

E0020

Methods, Hardware, and Software for High-Throughput and Remote Data Collection in Macromolecular Crystallography: the Brookhaven Experience. D.K. Schneider, H. Robinson, A. Héroux, A. Soares, A. Saxena, J. Skinner, R. Buono, M. Cowan, H. Bosshard, and R.M. Sweet, Biology Dept., Brookhaven National Laboratory, Upton, NY 11973 USA.

The PXRR (www.px.nsls.bnl.gov) operates six beam lines at the NSLS for macromolecular crystallography (PX). Two of these are high intensity insertion-device beam lines. We have defined a new paradigm for use of the synchrotron by structural biologists. Rapid Access is the norm for most beam line visits and daily open slots on our premier facilities are allocated over night to deserving projects or specimens. We implemented a mail-in service and promote a remote data collections capability with a resident PX-Operator staff that provides nearly 24h/7day facility support. To accomplish this we provide a pool of equipment, including ALS-style automounters, and software with very similar feel and layout across our facilities. An experiment-tracking database, PXdb, which carries information from beam time request to the final reduced data, is of critical importance in connecting dipole beam lines where users may screen specimens for quality, with ID lines where they may measure final data.

This work is supported by the NCRR of the National Institutes of Health, and the OBER of the US Department of Energy.