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Reducing data volume with X-ray Laue diffraction

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The X-ray Laue diffraction captures the crystal diffraction from white beam and can contain significant amount of structural information in comparison to monochromatic diffraction. In time-resolved study, the serial femtosecond crystallography (SFX) and serial synchrotron crystallography (SSX) are the mainstream approaches with the caveat of generating large data volume. Laue diffraction has great potential in mitigating the data volume challenge and has recently regain the interest by the community. Here, we share the preliminary works conducted at BL03HB Laue Micro-diffraction Beamline at Shanghai Synchrotron Radiation Facility (SSRF) to compare with conventional method. We crystallized an apo stilbene synthase (STS) with inherent loop conformation duality and collected diffraction data via (i) single-crystal, cryogenic, rotation approach with monochromatic beam, (ii) single-crystal, ambient, helical approach with white beam, and (iii) multi-crystal, ambient, single-frame approach with white beam. Compare to monochromatic diffraction, Laue diffraction dataset show increased content of structural information per image but with poor statistical metrics upon merging. Nevertheless, the solved structure from Laue diffraction dataset can resolve the duality of the loop conformation and reveal the loop conformational preference at productive state at ambient temperature. In short, Laue diffraction is a promising approach to explore in mitigating the data volume challenge.

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