MBG FOCUS TALK

hosted by Poul Nissen & Thomas Lykke-Møller Sørensen

MBG Focus Talks in Molecular Biology

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Online via Zoom

By Joao Ramos

Life Sciences Group, Institute Laue-Langevin, Grenoble, France
Dept. Drug Design and Pharmacology, University of Copenhagen, Denmark

Protein and water dynamics at the atomic level using neutron crystallography

Protein biological function is intimately related to structure as well as dynamics at the molecular and atomic scales. X-ray diffraction has contributed immensely to the understanding of protein function mainly through the description of structural properties. However, the study of atomic motion has been somewhat overlooked due to the limitations inherent to X-ray models and to the challenges faced in obtaining neutron diffraction data. Small-molecule studies have shown that neutron diffraction is capable of providing accurate information on atomic and molecular motion.
By pushing the current boundaries of neutron macromolecular crystallography to obtain anisotropic atomic displacement parameters (ADPs) for perdeuterated hen egg-white lysozyme (D-HEWL), we were able to study protein and water dynamics at the atomic level and the potential discrepancies between neutron and X-ray derived ADPs.
Atomic resolution neutron diffraction data was measured at room temperature for a 4 mm^3 D-HEWL crystal grown at the pH where the enzyme is fully active. This neutron data allowed the unambiguous assignment of H positions for protein residues and water molecules in the enzyme's active site, elucidating its configuration and underlying dynamics.
The preliminary analysis of room temperature and 100 K X-ray and neutron datasets of D-HEWL suggest differences in the ADPs derived from the X-ray and neutron models. Additionally, the neutron model seems to describe more accurately structural disorder, affecting less the modelling of the ADPs. The neutron ADPs seem to contain biologically relevant information that is more physically realistic than that which can be derived from the X-ray model.

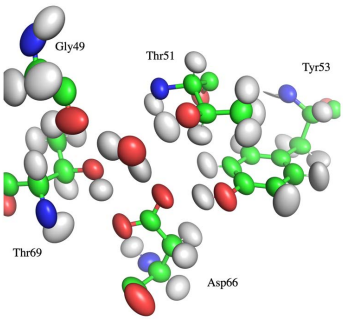

Figure – Ellipsoidal representation of anisotropic atomic displacement parameters in a region of perdeuterated hen egg-white lysozyme structure from neutron diffraction data. Carbon atoms colored in green, Oxygen in red, Nitrogen in blue and Deuterium in white.

Anyone interested is very welcome to attend.
Zoom link is available upon request to karenb@mbg.au.dk

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