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Structure and Conformation of a Virus from Single-particle X-ray Diffraction

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In the absence of extraneous and stochastic data artifacts, differences between X-ray diffraction snapshots of a biomolecule arise from changes in object orientation and conformation. Using the X-ray Free Electron Laser data from the PR772 virus, collected at SLAC National Laboratory, we show that a manifold embedding technique can extract the structure and map the conformational spectrum of this virus. The ability to determine and sort conformational heterogeneity is thus essential for a reliable determination of the three-dimensional structure in single-particle experiments.

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