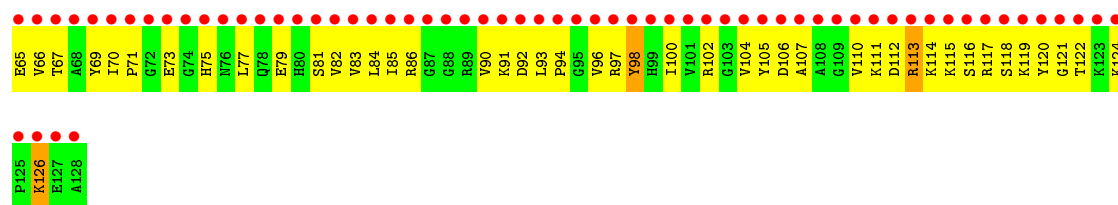


• Molecule 11: 30S ribosomal protein S11

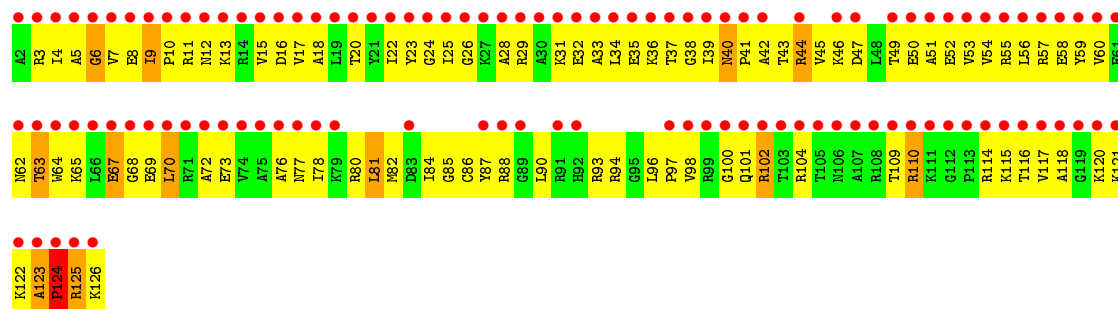


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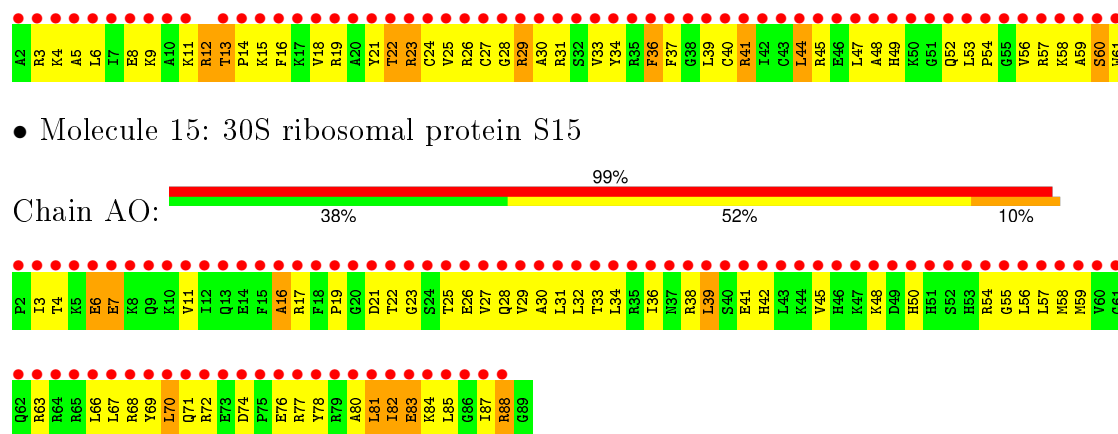




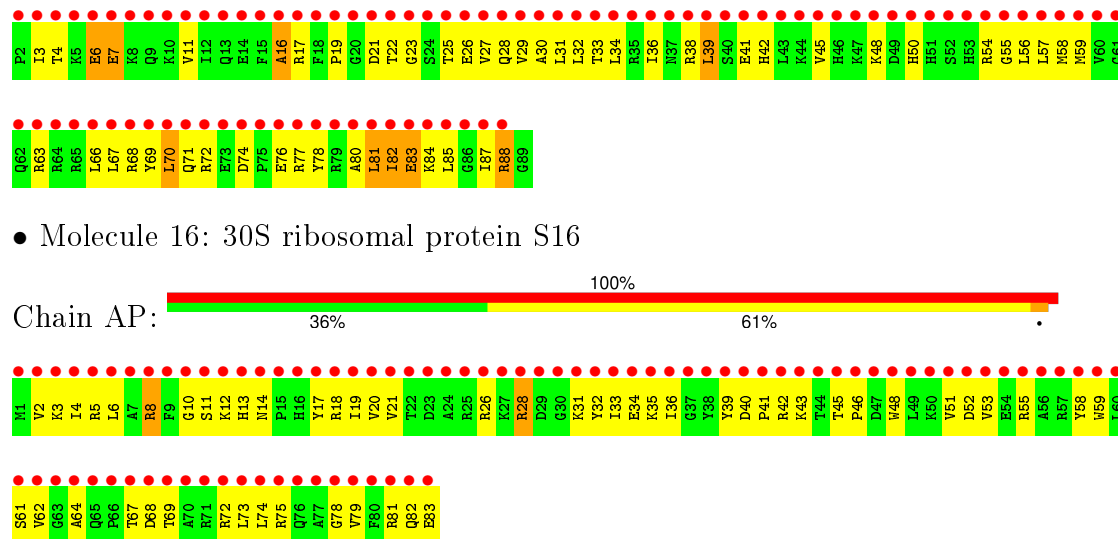
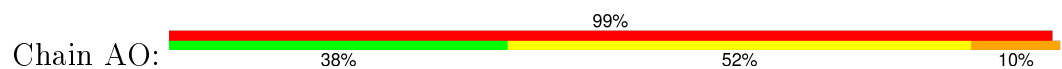
• Molecule 13: 30S ribosomal protein S13



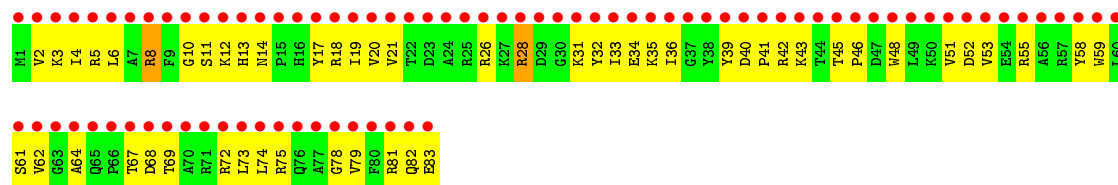
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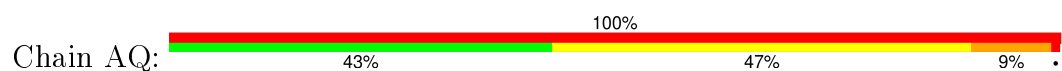
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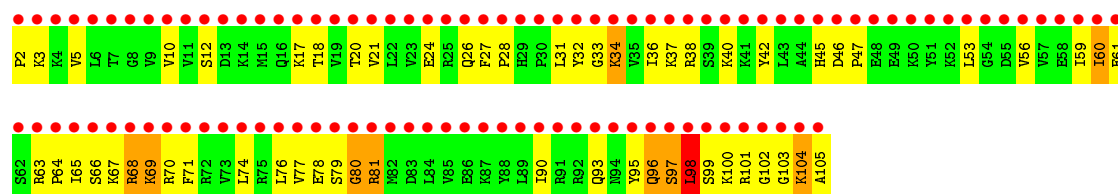


• Molecule 16: 30S ribosomal protein S16



• Molecule 17: 30S ribosomal protein S17





• Molecule 18: 30S ribosomal protein S18



• Molecule 19: 30S ribosomal protein S19



• Molecule 20: 30S ribosomal protein S20



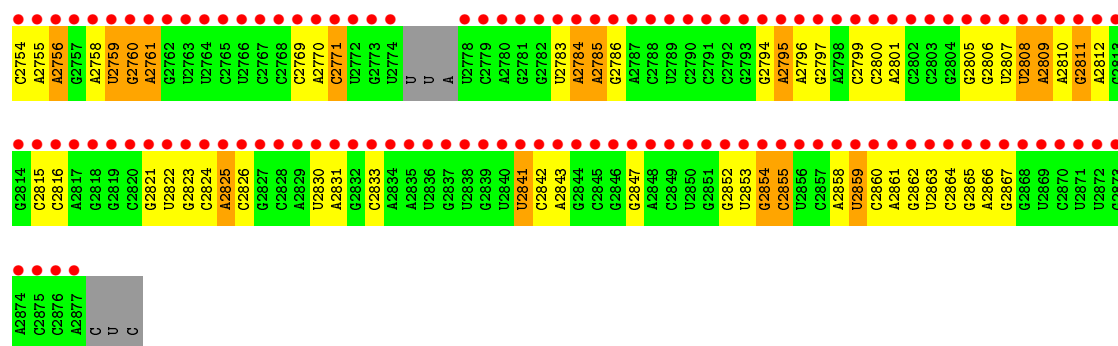
• Molecule 21: 23S RIBOSOMAL RNA



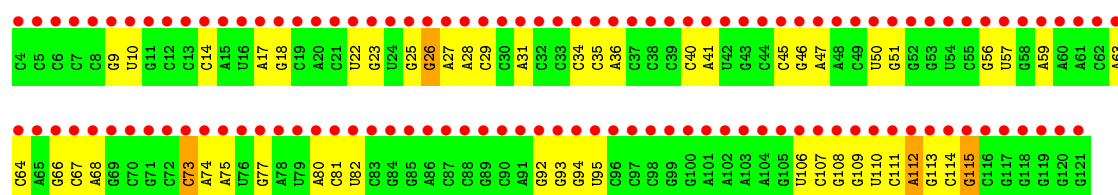
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G1024	A964	G903	G844	U784	C724	C664	U604	U544	G484	G424	G364	A304	G244	G184
A1025	U965	U904	U845	U785	G725	G665	G605	A545	G485	C425	U365	A305	C245	G185
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C1027	G967	U906	C847	G787	G727	U667	G607	U547	C487	C427	G367	C307	A247	U187
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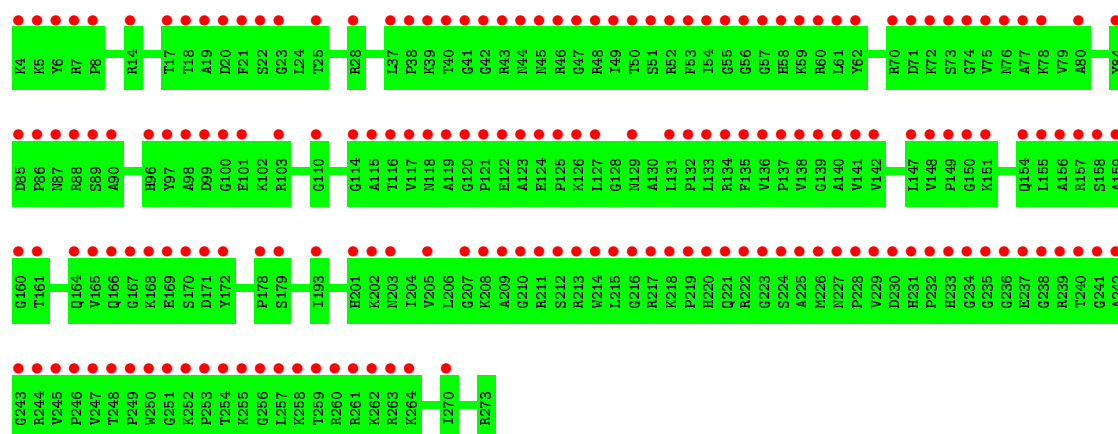
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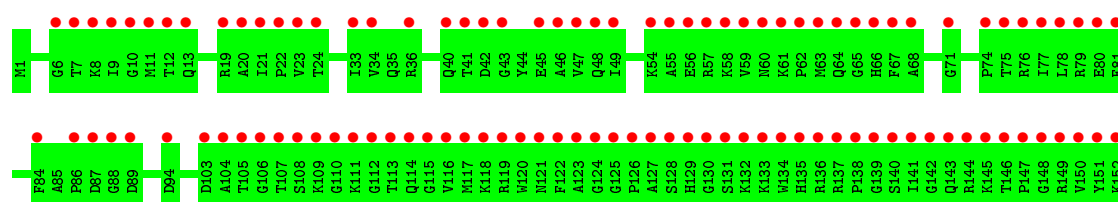
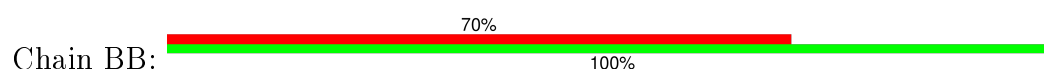
• Molecule 22: 5S RIBOSOMAL RNA

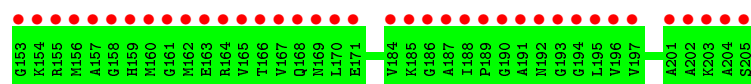


• Molecule 23: 50S ribosomal protein L2

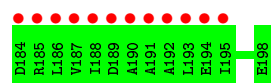
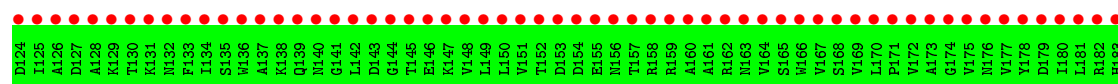
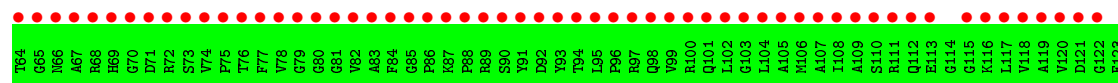
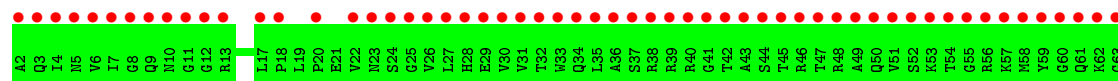


• Molecule 24: 50S ribosomal protein L3

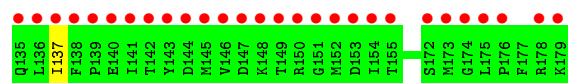
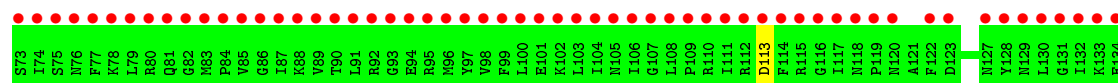
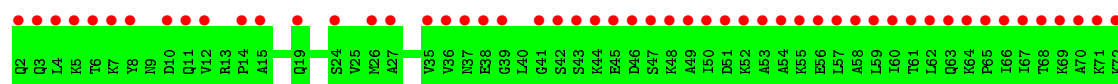
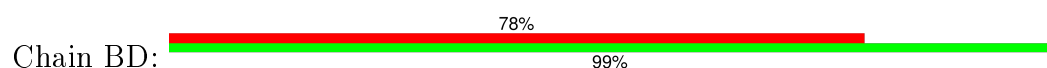




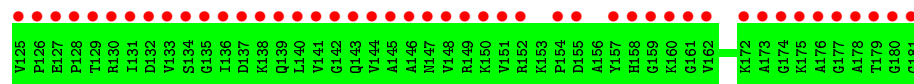
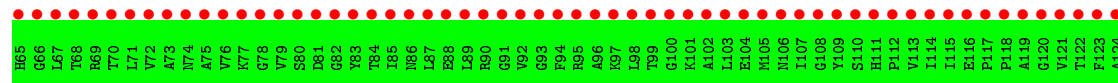
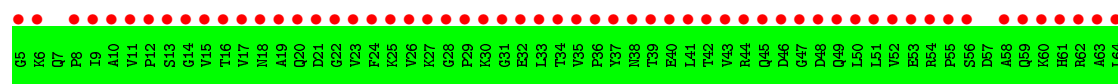
• Molecule 25: 50S ribosomal protein L4



• Molecule 26: 50S ribosomal protein L5

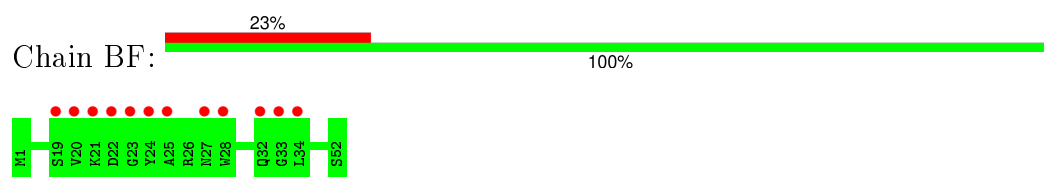


• Molecule 27: 50S ribosomal protein L6

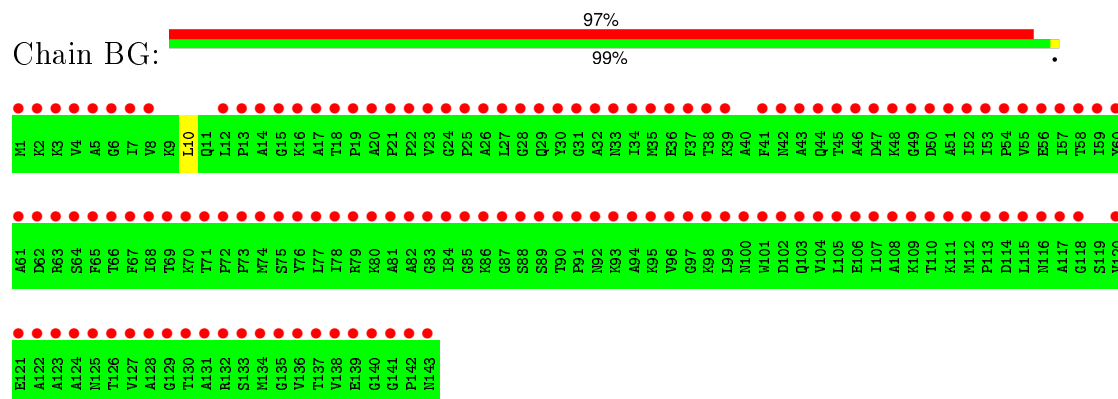


• Molecule 28: 50S ribosomal protein L9

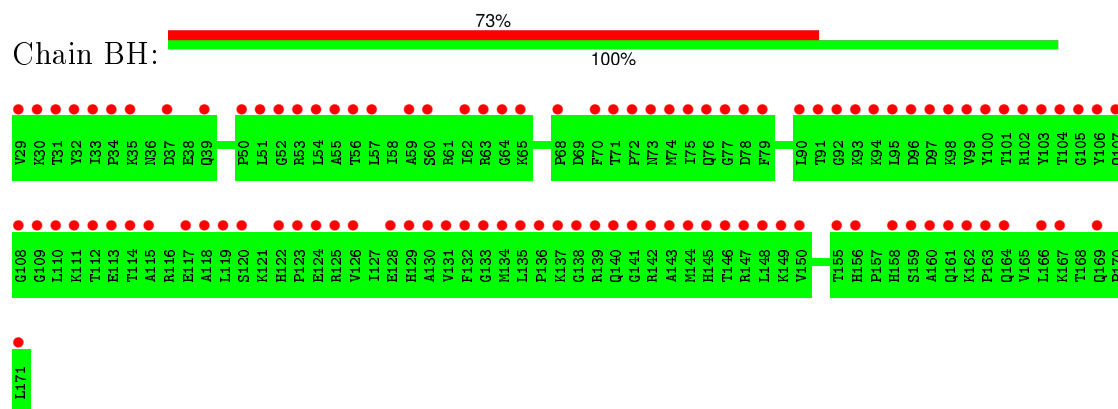




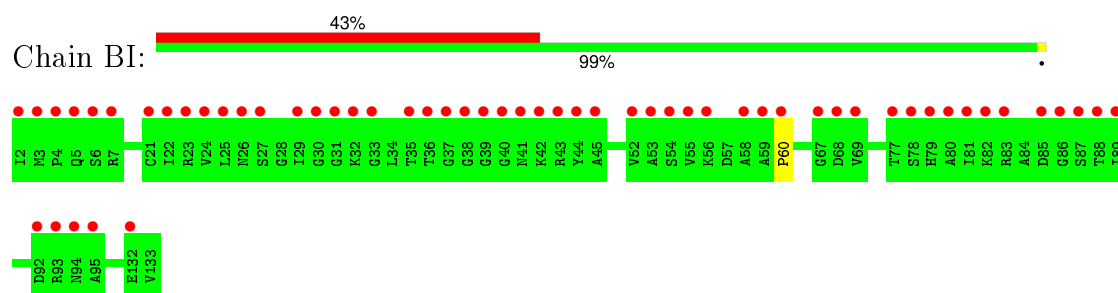
- Molecule 29: 50S ribosomal protein L11



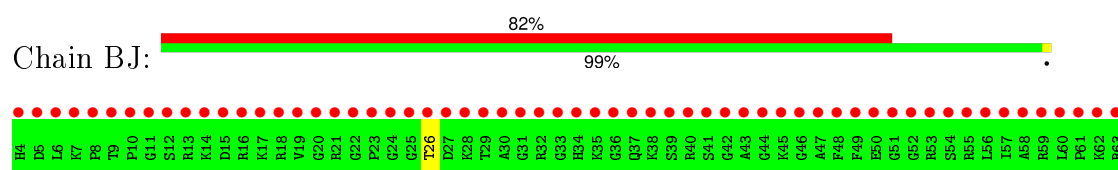
- Molecule 30: 50S ribosomal protein L13

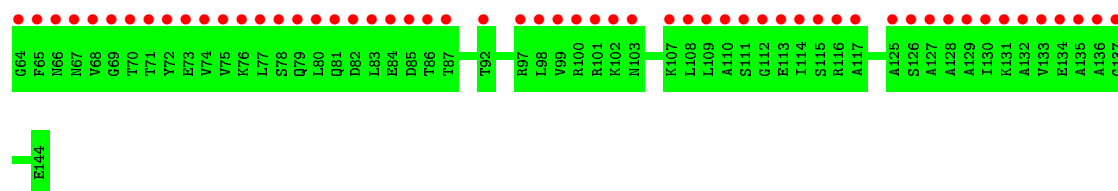


- Molecule 31: 50S ribosomal protein L14

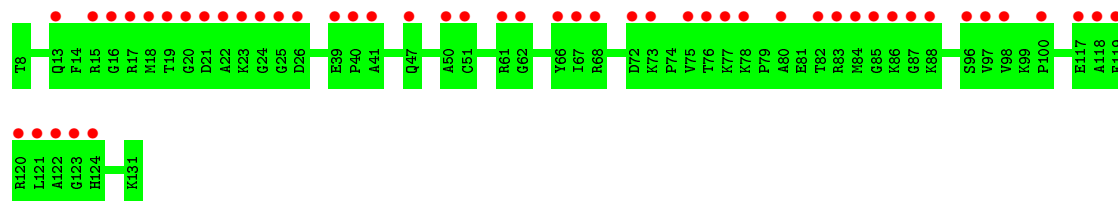
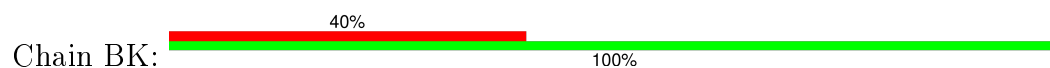


- Molecule 32: 50S ribosomal protein L15

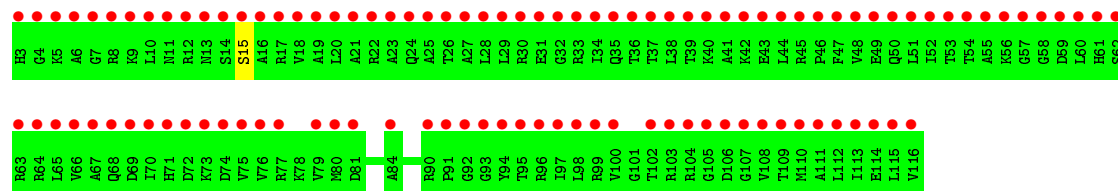




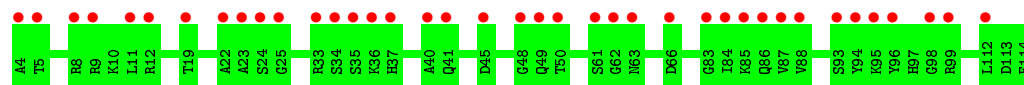
- Molecule 33: 50S ribosomal protein L16



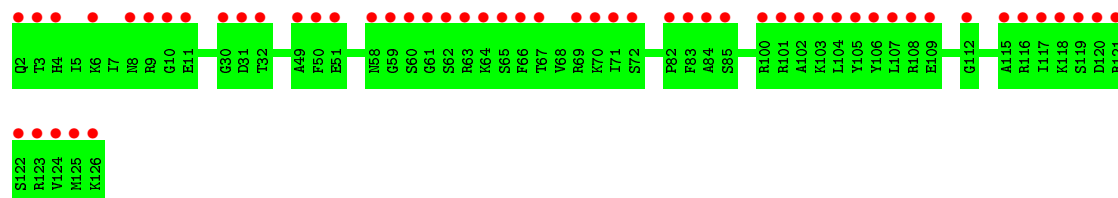
- Molecule 34: 50S ribosomal protein L17



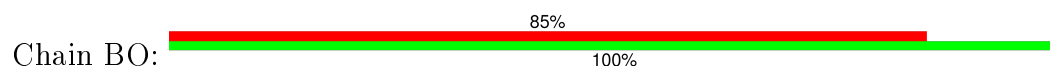
- Molecule 35: 50S ribosomal protein L18

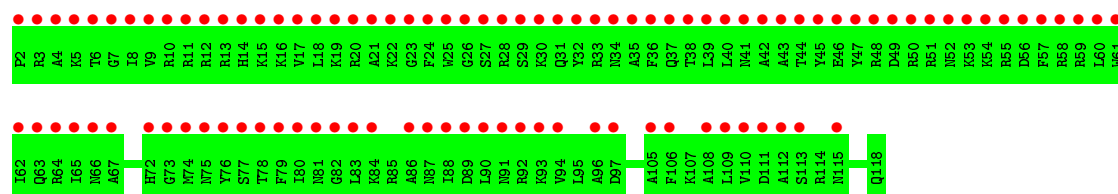


- Molecule 36: 50S ribosomal protein L19

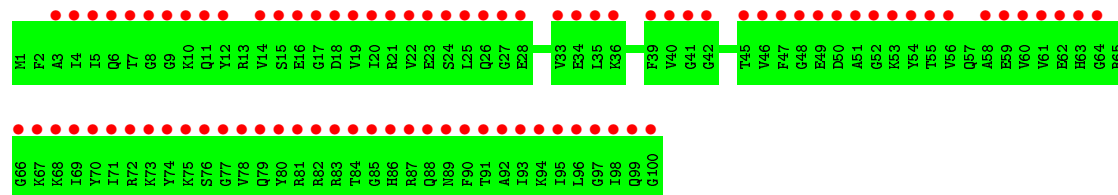


- Molecule 37: 50S ribosomal protein L20

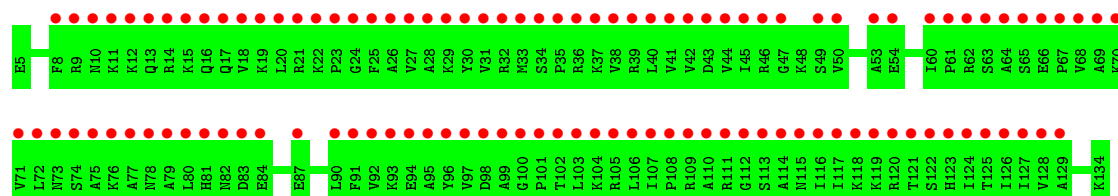
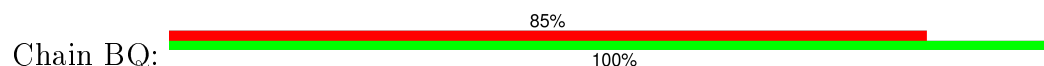




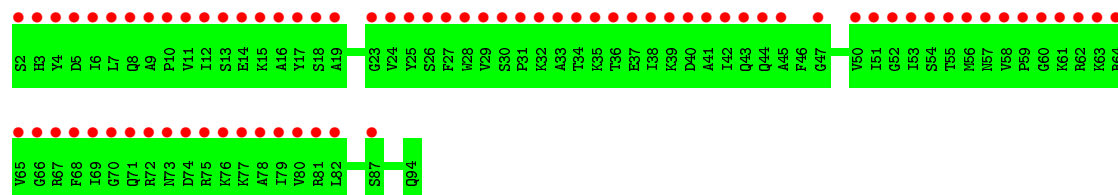
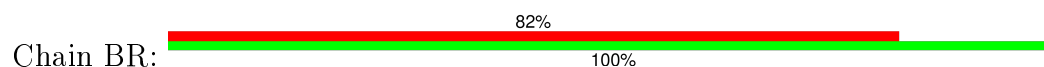
- Molecule 38: 50S ribosomal protein L21



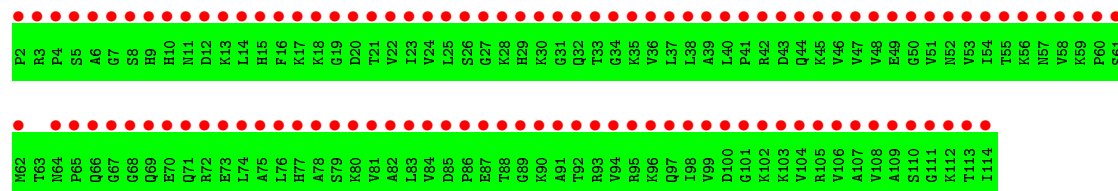
- Molecule 39: 50S ribosomal protein L22



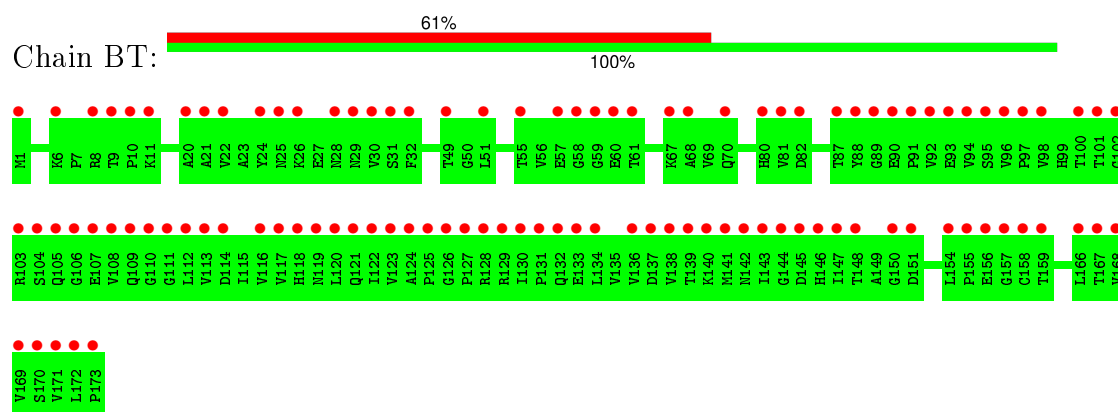
- Molecule 40: 50S ribosomal protein L23



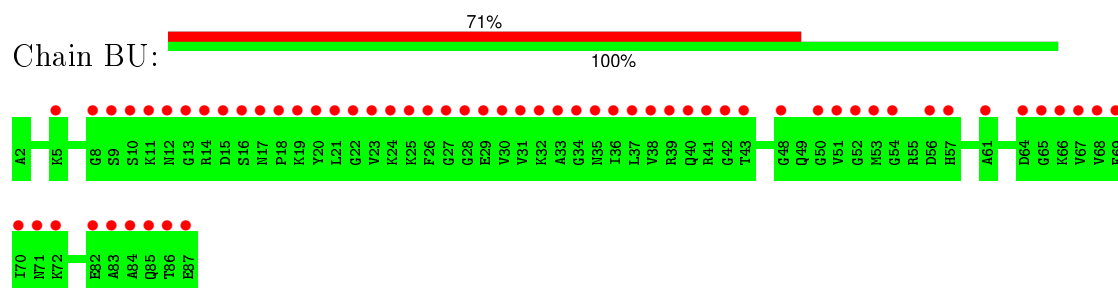
- Molecule 41: 50S ribosomal protein L24



- Molecule 42: general stress protein Ctc



- Molecule 43: 50S ribosomal protein L27

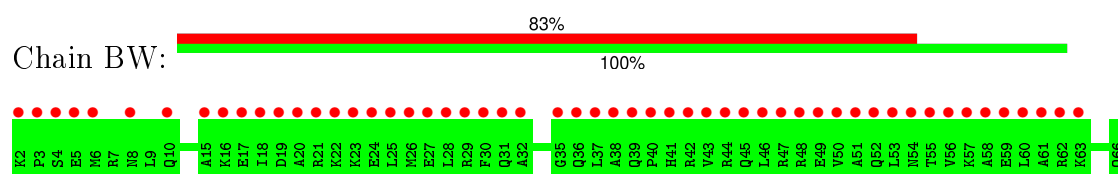


- Molecule 44: 50S RIBOSOMAL PROTEIN L28

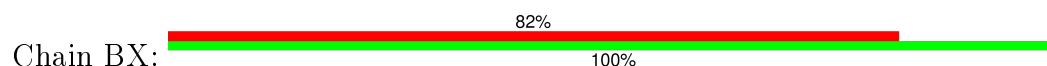


There are no outlier residues recorded for this chain.

- Molecule 45: 50S ribosomal protein L29



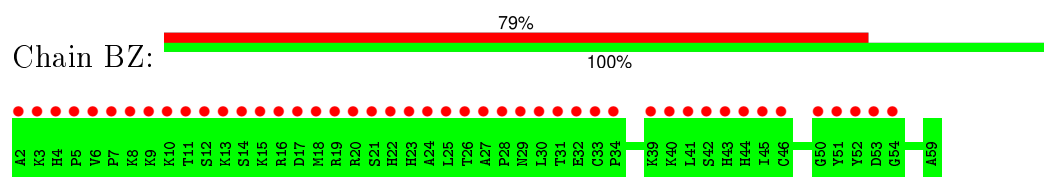
- Molecule 46: 50S ribosomal protein L30



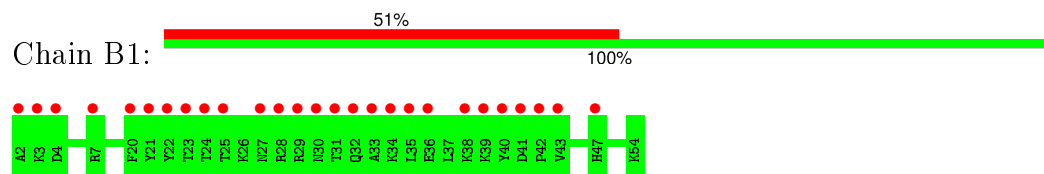
- Molecule 47: 50S ribosomal protein L31



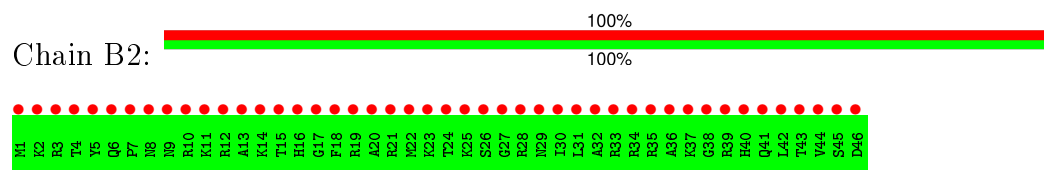
- Molecule 48: 50S ribosomal protein L32



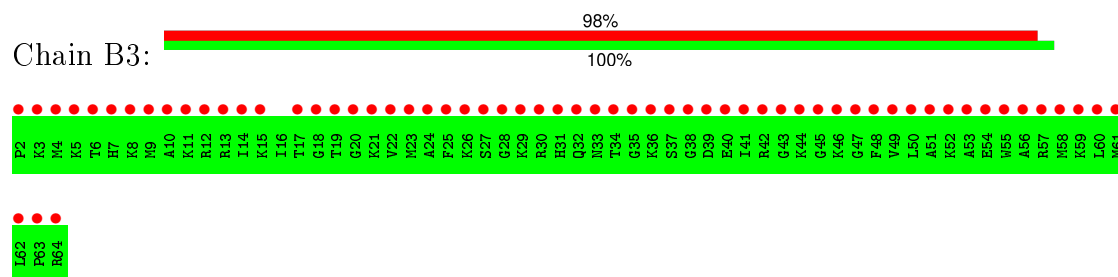
- Molecule 49: 50S ribosomal protein L33



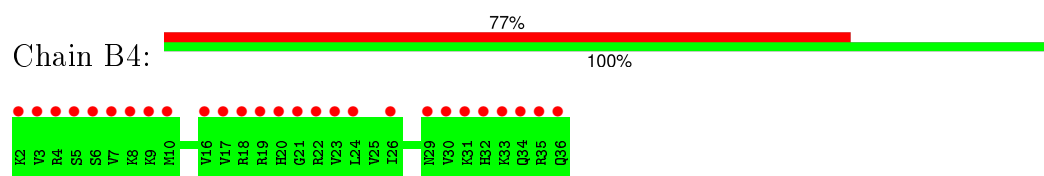
- Molecule 50: 50S ribosomal protein L34



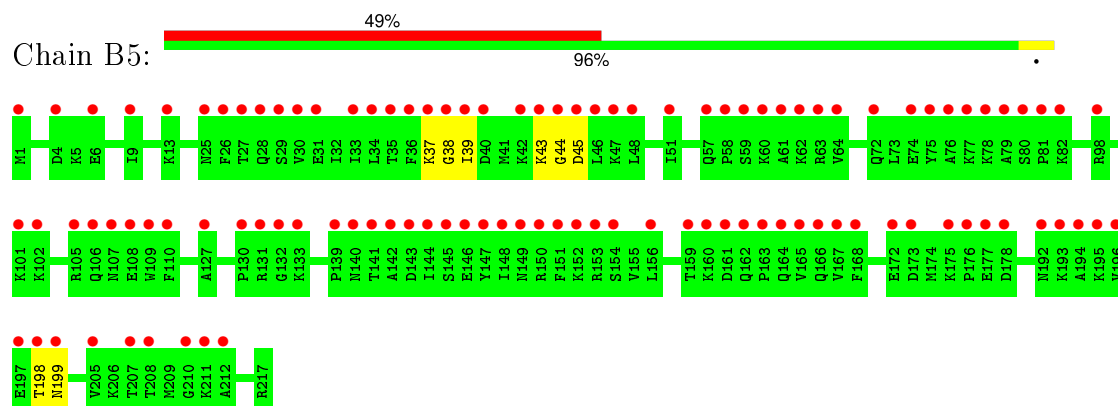
- Molecule 51: 50S ribosomal protein L35



- 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, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	9.49 (at 9.99Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.389 , 0.407 0.367 , 0.383	Depositor DCC
$R_{free}$ test set	1211 reflections (4.79%)	DCC
Wilson B-factor (Å <sup>2</sup> )	437.2	Xtriage
Anisotropy	0.460	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	1.31 , -10.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 26821 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	118711	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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%)	1	12
3	AC	204/206 (99%)	135 (66%)	40 (20%)	29 (14%)	0	6
4	AD	206/208 (99%)	166 (81%)	31 (15%)	9 (4%)	3	33
5	AE	148/150 (99%)	130 (88%)	13 (9%)	5 (3%)	5	40
6	AF	99/101 (98%)	79 (80%)	19 (19%)	1 (1%)	19	65
7	AG	153/155 (99%)	127 (83%)	16 (10%)	10 (6%)	1	25
8	AH	136/138 (99%)	125 (92%)	7 (5%)	4 (3%)	6	43
9	AI	125/127 (98%)	88 (70%)	27 (22%)	10 (8%)	1	19
10	AJ	96/98 (98%)	59 (62%)	20 (21%)	17 (18%)	0	4
11	AK	117/119 (98%)	88 (75%)	20 (17%)	9 (8%)	1	20
12	AL	120/124 (97%)	96 (80%)	15 (12%)	9 (8%)	1	21
13	AM	121/125 (97%)	87 (72%)	26 (22%)	8 (7%)	1	24
14	AN	58/60 (97%)	40 (69%)	11 (19%)	7 (12%)	0	8
15	AO	86/88 (98%)	70 (81%)	11 (13%)	5 (6%)	2	27
16	AP	81/83 (98%)	65 (80%)	15 (18%)	1 (1%)	16	61
17	AQ	102/104 (98%)	84 (82%)	10 (10%)	8 (8%)	1	20
18	AR	71/73 (97%)	62 (87%)	7 (10%)	2 (3%)	6	44
19	AS	78/80 (98%)	48 (62%)	19 (24%)	11 (14%)	0	6
20	AT	97/99 (98%)	65 (67%)	20 (21%)	12 (12%)	0	8
All	All	2330/2372 (98%)	1788 (77%)	361 (16%)	181 (8%)	1	20

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%)	8	35
3	AC	160/160 (100%)	142 (89%)	18 (11%)	7	33
4	AD	180/180 (100%)	172 (96%)	8 (4%)	35	69
5	AE	115/115 (100%)	100 (87%)	15 (13%)	5	28
6	AF	90/90 (100%)	88 (98%)	2 (2%)	60	83
7	AG	126/126 (100%)	122 (97%)	4 (3%)	46	76
8	AH	119/119 (100%)	109 (92%)	10 (8%)	14	48
9	AI	98/98 (100%)	90 (92%)	8 (8%)	14	49
10	AJ	88/88 (100%)	79 (90%)	9 (10%)	9	37
11	AK	90/90 (100%)	84 (93%)	6 (7%)	20	57
12	AL	104/104 (100%)	96 (92%)	8 (8%)	16	52
13	AM	100/100 (100%)	90 (90%)	10 (10%)	9	38
14	AN	49/49 (100%)	47 (96%)	2 (4%)	37	71
15	AO	79/79 (100%)	72 (91%)	7 (9%)	12	44
16	AP	72/72 (100%)	67 (93%)	5 (7%)	19	56
17	AQ	96/96 (100%)	90 (94%)	6 (6%)	22	59
18	AR	64/64 (100%)	61 (95%)	3 (5%)	32	68
19	AS	71/71 (100%)	68 (96%)	3 (4%)	36	70
20	AT	76/76 (100%)	69 (91%)	7 (9%)	11	43
All	All	1979/1979 (100%)	1826 (92%)	153 (8%)	16	52

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	82
21	B0	26
22	B9	2
12	AL	1
13	AM	1

The worst 5 of 112 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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	AA	1533/1537 (99%)	38.28	1533 (100%) 0 0	207, 548, 819, 940	0
2	AB	234/234 (100%)	1.53	77 (32%) 0 5	754, 754, 754, 754	0
3	AC	206/206 (100%)	5.67	168 (81%) 0 2	378, 378, 378, 378	0
4	AD	208/208 (100%)	14.87	202 (97%) 0 1	709, 709, 709, 709	0
5	AE	150/150 (100%)	14.91	150 (100%) 0 0	756, 756, 756, 756	0
6	AF	101/101 (100%)	1.33	22 (21%) 1 6	748, 748, 748, 748	0
7	AG	155/155 (100%)	4.41	106 (68%) 0 3	374, 374, 374, 374	0
8	AH	138/138 (100%)	7.39	131 (94%) 0 1	856, 856, 856, 856	0
9	AI	127/127 (100%)	7.38	79 (62%) 0 3	439, 439, 439, 439	0
10	AJ	98/98 (100%)	7.29	78 (79%) 0 2	430, 430, 430, 430	0
11	AK	119/119 (100%)	3.14	56 (47%) 0 4	652, 652, 652, 652	0
12	AL	124/124 (100%)	11.34	124 (100%) 0 0	423, 541, 541, 541	0
13	AM	125/125 (100%)	6.27	111 (88%) 0 2	378, 572, 572, 572	0
14	AN	60/60 (100%)	10.50	59 (98%) 0 0	378, 378, 378, 378	0
15	AO	88/88 (100%)	11.53	87 (98%) 0 0	740, 740, 740, 740	0
16	AP	83/83 (100%)	20.42	83 (100%) 0 0	781, 781, 781, 781	0
17	AQ	104/104 (100%)	12.31	104 (100%) 0 0	857, 857, 857, 857	0
18	AR	73/73 (100%)	3.63	41 (56%) 0 3	748, 748, 748, 748	0
19	AS	80/80 (100%)	3.13	44 (55%) 0 3	633, 633, 633, 633	0
20	AT	99/99 (100%)	13.47	99 (100%) 0 0	940, 940, 940, 940	0
21	B0	2825/2887 (97%)	61.95	2825 (100%) 0 0	462, 737, 737, 940	0
22	B9	118/118 (100%)	49.43	118 (100%) 0 0	772, 938, 938, 938	0
23	BA	270/270 (100%)	6.43	181 (67%) 0 3	737, 737, 737, 737	0
24	BB	205/205 (100%)	6.15	144 (70%) 0 3	737, 737, 737, 737	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	BC	197/197 (100%)	8.67	187 (94%) 0 1	737, 737, 737, 737	0
26	BD	178/178 (100%)	18.80	139 (78%) 0 2	938, 938, 938, 938	0
27	BE	177/177 (100%)	13.62	164 (92%) 0 1	737, 737, 737, 737	0
28	BF	52/52 (100%)	1.49	12 (23%) 1 6	737, 737, 737, 737	0
29	BG	143/143 (100%)	18.40	138 (96%) 0 1	907, 907, 907, 907	0
30	BH	143/143 (100%)	6.23	105 (73%) 0 3	737, 737, 737, 737	0
31	BI	132/132 (100%)	3.24	57 (43%) 0 4	737, 737, 737, 737	0
32	BJ	141/141 (100%)	10.89	116 (82%) 0 2	737, 737, 737, 737	0
33	BK	124/124 (100%)	2.54	50 (40%) 0 4	737, 737, 737, 737	0
34	BL	114/114 (100%)	7.36	105 (92%) 0 1	737, 737, 737, 737	0
35	BM	111/111 (100%)	1.89	39 (35%) 0 4	938, 938, 938, 938	0
36	BN	125/125 (100%)	2.78	55 (44%) 0 4	737, 737, 737, 737	0
37	BO	117/117 (100%)	13.14	99 (84%) 0 2	737, 737, 737, 737	0
38	BP	100/100 (100%)	6.22	87 (87%) 0 2	737, 737, 737, 737	0
39	BQ	130/130 (100%)	7.84	110 (84%) 0 2	737, 737, 737, 737	0
40	BR	93/93 (100%)	5.08	76 (81%) 0 2	737, 737, 737, 737	0
41	BS	113/113 (100%)	11.77	112 (99%) 0 0	737, 737, 737, 737	0
42	BT	173/173 (100%)	8.73	106 (61%) 0 3	737, 772, 772, 772	0
43	BU	86/86 (100%)	6.62	61 (70%) 0 3	737, 737, 737, 737	0
44	BV	0/16	-	-	-	-
45	BW	65/65 (100%)	6.20	54 (83%) 0 2	737, 737, 737, 737	0
46	BX	55/55 (100%)	7.98	45 (81%) 0 2	737, 737, 737, 737	0
47	BY	73/73 (100%)	4.45	47 (64%) 0 3	737, 737, 737, 737	0
48	BZ	58/58 (100%)	12.29	46 (79%) 0 2	737, 737, 737, 737	0
49	B1	53/53 (100%)	6.05	27 (50%) 0 4	737, 737, 737, 737	0
50	B2	46/46 (100%)	9.82	46 (100%) 0 0	737, 737, 737, 737	0
51	B3	63/63 (100%)	7.71	62 (98%) 0 0	737, 737, 737, 737	0
52	B4	35/35 (100%)	6.96	27 (77%) 0 2	737, 737, 737, 737	0
53	B5	213/217 (98%)	4.64	107 (50%) 0 4	940, 940, 940, 940	0
All	All	10433/10519 (99%)	27.61	8901 (85%) 0 2	207, 737, 938, 940	0

The worst 5 of 8901 RSRZ outliers are listed below:



Mol	Chain	Res	Type	RSRZ
21	B0	1989	C	315.0
21	B0	2624	G	251.3
21	B0	2480	C	226.1
21	B0	1988	A	218.6
21	B0	2425	G	216.0

## 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.