



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 09:31 PM 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

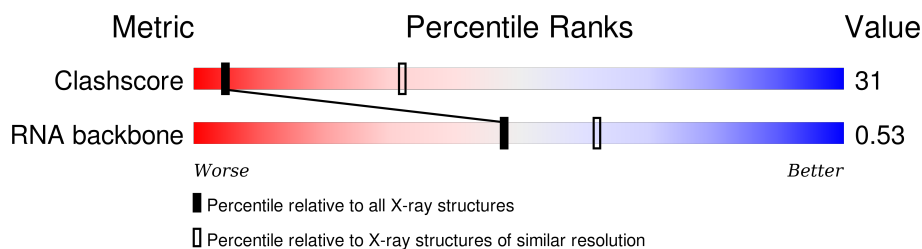
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 Å.

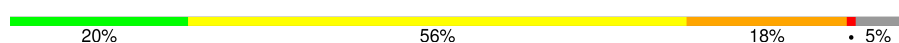
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1611 (3.50-3.30)
RNA backbone	2183	1041 (4.00-2.80)

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 ≥ 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% 56% 18% • 5%

2 Entry composition ⓘ

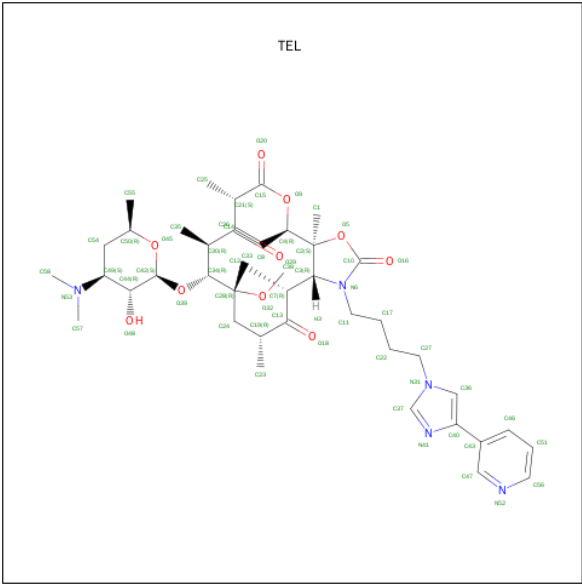
There are 2 unique types of molecules in this entry. The entry contains 58817 atoms, of which 0 are hydrogens and 0 are deuteriums.

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).



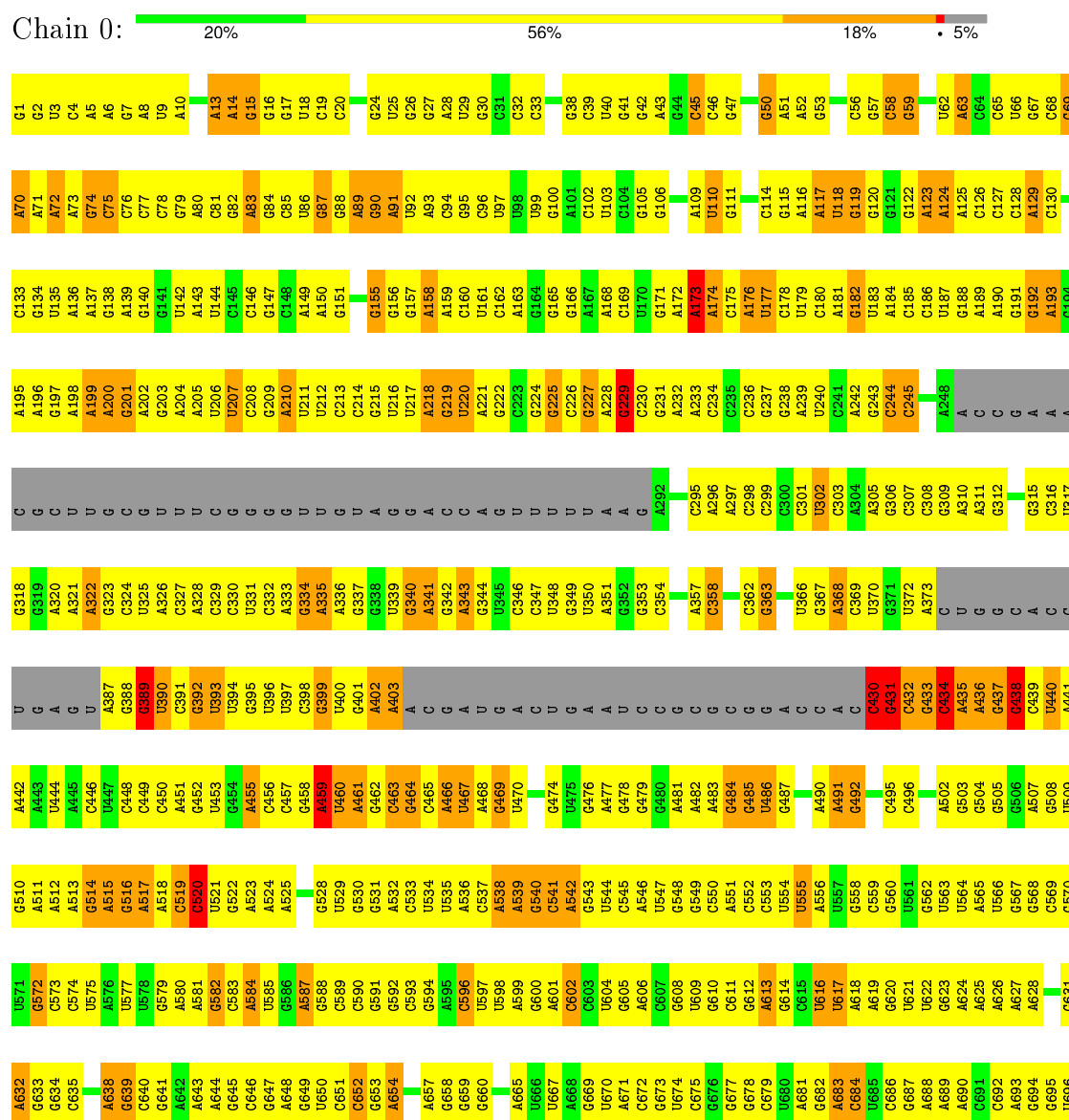
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	0	1	58	43	5	10	0	0

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 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 ($RSRZ > 2$). 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.

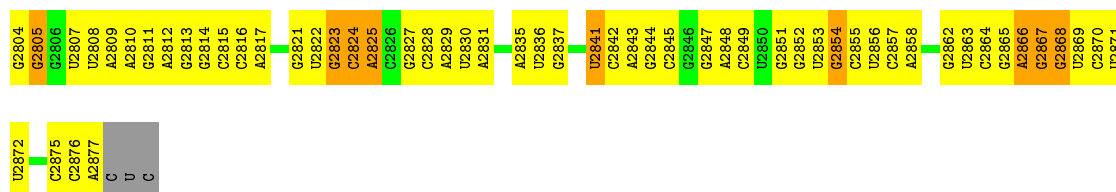
Note EDS was not executed.

• Molecule 1: 23S RIBOSOMAL RNA





G2741	C5678	A2544	C2480	U2410	A2348	U2212	G	U2081	G2015	C1948	U1811	A1750
G2742	G2679	A2545	G2481	A2411	G2349	G2213	G	C2082	A2016	A1949	A1812	A1751
G2743	U2680	G2546	A2482	A2412	G2350	G2214	C	G2083	U2017	C1950	A1813	U1752
G2744	A2681	C2547	U2483	A2413	G2351		A	G2084	G2018	G1951	A1814	A1753
A2745	G2684	G2548	G2484	A2414	A2352	G2217	A	G2085	C2019	A1952	G1815	G1754
G2746	A2685	G2549	U2485		G2353	G2218	C	U2086	G2020	A1953	G1816	G1755
G2747	C2686	C2550	C2486	A2418	G2354	U2219	G	U2087	G2021	A1954	U1817	C1756
G2748	A2687	A2551	G2487	C2419	A2355		G	U2088	C2022	G1955	U1818	C1757
A2749	G2687	C2552	G2488	C2420	A2356	U2222	U		C2023	G1956	U1819	C1758
C5753	G2688	G2553	C2489	C2421	A2357	U2223	A	C2091	U2024	C1957	A1820	A1759
C2754	C2689	C2554	U2490	C2422	G2358	U2224	G	U2092	A2025	G1958	A1821	G1760
A2755	G2690	G2555	G2491	G2423	A2359	G2225	A	G2093	C2026	U1959	G1822	G1761
A2756	C2691	A2556	G2492	G2424	C2360	A2226	A	C2094	G2027		G1823	G1762
A2757	A2692	G2557	U2493	G2425	G2361	C2227	U	G2095	C2028	C1962	C1824	G1763
A2758	U2693	C2558	G2494	A2426	G2362	U2228	A	U2096	G2029	G1963	C1825	A1764
U2759	G2694	U2559	A2495	G2427	G2363	G2229	C1517	A2097	U2030	A1964	U1826	C1765
C2760	C2695	G2560	U2496	U2428	C2364	G2230	C2158		A2031	U1965	G1827	U1766
A2761	G2697	G2561	A2497	A2429		G2231	A2159	G	G2032		A1901	G1767
G2762	G2698	C2565	U2498	A2430	A2367	G2232	C2160	A	C2033		C1828	
U2763	U2699	A2566	C2499	C2431	G2368	G2235	C2161	U	A2034	G1970	C1829	
C2764	A2700	G2567	C2505	U2432	G2369	U2236	C2162	A	G2035	C1971	C1830	U1770
C2765	G2701	C2633	G2506	G2433	A2370	G2237	A2168	G	C2038	G1904	G1831	A1771
U2766	G2702	U2635	C2507	G2434	C2371	C2238		G2104	G2039	G1905	A1832	C1772
C2767	C2703	G2570	U2507	C2435	A2372	G2239	U2105	U2105	G2040	U1906	G1833	C1773
U2768	U2704	G2571	G2508	U2436	C2373		U2171	G2106	A2041	C1907	G1834	A1774
C2769	A2705	U2572	A2509	G2437	C2374	G2240	U2172	G2107	A2042	U1976	C1835	A1775
A2770	U2706	C2573	A2510	U2438	U2377	U2241	G2173	G2108	A2043	C1977		A1776
C2771	G2707	G2574	C2511	C2440	G2378	G2242	C2174	A2109	A2044	U1978	G1838	U1777
U2772	U2708	U2575	A2512	U2441	A2379	C2243	A2175	G2110	G2045	A1980	A1839	U1778
G2773	C2709	G2576	A2513	C2442	U2380	G2244	U2176	C	A2046	U1914	C1779	A1780
U2774	U2710	A2577	G2514		A2381	A2245	U2177	U	C2047	A1915	C1781	
U	G2711	G2578	G2515	C2446	C2382	A2246	U2178	G	C2048	G1916	A1846	A1782
A	C2712	A2579	U2516	G2447	C2383	A2247	C2179	G	C2049	C1917	U1847	G1783
C2778	A2713	C2580	C2517	U2448	G2384	U2248	U2180	C	G2050	A1918	U1848	C1784
C2779	G2714	A2581	C2518	G2449	U2385	G2250	A2181	G	U2051	A1919	G1852	A1785
A2780	U2715	G2582	C2519	A2450	G2386	U2251	U2185	A2117	A1920	A1921	G1853	C1786
G2781	G2716	U2583	A2520	G2451	U2387	A2252	G2186	A2118	U1922	U1922	G1854	U1787
G2782	C2717	U2584	A2521		U2388	A2253		A2119	G2053	U1923	U1855	C1788
U2783	U2718	C2585	G2522	A2455	G2389	C2254	A2191	C2120	A2054	U1924	U1856	U1789
A2784	C2719	G2586	G2523	U2456	A2390	G2255	U1912	G2122	G2055	C1925		C1791
G2785	A2720	G2587		A2457	A2391	G2256	C2193	G2123	U2057	U1926	A1859	C1792
A2786	C2721	U2588	U2526	G2460	G2392	A2257	A2194	C2124	U2058	A1997	A1860	A1793
C2787	G2722	C2589	G2527	G2461	G2393		C2195	C2125	U2059	U1998	G1861	A1794
U2788	C2723	U2590	G2528	C2462	G2394	C2260	U2196	U	A2060	U1999	C1862	C1795
C2789	G2724	C2591	G2529	G2463	C2395	G2261	U2197	U	C2061	C1930	A1869	C1801
U2789	C2725	U2592	C2530	U2464	C2396	C2262	U2198	U	U2062	G2001	U1870	A1802
C2790	U2726	A2593	U2531	G2465	A2397	G2263	C2199	U	A2063	G1931	G1871	G1803
G2791	G2727	U2594	G2532	G2466	U2398	G2264	G2200	G		A2002	A1872	U1804
C2792	A2728		U2533	G2467	C2399	A2265	G2201		U2069	A2003	A1873	G1805
G2793	A2729	G2597	U2534	A2467	G2400	A2266	G2202	G2132	G2070	U2004	G1874	G1806
A2794	U2730	C2598	C2535	G2468	A2401	G2267	G2203	G2133	G2071	U2005	C1875	A1807
C2795	G2731	U2599	G2536	G2469	U2402	C2268	A2204	G2134	C2072	U1938	G1876	C1808
A2796	C2732	A2600	C2537	U2470	C2403	G2269	C2205	C2135	A2073	C2008	A1877	G1809
G2797	A2733		C2538		A2404	U2270	G2206	G2136	U2074	U2009	A1878	
A2798	U2734		C2539	C2475	U2405	C2271	G2207	G2137	U2075	G2010	G1879	G1806
C2799	C2735	G2605	A2540	A2476	A2406		U2208	U2138	G2076	U2011	C1872	A1807
U2800	U2736	G2606	U2541	C2477	G2407	C2274	G2209	G2139		A2012	C1876	C1808
A2801	A2737	A2608	U2542	C2478	G2408	C2275	C2210	G2140		U1946	C1877	G1809
		G2609	A2543	U2479	A2409	C2276	U2211	A	A2079	A2014	C1878	U1810



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be 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	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 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	-	59,62,62	3.36	29 (49%)	72,92,92	3.21	28 (38%)

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 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	0	2881	TEL	C37-N41	-2.35	1.30	1.35
2	0	2881	TEL	C1-C2	2.04	1.57	1.51
2	0	2881	TEL	C12-C7	2.17	1.58	1.53
2	0	2881	TEL	O18-C13	2.18	1.25	1.21
2	0	2881	TEL	O29-C26	2.23	1.25	1.21

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	0	2881	TEL	C3-N6-C10	-12.74	96.35	111.94
2	0	2881	TEL	O39-C34-C28	-6.34	91.39	106.32
2	0	2881	TEL	C11-N6-C10	-6.30	113.68	122.14
2	0	2881	TEL	C2-O5-C10	-6.12	104.19	109.28
2	0	2881	TEL	O20-C15-C21	-6.05	115.73	124.77

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 [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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.