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SGX-CAT: An Automated Synchrotron Beamline Dedicated to Mail-in Crystallography. David W. Smith, Stephen R. Wasserman, John W. Koss, Laura L. Morisco, Kevin L. D'Amico, SGX Pharmaceuticals, Inc., Advanced Photon Source, Argonne National Laboratory, 9700 S. Cass Ave, Argonne, IL 60439.

SGX Pharmaceuticals, Inc. developed and operates SGX-CAT, a beamline at the Advanced Photon Source whose sole mode of operation is mail-in crystallography. All samples, whether from the company, corporate partners, or general users, are assessed and collected by a staff of five based locally at the synchrotron. The beamline operations are linked to an Oracle database that tracks the crystals, their collection status, and the quality of the data from them. The initial descriptions of the crystals, including their provenance and likely properties, are entered into the database, either directly or through an electronic spreadsheet. Samples are identified by 1-D and 2-D barcodes that link the information in the database to the physical samples. Screening and collection utilize several automated processes, including generation of protocols for data collection, centering of loops, removal of surface ice, scoring of crystal quality, processing of data, and updating of the database. For most crystals, quality is evaluated and data are generated without a human examining a single diffraction image from the crystal. The high degree of automation permits the staff to operate and maintain the beamline while providing the crystallographic information. In 2005, 9000 crystals were screened and 4200 datasets were collected using these processes.