

25.1. SURVEY OF AVAILABLE PROGRAMS

ment, electron-density modification, structure refinement and structure comparison, and include many utility programs.

Location: <http://www-structure.bio.purdue.edu/~kvz/> (also includes references for individual programs). Operating systems: IBM RS/6000 and UNIX. Type: source code and binary. Distribution: free.

25.1.2.10. SOLVE

SOLVE (Terwilliger & Berendzen, 1999) is a complete program package designed for automated crystallographic structure solution for MIR and MAD. *SOLVE* can carry out all steps of macromolecular structure determination automatically using MIR and MAD methods, ranging from scaling data to calculation of an electron-density map. It scales data, solves Patterson functions, calculates difference Fourier maps, searches native Fourier maps for distinct solvent and protein regions, and scores partial MAD and MIR solutions to build up a complete solution.

Locations: <http://www.solve.lanl.gov/>, <ftp://solve.lanl.gov/pub/solve>. Operating systems: SGI, SUN, HP, DEC and LINUX. Type: binary. Distribution: minor licence fee for academic users.

25.1.2.11. USF

The Uppsala Software Factory (*USF*) comprises a large collection of programs written by Dr Gerard Kleywegt at Uppsala University. These programs have applications in many aspects of structure determination and analysis, including electron-density modification, multiple crystal forms and protein domain averaging, structure validation, error detection and recognition of spatial motifs in protein structures, and includes many utility programs and interface programs for program *O*. See Chapter 17.1 for more details.

Location: <http://alpha2.bmc.uu.se/~gerard/usf/>. Operating systems: UNIX and VAX/VMS. Type: binary. Distribution: free academic.

25.1.2.12. X-PLOR

X-PLOR (Brünger *et al.*, 1987; Brünger, 1992) is an integrated program package for structure determination of macromolecules using X-ray crystallography and NMR. The main features of *X-PLOR* related to X-ray crystallography include: (1) crystallographic refinement by the simulated-annealing method; (2) rigid-body refinement; (3) conventional positional refinement; (4) refinement of individual *B* factors, group *B* factors and overall anisotropic *B* factors; and (5) analysis of macromolecular structures. The new release, *X-PLOR98*, includes maximum-likelihood refinement as well.

Locations: for *X-PLOR98*, <http://www.msi.com/>; for *X-PLOR3.851*, <http://xplor.csb.yale.edu/xplor-info/>. Operating system: UNIX. Type: source code and binary. Distribution: commercial.

25.1.2.13. Xtal

The *Xtal* system (Hall *et al.*, 1999) is a comprehensive package of crystallographic software for structure determination, including applications for manipulation of diffraction data, structure solution, structure refinement, structure analysis and presentation of crystal structures. These programs are applicable to X-ray, neutron and electron diffraction analyses, including charge-density studies. The package contains a number of interactive graphics tools and is distributed as execution modules for most commonly available workstations and PCs.

Locations: <http://www.crystal.uwa.edu.au/xtal/>; <ftp://ftp.crystal.uwa.edu.au/xtal>. Operating systems: UNIX, VMS and Windows. Type: binary. Language: Fortran77. Distribution: commercial.

25.1.2.14. XtalView

XtalView (McRee, 1993) is a crystallographic software package for fitting electron-density maps and solving crystal structures of macromolecules by MIR and MAD methods. Applications include graphics, visualization, virtual reality, modelling and structure determination. It has a simple but comprehensive Windows-based interface. The main menu drives a suite of crystallographic modules by clicking on icons. Standard file formats are used, which facilitate communication between *XtalView* and programs such as *X-PLOR*, *TNT* and *MERLOT*.

Location: <http://www.scripps.edu/pub/dem-web/toc.html>. Operating systems: UNIX, SGI, SUN, DEC, IBM and LINUX. Type: source code and binary. Distribution: free academic.

25.1.3. Data collection and processing

25.1.3.1. DPS

The Data Processing Suite (*DPS*) (Rossmann & van Beek, 1999) is a complete package for processing X-ray diffraction data from crystals of proteins, viruses, nucleic acids and other large biological complexes. The emphasis is on diffraction data collected using synchrotron sources. Currently *DPS* consists of *dps_index* and *dps_scale*, and uses some of the programs from the *MOSFLM/CCP4* suite. The *dps_index* program uses Fourier analysis for the automatic indexing of oscillation images. The *dps_scale* program uses a scaling method that does not depend on the exclusive use of full reflections. See Chapters 11.1 and 11.5 for more details.

Location: <http://ultdev.chess.cornell.edu/MacCHESS/DPS>. Operating systems: UNIX, SGI and LINUX. Type: binary. Distribution: free academic.

25.1.3.2. HKL

The *HKL* program package (Otwinowski & Minor, 1996) is a complete set of data-processing programs for the analysis of X-ray diffraction data collected from single crystals. The package comprises three components: *XDISPLAY* for graphical visualization of the diffraction image; *DENZO* for autoindexing, reduction and integration of diffraction data; and *SCALEPACK* for scaling and merging of intensities from multiple images. See Chapter 11.4 for more details.

Location: <http://www.hkl-xray.com/>. Operating systems: SGI, DEC Alpha, SUN and HP-UX. Type: binary. Distribution: commercial.

25.1.3.3. LOCSCL

LOCSCL (Blessing, 1997) is a program used to optimize statistically local scaling of single-isomorphous-replacement and single-wavelength anomalous-scattering data.

Location: e-mail blessing@hwi.buffalo.edu. Operating systems: UNIX and Windows. Type: source code. Language: Fortran77. Distribution: free.

25.1.3.4. MOSFLM

MOSFLM is a general-purpose data-processing package developed by Dr Andrew Leslie at the MRC, England. The programs have two main applications: (1) determination of crystal orientation, cell parameters and possible space group; and (2) autoindexing of images, generation of reflection lists and integration of diffraction spots. *MOSFLM* is distributed as part of the *CCP4* suite and runs on multiple platforms. See Chapters 11.2 and 11.3 for more details.

Location: <ftp://ftp.mrc-lmb.cam.ac.uk/>. Operating systems: UNIX and VAX/VMS. Type: source code and binary. Distribution: free academic.