Menus

The menu items provide access to some of the more advanced features of CRYSTALS. You probably won't even need to use them for routine work.

The menus are arranged from left to right roughly in the order that you might carry out an analysis: data import, structure solution, refinement, analysis or results and publication tables.

Main Toolbar

The main toolbar contains just a few items that will come in very handy during a structure analysis. **Guide** starts up the guide to advise on the next appropriate step. **Fourier** finds peaks in the Fourier map and adds them into the model. **Add H** provides a quick way of comparing and choosing between geometrically placed H positions and difference map positions. **Kill Q's** and **Kill H's** remove Q and H atoms from the model. **Cameron** starts the graphics program for thermal ellipsoid plots and packing diagrams.

Model Toolbar

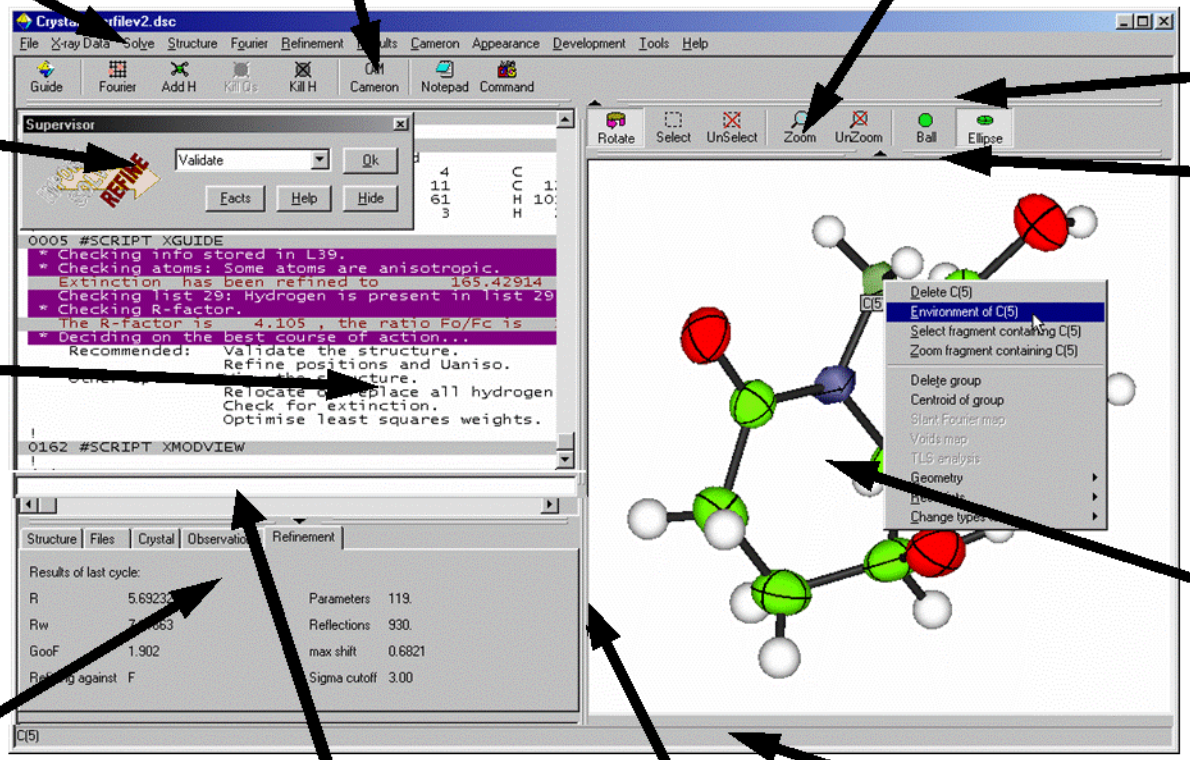
The model toolbar contains tools for interacting with the view of the model. **Rotate** is on by default—click and drag the model to rotate it. (Clicking atoms will also select them). **Select** gives you a selection rectangle for toggling the selection state of atoms. **Unselect** unselects all the atoms. **Zoom** excludes all atoms except the currently selected ones. **Unzoom** re-includes all atoms. **Ball** is on by default, and represents atoms at one quarter of their covalent radii. **Ellipse** represents atoms as their 50% probabilty thermal ellipsoids.

The Guide

The guide advises on the next step to take at every stage of the analysis. You can continue working while this window is displayed, or you can hide it away.

Collapsible bars

Click the arrows in the middle of these bars to hide or show their contents. In this case you can hide the toolbar.



Output

Summary of what is going on, results of calculations, and so on. You can scroll back if things whizz by too fast. The output sometimes includes hyperlinks, which may be clicked to launch external documents.

Model

Click and drag to rotate. Click atoms to select or unselect them. Right click in:

Empty space. A popup menu of general structure manipulating commands (also available in the Structure menu)

An un-selected atom. A menu of commands to carry out on that atom (e.g. Edit, Delete, Environment etc.)

A selected atom. A menu of commands that affect all the selected atoms. The availability varies depending on how many atoms are selected. (e.g. Slant Fourier map, restrain distance, restrain angle, etc.)

Hold down control and drag up and down to zoom in and out, or select some atoms and choose zoom from the toolbar.

Summary Info

Some important facts about the current structure. **Structure** gives the cell, formula and space group. **Files** the currently open files, including the more detailed *listing* file. **Crystal** has some data on the crystal. **Observations** - reflection limits and merging R. **Refinement** - R-factor, goodness of fit, parameters, observations, etc.

Command line

For CRYSTALS veterans. Also some scripts will ask for input and it may be typed in here. When typing (old style) commands into the program, clicking atoms appends their name here.

Resize bars

Drag to change relative sizes of the items either side.

Status Bar

Displays atom name of atom under mouse pointer, current status of program and progress during long calculations.