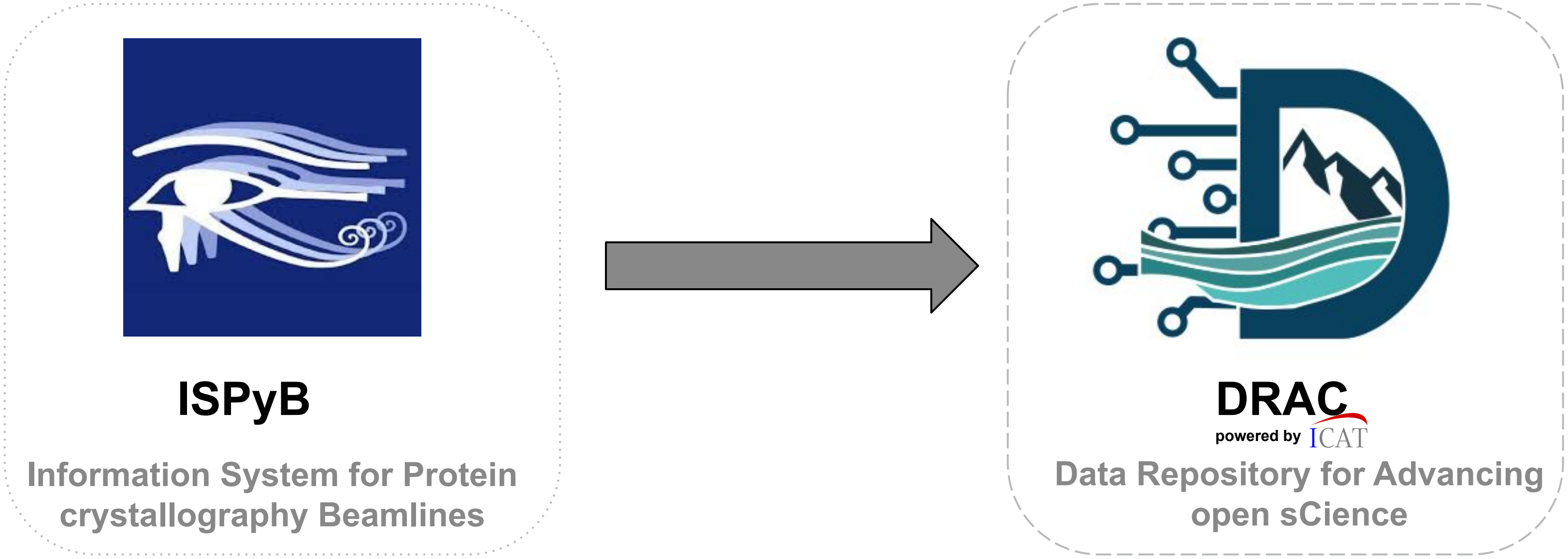
Transition from ISPyB to DRAC at ESRF (IV)

Alex DE MARIA
On behalf of
Software Group and Structural Biology group
DLS 17/11/2025

Goal



ISPyB

Information System for Protein crystallography Beamlines

DRAC

powered by ICAT

Data Repository for Advancing open sCience

Motivation

Overcome DB limitations
Reduce DB complexity
Modular
Scalable

FAIRness (i.e: DOI)
Data policy (i.e : embargo, sharing data)
Support non-SB techniques with rich metadata

Steps

March 2023

A proposal for a Next Generation of ISPyB Software

- Requested further evaluation and testing of the ICAT-based solution

ISPyB/MXCuBE Collaboration Meeting SOLEIL

Nov 2023

MX on ICAT

- Requested further development and deployment in real conditions

ISPyB/MXCuBE Collaboration Meeting ALBA

May 2024

Transition from ISPyB to ICAT at ESRF

- Shipment, sample tracking
- Ingestion of RAW and PROCESSED data from Beamlines

ISPyB/MXCuBE Collaboration Meeting MAXIV

Nov 2024

Transition from ISPyB to ICAT at ESRF (II)

- DRAC was born
- Oath2 (SSO) implemented on MXCuBE and session selection

ISPyB/MXCuBE Collaboration Meeting ELETTRA

May 2025

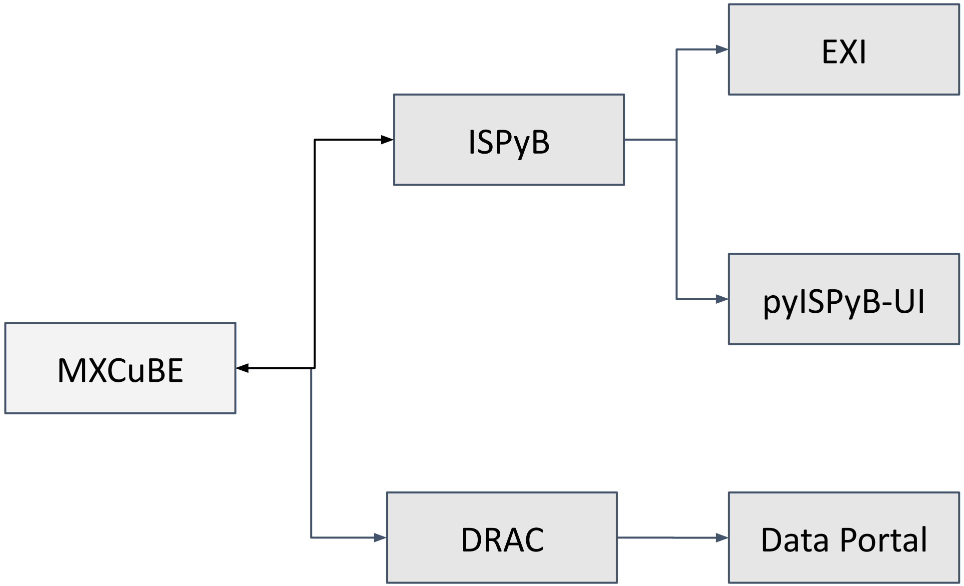
Transition from ISPyB to DRAC at ESRF (III)

- Dual synchronization of samples from MXCuBE

ISPyB/MXCuBE Collaboration Meeting DESY

Current status (November 2025)

Versions: backend|database & frontend?


MXCuBE

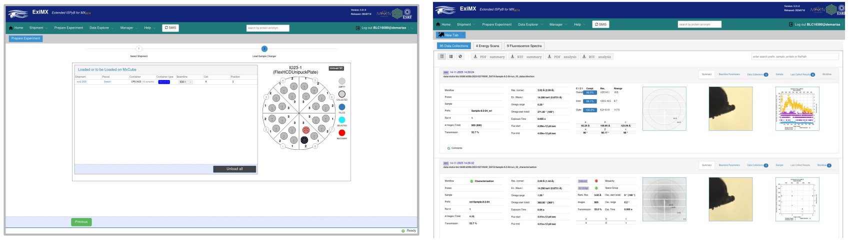
ISPyB

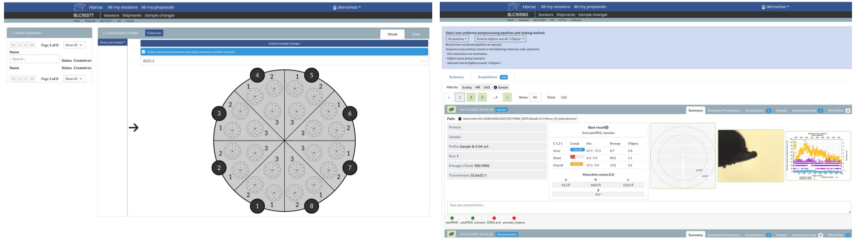
EXI

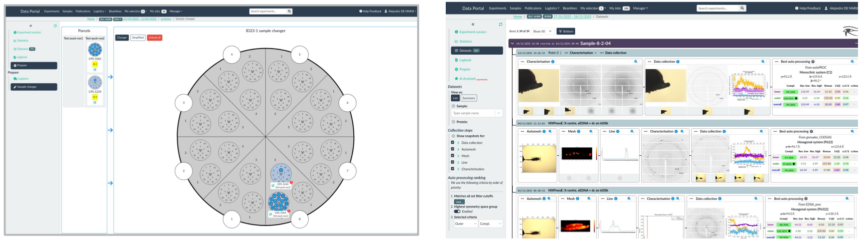
pyISPyB-UI

DRAC

Data Portal







Developments since last meeting (May to October 2025)

Work on improving the configuration of the experiment

Experiment Plan

Min .Rot. Angle
Tot. Rot. Angle
Initial Resolution
Mesh beam diameter
Collection beam diameter
Radiation sensitivity
Number of positions
etc…

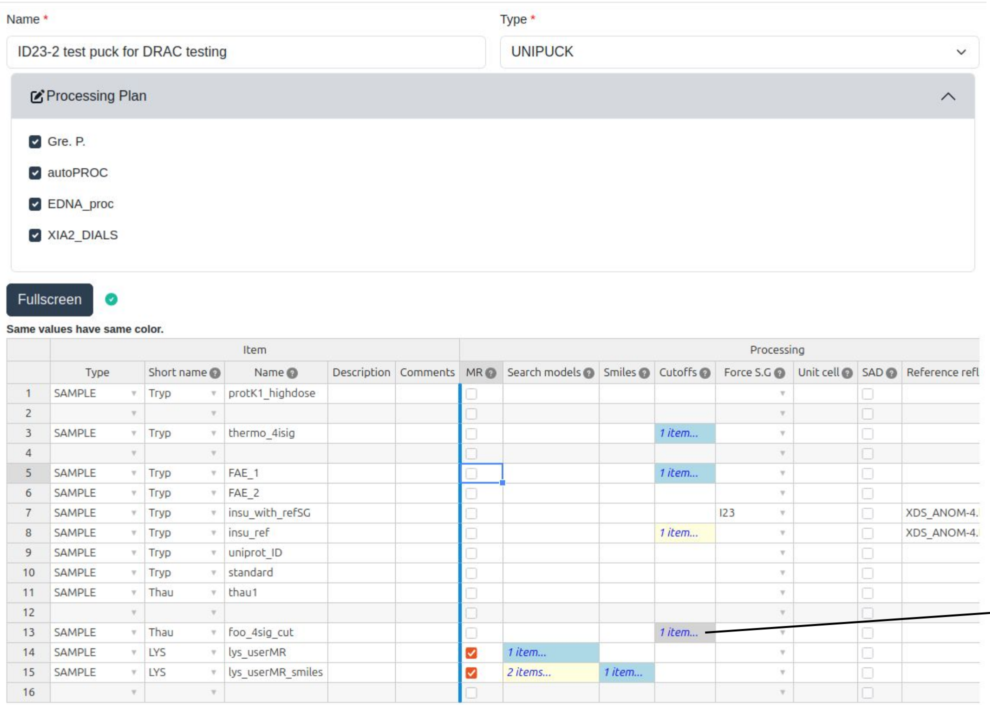
Processing Plan

Pipelines
    Grenades
    AutoPROC
    EDNA_proc
    XIA2_DIALS
Run Molecular Replacement
Search models/UniProt IDs
Smiles
Cutoffs
Force Space group
SAD
Reference reflection

- Users can configure the acquisition and processing parameters on a per-sample basis
- Spreadsheet integrated in DRAC
- Support for import/export CSV (currently still working on this)
- **Configurable for each beamline** (support of multiple techniques)

Developments since last meeting (May to October 2025)

Work on improving the configuration of the experiment



Name *

ID23-2 test puck for DRAC testing

Type *

UNIPUCK

Processing Plan

☑ Gre. P.

☑ autoPROC

☑ EDNA_proc

☑ XIA2_DIALS

Same values have same color.

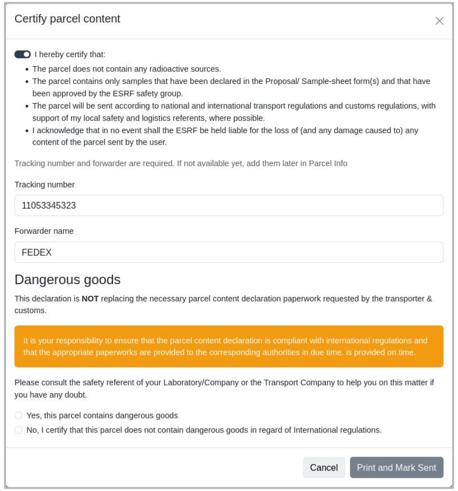
	Item					Processing							
	Type	Short name	Name	Description	Comments	MR	Search models	Smiles	Cutoffs	Force S.G	Unit cell	SAD	Reference refl
1	SAMPLE	Tryp	protK1_highdose			☐						☐	
2						☐						☐	
3	SAMPLE	Tryp	thermo_4isig			☐			*1 item...*			☐	
4						☐						☐	
5	SAMPLE	Tryp	FAE_1			☐			*1 item...*			☐	
6	SAMPLE	Tryp	FAE_2			☐						☐	
7	SAMPLE	Tryp	insu_with_refSG			☐				I23		☐	XDS_ANOM-4.
8	SAMPLE	Tryp	insu_ref			☐			*1 item...*			☐	XDS_ANOM-4.
9	SAMPLE	Tryp	uniprot_ID			☐						☐	
10	SAMPLE	Tryp	standard			☐						☐	
11	SAMPLE	Thau	thau1			☐						☐	
12						☐						☐	
13	SAMPLE	Thau	foo_4sig_cut			☐			*1 item...*			☐	
14	SAMPLE	LYS	lys_userMR			☑	*1 item...*					☐	
15	SAMPLE	LYS	lys_userMR_smiles			☑	*2 items...*	*1 item...*				☐	
16						☐						☐	

	Parameter	Value
1	Completeness	6
2	I/s(I)	9.5
3		
4		
5		
6		
7		
8		
9		
10		

Developments since last meeting (May to October 2025)

Work on improving the parcel tracking

- Improved workflow with the support of the user office and stores
- New labels



Certify parcel content

● I hereby certify that:

- The parcel does not contain any radioactive sources.
- The parcel contains only samples that have been declared in the Proposal/ Sample-sheet form(s) and that have been approved by the ESRF safety group.
- The parcel will be sent according to national and international transport regulations and customs regulations, with support of my local safety and logistics referents, where possible.
- I acknowledge that in no event shall the ESRF be held liable for the loss of (and any damage caused to) any content of the parcel sent by the user.

Tracking number and forwarder are required. If not available yet, add them later in Parcel Info

Tracking number: 11053345323

Forwarder name: FEDEX

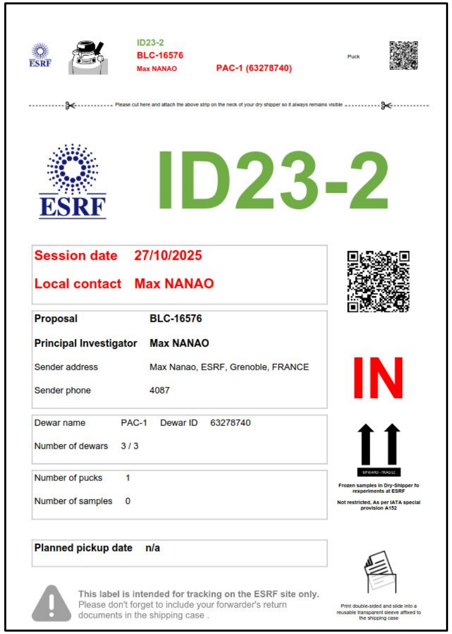
Dangerous goods

This declaration is **NOT** replacing the necessary parcel content declaration paperwork requested by the transporter & customs.

It is your responsibility to ensure that the parcel content declaration is compliant with international regulations and that the appropriate paperworks are provided to the corresponding authorities in due time. is provided on time.

Please consult the safety referent of your Laboratory/Company or the Transport Company to help you on this matter if you have any doubt.

○ Yes, this parcel contains dangerous goods
○ No, I certify that this parcel does not contain dangerous goods in regard of International regulations.



ESRF
ID23-2
BLC-16576
Max NANAO
PAC-1 (63278740)
Puck

Please cut here and attach the above strip on the neck of your dry shipper so it always remains visible

ESRF
ID23-2

Session date 27/10/2025
Local contact Max NANAO

Proposal BLC-16576
Principal Investigator Max NANAO
Sender address Max Nanao, ESRF, Grenoble, FRANCE
Sender phone 4087

Dewar name PAC-1 Dewar ID 63278740
Number of dewars 3 / 3

Number of pucks 1
Number of samples 0

Planned pickup date n/a

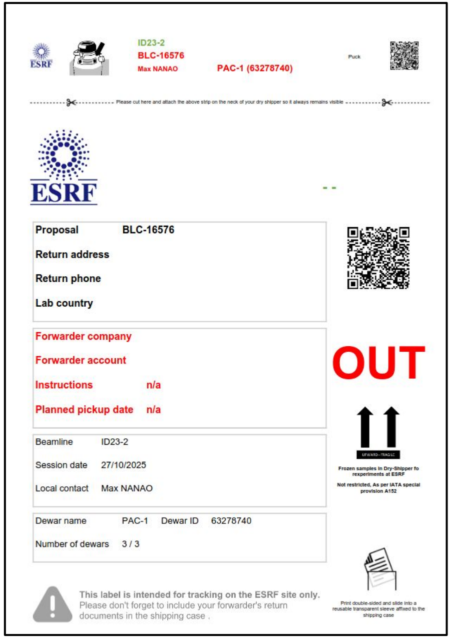
IN

Frozen samples in Dry-Shipper fo rexperiments at ESRF

Not restricted, As per IATA special provision A152

This label is intended for tracking on the ESRF site only.
Please don't forget to include your forwarder's return documents in the shipping case .

Print double-sided and slide into a reusable transparent sleeve affixed to the shipping case



ESRF
ID23-2
BLC-16576
Max NANAO
PAC-1 (63278740)
Puck

Please cut here and attach the above strip on the neck of your dry shipper so it always remains visible

ESRF
- -

Proposal BLC-16576
Return address
Return phone
Lab country

Forwarder company
Forwarder account
Instructions n/a
Planned pickup date n/a

Beamline ID23-2
Session date 27/10/2025
Local contact Max NANAO

Dewar name PAC-1 Dewar ID 63278740
Number of dewars 3 / 3

OUT

Frozen samples in Dry-Shipper fo rexperiments at ESRF

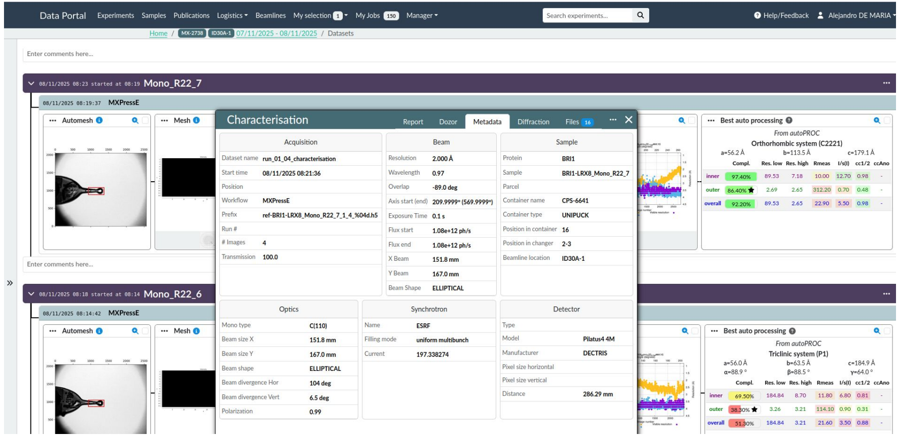
Not restricted, As per IATA special provision A152

This label is intended for tracking on the ESRF site only.
Please don't forget to include your forwarder's return documents in the shipping case .

Print double-sided and slide into a reusable transparent sleeve affixed to the shipping case

Developments since last meeting (May to October 2025)

Enrichment of the metadata linked to the experiments



Characterisation — Report | Dozor | Metadata | Diffraction | Files 16

Acquisition	
Dataset name	run_01_04_characterisation
Start time	08/11/2025 08:21:36
Position	
Workflow	MXPressE
Prefix	ref-BRI1-LRX8_Mono_R22_7_1_4_%04d.h5
Run #	
# Images	4
Transmission	100.0

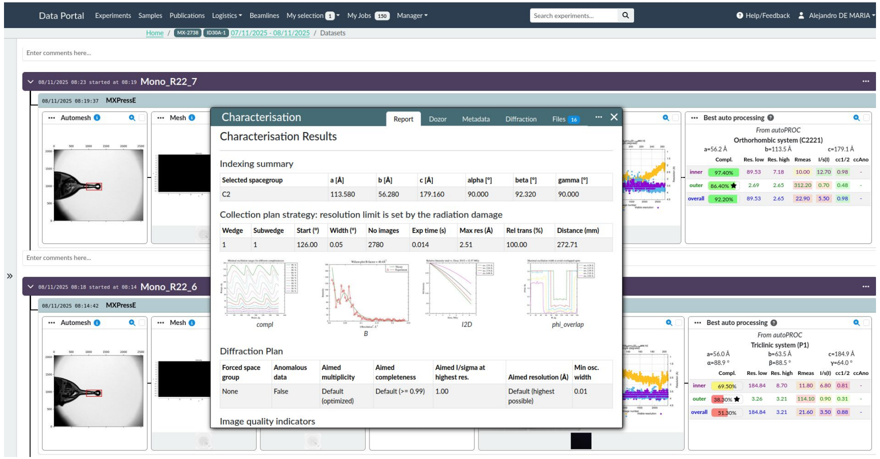
Beam	
Resolution	2.000 Å
Wavelength	0.97
Overlap	-89.0 deg
Axis start (end)	209.9999° (569.9999°)
Exposure Time	0.1 s
Flux start	1.08e+12 ph/s
Flux end	1.08e+12 ph/s
X Beam	151.8 mm
Y Beam	167.0 mm
Beam Shape	ELLIPTICAL

Sample	
Protein	BRI1
Sample	BRI1-LRX8_Mono_R22_7
Parcel	
Container name	CPS-6641
Container type	UNIPUCK
Position in container	16
Position in changer	2-3
Beamline location	ID30A-1

Optics	
Mono type	C(110)
Beam size X	151.8 mm
Beam size Y	167.0 mm
Beam shape	ELLIPTICAL
Beam divergence Hor	104 deg
Beam divergence Vert	6.5 deg
Polarization	0.99

Synchrotron	
Name	ESRF
Filling mode	uniform multibunch
Current	197.338274

Detector	
Type	
Model	Pilatus4 4M
Manufacturer	DECTRIS
Pixel size horizontal	
Pixel size vertical	
Distance	286.29 mm



Characterisation — Report | Dozor | Metadata | Diffraction | Files 16

Characterisation Results

Indexing summary

Selected spacegroup	a [Å]	b [Å]	c [Å]	alpha [°]	beta [°]	gamma [°]
C2	113.580	56.280	179.160	90.000	92.320	90.000

Collection plan strategy: resolution limit is set by the radiation damage

Wedge	Subwedge	Start (°)	Width (°)	No images	Exp time (s)	Max res (Å)	Rel trans (%)	Distance (mm)
1	1	126.00	0.05	2780	0.014	2.51	100.00	272.71

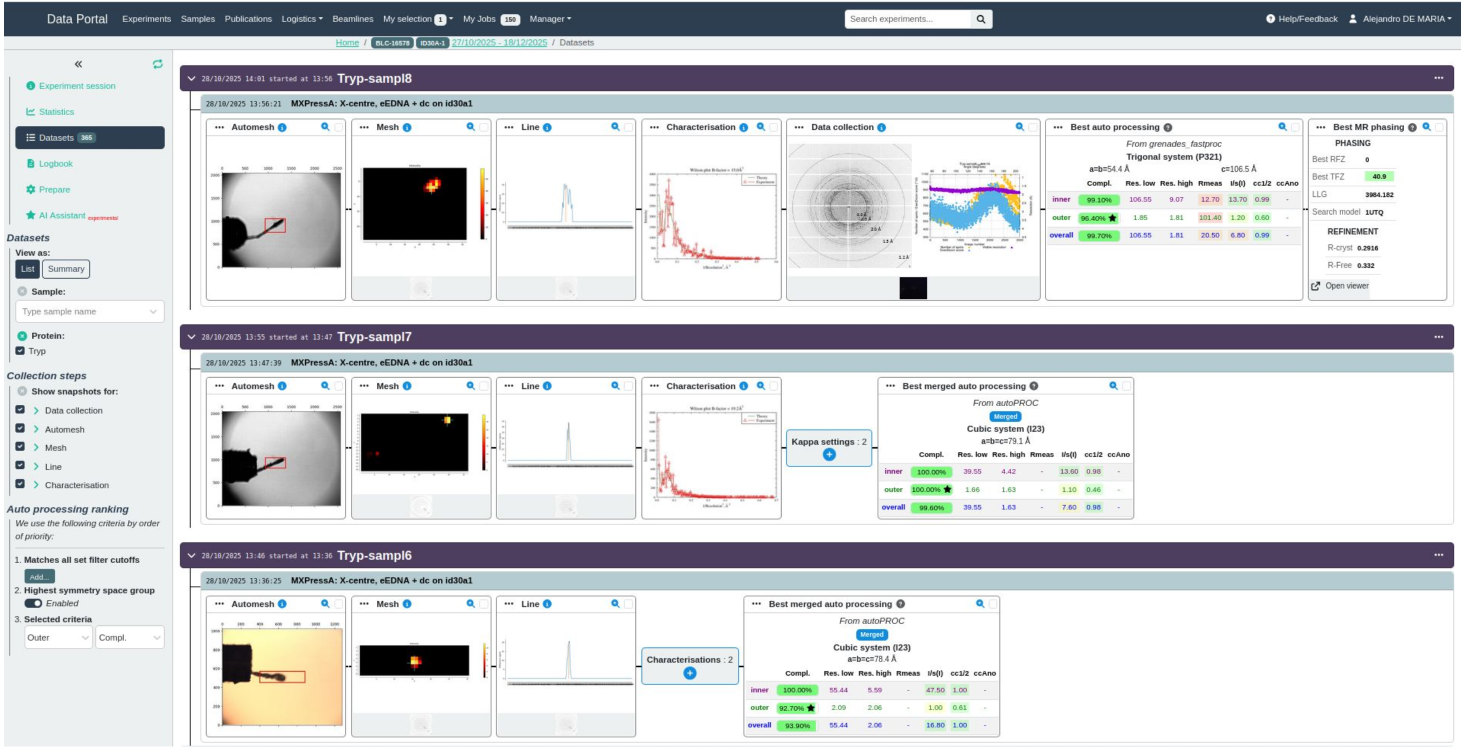
Diffraction Plan

Forced space group	Anomalous data	Aimed multiplicity	Aimed completeness	Aimed I/sigma at highest res.	Aimed resolution (Å)	Min osc. width
None	False	Default (optimized)	Default (>= 0.99)	1.00	Default (highest possible)	0.01

Image quality indicators

Developments since last meeting (May to October 2025)

- Real cases of dynamic grouping of the results



Datasets

View as: List | Summary

Sample: Type sample name

Protein:
☑ Tryp

Collection steps

Show snapshots for:
☑ Data collection
☑ Automesh
☑ Mesh
☑ Line
☑ Characterisation

Auto processing ranking

We use the following criteria by order of priority:

1. Matches all set filter cutoffs
2. Highest symmetry space group — *Enabled*
3. Selected criteria — Outer, Compl.

28/10/2025 14:01 started at 13:56 **Tryp-sampl8**

28/10/2025 13:56:21 MXPressA: X-centre, eEDNA + dc on id30a1

Best auto processing

From grenades_fastproc

Trigonal system (P321)

a=b=54.4 Å c=106.5 Å

	Compl.	Res. low	Res. high	Rmeas	I/s(I)	cc1/2	ccAno
inner	99.10%	106.55	9.07	12.70	13.70	0.99	-
outer	96.40% ★	1.85	1.81	101.40	1.20	0.60	-
overall	99.70%	106.55	1.81	20.50	6.80	0.99	-

Best MR phasing

PHASING

Best RFZ	0
Best TFZ	40.9
LLG	3984.182
Search model	1UTQ

REFINEMENT

R-cryst	0.2916
R-Free	0.332

28/10/2025 13:55 started at 13:47 **Tryp-sampl7**

28/10/2025 13:47:39 MXPressA: X-centre, eEDNA + dc on id30a1

Best merged auto processing

From autoPROC

Cubic system (I23)

a=b=c=79.1 Å

	Compl.	Res. low	Res. high	Rmeas	I/s(I)	cc1/2	ccAno
inner	100.00%	39.55	4.42	-	13.60	0.98	-
outer	100.00% ★	1.66	1.63	-	1.10	0.46	-
overall	99.60%	39.55	1.63	-	7.60	0.98	-

28/10/2025 13:46 started at 13:36 **Tryp-sampl6**

28/10/2025 13:36:25 MXPressA: X-centre, eEDNA + dc on id30a1

Best merged auto processing

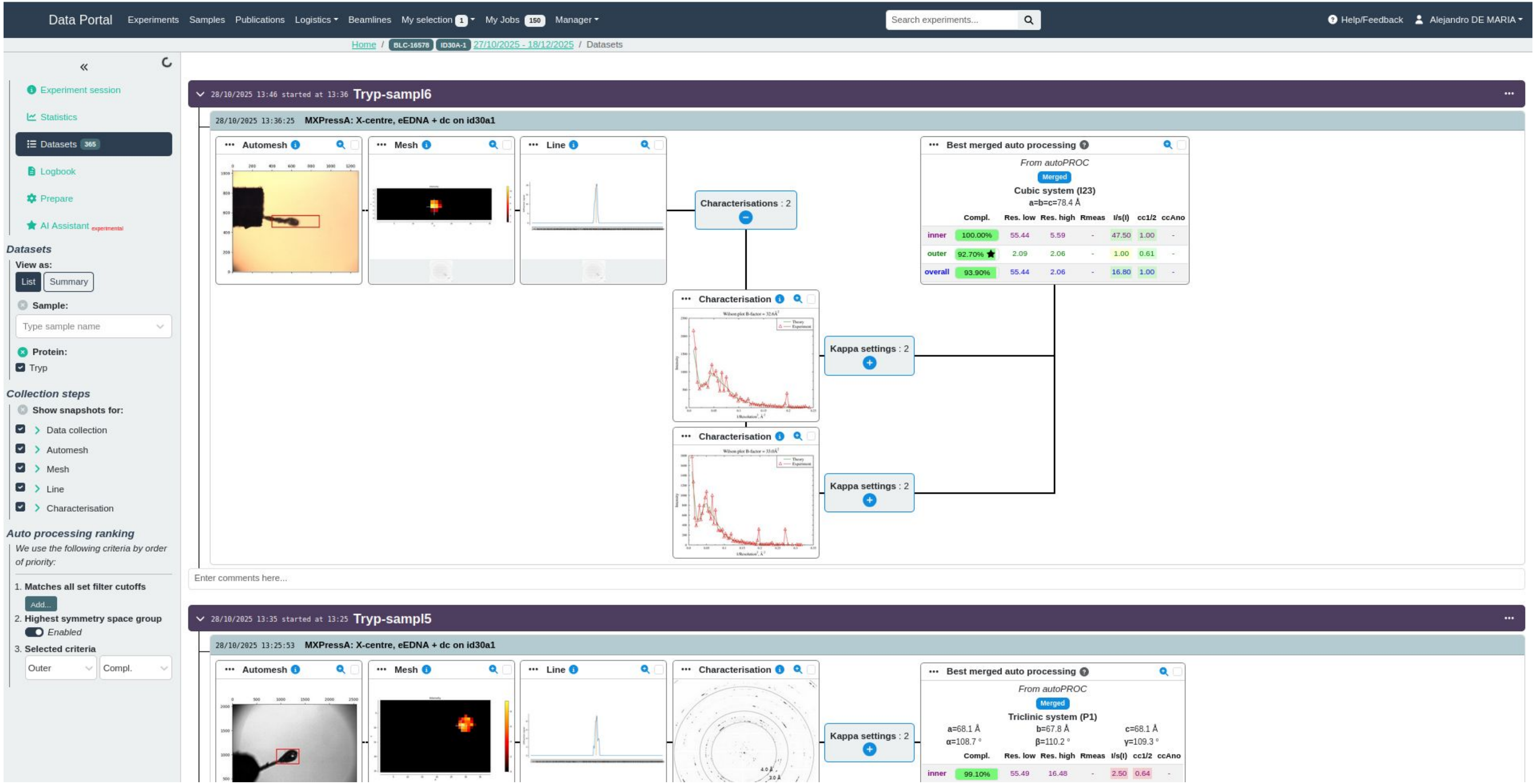
From autoPROC

Cubic system (I23)

a=b=c=78.4 Å

	Compl.	Res. low	Res. high	Rmeas	I/s(I)	cc1/2	ccAno
inner	100.00%	55.44	5.59	-	47.50	1.00	-
outer	92.70% ★	2.09	2.06	-	1.00	0.61	-
overall	93.90%	55.44	2.06	-	16.80	1.00	-

Developments since last meeting



Datasets

View as: List Summary

Sample: Type sample name

Protein:
☑ Tryp

Collection steps

Show snapshots for:
☑ Data collection
☑ Automesh
☑ Mesh
☑ Line
☑ Characterisation

Auto processing ranking

We use the following criteria by order of priority:

1. Matches all set filter cutoffs — Add...
2. Highest symmetry space group — *Enabled*
3. Selected criteria — Outer, Compl.

28/10/2025 13:46 started at 13:36 **Tryp-sampl6**

28/10/2025 13:36:25 **MXPressA: X-centre, eEDNA + dc on id30a1**

Best merged auto processing

From autoPROC

Merged

Cubic system (I23)

a=b=c=78.4 Å

	Compl.	Res. low	Res. high	Rmeas	I/s(I)	cc1/2	ccAno
inner	100.00%	55.44	5.59	-	47.50	1.00	-
outer	92.70% ★	2.09	2.06	-	1.00	0.61	-
overall	93.90%	55.44	2.06	-	16.80	1.00	-

Enter comments here...

28/10/2025 13:35 started at 13:25 **Tryp-sampl5**

28/10/2025 13:25:53 **MXPressA: X-centre, eEDNA + dc on id30a1**

Best merged auto processing

From autoPROC

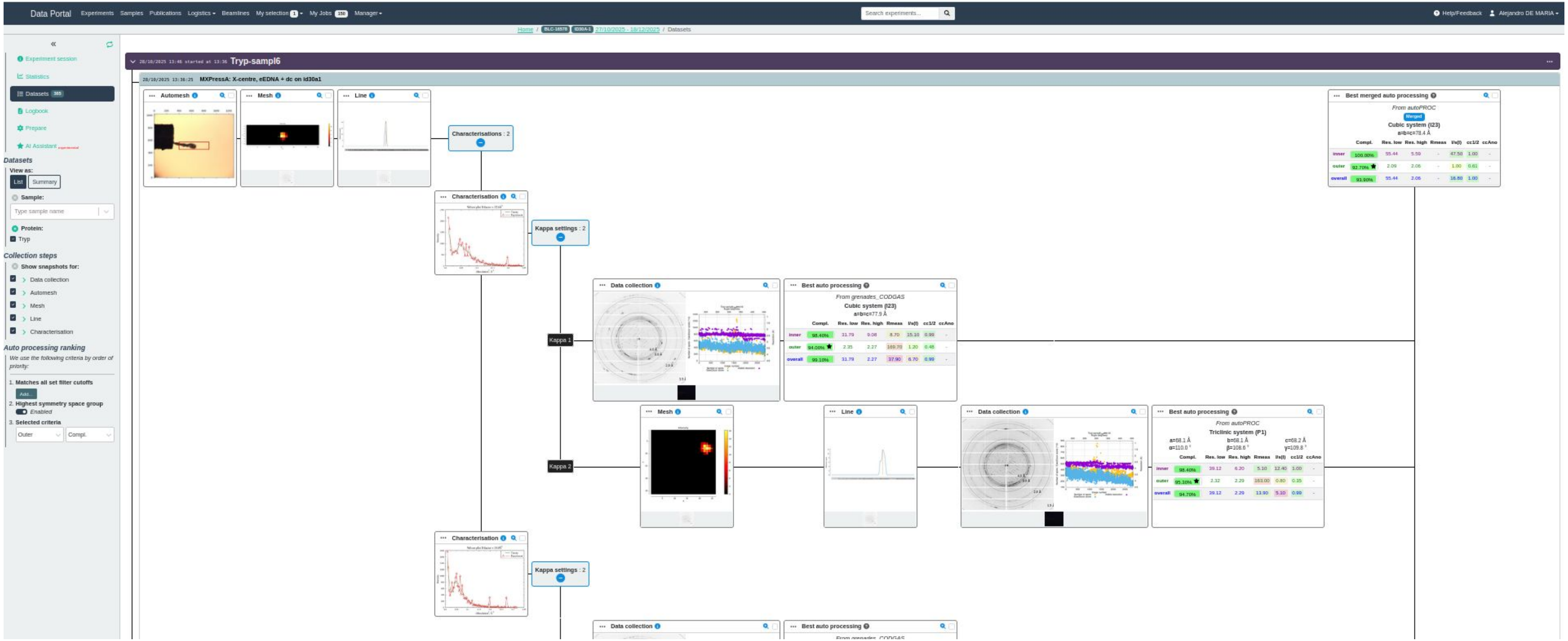
Merged

Triclinic system (P1)

a=68.1 Å b=67.8 Å c=68.1 Å
α=108.7 ° β=110.2 ° γ=109.3 °

	Compl.	Res. low	Res. high	Rmeas	I/s(I)	cc1/2	ccAno
inner	99.10%	55.49	16.48	-	2.50	0.64	-

Developments since last meeting



Datasets

View as: List Summary

Sample: Type sample name

Protein:

☑ Tryp

Collection steps

Show snapshots for:

☑ Data collection
☑ Automesh
☑ Mesh
☑ Line
☑ Characterisation

Auto processing ranking

We use the following criteria by order of priority:

1. Matches all set filter cutoffs
   Add...
2. Highest symmetry space group
   Enabled
3. Selected criteria
   Outer Compl.

Best merged auto processing

From autoPROC

Merged

Cubic system (I23)

a=b=c=78.4 Å

	Compl.	Res. low	Res. high	Rmeas	I/s(I)	cc1/2	ccAno
inner	100.00%	55.44	5.59	-	47.50	1.00	-
outer	92.70% ★	2.09	2.06	-	1.00	0.61	-
overall	93.90%	55.44	2.06	-	16.80	1.00	-

Best auto processing

From grenades_CODGAS

Cubic system (I23)

a=b=c=77.9 Å

	Compl.	Res. low	Res. high	Rmeas	I/s(I)	cc1/2	ccAno
inner	98.40%	31.79	9.08	8.70	15.10	0.99	-
outer	94.00% ★	2.35	2.27	169.70	1.20	0.48	-
overall	99.10%	31.79	2.27	37.90	6.70	0.99	-

Best auto processing

From autoPROC

Triclinic system (P1)

a=68.1 Å b=68.1 Å c=68.2 Å
α=110.0 ° β=108.6 ° γ=109.8 °

	Compl.	Res. low	Res. high	Rmeas	I/s(I)	cc1/2	ccAno
inner	98.40%	39.12	6.20	5.10	12.40	1.00	-
outer	95.30% ★	2.32	2.29	163.00	0.80	0.35	-
overall	94.70%	39.12	2.29	13.90	5.10	0.99	-

From grenades_CODGAS

Developments since last meeting

Better summary view

- Display of collected and uncollected positions
- Non declared containers

We use the following criteria by order of priority:

1. Matches all set filter cutoffs
2. Highest symmetry space group: Enabled
3. Selected criteria: Overall, Compl.

Selected statistics: Overall Compl.

66.791015625

Analyzed: 98 **Collected:** 48 **Autoprocessed:** 39

Puck: CPS-7423 - *Analyzed: 16 Collected: 0 Autoprocessed: 0*

Puck: CPS-7424 - *Analyzed: 11 Collected: 0 Autoprocessed: 0*

Puck: DLS500 - *Analyzed: 2 Collected: 1 Autoprocessed: 1*

Puck: DLS502 - *Analyzed: 16 Collected: 9 Autoprocessed: 9*

Puck: DLS503 - *Analyzed: 16 Collected: 16 Autoprocessed: 16*

Puck: DLS504 - *Analyzed: 16 Collected: 10 Autoprocessed: 8*

Puck: ITQB-101 - *Analyzed: 16 Collected: 8 Autoprocessed: 3*

Puck: ITQB-102 - *Analyzed: 4 Collected: 3 Autoprocessed: 2*

Before

We use the following criteria by order of priority:

1. Matches all set filter cutoffs
2. Highest symmetry space group: Enabled
3. Selected criteria: Overall, I/s(I)

Selected statistics: Overall I/s(I)

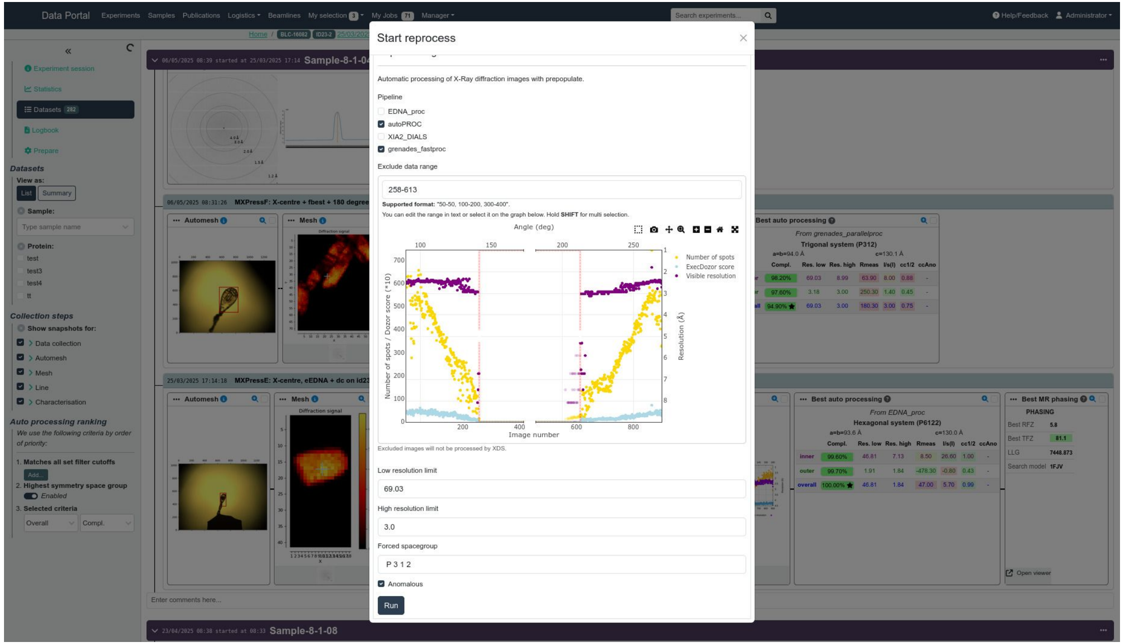
Analyzed: 98 **Collected:** 48 **Autoprocessed:** 39

DLS504
DLS503
DLS502
DLS500
ITQB-102
ITQB-101
CPS-7424
CPS-7423
NA

Now

Developments since last meeting

Reprocessing improvements



Start reprocess

Automatic processing of X-Ray diffraction images with prepopulate.

Pipeline

☐ EDNA_proc
☑ autoPROC
☐ XIA2_DIALS
☑ grenades_fastproc

Exclude data range: 258-613

Supported format: "50-50, 100-200, 300-400".

You can edit the range in text or select it on the graph below. Hold **SHIFT** for multi selection.

Excluded images will not be processed by XDS.

Low resolution limit: 69.03

High resolution limit: 3.0

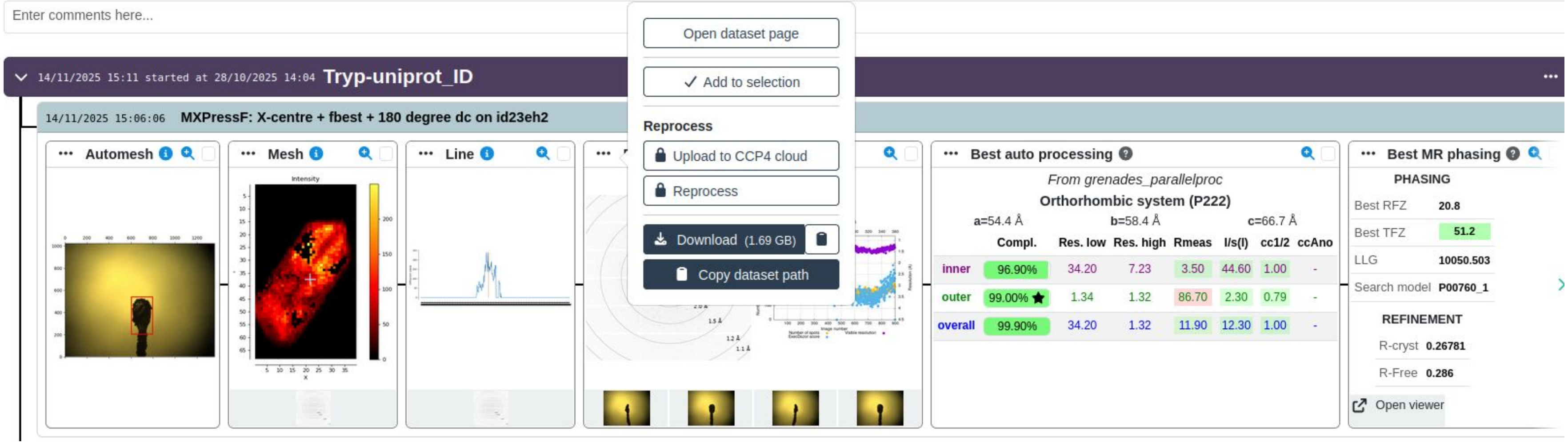
Forced spacegroup: P 3 1 2

☑ Anomalous

Run

- Reprocess your dataset via ewoks
- Range image selector
- Specify more parameters, i.e: resolution limits and space group

Reprocessing improvements



14/11/2025 15:11 started at 28/10/2025 14:04 **Tryp-uniprot_ID**

14/11/2025 15:06:06 **MXPressF: X-centre + fbest + 180 degree dc on id23eh2**

Best auto processing

From grenades_parallelproc

Orthorhombic system (P222)

a=54.4 Å b=58.4 Å c=66.7 Å

	Compl.	Res. low	Res. high	Rmeas	I/s(I)	cc1/2	ccAno
inner	96.90%	34.20	7.23	3.50	44.60	1.00	-
outer	99.00% ★	1.34	1.32	86.70	2.30	0.79	-
overall	99.90%	34.20	1.32	11.90	12.30	1.00	-

Best MR phasing

PHASING

Best RFZ	20.8
Best TFZ	51.2
LLG	10050.503
Search model	P00760_1

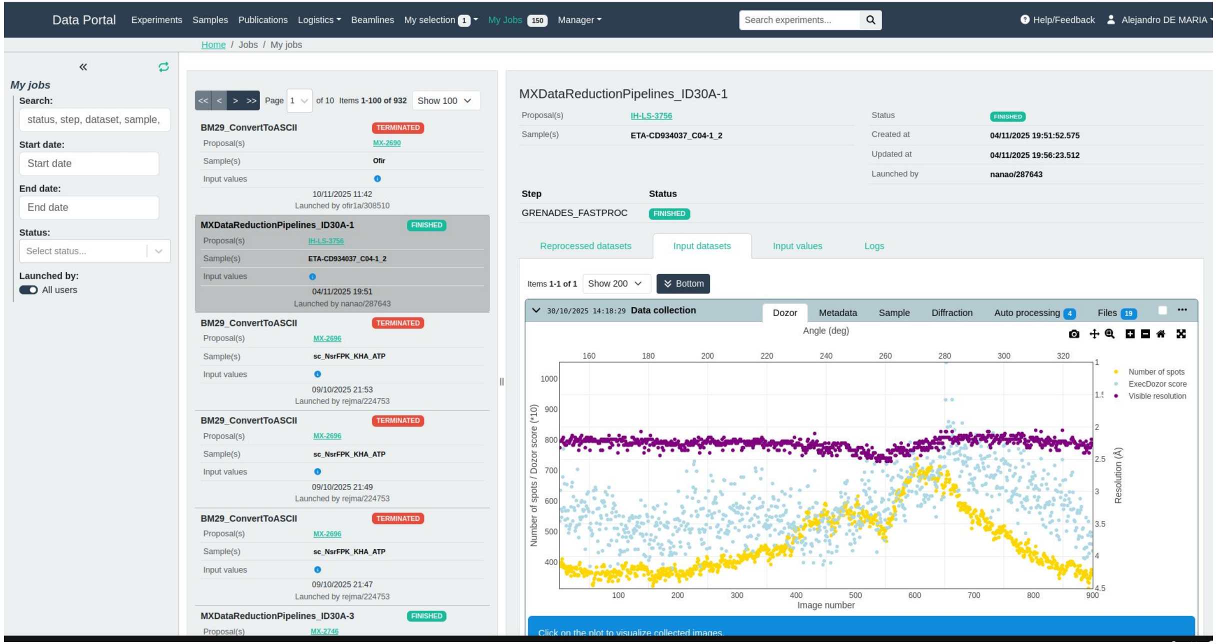
REFINEMENT

R-cryst	0.26781
R-Free	0.286

- Upload your dataset to the CCP4 Cloud automatically via Ewoks

Developments since last meeting

Reprocessing improvements



BM29_ConvertToASCII TERMINATED
Proposal(s) MX-2690
Sample(s) Ofir
Input values
10/11/2025 11:42
Launched by ofir1a/308510

MXDataReductionPipelines_ID30A-1 FINISHED
Proposal(s) IH-LS-3756
Sample(s) ETA-CD934037_C04-1_2
Input values
04/11/2025 19:51
Launched by nanao/287643

BM29_ConvertToASCII TERMINATED
Proposal(s) MX-2696
Sample(s) sc_NsrFPK_KHA_ATP
Input values
09/10/2025 21:53
Launched by rejma/224753

BM29_ConvertToASCII TERMINATED
Proposal(s) MX-2696
Sample(s) sc_NsrFPK_KHA_ATP
Input values
09/10/2025 21:49
Launched by rejma/224753

BM29_ConvertToASCII TERMINATED
Proposal(s) MX-2696
Sample(s) sc_NsrFPK_KHA_ATP
Input values
09/10/2025 21:47
Launched by rejma/224753

MXDataReductionPipelines_ID30A-3 FINISHED
Proposal(s) MX-2746

MXDataReductionPipelines_ID30A-1

Proposal(s) IH-LS-3756
Sample(s) ETA-CD934037_C04-1_2
Status FINISHED
Created at 04/11/2025 19:51:52.575
Updated at 04/11/2025 19:56:23.512
Launched by nanao/287643

Step	Status
GRENADES_FASTPROC	FINISHED

Reprocessed datasets | Input datasets | Input values | Logs

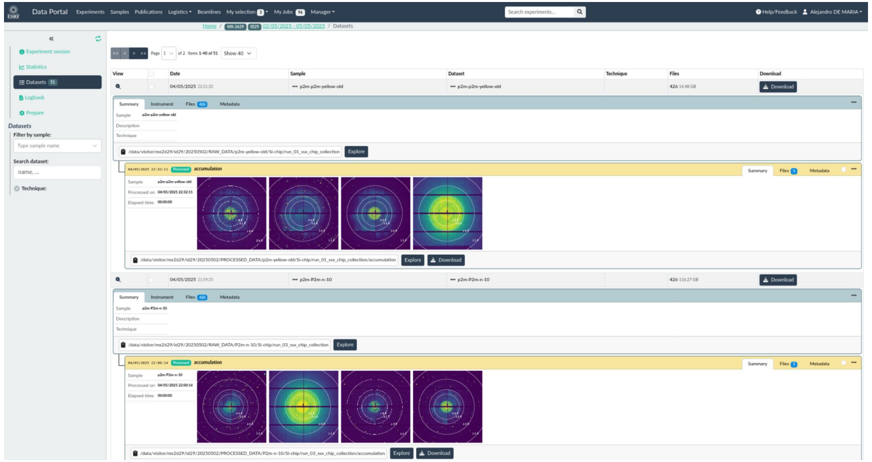
Items 1-1 of 1 Show 200 Bottom

30/10/2025 14:18:29 Data collection — Dozor | Metadata | Sample | Diffraction | Auto processing 4 | Files 19

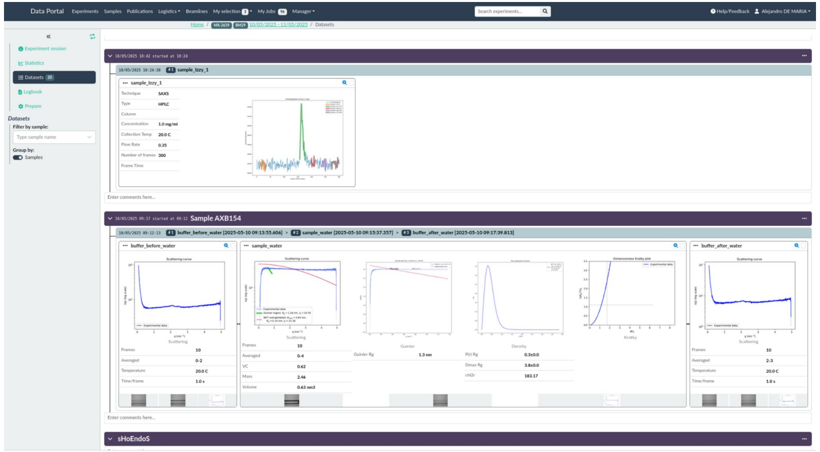
Click on the plot to visualize collected images.

- Better interface to manage the jobs that have been run

Developments on other techniques



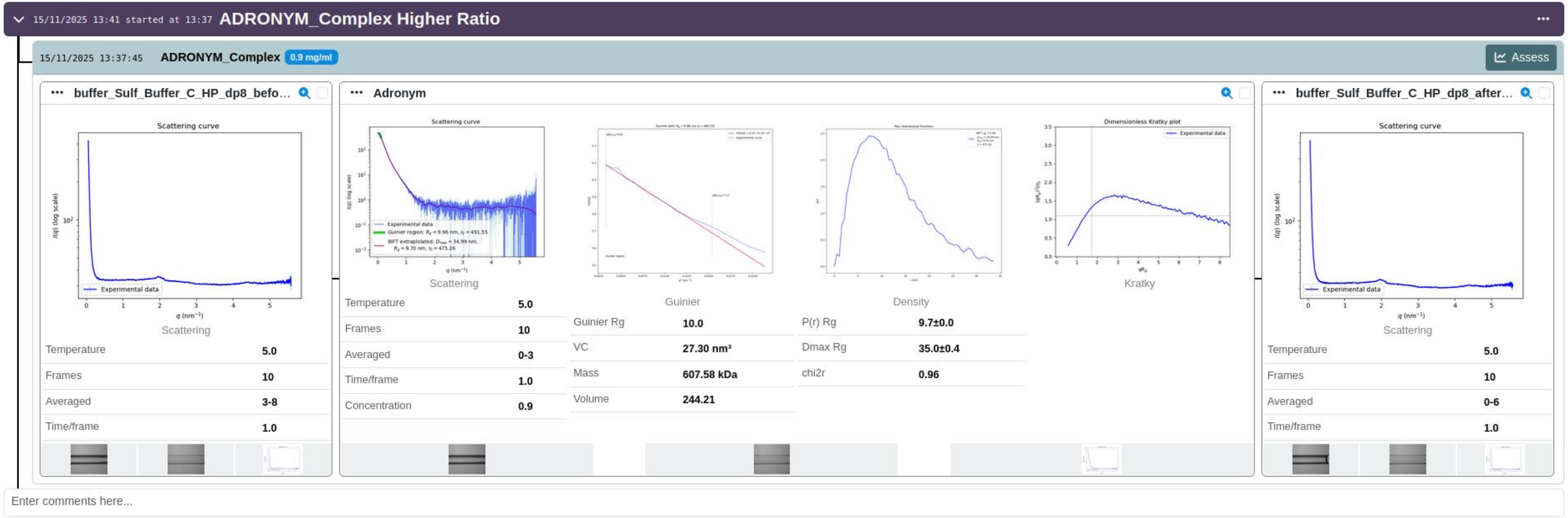
SSX Experiments



BioSAXS Experiments

- DRAC allows to change the presentation depending on the type of experiment
- As we catalog the metadata of new techniques, the data are presented appropriately.

Developments on other techniques



15/11/2025 13:41 started at 13:37 **ADRONYM_Complex Higher Ratio**

15/11/2025 13:37:45 **ADRONYM_Complex** 0.9 mg/ml

buffer_Sulf_Buffer_C_HP_dp8_befo…

Scattering

Temperature	5.0
Frames	10
Averaged	3-8
Time/frame	1.0

Adronym

Scattering

Temperature	5.0
Frames	10
Averaged	0-3
Time/frame	1.0
Concentration	0.9

Guinier

Guinier Rg	10.0
VC	27.30 nm³
Mass	607.58 kDa
Volume	244.21

Density

P(r) Rg	9.7±0.0
Dmax Rg	35.0±0.4
chi2r	0.96

Kratky

buffer_Sulf_Buffer_C_HP_dp8_after…

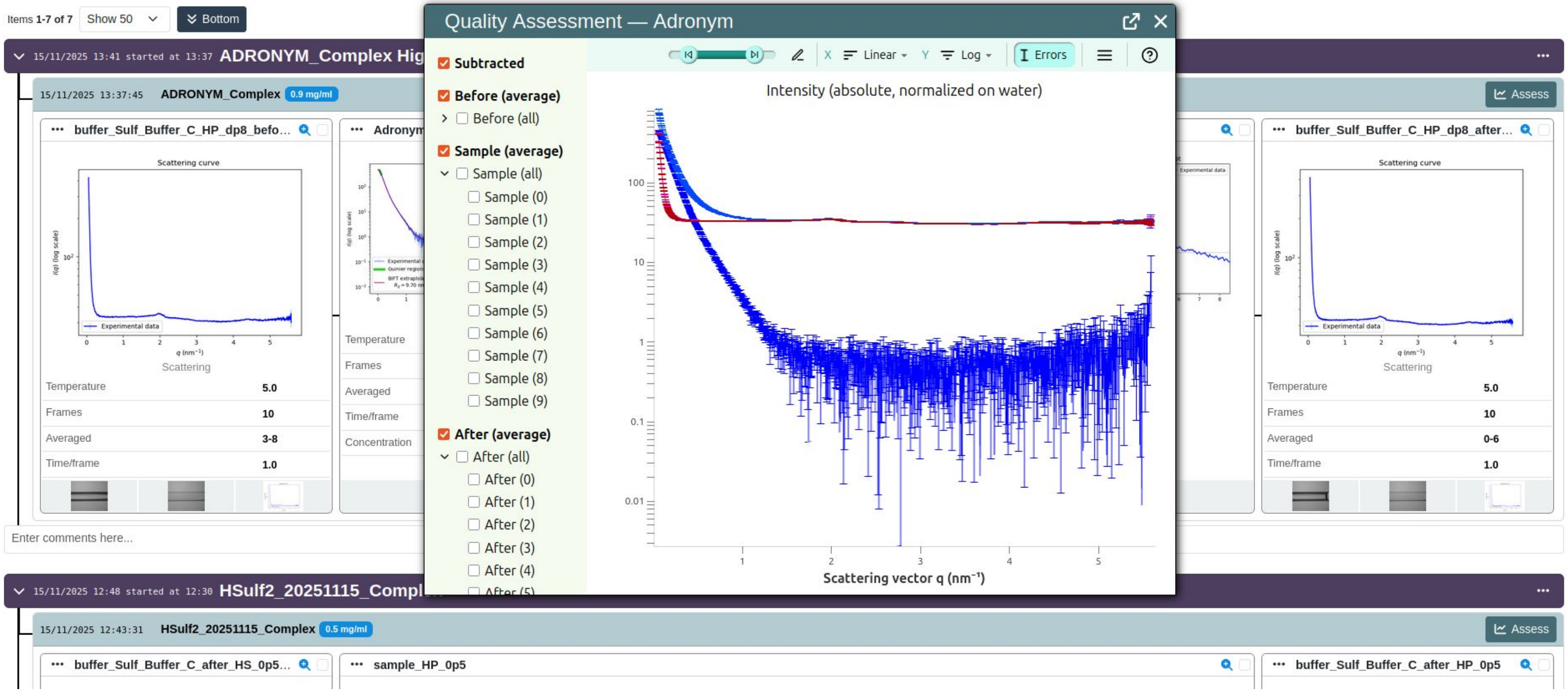
Scattering

Temperature	5.0
Frames	10
Averaged	0-6
Time/frame	1.0

Enter comments here...

- Visualization widgets have been developed and integrated for certain techniques
- Example: New feature for quick assessment of the data

Developments on other techniques



Items 1-7 of 7 Show 50 Bottom

15/11/2025 13:41 started at 13:37 ADRONYM_Complex Hig

15/11/2025 13:37:45 ADRONYM_Complex 0.9 mg/ml

buffer_Sulf_Buffer_C_HP_dp8_befo…

Temperature	5.0
Frames	10
Averaged	3-8
Time/frame	1.0

buffer_Sulf_Buffer_C_HP_dp8_after…

Temperature	5.0
Frames	10
Averaged	0-6
Time/frame	1.0

Enter comments here...

15/11/2025 12:48 started at 12:30 HSulf2_20251115_Compl

15/11/2025 12:43:31 HSulf2_20251115_Complex 0.5 mg/ml

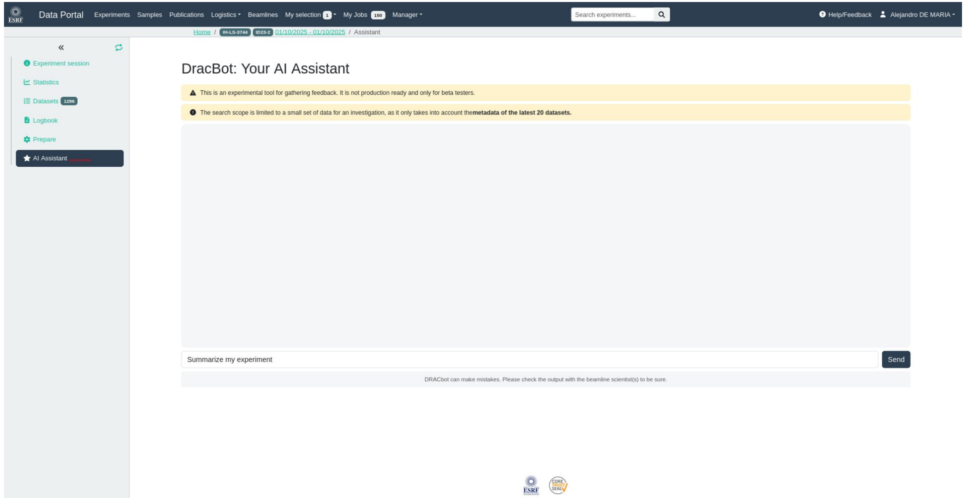
buffer_Sulf_Buffer_C_after_HS_0p5…

sample_HP_0p5

buffer_Sulf_Buffer_C_after_HP_0p5

- Integration of H5web plugin for BioSAXS

DRACBot: AI Assistant



DracBot: Your AI Assistant

This is an experimental tool for gathering feedback. It is not production ready and only for beta testers.

The search scope is limited to a small set of data for an investigation, as it only takes into account the**metadata of the latest 20 datasets.**

Summarize my experiment

DRACbot can make mistakes. Please check the output with the beamline scientist(s) to be sure.

POC

- A proof of concept deployed on 16th Oct
- Accessible to ESRF beamline staff only

RAG (Retrieval Augmented Generation)

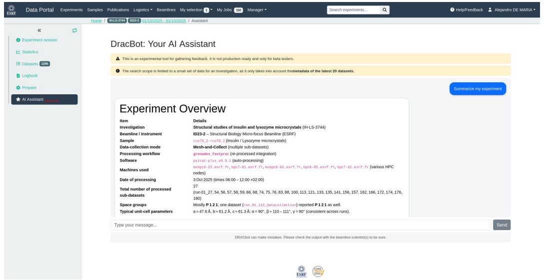
- Limited context send to the LLM
  - Metadata of latest datasets

- LLM: gpt-oss

Evaluation purposes only

- Gather feedback
- Inspiration about use cases

DRACBot: Example of “summarize my experiment”



DracBot: Your AI Assistant

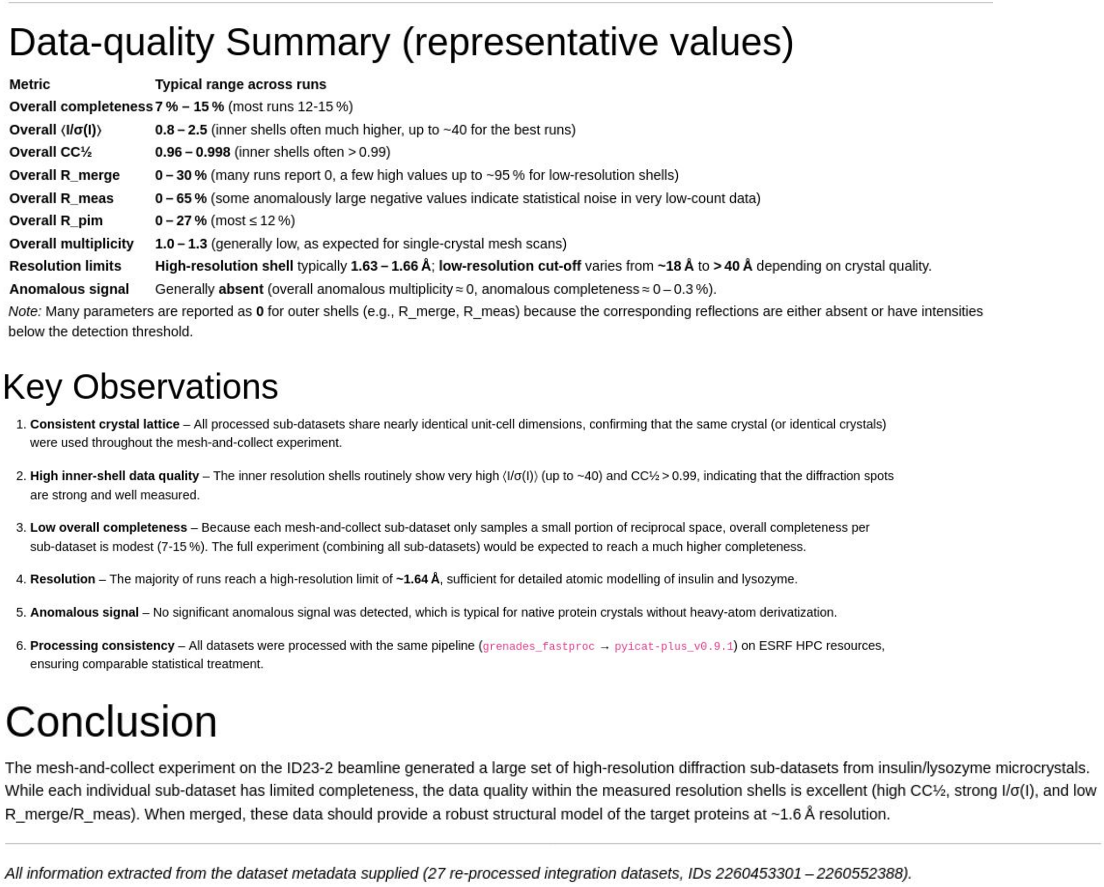
▲ This is an experimental tool for gathering feedback. It is not production ready and only for beta testers.

● The search scope is limited to a small set of data for an investigation, as it only takes into account the**metadata of the latest 20 datasets.**

Experiment Overview

Item	Details
Investigation	**Structural studies of insulin and lysozyme microcrystals** (IH-LS-3744)
Beamline / Instrument	**ID23-2** – Structural Biology Micro-focus Beamline (ESRF)
Sample	`rco78_2-rco78_2` (Insulin / Lysozyme microcrystals)
Data-collection mode	**Mesh-and-Collect** (multiple sub-datasets)
Processing workflow	`grenades_fastproc` (re-processed integration)
Software	`pyicat-plus_v0.9.1` (auto-processing)
Machines used	`mxhpc6-22.esrf.fr`, `hpc7-61.esrf.fr`, `mxhpc6-01.esrf.fr`, `hpc6-05.esrf.fr`, `hpc7-61.esrf.fr` (various HPC nodes)
Date of processing	3 Oct 2025 (times 06:00 – 12:00 +02:00)
Total number of processed sub-datasets	27 (run 01_27, 54, 56, 57, 58, 59, 66, 68, 74, 75, 76, 83, 88, 100, 113, 121, 133, 135, 141, 156, 157, 162, 166, 172, 174, 176, 180)
Space groups	Mostly **P 1 2 1**; one dataset (`run_01_113_datacollection`) reported **P 1 2 1** as well.
Typical unit-cell parameters	a ≈ 47.6 Å, b ≈ 61.2 Å, c ≈ 61.3 Å; α = 90°, β ≈ 110 – 111°, γ = 90° (consistent across runs).

DRACbot can make mistakes. Please check the output with the beamline scientist(s) to be sure.



Data-quality Summary (representative values)

Metric	Typical range across runs
Overall completeness	**7 % – 15 %** (most runs 12-15 %)
Overall ⟨I/σ(I)⟩	**0.8 – 2.5** (inner shells often much higher, up to ~40 for the best runs)
Overall CC½	**0.96 – 0.998** (inner shells often > 0.99)
Overall R_merge	**0 – 30 %** (many runs report 0, a few high values up to ~95 % for low-resolution shells)
Overall R_meas	**0 – 65 %** (some anomalously large negative values indicate statistical noise in very low-count data)
Overall R_pim	**0 – 27 %** (most ≤ 12 %)
Overall multiplicity	**1.0 – 1.3** (generally low, as expected for single-crystal mesh scans)
Resolution limits	**High-resolution shell** typically **1.63 – 1.66 Å**; **low-resolution cut-off** varies from **~18 Å** to **> 40 Å** depending on crystal quality.
Anomalous signal	Generally **absent** (overall anomalous multiplicity ≈ 0, anomalous completeness ≈ 0 – 0.3 %).

Note: Many parameters are reported as **0** for outer shells (e.g., R_merge, R_meas) because the corresponding reflections are either absent or have intensities below the detection threshold.

Key Observations

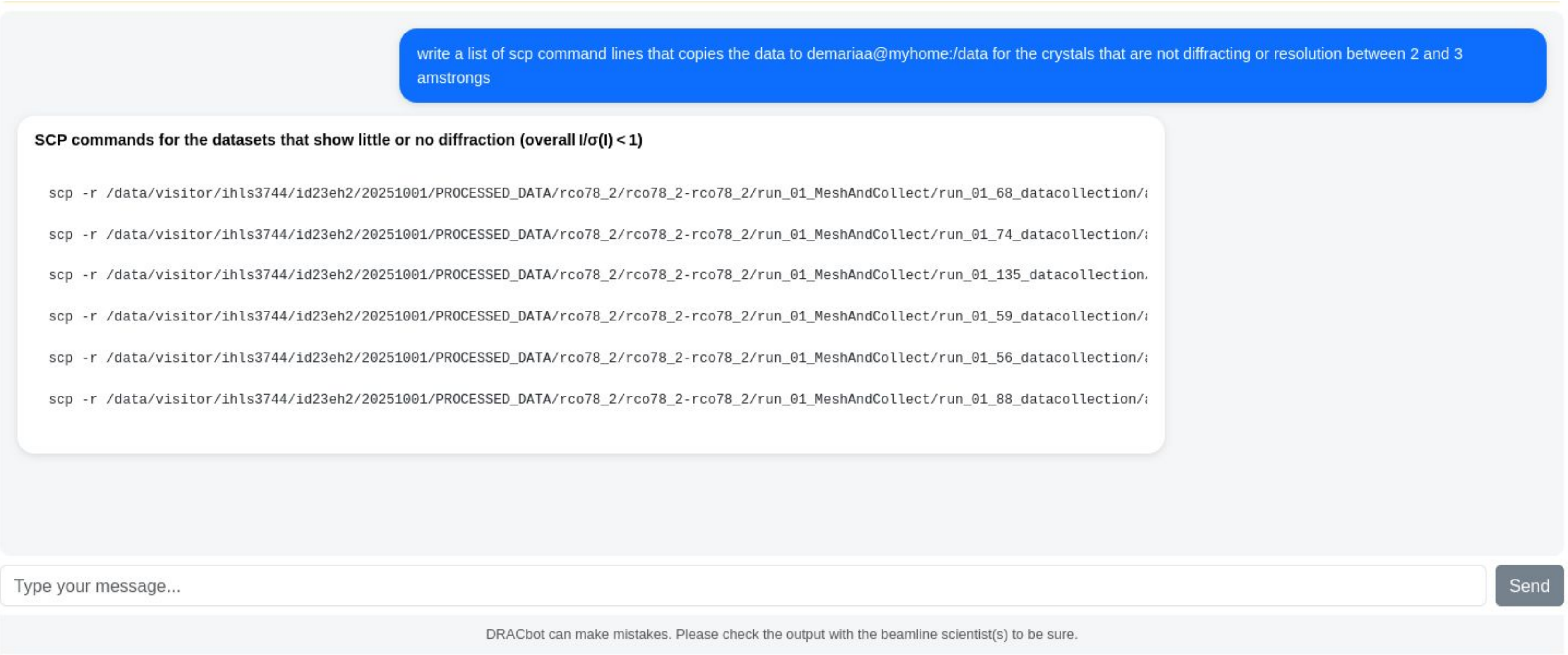
1. **Consistent crystal lattice** – All processed sub-datasets share nearly identical unit-cell dimensions, confirming that the same crystal (or identical crystals) were used throughout the mesh-and-collect experiment.
2. **High inner-shell data quality** – The inner resolution shells routinely show very high ⟨I/σ(I)⟩ (up to ~40) and CC½ > 0.99, indicating that the diffraction spots are strong and well measured.
3. **Low overall completeness** – Because each mesh-and-collect sub-dataset only samples a small portion of reciprocal space, overall completeness per sub-dataset is modest (7-15 %). The full experiment (combining all sub-datasets) would be expected to reach a much higher completeness.
4. **Resolution** – The majority of runs reach a high-resolution limit of **~1.64 Å**, sufficient for detailed atomic modelling of insulin and lysozyme.
5. **Anomalous signal** – No significant anomalous signal was detected, which is typical for native protein crystals without heavy-atom derivatization.
6. **Processing consistency** – All datasets were processed with the same pipeline (`grenades_fastproc` → `pyicat-plus_v0.9.1`) on ESRF HPC resources, ensuring comparable statistical treatment.

Conclusion

The mesh-and-collect experiment on the ID23-2 beamline generated a large set of high-resolution diffraction sub-datasets from insulin/lysozyme microcrystals. While each individual sub-dataset has limited completeness, the data quality within the measured resolution shells is excellent (high CC½, strong I/σ(I), and low R_merge/R_meas). When merged, these data should provide a robust structural model of the target proteins at ~1.6 Å resolution.

All information extracted from the dataset metadata supplied (27 re-processed integration datasets, IDs 2260453301 – 2260552388).

DRACBot: Utils



write a list of scp command lines that copies the data to demariaa@myhome:/data for the crystals that are not diffracting or resolution between 2 and 3 amstrongs

SCP commands for the datasets that show little or no diffraction (overall I/σ(I) < 1)

```
scp -r /data/visitor/ihls3744/id23eh2/20251001/PROCESSED_DATA/rco78_2/rco78_2-rco78_2/run_01_MeshAndCollect/run_01_68_datacollection/

scp -r /data/visitor/ihls3744/id23eh2/20251001/PROCESSED_DATA/rco78_2/rco78_2-rco78_2/run_01_MeshAndCollect/run_01_74_datacollection/

scp -r /data/visitor/ihls3744/id23eh2/20251001/PROCESSED_DATA/rco78_2/rco78_2-rco78_2/run_01_MeshAndCollect/run_01_135_datacollection

scp -r /data/visitor/ihls3744/id23eh2/20251001/PROCESSED_DATA/rco78_2/rco78_2-rco78_2/run_01_MeshAndCollect/run_01_59_datacollection/

scp -r /data/visitor/ihls3744/id23eh2/20251001/PROCESSED_DATA/rco78_2/rco78_2-rco78_2/run_01_MeshAndCollect/run_01_56_datacollection/

scp -r /data/visitor/ihls3744/id23eh2/20251001/PROCESSED_DATA/rco78_2/rco78_2-rco78_2/run_01_MeshAndCollect/run_01_88_datacollection/
```

DRACbot can make mistakes. Please check the output with the beamline scientist(s) to be sure.

Plans for the next six months

Final phase of replacing ISPyB with DRAC

From October 2025

- users are **encouraged** to use DRAC
- ISPyB expected as main LIMS

From January 2026

- Users are **requested** to use DRAC
- ISPyB can still be used (grace period)

From March 2026

- ISPyB can not be used for shipments
  - Ingestion of data will be stopped before end of 2026

Plans for the next six months

Strengthen Collaboration

EMBL:

Helping on the installation of DRAC software ecosystem in EMBL -HH
Helping on the development of the CRIMS-API

LNLS:

Work in progress adopting DRAC
Customization of sample tracking
Credits: Allan Pinto

SESAME:

DRAC was adopted few years ago

ALBA:

DRAC was adopted few years ago
ESRF is interested in adopting/collaborating with their new ingestion software

Work on improving the downloading of public data

"Pubic data" not really accessible (to me)?

Issue reported by Clemens 22/5/2025

- Restored data were not visible on Globus
- Prefers tar.gz files to zip because more robust
- (ESRF) PDB entries cite DOI for all data in session + not data only used for the reconstruction
- Globus is not an option for everyone - needs a login, would like a simple solution via command line

Ongoing improvements

1. Inform and follow-up with users to create bespoke DOIs with only data used in the reconstruction and cite the raw data DOIs in PDB
2. Provide a command line tool to download data in one command (aria2)
3. Automatically copy data to open area for Globus users
4. Implement restore request for data referenced in DOI directly in the data portal

- **What works -** restored open data can be downloaded with https if < 2GB and with Globus if requested (to be sure data are copied to the open area)
- **Why the problem(s) -** (1) we have a new archiving system which has slowed down the implementation of the improvements; (2) we need to train users to create bespoke DOIs and this takes time
- **A big thank you to Clemens** for testing and providing detailed feedback!
- **Our goal** remains FAIR data easily accessible to everyone!

Acknowledges

- Data Automation Unit
  - Marjolaine Bodin
  - Olof Svensson
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  - Matthew Bowler
  - Romain Talon
  - Andrew McCarthy
- MXCuBE
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  - Antonia Beteva
  - Yan Walesch
- Steering
  - Max Nanao
  - Andy Gotz
  - Vicente Rey