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Statistical mechanics of hydrophobic amino acids in aqueous solution: A joint experimental scattering and computational study LINGSHUANG SONG, Case Western Reserve University, LIN YANG, Brookhaven National Laboratory, WEI HUANG, Case Western Reserve University, JIE MENG, Peking University, SICHUN YANG, Case Western Reserve University — How hydrophobic amino acids interact with each other is still a fundamental question in understanding protein dynamics and folding. Here, we describe an integrative experimental-computational approach of combining x-ray solution scattering and atomistic molecular simulations to determine the molecular properties of a hydrophobic leucine amino acid in an aqueous solution. First, scattering data were acquired at a series of amino acid and salt concentrations and these scattering profiles were further used to calibrate atomistic molecular simulations via a single parameter for solute-solvent interaction. Second, these accurate data of atomistic leucine simulations were used to quantify the effective interacting potentials via a structural simplification of one-bead-per-residue and two-bead-per-residue representations. Third, comparative energetic analyses between the one-bead and two-bead representations were performed to reach a simple picture of residue-residue interactions with an accurate energy function. Taken together, this joint experimental-computational study provides critical insights into microscopic interactions of hydrophobic amino acids in solution with a profound application for studying molecular dynamics of, e.g., intrinsically disordered proteins and their folding.

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