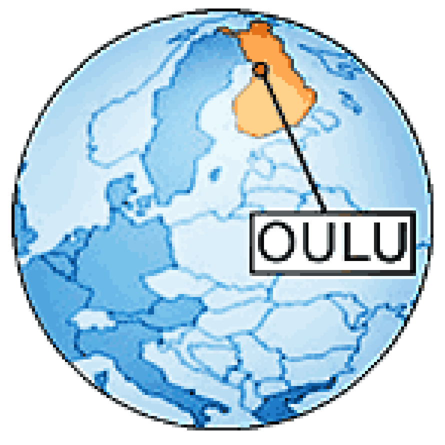


Towards standard APIs for the exchange of meta data between homelab LIMS software and ISPyB

ISPyB-developers meeting

Barcelona, June 30, 2020

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, Neil Smith, Dave Hall)

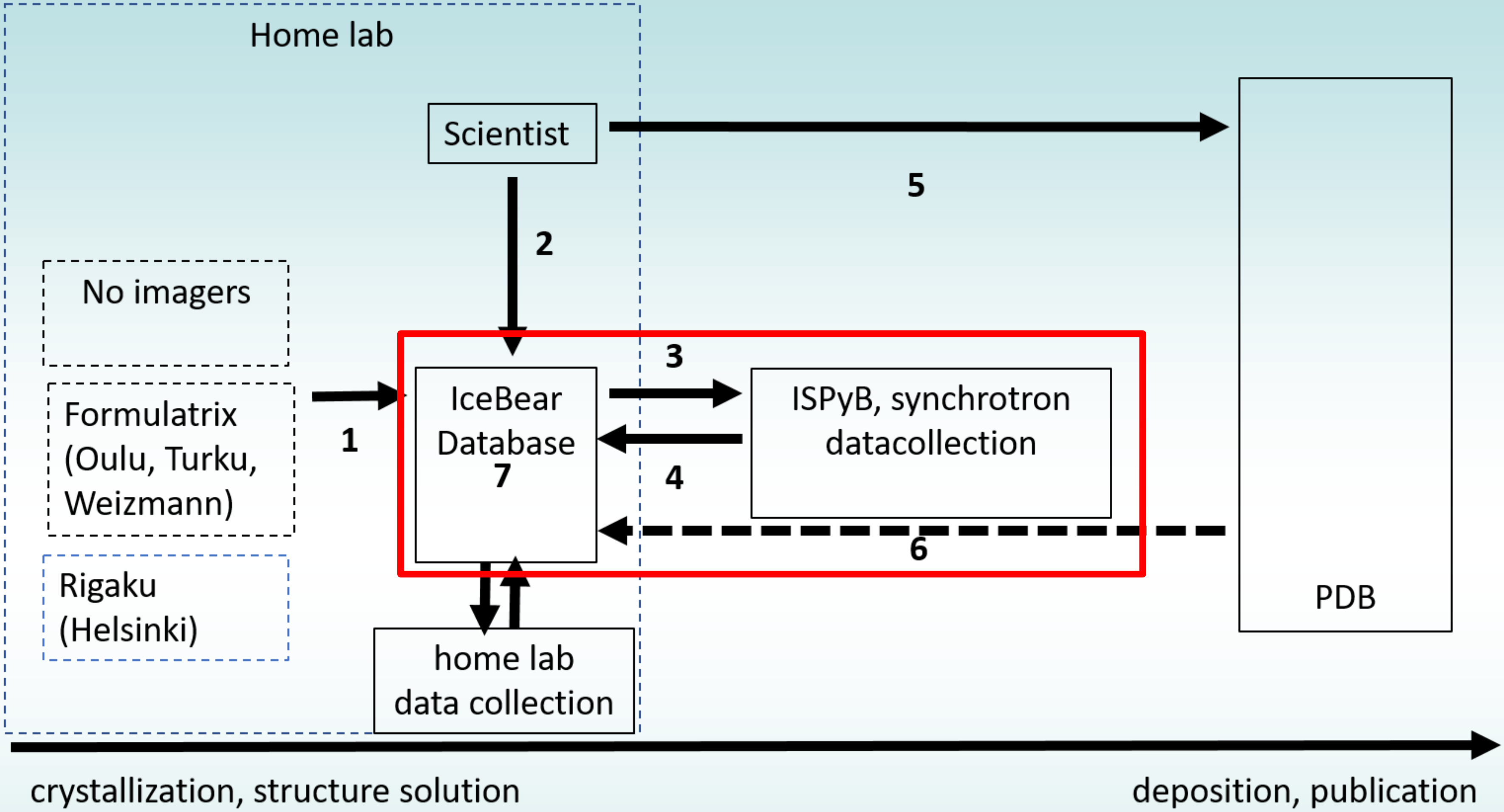
IceBear:

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 home lab, using a diverse range of crystallization setups and crystal treatment protocols.

Icebear version 1.1.0
Distributed under the **MIT Licence**



Home lab

Scientist

No imagers

Formulatrix (Oulu, Turku, Weizmann)

Rigaku (Helsinki)

IceBear Database

ISPyB, synchrotron datacollection

home lab data collection

PDB

1

2

3

4

5

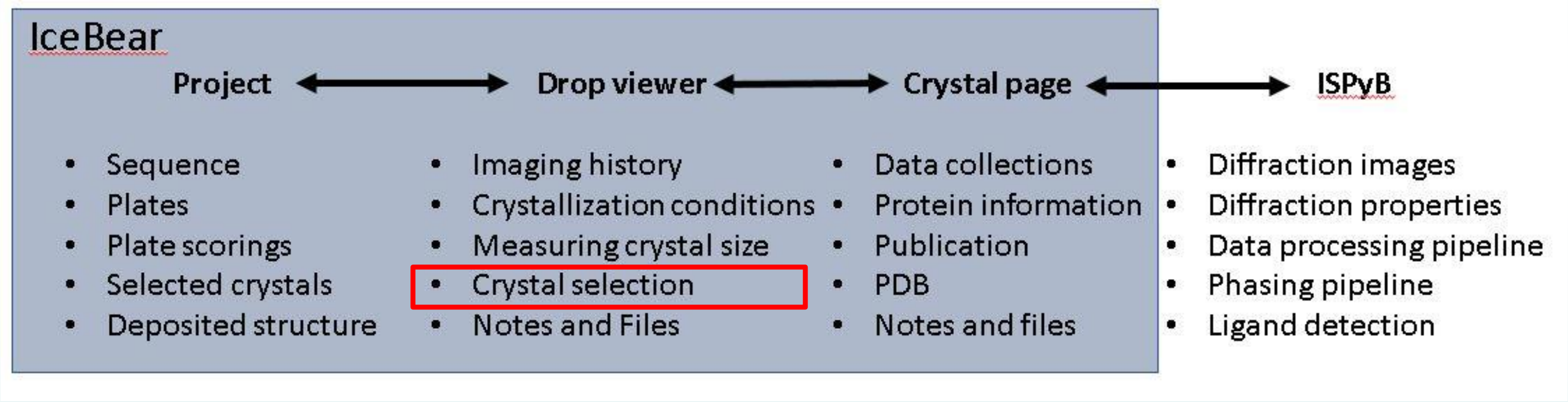
6

7

crystallization, structure solution

deposition, publication

1. Image and plate import
2. Project information
3. Uploading metadata to ISPyB
4. Diffraction information
5. Deposition, publication, archiving
6. Data tracking with PDB code
7. Data base on information from crystallization to deposition



Project ↔ **Drop viewer** ↔ **Crystal page** ↔ **ISPyB**

Project
- Sequence
- Plates
- Plate scorings
- Selected crystals
- Deposited structure

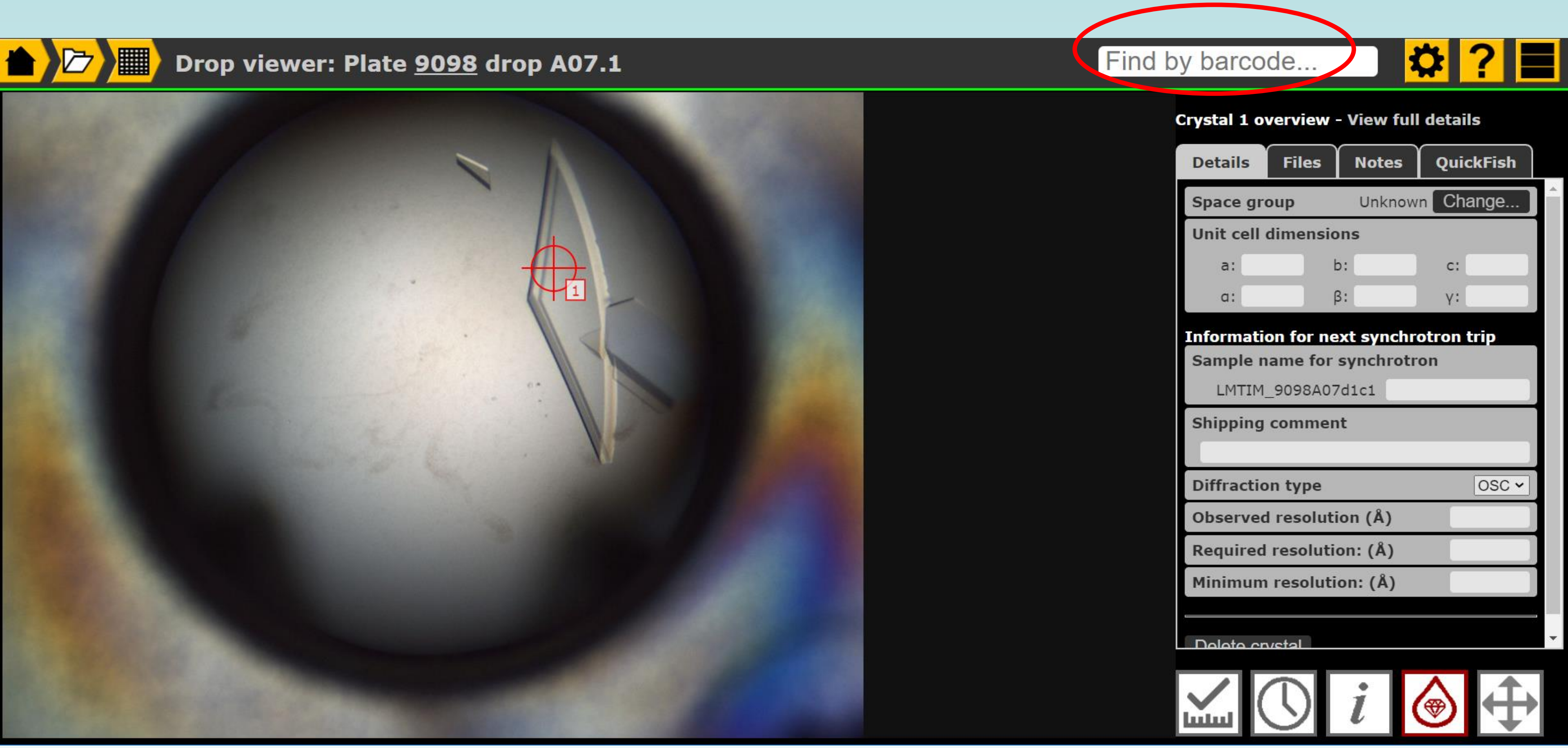
Drop viewer
- Imaging history
- Crystallization conditions
- Measuring crystal size
- Crystal selection
- Notes and Files

Crystal page
- Data collections
- Protein information
- Publication
- PDB
- Notes and files

ISPyB
- Diffraction images
- Diffraction properties
- Data processing pipeline
- Phasing pipeline
- Ligand detection

IceBear has several modules.
Central hubs are the Drop viewer and the Crystal page.
Several navigation options, using active links or using the search box, are available to reach these pages.

the search box



Drop viewer: Plate 9098 drop A07.1

Crystal 1 overview - View full details

Space group: Unknown

Unit cell dimensions
a:
b:
c:
α:
β:
γ:

Information for next synchrotron trip

Sample name for synchrotron: LMTIM_9098A07d1c1

Shipping comment:

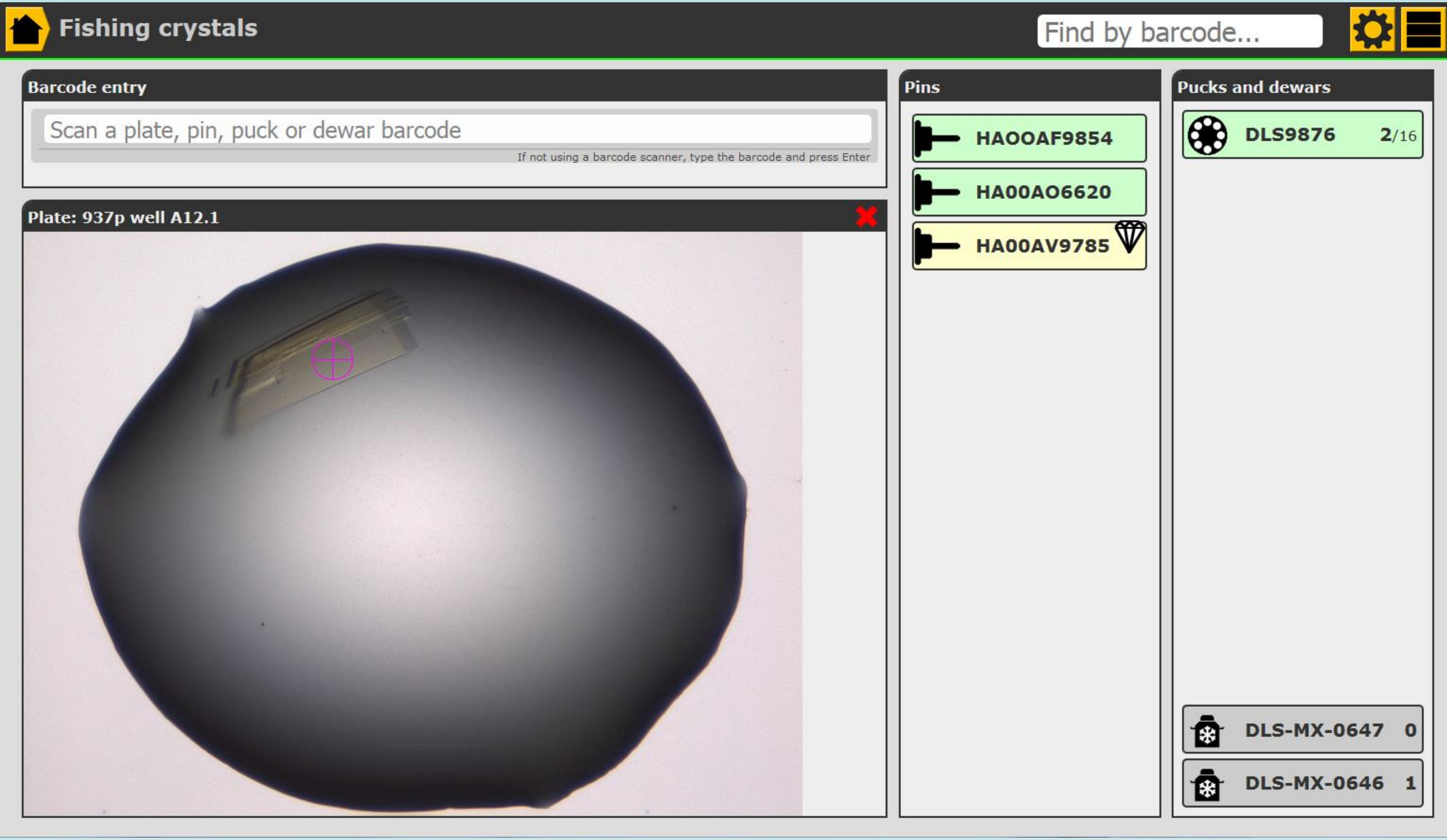
Diffraction type: OSC

Observed resolution (Å):

Required resolution: (Å):

Minimum resolution: (Å):

(selecting a crystal: crystal identifier/sample name: LMTIM_9098A07d1c1)



Fishing crystals

Find by barcode...

Barcode entry

Scan a plate, pin, puck or dewar barcode

If not using a barcode scanner, type the barcode and press Enter

Plate: 937p well A12.1

Pins

- HAOOAF9854
- HA00AO6620
- HA00AV9785

Pucks and dewars

DLS9876	2/16
DLS-MX-0647	0
DLS-MX-0646	1

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

Icebear crystal shipment manifest

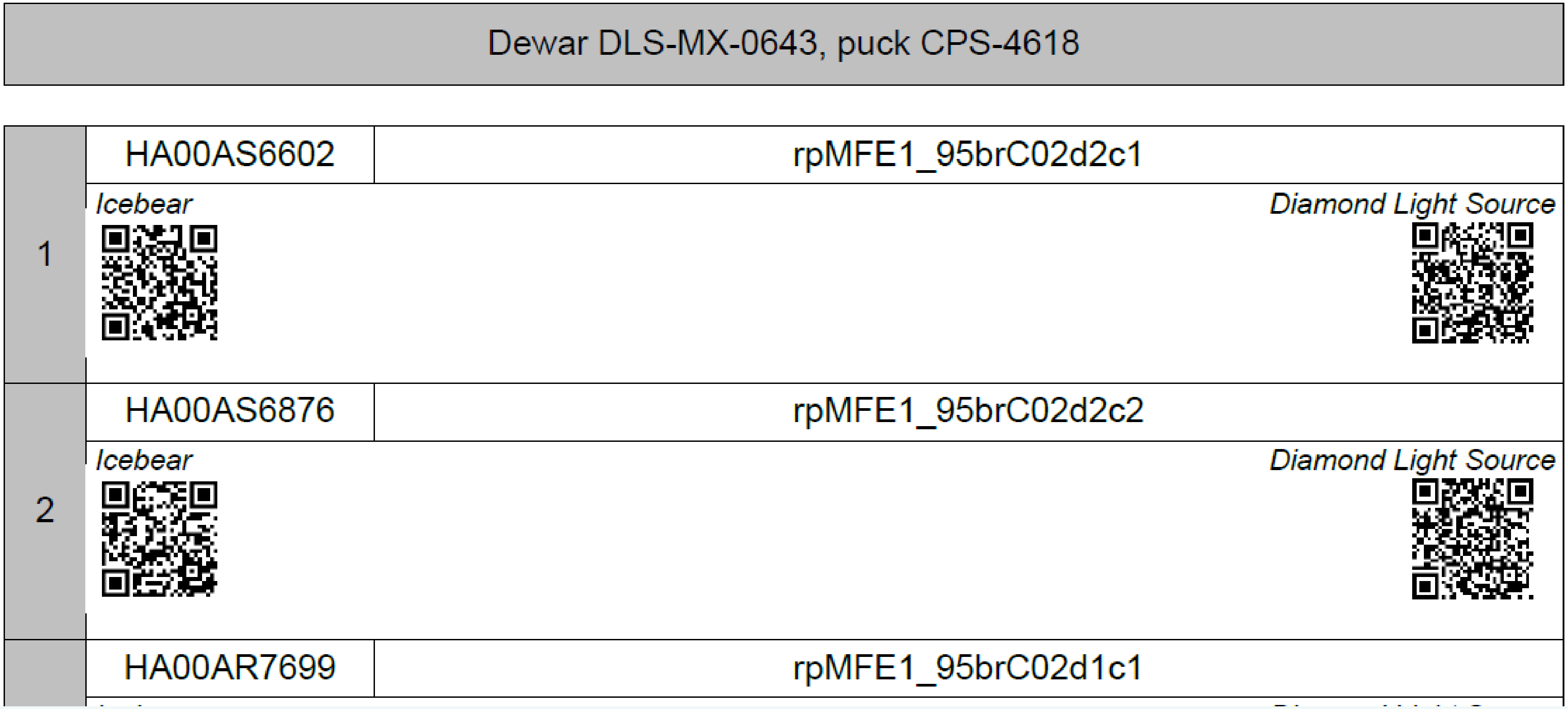
Icebear:
https://icebear.oulu.fi/shipment/13899966

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

Shipment: DLS 12 Oct Dewar 1

To: Diamond Light Source

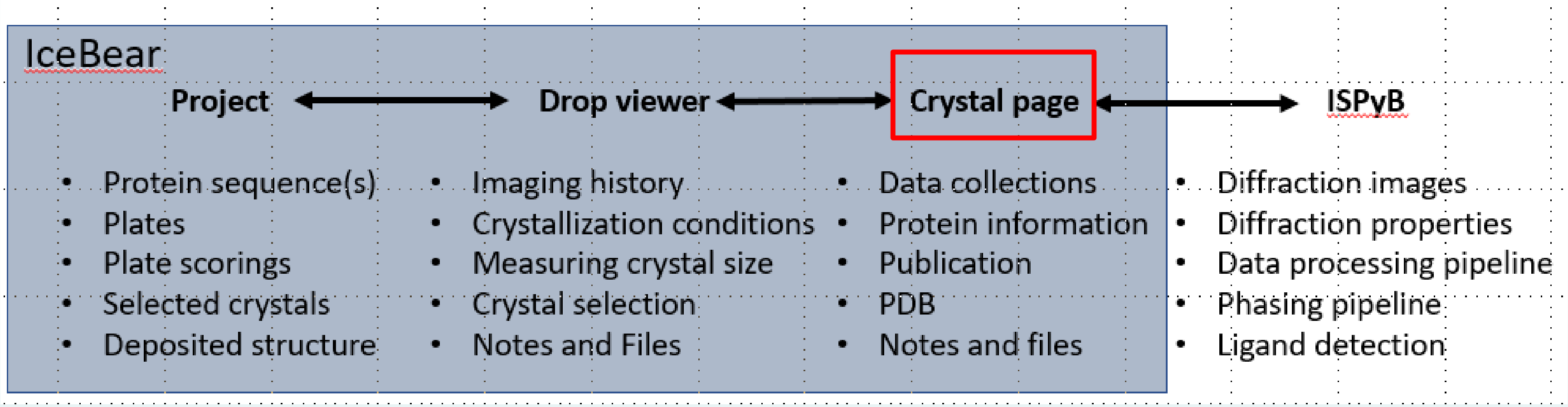
Shipped: 2019-10-04



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

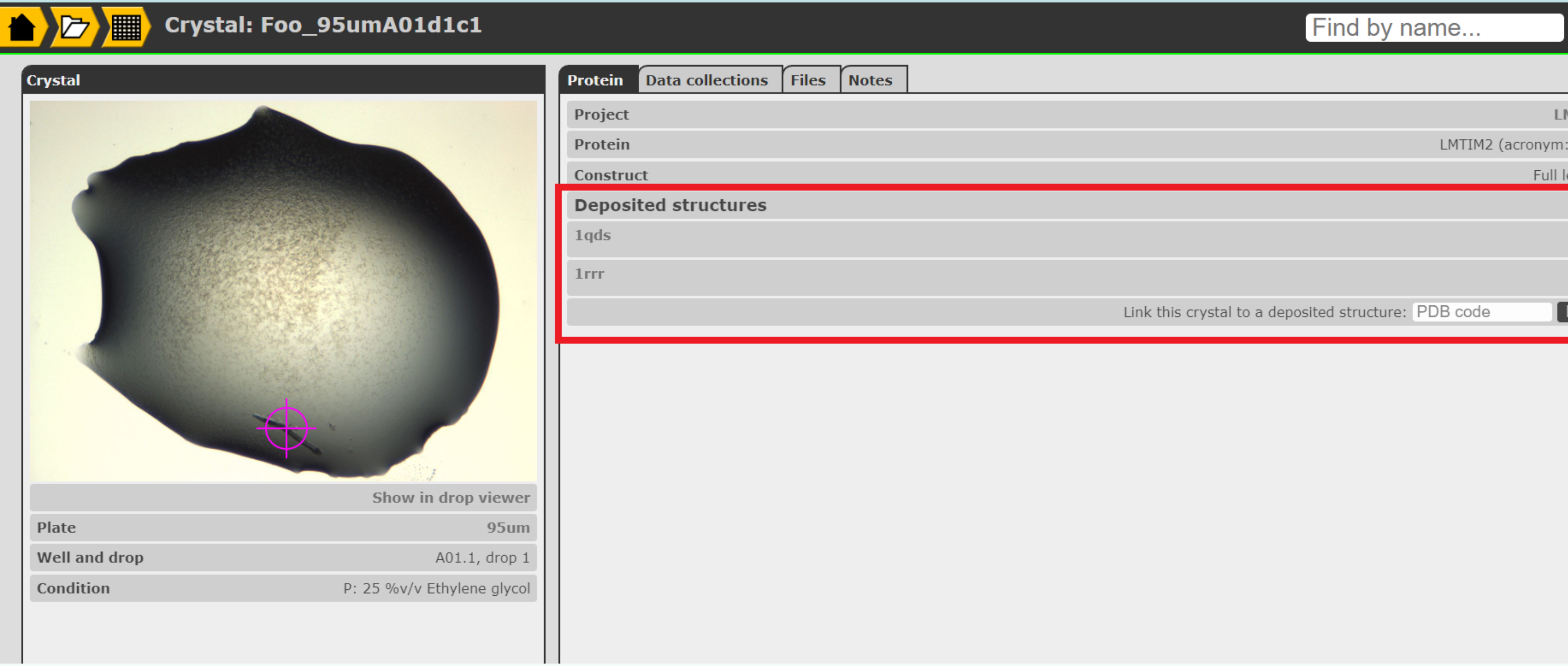
The shipping manifest



IceBear

Project	Drop viewer	Crystal page	ISPyB
Protein sequence(s)	Imaging history	Data collections	Diffraction images
Plates	Crystallization conditions	Protein information	Diffraction properties
Plate scorings	Measuring crystal size	Publication	Data processing pipeline
Selected crystals	Crystal selection	PDB	Phasing pipeline
Deposited structure	Notes and Files	Notes and files	Ligand detection

The crystal page communicates with ISPyB.



Crystal: Foo_95umA01d1c1

Crystal

Plate: 95um

Well and drop: A01.1, drop 1

Condition: P: 25 %v/v Ethylene glycol

Project: LI

Protein: LMTIM2 (acronym:

Construct: Full l

Deposited structures

1qds

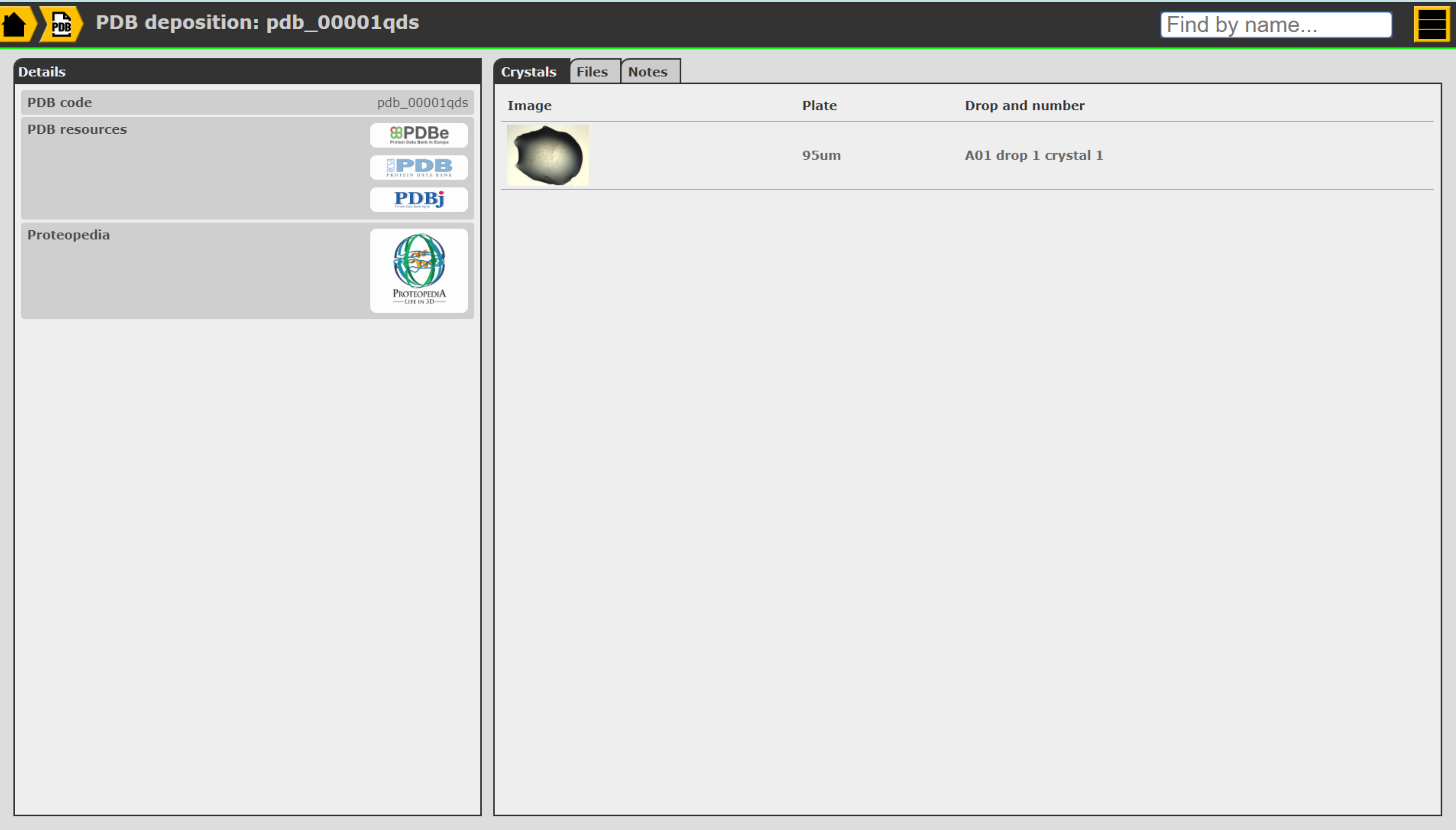
1rrr

Link this crystal to a deposited structure: PDB code

The crystal page

Crystal page can be found in various ways, including using the search box searching for the PDB code and the sample name.

If their exists a PDB deposited structure, then this information can be provided.
If one sample has resulted in several PDB structures then several PDB codes can be provided.

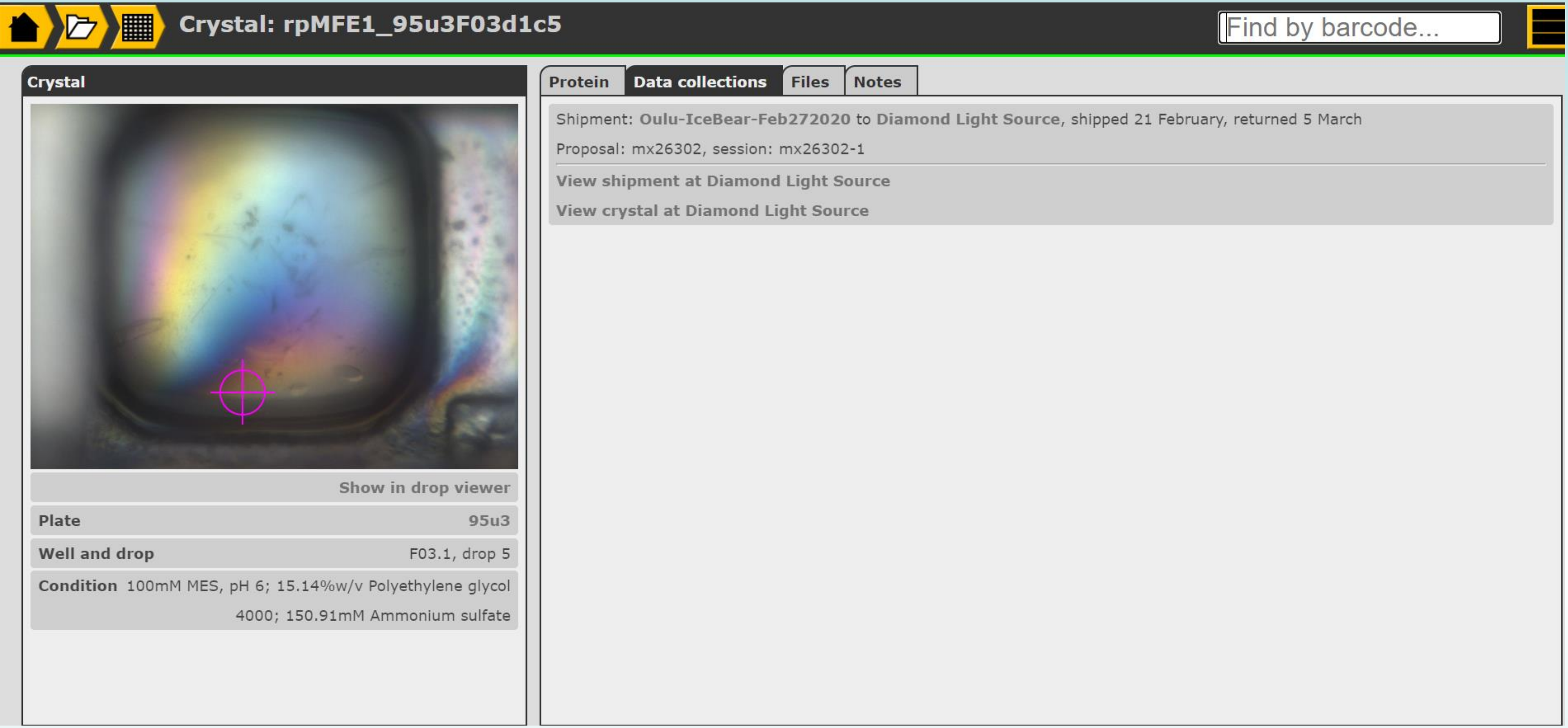


PDB deposition: pdb_00001qds

PDB code: pdb_00001qds

Image	Plate	Drop and number
	95um	A01 drop 1 crystal 1

The PDB page: if more than one crystal/sample has been used then this information can be provided



Crystal: rpMFE1_95u3F03d1c5

Shipment: **Oulu-IceBear-Feb272020** to **Diamond Light Source**, shipped 21 February, returned 5 March

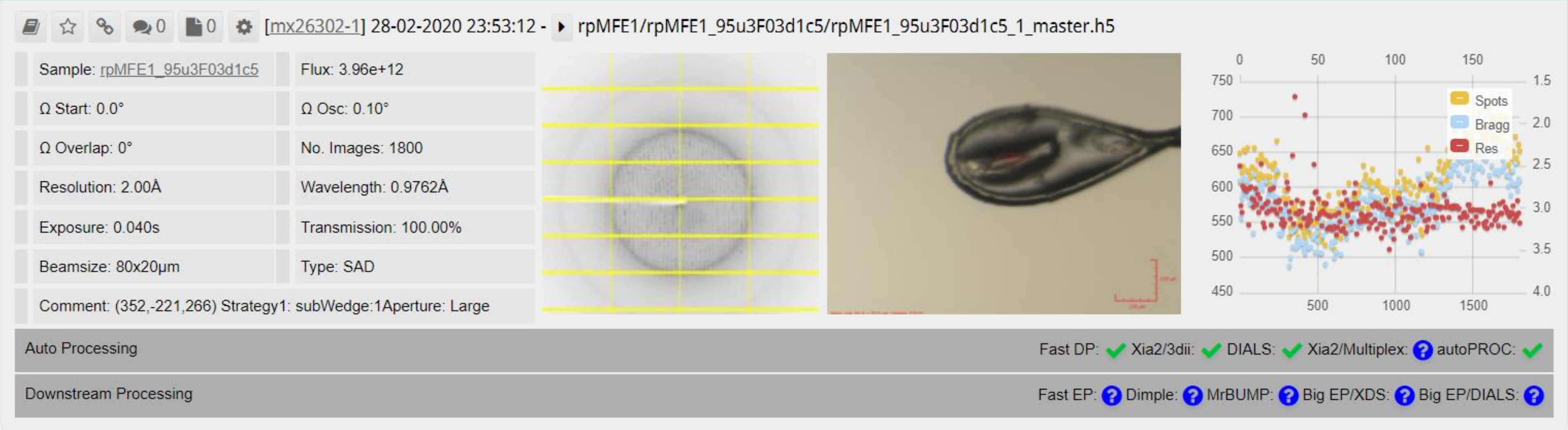
Proposal: mx26302, session: mx26302-1

View shipment at Diamond Light Source

View crystal at Diamond Light Source

Plate	95u3
Well and drop	F03.1, drop 5
Condition	100mM MES, pH 6; 15.14%w/v Polyethylene glycol 4000; 150.91mM Ammonium sulfate

On this page
-we can easily find the crystallization conditions
-we can easily find the diffraction information



[mx26302-1] 28-02-2020 23:53:12 - rpMFE1/rpMFE1_95u3F03d1c5/rpMFE1_95u3F03d1c5_1_master.h5

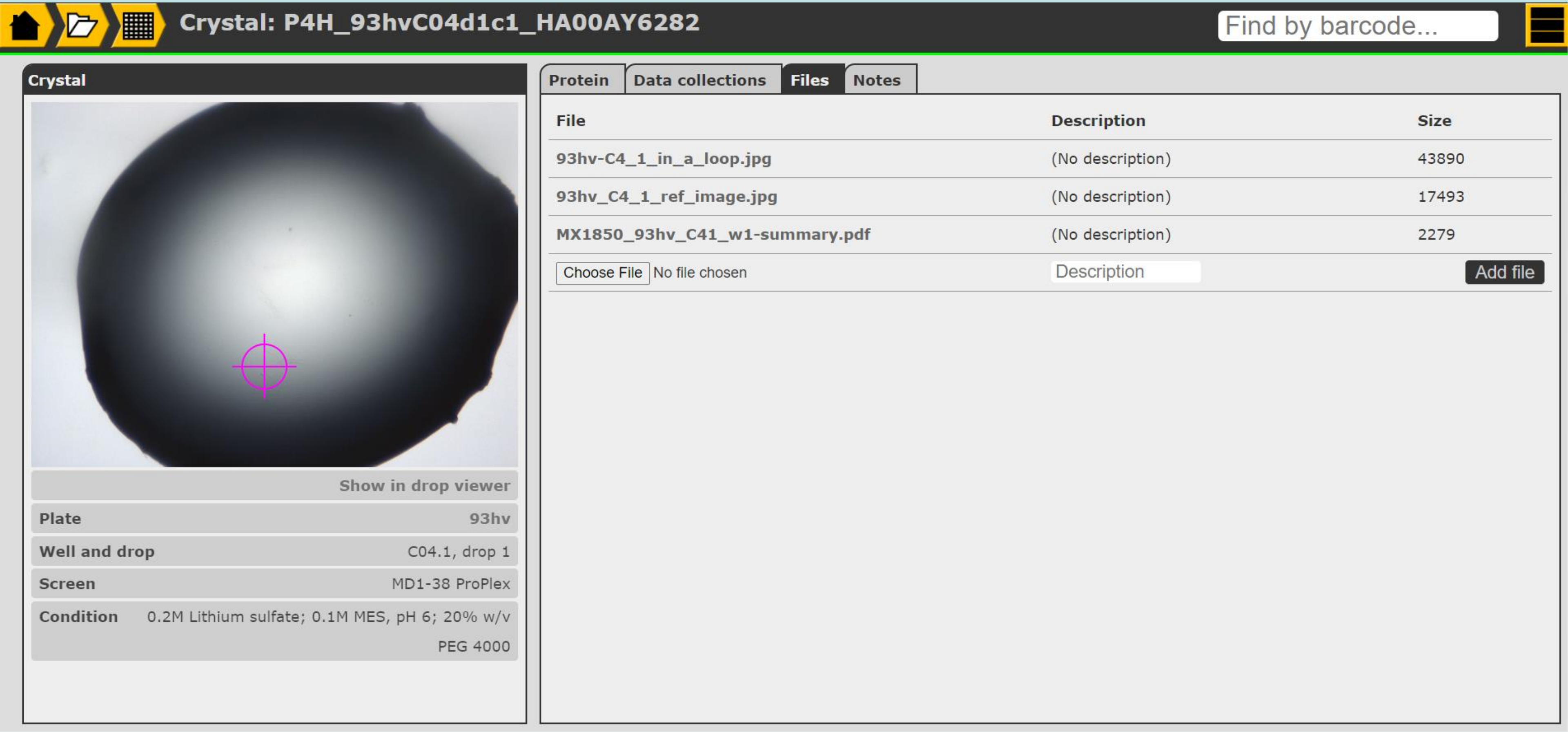
Sample: rpMFE1_95u3F03d1c5	Flux: 3.96e+12
Ω Start: 0.0°	Ω Osc: 0.10°
Ω Overlap: 0°	No. Images: 1800
Resolution: 2.00Å	Wavelength: 0.9762Å
Exposure: 0.040s	Transmission: 100.00%
Beamsize: 80x20μm	Type: SAD

Comment: (352,-221,266) Strategy1: subWedge:1Aperture: Large

Auto Processing — Fast DP: ✓ Xia2/3dii: ✓ DIALS: ✓ Xia2/Multiplex: ? autoPROC: ✓

Downstream Processing — Fast EP: ? Dimple: ? MrBUMP: ? Big EP/XDS: ? Big EP/DIALS: ?

When the Diamond-link is activated we reach the correct ISPyB-page:
-refinements of structures are very often done later, but with this functionality we can easily check resolution, radiation damage, anisotropy, cell dimensions, spacegroup etc



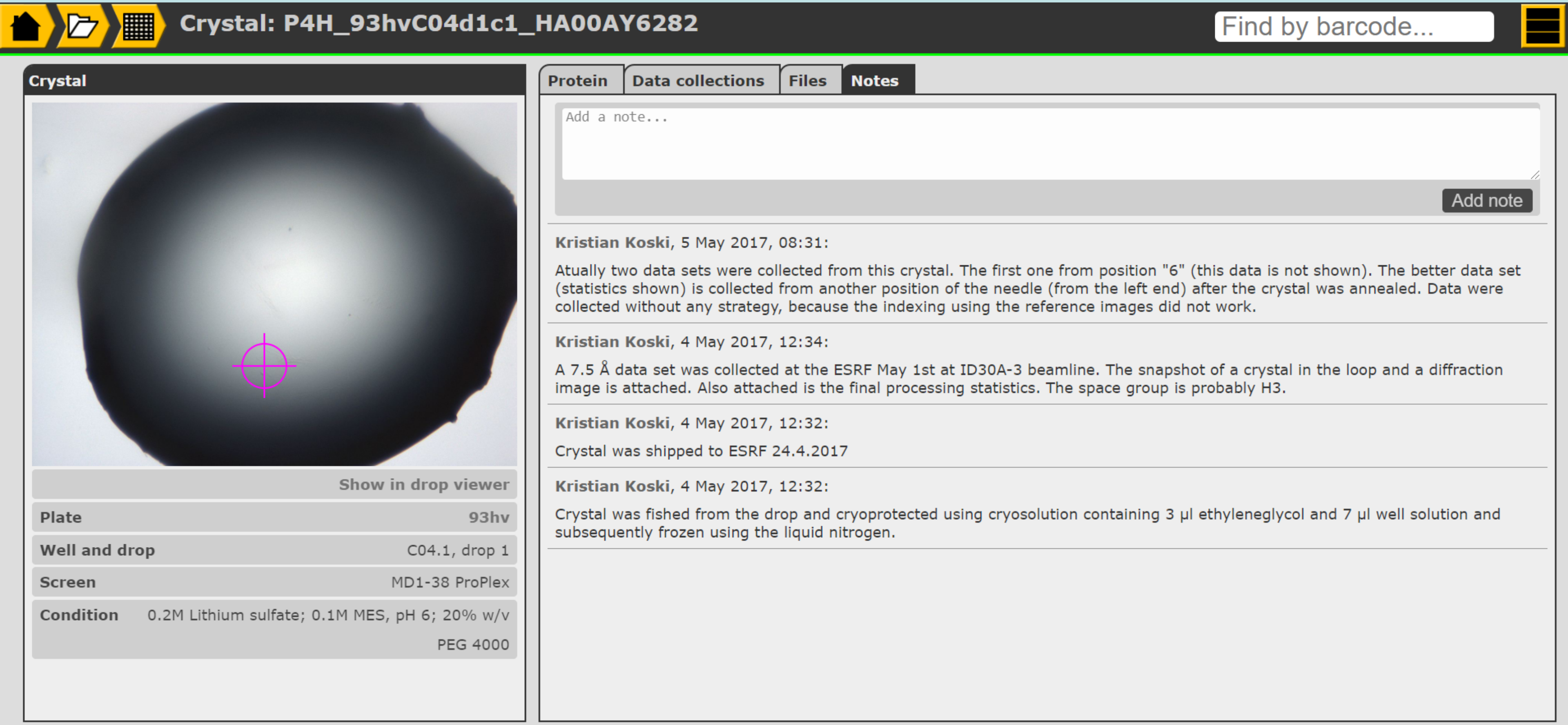
Crystal: P4H_93hvC04d1c1_HA00AY6282

Crystal

Plate	93hv
Well and drop	C04.1, drop 1
Screen	MD1-38 ProPlex
Condition	0.2M Lithium sulfate; 0.1M MES, pH 6; 20% w/v PEG 4000

File	Description	Size
93hv-C4_1_in_a_loop.jpg	(No description)	43890
93hv_C4_1_ref_image.jpg	(No description)	17493
MX1850_93hv_C41_w1-summary.pdf	(No description)	2279

Each project member (with write access) can make notes, which then can be seen by all project members. User management is very flexible.



Crystal: P4H_93hvC04d1c1_HA00AY6282

Plate	93hv
Well and drop	C04.1, drop 1
Screen	MD1-38 ProPlex
Condition	0.2M Lithium sulfate; 0.1M MES, pH 6; 20% w/v PEG 4000

Kristian Koski, 5 May 2017, 08:31:

Atually two data sets were collected from this crystal. The first one from position "6" (this data is not shown). The better data set (statistics shown) is collected from another position of the needle (from the left end) after the crystal was annealed. Data were collected without any strategy, because the indexing using the reference images did not work.

Kristian Koski, 4 May 2017, 12:34:

A 7.5 Å data set was collected at the ESRF May 1st at ID30A-3 beamline. The snapshot of a crystal in the loop and a diffraction image is attached. Also attached is the final processing statistics. The space group is probably H3.

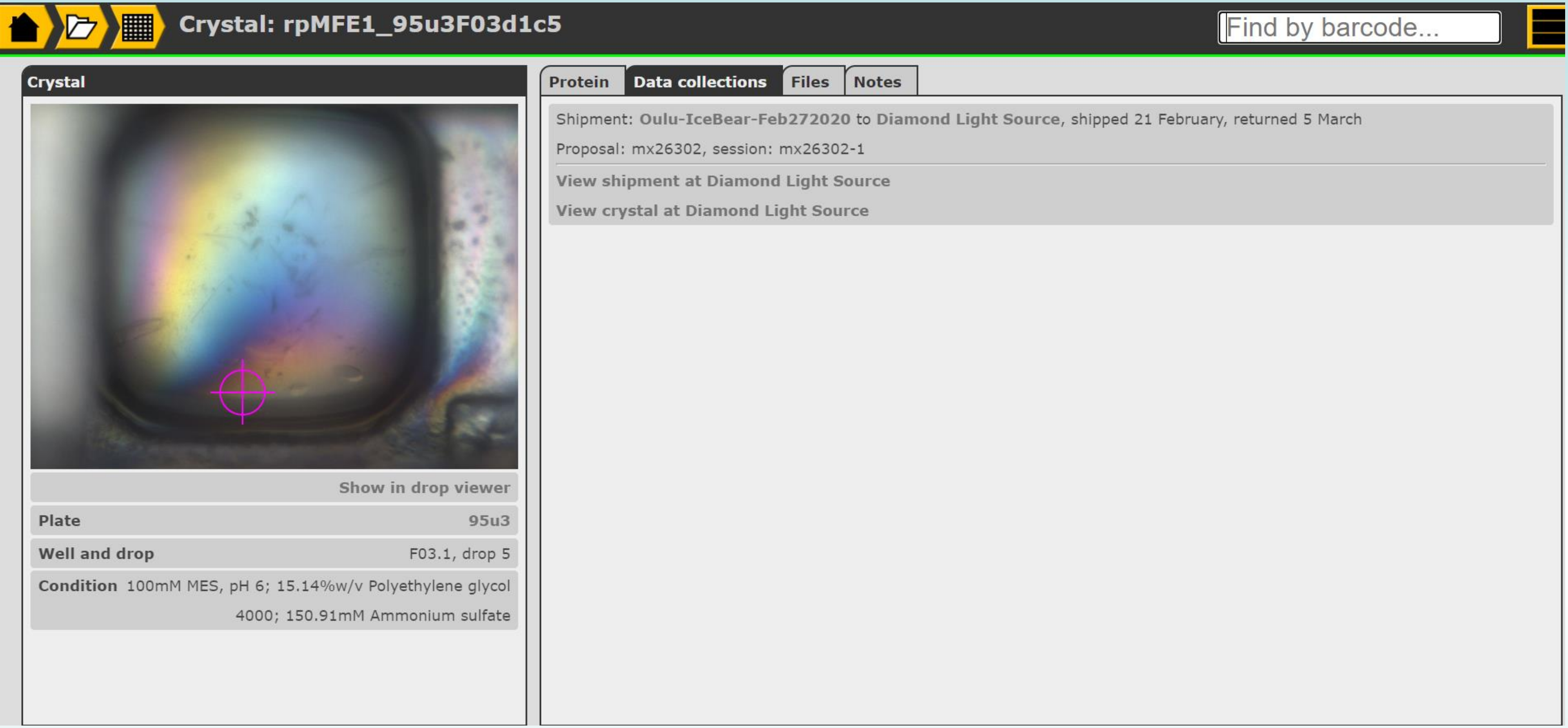
Kristian Koski, 4 May 2017, 12:32:

Crystal was shipped to ESRF 24.4.2017

Kristian Koski, 4 May 2017, 12:32:

Crystal was fished from the drop and cryoprotected using cryosolution containing 3 µl ethyleneglycol and 7 µl well solution and subsequently frozen using the liquid nitrogen.

Each project member (with write access) can make notes, which then can be seen by all project members



Crystal: rpMFE1_95u3F03d1c5

Crystal

Plate 95u3

Well and drop F03.1, drop 5

Condition 100mM MES, pH 6; 15.14%w/v Polyethylene glycol 4000; 150.91mM Ammonium sulfate

Shipment: **Oulu-IceBear-Feb272020** to **Diamond Light Source**, shipped 21 February, returned 5 March

Proposal: mx26302, session: mx26302-1

View shipment at Diamond Light Source

View crystal at Diamond Light Source

IceBear is under continuous development, being tested at Weizmann and DLS https://icebear.oulu.fi/help/

https://icebear.oulu.fi/ (demo/demo 9098)

Contact: Ed Daniel, Lari Lehtiö, Rik Wierenga

Acknowledgements

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

Kristian Koski, Mirko Maksimainen, Lari Lehtiö (Oulu)
Protein crystallography community in Oulu (Oulu)
FINStruct community in Finland (Finland)

Instruct-ULTRA (EU)
Diamond (UK)

instruct ULTRA

instruct ERIC
BF Biocenter Finland
FINStruct
ACADEMY OF FINLAND
diamond
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