Serial crystallography is an increasingly important approach to protein crystallography that exploits both X-ray free electron laser (XFEL) and synchrotron radiation. Serial crystallography recovers complete X-ray diffraction data by processing and merging diffraction images from thousands of randomly oriented non-uniform microcrystals, of which all observations are partial Bragg reflections. Random fluctuations in the XFEL pulse energy spectrum, variations in the size and shape of microcrystals, integrating over millions of weak partial observations and instabilities in the XFEL beam position lead to new types of experimental errors. The quality of Bragg intensity estimates deriving from serial crystallography are therefore contingent upon assumptions made while modeling these data. Here we observe that Serial Femtosecond Crystallography (SFX) Bragg reflections do not follow a unimodal Gaussian distribution and recommend that an idealized assumption of single Gaussian peak profiles be relaxed to incorporate apparent asymmetries when processing SFX data. We illustrate the phenomenon by reanalyzing data collected from microcrystals of the Blastochloris viridis photosynthetic reaction center and compare these intensity observations to conventional synchrotron data. Our results show that skewness in the SFX observations captures the essence of the Wilson plot and we suggest an empirical treatment that can help to separate the diffraction Bragg intensity from background.


Keywords: ex-Gaussian distribution, serial femtosecond crystallography, bragg reflections