

**W0046**

**Mogul - Rapid Retrieval of Molecular Geometry from the Cambridge Structural Database.** G.M. Battle, Cambridge Crystallographic Data Centre, 12 Union Rd., Cambridge, CB2 1EZ, UK.

Mogul is a knowledge base of molecular geometry derived from the Cambridge Structural Database1 (CSD) and provides extremely rapid access to information on the preferred values of bond lengths, valence angles and acyclic torsion angles.

Given the instruction to retrieve data for a particular geometric feature in an input molecule, e.g. a valence angle, Mogul will automatically generate atom- and bond-based keys that describe the environment of that feature. These keys are then used to retrieve all CSD entries that contain the feature of interest. Fast search speeds are achieved by use of a search tree and without the need for graph-based atom-by atom matching. The search tree also allows retrieval of similar geometric features ranked by a relevance score.

Histograms and summary statistics for retrieved CSD distributions can be viewed interactively in the program interface. Searches can also be run automatically *via* an instructions file, thus providing a way of utilising geometric information in other applications, e.g. during crystal structure refinement. By providing rapid access to molecular dimensions and conformational preferences, this methodology has many potential applications in the areas of geometry and conformational validation.

1. Allen, F.H. **2002**. *Acta Cryst.* B58, 380