



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 18, 2021 – 06:05 PM EST

PDB ID : 1P9X  
Title : THE CRYSTAL STRUCTURE OF THE 50S LARGE RIBOSOMAL SUB-UNIT FROM DEINOCOCCUS RADIODURANS COMPLEXED WITH TELITHROMYCIN KETOLIDE ANTIBIOTIC  
Authors : Berisio, R.; Harms, J.; Schlutzen, F.; Zarivach, R.; Hansen, H.A.; Fucini, P.; Yonath, A.  
Deposited on : 2003-05-13  
Resolution : 3.40 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.

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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)
Xtriage (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)	:	2.16

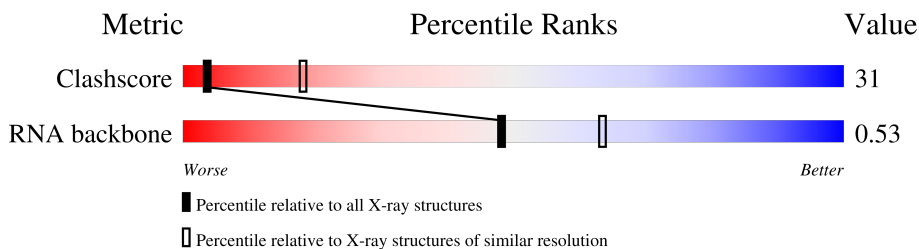
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.40 Å.

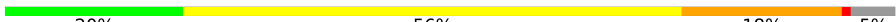
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1055 (3.48-3.32)
RNA backbone	3102	1006 (3.84-2.96)

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	 20% 56% 18% • 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
2	TEL	0	2881	X	-	-	-

2 Entry composition [i](#)

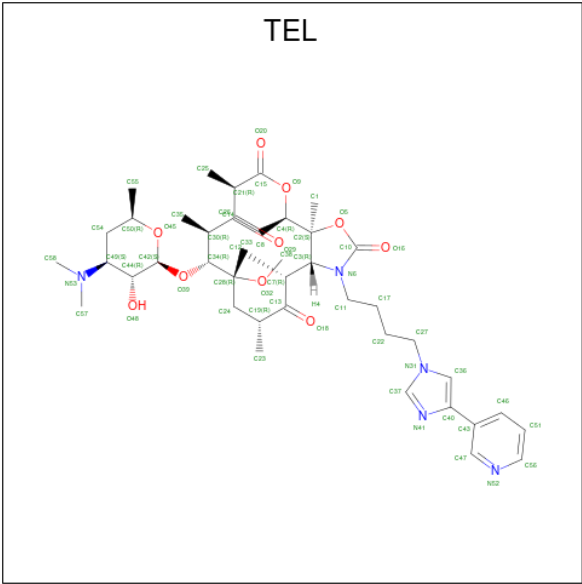
There are 2 unique types of molecules in this entry. The entry contains 58817 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	2738	58759	26211	10836	18975	2737	0	0	0

- Molecule 2 is TELITHROMYCIN (three-letter code: TEL) (formula: C<sub>43</sub>H<sub>65</sub>N<sub>5</sub>O<sub>10</sub>).



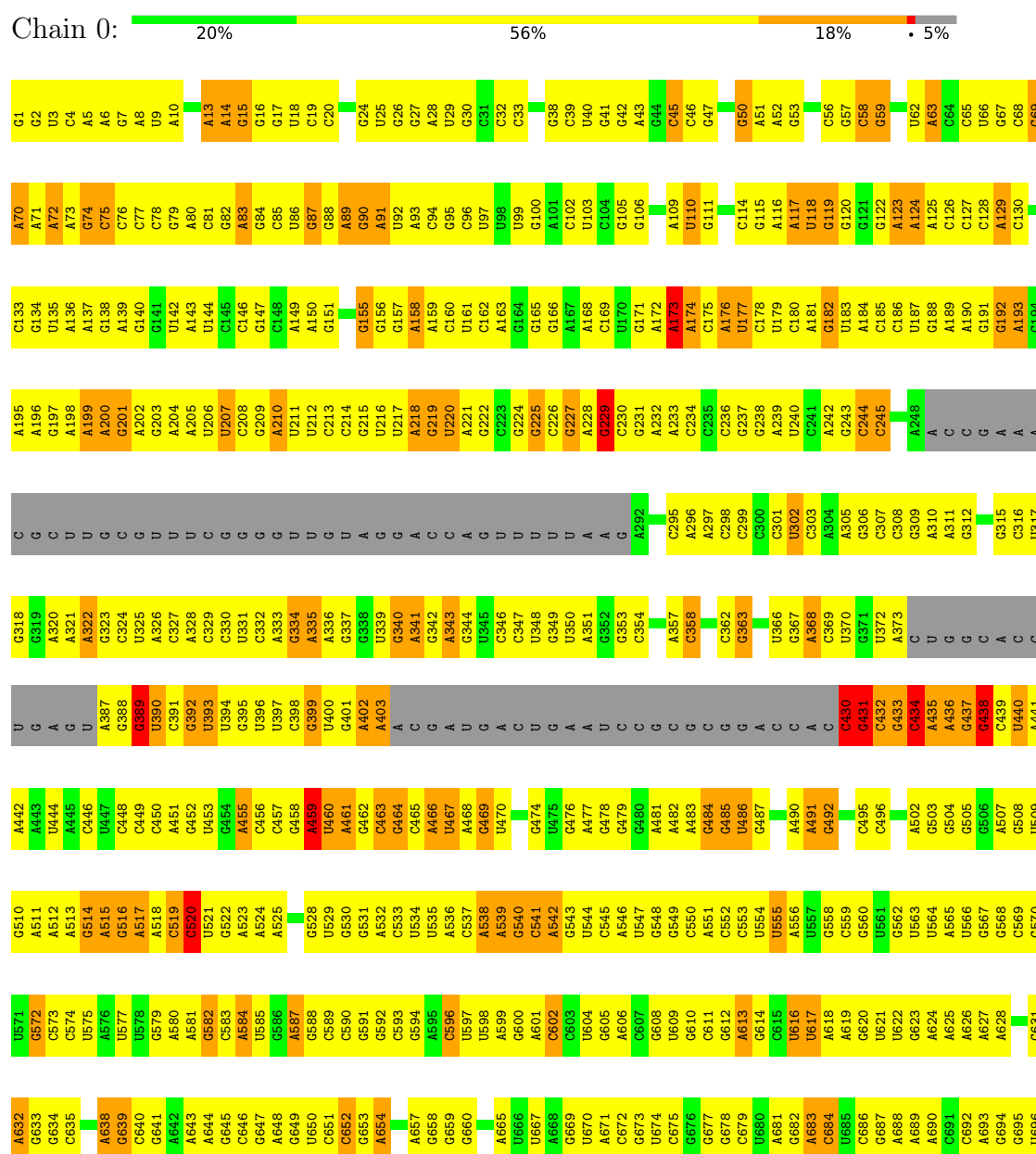
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	0	1	58	43	5	10	0	0

### 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 RNA



C1516	C1517	U1518	C1519	C1520	C1521	C1522	C1523	A1524	C1525	C1526	C1527	C1528	G1529	A1530	C1531	A1532	C1533	A1534	G1535	C1541	G1542	A1543	G1544	C1545	G1546	U1547	C1548	A1551	G1552	G1553	A1554	C1555	U1556	C1557	C1558	G1559	A1560	A1561	G1562	G1566	C1567	A1568	G1569	C1570	C1571	C1572	G1573	A1574	C1575	G1576	U1577	U1578	G1579	A1582	A1583	G1584	A1585	C1586	A1587	A1588	G1589	U1592	C1593	U1594	A1595	A1596	A1597	C1598	A1603	A1604	A1605	C1606	A1607	U1608	G1609	A1610	U1611	U1612	A1681	A1682	G1683	G1684																													
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G2624	A2556	G2492	G2424	C2360	U2289	A2226	C2094	C2027	C1962	C1892	G1823	G1762	C1698
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U2626	U2558	G2494	G2426	G2362	U2290	U2228	U2096	G2029	G1964	A1899	C1825	A1764	C1700
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U2640	G2572	U2379	U2380	C2382	G2309	U2242	G2110	G2046	A1981	U1914	A1839	C1779	G1716
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G2642	G2574	U2381	A2382	U2384	U2311	C2244	U	C2048	C1983	U1916	G1846	G1781	G1718
C2643	U2575	U2382	A2383	C2385	G2312	A2245	C	C2049	G1984	G1917	G1847	A1782	G1719
U2644	G2576	C2383	U2384	U2386	A2313	A2246	G	U2051	U1985	U1918	U1848	G1783	G1720
C2645	A2577	U2384	U2385	U2387	A2314	A2247	A2117	G2050	G1986	A1919	G1852	A1784	G1721
A2646	G2578	C2385	U2386	U2388	G2315	U2248	A2118	U2052	C1987	A1920	G1853	U1785	U1723
G2647	C2579	U2386	U2387	U2389	C2316	U2249	A2119	G2053	A1988	U1922	G1854	C1786	G1724
C2648	U2580	G2387	U2388	U2390	C2317	U2250	C2120	A2054	U1994	U1923	U1856	C1787	C1725
U2649	G2581	C2388	U2389	A2391	G2318	A2251	C2121	G2055	G1995	C1924	G1857	G1790	C1726
C2650	A2582	U2389	A2390	C2391	U2319	A2252	U	G2056	U1996	C1925	C1858	C1791	C1729
G2651	G2583	C2390	G2391	C2392	C2320	A2253	G2122	U2057	A1997	G1926	A1859	C1792	G1730
A2652	C2584	U2391	U2392	C2393	C2321	A2254	C2123	U2058	A1998	U1927	A1860	A1793	C1731
C2653	U2585	G2392	G2393	C2394	U2322	A2255	C2124	U2059	U1999	G1928	G1861	A1794	U1732
U2654	G2586	C2393	U2394	C2395	U2323	A2256	U	A2060	U2000	U1929	C1862	C1795	U1733
G2655	C2587	U2394	U2395	C2396	G2324	A2257	U	C2061	G2001	C1930	U1863	A1796	C1736
C2656	U2588	G2395	G2396	C2397	U2325	A2258	U	U2062	A2002	G1931	G1864	C1797	G1737
U2657	G2589	C2396	U2397	C2398	C2326	A2259	U	A2063	A2003	G1932	G1865	G1798	U1738
C2658	C2590	U2397	U2398	C2399	C2327	A2260	G	U2069	U2004	G1933	G1866	A1800	G1739
G2659	U2591	C2398	G2399	C2400	U2328	A2261	C2125	A2060	U2005	U1937	A1869	C1801	G1740
U2660	C2592	U2399	U2400	A2401	C2329	G2262	U	C2062	G2006	U1938	U1870	A1802	G1741
C2661	G2593	C2400	A2401	C2402	G2330	A2263	G	U2063	A2007	U1939	G1871	G1803	G
U2662	U2594	G2401	U2402	C2403	U2331	A2264	U	A2063	A2008	G1942	U1872	C1804	C1743
G2663	A2595	U2402	C2403	C2404	C2332	A2265	C2135	A2064	C2009	G1943	A1873	G1805	G1744
C2664	C2596	U2403	C2404	C2405	C2333	A2266	U	U2065	G2010	A1944	G1874	G1806	C1745
U2665	U2597	G2404	A2405	C2406	U2334	A2267	C2136	U2066	G2011	G1945	C1875	A1807	A1746
C2666	G2598	U2405	C2406	C2407	C2335	A2268	U	G2067	A2012	C1946	C1876	G1808	U1747
U2667	C2599	U2406	C2407	U2408	U2336	A2269	C2137	G2068	A2013	U1947	C1877	U1748	C1750
G2668	U2600	A2407	C2408	U2409	C2337	A2270	C2138	G2069	A2014	G1947	C1878	U1810	G1749
C2669	C2601	U2408	U2409	A2410	U2338	A2271	A	U2070	G2005	U1937	A1869	C1801	G1740
U2670	G2602	U2409	U2410	C2411	U2339	A2272	G	G2070	G2006	U1938	U1870	A1802	G1741
C2671	A2603	U2410	C2411	C2412	U2340	A2273	U	A2063	A2007	U1939	G1871	G1803	G
U2672	U2604	U2411	C2412	C2413	C2340	A2274	U	U2062	A2008	G1942	U1872	C1804	C1743
G2673	C2605	U2412	C2413	C2414	C2341	A2275	C2139	U2063	G2009	G1943	A1873	G1805	G1744
C2674	U2606	U2413	C2414	C2415	C2342	A2276	U	G2064	G2010	A1944	G1874	G1806	C1745
U2675	G2607	U2414	C2415	C2416	C2343	A2277	C2140	U2065	G2011	G1945	C1875	A1807	A1746
C2676	A2608	U2415	C2416	C2417	C2344	A2278	C2141	U2066	A2012	C1946	C1876	G1808	U1747
U2677	G2609	U2416	C2417	U2417	C2345	A2279	A	A2064	A2013	U1947	C1877	U1748	C1750
		U2417	U2418	U2419	C2346	A2280		U2065	A2014	G1947	C1878	U1810	G1749



## 4 Data and refinement statistics

Xtriage (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, $\alpha$ , $\beta$ , $\gamma$	170.00Å 414.50Å 693.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.40	Depositor
% Data completeness (in resolution range)	(Not available) (15.00-3.40)	Depositor
$R_{merge}$	0.18	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.273 , 0.340	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	58817	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	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: TEL

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	0.77	20/65792 (0.0%)	0.71	28/102613 (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	28

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	762	A	O3'-P	-8.05	1.51	1.61
1	0	1410	U	N1-C2	6.70	1.44	1.38
1	0	2493	U	N1-C2	-6.33	1.32	1.38
1	0	1276	U	N1-C2	6.27	1.44	1.38
1	0	2555	G	C5-C6	-6.20	1.36	1.42

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	1182	U	O4'-C1'-N1	13.88	119.30	108.20
1	0	2044	G	P-O3'-C3'	11.50	133.50	119.70
1	0	765	C	N1-C1'-C2'	11.09	128.42	114.00
1	0	2001	G	N9-C1'-C2'	-9.80	101.22	112.00
1	0	2041	A	OP1-P-OP2	-6.87	109.30	119.60

There are no chirality outliers.

5 of 28 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	229	G	Sidechain
1	0	389	G	Sidechain
1	0	431	G	Sidechain
1	0	438	G	Sidechain
1	0	459	A	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	58759	0	29615	2745	0
2	0	58	0	65	11	0
All	All	58817	0	29680	2746	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 31.

The worst 5 of 2746 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)
1:0:940:G:H3'	1:0:941:U:H5''	1.24	1.18
1:0:752:G:H5'	1:0:1775:A:H61	1.07	1.13
1:0:1572:C:H2'	1:0:1573:G:H5''	1.21	1.10
1:0:2451:G:H1'	1:0:2457:A:H61	1.16	1.09
1:0:387:A:H5'	1:0:436:A:H62	1.07	1.08

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	0	2727/2880 (94%)	580 (21%)	62 (2%)

5 of 580 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	13	A
1	0	14	A
1	0	15	G
1	0	45	C
1	0	50	G

5 of 62 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	1299	A
1	0	1617	G
1	0	2633	A
1	0	1338	G
1	0	1634	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 monosaccharides 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
2	TEL	0	2881	-	59,62,62	3.60	31 (52%)	77,92,92	3.46	33 (42%)

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
2	TEL	0	2881	-	1/1/19/19	23/73/108/108	0/4/5/5

The worst 5 of 31 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	0	2881	TEL	C30-C34	12.60	1.72	1.54
2	0	2881	TEL	C7-C3	8.59	1.65	1.54
2	0	2881	TEL	C24-C28	7.93	1.64	1.52
2	0	2881	TEL	O9-C15	7.30	1.51	1.34
2	0	2881	TEL	C47-C43	6.74	1.51	1.39

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	0	2881	TEL	O9-C15-C21	13.29	124.38	110.88
2	0	2881	TEL	C3-N6-C10	-11.45	96.35	111.69
2	0	2881	TEL	C42-O39-C34	7.20	128.76	116.25
2	0	2881	TEL	O20-C15-C21	-6.87	115.73	124.77
2	0	2881	TEL	C11-N6-C10	-6.78	113.68	122.25

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	0	2881	TEL	C21

5 of 23 torsion outliers are listed below:

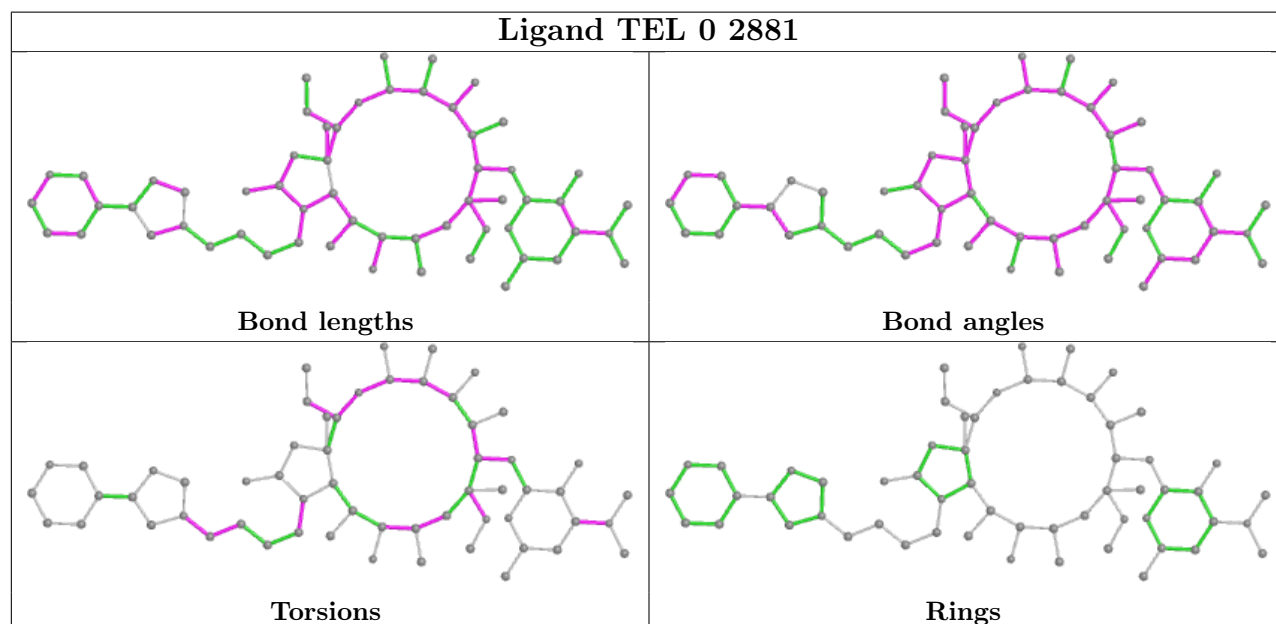
Mol	Chain	Res	Type	Atoms
2	0	2881	TEL	C7-C13-C19-C24
2	0	2881	TEL	O9-C15-C21-C25
2	0	2881	TEL	C25-C21-C26-O29
2	0	2881	TEL	C25-C21-C26-C30
2	0	2881	TEL	C26-C30-C34-C28

There are no ring outliers.

1 monomer is involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	0	2881	TEL	11	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.