



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 11:57 PM GMT

PDB ID : 1Z58
Title : Crystal structure of a complex of the ribosome large subunit with rapamycin
Authors : Amit, M.; Berisio, R.; Baram, D.; Harms, J.; Bashan, A.; Yonath, A.
Deposited on : 2005-03-17
Resolution : 3.80 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

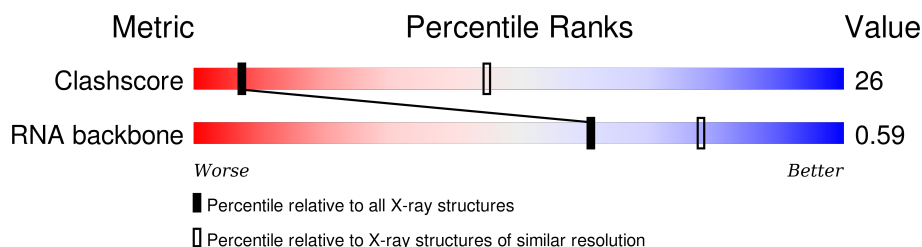
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 Å.

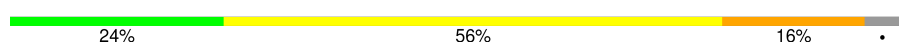
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1458 (4.10-3.50)
RNA backbone	2183	1070 (4.76-2.80)

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	2	2880	 24% 56% 16% .

2 Entry composition [i](#)

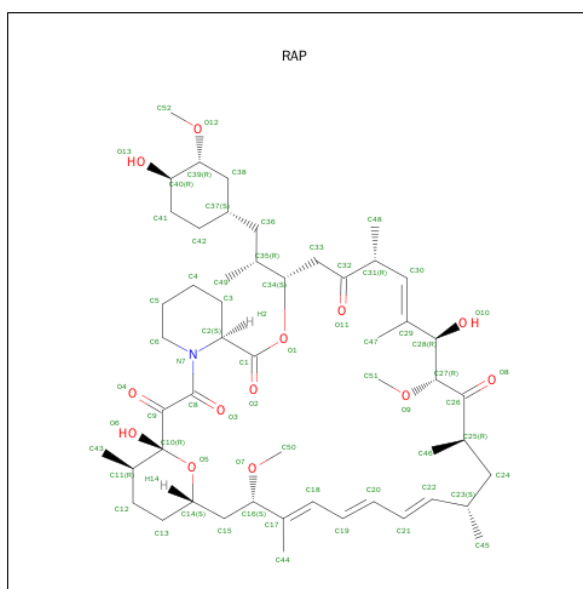
There are 2 unique types of molecules in this entry. The entry contains 59424 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	C	N	O	P			
1	2	2766	59359	26479	10949	19166	2765	0	0	0

- Molecule 2 is RAPAMYCIN IMMUNOSUPPRESSANT DRUG (three-letter code: RAP) (formula: C₅₁H₇₉NO₁₃).



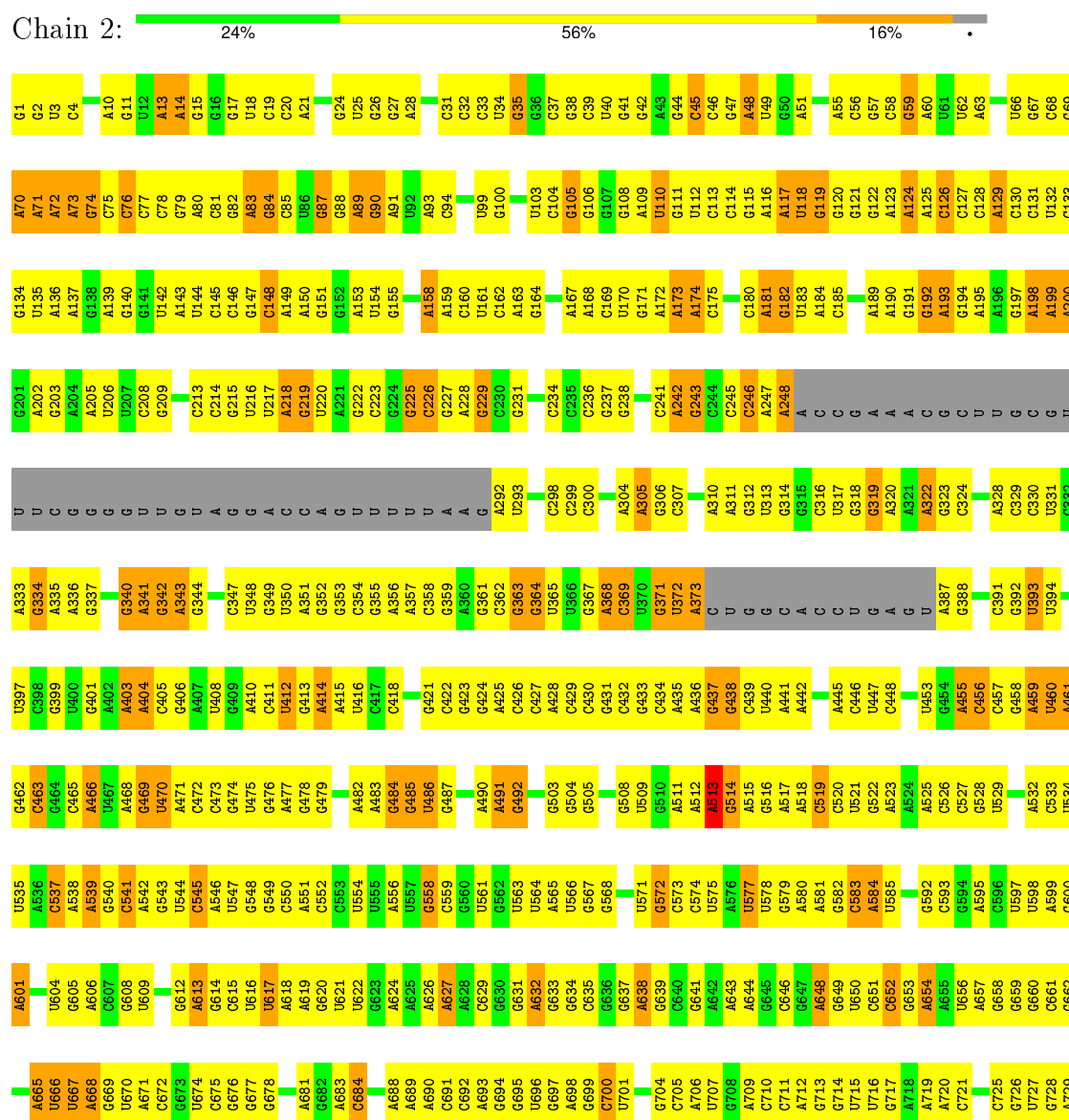
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	2	1	65	51	1	13	0	0

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



A1746	G1747	A1748	G1749	A1750	A1751	A1752	A1753	G1754	A1755	A1756	C1757	A1758	A1759	A1760	A1761	A1762	A1763	A1764	A1765	A1766	A1767	A1768	A1769	A1770	A1771	A1772	A1773	A1774	A1775	A1776	A1777	A1778	A1779	A1780	A1781	A1782	A1783	A1784	A1785	A1786	A1787	A1788	A1789	G1790	A1791	A1792	C1793	A1793	A1800	A1801	A1802	A1803	A1804	A1805	A1806	A1807	A1808	A1809	A1810																																																																																																																																																																																																																																																																																																																																											
C1677	A1678	A1679	A1680	A1681	A1682	A1683	A1684	A1685	A1686	A1687	A1688	A1689	A1690	A1691	A1694	A1695	A1696	A1697	A1698	A1699	A1700	C1701	A1702	A1703	A1704	A1705	A1706	A1707	A1708	A1709	A1710	A1711	A1712	A1713	A1714	A1715	A1716	A1717	A1718	A1719	A1720	A1721	A1722	A1723	A1724	A1725	A1726	A1727	A1728	A1729	A1730	A1731	A1732	A1737	A1738	A1742	A1743	A1744	A1745																																																																																																																																																																																																																																																																																																																																											
U1608	G1609	A1610	A1611	A1612	A1613	A1614	A1615	A1616	A1617	A1618	A1619	A1620	A1621	A1622	A1623	A1624	A1625	A1626	A1627	A1632	A1633	A1634	A1635	A1636	A1637	A1638	A1639	A1640	A1641	A1642	A1643	A1644	A1645	A1646	A1647	A1651	A1652	A1653	A1654	A1655	A1656	A1657	A1658	A1659	A1663	A1664	A1665	A1666	A1670	A1671	A1672	A1673	A1674	A1675	A1676																																																																																																																																																																																																																																																																																																																																															
A1538	A1539	A1540	A1541	A1544	A1545	A1546	A1549	A1550	A1551	A1552	A1557	A1558	A1559	A1560	A1561	A1562	A1563	A1564	A1565	A1566	A1567	A1568	A1569	A1570	A1571	A1572	A1573	A1574	A1577	A1578	A1579	A1580	A1583	A1584	A1585	A1586	A1587	A1588	A1591	A1592	A1593	A1594	A1595	A1596	A1597	A1600	A1601	A1602	A1603	A1604	A1605	A1606	A1607																																																																																																																																																																																																																																																																																																																																																	
U1473	A1474	A1475	A1476	A1479	A1480	A1481	A1482	A1483	A1484	A1485	A1486	A1487	A1488	A1489	A1490	A1492	A1493	A1494	A1495	A1496	A1497	A1498	A1499	A1500	A1501	A1502	A1503	A1504	A1505	A1506	A1507	A1508	A1509	A1510	A1511	A1512	A1513	A1514	A1515	A1516	A1517	A1518	A1519	A1520	A1521	A1522	A1523	A1524	A1525	A1526	A1527	A1528	A1529	A1530	A1531	A1532	A1533	A1534	A1537																																																																																																																																																																																																																																																																																																																																											
U1409	U1410	A1411	A1412	A1413	A1414	A1415	A1416	A1417	A1418	A1419	A1420	A1421	A1422	A1423	A1427	A1428	A1429	A1430	A1431	A1432	A1433	A1434	A1435	A1436	A1437	A1438	A1439	A1440	A1441	A1442	A1443	A1444	A1445	A1446	A1450	A1451	A1452	A1453	A1454	A1455	A1456	A1457	A1458	A1459	A1460	A1461	A1462	A1463	A1464	A1465	A1466	A1467	A1468	A1469	A1470	A1472																																																																																																																																																																																																																																																																																																																																														
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A1278	G1279	A1280	A1281	A1282	A1283	A1284	A1285	A1286	A1287	A1288	A1289	A1290	A1291	A1292	A1293	A1294	A1295	A1296	A1297	A1298	A1299	A1300	A1301	A1302	A1303	A1304	A1305	A1306	A1307	A1308	A1309	A1310	A1311	A1312	A1313	A1314	A1315	A1316	A1317	A1321	A1322	A1323	A1324	A1325	A1326	A1327	A1328	A1329	A1332	A1333	A1334	A1335	A1336	A1337	A1338	A1339	A1340																																																																																																																																																																																																																																																																																																																																													
G1210	G1211	U1212	U1213	U1214	A1215	A1216	U1217	A1218	A1219	U1220	A1221	A1222	A1223	A1224	A1225	A1226	A1227	A1233	A1234	A1235	A1236	A1243	A1244	A1245	A1246	A1247	A1248	A1249	A1250	A1251	A1252	A1253	A1254	A1255	A1256	A1257	A1258	A1259	A1260	A1261	A1262	A1263	A1264	A1265	A1266	A1267	A1268	A1269	A1270	A1271	A1272	A1273	A1274	A1275	A1276	A1277																																																																																																																																																																																																																																																																																																																																														
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G2747	C2747	A3585	G2630	G2555	G2487	C2420	A2352	C2271	C2205	G2140	G2076	A2014	C1948	C1878	A1811
G2748	C2748	C2686	G2621	A2556	G2488	C2421	G2353	C2271	C2206	A	G2077	G2015	A1949	G1879	U1812
A2749	G2749	G2687	G2622	G2557	C2489	G2422	G2354	C2274	G2207	G	U2080	G2016	G1951	G1880	A1813
G2750	A2623	G2688	A2623	G2558	U2490	G2423	A2355	U2275	U2208	C	U2081	U2017	G1951	U1881	G1814
C2751	G2624	C2689	G2625	U2559	C2491	G2424	A2356	C2276	G2209	C	U2082	C2018	A1952	G1882	G1815
G2752	U2625	G2690	U2625	G2560	G2492	G2425	A2357	A2280	G2210	A	C2082	C2019	A1953	A1883	G1816
C2753	U2626	G2691	U2626	G2561	U2493	G2426	C2358	C2281	U2211	A	G2083	G2020	A1954	U1817	U1817
G2754	G2627	A2692	G2627	G2562	C2494	A2427	U2359	G2282	U2212	C	G2084	G2021	G1955	C1885	G1818
A2755	G2628	U2693	G2628	U2563	G2495	U2428	C2360	G2283	G2213	G	G2085	C2022	G1956	G1886	U1819
G2756	U2629	G2694	U2629	C2496	C2496	A2429	G2361	U2284	G2214	U	U2086	C2023	G1957	G1887	G1820
C2757	C2630	C2695	C2630	C2565	A2497	A2429	G2362	U2285	G2215	U	U2087	U2024	C1957	C1888	A1821
A2758		A2696		A2566	U2498	A2432	G2363	G2286	G2216	G	U2088	A2025	G1962	G1889	C1822
U2759		G2697		G2567	C2499	G2433	C2364	G2287	G2217	A	C2089	C2026	G1963		
G2760	G2634	G2698	G2634	A2568	C2500	G2434	U2365	A2288	G2218	A	U2090		A1964	U1894	C1825
A2761	U2635	A2569	U2635	A2569	U2501	G2436	U2366	A2289	U2219	A	C2091	G2029	U1965	U1826	C1825
G2762	A2636	C2570	A2636	G2570	G2502	A2437	G2367	A2290	A2220	U	U2092	U2030	C1966	G1827	U1827
A2763	C2637	G2571	G2637	G2571	G2503	G2438	U2368	U2291	G2221	A	G2093	A2031	U1967	C1828	C1828
G2764	U2638	U2572	U2638	U2572	G2504		U2369	U2292	C2292	C	C2094	G2032	G1968	C1829	C1829
U2765		C2573		C2573	U2507	A2439	G2370	G2293	U2224	C	G2095	C2033	G1969	C1830	C1830
C2766	G2640	G2574	G2640	G2574	G2508	U2441	A2371	U2294	G2225	A	U2096	A2034	G1970	G1831	G1831
G2767	A2641	U2575	A2641	U2575	G2509	C2442	C2372	G2297	G2226	A	A2097	G2035	C1971	G1832	G1832
A2768	G2642	G2576	G2642	G2576	A2510	G2443	C2373	U2298	A2226	C	G	G2036	G1972	G1904	U1833
C2769	U2643	A2577	U2643	A2577	G2511	G2444	C2374	U2299	U2228	C	U2098	A2037	C1973	G1834	U1834
U2770	A2644	G2578	A2644	G2578	A2512	C2445	G2375	A2299	G2229	A	A	C2038	G1974	C1835	C1835
G2771	G2645	A2579	G2645	A2579	A2513	G2446	G2376	G2300	G2230	U	U2099	G2039	G1975	C1836	C1836
U2772	C2646	C2580	C2646	C2580	G2514	G2447	U2377	A2301	G2231	A	A		U1976		
G2773		A2581		A2581	U2515	A2448	G2378	G2302	G2235	A	G2103	A2042	C1977	A1910	A1840
U2774	A2649	G2582	A2649	G2582	U2516	G2449	G2379	C2303	G2236	A	G2104	A2043	U1978	G1841	G1841
	G2650	U2583	G2650	U2583	C2517	A2450	U2380	G2304	U2236	C	U2110	G2044	C1979	G1912	U1842
A2775	U2651	C2518	U2651	C2518	G2518		A2381	C2305	G2237	C	U2111	A2045	A1980	G1913	U1843
U2776	G2652	G2585	G2652	G2585	C2519	C2454	C2382	A2306	G2238	C	U2112	C2046	A1981	U1914	U1844
G2777	A2653	A2520	A2653	A2520	G2520	A2455	C2383	A2307	G2239	A	A2109	C2047	C1982	A1915	A1845
		U2521		U2521	A2521		G2384	A2308	G2240	C	G	C2048	G1983	G1916	A1846
		G2522		G2522	C2522	G2459	U2385	G2309	U2241	C	U2113	C2049	C1984	G1917	A1847
		G2523		G2523	G2523	G2460	U2386	G2310	G2242	U	U2114	G2050	G1985	G1918	U1848
		G2524		G2524	G2461	G2462	G2387	G2311	C2243	U	U2115	G2051	G1986	A1919	G1849
		U2525		U2525	G2463	G2464	A2390	U2312	A2245	C	G	G2052	G1987	A1920	G1850
		U2526		U2526	G2465	G2466	A2391	G2313	A2246	C	U2116	G2053	A1988		
		G2527		G2527	G2466	G2467	A2392	A2314	A2247	C	U2117	A2054	C1991	U1922	C1853
					G2467	G2468	C2395	G2315	A2248	C	A2118	G2055	G1992	U1923	G1854
					G2468	G2469	C2396	G2316	U2249	C	A2119	G2056	G1993	C1924	G1855
					G2470	G2471	A2397	G2317	G2250	C	U2120	U2057	C1925	U1856	U1856
					G2471	G2472	U2398	G2318	U2251	C	G2122	U2058	U1994	G1857	G1857
					G2472	G2473	U2399	G2319	A2252	C	G2123	U2059	U1927	C1858	C1858
					G2473	G2474	G2400	G2320	A2253	C	C2124	A2060	A1995	A1859	A1859
					G2474	G2475	G2401	G2321	A2254	C	C2125	G2061	A1996	G1928	
					G2475	G2476	U2402	G2322	G2255	U	U	U2062	U1934	U1934	A1860
					G2476	G2477	U2403	G2323	G2256	U	U	A2063	A1935	A1935	G1861
					G2477	G2478	A2404	G2324	G2257	U	U	U2064	A2002	A1936	C1862
					G2478	G2479	A2405	G2325	G2258	U	U	A2065	A2003	G1937	U1863
					G2479	G2480	A2406	G2326	G2259	U	U	G2066	U2004	U1938	C1864
					G2480	G2481	C2407	G2327	G2260	U	U	U2067	U2005	U1939	G1865
					G2481	G2482	G2408	G2328	G2261	U	U	C2068	G2006	C1940	A1867
					G2482	G2483	A2409	G2329	G2262	U	U	U2069	G2007	C1941	A1868
					U2410	U2411	U2410	G2330	G2263	U	U	G2070	C2008	G1942	U1869
					U2411	U2412	U2411	G2331	G2264	U	U	G2071	C2009	U2009	U1870
					U2412	U2413	U2412	G2332	G2265	U	U	G2072	G2010	C1944	G1871
					U2413	U2414	U2413	G2333	G2266	U	U	C2073	U2011	C1945	
					U2414	U2415	U2414	G2334	G2267	U	U	A2074	A2012	U1946	C1875
					U2415	U2416	U2415	G2335	G2268	U	U	U2075	A2013	G1947	
					U2416	U2417	U2416	G2336	G2269	U	U				
					U2417	U2418	U2417	G2337	G2270	U	U				
					U2418	U2419	U2418	G2338	G2271	U	U				
					U2419	U2420	U2419	G2339	G2272	U	U				
					U2420	U2421	U2420	G2340	G2273	U	U				
					U2421	U2422	U2421	G2341	G2274	U	U				
					U2422	U2423	U2422	G2342	G2275	U	U				
					U2423	U2424	U2423	G2343	G2276	U	U				
					U2424	U2425	U2424	G2344	G2277	U	U				
					U2425	U2426	U2425	G2345	G2278	U	U				
					U2426	U2427	U2426	G2346	G2279	U	U				
					U2427	U2428	U2427	G2347	G2280	U	U				
					U2428	U2429	U2428	G2348	G2281	U	U				
					U2429	U2430	U2429	G2349	G2282	U	U				
					U2430	U2431	U2430	G2350	G2283	U	U				
					U2431	U2432	U2431	G2351	G2284	U	U				
					U2432	U2433	U2432	G2352	G2285	U	U				
					U2433	U2434	U2433	G2353	G2286	U	U				
					U2434	U2435	U2434	G2354	G2287	U	U				
					U2435	U2436	U2435	G2355	G2288	U	U				
					U2436	U2437	U2436	G2356	G2289	U	U				
					U2437	U2438	U2437	G2357	G2290	U	U				
					U2438	U2439	U2438	G2358	G2291	U	U				
					U2439	U2440	U2439	G2359	G2292	U	U				
					U2440	U2441	U2440	G2360	G2293	U	U				
					U2441	U2442	U2441	G2361	G2294	U	U				
					U2442	U2443	U2442	G2362	G2295	U	U				
					U2443	U2444	U2443	G2363	G2296	U	U				
					U2444	U2445	U2444	G2364	G2297	U	U				
					U2445	U2446	U2445	G2365	G2298	U	U				
					U2446	U2447	U2446	G2366	G2299	U	U				
					U2447	U2448	U2447	G2367	G2300	U	U				
					U2448	U2449	U2448	G2368	G2301	U	U				
					U2449	U2450	U2449	G2369	G2302	U	U				
					U2450	U2451	U2450	G2370	G2303	U	U				
					U2451	U2452	U2451	G2371	G2304	U	U				
					U2452	U2453	U2452	G2372	G2305	U	U				
					U2453	U2454	U2453	G2373	G2306	U	U				
					U2454	U2455	U2454	G2374	G2307	U	U				
					U2455	U2456	U2455	G2375	G2308	U	U				
					U2456	U2457	U2456	G2376	G2309	U	U				
					U2457	U2458	U2457	G2377	G2310	U	U				
					U2458	U24									

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	168.50 Å 404.00 Å 689.00 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 3.80	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-3.80)	Depositor
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.273 , 0.368	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	59424	wwPDB-VP
Average B, all atoms (Å ²)	58.0	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: RAP

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	2	0.15	0/66467	0.63	1/103673 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	2	513	A	C2'-C3'-O3'	6.09	123.44	113.70

There are no chirality outliers.

There are no planarity outliers.

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	2	59359	0	29917	2275	0
2	2	65	0	79	20	0
All	All	59424	0	29996	2275	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 26.

The worst 5 of 2275 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)
1:2:1773:C:H41	2:2:2881:RAP:C15	1.42	1.32
1:2:1773:C:N4	2:2:2881:RAP:H151	1.54	1.20
1:2:700:C:H42	1:2:800:U:H4'	1.11	1.15
1:2:1663:C:H5'	1:2:1664:G:H5''	1.32	1.08
1:2:940:G:H3'	1:2:941:U:H5''	1.36	1.08

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	2	2757/2880 (95%)	529 (19%)	65 (2%)

5 of 529 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	14	A
1	2	35	G
1	2	45	C
1	2	48	A
1	2	49	U

5 of 65 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	1325	U
1	2	1632	A
1	2	2633	A
1	2	1345	G
1	2	1410	U

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$
2	RAP	2	2881	-	65,68,68	1.89	13 (20%)	65,96,96	1.43	8 (12%)

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
2	RAP	2	2881	-	-	0/81/124/124	0/2/4/4

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	2881	RAP	C8-C9	-8.00	1.42	1.53
2	2	2881	RAP	O1-C34	-3.28	1.40	1.46
2	2	2881	RAP	C13-C14	2.06	1.56	1.51
2	2	2881	RAP	C2-N7	2.58	1.50	1.47
2	2	2881	RAP	C38-C39	2.59	1.57	1.52

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	2	2881	RAP	O1-C1-O2	-2.74	118.24	123.89
2	2	2881	RAP	C3-C2-N7	-2.74	106.49	110.43
2	2	2881	RAP	C28-C29-C30	2.03	123.03	119.46
2	2	2881	RAP	C12-C13-C14	2.07	114.14	110.90
2	2	2881	RAP	C52-O12-C39	2.28	120.27	114.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	2	2881	RAP	20	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 ⓘ

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

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

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

6.4 Ligands ⓘ

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

6.5 Other polymers ⓘ

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