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Effect of protein crystal hydration on side chain conformational heterogeneity HAKAN ATAKISI, DAVID MOREAU, JESSE HOPKINS, ROBERT THORNE, Cornell University, ROBERT THORNE'S GROUP TEAM — The structure of protein crystals is determined in part by water-mediated interactions involving both protein surface-ordered (hydration) and bulk water, and so is sensitive to the relative humidity of the environment. Monoclinic lysozyme provides a remarkable model for studying structural changes induced by dehydration, as it maintains excellent order for relative humidities (r.h.) down to 5%, corresponding to solvent content of 9% by volume, much smaller than the 88% (22% by volume) at which lysozyme loses its enzymatic activity. Although the main chain conformation does not change significantly, the effect of dehydration on side chain conformations has not been systematically studied. High resolution (1.1 to 1.7 A) structural data sets for monoclinic lysozyme at r.h. between 99% and 11% have been analyzed to identify major and minor side chain conformers at each humidity, and to map out how the side chain conformational ensemble evolves with hydration. Modest dehydration produces comparable overall effects to cooling to T=100 K, but with conformational changes largely confined to solvent-exposed residues. The largest side chain conformation changes occur at humidities that deplete water within the first two hydration shells.

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