Mogul: A tool to analyze protein bound ligand structures

Sivakumar Sekharan¹, Jason Cole², Amy Sarjeant¹, Colin Groom²

¹Cambridge Crystallographic Data Centre, Piscataway, United States, ²Cambridge Crystallographic Data Centre, Cambridge, United Kingdom

E-mail: ssekharan@ccdc.cam.ac.uk

The Cambridge Structural Database (CSD) is the worldwide resource for dissemination of all published 3D structures of small molecule organic and metal-organic compounds. This presentation will showcase that chemical crystallography and macromolecular crystallography can be of mutual interest and benefit to macromolecular crystallographers, particularly those interested in protein-ligand binding. For example, how the CSD and associated software can aid in the protein-ligand complex validation and how the CSD could be further used in the generation of geometrical restraints for protein structure refinement will be presented for a discussion. In addition, the presentation will introduce the new changes to the knowledge-based Mogul software that is used for validation of small molecule crystal structures including fused and bridged ring systems as compared to entries in the CSD.


Keywords: crystallography, macromolecules, proteins