GI-MS48-P15 | WHEN ARE "BAD DATA" "GOOD" DATA?

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Over ten years of running the Chemical Crystallography Service in Oxford there have been a lot of apparently simple questions like, "What is the R-factor for this structure?" and "Is it publishable?". For some structures, the answer will be, "2%" and "Yes!", but it is often not as simple as that and there are usually follow up questions. More importantly, despite the best efforts of IUCr and checkCIF, crystallography is still an experimental science with real data which are never perfect: data quality can range from good to truly dreadful. Indeed, Murphy's Law [1] suggests that problems will be particularly complex when the science is most interesting, and in such cases, the answers to the Chemists' questions are rarely straight forward.

A selection of problem structures will be presented highlighting some of the challenges of working with "difficult data". The discussion will attempt to justify the premise that there is no such thing as unpublishable data, just data that are not fit for purpose.

[1] Roe, A., *Genet. Psychol. Monogr.*, 1951, 43(2), 121-235.