Seeing hydrogens in Crystal structures: Limitations and possibilities at 0.9 Å resolution X-ray structures – why do we still need Neutrons?

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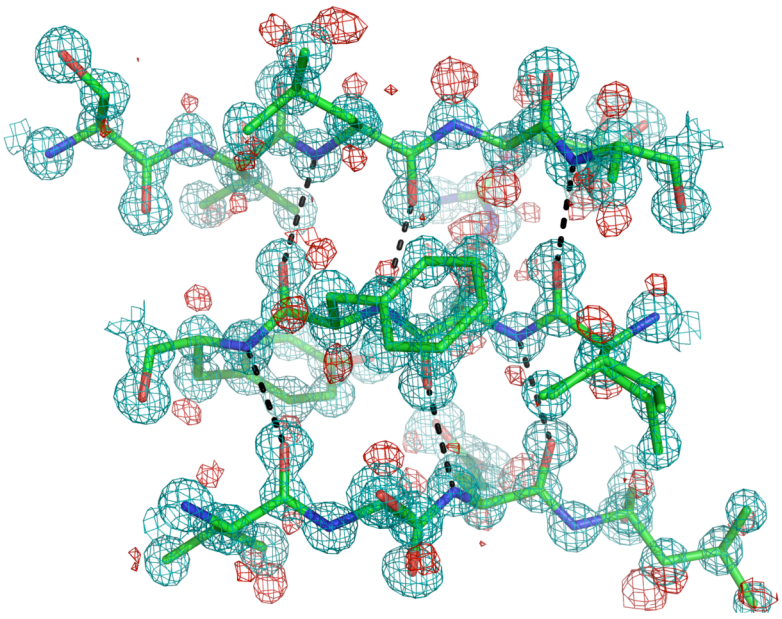
Protons and proton transfer pathways play a critical role in many enzyme mechanisms. Direct information on proton (hydrogen) positions may be obtained from neutron crystallographic data. Despite advances in neutron sources and detectors, the application of neutron diffraction has remained limited to large crystals with small unit cell dimensions. This has resulted in general in a paucity of information about the proton delivery mechanisms that are central to our understanding of many enzyme mechanisms. In our attempt to understand the underlying mechanism of proton transfer, we have adopted the approach of obtaining X-ray data to subatomic (<0.9 Å) resolution. Electron density maps from structures determined to such resolution can reveal the positions of crucial hydrogens within the active sites and on proton pathways. Details of hydrogen location in green nitrite reductase from *Achromobacter cycloclastes* (0.85 Å) [1], human Cu-Zn superoxide dismutase (0.88 Å) [2], cytochrome c' (CYTcp) (0.82 Å) from *Alcaligenes xylosoxidans*, Mn catalase from *Thermus thermophilus* (0.98 Å) and Cupin-like protein from *Aquifex aeolicus* VF5 with endogenously bound aspartate (0.9 Å) will be presented.



References

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2. R.W.Strange, S.V.Antonyuk, M.A.Hough, P.A. Doucette, J. Roderiguez, J.S. Valentine & S.S. Hasnain *J.Mol.Biol.*, 356, 1152 (2006)