Thermodynamics of Folding

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

- $\Delta G = 1.61 \text{ kcal/mol at } 54 \,^{\circ}\text{C}$
- $\Delta H = -43.80 \text{ kcal/mol}$
- $\Delta S = -138.8 \text{ cal/}(K \cdot \text{mol})$
- T_m = 42.4 °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 2 24Jun24-07-39-34 $\Delta G = 1.61$

Structural element	δG	Information
External loop	-0.21	4 ss bases & 1 closing helices.
Stack	-1.35	External closing pair is c ² -G ²⁹
Stack	-0.70	External closing pair is g ³ -C ²⁸
Stack	-0.70	External closing pair is t ⁴ -A ²⁷
Stack	-0.70	External closing pair is g ⁵ -C ²⁶
Helix	-3.45	5 base pairs.
Hairpin loop	5.27	Closing pair is t ⁶ -A ²⁵