

Poster Presentation

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Ultra-high resolution neutron and X-ray crystallography: structure of crambin

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Neutron diffraction data to 1.1 Å was collected on a crystal of the small protein crambin at the Protein Crystallography Station (PCS) at Los Alamos, the highest resolution neutron structure of a protein to date, and a technical benchmark for the instrument. 95 % of the hydrogen atoms in the protein structure were resolved. The data allowed for the refinement of anisotropic temperature factors for selected deuterium atoms within the protein. Hydrogen bonding networks ambiguous in room temperature, ultra-high resolution (0.84 Å) electron density maps are clarified in the nuclear density maps. The ultra-high resolution data also reveals unusual H/D exchange patterns and novel chemistry in the side chains and protein backbone. Complementary X-ray diffraction data was collected at 19-ID at the Advanced Photon Source, with extensive re-configuration of the beamline to allow for operation at higher energy settings.

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