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Stop! Don't throw that crystal away!

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We have developed methods for processing area detector data collected from samples containing several crystal lattices, and implemented these into the data processing program Mosflm and its GUI iMosflm [1]. In particular we have extended the following processes: (1) modified autoindexing routines recognize different lattices and display this information in iMosflm in a clear and concise way, allowing the user to choose how to proceed. (2) multiple lattice information is used to determine which data are used in refinement of crystal parameters and which (e.g. overlapped reflections) should be excluded. (3) observations are integrated in each lattice and flagged in the output reflection file (written in the MTZ format) to indicate whether they arise from a single lattice or from overlapped reflections from multiple lattices. The choice of lattice in the latter two stages of data processing is made simple in iMosflm. The information regarding reflection overlap can now be processed correctly in the merging and scaling steps by the programs Feckless, Pointless and Aimless [2]. The refinement program RefMac [3] has been modified to make use of the extra information from multiple lattices. We will discuss these improvements to processing and present early results from their implementation.

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