25.2.1.12.4. *Generic plot files and drivers*

The plot files created by *CTOUR* are generic in nature and are not directly displayable. One needs a driver program to convert the generic files to the format appropriate for the desired display device. The appropriate drivers for several popular display devices are provided within the package and are described below.

25.2.1.12.4.1. *GL displays*

For display on Silicon Graphics workstations, the interactive program *VIEWPLT* can be used to examine the generic plots created by *CTOUR*. Up to ten plots can be displayed simultaneously. It is particularly useful to display the various contoured Harker sections simultaneously during difference-Patterson interpretation.

25.2.1.12.4.2. *X-Window displays*

For display of *CTOUR* plots on monitors supporting the X-Window protocol, including most workstation monitors and X-terminals, the program *VIEWPLT_X* can be used instead of *VIEWPLT*. The functionality is identical to the GL version.

25.2.1.12.4.3. *PostScript files*

The interactive program *MKPOST* is provided to generate standard PostScript equivalents from the generic plot files produced by *CTOUR*. Multiple plot files can be generated in the same process. The PostScript files can be printed, viewed with a PostScript previewer, or incorporated into other documents.

25.2.1.12.4.4. *Tektronix output*

The interactive program *PLTTEK* can be used to display the generic plots created by *CTOUR* on any device supporting Tektronix 4010 emulation. While slow, this enables visualization of the plots on many 'dumb' terminals.

25.2.1.13. *Auxiliary programs*

In addition to the major programs already described, a number of auxiliary programs (all interactive) are provided in the package to aid the user in porting information to or from external software and to assess phasing methods. These programs are briefly described below.

25.2.1.13.1. *Coordinate conversions*

Within the package, fractional atomic coordinates are used extensively, and the program *PDB_CDS* is provided to convert from PDB (Protein Data Bank) to *PHASES* coordinate files and *vice versa*. The program prompts for input and output file names, the direction of the conversion, chain or residue ranges, and whether to reset occupancies and/or thermal factors to specified values. The coordinate ranges (both fractional and in PDB coordinates) spanned by the model are also listed.

25.2.1.13.2. *NC symmetry operator conversions*

The program *O_TO_SP* is provided to convert NC symmetry operators expressed in terms of a 3×3 rotation matrix and 1×3 translation vector to the *PHASES*-style spherical polar system described earlier. Although originally written to convert the transformation operator as defined in the *O* program (Jones *et al.*, 1991), the procedure works for any rotation or translation operator expressed in this form, provided that the operator is applicable to Cartesian coordinates in Å orthogonalized as in the Protein Data Bank (Bernstein *et al.*, 1977).

25.2.1.13.3. *Binary or formatted file conversions*

For efficiency, structure-factor files used within the package are binary; however, the program *RD*31 is provided to read these binary files and convert them to formatted files that can be examined and possibly edited by the user. The indices, amplitudes, phases, figures of merit, phase probability distribution coefficients, and markers indicating which reflections are centric along with the allowed phase values are thus made readily accessible. A corresponding program, *MK*31*B*, is also provided to reverse the process; it reads the formatted (and possibly edited) versions of the structure-factor files and generates the appropriate binary-file equivalents. Additionally, the program *XPL_PHI* is supplied to convert the binary structure-factor files to a form readable by the *X-PLOR* program (Brünger *et al.*, 1987) in order to facilitate complete model refinement. Phase and figure-of-merit information are also passed to the output file, allowing refinement with phase restraints if desired.

25.2.1.13.4. *Importing phase information*

The program *IMPORT* allows users to 'import' phase information obtained from programs external to the package so it can be used for subsequent calculations within the package. For example, one can use phase and probability distribution information obtained elsewhere to initiate solvent flattening, negative-density truncation and/or NC symmetry averaging within *PHASES*, or simply to generate and display maps with *MAPVIEW* or the other graphics programs. Reflection indices, the observed structure-factor amplitude, figure of merit, phase and phase probability distribution coefficients must be supplied, although free format can be used.

25.2.1.13.5. *Phase set comparisons*

The program *PSTATS* compares phases in two different structure-factor files. It lists mean phase differences as a function of *d* spacing for common reflections. The program is very useful for comparing results from different phasing strategies and for testing new procedures against error-free phases. It can also be used to check for convergence in iterative procedures or to assess the relative contributions of phase sets during phase combination.

25.2.2. *DM/DMMULTI* software for phase improvement by density modification

(K. D. Cowtan, K. Y. J. Zhang and P. Main)

25.2.2.1. *Introduction*

DM is an automated procedure for phase improvement by iterated density modification. It is used to obtain a set of improved phases and figures of merit, using as a starting point the observed diffraction amplitudes and some initial poor estimates for the phases and figures of merit. *DM* improves the phases through an alternate application of two processes: real-space electron-density modification and reciprocal-space phase combination. *DM* can perform solvent flattening, histogram matching, multi-resolution modification, averaging, skeletonization and Sayre refinement, as well as conventional or reflection-omit phase combination. Solvent and averaging masks may be input by the user or calculated automatically. Averaging operators may be refined within the program. Multiple averaging domains may be averaged using different operators.

DMMULTI is a modified version of the *DM* software that can perform density modification simultaneously across multiple crystal forms. The procedure is general, handling an arbitrary number of domains appearing in an arbitrary number of crystal forms. Initial phases may be provided for one or more crystal forms; however, improved phases are calculated in every crystal form.

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