

To Direct Or To Be Directed

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Reverse turns help proteins attain compact globular shape. Very often they play a role in protein function. They also play a role in protein folding. For instance, formation of a turn, in an unfolded protein, can bring together distant regions of the protein and promote folding. However, it is not always clear whether a turn actively played a role in the folding process or remained a mere passive player, played upon by the folding process. In this presentation, I shall talk about a particular turn from staphylococcal nuclease and our efforts to understand what makes it an active turn and what makes it a passive turn through molecular dynamics simulations.