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Quick Solution of Difficult Structures is not Necessarily an Oxymoron. W. Minor¹, M. Cymborowski¹, M. Chruszcz¹, Z. Otwinowski², D. Borek², ¹Univ. of Virginia, Charlottesville, VA 22903, USA, ²UT Southwestern Medical Center, Dallas, TX 7590, USA

The term difficult structure is very subjective and is quite often related to the time difference between the start of the project and PDB deposition. However, in many cases, the process of discovering what makes the structure resistant takes a long time, and when it is revealed, the structure is solved relatively fast. When an appropriate treatment of a particular problem can be coded in the structure solution system, a similar problem encountered next time does not pose a serious difficulty. For that reason, the frequently used term 'high-hanging fruit' is constantly redefined. We can define a difficult structure as one that has pathologies that are not easily recognizable by current methods or an experimenter's experience.

We have developed an expert system HKL-2000_ph, for semi-automatic or automatic analysis of X-ray diffraction data, which has been successfully used for more than 120 new structure determinations. The current system is oriented towards very fast structure solution, in order to provide feedback during the diffraction experiment. The typical end result is an interpretable electron density map with a partially built structure. The system recognizes sample or data pathologies, sets the optimal data collection strategy, and identifies and corrects for many experimental set-up errors. The most important corrections include, but are not limited to: absorption correction, spindle axis misalignment, uneven speed of spindle axis rotation, and vibration of the cryogenic loop with the frozen crystal during data collection. Examples of various pathologies and their successful (and sometimes unsuccessful) treatment will be presented and discussed.