Assuring Quality in Rietveld Refinements

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For work in small molecule single-crystal crystallography, obtaining a low R-factor provides a valuable indication that a structure has been determined properly. However, this one metric does not provide assurance that the resulting structure is the best possible description to match the observations. Likewise, the lack of a low R-factor does not prove that a structure is wrong. Life gets more complex in powder diffraction crystallography. As will be presented, no numerical metric exists that can be used as a guide for determination of quality in Rietveld refinements; one can obtain a low R-factor with a wrong structure and a high R- factor with an excellent structure. [Toby, B. H. (2006). *Powder Diffraction* 21(1): 67-70.] Nonetheless, this talk will present some criteria that can be used to discern fit quality, but this requires review of both the structural results [Kaduk, J. A. (2007). *Powder Diffraction* 22(1): 74-82; Kaduk, J. A. (2007). *Powder Diffraction* 22(3): 268-278.] and the observed and fitted patterns. One important note is that a full electronic documentation of a Rietveld refinement in a CIF will include a pdCIF description of the data and computed pattern. [Toby, B. H. (2005). *Int. Tables for Cryst. Vol. G*: 117-130; Toby, B. H. (2019). *Int. Tables for Cryst. Vol. H*: 515-521.] This provides the ability to reviewers to make a good consideration of refinement quality. [https://journals.iucr.org/https://publcif.iucr.org/services/tools/pdcifplot.php; Rowles, M. R. (2022). *J. Appl. Cryst.* 55: 631-637.] It will be argued that reviewers and editors should refuse publication for Rietveld structures that do not include such a full CIF.