



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 09:25 PM GMT

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

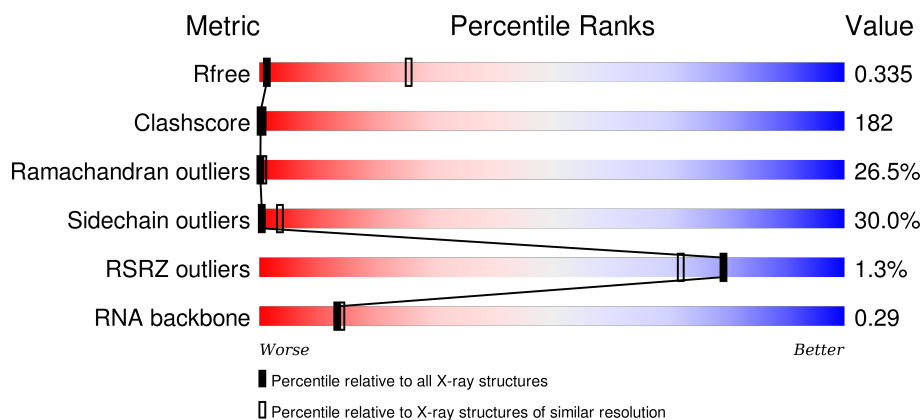
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*





The reported resolution of this entry is 5.00 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))
$R_{free}$	91344	1119 (6.22-3.60)
Clashscore	102246	1019 (6.22-3.66)
Ramachandran outliers	100387	1158 (6.22-3.60)
Sidechain outliers	100360	1136 (6.22-3.60)
RSRZ outliers	91569	1122 (6.22-3.60)
RNA backbone	2183	1097 (7.04-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	
2	AC	77	
3	AD	76	
4	AE	256	

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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	 A horizontal bar chart showing the quality of chain B8. The bar is divided into four segments: green (5%), yellow (54%), orange (38%), and red (5%). The segments are labeled with their respective percentages: 5%, 54%, 38%, and 5%.

## 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			

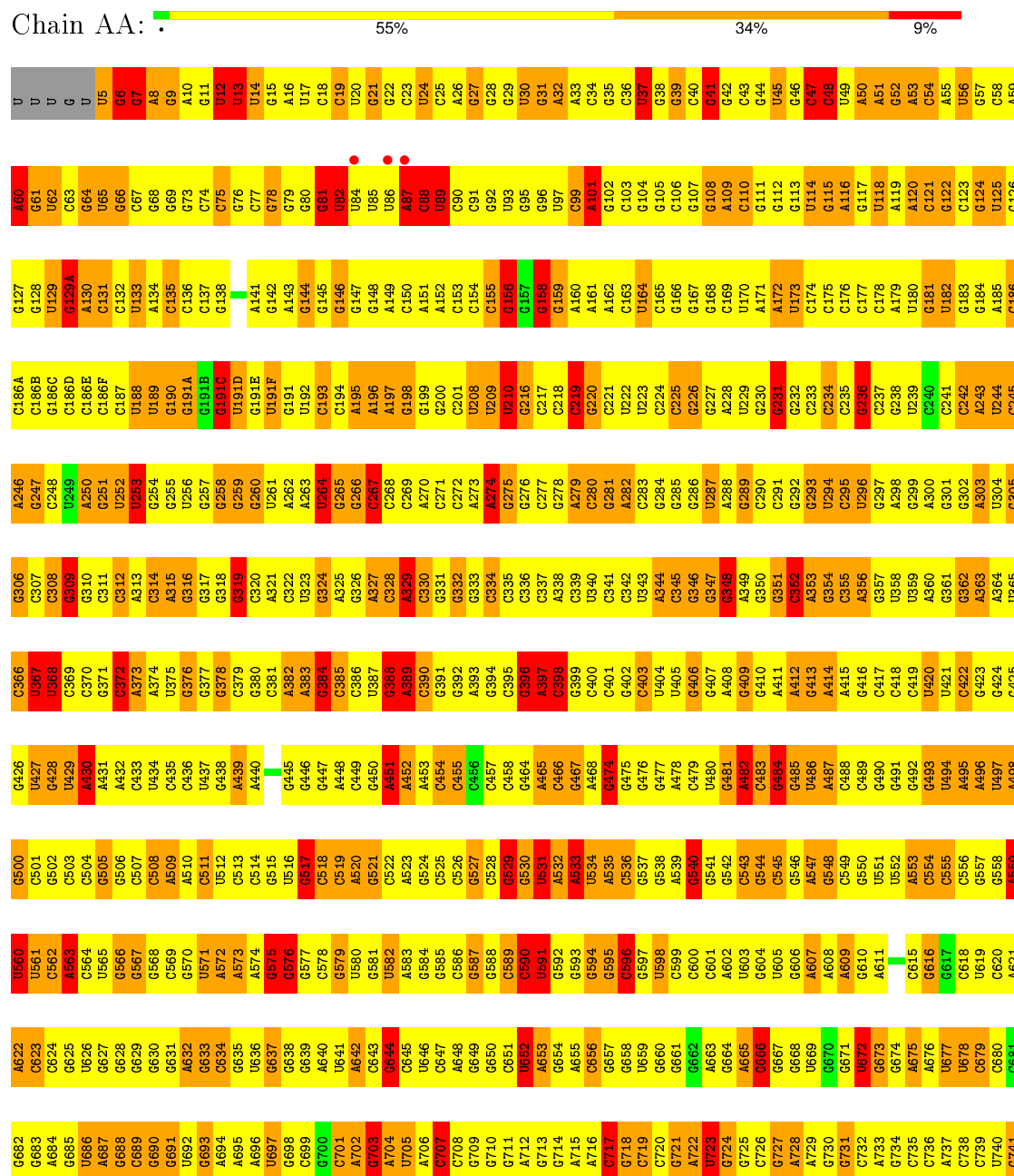
- Molecule 55 is a protein called 50S ribosomal protein L36.

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

### 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 errors 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 ( $\text{RSRZ} > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: 16S rRNA



G1529	G1469	C1404	U1345	A1285	A1225	G1164	G1104	A1044	C989	G929	C869	A802	G742
G1530	G1470	G1405	A1346	A1286	C1226	C1165	A1105	C1045	C990	C930	U870	G803	U743
A1531	G1471	U1406	G1347	A1287	A1227	A1166	A1106	A1046	U991	C931	U871	U804	C744
U1532	G1472	C1407	U1348	A1288	C1228	A1167	C1107	G1047	U992	G932	A872		C745
C1533	A1473	A1408	A1349	A1289	A1229	A1169	G1048	G993	G993	G933	A873	A807	A746
A1534	G1474	C1409	A1350	G1290	C1230	A1170	C1109	U1049	A994	G934	G874	C808	C747
C1535	G1475	G1410	U1351	G1291	G1231	G1171	A1110	G1050	C995	A935	C875	G809	C748
C1536	G1476	C1411	C1352	U1292	U1232	C1172	A1111	C1051	A996	C936	G876	C810	C749
U1537	G1477	G1412	G1353	G1293	G1233	G1173	C1112	U1052	U997	A937	C877	C811	G750
C1538	C1478	A1413	C1354	G1294	C1234	G1174	C1113	G1053	C998A	A938	G878	C812	U751
C1539	C1479	A1414	G1355	G1295	U1235	G1175	C1114	C1054	C998A	A939	C879	C813	G752
U1540	G1480	G1415	G1356	G1296	U1236	A1176	C1115	A1055	U999	C940	C880	A814	A753
U1541	U1481	G1416	A1357	C1297	C1237	G1177	C1116	U1056	A1000	G941	G881	A815	C754
U1542	G1482	G1417	U1358	C1298	A1238	G1178	G1117	G1057	G1001	G942	C882	A816	G755
C	A1483	A1418	C1359	A1299	A1239	A1179	C1118	G1058	C1002	U943	C883	C817	C756
U	C1484	G1419	A1360	G1300	U1240	A1180	C1119	C1059	G1003	U944	U884	G818	U757
	U1485	C1420	G1361	U1301	C1241	G1181	G1120	A1004	A1004	G945	G885	A819	G758
	G1486	G1421	C1362	U1302	G1242	G1182	U1121	C1060	A1005	A946	G886	U820	A759
	G1487	G1422	C1362A	C1303	C1243	A1183	U1122	U1062	C1006	G947	G887	G821	G760
	G1488	G1423	A1363	G1304	C1244	A1184	A1123	C1063	C1007	C948	G888	C822	G761
	G1489	C1424	A1364	G1305	A1245	G1185	G1124	G1064	C1008	A949	A889	G823	G762
	A1490	U1425	G1365	A1306	C1246	G1186	U1125	U1065	G1009	U950	G890	C824	G763
	G1491	C1426	C1366	U1307	U1247	G1187	U1126	C1066	G1010	G951	U891	G825	C764
	A1492	U1427	C1367	U1308	A1248	A1188	G1127	A1067	G1011	U952	A892	G826	G765
	A1493	A1428	G1368	G1309	C1249	C1189	C1128	G1068	U1012	G953	C893	U827	A766
	G1494	C1429	C1369	G1310	A1250	G1190	C1129	C1069	G1013	G954	G894	A828	A767
	U1495	C1430	G1370	G1311	A1251	A1191	A1130	U1070	A1014	U955	G895	G829	A768
	C1496	C1431	G1371	G1312	A1252	C1192	G1131	C1071	C1071	U956	C896	G830	G769
	G1497	G1432	U1372	U1313	G1253	G1193	C1132	G1072	A1016	U957	C897	U831	C770
	U1498	A1433	G1373	C1314	C1254	G1194	G1133	U1073	G1017	A958	C898	C832	G771
	A1499	A1434	A1374	G1315	G1255	G1195	G1134	G1074	C1018	A959	C899	U833	U772
	A1500	G1435	A1375	G1316	A1256	U1196	U1335	C1075	C1019	U860	A900	C834	G773
	C1501	U1436	C1376	C1317	U1257	G1197	U1136	C1076	U1020	U961	A901	U835	G774
	A1502	C1437	A1377	A1318	G1258	G1198	C1137	U1077	G1021	C962	G902	G836	G775
	G1503	G1438	G1378	A1319	C1259	U1199	G1138	U1078	G1022	G963	G903	G837	G776
	G1504	C1439	G1379	C1320	C1260	G1200	G1139	G1079	C1023	A964	C904	G838	A777
	U1505	G1440	U1380	C1321	A1261	A1201	C1140	A1080	G1024	A965	U905	U841	G778
	U1506	G1441	U1381	C1322	C1262	G1202	C1141	G1081	U1025	G966	G906	C842	G779
	A1507	G1442	C1382	G1323	C1263	C1203	G1142	G1082	G1026	C967	A907	U843	A780
	G1508	G1443	C1383	A1324	C1264	A1204	G1143	U1083	C1027	A968	A908	C848	A781
	C1509	A1446	C1384	C1325	G1265	U1205	G1144	G1084	C1028	A969	A909	C849	A782
	U1510	G1447	G1385	C1326	G1266	G1206	C1145	U1085	C1028A	C970	C910	U850	C783
	G1511	C1448	G1386	C1327	C1267	G1207	A1146	U1086	C1028B	G971	U911	G851	C784
	U1512	G1449	G1387	G1328	A1268	C1208	C1147	G1087	G1039	C972	C912	G852	G785
	A1513	U1450	C1388	A1329	A1269	C1209	U1148	G1088	C1030	G973	A913	G853	G786
	C1514	A1451	C1389	U1330	C1270	C1210	C1149	G1089	G1031	A974	A914	G854	A787
	G1515	C1452	U1390	G1331	G1271	U1211	U1150	U1090	A1032	A975	A915	G855	U788
	G1516	G1453	U1391	A1332	G1272	A1212	A1151	U1091	G1032A	G976	G916	C856	U789
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	A1518	U1393	G1393	G1334	G1274	C1214	C1153	A1093	G1033	A978	A918	G858	G791
	C1519	A1394	A1395	C1335	A1275	G1215	G1154	G1094	G1034	C979	A919	A859	A792
	G1520	A1460	C1396	C1336	G1276	G1216	G1155	U1095	A1035	C980	U920	A860	A793
	G1521	G1461	A1396	G1337	C1277	C1217	G1156	C1096	G1036	U981	U921	G861	A794
	U1522	G1462	C1397	G1338	U1278	C1218	A1157	C1097	C1037	U982	G922	C862	C795
	C1523	G1463	A1398	A1339	U1279	U1219	C1158	C1098	A983	A983	C924	U863	C796
	G1524	G1464	C1399	A1340	A1280	G1220	U1159	G1099	C1039	C984	A924	A864	C797
	U1525	C1465	C1400	U1341	U1281	G1221	G1160	G1100	U1040	C985	G925	A865	G798
	G1526	G1466	G1401	C1342	C1282	G1222	C1161	A1101	G1041	A986	G926	C866	G799
	U1527	G1467	C1402	G1343	G1283	C1223	C1162	A1102	G1042	G987	G927	G867	G800
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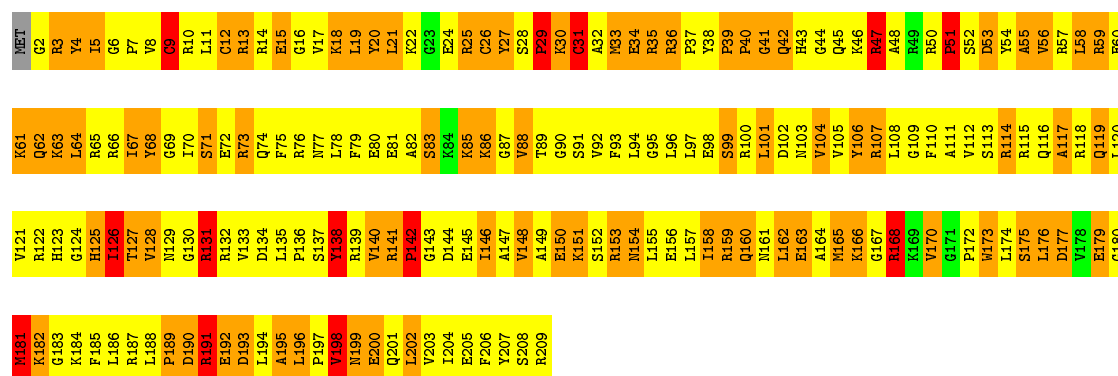
• Molecule 2: tRNA fMET (unmodified bases)

Chain AC:  45% 42% 10%

C1	G2	C3	G4	G5	G6	G7	G8	G9	G10	G11	G12	G13	A14	G15	G16	G17	U	G18	G19	G20	A21	G22	G23	U24	C25	G26	G27	G28	G29	G30	G31	C32	C33	C34	A35	U36	A37	A38	C39	C40	C41	C42	C43	C44	G45	G46	U47	G48	G49	U50	C51	G52	G53	U54	U55	C56	A57	A58	A59
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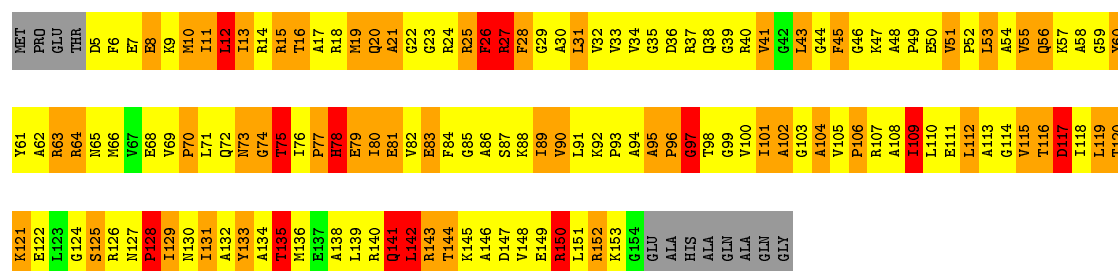






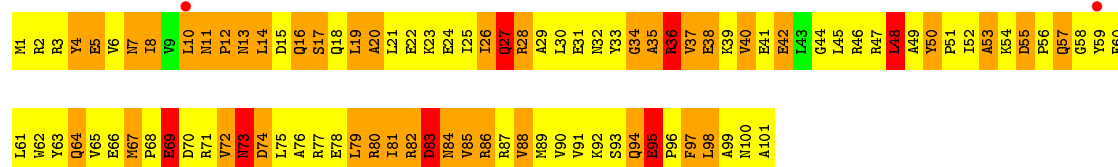
• Molecule 7: 30S ribosomal protein S5

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



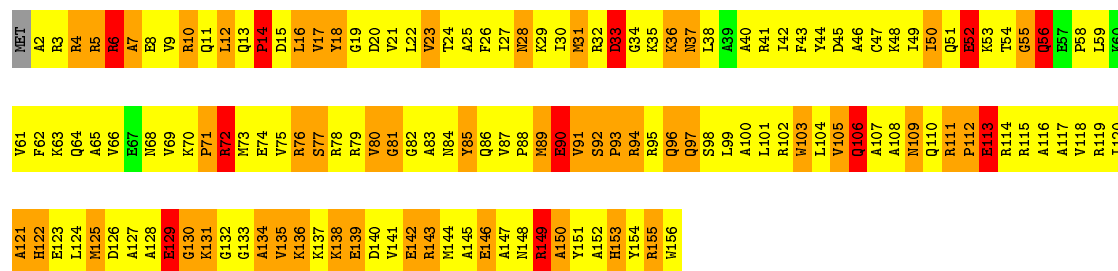
• Molecule 8: 30S ribosomal protein S6

Chain AI: . 2% 51% 40% 7%



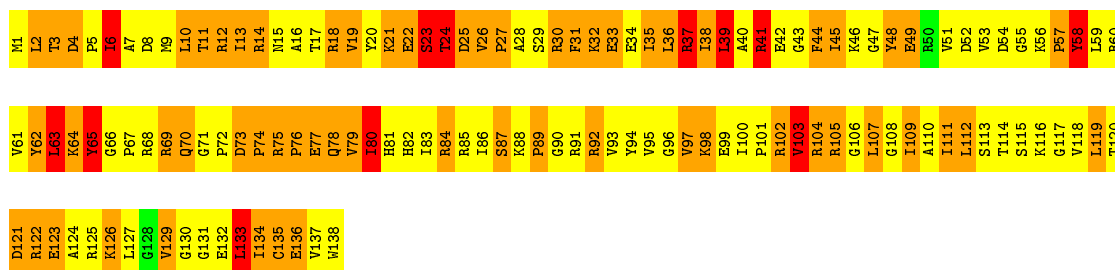
• Molecule 9: 30S ribosomal protein S7

Chain AJ: . 58% 31% 7%

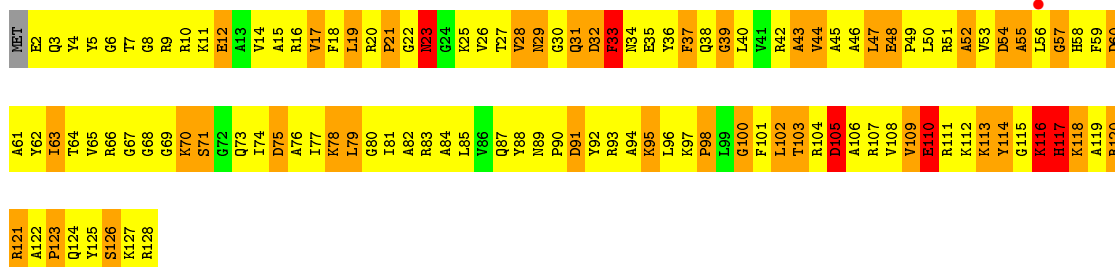


• Molecule 10: 30S ribosomal protein S8

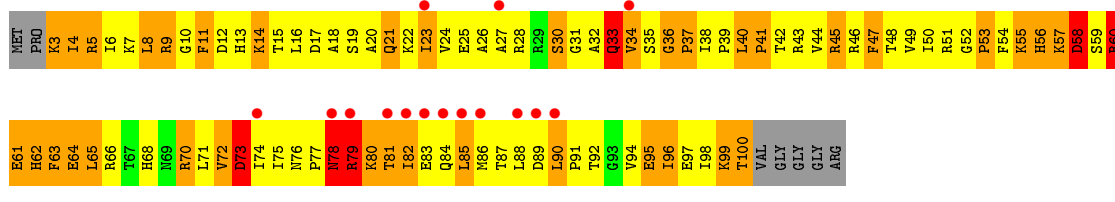
Chain AK: . 46% 43% 9%



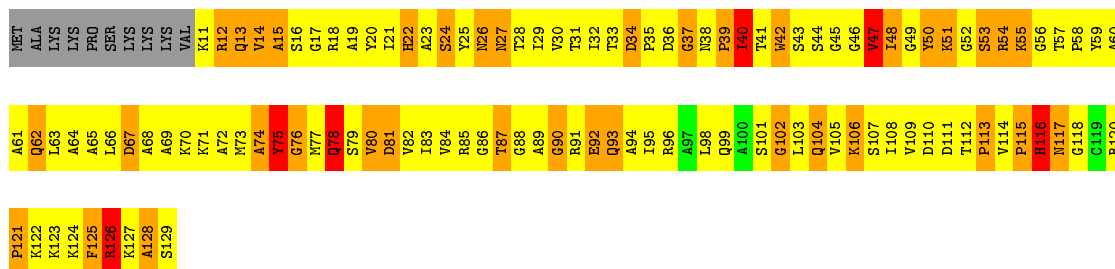
• Molecule 11: 30S ribosomal protein S9



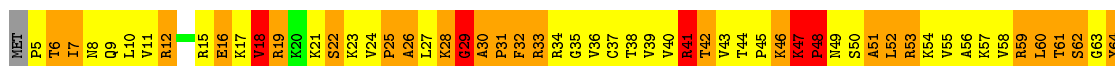
• Molecule 12: 30S ribosomal protein S10

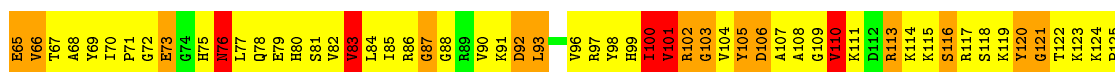


• Molecule 13: 30S ribosomal protein S11



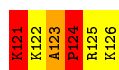
• Molecule 14: 30S ribosomal protein S12





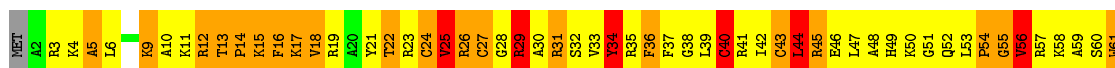
- Molecule 15: 30S ribosomal protein S13

Chain AP: 60% 31% 6%



- Molecule 16: 30S ribosomal protein S14

Chain AQ: 7% 49% 33% 10%



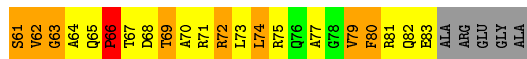
- Molecule 17: 30S ribosomal protein S15

Chain AR: 57% 35% 6%



- Molecule 18: 30S ribosomal protein S16

Chain AS: 5% 48% 36% 6%



- Molecule 19: 30S ribosomal protein S17

Chain AT: 56% 38% 6%





- Molecule 20: 30S ribosomal protein S18



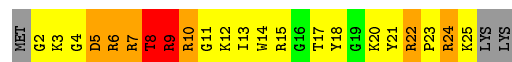
- Molecule 21: 30S ribosomal protein S19



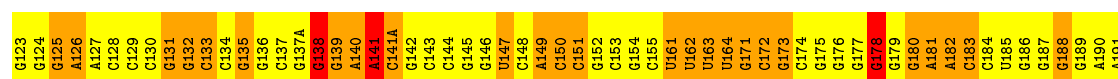
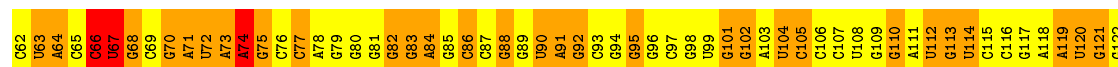
- Molecule 22: 30S ribosomal protein S20



- Molecule 23: 30S ribosomal protein Thx



- Molecule 24: 23S ribosomal RNA



U1094	G1034	C974A	C914	G853	A793	G733	G673	G635	G577	A515	A454	A394	C937	C277	G252	C192
A1095	U1035	G975	C915	G854	G794	A734	G674	G636	A578	C916	C485	U395	G338	A278	C253	U193
A1096	G1036	G976	G795	G855	G796	A735	A675	A637	C917	G517	C486	G396	U339	C279	G254	U194
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G1104	G1044	A984	A924	A863	U803	G743	C683	G645	C587	U525	U464	C404	A347	C287	A262	U202
U1105	A1045	C985	C925	G864	A804	G744	G684	A646	U588	A526	G465	U405	G348	C288	C263	C203
G1106	A1046	C986	A926	C865	G805	G745	A685	G647	C589	C527	A466	G406	G349	A289	C264	A204
G1107	G1047	G987	G928	A866	C806	A746	G686	G648	A590	A528	G467	G407	U850	G290	A265	G205
U1108	A1048	A988	G929	C867	U807	U747	C687	G649	A591	A529	G468	G408	G351	C291	G266	U206
C1109	C1049	G989	U930	U868	G808	G748	U688	C	C592	C530	G469	C409	G352	C292	C267	A207
A1110	A1050	A990	G931	G869	G809	C749	A689	G	U593	C531	A470	G410	G353	C293	C268	C208
G1111	G1051	G991	G932	A870	U810	A750	G690	C	U594	A532	A471	G411	G354	A294	U269	C209
C1112	C1052	C992	A933	U871	U811	A751	C691	A	C595	G533	A472	A412	G355	G295	A270	C210
U1113	C1053	G993	G934	A872	C812	A752	C692	A	U596	U534	G473	C413	G356	C296	A270A	A211
G1114	G1054	C994	C935	G873	U813	C753	C693	G	C597	C535	G474	C414	A357	C297	A270B	G212
G1115	G1055	C995	C936	G874	C814	C754	U694	C	U598	A536	U475	A415	U358	G298	A213	A213
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G1117	A1057	G997	G938	C876	C816	C756	G696	G	G600	G539	A477	C417	G360	A300	C270E	G215
C1118	G1058	C998	G939	U877	C817	U757	C697	G	C601	C540	A478	G418	G361	G301	U270F	A216
G1119	G1059	U999	G940	A878	G818	C758	C698	C	G602	C541	A479	G	U862	C302	C270G	G217
G1120	A1060	A1000	A941	G879	A819	G759	A699	C	A603	C542	A480	C419	G363	U303	C270H	A218
C1121	U1061	A1001	G942	G880	A820	G760	G700	C	G604	C543	G481	C420	A363A	G304	C270I	G219
A1122	G1062	G1002	U943	G881	A821	A761	G701	C	C605	C544	A482	U421	G363B	U305	G270J	G220
C1123	G1063	G1003	G944	G882	U822	U762	G702	A	U606	G545	A483	A422	G363C	U306	C270K	A221
G1124	C1064	A945	G945	G883	G823	G763	U703	C	U607	C546	C484	A423	G363D	G307	U270L	A222
C1125	U1065	G1005	G946	C884	A824	A764	G704	C	A608	A547	C485	G424	U863E	G308	U270M	A223
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A1128	G1068	A1008	A949	A887	U827	U767	G707	C	C610	U550	G489	U427	C365	G311	C270P	G226
C1129	C1069	G950	C950	C888	U828	G768	C708	C	C611	G551	G491	A428	C366	G312	C270Q	A227
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G1131	G1071	G952	G952	A890	G830	G770	G710	C	U613	U553	A493	C431	A371	A314	G270S	A229
A1132	C1072	A953	A953	G892	G831	G771	G711	G651	U614	U554	G494	A432	G372	G315	G270T	U230
U1133	A1073	G954	G954	C893	G832	C772	G712	C	G615	G556	G494	A433	U373	C316	C270U	C231
G1134	G1074	C955	C955	C894	U833	U773	G713	A653	A616	U557	G495	C433	A374	G317	G270V	G232
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C1137	A1077	U958	U958	C897	G836	G776	A716	G656	C618A	C560	G498	C436	C377	A320	G270Y	U235
G1138	U1078	A959	C959	C898	C837	A777	G717	U657	G619	G561	U499	G436	C378	G321	U270Z	C236
C1139	C1079	U1019	A960	A899	C838	G778	A718	C658	G620	U562	G500	G439	G379	A322	C271A	C237
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A1141	U1081	A1021	G962	A901	C940	G780	C720	G660	G622	C564	A502	U441	G381	A324	U271C	U239
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G2104	G2044	G1984	G1855	C1795	G1728	U1659	C1600	G1540	G1479	U1420	A1360	U1300	U1240	C1180
C2105	C2045	G1985	G1856	U1796	U1729	C1660	U1601	U1541	G1480	G1421	G1361	A1301	A1241	C1181
G2106	G2046	A1986	G1857	C1797	U1730	G1661	G1602	G1542	U1482	G1422	C1362	A1302	A1242	A1182
C2107	U2047	G1987	U1858	U1798	G1731	C1662	A1603	A1543	G1483	G1423	C1363	G1303	G1243	G1183
G2108	G2048	A1988	G1859	G1799	A1732	C1663	C1604	C1544	G1484	G1424	G1364	C1304	G1244	G1184
U2109	G2049	C1989	G1860	G1800	G1733	A1664	C1605	A1545	G1485	G1425	A1365	C1305	G1245	C1185
G2110	C2050	G1990	G1861	G1801	C1734	A1665	G1606	A1546A	A1486	G1426	A1366	C1306	A1246	G1186
C2111	A2051	U1991	G1862	A1802	C1735	G1666	C1607	U1546	G1487	A1427	A1367	A1307	A1247	G1187
G2112	G2052	G1992	G1863	A1803	C1741	G1667	A1608	C1547	G1488	C1428	G1368	A1308	G1248	U1188
U2113	C2053	U1993	U1864	C1804	G1742	A1668	A1609	C1548	U1489	G1429	G1369	U1249	U1249	A1189
A2114	A2054	C1994	G1869	U1805	G1743	A1669	A1610	C1549	A1490	C1430	C1370	G1310	G1250	G1190
C2115	C2055	U1995	C1870	C1806	G1746	G1670	C1611	C1550	G1491	U1431	G1371	G1311	C1251	G1191
G2116	G2056	A1996	A1871	G1807	G1747	U1671	C1612	C1551	G1492	C1432	U1372	U1312	G1252	G1192
A2117	A2057	G1997	U1872	U1808	G1748	C1672	G1613	G1552	C1493	U1433	A1373	U1313	A1253	G1193
U2118	A2058	A1998	G1878	A1809	A1749	U1673	A1614	A1553	A1494	A1434	G1374	C1314	A1254	A1194
A2119	A2059	C1999	C1879	A1810	G1750	G1674	C1615	A1554	A1495	G1435	C1375	C1315	U1255	G1195
G2120	G2060	G2000	C1880	G1811	C1751	C1675	A1616	G1555	A1496	G1436	C1376	U1316	G1256	C1196
C2121	G2061	A2001	C1881	A1812	G1752	A1677	C1617	C1556	U1497	C1437	G1377	A1317	G1257	G1197
A2122	A2062	G2002	C1882	G1813	G1753	A1678	A1618	C1557	G1498	U1438	A1378	C1318	G1258	U1198
G2123	C2063	C2003	G1883	G1814	C1754	G1678	G1619	A1558	C1499	A1439	A1379	G1319	G1259	U1199
C2124	C2064	G2004	A1884	A1815	A1755	U1679	G1620	G1559	G1500	G1440	C1320	G1260	G1260	C1200
G2125	C2065	A2005	A1885	G1816	G1756	U1680	U1621	G1560	G1441	G1381	A1321	C1261	G1261	C1201
A2126	C2066	C2006	C1886	G1817	U1757	G1681	G1622	G1561	C1502	G1382	A1322	A1262	G1262	C1202
G2127	G2067	C2007	C1887	U1818	G1758	G1682	G1623	A1562	U1503	G1383	U1323	U1263	G1263	G1203
C2128	U2068	C2008	A1888	A1819	A1759	G1683	G1624	G1563	C1504	G1444	A1384	G1324	G1264	A1204
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G2130	G2070	U1950	A1890	A1821	G1761	C1685	G1626	C1565	C1506	G1445	C1326	G1266	G1266	G1206
C2131	U2071	U2011	G1891	G1822	A1762	C1686	G1627	A1566	A1507	C1446	C1327	U1267	G1267	C1207
U2132	G2072	C2012	C1892	G1823	G1763	G1687	G1628	A1567	A1508	G1447	G1328	A1268	C1208	G1208
A2133	C2073	A2013	G1893	G1824	G1764	U1688	U1629	G1568	C1509	G1448	G1329	A1269	G1209	G1209
C2134	U2074	A1954	C1894	A1825	C1765	A1689	G1630	A1569	A1510	A1449	U1330	C1270	G1270	A1210
A2135	U2075	U1955	C1895	G1826	U1766	A1690	C1630A	A1570	A1511	G1449A	U1391	A1331	G1271	U1211
G2136	G2076	U1956	G1896	C1827	U1767	C1691	A1631	A1571	G1512	C1450	A1392	G1332	A1272	A1212
C2137	A2077	G1957	G1897	G1828	U1768	U1692	A1632	A1572	C1513	C1451	A1393	G1333	A1273	A1213
C2138	G2078	G1958	U1898	A1829	G1769	U1693	G1633	G1573	U1514	A1453	U1394	G1334	A1274	A1214

C2139	A2199	A2269	G2329	G2389	U2499	G2509	G2569	A2629	U2689	A2749	G2812	G2872
C2140	C2205	G2270	G2330	U2390	A2450	C2510	G2570	G2630	C2690	A2750	A2813	A2873
C2141	C2206	G2271	G2331	G2391	A2451	U2511	C2571	G2631	C2691	A2751	C2814	C2874
C2142	C2207	U2272	U2332	A2392	C2452	C2512	A2572	A2632	C2692	C2752	C2815	C2875
C2143	U2208	A2273	A2333	A2393	A2453	G2513	G2573	G2633	A2693	U2753	C2816	G2876
U2144	C2209	A2274	G2334	C2394	G2454	U2514	C2574	G2634	C2694	U2754	G2817	G2877
C2145	G2210	G2275	A2335	C2395	C2455	C2515	C2575	G2635	C2695	C2755	G2818	U2878
C2146	G2211	G2276	A2336	G2396	C2456	G2516	G2576	U2636	U2696	U2756	G2819	C2879
C2147	A2212	G2277	G2337	G2397	U2457	C2517	A2577	U2637	G2697	U2757	A2820	C2880
G2148	G2213	G2278	G2338	U2398	C2458	A2518	G2578	G2638	U2698	A2758	A2821	C2881
G2149	G2215	G2279	G2339	G2399	A2459	U2519	C2579	A2639	C2699	C2759	C2822	A2882
U2150	G2216	G2280	G2400	G2400	U2460	C2520	U2580	G2640	C2700	C2760	A2823	C2883
G2151	G2217	C2281	G2341	U2401	C2461	C2521	G2581	G2641	C2701	G2761	C2824	U2884
G2152	G2218	G2282	C2342	C2402	U2462	U2522	G2582	G2642	U2702	G2762	C2825	C2885
G2153	G2219	C2283	C2343	C2403	C2463	G2523	G2583	G2643	C2703	G2763	C2826	U2886
G2154	G2224	C2284	C2344	C2404	C2464	G2524	U2584	G2644	C2704	G2764	C2827	U2887
G2155	G2225	C2285	G2345	C2405	C2465	G2525	U2585	G2645	A2705	A2765	C2828	C2888
G2156	A2226	A2286	C2346	U2406	C2466	G2526	C2586	C2646	G2706	G2766	C2829	C2889
G2157	A2227	A2287	C2347	G2407	C2467	C2527	A2587	U2647	G2707	C2767	G2830	C2891
A2158	G2228	A2288	U2348	U2408	G2468	U2528	G2588	C2648	G2708	C2768	G2831	A2892
G2159	G2229	A2289	U2349	A2409	A2469	A2529	A2589	U2649	G2709	C2769	U2832	C2893
G2160	G2230	G2290	C2350	G2410	A2470	A2530	A2590	U2650	C2710	C2770	C2833	U2894
C2161	C2231	U2291	G2351	A2411	C2471	A2531	C2591	C2651	A2711	C2771	C2834	U2895
G2162	U2232	C2292	A2352	A2412	G2472	G2532	G2592	C2652	U2712	C2772	A2835	C2896
C2163	U2233	C2293	G2353	G2413	U2473	A2533	U2593	U2653	A2712A	C2773	U2836	U2897
C2164	G2234	C2294	G2354	G2414	C2474	A2534	C2594	A2654	A2713	C2774	G2837	U2898
G2165	G2235	C2295	C2355	G2415	C2475	G2535	G2595	U2655	G2714	A2775	G2838	C2899
G2166	C2236	U2296	C2356	A2416	A2476	G2536	U2596	U2656	G2715	C2776	C2839	A2900
U2167	G2237	C2297	U2357	C2417	C2477	U2537	C2597	A2657	U2716	G2777	C2840	C2901
G2168	G2238	A2298	G2358	A2418	A2478	C2538	A2598	C2658	G2717	C2778	C2841	C2902
A2169	G2239	G2299	C2359	U2419	G2479	C2539	U2599	G2659	G2718	U2779	G2842	C
A2170	C2240	G2300	A2360	C2420	C2480	C2540	A2600	A2660	G2719	G2780	G2843	C
A2171	A2241	C2301	A2361	A2421	C2481	A2541	A2601	A2661	A2720	A2781	A2844	U
U2172	A2242	G2302	C2362	A2422	G2482	A2542	A2602	A2662	A2721	G2782	C2845	C
A2173	U2243	G2303	C2363	U2423	C2483	G2543	G2603	G2663	G2722	C2783	G2846	G3
C2174	U2244	G2304	C2364	C2424	G2484	G2544	U2604	G2664	C2723	C2784	U2847	G3
C2175	U2245	A2305	G2365	A2425	G2485	G2545	U2605	A2665	C2724	G2785	G2848	U3
A2176	G2246	C2306	A2366	A2426	G2486	U2546	C2606	C2666	A2725	U2786	U2849	U3
C2177	A2247	G2307	G2367	C2427	G2487	U2547	G2607	C2667	U2726	C2787	A2850	G95
C2178	G2248	G2308	C2368	G2428	A2488	G2548	G2608	G2668	G2727	C2788	A2851	G97
C2179	U2249	A2309	A2369	G2429	G2489	G2549	U2609	G2669	U2728	C2789	C2852	G98
U2180	G2250	A2310	G2370	A2430	G2490	G2550	C2610	G2670	G2729	A2790	C2853	A99
G2181	G2251	A2311	G2371	U2431	U2491	C2551	U2611	G2671	C2730	U2791	G2854	G100
G2182	G2252	U2312	G2372	A2432	U2492	U2552	G2612	G2672	G2731	G2792	C2855	A101
C2183	G2253	C2313	G2373	A2433	U2493	G2553	U2613	G2673	G2732	G2793	C2856	A102
G2184	G2254	G2314	C2374	A2434	G2494	U2554	A2614	G2674	A2733	C2794	G2857	G103
C2185	G2255	G2315	G2375	A2435	C2495	U2555	U2615	A2675	A2734	G2795	C2858	A104
G2186	G2256	C2316	A2376	G2436	C2496	U2556	C2616	G2676	G2735	U2795	G2859	A45
G2187	U2257	C2317	A2377	U2437	A2497	G2557	G2617	G2677	C2736	C2796	G2860	G105
G2188	G2258	G2318	A2378	U2438	C2498	C2558	G2618	G2678	G2737	A2797	G2861	G106
U2189	G2259	G2319	G2379	A2439	C2499	C2559	C2619	A2679	U2739	A2799	G2862	U107
G2190	G2260	A2320	C2380	C2440	U2500	C2560	C2620	C2680	A2740	G2800	G2863	G108
G2191	C2261	C2321	C2381	C2441	C2501	A2561	A2621	C2681	A2741	C2801	G2864	G109
G2192	U2262	A2322	G2382	C2442	G2502	U2562	C2622	U2682	C2742	C2802	U2865	G110
G2193	G2263	G2323	C2383	G2443	A2503	U2563	C2623	C2683	C2743	G2803	G2866	A52
G2194	C2264	C2324	G2384	G2444	U2504	A2564	G2624	U2684	G2744	G2804	G2867	A53
C2195	U2265	G2325	C2385	G2445	G2505	A2565	G2625	G2685	C2745	U2805	A2868	G54
C2196	A2266	C2326	C2386	G2446	U2506	A2566	G2626	G2686	C2746	A2806	G2869	U55
U2197	A2267	G2327	C2387	G2447	C2507	G2567	G2627	U2687	U2747	A2810	C2870	G56
A2198	A2268	A2328	A2388	A2448	G2508	C2568	C2628	U2688	A2748	C2811	C2871	G117

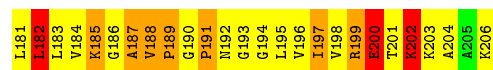
● Molecule 25: 5S ribosomal RNA

Chain BB:  46% 46% 7%

A-1	A59
A0	C60
U1	G61
C2	C62
C3	G63
C4	G64
C5	G65
C6	A66
G7	G67
U8	C68
G9	C69
C10	G70
C11	G71
C12	G72
A13	U73
U14	A74
G15	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
C28	C88
A29	G89
A30	A90A
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
U48	U107
C49	G108
G50	C109
G51	G110
A52	U111
A53	G112
G54	C113
U55	G114
G56	G115
A57	G116
A58	G117

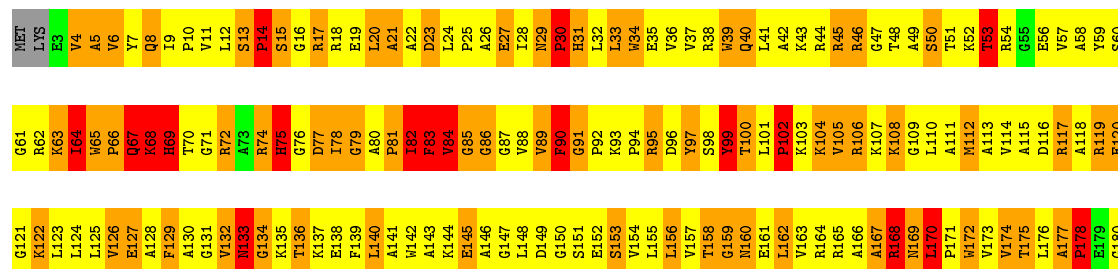






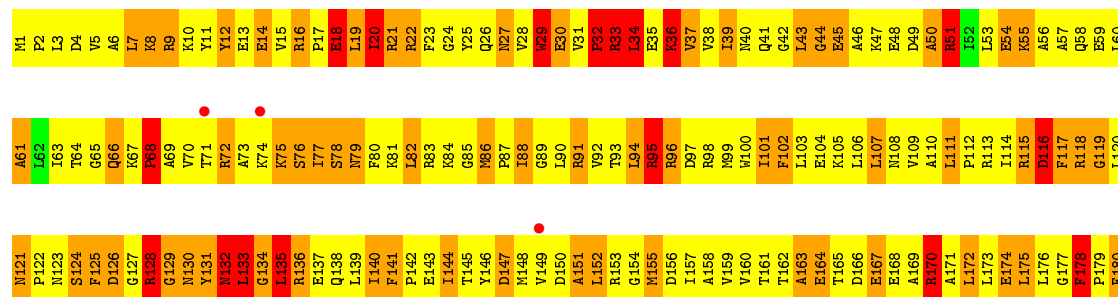
• Molecule 29: 50S ribosomal protein L4

Chain BF: . 50% 38% 9% .



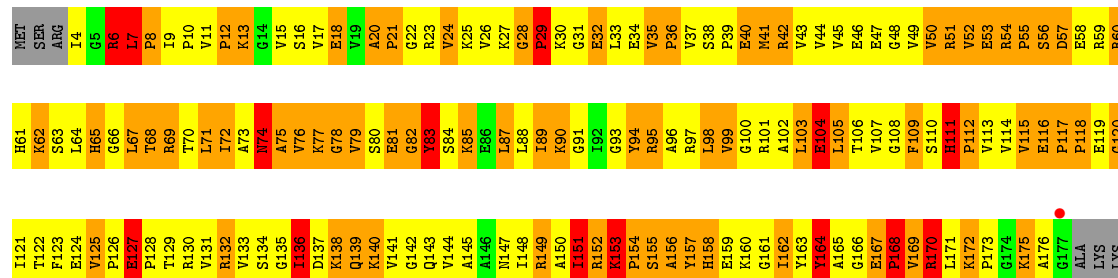
• Molecule 30: 50S ribosomal protein L5

Chain BG: . 2% 54% 35% 10%



• Molecule 31: 50S ribosomal protein L6

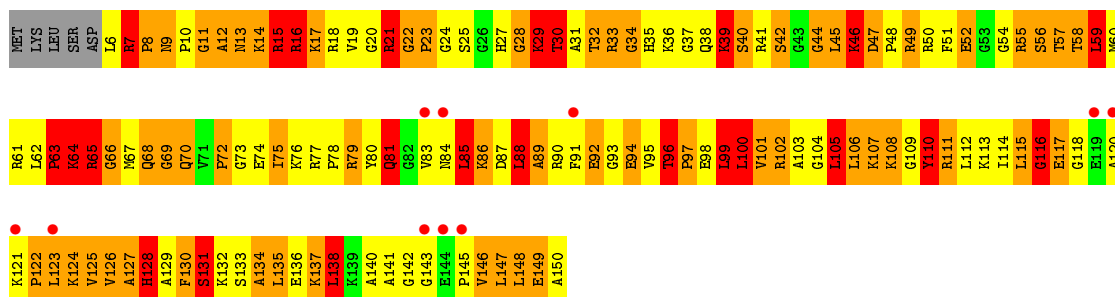
Chain BH: . 45% 39% 8% .



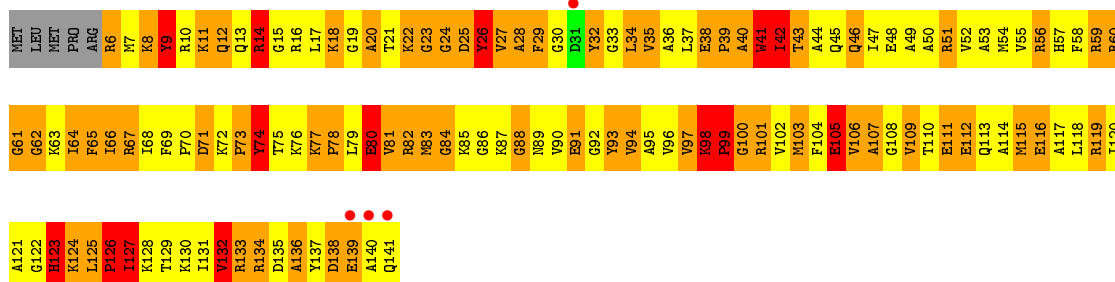
• Molecule 32: 50S ribosomal protein L9

Chain BK: . 57% 36% .





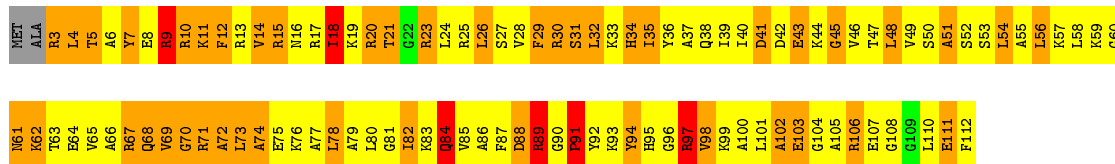
• Molecule 37: 50S ribosomal protein L16



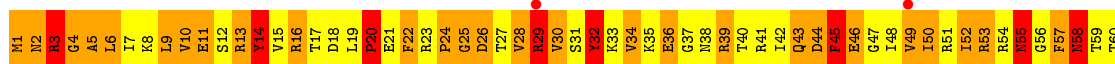
• Molecule 38: 50S ribosomal protein L17

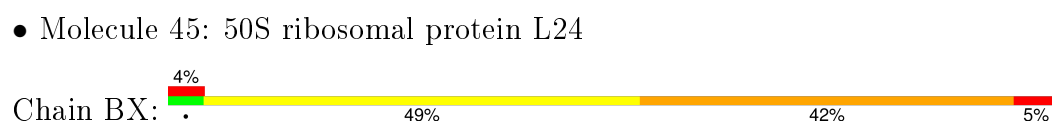


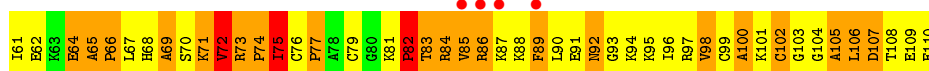
• Molecule 39: 50S ribosomal protein L18



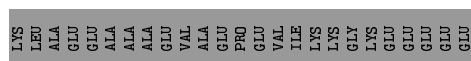
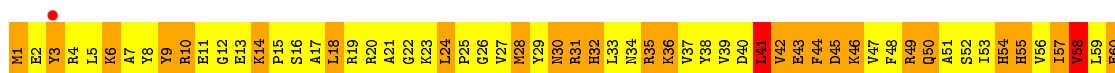
• Molecule 40: 50S ribosomal protein L19







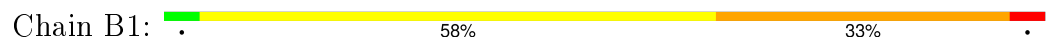
• Molecule 46: 50S ribosomal protein L25



• Molecule 47: 50S ribosomal protein L27



• Molecule 48: 50S ribosomal protein L29

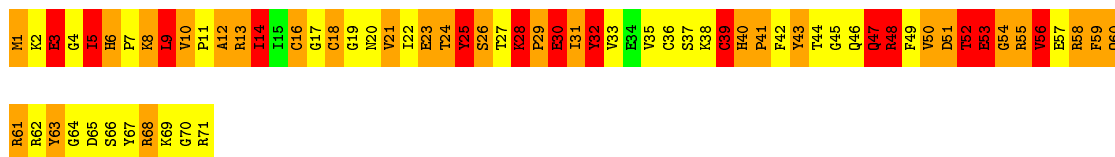


• Molecule 49: 50S ribosomal protein L30



• Molecule 50: 50S ribosomal protein L31

Chain B3:  39% 38% 20%



- Molecule 51: 50S ribosomal protein L32

Chain B4:  43% 33% 15% 5%



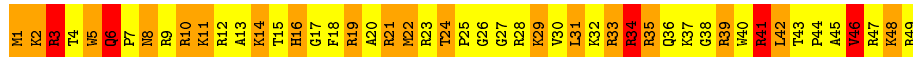
- Molecule 52: 50S ribosomal protein L33

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



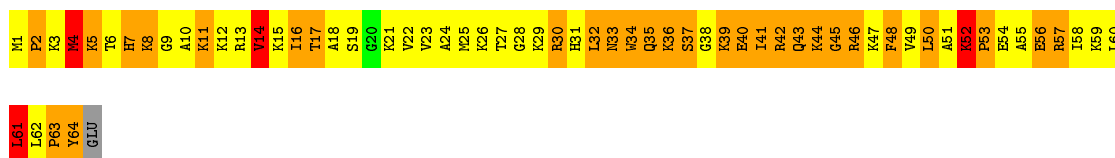
- Molecule 53: 50S ribosomal protein L34

Chain B6:  51% 39% 10%



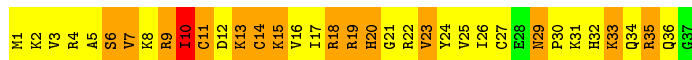
- Molecule 54: 50S ribosomal protein L35

Chain B7:  46% 45% 6%



- Molecule 55: 50S ribosomal protein L36

Chain B8:  5% 54% 38%



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	509.52Å 509.52Å 804.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	300.00 – 5.00 430.52 – 4.80	Depositor EDS
% Data completeness (in resolution range)	93.9 (300.00-5.00) 96.7 (430.52-4.80)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.09 (at 4.88Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.263 , 0.323 0.282 , 0.335	Depositor DCC
$R_{free}$ test set	10783 reflections (5.16%)	DCC
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> )	0.09 , 59.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.55$ , $\langle L^2 \rangle = 0.39$	Xtriage
Outliers	1 of 252174 reflections (0.000%)	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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	AA	0.94	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	2
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	2
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	2
14	AO	122/132 (92%)	60 (49%)	29 (24%)	33 (27%)	0	0
15	AP	123/126 (98%)	64 (52%)	33 (27%)	26 (21%)	0	2
16	AQ	58/61 (95%)	24 (41%)	16 (28%)	18 (31%)	0	0
17	AR	86/89 (97%)	43 (50%)	26 (30%)	17 (20%)	0	3
18	AS	81/88 (92%)	46 (57%)	22 (27%)	13 (16%)	0	5
19	AT	102/105 (97%)	63 (62%)	20 (20%)	19 (19%)	0	3
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	4
33	BL	136/147 (92%)	68 (50%)	38 (28%)	30 (22%)	0	2
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	5
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	2
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	3
48	B1	65/67 (97%)	30 (46%)	20 (31%)	15 (23%)	0	1
49	B2	57/60 (95%)	33 (58%)	12 (21%)	12 (21%)	0	2
50	B3	69/71 (97%)	20 (29%)	23 (33%)	26 (38%)	0	0
51	B4	55/60 (92%)	14 (26%)	22 (40%)	19 (34%)	0	0
52	B5	47/54 (87%)	15 (32%)	8 (17%)	24 (51%)	0	0
53	B6	47/49 (96%)	18 (38%)	14 (30%)	15 (32%)	0	0
54	B7	62/65 (95%)	23 (37%)	18 (29%)	21 (34%)	0	0
55	B8	35/37 (95%)	21 (60%)	6 (17%)	8 (23%)	0	1
All	All	5988/6337 (94%)	2879 (48%)	1522 (25%)	1587 (26%)	0	1

5 of 1587 Ramachandran outliers are listed below:

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

### 5.3.2 Protein sidechains ⓘ

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

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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	5
39	BR	87/88 (99%)	61 (70%)	26 (30%)	0	3
40	BS	105/127 (83%)	65 (62%)	40 (38%)	0	0
41	BT	93/94 (99%)	61 (66%)	32 (34%)	0	2
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	10
45	BX	91/91 (100%)	71 (78%)	20 (22%)	1	10
46	BY	159/179 (89%)	107 (67%)	52 (33%)	0	2
47	BZ	67/67 (100%)	49 (73%)	18 (27%)	0	5
48	B1	62/62 (100%)	49 (79%)	13 (21%)	1	11
49	B2	51/52 (98%)	37 (72%)	14 (28%)	0	4
50	B3	63/63 (100%)	42 (67%)	21 (33%)	0	2
51	B4	50/52 (96%)	33 (66%)	17 (34%)	0	2
52	B5	48/52 (92%)	32 (67%)	16 (33%)	0	2
53	B6	42/42 (100%)	29 (69%)	13 (31%)	0	3
54	B7	54/55 (98%)	39 (72%)	15 (28%)	0	4
55	B8	34/34 (100%)	25 (74%)	9 (26%)	0	5
All	All	5040/5237 (96%)	3528 (70%)	1512 (30%)	0	3

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

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

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

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

### 5.3.3 RNA ⓘ

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

5 of 1753 RNA backbone outliers are listed below:

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

5 of 436 RNA pucker outliers are listed below:

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

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

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

## 5.5 Carbohydrates ⓘ

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	2501:C	O3'	2502:G	P	1.90
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%)	-0.51	3 (0%) 95 94	88, 158, 260, 350	0
2	AC	76/77 (98%)	-0.53	0 100 100	133, 166, 216, 249	0
3	AD	76/76 (100%)	-0.33	0 100 100	219, 265, 316, 334	0
4	AE	234/256 (91%)	-0.04	10 (4%) 39 32	122, 163, 221, 265	0
5	AF	206/239 (86%)	-0.03	4 (1%) 70 62	143, 182, 210, 228	0
6	AG	208/209 (99%)	-0.75	0 100 100	106, 148, 170, 187	0
7	AH	150/162 (92%)	-0.36	0 100 100	114, 139, 171, 200	0
8	AI	101/101 (100%)	0.22	2 (1%) 68 60	121, 150, 168, 203	0
9	AJ	155/156 (99%)	-0.03	0 100 100	155, 180, 208, 214	0
10	AK	138/138 (100%)	-0.65	0 100 100	113, 133, 153, 160	0
11	AL	127/128 (99%)	-0.22	1 (0%) 87 82	161, 225, 247, 255	0
12	AM	98/105 (93%)	0.58	15 (15%) 3 4	146, 208, 237, 240	0
13	AN	119/129 (92%)	-0.26	0 100 100	114, 142, 176, 206	0
14	AO	124/132 (93%)	-0.13	0 100 100	96, 129, 162, 184	0
15	AP	125/126 (99%)	-0.50	0 100 100	167, 194, 223, 230	0
16	AQ	60/61 (98%)	-0.44	0 100 100	163, 188, 203, 206	0
17	AR	88/89 (98%)	-0.71	0 100 100	113, 131, 168, 183	0
18	AS	83/88 (94%)	-0.92	0 100 100	104, 128, 155, 185	0
19	AT	104/105 (99%)	-0.74	0 100 100	98, 126, 169, 215	0
20	AU	73/88 (82%)	-0.36	4 (5%) 29 24	109, 136, 190, 224	0
21	AV	80/93 (86%)	0.22	1 (1%) 79 72	175, 198, 217, 222	0
22	AW	99/106 (93%)	-0.61	0 100 100	105, 134, 163, 166	0
23	AX	24/27 (88%)	-0.84	0 100 100	168, 210, 224, 229	0
24	BA	2889/2916 (99%)	-0.50	0 100 100	63, 155, 266, 322	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	BB	123/123 (100%)	-0.43	0 100 100	146, 209, 257, 291	0
26	BC	228/229 (99%)	0.25	17 (7%) 17 15	220, 256, 308, 312	0
27	BD	272/276 (98%)	0.01	4 (1%) 76 68	80, 125, 153, 198	0
28	BE	206/206 (100%)	-0.37	1 (0%) 91 88	69, 117, 172, 224	0
29	BF	208/210 (99%)	-0.42	0 100 100	111, 179, 215, 231	0
30	BG	182/182 (100%)	-0.31	3 (1%) 74 66	160, 198, 226, 240	0
31	BH	174/180 (96%)	-0.29	1 (0%) 90 86	146, 186, 216, 238	0
32	BK	148/148 (100%)	-0.44	0 100 100	135, 161, 188, 190	0
33	BL	138/147 (93%)	0.99	33 (23%) 1 2	277, 307, 330, 334	0
34	BM	139/140 (99%)	-0.43	1 (0%) 89 84	107, 133, 167, 183	0
35	BN	122/122 (100%)	-0.30	0 100 100	78, 106, 140, 154	0
36	BO	145/150 (96%)	0.03	10 (6%) 20 16	106, 190, 227, 239	0
37	BP	136/141 (96%)	-0.13	4 (2%) 55 45	109, 141, 173, 186	0
38	BQ	117/118 (99%)	-0.47	0 100 100	91, 124, 157, 173	0
39	BR	110/112 (98%)	-0.69	0 100 100	152, 183, 210, 248	0
40	BS	117/146 (80%)	-0.13	2 (1%) 73 65	83, 127, 165, 184	0
41	BT	117/118 (99%)	-0.39	1 (0%) 85 80	100, 138, 152, 158	0
42	BU	101/101 (100%)	0.32	7 (6%) 20 16	104, 160, 186, 197	0
43	BV	110/113 (97%)	-0.39	0 100 100	110, 143, 179, 195	0
44	BW	94/96 (97%)	-0.31	0 100 100	153, 170, 232, 237	0
45	BX	110/110 (100%)	-0.22	4 (3%) 46 39	157, 199, 247, 273	0
46	BY	180/206 (87%)	0.37	6 (3%) 50 41	142, 190, 211, 226	0
47	BZ	85/85 (100%)	-0.65	0 100 100	139, 166, 181, 197	0
48	B1	67/67 (100%)	-0.18	0 100 100	172, 186, 199, 209	0
49	B2	59/60 (98%)	-0.36	0 100 100	127, 163, 188, 202	0
50	B3	71/71 (100%)	-0.70	0 100 100	127, 160, 176, 185	0
51	B4	57/60 (95%)	-0.46	0 100 100	96, 147, 217, 241	0
52	B5	49/54 (90%)	-0.19	1 (2%) 68 60	141, 163, 183, 198	0
53	B6	49/49 (100%)	-0.40	0 100 100	87, 145, 164, 188	0
54	B7	64/65 (98%)	-0.44	0 100 100	113, 131, 153, 165	0
55	B8	37/37 (100%)	-0.80	0 100 100	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%)	-0.35	135 (1%) 79 72	63, 160, 260, 350	0

The worst 5 of 135 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
31	BH	177	GLY	6.7
33	BL	17	ALA	6.0
4	AE	231	GLU	5.1
12	AM	81	THR	4.6
26	BC	126	LYS	4.3

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.