Electronic Supplementary Material (ESI) for RSC Advances.

Electronic Supplementary Information

OneG-Vali: A Computational tool for Detecting, Estimating and Validating Cryptic Intermediates of Proteins under Native Conditions

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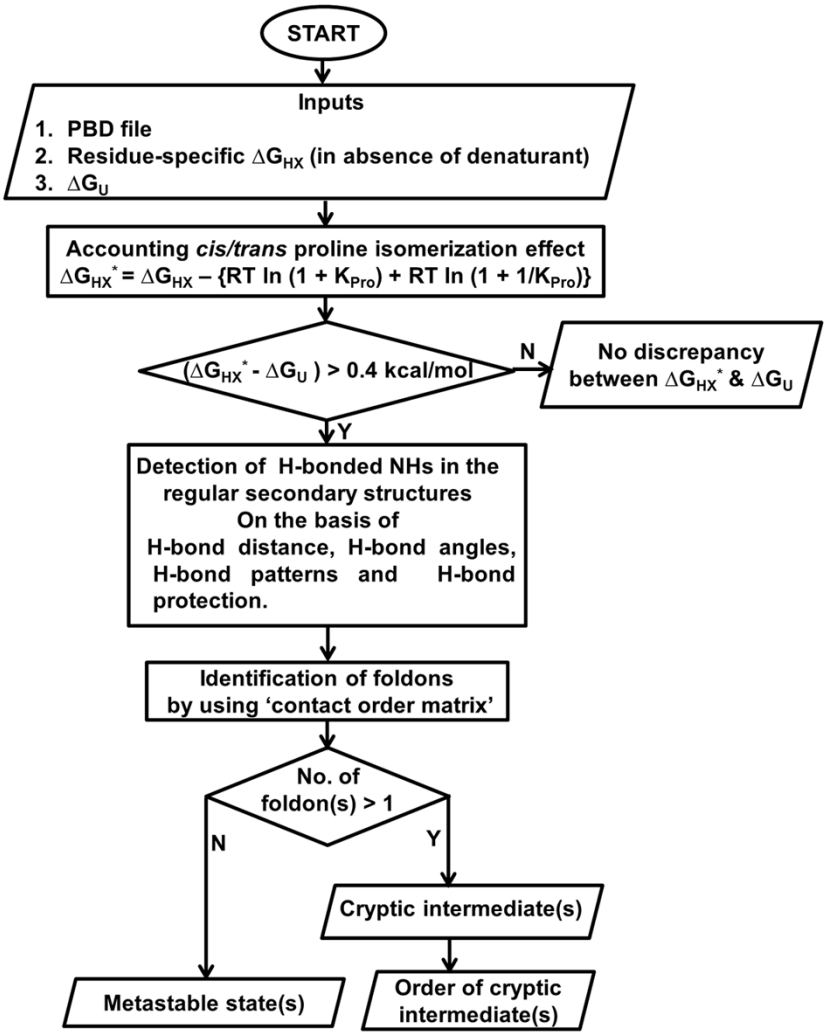
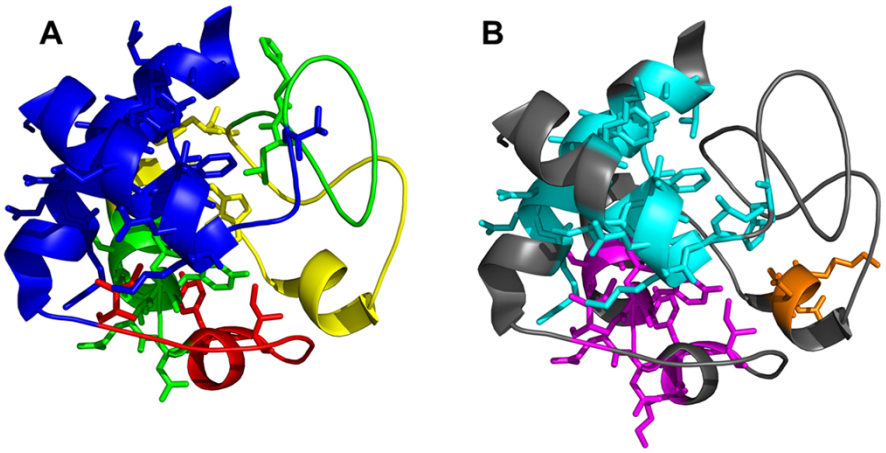
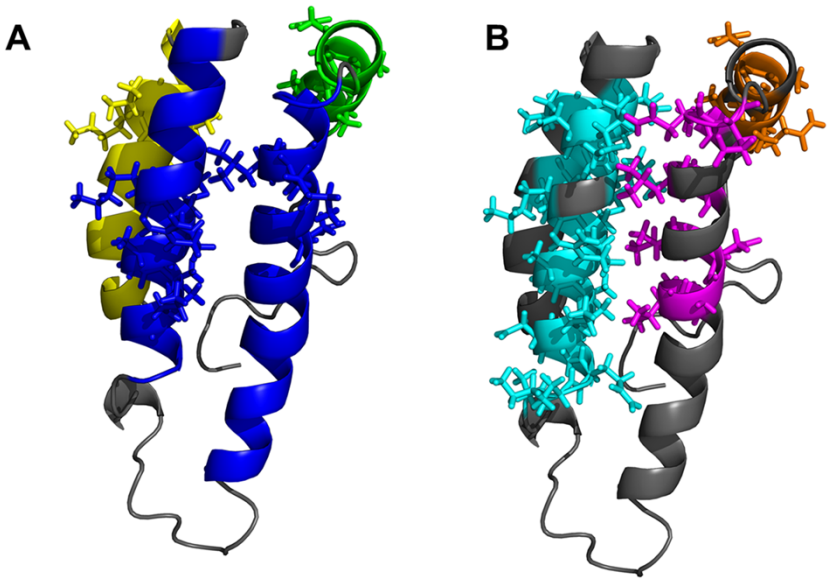


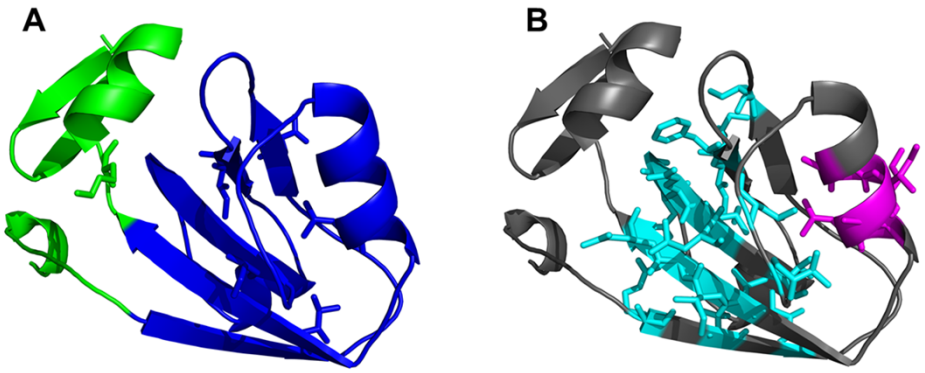
Supplementary Fig. S1: Workflow diagram of OneG. Flowchart outlines key-steps of the OneG used to predict cryptic intermediates/metastable states of proteins under native conditions.



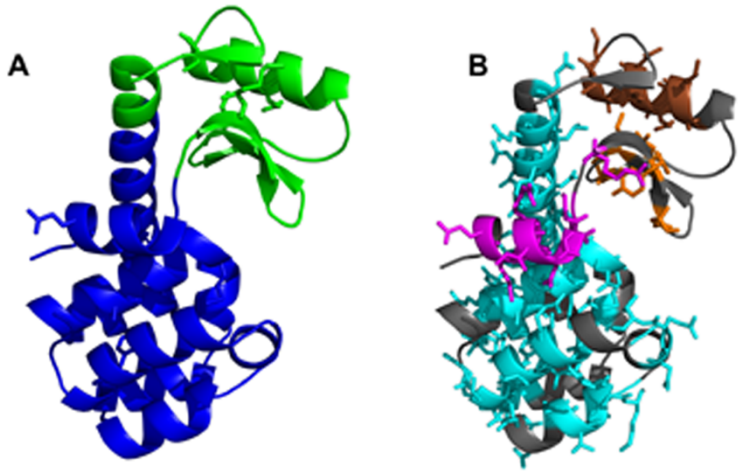
Supplementary Fig. S2: Figurative representations of various foldons in cytochrome c unfolding. The backbone structures of the protein and residues (for which exchange kinetics were observed by NS H/D exchange) representing each foldon are shown in ribbon and stick models, respectively (refer to Table 1). Figure S2A shows foldons detected by the NS H/D exchange method in blue (GUU), green (CI1), yellow (CI2) and red (CI3) colours. Figure S2B shows foldons predicted by the OneG-Vali tool in cyan (GUU), magenta (CI1) and orange (CI2) colours. Each CI is represented by residues defining its respective isotherm (refer to 'Methods').



Supplementary Fig. S3: Figurative representations of various foldons in apocytochrome b_{562} unfolding. The backbone structures of the protein and residues (for which exchange kinetics were observed by NS H/D exchange) representing each foldon are shown in ribbon and stick models, respectively (refer to Table 1). Figure S3A shows foldons detected by the NS H/D exchange method in blue (GUU), green (CI1) and yellow (CI2) colours. Figure S3B shows foldons predicted by the OneG-Vali tool in cyan (GUU), magenta (CI1) and orange (CI2) colours. Each CI is represented by residues defining its respective isotherm (refer to 'Methods').



Supplementary Fig. S4: Figurative representations of various foldons in third domain of PDZ unfolding. The backbone structures of the protein and residues (for which exchange kinetics were observed by NS H/D exchange) representing each foldon are shown in ribbon and stick models, respectively (refer to Table 1). Figure S4A shows foldons detected by the NS H/D exchange method in blue (GUU) and green (CI1) colours. Figure S4B shows foldons predicted by the OneG-Vali tool in cyan (GUU) and magenta (CI1) colours. Each CI is represented by residues defining its respective isotherm (refer to 'Methods').



Supplementary Fig. S5: Figurative representations of various foldons in T4 Lysozyme unfolding. The backbone structures of the protein and residues (for which exchange kinetics were observed by NS H/D exchange) representing each foldon are shown in ribbon and stick models, respectively (refer to Table 1). Figure S5A shows foldons detected by the NS H/D exchange method in blue (GUU) and green (CI1) colours. Figure S5B shows foldons predicted by the OneG-Vali tool in cyan (GUU), magenta (CI1), orange (CI2) and brown (CI3) colours. Each CI is represented by residues defining its respective isotherm (refer to 'Methods').