The structure of amino acids in aqueous solution: A combined neutron diffraction and empirical potential structure refinement study

Sylvia E. McLain ISIS Facility, Rutherford Appleton Labs, United Kingdom

The structure of amino acids or derivatives of biological in aqueous solutions have been investigated using **n**eutron **d**iffraction augmented with **i**sotopic **s**ubstitution (NDIS). NDIS is a well-proven technique for the determining the structure of hydrogen containing molecules in aqueous solution. The data collected were subsequently modeled using the disordered materials program Empirical **P**otential **s**tructural **r**efinement (EPSR) which provides a molecular structural model of the systems studied that is not only consistent with the measured diffraction data but also physically reasonable. Using this combination of NDIS and EPSR, site-specific information concerning the intermolecular interactions between the amino acid solute and the surrounding water solvent as well as the solvent-solvent interaction on a local level (1-10 Å scale) are elucidated. Several examples will be presented.