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Methods, Hardware, and Software for High-Throughput Data Collection in Macromolecular Crystallography: The Brookhaven Experience. R.M. Sweet, D. Schneider, H. Robinson, A. Héroux, A. Soares, M. Becker, J. Jiang, J. Skinner, R. Buono, M. Cowan. Biology Dept., Brookhaven Nat'l Lab, Upton, NY.

The PXRR (<http://www.px.nsls.bnl.gov>) operates six beamlines at the NSLS for macromolecular crystallography (PX). We have defined a new paradigm for use of the synchrotron by structural biologists. Rapid Access, sometimes very rapid, is the norm for most beam line visits. We implemented a mail-in (so-called FedEx) operation: investigators send frozen specimens; we do the work. We provide fluid access to all of our work stations and a consistent look-and-feel among them. It's not unusual for visitors to switch to a more appropriate beam line during a visit, or to operate two at once.

To accomplish this we provide a pool of equipment and personnel, especially overnight PX Operators and computing support. We have a long-standing drive to provide users with easy-to-use tools that let them focus on the crystallographic problem at hand. Software development is a central aspect of this; more recently we are installing ALS-style automounters. Now we are tying the whole process together in a high-throughput mode with our experiment-tracking database, PXDB, which carries information from the initial request for beam time to the final reduced data. All of this is supported by our numerous innovations in the field: the first electronic area-sensitive detector at a beamline in the US, the first graphical user interface for experiment control, on-site data reduction, automatic MAD data collection, web-based remote observation, and more.