



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 12, 2024 – 05:57 AM EDT

PDB ID : 2OGM
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 : 4.02b-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

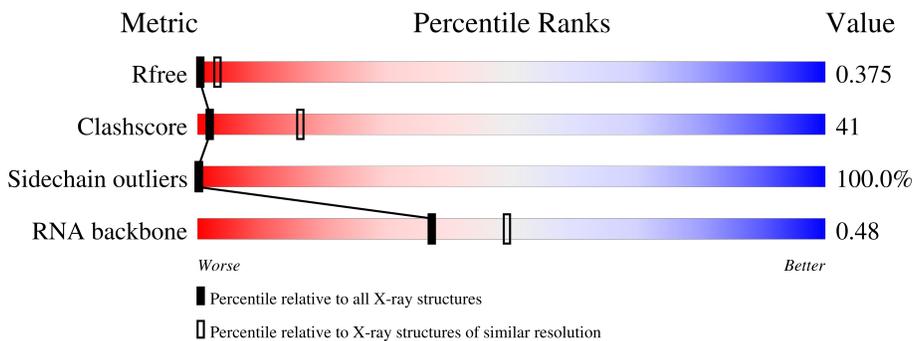
1 Overall quality at a glance i

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}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RNA backbone	3102	1002 (4.00-3.00)

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	
2	B	211	

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.

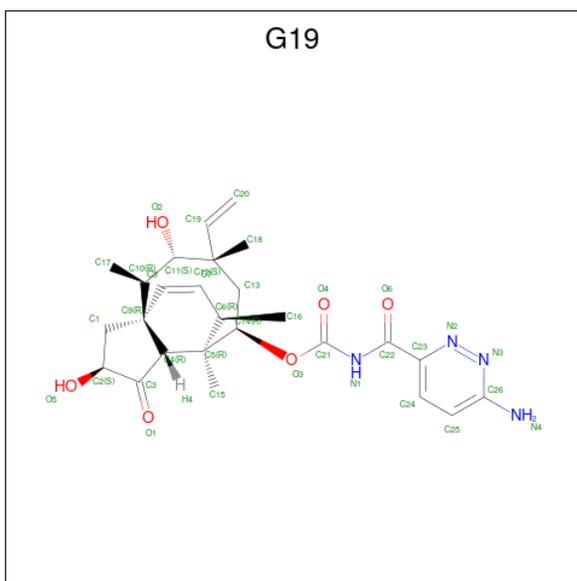
- Molecule 1 is a RNA chain called 23S ribosomal RNA.

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

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

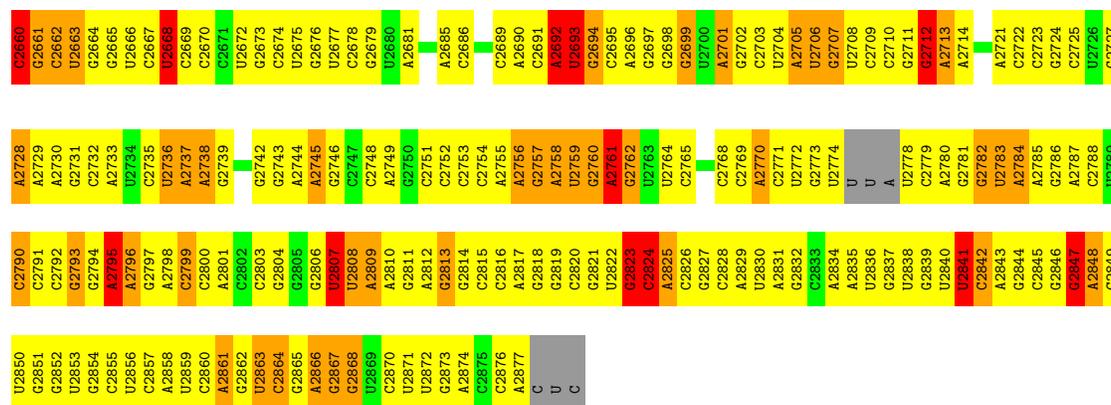
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	205	215	210	4	1	0	0	204

- Molecule 3 is (2S,3AR,4R,5S,6S,8R,9R,9AR,10R)-2,5-DIHYDROXY-4,6,9,10-TETRAMETHYL-1-OXO-6-VINYLDCAHYDRO-3A,9-PROP[1]ENOCYCLOPENTA[8]ANNULEN-8-YL [(6-AMINOPYRIDAZIN-3-YL)CARBONYL]CARBAMATE (three-letter code: G19) (formula: C₂₆H₃₄N₄O₆).



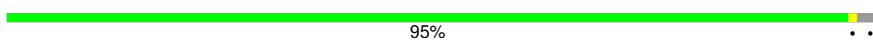
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	0	1	36	26	4	6	0	0

A1632	C1641	G1571	G1504	C1375	G1308	C1236	G1173	U108	A1039	U978	C	A842	G776	C710
A1633	G1642	C1572	U1505	G1380	G1309	G1236	G1174	U109	A1040	U979	A911	G843	A777	C711
A1634	G1643	G1573	C1506	G1381	C1310	G1237	A1175	G1109	G1041	G980	A912	G844	A778	A712
G1635	A1644	A1507	G1381	A1507	C1311	A1238	U1176	C1111	G1042	C981	A913	G845	G779	G713
G1636	G1645	C1575	G1508	G1382	G1312	A1239	U1177	C1112	A1043	C982	C914	A846	U780	G714
U1637	A1646	G1576	U1313	G1383	U1313	A1240	C1178	C1113	U1044	C983	C915	C847	G781	U715
C1641	G1647	G1577	A1314	G1448	A1314	G1241	A1179	G1117	G1045	A984	A918	A848	U785	U716
G1642	U1647	U1578	A1315	G1449	A1315	A1242	A1180	G1118	U1046	G986	U919	U786	U786	A718
A1643	C1648	C1579	G1316	G1387	A1316	A1243	C1181	U1119	C1052	G987	G920	A787	A787	A719
G1644	U1648	G1580	G1322	G1390	G1322	G1249	U1182	C1120	G1053	G988	A921	G854	G788	A720
A1645	G1649	A1512	G1323	A1391	G1323	A1250	G1185	G1121	U1054	G989	A922	G855	G789	
G1646	U1649	C1581	U1324	U1392	U1324	G1251	C1186	A1122	A1055	A990	A923	G856	A790	U727
U1647	A1650	G1517	U1325	U1393	U1325	G1252	A1187	G1123	U1056	A991	C924	U857	G728	G728
C1648	U1651	C1518	U1326	G1393	U1326	C1252	A1188	G1124	A1057	A992	U925	G858	A729	A729
U1651	G1652	C1522	C1327	A1397	C1327	C1253	G1189	G1125	A1058	C993	G926	U859	G794	G794
G1652	A1653	A1592	U1328	U1398	U1328	G1254	C1190	G1126	A1059	A993	G927	U860	A795	G732
C1653	A1654	C1524	U1329	G1399	U1329	G1255	G1191	A1127	U1060	A994	G928	U861	A796	G733
A1654	U1655	U1527	G1330	A1400	U1330	U1257	C1192	G1128	A1061	A995	A929	G862	A797	G734
C1655	G1656	G1527	G1331	A1401	G1331	G1258	G1193	A1129	G1062	C996	A930	C863	G798	G735
U1656	U1657	C1528	G1332	A1402	G1332	A1259	U1194	U1137	A1063	C998	G931	C864	G799	G736
G1657	A1658	U1529	U1333	G1403	U1333	A1260	U1195	A1138	C1064	A999	G932	U865	U800	U800
A1658	U1659	C1530	A1334	U1403	A1334	G1261	G1196	C1133	A1065	A999	G932	U866	A801	G738
G1659	U1660	U1531	U1335	C1404	U1335	U1262	U1197	G1135	G1066	A1001	A936	U867	A802	G739
G1660	U1661	C1531	G1336	A1405	U1336	G1263	C1198	A1136	G1067	C1002	G937	C803	A740	A740
A1661	U1662	A1532	U1337	A1406	U1337	C1264	U1199	A1137	A1068	C1003	G938	U871	C804	G741
U1662	G1663	G1533	G1338	A1407	U1338	G1265	G1200	A1138	G1069	A1004	G939	G872	G805	G742
A1663	U1664	C1534	U1339	A1408	U1339	G1266	A1201	C1145	C1070	U1005	G940	U873	A806	A743
G1664	U1665	G1535	G1340	U1409	U1340	A1267	U1202	G1146	U1071	C1006	G941	U874	A807	C744
U1665	U1666	C1536	C1341	U1410	G1341	U1268	A1203	A1140	U1072	U1019	G942	G875	C745	G745
A1666	U1667	U1537	U1342	U1411	U1342	G1269	G1204	G1142	G1073	C1008	G943	G876	C809	G746
G1667	U1668	C1538	U1343	C1411	U1343	G1270	G1205	A1143	G1074	C1009	G944	G877	U810	A747
U1668	U1669	G1539	C1344	G1414	U1344	G1271	A1208	U1144	C1075	U1010	G945	C878	A748	A748
A1669	U1670	C1540	G1345	C1415	U1345	G1272	U1209	G1145	U1076	A1011	G946	C879	A812	G750
U1670	U1671	G1541	C1346	A1416	U1346	C1273	A1208	C1146	U1077	A1012	G947	C880	A813	C751
A1671	U1672	G1542	C1347	C1417	U1347	G1274	C1210	G1147	A1078	G1013	C948	U886	G814	G752
U1672	U1673	U1543	G1348	C1418	U1348	G1277	G1211	G1148	G1079	G1014	A852	U887	A815	U753
C1673	U1674	C1544	A1349	G1419	U1349	A1278	U1212	G1149	A1080	U1015	A853	G888	U816	U754
U1674	U1675	G1545	G1350	A1420	U1350	G1279	U1213	C1150	A1081	C1016	G953	G889	A817	G755
C1675	U1676	C1546	C1351	A1421	U1351	U1280	C1214	U1151	G1082	C1017	G954	U890	C818	C756
U1676	U1677	G1547	G1352	C1422	U1352	A1281	A1215	C1152	C1083	C1018	G955	U891	U820	U757
U1677	U1678	C1548	A1353	A1423	U1353	A1282	G1216	A1153	C1086	U1019	A956	U892	A821	G758
U1678	U1679	U1549	A1354	U1424	U1354	G1283	U1217	G1154	C1087	A1020	G957	G	G	C759
U1679	U1680	G1550	A1355	G1425	U1355	G1284	C1218	A1155	U1087	A1021	G958	G	G	U760
U1680	U1681	C1552	G1356	U1426	U1356	A1285	C1219	G1156	A1088	A1022	C959	G	G	U761
A1681	U1682	U1553	U1357	U1427	U1357	U1286	G1220	A1158	C1089	U1023	U960	G	G	A762
G1682	U1683	G1554	C1358	G1428	U1358	A1287	C1221	U1159	G1090	G1024	G	C	C	A763
U1683	U1684	C1555	G1359	A1429	U1359	U1288	G1222	C1160	C1091	A1025	G	C	C	A764
G1684	U1685	U1556	G1360	G1430	U1360	A1289	G1223	U1161	U1092	U1026	G	C	C	C765
A1685	U1686	C1558	G1361	G1431	U1361	G1290	A1224	A1162	G1098	C1029	G	U	A	A766
C1687	U1687	G1559	A1362	U1434	U1362	A1291	G1225	C1163	G1098	C1030	C968	A	A	A766
U1688	U1689	C1560	C1363	U1435	U1363	A1292	A1226	C1164	A1099	U1030	C969	C	C	G767
U1689	U1690	G1562	C1364	G1436	U1364	A1300	A1227	G1165	G1100	C1031	U969	C	C	U768
U1690	U1691	U1563	U1365	U1437	U1365	U1301	G1228	A1166	U1101	A1032	A970	C	C	C769
C1692	U1692	C1564	U1366	G1438	U1366	C1302	C1229	A1167	G1102	G1033	A971	A	A	U770
A1693	U1693	U1565	U1370	U1439	U1370	U1303	C1230	A1168	G1103	C972	G972	C	C	C771
U1694	U1695	C1567	G1371	G1440	U1371	U1304	C1231	G1169	G1104	G1034	U974	U	U	G772
U1695	U1696	U1568	A1372	U1441	U1372	U1305	U1232	C1171	U1105	U1035	G975	U	U	A773
C1696	U1697	C1570	G1374	C1442	U1374	U1307	C1234	U1172	A1106	U1037	G976	A	A	U774
									A1107	U1038	G977	C	C	U775



- Molecule 2: 50S ribosomal protein L3

Chain B:



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 29.92 – 3.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (29.93-3.50) 92.8 (29.92-3.50)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 3.47Å)	Xtrriage
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	Xtrriage
Anisotropy	0.807	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.19 , 82.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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 i

5.1 Standard geometry i

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	0.61	6/66467 (0.0%)	0.82	100/103673 (0.1%)
2	B	0.11	0/10	0.42	0/11
All	All	0.61	6/66477 (0.0%)	0.82	100/103684 (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	121

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	700	C	N1-C2	9.14	1.49	1.40
1	0	788	G	N9-C4	7.37	1.43	1.38
1	0	1664	G	N9-C4	-5.84	1.33	1.38
1	0	1681	A	C5-C6	-5.47	1.36	1.41
1	0	2799	C	N1-C2	-5.33	1.34	1.40

The worst 5 of 100 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	985	G	N9-C1'-C2'	11.62	129.11	114.00
1	0	460	U	N1-C1'-C2'	10.14	127.18	114.00
1	0	1264	C	N1-C1'-C2'	10.06	127.08	114.00
1	0	788	G	N9-C1'-C2'	10.03	127.04	114.00
1	0	984	A	N9-C1'-C2'	9.21	125.98	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
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	3642	0
2	B	215	0	12	5	0
3	0	36	0	34	2	0
All	All	59610	0	29963	3646	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 3646 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%)	0	1 (100%)	0 0

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	144	ARG

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%)	618 (22%)	184 (6%)

5 of 618 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 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	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 Torsion 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
3	0	2881	G19	C9-C10-C11	4.71	116.85	112.46

There are no chirality outliers.

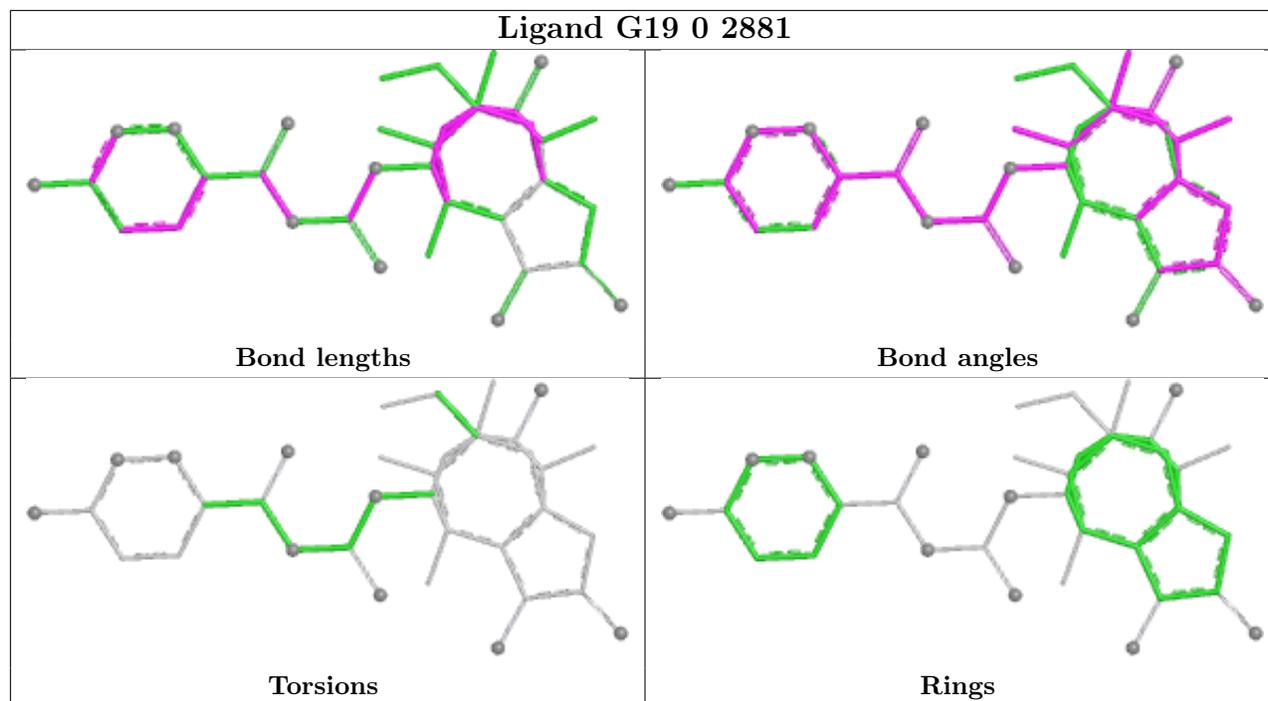
There are no torsion outliers.

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](#)

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

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

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

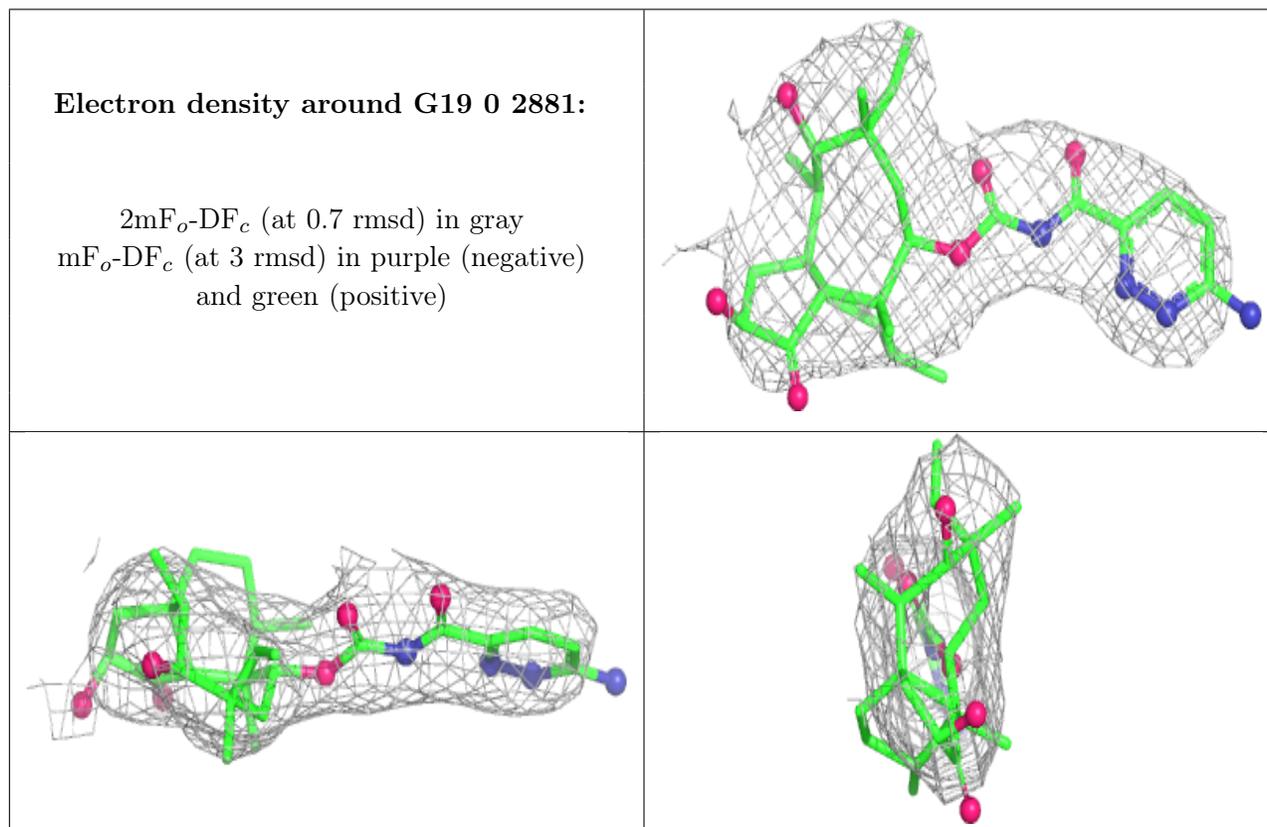
6.3 Carbohydrates [i](#)

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

6.4 Ligands [i](#)

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.