



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 05:38 PM GMT

PDB ID : 4IOA  
Title : Crystal structure of compound 4e bound to large ribosomal subunit (50S) from *Deinococcus radiodurans*  
Authors : Han, S.; Marr, E.S.  
Deposited on : 2013-01-07  
Resolution : 3.20 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

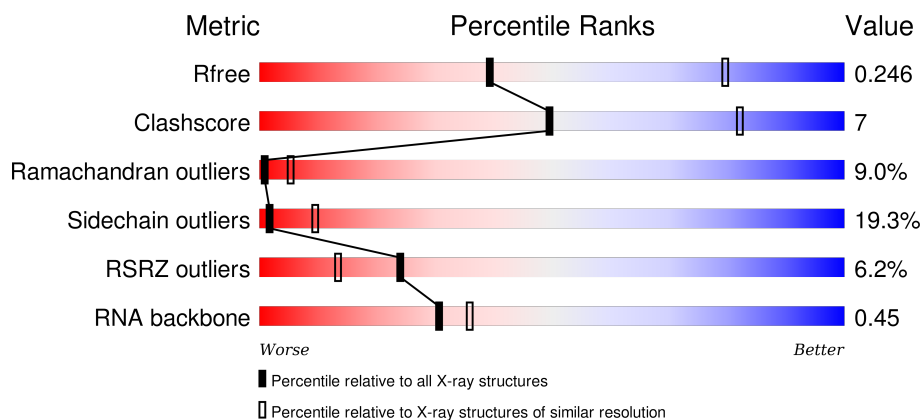
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)
RNA backbone	2183	1079 (3.70-2.70)

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> <div></div> <div>36%</div> <div>34%</div> <div>19%</div> <div>7%</div> </div> </div>
2	Y	123	<div> <div>2%</div> <div> <div></div> <div>40%</div> <div>42%</div> <div>15%</div> <div>••</div> </div> </div>
3	A	274	<div> <div>2%</div> <div> <div></div> <div>48%</div> <div>30%</div> <div>8%</div> <div>•</div> <div>12%</div> </div> </div>
4	B	211	<div> <div>%</div> <div> <div></div> <div>67%</div> <div>21%</div> <div>9%</div> <div>•</div> </div> </div>

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Mol	Chain	Length	Quality of chain
5	C	205	
6	D	180	
7	E	185	
8	F	144	
9	G	174	
10	H	134	
11	I	156	
12	J	141	
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	

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Mol	Chain	Length	Quality of chain
30	4	37	<div> <div>97%</div> <div>73%</div> <div>24%</div> </div>

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	2902	-	-	-	X
31	MG	X	2908	-	-	-	X
31	MG	X	2916	-	-	-	X
31	MG	X	2919	-	-	-	X
31	MG	X	2924	-	-	-	X
31	MG	X	2926	-	-	-	X
31	MG	X	2928	-	-	-	X
31	MG	Y	201	-	-	-	X

## 2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 83879 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 23S ribosomal 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 5S ribosomal 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	S	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			

- 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		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	0	0	53
			53 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

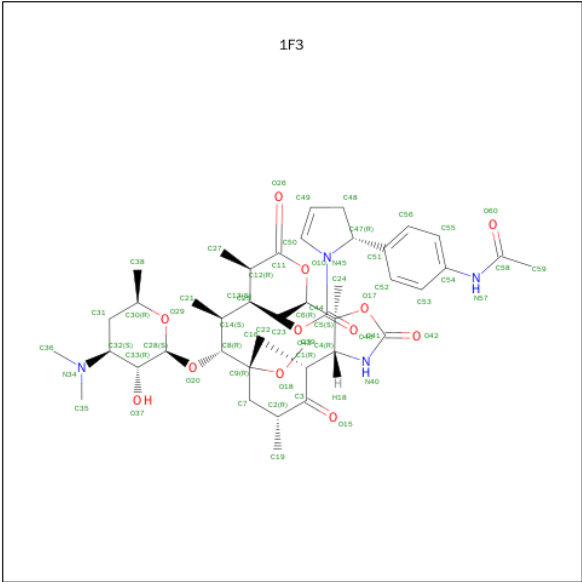
- Molecule 30 is a protein called 50S ribosomal protein L36.

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

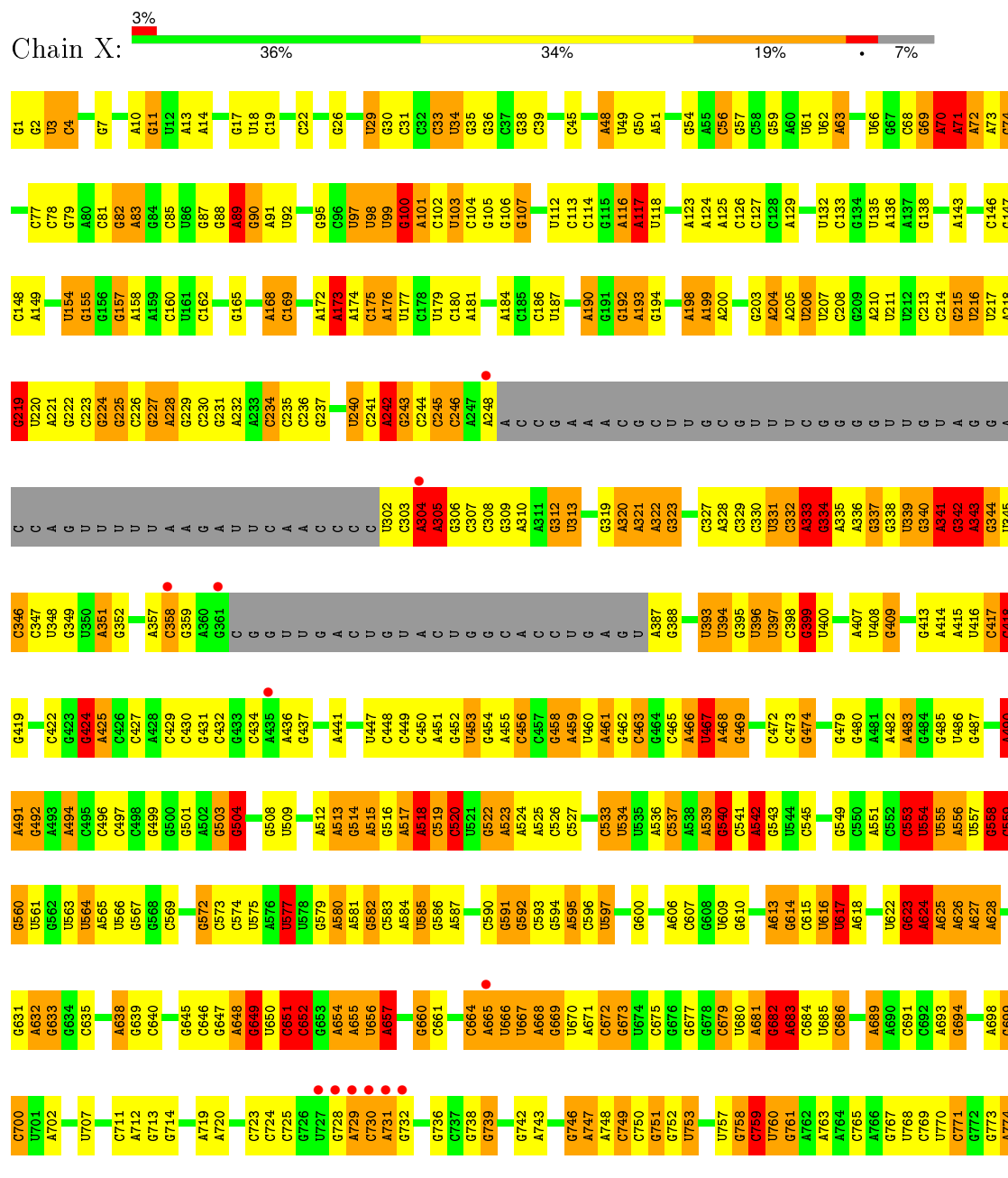
- Molecule 32 is (3AS,4R,7R,8S,9S,10R,11R,13R,15R,15AR)-4-ETHYL-11-METHOXY-3-A,7,9,11,13,15-HEXAMETHYL-2,6,14-TRIOXO-10-{{3,4,6-TRIDEOXY-3-(DIMETHYL AMINO)-BETA-D-XYLO-HEXOPYRANOSYL}OXY}TETRADECAHYDRO-2H-OXA CYCLOTETRADECINO[4,3-D][1,3]OXAZOL-8-YL (2R)-2-[4-(ACETYLAMINO)PHEN YL]-2,3-DIHYDRO-1H-PYRROLE-1-CARBOXYLATE (three-letter code: 1F3) (formula: C<sub>44</sub>H<sub>66</sub>N<sub>4</sub>O<sub>12</sub>).



### 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.

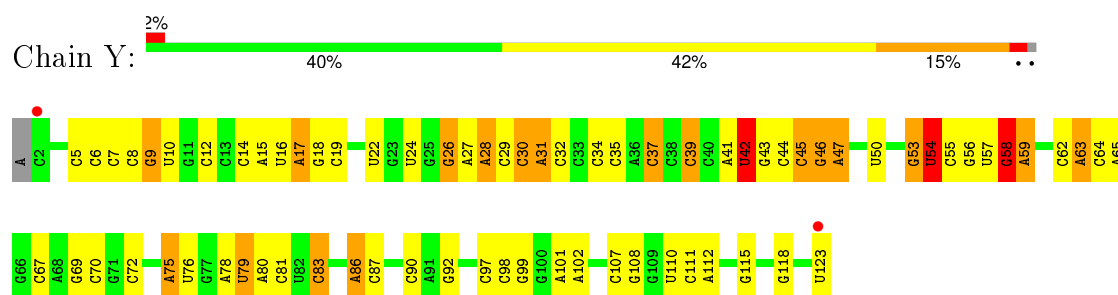
#### • Molecule 1: 23S ribosomal RNA



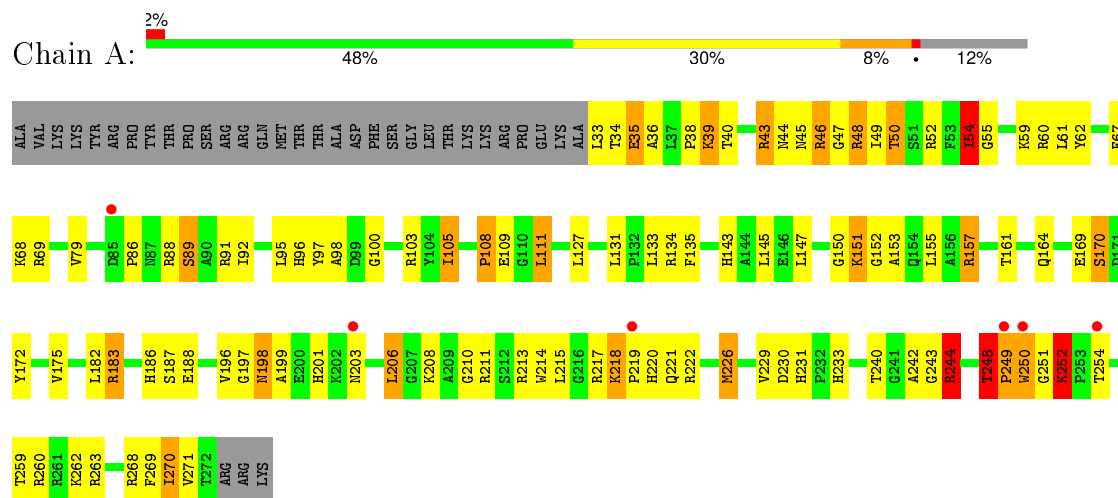
G1790	C1791	G1720	U1847	U1564	A1493	C1418	U1342	G1273	C1190	G1117	U1056	A984	U	A838	U776
C1792	A1793	G1721	C1648	A1567	G1494	U1421	C1343	C1274	G1191	G1118	A1057	G985	A	U839	G776
A1794	C1795	G1722	U1651	U1567	G1495	C1422	C1344	C1275	A1192	U1119	G1058	A986	C	U840	A777
G1796	A1796	U1723	G1652	C1570	C1497	U1426	C1346	U1276	U1194	G1121	C1060	A989	C	U842	G778
		G1724	G1571	G1572	A1499	G1427	C1347	A1278	U1195	G1122	G1063	A990	A911	G843	U779
		G1725	C1655	G1573	U1500	A1428	G1350	G1279	U1199	G1123	C1064	C993	U917	G844	G781
A1799	A1800	C1729	A1656	G1574	A1428	A1428	G1351	U1280	G1200	U1124	A1065	A994	A922	U845	U784
		G1730	C1575	G1575	U1505	G1430	C1352	A1281	G1201	C1127	G1066	A995	A923	U846	U785
G1803	U1804	C1731	G1659	G1576	U1506	U1431	C1353	A1282	U1202	G1128	G1067			C847	U786
U1805	G1806	U1732	G1660	G1577	A1507	G1432	C1354	A1283	C1210	U1129	A1068	C998	C926	C851	A787
		U1733	C1661	G1579	G1508	A1433	C1355	G1284		U1130	G1069	A999	C927	U852	G788
G1805	G1806	G1734	G1662	C1580	A1509	U1434	G1356	A1285	C1218	G1131	G1070	G1000	C928	C853	G789
G1806	A1807	G1735	C1581	C1581	A1510	U1437	C1358	U1286	C1219	C1132	U1071	A1001		U857	A790
G1807	C1808	G1736	G1664	A1582	G1513	G1438	C1367	A1287	U1202	G1133	G1072	C1002	G931	U858	G791
G1808	G1809	G1737	C1665	A1583	U1514	U1445	C1368	A1288	G1220	C1134	G1073	C1003		U859	U792
U1810			G1666	G1584	C1515	A1441	C1369	A1289	G1221	C1135	G1074	U1004	C937	C863	A794
U1811	U1812	G1741	A1667	A1585	U1515	C1442	C1365	G1291	G1223	G1136	C1075	U1005	C938	C864	A795
		G1742	G1668	A1586	G1519	G1443	U1366	A1292	A1224	A1137	U1076	C1006	C939	A796	
G1812	G1813	C1745	A1669		U1520	C1444	C1367	U1287	G1225	G1138	U1077	C1007	C940	A797	
G1814	G1815	A1746	C1670	G1445	U1521	A1445	G1368	A1288	G1226	C1139	G1078	C1008	C941	U865	A798
G1815	G1816	G1747	A1672	A1446	C1522	U1447	C1373	G1298	G1229	U1141	A1080	U1010	C942	U866	G798
U1817	G1818	U1748	C1673	A1448	U1523	U1447	A1378	A1299	C1230	G1142	C1081	A1011	C943	U867	C799
		G1749	G1674	A1448	C1524	A1448	A1379	A1300	A1231	C1143	G1082	A1012	C944	U868	U800
G1818	G1819	C1675	U1600	G1599	A1525		C1380	U1301	U1232	U1144	C1083	G1013	C945	C869	A801
U1819	G1820	G1676	U1601	U1526	C1527	C1451	A1378	U1302	A1233	C1145	C1084	G1014	C946	C870	A802
G1820	A1821	U1678	G1602	G1527	G1528	C1451	C1389	U1303	C1234	C1146	C1085	G1015	C947	U871	C803
A1821	G1822	G1754	A1603	C1528	U1544	U1454	G1390	U1304	C1235	G1149	C1086	C1016	C948	C872	C804
		G1755	C1529	G1529	U1458	U1458	G1384	U1305	G1236	C1150	C1087	C1017	C949	U873	C805
G1823	C1824	C1758	U1530	U1530	A1458	U1458	C1385	U1306	G1237	C1151	A1088	C1018	C951	A874	A806
U1825	G1826	G1762	A1532	A1532	U1459	G1460	C1385	U1307	A1238	C1152	C1089	C1019	C952	C875	C809
G1827	U1828	G1763	C1533	C1533	C1461	G1461	C1388	C1310	A1239	C1153	C1090	A1022	C953	C877	U810
G1828	C1829	C1764	A1534	C1535	G1465	G1465	C1389	C1311	G1240	A1153	C1091	U1023	C954	U878	G811
C1830	G1831	G1765	C1535	C1535	C1466	C1466	G1390	G1312	G1241	A1154	U1092	G1024	C955	A879	G812
U1832	G1833	U1766	U1539	U1539	U1467	U1467	C1391	G1312	A1242	G1155	C1093		C956	C880	A813
G1833	U1834	G1767	C1540	C1540	A1468	A1468	U1392	U1313	C1243	U1161	C1094	G1028	C957	U881	G814
U1834		U1770	G1541	G1541	U1469	U1469	C1396	A1314	U1244	C1164	A1095	C1029	C958	C882	A815
G1834		A1771	G1542	G1542	U1470	G1470	C1397	A1315	G1245		A1096	C1030	C959	A883	U816
		A1694	G1543	G1543	G1471	G1471	C1398	C1319	U1247	A1167	A1099	A1032	A964	C884	C818
G1838	A1839	C1772	A1544	A1544	C1472	C1472	C1399	G1324	G1248	C1168	U1101	G1033	C967	U890	C819
A1839	U1840	G1773	G1545	G1545	U1473	U1473	U1403	U1325	A1250	C1169	G1102	U1034	C968	A891	U820
G1841	C1842	C1627	C1546	C1546	A1474	A1474	C1404	G1326	C1251	U1170	C1103	G1035	C969	G	A821
U1843	G1844	G1629	U1547	U1547	U1475	U1475	C1405	C1327	C1252	A1171	C1103	G1036	A970	G	U823
		A1699	U1548	U1548	G1476	G1476	A1406	C1328	C1253	U1172	G1104	U1037	A971	G	U824
G1844		C1700	C1549	C1549	G1477	G1477	A1407	U1329	G1254	G1173	U1105	U1038	C972	G	C825
		G1703	U1550	U1550	U1478	U1478	G1407	G1330	A1255	G1174	A1106	U1038	U973	G	U826
A1845		C1703	C1551	C1551	U1482	U1482	A1408		C1256	C1181	A1107	A1043	U974	C	C827
		U1710	G1552	G1552	G1483	G1483	U1409	G1333	U1257	U1182	U1108	U1044	C975	C	C828
G1850		A1780	C1553	C1553	C1487	C1487	U1410	U1334	G1263	U1183	A1109	C1049	C976	U	C829
		C1781	G1554	G1554	G1488	G1488	C1411	A1335	U1264	C1184	G1110	C1049	C977	A	C830
C1853	G1854	G1713	U1637	U1637	C1489	C1489	U1412	G1336	G1265	G1184	C1111	U1051	U978	C	G831
		A1714	G1644	G1644	U1490	U1490	U1413	G1337	G1266	C1185	C1112	C1062	A979	C	A832
G1858		G1715	U1645	U1645	C1489	C1489	G1414	G1338	G1286	G1186	C1113	C1062	G980	A	A833
		U1787	G1646	G1646	U1491	U1491	C1415	U1339	A1267	A1187	C1114	C1063	C981	G	A834
		U1789			C1490	C1490	A1416	U1340	U1268	A1188	C1115	C1064	C982	C	U835
A1859			G1646	G1646	A1492	A1492	C1417	G1341	G1269	G1189	U1116	A1055	G983	U	

U2871	C2791	C2645	C2573	C2499	G2423	A2355	U2285	G2209	A	U2086	U2004	U1926	A1960
U2872	C2792	C2646	C2574	C2500	G2426	C2358	G2286	G2209	A	U2087	U2004	U1927	G1861
C2875	C2793	C2650	C2575	U2501	A2427	U2359	G2287	U2212	C	U2088	G2006	G1928	G1862
C2876	C2794	C2651	C2576	G2502	G2428	C2360	A2288	G2213	G	C2089	U2009	A1935	U1863
A2877	A2795	A2653	A2577	G2503	U2429	G2361	U2291	G2217	G	U2090	G2010	A1936	G1865
C	C2797	A2654	A2578	C2504	A2430	G2362	C2292	G2218	U	C	U2011	G1937	G1866
U	C2798	C2656	C2579	C2505	A2431	U2363	C2293	U2222	A	U	U2012	U1938	A1867
C	C2799	C2657	A2580	U2506	G2432	C2364	U2294	U2223	A	U	A2013	U1939	
C2800	U2583	U2583	U2583	A2509	U2433	U2366	U2296	U2223	U	C	A2014	C1940	U1870
G2805	G2587	G2587	G2587	G2514	U2439	G2370	G2297	A2226	U	U	G2015	A1943	G1871
G2806	U2588	U2588	U2588	G2515	C2440	A2371	U2298	C2227	C	U	A2016	A1872	A1872
U2807	C2662	C2662	C2662	U2516	U2441	A2372	A2299	U2228	C	G	U2017	C1944	A1873
U2808	U2663	U2663	U2663	C2517	C2442	A2373	G2300	G2229	A	G	G2018	C1945	G1874
A2809	U2666	U2666	U2666	G2522	C2444	C2374	G2302	G2231	C	U	C2019	U1946	
A2810	C2667	C2667	C2667	G2523	C2445	G2375	C2303	G2231	C	U		G1947	C1877
A2811	U2668	U2668	U2668	G2524	G2446	G2376	G2304	G2232	C	U	A2025	C1950	G1882
G2812	C2669	C2669	C2669	G2525	C2447	U2377	C2305	U2236	U	G	C2026	A1853	A1883
G2813	C2670	C2670	C2670	G2526	G2448	U2378	C2306	C2237	G	U	A2031	A1854	A1884
C2815	U2672	U2672	U2672	C2528	C2449	A2381	A2307	G2238	G	U	A2034	A1954	C1885
C2824	U2675	U2675	U2675	C2530	U2452	C2382	G2309	C2240	G	G	G2035	G1955	G1886
A2825	C2678	C2678	C2678	U2533	A2455	C2383	G2310	U2241	A	G	G2036	G1958	G1887
C2826	G2679	G2679	G2679	U2534	U2456	G2384	U2311	G2242	C	C	A2037	C1962	G
G2827	C2680	C2680	C2680	C2535	C2457	U2385	A2312	C2243	C	C	U2171	G1963	G
U2830	A2681	A2681	A2681	A2540	G2463	U2387	G2313	C2243	C	C	G2038	A1964	C
U2841	C2682	C2682	C2682	U2541	G2464	U2388	A2314	A2247	U	U	U1965	U1965	G
C2842	A2683	A2683	A2683	U2542	U2470	G2389	U2315	U2251	C	C	A2042	C1971	A
A2843	G2684	G2684	G2684	U2543	U2471	G2392	U2318	C2254	C	C	G2043	G1972	A
G2844	A2685	A2685	A2685	C2544	U2472	C2393	C2321	G2255	A	A	A2044	C1973	C
G2845	G2686	G2686	G2686	G2545	G2473	G2394	U2322	G2256	A	A	A2045	C1974	C
G2846	A2687	A2687	A2687	C2546	G2474	C2395	U2323	G2257	A	A	C2046	U1975	A
G2847	C2688	C2688	C2688	G2547	C2475	C2396	G2324	A2257	U	U	C2048	U1976	A
A2848	A2689	A2689	A2689	G2548	A2476	A2397	G2325	G2258	C	C	G2049	C1977	A
U2849	C2691	C2691	C2691	C2549	G2477	U2398	C2326	G2261	U	U	G2050	U1978	A
U2850	G2692	G2692	G2692	A2551	U2479	A2401	C2329	C2262	C	C	U2051	C1979	C
G2851	U2693	U2693	U2693	C2552	C2480	U2402	G2330	C2263	C	C	G2052	C1980	G
G2852	G2694	G2694	G2694	G2553	G2481	C2403	U2334	C2264	C	C	U2062	G1982	U
U2853	U2697	U2697	U2697	C2554	A2482	A2404	C2334	A2265	U	U	A2064	A1984	C
G2854	G2698	G2698	G2698	G2555	U2483	A2405	U2335	A2266	U	U		G1985	
C2855	U2699	U2699	U2699	A2556	G2484	C2406	G2336	A2267	C	C	U2067	G1986	
U2856	U2700	U2700	U2700	G2557	G2485	G2407	U2337	U2270	G	G	G2070	G1987	A1910
C2857	A2701	A2701	A2701	C2558	C2486	G2408	A2339	C2271	U	U		A1988	A1911
A2858	C2702	C2702	C2702	U2559	G2487	U2409	C2340	A2272	G	G	G2071	C1989	G1912
U2859	C2703	C2703	C2703	G2560	C2488	U2410	C2341	C2273	U	U	C2072	U1990	G1913
C2860	U2704	U2704	U2704	G2561	C2489	U2411	C2343	C2274	C	C		C1991	U1914
U2861	A2705	A2705	A2705	U2562	U2490	A2414	G2344	C2275	U	U	A2079	G1992	C
C2864	U2706	U2706	U2706	C2563	C2491	U2415	G2345	U2276	G	G	U2080	G1993	G1917
G2865	A2707	A2707	A2707	U2564	G2492	U2416	C2347	C2276	U	U	U2081	U1994	G1918
A2866	U2708	U2708	U2708	G2565	U2493	U2417	A2348	G2279	C	C	G2082	G1995	A1920
G2867	C2709	C2709	C2709	G2566	C2494	A2418	G2349	A2281	A	A	U2083	A1996	A1921
C2868	G2710	G2710	G2710	A2567	G2495	C2419	G2350	G2282	G	G	U2084	A1997	U1922
U2869	A2711	A2711	A2711	A2568	C2496	C2420	G2351	G2283	C	C	G2085	A1998	U1923
	G2712	G2712	G2712	A2569	A2497	C2421	G2352	U2284	G	G		U1999	U1924
	C2790	C2790	C2790	C2570	U2498	C2422	G2354		C	C		U2000	C1925

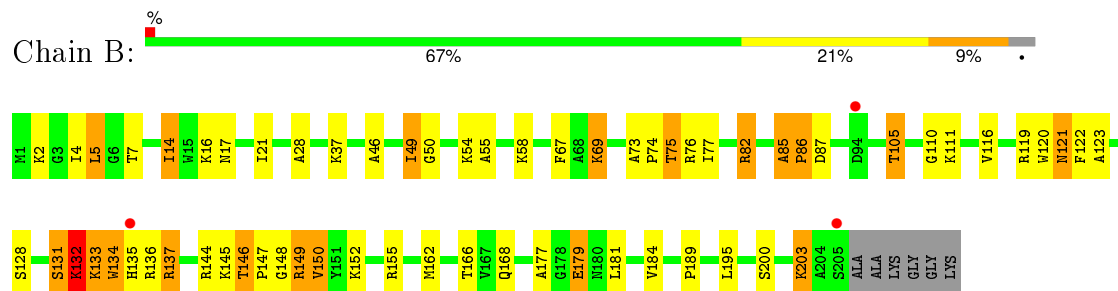
- Molecule 2: 5S ribosomal RNA



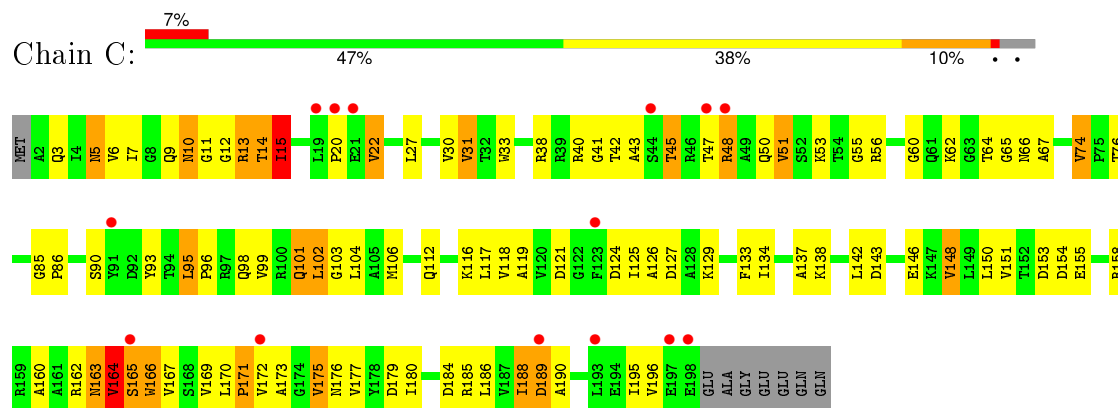
• Molecule 3: 50S ribosomal protein L2



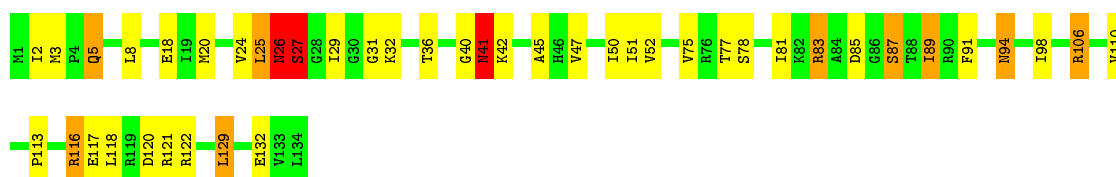
• Molecule 4: 50S ribosomal protein L3



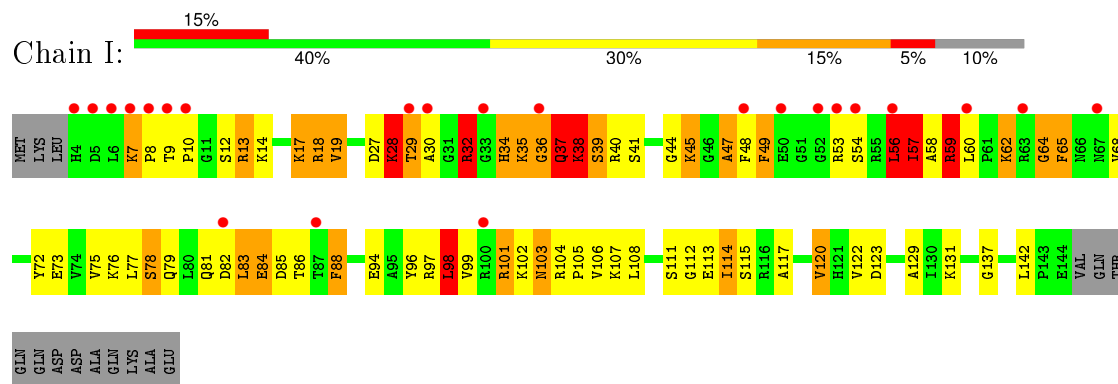
• Molecule 5: 50S ribosomal protein L4



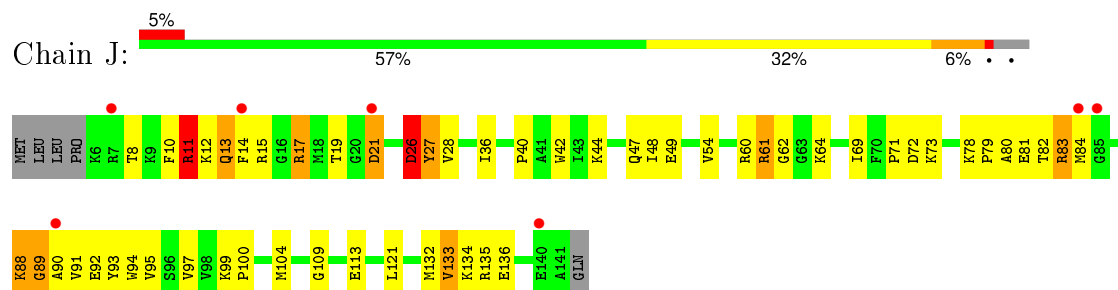




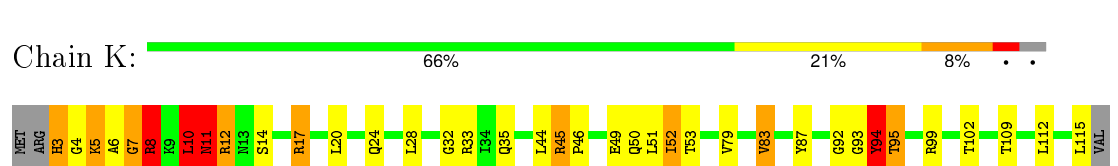
• Molecule 11: 50S ribosomal protein L15



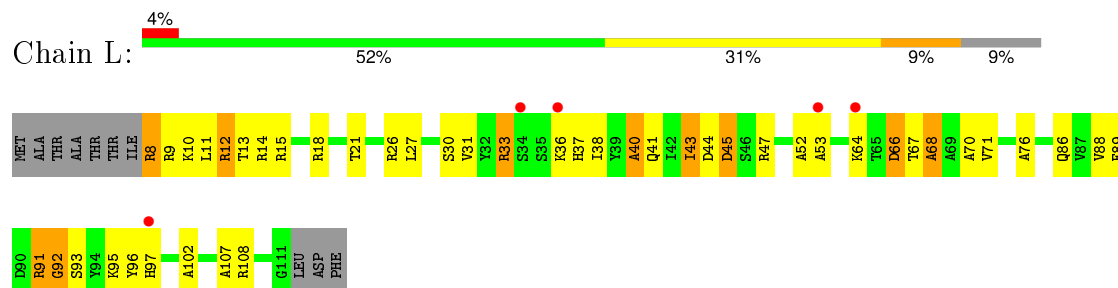
• Molecule 12: 50S ribosomal protein L16



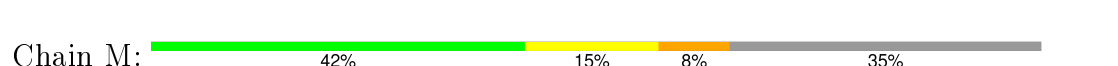
• Molecule 13: 50S ribosomal protein L17



• Molecule 14: 50S ribosomal protein L18

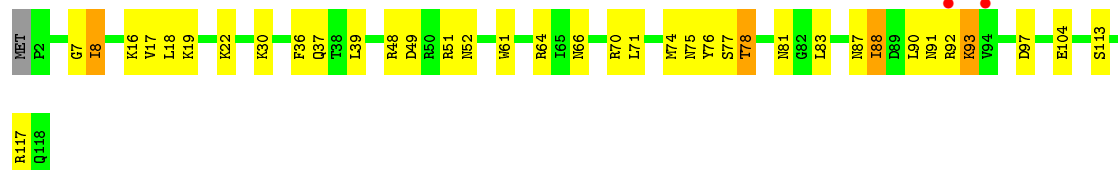


• Molecule 15: 50S ribosomal protein L19

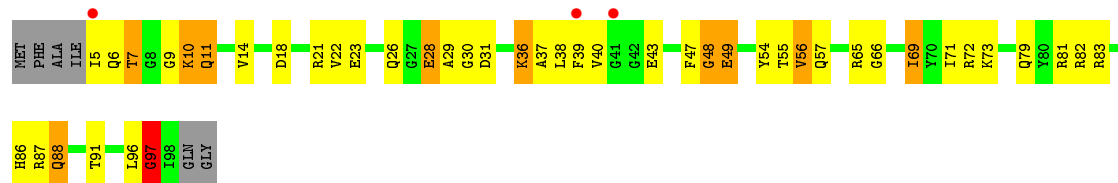




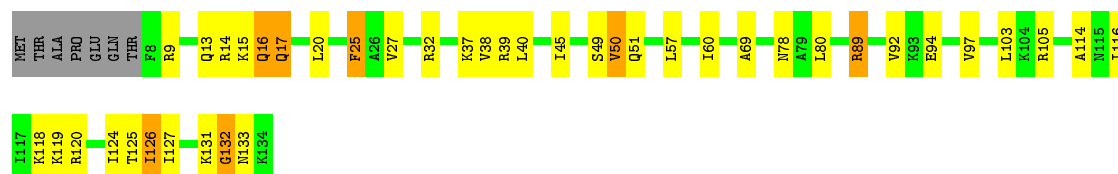
- Molecule 16: 50S ribosomal protein L20



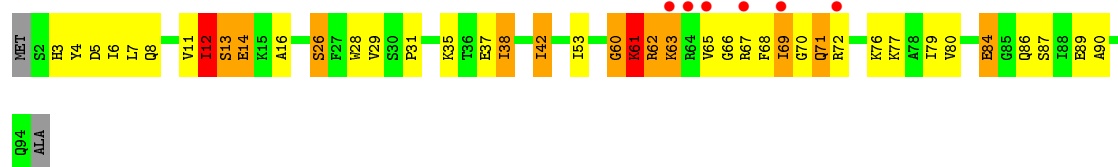
- Molecule 17: 50S ribosomal protein L21



- Molecule 18: 50S ribosomal protein L22



- Molecule 19: 50S ribosomal protein L23

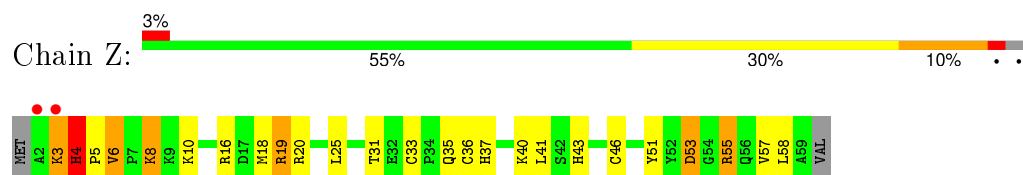


- Molecule 20: 50S ribosomal protein L24

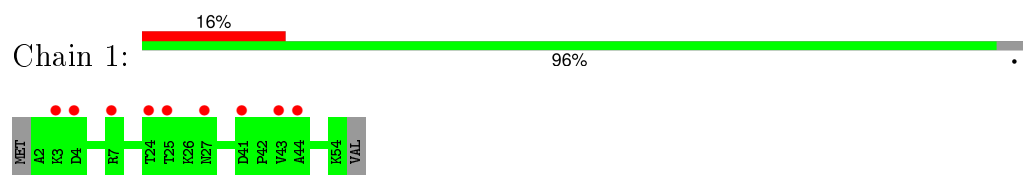




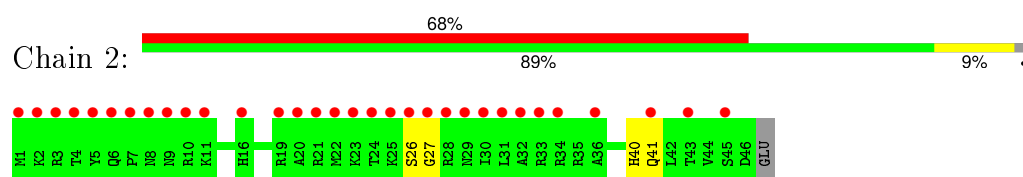
- Molecule 26: 50S ribosomal protein L32



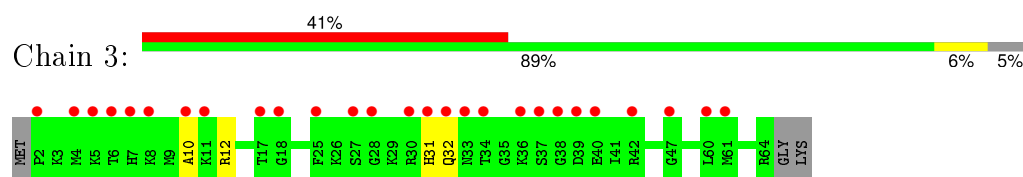
- Molecule 27: 50S ribosomal protein L33



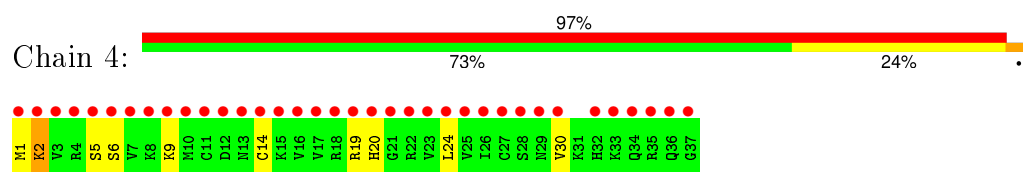
- Molecule 28: 50S ribosomal protein L34



- Molecule 29: 50S ribosomal protein L35



- Molecule 30: 50S ribosomal protein L36



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	169.77Å 406.66Å 696.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.20 30.38 – 3.23	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-3.20) 89.8 (30.38-3.23)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.51 (at 3.24Å)	Xtriage
Refinement program	autobuster	Depositor
R, $R_{free}$	0.197 , 0.230 0.211 , 0.246	Depositor DCC
$R_{free}$ test set	17364 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	80.0	Xtriage
Anisotropy	0.713	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.24 , 91.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 343784 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	83879	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% 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, 1F3

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	1.00	38/64561 (0.1%)	1.86	1965/100708 (2.0%)
2	Y	1.02	0/2904	1.68	66/4525 (1.5%)
3	A	0.62	0/1862	0.96	2/2510 (0.1%)
4	B	0.60	0/1567	0.96	2/2105 (0.1%)
5	C	0.63	0/1529	0.95	1/2070 (0.0%)
6	D	0.47	0/1419	0.67	0/1903
7	E	0.44	0/1308	0.68	0/1771
8	F	0.47	0/508	0.64	0/683
9	G	0.64	0/1138	1.01	4/1539 (0.3%)
10	H	0.55	0/1007	0.84	1/1352 (0.1%)
11	I	0.73	0/1081	1.11	8/1448 (0.6%)
12	J	0.65	0/1113	0.92	2/1486 (0.1%)
13	K	0.80	2/886 (0.2%)	0.99	3/1188 (0.3%)
14	L	0.57	0/785	0.95	1/1048 (0.1%)
15	M	0.65	1/884 (0.1%)	0.98	2/1186 (0.2%)
16	N	0.51	0/994	0.78	0/1323
17	O	0.56	0/750	0.96	1/1000 (0.1%)
18	P	0.56	0/1027	0.82	0/1373
19	Q	0.62	0/737	1.04	4/988 (0.4%)
20	R	0.64	0/835	0.99	0/1121
21	S	0.49	0/1370	0.73	0/1862
22	T	0.53	0/633	0.85	0/838
23	U	0.75	0/556	1.12	2/741 (0.3%)
24	V	0.47	0/537	0.69	0/714
25	W	0.46	0/426	0.79	0/568
26	Z	0.65	0/469	0.97	0/629
30	4	0.48	0/298	0.72	0/390
All	All	0.91	41/91184 (0.0%)	1.68	2064/137069 (1.5%)

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	6

The worst 5 of 41 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	540	G	C2-N3	9.96	1.40	1.32
1	X	774	A	C5-C4	9.11	1.45	1.38
1	X	774	A	N7-C5	-7.92	1.34	1.39
1	X	2018	G	N9-C8	7.57	1.43	1.37
1	X	542	A	N7-C5	-7.47	1.34	1.39

The worst 5 of 2064 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1288	A	C1'-O4'-C4'	-38.76	78.89	109.90
1	X	1288	A	C5'-C4'-O4'	20.93	134.22	109.10
1	X	1716	G	P-O3'-C3'	19.09	142.60	119.70
1	X	1288	A	C4'-C3'-C2'	-19.04	83.56	102.60
1	X	2808	U	O4'-C1'-N1	17.91	122.53	108.20

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	X	1288	A	Sidechain
1	X	219	G	Sidechain
1	X	474	G	Sidechain
1	X	683	A	Sidechain
1	X	739	G	Sidechain

## 5.2 Too-close contacts [i](#)

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	29049	431	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Y	2598	0	1328	17	0
3	A	1826	0	1885	62	0
4	B	1539	0	1600	62	0
5	C	1506	0	1525	57	0
6	D	1400	0	1481	22	0
7	E	1286	0	1336	9	0
8	F	503	0	520	3	0
9	G	1114	0	1144	63	0
10	H	997	0	1046	24	0
11	I	1067	0	1103	48	0
12	J	1090	0	1125	32	0
13	K	878	0	930	28	0
14	L	779	0	820	17	0
15	M	871	0	894	29	0
16	N	978	0	1020	25	0
17	O	741	0	756	30	0
18	P	1014	0	1096	20	0
19	Q	726	0	753	23	0
20	R	825	0	881	28	0
21	S	1345	0	1372	21	0
22	T	625	0	655	11	0
23	U	552	0	604	28	0
24	V	533	0	558	4	0
25	W	424	0	470	9	0
26	Z	457	0	462	16	0
27	1	53	0	0	0	0
28	2	46	0	0	2	0
29	3	63	0	0	2	0
30	4	297	0	330	5	0
31	X	30	0	0	0	0
31	Y	5	0	0	0	0
32	X	60	0	66	2	0
All	All	83879	0	54809	969	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 7.

The worst 5 of 969 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)
13:K:52:ILE:CD1	13:K:52:ILE:CG1	1.93	1.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:I:62:LYS:NZ	11:I:64:GLY:HA2	1.60	1.15
1:X:1333:G:N2	1:X:1344:C:H41	1.44	1.12
15:M:79:ARG:HH11	15:M:79:ARG:HG3	1.03	1.10
19:Q:29:VAL:HG11	19:Q:38:ILE:HD11	1.35	1.09

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%)	170 (71%)	39 (16%)	29 (12%)	0	2
4	B	203/211 (96%)	172 (85%)	17 (8%)	14 (7%)	1	10
5	C	195/205 (95%)	131 (67%)	37 (19%)	27 (14%)	0	1
6	D	175/180 (97%)	136 (78%)	26 (15%)	13 (7%)	1	9
7	E	169/185 (91%)	132 (78%)	29 (17%)	8 (5%)	3	22
8	F	69/144 (48%)	59 (86%)	8 (12%)	2 (3%)	6	36
9	G	140/174 (80%)	103 (74%)	23 (16%)	14 (10%)	1	4
10	H	132/134 (98%)	117 (89%)	9 (7%)	6 (4%)	3	24
11	I	139/156 (89%)	79 (57%)	34 (24%)	26 (19%)	0	0
12	J	134/141 (95%)	97 (72%)	26 (19%)	11 (8%)	1	7
13	K	111/116 (96%)	96 (86%)	7 (6%)	8 (7%)	1	10
14	L	102/114 (90%)	72 (71%)	20 (20%)	10 (10%)	1	4
15	M	106/166 (64%)	95 (90%)	7 (7%)	4 (4%)	4	28
16	N	115/118 (98%)	101 (88%)	10 (9%)	4 (4%)	4	31
17	O	92/100 (92%)	66 (72%)	13 (14%)	13 (14%)	0	1
18	P	125/134 (93%)	114 (91%)	5 (4%)	6 (5%)	3	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	Q	91/95 (96%)	59 (65%)	19 (21%)	13 (14%)	0	1
20	R	108/115 (94%)	66 (61%)	23 (21%)	19 (18%)	0	0
21	S	173/237 (73%)	145 (84%)	20 (12%)	8 (5%)	3	23
22	T	82/91 (90%)	64 (78%)	9 (11%)	9 (11%)	0	3
23	U	70/81 (86%)	39 (56%)	17 (24%)	14 (20%)	0	0
24	V	64/67 (96%)	57 (89%)	3 (5%)	4 (6%)	2	13
25	W	53/55 (96%)	49 (92%)	4 (8%)	0	100	100
26	Z	56/60 (93%)	47 (84%)	5 (9%)	4 (7%)	1	10
30	4	35/37 (95%)	28 (80%)	5 (14%)	2 (6%)	2	17
All	All	2977/3390 (88%)	2294 (77%)	415 (14%)	268 (9%)	1	5

5 of 268 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	60	ARG
3	A	151	LYS
3	A	170	SER
3	A	187	SER
3	A	199	ALA

### 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%)	144 (78%)	41 (22%)	1	5
4	B	155/157 (99%)	135 (87%)	20 (13%)	5	24
5	C	157/163 (96%)	125 (80%)	32 (20%)	1	7
6	D	153/156 (98%)	129 (84%)	24 (16%)	3	15
7	E	136/144 (94%)	117 (86%)	19 (14%)	4	20
8	F	51/107 (48%)	46 (90%)	5 (10%)	10	38
9	G	118/146 (81%)	95 (80%)	23 (20%)	2	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	H	103/103 (100%)	81 (79%)	22 (21%)	1	6
11	I	108/121 (89%)	72 (67%)	36 (33%)	0	0
12	J	110/115 (96%)	93 (84%)	17 (16%)	3	15
13	K	90/93 (97%)	73 (81%)	17 (19%)	2	10
14	L	74/82 (90%)	54 (73%)	20 (27%)	0	2
15	M	94/134 (70%)	75 (80%)	19 (20%)	1	7
16	N	96/97 (99%)	81 (84%)	15 (16%)	3	15
17	O	75/79 (95%)	60 (80%)	15 (20%)	1	8
18	P	109/115 (95%)	94 (86%)	15 (14%)	4	21
19	Q	75/76 (99%)	60 (80%)	15 (20%)	1	8
20	R	91/96 (95%)	71 (78%)	20 (22%)	1	6
21	S	149/192 (78%)	126 (85%)	23 (15%)	3	16
22	T	62/67 (92%)	53 (86%)	9 (14%)	4	19
23	U	57/66 (86%)	33 (58%)	24 (42%)	0	0
24	V	54/55 (98%)	44 (82%)	10 (18%)	2	10
25	W	48/48 (100%)	38 (79%)	10 (21%)	1	7
26	Z	51/53 (96%)	37 (72%)	14 (28%)	0	1
30	4	35/35 (100%)	31 (89%)	4 (11%)	7	31
All	All	2436/2715 (90%)	1967 (81%)	469 (19%)	2	9

5 of 469 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	I	98	LEU
14	L	33	ARG
24	V	13	ASP
11	I	114	ILE
12	J	134	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 52 such sidechains are listed below:

Mol	Chain	Res	Type
16	N	31	GLN
17	O	79	GLN
25	W	49	HIS

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Mol	Chain	Res	Type
16	N	66	ASN
16	N	81	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	X	2681/2880 (93%)	638 (23%)	238 (8%)
2	Y	121/123 (98%)	28 (23%)	5 (4%)
All	All	2802/3003 (93%)	666 (23%)	243 (8%)

5 of 666 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	X	2	G
1	X	3	U
1	X	4	C
1	X	13	A
1	X	14	A

5 of 243 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	X	1182	U
1	X	1531	C
1	X	2736	U
1	X	1223	G
1	X	1409	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 ⓘ

Of 36 ligands modelled in this entry, 35 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
32	1F3	X	2931	-	60,64,64	1.10	5 (8%)	82,96,96	1.83	18 (21%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	1F3	X	2931	-	-	0/78/119/119	0/5/5/5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	X	2931	1F3	C48-C47	-3.82	1.51	1.54
32	X	2931	1F3	O17-C5	-2.86	1.43	1.47
32	X	2931	1F3	C51-C47	-2.09	1.48	1.51
32	X	2931	1F3	C41-N40	2.31	1.37	1.33
32	X	2931	1F3	C50-N45	2.74	1.44	1.38

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	X	2931	1F3	C59-C58-N57	-5.79	106.72	114.97
32	X	2931	1F3	C28-O20-C8	-4.72	107.83	116.30
32	X	2931	1F3	C23-C6-C5	-4.63	108.42	115.25
32	X	2931	1F3	C5-O17-C41	-4.35	105.67	109.28
32	X	2931	1F3	C27-C12-C13	-3.01	106.28	112.97

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	X	2931	1F3	2	0

## 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%)	-0.19	77 (2%) 55 41	43, 87, 194, 279	0
2	Y	122/123 (99%)	-0.12	2 (1%) 74 62	82, 129, 165, 187	0
3	A	240/274 (87%)	0.06	6 (2%) 61 47	63, 107, 137, 156	0
4	B	205/211 (97%)	-0.33	3 (1%) 76 63	38, 68, 99, 145	0
5	C	197/205 (96%)	0.15	14 (7%) 19 10	55, 107, 150, 178	0
6	D	177/180 (98%)	0.47	16 (9%) 12 6	148, 178, 210, 216	0
7	E	171/185 (92%)	-0.14	4 (2%) 64 49	98, 139, 178, 188	0
8	F	71/144 (49%)	2.76	38 (53%) 0 0	221, 234, 251, 259	0
9	G	142/174 (81%)	0.08	8 (5%) 28 16	65, 89, 137, 149	0
10	H	134/134 (100%)	-0.50	0 100 100	49, 62, 88, 110	0
11	I	141/156 (90%)	0.79	23 (16%) 2 1	54, 120, 171, 195	0
12	J	136/141 (96%)	0.05	7 (5%) 32 18	83, 106, 147, 172	0
13	K	113/116 (97%)	-0.50	0 100 100	37, 53, 71, 99	0
14	L	104/114 (91%)	0.29	5 (4%) 34 21	91, 122, 149, 166	0
15	M	108/166 (65%)	-0.51	0 100 100	44, 64, 106, 128	0
16	N	117/118 (99%)	-0.28	2 (1%) 73 60	54, 86, 124, 152	0
17	O	94/100 (94%)	-0.14	3 (3%) 51 36	67, 106, 146, 160	0
18	P	127/134 (94%)	-0.48	0 100 100	48, 64, 103, 143	0
19	Q	93/95 (97%)	0.10	6 (6%) 22 12	69, 101, 156, 193	0
20	R	110/115 (95%)	0.41	12 (10%) 7 4	84, 113, 170, 173	0
21	S	175/237 (73%)	0.31	13 (7%) 17 10	119, 154, 178, 190	0
22	T	84/91 (92%)	0.81	16 (19%) 2 1	72, 103, 176, 195	0
23	U	72/81 (88%)	0.57	5 (6%) 20 11	86, 122, 146, 182	0
24	V	66/67 (98%)	0.79	8 (12%) 6 3	88, 128, 213, 230	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	W	55/55 (100%)	-0.29	0 100 100	76, 96, 123, 161	0
26	Z	58/60 (96%)	-0.25	2 (3%) 49 34	47, 64, 96, 108	0
27	1	53/55 (96%)	0.89	9 (16%) 2 1	6, 28, 62, 73	0
28	2	46/47 (97%)	2.89	32 (69%) 0 0	3, 10, 27, 42	0
29	3	63/66 (95%)	2.14	27 (42%) 0 0	3, 18, 41, 84	0
30	4	37/37 (100%)	8.19	36 (97%) 0 0	191, 239, 247, 252	0
All	All	5997/6561 (91%)	0.07	374 (6%) 24 13	3, 96, 193, 279	0

The worst 5 of 374 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
30	4	25	VAL	20.6
30	4	16	VAL	17.9
24	V	1	MET	17.0
8	F	114	ASP	16.1
30	4	29	ASN	15.8

## 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	2928	1/1	0.98	0.89	43.39	42,42,42,42	0
31	MG	X	2916	1/1	0.91	0.56	25.04	53,53,53,53	0
31	MG	X	2908	1/1	0.89	0.51	23.90	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
31	MG	X	2926	1/1	0.93	0.99	23.35	56,56,56,56	0
31	MG	X	2924	1/1	0.97	0.64	20.57	39,39,39,39	0
31	MG	Y	201	1/1	0.84	0.50	17.67	82,82,82,82	0
31	MG	X	2902	1/1	0.97	0.42	16.65	45,45,45,45	0
31	MG	X	2919	1/1	0.95	0.57	14.56	56,56,56,56	0
31	MG	X	2915	1/1	0.99	0.28	0.71	24,24,24,24	0
32	1F3	X	2931	60/60	0.97	0.23	0.04	38,60,90,99	0
31	MG	X	2907	1/1	0.98	0.42	-	53,53,53,53	0
31	MG	X	2906	1/1	0.87	0.40	-	79,79,79,79	0
31	MG	X	2909	1/1	0.95	1.00	-	37,37,37,37	0
31	MG	X	2927	1/1	0.84	0.49	-	106,106,106,106	0
31	MG	X	2929	1/1	0.80	0.36	-	77,77,77,77	0
31	MG	X	2901	1/1	0.83	0.39	-	110,110,110,110	0
31	MG	X	2921	1/1	0.97	0.47	-	18,18,18,18	0
31	MG	X	2913	1/1	0.80	0.56	-	66,66,66,66	0
31	MG	Y	202	1/1	0.94	0.48	-	54,54,54,54	0
31	MG	X	2920	1/1	0.97	0.62	-	38,38,38,38	0
31	MG	X	2904	1/1	0.55	0.55	-	90,90,90,90	0
31	MG	X	2911	1/1	0.99	0.43	-	35,35,35,35	0
31	MG	Y	204	1/1	0.95	0.19	-	67,67,67,67	0
31	MG	X	2903	1/1	0.96	0.12	-	82,82,82,82	0
31	MG	X	2925	1/1	0.94	0.46	-	39,39,39,39	0
31	MG	X	2917	1/1	0.98	0.85	-	37,37,37,37	0
31	MG	X	2910	1/1	0.78	0.18	-	85,85,85,85	0
31	MG	X	2914	1/1	0.96	0.59	-	51,51,51,51	0
31	MG	Y	203	1/1	0.75	0.49	-	87,87,87,87	0
31	MG	X	2930	1/1	0.86	0.98	-	71,71,71,71	0
31	MG	X	2922	1/1	0.64	0.87	-	81,81,81,81	0
31	MG	X	2912	1/1	0.90	0.29	-	60,60,60,60	0
31	MG	Y	205	1/1	0.79	0.33	-	77,77,77,77	0
31	MG	X	2918	1/1	0.98	0.60	-	32,32,32,32	0
31	MG	X	2905	1/1	0.70	0.54	-	104,104,104,104	0
31	MG	X	2923	1/1	0.98	0.81	-	74,74,74,74	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.