**ShelXle: a Qt graphical user interface for SHELXL**

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ShelXle [1] is a graphical user interface for SHELXL [2], currently the most widely used program for small-molecule structure refinement. It combines an editor with syntax highlighting for the SHELXL-associated .ins (input) and .res (output) files with an interactive graphical display for visualization of a three-dimensional structure including the electron density ($F_o$) and difference density ($F_o-F_c$) maps. Special features of ShelXle include intuitive atom (re-)naming, structure visualization and a novel way of displaying disorder extending over special positions. The DSR [3, 4] plugin can be of great help in mastering messy disorders. ShelXle is completely compatible with all features of SHELXL and is written entirely in C++ using the Qt4 and FFTW libraries. It is available at no cost for Windows, Linux and Mac-OS X and as source code. Since its release in 2011 it has been 47900 times downloaded.

![ShelXle's Icon](image)

**Fig. 1. ShelXle’s Icon**

References:


