

E0007

Spallation Neutron Protein Crystallography: Enzyme Mechanism Studies with D-Xylose Isomerase. **B. Leif Hanson***, **Paul Langan^**, **Xinmin Li^**, **Amy K. Katz#**, **Benno P. Schoenborn^**, **Jenny P. Glusker#**, and **Gerard J. Bunick*s**

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Neutron diffraction data have been measured at the recently commissioned LANSCE macromolecular neutron beamline at Los Alamos for the enzyme D-xylose isomerase (XI). This new neutron beam line provides us with an opportunity to collect diffraction data from higher molecular weight proteins using time-of-flight techniques. Large crystals (1-2 mm) of XI were grown in the EDCAM hardware developed by NASA for microgravity studies. The use of these devices facilitated the month-long H₂O/D₂O exchange process, during which the crystals showed no alterations. One crystal was used with 23 crystal orientations. The data were integrated using the Langan TOF version of D*Trek and normalized and scaled with LAUENORM and SCALA (82,261 reflections, 32,976 unique extending to 1.48 Å resolution with 42% completeness, 70% to 2.0 Å). Results from molecular refinement, currently underway, will be contrasted with structural information from an ultra-high resolution X-ray data structure measured by us. This structure determination of XI reinforces the idea that neutron diffraction is unsurpassed as a method for accurately locating the positions of hydrogen atoms. This represents the initial stage of a long-term study using inhibitor complexes and differing metal ions to help determine the mechanism of XI by locating key hydrogen atoms.

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