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Is radiation damage the limiting factor in high-resolution single particle imaging with X-ray free-electron lasers?

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The prospect of single particle imaging with atomic resolution is one of the scientific drivers for the development of X-ray free-electron lasers. The assumption since the beginning has been that damage to the sample caused by intense X-ray pulses is one of the limiting factors for achieving subnanometer X-ray imaging of single particles and that X-ray pulses need to be as short as possible. Based on the molecular dynamics simulations of proteins in X-ray fields, we show that the noise in the diffracted signal caused by radiation damage is less than what can be expected from other sources, such as sample inhomogeneity and X-ray shot-to-shot variations. These findings show a different aspect of the feasibility of high-resolution single particle imaging using free-electron lasers, where employing X-ray pulses of longer durations could still provide a useful diffraction signal above the noise due to the Coulomb explosion.

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