



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 04:28 am GMT

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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

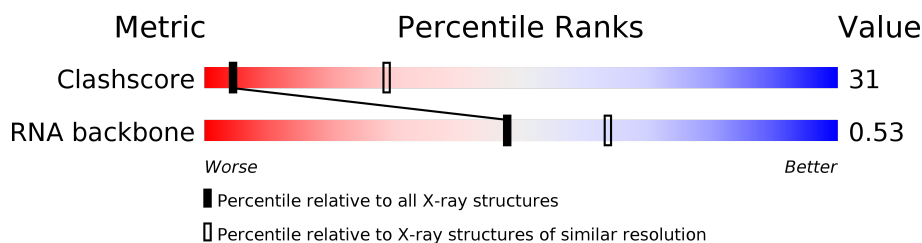
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 Å.

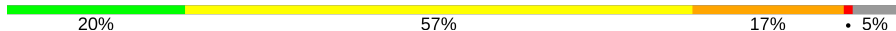
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	1832 (3.50-3.30)
RNA backbone	2435	1009 (3.96-2.84)

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 ≥ 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	0	2880	 20% 57% 17% • 5%

2 Entry composition [i](#)

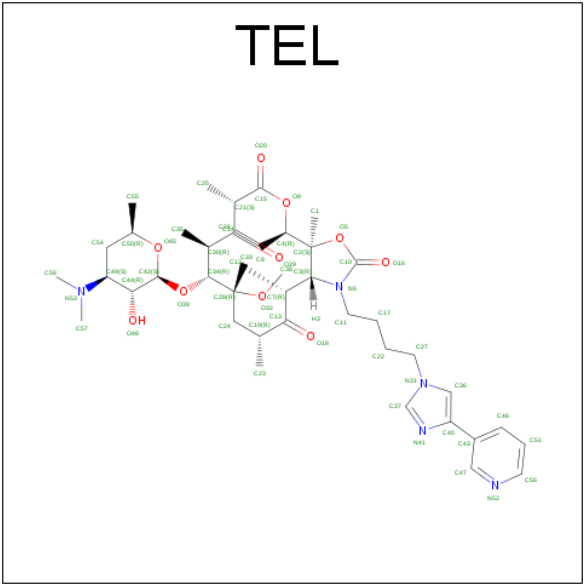
There are 2 unique types of molecules in this entry. The entry contains 58817 atoms, of which 0 are hydrogens and 0 are deuteriums.

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: C₄₃H₆₅N₅O₁₀).



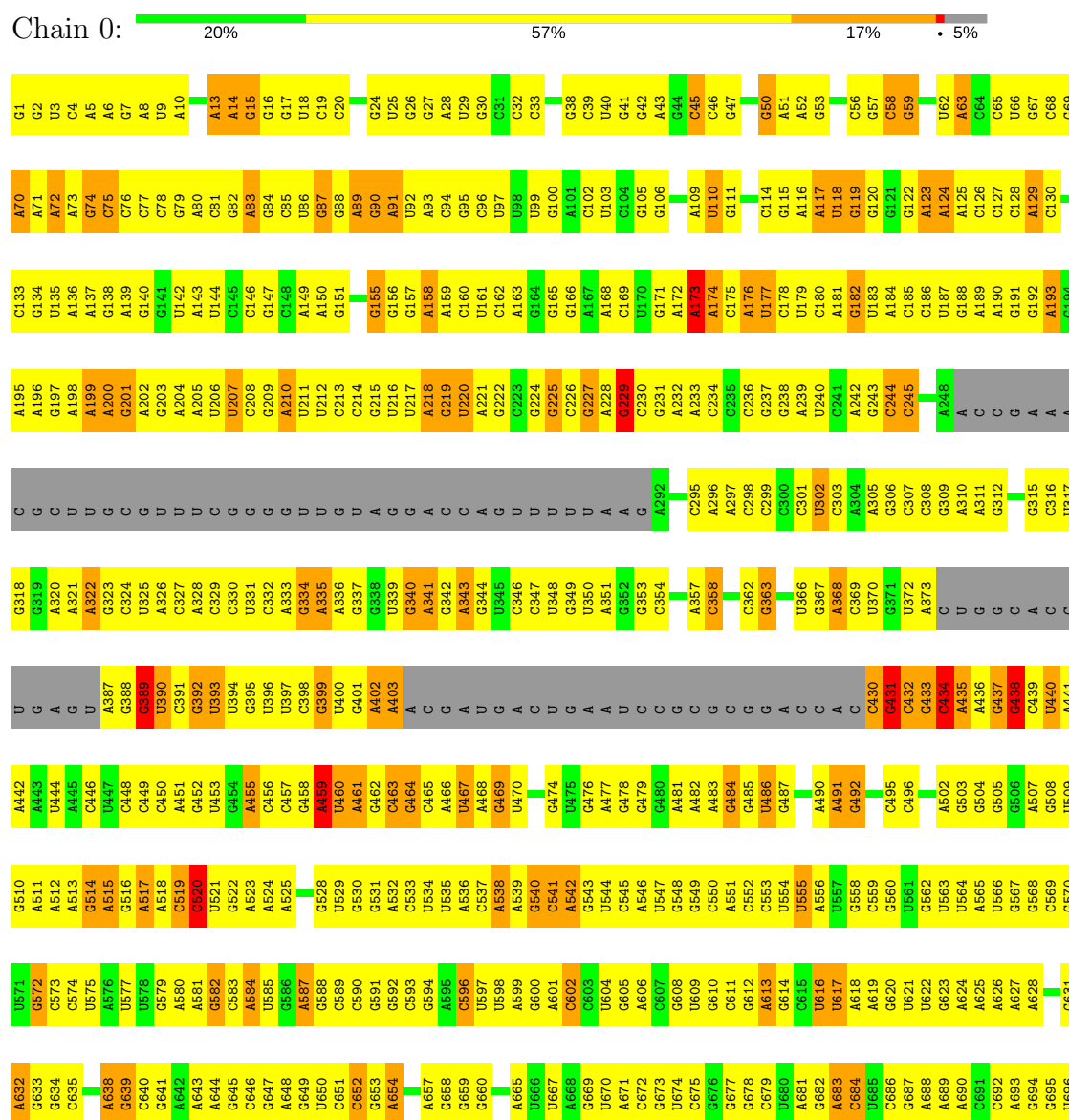
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	0	1	58	43	5	10	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

Note EDS was not executed.

• Molecule 1: 23S RIBOSOMAL RNA



WORLDWIDE
PDB
PROTEIN DATA BANK

G2741	C2678	A2544	C2480	U2410	A2348	A2277	U2212	G	U2081	G2015	C1948		A1811	A1751
G2742	G2679	A2545	G2481	A2411	G2349	A2278	G2213	G	C2082	A2016	A1949		U1812	A1751
G2743	U2680	A2546	A2482	A2412	G2350	G2279	G2214	C	G2083	U2017	C1950		A1813	A1752
A2681	A2681	C2547	U2483	A2413	G2351	A2280		A	G2084	G2018	G1951		A1814	A1753
		G2548	G2484	A2414	A2352	G2281	G2217	A	G2085	C2019	A1884		G1815	G1754
A2684	A2684	G2549	U2485		G2353	G2282	U2219	C	U2086	G2020	A1953		G1816	G1755
A2685	A2685	C2550	C2486	A2418	G2354	G2283		G	U2087	G2021	A1954		U1817	C1756
C2686	C2686	A2551	G2487	C2419	A2355	U2284	U2222	G	U2088	G2022	G1955		U1818	C1757
A2748	A2748	C2552	G2488	C2420	A2356	U2285	U2223	U	C2091	C2023	G1956		U1819	C1758
		G2553	C2489	C2421	A2357	G2286	U2224	G	U2092	U2024	G1957		G1820	A1759
C2753	C2688	C2554	U2490	G2422	C2358	G2287	U2225	A	C2093	A2025	G1958		A1821	G1760
C2754	C2689	G2555	C2491	G2423	U2359	A2288	G2226	A	C2094	C2026	U1959		G1822	G1761
A2755	C2691	A2556	G2492	G2424	C2360		A2226	A	C2095	C2027	G1823		G1823	C1762
A2756	A2692	G2557	U2493	G2425	G2361	C2292	C2227	U	U2096	C2028	C1962		C1824	G1763
G2757	G2693	C2558	C2494	G2426	G2362		U2228	A	U2097	G2029	G1963		C1825	A1764
A2758	G2694	U2559	A2427	A2427	G2363	U2296	U2229	C2157	A1899	U2030	A1964		U1826	C1765
C2695	C2695	G2560	U2496	U2428	C2364	G2297	G2230	C2158	U1900	A2031	U1965		G1827	U1766
A2696	A2696	G2561	A2497	A2429	A2367	U2298	G2231	A2159	A1901	G2032			C1828	G1767
A2761	G2697		U2498	A2430	G2368	U2299	G2232	C2160		C2033	G1970		C1829	
G2762	G2698	C2565	C2499	C2431	G2369	G2300		C2161		U2034	C1971		C1830	U1770
U2763	G2699	A2566	C2500	A2432	G2369	A2301	G2235	C2162		G2035	C1972		G1831	A1771
U2764	U2700	G2567		G2433	G2370	C2302	U2236		G2103		G1904		G1832	C1772
C2765	A2701	A2568	G2505	G2434	A2371	C2303	G2237	A2168	G2104	C2038	G1905		G1833	C1773
U2766	G2702	A2569	C2506	G2435	C2372		G2238	U2105	U2105	G2039	C1906		G1834	C1774
C2767	C2703	C2570	U2507	U2436	G2373	U2298	G2239	A2176	G2106	G2040	G1907		G1835	A1774
C2768	U2704	G2571	G2508	G2437	C2374	G2300	C2240	U2177	G2107	A2041	U1908			A1775
C2769			A2509	A2438		A2306	U2241	U2172			C1910			A1776
A2770	A2770	C2572	C2510	U2439	U2377	A2307	G2242	G2173		A2042	A1911		G1838	U1777
G2771	G2707	G2573	G2511	C2440	G2378	A2308	C2241	C2174		A2043	A1912		A1839	U1778
U2772	U2708	U2574	G2512	U2441	G2379	G2309	G2242	G2175		G2044	A1980		G1840	C1779
G2773	C2709	U2575	A2513	C2442	U2380	G2311	G2244	U2176	C	A2045	A1981		A1780	
U2774	C2710	G2576	G2514		U2381	A2312	A2245	U2177	C	C2046	C1982		C1781	
U		A2577	G2515		C2382	G2313	A2246	U2178	U	C2047	G1983		A1846	A1782
U2778		G2578	G2516	C2446	A2381	A2314	A2247	C2179	G	C2048	A1984		U1847	G1783
A2779	A2713	A2579	U2517	G2447	C2382	A2315	U2248	U2180	C	C2049	G1985		U1848	C1784
C2779	C2714	C2580	C2518	A2448	G2383	G2316	G2250	A2181		G2050	A1919		G1852	A1785
A2780	G2715	A2581	C2519	G2449	U2384		G2251	U2185		U2051	A1920		G1853	C1786
U2781	G2716	G2582	A2520	A2450	G2385	C2321	U2251	A2117		G2052	A1921		G1854	U1787
G2782	G2717	U2583	A2521	G2451	U2387	U2322	A2252	A2119		G2053	U1922		G1855	C1788
C2783	A2718	U2584	A2522	A2455	G2388	U2323	A2253	C2120		U2054	U1923		U1856	U1789
A2784	U2719	G2585	G2523	U2456	G2389	G2324	C2254	U2121		G2055	C1924		C1791	
G2785	C2720	G2586		A2457	A2390	A2325	G2255	G2122		C2056	C1925			
A2786	A2721	C2587	U2526	A2457	A2391	C2326	G2256	G2123		U2057	U1926		A1859	C1792
C2786	C2722	U2588	G2527	G2460	G2392	U2327	A2257	A2194		U2058	A1997		A1860	A1793
A2787	G2723	C2589	G2527	G2461	G2393	G2328		C2195		U2059	A1998		G1861	A1794
U2788	G2724	U2590	U2534	A2467	G2394	C2329	C2260	U2196		A2060	U1999		C1862	C1795
C2789	C2725	G2591	G2529	C2462	C2395	G2330	G2261	U2197		C2061	U2000		U1863	A1796
U2790	U2726	U2592	C2530	G2463	G2396		C2262	U2198		U2062	G2001		U1864	C1797
C2791	G2727	A2593	U2531	G2464	A2397	U2335	G2263	C2199		A2063	G1931		C1865	G1798
C2792	A2728	U2594	G2532	G2465	U2398	C2336	C2264	G2200			G1932		G1866	A1799
G2793			U2533	G2466	C2399	G2336	A2265	G2201		U2069	U2004			A1800
G2794	A2729	G2597	U2534	A2467	G2400	A2337	A2266	G2202		G2070	U2005		A1869	C1801
A2795	U2730	C2598	G2535	G2468	A2401	C2338	C2267	G2203		G2071	G2006		U1870	A1802
C2796	C2732	A2600	U2536	G2469	U2402	A2339	C2268	A2204		C2072	G2007		G1871	G1803
G2797	A2733		C2537	U2470	C2403	G2340	G2269	C2205		A2073	C2008		A1872	U1804
A2798	U2734		A2404		A2404	U2270	G2271	C2206		U2074	U2009		G1942	G1805
C2799	C2735		A2405		A2405	C2343		G2207		U2075	G2010		G1873	G1806
C2800	U2736		A2406		G2407	G2344		U2208		G2076	U2011		C1875	A1807
A2801	A2737		G2478		G2478	A2345	C2274	G2209			A2012		C1876	C1808
			U2479		A2409	G2346	C2275	C2210			A2013		C1877	G1809
						C2347	C2276	U2211			A2014		C1878	G1810

U2872	C2804	U2807	U2808	A2810	A2811	A2812	A2813	A2814	C2815	C2816	A2817	U2821	U2822	C2823	C2824	A2825	C2826	C2827	C2828	A2829	U2830	A2831	U2835	U2836	C2837	U2841	C2842	A2843	C2844	C2845	C2846	C2847	A2848	C2849	U2850	C2851	C2852	U2853	C2854	C2855	U2856	C2857	A2858	U2862	U2863	C2864	C2865	A2866	C2867	C2868	U2869	C2870	U2871
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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, α , β , γ	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 ²)	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	2726/2880 (94%)	580 (21%)	0

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

There are no RNA pucker outliers to report.

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
2	TEL	0	2881	-	60,62,62	3.57	30 (50%)	78,92,92	3.38	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	-	-	0/73/108/108	0/4/5/5

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	0	2881	TEL	C36-C40	-2.74	1.34	1.37
2	0	2881	TEL	C37-N41	-2.41	1.30	1.35
2	0	2881	TEL	C1-C2	2.15	1.57	1.51
2	0	2881	TEL	C12-C7	2.23	1.58	1.53
2	0	2881	TEL	O18-C13	2.27	1.25	1.21

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	0	2881	TEL	C3-N6-C10	-11.25	96.35	111.77
2	0	2881	TEL	C11-N6-C10	-6.81	113.68	122.31
2	0	2881	TEL	O20-C15-C21	-6.73	115.73	124.71
2	0	2881	TEL	C2-O5-C10	-6.31	104.19	109.32
2	0	2881	TEL	O39-C34-C28	-6.25	91.39	106.47

There are no chirality outliers.

There are no torsion outliers.

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

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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.