# py-ISPyB

## Framework
## &
## Serial crystallography use case

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# py-ISPyB Technical context

## New server side

- Technical redesign
- Implementation language changed from Java to Python
- Modern API (REST)
- Includes new administrative & scientific requirements
- Backwards compatibility + new features

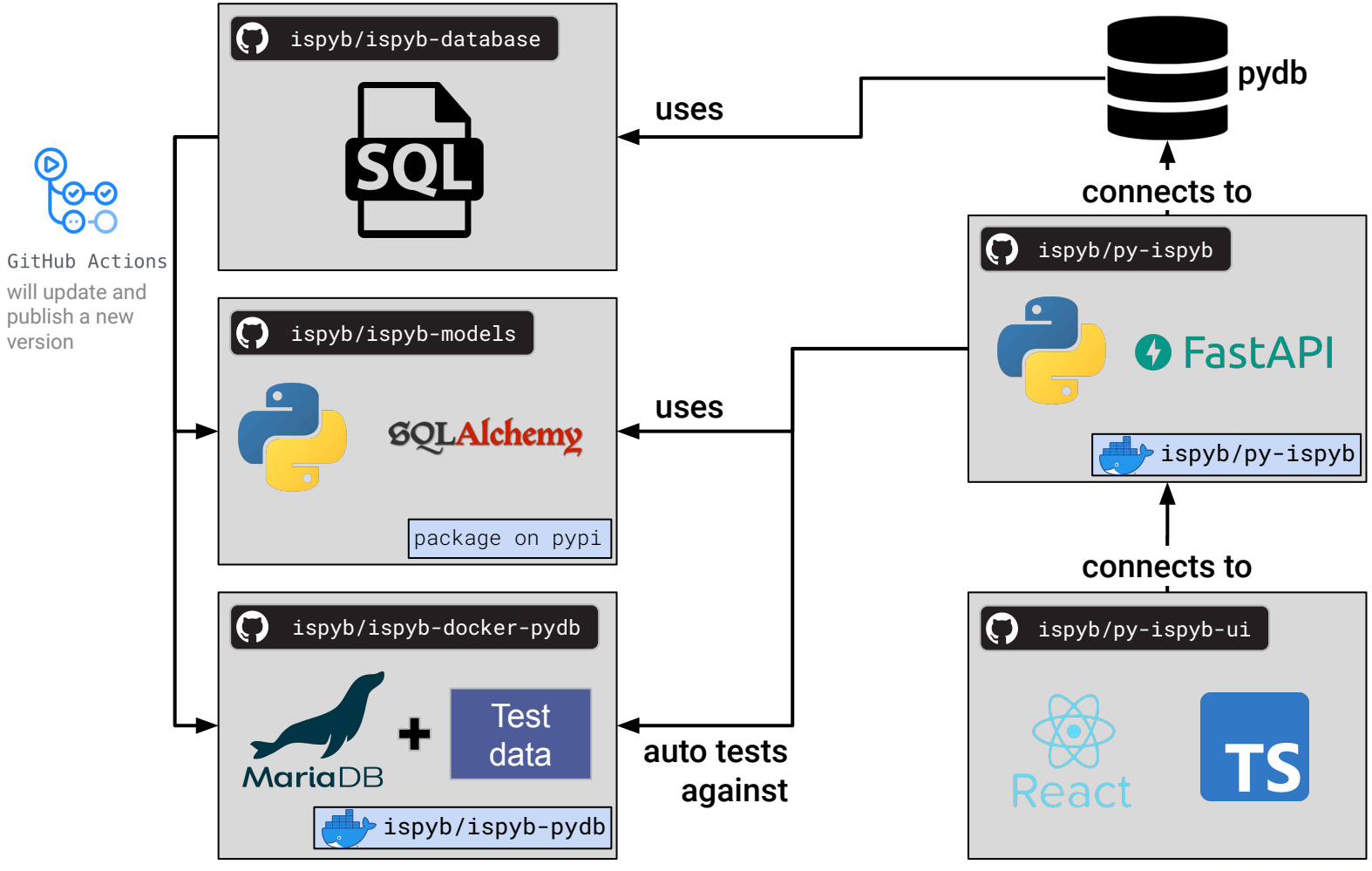
# py-ISPyB Technical context

## New user interface

- Latest frontend technologies (React v18)
- Easy to extend
- Backwards compatibility with limited functionalities

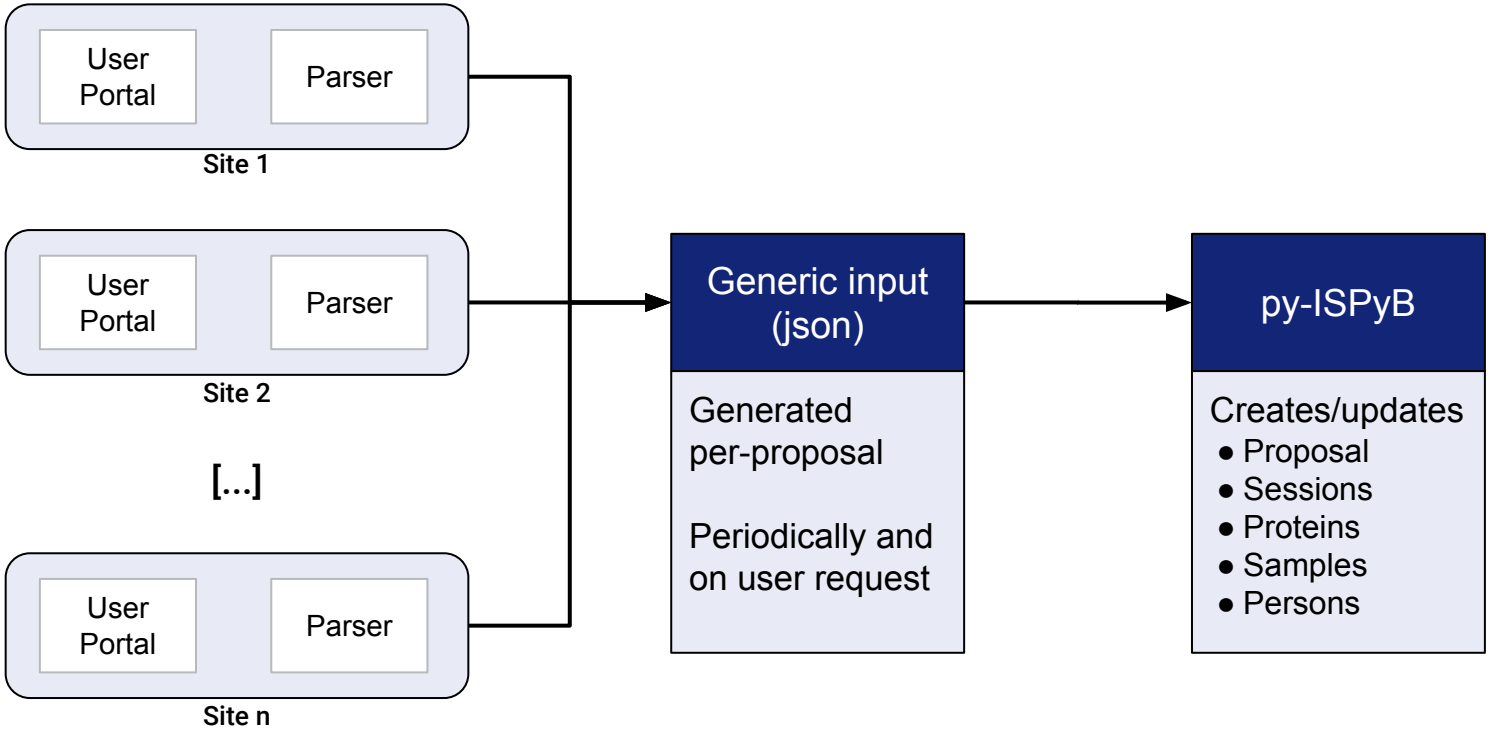
# Status

# Architecture

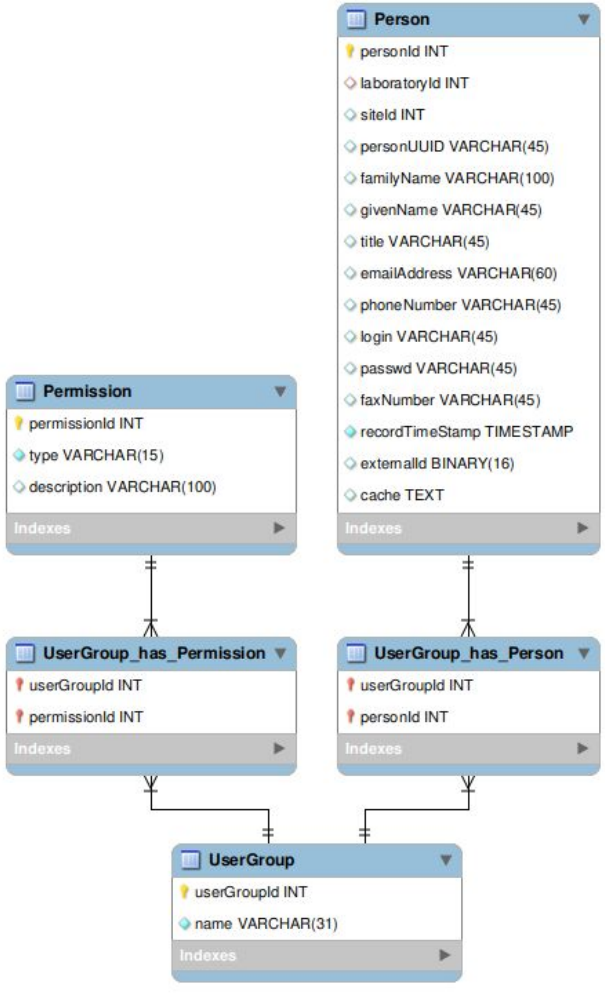


# User Portal Sync

Developed a generic mechanism to synchronize the data from the User Portal.

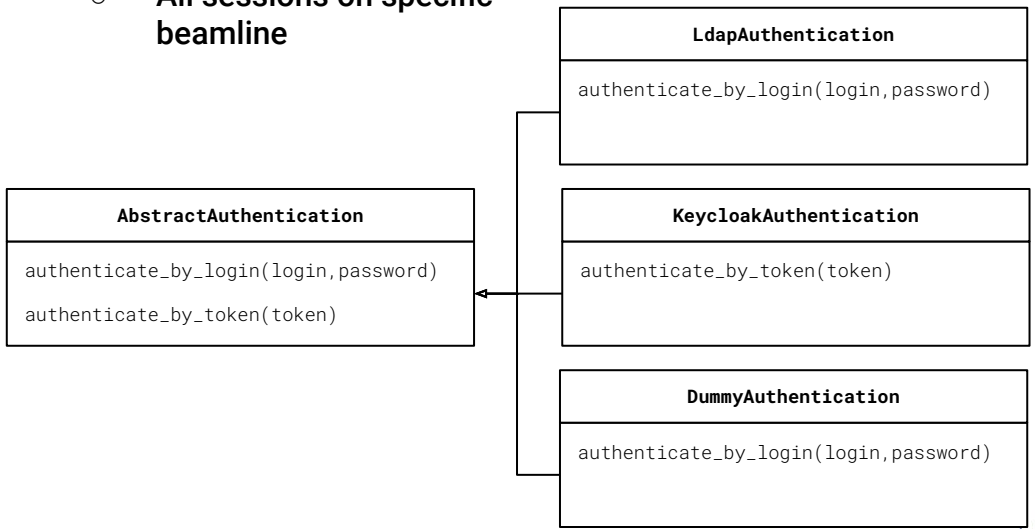


# Authentication/Authorization




- Groups & permission centralized in DB
- Multiple authentication mechanisms
  - Natively supports:
    - LDAP
    - Keycloak
    - Dummy *(For developments)*
  - Possibility to add your own auth ***via plugin***

- Authorization possible for:
  - **Whole proposal** *(from user portal)*
  - **Individual sessions** *(from user portal)*
  - **All sessions on specific beamline**

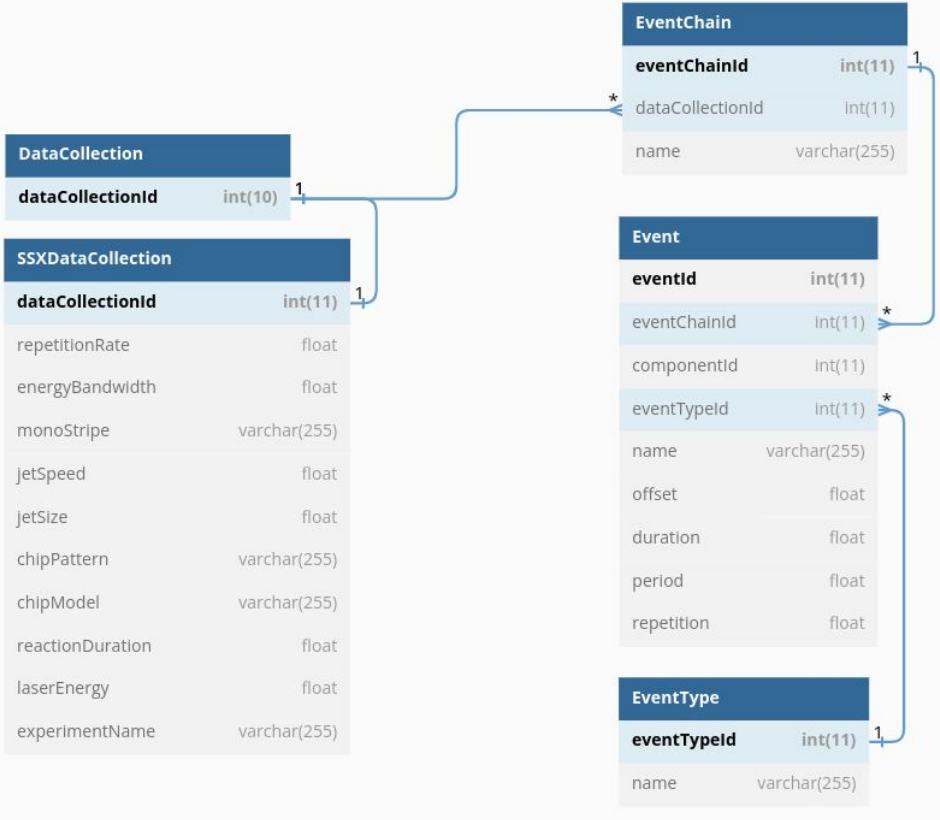


# First use case: Serial synchrotron crystallography

# MX VS SSX

| MX | SSX |
| --- | --- |
| 1 crystal | Many crystals |
| Many images | 1 image per crystal |
| Rotation | Static |
| Frozen loop | Chip or jet |

# Database extension - Experiment events



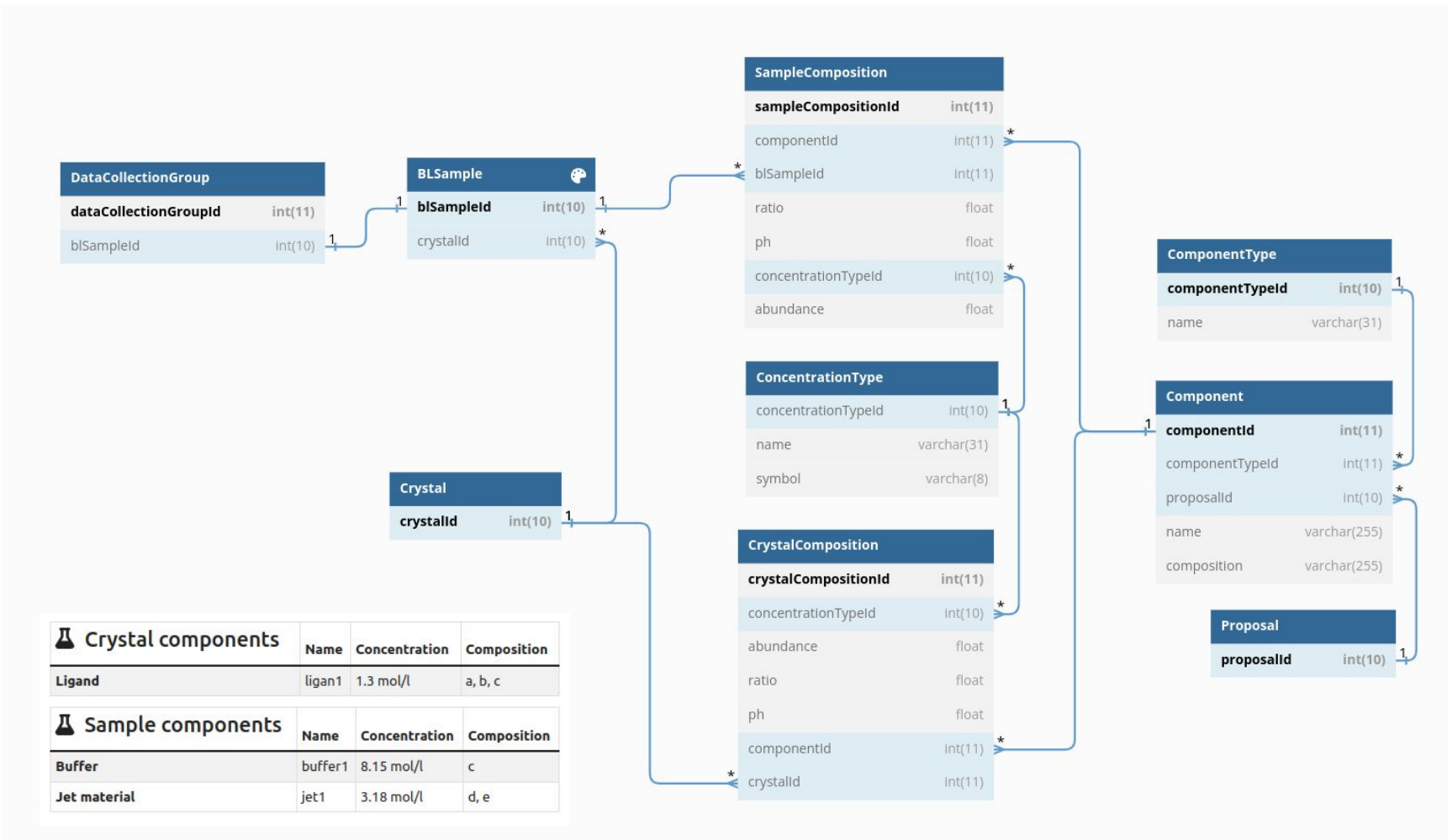

**Detections** 3 events

| offset | type | duration | period | repetition |
|---|---|---|---|---|
| 0.1 | Laser excitation | 0.5 | 1 | 10000 |
| 0.7 | Xray detection | 0.1 | 1 | 10000 |
| 0.9 | Xray detection | 0.1 | 1 | 10000 |

**Sample preparation** 3 events

| offset | type | name |
|---|---|---|
| -50 | Reaction trigger | mixed a |
| -50 | Reaction trigger | mixed b |
| 0 | Reaction trigger | mixed c |

# Database extension - Sample description




**Crystal components**

| Name | Concentration | Composition |
|---|---|---|
| Ligand | ligan1 | 1.3 mol/l | a, b, c |

**Sample components**

| Name | Concentration | Composition |
|---|---|---|
| Buffer | buffer1 | 8.15 mol/l | c |
| Jet material | jet1 | 3.18 mol/l | d, e |

# UI Demo

Home Calendar Proposals SSX1 gaonach Logout

Home » Proposals » SSX1 » Sessions » 10

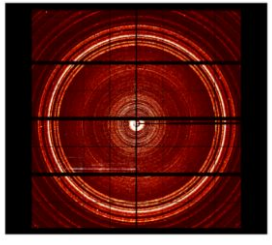
« 1 » Total: 16

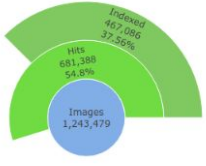
Summary | Parameters | 02/12/2022 16:44:51

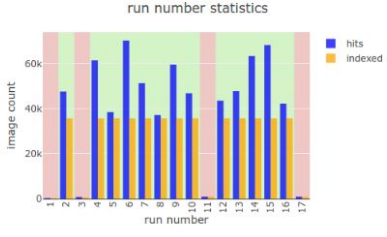
Protein: kljvz | Sample: laagq | Sample support: SSX-Chip | Experiment name: fvkhb | # Runs: 17

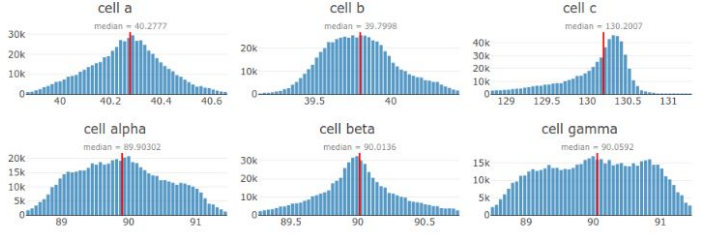
467,086 indexed (37.56%) | 214,302 non-indexed hits (17.23%) | 562,091 skipped images (45.2%)

## Cumulative summary

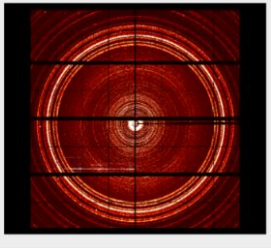




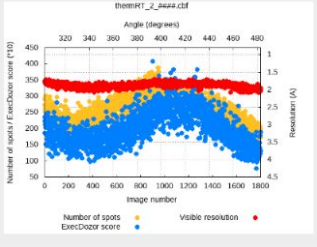



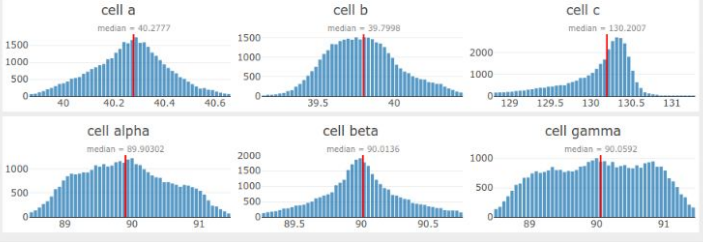

Run # #1 #2 #3 #4 #5 #6 #7 #8 #9 #10 #11 #12 #13 #14



### Run #3 summary (02/12/2022 16:44:56)

Images 63,021




02/12/2022 16:44:41

Protein: sxbyy | Sample: xdwtg | Sample support: SSX-Chip | Experiment name: gwhkj | # Runs: 14

429,610 indexed (42.32%) | 281,588 non-indexed hits (27.74%) | 303,970 skipped images (29.94%)



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Data Collections | Energy Scans | Flourescence Spectra

Summary | Analysis | Containers

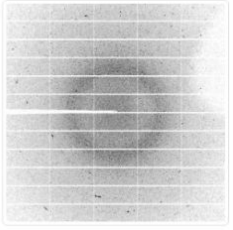
## 30/05/2018 16:52:11 OSC

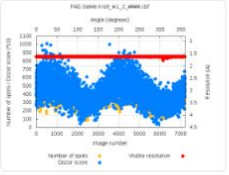
Summary | Beamline Parameters | Data Collections 1 | Sample | Results 31 | Workflow 0

| | | | |
|---|---|---|---|
| Workflow | | Res. (corner) | 2.01 Å (1.72 Å) |
| Protein | FAE | En. (Wave.) | 7.000 KeV (1.7712) |
| Sample | SeMe-Ins9 | Omega range | 0.05 ° |
| Prefix | FAE-SeMe-Ins9_w1 | Omega start (total) | ° (360.00) |
| Run | 1 | Exposure Time | 0.037 s |
| # Images (Total) | 7200 (7200) | Flux start | 7.94e+9 ph/sec |
| Transmission | 2.0095 % | Flux end | ph/sec |

| P 21 21 21 | Completeness | Res. | Rmerge |
|---|---|---|---|
| Overall | 87.5% | 113.1 - 1.7 | 6.8 |
| Inner | 100.0% | 113.4 - 4.7 | 4.3 |
| Outer | 14 | 1.8 - 1.7 | 22.6 |

| a | b | c |
|---|---|---|
| 65.3 Å | 108.5 Å | 113.2 Å |
| α | β | γ |
| 90.0 ° | 90.0 ° | 90.0 ° |





Comments

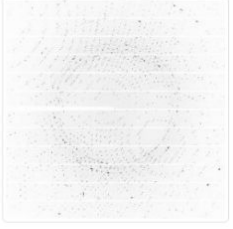
## 30/05/2018 16:49:37 Characterization

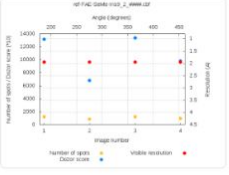
Summary | Beamline Parameters | Data Collections 1 | Sample | Results 0 | Workflow 1

| | | | |
|---|---|---|---|
| Workflow | Characterisation | Res. (corner) | 2.40 Å (1.96 Å) |
| Protein | FAE | En. (Wave.) | 7.000 KeV (1.7712) |
| Sample | SeMe-Ins9 | Omega range | 1.00 ° |
| Prefix | ref-FAE-SeMe-Ins9 | Omega start (total) | 184.32 ° (360.00) |
| Run | 1 | Exposure Time | 0.1 s |
| # Images (Total) | 4 (4) | Flux start | 5.48e+11 ph/sec |
| Transmission | 100 % | Flux end | 5.95e+11 ph/sec |

| | | | |
|---|---|---|---|
| Indexed | | Mosaicity | 0.1 |
| Strategy | | Space Group | P222 |
| Rank. Res. | | | 2.01 Å |
| Osc. start (total) | | | 0 ° (360 °) |
| Images | | | 7200 |
| Osc. range | | | 0.05 ° |
| Transmission | | | 2.9646 s |
| Exp. Time | | | 0.037 s |

| a | b | c |
|---|---|---|
| 65.23 Å | 108.35 Å | 112.99 Å |
| α | β | γ |
| 90 ° | 90 ° | 90 ° |





Comments

## 30/05/2018 16:47:00 Characterization

Summary | Beamline Parameters | Data Collections 1 | Sample | Results 0 | Workflow 1

# py-ISPyB UI features

*Supports both backends but…*

| With Java backend | | With Python backend |
|---|---|---|
| NA | | SSX Data collections |
| EM Data collections | | basic information |
| MX Data collections | need to log out and back in to switch backend | basic information |
| Prepare experiment | | NA |
| Shippings | | basic information |

**Confusing and not practical: we need to switch to all-python as soon as possible**

# Ongoing and future developments

- Serial synchrotron crystallography
  - Improve UI with experiment feedback
  - Develop experiment processing results

- Switch all techniques to py-ISPyB UI
  - Re-implement (with improvements) missing features from EXI
    - Missing bits of MX data collection visualization

- Switch all techniques to py-ISPyB
  - Re-implement (with improvements) missing features from Java
    - backend for techniques: MX, EM
    - backend for shipments
    - backend for experiment preparation

# Thank you!

Any question?