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Using the Pair Angle Distribution Function for Analysing Protein Structure.

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X-Ray Free Electron Lasers provide a means of conducting crystallography experiments with remarkable time and spatial resolution. These methods can directly recover the electron density of the materials analysed, however, stringent requirements such as crystal size, number density per exposure, and the crystal order can compromise data quality. Membrane proteins, which do not readily crystallise or meet these requirements [1], are particularly interesting to study as they comprise up to 50% of drug targets [2], but less than 10% of the protein structures in the Protein Data Bank [3]. The Pair Angle Distribution Function (PADF) describes the three and four body correlations of the electron density in a sample, and can be recovered from X-ray angular cross-correlation analysis [4]. Although it does not recover the electron density directly, it still contains significant information about the local three dimensional structure of the material. PADF analysis also has the potential to relax the stringent crystal requirements imposed by current XFEL experiments. We discuss the sensitivity of the PADF to different protein structures [5], and the correlations generated at different length scales; from atomic bonding to tertiary structure. Our aim is to develop PADF analysis to be used complementarily with conventional crystallography analysis, and to use changing angular correlations to measure conformational changes in proteins.

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