

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.

Data Collections for cm28127-4 on i19-1

Assign Containers Summary Auto Processing Visit Stats Users Dewars Sample Changer Reprocessing Beamline Status

i19-1 Webcams & Beamline Status

Ring Current 298.592	Refill 0	Hutch Locked	Port Shutter Open	Fast Shutter Closed	Energy 17.9937	Current Puck 4	Current Pin 3
ID Gap 5.1951							

2021-10-04 11:20:11

2021-10-04 11:20:11

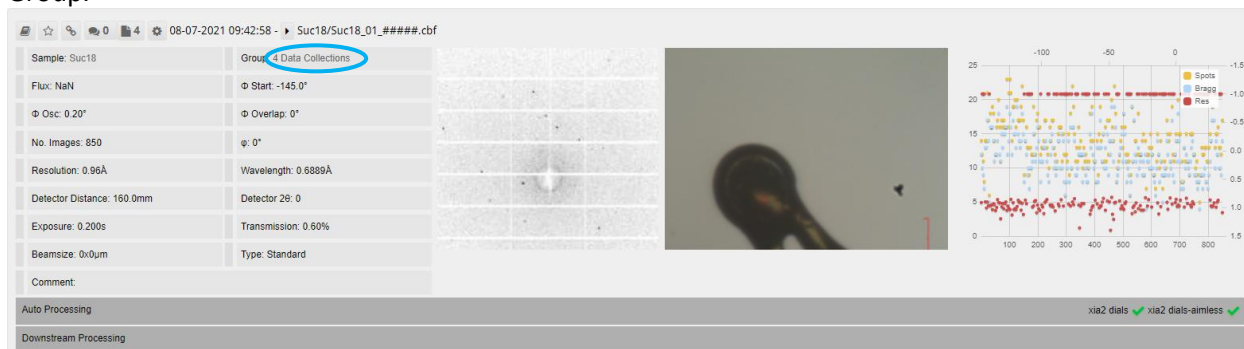
The status box displays include which sample is actually mounted and show when various shutters are open/closed - they are green when in a ready state and red when not.

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 μ m 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

Diffraction Image Viewer

Exposure: 0.200s Transmission: 0.20% Resolution: 0.96Å Wavelength: 0.6889Å Oscillation: 0.20°

View Full Screen

< 1 / 850 > Resolution Rings: Zoom: 167% Contrast: 0 Brightness: 0
Ice Rings: Invert: Threshold: Reset

Resolution: 1.16Å

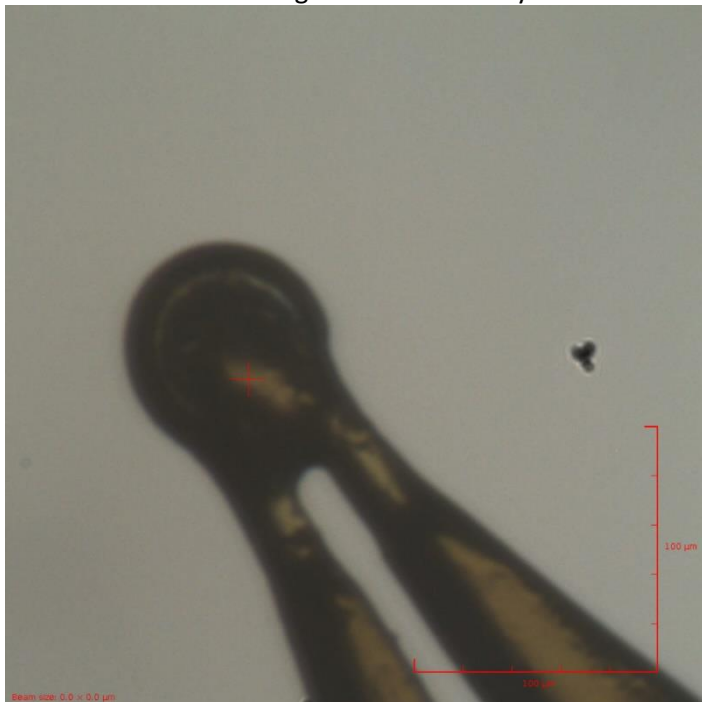
1.14Å
1.43Å
2.04Å
3.95Å

Close

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.



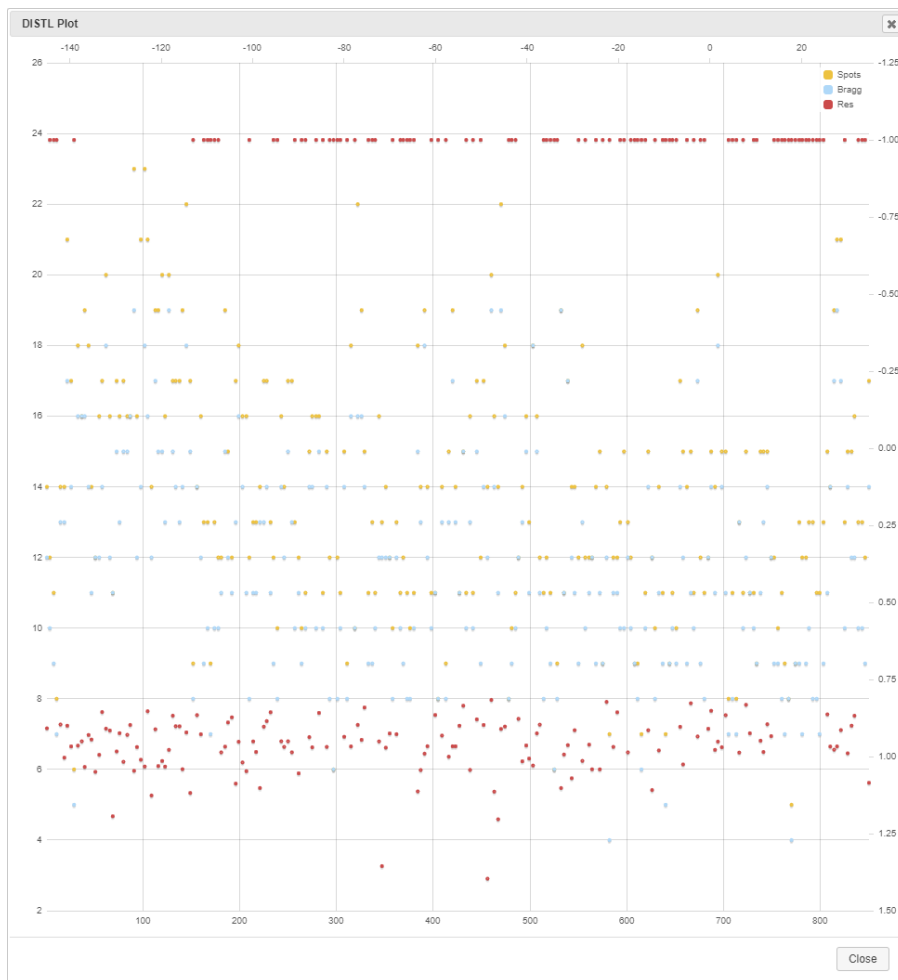
Remember, you can persuade the system to take more snapshots by clicking the “Make hutch safe” or “Prepare Sample Mount” buttons in the GDA and then starting the next data collection. As the backlight is put back in position, the GDA expects that the sample has been changed and will take another set 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).



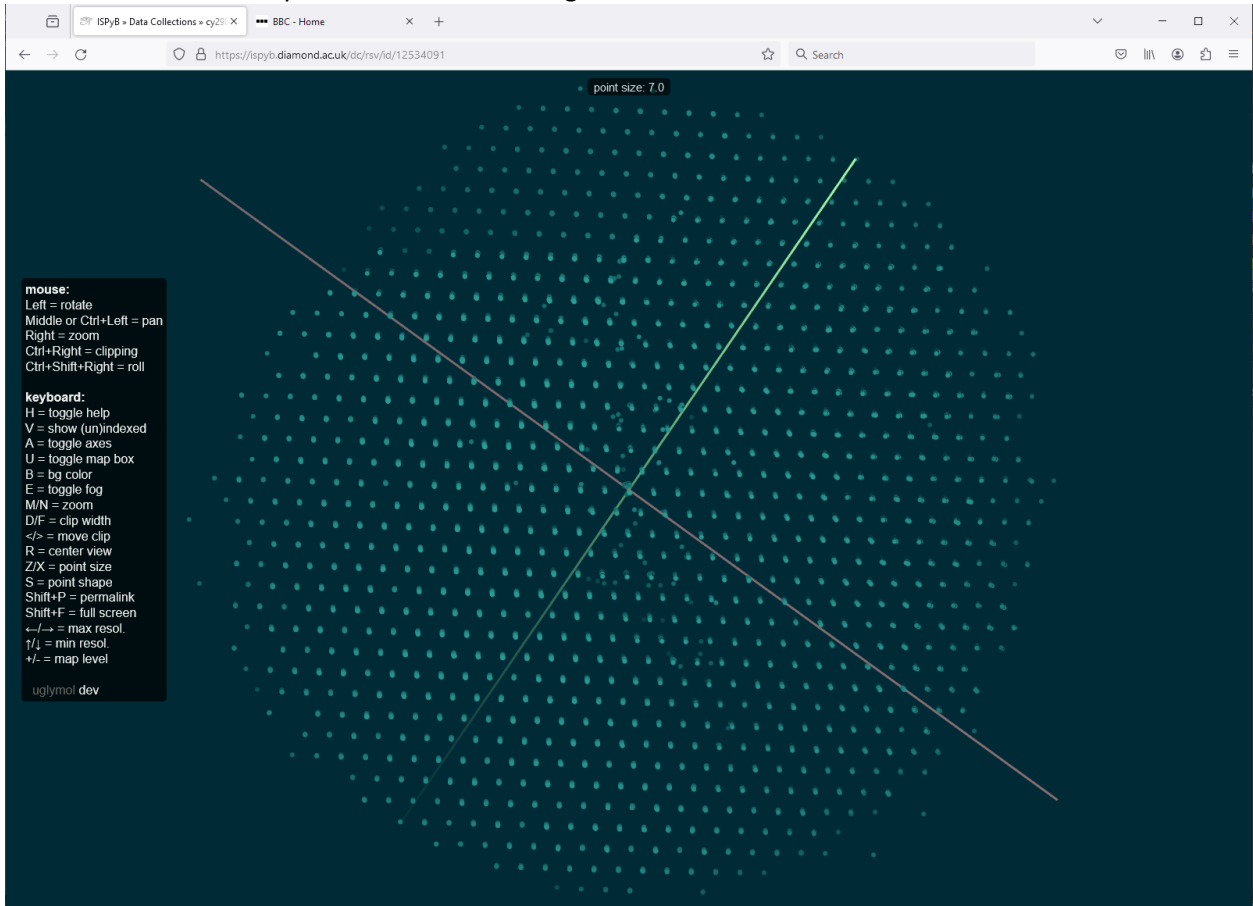
Reciprocal Lattice Viewer

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.

The screenshot shows a software interface. At the top, there is a toolbar with several icons: a document icon (circled in red), a star, a link, a speech bubble with '0', a gear, and a file name '08-07-2021 09:42:58 - Suc18/Suc18_01_#####.cbf'. Below the toolbar is a metadata panel with the following information:

Sample: Suc18	Group: 4 Data Collections
Flux: NaN	Φ Start: -145.0°
Φ Osc: 0.20°	Φ Overlap: 0°

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.

Sample:	Suc18	Group:	4 Data Collections
Flux:	NaN	Φ Start:	-145.0°
Φ Osc:	0.20°	Φ Overlap:	0°
No. Images:	850	ψ :	0°
Resolution:	0.96Å	Wavelength:	0.6889Å
Detector Distance:	160.0mm	Detector 2 θ :	0
Exposure:	0.200s	Transmission:	0.60%
Beamsize:	0x0µm	Type:	Standard

data	Resolution	Spacegroup	Mn(I)sg(I)P	Rmeas Inner	Rmeas Outer	Completeness	Cell	Status
xia2 diats-aimless	8.71 - 0.81	P 1 2 1 1	24.2	0.077	0.000	76.3	7.76 8.71 10.87 90.00 102.96 90.00	processing successful
xia2 diats	10.50 - 0.81	P 1 2 1 m 1	34.2	0.076	0.000	76.7	7.76 8.71 10.87 90.00 102.96 90.00	processing successful

Space Group	A	B	C	α	β	γ
P 1 2 1 1	7.76	8.71	10.87	90.00	102.96	90.00

Shell	Observations	Unique	Resolution	Rmeas	I/sig(I)	CC Half	Completeness	Multiplicity	Anom Completeness	Anom Multiplicity	CC Anom
outer:Shell	5	5	0.81 - 0.82	0.000	11.2	0.0	6.6	1.0	0.0	1.0	0.0
inner:Shell	232	86	2.10 - 0.71	0.077	28.8	1.0	100.0	2.7	04.9	1.6	0.1
overall	3129	1151	0.81 - 0.71	0.053	24.2	1.0	76.3	2.7	56.1	1.6	-0.1

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.

Auto Processing											xia2 dials-aimless ✓	xia2 dials undefined	
data	Resolution	Spacegroup	MvI/sigma$$	Rmeas Inner	Rmeas Outer	Completeness	Cell				Status		
4x multi-xia2 dials-aimless	10.80 - 0.58	P 1 21m 1	30.3	0.032	0.082	93.1	7.77	8.71	10.87	90.00	102.64	90.00	processing successful
4x multi-xia2 dials	10.80 - 0.59	P 1 21m 1	32.4	0.032	0.085	95.9	7.77	8.71	10.87	90.00	102.64	90.00	processing successful

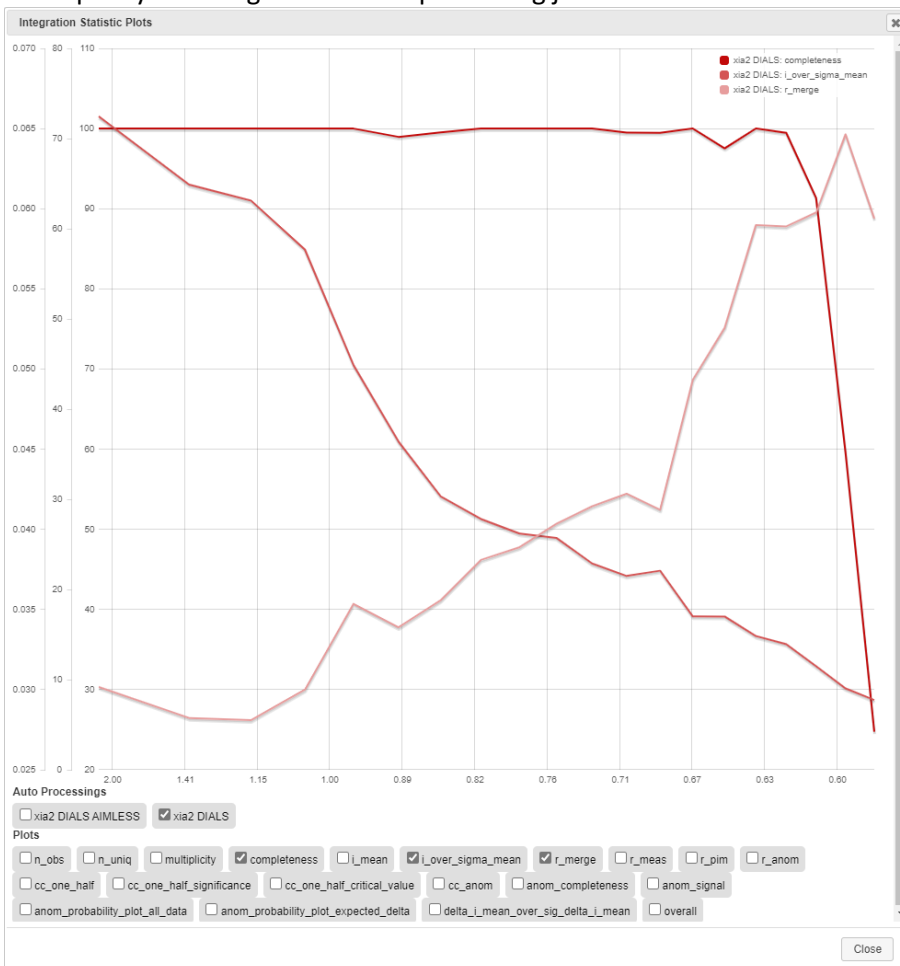
Space Group	A	B	C	α	β	γ
P 1 21m 1	7.77	8.71	10.87	90.00	102.64	90.00

Shell	Observations	Unique	Resolution	Rmeas	I/sig(I)	CC Half	Completeness	Multiplicity	Anom Completeness	Anom Multiplicity	CC Anom
outerShell	43	39	0.58 - 0.59	0.082	8.8	1.0	20.0	1.1	0.0	0.0	0.0
innerShell	1873	218	1.59 - 10.80	0.032	62.2	1.0	100.0	7.7	0.0	0.0	0.0
overall	1551	387	0.58 - 10.80	0.033	30.3	1.0	93.1	4.3	0.0	0.0	0.0

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, $I/\sigma(I)$ and multiplicity (these can also be found in Plots)
- Analysis by batch: summary of mean $I/\sigma(I)$ 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

Data Collections for cm28127-3 on i19-1

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i19-1 Webcams & Beamline Status

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.

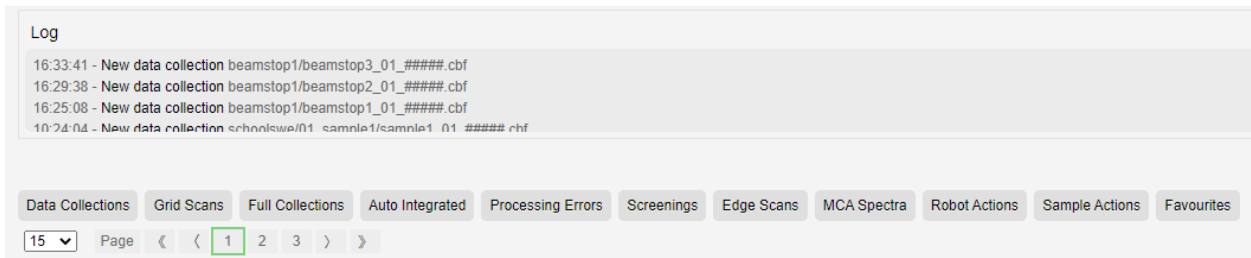
Reprocessing

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.

The image shows a screenshot of a web form. The top field is labeled "Sample Material or Protein" and contains the text "cytidine". Below it is a field labeled "Acronym" which contains the text "cyt". The "Acronym" label and its input field are circled in red. There is a small blue circular icon with a plus sign to the right of the "Acronym" input field.

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:

The screenshot shows the ISPyB interface. On the left, a sidebar menu contains various options: View All Data, Visits, Calendar, Assign Containers, Shipments, Registered Dewars, Registered Containers, Containers, Samples, Proteins (circled in red), Lab Contacts, Statistics, and Migrate. The main content area is titled 'Visit List' and includes a notification: 'The start of run 5 has been delayed.' Below this is a table with columns 'Start', 'End', and 'Number of Visits'. The table lists several visits with their respective dates and times. At the bottom, there is a pagination control showing 'Page 1'.

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.

Components

The screenshot shows the 'Components' page in ISPyB. A notification at the top states: 'This page lists all components associated with the currently selected proposal. Approved samples are highlighted in colour.' Below the notification are filter buttons for 'Protein', 'DNA', 'Small Molecule', and 'RNA', along with a '+ Add Component' button and a search box. The main content is a table with the following data:

Name	Acronym	Mass	Type	Samples	Data Collections	Risk Rating
cyt	cyt			3	0	GREEN
Fru	Fru			3	0	GREEN
Suc	Suc			10	0	GREEN

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.

The screenshot shows a web interface with a sidebar menu on the right. The menu items are: View All Data, Visits, Calendar, Assign Containers, Shipments, Registered Dewars, Registered Containers, Containers, Samples, Proteins, Lab Contacts (circled in red), Statistics, and Migrate. The main content area is titled 'Visit List' and contains a table with the following data:

Start	End	Number
09:00 23-10-2020	09:00 31-12-2020	
09:00 14-08-2020	09:00 23-10-2020	
09:00 22-05-2020	09:00 14-08-2020	
09:00 06-03-2020	09:00 22-05-2020	
13:50 06-01-2020	13:50 06-01-2020	
09:00 01-01-2020	09:00 06-03-2020	

At the bottom of the table, there is a pagination control showing '10' items per page and 'Page 1'.

The screenshot shows the 'Home Lab Contacts' page. At the top, there is a message: 'This page shows registered home laboratory contacts. This information is generally used to return shipments back after an experiment'. Below this is a search bar and a button '+ Add Home Lab Contact' (circled in red). The main content is a table with the following data:

Card Name	First Name	Surname	Address	City	Postcode	Country	Phone No.	Laboratory
Sarah Barnett	Sarah	Barnett	Harwell Science and Innovation Campus	Didcot	OX11 0DE	United Kingdom	01235778923	Diamond Light Source

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.

Add New Home Lab Contact

Card Name Name for the Contact Card	<input type="text"/>	Choose something that will be easily recognisable, e.g., your name, in the list of contacts
Contact Details		
Contact Family Name The person's family name	<input type="text"/>	
Contact First Name The person's first name	<input type="text"/>	
Contact Phone Number The person's phone number	<input type="text"/>	
Contact Email The person's email address	<input type="text"/>	
Contact Laboratory Details		
Laboratory Name The contact's laboratory name	<input type="text"/>	
Laboratory Street Address Street Address (excluding post code, city)	There is a line limit of 35 characters so add over multiple lines where necessary Only include address lines which are not required specifically elsewhere	
Laboratory City The contact's laboratory city	<input type="text"/>	
Laboratory Postcode The contact's laboratory postcode	<input type="text"/>	
Laboratory Country The contact's laboratory country	<input type="text" value="United Kingdom"/>	
Dewar Return Details The following information is used for each shipment associated with this contact		
Courier Company Courier company to use to return dewars to home lab	<input type="text"/>	This section should be left blank if using the Diamond Courier (only available for UK addresses)
Courier Account No. Courier account number for returning dewars to home lab	<input type="text"/>	
Billing Reference Billing reference to use when returning dewars to home lab	<input type="text"/>	
Average customs value of dewar The average customs value of a dewar	<input type="text"/>	
Average transport value of dewar The average transport value of a dewar	<input type="text"/>	
<input type="button" value="Add Home Lab Contact"/>	Click here to add the contact, or save changes, once done	

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.

Add New Dewar	
Facility Code	<input type="text"/>
Purchase Date When the dewar was purchased	<input type="text"/>
<input type="button" value="+ Add Dewar"/>	

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).

Registered Dewars

Registered Dewar not listed here? Ask your local contact to associate it with this proposal.

Orphaned

DLS-CY

<input type="checkbox"/>	Facility Code	Proposals	Created	# Uses	Last Use	Reports
<input type="checkbox"/>	DLS-CY-0001	cy22240	2019-10-15 21:32:59	3	09-03-2020	0
<input type="checkbox"/>	DLS-CY-0002	cm26454	2019-09-24 10:15:47	5	09-07-2020	0
<input type="checkbox"/>	DLS-CY-0006	cy21726	2019-04-29 09:46:48	7	24-09-2020	0
<input type="checkbox"/>	DLS-CY-0007	cy25064	2019-04-24 16:00:18	10	15-07-2020	0
<input type="checkbox"/>	DLS-CY-0008	mt20570	2020-11-17 09:48:24	0		0
<input checked="" type="checkbox"/>	DLS-CY-0009		2020-11-17 09:48:49	0		0
<input type="checkbox"/>	DLS-CY-0011	cy22240	2019-05-24 12:56:42	16	05-10-2020	0
<input type="checkbox"/>	DLS-CY-0013	cy21726	2019-05-21 16:34:17	9	16-10-2020	0
<input type="checkbox"/>	DLS-CY-0014	cy22240	2020-01-28 15:09:18	3	08-10-2020	0

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.

Add Proposal

26454

<input type="checkbox"/>	Code	Number	Visits	Title
<input type="checkbox"/>	cm	26454	6	I19-1 Commissioning Directory 2020

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+ Add to Proposal(s)

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.

Shipments

This page shows a list of shipments associated with the currently selected proposal

In order to register your samples you need to create a shipment. Shipments contain dewars, dewars contain containers, and containers individual samples. These can be created sequentially by viewing a particular shipment

+ Add Shipment

Name	Creation Date	Outgoing Contact	Return Contact	Status	# Comp	Comments
Sarah Barnett	18-06-2020	Sarah Barnett	Sarah Barnett	opened	2	

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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.

Add New Shipment

Name
Name for the shipment

Number of Dewars
Number of dewars to automatically create for this shipment

Facility Dewar Codes
Unique code for each dewar of the shipment. No facility codes listed? Make sure they are [Registered](#) to this proposal.

First Experiment / Scheduling
Select first experiment or if it's for an automated or responsive remote mail-in session

Safety Level
The safety level of the shipment

Comments
Comment for the shipment

Outgoing Lab Contact
Lab contact for outgoing transport | [Add](#)

Return Lab Contact
Lab contact for return transport | [Add](#)

Shipping Date
Date shipment will leave lab / be picked up

Pickup Location
Location where shipment can be picked up from. i.e. Reception

Ready by Time
Time shipment will be ready for pickup

Close Time
Time after which shipment cannot be picked up

Delivery Date
Estimated date of delivery at facility

Courier Name
Courier name for the return shipment

Courier Account Number
Courier account number for return shipment

Buttons: Add Shipment

Annotations:
 - "Please select one" dropdown for Facility Dewar Codes.
 - "Your Dewar should be listed here" text.
 - "Do NOT check either of these boxes" text with arrows pointing to "Automated / Imager" and "Responsive Remote / Mail-in" checkboxes.
 - "The shipping information should be filled in, if possible, at this stage, but it can be edited later" text.
 - "Assuming Diamond will be paying the shipping costs, the Courier Name is DHL, but the Courier Account Number should be left blank" text.

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.

Shipments

This page shows a list of shipments associated with the currently selected proposal

In order to register your samples you need to create a shipment. Shipments contain dewars, dewars contain containers, and containers individual samples. These can be created sequentially by viewing a particular shipment

[+ Add Shipment](#)

Name	Creation Date	Outgoing Contact	Return Contact	Status	# Comp	Comments
Test	17-11-2020	Sarah Barnett	Sarah Barnett	opened	1	
Sarah Barnett	18-06-2020	Sarah Barnett	Sarah Barnett	opened	2	

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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.

Shipment Contents

Select a dewar by clicking on the row in the table below. Dewar details are then shown below. Click the + icon to add a container to the selected dewar

+ Add Dewar

Name	Barcode	Facility Code	Weight (Kg)	First Experiment	Tracking # to	Tracking # from	Status	Location	Containers
Test	cm26454-5-i19-1-0044018	DLS-CY-0002	18	cm26454-5	Click to edit	Click to edit	opened		0

Dewar Details: **Test** + Add Container

This section shows contents and history for the selected dewar. Click the spyglass icon to view the contents of the container

No Containers for this dewar

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Date	Status	Location
No history available		
Origin	N/A	
Destination	N/A	

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Date	Status	Location	Signatory
No tracking available			

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.

Add New Container

+ Assign Containers

This page shows the contents of the selected container. Samples can be added and edited by clicking the pencil icon, and removed by clicking the x

Paste from Spreadsheet

Shipment: Test

Dewar: Test

Container Type: Puck I19 can only use pucks

Container Name: The label on the puck, e.g., all I19 owned pucks are named I19-0XXX

Registered Container: Please select one

Priority Processing: xia2/DIALS Other data reduction pipelines will run on a lower priority queue

Automated Collection: Do NOT check this box (for I03 only)

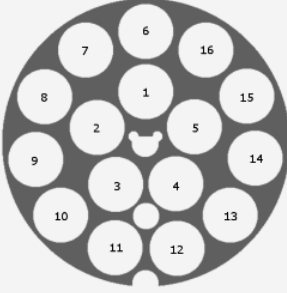
Owner: Sarah Barnett [You]

Comments:

+ Clone from First Sample + Extra Fields

Location	Protein Acronym	Name	Spacegroup	Barcode	Comment	Anomalous	Required Res
1							
2							
3							
16							

+ Add Container



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.

Container: I19-0064

This page shows the contents of the selected container. Samples can be added and edited by clicking the pencil icon, and removed by clicking the x

Shipment: [Test](#)

Dewar: Test

Container Type: Puck

Registered Container: [Click to edit](#)

Barcode: [Click to edit](#)

Priority Processing: xia2/DIALS

Automated Collection: Queue this container for Auto Collect

Comments: [Click to edit](#)

Location History

Date	Status	Location	Beamline
No history found			

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+ Extra Fields

Location	Protein Acronym	Name	Spacegroup	Barcode	Comment	Anomalous	Required Res	Status
1	cyt	C1						
2	cyt							
3	Fru	F1						
4	cyt	S1						
5	Suc							

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

Shipment Contents

Select a dewar by clicking on the row in the table below. Dewar details are then shown below. Click the + icon to add a container to the selected dewar

[+ Add Dewar](#)

Name	Barcode	Facility Code	Weight (Kg)	First Experiment	Tracking # to	Tracking # from	Status	Location	Containers
Test	cm26454-5-i19-1-0044018	DLS-CY-0002	18	cm26454-5	Click to edit	Click to edit	opened		4

Dewar Details: Test

[+ Add Container](#)

This section shows contents and history for the selected dewar. Click the spyglass icon to view the contents of the container

Date	Status	Location
No history available		

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I19-0064 (0 samples)	
I19-0066 (0 samples)	
I19-0065 (0 samples)	
I19-0064 (4 samples)	

15 ▾ Page < < 1 > >

Origin	N/A
Destination	N/A

Date	Status	Location	Signatory
No tracking available			

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.

Container: I19-0064

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	<input type="checkbox"/> 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	Click on this button to use the Diamond courier account Check and accept the terms and conditions
Declared Value	<input type="text" value="100"/>	GBP
Package Description	<input type="text" value="Dry shipper - not restricted as per IATA special provision A152"/>	

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

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.

Shipment Contents

Select a dewar by clicking on the row in the table below. Dewar details are then shown below. Click the + icon to add a container to the selected dewar

Name	Barcode	Facility Code	Weight (Kg)	First Experiment	Tracking # to	Tracking # from	Status	Location	Containers
Test	cm26454-5-i19-1-0044018	DLS-CY-0002	18	cm26454-5	Click to edit	Click to edit	opened		4

Dewar Details: Test

This section shows contents and history for the selected dewar. Click the spyglass icon to view the contents of the container

- I19-0069 (0 samples)
- I19-0066 (0 samples)
- I19-0065 (0 samples)
- I19-0064 (4 samples)

Date	Status	Location
17-11-2020 15:11	pickup booked	The Dewar location within Diamond is shown here
17-11-2020 15:11	awb created	

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Origin OXFORD-GBR
Destination OXFORD-GBR

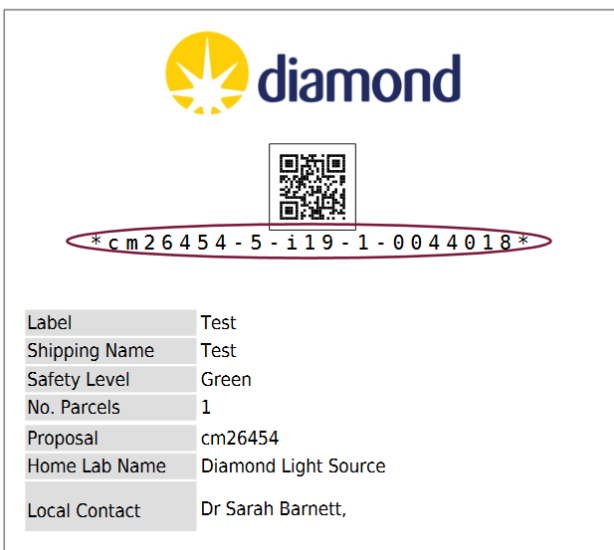
Date	Status	Location	Signatory
2020-11-18 09:59:00	Shipment pick up	OXFORD-GBR	DHL tracking details are listed here

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

The screenshot shows the ISPyB interface with a sidebar menu on the right. The menu items are: View All Data, Visits, Calendar, Assign Containers (circled in blue), Shipments, Registered Dewars, Registered Containers, Containers, Samples, Proteins, Lab Contacts, Statistics, and Migrate. The main content area shows a 'Visit List' table with columns for Start, End, and Number of Pucks. The table contains several rows of visit data, including dates and times. A notification at the top left states 'The start of run 5 has been delayed.' and another at the top right states 'Day 19th November.'

Click on the current visit from the potential list

The screenshot shows a dialog box titled 'Assign Containers: Select a Visit'. It contains a black instruction bar that reads 'Select a visit for which you want to assign samples to the beamline sample changer'. Below this, there is a single green button labeled 'cm26454-5: 119-1 - 09:00 23-10-2020', which is circled in blue.

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.

Container Allocation for cm26454-5 on i19-1 at 09:00 23-10-2020

This page allows you to allocate samples from ISPyB to the beamline sample changer. Drag and drop containers on to the locations on the beamline. Shipments and Dewars can be expanded by clicking on their titles

Unassign containers by dragging them to any shipment listed under "Unassigned Containers". The container will still belong to its original shipment.

Confirm Container Assignment ✕

Are you sure you want to assign "I19-0064" to sample changer position "1"?

Assigned Containers: Sample Changer

1	2	3	4	5
6	7	8	9	10
11	12	13	14	

Unassigned Containers + Add New Container

Page < < 1 > >

Test

I19-0064	I19-0065	I19-0066	I19-0068
----------	----------	----------	----------

Sarah Barnett

DLS-CY-0002

I19-0063

Pucks assigned in ISPyB:

Container Allocation for cm26454-5 on i19-1 at 09:00 23-10-2020

This page allows you to allocate samples from ISPyB to the beamline sample changer. Drag and drop containers on to the locations on the beamline. Shipments and Dewars can be expanded by clicking on their titles

Unassign containers by dragging them to any shipment listed under "Unassigned Containers". The container will still belong to its original shipment.

Data Collections

Assigned Containers: Sample Changer

I19-0064	I19-0065	I19-0066	I19-0068	
		I19-0063		

Unassigned Containers + Add New Container

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Test

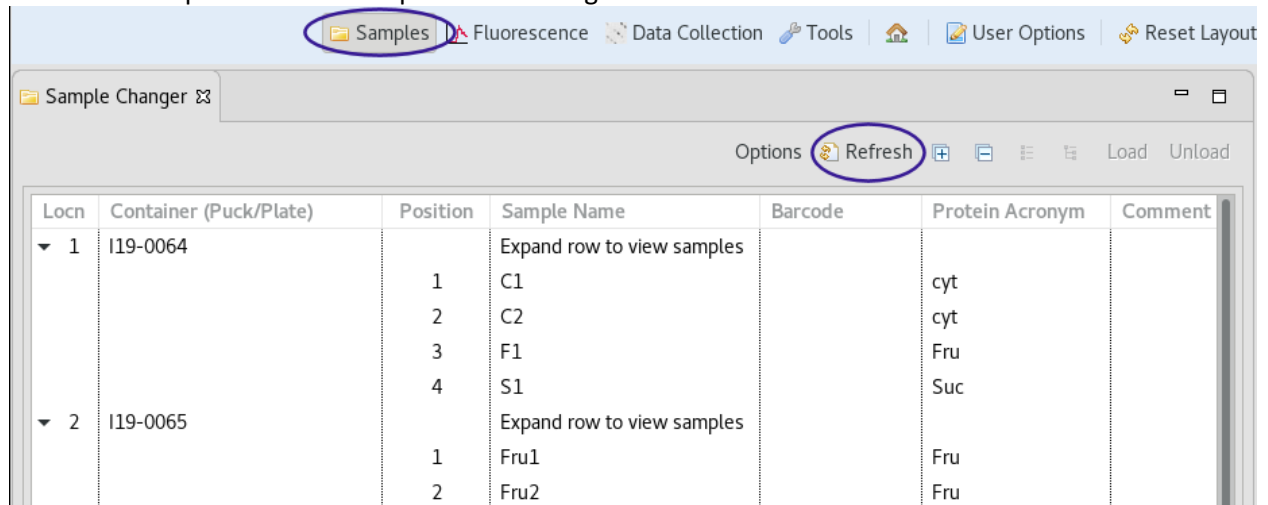
Test

Sarah Barnett

DLS-CY-0002

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

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)
1	Not-defined				Phi	0.00	0.00	0.00	0.100	0.00	45.00	Screening	450	0.100
2	Not-defined								0.200	0.00	180.00	Standard	900	0.200
3	Not-defined				Omega	0.00	30.00	-145.00	0.200	0.00	25.00	Standard	850	0.200
4	Not-defined				Omega	120.00	30.00	-145.00	0.200	0.00	25.00	Standard	850	0.200
5	Not-defined				Omega	240.00	30.00	-145.00	0.200	0.00	25.00	Standard	850	0.200

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

Sample Selection

Scope of Samples to Display: Samples in Changer

Locn	Position	Sample Name	Code	Protein Acron	Comment
1	1	cytidine-1		CYT	
1	2	cytidine-2		CYT	
1	3	cytidine-3		CYT	
1	4	cytidine-4		CYT	
1	5	cytidine-5		CYT	
1	6	cytidine-6		CYT	
1	7	cytidine-7		CYT	
1	8	cytidine-8		CYT	
1	9	cytidine-9		CYT	
1	10	cytidine-10		CYT	
1	11	cytidine-11		CYT	
1	12	cytidine-12		CYT	
1	13	cytidine-13		CYT	
1	14	cytidine-14		CYT	
1	15	cytidine-15		CYT	
1	16	cytidine-16		CYT	

Filter: RE Search: RE 16 Loaded - 16 Shown - 1 Selected - [Custom: -- Table Default -

Create Manual-Mount Sample: Duplicate Selected Sample and Edit Create and Edit Default Sample

Note: A Manual-Mount Sample is not assigned to a puck or into the Sample Changer

Cancel
OK

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