

The generation of the first electron density maps from the experimental data is the most exiting step of the structure determination process. In many cases this step is relatively easy and due to the advances in software development can be performed in a completely automatic way. However, sometimes the available set of experimental data is not of the highest quality. In such a case the automatic approach may fail or result in a poor quality electron density map. HKL-3000 provides an integrated and well tested pipeline that is usually run in a semi-automatic mode and could be used for both Molecular Replacement and *de novo* phasing [1]. The analysis of results from each step is used to optimize input parameters for every subsequent step. Therefore, in the case of an unsuccessful outcome for a particular step, the experimenter has the possibility to use a more sophisticated approach than that coded as a default in the system. For example, the system has the ability to import partial solutions from external programs. Similarly, the experimenter has the ability to adjust many parameters and test various phasing strategies relatively quickly. The examples of phasing using this approach for cases with non-optimal experimental data will be discussed.

1. Minor W., Cymborowski M., Otwinowski Z., Chruszcz M. "HKL -3000: the integration of data reduction and structure solution – from diffraction images to an initial model in minutes" Acta Cryst. 2006, D62, 859–866.