



wwPDB X-ray Structure Validation Summary Report ⓘ

May 15, 2020 – 04:18 pm BST

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

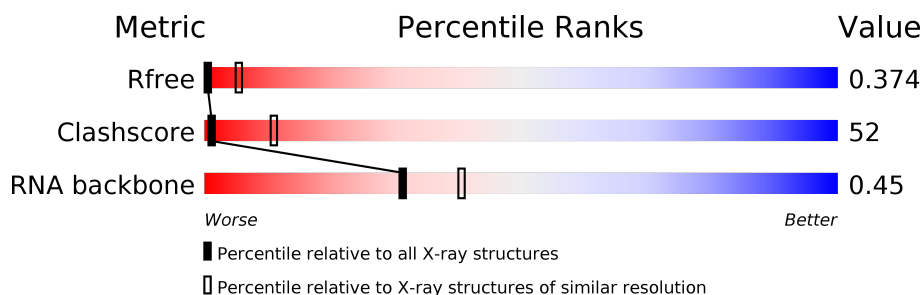
1 Overall quality at a glance

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}	130704	1557 (3.82-3.50)
Clashscore	141614	1037 (3.80-3.52)
RNA backbone	3102	1024 (4.30-3.00)

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 on 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 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.

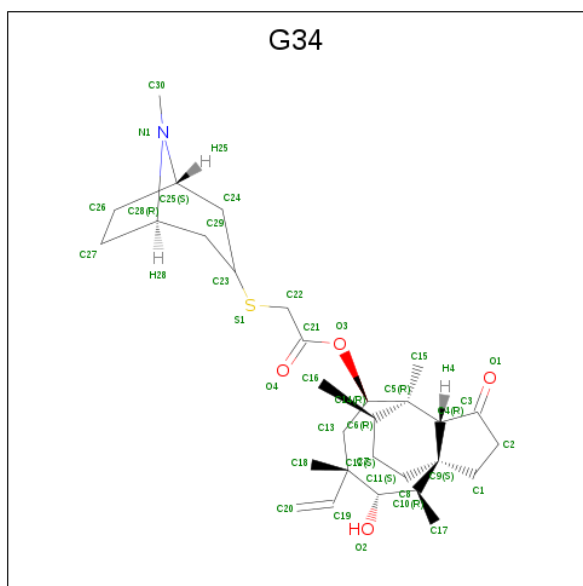
- Molecule 1 is a RNA chain called 23S ribosomal RNA.

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-EXO)-8-METHYL-8-AZABICYCLO[3.2.1]OCT-3-YL]THIO}ACETATE (three-letter code: G34) (formula: C₃₀H₄₇NO₄S).

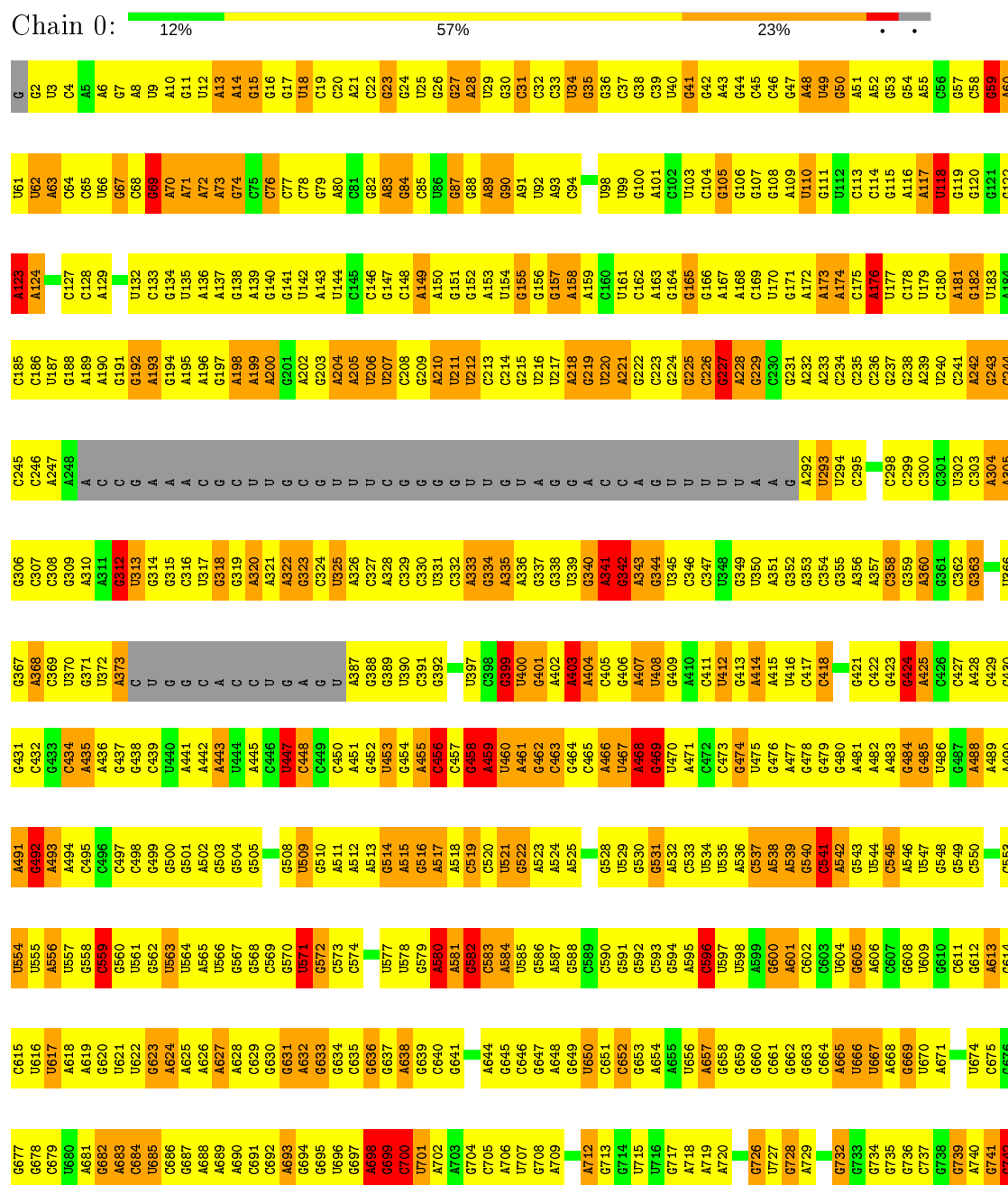


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	0	1	Total	C	N	O	S	0	0
			36	30	1	4	1		

3 Residue-property plots

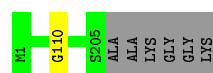
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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



U1676	C1616	U1551	C1491	A1429	U1365	C1305	U1244	C1183	U1119	G1058	A994	A929	A865	G805	A743
G1677	G1617	C1552	A1492	G1430	A1366	U1306	G1246	G1184	C1120	A1059	A995	A930	U866	A806	C744
G1678	G1618	C1553	A1493	U1431	A1367	U1307	G1247	C1185	G1121	C996	C997	G931	U868	A807	C746
U1679	G1620	G1554	G1494	G1432	G1368	C1308	U1248	A1186	A1122	A1061	C998	G932	U869	C808	
U1680	C1621	A1555	G1495	A1433		C1309	G1249	A1187	U1124	G1063	C999	G933	C869	C809	
A1681	C1622	G1559	G1496	U1434	G1371	C1310	A1249	A1188		G1064	A999	G934	C870	U810	C750
A1682	C1623	G1560	C1497	G1435	A1372	C1311	A1250	C1189	G1128	C1065	G1000	C935	U871	G811	C751
G1683	A1624	A1561	G1498	G1436	G1373	G1312	G1251	C1190		A1066	A1001	A936	G872	G812	C752
G1684	C1625	U1562	A1499	A1437	G1374	U1313	C1252	G1191	A1129	G1066	C1002	C937	U873	U753	
A1685	A1626	G1563	U1500	G1438	C1375	A1314	C1253	A1192	U1130	G1067	C1003	A874	C874	G814	
A1686	C1627	U1564	C1501	G1439	C1376	A1315	G1254	A1193	G1131	A1068	A1004	C939	G875	A815	C755
C1687	G1628	U1564	G1502	G1440	G1377	C1316	A1255	U1194	C1132	G1069	U1005	A876	G876	U816	C756
C1688	C1629	G1565	G1503	A1441	A1378	G1317	C1256	U1195	C1133	G1070	C1006	U941	G877	U757	
U1689		G1566	G1504	C1442	A1379	A1318	U1257	G1196	C1134	U1071	A1007	U942	C878	G818	C758
U1690	A1630		U1505	G1443	C1380	C1319	G1258	U1197	C1135	U1072	G1008	U943	A879	C819	C759
G1691	C1631	G1571	C1506	G1444	G1381	A1320	A1259	C1198	G1136	U1073	A879	A944	C880	U760	
C1692	A1632	C1572	A1507	U1445	G1382	U1326	A1260	U1199	A1137	G1074	U1010	G945	U881	G761	
G1693	C1633	G1573	G1508	A1446	C1383	C1327	G1261	G1200	A1138	C1075	A1011	U946	C882	A821	
A1694	A1634	A1574	A1509	U1447	G1384	G1323	U1262	G1201	A1139	U1076	C1012	C947	A883	U823	
U1695	G1635	G1575	A1510	A1448	C1385	G1324	G1263	U1202	A1140		G1013	C948	C884	A763	
C1696		G1576	A1511	C1449	A1386	U1325	C1264	U1203	A1141	G1079	G1014		A885	U824	
U1697	U1636		U1508	G1450	G1387	G1326	G1265	G1204	A1142	A1080	U766	A886	A886	C825	
C1698	G1637	U1577	A1512	C1451		C1327	G1266	G1205	A1143	A1081	C1016	U954	U887	G767	
U1699	U1638	G1578	U1513	U1452	A1391	C1328	A1267	U1144	U1144	C1082	C1017	C859	U889	U768	
A1699	C1639	G1579	C1514	A1453	U1392	U1329	U1268	G1145	G1146	C1083	C1018	G955	U890	C829	
C1700	C1640	C1580	U1515	U1454	U1392	G1330	G1269	G1147		A1084	U1019	A956	A891	C830	
C1701	C1641	C1581	A1516	U1454		G1331	G1270	G1148		C1085	A1020	G957	G	G831	
C1702	G1642	A1582	C1518	C1455	G1393	C1332	C1271	A1149		C1086	A1021	G958	G	C827	
C1703	A1644	G1583	G1519	A1458	G1394	G1333	G1272	C1150		C1087	A1022	C959	G	A833	
G1704	U1645	A1584	G1520	U1459	C1395	U1334	G1273	U1213		A1088	U1023		G	A834	
U1705	U1646	U1585	U1521	G1460	A1397	A1335	C1274	C1214		C1089	G1024	G962	G	U775	
A1706		A1586	U1522		G1398	G1336	A1275	A1215		A1092	A1025	G963	C	G776	
A1707	U1647	U1587	C1523	A1463	C1399	G1337		G1216		C1091	U1026	A964	C	U837	
C1708	A1648	A1588	A1524	A1464	A1400	G1338	A1278	G1217	A1153	U1093	C1027	G965	U	G778	
U1709	U1649	G1589	C1525	G1465	G1401	U1339	G1279	C1218	A1154	U1094			A	U779	
C1710	A1650	C1590	A1526	A1466	C1402	C1340	U1280	G1219	U1156	A1095			C	U840	
G1711	G1651	U1591	U1527	C1467	U1403	G1341	A1281	G1220		A1097	A1033	U969	C	G841	
G1712	G1652	U1592	G1528	U1467	C1404		A1282	C1221		A1098	U1034	A970	A	U782	
G1713	C1653	C1593	C1529	A1468		U1342	C1283	G1222	U1161	C1097	G1035	C972	G	G843	
A1714	A1654	U1594	U1530	U1469	A1405	C1343	G1284	G1223	A1162	G1098	C1036	A971	C	G844	
A1715	C1655	A1595	A1531	G1470	G1406	G1344	G1285	C1224	C1163	A1099	U1037	C973	C	U784	
G1716	U1656	A1596	C1532	G1471	A1407	G1345	A1286	G1225	C1164	G1100	U1038	U974	U	U845	
A1717	A1657	A1597	A1533	C1472	A1408	C1346	U1287	G1226	G1165	U1101	A1039	G975	A	U846	
A1718	A1658	C1598	G1533	U1473	U1409	C1347	A1287	A1227	A1166	G1102	C1040	C976	C	C847	
G1719	G1659	U1599	A1534	A1474	U1410	C1348	A1288	C1227		C1103	U1041	G977	C	A848	
	G1660	U1600	C1535	U1475	C1411	A1349	A1289	G1228	A1167	U1099	U1042	A911	C	G849	
U1723	C1661	U1601	G1536	G1476	C1412	G1350	A1290	C1229	G1168	G1104	A1043	A912		C850	
C1724	G1662	G1602	U1537	C1477		G1351	G1291	G1230	U1169	U1105	U1044	G980		G791	
C1725	C1663	A1603	A1538	U1478	A1406	G1352	A1292	A1231	U1170	A1106	U1045			U792	
	G1664	A1604	U1539	G1479	A1416	A1353	A1293	U1232	A1171	G1045	C981	U917		G793	
C1729	C1665	A1605	C1540	U1480	C1417	A1354	G1294	A1233	U1172	U1046	C982	U918		A794	
G1730	G1666	C1606	G1541	U1481	C1418	A1355	U1295	C1234	G1173	U1047	G983	U919		A795	
C1731	A1667	A1607	G1542	U1482	G1419	C1356	G1296	C1235		U1048	A984	G920		A796	
C1732	G1668	U1608	G1543	G1483	A1420	U1357	A1297	G1236	C1111	U1051	A985	A921		A797	
U1733	A1669	G1609	A1544	C1484	U1421	C1358	G1298	G1237	U1176	U1112	A986	A922		G798	
	G1670	A1610	G1545	U1485	C1422	G1359	A1299	A1238	U1177	C1113	C1052	G987		C799	
	A1671	C1610	C1546	U1486	A1423	G1360	A1298	A1239	C1178	A1114	G1053	A923		U859	
C1736	C1671	U1611	C1547	A1487	U1424	G1361	U1301	G1240	A1179	C1115	C1054	U925		U860	
G1737	A1672	U1612	U1547	C1487		A1362	C1302	G1241		U1116	A1055	A981		G861	
U1738	C1673	G1613	U1548	G1488		C1363	U1303	A1242	C1181		C927	C926		A862	
G1739	C1674	C1614	C1549	C1489		G1427		G1117	U1056		A1057	C933		C863	
G1740	C1675	C1615	C1550	U1490	G1428	C1364	U1304	G1243	U1182	G1118				C864	





4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 3.65Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.260 , 0.334 0.354 , 0.374	Depositor DCC
R_{free} test set	12167 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	135.2	Xtriage
Anisotropy	0.524	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.18 , 80.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	59577	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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: 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	-	40,40,40	2.53	11 (27%)	58,64,64	2.34	17 (29%)

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	G34	0	0	-	-	0/12/94/94	0/6/5/5

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	0	0	G34	C12-C11	7.56	1.62	1.55
3	0	0	G34	C5-C14	7.35	1.61	1.56
3	0	0	G34	C5-C6	4.96	1.64	1.56
3	0	0	G34	C10-C11	3.81	1.59	1.56
3	0	0	G34	O3-C14	3.34	1.52	1.46

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	0	0	G34	C18-C12-C11	8.93	113.28	108.06
3	0	0	G34	C4-C5-C6	-6.40	100.51	106.61
3	0	0	G34	O3-C21-C22	5.88	120.23	110.32
3	0	0	G34	C16-C6-C7	-3.81	104.63	110.37
3	0	0	G34	C9-C4-C3	-3.70	97.67	101.79

There are no chirality outliers.

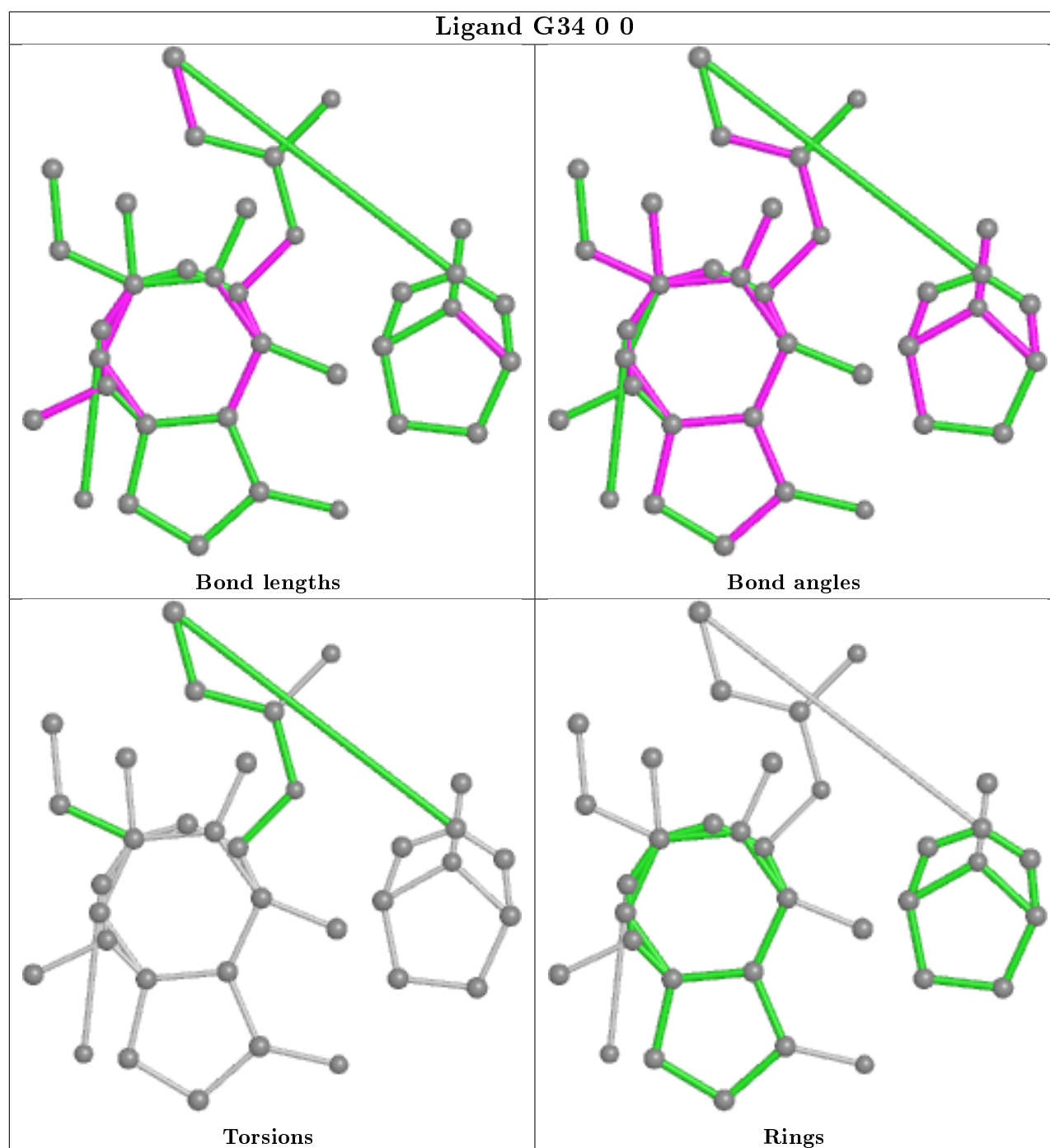
There are no torsion outliers.

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

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 ⓘ

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.

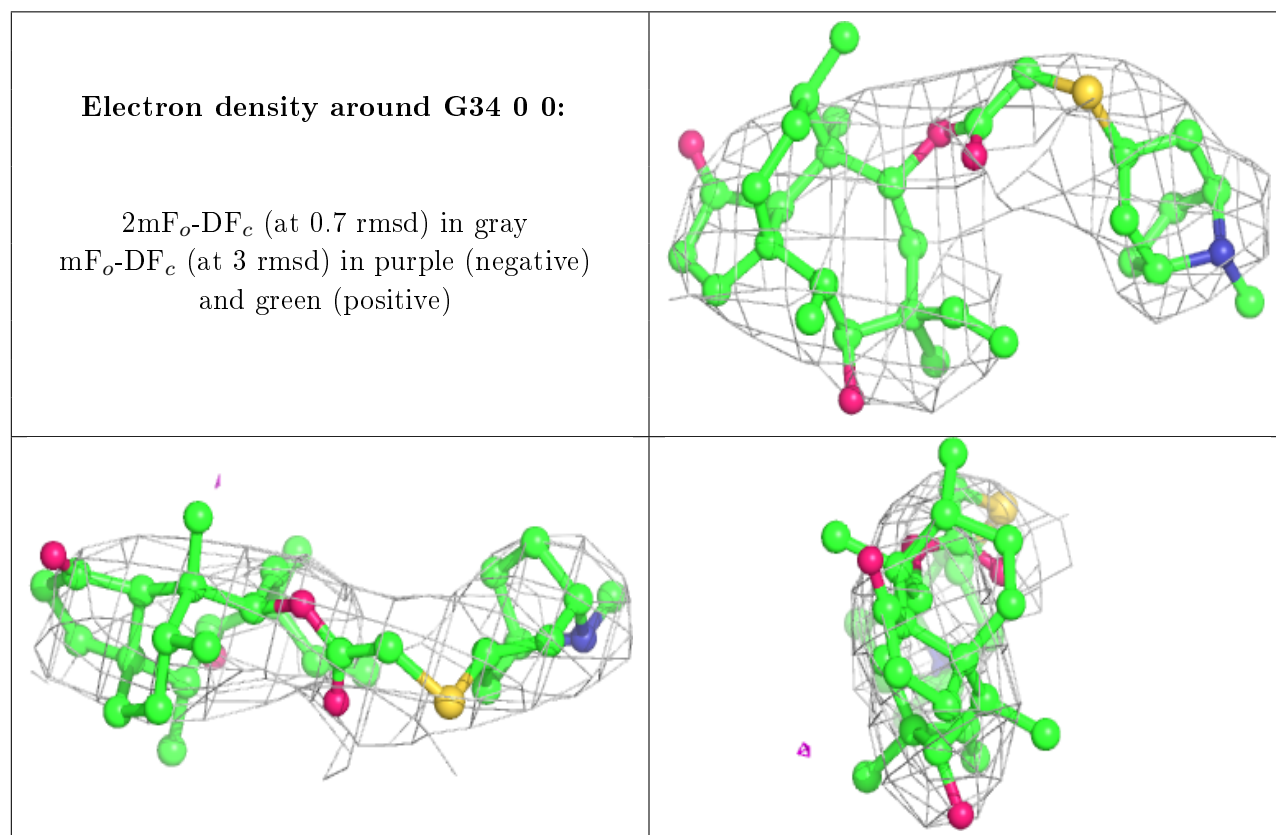
6.3 Carbohydrates ⓘ

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.