Thermodynamics of Folding

Thermodynamics of Folding: $\Delta G = \Delta H - T \Delta S$

- $\Delta G = 0.11 \text{ kcal/mol at } 54 \,^{\circ}\text{C}$
- $\Delta H = -60.40 \text{ kcal/mol}$
- $\Delta S = -184.9 \text{ cal/}(K \cdot \text{mol})$
- $T_m = 53.4$ °C assuming a 2 state model.
- linear DNA folding.
- Ionic conditions: [Na⁺] = 0.05 M, [Mg⁺⁺] = 0 M.
- Standard errors are roughly $\pm 5\%$, $\pm 10\%$, $\pm 11\%$ and 2-4 °C for free energy, enthalpy, entropy and T_m , respectively.

Structure 1 $0F_CGTGT_end$ $\Delta G = 0.11$

Structural element	δG	Information
External loop	0.00	1 ss bases & 1 closing helices.
Stack	-0.70	External closing pair is c ¹ -G ²⁵
Stack	-0.70	External closing pair is a ² -T ²⁴
Stack	-1.35	External closing pair is c ³ -G ²³
Stack	-0.56	External closing pair is g ⁴ -C ²²
Stack	-0.70	External closing pair is a ⁵ -T ²¹
Helix	-4.01	6 base pairs.
Hairpin loop	4.12	Closing pair is c ⁶ -G ²⁰