## Structure and ligand-mediated folding of the periplasmic domain of Acinetobacter Baumanii OmpA

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The periplasmic domain of OmpA from Acinetobacter baumannii (AbOmpA-PD) binds to diaminopimelate and anchors the outer membrane to the peptidoglycan layer in the cell wall. Although the crystal structure of AbOmpA-PD with its ligands has been reported, the mechanism of ligandmediated folding of AbOmpA remains elusive. Here, we report that in vitro refolded apo-AbOmpA-PD in the absence of ligand exists as a mixture of two partially folded forms in solution: mostly unfolded (apo-state I) and hololike (apo-state II) states. Binding of the diaminopimelate or glycine ligand induced complete folding of AbOmpA-PD. The apo-state I was highly flexible and contained some secondary structural elements, whereas the apo-state II closely resembled the holo-state in terms of both structure and backbone dynamics, except for the ligand-binding region. <sup>15</sup>N-relaxation-dispersion analyses for apo-state II revealed substantial motion on a millisecond timescale of residues in the H3 helix near the ligand-binding site, with this motion disappearing upon ligand binding. These results provide an insight into the ligand-mediated folding mechanism of AbOmpA-PD in solution.