

Data collection names		Buttons (summary / Processing/ exp details)	
Exp details	Autoprocessing summary	Max Projection	Hit map

TEMPLATE IDEA FOR SSX – DETAILS FOR THE OVERVIEW

Data collection names		Buttons (summary / sample / Processing/ exp details)	
EXP Details: Sample name Experiment type Support (delivery method) Exposure time Repetition rate Energy Flux Transmission Det. Distance	Autoprocessing summary <u>CrystFEL results should go here</u> <u>(see the last slide)</u>	Max Projection (the sum of all patterns)	Hit map (from pyFAI?) (can be 2D: sample map 1D: cumulative hit rate)

OTHER INFOS TO BE STORED AND PRESENTED

Sample	Experiment	Data collection	Processing
Protein	Experiment type	Exp time	Spacegroup
Preparation	Start time	Transmission	Completeness
Avg xtal size	Excitation wavelength	Flux	Pipeline input params (including crystfel command line)
Xtal concentration	Time delay (see “gleb” data model)	Repetition rate	Unit cell
Support (jet / 2d/ kind of matrix)	Temperature	Energy (bandwidth)	Hirate/indexing rate (at the end of collect)
crystal form		Flux	Quality stats of final dataset
ligand		Resolution	

BEAMLINE PARAMETERS

Helical 06-05-2022 14:15:20

/data/visitor/mx1816/id30a1/20220506/RAW_DATA/Lyso/Lyso-CD033084_H12-2

Workflow	MXPressR_180
Protein	
Sample	
Prefix	Lyso-CD033084_H12-2
Run #	1
# Images (Total)	900 (1100)
Transmission	55.1 %

Res. (corner)	2.00 Å (Å)
En. (Wave.)	NA keV (Å)
Omega range	0.20 °
Omega start (total)	45.00 ° (180°)
Exposure Time	0.02 s
Flux start	ph/sec
Flux end	ph/sec

Beamline name	
Detector Distance	mm
X Beam	mm
Y Beam	mm
Kappa	95.35
Phi	351.00

☒ Comments: Predefined parameters: no auto mesh; Very weak diffraction. Dynamic aperture set to 30 um Flux maintained at 7.00e+10

Summary

Beamline Parameters

Data Collections 3

Sample

Last Collect Results

Workflow 2

Synchrotron name	ESRF
Synchrotron filling mode	16 bunch
Synchrotron Current	
Undulator types	
Undulator gaps	

Focusing optics	Vertical CRL / Horizontal CRL
Monochromator type	C(110)
Beamline	
Beam size at Sample Hor (Vert)	
Beam divergence Hor (Vert)	104 (6.5) μ rad
Polarisation	0.99

Detector Type	PIXEL
Detector Model	Pilatus3_2M
Manufacturer	DECTRIS
Pixel Size Hor (Vert)	172 (172) μ m

Chopper modes/ Timing
Mono-strip

SAMPLE: DO WE KEEP IT?

OSC 06-05-2022 13:58:50

/data/visitor/mx1816/id30a1/20220506/RAW_DATA/Lyso/Lyso-CD033084_E11-2

Protein

Sample

Shipment

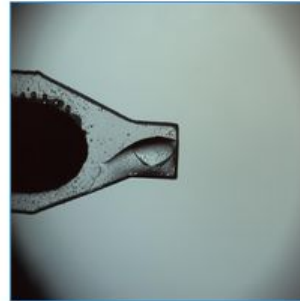
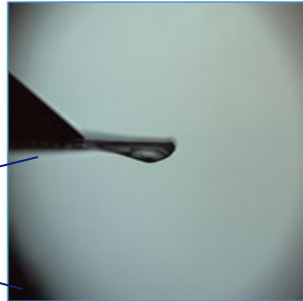
Parcel

Container / Position

Sample barcode

Beamline location

~~Sample changer location~~



☒ Comments: Predefined parameters: no auto mesh; Very weak diffraction. Dynamic aperture set to 100 um Flux maintained at 7.00e+10

PYFAI PARAMETERS!

Data	
0	"/usr/bin/peakfinder"
1	"-o"
2	"pyfai_run3.h5"
3	"-p"
4	"geometry.poni"
5	"-m"
6	"mask.msk"
7	"--dummy"
8	"65535"
9	"-P"
10	"0.99"
11	"--error-model"
12	"azimuthal"
13	"--cutoff-pick"
14	"3"
15	"lysozyme_Gd_4_1_data_000001.h5"
16	"--save-source"
17	"--save-powder"

Peaks per frame
Powder diffraction?

Sample definition

From MXCUBE

to be discussed also at the ISPYB meeting next week.

CRYSTFEL RESULTS?

For each data collection ID →
Automated CrystFEL run on pyFAI hits/peak list → Result →

#hits
#indexed
unit cell params (mode value)
 if #indexed > 1000,
 histogram plot with
 mode value?
lattice type
Estimated resolution (mode)

Need an object which can track and group data collection IDs and corresponding CrystFEL runs connected to the same projectID or SampleID

Task of this object –

1. Check if #indexed patterns > 1000 (for each data collection ID)
2. Launch Partialator to scale/merge over accumulated images in every 1000 indexed frames.
3. Return/Display CC* and Rsplit (with a slider) (what is being done in standard experiments CC1/2 and Rmerge)