

Software at the CMCF

Canadian Macromolecular Crystallography Facility



The CMCF beamlines are equipped with an integrated, state-of-the-art software system for data collection, experiment management, and automated data processing for both on-site and remote users. Developed in-house, CMCF software offers experiment-focused control of the beamline through an integrated graphical user interface, and experiment management through a web browser.

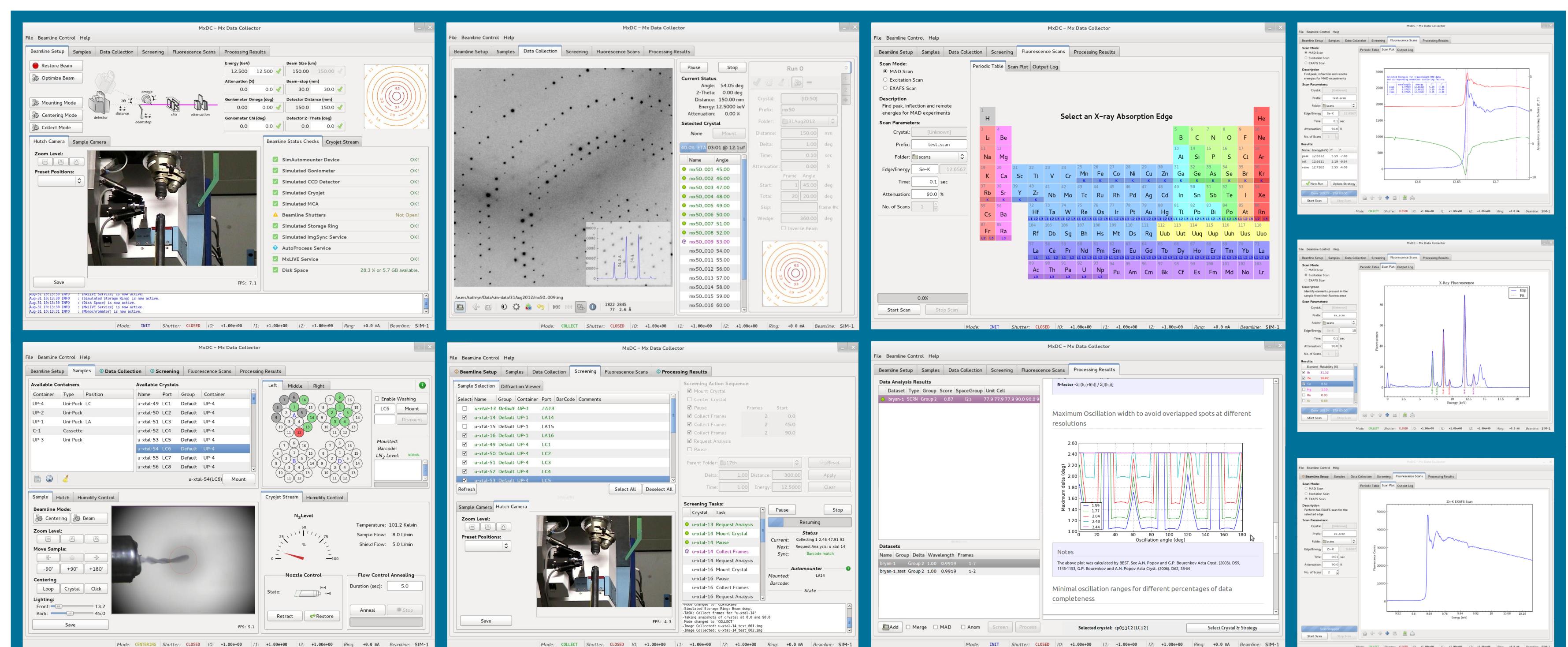
Learn More:



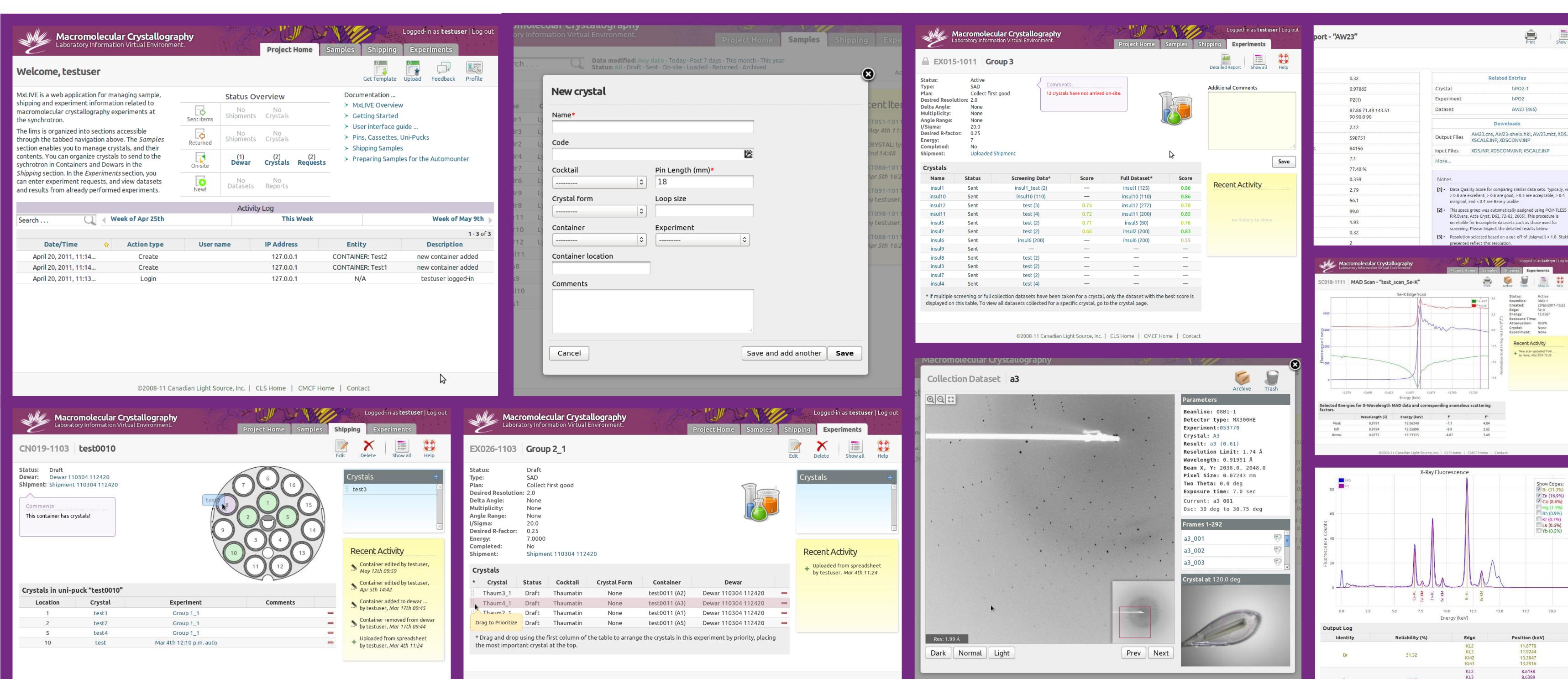
MxDC - Data Collection

A user-friendly interface and full integration with both MxLIVE and AutoProcess make MxDC a leader in crystallography data collection software. From beamline setup and sample management (with MxLIVE) to data collection and processing (with AutoProcess), MxDC is designed to guide users through their beamtime, putting the focus where it belongs – on the experiment.

MxDC is developed in the python programming language, using tools such as the Zope Component Architecture, the Twisted Framework, the Multicast DNS protocol, and the CTK+ toolkit.



MxLIVE - Experiment Management



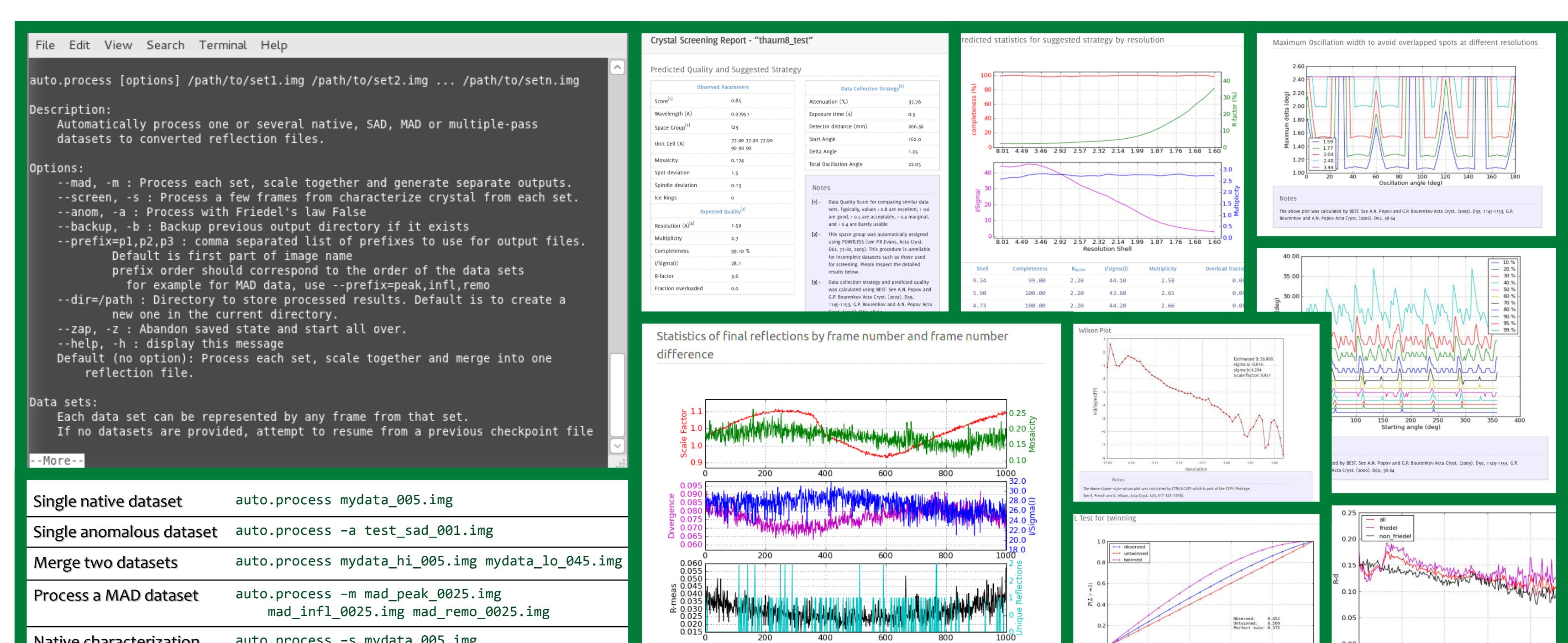
MxLIVE is an information management system that allows users to manage sample information, track shipments, view datasets, scans, and processing reports as they are completed on the beamline, and download processing files from any internet browser, anywhere in the world.

AutoProcess - Automated Data Processing

AutoProcess is a data processing pipeline that can be used from the command line with minimal input or remotely as a server. Starting with a single file name as input, the system presents users with a graphical data processing report as well as processed reflection output files in popular formats, without user intervention. These files can be used directly in users' favourite structure solution/refinement programs.

AutoProcess is a pipeline layered on the XDS data processing package and makes use of the BEST strategy calculation package from EMBL. A few CCP4 utilities for automatic space group selection and data quality evaluation such as POINTLESS and CTRUNCATE are also used. The system is developed in the Python programming language.

Technical Details



MxLIVE is developed using Django, a Python-based web framework, backed by a MySQL database. A combination of HTML and jQuery javascript form an interface supported on all major browsers. Using JSON-RPC to handle the integration with MxDC and AutoProcess, MxLIVE is deployed using Apache and is SSL secured.



Technical Details