



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 7, 2026 – 01:35 AM UTC

PDB ID : 3JQ4 / pdb_00003jq4
Title : The structure of the complex of the large ribosomal subunit from D. Radiodurans with the antibiotic lankacidin
Authors : Auerbach-Nevo, T.; Mermershtain, I.; Davidovich, C.; Bashan, A.; Rozenberg, H.; Yonath, A.
Deposited on : 2009-09-06
Resolution : 3.52 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

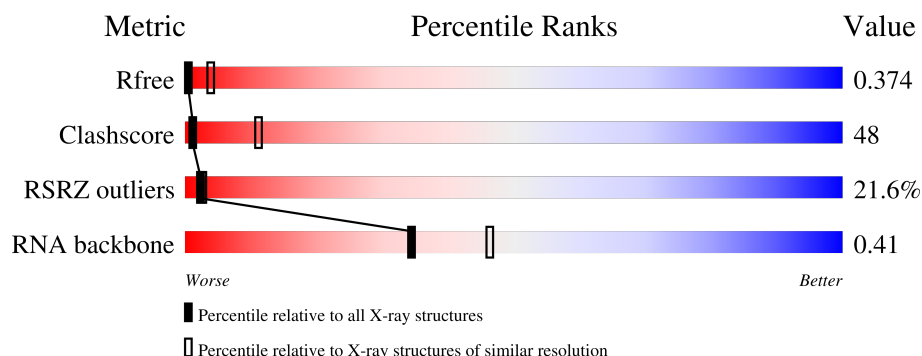
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.52 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	1025 (3.56-3.48)
Clashscore	190562	1079 (3.56-3.48)
RSRZ outliers	180081	1024 (3.56-3.48)
RNA backbone	3983	1018 (4.00-3.04)

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.

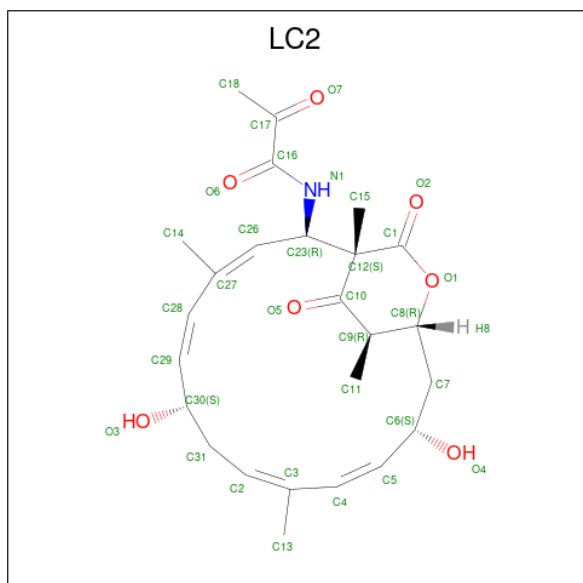
- Molecule 1 is a RNA chain called 23S ribosomal RNA.

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

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

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

- Molecule 3 is N-[(1S,2R,3E,5E,7S,9E,11E,13S,15R,19R)-7,13-dihydroxy-1,4,10,19-tetramethyl-17,18-dioxo-16-oxabicyclo[13.2.2]nonadeca-3,5,9,11-tetraen-2-yl]-2-oxopropanamide (CCD ID: LC2) (formula: C₂₅H₃₃NO₇).

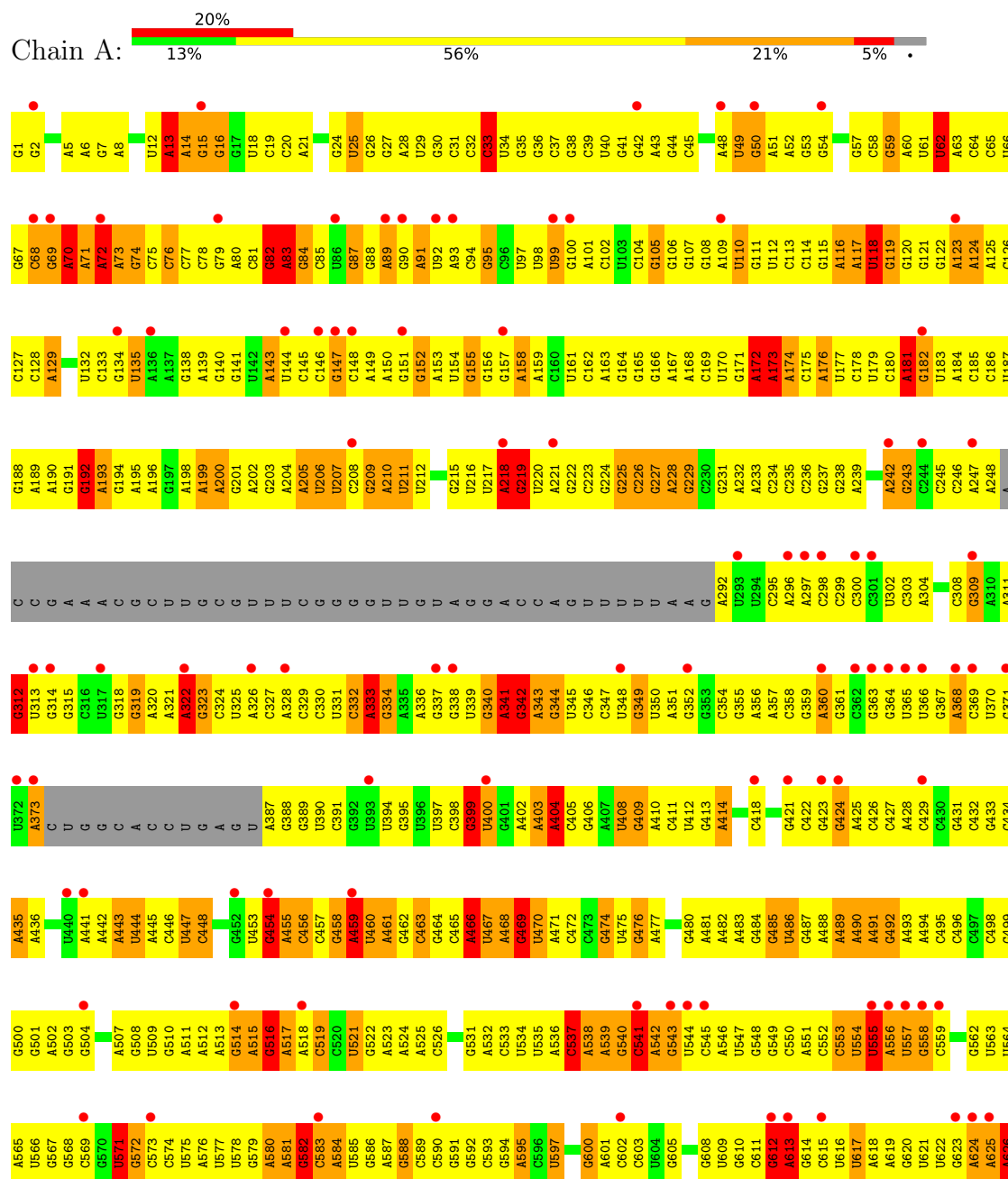


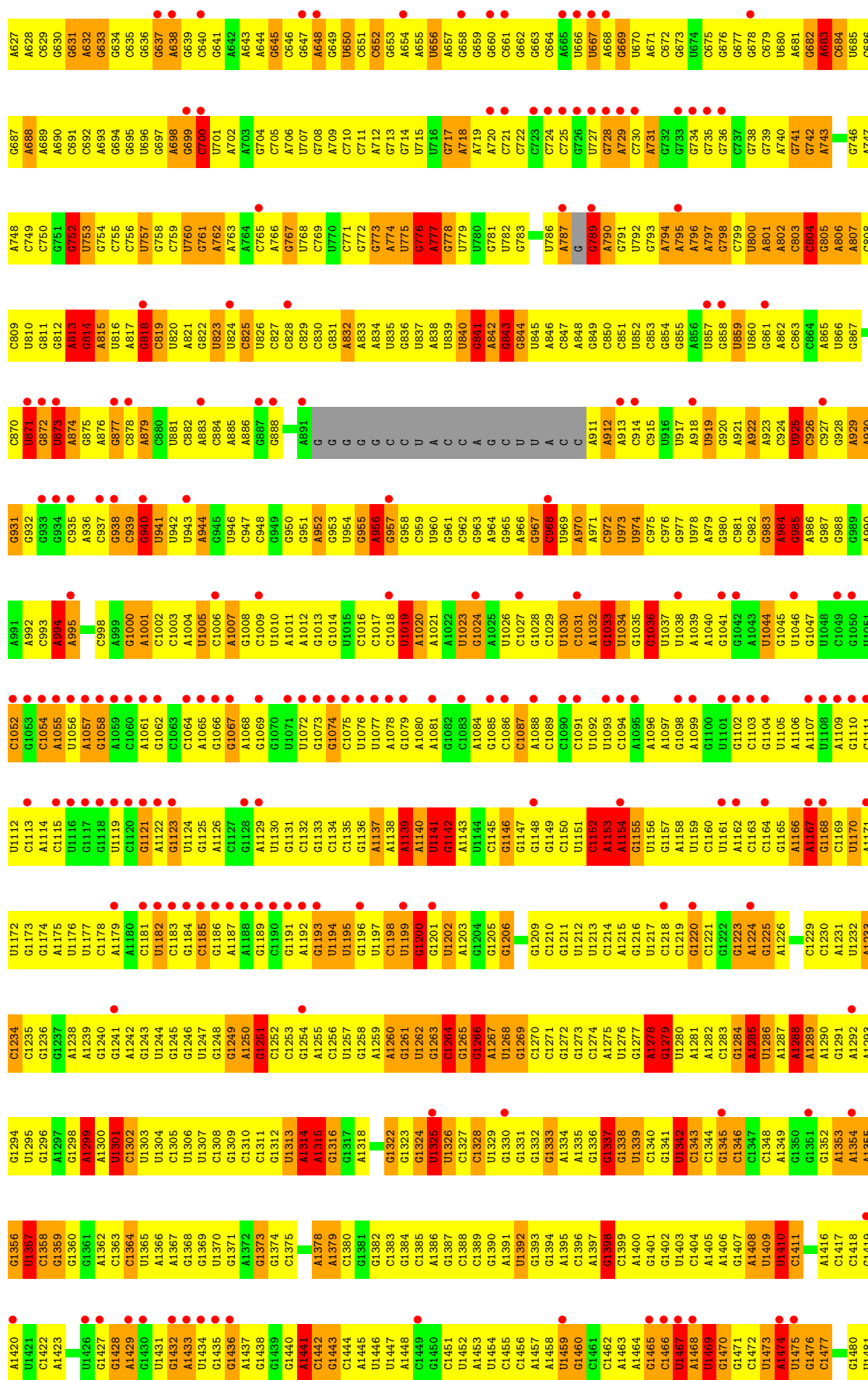
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			33	25	1	7		

3 Residue-property plots

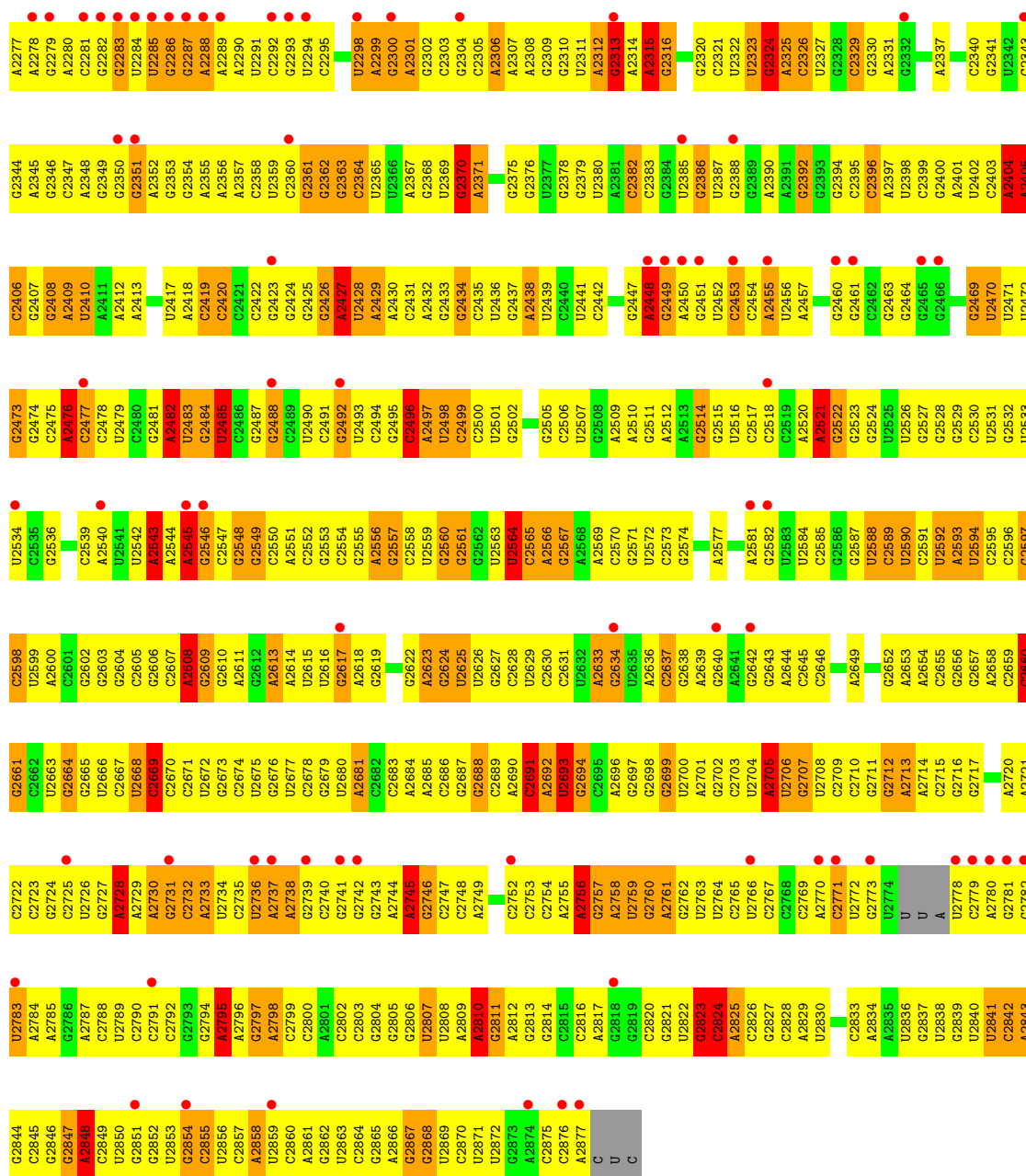
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

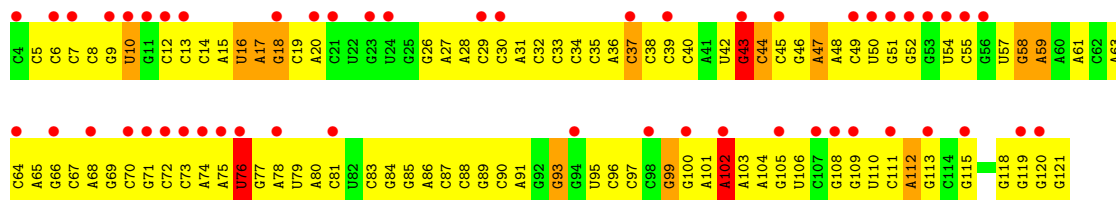




C2215	A	C2094	C2033	C1973	G1913	C1853	C1792	A1728	G1664	A1605	G1543	U1482
G2216	U	G2095	A2034	U1974	U1914	G1854	A1793	C1732	C1665	A1606	A1544	G1483
G2217	A	U2096	G2035	G1975	A1915	G1855	C1794	U1730	G1666	A1607	C1545	A1486
U2219	G	A2097	G2036	U1976	G1916	G1856	C1795	U1731	A1667	G1608	C1546	C1487
A2220	G	C2098	A2037	C1977	G1917	G1857	G1798	U1732	A1668	U1609	U1547	G1488
G2221	A	G2038	C2038	U1978	G1918	C1858	C1799	C1734	A1669	G1610	C1548	C1489
U2222	A	G2039	G2039	C1979	A1919	A1859	A1799	G1735	G1670	C1549	U1549	
U2223	A	A1980	A2040	A1980	A1920	A1860	A1800	C1736	A1671	C1550	U1550	
U2224	A	A1981	A2041	A1981	A1921	G1861	A1801	C1737	A1672	U1551	C1491	
G2225	G	A1982	A2042	G1982	U1922	U1862	A1802	U1738	C1673	G1613	A1492	
G2226	A	G1983	A2043	G1983	U1923	U1863	A1803	U1739	C1674	G1552	A1493	
A2227	A	A1984	G2044	A1984	C1924	G1864	U1804	G1740	C1675	G1554	G1494	
C2227	A	G1985	A2045	G1985	C1925	G1865	G1805	G1741	U1676	A1555	G1495	
U2228	A	G1986	C2046	G1986	U1926	G1866	G1806	G1742	C1677	A1556	G1496	
G2229	A	G1987	C2047	G1987	U1927	A1867	A1807	C1743	G1678	U1557	C1497	
G2230	A	A1988	C2048	A1988	U1928	A1868	A1808	C1744	G1679	C1558	G1498	
G2231	A	G1989	C2049	G1989	U1929	A1869	A1809	C1745	U1680	G1559	A1499	
G2232	C	U1990	G2050	U1990	C1930	U1870	U1810	G1746	A1681	A1560	U1500	
C2233	C	C1991	U2051	C1991	G1931	G1871	A1811	G1747	A1682	G1561	C1501	
G2234	U	G1992	G2052	G1992	G1932	A1872	U1812	U1748	G1683	C1623	G1502	
G2235	U	G1993	G2053	G1993	G1933	A1873	A1813	U1749	G1684	U1563	G1503	
U2236	U	U1994	A2054	U1994	U1934	G1874	G1814	A1750	A1685	A1624	U1504	
C2237	G	G1995	G2055	G1995	A1935	G1875	G1815	A1751	A1686	A1625	G1505	
G2238	A	A1996	C2056	A1996	A1936	C1876	G1816	U1752	C1687	A1626	U1506	
G2239	A	U1997	U2057	U1997	G1937	C1877	U1817	U1753	U1688	C1627	C1507	
C2240	A	A1998	U2058	A1998	U1938	C1878	G1818	G1754	U1689	G1628	A1507	
U2241	A	U1999	U2059	U1999	U1939	G1879	U1819	G1755	U1690	G1629	G1508	
C2242	A	U2000	A2060	U2000	C1940	G1880	G1820	C1756	G1691	A1630	A1509	
C2243	A	G2001	C2061	G2001	C1941	U1881	A1821	C1757	C1692	C1570	A1510	
C2244	A	A2002	C2062	A2002	G1942	G1882	C1822	G1760	A1693	C1572	A1512	
A2245	A	U2003	U2064	U2003	A1943	A1883	G1823	C1761	A1694	G1573	U1513	
A2246	U	U2005	A2065	U2005	C1945	A1884	C1824	C1762	U1695	A1574	C1514	
A2247	U	G2006	U2067	G2006	G1946	C1885	C1825	G1763	C1696	C1575	U1515	
U2248	U	G2007	C2068	G2007	G1947	G1886	G1826	U1764	U1697	G1576	A1516	
G2250	U	U2008	U2069	G2008	C1948	G1887	G1827	G1765	C1698	G1577	C1517	
U2251	U	U2009	G2070	U2009	A1949	C1888	C1828	U1766	A1699	U1639	C1518	
A2252	C	G2071	G2071	G2071	C1950	G1889	C1830	G1767	C1700	G1640	G1519	
A2253	G	C2072	C2072	U2011	G1951	G1890	C1831	C1768	C1701	C1641	G1520	
C2254	A	A2073	A2073	A2012	A1952	C1891	G1832	U1769	G1704	G1642	C1521	
G2255	A	U2074	U2074	A2013	A1953	G1893	U1833	U1770	U1705	A1582	U1522	
G2256	A	U2075	U2075	A2014	A1954	U1894	G1834	A1771	A1706	A1583	A1523	
U2257	A	G2076	G2076	G2015	G1955	A1895	C1835	C1772	A1707	G1585	A1524	
U2258	A	G2077	G2077	A2016	G1956	A1896	C1836	C1773		A1586	U1525	
U2259	A	G2078	G2078	U2017	C1957	C1897	G1837	A1774	U1710	A1587	U1526	
G2260	A	U2079	A2079	G2018	G1958	U1898	G1838	A1775	C1711	A1588	G1527	
G2261	A	U2080	U2080	C2019	U1959	A1899	G1839	A1776	G1712	A1588	C1528	
C2262	A	U2081	U2081	G2020	A1960	U1900	A1840	A1777	G1713	G1589	C1529	
C2263	A	C2082	C2082	G2021	A1961	U1901	G1841	U1778	A1714	U1591	C1531	
A2265	C	G2083	G2083	C2022	C1962	A1902	G1842		A1715	C1590	U1530	
A2266	C	G2084	G2084	C2023	G1963	C1903	U1843	C1761	G1716	C1653	A1532	
A2267	C	G2085	U2085	U2024	A1964	G1904	U1844	A1782	G1717	A1592	G1533	
G2268	A	A2086	A2086	A2025	U1965	G1905	A1845		U1718	C1593	A1534	
G2269	A	C2087	C2087	C2026	C1966	U1906	A1846	A1785	A1719	A1595	C1535	
U2270	C	C2088	C2088	C2027	U1967	G1907	G1847	G1786	G1719	A1596	G1536	
C2271	G	C2089	C2089	C2028	G1968	C1908	U1848	U1787	U1723	A1597	U1537	
A2272	U	U2090	U2090	G2029	G1969	U1909	G1849	C1788	C1724	A1598	A1538	
C2273	G	U2030	U2030	G2030	A1970	A1910	G1850	U1789	C1725	G1599	U1539	
C2274	G	A2031	A2031	C1971	A1911	A1911	A1851	G1790	C1726	U1600	C1540	
U2275	A	G1972	G1972	G1912	G1912	G1912	G1852	C1791	C1727	U1601	G1541	
C2276	A									C1663	G1542	



• 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, α , β , γ	169.80Å 410.30Å 694.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 3.52 8.00 – 3.52	Depositor EDS
% Data completeness (in resolution range)	89.8 (8.00-3.52) 83.7 (8.00-3.52)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 3.57Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.268 , 0.325 0.353 , 0.374	Depositor DCC
R_{free} test set	13457 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	106.6	Xtriage
Anisotropy	0.863	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 70.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.81	EDS
Total number of atoms	61885	wwPDB-VP
Average B, all atoms (Å ²)	118.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% 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: LC2

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	0.44	0/66440	0.85	172/103628 (0.2%)
2	B	0.35	0/2813	0.70	2/4384 (0.0%)
All	All	0.43	0/69253	0.84	174/108012 (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	124
2	B	0	1
All	All	0	125

There are no bond length outliers.

The worst 5 of 174 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	985	G	N9-C1'-C2'	10.71	130.07	114.00
1	A	1975	G	C2'-C3'-O3'	10.15	124.72	109.50
1	A	1154	A	N9-C1'-C2'	8.64	124.97	112.00
1	A	1337	G	N9-C1'-C2'	8.47	126.71	114.00
1	A	2660	C	C2'-C3'-O3'	8.32	121.98	109.50

There are no chirality outliers.

5 of 125 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	15	G	Sidechain

Continued on next page...

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Mol	Chain	Res	Type	Group
1	A	16	G	Sidechain
1	A	172	A	Sidechain
1	A	25	U	Sidechain
1	A	33	C	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	4288	0
2	B	2516	0	1286	151	0
3	A	33	0	33	1	0
All	All	61885	0	31226	4436	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 48.

The worst 5 of 4436 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:614:G:N2	1:A:634:G:H22	1.28	1.29
1:A:2194:A:H2'	1:A:2195:C:H5''	1.25	1.18
1:A:2691:C:C2'	1:A:2692:A:H5''	1.79	1.11
1:A:918:A:H2'	1:A:919:U:H5''	1.33	1.10
1:A:2198:U:H3'	1:A:2199:C:H4'	1.14	1.10

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	2756/2880 (95%)	677 (24%)	213 (7%)
2	B	117/118 (99%)	17 (14%)	2 (1%)
All	All	2873/2998 (95%)	694 (24%)	215 (7%)

5 of 694 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	13	A
1	A	14	A
1	A	45	C
1	A	49	U
1	A	50	G

5 of 215 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1575	C
1	A	1807	A
1	A	2668	U
1	A	1626	A
1	A	1691	G

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	LC2	A	2881	-	31,34,34	1.99	7 (22%)	35,49,49	2.10	11 (31%)

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	LC2	A	2881	-	-	1/35/61/61	0/0/2/2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2881	LC2	C12-C1	6.01	1.65	1.53
3	A	2881	LC2	C13-C3	4.85	1.60	1.50
3	A	2881	LC2	C2-C3	2.70	1.40	1.33
3	A	2881	LC2	C31-C30	2.36	1.62	1.54
3	A	2881	LC2	C16-C17	2.31	1.57	1.54

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2881	LC2	O7-C17-C16	-6.65	112.41	119.90
3	A	2881	LC2	O7-C17-C18	4.83	130.58	119.77
3	A	2881	LC2	C17-C16-N1	3.77	117.35	112.97
3	A	2881	LC2	C6-C5-C4	-2.98	118.51	124.73
3	A	2881	LC2	C8-C7-C6	2.83	121.60	113.97

There are no chirality outliers.

All (1) torsion outliers are listed below:

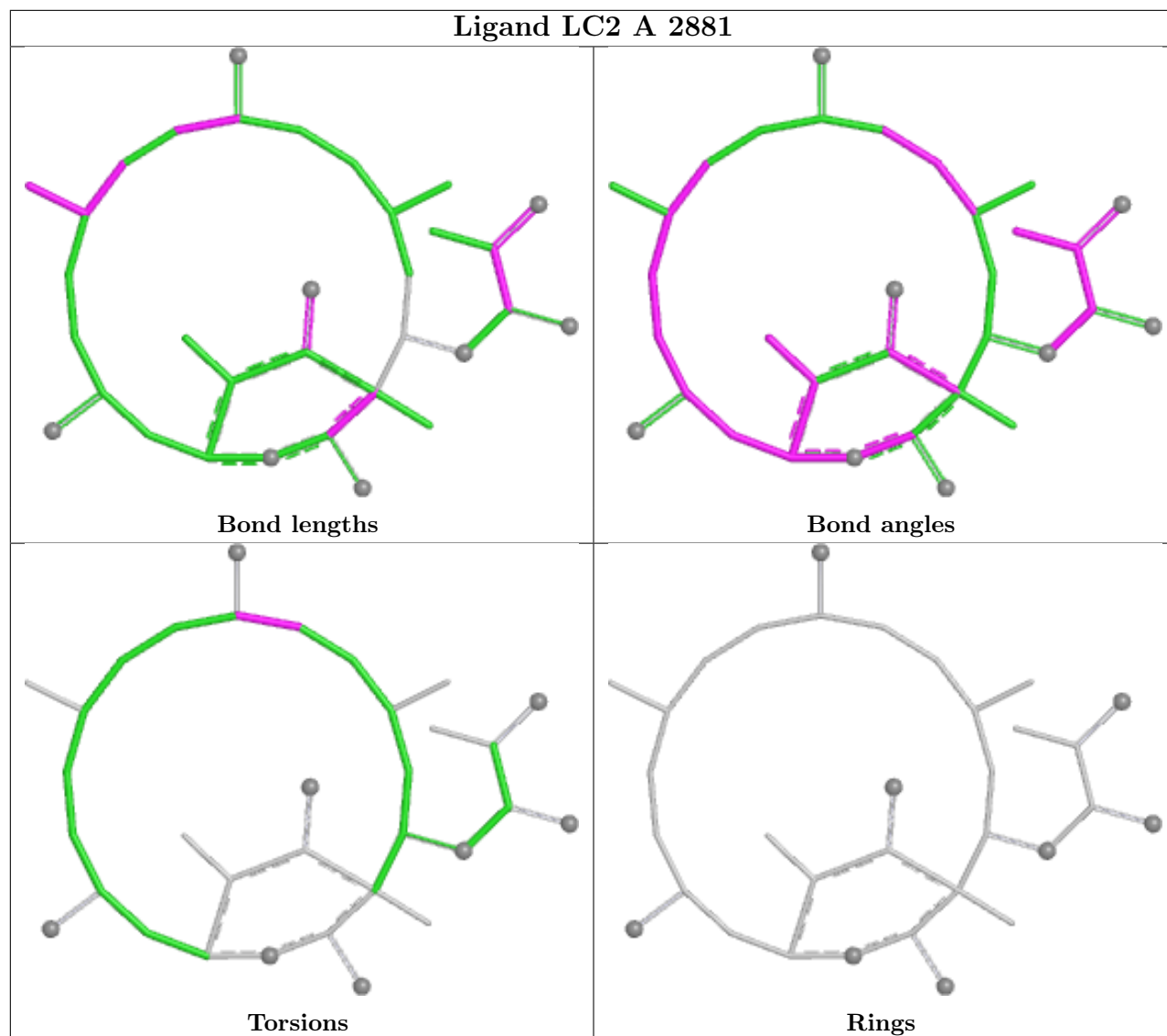
Mol	Chain	Res	Type	Atoms
3	A	2881	LC2	C28-C29-C30-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2881	LC2	1	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%)	1.23	571 (20%) 2 3	37, 107, 200, 200	0
2	B	118/118 (100%)	1.90	52 (44%) 0 1	100, 143, 183, 200	0
All	All	2883/2998 (96%)	1.26	623 (21%) 2 3	37, 108, 200, 200	0

The worst 5 of 623 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2199	C	7.3
1	A	625	A	7.0
2	B	75	A	6.9
1	A	1072	U	6.4
1	A	514	G	6.3

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](#)

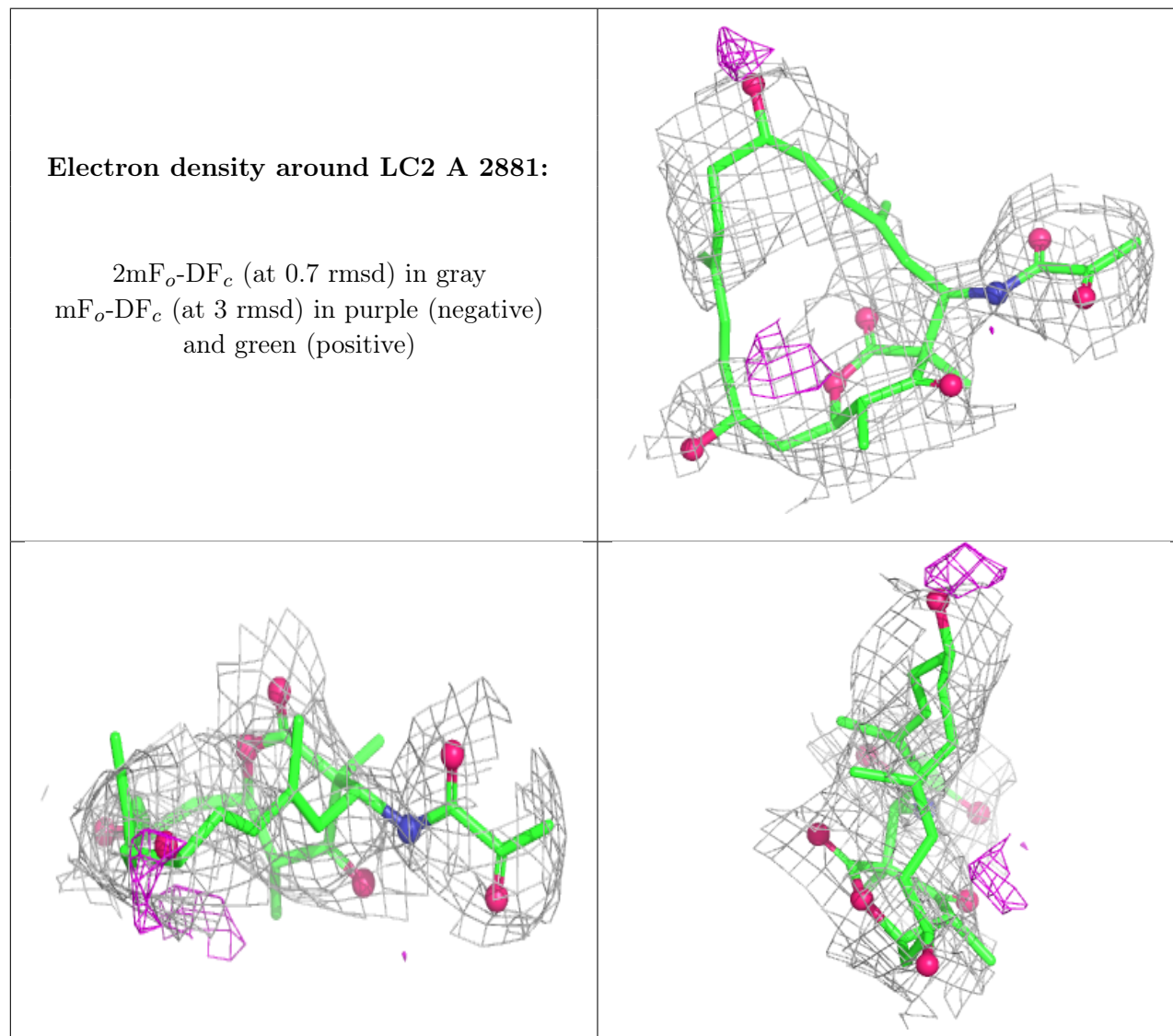
There are no oligosaccharides in this entry.

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	LC2	A	2881	33/33	0.93	0.14	88,88,88,88	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 ⓘ

There are no such residues in this entry.