StructMap: Method for mapping a set of electron-microscopy structures onto a space defined by their distances

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Single-particle electron microscopy has been shown to be very powerful for studying conformational flexibility of macromolecular complexes. To further analyze flexibility and start understanding dynamics of a complex, its distinct conformations are usually computed by analyzing images of coexisting multiple conformations of the complex. The resulting structures are then analyzed to explain flexibility. However, a quantitative analysis of dissimilarities (distances) among structures, placing the entire set of structures into a common space of comparison, is often lacking. We have recently developed an approach that provides an overall view of distances among given structures. The approach is based on statistical analysis of distances among elastically aligned structures, and results in visualizing structures as points in a lower-dimensional distance space. The configuration of these points can be analyzed to explore potential pathways of conformational changes. The method was tested with several sets of synthetic and experimental structures at different resolutions. In this abstract, we show one example of use of the method. The method and other examples of its use will be presented at the meeting.