Thermodynamics of Folding

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

- $\Delta G = 0.12 \text{ kcal/mol at 54 °C}$
- $\Delta H = -47.30 \text{ kcal/mol}$
- $\Delta S = -144.9 \text{ cal/(K·mol)}$
- $T_m = 53.1$ °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 $0F_CGTGT_end$ $\Delta G = 0.12$

Structural element	δG	Information
External loop	-0.37	1 ss bases & 1 closing helices.
Stack	-0.70	External closing pair is a ² -T ²⁶
Stack	-0.70	External closing pair is c ³ -G ²⁵
Stack	-0.70	External closing pair is a ⁴ -T ²⁴
Stack	-1.35	External closing pair is c ⁵ -G ²³
Stack	-0.56	External closing pair is g ⁶ -C ²²
Helix	-4.01	6 base pairs.
Hairpin loop	4.50	Closing pair is A ⁷ -T ²¹