HAPPy progress

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Work on the new experimental phasing system, HAPPy (Heavy Atom Phasing in Python), discussed in the previous newsletter, is progressing well. We are testing several packages for inclusion as phasing modules including MLPHARE and PHASER. HAPPy can now take a SAD dataset from the post data processing stage to a refined map with no interaction from the user after providing the initial problem description. The current priority is determining the optimal parameters for the major components and systematic testing and analysis of results to improve the quality of solutions obtained.

There has also been work on the history and data tracking for the next generation CCP4i database and the development of an experimental phasing datamodel for the database being developed by CCP4 in the BioXHIT framework.

The diagram on the right, generated automatically by the HAPPy tracking database, shows the flow of a simple example run. Note that this shows what happened for this particular run; the procedure can become more complicated depending on the dataset and options selected. In this example, HAPPy first ran SHELXD with various sets of resolution and anomalous difference limits, then chose the best resulting heavy atom solution for phasing with MLPHARE. After determining the correct hand for the heavy atom substructure by looking at variance maps of the MLPHARE output, the final map and phases were refined using PIRATE. The figure below shows a section of the final map in COOT.