

Introduction to XDisp Qt

The New HKL-2000 and HKL-3000 Diffraction Image Display

HKL-2000 and HKL-3000 have a new, sleeker way of displaying your diffraction data, because HKL is now distributed with XDisp Qt, the new version of the program that displays and interacts with diffraction images. This new version may not be the default version in your setup. To work with the new version, in the main menu select “**Options** → **XDisp** → **XDisp Qt**” (Figure 1). You can switch back and forth between the new and old versions of XDisp as you like. To ensure you work with the new version every time, select “**Options** → **Save Options**” while XDispQt is selected. Many of the new features of XDisp Qt will be intuitive for those familiar with the old version of XDisp.



Figure 1. Selecting XDispQt

As before, you can launch the new version of XDisp using either the “**Display**” button in the **Data** tab (Figure 2) or the “**Display**” or “**Peak Search**” button in the “**Index**” tab (Figure 3). If you use the “**Peak Search**” button, XDisp Qt will open and peaks will be picked with default settings, which are often sufficient (Figure 4). The automatic peak search button will pick peaks from several frames, using the number of frames set in the 3D window option. XDisp Qt will pick peaks from all the frames before displaying the image, so expect a slight lag if you set the 3D window high.



Figure 2. Display button from Data tab

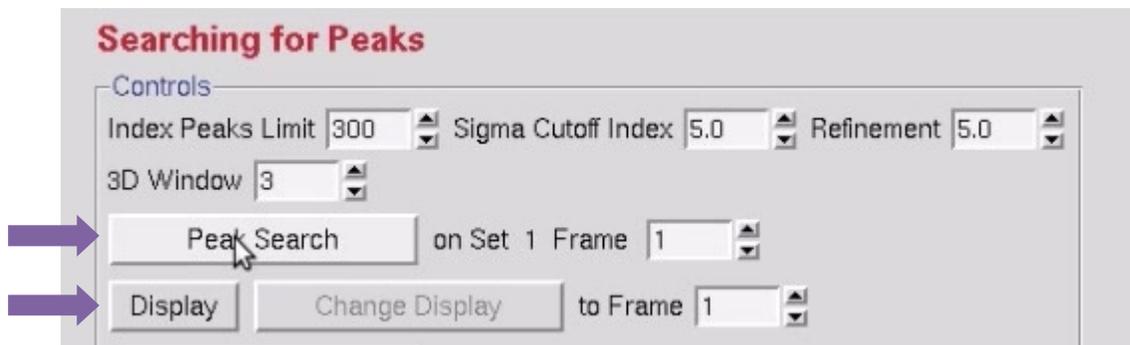


Figure 3. Display and Peak Search Button on the Index tab

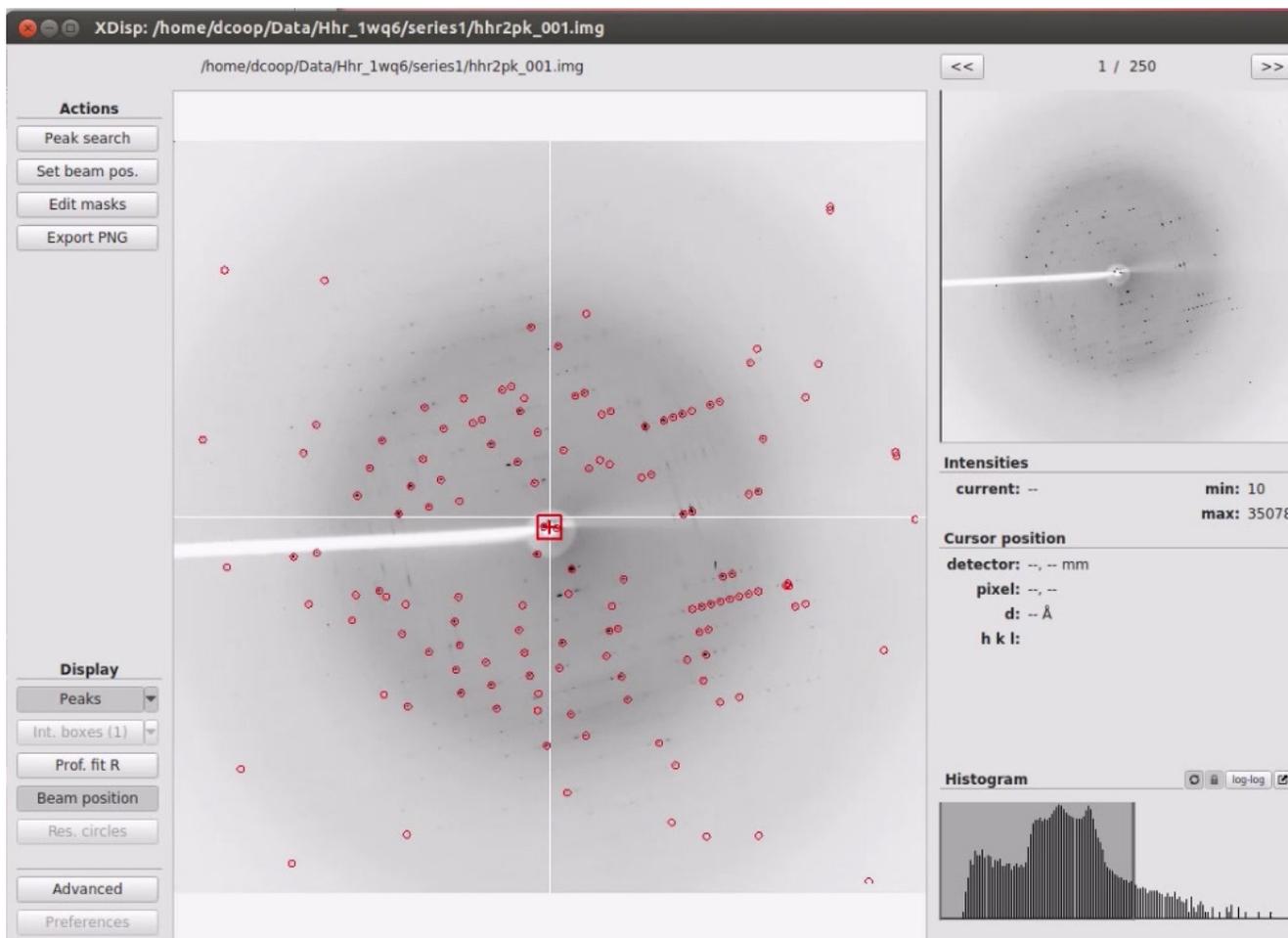


Figure 4. The main window showing an automatic peak search result

The new XDisp has many improvements. Notably, zooming is now controlled by the mouse wheel and will zoom the image using the mouse pointer as the center of the zoom (Figure 5). Push the wheel forward to zoom in. To scroll around the image, click and drag the image with the left mouse button or drag the zoom box around on the image thumbnail on the top right. The window can also be

resized using standard window manipulation methods. I prefer to use Alt-middle-click and drag method, which currently only works on Linux installations. For this, your mouse needs to be inside the window somewhere near a corner, and I find that much easier than either clicking and dragging the exact edge or right-clicking in the window's top panel and selecting “resize”. Zoom in far enough and the numeric intensity value for each pixel will be displayed. Click and drag with the right mouse button to show a cross-hair and intensity distribution for the vertical and horizontal lines displayed on their respective axis.

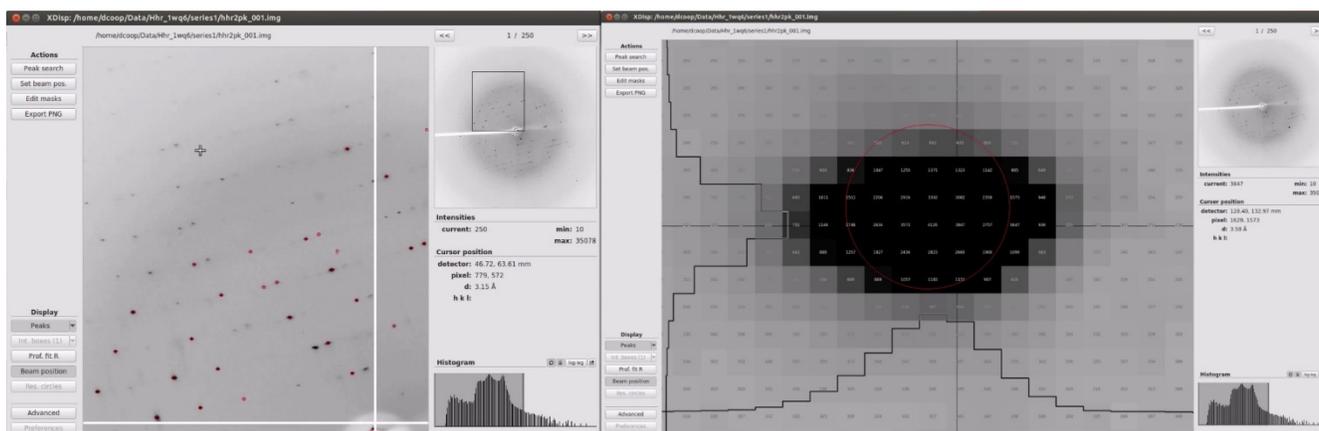


Figure 5. Zoom in the main window using the mouse wheel. Two zoom levels are shown.

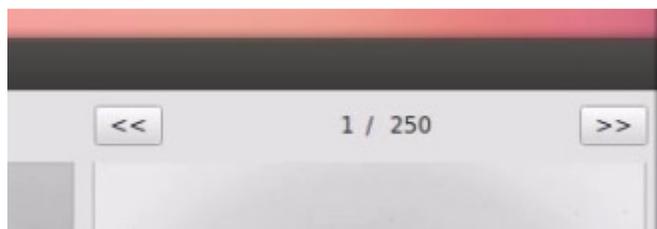


Figure 6. The frame up and down arrows are on the top right.

The *frame up* and *frame down* arrows are on the top right (Figure 6). Change the intensity maximum and minimum using the *intensity histogram* on the bottom right (Figure 7). Click and drag the shaded box to change the range of intensities or drag an edge when it turns yellow to change just the maximum or minimum intensity. If your screen update is too slow, turn off the *automatic refresh* button.

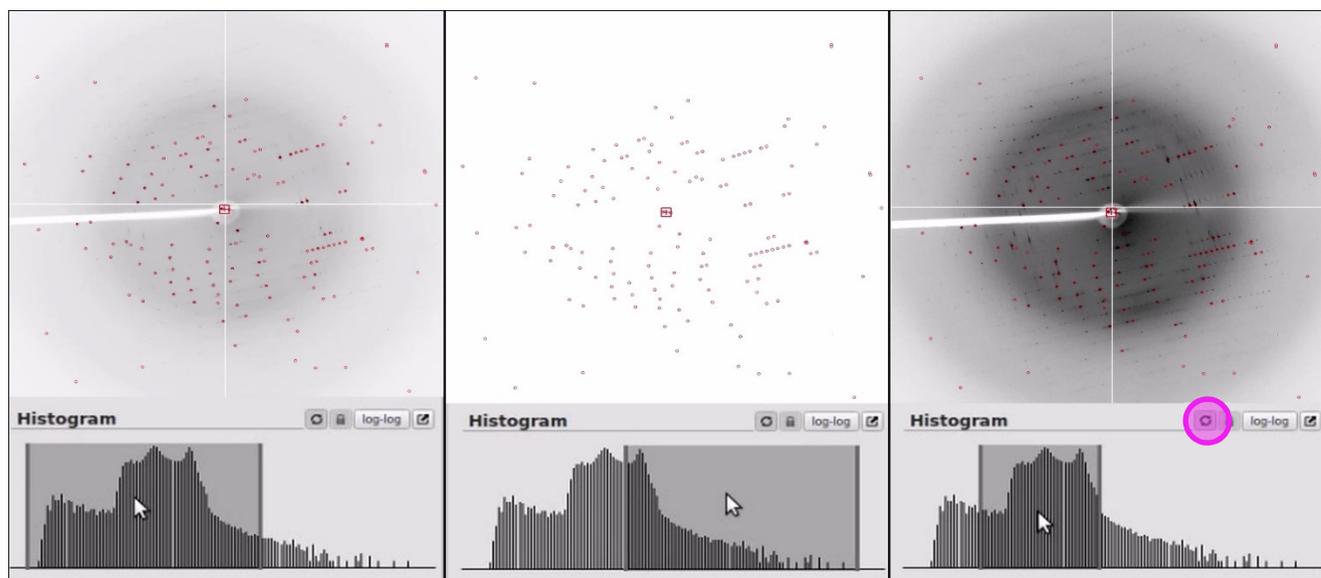


Figure 7. Change contrast with the histogram slider. An **Automatic Refresh Button** is highlighted.

The minimum and maximum intensities for the image are displayed on the right side of the display. The cursor position, intensity at the cursor, and the resolution at the cursor are also displayed when the cursor is in the main window.

To perform a manual peak search, use the peak search button in the top left (Figure 8). The buttons **More Peaks**, **Fewer Peaks**, **Bigger Peaks**, and **Smaller Peaks** work as before, and now have a pop-up description if you hover over the buttons. Use the frame up button to increase the number of frames that will be included in the peak search.

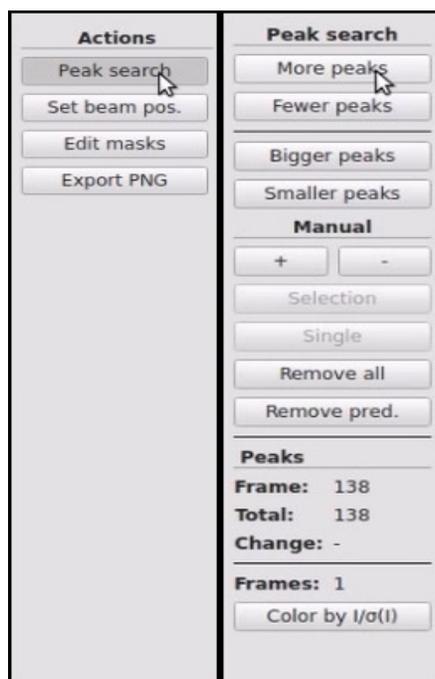


Figure 8. Select "**Peak search**" on the top left to launch the manual peak search. This opens the dialog shown here on the right.

If you want to manually change the peaks that are picked, use the + and - buttons to add or remove peaks. With the + button, click on a reflection to add it to the peak list. With the - button, you can either remove reflections one at a time, or use the selection button and click twice to define a rectangle of reflections that will be removed.

You also have the options of removing all the peaks so you can start over or coloring the peaks by their I/σ levels. *Reset*, *Cancel*, and *Finish* buttons are located at the bottom left. When performing a manual peak search, it is important to click the *Finish* button to save the peaks to a file so they can be used for indexing.

XDisp Qt also allows you to change the beam position using the *Set Beam Pos* button. You can either drag the beam center to a new position or click where you want the beam center to be. This is especially useful if you have collected data at a beamline where the beam center is visible through the beamstop. Xdisp Qt also has a built-in function to find the beam center that can sometimes determine the beam position automatically. This algorithm relies on the distribution of background scatter or ice rings, and doesn't always work. If you are really having trouble locating the beam center, perform a peak search and then use *Find Beam Position* in the *Index* tab of the main HKL window. This function will try to find the beam center by trying to index the image using different values for the beam center. *When it has finished rastering around, the hottest pixel will automatically be selected.* If you want to choose a different pixel, select it and click *Use current*. After that, you can opt to update the stored site information using *Update Site*.

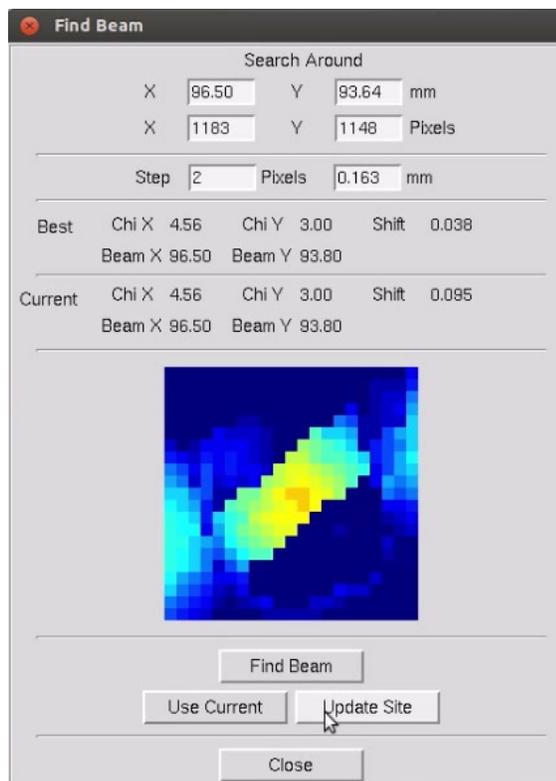


Figure 9. The end of the "Find Beam" process

The **Edit Masks** button provides an easy and intuitive way to define the beam stop or flag regions where a shadow appears on the image. To use this feature, click on a polygon and the corners appear as circles that can be dragged to fit the beamstop shadow. Circular regions have a single control circle on the edge that changes the diameter. The shapes can be moved by clicking inside the shape and dragging it to a new location. More than one mask can be created. To delete a mask, select it and then remove it. Select **Finish** when you are done.

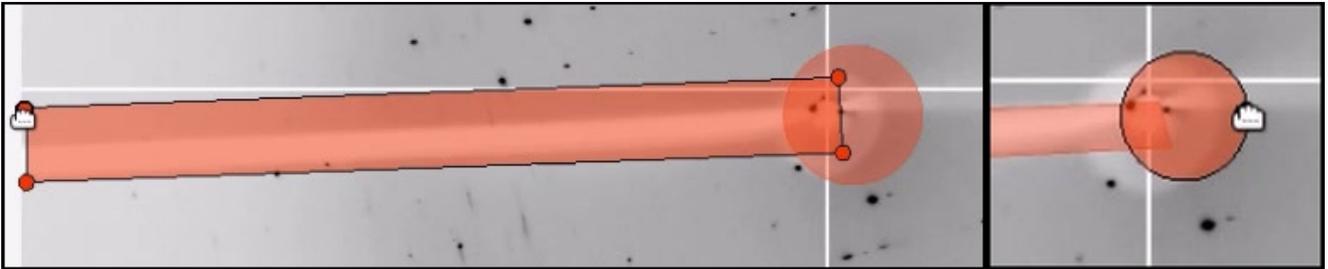


Figure 10. When editing a mask, select a polygon and drag a corner or select a circle and resize using the edge handle. Move either using "click and drag" with the mouse.

The **Export PNG** button is provided to give you an easy means of exporting your image into a lossless format. Simply select the directory and file name and click Save.

The remaining features of XDisp Qt require that you have indexed your data. See the HKL Research Indexing and Scaling video tutorial for details on how this is done. Briefly, I select the **Index** button, refine basic parameters while in P1, use "**fit all**" to refine all parameters, then revisit the **Bravais Lattice**.

Returning to XDisp Qt, you can toggle the predicted reflections on and off using the **predictions** button. The arrow next to the button is a drop down list that controls which reflections are displayed. The default is to show reflections that meet the sigma cutoff level you have set for refinement. By selecting all peaks, you can see how many predicted reflections do not meet this cutoff. You can also display the peaks found during the peak search again.

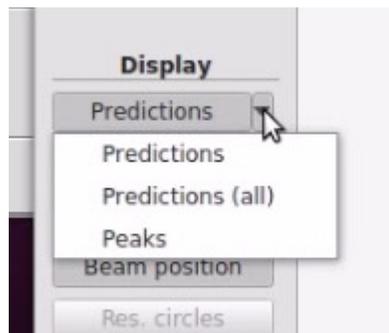


Figure 11. Toggle predicted reflections using the "Predictions" button. Select the type to display using the drop down arrow.

The *Integration boxes* button is also a toggle that will turn on or off the boxes that show the peak and box size. These can only be seen if you are zoomed in close enough. Pixels inside the inner circle are recorded as the peak, pixels between the two circles are the guard region and are not used. Pixels between the box edges and the outer circle are used for calculating the background for the reflection. Xdisp Qt has two ways of coloring the inner circle, which can be selected using the *Integration Boxes (1)* and *Integration Boxes (2)* options using the select dropdown associated with this toggle. Selecting the *Difference Vector* option will show difference vector between the peak maxima and the center of the predicted reflection.



Figure 12. Integration boxes can be displayed to show what is considered the peak, background, and guard region.

The *Profile Fitting Radius* button can be used to show the size of the area that is used to calculate the expected profile for each reflection. The *Beam position* button toggles the beam position crosshairs on and off. The *Res. Circles* button is used to toggle the circles that show various resolutions. These circles are initially displayed from the main HKL window, where you can choose the resolutions you want to display.

If you have questions or comments, please contact HKL Research at support@hkl-xray.com.

