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Title: Two molecular dynamics applications: (a) simulations of the Pdx1 homeodomain; (b) investigation of the  $\alpha$ -sheet secondary structure.

Name: Babin, Volodymyr

Affiliation: North Carolina State University

(a) Pancreatic and duodenal homeobox 1 (Pdx1) is a transcription factor that plays essential role in pancreatic endocrine/exocrine cell development and maintenance of adult islet  $\beta$ -cell function. We report on molecular dynamics simulations of the Pdx1/DNA complex in crystal environment and in aqueous solution. Crystal simulations satisfactorily reproduce the experimental structure (PDB code 2H1K) thus providing a validation for the force field used (ff99SB/parmbsc0). Results from the solution runs deliver additional insights on the protein/DNA contacts variability reported earlier. (b) The  $\alpha$ -sheet has been speculated to play a role as a toxic conformer in amyloid diseases. However, except for relatively short fragments, its detection has remained elusive. We report on molecular dynamics simulations that support the existence of the  $\alpha$ -sheet as a stable, metastable, or long-lived secondary structure in polyglutamine and, to a lesser extent, in polyasparagine aggregates.