



wwPDB X-ray Structure Validation Summary Report ⓘ

May 21, 2020 – 05:09 pm BST

PDB ID : 2ZJQ
Title : Interaction of L7 with L11 induced by Micrococin binding to the Deinococcus radiodurans 50S subunit
Authors : Harms, J.M.; Wilson, D.N.; Schlutzen, F.; Connell, S.R.; Stachelhaus, T.; Zaborowska, Z.; Spahn, C.M.T.; Fucini, P.
Deposited on : 2008-03-08
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

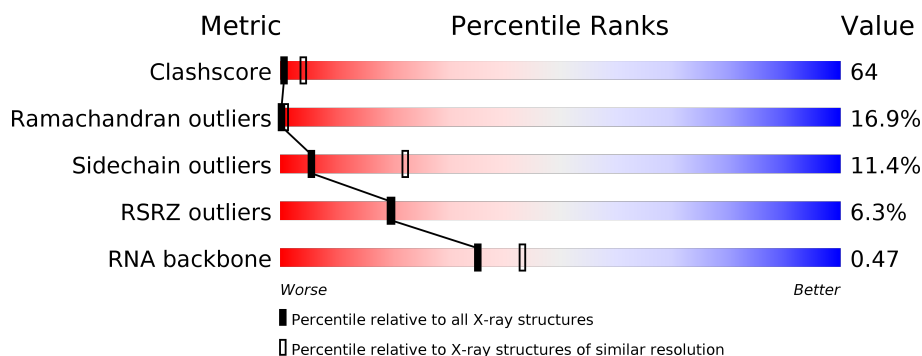
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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.



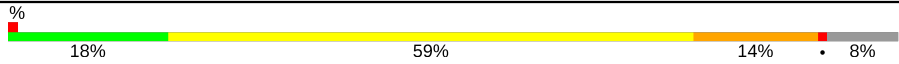

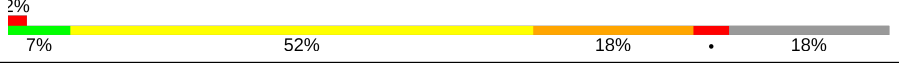
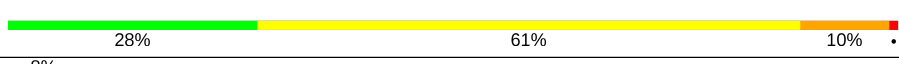
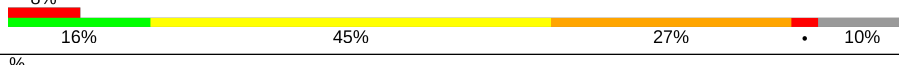
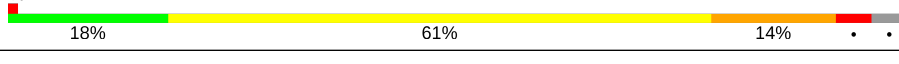
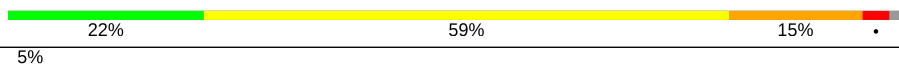


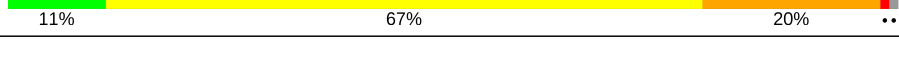

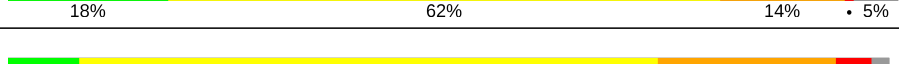
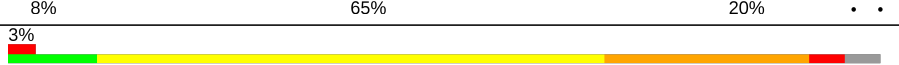
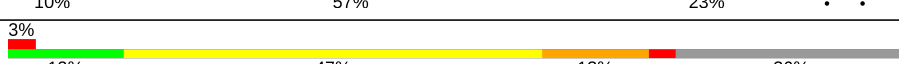

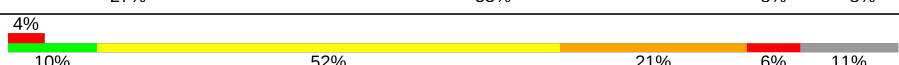
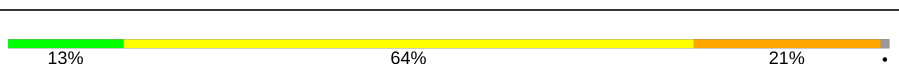
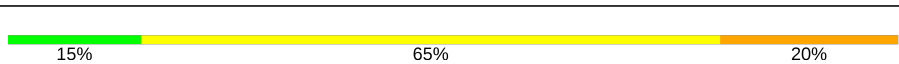
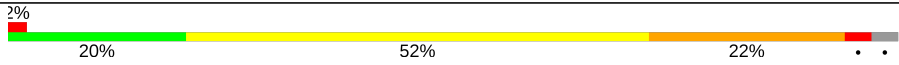
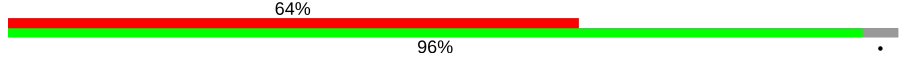
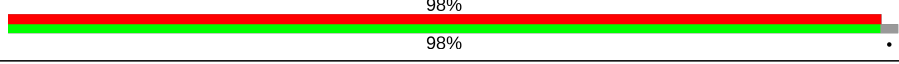
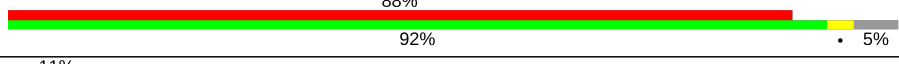
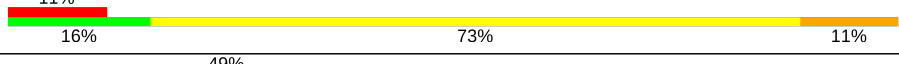
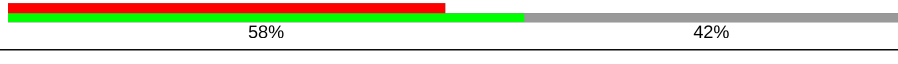

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)
RNA backbone	3102	1117 (3.70-2.90)

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

Mol	Chain	Length	Quality of chain
1	X	2880	<div> <div>%</div> <div> <div></div> <div>11%</div> <div>50%</div> <div>23%</div> <div>10%</div> <div>7%</div> </div> </div>
2	Y	122	<div> <div>2%</div> <div> <div></div> <div>16%</div> <div>69%</div> <div>14%</div> </div> <div>.</div> </div>
3	A	274	<div> <div>2%</div> <div> <div></div> <div>19%</div> <div>55%</div> <div>14%</div> <div>12%</div> </div> </div>
4	B	211	<div> <div>%</div> <div> <div></div> <div>25%</div> <div>56%</div> <div>13%</div> </div> <div>.</div> </div>
5	C	205	<div> <div>%</div> <div> <div></div> <div>14%</div> <div>54%</div> <div>24%</div> <div>5%</div> </div> <div>.</div> </div>
6	D	180	<div> <div>3%</div> <div> <div></div> <div>9%</div> <div>71%</div> <div>16%</div> </div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
7	E	185	
8	F	144	
9	G	174	
10	H	134	
11	I	156	
12	J	142	
13	K	116	
14	L	114	
15	M	166	
16	N	118	
17	O	100	
18	P	134	
19	Q	95	
20	R	115	
21	S	237	
22	T	91	
23	U	81	
24	V	67	
25	W	55	
26	Z	60	
27	1	55	
28	2	47	
29	3	66	
30	4	37	
31	5	122	

2 Entry composition

There are 31 unique types of molecules in this entry. The entry contains 84395 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 ribosomal 23S RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	2686	Total	C	N	O	P	0	0	0
			57651	25718	10642	18606	2685			

- Molecule 2 is a RNA chain called ribosomal 5S RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Y	122	Total	C	N	O	P	0	0	0
			2598	1161	476	840	121			

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	240	Total	C	N	O	S	0	0	0
			1826	1137	366	321	2			

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	205	Total	C	N	O	S	0	0	0
			1539	965	295	271	8			

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	197	Total	C	N	O	S	0	0	0
			1506	935	287	282	2			

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	D	177	Total	C	N	O	S	0	0	0
			1400	892	247	254	7			

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	E	171	Total	C	N	O	S	0	0	0
			1286	812	237	236	1			

- Molecule 8 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	F	144	Total	C	N	O	S	0	0	0
			1043	663	179	196	5			

- Molecule 9 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	G	142	Total	C	N	O	S	0	0	0
			1114	704	209	198	3			

- Molecule 10 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	H	134	Total	C	N	O	S	0	0	0
			997	614	198	180	5			

- Molecule 11 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	I	141	Total	C	N	O	0	0	0
			1067	655	216	196			

- Molecule 12 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	J	136	Total	C	N	O	S	0	0	0
			1090	696	202	185	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	1	MET	-	INITIATING METHIONINE	UNP Q9RXJ5

- Molecule 13 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	K	113	Total	C	N	O	S	0	0	0
			878	541	178	157	2			

- Molecule 14 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	L	104	Total	C	N	O		0	0	0
			779	476	161	142				

- Molecule 15 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	M	108	Total	C	N	O		0	0	0
			871	543	172	156				

- Molecule 16 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	N	117	Total	C	N	O	S	0	0	0
			978	608	210	159	1			

- Molecule 17 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	O	94	Total	C	N	O		0	0	0
			741	465	139	137				

- Molecule 18 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	P	127	Total	C	N	O	S	0	0	0
			1014	639	199	174	2			

- Molecule 19 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Q	93	Total	C	N	O	S	0	0	0
			726	458	136	130	2			

- Molecule 20 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	R	110	Total	C	N	O	S	0	0	0
			825	513	160	151	1			

- Molecule 21 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	S	175	Total	C	N	O	S	0	0	0
			1345	849	236	254	6			

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	T	84	Total	C	N	O	S	0	0	0
			625	393	122	109	1			

- Molecule 23 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	U	72	Total	C	N	O	S	0	0	0
			552	341	116	95				

- Molecule 24 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	V	66	Total	C	N	O	S	0	0	0
			533	327	107	96	3			

- Molecule 25 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	W	55	Total	C	N	O	S	0	0	0
			424	264	82	76	2			

- Molecule 26 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Z	58	Total	C	N	O	S	0	0	0
			457	281	94	77	5			

- Molecule 27 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
27	1	53	Total C 53 53	0	0	53

- Molecule 28 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
28	2	46	Total C 46 46	0	0	46

- Molecule 29 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
29	3	63	Total C 63 63	0	0	63

- Molecule 30 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
30	4	37	Total C N O S 297 179 66 47 5	0	0	0

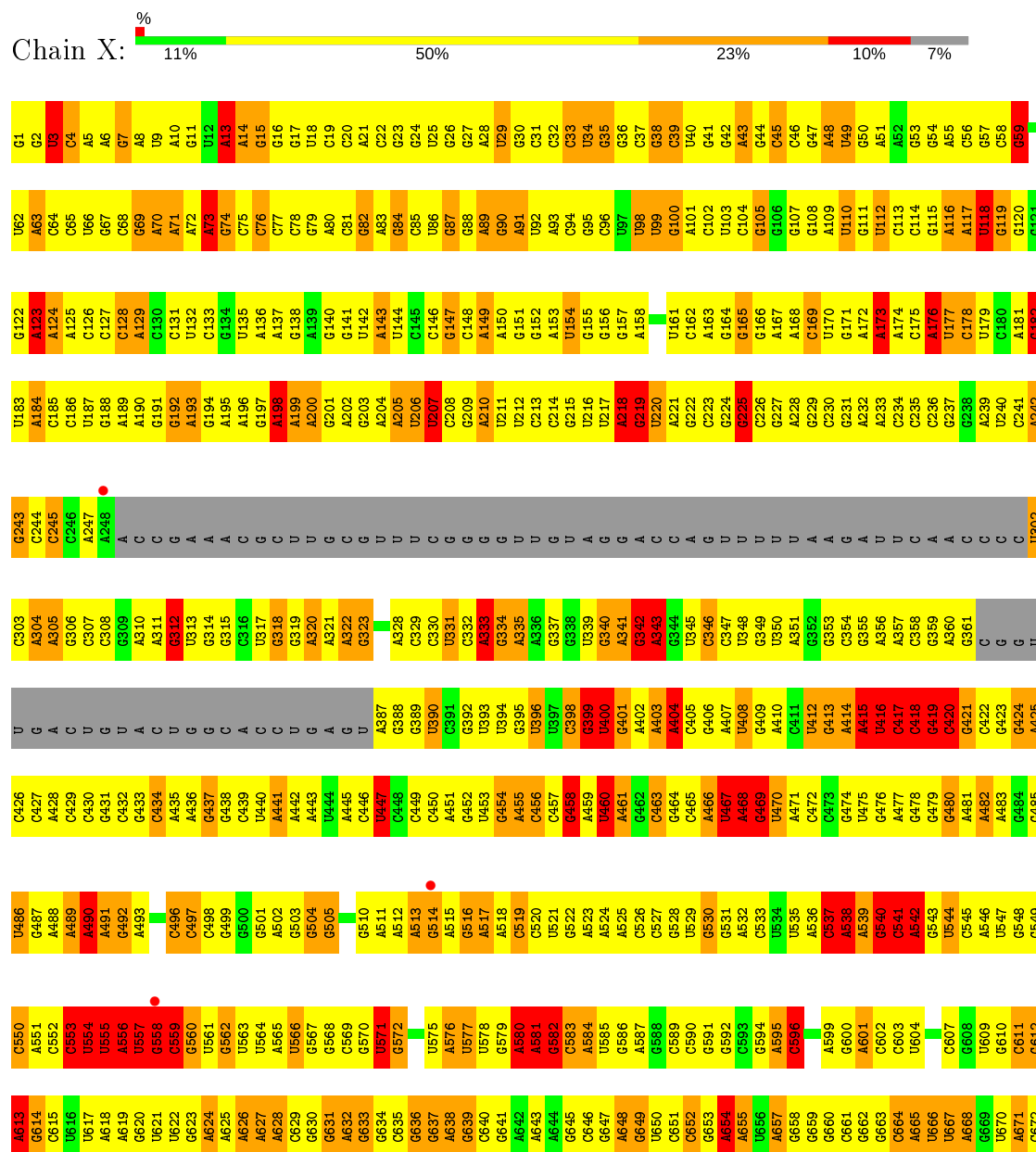
- Molecule 31 is a protein called 50S ribosomal protein L7/L12.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
31	5	71	Total C 71 71	0	0	71

3 Residue-property plots

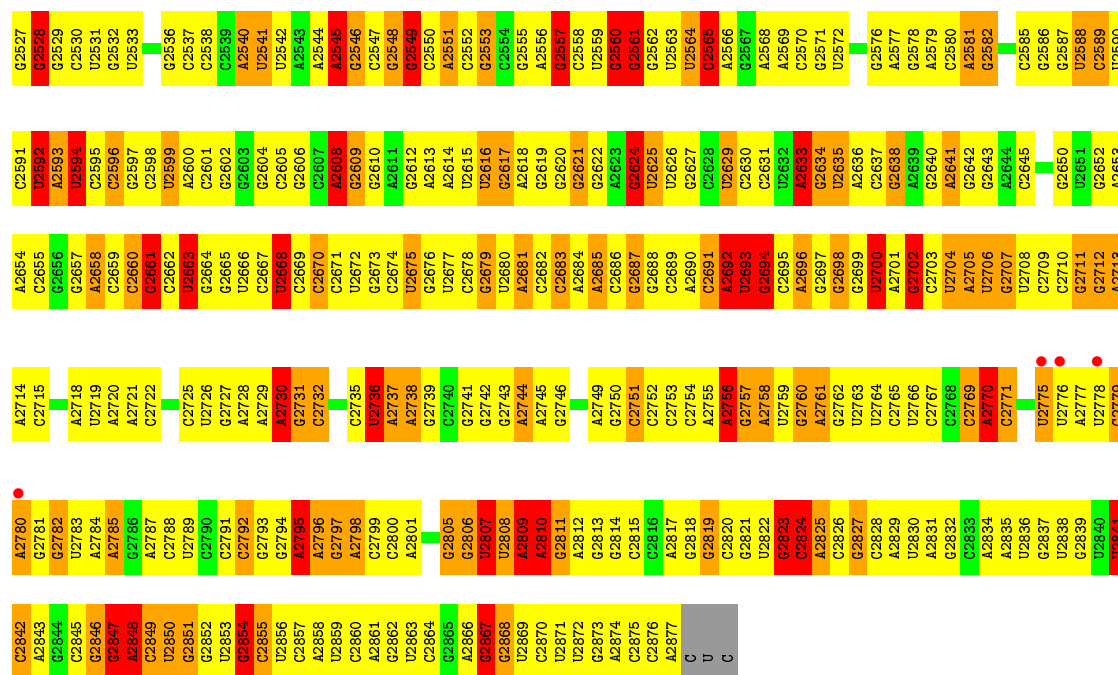
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

• Molecule 1: ribosomal 23S RNA

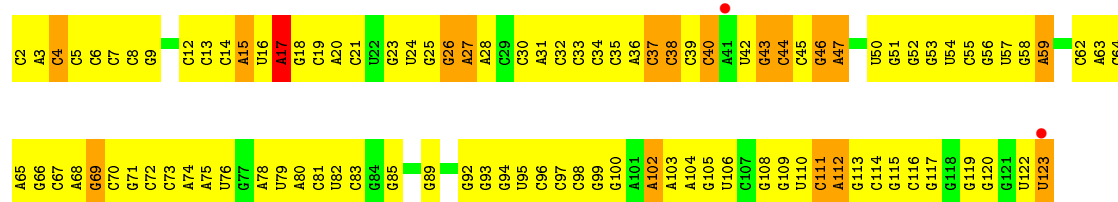


C1529	A1468	G1407	C1346	C1283	G1222	A1162	U1101	G1041	A979	G855	G793	G733	G673
U1530	U1469	A1408	C1347	G1284	G1223	C1163	G1102	G1042	G980	A856	A794	G734	U674
A1534	G1470	U1409	C1348	A1285	A1224	G1165	C1103	A1043	G981	U857	A795	G735	G675
C1535	G1471	U1410	C1349	U1286	G1166	G1166	C1104	U1044	C982	G858	A796	G736	G676
G1536	C1472	G1411	G1350	A1287	A1225	U1105	U1105	U1045	G983	U859	A797	G737	G677
U1537	G1473	G1412	G1351	A1288	A1226	A1167	A1106	U1046	A984	U860	G798	G738	G678
A1474	U1473	U1413	G1352	A1289	G1228	A1168	A1107	G1047	G985	C799	C799	G739	C679
U1475	A1353	G1414	A1354	A1290	C1229	C1169	U1108	U1048	A986	A862	U800	G740	U680
U1476	G1475	C1415	A1355	G1291	U1170	U1170	A1109	C1049	G988	A863	A801	G741	A681
C1477	G1476	A1416	A1356	A1292	A1171	U1172	A1171	U1050	C987	C984	A802	G742	G682
G1478	C1477	A1417	G1356	U1293	U1172	U1172	C1115	U1051	A994	C985	A803	G743	A683
G1479	A1418	U1418	U1357	G1294	C1233	G1173	C1113	C1052	A991	U866	C804	C744	U684
G1480	G1419	G1419	C1358	U1295	C1234	G1174	A1114	G1053	C993	C987	G805	C745	U685
U1481	U1420	A1420	G1359	G1296	C1235	A1175	C1115	C1054	C993	U868	A806	G746	C686
U1482	C1421	U1421	G1360	A1297	G1236	U1176	U1116	U1056	A994	C989	A807	A747	G687
G1483	G1422	G1422	G1361	G1298	G1237	U1177	U1116	U1057	A995	C990	C808	A748	A688
G1484	A1423	A1423	A1362	A1299	U1238	C1178	C1118	A1057	C996	U871	C749	A749	A689
U1547	U1424	U1424	C1363	A1300	A1239	U1119	U1119	C1058	C997	G872	U810	C750	A690
U1485	G1425	G1425	U1364	U1301	G1240	A1180	C1120	A1059	C998	U873	G811	C751	C691
A1486	U1426	U1426	U1365	C1302	G1241	C1181	G1121	C1060	A999	A874	G812	G752	C692
C1487	G1427	A1427	A1366	U1303	A1242	U1182	A1122	A1061	G1000	G875	A813	G753	A693
U1551	G1428	G1428	G1367	C1304	G1243	C1183	U1123	G1062	A1001	A876	G814	G754	G694
C1491	A1429	A1429	A1368	G1305	G1243	G1184	U1124	C1063	C1002	G877	A815	C755	G695
A1492	G1430	U1430	G1369	G1309	U1246	C1185	G1125	C1064	C1003	C878	U816	C756	U696
A1493	U1431	U1431	U1370	C1310	U1247	G1186	A1126	A1065	A1004	A879	A817	C757	U697
G1494	G1432	G1432	G1371	C1311	G1248	A1187	C1127	G1066	U1005	C880	C818	G758	A698
G1495	A1433	A1433	A1372	G1312	G1249	U1188	G1128	G1067	C1006	U943	C819	C759	G699
U1557	G1434	U1434	G1373	C1313	U1250	C1189	A1129	A1068	A1007	C882	U820	U760	C700
G1558	G1435	G1435	C1374	U1313	G1251	C1190	U1130	G1069	G1008	A883	A821	G761	U701
C1559	C1436	G1436	C1375	A1314	C1252	G1191	G1131	U1076	U1015	U890	G822	A762	A702
A1560	G1437	U1437	C1376	A1315	G1253	A1192	C1132	U1077	C1016	A952	C828	U768	G708
U1561	A1437	A1437	G1377	G1316	G1254	C1193	G1133	U1071	C1017	G953	C829	C769	A709
U1562	G1438	U1438	G1377	G1316	G1254	U1194	C1134	G1073	A1011	C948	C830	U770	C710
C1501	G1439	G1439	A1378	G1319	A1255	C1195	C1135	U1074	A1012	G949	C831	C771	C704
U1563	G1440	U1440	C1380	A1320	C1256	U1196	G1136	C1075	G1014	G950	A832	G772	C705
G1502	A1441	A1441	G1381	A1321	U1257	G1196	C1136	C1076	U1015	G951	A833	G773	A706
G1565	C1442	C1442	G1382	G1322	G1258	U1197	A1137	U1077	U1016	U891	C834	G774	G714
G1566	G1443	G1443	G1383	G1322	A1259	C1198	A1138	U1077	C1017	G954	U835	U775	U715
U1505	C1444	C1444	C1383	G1323	A1260	U1199	A1139	A1078	C1018	U964	U836	U776	U716
C1506	G1445	A1445	G1384	G1324	G1261	G1200	A1140	G1079	U1019	G955	U837	A777	G717
A1507	U1446	U1446	C1385	U1325	U1262	G1201	U1141	A1080	A1020	A956	A838	G778	A718
A1509	U1447	U1447	A1386	U1326	G1263	U1202	G1142	A1081	A1021	G957	U839	U779	A719
A1510	A1448	A1448	G1387	C1327	C1264	A1203	U1144	C1082	A1022	G958	U840	U780	A720
A1511	G1449	G1449	C1389	G1328	G1265	G1204	U1145	C1083	U1023	C959	C841	G781	G721
A1512	C1450	C1450	G1390	U1329	G1266	G1205	C1145	A1084	G1024	U960	A842	U782	C722
U1513	C1451	U1452	A1391	G1330	A1267	G1206	G1146	G1085	A1025	A964	U843	G783	C723
C1514	U1452	A1453	G1392	G1331	U1268	G1207	G1147	C1086	U1026	C965	C847	U784	C724
U1515	A1453	G1332	G1393	G1332	G1269	A1208	G1148	C1087	C1027	G966	U848	U785	C725
A1516	G1333	G1333	G1394	G1333	C1270	G1209	G1149	A1088	G1028	A966	A849	U786	G726
C1517	C1455	U1455	A1395	A1334	C1271	C1210	C1150	C1089	C1029	G967	C849	A787	U727
C1518	C1456	C1456	C1396	A1335	G1272	G1211	U1151	C1090	U1030	C968	U852	G788	G728
G1519	A1397	G1336	A1397	G1336	G1273	U1212	C1152	C1091	C1031	U969	C850	A789	A729
A1520	G1398	G1337	G1398	U1337	C1274	U1213	A1153	U1092	A1032	A970	C851	G790	C730
G1584	C1399	G1338	C1399	G1338	A1275	C1214	A1154	U1093	G1033	A971	C852	A791	G731
C1522	A1400	U1276	A1400	A1215	U1275	G1215	G1155	C1094	C1034	C972	A848	U789	A732
A1523	G1401	C1340	G1401	G1216	G1277	U1156	U1156	A1095	G1035	U973	A849	G790	G733
C1524	G1402	A1278	G1402	U1217	A1278	U1217	A1158	A1096	G1036	U974	C853	G791	G734
A1525	U1403	G1279	U1403	C1218	G1279	C1218	A1158	A1097	U1037	C975	C854	G792	G735
U1526	G1404	U1280	C1404	C1219	U1280	G1219	U1159	G1098	A1038	G976	C855	A793	G736
G1589	A1405	U1281	A1405	G1220	U1281	C1220	U1160	G1099	A1039	G977	U852	G794	G737
C1593	C1528	U1467	A1406	G1345	A1282	C1221	U1161	G1100	A1040	U978	C856	U792	G738

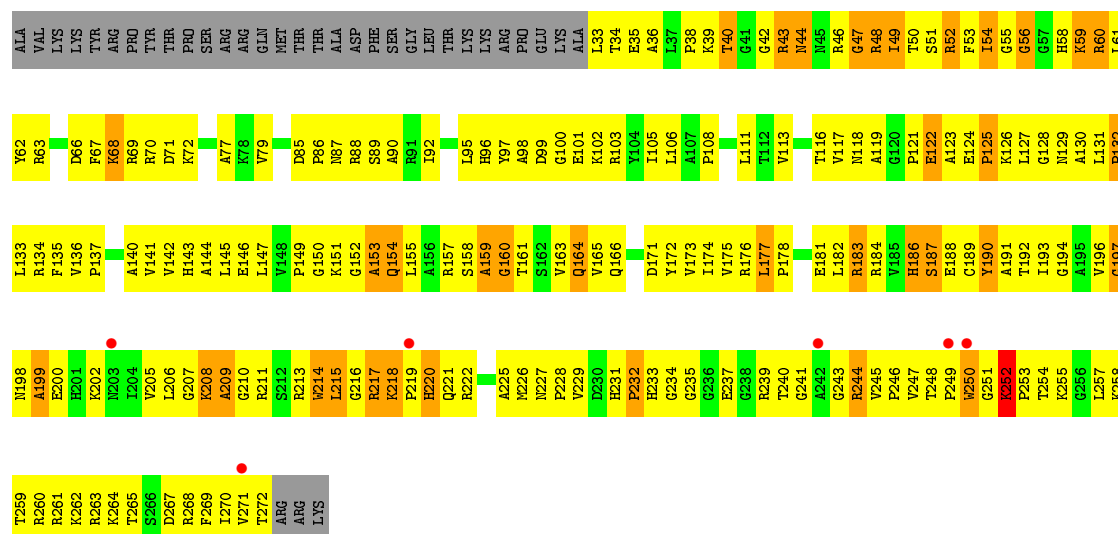
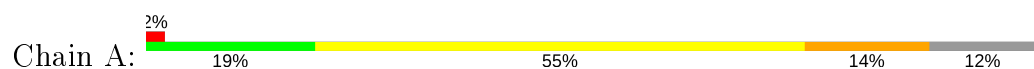




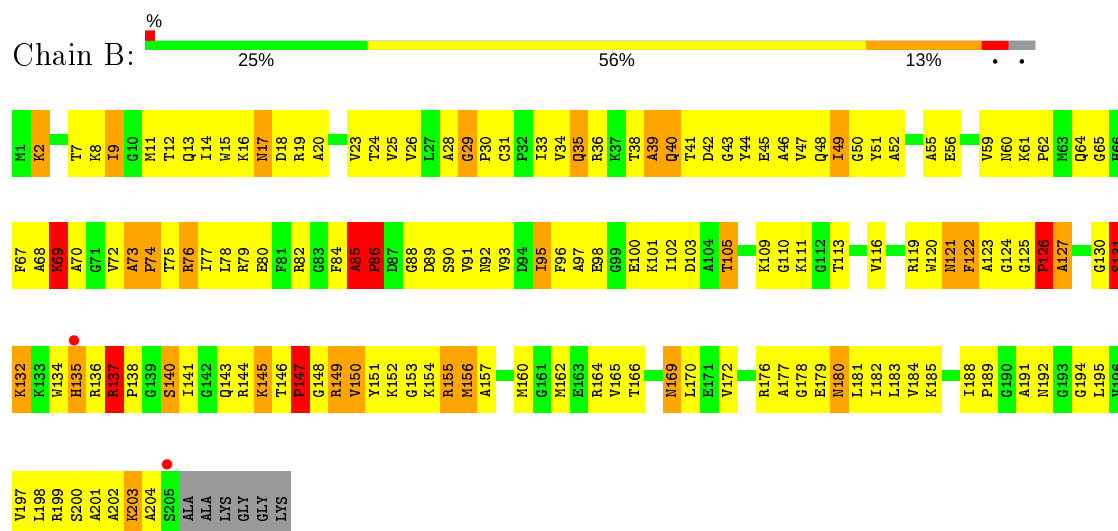
• Molecule 2: ribosomal 5S RNA



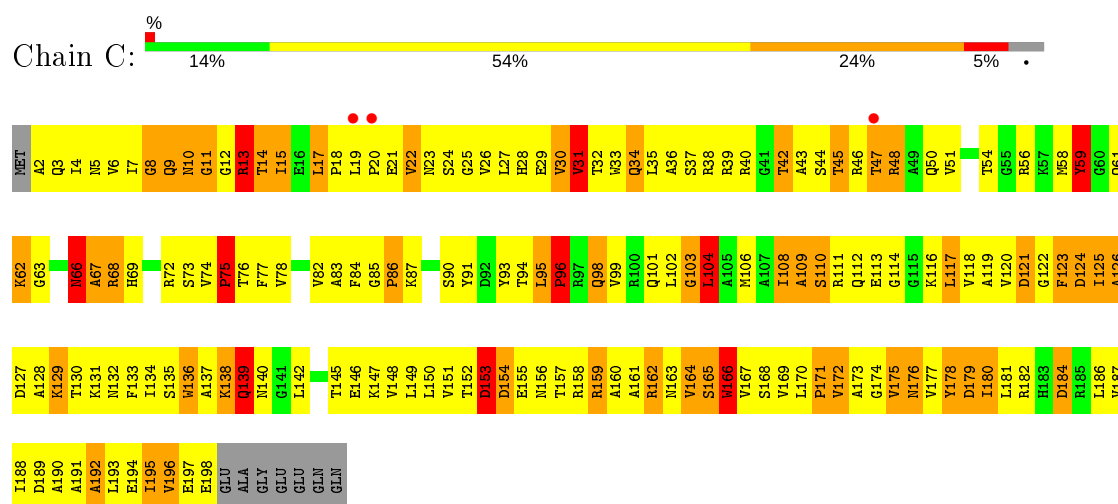
• Molecule 3: 50S ribosomal protein L2



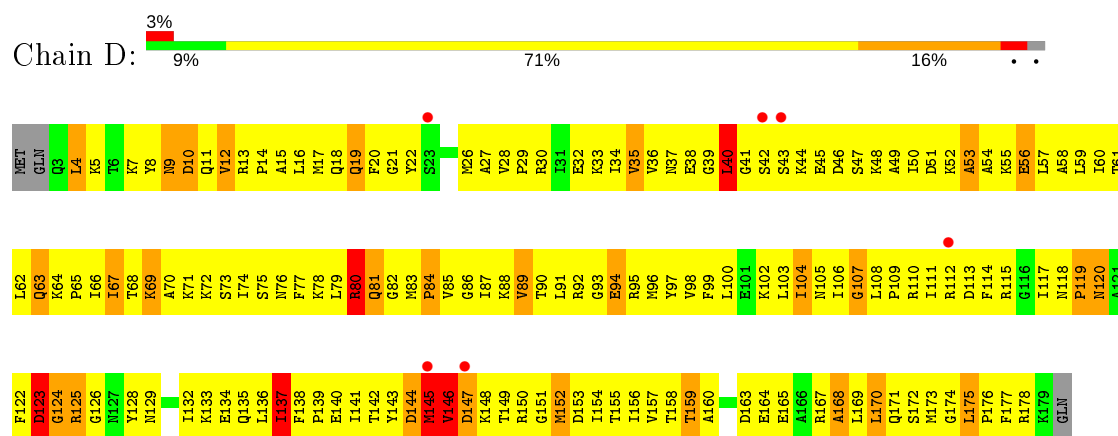
- Molecule 4: 50S ribosomal protein L3



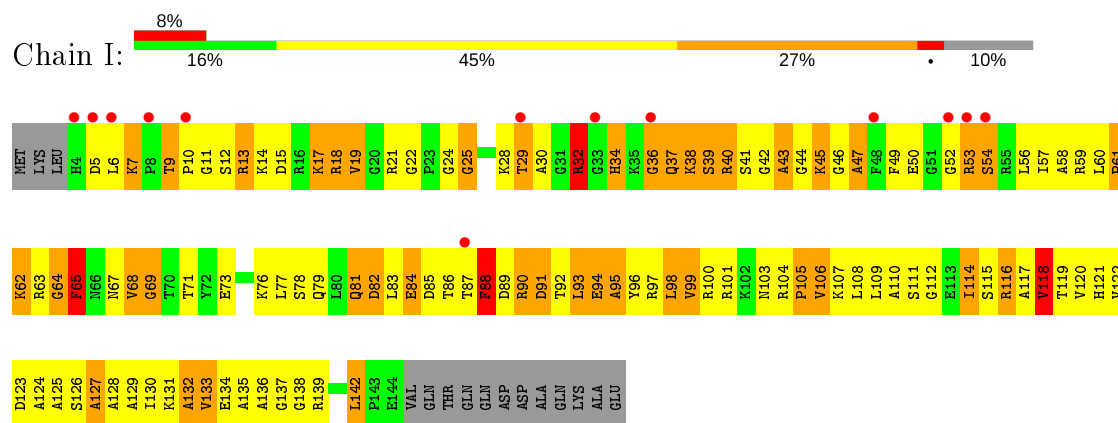
- Molecule 5: 50S ribosomal protein L4



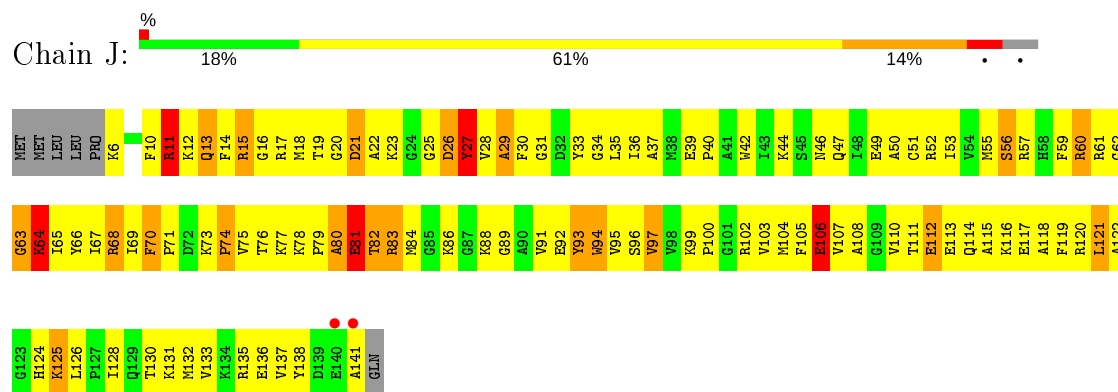
- Molecule 6: 50S ribosomal protein L5



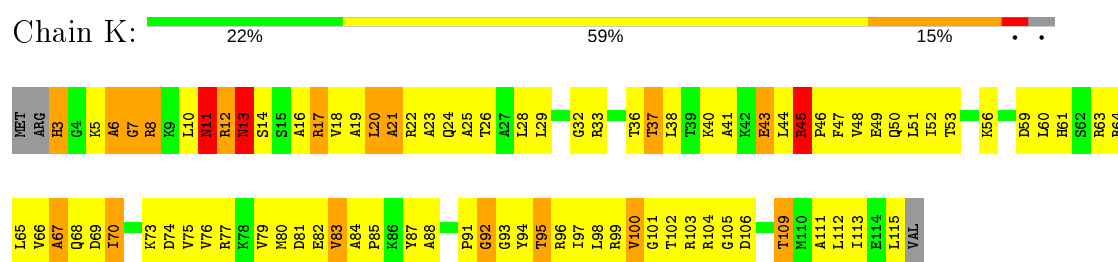
- Molecule 11: 50S ribosomal protein L15



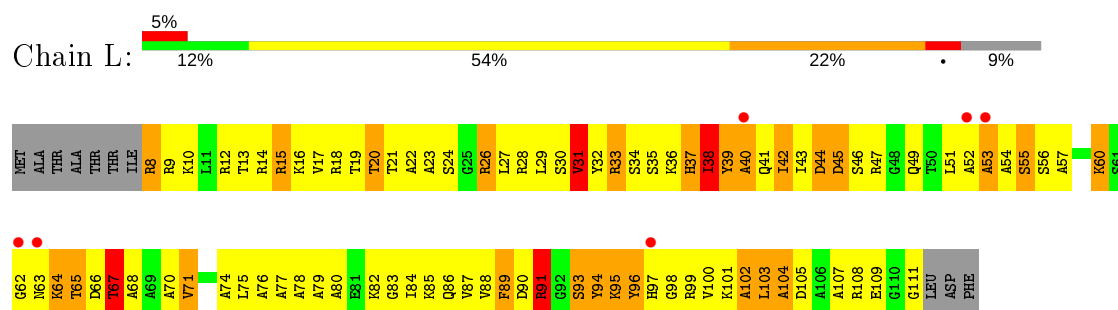
- Molecule 12: 50S ribosomal protein L16



- Molecule 13: 50S ribosomal protein L17

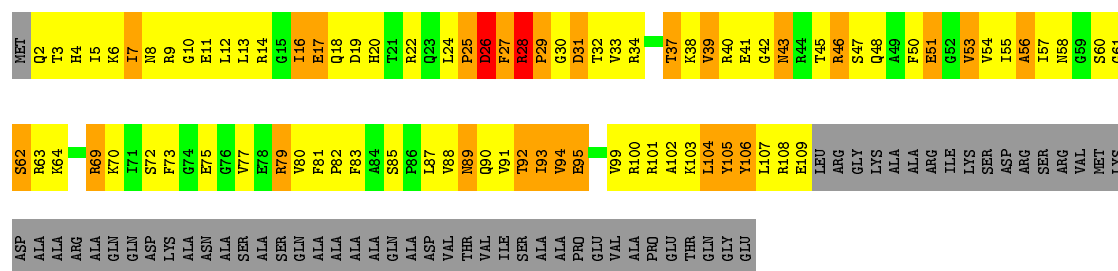


- Molecule 14: 50S ribosomal protein L18

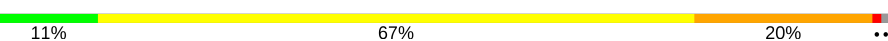


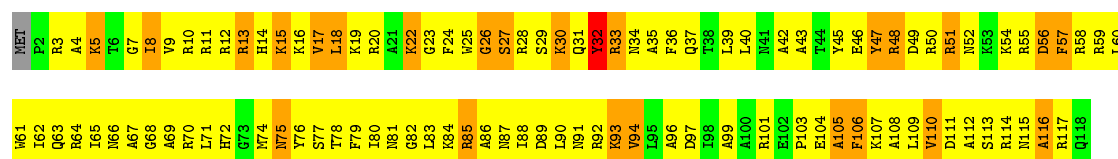
- Molecule 15: 50S ribosomal protein L19

Chain M: 



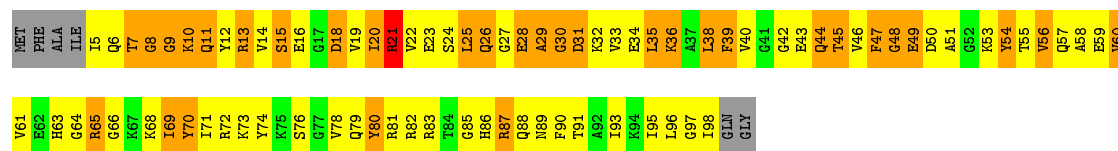
• Molecule 16: 50S ribosomal protein L20

Chain N: 

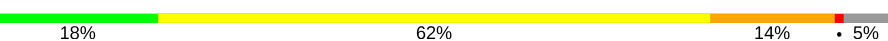


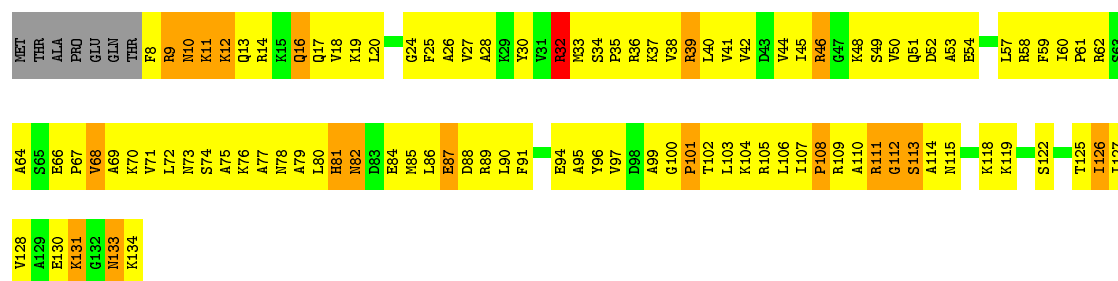
• Molecule 17: 50S ribosomal protein L21

Chain O: 

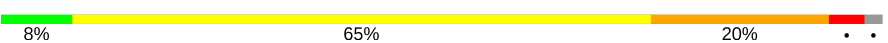


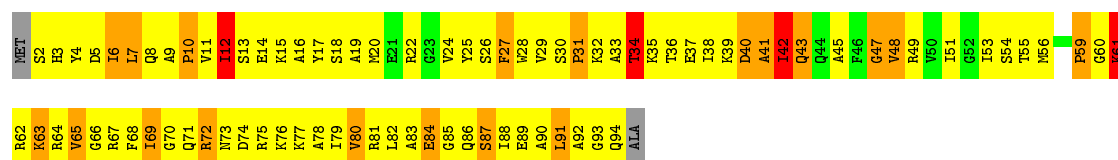
• Molecule 18: 50S ribosomal protein L22

Chain P: 

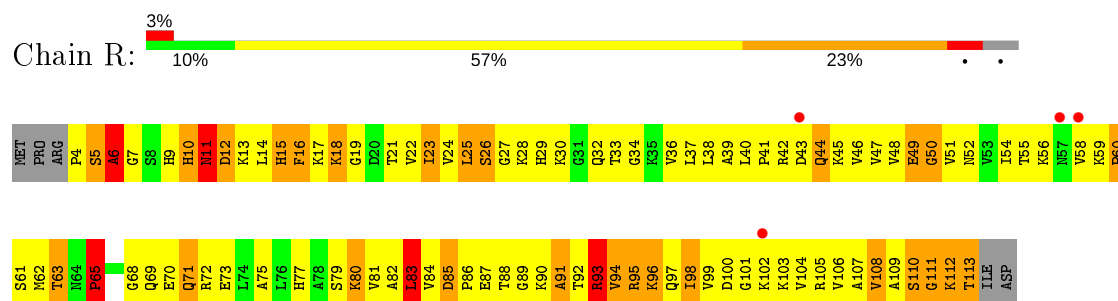


• Molecule 19: 50S ribosomal protein L23

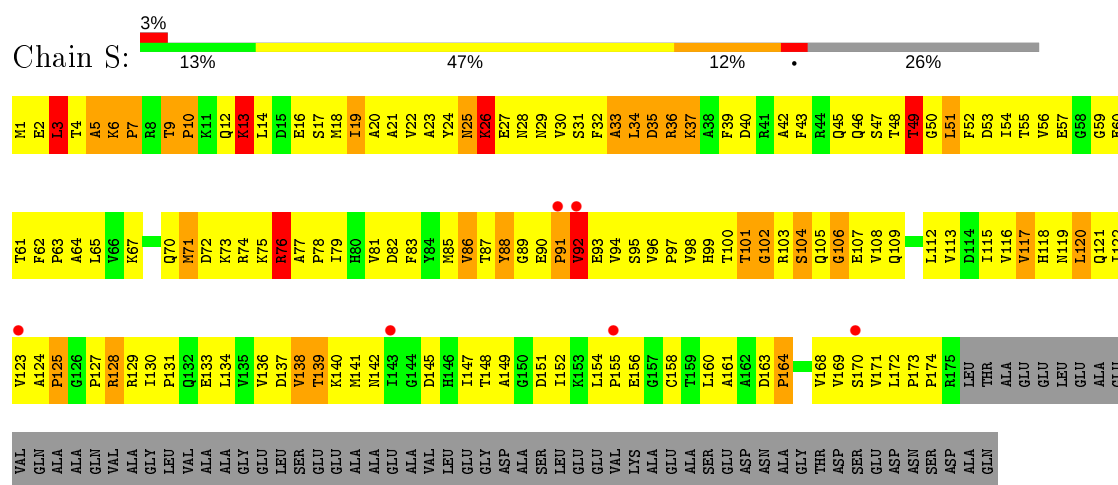
Chain Q: 



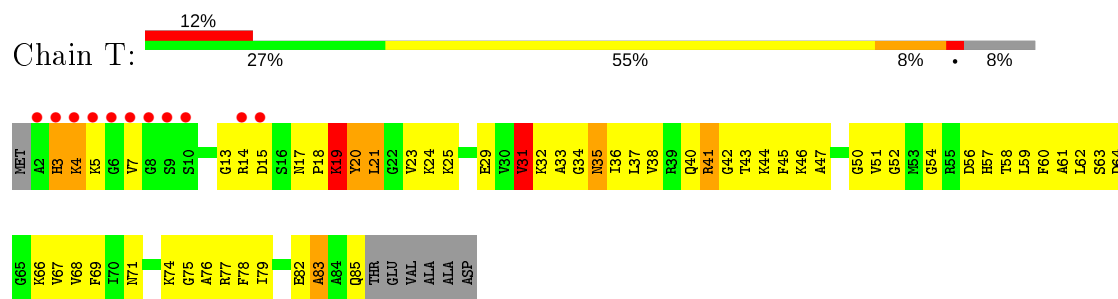
- Molecule 20: 50S ribosomal protein L24



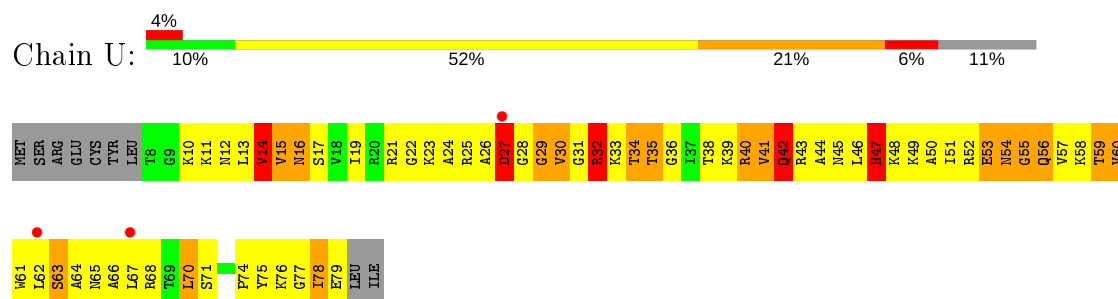
- Molecule 21: 50S ribosomal protein L25



- Molecule 22: 50S ribosomal protein L27



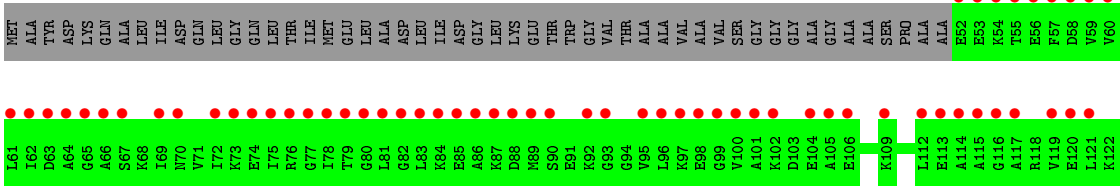
- Molecule 23: 50S ribosomal protein L28



- Molecule 24: 50S ribosomal protein L29



● Molecule 31: 50S ribosomal protein L7/L12



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	169.90Å 408.90Å 694.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.30 29.92 – 3.31	Depositor EDS
% Data completeness (in resolution range)	97.8 (30.00-3.30) 97.2 (29.92-3.31)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 3.31Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.302 , 0.339 0.274 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	73.4	Xtriage
Anisotropy	0.201	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.17 , 64.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	84395	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.69% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	X	0.90	77/64561 (0.1%)	1.04	462/100708 (0.5%)
2	Y	0.60	0/2904	0.77	0/4525
3	A	0.60	0/1862	0.83	0/2510
4	B	0.72	0/1567	0.95	2/2105 (0.1%)
5	C	0.63	0/1529	0.86	0/2070
6	D	0.60	0/1419	0.77	0/1903
7	E	0.55	0/1308	0.82	0/1771
8	F	0.23	0/1062	0.41	0/1440
9	G	0.65	0/1138	0.93	2/1539 (0.1%)
10	H	0.77	0/1007	0.85	0/1352
11	I	0.65	0/1081	0.93	1/1448 (0.1%)
12	J	0.68	0/1113	0.87	0/1486
13	K	0.80	0/886	0.95	0/1188
14	L	0.56	0/785	0.83	0/1048
15	M	0.73	0/884	0.97	2/1186 (0.2%)
16	N	0.60	0/994	0.81	0/1323
17	O	0.62	0/750	0.85	1/1000 (0.1%)
18	P	0.78	0/1027	0.89	0/1373
19	Q	0.67	0/737	0.94	1/988 (0.1%)
20	R	0.57	0/835	0.90	1/1121 (0.1%)
21	S	0.56	0/1370	0.79	0/1862
22	T	0.62	0/633	0.81	1/838 (0.1%)
23	U	0.58	0/556	0.94	0/741
24	V	0.54	0/537	0.75	0/714
25	W	0.55	0/426	0.82	0/568
26	Z	0.62	0/469	0.87	0/629
30	4	0.54	0/298	0.75	0/390
All	All	0.83	77/91738 (0.1%)	0.99	473/137826 (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	X	2	281
2	Y	0	2
5	C	0	1
9	G	0	1
16	N	0	1
17	O	0	1
22	T	0	1
All	All	2	288

The worst 5 of 77 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	1056	U	P-O5'	8.88	1.68	1.59
1	X	1750	A	C5-C6	-7.65	1.34	1.41
1	X	1688	U	C4-O4	7.39	1.29	1.23
1	X	2189	A	N9-C4	7.30	1.42	1.37
1	X	1981	A	C5-C6	-7.18	1.34	1.41

The worst 5 of 473 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1055	A	N9-C1'-C2'	-32.03	72.36	114.00
1	X	557	U	N1-C1'-C2'	19.61	139.50	114.00
1	X	417	C	N1-C1'-C2'	17.87	137.24	114.00
1	X	2323	U	O4'-C1'-N1	13.98	119.39	108.20
1	X	558	G	C3'-C2'-C1'	-13.92	90.37	101.50

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	X	1278	A	C1'
1	X	2592	U	C1'

5 of 288 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	X	13	A	Sidechain
1	X	15	G	Sidechain
1	X	29	U	Sidechain
1	X	43	A	Sidechain
1	X	59	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	X	57651	0	29046	4354	0
2	Y	2598	0	1328	184	0
3	A	1826	0	1885	379	0
4	B	1539	0	1600	236	0
5	C	1506	0	1525	356	0
6	D	1400	0	1481	400	0
7	E	1286	0	1336	249	0
8	F	1043	0	1088	71	0
9	G	1114	0	1144	282	0
10	H	997	0	1046	167	1
11	I	1067	0	1103	286	0
12	J	1090	0	1125	268	0
13	K	878	0	930	131	1
14	L	779	0	820	227	0
15	M	871	0	894	183	0
16	N	978	0	1020	234	0
17	O	741	0	756	200	0
18	P	1014	0	1096	184	0
19	Q	726	0	753	159	0
20	R	825	0	881	266	0
21	S	1345	0	1372	276	0
22	T	625	0	655	99	0
23	U	552	0	604	209	0
24	V	533	0	558	86	0
25	W	424	0	470	84	0
26	Z	457	0	464	81	0
27	1	53	0	0	0	0
28	2	46	0	0	0	0
29	3	63	0	0	2	0
30	4	297	0	330	69	0
31	5	71	0	0	0	0
All	All	84395	0	55310	8913	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 64.

The worst 5 of 8913 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)
1:X:1854:G:O2'	1:X:1855:G:H5'	1.31	1.28
1:X:2195:C:C5	1:X:2196:U:C5	2.22	1.28
1:X:729:A:H2'	1:X:730:C:O4'	1.19	1.25
1:X:2196:U:H2'	1:X:2197:U:C6	1.74	1.21
1:X:731:A:H2'	1:X:732:G:O4'	1.34	1.21

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)
10:H:125:LYS:NZ	13:K:82:GLU:OE2[8_555]	2.08	0.12

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	
3	A	238/274 (87%)	150 (63%)	62 (26%)	26 (11%)	0	2
4	B	203/211 (96%)	143 (70%)	29 (14%)	31 (15%)	0	1
5	C	195/205 (95%)	89 (46%)	60 (31%)	46 (24%)	0	0
6	D	175/180 (97%)	101 (58%)	44 (25%)	30 (17%)	0	1
7	E	169/185 (91%)	98 (58%)	43 (25%)	28 (17%)	0	1
8	F	142/144 (99%)	113 (80%)	22 (16%)	7 (5%)	2	14
9	G	140/174 (80%)	76 (54%)	35 (25%)	29 (21%)	0	0
10	H	132/134 (98%)	108 (82%)	16 (12%)	8 (6%)	1	10
11	I	139/156 (89%)	63 (45%)	36 (26%)	40 (29%)	0	0
12	J	134/142 (94%)	74 (55%)	39 (29%)	21 (16%)	0	1
13	K	111/116 (96%)	75 (68%)	20 (18%)	16 (14%)	0	1
14	L	102/114 (90%)	52 (51%)	31 (30%)	19 (19%)	0	1
15	M	106/166 (64%)	57 (54%)	32 (30%)	17 (16%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	N	115/118 (98%)	68 (59%)	30 (26%)	17 (15%)	0	1
17	O	92/100 (92%)	53 (58%)	14 (15%)	25 (27%)	0	0
18	P	125/134 (93%)	87 (70%)	20 (16%)	18 (14%)	0	1
19	Q	91/95 (96%)	46 (50%)	23 (25%)	22 (24%)	0	0
20	R	108/115 (94%)	57 (53%)	28 (26%)	23 (21%)	0	0
21	S	173/237 (73%)	99 (57%)	43 (25%)	31 (18%)	0	1
22	T	82/91 (90%)	48 (58%)	24 (29%)	10 (12%)	0	1
23	U	70/81 (86%)	35 (50%)	18 (26%)	17 (24%)	0	0
24	V	64/67 (96%)	32 (50%)	19 (30%)	13 (20%)	0	0
25	W	53/55 (96%)	36 (68%)	11 (21%)	6 (11%)	0	2
26	Z	56/60 (93%)	35 (62%)	13 (23%)	8 (14%)	0	1
30	4	35/37 (95%)	23 (66%)	6 (17%)	6 (17%)	0	1
All	All	3050/3391 (90%)	1818 (60%)	718 (24%)	514 (17%)	0	1

5 of 514 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	54	ILE
3	A	59	LYS
3	A	60	ARG
3	A	153	ALA
3	A	154	GLN

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	
3	A	185/215 (86%)	165 (89%)	20 (11%)	6	24
4	B	155/157 (99%)	140 (90%)	15 (10%)	8	29
5	C	157/163 (96%)	133 (85%)	24 (15%)	2	12
6	D	153/156 (98%)	137 (90%)	16 (10%)	7	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	E	136/144 (94%)	126 (93%)	10 (7%)	13	40
8	F	107/107 (100%)	105 (98%)	2 (2%)	57	77
9	G	118/146 (81%)	102 (86%)	16 (14%)	3	16
10	H	103/103 (100%)	90 (87%)	13 (13%)	4	19
11	I	108/121 (89%)	95 (88%)	13 (12%)	5	20
12	J	110/116 (95%)	99 (90%)	11 (10%)	7	27
13	K	90/93 (97%)	79 (88%)	11 (12%)	5	20
14	L	74/82 (90%)	57 (77%)	17 (23%)	1	3
15	M	94/134 (70%)	82 (87%)	12 (13%)	4	18
16	N	96/97 (99%)	87 (91%)	9 (9%)	8	30
17	O	75/79 (95%)	65 (87%)	10 (13%)	4	17
18	P	109/115 (95%)	103 (94%)	6 (6%)	21	52
19	Q	75/76 (99%)	66 (88%)	9 (12%)	5	20
20	R	91/96 (95%)	76 (84%)	15 (16%)	2	10
21	S	149/192 (78%)	131 (88%)	18 (12%)	5	20
22	T	62/67 (92%)	57 (92%)	5 (8%)	11	36
23	U	57/66 (86%)	46 (81%)	11 (19%)	1	6
24	V	54/55 (98%)	50 (93%)	4 (7%)	13	40
25	W	48/48 (100%)	42 (88%)	6 (12%)	4	19
26	Z	51/53 (96%)	41 (80%)	10 (20%)	1	5
30	4	35/35 (100%)	35 (100%)	0	100	100
All	All	2492/2716 (92%)	2209 (89%)	283 (11%)	5	22

5 of 283 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	I	142	LEU
14	L	44	ASP
23	U	70	LEU
12	J	60	ARG
13	K	12	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 87 such sidechains are listed below:

Mol	Chain	Res	Type
11	I	34	HIS
14	L	63	ASN
24	V	52	GLN
11	I	37	GLN
11	I	121	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	X	2680/2880 (93%)	695 (25%)	301 (11%)
2	Y	121/122 (99%)	23 (19%)	0
All	All	2801/3002 (93%)	718 (25%)	301 (10%)

5 of 718 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	X	4	C
1	X	13	A
1	X	14	A
1	X	34	U
1	X	35	G

5 of 301 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	X	1278	A
1	X	1581	C
1	X	2633	A
1	X	1313	U
1	X	1357	U

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](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	X	2686/2880 (93%)	-0.29	38 (1%) 75 75	11, 57, 103, 131	0
2	Y	122/122 (100%)	-0.04	2 (1%) 72 70	29, 81, 102, 108	0
3	A	240/274 (87%)	-0.04	6 (2%) 57 54	35, 65, 77, 90	0
4	B	205/211 (97%)	-0.27	2 (0%) 82 82	30, 53, 64, 77	0
5	C	197/205 (96%)	-0.25	3 (1%) 73 72	38, 60, 71, 83	0
6	D	177/180 (98%)	0.07	6 (3%) 45 43	54, 67, 76, 84	0
7	E	171/185 (92%)	-0.40	1 (0%) 89 90	50, 64, 75, 80	0
8	F	144/144 (100%)	2.13	74 (51%) 0 0	0, 0, 83, 88	0
9	G	142/174 (81%)	-0.15	4 (2%) 53 51	47, 59, 69, 77	0
10	H	134/134 (100%)	-0.29	0 100 100	27, 52, 62, 69	0
11	I	141/156 (90%)	0.34	13 (9%) 9 9	40, 63, 75, 83	0
12	J	136/142 (95%)	-0.22	2 (1%) 73 72	45, 61, 72, 78	0
13	K	113/116 (97%)	-0.24	0 100 100	37, 50, 60, 63	0
14	L	104/114 (91%)	0.04	6 (5%) 23 22	52, 63, 73, 78	0
15	M	108/166 (65%)	-0.33	0 100 100	23, 53, 65, 73	0
16	N	117/118 (99%)	-0.36	0 100 100	39, 57, 69, 75	0
17	O	94/100 (94%)	-0.40	0 100 100	42, 61, 72, 79	0
18	P	127/134 (94%)	-0.38	0 100 100	34, 52, 66, 76	0
19	Q	93/95 (97%)	-0.33	0 100 100	47, 58, 73, 78	0
20	R	110/115 (95%)	-0.05	4 (3%) 42 40	49, 62, 73, 85	0
21	S	175/237 (73%)	0.04	6 (3%) 45 43	55, 65, 76, 87	0
22	T	84/91 (92%)	0.27	11 (13%) 3 3	50, 61, 74, 80	0
23	U	72/81 (88%)	0.10	3 (4%) 36 34	52, 64, 73, 78	0
24	V	66/67 (98%)	-0.31	0 100 100	54, 63, 75, 81	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	W	55/55 (100%)	-0.51	0 100 100	48, 58, 70, 79	0
26	Z	58/60 (96%)	-0.26	1 (1%) 70 68	35, 53, 66, 69	0
27	1	53/55 (96%)	3.19	35 (66%) 0 0	53, 61, 68, 71	0
28	2	46/47 (97%)	6.59	46 (100%) 0 0	43, 56, 62, 63	0
29	3	63/66 (95%)	5.23	58 (92%) 0 0	50, 58, 65, 67	0
30	4	37/37 (100%)	0.34	4 (10%) 5 5	52, 63, 71, 76	0
31	5	71/122 (58%)	4.99	60 (84%) 0 0	0, 0, 0, 0	0
All	All	6141/6683 (91%)	0.04	385 (6%) 20 20	0, 60, 91, 131	0

The worst 5 of 385 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
31	5	101	ALA	22.2
29	3	37	SER	16.3
28	2	4	THR	13.3
31	5	97	LYS	12.9
31	5	104	GLU	12.8

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.