A conformational search method of protein systems by using genetic algorithm

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Proteins have the life functions by forming the characteristic tertiary structures. Therefore, the search of the stable states of proteins by molecular simulation is important to understand their functions and stabilities. However, getting the stable state by conformational search is difficult, because the energy landscape of the system is characterized by many local minima separated by high energy barriers. In order to overcome this difficulty, various sampling and optimization methods for conformations of proteins have been proposed. We also have performed the folding simulation of proteins by using our method [1]. In this study, we propose a new conformational search method for proteins by using genetic algorithm. We applied this method to several proteins (Fig.). As the results, the conformations obtained from the simulations were in good agreement with the experimental results.


Fig. Two structures obtained from the simulation (left) and the experiment (right) of Protein A (10-55 in 60 amino acids). The root mean square deviation (RMSD) is 1.707\text{Å}.