Molecular dynamics modeling of protein diffusion in an aqueous solution

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The movement of proteins in the cell cytoplasm plays an important role in the functioning of cells of living organisms. A quantitative characteristic of such processes is the diffusion coefficient. In this paper, the simplest model is considered for the quantitative description of the diffusion of a small lysozyme protein in an aqueous solution. At the first stage, the protein is released for relaxation in water, and then attempts are made to calculate the diffusion coefficient of this protein in water in various ways.
The first method is to use the Einstein relation

$$D = \mu k_b T$$

where D is the diffusion coefficient, μ is the protein mobility, and k_b is the Boltzmann constant, T is the absolute temperature of the system.
The second method is using the Stokes-Einstein formula

$$D = \frac{k_b T}{6\pi\eta r}$$

to estimate the diffusion coefficient. Here η is the viscosity coefficient of water at the desired temperature, r is the gyration radius of the protein (the characteristic size of the protein). The formula has this form, because in the work the whole protein moves translationally, possible rotations are not investigated.