



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 08:47 AM GMT

PDB ID : 3FWO  
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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

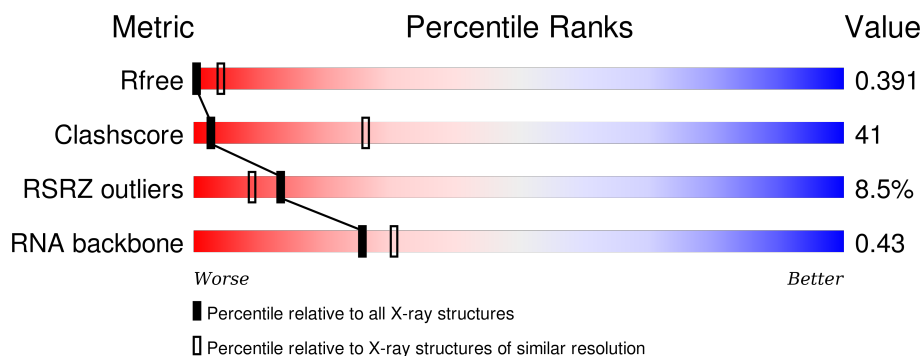
# 1 Overall quality at a glance

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))
$R_{free}$	91344	1129 (3.94-3.50)
Clashscore	102246	1252 (3.94-3.50)
RSRZ outliers	91569	1136 (3.94-3.50)
RNA backbone	2183	1067 (4.60-2.80)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MT9	A	2881	-	-	-	X

## 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.

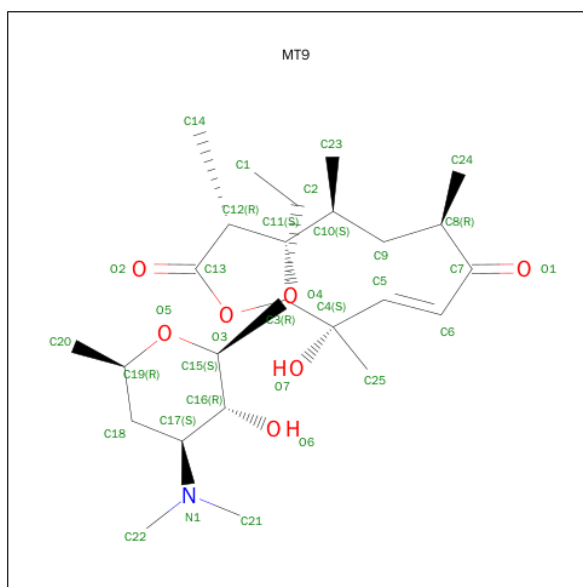
- Molecule 1 is a RNA chain called 23S RIBOSOMAL RNA.

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-DIOXOXYACYCLODODEC-9-EN-4-YL 3,4,6-TRIDEOXY-3-(DIMETHYLAMINO)-BETA-D-XYLO-HEXOPYRANOSIDE (three-letter code: MT9) (formula:  $C_{25}H_{43}NO_7$ ).

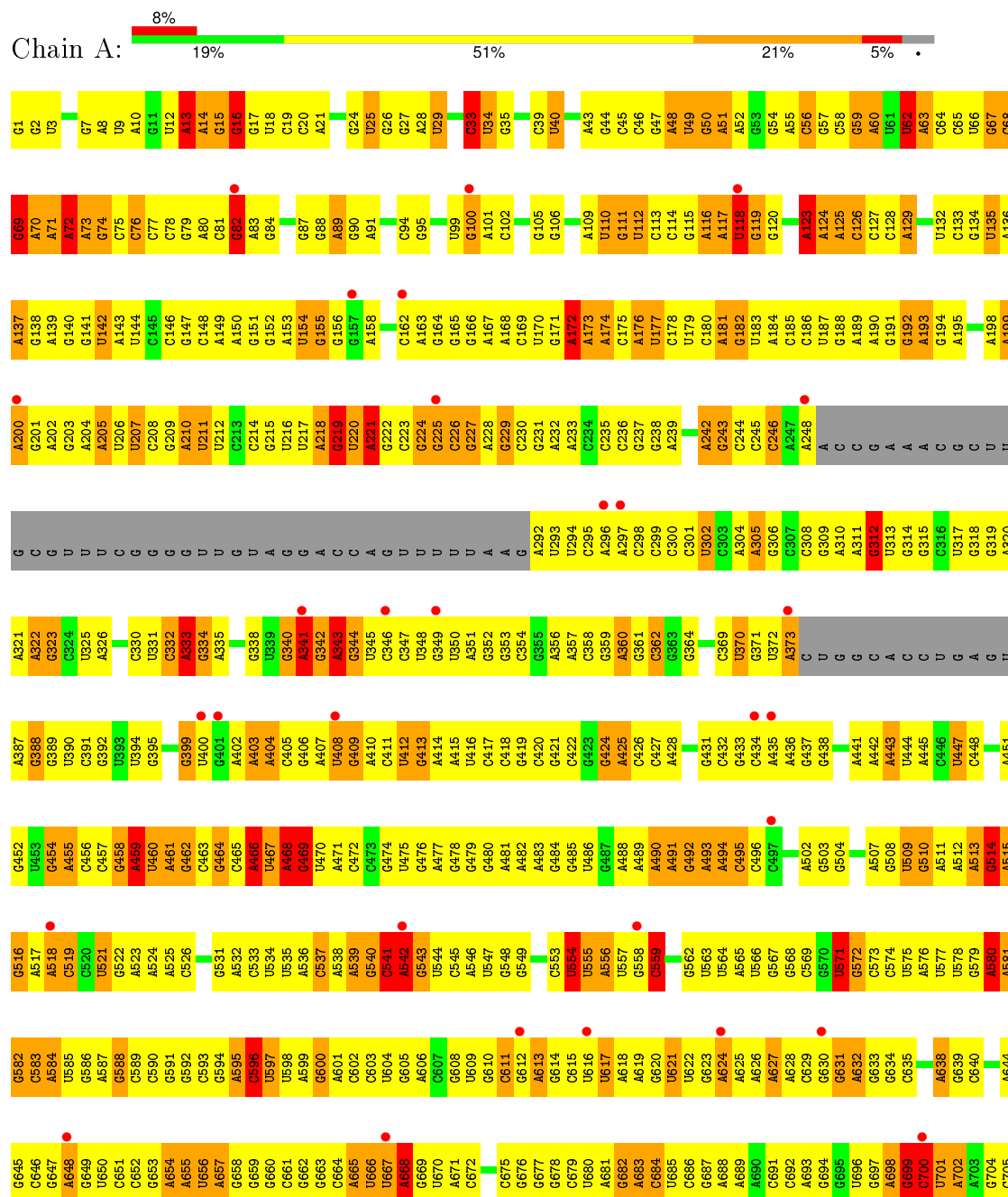


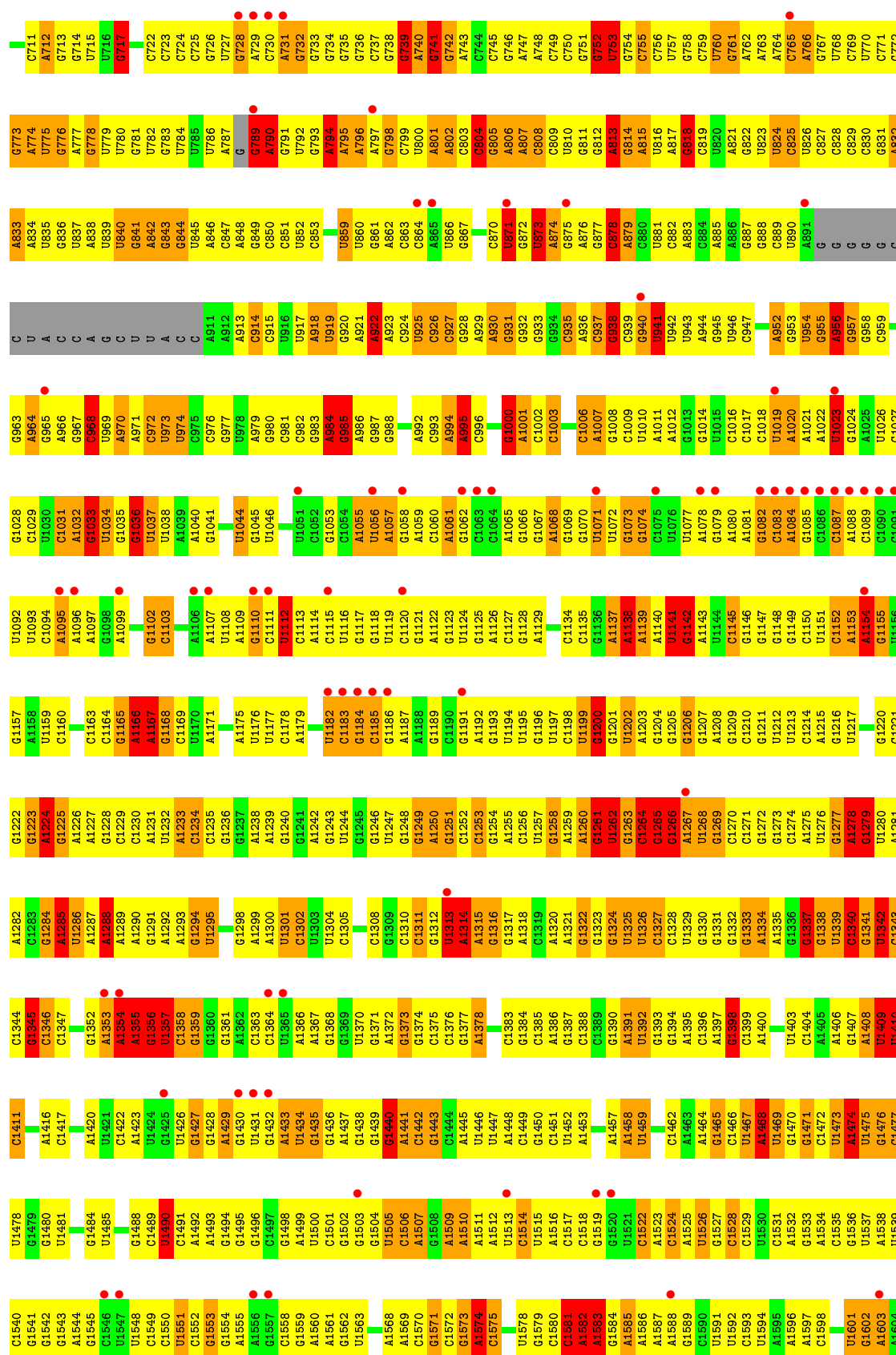
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	33	25	1	7	0	0

### 3 Residue-property plots

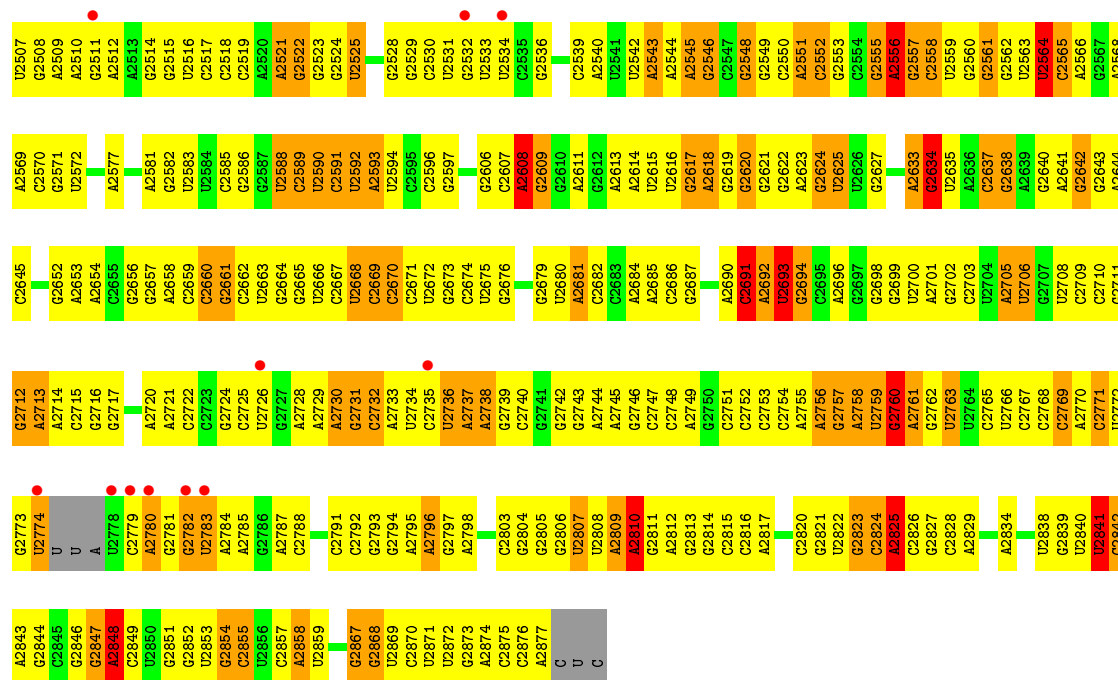
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ( $\text{RSRZ} > 2$ ). 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

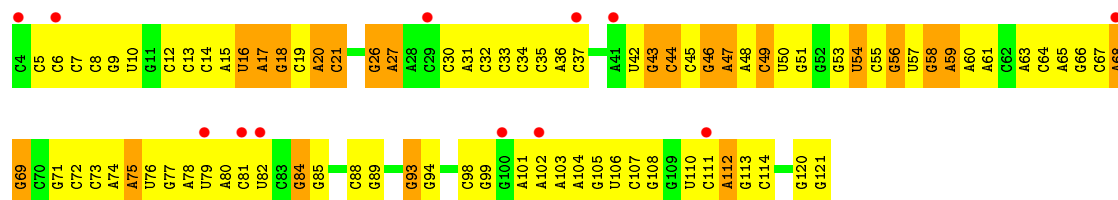




C2444	C2382	A2308	A2245	U2121	A1996	G1928	C1865	G1801	G1737	A1869	A1805
C2445	C2383	U2311	A2246	G2122	A1997	U1929	G1866	A1802	U1738	G1670	C1606
C2446	C2384	U2312	A2247	G2123	A1998	C1930	A1867	G1803	U1739	G1671	C1607
G2447	U2385	A2313	A2248	C2124	U1999	G1931	A1868	U1804	G1740	A1672	U1608
G2448	C2386	G2313	U2249	C2125	U2000	G1932	A1869	G1805	C1673	G1674	G1610
G2449	U2387	A2314	G2250	U	G2001	G1933	U1870	G1806	U1611	C1675	U1612
A2450	C2388	A2315	U2251	U	A2002	U1934	G1871	A1807	G1744	U1676	G1613
G2451	C2389	A2316	A2252	U	A2003	A1935	A1872	C1808	G1745	G1677	C1614
U2452	G2390	G2317	A2253	G	U2004	A1936	A1873	G1809	A1746	U1678	C1615
C2453	A2391	G2320	G2254	U	U2005	G1937	A1874	U1810	U1747	U1679	C1616
C2454	C2392	U2192	G2255	G	G2006	U1938	G1874	A1811	U1748	G1678	C1617
A2455	G2393	A2193	U2193	U	G2007	U1939	G1879	U1812	G1749	U1680	G1618
U2456	C2394	A2194	A2256	G2132	G2008	C1940	U1880	A1813	G1750	G1681	G1619
G2457	U2322	C2195	G2257	G2135	U2009	C1941	U1881	G1814	A1751	A1682	U1618
C2458	U2323	U2196	G2258	U2136	G2010	G1942	U1882	G1815	U1752	G1683	A1619
C2459	G2324	U2197	G2259	G2137	U2011	A1943	A1883	G1816	A1753	G1684	C1620
C2460	A2325	U2198	G2260	U2138	G2012	G1944	A1884	U1817	G1754	A1885	C1621
G2461	C2326	G2200	G2261	U2139	A2013	C1945	G1885	G1755	G1755	A1686	G1622
C2462	G2329	G2201	C2263	G2140	A2014	U1946	G1886	U1819	C1756	G1687	C1623
G2463	G2330	G2202	A2264	A	G2015	G1947	G1887	A1820	G1757	U1688	A1624
C2464	A2331	G2203	A2265	G	A2016	C1948	G1888	A1821	G1760	U1689	A1625
G2465	A2404	A2204	A2266	G	U2017	A1949	G1889	C1822	G1761	A1690	A1626
G2466	A2405	C2205	A2267	C	G2018	C1950	G1890	G1823	C1692	G1691	C1627
C2467	A2406	C2206	G2268	A	C2019	G1951	G1891	C1824	G1762	G1692	C1628
G2468	U2335	G2207	G2269	A	G2020	A1952	C1892	C1825	G1763	A1693	G1629
G2469	U2336	G2208	U2270	C	G2021	A1953	G1893	U1826	A1764	A1694	A1630
G2470	A2409	G2209	C2271	G	C2022	A1954	G1894	G1827	C1765	A1631	G1631
U2471	U2410	G2210	G2272	G	C2023	G1955	A1895	C1828	U1766	U1697	A1632
G2472	A2413	C2343	C2274	U	U2024	C1956	A1896	G1829	C1767	C1698	C1633
G2473	G2473	G2344	U2275	U	A2025	C1957	G1897	C1830	U1768	A1699	A1634
G2474	A2414	A2345	U2276	G	C2026	U1958	A1898	C1831	U1769	C1700	G1635
C2475	G2415	G2346	A2277	A	U1961	A1899	A1899	G1834	U1770	C1701	G1636
A2476	U2416	G2350	A2278	A	G2029	C1962	U1900	C1835	A1771	U1637	U1637
C2477	U2417	G2351	G2279	U	U2030	G1963	A1901	C1836	C1772	U1705	C1641
C2478	A2418	A2352	G2280	A	G2031	A1964	A1902	G1837	C1773	A1706	G1642
U2479	C2419	G2353	G2281	U	G2032	U1965	C1903	G1838	A1774	G1643	G1644
C2480	C2420	G2354	U2284	C2157	C2033	C1966	G1904	G1839	U1775	U1710	A1643
G2481	G2421	A2355	U2285	A2159	A2034	G1967	G1905	A1840	A1776	C1711	G1647
A2482	C2422	A2356	G2286	C2160	G2035	U1974	U1906	G1841	U1777	G1712	C1648
G2483	G2423	A2357	U2287	A	G2036	A1975	C1907	G1842	U1778	G1713	C1649
G2484	G2424	C2358	G2288	C2161	A2037	G1976	C1908	U1843	C1779	A1714	A1948
G2485	G2425	U2359	A2289	U2163	C2038	U1977	U1909	G1844	A1780	A1715	A1949
G2486	G2426	A2360	C2297	G2164	G2039	C1977	A1910	A1845	G1781	G1716	A1650
A2487	U2427	C2361	U2291	A2165	A2040	U1978	A1911	A1846	A1782	A1717	U1651
C2488	U2428	G2362	C2292	G2166	A2041	C1979	G1912	G1847	G1783	A1718	G1652
C2489	U2429	G2363	G2293	A2167	A2042	A1980	G1913	U1848	C1784	C1721	C1653
U2490	A2430	C2364	U2294	A2168	A2043	A1981	U1914	G1852	A1785	G1722	A1654
C2491	C2431	U2365	G2295	A2169	G2044	C1982	A1915	C1853	C1786	G1723	C1655
G2492	G2432	U2366	U2296	C2170	A2045	G1983	G1916	U1857	U1787	U1724	U1656
U2493	A2433	A2367	G2297	U2171	C2046	A1984	C1917	C1853	C1788	G1725	A1657
G2494	G2434	G2368	U2298	U2172	C2047	G1987	G1918	U1856	U1789	C1726	A1658
A2495	U2435	U2369	A2299	C	C2048	U1987	A1919	G1857	G1790	C1727	A1659
C2496	U2436	G2370	G2300	U	C2049	A1988	A1920	C1858	C1791	G1728	G1660
C2497	G2437	A2371	A2301	G	C2050	C1989	A1921	G1859	C1792	G1729	C1661
A2498	A2438	G2372	G2302	C	U2051	U1990	U1922	A1860	A1793	G1730	G1662
U2500	U2439	G2373	C2303	U2176	G2052	C1991	U1923	A1861	A1794	G1731	C1663
G2501	C2440	U2374	U2241	U2177	G2053	G1982	U1924	G1862	U1798	U1732	C1664
G2502	U2441	G2375	C2242	U2178	C2054	G1983	U1925	U1863	A1799	C1733	C1665
G2503	C2442	U2380	C2243	A2119	A2055	U1994	U1926	U1864	G1799	U1734	A1666
G2504	C2443	A2381	C2244	C2120	G1995	G1995	U1927	G1964	A1900	G1668	G1668



## • Molecule 2: 5S RIBOSOMAL RNA



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	172.50Å 415.69Å 701.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.71 38.32 – 3.71	Depositor EDS
% Data completeness (in resolution range)	94.7 (30.00-3.71) 94.7 (38.32-3.71)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.17	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.89 (at 3.66Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.278 , 0.337 0.368 , 0.391	Depositor DCC
$R_{free}$ test set	12486 reflections (5.24%)	DCC
Wilson B-factor (Å <sup>2</sup> )	128.9	Xtriage
Anisotropy	0.649	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.17 , 50.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 251070 reflections (0.000%)	Xtriage
$F_o, F_c$ correlation	0.83	EDS
Total number of atoms	61885	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

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



## 5 Model quality

### 5.1 Standard geometry

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	0.62	4/66440 (0.0%)	0.85	132/103628 (0.1%)
2	B	0.48	0/2813	0.78	0/4384
All	All	0.61	4/69253 (0.0%)	0.85	132/108012 (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	A	0	167

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	700	C	N1-C2	8.55	1.48	1.40
1	A	542	A	C5-C6	-5.95	1.35	1.41
1	A	824	U	N1-C2	5.53	1.43	1.38
1	A	1313	U	C2-N3	5.37	1.41	1.37

The worst 5 of 132 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	985	G	N9-C1'-C2'	12.79	130.63	114.00
1	A	514	G	N9-C1'-C2'	11.06	128.38	114.00
1	A	1279	G	N9-C1'-C2'	10.86	128.12	114.00
1	A	13	A	N9-C1'-C2'	10.38	127.49	114.00
1	A	2405	A	N9-C1'-C2'	9.29	126.08	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
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	3646	0
2	B	2516	0	1286	133	0
3	A	33	0	43	5	0
All	All	61885	0	31236	3782	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 3782 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 [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2757/2880 (95%)	676 (24%)	191 (6%)
2	B	117/118 (99%)	17 (14%)	5 (4%)
All	All	2874/2998 (95%)	693 (24%)	196 (6%)

5 of 693 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	1325	U
1	A	1651	U
1	A	2668	U
1	A	1338	G
1	A	1441	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	MT9	A	2881	-	32,34,34	1.95	8 (25%)	37,50,50	1.76	7 (18%)

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	-	-	0/46/62/62	0/1/2/2

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2881	MT9	C12-C11	2.08	1.60	1.55
3	A	2881	MT9	C9-C8	2.11	1.60	1.54
3	A	2881	MT9	C17-N1	2.27	1.53	1.48
3	A	2881	MT9	C6-C5	2.83	1.38	1.32
3	A	2881	MT9	O3-C13	2.86	1.41	1.34

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2881	MT9	O4-C15-O5	-5.20	97.53	110.68
3	A	2881	MT9	C3-O3-C13	-5.14	109.45	118.12
3	A	2881	MT9	O4-C11-C12	-3.27	104.99	111.10
3	A	2881	MT9	C18-C17-C16	-2.25	106.75	110.03
3	A	2881	MT9	C18-C17-N1	-2.25	109.04	115.70

There are no chirality outliers.

There are no torsion outliers.

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

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	2765/2880 (96%)	0.52	233 (8%) 14 9	61, 129, 200, 200	0
2	B	118/118 (100%)	0.39	12 (10%) 9 6	124, 171, 200, 200	0
All	All	2883/2998 (96%)	0.51	245 (8%) 13 9	61, 130, 200, 200	0

The worst 5 of 245 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	558	G	10.2
1	A	1936	A	8.6
1	A	2124	C	7.4
1	A	1871	G	7.3
1	A	1845	A	7.1

### 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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MT9	A	2881	33/33	0.70	0.59	9.32	156,163,166,166	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.