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Investigating conformational landscapes through alternative cryocrystallographic approaches

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Temperature plays a dominant role in the nature of the low energy conformational state(s) a protein can adopt; an understanding of which is essential to comprehending protein function. Historically observing the influence of temperature on both low energy conformational states and as well as the dynamic and static disorder of mobile elements have been difficult to investigate through traditional cryocrystallographic approaches. This difficulty unfortunately results in this energetic information being largely ignored in structural studies. Recent, albeit limited, accessibility of XFELs has opened a door to collect information on these conformational states through collecting high-resolution diffraction data at different temperatures while minimizing the concern associated with radiation damage. An alternative, perhaps more accessible approach to collection of data at various temperatures, is to use cryo-cooling methods to trap these temperature-dependant states. In our work, we examine this idea of cryo-trapping over a 60°C range to investigate the influence of temperature on the low-energy conformational state of several active site mobile loops. The studied enzyme, phosphoenolpyruvate carboxykinase, is a well characterized system which has many mobile elements that must adopt specific conformations for catalysis to occur. This offers a good model enzyme to understand the usefulness of this cryo-trapping approach to investigate an enzyme's conformational landscape.