



wwPDB X-ray Structure Validation Summary Report

Jun 16, 2014 – 07:31 PM BST

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 : 2006-06-27
Resolution : 5.50 Å (reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

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

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

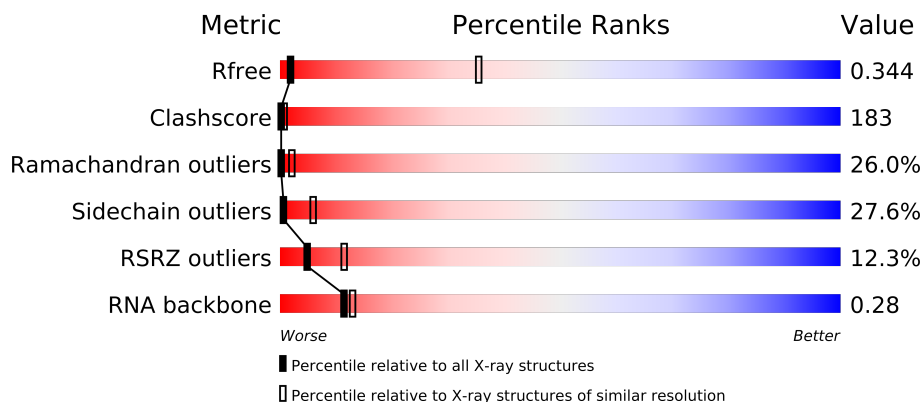
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1323
EDS : stable23397
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23397

1 Overall quality at a glance

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}	66092	1083 (7.50-3.50)
Clashscore	79885	1008 (7.40-3.52)
Ramachandran outliers	78287	1275 (7.50-3.50)
Sidechain outliers	78261	1251 (7.50-3.50)
RSRZ outliers	66119	1082 (7.50-3.50)
RNA backbone	1838	1040 (7.50-2.80)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	AA	1522	
2	A1	50	
3	AB	76	
3	AC	76	
3	AD	76	
4	AE	256	
5	AF	239	
6	AG	209	
7	AH	162	
8	AI	101	
9	AJ	156	
10	AK	138	

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Mol	Chain	Length	Quality of chain
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	
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>
54	B7	65	<div><div></div></div>
55	B8	37	<div><div></div></div>

2 Entry composition

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

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		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

- 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

- 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

- 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

- 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

- 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

- 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.

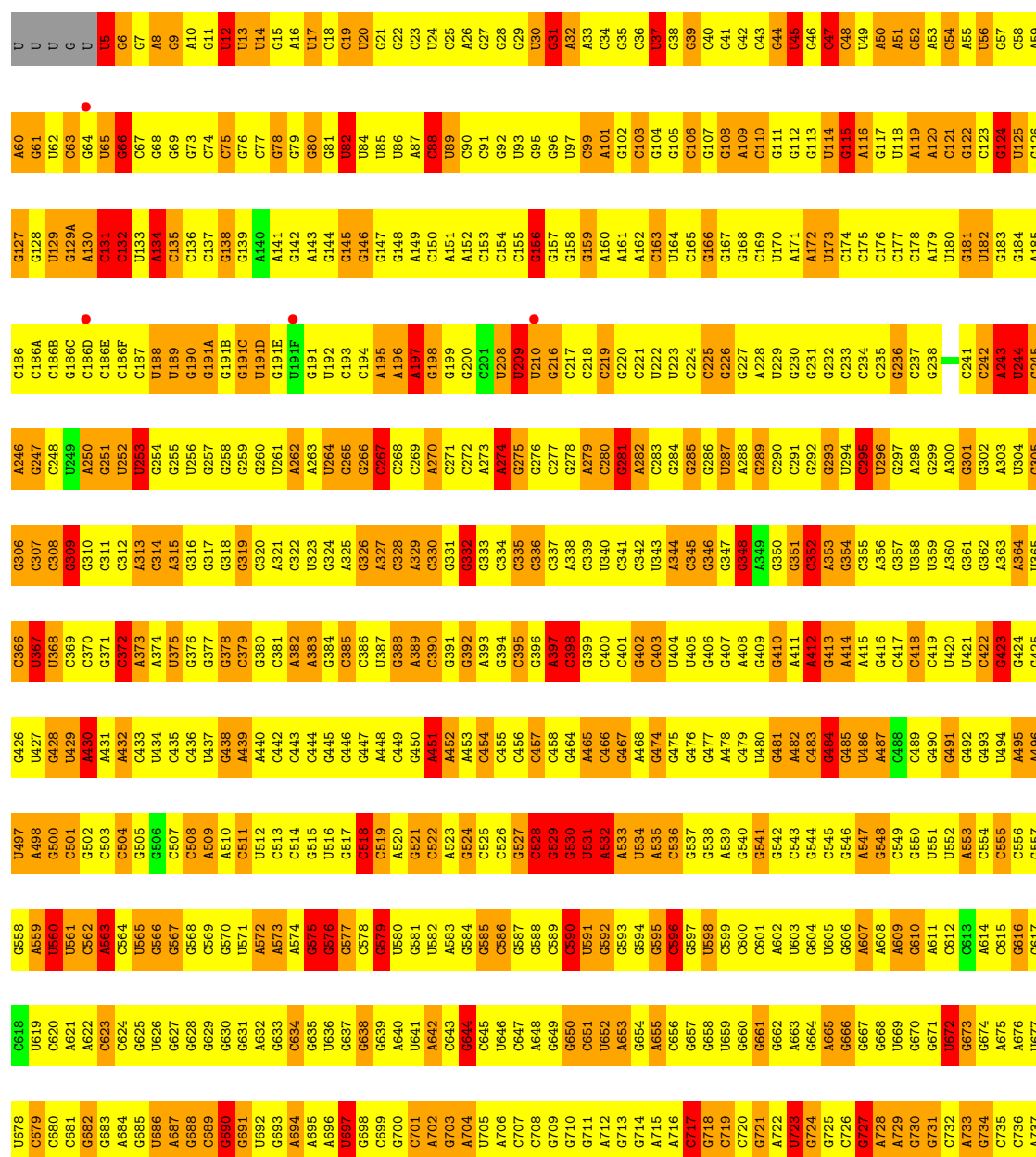
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	B8	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

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 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 ($RSRZ > 2$). 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

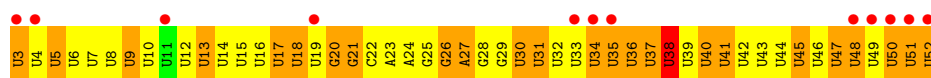
Chain AA: 



G1524	G1464	C1399	A1340	A1280	G1220	U1159	G1099	C924	A864	G798	C738
G1525	C1465	C1400	U1341	U1281	G1221	G1160	C1100	G925	A865	G799	C739
G1526	C1466	G1401	C1342	C1282	C1222	C1161	A1101	G926	C866	G800	U740
C1527	G1467	C1402	G1343	G1283	C1223	C1162	A1102	G927	G867	A986	G741
U1528	A1468	C1403	C1344	C1284	G1224	C1163	C1103	G928	C868	A802	G742
G1529	G1469	C1404	U1345	A1285	A1225	G1164	G1104	G929	C869	G803	U743
G1530	G1470	G1405	A1346	A1286	C1226	C1165	A1105	C930	U870	U804	C744
A1531	G1471	U1406	U1347	A1287	A1227	G1166	A1106	C931	U871	G805	C745
U1532	U1472	C1407	U1348	A1288	C1228	A1167	G1107	C932	A872	C806	A746
C1533	A1473	A1408	A1349	A1289	A1229	G1168	G1108	G933	A873	A807	C747
A1534	G1474	C1350	A1350	G1290	C1230	A1169	C1109	G934	G874	C808	C748
C1535	G1475	G1351	U1351	G1291	G1231	G1171	A1110	A934	C875	G809	C749
C1536	G1476	C1352	U1352	U1292	U1232	G1172	A1111	C935	C876	C810	G750
U1537	C1477	C1411	G1353	G1293	G1233	G1173	C1112	A936	C877	C811	U751
C1538	C1478	A1413	C1354	G1294	C1234	G1174	U1052	A937	G878	C812	G752
C1539	C1479	U1414	G1355	G1295	U1235	G1175	C1113	A938	G879	U813	A753
U1540	G1480	G1415	G1356	U1296	A1236	A1176	C1114	G939	C880	A814	C754
U1541	U1481	G1416	A1357	C1297	C1237	G1177	C1115	A940	C881	A815	G755
U1542	G1482	G1417	U1358	C1298	U1238	G1178	C1116	C941	C882	A816	C756
C	A1483	A1418	C1359	A1299	A1239	G1179	C1117	U942	C883	C817	U757
U	C1484	C1419	A1360	C1300	U1240	A1180	C1118	G944	U884	G818	G758
	U1485	C1420	G1361	U1301	G1241	G1181	C1119	A945	C885	A819	A759
	G1486	C1421	C1362	U1302	C1242	G1182	U1121	A946	G886	U820	G760
	G1487	G1422	A1362A	C1303	C1243	A1183	U1122	C947	G887	G821	G761
	G1488	G1423	C1363	G1304	C1244	G1184	A1123	U947	G888	C822	C762
	C1489	C1424	U1364	G1305	A1245	C1185	G1124	A949	A889	G823	G763
	C1490	U1425	C1365	A1306	U1246	G1186	U1125	U950	C890	C824	C764
	G1491	C1426	C1366	U1307	U1247	G1187	U1126	G951	U891	G825	G765
	A1492	U1427	C1367	U1308	A1248	A1188	G1127	U952	A892	C826	A766
	A1493	A1428	G1368	G1309	C1249	C1189	C1128	G953	C893	U827	A767
	G1494	C1429	C1369	G1310	A1250	G1190	C1129	G954	G894	A828	A768
	U1495	C1430	G1370	G1311	A1251	A1191	U1070	U955	G895	C829	G769
	C1496	C1431	G1371	G1312	A1252	A1192	A1014	U956	C896	C830	C770
	G1497	G1432	U1372	U1313	C1253	C1193	A1016	U957	C897	U831	G771
	A1498	A1433	C1373	C1314	C1254	G1194	G1017	A958	G898	C832	U772
	A1499	A1434	A1374	U1315	G1255	G1195	C1018	A959	C899	U833	G773
	U1500	G1435	A1375	G1316	A1256	U1196	G1074	U960	A900	C834	G774
	C1501	U1436	U1376	C1317	U1257	G1197	C1075	U961	A901	U835	G775
	A1502	C1437	A1377	G1318	G1258	G1198	C1076	C962	G902	G836	G776
	A1503	G1438	C1378	A1319	C1259	U1199	U1077	G963	G903	G837	A777
	G1504	C1439	G1379	C1320	C1260	C1200	G1078	A964	C904	G838	G778
	G1505	C1440	U1380	C1321	A1261	A1201	A1080	A965	U905	U841	C779
	U1506	G1441	U1381	C1322	C1262	G1202	G1081	G966	G906	C842	A780
	A1507	G1442	C1382	G1323	C1263	C1203	G1082	C967	A907	U843	A781
	G1508	G1443	C1383	A1324	C1264	A1204	U1083	A968	A908	C848	A782
	C1509	A1446	C1384	C1325	G1265	U1205	G1084	A969	A909	C849	C783
	U1510	G1447	G1385	C1326	G1266	G1206	U1085	C970	C910	U850	C784
	G1511	C1448	G1386	C1327	C1267	G1207	A1146	G971	U911	G851	G785
	U1512	C1449	G1387	C1328	A1268	C1208	U1086	C972	C912	G852	G786
	A1513	U1450	C1388	A1329	A1269	C1209	G1087	G973	A913	G853	A787
	C1514	A1451	C1389	U1330	C1270	C1210	U1088	A974	A914	C854	U788
	C1515	C1452	U1390	G1331	G1271	U1211	G1089	A975	A915	G855	U789
	G1516	G1453	U1391	U1212	G1272	U1212	U1090	A976	A916	C856	A790
	G1517	G1454	A1392	A1213	C1273	A1213	U1091	G977	G916	C857	G791
	A1518	G1455	U1393	G1334	G1274	C1214	A1092	A978	A917	G858	A792
	A1519	C1456	A1394	G1215	A1275	G1215	G1093	C979	A918	A859	U793
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	G1521	G1461	A1396	C1217	C1277	G1217	U1096	U981	U921	G861	C795
	U1522	G1462	C1397	C1218	U1278	A1157	C1097	U982	C862	C796	C797
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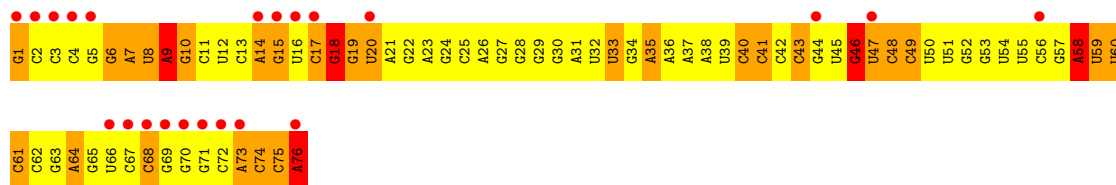
• Molecule 2: mRNA

Chain A1: 



- Molecule 3: tRNA PHE (unmodified bases)

Chain AC:



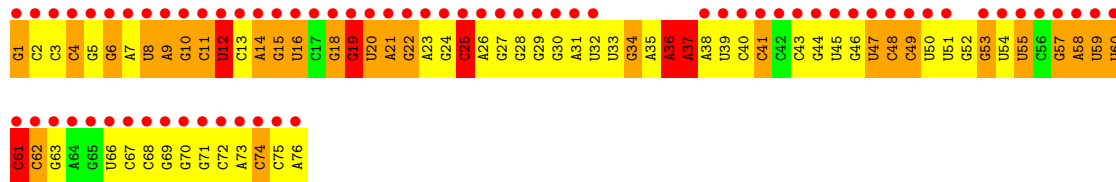
- Molecule 3: tRNA PHE (unmodified bases)

Chain AD:



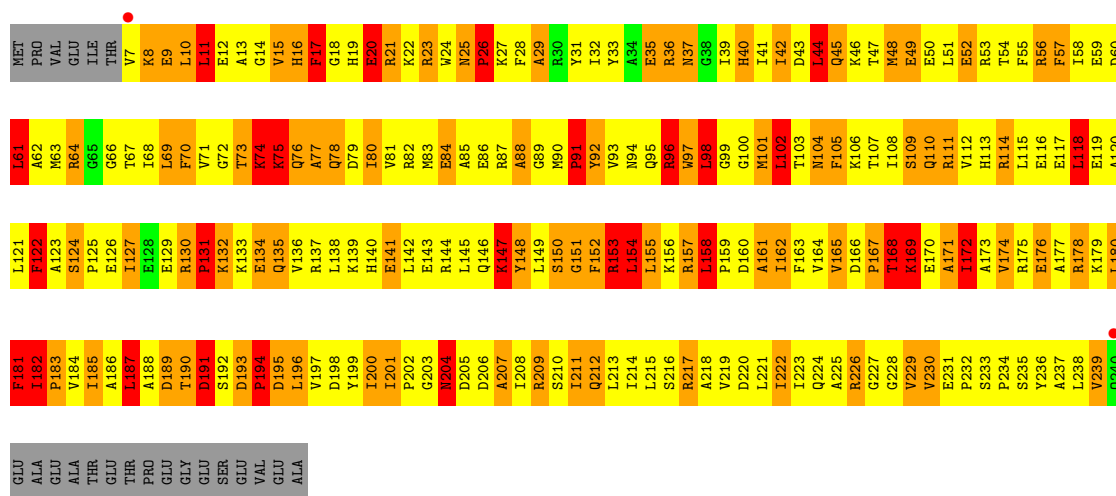
- Molecule 3: tRNA PHE (unmodified bases)

Chain AB:



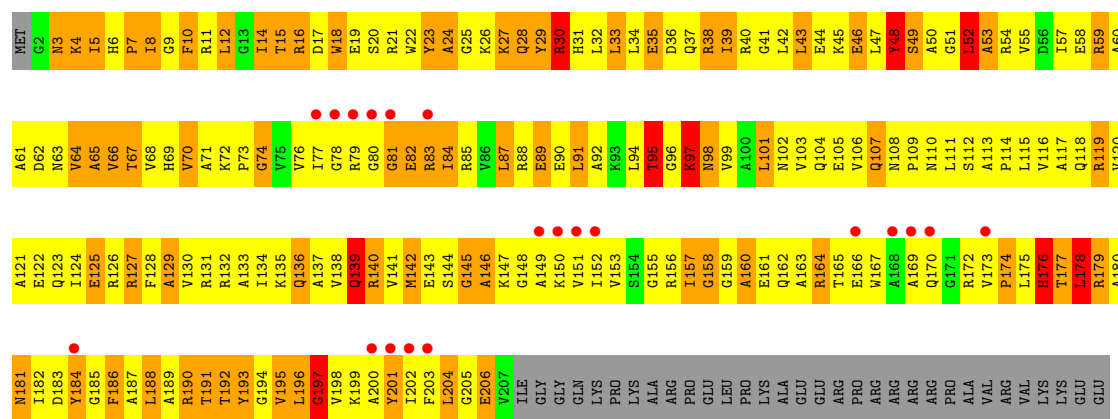
- Molecule 4: 30S ribosomal protein S2

Chain AE:



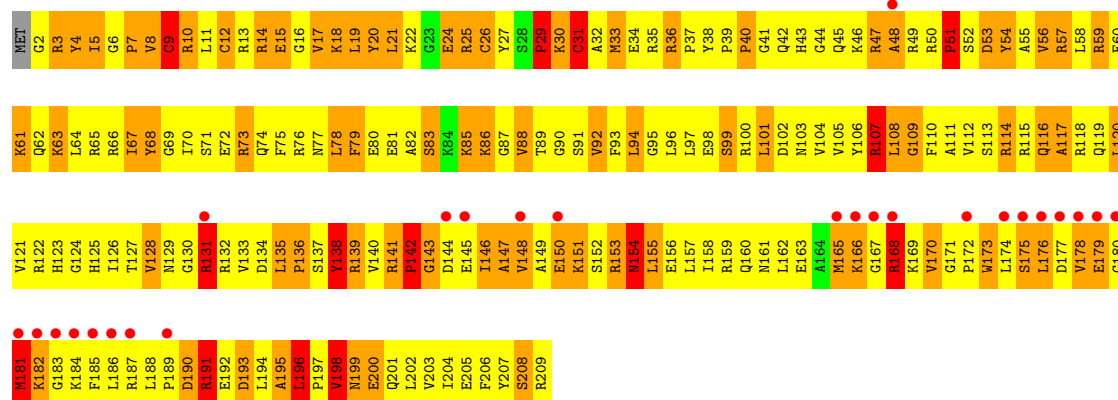
- Molecule 5: 30S ribosomal protein S3

Chain AF:



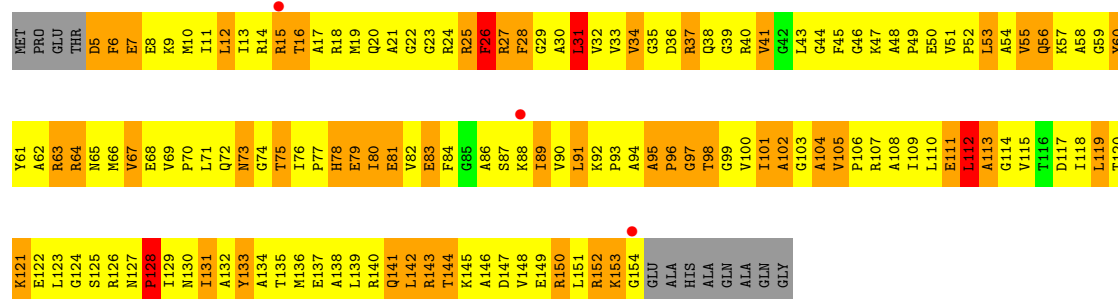
- Molecule 6: 30S ribosomal protein S4

Chain AG:



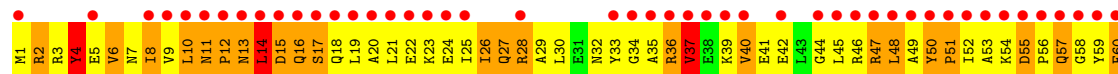
- Molecule 7: 30S ribosomal protein S5

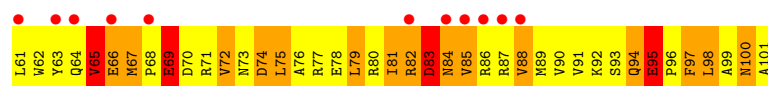
Chain AH:



- Molecule 8: 30S ribosomal protein S6

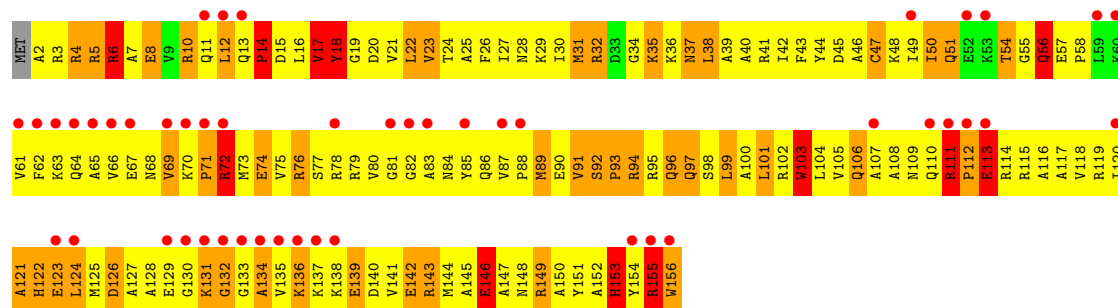
Chain AI:





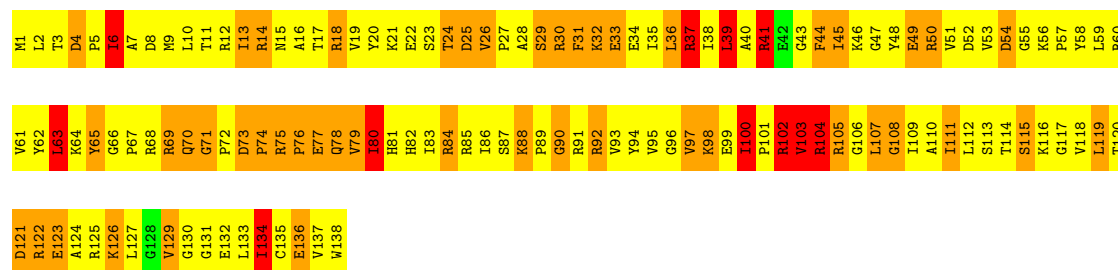
• Molecule 9: 30S ribosomal protein S7

Chain AJ:



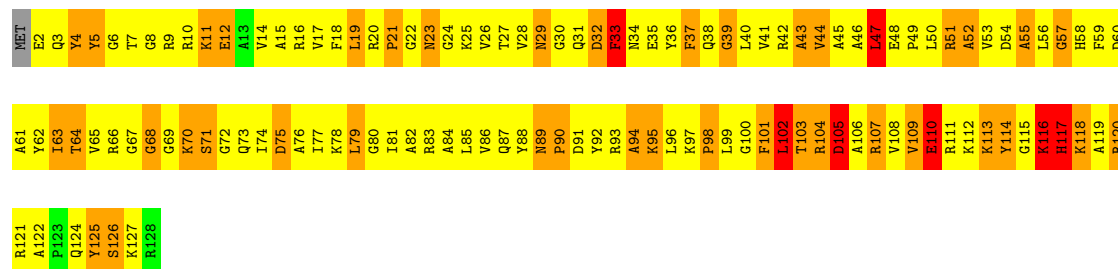
• Molecule 10: 30S ribosomal protein S8

Chain AK:



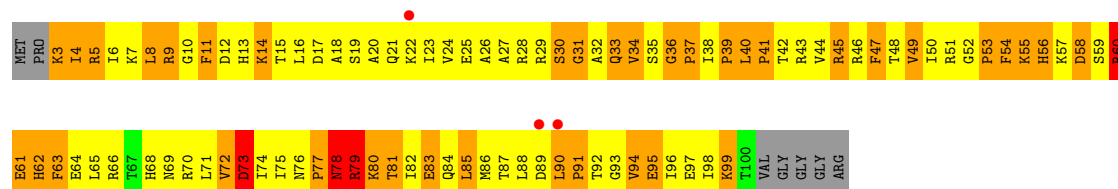
• Molecule 11: 30S ribosomal protein S9

Chain AL:



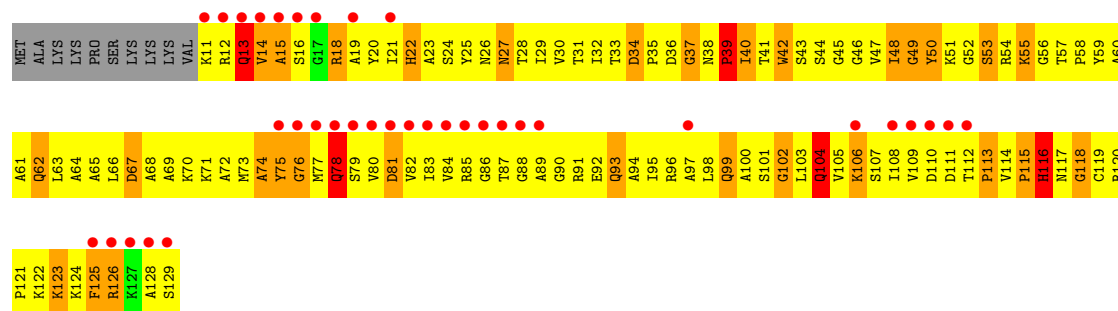
• Molecule 12: 30S ribosomal protein S10

Chain AM:



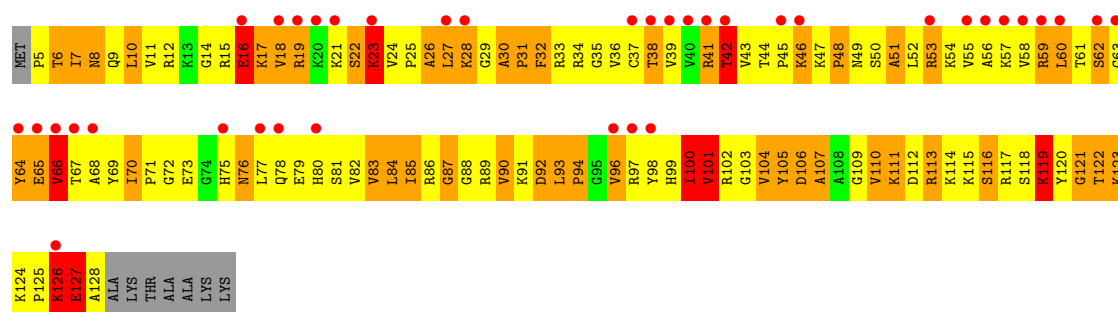
• Molecule 13: 30S ribosomal protein S11

Chain AN:



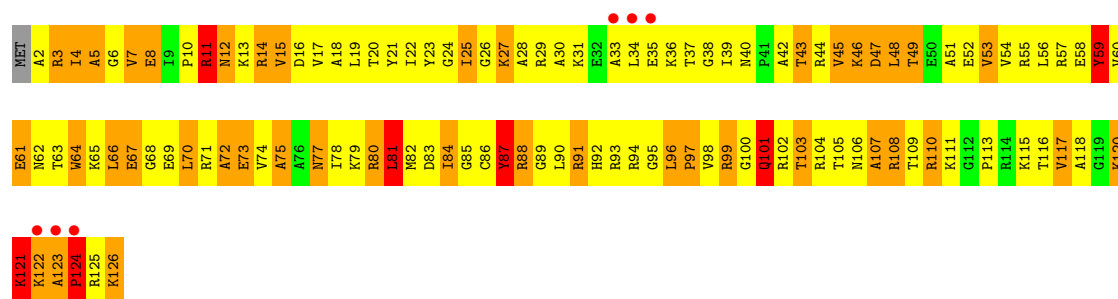
- Molecule 14: 30S ribosomal protein S12

Chain AO:



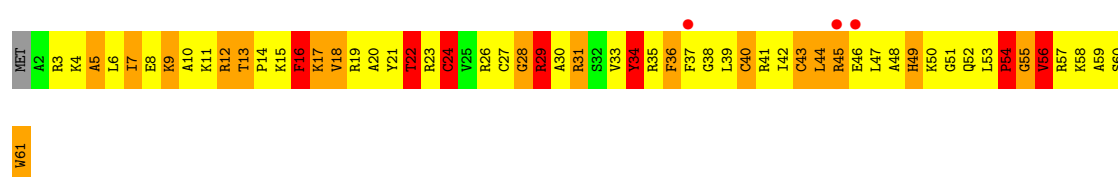
- Molecule 15: 30S ribosomal protein S13

Chain AP:



- Molecule 16: 30S ribosomal protein S14

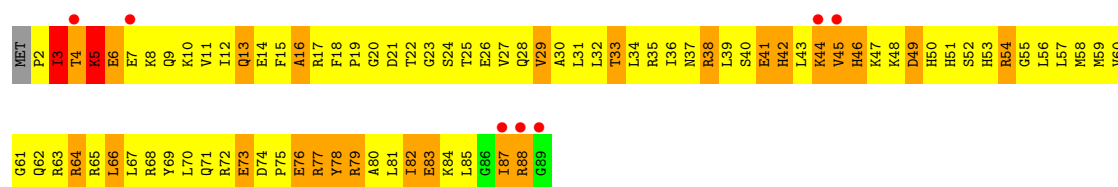
Chain AQ:



- Molecule 17: 30S ribosomal protein S15

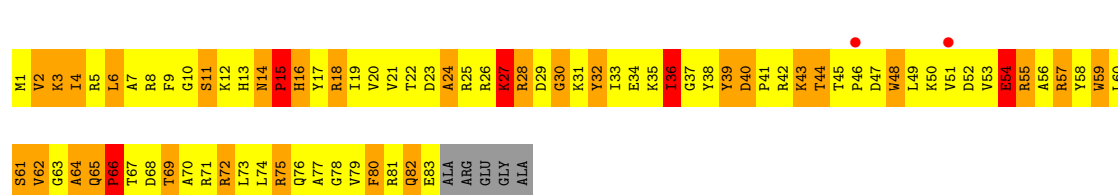
Chain AR:





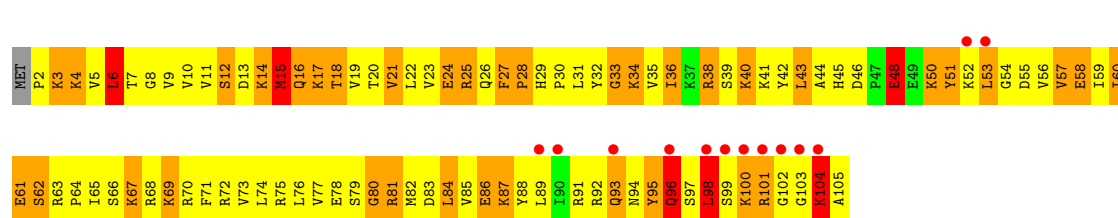
• Molecule 18: 30S ribosomal protein S16

Chain AS:



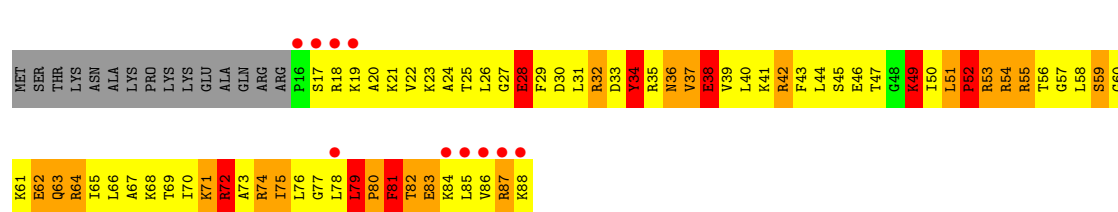
• Molecule 19: 30S ribosomal protein S17

Chain AT:



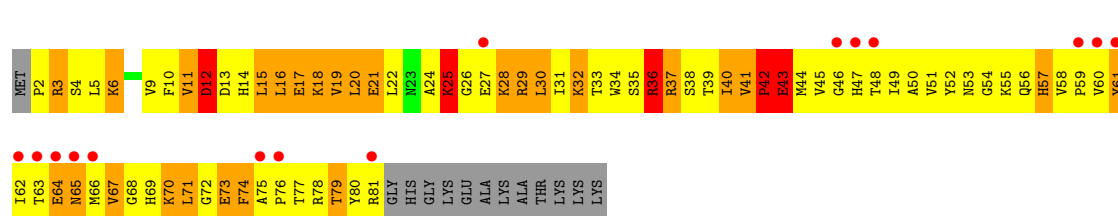
• Molecule 20: 30S ribosomal protein S18

Chain AU:



• Molecule 21: 30S ribosomal protein S19

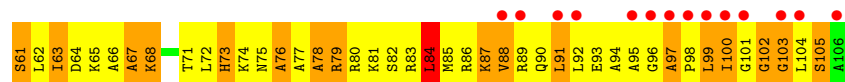
Chain AV:



• Molecule 22: 30S ribosomal protein S20

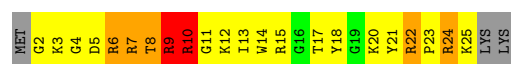
Chain AW:





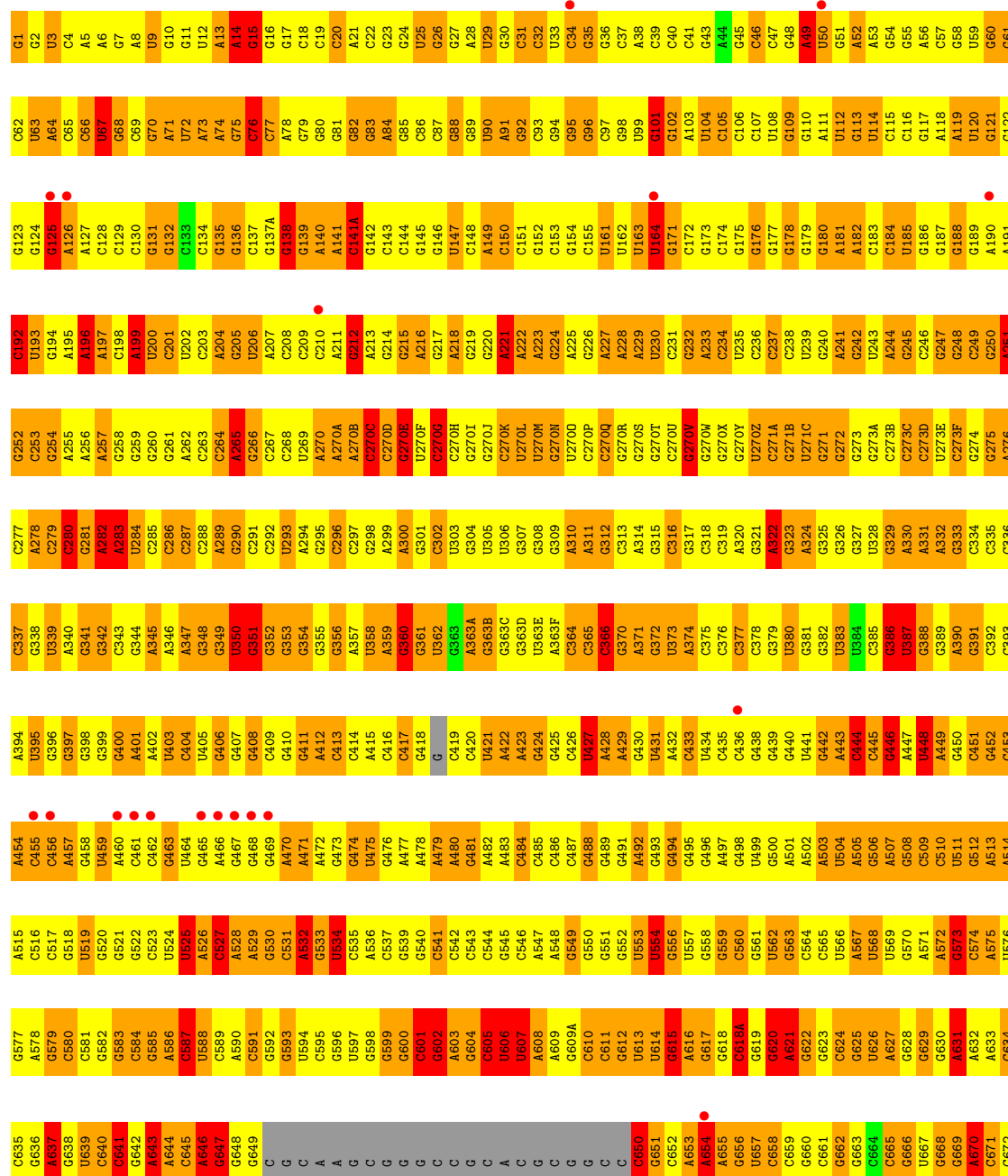
- Molecule 23: 30S ribosomal protein Thx

Chain AX:



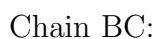
- Molecule 24: 23S ribosomal RNA

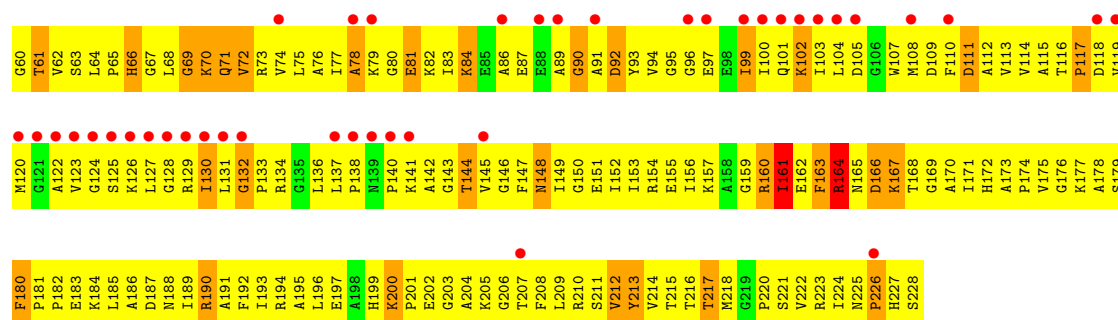
Chain BA:



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G1456	U1396	U1396	A1336	A1276	G1215	G1154	A1095	U1035	G975	C915	G854	G794	A734	G674
A1457	U1397	C1397	G1337	G1277	G1216	A1155	A1096	G1036	C976	C916	G855	C795	A735	A675
C1458	C1398	C1398	G1338	A1278	C1217	A1156	U1097	G1037	G977	A917	C856	C796	C736	A676
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G1461	G1401	G1401	U1341	G1282	C1221	U1159	C1100	C1040	A980	G920	G859	G799	G739	C679
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G1475	G1415	G1295	G1355	G1295	G1235	A1174	G1114	G1054	C994	C935	A873	U813	C753	C693
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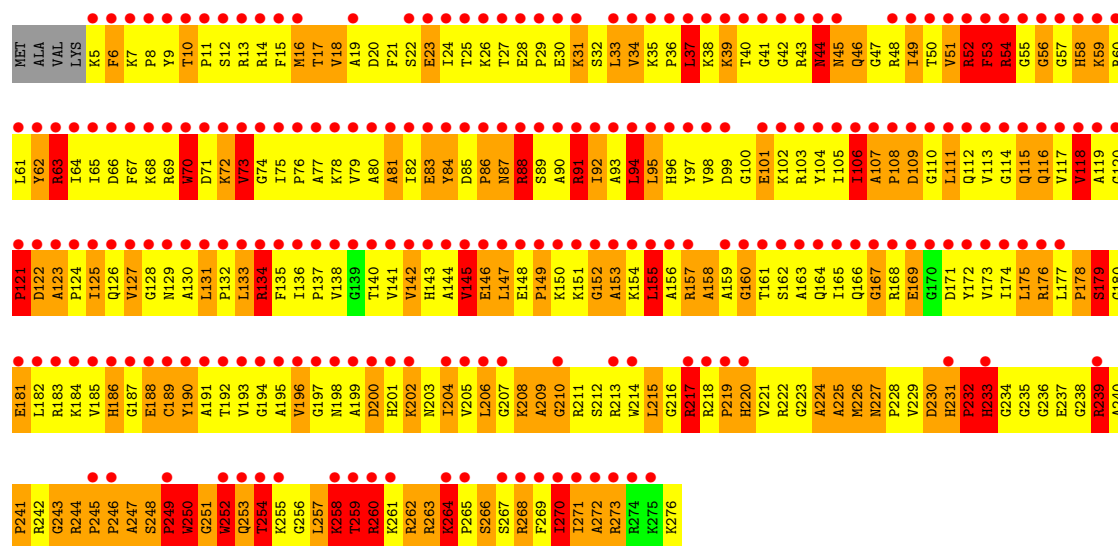
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U2079	U2080	U2081	U2082	U2083	U2084	U2085	U2086	U2087	U2088	U2089	U2090	U2091	U2092	U2093	G2094	G2095	U2096	U2097	U2098	U2099	U2100	U2101	U2102	U2103	C2104	C2105	C2106	U2107	U2108	U2109	U2110	C2111	C2112	U2113	U2114	C2115	C2116	U2117	U2118	C2119	C2120	C2121	U2122	C2123	C2124	C2125	C2126	U2127	U2128	C2129	U2130	C2131	U2132	C2133	C2134	U2135	C2136	U2137	C2138	U2139																									
A2019	A2020	C2021	G2022	G2023	G2024	G2025	C2026	G2027	G2028	G2029	A2030	A2031	G2032	A2033	G2034	G2035	C2036	G2037	G2038	A2039	C2040	U2041	U2042	C2043	C2044	C2045	C2046	U2047	G2048	G2049	C2050	G2051	G2052	C2053	A2054	C2055	C2056	G2057	A2058	C2059	A2060	C2061	C2062	C2063	C2064	C2065	C2066	G2067	U2068	G2069	G2070	C2071	C2072	C2073	U2074	U2075	C2076	C2077	C2078																										
G1959	G1960	C1961	G1962	C1963	G1964	G1965	A1966	G1967	G1968	A1969	C1970	C1971	G1972	G1973	C1974	G1975	U1976	A1977	G1978	C1979	G1980	C1981	C1982	G1983	G1984	G1985	C1986	G1987	C1988	G1989	C1990	U1991	G1992	U1993	C1994	U1995	G1996	G1997	G1998	C1999	G2000	A2001	C2002	G2003	C2004	A2005	C2006	C2007	G2008	G2009	G2010	U2011	C2012	A2013	C2014	A2015	U2016	U2017	C2018	C2019																									
H1899	A1900	C1901	G1902	C1903	G1904	C1905	G1906	C1907	G1908	C1909	C1910	C1911	A1912	C1913	C1914	C1915	A1916	C1917	A1918	C1919	C1920	C1921	C1922	C1923	G1924	C1925	U1926	C1927	C1928	C1929	C1930	C1931	C1932	G1933	C1934	C1935	A1936	A1937	C1938	C1939	U1940	C1941	C1942	U1943	C1944	C1945	U1946	C1947	G1948	G1949	C1950	C1951	C1952	C1953	G1954	C1955	U1956	C1957	C1958																										
C1830	C1831	C1832	U1833	C1834	G1835	C1836	C1837	C1838	G1839	C1840	U1841	C1842	C1843	C1844	G1845	C1846	C1847	C1848	A1849	C1850	C1851	C1852	C1853	C1854	G1855	C1856	G1857	C1858	C1859	C1860	C1861	C1862	C1863	C1864	C1865	C1866	C1867	C1868	C1869	C1870	C1871	C1872	C1873	C1874	C1875	C1876	C1877	C1878	C1879	C1880	C1881	C1882	C1883	C1884	C1885	C1886	C1887	C1888	C1889	C1890	C1891	C1892	C1893	C1894	C1895	C1896	C1897	C1898																	
G1770	C1771	C1772	C1773	C1774	U1775	G1776	U1777	C1778	U1779	C1780	C1781	C1782	C1783	C1784	C1785	C1786	C1787	C1788	C1789	C1790	C1791	C1792	C1793	C1794	G1795	U1796	C1797	U1798	C1799	C1800	C1801	A1802	C1803	C1804	U1805	C1806	C1807	C1808	C1809	C1810	C1811	C1812	C1813	C1814	C1815	C1816	C1817	C1818	C1819	U1820	C1821	C1822	C1823	C1824	C1825	C1826	C1827	C1828	C1829																										
C1684	C1685	C1686	C1687	C1688	C1689	C1690	C1691	C1692	C1693	C1694	C1695	C1696	C1697	C1698	C1699	C1700	C1701	C1702	C1703	C1704	C1705	C1706	C1707	C1708	C1709	C1710	C1711	C1712	C1713	C1714	C1715	C1716	C1717	C1718	C1719	C1720	C1721	C1722	C1723	C1724	C1725	C1726	C1727	C1728	C1729	C1730	C1731	C1732	C1733	C1734	C1735	C1736	C1737	C1738	C1739	C1740	C1741	C1742	C1743	C1744	C1745	C1746	C1747	C1748	C1749	C1750	C1751	C1752	C1753	C1754	C1755	C1756	C1757	C1758	C1759	C1760	C1761	C1762	C1763	C1764	C1765	C1766	C1767	C1768	C1769
A1634	C1635	C1636	C1637	C1638	C1639	C1640	C1641	C1642	C1643	C1644	C1645	C1646	C1647	C1648	C1649	C1650	C1651	C1652	C1653	C1654	C1655	C1656	C1657	C1658	C1659	C1660	C1661	C1662	C1663	C1664	C1665	C1666	C1667	C1668	C1669	C1670	C1671	C1672	C1673	C1674	C1675	C1676	C1677	C1678	C1679	C1680	C1681	C1682	C1683	C1684	C1685	C1686	C1687	C1688	C1689	C1690	C1691	C1692	C1693	C1694	C1695	C1696	C1697	C1698	C1699																				
C1574	C1575	C1576	C1577	C1578	C1579	C1580	C1581	C1582	C1583	C1584	C1585	C1586	C1587	C1588	C1589	C1590	C1591	C1592	C1593	C1594	C1595	C1596	C1597	C1598	C1599	C1600	C1601	C1602	C1603	C1604	C1605	C1606	C1607	C1608	C1609	C1610	C1611	C1612	C1613	C1614	C1615	C1616	C1617	C1618	C1619	C1620	C1621	C1622	C1623	C1624	C1625	C1626	C1627	C1628	C1629	C1630	C1631	C1632	C1633	C1634	C1635	C1636	C1637	C1638	C1639																				
C1515	C1516	C1517	C1518	C1519	C1520	C1521	C1522	C1523	C1524	C1525	C1526	C1527	C1528	C1529	C1530	C1531	C1532	C1533	C1534	C1535	C1536	C1537	C1538	C1539	C1540	C1541	C1542	C1543	C1544	C1545	C1546	C1547	C1548	C1549	C1550	C1551	C1552	C1553	C1554	C1555	C1556	C1557	C1558	C1559	C1560	C1561	C1562	C1563	C1564	C1565	C1566	C1567	C1568	C1569	C1570	C1571	C1572	C1573																											





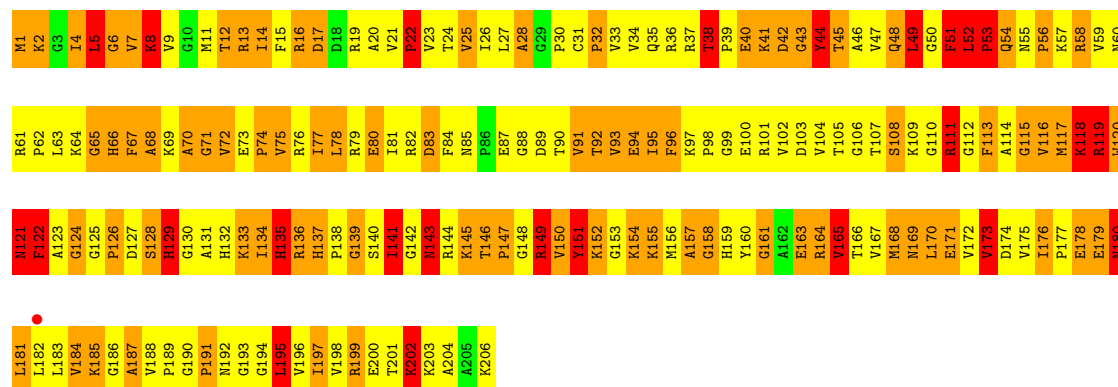
• Molecule 27: 50S ribosomal protein L2

Chain BD:



• Molecule 28: 50S ribosomal protein L3

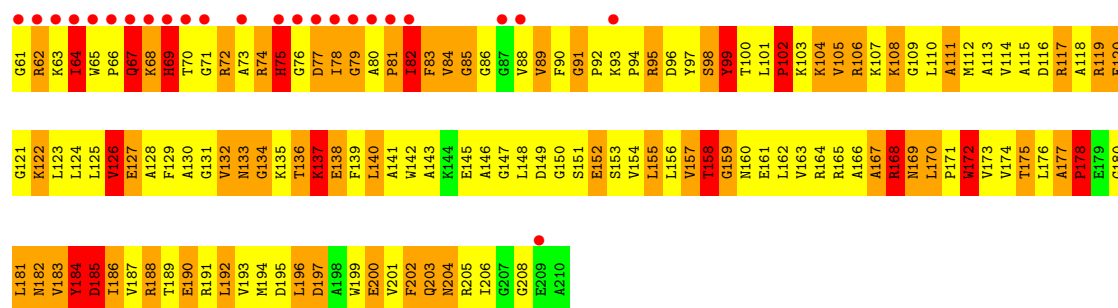
Chain BE:



• Molecule 29: 50S ribosomal protein L4

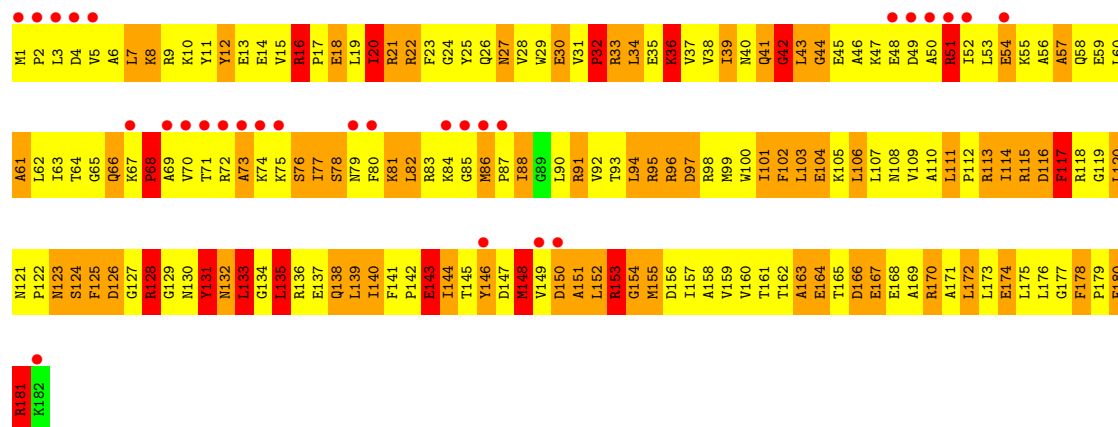
Chain BF:





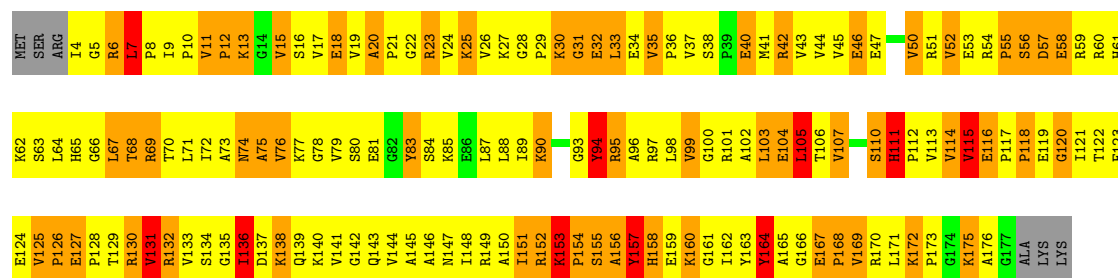
• Molecule 30: 50S ribosomal protein L5

Chain BG:



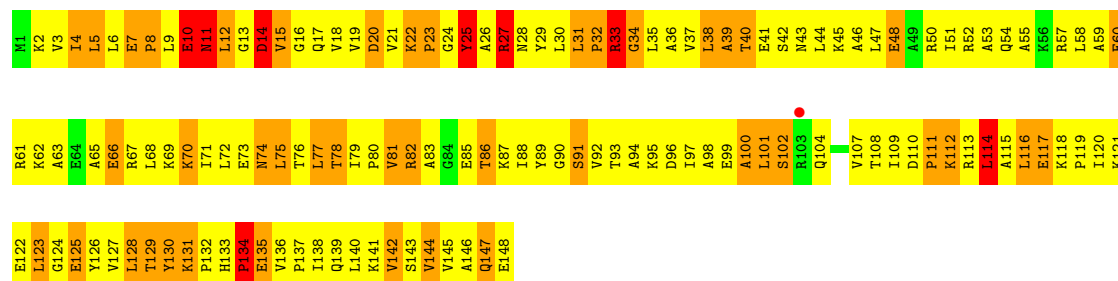
• Molecule 31: 50S ribosomal protein L6

Chain BH:



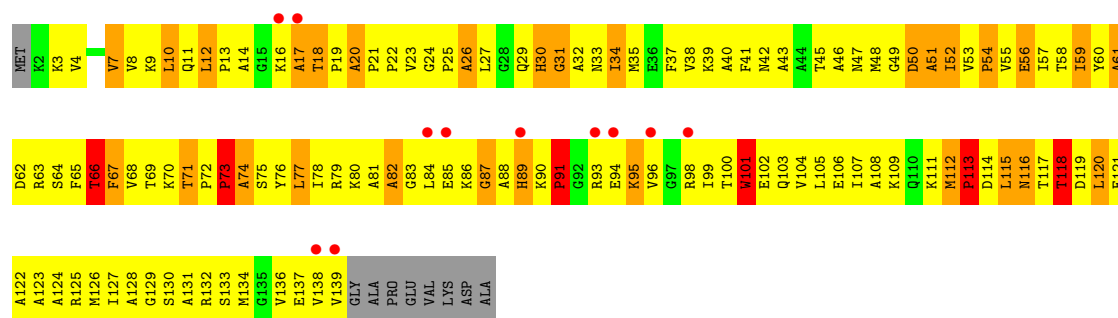
• Molecule 32: 50S ribosomal protein L9

Chain BK:



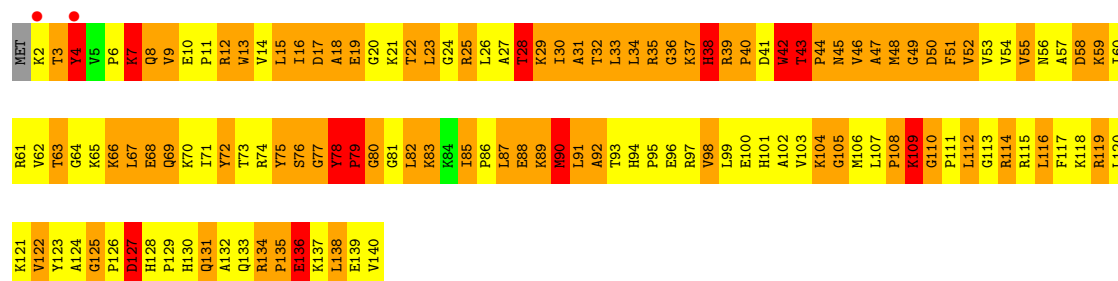
- Molecule 33: 50S ribosomal protein L11

Chain BL:



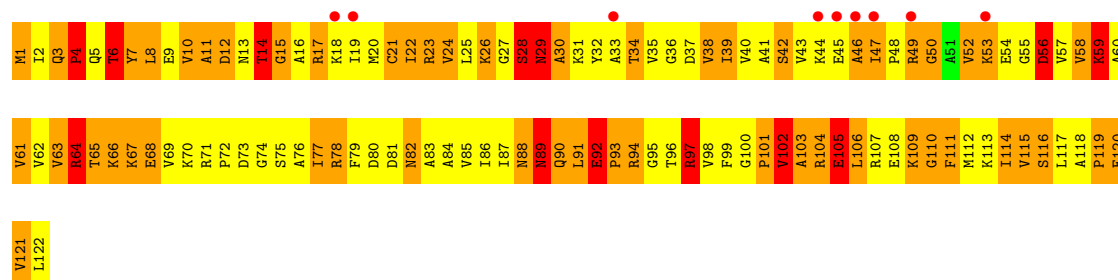
- Molecule 34: 50S ribosomal protein L13

Chain BM:



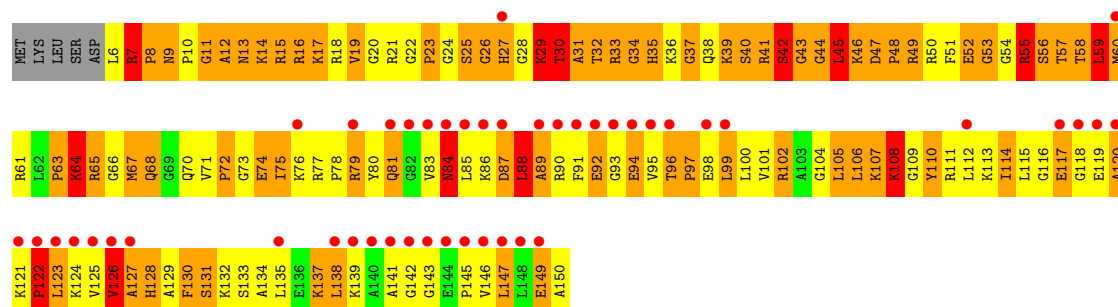
- Molecule 35: 50S ribosomal protein L14

Chain BN:



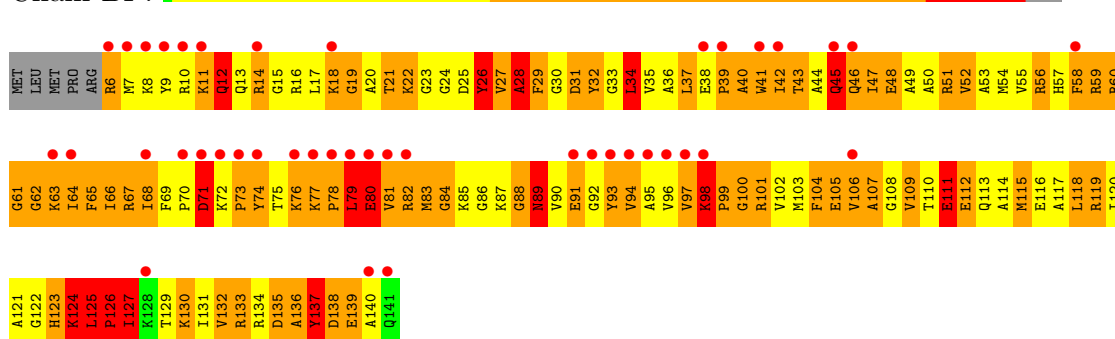
- Molecule 36: 50S ribosomal protein L15

Chain BO:



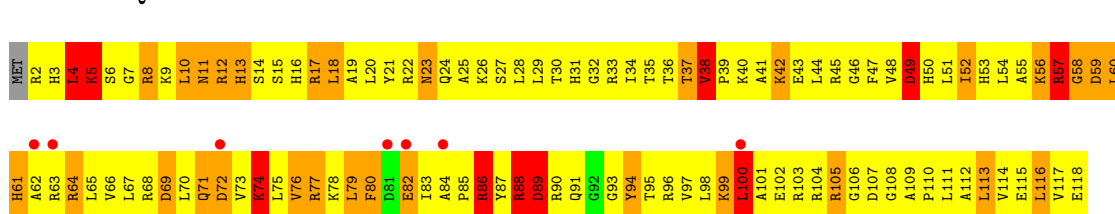
- Molecule 37: 50S ribosomal protein L16

Chain BP:



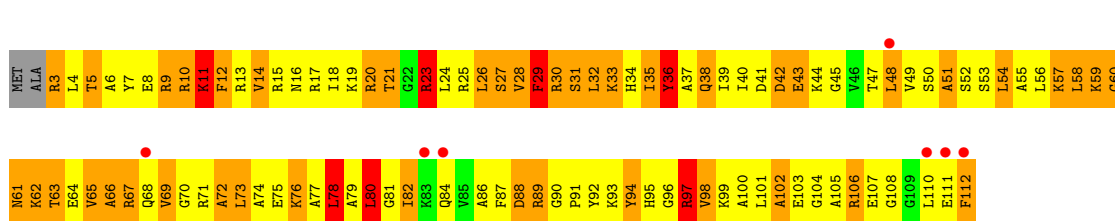
- Molecule 38: 50S ribosomal protein L17

Chain BQ:



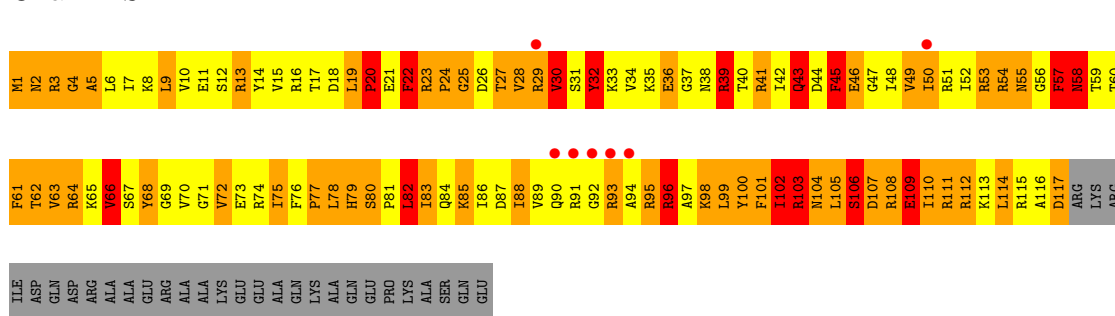
- Molecule 39: 50S ribosomal protein L18

Chain BR:



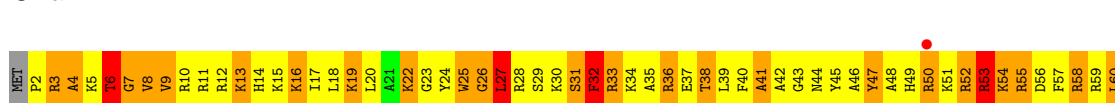
- Molecule 40: 50S ribosomal protein L19

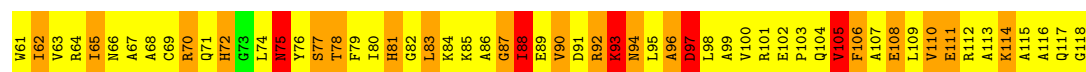
Chain BS:



- Molecule 41: 50S ribosomal protein L20

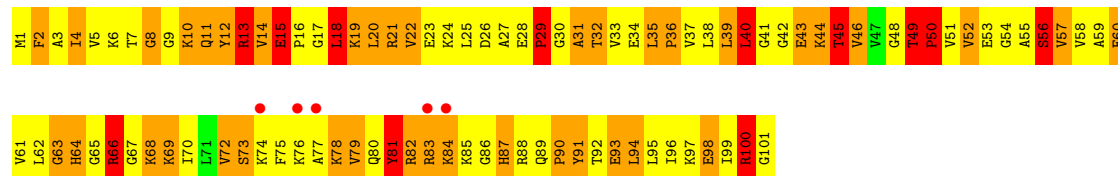
Chain BT:





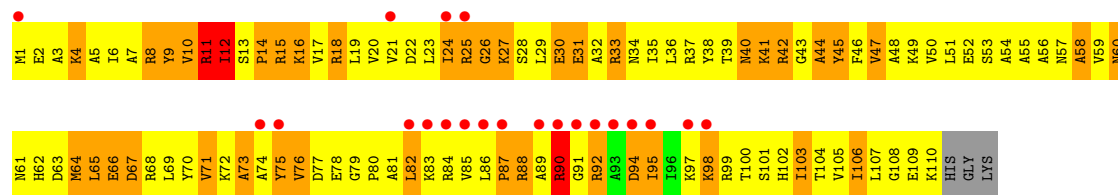
• Molecule 42: 50S ribosomal protein L21

Chain BU:



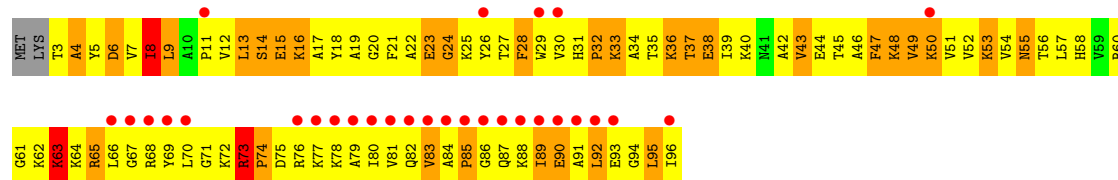
• Molecule 43: 50S ribosomal protein L22

Chain BV:



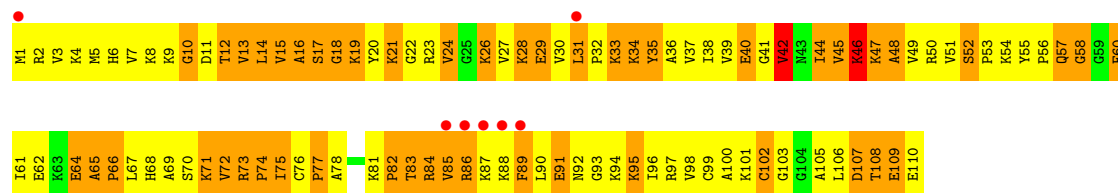
• Molecule 44: 50S ribosomal protein L23

Chain BW:



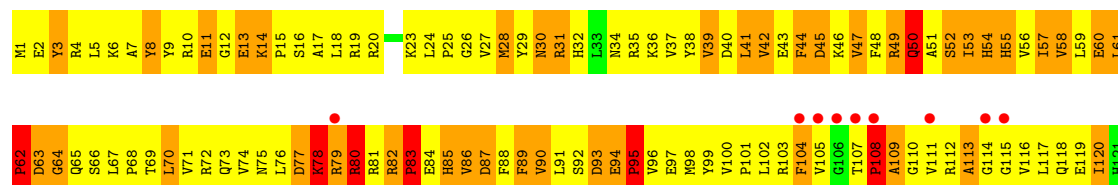
• Molecule 45: 50S ribosomal protein L24

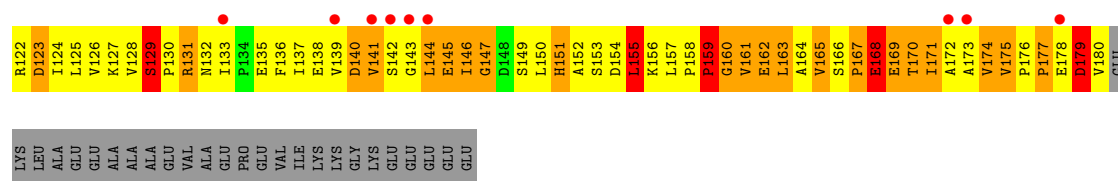
Chain BX:



• Molecule 46: 50S ribosomal protein L25

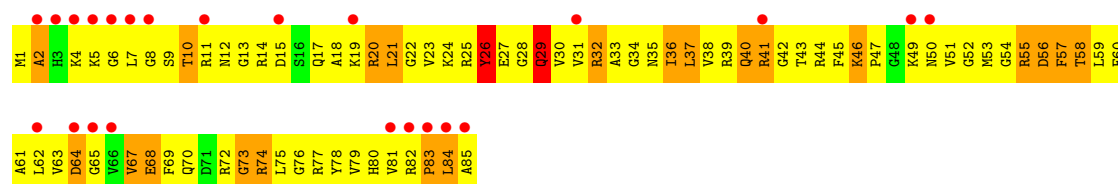
Chain BY:





• Molecule 47: Ribosomal protein L27

Chain BZ:



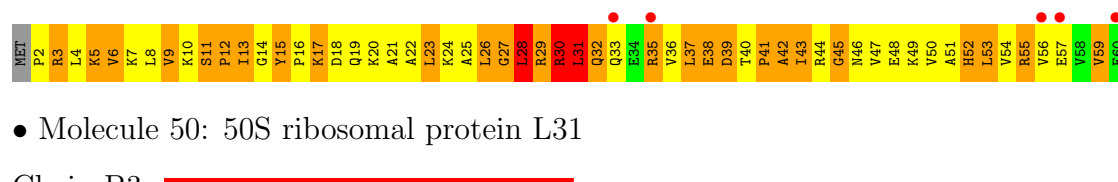
• Molecule 48: 50S ribosomal protein L29

Chain B1:



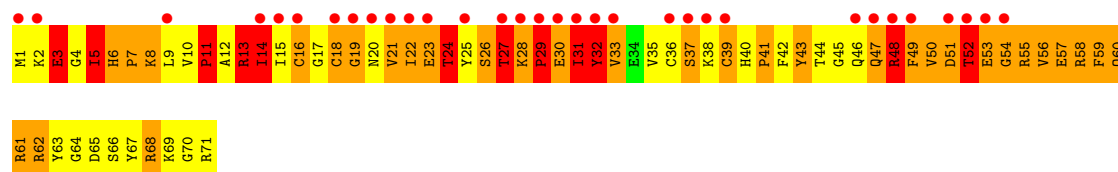
• Molecule 49: 50S ribosomal protein L30

Chain B2:



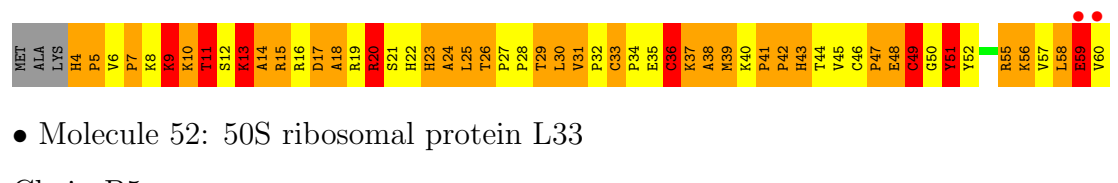
• Molecule 50: 50S ribosomal protein L31

Chain B3:



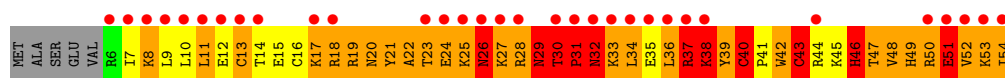
• Molecule 51: 50S ribosomal protein L32

Chain B4:



• Molecule 52: 50S ribosomal protein L33

Chain B5:



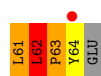
- Molecule 53: 50S ribosomal protein L34

Chain B6:



- Molecule 54: 50S ribosomal protein L35

Chain B7:



- Molecule 55: 50S ribosomal protein L36

Chain B8:



4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 4.88Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.243 , 0.326 0.306 , 0.344	Depositor DCC
R_{free} test set	7981 reflections (4.99%)	DCC
Wilson B-factor (Å ²)	108.9	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.07 , 22.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Outliers	1 of 226745 reflections (0.000%)	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	151691	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

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

Continued on next page...

Continued from previous page...

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	BM	1113	0	1183	782	0
35	BN	932	0	994	712	0
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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 183.

The worst 5 of 46416 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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	Distance(Å)	Clash(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	2
7	AH	148/162 (91%)	93 (63%)	38 (26%)	17 (12%)	1	15
8	AI	99/101 (98%)	58 (59%)	19 (19%)	22 (22%)	0	3
9	AJ	153/156 (98%)	73 (48%)	45 (29%)	35 (23%)	0	3
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	3
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	4
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	2
16	AQ	58/61 (95%)	24 (41%)	16 (28%)	18 (31%)	0	1
17	AR	86/89 (97%)	36 (42%)	35 (41%)	15 (17%)	0	6
18	AS	81/88 (92%)	42 (52%)	24 (30%)	15 (18%)	0	5
19	AT	102/105 (97%)	62 (61%)	23 (22%)	17 (17%)	0	7
20	AU	71/88 (81%)	26 (37%)	26 (37%)	19 (27%)	0	2
21	AV	78/93 (84%)	32 (41%)	23 (30%)	23 (30%)	0	1
22	AW	97/106 (92%)	38 (39%)	32 (33%)	27 (28%)	0	1
23	AX	22/27 (82%)	9 (41%)	6 (27%)	7 (32%)	0	1
26	BC	226/229 (99%)	155 (69%)	41 (18%)	30 (13%)	0	12
27	BD	270/276 (98%)	125 (46%)	59 (22%)	86 (32%)	0	1
28	BE	204/206 (99%)	117 (57%)	31 (15%)	56 (28%)	0	1
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	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	BH	172/180 (96%)	80 (46%)	46 (27%)	46 (27%)	0	2
32	BK	146/148 (99%)	91 (62%)	30 (20%)	25 (17%)	0	6
33	BL	136/147 (92%)	69 (51%)	38 (28%)	29 (21%)	0	4
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	1
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	7
39	BR	108/112 (96%)	48 (44%)	29 (27%)	31 (29%)	0	1
40	BS	115/146 (79%)	52 (45%)	26 (23%)	37 (32%)	0	1
41	BT	115/118 (98%)	35 (30%)	50 (44%)	30 (26%)	0	2
42	BU	99/101 (98%)	52 (52%)	19 (19%)	28 (28%)	0	1
43	BV	108/113 (96%)	63 (58%)	24 (22%)	21 (19%)	0	5
44	BW	92/96 (96%)	57 (62%)	16 (17%)	19 (21%)	0	4
45	BX	108/110 (98%)	43 (40%)	32 (30%)	33 (31%)	0	1
46	BY	178/206 (86%)	95 (53%)	44 (25%)	39 (22%)	0	3
47	BZ	83/85 (98%)	52 (63%)	21 (25%)	10 (12%)	1	14
48	B1	65/67 (97%)	36 (55%)	20 (31%)	9 (14%)	0	11
49	B2	57/60 (95%)	34 (60%)	8 (14%)	15 (26%)	0	2
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	1
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	1
All	All	5988/6337 (94%)	2955 (49%)	1476 (25%)	1557 (26%)	0	2

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	4
5	AF	160/188 (85%)	123 (77%)	37 (23%)	1	9
6	AG	180/181 (99%)	131 (73%)	49 (27%)	0	6
7	AH	115/123 (94%)	78 (68%)	37 (32%)	0	4
8	AI	90/90 (100%)	61 (68%)	29 (32%)	0	4
9	AJ	126/127 (99%)	93 (74%)	33 (26%)	1	7
10	AK	119/119 (100%)	86 (72%)	33 (28%)	0	6
11	AL	98/99 (99%)	73 (74%)	25 (26%)	1	8
12	AM	88/92 (96%)	67 (76%)	21 (24%)	1	9
13	AN	90/99 (91%)	74 (82%)	16 (18%)	2	19
14	AO	104/109 (95%)	81 (78%)	23 (22%)	1	11
15	AP	100/101 (99%)	75 (75%)	25 (25%)	1	8
16	AQ	49/50 (98%)	36 (74%)	13 (26%)	1	7
17	AR	79/80 (99%)	64 (81%)	15 (19%)	2	16
18	AS	72/74 (97%)	49 (68%)	23 (32%)	0	4
19	AT	96/97 (99%)	67 (70%)	29 (30%)	0	5
20	AU	64/77 (83%)	48 (75%)	16 (25%)	1	8
21	AV	71/80 (89%)	55 (78%)	16 (22%)	1	10
22	AW	76/82 (93%)	59 (78%)	17 (22%)	1	11
23	AX	19/22 (86%)	17 (90%)	2 (10%)	10	47
26	BC	180/181 (99%)	151 (84%)	29 (16%)	3	26
27	BD	215/218 (99%)	153 (71%)	62 (29%)	0	5
28	BE	166/166 (100%)	102 (61%)	64 (39%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	BF	164/166 (99%)	105 (64%)	59 (36%)	0	2
30	BG	156/156 (100%)	112 (72%)	44 (28%)	0	5
31	BH	143/148 (97%)	109 (76%)	34 (24%)	1	9
32	BK	124/124 (100%)	92 (74%)	32 (26%)	1	7
33	BL	105/111 (95%)	89 (85%)	16 (15%)	4	28
34	BM	118/119 (99%)	79 (67%)	39 (33%)	0	3
35	BN	100/100 (100%)	69 (69%)	31 (31%)	0	4
36	BO	111/116 (96%)	71 (64%)	40 (36%)	0	2
37	BP	106/111 (96%)	65 (61%)	41 (39%)	0	1
38	BQ	100/101 (99%)	71 (71%)	29 (29%)	0	5
39	BR	87/88 (99%)	63 (72%)	24 (28%)	0	6
40	BS	105/127 (83%)	68 (65%)	37 (35%)	0	2
41	BT	93/94 (99%)	64 (69%)	29 (31%)	0	4
42	BU	82/82 (100%)	57 (70%)	25 (30%)	0	5
43	BV	90/92 (98%)	64 (71%)	26 (29%)	0	5
44	BW	76/78 (97%)	57 (75%)	19 (25%)	1	8
45	BX	91/91 (100%)	72 (79%)	19 (21%)	1	12
46	BY	159/179 (89%)	120 (76%)	39 (24%)	1	8
47	BZ	67/67 (100%)	51 (76%)	16 (24%)	1	9
48	B1	62/62 (100%)	44 (71%)	18 (29%)	0	5
49	B2	51/52 (98%)	36 (71%)	15 (29%)	0	5
50	B3	63/63 (100%)	45 (71%)	18 (29%)	0	5
51	B4	50/52 (96%)	31 (62%)	19 (38%)	0	1
52	B5	48/52 (92%)	32 (67%)	16 (33%)	0	3
53	B6	42/42 (100%)	29 (69%)	13 (31%)	0	4
54	B7	54/55 (98%)	44 (82%)	10 (18%)	2	17
55	B8	34/34 (100%)	29 (85%)	5 (15%)	4	30
All	All	5040/5237 (96%)	3649 (72%)	1391 (28%)	0	6

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

Mol	Chain	Res	Type
28	BE	45	THR

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Mol	Chain	Res	Type
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 ⓘ

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 ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
24	BA	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1515/1522 (99%)	-0.21	16 (1%) 77 65	145, 221, 302, 356	0
2	A1	50/50 (100%)	1.67	12 (24%) 1 4	200, 320, 348, 357	0
3	AB	76/76 (100%)	18.41	70 (92%) 0 2	288, 351, 370, 374	0
3	AC	76/76 (100%)	1.12	22 (28%) 1 4	167, 214, 260, 284	0
3	AD	76/76 (100%)	0.63	11 (14%) 3 8	222, 271, 293, 316	0
4	AE	234/256 (91%)	-0.15	2 (0%) 81 70	189, 226, 271, 304	0
5	AF	206/239 (86%)	0.44	20 (9%) 8 15	222, 244, 266, 277	0
6	AG	208/209 (99%)	0.36	26 (12%) 5 11	168, 215, 233, 242	0
7	AH	150/162 (92%)	0.04	3 (2%) 62 51	174, 210, 235, 257	0
8	AI	101/101 (100%)	2.51	58 (57%) 0 3	191, 223, 236, 261	0
9	AJ	155/156 (99%)	1.39	47 (30%) 1 4	210, 240, 256, 275	0
10	AK	138/138 (100%)	-0.42	0 100 100	186, 208, 225, 232	0
11	AL	127/128 (99%)	-0.49	0 100 100	222, 261, 276, 287	0
12	AM	98/105 (93%)	0.16	3 (3%) 47 41	230, 260, 274, 282	0
13	AN	119/129 (92%)	1.57	36 (30%) 1 4	193, 212, 245, 267	0
14	AO	124/132 (93%)	1.56	38 (30%) 1 4	179, 199, 233, 267	0
15	AP	125/126 (99%)	0.07	6 (4%) 29 30	223, 243, 272, 278	0
16	AQ	60/61 (98%)	0.11	3 (5%) 28 29	215, 248, 259, 263	0
17	AR	88/89 (98%)	0.29	7 (7%) 12 19	186, 207, 231, 238	0
18	AS	83/88 (94%)	-0.05	2 (2%) 56 47	180, 201, 226, 249	0
19	AT	104/105 (99%)	0.65	13 (12%) 5 11	164, 193, 244, 277	0
20	AU	73/88 (82%)	0.18	10 (13%) 4 9	184, 209, 258, 287	0
21	AV	80/93 (86%)	0.66	15 (18%) 2 6	226, 252, 266, 270	0
22	AW	99/106 (93%)	1.08	29 (29%) 1 4	167, 195, 225, 241	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
23	AX	24/27 (88%)	-0.42	0 100 100	230, 249, 280, 288	0
24	BA	2889/2916 (99%)	-0.10	204 (7%) 16 21	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%)	1.23	44 (19%) 2 5	250, 281, 300, 313	0
27	BD	272/276 (98%)	4.12	222 (81%) 0 2	130, 199, 221, 259	0
28	BE	206/206 (100%)	-0.15	1 (0%) 88 80	148, 186, 232, 269	0
29	BF	208/210 (99%)	0.35	24 (11%) 5 12	164, 238, 263, 276	0
30	BG	182/182 (100%)	0.72	29 (15%) 3 8	212, 246, 268, 276	0
31	BH	174/180 (96%)	-0.38	0 100 100	196, 241, 260, 271	0
32	BK	148/148 (100%)	-0.20	1 (0%) 84 74	202, 227, 249, 257	0
33	BL	138/147 (93%)	0.20	11 (7%) 12 19	271, 298, 312, 327	0
34	BM	139/140 (99%)	-0.13	2 (1%) 72 60	167, 198, 224, 235	0
35	BN	122/122 (100%)	0.60	9 (7%) 14 21	148, 177, 209, 221	0
36	BO	145/150 (96%)	1.81	46 (31%) 1 4	166, 247, 276, 315	0
37	BP	136/141 (96%)	1.45	42 (30%) 1 4	166, 208, 234, 241	0
38	BQ	117/118 (99%)	0.38	7 (5%) 21 25	168, 192, 219, 226	0
39	BR	110/112 (98%)	0.45	7 (6%) 19 24	186, 235, 263, 289	0
40	BS	117/146 (80%)	0.49	7 (5%) 21 25	164, 194, 227, 242	0
41	BT	117/118 (99%)	-0.03	1 (0%) 81 70	183, 202, 220, 232	0
42	BU	101/101 (100%)	0.08	5 (4%) 28 29	168, 225, 246, 257	0
43	BV	110/113 (97%)	0.89	21 (19%) 2 5	180, 209, 237, 248	0
44	BW	94/96 (97%)	1.48	29 (30%) 1 4	212, 232, 280, 288	0
45	BX	110/110 (100%)	-0.08	7 (6%) 19 24	221, 255, 287, 305	0
46	BY	180/206 (87%)	0.47	18 (10%) 8 15	208, 246, 268, 279	0
47	BZ	85/85 (100%)	1.65	23 (27%) 1 4	211, 229, 242, 271	0
48	B1	67/67 (100%)	0.14	1 (1%) 70 58	218, 243, 263, 268	0
49	B2	59/60 (98%)	0.50	5 (8%) 11 18	204, 224, 249, 259	0
50	B3	71/71 (100%)	1.85	32 (45%) 1 3	199, 223, 238, 246	0
51	B4	57/60 (95%)	0.20	2 (3%) 42 38	164, 209, 264, 289	0
52	B5	49/54 (90%)	3.22	32 (65%) 0 3	206, 232, 242, 252	0
53	B6	49/49 (100%)	3.27	38 (77%) 0 2	162, 209, 221, 235	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
54	B7	64/65 (98%)	1.60	21 (32%) 1 4	164, 195, 225, 242	0
55	B8	37/37 (100%)	-0.53	0 100 100	205, 215, 224, 226	0
All	All	10893/11176 (97%)	0.49	1340 (12%) 5 11	129, 223, 295, 374	0

The worst 5 of 1340 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	AB	4	C	43.7
3	AB	3	C	43.3
3	AB	67	C	42.5
3	AB	2	C	42.1
3	AB	5	G	40.1

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.