SM-1 January 2018

Protein: N particles

u is a constant

One folded state: $E = -\varepsilon_b$

u^N unfolded states: $E = 0$

$P_u(T) \rightarrow$ fraction of unfolded protein molecules

a. Write down partition function.

$N = N_f + N_u$ $\quad$ $f \rightarrow$ folded $\quad$ $u \rightarrow$ unfolded

$E_T = -\varepsilon_b$

$$Z_N = u^N (e^{\beta 0}) + e^{\beta \varepsilon_b} = u^N + e^{\beta \varepsilon_b} = u^N + e^{\varepsilon_B / k_B T}$$

b. Find unfolding transition temperature $\rightarrow$ half particles are folded

$P_u(T) = \frac{1}{2}$

$$P_u(T) = \frac{u^N}{Z} = \frac{u^N}{u^N + e^{\varepsilon_B/k_B T}} = \frac{1}{2}$$

$$2u^N = u^N + e^{\varepsilon_B / k_B T} \Rightarrow u^N = e^{\varepsilon_B / k_B T}$$

$$N \ln(u) = -\frac{\varepsilon_B}{k_B T_t} \qquad T_t = \frac{\varepsilon_B}{N k_B \ln(u)} = \frac{-\varepsilon_B \ln(u)}{N k_B}$$

$[\varepsilon] = \frac{kg\, m^2}{s^2}$

$[k_B] = \frac{kg\, m^2}{s^2 K}$

$\left[\frac{\varepsilon}{k_B}\right] = K$ ✓ units are correct.

c. Compute width of unfolding transition

$$\delta T_t = \left(\frac{dP_u}{dT}\right)^{-1} \text{ at } T_t$$

$$\frac{d}{dt}\left(\frac{u^N}{u^N + e^{\varepsilon_B/k_B T}}\right) = \frac{d}{dt} u^N \left(u^N + e^{\varepsilon_B / k_B T}\right)^{-1} = -u^N \left(u^N + e^{\varepsilon_B / k_B T}\right)^{-2} \cdot \frac{\varepsilon_B}{k_B T^2} e^{\varepsilon_B / k_B T}$$

$$= \frac{-\varepsilon_B}{k_B T^2} \frac{u^N e^{\varepsilon_B / k_B T}}{(u^N + e^{\varepsilon_B / k_B T})^2}$$

$$\delta T_t = \frac{-T^2 k_B}{u^N \varepsilon_B} \frac{\left(\frac{u^N + e^{\varepsilon_B / k_B T}}{u^N}\right)^2}{e^{\varepsilon_B / k_B T}} = \frac{-T^2 k_B}{u^N \varepsilon_B}\left(u^N e^{-2\varepsilon_B / k_B T} + e^{-\varepsilon_B / k_B T}\right)^2$$

$u^N = e^{\varepsilon_B / k_B T}$

$T_t = \frac{-\varepsilon_B \ln u}{N k_B}$

$$= \frac{-k_B T^2}{u^N \varepsilon_B}\left(u^{-N} + u^{-N}\right)^2 = \frac{-4 k_B T^2}{u^N \varepsilon_B} u^{-4N} = \frac{-4 k_B T_t^2}{\varepsilon_B u^{3N}}$$

$$= \frac{4 \varepsilon_B (\ln u)^2}{N^2 k_B u^{3N}} \sim \frac{1}{N^2}$$

δT_t is smaller $\rightarrow$ sharper transition