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

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OLEX2: A portable molecular graphics toolset for crystallography

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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

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

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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

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

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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

and limitations of WAXS data will thus enhance both our ability to analyze WAXS experiments and their use as experimental tests of computational models of molecular systems.

Keywords: WAXS characterization, X-ray solution scattering, SAXS

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"Irena" software package for analysis and modeling of small-angle scattering data

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Availability of high-quality small-angle scattering (SAS) data is increasing with the proliferation of a wide range of high-performance user-friendly synchrotron and desktop small-angle X-ray scattering (SAXS) instruments. Similarly, neutron sources also provide an increasing number of quality and well-supported small-angle neutron scattering (SANS) instruments. As the barrier to quality data is decreasing, non-expert users - highly skilled experts in their particular fields with only limited small-angle scattering expertise - are applying the SAS techniques in their science. These users often need extensive help to be able to correctly apply the small-angle scattering methods and generate high-level science in their areas of expertise. The software package "Irena" was designed to be a comprehensive package with tools for most of the steps a user commonly needs to perform, balancing ease of use for non-expert users with the controls and complexity expert users need. "Irena" provides a number of data modeling and analysis tools, mostly applicable in such fields as materials science, polymers, and chemistry. A wide range of support tools are also included such as ones to enable input, output, manipulations with, and graphing of the data, as well as a scattering contrast calculator. As an example: one of the tools in Irena enables modeling of multiple non-interacting dilute systems with a choice of form factors and, when necessary, including one of five available structure factors. This model can be fitted to one or multiple input data sets (at once), enabling, for example, analysis of anomalous SAXS data or co-fitting of SAXS and SANS data. Other tools include "Unified fit" model, fractals model, "Debye-Bueche" model, and small-angle diffraction model.

Keywords: small-angle scattering, SAS modeling, SAS analysis

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ARP/wARP: From noisy electron densities of proteins to complete structures

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Structural interpretation of the provided experimental X-ray data, which have a low level of the information content, that therefore leads to a noisy and troublesome interpretable electron density map is a challenging task in the protein crystallography. An important carrier of the structural information in electron density maps of proteins is the repetitive chemical motif of the peptide unit that links the amino acids. One efficient way for the peptide recognition is implemented in the chain tracing module of the ARP/wARP suite, where an advanced template matching technique is applied to the shapes of the density. However, the success of the recognition process strongly depends on the level of informational content in the electron density map. Our on-going development concerns studying the functional p(x,y,z) which describes the electron density map corresponding to peptides and its relation to some distance functional r(x,y,z). The connection between them can be presented as radial density functional p(x,y,z)*r(x,y,z). The distribution of values of the radial density functional can then be applied to the recognition of the peptide pattern. The method is rotation invariant and its combination with the existing technique that uses the template matching improves the completeness of the protein structure provided by ARP/wARP.

Keywords: protein structure determination, electron density, pattern recognition

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Density modification by directed evolution of electron density maps

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There are numerous cases in macromolecular X-ray crystallography where current methods of density modification are not capable to yield an interpretable map. Since the performance of the automatic procedures for model building of the corresponding protein (e.g. RESOLVE, TEXTAL or ARP/wARP) strongly depends on the quality of the phases, reliable methods for modifying the density are absolutely essential. We are developing a new iterative density modification method which is based on directed evolution of the electron density map. One of the central aims for the new method is to be applicable to cases when the resolution of the data is lower than 3 Å. In a first step each grid point of the initially phased map is analysed by statistical and pattern recognition methods to define a likelihood whether the density value of the point should be changed. A small number of map points are subsequently 'mutated'. Finally, the phases from the mutated map are used to generate a new density distribution. First encouraging results with 3 Å resolution test cases have been obtained, where this iterative procedure lead to a reduction of the phase error of about 0.2° for each iterative step of the procedure. These will be presented and discussed. The application of the method to the crystallographic use of low resolution images from electron microscopy studies will also be presented.

Keywords: density modification, pattern recognition, protein crystallography

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Validation and correction of carbohydrate 3D structures

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Carbohydrate structures in PDB entries exhibit a rather high rate of errors [1,2]. Some errors, such as wrong residue names, surplus atoms in the glycosidic linkage, or wrong connectivities, can be