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Vagabond: a new project for macromolecular model refinement

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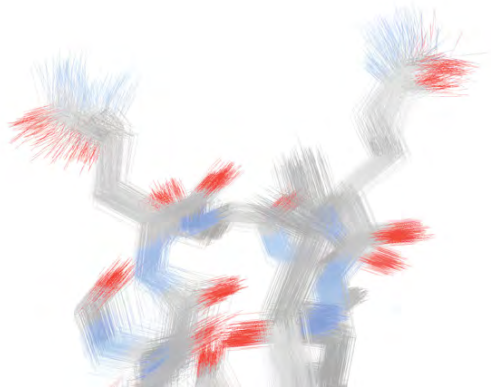
Model refinement for biomolecular crystallography, at present, relies on a model defined in atomic x, y, z parameters and associated B factors . Vagabond is a new refinement project which revisits the concept of refining in torsion space (1), defining the model in terms of bond lengths, angles and torsion angles. This significantly reduces the number of parameters required to describe most of the structure. However, it also incorporates a novel model for expressing flexibility in a chemically sensible manner, and is capable of describing weird and wonderful atomic distributions which are not accessible from isotropic or anisotropic B factor models. The combination of these features leads to a reduction in overfitting and increased clarity of maps



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Neutron protein crystallography at the Heinz Meier-Leibnitz Zentrum (MLZ): New developments and recent application examples

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With the advent of new instruments (e. g. Imagine at HFIR, MANDI at SNS and BIODIFF at FRMII) neutron protein crystallography has seen a resurrection from past pioneering work. New sample environment options at the instruments and a growing user community have greatly enhanced the outcome of the existing neutron diffractometers optimized for large unit cells. Measurements at 100 K in a nitrogen gas-stream (cryostream) are now routinely possible at most neutron diffractometers. Efforts to increase the flux at the sample position and to reduce the background at the detector make it possible to measure smaller and smaller protein crystals.

At the instrument BIODIFF latest developments allow to tilt the crystal to a kappa-geometry without the need to take it off from the goniometer head keeping it constantly at 100 K. The neutron single crystal diffractometer BIODIFF at the Heinz Maier-Leibnitz Zentrum (MLZ) is especially designed to collect data from crystals with large unit cells. The main field of application is the structural analysis of proteins, especially the determination of hydrogen atom positions. BIODIFF is a joint project of the Jülich Centre for Neutron Science (JCNS) and the FRM II. BIODIFF is designed as a monochromatic instrument with a narrow wavelength spread of less than 3 %. To cover a large solid angle the main detector of BIODIFF consists of a neutron imaging plate in a cylindrical geometry with online read-out capability. With a radius of 200 mm and a height of 450 mm it covers a solid angle of approximately 2π with a spatial resolution of up to 125 µm. An optical CCD-camera pointing at the sample position is used to quickly align the sample with respect to the neutron beam. The main advantage of BIODIFF is the possibility to adapt the wavelength to the size of the unit cell of the sample crystal while operating with a clean monochromatic beam that keeps the background level low. To illustrate the power of neutron protein crystallography, some recent application examples will be shown.

Keywords: Neutron, Monochromatic, Diffractometer