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.

Fig. 1. ShelXle's Icon

References:

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[3]D. Kratzert, I. Krossing, (2018) J. Appl. Cryst. , **51**, 928-934.

[4]D. Kratzert, J.J. Holstein, I. Krossing, (2015) J. Appl. Cryst. ***48***, 933-938.