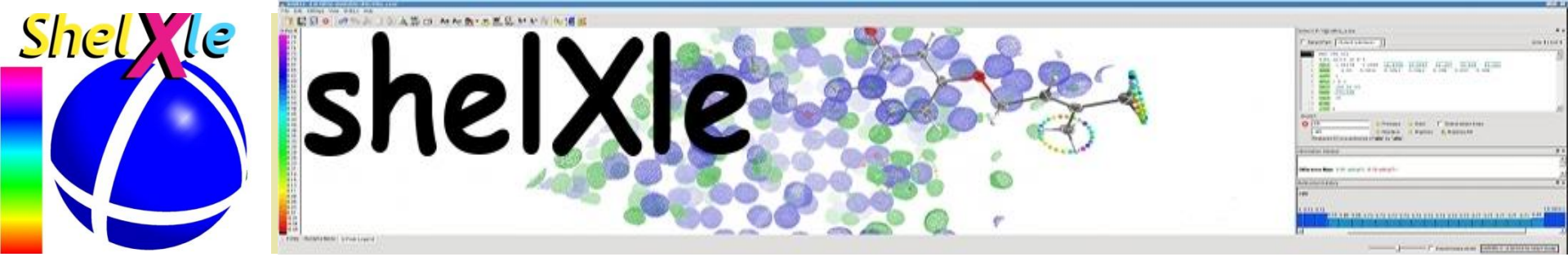

ShelXle: A cute GUI for *SHELXL*

Christian B. Hübschle

17.11.2011

GEORG-AUGUST-UNIVERSITÄT
GÖTTINGEN

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

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ShelXle: a Qt graphical user interface for *SHELXL*

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

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

ShelXle is a graphical user interface for *SHELXL* [Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 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_o) and difference density (F_o–F_c) maps. Special features of *ShelXle* include intuitive atom (re-)naming, 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 Qt4 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 lineprinter 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 in most small-molecule structure refinements.

More recently, a number of excellent graphical user interfaces (GUIs) [*e.g. WINGX* (Farrugia, 1999), *OLEX2* (Dolomanov *et al.*, 2009), *XSEED* (Barbour, 2001), *PLATON* and *SYSTEM-S* (Spek, 2009), and the Bruker programs *XP* (Nicolet, 1981) and *XSHELL* (Bruker, 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 awkward to integrate 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 of the original *SHELXL* flavour and capabilities. For this purpose, *ShelXle* was developed. *ShelXle* shares some concepts with earlier programs, such as *MoleCoolQt* (Hübschle & Dittrich, 2011), but most of the code was rewritten.

2. Technical description and functionality

ShelXle opens a *SHELX*-format .res file from a structure solution program or a *SHELXL* refinement. The .cif/.res file in *SHELX* 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 displayed 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 Qt4 (http://qt.nokia.com/products/) and the FFTW (*http://www.fftw.org/*) libraries, and so is able to exploit the latest developments in computer graphics as well as being highly portable.

2.1. Electron density maps

If the previous *SHELXL* refinement used the 'LIST 6' instruction, F_o and F_o–F_c maps are calculated and visualized as mesh-style isosurfaces. 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_o map is changed in the same way but using the shift key. Initial isocontour levels are 2.7 σ for the F_o–F_c map and 1.2σ for the F_o 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 deemed desirable, in order to simplify the view, it is possible to display only density within 1.41 Å ($2^{1/2}$) 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_o–F_c residual density that are higher than the current isosurface value.

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

Q peaks are visualized as small colour-coded icosahedra. 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 AFIX instructions in the file being edited. If the F_o–F_c map is available, the difference electron density may be used to find optimal positions for H atoms in CH_n 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 or following '!') are coloured in blue, while temporary comments (lines beginning with a space when the line before does not end with '=') are coloured dark blue and are underlined. Lines longer than 80 characters are flagged by a red background colour, since characters after column 80 (not compatible with punched cards) are ignored by *SHELXL*. After the first one or two characters of a new line have been entered, a code-completer function opens, suggesting commands beginning with the given letters. Accepting a suggestion by striking the 'enter' key inserts the command in capital letters (whether or not they were entered in upper case).

Care is taken to keep track of the 'free variables', a defining feature of *SHELXL*. When a number in the editor window implicitly references a free variable and the mouse pointer hovers over it for several seconds, a popup 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, right clicking in the selected area in the editor achieves atom selection. The editor is also equipped with a 'search and replace' tool that highlights matches in the editor in yellow. Entire parts ('PART') and residues ('RESI') 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 rearranging the windows. When desired, or prior to performing a refinement, the three-dimensional display and the editor are synchronized and the editor contents are saved. More esoteric *SHELXL* instructions – *e.g.* FRAG ... FEND or the third number on the L.S. command – can easily be added using the editor.

2.5. Refinement history facility

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

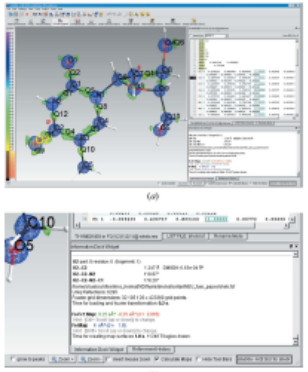


Figure 1
(*a*) The GUI of *ShelXle*, displaying the structure of thymidine at 20 K (Hübschle *et al.*, 2008). The F_o–F_c map at 0.25 e Å^{-3} shows features of bonding and lone-pair electron density. Atom O2 is currently selected. (*b*) An enlargement of the lower-right corner of the screenshot above.

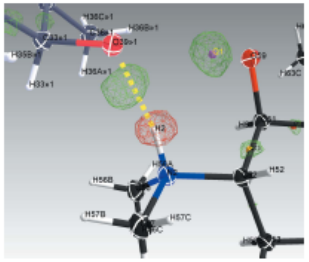
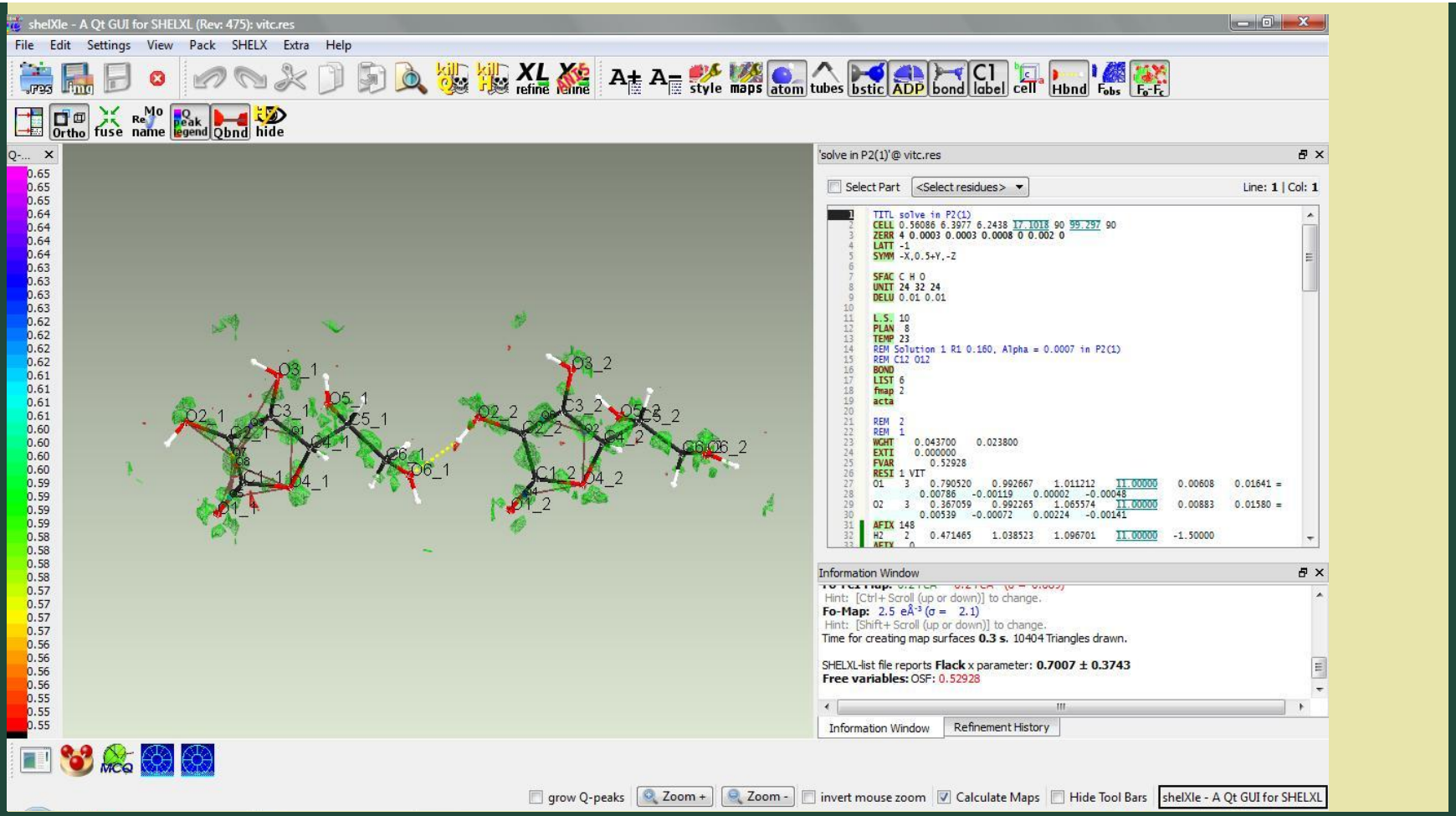
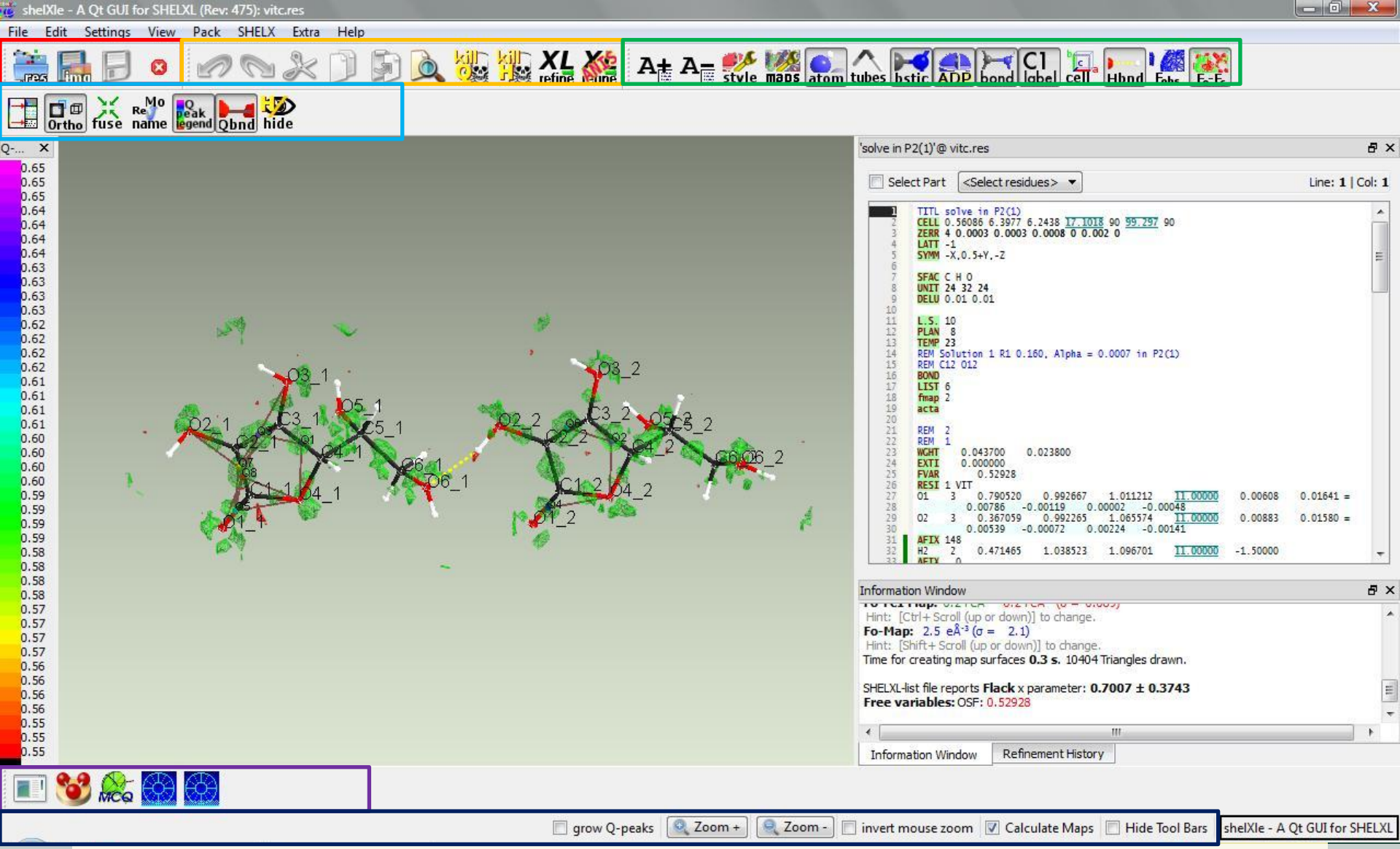


Figure 2
An early refinement state of roxithromycin (Hübschle *et al.*, 2010), showing difference electron density. Missing and erroneously placed H atoms are clearly visible.

The GUI


shelXle - A Qt GUI for SHELXL (Rev: 475): vitc.res
File Edit Settings View Pack SHELX Extra Help
'solve in P2(1)'@ vitc.res
Select Part
<Select residues>
Line: 1 | Col: 1
TITL solve in P2(1)
CELL 0.56086 6.3977 6.2438 17.1018 90 99.297 90
ZERR 4 0.0003 0.0003 0.0008 0 0.002 0
LATT -1
SYMM -X,0.5+Y,-Z
SFAC C H O
UNIT 24 32 24
DELU 0.01 0.01
L.S. 10
PLAN 8
TEMP 23
REM Solution 1 R1 0.160, Alpha = 0.0007 in P2(1)
REM C12 O12
BOND
LIST 6
fmap 2
acta
REM 2
REM 1
WGHT 0.043700 0.023800
EXTI 0.000000
FVAR 0.52928
RESI 1 VIT
O1 3 0.790520 0.992667 1.011212 11.00000 0.00608 0.01641 =
0.00786 -0.00119 0.00002 -0.00048
O2 3 0.367059 0.992265 1.065574 11.00000 0.00883 0.01580 =
0.00539 -0.00072 0.00224 -0.00141
AFIX 148
H2 2 0.471465 1.038523 1.096701 11.00000 -1.50000
Information Window
Hint: [Ctrl+Scroll (up or down)] to change.
Fo-Map: 2.5 eÅ-3 (σ = 2.1)
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 ± 0.3743
Free variables: OSF: 0.52928
Information Window
Refinement History
grow Q-peaks
Zoom +
Zoom -
invert mouse zoom
Calculate Maps
Hide Tool Bars
shelXle - A Qt GUI for SHELXL



File Tool Bar

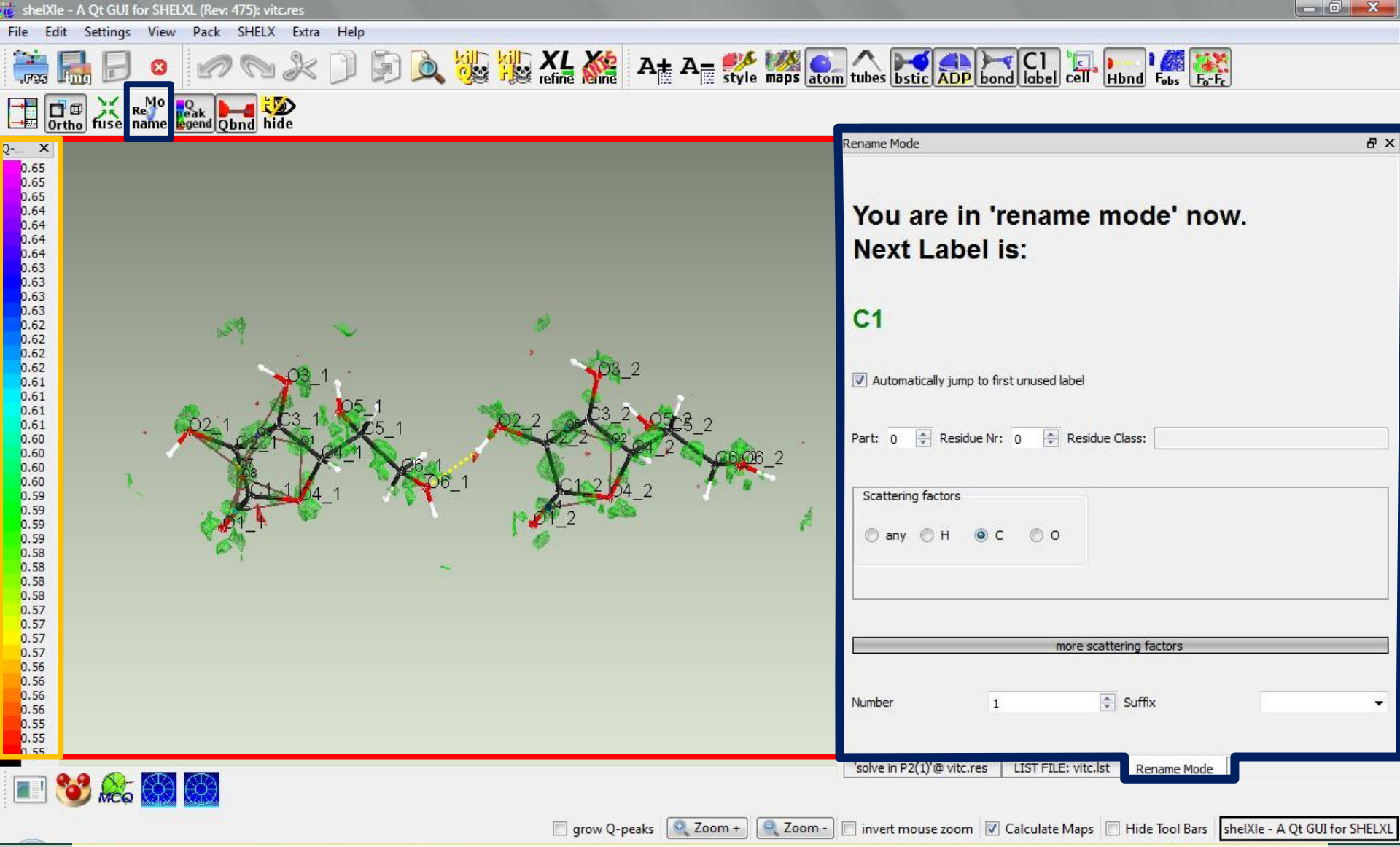
Selection Tool Bar

Editor Tool Bar

Extra Tool Bar

View Tool Bar

Status Bar



OpenGL view

Information Window

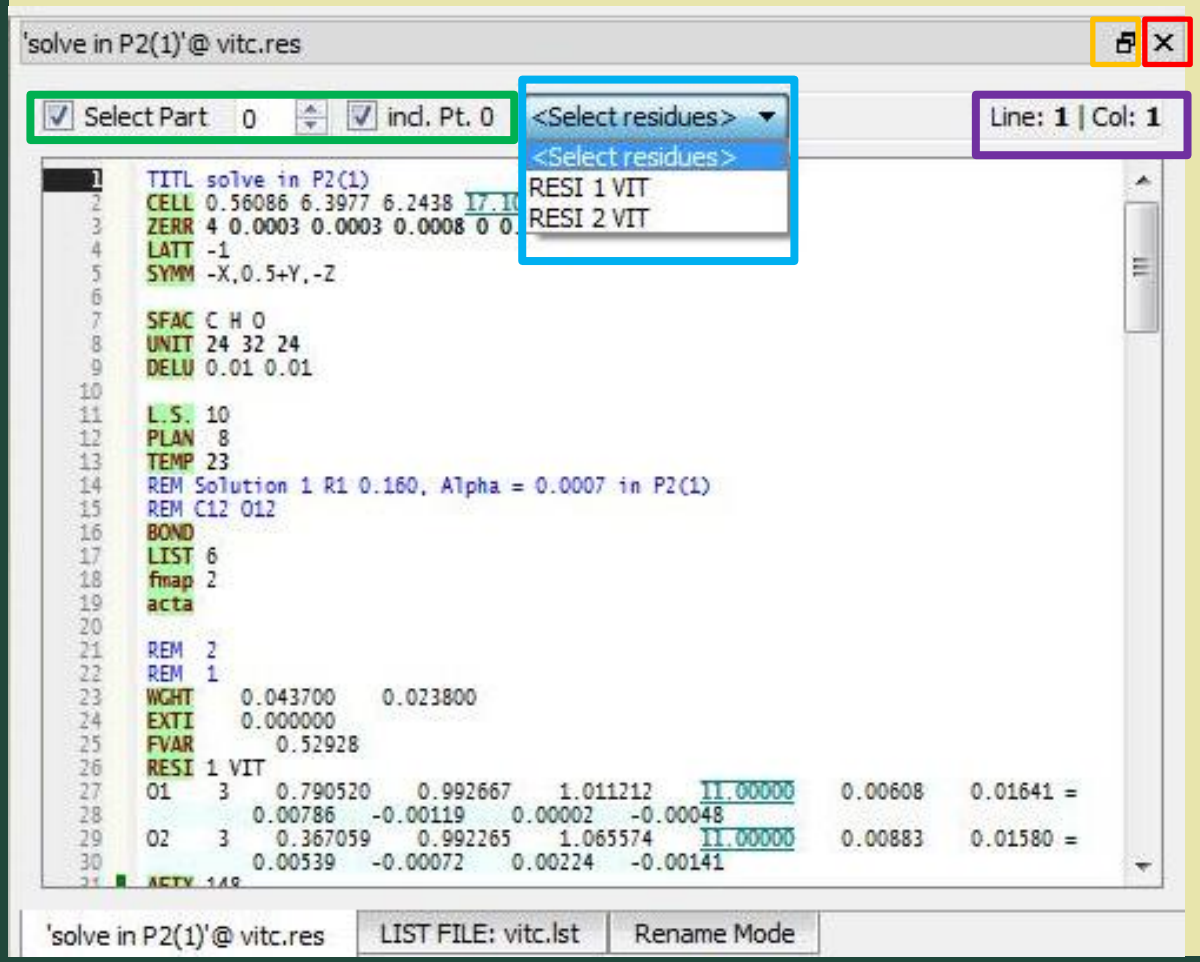
Q-Peak Legend

Refinement History

Editor window

Rename Mode

The Editor



Hide Button

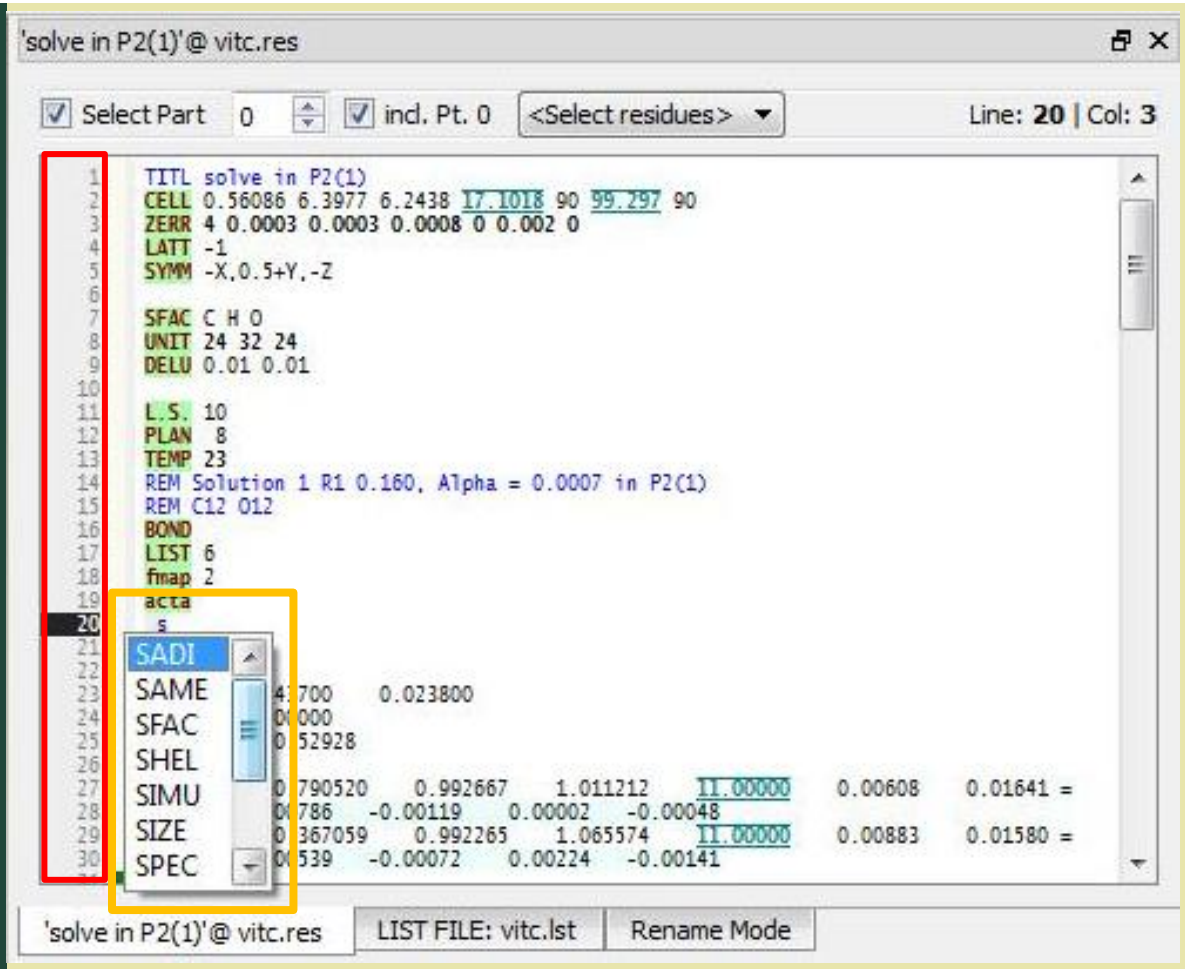
Float Button

Part selector

Residue selector

Cursor Position

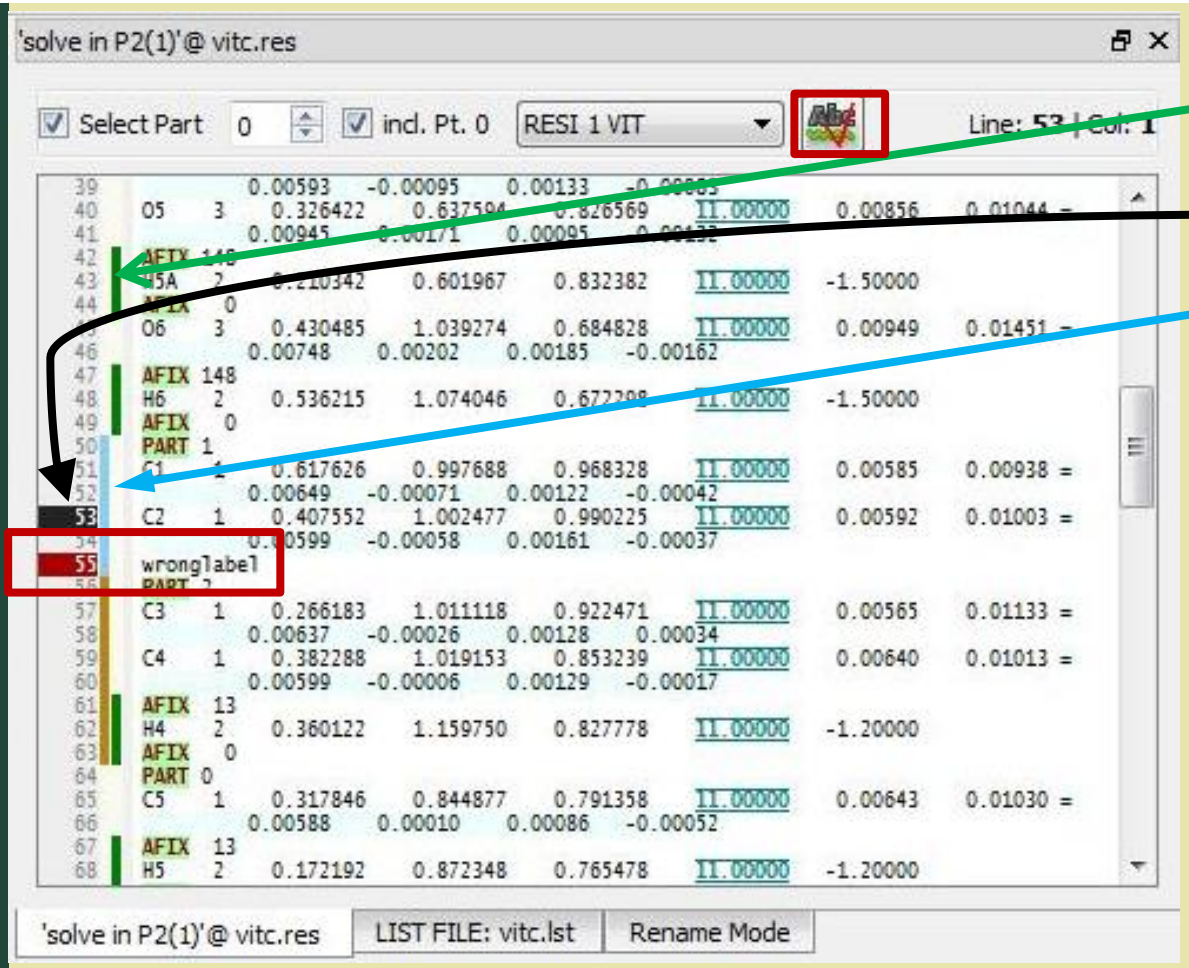
The Editor



Line number area

Code completer

The Editor


'solve in P2(1)'@ vitc.res
Select Part
0
incl. Pt. 0
RESI 1 VIT
Line: 53 | Col: 1
AFIX Highlighter
Current Line Indicator
Part Highlighter
Error Indicator
wronglabel
'solve in P2(1)'@ vitc.res
LIST FILE: vitc.lst
Rename Mode

The Editor

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

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

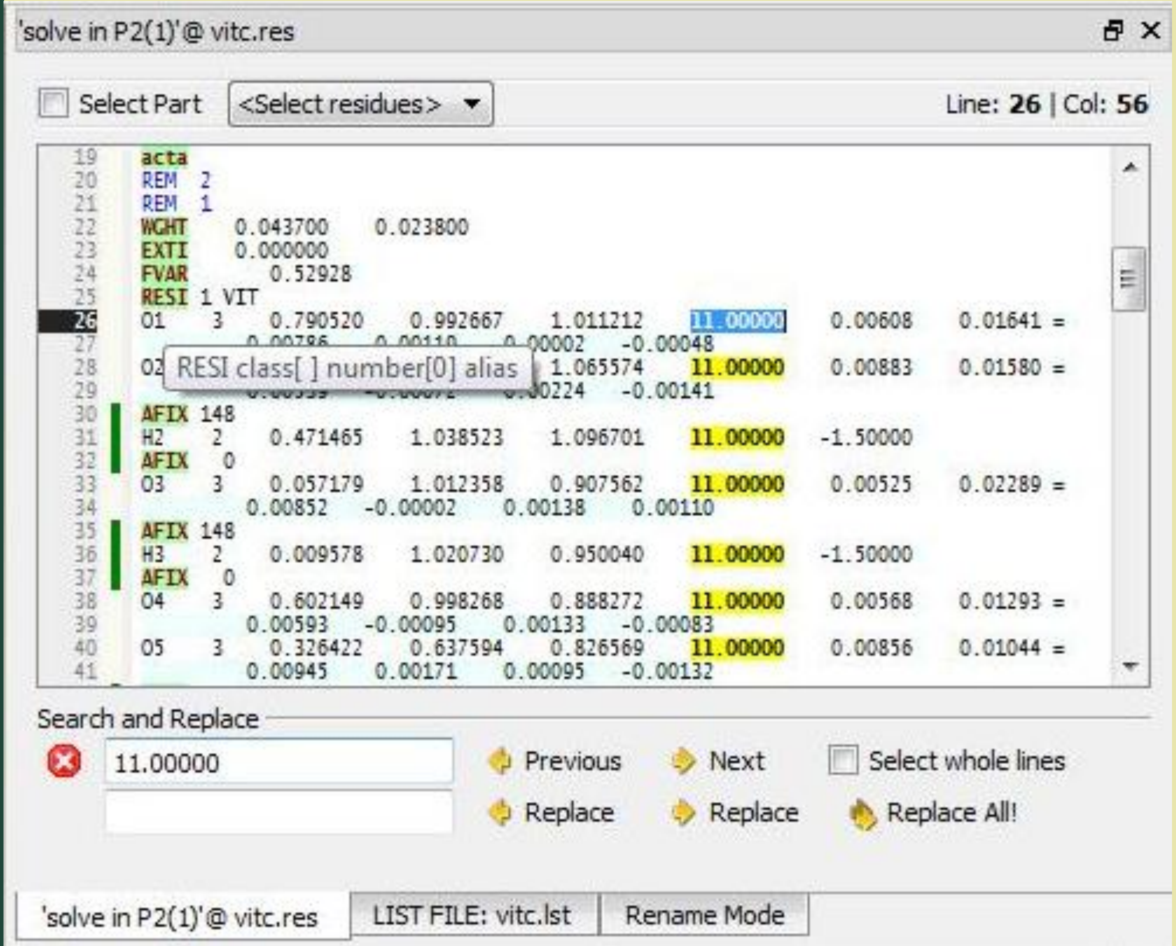
```
54   C3    1    0.266183    1.011118    0.922471    11.00000    0.00565    0.01133 =
55        0.00637   -0.00026    0.00128    0.00034
56   C4    1    0.382288    1.019153    0.853239    11.00000    0.00640    0.01013 =
57        0.00599   -0.00006    0.00129   -0.00017
58   AFIX  13
59   H4    2    0.360122    1.159750    0.827778    11.00000   -1.20000
60   AFIX   0
61
62   C5    1    0.317846    0.844877    0.791358    11.00000    0.00643    0.01030 =
63
64   AFIX  1
65   H5    2
66   AFIX
67   C6    1                                                              99 =
68
69   AFIX  2
70   H6A   2
71   H6B   2
72   AFIX
73   RESI  2
74   O1    3                                                              86 =
75
76   O2    3                                                              54 =
77
78   AFIX  14
79   H2    2
80   AFIX
81   O3    3                                                              58 =
82
83   AFIX  14
84   H3    2
```

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

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

Context Menu

The Editor

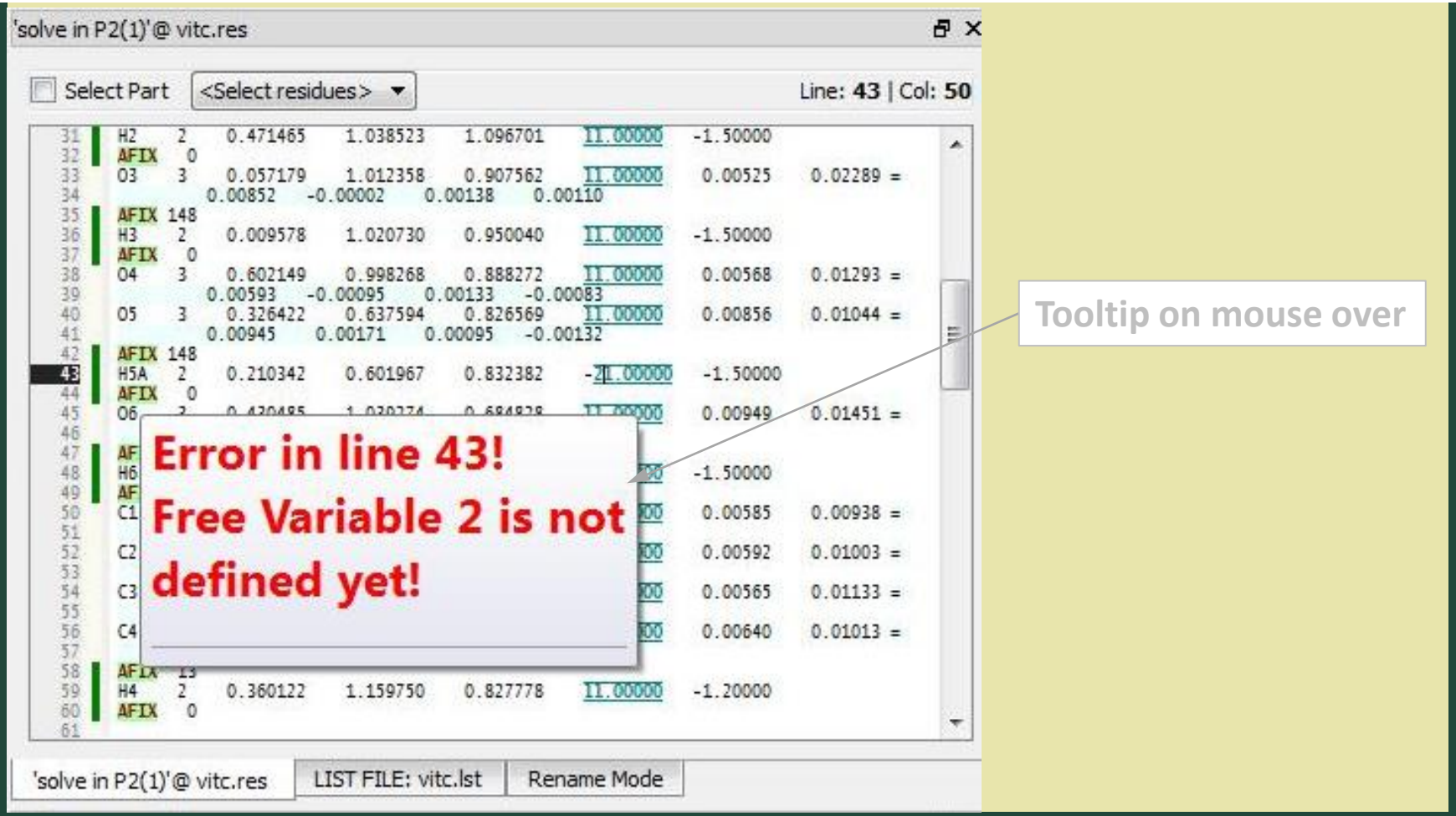


Search and Replace

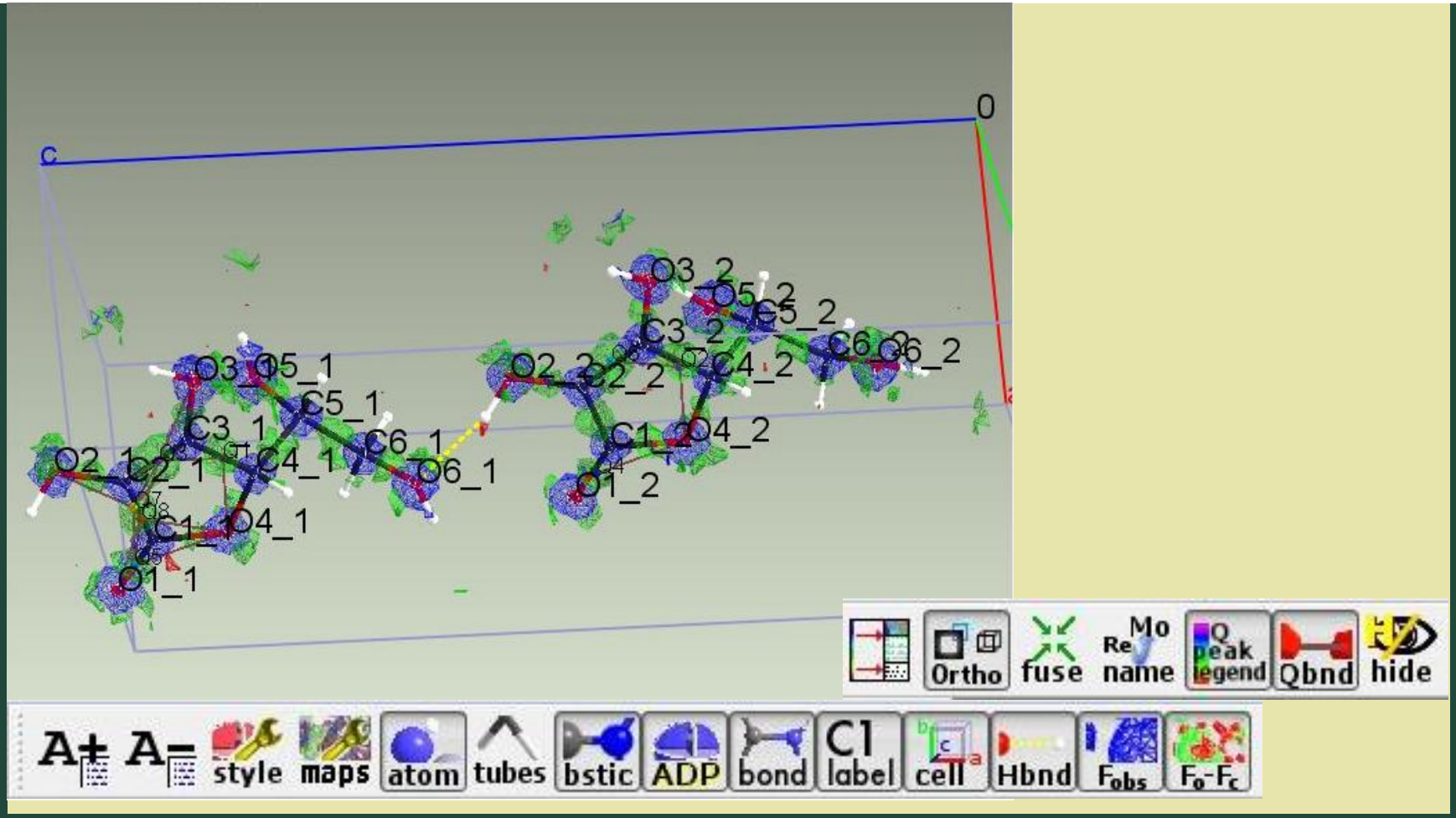
- Regular Expressions
- Highlighting of Hits
- [Ctrl+F] or [F3]

Tooltip on mouse over

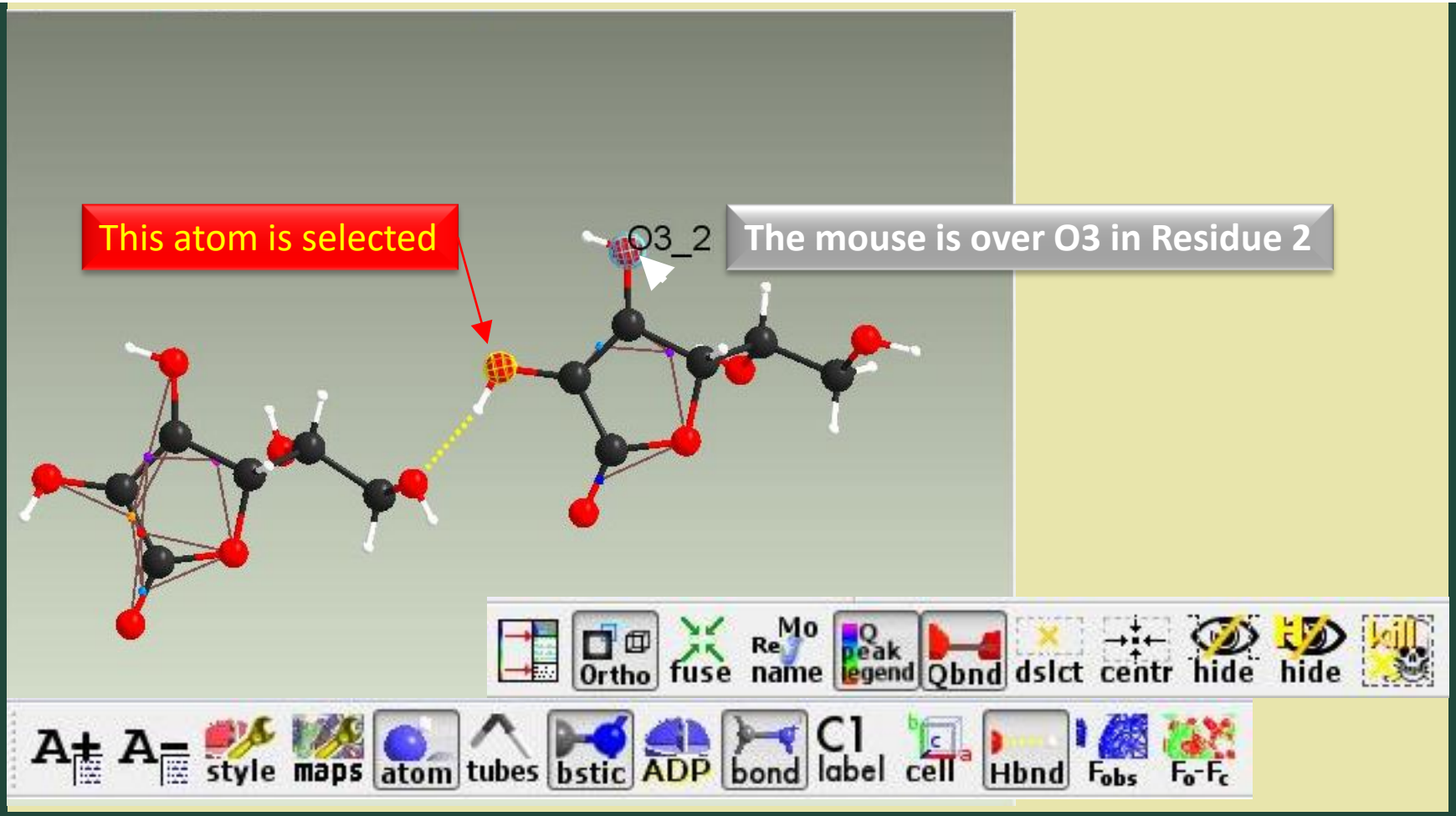
The Editor


'solve in P2(1)'@ vitc.res
Select Part
<Select residues>
Line: 43 | Col: 50
Error in line 43!
Free Variable 2 is not defined yet!
Tooltip on mouse over
'solve in P2(1)'@ vitc.res
LIST FILE: vitc.lst
Rename Mode

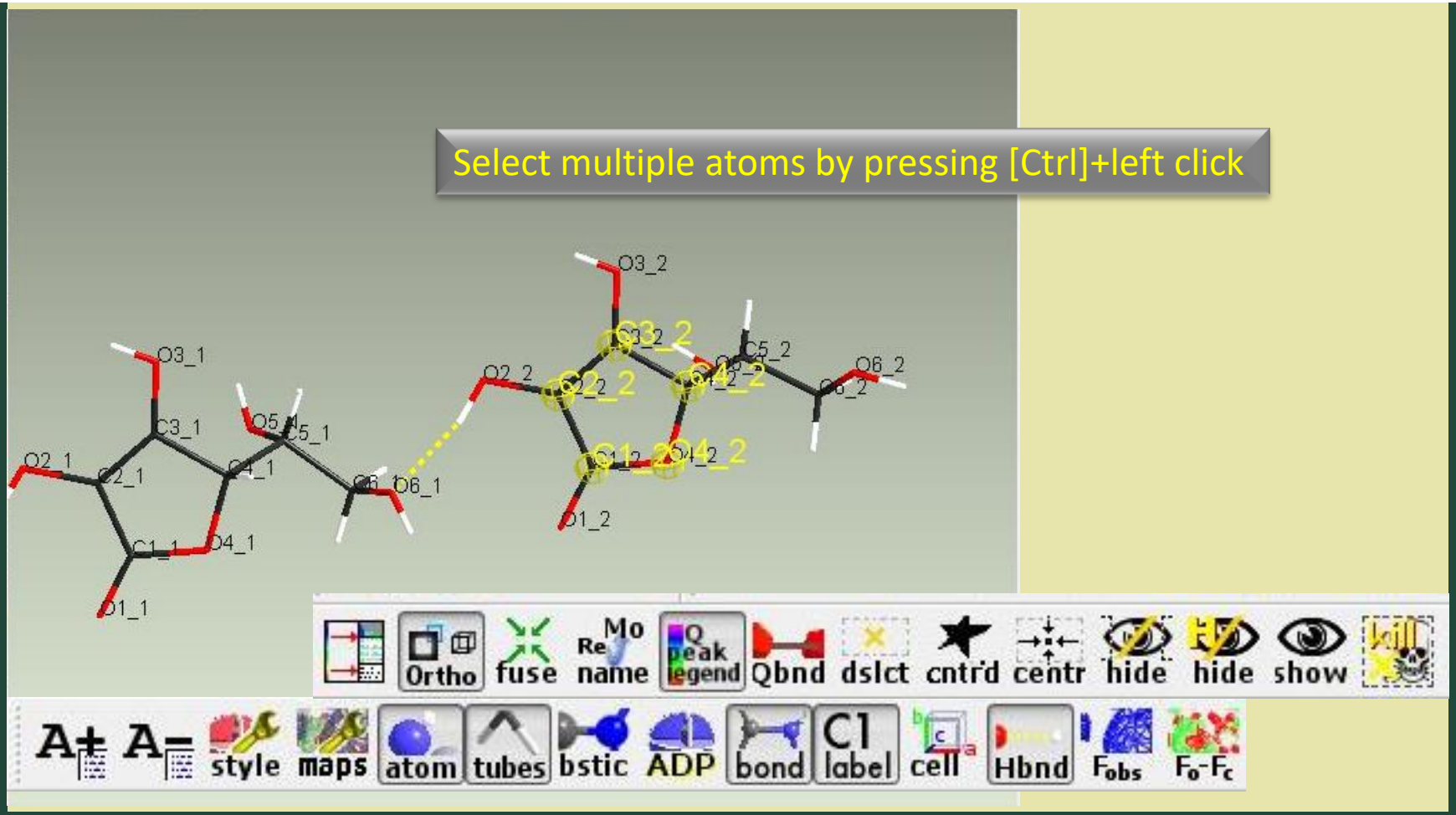
The OpenGL View



The OpenGL View



The OpenGL View



The Selection Tool Bar


Hides Information Window, Refinement History and Editor

Shows molecular graphics with central or orthographic Projection

Completes molecules in the asymmetric unit

Shows the asymmetric unit only

Enters/Exit Rename Mode

Shows/Hide Q-Peak Legend

Draws lines between Q-Peaks

Connects the two selected atoms

Disconnects the two selected atoms

Deselects the selected atoms

Adds a Centroid Dummy atom 

Sets rotation center to selected atom(s) 

Hides everything not selected 

Hides H-atoms 

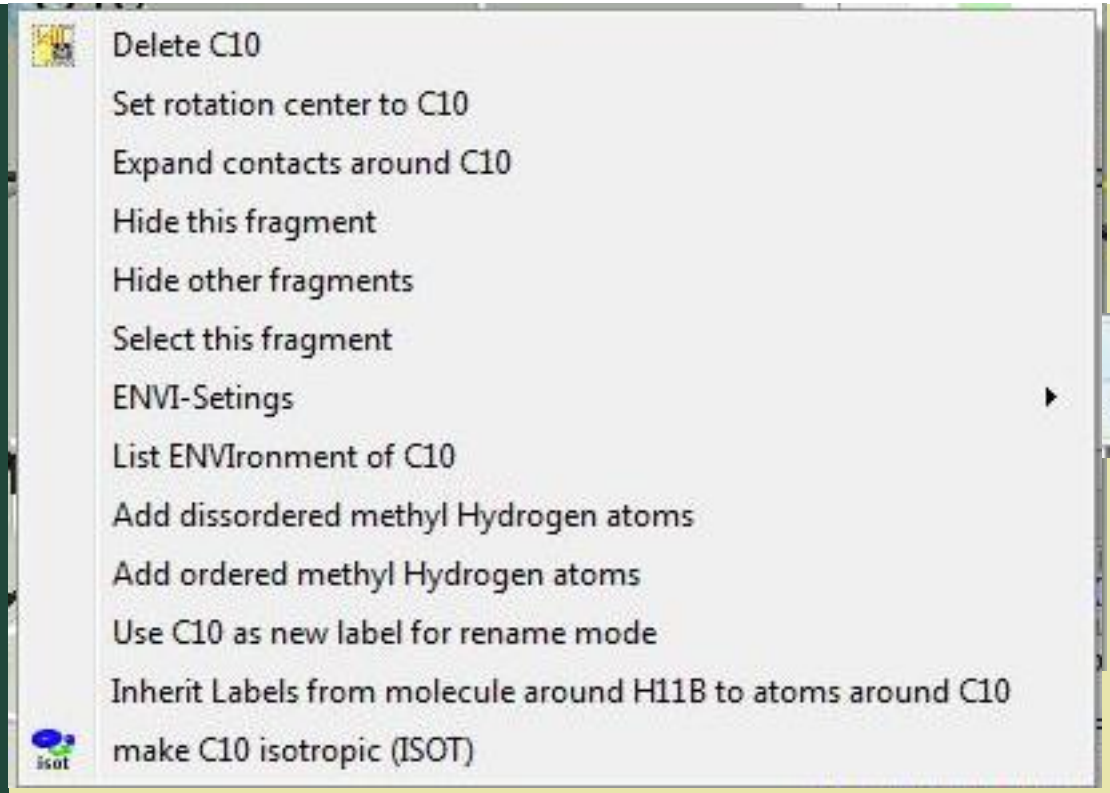
Indicates hidden objects 

Hides PART –N Ghosts 

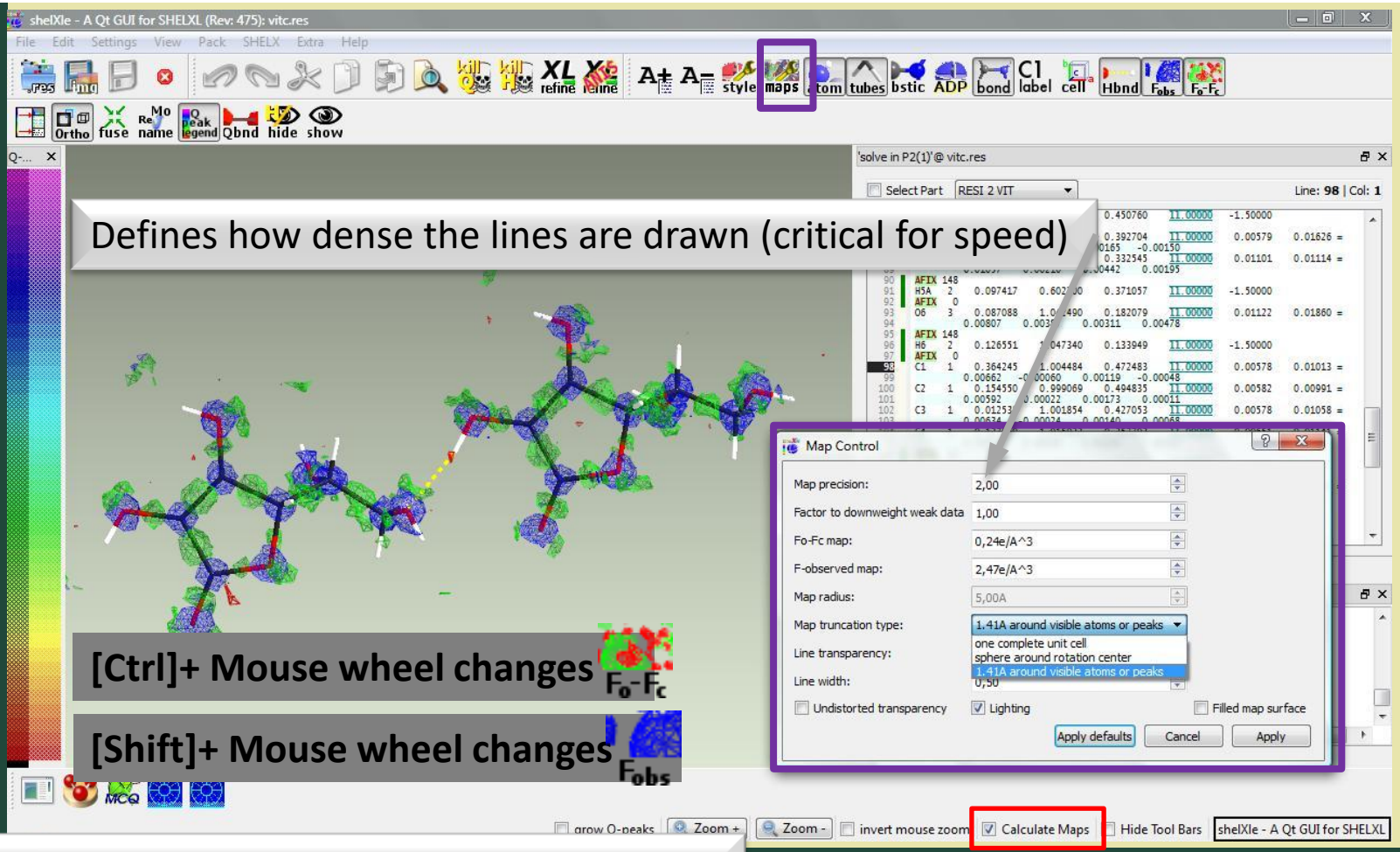
Highlights atoms in Parts 

Kills selected atoms [Ctrl]+[Del] 

Context Menu by right click on atom



Electron-Density Maps



Blue mesh: Observed data with model phases

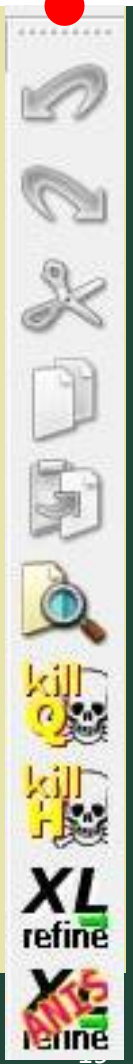
Red and green Mesh: Observed data minus model green+ red-

Customization

- Tool bars can be moved to different places

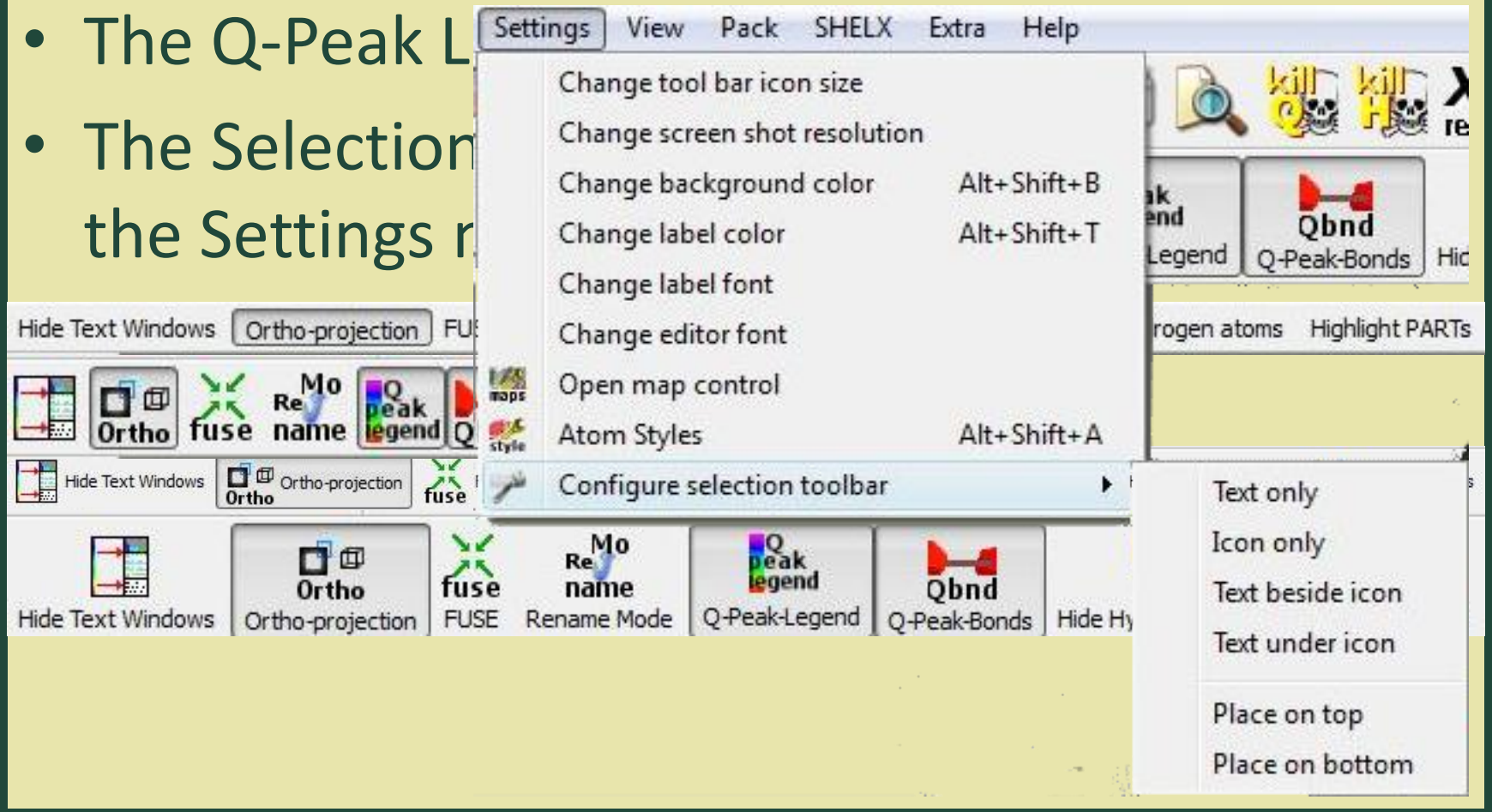
Grab here with the mouse and drag around.

- 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.

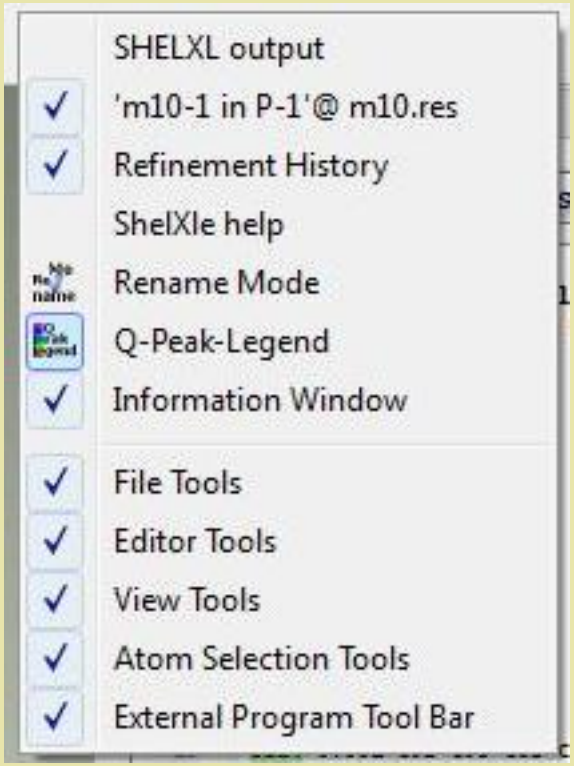


Customization

- The Q-Peak L
- The Selection
  the Settings r

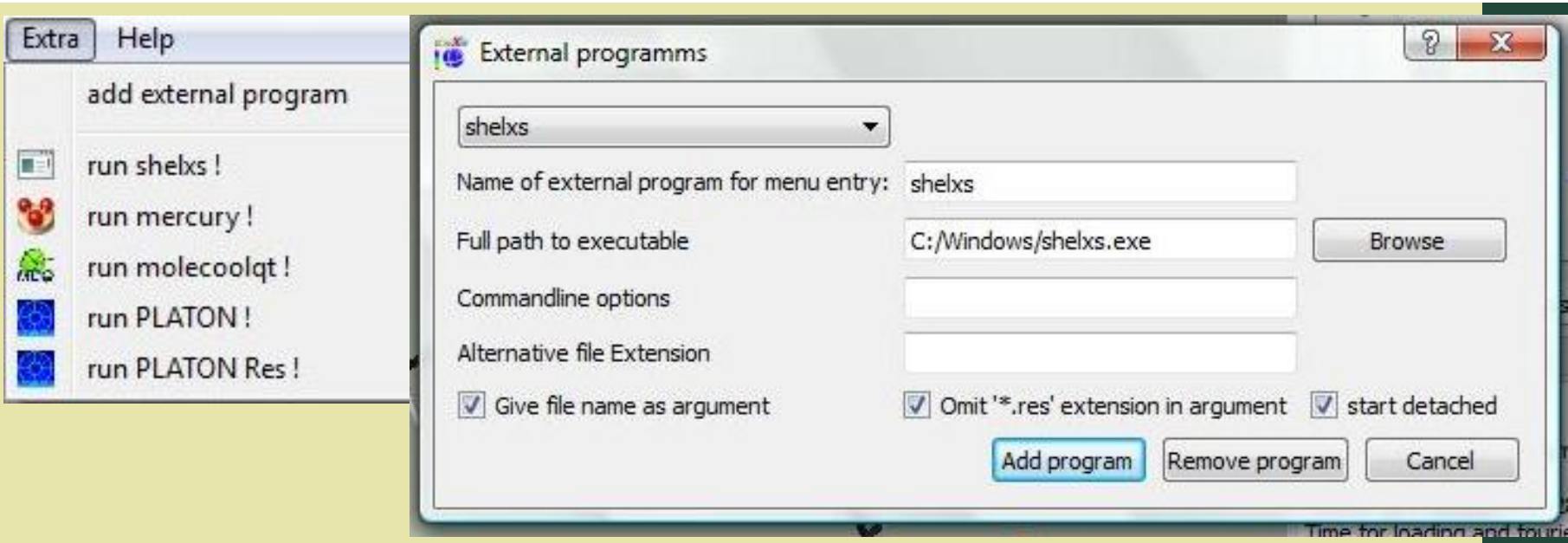


Customization



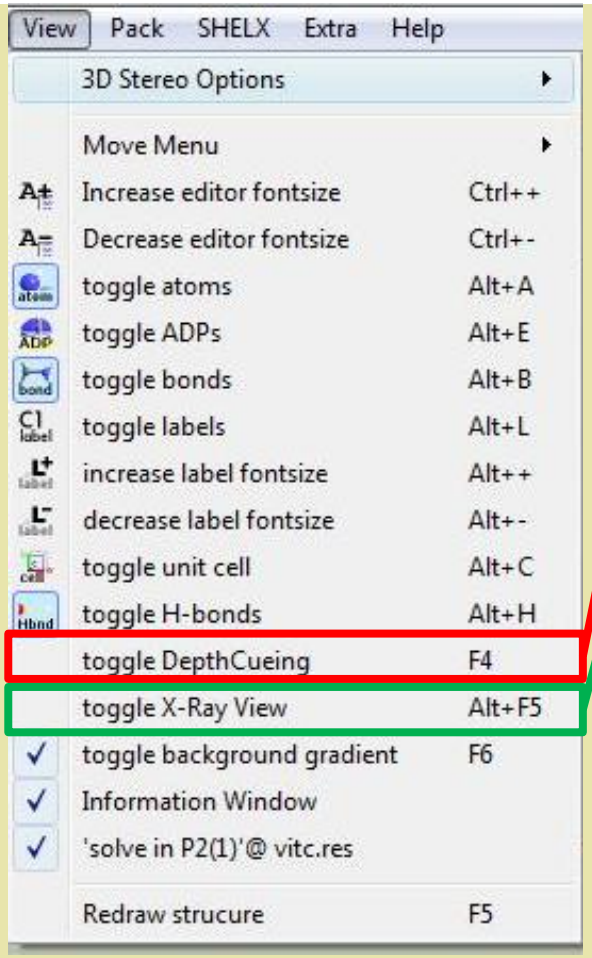
Right clicking on the menu or any tool bar shows this menu. Here any hidden tool bar or window can be recovered.
When Rename Mode is visible you are in Rename Mode and vice versa.

Customization - External Programs



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

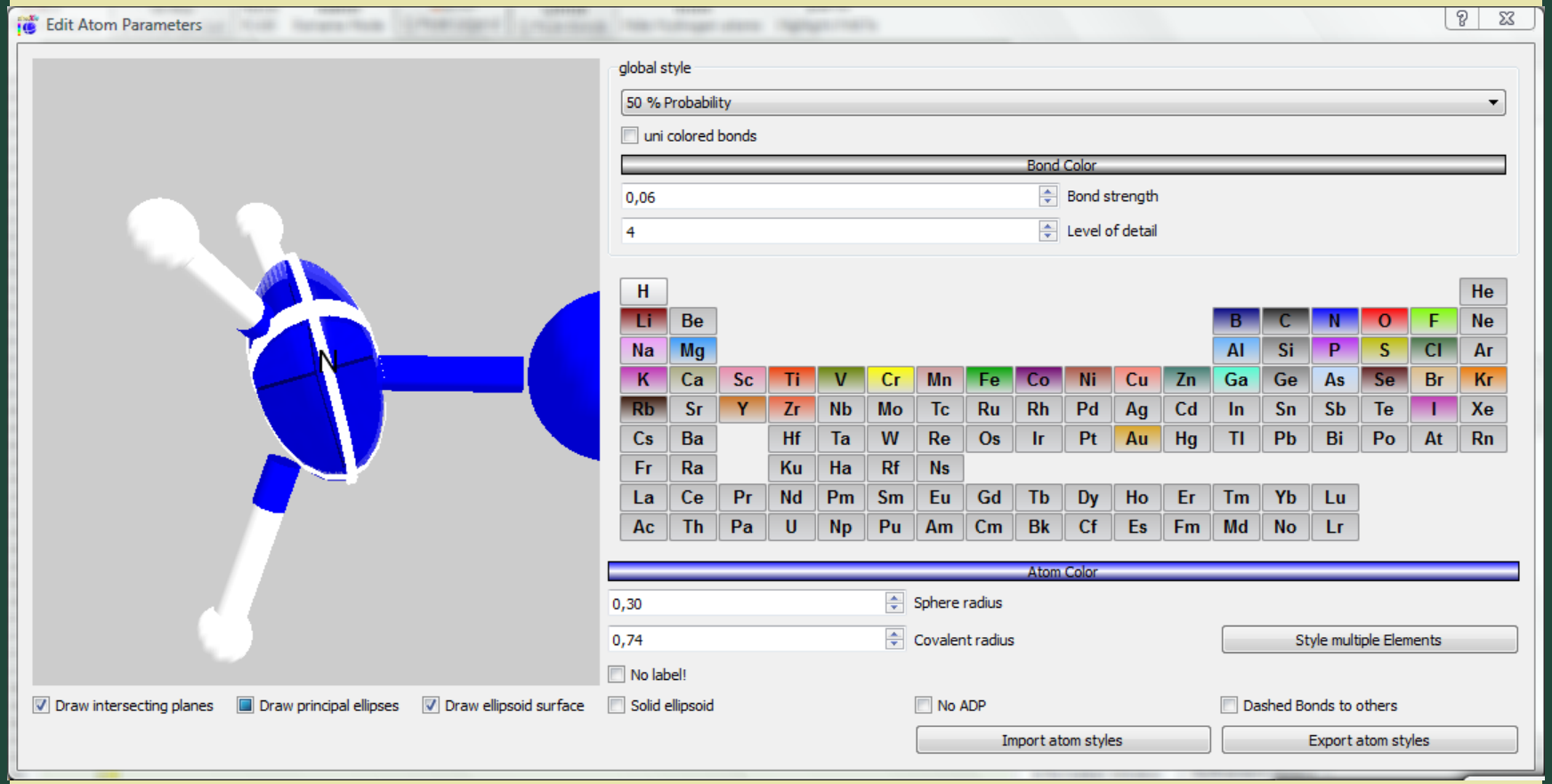
Customizing – View Menu



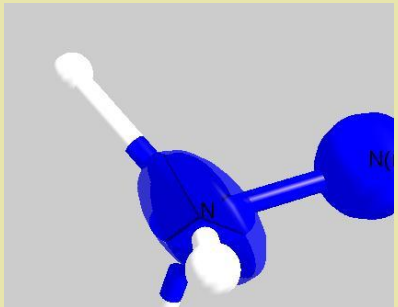
Toggles fog. Fog density by [Alt + Mouse wheel]

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)

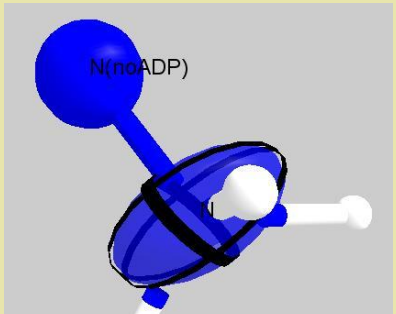
Atom-Styles Dialog



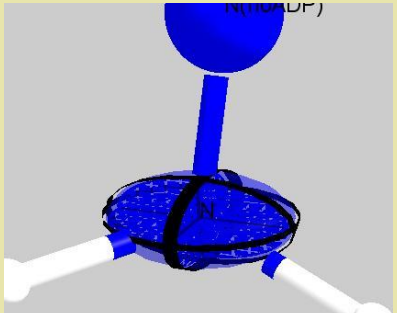
Atom-Styles Dialog



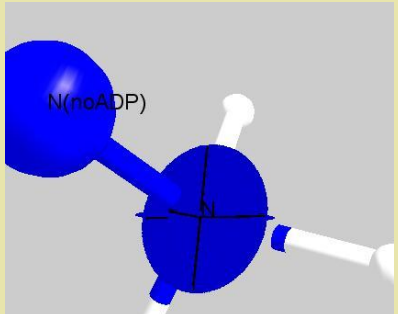
Intersect. Planes+ Surface



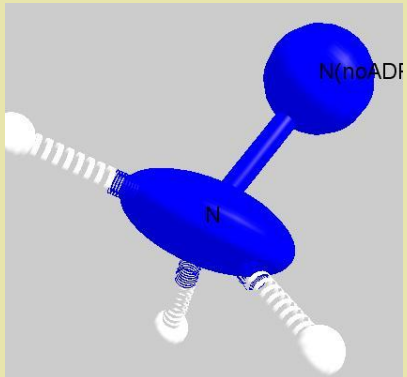
Principal ellipses2



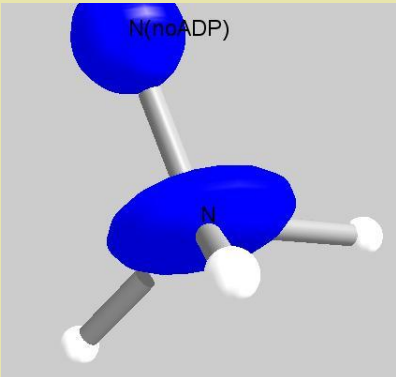
Intersect. planes2



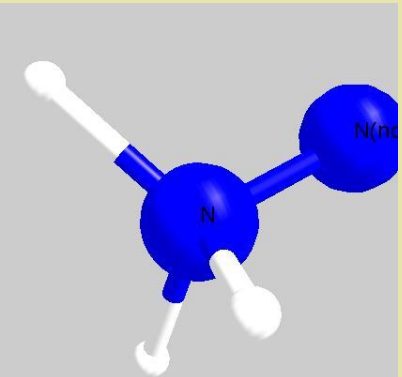
Intersect. planes



Dashed bonds to o



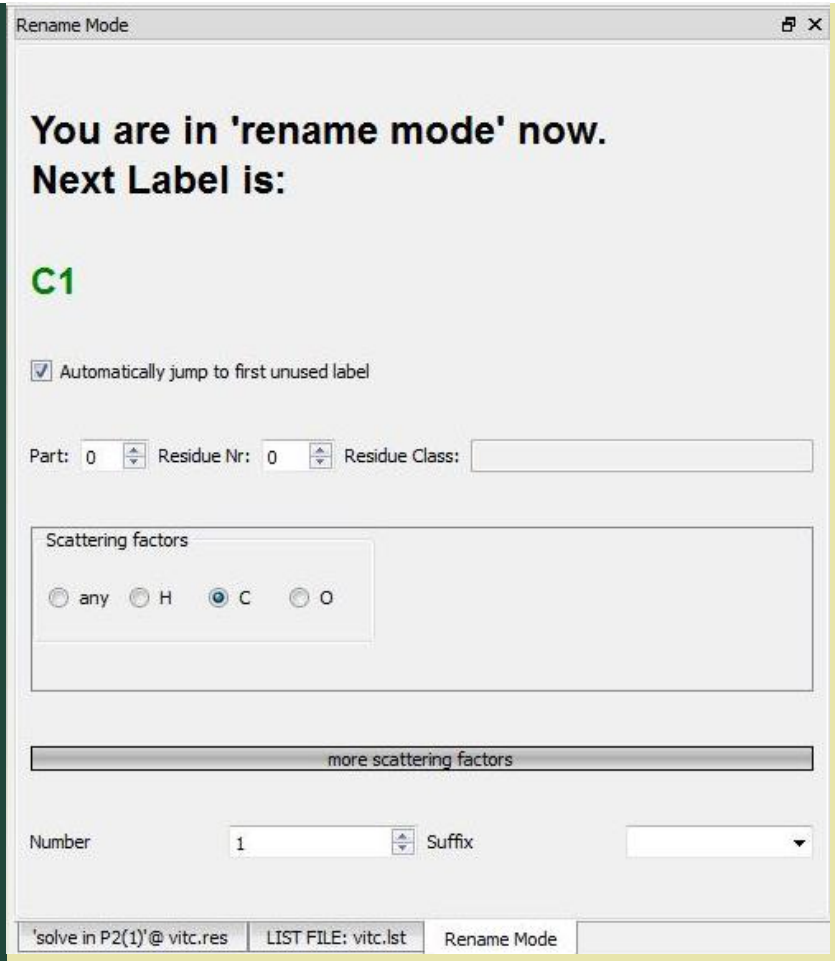
Uni color bonds

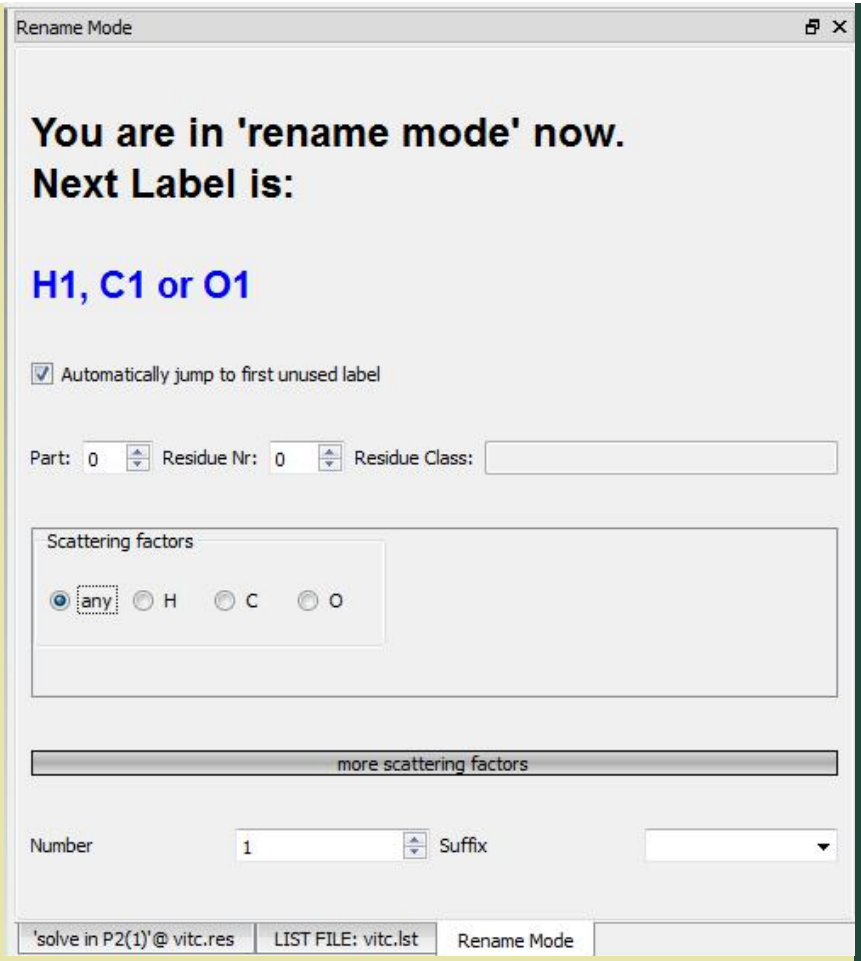


No ADP

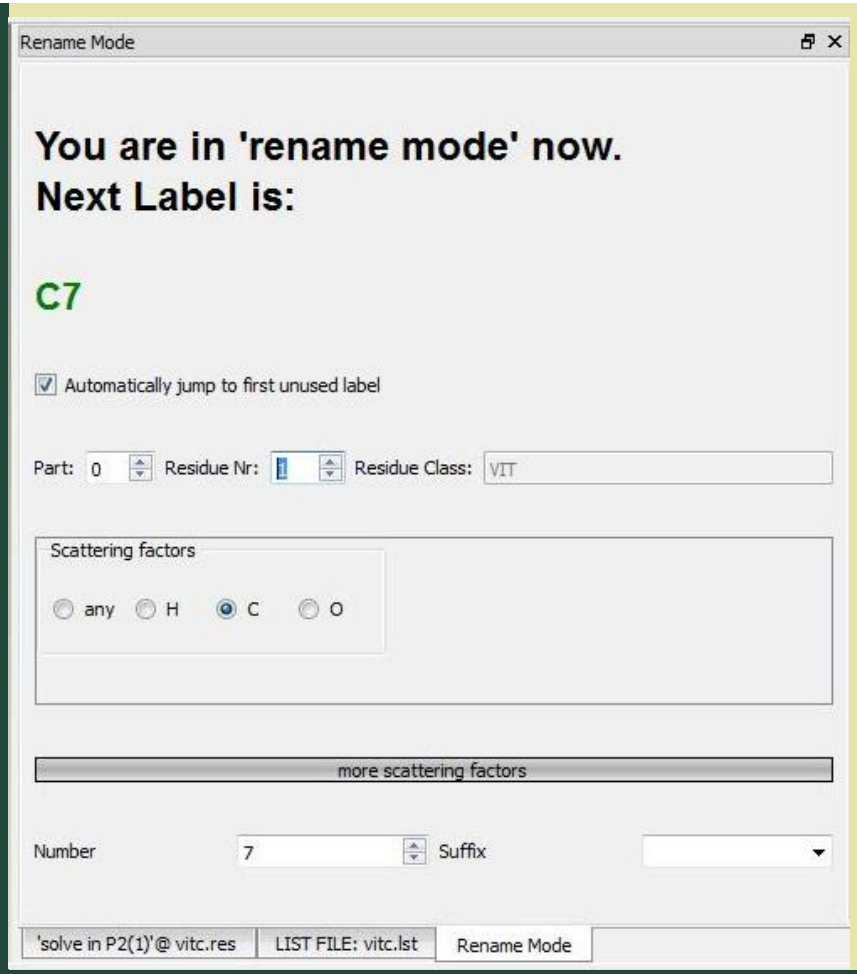
Play around with Checkboxes to figure out what you like best!

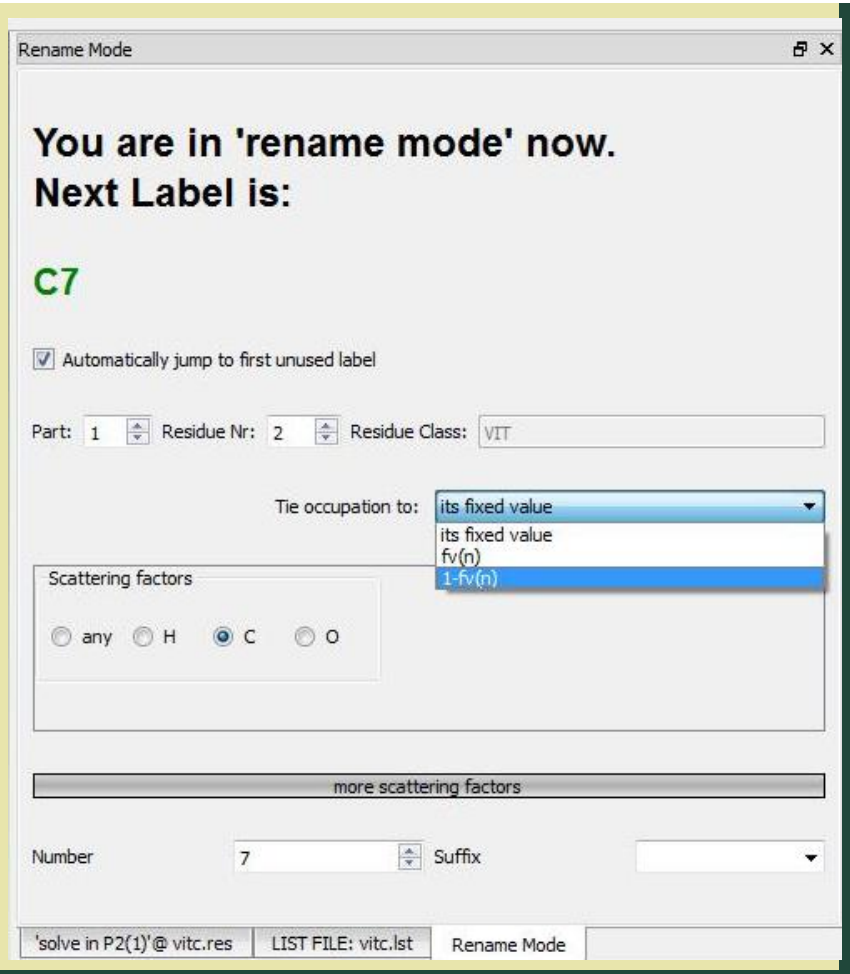
Rename Mode


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

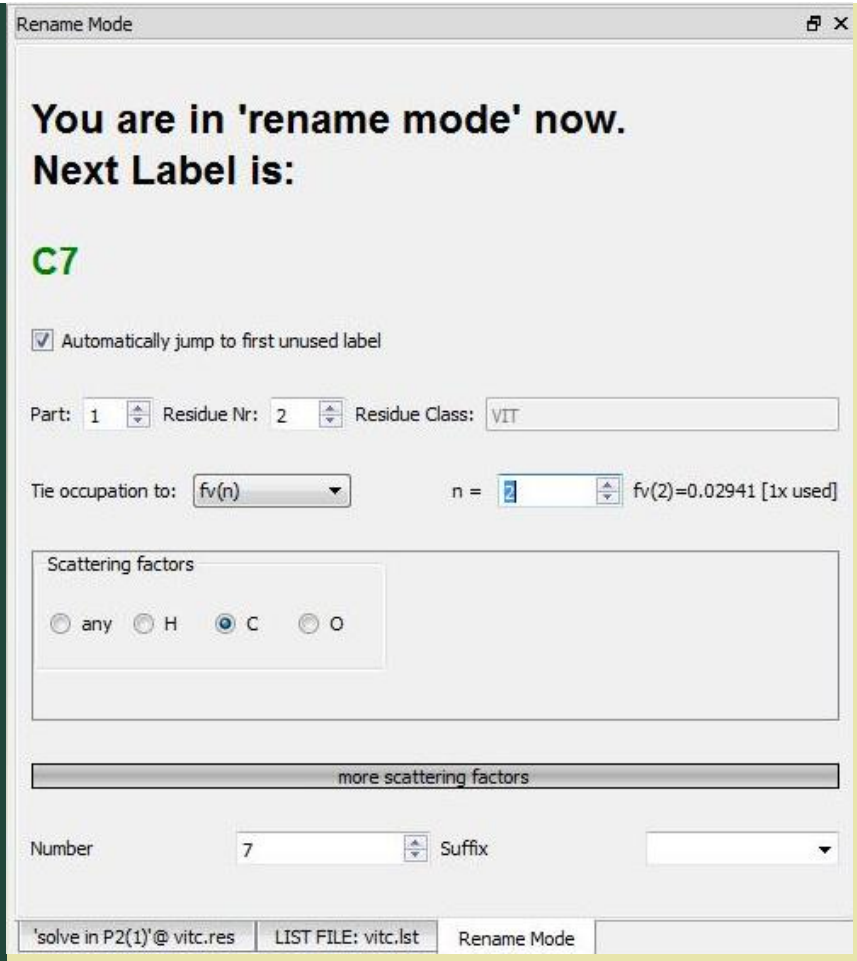

Rename Mode
You are in 'rename mode' now.
Next Label is:
H1, C1 or O1
Automatically jump to first unused label
Part: 0 Residue Nr: 0 Residue Class:
Scattering factors
any H C O
more scattering factors
Number 1 Suffix
'solve in P2(1)'@ vitc.res
LIST FILE: vitc.lst
Rename Mode

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



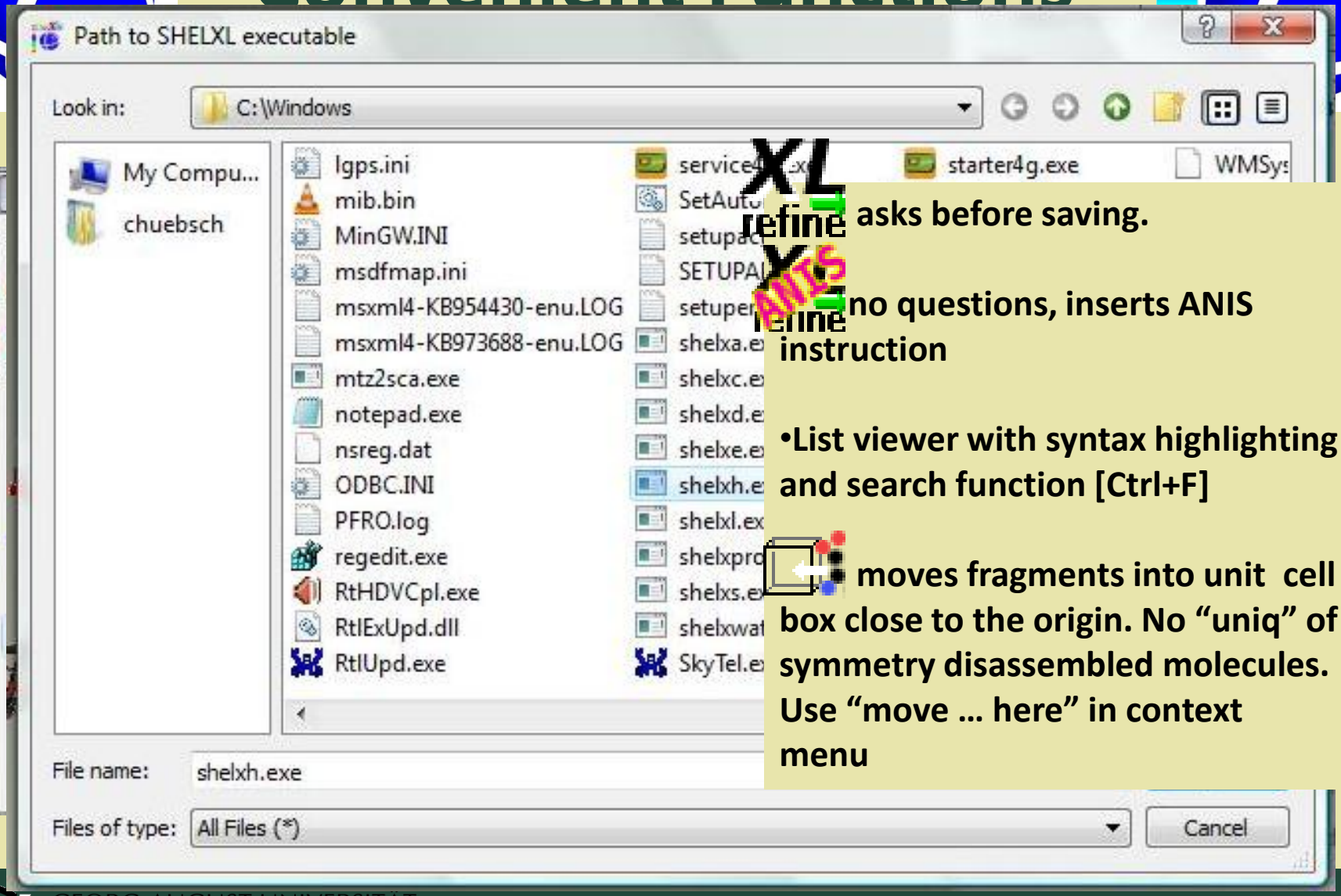
Residue Class can only be edited if ResiNr is not yet in use.

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



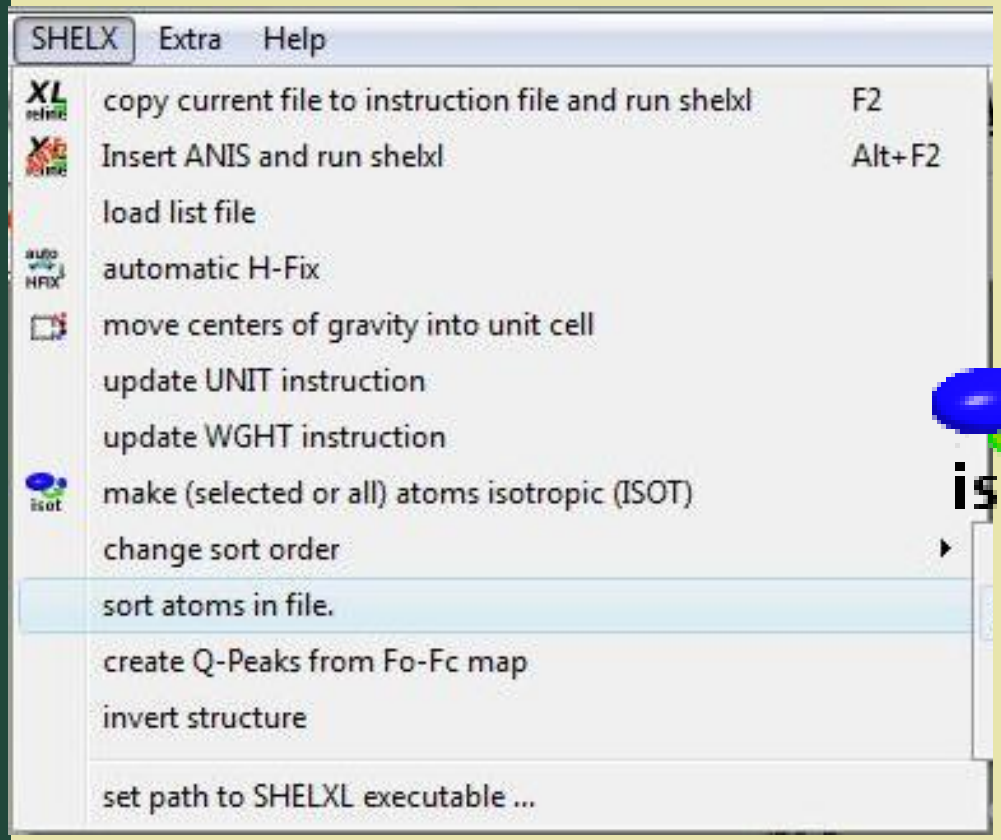
asks before saving.

no questions, inserts ANIS instruction

- **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

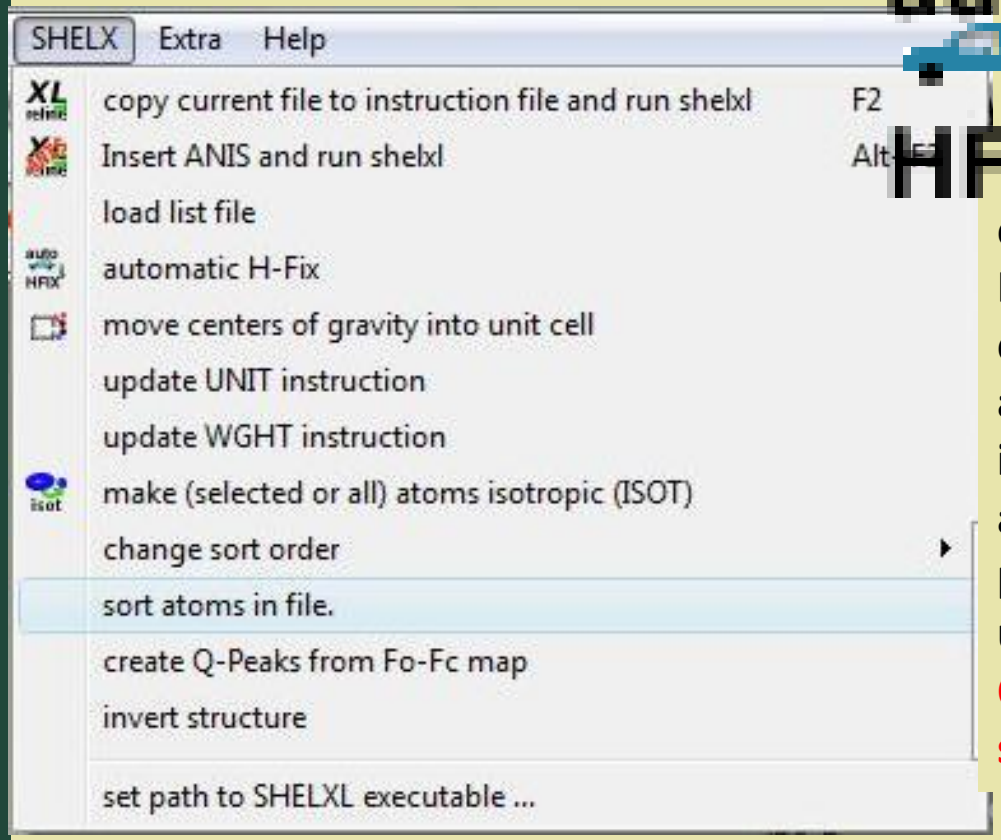
Convenient Functions



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.

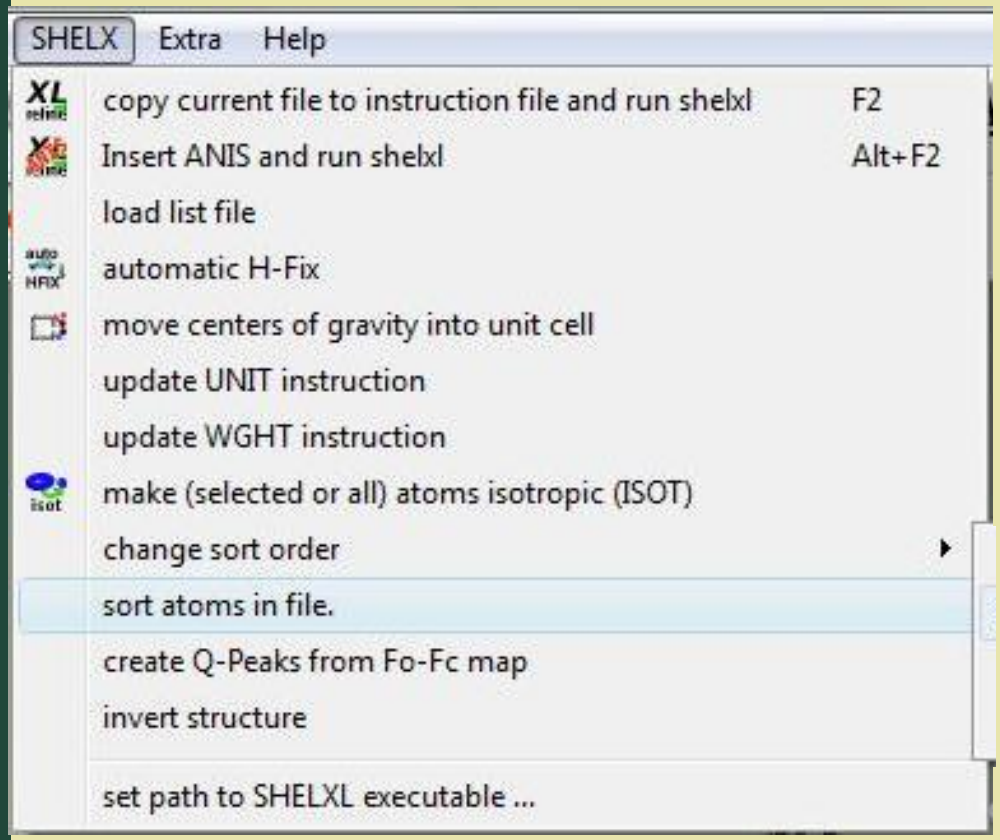
Convenient Functions



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!

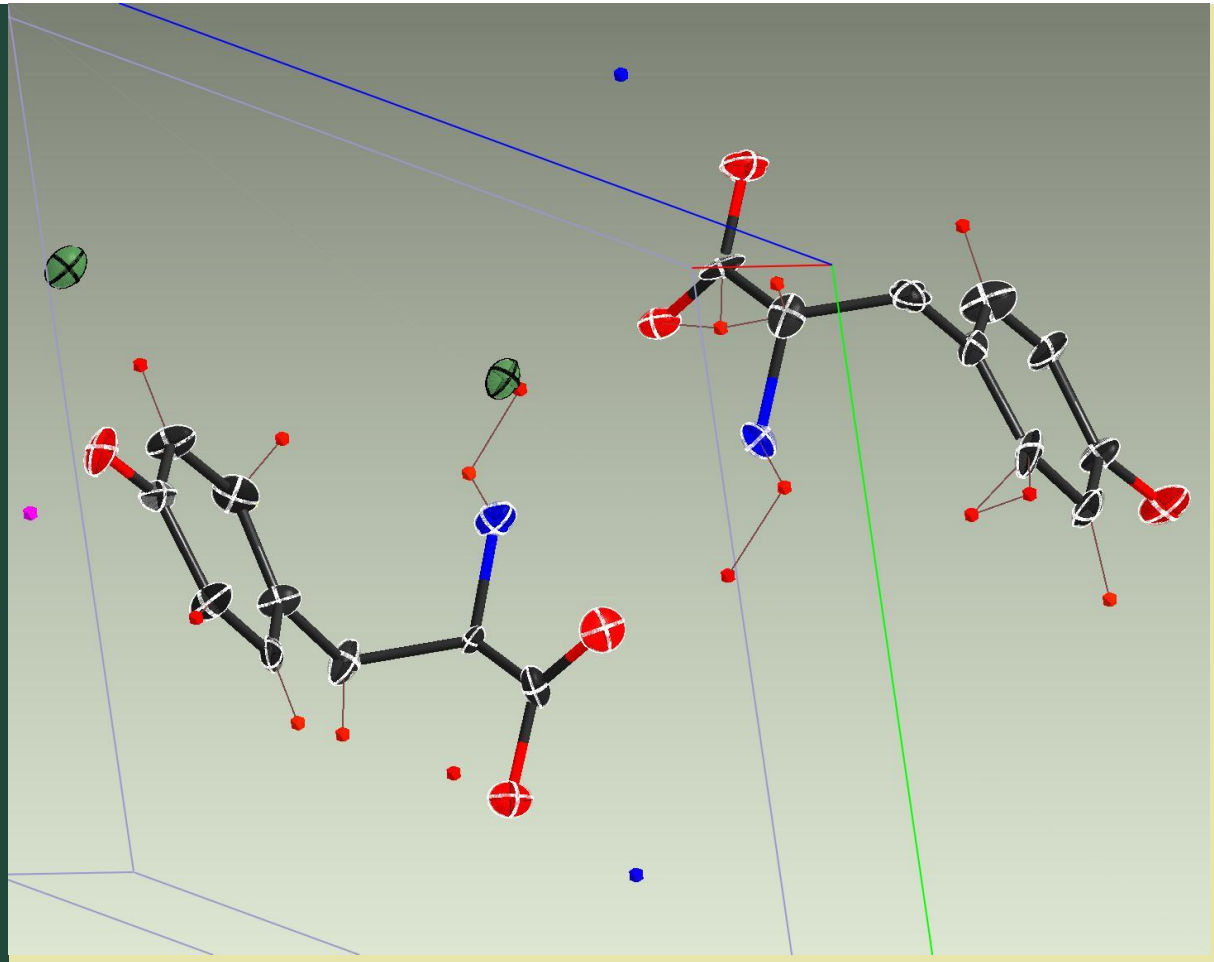
Convenient Functions

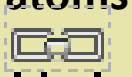


Inverting structure changes the space group if enantiomorphic. Origin is moved if necessary but move in cell might then be necessary

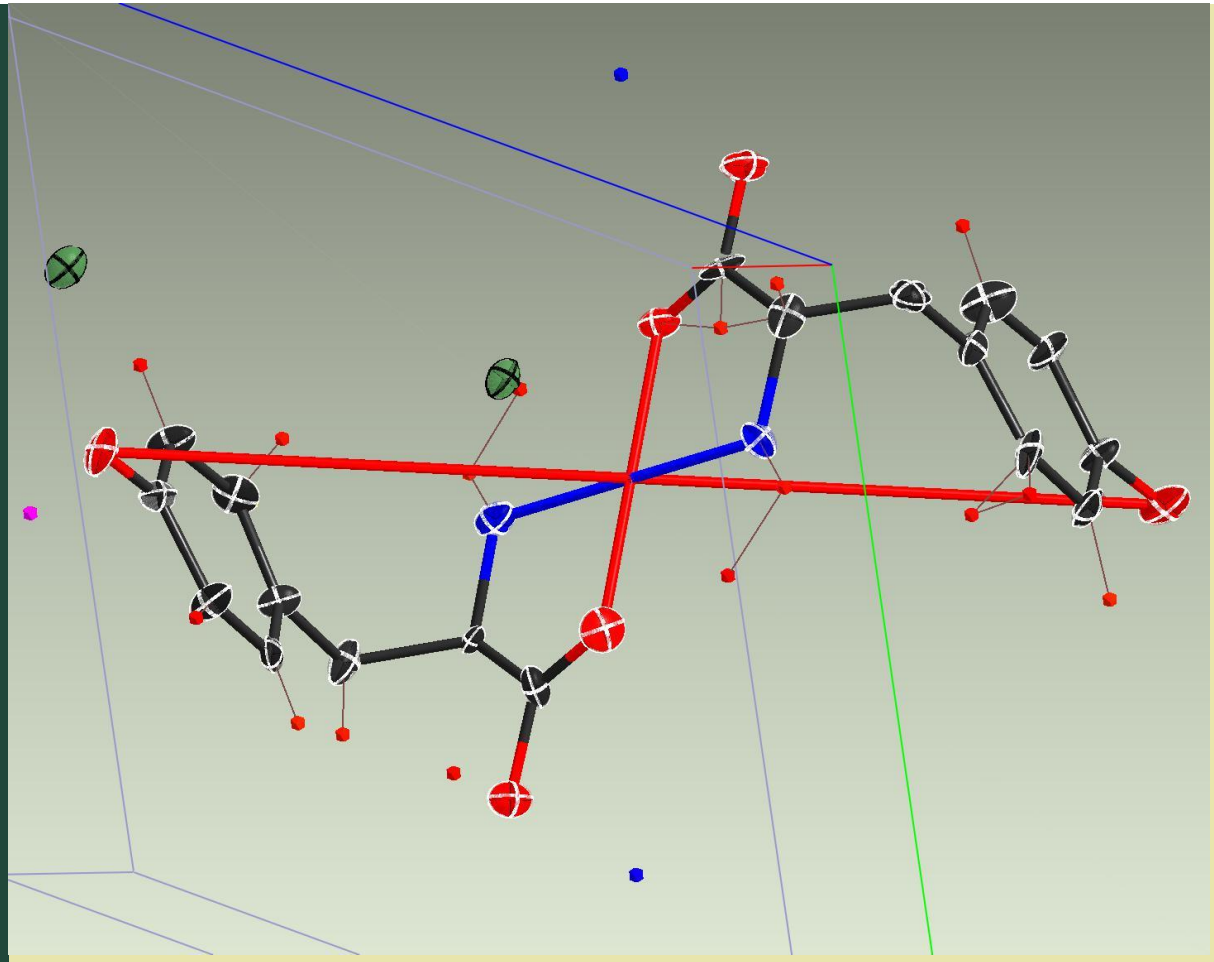
Use  **before and after!**

Example: Solved Structure in P1 which is P-1



1. Select pairs of chemical identical atoms and click on 

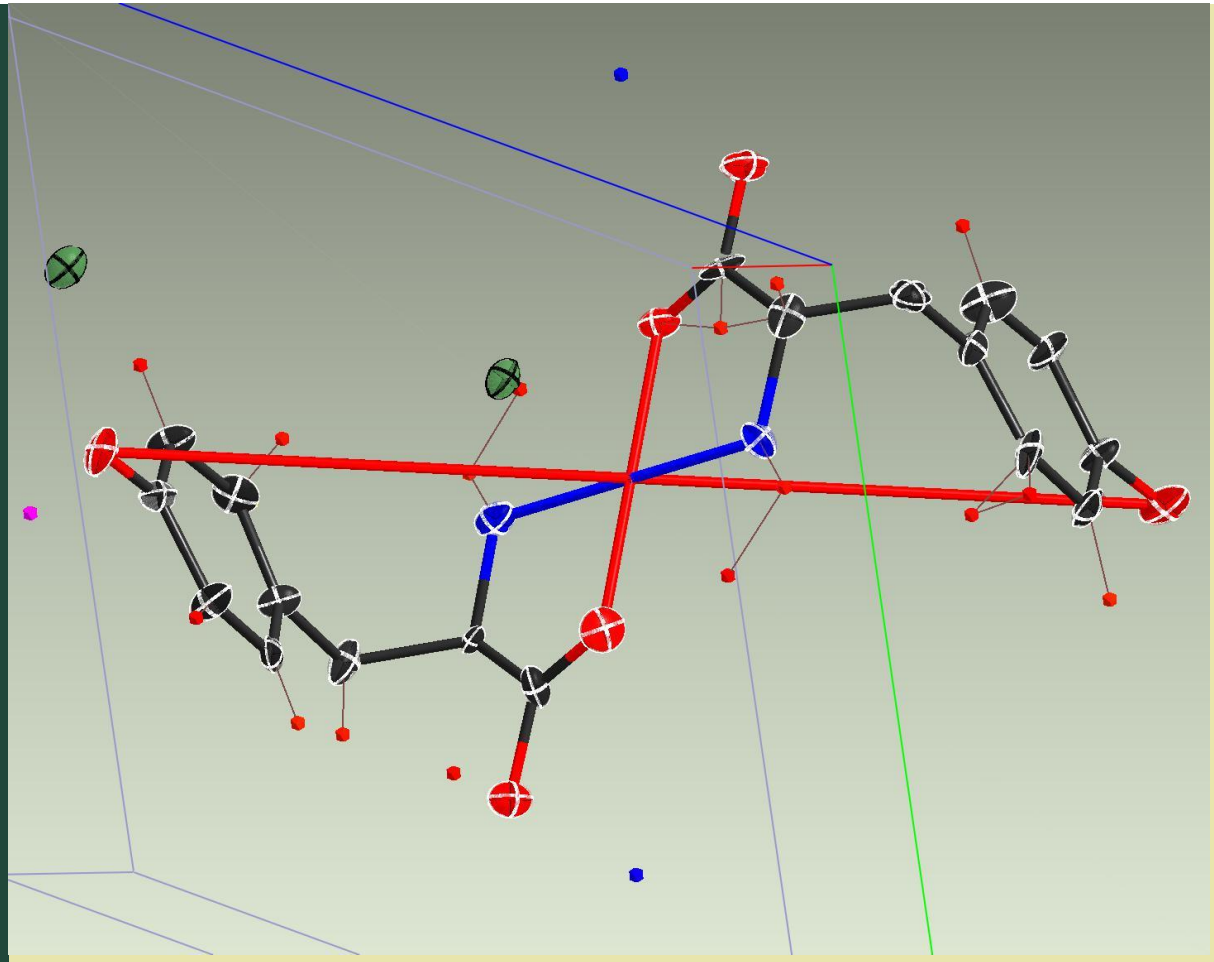
Example: Solved Structure in P1 which is P-1



1. Select pairs of chemical identical atoms and click on 

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 

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** 

Example: Solved Structure in P1 which is P-1

```
Cnt1 6   1.130679   0.261422   0.095238 10.000 0.001 ! centroid
REM Cnt1 was created from: C1, C2, C3, C4, C5, C6, C7, C8, C9, C10, C11, C12,
REM  C13, C14, C15, C16, C17, C18, O19, O20, O21, O22,
REM  O23, O24, N25, N26,
FREE Cnt1 C1 ! this might be needed for AFIX
FREE Cnt1 C2 ! this might be needed for AFIX
FREE Cnt1 C3 ! this might be needed for AFIX
FREE Cnt1 C4 ! this might be needed for AFIX
FREE Cnt1 C5 ! this might be needed for AFIX
FREE Cnt1 C6 ! this might be needed for AFIX
FREE Cnt1 C7 ! this might be needed for AFIX
FREE Cnt1 C8 ! this might be needed for AFIX
FREE Cnt1 C9 ! this might be needed for AFIX
FREE Cnt1 C10 ! this might be needed for AFIX
FREE Cnt1 C11 ! this might be needed for AFIX
FREE Cnt1 C12 ! this might be needed for AFIX
FREE Cnt1 C13 ! this might be needed for AFIX
FREE Cnt1 C14 ! this might be needed for AFIX
FREE Cnt1 C15 ! this might be needed for AFIX
FREE Cnt1 C16 ! this might be needed for AFIX
FREE Cnt1 C17 ! this might be needed for AFIX
FREE Cnt1 C18 ! this might be needed for AFIX
FREE Cnt1 O19 ! this might be needed for AFIX
FREE Cnt1 O20 ! this might be needed for AFIX
FREE Cnt1 O21 ! this might be needed for AFIX
FREE Cnt1 O22 ! this might be needed for AFIX
FREE Cnt1 O23 ! this might be needed for AFIX
FREE Cnt1 O24 ! this might be needed for AFIX
FREE Cnt1 N25 ! this might be needed for AFIX
FREE Cnt1 N26 ! this might be needed for AFIX
HKLF 4
```

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

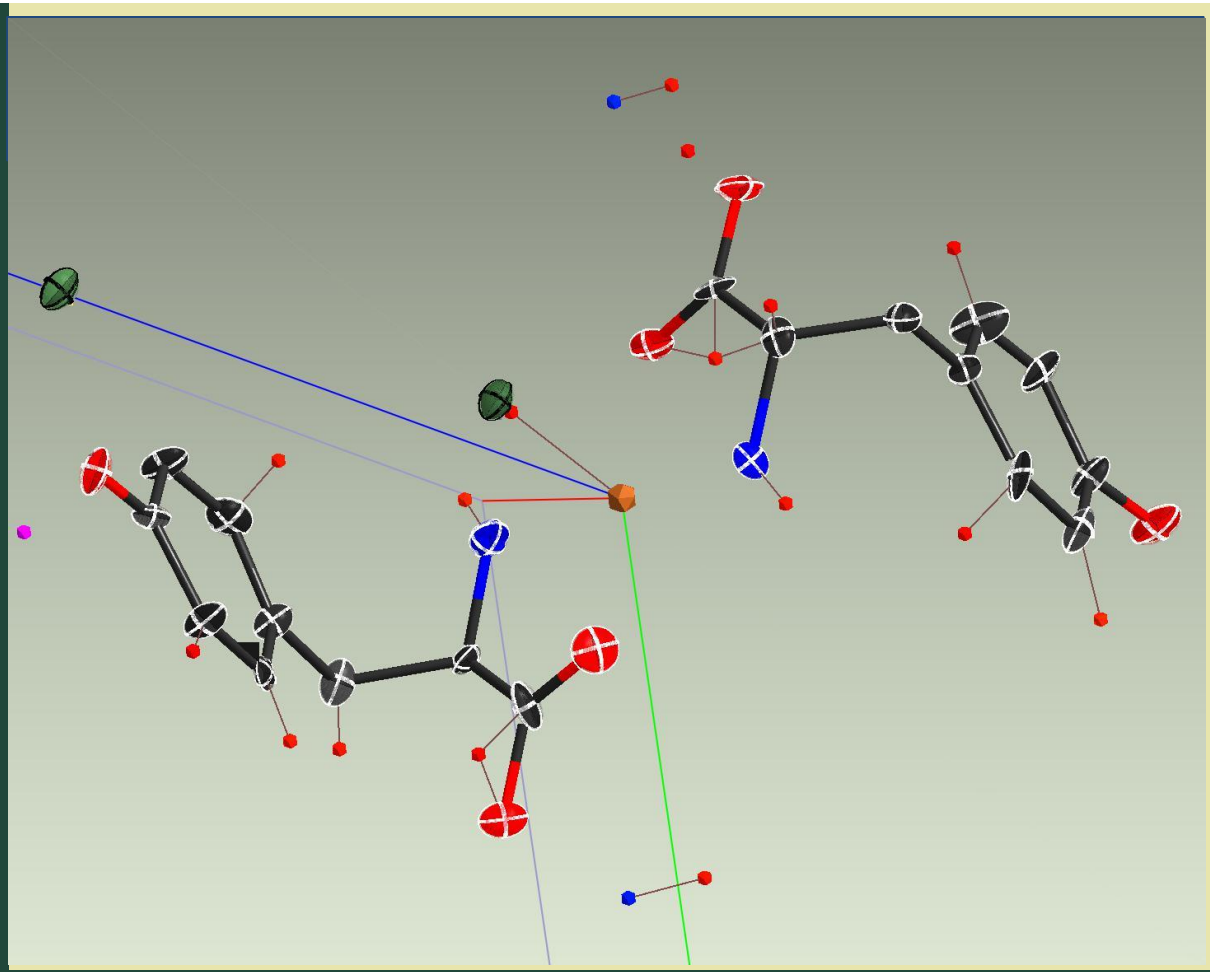
Example: Solved Structure in P1 which is P-1

```
Cnt1 6   1.130679   0.261422   0.095238 10.000 0.001 ! centroid
REM Cnt1 was created from: C1, C2, C3, C4, C5, C6, C7, C8, C9, C10, C11, C12,
REM  C13, C14, C15, C16, C17, C18, O19, O20, O21, O22,
REM  O23, O24, N25, N26
WGHT    0.100000
FVAR       0.80940
MOVE -1.130679   -0.261422   -0.095238 1
C1    1    1.055496    0.039846   -0.494321    11.00000    0.01628    0.02566 =
         0.02449    0.01886    0.01100    0.00772
FREE Cnt1 C6 ! this might be needed for AFIX
FREE Cnt1 C7 ! this might be needed for AFIX
FREE Cnt1 C8 ! this might be needed for AFIX
FREE Cnt1 C9 ! this might be needed for AFIX
FREE Cnt1 C10 ! this might be needed for AFIX
FREE Cnt1 C11 ! this might be needed for AFIX
FREE Cnt1 C12 ! this might be needed for AFIX
FREE Cnt1 C13 ! this might be needed for AFIX
FREE Cnt1 C14 ! this might be needed for AFIX
FREE Cnt1 C15 ! this might be needed for AFIX
FREE Cnt1 C16 ! this might be needed for AFIX
FREE Cnt1 C17 ! this might be needed for AFIX
FREE Cnt1 C18 ! this might be needed for AFIX
FREE Cnt1 O19 ! this might be needed for AFIX
FREE Cnt1 O20 ! this might be needed for AFIX
FREE Cnt1 O21 ! this might be needed for AFIX
FREE Cnt1 O22 ! this might be needed for AFIX
FREE Cnt1 O23 ! this might be needed for AFIX
FREE Cnt1 O24 ! this might be needed for AFIX
FREE Cnt1 N25 ! this might be needed for AFIX
FREE Cnt1 N26 ! this might be needed for AFIX
HKLF 4
```

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

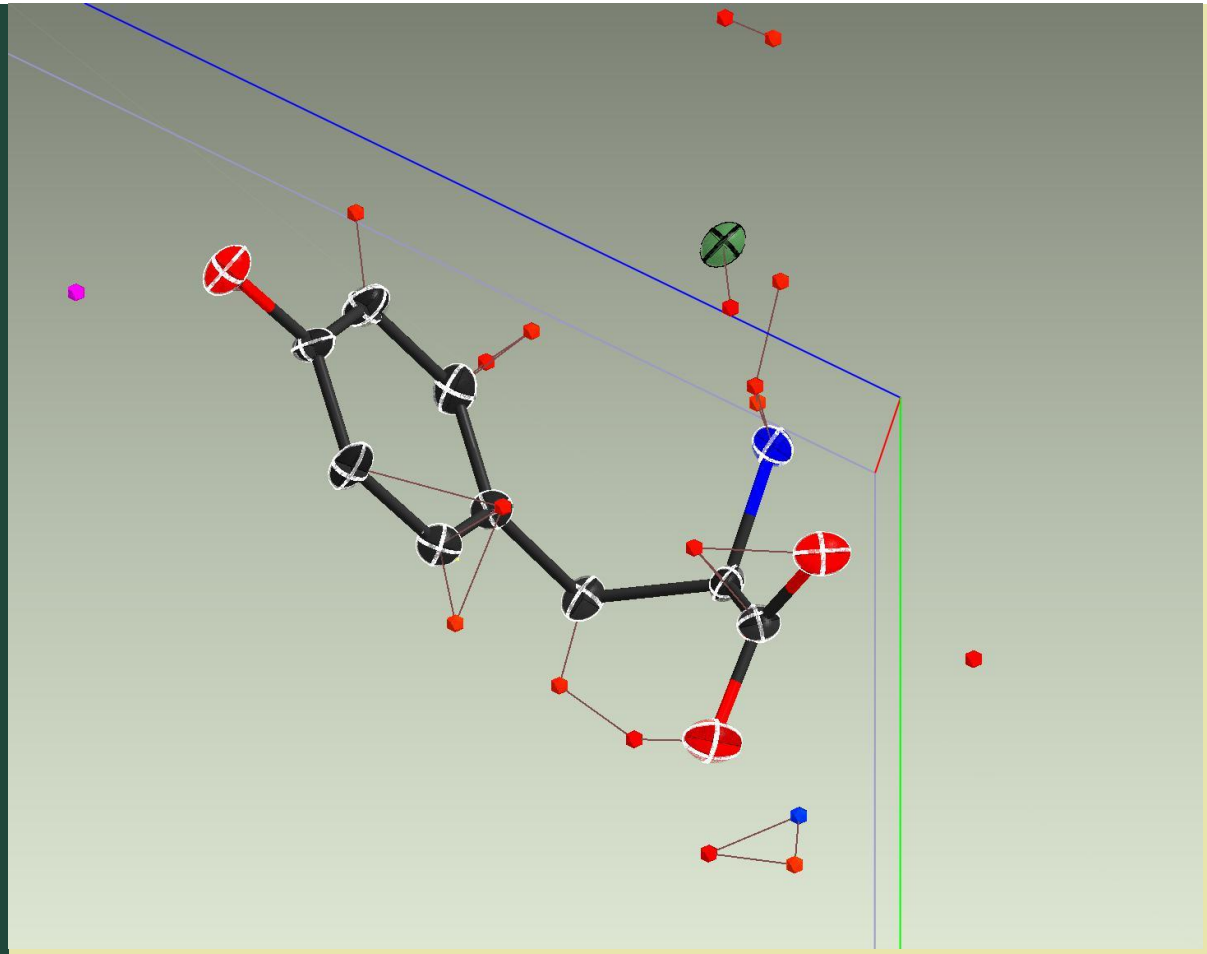
2. Select coordinates of the Cnt1 and copy to clipboard
3. Type in MOVE and paste the coordinates
4. Change the sign of the coordinates and add 1

Example: Solved Structure in P1 which is P-1



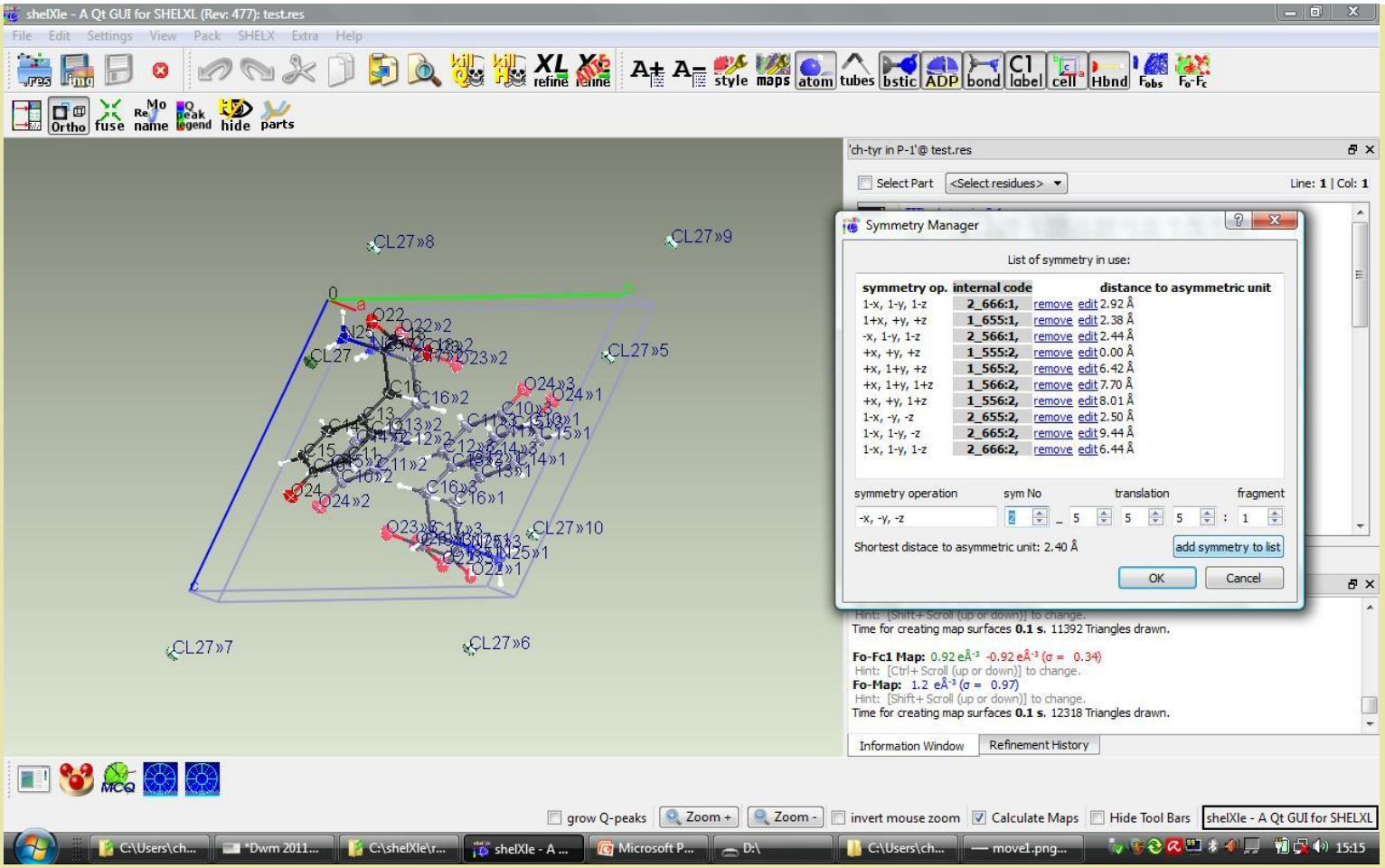
1. **Change the sign of the coordinates and add 1**
2. **Save and refine.**
3. **The Centroid dummy atom should no be at the origin.**
4. **Select the no longer needed fragment and delete them.**
5. **Delete the centroid dummy if you want**
6. **Change** LATT -1 **into** LATT 1 **and save + refine.**

Example: Solved Structure in P1 which is P-1

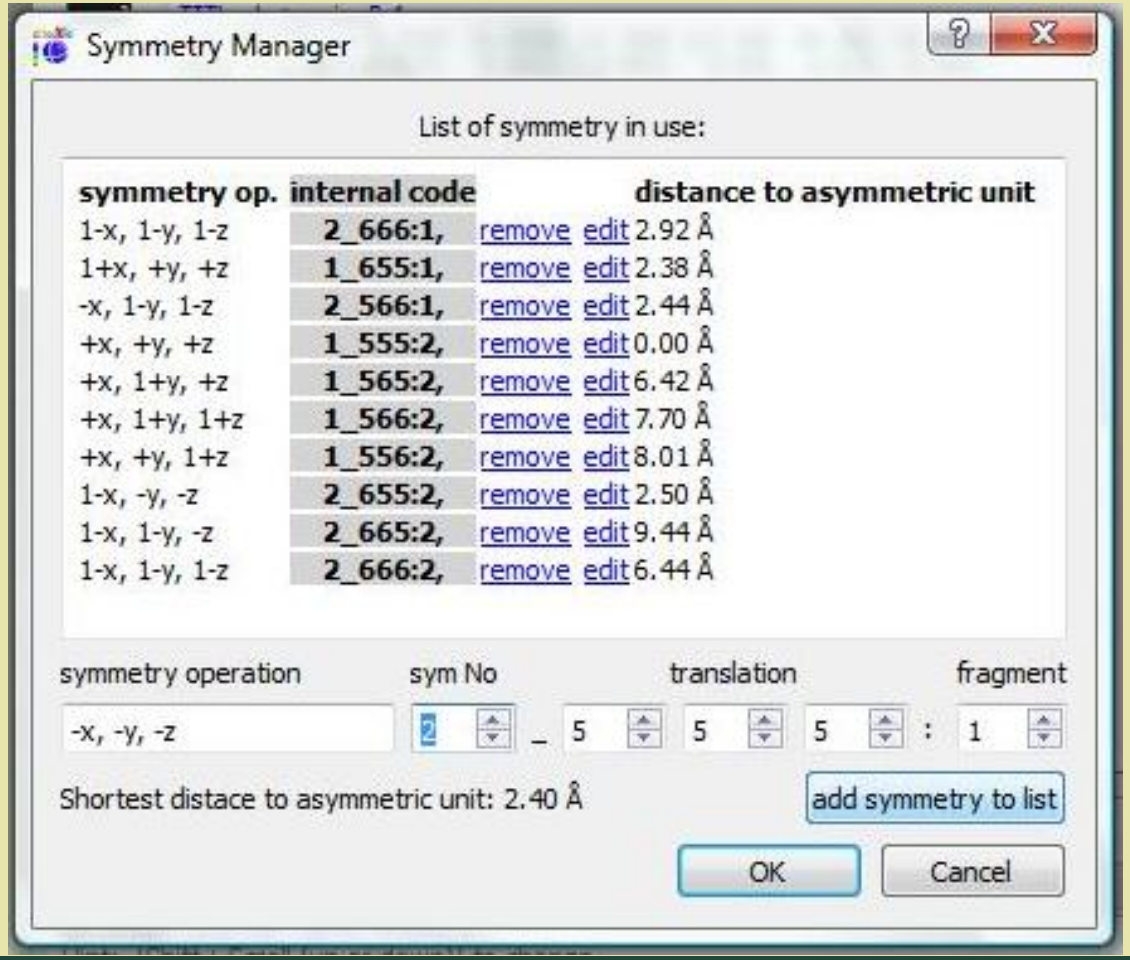


1. **Change the sign of the coordinates and add 1**
2. **Save and refine.**
3. **The Centroid dummy atom should no be at the origin.**
4. **Select the no longer needed fragment and delete them.**
5. **Delete the Centroid dummy if you want**
6. **Change** LATT -1 **into** LATT 1 **and save + refine.**

Symmetry manager



Symmetry manager



ENVI

Information Window

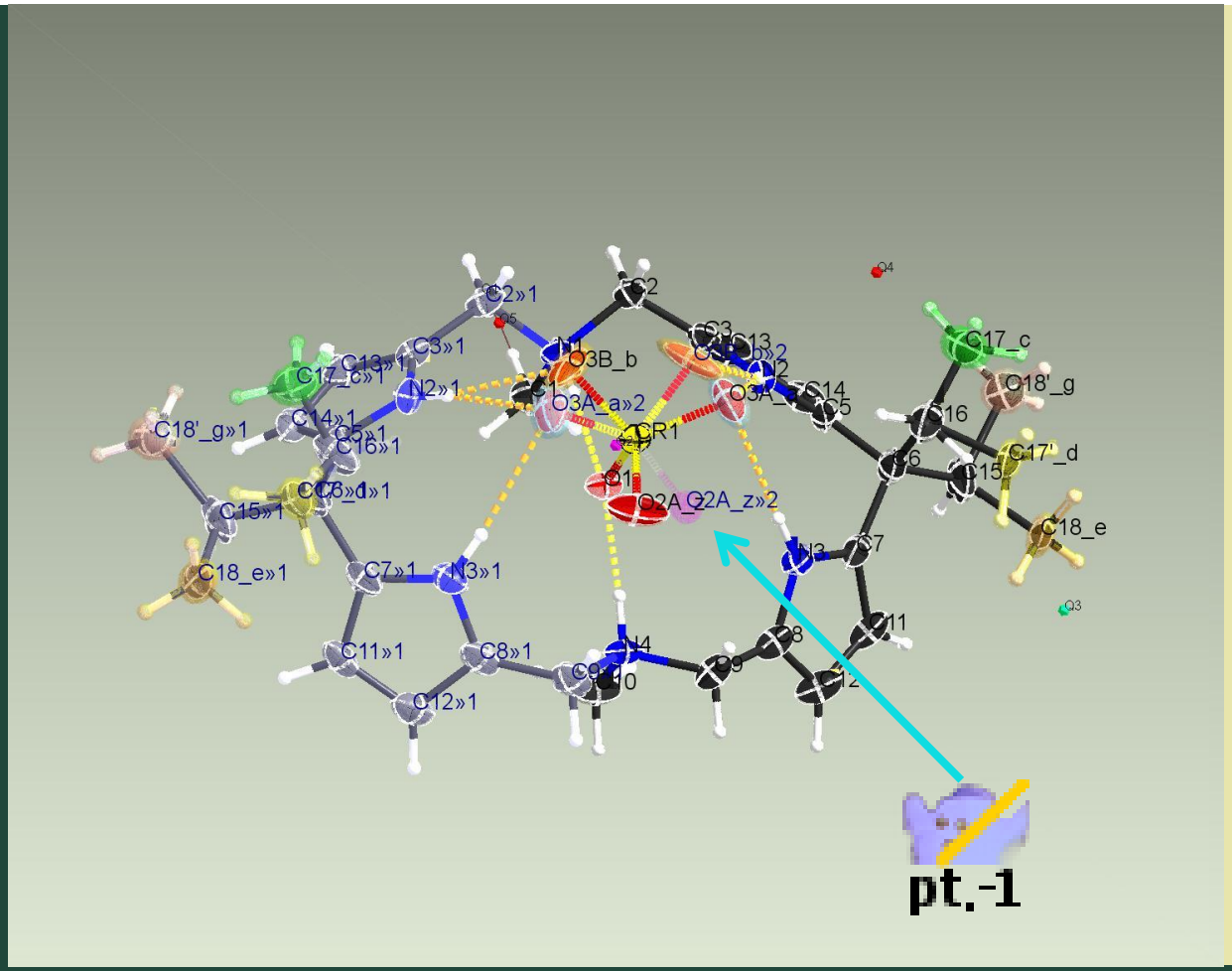
»3 : 1-x, -y, 1-z

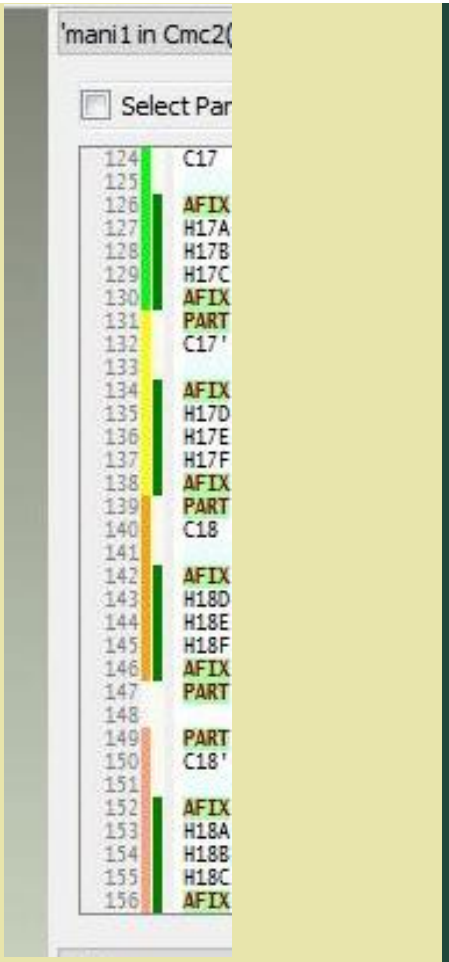
Environment of C17

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°	88.81°			
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°	36.83°	64.78°		
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°	22.29°	70.43°	15.87°	
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°	21.13°	95.78°	56.72°	41.08°
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°	35.23°	107.55°	71.77°	56.35°
		H17	N25	C18	C16	H25b	H25a	H25c	H16b	H16a	O23	O22	C13	O22»1	H12	C12

»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!)*