# Should we remediate small molecule structures? If so, who should do it?

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In principle, new reports of small molecule crystal structures should be error-free since most reputable journals require validation of crystallographic data with CheckCIF and this software is integrated into the CCDC deposition procedure. However, because some chemical journals appear to ignore or not even to use crystallographic referees, errors may not be pointed out. Furthermore, what should happen if authors are unable or unwilling to make corrections when required? Should an otherwise correct structure be rejected because a hydrogen atom has been incorrectly placed or disorder of a terminal methyl group has not been entered into the model? Should such a structure be published or deposited with a warning message, or should a corrected version be created by an external referee? These questions have particular force with regard to already published structures that have errors. An example from the author's early work shows that well-intentioned remediation can sometimes go wrong. Faults in structures have been corrected by "vigilantes" in their particular area of interest, such as space group symmetry [1] and misplaced hydrogen atoms [2,3]; but such coverage is inevitably limited. Can and should the crystallographic community organize a systematic validation and correction effort?

[1] R. E. Marsh (2009), *Acta Cryst.* B**65**, 782-783.

[2] I. Bernal & S. F. Watkins (2013), *Acta Cryst.* C**69**, 808-810.

[3] C. H. Schwalbe (2016) Abstract 01.11.01.12, 66th ACA Annual Meeting, Denver.