



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 07:13 AM GMT

PDB ID : 2ZJR  
Title : Refined native structure of the large ribosomal subunit (50S) from *Deinococcus radiodurans*  
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 : 2.91 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

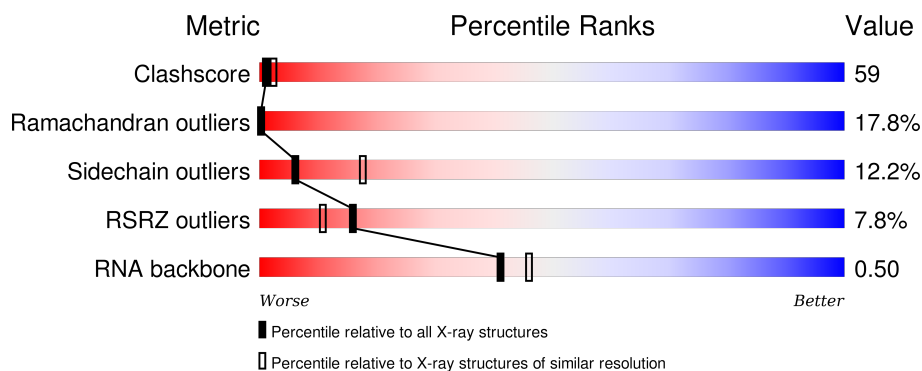
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.91 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	102246	1871 (2.94-2.90)
Ramachandran outliers	100387	1824 (2.94-2.90)
Sidechain outliers	100360	1826 (2.94-2.90)
RSRZ outliers	91569	1650 (2.94-2.90)
RNA backbone	2183	1004 (3.30-2.54)

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

Mol	Chain	Length	Quality of chain
1	X	2880	<div> <div>3%</div> <div>16% 46% 20% 10% 7%</div> </div>
2	Y	123	<div> <div>2%</div> <div>23% 59% 15% ..</div> </div>
3	A	274	<div> <div>8%</div> <div>16% 54% 16% 12%</div> </div>
4	B	211	<div> <div>29% 52% 12% ..</div> </div>
5	C	205	<div> <div>5%</div> <div>11% 56% 25% ..</div> </div>

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Mol	Chain	Length	Quality of chain
6	D	180	
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	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	MG	X	2882	-	-	-	X
31	MG	X	2888	-	-	-	X
31	MG	X	2899	-	-	-	X
31	MG	X	2906	-	-	-	X
31	MG	X	2908	-	-	-	X
31	MG	X	2910	-	-	-	X
31	MG	Y	124	-	-	-	X

## 2 Entry composition

There are 31 unique types of molecules in this entry. The entry contains 83819 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	71	Total	C	N	O	S	0	0	0
			503	310	91	99	3			

- 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

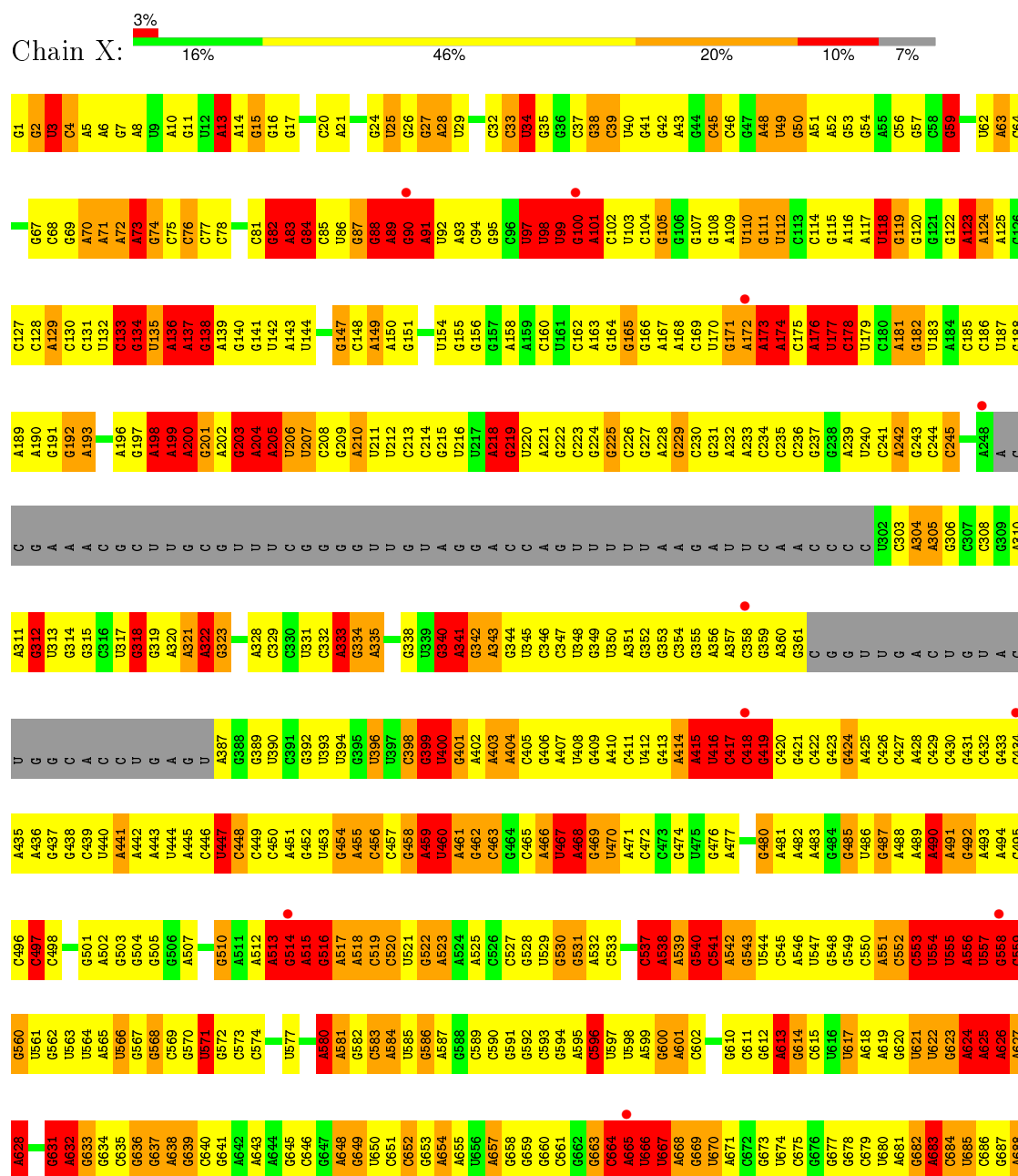
- Molecule 31 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	X	30	Total Mg 30 30	0	0
31	Y	5	Total Mg 5 5	0	0

### 3 Residue-property plots

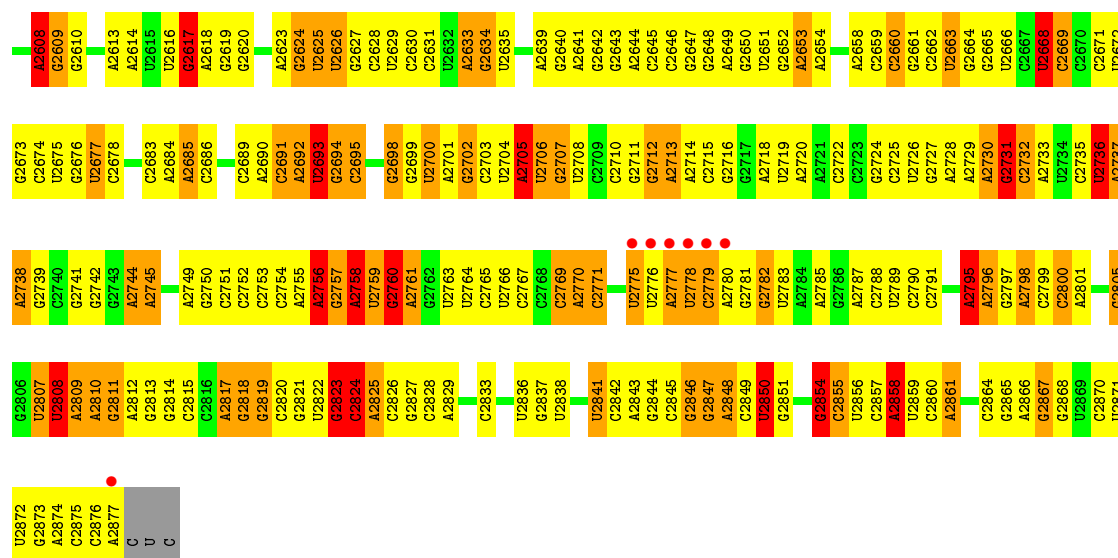
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

- Molecule 1: ribosomal 23S RNA

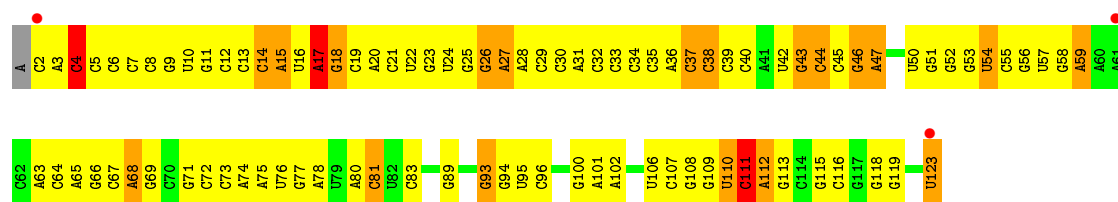


A1585	A1586	A1587	A1588	G1589	C1593	U1594	A1595	A1596	A1597	C1598	U1599	U1600	U1601	A1602	A1603	C1606	A1607	G1608	A1609	A1610	U1611	U1612	G1613	C1614	C1615	U1616	U1617	U1618	A1619	C1620	G1621	C1622	C1623	A1624	A1625	A1626	C1627	C1628	G1629	A1630	G1631	A1632	C1633	A1634	G1635	G1636	U1637	G1642	A1643	U1645	C1648	U1651	G1652																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
G1520	U1521	A1522	A1523	C1524	A1525	U1526	G1527	A1528	C1529	U1530	C1531	A1532	G1533		G1536	U1537	A1538	U1539	C1540	U1541	U1542	A1543	A1544	U1547	U1548	U1549	C1550	U1551	C1552	G1553	A1554	A1555	C1556	G1557	A1558	A1559	A1560	G1561	G1562	A1563	U1564	A1569	C1570	G1571	G1572	G1573	A1574	C1575	A1576	U1578	G1579	C1580	C1581	A1582	A1583	G1584																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
C1456	U1459	G1460	C1461	G1462	A1463	A1464	G1465	C1466	U1467	A1468	U1469	G1470	G1471	C1472	U1473	A1474	U1475	U1476	C1477	U1482	G1483	A1484	U1485	A1486	C1487	G1488	U1489	C1490	C1491	A1492	A1493	G1494	G1495	A1496	C1497	G1498	A1499	U1500	C1501	G1502	C1503	G1504	U1505	C1506	A1507	G1508	A1509	A1510	A1511	U1512	U1513	C1514	U1515	A1516	C1517	U1518																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
G1319	A1320	A1321	G1322	G1323	G1324	U1325	U1326	C1327	U1328	A1329	A1330	G1331	G1332	G1333	A1334	A1335	G1336	G1337	G1338	U1339	C1340	G1341	U1342	C1343	C1344	G1345	C1346	C1347	C1348	A1349	G1350	G1351	G1352	A1353	A1354	G1355	U1356	C1357	C1358	G1359	G1360	U1370	G1371	A1372	G1373	G1374	C1375	C1376	G1377	A1378	C1383	C1384	C1385	A1386	C1387	C1388	C1389																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												
G1390	A1391	U1392	G1393		A1397	G1398		G1402	U1403	C1404	A1405	A1406	G1407	A1408	U1409	U1410	A1411	C1412	G1413	G1414	U1415	A1416	C1417	G1418	G1419	A1420	U1421	C1422	C1423	U1424	G1425	U1426	G1427	A1428	A1429	G1430	U1431	G1432	U1433	U1434	G1435	G1436	A1437	G1438	U1439	U1440	C1441	C1442	G1443	C1444	A1448	C1449	G1450	C1451	U1452	A1453	U1454	C1455																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
C1456	U1459	G1460	C1461	G1462	A1463	A1464	G1465	C1466	U1467	A1468	U1469	G1470	G1471	C1472	U1473	A1474	U1475	U1476	C1477	U1482	G1483	A1484	U1485	A1486	C1487	G1488	U1489	C1490	C1491	A1492	A1493	G1494	G1495	A1496	C1497	G1498	A1499	U1500	C1501	G1502	C1503	G1504	U1505	C1506	A1507	G1508	A1509	A1510	A1511	U1512	U1513	C1514	U1515	A1516	C1517	U1518																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
G1251	C1252	C1253	G1254		G1258	A1259	A1260	C1261	U1262	G1263	C1264	G1265	G1266	A1267	U1268	C1269	C1270		G1273	C1274	A1275	U1276	G1277	A1278	C1279	U1280	C1281	A1282	C1283	G1284	A1285	U1286	C1287	A1288	A1289		A1293	G1294	U1295	C1296	A1297	G1298	C1299	A1300	U1301	C1302	U1303	U1304		G1309	C1310	C1311	G1312	U1313	C1314	A1315	C1316	G1317	A1318																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
A1187	A1188	C1189	G1190	G1191	A1192	U1193	U1194	U1195	G1196	U1197	C1198	U1199	G1200	A1201	U1202	A1203	G1204	G1205	G1206	G1207		U1211	U1212	U1213	C1214	A1215	C1218	C1219	C1220	C1221	G1222	C1223	A1224	G1225	A1226	U1227	G1228	C1229	C1230	A1231	U1232	A1233	U1234	C1235	G1236	G1237	A1238	U1239	G1240	U1241	A1242	G1243		G1246	U1247	C1248	G1249	A1250																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
U1124	G1125	A1126	G1127	G1128	A1129	U1130	G1131	G1132	G1133	U1134	C1135	G1136	A1137	A1138	U1139	A1140	U1141	G1142	A1143	U1144	C1145	U1146	G1147	G1148	G1149		U1151	C1152	A1153	A1154	G1155	U1156	G1157	A1162	C1163	C1164	G1165	A1166	A1167	G1168	C1169	U1170	A1171	U1172	G1173	G1174	A1175	U1176	U1177	C1178	A1179	U1180	C1181	U1182	C1183	G1184	C1185	G1186																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
C1064	A1065	C1066	G1067	A1068	G1069	G1070	U1071	U1072	G1073	U1074	C1075	U1076	U1077	A1078	U1079	A1080	A1081	G1082	C1083	A1084	C1085	G1086	C1087	A1088	C1089	C1090	C1091	U1092	C1093	C1094	A1095	A1096	A1097	G1098	A1099	G1100	U1101	G1102	C1103	G1104	U1105	A1106	A1107	U1108	A1109	U1110	G1111	G1112	C1113	U1114	C1115	U1116	U1117	C1118	U1119	C1120	A1121	A1122	C1123																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
U1004	U1005	C1006	A1007	G1008	C1009	U1010	A1011	A1012	G1013	A1014	U1015	U1016	C1017	C1018	U1019	A1020	A1021	A1022	U1023	A1024	C1025	G1026	C1027	G1028	C1029	U1030	A1031	A1032	C1033	C1034	G1035	G1036	U1037	U1038	A1039	A1040	G1041	G1042	A1043	U1044	G1045	A1046	U1047	U1048	C1049	G1050	U1051	A1052	C1053	A1054	U1055	C1056	U1057	C1058	A1059	G1060	A1061	G1062	C1063																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
U941	U942	U943	A944	U945	U946	C947	C948		G951	A952	G953	U954	G955	A956	G957	G958	C959	U960	G963	A964	G965	A966	G967	C968	U969	A970	A971	C972	U973	U974	A911	A912	A913	C914	C915		A918	U919	G920	A921	A922	A923	C924	U925	C926	U927	G928	A929	C930	G931	G932	U933	G934	C935	A936	C937	G938	C939	U940																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
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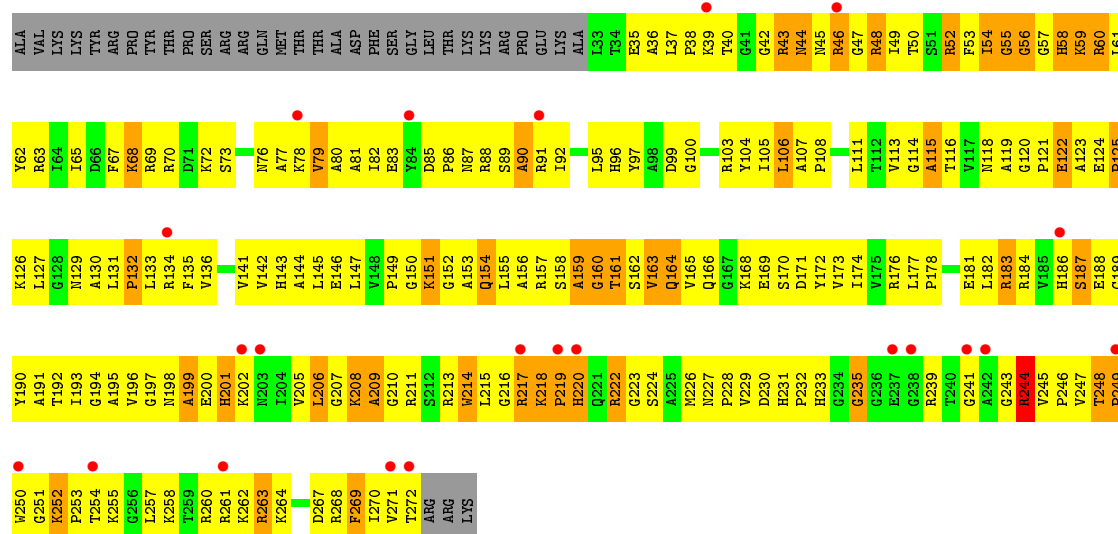
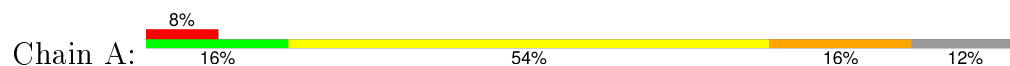
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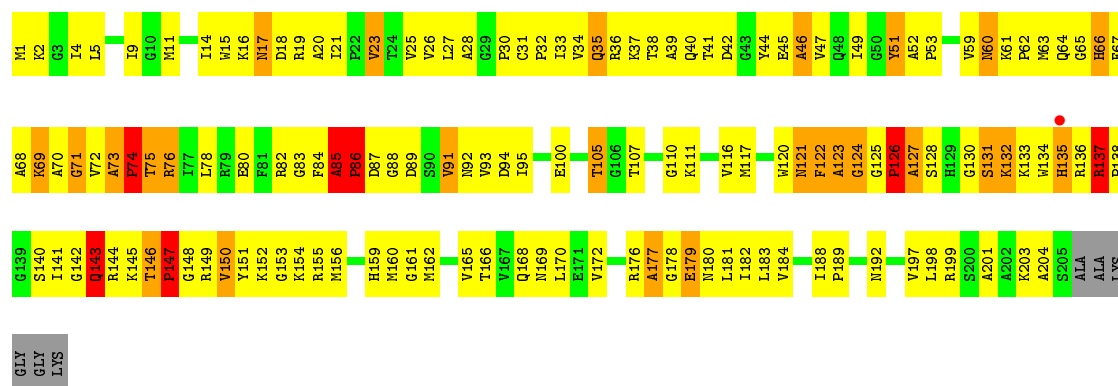


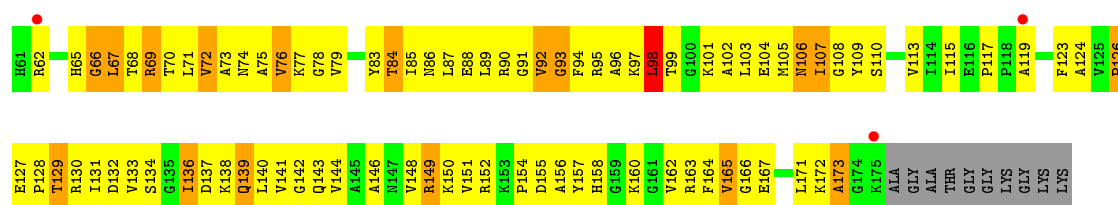
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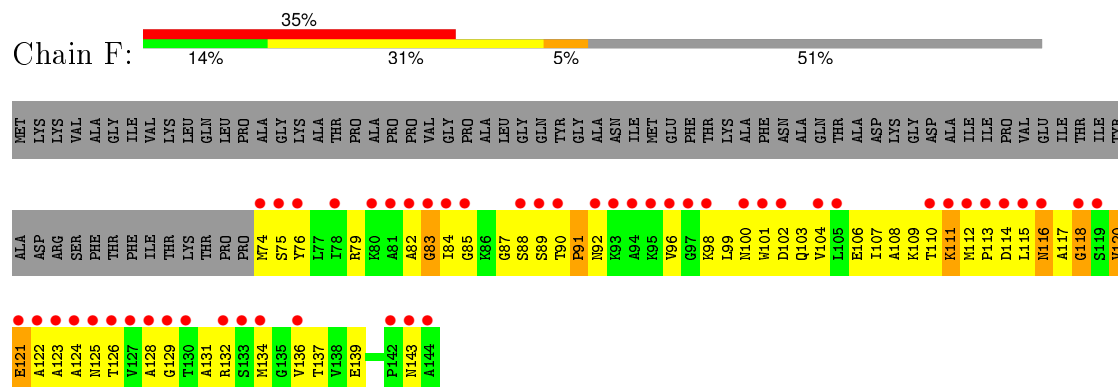
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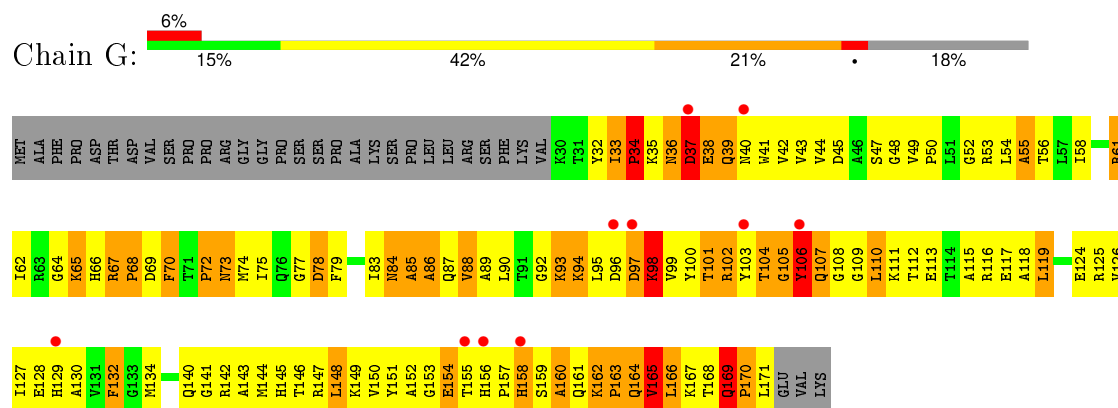




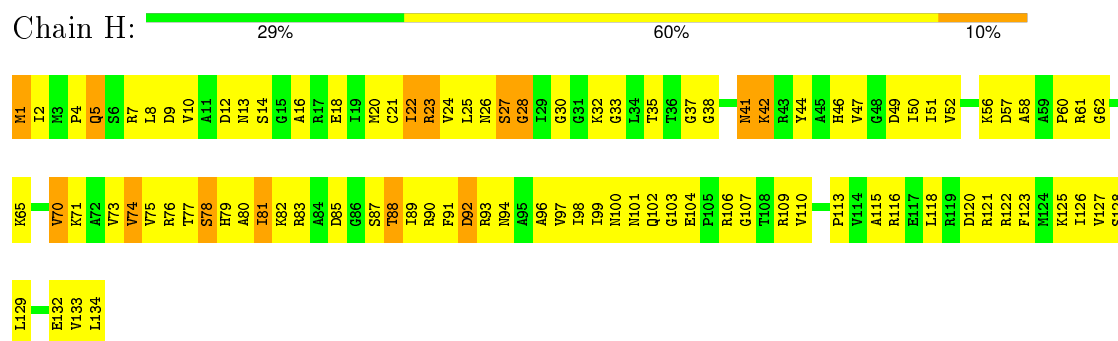
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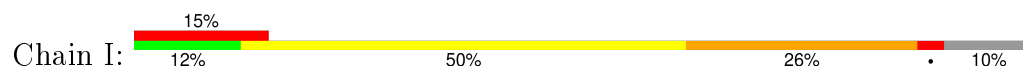
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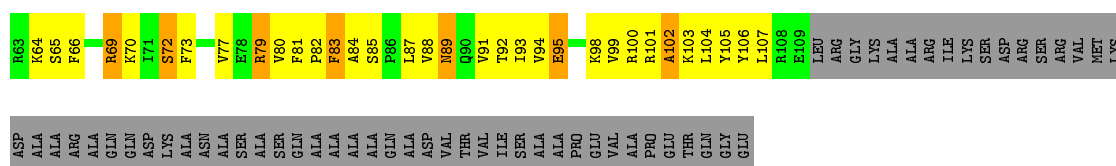


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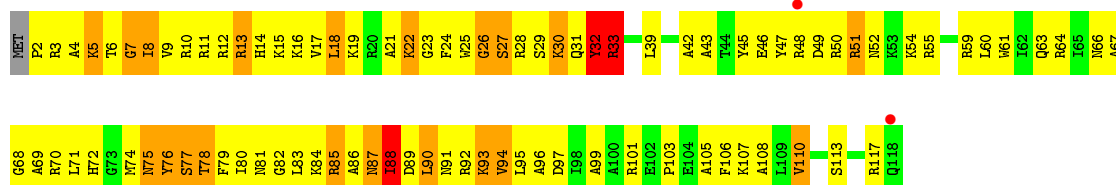




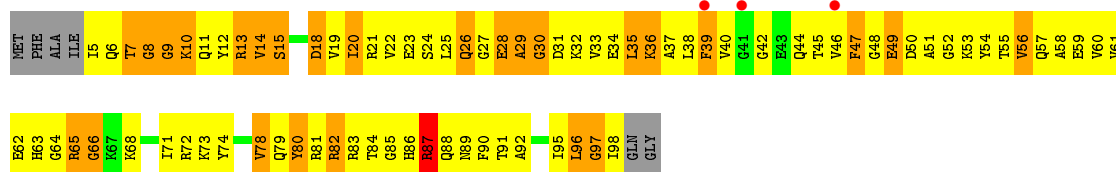
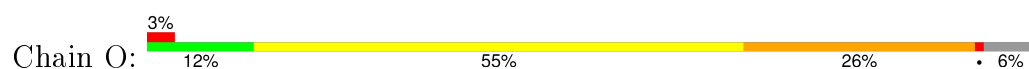




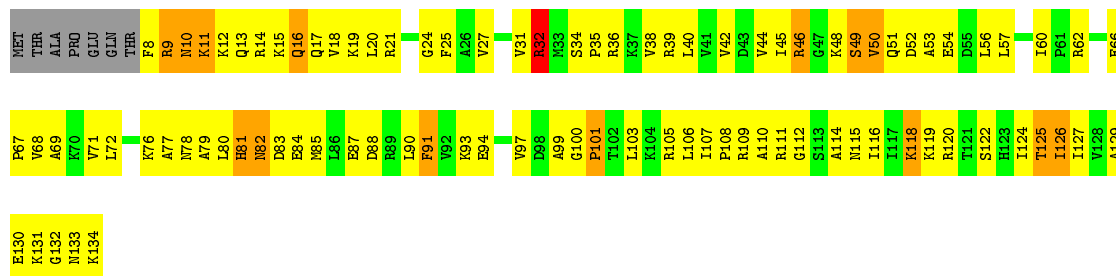
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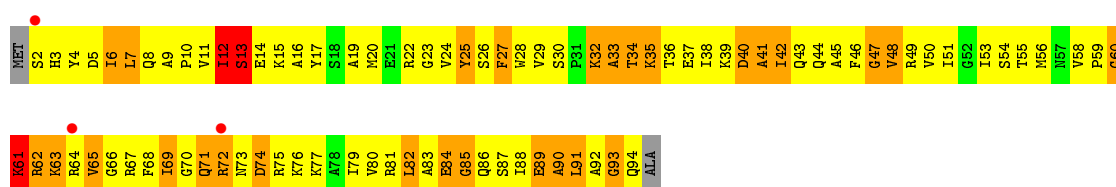
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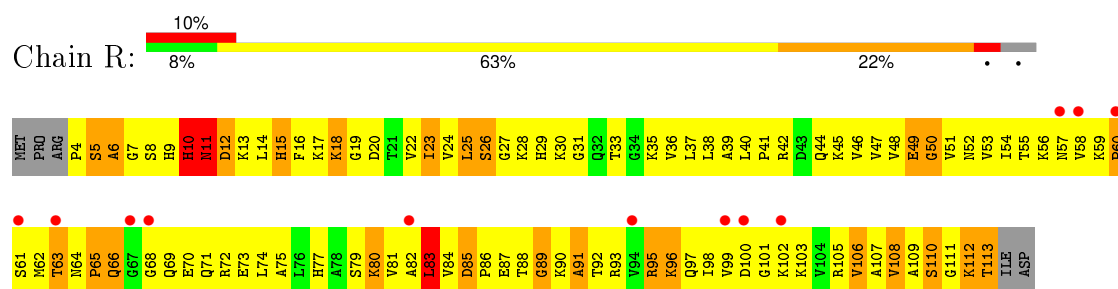
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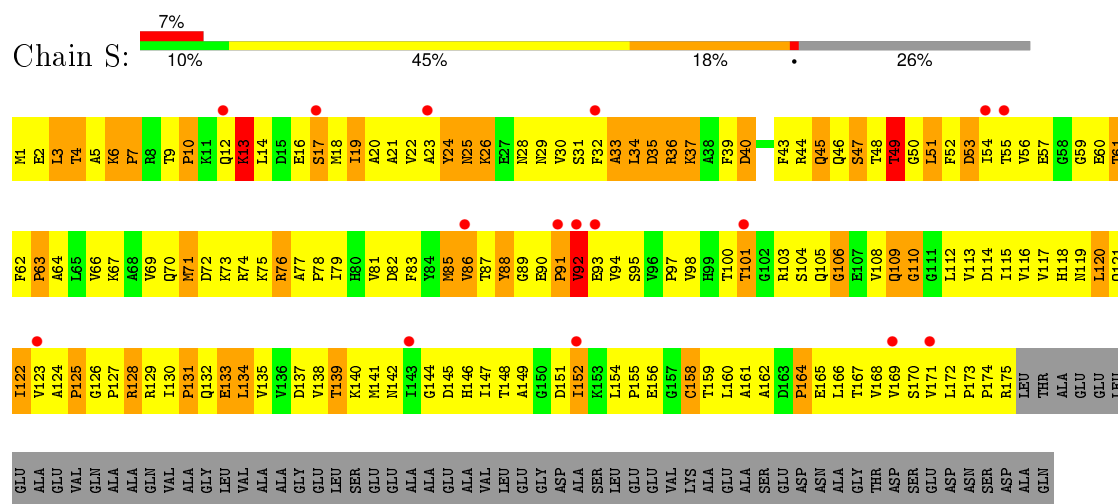
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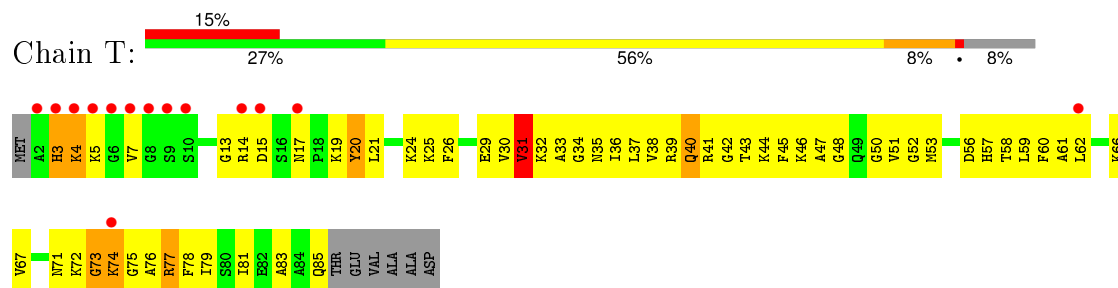
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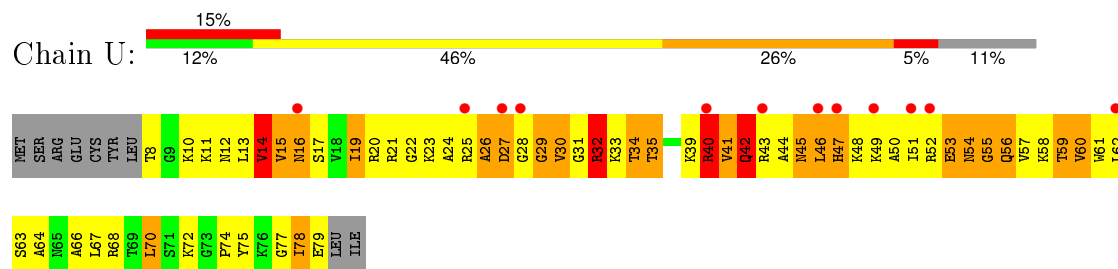
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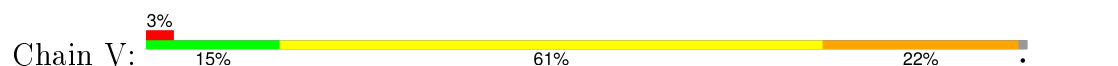
• Molecule 22: 50S ribosomal protein L27

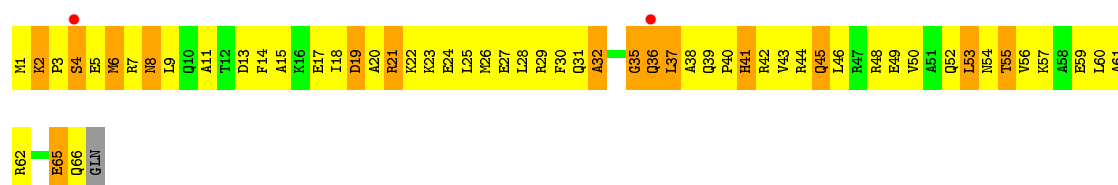


• Molecule 23: 50S ribosomal protein L28



• Molecule 24: 50S ribosomal protein L29





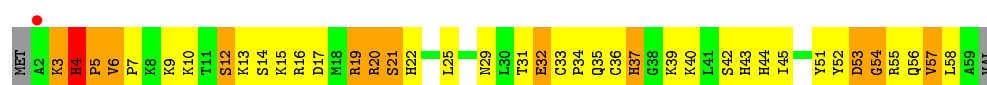
- Molecule 25: 50S ribosomal protein L30

Chain W: 25% 62% 13%



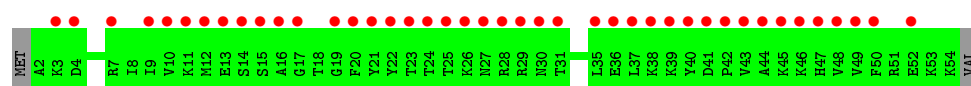
- Molecule 26: 50S ribosomal protein L32

Chain Z: 2% 30% 45% 20%



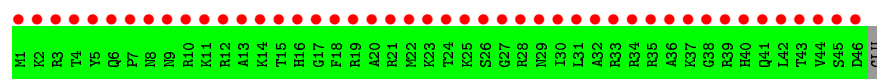
- Molecule 27: 50S ribosomal protein L33

Chain 1: 76% 96%



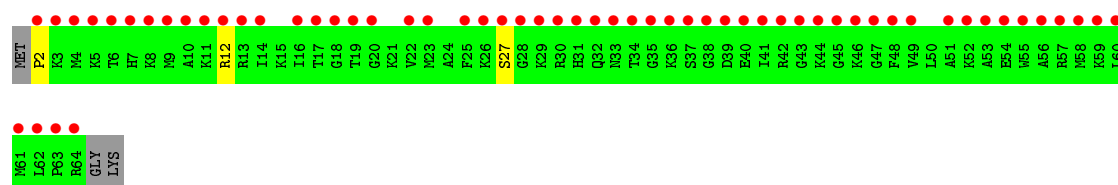
- Molecule 28: 50S ribosomal protein L34

Chain 2: 98% 98%



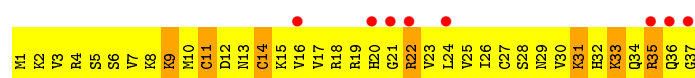
- Molecule 29: 50S ribosomal protein L35

Chain 3: 89% 91% 5% 5%



- Molecule 30: 50S ribosomal protein L36

Chain 4: 22% 81% 19%



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	169.90 Å   408.90 Å   694.50 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	29.90 – 2.91 29.92 – 2.91	Depositor EDS
% Data completeness (in resolution range)	94.1 (29.90-2.91) 94.1 (29.92-2.91)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.56 (at 2.90 Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.277   ,   0.311 0.267   ,   (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	52.9	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.17 , 46.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 493787 reflections	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	83819	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.87% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	156/64561 (0.2%)	1.15	809/100708 (0.8%)
2	Y	0.50	0/2904	0.73	0/4525
3	A	0.50	0/1862	0.82	0/2510
4	B	0.70	0/1567	0.99	6/2105 (0.3%)
5	C	0.60	0/1529	0.87	0/2070
6	D	0.47	0/1419	0.70	0/1903
7	E	0.46	0/1308	0.76	0/1771
8	F	0.65	0/508	1.11	2/683 (0.3%)
9	G	0.59	0/1138	0.92	2/1539 (0.1%)
10	H	0.72	0/1007	0.93	1/1352 (0.1%)
11	I	0.60	0/1081	0.89	0/1448
12	J	0.59	0/1113	0.86	1/1486 (0.1%)
13	K	0.83	0/886	1.04	1/1188 (0.1%)
14	L	0.48	0/785	0.82	1/1048 (0.1%)
15	M	0.72	0/884	1.15	6/1186 (0.5%)
16	N	0.54	0/994	0.80	0/1323
17	O	0.54	0/750	0.83	0/1000
18	P	0.73	0/1027	0.90	0/1373
19	Q	0.58	0/737	0.88	3/988 (0.3%)
20	R	0.48	0/835	0.84	0/1121
21	S	0.48	0/1370	0.71	0/1862
22	T	0.52	0/633	0.77	0/838
23	U	0.51	0/556	0.87	0/741
24	V	0.44	0/537	0.67	0/714
25	W	0.51	0/426	0.83	0/568
26	Z	0.68	0/469	0.95	1/629 (0.2%)
30	4	0.45	0/298	0.65	0/390
All	All	0.82	156/91184 (0.2%)	1.08	833/137069 (0.6%)

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	0	225
2	Y	0	4
9	G	0	1
16	N	0	1
19	Q	0	1
All	All	0	232

The worst 5 of 156 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	1123	G	C3'-O3'	14.43	1.62	1.42
1	X	1123	G	C4'-C3'	13.55	1.68	1.53
1	X	2322	U	C3'-O3'	12.22	1.59	1.42
1	X	1187	A	C2'-C1'	11.44	1.66	1.53
1	X	100	G	C3'-O3'	10.61	1.57	1.42

The worst 5 of 833 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1055	A	N9-C1'-C2'	-29.46	75.70	114.00
1	X	513	A	N9-C1'-C2'	24.54	145.90	114.00
1	X	2297	G	N9-C1'-C2'	21.75	142.27	114.00
1	X	557	U	N1-C1'-C2'	19.63	139.52	114.00
1	X	2298	U	N1-C1'-C2'	19.50	139.35	114.00

There are no chirality outliers.

5 of 232 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	X	13	A	Sidechain
1	X	15	G	Sidechain
1	X	32	C	Sidechain
1	X	34	U	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	29047	3656	0
2	Y	2598	0	1328	160	0
3	A	1826	0	1885	387	0
4	B	1539	0	1600	265	0
5	C	1506	0	1525	369	0
6	D	1400	0	1481	377	0
7	E	1286	0	1336	242	0
8	F	503	0	520	94	0
9	G	1114	0	1144	264	0
10	H	997	0	1046	152	0
11	I	1067	0	1103	273	0
12	J	1090	0	1125	254	0
13	K	878	0	930	120	0
14	L	779	0	820	236	0
15	M	871	0	894	198	0
16	N	978	0	1020	216	0
17	O	741	0	756	192	0
18	P	1014	0	1096	152	0
19	Q	726	0	753	183	0
20	R	825	0	881	263	0
21	S	1345	0	1372	294	0
22	T	625	0	655	97	0
23	U	552	0	604	201	0
24	V	533	0	558	107	0
25	W	424	0	470	67	0
26	Z	457	0	464	67	0
27	1	53	0	0	0	0
28	2	46	0	0	0	0
29	3	63	0	0	3	0
30	4	297	0	330	68	0
31	X	30	0	0	0	0
31	Y	5	0	0	0	0
All	All	83819	0	54743	8176	0

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 59.

The worst 5 of 8176 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:135:U:H2'	1:X:136:A:C8	1.59	1.37
1:X:2195:C:C5	1:X:2196:U:C5	2.22	1.28
1:X:623:G:N2	1:X:626:A:C2	2.01	1.26
1:X:1053:G:H2'	1:X:1054:C:C6	1.71	1.25
1:X:333:A:H3'	5:C:162:ARG:NH2	1.49	1.24

There are no symmetry-related clashes.

## 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	
3	A	238/274 (87%)	147 (62%)	53 (22%)	38 (16%)	0	0
4	B	203/211 (96%)	147 (72%)	31 (15%)	25 (12%)	0	1
5	C	195/205 (95%)	99 (51%)	48 (25%)	48 (25%)	0	0
6	D	175/180 (97%)	91 (52%)	59 (34%)	25 (14%)	0	0
7	E	169/185 (91%)	100 (59%)	39 (23%)	30 (18%)	0	0
8	F	69/144 (48%)	45 (65%)	19 (28%)	5 (7%)	1	3
9	G	140/174 (80%)	80 (57%)	28 (20%)	32 (23%)	0	0
10	H	132/134 (98%)	114 (86%)	11 (8%)	7 (5%)	2	7
11	I	139/156 (89%)	62 (45%)	33 (24%)	44 (32%)	0	0
12	J	134/142 (94%)	74 (55%)	36 (27%)	24 (18%)	0	0
13	K	111/116 (96%)	85 (77%)	12 (11%)	14 (13%)	0	1
14	L	102/114 (90%)	55 (54%)	22 (22%)	25 (24%)	0	0
15	M	106/166 (64%)	71 (67%)	21 (20%)	14 (13%)	0	1
16	N	115/118 (98%)	72 (63%)	25 (22%)	18 (16%)	0	0
17	O	92/100 (92%)	57 (62%)	16 (17%)	19 (21%)	0	0
18	P	125/134 (93%)	94 (75%)	20 (16%)	11 (9%)	1	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	Q	91/95 (96%)	44 (48%)	23 (25%)	24 (26%)	0	0
20	R	108/115 (94%)	60 (56%)	24 (22%)	24 (22%)	0	0
21	S	173/237 (73%)	94 (54%)	40 (23%)	39 (22%)	0	0
22	T	82/91 (90%)	48 (58%)	20 (24%)	14 (17%)	0	0
23	U	70/81 (86%)	35 (50%)	18 (26%)	17 (24%)	0	0
24	V	64/67 (96%)	32 (50%)	20 (31%)	12 (19%)	0	0
25	W	53/55 (96%)	42 (79%)	6 (11%)	5 (9%)	1	1
26	Z	56/60 (93%)	41 (73%)	7 (12%)	8 (14%)	0	0
30	4	35/37 (95%)	17 (49%)	9 (26%)	9 (26%)	0	0
All	All	2977/3391 (88%)	1806 (61%)	640 (22%)	531 (18%)	0	0

5 of 531 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	60	ARG
3	A	187	SER
3	A	209	ALA
3	A	217	ARG
3	A	220	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	
3	A	185/215 (86%)	167 (90%)	18 (10%)	10	30
4	B	155/157 (99%)	139 (90%)	16 (10%)	9	26
5	C	157/163 (96%)	132 (84%)	25 (16%)	3	8
6	D	153/156 (98%)	136 (89%)	17 (11%)	8	22
7	E	136/144 (94%)	124 (91%)	12 (9%)	12	35
8	F	51/107 (48%)	49 (96%)	2 (4%)	39	74
9	G	118/146 (81%)	101 (86%)	17 (14%)	4	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	H	103/103 (100%)	93 (90%)	10 (10%)	10	30
11	I	108/121 (89%)	91 (84%)	17 (16%)	3	9
12	J	110/116 (95%)	97 (88%)	13 (12%)	6	19
13	K	90/93 (97%)	73 (81%)	17 (19%)	2	5
14	L	74/82 (90%)	57 (77%)	17 (23%)	1	3
15	M	94/134 (70%)	81 (86%)	13 (14%)	4	12
16	N	96/97 (99%)	85 (88%)	11 (12%)	7	20
17	O	75/79 (95%)	66 (88%)	9 (12%)	6	18
18	P	109/115 (95%)	100 (92%)	9 (8%)	14	38
19	Q	75/76 (99%)	67 (89%)	8 (11%)	8	24
20	R	91/96 (95%)	79 (87%)	12 (13%)	5	14
21	S	149/192 (78%)	133 (89%)	16 (11%)	8	24
22	T	62/67 (92%)	58 (94%)	4 (6%)	21	51
23	U	57/66 (86%)	44 (77%)	13 (23%)	1	3
24	V	54/55 (98%)	48 (89%)	6 (11%)	8	22
25	W	48/48 (100%)	43 (90%)	5 (10%)	9	25
26	Z	51/53 (96%)	43 (84%)	8 (16%)	3	9
30	4	35/35 (100%)	33 (94%)	2 (6%)	25	58
All	All	2436/2716 (90%)	2139 (88%)	297 (12%)	6	18

5 of 297 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	J	11	ARG
14	L	37	HIS
23	U	70	LEU
12	J	64	LYS
13	K	13	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 90 such sidechains are listed below:

Mol	Chain	Res	Type
13	K	13	ASN
16	N	34	ASN
25	W	49	HIS

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Mol	Chain	Res	Type
14	L	37	HIS
14	L	97	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	X	2680/2880 (93%)	695 (25%)	324 (12%)
2	Y	121/123 (98%)	25 (20%)	1 (0%)
All	All	2801/3003 (93%)	720 (25%)	325 (11%)

5 of 720 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	X	2	G
1	X	4	C
1	X	13	A
1	X	14	A
1	X	25	U

5 of 325 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	X	1194	U
1	X	1439	G
1	X	2608	A
1	X	1249	G
1	X	1315	A

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 35 ligands modelled in this entry, 35 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	X	2686/2880 (93%)	-0.17	96 (3%) 46 39	3, 38, 98, 118	0
2	Y	122/123 (99%)	-0.00	3 (2%) 61 56	24, 67, 89, 101	0
3	A	240/274 (87%)	0.29	22 (9%) 11 7	17, 53, 65, 71	0
4	B	205/211 (97%)	-0.44	1 (0%) 91 90	2, 21, 43, 56	0
5	C	197/205 (96%)	0.03	10 (5%) 32 26	14, 43, 58, 66	0
6	D	177/180 (98%)	0.47	13 (7%) 18 12	50, 60, 67, 69	0
7	E	171/185 (92%)	-0.08	5 (2%) 55 49	38, 53, 64, 68	0
8	F	71/144 (49%)	2.92	51 (71%) 0 0	0, 77, 83, 85	0
9	G	142/174 (81%)	0.12	10 (7%) 19 14	24, 39, 53, 63	0
10	H	134/134 (100%)	-0.52	0 100 100	3, 17, 33, 42	0
11	I	141/156 (90%)	0.78	24 (17%) 2 1	21, 53, 62, 71	0
12	J	136/142 (95%)	-0.02	3 (2%) 65 61	28, 43, 60, 65	0
13	K	113/116 (97%)	-0.46	0 100 100	2, 10, 24, 34	0
14	L	104/114 (91%)	0.28	10 (9%) 10 6	38, 51, 58, 63	0
15	M	108/166 (65%)	-0.54	1 (0%) 85 84	3, 18, 43, 55	0
16	N	117/118 (99%)	-0.18	2 (1%) 73 70	5, 37, 54, 61	0
17	O	94/100 (94%)	-0.15	3 (3%) 51 44	22, 47, 59, 64	0
18	P	127/134 (94%)	-0.49	0 100 100	4, 18, 47, 59	0
19	Q	93/95 (97%)	0.01	3 (3%) 51 44	29, 42, 57, 68	0
20	R	110/115 (95%)	0.39	12 (10%) 7 4	35, 46, 61, 65	0
21	S	175/237 (73%)	0.65	16 (9%) 11 7	49, 58, 64, 68	0
22	T	84/91 (92%)	0.63	14 (16%) 2 1	26, 44, 59, 70	0
23	U	72/81 (88%)	0.76	12 (16%) 2 1	41, 53, 63, 67	0
24	V	66/67 (98%)	-0.10	2 (3%) 54 47	38, 52, 65, 67	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	W	55/55 (100%)	-0.38	0 100 100	21, 37, 49, 64	0
26	Z	58/60 (96%)	-0.41	1 (1%) 73 70	4, 16, 38, 44	0
27	1	53/55 (96%)	3.51	42 (79%) 0 0	37, 47, 56, 60	0
28	2	46/47 (97%)	6.30	46 (100%) 0 0	11, 27, 34, 37	0
29	3	63/66 (95%)	5.75	59 (93%) 0 0	21, 36, 46, 48	0
30	4	37/37 (100%)	1.01	8 (21%) 1 1	44, 52, 58, 59	0
All	All	5997/6562 (91%)	0.13	469 (7%) 16 11	0, 43, 85, 118	0

The worst 5 of 469 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
29	3	37	SER	16.8
29	3	38	GLY	16.5
29	3	39	ASP	11.7
29	3	33	ASN	11.7
29	3	43	GLY	11.1

## 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 ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
31	MG	X	2910	1/1	0.62	0.37	21.47	19,19,19,19	0
31	MG	X	2908	1/1	0.72	0.50	18.86	17,17,17,17	0
31	MG	Y	124	1/1	0.80	0.44	12.95	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
31	MG	X	2882	1/1	0.66	0.29	9.24	12,12,12,12	0
31	MG	X	2906	1/1	0.91	0.43	7.34	13,13,13,13	0
31	MG	X	2899	1/1	0.88	0.22	4.64	19,19,19,19	0
31	MG	X	2888	1/1	0.83	0.23	4.44	3,3,3,3	0
31	MG	X	2895	1/1	0.97	0.35	1.85	3,3,3,3	0
31	MG	X	2904	1/1	0.96	0.14	-0.56	3,3,3,3	0
31	MG	Y	128	1/1	0.83	0.15	-	41,41,41,41	0
31	MG	X	2897	1/1	0.93	0.52	-	3,3,3,3	0
31	MG	X	2909	1/1	0.86	0.12	-	3,3,3,3	0
31	MG	X	2907	1/1	0.96	0.17	-	58,58,58,58	0
31	MG	X	2894	1/1	0.95	0.39	-	15,15,15,15	0
31	MG	X	2886	1/1	0.51	0.33	-	41,41,41,41	0
31	MG	X	2891	1/1	0.99	0.51	-	12,12,12,12	0
31	MG	X	2883	1/1	0.76	0.19	-	49,49,49,49	0
31	MG	X	2881	1/1	0.83	0.24	-	59,59,59,59	0
31	MG	X	2901	1/1	0.93	0.28	-	3,3,3,3	0
31	MG	X	2892	1/1	0.87	0.19	-	22,22,22,22	0
31	MG	X	2898	1/1	0.92	0.42	-	3,3,3,3	0
31	MG	X	2889	1/1	0.98	0.37	-	3,3,3,3	0
31	MG	X	2902	1/1	0.98	0.11	-	60,60,60,60	0
31	MG	X	2885	1/1	0.84	0.53	-	56,56,56,56	0
31	MG	X	2905	1/1	0.92	0.28	-	6,6,6,6	0
31	MG	Y	125	1/1	0.97	0.20	-	9,9,9,9	0
31	MG	X	2900	1/1	0.83	0.40	-	3,3,3,3	0
31	MG	Y	127	1/1	0.90	0.17	-	12,12,12,12	0
31	MG	X	2896	1/1	0.92	0.25	-	3,3,3,3	0
31	MG	X	2893	1/1	0.83	0.21	-	13,13,13,13	0
31	MG	X	2890	1/1	0.84	0.20	-	49,49,49,49	0
31	MG	X	2903	1/1	0.93	0.24	-	24,24,24,24	0
31	MG	X	2884	1/1	0.52	0.42	-	55,55,55,55	0
31	MG	Y	126	1/1	0.74	0.29	-	25,25,25,25	0
31	MG	X	2887	1/1	0.94	0.15	-	3,3,3,3	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.