



# ShelXle – A Qt<sup>+</sup> GUI for SHELXL

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Qt  
© 2011 Nokia Corporation and/or its subsidiaries. Qt is the library ShelXle is using. Qt is spoken like the word 'cute'.

The 'selection toolbar' shows possible actions.

Q-Peaks are visualized as colored icosahedra. Each color refers to an electron-density peak height.

The 'Q-Peak Legend' can be used to locate and hide 'Q-Peaks'

ShelXle is available for Windows, Linux, MacOs and WeTab.

The text cursor of the editor jumps immediately to the clicked atom.

Sub-windows can be gathered together in tabs.

The Information Window gathers useful information that can be easily copied and pasted.

## Inherit labels

If you wish to assign same labels to chemical identical molecules in the asymmetric unit then click on any atom of the molecule with final labels. Then right click any atom of the other molecule and choose "Inherit labels..."

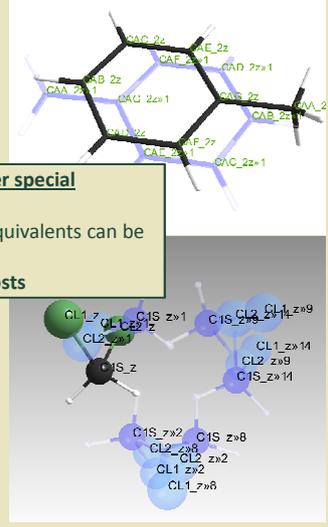
You can reassign atom labels by drag and drop the label icons of the target molecule

These are the final labels in this (left) column

In this example C5 gets labeled C15 (residue 1 VIT)

**Abstract:** ShelXle is a graphical user interface (GUI) for small-molecule refinements with SHELXL<sup>[1]</sup>. It is designed like an integrated development environment and combines an editor with syntax highlighting and auto completer with the graphical representation of the three dimensional structure. ShelXle is a tool for expert users of SHELXL giving them the full control over the \*.res/\*.ins input file. Non expert users can rapidly learn how to appreciate the full capability of SHELXL by exploring the functionality of ShelXle. The electron density and difference electron density maps ( $F_o$  and  $F_o - F_c$ ) can be visualized as wire framed iso-surfaces. A 'rename mode' provides the ability to re-label atoms including residues and/or parts and assigning free variables for occupation constraints. Molecules can be moved so that their centers of gravity lie inside of the unit cell by just one click. Identical molecules in the asymmetric unit can inherit their labels semi-automatically from a previous labeled molecule. The 'auto HFIX' function uses electron density ( $F_o - F_c$ ) for the placement of Hydrogen atoms with suitable constraints/restraints. For convenience functions to update the number of atoms in the cell (UNIT) and the weighting scheme (WGHT) are build in. A refinement history and a save history allow to go back to previous file versions. The three dimensional representation of the molecule is drawn using OpenGL. Several stereoscopic projection modes are available including one for Zalman Monitors. The ShelXle is written entirely in C++ using the Qt. The program has been thoroughly tested prior this launch. ShelXle is available for Windows (XP/Vista/7), MacOS X (10.5/10.6), Linux (SuSE [11.1-11.4] / Debian) and as source. On all systems it is easy to install. ShelXle is licensed under LGPL(2.1) and can be downloaded free of charge at <http://ewald.ac.chemie.uni-goettingen.de/shelx/>.

**Disorder over special positions:** Symmetry equivalents can be visualized as PART-N Ghosts



## Highly configurable atom and bond styles

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Difference electron-density maps can help finding missing or erroneous hydrogen positions.



Download ShelXle here: <http://ewald.ac.chemie.uni-goettingen.de/shelx/>

## Refinement and Save History

In the preview of the save history every line that is different to the current file version is highlighted in orange.

The interactive 'rename mode' allows you to assign free variables to occupancies of disordered parts and/or residue numbers and classes

The label here turns red if an atom with the same name already exists.

You can add atoms to the scattering factors by clicking on the periodic system