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Mogul: A tool to analyze protein bound ligand structures

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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.

1. Bruno, I. et al. J. Chem. Inf. Comput. Sci. (2004) 44, 2133-2144.
2. Cottrell, S. et al. J. Chem. Inf. Model. (2012) 52, 956-962.
3. Liebeschuetz, J. et al. J. Comput. Aided Mol. Des. (2012) 26,169–183.

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