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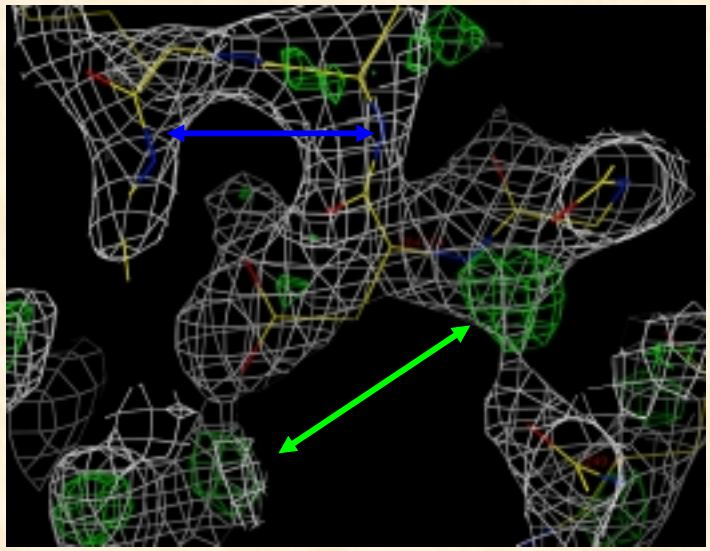
The neutron structure of the enzyme D-xylose isomerase (XI) has progressed to the calculations of neutron density maps. XI is the largest enzyme for which high-resolution neutron data has been measured by time-of-flight methods.

A Letter of Intent for developing a Macromolecular Neutron Diffractometer (MANDI) at BL 11B at the HPTS at SNS was submitted to the SNS Experimental Facilities Advisory Board. G. Bunick and L. Hanson are members of the submitting team.



A slice of **neutron** density of the D-xylose isomerase structure is shown at 2.5 Å resolution. The double-headed green arrow points to large positive neutron density (green) associated with deuterium atoms. A deuterium atom is bound to the amide nitrogen atom (blue) of aspartic acid 264. Positive density (white) extends from the deuterium atom to the carbonyl oxygen atom (red) of glutamine 249, suggesting hydrogen (or in this case a deuteron) bonds between the two atoms. This type of information is not revealed by X-ray structures, which show electron density. For contrast, the blue double-headed arrow points to amide nitrogen atoms in the main chain that do not indicate the presence of deuterium atoms, since the positive neutron density is not prominent off the nitrogen atoms. As more neutron reflections are added to the refinement and the resolution of the structure increases, it is likely that negative neutron density will appear at these locations revealing the presence of hydrogen atoms.