The science of diffraction data collection

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Due to technological advances in both hardware and software in recent years, collection of diffraction data from macromolecular crystals became ever easier and faster. Parallel advances have occurred in the subsequent steps of the analysis, such as phasing, refinement, and model building, where more powerful programs accelerate the process and make difficult cases more tractable. As all subsequent, mainly computational steps of structure analysis, become faster and easier, the primary data quality plays a more important role since data collection is the last experimental stage, often difficult to repeat. High data quality makes all subsequent steps easier and leads to more accurate atomic models. However, X-ray data collection is not a mere technicality and should be treated as an important scientific process. The factors involved are complex. Some can be treated in an automatic manner by the controlling software. Others require decisions to be made by the experimenter. Macromolecular crystals tremendously vary in their properties and similarly the characteristics of data collection facilities differ considerably from each other. It is always the responsibility of the experimenter to select the optimal conditions leading to the best quality of diffraction data measured with particular crystal and specific facility.