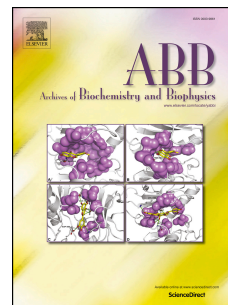


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## Neutron Protein Crystallography:

### A Complementary Tool for Locating Hydrogens in Proteins

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#### Highlights

- Hydrogen atoms are central to enzyme chemistry.
- Neutron protein crystallography (NPC) locates hydrogen atoms in protein structures.
- NPC is a powerful tool for investigating enzyme chemistry.

#### Abstract

Neutron protein crystallography is a powerful tool for investigating protein chemistry because it directly locates hydrogen atom positions in a protein structure. The visibility of hydrogen and deuterium atoms arises from the strong interaction of neutrons with the nuclei of these isotopes. Positions can be unambiguously assigned from diffraction at resolutions typical of protein crystals. Neutrons have the additional benefit to structural biology of not inducing radiation damage in protein crystals. The same crystal could be measured multiple times for parametric studies. Here, we review the basic principles of neutron protein crystallography. The information that can be gained from a neutron structure is presented in balance with practical considerations. Methods to produce isotopically-substituted proteins and to grow large crystals are provided in the context of neutron structures reported in the literature. Available instruments for data collection and software for data processing and structure refinement are described along with technique-specific strategies including joint X-ray/neutron structure refinement. Examples are given to illustrate, ultimately, the unique scientific value of the neutron protein crystal structure.

#### Introduction

Proteins, and more specifically enzymes, are the lifeblood of cellular processes. Enzymes catalyze a broad array of chemical reactions essential to life. No less than 20,000 distinctive enzyme-catalyzed reactions are likely across all living organisms [1], controlling processes as diverse as the capture and conversion of energy from light, cell signaling, DNA translation and

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