MS4 New developments in phasing and refinement

Chairs: Eleanor Dodson, Randy Read

MS4-P1 *ContaMiner*: a webserver for early identification of unwantedly crystallised protein contaminants

Stefan T. Arold[1], Arnaud Hungler[1], Afaque Momin[1], Kay Diederichs[2]

1. King Abdullah University of Science and Technology
2. Fachbereich Biologie, Universität Konstanz, M647, D-78457 Konstanz, Germany

email: stefan.arold@kaust.edu.sa

Solving the phase problem in protein X-ray crystallography relies heavily on the identity of the crystallised protein, especially when molecular replacement (MR) methods are used. Yet, it is not uncommon that a contaminant crystallises instead of the protein of interest. Such contaminants may be bacterial proteins, protein fusion tags or proteins added during the purification steps. Many contaminants easily co-purify, crystallise and give good diffraction data. Identification of contaminant crystals may take much time, since the presence of the contaminant is unexpected, and its identity unknown. We have established a webserver, titled '*ContaMiner*' that allows fast MR-based screening of crystallographic data against a database of currently 57 potential contaminants. The web-based *ContaMiner* (available at strube.cbrc.kaust.edu.sa/contaminer/) currently returns results in 2-4h. Alternatively, the program is available in a GitHub repository and can be installed locally. *ContaMiner* enables systematic screening of novel crystals at synchrotron beamlines, and it would be valuable as a routine safety check for 'crystallisation and preliminary X-ray analysis' publications. Thus, in addition to potentially saving X-ray crystallographers much time and efforts, *ContaMiner* might minimise the risk of publishing erroneous data.

Keywords: diffraction, contaminant, crystal, molecular replacement

MS4-P2 HKL2MAP 0.5 – new features for phasing with SHELXC/D/E

Fabio Dall'Antonia[1], Thomas R. Schneider[1]

1. European Molecular Biology Laboratory, Hamburg Outstation

email: fabio.dallantonia@embl-hamburg.de

Crystallographic phasing (SAD, MAD, SIR, SIRAS) with the programs SHELXC, -D and –E [1] is a widely used path in macromolecular structure determination, in particular at synchrotron beam-lines, due to the fast feedback on phasing success. Along with the introduction of novel and powerful SHELXC/D/E features during the last years – *e. g.* substructure site refinement and backbone auto-tracing – the graphical user interface (GUI) HKL2MAP [2] has evolved and became a very popular tool for the control of the SHELX suite workflow and the graphical visualization of results.

Here, we present the latest developments of HKL2MAP with a focus on input data preparation. Ultimately, the performance of substructure determination in experimental phasing (SHELXD) as well as the resulting protein phase quality, that is, interpretability of electron density maps after density modification (SHELXE), depend on the accuracy of the processed diffraction data – in particular for methods based on anomalous differences. In this context, HKL2MAP/SHELXC provide an interface between data processing software and the phasing tasks.

Yet unaccounted for in our software so far, the monitoring of accuracy criteria over the course of data collection (*i. e.*, frame number) and the justified rejection of frame regions are possible measures that can crucially improve the quality of data subjected to SHELXC/D/E – which is sometimes the vital step for phasing success. HKL2MAP 0.5 now employs a preprocessor module for graphical visualization of frame-based XDS [3] statistics, namely the mean unmerged $I/\sigma(I)$ vs. frame number and the derived R_{decay} [4] vs. frame distance. Furthermore, the new design of the GUI allows for truncation of frame ranges before submitting unmerged data to SHELXC. The new GUI and its functions are demonstrated and case studies of application presented.

HKL2MAP is free for academic users and can be obtained by online registration at webapps.embl-hamburg.de.

References:

[1] Sheldrick, G. M. (2010). *Acta Cryst.* **D66**, 479-485.

[2] Pape, T. & Schneider, T. R. (2004). *J. Appl. Cryst.* **37**, 843-844.

[3.a] Kabsch, W. (2010). *Acta Cryst.* **D66**, 125-132.

[3.b] Kabsch, W. (2010). *Acta Cryst.* **D66**, 133-144.

[4] Diederichs, K. (2006). *Acta Cryst.* **D62**, 96-101.

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