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HETEROGENEITY IN SINGLE-PARTICLE XFEL DATA FROM A VIRUS

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In the absence of extraneous and stochastic data artifacts, differences between XFEL diffraction snapshots stem from changes in particle orientation and conformation. Using data from the PR772 virus, we show that a manifold embedding technique is able to reveal and map the conformational spectrum of this virus. The ability to determine and sort conformational heterogeneity is thus essential for reliable determination of three-dimensional structure in single-particle experiments.