



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 13, 2017 – 03:49 PM EST

PDB ID : 4V4Y  
Title : Crystal structure of the 70S *Thermus thermophilus* ribosome with translocated and rotated Shine-Dalgarno Duplex.  
Authors : Jenner, L.; Yusupova, G.; Rees, B.; Moras, D.; Yusupov, M.  
Deposited on : unknown  
Resolution : 5.50 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030345



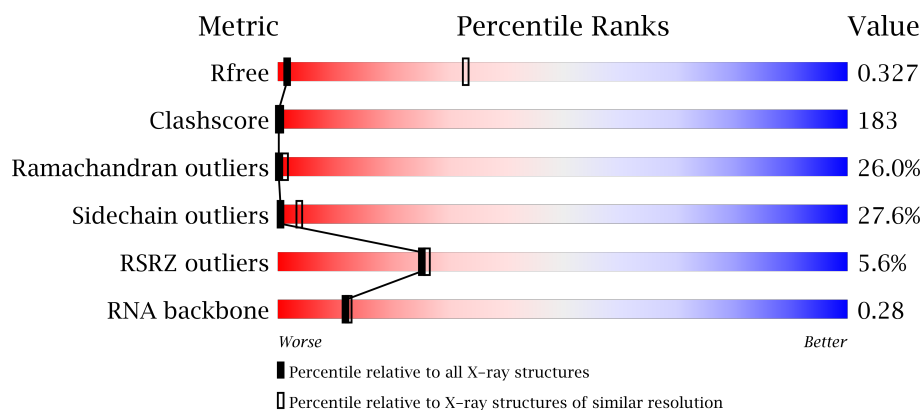
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 5.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	1052 (7.20-3.70)
Clashscore	112137	1021 (7.20-3.76)
Ramachandran outliers	110173	1082 (7.20-3.70)
Sidechain outliers	110143	1055 (7.20-3.70)
RSRZ outliers	101464	1061 (7.20-3.70)
RNA backbone	2435	1049 (7.80-2.90)

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

Mol	Chain	Length	Quality of chain
1	AA	1522	<div> <div>56%</div> <div>34%</div> <div>8%</div> </div>
2	A1	50	<div> <div>2%</div> <div>48%</div> <div>48%</div> <div>.</div> </div>
3	AB	76	<div> <div>89%</div> <div>7%</div> <div>50%</div> <div>36%</div> <div>8%</div> </div>
3	AC	76	<div> <div>13%</div> <div>59%</div> <div>34%</div> <div>7%</div> </div>

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

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

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Mol	Chain	Length	Quality of chain
53	B6	49	<div><div></div><div>43%</div><div>53%</div><div>37%</div><div>10%</div></div>
54	B7	65	<div><div></div><div>18%</div><div>52%</div><div>38%</div><div>8%</div><div></div></div>
55	B8	37	<div><div></div><div>8%</div><div>57%</div><div>30%</div><div>5%</div></div>



## 2 Entry composition

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

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

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

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

- Molecule 2 is a RNA chain called mRNA.

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

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

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

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

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

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

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

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



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

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

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

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

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

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

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

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

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

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

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

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

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

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



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

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

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

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

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

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

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

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

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

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

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

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

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

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



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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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



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

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

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

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

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

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

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

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

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

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

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

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

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

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



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

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

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

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

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

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

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

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

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

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

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

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

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

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



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

- Molecule 47 is a protein called Ribosomal protein L27.

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

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

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

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

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

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

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

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

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

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

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

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



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

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

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

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

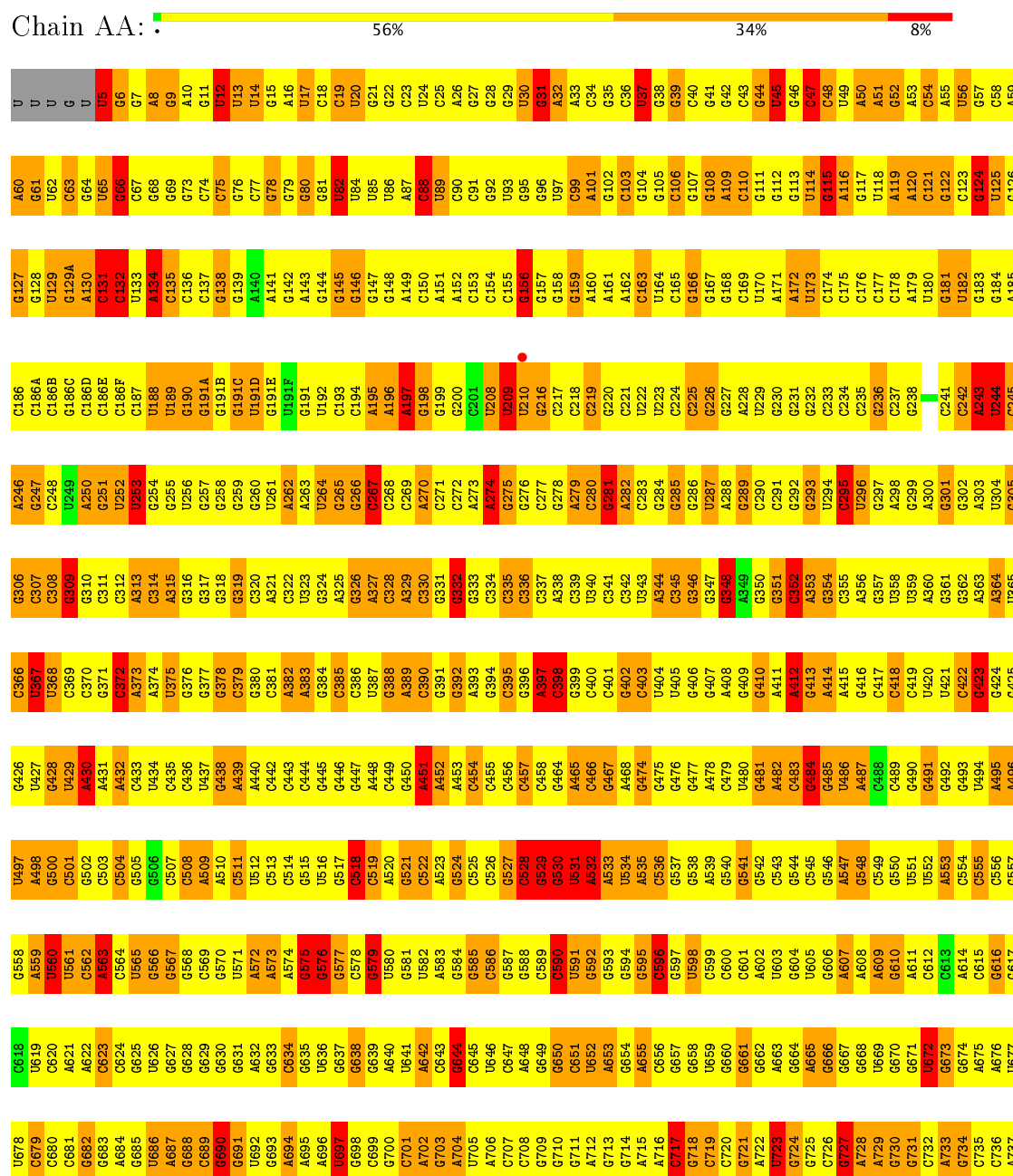
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	B8	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			



### 3 Residue-property plots

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

- Molecule 1: 16S ribosomal RNA





C1524	G1464	C1399	A1340	G1220	U1459	G1099	G1039	G984	C924	A864	G798	C738
G1525	C1465	C1400	U1341	G1221	G1460	C1100	U1040	C985	G925	A865	G799	C739
G1526	C1466	G1401	C1342	G1222	C1461	A1101	A1041	C986	G926	C866	G800	U740
G1527	G1467	C1402	G1343	C1223	C1462	A1102	G1042	G987	G927	G867	U801	G741
U1528	A1468	C1403	C1344	G1224	C1463	C1103	C1043	C988	G928	C868	A802	G742
G1529	G1469	C1404	U1345	A1285	G1464	G1104	A1044	C989	G929	C869	G803	U743
U1530	A1470	C1405	G1346	G1226	C1465	A1105	C1045	C990	C930	U870	U804	C744
A1531	G1471	U1406	C1347	A1227	G1466	A1106	A1046	C991	C931	U871	C806	C745
U1532	U1472	C1407	U1348	C1228	A1467	C1107	G1047	U992	C932	A872	C806	A746
C1533	A1473	A1408	A1349	A1229	A1468	G1108	U1048	G993	G933	A873	A807	C747
A1534	G1474	C1409	A1350	C1230	A1469	C1109	U1049	A994	C934	A874	C808	C748
C1535	G1475	G1231	U1351	G1231	G1470	A1110	G1050	C995	A935	C875	G809	C749
C1536	G1476	C1411	C1352	U1232	G1471	A1111	C1051	A996	C936	G876	C810	G750
U1537	C1477	C1412	G1353	G1233	G1472	C1112	U1052	U997	A937	C877	C811	U751
A1413	A1478	A1413	C1354	C1234	G1473	C1113	G1053	C998	A938	G878	C812	G752
C1414	U1479	U1414	G1355	U1235	G1474	C1114	C1054	C998A	G939	A879	U813	A753
U1480	G1481	G1415	G1356	A1236	A1476	C1115	A1055	U999	C940	C880	A814	C754
U1541	U1482	G1416	A1357	C1237	A1477	C1116	U1056	A1000	G941	G881	A815	G755
U1542	A1483	G1417	U1358	A1238	G1478	G1117	G1057	G1001	G942	C882	A816	C756
C	A1483	A1418	C1359	A1239	A1479	C1118	G1058	G1002	U943	C883	C817	U757
U	U1484	G1419	A1360	U1240	A1480	C1119	C1059	G1003	G944	U884	G818	G758
	U1485	U1420	G1361	C1241	G1481	G1120	G1060	A1004	G945	C885	A819	A759
	G1486	G1421	C1362	C1242	G1482	U1121	G1061	A1005	A946	G886	U820	G760
	G1487	G1422	C1362A	C1243	A1483	U1122	U1062	C1006	G947	G887	G821	G761
	G1488	G1423	A1363	C1244	G1484	A1123	C1063	C1007	C948	G888	C822	C762
	C1489	C1424	U1364	A1245	C1485	G1124	G1064	C1008	A949	A889	G823	G763
	U1490	U1425	G1365	C1246	G1486	U1125	U1065	G1009	U950	G890	C824	C764
	G1491	C1426	C1366	U1247	G1487	U1126	C1066	G1010	G951	U891	G825	G765
	A1492	U1427	C1367	A1248	A1488	G1127	A1067	G1011	U952	A892	C826	A766
	A1493	A1428	G1368	G1309	A1489	C1128	G1068	U1012	G953	C893	U827	A767
	G1494	C1429	C1369	G1310	A1490	C1129	C1069	G1013	G954	C894	A828	A768
	U1495	C1430	G1370	G1311	A1491	A1130	U1070	A1014	U955	G895	G829	G769
	C1496	C1431	G1371	A1251	A1492	C1131	C1071	A1015	U956	C896	G830	C770
	G1497	A1432	U1372	A1252	A1493	C1132	G1072	A1016	U957	C897	U831	G771
	A1498	A1433	C1373	C1254	U1494	G1133	U1073	G1017	A958	C898	C832	U772
	U1499	A1434	U1374	G1255	C1495	G1134	G1074	C1018	A959	C899	U833	G773
	A1500	G1435	A1375	A1256	U1496	U1135	C1075	C1019	U960	A900	C834	G774
	C1501	U1436	U1376	U1257	G1497	U1136	C1076	U1020	U961	A901	U835	G775
	A1502	C1437	A1377	G1258	G1498	C1137	U1077	G1021	C962	G902	G836	G776
	A1503	G1438	C1378	C1259	U1499	G1138	U1078	G1022	G963	G903	G837	A777
	G1504	C1439	G1379	C1260	C1200	G1139	G1079	G1023	A964	C904	G838	G778
	U1505	C1440	U1380	A1261	A1201	C1140	A1080	G1024	A965	U905	U841	C779
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	A1507	G1442	C1382	C1263	C1203	G1142	G1082	C1026	C967	A907	U843	A781
	G1508	G1443	C1383	C1264	A1204	G1143	U1083	C1027	A968	A908	C846	A782
	C1509	A1446	C1384	G1265	U1205	G1144	G1084	C1028	A969	A909	C849	C783
	U1510	G1447	G1385	G1266	G1206	C1145	U1085	C1028A	C970	C910	U850	C784
	G1511	C1448	G1386	C1267	G1207	A1146	U1086	C1028B	G971	U911	G851	G785
	U1512	C1449	G1387	A1268	C1208	C1147	G1087	G1029	C972	C912	G852	G786
	A1513	U1450	C1388	A1269	C1209	U1148	G1088	C1030	G973	A913	G853	A787
	C1514	A1451	C1389	C1270	C1210	C1149	G1089	G1031	A974	A914	G854	U788
	U1515	C1452	U1390	G1271	U1211	U1150	U1090	A1032	A975	A915	G855	U789
	G1516	U1391	A1332	G1272	U1212	A1151	U1091	G1032A	G976	A916	C856	A790
	G1517	G1454	C1392	G1273	A1213	A1152	U1092	G1032B	A977	C917	C857	G791
	A1518	G1455	U1393	G1334	G1214	C1153	A1093	G1033	A978	A918	G858	A792
	C1519	C1456	A1394	A1274	G1215	G1154	G1094	G1034	C979	A919	A859	U793
	G1520	A1460	C1395	G1275	G1216	G1155	U1095	A1035	C980	U920	A860	A794
	U1521	G1461	A1396	G1276	C1217	G1156	C1096	G1036	U981	U921	G861	C795
	U1522	C1397	G1397	U1278	C1218	A1157	C1097	C1037	U982	C922	C862	C796
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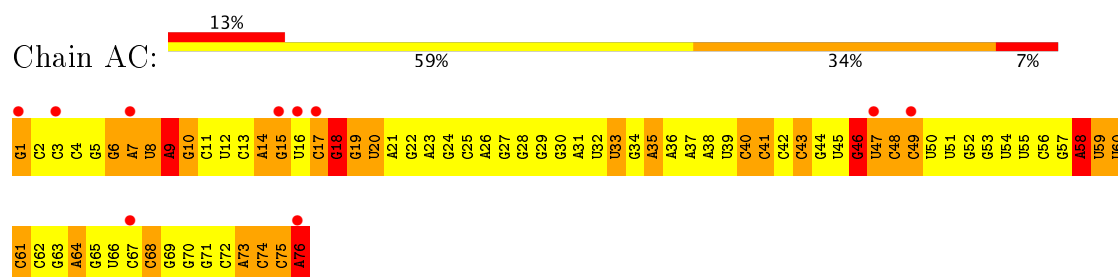
• Molecule 2: mRNA



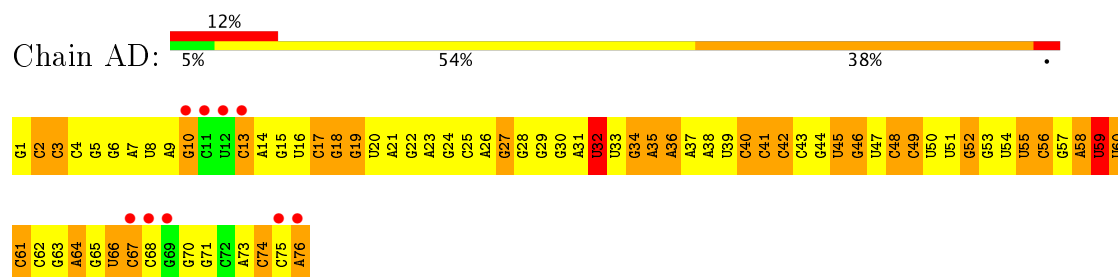
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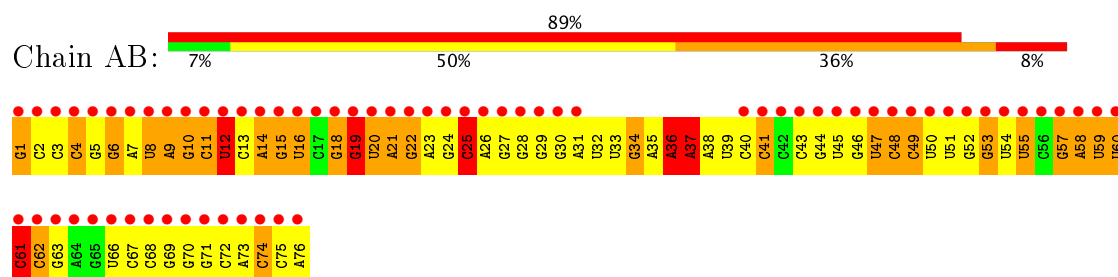
- Molecule 3: tRNA PHE (unmodified bases)



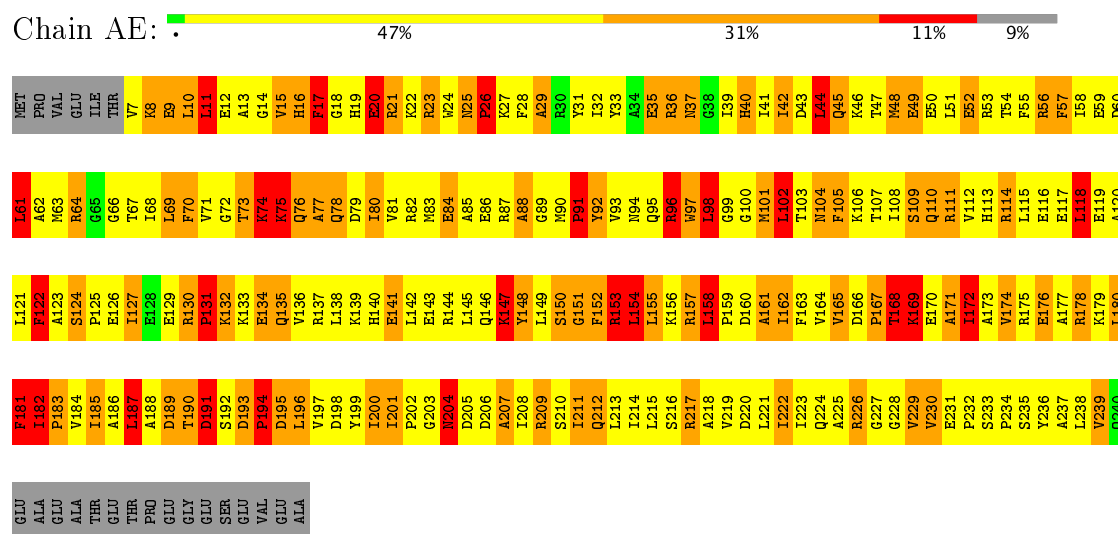
- Molecule 3: tRNA PHE (unmodified bases)



- Molecule 3: tRNA PHE (unmodified bases)

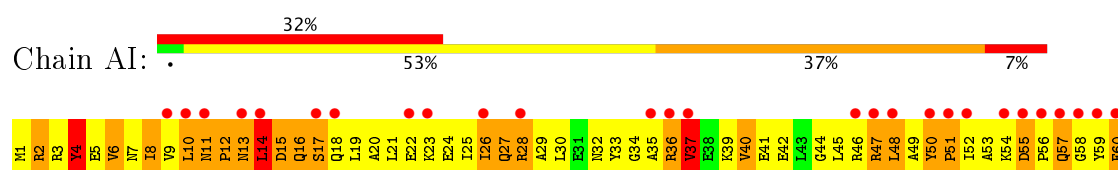


- Molecule 4: 30S ribosomal protein S2

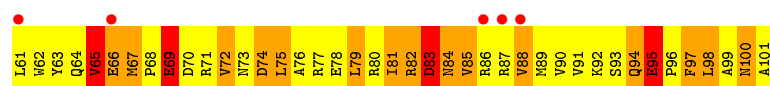


- Molecule 5: 30S ribosomal protein S3

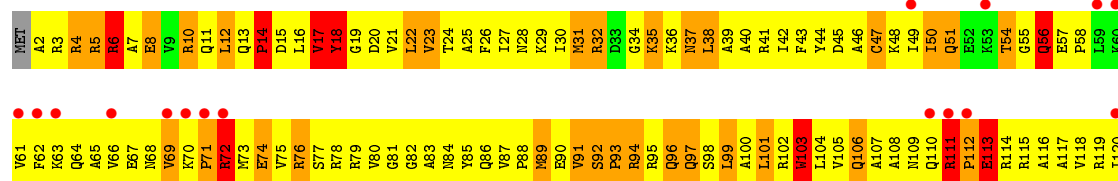








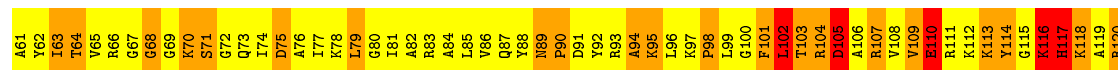
• Molecule 9: 30S ribosomal protein S7



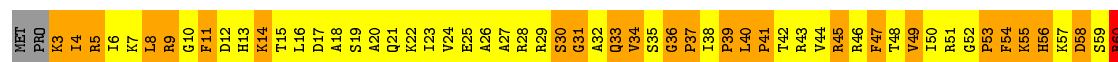
• Molecule 10: 30S ribosomal protein S8



• Molecule 11: 30S ribosomal protein S9



• Molecule 12: 30S ribosomal protein S10



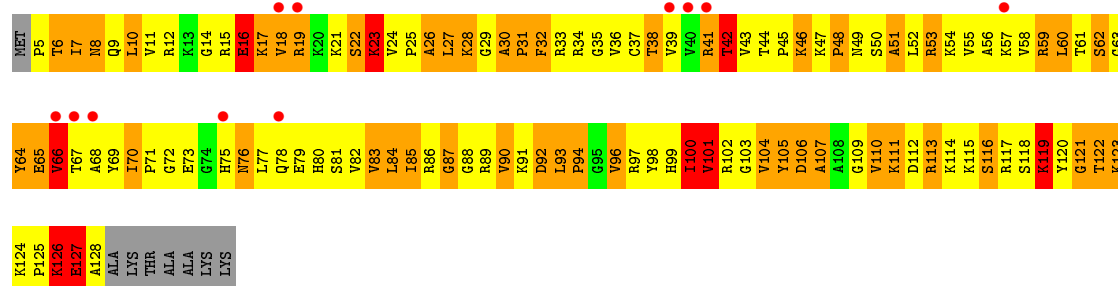




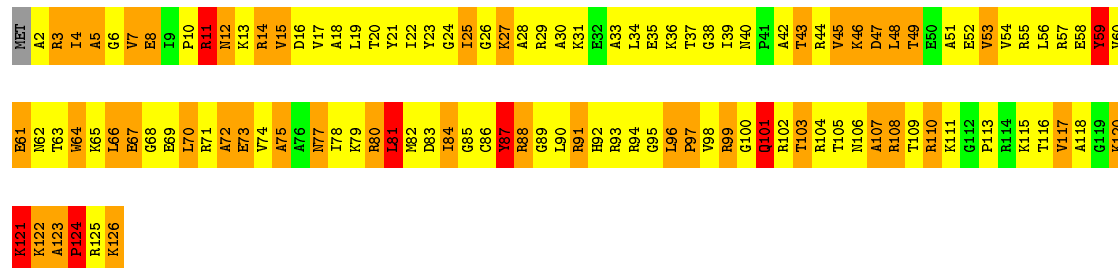
- Molecule 13: 30S ribosomal protein S11



- Molecule 14: 30S ribosomal protein S12



- Molecule 15: 30S ribosomal protein S13




- Molecule 16: 30S ribosomal protein S14





W61


- Molecule 17: 30S ribosomal protein S15

Chain AR: .  66% 28% ..

MET P2 I3 T4 R5 R6 E7 Q8 K9 K10 V11 I12 I13 Q14 F15 A16 R17 R18 F19 P19 G20 D21 D22 T22 G23 G24 S24 T25 E26 E27 I27 R28 Q28 V29 A30 L31 L32 L33 T33 L34 R35 R36 I36 I37 R38 L39 L40 S40 E41 E42 H42 L43 L44 V45 H46 K47 K48 D49 H50 H51 S52 S53 H54 G55 L56 L57 P58 P59 Y60

G61 Q62 R63 R64 R65 R66 L67 L68 Y69 L70 Q71 Q72 E73 D74 E75 E76 R77 Y78 Y79 A80 L81 I82 I83 E83 R84 L85 G86 G87 R88 R89

- Molecule 18: 30S ribosomal protein S16

Chain AS:  56% 33% 6% 6%

M1 V2 K3 K4 I4 R5 L6 A7 R8 F9 G10 A10 S11 K12 H13 H14 P15 H16 Y17 Y18 R19 I19 V20 V21 T22 D23 A24 R25 R26 R27 R28 D29 G30 K31 Y32 L33 E34 K35 I36 G37 Y38 Y39 D40 P41 R42 K43 T44 T45 P46 D47 W48 L49 K50 V51 D52 V53 E54 R55 A56 R57 Y58 P59 L60

S61 V62 G63 A64 Q65 P66 T67 D68 T69 A70 R71 R72 R73 L74 R75 Q76 A77 G78 V79 F80 R81 Q82 E83 A84 A85 A86 A87 A88 A89

- Molecule 19: 30S ribosomal protein S17

Chain AT: .  54% 35% 6% .

MET P2 K3 K4 V5 L6 T7 G8 V9 V10 V11 S12 D13 K14 R15 Q16 K17 T18 V19 T20 T21 L22 V23 E24 R25 Q26 F27 Y28 H29 P30 L31 Y32 G33 K34 V35 I36 K37 R38 S39 K40 K41 Y42 L43 A44 H45 D46 P47 E48 E49 K50 Y51 K52 L53 G54 D55 V56 V57 E58 I59 L60

E61 S62 R63 P64 I65 S66 K67 K68 K69 R70 F71 R72 V73 L74 R75 W76 V77 E78 S79 G80 R81 M82 D83 V84 V85 E86 K87 Y88 L89 I90 R91 R92 Q93 N94 Y95 Q96 S97 R98 S99 K100 R101 G102 G103 K104 A105

- Molecule 20: 30S ribosomal protein S18

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

MET SER THR LYS LYS ALA LYS PRO LYS LYS GLU ALA GLN ARG A16 S17 R18 K19 A20 K21 V22 T23 A24 T25 L26 G27 E28 R29 D30 D31 D32 R33 R34 R35 R36 V37 E38 V39 L40 L41 R42 F43 L44 S45 E46 T47 Q48 Q49 K50 L51 P52 R53 K54 K55 T56 G57 L58 S59 Y60

K61 E62 Q63 R64 I65 L66 A67 K68 T69 I70 K71 R72 A73 R74 L75 L76 G77 L78 L79 P80 F81 T82 E83 A84 K85 L86 V87 R88

- Molecule 21: 30S ribosomal protein S19

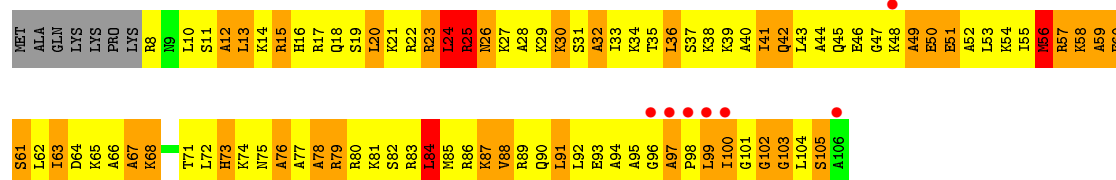
Chain AV: .  4% 48% 29% 5% 14%

MET P2 R3 S4 L5 K6 V9 F10 V11 D12 D13 H14 L15 L16 E17 K18 V19 L20 L21 L22 N23 A24 K25 G26 E27 R28 R29 L30 I31 K32 K33 W34 S35 R36 R37 S38 T39 L40 V41 P42 E43 E44 V45 G46 T48 T49 I49 A50 V51 Y52 N53 G54 K55 Q56 H57 V58 P59 V60 Y61

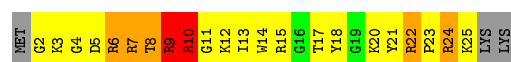




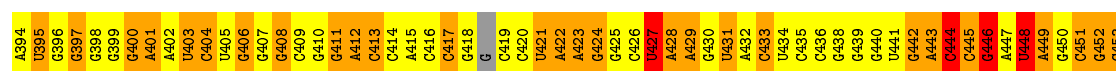
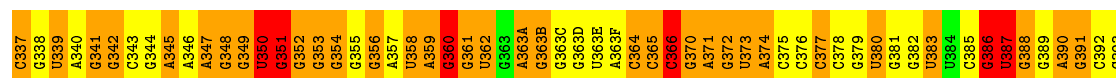
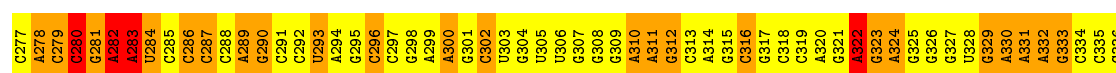
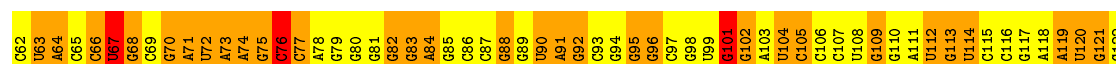
• Molecule 22: 30S ribosomal protein S20



• Molecule 23: 30S ribosomal protein Thx



• Molecule 24: 23S ribosomal RNA





U1335	A1275	A1214	C1153	U1094	G1034	C974A	C914	G853	A793	G733	C673	C635	G577	A516
A1336	A1276	G1215	G1154	A1095	U1035	G975	C915	G854	G794	A734	G674	G636	A578	C516
G1337	G1277	G1216	A1155	A1096	G1036	G976	G916	G855	G795	A735	A675	A637	A579	C517
G1338	G1278	C1217	A1156	U1097	G1037	G977	A917	G856	G796	C736	A676	G638	C580	A518
G1339	G1279		G1157	A1098	G1038	G978	A918	C857	G797	C737	A677	G639	C581	U519
U1340	G1280	A1220	G1158	G1099	G1039	G979	G919	U858	G798	C738	C678	C640	G582	G520
U1341	G1281	C1221	U1159	C1100	C1040	A980	G920	G859	G799	G739	C679	G641	G583	C521
A1342	U1282	C1222	G1160	U1101	C1041	A981	G921	U860	A800	G740	G680	G642	C584	G522
G1343	G1283	C1223	C1161	C1102	G1042	G982	U922	A861	G801	G741	G681	A643	G585	C523
A1344	G1284	G1224	A1162	A1103	C1043	A983	C923	G862	A802	G742	A682	A644	A586	U524
C1345	G1285	G1225	G1163	C1104	G1044	A984	C924	A863	U803	G743	C683	C645	C587	U525
A1346	A1286	G1226	U1164	U1105	A1045	G985	C925	G864	A804	G744	G684	A646	U588	A526
G1347	A1287	A1227	G1165	G1106	A1046	C986	A926	G865	G805	G745	A685	G647	C589	C527
G1348	U1288	G1228	C1166	G1107	G1047	G987	G928	A866	C806	A746	G686	G648	A590	A528
A1349	C1289	G1229	U1167	C1108	A1048	A988	G929	G867	U807	G747	C687	G649	C591	A529
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C1351	C1291	G1231	G1169	G1110	A1050	A990	G931	G869	G809	C749	A689	G	G593	C531
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C1353	C1293	C1233	G1171	G1112	C1052	C992	A933	U871	U811	A751	C691	A	C595	G533
A1354	U1294	U1234	A1173	U1113	C1053	G993	G934	A872	C812	A752	C692	A	G596	U534
G1355	G1295	G1235	A1174	G1114	A1054	C994	C935	G873	U813	C753	C693	G	U597	C535
G1356	G1296	G1236	U1175	G1115	G1055	C995	C936	G874	C814	C754	U694	C	G598	A536
U1357	C1297	G1237	G1176	C1116	G1056	A996	U937	G875	C815	C755	G695	G	G599	C537
G1358	G1298	G1238	A1177	G1117	A1057	G997	G938	C876	C816	C756	G696	G	G600	A539
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G1363	G1303	G1243	A1182	G1122	G1062	G1002	U943	G881	A821	A761	G701	C	C605	C544
G1364	G1304	G1244	G1183	C1123	G1063	G1003	G944	G882	U822	U762	G702	A	U606	A545
A1365	C1305	G1245	G1184	C1124	U1064	C1004	A945	G883	G823	G763	U703	C	U607	C546
C1306	C1306	A1246	C1185	G1125	U1065	C1005	G946	C884	A824	A764	G704	G	A608	A547
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G1393	C1333	U1273	G1212	G1151	C1092	A1032	A973	C912	U851	C791	C731	A633	A632	A575
U1394	G1334	A1274	A1213	C1152	G1093	U1033	G974	U913	G852	G792	C732	C672	C634	U576



C2205	C2140	U2079	A2019	G1959	G1899	G1830	G1770	C1694	A1634	C1574	C1515	U1454	A1395
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C2209	U2144	G2083	U2023	U1983	G1903	U1834	C1774	A1698	C1638	U1578	G1519	C1488	G1399
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G2218	G2152	U2091	A2031	A1971	U1911	U1842	G1782	U1706	C1646	A1587	G1527	G1466	U1407
G2219	G2153	U2092	G2032	A1972	A1912	C1843	A1783	G1707	G1647	C1588	A1528	C1467	C1408
G2224	G2154	G2093	A2033	G1973	A1913	C1844	A1784	C1708	C1648	C1589	A1529	C1468	C1409
A2225	G2155	U2094	U2034	C1974	C1914	G1845	A1785	U1709	G1649	U1590	G1530	A1469	G1410
C2226	G2156	C2095	G1975	U1915	U1915	G1846	A1786	U1710	G1650	G1591	C1531	G1470	C1411
A2227	U2096	U2096	G2035	G1976	A1916	A1847	A1787	C1711	G1651	C1592	C1532	A1471	A1412
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C2229	G2159	U2098	G2038	A1978	A1918	G1849	A1789	U1716	G1653	G1594	G1534	C1473	G1414
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G2235	G2165	G2104	C2044	G1984	C1924	G1855	C1795	G1728	U1659	C1600	G1540	U1420	U1420
C2236	C2166	C2105	C2045	G1985	C1925	G1856	U1796	A1729	G1660	G1601	U1541	G1480	G1421
G2237	U2167	G2106	G2046	A1986	U1926	G1857	C1797	U1730	G1661	U1602	U1542	G1482	G1422
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C2263	G2193	G2133	G2072	G2012	A1952	C1892	G1823	G1763	G1687	G1628	A1567	A1508	G1447
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A2266	C2196	C2136	U2075	A2015	U1955	C1895	G1826	U1766	A1690	C1630A	A1570	G1490A	G1449A
A2267	U2197	U2016	U2076	U2016	U1956	G1896	G1827	C1767	C1691	A1631	A1571	C1450	G1450
A2268	A2198	C2137	A2077	U2017	U1957	G1897	G1828	U1768	U1692	A1632	A1572	C1451	G1451
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A2750	G2691	G2630	G2570	A2450	U2390	G2330	G2270
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C2752	A2693	G2632	A2572	A2452	G2392	U2332	A2272
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G2754	C2695	G2634	G2574	G2454	C2394	G2334	A2274
C2755	U2696	G2635	C2575	G2455	C2395	A2335	C2275
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A2757	U2698	U2637	A2577	C2457	G2397	A2337	G2277
A2758	C2699	G2638	G2578	G2458	U2398	G2338	A2278
G2759	A2700	A2639	C2579	A2459	G2399	G2339	G2279
C2760	C2701	G2640	U2580	U2460	G2400	G2340	G2280
G2761	U2702	G2641	G2581	U2461	U2401	G2341	G2281
G2762	C2703	G2642	G2582	U2462	C2402	C2342	G2282
G2763	C2704	G2643	G2583	C2463	C2403	C2343	C2283
A2764	A2705	G2644	U2584	C2464	U2404	U2344	C2284
G2766	G2706	G2645	U2585	C2465	G2405	U2345	C2285
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C2769	G2709	C2648	G2588	G2468	U2408	U2348	A2288
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C2772	A2712A	C2652	C2591	C2471	A2411	G2351	U2291
G2773	A2713	U2653	U2593	G2472	A2412	A2352	C2292
C2774	G2714	A2654	C2594	U2473	G2413	G2353	C2293
A2775	C2715	G2655	G2595	C2474	G2414	G2354	C2294
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A2777	G2717	G2657	C2597	A2476	C2416	C2356	U2296
C2778	G2718	C2658	A2598	C2477	G2417	U2357	C2297
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G2784	G2724	G2664	U2604	C2483	U2423	G2363	G2303
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A2790	C2730	A2670	C2610	G2489	A2429	A2369	A2309
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G2794	G2734	A2675	A2614	U2493	A2433	G2373	C2313
U2795	G2735	C2676	U2615	G2494	A2434	C2374	C2314
G2797	G2736	G2677	C2616	G2495	A2435	G2375	G2315
C2798	G2737	C2678	C2617	C2496	G2436	A2376	C2316
A2799	A2738	A2679	G2618	A2497	U2437	G2377	C2317
G2800	U2739	C2680	C2619	G2498	U2438	A2378	G2318
C2801	G2740	G2681	C2620	C2499	A2439	G2379	G2319
G2802	A2741	U2682	A2621	U2500	C2440	C2380	A2320
C2803	G2804	C2683	C2622	C2501	G2441	G2381	G2321
U2804	C2742	U2684	G2623	G2502	C2442	A2382	A2322
G2805	G2743	G2685	U2624	A2503	C2443	G2383	G2323
C2806	G2744	G2686	G2625	U2504	G2444	G2384	C2324
G2807	C2745	U2687	C2626	G2505	G2445	G2385	G2325
U2808	U2746	U2688	U2627	U2506	G2446	C2386	C2326
A2809	A2747	U2689	G2628	C2507	G2447	U2387	A2327
G2810	G2748	U2690	A2629	G2508	A2448	A2388	A2328
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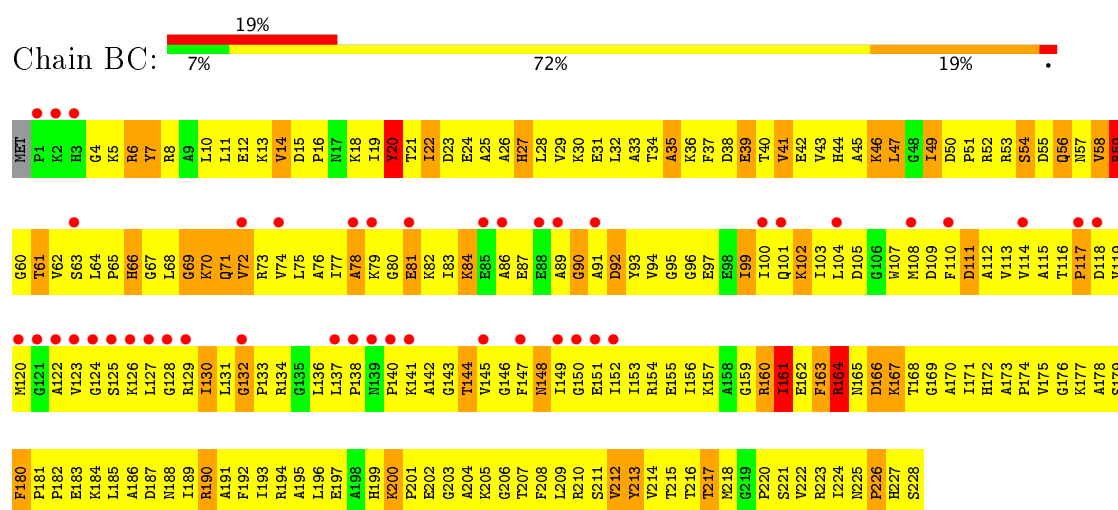
• Molecule 25: 5S ribosomal RNA

Chain BB:  51% 40% 9%

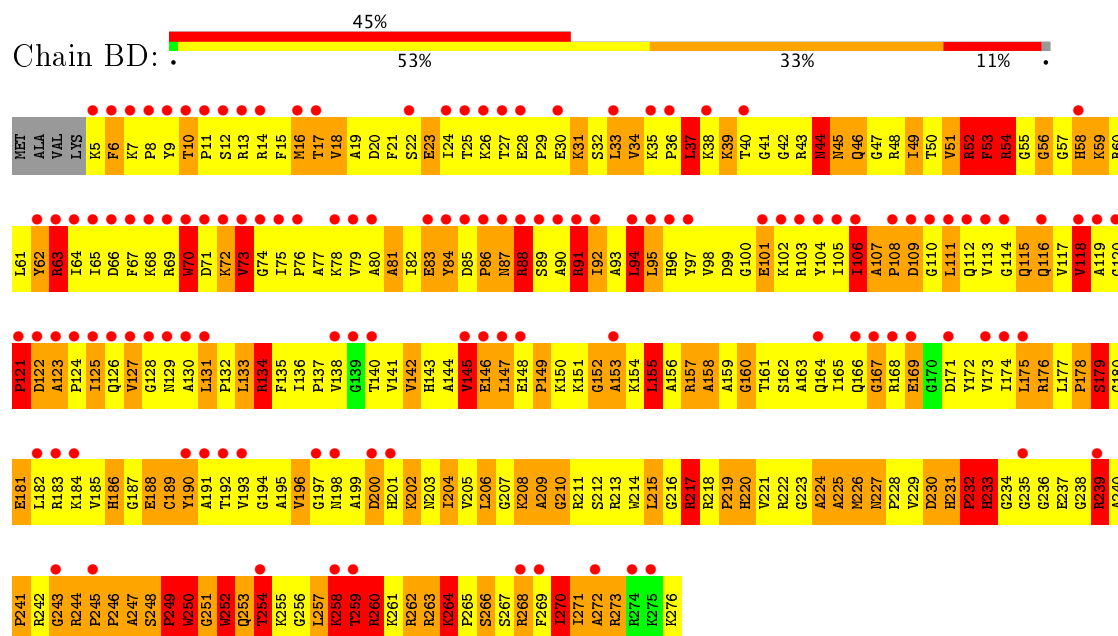
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A0	C60	A119
U1	G61	U120
C2	G62	
G3	G63	
C4	G64	
C5	G65	
C6	A66	
G7	G67	
U8	G68	
G9	A69	
G10	C70	
C11	G71	
G12	G72	
A13	A73	
U14	G74	
A15	G75	
G16	G76	
C17	U77	
G18	A78	
G19	C79	
C20	U80	
G21	G81	
U22	G82	
G23	G83	
C24	C84	
A25	G85	
A26	G86	
C27	G87	
G28	C88	
A29	G89	
C30	A89A	
C31	C90	
C32	G91	
G33	C92	
U34	C93	
U35	C94	
C36	U95	
C37	G96	
C38	G97	
A39	G98	
U40	A99	
U41	G100	
C42	A101	
C43	G102	
G44	U103	
A45	A104	
A46	G105	
C47	G106	
A48	U107	
C49	C108	
G50	G109	
G51	G110	
A52	U111	
A53	G112	
G54	C113	
U55	G114	
G56	G115	
A57	C116	
G58	G117	

• Molecule 26: 50S ribosomal protein L1



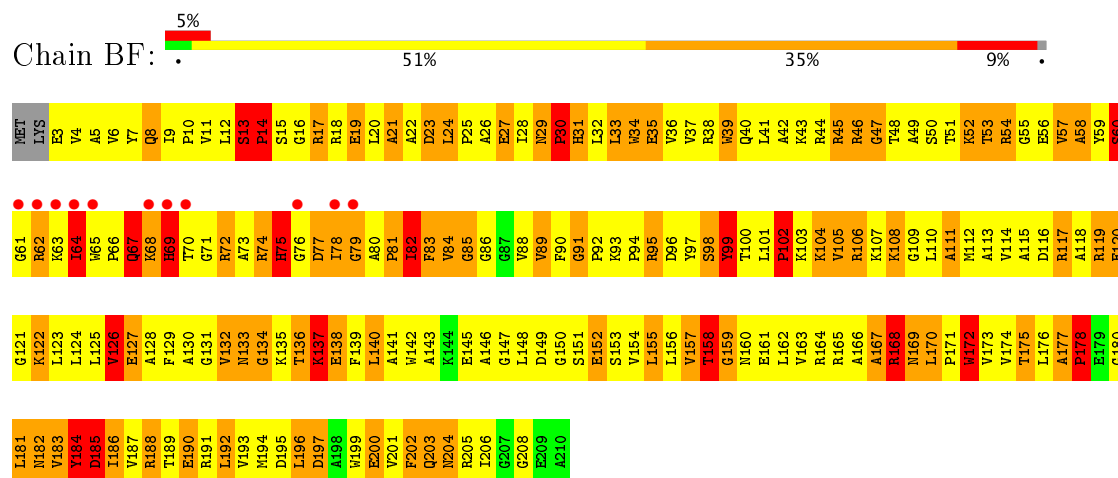


• Molecule 27: 50S ribosomal protein L2

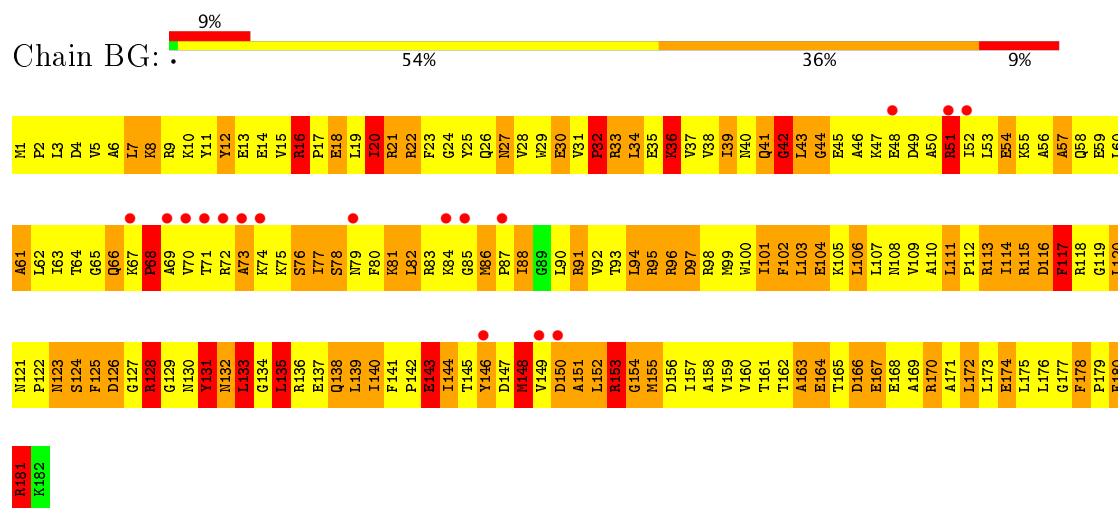




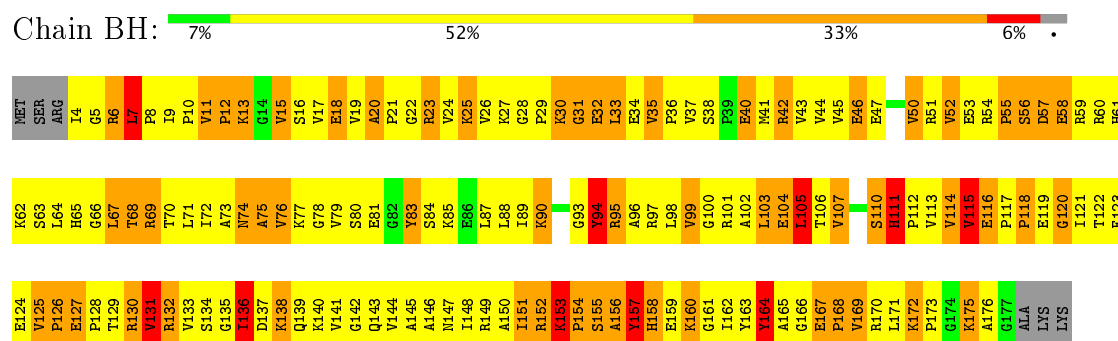
## • Molecule 29: 50S ribosomal protein L4



## • Molecule 30: 50S ribosomal protein L5



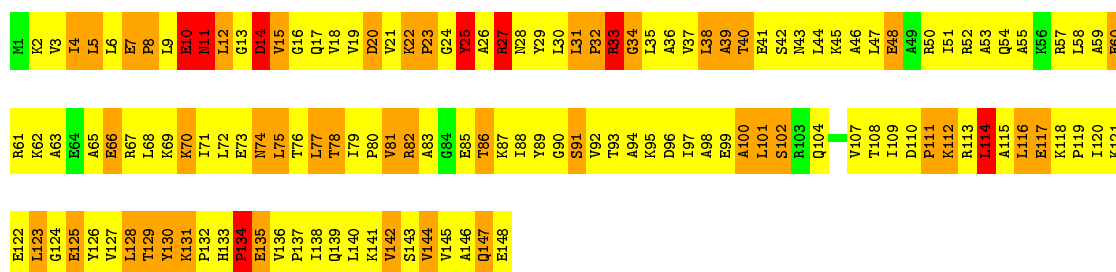
## • Molecule 31: 50S ribosomal protein L6



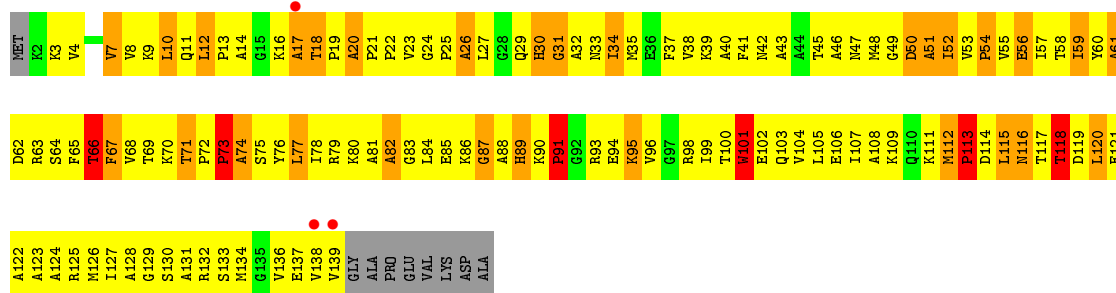
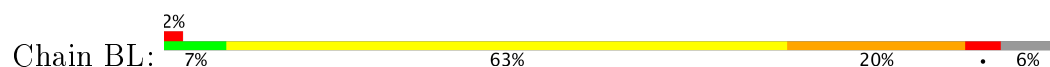
## • Molecule 32: 50S ribosomal protein L9



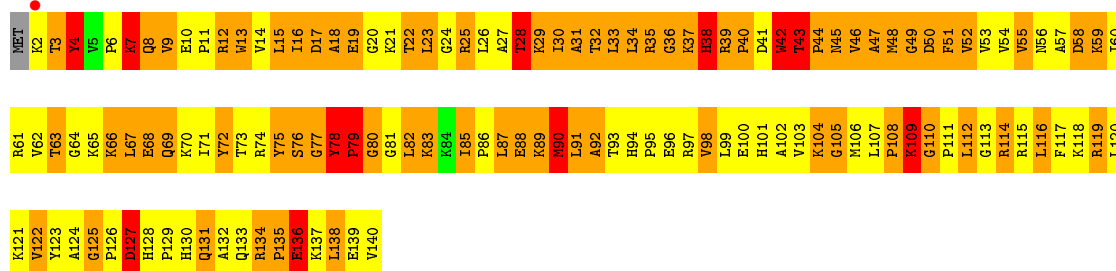




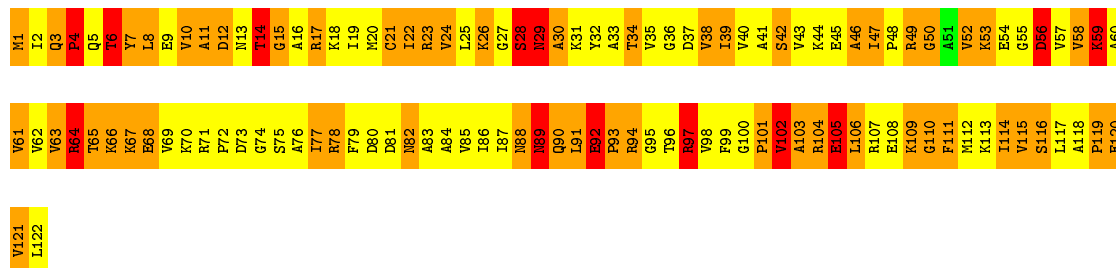
• Molecule 33: 50S ribosomal protein L11



• Molecule 34: 50S ribosomal protein L13



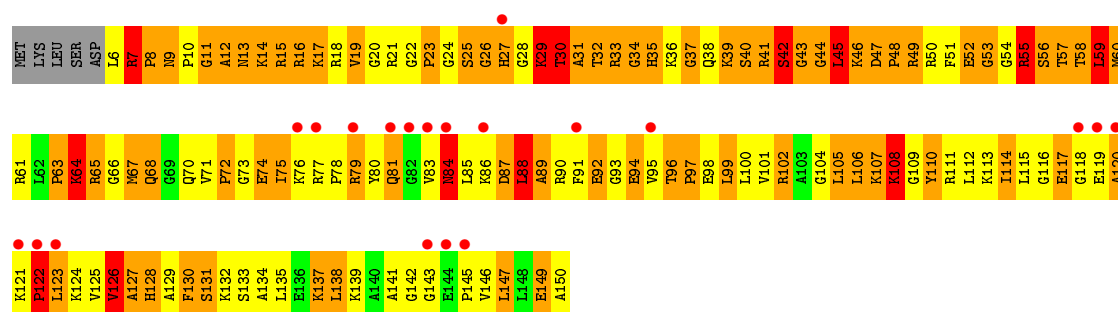
• Molecule 35: 50S ribosomal protein L14



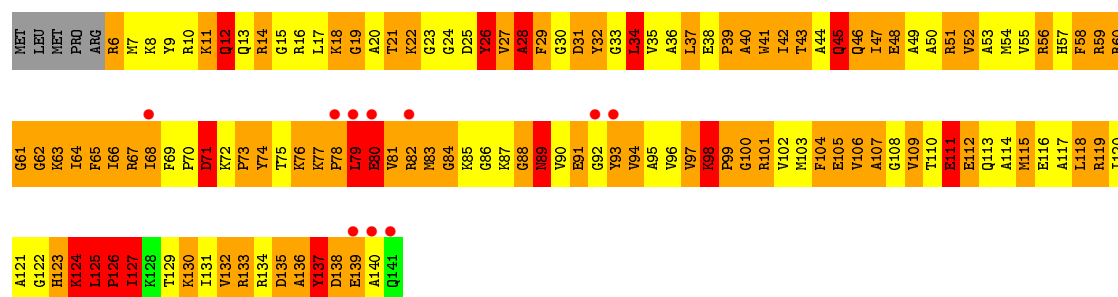
• Molecule 36: 50S ribosomal protein L15



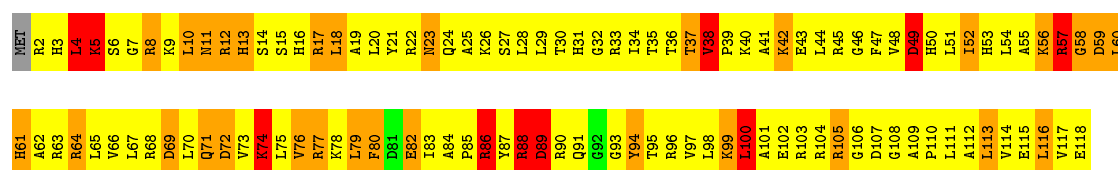




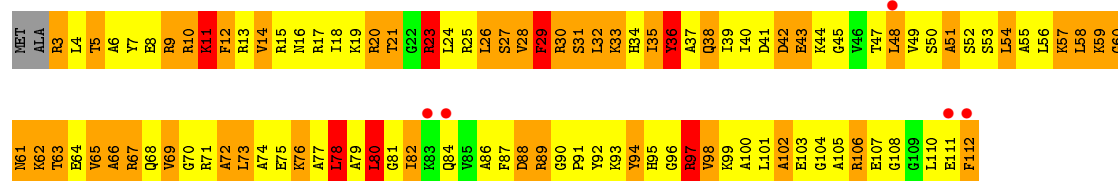
• Molecule 37: 50S ribosomal protein L16



• Molecule 38: 50S ribosomal protein L17



• Molecule 39: 50S ribosomal protein L18

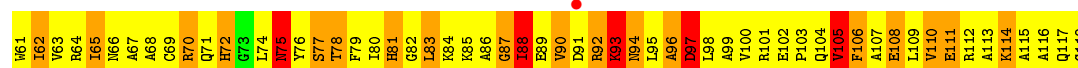
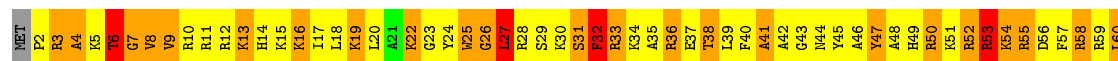


• Molecule 40: 50S ribosomal protein L19





- Molecule 41: 50S ribosomal protein L20



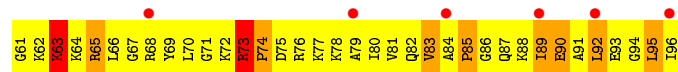
- Molecule 42: 50S ribosomal protein L21



- Molecule 43: 50S ribosomal protein L22



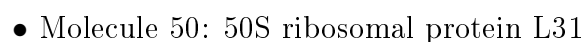
- Molecule 44: 50S ribosomal protein L23



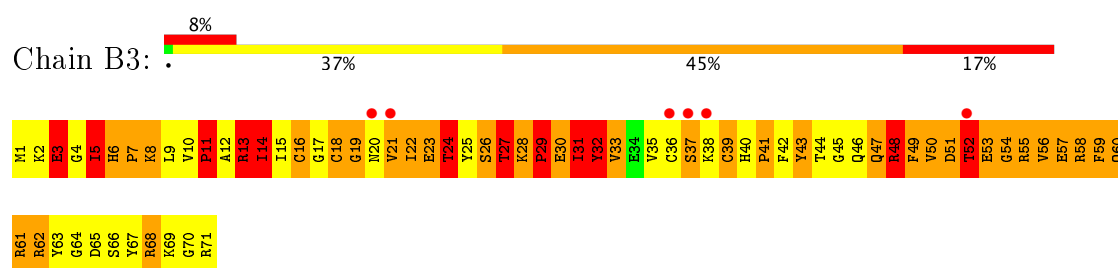
- Molecule 45: 50S ribosomal protein L24



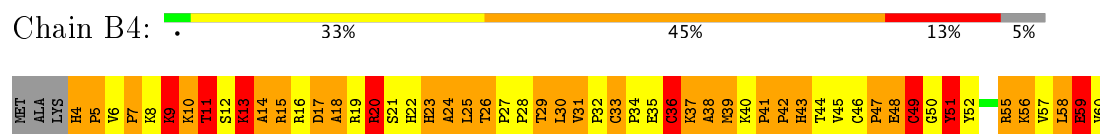




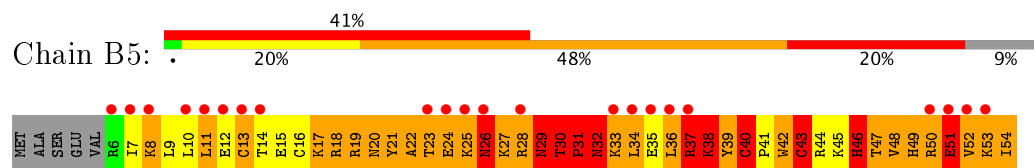




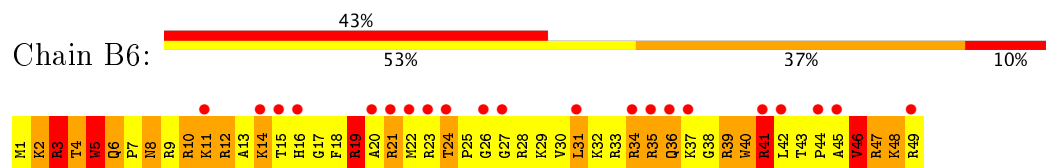
• Molecule 51: 50S ribosomal protein L32



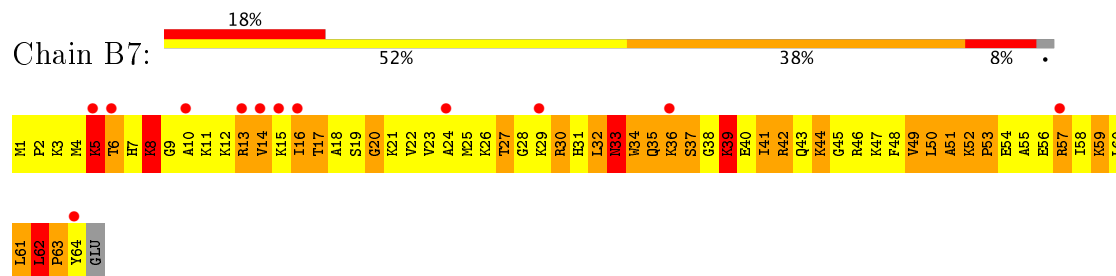
• Molecule 52: 50S ribosomal protein L33



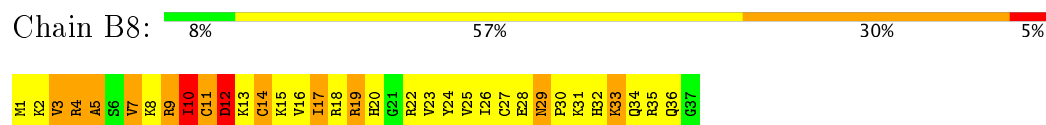
• Molecule 53: 50S ribosomal protein L34



• 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, $\alpha$ , $\beta$ , $\gamma$	508.54Å 508.54Å 806.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	300.00 – 5.50 430.13 – 4.98	Depositor EDS
% Data completeness (in resolution range)	96.7 (300.00-5.50) 99.1 (430.13-4.98)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.00 (at 4.88Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.243 , 0.326 0.280 , 0.327	Depositor DCC
$R_{free}$ test set	7981 reflections (4.99%)	DCC
Wilson B-factor (Å <sup>2</sup> )	108.9	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.07 , 78.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.53$ , $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	151691	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	226.0	wwPDB-VP

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

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



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

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AA	0	175
2	A1	0	3
3	AB	0	6
3	AC	0	8
3	AD	0	8
6	AG	0	1
8	AI	0	1
13	AN	0	1
15	AP	0	1
16	AQ	0	1
24	BA	0	463

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

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

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

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

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

There are no chirality outliers.

5 of 694 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	12	U	Sidechain
1	AA	17	U	Sidechain
1	AA	31	G	Sidechain
1	AA	37	U	Sidechain
1	AA	45	U	Sidechain



## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

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

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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 183.

The worst 5 of 46416 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:BA:2447:G:C8	24:BA:2500:U:H3'	1.23	1.61
24:BA:1202:C:C5	24:BA:1203:G:H1'	1.39	1.55
24:BA:1203:G:O6	24:BA:1240:U:C2	1.66	1.48
24:BA:2459:A:N3	24:BA:2460:U:H1'	1.38	1.38
24:BA:2596:U:H2'	27:BD:242:ARG:CZ	1.55	1.35

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BB:0:A:OP1	25:BB:0:A:OP1[15_545]	2.18	0.02



## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

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

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

5 of 1557 Ramachandran outliers are listed below:

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

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

### 5.3.2 Protein sidechains ⓘ

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

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

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	BE	166/166 (100%)	102 (61%)	64 (39%)	0	0
29	BF	164/166 (99%)	105 (64%)	59 (36%)	0	1
30	BG	156/156 (100%)	112 (72%)	44 (28%)	0	3
31	BH	143/148 (97%)	109 (76%)	34 (24%)	1	6
32	BK	124/124 (100%)	92 (74%)	32 (26%)	0	5
33	BL	105/111 (95%)	89 (85%)	16 (15%)	3	20
34	BM	118/119 (99%)	79 (67%)	39 (33%)	0	2
35	BN	100/100 (100%)	69 (69%)	31 (31%)	0	2
36	BO	111/116 (96%)	71 (64%)	40 (36%)	0	1
37	BP	106/111 (96%)	65 (61%)	41 (39%)	0	0
38	BQ	100/101 (99%)	71 (71%)	29 (29%)	0	3
39	BR	87/88 (99%)	63 (72%)	24 (28%)	0	4
40	BS	105/127 (83%)	68 (65%)	37 (35%)	0	1
41	BT	93/94 (99%)	64 (69%)	29 (31%)	0	2
42	BU	82/82 (100%)	57 (70%)	25 (30%)	0	2
43	BV	90/92 (98%)	64 (71%)	26 (29%)	0	3
44	BW	76/78 (97%)	57 (75%)	19 (25%)	1	5
45	BX	91/91 (100%)	72 (79%)	19 (21%)	1	8
46	BY	159/179 (89%)	120 (76%)	39 (24%)	1	5
47	BZ	67/67 (100%)	51 (76%)	16 (24%)	1	5
48	B1	62/62 (100%)	44 (71%)	18 (29%)	0	3
49	B2	51/52 (98%)	36 (71%)	15 (29%)	0	3
50	B3	63/63 (100%)	45 (71%)	18 (29%)	0	3
51	B4	50/52 (96%)	31 (62%)	19 (38%)	0	1
52	B5	48/52 (92%)	32 (67%)	16 (33%)	0	2
53	B6	42/42 (100%)	29 (69%)	13 (31%)	0	2
54	B7	54/55 (98%)	44 (82%)	10 (18%)	2	12
55	B8	34/34 (100%)	29 (85%)	5 (15%)	3	21
All	All	5040/5237 (96%)	3649 (72%)	1391 (28%)	0	4

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



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

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

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

### 5.3.3 RNA ⓘ

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

5 of 1812 RNA backbone outliers are listed below:

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

5 of 403 RNA pucker outliers are listed below:

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

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

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
24	BA	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	BA	2756:U	O3'	2757:A	P	1.77
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%)	-0.34	2 (0%) 95 94	145, 221, 302, 356	0
2	A1	50/50 (100%)	-0.06	1 (2%) 65 61	200, 320, 348, 357	0
3	AB	76/76 (100%)	14.23	68 (89%) 0 1	288, 351, 370, 374	0
3	AC	76/76 (100%)	0.60	10 (13%) 4 8	167, 214, 260, 284	0
3	AD	76/76 (100%)	0.08	9 (11%) 5 10	222, 271, 293, 316	0
4	AE	234/256 (91%)	-1.03	0 100 100	189, 226, 271, 304	0
5	AF	206/239 (86%)	-0.23	10 (4%) 30 31	222, 244, 266, 277	0
6	AG	208/209 (99%)	-0.41	4 (1%) 67 63	168, 215, 233, 242	0
7	AH	150/162 (92%)	-0.72	0 100 100	174, 210, 235, 257	0
8	AI	101/101 (100%)	1.27	32 (31%) 0 4	191, 223, 236, 261	0
9	AJ	155/156 (99%)	0.64	21 (13%) 3 8	210, 240, 256, 275	0
10	AK	138/138 (100%)	-1.13	0 100 100	186, 208, 225, 232	0
11	AL	127/128 (99%)	-0.97	0 100 100	222, 261, 276, 287	0
12	AM	98/105 (93%)	-0.53	2 (2%) 65 61	230, 260, 274, 282	0
13	AN	119/129 (92%)	0.79	17 (14%) 3 8	193, 212, 245, 267	0
14	AO	124/132 (93%)	0.42	11 (8%) 10 14	179, 199, 233, 267	0
15	AP	125/126 (99%)	-0.78	0 100 100	223, 243, 272, 278	0
16	AQ	60/61 (98%)	-0.92	0 100 100	215, 248, 259, 263	0
17	AR	88/89 (98%)	-0.57	1 (1%) 80 75	186, 207, 231, 238	0
18	AS	83/88 (94%)	-0.97	0 100 100	180, 201, 226, 249	0
19	AT	104/105 (99%)	-0.51	1 (0%) 82 77	164, 193, 244, 277	0
20	AU	73/88 (82%)	-0.41	6 (8%) 12 16	184, 209, 258, 287	0
21	AV	80/93 (86%)	-0.04	4 (5%) 30 30	226, 252, 266, 270	0
22	AW	99/106 (93%)	-0.22	7 (7%) 17 19	167, 195, 225, 241	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
23	AX	24/27 (88%)	-1.10	0 100 100	230, 249, 280, 288	0
24	BA	2889/2916 (99%)	-0.27	58 (2%) 65 61	129, 215, 297, 342	0
25	BB	123/123 (100%)	-0.50	0 100 100	199, 259, 293, 316	0
26	BC	228/229 (99%)	0.62	44 (19%) 1 6	250, 281, 300, 313	0
27	BD	272/276 (98%)	2.06	125 (45%) 0 3	130, 199, 221, 259	0
28	BE	206/206 (100%)	-0.55	3 (1%) 74 68	148, 186, 232, 269	0
29	BF	208/210 (99%)	-0.14	11 (5%) 27 28	164, 238, 263, 276	0
30	BG	182/182 (100%)	0.31	17 (9%) 9 14	212, 246, 268, 276	0
31	BH	174/180 (96%)	-0.90	0 100 100	196, 241, 260, 271	0
32	BK	148/148 (100%)	-0.88	0 100 100	202, 227, 249, 257	0
33	BL	138/147 (93%)	-0.39	3 (2%) 62 58	271, 298, 312, 327	0
34	BM	139/140 (99%)	-0.73	1 (0%) 87 84	167, 198, 224, 235	0
35	BN	122/122 (100%)	-0.27	0 100 100	148, 177, 209, 221	0
36	BO	145/150 (96%)	0.81	20 (13%) 3 8	166, 247, 276, 315	0
37	BP	136/141 (96%)	0.34	10 (7%) 15 18	166, 208, 234, 241	0
38	BQ	117/118 (99%)	-0.49	0 100 100	168, 192, 219, 226	0
39	BR	110/112 (98%)	-0.49	5 (4%) 34 33	186, 235, 263, 289	0
40	BS	117/146 (80%)	-0.11	3 (2%) 56 52	164, 194, 227, 242	0
41	BT	117/118 (99%)	-0.45	1 (0%) 84 79	183, 202, 220, 232	0
42	BU	101/101 (100%)	-0.27	3 (2%) 51 46	168, 225, 246, 257	0
43	BV	110/113 (97%)	0.28	12 (10%) 6 11	180, 209, 237, 248	0
44	BW	94/96 (97%)	0.26	7 (7%) 15 18	212, 232, 280, 288	0
45	BX	110/110 (100%)	-0.23	6 (5%) 26 27	221, 255, 287, 305	0
46	BY	180/206 (87%)	0.06	6 (3%) 47 43	208, 246, 268, 279	0
47	BZ	85/85 (100%)	0.48	9 (10%) 7 11	211, 229, 242, 271	0
48	B1	67/67 (100%)	-0.36	0 100 100	218, 243, 263, 268	0
49	B2	59/60 (98%)	0.06	2 (3%) 46 42	204, 224, 249, 259	0
50	B3	71/71 (100%)	0.38	6 (8%) 11 15	199, 223, 238, 246	0
51	B4	57/60 (95%)	-0.45	0 100 100	164, 209, 264, 289	0
52	B5	49/54 (90%)	1.81	22 (44%) 0 3	206, 232, 242, 252	0
53	B6	49/49 (100%)	1.70	21 (42%) 0 3	162, 209, 221, 235	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
54	B7	64/65 (98%)	0.98	12 (18%) 1 6	164, 195, 225, 242	0
55	B8	37/37 (100%)	-1.02	0 100 100	205, 215, 224, 226	0
All	All	10893/11176 (97%)	-0.07	613 (5%) 25 26	129, 223, 295, 374	0

The worst 5 of 613 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	AB	69	G	37.8
3	AB	67	C	32.8
3	AB	70	G	30.8
3	AB	68	C	30.1
3	AB	19	G	30.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.