

MXCuBE/ISPyB meeting

ISPyB in ICAT - MX UI

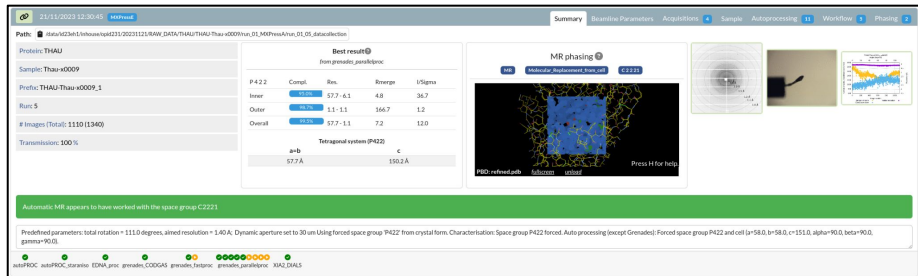
30/11/23

Maël Gaonach

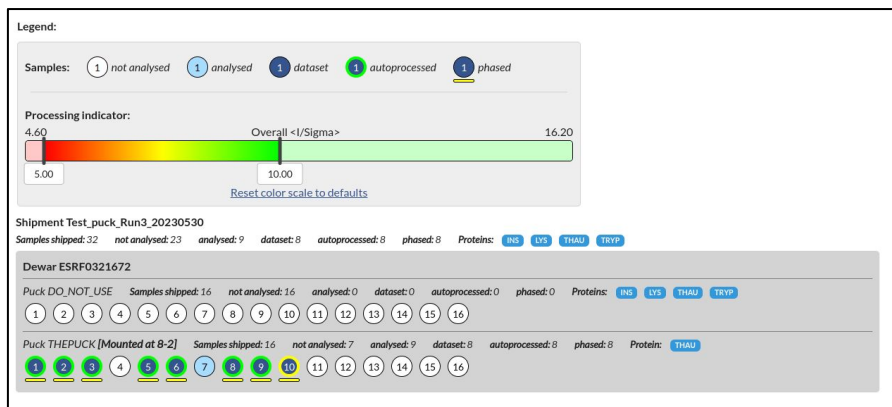
Software Engineer
Data Automation Unit
Software Group ESRF

Current state

Growing amount of essential features for SB



Specialized data visualisation



Data quality assessment

Editing container from: Test_puck_Run3_20230530 (Test_puck)

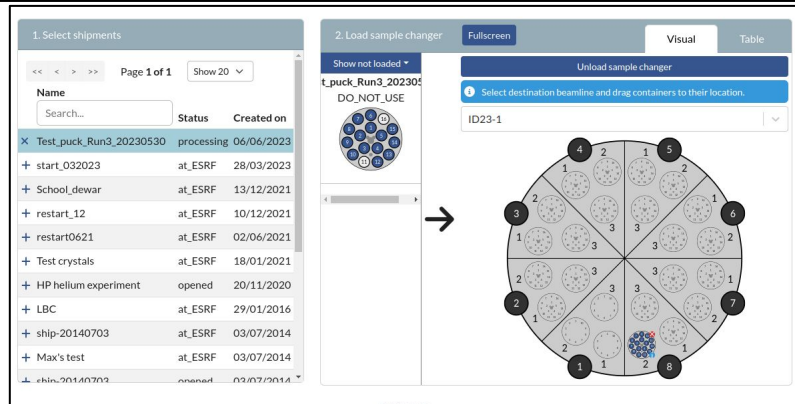
Name: THEPUCK Type: Unipuck Beamline: ID23-1 #Sample Changer: 23 Status: processing

Sample name field is mandatory and no special characters are allowed Protein + sample name should be unique for the whole proposal

#	Protein Acronym	Sample Name	Pin BarCode	Crystal Form	Exp. Type	Aimed resolution	Required resolution	Beam Diameter	Number of positions	Aimed multiplicity	Aimed Completeness	Forced Space G	Radiation Sensitivity	Smiles	Tot. Rot. Angle	Min Osc. Angle	Observed resolution	Comments	Ligands
1	THAU	Thauv0001		P422 - (58, 58, 151-90, 90, 90)	MXPressF	1.4									333				
2	THAU	Thauv0002		P422 - (58, 58, 151-90, 90, 90)	MXPressO	1.4									222				
3	THAU	Thauv0003		P422 - (58, 58, 151-90, 90, 90)	MXPressE	1.4									111				
4	THAU	Thauv0004		P422 - (58, 58, 151-90, 90, 90)	MXPressE	1.4									333				
5	THAU	Thauv0005		P422 - (58, 58, 151-90, 90, 90)	MXPressO	1.4									222				
6	THAU	Thauv0006		P422 - (58, 58, 151-90, 90, 90)	MXPressE	1.4									111				
7	THAU	Thauv0007		P422 - (58, 58, 151-90, 90, 90)	MXPressF	1.4									333				
8	THAU	Thauv0008		P422 - (58, 58, 151-90, 90, 90)	MXPressO	1.4									222				
9	THAU	Thauv0009		P422 - (58, 58, 151-90, 90, 90)	MXPressE	1.4									111				
10	THAU	Thauv0010		P422 - (58, 58, 151-90, 90, 90)	MXPressF	1.4									333				
11	THAU	Thauv0011		P422 - (58, 58, 151-90, 90, 90)	MXPressE	1.4									222				
12	THAU	Thauv0012		P422 - (58, 58, 151-90, 90, 90)	MXPressO	1.4									111				
13	THAU	Thauv0013		P422 - (58, 58, 151-90, 90, 90)	MXPressF	1.4									333				
14	THAU	Thauv0014		P422 - (58, 58, 151-90, 90, 90)	MXPressO	1.4									222				
15	THAU	Thauv0015		P422 - (58, 58, 151-90, 90, 90)	MXPressE	1.4									111				
16	THAU	Thauv0016		P422 - (58, 58, 151-90, 90, 90)	MXPressF	1.4									333				

✓ Data is synchronized with server.

Save Reset



Experiment preparation

The ESRF Data Portal

Data Portal My Data Open Data Closed Data Feedback Log out Anonymous

Open Data / 1003-5-0000 1023-1 11/11/2023-11/11/2023 Data collected for the ISPyB Collaboration

Dataset List 43 Logbook

For users that want to download large volume of experimental data (>2GB), ESRF users can access the Globus service, please read the documentation for proceeding: <https://confluence.esrf.fr/display/SCKB/Globus>

Filter by samples + X

Search

	Date	Sample	Dataset	Definition	Files	Size	Processed	Download
	11:00 14 Nov 2023	Sample-4-1-07	run_03_datacollection		22	2.3 GB	✓	Download
	10:58 14 Nov 2023	Sample-4-1-07	run_02_characterisation		20	585.0 MB	✓	Download

Summary Crystallography Instrument Files 20 Metadata List

Name	Resolution	Wavelength	Exposure Time	Flux start	Flux end	Transmission	X Beam	Y Beam
run_02_characterisation [2023-11-14 10:58:26]	1.3000423961627905 Å	0.8856033875217176 Å	0.01 s	4.543246778242394e+12	4.543246778242394e+12	100.0 %	154.4628559375 mm	166.17452587499997 mm

Start 10:58:26 AM

Sample Sample-4-1-07

Images 4

Prefix ref-opid231_1_04d.h5

diffraction_thumbnail_ref-opid231_1_0001 [2023-11-14 10:58:09] Processed

diffraction_thumbnail_ref-opid231_1_0002 [2023-11-14 10:58:16] Processed

diffraction_thumbnail_ref-opid231_1_0003 [2023-11-14 10:58:23] Processed

diffraction_thumbnail_ref-opid231_1_0004 [2023-11-14 10:58:33] Processed

characterisation [2023-11-14 10:58:57] Processed

dozor_plot [2023-11-14 10:59:09] Processed

/data/d223eh1/inhouse/opid231/20231114/RAW_DATA/Sample-4-1-07/run_02_characterisation Download

	Date	Sample	Dataset	Files	Size	Processed	Download
	10:56 14 Nov 2023	Sample-4-1-07	run_01_02_line	11	894.4 MB	✓	Download
	10:56 14 Nov 2023	Sample-4-1-07	run_01_01_mesh	14	1.9 GB	✓	Download

+ Tons of essential features for the whole facility (including SB!)

- Data policy implementation
- Data download
- Electronic logbook
- DOI minting
- Sample tracking
- Reprocessing

- Limited data visualization : list of parameters, images...

- Needs to support wide variety of techniques

The ESRF Data Portal

The screenshot shows the ESRF Data Portal interface. At the top, there's a navigation bar with 'Data Portal', 'My Data', 'Open Data', and 'Closed Data'. Below this, a 'Dataset List' section shows a table of datasets. A green box highlights a specific dataset, 'run_02_characterisation', and its details are shown in a sidebar. The details include parameters like Resolution, Wavelength, Exposure Time, Flux start, Flux end, X Beam, Y Beam, and Prefix. Below the details, there's a list of files, with a green box highlighting the first five files, which are thumbnails of diffraction patterns. A green arrow points from the highlighted files to a text box on the right. At the bottom, there's another table showing a list of datasets, with a green box highlighting the first two rows.

Date	Sample	Dataset	Definition	Files	Size	Processed	Download
11:00 14 Nov 2023	Sample-4-1-07	run_03_datacollection		22	2.3 GB	✓	Download
10:58 14 Nov 2023	Sample-4-1-07	run_02_characterisation		20	585.0 MB	✓	Download

Name	Resolution	Wavelength	Exposure Time	Flux start	Flux end	X Beam	Y Beam
run_02_characterisation [2023-11-14 10:58:26]	1.3000423961627905 Å	0.8856033875217176 Å	0.01 s	4.543246778242394e+12	4.543246778242394e+12	154.4628559375 mm	166.17452587499997 mm

File	Status
diffraction_thumbnail_ref-opid231_1_0001[2023-11-14 10:58:09]	Processed
diffraction_thumbnail_ref-opid231_1_0002[2023-11-14 10:58:16]	Processed
diffraction_thumbnail_ref-opid231_1_0003[2023-11-14 10:58:23]	Processed
diffraction_thumbnail_ref-opid231_1_0004[2023-11-14 10:58:33]	Processed
characterisation[2023-11-14 10:58:57]	Processed
dozor_plot[2023-11-14 10:59:09]	Processed

Date	Sample	Dataset	Files	Size	Processed	Download
10:56 14 Nov 2023	Sample-4-1-07	run_01_02_line	11	894.4 MB	✓	Download
10:56 14 Nov 2023	Sample-4-1-07	run_01_01_mesh	14	1.9 GB	✓	Download

+ Tons of essential features for the whole facility (including SB!)

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- Sample tracking
- Reprocessing

- Limited data visualization : list of parameters, images...

- Needs to support wide variety of techniques

But all the data we need is already there!

**Could we federate these
features?**

How to manage the diversity?

ISPyB focuses on SB and is already too complex. It would be impossible to manage an all-techniques monolith...

We need to split up things:

Generic features

Logbook

Sample
tracking

Core features

- User management
- Proposal/session management
- General navigation
- Data fetching
- Generic visualization

Specialized features

MX
visualization

Cryo EM/ET
visualization

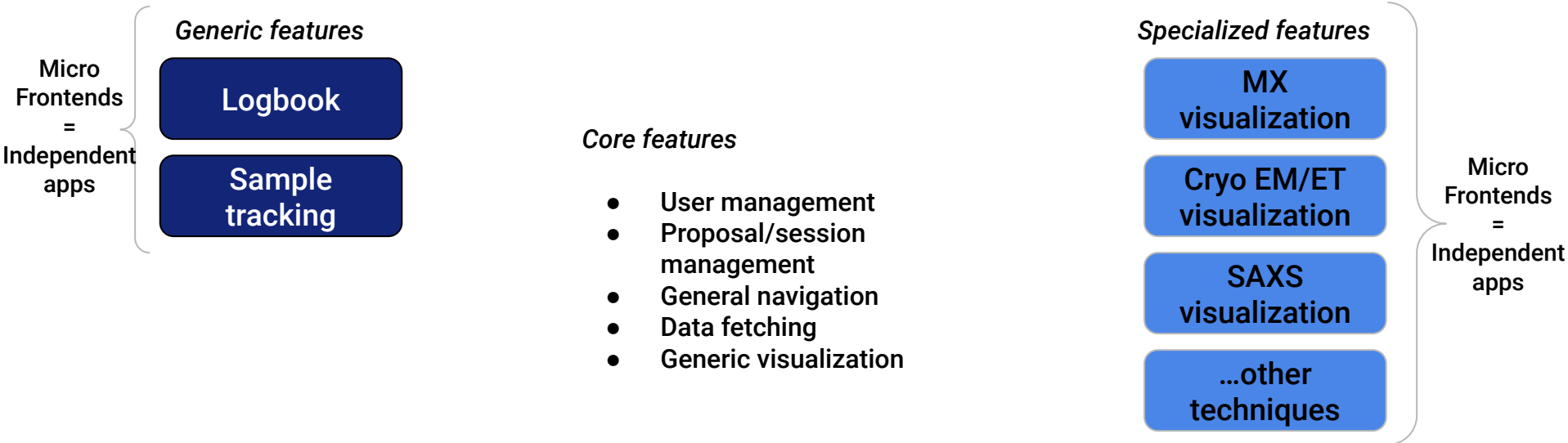
SAXS
visualization

...other
techniques

How to manage the diversity?

ISPyB focuses on SB and is already too complex. It would be impossible to manage an all-techniques monolith...

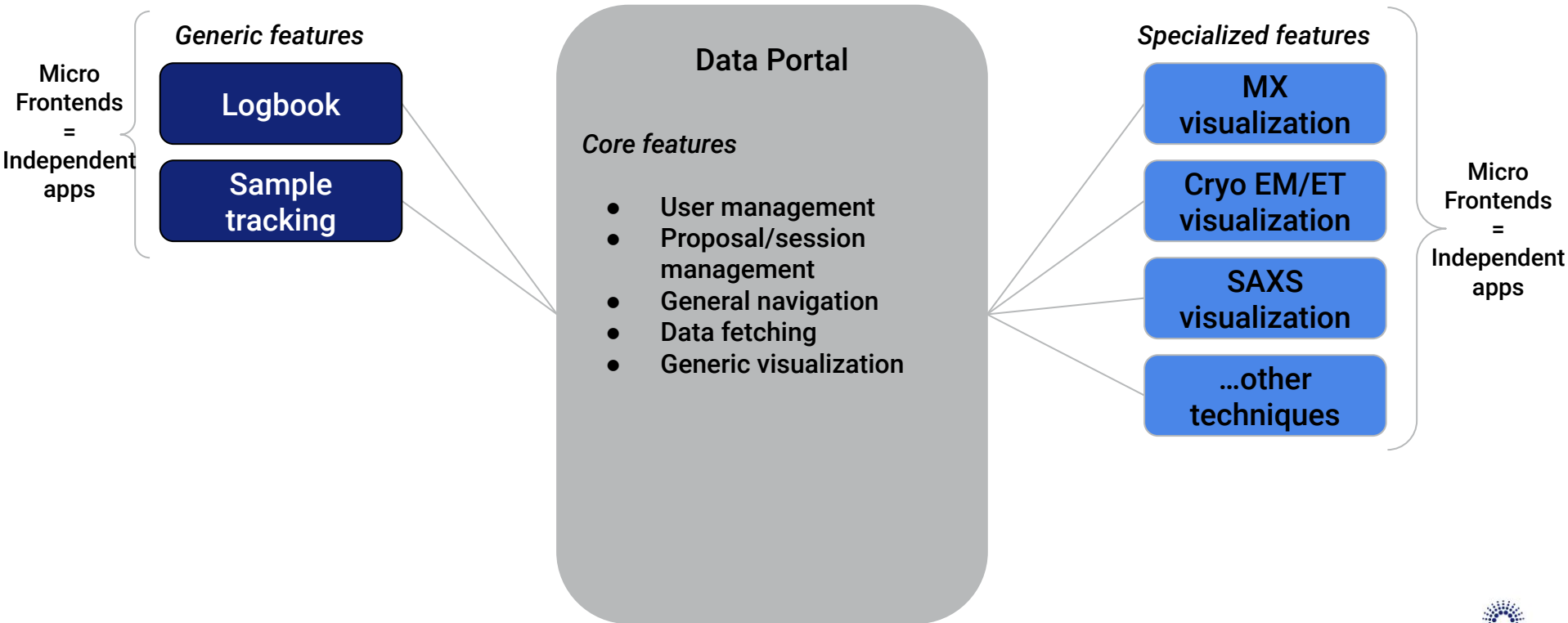
We need to split up things:



How to manage the diversity?

ISPyB focuses on SB and is already too complex. It would be impossible to manage an all-techniques monolith...

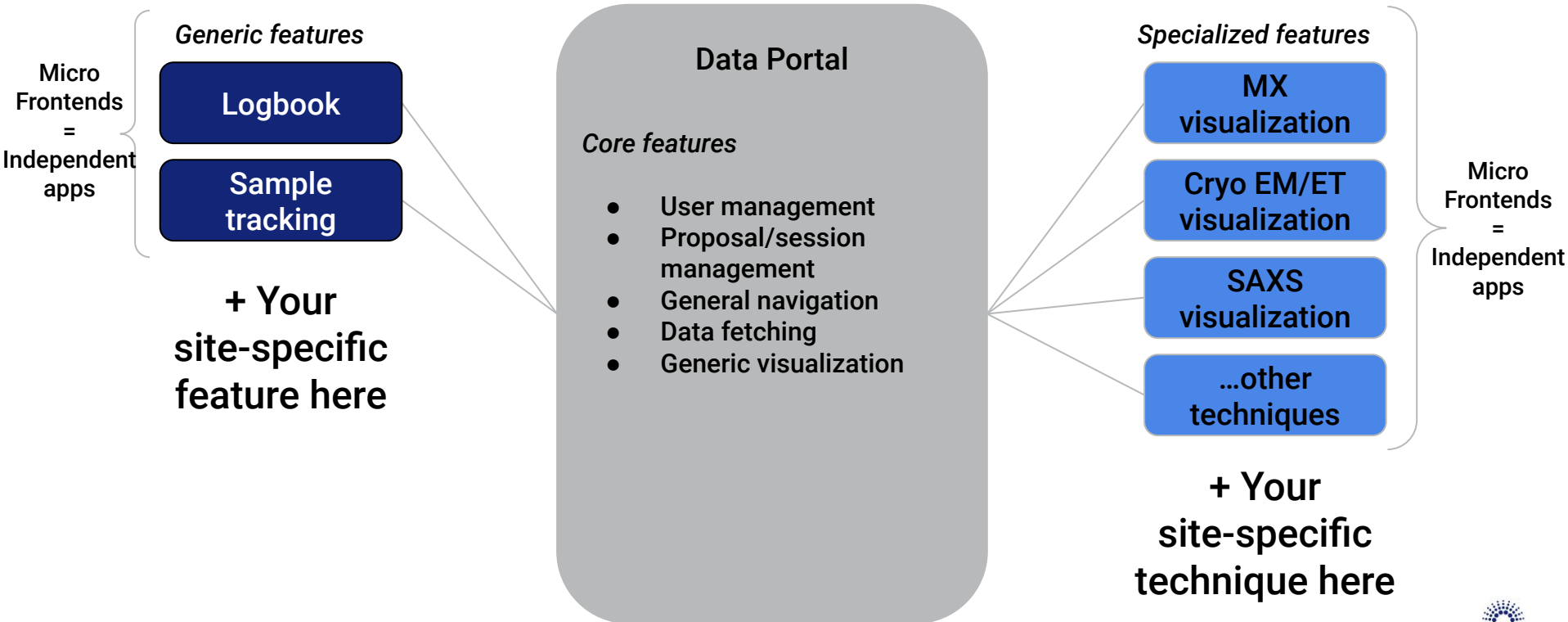
We need to split up things:



How to manage the diversity?

ISPyB focuses on SB and is already too complex. It would be impossible to manage an all-techniques monolith...

We need to split up things:



We can load the appropriate app depending on the session...

The screenshot shows the ESRF Data Portal interface. At the top, there's a navigation bar with links like Data, Logistics, Instruments, My selection, Datasets, Examples, My Jobs, and Admin. A search bar is on the right. Below the navigation bar, there's a sidebar on the left with filters for Data type (Investigations, Data collections, Documents), Search (name, title, abstract, DOI), Filter by (Public data, Embargoed data, My data), and Instrument. The main area displays a table of datasets with columns: Instrument, Start, Title, A-Form, Samples, Datasets, Files, Release, DOI, and Logbook. The table lists several datasets, including ID23-1, ES-1294, IH-ES-74, HC-4361, and HC-4062.

Portal

This includes all the portal features previously mentioned

CryoET

MX

This screenshot shows the dataset view for a CryoET session. The top navigation bar is the same as the previous screenshot. The sidebar on the left has links for Investigation, Experiment, Statistics, Datasets, Logbook, and Prepare. The main area displays a sample view for 'Insectcells-leica-g2-2, Position_1_test4'. It includes a 'Back to grid' button, a table of angles (total, step, range), and a 'Non-aligned micrographs movie' section with a video player showing a sequence of images. The video player has controls for speed (10 frames per second) and current angle (-70°).

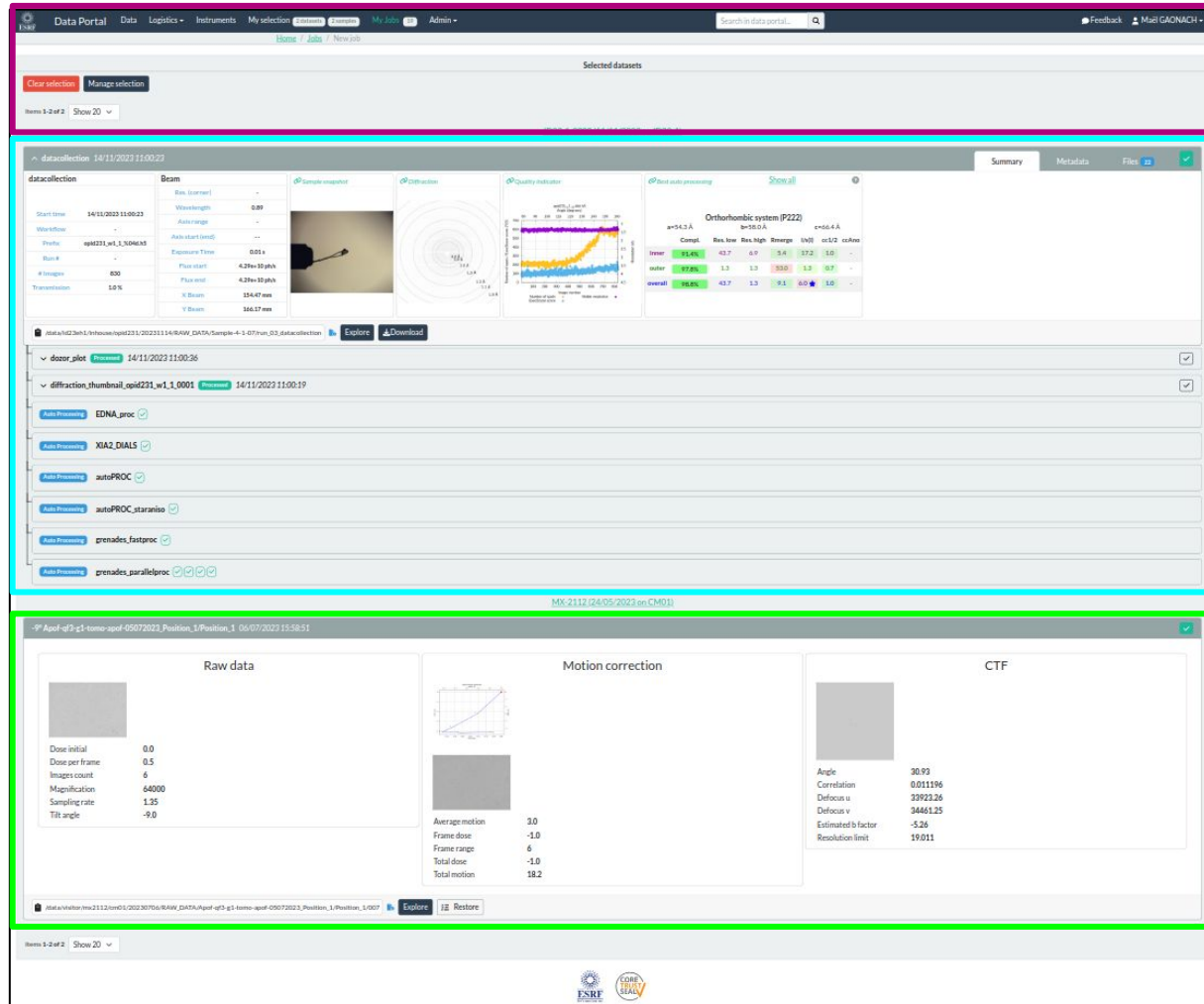
This screenshot shows the dataset view for an MX session. The top navigation bar is the same as the previous screenshot. The sidebar on the left has links for Investigation, Experiment, Statistics, Datasets, Logbook, and Prepare. The main area displays a sample view for 'Sample 4-1-07'. It includes a 'Back to grid' button, a table of angles (total, step, range), and a 'Non-aligned micrographs movie' section with a video player showing a sequence of images. The video player has controls for speed (10 frames per second) and current angle (-70°).

... Or mix them together

portal

MX

CryoET



These could be the same sample/protein analysed with different techniques on the same page.

Or fallback to a default 'generic' viewer

ESRF Data Portal

Home / HG-94 ID21 26/07/2019 - 06/02/2017 / Datasets

Investigation

- Experiment
- Statistics
- Datasets 16**
- Logbook
- Prepare

Datasets

Filter by sample:

Type sample name

For users who want to download large volume of experimental data (>2GB), ESRF users can access the Globus service, please read the [documentation](#) for proceeding.

Items 1-1 of 1 Show 20

ultramarine

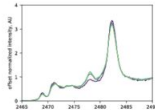
26/07/2019 15:38:43 dataset_RAD

Summary Files 2 Metadata

Sample ultramarine

Description

Technique XANES



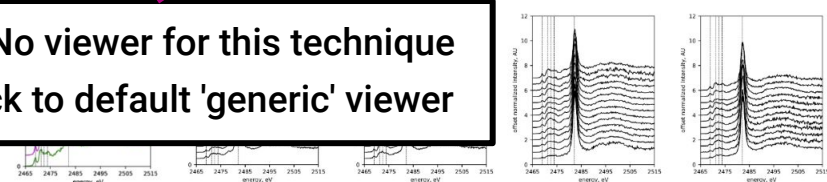
/data/id21/inhouse/ultramarine/HG94/ultramarine/dataset_RAD Explore Download

26/07/2019 15:38:22 dataset_33

Summary Files 23 Metadata

Created: Ultramarine

Processed: Ultramarine



/data/id21/inhouse/ultramarine/HG94/ultramarine/dataset_33 Explore Download

26/07/2019 15:38:07 dataset_32

Summary Files 2 Metadata

Sample ultramarine

portal

**XANES : No viewer for this technique
=> fallback to default 'generic' viewer**

ESRF

Implementation of the MX UI

<https://data2.esrf.fr/investigation/1405067863/datasets>

- New view of complex collections as a tree
- On-par with py-ISPb UI in terms of features
 - Except for phasing soon to come
- More freedom for the users to choose how and what they want to see
- Ongoing development - currently deployed on ID23-1 and MASSIF-1 for validation

Thank you!

(backup screenshots)

Investigation

Experiment

Statistics

Datasets 43

Logbook

Prepare

Datasets

View as:

List

Summary

Sample:

Type sample name

MX

Filter by type:

- ☐ Automesh
- ☐ Characterisation
- ☐ Datacollection
- ☐ Line
- ☐ Mesh

Ranking shell

Overall

Ranking parameter

I/s(I)

For users who want to download large volume of experimental data (>2GB), ESRF users can access the Globus service, please read the [documentation](#) for proceeding.

Items 1-7 of 7

Show 20

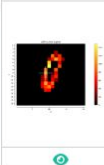
Sample-4-1-07

14/11/2023 10:56:10 X-ray centering on id23eh1 > Characterisation > Datacollection

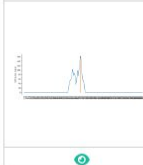
Sample snapshot



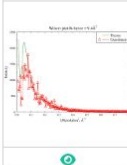
Mesh



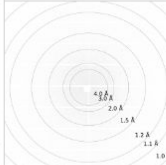
Line



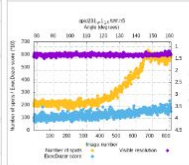
Characterisation



Diffraction



Quality indicator



Best auto processing

Show all

Orthorhombic system (P222)

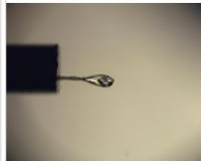
a=54.3 Å b=58.0 Å c=66.4 Å

	Compl.	Res. low	Res. high	Rmerge	I/s(I)	cc1/2	ccAno
inner	91.4%	43.7	6.9	5.4	17.2	1.0	-
outer	97.8%	1.3	1.3	53.0	1.3	0.7	-
overall	98.8%	43.7	1.3	9.1	6.0	1.0	-

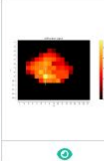
Sample-4-1-01

14/11/2023 10:46:19 X-ray centering on id23eh1 > Characterisation > Datacollection

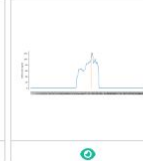
Sample snapshot



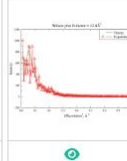
Mesh



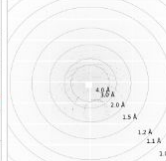
Line



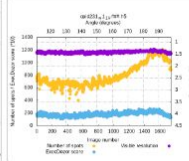
Characterisation



Diffraction



Quality indicator



Best auto processing

Show all

Tetragonal system (P422)

a=b=78.9 Å c=37.2 Å

	Compl.	Res. low	Res. high	Rmerge	I/s(I)	cc1/2	ccAno
inner	90.6%	78.9	6.8	5.8	25.7	1.0	-
outer	87.9%	1.3	1.2	97.3	1.3	0.4	-
overall	96.8%	78.9	1.2	7.5	10.1	1.0	-

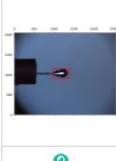
PRP4K-IAB161_x8

02/11/2023 18:32:58 MXPressA: X-centre, eDNA + dc on id30a1

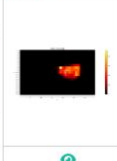
Sample snapshot



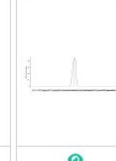
Automesh



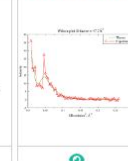
Mesh



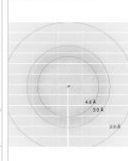
Line



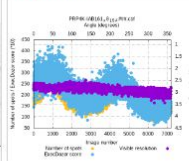
Characterisation



Diffraction



Quality indicator



Best auto processing

Show all

Monoclinic system (P2)

a=61.1 Å b=99.0 Å c=75.0 Å

 $\beta=110.9^\circ$

	Compl.	Res. low	Res. high	Rmerge	I/s(I)	cc1/2	ccAno
inner	99.3%	70.1	8.8	3.7	41.2	1.0	-
outer	98.5%	2.5	2.5	119.1	1.2	0.6	-
overall	99.5%	70.1	2.5	7.0	14.2	1.0	-

PRP4K-IAB161_x14

02/11/2023 19:15:24 MXPressA: X-centre, eDNA + dc on id30a1

Sample snapshot



Automesh



Mesh



Line



Characterisation



Line



Characterisation



Diffraction



Quality indicator



Best auto processing

Investigation

Experiment

Statistics

Datasets 43

Logbook

Prepare

Datasets

View as:

List

Summary

Sample:

Type sample name

MX

Filter by type:

- ☐ Automesh
- ☐ Characterisation
- ☐ Datacollection
- ☐ Line
- ☐ Mesh

Ranking shell :

Overall

Ranking parameter :

I/s(I)

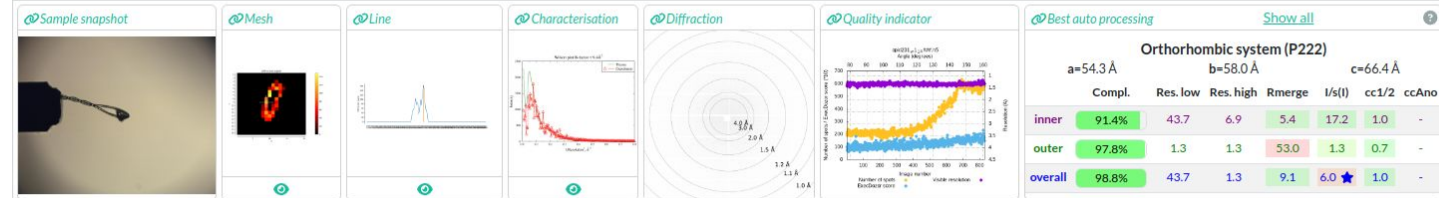
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Items 1-7 of 7

Show 20

Sample-4-1-07

14/11/2023 10:56:10 X-ray centering on id23eh1 > Characterisation > Datacollection



14/11/2023 11:00:23 Datacollection

14/11/2023 10:58:26 Characterisation

X-ray centering on id23eh1 2 actions

14/11/2023 10:56:47 Line

14/11/2023 10:56:10 Mesh

Summary

Metadata

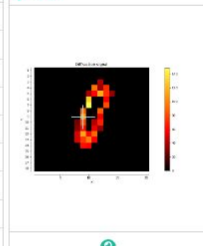
mesh

Beam

Mesh

Start time	14/11/2023 10:56:10
Workflow	XrayCentering
Prefix	mesh-opid231_1_1_%04d.h5
Run #	-
# Images	360
Transmission	52.8 %

Res. (corner)	-
Wavelength	0.89
Axis range	-
Axis start (end)	--
Exposure Time	0.019 s
Flux start	7.56e+11 ph/s
Flux end	7.56e+11 ph/s
X Beam	154.44 mm
Y Beam	166.21 mm



/data/id23eh1/inhouse/opid231/20231114/RAW_DATA/Sample-4-1-07/run_01_XrayCentering/run_01_01_mesh

Explore

Download

14/11/2023 10:56:16 Diffraction thumbnail Processed

14/11/2023 10:56:00 Diffraction thumbnail Processed

Investigation

Experiment

Statistics

Datasets 43

Logbook

Prepare

Datasets

View as:

List

Summary

Sample:

Type sample name

MX

Filter by type:

- ☐ Automesh
- ☐ Characterisation
- ☐ Datacollection
- ☐ Line
- ☐ Mesh

Ranking shell :

Overall

Ranking parameter :

I/s(I)

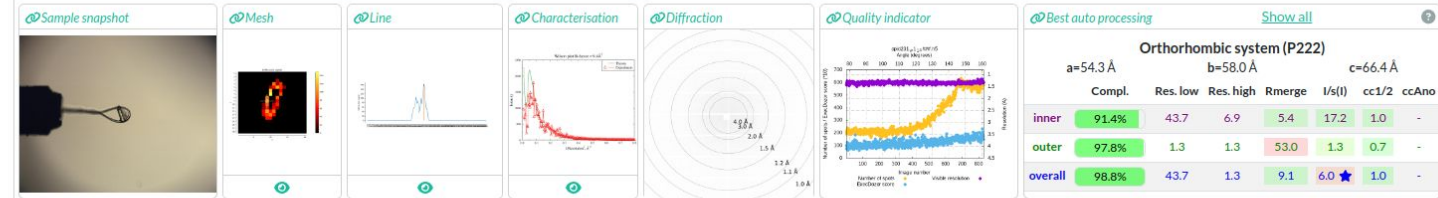
For users who want to download large volume of experimental data (>2GB), ESRF users can access the Globus service, please read the [documentation](#) for proceeding.

Items 1-7 of 7

Show 20

Sample-4-1-07







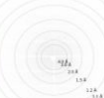

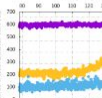


14/11/2023 10:56:10 X-ray centering on id23eh1 > Characterisation > Datacollection



14/11/2023 11:00:23 Datacollection

Summary

Metadata

	Beam	 Sample snapshot	 Diffraction	 Quality indicator	 All auto processing Show best										
	Res. (corner)	-			Program	a,b,c (Å)	α,β,γ (°)	Compl.	Res. low	Res. high	Rmerge	I/s(I)	cc1/2	ccAno	
23 11:00:23	Wavelength	0.89			 grenades_parallelproc	54.3	90.0	inner	91.4%	43.7	6.9	5.4	17.2	1.0	-
	Axis range	-				58.0	90.0	outer	97.8%	1.3	1.3	53.0	1.3	0.7	-
					P222	66.4	90.0	overall	98.8%	43.7	1.3	9.1	6.0	1.0	-
1_1%04d.h5	Axis start (end)	--			 grenades_parallelproc	54.3	90.0	inner	92.1%	43.7	6.9	5.5	17.2	1.0	-
	Exposure Time	0.01 s				58.0	90.0	outer	97.8%	1.3	1.3	53.1	1.3	0.7	-
					P212121	66.4	90.0	overall	98.9%	43.7	1.3	9.1	6.0	1.0	-
330	Flux start	4.29e+10 ph/s			 grenades_fastproc	54.3	90.0	inner	91.3%	43.7	6.5	5.5	17.0	1.0	-
	Flux end	4.29e+10 ph/s				58.0	90.0	outer	96.7%	1.2	1.2	62.8	1.1	0.6	-
					P222	66.4	90.0	overall	98.8%	43.7	1.2	9.7	5.4	1.0	-
0 %	X Beam	154.47 mm			 XIA2_DIALS	54.3	90.0	inner	95.4%	26.6	2.9	8.4	23.2	1.0	-
	Y Beam	166.17 mm				58.1	90.0	outer	85.6%	1.1	1.1	89.6	0.5	0.3	-
					P212121										

/data/id23eh1/inhouse/opid231/20231114/RAW_DATA/Sample-4-1-07/run_03_datacollection

Explore

Download

14/11/2023 11:00:36 Quality indicator

Processed

14/11/2023 11:00:19 Diffraction thumbnail

Processed

Auto Processing EDNA_proc

✓

Auto Processing XIA2_DIALS

✓

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Datasets

View as:

[List](#)[Summary](#)

MX

Ranking shell ⓘ:

Overall

Ranking parameter ⓘ:

I/s(I)

For users who want to download large volume of experimental data (>2GB), ESRF users can access the Globus service, please read the [documentation](#) for proceeding.

[Reset color scale to defaults](#)

Selected statistics: Overall I/s(I)



Legend:



not analysed



analysed



collected



autoprocessed

Samples:

FEM1B-FEM1B_GLYCEROL_3

Lysoz

PRP4K-IAB161_x14

PRP4K-IAB161_x8

Puck: puck_1

1

2

Puck: puck_2

1

ESRF

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Order

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Show 100

20/11/2023

12:34:46

Alejandro DE MARIA

Problem with crystal snapshots which are very dark

In order to save time, some collections performed in MASSIF-1 were done with frontlight only to save time.

PRP4K-IAB161_x8

MXPressA: X-centre, eED

Sample snapshot

For the demo purpose, it was agreed to replace by other snapshots. The samples affected (and their metadata) are:

Sample	ResourcesGallery	ResourcesGalleryFilePaths
PRP4K-IAB161_x8 id= 1388622710	6543df5ec6327c001b60f56a 6543df5edb4f3c0014e59d74 6543df5ed35cc30013d06f2a 6543df5ed4f15e0012ce2726 replaced by: 65534545750d1d0012b529c9 6553454573ff8d00139e3f9c 655345462ffe6b0012fa57ab 65534546373a190013907148	/data/id30a1/inhouse/opid30a1/20231102/RAW_DATA/PRP4K/PRP4K-IAB161_x8/run_01_MXPressA/run_01_05_datacollection/gallery/PRP4K-IAB161_x8_1_5_2.snapshot.jpeg,/data/id30a1/inhouse/opid30a1/20231102/RAW_DATA/PRP4K/PRP4K-IAB161_x8/run_01_MXPressA/run_01_05_datacollection/gallery/PRP4K-IAB161_x8_1_5_1.snapshot.jpeg,/data/id30a1/inhouse/opid30a1/20231102/RAW_DATA/PRP4K/PRP4K-IAB161_x8/run_01_MXPressA/run_01_05_datacollection/gallery/PRP4K-IAB161_x8_1_5_3.snapshot.jpeg,/data/id30a1/inhouse/opid30a1/20231102/RAW_DATA/PRP4K/PRP4K-IAB161_x8/run_01_MXPressA/run_01_05_datacollection/gallery/PRP4K-IAB161_x8_1_5_4.snapshot.jpeg
	6543e971d4f15e0012ce2a24 6542e971392b4d011996c7f2	

<<

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Parameter:

Volume

Accumulate:

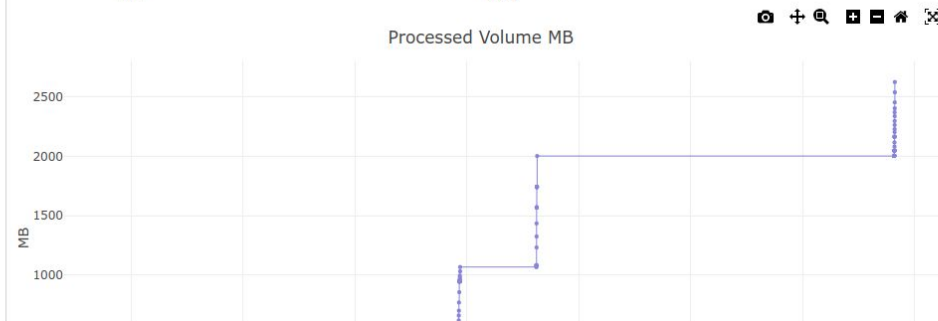
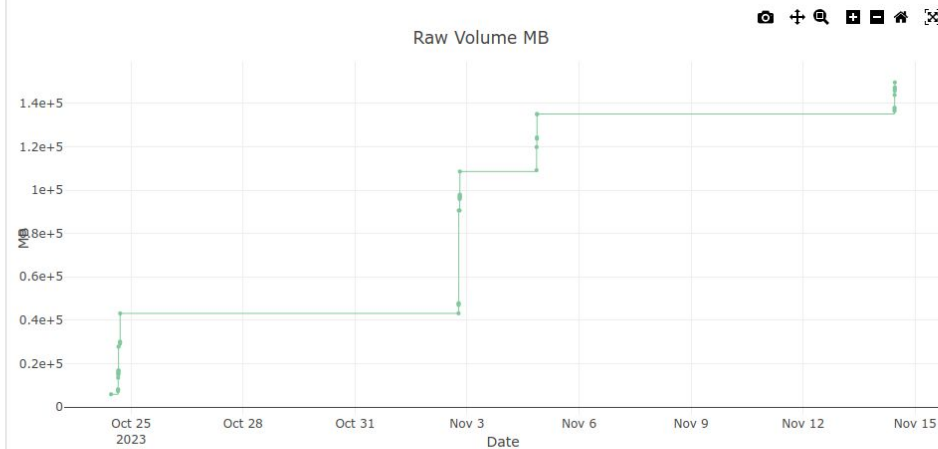


Data collected for the ISPyB Collaboration

Acquisition timeline



Session data statistics



Summary

Samples	7
Volume	148.78 GB
Datasets	173
Archived	ERROR

Datasets

Raw	43 (146.21 GB)
Processed	130 (2.57 GB)

«

Investigation

1 Experiment

Statistics

Datasets 43

Logbook

Prepare















Data collected for the ISPyB Collaboration

Proposal	Instrument	Start	End	Release date	DOI	Data Management Plan
ID23-1-0000	ID23-1	11/11/2023 05:54	11/11/2023 06:42	14/11/2023	DOI ESRF-DOI/ISPYB-12345567894	No DMP

Abstract

Proposal for software developments

Samples

Name	Description	Safety Mode	Datasets	Files	Edit
<div>Search...</div>					
FEM1B-FEM1B_GLYCEROL_1			13 12.8 GB 	1,985	 Edit
FEM1B-FEM1B_GLYCEROL_3			14 16.0 GB 	2,621	 Edit
Lysoz			46 45.8 GB 	7,497	 Edit
PRP4K-IAB161_x14			30 19.0 GB 	3,169	 Edit
PRP4K-IAB161_x8			22 50.2 GB 	8,126	 Edit
Sample-4-1-01			21 9.4 GB 	136	 Edit
Sample-4-1-07			27 6.5 GB 	177	 Edit

Items 1-7 of 7

Show 10 ▾

Selected datasets

Clear selection

Manage selection

Items 1-1 of 1 Show 20 ▾

[ID23-1-0000 \(11/11/2023 on ID23-1\)](#)

14/11/2023 11:00:23 Datacollection

Summary

Metadata

✓

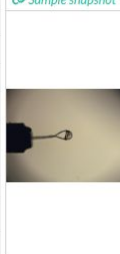
datacollection

Start time	14/11/2023 11:00:23
Workflow	-
Prefix	opid231_w1_1_004d.h5
Run #	-
# Images	830
Transmission	1.0%

Beam

Res. (corner)	-
Wavelength	0.89
Axis range	-
Axis start (end)	--
Exposure Time	0.01 s
Flux start	4.29e+10 ph/s
Flux end	4.29e+10 ph/s
X Beam	154.47 mm
Y Beam	166.17 mm

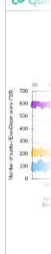
Sample snapshot



Diffraction



Quick



/data/id23eh1/inhouse/opid231/20231114/RAW_DATA/Sample-4-1-07/run_03_datacollection

Explore

Download

14/11/2023 11:00:36 Quality indicator Processed

✓

14/11/2023 11:00:19 Diffraction thumbnail Processed

✓

Auto Processing EDNA_proc ✓

Auto Processing XIA2_DIALS ✓

Auto Processing autoPROC ✓

Auto Processing autoPROC_stارانiso ✓

Auto Processing grenades_fastproc ✓

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Minting the DOI makes the datasets public immediately.

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Abstract*

Authors*

+ New author

Clear all authors

≡

Name*

Author1

Surname*

Author1

✗

≡

Name*

Author2

Surname*

Author2

✗

Mint DOI