

Rigid groups, model restraints, elusive H atoms... practical examples of using CSD entries to help with difficult structures

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Problematic structural features such as twinning, disorder, and pseudosymmetry can hamper the solution, refinement, and/or interpretation of a crystal structure. The CSD provides a wealth of structural information that can help find a way round these problems. Fragments of ideal geometry from reliable known structures may be suitable models for a Patterson search approach when traditional direct methods and dual-space procedures fail; alternatively they may help extract a useful partial structure from the mess of an electron density map corresponding to the superposition of two or more intersecting disorder components. Known structures are a useful source of suitable geometrical restraints for the refinement of disordered or poorly resolved molecules. In cases where the location of hydrogen atoms is important but they are not clearly seen in difference maps or not well-behaved in unrestrained refinement, well-determined comparable structures in the CSD can suggest appropriate restraints or constraints as well as good starting positions. Comparison with relevant known structures is part of structure validation alongside tools such as PLATON/CheckCIF, and the CCDC software Mogul is particularly valuable for this.

This talk will include some particular examples of these approaches, including a recent key structure in a project investigating substituted fused borane clusters that is afflicted by both twinning and extensive disorder, for which a definitive and assuredly correct result could be obtained by combined crystallographic, spectroscopic and theoretical approaches including the use of results from the CSD.