Useful Olex2 Commands

I've listed a few olex2 commands that I've found useful for a structure refinement. This list is incomplete (a complete list of olex2 commands can be located in the file help.xld). Global restraints/constraints can be added from the command prompt by selecting groups of bonds (Graphics, select the group) and typing the constraint/restraint (eg. DFIX 1.52 0.01). AFIX instructions can also be added by selecting a group of atoms and typing the AFIX command.

1) **sel $Q** ($C, etc); **sel C1 > C20**

Selects all the Q-peaks ($C, etc); Selects all the C-atoms C1 through to C20.

2) **kill $Q** ($C, etc)

Kills all the Q-peaks ($C, etc).

3) **fuse**

Show the asymmetric unit only.

4) **isot/anis**

Makes selected atoms isotropic/anisotropic.

5) **mpln** (selected atoms) **–n**

The best plane of view is calculated for all the atoms or selected atoms. If -n is specified, the best plane of view is calculated and the molecule is rotated accordingly.

6) **telp 30 (50, etc.)**

Shows ellipoidsat 30 (50, etc.)% probability level.

7) **labels**

Turns labels ON/OFF.

8) **/** Shelx instruction

Adds any instruction to the header of the ins file (eg. / ACTA adds the ACTA command to the ins file).

9) **ESC**

Unselects the current selected atoms (/selection). It also exits from a MODE.

10) **split sel** ; **split –r=EADP**(/SIMU) **sel**

Splits an atom into two positions corresponding to the foci of its thermal ellipsoid. Useful for splitting whole disordered groups of atoms.

11) **compaq** (various options)

Assembles fragments of molecules together. Compaq –c is useful for assembling bonded fragments, and often works when compaq –a does not.

12) **help** command

Information on an olex2 command.

13) **ShowP 1** (2, …)

Show Part 1 (2, ..) only. Useful for viewing disorder, only specified parts are shown. ShowP on its own unhides hidden fragments.

14) **htab grow**

Generates h-bond tables of the grown structure and writes these to the CIF.

15) **conn 6**(0, etc.) **$W ($C, etc)**.

Sets the maximum number of bonds W (($C, etc). can have to 6(0, etc.).

16) **sel wbox**

Generates a re-sizable,movable box. This is a useful time saving tool since electron density, void maps are calculated for the region inside the box.

17) **mode grow –shells**

Grows molecules by single atoms. Useful for polymeric, bridged molecules.

18) **mode fit**

Running this command after atoms have been selected allows these atoms to be rotated and translated. Useful for modeling disorder – atoms can be dragged to positions where they are meant to be!

19) Right clicking on a bond (eg C-H), selecting Graphics, Select Group selects ALL C-H bonds. A global constraint/restraint can then be applied.

20) **editatom**

Typing this command after an individual atom or a group atoms (eg. a PART of a disordered group), will open a text window with the shelx representation of only the selected atoms (and their dependencies). The individual properties of the atoms can then be edited with the text editor.