Statistical mechanics of hydrophobic amino acids in aqueous solution: A joint experimental scattering and computational study LING-SHUANG 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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