Thermodynamics of Folding

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

- $\Delta G = -0.06 \text{ kcal/mol at 54 °C}$
- $\Delta H = -58.40 \text{ kcal/mol}$
- $\Delta S = -178.3 \text{ cal/(K·mol)}$
- $T_m = 54.3$ °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 24Jun24-07-42-23 $\Delta G = -0.06$

Structural element	δG	Information
External loop	0.00	3 ss bases & 1 closing helices.
Stack	-1.35	External closing pair is c ¹ -G ²⁴
Stack	-0.70	External closing pair is g ² -C ²³
Stack	-0.70	External closing pair is t ³ -A ²²
Stack	-0.70	External closing pair is g ⁴ -C ²¹
Stack	-0.70	External closing pair is t ⁵ -A ²⁰
Helix	-4.15	6 base pairs.
Hairpin loop	4.09	Closing pair is g ⁶ -C ¹⁹