We have come to rely on checkCIF for the validation of crystal structures, but sometimes structures determined using powder data can present more challenges than the usual single crystal structure. Using PLATON directly (with more control over tolerances) can prove helpful, but other things can go wrong. Trirubidium citrate provides an example of traditional “Marshing”; the true space group is $Pnma$, even though the apparent space group was $Pna2_1$. Comparing the result of a Rietveld refinement to a density functional geometry optimization of the crystal structure is a powerful way of detecting errors. The original structure of paliperidone palmitate did not agree well with the DFT, providing a hint that the molecule was in the wrong conformation. A similar DFT comparison showed that for 17α-dihydroequilin, the crystal structure was solved using the wrong molecular structure. DFT calculations, like least squares refinements, find a local minimum, but provide no assurance that the global minimum has been obtained. The structure of nilotinib provides an example, in which rotation of a ring yielded a lower-energy structure with a better hydrogen bonding pattern. The DFT calculation can also be wrong; the first calculation on sitagliptin dihydrogen phosphate monohydrate was carried out using incorrect hydrogen positions. The structure of telaprevir provides an example of how a Mogul analysis (and many other signs) during the refinement can point out a suspect structure.