What is the Issue with Autodeposit?

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In macromolecular crystallographic structure solution the flow of information between stages is the key component of success. The final model is deposited in the PDB together with the information collected during the process. The dispersion of information between different formats of different programs makes the data organization and the automation of deposition a hard to achieve task. The main issue is still deciding which information is the most valuable and should be deposited. The answer depends on the view of the PDB role. The Protein Data Bank is not only the structural models repository, but it also contains a limited description of facts related to structure determination. The question is: should we enhance this information and can we achieve it using automatic tools?

The important facts missing from the PDB are: the increase in temperature factor, comments about twinning, diffuse scattering, use of multiple crystals for a single data set. Log files from numerical calculations are mostly of interest to the process of structure determination; however, it is not clear how this information would enhance the PDB deposits.

Overall, we should concentrate on how to improve the process of structure determination, which is challenging due to diversity of problems and approaches. The issue of autodeposit is subordinated to an overall improvement in crystallographic computational and database methods.

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