Thermodynamics of Folding

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

- $\Delta G = 0.42 \text{ kcal/mol at 54 °C}$
- $\Delta H = -47.30 \text{ kcal/mol}$
- $\Delta S = -145.8 \text{ cal/}(K \cdot \text{mol})$
- $T_m = 51.1$ °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 $0F_CGTGT_end$ $\Delta G = 0.42$

Structural element	δG	Information
External loop	-0.07	0 ss bases & 1 closing helices.
Stack	-0.70	External closing pair is a ¹ -T ²⁵
Stack	-0.70	External closing pair is c ² -G ²⁴
Stack	-0.70	External closing pair is a ³ -T ²³
Stack	-1.35	External closing pair is c ⁴ -G ²²
Stack	-0.56	External closing pair is g ⁵ -C ²¹
Helix	-4.01	6 base pairs.
Hairpin loop	4.50	Closing pair is A ⁶ -T ²⁰