

## Poster Presentation

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### *Perdeuteration: Vital to visualising solvent in neutron crystallography?*

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Early neutron crystallography studies replaced hydrogen with deuterium by soaking the crystal in heavy water prior to data collection, which exchanged labile hydrogen atoms (OH, NH, and SH) and solvent molecules only. Carbon bonded hydrogen atoms were not replaced, and their negative scattering density resulted in cancellation in nuclear density maps with resolution worse than 1.8 Å. Furthermore complications arise due to partial exchange, where deuterium is present in some unit cells and hydrogen in others. More recently it has become possible to completely replace hydrogen with deuterium through expression in a deuterated medium, using facilities such as the Deuteration Laboratory (DLAB) in Grenoble. As this is a complex and expensive task, the question arises as to the importance of its use. As well as allowing the study of radically smaller crystals (<0.05mm<sup>3</sup>), it also has the possibility to avoid the cancellation problems discussed above. We have obtained data from high quality crystals of partially hydrogenated type III antifreeze protein, where methyl protonated valine and leucine residues were incorporated into the perdeuterated protein. This provides an excellent opportunity to assess the effects of negative scattering from hydrogen atoms not only on the visibility of neighbouring carbon atoms but also on water molecules in close vicinity. The observation of these cancellation effects gives a further reason to use full deuteration in neutron protein crystallography.

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