Using Mogul with CRYSTALS

February 2004

The Cambridge Crystallographic Data Centre
Registered Charity No 800579

1 Using Mogul with CRYSTALS

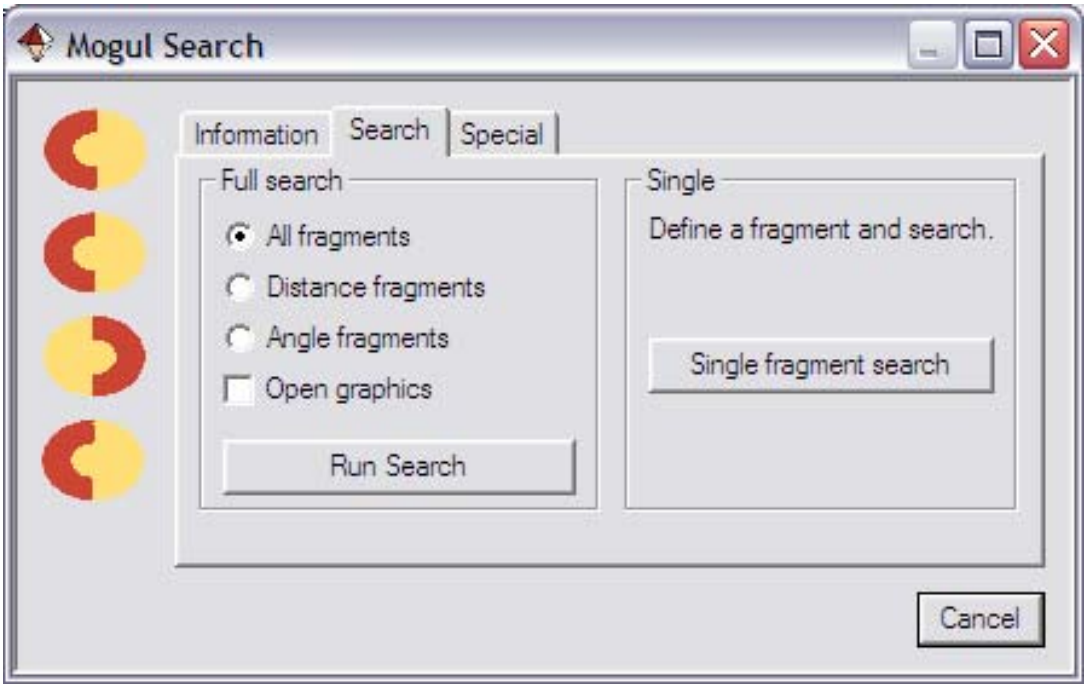
- CRYSTALS is a package for X-ray structure refinement and analysis distributed by the Chemical Crystallography Laboratory, University of Oxford, UK.
- CRYSTALS will interface to Mogul enabling CRYSTALS to retrieve bond-length and angle statistics from the CSD for a partially refined structure. The retrieved data can then be used to help identify misplaced atoms and set up least-squares refinement restraints within CRYSTALS.
- This section contains details about the using Mogul from within CRYSTALS.

- For further information about CRYSTALS, including details about availability, see:

  http://www.xtl.ox.ac.uk/crystals.html

1.1 Running Mogul Searches from CRYSTALS

- It is assumed that you have a CRYSTALS session open with a fully or partially refined structure loaded.
- Select the top-level menu option **Analyse** and pick **Mogul Geometry Check** from the resulting pull-down menu. This will open the *Mogul Search* dialogue box. Select the *Search* tab:

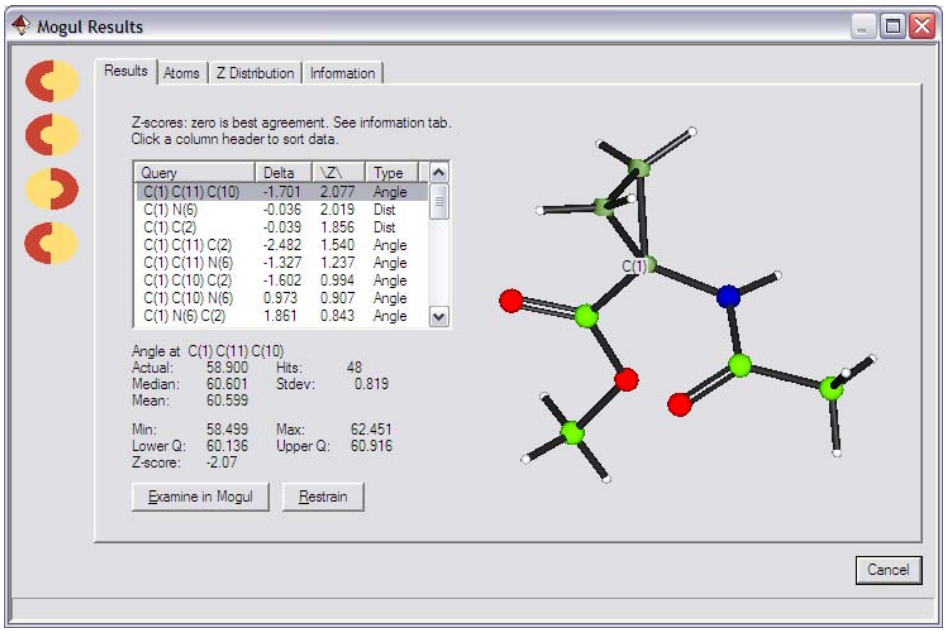


- Switch on **Distance Fragments**, **Angle fragments** or **All fragments**, depending on whether you wish to request Mogul searches for all the bonds in your structure, all the valence angles, or both.

- Then hit **Run Search** to run the Mogul searches.

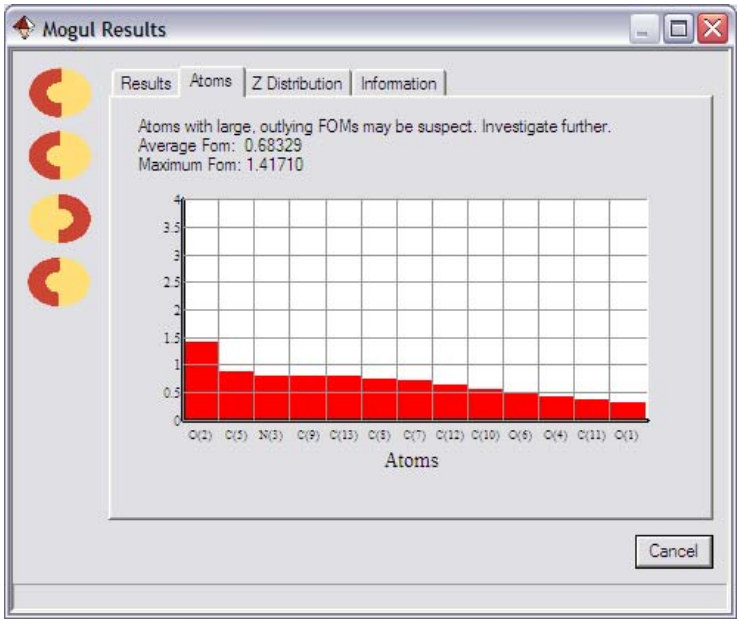
1.2 Using the Results of Mogul Searches

- Once the Mogul searches you have requested have run, the *Mogul Results* dialogue box will open. It should look something like this:

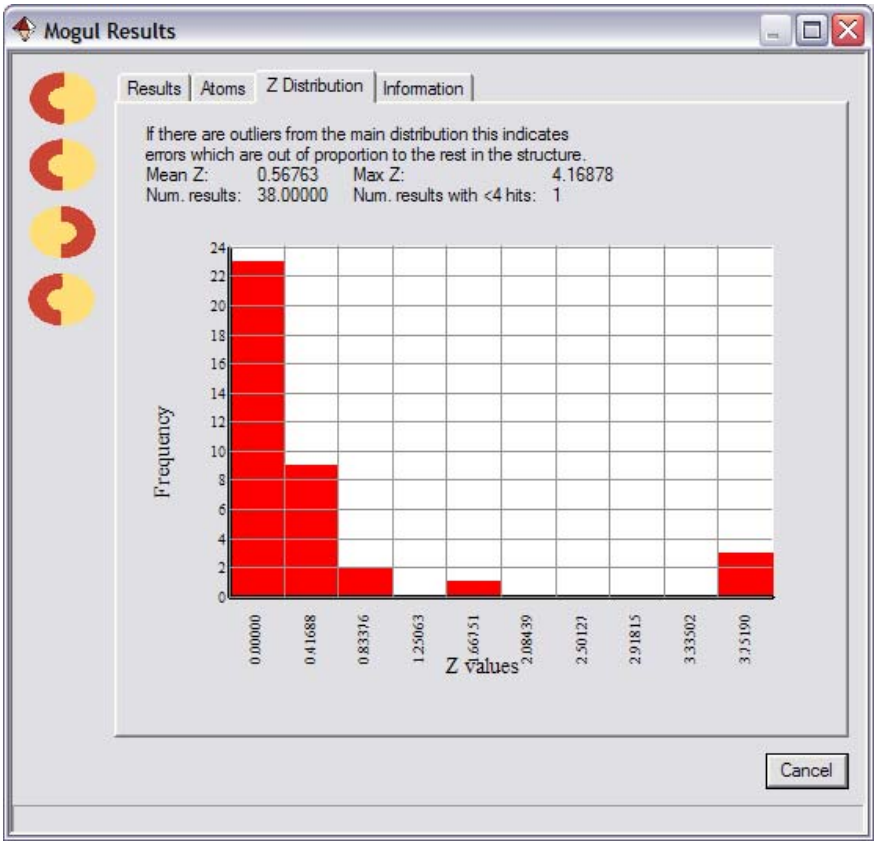


- The first column displays the bond or angle that was searched for in Mogul. The currently selected bond or angle is highlighted in the model on the right, and the geometrical results obtained from Mogul are displayed in the area below the list.
- The second column, *Delta*, lists (*obs* - *median*), the difference between the bond length or angle in the structure and the median of the Mogul distribution (i.e. if *Delta* is negative, a bond may be too short, or an angle too acute).
- The third column lists absolute Z values, computed as |*obs* - *median*|/*sd*, where *obs* is the value observed for that bond length or angle in your crystal structure, *median* is the median value of that type of bond length or angle in Mogul (i.e. in the CSD), and *sd* is the standard deviation of the Mogul distribution. By default this column is sorted in descending order of |Z| when the *Mogul Results* dialogue box appears.
- Absolute values of Z greater than about 2 to 3 indicate a bond length or angle that is sufficiently unusual, compared with the data from Mogul, that it is worth your attention.
- Hit the **Restrain** button to restrain the currently selected distance or angle, using the Mogul value as the restraint target.
- Hit the **Restrain Everything** button to restrain all distances and/or angles for which Mogul searches were performed, using Mogul values as the restraint target.

- Hit **Examine in Mogul** to look in detail at the Mogul search results for the currently selected bond length or angle.
- Select the *Atoms* tab to get a bar chart displaying a figure of merit per atom, based on the collected statistics:



- The Z-scores are limited to the range 1.0->10.0; bonds or angles for which no hits were found in Mogul are assigned an arbitrary Z-score of 2.0. The figure of merit is calculated by taking the geometric mean of all relevant Z-scores for an atom. It rises rapidly for atoms which are involved in more than one suspicious geometry and helps to pinpoint the location of any problem.
- Select the *Z Distribution* tab to get a bar chart of the Z values for all the bond lengths and/or angles for which you retrieved Mogul data.



- Look out for outliers from the main distribution of errors.

- If Mogul did not return any results for a given bond or angle, the most likely reasons are:
  - The bond or angle involves a metal or hydrogen atom – Mogul currently does not contain data for these.
  - The bond or angle is chemically unusual and no similar examples occur in the CSD.
  - Bond types do not conform to CCDC conventions or hydrogens are incorrect (see Section 1.3, page 4).

1.3 Bond Types, Hydrogens and Mogul

- Mogul requires bond type information that conforms to CCDC conventions. Mogul will attempt to guess unknown bond types and standardise to CCDC conventions for you but this is not always perfect. If you want to specify your own bond types before loading the molecule into Mogul you can do this within CRYSTALS. See the CRYSTALS user guide for details about changing bond types in CRYSTALS and the Mogul user guide for information about CCDC bonding conventions.
- Mogul also requires that hydrogens are present in the input molecule. If Mogul does not detect any hydrogens in the input molecule, it will attempt to guess these. To specify hydrogens in CRYSTALS, see the CRYSTALS user guide.