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Water in Protein Crystals IREM ALTAN, Duke University, DIANA FUSCO, University of California, Berkeley, PAVEL AFONINE, Lawrence Berkeley Laboratories, PATRICK CHARBONNEAU, Duke University — Water is both the solvent and an active component of biological processes. Protein crystals contain up to 80% water by volume. Yet water-protein interactions are challenging to probe by X-ray diffraction because of the probabilistic nature of solvation, the mosaic of hydrophilic and hydrophobic residues on the protein surface, and the complexity of the protein surface. We compare the solvent structure obtained from diffraction data for which experimental phasing is available to that obtained from constrained molecular dynamics (MD) simulations. The resulting spatial density maps show that MD water models capture the radial extent of biomolecular solvation fairly well, irrespective of the choice of MD water, but cannot reproduce the real space distribution of solvent with a comparable accuracy. MD simulations can predict only a fraction of the assigned crystal waters. These differences are due to shortcomings of both the water models and the protein force fields. Our findings nonetheless suggest that MD-derived densities can be utilized to infer the protonation states of side chains, provided that they are sufficiently solvent-exposed. Our work also paves the way to treating waters contribution to protein refinement more accurately through the development of hybrid models.

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