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MrBUMP, an Automated Framework for Doing Molecular Replacement in Protein Crystallography. R.M. Keegan, M. D. Winn, CCP4 group, CCLRC Daresbury Laboratory, Warrington, Cheshire, WA4 4AD, U.K.

The number of models of macromolecular structure deposited in the Protein Data Bank continues to grow apace. Mostly this reflects advances in crystallography, although other techniques such as NMR are also maturing. As well as providing input to further theoretical modelling or experiment design, the PDB increasingly supports further structure determination through the technique of Molecular Replacement (MR). As the size of the PDB increases, the relative significance of the MR technique is widely expected to grow. Although there continue to be advances in the underlying algorithms, the software effort in macromolecular structure determination is increasingly turning towards the development of automation schemes which link together several steps of the structure solution pipeline. Part of the reason is to make the application of crystallographic techniques easier so that scientists can focus on the biology, but automation also allows a more exhaustive search of relevant methods and parameters which may increase the quality of the solution. In the context of MR, a crystallographer may have to try a large number of search models and MR programs before finding the optimum solution, or indeed any solution, and this aspect is clearly ripe for automation. Here, we describe an automated package for structure solution by molecular replacement, called MrBUMP. In essence, the package consists of a set of Python scripts which link together established programs. We believe that MrBUMP differs from other molecular replacement pipelines in two ways: Firstly, there is a greater emphasis on the discovery of potential search models. A list of search models is generated and many are tried in molecular replacement with the aim of finding the optimum model. Secondly, MrBUMP is intended for general use within the CCP4 software suite (the Collaborative Computational Project No. 4, a UK-based software project that provides a suite of programs for the determination of macromolecular structures via X-ray crystallography), and is designed to be portable and flexible.