SciCat Development

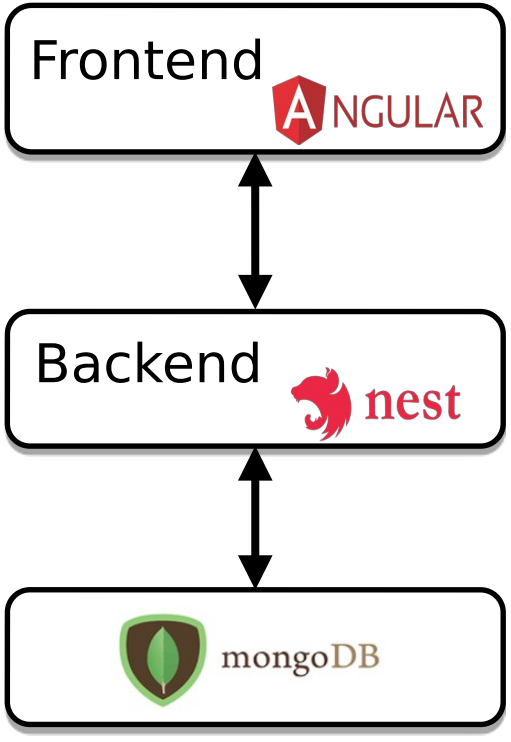
Max Novelli
max.novelli@ess.eu
SciCat Project Leader

Senior Data Curation Scientist
European Spallation Source, DMSC
Copenhagen, Denmark

MXCuBE ISPyB 2024, Trieste, Italy, 2024/11/20

SciCat Project

Open Source Scientific Metadata Catalog



https://scicatproject.github.io/

https://github.com/scicatproject

https://scicatproject.github.io/documentation

European Spallation Source

Paul Scherrer Institut

MAX IV

Rosalind Franklin Institute

Heinz Maier-Leibnitz Zentrum

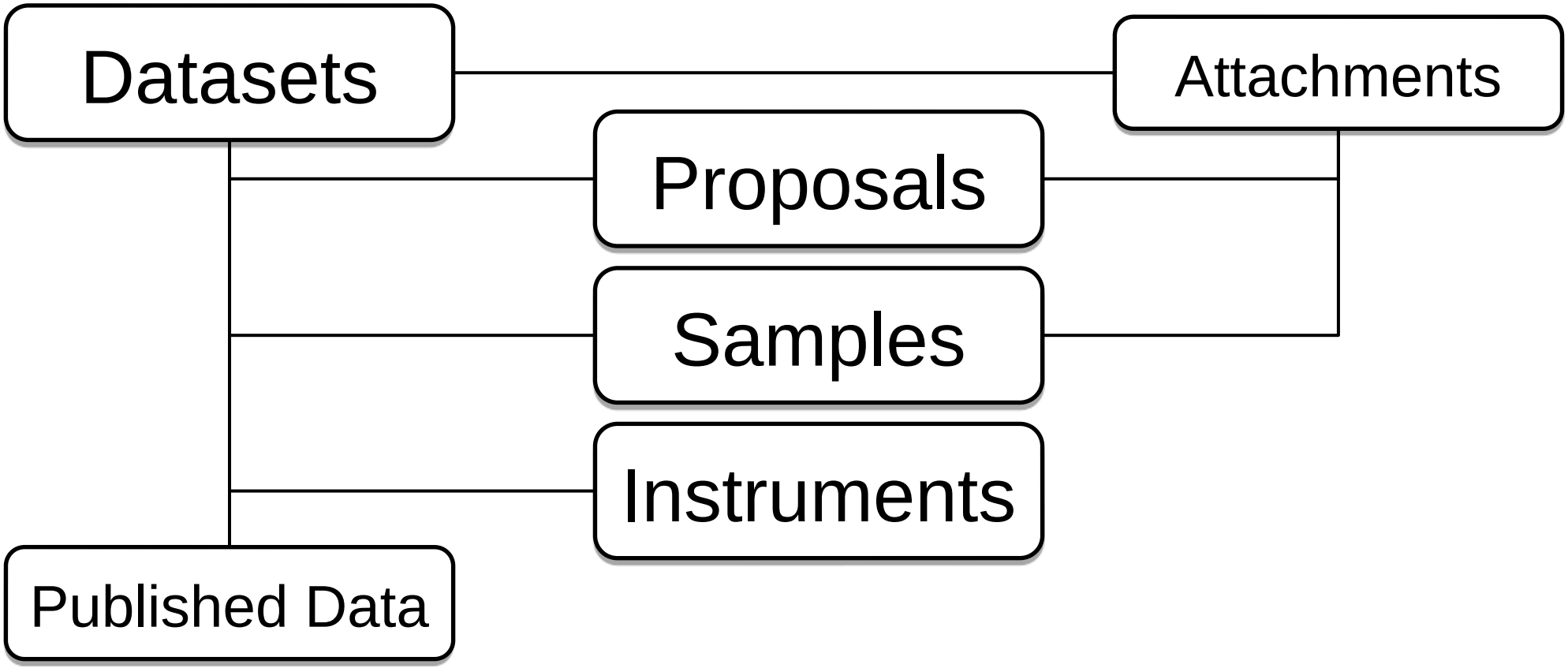
Advanced Light Source

Deutsches Elektronen-Synchrotron DESY

Synchrotron SOLEIL

DAta from PHoton and Neutron Experiments

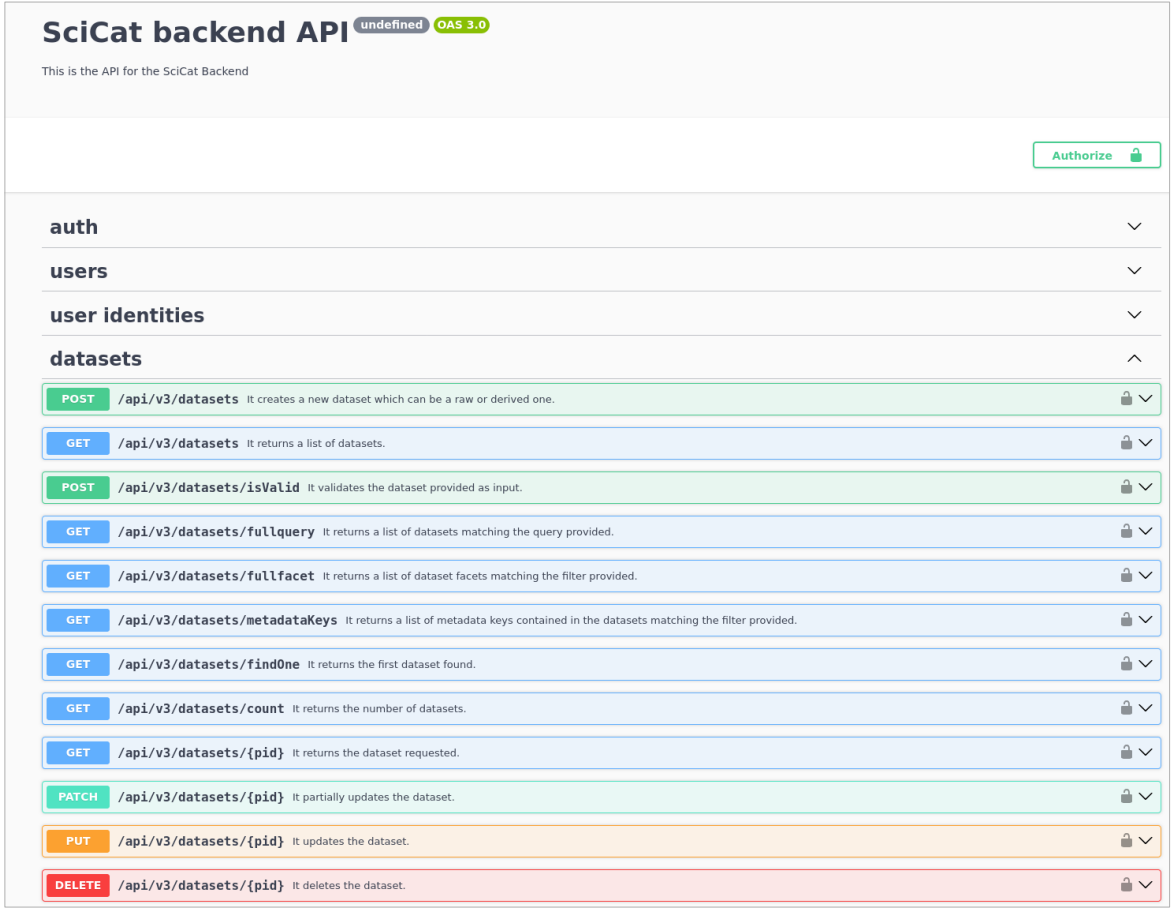
SciCat Sub-Systems



Backend Interface

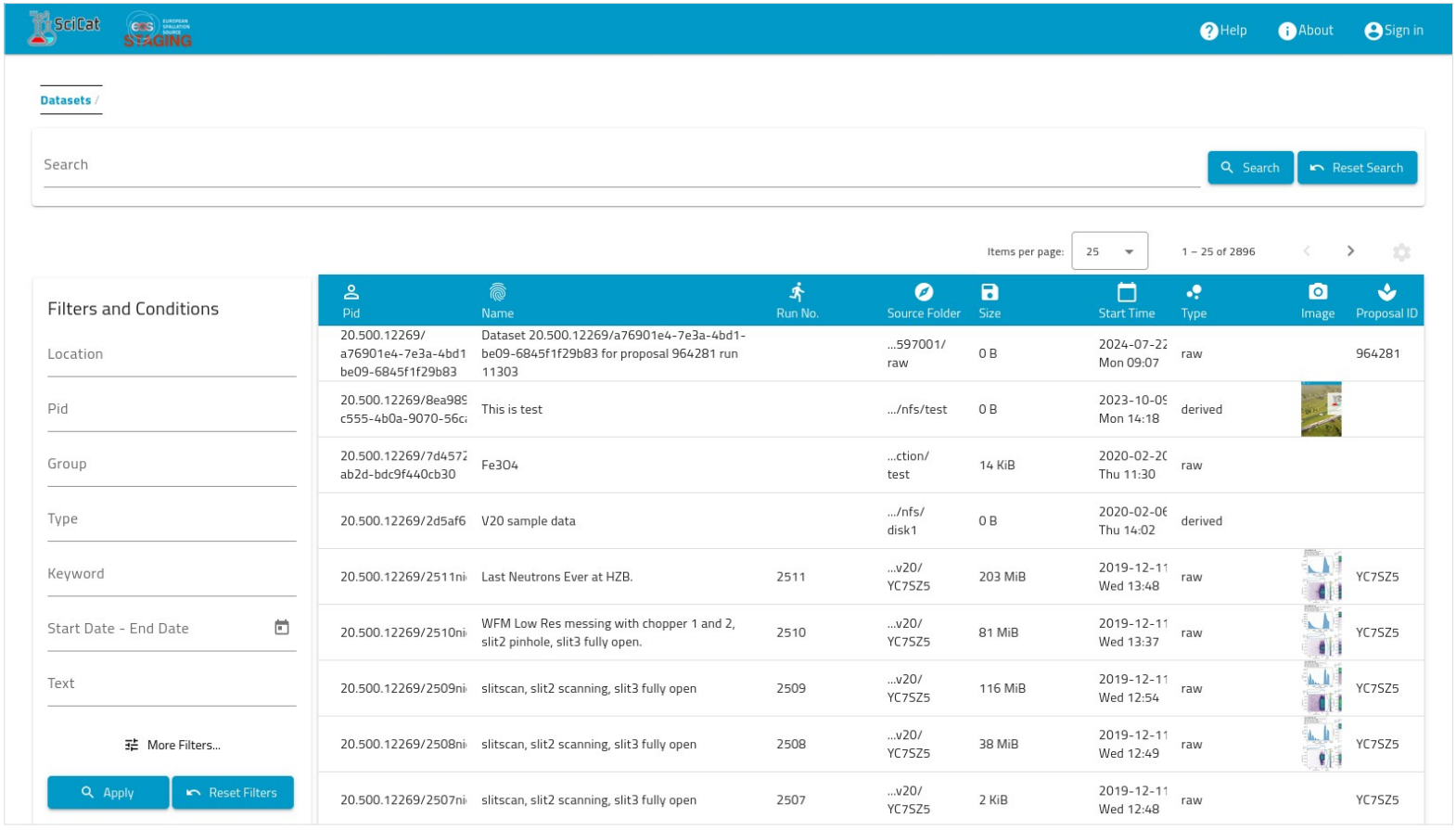
REST API

Swagger™



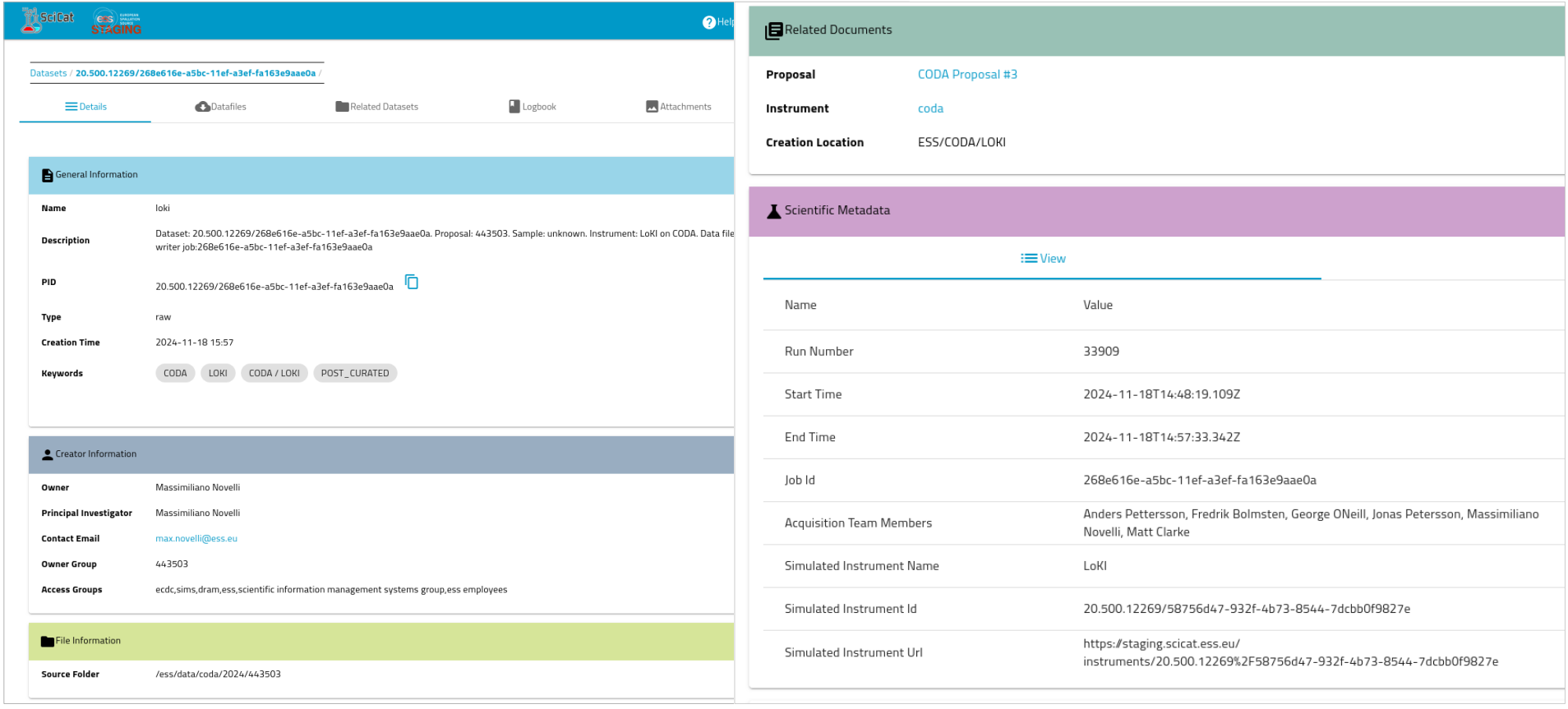
Frontend Interfaces

Datasets list



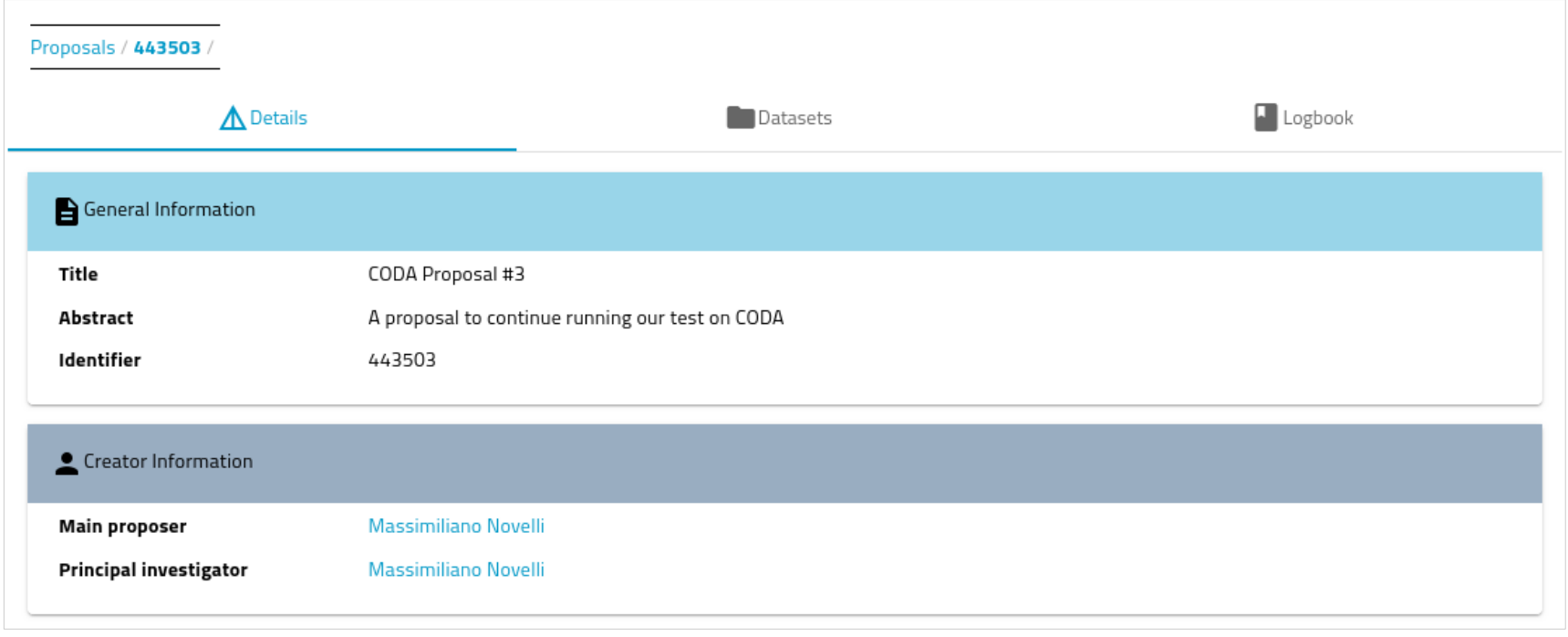
Frontend Interfaces

Datasets details



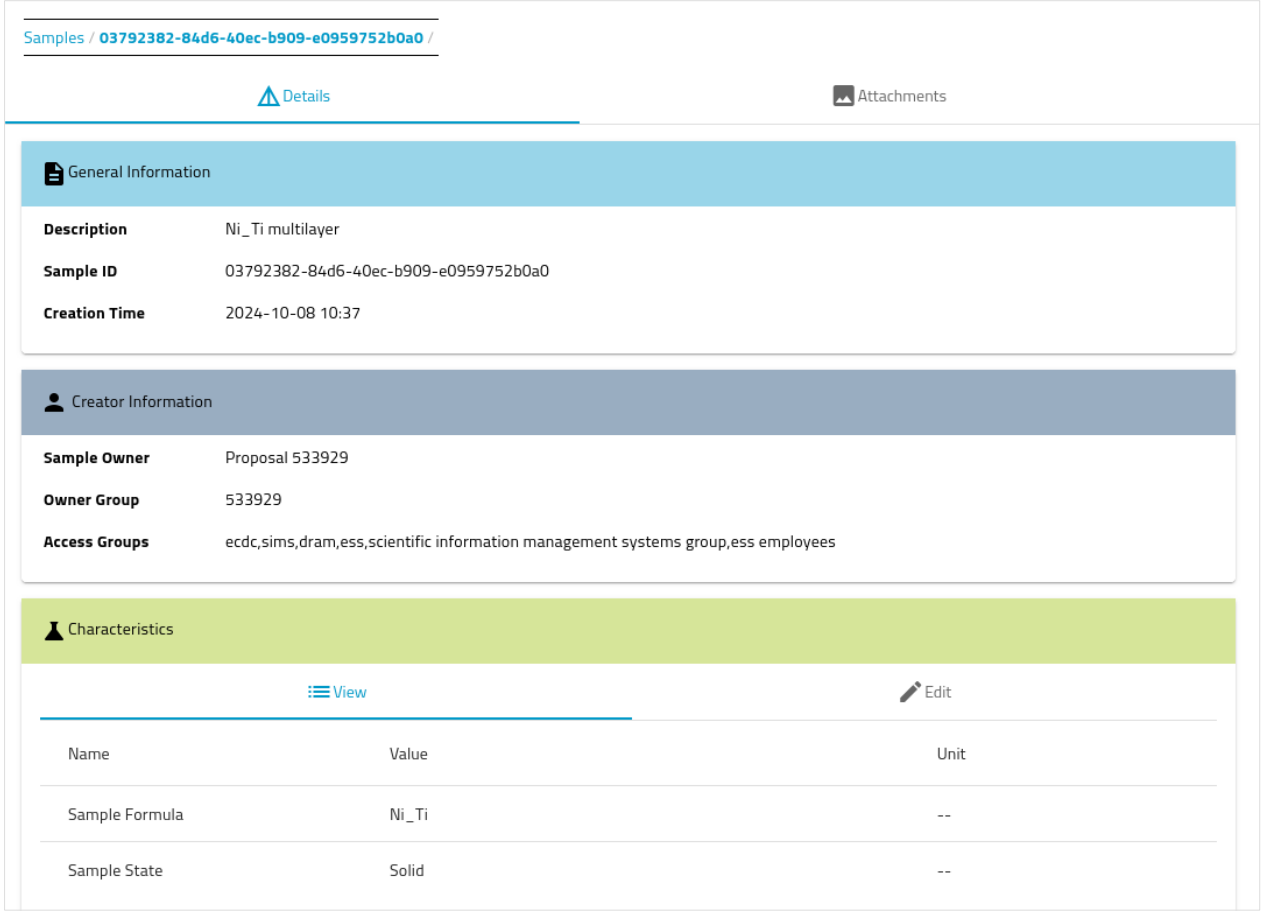
Frontend Interfaces

Proposal



Frontend Interfaces

Samples



Development

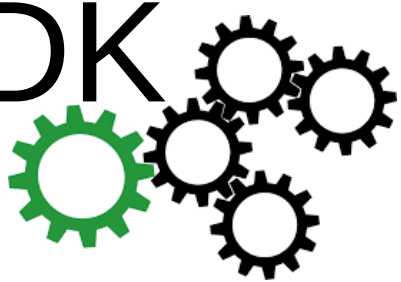
Jobs

ES Integration

Search UI

SciCatLive

SDK



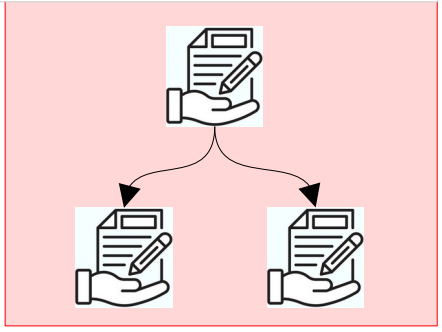
Proposals

Current Development (2)

Proposals

Flat → Hierarchical

Dedicated Metadata



Proposals / 443503 /

Details | Datasets | Logbook

General Information

Title	CODA Proposal #3
Abstract	A proposal to continue running our test on CODA
Identifier	443503

Parent Proposal

Creator Information

Main proposer	Massimiliano Novelli
Principal investigator	Massimiliano Novelli

Characteristics

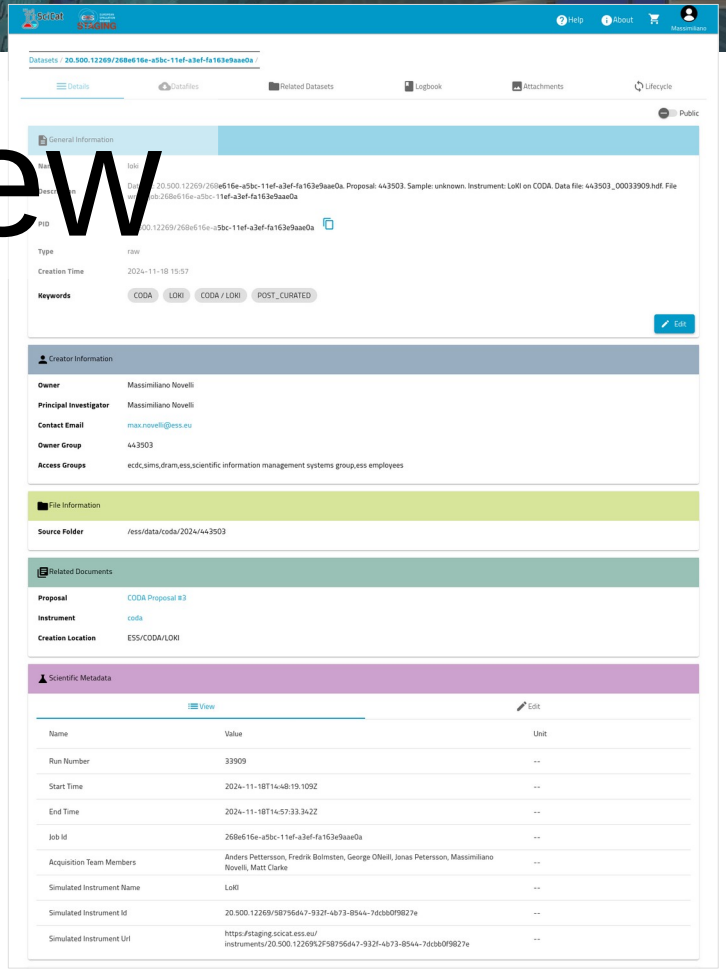
View | Edit

Name	Value	Unit
Sample Formula	Ni_Ti	--
Sample State	Solid	--

Future Development

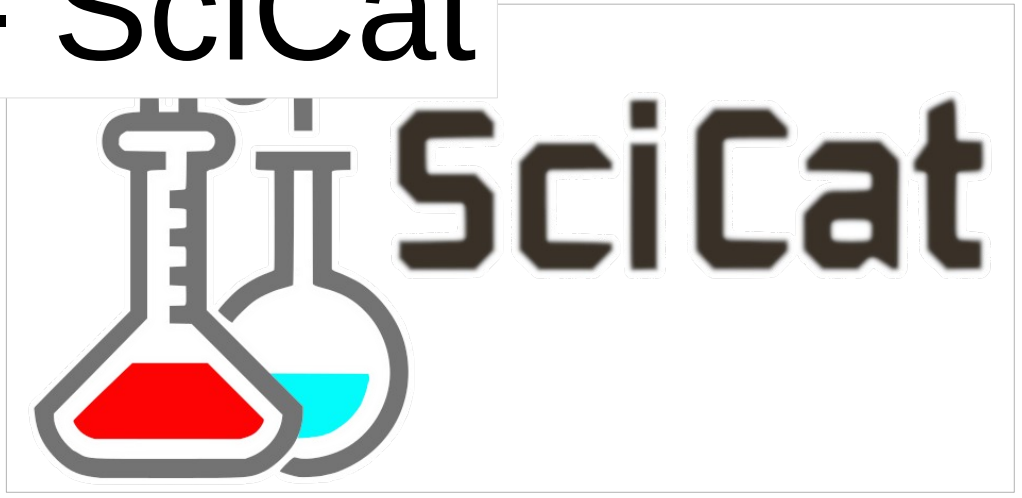
Dataset Details View

- Flexible
- Customizable
- Selectable



Integration

ISPyB - SciCat

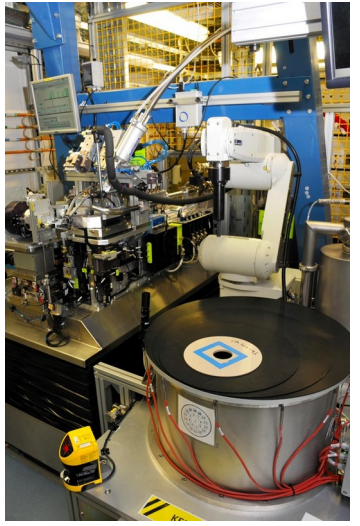


SciCat

ISPyB

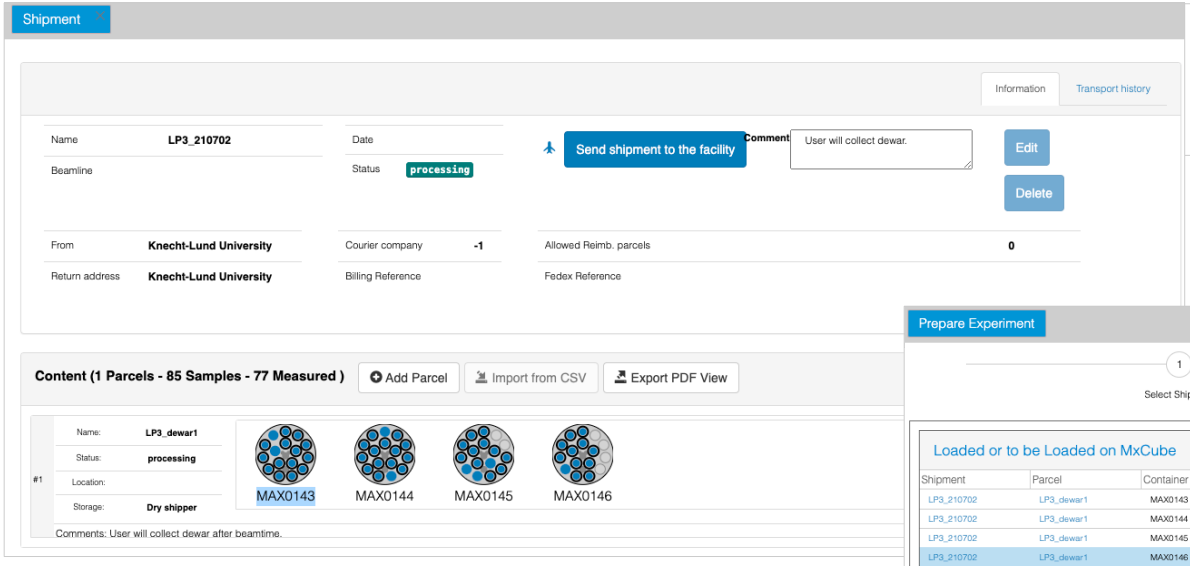
Sample Management

- Sample Shipment ✓
- Sample Declaration ✓
- Puck Layout ✓
- Metadata Catalogue ✓

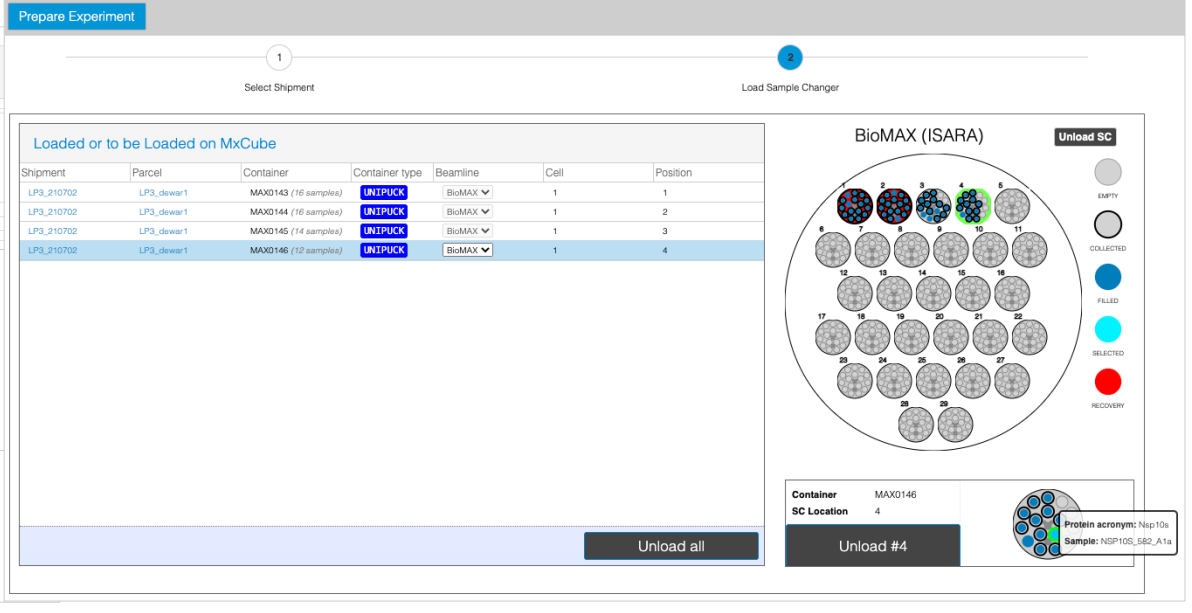


ISPyB Sample

Shipment Management



Puck Layout



Sample: ISPyB to SciCat (1)

Sample → Sample Item

Flat → Hierarchical

Single Type → Multiple Types

Sample: ISPyB to SciCat (2)

Shipment

- All Sample Items
- Different Types
- Properties in Metadata
- Use metadata schema

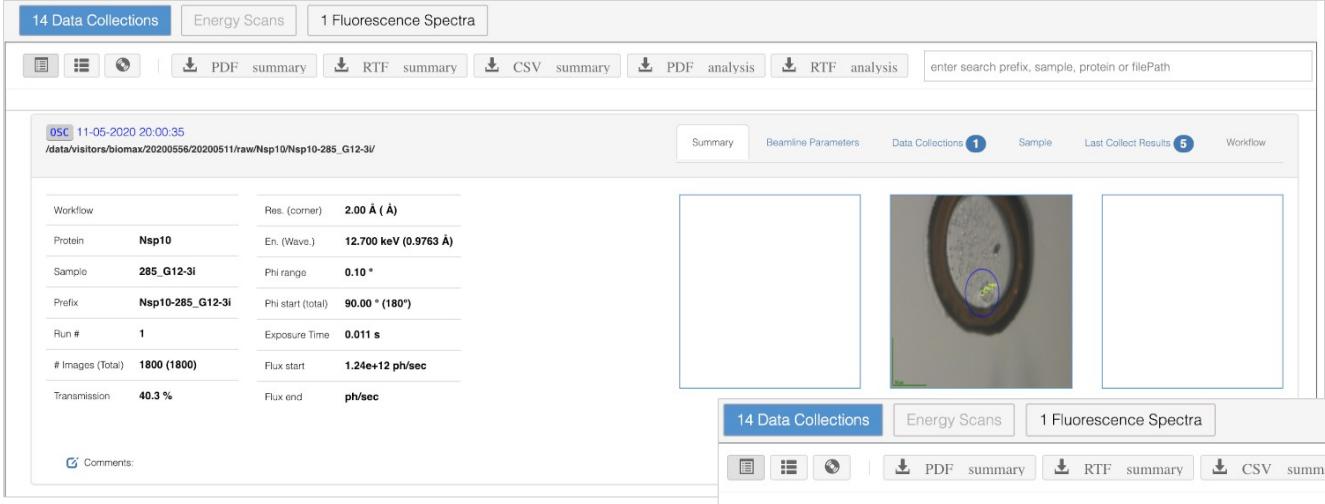
Sample

PUCK

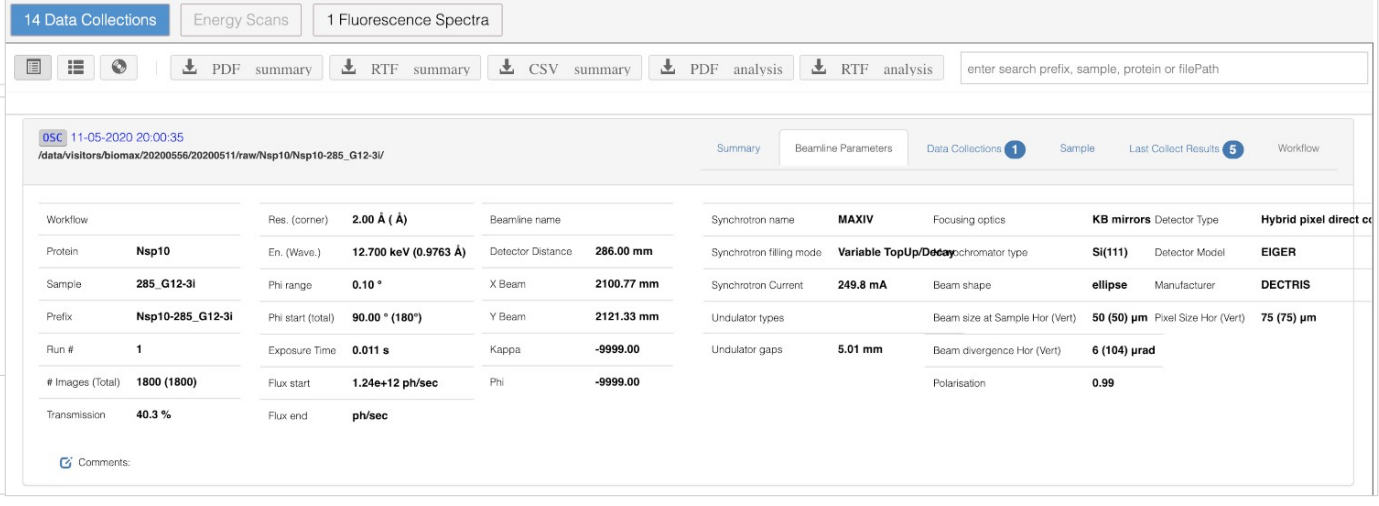
Sample Charger

ISPyB Datasets

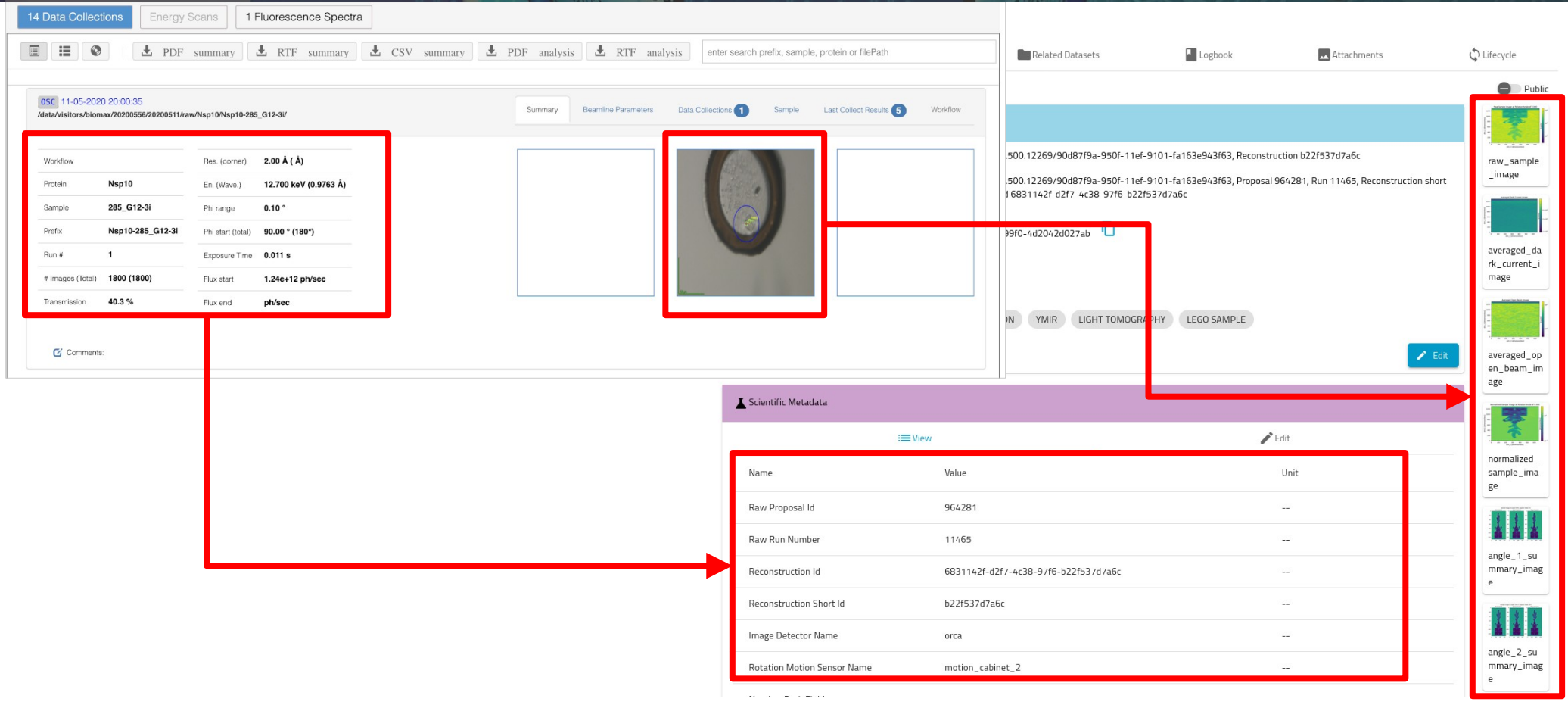
Dataset Overview



Dataset Metadata

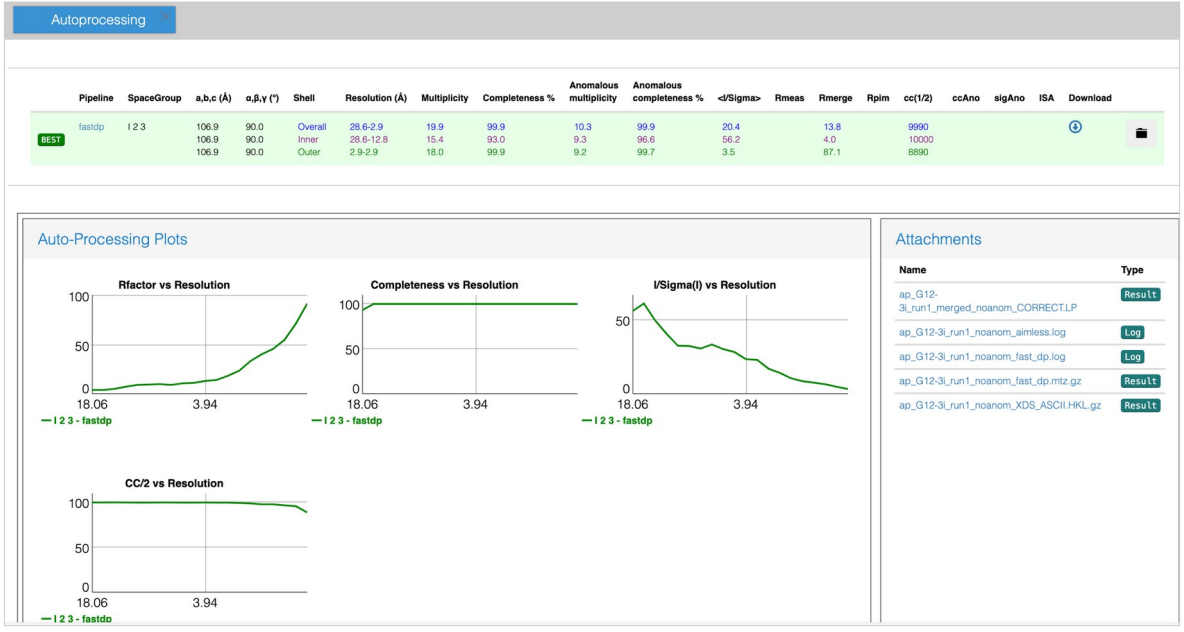


Datasets: ISPyB to SciCat

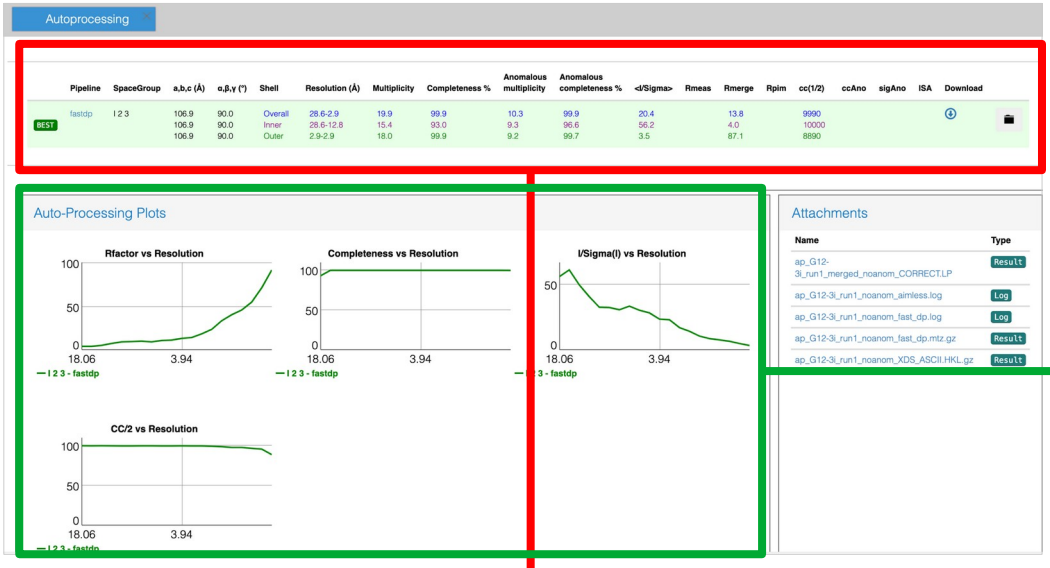


ISPyB Autoprocessing

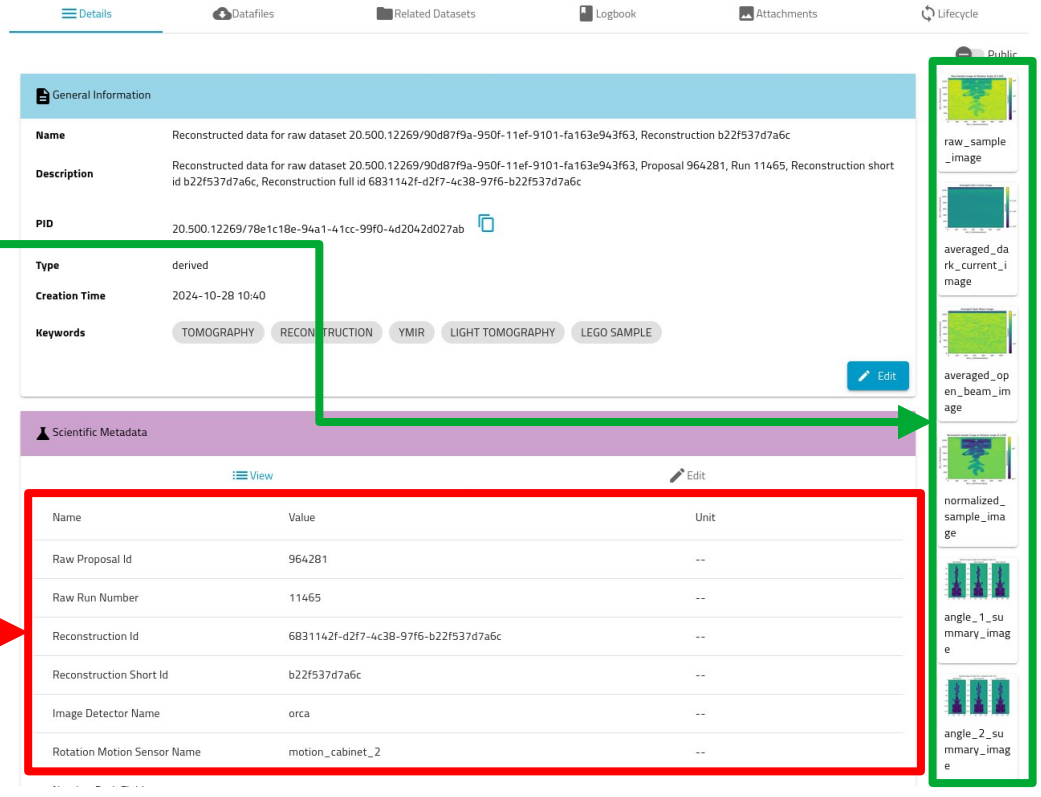
Upon data collection,
automatic reduction pipelines are triggered



Autoproc.: ISPyB to SciCat



Jobs



Roadmap

Action items

- Data mapping
- SciCat backend features
- Refactor current ISPyB UIs
  to use SciCat BE leveraging SDK
- Dedicated datasets details view in SciCat UI

Effort

All effort available within the SciCat project is currently allocated.

SciCat collaborators and ESS will be excited to assist, support and manage the effort.

Additional resources needs to be found and allocated for this integration

Thank you

Massimiliano (Max) Novelli
max.novelli@ess.eu

EUROPEAN SPALLATION SOURCE

Thanks to all SciCat contributors