[MS04-P03] HKL2MAP. An Updated Version Compatible with SHELX-2013.
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HKL2MAP [1] is a graphical user interface designed for the semi-automatic operation of the command-line-driven programs SHELXC/D/E [2]. The typical workflow of macromolecular crystallographic phasing using the SAD, MAD or SIRAS methods is separated into three task modules related to the respective SHELX programs. HKL2MAP allows for the selection of input files with diffraction data in various formats and automatically extracts unit cell parameters and space group for FA data preparation with SHELXC. The expected number of sites for heavy, respectively anomalously scattering, atoms is the sole essential user input to SHELXD for substructure determination. HKL2MAP can estimate the solvent content of the crystal structure from the number of amino acid residues and provides this parameter to SHELXE for phase calculation, solvent flattening and peptide backbone auto-tracing. Output produced by the SHELX programs is visualized by means of various graphs in order to facilitate decisions like FA data truncation and to monitor the phasing success.
The updated version HKL2MAP 0.3 has been refurbished in order to integrate with the recently released versions of SHELXC/D/E (http://shelx.uni-ac.gwdg.de/SHELX/). It supports the use of the multi-processor version of SHELXD and allows to control recently introduced features of SHELXE. Firstly, the optimization of the heavy atom substructure prior to the initial phase calculation, a choice that has often found to be critical for the structure solution, can be activated. Secondly, alternate cycles of poly-Ala auto-tracing – optionally with initial search for secondary structure – and solvent flattening are introduced for an iterative improvement of density-modified phases. Thirdly, HKL2MAP now employs COOT [3] as the graphical display program, so that the final poly-Ala model and electron density map derived from SHELXE phases can be readily inspected.
In addition to demonstrating the general usage of HKL2MAP with a focus on the new features, cases of successful structure determination starting from weak anomalous signal and/or borderline diffraction data quality are presented. HKL2MAP is freely available for academic usage and can be downloaded from http://webapps.embl-hamburg.de.

[1] T. Pape & T. R. Schneider (2004). *J. Appl. Cryst.* 37, 843-844.
[2] G. M. Sheldrick (2010). *Acta Cryst.* D66, 479-485.
[3] P. Emsley, B. Lohkamp, W. G. Scott & K. Cowtan (2010). *Acta Cryst*. D66, 486-501.

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