mmCIF and Modern Macromolecular Structure Determination Software: Status and Perspectives

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As developers in the *Phenix* project [1], we are confronted with *mmCIF* in two ways. Firstly, our algorithms produce results that need to be archived. Secondly, access to information stored in databases, such as the PDB [2], is often invaluable in the development and testing of new methods. In contrast to most traditional, static file formats, *mmCIF* is highly flexible. Therefore we have the opportunity to export parameters and results of ever more complex algorithms in a uniform framework. However, it is non-trivial to import information from *mmCIF* files since their processing requires very sophisticated tools. Unfortunately, in many contexts adequate practical tools are not available. The limitations of traditional software development technology are probably the most important factors giving rise to this situation. Fortunately, many in the crystallographic methods development community have begun a transition to modern software technology. Database developers, most notably at the PDB, have already published comprehensive *mmCIF* libraries. Further development of such libraries in a collaborative effort with an open two-way exchange between the communities has the potential to stimulate a much wider use of *mmCIF* in the future.

[1] Adams P.D., Gopal K., Grosse-Kunstleve R.W., Hung L.-W., Ioerger T.R., McCoy A.J., Moriarty N.W., Pai R.K., Read R.J., Romo T.D., Sacchettini J.C., Sauter N.K., Storoni L.C., Terwilliger T.C., *J. Synchrotron Rad.*, 2004, **11**, 53-55. [2] Berman H.M., Westbrook J., Feng Z., Gilliland G., Bhat T.N., Weissig H., Shindyalov I.N., Bourne P.E., *Nucleic Acids Research*, 2000, **28**, 235-242.

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