

equations_main

May 19, 2021

$$V_{native} = V_{native, bonded} + V_{native, excluded\ volume} + V_{native, non-bonded} + V_{native, DH}$$

$$V_{native, bonded} = \sum_{bonds} k_{bond} (b_{ij} - b_{ij}^0)^2 + \sum_{angle} k_{angle} (b_{ijk} - b_{ijk}^0)^2 + \sum_{DH} k_{DH} (b_{ijkl} - b_{ijkl}^0)^2$$

$$V_{native, excluded\ volume} = \sum_{i < j-3} k_{excluded\ volume} \left(\frac{\sigma_{ij}}{r_{ij}} \right)^{12}$$

$$V_{native, non-bonded} = \sum_{i \neq j} k_{native} \left[5 \left(\frac{A_{ij}}{r_{ij}} \right)^{12} - 6 \left(\frac{A_{ij}}{r_{ij}} \right)^{10} \right]$$

$$V_{native, DH} = K_{Coulomb} B(\kappa) \sum_{i \neq j} \frac{q_i q_j e^{-\kappa r_{ij}}}{\epsilon r_{ij}},$$

$$K_{Coulomb} = 332\ kcal \cdot mol^{-1}, \epsilon = 70\ F \cdot m^{-1}$$

For dilute solutions and monovalent ions:

$$B(\kappa) \approx 1, \quad -\kappa \approx 0.32 \sqrt{C_s}, \quad C_s = 0.5 \sum_{i=1}^{n_i} c_i$$