Structure and dynamics of chloride ion pumping rhodopsin revealed by time resolved SFX and atomic molecular dynamics simulations

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The chloride ion pumping rhodopsin was studied with the powerful X-ray lasers and supercomputers, to reveal the molecular mechanism of proteins. The chloride ion pumping rhodopsin (ClIR) utilizes energies from light to actively transport Cl- ions through membranes. In this study, we report, for the first time, an atomic structure determined at room temperature using serial femtosecond X-ray Crystallography (SFX) method. The atomic structure determined using SFX method is very consistent with the structure solved at synchrotrons. Furthermore, using pump-probe method, time-resolved crystallography method was applied to determine structures at several time point after photoactivation. Extensive molecular dynamics simulations have been carried out to study the pathway of Cl- ions through the rhodopsin channel. By using all-atom molecular dynamics simulation method, the plausible pathways of Cl- ion were observed (Figure 1d,e). The residues that undergo substantial conformational changes during the ion transportation have been identified.

Figure 1. SFX experimental data and simulation results. Microcrystals in syringe (a) and in plate (b) both in LCP medium. (c) A representative diffraction pattern collected at CXI. (d) Steered molecular dynamics simulation reveals intermediate states as Cl- ion moves through the channel, each curve shows a simulated transportation process. (e) A plausible pathway for ion transportation (orange sphere, Cl- ion) and the key residues identified in the simulations.

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