



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 12, 2024 – 06:41 AM EDT

PDB ID : 2OGN
Title : The crystal structure of the large ribosomal subunit from *Deinococcus radiodurans* complexed with the pleuromutilin derivative SB-280080
Authors : Davidovich, C.; Bashan, A.; Auerbach-Nevo, T.; Yonath, A.
Deposited on : 2007-01-07
Resolution : 3.56 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

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

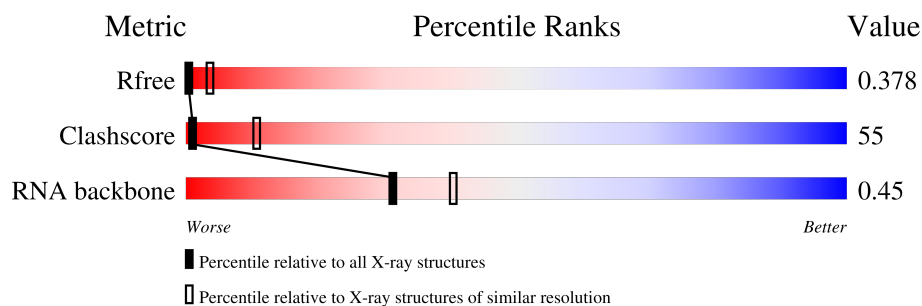
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


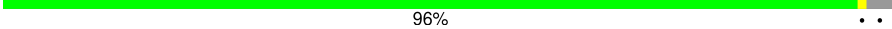
The reported resolution of this entry is 3.56 Å.

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}	130704	1020 (3.62-3.50)
Clashscore	141614	1100 (3.62-3.50)
RNA backbone	3102	1008 (4.10-3.00)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	0	2880	 11% 59% 22% . .
2	B	211	 96% . .

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 59597 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.

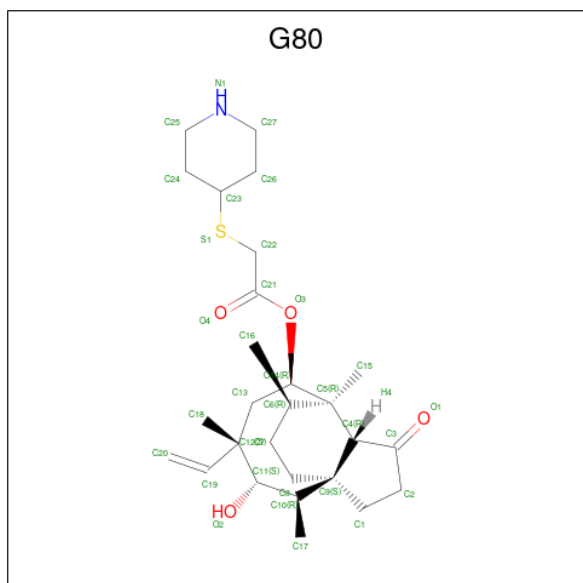
- Molecule 1 is a RNA chain called 23S ribosomal RNA.

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

- 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 (PIPERIDIN-4-YLTHIO)ACETATE (three-letter code: G80) (formula: C₂₇H₄₃NO₄S).

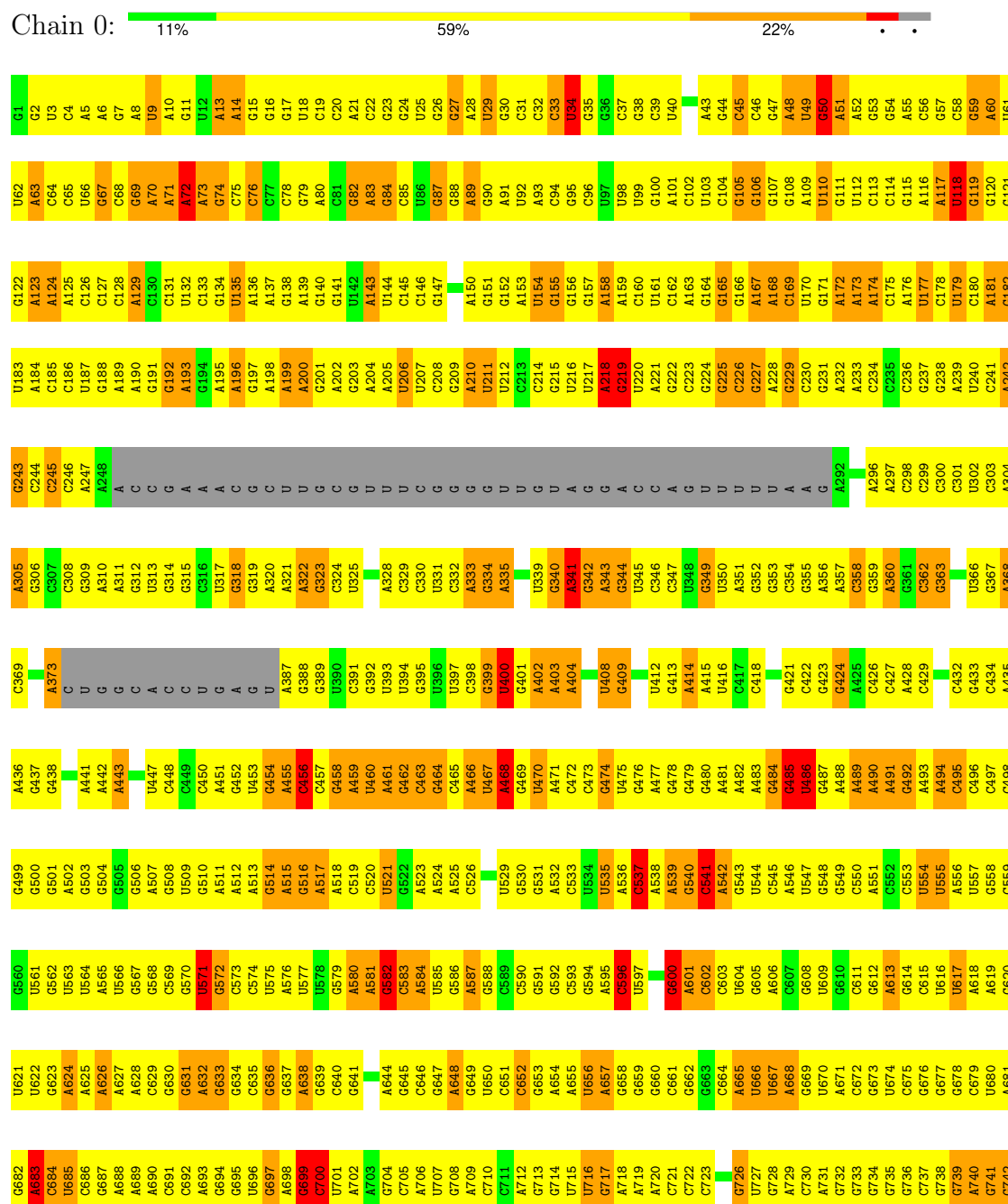


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	0	1	Total	C	N	O	S	0	0
			33	27	1	4	1		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: 23S ribosomal RNA



C1616	G1554	G1368	U1303	A1242	C1181	U1116	G1053	C927	A865	G805	A743
G1617	A1555	G1369	U1304	G1243	U1182	G1117	C1054	G928	U866	A806	G746
A1618	C1558	U1370	C1305	A1244	C1185	G1118	A1055	A929	A992	A807	A747
A1619	G1495	G1371	U1306	G1245	C1186	U1119	U1056	A930	C993	C808	A748
C1620	G1496	A1372	C1307	G1246	C1187	G1120	A1057	G931	U871	C809	C749
C1621	G1497	G1372	U1308	G1247	A1187	C1121	G1058	G932	G872	U810	G750
G1622	C1498	G1373	C1309	G1248	A1188	A1122	A1059	G933	U873	G811	C751
A1623	G1438	C1374	G1309	G1249	G1189	G1123	C1060	G934	A874	G812	G752
G1624	U1500	C1375	C1310	A1250	C1190	U1124	A1061	C995	A875	A813	G753
A1625	G1376	G1311	C1312	G1251	C1191	G1125	G1062	A936	A876	G814	G754
C1626	A1440	G1377	U1313	C1252	A1192	G1126	C1063	C937	G877	A815	G755
G1627	G1442	A1378	A1314	G1253	G1193	G1128	G1066	G938	A878	U816	C756
C1628	G1443	C1379	A1315	G1254	U1194	A1129	G1067	C939	A879	C817	C757
G1629	C1444	G1381	G1316	A1255	U1195	U1130	A1068	G940	C880	G818	U757
A1630	U1445	C1382	C1322	C1256	G1196	G1133	G1069	U941	U881	C819	G758
C1631	A1446	G1383	G1323	U1257	U1197	C1134	G1070	U942	C882	U820	C759
A1632	U1447	G1384	C1324	G1258	C1198	G1135	U1071	U943	A883	A821	U760
C1633	C1572	C1385	G1324	A1259	U1199	G1142	U1072	A944	C884	G822	G761
A1634	G1573	A1386	U1325	G1260	G1200	A1137	G1073	G945	A885	U823	A762
G1635	U1451	C1387	U1326	G1261	G1201	A1138	G1074	U946	A886	U824	A763
C1636	U1452	C1388	C1327	A1262	U1202	A1139	C1075	C947	G887	C825	A764
A1637	A1453	C1389	U1328	G1263	A1203	U1140	U1076	U948	U888	U826	C765
G1638	U1454	A1391	C1329	C1264	G1204	U1141	A1077	G949	C889	C827	A766
C1639	U1515	G1392	U1330	G1265	G1205	G1142	G1079	G950	C890	U890	G767
G1640	C1455	G1393	C1331	G1266	G1206	A1143	A1080	G951	A891	C829	U768
C1641	C1456	G1394	G1332	A1267	G1207	U1144	A1081	A952	G	C830	C769
A1642	A1457	C1395	C1333	U1268	A1208	C1145	G1082	G953	G	G831	G772
A1643	U1458	C1396	A1334	G1269	C1209	G1146	C1083	U954	G	A832	G773
G1644	A1460	A1397	C1335	C1270	C1210	U1147	A1084	G955	G	A833	G774
U1645	C1461	G1398	U1336	C1271	G1211	G1148	G1085	A956	G	A834	A774
A1646	C1462	C1399	C1337	C1272	U1212	G1149	C1086	G957	C	U835	U775
C1647	A1463	A1400	U1339	G1273	U1213	C1150	C1087	C958	C	G836	G776
U1648	A1464	G1401	C1340	C1274	C1214	U1151	A1088	C959	U	U837	A777
G1649	G1465	G1402	U1342	C1275	A1215	C1152	C1089	U960	A	A838	G778
A1650	C1466	A1403	C1341	A1276	G1216	A1153	C1090	C1023	C	U839	U779
C1651	U1467	C1404	C1343	A1278	U1217	A1154	C1091	A964	C	U840	U780
A1652	A1468	A1405	C1344	G1279	U1218	G1155	U1092	G965	A	G841	G781
C1653	U1469	A1406	G1345	U1280	C1219	C1156	C1093	A966	G	A842	U782
A1654	G1470	G1407	C1346	A1281	G1220	U1159	C1094	G967	C	G843	G783
C1655	C1471	A1408	C1347	A1282	C1221	C1160	A1095	C968	U	G844	U784
U1656	G1472	U1409	C1348	G1283	G1222	U1161	A1096	U969	U	U845	U785
A1657	U1473	U1410	A1349	C1284	G1223	A1162	A1097	A970	A	A846	U786
C1658	A1474	C1411	G1350	A1285	A1224	C1163	G1098	A971	C	C847	A787
G1659	U1475	C1412	G1351	U1286	G1225	C1164	A1099	C972	C	A848	G788
C1660	G1476	U1413	C1352	A1287	A1226	G1165	G1100	U973	A911	G849	G789
A1661	C1477	G1414	A1353	G1288	A1227	A1166	U1101	U974	A912	C850	A790
C1662	U1478	C1415	C1354	A1289	G1228	A1167	G1102	C975	A913	C851	A791
G1663	G1479	A1416	A1355	A1290	C1229	G1168	G1037	C976	A914	U852	G792
A1664	G1480	C1417	G1356	G1291	C1230	C1169	C1103	G977	C915	C853	U793
C1665	U1481	C1418	U1357	A1292	A1231	U1170	U1105	U978	U916	G854	A794
G1666	U1482	G1419	C1358	A1293	U1232	A1171	A1106	A979	U917	G855	A795
A1667	A1420	A1420	G1359	G1294	A1233	U1172	A1107	G980	A918	U856	A796
C1668	U1421	U1421	G1360	U1295	C1234	G1173	U1108	C981	U919	U857	A797
A1669	U1485	C1422	G1361	G1296	C1235	G1174	A1109	C982	G920	U858	G798
C1670	A1486	A1423	C1362	A1297	G1236	U1175	U1044	A983	A921	U859	C799
G1671	C1487	C1363	C1363	G1298	G1237	A1176	G1110	G984	A922	U860	U800
A1672	G1427	C1364	C1364	A1299	A1238	U1177	U1112	C985	A923	C861	A801
C1673	G1428	U1365	U1365	A1300	A1239	C1178	C1113	A986	C924	A862	A802
G1674	U1429	A1366	U1366	U1301	G1240	A1179	A1114	G987	U925	C863	A803
C1675	C1491	G1430	A1367	C1302	G1241	A1180	C1115	G988	C926	C864	C804

C2547	G2487	G2434	C2360	A2299	C2239	U2178	G	G2050	C1939	U1929	G1864	A1799	G1737	U1676
G2548	G2488	G2425	G2361	G2300	C2240	C2179	C	U2061	U1990	C1930	C1865	A1800	U1738	C1677
G2549	G2489	G2426	G2362	A2301	U2241	U2190	G	G2052	C1991	G1931	C1866	A1990	G1678	C1678
C2550	G2490	A2427	G2363	G2302	C2242	A2181	A2117	G2053	C1992	G1932	A1867	A1802	U1679	U1679
A2551	G2491	U2428	C2364	C2303	C2243	A2182	A2118	G2054	C1993	G1933	A1868	U1803	G1742	U1680
C2552	G2492	U2429	C2365	C2306	C2244	C2183	A2119	G2055	C1994	G1934	A1869	U1804	C1743	A1681
G2553	U2493	A2430	U2366	A2307	A2245	C2184		U2058	C1995	A1935	U1870	G1805	G1744	A1682
C2554	G2494	C2431	A2367	A2308	A2246	C2185	G2123	U2059	A1996	A1936	A1871	G1806	C1745	G1683
G2555	G2495	A2432	G2368	A2309	A2247	U2186	C2124	U2058	A1997	G1937	A1872	A1807	A1746	G1684
A2556	G2496	G2433	U2369	G2310	A2248	A2187	G2125	U2059	A1998	U1938	G1747	C1808	G1747	A1685
C2557	U2497	G2434	G2370	G2311	U2249	A2188	U	C2061	U1999	G1939	A1873	A1809	U1748	A1686
U2498	U2498	U2435	A2371	U2311	G2250	A2189	U	U2062	U2000	C1940	G1878	U1810	G1749	C1687
U2499	U2499	U2436	A2372	A2312	G2251	A2190	U	A2063	G2001	C1941	G1879	A1811	A1750	U1688
G2500	G2499	G2437	C2373	G2313	A2252	A2191	U	U2064	A2002	G1942	G1880	U1812	A1751	U1689
U2501	A2498	A2438	G2374	A2314	A2253	U2192	U	A2065	A2003	G1943	U1881	U1813	U1752	U1690
G2502	G2503	U2439	G2375	A2315	C2254	C2193	G	G2066	U2004	C1944	G1882	A1814	A1753	C1691
G2503	G2504	G2440	G2376	C2316	G2255	G2194	G2132	U2067	U2005	C1945		G1815	C1692	C1692
G2504	U2441	U2441	U2377	G2317	G2256	A2195	G2133	C2068	U2006	U1946		G1816	G1755	A1693
G2505	C2442	C2442	U2377	U2318	A2257	U2196	U2134	U2069	G2007	G1947	G1886	U1817	C1756	A1694
G2506	C2443	C2443	A2381	G2319	A2258	U2197		G2070	C2008	C1948	G1887	U1818	C1757	U1695
U2507			C2382	G2320	G2259	U2198	G2137	G2071	U2009	A1949	C1888	U1819	C1758	C1702
A2508	G2447	G2447	C2383	C2321	G2260	C2199	U2138	C2072	G2010	C1950	A1759	A1820	A1759	U1697
A2509	A2448	A2448	G2384	G2322	G2261	G2200	G2139	A2073	U2011	G1951	G1889	A1821	G1760	C1698
A2510	G2449	G2449	U2385	G2323	G2262	G2201	G2140	U2074	A2012	A1952	C1891	C1822	G1761	C1699
G2511	A2450	A2450	G2386	U2334	C2263	G2202	A	U2075	A2013	A1953	C1892	G1823	G1762	C1700
A2512	G2451	G2451	C2264	A2355	C2264	G2283	G	G2076	A2014	A1954	G1893	C1824	G1763	C1701
C2513			A2265	C2326	A2266	A2204	G	G2077	G2015	G1955	C1894	C1825	A1764	C1702
G2514	C2454	C2454	G2266	U2327	A2267	C2205	C	G2078	A2016	G1956	A1895	U1826	C1765	C1703
G2515	A2455	A2455	G2267	G2328	A2267	C2206	A	A2079	U2017	C1957	A1896	G1897	U1766	G1704
U2516	U2456	U2456	G2268	G2329	G2268	G2207	A	U2080	G2018	G1958	C1897	U1767	U1705	U1705
C2517	A2457	A2457	G2269	G2330	G2269	U2208	C	U2081	C2019	U1959	U1898	A1706	U1768	A1706
G2518	U2458	U2458	U2270	A2331	G2270	C2209	C	C2082	G2020	A1960	A1899	U1707	U1769	A1707
C2519	C2459	C2459	C2271	G2332	C2271	C2210	G	G2083	G2021	A1961	U1900	G1832	U1770	C1708
A2520	G2460	G2460	A2272	A2333	A2272	U2211	U	G2084	C2022	C1962	A1901	U1833	A1771	U1709
A2581	G2461	G2461	C2273	C2334	C2273	U2212	G	G2085	C2023	G1963		G1834	A1772	U1710
G2582	C2462	C2462	C2274	U2335	C2274	G2213	A	U2086	U2024	A1964	G1904	C1835	C1773	C1711
	G2463	G2463	U2275	G2336	U2275	G2214	A		A2025	A1965	G1905	C1836	A1774	G1712
	G2464	G2464	G2276	A2337	C2276	G2215	A		C2026	C1966	U1906	G1837	A1775	G1713
G2586	U2525	G2465	A2277	C2338	A2277	G2216	U	C2091		U1967	C1907	G1838	A1776	A1714
G2587	U2526	G2466	A2278	A2339	A2278	G2217	A	G2092	G2029	G1968	G1908	A1839	A1777	A1715
U2588	G2527	G2467	G2279	C2340	G2279	G2218	C2157	C2094	U2030	G1969	C1909	A1840	U1778	G1716
G2589	G2528	G2468	A2280	G2341	A2280	U2219	C2158	G2095	A2031	G1970	U1909	A1841	C1779	A1717
U2590	G2529	G2469	G2281	U2342	G2281	A2220	A2159	U2096	G2032	C1971	A1911	G1842	A1780	A1718
C2591	G2530	U2470	G2282	C2343	G2282	G2221	C2160	A2097	U2033	G1972	G1912	A1845	G1719	G1719
U2531	U2471	U2471	G2283	G2344	G2283	U2222	C2161	G	A2034	C1973	G1913	A1846	G1720	G1720
G2532	U2472	U2472	U2284	A2345	U2284	U2223	C2162	G	G2035	U1974	U1914	G1847	G1721	G1721
U2533	G2473	G2473	U2285	G2346	U2285	U2224	U2163	A	G2036	G1975	A1915	U1848	G1783	G1783
U2534	G2474	G2474	G2286	C2347	G2286	G2225	G2164	U	A2037	U1976	G1916	G1849	G1784	G1722
C2585	C2475	C2475	G2287	A2348	G2287	A2226	A2165	A	C2038	C1977	C1917	G1850	U1785	U1723
U2535	U2476	U2476	A2288	G2349	G2288	C2227			G2039	U1978	G1918	G1851	C1724	C1724
G2536	C2477	C2477	A2289	G2350	A2289	U2228	A2168	G2103	A2040	C1979	A1919	G1854	C1726	C1726
C2537	U2478	U2478	A2290	G2351	A2290	G2229	A2169	G2104	A2041	G1980	A1920	G1855	C1727	C1727
C2538	U2479	U2479	U2291	A2352	U2291		C2170	U2105	A1980	G1981	A1921	U1856	U1789	U1789
A2600	G2480	G2480	G2292	G2353	C2292	G2232	U2171	G2106	A2042	A1981	A1922	U1857	G1790	A1728
C2601	U2541	G2481	G2293	G2354	G2293	C2233	U2172	G2107	A2043	G1982	U1922	G1857	C1791	C1729
G2602	U2542	U2542	G2294	A2355	U2294	G2234	U2173	G2108	G2044	G1983	U1923	C1858	C1792	C1792
G2603	U2543	U2543	G2295	A2356	G2295	G2235	G2174	A2109	A2045	A1984	C1924	A1859	A1793	G1730
G2604	U2544	U2544	A2357	A2357	U2296	G2236	C2175	G2110	C2046	G1985	C1925	A1860	A1794	U1733
C2605	U2545	U2545	U2297	A2358	G2297	C2237	A2176	C	C2047	G1986	U1926	G1861	C1797	C1734
G2606	U2546	U2546	C2297	U2358	G2297	C2237	U2176	U	C2048	G1987	U1927	C1862	C1797	C1734
C2607	G2546	G2546	U2298	U2359	U2298	G2238	U2177		C2049	A1988	G1928	U1863	G1798	C1736

4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	170.47Å 412.74Å 696.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.96 – 3.56 29.95 – 3.56	Depositor EDS
% Data completeness (in resolution range)	90.5 (29.96-3.56) 90.6 (29.95-3.56)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 3.56Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.276 , 0.338 0.359 , 0.378	Depositor DCC
R_{free} test set	13101 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	97.3	Xtriage
Anisotropy	0.737	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.15 , 79.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.80	EDS
Total number of atoms	59597	wwPDB-VP
Average B, all atoms (Å ²)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.23% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: G80

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	0.62	9/66467 (0.0%)	0.83	95/103673 (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	0	0	158

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	788	G	N9-C4	8.60	1.44	1.38
1	0	700	C	N1-C2	8.52	1.48	1.40
1	0	788	G	C5-C6	6.89	1.49	1.42
1	0	824	U	N1-C2	6.74	1.44	1.38
1	0	788	G	C2-N3	5.96	1.37	1.32

The worst 5 of 95 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	1342	U	N1-C1'-C2'	10.68	127.89	114.00
1	0	985	G	N9-C1'-C2'	10.52	127.68	114.00
1	0	2497	A	N9-C1'-C2'	10.09	127.12	114.00
1	0	1975	G	N9-C1'-C2'	9.37	126.19	114.00
1	0	2660	C	N1-C1'-C2'	9.30	126.09	114.00

There are no chirality outliers.

5 of 158 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	118	U	Sidechain
1	0	154	U	Sidechain
1	0	29	U	Sidechain
1	0	50	G	Sidechain
1	0	67	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	59359	0	29917	4825	0
2	B	205	0	0	2	0
3	0	33	0	43	7	0
All	All	59597	0	29960	4828	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 55.

The worst 5 of 4828 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)
1:0:2040:A:H2'	1:0:2041:A:C8	1.52	1.42
1:0:2040:A:C2'	1:0:2041:A:H8	1.48	1.27
1:0:2564:U:O2'	1:0:2565:C:H5'	1.34	1.26
1:0:2418:A:H1'	1:0:2565:C:O2'	1.31	1.24
1:0:2810:A:C6	1:0:2854:G:C8	2.27	1.22

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	2757/2880 (95%)	664 (24%)	167 (6%)

5 of 664 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	9	U
1	0	13	A
1	0	14	A
1	0	27	G
1	0	33	C

5 of 167 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	1921	A
1	0	2428	U
1	0	1963	G
1	0	2161	C
1	0	2589	C

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 monosaccharides 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	G80	0	2881	-	36,36,36	4.14	22 (61%)	55,56,56	2.77	19 (34%)

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	G80	0	2881	-	-	1/12/81/81	0/4/4/4

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	0	2881	G80	C12-C11	12.11	1.67	1.55
3	0	2881	G80	C5-C14	10.66	1.64	1.56
3	0	2881	G80	C5-C6	9.24	1.70	1.56
3	0	2881	G80	C10-C11	7.71	1.63	1.56
3	0	2881	G80	C8-C7	5.31	1.64	1.53

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	0	2881	G80	C4-C5-C6	-8.57	97.21	106.87
3	0	2881	G80	C12-C11-C10	-7.08	107.83	114.75
3	0	2881	G80	C7-C6-C5	6.30	118.59	111.57
3	0	2881	G80	O3-C21-C22	5.72	119.95	110.52
3	0	2881	G80	C18-C12-C11	5.31	111.80	108.16

There are no chirality outliers.

All (1) torsion outliers are listed below:

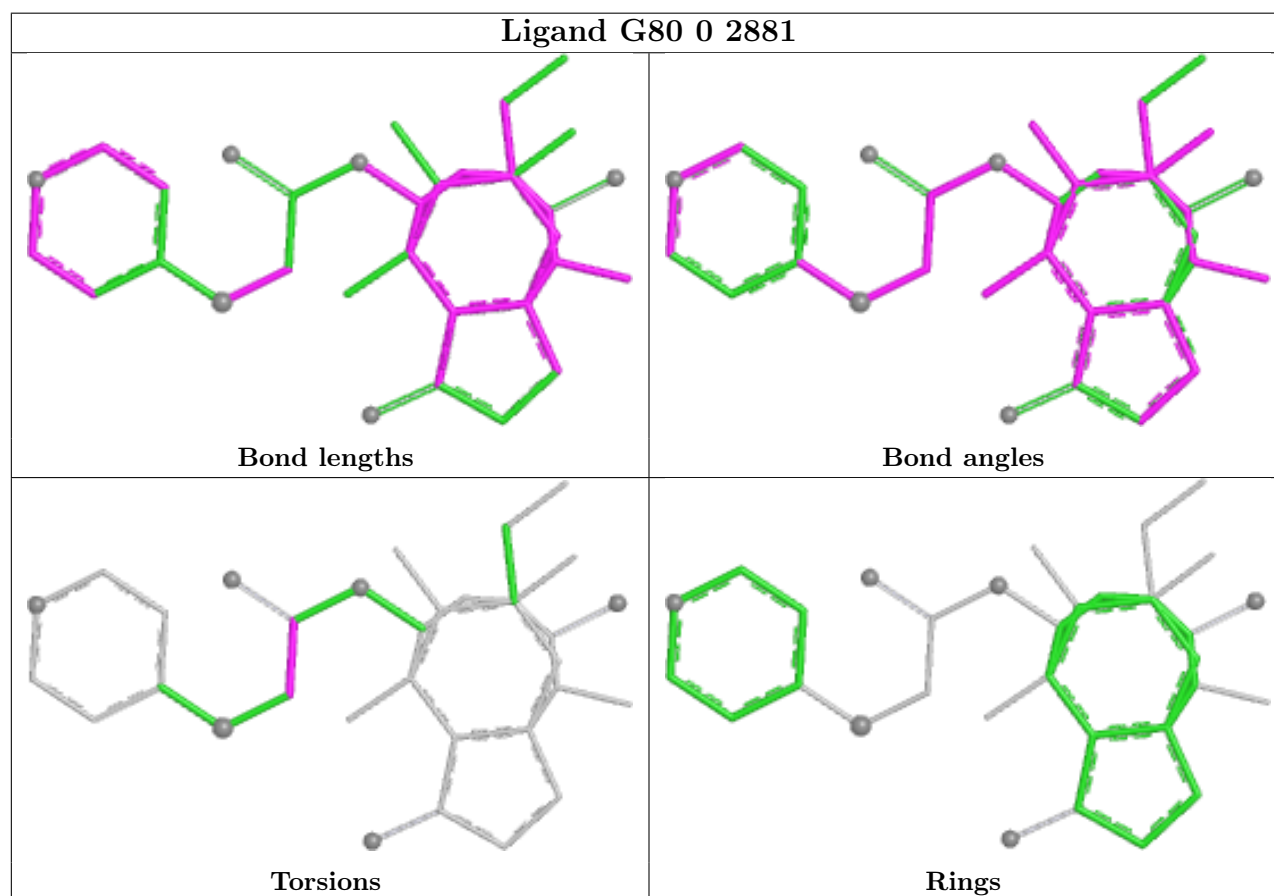
Mol	Chain	Res	Type	Atoms
3	0	2881	G80	O3-C21-C22-S1

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	0	2881	G80	7	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

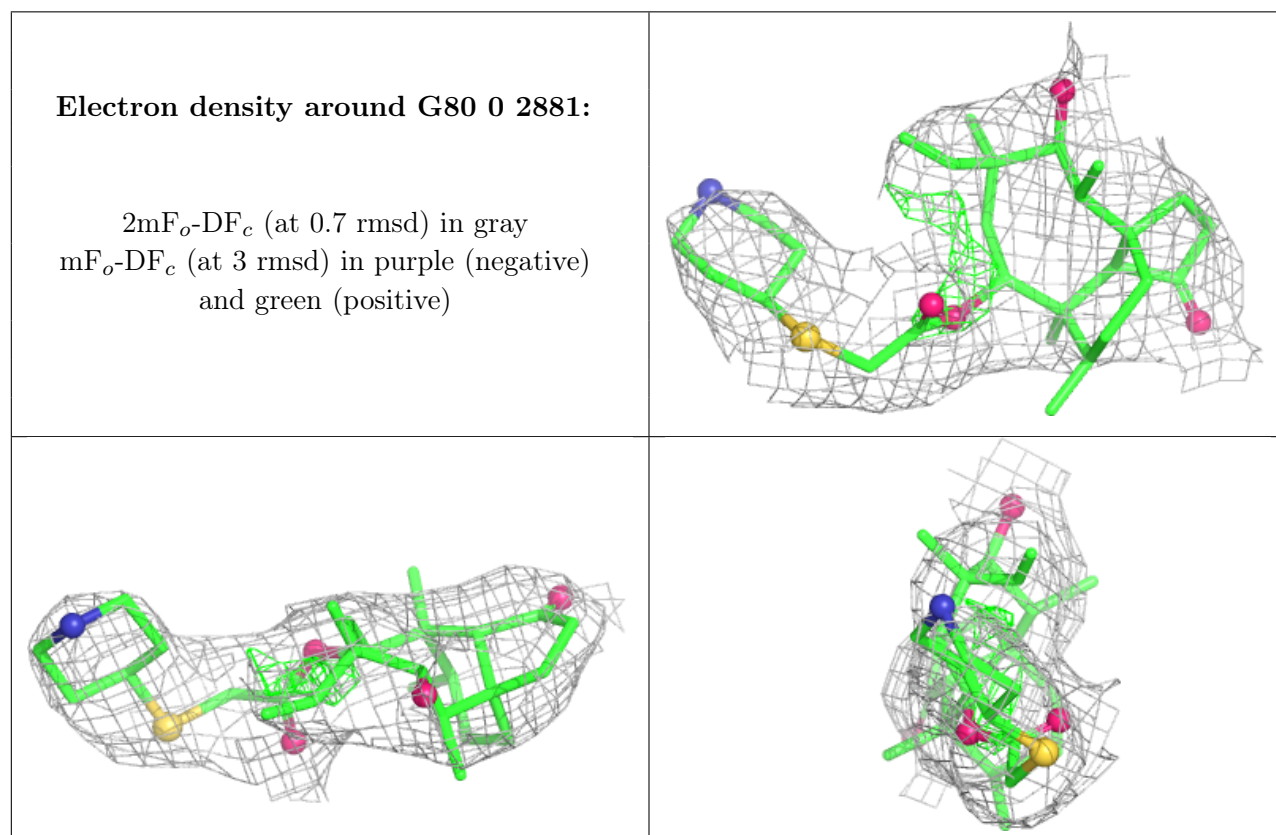
6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.