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*DSR- A tool for disorder refinements with SHELXL*

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X-ray crystallography as a method used for identifying the atomic and molecular structure of a crystal has led to a better understanding of chemical bonds. It is an essential tool to determine the absolute configuration of molecules, has been important for the characterization of coordination complexes, as well as identifying supramolecular assemblies in biology and material science. Being so successful, one of the remaining problems in practical crystallography is the description of disorder in crystal structures. The Cambridge Structural Database includes 23% of disordered structures in its collection of nearly 700000.[1] The program described here is able to simplify many aspects of disorder modelling.   The modelling of disorder with SHELXL is possible since its early stages. SHELXL is able to treat almost every possible kind of disorder but with a lot of manual work. It needs a free variable and a part number in combination of displacement parameters and bond length restraints. DSR (Disordered Solvent Refinement) transfers a molecular fragment from a database of molecular fragments to the desired position in the unit cell automatically and generates restraints to stabilize the model (Figure 1). In practice, the user writes a command line into the SHELXL .res file, which subsequently is interpreted by DSR. The command line's main purpose is to tell DSR, which source atom of the fragment should go on which target coordinates in the .res file. The user has to choose a minimum of three atoms from the database fragment (source atoms) and the same amount of target positions (target atoms) where the fitting fragment should be placed on. Molecular fragments can be either imported directly from the GRADE server of Globalphasing Ltd.[4], from existing crystal structures or from ab initio calculations. DSR offers several more options available to make disorder modelling a convenient process. DSR can be obtained from http://goo.gl/BL6wP1.

[1] http://www.ccdc.cam.ac.uk/Lists/ResourceFileList/2014_stats_entries.pdf, [2] G. M. Sheldrick, Acta Crystallogr. 2008, A64, 112-122., [3] Grade Web Server, Global Phasing Ltd. http://grade.globalphasing.org.
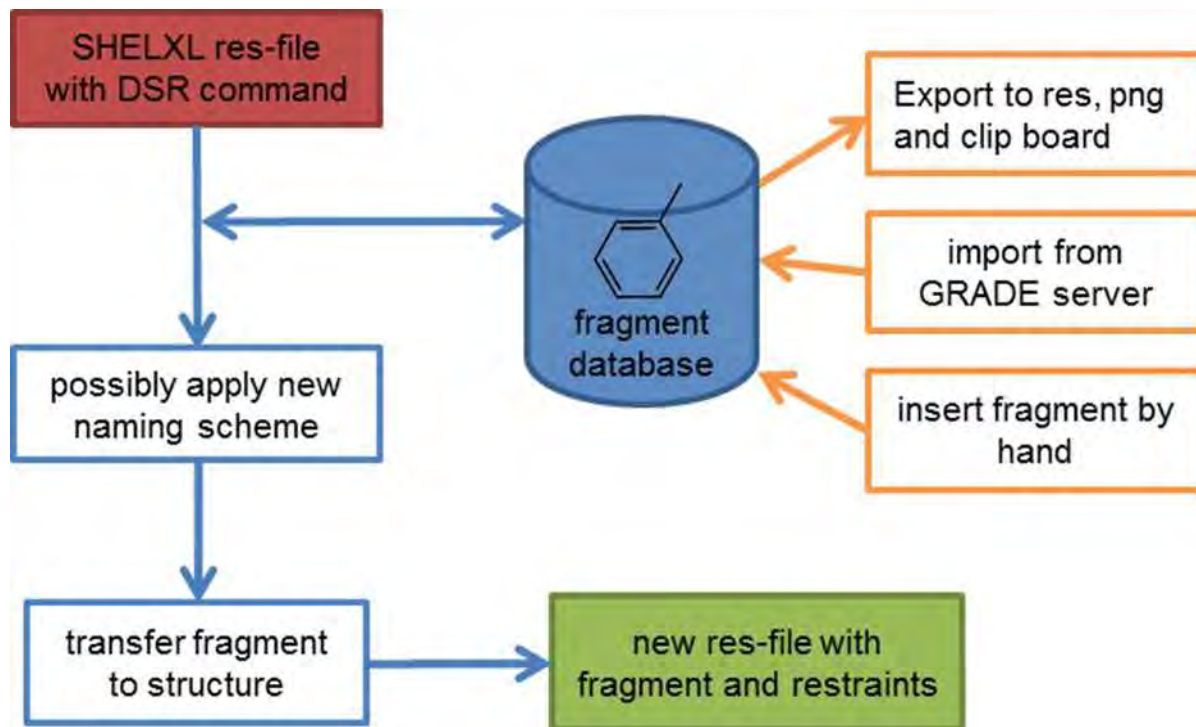
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