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Design rules for the self-assembly of a protein crystal THOMAS HAXTON, STEPHEN WHITELAM, Lawrence Berkeley National Laboratory — The need to crystallize proteins for X-ray studies has motivated theories of protein crystallization. These theories, based largely on the behavior of isotropic spheres that form close-packed crystals, predict that assembly is enhanced near the metastable critical point associated with phase separating into a vapor of proteins (protein-poor solution) and a liquid of proteins (protein-rich solution). However, most protein crystals are open structures stabilized by anisotropic interactions, and many assemble best above the critical point. Using theory and simulation, we show that optimal assembly of one such crystal, a model surface-layer protein crystal, is not predicted by the critical point but can be predicted by a combination of two design rules: the thermodynamic driving force must be on the order of the thermal energy, and interactions must be made as nonspecific as possible without promoting liquid-vapor phase separation. In experimental terms, our results suggest adjusting solution conditions in order to impose a defined supersaturation at the liquid-vapor critical point. Our findings suggest that self-assembly of open crystals is more akin to viral capsid self-assembly than to the crystallization of spherical colloids.

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