

ISPyB status report



ISPyB status

- ISPyB up and running since 2015.
- Two Dell R330 servers installed with enterprise iDRAC (CentOS 7.3).
- DRBD: synchronizing data across nodes.
- NAGIOS for monitoring of hw/sw (emails if errors occur).
- RAID 5e.
- Crystals, samples, sessions from SMIS user portal.
- 1144 core cluster with SLURM for offline processing (EDNAproc and AutoProc).

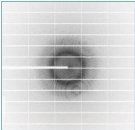
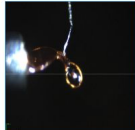
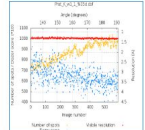
Method	Peak Group	Cell A	Cell B	Cell C	Cell Alpha	Cell Beta	Cell Gamma
Autoprocessing Summary (link to an entry for more details)							
Autoproc_Overview	P 41 21 2	68	68	102	90	90	90
KXZ_DALS	P 41 21 2	68	68	102	90	90	90
Autoproc	P 41 21 2	68	68	102	90	90	90
EDNA_proc	P 4	68	68	102	90	90	90

Pipeline	SpecGroup	a1(a)	a2(a)	a3(a)	a4(a)	a5(a)	a6(a)	a7(a)	a8(a)	a9(a)	a10(a)	Resolution (Å)	Multiplicity
Autoproc	P 41 21 2	68	68	102	90	90	90	90	90	90	90	41.1	42
Autoproc_Overview	P 41 21 2	68	68	102	90	90	90	90	90	90	90	41.1	41
KXZ_DALS	P 41 21 2	68	68	102	90	90	90	90	90	90	90	41.1	42
EDNA_proc	P 4	68	68	102	90	90	90	90	90	90	90	41.1	42

03-09-2018 10:11:26
icsP1320181095_206pompidor0218093RAW_DATAProt_K

Summary | Beamline Parameters | Data Collection | Sample | Last Collect Results | Workflow

Workflow	Res. (corner)	1.15 Å (Å)	P 41 21 2	Completeness	98.4%	Res.	43.5-1.2	Rmerge	6.7
Protein	En. (Wave)	12.700 keV (0.9763 Å)	Overall	98.4%	43.5-3.3	2.3			
Sample	Phi range	0.10°	Inner	94.5%	1.22-1.20	58.0			
Prot. K_w1	Phi start (total)	132.00° (59°)	Outer	99.6%					
Run #	Exposure Time	0.04 s							
# Images (Total)	Flux start	5.25e+11 ph/sec							
Transmission	Flux end	5.25e+11 ph/sec							

Comments:

ISPyB GUI status

- Old (html) gui works **ispyb.embl-hamburg.de** and is used, but is slow and do not cope with evolving collection methods.
- EXI available at **exi.embl-hamburg.de**
 1. EXI is faster and is more user friendly.
 2. Needs site specific adjustments.
- After slight adjustment of the current ISPyB installation Synchronweb is locally available at **synchweb.embl-hamburg.de**. Main work done to support synchweb is:
 1. Added missing tables, columns in the data base.
 2. Custom made SQL scripts to fill columns used by synchweb.
 3. Slightly modified MXCuBE ISPyBClient hardware objects and EDNA ISPyB plugin to fill the columns used by synchweb.
 4. Learn PHP.

Thank you for your attention!

Acknowledgments:

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- IT Group: A. D. Amato
- ISPyB community.