by *Solve* by finding the shift that best maps the trial solution onto the (known) correct solution.

14.2.2.9. *Conclusions*

The *Solve* algorithm is very useful for solving macromolecular structures by the MIR and MAD methods. It has been used to solve MAD structures with as many as 56 selenium atoms in the asymmetric unit (W. Smith & C. Janson, personal communication). From the user's point of view, the algorithm is very simple. Only a few input parameters are needed in most cases, and the *Solve* algorithm carries out the entire process automatically. In principle, the procedure can be very thorough as well, so that many trial starting solutions can be examined and difficult heavy-atom structures can be found. Additionally, for the most difficult structure-solution cases, the failure to find a solution can be useful in confirming that additional information is needed.

14.2.2.10. *Software availability*

The *Solve* software and complete documentation can be obtained from the web site http://solve.lanl.gov.

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