



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 07:54 AM UTC

PDB ID : 4V4Z / pdb_00004v4z
Title : 70S Thermus thermophilus ribosome functional complex with mRNA and E- and P-site tRNAs at 4.5Å.
Authors : Jenner, L.; Yusupova, G.; Rees, B.; Moras, D.; Yusupov, M.
Deposited on : 2006-06-27
Resolution : 4.51 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

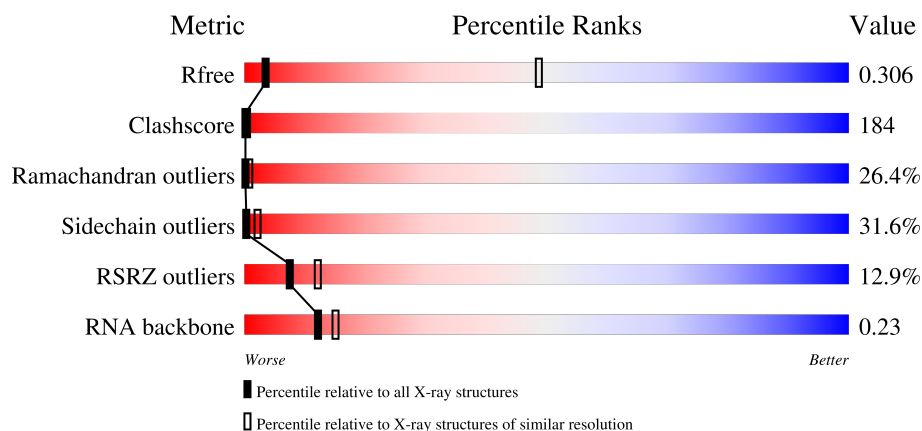
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.51 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}	180053	1131 (5.14-3.90)
Clashscore	190562	1005 (5.10-3.94)
Ramachandran outliers	187476	1061 (5.12-3.90)
Sidechain outliers	187428	1044 (5.12-3.90)
RSRZ outliers	180081	1126 (5.14-3.90)
RNA backbone	3983	1039 (5.90-3.10)

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 of 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	54% 33% 12%
2	AC	76	4% 51% 37% 12%
3	AD	76	8% 45% 46% 7%
4	A1	27	30% 11% 48% 22% 19%

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Mol	Chain	Length	Quality of chain
5	AE	256	
6	AF	239	
7	AG	209	
8	AH	162	
9	AI	101	
10	AJ	156	
11	AK	138	
12	AL	128	
13	AM	105	
14	AN	129	
15	AO	132	
16	AP	126	
17	AQ	61	
18	AR	89	
19	AS	88	
20	AT	105	
21	AU	88	
22	AV	93	
23	AW	106	
24	AX	27	
25	BA	2916	
26	BB	123	
27	BC	229	
28	BD	276	
29	BE	206	

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Mol	Chain	Length	Quality of chain
30	BF	210	
31	BG	182	
32	BH	180	
33	BK	148	
34	BL	147	
35	BM	140	
36	BN	122	
37	BO	150	
38	BP	141	
39	BQ	118	
40	BR	112	
41	BS	146	
42	BT	118	
43	BU	101	
44	BV	113	
45	BW	96	
46	BX	110	
47	BY	206	
48	BZ	85	
49	B1	67	
50	B2	60	
51	B3	71	
52	B4	60	
53	B5	54	
54	B6	49	

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Mol	Chain	Length	Quality of chain
55	B7	65	11% 32% 51% 15%
56	B8	37	5% 41% 46% 11%

2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 149640 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
1	AA	1515	Total	C	N	O	P	0	0	0
			32554	14490	6022	10527	1515			

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

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

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

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

- Molecule 4 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A1	27	Total	C	N	O	P	0	0	0
			596	267	127	175	27			

- Molecule 5 is a protein called 30S ribosomal protein S2.

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

- Molecule 6 is a protein called 30S ribosomal protein S3.

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

- Molecule 7 is a protein called 30S ribosomal protein S4.

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

- Molecule 8 is a protein called 30S ribosomal protein S5.

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

- Molecule 9 is a protein called 30S ribosomal protein S6.

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

- Molecule 10 is a protein called 30S ribosomal protein S7.

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

- Molecule 11 is a protein called 30S ribosomal protein S8.

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

- Molecule 12 is a protein called 30S ribosomal protein S9.

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

- Molecule 13 is a protein called 30S ribosomal protein S10.

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

- Molecule 14 is a protein called 30S ribosomal protein S11.

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

- Molecule 15 is a protein called 30S ribosomal protein S12.

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

- Molecule 16 is a protein called 30S ribosomal protein S13.

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

- Molecule 17 is a protein called 30S ribosomal protein S14.

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

- Molecule 18 is a protein called 30S ribosomal protein S15.

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

- Molecule 19 is a protein called 30S ribosomal protein S16.

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

- Molecule 20 is a protein called 30S ribosomal protein S17.

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

- Molecule 21 is a protein called 30S ribosomal protein S18.

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

- Molecule 22 is a protein called 30S ribosomal protein S19.

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

- Molecule 23 is a protein called 30S ribosomal protein S20.

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

- Molecule 24 is a protein called 30S ribosomal protein Thx.

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

- Molecule 25 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	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 26 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	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 27 is a protein called 50S RIBOSOMAL PROTEIN L1.

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

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L2.

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

- Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L3.

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

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L4.

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

- Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L5.

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

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L6.

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

- Molecule 33 is a protein called 50S RIBOSOMAL PROTEIN L9.

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

- Molecule 34 is a protein called 50S RIBOSOMAL PROTEIN L11.

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

- Molecule 35 is a protein called 50S RIBOSOMAL PROTEIN L13.

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

- Molecule 36 is a protein called 50S RIBOSOMAL PROTEIN L14.

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

- Molecule 37 is a protein called 50S RIBOSOMAL PROTEIN L15.

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

- Molecule 38 is a protein called 50S RIBOSOMAL PROTEIN L16.

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

- Molecule 39 is a protein called 50S RIBOSOMAL PROTEIN L17.

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

- Molecule 40 is a protein called 50S RIBOSOMAL PROTEIN L18.

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

- Molecule 41 is a protein called 50S RIBOSOMAL PROTEIN L19.

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

- Molecule 42 is a protein called 50S RIBOSOMAL PROTEIN L20.

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

- Molecule 43 is a protein called 50S RIBOSOMAL PROTEIN L21.

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

- Molecule 44 is a protein called 50S RIBOSOMAL PROTEIN L22.

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

- Molecule 45 is a protein called 50S RIBOSOMAL PROTEIN L23.

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

- Molecule 46 is a protein called 50S RIBOSOMAL PROTEIN L24.

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

- Molecule 47 is a protein called 50S RIBOSOMAL PROTEIN L25.

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

- Molecule 48 is a protein called 50S RIBOSOMAL PROTEIN L27.

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

- Molecule 49 is a protein called 50S RIBOSOMAL PROTEIN L29.

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

- Molecule 50 is a protein called 50S RIBOSOMAL PROTEIN L30.

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

- Molecule 51 is a protein called 50S RIBOSOMAL PROTEIN L31.

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

- Molecule 52 is a protein called 50S RIBOSOMAL PROTEIN L32.

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

- Molecule 53 is a protein called 50S RIBOSOMAL PROTEIN L33.

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

- Molecule 54 is a protein called 50S RIBOSOMAL PROTEIN L34.

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

- Molecule 55 is a protein called 50S RIBOSOMAL PROTEIN L35.

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

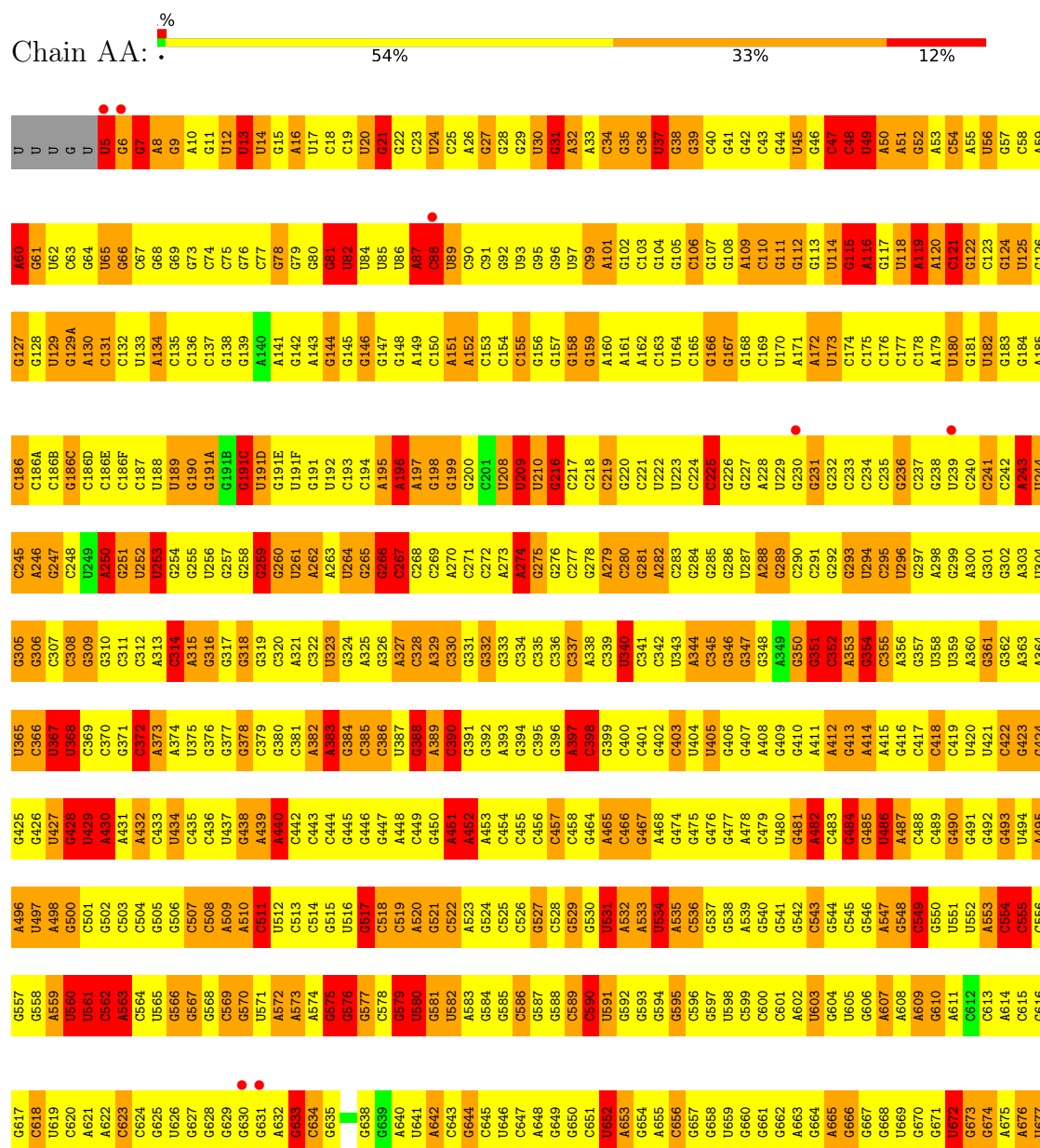
- Molecule 56 is a protein called 50S RIBOSOMAL PROTEIN L36.

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

3 Residue-property plots

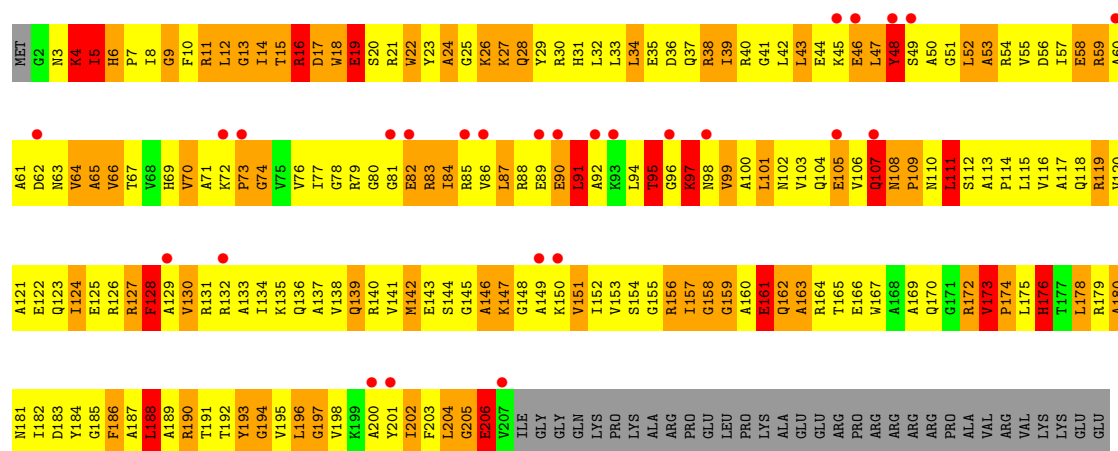
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

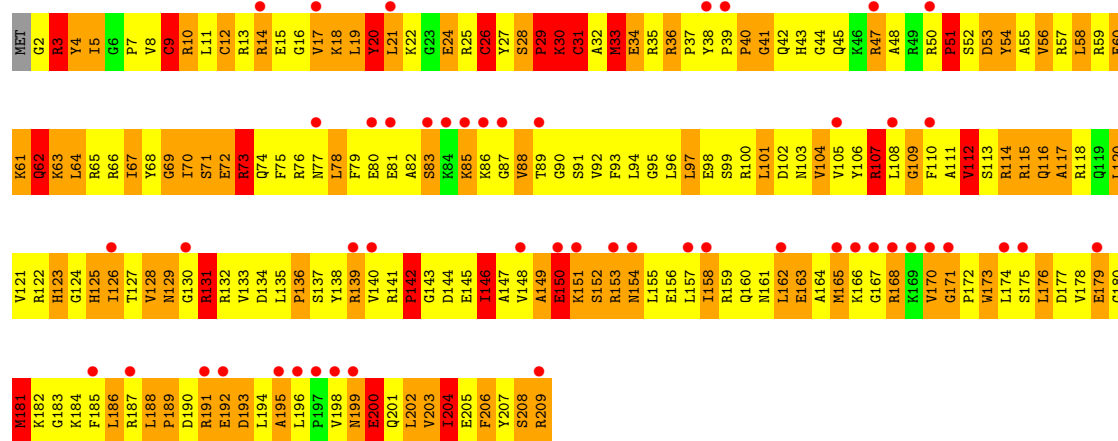


G1525	C1465	U1281	G1221	G1160	C1100	U1040	C985	G925	A864	G798	C738	U678
G1526	C1466	C1282	G1222	C1161	A1101	A1041	A986	G926	A865	G799	C739	C679
C1527	G1467	G1283	C1223	C1162	A1102	G1042	G987	G927	C866	G800	C740	C680
U1528	C1468	C1284	G1224	C1163	C1103	G1043	G988	C928	C867	U801	G741	C681
G1529	G1469	A1285	A1225	C1164	A1104	A1044	C989	G929	C868	A802	G742	C682
G1530	G1470	A1286	C1226	C1165	G1105	G1045	C990	C930	C869	A803	G743	G683
A1531	G1471	A1287	A1227	C1166	G1106	A1046	U991	C931	U870	U804	C744	A684
U1466	C1472	A1288	C1228	A1167	C1107	G1047	U992	C932	U871	C805	C745	A685
C1407	A1408	A1289	A1229	G1169	G1108	G1048	G993	G933	A872	C806	C746	U686
A1408	G1473	G1290	C1230	A1170	C1109	U1049	A994	C934	A873	A807	C747	A687
G1409	G1474	G1291	G1231	C1171	A1110	G1050	C995	A935	C874	C808	C748	G688
C1534	G1475	U1291	G1231	C1171	A1110	G1050	A995	A935	C875	C809	C749	C689
C1535	C1411	U1292	U1232	C1172	A1111	U1051	A996	C936	C876	C810	G750	G690
G1476	C1412	G1293	G1233	C1173	C1112	U1052	U997	A937	C877	C811	U751	C691
C1477	G1353	G1294	G1234	C1174	C1113	G1053	G998	A938	C877	C812	G752	C692
C1478	C1354	G1295	U1235	G1175	C1114	C1054	G999A	G939	C878	U813	A753	G693
C1479	G1355	G1296	U1236	A1176	C1115	A1055	U999	C940	C879	U814	C754	A694
G1415	G1356	C1297	A1237	G1177	C1116	U1056	A1000	G941	C880	A814	G755	A695
G1416	A1357	C1297	A1238	C1178	G1117	G1057	G1001	G942	C881	A815	G756	A696
G1417	U1358	C1298	G1239	C1179	G1118	G1058	G1002	U943	C882	A816	U757	U697
A1418	C1359	A1299	U1240	A1180	C1119	G1059	G1003	G944	C883	C817	G758	G698
C1419	A1360	G1300	U1241	G1181	G1120	C1060	A1004	G945	U884	C818	G759	C699
C1420	C1362	U1302	C1242	G1182	U1121	U1062	A1006	A946	C885	A819	A760	G700
G1421	C1362A	C1303	C1243	A1183	U1122	U1063	C1006	G947	C886	U820	G760	C701
G1422	A1363	G1304	C1244	G1184	A1123	G1064	C1007	C948	C887	C821	G761	C702
G1423	G1364	G1305	C1245	G1185	G1124	U1065	G1008	A949	C888	C822	G762	A703
C1424	G1365	A1306	C1246	G1186	U1125	U1066	G1009	U950	A889	G823	G763	G703
U1425	C1366	U1307	U1247	G1187	U1126	C1066	G1010	G951	C890	C824	C764	A704
U1426	C1367	U1308	A1248	A1188	G1127	A1067	G1011	U952	U891	G825	G765	U705
U1427	A1368	G1309	G1249	C1189	C1128	G1068	U1012	G953	A892	C826	A766	A706
A1428	G1369	G1310	A1250	G1190	C1129	C1069	G1013	G954	C893	A767	C707	C707
C1429	C1370	G1311	A1251	A1191	A1130	U1070	A1014	U955	C894	A828	A768	C708
C1430	G1371	G1312	A1252	C1192	G1131	C1071	A1015	U956	C895	C829	G769	G709
C1431	U1372	U1313	G1253	C1193	C1132	G1072	A1016	U957	C896	U830	C770	G710
G1432	C1373	C1314	C1254	U1194	G1133	U1073	G1017	A958	C897	U831	G771	G711
A1433	A1374	U1315	G1255	C1195	G1134	C1074	C1018	U960	C898	C832	U772	A712
A1434	A1375	G1316	U1256	U1196	U1135	C1075	C1019	U1020	C899	U833	G773	G713
G1435	U1376	C1317	U1257	G1197	U1136	G1076	U1021	C962	A901	C834	G774	G714
U1436	U1377	A1318	G1258	G1198	C1137	G1077	G1022	G963	A902	U835	G775	A715
C1437	C1378	A1319	C1259	U1199	G1138	U1078	G1023	A964	G903	G836	A776	A716
G1438	G1379	C1320	C1260	C1200	G1139	G1079	G1024	A965	G906	U837	A777	C717
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C1440	U1381	C1322	C1262	G1202	C1141	G1081	U1026	C967	A907	C842	A780	C720
G1441	G1382	G1323	C1263	C1203	G1142	G1082	C1027	A968	A908	U843	A781	G721
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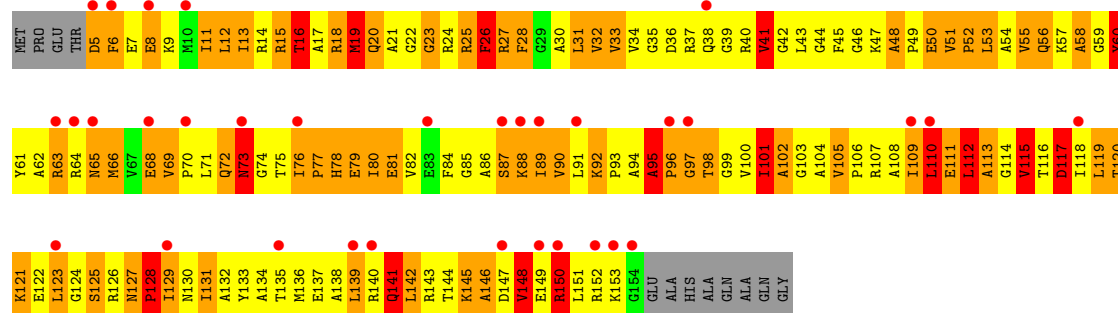
• Molecule 2: tRNA fMET (unmodified bases)



• Molecule 7: 30S ribosomal protein S4

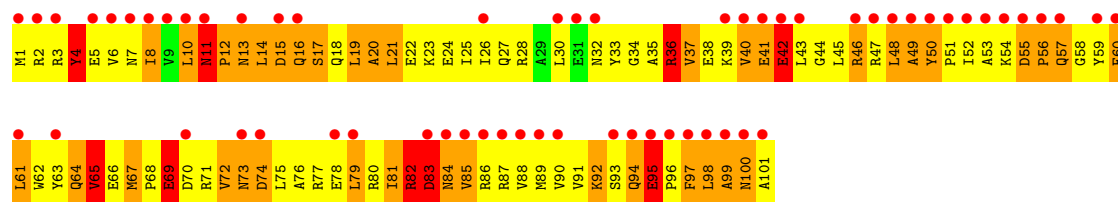


• Molecule 8: 30S ribosomal protein S5

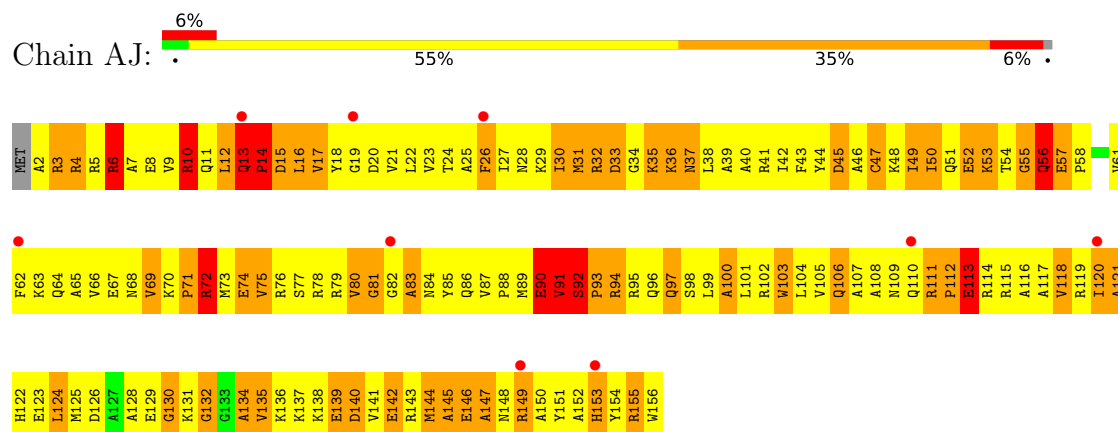


• Molecule 9: 30S ribosomal protein S6

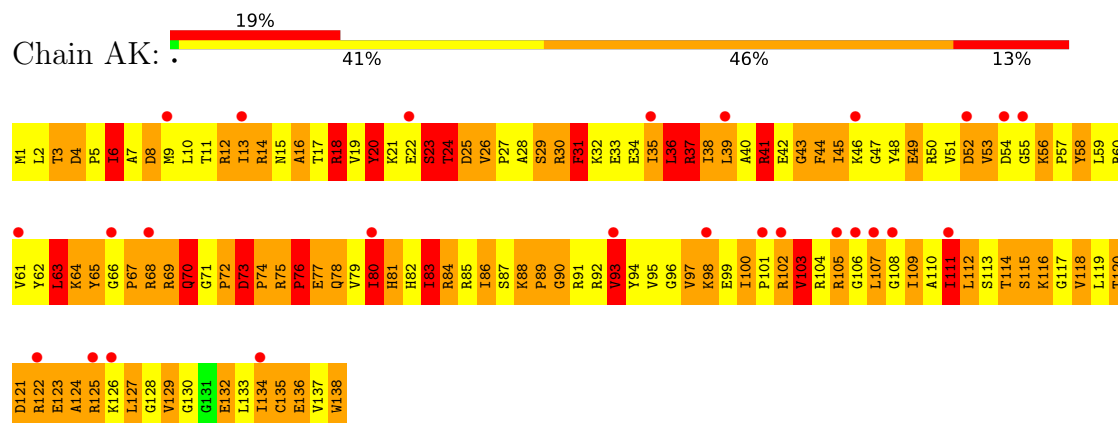




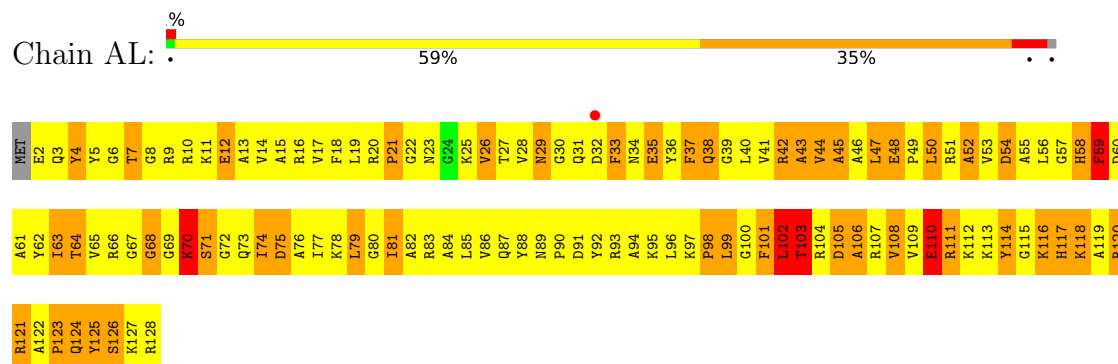
• Molecule 10: 30S ribosomal protein S7



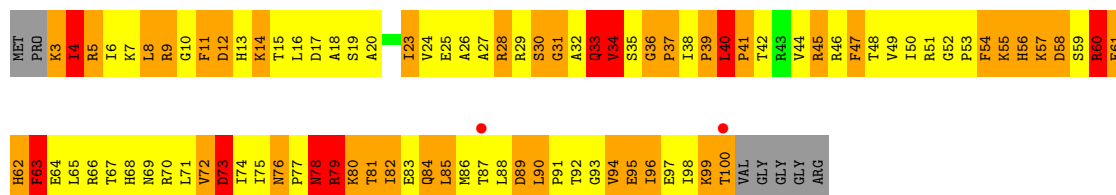
• Molecule 11: 30S ribosomal protein S8



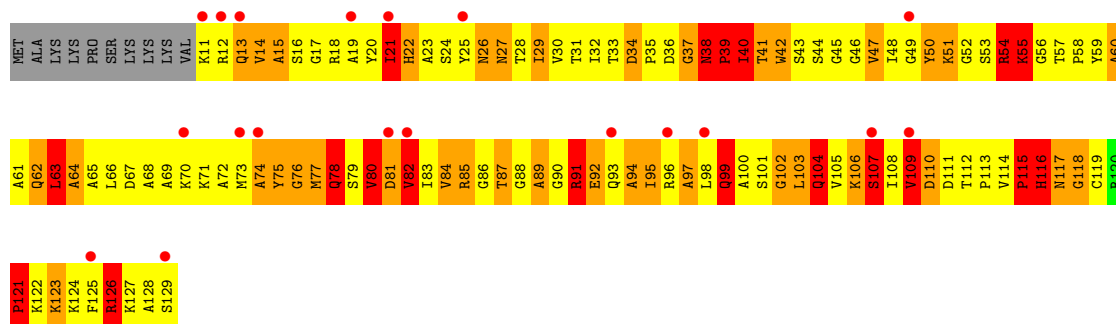
• Molecule 12: 30S ribosomal protein S9



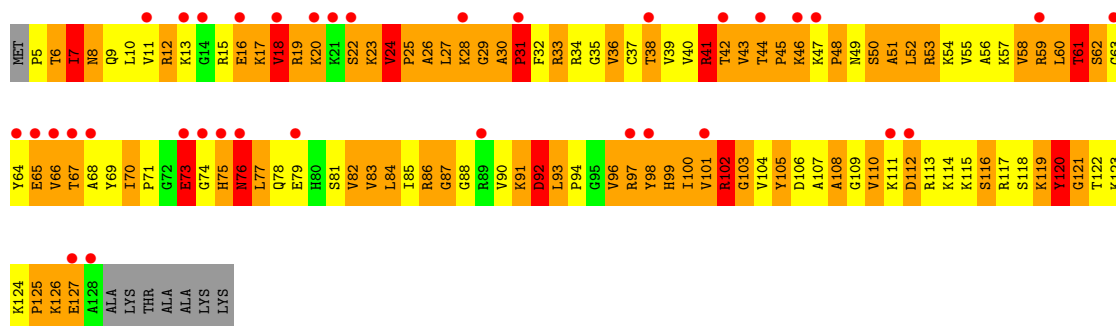
• Molecule 13: 30S ribosomal protein S10



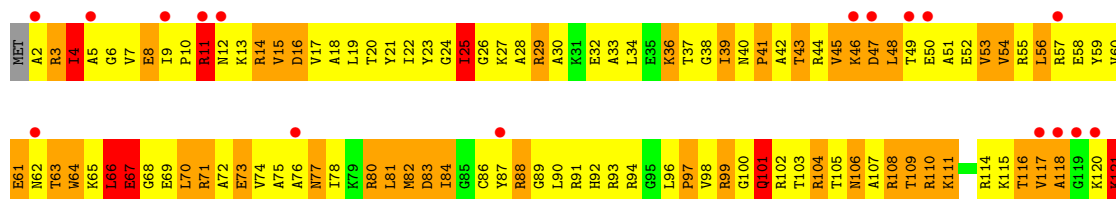
• Molecule 14: 30S ribosomal protein S11

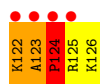


• Molecule 15: 30S ribosomal protein S12



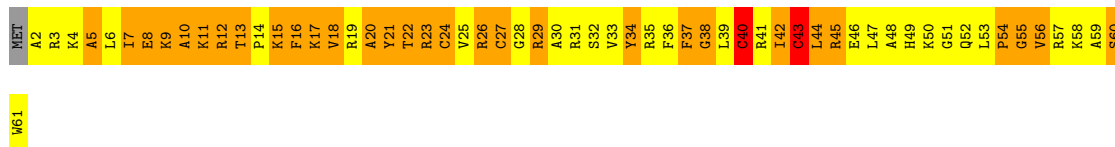
• Molecule 16: 30S ribosomal protein S13





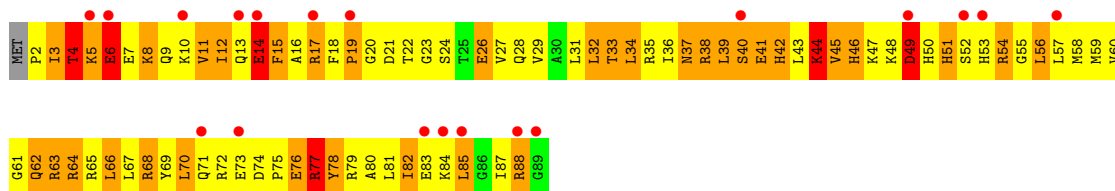
• Molecule 17: 30S ribosomal protein S14

Chain AQ: 46% 49%



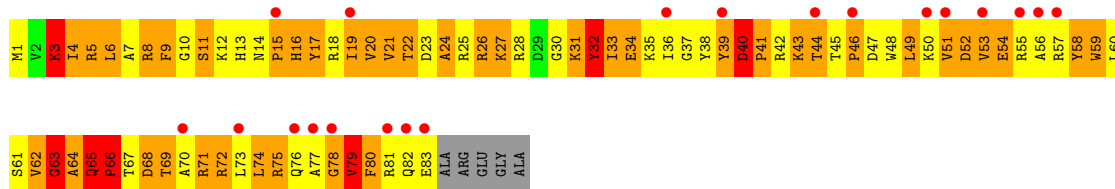
• Molecule 18: 30S ribosomal protein S15

Chain AR: 21% 49% 38% 7%



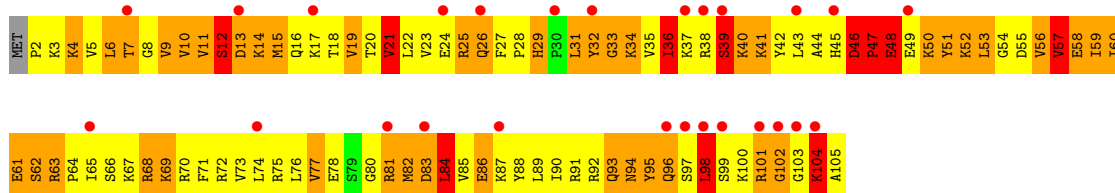
• Molecule 19: 30S ribosomal protein S16

Chain AS: 23% 38% 47% 8% 6%



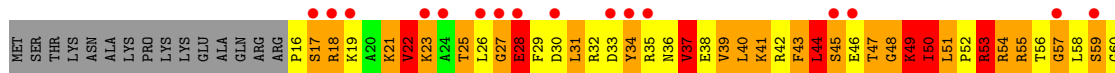
• Molecule 20: 30S ribosomal protein S17

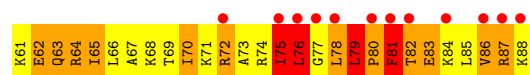
Chain AT: 25% 46% 41% 10%



• Molecule 21: 30S ribosomal protein S18

Chain AU: 32% 32% 36% 13% 17%

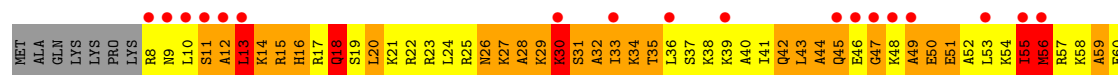




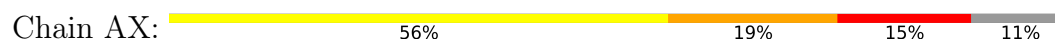
- Molecule 22: 30S ribosomal protein S19



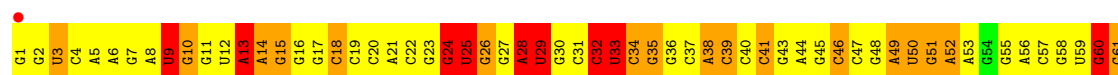
- Molecule 23: 30S ribosomal protein S20



- Molecule 24: 30S ribosomal protein Thx



- Molecule 25: 23S rRNA



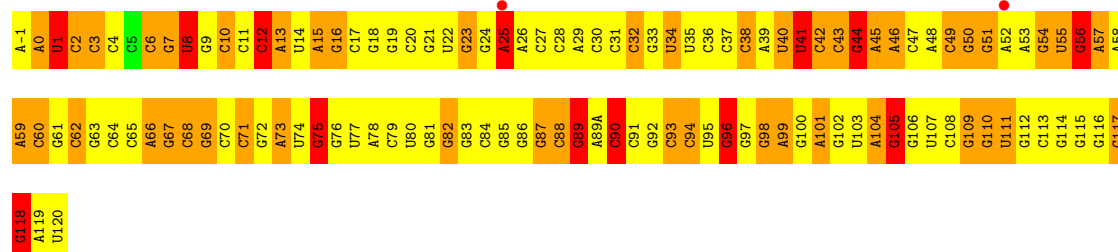
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A1098	G1038	G976	C916	G855	C795	A735	A675	A637	A579	C517	C456	U339	U339	C279	C254
G1099	C1039	G977	A917	G856	C796	C736	A676	G638	C580	C518	A457	G397	A340	C280	A255
C1100	G1040	G978	A918	G857	C797	C737	A677	G639	C581	U519	G458	G398	G342	G281	A256
U1101	C1041	G979	G919	U858	C798	G738	C678	G640	G582	G520	U459	G399	G342	A282	A257
C1102	G1042	A980	G920	G859	G799	G739	C679	G641	G583	G521	A460	G400	G343	A283	G258
A1103	C1043	A981	G921	U860	A800	G740	G680	G642	C584	G522	C461	A401	C344	U284	G259
C1104	G1044	C982	U922	A861	G801	G741	G681	A643	C585	C523	C462	A402	A345	C285	G260
U1105	A1045	A983	C923	G862	A802	G742	G682	A644	A586	U524	G463	U403	A346	C286	G261
G1106	A1046	A984	C924	A863	U803	G743	C683	C645	C587	U525	U464	C404	A347	C287	A262
U1107	G1047	C985	A925	G864	A804	G744	G684	A646	U588	A526	G465	U405	A348	C288	C263
U1108	A1048	C986	A926	C865	G805	G745	A685	G647	C589	C527	A466	G406	G349	A289	C264
C1109	C1049	C987	G928	A866	C806	A746	G686	G648	A590	A528	C467	G407	U350	G290	A265
G1110	A1050	A988	G929	C867	U807	G747	U687	G649	C591	A529	G468	G408	G351	C291	G266
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G1112	C1052	A990	G931	G869	A809	C749	A689	C	G593	C531	A470	C410	G354	U293	C268
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G1114	A1054	C992	A933	U871	U811	A751	C691	A	C595	G533	A472	A412	G355	G295	A270
G1115	G1055	G993	G934	A872	C812	A752	C692	A	G596	U534	C473	C413	G356	C296	A270A
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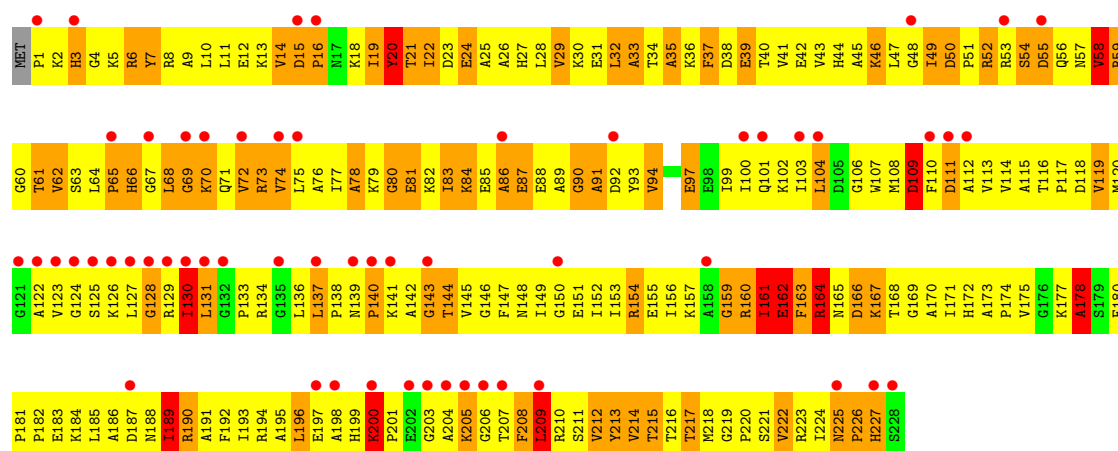
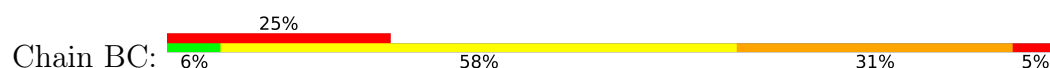
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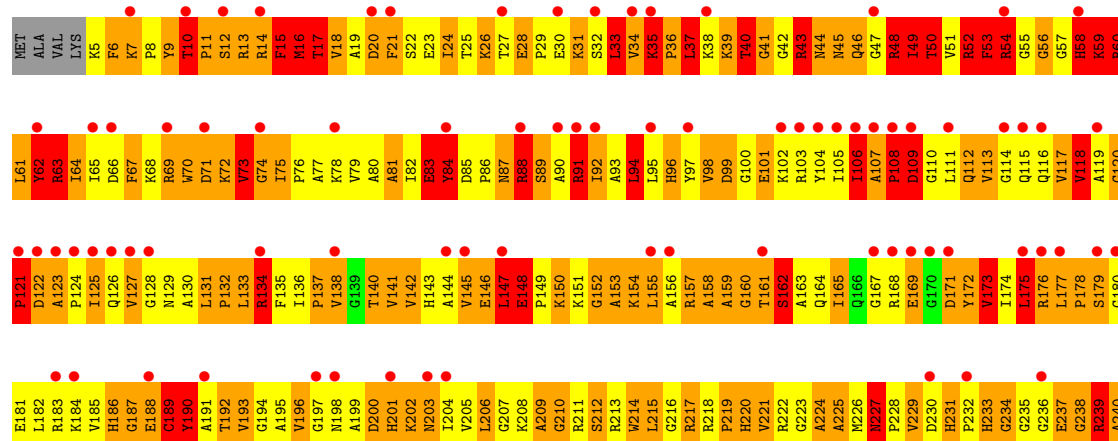
• Molecule 26: 5S rRNA

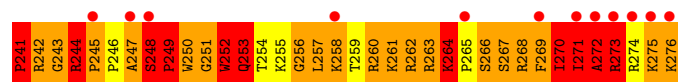


• Molecule 27: 50S RIBOSOMAL PROTEIN L1

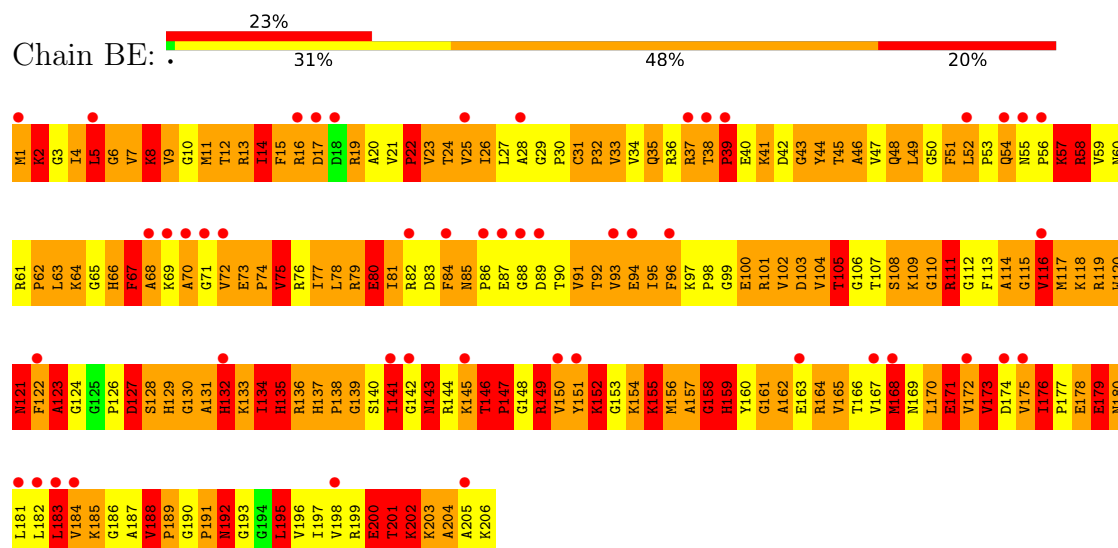


• Molecule 28: 50S RIBOSOMAL PROTEIN L2

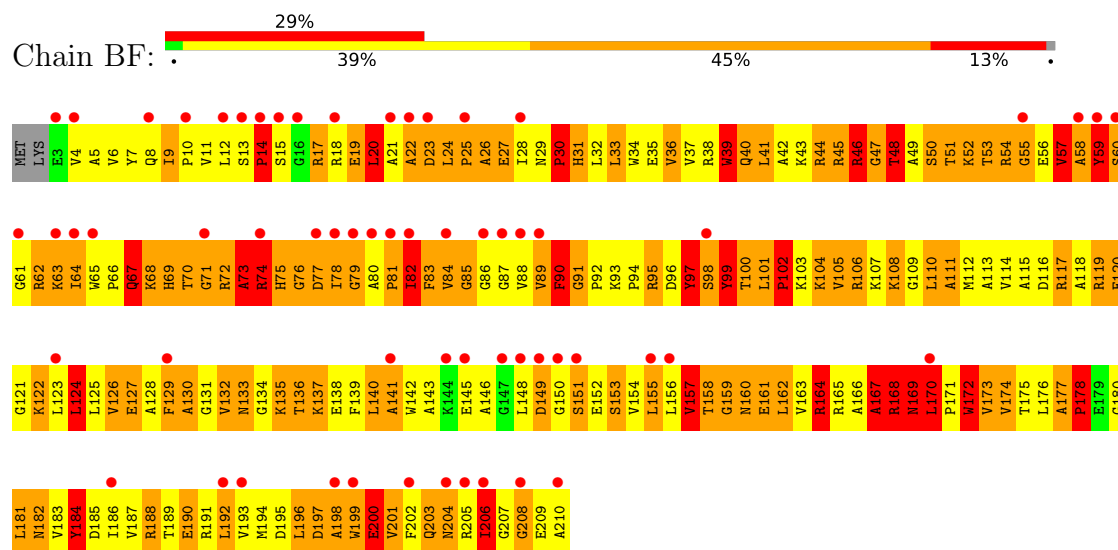




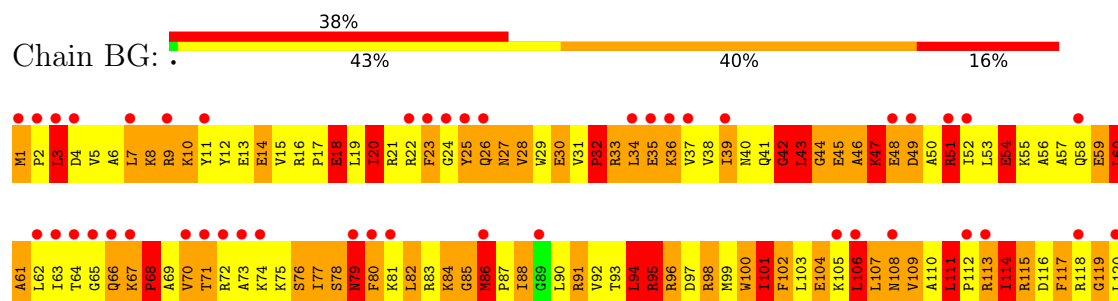
• Molecule 29: 50S RIBOSOMAL PROTEIN L3

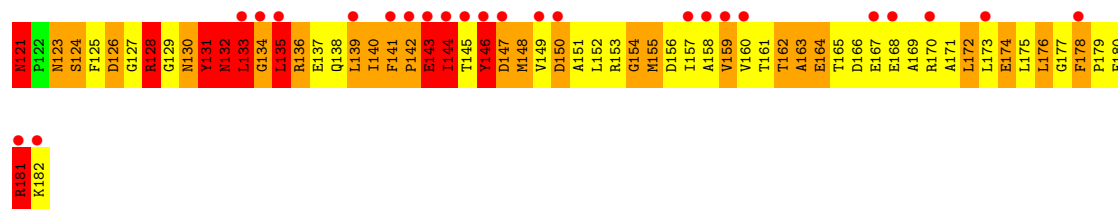


• Molecule 30: 50S RIBOSOMAL PROTEIN L4

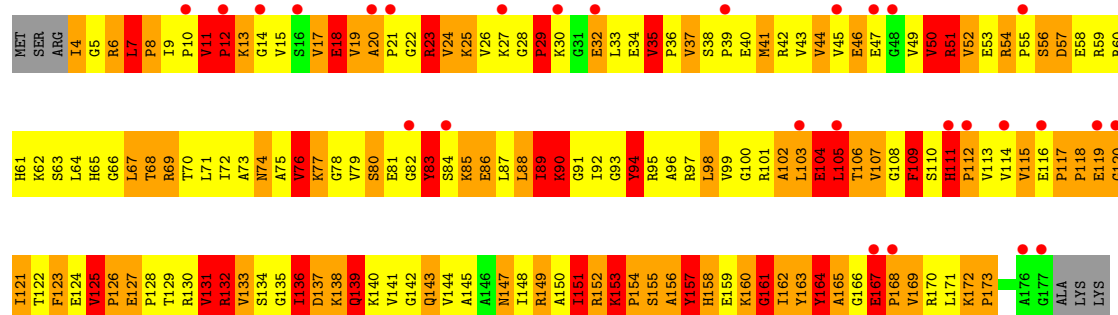


• Molecule 31: 50S RIBOSOMAL PROTEIN L5

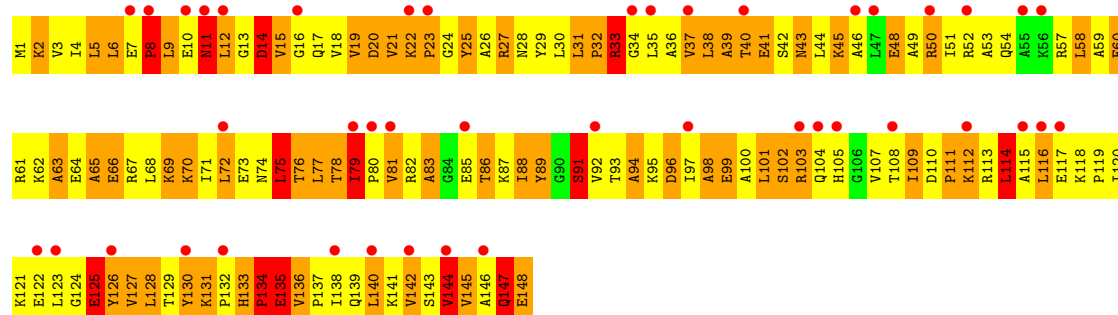




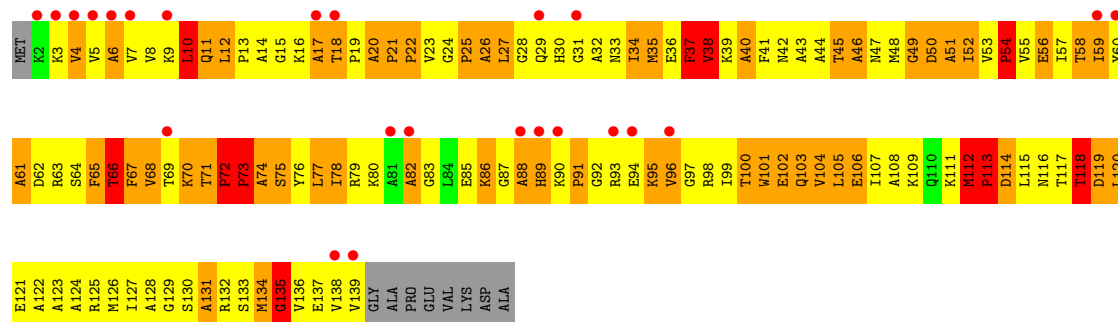
• Molecule 32: 50S RIBOSOMAL PROTEIN L6



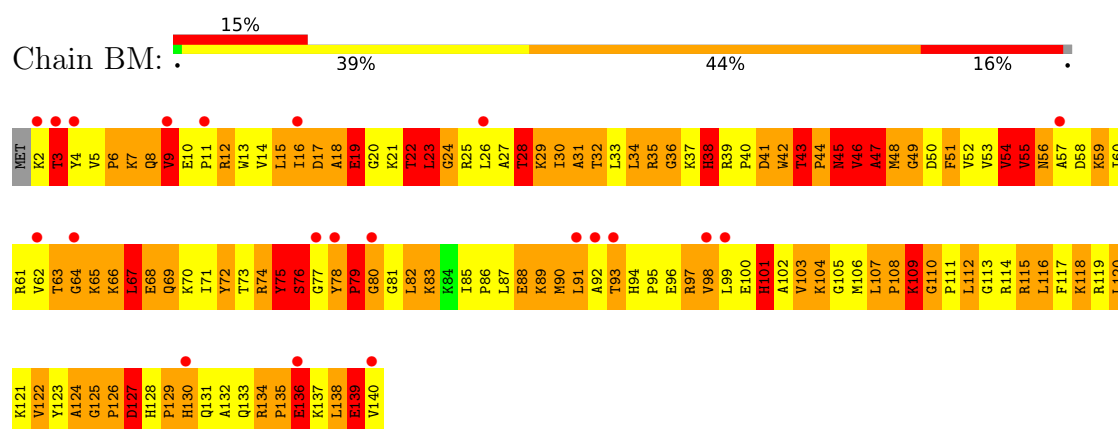
• Molecule 33: 50S RIBOSOMAL PROTEIN L9



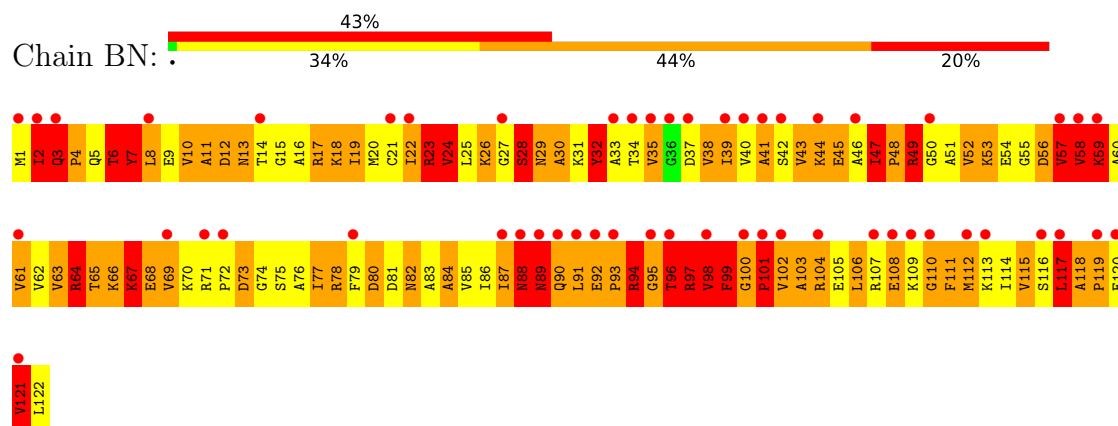
• Molecule 34: 50S RIBOSOMAL PROTEIN L11



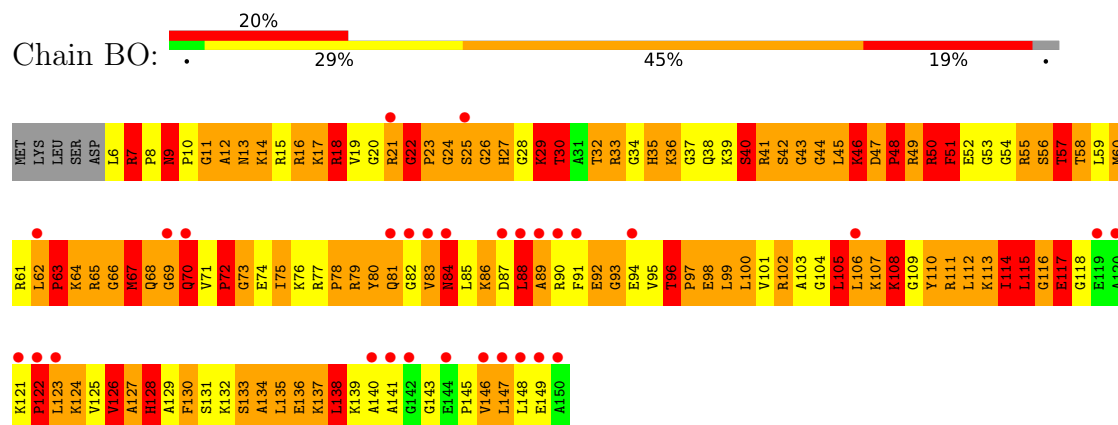
• Molecule 35: 50S RIBOSOMAL PROTEIN L13



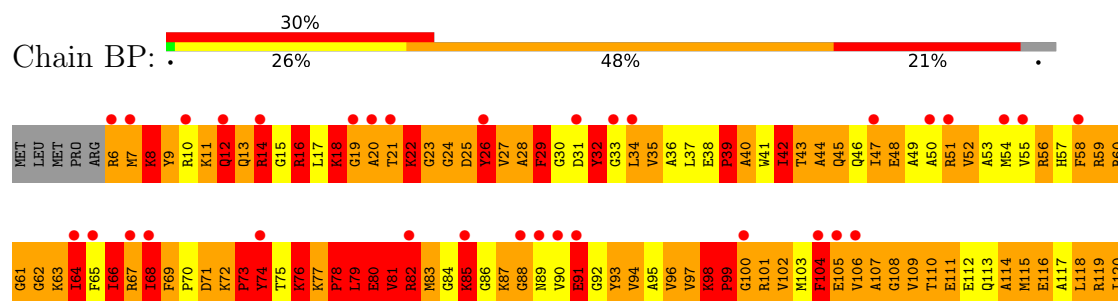
• Molecule 36: 50S RIBOSOMAL PROTEIN L14



• Molecule 37: 50S RIBOSOMAL PROTEIN L15



• Molecule 38: 50S RIBOSOMAL PROTEIN L16

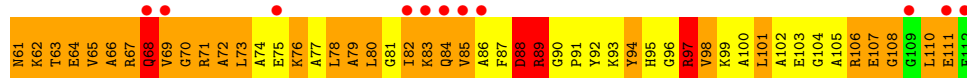




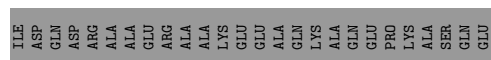
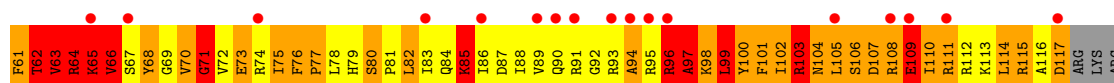
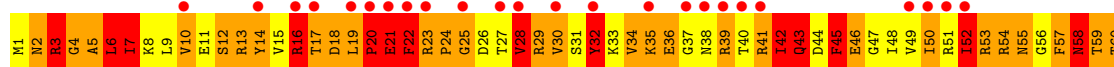
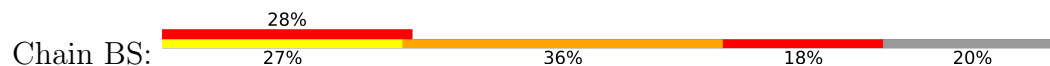
• Molecule 39: 50S RIBOSOMAL PROTEIN L17



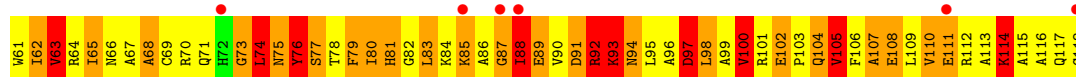
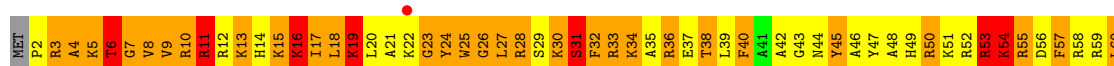
• Molecule 40: 50S RIBOSOMAL PROTEIN L18



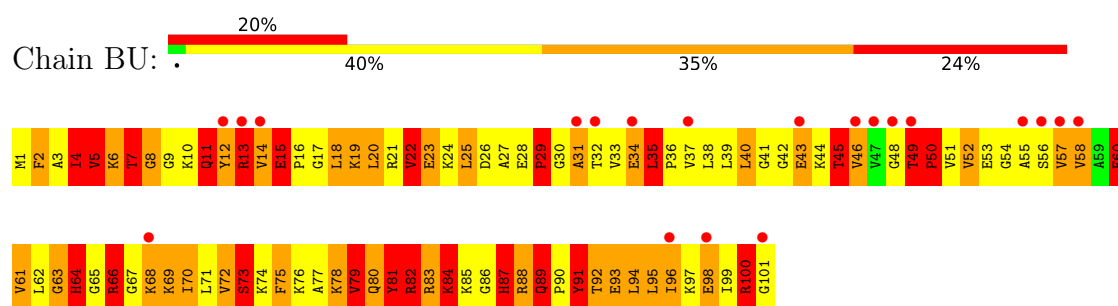
• Molecule 41: 50S RIBOSOMAL PROTEIN L19



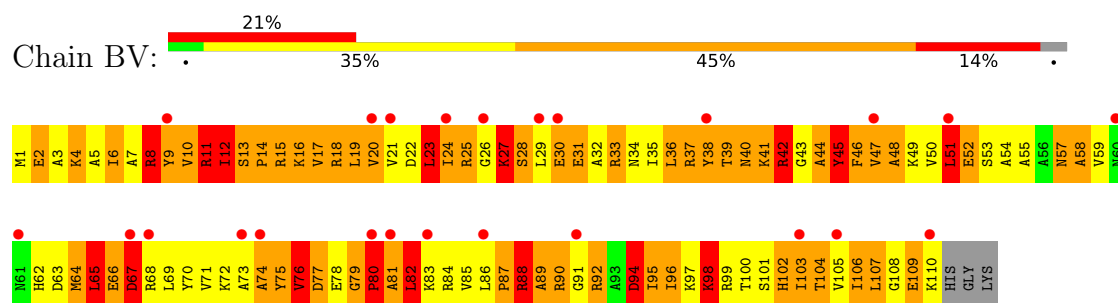
• Molecule 42: 50S RIBOSOMAL PROTEIN L20



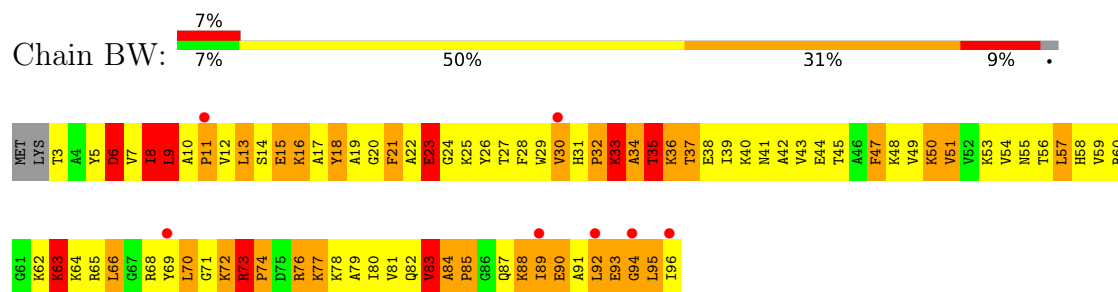
• Molecule 43: 50S RIBOSOMAL PROTEIN L21



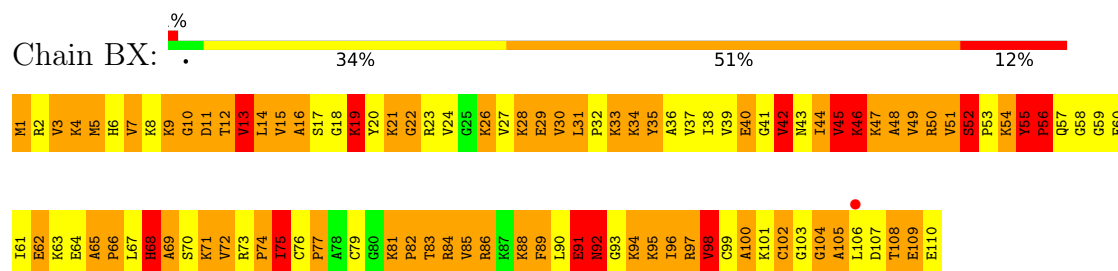
• Molecule 44: 50S RIBOSOMAL PROTEIN L22



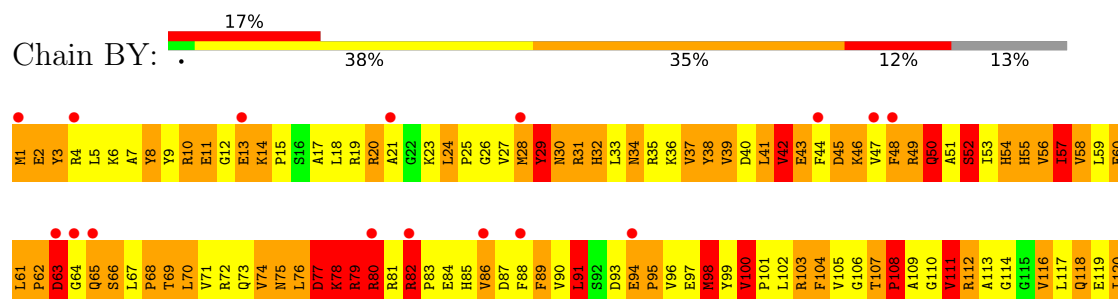
• Molecule 45: 50S RIBOSOMAL PROTEIN L23

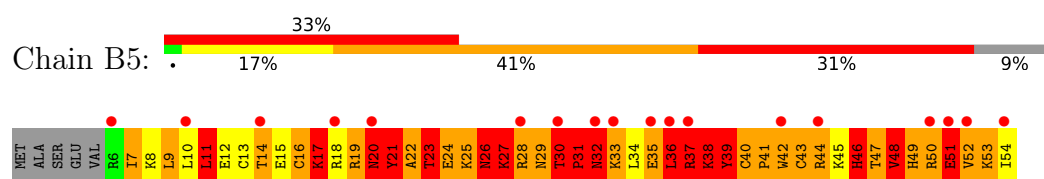


• Molecule 46: 50S RIBOSOMAL PROTEIN L24

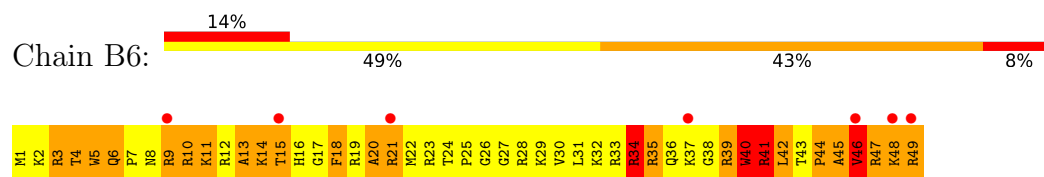


• Molecule 47: 50S RIBOSOMAL PROTEIN L25

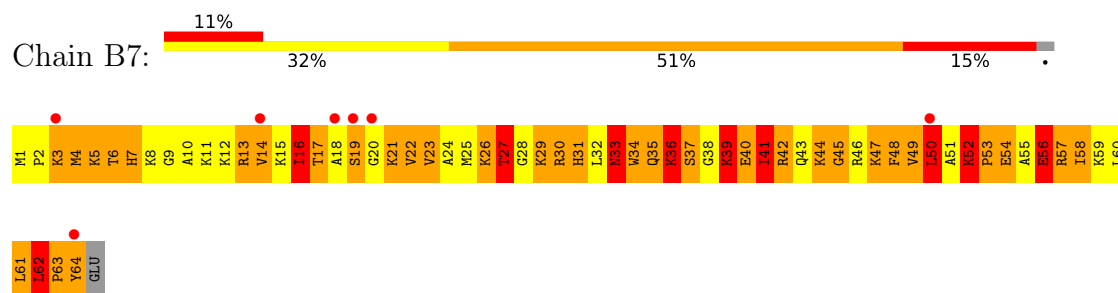




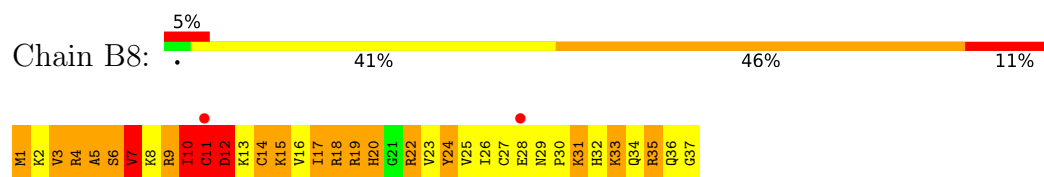
- Molecule 54: 50S RIBOSOMAL PROTEIN L34



- Molecule 55: 50S RIBOSOMAL PROTEIN L35



- Molecule 56: 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	508.65Å 508.65Å 803.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	300.00 – 4.51 300.00 – 4.51	Depositor EDS
% Data completeness (in resolution range)	90.3 (300.00-4.51) 95.0 (300.00-4.51)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 4.02Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.298 , 0.345 0.264 , 0.306	Depositor DCC
R_{free} test set	21439 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	198.7	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.13 , 22.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.55$, $\langle L^2 \rangle = 0.39$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	149640	wwPDB-VP
Average B, all atoms (Å ²)	252.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.62% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	AA	0.63	7/36438 (0.0%)	1.04	177/56869 (0.3%)
2	AC	0.65	0/1814	1.04	10/2825 (0.4%)
3	AD	0.78	2/1813 (0.1%)	0.92	4/2823 (0.1%)
4	A1	0.56	0/673	1.00	5/1048 (0.5%)
5	AE	0.85	0/1935	1.52	42/2609 (1.6%)
6	AF	0.72	0/1636	1.37	22/2205 (1.0%)
7	AG	0.88	4/1733 (0.2%)	1.62	36/2318 (1.6%)
8	AH	0.98	2/1162 (0.2%)	1.52	23/1564 (1.5%)
9	AI	0.88	0/856	1.38	12/1154 (1.0%)
10	AJ	0.71	0/1276	1.33	16/1709 (0.9%)
11	AK	0.95	0/1136	1.57	25/1527 (1.6%)
12	AL	0.71	0/1029	1.17	11/1379 (0.8%)
13	AM	0.69	0/807	1.27	8/1085 (0.7%)
14	AN	0.89	0/900	1.54	22/1213 (1.8%)
15	AO	0.87	1/986 (0.1%)	1.59	18/1320 (1.4%)
16	AP	0.71	0/1008	1.36	14/1347 (1.0%)
17	AQ	0.72	0/501	1.46	8/664 (1.2%)
18	AR	0.92	0/745	1.35	7/992 (0.7%)
19	AS	0.99	0/716	1.51	18/963 (1.9%)
20	AT	0.90	0/870	1.54	21/1159 (1.8%)
21	AU	0.91	0/603	1.64	14/799 (1.8%)
22	AV	0.69	0/661	1.23	8/890 (0.9%)
23	AW	0.96	0/765	1.49	17/1007 (1.7%)
24	AX	0.75	2/212 (0.9%)	1.22	2/277 (0.7%)
25	BA	0.71	28/69685 (0.0%)	1.15	585/108786 (0.5%)
26	BB	0.56	0/2954	0.98	10/4606 (0.2%)
27	BC	0.75	0/1775	1.37	33/2393 (1.4%)
28	BD	1.13	6/2174 (0.3%)	1.90	85/2927 (2.9%)
29	BE	1.20	7/1611 (0.4%)	1.96	67/2171 (3.1%)
30	BF	1.00	3/1660 (0.2%)	1.67	44/2247 (2.0%)
31	BG	0.84	2/1507 (0.1%)	1.61	36/2027 (1.8%)
32	BH	0.90	4/1354 (0.3%)	1.59	39/1831 (2.1%)
33	BK	0.91	1/1170 (0.1%)	1.69	33/1581 (2.1%)
34	BL	0.79	0/1044	1.46	27/1415 (1.9%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
35	BM	1.12	4/1140 (0.4%)	1.66	27/1537 (1.8%)
36	BN	1.36	4/942 (0.4%)	2.08	44/1268 (3.5%)
37	BO	1.06	5/1123 (0.4%)	1.89	40/1493 (2.7%)
38	BP	1.09	3/1100 (0.3%)	1.76	33/1470 (2.2%)
39	BQ	0.97	1/974 (0.1%)	1.49	17/1302 (1.3%)
40	BR	1.06	3/887 (0.3%)	1.68	23/1180 (1.9%)
41	BS	1.31	6/990 (0.6%)	2.08	44/1325 (3.3%)
42	BT	1.07	1/982 (0.1%)	1.67	31/1306 (2.4%)
43	BU	1.24	4/790 (0.5%)	2.11	32/1057 (3.0%)
44	BV	1.00	0/886	1.79	37/1189 (3.1%)
45	BW	0.80	0/756	1.44	11/1015 (1.1%)
46	BX	0.85	2/857 (0.2%)	1.64	23/1142 (2.0%)
47	BY	0.91	2/1467 (0.1%)	1.69	44/1992 (2.2%)
48	BZ	0.87	0/679	1.46	10/902 (1.1%)
49	B1	0.83	0/569	1.21	4/751 (0.5%)
50	B2	0.97	1/474 (0.2%)	1.55	12/635 (1.9%)
51	B3	1.36	6/594 (1.0%)	2.02	35/795 (4.4%)
52	B4	1.15	2/459 (0.4%)	1.89	15/621 (2.4%)
53	B5	1.27	1/433 (0.2%)	2.16	24/576 (4.2%)
54	B6	1.06	0/438	1.39	5/575 (0.9%)
55	B7	0.97	0/523	1.95	19/690 (2.8%)
56	B8	0.97	0/310	1.61	10/407 (2.5%)
All	All	0.78	114/162582 (0.1%)	1.27	2039/242958 (0.8%)

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	241
2	AC	0	9
3	AD	0	12
4	A1	0	5
7	AG	0	1
8	AH	0	1
11	AK	0	2
14	AN	0	1
15	AO	0	1
20	AT	0	1
24	AX	0	1
25	BA	0	610

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Mol	Chain	#Chirality outliers	#Planarity outliers
26	BB	0	20
28	BD	0	1
30	BF	0	1
32	BH	0	3
36	BN	0	2
38	BP	0	3
41	BS	0	2
42	BT	0	1
43	BU	0	2
44	BV	0	1
51	B3	0	2
52	B4	0	1
53	B5	0	1
56	B8	0	1
All	All	0	926

The worst 5 of 114 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	BA	1203	G	O3'-P	-27.77	1.19	1.61
25	BA	1202	C	O3'-P	23.92	1.97	1.61
25	BA	2447	G	O3'-P	-17.04	1.35	1.61
25	BA	2601	C	O3'-P	15.73	1.84	1.61
25	BA	2756	U	O3'-P	15.35	1.84	1.61

The worst 5 of 2039 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	BA	2448	A	C5'-C4'-O4'	-21.86	76.31	109.10
25	BA	1203	G	P-O3'-C3'	21.85	152.97	120.20
53	B5	24	GLU	N-CA-C	19.82	138.49	111.74
43	BU	49	THR	CA-C-N	18.81	143.35	119.84
43	BU	49	THR	C-N-CA	18.81	143.35	119.84

There are no chirality outliers.

5 of 926 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	12	U	Sidechain
1	AA	16	A	Sidechain
1	AA	21	G	Sidechain

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Mol	Chain	Res	Type	Group
1	AA	24	U	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	6684	0
2	AC	1624	0	826	330	0
3	AD	1623	0	809	306	0
4	A1	596	0	296	66	0
5	AE	1900	0	1951	962	0
6	AF	1612	0	1677	682	0
7	AG	1703	0	1763	836	0
8	AH	1146	0	1207	497	0
9	AI	843	0	857	410	0
10	AJ	1257	0	1296	543	0
11	AK	1116	0	1177	680	0
12	AL	1010	0	1037	467	0
13	AM	794	0	840	335	0
14	AN	885	0	904	425	0
15	AO	970	0	1057	422	0
16	AP	997	0	1072	482	0
17	AQ	492	0	529	278	0
18	AR	734	0	771	364	0
19	AS	700	0	720	356	0
20	AT	857	0	930	397	0
21	AU	597	0	668	363	0
22	AV	647	0	673	255	0
23	AW	763	0	861	340	0
24	AX	208	0	221	89	0
25	BA	62218	0	31354	15681	0
26	BB	2641	0	1337	598	0
27	BC	1742	0	1796	780	0
28	BD	2124	0	2207	1457	0
29	BE	1578	0	1647	1143	0
30	BF	1625	0	1666	889	0
31	BG	1482	0	1546	864	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	BH	1328	0	1408	690	0
33	BK	1155	0	1244	590	0
34	BL	1025	0	1074	431	0
35	BM	1113	0	1183	739	0
36	BN	932	0	994	723	0
37	BO	1106	0	1183	820	0
38	BP	1080	0	1127	708	0
39	BQ	960	0	1021	514	0
40	BR	877	0	938	488	0
41	BS	976	0	1033	721	0
42	BT	964	0	1022	729	0
43	BU	779	0	852	642	0
44	BV	876	0	941	431	0
45	BW	742	0	800	343	0
46	BX	844	0	930	498	0
47	BY	1435	0	1463	707	0
48	BZ	670	0	700	378	0
49	B1	567	0	621	314	0
50	B2	469	0	518	306	0
51	B3	581	0	577	382	0
52	B4	445	0	459	280	0
53	B5	426	0	452	310	0
54	B6	430	0	480	280	0
55	B7	515	0	587	424	0
56	B8	307	0	335	129	0
All	All	149640	0	102066	46153	0

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 184.

The worst 5 of 46153 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)
25:BA:1204:A:C2	30:BF:188:ARG:HA	1.17	1.61
25:BA:2459:A:N3	25:BA:2460:U:H1'	1.22	1.46
25:BA:1204:A:C2	30:BF:188:ARG:CA	1.98	1.45
25:BA:2745:C:N4	25:BA:2756:U:C5	1.85	1.45
25:BA:1475:G:H1	25:BA:1477:A:N6	1.11	1.44

There are no symmetry-related clashes.

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	
5	AE	232/256 (91%)	112 (48%)	47 (20%)	73 (32%)	0	0
6	AF	204/239 (85%)	115 (56%)	43 (21%)	46 (22%)	0	1
7	AG	206/209 (99%)	103 (50%)	61 (30%)	42 (20%)	0	1
8	AH	148/162 (91%)	92 (62%)	34 (23%)	22 (15%)	0	3
9	AI	99/101 (98%)	58 (59%)	19 (19%)	22 (22%)	0	1
10	AJ	153/156 (98%)	74 (48%)	40 (26%)	39 (26%)	0	1
11	AK	136/138 (99%)	71 (52%)	32 (24%)	33 (24%)	0	1
12	AL	125/128 (98%)	64 (51%)	33 (26%)	28 (22%)	0	1
13	AM	96/105 (91%)	55 (57%)	14 (15%)	27 (28%)	0	0
14	AN	117/129 (91%)	62 (53%)	30 (26%)	25 (21%)	0	1
15	AO	122/132 (92%)	62 (51%)	22 (18%)	38 (31%)	0	0
16	AP	123/126 (98%)	63 (51%)	36 (29%)	24 (20%)	0	2
17	AQ	58/61 (95%)	28 (48%)	14 (24%)	16 (28%)	0	0
18	AR	86/89 (97%)	40 (46%)	33 (38%)	13 (15%)	0	3
19	AS	81/88 (92%)	45 (56%)	21 (26%)	15 (18%)	0	2
20	AT	102/105 (97%)	63 (62%)	22 (22%)	17 (17%)	0	2
21	AU	71/88 (81%)	30 (42%)	18 (25%)	23 (32%)	0	0
22	AV	78/93 (84%)	32 (41%)	18 (23%)	28 (36%)	0	0
23	AW	97/106 (92%)	32 (33%)	36 (37%)	29 (30%)	0	0
24	AX	22/27 (82%)	9 (41%)	8 (36%)	5 (23%)	0	1
27	BC	226/229 (99%)	137 (61%)	52 (23%)	37 (16%)	0	3
28	BD	270/276 (98%)	129 (48%)	49 (18%)	92 (34%)	0	0
29	BE	204/206 (99%)	106 (52%)	39 (19%)	59 (29%)	0	0
30	BF	206/210 (98%)	100 (48%)	47 (23%)	59 (29%)	0	0
31	BG	180/182 (99%)	79 (44%)	42 (23%)	59 (33%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	BH	172/180 (96%)	89 (52%)	41 (24%)	42 (24%)	0	1
33	BK	146/148 (99%)	88 (60%)	32 (22%)	26 (18%)	0	2
34	BL	136/147 (92%)	66 (48%)	32 (24%)	38 (28%)	0	0
35	BM	137/140 (98%)	66 (48%)	31 (23%)	40 (29%)	0	0
36	BN	120/122 (98%)	63 (52%)	21 (18%)	36 (30%)	0	0
37	BO	143/150 (95%)	60 (42%)	31 (22%)	52 (36%)	0	0
38	BP	134/141 (95%)	51 (38%)	35 (26%)	48 (36%)	0	0
39	BQ	115/118 (98%)	64 (56%)	33 (29%)	18 (16%)	0	3
40	BR	108/112 (96%)	45 (42%)	30 (28%)	33 (31%)	0	0
41	BS	115/146 (79%)	53 (46%)	26 (23%)	36 (31%)	0	0
42	BT	115/118 (98%)	49 (43%)	39 (34%)	27 (24%)	0	1
43	BU	99/101 (98%)	51 (52%)	22 (22%)	26 (26%)	0	1
44	BV	108/113 (96%)	69 (64%)	15 (14%)	24 (22%)	0	1
45	BW	92/96 (96%)	59 (64%)	14 (15%)	19 (21%)	0	1
46	BX	108/110 (98%)	41 (38%)	27 (25%)	40 (37%)	0	0
47	BY	178/206 (86%)	93 (52%)	48 (27%)	37 (21%)	0	1
48	BZ	83/85 (98%)	50 (60%)	14 (17%)	19 (23%)	0	1
49	B1	65/67 (97%)	27 (42%)	26 (40%)	12 (18%)	0	2
50	B2	57/60 (95%)	32 (56%)	16 (28%)	9 (16%)	0	3
51	B3	69/71 (97%)	26 (38%)	19 (28%)	24 (35%)	0	0
52	B4	55/60 (92%)	16 (29%)	12 (22%)	27 (49%)	0	0
53	B5	47/54 (87%)	13 (28%)	7 (15%)	27 (57%)	0	0
54	B6	47/49 (96%)	16 (34%)	16 (34%)	15 (32%)	0	0
55	B7	62/65 (95%)	29 (47%)	11 (18%)	22 (36%)	0	0
56	B8	35/37 (95%)	20 (57%)	4 (11%)	11 (31%)	0	0
All	All	5988/6337 (94%)	2997 (50%)	1412 (24%)	1579 (26%)	0	1

5 of 1579 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	AE	13	ALA
5	AE	15	VAL
5	AE	17	PHE

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Mol	Chain	Res	Type
5	AE	19	HIS
5	AE	20	GLU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	AE	202/220 (92%)	132 (65%)	70 (35%)	0	2
6	AF	160/188 (85%)	119 (74%)	41 (26%)	0	4
7	AG	180/181 (99%)	134 (74%)	46 (26%)	0	4
8	AH	115/123 (94%)	66 (57%)	49 (43%)	0	0
9	AI	90/90 (100%)	61 (68%)	29 (32%)	0	2
10	AJ	126/127 (99%)	103 (82%)	23 (18%)	2	10
11	AK	119/119 (100%)	74 (62%)	45 (38%)	0	1
12	AL	98/99 (99%)	80 (82%)	18 (18%)	1	10
13	AM	88/92 (96%)	65 (74%)	23 (26%)	0	4
14	AN	90/99 (91%)	59 (66%)	31 (34%)	0	2
15	AO	104/109 (95%)	75 (72%)	29 (28%)	0	3
16	AP	100/101 (99%)	76 (76%)	24 (24%)	1	5
17	AQ	49/50 (98%)	38 (78%)	11 (22%)	1	6
18	AR	79/80 (99%)	51 (65%)	28 (35%)	0	1
19	AS	72/74 (97%)	48 (67%)	24 (33%)	0	2
20	AT	96/97 (99%)	66 (69%)	30 (31%)	0	2
21	AU	64/77 (83%)	43 (67%)	21 (33%)	0	2
22	AV	71/80 (89%)	59 (83%)	12 (17%)	2	11
23	AW	76/82 (93%)	52 (68%)	24 (32%)	0	2
24	AX	19/22 (86%)	14 (74%)	5 (26%)	0	3
27	BC	180/181 (99%)	144 (80%)	36 (20%)	1	8
28	BD	215/218 (99%)	145 (67%)	70 (33%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	BE	166/166 (100%)	97 (58%)	69 (42%)	0	0
30	BF	164/166 (99%)	105 (64%)	59 (36%)	0	1
31	BG	156/156 (100%)	111 (71%)	45 (29%)	0	3
32	BH	143/148 (97%)	92 (64%)	51 (36%)	0	1
33	BK	124/124 (100%)	84 (68%)	40 (32%)	0	2
34	BL	105/111 (95%)	83 (79%)	22 (21%)	1	6
35	BM	118/119 (99%)	78 (66%)	40 (34%)	0	2
36	BN	100/100 (100%)	62 (62%)	38 (38%)	0	1
37	BO	111/116 (96%)	65 (59%)	46 (41%)	0	0
38	BP	106/111 (96%)	52 (49%)	54 (51%)	0	0
39	BQ	100/101 (99%)	66 (66%)	34 (34%)	0	2
40	BR	87/88 (99%)	53 (61%)	34 (39%)	0	1
41	BS	105/127 (83%)	69 (66%)	36 (34%)	0	2
42	BT	93/94 (99%)	62 (67%)	31 (33%)	0	2
43	BU	82/82 (100%)	55 (67%)	27 (33%)	0	2
44	BV	90/92 (98%)	54 (60%)	36 (40%)	0	1
45	BW	76/78 (97%)	54 (71%)	22 (29%)	0	3
46	BX	91/91 (100%)	66 (72%)	25 (28%)	0	3
47	BY	159/179 (89%)	106 (67%)	53 (33%)	0	2
48	BZ	67/67 (100%)	51 (76%)	16 (24%)	1	5
49	B1	62/62 (100%)	43 (69%)	19 (31%)	0	2
50	B2	51/52 (98%)	33 (65%)	18 (35%)	0	1
51	B3	63/63 (100%)	43 (68%)	20 (32%)	0	2
52	B4	50/52 (96%)	33 (66%)	17 (34%)	0	2
53	B5	48/52 (92%)	35 (73%)	13 (27%)	0	3
54	B6	42/42 (100%)	33 (79%)	9 (21%)	1	6
55	B7	54/55 (98%)	35 (65%)	19 (35%)	0	1
56	B8	34/34 (100%)	25 (74%)	9 (26%)	0	3
All	All	5040/5237 (96%)	3449 (68%)	1591 (32%)	0	2

5 of 1591 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
33	BK	60	GLU
38	BP	126	PRO
34	BL	4	VAL
33	BK	58	LEU
36	BN	80	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 186 such sidechains are listed below:

Mol	Chain	Res	Type
33	BK	105	HIS
42	BT	44	ASN
35	BM	69	GLN
38	BP	13	GLN
44	BV	40	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1515/1522 (99%)	481 (31%)	151 (9%)
2	AC	75/76 (98%)	30 (40%)	7 (9%)
25	BA	2888/2916 (99%)	1252 (43%)	313 (10%)
26	BB	122/123 (99%)	46 (37%)	5 (4%)
3	AD	75/76 (98%)	27 (36%)	3 (4%)
4	A1	26/27 (96%)	11 (42%)	1 (3%)
All	All	4701/4740 (99%)	1847 (39%)	480 (10%)

5 of 1847 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 480 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	BA	687	C
25	BA	2610	C
25	BA	1197	G

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Mol	Chain	Res	Type
25	BA	2566	A
25	BA	2879	C

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 oligosaccharides 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
25	BA	6
1	AA	2

The worst 5 of 8 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	BA	1202:C	O3'	1203:G	P	1.97
1	AA	173:U	O3'	174:C	P	1.84
1	BA	2601:C	O3'	2602:A	P	1.84
1	BA	2756:U	O3'	2757:A	P	1.84
1	BA	2755:C	O3'	2756:U	P	1.75

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%)	-0.13	13 (0%) 81 67	188, 245, 349, 445	0
2	AC	76/76 (100%)	0.28	3 (3%) 43 37	213, 249, 283, 294	0
3	AD	76/76 (100%)	0.42	6 (7%) 18 21	301, 334, 358, 368	0
4	A1	27/27 (100%)	1.42	8 (29%) 1 4	225, 347, 415, 416	0
5	AE	234/256 (91%)	0.20	12 (5%) 33 31	218, 248, 286, 307	0
6	AF	206/239 (86%)	0.59	27 (13%) 7 12	246, 269, 288, 296	0
7	AG	208/209 (99%)	1.22	51 (24%) 2 5	202, 233, 251, 265	0
8	AH	150/162 (92%)	1.17	33 (22%) 2 6	202, 220, 245, 262	0
9	AI	101/101 (100%)	2.83	60 (59%) 0 1	219, 237, 254, 271	0
10	AJ	155/156 (99%)	0.35	9 (5%) 29 29	250, 273, 285, 301	0
11	AK	138/138 (100%)	0.91	26 (18%) 3 8	203, 222, 236, 246	0
12	AL	127/128 (99%)	-0.18	1 (0%) 82 69	247, 317, 349, 353	0
13	AM	98/105 (93%)	-0.09	2 (2%) 65 51	256, 296, 311, 317	0
14	AN	119/129 (92%)	0.87	19 (15%) 5 9	214, 234, 252, 279	0
15	AO	124/132 (93%)	1.46	35 (28%) 1 5	189, 217, 243, 263	0
16	AP	125/126 (99%)	0.86	21 (16%) 4 9	253, 281, 302, 306	0
17	AQ	60/61 (98%)	-0.26	0 100 100	243, 273, 286, 290	0
18	AR	88/89 (98%)	1.12	19 (21%) 2 6	199, 222, 244, 251	0
19	AS	83/88 (94%)	0.99	20 (24%) 2 5	192, 212, 232, 267	0
20	AT	104/105 (99%)	1.11	26 (25%) 2 5	192, 218, 252, 296	0
21	AU	73/88 (82%)	1.64	28 (38%) 1 3	192, 228, 254, 276	0
22	AV	80/93 (86%)	0.36	4 (5%) 34 31	251, 287, 306, 310	0
23	AW	99/106 (93%)	1.55	33 (33%) 1 4	200, 228, 250, 254	0
24	AX	24/27 (88%)	-0.58	0 100 100	268, 289, 303, 306	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	BA	2889/2916 (99%)	0.09	108 (3%) 45 37	168, 241, 340, 398	0
26	BB	123/123 (100%)	-0.06	2 (1%) 70 55	236, 293, 329, 343	0
27	BC	228/229 (99%)	1.40	57 (25%) 2 5	299, 326, 342, 347	0
28	BD	272/276 (98%)	1.95	92 (33%) 1 4	184, 216, 235, 256	0
29	BE	206/206 (100%)	1.17	48 (23%) 2 6	155, 205, 250, 276	0
30	BF	208/210 (99%)	1.13	61 (29%) 1 4	186, 255, 283, 288	0
31	BG	182/182 (100%)	1.76	69 (37%) 1 3	247, 283, 306, 311	0
32	BH	174/180 (96%)	0.78	28 (16%) 4 9	230, 260, 278, 284	0
33	BK	148/148 (100%)	1.47	43 (29%) 1 4	212, 241, 261, 265	0
34	BL	138/147 (93%)	0.93	24 (17%) 4 8	305, 358, 399, 403	0
35	BM	139/140 (99%)	0.77	21 (15%) 5 10	187, 217, 245, 270	0
36	BN	122/122 (100%)	1.93	53 (43%) 0 2	172, 201, 228, 240	0
37	BO	145/150 (96%)	1.04	30 (20%) 2 6	189, 271, 304, 346	0
38	BP	136/141 (96%)	1.39	42 (30%) 1 4	199, 234, 257, 266	0
39	BQ	117/118 (99%)	0.44	8 (6%) 23 25	195, 214, 246, 256	0
40	BR	110/112 (98%)	1.15	25 (22%) 2 6	232, 266, 293, 300	0
41	BS	117/146 (80%)	1.65	41 (35%) 1 3	182, 205, 238, 244	0
42	BT	117/118 (99%)	0.36	7 (5%) 27 28	191, 221, 241, 250	0
43	BU	101/101 (100%)	0.98	20 (19%) 3 7	190, 244, 272, 277	0
44	BV	110/113 (97%)	1.18	24 (21%) 2 6	203, 226, 250, 260	0
45	BW	94/96 (97%)	0.28	7 (7%) 20 23	237, 253, 304, 309	0
46	BX	110/110 (100%)	0.21	1 (0%) 81 67	244, 282, 303, 312	0
47	BY	180/206 (87%)	1.08	34 (18%) 3 8	235, 267, 281, 287	0
48	BZ	85/85 (100%)	1.21	17 (20%) 3 7	236, 258, 272, 289	0
49	B1	67/67 (100%)	-0.09	0 100 100	251, 264, 276, 281	0
50	B2	59/60 (98%)	1.13	12 (20%) 3 6	208, 244, 261, 268	0
51	B3	71/71 (100%)	1.62	23 (32%) 1 4	212, 239, 259, 276	0
52	B4	57/60 (95%)	1.09	10 (17%) 4 8	200, 227, 276, 299	0
53	B5	49/54 (90%)	1.91	18 (36%) 1 3	211, 247, 269, 277	0
54	B6	49/49 (100%)	0.63	7 (14%) 6 11	189, 228, 244, 250	0
55	B7	64/65 (98%)	0.68	7 (10%) 10 15	201, 220, 235, 247	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
56	B8	37/37 (100%)	0.19	2 (5%) 31 30	212, 230, 240, 244	0
All	All	10794/11077 (97%)	0.59	1397 (12%) 7 12	155, 245, 336, 445	0

The worst 5 of 1397 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
27	BC	125	SER	14.9
40	BR	85	VAL	11.2
27	BC	126	LYS	11.1
16	AP	124	PRO	11.0
28	BD	170	GLY	10.2

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 oligosaccharides 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.