



wwPDB EM Validation Summary Report ⓘ

Mar 23, 2026 – 11:51 AM UTC

PDB ID : 1C2W / pdb_00001c2w
Title : 23S RRNA STRUCTURE FITTED TO A CRYO-ELECTRON MICRO-
SCOPIC MAP AT 7.5 ANGSTROMS RESOLUTION
Authors : Brimacombe, R.; Mueller, F.
Deposited on : 1999-07-28
Resolution : 7.50 Å(reported)
Based on initial models : 1CSV, 1CSX

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

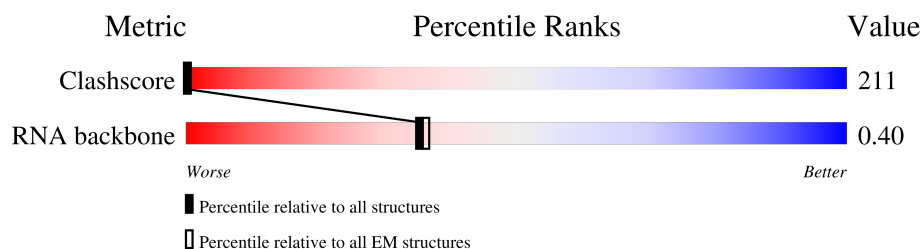
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 7.50 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)	EM structures (#Entries)
Clashscore	229148	23984
RNA backbone	8273	3508

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

Mol	Chain	Length	Quality of chain
1	B	2904	

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
1	5MU	B	1915	-	-	X	-
1	5MU	B	1939	X	-	X	-
1	7MG	B	2069	-	-	X	-
1	5MU	B	2449	X	-	X	-
1	5MC	B	2498	X	-	X	-
1	7MG	B	745	-	-	X	-
1	PSU	B	746	-	-	X	-
1	5MU	B	747	-	-	X	-

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 62371 atoms, of which 23 are hydrogens and 0 are deuteriums.

In the tables below, 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.

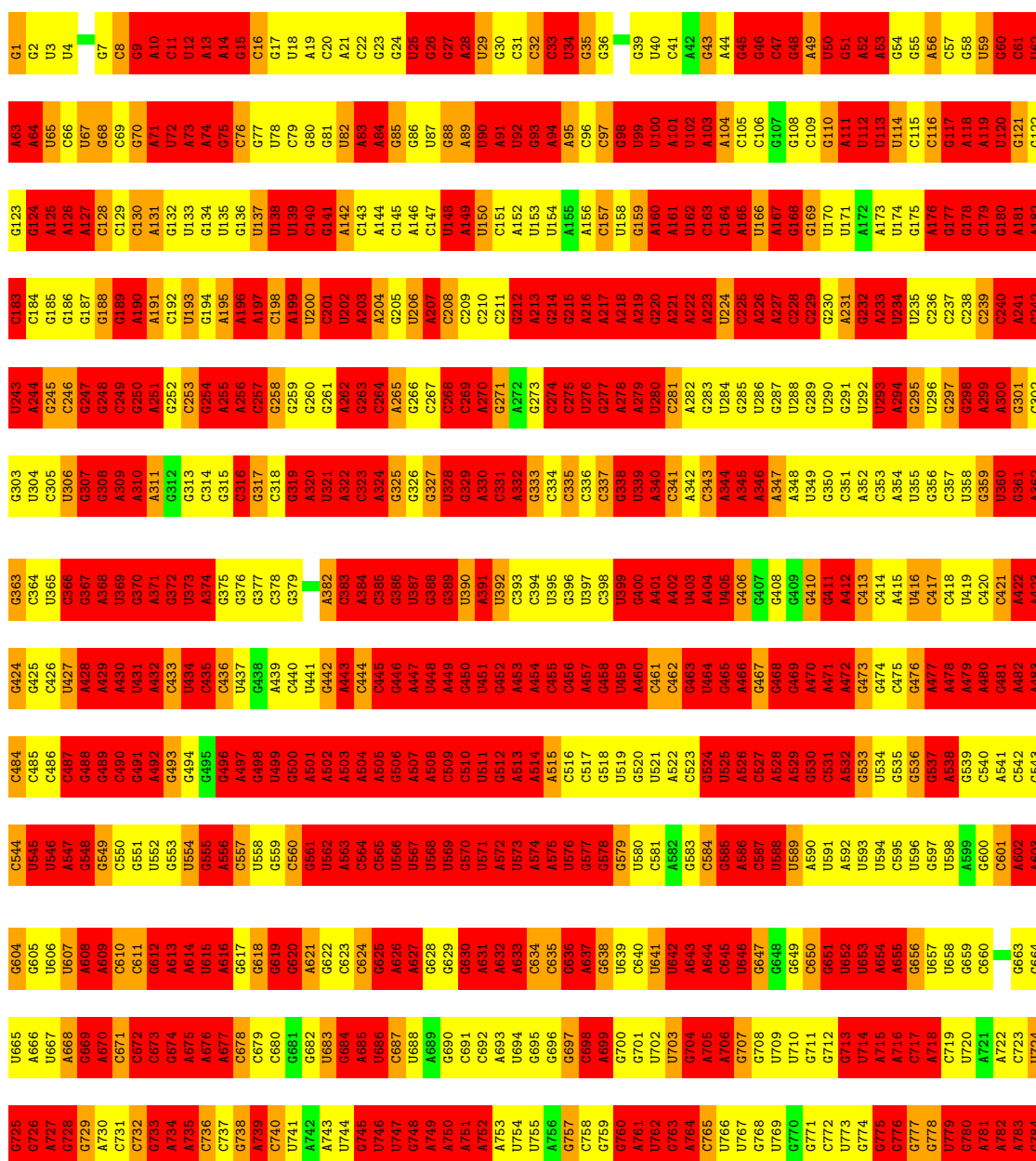
Mol	Chain	Residues	Atoms						AltConf	Trace
1	B	2904	Total	C	H	N	O	P	0	0
			62371	27819	23	11467	20158	2904		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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

Chain B: 



G1697	U1636	U1576	G1516	A1453	A1593	C1330	A1269	U1209	U1148	A1088	A1028	C968	A905	U845	G785
A1696	A1637	C1577	G1517	C1454	U1594	G1331	C1270	G1210	G1149	A1089	A1029	G969	U906	U846	C786
G1699	C1638	A1578	C1518	G1455	A1395	G1332	A1271	G1211	C1150	A1090	C1030	U970	U907	U847	C787
A1700	C1639	A1579	G1519	G1456	A1396	G1333	A1272	G1212	C1151	A1091	C1031	C908	C908	C848	A788
G1701	A1640	A1580	U1520	U1457	U1397	G1334	U1273	A1213	C1152	A1092	A1032	A972	A910	A849	A789
A1702	G1641	G1581	G1521	U1458	C1398	G1335	A1274	A1214	G1153	A1093	U1033	A973	A911	U850	U790
G1703	G1642	C1592	A1522	G1459	C1399	U1335	A1275	G1215	G1154	U1094	G1034	G974	C912	C851	C791
C1704	G1643	U1523	U1523	U1460	U1400	G1339	A1276	G1216	A1155	A1095	U1035	A975	C913	U852	A792
A1705	G1644	U1584	G1524	C1461	U1401	G1340	A1277	U1217	A1156	A1096	G1036	G976	U913	C853	A793
G1706	G1645	A1585	A1525	A1462	U1402	G1341	C1278	G1218	G1157	A1097	G1037	G977	C914	C854	A794
G1707	C1646	A1586	C1526	C1463	A1403	A1342	U1219	U1219	C1158	A1098	G1038	G978	C915	G855	C795
C1708	U1647	G1587	G1527	G1464	U1404	G1343	U1281	G1220	U1159	A1099	A1039	A979	G916	G856	C796
U1709	U1648	A1588	A1528	G1465	U1405	U1344	U1282	C1221	G1160	C1100	A1040	A980	A917	G857	C797
G1710	G1649	U1589	G1529	U1466	U1406	C1345	G1283	U1222	C1161	U1101	G1041	A981	A918	C858	C798
A1711	A1650	A1590	G1530	U1467	G1407	C1346	G1284	G1223	G1162	C1102	G1042	C982	U919	C859	G799
U1712	G1651	A1591	C1531	U1468	A1408	A1347	A1285	U1224	G1163	A1103	C1043	A983	A920	U860	A800
A1713	A1652	C1592	A1532	A1469	U1409	C1348	A1286	G1225	C1164	C1104	G1044	A984	C921	A861	A801
U1714	C1653	A1593	C1533	A1470	U1410	C1349	A1287	A1226	A1165	U1105	C1045	C985	C922	G862	A802
G1715	A1654	U1594	U1534	G1471	U1411	C1350	G1288	G1227	G1166	G1106	A1046	C986	U930	A863	U803
A1716	A1655	A1595	A1535	C1472	U1412	C1351	C1289	G1228	C1167	G1107	G1047	C987	U926	C864	A804
U1717	C1656	A1596	C1536	G1473	A1413	U1352	C1290	C1229	G1168	U1108	A1048	A988	A927	C865	G805
G1718	U1657	A1597	G1537	U1474	C1414	A1353	G1291	U1230	A1169	C1109	C1049	G989	A928	A866	C806
G1719	A1658	A1598	G1538	G1475	U1415	A1354	C1292	U1231	C1170	G1110	A1050	A990	U929	C867	U807
U1720	C1659	U1599	U1539	U1476	G1416	G1355	C1293	G1232	G1171	A1111	G1051	C991	G930	U868	G808
G1721	G1661	C1600	G1540	A1477	C1417	G1356	U1294	C1233	G1172	C1112	C1052	C992	U931	G869	G809
A1722	U1662	G1601	C1541	G1478	G1418	C1357	C1295	U1234	U1173	U1113	C1053	G993	U932	U870	U810
G1723	G1663	A1602	U1542	G1479	A1419	G1358	G1296	G1235	U1174	C1114	A1054	C994	A933	U871	U811
G1724	A1664	A1603	G1543	C1480	A1420	A1359	G1297	G1236	A1175	G1115	C1055	C995	U934	U872	C812
A1725	A1665	C1604	A1544	U1481	G1421	G1360	C1298	A1237	U1176	G1116	G1056	A996	C935	C873	U813
C1726	G1666	G1605	A1545	G1482	G1422	G1361	G1299	G1238	G1177	A1057	G1057	G997	A936	G874	C814
G1727	G1667	C1606	G1546	G1483	G1423	C1362	G1300	G1239	C1178	C1118	G1058	C998	C937	G875	C815
C1728	A1668	C1607	C1547	U1484	G1424	C1363	A1301	U1240	C1179	U1119	G1059	U999	G938	C876	C816
U1729	A1669	A1608	A1548	U1485	G1425	G1364	A1302	A1241	U1180	G1120	U1060	A1000	G939	A877	C817
G1730	C1670	A1609	C1549	U1486	G1426	A1365	G1303	U1242	U1181	C1121	U1061	G940	G941	A878	G818
G1731	U1671	A1610	C1550	U1487	A1427	A1366	A1304	C1243	G1182	G1122	G1062	A1002	A941	G879	A819
G1732	A1672	C1611	A1551	C1488	C1428	A1367	C1305	G1244	U1183	C1123	G1063	G1003	G942	G880	A820
G1733	G1673	G1612	A1552	C1489	G1429	G1368	C1306	G1245	U1184	G1124	G1064	U1004	A943	G881	A821
C1734	G1674	G1613	A1553	A1490	C1430	G1369	A1307	A1246	G1185	G1125	U1065	C1005	C944	G882	G822
A1735	C1675	A1614	U1554	G1491	G1431	C1370	A1308	A1247	G1186	A1126	U1066	A945	A945	G883	C823
G1736	A1676	C1615	G1555	G1492	G1432	G1371	C1309	G1248	G1187	A1127	A1067	C1007	C946	U894	U824
G1737	C1677	A1616	C1556	C1493	A1433	U1372	G1310	U1249	U1188	G1128	G1068	A1008	A947	C885	A825
G1738	A1678	C1617	C1557	A1494	A1434	A1373	G1311	G1250	A1189	A1129	A1069	A1009	C948	U896	U826
A1739	A1679	A1618	G1558	A1495	G1435	G1374	U1312	C1251	U1190	U1130	A1070	A1010	G949	U897	U827
G1740	U1680	U1559	A1496	U1496	G1436	U1375	U1313	G1252	U1191	G1131	G1071	G1011	G950	C898	U828
C1741	G1681	G1620	G1560	U1497	C1437	C1376	C1314	A1253	G1193	U1132	C1072	U1012	C951	C899	A829
U1742	G1682	U1621	C1561	C1498	U1438	G1377	C1315	A1254	A1194	A1133	A1073	C1013	U954	G890	G830
G1743	U1683	G1622	U1562	C1499	A1439	A1378	U1316	U1255	G1195	G1074	G1074	A1014	U955	G891	G831
A1744	G1684	G1623	U1563	G1500	U1440	U1379	G1317	G1256	C1196	C1135	C1075	G1015	U956	A892	U832
A1745	C1685	U1624	C1564	U1501	G1441	G1380	U1318	C1257	G1197	G1136	C1076	G1016	U957	C893	A833
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C1748	U1688	G1627	G1567	C1507	U1444	A1383	A1321	A1260	C1200	G1139	C1079	U1019	A959	A896	G836
A1749	A1689	G1628	A1568	A1508	G1445	A1384	A1322	C1261	U1201	C1140	A1080	A1020	A960	C897	G837
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U1751	C1691	A1630	G1510	C1447	G1447	C1386	G1324	U1263	U1203	A1142	U1082	G1022	G962	A899	U839
C1752	G1692	G1631	A1571	G1511	C1448	U1325	U1326	A1264	A1204	A1143	U1083	U1023	U963	A900	C840
G1753	U1693	A1632	A1572	C1512	G1449	U1389	U1326	A1265	A1205	A1144	A1084	G1024	C964	C901	C841
A1754	C1694	G1633	G1573	U1513	G1450	U1390	A1327	G1266	G1206	C1145	A1085	G1025	C965	C902	U842
U1755	G1695	A1634	C1574	G1514	U1451	U1391	A1328	G1267	C1207	C1146	A1086	G1026	G966	C903	G843
G1756	C1696	A1635	C1575	A1515	G1452	A1392	U1329	A1268	C1208	A1147	G1087	A1027	U967	G904	A844

G2668	G2606	G2546	G2484	G2363	G2302	G2239	C2178	U2118	A2058	C1997	A1937	A1877	G1817	A1757
G2671	G2607	A2547	G2485	C2364	G2303	U2240	C2179	A2119	A2059	A1998	A1938	G1878	U1818	U1758
G2672	G2608	U2548	G2486	G2365	G2304	A2241	U2180	A2120	A2060	A1999	U1939	G1879	A1819	A1759
G2673	G2610	G2549	G2487	A2366	U2305	G2242	G2120	G2121	G2061	C2000	U1940	U1880	U1820	C1760
G2674	G2611	G2550	G2488	G2367	G2306	U2243	U2182	U2122	G2062	C2001	C1941	U1881	A1821	C1761
A2675	G2612	G2551	G2489	G2368	G2307	U2244	A2183	G2123	C2063	U1882	C1942	U1882	C1822	A1762
G2676	G2613	U2552	G2490	A2369	G2308	U2245	A2184	G2124	C2064	G2004	U1943	U1883	G1823	G1763
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U2680	G2617	G2556	A2433	G2373	U2312	U2249	U2188	G2128	C2008	C2008	C1947	G1887	U1827	U1767
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A2682	G2619	G2375	G2376	G2377	G2316	G2251	G1900	U2130	A2070	G2010	G1949	A1889	A1829	U1769
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G2685	G2622	G2378	G2381	G2378	G2319	C2254	G2193	G2133	C2073	A1952	C1892	C1892	C1832	A1772
G2686	G2623	U2440	G2379	G2382	G2320	G2255	A2194	A2134	U2074	A2014	A1953	C1893	C1833	A1773
G2687	G2624	U2441	G2380	G2383	G2321	G2256	U2195	A2135	U2075	A2015	G1954	C1894	U1834	C1774
G2688	G2625	G2442	A2381	U2321	U2321	U2257	G2196	G2136	U2076	U2016	U1955	C1895	G1835	U1775
G2689	G2626	G2443	G2382	A2322	G2288	U2258	U2197	U2137	A2077	U2017	U1956	G1896	C1836	G1776
G2690	G2627	G2444	G2383	G2323	A2289	C2259	A2198	G2138	C2078	G2018	C1957	G1897	C1837	U1777
G2691	G2628	G2445	U2384	U2324	C2260	C2260	A2199	U2139	U2079	A2019	G1958	U1898	C1838	U1778
U2692	U2629	G2446	C2385	G2325	C2261	G2261	C2200	G2140	A2080	A2020	G1959	A1899	G1839	U1779
G2693	G2630	A2386	A2387	G2326	U2262	U2262	G2201	G2141	U2081	C2021	A1960	A1900	G1840	U1780
G2694	G2631	U2387	U2387	A2327	C2263	C2263	U2202	A2142	A2082	U2022	G1961	A1901	U1841	A1781
U2695	G2632	A2388	A2388	A2328	C2264	C2264	U2203	C2143	C2083	C2023	C1962	C1902	G1842	U1782
G2696	A2635	G2389	U2389	A2329	U2265	U2265	G2204	G2144	C2084	G2024	U1963	G1903	C1843	A1783
G2697	G2636	A2451	G2390	G2330	A2266	A2266	U2205	C2145	U2085	C2025	G1964	G1904	C1844	A1784
G2698	U2637	G2574	G2391	G2331	A2267	A2267	C2206	C2146	U2086	G2026	C1965	C1905	G1845	A1785
U2700	G2638	G2575	A2453	G2332	A2268	C2267	G2207	A2147	G2087	G2027	A1966	G1906	G1846	A1786
A2699	A2639	G2576	G2454	U2333	G2269	G2269	C2208	G2148	A2088	U2028	C1967	G1907	A1847	U1787
G2702	G2640	A2577	G2455	U2334	A2270	A2270	G2209	U2149	C2089	C2029	C1968	C1908	A1848	C1788
G2703	G2641	G2578	C2456	A2335	G2271	G2271	U2210	C2150	A2090	A2030	A1969	C1909	G1849	A1789
C2704	G2642	C2579	U2457	A2336	U2272	U2272	A2211	U2151	C2091	A2031	G1850	G1910	C1850	C1790
A2705	G2643	U2580	G2458	G2337	A2273	A2273	A2212	G2152	U2092	G2032	U1971	U1911	U1851	A1791
G2706	G2644	G2582	U2460	U2338	A2274	C2274	U2213	C2153	G2093	A2033	G1972	A1912	U1852	G1792
G2645	G2645	G2583	A2461	G2339	C2275	C2275	C2214	A2154	A2094	U2034	G1973	A1913	A1853	C1793
G2708	G2646	U2584	C2462	G2400	A2340	G2276	C2215	U2155	A2095	G2035	C1974	C1914	A1854	A1794
G2709	U2647	U2585	U2463	U2401	G2341	G2277	G2218	G2156	C2096	C2036	G1975	U1915	U1855	C1795
C2710	G2648	U2586	G2464	C2403	U2343	C2282	U2219	A2158	A2097	A2037	U1976	A1916	U1856	U1796
A2711	G2649	A2587	G2465	U2404	U2344	C2283	U2220	G2159	U2098	G2038	A1977	U1917	G1857	G1797
G2712	U2650	G2588	C2466	G2405	U2345	A2284	G2221	C2160	U2099	U2039	A1978	A1918	A1858	U1798
U2713	C2651	A2589	G2467	A2406	A2346	C2285	G2222	G2161	G2101	G2041	U1979	A1919	U1859	G1799
G2714	C2652	A2590	A2468	A2407	C2347	G2286	G2223	G2162	G2102	A2042	A1981	G1921	G1860	C1800
C2715	U2653	G2591	A2469	U2408	U2348	A2287	C2224	A2163	C2103	C2043	U1982	G1922	G1861	A1801
G2716	A2654	G2592	G2470	G2409	G2349	A2288	A2225	C2164	C2104	C2044	U1983	G1923	G1862	A1802
C2717	G2655	U2593	A2471	G2410	G2350	G2289	C2226	C2165	U2105	C2045	G1984	C1924	G1863	A1803
G2718	U2656	C2594	G2472	A2411	G2351	G2290	A2227	U2166	U2106	G2046	C1985	U1925	U1864	C1804
G2719	C2657	G2595	U2473	A2412	A2352	U2291	G2228	U2167	G2107	C2047	C1986	U1926	U1865	A1805
U2720	G2658	U2596	U2474	G2413	G2353	U2292	U2229	G2168	A2108	G2048	A1987	A1927	A1866	C1806
A2721	U2659	G2597	G2475	G2414	C2354	G2293	U2230	A2169	U2109	G2049	G1988	A1928	G1867	G1807
G2722	A2660	A2598	A2476	G2415	G2355	G2294	U2231	A2170	G2110	C2050	G1989	G1929	G1868	A1808
C2723	G2661	G2599	U2477	C2416	U2356	C2295	U2232	A2171	U2111	A2051	C1990	G1930	G1869	A1809
U2724	A2662	A2600	G2478	C2417	G2357	U2296	U2233	G2172	G2122	A2052	U1991	U1931	C1870	A1810
A2725	G2663	G2601	U2479	A2418	A2358	G2297	G2234	U2173	U2113	G2053	G1992	A1932	A1871	G1811
A2726	G2664	A2542	C2480	U2419	C2359	A2298	G2235	C2174	A2114	A2054	U1993	G1933	G1873	G1813
G2727	A2665	G2603	G2481	C2420	G2360	U2299	U2236	C2175	G2115	C2055	C1994	G1934	C1874	G1814
U2728	G2666	U2604	A2482	G2421	G2361	G2300	U2237	A2176	G2116	G2056	U1995	G1935	G1875	A1815
G2729	C2667	U2605	C2483	C2422	G2362	C2301	G2238	C2177	A2117	C2057	C1996	A1936	A1876	C1816

A2850	A2851	G2852	C2853	G2854	C2855	A2856	G2857	C2858	G2859	A2860	U2861	G2862	C2863	G2864	U2865	U2866	G2867	A2868	G2869	C2870	U2871	A2872	A2873	C2874	C2875	G2876	G2877	U2878	A2879	C2880	U2881	A2882	A2883	U2884	G2885	A2886	A2887	C2888	C2889	G2890	U2891	G2892	A2893	G2894	G2895	C2896	U2897	U2898	A2899	A2900	C2901	U2902	U2903	U2904					
U2790	G2791	A2792	C2793	G2794	C2795	U2796	U2797	U2798	A2799	A2800	G2801	G2802	G2803	U2804	C2805	U2806	U2807	G2808	A2809	A2810	G2811	C2812	A2813	A2814	C2815	G2816	U2817	U2818	G2819	A2820	A2821	G2822	A2823	C2824	G2825	A2826	C2827	G2828	A2829	C2830	G2831	U2832	U2833	G2834	A2835	U2836	A2837	G2838	G2839	C2840	C2841	G2842	G2843	G2844	U2845	G2846	U2847	G2848	U2849
C2730	G2731	G2732	A2733	A2734	G2735	A2736	G2737	A2738	U2739	A2740	A2741	G2742	U2743	G2744	C2745	U2746	G2747	A2748	A2749	A2750	C2751	C2752	A2753	U2754	C2755	U2756	A2757	U2758	G2759	C2760	A2761	C2762	G2763	A2764	G2765	A2766	C2767	U2768	U2769	G2770	C2771	C2772	C2773	C2774	G2775	A2776	G2777	A2778	U2779	G2780	A2781	G2782	U2783	U2784	C2785	U2786	C2787	G2788	C2789

4 Data and refinement statistics

Xtriage (Phenix) and EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	1.00Å 1.00Å 1.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 7.50	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-7.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	ERNA-3D	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	62371	wwPDB-VP
Average B, all atoms (Å ²)	0.0	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: 1MA, 7MG, PSU, 5MU, 5MC

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	B	4.62	6615/69489 (9.5%)	3.04	5838/108346 (5.4%)

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	B	466	117

The worst 5 of 6615 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	2848	G	C1'-N9	60.90	2.39	1.48
1	B	1888	G	C1'-N9	51.99	2.25	1.48
1	B	857	G	C1'-N9	46.01	2.17	1.48
1	B	396	G	O3'-P	-41.94	0.98	1.61
1	B	2258	C	O3'-P	39.41	2.20	1.61

The worst 5 of 5838 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	396	G	O3'-P-O5'	44.13	170.19	104.00
1	B	913	U	P-O5'-C5'	37.95	177.83	120.90
1	B	2849	U	P-O5'-C5'	37.95	177.83	120.90
1	B	2887	A	P-O5'-C5'	37.75	177.52	120.90
1	B	1680	U	P-O5'-C5'	37.34	176.90	120.90

5 of 466 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	10	A	C4'
1	B	12	U	C4'
1	B	15	G	C4'
1	B	27	G	C4',C3'
1	B	28	A	C4'

5 of 117 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	10	A	Sidechain
1	B	14	A	Sidechain
1	B	52	A	Sidechain
1	B	53	A	Sidechain
1	B	64	A	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	B	62348	23	31477	19787	0
All	All	62348	23	31477	19787	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 211.

The worst 5 of 19787 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:B:69:C:H4'	1:B:85:G:C4'	1.23	1.68
1:B:318:C:H5'	1:B:319:G:C8	1.24	1.68
1:B:1853:A:C5'	1:B:1853:A:H4'	1.23	1.68
1:B:1627:G:H1'	1:B:1641:A:C8	1.27	1.67
1:B:901:C:H5'	1:B:902:C:C5	1.19	1.66

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein molecules in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein molecules in this entry.

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	B	2903/2904 (99%)	1526 (52%)	1147 (39%)

5 of 1526 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	B	9	G
1	B	10	A
1	B	11	C
1	B	12	U
1	B	13	A

5 of 1147 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	B	2327	A
1	B	2903	U
1	B	2405	G
1	B	2326	C
1	B	2644	G

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

13 non-standard protein/DNA/RNA residues are 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
1	PSU	B	1917	1	18,21,22	0.67	0	21,30,33	0.81	0
1	7MG	B	745	1	23,26,27	7.34	6 (26%)	27,39,42	2.43	4 (14%)
1	7MG	B	2251	1	23,26,27	7.52	6 (26%)	27,39,42	1.86	2 (7%)
1	5MU	B	1915	1	19,22,23	0.45	0	27,32,35	1.42	3 (11%)
1	5MU	B	747	1	19,22,23	0.65	1 (5%)	27,32,35	1.10	3 (11%)
1	PSU	B	746	1	18,21,22	0.90	0	21,30,33	1.07	1 (4%)
1	5MU	B	1939	1	19,22,23	0.98	2 (10%)	27,32,35	1.54	4 (14%)
1	1MA	B	2030	1	21,25,26	3.67	4 (19%)	30,37,40	1.23	4 (13%)
1	7MG	B	2069	1	23,26,27	2.71	3 (13%)	27,39,42	1.82	2 (7%)
1	5MC	B	2498	1	19,22,23	3.23	4 (21%)	26,32,35	2.52	5 (19%)
1	1MA	B	1618	1	21,25,26	3.65	4 (19%)	30,37,40	1.18	4 (13%)
1	PSU	B	1911	1	18,21,22	0.58	0	21,30,33	0.79	0
1	5MU	B	2449	1	19,22,23	2.42	3 (15%)	27,32,35	2.25	4 (14%)

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
1	PSU	B	1917	1	-	1/7/25/26	0/2/2/2
1	7MG	B	745	1	-	2/7/37/38	0/3/3/3
1	7MG	B	2251	1	-	2/7/37/38	0/3/3/3
1	5MU	B	1915	1	-	0/7/25/26	0/2/2/2
1	PSU	B	746	1	-	1/7/25/26	0/2/2/2
1	7MG	B	2069	1	-	0/7/37/38	0/3/3/3
1	5MU	B	1939	1	2/2/5/5	2/7/25/26	0/2/2/2
1	1MA	B	2030	1	-	3/7/25/26	0/3/3/3
1	5MC	B	2498	1	1/1/5/5	2/7/25/26	0/2/2/2
1	1MA	B	1618	1	-	2/7/25/26	0/3/3/3
1	5MU	B	747	1	-	2/7/25/26	0/2/2/2
1	5MU	B	2449	1	1/1/5/5	5/7/25/26	0/2/2/2
1	PSU	B	1911	1	-	0/7/25/26	0/2/2/2

The worst 5 of 33 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	2251	7MG	C1'-N9	32.95	2.06	1.46
1	B	745	7MG	C1'-N9	31.79	2.04	1.46
1	B	2030	1MA	C1'-N9	15.44	1.91	1.47
1	B	1618	1MA	C1'-N9	15.20	1.90	1.47
1	B	2251	7MG	C8-N9	-12.35	1.37	1.45

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2449	5MU	O4'-C4'-C5'	-8.27	82.84	109.33
1	B	2498	5MC	C1'-N1-C6	7.87	134.11	121.15
1	B	2069	7MG	N9-C8-N7	7.51	114.01	103.37
1	B	745	7MG	N9-C8-N7	7.43	113.90	103.37
1	B	2251	7MG	N9-C8-N7	7.42	113.88	103.37

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	1939	5MU	C4'
1	B	1939	5MU	C3'
1	B	2449	5MU	C4'
1	B	2498	5MC	C4'

5 of 22 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	2030	1MA	O4'-C4'-C5'-O5'
1	B	2449	5MU	O4'-C4'-C5'-O5'
1	B	2449	5MU	C4'-C5'-O5'-P
1	B	2498	5MC	C4'-C5'-O5'-P
1	B	1939	5MU	C3'-C4'-C5'-O5'

There are no ring outliers.

13 monomers are involved in 159 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	1917	PSU	6	0
1	B	745	7MG	18	0
1	B	2251	7MG	1	0
1	B	1915	5MU	10	0
1	B	747	5MU	26	0
1	B	746	PSU	22	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	1939	5MU	41	0
1	B	2030	1MA	3	0
1	B	2069	7MG	14	0
1	B	2498	5MC	17	0
1	B	1618	1MA	1	0
1	B	1911	PSU	1	0
1	B	2449	5MU	14	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1566

The worst 5 of 1566 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	75:G	O3'	76:C	P	2.66
1	B	2023:C	O3'	2024:G	P	2.65
1	B	87:U	O3'	88:G	P	2.57
1	B	1004:U	O3'	1005:C	P	2.55
1	B	2652:C	O3'	2653:U	P	2.55