Thermodynamics of Folding

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

- $\Delta G = 1.19 \text{ kcal/mol at } 54 \,^{\circ}\text{C}$
- $\Delta H = -43.20 \text{ kcal/mol}$
- $\Delta S = -135.6 \text{ cal/(K·mol)}$
- $T_m = 45.2$ °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 4 $0F_CGTGT_end$ $\Delta G = 1.19$

| Structural element | δG | Information |
|--------------------|-------|--|
| External loop | 0.00 | 1 ss bases & 1 closing helices. |
| Stack | -0.70 | External closing pair is c ¹ -G ²³ |
| Stack | -0.70 | External closing pair is a ² -T ²² |
| Stack | -1.35 | External closing pair is c ³ -G ²¹ |
| Stack | -0.56 | External closing pair is g ⁴ -C ²⁰ |
| Helix | -3.31 | 5 base pairs. |
| Hairpin loop | 4.50 | Closing pair is A ⁵ -T ¹⁹ |