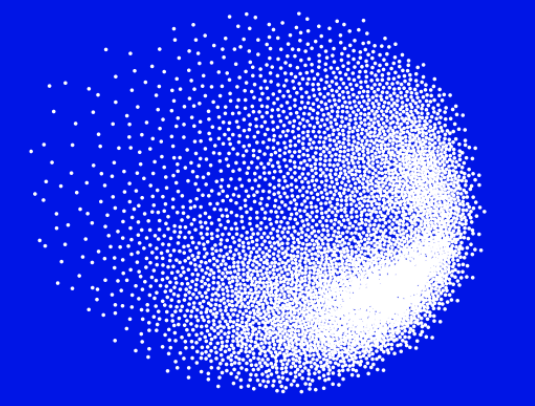




PSI

Center for
Photon Science



AARE

Advanced softwARE for
macromolecular
crystallography at
Swiss Light Source 2.0

Automation at the SLS 2.0 Macromolecular Crystallography (MX) Beamlines

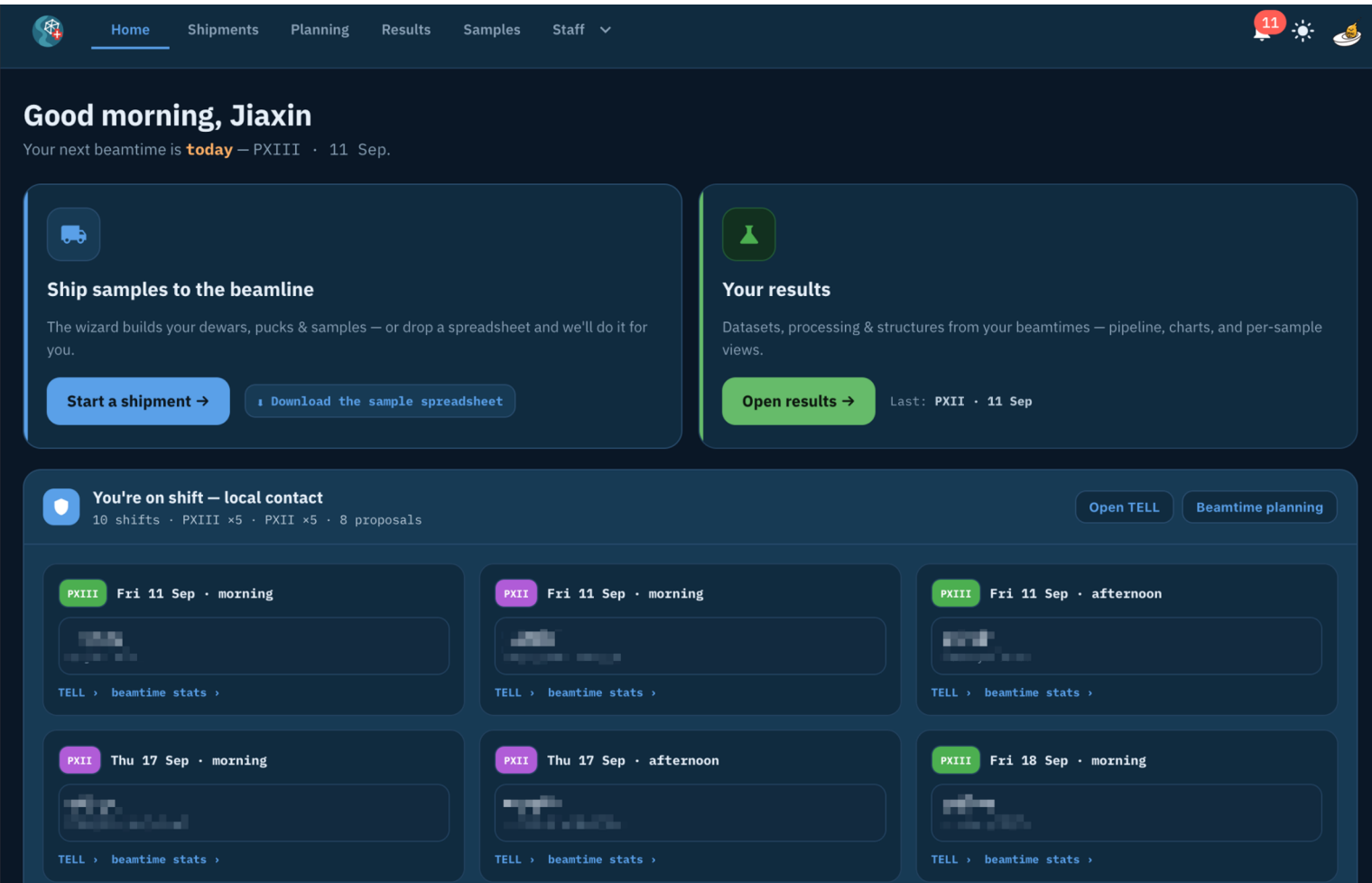
J. Duan¹, G. Gotthard,¹ A. Martin,¹ B. Dominik,¹ V. Olieric,¹ F. Leonarski,^{1,*} M. Wang^{1,*} & Claude^{*} : (Not sponsored, unfortunately

[1] Center for Photon Science, Paul Scherrer Institute, Forschungsstrasse 111, 5232 Villigen PSI, Switzerland

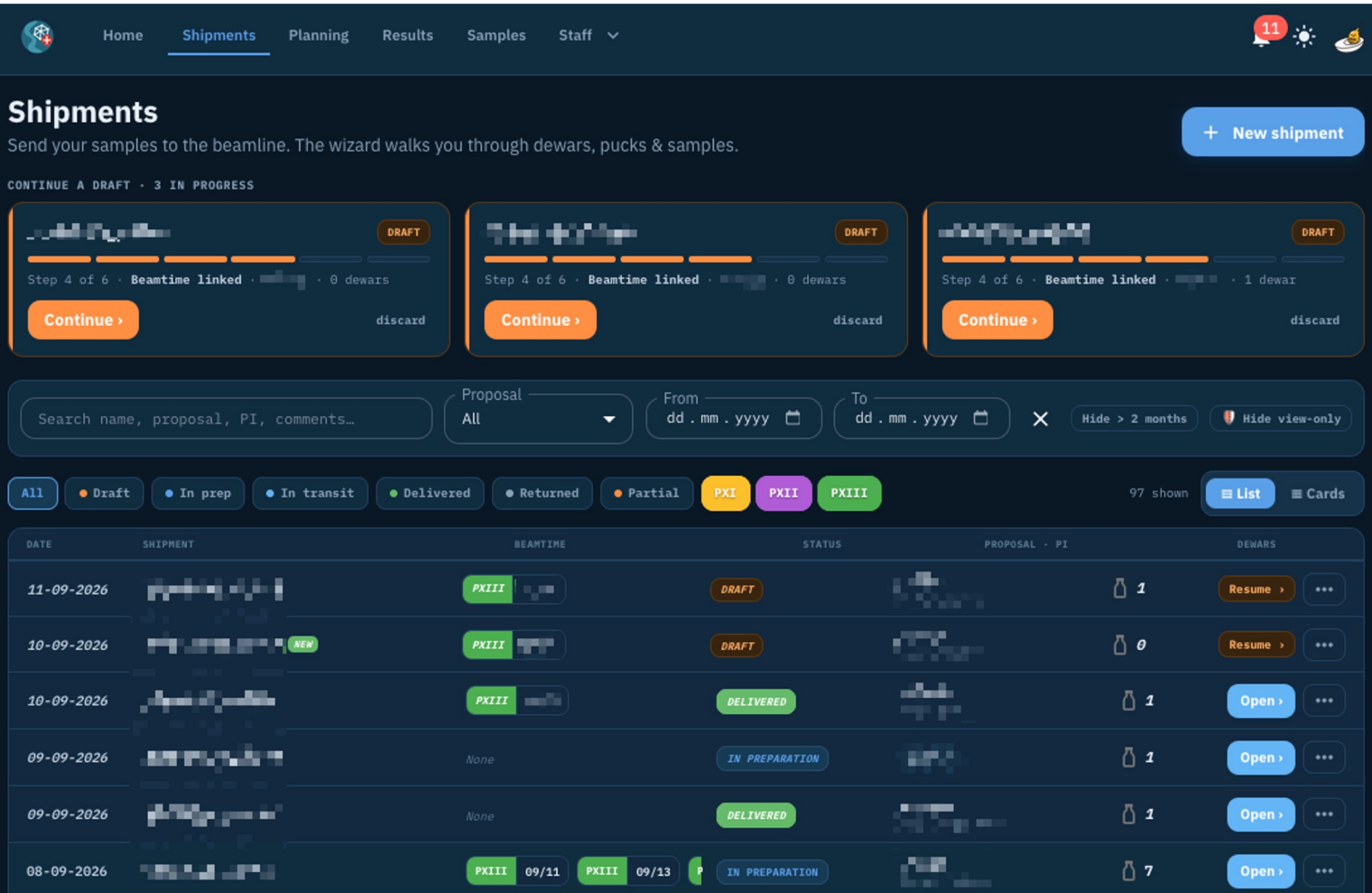
Contact: mx-software@psi.ch

If you want to try all these? Become our user =)

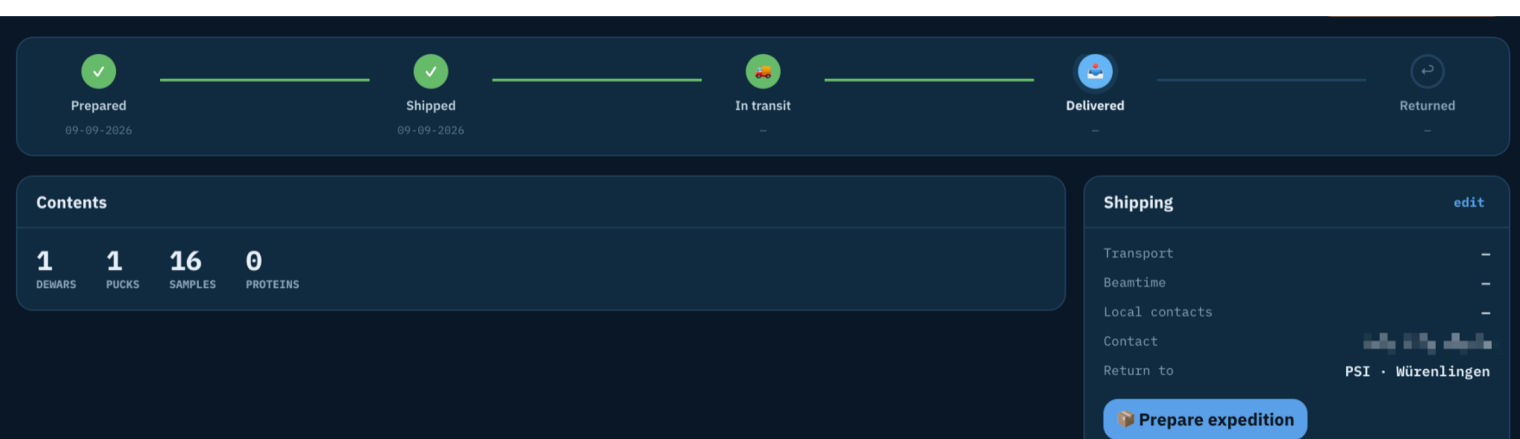
Web GUI for User, Local Contacts & Logistics



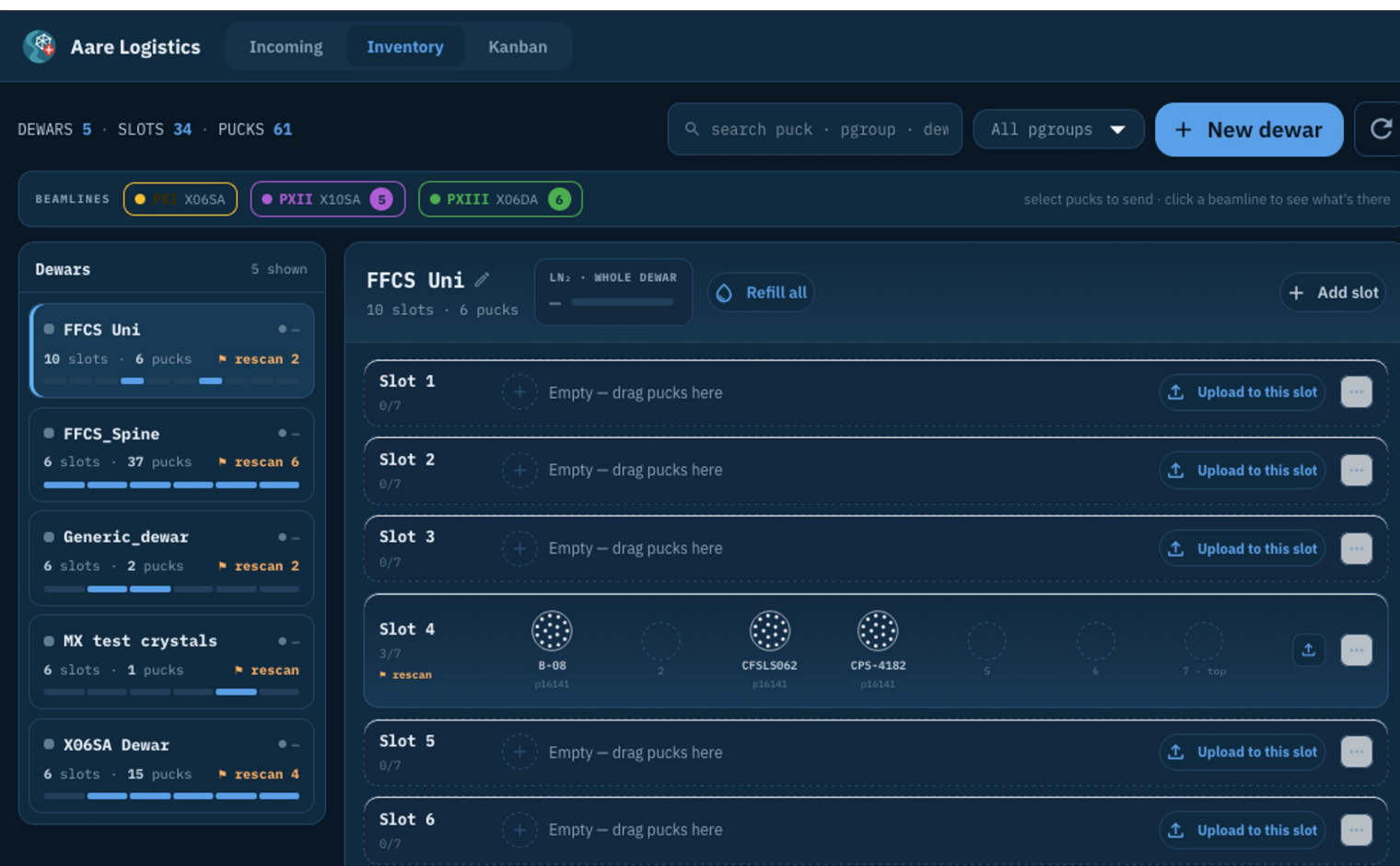
Prepare shipments



Tracking shipments



Monitoring dewards

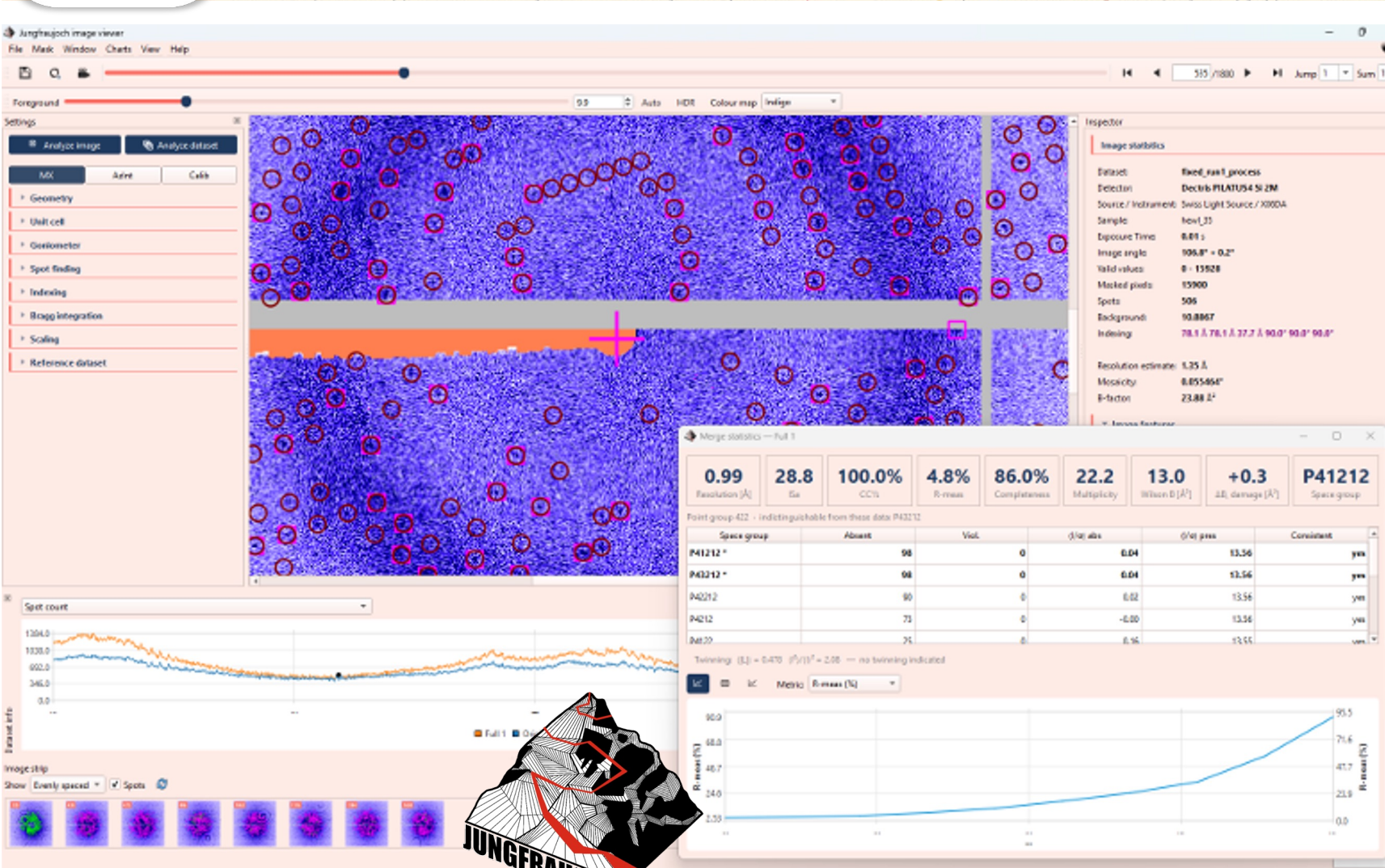
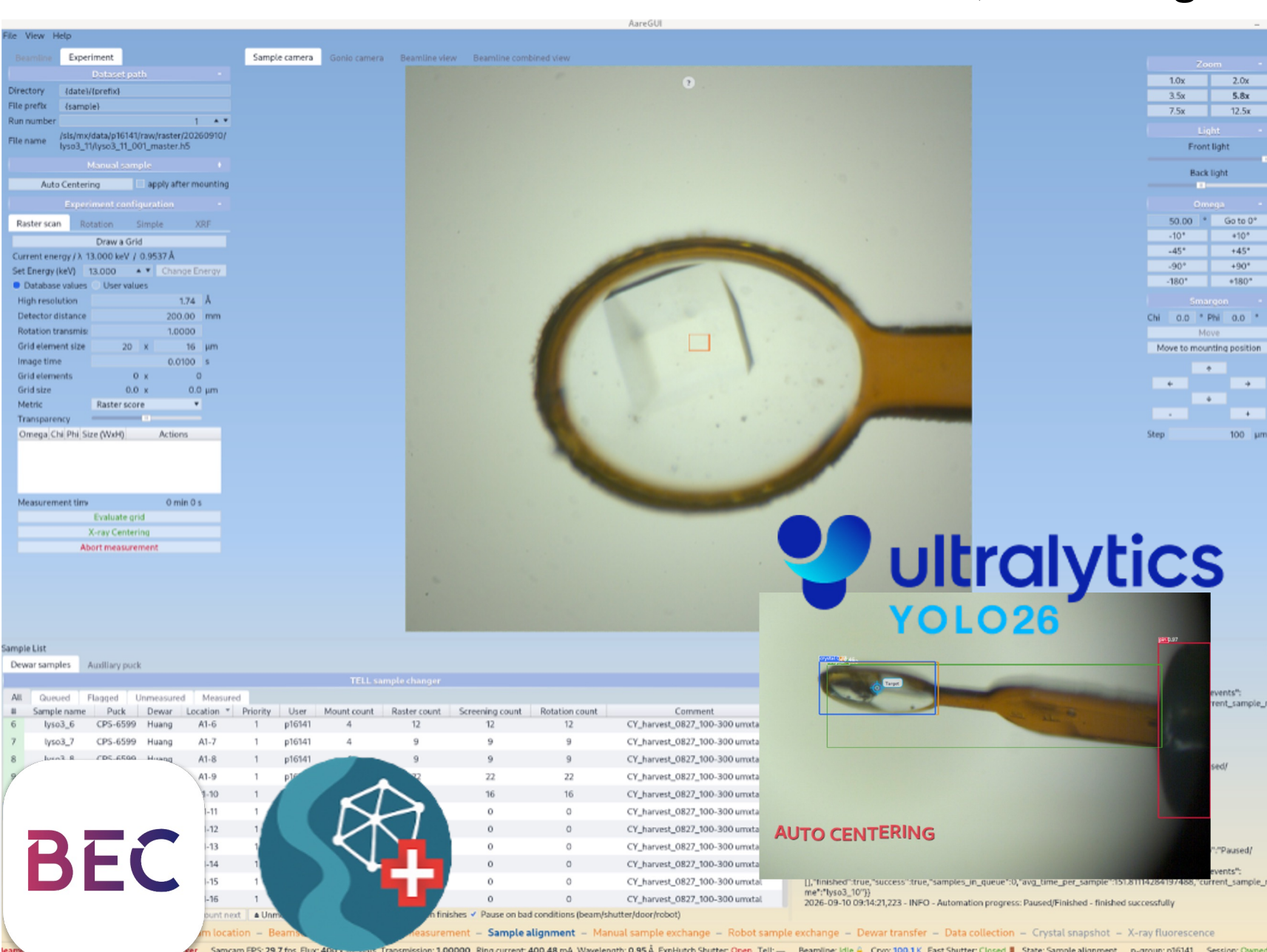


Planning beamtime and logo contact shift (sync with DUO)



During beamtime

User/loco interact with AareGUI on the consoles, BEC integrated

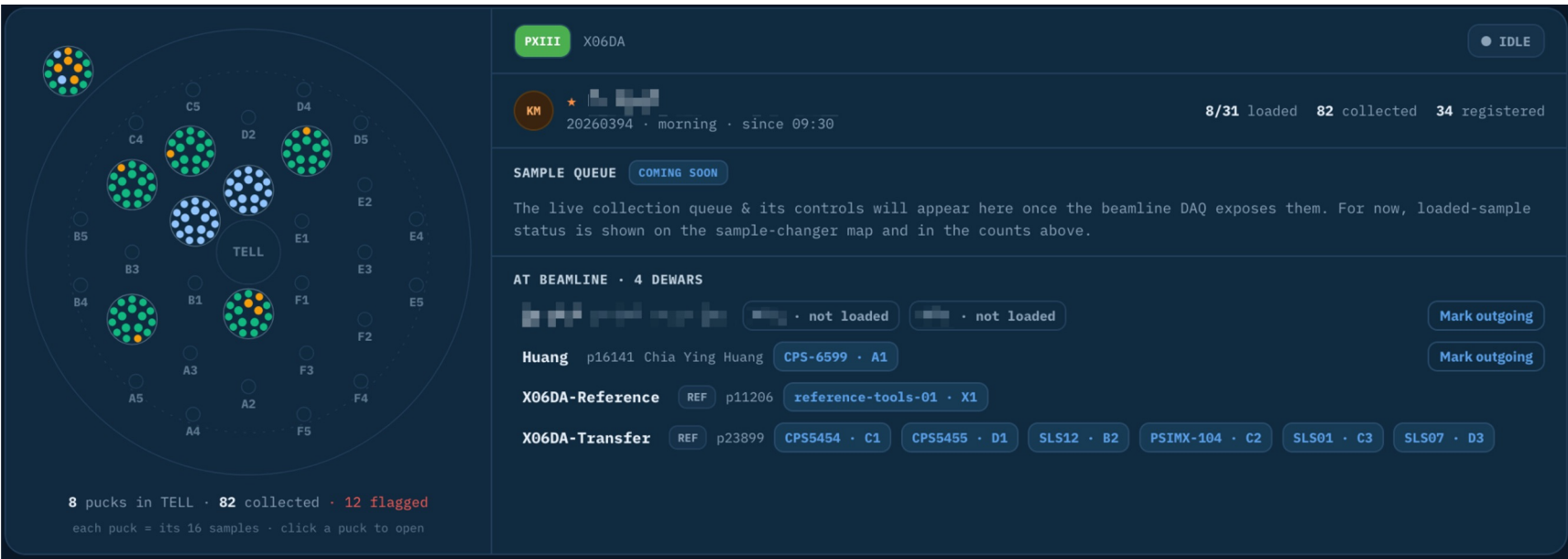


<https://gitea.psi.ch/mx/JungfrauJoch/releases>

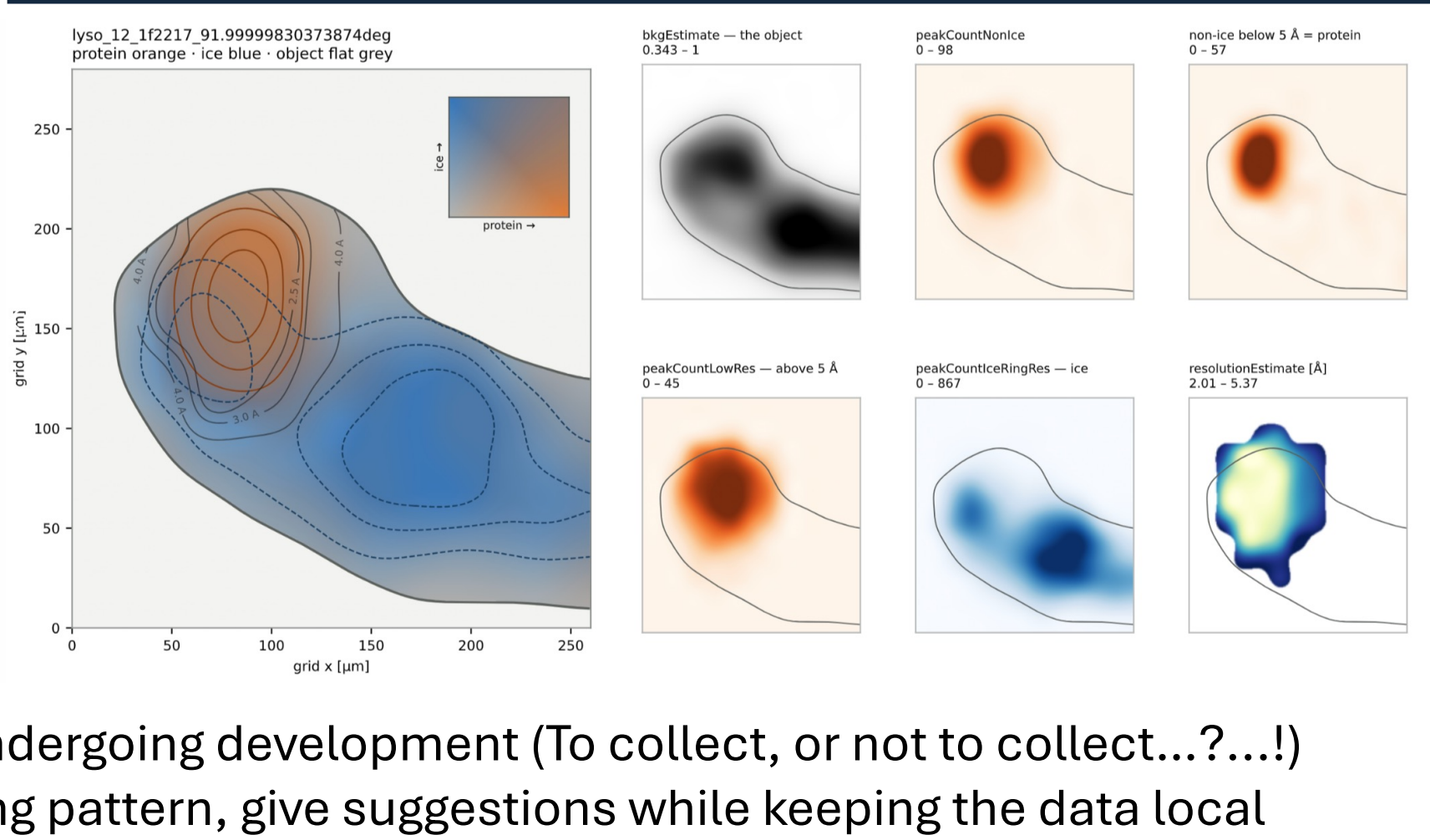
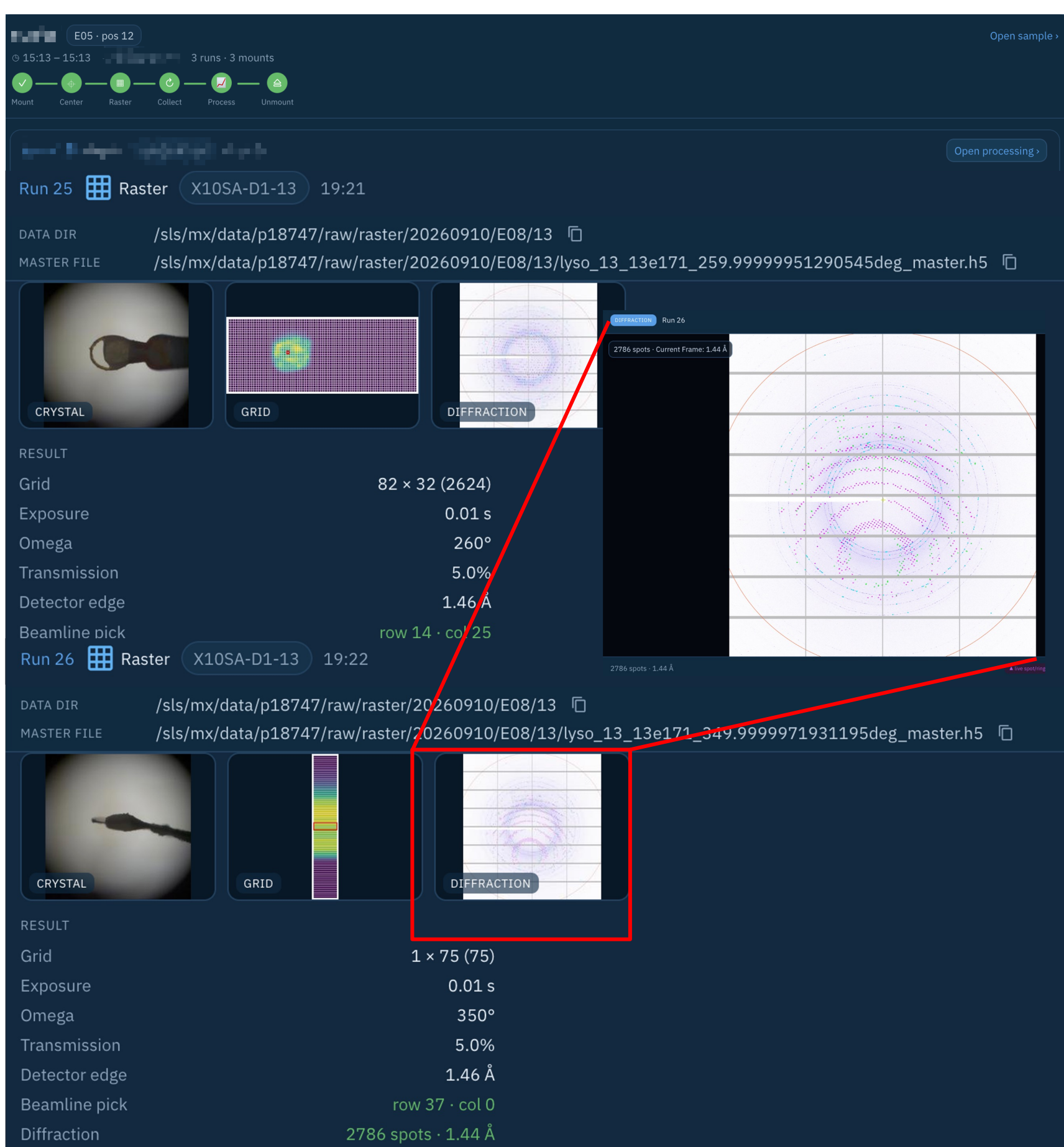
ML/AI-integration in our workflow

- Loop centering with Yolo26
- X-ray raster scan centering with AI-assisted grid evaluation undergoing development (To collect, or not to collect...?..!)
- Local model providing insights to our beamtime, identify failing pattern, give suggestions while keeping the data local

Real-time dewar monitoring



Following the experiment almost in realtime



Data processing result monitoring



Smart report powered by local LLM

Ice contamination and detector edge limited most runs; best data came from lyso_bromid_32

Automated summary of every run collected in this beamtime. No narrative was generated.

15 Jun 2024 0.0% of runs carry a human rating (0 of 78). Ratings are optional and do not enter the ranking.

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