Keywords: data collection, data analysis, macromolecular crystallography, DIALS, automation, pipelines



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Serial Femtosecond Crystallography using X-ray free electron lasers has established itself as a technique ideally suited to the study small and radiation sensitive crystals by outrunning radiation damage, and for probing protein dynamics with sub-picosecond time resolution. A typical experiment involves exposing a stream of crystals to millions of individual femtosecond duration X-ray pulses, resulting in measurable diffraction patterns from thousands of individual protein micro- or nano-crystals each of which is exposed to the intense X-ray beam only once before being discarded. Combining these diffraction patterns yields intensity measurements for structure analysis, for example reflection intensities for conventional crystallographic analysis. In some cases it can also reveal hidden gems including diffraction beyond the resolution of observable Bragg peaks and continuous diffraction from individual asymmetric units. This has required the development of new data analysis techniques.

Keywords: serial femtosecond crystallography, Free electron laser, data processing