

Microsymposium

MS099.001

What makes a structure report valid?

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The number of crystal structures archived in the Cambridge Crystallographic Database will soon reach 1 million. Their quality ranges from questionable to excellent. Obviously, it is from the scientific viewpoint always best to go for the best attainable data quality. In practice, the attainable data quality might be only acceptable for the purpose of the study. For that reason, the archival of just the model parameters (nowadays in CIF format) might be insufficient to properly validate the result of a structure study. Essentially, it is more a report of the author's interpretation of the experimental data. Possible errors are difficult to detect, to investigate and to correct. What is needed for that is to also archive the experimental (reflection) data along with the refinement model used. Modern refinement packages now implement (options to include) those data automatically into the archived CIF. In that way, automated extended structure validation is possible. In addition, independent analysis of unusual results and follow-up use of the (possibly difficult to obtain or unique) data will be possible as well. This talk will discuss some of the validation tools that are available in the program PLATON[1].

[1] Spek, A.L. (2015). Acta Cryst. C71, 9-18.

Keywords: [structure validation](#)