



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 25, 2026 – 09:06 AM EDT

PDB ID : 2OGN / pdb_00002ogn
Title : The crystal structure of the large ribosomal subunit from *Deinococcus radiodurans* complexed with the pleuromutilin derivative SB-280080
Authors : Davidovich, C.; Bashan, A.; Auerbach-Nevo, T.; Yonath, A.
Deposited on : 2007-01-07
Resolution : 3.56 Å (reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (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

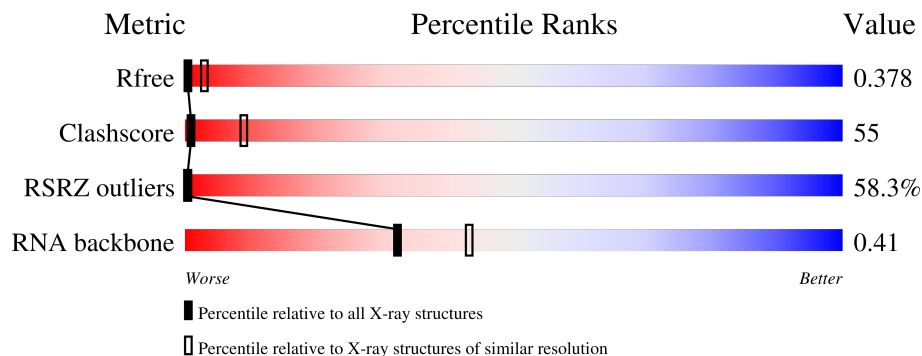
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.56 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1410 (3.62-3.50)
Clashscore	190562	1480 (3.62-3.50)
RSRZ outliers	180081	1409 (3.62-3.50)
RNA backbone	3983	1006 (4.02-3.06)

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	
2	B	211	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 59597 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

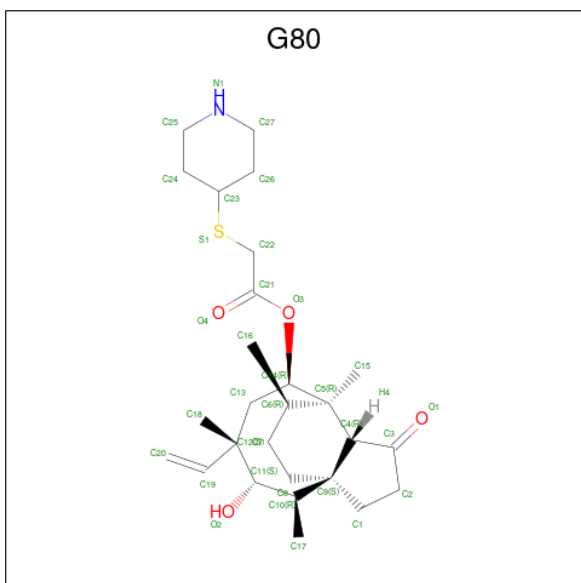
- Molecule 1 is a RNA chain called 23S ribosomal RNA.

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

- Molecule 3 is (3AS,4R,5S,6S,8R,9R,9AR,10R)-5-HYDROXY-4,6,9,10-TETRAMETHYL-1-OXO-6-VINYLDECAHYDRO-3A,9-PROPANOCYCLOPENTA[8]ANNULEN-8-YL (PIPERIDIN-4-YLTHIO)ACETATE (CCD ID: G80) (formula: C₂₇H₄₃NO₄S).

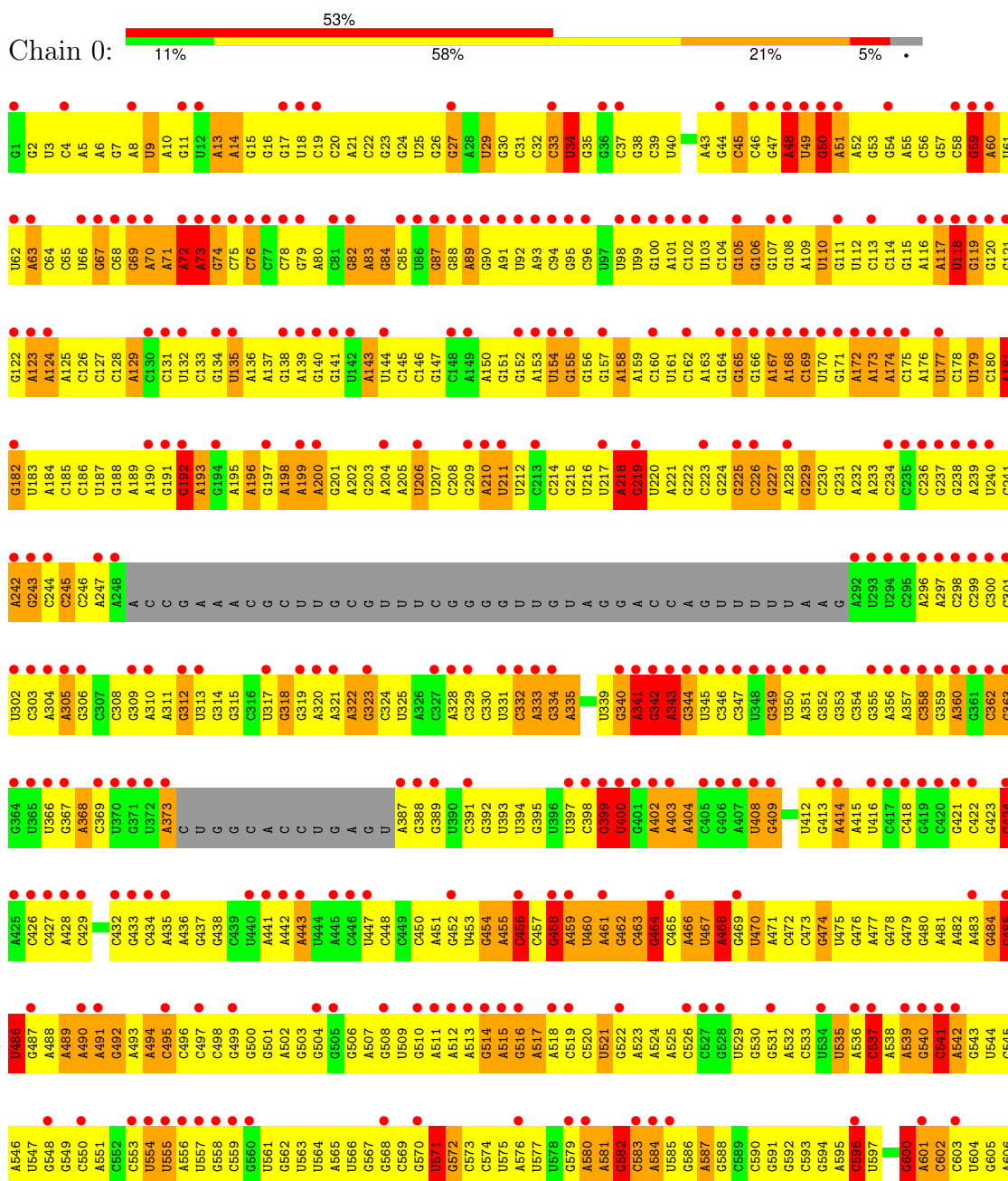


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
3	0	1	33	27	1	4	1	0	0

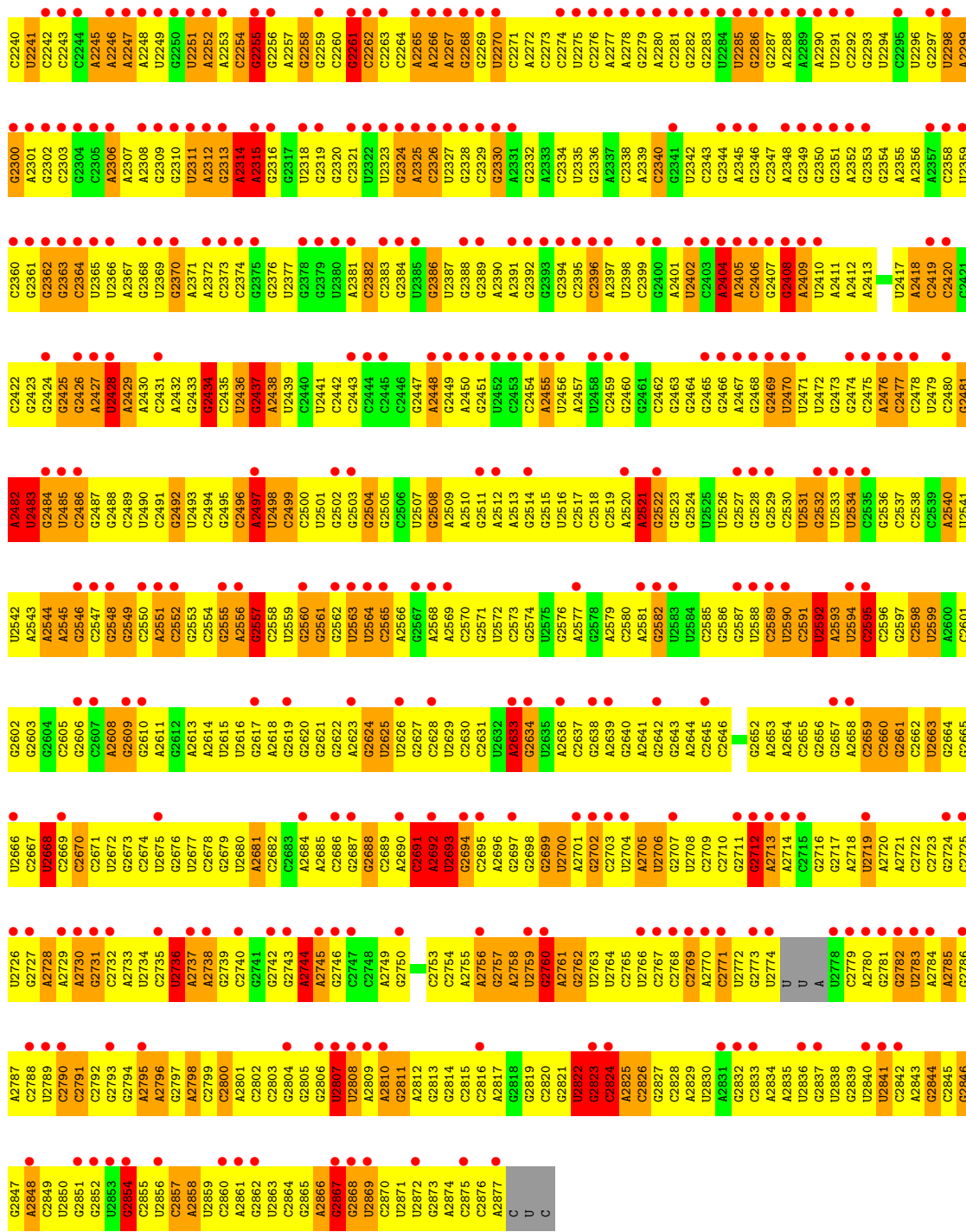
3 Residue-property plots

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 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.

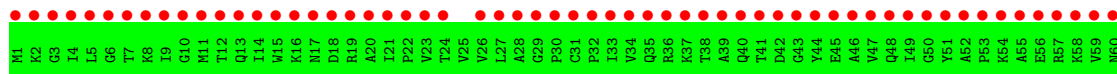
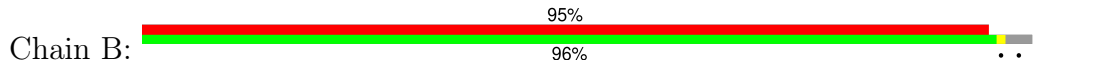
• Molecule 1: 23S ribosomal RNA



G1388	C1399	A1400	G1401	G1402	G1403	C1404	A1405	G1406	G1407	A1408	G1409	G1410	C1411	G1412	G1413	G1414	G1415	A1416	C1417	G1418	G1419	G1420	A1421	G1422	A1423	G1424	G1425	G1426	G1427	G1428	A1429	G1430	G1431	G1432	A1433	G1434	G1435	G1436	A1437	G1438	G1439	G1440	A1441	C1442	G1443	G1444	A1445	G1446	G1447	G1450	G1451	G1452	A1453	G1454	G1455	G1456	A1457	A1458		
G1337	G1338	G1339	G1340	G1341	G1342	G1343	C1344	G1345	G1346	G1347	G1348	A1349	G1350	G1351	G1352	A1353	G1354	A1355	G1356	G1357	G1358	G1359	G1360	G1361	A1362	G1363	G1364	G1365	G1366	G1367	G1368	G1369	G1370	G1371	A1372	G1373	G1374	G1375	G1376	G1377	G1378	A1379	G1380	G1381	G1382	G1383	G1384	G1385	A1386	G1387	G1388	G1391	G1392	G1393	G1394	A1395	G1396	A1397		
G1273	G1274	A1275	G1276	G1277	G1278	G1279	G1280	A1281	A1282	G1283	G1284	A1285	G1286	A1287	G1288	A1289	G1290	G1291	A1292	G1293	G1294	G1295	G1296	A1297	G1298	A1299	G1300	A1301	G1302	G1303	G1304	G1305	G1306	G1307	G1308	G1309	G1310	G1311	G1312	G1313	A1314	G1315	G1316	G1317	A1321	G1322	G1323	G1324	G1325	G1326	G1327	C1328	G1329	G1330	G1331	G1332	G1333	G1334		
U1213	C1214	A1215	G1216	G1217	G1218	G1219	G1220	G1221	G1222	G1223	A1224	G1225	A1226	A1227	G1228	G1229	C1230	A1231	U1232	G1233	G1234	G1235	G1236	G1237	A1238	G1239	G1240	G1241	G1242	G1243	U1244	G1245	G1246	G1247	G1248	G1249	A1250	G1251	C1252	G1253	G1254	A1255	C1256	U1257	G1258	A1259	G1260	G1261	U1262	G1263	G1264	G1265	G1266	A1267	G1268	G1269	C1270	G1271	G1272	
U1092	U1093	C1094	U1095	G1096	A1097	G1098	A1099	G1100	G1101	G1102	A1103	G1104	U1105	A1106	U1107	U1108	A1109	G1110	C1111	U1112	C1113	A1114	C1115	U1116	G1117	G1118	U1119	C1120	G1121	A1122	G1123	U1124	G1125	G1126	G1127	G1128	A1129	U1130	G1131	C1132	G1133	C1134	U1137	A1138	A1139	A1140	U1141	G1142	A1143	U1144	G1145	G1146	G1147	A1148	G1149	C1150	U1151	C1152		
A1032	G1033	U1034	G1035	G1036	G1037	U1038	A1039	A1040	G1041	G1042	A1043	U1044	G1045	U1046	G1047	U1048	C1049	G1050	U1051	C1052	G1053	C1054	A1055	U1056	A1057	G1058	U1059	C1060	A1061	G1062	G1063	C1064	A1065	G1066	G1067	A1068	G1069	U1070	U1071	G1072	G1073	A1074	G1075	U1076	U1077	A1078	G1079	A1080	A1081	G1082	G1083	A1084	G1085	G1086	C1087	A1088	C1089	A1090	C1091	
C972	U973	U974	C975	G976	G977	U978	A979	G980	C981	G982	G983	A984	G985	A986	G987	G988	G989	A990	A991	A992	C993	A994	G995	G996	G997	C998	U999	A1000	A1001	C1002	C1003	A1004	U1005	C1006	A1007	G1008	C1009	U1010	A1011	A1012	G1013	A952	G953	U954	G955	A956	C957	G958	A959	U960	A964	G965	A966	C967	G968	U969	A970	C1031		
A848	G849	C850	G851	U852	C853	G854	G855	A856	G857	G858	U859	G860	A861	A862	C863	G864	A865	U866	G867	U871	G872	U873	U874	G875	A876	G877	C878	A879	C880	U881	C882	A883	C884	A885	U886	G887	G888	U889	C890	A891	G	G	G	A832	A833	A834	U835	G836	U837	A838	U839	U840	A841	A842	G843	G844	U845	U846	U847	C
G788	G789	A790	G791	U792	G793	A794	A795	A796	A797	G798	C799	U800	A801	A802	C803	G804	A805	U806	A807	C808	C809	U810	G811	G812	A813	G814	A815	U816	C817	U818	C819	U820	A821	U822	U823	U824	C825	U826	C827	C828	C829	U830	G831	A832	A712	A713	G714	U715	U716	A717	G718	U719	U720	A721	C722	G723	U724	U725	U726	C947
U667	A668	G669	U670	A671	G672	C673	U674	G675	G676	G677	G678	U679	U680	A681	G682	A683	C684	U685	G686	G687	C688	G689	C700	U701	A702	G703	U704	C705	U706	U707	U708	A709	C710	G711	A712	G713	U714	U715	U716	A717	U718	A719	A720	G721	C722	G723	U724	U725	U726	C947										
U727	G728	A729	C730	G731	G732	G733	G734	G735	G736	C737	G738	U739	A740	G741	G742	A743	C744	C745	G746	A747	A748	C749	C750	G751	G752	U753	G754	C755	C756	U757	G758	C759	U760	G761	A762	A763	A764	C765	U766	U767	U768	C769	G772	G773	A774	U775	G776	A777	G778	U779	U780	A781	U782	G783	U784	U785	U786	U787		



● 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	170.47Å 412.74Å 696.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.96 – 3.56 29.96 – 3.56	Depositor EDS
% Data completeness (in resolution range)	90.5 (29.96-3.56) 90.4 (29.96-3.56)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 3.56Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.276 , 0.338 0.359 , 0.378	Depositor DCC
R_{free} test set	13101 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	97.3	Xtrriage
Anisotropy	0.737	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.16 , 89.3	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	0.80	EDS
Total number of atoms	59597	wwPDB-VP
Average B, all atoms (Å ²)	92.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: G80

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	0	0.46	0/66467	0.87	193/103673 (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	158

There are no bond length outliers.

The worst 5 of 193 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	0	985	G	N9-C1'-C2'	10.45	127.68	112.00
1	0	1975	G	C2'-C3'-O3'	10.35	125.03	109.50
1	0	1342	U	N1-C1'-C2'	9.26	127.89	114.00
1	0	956	A	C2'-C3'-O3'	9.16	123.23	109.50
1	0	813	A	N9-C1'-C2'	8.76	125.15	112.00

There are no chirality outliers.

5 of 158 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	118	U	Sidechain
1	0	154	U	Sidechain
1	0	29	U	Sidechain
1	0	50	G	Sidechain
1	0	67	G	Sidechain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	59359	0	29917	4815	0
2	B	205	0	0	2	0
3	0	33	0	43	7	0
All	All	59597	0	29960	4818	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 55.

The worst 5 of 4818 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2040:A:H2'	1:0:2041:A:C8	1.52	1.42
1:0:2040:A:C2'	1:0:2041:A:H8	1.48	1.27
1:0:2564:U:O2'	1:0:2565:C:H5'	1.34	1.26
1:0:2418:A:H1'	1:0:2565:C:O2'	1.31	1.24
1:0:2810:A:C6	1:0:2854:G:C8	2.27	1.22

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

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

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2757/2880 (95%)	667 (24%)	167 (6%)

5 of 667 RNA backbone outliers are listed below:

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

5 of 167 RNA pucker outliers are listed below:

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

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no 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	G80	0	2881	-	36,36,36	4.14	22 (61%)	55,56,56	2.77	19 (34%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	G80	0	2881	-	-	1/12/81/81	0/4/4/4

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

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

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

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

There are no chirality outliers.

All (1) torsion outliers are listed below:

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

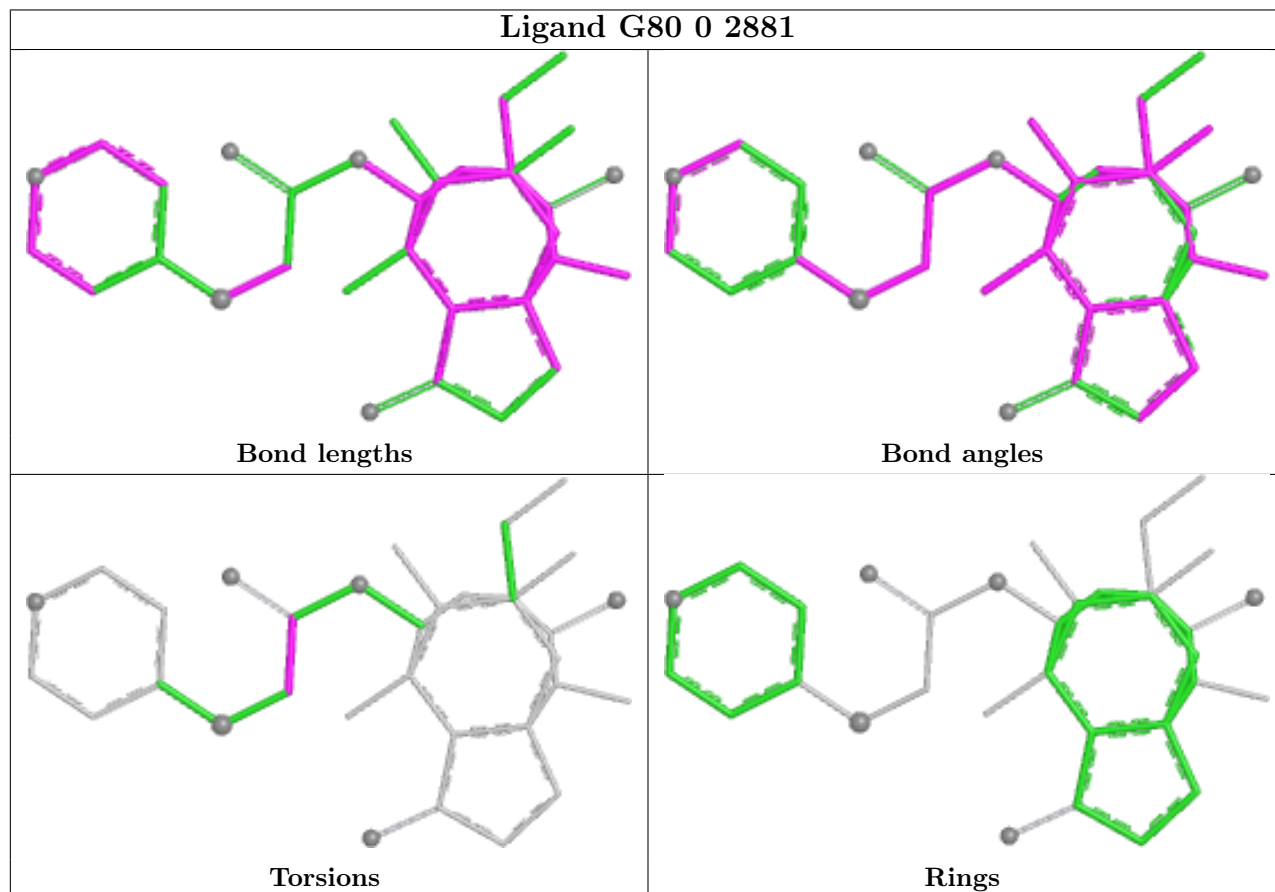
There are no ring outliers.

1 monomer is involved in 7 short contacts:

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

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [\(i\)](#)

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%)	2.74	1531 (55%) 0 0	12, 79, 200, 200	0
2	B	205/211 (97%)	11.52	200 (97%) 0 0	3, 58, 141, 202	0
All	All	2971/3091 (96%)	3.35	1731 (58%) 0 0	3, 77, 200, 202	0

The worst 5 of 1731 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	84	PHE	34.7
2	B	87	ASP	34.7
2	B	2	LYS	34.4
2	B	86	PRO	32.7
2	B	120	TRP	29.4

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](#)

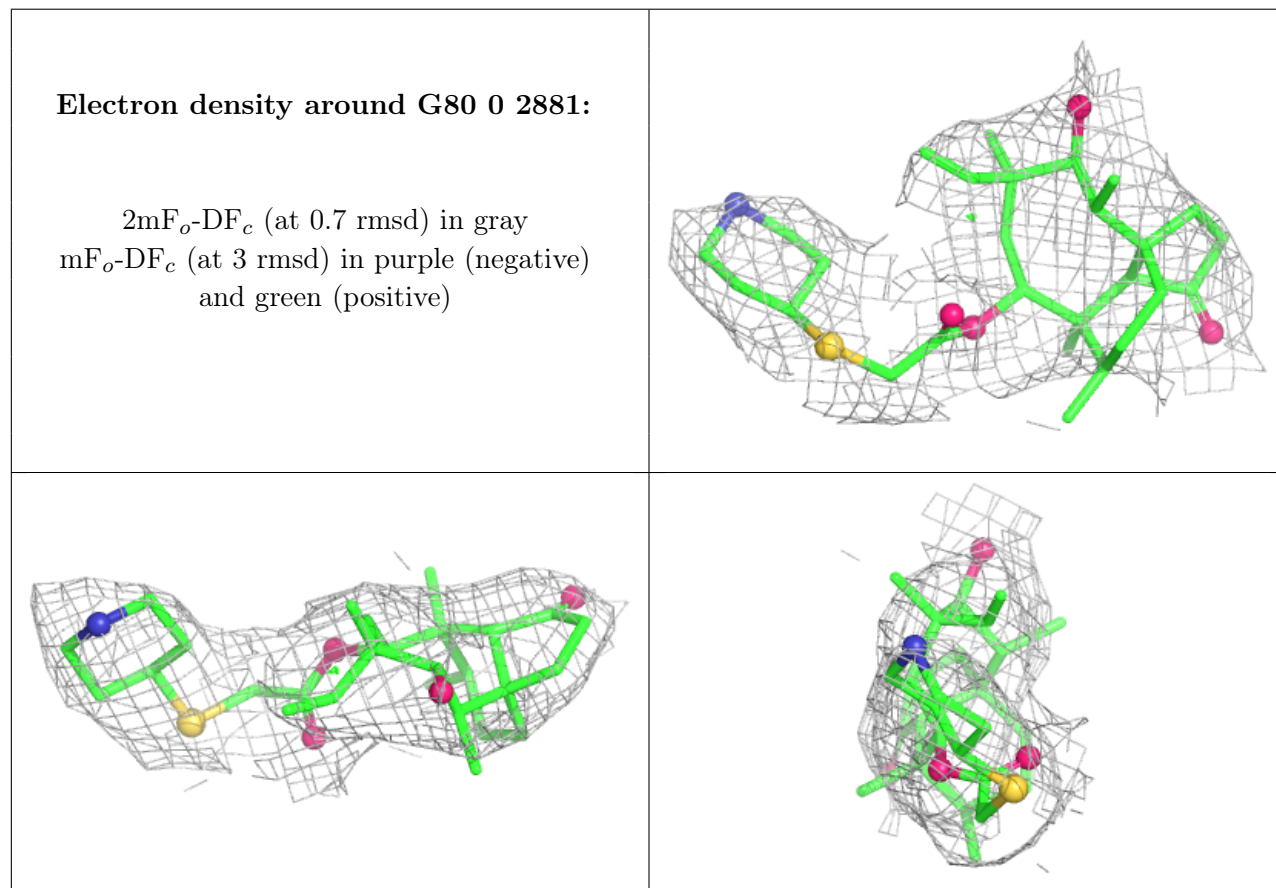
There are no oligosaccharides in this entry.

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(\AA^2)	Q<0.9
3	G80	0	2881	33/33	0.90	0.22	62,62,62,62	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.