CCDC
advancing structural science

Validate your experimental or predicted structures using experimentally-derived, peer-reviewed data.

Mogul

Display distributions of important geometries based on the bond lengths, angles, ring geometries, and torsions of the curated structures in the CSD.

- **Quick assessment of molecular geometries against the CSD.**
  - Build confidence in your structures by quickly identifying any unusual features, like torsions.
  - Colour code potentially concerning features for further analysis and understand what parts of the structure are unusual at a glance.
- **Visually display the distribution of the geometrical features.**
  - Compare observed features in your structure to averages found in the CSD.
  - Have confidence in your results, which are based on up to 10,000 randomized structures from the CSD.
  - Leverage the latest data in your analysis with the Mogul library, which is updated quarterly. Can also leverage your own data.
- **Drill into each of the individual structures behind a distribution.**
  - Develop a deep understanding of your structure with quick access to each experimentally derived, peer-reviewed structure that is behind an analysis.
- **Focus on the individual features of a molecule or generate reports.**
  - Tailor your analysis to a general or targeted review based on your research goals.
- **Run reports programmatically via the CSD Python API or use CCDC's Mercury or Hermes visualization tools.**
  - Assess the quality of intramolecular geometries as part of a standard workflow or run custom checks.

FAQs

Can I include my own in-house database alongside the CSD as a supplemental knowledge base?

Contact us at hello@ccdc.cam.ac.uk to discuss if this is a requirement.

How does Mogul describe unusual torsion angles?

Mogul uses “local density” to quantify the unusualness of torsion angles. Specifically, this refers to the percentage of observed values within a user-defined tolerance. By default, Mogul will classify as “unusual” any torsion angles where less than 5% of the distribution is within 10 degrees of the query value. This is different from the statistical approach to quantify unusualness for bond lengths and covalent bond angles, which uses the | z-score |. | z-score | is the number of standard deviations from the mean. As a standard, it uses a threshold of 2.0—meaning any bonds or angles with a z-score greater than 2.0 are classed as unusual.

How does Mogul’s “generalized” search functionality work?

Mogul has the ability to complete a generalized search for any related fragments if there are not enough hits to match the exact query fragment in question. You can configure the generalization settings, which allows you to decide if the results from a generalized search are applicable to your particular chemistry.

How do I know what structures Mogul used for a particular distribution?

You are able to drill down into each report to see the individual structures driving the results. In addition, the exact number of structures that went into each report is provided and can include up to 10,000 experimentally derived and peer-reviewed structures housed in the CSD.

What file formats does Mogul accept? Can you draw a molecule for Mogul?

Mogul accepts Crystallographic Information Files (CIFs), MOL2, PDB, RES, MOL, and .con (ConQuest 2D chemical diagrams) file formats as inputs. If running from Mercury, more file formats are available. There is also a draw function that generates a histogram with hits based on the structure you specified. However, drawn structures do not have an input conformation to check against the data. Mogul cannot identify unusual or usual geometries for drawn molecules since they do not have a 3D geometry to assess.

Learn More

- Email hello@ccdc.cam.ac.uk to ask a question or request an online demo.
- Visit our Mogul website page for more information.
- Free online training course teaching the basics of Mogul.
- How to video using Mogul.