

ABSTRACT

The Light Harvesting Complex LHC of photosystem II (LHC-II) collects and transmits the solar energy for photosynthesis in chloroplast membranes and it has an essential role in regulating photosynthesis and photoprotection, when there is excess light radiation. The 2.5 Å structure of pea LHC-II has been determined by X-ray crystallography of stacked two-dimensional crystals. It is believed that LHCII can change its function by switching between different conformations. To determine the structural changes involved in the switch and to identify potential quenching sites, we have explored the structural dynamics of LHCII (protein database code: 2BHW). Molecular Dynamics Simulations were run with the use of different software packages for the preparation and simulations. Two different protonation states were used, one with low pH and one with high pH at the lumen site of the chloroplasts. In each protonation case, two distinct cases were also determined regarding a KCL salt concentration gradient, one with a high gradient (0.5M) and one with lower. The gradient was attained by adding salts only to the lumen side of the membrane. This simulated the protein's response to protons and KCl presence. Samples were run in Classic Molecular Dynamics trajectories. We observe a larger conformational change for the low pH/ high salt content sample and especially for helix-5.