



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 04:46 AM GMT

PDB ID : 2O44  
Title : Structure of 23S rRNA of the large ribosomal subunit from *Deinococcus radiodurans* in complex with the macrolide josamycin  
Authors : Pyetan, E.; Daram, D.; Auerbach-Nevo, T.; Yonath, A.  
Deposited on : 2006-12-03  
Resolution : 3.30 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) : **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

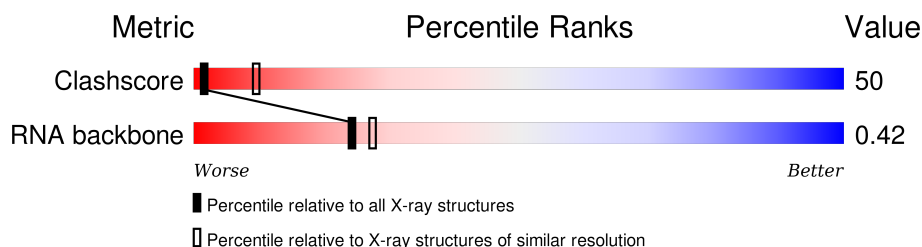
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 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	1058 (3.38-3.22)
RNA backbone	2183	1005 (3.82-2.78)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	2880	

2 Entry composition ⓘ

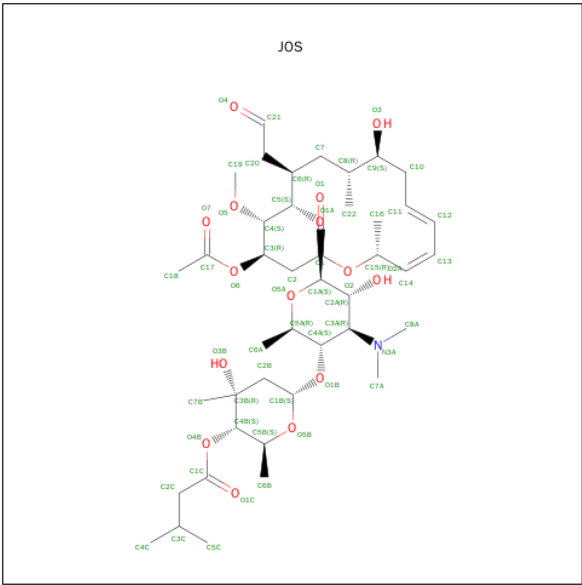
There are 2 unique types of molecules in this entry. The entry contains 59417 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	A	2766	59359	26479	10949	19166	2765	0	0	0

- Molecule 2 is (2S,3S,4R,6S)-6-([(2R,3S,4R,5R,6S)-6-([(4R,5S,6S,7R,9R,10S,12E,14Z,16R)-4-(ACETYLOXY)-10-HYDROXY-5-METHOXY-9,16-DIMETHYL-2-OXO-7-(2-OXOETHYL)OXACYCLOHEXADECA-12,14-DIEN-6-YL]OXY}-4-(DIMETHYLAMINO)-5-HYDROXY-2-METHYLTETRAHYDRO-2H-PYRAN-3-YL]OXY}-4-HYDROXY-2,4-DIMETHYLTETRAHYDRO-2H-PYRAN-3-YL 3-METHYLBUTANOATE (three-letter code: JOS) (formula: C<sub>42</sub>H<sub>69</sub>NO<sub>15</sub>).



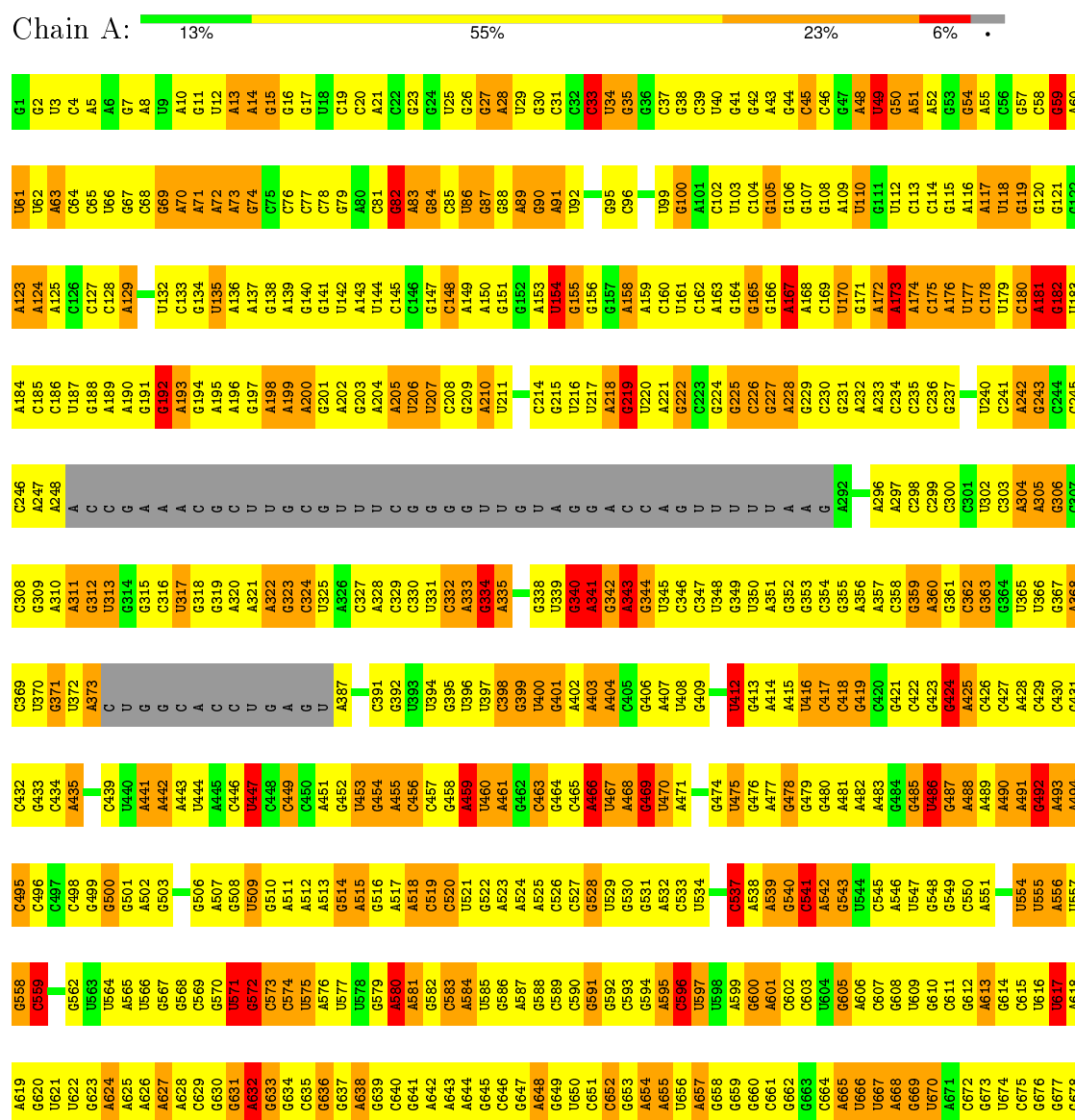
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	58	42	1	15	0	0

### 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 rRNA



U1601	G1541	G1479	G1418	G1352	A1292	C1169	U1108	G1047	A984	A923	C863	A802	G741	C679
G1602	G1542	G1480	G1419	A1353	A1293	U1170	A1109	U1048	G985	C924	C864	C803	G742	U680
A1603	G1543	U1481	A1420	A1354	G1294	A1171	C1110	C1049	A986	U925	A865	C804	U743	A682
A1604	A1544	U1482	A1421	A1355	U1295	U1172	C1111	G1050	G987	C926	U866	8805	C744	U683
A1605	G1545	G1483	A1422	A1356	G1296	G1173	U1112	G1051	G988	C927	G867	A806	G745	A683
C1606	G1546	G1484	A1423	U1357	A1297	G1174	C1113	C1052	G989	C928	U868	A807	G746	C684
A1607	U1547	U1485	U1424	C1358	G1298	A1175	A1114	G1053	G992	A929	C869	C808	A747	U685
U1608	A1486	G1425	G1425	G1358	A1299	U1176	C1115	C1054	A993	A930	C870	C809	A748	U686
G1609	G1548	G1487	U1426	G1361	A1300	U1177	U1116	A1055	C995	G931	U871	U810	C749	G687
A1610	C1550	G1488	G1427	A1362	U1301	C1178	G1117	U1056	A994	G932	G872	G811	G750	A688
U1611	U1551	G1489	G1428	C1363	C1302	A1179	G1118	A1057	A995	G933	U873	G812	G751	A689
C1614	G1552	U1490	G1364	U1303	U1303	A1180	U1119	G1058	C996	G934	A874	A813	G752	A690
U1618	C1553	G1491	G1430	U1365	U1304	C1181	C1120	A1059	G997	C935	G875	G814	G753	C691
A1619	G1554	A1492	U1431	A1366	C1305	U1182	G1121	C1060	G1000	A936	A876	A815	G754	C692
A1620	A1555	G1493	G1432	A1367	U1306	C1183	A1122	A1061	G1001	C937	G877	U816	C755	A693
A1621	G1557	G1496	U1434	G1369	G1308	G1184	G1123	G1062	C1002	U938	C878	A817	C756	G694
C1622	C1558	C1497	G1435	U1370	C1309	C1185	U1124	C1063	C1003	C939	A879	G818	G757	U695
G1623	U1559	C1497	G1436	G1371	C1310	A1186	G1125	C1064	A1004	G940	C880	C819	U757	A698
A1624	A1560	G1498	A1437	A1372	G1311	A1187	A1126	A1065	U1005	U941	U881	C819	G758	C699
A1625	G1561	A1499	G1438	A1373	C1312	A1188	A1129	G1066	C1006	U942	C882	G822	C759	A698
A1626	U1562	U1500	G1374	U1313	C1253	G1189	U1130	G1067	A1007	U943	U883	U824	U760	C700
C1627	U1563	C1501	G1440	C1375	G1254	C1190	U1131	A1068	G1008	A944	C884	U824	A762	A702
C1631	U1564	G1502	A1441	G1376	A1255	A1192	C1132	G1069	C1009	G945	A885	C825	A763	A703
C1632	G1565	G1503	A1442	G1377	G1316	G1193	G1133	G1070	U1010	U946	A886	U826	A764	G704
C1633	G1566	G1504	G1443	A1378	U1257	U1194	C1134	U1072	A1011	C947	G887	C827	C765	C705
C1634	A1567	U1505	C1444	A1379	A1318	U1195	C1135	G1073	G1013	G949	C888	C828	A766	A706
C1635	A1568	C1506	C1445	C1380	C1319	G1196	G1136	G1074	G1014	G950	U890	C830	G767	U707
G1638	U1569	A1507	U1447	G1381	A1320	U1197	A1137	C1075	U1015	G951	A891	G831	C769	A709
U1639	G1570	G1508	A1448	G1382	A1321	C1198	A1138	U1076	C1016	A952	G	A832	G772	C710
C1640	C1571	A1509	C1449	C1383	G1322	U1199	A1139	U1077	C1017	G953	G	A833	G773	G711
C1641	U1572	A1510	G1450	G1384	G1323	G1200	A1140	U1078	C1018	U954	G	A834	G774	A712
G1642	G1573	U1512	A1451	C1385	C1324	G1201	U1141	G1079	U1019	G955	G	U835	A775	G713
A1643	C1574	U1513	A1452	U1386	U1325	U1202	G1142	A1080	A1020	A956	G	U836	U776	G714
G1644	U1575	U1514	A1453	G1387	U1326	A1203	A1143	A1081	A1021	G957	C	U837	A777	U715
U1645	G1576	C1514	U1454	G1388	C1327	G1204	U1144	G1082	A1022	G958	C	A838	A778	U716
U1646	U1577	U1515	C1455	C1389	C1328	G1205	G1145	C1083	U1023	C959	U	U839	G779	G717
G1647	U1578	A1516	G1456	G1390	U1329	G1206	G1146	A1084	G1024	U960	A	U840	U779	A718
U1648	G1580	G1520	A1457	A1391	G1330	G1207	G1147	C1085	U1025	G963	C	8841	U780	A719
A1649	C1581	U1521	U1458	U1392	G1331	A1208	G1148	C1086	U1026	A964	C	A842	G781	A720
A1650	A1582	C1522	G1460	G1393	G1332	G1209	G1149	C1087	G1027	A965	A	8843	U782	G721
U1651	A1583	A1523	C1461	G1394	G1333	C1210	C1150	A1088	G1028	G965	G	8844	G783	G722
C1652	U1584	C1524	C1462	A1397	A1335	G1211	U1151	C1089	C1029	A966	C	U845	U784	C723
G1653	A1585	U1526	A1463	G1398	A1336	U1212	G1152	C1090	U1030	G967	U	A846	U785	C724
A1654	U1586	G1527	G1465	G1402	G1337	U1213	A1153	C1093	C968	C968	U	C847	U786	C725
C1655	A1587	C1528	C1466	U1403	G1338	C1214	A1154	A1093	A1032	C969	A	A848	A787	G726
C1656	U1588	U1529	U1467	G1407	A1339	A1215	G1155	C1094	G1033	A970	C	8849	G788	U727
U1657	G1590	U1530	A1468	A1407	C1341	U1217	G1157	A1095	U1034	A971	C	C850	G789	G728
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C1659	U1592	A1532	U1470	U1409	C1343	C1219	U1159	G1098	U1037	U974	A912	U852	G791	C730
G1660	C1593	G1533	G1471	C1410	G1344	G1220	C1160	A1099	U1038	U975	C914	C853	U792	A731
C1661	U1594	A1534	C1472	C1411	C1345	G1284	U1161	G1100	A1039	C976	C915	8855	G793	A732
C1662	A1595	G1535	U1473	C1412	G1346	U1285	A1162	U1101	A1040	G977	C916	A856	A794	G733
C1663	U1596	C1536	A1474	U1413	C1347	U1287	C1164	G1102	G1041	U978	U917	U857	A795	G734
C1664	A1597	U1537	U1475	G1414	G1348	A1288	G1165	C1103	G1042	A979	A918	8858	A796	G735
C1665	G1598	U1538	G1476	C1415	A1349	A1226	U1166	G1104	G1043	G980	U919	U859	G798	C737
C1666	U1600	C1540	U1477	A1416	A1350	A1227	A1167	U1105	U1044	C981	U920	U860	G799	G738
			U1478	C1417	G1351	C1228	A1167	A1106	G1045	C982	A921	8861	U800	G739
						C1229	G1168	A1107	U1046	G983	A922	A862	A801	A740

A2613	G2548	U2483	C2422	A2357	G2297	G2234	U2171	C	G2050	A1984	U1856	A1794	G1730	A1667
A2614	G2549	G2484	G2423	C2358	U2296	G2235	U2172	C	U2051	A1985	G1897	C1795	C1731	G1668
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G2620	C2364	U2490	U2429	C2364	G2304	U2241	U2178	A2117	U2057	U1991	U1863	C1801	C1674	C1675
A2621	U2365	G2492		U2365	C2305	C2242	C2179	A2118	U2058	G1992	U1864	A1802	C1675	U1676
G2622	U2366	U2493	A2432	C2366	A2306	G2243	U2180	A2119	U2059	G1993	G1865	U1738	G1739	U1677
A2623	C2367	G2494	G2433	A2367	A2307	C2244	U2181	A2120	A2060	U1994	G1866	G1740	G1740	G1677
G2624	G2368	G2495	G2434	G2368	A2308	A2245		G2122	A2061	U1995	A1867	G1741	G1741	G1678
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U2626	G2370	U2497	U2436	G2370	G2310	A2247	U2182	C2124	U2063	A1997	A1869	C1743	U1680	U1680
G2627	A2371	U2498	G2437	A2371	U2311	A2248	U2183	U	U2064	A1998	U1870	G1744	A1681	A1681
C2628	A2372	U2499	A2438	A2372	A2312	U2249	A2187	U	U2065	U1999	G1871	C1745	G1683	G1683
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G2630	G2374	U2501	U2440	U2374	G2314	U2251	A2189	U	G2067	U1999	A1873	G1747	U1685	U1685
C2631	U2375	G2502	U2441	U2375	A2315		A2190	U	U2068	A2002	G1874	U1748	A1685	A1685
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A2633	U2381	G2504	C2443	U2381	G2317	G2255	U2192	U	G2070	U2004	C1876	U1750	C1687	C1687
G2634	C2382	U2505	C2444	C2382	U2318		C2193	G	C2071	U2005	U1817	A1751	U1688	U1688
U2635	C2383	G2506	C2445	C2383	G2319	G2259	A2194	G	C2072	G2006	G1818	U1752	U1689	U1689
A2636	G2384	U2507	G2446	G2384	G2320	G2260	C2195	U	U2074	G2007	U1819	G1753	U1690	U1690
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G2638	G2386		A2448	G2386	U2322	C2262	U2197	G	G2076	U2009	A1885	G1755	C1692	C1692
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A2641	G2389	U2512	G2451	G2389	A2325	U2270	G2200	C	U2079	G1891	G1888	C1763	A1699	A1699
G2642	A2390	G2513	U2452	G2390	G2326	A2265	G2201	A	U2080	A2013	C1889	C1765	C1700	C1700
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G2645	C2393	U2517	A2455	C2393	G2329	G2269	A2204	G	G2083	G2016	C1892	U1770	U1705	U1705
C2646	U2394	G2518	U2456	G2394	G2330	C2270	G2205	C	G2084	G1955	G1893	A1771	A1706	A1706
G2647	C2395	U2519	A2457	G2395	A2331	U2271	C2206	A	G2085	U2017	G1894	C1772	C1708	C1708
A2648	U2396	A2520	U2458	G2396	G2332	A2272	G2207	C	U2086	G1958	G1895	C1773	U1709	U1709
G2649	A2397	G2521	C2459	A2397	A2333	C2273	U2208	G	U2087	U1959	G1896	A1774	U1710	U1710
G2650	U2398	U2522	G2460	U2398	C2334	C2274	G2209	U	U2088	A1960	C1897	A1775	G1710	G1710
U2651	G2399	U2523	G2461	G2399	U2335	U2275	C2210	G	C2089	A1961	U1898	A1776	G1712	G1712
G2652	U2402	U2526	G2462	U2402	G2336	C2276	U2211	U	U2090	G1962	A1899	A1777	G1713	G1713
A2653	C2403	G2529	G2463	C2403	A2337	A2277	U2212	G	C2091	G1963	U1900	U1778	A1714	A1714
U2654	U2404	U2530	G2464	U2404	A2338	G2278	G2213	A	U2092	A1964	A1901	C1779	A1715	A1715
G2655	A2405	U2531	G2465	A2405	A2339	G2279	U2223	A	G2093	U1965	A1902	A1774	U1716	U1716
C2656	C2406	G2530	A2466	C2406	G2341	C2280	G2217	U	C2094	C1903	A1839	A1775	A1717	A1717
G2657	G2407	U2532	U2467	G2407	U2342	C2281	G2218	A	G2095	G1904	A1840	A1776	G1712	G1712
A2658	C2408	U2533	G2468	G2408	U2343	G2282	U2219	G	U2096	G1905	A1841	A1777	G1713	G1713
C2659	A2409	U2534	G2469	A2409	G2344	U2284	A2220	C2157	G1906	U1906	G1842	U1778	A1714	A1714
G2660	U2410	U2535	U2470	U2410	G2344	U2285	G2221	C2158	C2037	C1907	U1843	C1779	A1715	A1715
U2661	A2411	G2536	U2471	A2411	A2345	U2286	U2222	A	G1907	G1908	C1844	A1780	G1716	G1716
C2662	U2412	C2537	G2472	U2412	G2346	G2286	U2223	C2160	A	U1909	A1845	C1781	A1717	A1717
G2665	A2413	U2538	G2473	A2413	C2347	G2287	U2224	C2161	U	U1910	A1846	A1782	G1721	G1721
U2666	G2414	C2539	G2474	C2414	A2348	A2288	G2225	C2162	A	A1911	G1847	C1786	U1722	U1722
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U2668	A2416	U2541	A2476	A2416	G2350	G2290	C2227	C2163	C2044	C1977	G1913	U1788	G1724	G1724
G2669	U2417	G2542	C2477	U2417	G2351	U2291	U2228	G2043	U1978	U1978	G1850	C1788	C1725	C1725
A2670	U2418	U2543	G2478	U2418	A2352	C2292	G2223	A2045	G1979	G1979	A1851	G1789	C1726	C1726
U2671	C2419	U2544	U2479	C2419	G2353	G2293	G2230	C2046	A1980	A1980	G1852	U1790	C1727	C1727
G2672	U2420	U2545	G2480	U2420	G2354	U2294	G2231	C2047	A1981	A1981	G1853	C1791	A1728	A1728
C2673	A2482	C2547	A2482	C2421	A2356	U2296	C2233	C2049	G1983	G1983	A1919	A1793	C1729	C1729

A2858	A2796	C2674	U2736	A2696	U2675
U2859	G2797	A2737	A2738	G2697	
A2860	A2798	A2739	A2738	G2698	
A2861	C2799	G2740	G2739	G2699	
G2862	C2800	G2741	G2740	U2700	
U2863	A2801	G2742	G2741	A2701	
C2864	C2802	G2743	G2742	G2702	
G2865	C2803	A2744	G2743	G2703	
A2866	G2804	A2745	A2744	U2704	
G2867	G2805	G2746	A2745	A2705	
G2868	G2806	G2747	G2746	U2706	
	U2807	G2748	G2747	G2707	
	U2808	C2749	G2748	U2708	
U2872	A2809	A2750	A2749	C2709	
G2873	A2810	G2751	A2750	C2710	
A2874	G2811	C2752	G2751	G2711	
C2875	A2812	G2753	G2752	G2712	
G2876	G2813	C2754	G2753	A2713	
A2877	G2814	A2755	G2754	A2714	
C	C2815	A2756	A2755	G2715	
U	C2816	G2757	A2756	G2716	
C	A2817	A2758	G2757	G2717	
	G2818	U2759	A2758	U2718	
	G2819	G2760	U2759	C2719	
	C2820	A2761	G2760	A2720	
	G2821	G2762	A2761	A2721	
	U2822	U2763	G2762	C2722	
	G2823	U2764	U2763	G2723	
	C2824	U2765	U2764	G2724	
	A2825	U2766	U2765	C2725	
	C2826	G2767	U2766	U2726	
	G2827	C2768	G2767	G2727	
	C2828	A2769	C2768	A2728	
	A2829	C2770	A2769	A2729	
	U2830	C2771	C2770	A2730	
	A2831	U2772	C2771	G2731	
	G2832	G2773	U2772	C2732	
	C2833	U2774	G2773	A2733	
	A2834	U	U2774	U2734	
	A2835	U	U	U2735	
	U2836	A	A		
	G2837	U2778	U2778		
	U2838	C2779	C2779		
	C2839	A2780	A2780		
	U2840	G2781	G2781		
	C2841	G2782	G2782		
	A2842	U2783	U2783		
	G2843	A2784	A2784		
	U2844	G2785	G2785		
	C2845	G2786	G2786		
	G2846	A2787	A2787		
	G2847	C2788	C2788		
	A2848	U2789	U2789		
	C2849	C2790	C2790		
		G2791	G2791		
		C2792	C2792		
		G2793	G2793		
		U2794	U2794		
		A2795	A2795		

## 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, $\alpha$ , $\beta$ , $\gamma$	172.80Å 411.48Å 697.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 3.30	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-3.30)	Depositor
$R_{merge}$	0.18	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.282 , 0.331	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	59417	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	83.0	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: JOS

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	A	0.67	4/66467 (0.0%)	0.85	130/103673 (0.1%)

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	A	1	200

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1711	C	N1-C2	6.95	1.47	1.40
1	A	528	G	C5-C6	-6.20	1.36	1.42
1	A	2566	A	C5-C6	-5.34	1.36	1.41
1	A	475	U	N1-C2	-5.10	1.33	1.38

The worst 5 of 130 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2044	G	N9-C1'-C2'	11.61	129.09	114.00
1	A	2237	C	N1-C1'-C2'	9.82	126.77	114.00
1	A	2045	A	N9-C1'-C2'	9.68	126.58	114.00
1	A	219	G	N9-C1'-C2'	9.26	126.04	114.00
1	A	841	G	N9-C1'-C2'	9.26	126.04	114.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	541	C	C1'

5 of 200 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	154	U	Sidechain
1	A	49	U	Sidechain
1	A	54	G	Sidechain
1	A	59	G	Sidechain
1	A	86	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	A	59359	0	29916	4363	0
2	A	58	0	68	7	0
All	All	59417	0	29984	4365	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 50.

The worst 5 of 4365 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:A:1435:G:C2	1:A:1436:G:H1'	1.70	1.25
1:A:2094:C:N4	1:A:2162:C:H42	1.40	1.19
1:A:793:G:H21	1:A:796:A:N6	1.41	1.17
1:A:1463:A:H1'	1:A:1543:G:N2	1.59	1.17
1:A:2498:U:H4'	1:A:2499:C:OP1	1.40	1.14

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	A	2757/2880 (95%)	718 (26%)	224 (8%)

5 of 718 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	13	A
1	A	14	A
1	A	23	G
1	A	28	A
1	A	33	C

5 of 224 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1264	C
1	A	1442	C
1	A	2593	A
1	A	1278	A
1	A	1324	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 ⓘ

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	JOS	A	2881	-	59,60,60	2.78	16 (27%)	68,85,85	1.94	19 (27%)

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	JOS	A	2881	-	-	0/65/104/104	0/2/3/3

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2881	JOS	C10-C11	-5.87	1.30	1.50
2	A	2881	JOS	C13-C12	-3.62	1.33	1.44
2	A	2881	JOS	C6A-C5A	-3.35	1.43	1.51
2	A	2881	JOS	C2B-C1B	2.03	1.56	1.51
2	A	2881	JOS	C8A-N3A	2.15	1.54	1.46

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2881	JOS	O3-C9-C10	-3.65	100.87	109.34
2	A	2881	JOS	C10-C11-C12	-3.38	120.64	125.34
2	A	2881	JOS	C4A-C3A-N3A	-3.16	103.98	111.70
2	A	2881	JOS	C19-O5-C4	-2.98	106.16	114.59
2	A	2881	JOS	C22-C8-C7	-2.93	106.20	110.76

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2881	JOS	7	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.