



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 09:41 PM UTC

PDB ID : 3FWO / pdb_00003fwo
Title : The large ribosomal subunit from *Deinococcus radiodurans* complexed with Methymycin
Authors : Auerbach, T.; Mermershtain, I.; Bashan, A.; Davidovich, C.; Rozenberg, H.; Sherman, D.H.; Yonath, A.
Deposited on : 2009-01-19
Resolution : 3.71 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

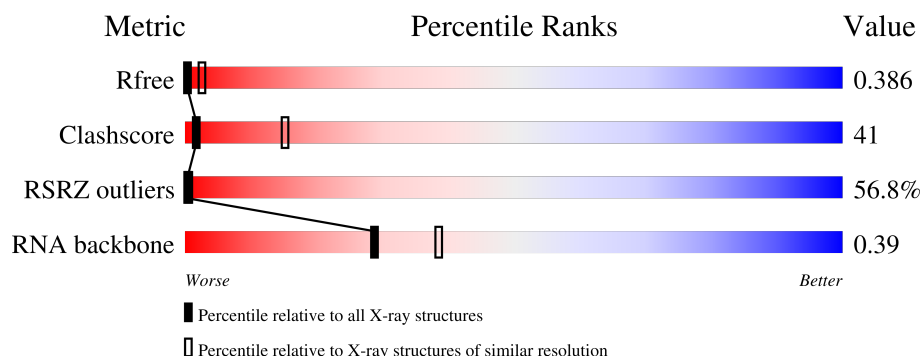
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.71 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	1182 (3.84-3.60)
Clashscore	190562	1222 (3.84-3.60)
RSRZ outliers	180081	1181 (3.84-3.60)
RNA backbone	3983	1007 (4.30-3.08)

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	A	2880	
2	B	118	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 61885 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.

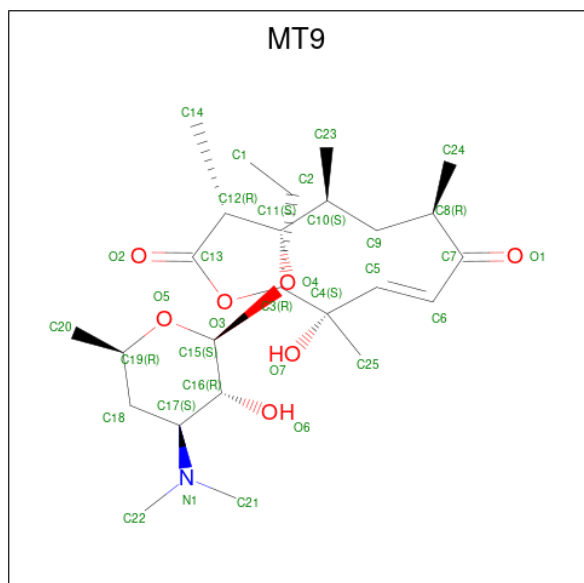
- Molecule 1 is a RNA chain called 23S RIBOSOMAL RNA.

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

- Molecule 2 is a RNA chain called 5S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	B	118	2516	1124	464	811	117	0	0	0

- Molecule 3 is (3R,4S,5S,7R,9E,11S,12R)-12-ethyl-11-hydroxy-3,5,7,11-tetramethyl-2,8-dioxoxacyclododec-9-en-4-yl 3,4,6-trideoxy-3-(dimethylamino)-beta-D-xylo-hexopyranoside (CCD ID: MT9) (formula: C₂₅H₄₃NO₇).

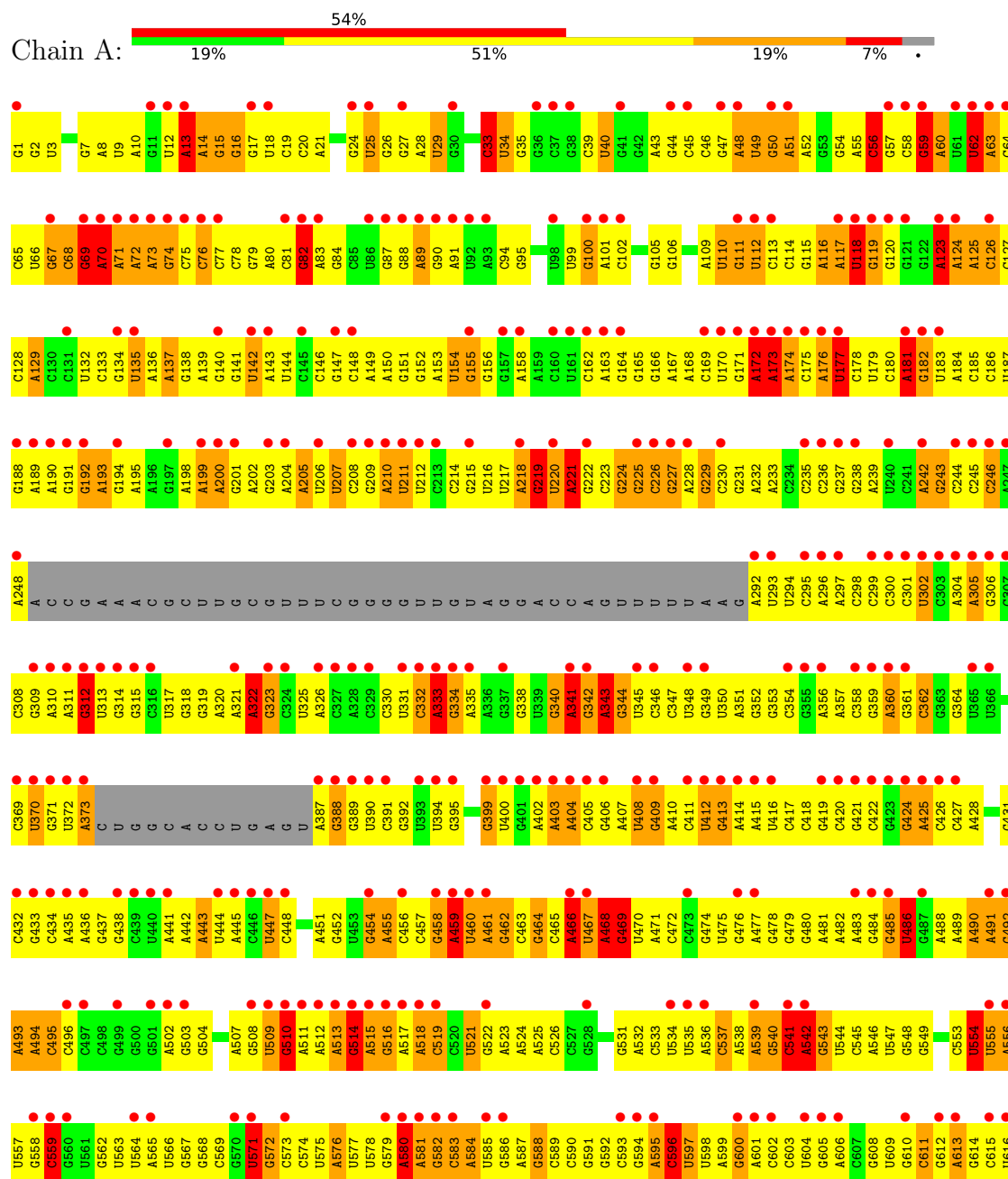


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	33	25	1	7	0	0

3 Residue-property plots

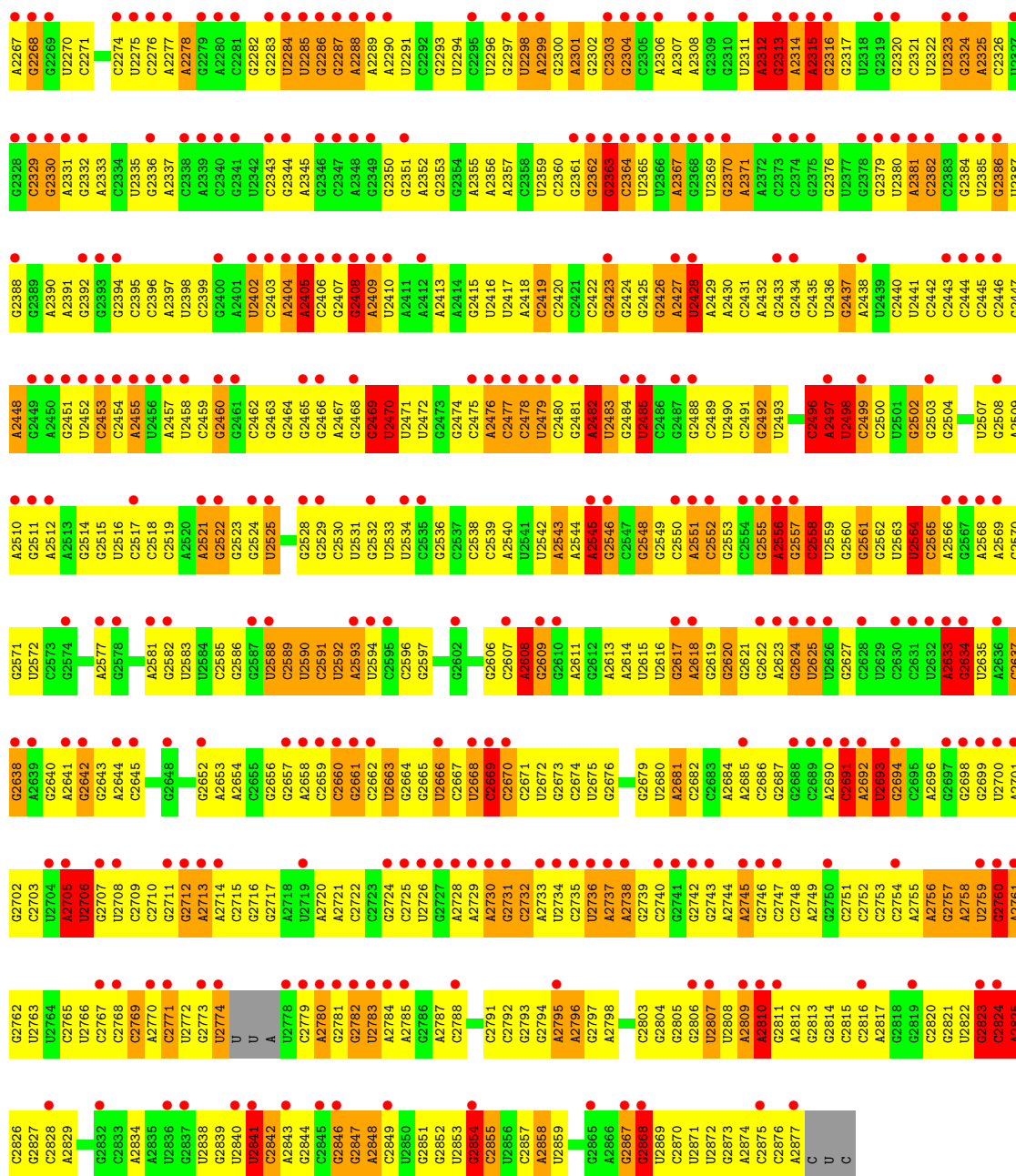
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



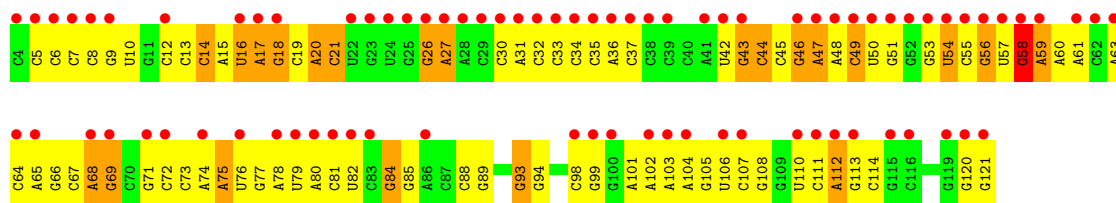
U1409	C1348	A1288	G1228	G1165	U1105	G1045	G985	A923	A862	A801	G741	C678	U617
U1410	A1289	A1290	C1229	A1166	A1106	U1046	A986	C924	C863	A802	G742	C679	A618
C1411	G1352	G1291	C1230	A1167	A1107	G1047	A987	U925	C864	C803	G743	C680	A619
G1414	A1353	A1292	A1231	G1168	U1108	U1048	G988	C926	A865	C804	C744	A681	G620
C1415	A1354	A1293	U1232	C1169	A1109	U1049	G989	C927	U866	G805	C745	G682	U621
A1416	A1355	A1294	A1233	U1170	G1110	G1050	A990	G928	C867	A806	G746	A683	G622
C1417	G1356	U1295	C1234	A1171	C1111	U1051	A991	A929	C870	C807	A747	C684	G623
G1418	U1357	G1296	G1236	U1176	A1113	C1053	C993	A930	U871	C808	A748	U685	A624
C1419	A1358	A1297	A1237	U1177	A1114	G1054	A994	G932	G872	C809	C749	C686	A625
U1420	G1359	G1298	A1238	U1178	U1115	A1055	A995	G933	U873	G811	G751	A688	A627
U1421	A1360	A1299	A1239	C1179	U1116	U1056	C996	G934	A874	G812	G752	A689	A628
C1422	G1361	U1300	G1240	A1179	G1117	A1057	C997	C935	G875	A813	U753	A690	C629
A1423	A1362	U1301	G1241	A1180	G1118	G1058	C998	A936	A876	G814	G754	C691	G630
U1424	C1363	C1302	A1242	C1181	U1119	A1059	A999	C937	G877	A815	C755	C692	G631
G1425	U1364	U1303	G1243	U1182	C1120	C1060	G1000	C938	A878	U816	C756	A693	G632
U1426	C1365	U1304	U1244	C1183	G1121	A1061	A1001	G939	A879	G694	U757	G694	G633
G1427	A1366	C1305	G1245	G1184	A1122	G1062	C1002	G940	C880	G818	G758	G695	G634
U1428	A1367	U1306	G1246	C1185	G1123	C1063	C1003	U941	U881	C819	C759	U696	C635
A1429	G1368	A1307	U1247	A1186	U1124	C1064	U820	U942	C882	U820	U760	G697	G636
G1430	U1369	C1308	G1248	A1187	U1125	A1065	U1005	U943	A883	A821	G761	A698	G637
U1431	U1370	G1309	G1249	A1188	A1126	G1066	C1006	A944	C884	G822	A762	C699	G638
G1432	C1371	C1310	A1250	G1189	G1127	G1067	A1007	U945	A885	U823	A763	C700	G640
A1433	A1372	C1311	G1251	G1190	C1128	A1068	G1008	U946	A886	U824	A764	U701	G641
U1434	G1373	G1312	C1252	G1191	A1129	G1069	C1009	C947	G887	C825	C765	A702	G642
G1435	C1374	U1313	G1253	A1192	U1130	U1070	U1010	G949	G888	U826	A766	G704	A643
A1436	A1375	A1314	C1254	G1193	G1131	G1071	A1011	U948	C889	U827	G767	G704	A644
U1437	C1376	A1315	A1255	U1194	C1132	U1072	U1012	G950	U890	C828	U768	C705	G645
G1438	G1377	G1316	C1256	U1195	G1133	G1073	G1013	G951	A891	C829	G769	G646	G646
U1439	A1378	G1317	U1257	G1196	C1134	G1074	G1014	A952	G	C830	U770	G708	G647
A1440	U1379	A1318	G1258	U1197	G1135	C1075	U1015	U953	G	G831	G771	A648	G648
U1441	C1380	C1319	A1259	C1198	G1136	U1076	C1016	U954	G	A832	G772	C711	G649
G1442	G1381	A1320	C1260	U1199	A1137	U1077	C1017	G955	G	A833	G773	A712	U650
A1443	C1382	C1321	G1261	G1200	A1138	U1078	C1018	A956	G	A834	A774	G713	C651
G1444	C1383	G1322	U1262	G1201	A1139	G1079	U1019	G957	C	U835	U775	G714	C652
A1445	G1384	C1323	G1263	U1202	A1140	A1080	A1020	G958	C	G836	G776	U715	G653
U1446	C1385	G1324	C1264	A1203	U1141	A1081	A1021	C963	A	U837	A777	G716	A654
G1447	A1386	U1325	G1265	G1204	G1142	C1083	U1023	G963	C	A838	G778	A718	A655
U1448	C1387	A1326	G1266	G1205	A1143	C1084	G1024	U963	C	U839	U779	U656	U657
C1449	U1388	C1327	A1267	G1206	U1144	A1084	A1025	G965	A	U840	G780	C721	G658
G1450	C1389	C1328	U1268	G1207	G1145	G1085	A1026	G966	C	G841	G781	G722	G659
U1451	G1390	U1329	G1269	A1208	G1146	C1086	U1026	A966	A	A842	U782	C723	G660
A1452	A1391	C1330	C1270	G1209	G1147	C1087	U1027	G967	C	G843	G783	C724	C661
U1453	U1392	G1331	C1271	C1210	G1148	A1088	G1028	C968	U	G844	U784	C725	G662
C1454	C1393	A1332	G1272	G1211	G1149	C1089	C1029	U969	A	U845	G785	G726	G663
U1455	G1394	G1333	G1273	U1212	C1150	C1090	U1030	A970	U	A846	U786	G727	G664
C1456	A1395	A1334	C1274	U1213	U1151	C1091	C1031	A971	C	C847	A787	U727	C664
U1457	C1396	A1335	A1275	C1214	G1152	U1092	A1032	C972	C	A848	G	G728	A665
A1458	A1397	G1336	U1276	A1215	C1153	U1093	G1033	U973	A911	U848	G789	A729	U666
U1459	C1398	G1337	G1277	G1216	A1154	C1094	U1034	G974	A912	C850	U790	C730	U667
G1460	C1399	A1338	A1278	U1217	G1155	A1095	G1035	C975	A913	C851	A791	A731	A668
U1461	A1400	G1401	G1279	U1156	U1156	A1096	G1036	C976	C914	U852	G792	G732	G669
C1462	C1401	C1340	U1280	G1220	G1157	A1097	U1037	G977	C915	C853	G793	G733	U670
A1463	G1402	G1341	A1281	C1221	A1158	G1098	U1038	U976	U916	G854	A793	G734	A671
U1464	U1403	A1342	A1282	G1222	U1159	A1099	A1039	G980	U917	G	G789	G735	C672
G1465	A1404	C1343	C1283	G1223	G1160	A1100	A1040	A918	A918	U857	A795	G736	C673
C1466	A1405	A1284	G1285	A1224	U1161	G1101	G1041	C981	U919	C850	A796	G737	U674
U1467	A1406	G1345	A1285	G1225	A1162	U1102	G1042	C982	G920	U859	A797	G738	C675
A1468	G1407	C1346	U1286	A1226	C1163	A1103	G1043	G983	A921	U860	G798	G739	G676
U1469	A1408	C1347	A1287	G1227	C1164	G1104	A1044	C984	C922	C961	U900	A740	C677





• Molecule 2: 5S RIBOSOMAL RNA

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	172.50Å 415.69Å 701.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.71 30.00 – 3.71	Depositor EDS
% Data completeness (in resolution range)	94.7 (30.00-3.71) 94.7 (30.00-3.71)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.17	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 3.66Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.278 , 0.337 0.363 , 0.386	Depositor DCC
R_{free} test set	12496 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	128.9	Xtriage
Anisotropy	0.649	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , 69.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	61885	wwPDB-VP
Average B, all atoms (Å ²)	138.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.05% 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: MT9

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	A	0.48	0/66440	0.88	223/103628 (0.2%)
2	B	0.41	0/2813	0.74	2/4384 (0.0%)
All	All	0.48	0/69253	0.87	225/108012 (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	A	0	167

There are no bond length outliers.

The worst 5 of 225 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	985	G	N9-C1'-C2'	11.09	130.63	114.00
1	A	1975	G	C2'-C3'-O3'	10.36	125.04	109.50
1	A	956	A	C2'-C3'-O3'	9.72	124.09	109.50
1	A	514	G	N9-C1'-C2'	9.58	128.38	114.00
1	A	1279	G	N9-C1'-C2'	9.41	128.12	114.00

There are no chirality outliers.

5 of 167 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	16	G	Sidechain
1	A	25	U	Sidechain
1	A	29	U	Sidechain

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Mol	Chain	Res	Type	Group
1	A	33	C	Sidechain
1	A	40	U	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	A	59336	0	29907	3635	0
2	B	2516	0	1286	132	0
3	A	33	0	43	5	0
All	All	61885	0	31236	3770	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 3770 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:A:987:G:H5'	1:A:1167:A:N6	1.56	1.19
1:A:1714:A:H5'	1:A:1715:A:H5''	1.21	1.17
1:A:2172:U:H2'	1:A:2173:G:H5''	1.25	1.16
1:A:1153:A:O2'	1:A:1154:A:H3'	1.44	1.16
1:A:623:G:H4'	1:A:626:A:H62	1.10	1.15

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein molecules in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein molecules in this entry.

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2757/2880 (95%)	679 (24%)	191 (6%)
2	B	117/118 (99%)	17 (14%)	5 (4%)
All	All	2874/2998 (95%)	696 (24%)	196 (6%)

5 of 696 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	13	A
1	A	14	A
1	A	15	G
1	A	33	C
1	A	34	U

5 of 196 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1710	U
1	A	2045	A
1	A	1749	G
1	A	1923	U
1	A	2237	C

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	MT9	A	2881	-	33,34,34	2.15	10 (30%)	44,50,50	1.87	9 (20%)

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	MT9	A	2881	-	-	11/46/62/62	0/1/2/2

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2881	MT9	C10-C11	6.74	1.65	1.53
3	A	2881	MT9	C4-C5	4.75	1.56	1.51
3	A	2881	MT9	C9-C10	4.20	1.60	1.54
3	A	2881	MT9	C8-C7	3.79	1.57	1.51
3	A	2881	MT9	O3-C13	2.96	1.41	1.34

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2881	MT9	C3-O3-C13	-5.01	109.45	118.20
3	A	2881	MT9	O4-C15-O5	-5.00	97.53	110.69
3	A	2881	MT9	C8-C9-C10	4.84	123.77	115.09
3	A	2881	MT9	O4-C11-C12	-3.66	104.99	111.16
3	A	2881	MT9	C9-C8-C7	2.73	117.14	110.64

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

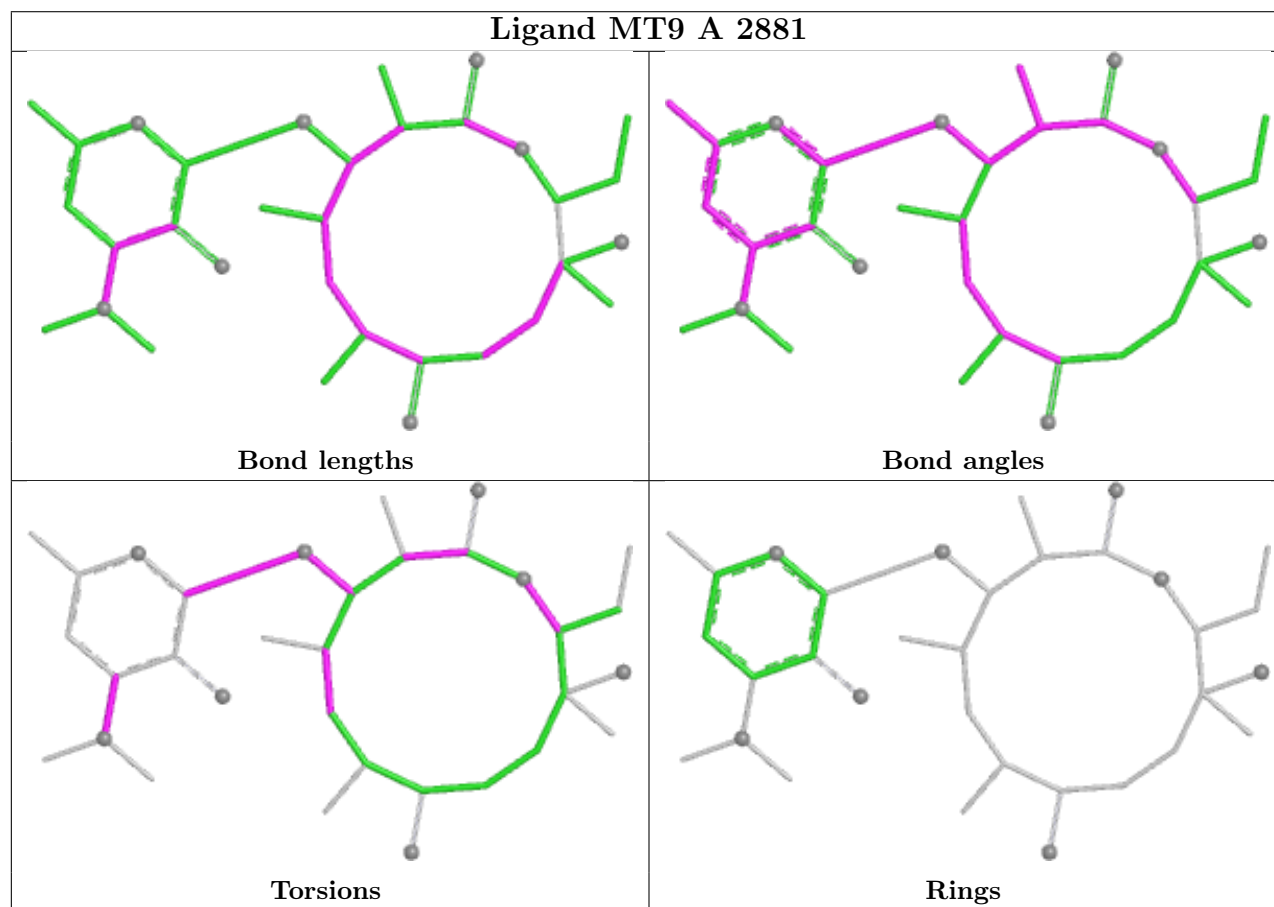
Mol	Chain	Res	Type	Atoms
3	A	2881	MT9	C11-C12-C13-O3
3	A	2881	MT9	C11-C12-C13-O2
3	A	2881	MT9	C12-C11-O4-C15
3	A	2881	MT9	C10-C11-O4-C15
3	A	2881	MT9	C23-C10-C9-C8

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2881	MT9	5	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	A	2765/2880 (96%)	2.55	1557 (56%) 0 0	61, 129, 200, 200	0
2	B	118/118 (100%)	2.88	80 (67%) 0 0	124, 171, 200, 200	0
All	All	2883/2998 (96%)	2.57	1637 (56%) 0 0	61, 130, 200, 200	0

The worst 5 of 1637 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1922	U	15.7
1	A	558	G	14.2
1	A	1921	A	13.8
1	A	940	G	13.2
1	A	2092	U	12.7

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](#)

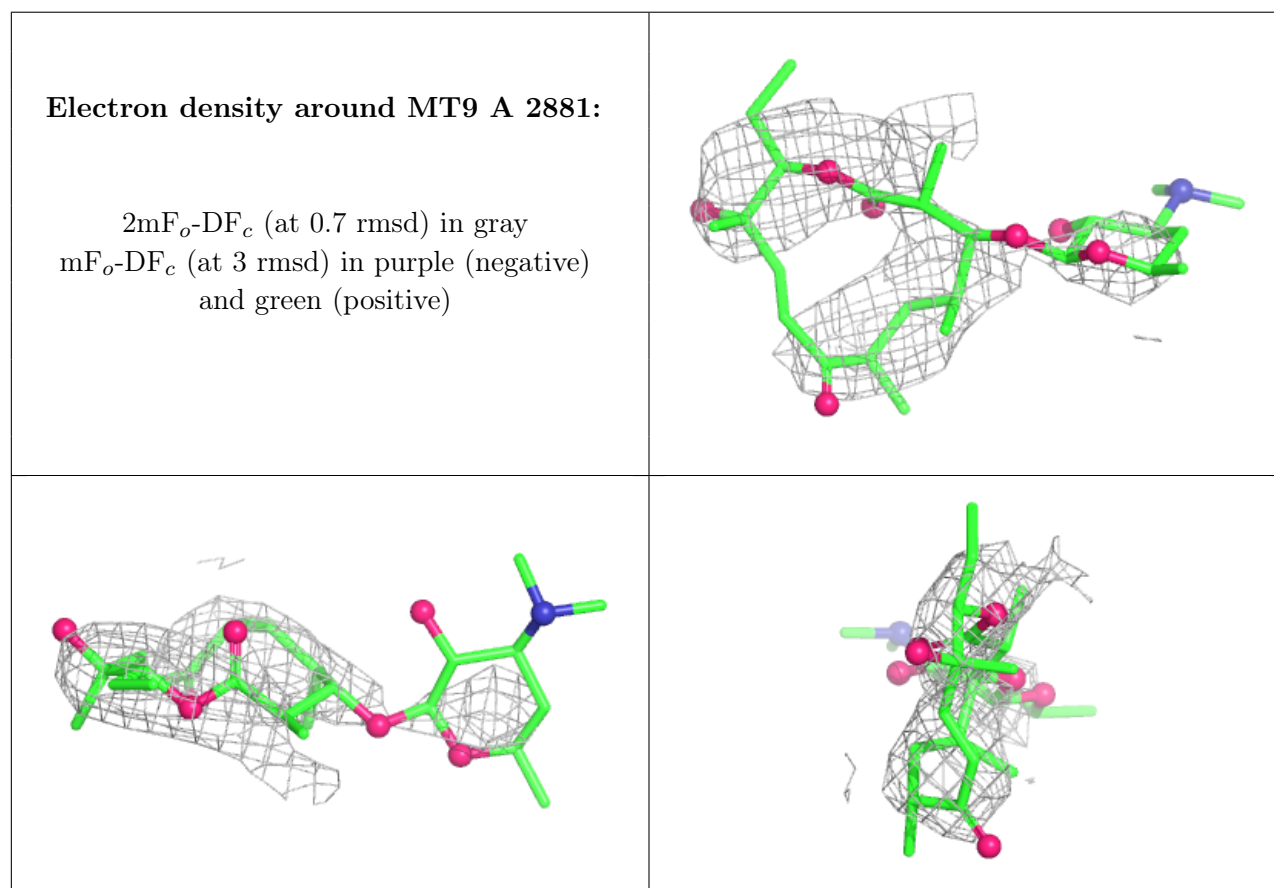
There are no oligosaccharides in this entry.

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	MT9	A	2881	33/33	0.86	0.37	156,163,166,166	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.