



# Crystal Structure Refinement: A Crystallographer's Guide to SHELXL (International Union of Crystallography Texts on Crystallography)

*By Peter Müller, Regine Herbst-Irmer, Anthony Spek, Thomas Schneider, Michael Sawaya*

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Crystal Structure Refinement is a mixture of textbook and tutorial. As A Crystallographers Guide to SHELXL it covers advanced aspects of practical crystal structure refinement, which have not been much addressed by textbooks so far. After an introduction to SHELXL in the first chapter, a brief survey of crystal structure refinement is provided. Chapters three and higher address the various aspects of structure refinement, from the treatment of hydrogen atoms to the assignment of atom types, to disorder, to non-crystallographic symmetry and twinning. One chapter is dedicated to the refinement of macromolecular structures and two short chapters deal with structure validation (one for small molecule structures and one for macromolecules). In each of the chapters the book gives refinement examples, based on the program SHELXL, describing every problem in detail. It comes with a CD-ROM with all files necessary to reproduce the refinements.

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### Review

"A key purchase for a wide population of scientists engaged in crystal structure determination...The depth of coverage of important topics such as twinning and disorder will be very valuable to structural scientists, and will provide information and an approach that is not currently available."--*Alexander J. Blake, University of Nottingham*

"A high quality text."--*David J. Watkin, University of Oxford*

### About the Author

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Peter Müller has worked in George Sheldrick's research group for over five years, where he received a thorough crystallographic education. He studied chemistry and crystallography (M.S. in 1997) and received his Ph.D. with George Sheldrick in 2001 on a thesis entitled "Problems of Modern High-Resolution Single-Crystal X-Ray Structure Determination" From 2001 to 2004, he spent three years in Los Angeles as a postdoc in David Eisenberg's group at UCLA. There he worked in the field of molecular and structural biology. Currently, he is the director of the X-ray diffraction facility at MIT.

Dr. Müller taught basic and advanced crystallography (both theory and lab classes) in Göttingen, Los Angeles and now at MIT, and has held several structure refinement workshops around the USA and in Germany.

For further details please see also online CV: <http://web.mit.edu/x-ray/pmueller/CV.html>>

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