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Phase Diagram for Urate Oxidase NATHANIEL WENTZEL, JAMES D. GUNTON, Lehigh University — Urate Oxidase from Asperigillus flavus has been shown to be a model protein in terms of understanding the effects of PEG on the crystallization of large proteins. Extensive experimental studies based on SAXS (Vivares et al, J. Phys. Chem. B 108, 6498 (2004)) have determined the effects of salt, pH, temperature, and most importantly polyethylene glycol (PEG), on the crystallization of this protein. Recently, some aspects of the phase diagram have also been determined. In this paper we use Monte Carlo techniques to predict phase diagrams for urate oxidase in solution with PEG. The model used includes an electrostatic interaction, van der Waals attraction, and a polymer-induced depletion interaction (Vivares et al, Eur. Phys. J. E 9, 15 (2002)). Results of the simulation are compared with experimental results.

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