

Neutron Macromolecule Crystallography with LADI

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Protons and water molecules play critical roles in the enzymatic mechanism of many enzymes. Direct information on hydrogen positions can be obtained from ultra-high resolution X-ray crystallographic data or from neutron crystallographic data at more modest resolutions of 1.5 – 2.0 Å. Neutron crystallography is therefore a useful experimental tool to address specific problems where direct visualisation of hydrogen atoms is crucial. However, neutron macromolecule crystallography raises many challenges. Unusually large crystals (> 1 mm³) are required to compensate the weak flux of available neutron beams. Moreover, the large hydrogen incoherent scattering background significantly reduces the signal to noise.

Recent advances in instrument technologies in parallel with the development of the preparation of 100% D-labelled macromolecules make neutron crystallography an appealing technique to address mechanistic and hydration questions on larger biological system and smaller crystal than previously possible.

We will discuss recent examples of neutron protein structures determined with the Laue Diffractometer (LADI) neutron-sensitive image plate detector at the ILL. The upgrade of the LADI, producing a minimum 6-fold gain will be presented.