Flight Path 15

PCS *Fact Sheet*

Protein Crystallography Station

The Bioscience Division has built a Protein Crystallography Station (PCS) at the Lujan Neutron Scattering Center for the international structural biology community to investigate the structure and dynamics of proteins, biological polymers, and membranes. Information relating to structurally and functionally important water molecules, hydrogen atoms, and protonation states can only be obtained using neutrons, making neutron crystallography especially useful for resolving enzyme reaction mechanisms. Despite the utility of macromolecular neutron crystallography, the number of studies are limited by access to neutron sources and appropriate instrumentation. The PCS, funded by the DOE Office of Biological and Environmental Research, is the first such instrument to be built at a spallation neutron source. Recent target and moderator improvements have resulted in increased flux, making it feasible to collect high-quality data on relatively small sample sizes (~0.3 mm^3). Approximately 20 experiments are accommodated each year during a 5-6 month run cycle. The PCS also offers full "gene to structure" support for users, including a biodeuteration facility, in-house X-ray diffractometer, and protein expression and purification equipment, housed in a brand new, state-of-the-art laboratory space.

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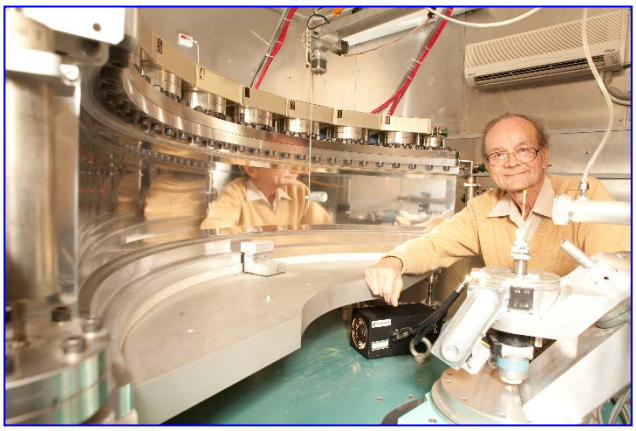
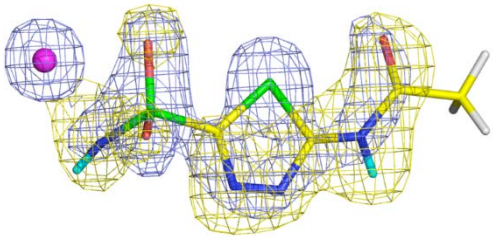
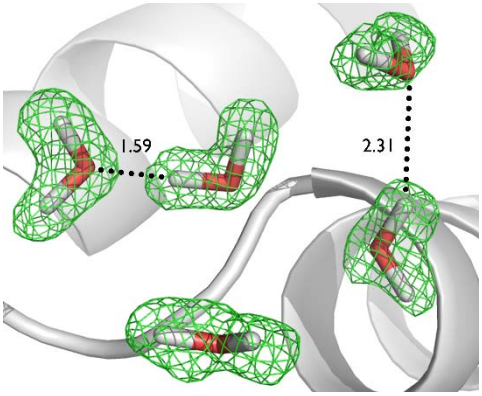
Specifications	
Unit cell size	150 Å
Sample size	0.3 mm^3
d-spacing	1 Å – 250 Å
Wavelength shaping	T_0 and T_1 choppers and tail cutter
Wavelength range	1 Å – 5 Å
Sample-to-detector distance	700 mm
Beam size	5 mm on detector
Resolution	1.2 mm
Detector area	2930 cm^2
Counting rate	> 1,000,000 c/s



The PCS neutron detector (above) consists of an electrode structure contained in an aluminum pressure vessel. The pressure vessel is filled with a mixture of ^3He and propane. The ^3He has an extremely high cross-section for thermal neutron absorption. Neutrons diffracted by the sample are absorbed by the ^3He, creating a proton and triton. These primary ionization products drift toward the nearest electrode-anode wire where they multiply in the high electric field near the wire surface. The charges induced over different electrodes allow for the spatial detection of an event.



Electron (blue) and nuclear (yellow) density for the drug acetazolamide bound to human carbonic anhydrase (Fisher, et al. **JACS 134,** 14726-9, 2012).



Left: 1.1 Å nuclear density map for D_2O molecules associated with crambin (Chen, et al. **PNAS 109,** 15301-6, 2012). *Right:* Capillary mounted crystal of crambin (10 mm^3).