ISPyB

ISPyB is where all the details about your samples, data collections and processing results are collated, including:

- sample registration
- shipment of samples
- data collection details
- access to diffraction images, crystal snapshots and reciprocal lattice views
- results from auto processing and ability to download pertinent files
- reprocessing of data using xia2

Access to visits you are associated with is unlimited, so details for both current and historic visits are always available.

Navigate to https://ispyb.diamond.ac.uk or click on the links from either the internet or intranet (if available) and log in using your FedID and password. ISPyB can be accessed from anywhere and on any device.

Data Collections

During an active visit, from the home page, click on the current visit to get to the Data Collections page. This page can also be reached by selecting Visits from the visit menu and choosing the appropriate visit.

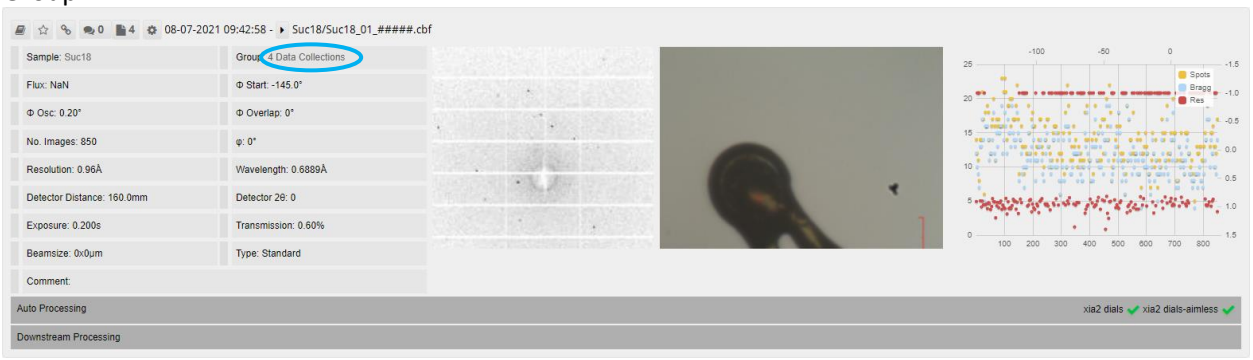
Clicking on the words **i19-1 Webcams & Beamline Status** will bring up a series of status boxes and *should* display the 2 hutch webcams – this section times out after 10 minutes so will need refreshing when required.

The status box displays include which sample is actually mounted and show when various shutters are open/closed - they are green when in a ready state and red when not.
NOTE: this option is only available just before and during your beamtime - it will stop working as soon as the visit officially ends.

When running remotely, do pay attention to the status boxes as they give the best indication of the current beam status. For there to be user beam:

- The ring current should (normally) be ~300 mA
- Beam is (normally) only available when the Refill (top-up) is active
- The Port shutter is open

At any time, the log window and the beamtime history are available to view. Full data collections consisting of multiple sweeps are grouped (with a somewhat random selection of details across the full collection shown on the summary page) but all runs can be accessed by clicking on the link next to Group.



Table

The table on the left-hand side shows the basic information for each sweep of data, including the goniometer positions, image step size, time per image, transmission used, wavelength and experiment type.

If the Sample ID is set correctly in the GDA data collection table (only applicable when samples have been pre-registered in ISPyB – see page 53) then the sample entry should match the sample as registered in the shipment. This means any data collections are linked to that sample.
If comments have been added to the comments column of the GDA data collection table, they will also be reported here.

NOTE: The beamsize is actually 100 µm and there is flux!

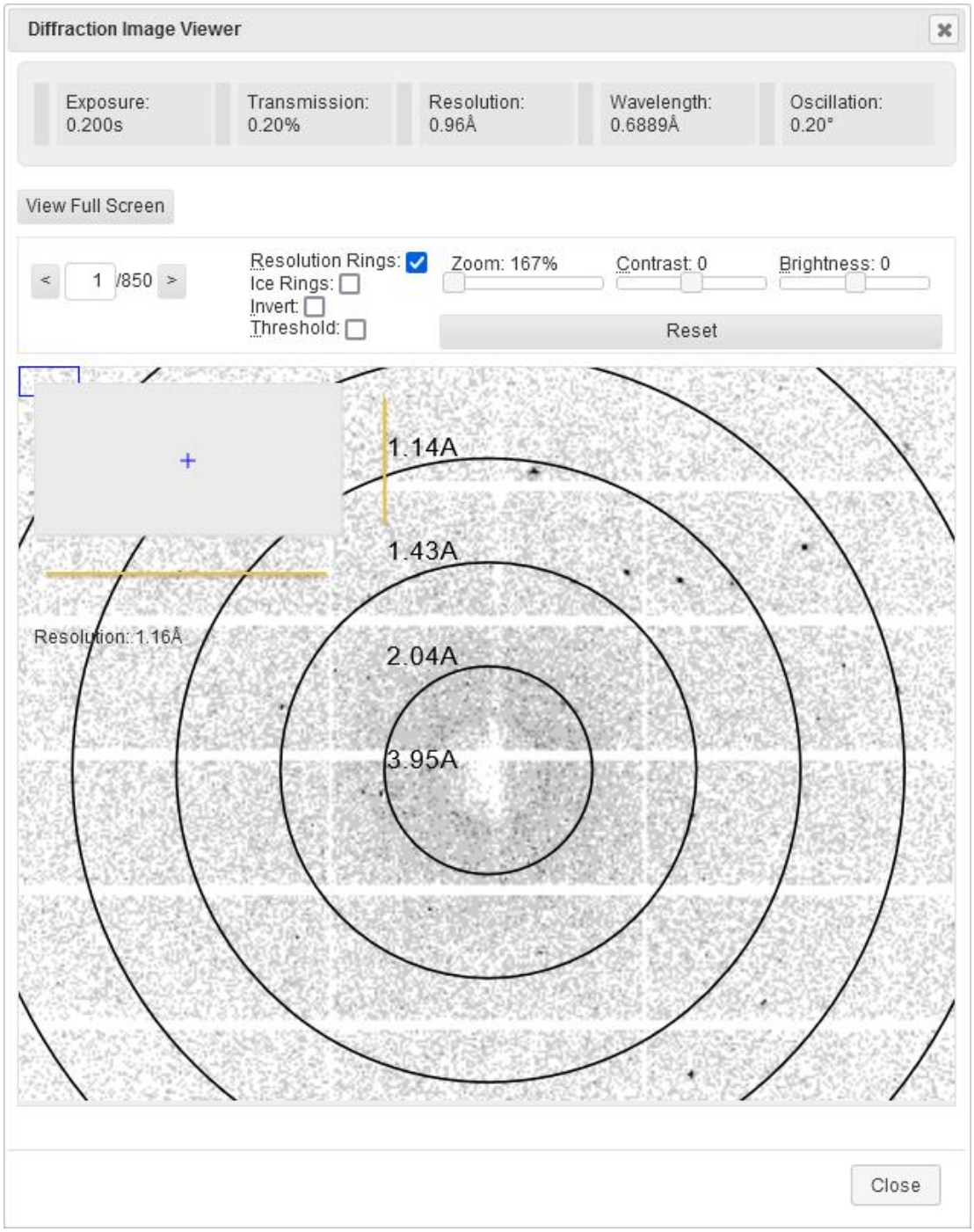
Diffraction Image

Just the first image is displayed in the summary, but by clicking on the image a new Diffraction Image Viewer window opens and it is possible to click through or select specific images.

If there are powder rings, checking the box for ice rings will show the expected locations for ice rings and is a quick and easy way to see if the powder rings are due to ice or the sample (or, occasionally, beam conditioning components – if you suspect this to be the case, request assistance from your local contact).

Notes:

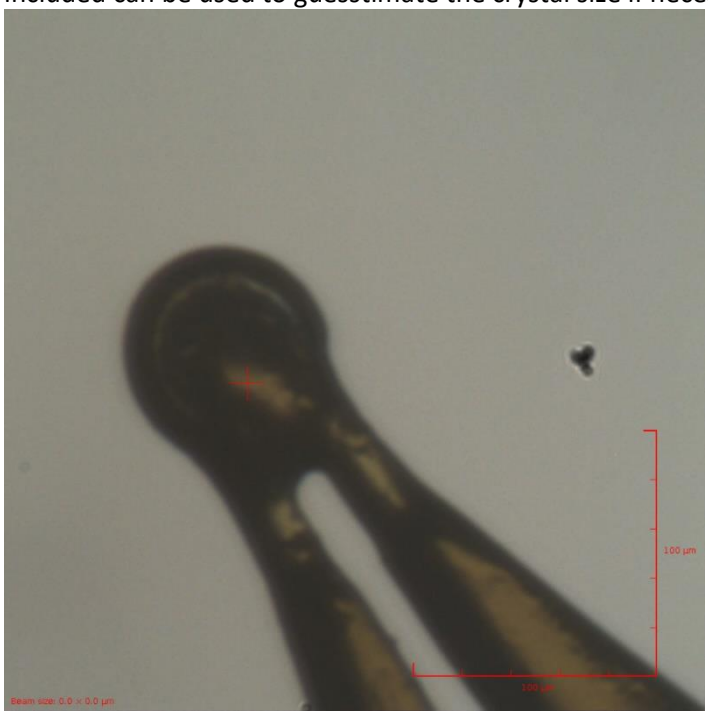
- The images are converted to jpgs so the contrast and brightness functions don't work usefully
- Resolution and ice rings are only located accurately for images collected with 2 theta at 0



Crystal Snapshots

Snapshots are taken of the crystal at 90 degree intervals (0°, 90°, 180° and 270°) between centring and data collection starting. As snapshots are only taken before the start of a data collection if the light is already in, pictures are normally only produced for the first screening run and they are only displayed for that collection.

Click on the picture to view it in full and use the arrows to move on to the next image. The scale included can be used to guesstimate the crystal size if necessary.



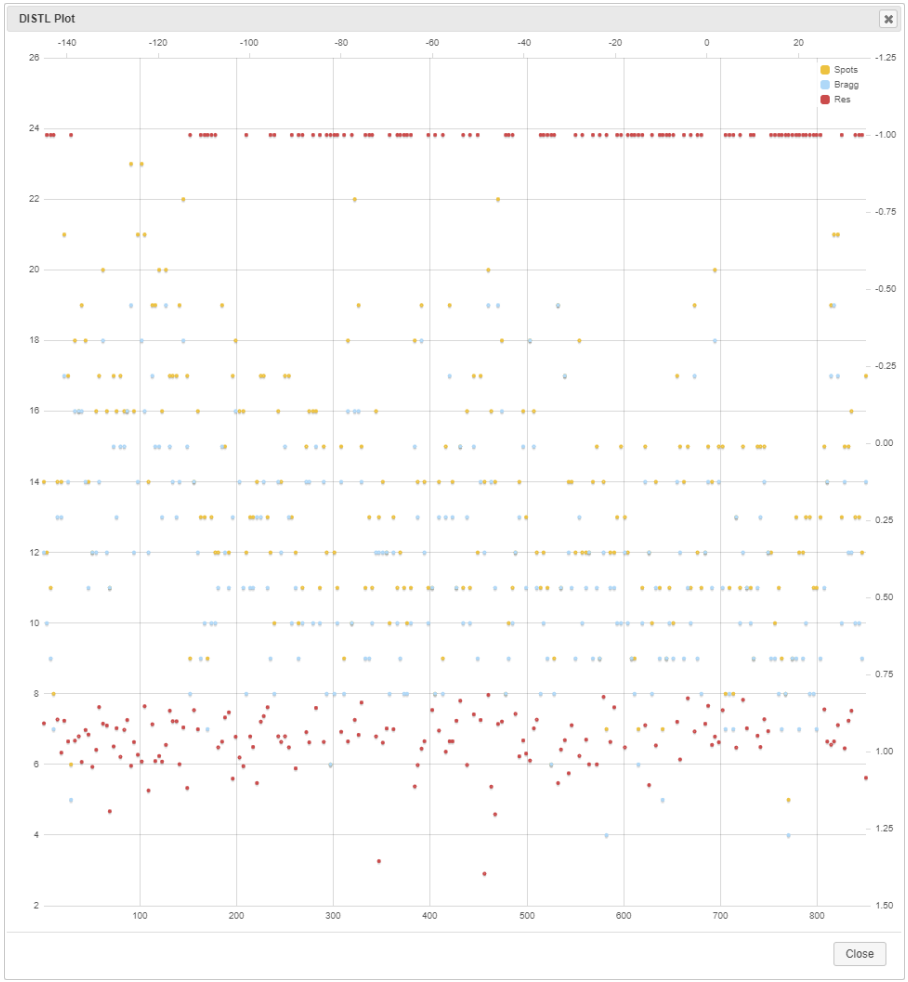
Remember, you can persuade the system to take more snapshots by clicking the “Make hutch safe” or “Prepare Sample Mount” buttons in the GDA and then starting the next data collection. As the backlight is put back in position, the GDA expects that the sample has been changed and will take another set of snapshots before the subsequent data collection starts. If you just want before and after shots, the "after" data collection could just be a single diffraction image.

Spotty Plot

The plot on the right-hand side gives an indication of the diffraction quality.

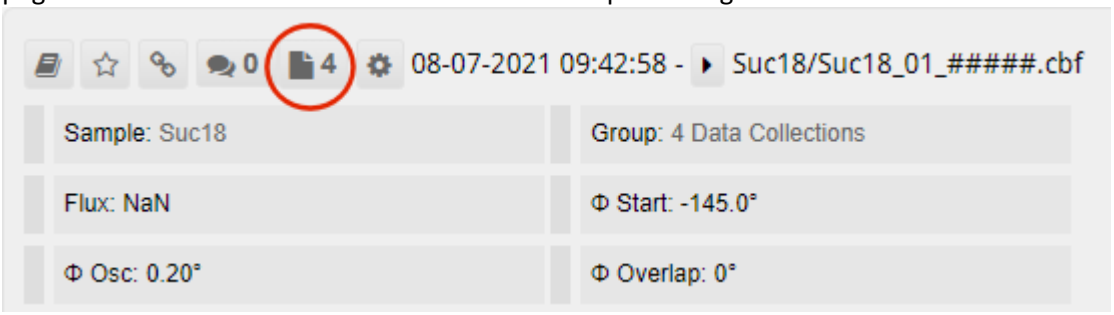
The yellow spots indicate the number of reflection-like features found per image – left hand axis.
The difference between yellow spots and blue spots is not obvious.

The red spots show the resolution of the reflection features found per image – it does *not* show the maximum resolution but that of the highest resolution shell with more than some number of reflections. For clean diffraction patterns and small unit cells, the reported resolution is often -1 (null) as there are not enough reflections above the threshold (which was defined for proteins).

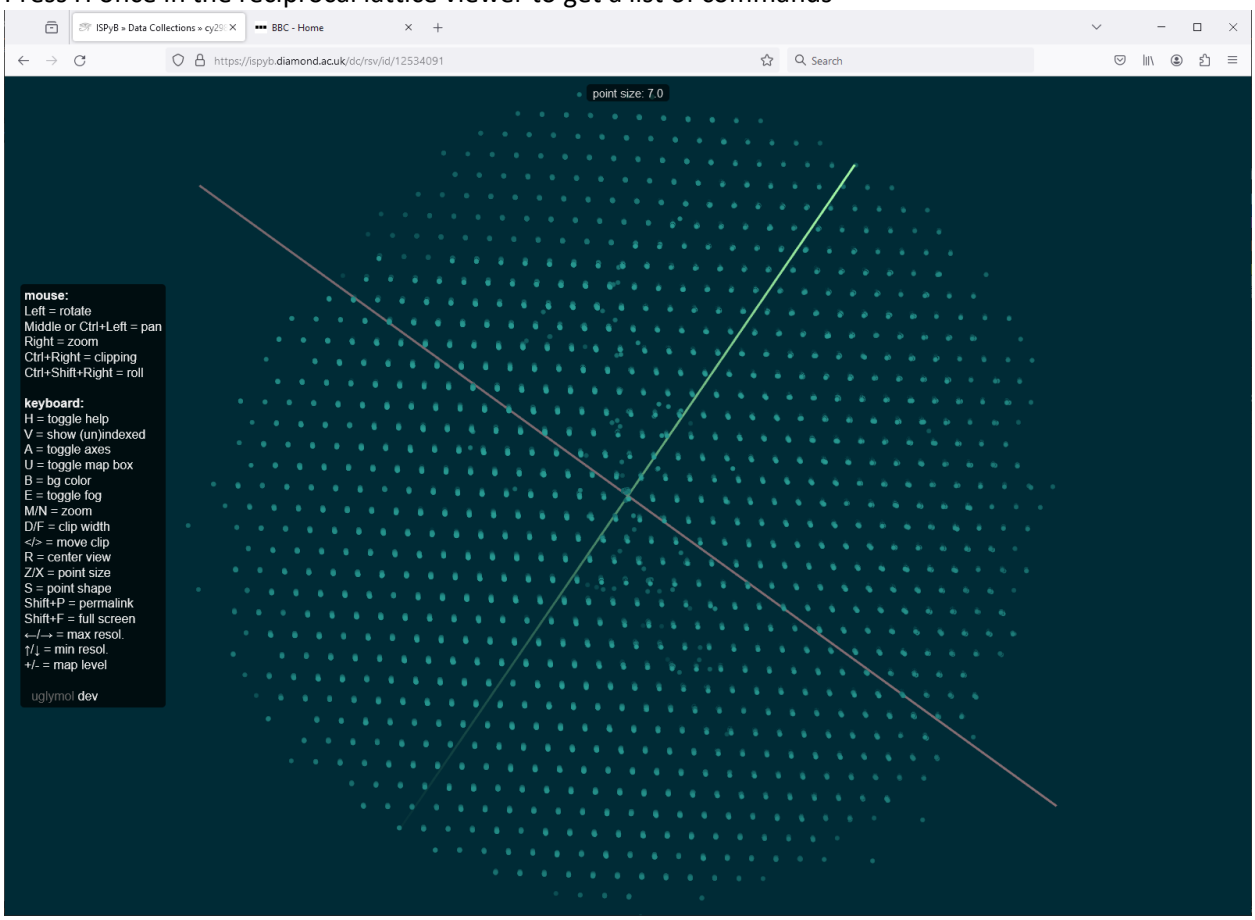


Reciprocal Lattice Viewer

To see the lattice for any given run, click on the page with the turned over corner to open an "Attachments" window and then click on Reciprocal Space Viewer for the desired run. Note that the page turns into a snowflake once a certain level of processing has been reached.



Press H once in the reciprocal lattice viewer to get a list of commands

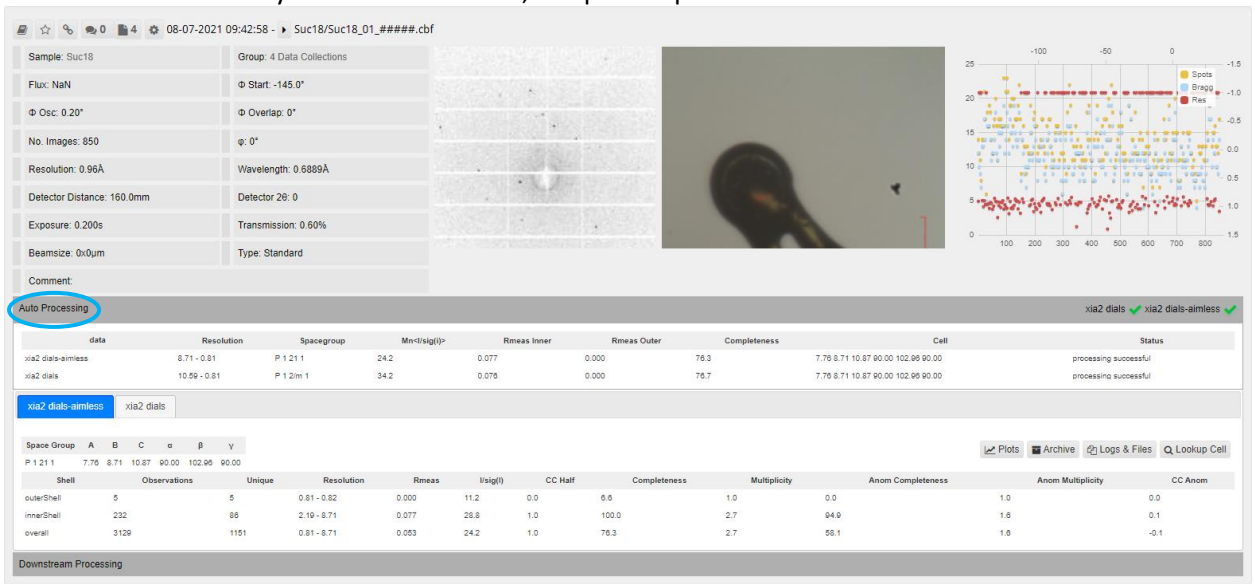


Once you have finished viewing the reciprocal lattice, click on the browser back arrow to return to the home page - do not be tempted to click on the close button as this will exit all of ISPyB.

It is not possible to view multiple sweeps in the same view here. This can be done *via* DIALS (page 81).

Auto Processing

A summary of the auto processing results is given in the Auto Processing tab – click on Auto Processing for the data collection you are interested in, to open it up.



Auto processing is run twice, once using aimless for the absorption correction and once using dials.scale. If a space group and unit cell have been provided for that sample (as part of the puck filling process) then auto processing will also be run for each scaling process, but with the cell information included.

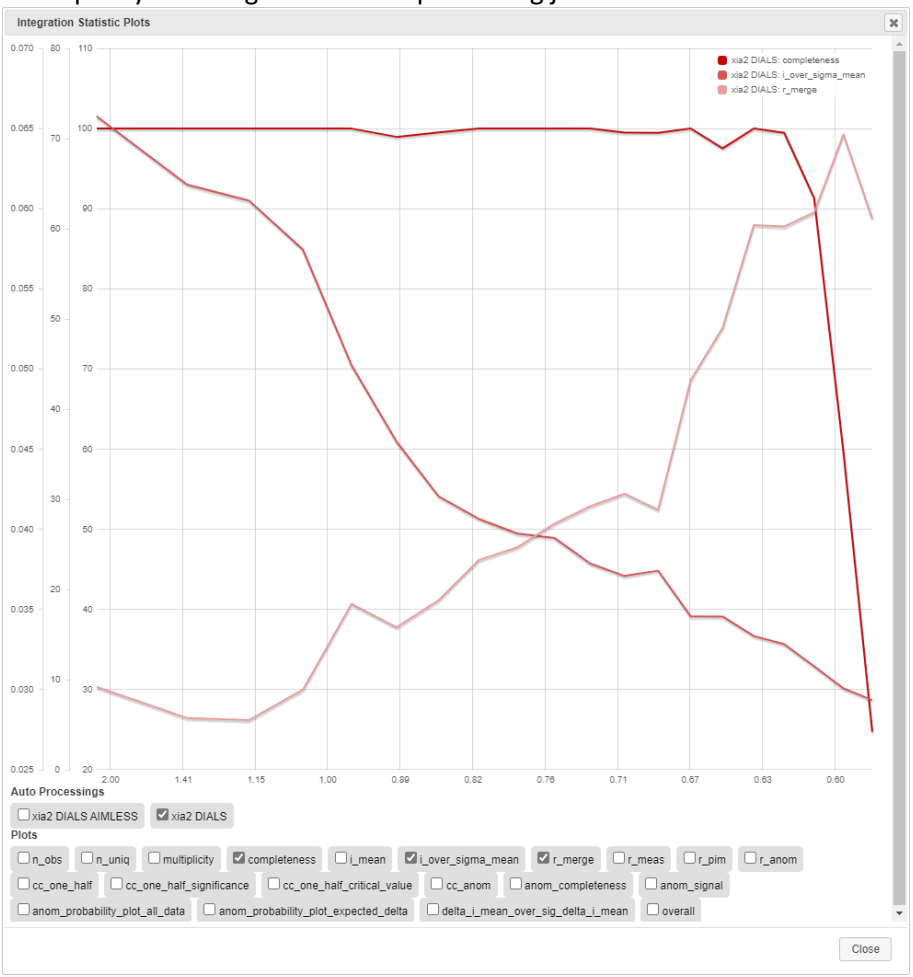
Generally, xia2 dials gives better results than xia2 dials-aimless but sometimes one will work when the other fails, as indicated by green ticks or red crosses. Note that there is a bug where processing jobs run including the unit cell information are classified as undefined.

The processing is run on all of the images collected so far so, within the group for a data collection, the final sweep will have the processing results for all data collected.

The tab title clearly indicates how many sweeps of data have been used. Sometimes, this number will be less than expected due to one or more sweeps failing to integrate successfully.

Plots

Completeness, mean I/σ and Rmerge are plotted by default but it is easy to display other options by swapping which check boxes are ticked. It is also possible to compare the results for multiple processing attempts by selecting the relevant processing jobs.



Lookup Cell

Clicking on this will produce a list of all auto processing results, across all visits you are associated with, which match the unit cell of the dataset you are looking at.

Logs and Files

Opening the Logs and Files will give a list of files associated with the processing job – these are always available to view or download even after the visit has been archived.

Below are some of the potentially more useful files.

shelxt.ins and shelxt.hkl
Although shelxt is run automatically on these files, the resulting res files are not available in this list.
It may, therefore, be easiest to download these input files and rerun shelxt (or other structure solution software) manually on your local system as this is likely to have write access.

It also gives you the opportunity to include the relevant atom types which obviously leads to a greater chance of a successful solution. At the moment, it is not possible to push this knowledge through to the auto processing.

xia2.cif
xia2.cif contains information regarding the software, versions and references used for the auto processing. It also contains the appropriate cif entries and references for the use of EH1, including
_diffrn_radiation_wavelength
_diffrn_measurement_device
etc.

NOTE: The hkl ranges and _diffrn_reflns_number are not calculated correctly so these should be obtained from the raw data in the hkl file.

xxxxx_merging-statistics.txt
This file gives an xprep style output table showing multiplicity, Rmerge, completeness etc. per resolution shell. The same information can be obtained from the plots, so it is just an alternative view depending on whether you find the table or graphs easier to interpret. At the top, there is a useful summary of the overall statistics.

xia2.html
Information from the merging-statistics and xia2.txt are combined and summarised here.
The Summary tab gives the same information as found at the top of the merging statistics file with values for all data (and outer resolution shell). The “xia2 output” button opens the xia2.txt file.
The Dataset SAD tab shows the table produced at the bottom of the xia2.txt file. Opening Resolution shells reveals the whole table from the merging-statistics file.
There are a number of plots available:

- Analysis by resolution: these are the most useful plots to protein crystallographers but do include completeness, I/σ(I) and multiplicity (these can also be found in Plots)
- Analysis by batch: summary of mean I/σ(I) and Rmerge shown per image and with sweeps highlighted
- Miscellaneous: information about the number and location of reflection multiplicities

xia2.txt
The xia2.txt file summarises the processing information, starting with spot finding, then indexing, then integration and finally cell refinement.

Options

Assign Containers
A short cut to the page for assigning the puck positions within the robot Dewar.

Summary
Produces a table of results for the data collections shown on the front page, so only the first sweep of multirun data collections. It includes unit cell parameters and some useful statistics, although they would probably be more useful if they were for the results from the full data collection.

Auto Processing
Auto Processing simply shows which data collections were processed successfully but again, only for the first sweep.

Visit Stats
Here, the proportion of time spent completing various tasks, including time the robot is in action, time spent centring and time spent collecting data can be seen as a function of the shift. This can be looked at in more detail by drawing a box around the period of interest.
Totals for the visit are also displayed including "Thinking" time – note that manual sample mounting counts and centring count under “Thinking”.

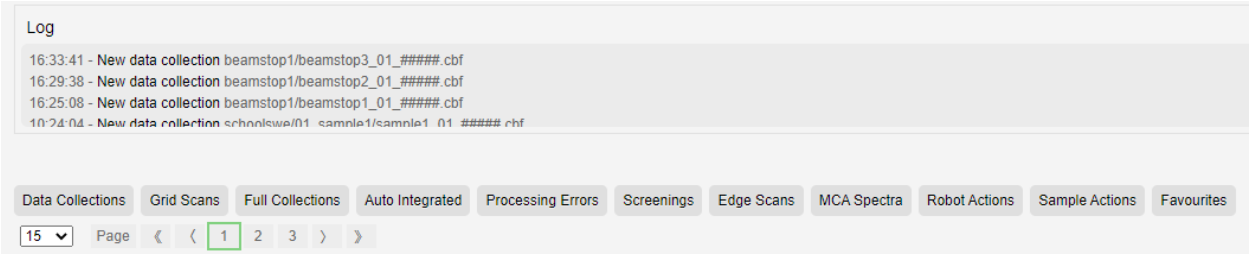
Users
A drop down appears showing the users on the visit and who the local contacts are.

Dewars
A drop down shows which Dewars (if any) are associated with the current visit and their current status.

Sample Changer
Sample Changer opens a new page with a pictorial overview of the maximal status of the samples, e.g., which ones have been loaded only, which have had data collected and which have had data collected and been successfully auto processed. At the moment, the screening flag doesn’t work as screening is not differentiated from data collections.
To make the view more user friendly make the browser window as narrow as possible, refresh the view and then maximise the window again – this should make the padding for each sample representation smaller and make it possible to see more samples at once.
Clicking on a sample will show all actions performed on that sample (as shown on the home data collections page) at the bottom of the screen.

Reprocessing
Reprocessing opens a window showing a list of current and completed reprocessing jobs with any input commands set, e.g., resolution, unit cell information and which images were used.
Click on the relevant line (the top line has the results for all included sweeps) under files to be taken to the results of the processing job.
This will appear as another result in the Auto Processing section for that data collection. The 2 chasing arrows show that this is a manual reprocessing job rather than an auto processing job. All options for the reprocessed job match those of the auto processing.

Filters



These buttons are used to filter the items on Data Collections page, so you just see the data collections or robot actions etc.

At the moment, no distinction is made between Data collections and Full collections, so the lists are the same.

Screenings are not registered as such at the moment, so this list is empty.

Grid scans, Edge scans, MCA spectra and Sample actions are not performed on I19.

Auto Integrated will filter down to list of data collections where auto processing has successfully completed for the first scan.

Robot actions will just show sample loads.

To go back to see the full list of everything, go to the visit tab, then click on Visits and choose the current visit.

View All Data will show every action and data collection for the whole proposal (multiple visits) but will not have the I19-1 Webcams & Beamline Status section even if the current visit is live.

Pre-Registering And Shipping Samples

The robot can only be used with samples which have been pre-registered in ISPyB, and the puck positions assigned.

It is possible to create shipments with pucks and samples, without actually needing to courier the Dewar to Diamond. Therefore, it is possible to set up pucks to use with the robot whilst on site during an active visit. It is also possible to create virtual pucks of samples – this may be useful as crystal information, such as space group and unit cell, can be added in ISPyB which is then used by the auto processing. The set-up process in ISPyB is the same.

Before Beamtime

Recommended Timeframe: For remote access, there are several extra steps which need to be completed before the start of your beamtime, summarised in the table below.

Action	When
Register samples in UAS and submit ERA for grading (don't forget to include an acronym!)	at least 2 weeks before beamtime
Register all users – make sure all remote users are listed and designated as remote	at least 2 weeks before beamtime
Check all samples registered in the UAS are listed in ISPyB Speak to your local contact if there are issues	1 day after ERA grading notification
Prepare samples in pucks	to be completed at least 4 working days before beamtime
Add shipment and samples in ISPyB	to be completed at least 4 working days before beamtime
Prepare shipping information and print labels	at least 4 working days before beamtime
Ship Dewar to Diamond	at least 3 working days before beamtime
Receive notification of Dewar arrival at Diamond – if not check Dewar tracking in ISPyB and the courier company	at least 2 working days before beamtime

Shipping Dates: We recommend following the shipping timetable below to ensure Dewars are at Diamond ready for the time they are required.

Beamtime	Latest Arrival at Diamond	Ship By
Monday	Friday 4pm (previous week)	Wednesday (previous week)
Tuesday	Monday 4pm	Thursday (previous week)
Wednesday	Tuesday 4pm	Friday (previous week)
Thursday	Wednesday 4pm	Monday
Friday	Thursday 4pm	Tuesday
Saturday	Friday 4pm	Wednesday
Sunday	Friday 4pm	Wednesday

Please try to ensure Dewars arrive at least 48 hours before the start of beamtime - this will allow flexibility around puck loading and for unexpected delays by DHL.

NOTE: Goods handling is only available for deliveries on weekdays.

Register Samples

For experiments using pre-mounted samples for loading by the robot, all samples must be identified in ISPyB.

ISPyB can be found at https://ispyb.diamond.ac.uk (or links to it are available from both the internal and external Diamond websites) and is accessed using your FedID and password.

ISPyB can be accessed from anywhere, on any computer, tablet or mobile device and does not need to be operated from within "Diamond". You will need to be registered on any visit you wish to be able to access – it doesn't matter if you are registered as attending site or as a remote user.

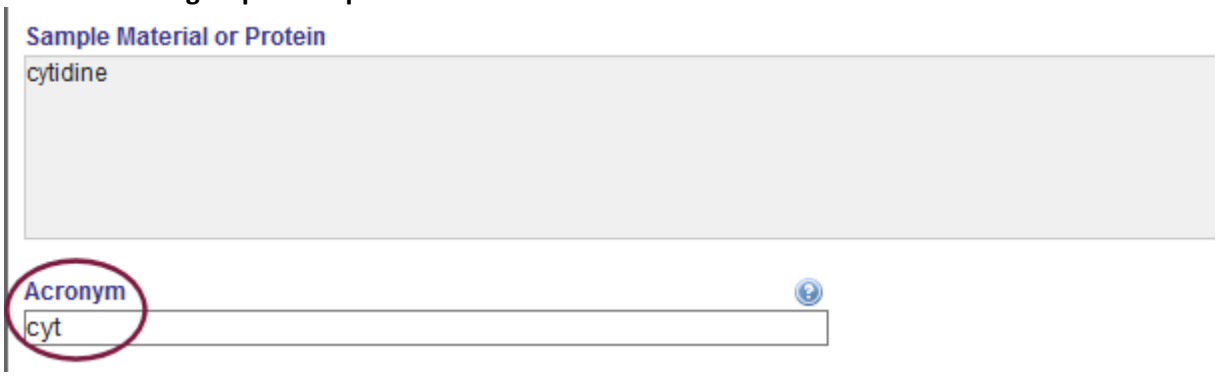
ISPyB is the database where all of the information about your samples is stored, and features include:

- Sample identification – *i.e.*, sample type and location within a puck
- Puck location within the robot Dewar
- Dewar shipping and tracking (including at Diamond)
- Monitoring of data collections
- Ability to reprocess data

Register Samples in the UAS

In order for samples to be available in ISPyB for allocation to a shipment, they MUST be registered and graded in the UAS first.

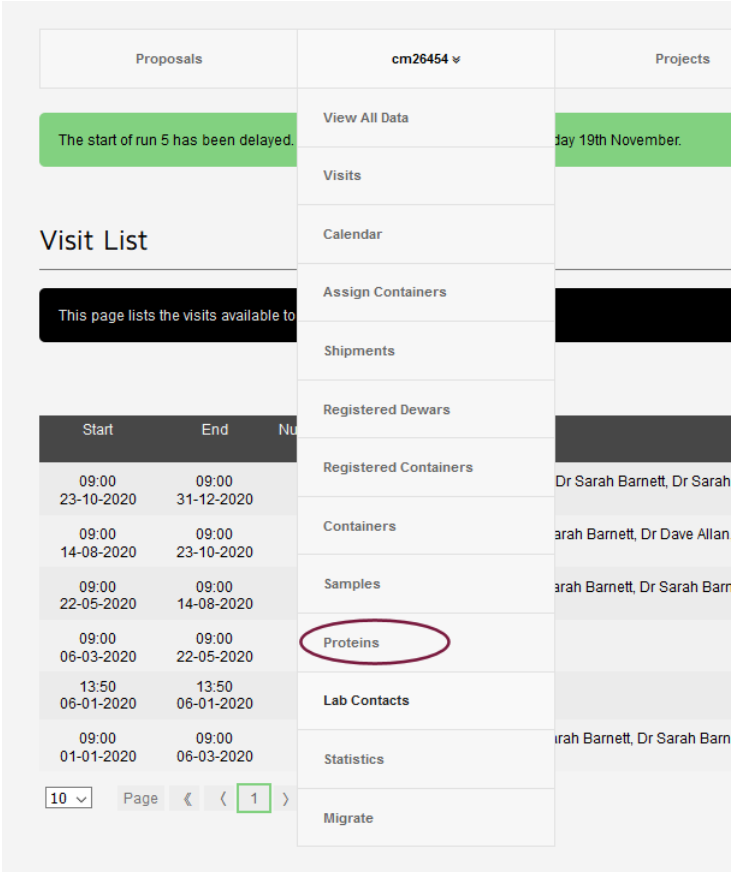
ISPyB only "sees" samples which have the acronym field in the UAS populated, so make sure a unique name for each group of samples is added here.



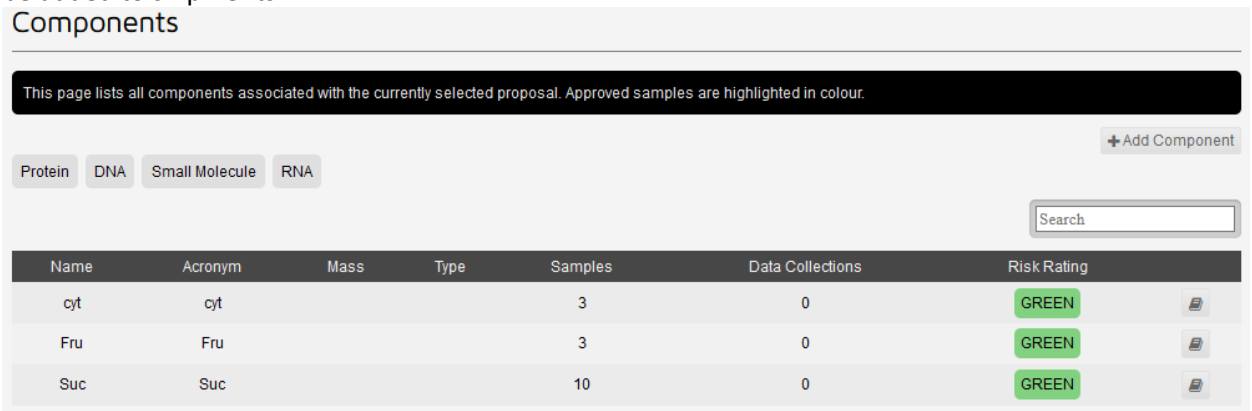
Please note, this is *not* a mandatory field so you will not be prompted to complete this for submission of the sample. Please remember to do this at the start as otherwise the samples will need to be checked out, have this information added, and then resubmitted for grading, causing delays.
ISPyB sample collections are run hourly, so there may be a short delay between the ERA being graded and the samples appearing in ISPyB. In case of any issues with the ERA grading or ISPyB sample harvesting we recommend the ERA is submitted as soon as possible.

Check for Samples in ISPyB

Once you have received the ERA grading from the Health and Safety team, start checking to see if the samples have been picked up in ISPyB. To view the list of available compounds, navigate to the **Proteins** page from the visit menu:



Samples which have been graded and successfully pulled into ISPyB will have a colour-coded risk rating – only samples graded low (green) or medium (yellow) risk on the ERA will be collected by ISPyB and can be added to shipments.



If some, or all, of your samples are not in the list 24 hours after receiving the safety rating from the Diamond Health and Safety team, and you are sure all samples were given an acronym in the UAS, please inform your local contact as soon as possible to resolve any issues.

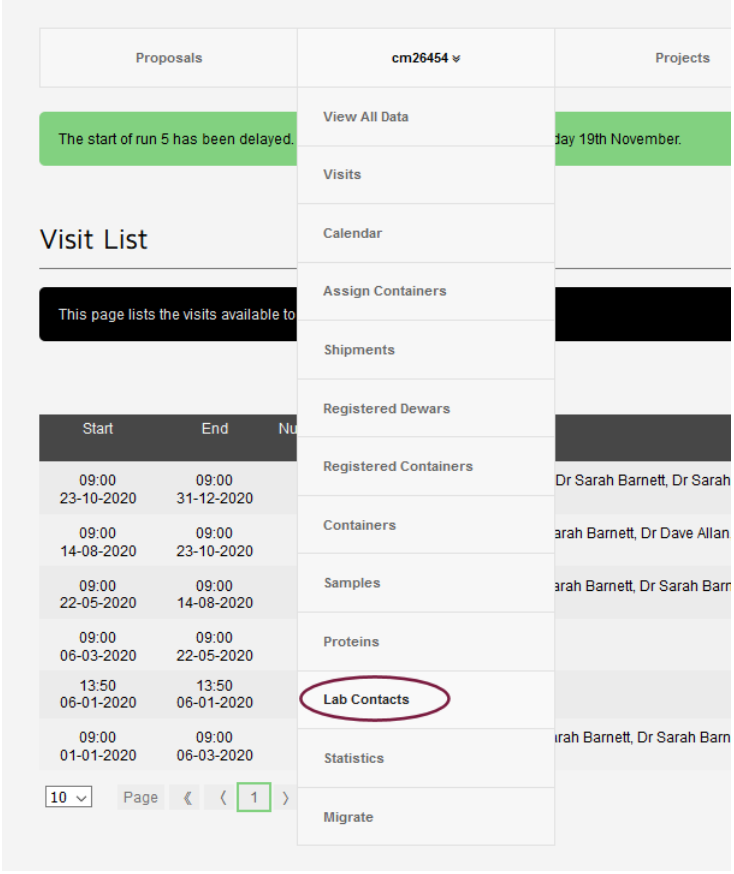
DO NOT try to make samples manually in ISPyB from the Proteins/Components page – these are not valid samples and can not be used to populate pucks.

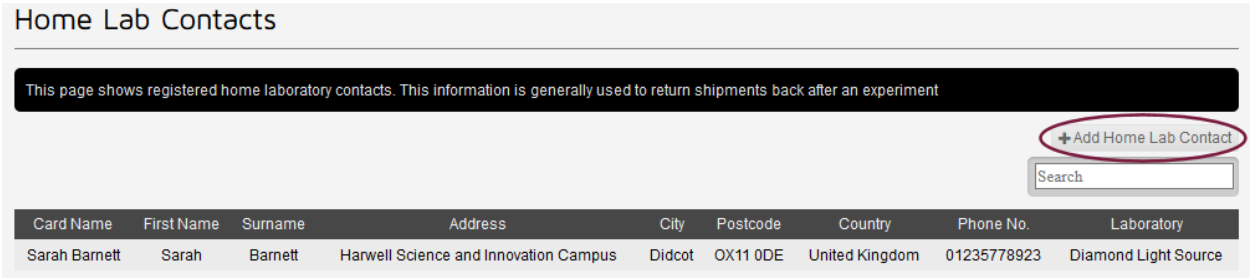
Create A Shipment

Log in to ISPyB using your FedID and password.
Navigate to the relevant visit by either selecting it from the Home Page or navigate to it from the list of proposals found in the "Proposals" section.

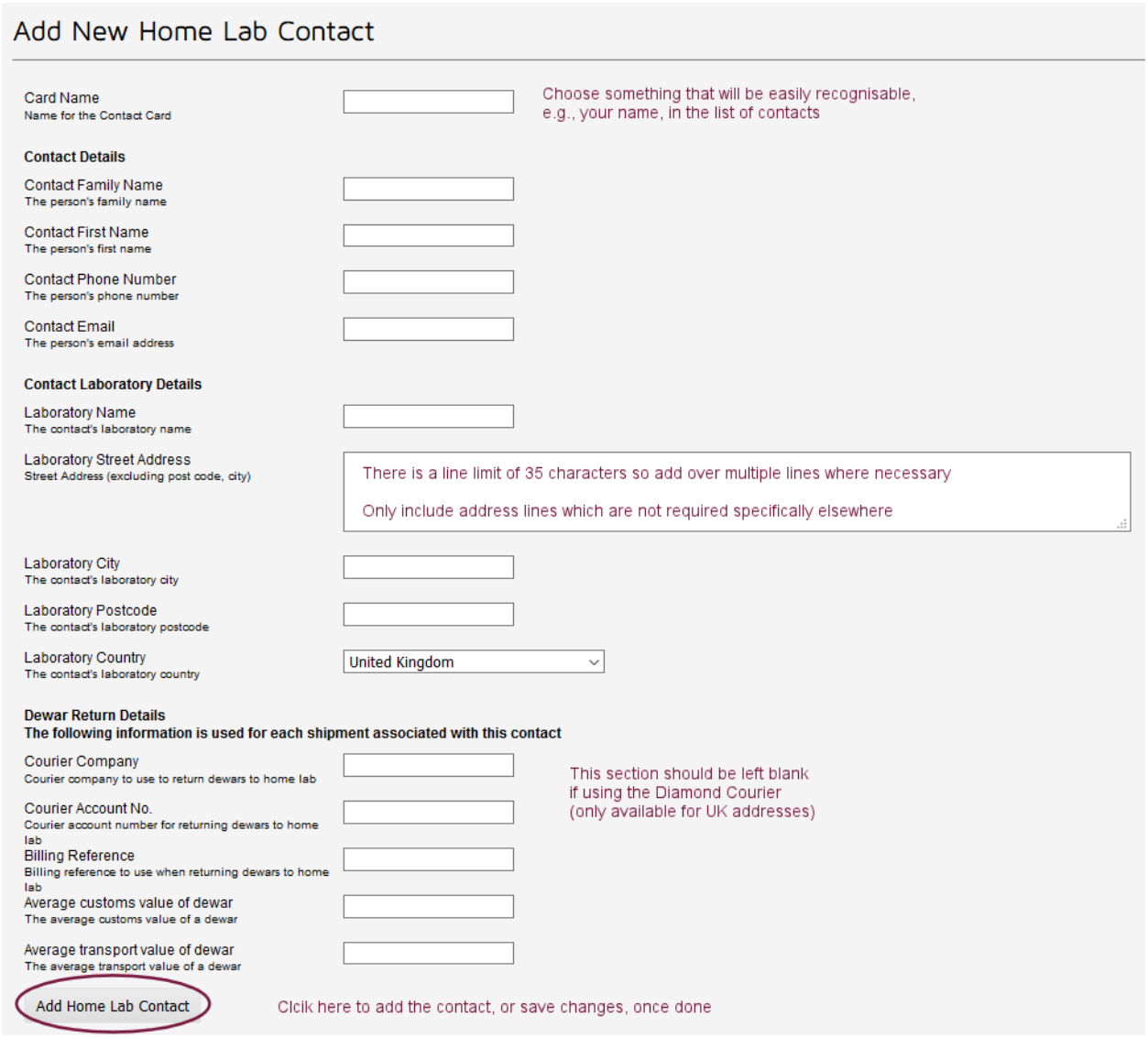
Lab Contact

Add a Lab contact – this should be the person who will be responsible for ensuring the Dewar is ready to go and in the right place for collection. From the Visit Menu, select Lab Contacts.





Here, you can edit the details of an existing contact or add more contacts by clicking on the button to add a home lab contact.



Register Dewars

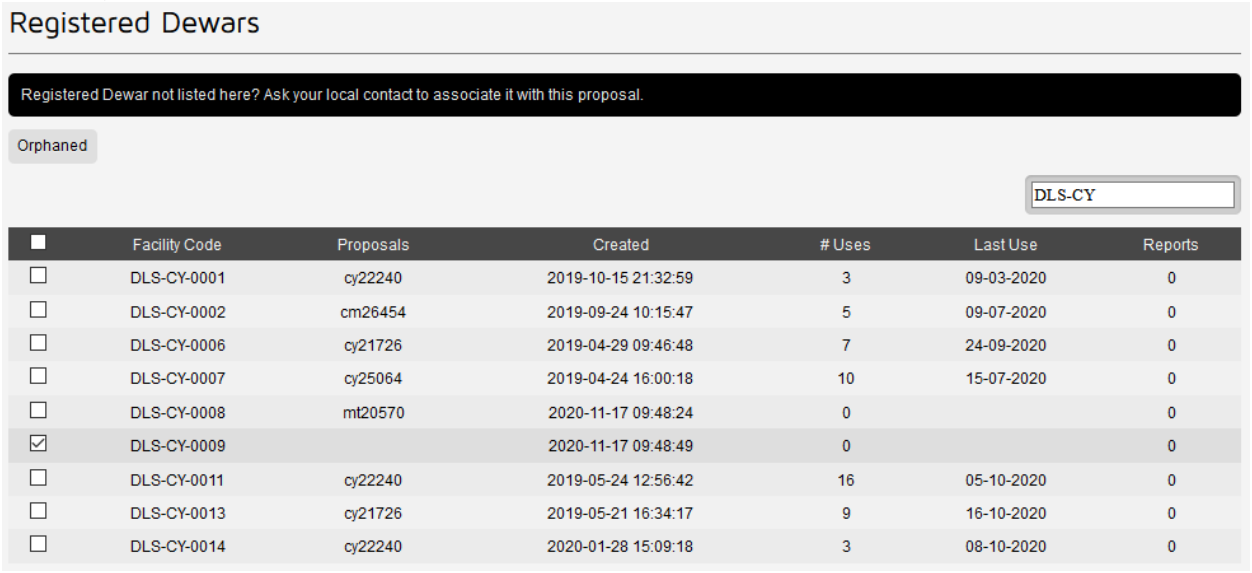
All Dewars must be registered in ISPyB as only registered Dewars can be added to a shipment in ISPyB and only Dewars registered with Diamond ID's will qualify for shipping using Diamond's courier. Dewars for use on I19 will be given a facility code in the form of **DLS-CY-00XX**.

If you have borrowed a Dewar from I19, or you are preparing a virtual shipment, then the Dewar should have been pre-registered by I19 staff, ready for use. If you have purchased a new Dewar, you will need to request a code from I19 staff (the Dewar will be labelled appropriately on arrival at Diamond) and register it.

From the visit menu, navigate to the Registered Dewars page and then scroll to the very bottom of this page to find the section to add a new Dewar.

Type in the facility code and the purchase date and then click on the "**+** Add Dewar" button.

The Dewar now needs to be associated with the correct proposal. Find the Dewar in the list of registered Dewars at the top of the page and check the box for your Dewar (it may be quicker to use the search function).

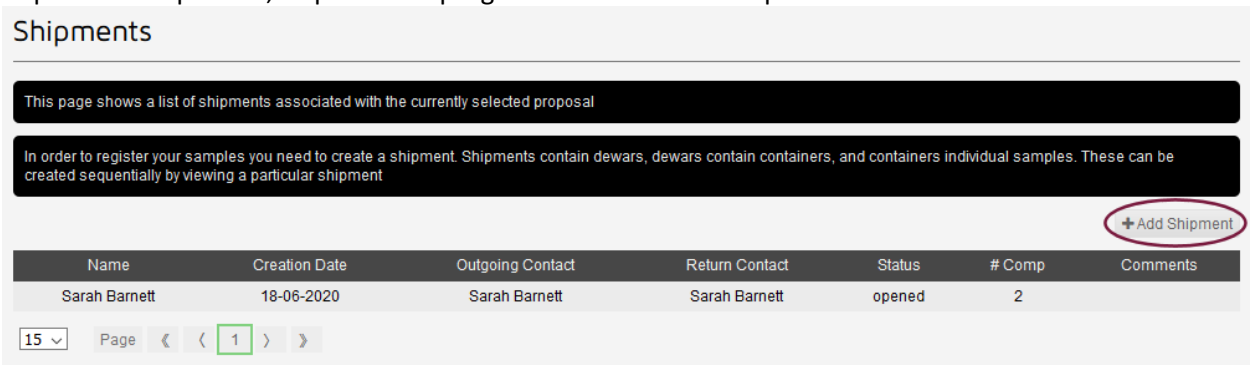


Then find your proposal in the section below, check the box for the appropriate proposal and click on the "**+** Add to Proposal" button. This should have associated your new Dewar with your visit.

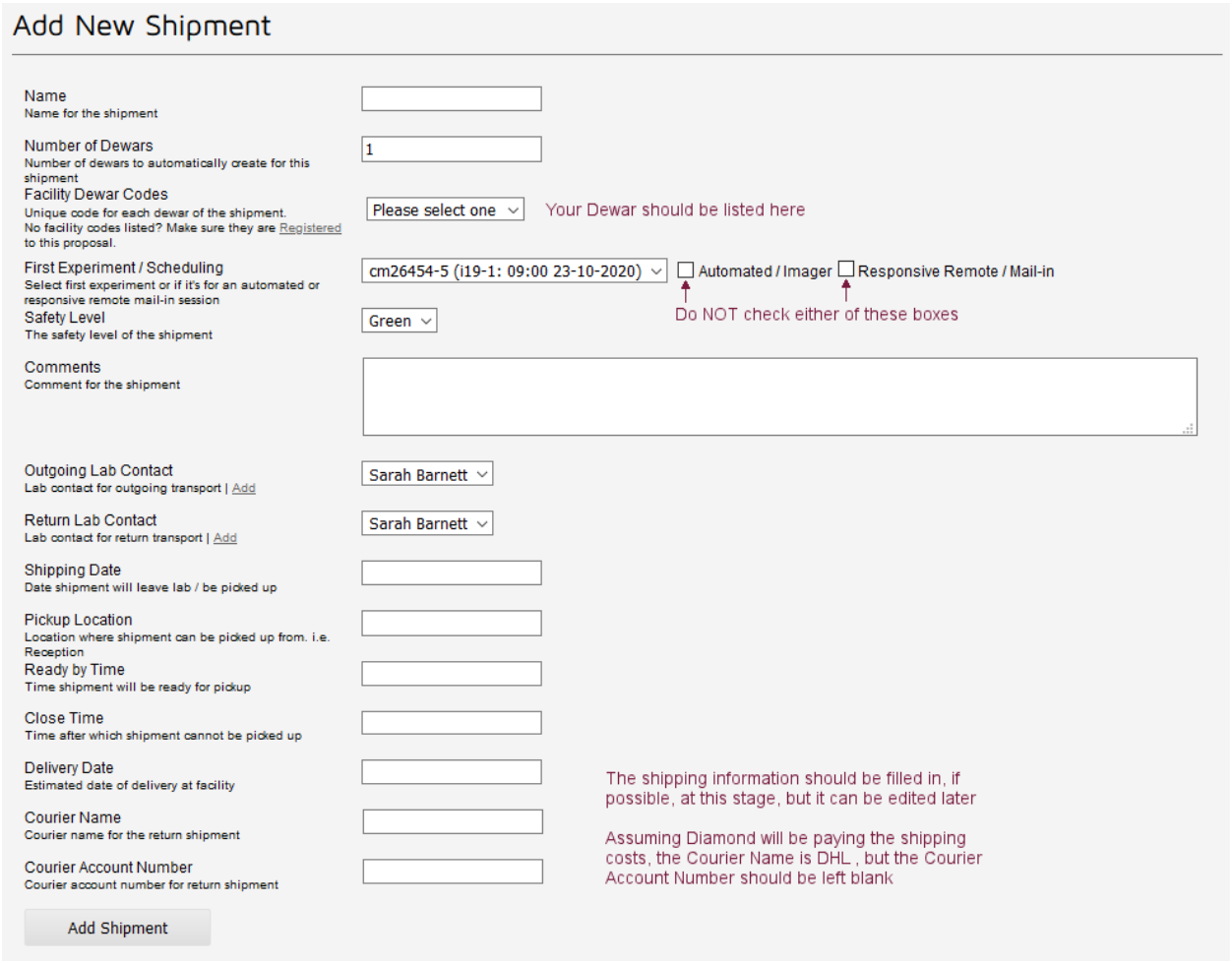
If you have any issues with trying to add, or use, a particular Dewar, please let I19 staff know.

Create Shipment

Create a new shipment by navigating to the shipments page from the visit menu. Here, you can see a list of previous shipments, shipments in progress and add a new shipment.



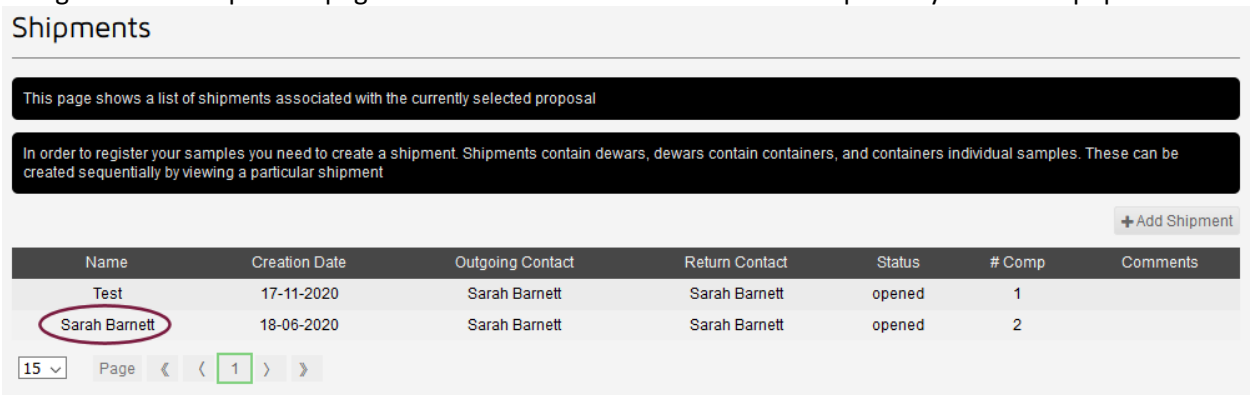
At the start of each visit a new shipment will need to be created so click on the "**+** Add Shipment" button and fill in the details on the form. Click on "Add Shipment" at the bottom, once the form is complete.



This new shipment will be added to the list of shipments for the proposal and is now ready to be edited and populated with samples.
Note – once a shipment has been created, it can not be deleted. (It is fine to create a test shipment, just don't actually ship it! – please do let your local contact know as soon as possible if any mistakes are made.)

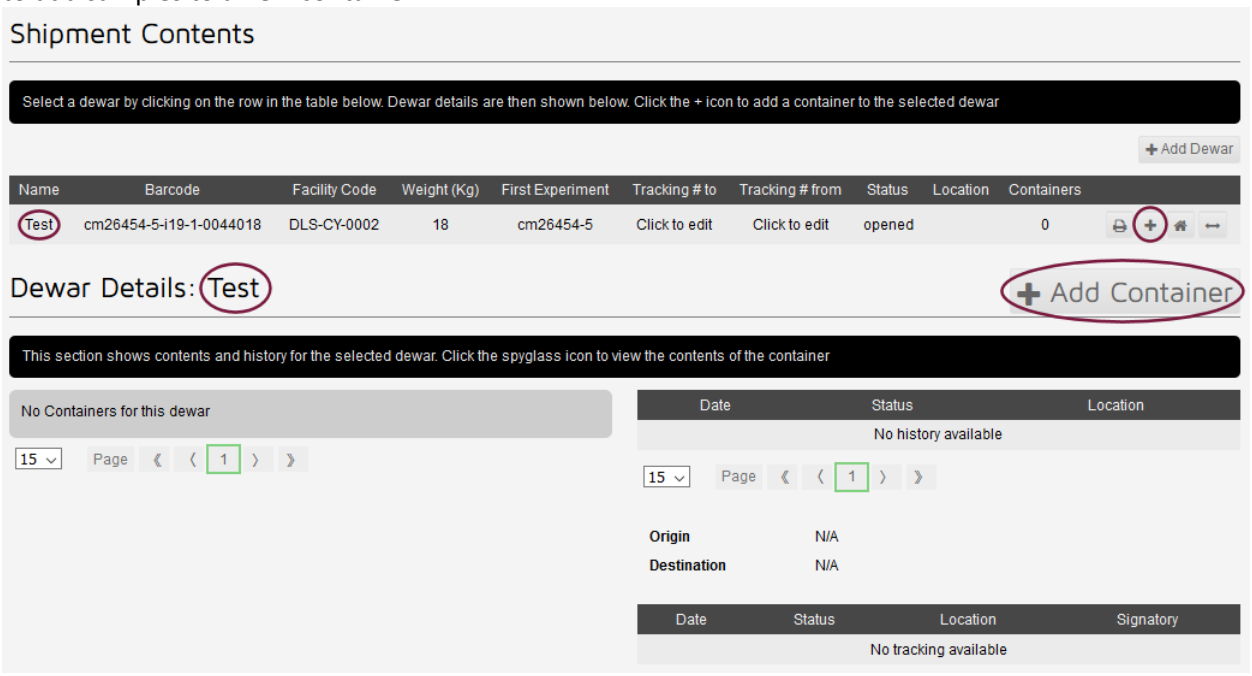
Add Samples to a Shipment

Navigate to the Shipments page from the Visit Menu and select the shipment you wish to populate.

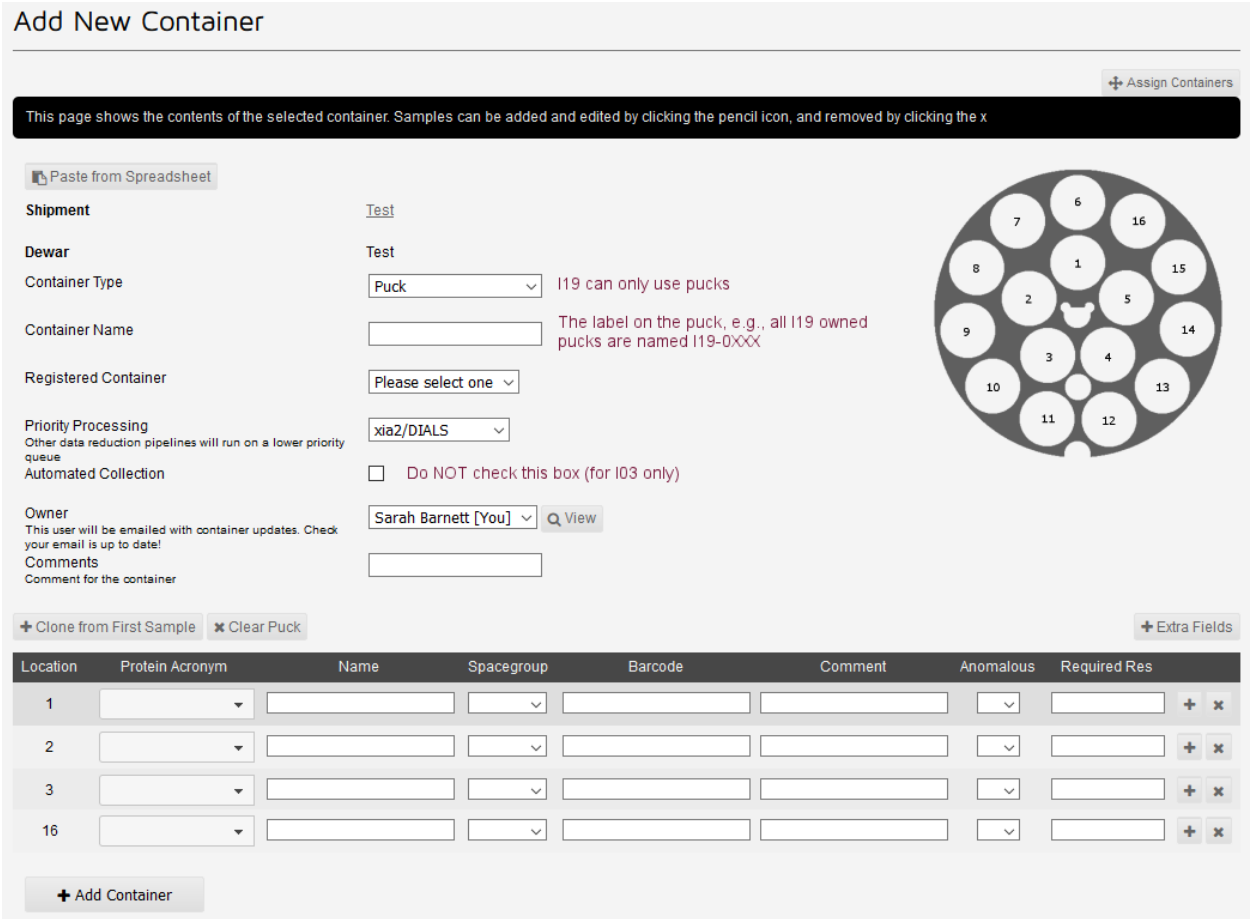


The top section shows the details given when the shipment creation form was completed. These can all be edited or updated here. The lower section lists the Dewars associated with this shipment. If you have more than one Dewar available, check you are adding samples to the correct Dewar; the name after Dewar details should match the name of the Dewar.

Click on either the "**+** Add Container" button or the "**+**" button on the right-hand side of the shipment to add samples to a new container.



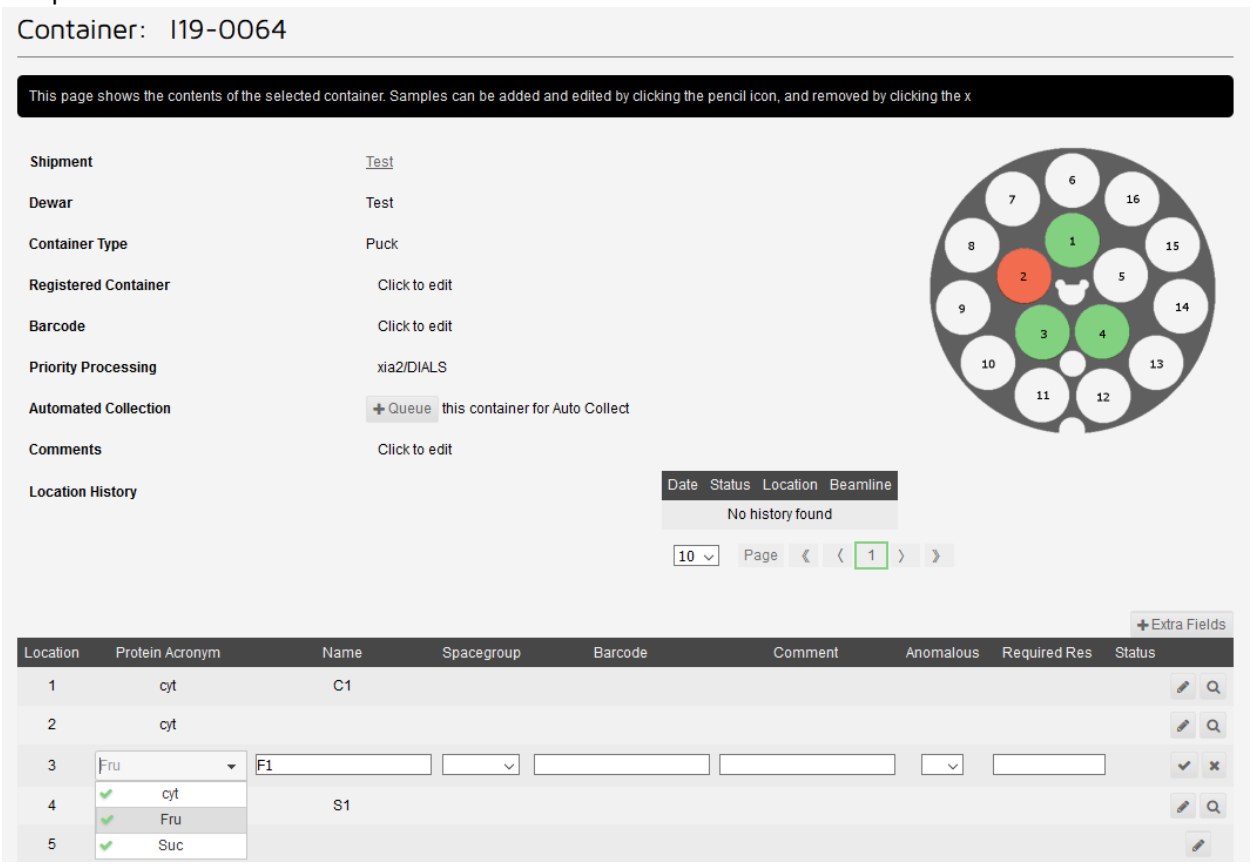
The I19 robot is only set up to take pucks so make sure this is selected from the dropdown. All pucks should have been labelled with a unique name at the time of purchase – use this label for the container name. Pucks which have barcodes are registered and should be selected from the list. However, for containers which are not registered, just make sure the hyphen is shown.



Please do NOT check the Automated Collection box – this is only available on MX and will cause much confusion to their system if it is checked.

Now click on the "**+** Add Container" button – this should create the container and give you the option to create the next container. Sometimes, this action will fail with the Registered Container section being highlighted in red and the instruction that "Container registry ID must be a number" - for unregistered pucks just select the hyphen from the dropdown and try adding the container again.

Once the container (puck) has been successfully added to the shipment, it can be populated with samples.



To add or edit a sample, click on the pen symbol on the right-hand side for the relevant pin position.

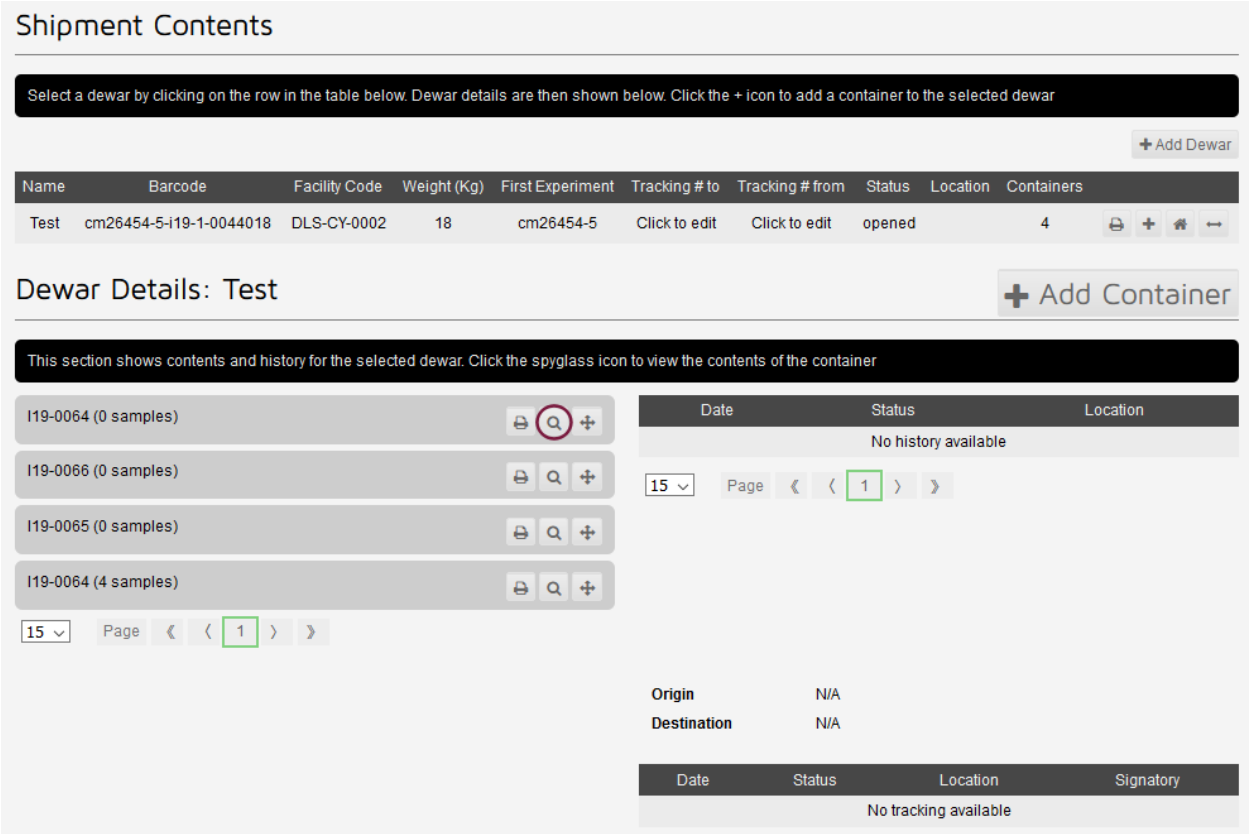
Samples MUST be identified by the Protein Acronym – samples can only be selected from the dropdown list. This box must be completed and is not editable. The sample name can be anything relevant to identify the sample and is also mandatory.

Other sections can be completed if desired and known - the space group and unit cell information (click on Extra Fields at the top right of the table), if provided, should be carried through to inform the data auto processing.

Click on the tick mark once finished to save all changes. Successful sample entries are shown in the puck diagram in green, whilst incomplete entries are red. Empty (or not yet completed positions) are white. (Whilst samples can be edited if you make a mistake, I am unable to delete samples if I made a location error in an incomplete puck as the acronym box seems to be impossible to clear – the sample name can be cleared by deleting the contents and then pressing the cross rather than the tick.)

It is possible to edit the samples and containers from the shipments pages, so mistakes can be fixed or more samples added to the pucks in ISPyB as samples are added to the real pucks.

Clicking on the spyglass for the relevant puck will open up the page to add samples



It is also possible to rename the puck, *e.g.*, if you realise you have mistakenly added two pucks with the same name, or assigned a set of samples to the wrong puck and it might be easier to swap the puck names than redo all the samples.

Simply click on the pen symbol and correct the puck name.

NOTE: Quite a lot of things are editable – just hover the mouse over items to see if the pen symbol appears.

Ship The Dewar To Diamond

Create Airway Bill

Once all samples have been added to the Dewar and ISPyB has been updated to reflect this, the Dewar can be shipped to Diamond.

Please Note: Samples should (can?) not be added to shipments in ISPyB after the Dewar has been shipped!

Click on the “Create Airway Bill” button.

Make sure all fields are completed correctly – all are editable if any errors are found. Click on “Create Airway Bill” at the bottom of the form once finished.

Shipment: Test

This page shows details and contents of the selected shipment. Most parameters can be edited by simply clicking on them.

Shipments need to have an outgoing and return home lab contact before shipment labels can be printed

You can now book your shipment with DHL using "Create Airway Bill" below

Mark as Sent | Create Airway Bill | Print Shipment Labels | Print Contents

Created	17-11-2020
Status	opened
Outgoing Lab Contact	Sarah Barnett
Return Lab Contact	Sarah Barnett
Safety Level	Green

Create Airway Bill: To Facility

Shipment Details

Shipment	Test
Dewars	☐ DLS-CY-0002 Check this is the correct Dewar and then check the box
Weight	0 Kg
DHL Account Number	Click to edit Use Facility Account
Declared Value	100 GBP
Package Description	Dry shipper - not restricted as per IATA special provision A152

Click on this button to use the Diamond courier account
Check and accept the terms and conditions

Contact Details

Contact	Sarah Barnett
Contact Phone Number	01235778923
Contact Email	sarah.barnett@diamond.ac.uk

Laboratory Details

Laboratory Name	Diamond Light Source
Laboratory Address (excluding post code)	Harwell Science and Innovation Campus
Laboratory City	Didcot
Laboratory Postcode	OX11 0DE
Laboratory Country	United Kingdom [Free For: Austria, Belgium, Bulgaria, Croatia, Cyprus, Czech Republic, The, Denmark, Estonia, Finland, France, Germany, Greece, Hungary, Iceland, Ireland, Republic Of, Italy, Latvia, Liechtenstein, Lithuania, Luxembourg, Malta, Netherlands, The, Norway, Poland, Portugal, Romania, Slovakia, Slovenia, Spain, Sweden, United Kingdom]

Pickup Details

Package Location **Location where shipment can be picked up from**	Click to edit
Shipping Date	00-00-0000
Ready By **Time shipment will be ready for pickup**	Click to edit
Close Time **Time after which shipment cannot be picked up**	Click to edit

Make sure all of this section is filled in as this information is passed onto the shipping company

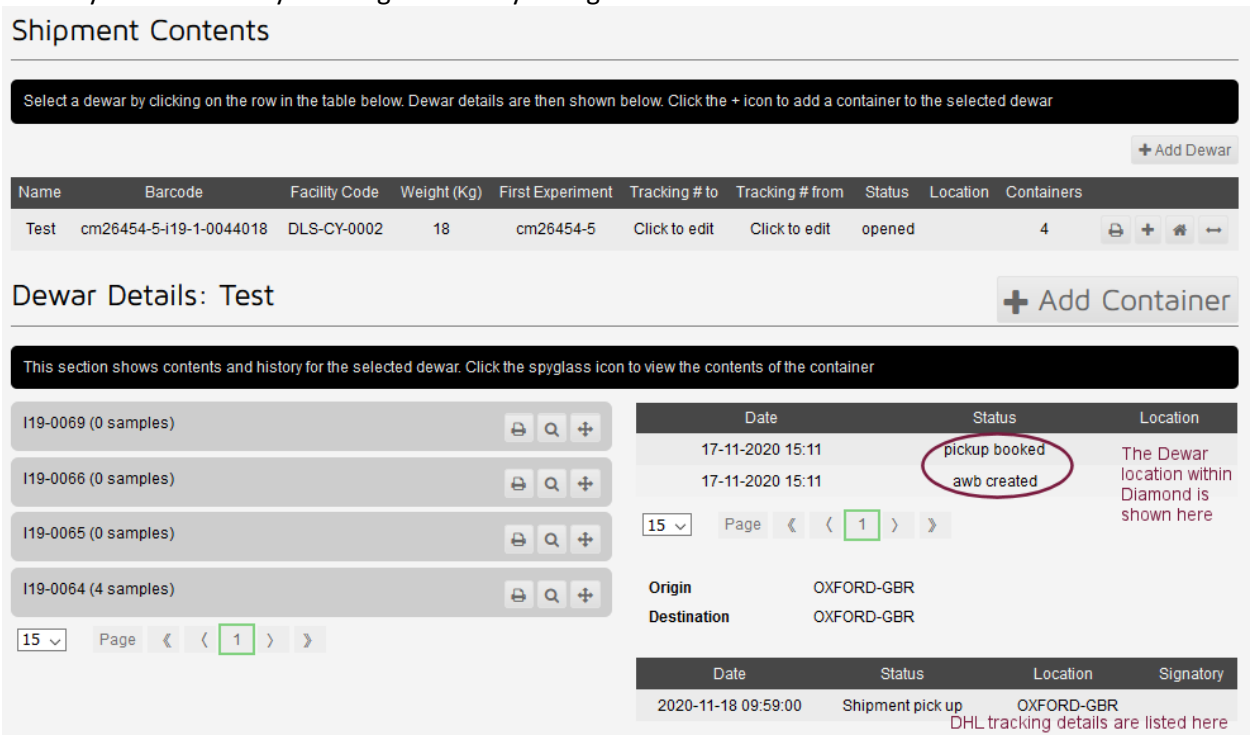
Terms & Conditions

I understand that use of DHL's services is entirely at my own risk and that Diamond makes no representations or warranties of any kind (express or implied)about the reliability or availability of the DHL service. Any reliance that I place on the DHL service is strictly at my own risk. It is my responsibility to ensure that I am authorised to use the DHL account that I provide to Diamond and to ensure that the samples arrive at Diamond in advance of any beamtime that Diamond may have awarded me. I hereby indemnify and hold Diamond harmless for any loss or damage arising out of my use of DHL's services.

Get Quote

This will update to Create Airway Bill if "Use Facility Account" is selected

Check at the bottom of the shipments page, that both “awb created” and “pickup booked” appear. If the pickup has not been booked, then the shipping request has not gone through properly and DHL will not collect your Dewar – try creating the airway bill again.



Print Shipment Labels

Now print the shipping labels, by clicking on the button "Print Shipment Labels".
Please make sure you print the labels on separate sheets!

Label 1 should be attached to the actual Dewar – **make sure any old labels are removed first.** The barcode generated is unique to each particular shipment - old labels will confuse the system and require manual intervention as the Dewar will be associated with a different visit and shipment to the case. (The Dewar is not necessarily stored in the case once it arrives at Diamond!)

1. Dewar Tracking Label

Label 2 (Outgoing Address Label) should be stuck on the Dewar case.
Label 3 (Return Address Label) should be placed in the case.

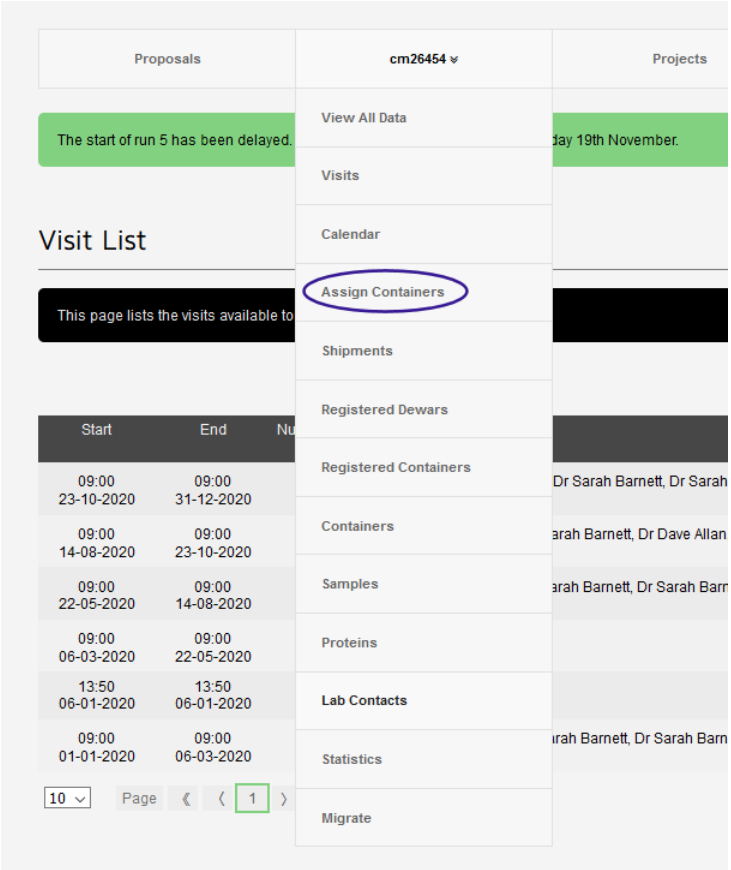
The Dewar is now ready to be collected.

Assign Pucks

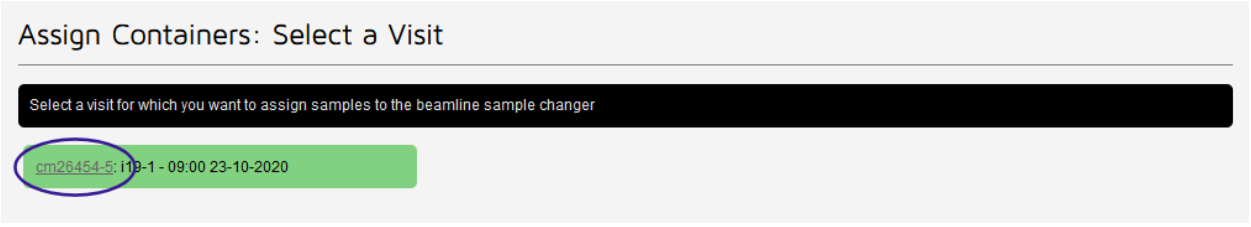
ISPyB

If not assigned by beamline staff, check the white board at the back of the hutch (webcam-11) to see where the pucks have been placed in the Dewars. Virtual pucks can be assigned to any unoccupied position as directed by the local contact.

In ISPyB, select Assign Containers, from the visit menu



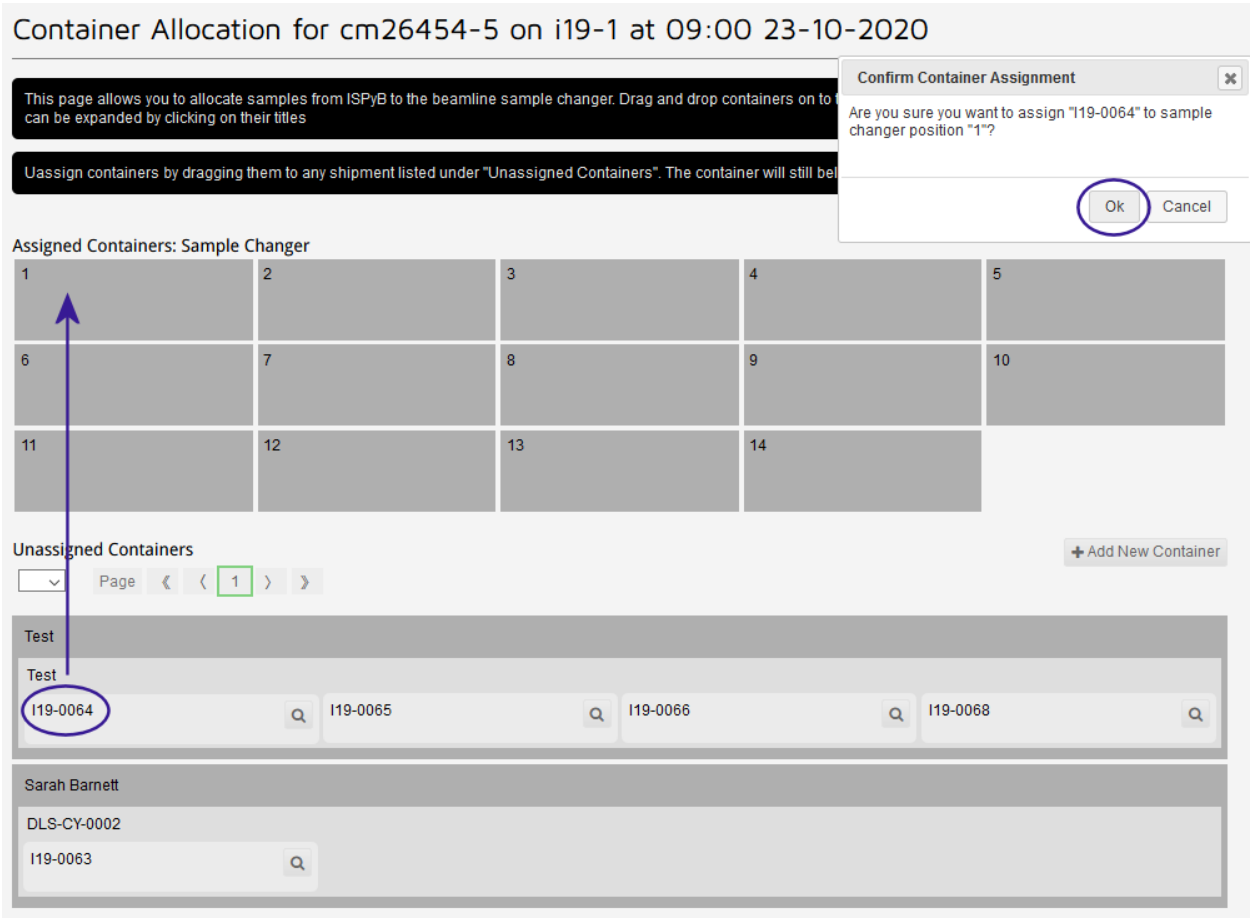
Click on the current visit from the potential list



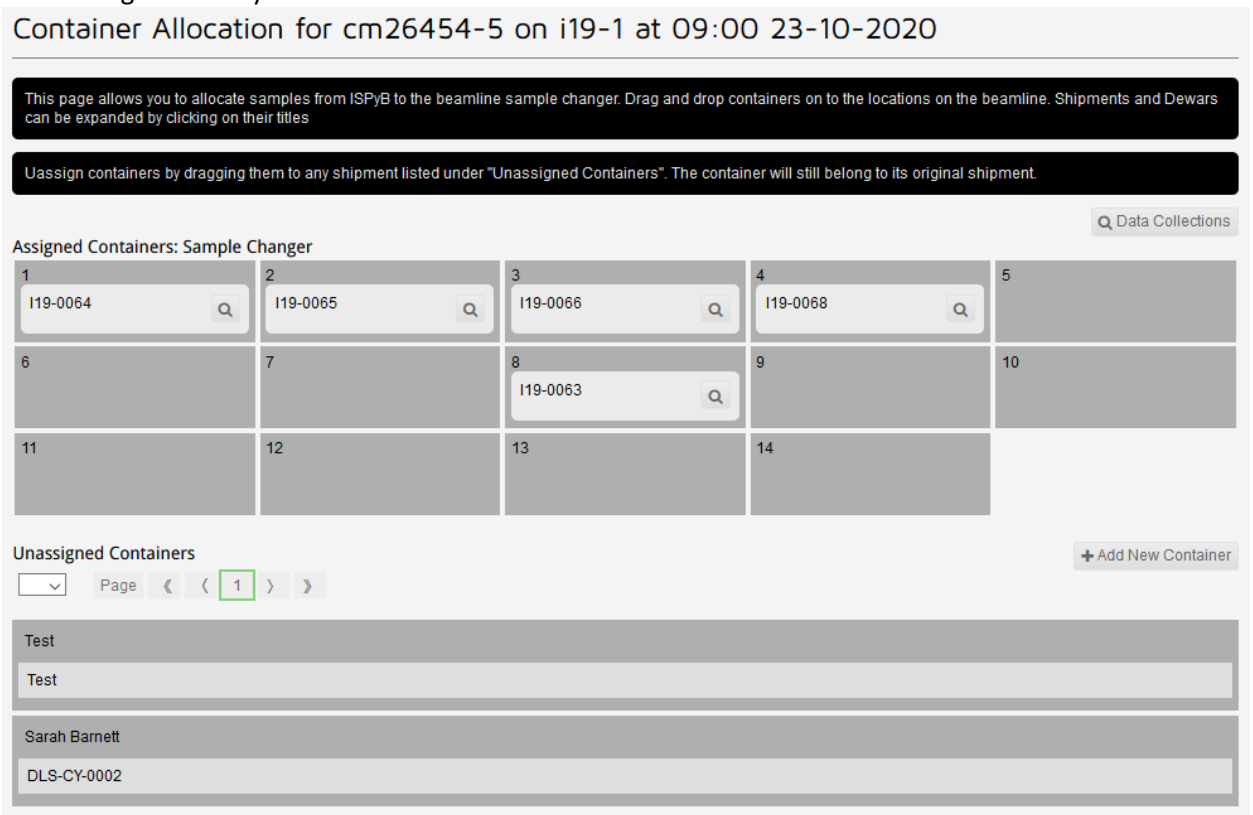
This will take you to the page where all available puck positions are shown.
Note positions 1-7 are in Dewar 1 and 8-14 are in Dewar 2.

The pucks are listed in the appropriate shipment and all shipments associated with the visit should be shown.

Click on the puck and drag it to the correct position in the Dewars. Click “Ok” to confirm the container assignment. If you mis-place a puck, just drag the puck to the correct place and click “Ok” to confirm its new position.

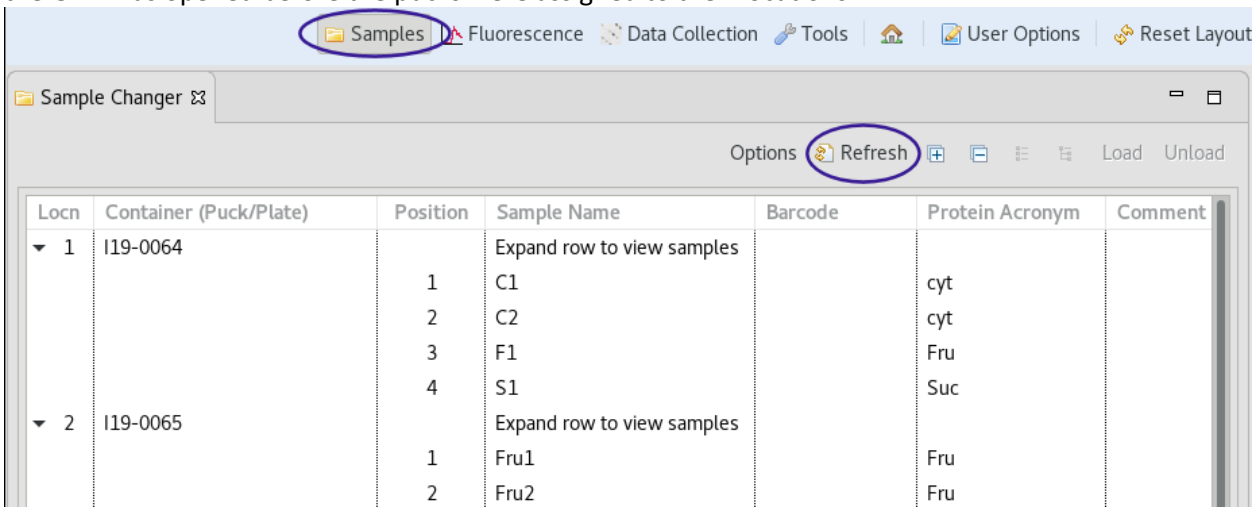


Pucks assigned in ISPyB:



GDA

In the GDA – click on the Samples tab. You may need to click on the "Refresh" button to update the list if the GDA was opened before the pucks were assigned to their locations.

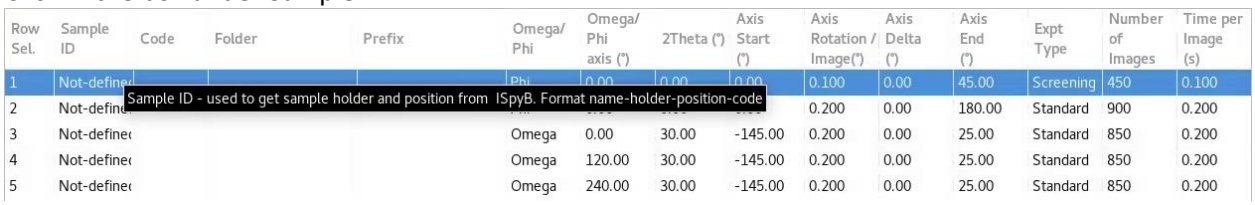


Please Note: Whilst staff will try to place all pucks for any given visit in one Dewar, they may sometimes need to be split between the 2 Dewars. It is recommended to work through the pucks in one Dewar, unload the last sample (to force a gripper dry) and then work through the pucks in the other Dewar. Measures in place to ensure the robot doesn't drive through the side of the Dewar when moving from one Dewar to the other, mean the robot briefly sits at the wait position and then re-soaks in the new Dewar if you go directly from one to the other – there is a higher risk of icing doing it this way.

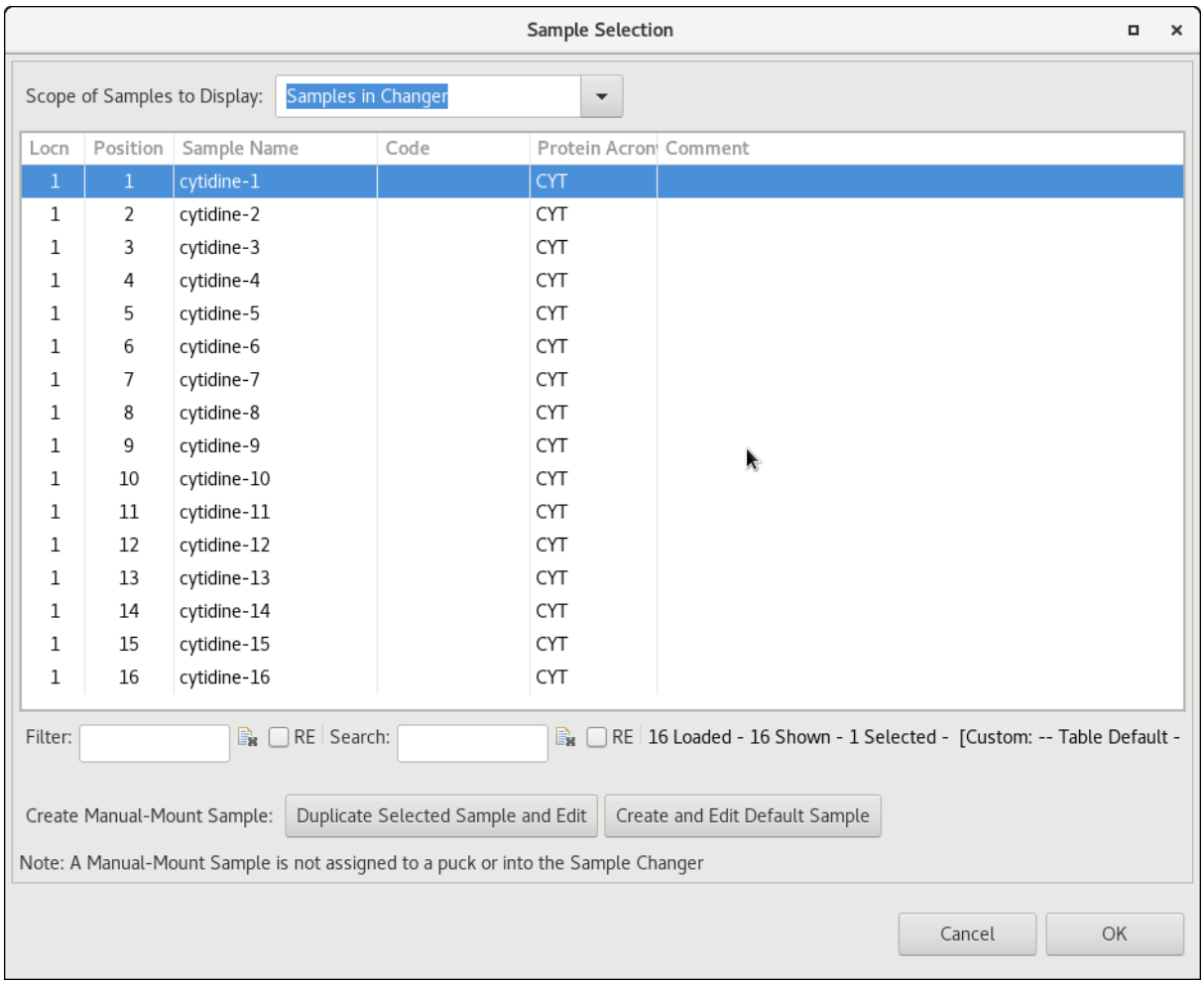
Selecting a sample in GDA, when NOT using the robot

If not using pucks/robot and just need the sample information, to be used for auto processing, then the appropriate sample can be selected from the list in the data collection table.

Click in the box under Sample ID



This will open a list of samples, as assigned in ISPyB – select the appropriate sample from the list.



You will need to do this manually, for all rows in the data collection table.

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)	Transmis (%)
1	cytidine-1				Phi	0.00	0.00	0.00	0.100	0.00	45.00	Screening	450	0.100	2.3793	160.0	1.000000
2	cytidine-1				Phi	0.00	0.00	0.00	0.200	0.00	180.00	Standard	900	0.200	2.3793	160.0	1.000000
3	cytidine-1				Omega	0.00	30.00	-145.00	0.200	0.00	25.00	Standard	850	0.200	2.3793	160.0	1.000000
4	cytidine-1				Omega	120.00	30.00	-145.00	0.200	0.00	25.00	Standard	850	0.200	2.3793	160.0	1.000000
5	cytidine-1				Omega	240.00	30.00	-145.00	0.200	0.00	25.00	Standard	850	0.200	2.3793	160.0	1.000000