



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 11:33 PM GMT

PDB ID : 1XBP
Title : Inhibition of peptide bond formation by pleuromutilins: The structure of the 50S ribosomal subunit from *Deinococcus radiodurans* in complex with Tiamulin
Authors : Schlunzen, F.; Pyetan, E.; Fucini, P.; Yonath, A.; Harms, J.M.
Deposited on : 2004-08-31
Resolution : 3.50 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
<http://wwpdb.org/validation/2016/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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

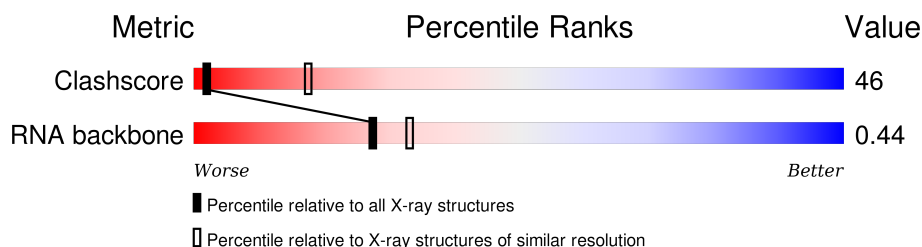
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1157 (3.60-3.40)
RNA backbone	2183	1050 (4.20-2.80)

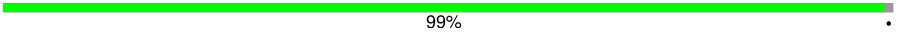

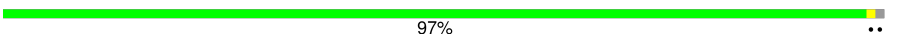


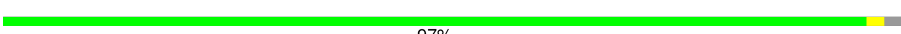









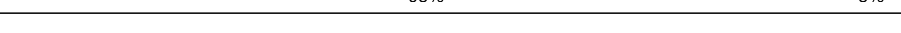
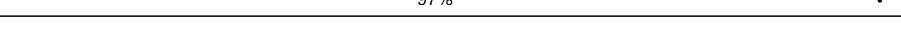
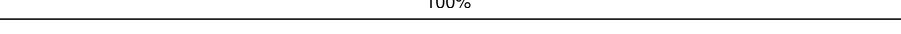
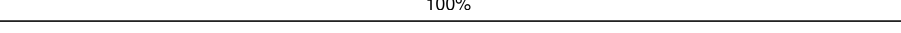
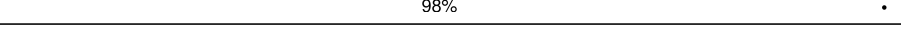
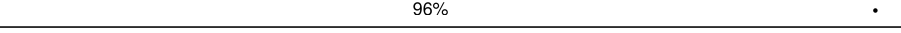
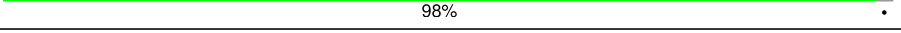
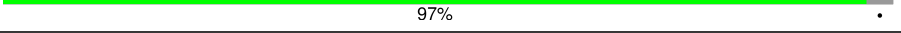
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	0	2880	
2	9	124	
3	A	274	
4	B	211	
5	C	204	
6	D	180	
7	E	185	
8	F	146	

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Mol	Chain	Length	Quality of chain
9	G	144	
10	H	174	
11	I	134	
12	J	156	
13	K	141	
14	L	116	
15	M	113	
16	N	166	
17	O	118	
18	P	100	
19	Q	134	
20	R	94	
21	S	115	
22	T	237	
23	U	91	
24	W	67	
25	X	55	
26	Y	73	
27	Z	59	
28	1	55	
29	2	47	
30	3	65	
31	4	37	

2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 65328 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	0	2766	Total	C	N	O	P	0	0	0
			59359	26479	10949	19166	2765			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	9	118	Total	C	N	O	P	0	0	0
			2516	1124	464	811	117			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
3	A	270	Total	C	0	0	270
			270	270			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
4	B	205	Total	C	0	0	205
			205	205			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
5	C	197	Total	C	0	0	197
			197	197			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
6	D	178	Total	C	0	0	178
			178	178			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
7	E	177	Total	C	0	0	177
			177	177			

- Molecule 8 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
8	F	52	Total	C	0	0	52
			52	52			

- Molecule 9 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
9	G	143	Total	C	0	0	143
			143	143			

- Molecule 10 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
10	H	143	Total	C	0	0	143
			143	143			

- Molecule 11 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
11	I	132	Total	C	0	0	132
			132	132			

- Molecule 12 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
12	J	141	Total	C	0	0	141
			141	141			

- Molecule 13 is a protein called ribosomal protein L16.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
13	K	124	Total	C	0	0	124
			124	124			

- Molecule 14 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
14	L	114	Total	C	0	0	114
			114	114			

- Molecule 15 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
15	M	111	Total	C	0	0	111
			111	111			

- Molecule 16 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
16	N	125	Total	C	0	0	125
			125	125			

- Molecule 17 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
17	O	117	Total	C	0	0	117
			117	117			

- Molecule 18 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
18	P	100	Total	C	0	0	100
			100	100			

- Molecule 19 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
19	Q	127	Total	C	0	0	127
			127	127			

- Molecule 20 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
20	R	93	Total	C	0	0	93
			93	93			

- Molecule 21 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
21	S	113	Total C 113 113	0	0	113

- Molecule 22 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
22	T	223	Total C 223 223	0	0	223

- Molecule 23 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
23	U	86	Total C 86 86	0	0	86

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
24	W	65	Total C 65 65	0	0	65

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
25	X	55	Total C 55 55	0	0	55

- Molecule 26 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
26	Y	73	Total C 73 73	0	0	73

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
27	Z	58	Total C 58 58	0	0	58

- Molecule 28 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
28	1	53	Total C 53 53	0	0	53

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
29	2	46	Total C 46 46	0	0	46

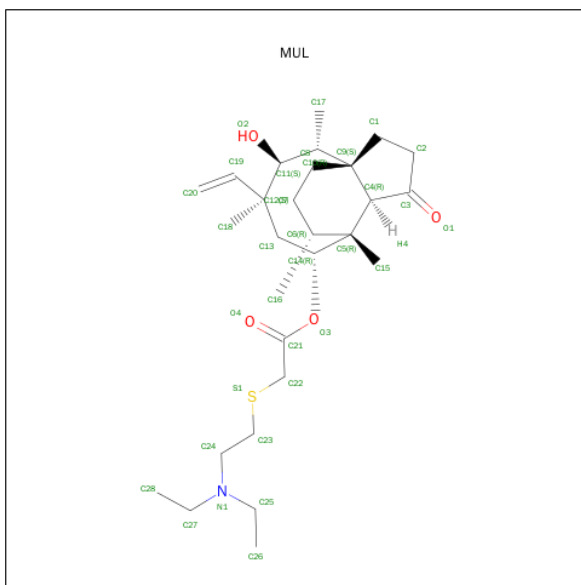
- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
30	3	63	Total C 63 63	0	0	63

- Molecule 31 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
31	4	35	Total C 35 35	0	0	35

- Molecule 32 is TIAMULIN (three-letter code: MUL) (formula: C₂₈H₄₇NO₄S).



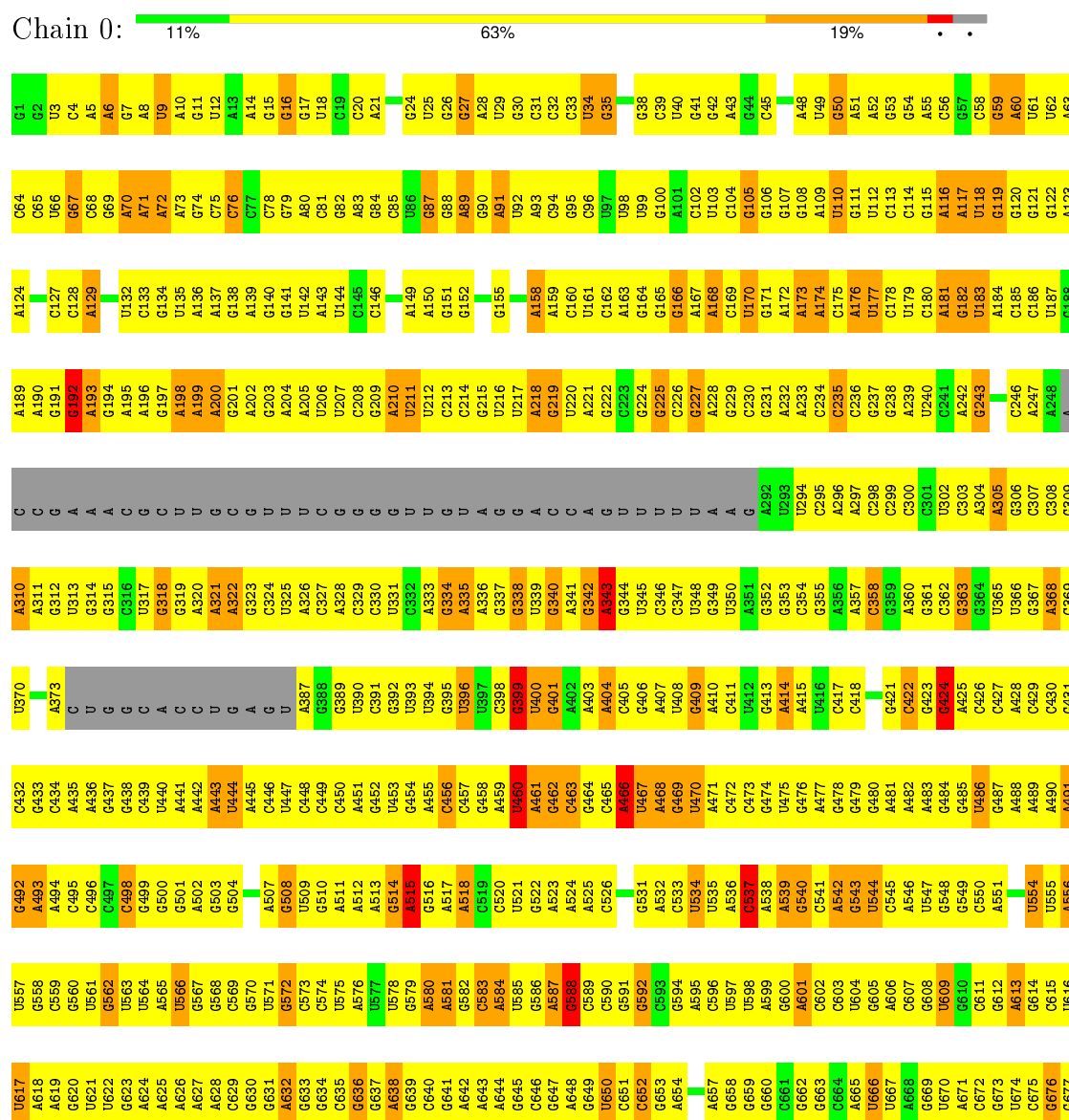
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	0	1	Total C N O S 34 28 1 4 1	0	0

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 ($RSRZ > 2$). 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.

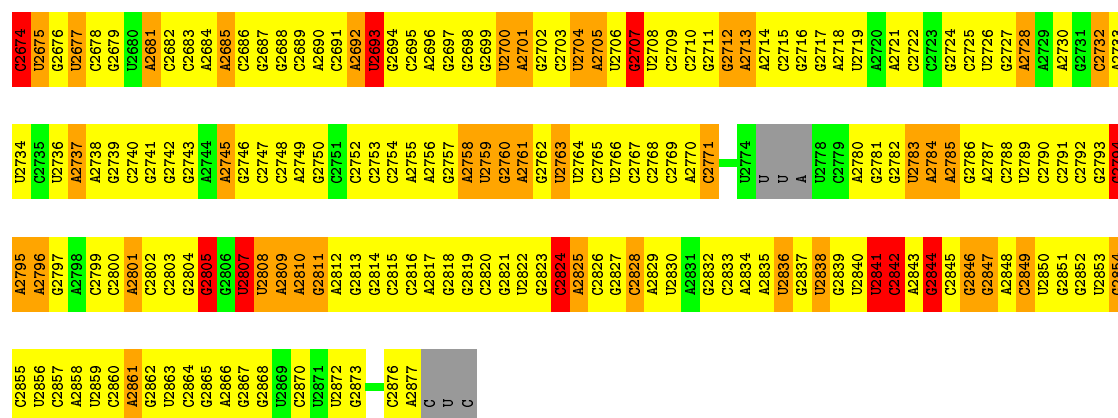
Note EDS was not executed.

• Molecule 1: 23S RIBOSOMAL RNA



A1610	G1545	U1481	A1416	G1356	G1296	C1234	U1172	G1110	U1044	G983	A922	G861	A801	A740	G678
U1611	C1546	U1482	C1417	U1357	A1297	C1235	G1173	C1111	G1045	A984	A923	A862	A802	G741	C679
U1612	U1547	G1483	U1483	G1358	G1298	G1236	G1174	U1112	G1046	G985	C924	C863	C803	G742	U680
G1613	U1548	G1484	U1424	G1359	G1299	U1236	A1175	C1113	G1047	A986	U925	C864	C804	A743	A681
C1549	C1549	U1485	G1425	G1360	A1301	A1239	U1176	A1114	U1048	G987	C926	A865	A805	C744	G682
G1582	G1582	A1486	G1426	G1361	U1302	G1241	U1177	C1115	U1049	G988	C927	U866	A806	C745	A683
G1583	G1583	C1487	G1427	A1362	G1302	G1242	U1178	U1116	C1049	G989	C928	C867	A807	G746	C684
U1584	U1584	G1488	G1428	C1363	A1242	U1243	C1181	G1117	C1052	A990	A929	U868	C808	A747	U685
G1585	G1585	C1489	G1429	C1364	U1303	A1243	U1182	G1118	G1053	A991	A930	C869	C809	A748	G686
A1586	A1586	U1490	G1430	U1365	U1304	G1243	C1183	U1119	C1054	A992	C931	C870	U810	C749	G687
C1587	C1587	C1491	U1431	A1366	U1306	G1244	G1184	C1120	A1055	C993	C932	U871	U811	C750	A688
G1622	G1622	A1492	G1432	A1367	U1307	U1245	C1185	G1121	U1056	A994	C933	G872	G812	G751	A689
C1623	C1623	U1493	A1433	G1368	C1308	G1248	C1186	U1122	A1057	A995	C934	U873	G813	G752	A690
U1590	U1590	G1496	U1434	G1369	G1309	G1249	A1187	G1125	G1058	C996	C935	A874	G814	U753	C691
A1591	A1591	C1497	G1435	U1370	C1310	A1250	A1188	A1126	A1059	C997	A936	G875	A815	G754	C692
G1592	G1592	G1498	G1436	G1371	C1311	G1251	G1189	C1127	C1060	C998	C937	A876	U816	G755	A693
U1593	U1593	A1499	A1437	A1372	G1312	C1252	C1190	G1128	U1061	A999	U942	G877	A817	C756	G694
C1594	C1594	U1500	G1438	G1373	U1313	G1253	G1191	A1129	C1062	A1001	U943	C878	A818	C757	G695
U1595	U1595	C1501	G1439	G1374	A1314	G1254	A1192	U1130	A1064	U1001	U944	A879	C819	G758	U696
G1596	G1596	G1502	G1440	C1375	A1315	A1255	G1193	G1131	A1065	C1002	U945	C880	U820	G759	G697
A1597	A1597	U1503	A1441	G1376	G1316	C1256	U1194	C1132	G1066	C1003	U946	U881	A821	U760	A698
C1631	C1631	G1504	G1442	G1377	G1317	U1257	U1195	G1133	G1067	A1004	C945	C882	U822	G761	G700
A1568	A1568	U1505	G1443	A1378	G1318	G1258	G1196	C1134	A1068	U1005	U946	A883	U823	A762	C701
G1633	G1633	C1506	G1444	A1379	U1259	A1260	U1197	G1135	G1069	C1006	U947	U884	U824	A763	U701
A1634	A1634	U1507	A1445	C1380	A1320	A1261	C1198	G1136	U1072	A1007	C947	A886	C825	A764	A702
G1635	G1635	G1508	U1446	G1381	A1321	G1262	U1199	A1137	U1073	G1008	C948	C887	U826	C765	A703
U1636	U1636	A1509	U1447	C1382	G1322	U1263	G1200	A1138	G1074	C1009	C949	G888	C827	A766	G704
G1637	G1637	U1510	G1448	G1383	G1323	C1264	G1201	U1139	G1075	U1010	C950	C889	C828	G767	C705
U1638	U1638	C1511	C1449	G1384	U1324	C1265	U1202	A1140	C1076	U1011	C951	U890	C829	U768	A706
G1639	G1639	A1512	G1450	G1385	G1325	G1266	A1203	U1141	U1077	A1012	A952	A891	C830	U770	U707
C1640	C1640	U1513	C1451	A1386	U1326	G1267	G1204	G1142	G1078	G1013	C953	G	C831	G771	G708
U1578	U1578	C1514	A1452	G1387	C1327	A1267	G1205	A1143	A1079	U1014	U954	G	A832	G772	A709
G1641	G1641	U1515	U1453	C1388	G1328	U1268	G1206	U1144	C1080	U1015	C955	G	A833	G773	C710
A1580	A1580	A1516	A1454	G1389	U1329	G1269	G1207	C1145	A1081	A1016	C956	G	U834	A774	C711
G1644	G1644	C1517	G1455	G1390	G1330	C1270	A1208	C1146	C1082	C1017	C957	G	U835	U775	A712
U1645	U1645	U1518	C1456	A1391	G1331	C1271	G1209	G1147	G1083	C1018	C958	C	U836	G776	G713
A1583	A1583	G1519	A1457	U1392	G1332	G1272	C1210	G1148	C1084	U1019	C959	C	U837	A777	G714
G1584	G1584	U1520	A1458	G1393	G1333	G1273	G1211	G1149	U1084	A1020	U960	U	A838	G778	U715
C1648	C1648	U1521	U1459	G1394	C1274	A1275	U1212	C1150	G1085	A1021	C961	A	U839	U779	U716
A1586	A1586	C1522	G1460	A1395	A1275	A1276	U1213	U1151	C1086	A1022	C962	C	U840	U780	G717
U1587	U1587	A1523	C1461	G1396	G1336	U1277	C1214	C1152	C1087	U1023	C963	C	A841	G781	A718
A1588	A1588	C1524	C1462	A1397	G1337	G1277	A1215	A1153	A1088	G1024	A964	A	A842	U782	A719
G1652	G1652	U1525	A1463	G1398	G1338	A1278	G1216	G1154	C1089	A1025	C965	G	G843	G783	A720
C1653	C1653	C1527	A1464	C1399	U1339	G1279	U1217	U1155	C1090	U1026	A966	C	G844	U784	C721
U1591	U1591	G1528	G1465	A1400	C1340	U1280	C1218	U1156	C1091	C1027	C967	U	U845	U785	C722
U1592	U1592	U1529	C1466	G1401	G1341	A1281	C1219	G1157	U1092	G1028	C968	U	A846	U786	G723
C1593	C1593	U1530	U1467	G1402	U1342	A1282	G1220	A1158	C1094	C1029	U969	A	C847	A787	U727
U1594	U1594	C1531	A1468	U1403	C1343	C1283	C1221	U1159	A1095	U1030	A970	C	A848	G788	G728
A1595	A1595	A1532	U1469	C1404	G1344	G1284	G1222	G1160	A1096	C1031	A971	C	G849	G789	U727
G1658	G1658	G1533	G1470	A1405	G1345	A1285	U1223	U1161	A1097	A1032	C972	A911	C850	A790	G728
C1598	C1598	U1534	G1471	U1406	C1346	U1286	A1224	A1162	G1098	G1033	U973	A912	C851	G791	A729
G1659	G1659	G1535	C1472	G1407	C1347	A1287	G1225	C1163	A1099	U1034	U974	A913	U852	U792	C730
C1661	C1661	U1537	U1473	U1408	C1348	A1288	A1226	C1164	U1102	G1035	C975	C914	C853	G793	G733
G1662	G1662	A1538	A1474	A1409	C1349	A1289	G1228	G1165	G1036	C976	C976	C915	C854	A794	G734
C1663	C1663	U1539	U1475	U1410	G1350	A1290	G1229	A1166	U1037	G1037	C977	U916	C855	A795	G735
G1664	G1664	A1540	G1476	C1411	G1351	G1291	C1229	A1167	G1104	U1038	U978	U917	A856	A796	G736
A1605	A1605	C1412	C1477	C1412	G1352	A1292	C1230	G1168	U1105	A1039	A979	A918	U857	A797	G737
G1606	G1606	U1541	U1478	U1413	G1353	A1293	A1231	U1169	U1106	A1040	C980	U919	G858	G798	G738
A1607	A1607	G1542	G1479	G1414	A1354	G1294	U1232	U1170	A1107	G1041	C982	G920	U859	G799	G739
G1608	G1608	C1543	A1480	C1415	A1355	U1295	A1233	A1171	U1107	U1041	C982	A921	U860	U800	G739

G2612	A2429	G2368	A2308	C2243	U2178	G	G2053	G1983	U1856	C1792	C1731	G1670
A2613	A2430	U2369	G2309	C2244	U2179	C	A2054	U1994	G1857	A1793	U1732	A1671
A2614	G2431	G2370	G2310	A2245	A2181	G	G2055	U1995	A1858	A1794	C1734	A1672
A2615	A2432	A2371	U2311	A2246	A2182	A2117	C2056	A1996	A1859	C1795	C1735	C1673
G2616	G2433	A2372	A2312	A2247	C2183	A2118	U2057	A1997	A1860	A1796	G1736	C1674
G2617	G2434	C2373	G2313	A2248	C2184	A2119	U2058	A1998	G1861	C1797	C1737	C1675
A2618	G2435	C2374	A2314	U2249	U2185	U	U2059	U1999	C1862	G1798	U1676	U1676
G2619	U2436	G2375	A2315	G2250	G2186	G2122	A2060	U1939	U1863	A1799	U1738	C1677
G2620	G2437	G2376	G2316	U2251	U	G2123	C2061	U1940	G1864	A1800	G1739	G1678
G2621	U2438	U2377	G2317	A2191	A2191	C2124	U2062	C2061	C1865	C1801	G1740	U1679
G2622	U2439	G2378	U2318	A2252	C2124	C2125	A2063	A2003	G1866	A1802	G1741	U1680
G2623	G2440	G2379	G2319	A2253	U	U	U2064	A1943	A1867	U	G1742	A1681
G2624	U2441	U2380	G2320	G2254	C2193	U	A2065	U2005	A1868	G1805	G1743	A1682
U2625	C2442	A2381	C2321	G2256	C2195	U	G2066	C2006	A1869	G1806	G1744	G1683
U2626	C2443	C2382	U2322	U2257	U2196	U	U2067	G2007	U1870	A1807	C1745	G1684
U2627	C2444	C2383	U2323	G2259	U2197	G	C2068	U2008	G1871	C1808	C1746	A1685
G2628	C2445	G2384	G2324	C2260	U2198	G	U2069	U2009	G1872	A1809	G1747	A1686
U2629	C2446	U2385	A2325	C2261	C2199	G2132	G2070	A1949	C1876	U1810	U1748	C1687
C2630	G2447	G2386	C2326	C2262	G2200	G2133	G2071	U2011	C1877	A1811	G1749	U1688
U2631	A2448	U2387	U2327	C2263	G2201	U2138	C2072	A2012	C1878	U1812	A1750	U1689
G2632	G2449	G2388	G2328	U2271	G2202	A2139	A2073	A1952	U	A1813	A1751	U1690
U2633	A2450	G2389	C2329	A2266	G2203	G2139	U2074	A1953	U1881	G1814	U1752	G1691
U2634	G2451	A2390	G2330	A2267	A2204	G2140	U2075	A1954	G1882	G1815	A1753	C1692
G2635	U2452	A2391	A2331	G2268	C2205	A	G2076	A1955	A1883	G1816	G1754	A1693
C2636	C2453	G2392	G2332	G2269	C2206	G	G2077	G1956	A1884	U1817	G1755	A1694
G2638	C2454	G2393	A2333	U2270	G2207	G	G2078	G1956	C1885	G1818	C1756	U1695
U2639	A2455	G2394	C2334	C2271	U2208	C	A2079	U1959	G1886	U1819	C1757	C1696
G2640	U2456	C2395	U2335	G2272	C	A	G2080	U1960	G1887	G2020	U	U1697
A2641	G2457	C2396	G2336	C2273	G2209	U	U2081	A1961	C1888	A1821	G1760	C1698
U2642	U2458	A2397	A2337	U2275	C2210	C	G2082	C2022	C1889	G1822	G1761	A1699
G2643	C2459	U2398	G2338	C2276	U2211	A	G2083	C1962	U	G1823	C1762	C1700
A2644	U2460	C2399	A2339	A2277	U2212	G	G2084	U2024	C1892	C1824	G1763	C1701
C2645	G2461	G2400	C2340	C2278	U2213	U	G2085	A2025	U1900	G1825	A1764	C1702
G2646	U2462	A2401	G2341	G2279	G	A	U2086	C2026	G1966	U1826	C1765	C1703
U2647	G2463	C2402	U2342	C2280	U2217	A	U2087	C2027	U1967	G1827	U1766	G1704
A2649	G2464	U2403	C2343	C2281	G2218	A	U2090	C2028	G1968	C1828	G1767	U1705
G2650	A2465	A2404	G2344	G2282	U2219	U	G2091	G1969	C1908	C1829	U1768	A1706
U2651	G2466	A2405	A2345	G2283	A2220	A	C2092	U2030	U1909	C1830	U1769	A1707
G2652	U2467	C2406	G2346	U2284	G2221	A	U2093	A2031	A1910	G1831	U1770	C1708
A2653	G2468	G2407	C2347	G2285	U2222	C2157	G2094	C2032	A1911	G1832	A1771	U1709
G2654	U2470	A2408	A2348	G2286	U2223	C2158	C2095	C2033	G1912	U1833	C1772	U1710
C2655	U2471	G2409	G2349	G2287	U2224	A2159	U2096	A2034	G1913	U	C1773	C1711
G2656	U2472	U2410	G2350	G2288	G2225	C2160	U2097	G2035	U1914	G1837	A1774	G1712
U2657	G2473	A2411	G2351	A2289	A2226	G2161	A2097	U1976	A1915	G1838	U1775	G1713
G2658	G2474	G2412	A2352	U2289	C2227	C2162	G	C1977	G1916	A1839	A1776	A1714
C2659	C2475	A2413	G2353	C2292	U2228	A	U2098	U1978	C1917	A1840	U1777	A1715
U2660	U2476	A2414	G2354	G2293	G2229	G2163	A	C2039	G1918	G1841	U1778	G1716
G2661	G2477	G2415	A2355	U2294	G2230	A2165	U	A1980	A1919	G1842	C1779	A1717
U2662	U2478	C2416	A2356	G2295	G2231	G2166	A	A1921	A1920	U1843	A1780	A1718
G2663	G2479	U2417	A2357	U2296	G2232	A2167	G2103	C1982	A1921	C1844	C1781	G1719
U2664	A2480	C2418	C2357	G2297	G2233	A2168	G2104	G1983	U1922	A1845	A1782	G1720
G2665	G2481	U2419	C2358	U2298	C2234	A2169	U2105	A1984	U1923	G1846	G1721	U1721
U2666	A2482	C2420	U2359	A2299	G2235	C2170	G2106	G1985	C1924	G1847	C1784	G1722
C2667	U2483	G2421	C2360	G2300	U2236	C2171	G2107	G1986	C1925	U1848	U1785	U1723
G2668	A2484	C2422	G2361	A2301	U2237	U2171	G2108	G1987	C2047	C1926	C1786	C1724
U2669	U2485	G2423	G2362	G2302	G2237	G2172	A2109	U1927	U1927	A1851	U1787	C1725
G2670	C2486	G2424	G2363	C2303	G2238	G2173	G2110	C1988	G1928	G1852	C1788	C1726
U2671	G2487	U2425	C2364	G2304	C2239	G2174	C	C1989	U1929	G1853	C1789	C1727
C2672	U2488	G2426	U2365	C2305	C2240	A2175	U	U1990	C1930	G1854	G1790	U1730
G2673	A2489	A2427	U2366	C2306	U2241	C	C	U2051	G1931	G1855	C1791	G1730



- Molecule 2: 5S RIBOSOMAL RNA

Chain 9: 13% 69% 14% 5%



- Molecule 3: 50S ribosomal protein L2

Chain A: 98% ..



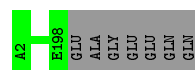
- Molecule 4: 50S ribosomal protein L3

Chain B: 96% ..



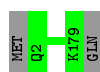
- Molecule 5: 50S ribosomal protein L4

Chain C: 97% .



- Molecule 6: 50S ribosomal protein L5

Chain D: 99% .



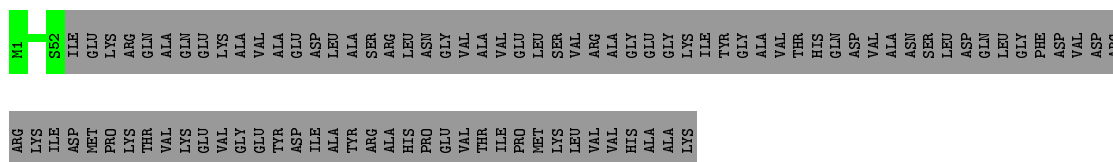
- Molecule 7: 50S ribosomal protein L6

Chain E: 95%



- Molecule 8: 50S ribosomal protein L9

Chain F: 36% 64%



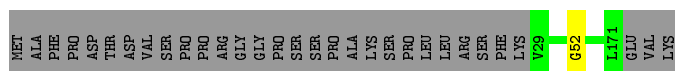
- Molecule 9: 50S ribosomal protein L11

Chain G: 99%



- Molecule 10: 50S ribosomal protein L13

Chain H: 82% 18%



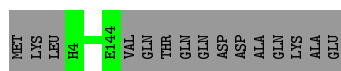
- Molecule 11: 50S ribosomal protein L14

Chain I: 97%



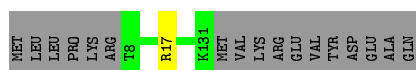
- Molecule 12: 50S ribosomal protein L15

Chain J: 90% 10%



- Molecule 13: ribosomal protein L16

Chain K: 87% 12%



- Molecule 14: 50S ribosomal protein L17

Chain L: 97%



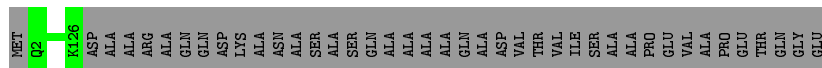
- Molecule 15: 50S ribosomal protein L18

Chain M: 98%



- Molecule 16: 50S ribosomal protein L19

Chain N: 75%



- Molecule 17: 50S ribosomal protein L20

Chain O: 99%



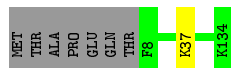
- Molecule 18: 50S ribosomal protein L21

Chain P: 100%

There are no outlier residues recorded for this chain.

- Molecule 19: 50S ribosomal protein L22

Chain Q: 94%



- Molecule 20: 50S ribosomal protein L23

Chain R: 97%



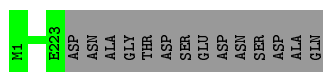
- Molecule 21: 50S ribosomal protein L24

Chain S:  98% .



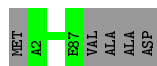
- Molecule 22: 50S ribosomal protein L25

Chain T:  94% 6%



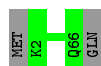
- Molecule 23: 50S ribosomal protein L27

Chain U:  95% 5%



- Molecule 24: 50S ribosomal protein L29

Chain W:  97% .



- Molecule 25: 50S ribosomal protein L30

Chain X:  100%

There are no outlier residues recorded for this chain.

- Molecule 26: 50S ribosomal protein L31

Chain Y:  100%

There are no outlier residues recorded for this chain.

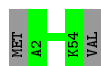
- Molecule 27: 50S ribosomal protein L32

Chain Z:  98% .



- Molecule 28: 50S ribosomal protein L33

Chain 1:  96% .



- Molecule 29: 50S ribosomal protein L34

Chain 2:  98% .



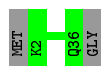
- Molecule 30: 50S ribosomal protein L35

Chain 3:  97% .



- Molecule 31: 50S ribosomal protein L36

Chain 4:  95% 5%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	168.70 Å 405.00 Å 693.00 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.50	Depositor
% Data completeness (in resolution range)	88.3 (15.00-3.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.290 , 0.360	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	65328	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0	0.79	21/66467 (0.0%)	0.82	43/103673 (0.0%)
2	9	0.44	0/2813	0.73	0/4384
All	All	0.78	21/69280 (0.0%)	0.82	43/108057 (0.0%)

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	0	0	260

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	1646	G	C5-C6	-7.94	1.34	1.42
1	0	2570	C	N1-C2	6.85	1.47	1.40
1	0	2801	A	C5-C6	-6.62	1.35	1.41
1	0	2673	G	C5-C6	-6.49	1.35	1.42
1	0	2222	U	N3-C4	-6.45	1.32	1.38

The worst 5 of 43 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2482	A	N9-C1'-C2'	8.75	125.37	114.00
1	0	460	U	N1-C1'-C2'	7.48	123.72	114.00
1	0	859	U	N1-C1'-C2'	-7.43	103.83	112.00
1	0	1710	U	N1-C1'-C2'	7.14	123.28	114.00
1	0	1266	G	N9-C1'-C2'	6.48	122.43	114.00

There are no chirality outliers.

5 of 260 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	16	G	Sidechain
1	0	27	G	Sidechain
1	0	6	A	Sidechain
1	0	67	G	Sidechain
1	0	9	U	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	0	59359	0	29916	4247	0
2	9	2516	0	1286	144	0
3	A	270	0	0	2	0
4	B	205	0	0	3	0
5	C	197	0	0	0	0
6	D	178	0	0	0	0
7	E	177	0	0	1	0
8	F	52	0	0	0	0
9	G	143	0	0	0	0
10	H	143	0	0	1	0
11	I	132	0	0	2	0
12	J	141	0	0	0	0
13	K	124	0	0	1	0
14	L	114	0	0	3	0
15	M	111	0	0	0	0
16	N	125	0	0	0	0
17	O	117	0	0	0	0
18	P	100	0	0	0	0
19	Q	127	0	0	1	0
20	R	93	0	0	1	0
21	S	113	0	0	0	0
22	T	223	0	0	0	0
23	U	86	0	0	0	0
24	W	65	0	0	0	0
25	X	55	0	0	0	0
26	Y	73	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	Z	58	0	0	0	0
28	1	53	0	0	0	0
29	2	46	0	0	0	0
30	3	63	0	0	0	0
31	4	35	0	0	0	0
32	0	34	0	47	4	0
All	All	65328	0	31249	4383	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 46.

The worst 5 of 4383 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)
1:0:584:A:H4'	1:0:2038:C:N4	1.53	1.23
1:0:1621:C:H4'	1:0:1626:A:N6	1.57	1.19
1:0:918:A:H2'	1:0:919:U:H5''	1.24	1.18
1:0:1339:U:H5''	1:0:1994:U:H1'	1.21	1.18
1:0:1938:U:O2'	1:0:1939:U:H5'	1.42	1.18

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2757/2880 (95%)	512 (18%)	39 (1%)
2	9	117/124 (94%)	17 (14%)	1 (0%)
All	All	2874/3004 (95%)	529 (18%)	40 (1%)

5 of 529 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	34	U
1	0	35	G
1	0	45	C
1	0	48	A
1	0	49	U

5 of 40 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	1634	A
1	0	1698	C
1	0	2482	A
1	0	1664	G
1	0	1820	G

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

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	MUL	0	2881	-	31,36,36	0.83	1 (3%)	28,55,55	1.18	3 (10%)

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	MUL	0	2881	-	-	0/16/79/79	0/1/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	0	2881	MUL	O3-C14	2.21	1.50	1.46

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	0	2881	MUL	C16-C6-C7	-2.77	105.97	110.44
32	0	2881	MUL	C7-C8-C9	2.05	117.00	112.92
32	0	2881	MUL	O3-C21-C22	3.23	119.56	111.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	0	2881	MUL	4	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 [i](#)

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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.