



wwPDB X-ray Structure Validation Summary Report ⓘ

May 25, 2020 – 07:59 am BST

PDB ID : 4V4X
Title : Crystal structure of the 70S *Thermus thermophilus* ribosome showing how the 16S 3'-end mimicks mRNA E and P codons.
Authors : Jenner, L.; Yusupova, G.; Rees, B.; Moras, D.; Yusupov, M.
Deposited on : 2006-06-27
Resolution : 5.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

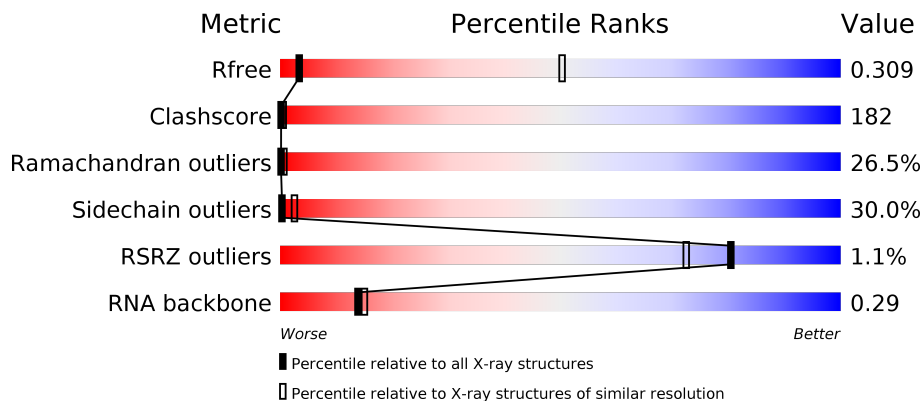
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 5.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



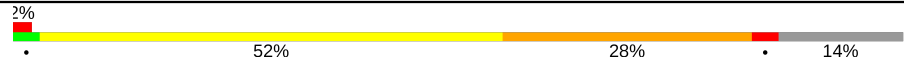
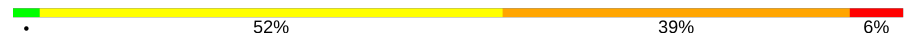
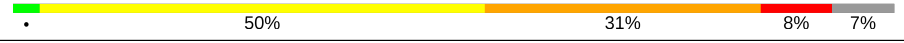
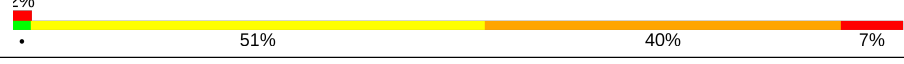
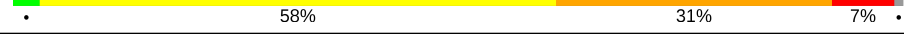

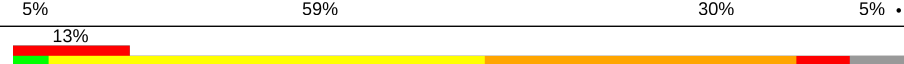
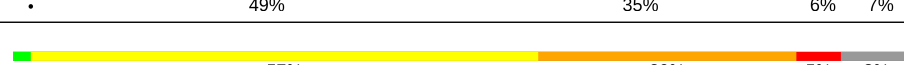

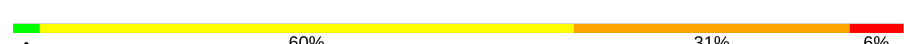
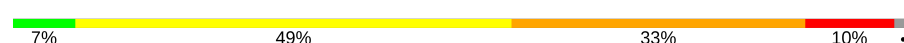


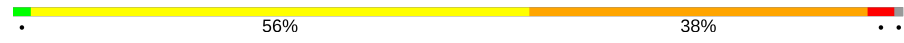





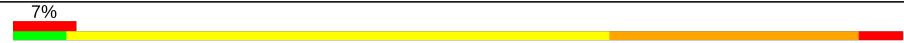





Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1140 (6.20-3.80)
Clashscore	141614	1000 (6.16-3.82)
Ramachandran outliers	138981	1146 (6.20-3.80)
Sidechain outliers	138945	1122 (6.20-3.80)
RSRZ outliers	127900	1010 (6.22-3.72)
RNA backbone	3102	1068 (7.00-3.00)

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

Mol	Chain	Length	Quality of chain
1	AA	1522	 4% 55% 34% 9%
2	AC	77	 45% 42% 10%
3	AD	76	 54% 42%
4	AE	256	 4% 48% 34% 7% 9%

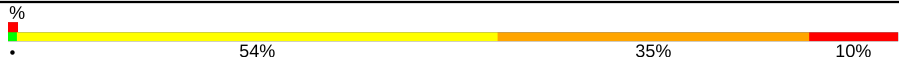

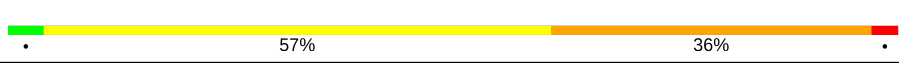
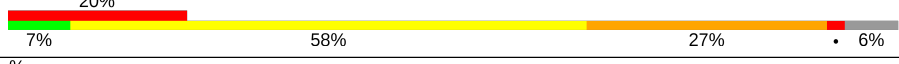
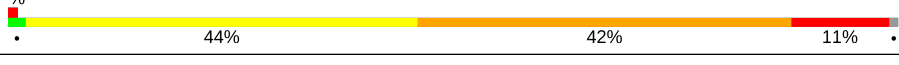



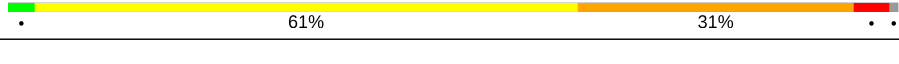
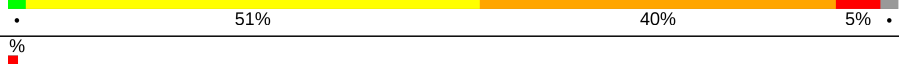
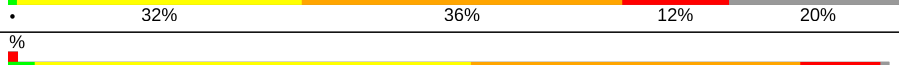


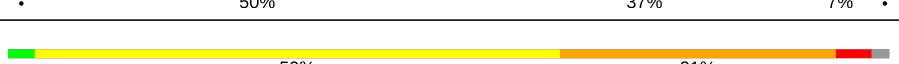


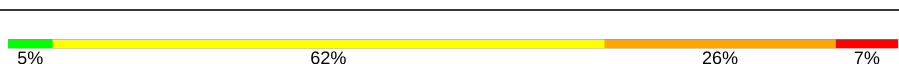
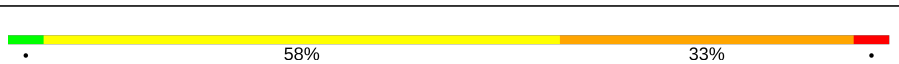
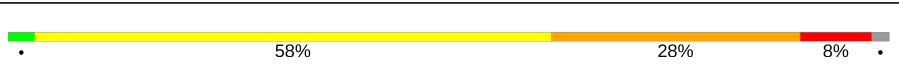


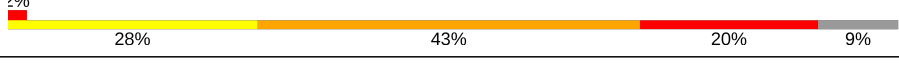



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Mol	Chain	Length	Quality of chain
5	AF	239	
6	AG	209	
7	AH	162	
8	AI	101	
9	AJ	156	
10	AK	138	
11	AL	128	
12	AM	105	
13	AN	129	
14	AO	132	
15	AP	126	
16	AQ	61	
17	AR	89	
18	AS	88	
19	AT	105	
20	AU	88	
21	AV	93	
22	AW	106	
23	AX	27	
24	BA	2916	
25	BB	123	
26	BC	229	
27	BD	276	
28	BE	206	
29	BF	210	


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Mol	Chain	Length	Quality of chain
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	
53	B6	49	
54	B7	65	

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Mol	Chain	Length	Quality of chain
55	B8	37	 5% 54% 38%

2 Entry composition [i](#)

There are 55 unique types of molecules in this entry. The entry contains 149044 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 rRNA.

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

- Molecule 2 is a RNA chain called tRNA fMET (unmodified bases).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	AC	76	1624	723	295	530	76	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BA	496	G	-	INSERTION	GB 48268

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

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BB	-1	A	-	INSERTION	GB 48271
BB	120	U	-	INSERTION	GB 48271

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
40	BS	117	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
			Total	C	N	O	S			
41	BT	117	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
			Total	C	N	O	S			
42	BU	101	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
			Total	C	N	O	S			
43	BV	110	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
			Total	C	N	O			
44	BW	94	742	483	133	126	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
45	BX	110	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
			Total	C	N	O	S			
46	BY	180	1435	916	256	260	3	0	0	0

- Molecule 47 is a protein called 50S ribosomal protein L27.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

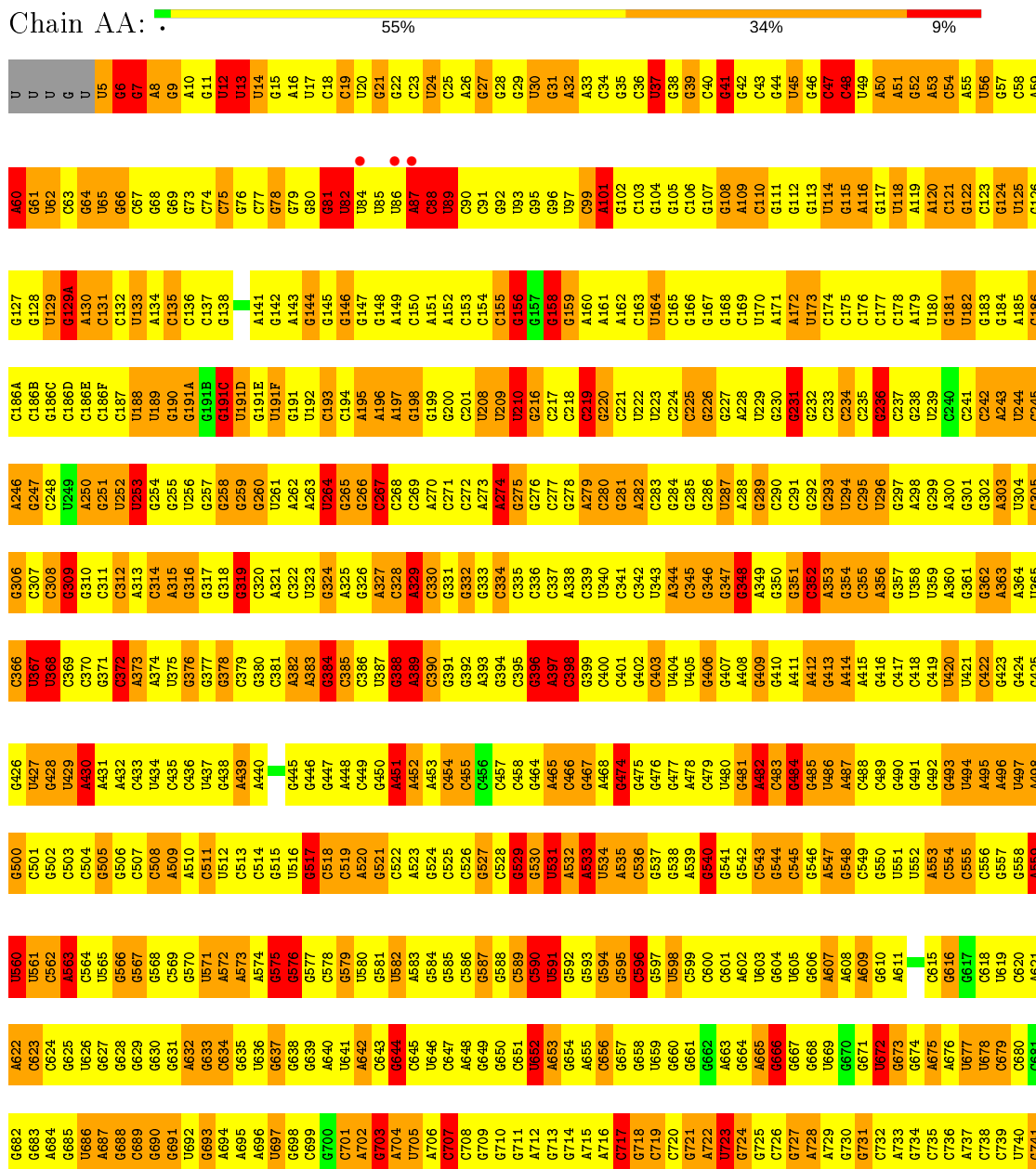
- Molecule 55 is a protein called 50S ribosomal protein L36.

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

3 Residue-property plots

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

- Molecule 1: 16S rRNA



G1529	G1469	G1404	U1345	A1285	A1225	G1164	G1104	A1044	C989	C929	G869	A802	G742
G1530	G1470	G1405	A1346	A1286	C1226	C1165	A1105	C1045	C990	C930	U870	G803	U743
A1531	G1471	U1406	G1347	A1287	A1227	A1166	A1106	A1046	U991	C931	A871	U804	C744
U1532	G1472	U1407	U1348	A1288	C1228	A1167	C1107	G1047	U992	C932	U872	G805	C745
C1533	A1473	A1408	A1349	A1289	A1229	A1169	G1108	G1048	G993	G933	A873	A807	C746
A1534	G1474	G1409	G1350	G1290	G1230	A1170	C1109	U1049	A994	C934	G874	G808	C747
C1535	G1475	G1410	U1351	G1291	G1231	G1171	A1110	G1050	C995	A935	C875	G809	C748
U1536	G1476	C1411	C1352	U1292	U1232	C1172	A1111	C1051	A996	C936	G876	C810	C749
U1537	C1477	C1412	C1353	G1293	G1233	A1173	G1112	U1052	U997	A937	C877	C811	G750
C1538	A1478	A1413	C1354	G1294	G1234	G1174	C1113	G1053	G998	A938	G878	C812	U751
C1539	C1479	U1414	C1355	G1295	U1235	G1175	C1114	C1054	C999A	G939	C879	U813	G752
U1540	G1480	G1415	G1356	C1296	A1236	A1176	G1115	A1055	U999	C940	G880	A814	A753
U1541	U1481	G1416	A1357	C1297	C1237	G1177	C1116	U1056	A1000	C941	G881	A815	C754
U1542	G1482	G1417	U1358	C1298	A1238	G1178	G1117	G1057	G1001	G942	C882	A816	G755
C	A1483	A1418	C1359	A1299	A1239	A1179	C1118	G1058	G1002	U943	C883	C817	C756
U	C1484	G1419	A1360	G1300	U1240	A1180	C1119	C1059	G1003	G944	U884	G818	U757
C	U1485	C1420	G1361	U1301	G1241	G1181	C1120	C1060	A1004	G945	G885	A819	G758
C	G1486	G1421	C1362	U1302	C1242	G1182	U1121	G1061	A1005	A946	G886	U820	A759
C	G1487	G1422	C1362A	C1303	C1243	A1183	U1122	U1062	C1006	G947	G887	G821	G760
C	G1488	G1423	A1363	G1304	C1244	G1184	A1123	C1063	C1007	C948	G888	G822	G761
C	G1489	G1424	U1364	U1305	A1245	G1185	G1124	G1064	C1008	U949	G889	G823	G762
C	A1490	U1425	C1365	A1306	C1246	G1186	U1125	U1065	G1009	U950	G890	G824	G763
C	G1491	C1426	C1366	U1307	U1247	G1187	U1126	C1066	G1010	G951	U891	G825	C764
C	A1492	U1427	C1367	U1308	A1248	A1188	G1127	A1067	G1011	U952	A892	C826	G765
C	G1493	A1428	G1368	G1309	G1249	G1189	C1128	G1068	U1012	C953	C893	U827	A766
C	G1494	C1429	C1369	G1310	A1250	G1190	C1129	C1069	G1013	G954	G894	A828	A767
C	U1495	A1430	G1370	G1311	A1251	A1191	A1130	A1070	A1014	U955	G895	G829	A768
C	C1496	C1431	C1371	G1312	A1252	C1192	G1131	C1071	A1015	U956	C896	G830	G769
C	G1497	G1432	U1372	U1313	G1253	G1193	C1132	G1072	A1016	U957	C897	U831	C770
C	U1498	A1433	G1373	C1314	G1254	U1194	G1133	U1073	G1017	A958	G898	C832	G771
C	A1499	A1434	A1374	U1315	G1255	G1195	G1134	G1074	C1018	A959	G899	U833	U772
C	A1500	G1435	A1375	G1316	A1256	U1196	U1135	G1075	C1019	U960	A900	G834	G773
C	C1501	U1436	U1376	G1317	U1257	G1197	U1136	C1076	U1020	U961	A901	U835	G774
C	A1502	A1437	C1377	A1318	G1258	U1198	C1137	G1077	G1021	G962	G902	G836	G775
C	G1503	G1438	C1378	A1319	G1259	U1199	C1138	U1078	G1022	G963	G903	G837	G776
C	G1504	C1439	G1379	C1320	C1260	G1200	G1139	G1079	G1023	A964	C904	G838	A777
C	G1505	G1440	U1380	C1321	A1261	A1201	C1140	A1080	G1024	A965	U905	U841	G778
C	U1506	G1441	U1381	C1322	C1262	G1202	C1141	G1081	U1025	C966	G906	C842	G779
C	A1507	G1442	C1382	C1323	C1263	C1203	G1142	G1082	G1026	C967	A907	U843	A780
C	C1508	G1443	C1383	A1324	G1264	A1204	G1143	U1083	C1027	A968	A908	C848	A781
C	C1509	A1446	C1384	C1325	G1265	U1205	G1144	G1084	G1028	A969	A909	C849	A782
C	U1510	G1447	G1385	C1326	G1266	G1206	C1145	U1085	C1028A	C970	C910	U850	C783
C	U1511	C1448	G1386	C1327	C1267	G1207	A1146	U1086	U1028B	G971	U911	G851	C784
C	U1512	G1449	G1387	C1328	A1268	C1208	C1147	G1087	G1028B	C972	C912	G852	G785
C	A1513	U1450	C1388	A1329	A1269	C1209	U1148	G1088	C1030	G973	A913	G853	G786
C	C1514	A1451	C1389	U1330	C1270	C1210	C1149	G1089	G1031	A974	A914	G854	U787
C	C1515	C1452	U1390	G1331	G1271	U1211	U1150	U1090	A1032	A975	A915	G855	A788
C	G1516	G1453	G1391	A1332	G1272	U1212	A1151	U1091	G1032A	G976	G916	C856	U789
C	G1517	G1454	G1392	A1333	G1273	A1213	A1152	A1092	G1032B	A977	G917	C857	A790
C	A1518	G1455	U1393	G1334	G1274	C1214	C1153	A1093	G1033	A978	A918	G858	G791
C	A1519	C1456	A1394	C1335	A1275	G1215	G1154	G1094	G1034	C979	A919	A859	A792
C	G1520	A1460	C1395	U1336	G1276	G1216	G1155	U1095	A1035	C980	U920	A860	U793
C	G1521	G1461	A1396	G1337	C1277	C1217	U1156	C1096	G1036	U981	U921	G861	A794
C	U1522	G1462	C1397	U1338	U1278	C1218	A1157	C1097	C1037	U982	G922	C862	C795
C	G1523	G1463	A1398	A1339	A1279	G1219	G1158	G1098	C1038	A983	A923	C863	C796
C	U1524	G1464	C1399	A1340	A1280	G1220	U1159	G1099	C1039	C984	C924	U864	C797
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C	G1526	G1466	G1401	C1342	G1282	G1222	C1161	C1101	A1041	A986	G926	G866	G799
C	G1527	G1467	C1343	G1343	G1283	C1223	C1162	A1102	G1042	G987	G927	G867	G800
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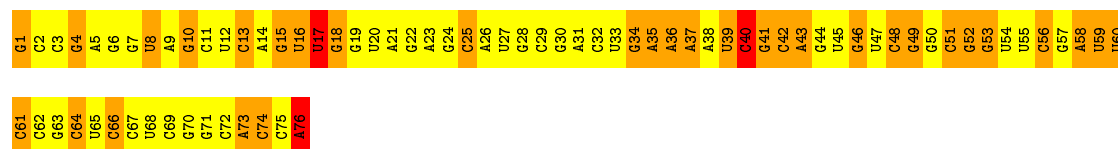
● Molecule 2: tRNA fMET (unmodified bases)

Chain AC:  45% 42% 10%

C1	C6	C11	C16	C21	C26	C31	C36	C41	C46	C51	C56	C61	C66	C71	C76	C81	C86	C91	C96	C101	C106	C111	C116	C121	C126	C131	C136	C141	C146	C151	C156	C161	C166	C171	C176	C181	C186	C191	C196	C201	C206	C211	C216	C221	C226	C231	C236	C241	C246	C251	C256	C261	C266	C271	C276	C281	C286	C291	C296	C301	C306	C311	C316	C321	C326	C331	C336	C341	C346	C351	C356	C361	C366	C371	C376	C381	C386	C391	C396	C401	C406	C411	C416	C421	C426	C431	C436	C441	C446	C451	C456	C461	C466	C471	C476	C481	C486	C491	C496	C501	C506	C511	C516	C521	C526	C531	C536	C541	C546	C551	C556	C561	C566	C571	C576	C581	C586	C591	C596	C601	C606	C611	C616	C621	C626	C631	C636	C641	C646	C651	C656	C661	C666	C671	C676	C681	C686	C691	C696	C701	C706	C711	C716	C721	C726	C731	C736	C741	C746	C751	C756	C761	C766	C771	C776	C781	C786	C791	C796	C801	C806	C811	C816	C821	C826	C831	C836	C841	C846	C851	C856	C861	C866	C871	C876	C881	C886	C891	C896	C901	C906	C911	C916	C921	C926	C931	C936	C941	C946	C951	C956	C961	C966	C971	C976	C981	C986	C991	C996	C1001	C1006	C1011	C1016	C1021	C1026	C1031	C1036	C1041	C1046	C1051	C1056	C1061	C1066	C1071	C1076	C1081	C1086	C1091	C1096	C1101	C1106	C1111	C1116	C1121	C1126	C1131	C1136	C1141	C1146	C1151	C1156	C1161	C1166	C1171	C1176	C1181	C1186	C1191	C1196	C1201	C1206	C1211	C1216	C1221	C1226	C1231	C1236	C1241	C1246	C1251	C1256	C1261	C1266	C1271	C1276	C1281	C1286	C1291	C1296	C1301	C1306	C1311	C1316	C1321	C1326	C1331	C1336	C1341	C1346	C1351	C1356	C1361	C1366	C1371	C1376	C1381	C1386	C1391	C1396	C1401	C1406	C1411	C1416	C1421	C1426	C1431	C1436	C1441	C1446	C1451	C1456	C1461	C1466	C1471	C1476	C1481	C1486	C1491	C1496	C1501	C1506	C1511	C1516	C1521	C1526	C1531	C1536	C1541	C1546	C1551	C1556	C1561	C1566	C1571	C1576	C1581	C1586	C1591	C1596	C1601	C1606	C1611	C1616	C1621	C1626	C1631	C1636	C1641	C1646	C1651	C1656	C1661	C1666	C1671	C1676	C1681	C1686	C1691	C1696	C1701	C1706	C1711	C1716	C1721	C1726	C1731	C1736	C1741	C1746	C1751	C1756	C1761	C1766	C1771	C1776	C1781	C1786	C1791	C1796	C1801	C1806	C1811	C1816	C1821	C1826	C1831	C1836	C1841	C1846	C1851	C1856	C1861	C1866	C1871	C1876	C1881	C1886	C1891	C1896	C1901	C1906	C1911	C1916	C1921	C1926	C1931	C1936	C1941	C1946	C1951	C1956	C1961	C1966	C1971	C1976	C1981	C1986	C1991	C1996	C2001	C2006	C2011	C2016	C2021	C2026	C2031	C2036	C2041	C2046	C2051	C2056	C2061	C2066	C2071	C2076	C2081	C2086	C2091	C2096	C2101	C2106	C2111	C2116	C2121	C2126	C2131	C2136	C2141	C2146	C2151	C2156	C2161	C2166	C2171	C2176	C2181	C2186	C2191	C2196	C2201	C2206	C2211	C2216	C2221	C2226	C2231	C2236	C2241	C2246	C2251	C2256	C2261	C2266	C2271	C2276	C2281	C2286	C2291	C2296	C2301	C2306	C2311	C2316	C2321	C2326	C2331	C2336	C2341	C2346	C2351	C2356	C2361	C2366	C2371	C2376	C2381	C2386	C2391	C2396	C2401	C2406	C2411	C2416	C2421	C2426	C2431	C2436	C2441	C2446	C2451	C2456	C2461	C2466	C2471	C2476	C2481	C2486	C2491	C2496	C2501	C2506	C2511	C2516	C2521	C2526	C2531	C2536	C2541	C2546	C2551	C2556	C2561	C2566	C2571	C2576	C2581	C2586	C2591	C2596	C2601	C2606	C2611	C2616
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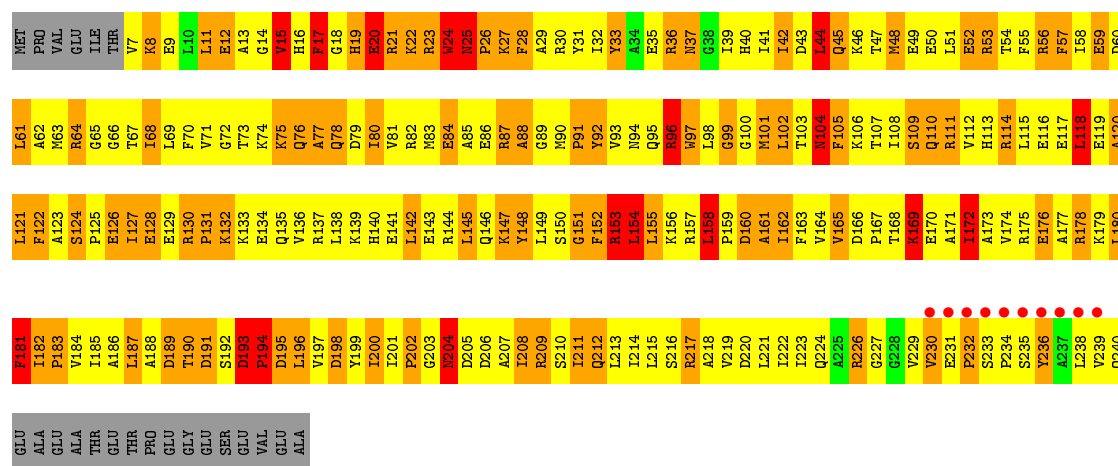
- Molecule 3: tRNA PHE (unmodified bases)

Chain AD: 



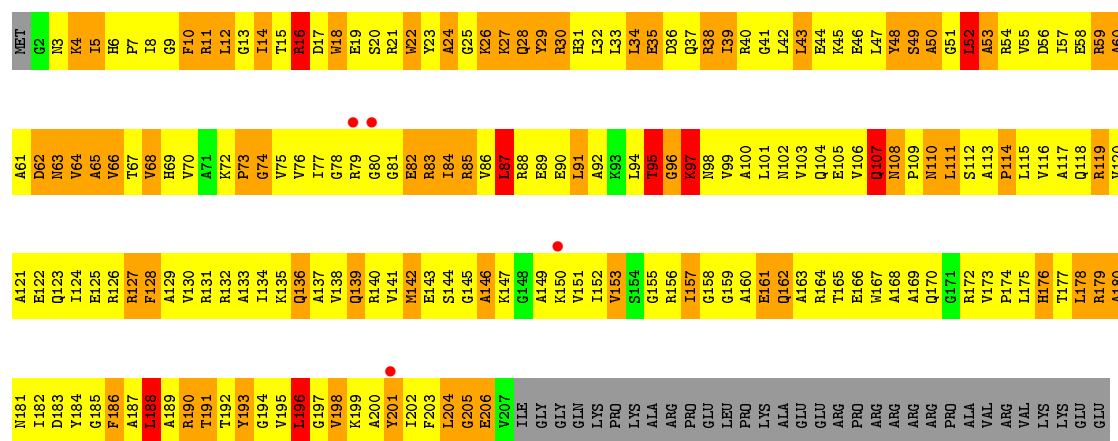
- Molecule 4: 30S ribosomal protein S2

Chain AE: 



- Molecule 5: 30S ribosomal protein S3

Chain AF: 



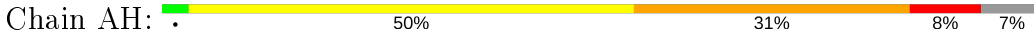
- Molecule 6: 30S ribosomal protein S4

Chain AG: 



K61	K62	K63	L64	R65	R66	L67	V68	G69	S70	S71	E72	R73	Q74	F75	R76	R77	N78	F79	E80	E81	A82	S83	K84	K85	K86	G87	V88	T89	G90	S91	V92	F93	L94	G95	L96	L97	E98	S99	R100	L101	D102	N103	V104	V105	Y106	R107	L108	G109	F110	A111	V112	S113	R114	R115	Q116	A117	R118	Q119	L120
V121	R122	H123	G124	H125	L126	V127	V128	N129	R130	R131	R132	V133	D134	L135	P136	S137	V138	R139	V140	R141	P142	G143	D144	E145	L146	A147	V148	A149	E150	K151	S152	R153	N154	L155	E156	L157	L158	R159	Q160	M161	L162	L163	A164	M165	R166	G167	R168	G169	V170	G171	P172	W173	L174	S175	L176	D177	V178	E179	G180
K181	K182	G183	K184	F185	L186	L187	L188	P189	D190	R191	E192	D193	L194	A195	L196	P197	V198	N199	E200	Q201	L202	V203	I204	E205	F206	Y207	R208																																

• Molecule 7: 30S ribosomal protein S5



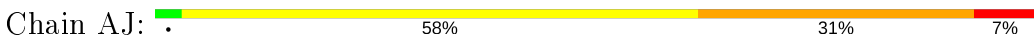
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Y61	A62	R63	R64	Y65	M66	V67	E68	V69	M70	L71	Q72	L73	G74	T75	T76	P77	H78	R79	I80	E81	G82	E83	F84	G85	A86	S87	K88	I89	V90	L91	K92	P93	A94	A95	P96	G97	T98	G99	V100	L101	A102	G103	A104	V105	P106	R107	A108	I109	L110	E111	L112	A113	K54	V55	D117	L118	L119	T120	
K121	E122	L123	G124	S125	L126	V127	P128	L129	M130	I131	Q132	A133	L134	T135	M136	E137	L138	L139	R140	Q141	L142	R143	T144	K145	A146	D147	V148	E149	R150	L151	R152	K153	G154	ALA	ALA	HIS	ALA	ALA	GLN	GLN	GLY																		

• Molecule 8: 30S ribosomal protein S6



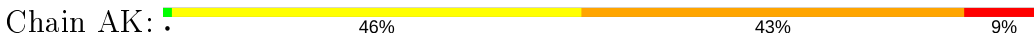
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L61	M62	Q63	Q64	A65	V66	M67	P68	E69	R70	R71	V72	M73	D74	L75	A76	R77	E78	L79	R80	L81	E82	D83	N84	V85	R86	R87	V88	M89	V90	V91	K92	S93	Q94	E95	P96	F97	L98	A99	M100	A101											

• Molecule 9: 30S ribosomal protein S7

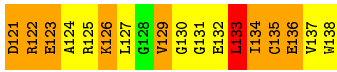


MET	A2	R3	R4	R5	R6	A7	E8	V9	R10	Q11	R12	Q13	P14	D15	L16	V17	Y18	G19	D20	V21	L22	V23	T24	A25	F26	L27	R28	K29	I30	M31	R32	D33	G34	K35	K36	N37	L38	A39	A40	R41	I42	F43	Y44	D45	A46	C47	K48	I49	I50	Q51	E52	K53	T54	G55	R56	E57	P58	L59	K60	
V61	F62	K63	Q64	A65	V66	E67	M68	V69	K70	Q71	P72	M73	E74	V75	R76	S77	R78	R79	V80	G81	E82	G83	N84	Y85	Q86	R87	P88	M89	E90	V91	S92	P93	R94	R95	Q96	Q97	S98	L99	A100	L101	R102	W103	L104	V105	Q106	A107	A108	N109	Q110	R111	P112	E113	R114	G55	R115	A116	A117	V118	R119	I120
A121	H122	E123	L124	M125	L126	A127	A128	E129	G130	K131	G132	G133	A134	V135	K136	K137	K138	E139	D140	V141	E142	R143	M144	A145	E146	M148	R149	A150	Y151	A152	H153	E33	Y94	I35	L36	W156																								

• Molecule 10: 30S ribosomal protein S8



M1	L2	T3	D4	P5	A6	A7	D8	M9	L10	T11	R12	L13	R14	M15	A16	T17	R18	V19	Y20	K21	E22	S23	T24	D25	V26	P27	K28	A28	S29	R30	F31	K32	E33	E34	I35	L36	R37	I38	L39	A40	R41	E42	G43	F44	I45	K46	G47	Y48	E49	R50	V51	D52	V53	T114	D54	G55	K56	P57	Y58	L119	R60
V61	Y62	L63	K64	V65	P66	P67	M68	R69	Q70	G71	P72	D73	F74	R75	E76	E77	Q78	V79	R80	H81	H82	I83	R84	R85	I86	S87	K88	P89	G90	R91	R92	V93	Y94	V95	G96	V97	K98	E99	I100	P101	R102	W103	R104	L105	G106	G108	I109	A110	I111	L112	S113	T114	S115	K116	G117	V118	L119	T120			



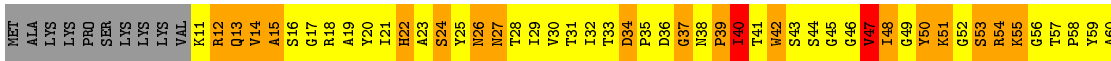
• Molecule 11: 30S ribosomal protein S9



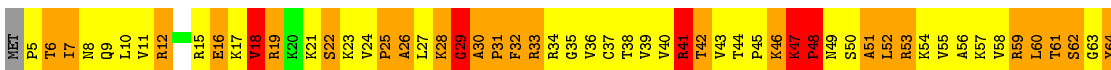
• Molecule 12: 30S ribosomal protein S10



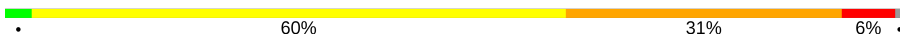
• Molecule 13: 30S ribosomal protein S11

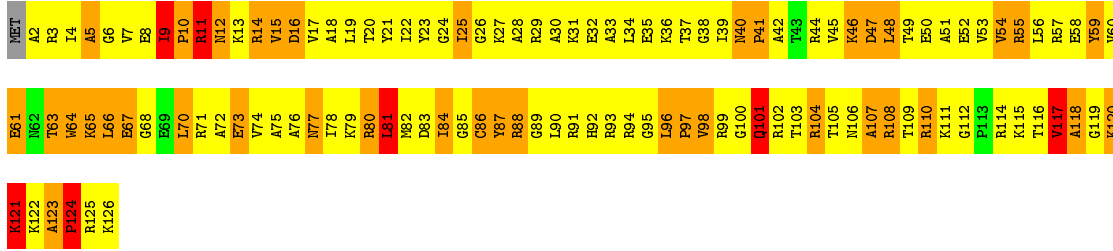


• Molecule 14: 30S ribosomal protein S12



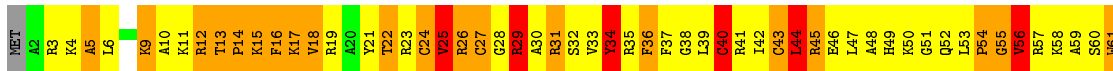
- Molecule 15: 30S ribosomal protein S13

Chain AP:  60% 31% 6%



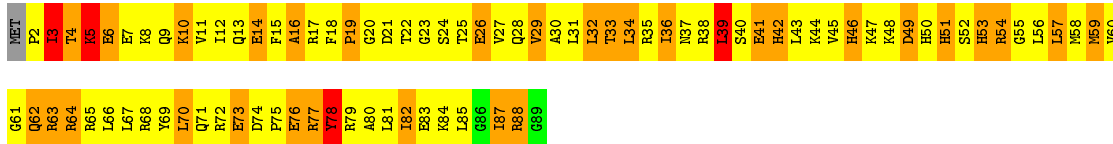
- Molecule 16: 30S ribosomal protein S14

Chain AQ:  7% 49% 33% 10%

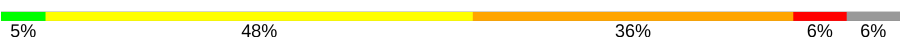


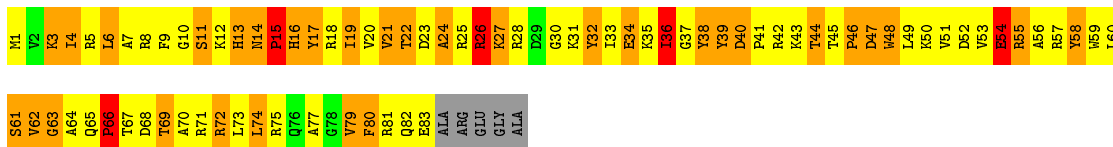
- Molecule 17: 30S ribosomal protein S15

Chain AR:  57% 35%

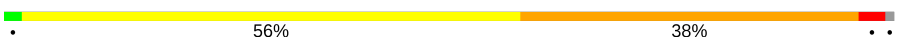


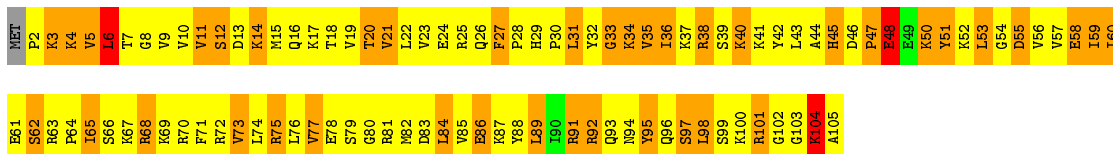
- Molecule 18: 30S ribosomal protein S16

Chain AS:  5% 48% 36% 6% 6%



- Molecule 19: 30S ribosomal protein S17

Chain AT:  56% 38%



- Molecule 20: 30S ribosomal protein S18

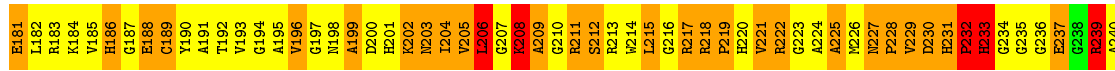
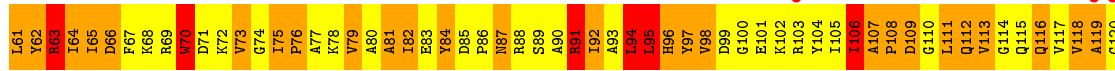
Chain AU:  5% 45% 26% 7% 17%



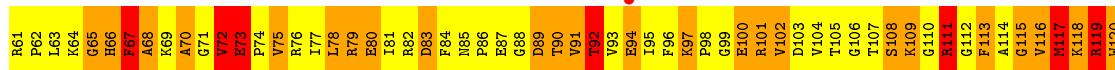
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A1336	A1276	G1216	A1155	A1095	U1035	G975	C915	G854	G794	A734	G674	C636	A578	C516	C455	U395	G338
G1337	A1277	G1217	A1156	A1096	G1036	C976	G916	G855	C795	A735	A675	A637	G579	C517	C456	G396	U339
G1338	A1278	C1218	G1157	U1097	G1037	G977	G917	G856	C796	A736	A676	C638	C580	G518	A457	G397	A340
G1339	A1279	G1219	A1158	A1098	G1038	G978	G918	G857	C797	A737	A677	U639	C581	U519	G458	G398	G341
U1340	G1280	A1220	U1159	G1099	G1039	G979	G919	U858	G798	G738	G678	U640	C582	G520	U459	G399	G342
U1341	G1281	C1221	G1160	C1100	C1040	A880	G920	G859	G799	G739	G679	G641	C583	G521	A460	G400	C343
G1342	U1282	C1222	C1161	U1101	G1041	A881	G921	U860	A800	G740	G680	G642	C584	G522	C461	A401	G344
G1343	G1283	C1223	G1162	C1102	G1042	C982	G922	A861	G801	G741	G681	A643	C585	C523	C462	A402	A345
G1344	A1284	G1224	A1163	A1103	C1043	A883	C923	G862	A802	G742	G682	A644	C586	U524	G463	U403	A346
C1345	G1285	G1225	G1164	G1104	G1044	A884	C924	A863	U803	G743	G683	C645	C587	U525	U464	C404	A347
G1346	A1286	G1226	U1165	U1105	A1045	C985	C925	G864	A804	G744	G684	A646	U588	A526	G465	U405	G348
G1347	A1287	A1227	C1166	G1106	A1046	C986	A926	C865	G805	G745	A685	G647	C589	C527	U466	G406	G349
G1348	U1288	G1228	U1167	G1107	G1047	G987	G928	A866	C806	A746	G686	G648	A590	A528	G467	G407	U350
A1349	G1289	G1229	G1168	U1108	A1048	A988	G929	C867	U807	A747	G687	G649	C591	A529	G468	G408	G351
C1350	C1290	C1230	G1169	C1109	C1049	G989	U930	U868	G808	G748	G688	C	C	G530	G469	C409	G352
C1351	G1291	G1231	G1170	A1110	A1050	A990	G931	A869	C809	C749	A689	C	G593	C531	A470	G410	G353
U1352	U1292	G1232	A1171	G1111	G1051	C991	G932	G870	U810	A750	G690	C	U594	A532	A471	G411	G354
A1353	C1293	C1233	G1173	G1112	C1052	C992	A933	U871	U811	A751	C691	A	C595	G533	A472	A412	G355
A1354	U1294	U1234	A1174	U1113	C1053	G993	G934	A872	C812	A752	C692	A	G596	U534	G473	C413	G356
G1355	C1295	G1235	U1175	G1114	A1054	C994	C935	G873	U813	C753	C693	G	U597	C535	G474	C414	A357
G1356	G1296	G1236	G1176	G1115	G1055	C995	C936	G874	C814	C754	U694	C	G598	A536	U475	A415	U358
U1357	C1297	A1237	A1177	C1116	G1056	A996	U937	G875	C815	C755	G695	C	G599	C537	G476	C416	A359
G1358	G1298	G1238	C1178	G1117	A1057	C997	G938	C876	C816	C756	G696	C	G600	G539	A477	G417	G360
A1359	G1299	G1239	C1179	C1118	G1058	C998	G939	U877	C817	U757	G697	G	G601	G540	A478	G418	G361
A1360	U1300	U1240	C1180	G1119	G1059	U999	G940	A878	G818	C758	C698	C	G602	C541	A479	G	U362
G1361	A1301	A1241	C1181	A1120	U1060	A1000	A941	G879	A819	G759	A699	C	A603	C542	A480	C419	G363
C1362	A1302	A1242	A1182	C1121	U1061	A1001	G942	G880	A820	G760	G700	C	G604	C543	G481	C420	A363A
G1363	G1303	G1243	G1183	G1122	G1062	G1002	U943	G881	A821	A761	G701	C	C605	C544	A482	U421	G363B
G1364	C1304	G1244	C1184	C1123	G1063	G1003	G944	G882	U822	U762	G702	A	U606	C545	A483	A422	G363C
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A1367	A1307	A1247	G1187	A1126	U1066	C1006	G947	C885	C825	G765	A705	C	A609	A548	C486	G425	A363F
G1368	G1308	G1248	A1188	A1127	A1068	C1007	G948	C886	U826	G766	A706	G	G609A	G549	C487	G426	C364
G1369	G1309	U1249	A1189	A1128	G1069	C1008	C949	A887	U827	U767	G707	G	G610	G550	G488	U427	C365
C1370	G1310	G1250	A1190	A1129	A1069	A1009	G950	C888	U828	G768	C708	C	C611	G551	G489	A428	G366
G1371	G1311	C1251	G1191	U1130	A1070	A1010	C951	C889	A829	G769	U709	C	G612	G552	G491	A429	G370
U1372	U1312	G1252	G1192	G1131	G1071	G1011	G952	A890	G830	G770	G710	C	U613	U553	A492	G430	A371
A1373	U1313	A1253	G1193	A1132	C1072	U1012	A953	G892	G831	G771	G711	C	U614	U554	G493	U431	G372
G1374	C1314	A1254	A1194	U1133	A1073	C1013	G954	C893	G832	C772	G712	C	G615	G556	G494	A432	U373
C1375	G1315	U1255	G1195	G1134	G1074	U1014	C955	U894	U833	U773	G713	C	A616	G557	G495	C433	A374
C1376	U1316	G1256	C1196	C1135	C1075	G1015	G956	C895	C834	A774	U714	C	G617	G558	G496	U434	C375
A1377	A1317	C1257	G1197	G1136	C1076	A1016	A957	A896	A835	G775	G715	C	G618	G559	A497	C435	G376
G1378	G1318	C1258	U1198	G1137	A1077	G1017	U958	C897	G836	G776	A716	C	G618A	C560	G498	C436	C377
A1379	G1319	G1259	U1199	C1138	A1078	C1018	A959	C898	C837	A777	G717	C	G619	G561	U499	G438	C378
C1320	C1320	G1260	C1200	G1139	C1079	U1019	A960	A899	C838	G778	A718	C	G620	U562	G500	G439	G379
A1321	A1321	C1261	C1201	C1140	C1080	A1020	C961	A900	U839	U779	C719	C	A621	G563	A501	G440	U380
A1322	C1322	U1262	G1202	U1141	U1081	A1021	G962	A901	C840	G780	C720	C	G622	C564	A502	U441	G381
C1323	U1323	A1263	U1142	U1142	U1082	G1022	U963	C902	A841	A781	C721	C	G623	C565	A503	G442	G382
A1324	G1324	G1264	A1204	A1142A	U1083	U1023	C964	C903	G842	A782	A722	C	G624	U566	U504	A443	U383
G1325	G1325	A1265	U1205	A1143	A1084	G1024	C965	C904	G843	A783	G723	C	G625	A567	A505	C444	U384
U1326	U1326	G1266	G1206	G1144	A1085	G1025	G966	U905	C844	A784	U724	C	U626	U568	G506	C445	C385
C1327	C1327	U1267	C1145	C1145	A1086	U1026	G967	G906	G845	G785	G725	C	G627	U569	A507	G446	G386
G1328	G1328	A1268	C1208	G1146	G1087	A1027	G968	U907	G846	G786	G726	C	G628	G570	G508	A447	U387
U1329	U1329	A1269	C1209	A1148	G1088	A1028	G969	C908	U847	U787	A727	C	G629	A571	C509	U448	G388
C1330	C1330	C1270	A1210	G1089	G1089	A1029	C970	A909	G848	A788	G728	C	G630	A572	C510	U449	G389
A1331	A1331	G1271	U1211	C1150	U1090	G1030	C971	A910	A849	A789	G729	C	A631	G573	U511	G450	A390
G1332	G1332	U1272	C1212	C1151	C1091	G1032	G972	A911	C850	C790	G730	C	A632	C574	A512	G451	G391
A1333	C1333	C1273	A1213	C1152	C1092	A1032	A973	C912	U851	C791	G731	C	A633	A575	A513	G452	C392
G1334	G1334	A1274	A1214	C1153	G1093	U1033	G974	U913	G852	G792	C732	C	C634	U576	A514	C453	C393



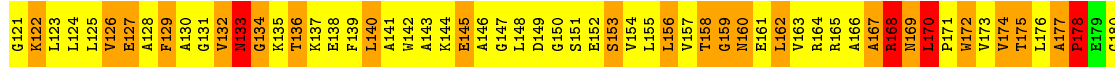
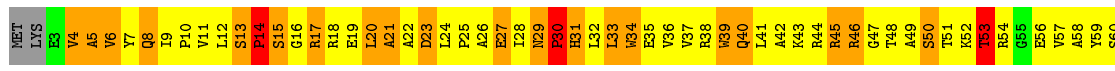
• Molecule 27: 50S ribosomal protein L2



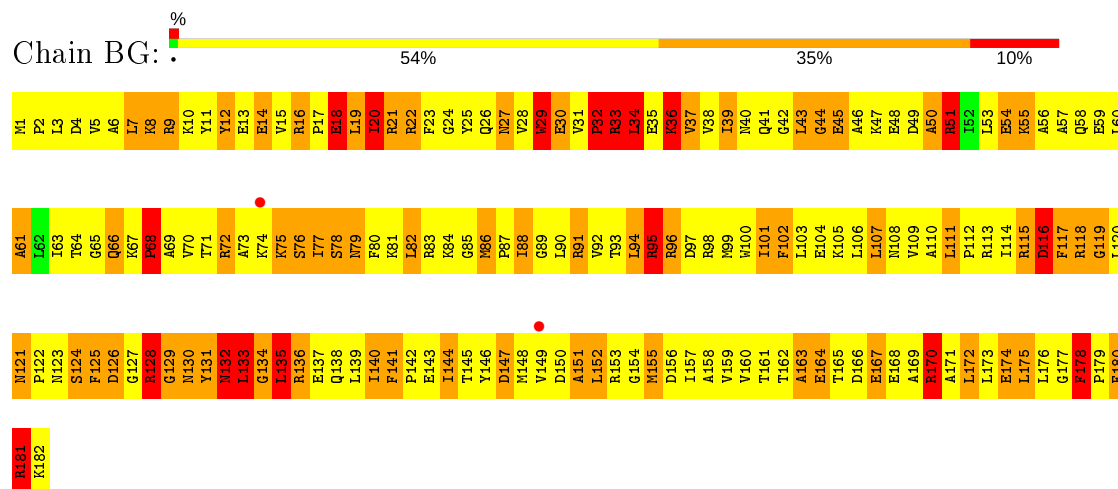
• Molecule 28: 50S ribosomal protein L3



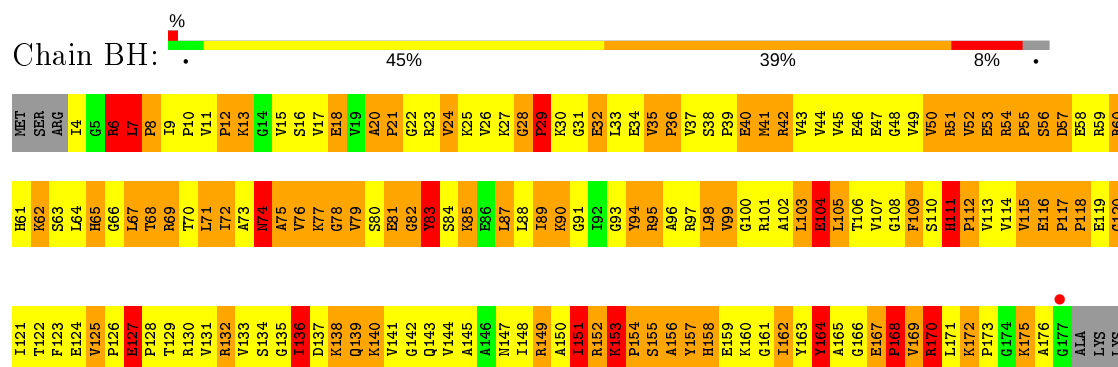
• Molecule 29: 50S ribosomal protein L4



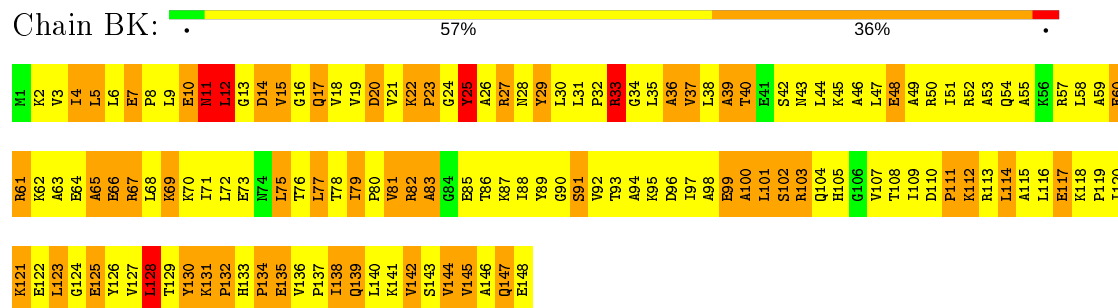
- Molecule 30: 50S ribosomal protein L5



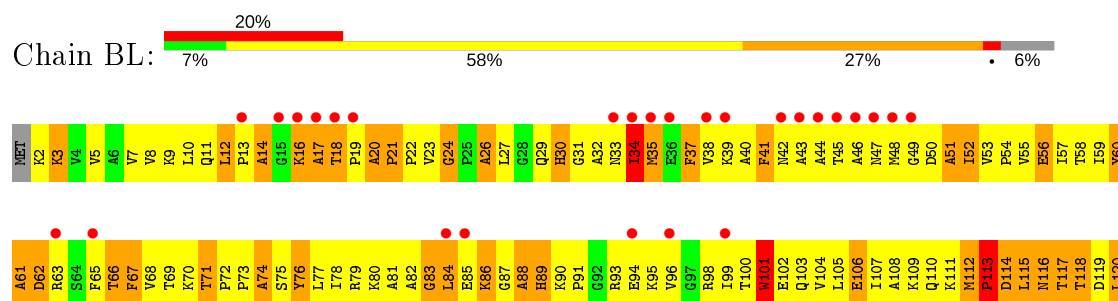
- Molecule 31: 50S ribosomal protein L6

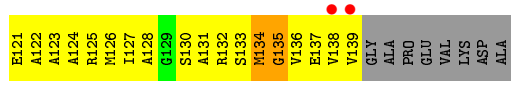


- Molecule 32: 50S ribosomal protein L9

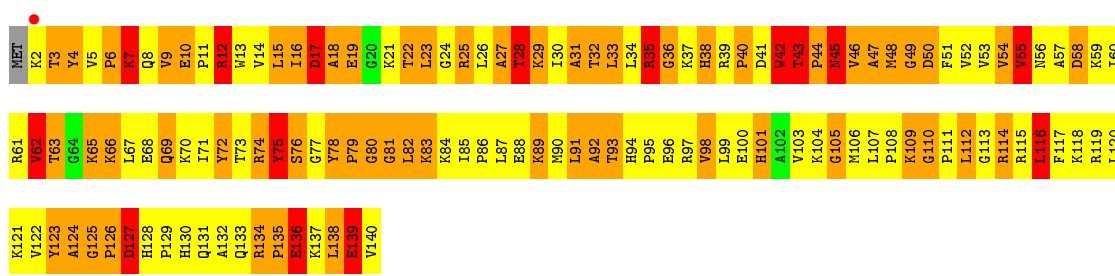


- Molecule 33: 50S ribosomal protein L11

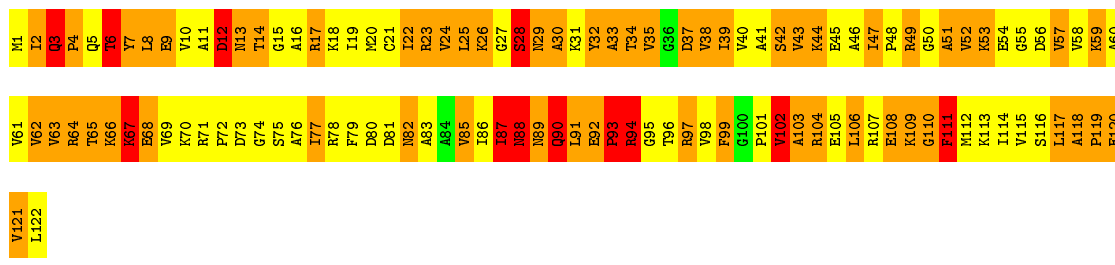
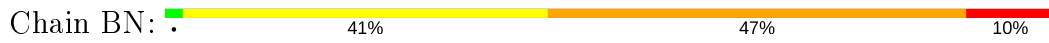




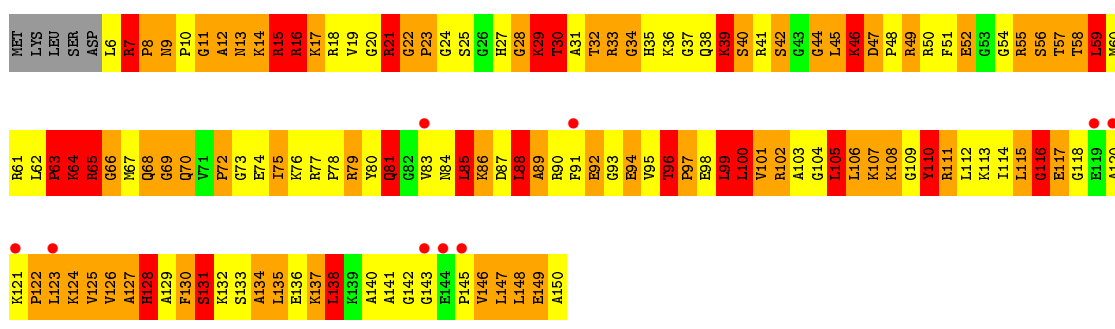
• Molecule 34: 50S ribosomal protein L13



• Molecule 35: 50S ribosomal protein L14



• Molecule 36: 50S ribosomal protein L15



• Molecule 37: 50S ribosomal protein L16

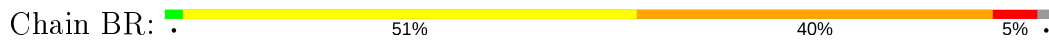




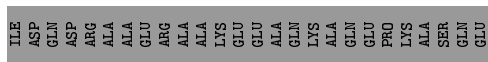
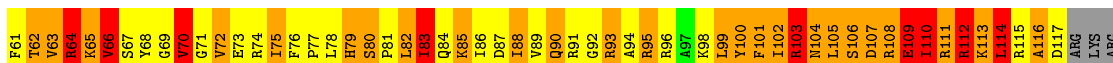
- Molecule 38: 50S ribosomal protein L17



- Molecule 39: 50S ribosomal protein L18



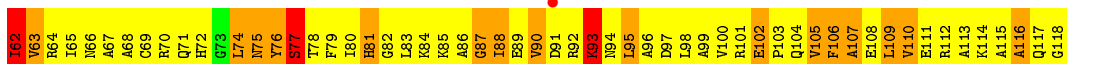
- Molecule 40: 50S ribosomal protein L19



- Molecule 41: 50S ribosomal protein L20

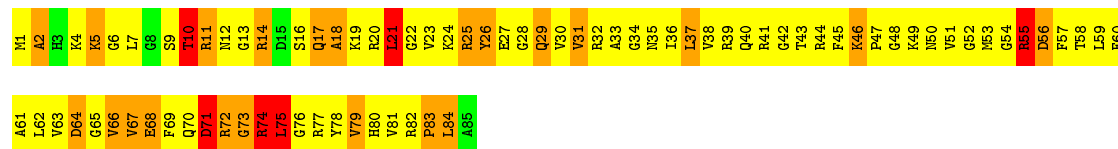


- Molecule 42: 50S ribosomal protein L21



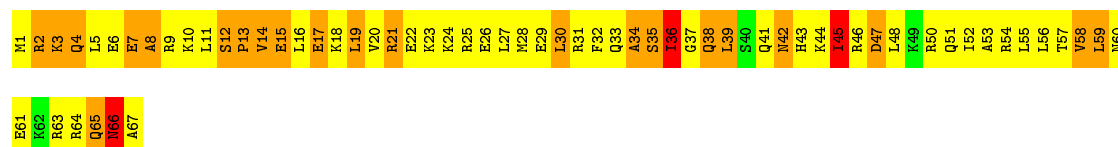
- Molecule 47: 50S ribosomal protein L27

Chain BZ: 5% 62% 26% 7%



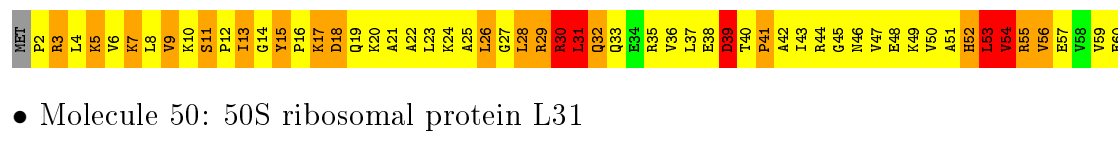
- Molecule 48: 50S ribosomal protein L29

Chain B1: 58% 33%



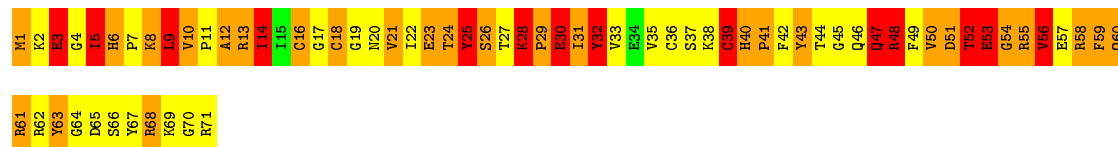
- Molecule 49: 50S ribosomal protein L30

Chain B2: 58% 28% 8%



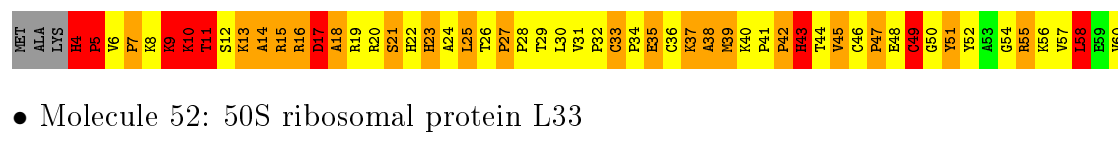
- Molecule 50: 50S ribosomal protein L31

Chain B3: 39% 38% 20%



- Molecule 51: 50S ribosomal protein L32

Chain B4: 43% 33% 15% 5%



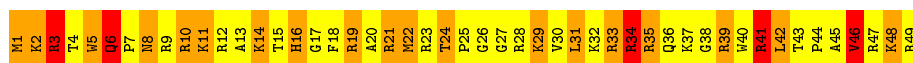
- Molecule 52: 50S ribosomal protein L33

Chain B5: 2% 28% 43% 20% 9%



- Molecule 53: 50S ribosomal protein L34

Chain B6: 51% 39% 10%



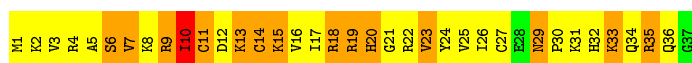
- Molecule 54: 50S ribosomal protein L35

Chain B7: 46% 45% 6%



- Molecule 55: 50S ribosomal protein L36

Chain B8: 5% 54% 38%



4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	509.52Å 509.52Å 804.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	300.00 – 5.00 430.52 – 4.80	Depositor EDS
% Data completeness (in resolution range)	93.9 (300.00-5.00) 96.7 (430.52-4.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.09 (at 4.88Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.263 , 0.323 0.257 , 0.309	Depositor DCC
R_{free} test set	10840 reflections (4.30%)	wwPDB-VP
Wilson B-factor (Å ²)	99.7	Xtrriage
Anisotropy	0.066	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.09 , 59.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.55$, $\langle L^2 \rangle = 0.39$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	149044	wwPDB-VP
Average B, all atoms (Å ²)	167.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.30% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

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	0.94	48/36438 (0.1%)	1.12	150/56869 (0.3%)
2	AC	1.00	1/1814 (0.1%)	0.92	3/2825 (0.1%)
3	AD	0.80	1/1813 (0.1%)	0.94	3/2823 (0.1%)
4	AE	0.65	0/1935	1.02	3/2609 (0.1%)
5	AF	0.55	0/1636	0.98	4/2205 (0.2%)
6	AG	0.68	1/1733 (0.1%)	1.07	5/2318 (0.2%)
7	AH	0.68	0/1162	1.06	2/1564 (0.1%)
8	AI	0.68	0/856	1.01	3/1154 (0.3%)
9	AJ	0.60	0/1276	0.90	0/1709
10	AK	0.68	0/1136	1.10	5/1527 (0.3%)
11	AL	0.54	0/1029	0.87	0/1379
12	AM	0.49	0/807	0.88	0/1085
13	AN	0.73	0/900	1.06	3/1213 (0.2%)
14	AO	0.67	0/986	1.12	6/1320 (0.5%)
15	AP	0.53	0/1008	0.90	2/1347 (0.1%)
16	AQ	0.57	0/501	1.01	1/664 (0.2%)
17	AR	0.71	0/745	1.00	1/992 (0.1%)
18	AS	0.72	0/716	1.05	3/963 (0.3%)
19	AT	0.73	0/870	1.07	2/1159 (0.2%)
20	AU	0.64	0/603	1.02	3/799 (0.4%)
21	AV	0.55	0/661	0.94	0/890
22	AW	0.77	0/765	1.03	1/1007 (0.1%)
23	AX	0.48	0/212	0.85	1/277 (0.4%)
24	BA	1.06	154/69685 (0.2%)	1.16	463/108786 (0.4%)
25	BB	0.86	4/2954 (0.1%)	1.01	8/4606 (0.2%)
26	BC	0.50	0/1775	0.89	2/2393 (0.1%)
27	BD	0.83	3/2174 (0.1%)	1.25	12/2927 (0.4%)
28	BE	0.86	2/1611 (0.1%)	1.29	13/2171 (0.6%)
29	BF	0.69	0/1660	1.11	8/2247 (0.4%)
30	BG	0.63	0/1507	1.05	4/2027 (0.2%)
31	BH	0.62	0/1354	1.06	5/1831 (0.3%)
32	BK	0.69	0/1170	1.08	2/1581 (0.1%)
33	BL	0.49	0/1044	0.90	1/1415 (0.1%)
34	BM	0.83	1/1140 (0.1%)	1.19	8/1537 (0.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
35	BN	1.00	0/942	1.39	8/1268 (0.6%)
36	BO	0.79	0/1123	1.27	15/1493 (1.0%)
37	BP	0.85	1/1100 (0.1%)	1.27	6/1470 (0.4%)
38	BQ	0.69	0/974	1.08	2/1302 (0.2%)
39	BR	0.78	0/887	1.11	2/1180 (0.2%)
40	BS	0.95	0/990	1.44	13/1325 (1.0%)
41	BT	0.79	0/982	1.18	6/1306 (0.5%)
42	BU	0.90	1/790 (0.1%)	1.44	11/1057 (1.0%)
43	BV	0.78	0/886	1.11	2/1189 (0.2%)
44	BW	0.57	0/756	0.91	0/1015
45	BX	0.53	0/857	1.09	4/1142 (0.4%)
46	BY	0.66	0/1467	1.13	6/1992 (0.3%)
47	BZ	0.72	0/679	1.11	2/902 (0.2%)
48	B1	0.64	0/569	0.91	0/751
49	B2	0.63	0/474	1.08	1/635 (0.2%)
50	B3	1.00	2/594 (0.3%)	1.37	8/795 (1.0%)
51	B4	0.74	1/459 (0.2%)	1.12	2/621 (0.3%)
52	B5	0.91	0/433	1.61	7/576 (1.2%)
53	B6	0.81	0/438	1.03	1/575 (0.2%)
54	B7	0.70	0/523	1.23	3/690 (0.4%)
55	B8	0.69	0/310	1.19	2/407 (0.5%)
All	All	0.93	220/161909 (0.1%)	1.13	828/241910 (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	217
2	AC	0	13
3	AD	0	7
5	AF	0	1
10	AK	0	1
13	AN	0	1
24	BA	0	546
25	BB	0	16
27	BD	0	2
28	BE	0	1
29	BF	0	1
31	BH	0	1
37	BP	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
40	BS	0	2
42	BU	0	2
43	BV	0	1
44	BW	0	1
50	B3	0	2
All	All	0	818

The worst 5 of 220 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	607	U	N3-C4	-31.59	1.10	1.38
24	BA	2501	C	O3'-P	24.61	1.90	1.61
24	BA	607	U	C2-N3	-22.10	1.22	1.37
1	AA	173	U	O3'-P	19.93	1.85	1.61

The worst 5 of 828 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1064	G	N1-C2-N2	-70.70	52.57	116.20
1	AA	1064	G	N3-C2-N2	58.69	160.98	119.90
24	BA	607	U	N3-C4-O4	-29.32	98.87	119.40
24	BA	1203	G	P-O3'-C3'	27.75	153.00	119.70
1	AA	1064	G	N1-C2-N3	-25.80	108.42	123.90

There are no chirality outliers.

5 of 818 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	12	U	Sidechain
1	AA	21	G	Sidechain
1	AA	24	U	Sidechain
1	AA	6	G	Sidechain
1	AA	7	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	32554	0	16429	6468	0
2	AC	1624	0	826	363	0
3	AD	1623	0	821	385	0
4	AE	1900	0	1951	934	0
5	AF	1612	0	1677	695	0
6	AG	1703	0	1763	800	0
7	AH	1146	0	1207	493	0
8	AI	843	0	857	370	0
9	AJ	1257	0	1296	561	0
10	AK	1116	0	1177	644	0
11	AL	1010	0	1037	460	0
12	AM	794	0	840	363	0
13	AN	885	0	904	407	0
14	AO	970	0	1057	440	0
15	AP	997	0	1072	511	0
16	AQ	492	0	529	255	0
17	AR	734	0	771	300	0
18	AS	700	0	720	308	0
19	AT	857	0	930	415	0
20	AU	597	0	668	331	0
21	AV	647	0	673	300	0
22	AW	763	0	861	356	0
23	AX	208	0	221	83	0
24	BA	62218	0	31353	15020	0
25	BB	2641	0	1337	589	1
26	BC	1742	0	1796	854	0
27	BD	2124	0	2207	1514	0
28	BE	1578	0	1647	1071	0
29	BF	1625	0	1666	891	0
30	BG	1482	0	1546	966	0
31	BH	1328	0	1408	737	0
32	BK	1155	0	1244	550	0
33	BL	1025	0	1074	489	0
34	BM	1113	0	1183	765	0
35	BN	932	0	994	688	0
36	BO	1106	0	1183	834	0
37	BP	1080	0	1127	704	0
38	BQ	960	0	1021	511	0
39	BR	877	0	938	586	0
40	BS	976	0	1033	667	0
41	BT	964	0	1022	665	0
42	BU	779	0	852	580	0
43	BV	876	0	941	448	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	BW	742	0	800	376	0
45	BX	844	0	930	504	0
46	BY	1435	0	1463	735	0
47	BZ	670	0	700	371	0
48	B1	567	0	621	314	0
49	B2	469	0	518	304	0
50	B3	581	0	577	360	0
51	B4	445	0	459	296	0
52	B5	426	0	452	291	0
53	B6	430	0	480	261	0
54	B7	515	0	587	388	0
55	B8	307	0	335	148	0
All	All	149044	0	101781	45453	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 182.

The worst 5 of 45453 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)
46:BY:27:VAL:HG23	46:BY:85:HIS:CE1	1.45	1.50
46:BY:27:VAL:CG2	46:BY:85:HIS:CE1	1.95	1.45
35:BN:64:ARG:HH11	35:BN:68:GLU:N	1.15	1.44
24:BA:775:G:H2'	24:BA:794:G:C8	1.54	1.42
24:BA:1201:C:N4	24:BA:1241:A:H61	1.15	1.39

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:-1:A:O2'	25:BB:-1:A:O2'[15_545]	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	
4	AE	232/256 (91%)	119 (51%)	48 (21%)	65 (28%)	0	0
5	AF	204/239 (85%)	117 (57%)	41 (20%)	46 (22%)	0	1
6	AG	206/209 (99%)	99 (48%)	52 (25%)	55 (27%)	0	0
7	AH	148/162 (91%)	89 (60%)	26 (18%)	33 (22%)	0	1
8	AI	99/101 (98%)	62 (63%)	14 (14%)	23 (23%)	0	1
9	AJ	153/156 (98%)	65 (42%)	45 (29%)	43 (28%)	0	0
10	AK	136/138 (99%)	71 (52%)	28 (21%)	37 (27%)	0	0
11	AL	125/128 (98%)	57 (46%)	38 (30%)	30 (24%)	0	1
12	AM	96/105 (91%)	53 (55%)	21 (22%)	22 (23%)	0	1
13	AN	117/129 (91%)	63 (54%)	28 (24%)	26 (22%)	0	1
14	AO	122/132 (92%)	60 (49%)	29 (24%)	33 (27%)	0	0
15	AP	123/126 (98%)	64 (52%)	33 (27%)	26 (21%)	0	2
16	AQ	58/61 (95%)	24 (41%)	16 (28%)	18 (31%)	0	0
17	AR	86/89 (97%)	43 (50%)	26 (30%)	17 (20%)	0	2
18	AS	81/88 (92%)	46 (57%)	22 (27%)	13 (16%)	0	3
19	AT	102/105 (97%)	63 (62%)	20 (20%)	19 (19%)	0	2
20	AU	71/88 (81%)	29 (41%)	23 (32%)	19 (27%)	0	0
21	AV	78/93 (84%)	32 (41%)	24 (31%)	22 (28%)	0	0
22	AW	97/106 (92%)	31 (32%)	43 (44%)	23 (24%)	0	1
23	AX	22/27 (82%)	11 (50%)	5 (23%)	6 (27%)	0	0
26	BC	226/229 (99%)	110 (49%)	62 (27%)	54 (24%)	0	1
27	BD	270/276 (98%)	110 (41%)	66 (24%)	94 (35%)	0	0
28	BE	204/206 (99%)	108 (53%)	40 (20%)	56 (28%)	0	0
29	BF	206/210 (98%)	106 (52%)	45 (22%)	55 (27%)	0	0
30	BG	180/182 (99%)	71 (39%)	52 (29%)	57 (32%)	0	0
31	BH	172/180 (96%)	75 (44%)	50 (29%)	47 (27%)	0	0
32	BK	146/148 (99%)	85 (58%)	36 (25%)	25 (17%)	0	3
33	BL	136/147 (92%)	68 (50%)	38 (28%)	30 (22%)	0	1
34	BM	137/140 (98%)	63 (46%)	28 (20%)	46 (34%)	0	0
35	BN	120/122 (98%)	60 (50%)	24 (20%)	36 (30%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	BO	143/150 (95%)	52 (36%)	40 (28%)	51 (36%)	0	0
37	BP	134/141 (95%)	53 (40%)	36 (27%)	45 (34%)	0	0
38	BQ	115/118 (98%)	60 (52%)	37 (32%)	18 (16%)	0	4
39	BR	108/112 (96%)	43 (40%)	35 (32%)	30 (28%)	0	0
40	BS	115/146 (79%)	55 (48%)	27 (24%)	33 (29%)	0	0
41	BT	115/118 (98%)	46 (40%)	40 (35%)	29 (25%)	0	1
42	BU	99/101 (98%)	53 (54%)	19 (19%)	27 (27%)	0	0
43	BV	108/113 (96%)	64 (59%)	20 (18%)	24 (22%)	0	1
44	BW	92/96 (96%)	53 (58%)	18 (20%)	21 (23%)	0	1
45	BX	108/110 (98%)	39 (36%)	34 (32%)	35 (32%)	0	0
46	BY	178/206 (86%)	85 (48%)	50 (28%)	43 (24%)	0	1
47	BZ	83/85 (98%)	48 (58%)	20 (24%)	15 (18%)	0	2
48	B1	65/67 (97%)	30 (46%)	20 (31%)	15 (23%)	0	1
49	B2	57/60 (95%)	33 (58%)	12 (21%)	12 (21%)	0	2
50	B3	69/71 (97%)	20 (29%)	23 (33%)	26 (38%)	0	0
51	B4	55/60 (92%)	14 (26%)	22 (40%)	19 (34%)	0	0
52	B5	47/54 (87%)	15 (32%)	8 (17%)	24 (51%)	0	0
53	B6	47/49 (96%)	18 (38%)	14 (30%)	15 (32%)	0	0
54	B7	62/65 (95%)	23 (37%)	18 (29%)	21 (34%)	0	0
55	B8	35/37 (95%)	21 (60%)	6 (17%)	8 (23%)	0	1
All	All	5988/6337 (94%)	2879 (48%)	1522 (25%)	1587 (26%)	0	1

5 of 1587 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	AE	13	ALA
4	AE	15	VAL
4	AE	17	PHE
4	AE	20	GLU
4	AE	42	ILE

5.3.2 Protein sidechains [i](#)

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%)	142 (70%)	60 (30%)	0	2
5	AF	160/188 (85%)	122 (76%)	38 (24%)	0	5
6	AG	180/181 (99%)	130 (72%)	50 (28%)	0	3
7	AH	115/123 (94%)	70 (61%)	45 (39%)	0	0
8	AI	90/90 (100%)	59 (66%)	31 (34%)	0	1
9	AJ	126/127 (99%)	97 (77%)	29 (23%)	1	5
10	AK	119/119 (100%)	76 (64%)	43 (36%)	0	1
11	AL	98/99 (99%)	74 (76%)	24 (24%)	0	4
12	AM	88/92 (96%)	61 (69%)	27 (31%)	0	2
13	AN	90/99 (91%)	70 (78%)	20 (22%)	1	6
14	AO	104/109 (95%)	79 (76%)	25 (24%)	0	5
15	AP	100/101 (99%)	73 (73%)	27 (27%)	0	3
16	AQ	49/50 (98%)	36 (74%)	13 (26%)	0	4
17	AR	79/80 (99%)	56 (71%)	23 (29%)	0	3
18	AS	72/74 (97%)	45 (62%)	27 (38%)	0	1
19	AT	96/97 (99%)	69 (72%)	27 (28%)	0	3
20	AU	64/77 (83%)	50 (78%)	14 (22%)	1	6
21	AV	71/80 (89%)	57 (80%)	14 (20%)	1	8
22	AW	76/82 (93%)	57 (75%)	19 (25%)	0	4
23	AX	19/22 (86%)	16 (84%)	3 (16%)	2	15
26	BC	180/181 (99%)	145 (81%)	35 (19%)	1	9
27	BD	215/218 (99%)	146 (68%)	69 (32%)	0	2
28	BE	166/166 (100%)	95 (57%)	71 (43%)	0	0
29	BF	164/166 (99%)	106 (65%)	58 (35%)	0	1
30	BG	156/156 (100%)	113 (72%)	43 (28%)	0	3
31	BH	143/148 (97%)	91 (64%)	52 (36%)	0	1
32	BK	124/124 (100%)	88 (71%)	36 (29%)	0	3
33	BL	105/111 (95%)	86 (82%)	19 (18%)	1	11
34	BM	118/119 (99%)	82 (70%)	36 (30%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	BN	100/100 (100%)	60 (60%)	40 (40%)	0	0
36	BO	111/116 (96%)	66 (60%)	45 (40%)	0	0
37	BP	106/111 (96%)	68 (64%)	38 (36%)	0	1
38	BQ	100/101 (99%)	73 (73%)	27 (27%)	0	3
39	BR	87/88 (99%)	61 (70%)	26 (30%)	0	2
40	BS	105/127 (83%)	65 (62%)	40 (38%)	0	1
41	BT	93/94 (99%)	61 (66%)	32 (34%)	0	1
42	BU	82/82 (100%)	55 (67%)	27 (33%)	0	2
43	BV	90/92 (98%)	56 (62%)	34 (38%)	0	1
44	BW	76/78 (97%)	59 (78%)	17 (22%)	1	6
45	BX	91/91 (100%)	71 (78%)	20 (22%)	1	6
46	BY	159/179 (89%)	107 (67%)	52 (33%)	0	2
47	BZ	67/67 (100%)	49 (73%)	18 (27%)	0	3
48	B1	62/62 (100%)	49 (79%)	13 (21%)	1	7
49	B2	51/52 (98%)	37 (72%)	14 (28%)	0	3
50	B3	63/63 (100%)	42 (67%)	21 (33%)	0	2
51	B4	50/52 (96%)	33 (66%)	17 (34%)	0	1
52	B5	48/52 (92%)	32 (67%)	16 (33%)	0	2
53	B6	42/42 (100%)	29 (69%)	13 (31%)	0	2
54	B7	54/55 (98%)	39 (72%)	15 (28%)	0	3
55	B8	34/34 (100%)	25 (74%)	9 (26%)	0	4
All	All	5040/5237 (96%)	3528 (70%)	1512 (30%)	0	2

5 of 1512 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
28	BE	57	LYS
31	BH	52	VAL
48	B1	7	GLU
28	BE	119	ARG
29	BF	119	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 190 such sidechains are listed below:

Mol	Chain	Res	Type
26	BC	56	GLN
29	BF	169	ASN
50	B3	20	ASN
26	BC	225	ASN
28	BE	54	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1515/1522 (99%)	430 (28%)	157 (10%)
2	AC	75/77 (97%)	29 (38%)	6 (8%)
24	BA	2888/2916 (99%)	1218 (42%)	265 (9%)
25	BB	122/123 (99%)	49 (40%)	4 (3%)
3	AD	75/76 (98%)	27 (36%)	4 (5%)
All	All	4675/4714 (99%)	1753 (37%)	436 (9%)

5 of 1753 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	6	G
1	AA	8	A
1	AA	9	G
1	AA	13	U
1	AA	14	U

5 of 436 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
24	BA	350	U
24	BA	776	G
24	BA	2491	U
24	BA	442	G
24	BA	620	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	4
1	AA	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	BA	2501:C	O3'	2502:G	P	1.90
1	AA	173:U	O3'	174:C	P	1.85
1	BA	2446:G	O3'	2447:G	P	1.40
1	BA	2499:C	O3'	2500:U	P	1.38
1	BA	1203:G	O3'	1204:A	P	1.19

6 Fit of model and data i

6.1 Protein, DNA and RNA chains i

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%)	-0.53	3 (0%) 95 93	88, 158, 260, 350	0
2	AC	76/77 (98%)	-0.55	0 100 100	133, 166, 216, 249	0
3	AD	76/76 (100%)	-0.37	0 100 100	219, 265, 316, 334	0
4	AE	234/256 (91%)	-0.08	10 (4%) 35 30	122, 163, 221, 265	0
5	AF	206/239 (86%)	-0.08	4 (1%) 66 58	143, 182, 210, 228	0
6	AG	208/209 (99%)	-0.76	0 100 100	106, 148, 170, 187	0
7	AH	150/162 (92%)	-0.39	0 100 100	114, 139, 171, 200	0
8	AI	101/101 (100%)	0.17	2 (1%) 65 56	121, 150, 168, 203	0
9	AJ	155/156 (99%)	-0.08	0 100 100	155, 180, 208, 214	0
10	AK	138/138 (100%)	-0.67	0 100 100	113, 133, 153, 160	0
11	AL	127/128 (99%)	-0.26	1 (0%) 86 79	161, 225, 247, 255	0
12	AM	98/105 (93%)	0.51	14 (14%) 2 3	146, 208, 237, 240	0
13	AN	119/129 (92%)	-0.30	0 100 100	114, 142, 176, 206	0
14	AO	124/132 (93%)	-0.17	0 100 100	96, 129, 162, 184	0
15	AP	125/126 (99%)	-0.52	0 100 100	167, 194, 223, 230	0
16	AQ	60/61 (98%)	-0.46	0 100 100	163, 188, 203, 206	0
17	AR	88/89 (98%)	-0.73	0 100 100	113, 131, 168, 183	0
18	AS	83/88 (94%)	-0.93	0 100 100	104, 128, 155, 185	0
19	AT	104/105 (99%)	-0.75	0 100 100	98, 126, 169, 215	0
20	AU	73/88 (82%)	-0.39	4 (5%) 25 22	109, 136, 190, 224	0
21	AV	80/93 (86%)	0.16	1 (1%) 77 68	175, 198, 217, 222	0
22	AW	99/106 (93%)	-0.63	0 100 100	105, 134, 163, 166	0
23	AX	24/27 (88%)	-0.85	0 100 100	168, 210, 224, 229	0
24	BA	2889/2916 (99%)	-0.53	0 100 100	63, 155, 266, 322	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	BB	123/123 (100%)	-0.46	0 100 100	146, 209, 257, 291	0
26	BC	228/229 (99%)	0.19	16 (7%) 16 13	220, 256, 308, 312	0
27	BD	272/276 (98%)	-0.04	3 (1%) 80 72	80, 125, 153, 198	0
28	BE	206/206 (100%)	-0.39	1 (0%) 91 85	69, 117, 172, 224	0
29	BF	208/210 (99%)	-0.45	0 100 100	111, 179, 215, 231	0
30	BG	182/182 (100%)	-0.34	2 (1%) 80 72	160, 198, 226, 240	0
31	BH	174/180 (96%)	-0.33	1 (0%) 89 83	146, 186, 216, 238	0
32	BK	148/148 (100%)	-0.47	0 100 100	135, 161, 188, 190	0
33	BL	138/147 (93%)	0.90	29 (21%) 1 1	277, 307, 330, 334	0
34	BM	139/140 (99%)	-0.46	1 (0%) 87 82	107, 133, 167, 183	0
35	BN	122/122 (100%)	-0.33	0 100 100	78, 106, 140, 154	0
36	BO	145/150 (96%)	-0.02	9 (6%) 20 17	106, 190, 227, 239	0
37	BP	136/141 (96%)	-0.17	3 (2%) 62 52	109, 141, 173, 186	0
38	BQ	117/118 (99%)	-0.50	0 100 100	91, 124, 157, 173	0
39	BR	110/112 (98%)	-0.70	0 100 100	152, 183, 210, 248	0
40	BS	117/146 (80%)	-0.17	1 (0%) 84 77	83, 127, 165, 184	0
41	BT	117/118 (99%)	-0.42	1 (0%) 84 77	100, 138, 152, 158	0
42	BU	101/101 (100%)	0.27	6 (5%) 22 19	104, 160, 186, 197	0
43	BV	110/113 (97%)	-0.42	0 100 100	110, 143, 179, 195	0
44	BW	94/96 (97%)	-0.34	0 100 100	153, 170, 232, 237	0
45	BX	110/110 (100%)	-0.25	3 (2%) 54 45	157, 199, 247, 273	0
46	BY	180/206 (87%)	0.31	4 (2%) 62 52	142, 190, 211, 226	0
47	BZ	85/85 (100%)	-0.67	0 100 100	139, 166, 181, 197	0
48	B1	67/67 (100%)	-0.21	0 100 100	172, 186, 199, 209	0
49	B2	59/60 (98%)	-0.38	0 100 100	127, 163, 188, 202	0
50	B3	71/71 (100%)	-0.71	0 100 100	127, 160, 176, 185	0
51	B4	57/60 (95%)	-0.49	0 100 100	96, 147, 217, 241	0
52	B5	49/54 (90%)	-0.22	1 (2%) 65 56	141, 163, 183, 198	0
53	B6	49/49 (100%)	-0.42	0 100 100	87, 145, 164, 188	0
54	B7	64/65 (98%)	-0.47	0 100 100	113, 131, 153, 165	0
55	B8	37/37 (100%)	-0.82	0 100 100	146, 157, 169, 172	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	10767/11051 (97%)	-0.38	120 (1%) 80 72	63, 160, 260, 350	0

The worst 5 of 120 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
31	BH	177	GLY	6.3
33	BL	17	ALA	5.5
4	AE	231	GLU	4.8
12	AM	81	THR	4.3
26	BC	126	LYS	4.2

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.