

MS2-O3 Improving resolution in serial crystallography

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In Serial Femtosecond Crystallography (SFX), the diffraction pattern from a series of small crystals streaming past the X-ray focus is recorded. For some samples, along with Bragg peaks and liquid background, additional scattering is observed at high resolution. We show that, with certain assumptions, this can be used to improve the resolution and quality of the final structure using iterative phasing techniques. With some real-world data collected at the Linac Coherent Light Source (LCLS), we demonstrate this method and show structural improvement, and discuss the general applicability of this method.

Keywords: serial femtosecond crystallography, XFEL

MS2-O4 Identification of rogue datasets in serial crystallography

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Advances in beamline optics, detectors and synchrotron sources allow new methods of crystallographic data collection. In serial crystallography, a large number of partial data sets from crystals with a small diffraction volume are measured. The general assumption underlying merging of data sets from different crystals in order to enhance x-ray data quality is only valid if the crystals are isomorphous, thus are structurally identical. Identification and exclusion of non-isomorphic data sets is therefore indispensable for merging and should be done by means of suitable data quality indicators. In our approach, CC1/2 [1], the correlation coefficient between two half-data sets composed of randomly assigned partial datasets is used as a quality indicator to identify rogue data sets. Remarkably, it was found that rejecting those data sets that reduce the overall CC1/2 significantly improved the PDB model obtained from the remaining datasets. This was verified by refinements of structures against the newly formed merged isomorphous data. Analysis of CC1/2 is therefore a sensible method to identify data sets containing systematic errors (displaying non-isomorphism) in comparison to conventional quality indicators such as Rmerge, which only accounts for the precision of the measurements and misleadingly discards weak data sets [1].

[1] Karplus P.A., Diederichs, K. (2012) Linking crystallographic model and data quality. *Science* 336, 1030-1033.

Keywords: Isomorphism, data quality, correlation coefficient, outlier rejection, serial crystallography