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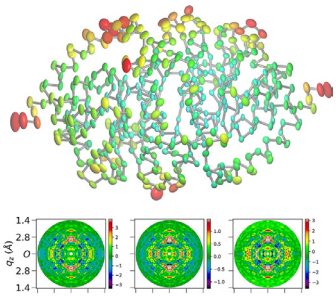
Data, theory, and analysis reveal signatures of atomic motions in diffuse X-ray scattering, an emerging crystallography signal.



Bragg peaks, the main source of structure information in X-ray crystallography, only reveal the average electron density of a crystal's unit cell. The signal between Bragg peaks, known as diffuse scattering, shows spatial correlations in electron density variations. Diffuse scattering could be used to model protein dynamics, but this signal is trickier to detect than Bragg peaks, and little is known about its reproducibility.

Su et al. investigated the reproducibility of diffuse scattering data, examining nine datasets of crystalline isocyanide hydratase (ICH) in three forms, its wild type and two mutants. They found the replicate datasets were similar, suggesting single-crystal diffuse scattering datasets can be reproducibly measured.

Developing a data analysis pipeline with a modular design, the authors evaluated, step by step, how processing choices affect data quality. The results emphasized the importance of background subtraction and defined other best practices.

The authors analyzed diffuse data using a liquid-like motions model of protein dynamics, extending the theory to include individual atomic displacement parameters (ADPs or B factors) from the crystal structure. The diffuse data were more sensitive than the Bragg data to differences in ADPs and could be used to identify more plausible anisotropic motions.

"The work is important, because it develops ICH as an experimental system, generates recommendations for best practices in data collection and processing, and demonstrates that diffuse data can be used to select a preferred atomic displacement parameter model," said author Michael Wall.

In addition to informing diffuse scattering experiment design, this work brings the X-ray crystallography field closer to combining diffuse and Bragg data to develop models of protein structure and dynamics.

Source: "Reproducibility of protein x-ray diffuse scattering and potential utility for modeling atomic displacement parameters," by Zhen Su, Medhanjali Dasgupta, Frédéric Poitevin, Irimpan I. Mathews, Henry van den Bedem, Michael E. Wall, Chun Hong Yoon, and Mark A. Wilson, *Structural Dynamics* (2021). The article can be accessed at https://aip.scitation.org/doi/full/10.1063/4.0000087.