Atomic structure of a single large biomolecule from diffraction patterns of random orientations

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The short and intense pulses of the new X-ray free electron lasers, now operational or under construction, may make possible diffraction experiments on single molecule-sized objects with high resolution, before radiation damage destroys the sample. In a single molecule imaging (SMI) experiment thousands of diffraction patterns of single molecules with random orientations are recorded. One of the most challenging problems of SMI is how to assemble these noisy patterns of unknown orientations into a consistent single set of diffraction data. Here we present a new method which can solve the orientation problem of SMI efficiently even for large biological molecules and in the presence of noise. We show on simulated diffraction patterns of a large protein molecule, how the orientations of the patterns can be found and the structure to atomic resolution can be solved. The concept of our algorithm could be also applied to experiments where images of an object are recorded in unknown orientations and/or positions like in cryoEM or tomography.

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