



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 04:47 AM GMT

PDB ID : 2O45
Title : Structure of the 23S rRNA of the large ribosomal subunit from *Deinococcus Radiodurans* in complex with the macrolide RU-69874
Authors : Baram, D.; Pyetan, E.; Auerbach-Nevo, T.; Yonath, A.
Deposited on : 2006-12-03
Resolution : 3.60 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

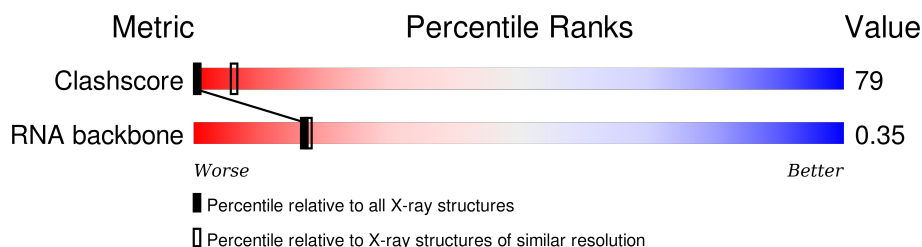
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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	1010 (3.74-3.46)
RNA backbone	2183	1058 (4.40-2.80)

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	A	2880	

2 Entry composition ⓘ

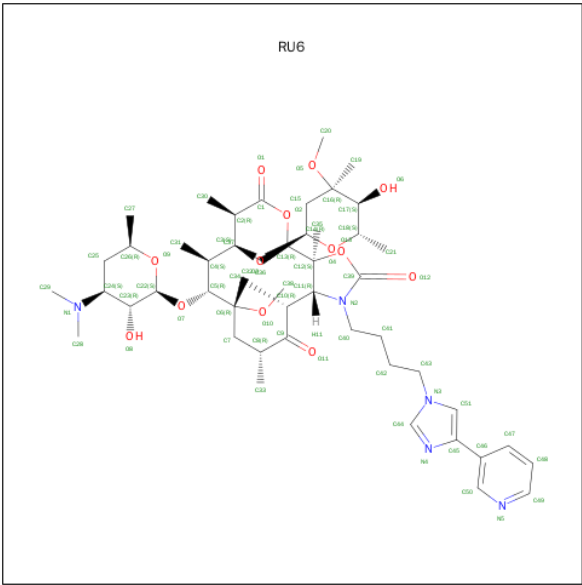
There are 2 unique types of molecules in this entry. The entry contains 59428 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (3AS,4R,7R,8S,9S,10R,11R,13R,15R,15AR)-4-ETHYL-11-METHOXY-3A,7,9,11,13,15-HEXAMETHYL-2,6,14-TRIOXO-1-[4-(4-PYRIDIN-3-YL-1H-IMIDAZOL-1-YL)BUTYL]-10-{[3,4,6-TRIDEOXY-3-(DIMETHYLAMINO)-BETA-D-XYLO-HEXOPYRANOSYL]OXY}TETRADECAHYDRO-2H-OXACYCLOTETRADECINO[4,3-D][1,3]OXAZOL-8-YL 2,6-DIDEOXY-3-C-METHYL-3-O-METHYL-ALPHA-L-RIBO-HEXOPYRANOSIDE (three-letter code: RU6) (formula: C₅₁H₈₁N₅O₁₃).



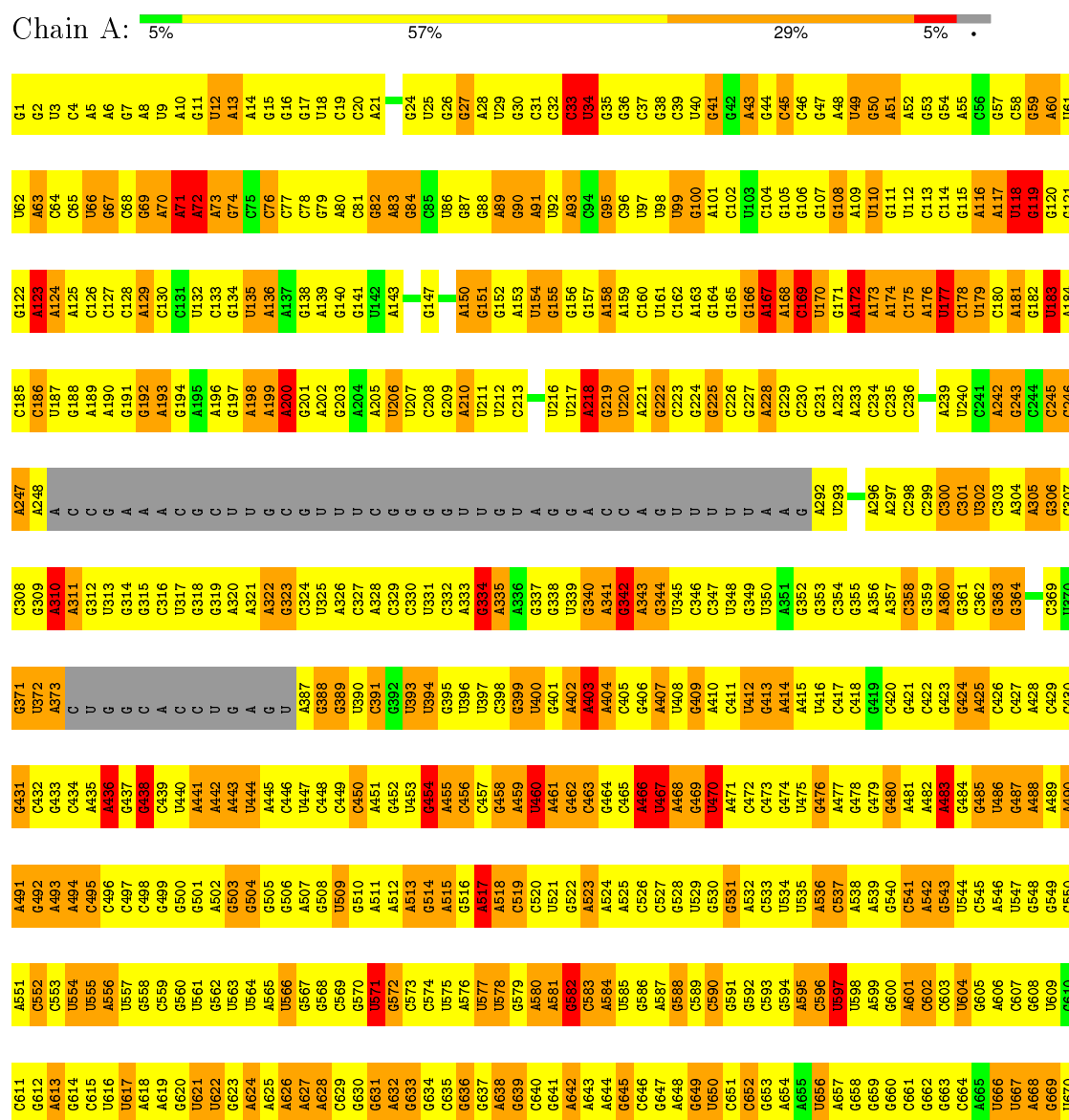
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	69	51	5	13	0	0

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 ($\text{RSRZ} > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

• Molecule 1: 23S rRNA



G1577	G1578	G1579	G1580	G1581	G1582	G1583	G1584	G1585	G1586	G1587	G1588	G1589	G1590	G1591	G1592	G1593	G1594	G1595	G1596	G1597	G1598	G1599	G1600	G1601	G1602	G1603	G1604	G1605	G1606	G1607	G1608	G1609	G1610	G1611	G1612	G1613	G1614	G1615	G1616	G1617	G1618	G1619	G1620	G1621	G1622	G1623	G1624	G1625	G1626	G1627	G1628	G1629	G1630	G1631	G1632	G1633	G1634	G1635	G1636																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
C1517	C1518	C1519	C1520	C1521	C1522	C1523	C1524	C1525	C1526	C1527	C1528	C1529	C1530	C1531	C1532	C1533	C1534	C1535	C1536	C1537	C1538	C1539	C1540	C1541	C1542	C1543	C1544	C1545	C1546	C1547	C1548	C1549	C1550	C1551	C1552	C1553	C1554	C1555	C1556	C1557	C1558	C1559	C1560	C1561	C1562	C1563	C1564	C1565	C1566	C1567	C1568	C1569	C1570	C1571	C1572	C1573	C1574	C1575	C1576																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
A1457	A1458	A1459	A1460	A1461	A1462	A1463	A1464	A1465	A1466	A1467	A1468	A1469	A1470	A1471	A1472	A1473	A1474	A1475	A1476	A1477	A1478	A1479	A1480	A1481	A1482	A1483	A1484	A1485	A1486	A1487	A1488	A1489	A1490	A1491	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																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
G1337	G1338	G1339	G1340	G1341	G1342	G1343	G1344	G1345	G1346	G1347	G1348	G1349	G1350	G1351	G1352	G1353	G1354	G1355	G1356	G1357	G1358	G1359	G1360	G1361	G1362	G1363	G1364	G1365	G1366	G1367	G1368	G1369	G1370	G1371	G1372	G1373	G1374	G1375	G1376	G1377	G1378	G1379	G1380	G1381	G1382	G1383	G1384	G1385	G1386	G1387	G1388	G1389	G1390	G1391	G1392	G1393	G1394	G1395	G1396																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
U1276	U1277	U1278	U1279	U1280	U1281	U1282	U1283	U1284	U1285	U1286	U1287	U1288	U1289	U1290	U1291	U1292	U1293	U1294	U1295	U1296	U1297	U1298	U1299	U1300	U1301	U1302	U1303	U1304	U1305	U1306	U1307	U1308	U1309	U1310	U1311	U1312	U1313	U1314	U1315	U1316	U1317	U1318	U1319	U1320	U1321	U1322	U1323	U1324	U1325	U1326	U1327	U1328	U1329	U1330	U1331	U1332	U1333	U1334	U1335	U1336																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														
G1216	G1217	G1218	G1219	G1220	G1221	G1222	G1223	G1224	G1225	G1226	G1227	G1228	G1229	G1230	G1231	G1232	G1233	G1234	G1235	G1236	G1237	G1238	G1239	G1240	G1241	G1242	G1243	G1244	G1245	G1246	G1247	G1248	G1249	G1250	G1251	G1252	G1253	G1254	G1255	G1256	G1257	G1258	G1259	G1260	G1261	G1262	G1263	G1264	G1265	G1266	G1267	G1268	G1269	G1270	G1271	G1272	G1273	G1274	G1275																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
G1155	G1156	G1157	G1158	G1159	G1160	G1161	G1162	G1163	G1164	G1165	G1166	G1167	G1168	G1169	U1170	G1171	G1172	G1173	G1174	G1175	U1176	G1177	G1178	G1179	G1180	G1181	U1182	G1183	G1184	G1185	G1186	G1187	G1188	G1189	G1190	G1191	G1192	G1193	G1194	G1195	G1196	G1197	G1198	G1199	G1200	G1201	G1202	G1203	G1204	G1205	G1206	G1207	G1208	G1209	G1210	G1211	G1212	G1213	G1214	G1215	G1216																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
C1094	C1095	C1096	C1097	G1098	G1099	G1100	G1101	G1102	G1103	G1104	G1105	G1106	G1107	G1108	G1109	G1110	G1111	G1112	G1113	G1114	G1115	G1116	G1117	G1118			G1121	G1122	G1123	U1124	G1125	G1126	G1127	G1128	G1129	G1130	G1131	G1132	G1133	G1134	G1135	G1136	G1137	G1138	G1139	G1140	G1141	G1142	G1143	G1144	G1145	G1146	G1147	G1148	G1149	G1150	G1151	G1152	G1153	G1154																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														
G1033	G1034	G1035	G1036	U1037	U1038	G1039	G1040	G1041	G1042	G1043	G1044	G1045	G1046	G1047	U1048	G1049		G1052	G1053	G1054	G1055	G1056	G1057	G1058	G1059	G1060	G1061	G1062	G1063	G1064	G1065	G1066	G1067	G1068	G1069	G1070	G1071	G1072	G1073	G1074	G1075	G1076	G1077	G1078	U1079	G1080	G1081	G1082	G1083	G1084	G1085	G1086	G1087	G1088	G1089	G1090	G1091	U1092	U1093	U1094	U1095	U1096	U1097	U1098	U1099	U1100	U1101	U1102	U1103	U1104	U1105	U1106	U1107	U1108	U1109	U1110	U1111	U1112	U1113	U1114	U1115	U1116	U1117	U1118	U1119	U1120	U1121	U1122	U1123	U1124	U1125	U1126	U1127	U1128	U1129	U1130	U1131	U1132	U1133	U1134	U1135	U1136	U1137	U1138	U1139	U1140	U1141	U1142	U1143	U1144	U1145	U1146	U1147	U1148	U1149	U1150	U1151	U1152	U1153	U1154	U1155	U1156	U1157	U1158	U1159	U1160	U1161	U1162	U1163	U1164	U1165	U1166	U1167	U1168	U1169	U1170	U1171	U1172	U1173	U1174	U1175	U1176	U1177	U1178	U1179	U1180	U1181	U1182	U1183	U1184	U1185	U1186	U1187	U1188	U1189	U1190	U1191	U1192	U1193	U1194	U1195	U1196	U1197	U1198	U1199	U1200	U1201	U1202	U1203	U1204	U1205	U1206	U1207	U1208	U1209	U1210	U1211	U1212	U1213	U1214	U1215	U1216	U1217	U1218	U1219	U1220	U1221	U1222	U1223	U1224	U1225	U1226	U1227	U1228	U1229	U1230	U1231	U1232	U1233	U1234	U1235	U1236	U1237	U1238	U1239	U1240	U1241	U1242	U1243	U1244	U1245	U1246	U1247	U1248	U1249	U1250	U1251	U1252	U1253	U1254	U1255	U1256	U1257	U1258	U1259	U1260	U1261	U1262	U1263	U1264	U1265	U1266	U1267	U1268	U1269	U1270	U1271	U1272	U1273	U1274	U1275	U1276	U1277	U1278	U1279	U1280	U1281	U1282	U1283	U1284	U1285	U1286	U1287	U1288	U1289	U1290	U1291	U1292	U1293	U1294	U1295	U1296	U1297	U1298	U1299	U1300	U1301	U1302	U1303	U1304	U1305	U1306	U1307	U1308	U1309	U1310	U1311	U1312	U1313	U1314	U1315	U1316	U1317	U1318	U1319	U1320	U1321	U1322	U1323	U1324	U1325	U1326	U1327	U1328	U1329	U1330	U1331	U1332	U1333	U1334	U1335	U1336	U1337	U1338	U1339	U1340	U1341	U1342	U1343	U1344	U1345	U1346	U1347	U1348	U1349	U1350	U1351	U1352	U1353	U1354	U1355	U1356	U1357	U1358	U1359	U1360	U1361	U1362	U1363	U1364	U1365	U1366	U1367	U1368	U1369	U1370	U1371	U1372	U1373	U1374	U1375	U1376	U1377	U1378	U1379	U1380	U1381	U1382	U1383	U1384	U1385	U1386	U1387	U1388	U1389	U1390	U1391	U1392	U1393	U1394	U1395	U1396	U1397	U1398	U1399	U1400	U1401	U1402	U1403	U1404	U1405	U1406	U1407	U1408	U1409	U1410	U1411	U1412	U1413	U1414	U1415	U1416	U1417	U1418	U1419	U1420	U1421	U1422	U1423	U1424	U1425	U1426	U1427	U1428	U1429	U1430	U1431	U1432	U1433	U1434	U1435	U1436	U1437	U1438	U1439	U1440	U1441	U1442	U1443	U1444	U1445	U1446	U1447	U1448	U1449	U1450	U1451	U1452	U1453	U1454	U1455	U1456	U1457	U1458	U1459	U1460	U1461	U1462	U1463	U1464	U1465	U1466	U1467	U1468	U1469	U1470	U1471	U1472	U1473	U1474	U1475	U1476	U1477	U1478	U1479	U1480	U1481	U1482	U1483	U1484	U1485	U1486	U1487	U1488	U1489	U1490	U1491	U1492	U1493	U1494	U1495	U1496	U1497	U1498	U1499	U1500	U1501	U1502	U1503	U1504	U1505	U1506	U1507	U1508	U1509	U1510	U1511	U1512	U1513	U1514	U1515	U1516	U1517	U1518	U1519	U1520	U1521	U1522	U1523	U1524	U1525	U1526	U1527	U1528	U1529	U1530	U1531	U1532	U1533	U1534	U1535	U1536	U1537	U1538	U1539	U1540	U1541	U1542	U1543	U1544	U1545	U1546	U1547	U1548	U1549	U1550	U1551	U1552	U1553	U1554	U1555	U1556	U1557	U1558	U1559	U1560	U1561	U1562	U1563	U1564	U1565	U1566	U1567	U1568	U1569	U1570	U1571	U1572	U1573	U1574	U1575	U1576	U1577	U1578	U1579	U1580	U1581	U1582	U1583	U1584	U1585	U1586	U1587	U1588	U1589	U1590	U1591	U1592	U1593	U1594	U1595	U1596	U1597	U1598	U1599	U1600	U1601	U1602	U1603	U1604	U1605	U1606	U1607	U1608	U1609	U1610	U1611	U1612	U1613	U1614	U1615	U1616	U1617	U1618	U1619	U1620	U1621	U1622	U1623	U1624	U1625	U1626	U1627	U1628	U1629	U1630	U1631	U1632	U1633	U1634	U1635	U1636
C851	C852	C853	C854	C855	C856	U857	C858	U859	C860	C861	C862	C863	C864	C865	C866	C867	C868	C869	C870	U871	C872	C873	C874	C875	C876	C877	C878	C879	C880	C881	C882	C883	C884	C885	C886	C887	C888	C889	U890	C891	C892	C893	C894	C895	C896	C897	C898	C899	C900	C901	C902	C903	C904	C905	C906	C907	C908	C909	C910	C911	C912	C913	C914	C915	C916	C917	C918	C919	C920	C921	C922	C923	C924	C925	C926	C927	C928	C929	C930	C931	C932	C933	C934	C935	C936	C937	C938	C939	C940	C941	C942	C943	C944	C945	C946	C947	C948	C949	C950	C951	C952	C953	C954	C955	C956	C957	C958	C959	C960	C961	C962	C963	C964	C965	C966	C967	C968	C969	C970	C971	C972	C973	C974	C975	C976	C977	C978	C979	C980	C981	C982	C983	C984	C985	C986	C987	C988	C989	C990	C991	C992	C993	C994	C995	C996	C997	C998	C999	C1000	C1001	C1002	C1003	C1004	C1005	C1006	C1007	C1008	C1009	C1010	C1011	C1012	C1013	C1014	C1015	C1016	C1017	C1018	C1019	C1020	C1021	C1022	C1023	C1024	C1025	C1026	C1027	C1028	C1029	C1030	C1031	C1032	C1033	C1034	C1035	C1036	C1037	C1038	C1039	C1040	C1041	C1042	C1043	C1044	C1045	C1046	C1047	C1048	C1049	C1050	C1051	C1052	C1053	C1054	C1055	C1056	C1057	C1058	C1059	C1060	C1061	C1062	C1063	C1064	C1065	C1066	C1067	C1068	C1069	C1070	C1071	C1072	C1073	C1074	C1075	C1076	C1077	C1078	C1079	C1080	C1081	C1082	C1083	C1084																																																																																																																																																																																																																																																																																																																																																																																	

U2541	G2481	C2421	G2361	A2301	U2241	A2181	U2121	A2060	U2000	C1940	G1879	G1818	C1757	U1697	U1637
U2542	A2482	C2422	G2362	G2302	C2242	A2182	G2122	C2061	G2001	C1941	G1880	U1819	C1758	C1698	G1638
A2543	U2483	G2423	G2363	G2303	C2243	C2183	G2123	A2062	A2002	U1942	U1881	G1820	G1759	A1699	U1639
U2544	G2484	G2424	G2364	G2304	C2244	C2184	C2124	A2063	A2003	A1943	U1882	G1821	G1760	C1700	C1640
U2545	U2485	G2425	U2365	C2305	A2245	G2185	C2125	U2064	U2004	C1944	A1883	G1822		C1701	C1641
C2546	C2486	G2426	U2366	A2306	A2246	G2186	U	A2065	U2005	C1945	A1884	G1823	G1763	G1702	C1642
G2547	A2487	A2427	U2367	A2307	A2247	A2187	U	G2066	G2006	U1946	C1885	C1824	A1764	C1703	A1643
G2548	G2488	U2428	G2368	G2308	A2248	A2188	U	G2067	G2007	C1947	G1886	C1825	C1765	G1704	G1644
G2549	C2489	U2429	U2369	G2309	U2249	A2189	U	C2068	C2008	C1948	G1887	U1826	U1766	U1705	U1645
C2550	U2490	G2430	G2370	G2310	G2250	A2190	G	U2069	U2009	A1949	C1888	G1827	G1767	A1706	G1646
A2551	C2491	C2431	A2371	G2311	U2251	A2191	U	G2070	G2010	C1950	U1768	C1828	U1768	A1707	U1647
C2552	G2492	A2432	A2372	A2312	U2252	U2192	G2132	G2071	U2011	G1951	G1890	C1829	U1769	G1708	C1648
G2553	C2493	G2433	C2373	G2313	A2253	C2193	G2133	G2072	A2012	A1952	C1891	G1830	U1770	U1709	A1649
C2554	C2494	A2434	C2374	A2314	C2254	A2194	U2134	A2073	A2013	A1953	C1892	G1831	A1771	U1710	A1650
G2555	G2495	G2435	G2375	A2315	G2255	C2195	U2135	U2074	A2014	A1954	G1893	G1832	C1772	G1711	U1651
C2556	C2496	G2436	G2376	G2316	G2256	U2196	G2136	U2075	G2015	A1955	U1894	U1833	C1773	G1712	G1652
G2557	A2497	U2437	U2377	G2317	G2257	U2197	G2137	G2076	A2016	G1956	A1895	G1834	A1774	G1713	C1653
C2558	U2498	G2438	G2378	U2318	G2258	U2198	U2138	G2077	U2017	C1957	A1896	G1835	A1775	A1714	A1654
U2559	C2499	U2439	G2379	G2319	G2259	C2199	G2139	G2078	G2018	G1958	C1897	G1836	A1776	A1715	C1655
G2560	C2500	U2440	U2380	G2320	G2260	G2200	G2140	A2079	C2019	U1959	U1898	G1837	A1777	U1716	U1656
U2561	U2501	U2441	A2381	C2321	G2261	G2201	A	U2080	G2020	A1960	A1899		U1778	A1717	A1657
G2562	C2502	C2442	C2382	U2322	C2262	G2202	G	G2081	G2021	A1961	U1900	A1840	C1779	A1718	A1658
U2563	G2503	C2443	C2383	U2323	C2263	G2203	G	C2082	C2022	C1962	A1901	G1841	U1780	G1719	G1659
G2564	G2504	G2444	G2384	G2324	C2264	A2204	C	G2083	C2023	G1963	G1904	G1842	C1781	G1720	G1660
C2565	U2505	C2445	U2385	A2325	G2265	C2205	A	G2084	U2024	A1964	G1905	U1843	A1782	G1721	C1661
A2566	C2506	C2446	G2386	C2326	A2266	C2206	A	G2085	A2025	U1965	U1906	C1844	G1783	G1722	G1662
U2567	U2507	G2447	U2387	U2327	A2267	G2207	C	U2086	C2026	C1966	A1907	A1845	C1784	U1723	C1663
A2568	G2508	U2448	G2388	G2328	G2268	U2208	G	U2087	C2027	U1967	C1907	A1846	C1724	G1724	G1664
A2569	A2509	G2449	G2389	C2329	G2269	G2209	U	G2088	C2028	G1968	C1908	G1847	C1786	G1725	C1665
C2570	U2510	U2450	A2390	G2330	U2270	G2210	U	U2089	G2029	G1969	U1909	U1848	U1787	C1726	G1666
G2571	G2511	G2451	A2391	A2331	C2271	U2211	G	C2091	U2030	G1970	A1910	G1849	C1788	C1727	A1667
A2572	A2512	U2452	G2392	C2332	A2272	U2212	A	U2092	A2031	C1971	A1911	G1850	U1789	A1728	G1668
C2573	C2513	C2453	G2393	C2333	C2273	G2213	A	G2093	G2032	U1972	G1912	A1851	U1790	C1729	A1669
G2574	G2514	G2454	G2394	U2334	C2274	G2214	A	C2094	C2033	C1973	G1913	G1852	C1791	G1730	G1670
U2575	A2515	A2455	C2395	U2335	U2275	G2215	U	U2095	A2034	U1974	U1914	G1853	C1792	C1731	A1671
G2576	U2516	U2456	C2396	G2336	C2276	G2216	A	U2096	G2035	G1975	A1915	G1854	A1793	U1732	A1672
U2577	C2517	A2457	A2397	A2337	A2277	G2217		A2097	G2036	U1976	G1916	G1855	A1794	U1733	C1673
G2578	C2518	U2458	U2398	C2338	A2278	G2218	C2157	G	A2037	C1977	C1917	U1856	C1795	C1734	C1674
A2579	C2519	C2459	C2399	A2339	G2279	U2219	C2158	G	C2038	U1978	G1918	G1857	A1796	C1735	U1675
C2580	U2520	G2460	C2400	C2340	A2280	A2220	A2159	A	G2039	C1979	A1919	C1858	C1797	G1736	U1676
A2581	A2521	G2461	A2401	G2341	C2281	U2221	U	U2081	A2040	A1980	A1920	A1859	G1798	G1737	C1677
G2582	C2522	C2462	U2402	U2342	G2282	U2222	C2161	U	A2041	A1981	A1921	A1860	A1799	U1738	G1678
U2583	G2523	G2463	C2403	G2343	U2283	U2223	C2162	A	A2042	C1982	U1922	G1861	A1800	G1739	U1679
C2584	U2524	G2464	A2404	G2344	G2284	U2224	G2163	G2103	A2043	G1983	U1923	C1862	C1801	G1740	U1680
U2525	U2525	A2345	A2405	A2345	U2285	G2225	A2164	G2104	G2044	A1984	C1924	U1863	A1802	G1741	A1681
G2586	U2526	G2466	C2406	G2346	G2286	A2226	A2165	U2105	A2045	G1985	C1925	G1864	G1803	G1742	A1682
U2527	G2527	A2467	G2407	C2347	G2287	U2227	A2167	G2106	C2046	G1986	U1926	C1865	U1804	C1743	G1683
G2528	C2528	G2468	G2408	A2348	A2288	U2228	A2168	G2108	C2047	G1987	U1927	G1866	G1805	G1744	G1684
C2589	G2529	A2469	A2409	G2349	A2289	U2229	A2169	A2109	C2048	A1988	G1928	A1867	G1806	C1745	A1685
U2590	U2410	U2470	G2350	G2350	A2290	G2230	C2170	G2110	C2049	C1989	U1929	A1868	A1807	A1746	A1686
U2591	A2411	U2471	A2411	G2351	U2291	G2231	U2171	C	G2050	U1990	C1930	A1869	C1808	G1747	C1687
G2592	U2412	U2472	A2412	A2352	C2292	U2232	C	U2051	U2051	C1991	G1931	A1870	C1809	U1748	U1688
A2593	G2413	G2473	G2413	G2353	G2293	C2233	U2172	U	G2052	G1992	G1932	G1871	U1810	G1749	U1689
U2594	A2414	G2474	A2414	G2354	U2294	G2234	G2173	U	G2053	G1993	G1933	A1872	A1811	A1750	U1690
C2595	G2415	A2355	G2415	A2355	C2295	U2235	C2174	G	A2054	U1994	A1934	A1873	U1812	A1751	G1691
G2596	U2416	U2476	U2416	A2356	U2296	U2236	A2175	G	G2055	G1995	U1935	G1874	U1813	U1752	C1692
C2597	U2417	G2477	G2417	A2357	G2297	U2237	U2176	A2117	C2056	A1996	A1936	C1875	G1814	A1753	A1693
C2598	U2418	U2478	A2418	C2358	U2298	G2238	U2177	A2118	U2057	A1997	G1937	C1876	G1815	G1754	A1694
U2599	C2419	U2479	C2419	U2359	A2299	G2239	C2178	A2119	U2058	U1998	U1938	C1877	G1816	G1755	U1695
A2600	U2540	C2480	C2420	C2360	G2300	C2240	U2180	C2120	U2059	U1999	U1939	C1878	U1817	C1756	C1696

U2841	G2781	A2721	G2661	G2601
C2842	G2782	C2722	C2662	G2602
A2843	U2783	G2723	U2663	G2603
G2844	A2784	G2724	G2664	G2604
C2845	A2785	G2725	G2665	C2605
G2846	G2786	U2726	U2666	G2606
G2847	A2787	G2727	C2667	C2607
A2848	C2788	A2728	U2668	A2608
C2849	U2789	A2729	C2669	G2609
U2850	G2790	A2730	C2670	G2610
G2851	C2791	G2731	C2671	A2611
G2852	G2792	C2732	U2672	G2612
U2853	G2793	A2733	G2673	A2613
G2854	G2794	U2734	C2674	A2614
C2855	A2795	C2735	U2675	U2615
U2856	A2796	U2736	G2676	U2616
C2857	G2797	A2737	U2677	G2617
A2858	U2798	A2738	C2678	A2618
U2859	C2799	G2739	G2679	G2619
C2860	C2800	C2740	U2680	G2620
A2861	A2801	G2741	A2681	G2621
G2862	C2802	G2742	C2682	G2622
U2863	C2803	G2743	C2683	A2623
C2864	G2804	A2744	A2684	G2624
G2865	G2805	A2745	A2685	U2625
A2866	G2806	G2746	C2686	U2626
G2867	U2807	C2747	G2687	G2627
G2868	U2808	C2748	G2688	C2628
U2869	A2809	A2749	C2689	U2629
C2870	A2810	G2750	A2690	C2630
U2871	G2811	C2751	C2691	C2631
U2872	A2812	C2752	A2692	U2632
G2873	G2813	C2753	U2693	A2633
A2874	G2814	C2754	G2694	G2634
C2875	C2815	A2755	C2695	U2635
C2876	C2816	A2756	A2696	A2636
A2877	A2817	G2757	G2697	C2637
C	G2818	A2758	G2698	G2638
U	G2819	U2759	C2699	A2639
C	C2820	G2760	U2700	G2640
	G2821	A2761	A2701	A2641
	U2822	G2762	G2702	G2642
	G2823	U2763	C2703	G2643
	C2824	U2764	U2704	A2644
	A2825	C2765	A2705	C2645
	C2826	U2766	U2706	C2646
	G2827	C2767	G2707	G2647
	C2828	C2768	U2708	G2648
	A2829	C2769	C2709	A2649
	U2830	A2770	C2710	G2650
	A2831	C2771	G2711	U2651
	G2832	U2772	U2712	G2652
	C2833	G2773	A2713	A2653
	A2834	U2774	A2714	A2654
	A2835	U	C2715	C2655
	U2836	U	G2716	G2656
	G2837	A	G2717	G2657
	U2838	U2778	U2718	A2658
	G2839	C2779	U2719	C2659
	U2840	A2780	A2720	C2660

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	170.01Å 411.48Å 697.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 3.60	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-3.60)	Depositor
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.283 , 0.364	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	59428	wwPDB-VP
Average B, all atoms (Å ²)	81.0	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: RU6

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	9/66467 (0.0%)	0.88	121/103673 (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	4	204

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	803	C	C3'-O3'	7.88	1.53	1.42
1	A	2589	C	C3'-C2'	-6.84	1.45	1.52
1	A	700	C	N1-C2	6.48	1.46	1.40
1	A	803	C	C3'-C2'	6.40	1.59	1.52
1	A	788	G	N9-C4	6.20	1.43	1.38

The worst 5 of 121 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2810	A	N9-C1'-C2'	14.02	132.22	114.00
1	A	2589	C	O4'-C1'-N1	12.82	118.46	108.20
1	A	985	G	N9-C1'-C2'	11.79	129.33	114.00
1	A	2588	U	O3'-P-O5'	10.97	124.85	104.00
1	A	1692	C	N1-C1'-C2'	10.55	127.72	114.00

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	765	C	C1'
1	A	1139	A	C1'
1	A	1685	A	C1'
1	A	2810	A	C1'

5 of 204 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	33	C	Sidechain
1	A	34	U	Sidechain
1	A	66	U	Sidechain
1	A	67	G	Sidechain
1	A	71	A	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	29917	6937	0
2	A	69	0	80	8	0
All	All	59428	0	29997	6939	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 79.

The worst 5 of 6939 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:2426:G:C4'	1:A:2427:A:H5''	1.53	1.35
1:A:2426:G:H4'	1:A:2427:A:C5'	1.57	1.34
1:A:968:C:N4	1:A:970:A:H1'	1.51	1.26
1:A:43:A:N6	1:A:446:C:H42	1.38	1.20
1:A:1733:U:H5'	1:A:1734:C:C5	1.78	1.17

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%)	853 (30%)	190 (6%)

5 of 853 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	12	U
1	A	13	A
1	A	27	G
1	A	33	C
1	A	43	A

5 of 190 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1301	U
1	A	1634	A
1	A	2633	A
1	A	1324	G
1	A	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 ⓘ

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	RU6	A	2881	-	71,74,74	2.42	25 (35%)	98,111,111	2.56	33 (33%)

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	RU6	A	2881	-	-	1/80/134/134	0/6/6/6

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2881	RU6	C10-C9	-5.72	1.43	1.52
2	A	2881	RU6	O11-C9	-3.36	1.15	1.21
2	A	2881	RU6	C2-C1	-3.05	1.44	1.51
2	A	2881	RU6	C2-C3	-2.63	1.48	1.55
2	A	2881	RU6	C25-C24	2.08	1.58	1.53

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2881	RU6	C40-N2-C39	-11.89	106.17	122.14
2	A	2881	RU6	C12-C11-N2	-6.53	89.28	99.98
2	A	2881	RU6	O5-C16-C15	-5.19	104.68	113.00
2	A	2881	RU6	C25-C24-C23	-5.08	102.63	110.03
2	A	2881	RU6	O10-C6-C5	-4.98	99.38	108.14

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2881	RU6	C20-O5-C16-C17

There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2881	RU6	8	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.