renaming copies of files. The metadata module automatically collates information from the data collection and processing steps. This can then be edited and added to, before merging with the information generated by the refinement program employed to create a complete and correct cif file, if possible. The precompiled Olex2 executable can be downloaded free of charge by academic users from http://www.olex2.org.
1. http://sourceforge.net/projects/olex2.

Keywords: crystallographic software, small molecules, graphical display and rendering of molecules

P03.01.03

Acta Cryst. (2008). A**64**, C219

OLEX2: A portable molecular graphics toolset for crystallography

Oleg V Dolomanov, Luc Bourhis, Horst Puschmann, Richard Guildea, Judith A.K. Howard
Durham University, Chemistry, CG 72, Durham, Durham Co, DH1 3LE, UK, E-mail：oleg_dolomanov@hotmail.com

Olex2 consists of two main parts: a flexible and easy-to-use Graphical User Interface (GUI) and comprehensive crystallographic library. The GUI provides intuitive access to all aspects of the underlying crystallographic library as well as external programs and libraries such as the computational crystallographic toolbox (cctbx)[1] and the ShelX[2] package. It is designed to make working with crystal structures as easy as possible for users with different experience. The GUI is easily extensible and written in extended HTML; it is designed to highlight possible problems with the structure and implements an easy to follow solve-refine-report workflow. Many other, more specialised tools, can be accessed through the GUI also, and a fully functional, command-line interface is provided at all times. Many of these tools are written in the Python scripting language and can be modified and extended by the user. The Olex2 GUI is also portable (currently tested to work on MS Windows and several 32/64 bit versions of Linux). The crystallographic library provides a portable platform for crystallographic software development and contains various tools for file I/O and structure model manipulation. Apart from these basic features, many more high-level features are included: geometric hydrogen placement, space group determination, tests for missing symmetry elements, calculation of voids and surfaces, pattern matching, report generation are only a few to mention. Olex2 is an open source project located at www.sourceforge.net. The Windows distribution is maintained by us and compiled executables are available from www.olex2.org. We acknowledge the financial support of EPSRC (EP/C536274/1).
1. CCTBX: http://cctbx.sourceforge.net
2. ShelX: G.M. Sheldrick, Acta Cryst. (2008). A64, 112-122

Keywords: visualisation, GUI, crystallographic programming library

P03.01.04

Acta Cryst. (2008). A**64**, C219

NORM - a program for performing normal probability plots and half-normal probability plots

Ferdinand Belaj
Karl-Franzens-Universitat Graz, Institut fur Chemie, Schubertstr. 1, Graz, Styria, 8042, Austria, E-mail：ferdinand.belaj@uni-graz.at

The program NORM primarily was written to obtain normal probability plots [1] from the data contained in a .FCF-file of the wide-spread used SHELXL program [2]. Furthermore normal probability plots and half-normal probability plots of arbitrary quantities can be obtained. Therefore the program can be used to estimate the reliability of the standard deviations and to identify significant geometric differences of two similar molecules in the asymmetric unit or of the same molecule in two different crystal structure determinations [3]. The difference between two independently determined interatomic distances generally is normally distributed and crystallographically independent molecular geometries can be compared using the powerful method of normal probability plot analysis [4]. Further capabilities of NORM are to plot $\Delta(F^2)/\sigma(F^2)$ vs. $F_c^2/\max(F_c^2)$ or to plot $\mathrm{SQRT}(w)\Delta(F^2)$ vs. $\sin(\theta)/\lambda$. Finally a normal probability plot of $\Delta m = (F1\text{-}K*F2)/\mathrm{SQRT}[\sigma(F1)^2+K2*\sigma(F2)^2]$ can be obtained in order to compare the observed structure factors F1 and F2 (or measured intensities) of two data sets, e. g. the measurements of two crystals of the same compound [1]. The scale factor K between the two data sets is computed to minimize $\Sigma(\Delta m)^2$. The plots produced by NORM can be viewed on the screen or included into Microsoft Word. Some examples for the use of NORM will be discussed.
[1] Abrahams S. C., Keve E. T., Acta Cryst., 1971, A27, 157. [2] Sheldrick, G. M., SHELXL-97. Program for the Refinement of Crystal Structures. Univ. of Göttingen, Germany, 1997. [3] Johansson M. H., Otto S., Oskarsson Å., Acta Cryst., 2002, B58, 244. [4] Albertsson J., Schultheiss P. M., Acta Cryst., 1974, A30, 854.

Keywords: data analysis, normal probability plot, software

P03.01.06

Acta Cryst. (2008). A**64**, C219–220

Computational challenges in wide-angle X-ray solution scattering (WAXS)

Jaydeep P Bardhan[1,2], Lee Makowski[2], Sanghyun Park[2]
[1]Argonne National Lab, Mathematics and Computer Science Division, 701 W. Buckingham Place, Chicago, IL, 60657, USA, [2]Argonne National Lab, 9700 S. Cass Ave, Argonne IL 60439, USA, E-mail：jbardhan@alum.mit.edu

The advent of third-generation high-brilliance synchrotrons brings not only opportunities for investigating molecular structure, but also challenges for data analysis. Measurements of X-ray scattering from proteins in solution, for instance, are now of high quality even at wide angles. Presently, WAXS experiments represent a valuable, but largely complementary tool to other experimental methods. Realizing the full potential of WAXS rests on meeting two primary challenges: characterizing the structural information contained in WAXS data, and developing methods to enable quantitative interpretation in terms of molecular structure. We address these challenges simultaneously using an integrated approach that combines experiment with molecular modeling. We have investigated several computational approaches for calculating the scattering from a protein in solution, given either a single set of atomic coordinates or sets of coordinates as calculated using techniques like molecular dynamics. Although calculating small-angle scattering patterns from structures is well established, our focus is development of techniques flexible and efficient enough to allow an exploration of a wide range of models for scattering (e.g., structure of the hydration layer) with sufficient accuracy at wide angles that the simulated patterns are truly representative of the molecular model under consideration. This will substantially increase the power of WAXS as a tool for biophysical characterization of protein structure and dynamics. Improving our understanding of the nature