Radius of Gyration

$$R_g^2 = \frac{1}{N}\sum_{i=1}^{N}\langle |r_i - R_G| \rangle \equiv \frac{1}{2N^2}\sum_{i=1}^{N}\sum_{j=1}^{N}|r_i - r_j|^2 \qquad (1)$$

where N is the number of steps in a structure, R_G is the center of mass given by,

$$R_G = \frac{1}{N}\sum_{i=1}^{N} r_i \qquad (2)$$

r_i is a vector from an arbitrary starting point to step "i". The definition in (1) can be shown by expanding the last double summation using R_G,

$$\begin{aligned}\sum_{i=1}^{N}\sum_{j=1}^{N}|r_i - r_j|^2 &= \sum_{i=1}^{N}\sum_{j=1}^{N}\left|(r_i - R_G) - (r_j - R_G)\right|^2 = \left|\left(N\sum_{i=1}^{N}(r_i - R_G)\right) - \left(N\sum_{j=1}^{N}(r_j - R_G)\right)\right|^2 \\ &= \left|\left(N\sum_{i=1}^{N}(r_i - R_G)\right)^2 + \left(N\sum_{j=1}^{N}(r_j - R_G)\right)^2 - 2N^2\sum_{i=1}^{N}(r_i - R_G)\sum_{j=1}^{N}(r_j - R_G)\right| \\ &= \left|2N\left(\sum_{i=1}^{N}(r_i - R_G)\right)^2 - \left(\sum_{j=1}^{N}(r_j) - NR_G\right)^2\right|\end{aligned} \qquad (3)$$

Eq. (2) can be rewritten,

$$\sum_{i=1}^{N} r_i - NR_G = 0 \qquad (4)$$

so eq. (3) becomes,

$$\sum_{i=1}^{N}\sum_{j=1}^{N}|r_i - r_j|^2 = \left|2N\left(\sum_{i=1}^{N}(r_i - R_G)\right)^2\right| \qquad (5)$$

which verifies eq. (1).