SHELX Workshop, ACA2007

SHELXPRO

Salt Lake City, July 21st 2007

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http://shelx.uni-ac.gwdg.de/SHELX/

SHELXPRO - Options

SHELXPRO was included in the 1997 release to provide an interface to SHELX for macromolecular users. It is basically a collection of 26 more or less independent routines that at the time were needed. When the program is started a menu appears:

```
SHELXPRO - SHELX interface for protein applications - Version 97-3
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[F] New output filename                          [V] R(free) files
[A] Anisotropic scaling (Hope & Parkin)          [I] .ins from PDB file
[P] Progress of LS refinement diagram            [L] Luzzati plot
[T] Thermal displacement analysis                [E] Esd analysis
[U] Update .res (and .pdb) to .ins file          [N] NCS analysis
[R] Ramachandran Phi-Psi plot                    [K] Kleywegt NCS plot
[M] Map file for O from .fcf                     [O] PDB file for O
[H] .hkl file from other data formats            [Y] X-PLOR/CNS .fob to .hkl
[D] Convert DENZO/SCALEPACK .sca to .hkl         [C] Color plots (now on)
[X] Write XtalView map coefficients              [W] Write Turbo-Frodo map
[S] Reflection statistics from .fcf              [Z] Least-squares fit
[J] Generate restraints from model               [B] PDB deposition
[G] Generate PDB file from .res or .pdb          [Q] Quit

Enter option:
```

SHELXPRO - Documentation

On entering one of the code letters, a short description appears of the option chosen. The user can choose to answer 'N' to select another option, or <CR> to continue:

```
Enter option: j

Reads a .ins, .res, PDB or Cambridge Data Base .dat format file and generates
DFIX and DANG restraints for use by SHELXL. An orthogonal fragment may be set
up for least-squares fitting in SHELXL prior to refinement; this fragment may
be plotted using the XP program in the Bruker SHELXTL system (CELL 1, then
READ ..., FMOL, MPLN and TELP etc.). All the restraints generated from the
model apply to the same residue type; it may be necessary to add FLAT and
CHIV restraints by hand. The atom names should be the same in the model file
and in the structure to be refined. Note that where the input is from a CSD
file, atom names beginning with 'H' will be interpreted as hydrogen and hence
ignored. DANG instructions may be duplicated for 1,3-distances across
four-membered rings, but this is harmless.

Enter N to abort option, <Enter> to continue:
```

Obsolete options

Many options are now obsolete because in the meantime better programs have become available. These include:

All map options (M, O, W. X). It is much better to read the *.fcf* file from SHELXL or the *.phs* file from SHELXE into Coot!

Options K, R, T, Z: read the *.res* file into the next version of Coot!

All operations on reflection lists: use XPREP, mtz2hkl or mtz2sca (the latter two programs by Tim Grüne are available from the SHELX server, but at the moment only for Linux).

Anisotropic scaling (A): use the HOPE instruction in SHELXL or the anisotropic scaling in XPREP.

Options that are still useful

I: generate a SHELXL .ins file from a PDB file, inserting the restraints for standard amino-acids and disulfide bridges, and renumbering residues (since SHELXL does not use chains, it is usual to start chain A at 1001, chain B at 2001 etc).

U: update the .res file to the .ins file for the next refinement job. This is better than 'I' for this purpose because all special SHELX instructions are retained. Possibly this option will be made redundant by a future version of Coot.

J: extract suitable bond length and angle distance restraints from a small molecule structure (e.g. of a ligand).

E, L, P, R, S, (T): Tables and Postscript plots based mainly on the .lst listing file from the final refinement. These could also be incorporated into a future version of Coot.

B; prepare PDB file for deposition with the RCSB.

Desirable improvements in SHELXL

A multi-CPU version, adapted by Kay Diederichs, achieves a high speedup for CGLS refinement and is available from the SHELX download server. This needs optimizing for full-matrix refinement and 64-bit operation.

SHELXL is inferior to REFMAC at modest and low resolution. My analysis shows that this is primarily due to the better solvent model in REFMAC and the lack of torsion angle restraints (for the side-chains) in SHELXL. The antibumping model in SHELX is also very crude and needs explicit hydrogen bonds.

The riding model for hydrogens is not very suitable for neutron diffraction data. It would be better to use restraints that could be generated automatically.

When SHELXL was written, computer memory was a scarce commodity. The program could be speeded up by not using scratch files and rewriting the instruction file parser (the current algorithm that converts characters to reals is very inefficient).

All of this would require a major rewrite!