s3.m1.o3 **Structure Validation: A Moving Target.** D.J. Watkin, R. Cooper & C.K. Prout. *Chemical Crystallography Laboratory, 9 Parks Road, OXFORD, OX1 3PD, UK.*
Keywords: computing, hot topics.

The 'Moving Target' referred to in the title is *not* the battery of standards set by the IUCr Checkcif utility, though they may represent the final 'Seal of Approval' to be applied to a structure analysis.

The important targets are those set by crystallographers themselves, and the people who rely on crystallographic evidence in other branches of science, in response to the revolution in data acquisition. Given a suitable supply of 'good' crystals, a modern diffractometer has the potential for 1 to 12 data sets per 24 hours - perhaps 30 data sets per week. Good data sets from good crystals usually yield a trial structure from a modern structure solution program - in fact, these programs are now so powerful that they will produce a recognisable structure even from quite poor data sets.

Until recently, it has been the task of the crystallographer to ensure that the development and refinement of the structure has been performed correctly. Because of the flood of diffraction data now available, this traditional pattern of working becomes increasingly impossible, and the burden of maintaining standards must be born by software. It is the duty of programs which develop and refine these structures to ensure that the best use is made of the available data.

To maximise the through-put of structure analyses, many of the routine cases must be processed by non-professional analysts. The definition of 'routine' will depend largely on the software. More 'knowledgable' software will be able to treat more difficult cases as routine.

The new version of CRYSTALS has several features to assist in the evaluation of an analysis *as it proceeds.* The advantage of this is that problems can be identified early on, rather than when a disappointing reply is returned from Checkcif. Two features which can be adapted to suit changing circumstances, without recompiling CRYSTALS, are:

1 Validation of the structure against similar structures in the Cambridge Data Base. CRYSTALS prepares search queries based on the current structure, and uses the replies from QUEST to build a library of target geometries.

2 User-writable SCRIPTS (macros) which can interrogate the CRYSTALS data-base, and take or suggest appropriate action to deal with abnormal refinements.

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s3.m1.o4 **Structure Solution with PATSEE: Where are the limits?** K. Wagner, S. Rühl, E. Egert, *Institut für Organische Chemie der Goethe-Universität, Marie-Curie-Straße 11, D-60439 Frankfurt, Germany.*
Keywords: molecular replacement, Patterson search, PATSEE

Patterson search is a powerful tool for solving difficult crystal structures since it actively uses chemical information and so can compensate for mediocre precision and resolution of the X-ray data [1]. Our program PATSEE [2], which attempts to combine the merits of both Patterson and direct methods in order to locate a fragment with known geometry in the unit cell, has solved a large number of crystal structures during the last decade and proved to be reliable and widely applicable. As far as "small" molecules are concerned, our experience with many problem structures has clearly shown that the chances of a successful structure solution with PATSEE are indeed very good if a reliable search model and reasonably good experimental data are available.

In order to find both the optimum solution strategy and the limits of the method we have systematically tested PATSEE under various conditions and tried to answer the following questions:

- How large does a search fragment have to be?
- What accuracy is required for a search fragment?
- Are fragments with calculated geometries as well suited as those derived from related crystal structures?
- Is PATSEE able to solve larger structures with several hundred atoms?
- Can PATSEE solve structures from powder diffraction data?

As a result of a thorough investigation, the first three questions have been answered satisfactorily [3]. We have also demonstrated that crystal structures of oligonucleotides with up to 500 atoms can be solved with PATSEE under realistic conditions, i. e. with data of limited resolution [4]. PATSEE has already solved several crystal structures from powder data; at present we are trying to optimize the search strategy so that it can be applied routinely.

[1] E. Egert, *Acta Cryst.* A**39**, 936-940 (1983).
[2] E. Egert, G. M. Sheldrick, *Acta Cryst.* A**41**, 262-268 (1985).
[3] K. Wagner, J. Hirschler, E. Egert, submitted for publication.
[4] K. Wagner, E. Egert, in preparation.