

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

ISPyB-developers meeting

Berlin, October 2019

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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:

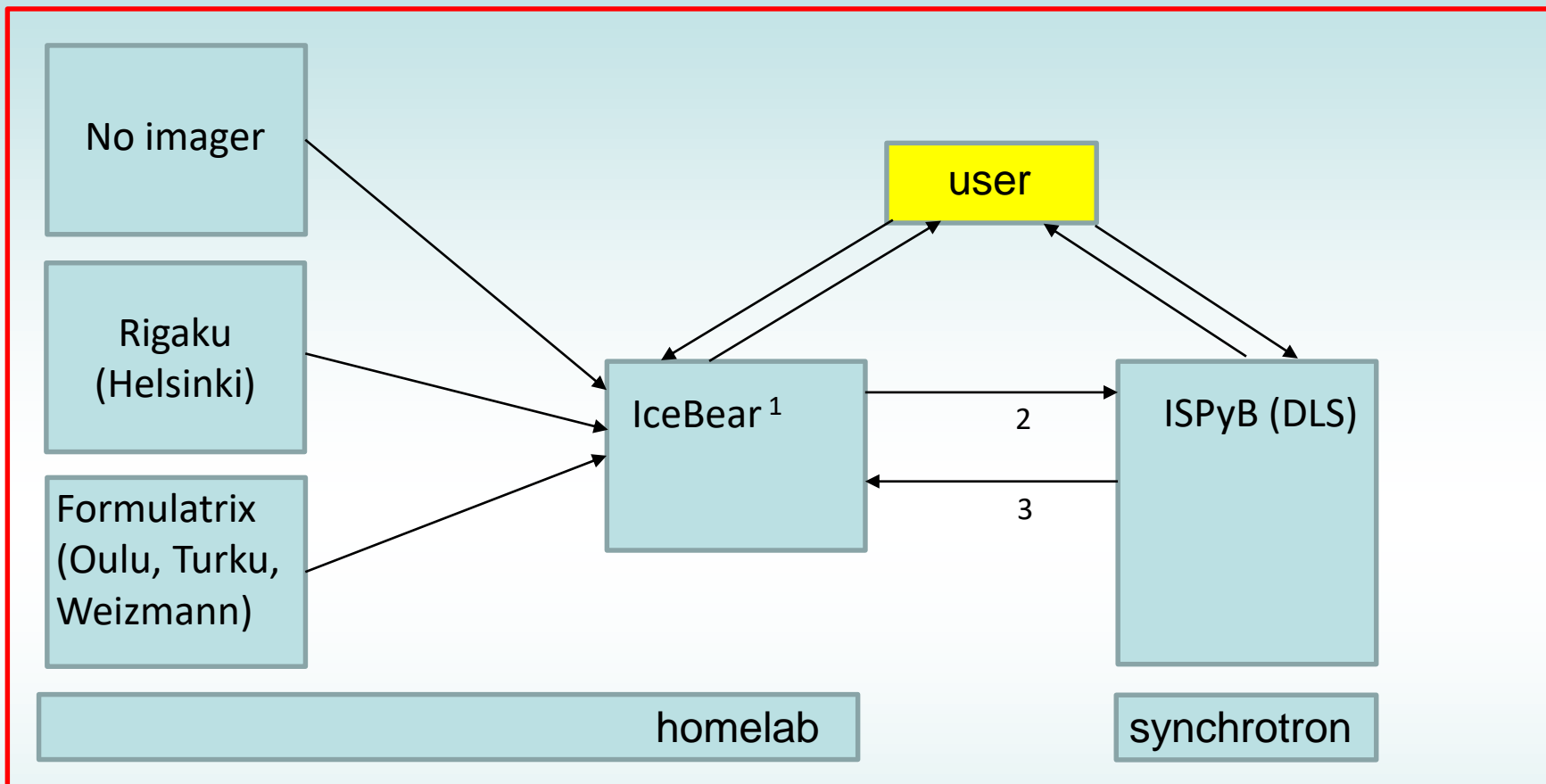
Integrated **C**ystal-data-tracking **E**nhancing **B**iochemistry **E**ducation **A**nd **R**esearch

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.



Icebear version 1.1.0
Distributed under the MIT Licence



- 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
	<i>Icebear</i> 	<i>Diamond Light Source</i> 
2	HA00AS6876	rpMFE1_95brC02d2c2
	<i>Icebear</i> 	<i>Diamond Light Source</i> 
	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:



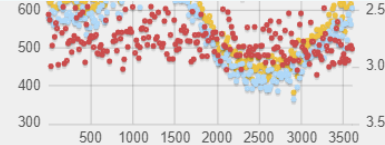
Proposal numbers, session numbers, beamline, data collection dates can be recorded. Any PDB-ident can be connected to where and when the data set was collected. Better use of the processing and structure determination pipelines.

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 downloaded 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**).

Resolution: 2.00Å	Wavelength: 0.9763Å			
Exposure: 0.004s	Transmission: 100.00%			
Beamsize: 80x20µm	Type: SAD			
Comment: (384,657,208) Strategy1: subWedge:1Aperture: Large				

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

Type	Resolution	Spacegroup	Mn$I/\sigma(I)$	Rmeas Inner	Rmeas Outer	Completeness	Cell	Status
xia2 dials	65.30 - 2.17	P 1 21 1	8.6	0.036	1.321	99.1	65.30 224.76 126.24 90.00 90.07 90.00	processing successful
xia2 3dii	56.23 - 2.21	P 21 21 21	15.0	0.028	1.729	100.0	65.32 126.32 224.92 90.00 90.00 90.00	processing successful
autoPROC	112.51 - 2.17	P 21 21 21	14.0	0.029	2.224	99.9	65.34 126.35 225.02 90.00 90.00 90.00	processing successful
fast_dp	29.13 - 2.33	P 2 2 2	19.5	0.022	0.858	99.2	65.31 126.30 224.90 90.00 90.00 90.00	processing successful
autoPROC+STARANISO	112.51 - 2.08	P 21 21 21	15.4	0.029	1.249	95.6	65.34 126.35 225.02 90.00 90.00 90.00	processing successful

[xia2 dials](#) [xia2 3dii](#) [autoPROC](#) [fast_dp](#) [autoPROC+STARANISO](#)

Beam Centre	X	Y
Start	156.38	168.98
Refined	156.42	168.95
Δ	-0.04	0.03

[Plots](#) [Archive](#) [Logs & Files](#) [Q Lookup Cell](#)

Space Group	A	B	C	α	β	γ
P 1 21 1	65.30	224.76	126.24	90.00	90.07	90.00

Shell	Observations	Unique	Resolution	Rmeas	$I/\sigma(I)$	CC Half	Completeness	Multiplicity	Anom Completeness	Anom Multiplicity	CC Anom
outerShell	31550	8917	2.17 - 2.21	1.321	1.0	0.3	93.6	3.5	88.8	1.8	-0.0
innerShell	33366	9702	5.88 - 65.33	0.036	23.9	1.0	100.0	3.4	93.9	1.8	-0.5
overall	661228	190033	2.17 - 65.30	0.070	8.6	1.0	99.1	3.5	93.5	1.8	-0.4

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

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


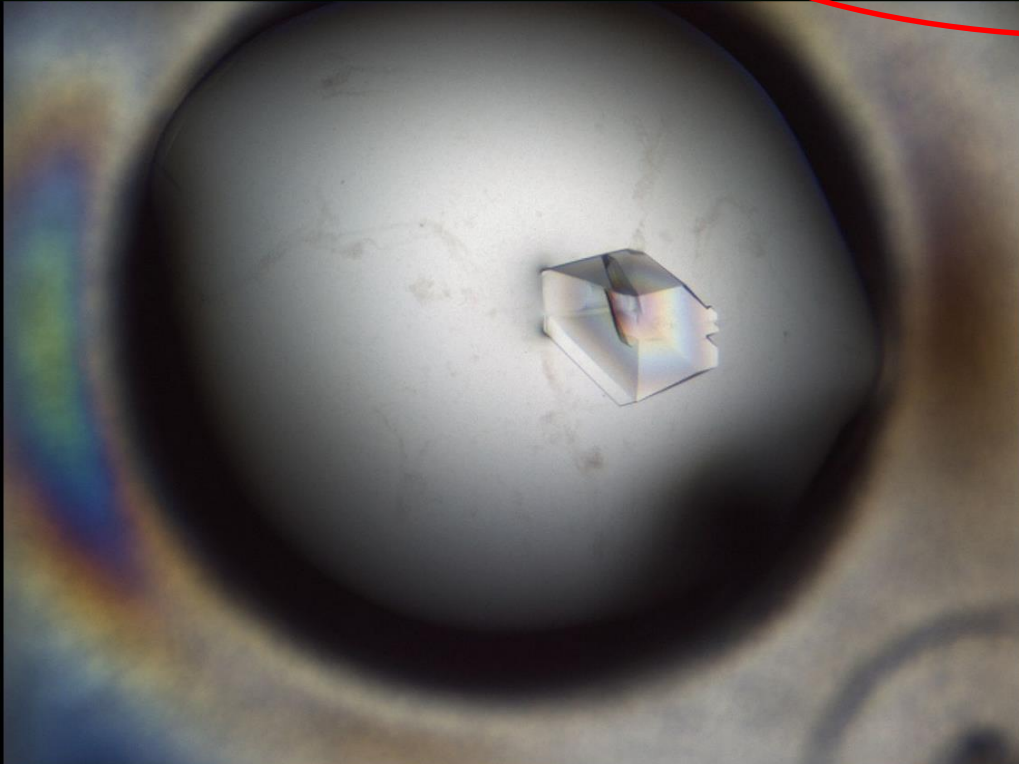
Well solution
1.75M (NH4)2HPO4
Screen: Factorial1

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

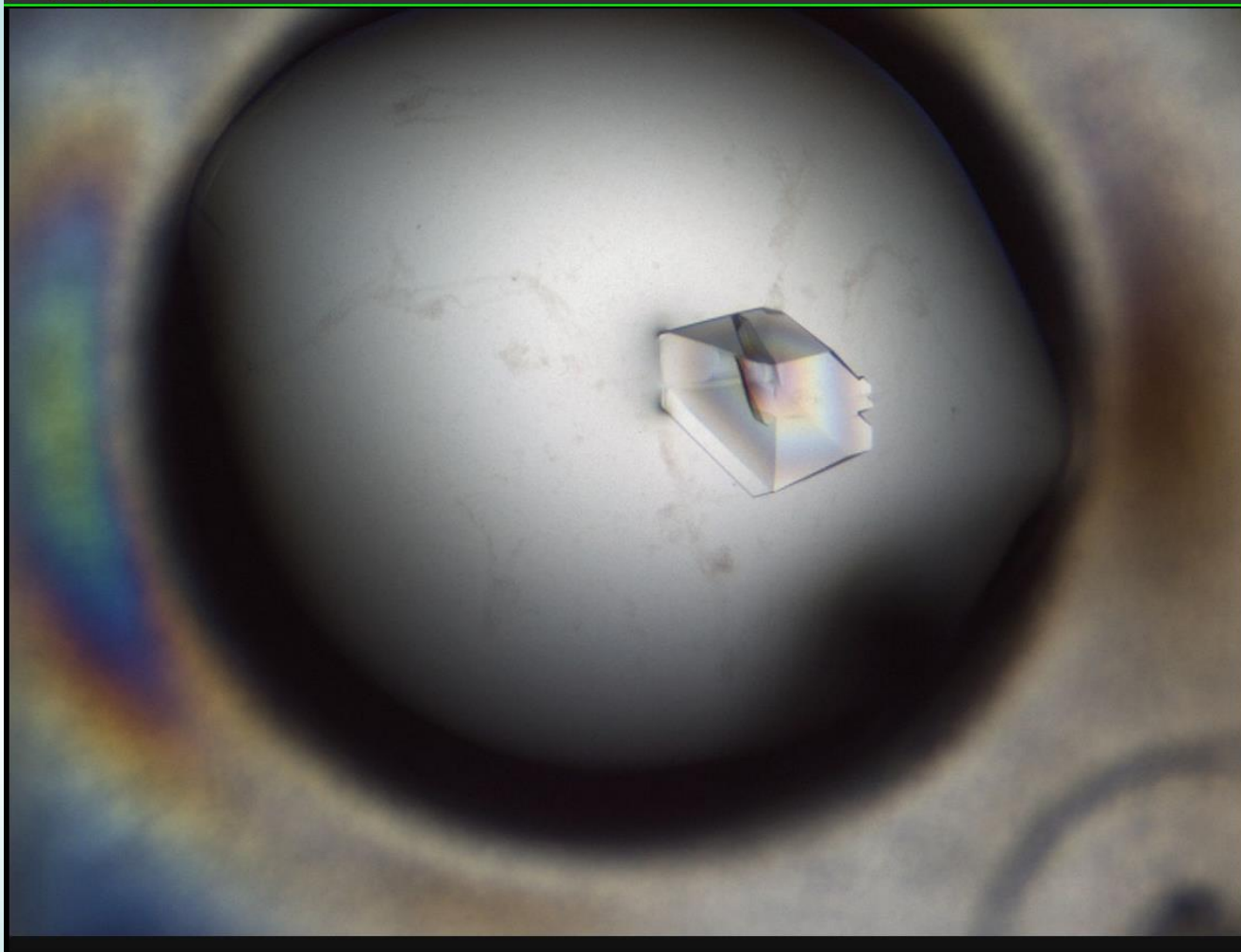
Incubation
Imager: +20 R154
Temperature: 20°C





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



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.

(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



Freezing crystals:


barcode reader is used to identify pins, pucks and dewars

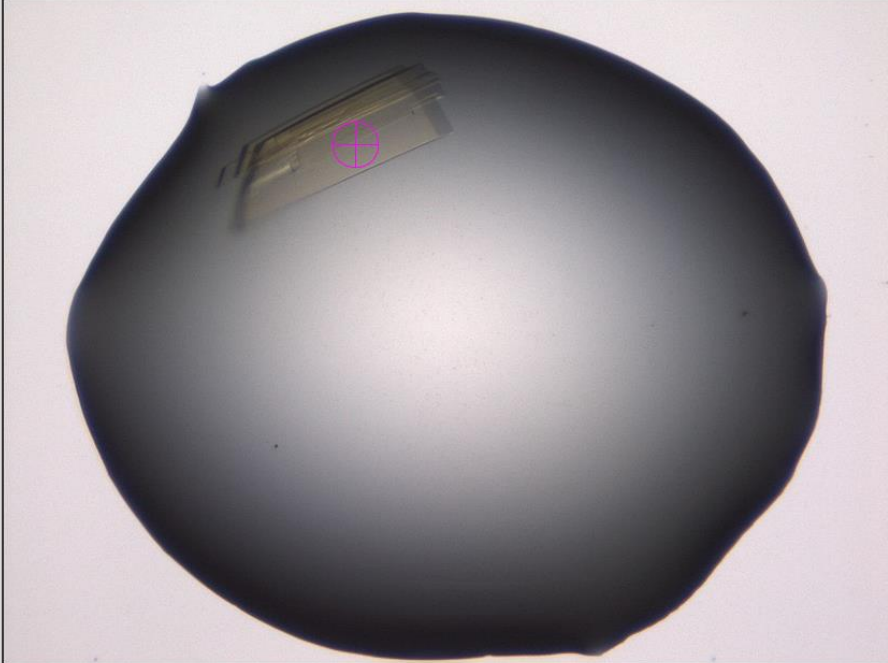
touch screen (or mouse) is used to record that a crystal has been attached to a pin

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

-  HA00AF9854
-  HA00A06620
-  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

Shipment details	
Name	Shipment for test <small>The name of the shipment</small>
Destination	Diamond Synchweb Live <small>Where the shipment is sent</small>
Shipper	System Administrator <small>The local person responsible for the shipment</small>
Date shipped	Today

Your shipment at Diamond Synchweb Live

[Open shipment in new tab](#)

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

Proposals	No Proposal ▾	Feedback	Help
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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?](#)

Diamond Light Source ©2013-2019



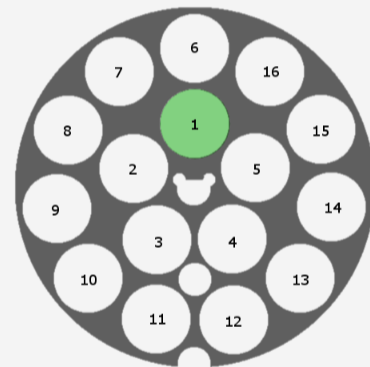
Proposals	mx4025 ▾	Projects	Unit Cell Search	Feedback	Help
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Please note that all dewars must now be registered before creating a shipment. Please see the updated help pages for details of the new process. ✕

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	<table border="1"> <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>	Date	Status	Location	Beamline	No history found			
Date	Status	Location	Beamline						
No history found									



Location	Protein Acronym	Name	Spacegroup	Barcode	Comment	Anomalous	Abundance	Components	Required Res	Unit Cell	Status												
1	LMTIM	LMTIM_9098B02d1c1	C222	OUL99XX9999	Shoot this one first					<table border="1"> <thead> <tr> <th>A</th> <th>B</th> <th>C</th> <th>α</th> <th>β</th> <th>γ</th> </tr> </thead> <tbody> <tr> <td>100</td> <td>100</td> <td>100</td> <td>90</td> <td>90</td> <td>90</td> </tr> </tbody> </table>	A	B	C	α	β	γ	100	100	100	90	90	90	
A	B	C	α	β	γ																		
100	100	100	90	90	90																		
2																							
3																							
4																							
5																							
6																							



Icebear crystal shipment manifest

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Diamond Light Source:

<https://ispyb.diamond.ac.uk/shipments/sid/31948>







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To: Diamond Light Source

Shipped: 2019-10-04

Dewar DLS-MX-0643, puck CPS-4618

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	<i>Icebear</i> 	<i>Diamond Light Source</i> 
2	HA00AS6876	rpMFE1_95brC02d2c2
	<i>Icebear</i> 	<i>Diamond Light Source</i> 
	HA00AR7699	rpMFE1_95brC02d1c1

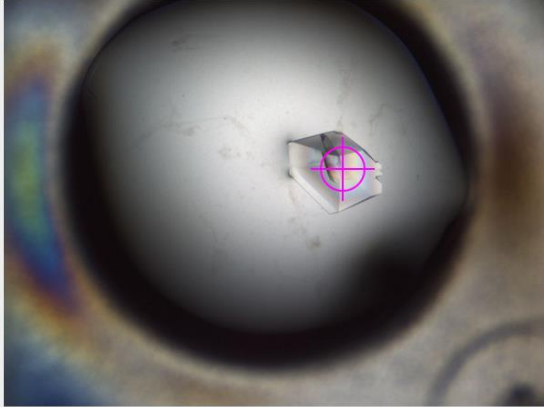
File Edit View History Bookmarks Tools Help

Crystal: rpMFEI_95bC02d2c2 Crystal: LMTIM_9098A01d1c1

icebear@id/crystal/29069800#

Crystal: LMTIM_9098A01d1c1 Find by barcode...

Crystal



Show in drop viewer

Plate 9098

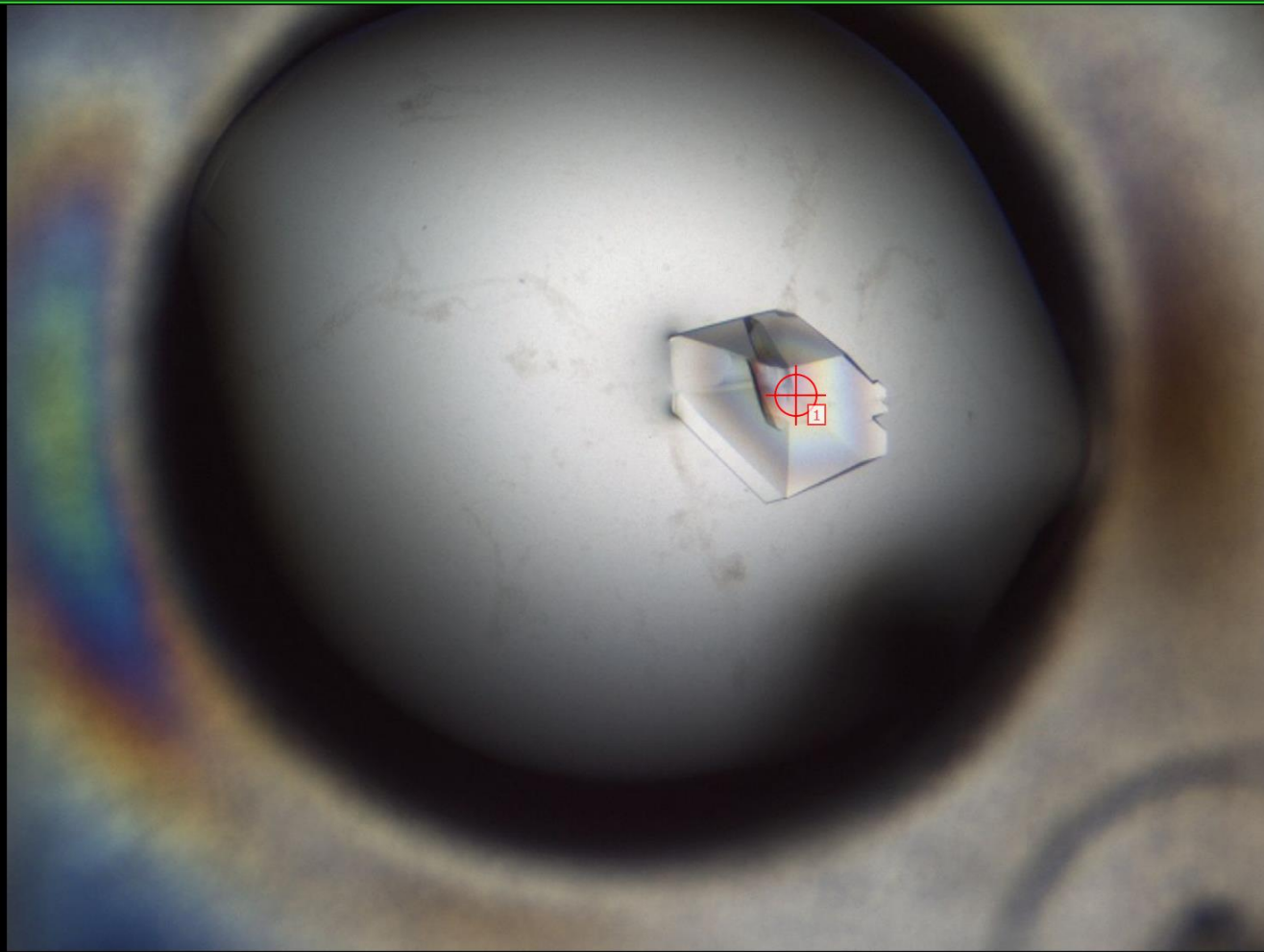
Protein Data collections Files Notes

Shipment: Shipment for test to Diamond Synchweb Live, shipped 12 May, returned 13 May

[View shipment at Diamond Synchweb Live](#)

[View crystal at Diamond Synchweb Live](#)

The crystal page



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
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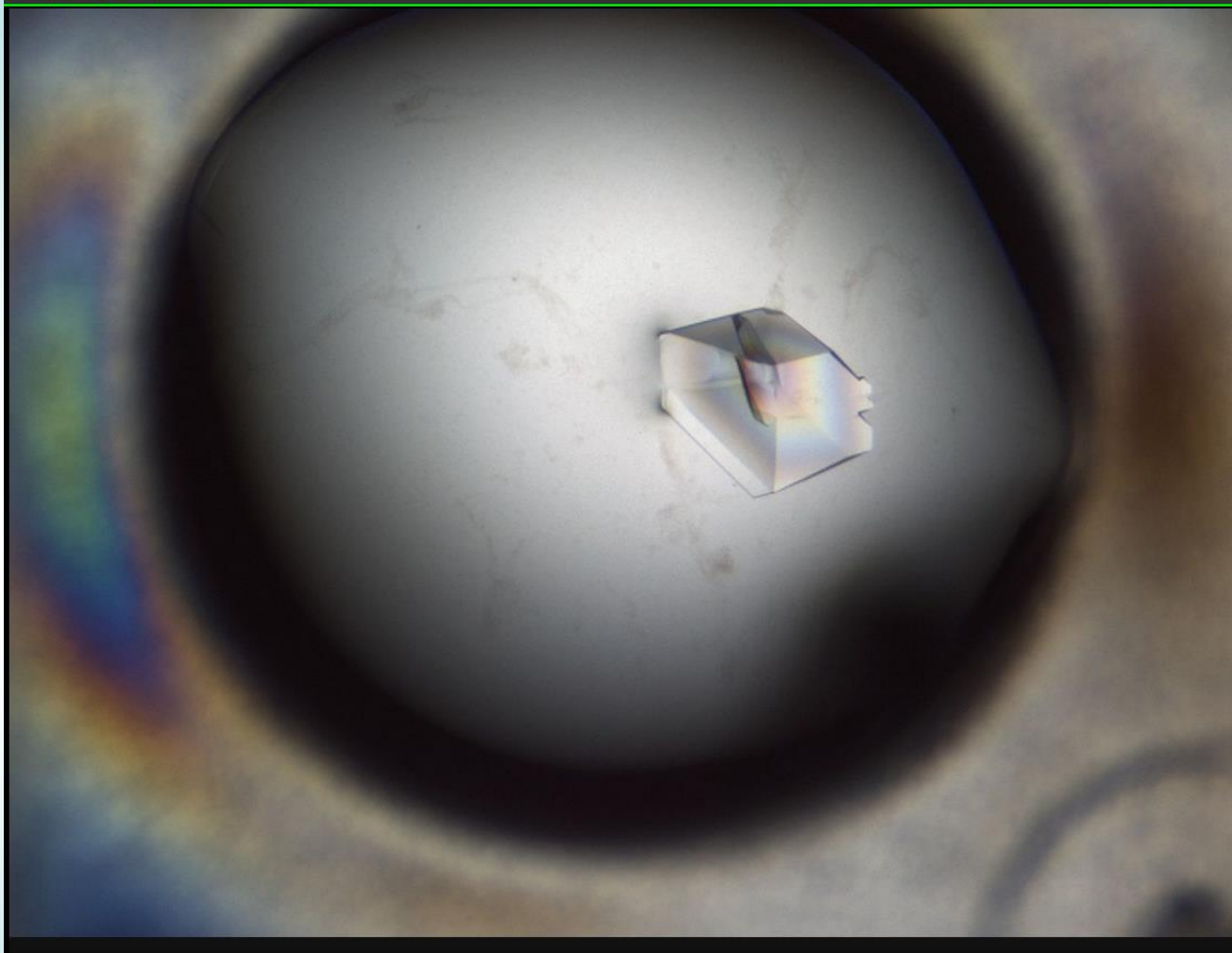
Minimum resolution (Å) 1.5

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LmTIM
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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



IceBear WWW-based viewer of the crystallization results



⊖ Dewar DEWAR1: 1 puck is still in this dewar.

⊖ Puck PUCK1: Crystals to keep, in puck: 2 Pins to wash: 5

Remove puck from dewar

Pos	Pin	Crystal	Protein	Action on return
1	PIN1	w_4000B01d1c1	LMTIM	Wash pin Remove and <input type="button" value="Keep crystal"/> <input type="button" value="Wash pin"/>
2	PIN2	w_4000B01d1c2	LMTIM	Keep crystal Remove and <input type="button" value="Keep crystal"/> <input type="button" value="Wash pin"/>
3	PIN3	w_4000B01d1c3	LMTIM	Wash pin Remove and <input type="button" value="Keep crystal"/> <input type="button" value="Wash pin"/>
4	PIN4	w_4000B01d1c4	LMTIM	Keep crystal Remove and <input type="button" value="Keep crystal"/> <input type="button" value="Wash pin"/>
5	(no barcode)	w_4000B01d1c5	LMTIM	Wash pin Non-barcoded pin. <input type="button" value="Remove and wash"/>
6	(no barcode)	w_4000B01d1c6	LMTIM	Wash pin Non-barcoded pin. <input type="button" value="Remove and wash"/>
7	(no barcode)	w_4000B01d1c7	LMTIM	Wash pin Non-barcoded pin. <input type="button" value="Remove and wash"/>
8	(no barcode)	w_4000B01d1c8	LMTIM	Wash pin Pin removed and washed.
9				
10				
11				
12				
13				
14				
15				
16				

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)

