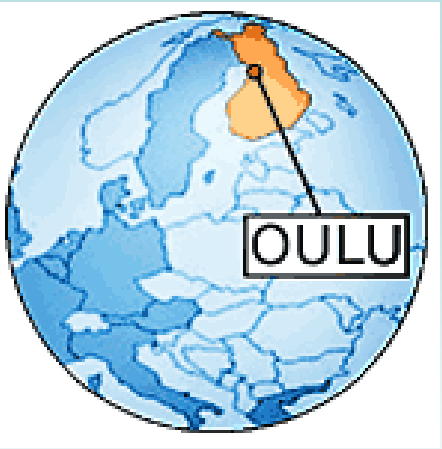


Towards standard APIs for the exchange of meta data between homelab LIMS software and ISPyB

ISPyB-developers meeting

Berlin, October 2019

Rik Wierenga
FBMM, BCO
University of Oulu
Oulu
Finland

Towards standard APIs for the exchange of meta data between homelab LIMS software and ISPyB

Oulu (Rik Wierenga)

Weizmann (Joel Sussman)

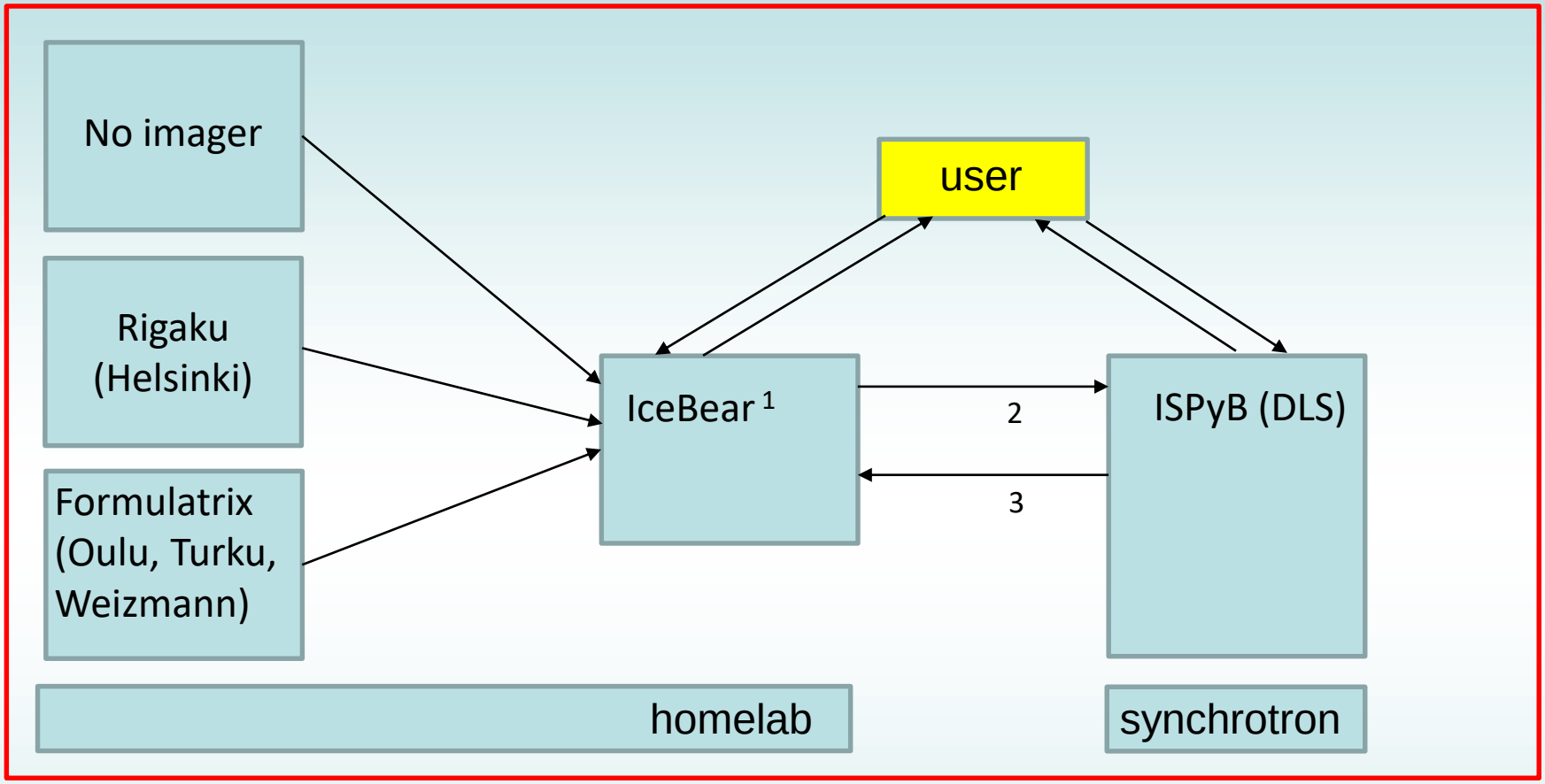
Diamond (Alun Ashton)

IceBear:

Integrated **C**rystal-data-tracking **E**nhancing **B**iochemistry **E**ducation **A**nd **R**esearch

Developed by Ed Daniel (University of Oulu)

Addressing the needs of the researchers of a homelab, using a diverse range of crystallization setups and crystal treatment protocols.



1 Crystallization and diffraction meta data in one data base

2 Meta data of crystals-on-pins

3 Link from the ISPyB shipment is stored in the homelab data base

We need to capture the workflow for cryofreezing selected crystals of selected drops
--connecting crystals to pins(barcoded/puckpositioned)
--cleaning/recycling dewar contents when the dewar comes back

We need to upload the meta data to ISPyB such that data collection can be done

We want to retrieve the link where ISPyB will store the diffraction information

We use barcoded pins, but the protocol will also work with non-barcoded pins

We have written a rapid-access proposal to Diamond to test these protocols on the live-server at Diamond and we have tested this now in two sessions.

Icebear crystal shipment manifest

Icebear:
https://icebear.oulu.fi/shipment/13899966

Diamond Light Source:
https://ispyb.diamond.ac.uk/shipments/sid/31948

Shipment: DLS 12 Oct Dewar 1

To: Diamond Light Source

Shipped: 2019-10-04

Dewar DLS-MX-0643, puck CPS-4618		
1	HA00AS6602	rpMFE1_95brC02d2c1
	Icebear 	*Diamond Light Source* 
2	HA00AS6876	rpMFE1_95brC02d2c2
	Icebear 	*Diamond Light Source* 
	HA00AR7699	rpMFE1_95brC02d1c1

Advantages, from the homelab perspective:

In Oulu there are about 30 researchers, newcomers very regularly starting

All researchers have direct access to the crystallization facility

Education: the information now provided by the system makes it much easier for supervisors to monitor/discuss the crystallization results and diffraction information as well as using the power of the processing and structure determination pipelines running at the ESRF and DLS

Research: All important data of the structure determination pipeline can now be recorded in one data base and are then available when writing publications

One person is needed to coordinate the shipment.
Inexperienced users are easily trained. Returning dewars are routinely cleaned.

Advantages, from the synchrotron perspective:

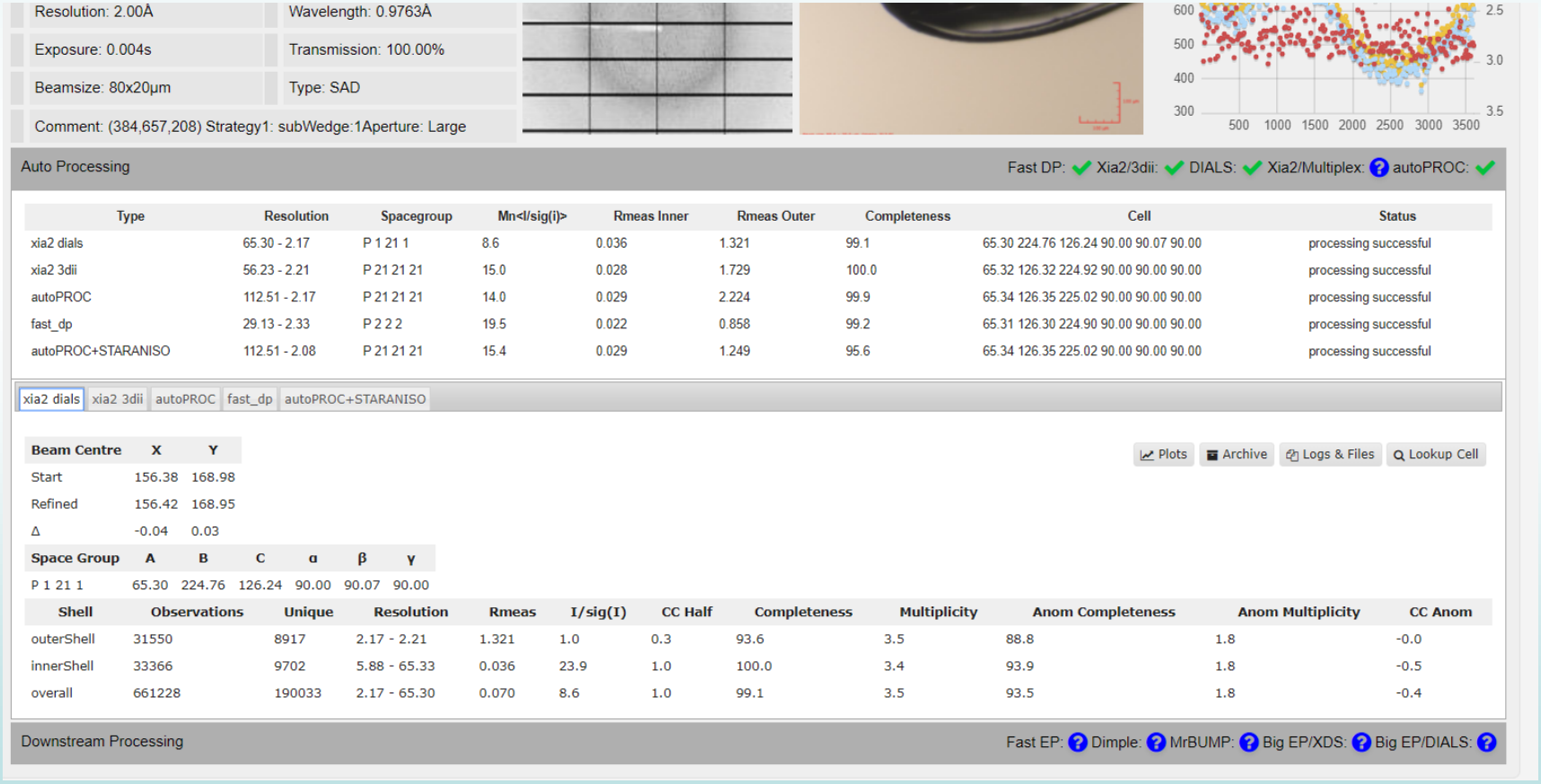
Proposal numbers, session numbers, beamline, data collection dates can be recorded. Any PDB-ident can be connected to where and when the data set was collected. Better use of the processing and structure determination pipelines.

The optimal use concerns a lab that has Formulatrix imagers driven by Rockmaker.

The software can be installed remotely using an installer.

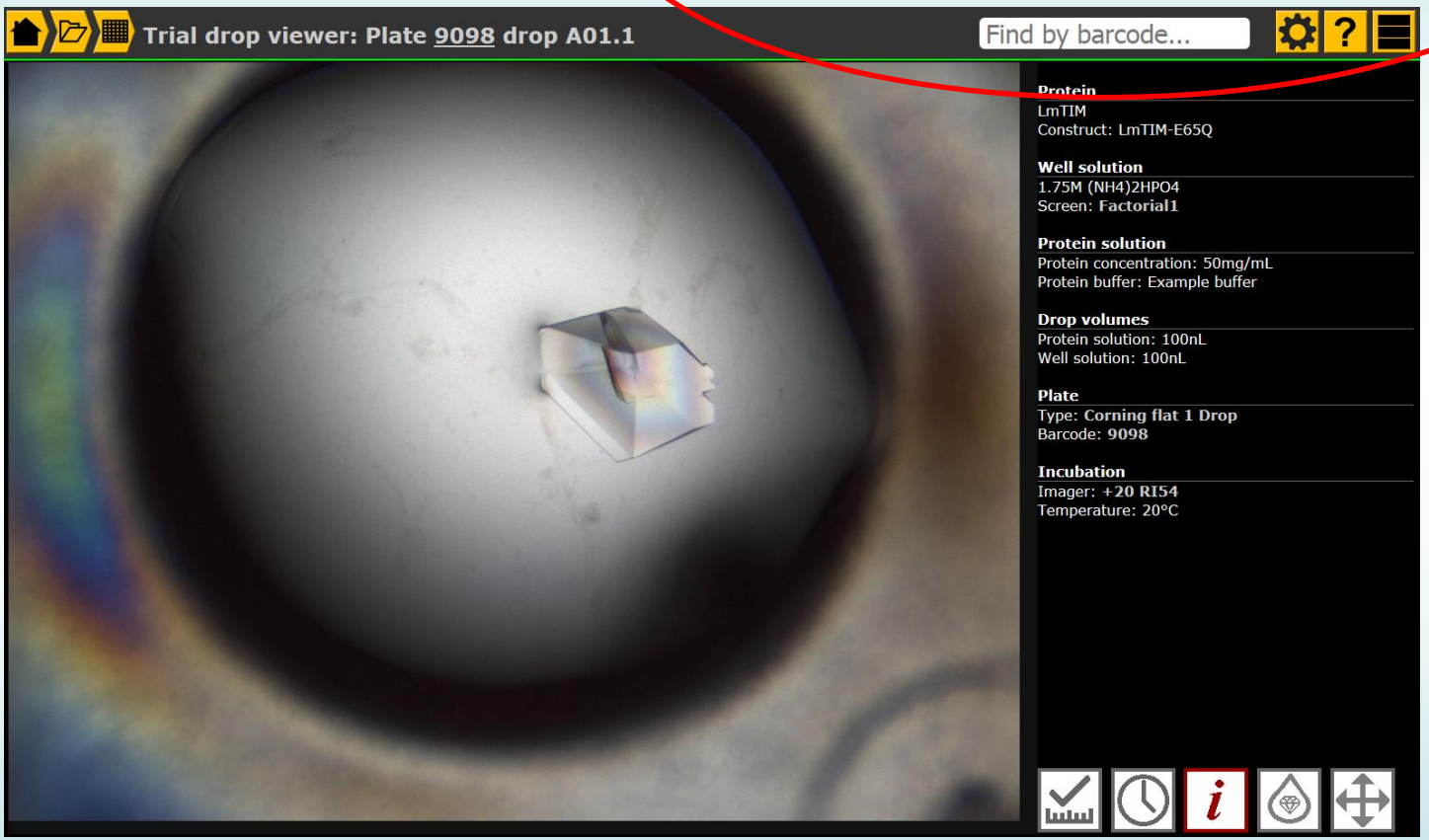
Upgrades can be dowloaded and implemented easily.

-we would like to upload more information: to optimally benefit from the data-processing-pipelines and the structure-determination-pipelines at the ESRF and DLS (sequence, structure/PDB-chain, ligand).



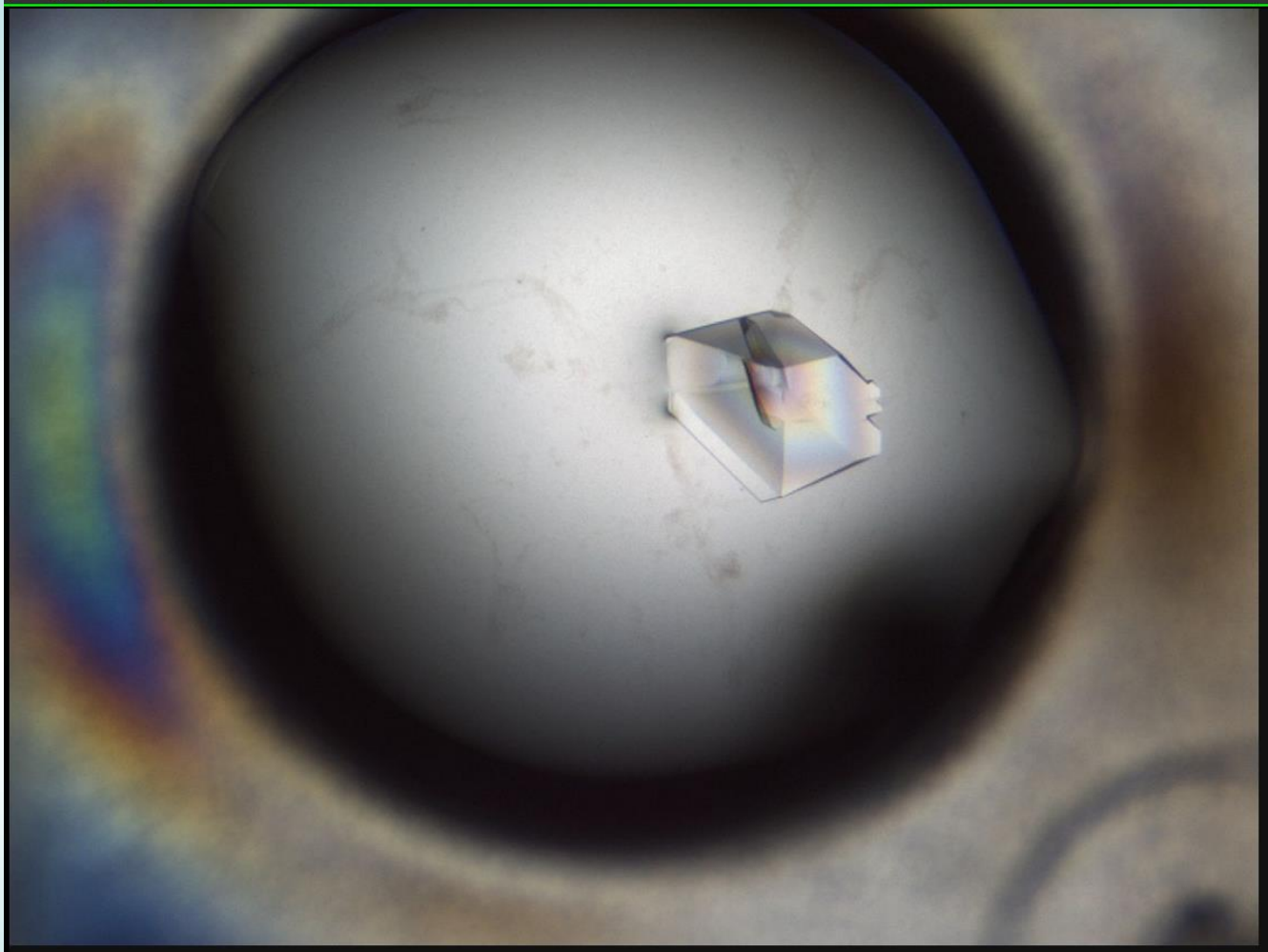
Practical aspects of how the work flow is captured

Search for plates, but also for dewars, crystal-identifiers, pin-barcodes



Trial drop viewer: Plate 9098 drop A01.1

Find by barcode...



Protein
LmTIM
Construct: LmTIM-E65Q

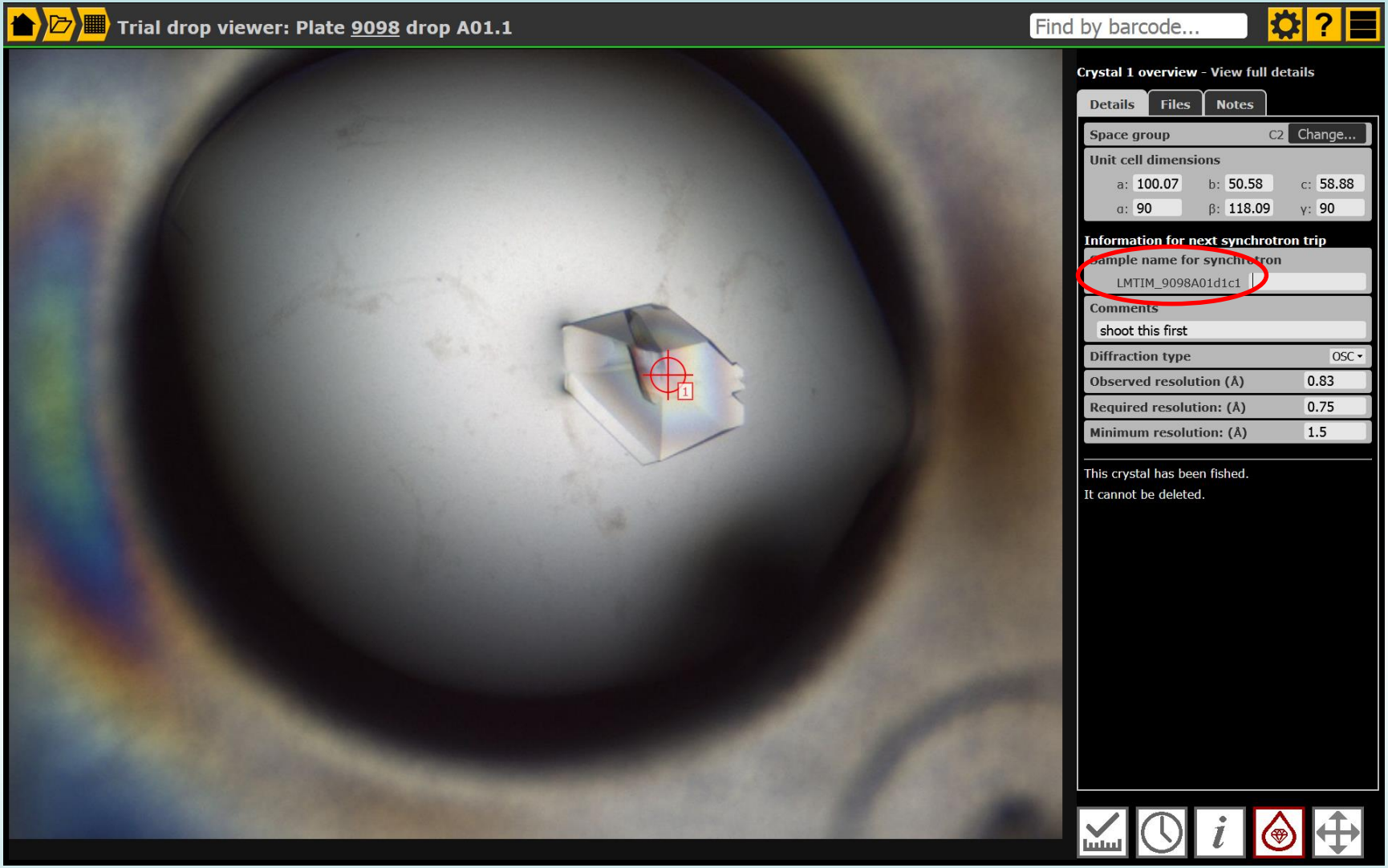
Well solution
1.75M (NH4)2HPO4
Screen: **Factorial1**

Protein solution
Protein concentration: 50mg/mL
Protein buffer: Example buffer

Drop volumes
Protein solution: 100nL
Well solution: 100nL

Plate
Type: **Corning flat 1 Drop**
Barcode: **9098**

Incubation
Imager: **+20 RI54**
Temperature: 20°C



(selecting a crystal: crystal identifier/sample name: LMTIM_9098A01d1c1)

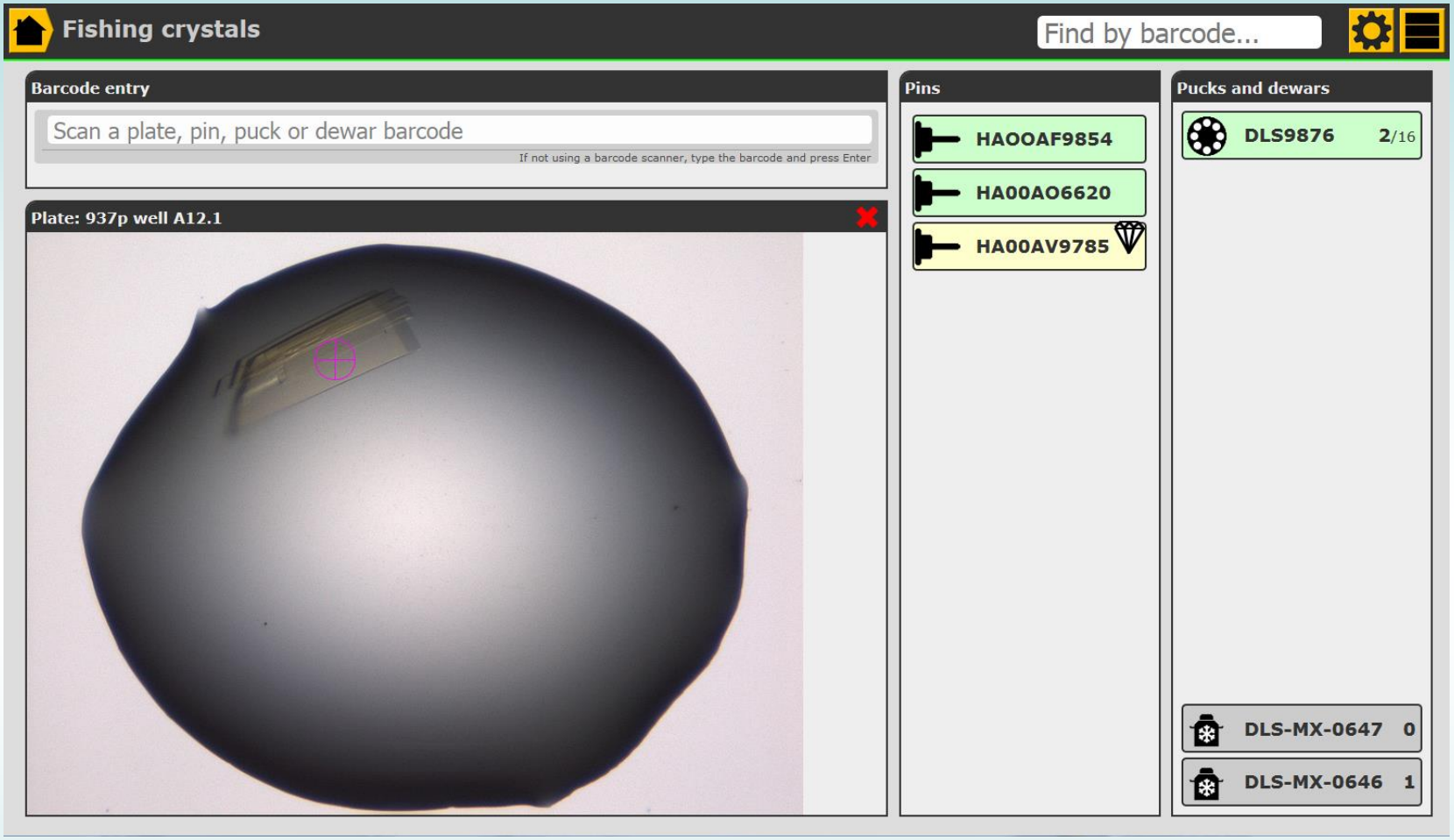
”fishing” module: we need to connect a crystal to a pin-barcode / position-in-puck

”shipment” module: to sent the meta data to ISPyB and clean the returning dewar

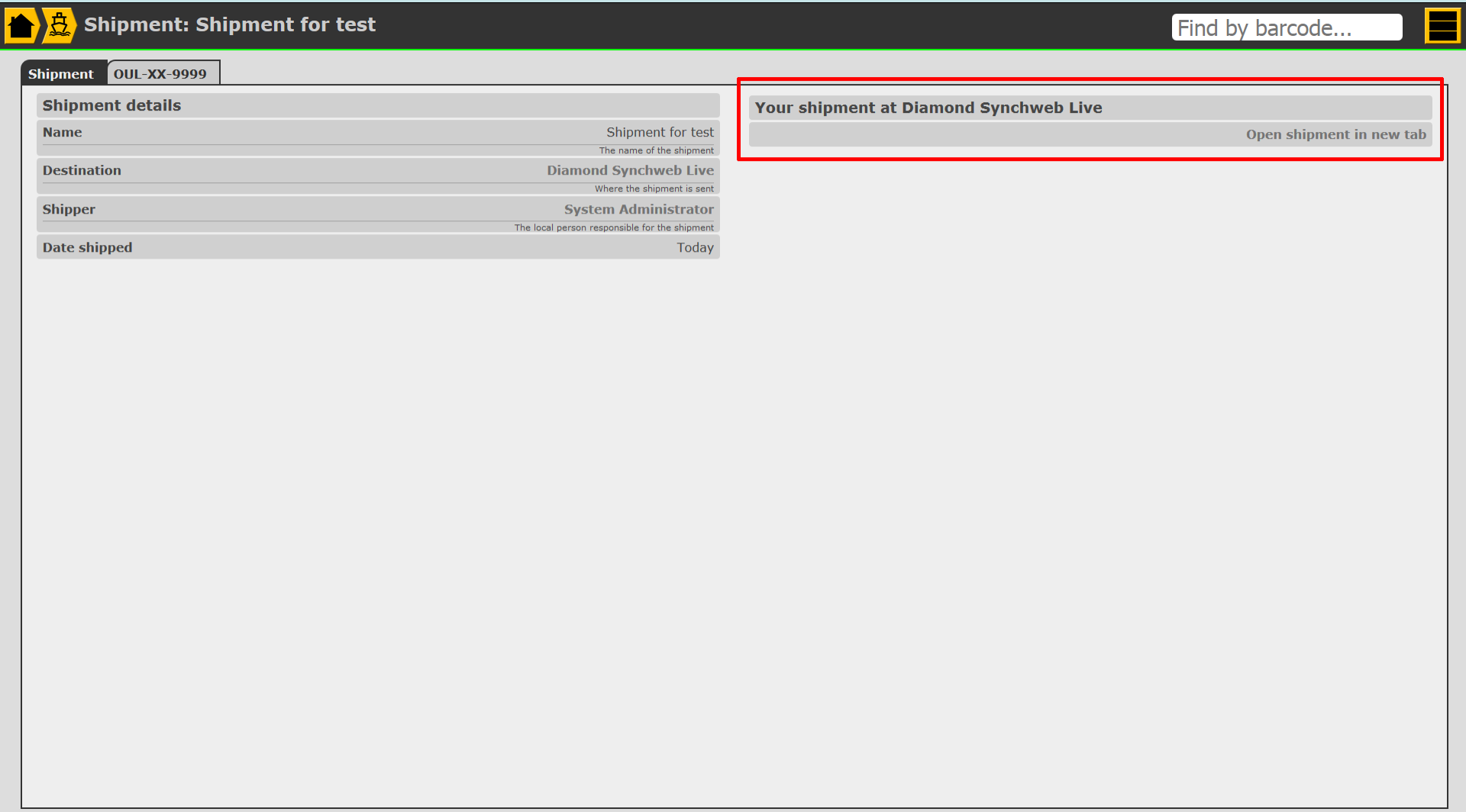
”crystal-page” module: to make accessible the ISPyB-link, DOI of the raw data, PDB entry

iNEXT course, 2019

Freezing crystals:
barcode reader is used to identify pins, pucks and dewars
touch screen (or mouse) is used to record that a crystal has been attached to a pin



Using IceBear when freezing crystals:
a crystal gets associated with a pin/pinbarcode or pin/puck position



ISPyB link is recorded in the data base. Other info (proposal-ID, session-ID, beamline-ID) can also be recorded.

Home Logout

diamond

» Login

Proposals | No Proposal | Feedback | Help

Please note that all dewars must now be registered before creating a shipment. Please see the updated help pages for details of the new process.

Login

Username (FedID)

Password

Login

SynchWeb? What is This?

Home Logout

diamond

» Shipments » Shipment for test » Containers » OUL-9999

Proposals | mx4025 | Projects | Unit Cell Search | | Feedback | Help

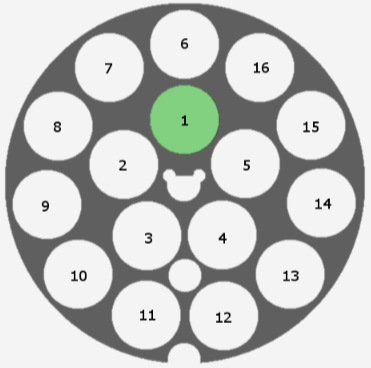
Please note that all dewars must now be registered before creating a shipment. Please see the updated help pages for details of the new process.

Container: OUL-9999

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	Shipment for test
Dewar	OUL-XX-9999
Container Type	Puck
Registered Container	Click to edit
Barcode	OUL-9999
Automated Collection	+ Queue this container for Auto Collect
Comments	Click to edit
Location History	Date Status Location Beamline No history found

10 Page ⟪ ⟨ 1 ⟩ ⟫



Extra Fields

Location	Protein Acronym	Name	Spacegroup	Barcode	Comment	Anomalous	Abundance	Components	Required Res	Unit Cell						Status
										A	B	C	α	β	γ	
1	LMTIM	LMTIM_9098B02d1c1	C222	OU99XX9999	Shoot this one first					100	100	100	90	90	90	
2																
3																
4																
5																
6																

Icebear crystal shipment manifest

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Shipment: DLS 12 Oct Dewar 1

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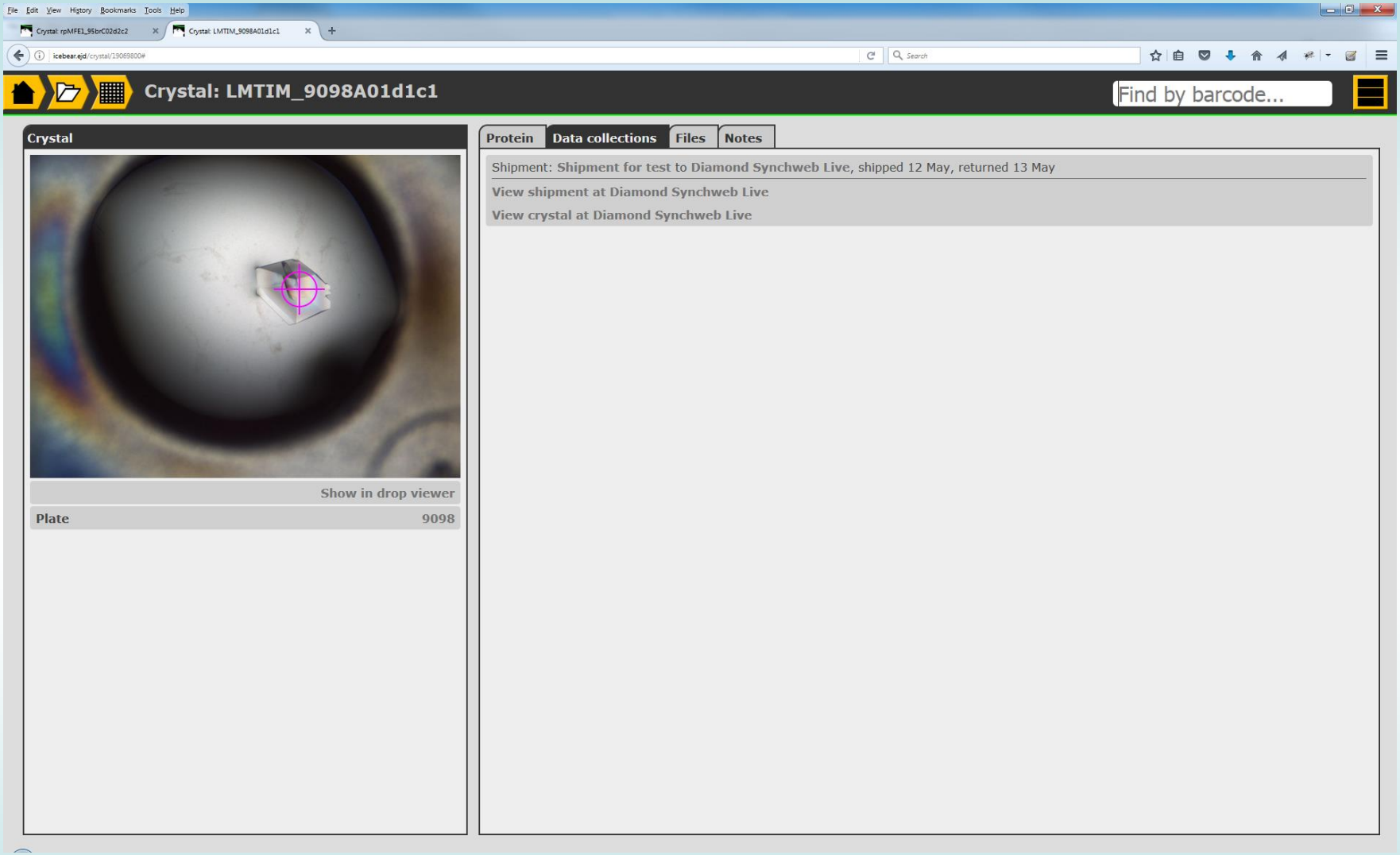
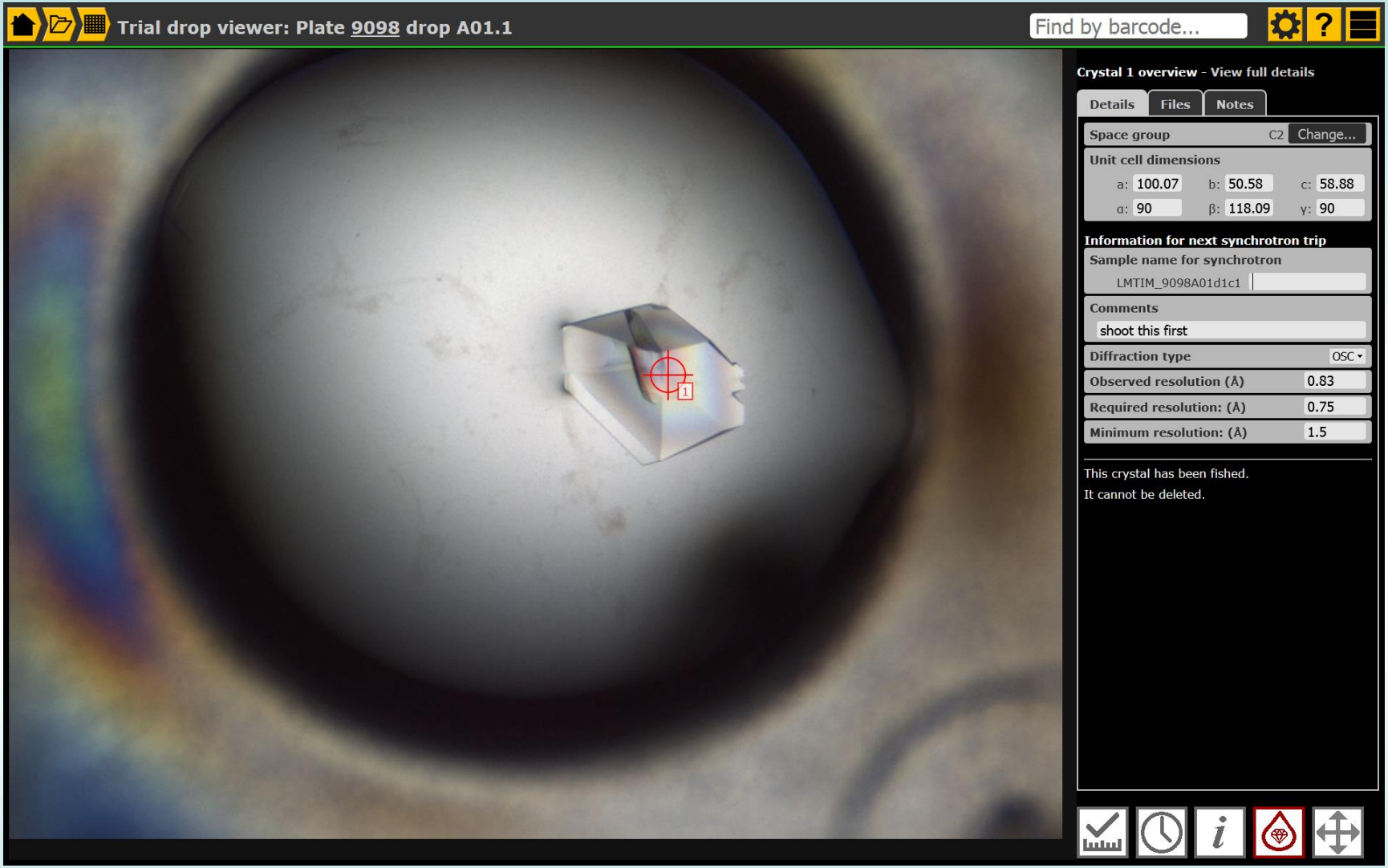
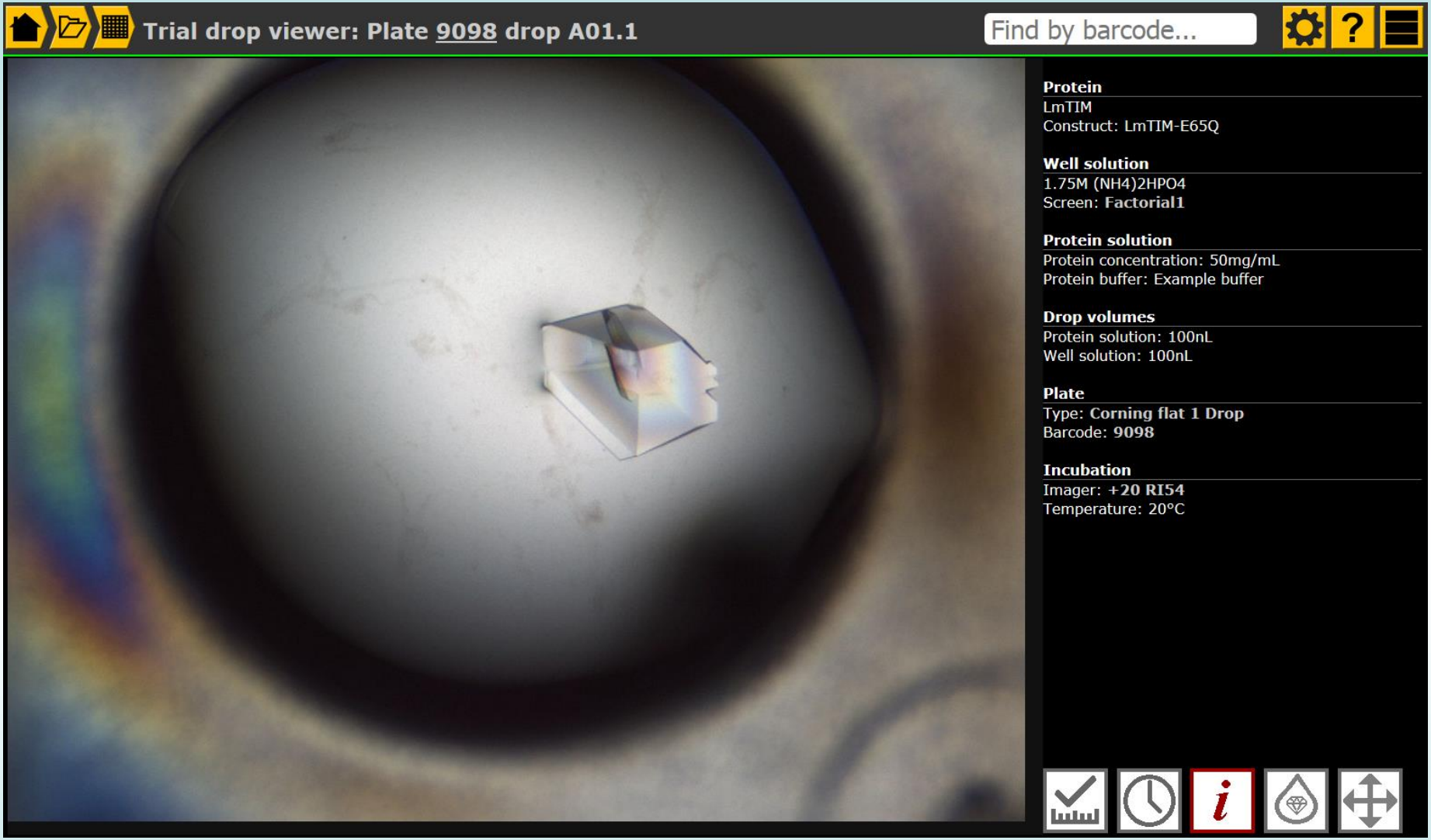
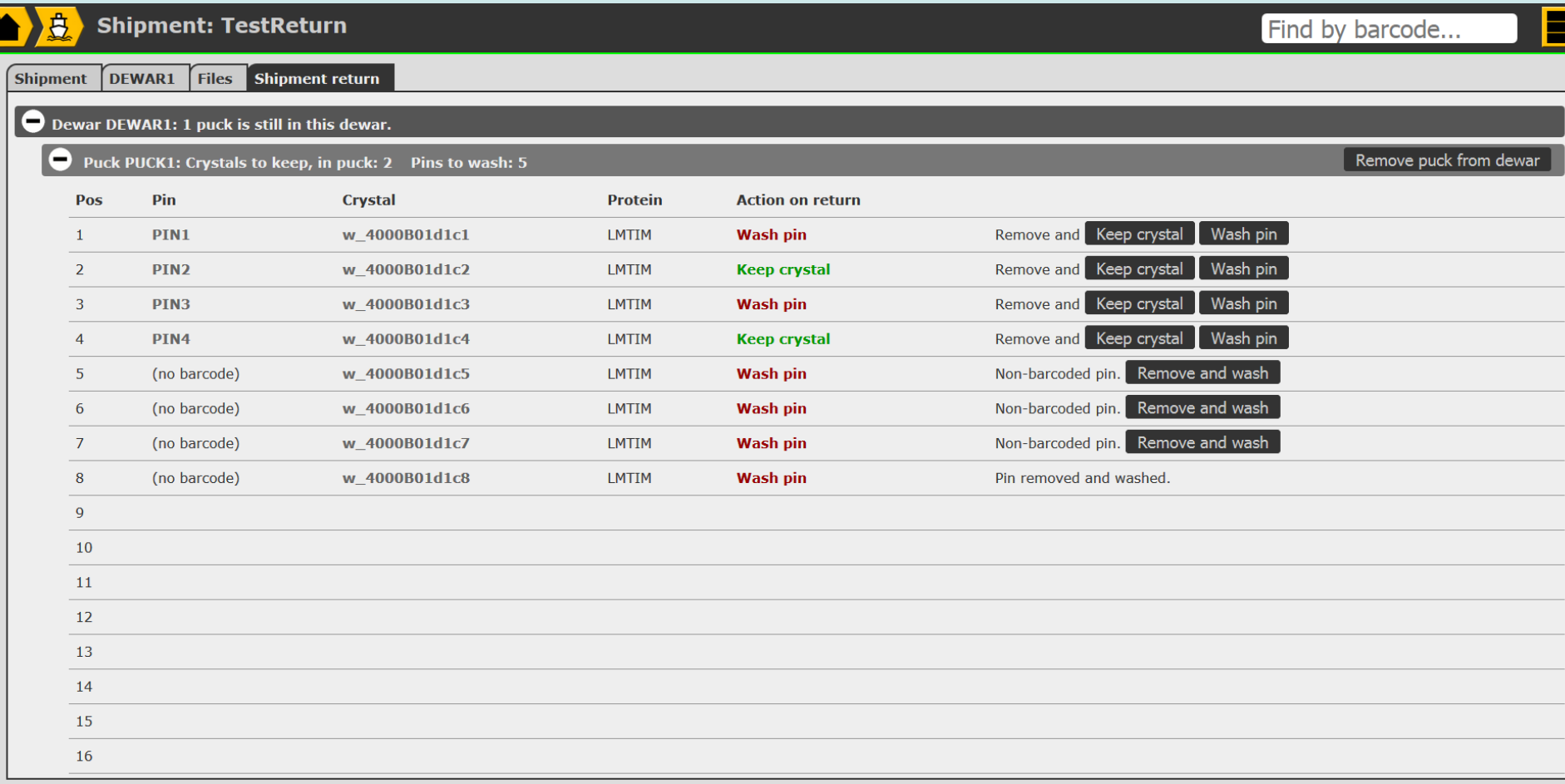


The crystal page


Trial drop viewer: Plate 9098 drop A01.1
Find by barcode...
Crystal 1 overview - View full details
Details
Files
Notes
Space group
C2
Change...
Unit cell dimensions
a: 100.07
b: 50.58
c: 58.88
α: 90
β: 118.09
γ: 90
Information for next synchrotron trip
Sample name for synchrotron
LMTIM_9098A01d1c1
Comments
shoot this first
Diffraction type
OSC
Observed resolution (Å)
0.83
Required resolution: (Å)
0.75
Minimum resolution: (Å)
1.5
This crystal has been fished.
It cannot be deleted.



IceBear WWW-based viewer of the crystallization results



Cleaning/recycling of the dewar and its contents when the dewar returns to the lab

In Finland Instruct-FI (Biocenter Finland, coordinated by Butcher, Lehtiö) has submitted a national infrastructure grant proposal aimed at getting a central installation at the CSC for each of the structural biology nodes. This can be extended to other Nordic countries.

Can we get this to work also for other synchrotrons?
Can we upload also info on sequence, structure and ligand?

Acknowledgements

Ed Daniel (Oulu)
Neil Smith, Karl Levik, Alun Ashton (Diamond)
Joel Sussman, Orly Dym (Weizmann)

Kristian Koski, Mirko Maksimainen, Lari Lehtiö (Oulu)
Protein crystallography community in Oulu (Oulu)
Instruct-FI community in Finland (Finland)

Instruct-ULTRA (EU)
Diamond (UK)