

Diffuse Scattering in Protein X-Ray Crystallography

Protein structures obtained through X-ray crystallography represent an average conformation of all protein molecules in a crystal. In reality, proteins are very flexible and dynamic. Even in a crystal, they can adopt many different conformations. Clues about their disorder can be captured during X-ray diffraction experiments, in the form of diffuse scattering. Here, we model experimentally observed diffuse scattering by simulating correlated motions inside a supercell.

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