



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 7, 2023 – 09:13 PM EDT

PDB ID : 1NWY  
Title : COMPLEX OF THE LARGE RIBOSOMAL SUBUNIT FROM DEINOCOCCUS RADIODURANS WITH AZITHROMYCIN  
Authors : Schluenzen, F.; Harms, J.; Franceschi, F.; Hansen, H.A.S.; Bartels, H.; Zariwach, R.; Yonath, A.  
Deposited on : 2003-02-07  
Resolution : 3.30 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

<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>.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35

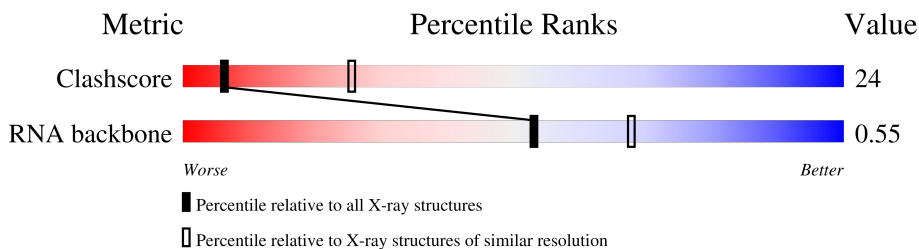
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 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))
Clashscore	141614	1205 (3.34-3.26)
RNA backbone	3102	1117 (3.70-2.90)

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  $\geq 3$ , 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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	0	2880	26% 57% 13% .
2	9	124	19% 59% 18% 5%
3	A	274	99% .
4	B	211	96% ..
5	C	204	96% .
6	D	180	98% ..
7	E	185	95% . .
8	F	146	34% 64%
9	G	144	99% .

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Mol	Chain	Length	Quality of chain
10	H	174	82% 18%
11	I	134	99%
12	J	156	90% 10%
13	K	141	87% 12%
14	L	116	97%
15	M	113	97%
16	N	166	75% 25%
17	O	118	99%
18	P	100	100%
19	Q	134	97%
20	R	94	99%
21	S	115	98%
22	T	237	94% 6%
23	U	91	95% 5%
24	W	67	97%
25	X	55	100%
26	Y	73	100%
27	Z	59	97%
28	1	55	96%
29	2	47	98%
30	3	65	97%
31	4	37	95% 5%

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
32	ZIT	0	2881	-	-	X	-
32	ZIT	0	2882	-	-	X	-

## 2 Entry composition [i](#)

There are 32 unique types of molecules in this entry. The entry contains 65404 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 RRNA.

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 RNA chain called 5S RIBOSOMAL RRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	9	118	2519	1124	464	813	118	0	0	0

- Molecule 3 is a protein called ribosomal protein L2.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
3	A	270	Total	C	0	0	270
			270	270			

- Molecule 4 is a protein called ribosomal protein L3.

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

- Molecule 5 is a protein called ribosomal protein L4.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
5	C	197	Total	C	0	0	197
			197	197			

- Molecule 6 is a protein called ribosomal protein L5.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
6	D	178	Total	C	0	0	178
			178	178			

- Molecule 7 is a protein called ribosomal protein L6.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
7	E	177	Total C 177 177	0	0	177

- Molecule 8 is a protein called ribosomal protein L9.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
8	F	52	Total C 52 52	0	0	52

- Molecule 9 is a protein called ribosomal protein L11.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
9	G	143	Total C 143 143	0	0	143

- Molecule 10 is a protein called ribosomal protein L13.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
10	H	143	Total C 143 143	0	0	143

- Molecule 11 is a protein called ribosomal protein L14.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
11	I	132	Total C 132 132	0	0	132

- Molecule 12 is a protein called ribosomal protein L15.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
12	J	141	Total C 141 141	0	0	141

- Molecule 13 is a protein called ribosomal protein L16.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
13	K	124	Total C 124 124	0	0	124

- Molecule 14 is a protein called ribosomal protein L17.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
14	L	114	Total C 114 114	0	0	114

- Molecule 15 is a protein called ribosomal protein L18.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
15	M	111	Total C 111 111	8	0	111

- Molecule 16 is a protein called ribosomal protein L19.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
16	N	125	Total C 125 125	0	0	125

- Molecule 17 is a protein called ribosomal protein L20.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
17	O	117	Total C 117 117	16	0	117

- Molecule 18 is a protein called ribosomal protein L21.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
18	P	100	Total C 100 100	0	0	100

- Molecule 19 is a protein called ribosomal protein L22.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
19	Q	130	Total C 130 130	0	0	130

- Molecule 20 is a protein called ribosomal protein L23.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
20	R	93	Total C 93 93	0	0	93

- Molecule 21 is a protein called ribosomal protein L24.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
21	S	113	Total C 113 113	0	0	113

- Molecule 22 is a protein called general stress protein Ctc.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
22	T	223	Total C 223 223	43	0	223

- Molecule 23 is a protein called ribosomal protein L27.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
23	U	86	Total C 86 86	0	0	86

- Molecule 24 is a protein called ribosomal protein L29.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
24	W	65	Total C 65 65	0	0	65

- Molecule 25 is a protein called ribosomal protein L30.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
25	X	55	Total C 55 55	4	0	55

- Molecule 26 is a protein called ribosomal protein L31.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
26	Y	73	Total C 73 73	0	0	73

- Molecule 27 is a protein called ribosomal protein L32.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
27	Z	58	Total C 58 58	0	0	58

- Molecule 28 is a protein called ribosomal protein L33.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
28	1	53	Total C 53 53	0	0	53

- Molecule 29 is a protein called ribosomal protein L34.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
29	2	46	Total C 46 46	0	0	46

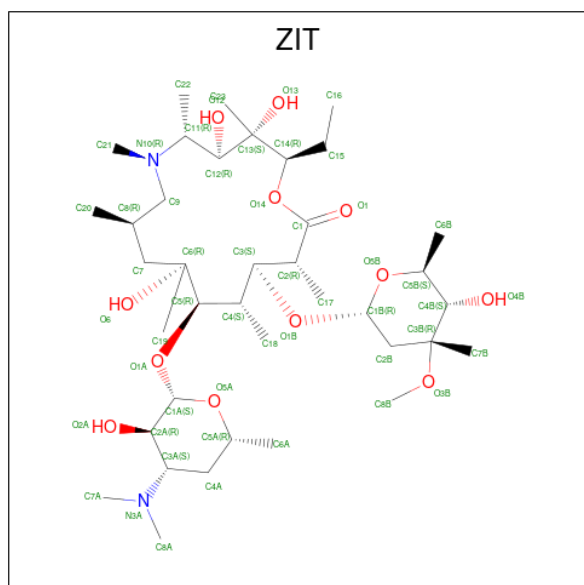
- Molecule 30 is a protein called ribosomal protein L35.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
30	3	63	Total C 63 63	0	0	63

- Molecule 31 is a protein called ribosomal protein L36.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
31	4	35	Total C 35 35	0	0	35

- Molecule 32 is AZITHROMYCIN (three-letter code: ZIT) (formula:  $C_{38}H_{72}N_2O_{12}$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	0	1	Total C N O 52 38 2 12	0	0

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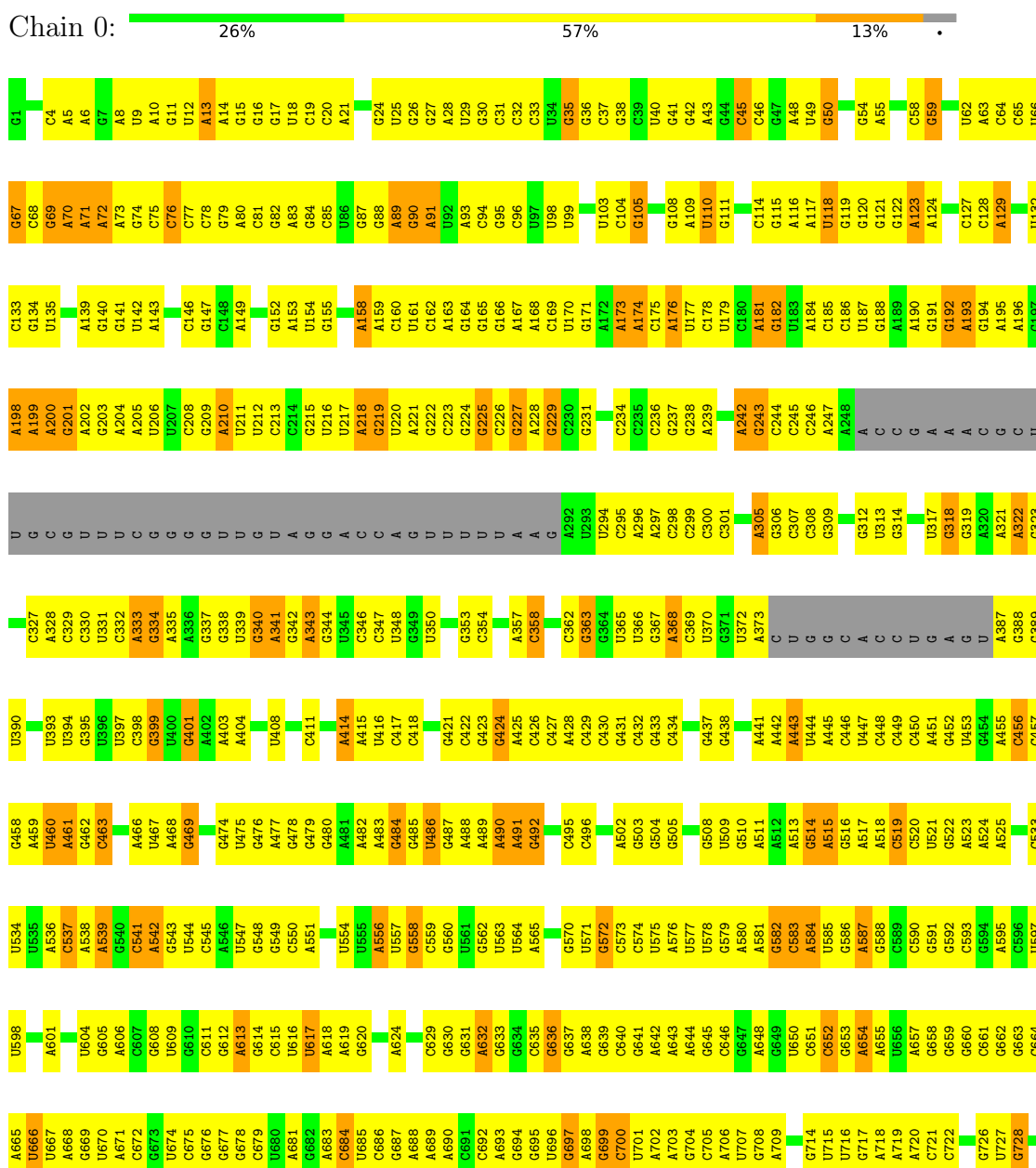
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
32	0	1	52	38	2	12	0	0

### 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.

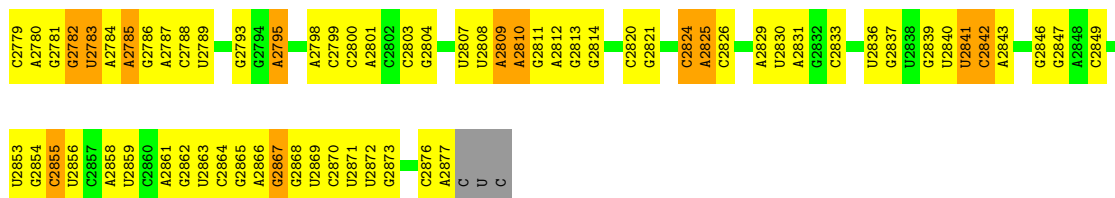
Note EDS was not executed.

- Molecule 1: 23S RIBOSOMAL RRNA

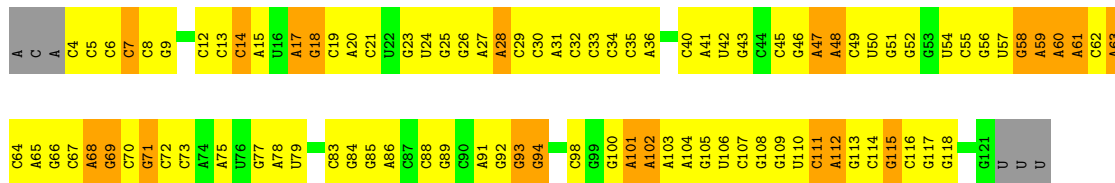
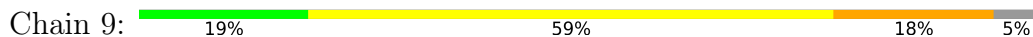


G1691	C1692	A1693	A1694	U1695	C1696	U1697	C1698	A1699	G1622	C1623	A1624	A1625	A1626	C1627	U1628	A1629	A1630	C1631	A1632	C1633	A1634	G1635	G1636	A1637	A1638	A1639	A1640	A1641	A1642	A1643	A1644	A1645	A1646	A1647	A1648	A1649	A1650	A1651	A1652	A1653	A1654	A1655	A1656	A1657	A1658	A1659	A1660	A1661	A1662	A1663	A1664	A1665	A1666	A1667	A1668	A1669	G1670	A1671	A1672	C1673	C1674	G1675	A1676	A1677	A1678	A1679	U1680	A1681	A1682	A1683	A1684	A1685	A1686	A1687	A1688	A1689	C1690	C1691	C1692	C1693	C1694	C1695	C1696	C1697	C1698	C1699	C1700	C1701	C1702	C1703	C1704	C1705	C1706	C1707	C1708	U1709	G1710	A1711	A1712	G1713	A1714	A1715	G1716	A1717	A1718	G1719	G1720	A1721	G1722	G1723	A1724	C1725	G1726	C1727	G1728	A1729	G1730	C1731	C1732	C1733	G1734	A1735	A1736	A1737	A1738	G1739	G1740	G1741	G1742	C1743	G1744	U1745	A1746	A1747	A1748	A1749	A1750	A1751	U1752	A1753	A1754	G1755	C1756	C1757	C1758	C1759	C1760	C1761	A1762	A1763	C1764	C1765	A1766	C1767	U1768	C1769	U1770	C1771	G1772	G1773	A1774	U1775	G1776	A1777	G1778	G1779	G1780	G1781	G1782	G1783	U1784	U1785	U1786	A1787	A1788	G1789	A1790	G1791	U1792	U1793	G1794	G1795	A1796	A1797	A1798	A1799	A1800	A1801	A1802	A1803	C1804	C1805	A1806	A1807	C1808	C1809	U1810	G1811	G1812	A1813	A1814	A1815	C1816	A1817	C1818	C1819	U1820	A1821	U1822	C1823	C1824	C1825	U1826	C1827	C1828	C1829	C1830	G1831	A1832	C1833	C1834	C1835	C1836	C1837	C1838	C1839	C1840	C1841	A1842	C1843	C1844	C1845	C1846	C1847	A1848	C1849	C1850	C1851	C1852	C1853	C1854	C1855	C1856	C1857	C1858	A1859	A1860	A1861	A1862	A1863	A1864	A1865	A1866	A1867	A1868	A1869	A1870	A1871	A1872	A1873	A1874	A1875	A1876	A1877	A1878	A1879	A1880	A1881	A1882	A1883	A1884	A1885	A1886	A1887	A1888	A1889	A1890	A1891	A1892	A1893	A1894	A1895	A1896	A1897	A1898	A1899	A1900	A1901	A1902	A1903	A1904	A1905	A1906	A1907	A1908	A1909	A1910	A1911	A1912	A1913	A1914	A1915	A1916	A1917	A1918	A1919	A1920	A1921	A1922	A1923	A1924	A1925	A1926	A1927	A1928	A1929	A1930	A1931	A1932	A1933	A1934	A1935	A1936	A1937	A1938	A1939	A1940	A1941	A1942	A1943	A1944	A1945	A1946	A1947	A1948	A1949	A1950	A1951	A1952	A1953	A1954	A1955	A1956	A1957	A1958	A1959	A1960	A1961	A1962	A1963	A1964	A1965	A1966	A1967	A1968	A1969	A1970	A1971	A1972	A1973	A1974	A1975	A1976	A1977	A1978	A1979	A1980	A1981	A1982	A1983	A1984	A1985	A1986	A1987	A1988	A1989	A1990	A1991	A1992	A1993	A1994	A1995	A1996	A1997	A1998	A1999	A2000	A2001	A2002	A2003	A2004	A2005	A2006	A2007	A2008	A2009	A2010	A2011	A2012	A2013	A2014	A2015	A2016	A2017	A2018	A2019	A2020	A2021	A2022	A2023	A2024	A2025	A2026	A2027	A2028	A2029	A2030	A2031	A2032	A2033	A2034	A2035	A2036	A2037	A2038	A2039	A2040	A2041	A2042	A2043	A2044	A2045	A2046	A2047	A2048	A2049	A2050	A2051	A2052	A2053	A2054	A2055	A2056	A2057	A2058	A2059	A2060	A2061	A2062	A2063	A2064	A2065	A2066	A2067	A2068	A2069	A2070	A2071	A2072	A2073	A2074	A2075	A2076	A2077	A2078	A2079	A2080	A2081	A2082	A2083	A2084	A2085	A2086	A2087	A2088	A2089	A2090	A2091	A2092	A2093	A2094	A2095	A2096	A2097	A2098	A2099	A2100	A2101	A2102	A2103	A2104	A2105	A2106	A2107	A2108	A2109	A2110	A2111	A2112	A2113	A2114	A2115	A2116	A2117	A2118	A2119	A2120	A2121	A2122	A2123	A2124	A2125	A2126	A2127	A2128	A2129	A2130	A2131	A2132	A2133	A2134	A2135	A2136	A2137	A2138	A2139	A2140	A2141	A2142	A2143	A2144	A2145	A2146	A2147	A2148	A2149	A2150	A2151	A2152	A2153	A2154	A2155	A2156	A2157	A2158	A2159	A2160	A2161	A2162	A2163	A2164	A2165	A2166	A2167	A2168	A2169	A2170	A2171	A2172	A2173	A2174	A2175	A2176	A2177	A2178	A2179	A2180	A2181	A2182	A2183	A2184	A2185	A2186	A2187	A2188	A2189	A2190	A2191	A2192	A2193	A2194	A2195	A2196	A2197	A2198	A2199	A2200	A2201	A2202	A2203	A2204	A2205	A2206	A2207	A2208	A2209	A2210	A2211	A2212	A2213	A2214	A2215	A2216	A2217	A2218	A2219	A2220	A2221	A2222	A2223	A2224	A2225	A2226	A2227	A2228	A2229	A2230	A2231	A2232	A2233	A2234	A2235	A2236	A2237	A2238	A2239	A2240	A2241	A2242	A2243	A2244	A2245	A2246	A2247	A2248	A2249	A2250	A2251	A2252	A2253	A2254	A2255	A2256	A2257	A2258	A2259	A2260	A2261	A2262	A2263	A2264	A2265	A2266	A2267	A2268	A2269	A2270	A2271	A2272	A2273	A2274	A2275	A2276	A2277	A2278	A2279	A2280	A2281	A2282	A2283	A2284	A2285	A2286	A2287	A2288	A2289	A2290	A2291	A2292	A2293	A2294	A2295	A2296	A2297	A2298	A2299	A2300	A2301	A2302	A2303	A2304	A2305	A2306	A2307	A2308	A2309	A2310	A2311	A2312	A2313	A2314	A2315	A2316	A2317	A2318	A2319	A2320	A2321	A2322	A2323	A2324	A2325	A2326	A2327	A2328	A2329	A2330	A2331	A2332	A2333	A2334	A2335	A2336	A2337	A2338	A2339	A2340	A2341	A2342	A2343	A2344	A2345	A2346	A2347	A2348	A2349	A2350	A2351	A2352	A2353	A2354	A2355	A2356	A2357	A2358	A2359	A2360	A2361	A2362	A2363	A2364	A2365	A2366	A2367	A2368	A2369	A2370	A2371	A2372	A2373	A2374	A2375	A2376	A2377	A2378	A2379	A2380	A2381	A2382	A2383	A2384	A2385	A2386	A2387	A2388	A2389	A2390	A2391	A2392	A2393	A2394	A2395	A2396	A2397	A2398	A2399	A2400	A2401	A2402	A2403	A2404	A2405	A2406	A2407	A2408	A2409	A2410	A2411	A2412	A2413	A2414	A2415	A2416	A2417	A2418	A2419	A2420	A2421	A2422	A2423	A2424	A2425	A2426	A2427	A2428	A2429	A2430	A2431	A2432	A2433	A2434	A2435	A2436	A2437	A2438	A2439	A2440	A2441	A2442	A2443	A2444	A2445	A2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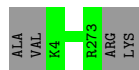




• Molecule 2: 5S RIBOSOMAL RRNA



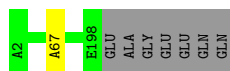
• Molecule 3: ribosomal protein L2



• Molecule 4: ribosomal protein L3



• Molecule 5: ribosomal protein L4



• Molecule 6: ribosomal protein L5

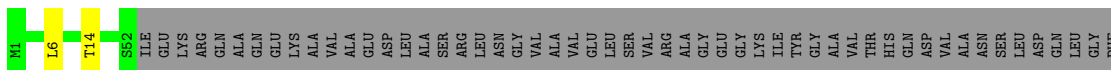


• Molecule 7: ribosomal protein L6





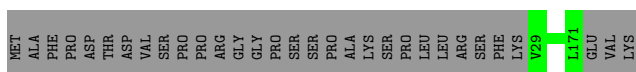
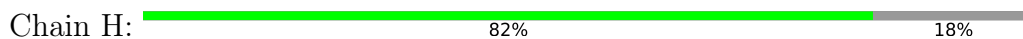
- Molecule 8: ribosomal protein L9



- Molecule 9: ribosomal protein L11



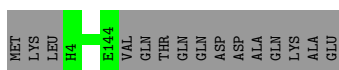
- Molecule 10: ribosomal protein L13



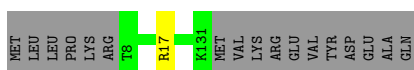
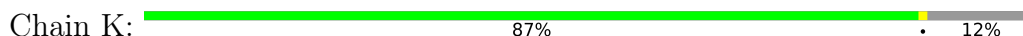
- Molecule 11: ribosomal protein L14



- Molecule 12: ribosomal protein L15



- Molecule 13: ribosomal protein L16



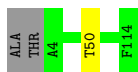
- Molecule 14: ribosomal protein L17

Chain L:  97% ..



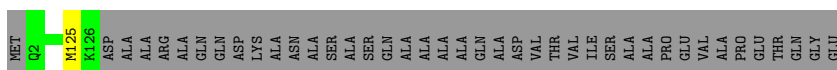
- Molecule 15: ribosomal protein L18

Chain M:  97% ..



- Molecule 16: ribosomal protein L19

Chain N:  75% . 25%



- Molecule 17: ribosomal protein L20

Chain O:  99% .



- Molecule 18: ribosomal protein L21

Chain P:  100%

There are no outlier residues recorded for this chain.

- Molecule 19: ribosomal protein L22

Chain Q:  97% .



- Molecule 20: ribosomal protein L23

Chain R:  99% .



- Molecule 21: ribosomal protein L24

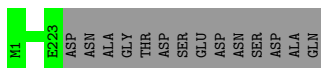
Chain S:  98% .





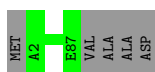
- Molecule 22: general stress protein Ctc

Chain T: 94% 6%



- Molecule 23: ribosomal protein L27

Chain U: 95% 5%



- Molecule 24: ribosomal protein L29

Chain W: 97%



- Molecule 25: ribosomal protein L30

Chain X: 100%

There are no outlier residues recorded for this chain.

- Molecule 26: ribosomal protein L31

Chain Y: 100%

There are no outlier residues recorded for this chain.

- Molecule 27: ribosomal protein L32

Chain Z: 97%



- Molecule 28: ribosomal protein L33

Chain 1: 96%



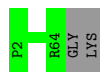
- Molecule 29: ribosomal protein L34

Chain 2:  98% .



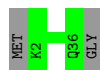
- Molecule 30: ribosomal protein L35

Chain 3:  97% .



- Molecule 31: ribosomal protein L36

Chain 4:  95% 5%



## 4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	170.80Å 409.50Å 695.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.30	Depositor
% Data completeness (in resolution range)	(Not available) (15.00-3.30)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.11	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.279 , 0.304	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	65404	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

## 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: ZIT

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	0.23	0/66467	0.67	0/103673
2	9	0.59	0/2816	0.81	1/4388 (0.0%)
All	All	0.26	0/69283	0.67	1/108061 (0.0%)

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	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	9	94	G	N9-C1'-C2'	-6.58	104.76	112.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	1342	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	0	59359	0	29917	2160	0
2	9	2519	0	1285	147	0
3	A	270	0	0	0	0
4	B	205	0	0	3	0
5	C	197	0	0	1	0
6	D	178	0	0	1	0
7	E	177	0	0	1	0
8	F	52	0	0	1	0
9	G	143	0	0	0	0
10	H	143	0	0	0	0
11	I	132	0	0	0	0
12	J	141	0	0	0	0
13	K	124	0	0	1	0
14	L	114	0	0	1	0
15	M	111	0	0	1	0
16	N	125	0	0	1	0
17	O	117	0	0	0	0
18	P	100	0	0	0	0
19	Q	130	0	0	0	0
20	R	93	0	0	0	0
21	S	113	0	0	0	0
22	T	223	0	0	0	0
23	U	86	0	0	0	0
24	W	65	0	0	0	0
25	X	55	0	0	0	0
26	Y	73	0	0	0	0
27	Z	58	0	0	1	0
28	1	53	0	0	0	0
29	2	46	0	0	0	0
30	3	63	0	0	0	0
31	4	35	0	0	0	0
32	0	104	0	144	47	0
All	All	65404	0	31346	2342	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 24.

The worst 5 of 2342 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)
32:0:2882:ZIT:H6A1	32:0:2882:ZIT:C6B	1.61	1.30
32:0:2881:ZIT:H6A1	32:0:2881:ZIT:C6B	1.61	1.29
1:0:1679:U:H2'	1:0:1680:U:H5''	1.27	1.16
1:0:2058:U:H1'	1:0:2576:G:H21	1.10	1.14
1:0:2548:G:H2'	1:0:2549:G:H5''	1.26	1.14

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%)	485 (17%)	43 (1%)
2	9	117/124 (94%)	23 (19%)	1 (0%)
All	All	2874/3004 (95%)	508 (17%)	44 (1%)

5 of 508 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	13	A
1	0	35	G
1	0	45	C
1	0	48	A
1	0	49	U

5 of 44 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	2015	G
1	0	2377	U

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	0	2018	G
1	0	2204	A
1	0	2560	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

2 ligands are 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
32	ZIT	0	2881	-	54,54,54	0.84	1 (1%)	82,83,83	1.27	6 (7%)
32	ZIT	0	2882	-	54,54,54	0.84	2 (3%)	82,83,83	1.27	5 (6%)

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
32	ZIT	0	2881	-	-	3/72/107/107	0/3/3/3
32	ZIT	0	2882	-	-	5/72/107/107	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	0	2881	ZIT	C3A-N3A	-2.32	1.42	1.48
32	0	2882	ZIT	C3A-N3A	-2.23	1.42	1.48
32	0	2882	ZIT	C1A-C2A	2.04	1.58	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	0	2882	ZIT	C1A-O1A-C5	-7.16	103.82	116.25
32	0	2881	ZIT	C1A-O1A-C5	-7.09	103.94	116.25
32	0	2881	ZIT	C4A-C3A-C2A	-3.16	105.42	109.97
32	0	2882	ZIT	C4A-C3A-C2A	-3.12	105.47	109.97
32	0	2882	ZIT	O1B-C3-C4	2.68	111.45	108.22

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	0	2882	ZIT	C13-C14-C15-C16
32	0	2881	ZIT	O5A-C1A-O1A-C5
32	0	2882	ZIT	O5A-C1A-O1A-C5
32	0	2882	ZIT	O14-C14-C15-C16
32	0	2881	ZIT	C4-C5-O1A-C1A

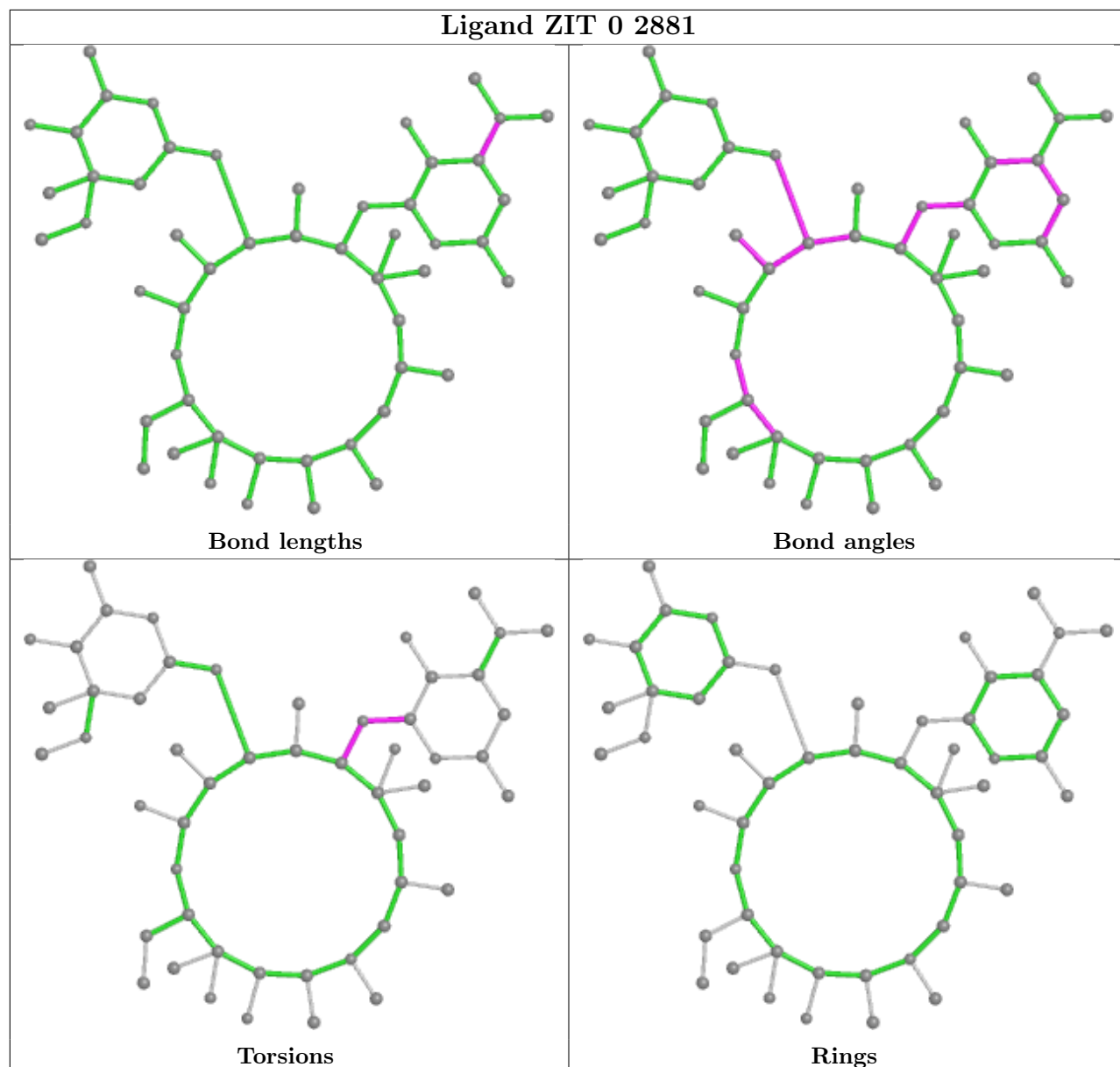
There are no ring outliers.

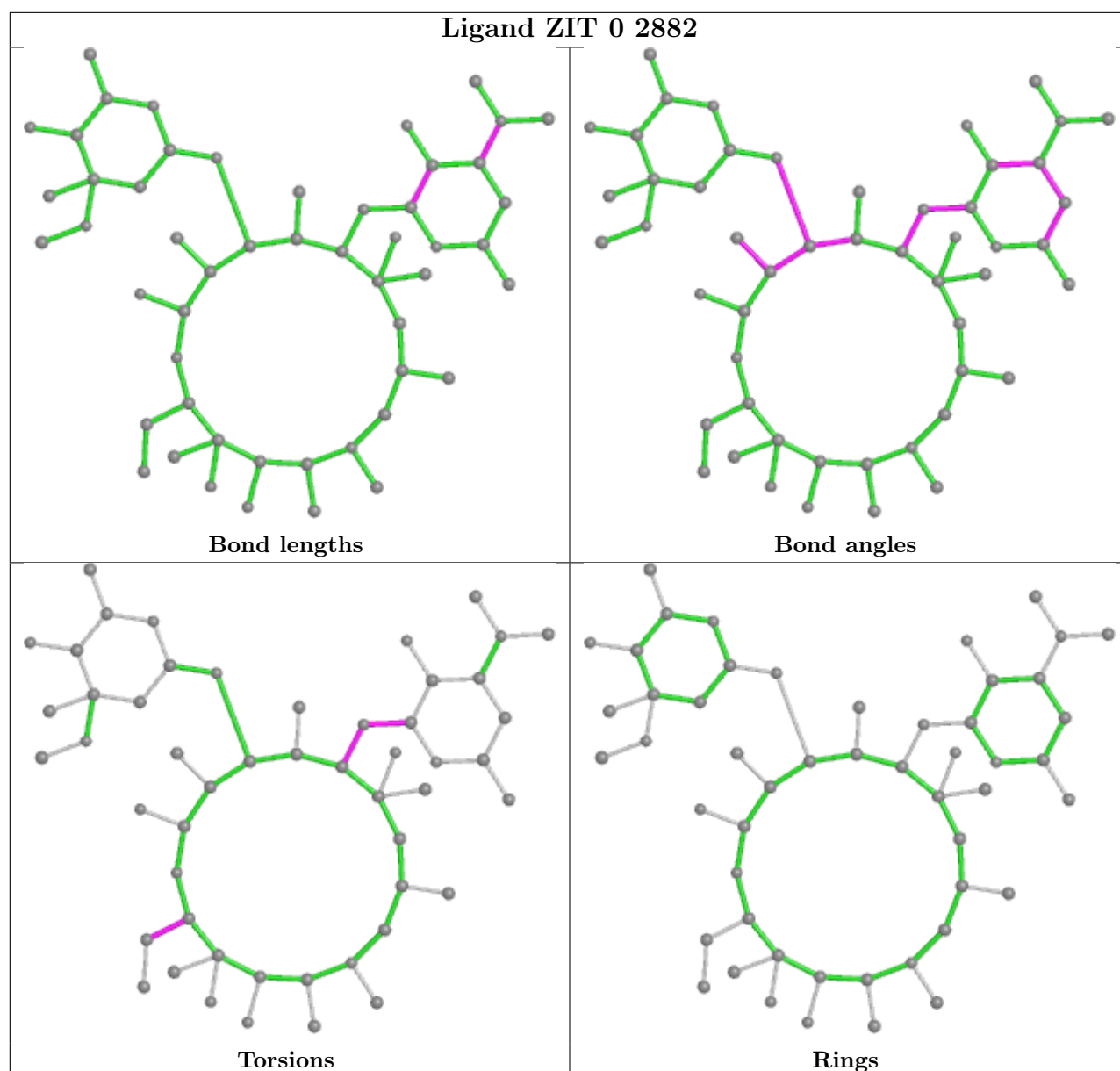
2 monomers are involved in 47 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	0	2881	ZIT	21	0
32	0	2882	ZIT	26	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](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.