



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2026 – 02:22 PM UTC

PDB ID : 2OGM / pdb_00002ogm
Title : The crystal structure of the large ribosomal subunit from *Deinococcus radiodurans* complexed with the pleuromutilin derivative SB-571519
Authors : Davidovich, C.; Bashan, A.; Auerbach-Nevo, T.; Yonath, A.
Deposited on : 2007-01-07
Resolution : 3.50 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

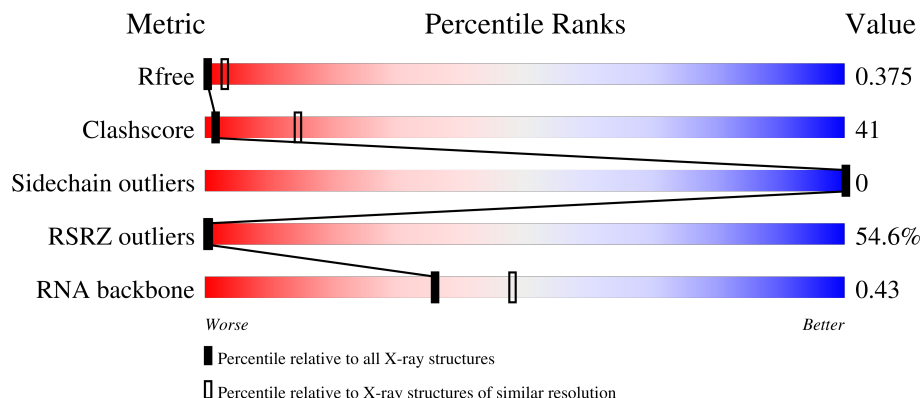
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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}	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)
RNA backbone	3983	1010 (3.98-3.02)

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 $\leq 5\%$. 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	49% 17% 55% 18% 6% .
2	B	211	97% 95% . .

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 59610 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.

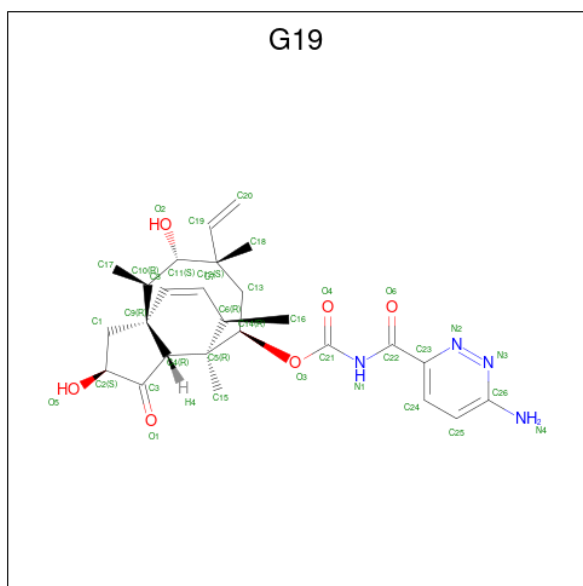
- Molecule 1 is a RNA chain called 23S ribosomal RNA.

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	N	O	0	0	204
			215	210	4	1			

- Molecule 3 is (2S,3AR,4R,5S,6S,8R,9R,9AR,10R)-2,5-DIHYDROXY-4,6,9,10-TETRAMETHYL-1-OXO-6-VINYLBENZOIC ACID 3-AMINOPYRIDAZIN-5-YL [(6-AMINOPYRIDAZIN-3-YL)CARBONYL]CARBAMATE (CCD ID: G19) (formula: $C_{26}H_{34}N_4O_6$).

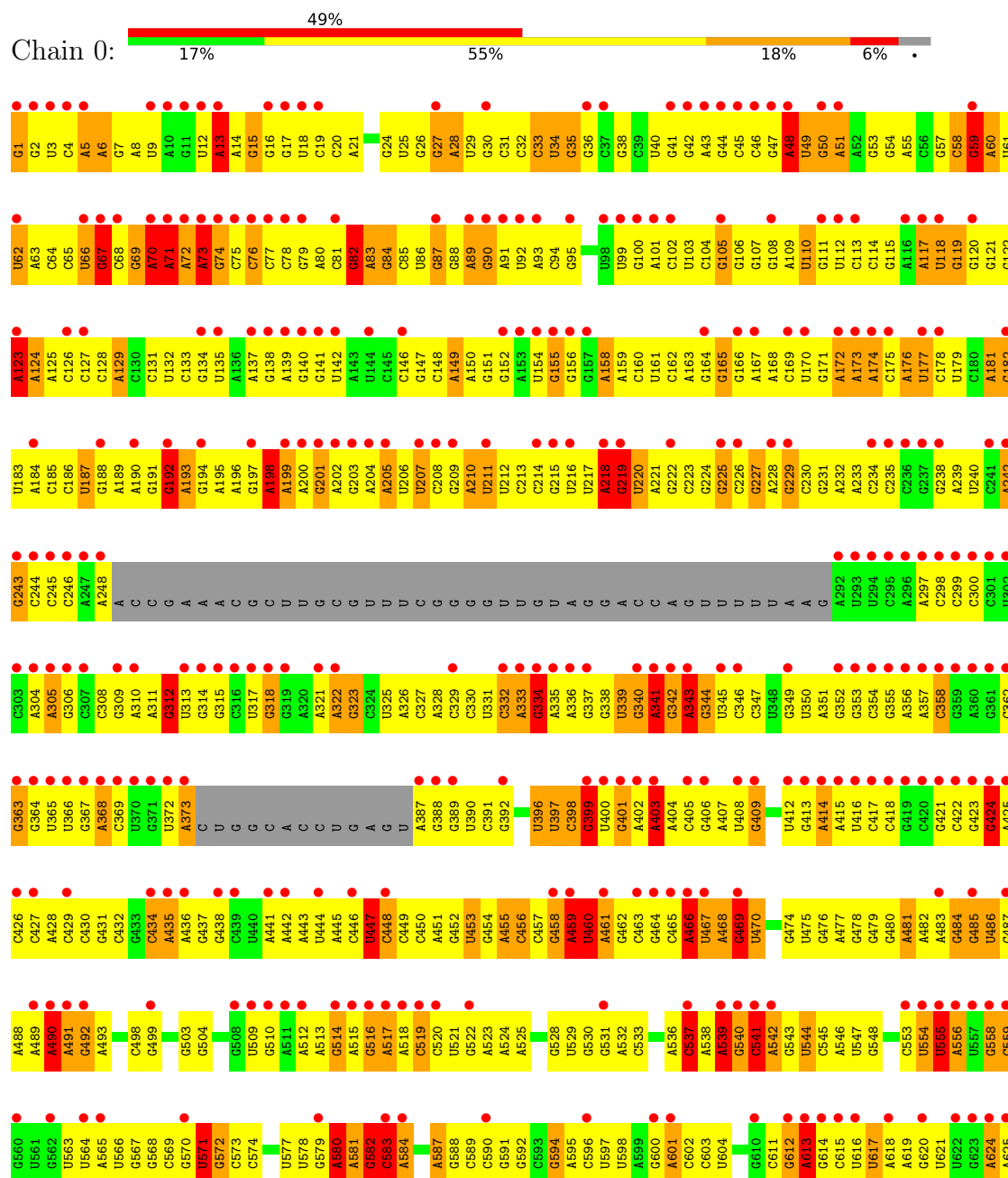


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	0	1	Total	C	N	O	0	0
			36	26	4	6		

3 Residue-property plots

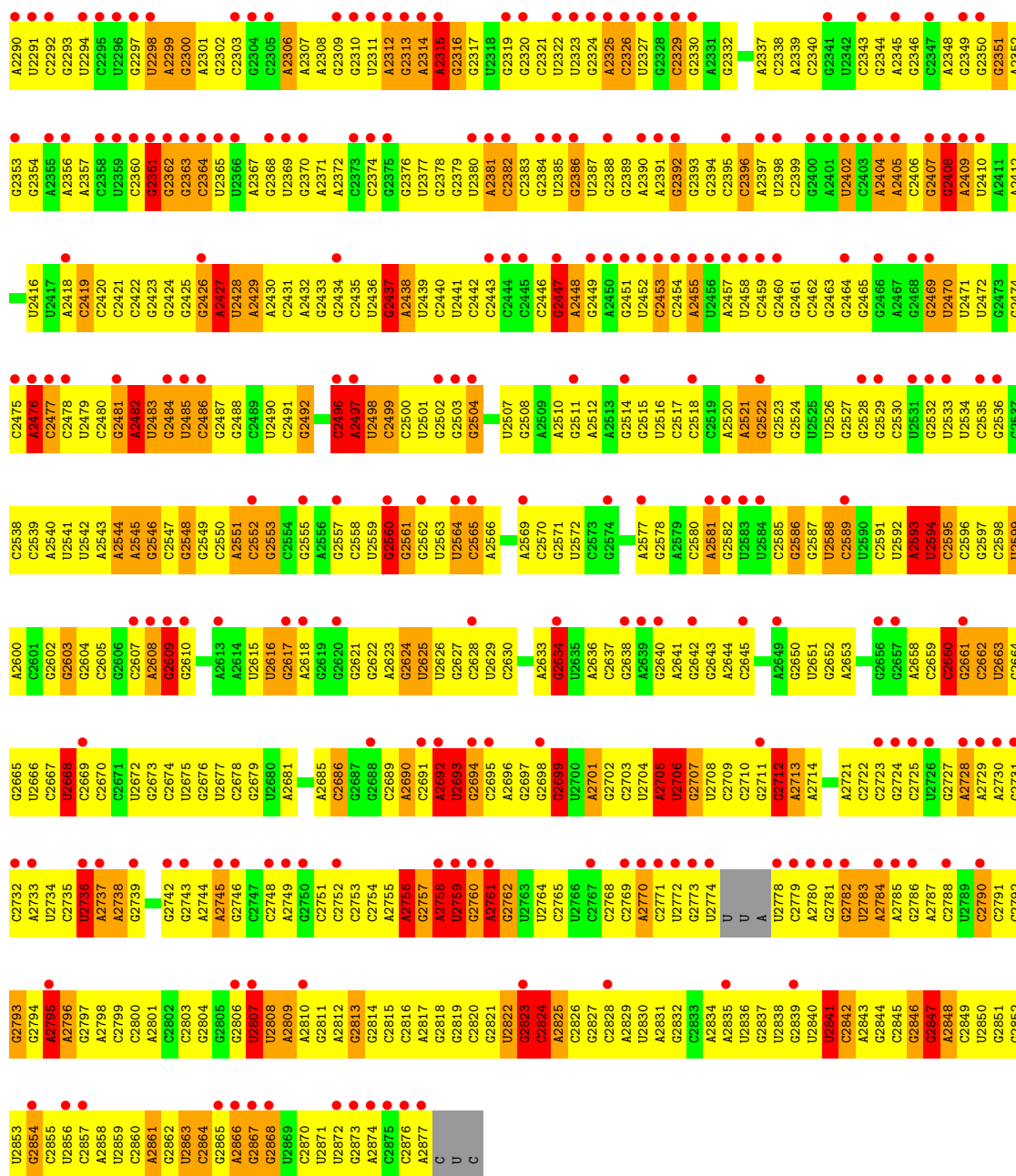
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

• Molecule 1: 23S ribosomal RNA

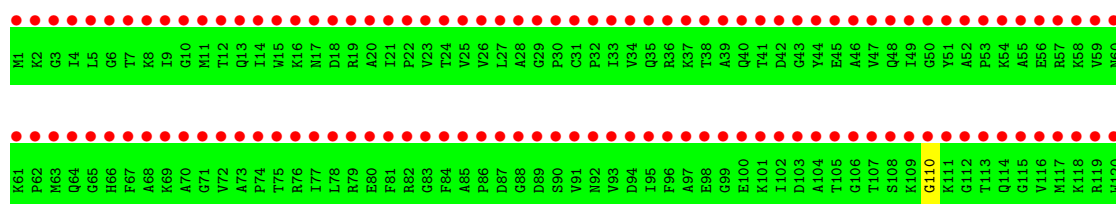


G1436	G1437	A1438	G1439	G1440	A1441	A1442	G1443	A1444	G1445	A1446	G1447	A1448	G1449	G1450	A1451	A1452	A1453	A1454	A1455	A1456	A1457	A1458	A1459	G1460	A1463	A1464	A1465	G1466	A1467	A1468	A1469	G1470	G1471	A1472	G1473	A1474	G1475	A1476	G1477	A1478	G1479	A1480	A1481	A1482	G1483	G1484	A1485	A1486	A1487	G1488	G1489	A1490	A1491	A1492	A1493	A1494	A1495	A1496																																																																																																																																																																																																																																																																																																																																																																														
C1376	G1377	A1378	A1379	C1380	G1381	G1382	C1383	G1384	C1385	A1386	G1387	C1388	G1389	G1390	A1391	G1392	G1393	G1394	A1395	A1396	A1397	G1398	C1399	A1400	G1401	G1402	C1403	C1404	A1405	A1406	G1407	A1408	U1409	U1410	C1411	C1412	G1413	G1414	A1415	A1416	G1417	G1418	A1419	A1420	G1421	C1422	A1423	A1424	G1425	G1426	A1427	G1428	A1429	G1430	A1431	A1432	A1433	A1434	A1435																																																																																																																																																																																																																																																																																																																																																																													
U1313	A1314	A1315	G1316	A1321	G1322	G1323	G1324	U1325	U1326	C1327	C1328	U1329	G1330	G1331	G1332	G1333	A1334	A1335	G1336	G1337	G1338	G1339	C1340	G1341	U1342	C1343	C1344	G1345	C1346	C1347	G1348	A1349	G1350	G1351	G1352	A1353	A1354	A1355	G1356	U1357	C1358	G1359	G1360	G1361	A1362	C1363	C1364	U1365	A1366	G1367	G1368	G1369	U1370	G1371	A1372	G1373	G1374	G1375																																																																																																																																																																																																																																																																																																																																																																														
A1242	G1243	U1244	G1245	G1246	G1249	A1250	G1251	C1252	C1253	G1254	U1257	G1258	G1259	A1260	G1261	U1262	G1263	G1264	G1265	G1266	A1267	U1268	G1269	G1272	G1273	C1274	G1277	A1278	G1279	U1280	A1281	A1282	C1283	G1284	A1285	U1286	A1287	A1288	A1289	G1298	A1299	A1300	U1301	C1302	U1303	U1304	C1305	U1306	U1307	C1308	G1309	C1310	C1311	G1312																																																																																																																																																																																																																																																																																																																																																																																		
U1182	C1183	G1184	C1185	G1186	A1187	A1188	G1189	C1190	A1191	A1192	U1193	U1194	U1195	G1196	U1197	G1198	U1199	G1200	A1139	A1140	A1141	A1202	A1203	G1265	G1266	G1267	G1268	G1269	G1270	G1271	A1272	A1273	A1274	A1275	A1276	A1277	A1278	A1279	A1280	A1281	A1282	A1283	A1284	A1285	A1286	A1287	A1288	A1289	A1290	A1291	A1292	A1293	A1294	A1295	A1296	A1297	A1298	A1299	A1300	A1301	A1302	A1303	A1304	A1305	A1306	A1307	A1308	A1309	A1310	A1311	A1312																																																																																																																																																																																																																																																																																																																																																																	
G1121	A1122	G1123	U1124	G1125	A1126	C1127	G1128	A1129	U1130	U1131	G1132	G1133	G1134	C1135	G1136	A1137	A1138	A1139	A1140	A1141	A1142	A1143	U1144	G1145	G1146	G1147	G1148	G1149	C1150	U1151	C1152	A1153	A1154	G1155	A1158	U1159	C1160	U1161	A1162	C1163	C1164	G1165	A1166	A1167	G1168	C1169	U1170	A1171	U1172	G1173	G1174	A1175	U1176	U1177	C1178	A1179	A1180	U1181	C1181																																																																																																																																																																																																																																																																																																																																																																													
A1061	G1062	C1063	A1064	A1065	G1066	C1067	A1068	G1069	U1070	U1071	U1072	G1073	G1074	C1075	U1076	C1077	A1078	G1079	A1080	G1081	G1082	C1083	A1084	G1085	C1086	C1087	A1088	G1089	C1090	U1091	U1092	U1093	C1094	A1095	A1096	A1097	G1098	A1099	G1100	U1101	C1102	G1103	G1104	U1105	U1106	U1107	U1108	A1109	G1110	C1111	U1112	C1113	A1114	C1115	U1116	G1117	U1118	U1119	C1120																																																																																																																																																																																																																																																																																																																																																																													
A1001	C1002	C1003	A1004	U1005	C1006	A1007	G1008	C1009	U1010	A1011	A1012	G1013	G1014	U1015	U1016	C1017	A1018	U1019	A1020	C1021	U1022	U1023	A1024	A1025	U1026	C1027	G1028	C1029	U1030	C1031	A1032	G1033	U1034	G1035	G1036	U1037	U1038	A1039	A1040	G1041	G1042	A1043	U1044	G1045	U1046	G1047	U1048	C1049	G1050	U1051	U1052	C1053	A1054	U1055	U1056	A1057	G1058	C1059	C1060																																																																																																																																																																																																																																																																																																																																																																													
C939	G940	U941	U942	A943	U944	G945	U946	C947	G948	G949	G950	G951	A952	G953	U954	G955	A956	G957	G958	C959	U960	A964	G965	A966	G967	C968	U969	A970	A971	C972	U973	C974	C975	G976	G977	U978	A979	G980	C981	C982	G983	A984	G985	A986	G987	G988	G989	A990	A991	A992	C993	A994	A995	C996	C997	C998	A999	G1000																																																																																																																																																																																																																																																																																																																																																																														
G877	C878	A879	C880	U881	A882	C883	C884	A885	C886	G887	G888	C889	U890	A891	G	G	G	G	C	C	U	U	A	C	A	G	C	U	U	A	C	A911	A912	A913	C914	C915	U916	G917	U918	A919	U920	U921	A922	A923	C924	U925	C926	C927	G928	A929	A930	G931	G932	A936	C937	A938	G938																																																																																																																																																																																																																																																																																																																																																																															
U810	G811	G812	A813	G814	A815	U816	A817	U818	C819	U820	A821	G822	U823	C824	C825	C830	G831	A832	A833	A834	U835	G836	U837	A838	U839	U840	A841	A842	G843	G844	U845	A846	C847	A848	U852	C853	G854	G855	A856	U857	G858	U859	U860	A861	C862	C863	C864	A865	U866	G867	U868	U869	A870	A871	U872	A873	U874	U875	U876	U877	U878	U879	U880	U881	U882	U883	U884	U885	U886	U887	U888	U889	U890	U891	U892	U893	U894	U895	U896	U897	U898	U899	U900	U901	U902	U903	U904	U905	U906	U907	U908	U909	U910	U911	U912	U913	U914	U915	U916	U917	U918	U919	U920	U921	U922	U923	U924	U925	U926	U927	U928	U929	U930	U931	U932	U933	U934	U935	U936	U937	U938	U939	U940	U941	U942	U943	U944	U945	U946	U947	U948	U949	U950	U951	U952	U953	U954	U955	U956	U957	U958	U959	U960	U961	U962	U963	U964	U965	U966	U967	U968	U969	U970	U971	U972	U973	U974	U975	U976	U977	U978	U979	U980	U981	U982	U983	U984	U985	U986	U987	U988	U989	U990	U991	U992	U993	U994	U995	U996	U997	U998	U999	U1000	U1001	U1002	U1003	U1004	U1005	U1006	U1007	U1008	U1009	U1010	U1011	U1012	U1013	U1014	U1015	U1016	U1017	U1018	U1019	U1020	U1021	U1022	U1023	U1024	U1025	U1026	U1027	U1028	U1029	U1030	U1031	U1032	U1033	U1034	U1035	U1036	U1037	U1038	U1039	U1040	U1041	U1042	U1043	U1044	U1045	U1046	U1047	U1048	U1049	U1050	U1051	U1052	U1053	U1054	U1055	U1056	U1057	U1058	U1059	U1060	U1061	U1062	U1063	U1064	U1065	U1066	U1067	U1068	U1069	U1070	U1071	U1072	U1073	U1074	U1075	U1076	U1077	U1078	U1079	U1080	U1081	U1082	U1083	U1084	U1085	U1086	U1087	U1088	U1089	U1090	U1091	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
A626	A627	A628	C629	G630	A631	A632	A633	A634	C635	G636	G637	A638	C639	G640	G641	A644	G645	G646	G647	A648	C649	U650	C651	C652	C653	A654	A655	U656	U657	C658	C659	C660	C661	G662	G663	C664	A665	U666	U667	A668	U669	U670	A671	U674	C675	G676	G677	C678	U669	U680	A681	G682	A683	C684	U685	G686	G687	A748																																																																																																																																																																																																																																																																																																																																																																														

G2230	G2170	G2110	G2050	G1989	U1926	G1866	G1806	G1744	A1681	G1617	G1557	C1497
G2231	U2171	C	U2051	G1992	U1927	A1867	A1807	C1745	A1682	U1618	C1558	C1498
G2232	G2172	C	G2052	G1993	G1928	A1868	G1808	G1746	A1683	G1619	C1559	A1499
G2233	G2173	U	G2053	G1994	G1929	A1869	G1809	A1747	G1684	C1620	A1560	U1500
G2234	G2174	C	A2054	U1994	C1930	U1870	U1810	U1748	A1685	A1561	C1501	C1501
G2235	A2175	G	G2055	G1995	G1931	G1871	A1811	G1749	A1686	G1622	G1562	G1502
U2236	U2176	G	C2056	A1996	G1932	A1872	U1812	A1750	C1687	C1623	U1563	G1503
G2237	U2177	A2117	U2057	A1997	G1933	A1873	A1813	A1753	U1690	A1624	U1564	G1504
G2238	U2178	A2118	U2058	A1998	U1934	G1874	G1814	G1754	G1691	A1625	G1565	U1505
C2239	C2179	A2119	U2059	A1999	A1935	G1875	G1815	G1755	C1692	C1626	G1566	C1506
C2240	U2180	C2120	A2060	U2000	A1936	G1876	G1816	G1756	G1693	C1627	A1567	C1507
C2241	A2181	U2121	C2061	G2001	G1937	C1877	U1817	G1757	A1694	G1628	A1568	G1508
C2242	A2182	G2122	U2062	A2002	U1938	C1878	G1818	C1757	U1685	G1629	A1569	A1509
C2243	C2183	G2123	A2063	A2003	U1939	G1879	U1819	G1758	U1686	A1630	C1570	A1510
C2244	U2184	C2124	U2064	U2004	C1940	G1880	A1820	A1759	C1697	C1631	G1571	A1511
A2245	U2185	C2125	A2065	U2005	C1941	U1881	A1821	G1760	U1697	A1632	C1572	A1512
A2246	C2186	U	G2066	G2006	G1942	G1882	C1822	G1761	C1698	C1533	A1574	U1513
A2247	A2187	U	U2067	G2007	A1943	A1883	C1823	C1762	A1699	A1634	A1574	C1514
A2248	A2188	U	C2068	C2008	C1944	A1884	C1824	G1763	C1700	G1635	C1575	U1515
U2249	A2189	U	U2069	U2009	C1945	A1885	C1825	A1764	C1701	G1636	G1576	A1516
G2250	A2190	G	G2070	G2010	U1946	G1886	U1826	C1765	C1702	U1637	G1577	C1517
U2251	A2191	G	G2071	A2012	C1947	G1887	G1827	U1766	G1703	C1641	U1578	G1518
A2252	U2192	G	C2072	A2012	C1948	C1888	G1828	G1767	U1704	G1642	G1579	C1519
A2253	C2193	U2133	A2073	A2013	A1949	U1768	C1829	U1769	U1705	A1643	C1580	U1521
C2254	U2134	U2134	U2074	A2014	C1950	G1889	C1830	U1770	A1706	G1644	C1581	C1522
G2255	C2135	C2135	U2075	G2015	G1951	C1891	G1831	U1771	A1707	U1645	A1582	A1523
G2256	U2196	G2136	G2076	A2016	A1952	C1892	U1832	C1772	U1708	G1646	A1583	C1524
A2257	U2197	G2137	G2077	U2017	A1953	G1893	U1833	C1773	U1709	A1654	C1590	U1530
G2258	U2198	U2138	G2078	G2018	A1954	A1894	C1834	C1774	U1710	A1655	U1591	C1531
G2259	C2199	U2139	A2079	C2019	G1955	A1895	C1835	A1774	C1711	A1586	C1592	A1532
C2260	G2200	C2140	U2080	G2020	G1956	A1896	C1836	A1775	G1712	G1648	C1587	U1526
G2261	U2201	A	U2081	G2021	C1957	C1897	C1837	A1776	G1713	U1651	A1588	C1528
C2262	G2202	G	C2082	C2022	G1958	U1898	G1838	A1777	A1714	G1652	C1589	C1529
C2263	G2203	G	G2083	G2023	U1959	A1899	A1839	U1778	A1715	C1653	C1590	U1530
C2264	A2204	C	G2084	U2024	A1960	U1900	A1840	C1779	G1716	A1654	C1591	C1531
A2265	C2205	A	U2085	A2025	A1961	A1901	G1841	C1780	A1717	C1655	C1592	A1532
A2266	U2086	A	G2086	C2026	C1962	A1902	G1842	C1781	A1718	U1656	C1593	G1533
A2267	U2087	C	U2087	C2027	G1963	C1903	U1843	A1782	G1722	A1657	U1594	A1534
G2268	U2088	G	G2088	G2028	A1964	G1904	C1844	C1783	G1723	A1658	A1595	C1535
G2269	C2089	G	C2089	G2029	U1965	G1905	A1845	C1784	U1724	G1659	A1596	G1536
U2270	U2090	U	U2090	U2030	C1966	U1906	A1846	A1785	C1724	G1660	A1597	U1537
C2271	C2091	G	C2091	A2031	U1967	C1907	G1847	C1786	C1725	C1661	C1598	A1538
C2272	A	A	U2092	G2032	G1968	U1908	U1848	U1787	C1726	G1662	G1599	U1539
G2273	G2213	A	G2093	C2033	G1969	U1909	G1849	C1788	G1727	C1663	U1600	C1540
C2274	G2214	A	C2094	A2034	G1970	A1910	G1850	U1789	A1728	G1664	U1601	G1541
U2275	C2215	U	G2095	G2035	C1973	A1911	A1851	C1790	C1729	C1665	G1602	G1542
C2276	G2216	A	U2096	G2036	G1974	G1912	G1852	C1791	G1730	G1666	A1603	G1543
A2277	G2217	C2157	G	A2037	G1975	G1913	C1853	C1792	C1731	A1667	A1604	A1544
U2278	U2218	A2158	A	G2038	U1976	A1914	G1854	A1793	U1732	G1668	A1605	G1545
G2279	U2219	A2159	G	G2039	C1977	A1915	G1855	A1794	U1733	A1669	C1606	C1546
A2280	A2220	C2160	A	A2040	C1978	C1917	U1856	C1797	C1734	G1670	A1607	U1547
C2281	G2221	C2161	U	A2041	U1978	G1917	G1857	A1671	G1735	U1608	U1608	U1548
G2282	U2222	C2162	A	A2042	C1979	G1918	A1858	G1798	C1736	A1672	G1609	C1549
G2283	U2223	U2163	A	A2043	A1980	A1919	A1859	A1799	G1737	C1673	A1610	C1550
U2284	U2224	G2164	G2104	G2044	A1981	A1920	A1860	A1800	U1738	C1674	U1611	U1551
G2285	G2225	A2165	U2105	A2045	C1982	A1921	G1861	C1801	G1739	C1675	U1612	C1552
G2286	A2226	G2166	G2106	C2046	G1983	U1922	C1862	A1802	G1740	U1676	G1613	G1553
A2287	U2227	A2167	G2107	C2047	C1987	U1923	U1863	A1803	G1741	C1614	C1614	G1554
A2288	U2228	C2168	G2108	C2048	G1987	C1924	G1864	U1804	G1742	U1679	C1615	A1555
A2289	G2229	A2169	A2109	C2049	A1988	C1925	C1865	G1805	C1743		C1616	A1556



• Molecule 2: 50S ribosomal protein L3





4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	170.40Å 405.83Å 703.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.93 – 3.50 29.93 – 3.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (29.93-3.50) 92.6 (29.93-3.50)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 3.47Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.275 , 0.334 0.356 , 0.375	Depositor DCC
R_{free} test set	14021 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	86.3	Xtriage
Anisotropy	0.807	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , 94.4	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	0.78	EDS
Total number of atoms	59610	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.31% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: G19

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	0.46	0/66467	0.86	217/103673 (0.2%)
2	B	0.14	0/10	0.66	0/11
All	All	0.46	0/66477	0.86	217/103684 (0.2%)

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	121

There are no bond length outliers.

The worst 5 of 217 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	985	G	N9-C1'-C2'	10.07	129.11	114.00
1	0	788	G	N9-C1'-C2'	10.03	127.04	112.00
1	0	2237	C	C4'-C3'-O3'	-9.67	98.50	113.00
1	0	2660	C	C2'-C3'-O3'	9.09	123.14	109.50
1	0	460	U	N1-C1'-C2'	8.79	127.18	114.00

There are no chirality outliers.

5 of 121 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	13	A	Sidechain
1	0	15	G	Sidechain
1	0	48	A	Sidechain

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Mol	Chain	Res	Type	Group
1	0	67	G	Sidechain
1	0	82	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	3636	0
2	B	215	0	12	5	0
3	0	36	0	34	2	0
All	All	59610	0	29963	3640	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 41.

The worst 5 of 3640 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)
1:0:1280:U:C5	1:0:1995:G:C2	2.04	1.44
1:0:1440:G:H3'	1:0:1441:A:C5'	1.66	1.25
1:0:699:G:N2	1:0:801:A:H2	1.40	1.18
1:0:1440:G:C3'	1:0:1441:A:H5''	1.75	1.16
1:0:2205:C:O2'	1:0:2206:C:H5'	1.42	1.16

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](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	1/157 (1%)	1 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2757/2880 (95%)	622 (22%)	184 (6%)

5 of 622 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	5	A
1	0	6	A
1	0	13	A
1	0	28	A
1	0	35	G

5 of 184 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	1698	C
1	0	2204	A
1	0	1723	U
1	0	1963	G
1	0	2408	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 oligosaccharides 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	G19	0	2881	-	35,39,39	4.41	14 (40%)	49,62,62	2.61	19 (38%)

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 Torsions and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	G19	0	2881	-	-	0/15/79/79	0/4/4/4

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	0	2881	G19	C7-C8	18.74	1.58	1.32
3	0	2881	G19	C5-C14	9.03	1.63	1.56
3	0	2881	G19	C12-C11	8.62	1.64	1.55
3	0	2881	G19	C10-C11	7.09	1.63	1.56
3	0	2881	G19	O3-C21	5.55	1.45	1.35

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	0	2881	G19	C18-C12-C11	7.50	113.29	108.16
3	0	2881	G19	O3-C21-N1	6.24	117.46	107.97
3	0	2881	G19	O3-C21-O4	-5.48	116.49	124.55
3	0	2881	G19	C14-O3-C21	4.81	123.79	116.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	0	2881	G19	C9-C10-C11	4.71	116.85	112.46

There are no chirality outliers.

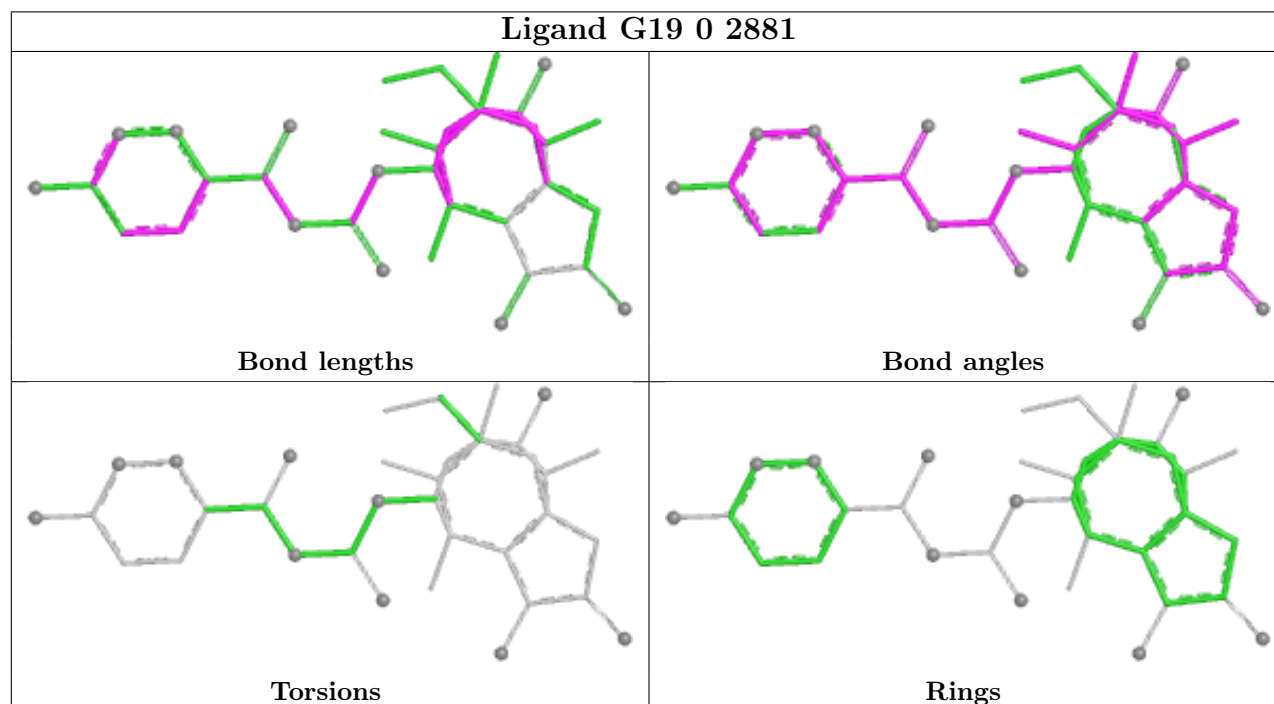
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	0	2881	G19	2	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 [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, 95th 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 ²)	Q<0.9
1	0	2766/2880 (96%)	2.67	1419 (51%) 0 1	9, 69, 200, 200	0
2	B	205/211 (97%)	10.76	204 (99%) 0 0	4, 52, 147, 201	0
All	All	2971/3091 (96%)	3.22	1623 (54%) 0 0	4, 67, 200, 201	0

The worst 5 of 1623 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	87	ASP	29.9
2	B	15	TRP	25.8
2	B	2	LYS	23.9
2	B	89	ASP	23.8
2	B	93	VAL	23.6

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](#)

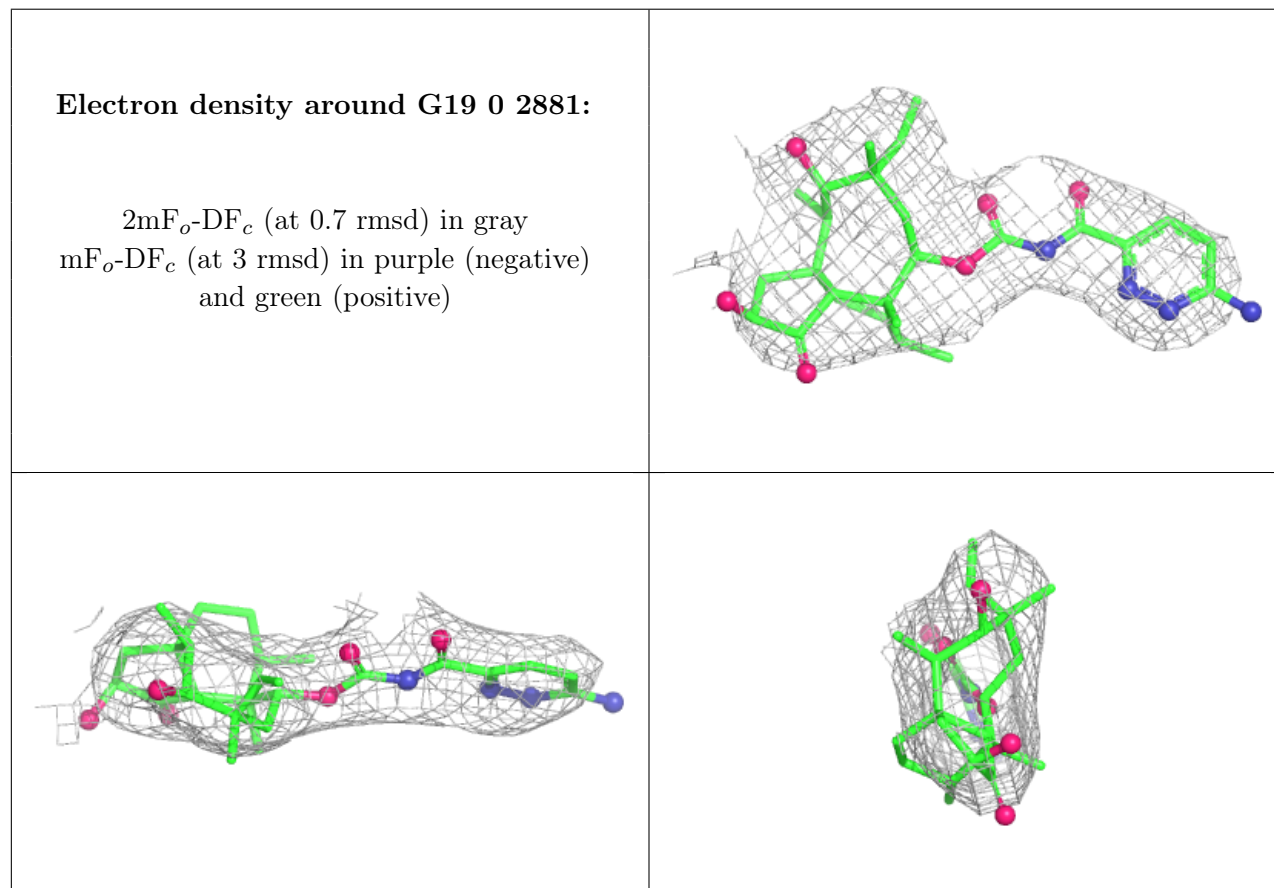
There are no oligosaccharides in this entry.

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. The B-factors column lists the minimum, median, 95th 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	B-factors($\text{\AA}^2$)	Q<0.9
3	G19	0	2881	36/36	0.90	0.23	70,70,70,70	0

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 [i](#)

There are no such residues in this entry.