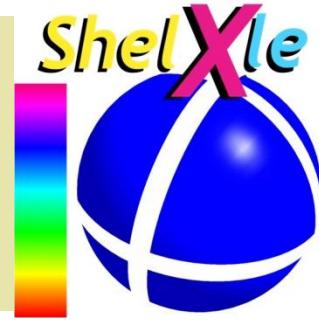


ShelXle: A cute GUI for *SHELXL*

Christian B. Hübschle

17.11.2011



Outline

- Main Features
 - Editor
 - OpenGL representation of the structure
 - Electron-density maps
- Customization
- Renaming Function
- Convenient Functions
- New Functions
- Plans





The paper is published!

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computer programs

ShelXle: a Qt graphical user interface for SHELXL

Christian B. Hübchle,* George M. Sheldrick and Birger Dittrich

Institut für Anorganische Chemie, Georg-August-Universität Göttingen, Göttingen, Germany. Correspondence e-mail: chubchle@molins.de

ShelXle is a graphical user interface for *SHELXL* [Sheldrick, G.M. (2008). *Acta Cryst.* A64, 112–122], 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_d) and difference density (F_{d-F}) maps. Special features of *ShelXle* include initiative atom (π -jamming), a strongly coupled editor, structure visualization in various mono and stereo modes, and a novel way of displaying disorder extending over special positions. *ShelXle* is completely compatible with all features of *SHELXL* and is written entirely in C++ using the Q4 and FFTW libraries. It is available at no cost for Windows, Linux and Mac-OS X and as source code.

1. Introduction

The *SHELX* programs as originally developed in the 1970s were intended for use with photographic intensity data, punched cards and computers multiple orders of magnitude slower than even the most basic models on the market today (Sheldrick, 2008). In the early days of *SHELX*, a crystal structure refinement usually involved examining a Imprintor output – i.e. drawing lines between the numbers to create a ‘picture’ of the structure – followed by editing a few of the input and output cards with a card-punch and combining the cards to create the input deck for the next refinement job, which usually ran overnight. The way crystal structure determinations are performed today is clearly different, but – somewhat surprisingly – *SHELXL* is still used frequently.

More recently, a number of other graphical user interfaces (GUIs) (e.g. WINGX (Barbour, 1999), OLEX2 (Dolomonev *et al.*, 2009), XSEED (Barbour, 2008), PLATON and SYSTEM-3 (Spek, 2009), and the Broker programs XP (Neuillet, 1988) and XSHELL (Bruylants, 2000)) have been developed to facilitate structure refinement with *SHELXL* as the underlying program, but in general the punched-card way of thinking that was central to the design of *SHELXL* has proven a hindrance to integrating it into a modern interactive computer-graphics environment without losing at least some of the unique capabilities of the original program. Despite the availability of a very informative International Union of Crystallography monograph (Müller *et al.*, 2006) describing the application of *SHELXL*, we felt that there was still a need for a simple, intuitive and robust GUI that uses state-of-the-art programming techniques but retains as much as possible the original *SHELXL* flavour and capabilities. For this purpose, *ShelXle* was developed. *ShelXle* shares some concepts with earlier programs, such as *MacCoy3D* (Hübchle & Dittrich, 2011), but most of the code was rewritten.

2. Technical description and functionality

ShelXle opens a *SHELXL*-format .ins file from a structure solution program or a *SHELXL* refinement. The .ins and .res file in *SHELXL* format is shown in an interactive editor window (on the right side of the graphical interface) and (on the left side) the mono or stereo

visualization of the three-dimensional structure is displayed. The display and editor are strongly coupled. The editor uses colour highlighting to identify the currently chosen atom and also possible syntax errors. Clicking on an atom in the display structure moves the text cursor to the corresponding atom in the editor. An atom can also be selected by right-clicking on a line in the editor containing an atom, which is then centred in the display. The GUI is controlled by menus and toolbars; command-line input is neither required nor implemented. Fig. 1 gives a general impression of the appearance and functionality of *ShelXle*. *ShelXle* is written entirely in C++ using the Q4 (<http://q4.sourceforge.net/products/>) and the FFTW (<http://www.fftw.org/>) libraries, and is able to exploit the latest developments in computer graphics as well as being highly portable.

2.1. Electron density map

If the previous *SHELXL* refinement used the ‘LIST 6’ instruction, F_d and F_{d-F} maps are calculated and visualized as mesh-style isovalues. The colour scheme used is the same as in the program COOT (Emsley *et al.*, 2010). The isocontour level of such maps can be controlled by using either the mouse wheel or a dialogue window. The contour level of the difference map may be changed with the mouse wheel while pressing the control key (or the command key under Mac-OS), and the contour level of the F_d map is changed in the same way but using the shift key. Initial isocontour levels are 2.7σ for the F_d map and 1.2σ for the F_{d-F} map, where σ is the square root of the average variance of the density. These maps are in principle infinite in all directions, but the region displayed is restricted by clipping planes perpendicular to the viewing direction. If desired, it is possible to change the view settings to display only density within 141 \AA (2.0σ) of any visible atom or ‘Q peak’ (difference electron density peak from *SHELXL*).

It may sometimes occur that the parameters of the *SHELXL* PLAN instruction are not sufficient to generate a Q peak at a desired position, for example when dominant heavy atoms are present. In such cases *ShelXle* can generate further Q peaks by searching for peaks in the F_{d-F} residual density that are higher than the current isocontour value.

computer programs

2.2. Special handling of difference electron density maxima (‘Q peaks’)

Q peaks are visualized as small colour-coded isosurfaces. The colour of a *Q* peak corresponds to the peak height. A separate *Q*-peak list shows the correspondence between colours and peak heights. By moving the mouse over this list, labels of *Q* peaks with the same peak height are highlighted. If the mouse pointer hovers over a *Q* peak, the region representing its height is highlighted in the list. *Q* peaks below a certain threshold may be hidden temporarily by clicking on the *Q*-peak list. Once some of the *Q* peaks have been hidden in this way, the cutoff value can be adjusted by scrolling with the mouse wheel while the mouse pointer is over the list.

2.3. Adding H atoms

The ‘Add H atoms’ function in *ShelXle* places hydrogen atoms automatically by generating the corresponding APTIX instructions in the file being edited. If the F_{d-F} map is available, the difference electron density may be used to find optimal positions for H atoms in CH_3 groups in a similar manner to the way in which the HFIX 137 command in *SHELXL* operates. As methyl groups are often disordered, there is a facility to place six H atoms in idealized positions and to refine an occupancy parameter to describe the disorder using one additional free variable that is generated automatically. Fig. 2 illustrates the usefulness of the difference electron density in placing the H atoms correctly.

2.4. The editor: syntax highlighting and codeword completion

One of the core functionalities of *ShelXle* is the editor and its ability to perform syntax highlighting. All known *SHELXL* commands are highlighted in the same way (dark red over light green). Permanent comments (REM cards following ‘#’) are coloured in blue, while temporary comments (lines beginning with a space when the line does not end with ‘#’) are coloured dark blue and are underlined. Lines longer than 80 characters are wrapped to a new line and each word is highlighted in blue (not complete words in a single line) as is typical for *SHELXL*. After finding one or two characters of a new line have been entered, a code-completion function opens, suggesting commands beginning with the given letters. A suggestion by striking the ‘enter’ key twice on the command in capital letters (whether or not they were entered in uppercase).

Code is taken to keep track of the ‘free variables’, a defining feature of *SHELXL*. When a number is the editor window implicitly references a free variable and the mouse pointer hovers over it for several seconds a pop-up window appears with the interpretation.

Analogously, a brief description of each *SHELXL* command is given when the mouse is placed over a line starting with a command. If lines containing atoms are selected in the editor window, clicking in the selection area is also interpreted as a selection. The editor is also equipped with a search and replace tool that highlights matches in the editor in yellow. Bsite parts (PART) and residues (RBSI) can also be selected. This function allows the selection of disordered PARTs, either separately or in combination with the ordered PART. Unselected atoms can optionally be hidden. A residue may also be selected using a residue list. In addition, facilities are provided for managing the windows. When deleted, or prior to performing a refinement, the three-dimensional display and the editor are synchronized and the editor contents are saved. More exotic *SHELXL* instructions – e.g. FRAG... FEND or the third number on the LS command – can easily be added using the editor.

2.5. Refinement history facility

Like *OLEX2* (Dolomonev *et al.*, 2009), *ShelXle* is equipped with a refinement history, where every refinement step is saved and reproto-

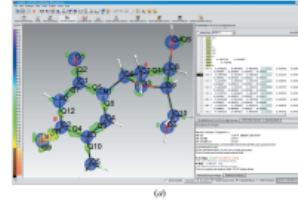


Figure 1
(a) The GUI of *ShelXle* displaying the structure of thymidine at 20 K (Hübchle *et al.*, 2011). The F_{d-F} map at 0.25 \AA^{-3} shows features of bonding and lone-pair electron density. Atom C1 is currently selected. (b) An enlargement of the lower-right corner of the molecular lattice.

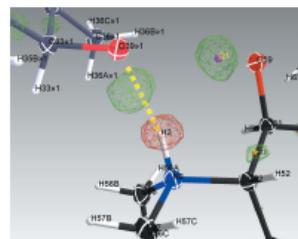
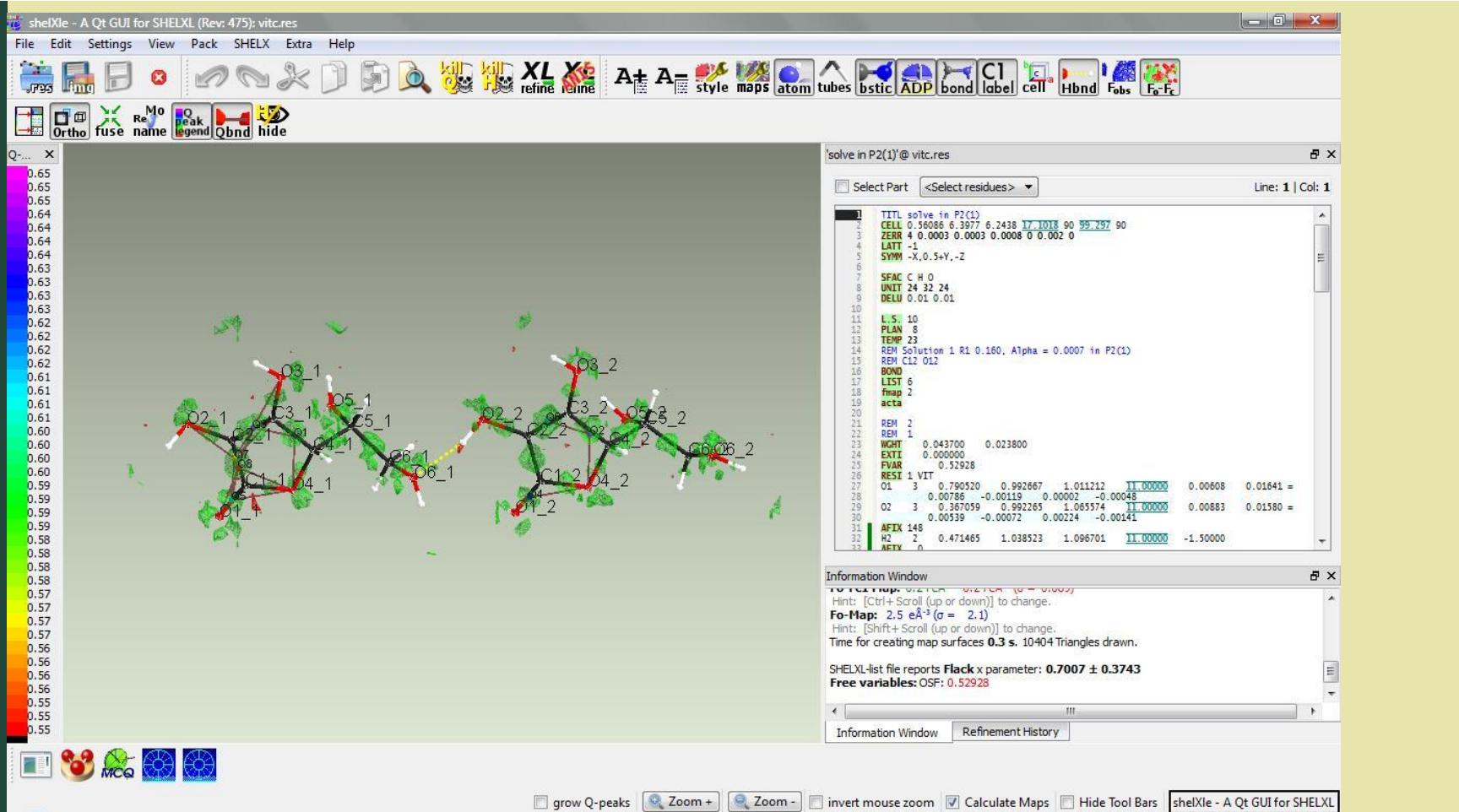
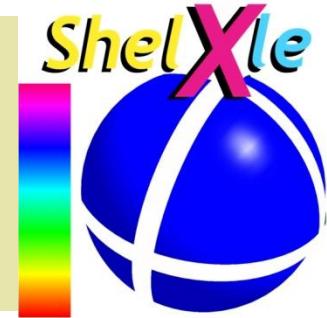


Figure 2
An early refinement state of methionine (Olson *et al.*, 2010), showing difference electron density. Mating and amineally phased H atoms are clearly visible.



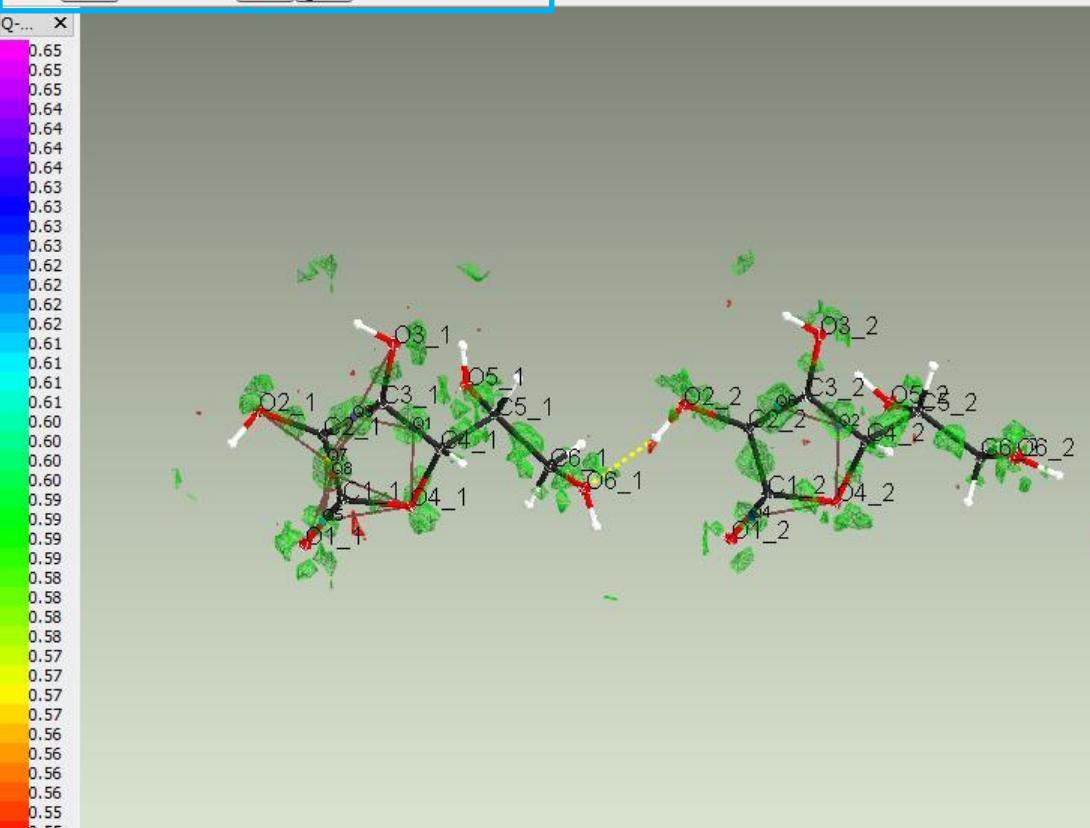


The GUI



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GÖTTINGEN

J. Appl. Cryst., **44**, (2011) 1281–1284



'solve in P2(1)'@ vitsc

Select Part <Select residues>

Line: 1 | Col: 1

```

1 TITL solve in P2(1)
2 CELL 0.56086 6.3977 6.2438 17.1018 90 99.297 90
3 ZERR 4 0.0003 0.0003 0.0008 0 0.002 0
4 LATT -1
5 SYMM -X,0.5+Y,-Z
6
7 SFAC C H O
8 UNIT 24 32 24
9 DELU 0.01 0.01
10
11 L.S. 10
12 PLAN 8
13 TEMP 23
14 REM Solution 1 R1 0.160, Alpha = 0.0007 in P2(1)
15 REM C12 O12
16 BOND
17 LIST 6
18 fmap 2
19 acta
20
21 REM 2
22 REM 1
23 WGT 0.043700 0.023800
24 EXTI 0.000000
25 FVAR 0.52928
26 RESI 1 VIT
27 O1 3 0.790520 0.992667 1.011212 11.00000 0.00608 0.01641 =
28 0.00786 -0.00119 0.00002 -0.00048
29 O2 3 0.367059 0.992265 1.065574 11.00000 0.00883 0.01580 =
30 0.00539 -0.00072 0.00224 -0.00141
31 AFIX 148
32 H2 2 0.471465 1.038523 1.096701 11.00000 -1.50000
33 AFXY 0

```

Information Wind

תְּמִימָה 0.216 0.216 0.216

Hint: [Ctrl+ Scroll (up or down)]

Hint: [Shift + Scroll (up or down)] to change

Time for creating map surfaces 0.3 s. 10404 Triangles drawn

SHELXL-list file reports Flack x parameter: **0.7007 ± 0.374**

Free variables: OSF: 0.52%

◀ ▶

Information Window



grow O-peaks Zoom + Zoom - invert mouse zoom Calculate Maps Hide Tool Bar

shelXle - A Qt GUI for SHELXL

File Tool Bar

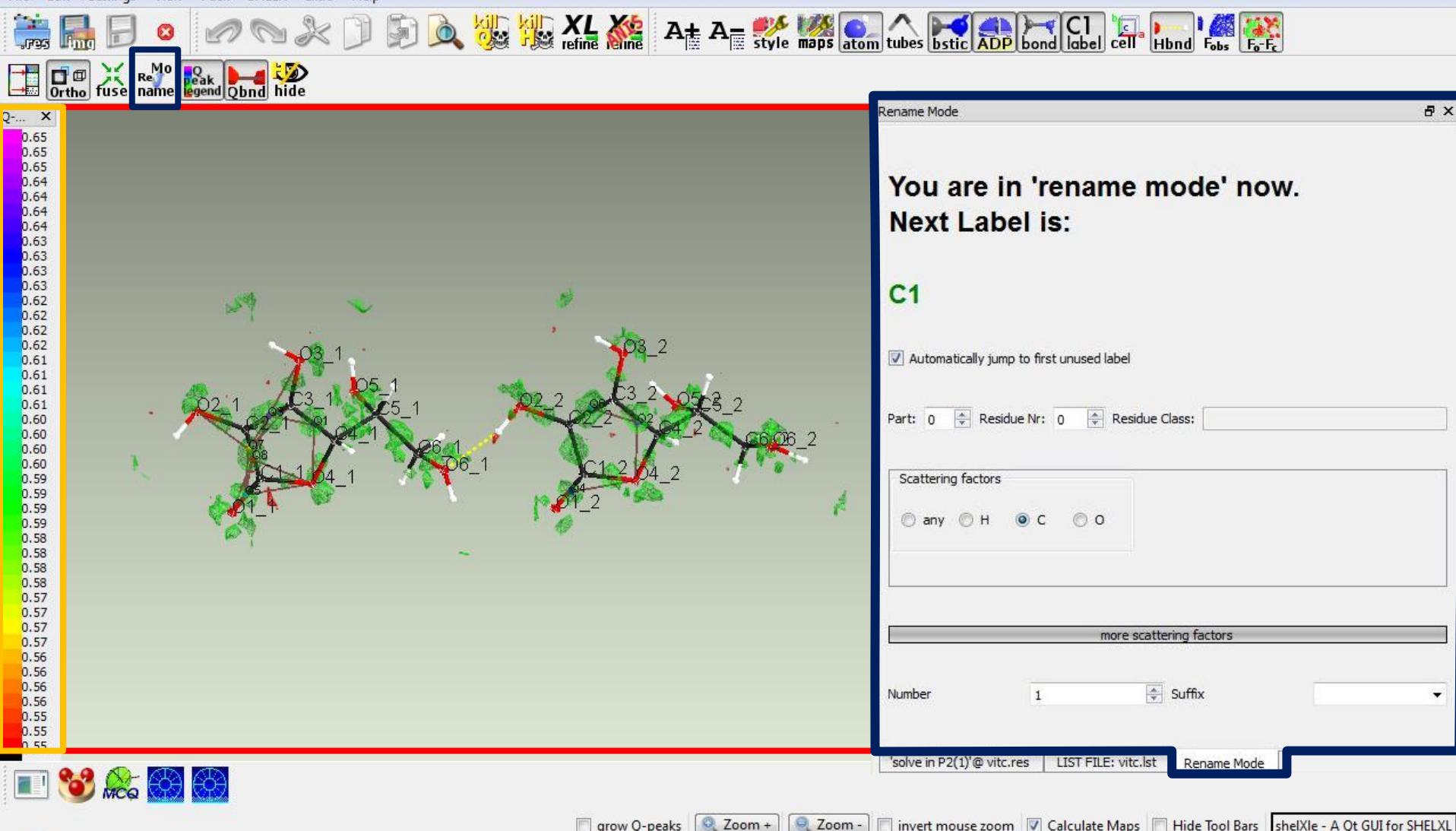
Selection Tool Bar

Editor Tool Bar

Extra Tool Bar

View Tool Bar

Status Bar *J. Appl. Cryst.*, **44**, (2011) 1281-128



OpenGL view

Q-Peak Legend

Editor window

Information Window

Refinement History

Rename Mode



The Editor

```
'solve in P2(1)'@ vitc.res
Select Part 0 ind. Pt. 0
<Select residues>
<Select residues>
RESI 1 VIT
RESI 2 VIT
Line: 1 | Col: 1

1 TITL solve in P2(1)
2 CELL 0.56086 6.3977 6.2438 17.10
3 ZERR 4 0.0003 0.0003 0.0008 0 0
4 LATT -1
5 SYMM -X,0.5+Y,-Z
6
7 SFAC C H O
8 UNIT 24 32 24
9 DELU 0.01 0.01
10
11 L.S. 10
12 PLAN 8
13 TEMP 23
14 REM Solution 1 R1 0.160, Alpha = 0.0007 in P2(1)
15 REM C12 O12
16 BOND
17 LIST 6
18 fmap 2
19 acta
20
21 REM 2
22 REM 1
23 WGHT 0.043700 0.023800
24 EXTI 0.000000
25 FVAR 0.52928
26 RESI 1 VIT
27 O1 3 0.790520 0.992667 1.011212 11.000000 0.00608 0.01641 =
28 0.00786 -0.00119 0.00002 -0.00048
29 O2 3 0.367059 0.992265 1.065574 11.000000 0.00883 0.01580 =
30 0.00539 -0.00072 0.00224 -0.00141
31 ACTV 1.00
```

Hide Button
Float Button
Part selector
Residue selector
Cursor Position





The Editor

'solve in P2(1)'@ vitc.res

Select Part 0 incl. Pt. 0 <Select residues> Line: 20 | Col: 3

```
1 TITL solve in P2(1)
2 CELL 0.56086 6.3977 6.2438 17.1018 90 99.297 90
3 ZERR 4 0.0003 0.0003 0.0008 0 0.002 0
4 LATT -1
5 SYMM -X,0.5+Y,-Z
6
7 SFAC C H O
8 UNIT 24 32 24
9 DELU 0.01 0.01
10
11 L.S. 10
12 PLAN 8
13 TEMP 23
14 REM Solution 1 R1 0.160, Alpha = 0.0007 in P2(1)
15 REM C12 O12
16 BOND
17 LIST 6
18 fmap 2
19 acta
20 SADI
21 SAME 4.700 0.023800
22 SFAC 0.000
23 SHEL 0.52928
24 SIMU 0.790520 0.992667 1.011212 11.00000 0.00608 0.01641 =
25 SIZE 0.786 -0.00119 0.00002 -0.00048
26 SPEC 0.367059 0.992265 1.065574 11.00000 0.00883 0.01580 =
27
28
29
30
```

'solve in P2(1)'@ vitc.res LIST FILE: vitc.lst Rename Mode

Line number area
Code completer





The Editor

'solve in P2(1)'@ vitc.res

Select Part 0 ind. Pt. 0 RESI 1 VIT Line: 53 | col. 1

| | | | | | | | | |
|----|------------|---------|----------|----------|----------|-----------------|----------|-----------|
| 39 | | 0.00593 | -0.00095 | 0.00133 | -0.00095 | | | |
| 40 | 05 | 3 | 0.326422 | 0.637594 | 0.826569 | <u>11.00000</u> | 0.00856 | 0.01044 = |
| 41 | | | 0.00945 | 0.00171 | 0.00095 | 0.00132 | | |
| 42 | AFIX | 149 | | | | | | |
| 43 | H5 | 2 | 0.210342 | 0.601967 | 0.832382 | <u>11.00000</u> | -1.50000 | |
| 44 | AFIX | 0 | | | | | | |
| 45 | H6 | 3 | 0.430485 | 1.039274 | 0.684828 | <u>11.00000</u> | 0.00949 | 0.01451 = |
| 46 | | | 0.00748 | 0.00202 | 0.00185 | -0.00162 | | |
| 47 | AFIX | 148 | | | | | | |
| 48 | H6 | 2 | 0.536215 | 1.074046 | 0.672208 | <u>11.00000</u> | -1.50000 | |
| 49 | AFIX | 0 | | | | | | |
| 50 | PART | 1 | | | | | | |
| 51 | C1 | 1 | 0.617626 | 0.997688 | 0.968328 | <u>11.00000</u> | 0.00585 | 0.00938 = |
| 52 | | | 0.00649 | -0.00071 | 0.00122 | -0.00042 | | |
| 53 | C2 | 1 | 0.407552 | 1.002477 | 0.990225 | <u>11.00000</u> | 0.00592 | 0.01003 = |
| 54 | | | 0.00599 | -0.00058 | 0.00161 | -0.00037 | | |
| 55 | wronglabel | | | | | | | |
| 56 | PART | 1 | | | | | | |
| 57 | C3 | 1 | 0.266183 | 1.011118 | 0.922471 | <u>11.00000</u> | 0.00565 | 0.01133 = |
| 58 | | | 0.00637 | -0.00026 | 0.00128 | 0.00034 | | |
| 59 | C4 | 1 | 0.382288 | 1.019153 | 0.853239 | <u>11.00000</u> | 0.00640 | 0.01013 = |
| 60 | | | 0.00599 | -0.00006 | 0.00129 | -0.00017 | | |
| 61 | AFIX | 13 | | | | | | |
| 62 | H4 | 2 | 0.360122 | 1.159750 | 0.827778 | <u>11.00000</u> | -1.20000 | |
| 63 | AFIX | 0 | | | | | | |
| 64 | PART | 0 | | | | | | |
| 65 | C5 | 1 | 0.317846 | 0.844877 | 0.791358 | <u>11.00000</u> | 0.00643 | 0.01030 = |
| 66 | | | 0.00588 | 0.00010 | 0.00086 | -0.00052 | | |
| 67 | AFIX | 13 | | | | | | |
| 68 | H5 | 2 | 0.172192 | 0.872348 | 0.765478 | <u>11.00000</u> | -1.20000 | |

'solve in P2(1)'@ vitc.res LIST FILE: vitc.lst Rename Mode

AFIX Highlighter

Current Line Indicator

Part Highlighter

Error Indicator





The Editor



'solve in P2(1)'@ vitc.res

Select Part RESI 1 VIT Line: 62 | Col: 7

| | | | | | | | | |
|----|------|----|----------|----------|----------|-----------------|----------|-----------|
| 54 | C3 | 1 | 0.266183 | 1.011118 | 0.922471 | <u>11.00000</u> | 0.00565 | 0.01133 = |
| 55 | | | 0.00637 | -0.00026 | 0.00128 | 0.00034 | | |
| 56 | C4 | 1 | 0.382288 | 1.019153 | 0.853239 | <u>11.00000</u> | 0.00640 | 0.01013 = |
| 57 | | | 0.00599 | -0.00006 | 0.00129 | -0.00017 | | |
| 58 | AFIX | 13 | | | | | | |
| 59 | H4 | 2 | 0.360122 | 1.159750 | 0.827778 | <u>11.00000</u> | -1.20000 | |
| 60 | AFIX | 0 | | | | | | |
| 61 | | | | | | | | |
| 62 | C5 | 1 | 0.317846 | 0.844877 | 0.701358 | <u>11.00000</u> | 0.00643 | 0.01030 = |
| 63 | AFIX | 1 | | | | | | |
| 64 | H5 | 2 | | | | | | |
| 65 | AFIX | 1 | | | | | | |
| 66 | C6 | 1 | | | | | | |
| 67 | | | | | | | | |
| 68 | AFIX | 2 | | | | | | |
| 69 | H6A | 2 | | | | | | |
| 70 | H6B | 2 | | | | | | |
| 71 | AFIX | 1 | | | | | | |
| 72 | RESI | 2 | | | | | | |
| 73 | O1 | 3 | | | | | | |
| 74 | O2 | 3 | | | | | | |
| 75 | | | | | | | | |
| 76 | | | | | | | | |
| 77 | AFIX | 14 | | | | | | |
| 78 | H2 | 2 | | | | | | |
| 79 | AFIX | 1 | | | | | | |
| 80 | O3 | 3 | | | | | | |
| 81 | | | | | | | | |
| 82 | | | | | | | | |
| 83 | AFIX | 14 | | | | | | |
| 84 | H3 | 2 | | | | | | |

Context Menu

- Undo
- Redo
- Cut
- Copy
- Paste
- Delete
- Select All Ctrl+A
- locate C5 in structure
- select atoms in structure found in selected text

LIST FILE: vitc.lst Rename Mode





The Editor



'solve in P2(1)'@ vitc.res

Select Part <Select residues> ▾ Line: 26 | Col: 56

```
19 acta
20 REM 2
21 REM 1
22 WGT 0.043700 0.023800
23 EXTI 0.000000
24 FVAR 0.52928
25 RESI 1 VIT
26 O1 3 0.790520 0.992667 1.011212 11.00000 0.00608 0.01641 =
27 0.00796 0.00110 0.0002 -0.00048
28 O3 RESI class[ ] number[0] alias 1.06574 11.00000 0.00883 0.01580 =
29 0.00555 0.00072 0.0224 -0.00141
30 AFIX 148
31 H2 2 0.471465 1.038523 1.096701 11.00000 -1.50000
32 AFIX 0
33 O3 3 0.057179 1.012358 0.907562 11.00000 0.00525 0.02289 =
34 0.00852 -0.00002 0.00138 0.00110
35 AFIX 148
36 H3 2 0.009578 1.020730 0.950040 11.00000 -1.50000
37 AFIX 0
38 O4 3 0.602149 0.998268 0.888272 11.00000 0.00568 0.01293 =
39 0.00593 -0.00095 0.00133 -0.00083
40 O5 3 0.326422 0.637594 0.826569 11.00000 0.00856 0.01044 =
41 0.00945 0.00171 0.00095 -0.00132
```

Search and Replace

11.00000 Select whole lines

'solve in P2(1)'@ vitc.res LIST FILE: vitc.lst Rename Mode

Search and Replace

- Regular Expressions
- Highlighting of Hits
- [Ctrl+F] or [F3]

Tooltip on mouse over





The Editor

'solve in P2(1)'@ vitc.res

Select Part <Select residues> Line: 43 | Col: 50

| | | | | | | | |
|----|------|-----|----------|----------|----------|-----------|----------|
| 31 | H2 | 2 | 0.471465 | 1.038523 | 1.096701 | 11.00000 | -1.50000 |
| 32 | AFIX | 0 | | | | | |
| 33 | O3 | 3 | 0.057179 | 1.012358 | 0.907562 | 11.00000 | 0.00525 |
| 34 | | | 0.00852 | -0.00002 | 0.00138 | 0.00110 | |
| 35 | AFIX | 148 | | | | | |
| 36 | H3 | 2 | 0.009578 | 1.020730 | 0.950040 | 11.00000 | -1.50000 |
| 37 | AFIX | 0 | | | | | |
| 38 | O4 | 3 | 0.602149 | 0.998268 | 0.888272 | 11.00000 | 0.00568 |
| 39 | | | 0.00593 | -0.00095 | 0.00133 | -0.00083 | |
| 40 | O5 | 3 | 0.326422 | 0.637594 | 0.826569 | 11.00000 | 0.00856 |
| 41 | | | 0.00945 | 0.00171 | 0.00095 | -0.00132 | |
| 42 | AFIX | 148 | | | | | |
| 43 | H5A | 2 | 0.210342 | 0.601967 | 0.832382 | -21.00000 | -1.50000 |
| 44 | AFIX | 0 | | | | | |
| 45 | O6 | 2 | 0.420495 | 1.020174 | 0.694979 | 11.00000 | 0.00949 |
| 46 | | | | | | | 0.01451 |
| 47 | AF | | | | | | |
| 48 | H6 | | | | | | |
| 49 | AF | | | | | | |
| 50 | C1 | | | | | | |
| 51 | | | | | | | |
| 52 | C2 | | | | | | |
| 53 | | | | | | | |
| 54 | C3 | | | | | | |
| 55 | | | | | | | |
| 56 | C4 | | | | | | |
| 57 | | | | | | | |
| 58 | AFLA | 13 | | | | | |
| 59 | H4 | 2 | 0.360122 | 1.159750 | 0.827778 | 11.00000 | -1.20000 |
| 60 | AFIX | 0 | | | | | |
| 61 | | | | | | | |

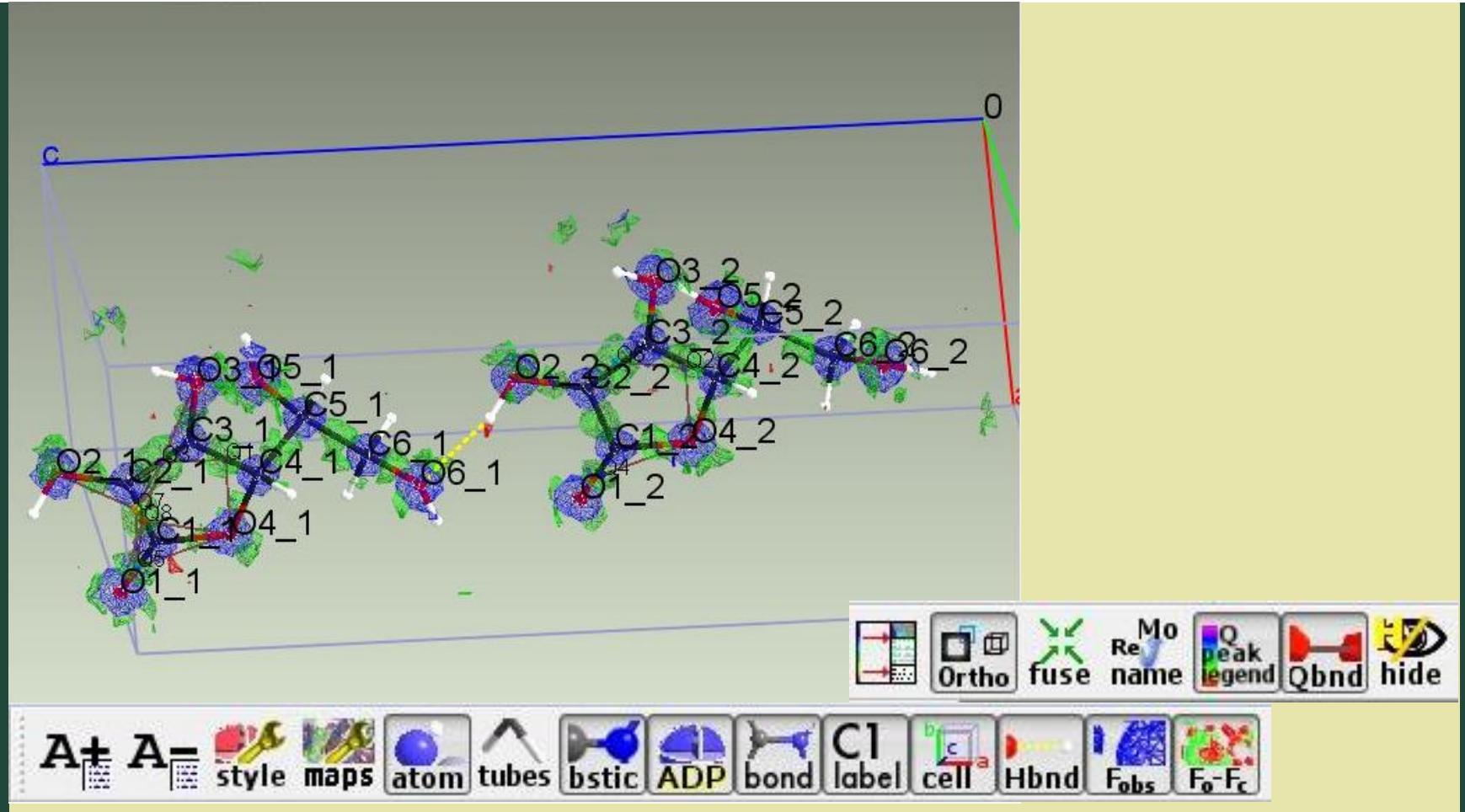
Error in line 43!
Free Variable 2 is not
defined yet!

'solve in P2(1)'@ vitc.res LIST FILE: vitc.lst Rename Mode

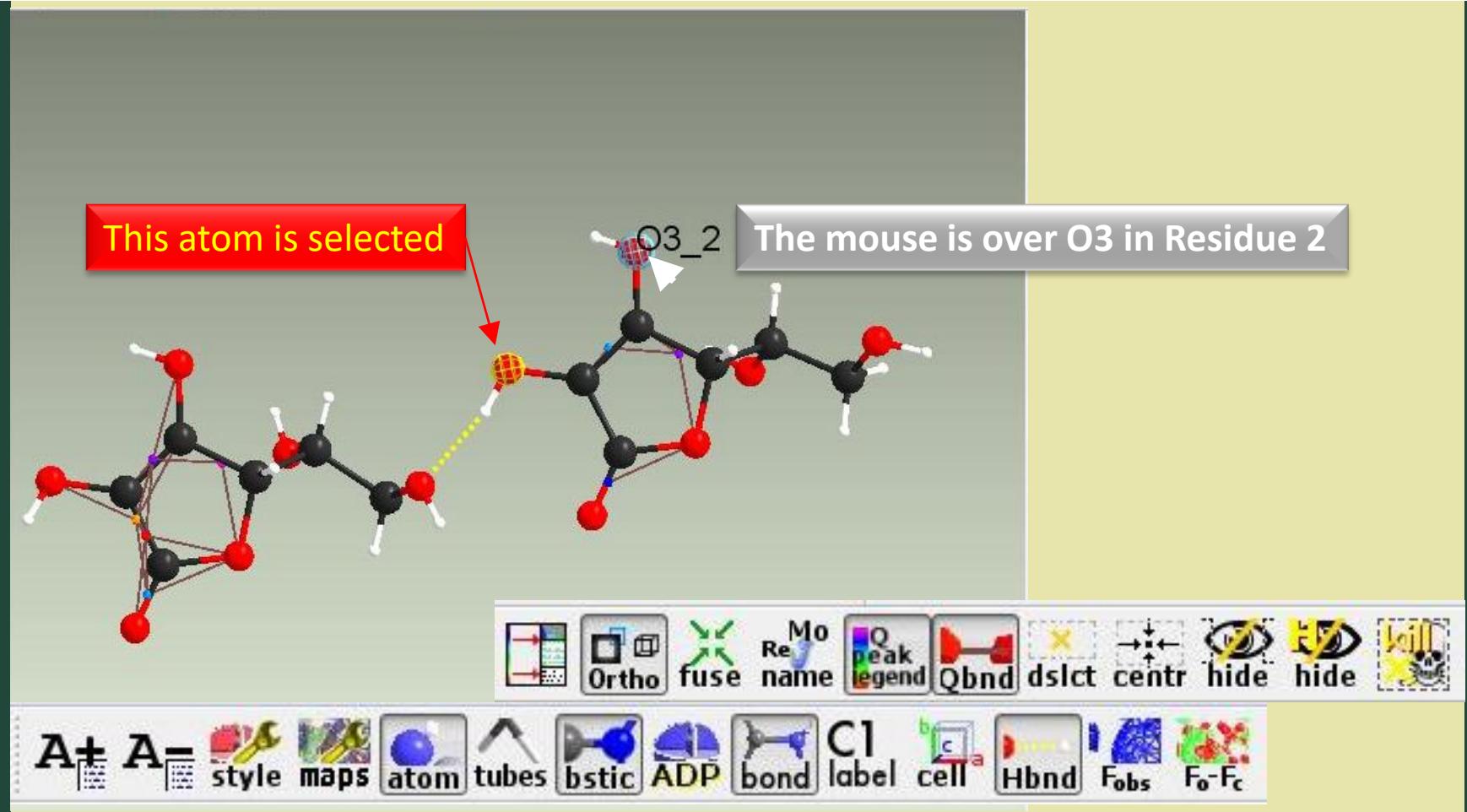
Tooltip on mouse over



The OpenGL View



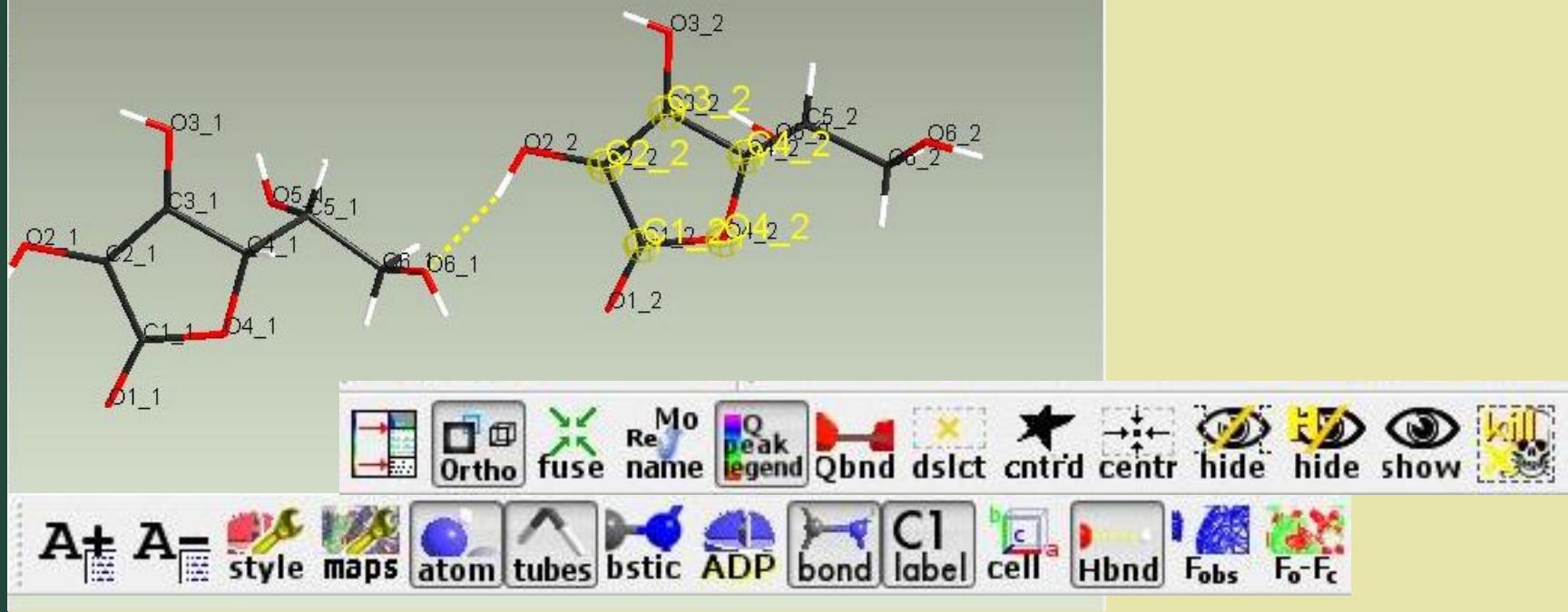
The OpenGL View





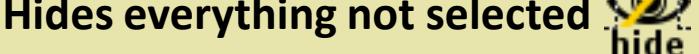
The OpenGL View

Select multiple atoms by pressing [Ctrl]+left click





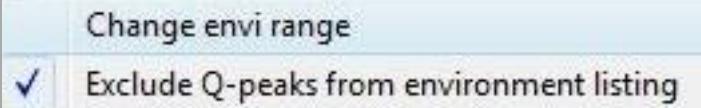
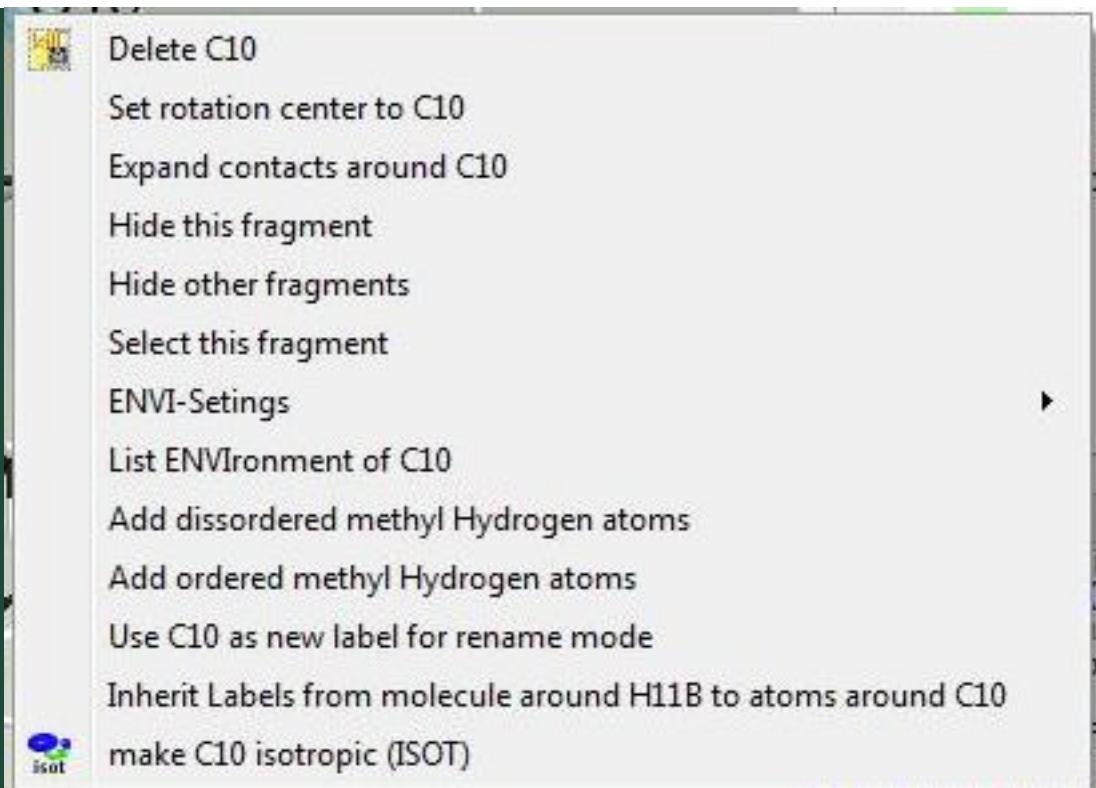
The Selection Tool Bar

-  Hides Information Window, Refinement History and Editor
-  Shows molecular graphics with central or orthographic Projection
Ortho
-  Completes molecules in the asymmetric unit
grow
-  Shows the asymmetric unit only
fuse
-  Enters/Exit Rename Mode
Mo
Re
name
-  Shows/Hide Q-Peak Legend
Q
peak
legend
-  Draws lines between Q-Peaks
Qbnd
-  Connects the two selected atoms
bind
-  Disconnects the two selected atoms
free
-  Deselects the selected atoms
dslect
-  Adds a Centroid Dummy atom
cntrd
-  Sets rotation center to selected atom(s)
-  Hides everything not selected
-  Hides H-atoms
-  Indicates hidden objects
-  Hides PART -N Ghosts
-  Highlights atoms in Parts
-  Kills selected atoms [Ctrl]+[Del]





Context Menu by right click on atom





Electron-Density Maps

Defines how dense the lines are drawn (critical for speed)

[Ctrl]+ Mouse wheel changes $F_{\text{O}} - F_{\text{c}}$

[Shift]+ Mouse wheel changes F_{obs}

Blue mesh: Observed data with model phases

Red and green Mesh: Observed data minus model green+ red-

Map Control settings:

- Map precision: 2,00
- Factor to downweight weak data: 1,00
- Fo-Fc map: 0,24e/A³
- F-observed map: 2,47e/A³
- Map radius: 5,00A
- Map truncation type: 1,41A around visible atoms or peaks
one complete unit cell
sphere around rotation center
1,41A around visible atoms or peaks
- Line transparency: 0,50
- Line width: 1,40
- Undistorted transparency:
- Lighting:
- Filled map surface:

Calculate Maps

shelXle - A Qt GUI for SHELXL (Rev: 475): vtc.res

File Edit Settings View Pack SHELX Extra Help

XL XE refine refine style maps atom tubes bistic ADP bond C1 label cell Hbnd Fobs F_O-F_C

Ortho fuse Re peak name Qbnd hide show

Q... x

'solve in P2(1)'@ vtc.res Line: 98 | Col: 1

| | | | | | | | | | |
|-----|------|-----|----------|----------|----------|----------|----------|-----------|--|
| 90 | AFIX | 148 | 2 | 0.097417 | 0.60230 | 0.371057 | 11.00000 | -1.50000 | |
| 91 | H5A | 2 | 0.097417 | 0.60230 | 0.371057 | 11.00000 | 0.00579 | 0.01626 = | |
| 92 | AFIX | 0 | | | | | 0.392704 | 11.00000 | |
| 93 | 06 | 3 | 0.087088 | 1.01490 | 0.182079 | 11.00000 | 0.01101 | 0.01114 = | |
| 94 | | | | 0.00807 | 0.00311 | 0.00478 | 0.332545 | 11.00000 | |
| 95 | AFIX | 148 | 2 | 0.126551 | 0.047340 | 0.133949 | 11.00000 | -1.50000 | |
| 96 | H6 | 1 | 0.364245 | 0.004884 | 0.472483 | 11.00000 | 0.00578 | 0.01880 = | |
| 97 | AFIX | 0 | | 0.00662 | -0.00060 | 0.00119 | -0.00048 | 11.00000 | |
| 98 | C1 | 1 | 0.154550 | 0.999069 | 0.494835 | 11.00000 | 0.00582 | 0.00991 = | |
| 99 | C2 | 1 | 0.00592 | 0.00022 | 0.00173 | 0.00011 | 11.00000 | | |
| 100 | | | | | | | 0.00578 | 0.01058 = | |
| 101 | C3 | 1 | 0.01253 | 1.001854 | 0.427053 | 11.00000 | | | |
| 102 | | | | 0.00634 | -0.00034 | 0.01140 | 0.00068 | | |
| 103 | | | | | | | | | |



Customization

- Tool bars can be moved to different places



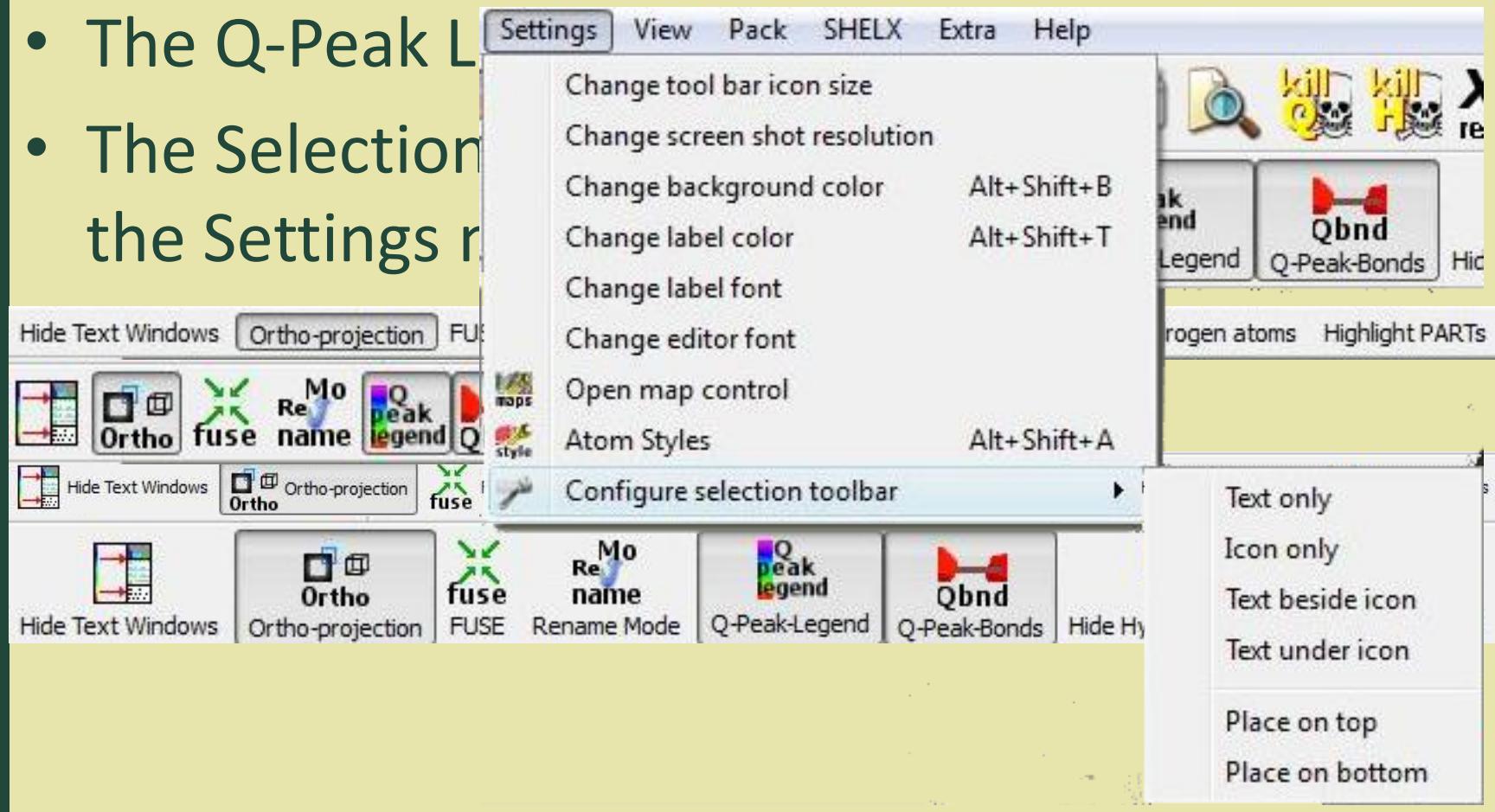
Grab here with the mouse and drag around.

- Sub windows can be detached and moved to different places. If a sub window is moved over a existing one the windows get stacked and a tab appears to bring one of them in front.



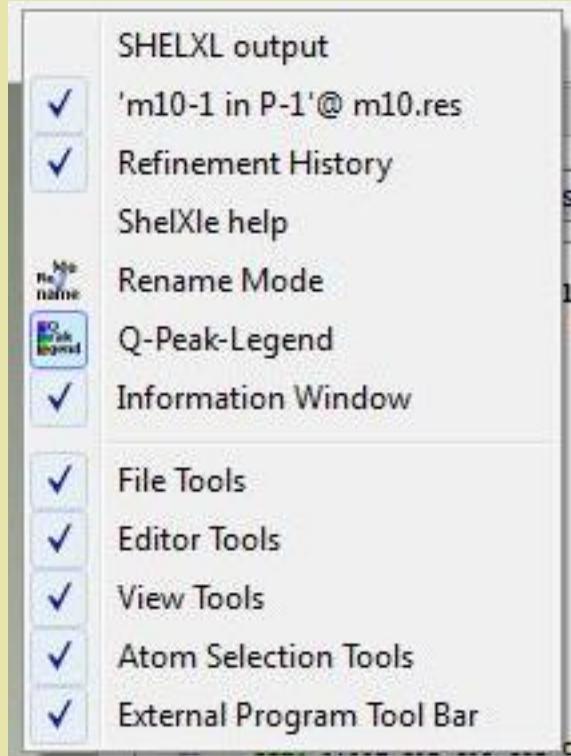
Customization

- The Q-Peak Legend
- The Selection toolbar
the Settings menu





Customization

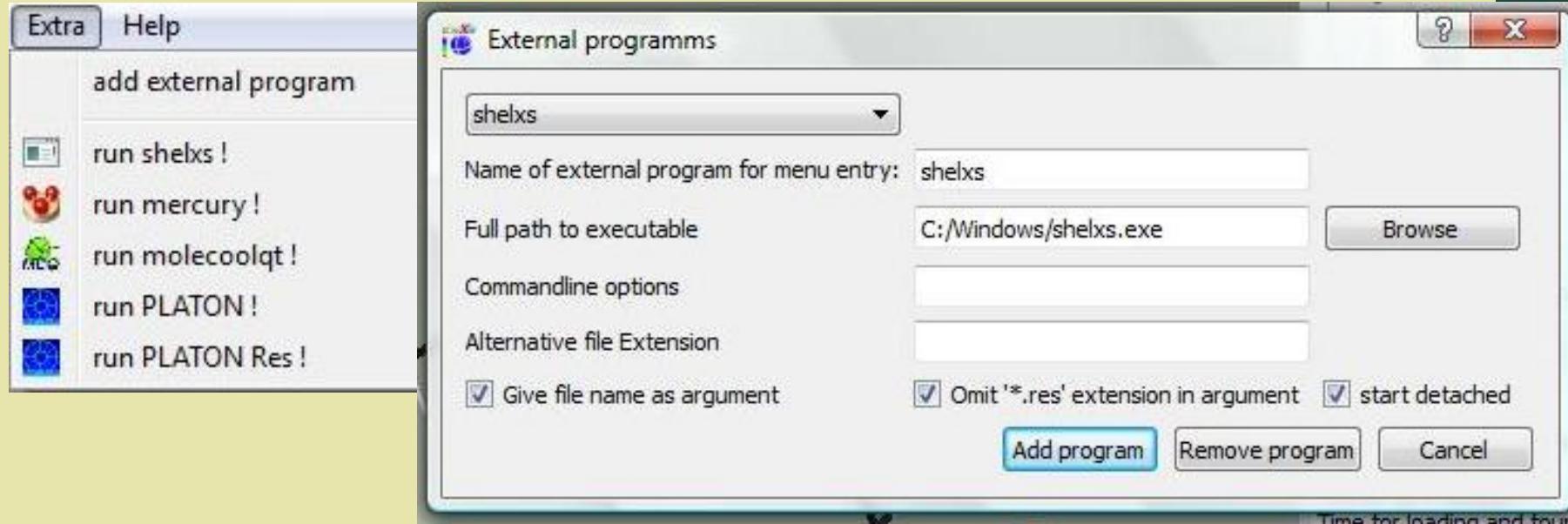


**Right clicking on the menu or any tool bar shows this menu. Here any hidden tool bar or window can be recovered.
When Rename Mode is visible you are in Rename Mode and vice versa.**





Customization - External Programs

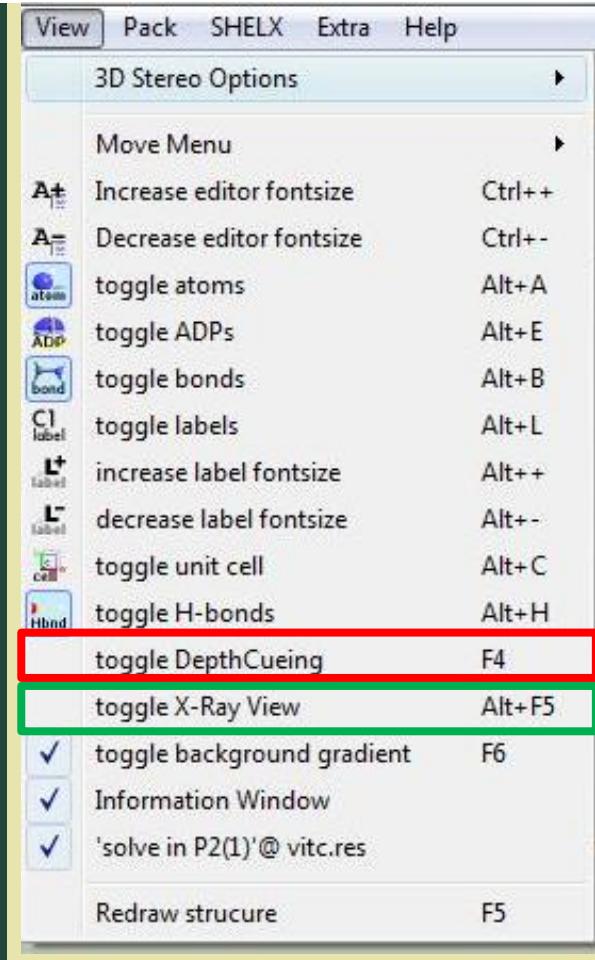


**Detached program run independently from ShelXle
for others a dialog box with output is provided.**





Customizing – View Menu



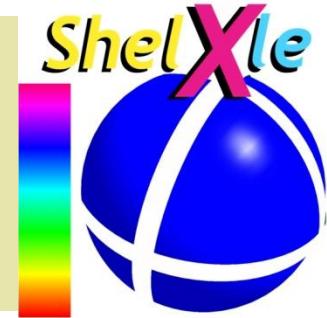
Toggles fog. Fog density by
[Alt + Mouse wheel]

Cuts out a wedge from the front side of the
OpenGL View so that the inside of a
complicated structure becomes visible
(currently only with central perspective)





Atom-Styles Dialog

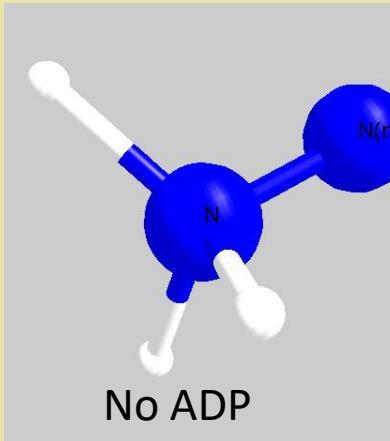
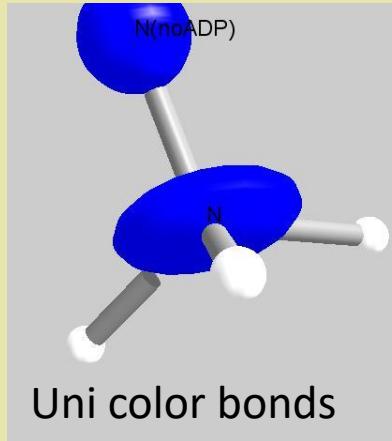
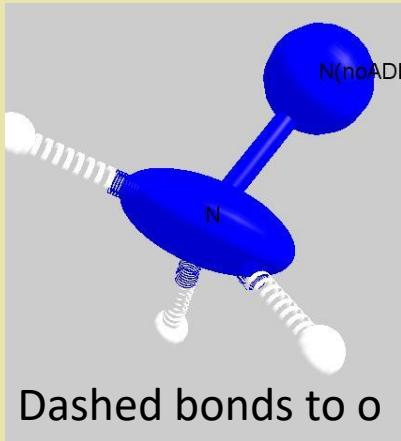
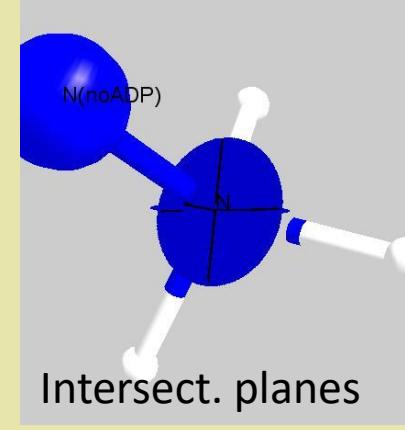
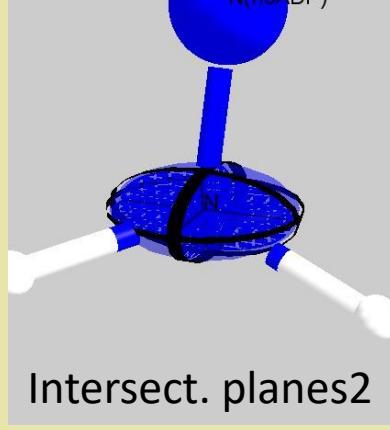
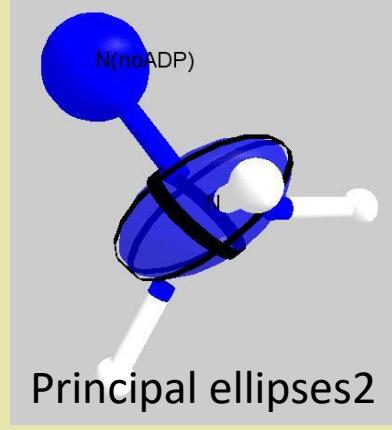
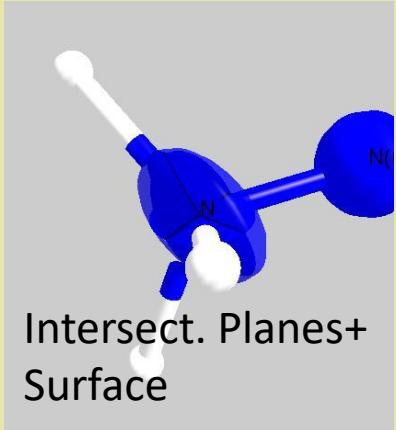


The screenshot shows a software interface titled "Edit Atom Parameters". On the left, there is a 3D visualization of a molecule consisting of blue spheres representing atoms and white lines representing bonds. The molecule has a complex, branched structure. To the right of the visualization are several control panels:

- global style**: A dropdown menu set to "50 % Probability".
 - uni colored bonds
- Bond Color**: A color bar with a slider at 0,06 and controls for "Bond strength" (up/down arrows) and "Level of detail" (up/down arrows).
- Atom Color**: A color bar with a slider at 0,30 and controls for "Sphere radius" (up/down arrows), "Covalent radius" (up/down arrows), and a button for "Style multiple Elements".
- Element Periodic Table**: A grid of elements from Hydrogen (H) to Helium (He). Elements are color-coded by group: Alkali metals (Li, Na, K, Rb, Cs, Fr) are pink; Alkaline earth metals (Be, Mg, Ca, Sr, Ba, Ra) are light blue; Transition metals (Sc, Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Zn, Y, Zr, Nb, Mo, Tc, Ru, Rh, Pd, Ag, Cd, Hf, Ta, W, Re, Os, Ir, Pt, Au, Hg, Ku, Ha, Rf, Ns) are orange/yellow; Post-transition metals (B, C, N, O, F, Ne, Al, Si, P, S, Cl, Ar, Ge, As, Se, Br, Kr, In, Sn, Sb, Te, I, Xe, Pb, Bi, Po, At, Rn) are green/blue/purple.
- Modeling Options**: A row of checkboxes:
 - Draw intersecting planes
 - Draw principal ellipses
 - Draw ellipsoid surface
 - Solid ellipsoid
 - No label!
 - No ADP
 - Dashed Bonds to others
- Import/Export Buttons**: Buttons for "Import atom styles" and "Export atom styles".



Atom-Styles Dialog



Play around with
Checkboxes to
figure out what
you like best!



Rename Mode

Rename Mode

You are in 'rename mode' now.
Next Label is:

C1

Automatically jump to first unused label

Part: 0 Residue Nr: 0 Residue Class:

Scattering factors
 any H C O

[more scattering factors](#)

Number Suffix

'solve in P2(1)'@ vitc.res LIST FILE: vitc.lst Rename Mode

Rename Mode

You are in 'rename mode' now.
Next Label is:

H1, C1 or O1

Automatically jump to first unused label

Part: 0 Residue Nr: 0 Residue Class:

Scattering factors
 any H C O

[more scattering factors](#)

Number Suffix

'solve in P2(1)'@ vitc.res LIST FILE: vitc.lst Rename Mode





Rename Mode

Rename Mode

You are in 'rename mode' now.
Next Label is:

C7

Automatically jump to first unused label

Part: 0 Residue Nr: 1 Residue Class: VIT

Scattering factors
 any H C O

more scattering factors

Number 7 Suffix

'solve in P2(1)'@ vitc.res LIST FILE: vitc.lst Rename Mode

Rename Mode

You are in 'rename mode' now.
Next Label is:

C7

Automatically jump to first unused label

Part: 1 Residue Nr: 2 Residue Class: VIT

Tie occupation to: **its fixed value**
its fixed value
fv(n)
1-fv(n)

Scattering factors
 any H C O

more scattering factors

Number 7 Suffix

'solve in P2(1)'@ vitc.res LIST FILE: vitc.lst Rename Mode





Rename Mode

Rename Mode

You are in 'rename mode' now.
Next Label is:

C7

Automatically jump to first unused label

Part: 1 Residue Nr: 2 Residue Class: VIT

Tie occupation to: fv(n) n = 2 fv(2)=0.02941 [1x used]

Scattering factors
 any H C O

more scattering factors

Number 7 Suffix

'solve in P2(1)'@ vitz.res LIST FILE: vitz.lst Rename Mode

Residue Class can only be edited if ResiNr is not yet in use.

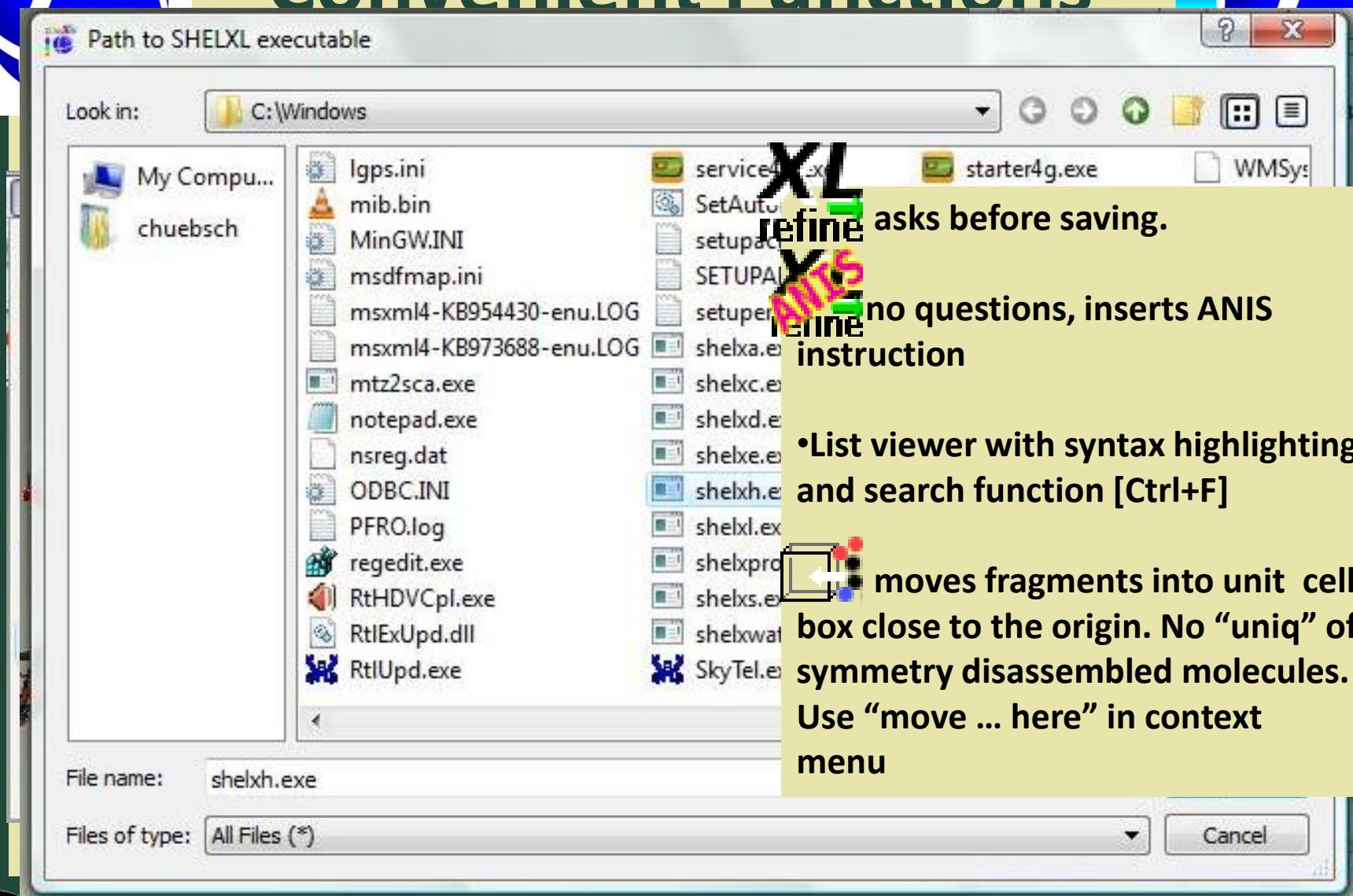
n can vary from 2 to N+1. With N the number of existing Free Variables. If there is one unused in between n can also not be greater.

If the Label number is -1 no Number is used in the Label.

If Scattering factor is “any” then no check of usage of that Label can be done.



Convenient Functions

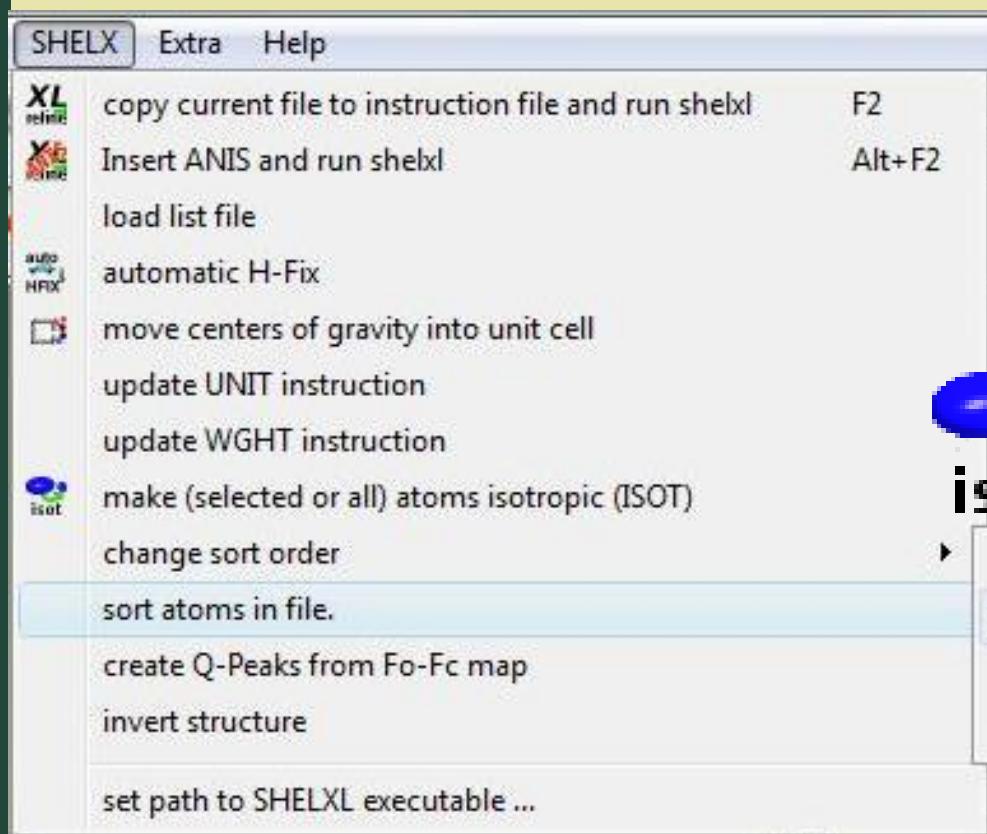


- List viewer with syntax highlighting and search function [Ctrl+F]

 moves fragments into unit cell box close to the origin. No “uniq” of symmetry disassembled molecules. Use “move ... here” in context menu



Convenient Functions



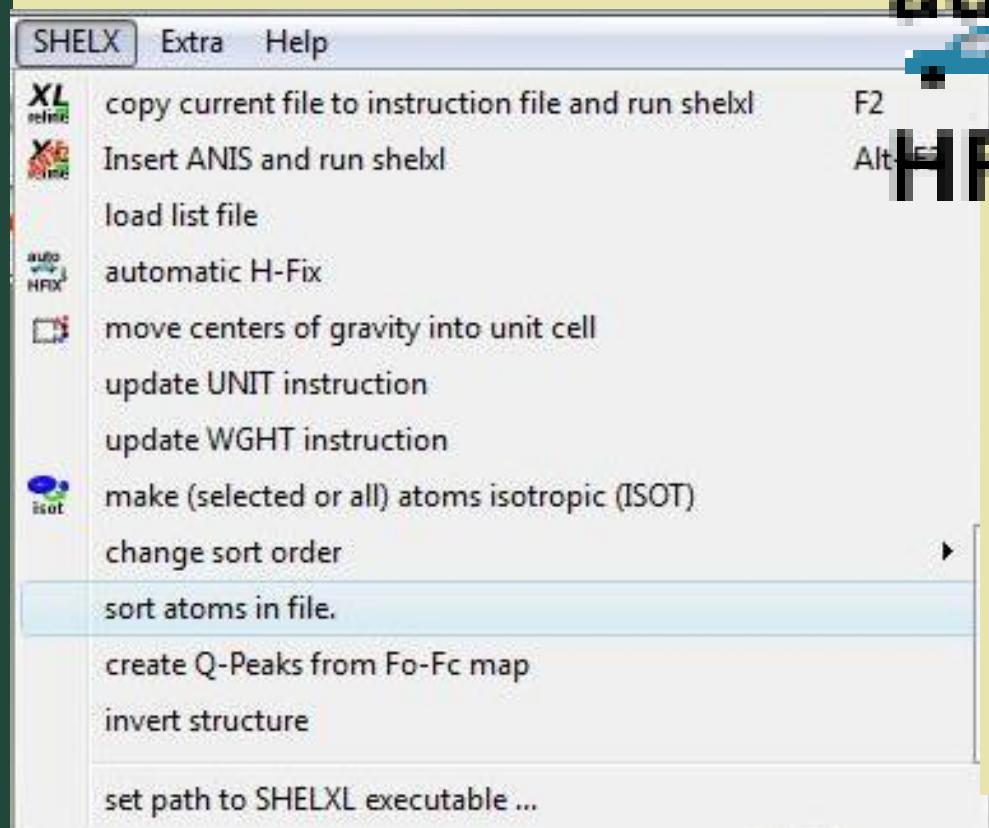
isot is only present when atoms with refined U_{ij} s are present.

“create Q-Peaks from Fo-Fc map” is useful if density close to existing atoms is present.





Convenient Functions

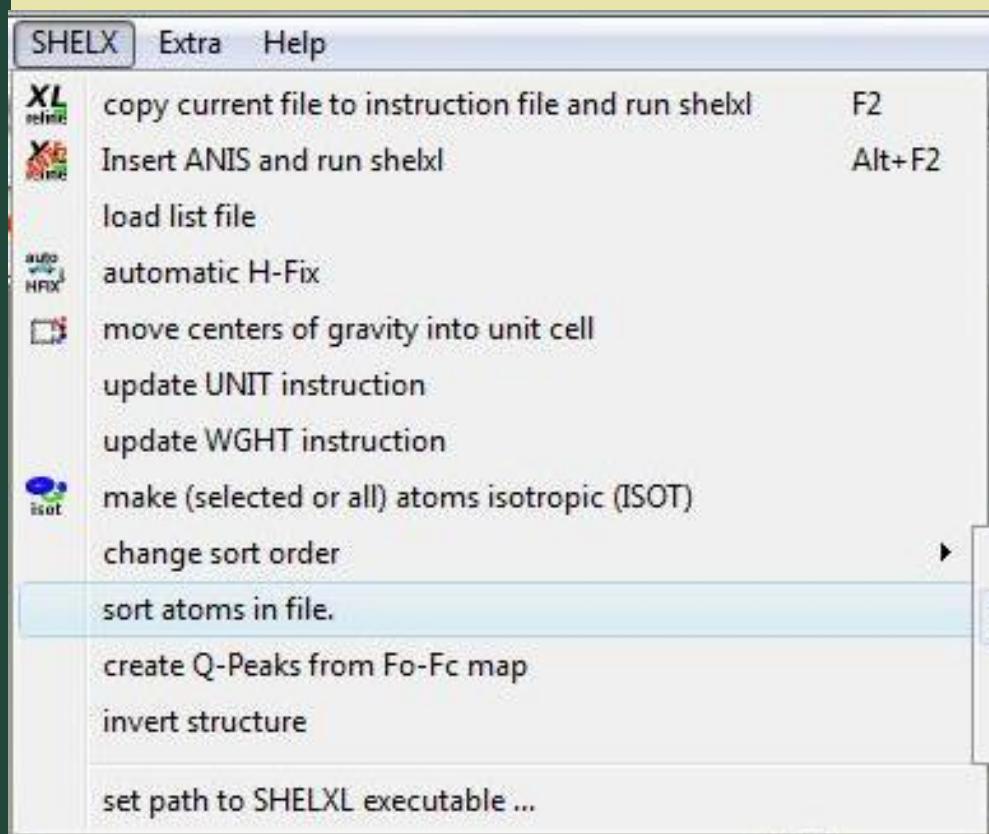


adds H-atoms including corresponding AFIX instructions. If electron-density maps are calculated the position of methyl H-atoms is optimized and hydrogens in O-H...contacts (excluding water) are generated. Increasing map precision might help. Repeated usage might find more H's
Only available on freshly loaded or saved files!





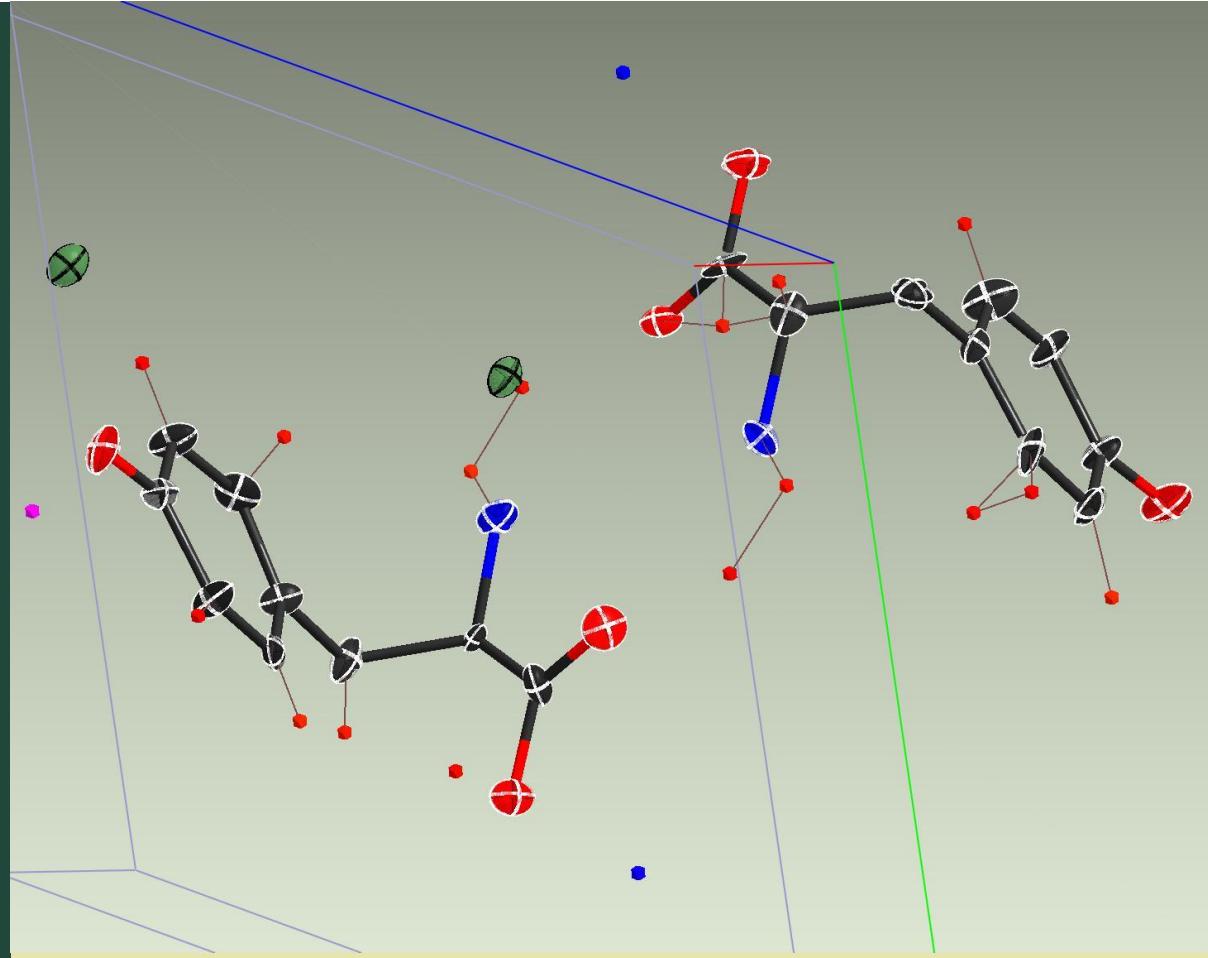
Convenient Functions



Inverting structure changes the space group if enantiomorphous. Origin is moved if necessary but move in cell might then be necessary
Use before and after!

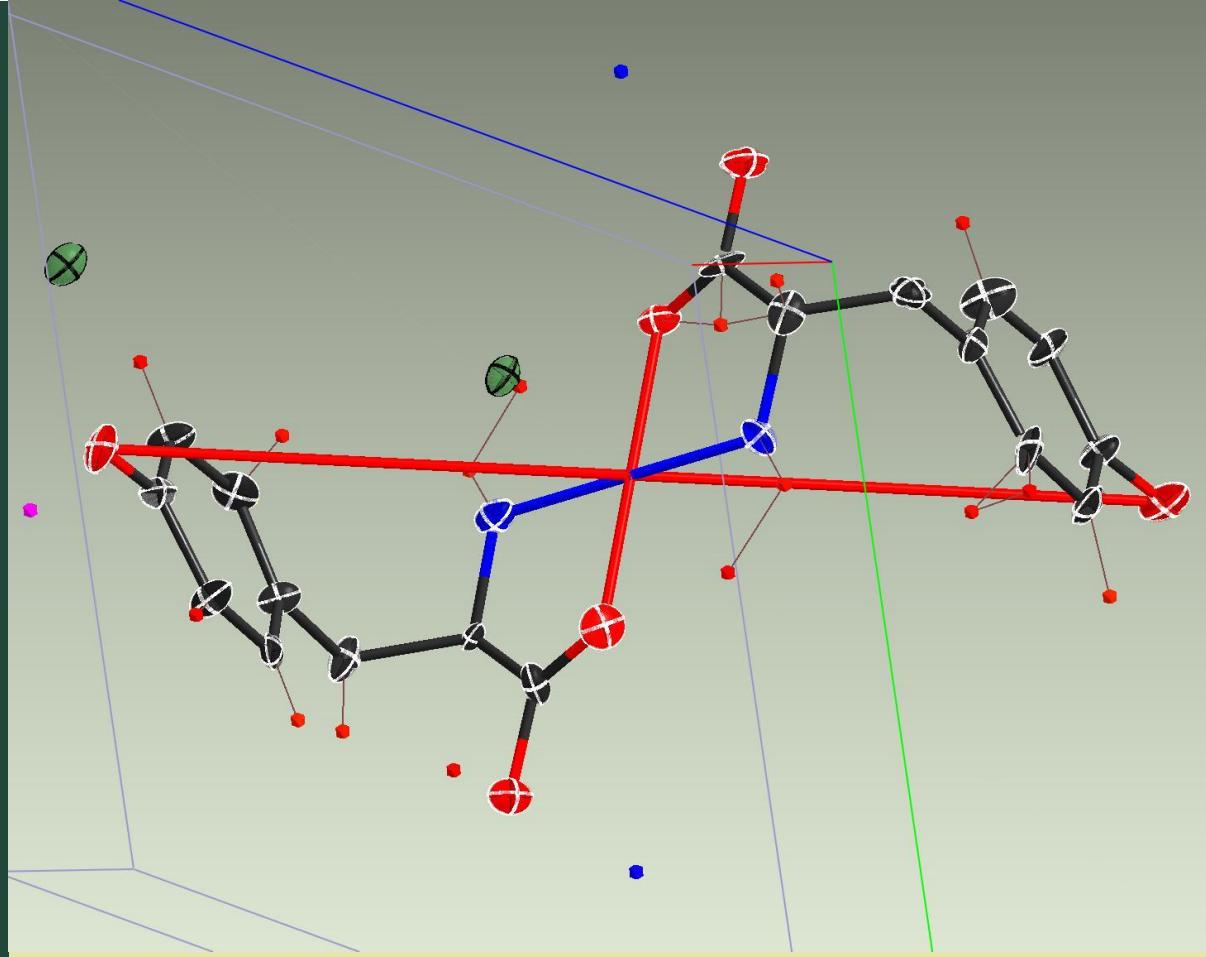
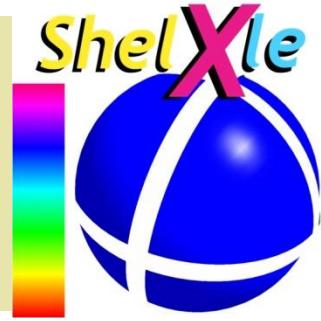


Example: Solved Structure in P1 which is P-1



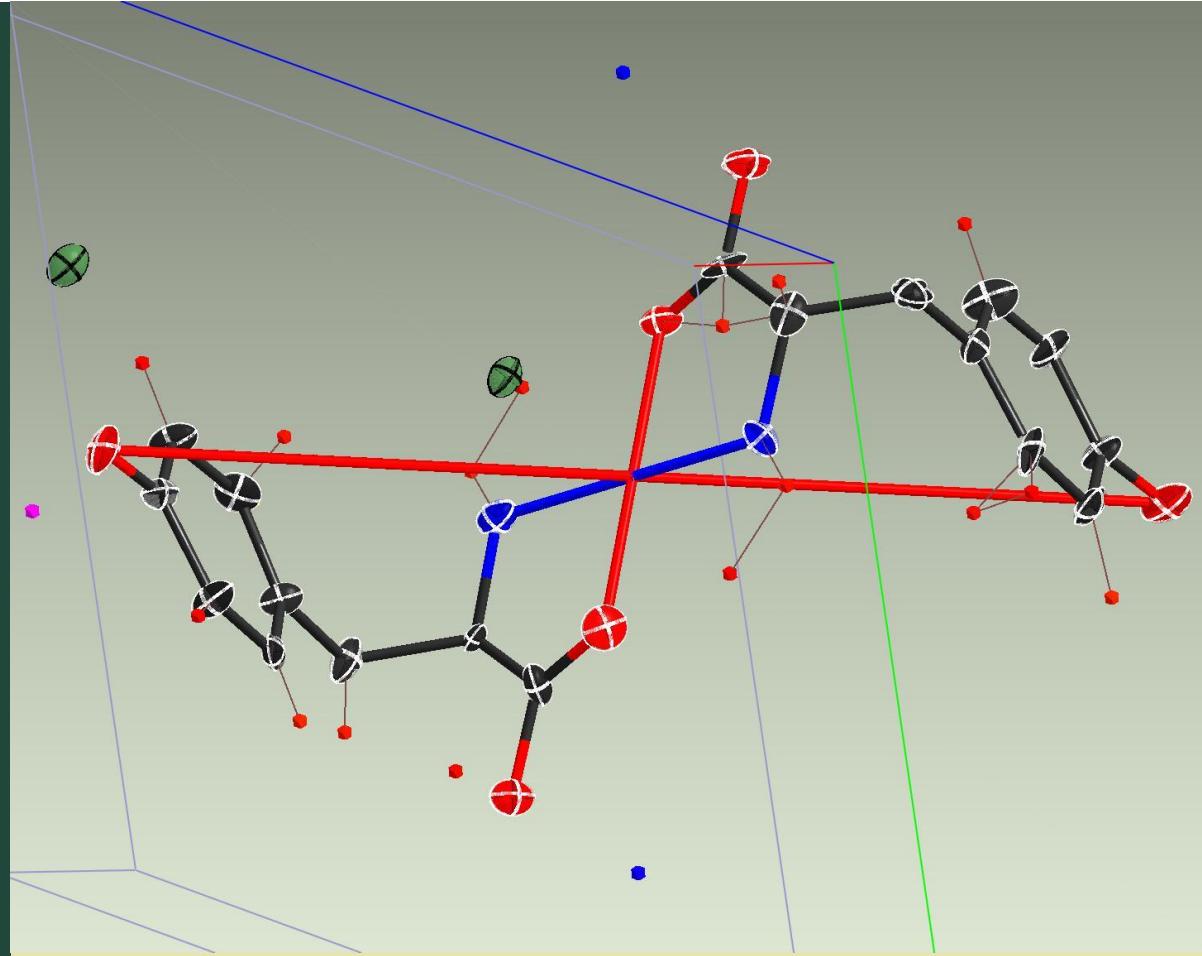
1. Select pairs of chemical identical atoms and click on  bind

Example: Solved Structure in P1 which is P-1



1. Select pairs of chemical identical atoms and click on  bind
2. If the bonds cross each other in one point then structure is P-1!

Example: Solved Structure in P1 which is P-1



1. Select pairs of chemical identical atoms and click on  bind
2. If the bonds cross each other in one point then structure is P-1!
3. Select all or at least one pair of chemical identical atoms and click on  cntrd



Example: Solved Structure in P1 which is P-1



```
72 Cnt1 6 1.130679 0.261422 0.095238 10.000 0.001 ! centroid
73 REM Cnt1 was created from: C1, C2, C3, C4, C5, C6, C7, C8, C9, C10, C11, C12,
74 REM C13, C14, C15, C16, C17, C18, O19, O20, O21, O22,
75 REM O23, O24, N25, N26,
76 FREE Cnt1 C1 ! this might be needed for AFIX
77 FREE Cnt1 C2 ! this might be needed for AFIX
78 FREE Cnt1 C3 ! this might be needed for AFIX
79 FREE Cnt1 C4 ! this might be needed for AFIX
80 FREE Cnt1 C5 ! this might be needed for AFIX
81 FREE Cnt1 C6 ! this might be needed for AFIX
82 FREE Cnt1 C7 ! this might be needed for AFIX
83 FREE Cnt1 C8 ! this might be needed for AFIX
84 FREE Cnt1 C9 ! this might be needed for AFIX
85 FREE Cnt1 C10 ! this might be needed for AFIX
86 FREE Cnt1 C11 ! this might be needed for AFIX
87 FREE Cnt1 C12 ! this might be needed for AFIX
88 FREE Cnt1 C13 ! this might be needed for AFIX
89 FREE Cnt1 C14 ! this might be needed for AFIX
90 FREE Cnt1 C15 ! this might be needed for AFIX
91 FREE Cnt1 C16 ! this might be needed for AFIX
92 FREE Cnt1 C17 ! this might be needed for AFIX
93 FREE Cnt1 C18 ! this might be needed for AFIX
94 FREE Cnt1 O19 ! this might be needed for AFIX
95 FREE Cnt1 O20 ! this might be needed for AFIX
96 FREE Cnt1 O21 ! this might be needed for AFIX
97 FREE Cnt1 O22 ! this might be needed for AFIX
98 FREE Cnt1 O23 ! this might be needed for AFIX
99 FREE Cnt1 O24 ! this might be needed for AFIX
100 FREE Cnt1 N25 ! this might be needed for AFIX
101 FREE Cnt1 N26 ! this might be needed for AFIX
102 HKLF 4
```

1. Select all or at least one pair of chemical identical atoms and click on **cntrd**

id dummy





Example: Solved Structure in P1 which is P-1

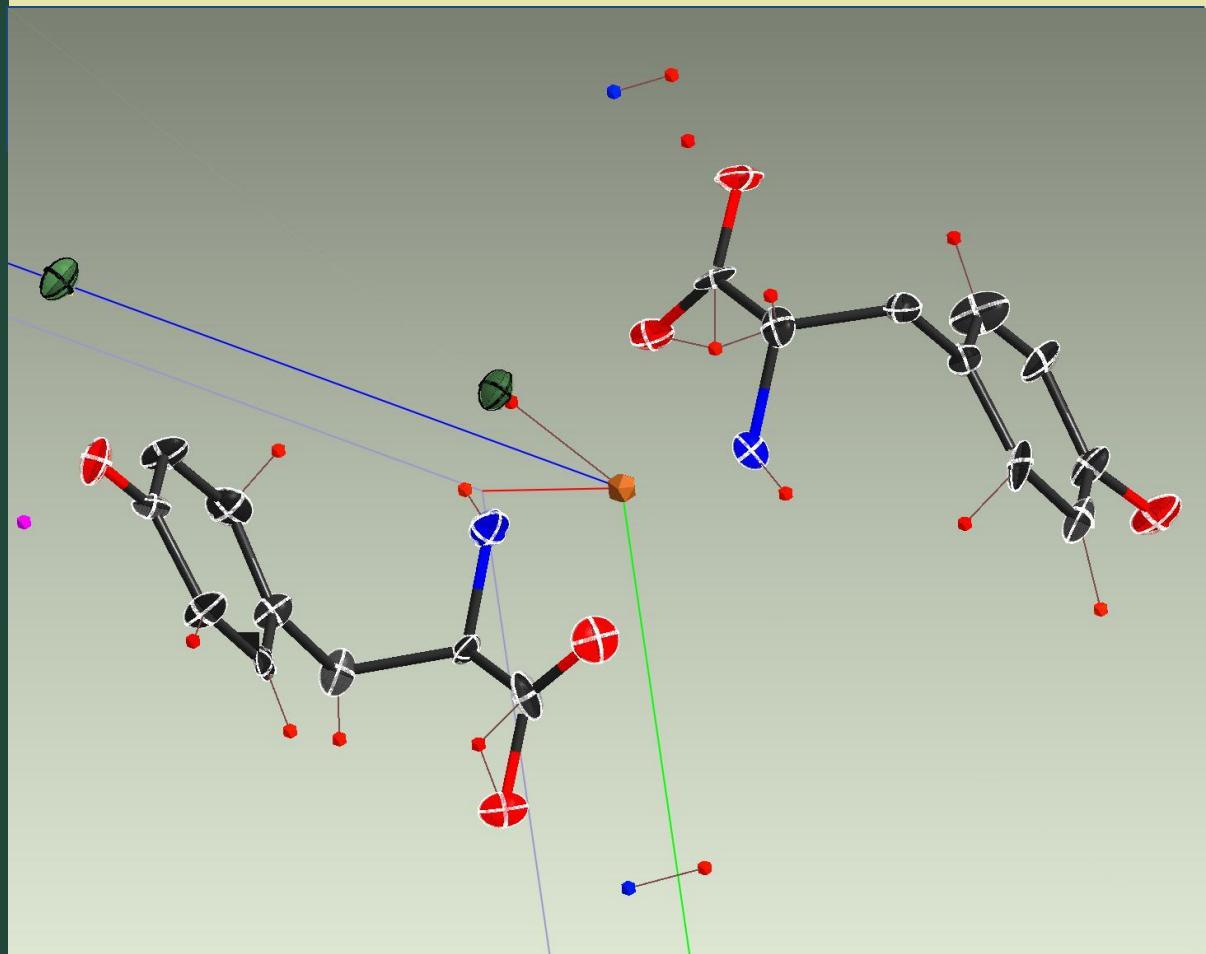


```
72 Cnt1 6 1.130679 0.261422 0.095238 10.000 0.001 ! centroid
73 REM Cnt1 was created from: C1, C2, C3, C4, C5, C6, C7, C8, C9, C10, C11, C12,
74 REM C13, C14, C15, C16, C17, C18, O19, O20, O21, O22,
75 REM O23 O24 N25 N26
14 WCHT 0.100000
15 FVAR 0.80940
16 MOVE -1.130679 -0.261422 -0.095238 1
17 C1 1 1.055496 0.039846 -0.494321 11.00000 0.01628 0.02566 =
18 0.02449 0.01886 0.01100 0.00772
81 FREE Cnt1 C6 ! this might be needed for AFIX
82 FREE Cnt1 C7 ! this might be needed for AFIX
83 FREE Cnt1 C8 ! this might be needed for AFIX
84 FREE Cnt1 C9 ! this might be needed for AFIX
85 FREE Cnt1 C10 ! this might be needed for AFIX
86 FREE Cnt1 C11 ! this might be needed for AFIX
87 FREE Cnt1 C12 ! this might be needed for AFIX
88 FREE Cnt1 C13 ! this might be needed for AFIX
89 FREE Cnt1 C14 ! this might be needed for AFIX
90 FREE Cnt1 C15 ! this might be needed for AFIX
91 FREE Cnt1 C16 ! this might be needed for AFIX
92 FREE Cnt1 C17 ! this might be needed for AFIX
93 FREE Cnt1 C18 ! this might be needed for AFIX
94 FREE Cnt1 O19 ! this might be needed for AFIX
95 FREE Cnt1 O20 ! this might be needed for AFIX
96 FREE Cnt1 O21 ! this might be needed for AFIX
97 FREE Cnt1 O22 ! this might be needed for AFIX
98 FREE Cnt1 O23 ! this might be needed for AFIX
99 FREE Cnt1 O24 ! this might be needed for AFIX
100 FREE Cnt1 N25 ! this might be needed for AFIX
101 FREE Cnt1 N26 ! this might be needed for AFIX
102 HKLF 4
```

1. Select all or at least one pair of chemical identical atoms and click on **cntFd**
2. Select coordinates of the Cnt1 and copy to clipboard
3. Type in MOVE and paste the coordinates
4. Change the sign of the coordinates and add 1

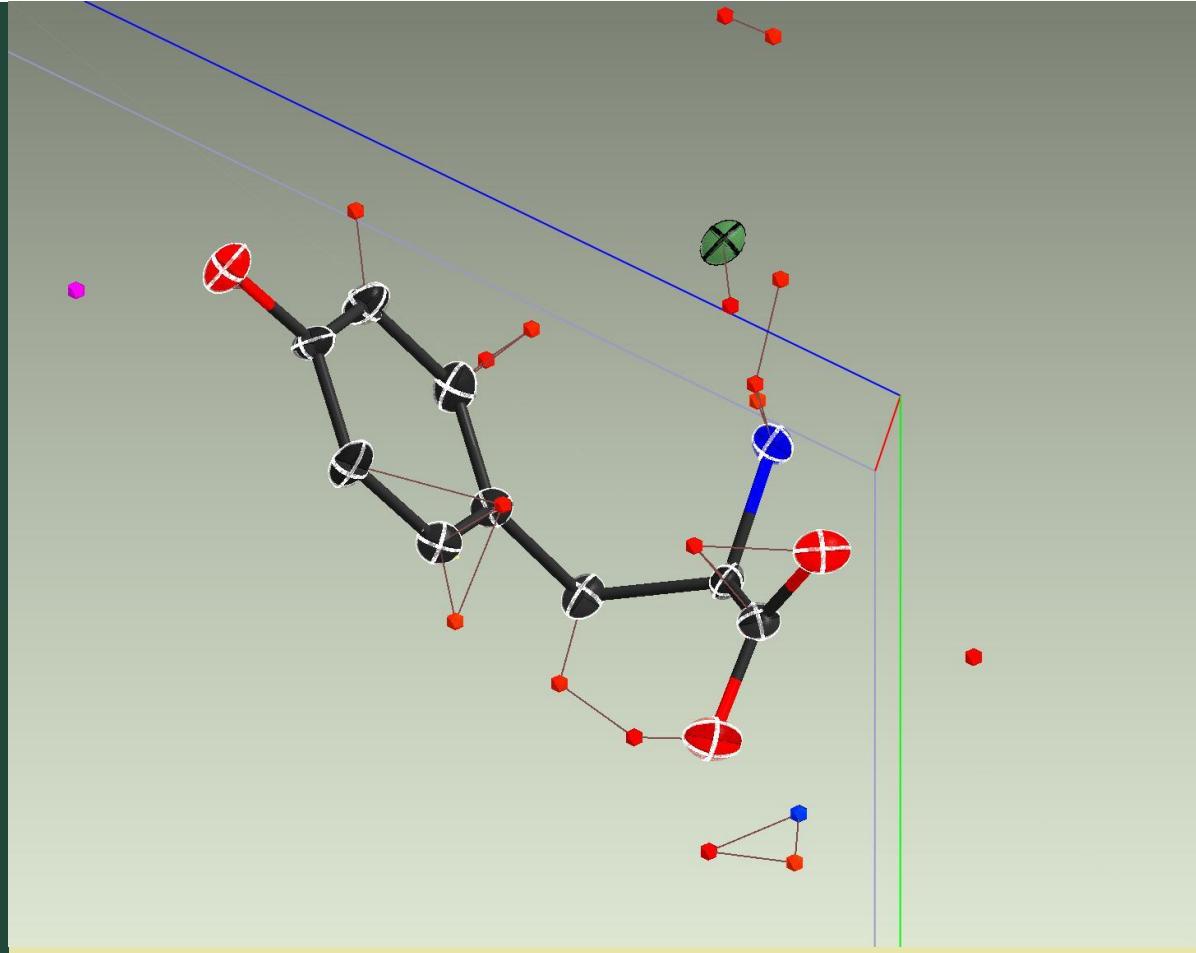


Example: Solved Structure in P1 which is P-1



1. Change the sign of the coordinates and add 1
2. Save and refine.
3. The Centroid dummy atom should no be at the origin.
4. Select the no longer needed fragment and delete them.
5. Delete the centroid dummy if you want
6. Change LATT -1 into LATT 1 and save + refine.

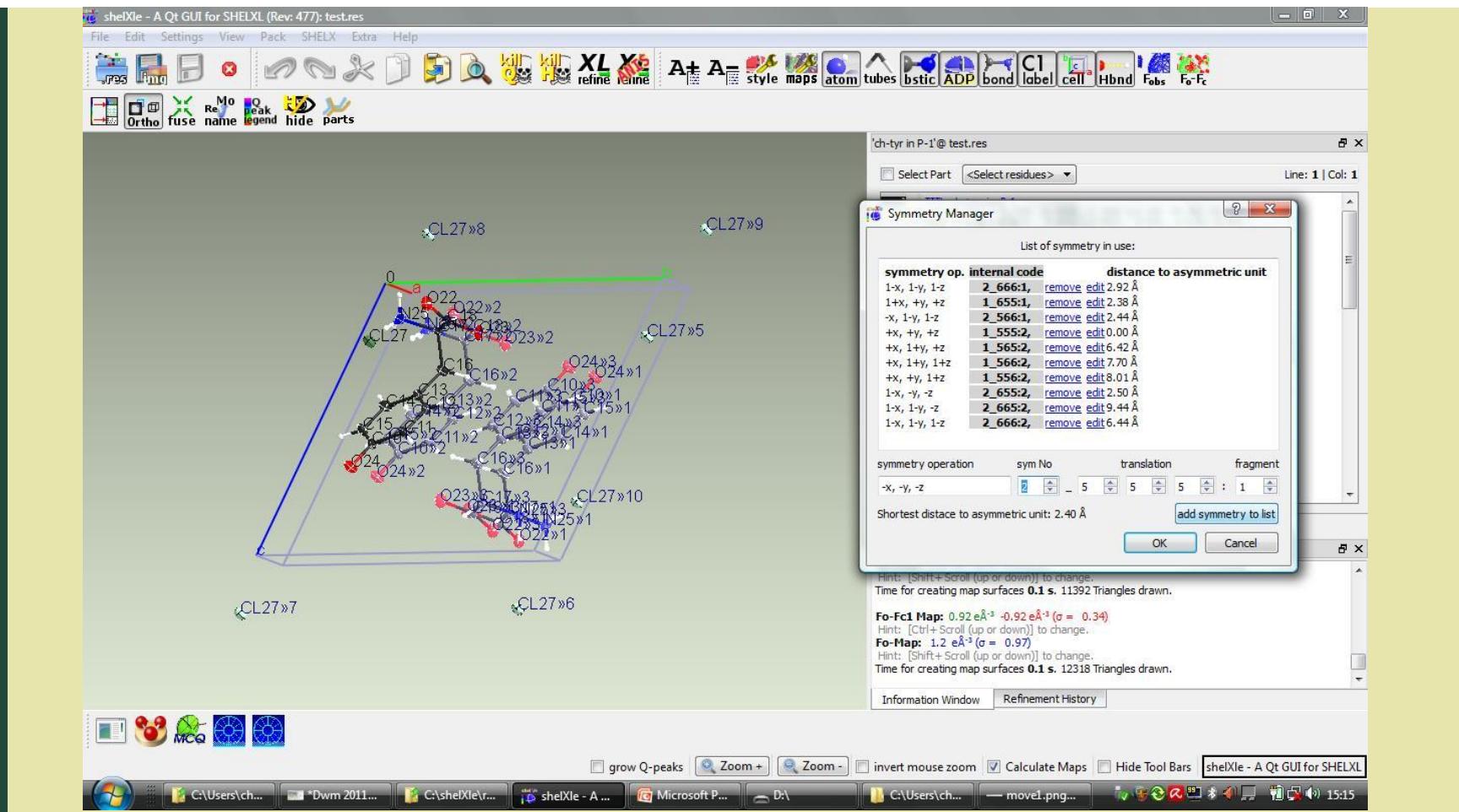
Example: Solved Structure in P1 which is P-1



1. Change the sign of the coordinates and add 1
2. Save and refine.
3. The Centroid dummy atom should no be at the origin.
4. Select the no longer needed fragment and delete them.
5. Delete the Centroid dummy if you want
6. Change LATT -1 into LATT 1 and save + refine.



Symmetry manager



GEORG-AUGUST-UNIVERSITÄT
GÖTTINGEN

J. Appl. Cryst., 44, (2011) 1281-1284



Symmetry manager

Symmetry Manager

List of symmetry in use:

| symmetry op. | internal code | distance to asymmetric unit |
|---------------|---|-----------------------------|
| 1-x, 1-y, 1-z | 2_666:1, remove edit 2.92 Å | |
| 1+x, +y, +z | 1_655:1, remove edit 2.38 Å | |
| -x, 1-y, 1-z | 2_566:1, remove edit 2.44 Å | |
| +x, +y, +z | 1_555:2, remove edit 0.00 Å | |
| +x, 1+y, +z | 1_565:2, remove edit 6.42 Å | |
| +x, 1+y, 1+z | 1_566:2, remove edit 7.70 Å | |
| +x, +y, 1+z | 1_556:2, remove edit 8.01 Å | |
| 1-x, -y, -z | 2_655:2, remove edit 2.50 Å | |
| 1-x, 1-y, -z | 2_665:2, remove edit 9.44 Å | |
| 1-x, 1-y, 1-z | 2_666:2, remove edit 6.44 Å | |

symmetry operation sym No translation fragment

-x, -y, -z 2 - 5 5 5 : 1

Shortest distance to asymmetric unit: 2.40 Å [add symmetry to list](#)

[OK](#) [Cancel](#)





ENVI

Information Window

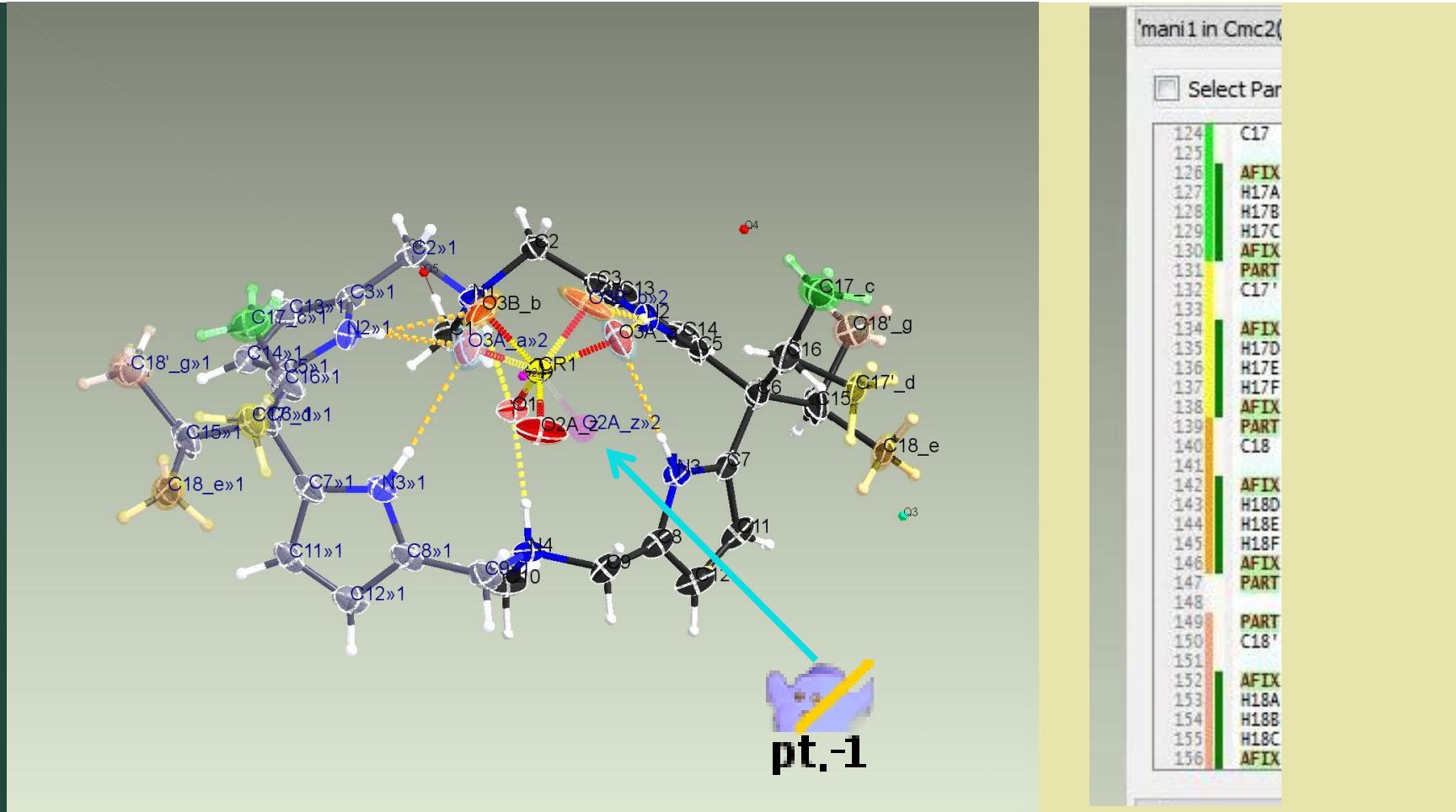
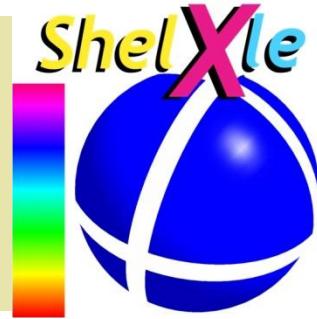
»3 : 1-x, -y, 1-z

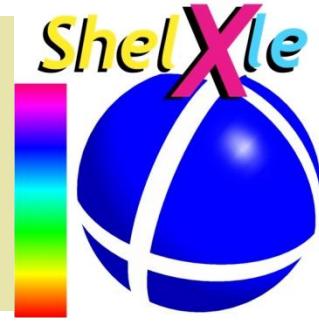
| Environment of C17 | | | | | | | | | | | | |
|--------------------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|
| H17 | 0.980 Å | | | | | | | | | | | |
| N25 | 1.492 Å | 111.18° | | | | | | | | | | |
| C18 | 1.509 Å | 107.46° | 108.09° | | | | | | | | | |
| C16 | 1.531 Å | 103.98° | 111.30° | 114.74° | | | | | | | | |
| H25b | 1.976 Å | 100.00° | 25.13° | 133.10° | 93.75° | | | | | | | |
| H25a | 1.976 Å | 95.03° | 25.13° | 96.31° | 135.74° | 43.16° | | | | | | |
| H25c | 1.976 Å | 136.05° | 25.13° | 92.87° | 101.84° | 43.16° | 43.16° | | | | | |
| H16b | 2.057 Å | 90.47° | 137.85° | 98.38° | 26.55° | 118.96° | 161.98° | 125.34° | | | | |
| H16a | 2.057 Å | 88.27° | 98.33° | 140.98° | 26.55° | 75.40° | 118.16° | 100.01° | 44.75° | | | |
| O23 | 2.378 Å | 92.88° | 138.96° | 31.04° | 93.28° | 163.39° | 125.65° | 120.49° | 71.01° | 115.75° | | |
| O22 | 2.390 Å | 116.00° | 82.58° | 25.65° | 129.41° | 107.69° | 71.76° | 70.02° | 120.83° | 153.80° | 56.69° | |
| C13 | 2.551 Å | 136.15° | 92.20° | 99.00° | 32.22° | 85.65° | 116.42° | 74.65° | 50.82° | 50.82° | 92.35° | 103.03° |
| O22»1 | 3.193 Å | 127.54° | 86.75° | 24.18° | 114.76° | 110.81° | 81.32° | 68.99° | 108.71° | 139.30° | 52.61° | 14.71° |
| H12 | 3.364 Å | 131.68° | 116.35° | 65.68° | 50.77° | 119.54° | 132.55° | 92.08° | 47.54° | 77.10° | 55.71° | 79.09° |
| C12 | 3.373 Å | 141.28° | 103.12° | 77.16° | 44.82° | 103.78° | 123.11° | 80.34° | 51.24° | 69.08° | 71.29° | 85.14° |
| C14 | 3.431 Å | 136.23° | 72.77° | 112.43° | 42.49° | 64.54° | 97.75° | 59.38° | 66.94° | 49.01° | 112.37° | 107.76° |
| H14 | 3.462 Å | 124.80° | 64.53° | 126.69° | 46.94° | 51.44° | 89.47° | 57.64° | 73.38° | 43.53° | 127.48° | 117.56° |
| | | H17 | N25 | C18 | C16 | H25b | H25a | H25c | H16b | H16a | O23 | O22 |
| | | | | | | | | | | | | |
| »1 : -1+x, +y, +z | | | | | | | | | | | | |





Part Highlighting

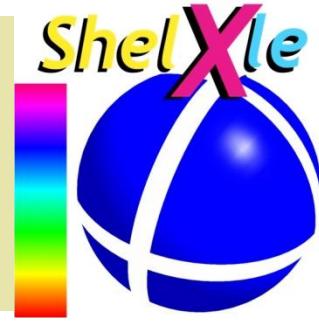




Plans:

- DISP from wavelength
- FREE and BIND instructions in file after clicking these functions in Selection Tool Bar
- Help! FAQ, more Videos.
- Linux distributions
- More sort options
- ENVI with graphics
- ...getting cited.





Credits

- George M Sheldrick,
 - Birger Dittrich, Kevin Pröpper, Julian Holstein,
 - Krzysztof Radacki, Håkon Hope, Daniel Kratzert
Joseph H. Reibenspies, Frederik J Holander and
many other testers and users.
-
- **Thank YOU!**
 - *(yesterday 16:00 2031 downloads!)*

