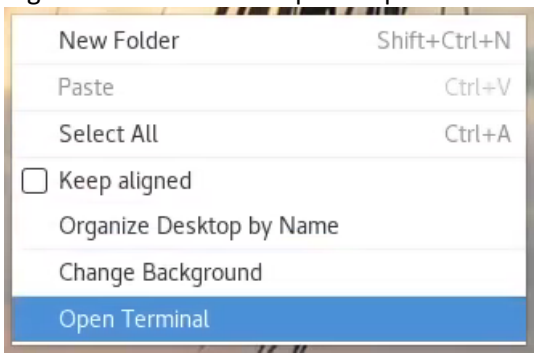
Data Collection

Starting Up

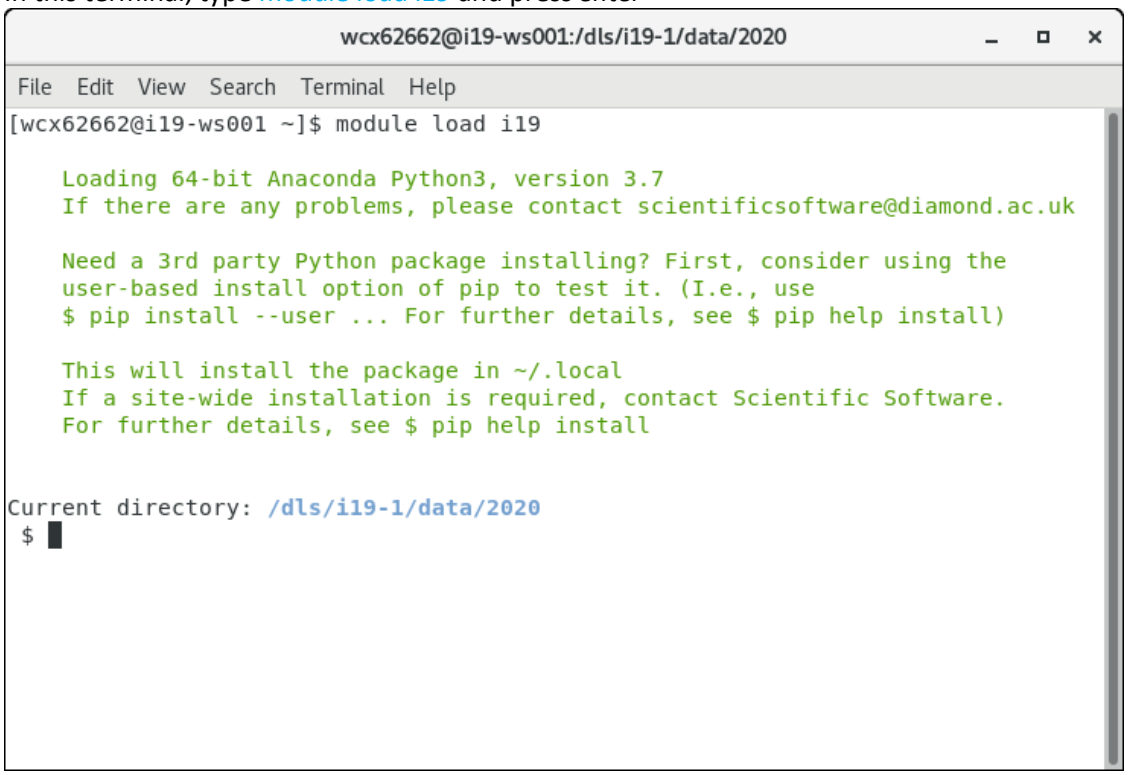
Login to the computers (Linux and Windows) using your FedID (in the form abc12345) and password.

On the Linux machines, we recommend doing the following to make things easier – it should only need to be done once.
Right click on the desktop and open a terminal



This should open a window like below, with your FedID

In this terminal, type module load i19 and press *enter*



This will automatically redirect the terminal to the current visit directory and mean programmes such as DIALS and Albula are ready for use.

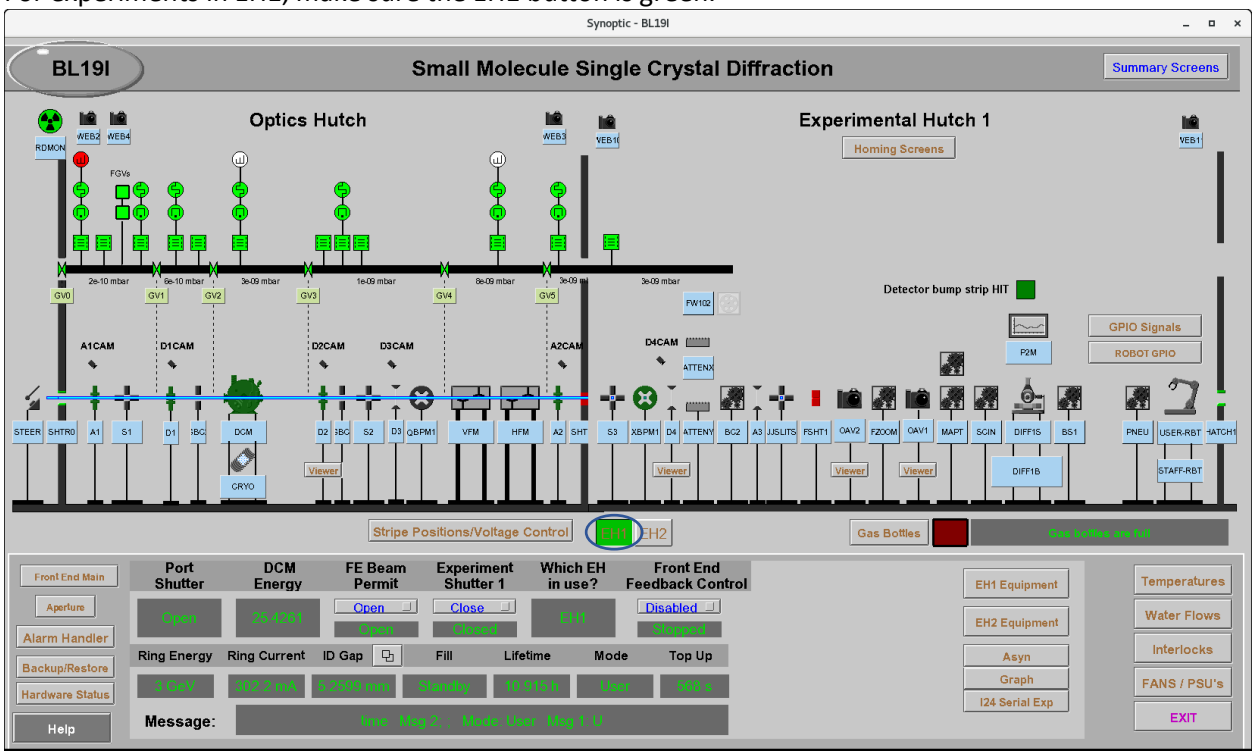
You can then type i19.install_to_profile and press *enter*

This will update your .bashrc file and means the I19 functions are present for any new terminal opened.

Your data are in:
/dls/i19-1/data/YEAR/cyxxxxx (old visits on I19 were mtxxxxx)

Opening The EPICS Synoptic

Click on the Diamond icon  in the top right-hand corner of a Linux workstation (or type Launcher in a terminal if it is unavailable). Select Beamlines from the resulting drop-down menu, followed by BL19I Small Molecule Single Crystal Diffraction. This will open the I19 EPICS Synoptic.
For experiments in EH1, make sure the EH1 button is green.



Cameras

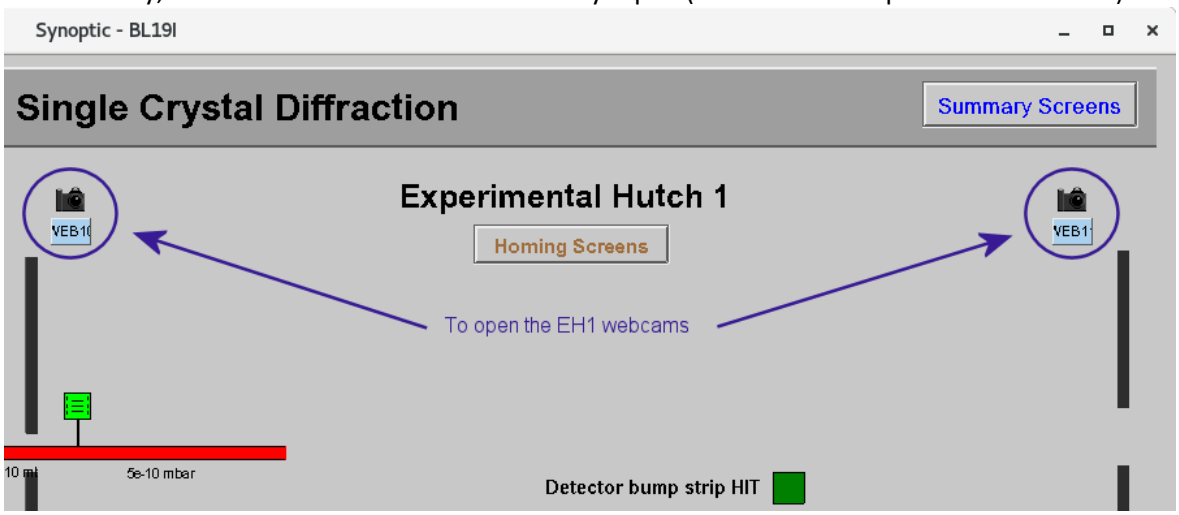
When running experiments from I19, all necessary cameras should already be up and running, however, the information below may be useful if there are any issues, or when not running locally.

Webcams

The 2 webcams in EH1 can be accessed by typing the following URL's in a Firefox window:
i19-webcam10.diamond.ac.uk - to view the sample position
i19-webcam11.diamond.ac.uk - to watch the robot or just for a general view of the hutch

The username and password for both are *i19*

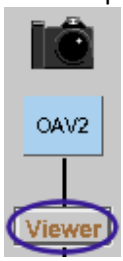
Alternatively, click on WEB10 and WEB11 in the synoptic (either side of Experimental Hutch 1)

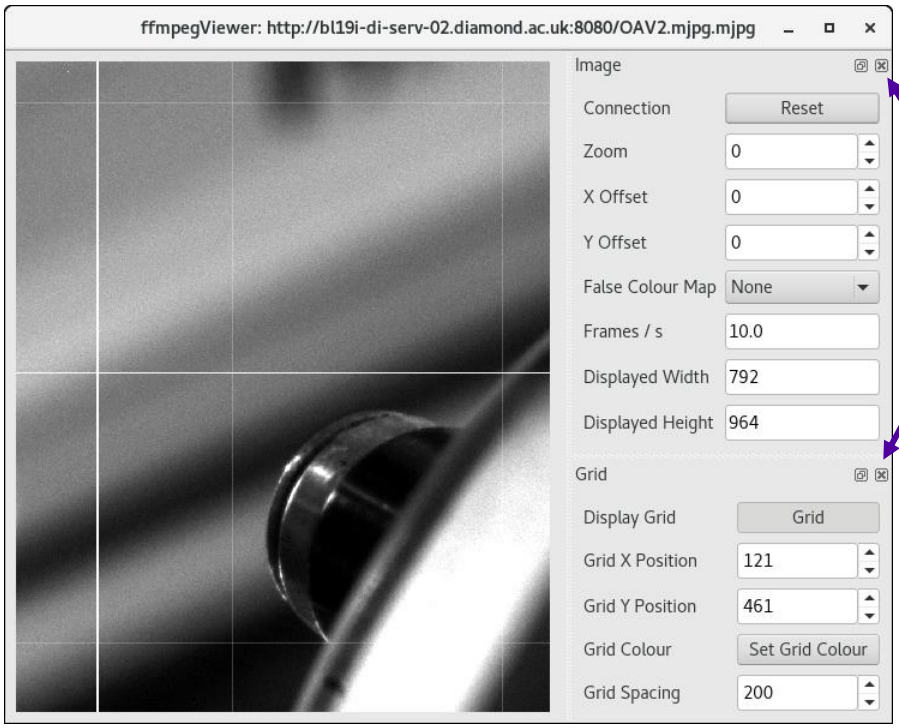


And decide whether to open using Firefox for camera control or as image only – the image only option can be better as it is less demanding over the network, but there are no drive or zoom functions in the view.

Sample position Camera

It is highly recommended to have OAV2 open at all times as it lets you easily see if there is a sample loaded or not and gives a good indication of where to move the sample if it isn't visible on the OAV View. It also gives a good view of the robot loading/unloading, in case there are any issues. The sample position camera is opened through the synoptic by clicking on Viewer, under OAV2.





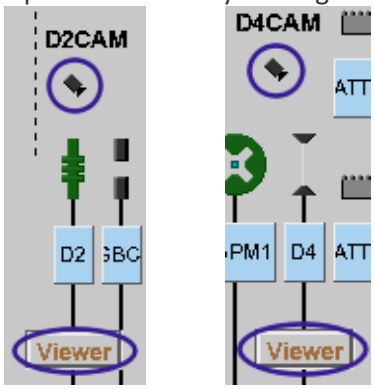
The sections on the right side of the camera view can be closed to make the window smaller and the window can be resized to fit the space available.

If no image is visible, check the camera is on by clicking on the picture of the camera  above the word OAv2 and checking the box next to Acquire is bright green - press Start if necessary to start the camera (see D2, below, for example).

Beam Position Cameras

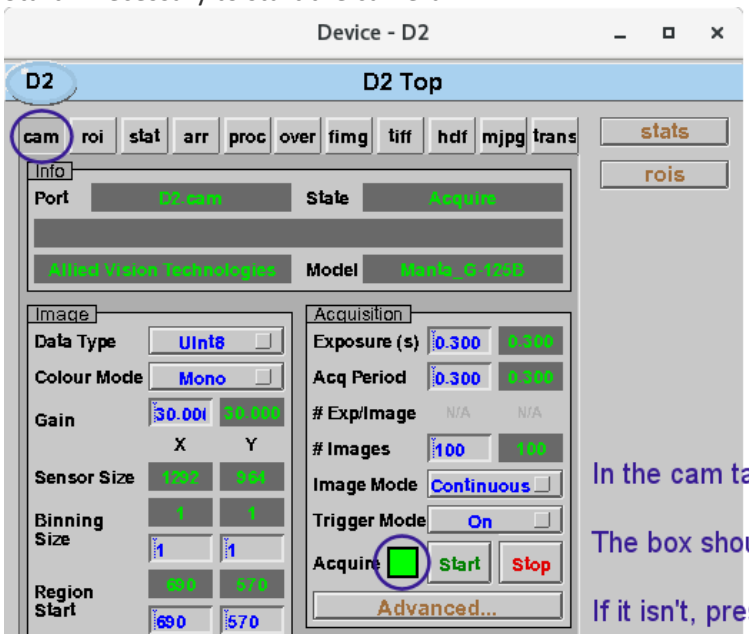
D2 shows the beam in the optics hutch, just after the DCM and D4 shows the beam in EH1, between the attenuators – it may be necessary to remove attenuation in order to see the beam on D4.

Open D2 and D4 by clicking on the Viewer buttons underneath the appropriate name



The sections on the right-hand side of the camera view can be closed to make the window smaller and the window can be resized to fit the space available.

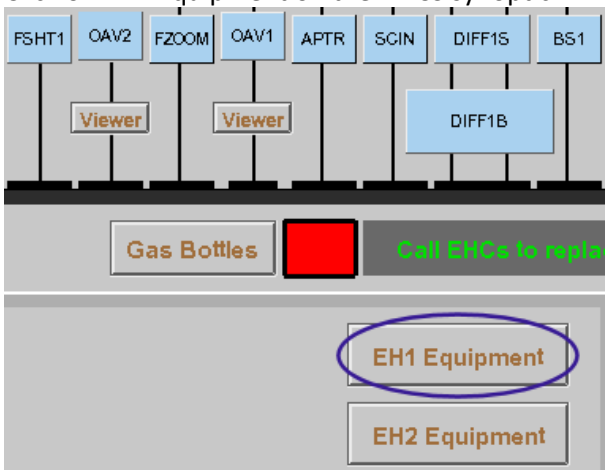
If no image is visible, check the camera is on by clicking on the picture of the camera below the name of the camera to bring up the controls. In the cam tab, check the box next to Acquire is bright green - press Start if necessary to start the camera.



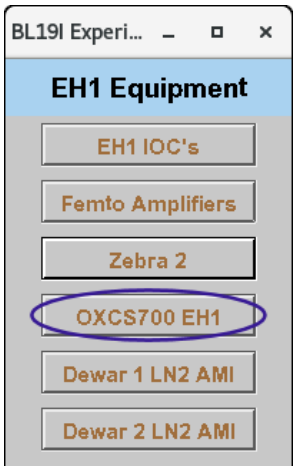
If the camera is still not working, see page 23 of the troubleshooting section.

Cryostream

Click on EH1 Equipment on the EPICS synoptic

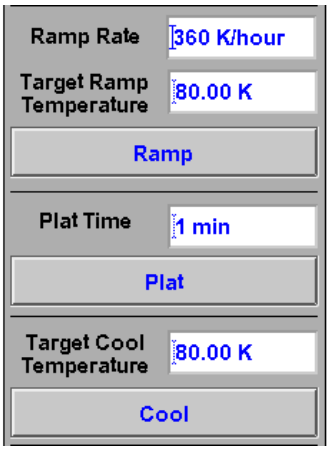


Then select OXCS700 EH1 from the menu to bring up the control interface for the EH1 cryostream.



Type the required value into the Ramp Rate box and press *enter*
Type the required temperature into the Target Ramp Temperature box and press *enter*

Click on the Ramp button



Cooling is quicker than ramping but the temperature does not change at a steady rate

Type the required temperature into the Target Cool Temperature and press *enter*

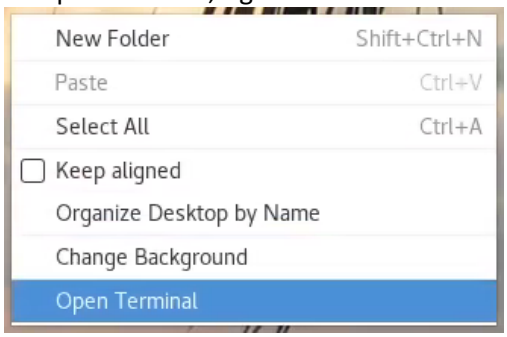
Click on the Cool button

NOTE: The values typed into EPICS boxes will only be updated if the Enter key is pressed afterwards.
The cryostream can also be controlled via the GDA – see page 15.

Opening the GDA

GDA Log

To open the GDA, right click on the desktop to open a terminal.

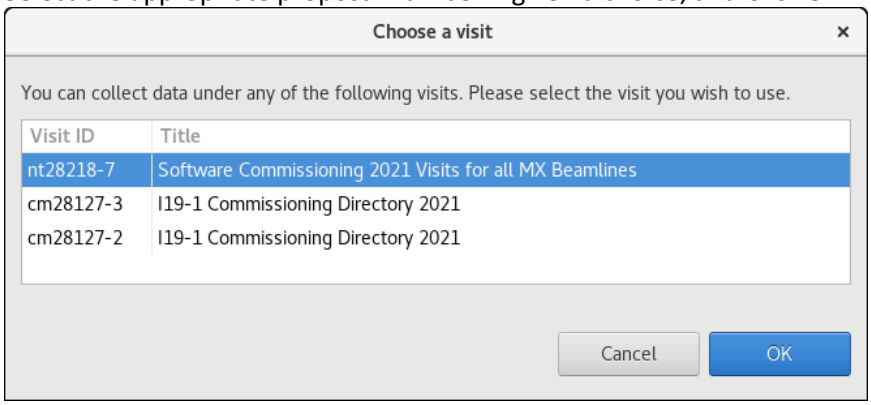


In the terminal window:
Type gdalog1 and then press *enter*

This opens a log panel showing details of all GDA processes and is useful to have available, particularly when using the robot, as a lot more details are shown in the log panel than appear in the Jython console of the GDA. Change the log level to DEBUG for maximum output. Actions are only shown in the log if the log panel is open before they happen, so it is a good idea to have it open all the time. It can be minimised while everything is working.

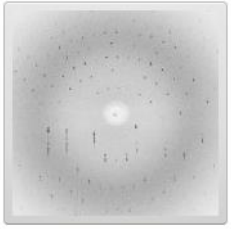
GDA Client

Open a second terminal window:
Type gdaclient1 and then press *enter*
Select the appropriate proposal number if given a choice, and Click *OK*



Occasionally, an old client can become stuck and a new one can't opened – there will be a pop-up prompt for this suggesting it can be resolved by typing:
gdaclient –reset (minus minus reset without spaces)
Note for EH1 experiments, this needs to be gdaclient1 -- reset

Then click on the *Data Collection* icon:



GDA Servers

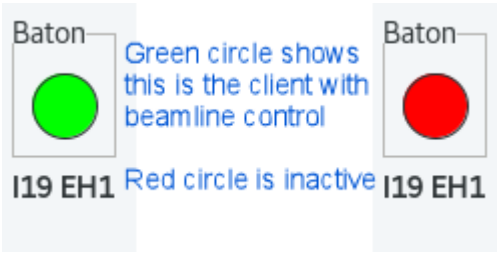
NOTE: There should be no need to restart the GDA servers as this will have been done by beamline staff at the start of the visit. Restarting the servers will close any clients that are open, potentially causing confusion and irritation if other remote colleagues are already logged in.
The servers may need to restarted if:

1. The GDA crashes and a restart is deemed sensible to try and clear the fault
2. A member of the group has left without passing on the baton – restarting the servers closes all clients leaving the baton free for the first person to open a client.

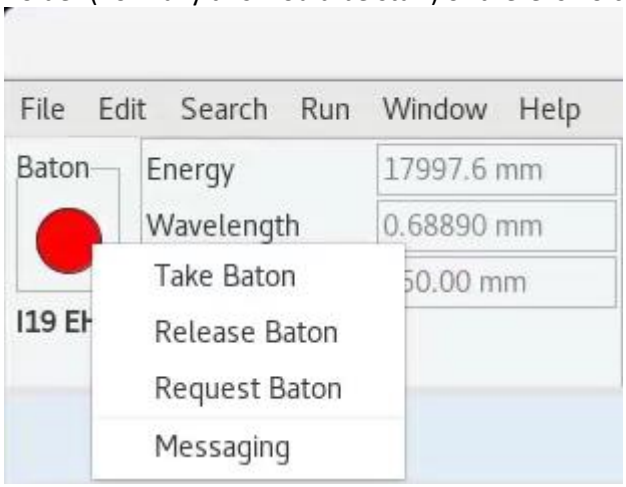
To restart the GDA servers, type gdaservers1 in a terminal and press *enter*
Wait until the box with the bouncing bar disappears and the terminal reads "GDA Server Started" and then open a client with gdaclient1.

Baton Control

Anyone with the GDA open can see what is happening, but only the active GDA client can control the beamline.
Control is passed by means of holding the baton - the active client is green, whilst inactive versions are red.



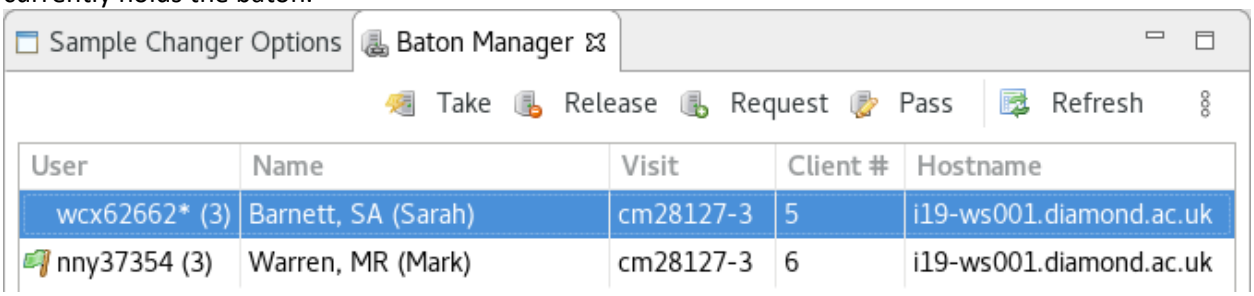
Right click on the circle to bring up the menu.
When switching control either request or take the baton - requesting lets the current user know you are looking to take control. You can only take the baton if you have greater privileges than the current baton holder (normally this would be staff) or there is no current holder.



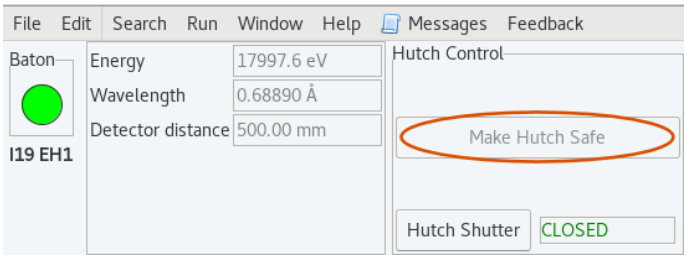
If running as part of a combined access visit, release the baton when you have finished to make things easier for the rest of the team.

Messaging brings up a new tab in the GDA window which can used for group conversations and interaction with the local contact - the local contact will also have a version of the GDA running and will be checking periodically for messages and errors.

The Baton Manager tab shows which users are currently connected to the session. It also shows who the users are, as people are only identified by their FedID in the Messages window. The flag indicates who currently holds the baton.



Crystal Centring



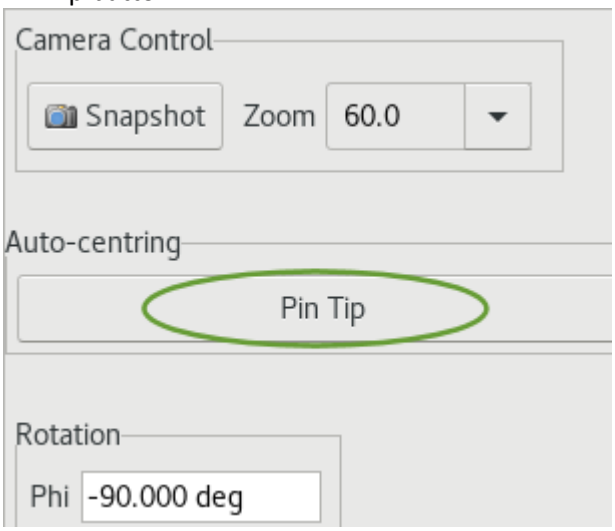
Press 

to close the hutch shutter and move the goniometer into a suitable position to exchange/load a sample.

Open up the hutch, mount the sample, and then interlock the hutch.

Auto Centring

If the robot has loaded a sample, an initial centring attempt starts automatically.
If the sample has been loaded manually, then the auto centring routine can be started by pushing the Pin Tip button.



The auto centring uses image recognition on OAV2 to put the left-most thing it can see on a set crosshair. This is then followed by a similar routine using the on-axis camera (OAV1).

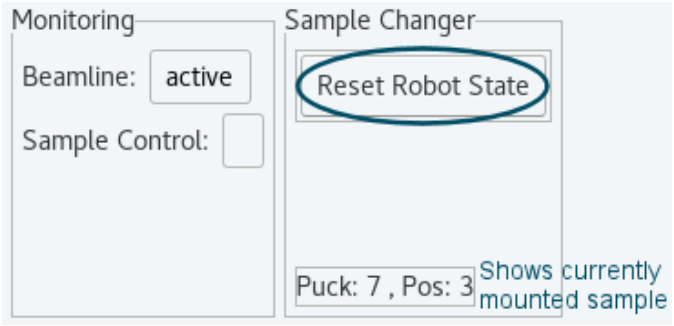
NOTE: The centring should always be checked manually as the auto centring is not guaranteed to do an accurate job.

There are 3 main causes of failure:

1. The sample-Z stage is in an error state - pressing the + or – button in the DIFF1S window from the synoptic normally works to clear it – see the troubleshooting section, 24. Click on the Pin Tip button to rerun the auto centring script once the error is cleared.
2. The sample is contaminated with fluff or the loop is missing and the routine tries to put this on the crosshair, but it needs to move the sample stages beyond the limit. In this case the sample will need to be centred manually – see below.
3. The lighting changed (due to the hutch being interlocked) meaning the sample stopped being visible on the camera - click on the Pin Tip button to rerun the auto centring script once the hutch lights are back on.

Manual Centring

NOTE: If the sample has been loaded by the robot, you may need to click on the "Reset Robot State" button to change the robot status and give GDA control of the sample stages – this button can be found on the far right of the top banner of the GDA (same section as the baton).

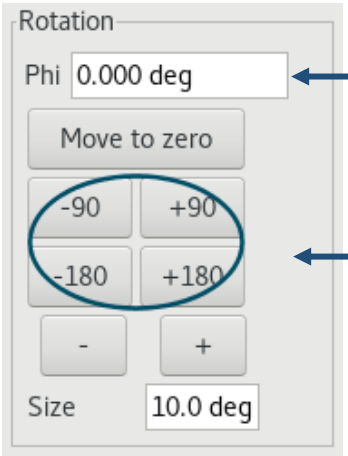


Centre the crystal in GDA in the 

tab by left clicking on the centre of the crystal to bring it to the crosshair.

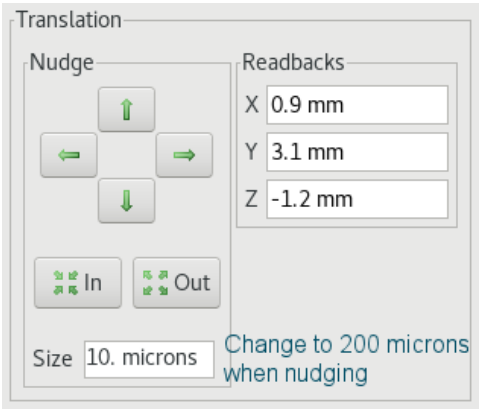
Generally, it helps to start at zoom level 30 and then make final adjustments at zoom level 90. Click on the down arrow to select the required zoom level from the dropdown list 

The camera view can be optimised to fit the window space by clicking on 



Keep an eye on the phi angle – the limits are set to +/- 1000 but phi will unwind before the data collection starts.

Use the +/-90 and +/-180 buttons to check the centring at 90 degree offsets, e.g., 0°, 90°, 180° and 270°, but the centring will work from any starting angle.



If you cannot see the crystal on the OAV View, at zoom 30, use OAV2 as a guide and either click in the OAV View window or use the nudge buttons to steer the sample towards the cross-hair (the directions of movement are the same for both cameras).

Rotate phi 90 degrees to see if the sample comes into view.
If it doesn't, again nudge the sample towards the crosshair on OAV2 until it is visible in the OAV View.

NOTE: The crosshair positions on OAV2 and in the GDA are a guide to the position of the centre of rotation of the goniometer and are usually very close, but it is possible that the true centre is slightly off the crosshair – note that the centring position changes when the temperature is changed. Try to align the crystal so that its centre of mass does not move as the crystal is rotated.

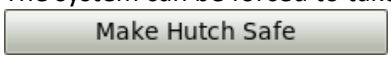
Crystal Measuring

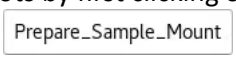
Once the crystal is fully in view, it can be measured by left-clicking the mouse and dragging a line along the length of the crystal – be careful not to just click and move the sample!
For more accurate measurements, change the phi angle so the crystal is aligned with the camera first.
If the red text showing the size is too small and blurred, try scrolling on the image to zoom in - this should make the text more legible.

TIP: As it is very easy to just click rather than click and drag the mouse, it may be better to measure the crystal before fine tuning the crystal centring.

Crystal Snapshots

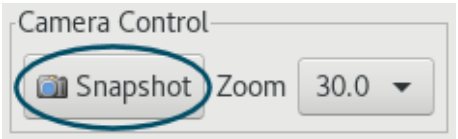
Auto Mode: A series of 4 snapshots are automatically taken at 90° intervals (0°, 90°, 180°, 270°) at the start of a data collection, as long as the collection is started from a position where the backlight is in. These images are visible in ISPyB.

Usually, the snapshots will be associated with the first screening run, but not retaken for subsequent data collections on the same crystal.
The system can be forced to take another set of snapshots by first clicking on either the 

button, or running the 

script (Axis Control tab) to move the goniometer to a position where the backlight comes back in, and then setting the data collection running - this could just be a single image if snapshots are required at the end of an experiment.

Manual Mode: It is also possible to take snapshots manually by clicking on the Snapshot button within Camera Control.

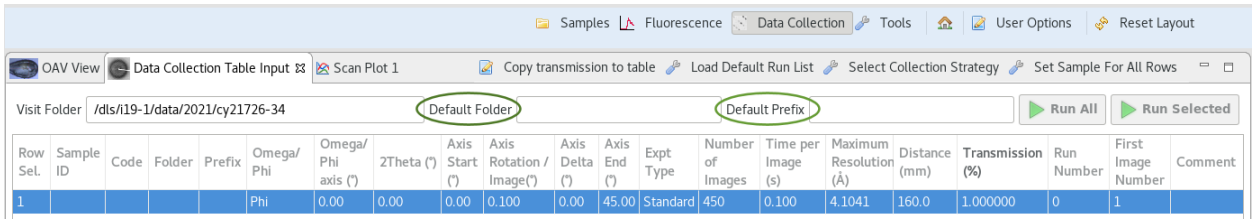


Images can only be saved within the jpegs folder of your visit directory (this is where the snapshots taken automatically are also saved).

Unfortunately, any measurements added are not saved.

Data Collection

Once the crystal is centred and measured, change to the Data Collection Tab by clicking on



All data will be collected within your visit directory, as indicated by the Visit Folder, and only users identified on the visit in the UAS will have access to this data.

The Default Folder box defines the folder within the visit where the images will be saved - it is possible to include multiple levels using /
e.g., SampleA/Crystal1/100K..... SampleA/Crystal3/300K

The Default Prefix is what the images will be called within that directory. The run numbers and image numbers are added automatically based on the values given in the table.

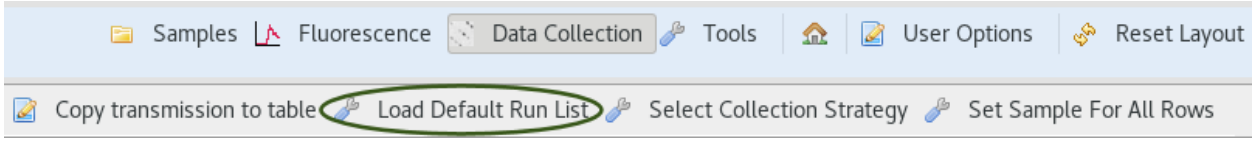
Any name, using less than 23 characters (but not certain ones) can be typed into the Default Folder and Prefix boxes.

Crystal Screening

Normally, the first collection on a new sample will be a screening run to determine the optimum level of attenuation as it is important to ensure reflections on the detector are not overloaded.

The top line of any pre-defined run list is a screening run (Experiment Type = Screening) and is a phi scan consisting of 450 0.1° images. The default transmission for screening is set to 1% but this can/should be adjusted in the table once you have a feel for what an appropriate level is likely to be.

The standard sphere can be loaded by clicking on the "Load Default Run List" button



Row Sel.	Sample ID	Code	Folder	Prefix	Omega/ Phi	Omega/ Phi axis (°)	2Theta (°)	Axis Start (°)	Axis Rotation / Image(°)	Axis Delta (°)	Axis End (°)	Expt Type	Number of Images	Time per Image (s)	Maximum Resolution (Å)	Distance (mm)	Transmission (%)	Run Number	First Image Number
1	Fru17				Phi	0.00	0.00	0.00	0.100	0.00	45.00	Screening	450	0.100	2.0000	160.0	1.000000	1	1
2	Fru17				Phi	0.00	0.00	0.00	0.200	0.00	180.00	Standard	900	0.200	2.0000	160.0	1.000000	1	1
3	Fru17				Omega	0.00	30.00	-145.00	0.200	0.00	25.00	Standard	850	0.200	2.0000	160.0	1.000000	2	1
4	Fru17				Omega	120.00	30.00	-145.00	0.200	0.00	25.00	Standard	850	0.200	2.0000	160.0	1.000000	3	1
5	Fru17				Omega	240.00	30.00	-145.00	0.200	0.00	25.00	Standard	850	0.200	2.0000	160.0	1.000000	4	1

Click on the row number under Row Sel. in the table to highlight this row and then click on “Run Selected”, above the table, to collect these images.

Use the output from Screen19 to determine what transmission should be used for the full data collection, and how long images should be collected for. Screen19 will suggest the optimal level of attenuation based on the cell it calculates. Aim for no more than 25% on the pixel intensities plot but remember, **25% is the maximum and not a target level** – if there is good data to the required resolution, then there is no need to increase the transmission.

See page 27 for details on using Screen19 and interpreting the screening results.

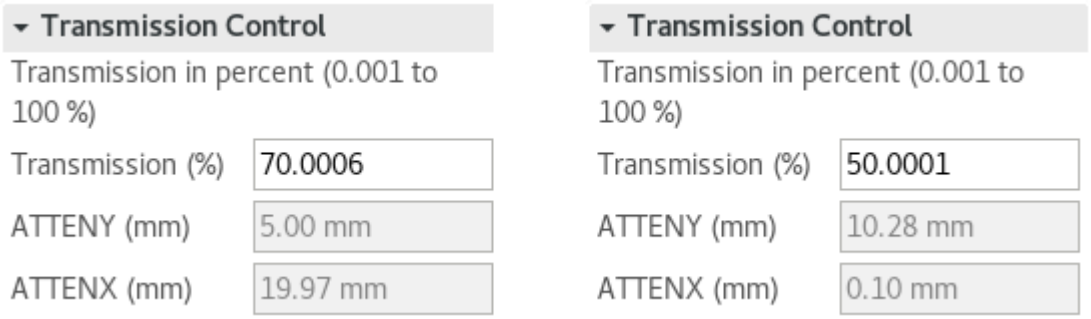
Multiple screening runs may be needed to decide on the best attenuation level, and they should be collected in separate directories to ensure Screen19 runs on images with a single transmission setting.

The screening output also provides a summary table of the exposure factor needed to reach various data resolutions - this should be used in conjunction with the histogram to decide the best attenuation level and collection time.
NOTE: It may be necessary to increase the collection time per image in order to obtain strong enough data to the required resolution as the detector threshold (25%) should not be breached.

Transmission

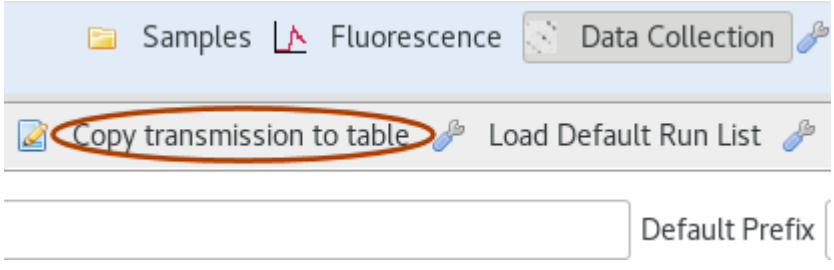
The transmission for a data collection is set using the transmission column in the GDA data collection table.
NOTE: The transmission set in the data collection table will override the transmission value set anywhere else.

The attenuation is driven by specifying the **percentage transmission** required – the wedge positions are shown in the Axis control tab. The level of transmission required will determine which wedge is used - higher levels are achieved using the resin wedge (ATTENX) whilst lower levels are achieved using the aluminium wedge (ATTENY).

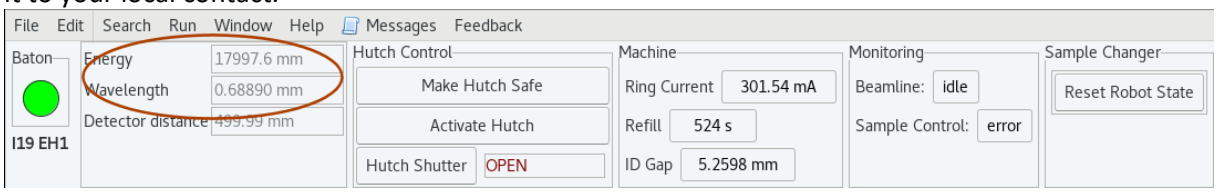


For example, at a wavelength of 0.6889 Å, 50% of the incident beam transmission is achieved by inserting a thickness of 0.5 mm of Al into the beam. This is the thickness of the wedge when ATTENY is set to 10.28 mm.
Note that ATTENX is out of the beam at 0.10 mm, whereas ATTENY is out of the beam at 5.00 mm.

Clicking on the “Copy transmission to table” button will update the transmission for all scans in the data collection table to match the value currently set in the Transmission Control box.



The transmission is calculated using the set wavelength so it is worth checking this is reported correctly in the top menu of the GDA – if the wavelength shown doesn't match the expected value, please report it to your local contact.



See page 29 for more details on how the attenuation works.

Collection Strategies

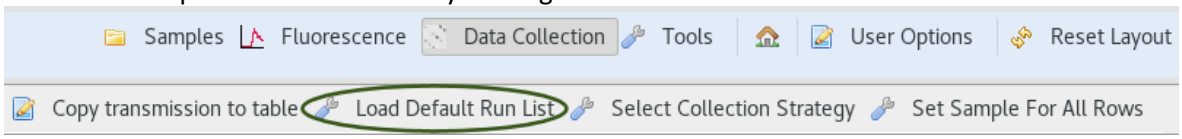
Several run lists are available in the GDA giving coverage with the detector set to either 160 mm (in practice, this is as close in as possible for a reasonable omega sweep) and further back at 300 mm.

At a detector distance of 160 mm, 2θ=30° is the maximum value where the beamstop is still visible.
At a detector distance of 300 mm, 2θ=20° is the maximum value where the beamstop is still visible.

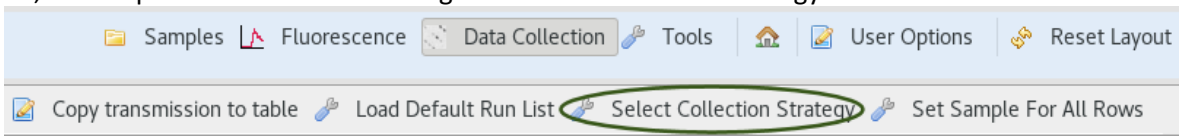
Run lists do not need to be used in their entirety – just select the rows required to be collected.

The section on Strategies, page 30, should provide some guidance to each run list and can used to modify or prepare your own run list.

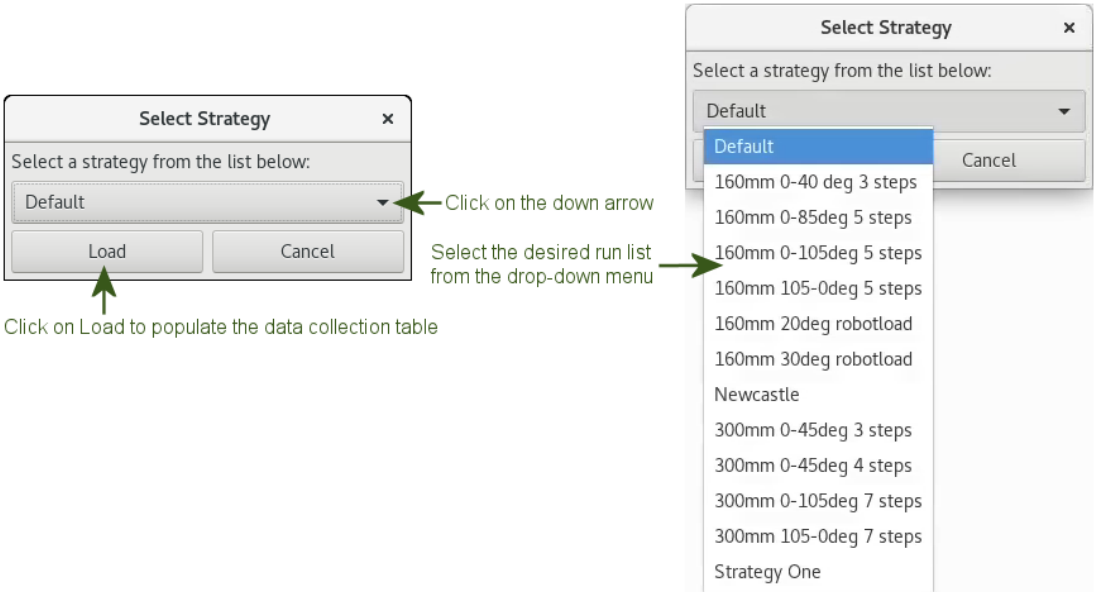
The standard sphere can be loaded by clicking on the "Load Default Run List" button



Or, other options can be loaded using the "Select Collection Strategy" button.



This will open a window towards the top left of the screen – Default is always top of the list.



NOTE: The run list selected will be overwrite any existing runs in the table.

Things to consider:

1. Check the folder and prefix fields in the data collection table are empty on loading the run list. Over time, these can become populated and the values in the table take precedence over the names given in the default fields above. Please let a member of staff know if this happens so that it can be fixed.
2. The first line of all run lists is a screening run consisting of 450 0.1° images – this should not be collected as part of the full dataset.
3. The transmission setting is not the same for all run lists – typically the high angle run lists have the transmission set to 100% while the others have the default set at 1% - remember to update the transmission to the appropriate value for the sample.
4. The time per image is not consistent for all run lists – generally this is set to 0.2 seconds but the time per image has been increased for the high angle collections - change the image collection times as appropriate.

Collecting Data

Once the collection strategy and transmission have been set, make sure the run numbers are set incrementally for the sweeps to be collected, and then highlight the required runs by clicking on the numbers in the Row Sel. column. Then click on the “Run Selected” button to start the data collection.

Note that, if the data collection is being added to a queue, this button will change to say “Queue Selected”.

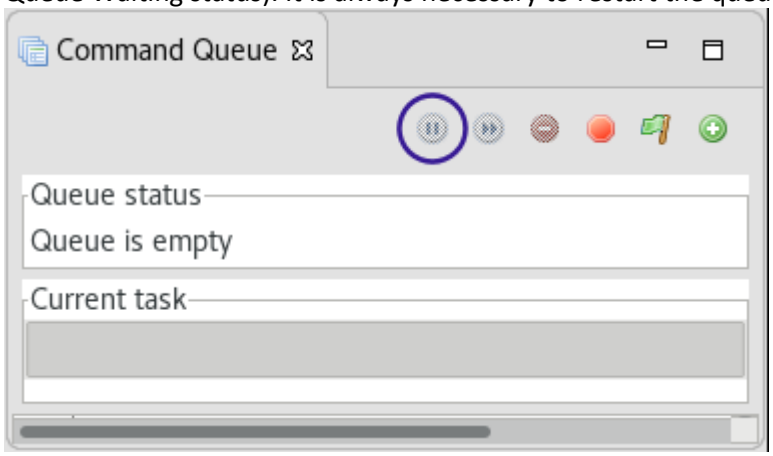
Stopping Data Collection

If you want/need to stop the data collection (or anything at any time):

Press the button with the little red circle next to the word Stop All 

This is located towards the centre of the bar at the very bottom of the GDA window

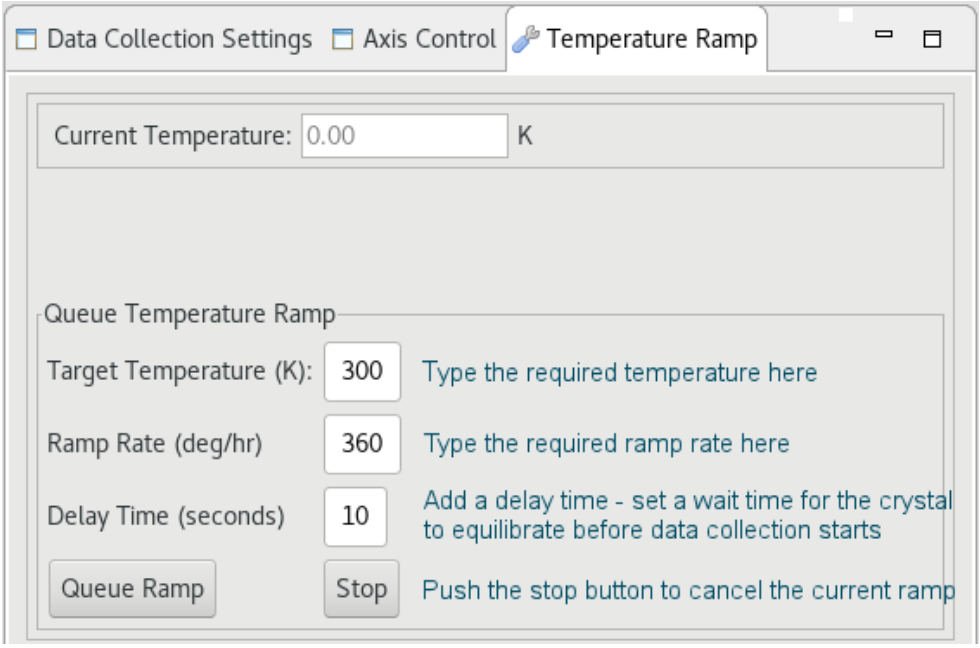
One side effect of the “Stop All” button is that it will pause the queue, indicated in the bottom right-hand corner of GDA with a paused status in red. The pause button in the Command Queue tab (in the purple circle, below) will turn into a play button and this should be pressed twice to get back to the Queue Waiting status). It is always necessary to restart the queue after a Stop All.



NOTE: the Stop All button has no effect on the robot

Cryostream Control

The cryostream can be controlled via the GDA – this means it is easy to queue temperature changes between data collections.
Select Temperature Ramp from the series of tabs on the right-hand side of the GDA.



Click the “Queue Ramp” button - this will add the temperature change to the end of the list of queued jobs or, start it immediately if the queue is empty.
NOTE: If the temperature change is queued via the GDA, then any other commands set by the GDA will be queued to start once the temperature ramp is completed. Therefore, on some occasions it may be more efficient to use EPICS (see page 5) to control the temperature in order to keep the GDA free for other tasks.

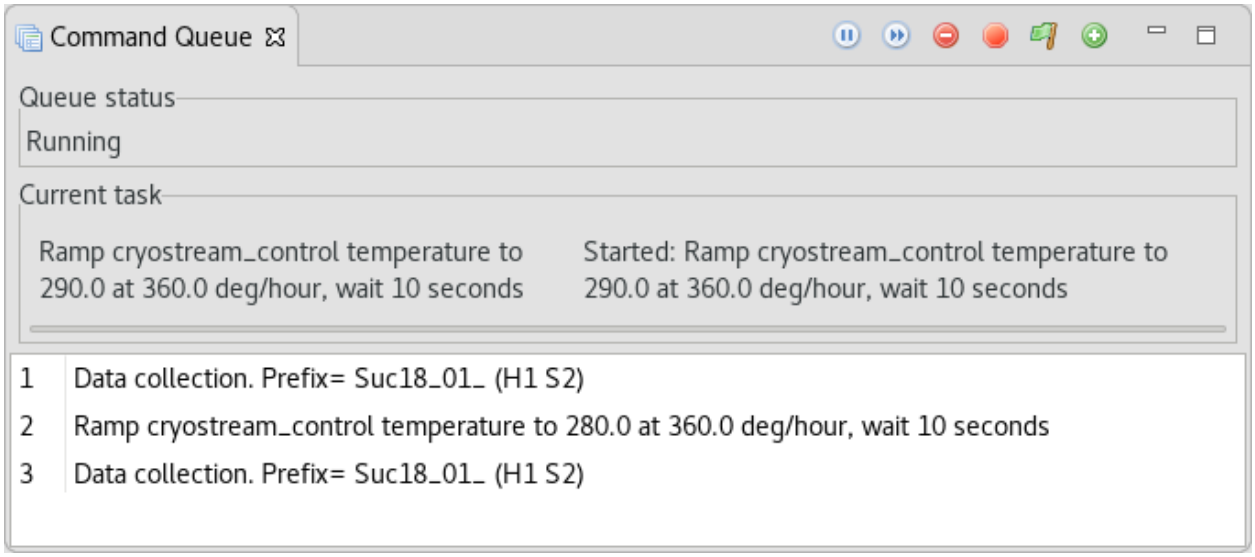
Notes:
1) The Mitegen mounts change length depending on the temperature, so it is important to check the crystal centring at regular intervals, e.g., every 30K. Anecdotally, this change is less when using the tall copper mounts.
2) There is an optical effect which means the centre position will appear to move when the cryostream is at different temperatures – make sure to centre the crystal on the centre of mass as it will be impossible to maintain the centre on the crosshair.

Queuing Tasks

It is possible to queue many actions, including data collections, robot actions and temperature ramps.

All queued items can be viewed in the Command Queue window and items can be moved and deleted from here.

It is also possible perform actions on the queue according to the buttons at the top of the box.



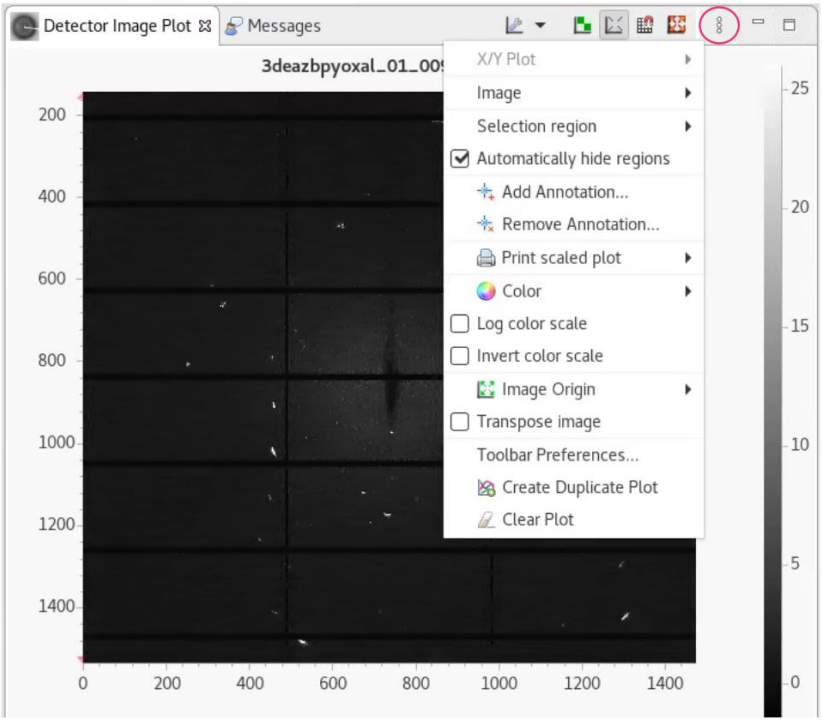
If the GDA window is wide enough, the colour-coded queue status is displayed in the bottom bar of the GDA, e.g., waiting, running or paused.

Viewing Images

GDA

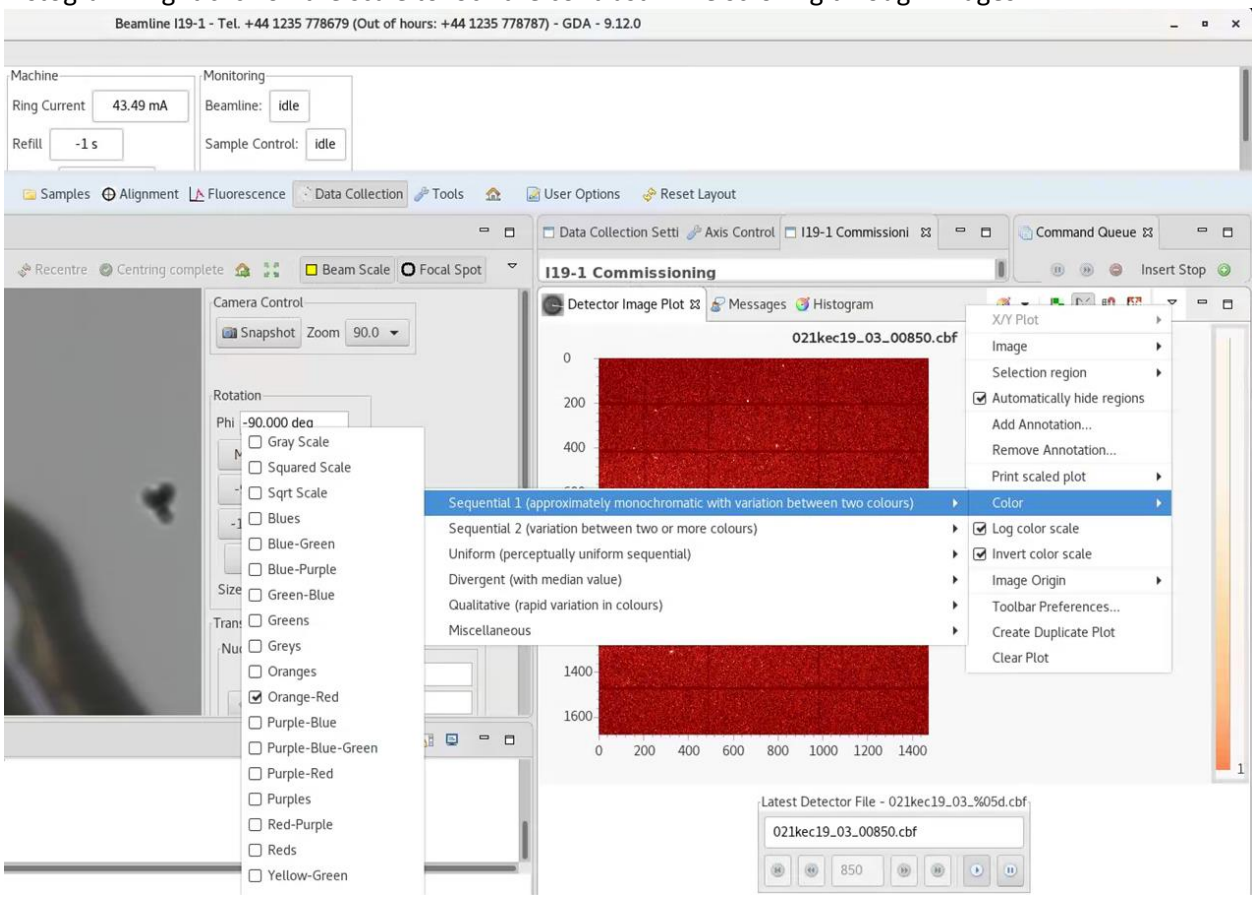
During data collection, some images will be displayed in the GDA in the Detector Image Plot window. It is possible to modify the image settings to make this more useful.

Click on the vertical array of dots to bring up the list of image options – e.g., invert the image colour scale.



You can also change the colour scheme - click on the arrow next to colour to have a look (and a play). Below is orange-red and above is grey scale from sequential 1, for example.

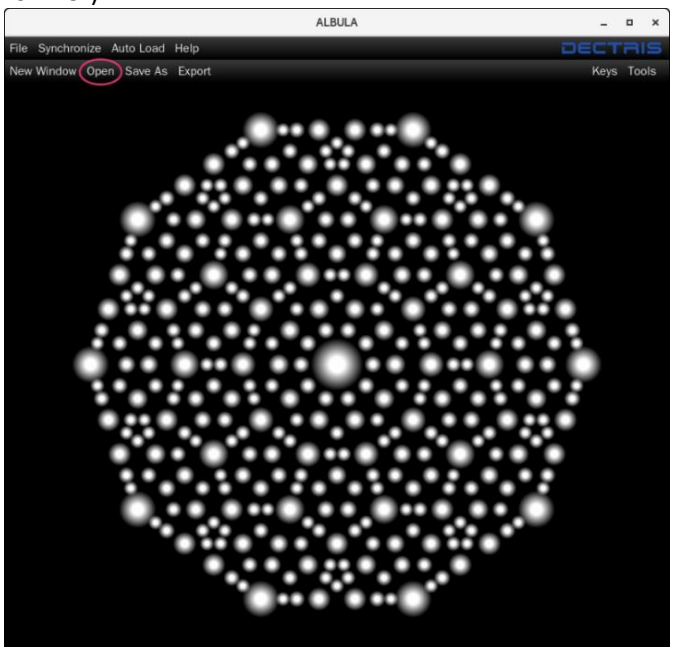
Click on the scale on the right-hand side and scroll to change contrast. The  button will auto-histogram. Right click on the scale to lock the contrast while scrolling through images.



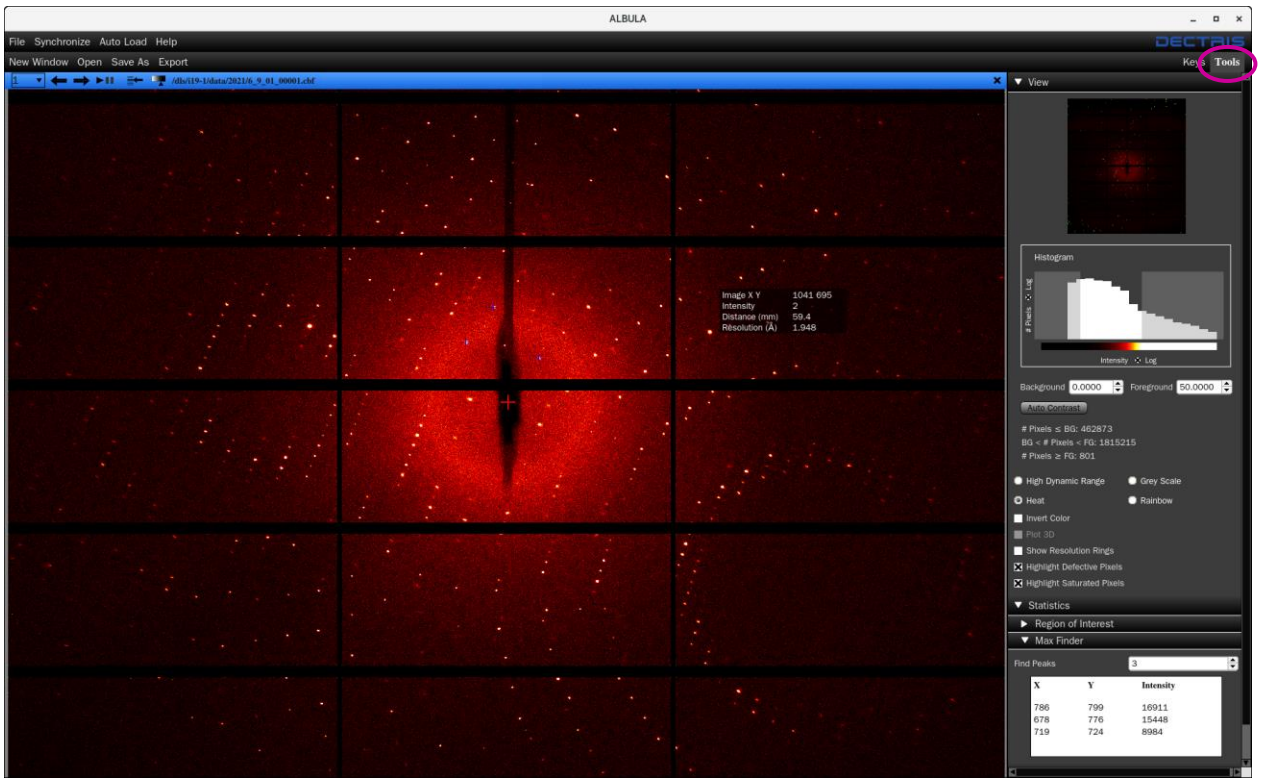
You might need to look in preferences to find the box to make your changes stick, but once set they should be remembered and then be sensible in the future.

Albula

To view images in Albula (Dectris software), open a terminal window and type albula, then press *enter.* (You may need to type module load i19 or module load albula first, if the terminal has not been set up for I19.)



Click Open in the top left-hand corner and navigate to the desired dataset - bear in mind that a folder containing a lot of images will take a while to load in.



The Tool menu shown on the right had side is opened by clicking on Tools in the top right-hand corner. There are a number of image viewing options, for example:

1. High Dynamic Range highlights the strongest reflections with red dots – **important note**: this is not related to the detector threshold and does not mean these reflections are overloaded.
2. Heat gives yellow and red images, similar to the standard display in Apex and is usually the clearest option to see the reflections.

The contrast of the image can be changed by:

1. Dragging the bars on the histogram plot (within the Tool menu)
2. Changing the Background and/or Foreground values
3. Clicking on the icon in the blue menu bar and dragging the line across - the Auto Contrast button often gives a good starting place

The image can be zoomed by simply rolling the mouse wheel.
Opening the Statistics section of the Tool bar gives you the option to highlight the strongest reflections with blue crosses (choose how many by typing the number in the box, e.g., 3 in the screenshot above).

Resolution rings can be checked, but it is important to note that they are only accurate for the 2 theta=0 scans. For 2 theta=30° scans, the edge of the second column of sensors is about 0.8 Å resolution when at a wavelength of 0.6889 Å.

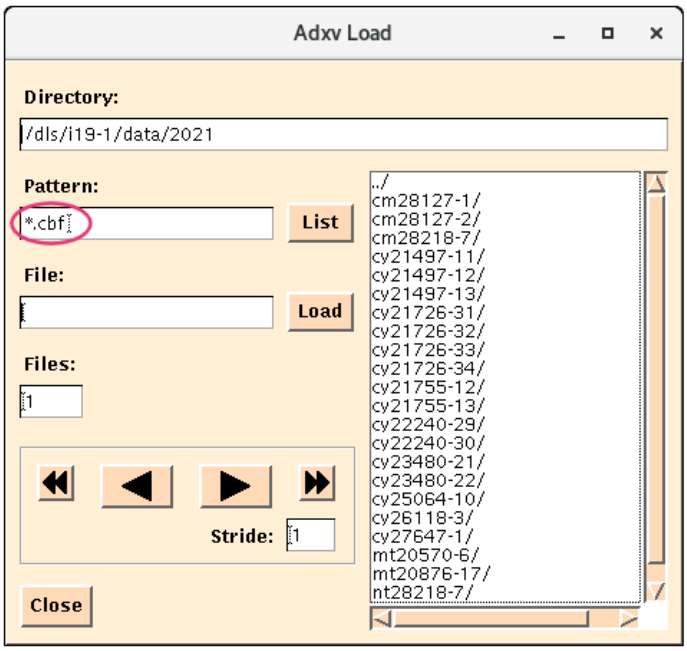
To move through the images, click on the arrow buttons , or the play/pause button to auto-play. The number of images viewed can also be changed if you don't want to see every one – click on the down arrow and select the step-size required .

ADXV

Another option which may be useful, particularly if you are accessing the beamline remotely, is ADXV (Albula can run slowly and the images end up very pixelated.)
ADXV is not included in the list of programs loaded by module load i19, so needs to be done separately.

In a terminal, type module load adxv and press *enter*
Then type adxv and press *enter*

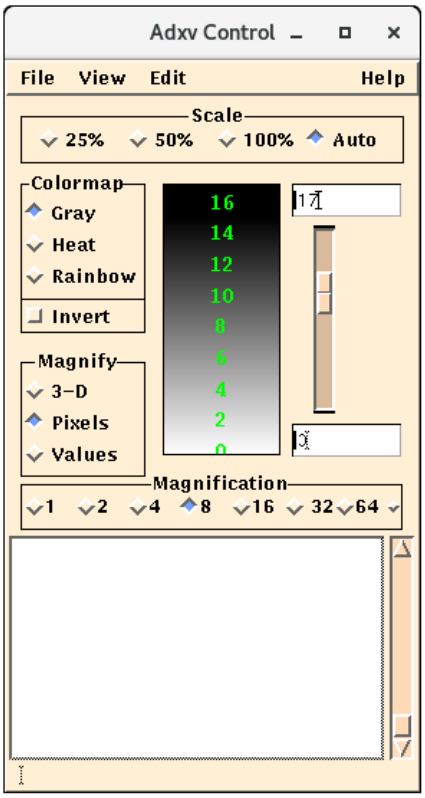
Three windows should open:



Change the Pattern from *.img to *.cbf to match the image format

Browse to your visit and the required visit directory.
Double click on the image to open it.

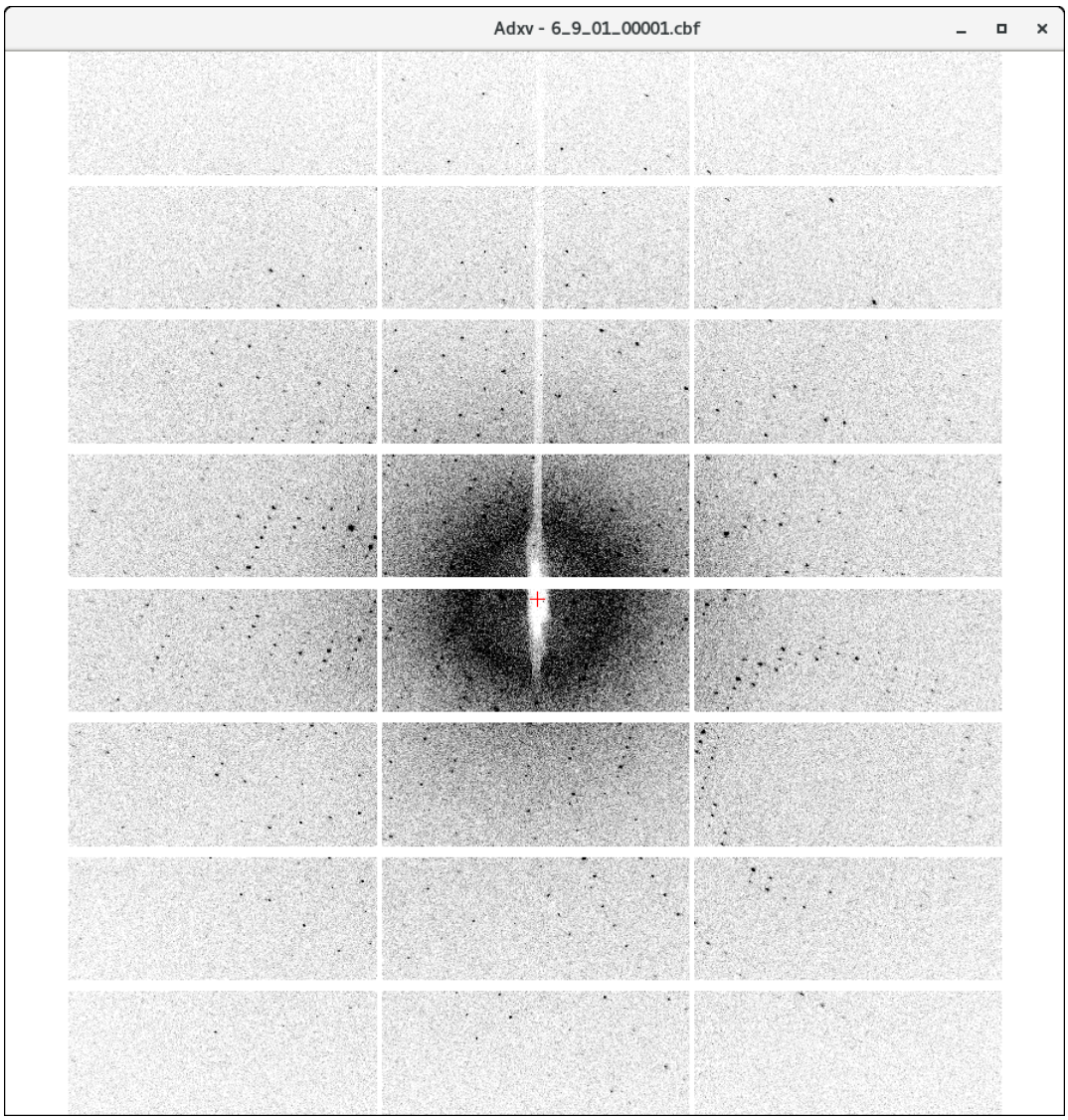
Use the arrows to move through the images
The double arrow buttons play throught the images
Stride can be set to e.g., 5 to just view every 5th image



Scale is best left on Auto as this resizes the image to best fit the window size, although 50% and 100% may be useful for zooming in

The image appearance can be changed using the ADXV Control window
e.g., change from grey scale to heat
It is also possible to change the contrast, although this is often not that useful

From the Edit Menu, select properties - in this window check the box to add resolution rings. Again, these will only be correct when 2 theta is at 0.



DIALS

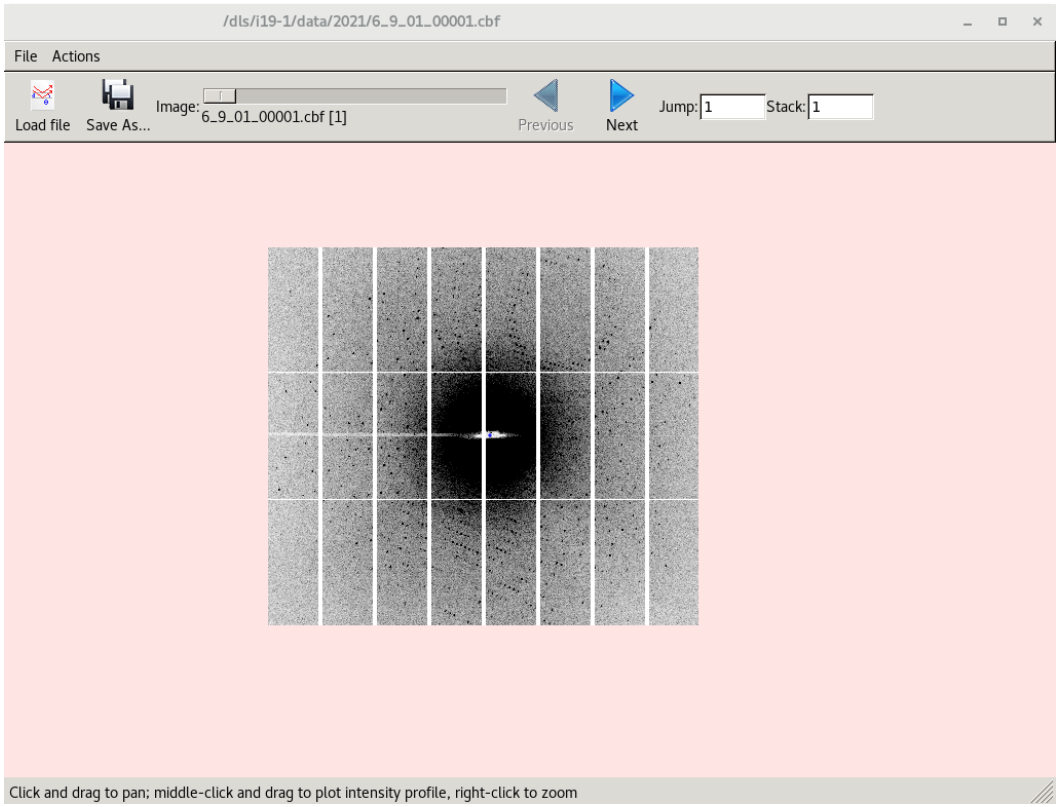
One very useful feature of the DIALS image viewer is that the resolution rings take into account the angle of 2 theta.

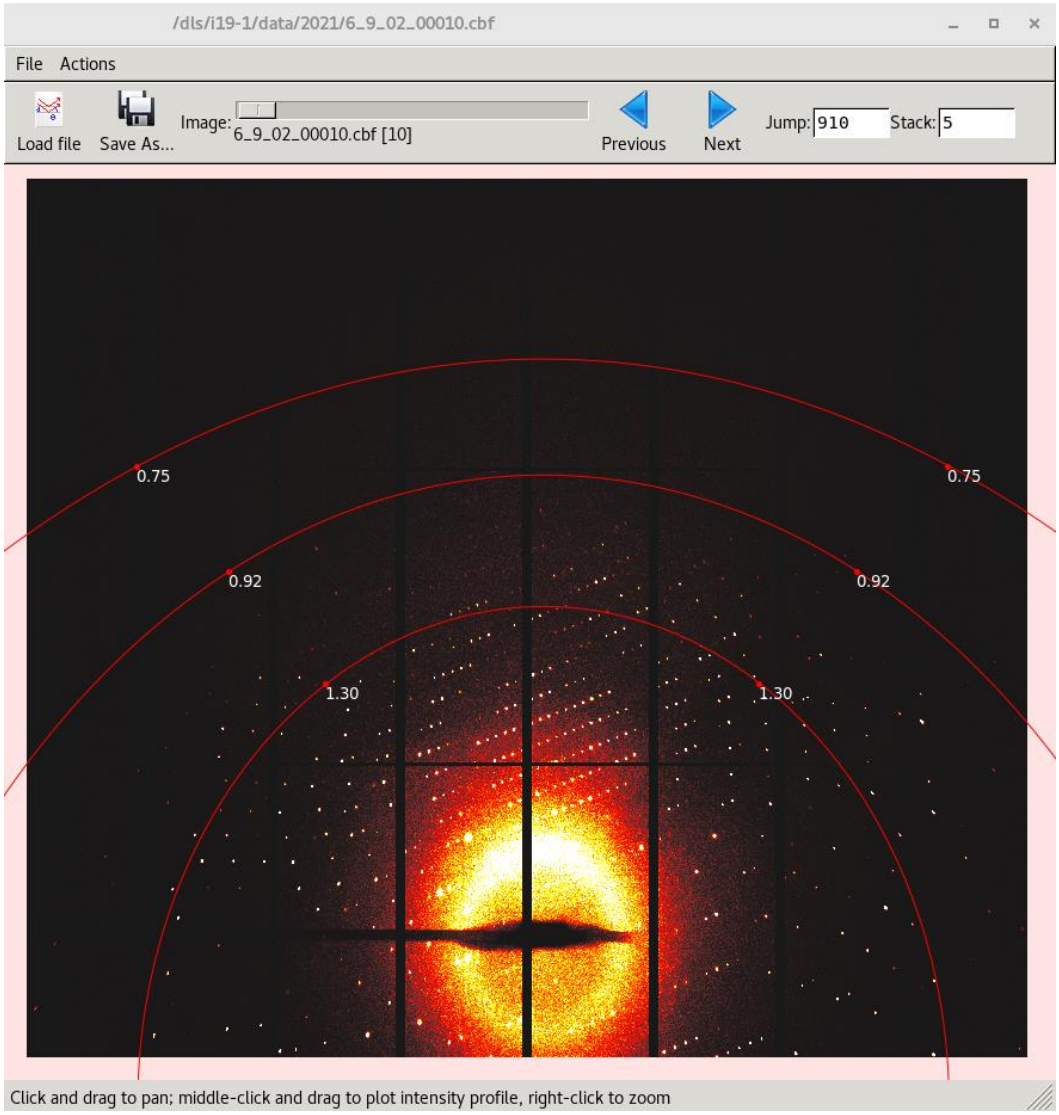
To open all images in a folder from the location of the images type:
dials.image_viewer *.cbf

Alternatively, from anywhere type:
dials.image_viewer /dls/i19-1/data/YEAR/VISIT/path/to/images *.cbf

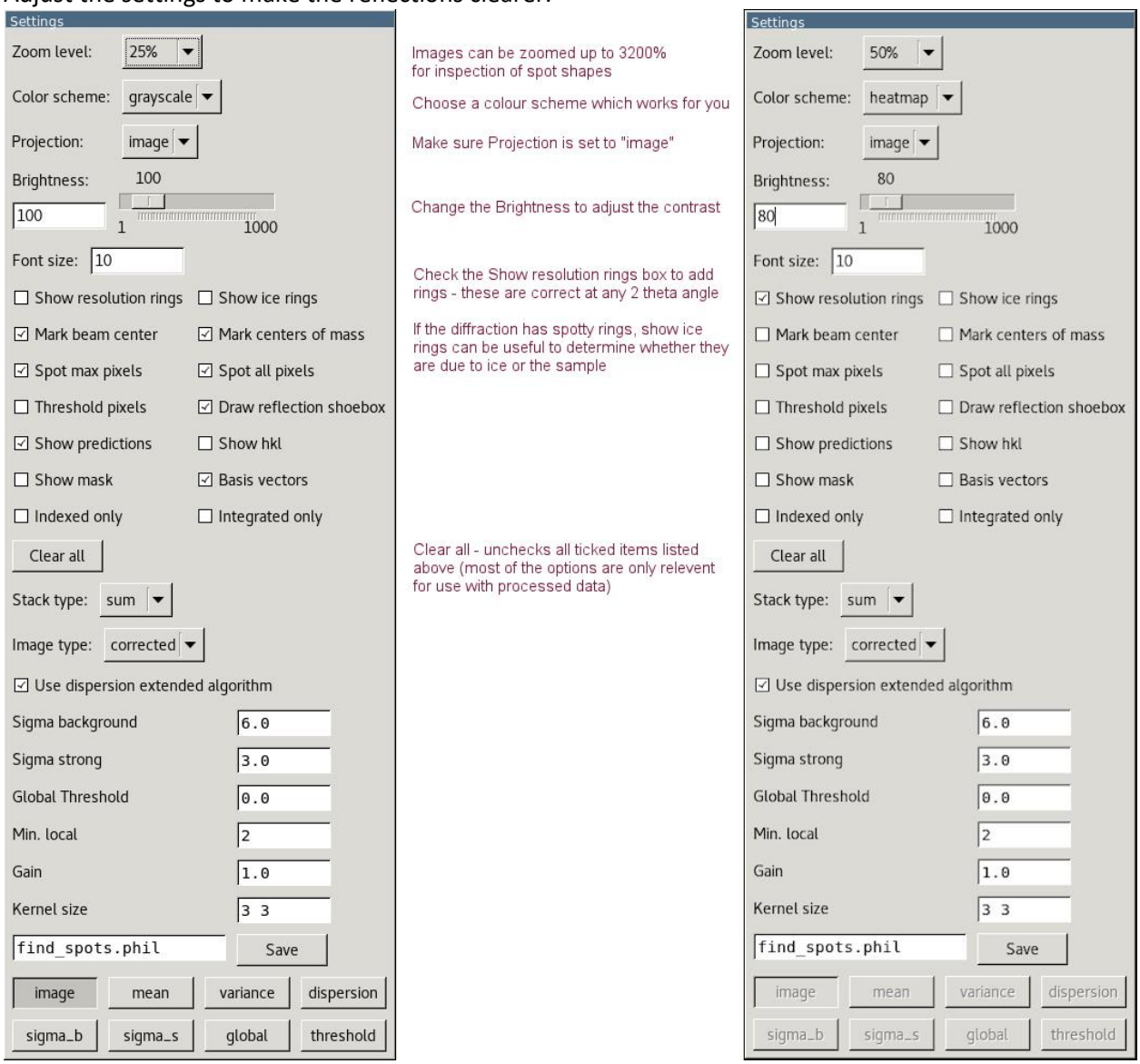
To just open a single run, use *_04*.cbf for example, to just look at run 4

The Image and Settings windows should open.


/dls/i19-1/data/2021/6_9_01_00001.cbf
File Actions
Load file
Save As...
Image:
6_9_01_00001.cbf [1]
Previous
Next
Jump: 1
Stack: 1
Click and drag to pan; middle-click and drag to plot intensity profile, right-click to zoom


/dls/i19-1/data/2021/6_9_02_00010.cbf
File Actions
Load file
Save As...
Image:
6_9_02_00010.cbf [10]
Previous
Next
Jump: 910
Stack: 5
0.75
0.75
0.92
0.92
1.30
1.30
Click and drag to pan; middle-click and drag to plot intensity profile, right-click to zoom

Adjust the settings to make the reflections clearer.



Use Next/Previous to move on/back a single image. Use the scroll bar to move very quickly to another image or type the image number in the Jump box to view a specific image. Jump is based on the total number of images in the dataset with no regard for the run number so for the default run list, the final image of the dataset is 3450.

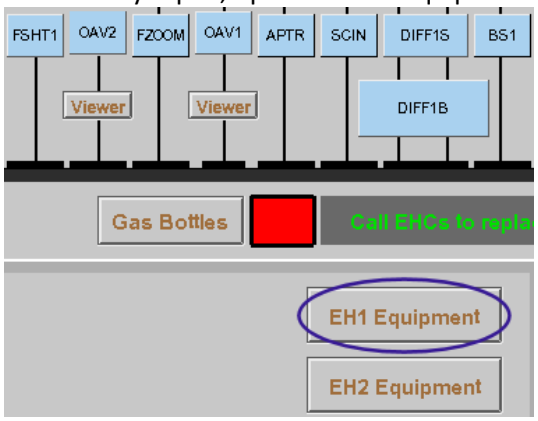
Stack will sum adjacent images so, for example, 5 x 0.2° images will stack to show the equivalent of a 1° image.

Troubleshooting

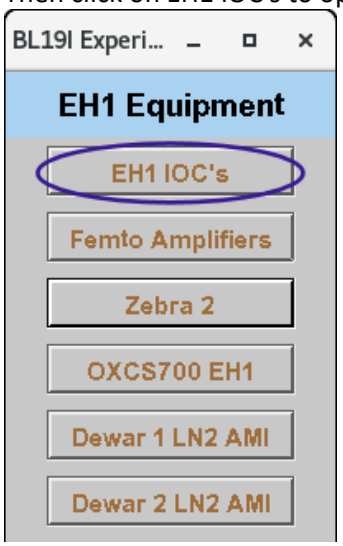
OAV (in GDA) camera and/or OAV2, D2, D4 stops updating

Check the camera is acquiring (see page 4) and press Start if required. If that doesn't fix things, restart the camera IOC.

From the synoptic, open the EH1 Equipment menu:

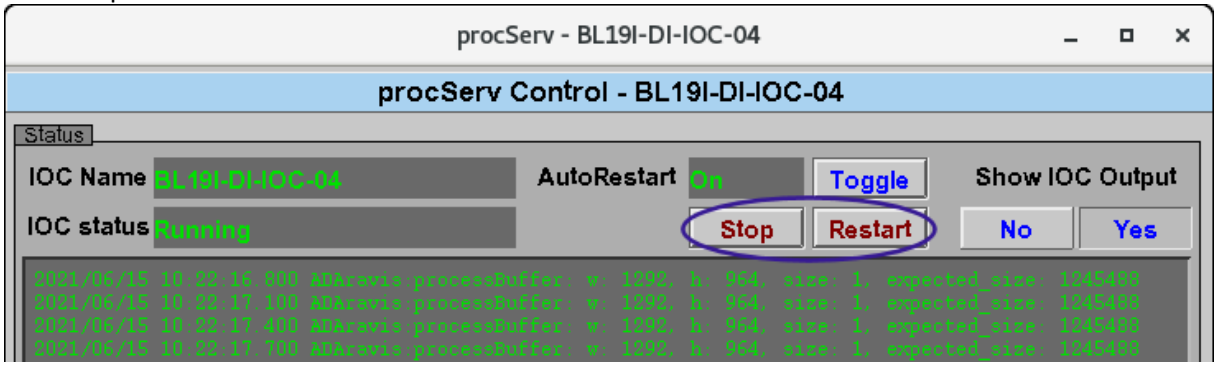


Then click on EH1 IOC's to open up the full list of IOCs.



Click on the Start/Stop button for the EH1 GigE Cameras

Then Stop and Restart the camera



Drifting of sample stages

This sometimes happens after a sample change as ice can get trapped between the sample and the mount. Wait for a couple of minutes and the drifting should stop once the ice has melted.
If the drifting continues as you try to centre, check that the sample pin is securely glued into the magnetic base.

Can not centre the sample

There are 3 likely causes for manual centring not working:

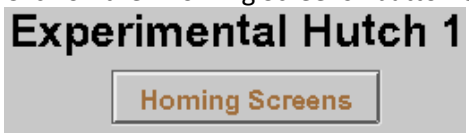
a) One of the centre axes is in an error state

Check the status of the axes in EPICS:
Click on DIFF1S to open all of the axes

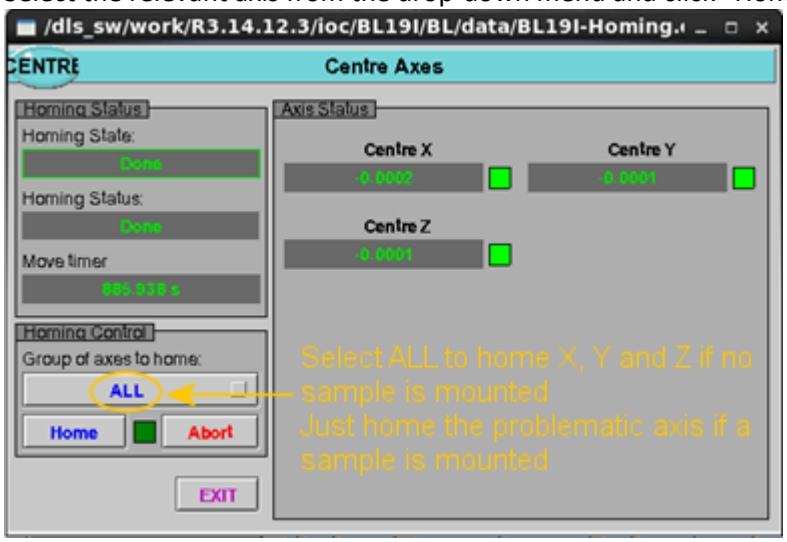
If any of the centring axes (Centre X, Y, Z) are flashing red, click on any of the buttons for the affected axis

Normally, this will be enough and the motor should work again.

However, if there is still an issue, then the axis will need rehoming.
Click on the “Homing Screens” button on the synoptic and select Centre Axes from the list that appears.



Select the relevant axis from the drop-down menu and click “Home”



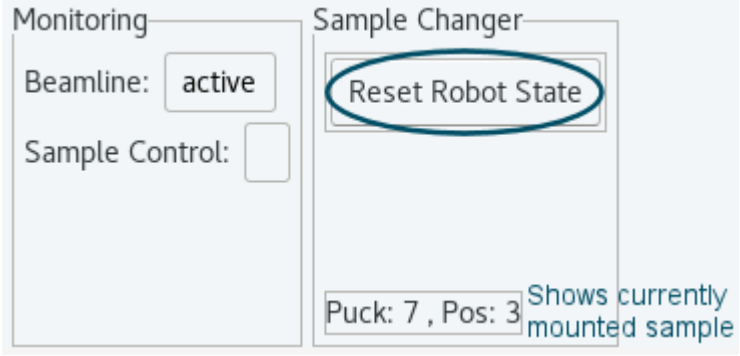
A good starting point for crystal centring is x=0.9, y=3.1, z=-1.2. Type these numbers in the DIFF1S window, in the relevant boxes with the blue numbers and press *enter*.

b) The sample has not been loaded squarely on the magnet

If the sample is not mounted squarely on the magnet, the centre position can end up outside the range of travel of the sample stages. The sample will need to be adjusted so that it sits straight.

c) The robot is still active

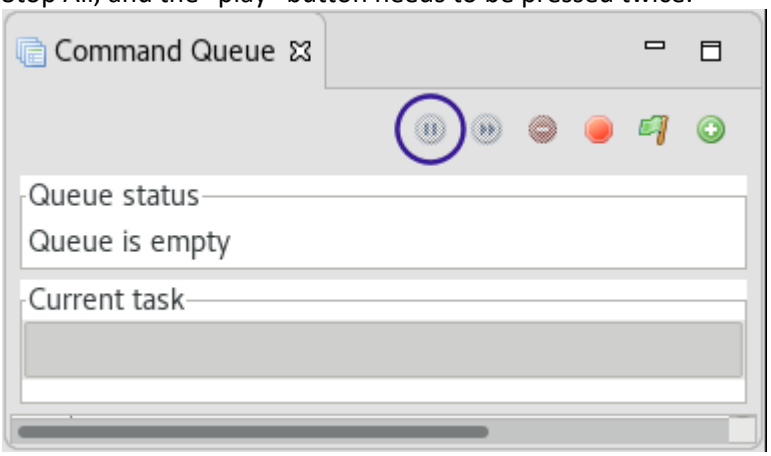
Click on the “Reset Robot State” button to deactivate the robot and pass control back to the GDA. (There is never any harm in pressing this button, even if that wasn't the cause.)



NOTE: this can be an issue even if you are not using the robot as it can be a hangover from the previous user.

Data collection won't start

a) Check that the GDA queue is not paused; see bottom right-hand corner of GDA where a paused status will be indicated in red. If it is paused, the “pause” button in the purple circle is a “play” button - press the “play” button in the command queue tab. It is always necessary to restart the queue after a Stop All, and the “play” button needs to be pressed twice.



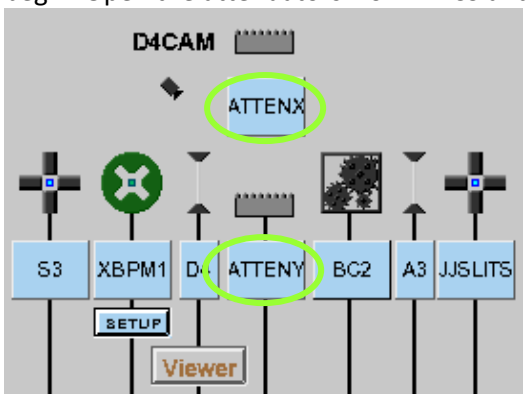
b) Check that you are not trying to write image names that already exist – this will be indicated in the error message that appears in the Jython Console tab. Change the name of the Default Folder and try again.

c) Check the beamstop is mounted correctly - the data collection won’t start if direct beam is detected on the diode - again this should be reported in the Jython Console

d) Check there is beam in the ring and optics hutch (check for beam on D2 or check the status of the Port Shutter in ISPyB) - the data collection won’t start if no beam is detected on the pre-shutter diode - this should be reported in the Jython Console

e) Check that the beamstop check has run to completion – there are a number of steps which need to be performed and, if any of the motors fail to reach position, the check will fail. If this is the case, just restart the data collection again.
NOTE: If the restarted data collection starts from a position where the backlight it out, the crystal snapshots will not be retaken and the snapshots from the aborted collection will not appear in ISPyB – they can be found in the jpegs directory.

f) Check that the wedge attenuator is not stuck. The wedge is driven as part of the check for beam to ensure the beamstop is in. If the wedge can't move, then this check fails and data collection will not begin. Open the attenuators from EPICS and check the motor state - it will be red if it is in an error state.



Try to move it to the required value (do not move ATTENY to a value less than 5 or ATTENX to a value below 0.1) by typing a number in the box with the blue numbers and pressing *Enter*. Then restart the data collection.

Last Resort
If nothing seems to fix the problem, restart the GDA - close the client and then restart both the servers and then the client – see pages 6-7 on restarting the GDA
Bear in mind that this will disconnect all users currently using the GDA.

APPENDIX

Screen19

The results from Screen19 are best viewed in a terminal window (right click on the desktop and open a new terminal window) where the results will be displayed automatically when running i19.tail.

If the terminal does not automatically open in your current visit directory:
type module load i19 and press enter, then
type i19.tail at the prompt and press enter

If the terminal window opens with the prompt showing your current visit directory, you should be able to go straight to the i19.tail step.

(The program may time out if the wait for the first set of images to be collected takes too long – just type it again if this happens.)

Screen19 is run on every full scan of data collected, not just the screening run. These results can be found in the "processed" directory if needed:
Processed/foldername/imagename_runnumber__sweep/screen19

Type gedit screen19.log once in the appropriate directory to view the log file [Ctrl C to exit]

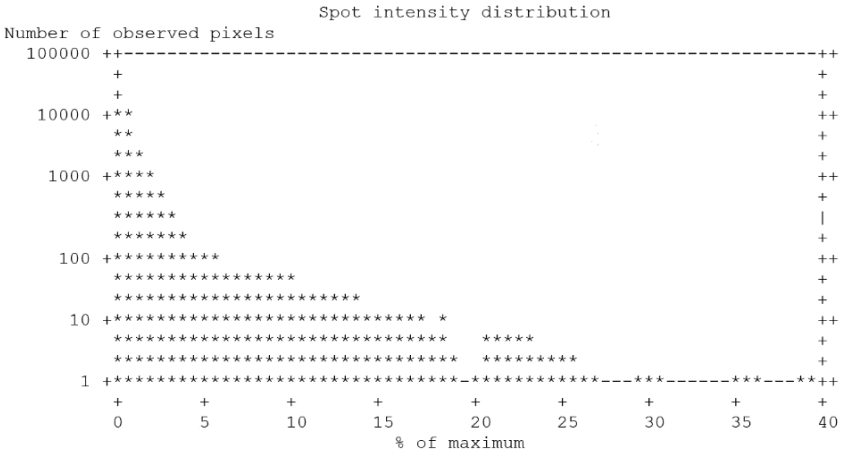
NOTE: the other output files from the auto processing are only stored for one week in the tmp directory. These can be found in /tmp/zocalo/foldername/imagename_runnumber__sweep/screen19

Results

If the program has worked, the final section of the output is a list of possible unit cells. Check that the unit cell found looks sensible with a reasonable metric fit.

```
Refining bravais settings...
---------------------------------------------------------------------------------------------------------------
Solution Metric fit  rmsd  min/max cc #spots lattice                                  unit_cell volume cb_op
---------------------------------------------------------------------------------------------------------------
*      2     0.0151 0.040 0.645/0.645   2226      mP  11.56  13.40  29.85  90.00  95.20  90.00   4606 a,b,c
*      1     0.0000 0.039         -/-   2217      aP  11.56  13.40  29.86  89.99  95.21  90.02   4605 a,b,c
---------------------------------------------------------------------------------------------------------------
```

Scroll back up and find the plot showing the spot intensity distribution.
Note the value given for the maximum percentage of the detector count rate limit and the shape of the histogram - the final column of points in the histogram should be ignored.




```
Strongest pixel (191190 counts) reaches 38.8% of the detector count rate limit
The photon incidence rate is outside the linear response region of the detector (<25%).
The built-in detector count rate correction should be able to adjust for this.
Total sum of counts in dataset: 5702649689
```

Also consider what the diffraction limit looks like from the Wilson plot - the table below gives an indication of the transmission required to get good quality data to various resolution levels.

```
Estimating lower exposure bound...
                        Wilson plot
  100000 ++-----------------------------------------------++
         +                                                 +
         *********                                         +
         **********                                        +
         ************    *  *                             |
   10000 +*************  *** ***                           ++
         ************* ********    * *                     +
         ************************* ***                     +
         ******************************* ******            +
         ************************************* ****    * |
    1000 +*****************************************************++
         ************************************************
         ************************************************
         +                                                 +
         |                                                 |
     100 ++-------+-----------+-----------------------------++
                 +           +
                 2          1.5
                d (Angstrom) (inverse-square scale)
Fitted isotropic displacement parameter, B = 6.94 Ã…Â²

Recommendations, summarised:
================  =================
  Resolution (Ã…)          Suggested
                     exposure factor
================  =================
            1.0             0.0829
            0.84            0.352
            0.76            1.0
            0.6            39.5
            0.4             6.74e+06
================  =================
Exposure is flux Ã— exposure time.
You can achieve your desired exposure factor by modifying transmission and/or exposure time.
Successfully completed (0.7 sec)
```

What the results indicate:
For the example above, if there is strong diffraction beyond 0.84Å, i.e., there are clear diffraction spots to the edge of the detector for the screening run (check the images visually!), then the spot intensity histogram (detector limit) recommends decreasing the transmission by about 1/3 (2/3 of 36 = 24%). The table suggests that 1/3 of the current transmission is sufficient to obtain good data to 0.84Å so collecting with 2/3 of the current transmission would be fine.

1.) If there is little evidence of diffraction to this required limit, then sticking with the attenuation level used for the screen will be fine in this instance because the built-in detector count rate correction should be able to adjust for the few reflections which are too strong.
2.) If the suggested transmission to achieve the required resolution is greater than the transmission recommended by the detector count rate limit, then the data collection time needs to be increased in order to collect stronger data. For example, to collect weaker spots it may be appropriate to halve the speed of data collection by collecting 0.2° images in 0.4 seconds (rather than the default 0.2° in 0.2 seconds). **Do not go over the detector threshold.**

Running Screen19 Manually

If, for any reason, screen19 does not run automatically, it can be run manually in the following way: Navigate to the “processing” directory – note that this is the only place you have permission to write files.

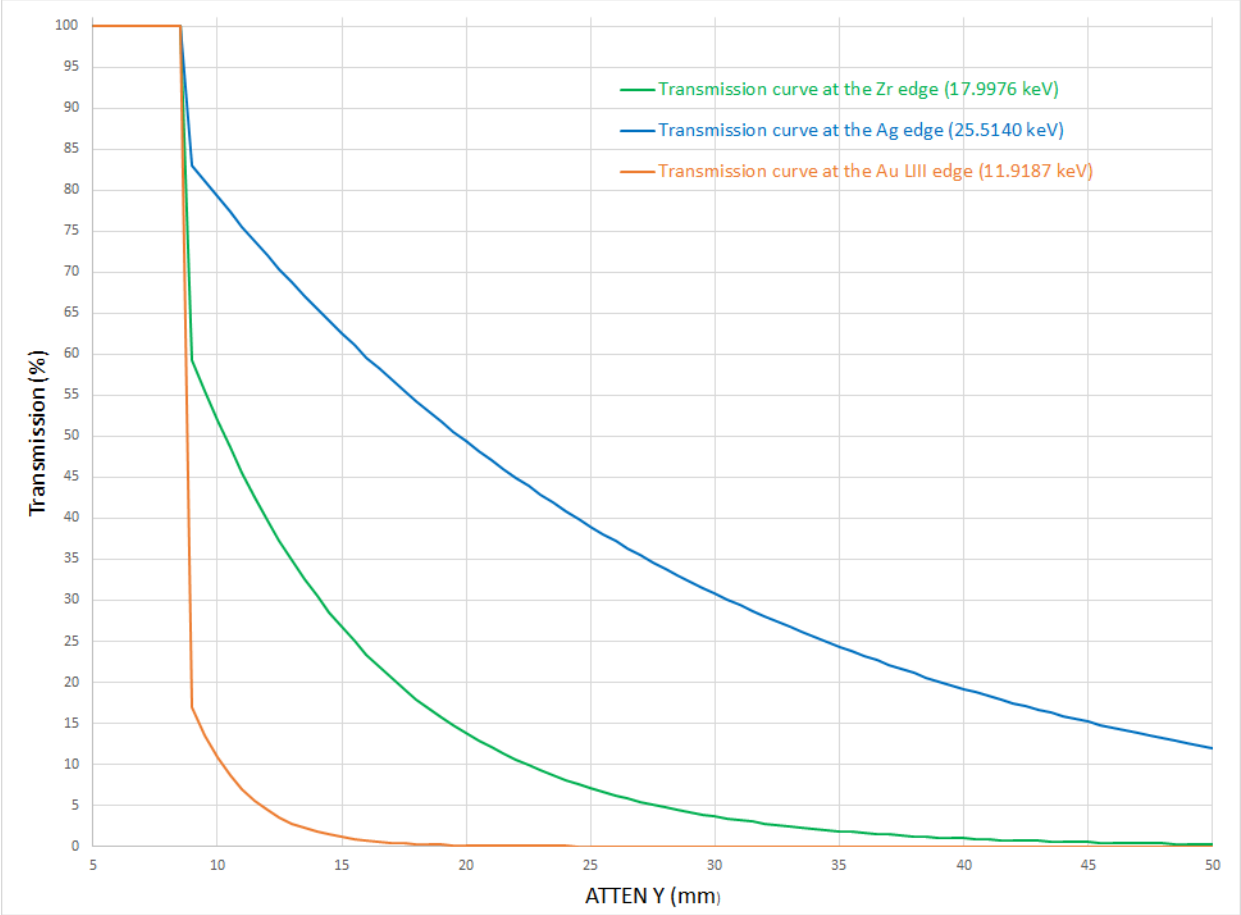
Create a suitably named directory (mkdir *foldername*) and enter it (cd *foldername*)

Type screen19 /dls/i19-1/data/YEAR/cyxxxxx-x/samplename/*.cbf
(the path to where the images are saved)

Attenuation

By placing materials in the path of the X-ray beam, and reducing the number of incident photons, it is possible to ensure that the maximum count rate of the detector is not exceeded. If photons arrive at the detector at a rate faster than the electronics for the affected pixel can process them, then some of the photons will not be counted. If this happens, then the brightest reflections will not be measured accurately, and this will reduce the quality of the data.

The attenuation devices are driven by specifying the **percentage transmission** required. The transmission is wavelength dependent so for a given thickness of material, the percentage transmission will be greater for shorter wavelengths than for longer ones. The plot below shows how the transmission varies at different energies as the thickness of the aluminium wedge increases.



For example, at Zr (0.6889 Å) 50% of the incident beam transmission is achieved by inserting a thickness of 0.5 mm of Al into the beam. This is the thickness of the wedge when ATTEN Y is set to 10.28 mm. However, at Ag (0.4859 Å) the transmission at this setting of ATTEN Y would be 78% and at Au LIII (1.0402 Å) the transmission would be 10%.

As there are gaps in the transmission options at both extremes of the energy range when using just the aluminium wedge, there are additional attenuation devices available to cover high transmission requests at lower energy, and low transmission requirements at higher energy.

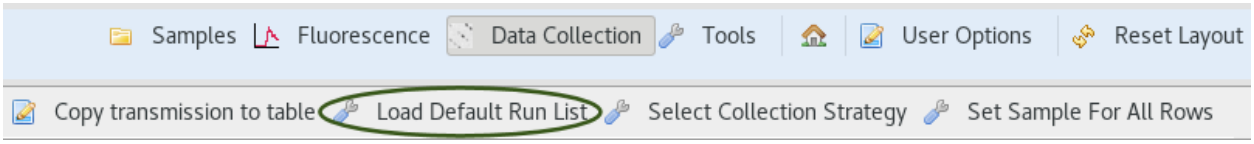
The GDA will automatically select the attenuation settings to provide the requested percentage transmission.

Strategies

The tables below show the resolution achievable by collecting data to the 2 theta settings indicated at various wavelengths. Also included is the minimum wavelength required to reach 0.84 A resolution for that run list.

Default

This can also be imported using the "Load Default Run List" button just above the right-hand corner of the data collection table.



Wavelength (Å)	Energy (keV)	Resolution to the detector edge (Å) at 2θ=30° [*not* corners]
0.4859 (Ag)	25.514	0.43
0.6889 (Zr)	17.9996	0.62
0.9028 (Au LII)	13.7336	0.81
0.9430		0.84

160mm 0-40 deg 3 steps

Wavelength (Å)	Energy (keV)	Resolution to detector edge (Å) at 2θ=20°	Resolution to detector edge (Å) at 2θ=40°
0.4859 (Ag)	25.514	0.50	0.38
0.6889 (Zr)	17.9996	0.71	0.55
0.9028 (Au LII)	13.7336	0.93	0.72
0.8150		0.84	0.65
1.0550		1.08	0.84

Note: If data is being collected at 2θ=40°, then the 2θ=20° scans are also required to make sure the inner sphere is adequately covered, the phi scan at 2θ=0° is not necessarily enough to ensure there is good scaling.

160mm 0-85deg 5 steps

Wavelength (Å)	Energy (keV)	Resolution to detector edge (Å) at 2θ=65°	Resolution to detector edge (Å) at 2θ=85°
0.4859 (Ag)	25.514	0.31	0.28
0.6889 (Zr)	17.9996	0.44	0.39
0.9028 (Au LII)	13.7336	0.58	0.51
1.2837 (Zn)	9.6586	0.82	0.73
1.3808 (Cu)	8.9789	0.88	0.78
1.3150		0.84	0.75
1.4750		0.94	0.84

160mm 0-105deg 5 steps

Wavelength (Å)	Energy (keV)	Resolution to detector edge (Å) at 2θ=80	Resolution to detector edge (Å) at 2θ=105°
0.4859 (Ag)	25.514	0.28	0.26
0.6889 (Zr)	17.9996	0.40	0.37
0.9028 (Au LII)	13.7336	0.53	0.48
1.2837 (Zn)	9.6586	0.75	0.68
1.3808 (Cu)	8.9789	0.80	0.73
1.4879 (Ni)	8.3328	0.87	0.78
1.6083 (Co)	7.7089	0.94	0.85
1.7433 (Fe)	7.1120	1.01	0.92
1.8961 (Mn)	6.5390	1.10	1.00
1.4350		0.84	0.76
1.5900		0.93	0.84

160mm 105-0deg 5 steps

This is the same as **160mm 0-105deg 5 steps** but with the 2 theta steps in reverse so the high angle data is collected first. This could be useful if radiation damage affecting the high angle data is likely to be an issue.

300mm 0-45deg 3 steps

Wavelength (Å)	Energy (keV)	Resolution to detector edge (Å) at 2θ=20°	Resolution to detector edge (Å) at 2θ=45
0.4859 (Ag)	25.514	0.67	0.43
0.6889 (Zr)	17.9996	0.94	0.62
0.9028 (Au LII)	13.7336	1.24	0.81
0.613		0.84	0.67
0.935		0.93	0.84

The overlap between the 2θ=20° and 2θ=45° is a bit small, but this could be worth a try if radiation damage is likely to cause more issues than scaling.

For wavelengths between 0.75 Å and 0.87 Å, changing the 2θ=45°set of scans to 2θ=40° should work better as this will still give a resolution of 0.84 Å, but with better detector overlap

– Remember to update the start axis to omega = -135°!
(Or use the start of the **300mm 0-105deg 7 steps** option)

300mm 0-45deg 4 steps

Wavelength (Å)	Energy (keV	Resolution to detector edge (Å) at 2θ=30	Resolution to detector edge (Å) at 2θ=45°
0.4859 (Ag)	25.514	0.55	0.43
0.6889 (Zr)	17.9996	0.77	0.62
0.9028 (Au LII)	13.7336	1.01	0.81
0.745		0.84	0.67
0.935		1.05	0.84

This option gives better overlap between scans up to 2θ=45° than **300mm 0-45deg 3 steps**.

300mm 0-105deg 7 steps

Wavelength (Å)	Energy (keV)	Resolution (Å) at 2θ=75°	Resolution (Å) at 2θ=90°	Resolution (Å) at 2θ=105°
0.4859 (Ag)	25.514	0.32	0.29	0.27
0.6889 (Zr)	17.9996	0.46	0.41	0.38
0.9028 (Au LII)	13.7336	0.6	0.54	0.50
1.2837 (Zn)	9.6586	0.85	0.77	0.71
1.3808 (Cu)	8.9789	0.92	0.83	0.77
1.4879 (Ni)	8.3328	0.99	0.89	0.83
1.6083 (Co)	7.7089	1.07	0.96	0.89
1.7433 (Fe)	7.1120	1.16	1.05	0.97
1.8961 (Mn)	6.5390	1.26	1.14	1.06
1.2650		0.84	0.76	0.71
1.3950		0.93	0.84	0.78
1.5050		1.00	0.90	0.84

300mm 105-0deg 7 steps

This has the same coverage as **300mm 0-105deg 7 steps** but with the 2 theta steps in reverse, so the high angle data is collected first. This could be useful if radiation damage affecting the high angle data is likely to be an issue.

Others

There are also some options available which include extra omega sweeps for increased redundancy.