MS08-2-4 Development of metric(s) for validation of automated processing of X-ray free-electron SFX data
#MS08-2-4

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Abstract
Data processing in Serial Femtosecond X-ray Crystallography(SFX) collected at X-ray free-electron laser sources is carried out using software packages such as OnDA [1], Cheetah [2] and CrystFEL [3]. At the European X-Ray Free-Electron Laser (EuXFEL) Facility, an in-house automated analysis software package based on CrystFEL is used for offline analysis of calibrated detector data. The in-house or other automated pipelines offer a robust implementation of processing subsets for offline SFX data on different worker nodes in a cluster computing systems. They provide advantages such as ease of use and firsthand results. However, the trade-off between simplicity in usage and processing success rate when using these pipelines in comparison to manual data analysis is yet to be fully understood. To explore this-, a metric, or a combination of metrics, is being developed which can be used to evaluate the success rate of the data processing. Metric(s) such as CC^*, $CC\_1/2$, and R_split computed after the data processing step as well as the phase error computed after the phasing step in the structure solution process are currently under study towards this aim. In later stages, these metrics are used to validate the success rate of automated and manual processing.

References
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