

## **A Relational Database Approach to Report Generation**

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As the throughput of X-ray diffraction laboratories increases and the groups of users diversify, the need for an automatic report generation system becomes more apparent. Although the type of report varies depending on the user's objectives, the data in the report is always based on information gathered throughout the experiment.

We present a relational database approach to report generation. For each step of the structure determination the relevant pieces of information are recorded, such as the type of operation, input and output data, software version, user name, date and time. Furthermore, by linking the input of an operation to the output of the preceding steps, each piece of information is put into context as and when it becomes available. From the emerging tree structure it is possible to create a report from the beginning of the experiment to any step in the experiment. Wrong paths that did not lead to the final result are preserved too.

Reports come in different shapes and sizes: various formats (e.g. CIF, mmCIF, HTML, and proprietary formats), various purposes (e.g. publication, archiving, or visualization), and varying degrees of detail. In order to serve this wide spectrum of needs we have developed a template language that describes which data is extracted from the database and how it is formatted.

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