



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 22, 2024 – 01:55 PM EDT

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](mailto: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>.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

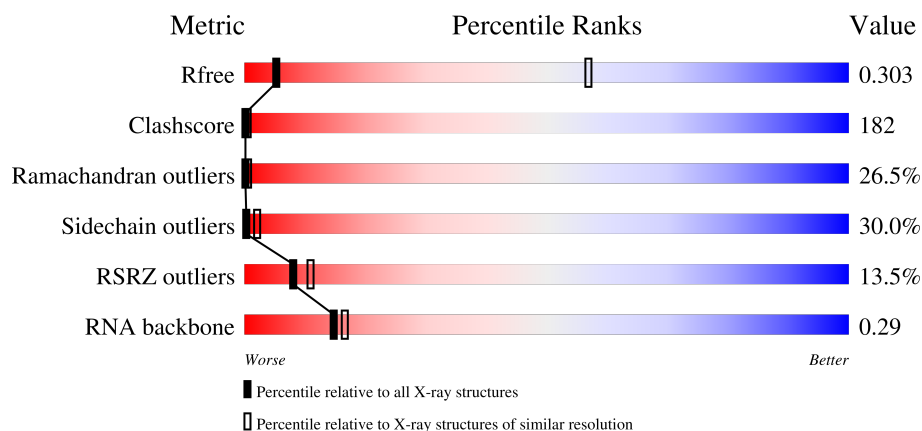
# 1 Overall quality at a glance

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))
$R_{free}$	164625	1015 (6.06-3.94)
Clashscore	180529	1031 (6.04-3.96)
Ramachandran outliers	177936	1102 (6.10-3.90)
Sidechain outliers	177891	1081 (6.10-3.90)
RSRZ outliers	164620	1011 (6.06-3.94)
RNA backbone	3690	1166 (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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	<div> <div>55%</div> <div>34%</div> <div>9%</div> </div>
2	AC	77	<div> <div>5%</div> <div>45%</div> <div>42%</div> <div>10%</div> </div>
3	AD	76	<div> <div>14%</div> <div>54%</div> <div>42%</div> </div>
4	AE	256	<div> <div>7%</div> <div>48%</div> <div>34%</div> <div>7%</div> <div>9%</div> </div>

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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	<div><div></div><div>11%</div><div>5%</div><div>54%</div><div>38%</div><div></div></div>

## 2 Entry composition

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
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 protein called 30S ribosomal protein S2.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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



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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

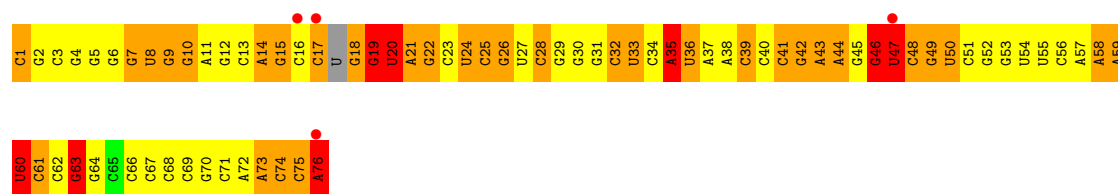
- Molecule 55 is a protein called 50S ribosomal protein L36.

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

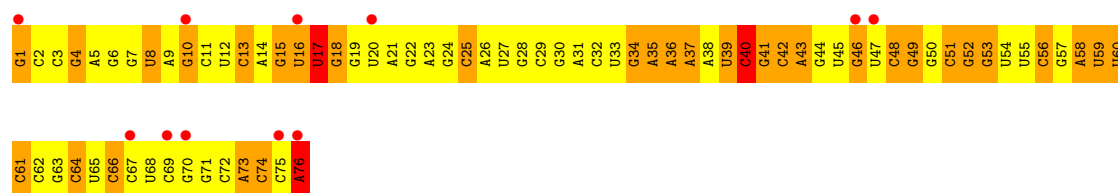


G1529	G1530	A1531	U1532	C1533	A1534	C1535	C1536	C1537	C1538	C1539	U1540	U1541	U1542	C	U
G1469	G1470	G1471	U1472	A1473	G1474	G1475	G1476	G1477	C1478	C1479	G1480	U1481	G1482	A1483	A1484
G1404	G1405	U1406	C1407	A1408	C1409	G1410	G1411	C1412	A1413	A1414	G1415	G1416	G1417	A1418	A1419
G1345	A1346	G1347	U1348	A1349	A1350	U1351	C1352	G1353	C1354	G1355	G1356	A1357	U1358	C1359	A1360
G1285	A1286	A1287	A1288	A1289	G1290	G1291	U1292	G1293	G1294	G1295	C1296	G1297	U1298	A1299	G1300
A1225	C1226	C1227	C1228	A1229	C1230	G1231	U1232	G1233	C1234	U1235	C1236	A1237	A1238	A1239	U1240
G1164	C1165	A1166	A1167	A1169	C1170	G1171	C1172	G1173	G1174	C1175	G1176	A1177	G1178	A1179	G1180
G1104	A1105	G1106	C1107	G1108	C1109	A1110	C1111	G1112	C1113	G1114	C1115	G1116	G1117	C1118	G1119
A1044	C1045	A1046	G1047	U1048	G1049	G1050	C1051	U1052	C1053	C1054	A1055	U1056	G1057	G1058	C1059
C989	C990	U991	U992	G993	A994	C995	A996	U997	G998	C998A	U999	A1000	G1001	G1002	G1003
C929	C930	C931	C932	G933	C934	A935	C936	U937	A938	C939	C940	G941	C942	C943	U944
G889	U890	U891	A892	G893	G894	C895	C896	C897	C898	C899	G900	C901	C902	U903	U904
G802	G803	U804	C805	G806	G807	G808	C809	C810	C811	C812	A813	A814	A815	A816	C817
G742	U743	C744	C745	A746	C747	C748	C749	C750	C751	C752	A753	C754	C755	C756	C757
G760	C761	C762	G763	C764	C765	A766	C767	C768	C769	C770	C771	U772	C773	C774	C775
G776	C777	C778	C779	A780	C781	C782	C783	C784	C785	C786	C787	C788	C789	C790	C791
U801	C868	C869	C870	C871	C872	C873	C874	C875	C876	C877	C878	C879	C880	C881	C882
C928	C929	C930	C931	C932	C933	C934	C935	C936	C937	C938	C939	C940	C941	C942	C943
C988	C989	C990	C991	C992	C993	C994	C995	C996	C997	C998	C999	C1000	C1001	C1002	C1003
C1043	C1044	C1045	C1046	C1047	C1048	C1049	C1050	C1051	C1052	C1053	C1054	C1055	C1056	C1057	C1058
C1103	C1104	C1105	C1106	C1107	C1108	C1109	C1110	C1111	C1112	C1113	C1114	C1115	C1116	C1117	C1118
C1163	C1164	C1165	C1166	C1167	C1168	C1169	C1170	C1171	C1172	C1173	C1174	C1175	C1176	C1177	C1178
C1224	C1225	C1226	C1227	C1228	C1229	C1230	C1231	C1232	C1233	C1234	C1235	C1236	C1237	C1238	C1239
C1284	C1285	C1286	C1287	C1288	C1289	C1290	C1291	C1292	C1293	C1294	C1295	C1296	C1297	C1298	C1299
C1344	C1345	C1346	C1347	C1348	C1349	C1350	C1351	C1352	C1353	C1354	C1355	C1356	C1357	C1358	C1359
C1403	C1404	C1405	C1406	C1407	C1408	C1409	C1410	C1411	C1412	C1413	C1414	C1415	C1416	C1417	C1418
C1468	C1469	C1470	C1471	C1472	C1473	C1474	C1475	C1476	C1477	C1478	C1479	C1480	C1481	C1482	C1483
C1528	C1529	C1530	C1531	C1532	C1533	C1534	C1535	C1536	C1537	C1538	C1539	C1540	C1541	C1542	C1543
C1598	C1599	C1600	C1601	C1602	C1603	C1604	C1605	C1606	C1607	C1608	C1609	C1610	C1611	C1612	C1613
C1668	C1669	C1670	C1671	C1672	C1673	C1674	C1675	C1676	C1677	C1678	C1679	C1680	C1681	C1682	C1683
C1738	C1739	C1740	C1741	C1742	C1743	C1744	C1745	C1746	C1747	C1748	C1749	C1750	C1751	C1752	C1753
C1808	C1809	C1810	C1811	C1812	C1813	C1814	C1815	C1816	C1817	C1818	C1819	C1820	C1821	C1822	C1823
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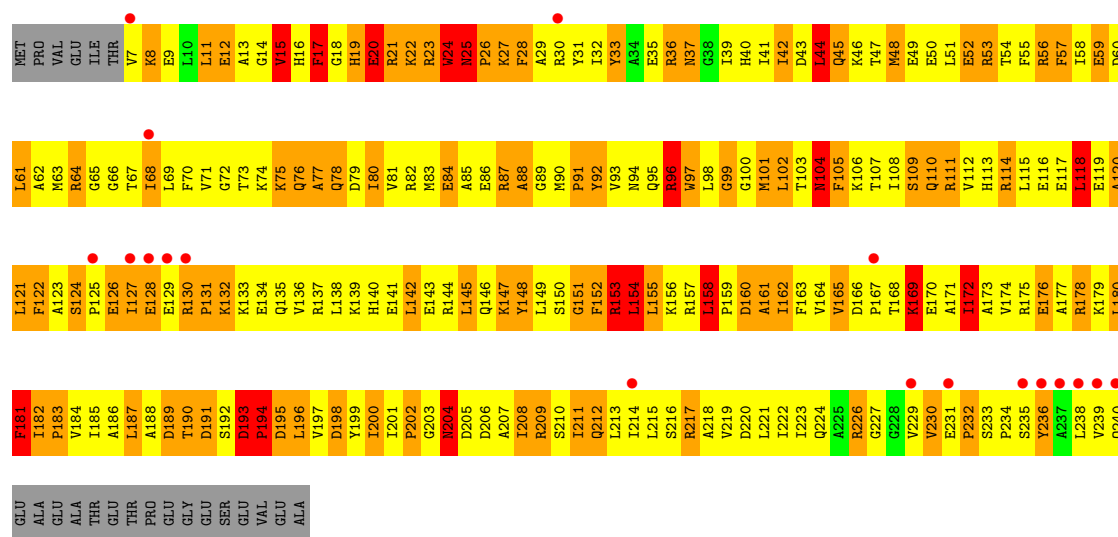




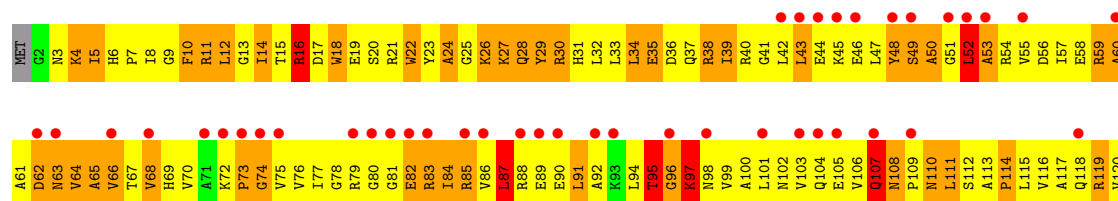
• Molecule 3: tRNA PHE (unmodified bases)

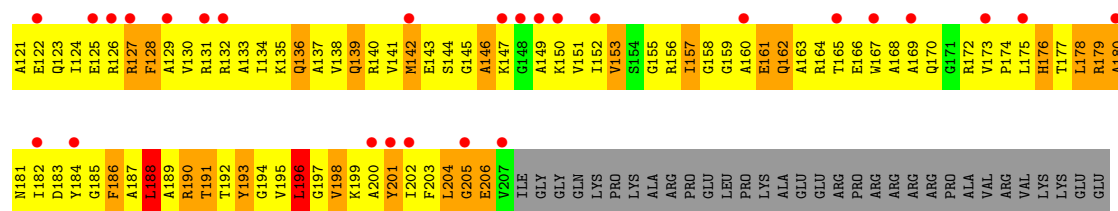


• Molecule 4: 30S ribosomal protein S2



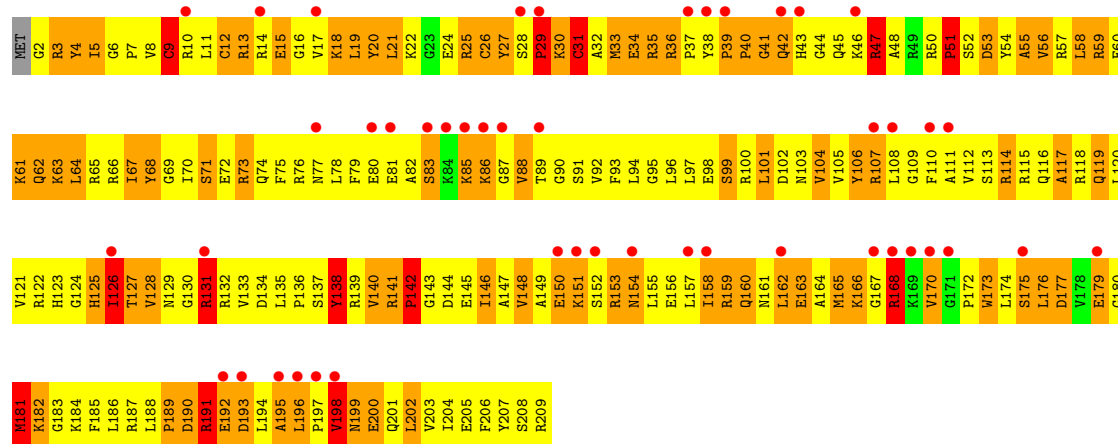
• Molecule 5: 30S ribosomal protein S3





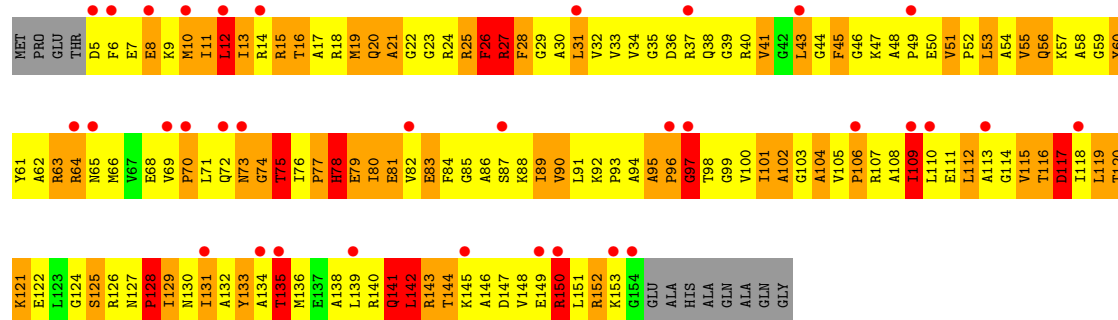
• Molecule 6: 30S ribosomal protein S4

Chain AG: . 22% 52% 39% 6%



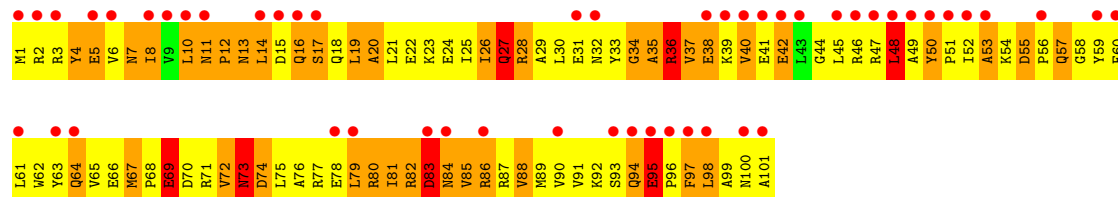
• Molecule 7: 30S ribosomal protein S5

Chain AH: . 21% 50% 31% 8% 7%

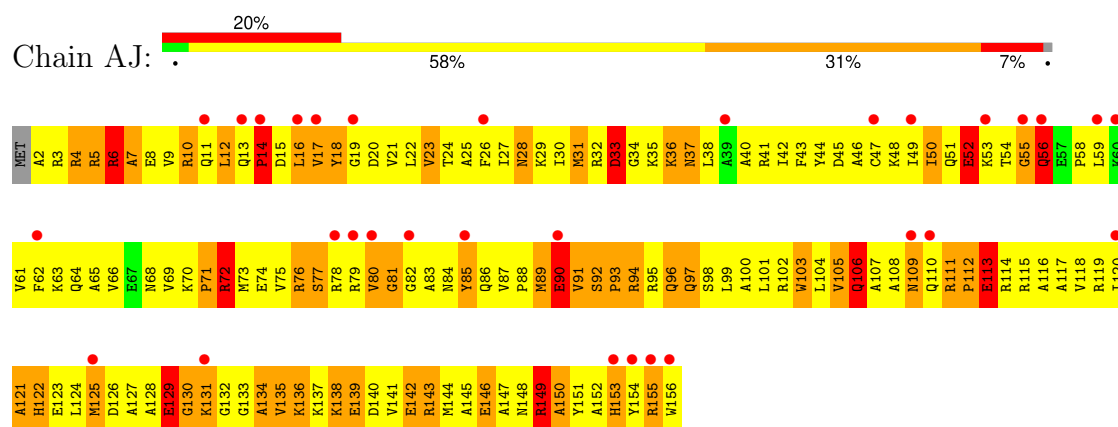


• Molecule 8: 30S ribosomal protein S6

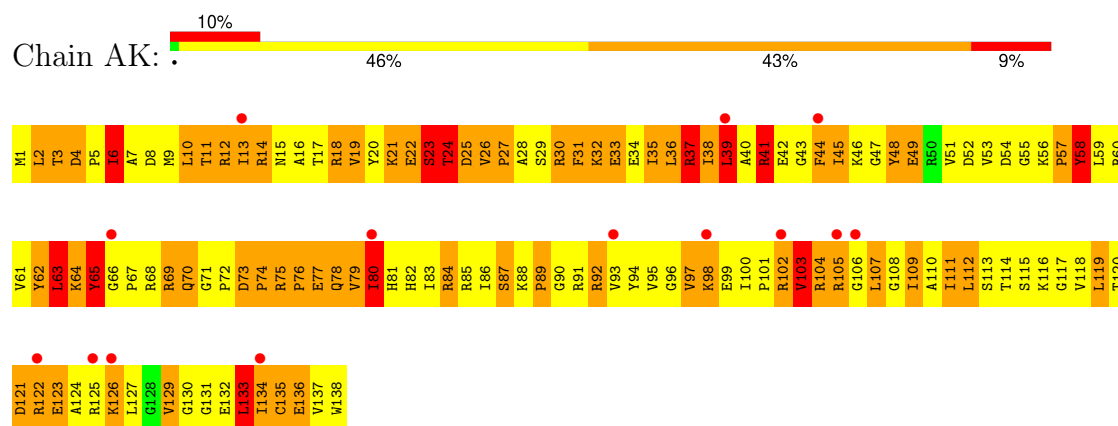
Chain AI: . 50% 51% 40% 7%



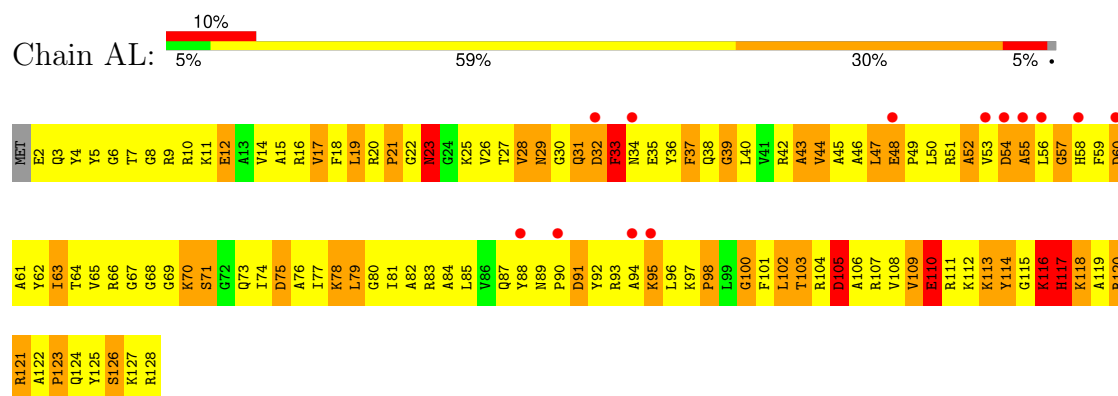
• Molecule 9: 30S ribosomal protein S7



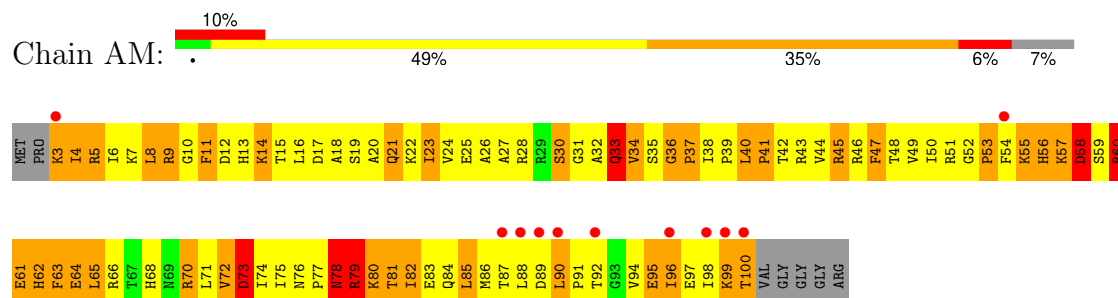
## ● Molecule 10: 30S ribosomal protein S8



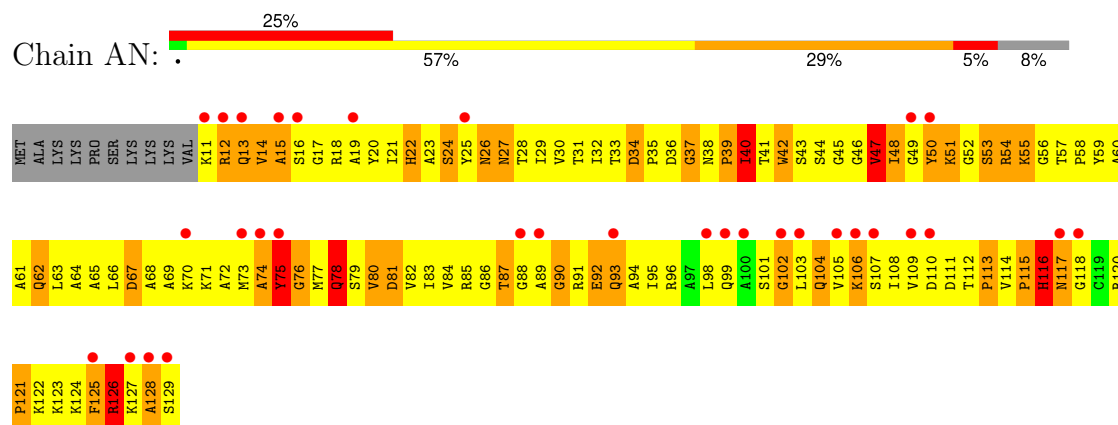
## ● Molecule 11: 30S ribosomal protein S9



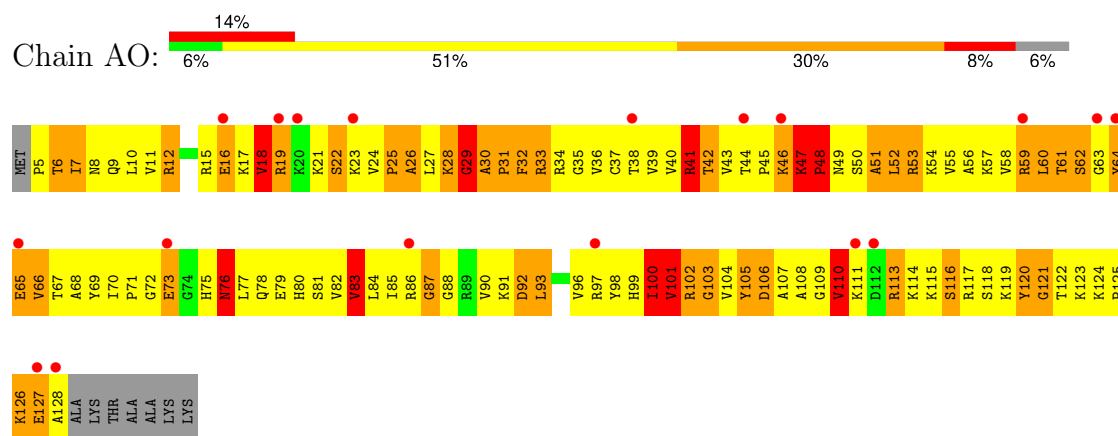
## ● Molecule 12: 30S ribosomal protein S10



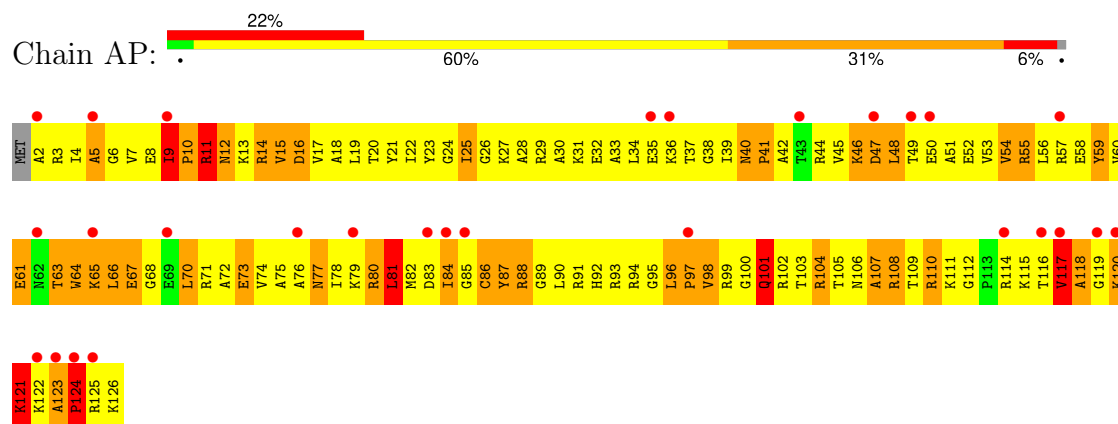
- Molecule 13: 30S ribosomal protein S11



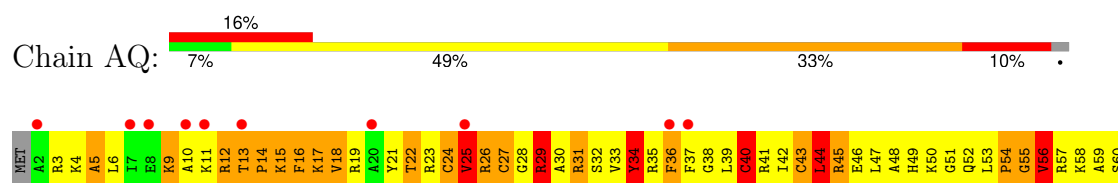
- Molecule 14: 30S ribosomal protein S12



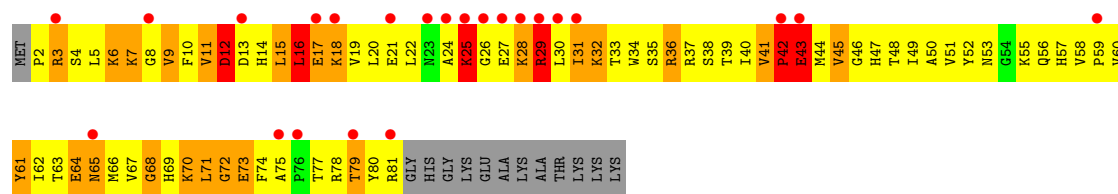
- Molecule 15: 30S ribosomal protein S13



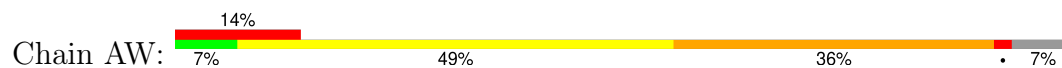
- Molecule 16: 30S ribosomal protein S14







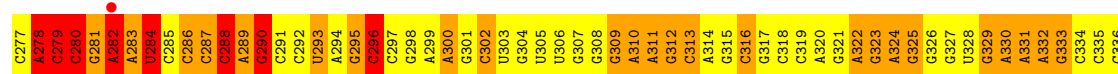
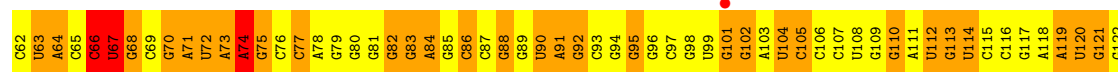
• Molecule 22: 30S ribosomal protein S20



• Molecule 23: 30S ribosomal protein Thx



• Molecule 24: 23S ribosomal RNA



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A1155	A1095	U1035	G975	C915	G854	G794	A734	G674	G636	A678	C516	C455	U395	G338
A1156	A1096	G1036	C976	G916	G855	C795	A735	A675	A637	G579	G517	C456	G396	U339
A1157	U1097	G1037	G977	A917	G856	C796	A736	A676	G638	C580	G317	A457	G397	A340
C1158	A1098	G1038	G978	A918	C857	C797	C737	A677	U639	C581	U519	G458	G398	G341
U1159	G1099	G1039	G979	A919	U858	C798	G738	A678	C640	G582	U520	U459	G399	G342
G1160	C1100	G1040	A980	G920	G859	C799	G739	G679	C641	G583	G521	A460	G400	C343
C1161	U1101	C1041	A981	G921	U860	A800	U740	G680	G642	C584	G522	C461	A401	G344
G1162	C1102	C982	C982	U922	A861	C801	G741	G681	A643	G585	C523	C462	A402	A345
G1163	C1043	A983	A983	C923	G862	U803	G742	G682	A586	C524	G524	G463	U403	A346
G1164	C1044	A984	A984	C924	A863	U803	G743	G683	C645	C587	U525	U464	C404	A347
U1165	A1045	C985	C985	C925	G864	A804	G744	G684	A646	U588	A526	G465	U405	G348
C1166	A1046	C986	C986	A926	C865	G805	G745	A685	G647	C589	C527	A466	G406	G349
U1167	G1047	C987	C987	G928	A866	C806	A746	G686	G648	A590	A528	G467	G407	U350
G1168	A1048	A988	A988	G929	C867	U807	U747	G687	G649	C591	A529	G468	G408	G351
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G1171	G1101	G1051	C991	G932	A870	U810	A750	G690	C	U594	A532	A471	G411	G354
G1172	U1112	C1052	C992	A933	U871	U811	A751	C691	A	C595	G533	A472	A412	G355
A1173	G1113	C1053	G993	G934	A872	C812	A752	C692	A	G596	U534	G473	C413	G356
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G1175	G1115	G1055	C995	C936	G874	U814	C754	U694	C	G598	A536	U475	A415	U358
G1176	C1116	G1056	A996	U937	G875	C815	C755	G695	G	G599	C537	G476	C416	A359
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C1180	G1120	U1060	A1000	A941	G879	A819	G759	A699	C	A603	C542	A480	C419	G363
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G1183	C1123	G1063	G1003	G944	G882	U822	U762	G702	A	U606	G545	A483	A422	G363C
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G1190	U1130	A1070	A1010	C951	C889	A829	G769	U709	C	G612	G552	G491	A429	G367
G1191	G1131	G1071	G1011	G952	A890	G830	G770	G710	C850	U613	U553	A492	C430	A371
G1192	A1132	C1072	U1012	A953	G892	G831	G771	G711	G651	U614	U554	G493	U431	G372
G1193	U1133	A1073	C1013	G954	C893	G832	C772	G712	C652	G615	G556	G494	A432	U373
G1195	G1134	G1074	U1014	G955	C894	U833	U773	G713	A653	A616	U557	G495	C433	G375
C1196	C1135	C1075	G1015	G956	U895	C834	A774	U714	A654	G617	G558	G496	U434	A374
G1197	G1136	C1076	G1016	A957	A896	A835	G775	G715	G655	G618	G559	A497	C435	C376
U1198	G1137	A1077	G1017	U958	C897	C836	G776	A716	G656	C618A	C560	G498	C436	C377
U1199	G1138	A1078	C1018	A959	C898	C837	A777	G717	U657	G619	G561	U499	G438	C378
C1200	G1139	C1079	U1019	A960	A899	C838	G778	A718	C658	G620	U562	G500	G379	G379
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C1202	U1141	U1081	A1021	G962	A901	C840	G780	C720	G660	G622	C564	A502	U441	G381
U1142	U1142	U1082	G1022	U963	C902	A841	A781	C721	C661	G623	C565	A503	G442	G382
A1142A	A1204	U1083	U1023	C964	C903	G842	A782	A722	G662	G624	U566	U504	A443	U383
A1143	G1144	A1084	G1024	C965	C904	G843	A783	G723	G663	G625	A567	A505	C444	U384
G1206	C1145	A1085	G1025	G966	U905	C844	A784	U724	C664	U626	U568	G506	C445	C385
C1207	G1146	G1086	U1026	C967	G906	G845	G785	G725	C665	A627	U569	A507	G446	C386
G1208	U1147	G1087	A1027	G968	U907	C846	G786	G726	G666	G628	G570	G508	G447	U387
G1209	C1208	A1088	A1028	U969	C908	U847	A787	A727	U667	G629	A571	C509	U448	G388
G1210	G1149	G1089	A1029	C970	A909	C848	A788	G728	G668	G630	A572	C510	A449	G389
U1211	C1150	U1090	G1030	C971	A910	A849	A789	G729	G669	A631	G573	U511	G450	A390
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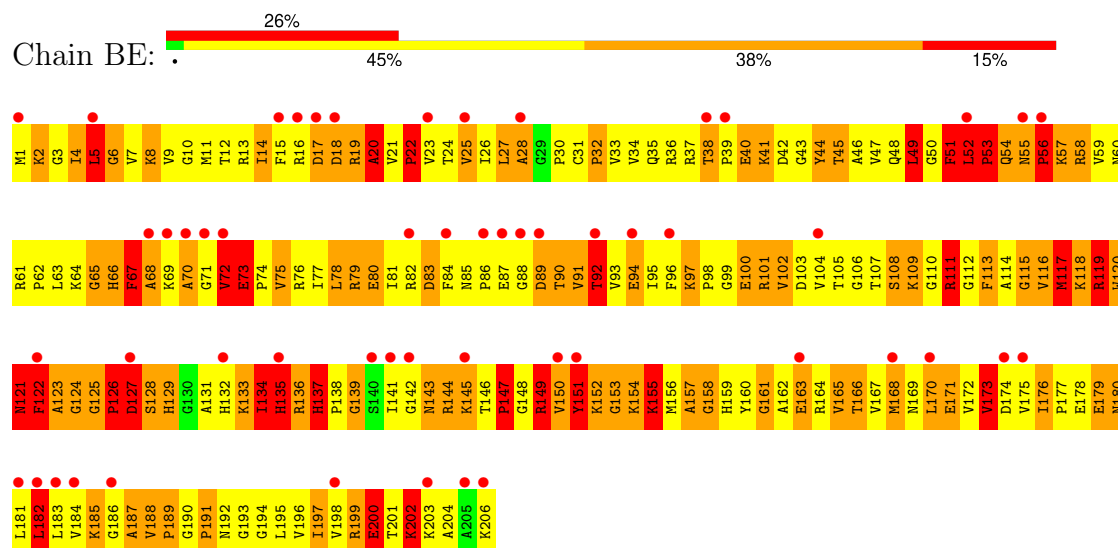
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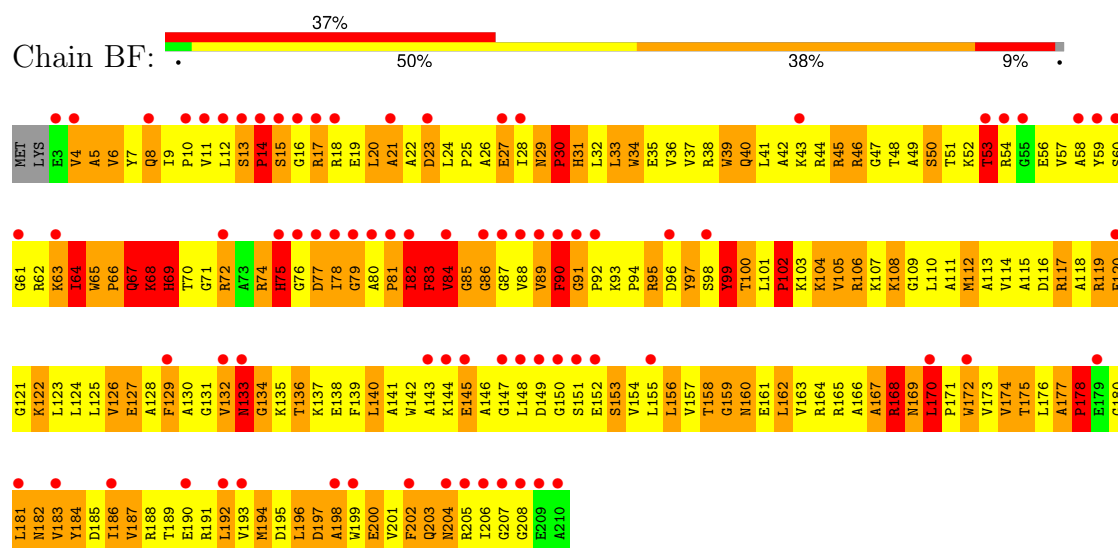
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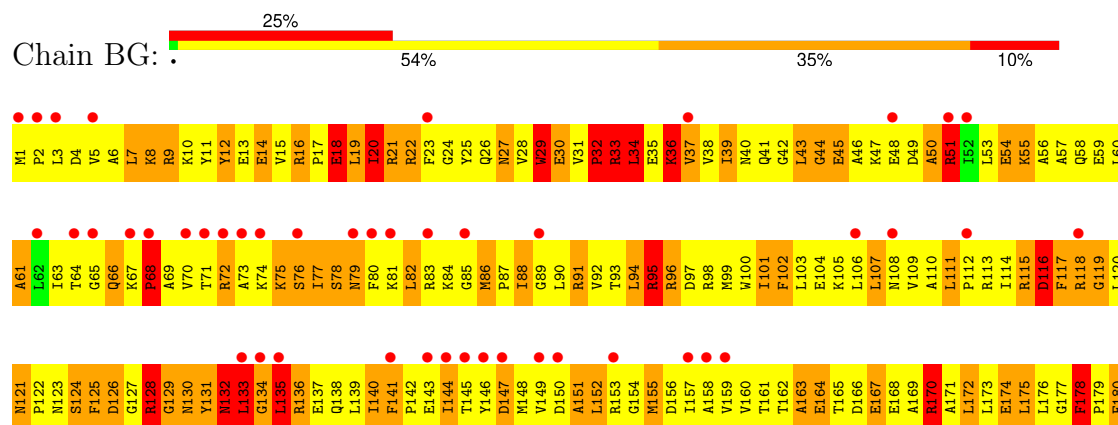
• Molecule 28: 50S ribosomal protein L3



• Molecule 29: 50S ribosomal protein L4

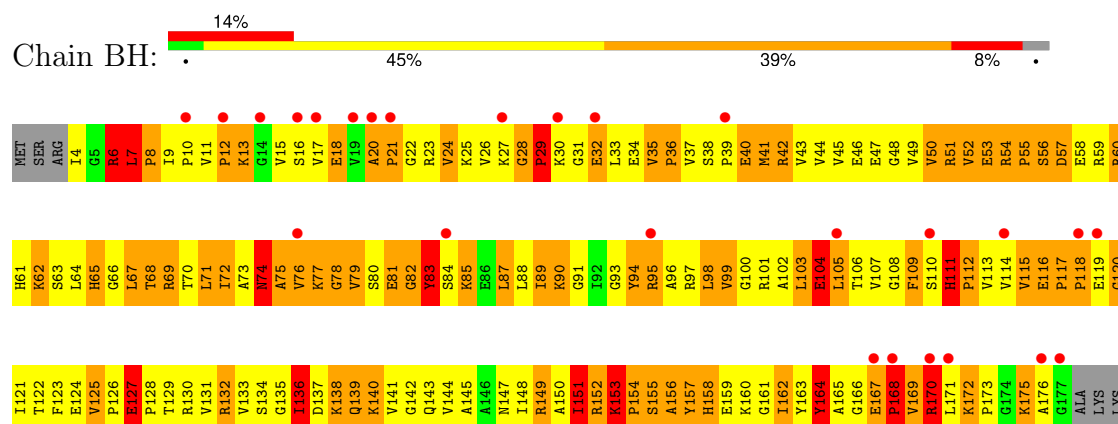


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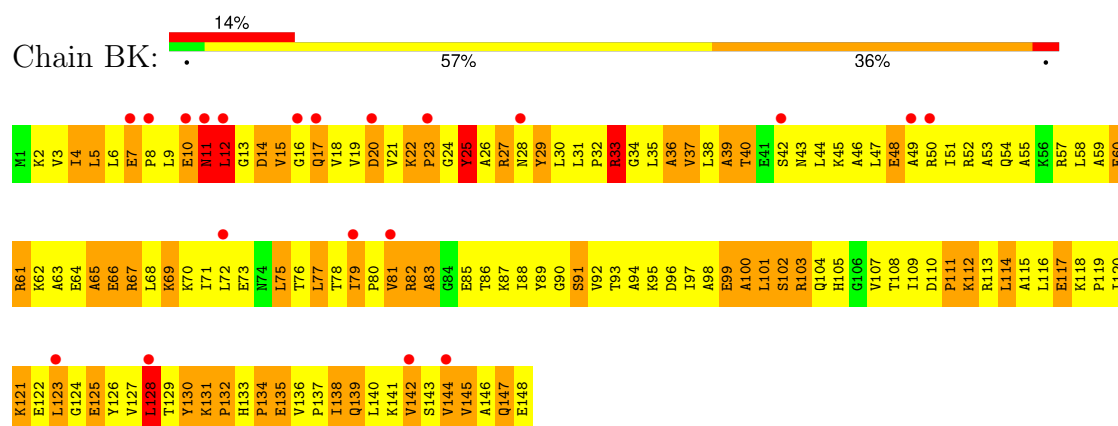




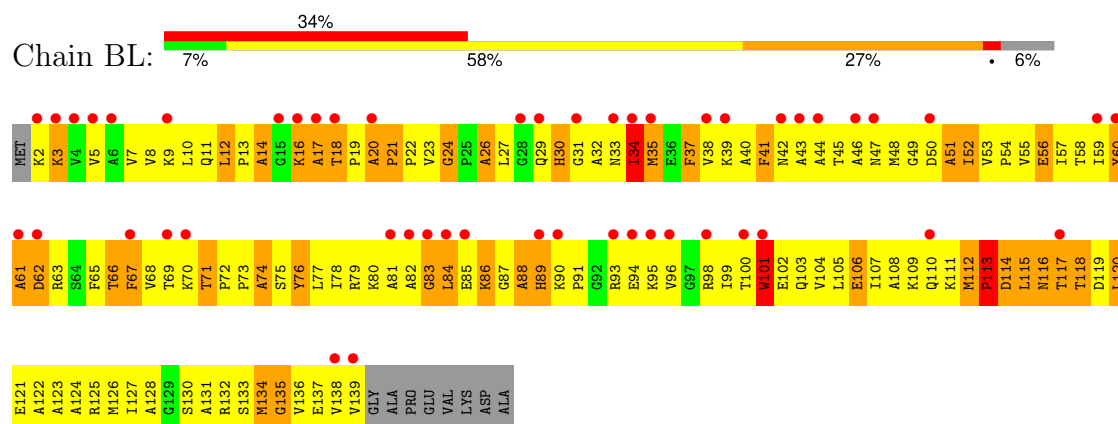
• Molecule 31: 50S ribosomal protein L6



• Molecule 32: 50S ribosomal protein L9

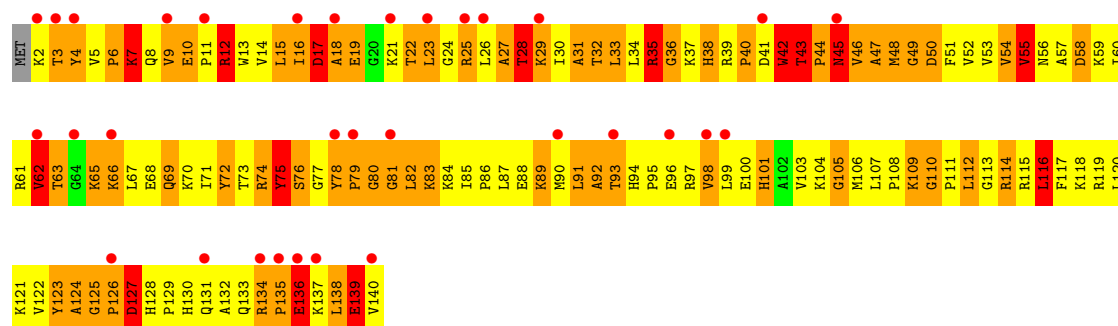


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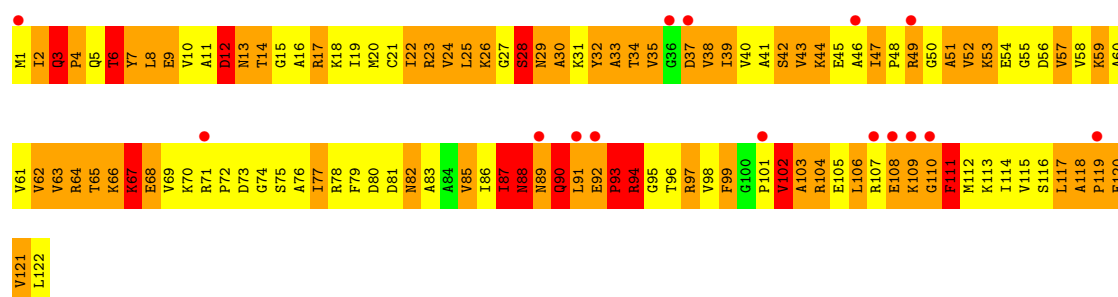


• Molecule 34: 50S ribosomal protein L13

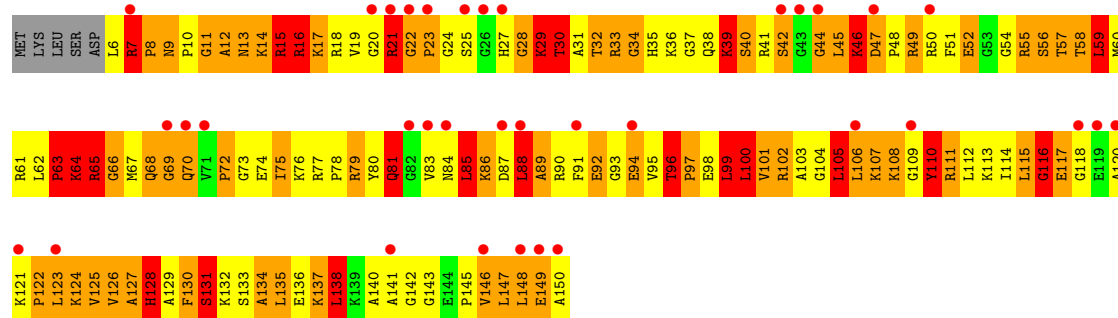




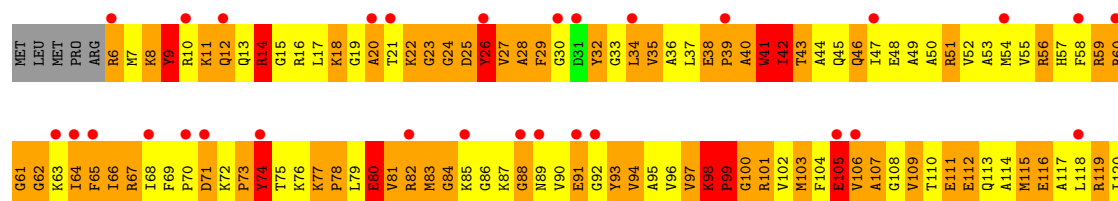
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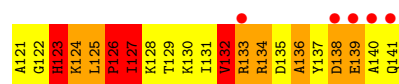


• Molecule 36: 50S ribosomal protein L15

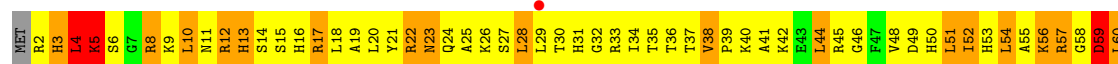


• Molecule 37: 50S ribosomal protein L16





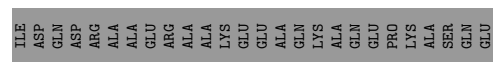
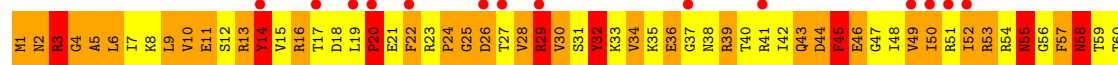
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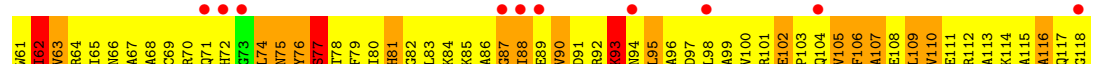
• Molecule 39: 50S ribosomal protein L18



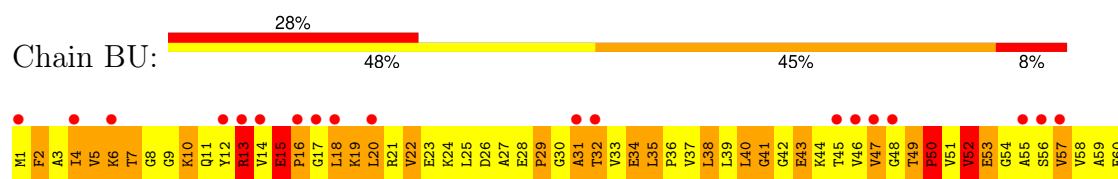
• Molecule 40: 50S ribosomal protein L19



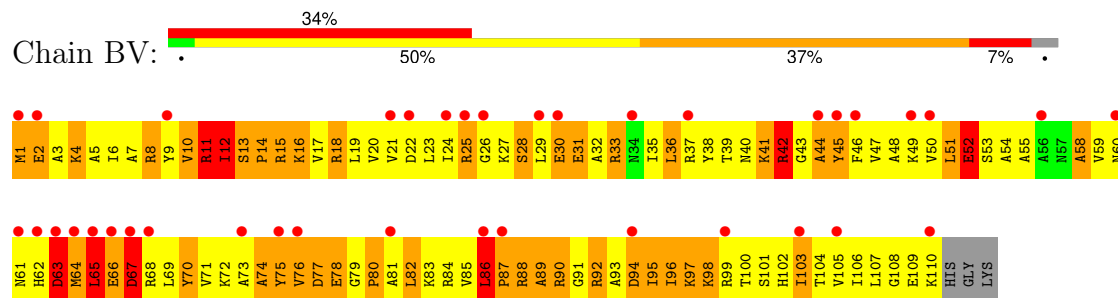
• Molecule 41: 50S ribosomal protein L20



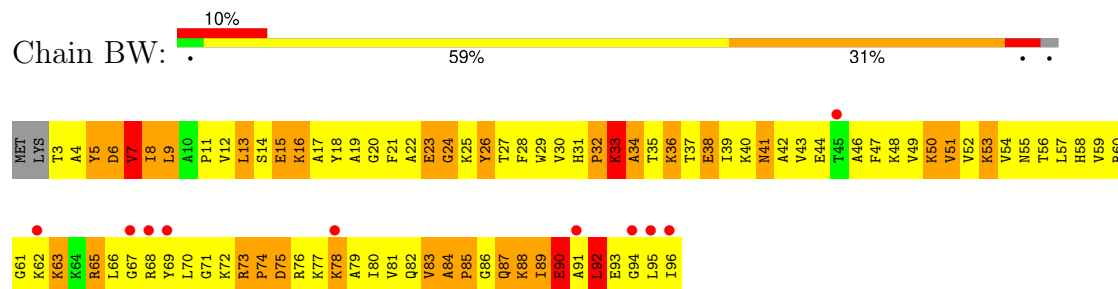
• Molecule 42: 50S ribosomal protein L21



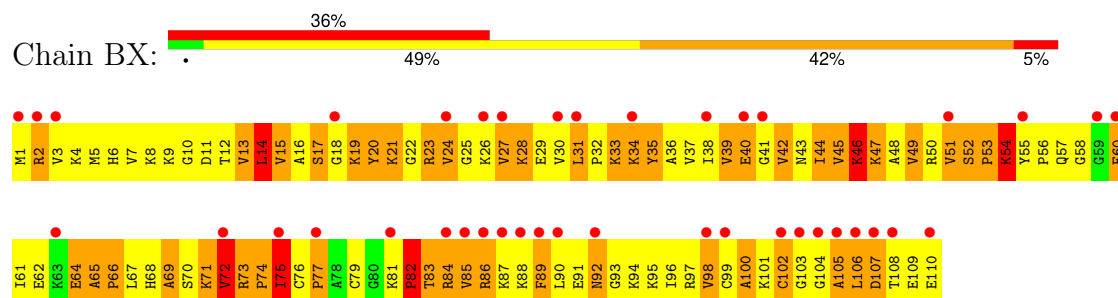
• Molecule 43: 50S ribosomal protein L22



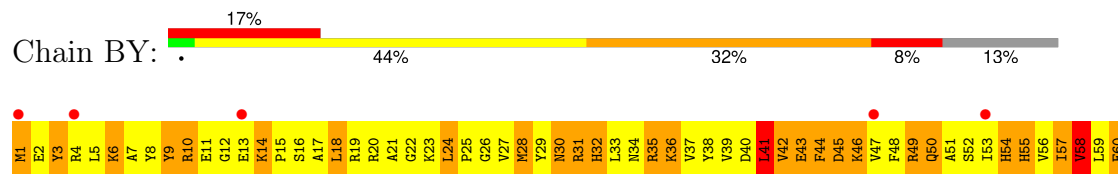
• Molecule 44: 50S ribosomal protein L23

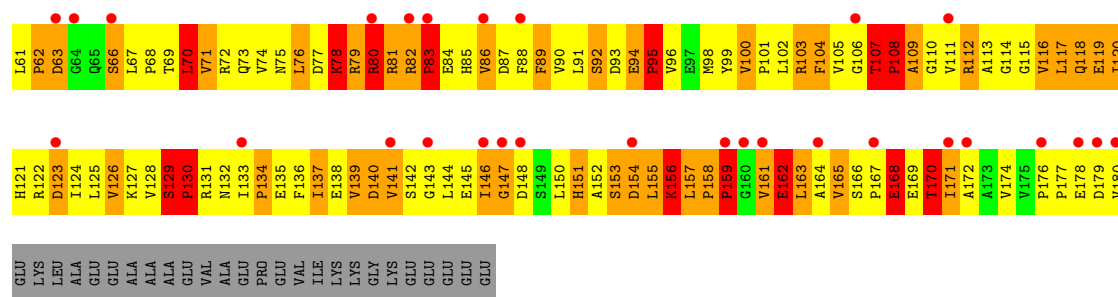


• Molecule 45: 50S ribosomal protein L24

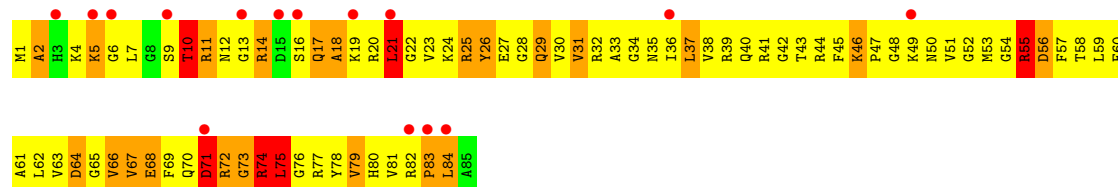
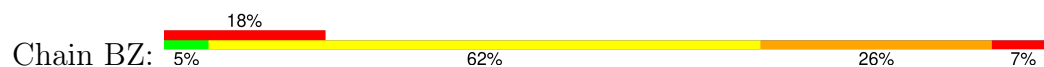


• Molecule 46: 50S ribosomal protein L25

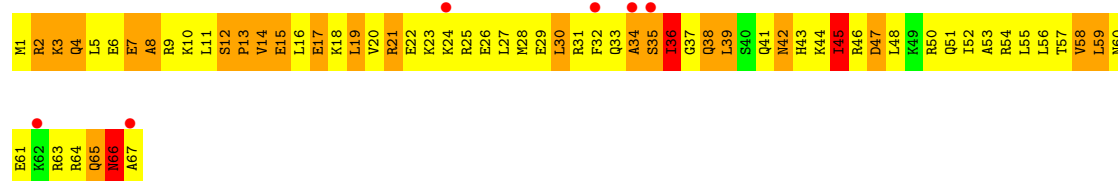




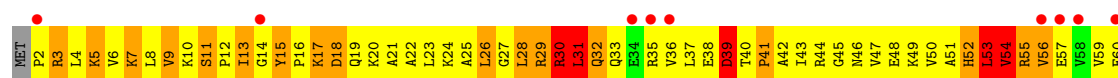
• Molecule 47: 50S ribosomal protein L27



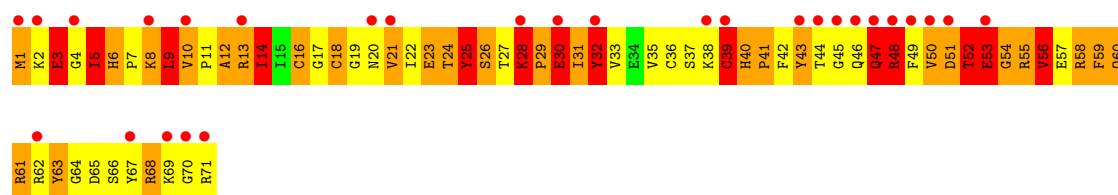
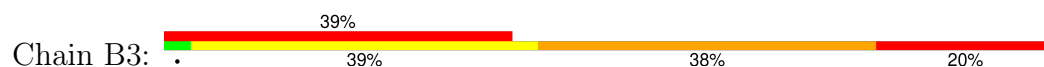
• Molecule 48: 50S ribosomal protein L29



• Molecule 49: 50S ribosomal protein L30

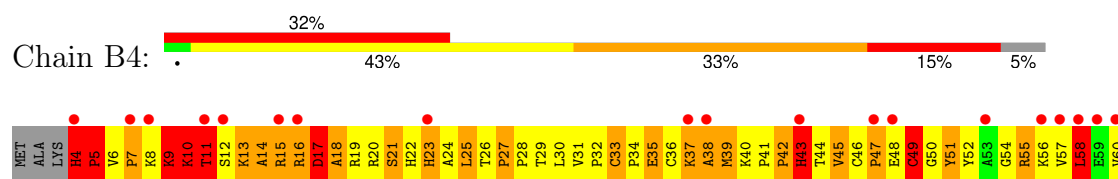


• Molecule 50: 50S ribosomal protein L31

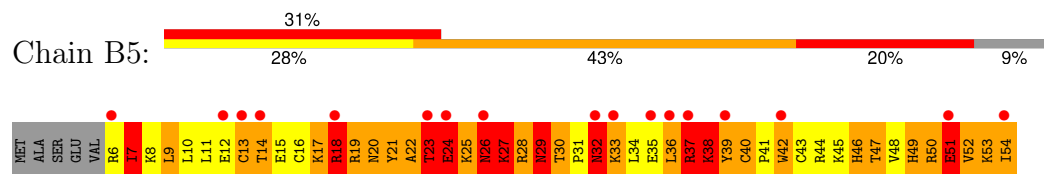


• Molecule 51: 50S ribosomal protein L32

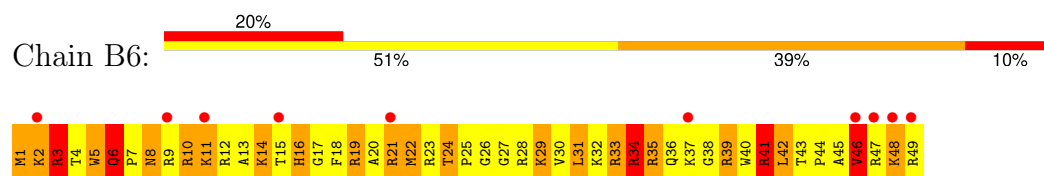




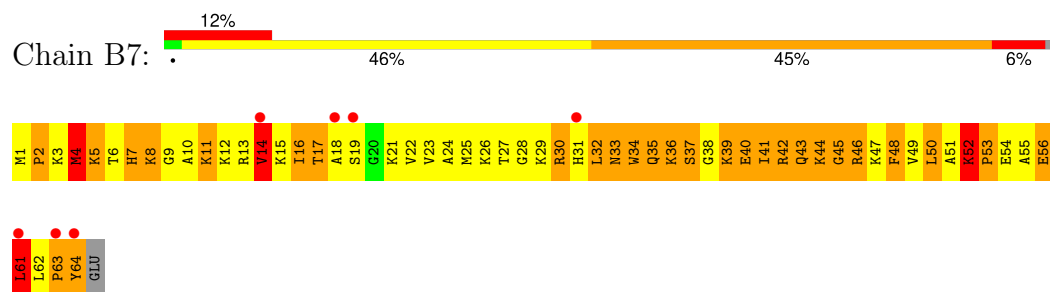
- Molecule 52: 50S ribosomal protein L33



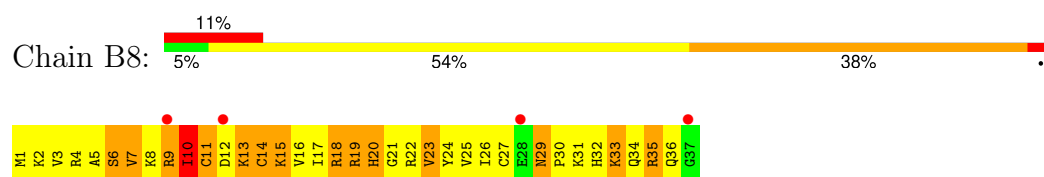
- Molecule 53: 50S ribosomal protein L34



- Molecule 54: 50S ribosomal protein L35



- Molecule 55: 50S ribosomal protein L36



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	509.52Å 509.52Å 804.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	300.00 – 5.00 300.00 – 5.00	Depositor EDS
% Data completeness (in resolution range)	93.9 (300.00-5.00) 97.3 (300.00-5.00)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.09 (at 4.88Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.263 , 0.323 0.250 , 0.303	Depositor DCC
$R_{free}$ test set	10783 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	99.7	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.08 , 0.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.55$ , $\langle L^2 \rangle = 0.39$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	149044	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	167.0	wwPDB-VP

Xtriage'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.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 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	0.94	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	1
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	2
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	3
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	1
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	0

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 ⓘ

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	4
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%)	0	4
10	AK	119/119 (100%)	76 (64%)	43 (36%)	0	1
11	AL	98/99 (99%)	74 (76%)	24 (24%)	0	3
12	AM	88/92 (96%)	61 (69%)	27 (31%)	0	2
13	AN	90/99 (91%)	70 (78%)	20 (22%)	1	5
14	AO	104/109 (95%)	79 (76%)	25 (24%)	0	4
15	AP	100/101 (99%)	73 (73%)	27 (27%)	0	3
16	AQ	49/50 (98%)	36 (74%)	13 (26%)	0	3
17	AR	79/80 (99%)	56 (71%)	23 (29%)	0	2
18	AS	72/74 (97%)	45 (62%)	27 (38%)	0	0
19	AT	96/97 (99%)	69 (72%)	27 (28%)	0	2
20	AU	64/77 (83%)	50 (78%)	14 (22%)	1	5
21	AV	71/80 (89%)	57 (80%)	14 (20%)	1	7
22	AW	76/82 (93%)	57 (75%)	19 (25%)	0	3
23	AX	19/22 (86%)	16 (84%)	3 (16%)	2	11
26	BC	180/181 (99%)	145 (81%)	35 (19%)	1	7
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	2
33	BL	105/111 (95%)	86 (82%)	19 (18%)	1	8
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	0
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	0
44	BW	76/78 (97%)	59 (78%)	17 (22%)	1	5
45	BX	91/91 (100%)	71 (78%)	20 (22%)	1	5
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	5
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	3
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
33	BL	34	ILE
39	BR	88	ASP
34	BM	33	LEU
33	BL	30	HIS
36	BO	81	GLN

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

Mol	Chain	Res	Type
32	BK	105	HIS
40	BS	55	ASN
33	BL	42	ASN
36	BO	13	ASN
41	BT	117	GLN

### 5.3.3 RNA ⓘ

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	686	G
24	BA	1248	G
24	BA	2481	G
24	BA	745	G
24	BA	945	A

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

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
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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å <sup>2</sup> )	Q < 0.9
1	AA	1515/1522 (99%)	-0.09	12 (0%)	82 68	88, 158, 260, 350	0
2	AC	76/77 (98%)	0.59	4 (5%)	33 27	133, 166, 216, 249	0
3	AD	76/76 (100%)	1.32	11 (14%)	7 10	219, 265, 316, 334	0
4	AE	234/256 (91%)	0.57	18 (7%)	21 19	122, 163, 221, 265	0
5	AF	206/239 (86%)	1.77	69 (33%)	1 3	143, 182, 210, 228	0
6	AG	208/209 (99%)	1.27	46 (22%)	3 5	106, 148, 170, 187	0
7	AH	150/162 (92%)	1.22	34 (22%)	3 5	114, 139, 171, 200	0
8	AI	101/101 (100%)	2.16	50 (49%)	0 2	121, 150, 168, 203	0
9	AJ	155/156 (99%)	1.06	31 (20%)	3 7	155, 180, 208, 214	0
10	AK	138/138 (100%)	0.62	14 (10%)	14 15	113, 133, 153, 160	0
11	AL	127/128 (99%)	0.65	13 (10%)	13 14	161, 225, 247, 255	0
12	AM	98/105 (93%)	0.85	11 (11%)	11 13	146, 208, 237, 240	0
13	AN	119/129 (92%)	1.32	32 (26%)	2 4	114, 142, 176, 206	0
14	AO	124/132 (93%)	1.15	18 (14%)	7 10	96, 129, 162, 184	0
15	AP	125/126 (99%)	1.25	28 (22%)	3 5	167, 194, 223, 230	0
16	AQ	60/61 (98%)	0.85	10 (16%)	5 8	163, 188, 203, 206	0
17	AR	88/89 (98%)	0.84	8 (9%)	16 16	113, 131, 168, 183	0
18	AS	83/88 (94%)	0.54	5 (6%)	29 25	104, 128, 155, 185	0
19	AT	104/105 (99%)	0.75	11 (10%)	13 14	98, 126, 169, 214	0
20	AU	73/88 (82%)	1.51	24 (32%)	1 3	109, 136, 190, 224	0
21	AV	80/93 (86%)	1.18	23 (28%)	1 4	175, 198, 217, 222	0
22	AW	99/106 (93%)	0.96	15 (15%)	6 10	105, 134, 163, 166	0
23	AX	24/27 (88%)	0.02	0	100 100	168, 210, 224, 229	0
24	BA	2889/2916 (99%)	0.26	94 (3%)	49 38	63, 155, 266, 322	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å²)	Q<0.9	
25	BB	123/123 (100%)	-0.24	0	100	100	146, 209, 257, 291	0
26	BC	228/229 (99%)	1.98	98 (42%)	1	2	220, 256, 308, 312	0
27	BD	272/276 (98%)	1.52	68 (25%)	2	5	80, 125, 153, 198	0
28	BE	206/206 (100%)	1.20	53 (25%)	2	5	69, 117, 172, 224	0
29	BF	208/210 (99%)	1.73	77 (37%)	1	3	111, 179, 215, 231	0
30	BG	182/182 (100%)	1.17	46 (25%)	2	5	160, 198, 226, 240	0
31	BH	174/180 (96%)	0.92	26 (14%)	7	10	146, 186, 216, 238	0
32	BK	148/148 (100%)	1.05	20 (13%)	8	11	135, 161, 188, 190	0
33	BL	138/147 (93%)	1.57	50 (36%)	1	3	277, 307, 330, 334	0
34	BM	139/140 (99%)	1.27	32 (23%)	2	5	107, 133, 167, 183	0
35	BN	122/122 (100%)	1.05	15 (12%)	9	12	78, 106, 140, 154	0
36	BO	145/150 (96%)	1.19	35 (24%)	2	5	106, 190, 227, 239	0
37	BP	136/141 (96%)	1.41	35 (25%)	2	5	109, 141, 173, 186	0
38	BQ	117/118 (99%)	0.55	4 (3%)	48	36	91, 124, 157, 173	0
39	BR	110/112 (98%)	0.39	7 (6%)	27	24	152, 183, 210, 248	0
40	BS	117/146 (80%)	1.17	22 (18%)	4	7	83, 127, 165, 184	0
41	BT	117/118 (99%)	0.79	14 (11%)	10	12	100, 138, 152, 158	0
42	BU	101/101 (100%)	1.47	28 (27%)	2	4	104, 160, 186, 197	0
43	BV	110/113 (97%)	1.62	38 (34%)	1	3	110, 143, 179, 195	0
44	BW	94/96 (97%)	0.80	10 (10%)	13	14	153, 170, 232, 237	0
45	BX	110/110 (100%)	1.64	40 (36%)	1	3	157, 199, 247, 273	0
46	BY	180/206 (87%)	1.09	34 (18%)	4	7	142, 190, 211, 226	0
47	BZ	85/85 (100%)	0.93	15 (17%)	4	7	139, 166, 181, 197	0
48	B1	67/67 (100%)	0.63	6 (8%)	17	16	172, 186, 199, 209	0
49	B2	59/60 (98%)	1.05	9 (15%)	6	9	127, 163, 188, 202	0
50	B3	71/71 (100%)	2.07	28 (39%)	1	2	127, 160, 176, 185	0
51	B4	57/60 (95%)	1.54	19 (33%)	1	3	96, 147, 217, 241	0
52	B5	49/54 (90%)	1.67	17 (34%)	1	3	141, 163, 183, 198	0
53	B6	49/49 (100%)	1.31	10 (20%)	3	6	87, 145, 164, 188	0
54	B7	64/65 (98%)	0.99	8 (12%)	9	12	113, 131, 153, 165	0
55	B8	37/37 (100%)	0.72	4 (10%)	12	14	146, 157, 169, 172	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
All	All	10767/11051 (97%)	0.74	1449 (13%) <b>8</b> <b>11</b>	63, 160, 260, 350	0

The worst 5 of 1449 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
15	AP	123	ALA	11.8
27	BD	275	LYS	11.3
5	AF	201	TYR	10.8
26	BC	127	LEU	10.8
26	BC	126	LYS	10.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides 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.