

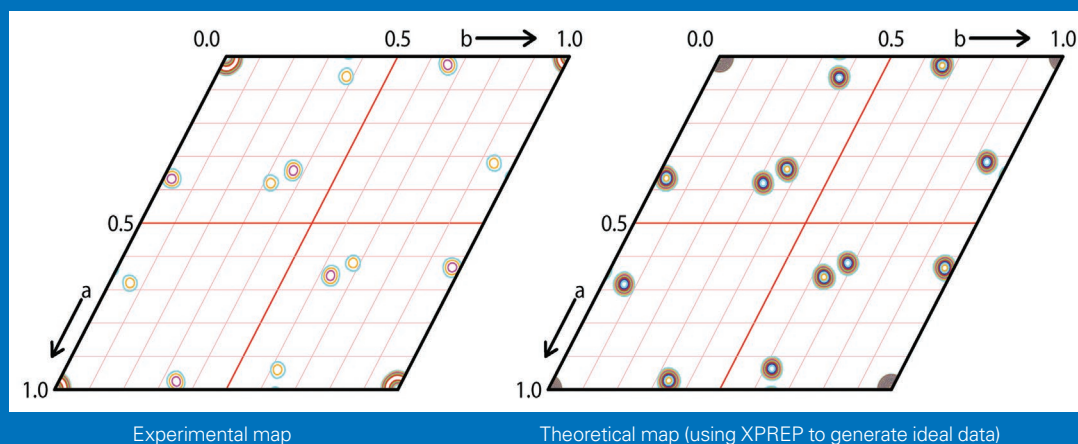
Product Sheet SC-XRD 46

XPREP

Versatile Data Analysis Tool for Macromolecular Crystallography

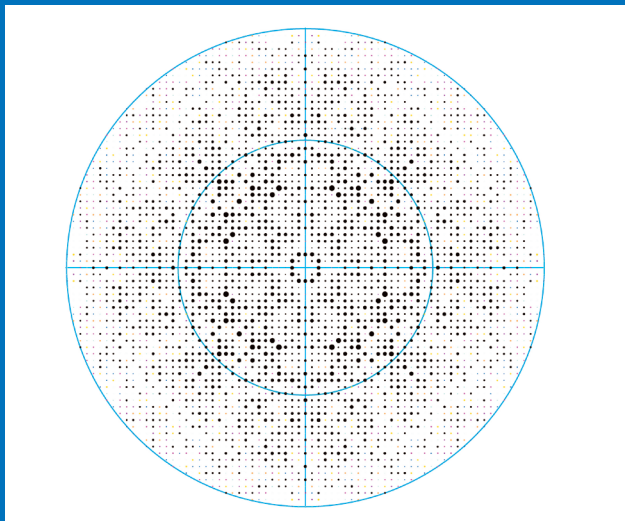
XPREP can read and write single crystal diffraction data in a variety of formats. XPREP automatically determines space groups displaying relevant symmetry information along the way. It easily allows the user to statistically evaluate and prepare the data for the next step. XPREP also calculates all the coefficients and input files required for structure solution using the SHELX suite. All numerical output is stored in a detailed log file and all graphical output may be saved as PostScript files as well as being displayed in the graphical

Harker section of a FA-Patterson map 2-site gold SAD data set collected on a Bruker X8 PROSPECTOR



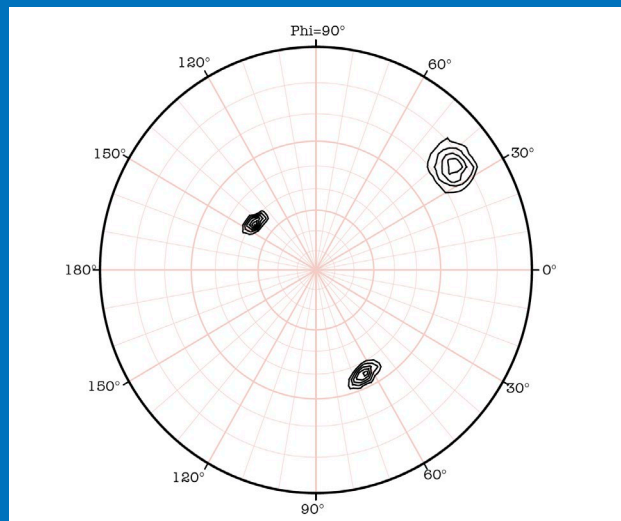
user interface. Compatible with any in-house or beamline data, XPREP provides many tools for data analysis and manipulation that greatly simplify the transition from data reduction to structure determination and refinement.

Reciprocal space display from experimental data



The reciprocal space display visualizes intensities and standard uncertainties of layers of reflections

Self-rotation function of triclinic protein



Self-rotation function of a triclinic protein showing three two-fold axes 90 degrees from each other (local 222 non-crystallographic symmetry).

Key features include:

- Automatic space group determination, if necessary transforming to a standard unit cell in the process.
- All operations can handle reflections in any order and take equivalents into account, using the space group to distinguish between Friedel mates and true symmetry equivalents.
- Generates statistics and graphs for input data sets. Provides all the standard data correlation coefficients as well as quality indicators for anomalous scattering information.
- Outputs HKL files in various formats including: SHELX, Scalepack and CNS.
- Outputs coefficients for MAD, SIR, SAD and SIRAS experiments. Can be used for either in-house or synchrotron data.
- Generates Patterson Harker sections and peak lists. This is especially useful for identifying heavy atom sites.
- Creates reciprocal space displays, with or without generation of symmetry equivalent reflections. This is useful for checking data completeness and also for visualizing data artifacts.
- Provides tools for detecting twinned data.
- Generates free R flags either randomly or in thin shells. Transfers free R flags from one dataset to another.

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