



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 09:25 PM GMT

PDB ID : 4V4Y
Title : Crystal structure of the 70S *Thermus thermophilus* ribosome with translocated and rotated Shine-Dalgarno Duplex.
Authors : Jenner, L.; Yusupova, G.; Rees, B.; Moras, D.; Yusupov, M.
Deposited on : 2006-06-27
Resolution : 5.50 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

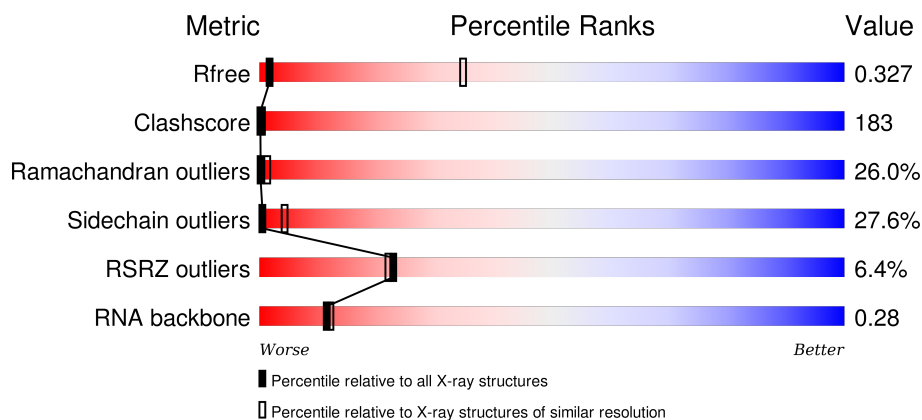
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 5.50 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 (7.38-3.62)
Clashscore	102246	1020 (7.10-3.70)
Ramachandran outliers	100387	1014 (7.36-3.64)
Sidechain outliers	100360	1013 (7.38-3.62)
RSRZ outliers	91569	1014 (7.38-3.62)
RNA backbone	2183	1101 (7.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	AA	1522	
2	A1	50	
3	AB	76	
3	AC	76	

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Mol	Chain	Length	Quality of chain
3	AD	76	
4	AE	256	
5	AF	239	
6	AG	209	
7	AH	162	
8	AI	101	
9	AJ	156	
10	AK	138	
11	AL	128	
12	AM	105	
13	AN	129	
14	AO	132	
15	AP	126	
16	AQ	61	
17	AR	89	
18	AS	88	
19	AT	105	
20	AU	88	
21	AV	93	
22	AW	106	
23	AX	27	
24	BA	2916	
25	BB	123	
26	BC	229	
27	BD	276	

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Mol	Chain	Length	Quality of chain
28	BE	206	
29	BF	210	
30	BG	182	
31	BH	180	
32	BK	148	
33	BL	147	
34	BM	140	
35	BN	122	
36	BO	150	
37	BP	141	
38	BQ	118	
39	BR	112	
40	BS	146	
41	BT	118	
42	BU	101	
43	BV	113	
44	BW	96	
45	BX	110	
46	BY	206	
47	BZ	85	
48	B1	67	
49	B2	60	
50	B3	71	
51	B4	60	
52	B5	54	

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Mol	Chain	Length	Quality of chain
53	B6	49	<div><div></div><div>45%</div><div></div><div>53%</div><div></div><div>37%</div><div></div><div>10%</div></div>
54	B7	65	<div><div></div><div>18%</div><div></div><div>52%</div><div></div><div>38%</div><div></div><div>8%</div><div></div></div>
55	B8	37	<div><div></div><div>8%</div><div></div><div>57%</div><div></div><div>30%</div><div></div><div>5%</div></div>

2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 151691 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1515	Total	C	N	O	P	0	0	0
			32554	14490	6022	10527	1515			

- Molecule 2 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A1	50	Total	C	N	O	P	0	0	0
			1025	459	128	388	50			

- Molecule 3 is a RNA chain called tRNA PHE (unmodified bases).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	76	Total	C	N	O	P	0	0	0
			1623	723	290	534	76			
3	AD	76	Total	C	N	O	P	0	0	0
			1623	723	290	534	76			
3	AB	76	Total	C	N	O	P	0	0	0
			1623	723	290	534	76			

- Molecule 4 is a protein called 30S ribosomal protein S2.

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

- Molecule 5 is a protein called 30S ribosomal protein S3.

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

- Molecule 6 is a protein called 30S ribosomal protein S4.

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

- Molecule 7 is a protein called 30S ribosomal protein S5.

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

- Molecule 8 is a protein called 30S ribosomal protein S6.

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

- Molecule 9 is a protein called 30S ribosomal protein S7.

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

- Molecule 10 is a protein called 30S ribosomal protein S8.

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

- Molecule 11 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AL	127	Total	C	N	O	S	0	0	0
			1010	639	197	174				

- Molecule 12 is a protein called 30S ribosomal protein S10.

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

- Molecule 13 is a protein called 30S ribosomal protein S11.

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

- Molecule 14 is a protein called 30S ribosomal protein S12.

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

- Molecule 15 is a protein called 30S ribosomal protein S13.

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

- Molecule 16 is a protein called 30S ribosomal protein S14.

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

- Molecule 17 is a protein called 30S ribosomal protein S15.

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

- Molecule 18 is a protein called 30S ribosomal protein S16.

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

- Molecule 19 is a protein called 30S ribosomal protein S17.

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

- Molecule 20 is a protein called 30S ribosomal protein S18.

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

- Molecule 21 is a protein called 30S ribosomal protein S19.

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

- Molecule 22 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AW	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

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

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

- Molecule 24 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	BA	2889	Total	C	N	O	P	0	0	0
			62218	27691	11629	20009	2889			

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 25 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	BB	123	Total	C	N	O	P	0	0	0
			2641	1175	488	855	123			

There are 2 discrepancies between the modelled and reference sequences:

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

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Chain	Residue	Modelled	Actual	Comment	Reference
BB	120	U	-	INSERTION	GB 48271

- Molecule 26 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	BC	228	Total	C	N	O	S	0	0	0
			1742	1102	318	319	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	BD	272	Total	C	N	O	S	0	0	0
			2124	1339	424	358	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	BE	206	Total	C	N	O	S	0	0	0
			1578	997	302	273	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	BF	208	Total	C	N	O	S	0	0	0
			1625	1034	303	286	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	BG	182	Total	C	N	O	S	0	0	0
			1482	947	269	261	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	BH	174	Total	C	N	O	S	0	0	0
			1328	844	248	235	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BK	148	Total	C	N	O	S	0	0	0
			1155	737	205	212	1			

- Molecule 33 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BL	138	Total	C	N	O	S	0	0	0
			1025	654	181	185	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BM	139	Total	C	N	O	S	0	0	0
			1113	717	207	186	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BN	122	Total	C	N	O	S	0	0	0
			932	587	171	170	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BO	145	Total	C	N	O	S	0	0	0
			1106	688	226	190	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BP	136	Total	C	N	O	S	0	0	0
			1080	688	204	183	5			

- Molecule 38 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
38	BQ	117	Total	C	N	O	0	0	0
			960	599	202	159			

- Molecule 39 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
39	BR	110	Total	C	N	O			
			877	553	175	149	0	0	0

- Molecule 40 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BS	117	Total	C	N	O	S			
			976	614	197	164	1	0	0	0

- Molecule 41 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BT	117	Total	C	N	O	S			
			964	610	202	151	1	0	0	0

- Molecule 42 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BU	101	Total	C	N	O	S			
			779	501	142	135	1	0	0	0

- Molecule 43 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BV	110	Total	C	N	O	S			
			876	552	171	151	2	0	0	0

- Molecule 44 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
44	BW	94	Total	C	N	O			
			742	483	133	126	0	0	0

- Molecule 45 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BX	110	Total	C	N	O	S			
			844	539	158	141	6	0	0	0

- Molecule 46 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BY	180	Total	C	N	O	S	0	0	0
			1435	916	256	260	3			

- Molecule 47 is a protein called Ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	BZ	85	Total	C	N	O	S	0	0	0
			670	415	141	112	2			

- Molecule 48 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	B1	67	Total	C	N	O	S	0	0	0
			567	350	116	99	2			

- Molecule 49 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	B2	59	Total	C	N	O	S	0	0	0
			469	298	90	81				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	B3	71	Total	C	N	O	S	0	0	0
			581	364	108	104	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	B4	57	Total	C	N	O	S	0	0	0
			445	279	87	74	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	B5	49	Total	C	N	O	S	0	0	0
			426	265	87	70	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	B6	49	Total	C	N	O	S	0	0	0
			430	263	108	57	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	B7	64	Total	C	N	O	S	0	0	0
			515	331	102	79	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	B8	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

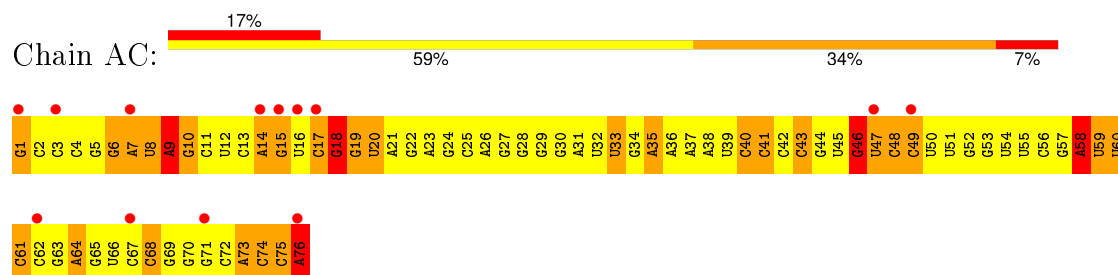
C1399	C1340	G1220	U1559	G1099	C1039	C924	A864	G798	C738
C1400	U1341	G1221	G1160	C1100	U1040	G925	A865	G799	C739
C1401	C1342	G1222	C1161	A1101	A1041	G926	C866	G800	U740
C1402	G1343	C1223	C1162	A1102	G1042	G927	G867	U801	G741
C1403	C1344	G1224	C1163	C1103	C1043	G928	C868	A802	G742
C1404	U1345	A1285	G1164	G1104	A1044	G929	C869	G803	U743
C1405	A1346	G1226	C1165	A1105	C1045	C930	C870	U804	C744
U1406	G1347	A1227	G1166	A1106	A1046	C931	C871	C805	C745
U1407	U1348	C1228	C1167	C1107	G1047	C932	A872	C806	A746
C1408	A1349	A1229	A1169	G1108	G933	G933	A873	A807	C747
C1409	A1350	C1230	A1170	C1109	U1048	G934	A874	C808	C748
C1410	U1351	G1231	G1171	A1110	G1050	A935	C875	G809	C749
C1411	C1352	U1232	C1172	A1111	C1051	C936	G876	C810	G750
C1412	G1353	G1233	G1173	C1112	U1052	A937	C877	C811	U751
C1413	C1354	C1234	G1174	C1113	G1053	A938	G878	C812	G752
U1414	G1355	U1235	G1175	C1114	C1054	G939	C879	U813	A753
G1415	G1356	A1236	A1176	C1115	A1055	C940	C880	A814	C754
G1416	A1357	C1237	G1177	C1116	U1056	G941	G881	A815	G755
G1417	U1358	A1238	G1178	G1117	G1057	G942	C882	A816	C756
C1418	C1359	A1239	A1179	C1118	G1058	U943	C883	C817	U757
C1419	A1360	U1240	A1180	C1119	C1059	G944	U884	G818	G758
U1420	G1361	G1241	G1181	G1120	A1060	G945	C885	A819	A759
G1421	C1362	C1242	G1182	U1121	G1061	A946	G886	U820	G760
G1422	C1362A	C1243	A1183	U1122	U1062	G947	G887	G821	G761
G1423	A1363	G1244	G1184	A1123	C1063	C948	G888	C822	C762
C1424	U1364	A1245	G1185	G1124	G1064	A949	A889	G823	G763
U1425	G1365	C1246	G1186	U1125	U1065	U950	G890	C824	C764
U1426	C1366	U1247	G1187	U1126	C1066	G951	G891	G825	G765
U1427	C1367	A1248	A1188	G1127	A1067	U952	A892	C826	A766
A1428	G1368	G1249	C1189	C1128	G1068	G953	C893	U827	A767
C1429	C1369	G1310	G1190	C1129	C1069	G954	G894	A828	A768
C1430	G1370	G1311	A1191	A1130	U1070	U955	G895	G829	G769
C1431	G1371	A1312	C1192	C1131	C1071	U956	C896	G830	C770
C1432	U1372	U1313	G1193	C1132	G1072	U957	C897	U831	G771
A1433	G1373	C1314	U1194	G1133	U1073	A958	C898	C832	U772
A1434	A1374	G1254	C1195	G1134	G1074	A959	C899	U833	G773
G1435	U1375	A1255	U1196	U1135	C1075	U960	A900	C834	G774
U1436	U1376	U1257	G1197	U1136	C1076	U961	A901	U835	G775
C1437	A1377	G1258	G1198	C1137	U1077	C962	G902	G836	G776
C1438	C1378	C1259	U1199	G1138	U1078	G963	G903	G837	A777
C1439	G1379	C1260	C1200	G1139	G1079	A964	C904	G838	G778
C1440	U1380	A1261	A1201	C1140	A1080	A965	U905	U841	C779
G1441	U1381	C1322	G1202	G1141	G1081	G966	G906	C842	A780
G1442	C1382	G1263	C1203	G1142	G1082	C967	A907	U843	A781
C1443	C1383	A1324	A1204	G1143	U1083	A968	A908	C846	A782
A1446	C1384	G1265	U1205	G1144	G1084	A969	A909	C849	C783
G1447	G1385	G1266	G1206	C1145	U1085	C970	C910	U850	C784
C1448	G1386	C1267	G1207	A1146	U1086	G971	U911	G851	G785
C1449	G1387	A1268	C1208	C1147	G1087	C972	C912	G852	G786
U1450	C1388	A1269	C1209	U1148	G1088	G973	A913	G853	A787
A1451	C1389	U1330	C1210	C1149	G1089	A974	A914	G854	U788
C1452	U1390	G1331	U1211	U1150	U1090	A975	A915	G855	U789
G1453	U1391	A1332	U1212	A1151	U1091	G976	G916	C856	A790
G1454	C1392	G1273	A1213	A1152	U1092	A977	G917	C857	G791
C1455	U1393	G1334	G1214	C1153	A1093	A978	A918	G858	A792
C1456	A1394	A1274	G1215	G1154	G1094	C979	A919	A859	U793
C1459	C1395	G1275	G1216	G1155	U1095	C980	U920	A860	A794
A1460	G1396	G1276	C1217	G1156	C1096	U981	U921	G861	C795
G1461	A1396	U1277	C1218	A1157	C1097	U982	U922	C862	C796
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• Molecule 2: mRNA

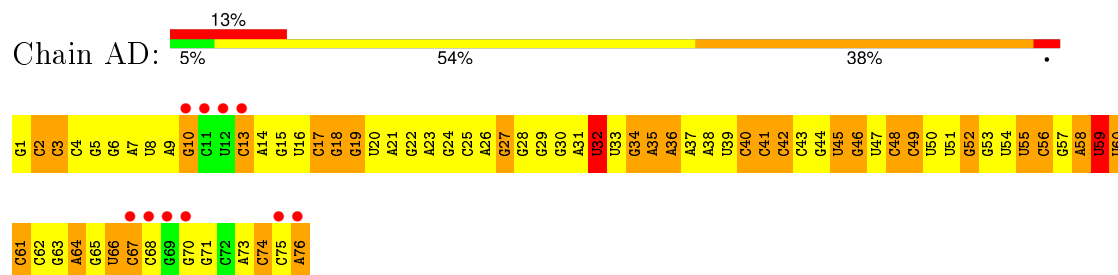


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----	----	----	----	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

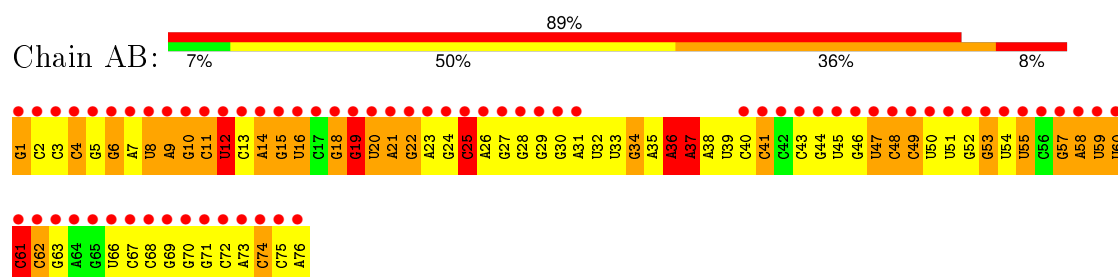
- Molecule 3: tRNA PHE (unmodified bases)



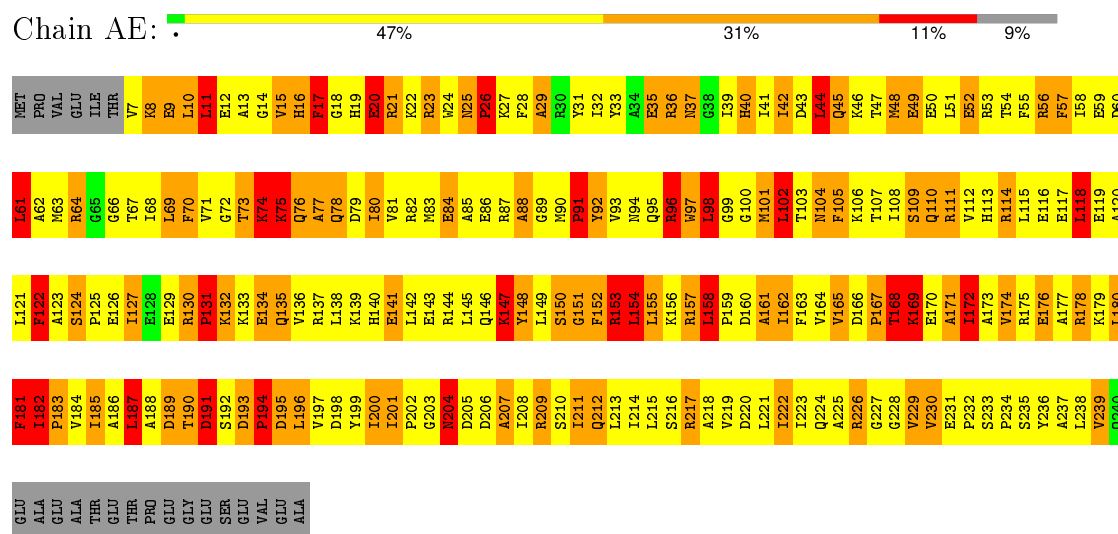
- Molecule 3: tRNA PHE (unmodified bases)



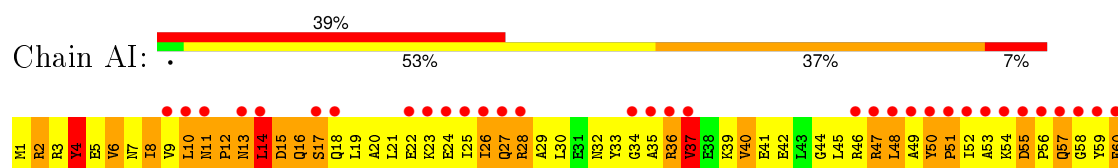
- Molecule 3: tRNA PHE (unmodified bases)

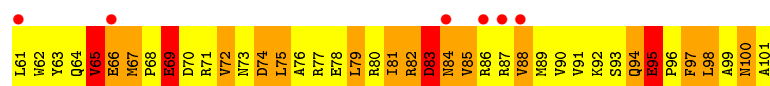


- Molecule 4: 30S ribosomal protein S2

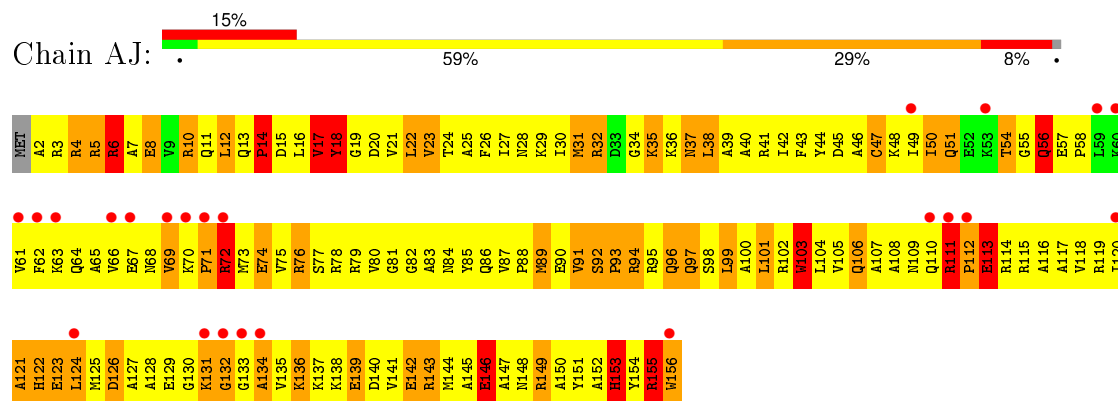


- Molecule 5: 30S ribosomal protein S3

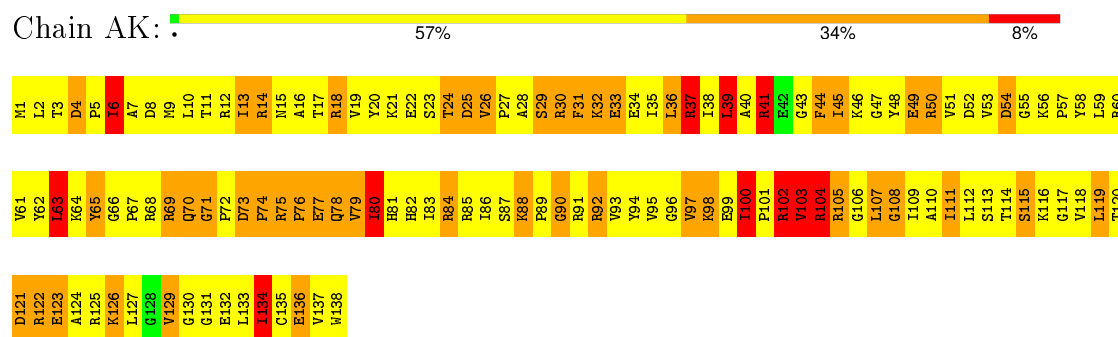




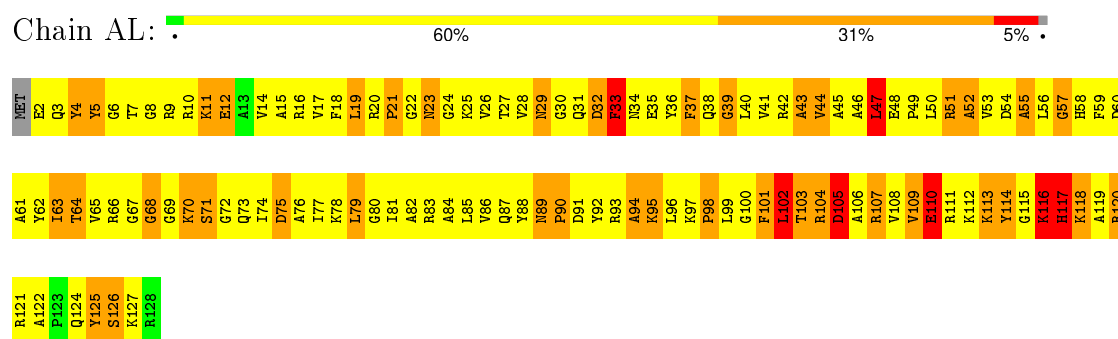
• Molecule 9: 30S ribosomal protein S7



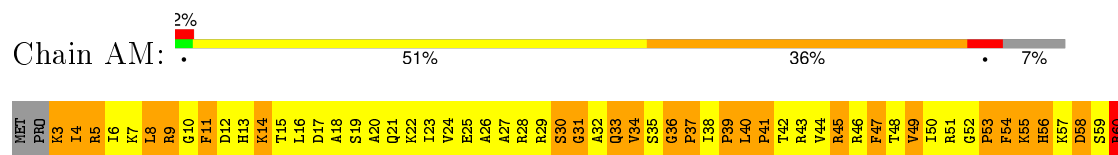
• Molecule 10: 30S ribosomal protein S8

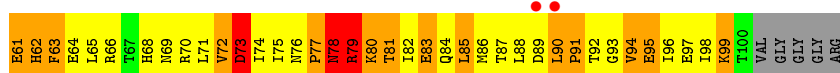


• Molecule 11: 30S ribosomal protein S9

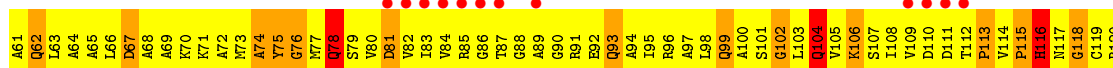


• Molecule 12: 30S ribosomal protein S10

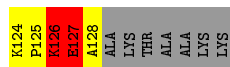
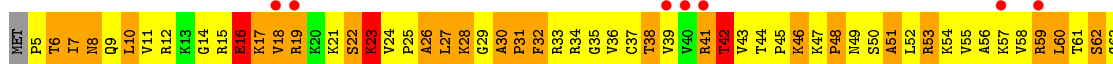




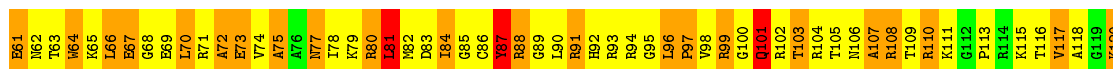
• Molecule 13: 30S ribosomal protein S11



• Molecule 14: 30S ribosomal protein S12



• Molecule 15: 30S ribosomal protein S13




• Molecule 16: 30S ribosomal protein S14



W61


- Molecule 17: 30S ribosomal protein S15

Chain AR:  66% 28% 6%

MET P2 I3 T4 R5 E6 E7 Q8 Q9 K10 V11 S11 I12 I13 E14 F15 A16 R17 R77 F18 P19 G20 I21 D21 T22 G23 G24 S24 T25 E26 V27 I27 Q28 V29 A30 L31 L32 T33 L34 R35 R36 I36 I37 R38 L39 S40 S41 E41 H42 H43 L44 K44 V45 H46 K47 K48 D49 H50 H51 S52 S53 R54 G55 L56 L57 P58 P59 V60

G61 Q62 R63 R64 R65 L66 L67 Y69 L70 Q71 R72 E73 D74 E76 E77 Y78 R79 A80 L81 I82 I83 E83 G84 L85 G86 I87 R88 G89

- Molecule 18: 30S ribosomal protein S16

Chain AS:  56% 33% 6% 6%

M1 V2 K3 K4 I4 R5 L6 A7 R8 F9 G10 A11 K12 H13 P15 H16 Y17 R18 I19 V20 V21 T22 D23 A24 R25 R26 R27 D29 D30 K31 Y32 I33 E34 K35 I36 G37 Y38 Y39 D40 P41 R42 K43 T44 T45 P46 D47 W48 L49 K50 V51 D52 V53 E54 R55 A56 R57 Y58 P59 L60

S61 V62 G63 A64 Q65 P66 T67 D68 T69 A70 R71 R72 H73 L74 R75 Q76 A77 G78 V79 F80 A81 Q82 E83 ALA A84 ARG GLY ALA

- Molecule 19: 30S ribosomal protein S17

Chain AT:  54% 35% 6% 2%

MET P2 K3 K4 V5 L6 T7 G8 V9 V10 V11 S12 D13 K14 R15 Q16 K17 V18 T19 T20 V21 V22 V23 E24 R25 Q26 Q27 F28 R29 P30 P31 Y32 G33 K34 Y35 Y36 I36 I37 R38 S39 K40 K41 K42 L43 L44 H45 D46 P47 E48 E49 K50 Y51 K52 L53 G54 D55 V56 N57 E58 I59 G60

E61 S62 R63 P64 I65 S66 K67 R68 R69 F70 F71 R72 V73 L74 R75 L76 V77 E78 S79 G80 R81 N82 D83 L84 V85 E86 K87 Y88 L89 I90 R91 R92 Q93 N94 Y95 Q96 I96 I97 R98 S99 K100 K101 G102 G103 K104 A105

- Molecule 20: 30S ribosomal protein S18

Chain AU:  50% 22% 9% 17% 7%

MET SER THR LYS ASN ALA LYS PRQ LYS LYS GLU ALA GLN ARG ARG P16 S17 R18 K19 A20 A21 K21 V22 K23 A24 T25 L26 G27 E28 F29 D30 L31 R32 D33 Y34 R35 R36 V37 E38 V39 L40 L41 K42 F43 L44 S45 E46 T47 G48 K49 K50 L51 P52 R53 R54 R55 T56 G57 S58 S59 G60

K61 E62 Q63 R64 I65 L66 A67 K68 T69 I70 K71 R72 A73 R74 L75 L76 G77 L78 L79 P80 F81 T82 E83 K84 L85 V86 R87 K88

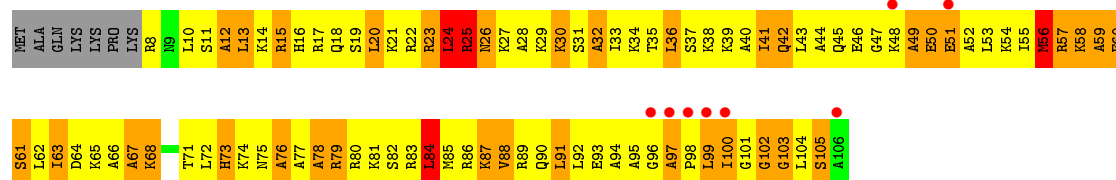
- Molecule 21: 30S ribosomal protein S19

Chain AV:  48% 29% 5% 14% 6%

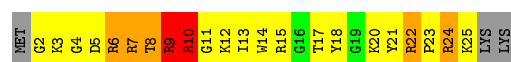
MET P2 R3 S4 L5 K6 V9 V10 V11 D12 D13 H14 L15 L16 K18 V19 L20 E21 L22 N23 A24 R25 G26 E27 R28 R29 L30 L31 K32 T33 W34 S35 R36 R37 S38 T39 I40 V41 P42 E43 M44 V45 G46 H47 T48 I49 A50 V51 Y52 N53 G54 K55 Q56 H57 V58 P59 V60 Y61



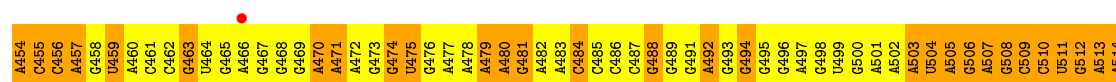
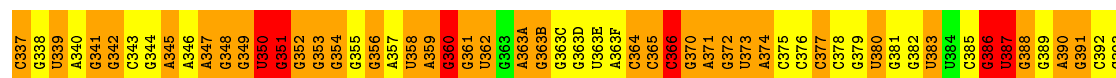
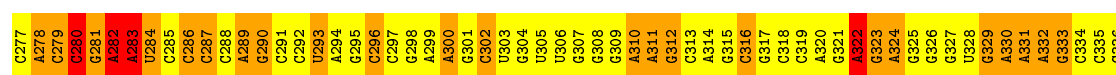
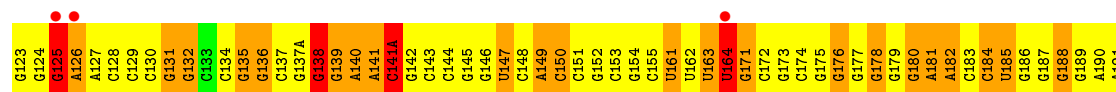
• Molecule 22: 30S ribosomal protein S20



• Molecule 23: 30S ribosomal protein Thx



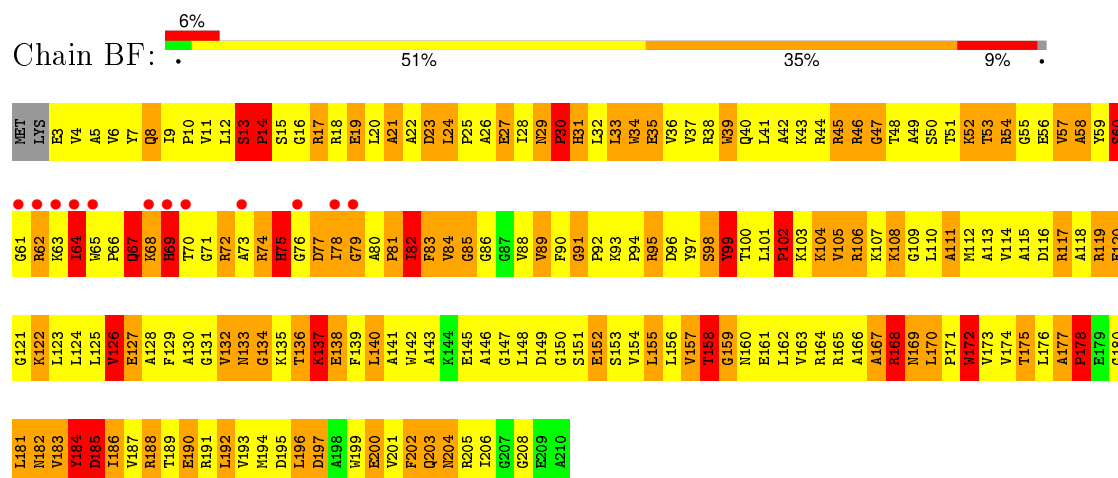
• Molecule 24: 23S ribosomal RNA



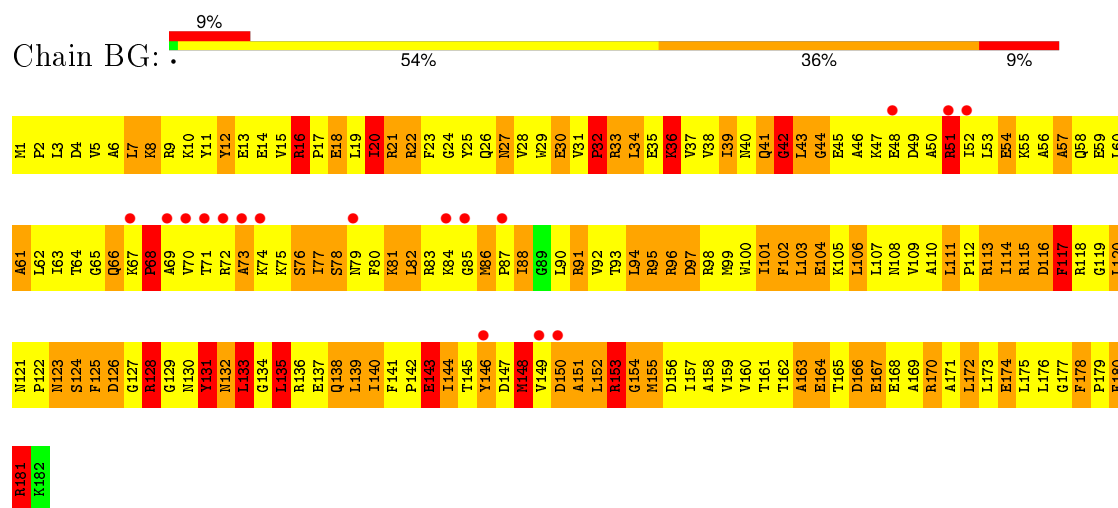
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G1337	G1277	G1216	A1155	A1096	G1036	G976	G916	G855	G795	A735	A675	A637	A579	C517
G1338	G1278	C1217	A1156	U1097	G1037	G977	A917	C856	G796	C736	A676	G638	C580	A518
G1339	G1279		G1157	A1098	G1038	G978	G918	C857	G797	C737	A677	G639	C581	U519
U1340	G1280	A1220	G1158	G1099	G1039	G979	G919	C858	G798	C738	C678	C640	G582	G520
U1341	G1281	C1221	U1159	C1100	C1040	A980	G920	G859	G799	G739	C679	G641	G583	C521
A1342	U1282	C1222	G1160	U1101	G1041	A981	G921	C860	A800	G740	G680	G642	C584	G522
G1343	G1283	C1223	C1161	C1102	G1042	C982	U922	A861	G801	G741	G681	A643	G585	C523
G1344	A1284	G1224	A1162	A1103	C1043	A983	C923	G862	A802	G742	A682	A644	A586	U524
C1345	G1285	G1225	G1163	C1104	G1044	A984	C924	A863	A803	G743	C683	C645	C587	U525
G1346	A1286	G1226	U1164	U1105	A1045	G985	G925	C864	A804	G744	G684	A646	U588	A526
G1347	G1287	A1227	G1165	G1106	A1046	C986	A926	C865	G805	G745	A685	G647	C589	C527
G1348	U1288	G1228	C1166	G1107	G1047	G987	G928	A866	C806	A746	G686	G648	A590	A528
A1349	C1289	G1229	U1167	U1108	A1048	A988	G929	U868	U807	U747	C687	G649	C591	A529
C1350	C1290	C1230	G1168	C1109	C1049	G989	U930	U868	G808	G748	G688	C	G592	A530
C1351	C1291	G1231	G1169	G1110	A1050	A990	G931	G869	G809	C749	A689	G	G593	C531
U1352	U1292	G1232	A1170	A1111	G1051	C991	G932	A870	U810	A750	G690	C	U594	A532
C1353	C1293	C1233	G1171	G1112	C1052	C992	A933	U871	U811	A751	C691	A	C595	G533
U1354	U1294	U1234	A1173	U1113	C1053	G993	G934	A872	C812	A752	C692	A	G596	U534
G1355	A1295	G1235	A1174	G1114	A1054	C994	C935	G873	U813	G753	C693	G	U597	C535
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G1358	G1298	G1238	A1177	G1117	A1057	G997	G938	C876	C816	C756	G696	G	G600	A539
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C2231	C2161	G2100	C2040	G1980	C1920	U1851	A1791	G1718	A1655	A1596	A1536	G1475	G1416
U2232	C2162	G2101	U2041	A1981	G1921	C1852	G1792	G1725	C1656	A1597	C1537	C1476	C1417
U2233	C2163	U2102	A2042	C1982	G1922	A1853	C1793	G1726	C1657	C1598	G1538	A1477	G1418
G2234	C2164	C2103	C2043	C1983	U1923	A1854	U1794	U1727	C1658	C1599	G1539	G1478	A1419
G2235	G2165	G2104	C2044	G1984	C1924	G1855	C1795	G1728	U1659	C1600	G1540	U1420	U1420
C2236	C2166	C2105	C2045	G1985	C1925	G1856	U1796	A1729	G1660	G1601	U1541	G1480	G1421
G2237	U2167	G2106	G2046	A1986	U1926	G1857	C1797	U1730	G1661	U1602	U1542	G1482	G1422
G2238	C2168	C2107	U2047	G1987	A1927	G1858	U1798	G1731	C1662	A1603	G1543	G1483	G1423
G2239	A2169	G2108	G2048	C1988	A1928	A1859	G1799	A1732	C1663	C1604	C1544	G1484	G1424
C2240	A2170	C2109	G2049	G1989	G1929	G1860	G1800	G1733	A1664	C1605	A1545	G1485	G1425
A2241	A2171	C2110	C2050	C1990	G1930	G1861	G1801	C1734	A1665	G1606	A1545A	A1486	G1426
G2242	U2172	G2112	A2051	U1991	U1931	G1862	A1802	C1735	G1666	C1607	C1546	G1487	A1427
U2243	C2173	U2113	G2052	C1992	A1932	G1863	A1803	C1742	G1667	A1608	C1547	G1488	G1428
U2244	C2174	A2114	G2053	U1993	G1933	G1864	C1804	G1743	A1668	A1609	C1548	U1489	G1429
U2245	C2175	G2115	A2054	C1994	C1934	G1869	U1805	G1746	A1669	A1610	C1549	A1490	C1430
G2246	A2176	G2116	G2055	U1995	G1935	C1870	C1806	G1746	G1670	C1611	C1550	G1491	U1431
A2247	C2177	A2117	G2056	C1996	A1936	A1871	G1807	G1747	U1671	C1612	C1551	G1492	C1432
C2248	C2178	U2118	A2057	G1997	A1937	A1872	U1808	G1748	C1672	G1613	G1552	C1493	U1433
U2249	C2179	A2119	A2058	C1998	A1938	G1878	A1809	A1749	U1673	A1614	A1553	A1494	A1434
G2250	U2180	G2120	C2059	C1999	U1939	C1879	A1810	G1750	G1674	C1615	A1554	A1495	G1435
G2251	G2181	G2121	A2060	G2000	U1940	C1880	G1811	C1751	G1675	A1616	G1555	A1496	G1436
G2252	C2182	U2122	G2061	A2001	C1941	C1881	A1812	C1752	A1676	C1617	C1556	U1497	U1437
G2253	C2183	G2123	A2062	C2002	C1942	C1882	G1813	G1753	A1677	A1618	C1557	C1498	U1438
C2254	G2184	G2124	C2063	G2003	U1943	G1883	G1814	C1754	G1678	G1619	A1558	C1499	A1439
G2255	C2185	G2125	C2064	G2004	U1944	A1884	A1815	A1755	U1679	G1620	G1559	G1500	G1440
G2256	A2186	A2126	C2065	A2005	G1945	G1885	G1756	G1756	U1680	U1621	G1560	C1501	G1441
U2257	G2187	G2127	C2066	C2006	U1946	C1886	G1817	U1757	G1681	G1622	G1561	C1502	G1442
C2258	C2188	C2128	G2067	C2007	C1947	C1887	U1818	G1758	G1682	G1623	A1562	U1503	G1443
G2259	U2189	C2129	U2068	C2008	G1948	G1888	A1819	A1759	C1683	G1624	C1563	C1504	G1444
C2260	G2190	U2130	G2069	G2009	G1949	A1889	U1820	A1760	C1684	C1625	C1564	C1505	A1444A
C2261	G2191	G2131	G2070	G2010	G1950	A1890	A1821	C1761	C1685	G1626	C1565	C1506	G1445
U2262	G2192	U2132	A2071	U2011	U1951	G1891	A1762	A1762	C1686	G1627	A1566	A1507	G1446
C2263	G2193	G2133	G2072	G2012	A1952	C1892	G1823	G1763	G1687	G1628	A1567	A1508	G1447
G2264	G2194	A2134	C2073	A2013	A1953	C1893	G1824	G1764	U1688	G1629	G1568	A1509	G1448
U2265	C2195	A2135	C2074	A2014	G1954	C1894	A1825	C1765	A1689	G1630	A1510	A1449	A1449
A2266	C2196	C2136	U2075	A2015	U1955	C1895	G1826	U1766	A1690	C1630A	A1511	G1450	G1449A
A2267	U2197	U2016	U2076	U2016	U1956	G1896	G1827	C1767	C1691	A1631	A1512	C1451	G1450
A2268	C2198	C2137	A2077	U2017	U1957	G1897	G1828	U1768	U1692	A1632	A1572	C1452	G1451
A2269	A2199	C2139	C2078	G2018	C1958	U1998	A1829	G1769	U1693	G1633	G1573	U1514	A1453

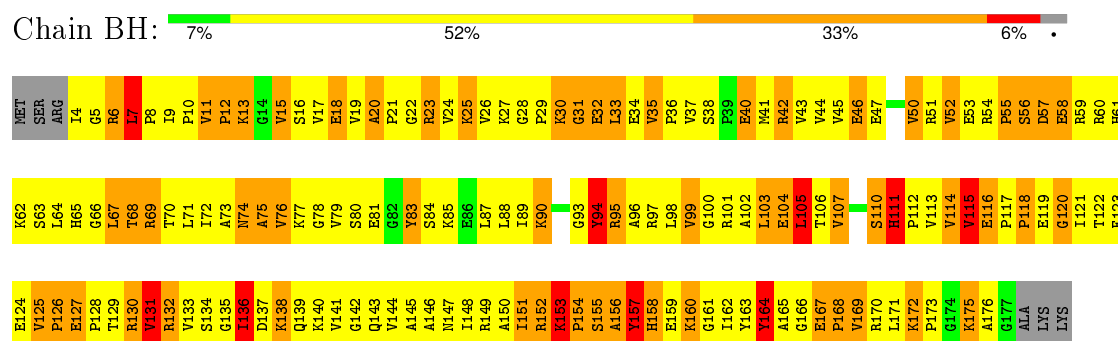
- Molecule 29: 50S ribosomal protein L4



- Molecule 30: 50S ribosomal protein L5

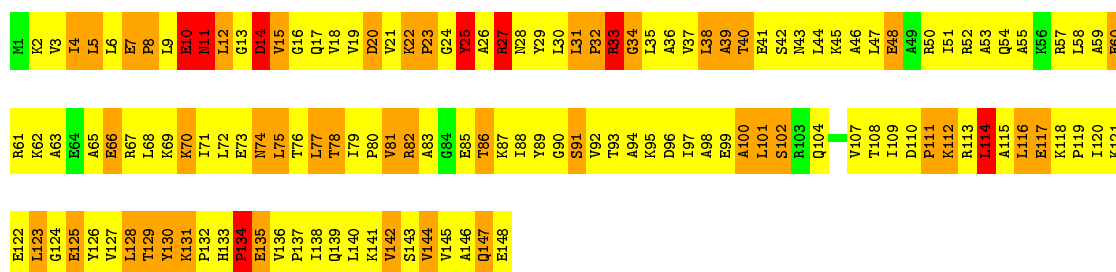


- Molecule 31: 50S ribosomal protein L6

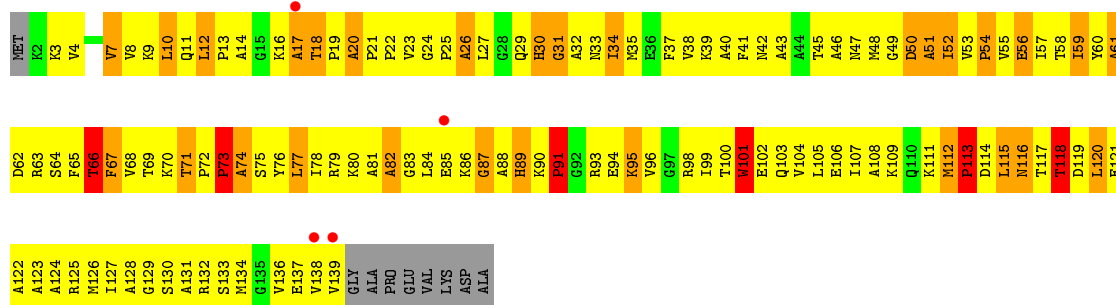
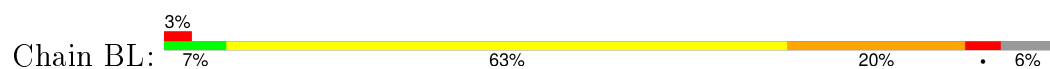


- Molecule 32: 50S ribosomal protein L9

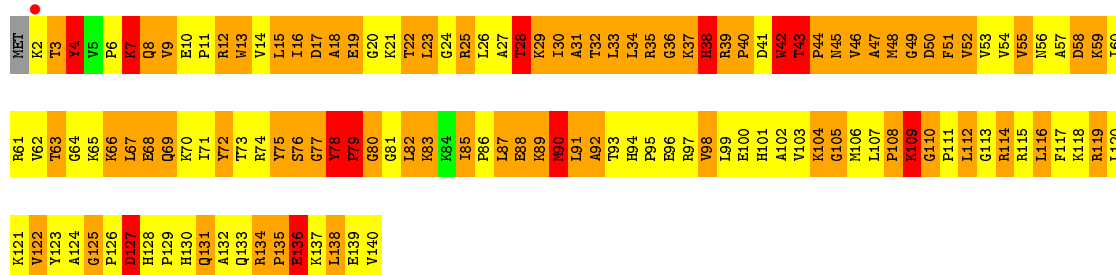




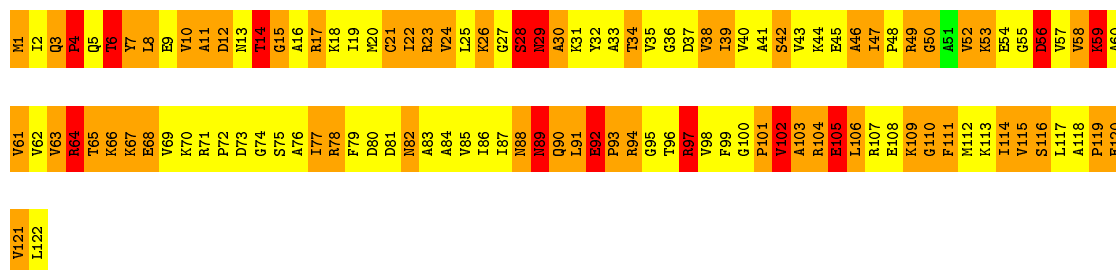
• Molecule 33: 50S ribosomal protein L11



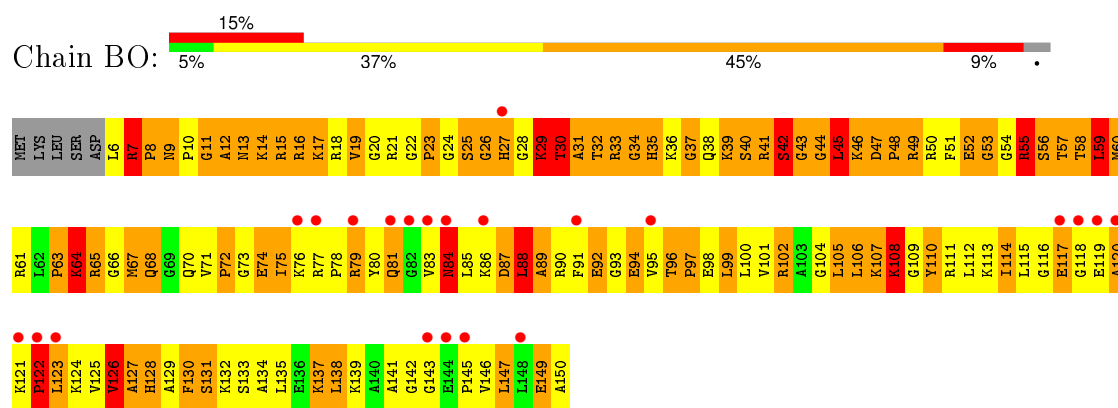
• Molecule 34: 50S ribosomal protein L13



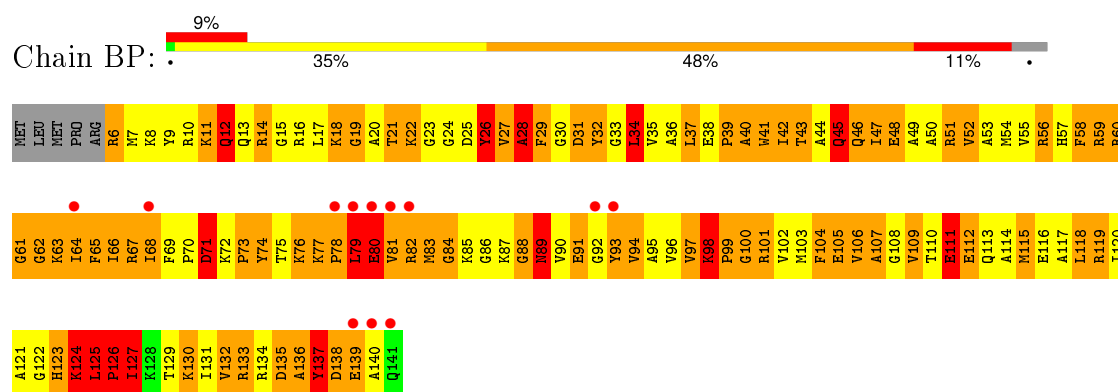
• Molecule 35: 50S ribosomal protein L14



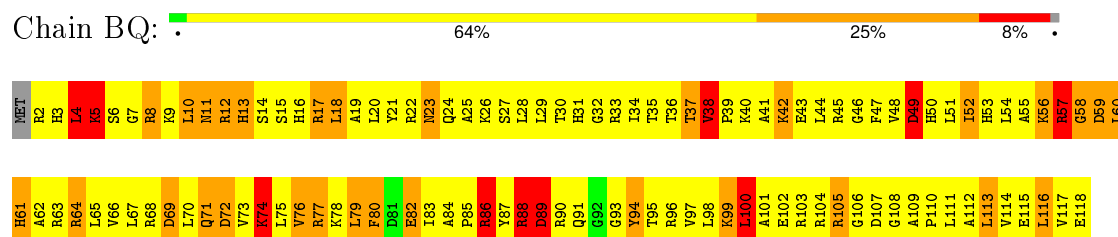
• Molecule 36: 50S ribosomal protein L15



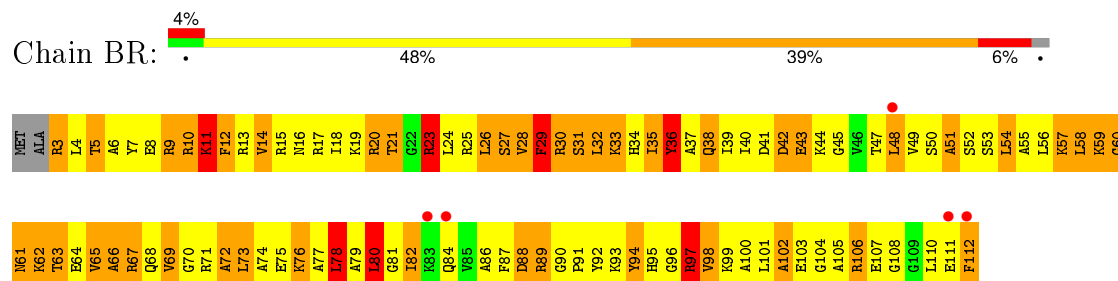
• Molecule 37: 50S ribosomal protein L16



• Molecule 38: 50S ribosomal protein L17



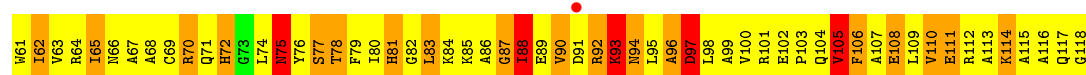
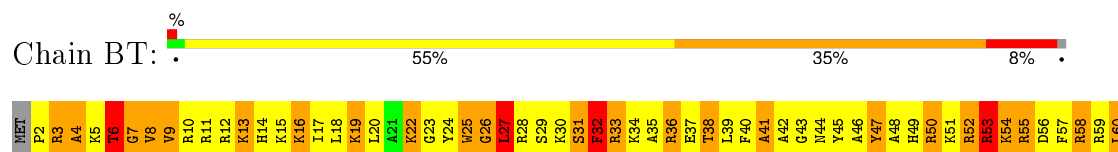
• Molecule 39: 50S ribosomal protein L18



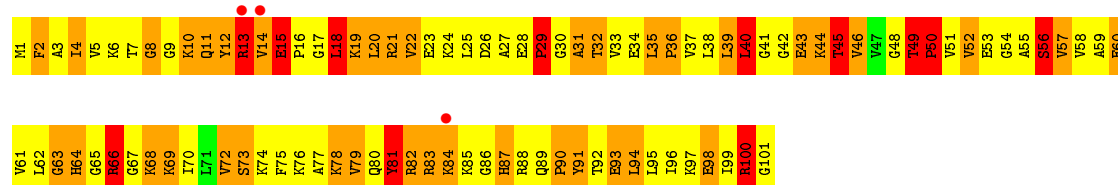
• Molecule 40: 50S ribosomal protein L19



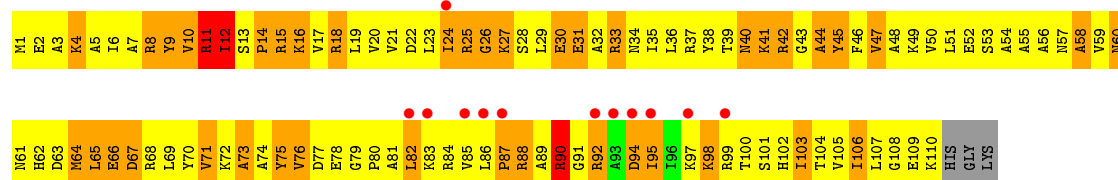
- Molecule 41: 50S ribosomal protein L20



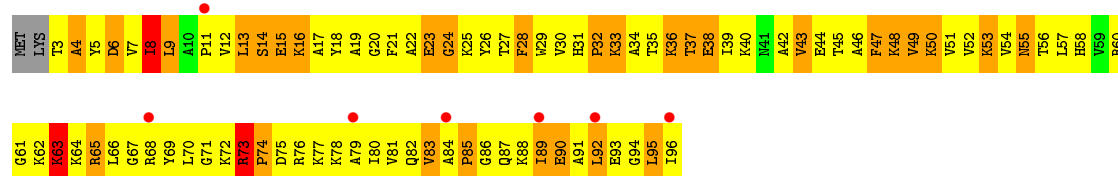
- Molecule 42: 50S ribosomal protein L21



- Molecule 43: 50S ribosomal protein L22

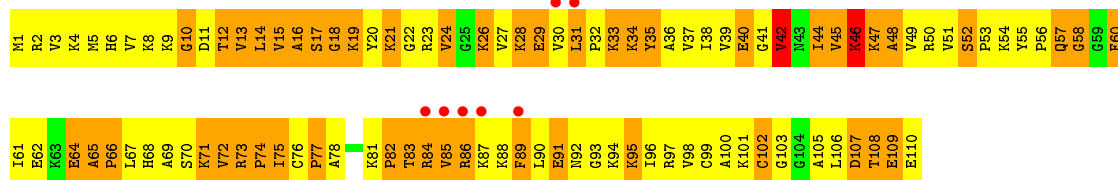


- Molecule 44: 50S ribosomal protein L23



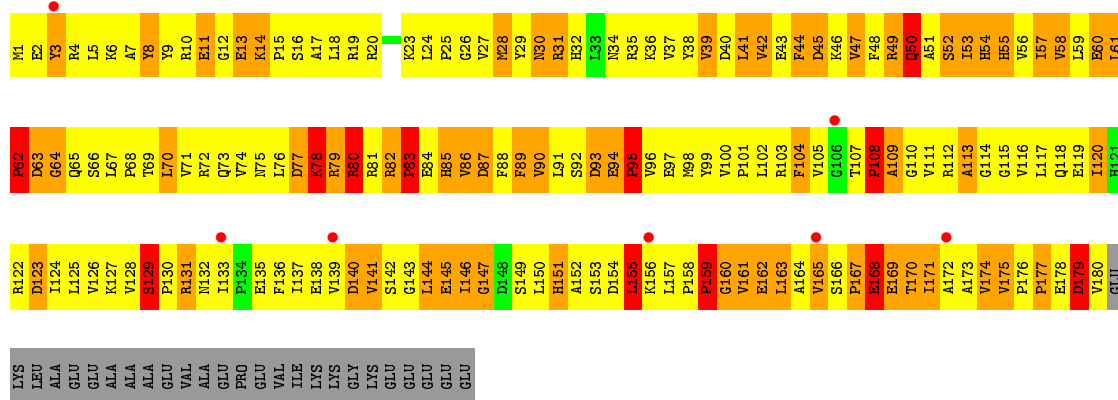
- Molecule 45: 50S ribosomal protein L24

Chain BX:  6% 48% 44%




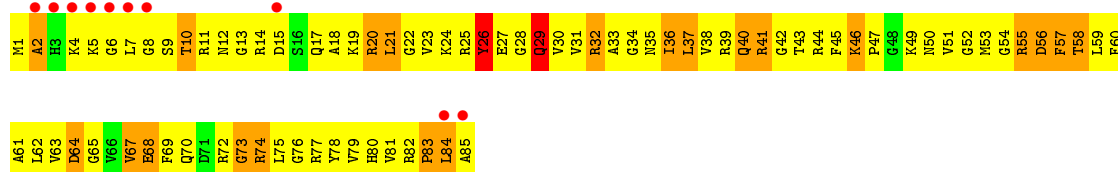
• Molecule 46: 50S ribosomal protein L25

Chain BY:  3% 49% 30% 6% 13%



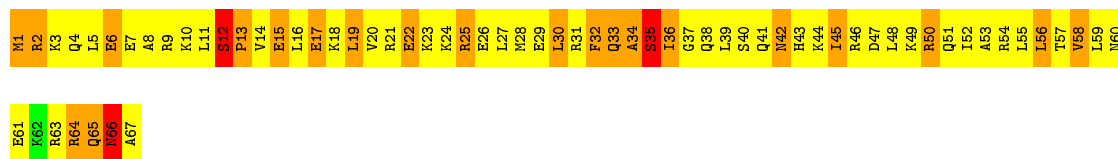
• Molecule 47: Ribosomal protein L27

Chain BZ:  12% 6% 67% 25%




• Molecule 48: 50S ribosomal protein L29

Chain B1:  63% 31%

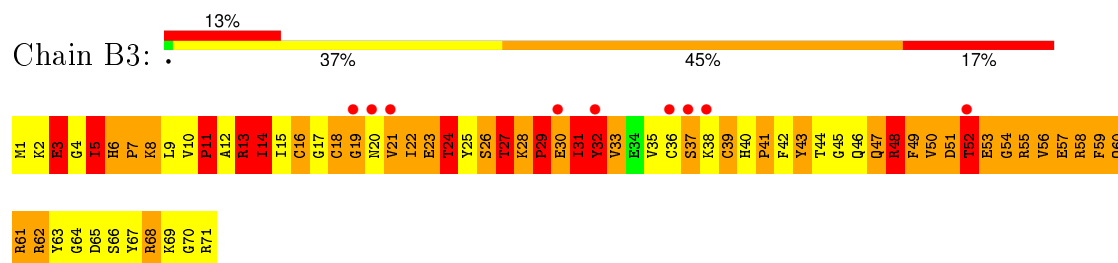


• Molecule 49: 50S ribosomal protein L30

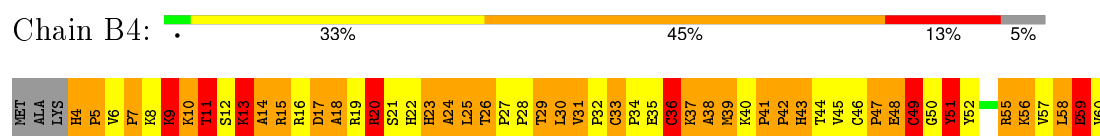
Chain B2:  3% 5% 45% 43% 5%



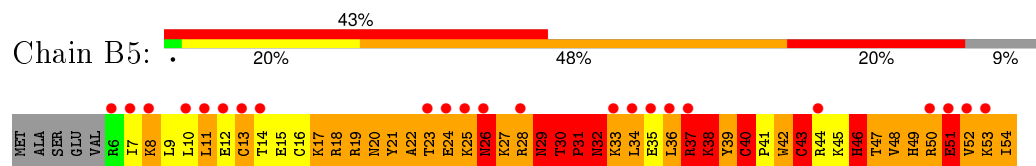
- Molecule 50: 50S ribosomal protein L31



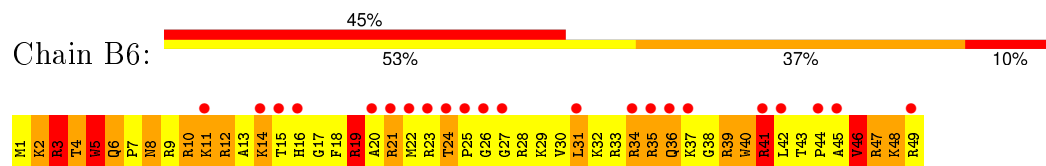
- Molecule 51: 50S ribosomal protein L32



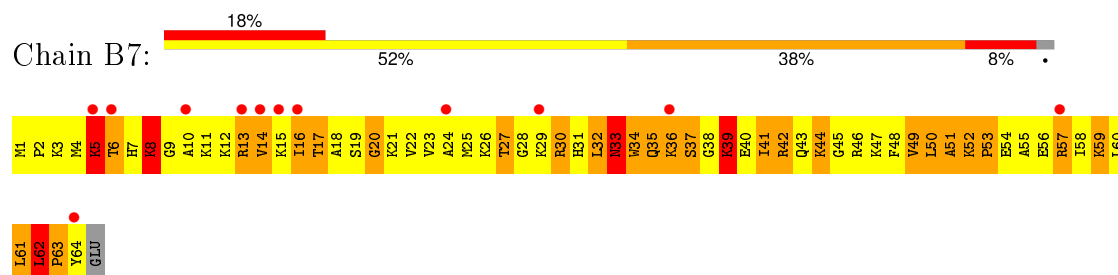
- Molecule 52: 50S ribosomal protein L33



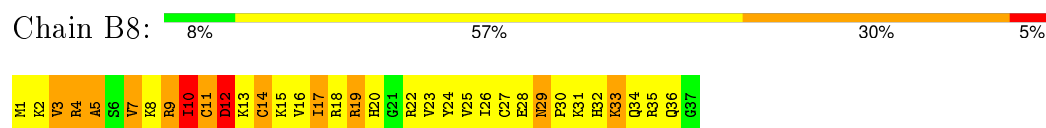
- Molecule 53: 50S ribosomal protein L34



- Molecule 54: 50S ribosomal protein L35



- Molecule 55: 50S ribosomal protein L36



4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	508.54Å 508.54Å 806.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	300.00 – 5.50 430.13 – 4.98	Depositor EDS
% Data completeness (in resolution range)	96.7 (300.00-5.50) 99.1 (430.13-4.98)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 4.88Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.243 , 0.326 0.280 , 0.327	Depositor DCC
R_{free} test set	8057 reflections (5.04%)	DCC
Wilson B-factor (Å ²)	108.9	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.07 , 78.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Outliers	1 of 226745 reflections (0.000%)	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	151691	wwPDB-VP
Average B, all atoms (Å ²)	226.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.63% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	0.87	32/36438 (0.1%)	1.08	147/56869 (0.3%)
2	A1	0.67	1/1133 (0.1%)	0.93	2/1753 (0.1%)
3	AB	0.70	1/1813 (0.1%)	1.02	9/2823 (0.3%)
3	AC	0.98	2/1813 (0.1%)	0.93	2/2823 (0.1%)
3	AD	0.69	1/1813 (0.1%)	0.92	2/2823 (0.1%)
4	AE	0.64	0/1935	1.00	4/2609 (0.2%)
5	AF	0.55	0/1636	0.92	4/2205 (0.2%)
6	AG	0.64	1/1733 (0.1%)	0.98	3/2318 (0.1%)
7	AH	0.63	0/1162	1.01	3/1564 (0.2%)
8	AI	0.60	0/856	0.95	0/1154
9	AJ	0.57	0/1276	0.90	3/1709 (0.2%)
10	AK	0.62	0/1136	1.01	3/1527 (0.2%)
11	AL	0.54	0/1029	0.83	0/1379
12	AM	0.48	0/807	0.89	1/1085 (0.1%)
13	AN	0.62	0/900	0.98	0/1213
14	AO	0.60	0/986	1.00	3/1320 (0.2%)
15	AP	0.50	0/1008	0.91	2/1347 (0.1%)
16	AQ	0.55	0/501	0.96	1/664 (0.2%)
17	AR	0.62	0/745	0.95	0/992
18	AS	0.62	0/716	0.95	1/963 (0.1%)
19	AT	0.68	1/870 (0.1%)	0.99	2/1159 (0.2%)
20	AU	0.59	0/603	1.01	1/799 (0.1%)
21	AV	0.51	0/661	0.92	0/890
22	AW	0.65	0/765	1.00	2/1007 (0.2%)
23	AX	0.45	0/212	0.80	0/277
24	BA	0.98	108/69685 (0.2%)	1.10	361/108786 (0.3%)
25	BB	0.83	4/2954 (0.1%)	0.99	7/4606 (0.2%)
26	BC	0.54	0/1775	0.86	0/2393
27	BD	0.72	2/2174 (0.1%)	1.19	12/2927 (0.4%)
28	BE	0.75	0/1611	1.16	13/2171 (0.6%)
29	BF	0.64	0/1660	1.03	4/2247 (0.2%)
30	BG	0.62	0/1507	1.06	4/2027 (0.2%)
31	BH	0.59	0/1354	0.99	4/1831 (0.2%)
32	BK	0.60	0/1170	1.02	4/1581 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	BL	0.61	0/1044	0.94	1/1415 (0.1%)
34	BM	0.77	1/1140 (0.1%)	1.16	8/1537 (0.5%)
35	BN	0.92	1/942 (0.1%)	1.31	10/1268 (0.8%)
36	BO	0.71	0/1123	1.12	5/1493 (0.3%)
37	BP	0.72	0/1100	1.19	8/1470 (0.5%)
38	BQ	0.70	0/974	1.06	2/1302 (0.2%)
39	BR	0.72	0/887	1.06	4/1180 (0.3%)
40	BS	0.85	0/990	1.31	9/1325 (0.7%)
41	BT	0.76	0/982	1.08	0/1306
42	BU	0.87	1/790 (0.1%)	1.28	9/1057 (0.9%)
43	BV	0.66	0/886	1.04	1/1189 (0.1%)
44	BW	0.57	0/756	0.93	0/1015
45	BX	0.54	0/857	1.04	2/1142 (0.2%)
46	BY	0.66	0/1467	1.11	7/1992 (0.4%)
47	BZ	0.65	0/679	1.04	1/902 (0.1%)
48	B1	0.59	0/569	0.88	0/751
49	B2	0.59	0/474	1.09	2/635 (0.3%)
50	B3	0.84	1/594 (0.2%)	1.31	8/795 (1.0%)
51	B4	0.71	0/459	1.16	3/621 (0.5%)
52	B5	0.85	1/433 (0.2%)	1.36	5/576 (0.9%)
53	B6	0.73	0/438	1.01	0/575
54	B7	0.60	0/523	1.14	5/690 (0.7%)
55	B8	0.59	0/310	1.08	1/407 (0.2%)
All	All	0.86	158/164854 (0.1%)	1.07	695/246484 (0.3%)

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	0	175
2	A1	0	3
3	AB	0	6
3	AC	0	8
3	AD	0	8
6	AG	0	1
8	AI	0	1
13	AN	0	1
15	AP	0	1
16	AQ	0	1
24	BA	0	463

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Mol	Chain	#Chirality outliers	#Planarity outliers
25	BB	0	18
26	BC	0	1
28	BE	0	1
34	BM	0	1
37	BP	0	1
40	BS	0	1
42	BU	0	1
50	B3	0	1
51	B4	0	1
All	All	0	694

The worst 5 of 158 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	BA	1203	G	O3'-P	-34.70	1.19	1.61
24	BA	2500	U	C4-O4	18.52	1.38	1.23
24	BA	2500	U	O3'-P	-15.17	1.43	1.61
24	BA	607	U	N3-C4	-14.53	1.25	1.38
24	BA	2448	A	O3'-P	-14.42	1.43	1.61

The worst 5 of 695 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1064	G	N1-C2-N2	-71.65	51.71	116.20
1	AA	1064	G	N3-C2-N2	57.72	160.30	119.90
24	BA	1203	G	P-O3'-C3'	27.70	152.94	119.70
24	BA	2448	A	C5'-C4'-O4'	-27.31	76.33	109.10
1	AA	1064	G	N1-C2-N3	-25.51	108.59	123.90

There are no chirality outliers.

5 of 694 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	12	U	Sidechain
1	AA	17	U	Sidechain
1	AA	31	G	Sidechain
1	AA	37	U	Sidechain
1	AA	45	U	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	32554	0	16431	6724	0
2	A1	1025	0	511	175	0
3	AB	1623	0	821	225	0
3	AC	1623	0	821	322	0
3	AD	1623	0	821	288	0
4	AE	1900	0	1951	1040	0
5	AF	1612	0	1677	721	0
6	AG	1703	0	1763	869	0
7	AH	1146	0	1207	588	0
8	AI	843	0	857	384	0
9	AJ	1257	0	1296	577	0
10	AK	1116	0	1177	735	0
11	AL	1010	0	1037	470	0
12	AM	794	0	840	358	0
13	AN	885	0	904	471	0
14	AO	970	0	1057	512	0
15	AP	997	0	1072	521	0
16	AQ	492	0	529	278	0
17	AR	734	0	771	332	0
18	AS	700	0	720	353	0
19	AT	857	0	930	450	0
20	AU	597	0	668	369	0
21	AV	647	0	673	312	0
22	AW	763	0	861	374	0
23	AX	208	0	221	83	0
24	BA	62218	0	31356	15296	0
25	BB	2641	0	1337	605	1
26	BC	1742	0	1796	739	0
27	BD	2124	0	2207	1491	0
28	BE	1578	0	1647	1084	0
29	BF	1625	0	1666	822	0
30	BG	1482	0	1546	898	0
31	BH	1328	0	1408	697	0
32	BK	1155	0	1244	502	0
33	BL	1025	0	1074	441	0
34	BM	1113	0	1183	782	0
35	BN	932	0	994	712	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	BO	1106	0	1183	795	0
37	BP	1080	0	1127	752	0
38	BQ	960	0	1021	603	0
39	BR	877	0	938	517	0
40	BS	976	0	1033	636	0
41	BT	964	0	1022	742	0
42	BU	779	0	852	574	0
43	BV	876	0	941	459	0
44	BW	742	0	800	360	0
45	BX	844	0	930	421	0
46	BY	1435	0	1463	720	0
47	BZ	670	0	700	354	0
48	B1	567	0	621	312	0
49	B2	469	0	518	320	0
50	B3	581	0	577	397	0
51	B4	445	0	459	277	0
52	B5	426	0	452	279	0
53	B6	430	0	480	273	0
54	B7	515	0	587	396	0
55	B8	307	0	335	150	0
All	All	151691	0	103113	46416	1

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 183.

The worst 5 of 46416 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)
24:BA:2447:G:C8	24:BA:2500:U:H3'	1.23	1.61
24:BA:1202:C:C5	24:BA:1203:G:H1'	1.39	1.55
24:BA:1203:G:O6	24:BA:1240:U:C2	1.66	1.48
24:BA:2459:A:N3	24:BA:2460:U:H1'	1.38	1.38
24:BA:2596:U:H2'	27:BD:242:ARG:CZ	1.55	1.35

All (1) 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)
25:BB:0:A:OP1	25:BB:0:A:OP1[15_545]	2.18	0.02

5.3 Torsion angles

5.3.1 Protein backbone

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	
4	AE	232/256 (91%)	114 (49%)	42 (18%)	76 (33%)	0	0
5	AF	204/239 (85%)	107 (52%)	46 (22%)	51 (25%)	0	2
6	AG	206/209 (99%)	96 (47%)	57 (28%)	53 (26%)	0	1
7	AH	148/162 (91%)	93 (63%)	38 (26%)	17 (12%)	0	9
8	AI	99/101 (98%)	58 (59%)	19 (19%)	22 (22%)	0	2
9	AJ	153/156 (98%)	73 (48%)	45 (29%)	35 (23%)	0	2
10	AK	136/138 (99%)	68 (50%)	35 (26%)	33 (24%)	0	2
11	AL	125/128 (98%)	62 (50%)	33 (26%)	30 (24%)	0	2
12	AM	96/105 (91%)	52 (54%)	20 (21%)	24 (25%)	0	2
13	AN	117/129 (91%)	65 (56%)	29 (25%)	23 (20%)	0	3
14	AO	122/132 (92%)	50 (41%)	30 (25%)	42 (34%)	0	0
15	AP	123/126 (98%)	56 (46%)	34 (28%)	33 (27%)	0	1
16	AQ	58/61 (95%)	24 (41%)	16 (28%)	18 (31%)	0	0
17	AR	86/89 (97%)	36 (42%)	35 (41%)	15 (17%)	0	4
18	AS	81/88 (92%)	42 (52%)	24 (30%)	15 (18%)	0	3
19	AT	102/105 (97%)	62 (61%)	23 (22%)	17 (17%)	0	5
20	AU	71/88 (81%)	26 (37%)	26 (37%)	19 (27%)	0	1
21	AV	78/93 (84%)	32 (41%)	23 (30%)	23 (30%)	0	0
22	AW	97/106 (92%)	38 (39%)	32 (33%)	27 (28%)	0	0
23	AX	22/27 (82%)	9 (41%)	6 (27%)	7 (32%)	0	0
26	BC	226/229 (99%)	155 (69%)	41 (18%)	30 (13%)	0	7
27	BD	270/276 (98%)	125 (46%)	59 (22%)	86 (32%)	0	0
28	BE	204/206 (99%)	117 (57%)	31 (15%)	56 (28%)	0	0
29	BF	206/210 (98%)	109 (53%)	46 (22%)	51 (25%)	0	2
30	BG	180/182 (99%)	79 (44%)	47 (26%)	54 (30%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	BH	172/180 (96%)	80 (46%)	46 (27%)	46 (27%)	0	1
32	BK	146/148 (99%)	91 (62%)	30 (20%)	25 (17%)	0	4
33	BL	136/147 (92%)	69 (51%)	38 (28%)	29 (21%)	0	3
34	BM	137/140 (98%)	64 (47%)	28 (20%)	45 (33%)	0	0
35	BN	120/122 (98%)	59 (49%)	23 (19%)	38 (32%)	0	0
36	BO	143/150 (95%)	57 (40%)	36 (25%)	50 (35%)	0	0
37	BP	134/141 (95%)	49 (37%)	33 (25%)	52 (39%)	0	0
38	BQ	115/118 (98%)	57 (50%)	39 (34%)	19 (16%)	0	5
39	BR	108/112 (96%)	48 (44%)	29 (27%)	31 (29%)	0	0
40	BS	115/146 (79%)	52 (45%)	26 (23%)	37 (32%)	0	0
41	BT	115/118 (98%)	35 (30%)	50 (44%)	30 (26%)	0	1
42	BU	99/101 (98%)	52 (52%)	19 (19%)	28 (28%)	0	0
43	BV	108/113 (96%)	63 (58%)	24 (22%)	21 (19%)	0	3
44	BW	92/96 (96%)	57 (62%)	16 (17%)	19 (21%)	0	3
45	BX	108/110 (98%)	43 (40%)	32 (30%)	33 (31%)	0	0
46	BY	178/206 (86%)	95 (53%)	44 (25%)	39 (22%)	0	2
47	BZ	83/85 (98%)	52 (63%)	21 (25%)	10 (12%)	0	8
48	B1	65/67 (97%)	36 (55%)	20 (31%)	9 (14%)	0	6
49	B2	57/60 (95%)	34 (60%)	8 (14%)	15 (26%)	0	1
50	B3	69/71 (97%)	23 (33%)	16 (23%)	30 (44%)	0	0
51	B4	55/60 (92%)	14 (26%)	19 (34%)	22 (40%)	0	0
52	B5	47/54 (87%)	14 (30%)	7 (15%)	26 (55%)	0	0
53	B6	47/49 (96%)	20 (43%)	12 (26%)	15 (32%)	0	0
54	B7	62/65 (95%)	23 (37%)	18 (29%)	21 (34%)	0	0
55	B8	35/37 (95%)	20 (57%)	5 (14%)	10 (29%)	0	0
All	All	5988/6337 (94%)	2955 (49%)	1476 (25%)	1557 (26%)	0	1

5 of 1557 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	AE	8	LYS
4	AE	11	LEU
4	AE	13	ALA

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Mol	Chain	Res	Type
4	AE	15	VAL
4	AE	16	HIS

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	
4	AE	202/220 (92%)	138 (68%)	64 (32%)	0	3
5	AF	160/188 (85%)	123 (77%)	37 (23%)	1	8
6	AG	180/181 (99%)	131 (73%)	49 (27%)	0	5
7	AH	115/123 (94%)	78 (68%)	37 (32%)	0	2
8	AI	90/90 (100%)	61 (68%)	29 (32%)	0	2
9	AJ	126/127 (99%)	93 (74%)	33 (26%)	0	5
10	AK	119/119 (100%)	86 (72%)	33 (28%)	0	4
11	AL	98/99 (99%)	73 (74%)	25 (26%)	1	6
12	AM	88/92 (96%)	67 (76%)	21 (24%)	1	7
13	AN	90/99 (91%)	74 (82%)	16 (18%)	2	16
14	AO	104/109 (95%)	81 (78%)	23 (22%)	1	9
15	AP	100/101 (99%)	75 (75%)	25 (25%)	1	6
16	AQ	49/50 (98%)	36 (74%)	13 (26%)	0	5
17	AR	79/80 (99%)	64 (81%)	15 (19%)	2	13
18	AS	72/74 (97%)	49 (68%)	23 (32%)	0	2
19	AT	96/97 (99%)	67 (70%)	29 (30%)	0	3
20	AU	64/77 (83%)	48 (75%)	16 (25%)	1	6
21	AV	71/80 (89%)	55 (78%)	16 (22%)	1	9
22	AW	76/82 (93%)	59 (78%)	17 (22%)	1	9
23	AX	19/22 (86%)	17 (90%)	2 (10%)	8	37
26	BC	180/181 (99%)	151 (84%)	29 (16%)	3	21
27	BD	215/218 (99%)	153 (71%)	62 (29%)	0	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	BE	166/166 (100%)	102 (61%)	64 (39%)	0	0
29	BF	164/166 (99%)	105 (64%)	59 (36%)	0	1
30	BG	156/156 (100%)	112 (72%)	44 (28%)	0	3
31	BH	143/148 (97%)	109 (76%)	34 (24%)	1	7
32	BK	124/124 (100%)	92 (74%)	32 (26%)	0	6
33	BL	105/111 (95%)	89 (85%)	16 (15%)	3	23
34	BM	118/119 (99%)	79 (67%)	39 (33%)	0	2
35	BN	100/100 (100%)	69 (69%)	31 (31%)	0	3
36	BO	111/116 (96%)	71 (64%)	40 (36%)	0	1
37	BP	106/111 (96%)	65 (61%)	41 (39%)	0	0
38	BQ	100/101 (99%)	71 (71%)	29 (29%)	0	3
39	BR	87/88 (99%)	63 (72%)	24 (28%)	0	4
40	BS	105/127 (83%)	68 (65%)	37 (35%)	0	1
41	BT	93/94 (99%)	64 (69%)	29 (31%)	0	3
42	BU	82/82 (100%)	57 (70%)	25 (30%)	0	3
43	BV	90/92 (98%)	64 (71%)	26 (29%)	0	3
44	BW	76/78 (97%)	57 (75%)	19 (25%)	1	6
45	BX	91/91 (100%)	72 (79%)	19 (21%)	1	10
46	BY	159/179 (89%)	120 (76%)	39 (24%)	1	6
47	BZ	67/67 (100%)	51 (76%)	16 (24%)	1	7
48	B1	62/62 (100%)	44 (71%)	18 (29%)	0	3
49	B2	51/52 (98%)	36 (71%)	15 (29%)	0	3
50	B3	63/63 (100%)	45 (71%)	18 (29%)	0	3
51	B4	50/52 (96%)	31 (62%)	19 (38%)	0	1
52	B5	48/52 (92%)	32 (67%)	16 (33%)	0	2
53	B6	42/42 (100%)	29 (69%)	13 (31%)	0	3
54	B7	54/55 (98%)	44 (82%)	10 (18%)	2	15
55	B8	34/34 (100%)	29 (85%)	5 (15%)	4	24
All	All	5040/5237 (96%)	3649 (72%)	1391 (28%)	0	4

5 of 1391 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
28	BE	45	THR
30	BG	174	GLU
48	B1	32	PHE
28	BE	119	ARG
29	BF	106	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 180 such sidechains are listed below:

Mol	Chain	Res	Type
26	BC	148	ASN
30	BG	40	ASN
52	B5	20	ASN
26	BC	188	ASN
28	BE	55	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1515/1522 (99%)	463 (30%)	137 (9%)
2	A1	49/50 (98%)	21 (42%)	4 (8%)
24	BA	2888/2916 (99%)	1204 (41%)	253 (8%)
25	BB	122/123 (99%)	46 (37%)	3 (2%)
3	AB	75/76 (98%)	32 (42%)	1 (1%)
3	AC	75/76 (98%)	23 (30%)	4 (5%)
3	AD	75/76 (98%)	23 (30%)	1 (1%)
All	All	4799/4839 (99%)	1812 (37%)	403 (8%)

5 of 1812 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	6	G
1	AA	8	A
1	AA	9	G
1	AA	14	U
1	AA	19	C

5 of 403 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
24	BA	503	A
24	BA	944	G

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Mol	Chain	Res	Type
24	BA	2571	C
24	BA	530	G
24	BA	745	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
24	BA	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	BA	1203:G	O3'	1204:A	P	1.19

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1515/1522 (99%)	-0.30	2 (0%) 95 95	145, 221, 302, 356	0
2	A1	50/50 (100%)	0.02	1 (2%) 68 62	200, 320, 348, 357	0
3	AB	76/76 (100%)	15.85	68 (89%) 0 1	288, 351, 370, 374	0
3	AC	76/76 (100%)	0.75	13 (17%) 2 6	167, 214, 260, 284	0
3	AD	76/76 (100%)	0.17	10 (13%) 4 8	222, 271, 293, 316	0
4	AE	234/256 (91%)	-1.03	0 100 100	189, 226, 271, 304	0
5	AF	206/239 (86%)	-0.19	11 (5%) 30 29	222, 244, 266, 277	0
6	AG	208/209 (99%)	-0.38	4 (1%) 70 64	168, 215, 233, 242	0
7	AH	150/162 (92%)	-0.71	0 100 100	174, 210, 235, 257	0
8	AI	101/101 (100%)	1.38	39 (38%) 0 3	191, 223, 236, 261	0
9	AJ	155/156 (99%)	0.72	23 (14%) 3 7	210, 240, 256, 275	0
10	AK	138/138 (100%)	-1.14	0 100 100	186, 208, 225, 232	0
11	AL	127/128 (99%)	-0.97	0 100 100	222, 261, 276, 287	0
12	AM	98/105 (93%)	-0.50	2 (2%) 68 62	230, 260, 274, 282	0
13	AN	119/129 (92%)	0.88	19 (15%) 3 7	193, 212, 245, 267	0
14	AO	124/132 (93%)	0.48	14 (11%) 7 10	179, 199, 233, 267	0
15	AP	125/126 (99%)	-0.77	0 100 100	223, 243, 272, 278	0
16	AQ	60/61 (98%)	-0.91	0 100 100	215, 248, 259, 263	0
17	AR	88/89 (98%)	-0.55	1 (1%) 82 78	186, 207, 231, 238	0
18	AS	83/88 (94%)	-0.97	0 100 100	180, 201, 226, 249	0
19	AT	104/105 (99%)	-0.49	2 (1%) 70 64	164, 193, 244, 277	0
20	AU	73/88 (82%)	-0.38	6 (8%) 14 16	184, 209, 258, 287	0
21	AV	80/93 (86%)	0.01	6 (7%) 17 19	226, 252, 266, 270	0
22	AW	99/106 (93%)	-0.18	8 (8%) 15 17	167, 195, 225, 241	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
23	AX	24/27 (88%)	-1.10	0 100 100	230, 249, 280, 288	0
24	BA	2889/2916 (99%)	-0.22	86 (2%) 54 47	129, 215, 297, 342	0
25	BB	123/123 (100%)	-0.48	0 100 100	199, 259, 293, 316	0
26	BC	228/229 (99%)	0.70	50 (21%) 1 5	250, 281, 300, 313	0
27	BD	272/276 (98%)	2.20	136 (50%) 0 3	130, 199, 221, 259	0
28	BE	206/206 (100%)	-0.53	3 (1%) 76 70	148, 186, 232, 269	0
29	BF	208/210 (99%)	-0.10	12 (5%) 26 25	164, 238, 263, 276	0
30	BG	182/182 (100%)	0.37	17 (9%) 11 14	212, 246, 268, 276	0
31	BH	174/180 (96%)	-0.90	0 100 100	196, 241, 260, 271	0
32	BK	148/148 (100%)	-0.87	0 100 100	202, 227, 249, 257	0
33	BL	138/147 (93%)	-0.36	4 (2%) 55 49	271, 298, 312, 327	0
34	BM	139/140 (99%)	-0.71	1 (0%) 89 85	167, 198, 224, 235	0
35	BN	122/122 (100%)	-0.23	0 100 100	148, 177, 209, 221	0
36	BO	145/150 (96%)	0.89	22 (15%) 3 7	166, 247, 276, 315	0
37	BP	136/141 (96%)	0.40	12 (8%) 12 15	166, 208, 234, 241	0
38	BQ	117/118 (99%)	-0.46	0 100 100	168, 192, 219, 226	0
39	BR	110/112 (98%)	-0.47	5 (4%) 37 34	186, 235, 263, 289	0
40	BS	117/146 (80%)	-0.07	3 (2%) 59 54	164, 194, 227, 242	0
41	BT	117/118 (99%)	-0.42	1 (0%) 85 81	183, 202, 220, 232	0
42	BU	101/101 (100%)	-0.24	3 (2%) 54 47	168, 225, 246, 257	0
43	BV	110/113 (97%)	0.35	12 (10%) 7 11	180, 209, 237, 248	0
44	BW	94/96 (97%)	0.33	7 (7%) 17 19	212, 232, 280, 288	0
45	BX	110/110 (100%)	-0.20	7 (6%) 23 22	221, 255, 287, 305	0
46	BY	180/206 (87%)	0.11	7 (3%) 43 39	208, 246, 268, 279	0
47	BZ	85/85 (100%)	0.55	10 (11%) 6 10	211, 229, 242, 271	0
48	B1	67/67 (100%)	-0.33	0 100 100	218, 243, 263, 268	0
49	B2	59/60 (98%)	0.10	2 (3%) 49 44	204, 224, 249, 259	0
50	B3	71/71 (100%)	0.43	9 (12%) 5 9	199, 223, 238, 246	0
51	B4	57/60 (95%)	-0.43	0 100 100	164, 209, 264, 289	0
52	B5	49/54 (90%)	1.92	23 (46%) 0 3	206, 232, 242, 252	0
53	B6	49/49 (100%)	1.81	22 (44%) 0 3	162, 209, 221, 235	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
54	B7	64/65 (98%)	1.06	12 (18%) 2 5	164, 195, 225, 242	0
55	B8	37/37 (100%)	-1.01	0 100 100	205, 215, 224, 226	0
All	All	10893/11176 (97%)	-0.01	695 (6%) 23 22	129, 223, 295, 374	0

The worst 5 of 695 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	AB	69	G	42.1
3	AB	67	C	37.1
3	AB	70	G	34.4
3	AB	68	C	34.1
3	AB	13	C	33.9

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.