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Influence of Crystal Packing on Global Protein Conformation LOGAN AHLSTROM, OSAMU MIYASHITA, Department of Chemistry and Biochemistry, University of Arizona — X-ray crystallography is the most robust method for solving protein structure. However, packing forces in the crystal lattice select just a snapshot of a protein's conformational ensemble, whereas proteins are flexible and can adopt different conformations. Here we compare molecular dynamics (MD) simulations in solution and the crystal lattice to add dynamical insight to the static X-ray images of proteins. As a model system, we consider the λ Cro dimer, whose solved X-ray structures range from a "closed" to an "open" global conformation. Free energy profiles depicting the conformational space sampled by the dimer in solution show some reported structures correspond to stable states. Yet other conformations, while accessible, lie higher in energy, indicating the effect of crystal packing. Subsequent crystal MD simulations estimated the strength of packing interfaces in the lattice, showing the influence of crystal form and mutation in stabilizing different dimer conformations. Our quantitative results will aid analysis of X-ray data in establishing protein structure-function relationships.

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