$$
\begin{aligned}
V_T &= V_{FENE} + V_{NB}^{ATT} + V_{NB}^{REP} \\
V_{FENE} &= \sum_{i=1}^{N-1} \frac{k}{2} R_0^2 log \left(1 - \frac{\left(r_{i,i+1} - r_{i,i+1}^0 \right)^2}{R_0^2} \right) \\
V_{NB}^{ATT} &= \sum_{i=1}^{N-3} \sum_{j=i+3}^{N} \epsilon_h \left[\left(\frac{r_{ij}^0}{r_{ij}} \right)^{12} - 2 \left(\frac{r_{ij}^0}{r_{ij}} \right)^{6} \right] \Delta_{ij} \\
V_{NB}^{REP} &= \sum_{i=1}^{N-2} \epsilon_1 \left(\frac{\sigma_{i,i+2}}{r_{i,i+2}} \right)^6 + \sum_{i=1}^{N-3} \sum_{j=i+3}^{N} \epsilon_1 \left(\frac{\sigma}{r_{ij}} \right)^6 \times \left(1 - \Delta_{ij} \right)
\end{aligned}
$$