The ideal crystal for structural biology

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The ideal crystal for structural biology can be defined as one that diffracts to sufficient resolution and completeness to answer the biological question being asked. While simply stated, that question can be asked in many ways and there is no single ideal. Single crystal studies can be used to build up a static picture of the structure from a synchrotron or laboratory source, serial crystallography can be used for those systems that may be radiation or time-sensitive. For work with X-ray free-electron lasers, crystals measured in terms of the number of unit cells may provide useful data. The ideal crystals span two extremes, macrocrystals for neutron studies probing hydrogens or charge state, and nanocrystals for electron diffraction where ideal crystal dimensions are measured in hundreds of nanometers. This talk discusses the crystallization experiment and how the first crystallization outcomes can be tailored to achieve the ideal outcome for the technique used for the final analysis. The knowledge of the behavior of proteins and their phase diagrams, and how different experimental conditions and techniques modulate nucleation and growth phases, are essential to optimize crystal size without expending on crystal quality. Our current knowledge is vast and distilling it to a set of useable and workable concepts is imperative given the expansion of techniques requiring appropriate crystals and the divergent requirements.