



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 04:52 AM GMT

PDB ID : 2OGO  
Title : The crystal structure of the large ribosomal subunit from *Deinococcus radiodurans* complexed with the pleuromutilin derivative retapamulin (SB-275833)  
Authors : Davidovich, C.; Bashan, A.; Auerbach-Nevo, T.; Yonath, A.  
Deposited on : 2007-01-07  
Resolution : 3.66 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) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

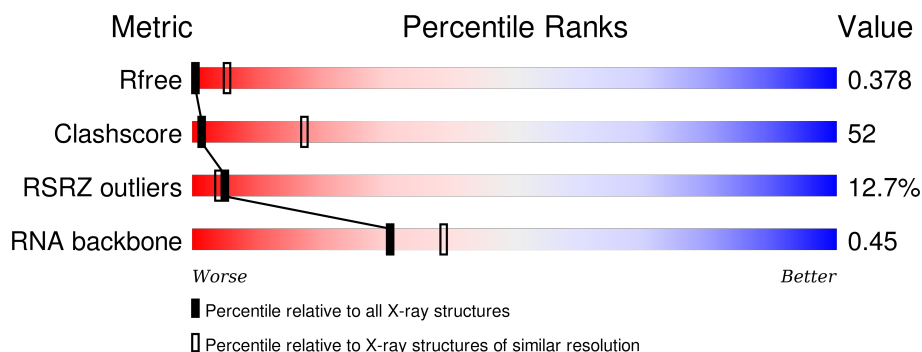
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.66 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))
$R_{free}$	91344	1010 (3.82-3.50)
Clashscore	102246	1125 (3.82-3.50)
RSRZ outliers	91569	1017 (3.82-3.50)
RNA backbone	2183	1066 (4.52-2.80)

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  $\geq 3$ , 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.

Mol	Chain	Length	Quality of chain
1	0	2880	
2	B	211	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 59577 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

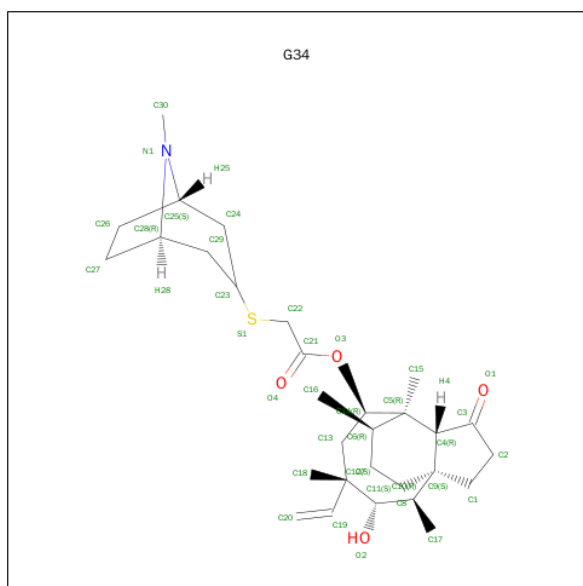
- Molecule 1 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	0	2765	Total	C	N	O	P	0	0	0
			59336	26469	10944	19159	2764			

- Molecule 2 is a protein called 50S ribosomal protein L3.

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

- Molecule 3 is (3AS,4R,5S,6S,8R,9R,9AR,10R)-5-HYDROXY-4,6,9,10-TETRAMETHYL-1-OXO-6-VINYLDECAHYDRO-3A,9-PROPANOCYCLOPENTA[8]ANNULEN-8-YL {[ (3-E XO)-8-METHYL-8-AZABICYCLO[3.2.1]OCT-3-YL]THIO}ACETATE (three-letter code: G34) (formula: C<sub>30</sub>H<sub>47</sub>NO<sub>4</sub>S).

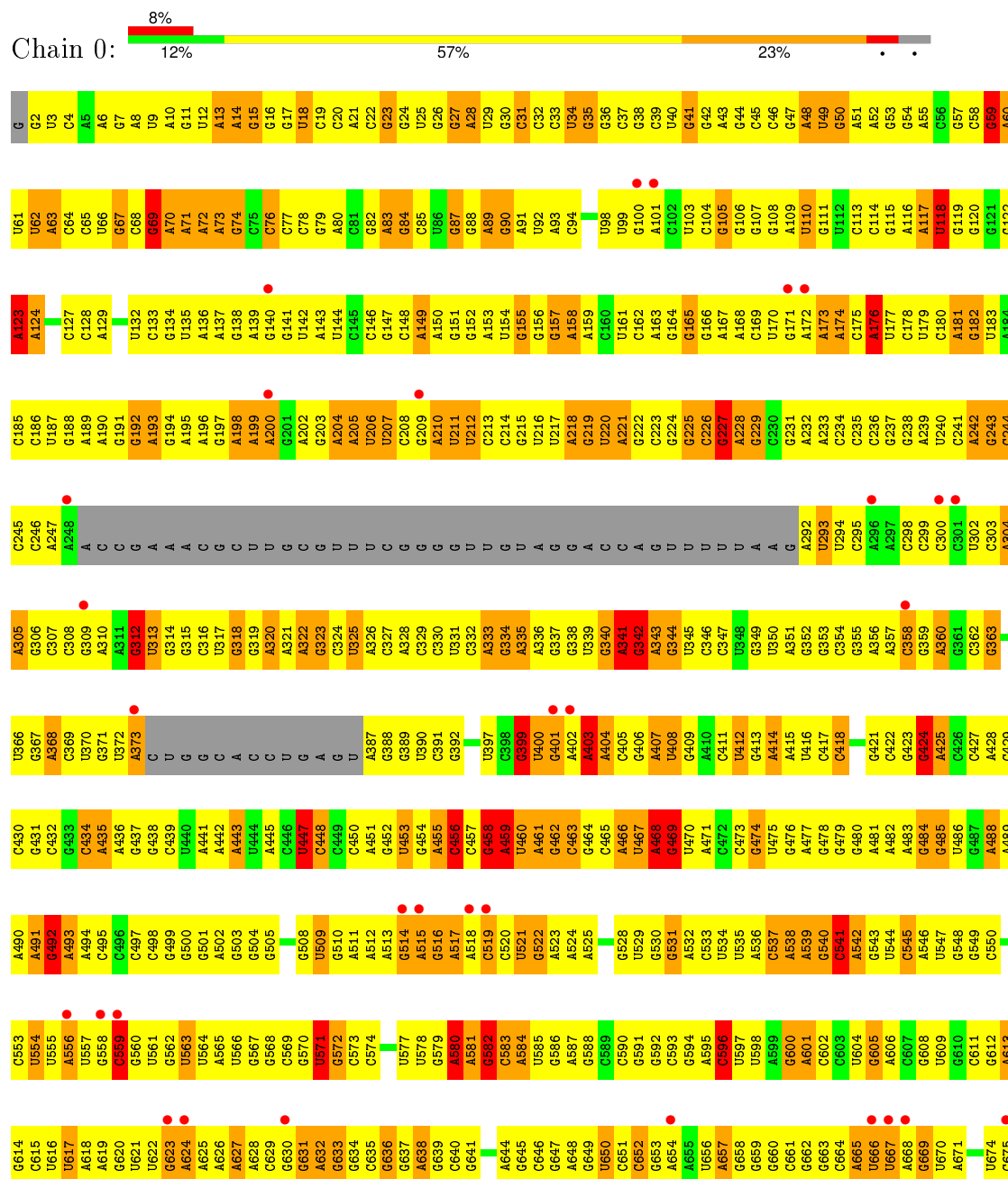


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	0	1	Total	C	N	O	S	0	0
			36	30	1	4	1		

### 3 Residue-property plots

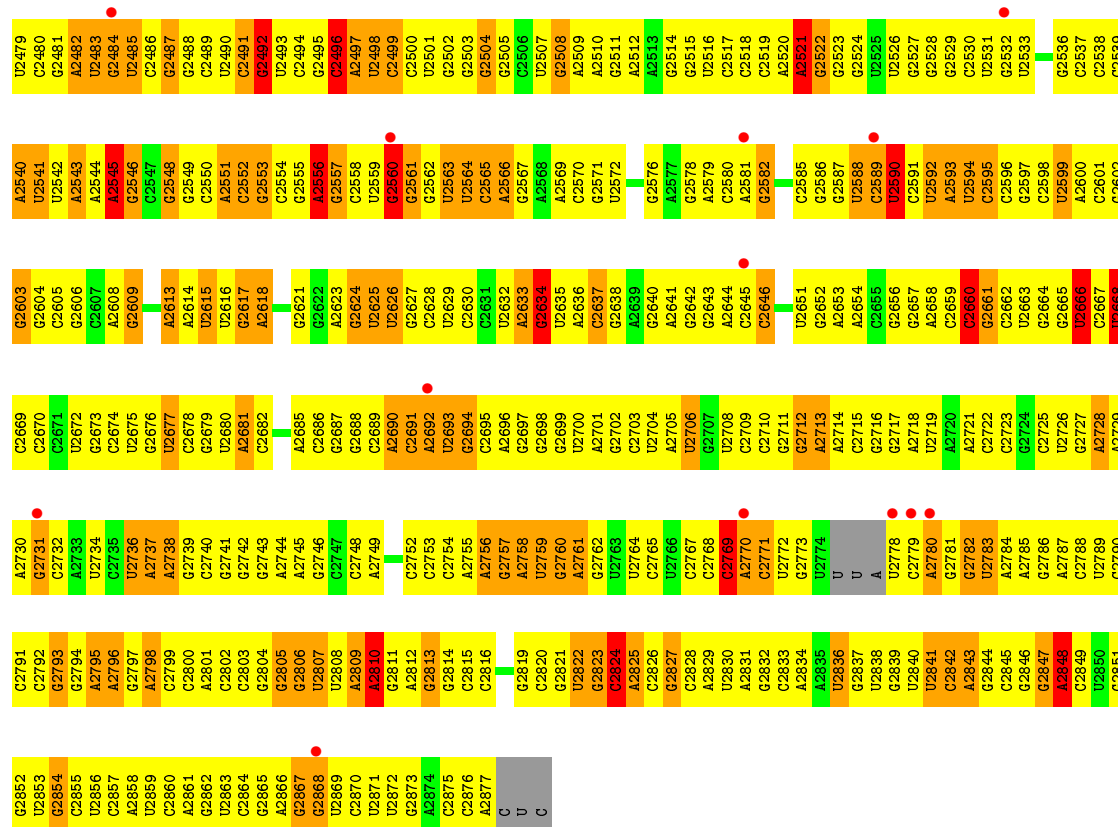
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

- Molecule 1: 23S ribosomal RNA



A1544	G1484	C1422	G1359	G1299	A1238	U1177	G1053	G988	C924	G861	A801	G739	G676
G1546	U1485	A1423	G1360	A1300	A1239	C1178	C1054	A991	U925	A862	A802	A740	G677
U1547	C1486	G1424	A1361	U1301	G1240	A1179	A1055	A992	C926	C863	C803	A741	G678
G1488	C1487	G1425	G1362	C1302	G1241	U1116	U1056	A993	C927	C864	G804	G742	C679
C1549	G1488	U1426	C1363	U1303	A1242	G1117	A1057	C993	A928	A865	G805	A743	U680
U1550	C1489	G1427	C1364	U1304	G1243	G1118	G1058	A994	G929	U866	A806	G744	A681
C1551	U1490	G1428	U1365	C1305	U244	U1119	A1059	A995	A930	G867	A807	G745	G682
U1552	A1491	G1429	A1366	U1306	G1245	G1120	C1060	C996	G931	U868	C808	G746	A683
G1553	C1492	G1430	A1367	U1307	U1246	G1121	A1061	C997	G932	C869	C809		C684
U1554	A1493	U1431	G1368	C1308	U1247	A1122	C1062	C998	G933	C870	U810		U685
G1494	C1493	G1432	G1369	U1309	A1187	G1123	C1063	A999	G934	U871	G811		G686
G1495	A1493	A1433	C1310	C1311	U1249	U1124	C1064	G1000	C935	G872	G812		G687
U1496	C1494	U1434	A1372	A1250	G1250		A1065	A1001	A936	U873	A813		A688
C1497	G1495	G1373	G1312	G1251	G1251		G1066	C1002	C937	A874	G814		A689
A1500	G1498	G1374	U1313	C1252	U1129		G1067	C1003	G938	G875			A690
U1501	A1499	A1437	A1314	A1192	U1130		A1068	A1004	C939	A876	U816		C691
G1502	U1500	G1438	A1315	G1193	G1131		G1069	U1005	G940	G877	A817		C692
U1503	C1501	G1439	C1316	U1194	U1194		G1070	C1006	U941	C878	G818		A693
G1504	G1502	A1440	A1378	G1317	C1256		U1071	A1007	U942	A879	C819		G694
U1505	G1503	A1441	A1379	U1257	U1257		U1072	G1008	U943	C880	U820		G695
G1506	U1504	C1442	C1380	C1319	U1258		G1073	G1009	A944	U881	G821		U696
A1507	C1506	G1443	G1381	A1320	A1259		C1074	A1010	G945	C882	U822		A698
G1571	A1507	C1444	G1382	A1321	U1199		C1075	A1011	U946	A883	G823		A763
G1572	U1508	A1445	C1383	G1322	G1200		U1076	A1012	C947	C884	U824		A764
A1573	A1509	U1446	G1384	G1323	U1262		U1077	G1013	C948	A885	C825		C700
C1575	A1510	U1447	C1385	G1324	G1263		A1078	G1034		A886	U826		U701
G1576	A1511	G1448	A1386	U1325	C1264		G1079	U1015	A952		C827		A702
U1577	G1512	C1449	G1387	C1326	G1265		A1080	C1016	G953	C889	C828		A703
G1578	A1514	U1452	G1390	C1327	G1266		A1081	C1017	G704	U890	C829		C769
U1579	U1515	U1453	A1391	C1328	A1267		G1082	C1018	G955	U770	C830		C705
C1580	A1516	U1454	U1392	G1330	G1269		A1084	A1020	A956	G	G831		U706
A1581	C1517	G1455	G1393	G1331	C1270		G1085	A1021	G957	G	A833		G708
U1582	G1518		G1394	G1332	G1271		C1086	U1022	C959	G	A834		A709
A1583	U1519	U1458	C1396	A1334	G1273		A1088	G1024	C962	C	G836		A712
G1584	U1520	U1459	A1397	A1335	G1274		C1089	A1025	G963	C	U837		G713
A1585	U1521	G1460	G1398	G1336	A1275		C1090	U1026	A964	U	A838		G714
A1586	C1522		A1400	G1337			C1091	C1027	G965		U839		U715
A1587	C1523	A1463	C1399	G1338	A1278		U1092	A1032	C968	C	U840		U716
A1588	C1524	A1464	G1401	U1339	G1279		U1093	G1033	U969	C	G841		G717
G1589	A1525	G1465	C1402	C1340	U1280		C1094	A1039	A971	A	A842		A718
C1590	U1526	C1466	U1403	G1341	G1281		A1095	U1034	A970	G	G843		A719
U1591	G1527	U1467	C1404	U1342	A1282		A1096	G1035	C971	C	G844		A720
C1592	C1528	A1468	A1405	C1343	C1283		A1097	U1036	C972	U	U845		C722
U1594	U1530	U1469	A1506	G1344	G1284		G1098	U1037	U973	A	A846		G726
A1595	C1531	G1470	G1407	G1345	A1285		A1099	U1038	U974	A	C847		G727
A1596	A1532	C1471	A1408	C1346	U1286		G1100	A1039	C975	C	G848		G728
U1597	G1533	U1473	U1409	C1347	A1287		U1101	A1040	C976	C	G849		A729
C1598	A1534	A1474	U1410	C1348	A1288		G1102	G1041	G977	A911	C850		G729
G1599	U1535	U1475	C1411	A1349	A1289		C1103	G1042	U978	A912	C851		C730
U1600	G1536	G1476	C1412	G1350	A1290		G1104	A1043	A979	A913	U852		A731
U1601	U1537	C1477	C1415	G1351	U1291		U1105	U1044	G980	U917	C853		G732
A1602	G1603	U1478	A1416	C1352	A1292		A1106	G1045	C981	A918	G854		G733
G1603	U1639	G1479	C1417	A1353	G1293		A1107	U1046	C982	U919	G855		G734
A1604	C1540	G1480	C1418	A1354	G1294		U1108	G1047	G983	G820	A856		G735
A1605	U1481	U1482	A1355	U1295	U1295		A1109	U1048	A984	U857	G858		G736
C1606	G1542	U1483	G1356	G1296	G1296		C1110	U1051	A986	A921	G859		C737
A1607	G1543	G1483	C1358	G1298	G1298		U1112	C1052	G987	A922	U860		G738

U2417	U2285	U2223	C2162	A	A2042	A1981	G1916	G1853	C1792	U1732	G1668	U1608
A2418	G2286	U2224	U2163	G2103	A2043	C1982	C1917	G1854	A1793	U1733	A1669	G1609
C2419	A2287	G2225	A2164	G2104	G2044	G1983	A1918	G1855	A1794	C1734	G1670	A1610
C2420	A2288	G2226	A2165	U2105	A2045	A1984	A1919	A1856	C1795	G1735	A1671	U1611
C2421	A2289	C2227	A2166	G2106	C2046	G1987	A1920	G1857	A1796	G1736	A1672	U1612
C2422	A2290	U2228	A2167	G2107	C2047	A1988	A1921	C1858	C1797	G1737	A1673	G1613
C2423	U2281	G2229	A2168	G2108	C2048	C1989	U1922	A1859	A1798	G1738	C1674	C1614
G2424	C2282	G2230	A2169	A2109	C2049	C1990	U1923	A1860	A1799	G1739	C1675	C1615
G2425	U2294	G2231	C2170	G2110	G2050	U1990	C1924	G1861	A1800	G1740	U1676	C1616
G2426	C2360	G2232	U2171	C	G2051	G1991	U1925	A1862	C1801	C1741	C1677	G1617
A2427	C2295	G2233	U2172	C	G2052	G1992	U1926	U1863	A1802	G1742	G1678	U1618
U2428	U2296	G2234	G2173	U	G2053	U1993	U1927	G1864	G1803	C1743	U1679	A1619
A2429	G2297	G2235	G2174	G	A2054	U1994	G1927	C1865	U1804	G1744	U1680	C1620
A2430	U2298	U2236	A2175	C	G2055	G1995	G1931	G1866	G1805	C1745	A1681	C1621
C2431	A2299	C2237	U2176	G	C2056	A1996	G1932	A1867	G1806	A1746	G1682	G1622
A2432	G2300	G2238	U2177	A2117	U2057	A1997	G1933	A1868	A1807	G1747	G1683	C1623
C2433	A2301	C2239	U2178	A2118	U2058	A1998	G1934	A1869	C1808	U1748	G1684	A1624
G2434	G2302	C2240	C2179	A2119	U2059	U1999	A1935	U1870	G1809	G1749	A1685	A1625
C2435	C2303	U2241	U2180	A2120	A2060	U2000	A1936	G1871	U1810	A1750	A1686	A1626
U2436	A2306	C2242	A2181	U2121	C2061	G2001	G1937	A1872	A1811	A1751	C1687	C1627
G2437	A2307	C2243	A2182	G2122	U2062	A2002	U1938	A1873	U1812	U1752	U1688	C1628
A2438	A2308	C2244	C2183	G2123	A2063	A2003	U1939	G1876	A1813	G1753	U1689	G1629
U2439	G2309	A2245	C2184	C2124	U2064	U2004	G1940	G1877	G1814	A1754	U1690	A1630
C2440	G2310	A2246	U2185	C2125	A2065	U2005	G1941	C1877	G1815	G1755	G1691	C1631
U2441	C2303	U2247	G2186	U	G2066	G2006	G1942	C1878	G1816	G1756	C1692	A1632
G2442	U2311	G2248	A2187	U	U2067	G2007	A1943	G1879	U1817	C1757	A1693	C1633
C2443	A2312	U2251	A2188	U	C2068	C2008	C1944	G1880	G1818	C1758	A1694	A1634
C2444	G2313	A2252	A2189	U	U2069	U2009	C1945	U1881	U1819	A1759	U1695	G1635
C2445	A2314	A2253	A2190	G	G2070	U2010	U1946	G1882	U1820	C1760	C1696	G1636
G2446	A2315	C2254	A2191	G	G2071	U2011	G1947	A1883	A1821	G1761	U1697	U1637
C2447	G2316	G2255	U2192	U	C2072	A2012	C1948	A1884	G1822	C1762	C1698	G1638
U2448	G2316	G2256	C2193	G2132	A2073	A2013	C1949	C1885	G1823	G1763	A1699	U1639
G2449	G2319	A2257	A2194	G2133	U2074	A2014	G1950	G1886	C1824	C1764	C1700	C1640
A2450	G2320	G2258	U2195	C2135	U2075	G2015	G1951	G1887	U1825	C1765	C1701	G1641
C2451	C2321	C2259	U2196	G2136	G2076	A2016	A1952	C1888	U1826	U1766	C1702	G1642
C2452	U2322	G2260	U2197	G2137	G2077	U2017	A1953	G1889	G1827	G1767	C1703	G1643
G2453	U2323	C2261	U2198	U2138	G2078	G2018	A1954	G1890	C1828	U1768	G1704	A1644
C2454	G2324	C2262	C2199	G2139	A2079	C2019	G1955	G1893	C1829	U1769	U1705	U1645
A2455	A2325	C2263	G2200	G2140	U2080	G2020	G1956	A1894	C1830	U1770	A1706	G1646
U2456	C2326	C2264	G2201	A	U2081	G2021	C1957	A1895	G1831	A1771	U1707	U1647
A2457	G2329	A2265	G2202	G	C2082	C2022	G1958	A1896	G1832	C1772	C1708	C1648
G2460	A2330	A2266	C2203	G	G2083	C2023	U1959	C1897	U1833	C1773	U1709	A1649
C2461	G2331	A2267	A2204	C	G2084	U2024	A1960	U1898	G1834	A1774	U1710	A1650
G2462	A2331	G2268	C2205	A	G2085	A2025	A1961	U1899	C1835	A1775	C1711	U1651
C2463	U2337	G2269	C2206	A	U2086	C2026	C1962	U1900	C1836	A1776	G1712	G1652
G2464	U2338	U2270	G2207	C	U2087	C2027	G1963	A1901	G1837	A1777	G1713	C1653
G2465	G2335	C2271	U2208	G	U2088	C2028	A1964	C1903	G1840	U1778	A1714	A1654
C2466	A2337	G2272	G2209	U	C2089	G2029	U1965	G1904	G1841	C1779	A1715	C1655
A2467	C2338	C2273	C2210	G	U2090	U2030	G1970	G1905	U1842	A1780	G1716	U1656
G2468	A2339	C2274	U2211	A	C2091	A2031	C1971	U1906	U1843	A1781	A1717	A1657
U2469	C2340	U2275	U2212	A	U2092	G2032	C1972	U1907	C1844	G1782	A1718	A1658
G2470	G2341	C2276	G2213	A	G2093	C2033	C1973	C1908	C1845	G1783	G1719	G1659
U2471	U2342	A2277	G2216	U	C2094	A2034	U1974	U1909	A1846	C1784	U1710	G1660
C2472	C2343	G2278	G2217	U	G2095	C2035	U1975	A1910	A1847	A1785	U1723	C1661
A2473	A2344	G2279	G2218	A	U2096	G2036	G1976	A1911	U1848	C1786	C1724	G1662
G2474	G2345	U2280	U2219	A	U2097	A2037	U1977	A1912	G1849	U1787	C1725	C1663
C2475	A2411	C2281	A2220	G	C2098	C2038	C1977	G1913	G1850	C1788	G1729	G1664
U2476	G2347	G2282	A2221	A	G	G2039	U1978	U1914	G1851	U1789	C1730	G1665
C2477	A2412	C2283	C2221	U	A	A2040	C1979	A1980	G1852	G1790	G1666	A1667
G2478	G2350	U2284	U2222	U	C2161	A2041	A1980	A1915		C1791		



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	170.12Å 405.87Å 695.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.96 – 3.66 29.96 – 3.66	Depositor EDS
% Data completeness (in resolution range)	93.0 (29.96-3.66) 93.1 (29.96-3.66)	Depositor EDS
$R_{merge}$	0.19	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.21 (at 3.65Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.260 , 0.334 0.356 , 0.378	Depositor DCC
$R_{free}$ test set	12167 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	135.2	Xtriage
Anisotropy	0.524	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.18 , 80.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 243559 reflections	Xtriage
$F_o, F_c$ correlation	0.84	EDS
Total number of atoms	59577	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	122.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.92% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.



## 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: G34

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	0	0.63	13/66441 (0.0%)	0.82	109/103632 (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	0	0	145

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	700	C	N1-C2	6.31	1.46	1.40
1	0	538	A	C5-C6	-6.22	1.35	1.41
1	0	2485	U	C1'-N1	-6.20	1.38	1.46
1	0	1711	C	N1-C2	6.13	1.46	1.40
1	0	2000	U	N1-C2	-6.11	1.33	1.38

The worst 5 of 109 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2485	U	C5'-C4'-O4'	-10.78	96.16	109.10
1	0	2426	G	N9-C1'-C2'	9.36	126.16	114.00
1	0	1749	G	N9-C1'-C2'	8.80	125.44	114.00
1	0	843	G	N9-C1'-C2'	8.64	125.23	114.00
1	0	2426	G	O4'-C1'-N9	8.58	115.06	108.20

There are no chirality outliers.

5 of 145 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	15	G	Sidechain
1	0	18	U	Sidechain
1	0	41	G	Sidechain
1	0	67	G	Sidechain
1	0	69	G	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	0	59336	0	29905	4618	0
2	B	205	0	0	1	0
3	0	36	0	47	12	0
All	All	59577	0	29952	4621	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 52.

The worst 5 of 4621 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:984:A:H1'	1:0:1202:U:C6	1.63	1.33
1:0:2691:C:H2'	1:0:2692:A:C5'	1.60	1.29
1:0:2691:C:C2'	1:0:2692:A:H5''	1.64	1.25
1:0:983:G:OP2	1:0:985:G:H5''	1.34	1.25
1:0:1279:G:O2'	1:0:1280:U:OP2	1.53	1.23

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

### 5.3.2 Protein sidechains [i](#)

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

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2756/2880 (95%)	667 (24%)	192 (6%)

5 of 667 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	13	A
1	0	14	A
1	0	23	G
1	0	28	A
1	0	34	U

5 of 192 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	1337	G
1	0	1690	U
1	0	2668	U
1	0	1345	G
1	0	1582	A

## 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
3	G34	0	0	-	34,40,40	1.85	9 (26%)	35,64,64	2.02	10 (28%)

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
3	G34	0	0	-	-	0/10/94/94	0/1/5/5

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	0	0	G34	C8-C9	2.01	1.60	1.54
3	0	0	G34	C25-N1	2.14	1.50	1.48
3	0	0	G34	C8-C7	2.86	1.59	1.53
3	0	0	G34	C28-N1	2.96	1.51	1.48
3	0	0	G34	C17-C10	3.09	1.60	1.53

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	0	0	G34	C24-C25-C26	-5.34	107.64	112.61
3	0	0	G34	C29-C28-C27	-4.94	108.01	112.61
3	0	0	G34	C16-C6-C7	-3.61	104.63	110.44
3	0	0	G34	C30-N1-C25	-2.61	108.14	113.24
3	0	0	G34	C30-N1-C28	-2.48	108.40	113.24

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	0	0	G34	12	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](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
1	0	2765/2880 (96%)	0.43	235 (8%)	13   8	49, 113, 200, 200	0
2	B	205/211 (97%)	3.69	142 (69%)	0   1	33, 87, 155, 200	0
All	All	2970/3091 (96%)	0.66	377 (12%)	5   4	33, 111, 200, 200	0

The worst 5 of 377 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	129	HIS	23.6
2	B	147	PRO	17.3
2	B	144	ARG	16.7
2	B	131	SER	14.9
2	B	169	ASN	11.9

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	G34	0	0	36/36	0.91	0.30	1.79	102,102,102,102	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.