

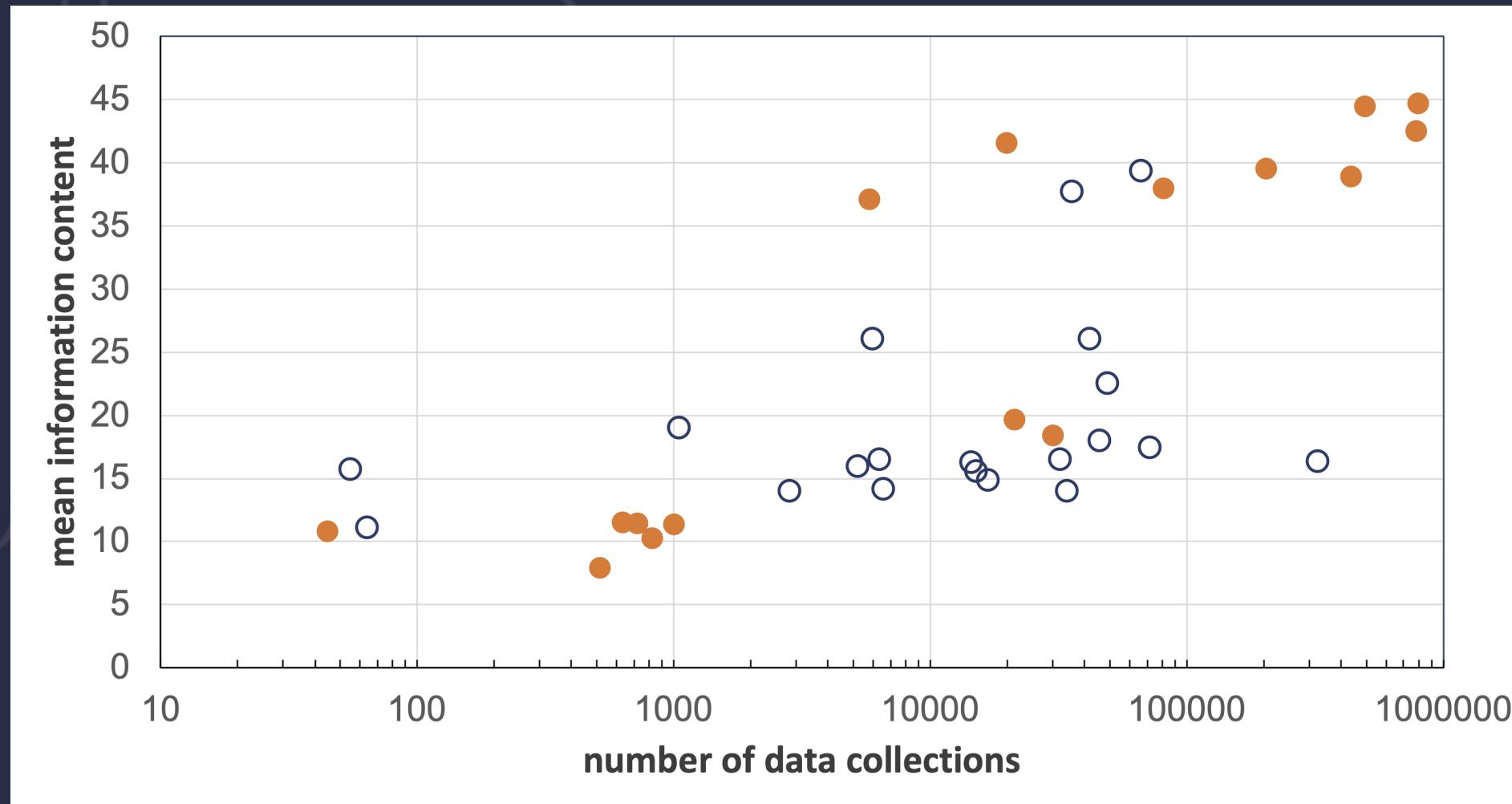
An introduction to ISPyB

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I19 EH-1 Remote Users Workshop February 2023



What is ISPyB and why do we need it?



And that's just the data collection

- What *is* this sample?
- Where did it come from?
- Whose is it?
- What did the results look like?

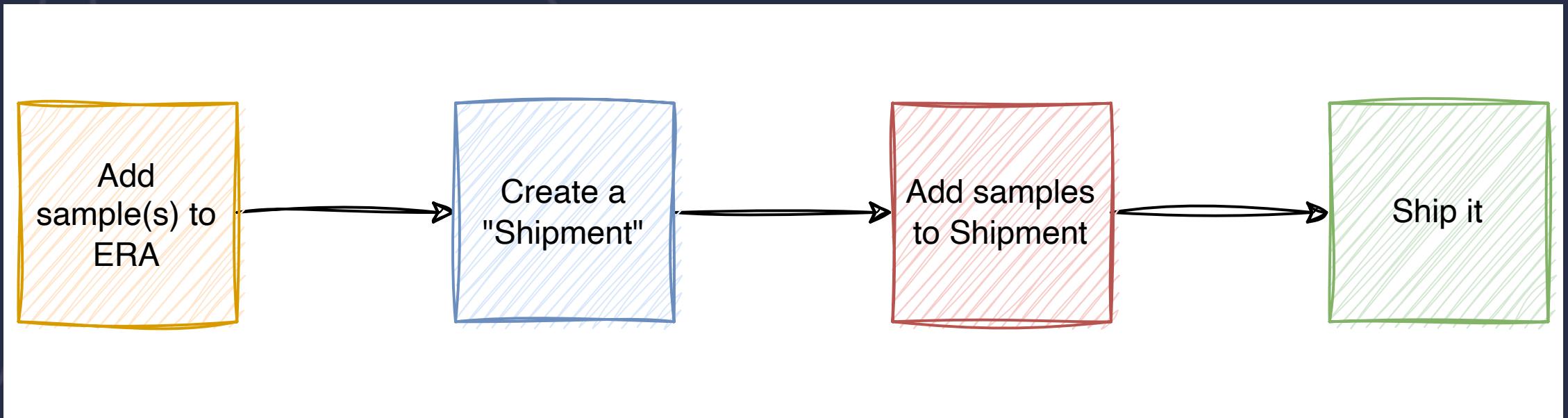
ISPyB is:

-  a stable, efficient database supporting many beamlines at Diamond

ISPyB is not:

-  specifically made for small molecule crystallography

Process Overview



<https://www.diamond.ac.uk/Instruments/Crystallography/I19/Manual/EH1.html>

Step 1: Add Sample(s) to ERA

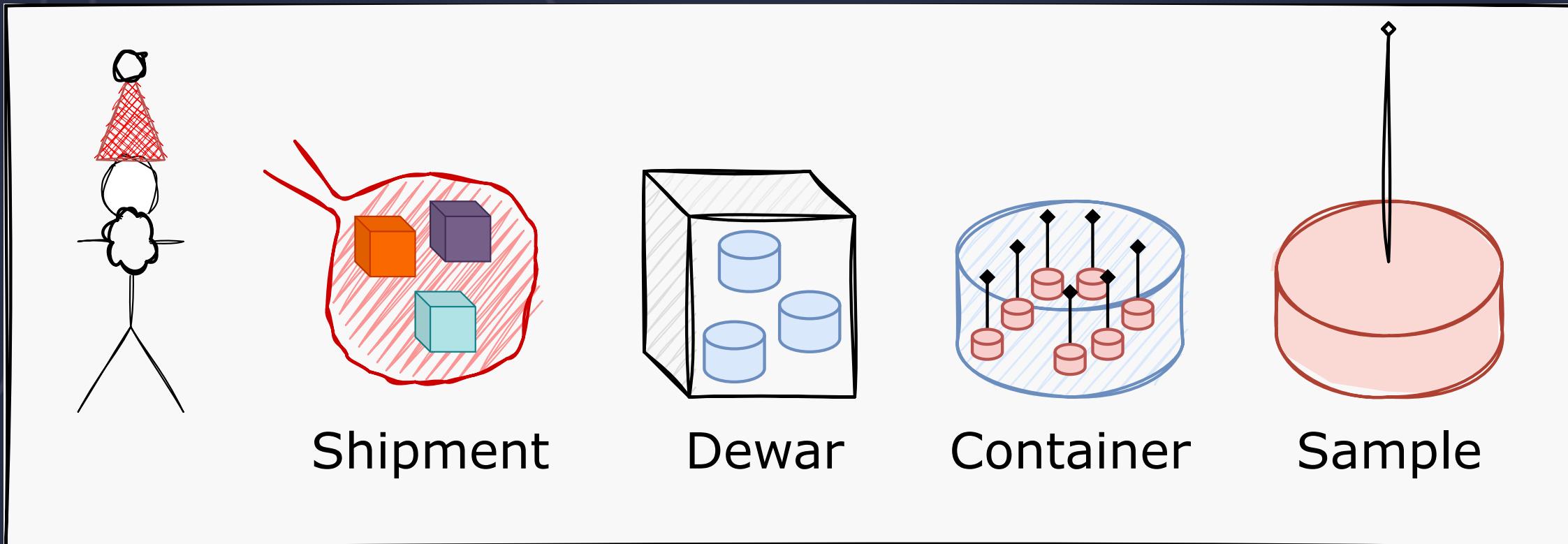
1. uas.diamond.ac.uk
2. Add your samples to the ERA as usual
3. Add an acronym

Sample Material or Protein
cytidine

Acronym
cyt

Step 1a: Wait for ERA to be validated
(...and then 3 hours more)

A couple of definitions



Step 2: Create the Shipment

1. ispyb.diamond.ac.uk
2. Log in and find the relevant proposal
3. Create a *Lab Contact*

Proposals	cm26454 ▾	Projects
The start of run 5 has been delayed.	View All Data	day 19th November.
	Visits	
	Calendar	
	Assign Containers	
	Shipments	
	Registered Dewars	
	Registered Containers	Dr Sarah Barnett, Dr Sarah
	Containers	sarah Barnett, Dr Dave Allan
	Samples	sarah Barnett, Dr Sarah Barr
	Proteins	
	Lab Contacts	
	Statistics	sarah Barnett, Dr Sarah Barn
	Migrate	

Visit List

This page lists the visits available to

Start	End	Nu
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	

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2a: Create a lab contact

The lab contact is the name and address of the person sending the samples to Diamond



Add New Home Lab Contact

Card Name
Name for the Contact Card 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

Contact First Name
The person's first name

Contact Phone Number
The person's phone number

Contact Email
The person's email address

Contact Laboratory Details

Laboratory Name
The contact's laboratory name

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

Laboratory Postcode
The contact's laboratory postcode

Laboratory Country
The contact's laboratory country 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

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

Billing Reference
Billing reference to use when returning dewars to home
lab

Average customs value of dewar
The average customs value of a dewar

Average transport value of dewar
The average transport value of a dewar

Add Home Lab Contact

Click here to add the contact, or save changes, once done

2a: Create a lab contact

The lab contact is the name and address of the person sending the samples to Diamond



2b: Register Dewars

Dewars need to be registered in the database to be usable. DLS-owned Dewars will already have been registered and so will have an identifier of the form

DLS-CY-00XX

If you are using your own Dewar, you will need to register it yourself



2c: Create 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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Step 3: Add Samples to Shipment

You've created a Shipment. Now lets add some samples to it



3a: Create 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		

15 ▾ Page < (**1**) >

Origin N/A

Destination N/A

Date	Status	Location	Signatory
No tracking available			

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	<table><thead><tr><th>Date</th><th>Status</th><th>Location</th><th>Beamline</th></tr></thead><tbody><tr><td colspan="4">No history found</td></tr></tbody></table> <p>10 Page « ‹ 1 › »</p>	Date	Status	Location	Beamline	No history found			
Date	Status	Location	Beamline						
No history found									
Location	Protein Acronym	Name	Spacegroup	Barcode	Comment	Anomalous	Required Res	Status	+ Extra Fields
1	cyt	C1							
2	cyt								
3	Fru	F1							
4	<input checked="" type="checkbox"/> cyt								
4	<input checked="" type="checkbox"/> Fru	S1							
5	<input checked="" type="checkbox"/> Suc								

3b: Put samples in Container

1. Dewar Tracking Label



diamond



Sample ID	2020-5-i19	00018*
Label		
Shipp. Name		
Safety Level	green	
No. Pcs	1	
Dropoff	cm26454	
Home Lab Name	Diamond Light Source	
Local Contact	Dr Sarah Barnett,	

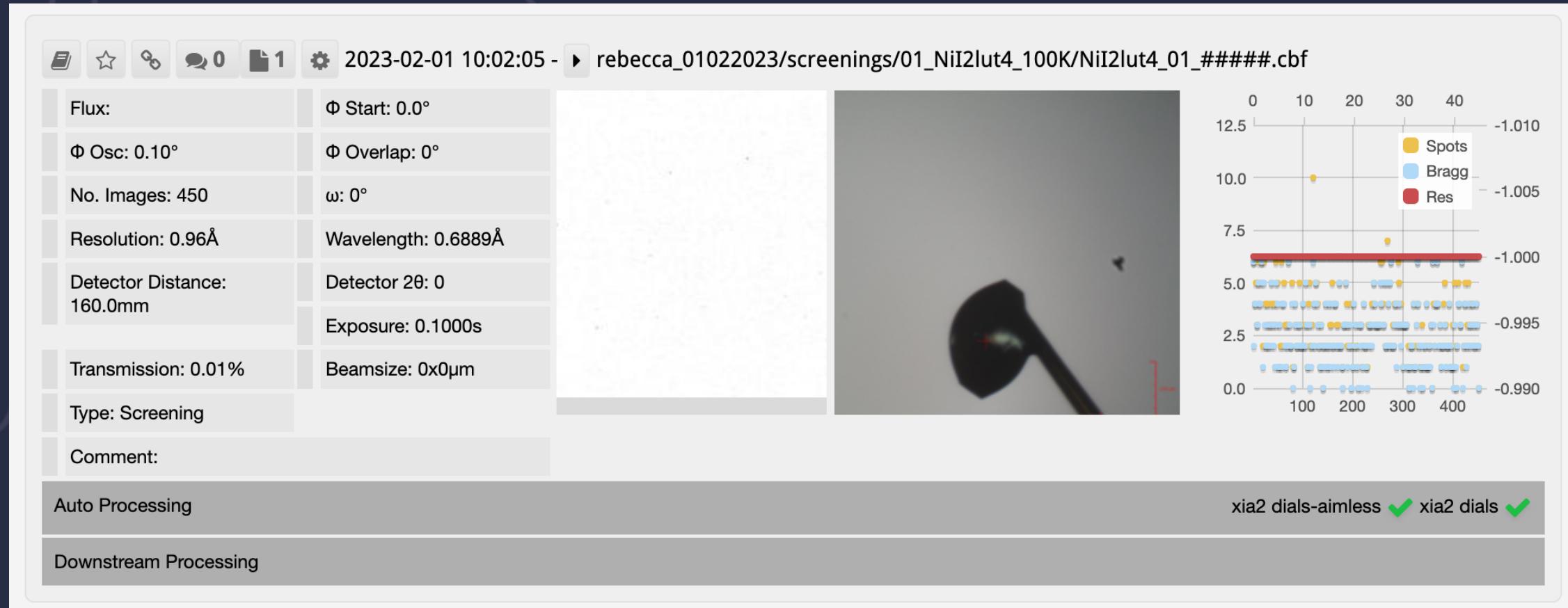
Using ISPyB during your experiment

During the visit you can see what's going on

The screenshot shows a web browser window for the ISPyB Data Collections interface at <https://ispyb.diamond.ac.uk/dc/visit/cm33867-1>. The title bar reads "Data Collections for cm33867-1 on i19-1". Below the title bar is a navigation bar with links: Assign Containers, Summary, Auto Processing, Visit Stats, Users, Dewars, Sample Changer, Reprocessing, and Beamline Status. A progress bar at the top is divided into three colored segments: yellow, purple, and red. The main content area is titled "i19-1 Webcams & Beamline Status". It displays various status indicators in green rounded rectangular boxes: Ring Current (299.853), Refill (289.727), Hutch Locked, Port Shutter Open, Fast Shutter Closed (red background), Energy (25.4926), Current Puck (0), and Current Pin (0). Below these are two green sections labeled "Machine Status 1" and "Machine Status 2". At the bottom, there are two video thumbnails showing the beamline setup. The left thumbnail shows a close-up of a metal pipe and a circular opening. The right thumbnail shows a wider view of the beamline equipment, including a robotic arm and various instruments.



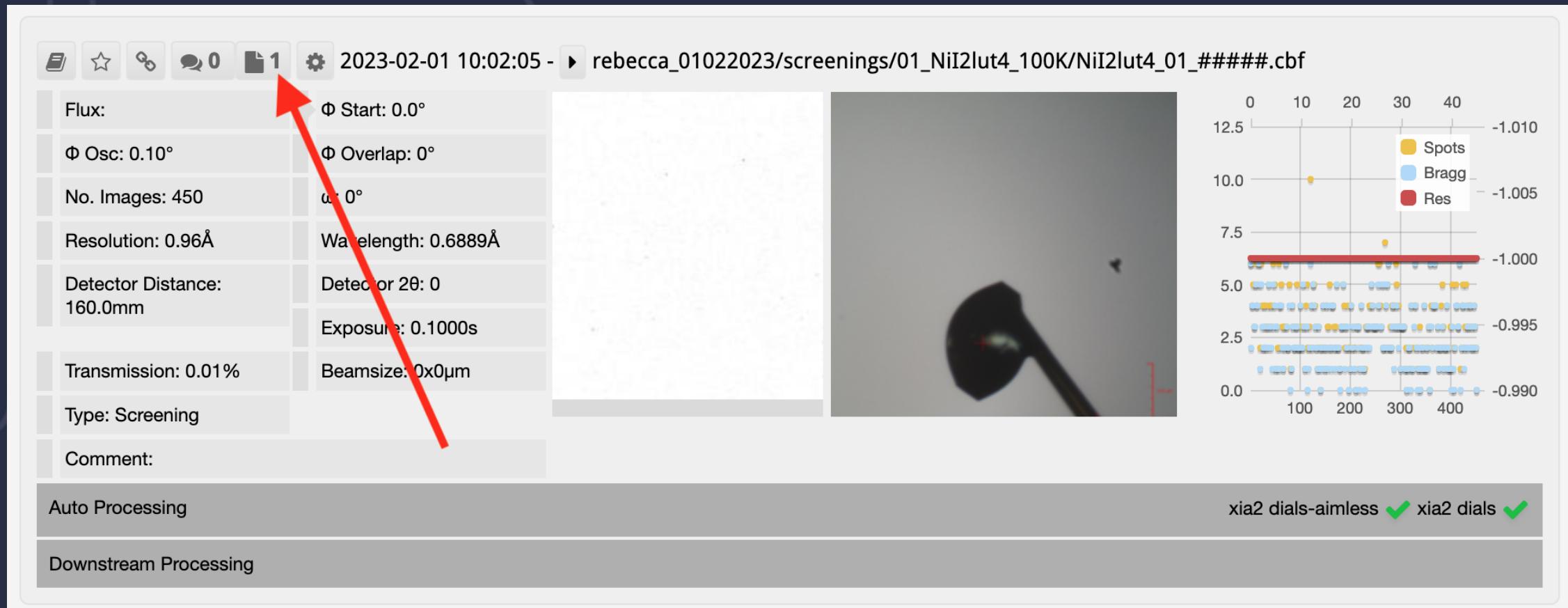
Data Collections Page, the distl plot



The concept of a data collection group



the reciprocal lattice viewer







A scatter plot showing a large number of teal-colored data points forming a roughly triangular shape. Two thick, intersecting lines are overlaid on the plot: a light green line sloping down from left to right, and a light red line sloping up from left to right. They intersect at approximately the center of the data cluster. In the bottom-left corner, the text "Press h for help" is displayed in a white, sans-serif font.
Press h for help

Processing Summary



Dials / Processing output

Auto Processing

xia2 dials-aimless ✓ xia2 dials ✓

Type	Resolution	Spacegroup	Mn< sig(i) >	Rmeas Inner	Rmeas Outer	Completeness	Cell	Status
xia2 dials-aimless	7.68 - 0.82	P 4/n n c	7.0	0.096	1.581	93.9	12.02 12.02 9.98 90.00 90.00 90.00	processing successful
xia2 dials	8.50 - 0.82	P 4/m m m	11.2	0.080	1.578	76.8	12.02 12.02 9.98 90.00 90.00 90.00	processing successful

xia2 dials-aimless xia2 dials

Space Group	A	B	C	α	β	γ	Plots	Archive	Logs & Files	Lookup Cell
P 4/n n c	12.02	12.02	9.98	90.00	90.00	90.00				

Shell	Observations	Unique	Resolution	Rmeas	I/sig(I)	CC Half	Completeness	Multiplicity	Anom Completeness	Anom Multiplicity	CC Anom
outerShell	9	8	0.82 - 0.84	1.581	3.5	0.0	22.9	1.1	0.0	0.0	0.0
innerShell	113	47	2.22 - 7.68	0.096	10.3	1.0	100.0	2.4	0.0	0.0	0.0
overall	1526	643	0.82 - 7.68	0.083	7.0	1.0	93.9	2.4	0.0	0.0	0.0

Downstream Processing

Imminent Improvements

There are some improvements coming soon which should hopefully make ispyb even more useful 

- Use the supplied formula in shelxt solve
- Attach shelxt outputs correctly as processing outputs