

GI-MS48-03 | THE DIFFERENCE ELECTRON DENSITY MAP AS A CRYSTAL STRUCTURE

VALIDATION TOOL

Spek, Ton (Utrecht University, Utrecht)

Structure validation as implemented by the IUCr aims at providing authors, referees, readers and users a tool to evaluate the results of a crystal structure report. The WEB based checkCIF tool offers a list of alerted for issues, ALERTS, to be inspected, acted or commented upon. ALERTS may report issues ranging from potentially serious (i.e. A-level ALERTS) to interesting info but not necessarily erroneous (i.e. G-level ALERTS). The messages are short assuming sufficient crystallographic knowledge of their meaning. For each ALERT there is also some explanatory WEB-based text available. Most ALERTS have their origin with issues encountered in the past with papers submitted to Acta Crystallographica journals. The set of ALERTS is frequently extended and finetuned on the basis reported new issues. Several ALERTS are based on information that can be derived from a difference electron density map. Alternatively, a significantly number of ALERTS are based on the analysis of the FCF file. Details with examples of this tool along with those of some other tools will be discussed in this talk.