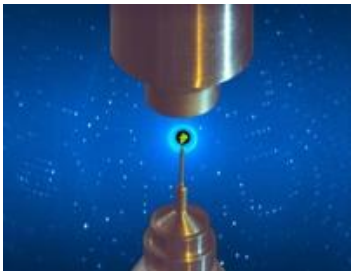

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Protein and water dynamics at the atomic level

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Despite of the pivotal role that hydrogen (H) atoms play in protein biological function, and the fact these comprise approximately 50% of all protein atoms, their observation through X-ray diffraction remains elusive. Conversely, neutron diffraction data at resolutions better than 2.5 Å allows the determination of H positions, providing unique insight to the catalytic mechanisms of enzymes. Additionally, neutron diffraction is uniquely suited for the study of atomic thermal motion, as routinely done for small molecules, since neutrons scatter from atomic nuclei, while X-rays interact with electrons.
Our study focuses on the description of protein and water structure and dynamics, through neutron crystallography. Perdeuterated hen egg-white lysozyme (D-HEWL) was produced recombinantly with the aim of growing crystals of several mm3. Complete neutron diffraction datasets were collected at D19, Institute Laue-Langevin, to a resolution of 1.0 Å on D-HEWL crystals at both 100 and 298 K.
The D-HEWL 298 K neutron structure provided a clear and complete picture of lysozyme's active site in its active state (room temperature and pH close the enzyme's optimal pH). The unambiguous assignment of H positions allowed the determination of the orientations of protein residues and waters molecules, and of the protonation states of the catalytic residues. Furthermore, atomic motion is analyzed based on anisotropic ADPs obtained from neutron and X-ray diffraction data at both 100 and 298 K.

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