

Abstract Submitted
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The role of crystal contacts in protein crystallization: soft matter characterization of two protein families¹ DIANA FUSCO, JEFFREY HEADD, Duke University, ALFONSO DE SIMONE, Imperial College London, JUN WANG, PATRICK CHARBONNEAU, Duke University — Crystallizing proteins is the bottleneck to systematically determining their structures, which are key to understanding certain biological processes and engineering bio-inspired materials. Identifying the conditions under which proteins crystallize should be equivalent to determining their phase diagram, but one typically resorts to combinatorial rather than physics-based sampling of solution conditions to tackle this difficult problem. Although several soft matter “patchy particle” models have been suggested to rationalize the phase behavior of proteins, the interactions that drive crystallization are insufficiently characterized for them to be of much use. We use atomistic simulations of solvated proteins of the rubredoxin family to parameterize patchy models. Their phase diagram is then compared with experimental crystallization conditions. The agreement between model and experiment supports the suitability of patchy models to describe globular protein crystallization and provides physical guidelines to systematically improve protein crystallization experiments. An analogous analysis of ubiquitin, which crystallizes in multiple crystal forms, further clarifies the role of competing patches in controlling crystal assembly.

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Diana Fusco
Duke University

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