

Macromolecular Crystallography Software

This page describes all software packages that are available at GM/CA. **Supported** programs and packages are regularly updated and thoroughly tested in the beamline computer environment. **Unsupported** programs are also available to the users, but support staff cannot guarantee that they are up to date or that local expertise exists for these programs.

Data Processing

- [HKL2000](#) The HKL2000 suite of programs contains Denzo, XdisplayF, Scalepack, STRAT (program for strategy and simulation). **Supported**
- [d*trek](#) The d*trek suite of programs from Jim Pflugrath of RIGAKU for indexing, visualization, strategy and processing data. **Supported**
- [Mosflm](#) A program for visualization, indexing and integrating single crystal diffraction data from area detectors. **Supported**
- [HKL \(Denzo/Scalepack\)](#) Programs for processing (index, integrate and scale) single crystal diffraction data. **Supported**
- [XDS](#) The XDS suite of programs from Wolfgang Kabsch for strategy and data processing. **Unsupported**
- [X-GEN](#) A Data Processing Software Package for Crystallographic Area Detector Data by Andy Howard. **Unsupported**
- [Labelit](#) A robust autoindexing program from Nick Sauter at LBNL. **Unsupported**

Data Scaling

- [CCP4](#) The CCP4 program suite for crystallographic software. **Supported**

Phasing and Refinement

- [CCP4](#) The CCP4 suite is a set of programs which communicate via standard data files. It has several programs for data manipulation, phasing, and refinement of macromolecules. **Supported**
- [SOLVE & RESOLVE](#) SOLVE program can carry out steps of macromolecular structure determination from scaling of the data sets to the calculation of an electron density map automatically. The companion program RESOLVE improves the electron density maps obtained from SOLVE or other phasing programs. **Supported**.
- [SHELX](#) SHELX is a set of programs for crystal structure determination from single-crystal diffraction data. This suite can also perform structure refinement. **Unsupported**
- [SnB](#) SnB program is based on Shake-and-Bake, a dual-space direct-methods procedure for determining crystal structures from X-ray diffraction data. **Unsupported**
- [BnP](#) BnP ("Buffalo and Pittsburgh" program is based on Shake-and-Bake and Phases from Charles Weeks and Bill Furey and **Unsupported**
- [CNS](#) Performs phasing, density modification, and refinement of macromolecules. **Unsupported**
- [ARP/wARP](#) ARP/wARP is a software suite for improvement and objective interpretation of crystallographic electron density maps. It also performs automatic tracing and refinement of macromolecular models. **Unsupported**

Model Building and Molecular Graphics

- [O](#) O is a program for model building using electron density maps and model manipulation. **Supported**
- [Coot](#) Coot is a GPL program for model building and validation. **Supported**
- [PyMOL](#) PyMOL program is a molecular graphics program with high-quality rendering, animations and other common molecular graphics activities. **Unsupported**
- [RasMol](#) A molecular graphics program intended for the visualisation of macromolecules and small molecules. **Unsupported**
- [Raster3D](#) A set of tools for generating high quality raster images for proteins or other molecules. **Unsupported**