



Contribution ID: 394

Type: **Talk**

AUSPEX: a diagnostic tool for graphical X-ray data analysis

Monday, 17 September 2018 15:27 (16 minutes)

Ice diffraction is a much bigger and more widespread problem in protein crystallography than commonly recognized [1]. 'Ice rings' are notoriously difficult to account for in integration [2]. The resulting experimental structure factor errors can affect the modelling of macromolecular structures and may even prevent their solution. Furthermore, ice rings are hard to recognize from diffraction images produced by modern pixel detectors, and even harder to identify in already processed data [1].

In order to address this problem, a new software tool, AUSPEX, has been developed. Here, it will be demonstrated how AUSPEX facilitates the detection of common problems in data collection and processing [3], allowing for visual inspection of the observed intensity (or amplitudes) distribution versus resolution and automatic ice ring detection. AUSPEX can also be used to investigate the structure and distribution of errors within crystallographic data sets; this reveals a number of additional pathologies in the processing and conversion of X-ray and neutron data.

AUSPEX will be available via CCP4 and as a web service.

[1] Thorn, A., Parkhurst, J.M., Emsley, P., Nicholls, R., Vollmar, M., Evans, G. & Murshudov, G.N. (2017) *Acta Cryst D* 73, 729-737.

[2] Parkhurst, J.M., Thorn, A., Vollmar, M., Winter, G., Waterman, D.G., Fuentes-Montero, L., Gildea, R.J., Murshudov G.N. & Evans, G. (2017), *IUCr J* 4, 626-638.

[3] Garman, E. F. & Mitchell, P. E. (1994) *J. Appl. Cryst.* 27, 1070-1074.

Primary author: THORN, Andrea (Julius-Maximilians-Universität Würzburg)

Co-authors: Dr PARKHURST, James (Diamond Light Source, Didcot, UK); Dr EMSLEY, Paul (MRC Laboratory of Molecular Biology, Cambridge, UK); Dr NICHOLLS, Robert (MRC Laboratory of Molecular Biology, Cambridge, UK); Dr VOLLMAR, Melanie (Diamond Light Source, Didcot, UK); Dr EVANS, Gwyndaf (Diamond Light Source, Didcot, UK); Dr MURSHUDOV, Garib (MRC Laboratory of Molecular Biology, Cambridge, UK)

Presenter: THORN, Andrea (Julius-Maximilians-Universität Würzburg)

Session Classification: Micro symposium 2

Track Classification: MS2 Structural biology: Instrumentation and methods, current trends and topics