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How to Make the Structure Difficult. Z. Dauter, Synchrotron Radiation Research Section, MCL, NCI, Argonne National Laboratory, Argonne, IL 60439, USA.

Classification of a particular structure as easy or difficult is very subjective, since its solution might be an easy task for one investigator and a difficult one for another. Taking as a criterion the time and effort spent on structure solution, the most difficult of all was the structure of hemoglobin, solved by Perutz through an effort that took 20 years. That structure would nowadays probably require no more than a few hours and a personal computer. Obviously, the most difficult structures are those that have never been successfully solved, but they are very rarely publicized. The factors contributing to the total “difficulty” depend on diffraction properties of the crystals, peculiarities of molecular packing, availability of appropriate software, the experience of investigators, and, last but not least, a measure of good luck. The most serious difficulties may reside in various steps of the whole procedure; some macromolecules are difficult to crystallize, some cannot be derivatized, and some crystals display atypical diffraction properties such as twinning or pseudosymmetry. If these factors are not understood and properly dealt with, difficulties arise. Various examples of different kinds of such problems will be presented and discussed.