

ISPyB status report

Global Phasing

MXCuBE/ISPyB Meeting, Diamond, 17 November 2025



GPhL and ISPyB

- We have no beamlines and do not run a LIMS
- Our software (Workflow, autoPROC, ...) runs at beamlines, takes inputs from beamline LIMS and sends outputs to beamline LIMS and viewers
- Our users depend on getting their data and metadata out of synchrotrons
- Our software provides added value (multi-sweep data sets, customised strategies, in-depth analysis) and we depend on optimal execution and full display of results going beyond the lowest common denominator.



LIMS standardisation

- Our software and users work at multiple synchrotrons and need uniformity of LIMS access and result viewers
- The increasing fragmentation of the synchrotron LIMS landscape works against standardisation, and forces people to access each synchrotron in a different way.
- Given the well-established impossibility of having uniform LIMS systems at different synchrotrons, we put our hopes in having a common API and exchange format: MXLIMS





- MXLIMS provides a flexible, adaptable data model and API, a well-defined data exchange format, and the underpinnings for in-memory implementation, currently with Pydantic, potentially with a noSQL database.
- The model is limited to MX for now but could be extended to e.g. SSX if desired.
- As an API and exchange format, MXLIMS can serve as a common standard without constraining the implementation of site-specific LIMS systems



Future development

- MXLIMS is currently being developed mostly by a 'coalition of the willing'. As more people commit to it, it will be formalised into a collaboration governed by the stakeholders, with procedures for version changes etc.
- There will be more detailed presentations on Day 2 of the meeting in relation to theme of Interoperability
- We invite you to consider what MXLIMS can do for synchrotron LIMS collaboration - and for you



END