

Thermodynamics of Folding

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

- $\Delta G = 1.12$ kcal/mol at 54 °C
- $\Delta H = -45.00$ kcal/mol
- $\Delta S = -140.9$ 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 3

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$\Delta G = 1.12$

Structural element	δG	Information
External loop	0.00	3 ss bases & 1 closing helices.
Stack	-1.35	External closing pair is c ¹ -G ²³
Stack	-0.70	External closing pair is g ² -C ²²
Stack	-0.70	External closing pair is t ³ -A ²¹
Stack	-0.70	External closing pair is g ⁴ -C ²⁰
Helix	-3.45	5 base pairs.
Hairpin loop	4.57	Closing pair is t ⁵ -A ¹⁹
