

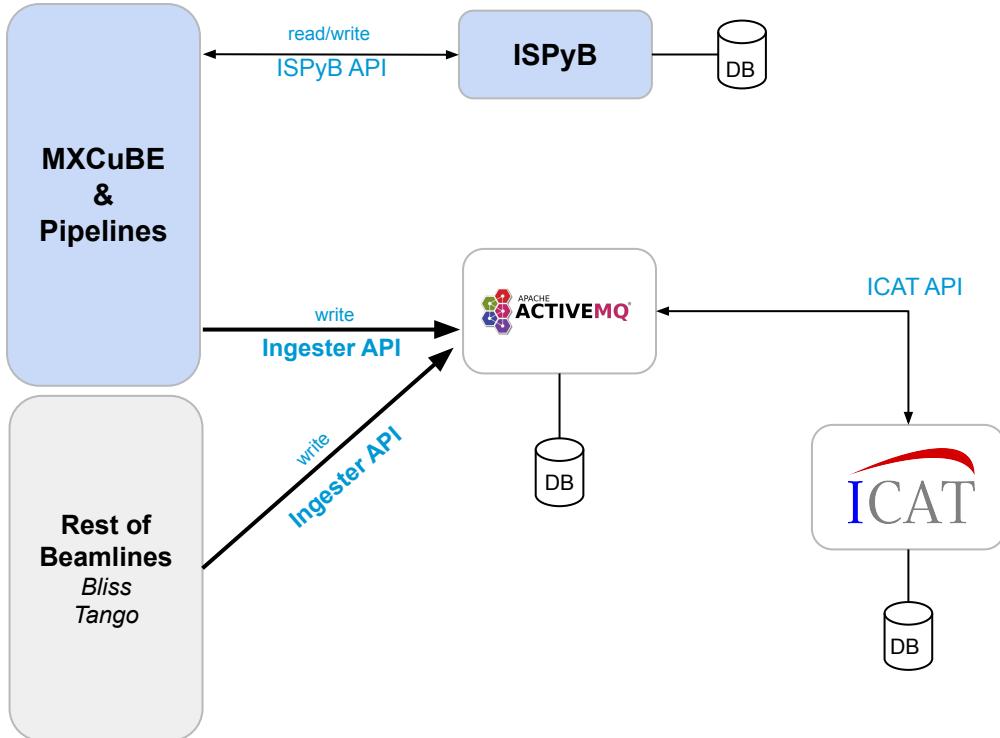
Transition from ISPyB to ICAT at ESRF

Alex DE MARIA
Data Manager
On behalf of
Software Group and Structural Biology group
MAXIV 28/05/2024

- March 2023 at Soleil
 - “**A proposal for a Next Generation of ISPyB Software**”
 - How a generic metadata catalog could replace ISPyB
 - Requested further evaluation and testing of a solution based on ICAT
- November 2023 at ALBA
 - “**MX on ICAT**”
 - Evaluation was satisfactory
 - Further development and deployment in real conditions
- Since last meeting
 - Weekly meetings with scientists
 - Deep discussions on how to present the data
 - Many iterations of the UI
 - Extending metadata
 - Integration with MXCuBE
 - Deployment on few beamlines

- Architecture
- New UI features
- Integration with MXCuBE
- Future developments and plans

Architecture: data ingestion



Ingestor API consists on

- a single endpoint
- STOMP Protocol

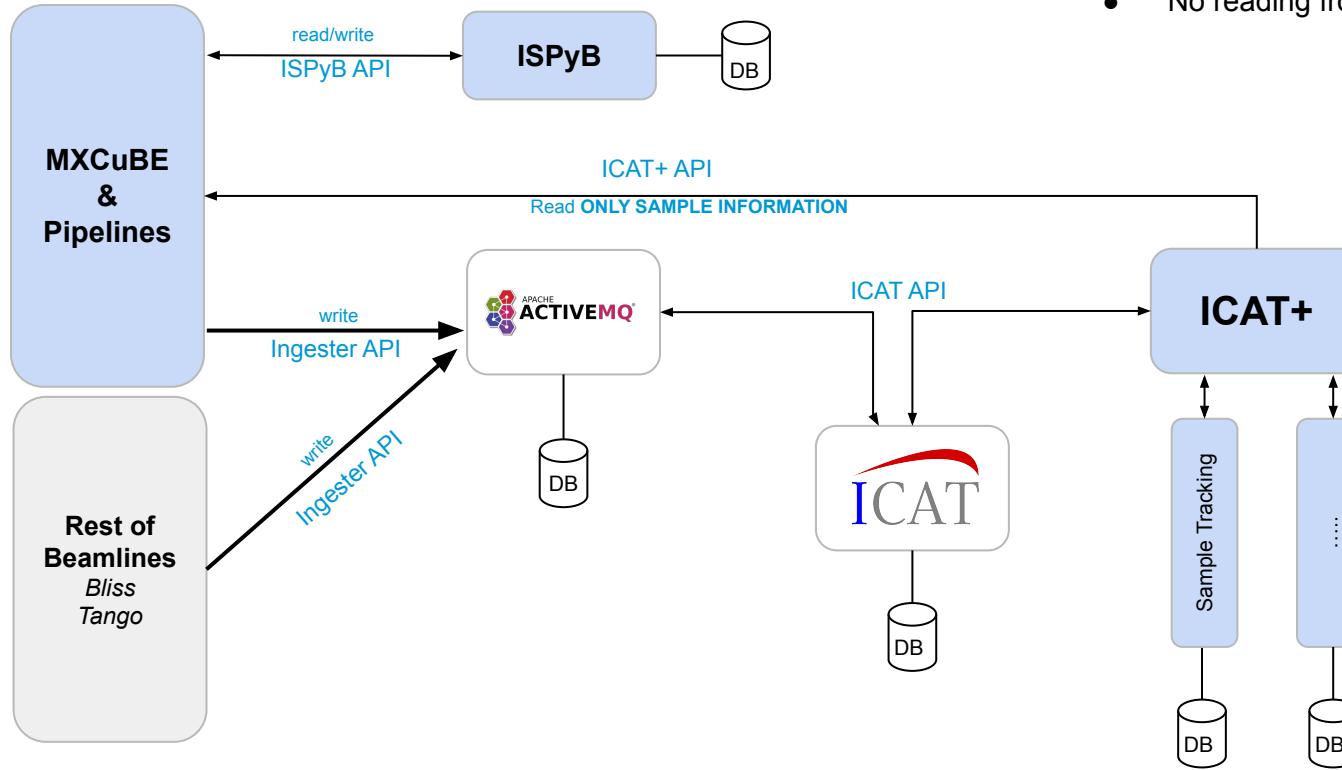
for:

- All beamlines
- Raw and processed

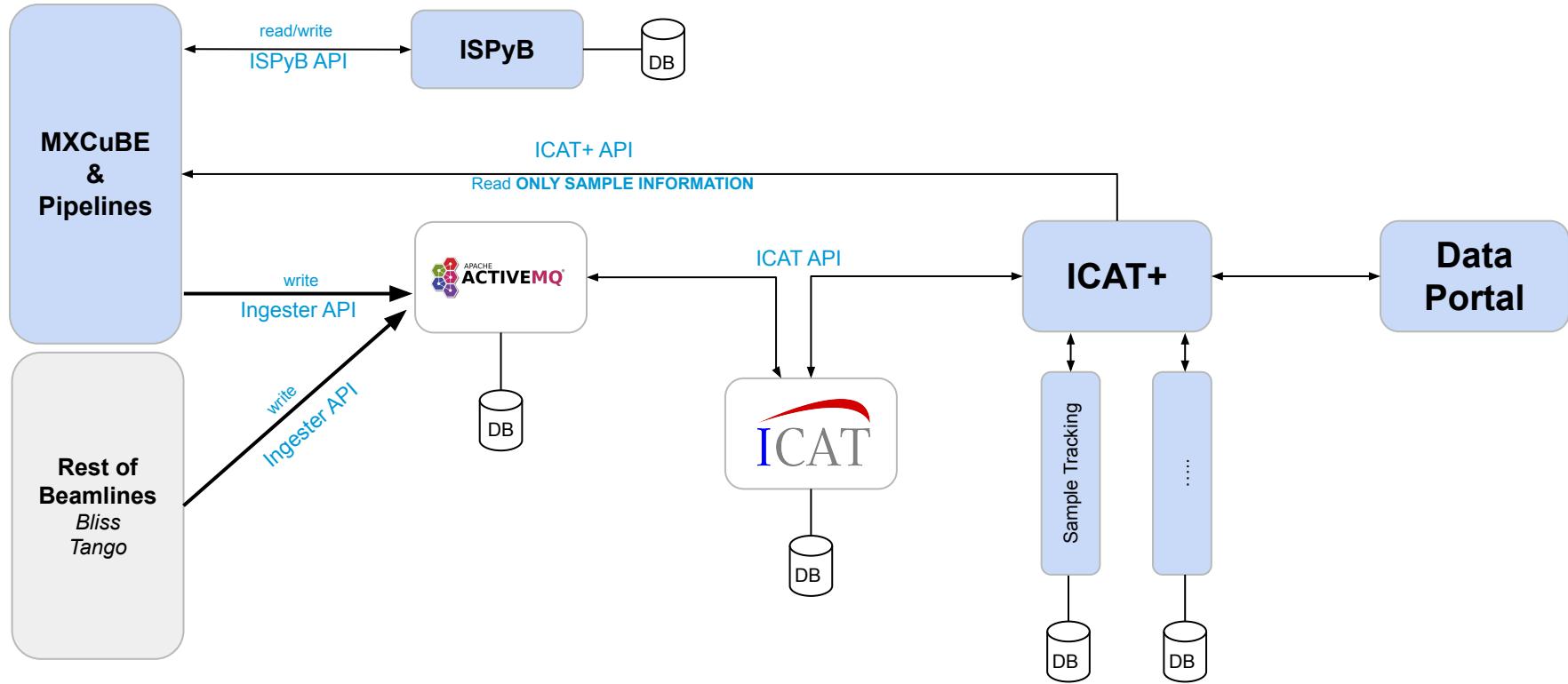
No developments done on:

- ICAT:
 - maintained by STFC
- ActiveMQ:
 - Apache

Architecture: sample synchronization

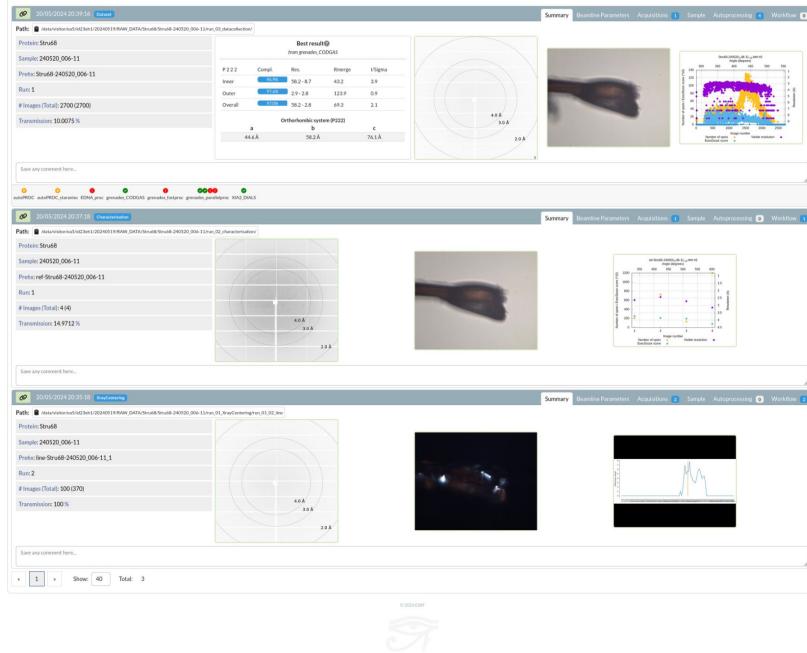


Architecture: user interface



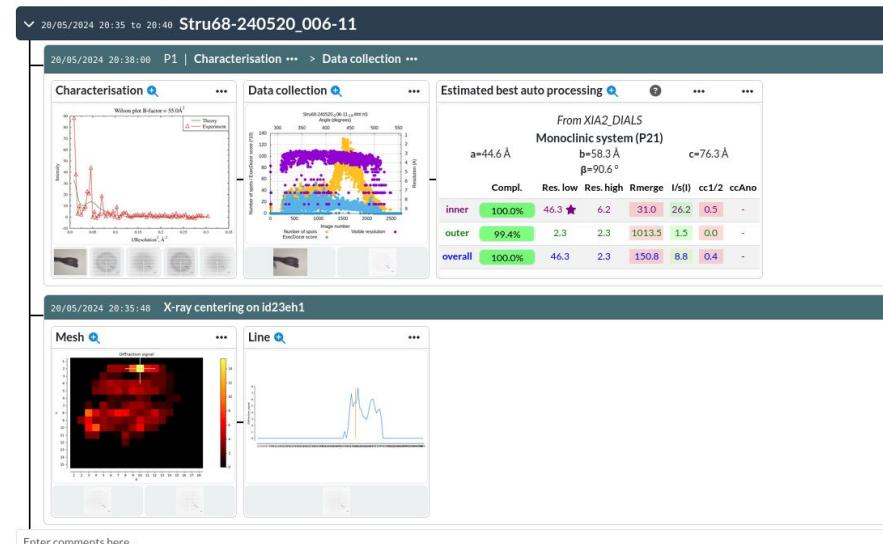
New UI features

A new display of the data



Visualization on py-ispyb

Example



Visualization on the Data portal

Grouped by sample and manual action

ESRF Data Portal Data Logistics Instruments My selection 2 My Jobs 7 Manager

Home / 04-3 [ID23-1] 19/05/2024 - 22/05/2024 / Datasets

Search in data portal... Help Alejandro DE MARIA

Sample: Stru68-240520_006-11

Items 1-1 of 1 Show 20

28/05/2024 20:38:00 P1 Characterisation ... > Data collection ...

Characterisation ... Data collection ... Estimated best auto processing ...

From XIA2_DIALS
Monoclinic system (P21)
 $a=44.6 \text{ \AA}$ $b=58.3 \text{ \AA}$ $c=76.3 \text{ \AA}$
 $\beta=90.6^\circ$

| | Compl. | Res. low | Res. high | Rmerge | $\lambda/\langle\lambda\rangle$ | cc1/2 | ccAno |
|---------|--------|----------|-----------|--------|---------------------------------|-------|-------|
| inner | 100.0% | 46.3 | 6.2 | 31.0 | 26.2 | 0.5 | - |
| outer | 99.4% | 2.3 | 2.3 | 1013.5 | 1.5 | 0.0 | - |
| overall | 100.0% | 46.3 | 2.3 | 150.8 | 8.8 | 0.4 | - |

28/05/2024 20:35:48 X-ray centering on id23eh1

Mesh ... Line ...

Enter comments here...

Items 1-1 of 1 Show 20 Add...

Investigation

- Experiment
- Statistics
- Samples 116
- Logbook
- Prepare

Datasets

View as:

- List
- Summary

Sample: Stru68-240520_006...

MX

Filter by type:

- Characterisation
- Datacollection
- Diffraction thumbnail
- Integration
- Line
- Mesh
- Quality indicator

Ranking shell:

- Inner

Ranking parameter:

- Res. low

Filter cutoffs:

- Add...

ESRF CORE INSTITUTE SEAL

Example

Data associated to datasets displayed as windows

ESRF Data Portal Data Logistics Instruments My selection 2 My Jobs 7 Manager

Search in data portal... Help Alejandro DE MARIA

Home / OA-5 ID23-1 19/05/2024 - 22/05/2024 / Datasets

Investigation

Experiment

Statistics

Samples 116

Logbook

Prepare

Datasets

View as: List Summary

Sample: Stru68-240520_006...

MX

Filter by type:

- Characterisation
- Datacollection
- Diffraction thumbnail
- Integration
- Line
- Mesh
- Quality indicator

Ranking shell:

Inner

Ranking parameter:

Res. low

Filter cutoffs:

Add...

Sample: Stru68-240520_006-11

Items 1-1 of 1 Show 20

20/05/2024 20:35 to 20:40 Stru68-240520_006-11

20/05/2024 20:38:00 P1 | Characterisation ... > Data collection ...

Characterisation

... Data collection

20/05/2024 20:35:48 X-ray centering on id23eh1

Mesh

Line

Enter comments here...

Characterisation

Report Dozor Metadata Sample Diffraction Files 17 ...

Characterisation Results

Indexing summary

| Selected spacegroup | a [Å] | b [Å] | c [Å] | alpha [°] | beta [°] | gamma [°] |
|---------------------|--------|--------|--------|-----------|----------|-----------|
| P2 | 44.560 | 58.310 | 76.500 | 90.000 | 91.470 | 90.000 |

Collection plan strategy: resolution limit is set according to the given max.time

| Wedge | Subwedge | Start (s) | Width (°) | No Images | Exp time (s) | Max res (Å) | Rel trans (%) | Distance (mm) |
|-------|----------|-----------|-----------|-----------|--------------|-------------|---------------|---------------|
| 1 | 1 | 69.00 | 0.25 | 616 | 0.035 | 3.21 | 14.97 | 543.26 |

Wavelength range vs diffraction angles

Wilson plot B factor = 55.0 Å²

Relative Intensity (a.u.) vs Resolution (Å)

Wilson plot B factor = 50.0 Å²

Relative Intensity (a.u.) vs Resolution (Å)

Wilson plot B factor = 50.0 Å²

Relative Intensity (a.u.) vs Resolution (Å)

phi_overlap

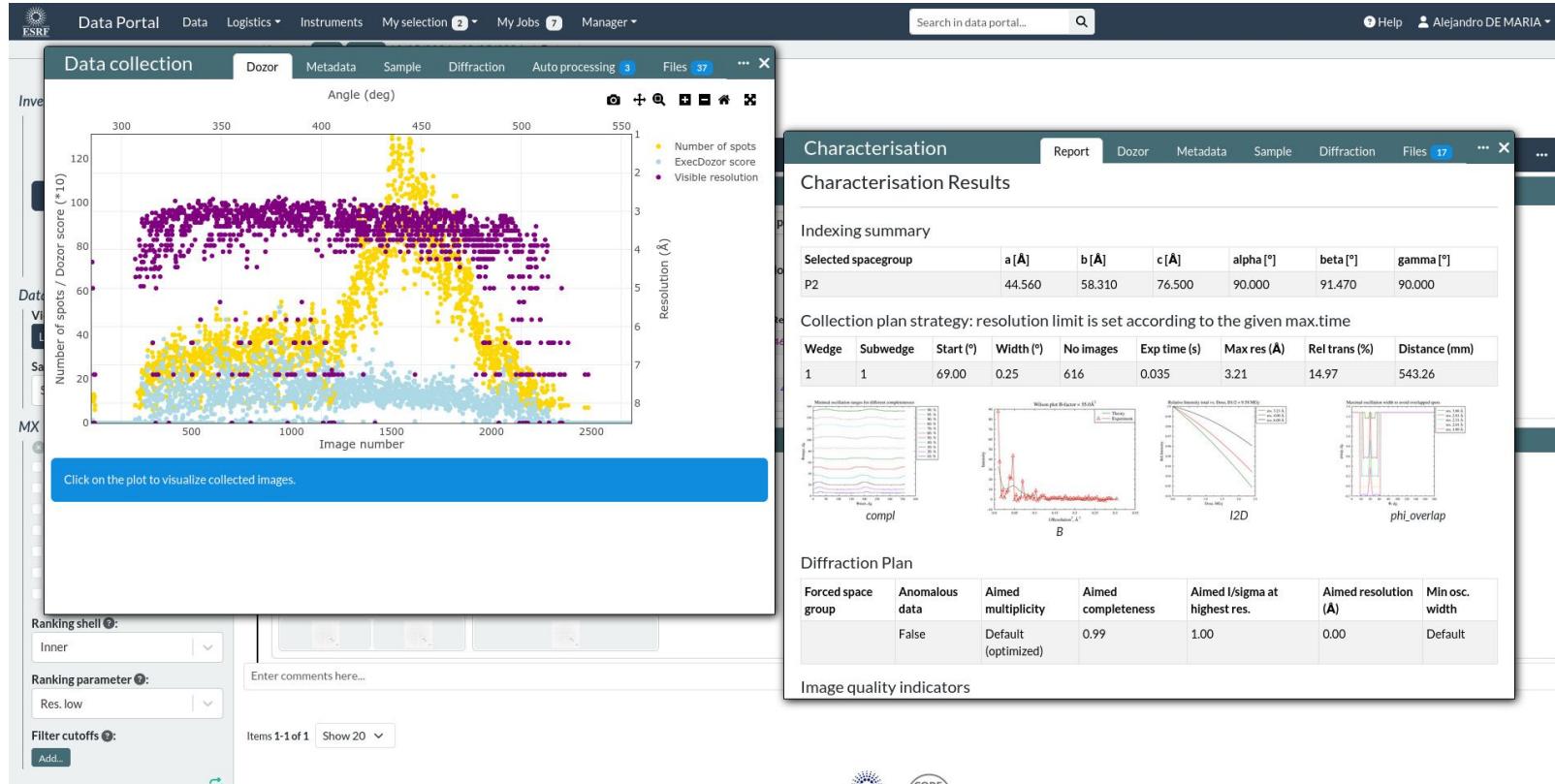
Diffraction Plan

| Forced space group | Anomalous data | Aimed multiplicity | Aimed completeness | Aimed I/sigma at highest res. | Aimed resolution (Å) | Min osc. width |
|--------------------|----------------|---------------------|--------------------|-------------------------------|----------------------|----------------|
| | False | Default (optimized) | 0.99 | 1.00 | 0.00 | Default |

Image quality indicators

Example

Data associated to datasets displayed as windows



Example

Filtering

ESRF Data Portal Data Logistics Instruments My selection 2 My Jobs 7 Manager

Home / MX ID30a-1 18/05/2024 – 18/05/2024 / Datasets

Search in data portal...

Help Alejandro DE MARIA

Investigation

Experiment Statistics Samples 31 Logbook Prepare

View as: List Summary

Sample: Type sample name

MX

Filter by type: Autoshell Characterisation Datacollection Diffraction thumbnail Integration Line Mesh Quality indicator

Ranking shell: Overall

Ranking parameter: Res. high

Filter cutoffs: Outer compl. < 99.5 Add...

Outer compl. < 99.5

Datacollection Outer compl. < 99.5

Page 1 of 2 Items 1-20 of 31 Show 20

17/05/2024 23:15 to 23:25 JNK1-CD040281_A05-1_3

17/05/2024 23:15:58 MXPressA: X-centre, eEDNA + dc on id30a1

Data collection

From XDSAPP Trigonal system (P3221)
 $a=b=136.8 \text{ \AA}$ $c=62.4 \text{ \AA}$

| | Compl. | Res. low | Res. high | Rmerge | I/s(l) | cc1/2 | ccAno |
|---------|--------|----------|-----------|--------|--------|-------|-------|
| inner | 99.5% | 46.1 | 8.3 | 5.7 | 30.4 | 1.0 | - |
| outer | 99.9% | 4.2 | 3.7 | 223.8 | 0.9 | 0.5 | - |
| overall | 99.9% | 46.1 | 3.7 | 32.2 | 5.9 | 1.0 | - |

Enter comments here...

17/05/2024 23:04 to 23:13 JNK1-CD040281_A05-1_2

17/05/2024 23:04:43 MXPressA: X-centre, eEDNA + dc on id30a1

Data collection

From grenades_parallelproc Hexagonal system (P622)
 $a=b=137.3 \text{ \AA}$ $c=64.2 \text{ \AA}$

| | Compl. | Res. low | Res. high | Rmerge | I/s(l) | cc1/2 | ccAno |
|---------|--------|----------|-----------|--------|--------|-------|-------|
| inner | 99.9% | 68.6 | 8.7 | 53.1 | 8.4 | 1.0 | - |
| outer | 100.0% | 3.3 | 3.1 | 291.2 | 0.9 | 0.3 | - |
| overall | 100.0% | 68.6 | 3.1 | 70.7 | 4.9 | 1.0 | - |

Enter comments here...

17/05/2024 22:57 to 23:02 JNK1-CD041648_G10-1_3

17/05/2024 22:57:30 MXPressA: X-centre, eEDNA + dc on id30a1

Example

Ranking of the results

Data Portal Data Logistics Instruments My selection 2 My Jobs 7 Manager Search in data portal... Help Alejandro DE MARIA

Home / MX-252 MX30A-1 18/05/2024 - 18/05/2024 / Datasets

Investigation

- Experiment
- Statistics
- Samples 31
- Logbook
- Prepare

Datasets

View as: List Summary

Sample: Type sample name

MX

Filter by type:

- Automesh
- Characterisation
- Datacollection
- Diffraction thumbnail
- Integration
- Line
- Mesh
- Quality indicator

Ranking shell:

Outer

Ranking parameter:

Res. high

Filter cutoffs:

Add...

Enter comments here...

Estimated best auto processing

| Program | a,b,c(Å) | α,β,γ(°) | Compl. | Res. low | Res. high | Rmerge | I/s() | cc1/2 | ccAno |
|-----------------------|----------|----------|----------------|----------|-----------|--------|-------|-------|-------|
| 17/05/2024 23:29 | 136.7 | 90.0 | inner 100.0% | 68.4 | 10.0 | 7.3 | 24.9 | 1.0 | - |
| XIA2_DIALS | 136.7 | 90.0 | outer 99.2% | 3.7 | 3.7 ★ | 372.5 | 0.2 | 0.3 | - |
| P3121 | 62.4 | 120.0 | overall 100.0% | 68.3 | 3.7 | 34.1 | 3.5 | 1.0 | - |
| 17/05/2024 23:27 | 136.8 | 90.0 | inner 99.5% | 46.1 | 8.3 | 5.7 | 30.4 | 1.0 | - |
| XDSAPP | 136.8 | 90.0 | outer 99.9% | 4.2 | 3.7 ★ | 223.8 | 0.9 | 0.5 | - |
| P3221 | 62.4 | 120.0 | overall 99.9% | 46.1 | 3.7 | 32.2 | 5.9 | 1.0 | - |
| 17/05/2024 23:26 | 136.4 | 90.0 | inner 97.0% | 46.0 | 15.7 | 6.4 | 25.9 | 1.0 | - |
| EDNA_proc | 136.4 | 90.0 | outer 100.0% | 4.2 | 4.1 ★ | 225.5 | 0.9 | 0.5 | - |
| P3121 | 62.3 | 120.0 | overall 99.9% | 46.0 | 4.1 | 25.8 | 6.1 | 1.0 | - |
| 17/05/2024 23:26 | 136.3 | 90.0 | inner 99.7% | 68.1 | 9.1 | 6.5 | 26.4 | 1.0 | - |
| grenades_fastproc | 136.3 | 90.0 | outer 99.9% | 4.6 | 4.1 ★ | 153.3 | 1.3 | 0.7 | - |
| P321 | 62.2 | 120.0 | overall 99.9% | 68.1 | 4.1 | 25.4 | 6.2 | 1.0 | - |
| 17/05/2024 23:28 | 136.6 | 90.0 | inner 99.8% | 68.3 | 9.4 | 5.9 | 28.2 | 1.0 | - |
| grenades_parallelproc | 136.6 | 90.0 | outer 99.0% | 4.7 | 4.2 ★ | 116.1 | 1.7 | 0.8 | - |
| P3121 | 62.3 | 120.0 | overall 99.7% | 68.3 | 4.2 | 23.0 | 7.1 | 1.0 | - |
| 17/05/2024 23:27 | 136.7 | 90.0 | inner 99.5% | 68.5 | 13.2 | 51.9 | 3.2 | 0.9 | - |
| grenades_parallelproc | 237.3 | 90.0 | outer 98.5% | 6.6 | 5.9 ★ | 82.9 | 1.1 | 0.8 | - |
| C222 | 62.4 | 90.0 | overall 99.5% | 68.5 | 5.9 | 65.6 | 2.1 | 0.9 | - |
| 17/05/2024 23:33 | 237.3 | 90.0 | inner 99.8% | 68.5 | 14.1 | 6.1 | 8.1 | 1.0 | - |
| autoPROC_staransio | 136.6 | 90.3 | outer 58.4% | 4.5 | 3.8 ★ | 71.7 | 1.8 | 0.7 | - |
| C2 | 62.4 | 90.0 | overall 81.5% | 68.5 | 3.8 | 17.9 | 3.7 | 1.0 | - |
| 17/05/2024 23:33 | 237.3 | 90.0 | inner 99.9% | 68.5 | 11.6 | 5.9 | 8.2 | 1.0 | - |
| autoPROC | 136.6 | 90.3 | outer 99.8% | 4.4 | 4.3 ★ | 171.8 | 0.6 | 0.4 | - |
| C2 | 62.4 | 90.0 | overall 99.9% | 68.5 | 4.3 | 32.9 | 2.5 | 1.0 | - |
| 17/05/2024 23:27 | 62.1 | 119.9 | inner 97.2% | 68.1 | 11.8 | 3.6 | 13.7 | 1.0 | - |

Data collection

Estimated best auto processing

From XIA2_DIALS
Trigonal system (P3121)
a=b=136.7 Å c=62.4 Å

| inner | outer | overall | Compl. | Res. low | Res. high | Rmerge | I/s() | cc1/2 | ccAno |
|--------|-------|---------|--------|----------|-----------|--------|-------|-------|-------|
| 100.0% | 99.2% | 100.0% | 68.4 | 10.0 | 7.3 | 24.9 | 1.0 | - | - |
| 99.2% | 3.7 | 3.7 | 3.7 ★ | 372.5 | 0.2 | 0.3 | - | - | - |
| 100.0% | 68.3 | 3.7 | 34.1 | 3.5 | 1.0 | - | - | - | - |

Data collection

Estimated best auto processing

From grenades_parallelproc
Hexagonal system (P622)
a=b=137.3 Å c=64.2 Å

| inner | outer | overall | Compl. | Res. low | Res. high | Rmerge | I/s() | cc1/2 | ccAno |
|--------|--------|---------|--------|----------|-----------|--------|-------|-------|-------|
| 99.9% | 100.0% | 99.9% | 68.6 | 8.7 | 53.1 | 8.4 | 1.0 | - | - |
| 100.0% | 3.3 | 3.1 | 3.1 ★ | 291.2 | 0.9 | 0.3 | - | - | - |
| 100.0% | 68.6 | 3.1 | 70.7 | 4.9 | 1.0 | - | - | - | - |

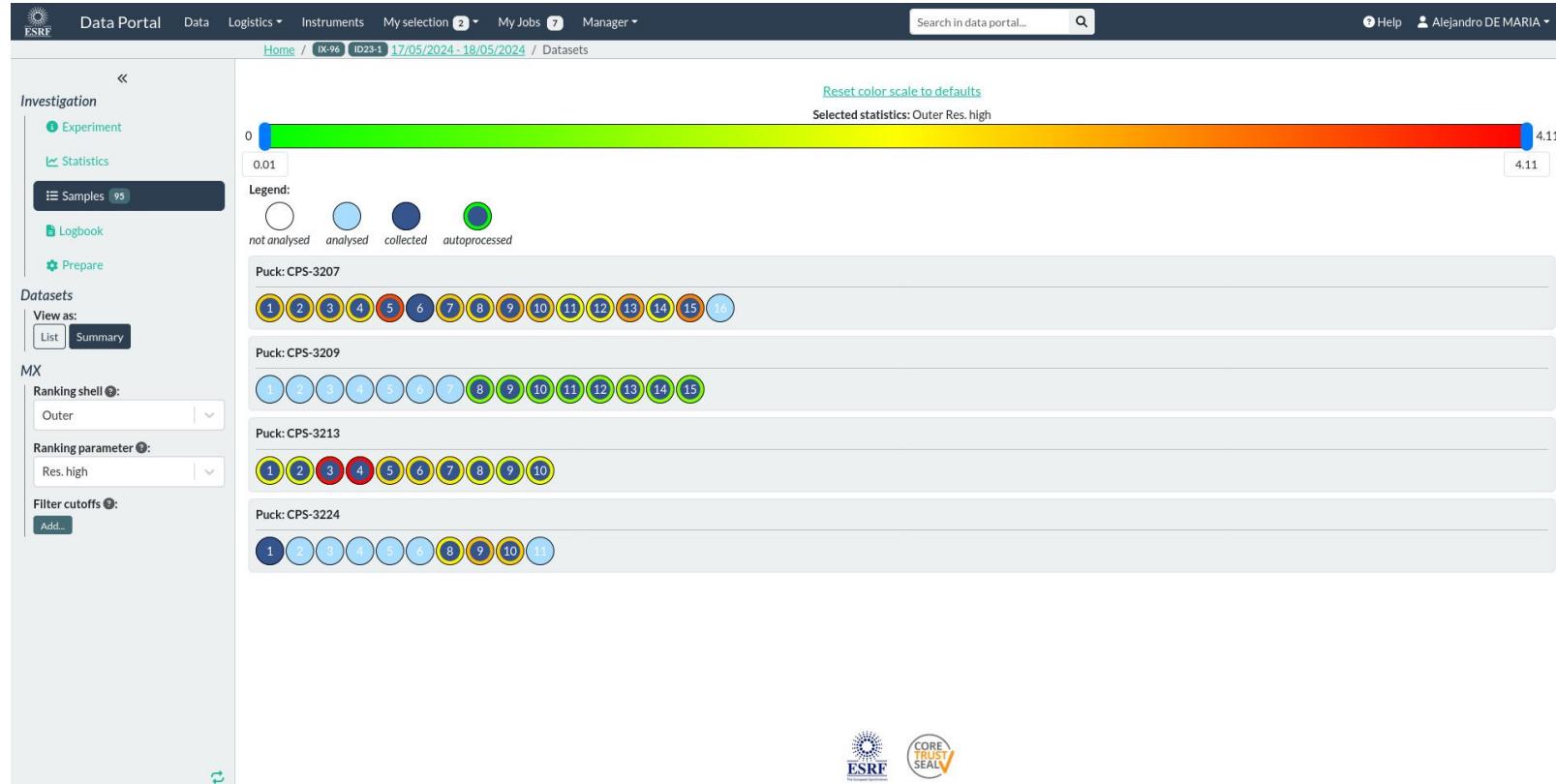
Enter comments here...

17/05/2024 22:57 to 23:02 JNK1-CD041648_G10-1_3

17/05/2024 22:57:30 MXPressA: X-centre, eEDNA + dc on id30a1

Example

Summary view



Example



File Browser

ESRF Data Portal Data Logistics Instruments My selection 2 My Jobs 7 Manager Search in data portal... Help Alejandro DE MARIA

Home / OA-5 ID23-1 190 Data collection Dozor Metadata Sample Diffraction Auto processing 3 Files 37

Investigation

- Experiment
- Statistics
- Samples 116
- Logbook
- Prepare

View as:

- List
- Summary

Sample: Stru68-240520_006...

MX

- Filter by type:
 - Characterisation
 - Datacollection
 - Diffraction thumbnail
 - Integration
 - Line
 - Mesh
 - Quality indicator

Ranking shell:

- Inner

Ranking parameter:

- Res. low

Filter cutoffs:

- Add...

Enter comments here...

Items 1-1 of 1 Show 20

Sample: Stru68-240520_006-11

28/05/2024 20:35 to 28/05/2024 20:38:00 P1

Characterisation

Wilson plot B-factor = 55.08

28/05/2024 20:35:48 X-ray

Mesh

Diffractogram

Enter comments here...

Items 1-1 of 1 Show 20

Search for a file

- Stru68-240520_006-11_1_1_data_000001.h5
- Stru68-240520_006-11_1_1_data_000002.h5
- Stru68-240520_006-11_1_1_data_000003.h5
- Stru68-240520_006-11_1_1_data_000004.h5
- Stru68-240520_006-11_1_1_data_000005.h5
- Stru68-240520_006-11_1_1_data_000006.h5
- Stru68-240520_006-11_1_1_data_000007.h5
- Stru68-240520_006-11_1_1_data_000008.h5
- Stru68-240520_006-11_1_1_data_000009.h5
- Stru68-240520_006-11_1_1_data_000010.h5
- Stru68-240520_006-11_1_1_data_000011.h5
- Stru68-240520_006-11_1_1_data_000012.h5
- Stru68-240520_006-11_1_1_data_000013.h5
- Stru68-240520_006-11_1_1_data_000014.h5
- Stru68-240520_006-11_1_1_data_000015.h5
- Stru68-240520_006-11_1_1_data_000016.h5
- Stru68-240520_006-11_1_1_data_000017.h5
- Stru68-240520_006-11_1_1_data_000018.h5
- Stru68-240520_006-11_1_1_data_000019.h5
- Stru68-240520_006-11_1_1_data_000020.h5
- Stru68-240520_006-11_1_1_data_000021.h5
- Stru68-240520_006-11_1_1_data_000022.h5
- Stru68-240520_006-11_1_1_data_000023.h5
- Stru68-240520_006-11_1_1_data_000024.h5
- Stru68-240520_006-11_1_1_data_000025.h5
- Stru68-240520_006-11_1_1_data_000026.h5
- Stru68-240520_006-11_1_1_data_000027.h5
- Stru68-240520_006-11_1_1_master.h5

gallery

- Stru68-240520_006-11_1_1.snapshot.jpeg

process

- x_geo_corr.cbf.bz2
- y_geo_corr.cbf.bz2
- hk12000_Stru68-240520_006-11_run1_1.def.site

Items 1-1 of 1 Show 20

File collection

Dozor

Metadata

Sample

Diffraction

Auto processing

Feedback

Matrix Line Heatmap

data

4.295e+9

4e+3
2e+3
0

0 1e+3 2e+3 3e+3 4e+3

Open viewer

ESRF CORE

Example

Sample Changer/Prepare Experiment

- No shipments
- Independent parcels status
- Processing plans

The screenshot shows the ESRF Data Portal interface with the 'Prepare' tab selected. On the left, there's a sidebar with 'Parcels' and search/filter options. The main area displays three parcels:

| Name | Items # | Status | Dangerous goods | After experiment | Sender |
|---------------|---------|-----------|-----------------|------------------|---|
| My 3rd parcel | 1 | SCHEDULED | No | Destroy | John Doe European Synchrotron Radiation Facility (ESRF) 71 Av des Martyrs 38000 Grenoble France |
| My 2nd Parcel | 2 | STORES | No | Destroy | John Doe European Synchrotron Radiation Facility (ESRF) 71 Av des Martyrs 38000 Grenoble France |
| My 1st Parcel | 1 | SENT | No | Destroy | John Doe European Synchrotron Radiation Facility (ESRF) 71 Av des Martyrs 38000 Grenoble France |

At the bottom right, there are logos for ESRF, CORE, and SEAL.

Example

Sample Changer/Prepare Experiment

ESRF Data Portal Data Logistics Instruments My selection 2 My Jobs 7 Manager Search in data portal... Help Alejandro DE MARIA

Home / ID23-12401 ID23-1 10/01/2024- 10/02/2024 / Logistics / Sample changer

Investigation < Investigation

- Experiment
- Statistics
- Samples
- Logbook
- Prepare**

Prepare

- Logistics
- Sample changer**

Parcels

My 1st Parcel My 2nd Parcel My 3rd parcel

SPINE1 test 3-3

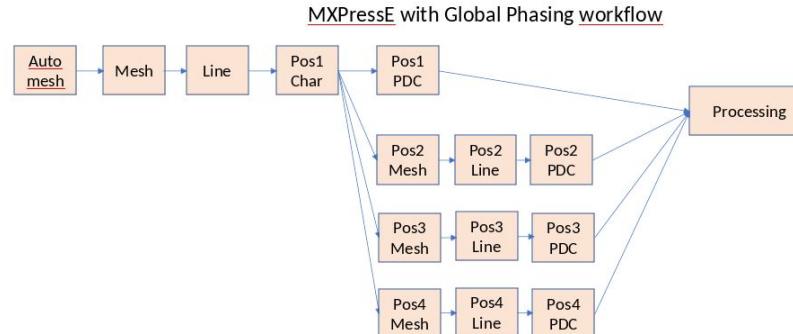
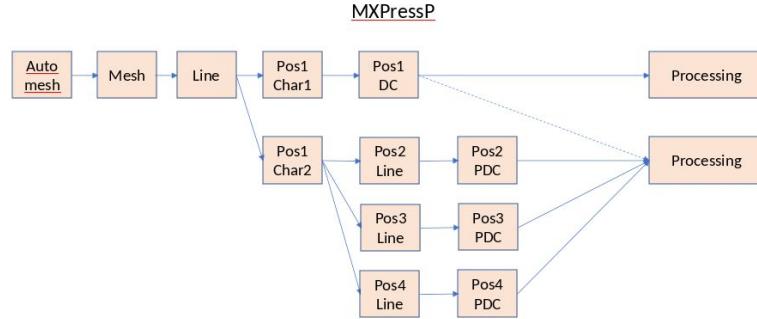
ID23-1 sample changer

Changer Simplified Unload all

[My 3rd parcel]

Example

Merging of multi sweep data



Example

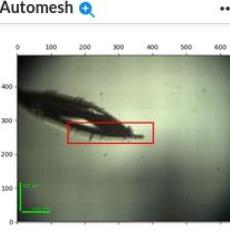
Merging of multi sweep data

MXPress P: performs a pseudo-helical data collection on positions determined within a crystal

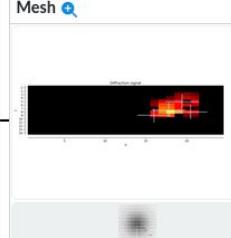
03/04/2024 10:47 to 10:57 **2024-04-03-8** ...

03/04/2024 10:47:36 MXPressP: Pseudo helical on id30a2

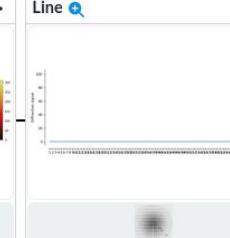
Automesh ...



Mesh ...



Line ...



2 characterisations
3 positions +

Estimated best merged auto processing ...

From autoPROC Merged

Trigonal system (P3112)

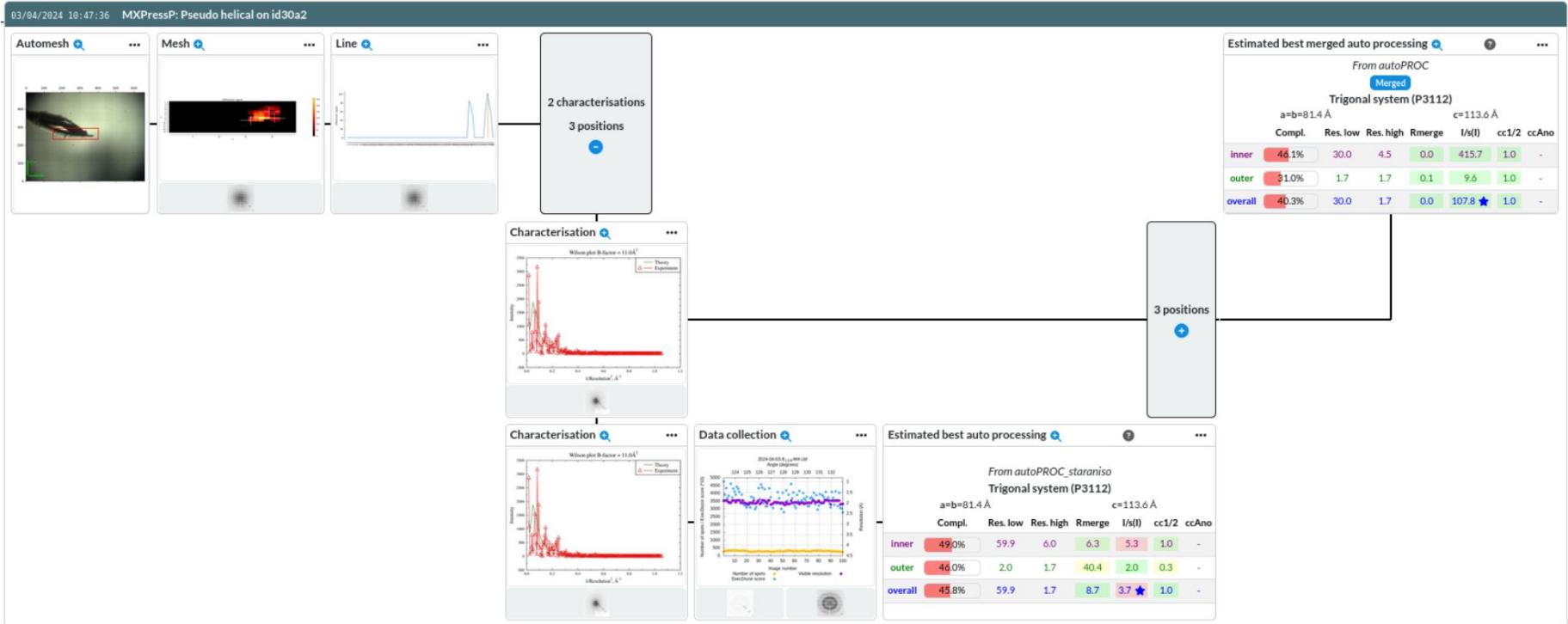
| | a=b=81.4 Å | c=113.6 Å |
|---------|------------|----------------------------|
| Compl. | | |
| inner | 46.1% | 30.0 4.5 0.0 415.7 1.0 - |
| outer | 31.0% | 1.7 1.7 0.1 9.6 1.0 - |
| overall | 40.3% | 30.0 1.7 0.0 107.8 ★ 1.0 - |

Enter comments here...

Example

Merging of multi sweep data

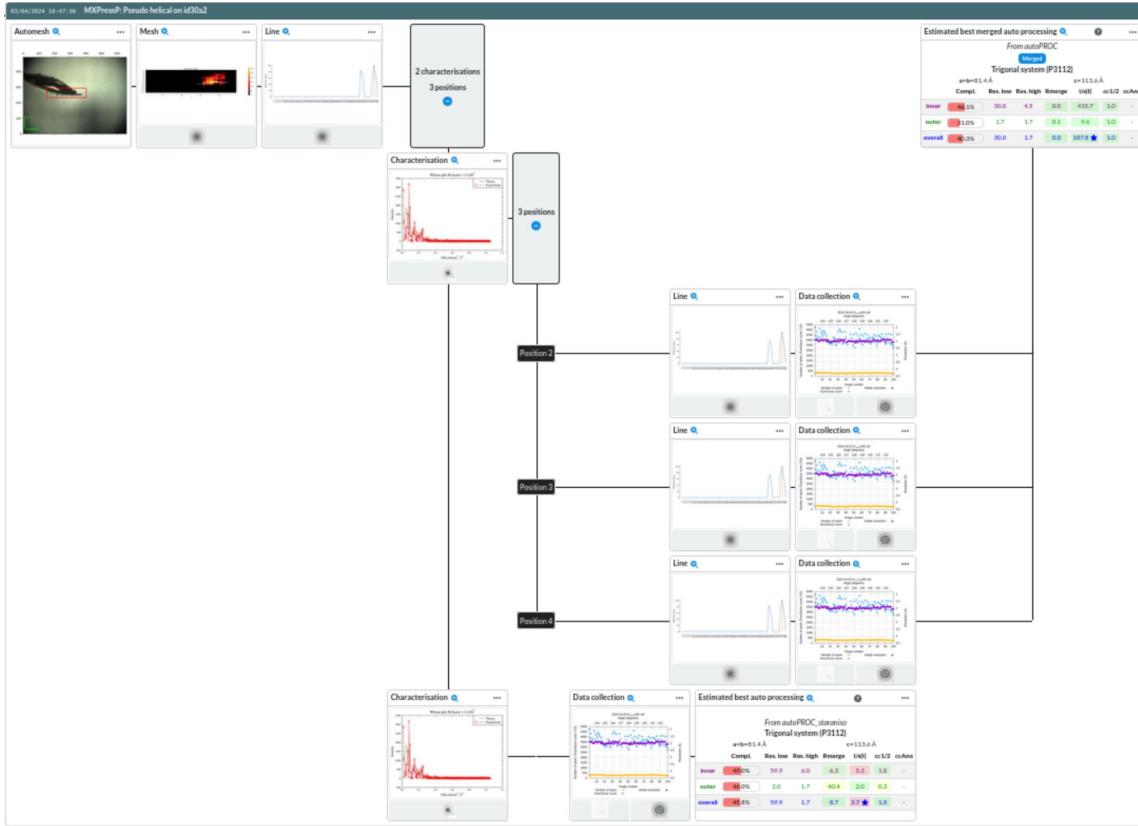
MXPress P: performs a pseudo-helical data collection on positions determined within a crystal



Example

Merging of multi sweep data

MXPress P: performs a pseudo-helical data collection on positions determined within a crystal



Multiple positions with low symmetry and kappa open

ESRF Data Portal Data Logistics Instruments My selection 1 My Jobs 97 Manager

Search in data portal...

Help adminFullName

Home / MX-2112 ID30a-2 05/07/2023 / Datasets

Sample: 2024-04-03-6

Items 1-1 of 1 Show 20

Investigation

Experiment

Statistics

Samples 231

Jobs 83

Logbook

Prepare

Datasets

View as: List Summary

Sample: 2024-04-03-6

MX

Filter by type: Helical Mesh Os c Automesh Characterisation Datacollection Line Mesh

Ranking shell: Overall

Ranking parameter: $I(s)$

Filter cutoffs: Add...

2024-04-03-6

03/04/2024 10:27:13 MXPressA: X-centre, eEDNA + dc on id30a2

Automesh Mesh 4 kappa settings 2 positions

Line Characterisation Position 1

Line Characterisation Position 2

Estimated best merged auto processing

From autoPROC Merged Trigonal system (P3112) $a=b=81.4\text{\AA}$ $c=113.6\text{\AA}$

| | Compl. | Res. low | Res. high | Rmerge | $I(s)/0$ | $c\bar{c}Ano$ |
|---------|--------|----------|-----------|--------|----------|---------------|
| inner | 45% | 44.2 | 4.5 | 0.0 | 236.6 | 1.0 |
| outer | 34.1% | 1.7 | 1.7 | 0.2 | 4.5 | 0.9 |
| overall | 41.7% | 44.2 | 1.7 | 0.0 | 57.3 | 1.0 |

Enter comments here...

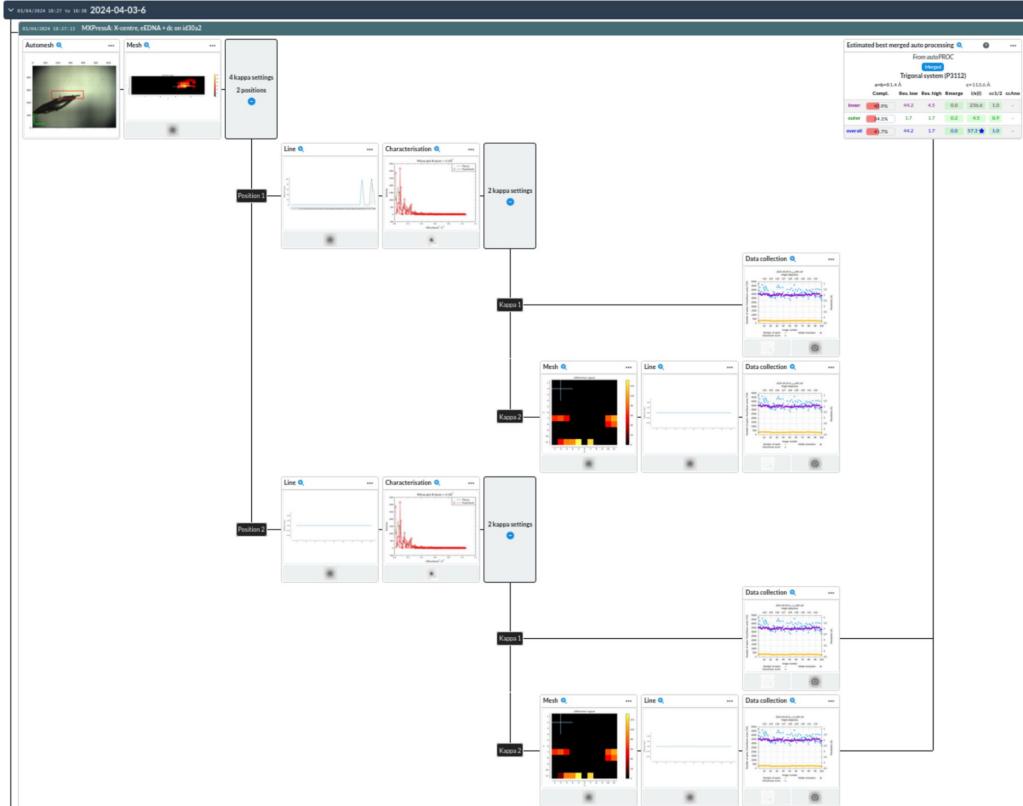
Items 1-1 of 1 Show 20

The screenshot shows the ESRF Data Portal interface. On the left, there's a sidebar with navigation links like 'Investigation', 'Samples', 'Jobs', 'Logbook', 'Prepare', and 'Datasets'. Under 'Datasets', it shows a sample named '2024-04-03-6'. The main area displays a timeline from '03/04/2024 10:27:13' to 'MXPressA: X-centre, eEDNA + dc on id30a2'. Below this, there are several processing steps: 'Automesh' (with a thumbnail of a protein structure), 'Mesh' (with a thumbnail of a density map), '4 kappa settings 2 positions' (with a large central box), 'Line' (with a plot of intensity vs. scattering vector), and 'Characterisation' (with two plots of intensity vs. scattering vector). To the right, there's a summary table for 'Estimated best merged auto processing' from 'autoPROC' for a 'Trigonal system (P3112)' with unit cell parameters $a=b=81.4\text{\AA}$ and $c=113.6\text{\AA}$. The table includes columns for 'Compl.', 'Res. low', 'Res. high', 'Rmerge', ' $I(s)/0$ ', and ' $c\bar{c}Ano$ '. It shows data for 'inner' (45%), 'outer' (34.1%), and 'overall' (41.7%) shells. At the bottom, there's a text input field for 'Enter comments here...'.

Example



Multiple positions with low symmetry and kappa open



Example

Integration with ICAT

- Selected based on experiment session instead of proposal
- Richer metadata. E.g:
 - Crystal position
 - Characterisation Identifier
- Possibility to select a session from:
 - Different time slot
 - Different beamline (when configured)
- ICAT Synchronization (ongoing)

MXCuBE-Web (osc)

Beamline Actions ▾ Energy: 12.4000 keV Res...
Wavelength: 1.00 Å Det...

Phase Control: Centring
Beam size: 10
Omega: 311.10 ▾ 90.0 °
Kappa: 11.0 ▾ 0.1 °
Kappa Phi: 22.0 ▾ 0.1 °
Sample alignment: Show motors ▾

50 μm

Samples Data collection Equipment System log Help Remote Select proposal (None/None) Sign out (demariaa)

Sample Changer Fast Shutter Safety shutter Ring Current
READY CLOSED CLOSED 189.0 mA

Settings Queued Samples (0)

Select a session

Scheduled Non scheduled

OA6 [REDACTED]
Start Date: 20/02/2024 09:30:00 End Date: 23/02/2024 08:00:00 Shortcuts: [Portal](#) [A-Form](#) [Logbook](#)

OA5 [REDACTED]
Start Date: 20/02/2024 09:30:00 End Date: 23/02/2024 08:00:00 Shortcuts: [Portal](#) [A-Form](#) [Logbook](#)

OA4 [REDACTED]
Start Date: 20/02/2024 09:30:00 End Date: 23/02/2024 08:00:00 Shortcuts: [Portal](#) [A-Form](#) [Logbook](#)

OA3 [REDACTED]
Start Date: 20/02/2024 09:30:00 End Date: 23/02/2024 08:00:00 Shortcuts: [Portal](#) [A-Form](#) [Logbook](#)

Cancel Select Proposal

Log messages:

Allows to beamline manager to reschedule or move experiment sessions

MXCuBE-Web (osc)

Energy: 12.4000 keV Wavelength: 1.00 Å

Samples Data collection Environment System icon Help Remote Select proposal (NoneNone) Sign out (demariaa)

Beamline Actions Samples Data collection Environment System icon Help Remote Select proposal (NoneNone) Sign out (demariaa)

Phase Control: Centring Beam size: 10 Omega: 311.10 Kappa: 11.0 Kappa Phi: 22.0

Sample alignment:

50 µm

Select a session

Scheduled Non scheduled

IX98 [REDACTED]

| | | | |
|---------------------|---------------------|----------|---|
| Start Date | End Date | Beamline | Shortcuts |
| 17/02/2024 17:00:00 | 18/02/2024 01:00:00 | ID23-1 | Portal A-Form Logbook |

FX29 [REDACTED]

| | | | |
|---------------------|---------------------|----------|---|
| Start Date | End Date | Beamline | Shortcuts |
| 22/02/2024 09:30:00 | 22/02/2024 17:00:00 | ID30A-1 | Portal A-Form Logbook |

MX2503 PROTEINS RELATED TO PATHOGENESIS OF DISEASES, VIRAL PROTEINS, CELL DIVISION, SIGNALLING AND CHROMATIN PROCESSES

| | | | |
|---------------------|---------------------|----------|---|
| Start Date | End Date | Beamline | Shortcuts |
| 17/02/2024 09:30:00 | 18/02/2024 01:00:00 | ID30A-1 | Portal A-Form Logbook |

Cancel Select Proposal

Log messages:

Sample Changer Fast Shutter Safety shutter Ring Current

READY CLOSED CLOSED 185.5 mA

Settings Queued Samples (0)

Missing bits and future plans

- Data catalog/LIMS
 - Add Phasing and SAD (ongoing)
 - Add missing metadata
 - Test with friendly users
- MXCuBE
 - ICAT sample synchronization (ongoing)
 - Do some abstraction that allows to send data to both ISPyB and ICAT (ongoing)
- Plans
 - Roll out with full functionality on the beamlines by September
 - Use both ISPyB/ICAT in parallel for the time being
 - Help other partners willing to adopt this software solution

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Architecture and services

