

# Thermodynamics of Folding

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

- $\Delta G = 0.37$  kcal/mol at 54 °C
- $\Delta H = -47.30$  kcal/mol
- $\Delta S = -145.7$  cal/(K·mol)
- $T_m = 51.4$  °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 1

0F\_CGTGT\_end

$\Delta G = 0.37$

Structural element	$\delta G$	Information
External loop	-0.07	0 ss bases & 1 closing helices.
Stack	-0.70	External closing pair is a <sup>1</sup> -T <sup>26</sup>
Stack	-0.70	External closing pair is c <sup>2</sup> -G <sup>25</sup>
Stack	-0.70	External closing pair is a <sup>3</sup> -T <sup>24</sup>
Stack	-1.35	External closing pair is c <sup>4</sup> -G <sup>23</sup>
Stack	-0.56	External closing pair is g <sup>5</sup> -C <sup>22</sup>
<b>Helix</b>	-4.01	6 base pairs.
Hairpin loop	4.45	Closing pair is a <sup>6</sup> -T <sup>21</sup>

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