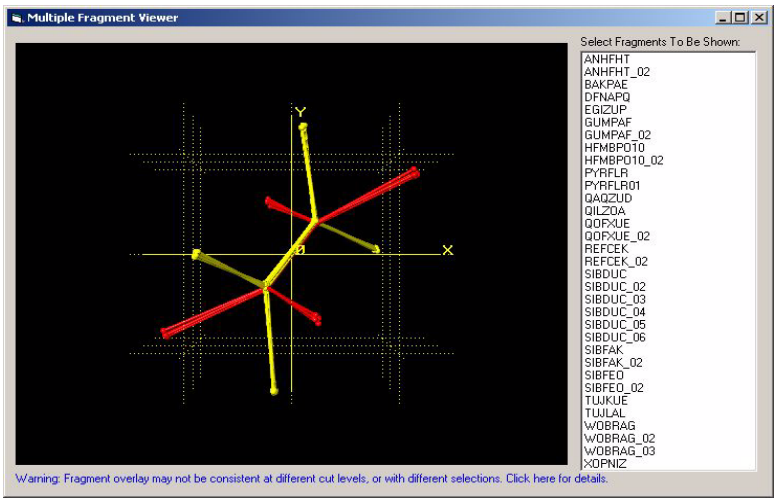
Using the Fragment Viewer



In order to gain an understanding of the analysis, it is very useful to be able to visualise the 3D structure of the distinct fragments. In *d*SNAP this can be done using the Multiple Fragments Viewer. To use this, the relevant fragments must first be selected.

This option can only be accessed when the Dendrogram is displayed.

To select one fragment: Click on the fragment box using the left mouse button.

To select multiple fragments: Click on the fragment, then holding the *Control* key click on the other fragments you wish to select.

To select a series of fragments in sequence: Click on the first fragment then holding the *Shift* key click on the last fragment in the sequence.

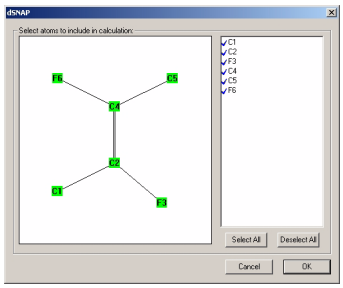
You may wish to view an entire cluster at once to try and understand why they have been grouped together and if this is sensible. You can also view fragments from different clusters to verify that the geometries are different between the different clusters and to see where these differences lie.

Opening the Fragment Viewer:

Once the desired fragments have been selected the fragment viewer window is opened by selecting *View selected fragments in the 3D visualiser...* from the *Tools* menu or by using the *F1* shortcut key.

A window appears to let you select/deselect atoms. By default, all atoms are selected so the entire fragment is optimally orientated and overlayed to allow for differences in structure to be seen. Optionally, you can

leave a just a subset of the entire fragment selected, and in that case *d*SNAP will only try to superimpose only those selected atoms.



Features of the Fragment viewer:

If multiple fragments were selected then these are initially overlaid on each other. This display can be rotated and zoomed in the same way as other graphics displays. A list of all the fragments is presented in a scroll-box on the right hand side of the window. Clicking on a fragment in the list will change the display so as to show that fragment only. Multiple fragments from the list can be selected and overlaid on each other by using the *Ctrl* or *Shift* key in the same fashion as when selecting the fragments to be displayed.

By right-clicking on the display further options can be accessed. Most useful is *Colour atoms by...* which allows the user to toggle between having the atoms on the fragment coloured according to the cluster the fragment belongs to (the default) or the by the element type of the atoms. Each individual fragment can also be coloured differently. This allows interpretation of the differences and similarities between different fragments.

It is also possible to view the atom numbering, again, by right-clicking on the display. The displayed fragment can be labelled either the numbering scheme of the search fragment (*Label atoms by > Number*) or the numbering scheme in the published CSD structure (*Label Atoms By > Name*).

Warning:

The fragment viewer works by arranging the selected fragments so that they are maximally overlapped for display. This helps to highlight differences or similarities between different clusters. However, as this calculation is done on the fly each time for whichever fragments are currently selected at a given cut level, it is therefore generally not meaningful to compare the fragment overlay from different selections of fragments. For this reason, only one 3D fragment viewer can be opened at a time.

Visualising entire hit structures:

The entire structures of individual selected fragments can also be visualised by viewing them in an external viewing program (*Mercury* or *ConQuest*). To do this selected the fragments and then select *Show Selected Hits in Database Viewer...* from the *Tools* menu or by using the *F3* shortcut key. *Mercury* is the default viewer.