W0356

An Anthropological Review of the Development of mmCIF. Paula M. D. Fitzgerald[1], J. Westbrook[2], [1]Merck Research Laboratories, Rahway, NJ, [2]Rutgers, State Univ. of New Jersey, Dept. of Chemistry and Chemical Biology, Piscataway, NJ.

The creation of the mmCIF dictionary was a community-based project, with input from many individuals within the crystallographic and related communities. As with any such project, particularly one that generated such a large and complicated data structure, there were many changes of direction along the way, and keeping the project moving forward was at times a major challenge.

The core team that guided the development of the dictionary consisted of Paula Fitzgerald, John Westbrook, Brian McMahon, Phil Bourne, Keith Watenpaugh, and our Buerger award winning Helen Berman. This presentation will focus on the human aspects of the project, in which Helen played a key role – particularly the fall weekends spent at Rutgers hammering out the original data model, followed over the next few years by workshops at York, Brussels, Tarrytown, and Rutgers elaborating the model and changing it to meet the desires of the community.

The mmCIF data model has now been fully vetted and published in the recent volume International Table of Crystallography Volume G: Definition and exchange of crystallographic data. The data model has been widely adopted, and this presentation will also survey the many ways in which the data model has facilitated the development of software that allows crystallographic commuting, structural bioinformatics, and data archiving to evolve while working in the context of a well-defined data structure.