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Completing the library of amino-acid neutron structures

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Accurate neutron structures of the 20 naturally occurring amino acids that are the building blocks of proteins are key to investigations of polymorphism, condensed-phase NMR analysis, periodic density-functional-theory calculations, as restraints in X-ray protein refinements, and as initial structures in the computer modelling of proteins. The first 16 members of the family were determined in the 1970s by groups at Brookhaven National Laboratory and the Indian Atomic Energy Laboratory, but the last four proved to be elusive due to the lack of single crystals large enough for the monochromatic neutron diffractometers of the time. State-of-the-art reactor-based neutron Laue diffractometers, such as Koala on OPAL, allow high-precision structural investigations of single crystals with volumes around 0.1 mm³. This opens the door to completing the library of high-precision amino-acid neutron structures.

Here we describe variable-temperature studies of three naturally-occurring amino acids using Koala, L-leucine [1] which is one of the four missing members and the two polymorphs of L-histidine. The data on the orthorhombic form of L-histidine greatly improve on the precision of a previous monochromatic neutron study. The second, monoclinic, form has been studied with neutrons for the first time [2]. Both studies were complemented by interaction-energy calculations using the Pixel method, and, for L-histidine, Hirshfeld Atom Refinement against X-ray data at the same temperatures. The resulting neutron structures yield geometric parameters with sufficient precision and accuracy for inclusion in restraint libraries of macromolecular structure refinements.

The search continues for neutron-quality crystals of L-isoleucine, L-methionine and L-tryptophan.

[1] J. Binns et al. *Acta Cryst. B*72 (2016) 885.

[2] G. Novelli et al. *Acta Cryst B*. In press.

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Australian Centre for Neutron Scattering

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