WinGX and *ORTEP for Windows*: an update
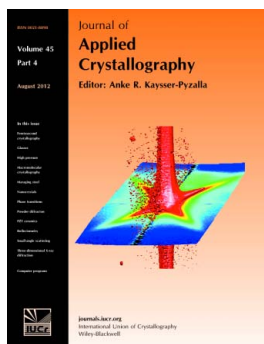
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WinGX and ORTEP for Windows: an update

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The *WinGX* suite provides a complete set of programs for the treatment of small-molecule single-crystal diffraction data, from data reduction and processing, structure solution, model refinement and visualization, and metric analysis of molecular geometry and crystal packing, to final report preparation in the form of a CIF. It includes several well known pieces of software and provides a repository for programs when the original authors no longer wish to, or are unable to, maintain them. It also provides menu items to execute external software, such as the *SIR* and *SHELX* suites of programs. The program *ORTEP for Windows* provides a graphical user interface (GUI) for the classic *ORTEP* program, which is the original software for the illustration of anisotropic displacement ellipsoids. The GUI code provides input capabilities for a wide variety of file formats, and extra functionality such as geometry calculations and ray-traced outputs. The programs *WinGX* and *ORTEP for Windows* have been distributed over the internet for about 15 years, and this article describes some of the more modern features of the programs.

1. Introduction

Easy access to computing facilities, especially the arrival of the personal computer during the 1980s, has revolutionized science in general and X-ray crystallography in particular. This branch of science has always been heavily dependent on computational facilities, and the lack of easy access to this resource greatly inhibited its advance until the late 1960s and early 1970s. Crystallographic laboratories originally relied heavily on home-written software, which often had incompatible input and output formats. The advent of general crystallographic codes such as *XRAY72* (Stewart *et al.*, 1972), the Oak Ridge program suite *ORTEP* (Johnson, 1965), *ORFFE* and *ORFLS* (Busing *et al.*, 1962, 1964), and *SHELX76* (Sheldrick, 2008) provided most of the necessary computational operations in a single program or suite of programs. One of these home-written codes was the *GX* suite of programs (Mallinson & Muir, 1985), in use in the Glasgow crystallographic laboratories since the early 1980s. At the time, this was one of the most complete sets of programs for undertaking a single-crystal X-ray structural analysis. The *GX* program was written in Fortran77 and was originally designed to run on a Gould SEL 32/27 minicomputer, with 750 kB RAM and a 32 MB hard disk. To place the expense of such computational equipment into some perspective for the modern reader, the author recalls that a replacement 50 MB Winchester disk storage unit for this computer cost the equivalent of more than US$16 000.

With the arrival in the early 1990s of desktop personal computers with sufficient computing power to run least-squares refinements comfortably, it was clear that the future for small-molecule crystallographic computing lay in this direction. The *GX* code was first ported to the MS-DOS environment and then to the Windows environment, becoming the *WinGX* program (Farrugia, 1999). The initial versions of *WinGX* used the *RBLS* least-squares refinement program from the *GX* suite, but with the release of the refinement program *SHELXL93*, and subsequently *SHELXL97* (Sheldrick, 2008), which had a much more sophisticated implementation of

constraints and restraints, it was decided to use the latter as the refinement engine for *WinGX*. This necessitated a move to the *SHELX* file format for holding the structural model information. It was at this stage that *WinGX* was first publicly released on the internet in 1997 (Farrugia, 1999). Originally written as a monolithic executable program, it incorporated a number of other publicly accessible crystallographic codes, including the *PLATON* program by Ton Spek (Spek, 2003). At a later stage, the monolithic executable was split into a controlling graphical user interface (GUI) component (`wgxMain.exe`) and a number of separate executables. The current version of *WinGX* has around 100 separate executables. *WinGX* (including the GUI) and almost all of the other code is written in Fortran77, using many Fortran95 extensions. Apart from the Fourier and geometric calculations, little of the original *GX* code actually remains. *WinGX* also acts as a repository for tried and tested crystallographic software, such as *DIRDIF2008* (Beurskens *et al.*, 2008) and *THMA* (Schomaker & Trueblood, 1968), in cases where the original authors no longer wish to, or are unable to, maintain them.

The *ORTEP for Windows* program, although released as a stand-alone program, was designed to work within the *WinGX* environment. It provides an extensive GUI framework for the *ORTEP* crystallographic program (Burnett & Johnson, 1996), which originated in the 1960s and was written in an early dialect of Fortran. Despite its age, *ORTEP* is still the industry standard for drawing displacement ellipsoid plots because of its careful design. The GUI code allows input from a large variety of crystallographic (and noncrystallographic) file formats in a seamless manner and also includes extra functionality, such as geometry calculations and output in the ray-tracing *POV-Ray* format (http://www.povray.org). *WinGX* and *ORTEP for Windows* have been available on the internet for some 15 years, with many tens of thousands of registered users worldwide. It now seems appropriate to describe some of the more modern features of these programs, which were not discussed in the original short computer program abstracts (Farrugia, 1997, 1999).

computer programs

2. Program descriptions

The *WinGX* program suite consists of the controlling GUI (`wgxMain.exe`), from which the user selects the appropriate program module (most of which are separate executables) *via* standard drop-down menus. The order of the main menu items from left to right, File, Model, Data *etc.*, follows the logical progression in a crystal structure analysis. There are several ways to initiate a structural analysis in *WinGX*, including semi-automatic input from diffractometer data files (Nonius KappaCCD, Bruker SMART or SAINT, or Rigaku files) or from *SHELX* files (Sheldrick, 2008). In the latter case, all that is required is a *SHELX*-format reflection file and an associated *SHELX* `.ins` file, present in the working directory. The `.ins` file need only contain the most basic information, *i.e.* cell constants and their errors, Z, elemental types, the numbers of atoms of each type in the cell (not essential) and any known space-group information, in the standard *SHELX* format.

The *ORTEP for Windows* program is similarly controlled from an intuitive set of drop-down menus, and users should rarely need to consult the manual. Default views are displayed automatically from the input coordinates (and displacement parameters if present) and standard mouse-controlled scrolling is provided to change the viewpoint. Accepted input file formats include *SHELX*, CIF, *ORTEP* instruction files, PDB (Protein Data Bank; http://www.pdb.org/pdb/home/home.do), *XD*, *XYZ*, *GX*, *GSAS* (Larson & Von Dreele, 1994), and output files from the quantum programs *GAUSSIAN* (Gaussian Inc., Pittsburgh, Pennsylvania, USA) and *GAMESS-UK* (Computing for Science Ltd, Daresbury Laboratory, Warrington, England). Output graphic formats include HPGL, PostScript and *POV-Ray*, as well as direct printing. All options of the original *ORTEPIII* program remain available, as well as other features derived from the GUI, *e.g.* geometry calculations and automatic hydrogen-bond generation.

2.1. Data reduction and processing

One of the intentions of the *WinGX* suite was to provide software that allowed the expert user as much control as possible over all stages of a crystal structure analysis. Since the original release of *WinGX*, the experimental measurement of X-ray diffraction data has been transformed. From using time-consuming serial-counting devices, most crystallographic laboratories have now adopted area detectors, capable of measuring several reflections in a single image. This has effectively meant a return to photographic techniques, but using digital technology. As a result, the treatment of the experimental data, *i.e.* the digital images, has become more complicated by at least an order of magnitude, owing to the increased size of the resultant data sets. There are several programs in the *WinGX* suite that process the data files from Nonius CAD-4 and Syntex/Siemens diffractometers with serial detectors, but there are none for the integration of digital images and the production of a set of raw intensities from area detectors. This job is left to specialist integration programs, generally supplied by the diffractometer manufacturers, *e.g. SAINT* (Bruker, 2012) or *HKL-2000* (Otwinowski & Minor, 1997). However, there are a number of tools in *WinGX* to deal with the resultant integrated data files and to merge the many thousands of individual measurements into a unique set of experimental structure factors. The primary tool is *SORTAV* (Blessing, 1987), which is able to correct data for absorption effects by fitting an empirical transmission surface to multiple equivalent reflections (Blessing, 1995), correct data for radiation damage using a similar empirical fitting, scale individual frames and batches, average equivalent reflections, and improve estimates of the experimental errors and errors on the means through analysis of variance.

The *HKLTOOL* module analyses the statistics of reflection data sets, calculates R_{merge} for all Laue symmetries, checks the systematic absences and provides an automated determination of the space group. The statistics of the normalized structure factors (*E-STATISTICS* module) can be useful to verify the presence of an inversion centre, although the user must be aware of the limitations of these statistics (Marsh, 1995). A variety of plotting options are available for easy visualization of the data quality. Many of these compare F_{obs} with F_{calc} in various ways (menu item Analyse – Data Plots), which of course relies on having a model structure, but some may usefully be applied to the raw intensity data without reference to any model. For example, when the absences have been specified during data-processing with *SORTAV*, one may obtain a scatter plot of the measured intensities of the systematic absences. Fig. 1 shows two such plots, where the intensities (I) of the systematic absences in a data set of monoclinic symmetry are plotted *versus* $I/\sigma(I)$, and where two options have been applied in the data-processing procedure. In Fig. 1(*a*), no correction has been applied for the effect of $\lambda/2$ contamination, which can give rise to anomalously high intensities for weak reflections (Kirschbaum *et al.*, 1997). A number of quite weak reflections have positive $I/\sigma(I)$ values well in excess of 3.0, and an automatic analysis of the systematic absences could erroneously flag these as non-absent. After application of the $\lambda/2$ correction (Fig. 1*b*), these reflections no longer have such large $I/\sigma(I)$ values. In fact, many now have significantly negative $I/\sigma(I)$ values. These plots also provide clear visual evidence that the data-integration procedure has treated these absent reflections in a statistically sensible manner, as there are approximately equal numbers of positive and negative intensities.

Two ASCII formats are used to store reflection data in the *WinGX* suite, the standard *SHELX* format files (with extension `.hkl`) used
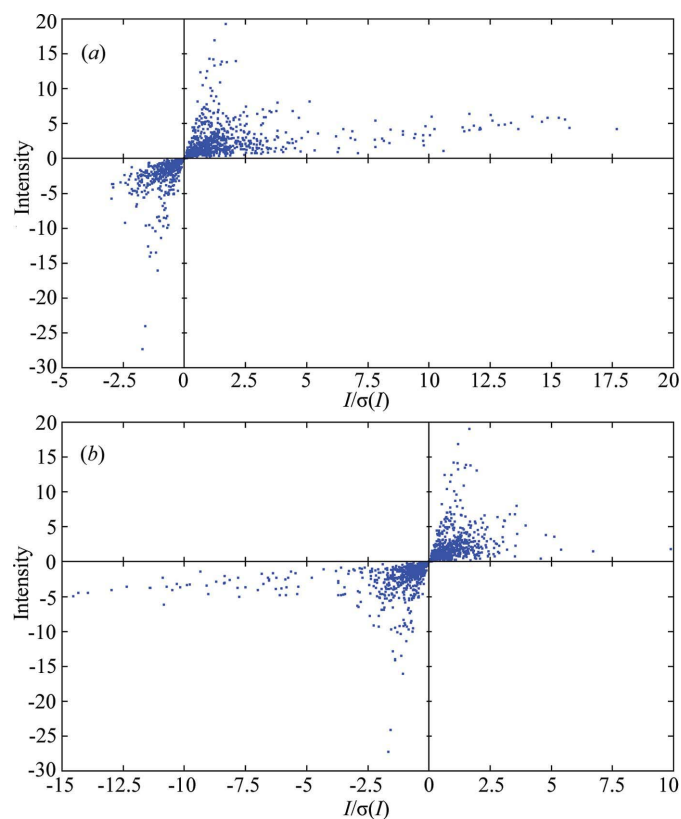

Figure 1
Distribution of intensity data for 1495 systematic absence intensities for two data-processing options (see text).

for refinement calculations and the intermediate *SORTAV* format files (called `*_hkl.sortav`), which are used as input for the *SORTAV* data-processing module. Many of the data-processing options allow the use of either format, although the *SORTAV* format is recommended. Absorption effects are one of the most important sources of experimental error in measured structure factors. A number of absorption corrections are maintained in *WinGX*, of varying rigour from empirical (ψ scan) and semi-empirical (*DIFABS*; Walker & Stuart, 1983) to fully accurate analytical or Gaussian methods. Several of these are now essentially of historical interest only. With the advent of area detectors, the great majority of reported structural analyses use the so-called multi-scan method (Blessing, 1995), as implemented in *SORTAV* or *SADABS* (Sheldrick, 2012). This method relies on the measurement of multiple equivalents to calculate an absorption surface, and is quite satisfactory except for strongly absorbing samples, when only a rigorous analytical (or Gaussian quadrature) method based on indexed crystal faces is viable. In many cases, the absorption correction will have been carried out at the data-reduction stage, but information such as the maximum and minimum transmission coefficients needs to be carried forward to prepare the final archive of the structural analysis.

2.2. Structure solution

The solution of the phase problem in crystallography, once a serious obstacle to X-ray structural analysis, is now routine and usually very fast for small-molecule data sets. The philosophy of *WinGX* is to provide as many approaches as possible and it is considered worthwhile to continue supporting fairly old structure-solution programs, such as *SHELXS86* (Sheldrick, 2008) and *SIR92* (Altomare *et al.*, 1993). There may well be the odd case where these old programs can solve structures that more modern programs cannot. Two major applications for structure solution are the *SHELX* suite of Sheldrick (2008) and the *SIR* suite of Giacovazzo and co-workers (Burla *et al.*, 2012). Executables for these programs are not provided with the *WinGX* release, although they may be obtained from the program authors, free of charge for academic users. *WinGX* provides GUI menu items linking to the *SHELX* suite, which currently contains two major programs for structure solution, *SHELXS* and *SHELXD*. The latter is intended primarily for macromolecules, although it works equally well for small molecules. Similarly, if *WinGX* detects that the programs have been installed, it will also provide GUI menu items for *SIR97* (Altomare *et al.*, 1999), *SIR2002* (Burla *et al.*, 2003), *SIR2004* (Burla *et al.*, 2005), *SIR2008* (Burla *et al.*, 2007) and recently for *SIR2011* (Burla *et al.*, 2012). These menu items create the necessary input files to run the *SIR* programs. Only quite basic versions of the instruction files are created (usually sufficient to solve the structure), but the user may edit these manually in difficult cases in order to access more sophisticated options in these programs.

In addition to these external 'plug-in' programs, several other structure-solution packages are supplied in the *WinGX* release, thanks to the agreement of the original authors. These include a Windows version of the original *SIR92* program (Altomare *et al.*, 1993), the *SUPERFLIP* program (Palatinus & Chapuis, 2007) and *DIRDIF2008* (Beurskens *et al.*, 2008). *SIR92* works remarkably well in the majority of cases when the space group and cell contents are known with certainty, but users are encouraged to try more recent and more sophisticated versions of *SIR*, such as *SIR2011* (Burla *et al.*, 2012), which includes the novel VLD algorithm (Burla *et al.*, 2010). *SUPERFLIP* employs the charge-flipping algorithm (Oszlányi & Sütő, 2005) and is a particularly useful program in cases where the

space group is uncertain. Since the retirement of its main author, Paul Beurskens, the *DIRDIF* program suite is now maintained only through the *WinGX* implementation of *DIRDIF2008*. The collection of structure-solution programs in *WinGX* is almost certain to work on any small-molecule structure; if none of them succeeds, then there is likely to be some problem with the data set (twinning, wrongly assigned Laue symmetry *etc.*) which will need careful consideration.

2.3. Structure refinement

The default refinement program for *WinGX* is currently *SHELXL97* (Sheldrick, 2008). This is probably the most widely used refinement program for small molecules, and an excellent monograph has been written, guiding the inexperienced in the use of this program (Müller *et al.*, 2006). The executable is not supplied with the *WinGX* release, but may be obtained from the program author. GUI menu items are also provided for refinements using *CRYSTALS* (Betteridge *et al.*, 2003) or *JANA* (Petříček *et al.*, 2006), carried out in subdirectories of the main working directory. The results may be transferred back for analysis with *WinGX*. Full documentation for the *SHELX* programs (and indeed all other programs) is supplied in *WinGX* in PDF format, and is accessed through the *WinGX* documentation tree structure (Fig. 2). The analysis modules of *WinGX* read the refined atomic parameters from the `.res` file from the *SHELXL* refinement and also from the *SHELXL* listing file, as this contains the errors on the refined parameters (not stored in the `.res` file).

For expert users who are well versed in the elaborate instruction set of the *SHELXL* program, a structural refinement can be undertaken in the 'traditional' manner by manual editing of the `.ins` file. For users more used to GUI interfaces, the refinement can also be followed using the *SXGRAPH* editor, which reads in a `.res` file and writes out an updated `.ins` file for further cycles of refinement
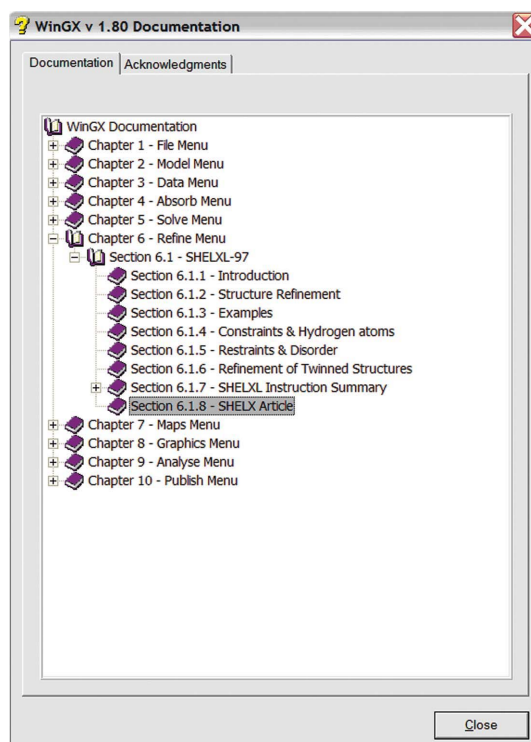

Figure 2
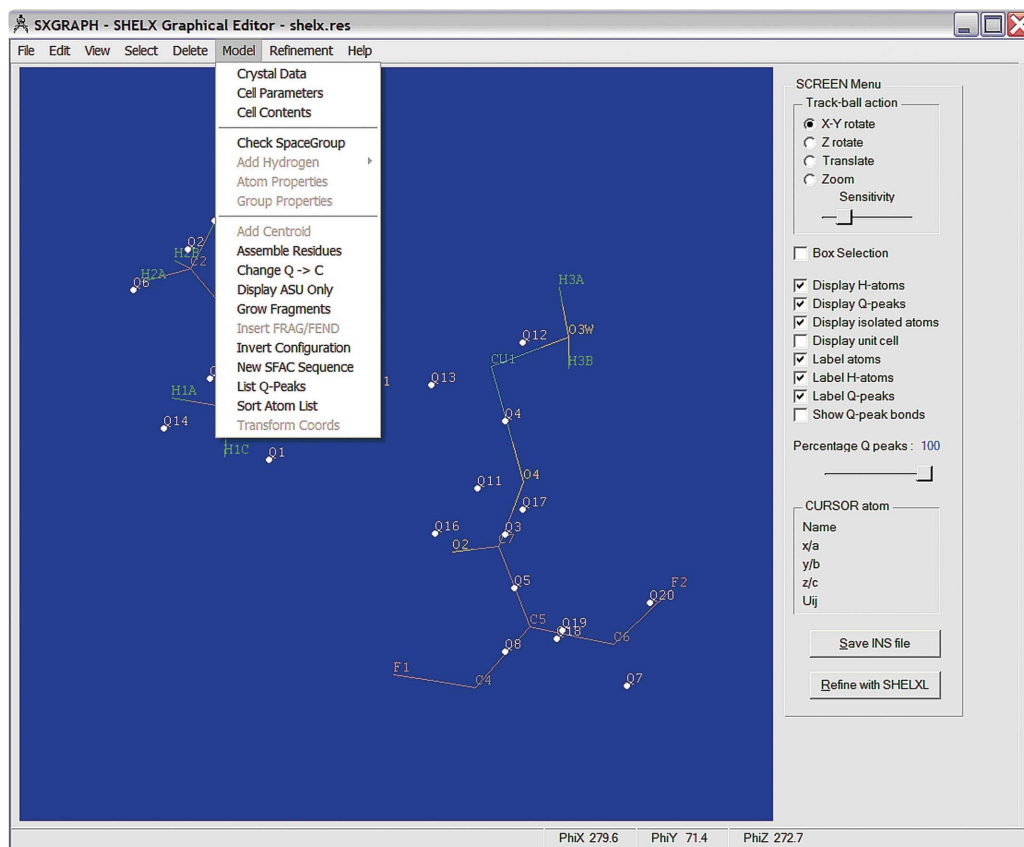The tree structure of the *WinGX* documentation files.

Figure 3
The interface of the *SXGRAPH* model editor for *SHELX* files.

(Fig. 3). This editor is effectively a GUI for *SHELXL*. The structural representation is kept deliberately simple, as in this way structures with many thousands of atoms can be quickly manipulated. Most of the facilities in *SHELXL* are available from this GUI, including many of the useful restraints and constraints.

The use of Fourier maps to visualize the electron density was an essential part of early X-ray structural analyses. With the advent of computer programs that searched Fourier maps automatically and printed out just the peak and hole positions (such as *SHELXL*), the routine visual examination of Fourier maps fell out of common usage. Nevertheless, visual examination of such maps, through the *MAPVIEW* module in *WinGX*, is highly informative in cases of disorder or incorrect refinement. For instance, Fig. 4 shows an $F_{obs} - F_{calc}$ difference Fourier map in a plane through the calculated positions of methyl H atoms, after using one of the options in *SHELXL* to place these in an idealized staggered geometry relative to the rest of the molecule. As can easily be seen, these calculated positions are actually incorrect. The true positions show up as positive peaks, while there are holes in the calculated positions. In this case, as the data quality is good, the correct H-atom positions are better obtained using the AFIX 137 option in *SHELXL*, which utilizes an initial circular Fourier search to optimize the H-atom positions.

2.4. Structure visualization, analysis and validation

One of the difficulties facing beginner students is knowing when a refined structural model is satisfactory, and *WinGX* provides a
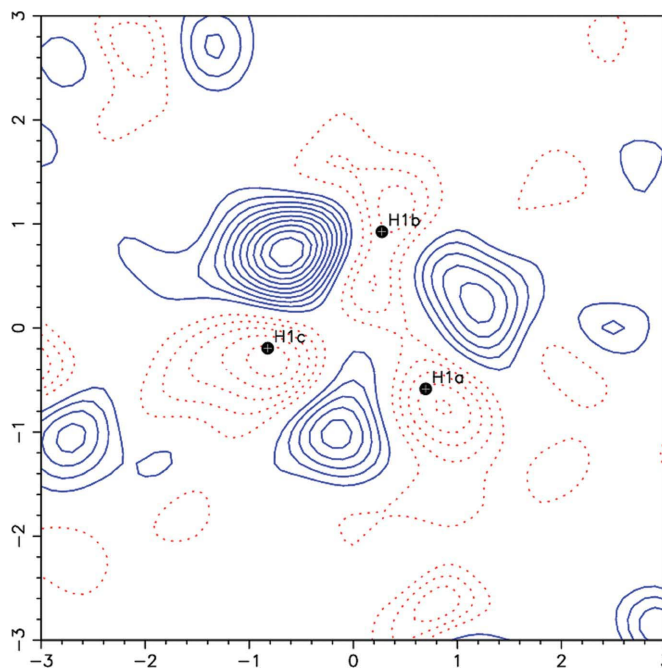

Figure 4
A difference Fourier map through the plane of calculated methyl H atoms, showing their true positions. Positive contours are in solid blue and negative ones in broken red lines, at intervals of 0.05 e Å^{-3}.
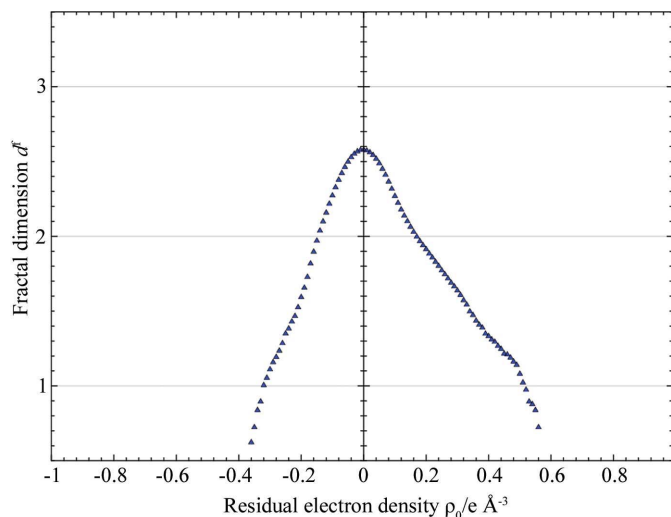
Figure 5
A fractal dimension plot, showing the deviation from an idealized Gaussian distribution of map pixels.

Figure 6
An example of a ray-traced '*ORTEP*' plot produced by *ORTEP for Windows*.

number of tools to help with this. Of course, the R values computed from least-squares refinements are a good guide, but it is also important to examine the difference Fourier maps to see if unmodelled features remain. This is normally done by looking for the peaks and holes in the map and considering whether these have any chemical significance. The module *MAPVIEW*, in conjunction with *FOURIER MAP*, allows the user to examine the residual density (or indeed the total density) in the entire cell or through arbitrary planes.

Another way is to examine the distribution of electron density throughout the entire map using fractal dimension plots (Meindl & Henn, 2008). If no unmodelled features remain in the experimental data, the difference map, calculated to sufficient resolution, should have a Gaussian distribution of map pixels centred on zero. The fractal dimension plot (module *PIXELSTATS*) should then correspond to a parabola, and the example shown in Fig. 5 has this fundamental distribution, although there is a noticeable 'bulge' at positive density, which indicates that some unmodelled features remain in the data. In this case, as the data quality is good and the resolution reasonably high at 0.7 Å^{-1}, these unmodelled features arise from the charge-density effects of covalent chemical bonding. They appear because of the inadequacy of the spherical atom scattering factors used in the *SHELXL* program.

Once the refinement is complete, the final results are collated together in the form of the archive CIF. This is created using the CIF written by *SHELXL* (or other refinement programs) and others written by *WinGX* through the structural analysis, *i.e.* `dreduc.cif` (from the data-reduction process), `struct.cif` (from the initialization process in *WinGX*) and `sortav.cif`, or possibly others prepared by the user. The collation process essentially involves filling in all the missing information from the refinement CIF. It creates an `archive.cif` in a form suitable for journal submission and structural archiving. The *WinGX* module producing this CIF is driven by a user-modifiable request list, a list of all possible CIF data items required for the final archive. Many journals now require that the crystallographic content of a paper has been automatically validated by dedicated software. The validation process demonstrates that the crystallographic content is complete and correct and that the quality of the analysis is acceptable. The *WinGX* module *IUCRVAL* checks whether the archive CIF is consistent with the original IUCr publication crite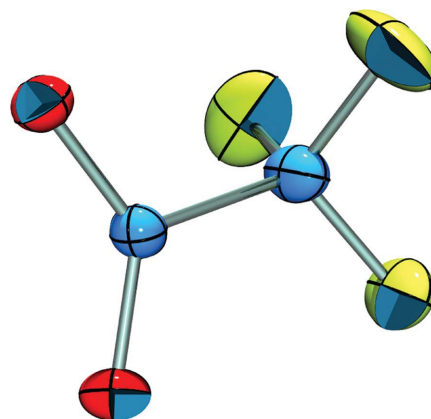ria, but much more extensive checks are undertaken by the *PLATON VALIDATE* module, which uses the CIF checking routines in the *PLATON* program (Spek, 2009).

The anisotropic displacement parameters (ADPs) are well known to act as a 'sink' for errors in the crystallographic data and analysis, so a careful investigation of these provides a useful check on the quality of the structural analysis (Spek, 2009). Highly anisotropic or non-positive definite ADPs are a sign of significant problems in the structural analysis, and their presence should lead to a careful reconsideration of the structural model. *ORTEP for Windows* allows the user to check for any unusual features of the ADPs, and of course provides the essential labelled molecular illustration for publication. The original graphic routines in *ORTEP* produced simple monochrome line drawings, but a full-colour ray-traced output of the displacement ellipsoids is also possible with *ORTEP for Windows* (Fig. 6). The rigid-body motion implied by the ADPs can also be analysed numerically using the **TLS** model (Dunitz *et al.*, 1988) using the *THMA* module (Schomaker & Trueblood, 1968). This provides another check on the veracity of the ADPs.

3. Availability

WinGX and *ORTEP for Windows* are supplied as pre-compiled executables only for the MS Windows environment. They will run on essentially any 32-bit version of this operating system (7, Vista, XP, 2000, 98 or NT) and the supplied 32-bit executables will also run on 64-bit Windows 7/Vista machines. Users have reported that they work satisfactorily on Linux systems under *Wine* emulation (although there is absolutely no support for this mode of operation). The executables and associated file systems may be downloaded from http://www.chem.gla.ac.uk/~louis/software and are free of charge for academic users. Licence files are required to run the programs, but these can be freely obtained from the same web site and are only used to keep track of all downloads.

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