Thermodynamics of Folding

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

- $\Delta G = 1.19 \text{ kcal/mol at } 54 \,^{\circ}\text{C}$
- $\Delta H = -47.50 \text{ kcal/mol}$
- $\Delta S = -148.8 \text{ cal/(K·mol)}$
- $T_m = 46$ °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 2 $0F_CGTGT_end$ $\Delta G = 1.19$

Structural element	δG	Information
External loop	-0.07	0 ss bases & 1 closing helices.
Stack	-0.70	External closing pair is a ¹ -T ³¹
Stack	-0.70	External closing pair is c ² -G ³⁰
Stack	-0.70	External closing pair is a ³ -T ²⁹
Stack	-1.35	External closing pair is c ⁴ -G ²⁸
Stack	-0.56	External closing pair is g ⁵ -C ²⁷
Helix	-4.01	6 base pairs.
Hairpin loop	5.27	Closing pair is a ⁶ -T ²⁶