

RLATT (Reciprocal Lattice Display Program) Version 3.0

1. Introduction

RLATT is a Windows NT program developed by Bruker-AXS for displaying X-ray diffraction reflections in reciprocal space. RLATT can display reflections from SMART .P4P and .SPIN files (indexing not necessary), from SHELXTL type ASCII files (.HKL, .RAW, ._RF, .POW), or from SAINT binary files (._RB). The reflections are displayed with varying brightness levels corresponding to the reflection intensities.

2. Reflection Color Description

.P4P / .SPIN Files	.RAW, .HKL, ._RF & ._RB Files
White -- Has all flags (ACHS)	Cyan -- SAINT or SHELXTL files
Magenta -- Missing C and H flags	
Yellow -- Missing A flag	
Red -- Missing C flag	
Green -- Missing H flag	
Blue -- Missing S flag	

The reflection color dependency is ranked by priority in this table. For example: if a reflection from a parameter (.P4P / .SPIN) file has only an S flag it will appear magenta rather than yellow because missing the C and H flags takes precedence over missing the A flag. The A flag implies that the angles are known, the C flag implies that the reflection was centered (observed on more than one frame), the H flag implies that the reflection was indexed and the S flag implies that the frame was unwarped. Use the Help > Quick Color Reference menu item to display the above color reference on-screen.

3. Mouse and Keyboard Commands: Operation Modes

There are three distinct operation modes in RLATT that control the outcome of depressing the left mouse button or a keyboard key. You can choose among the rotation, the measurement, or the graphical editing modes. You choose which mode is in effect by selecting an option from the RLATT menu. A check mark is displayed by the option chosen.

Rotation Mode (Display > Rotate)

Note: Holding down the Shift key before pressing the following keys will speed up rotation, whereas holding down the / key will slow down rotation. (All rotation occurs around the axes of the plane of the screen.)

Left Arrow -- Left-handed rotation around the Y-axis.
 Right Arrow -- Right-handed rotation around the Y-axis.
 Up Arrow -- Left-handed rotation around the X-axis.
 Down Arrow -- Right-handed rotation around the X-axis.
 Insert -- Left-handed rotation around the Z-axis.
 Delete -- Right-handed rotation around the Z-axis.
 F1 -- Right-handed rotation of 90 degrees around the X-axis.
 F2 -- Right-handed rotation of 90 degrees around the Y axis.
 F3 -- Right-handed rotation of 90 degrees around the Z axis.
 Shift + F5-F8 -- Store the current orientation of the reflections.
 F5-F8 -- Restore a previously saved orientation.
 + -- Zooms in.
 - (Minus) -- Zooms out.

Holding down the middle mouse button while dragging the mouse backward zooms in on the reflections, while pushing the mouse forwards zooms out. If there the user does not have a functioning middle mouse button then pressing and holding both the Ctrl and Alt key followed by the left mouse button will achieve the same results. Panning the structure can be accomplished by dragging the mouse while the right button is being pressed, or, if the user has no functioning right mouse button, by dragging the mouse while the Ctrl key and the left mouse button are being pressed.

Measurement Mode (Display > Measure distance)

In this mode you can measure distances corresponding to the displayed lattice. Choose a start point on the screen, click and hold the left mouse button down, drag the mouse to an end point on the screen, then release the left button. RLATT will measure (in reciprocal angstroms) the distance between the two points on the screen. By pressing the + key, you can subdivide the current measurement. RLATT will then measure the distance between these subdivided planes. Pressing the - key will reduce the number of subdivisions by one. Pressing the Page Up key will add extra subdivisions onto the ends of the measurement based on the current distance between subdivisions. Note that since these additional subdivisions are of the same length as the previous subdivisions the measurement distance will not be affected by them. Hence these subdivisions are only useful for ensuring that you have properly placed the measuring tool. Pressing the Page Down key removes the two outermost subdivisions. In this mode the arrow keys maneuver the measurement tool within the plane of the screen.

Graphical Editing Mode (Edit > Delete or Add a flag)

You invoke this tool by choosing an option from the edit menu. If selection box editing is currently selected, then clicking and holding the left mouse button while dragging the mouse creates a box. Once you release

the left mouse button the box holds its position. If you then press the enter key, the action chosen is performed (adding or deleting particular reflection flags). Changing the reflection flags will often alter the color of the displayed reflections (see the color description above).

If lattice overlay editing is selected, then clicking and dragging the mouse functions identically to the measurement tool. The +, -, Page Up, and Page Down keys are used to control the subdivisions of the lattice overlay, and the arrow keys are used to adjust its position within the plane of the screen. In this mode any reflections touched by the parallel planes of the overlay are altered according to the current flag-editing menu selection.

5. Intensity Scaling

You can alter the displayed intensity of all the reflections by adjusting the slider bar on the right-hand side of the screen. Moving the slider up multiplies all reflection intensities by the same amount. Reflections represented by square, over-sized spots indicate that the screen intensity is maximized for those reflections.

6. Toggling and Filtering Reflections

There are two methods for toggling reflections on and off. The simplest method for toggling reflections by color is to press the key corresponding to the first letter of their displayed color. Press W to toggle white reflections, R for red, Y for yellow, G for green, C for cyan, and B for blue. The second method for selectively displaying reflections is to use the Filter menu option to open up the reflection filter dialog box. You can filter the reflections by choosing any combination of flags, indices or resolution parameters. There is also an option in the Filter menu for displaying the reflections scaled by the intensity divided by the estimated standard deviation in intensity, $I/\Sigma(I)$, instead of the intensity. Because the reflections obtained from a parameter file do not have Σ s available, choosing the $I/\Sigma(I)$ option will suppress all parameter file reflections.

7. Adding Reflections to the Display and Saving Results

Add reflections to the display by choosing the File > Add Reflections option. There is no limit to the number of reflections that can be added to the display by multiple file inputs, but the number of reflections shown while the lattice is being rotated with the mouse is limited to the 2000 most intense reflections (for performance purposes). A parameter file must be read before a .HKL, .RAW, ._RF, .HKL or ._RB file can be read (the parameter file is needed

for the orientation matrix). The display will be re-scaled for the reflection intensity each time a new data file is read, but hidden reflections will be ignored. Remove all stored reflections (displayed and hidden) by choosing the File > Clear Reflections option.

You can save your reflections to a parameter file by choosing the File > Save Results option. The parameter file saved will include the parameters from the last .P4P or .SPIN file read and will also include all the reflections read from other parameter files (but not SAINT or SHELXTL output files). The saved reflection flags depend upon the results of any graphical editing you have done. You can choose whether to include or exclude hidden (filtered or toggled) reflections by checking or unchecking the box marked "Include Hidden Reflections" in the Save menu.

8. Background and Axes Options

The background color and brightness can be adjusted from the Display > Background Color menu. You can display either direct space, reciprocal space or laboratory axes by choosing the appropriate option from the Display menu.