



wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 16, 2023 – 01:45 PM EST

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 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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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

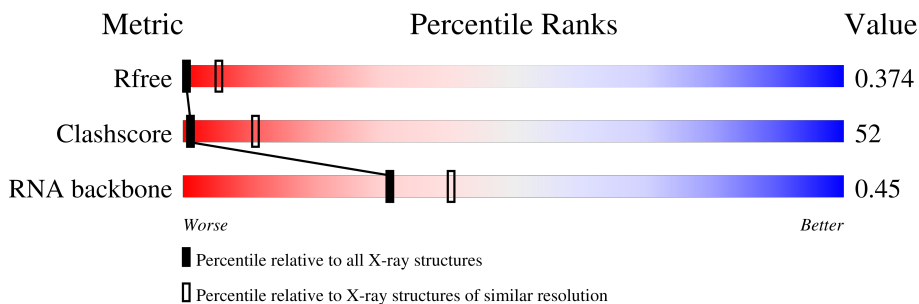
1 Overall quality at a glance

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 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	 12% 57% 22% . .
2	B	211	 97% .

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.

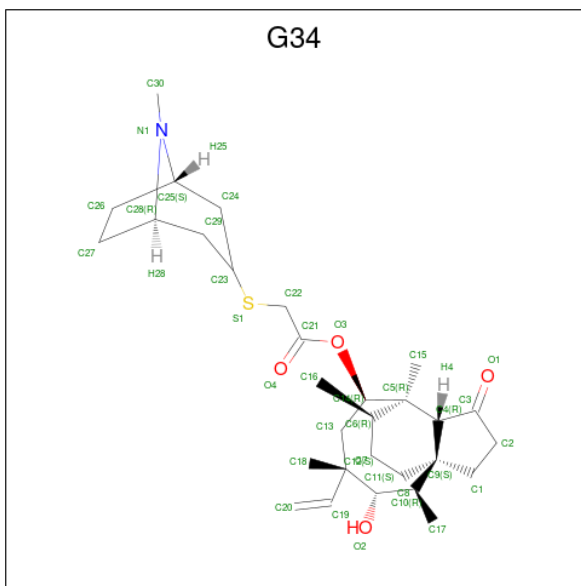
- Molecule 1 is a RNA chain called 23S ribosomal RNA.

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

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

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

- Molecule 3 is Retapamulin (three-letter code: G34) (formula: C₃₀H₄₇NO₄S).

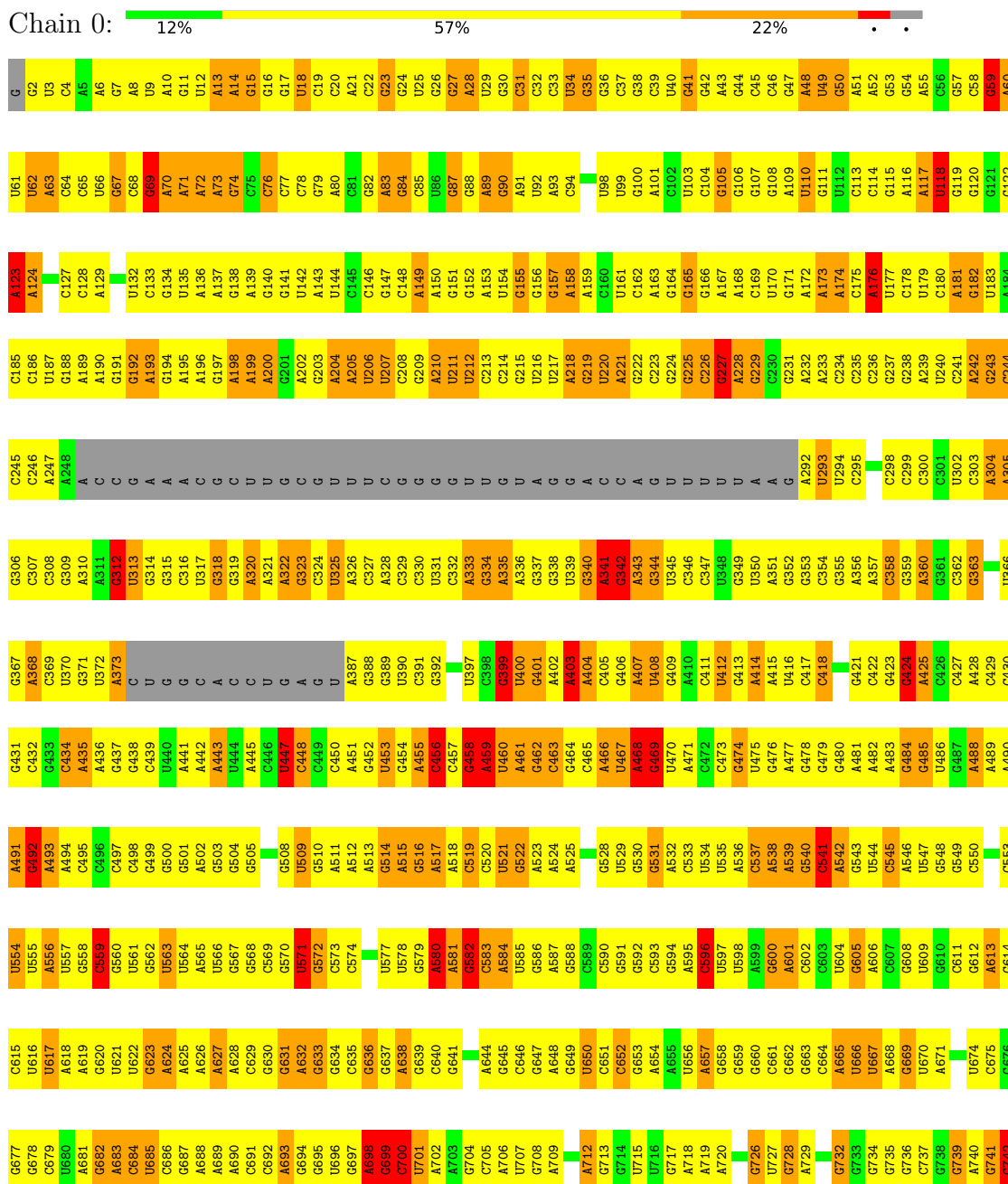


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
3	0	1	36	30	1	4	1	0	0

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



U1676	C1677	C1678	U1679	C1680	C1681	C1682	C1683	C1684	C1685	C1686	C1687	C1688	C1689	C1690	C1691	C1692	C1693	C1694	C1695	C1696	C1697	C1698	C1699	C1700	C1701	C1702	C1703	C1704	C1705	C1706	C1707	C1708	C1709	C1710	C1711	C1712	C1713	C1714	C1715	C1716	C1717	C1718	C1719	C1720	C1721	C1722	C1723	C1724	C1725	C1726	C1727	C1728	C1729	C1730	C1731	C1732	C1733	C1734	C1735	C1736	C1737	C1738	C1739	C1740																																																																							
U1429	U1430	U1431	U1432	U1433	U1434	U1435	U1436	U1437	U1438	U1439	U1440	U1441	U1442	U1443	U1444	U1445	U1446	U1447	U1448	U1449	U1450	U1451	U1452	U1453	U1454	U1455	U1456	U1457	U1458	U1459	U1460	U1461	U1462	U1463	U1464	U1465	U1466	U1467	U1468	U1469	U1470	U1471	U1472	U1473	U1474	U1475	U1476	U1477	U1478	U1479	U1480	U1481	U1482	U1483	U1484	U1485	U1486	U1487	U1488	U1489	U1490																																																																										
U1365	U1366	U1367	U1368	U1369	U1370	U1371	U1372	U1373	U1374	U1375	U1376	U1377	U1378	U1379	U1380	U1381	U1382	U1383	U1384	U1385	U1386	U1387	U1388	U1389	U1390	U1391	U1392	U1393	U1394	U1395	U1396	U1397	U1398	U1399	U1400	U1401	U1402	U1403	U1404	U1405	U1406	U1407	U1408	U1409	U1410	U1411	U1412	U1413	U1414	U1415	U1416	U1417	U1418	U1419	U1420	U1421	U1422	U1423	U1424	U1425	U1426	U1427	U1428	U1429																																																																							
U1305	U1306	U1307	U1308	U1309	U1310	U1311	U1312	U1313	U1314	U1315	U1316	U1317	U1318	U1319	U1320	U1321	U1322	U1323	U1324	U1325	U1326	U1327	U1328	U1329	U1330	U1331	U1332	U1333	U1334	U1335	U1336	U1337	U1338	U1339	U1340	U1341	U1342	U1343	U1344	U1345	U1346	U1347	U1348	U1349	U1350	U1351	U1352	U1353	U1354	U1355	U1356	U1357	U1358	U1359	U1360	U1361	U1362	U1363	U1364																																																																												
U1244	U1245	U1246	U1247	U1248	U1249	U1250	U1251	U1252	U1253	U1254	U1255	U1256	U1257	U1258	U1259	U1260	U1261	U1262	U1263	U1264	U1265	U1266	U1267	U1268	U1269	U1270	U1271	U1272	U1273	U1274	U1275	U1276	U1277	U1278	U1279	U1280	U1281	U1282	U1283	U1284	U1285	U1286	U1287	U1288	U1289	U1290	U1291	U1292	U1293	U1294	U1295	U1296	U1297	U1298	U1299	U1300	U1301	U1302	U1303	U1304																																																																											
C1183	C1184	C1185	C1186	C1187	C1188	C1189	C1190	C1191	C1192	C1193	C1194	C1195	C1196	C1197	C1198	C1199	C1200	C1201	C1202	C1203	C1204	C1205	C1206	C1207	C1208	C1209	C1210	C1211	C1212	C1213	C1214	C1215	C1216	C1217	C1218	C1219	C1220	C1221	C1222	C1223	C1224	C1225	C1226	C1227	C1228	C1229	C1230	C1231	C1232	C1233	C1234	C1235	C1236	C1237	C1238	C1239	C1240	C1241	C1242	C1243																																																																											
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A885	A886	A887	A888	A889	A890	A891	A892	A893	A894	A895	A896	A897	A898	A899	A900	A901	A902	A903	A904	A905	A906	A907	A908	A909	A910	A911	A912	A913	A914	A915	A916	A917	A918	A919	A920	A921	A922	A923	A924	A925	A926	A927	A928	A929	A930	A931	A932	A933	A934	A935	A936	A937	A938	A939	A940	A941	A942	A943	A944	A945	A946	A947	A948	A949	A950	A951	A952	A953	A954	A955	A956	A957	A958	A959	A960	A961	A962	A963	A964	A965	A966	A967	A968	A969	A970	A971	A972	A973	A974	A975	A976	A977	A978	A979	A980	A981	A982	A983	A984	A985	A986	A987	A988	A989	A990	A991	A992	A993	A994	A995	A996	A997	A998	A999	A1000																				
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A743	C744	C745	C746	C747	C748	C749	C750	C751	C752	C753	C754	C755	C756	C757	C758	C759	C760	C761	C762	C763	C764	C765	C766	C767	C768	C769	C770	C771	C772	C773	C774	C775	C776	C777	C778	C779	C780	C781	C782	C783	C784	C785	C786	C787	C788	C789	C790	C791	C792	C793	C794	C795	C796	C797	C798	C799	C800	C801	C802	C803	C804																																																																										

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G2570	G2515	G2454	U2387	C2322	C2259	U2196	U2074	A2014	A1883	U1819	A1759
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G2573	G2518	U2457	A2390	G2324	C2262	U2199	G2077	U2017	G1886	G1823	G1763
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G2579	G2524	U2465	A2397	A2331	G2268	G2205	G2083	C2023	A1895	C1829	U1769
G2580	U2525	G2466	U2398	G2332	C2269	C2206	G2084	U2024	A1896	U1770	U1770
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G2584	G2529	U2470	C2404	G2338	C2273	C2210	U2090	G2028	A1900	G1834	A1774
G2585	U2530	U2471	A2405	A2339	C2274	U2211	C2091	G2029	U1901	C1835	A1775
G2586	U2531	U2472	C2406	G2340	U2275	U2212	G2092	U2030	G1904	G1836	A1776
G2587	G2532	U2473	G2407	U2342	C2276	G2213	A	A2031	G1905	G1837	A1777
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G2592	G2537	U2478	A2412	C2347	C2282	A2220	G	G2036	U1909	U1844	A1782
G2593	G2538	G2479	A2413	C2347	G2283	G2221	A	A2037	A1910	C1845	G1783
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G2597	U2542	U2420	G2420	G2353	G2287	U2163	A	A2041	U1914	U1848	C1787
G2598	U2543	C2421	C2421	G2354	A2288	G2164	G2103	A2042	G1915	G1849	C1788
G2599	U2544	C2422	C2422	G2355	A2289	A2165	G2104	A2043	A1916	U1769	U1769
G2600	G2545	G2423	G2423	G2356	A2290	G2166	U2105	G2044	C1917	A1851	G1790
G2601	G2546	G2424	G2424	G2357	U2291	G2167	G2106	A2045	G1918	G1852	C1792
G2602	G2547	G2425	G2425	G2358	C2292	A2168	G2107	C2046	A1919	C1853	C1792
G2603	G2548	G2426	G2426	G2359	G2293	A2169	G2108	C2047	A1920	G1854	U1792
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G2607	G2552	U2492	A2429	G2363	U2297	G2174	C	U2051	U1990	G1857	C1797
G2608	G2553	U2493	U2430	G2364	U2298	A2175	U	G2052	G1992	A1859	G1798
G2609	G2554	C2494	G2431	G2365	U2299	U2176	C	G2053	G1993	A1860	A1799
G2610	G2555			U2365	A2299			A2054	U1994	G1861	A1800

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G2687	C2747	U2808	U2869
G2688	A2748	A2809	C2870
A2690	A2749	A2810	U2871
C2691	C2752	G2811	U2872
A2692	C2753	A2812	G2873
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G2694	A2755	G2814	C2875
C2695	A2756	C2815	A2876
A2696	G2757	C2816	C
G2697	A2758	G2819	U
G2698	U2759	C2820	C
G2699	G2760	G2821	
U2700	A2761	U2822	
A2701	G2762	G2823	
G2702	U2763	A2824	
C2703	U2764	A2825	
U2704	C2765	C2826	
A2705	U2766	G2827	
U2706	C2767	C2828	
G2707	C2768	A2829	
U2708	C2769	U2830	
C2709	A2770	A2831	
G2710	C2771	G2832	
G2711	U2772	C2833	
G2712	G2773	A2834	
A2713	U2774	A2835	
A2714	U	U2836	
C2715	U	G2837	
G2716	A	U2838	
G2717		G2839	
A2718		U2840	
U2719		U2841	
U2720		C2842	
A2721		A2843	
C2722		G2844	
C2723		C2845	
G2724		G2846	
U2725		G2847	
U2726		A2848	
G2727		C2849	
A2728		U2850	
A2729		G2851	
A2730		G2852	
G2731		U2853	
C2732		G2854	
U2733		C2855	
A2734		U2856	
U2735		C2857	
C2736		A2858	
A2737		U2859	
A2738		C2860	
G2739		A2861	
C2740		G2862	
G2741		U2863	
G2742		C2864	
G2743		G2865	
A2744		A2866	
A2745		G2867	

- Molecule 2: 50S ribosomal protein L3

Chain B:  97%

H1
G110
S205
ALA
ALA
LYS
GLY
GLY
LYS

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)	Xtrriage
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	Xtrriage
Anisotropy	0.524	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.18 , 80.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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	1777	A
1	0	2204	A
1	0	1913	G
1	0	2005	U
1	0	2299	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 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	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 Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	G34	0	0	-	-	0/12/94/94	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.

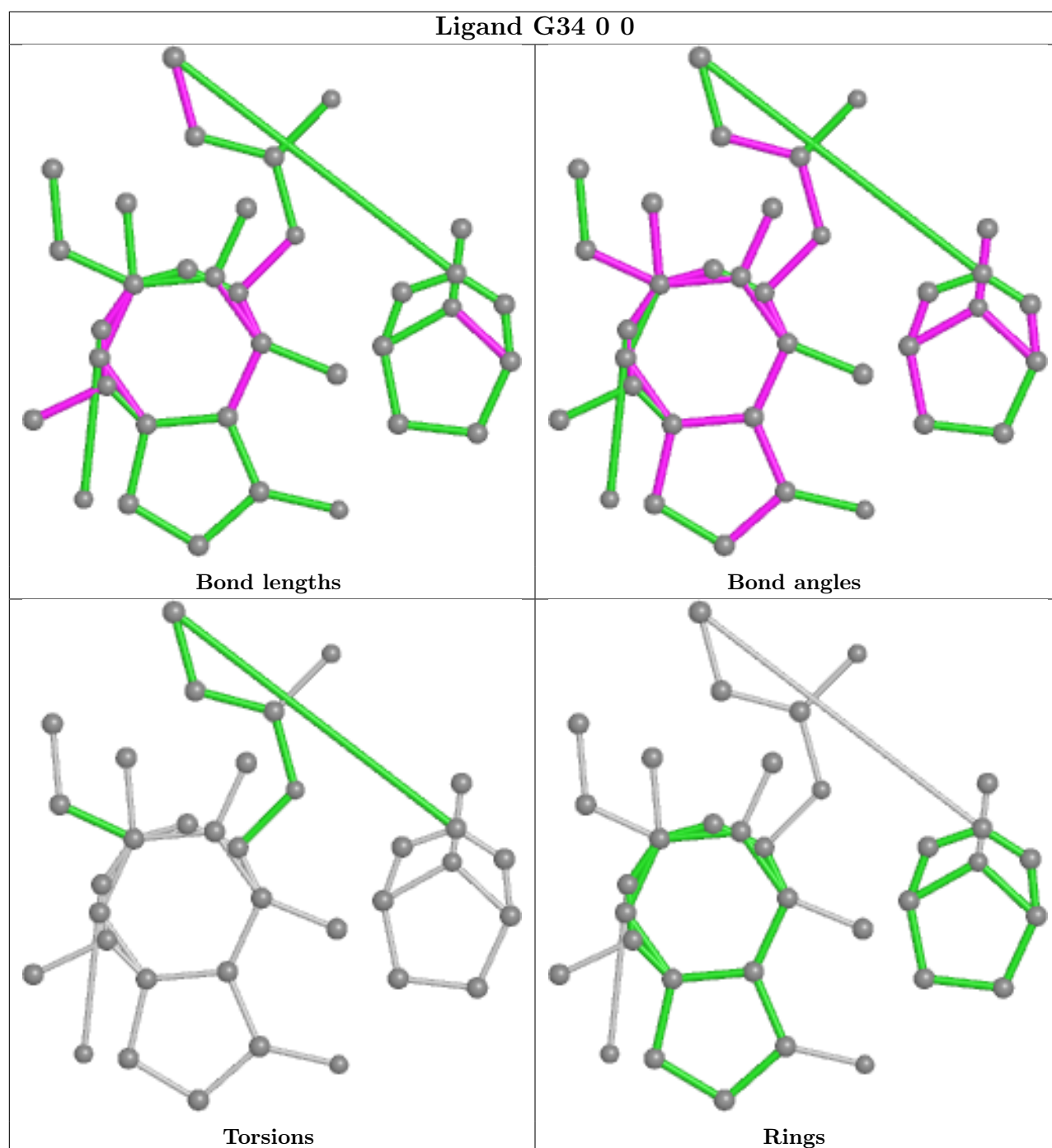
There are no torsion outliers.

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 [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.

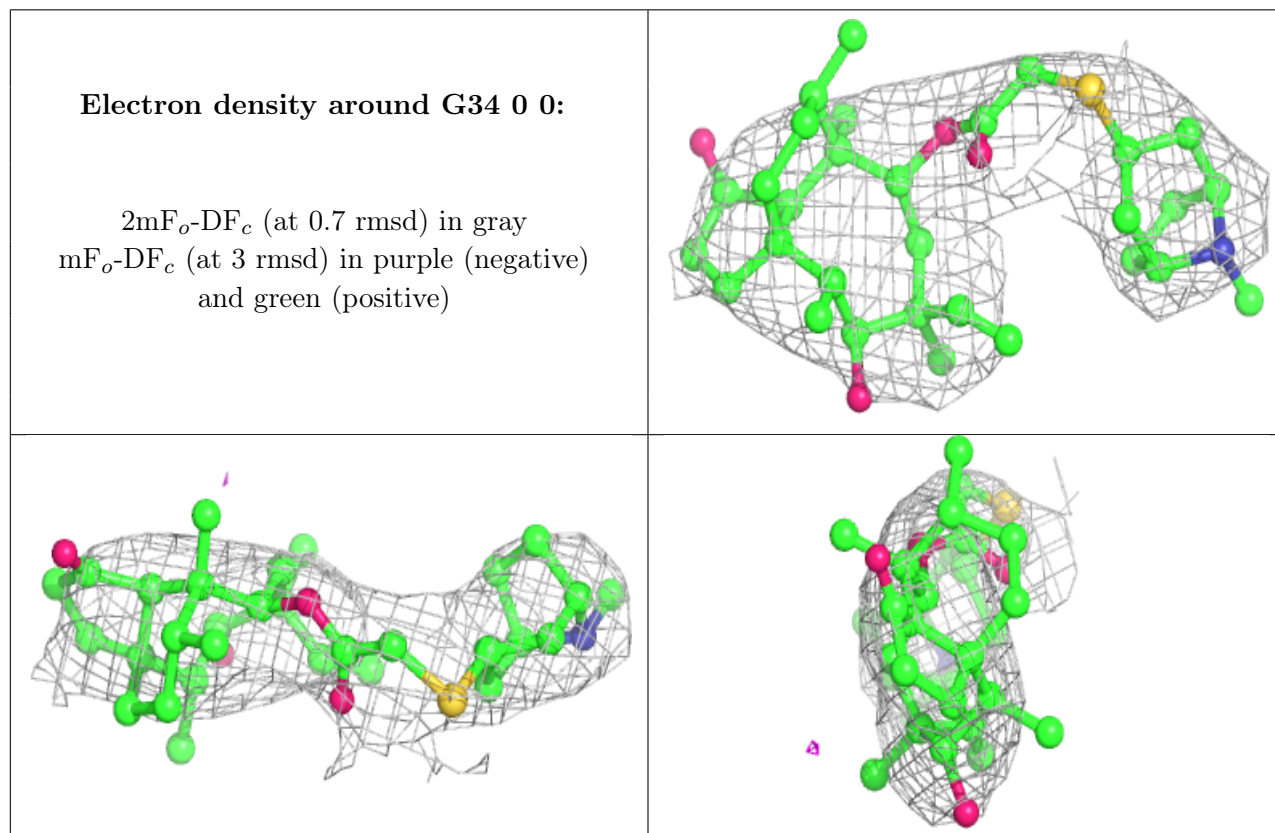
6.3 Carbohydrates [i](#)

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.