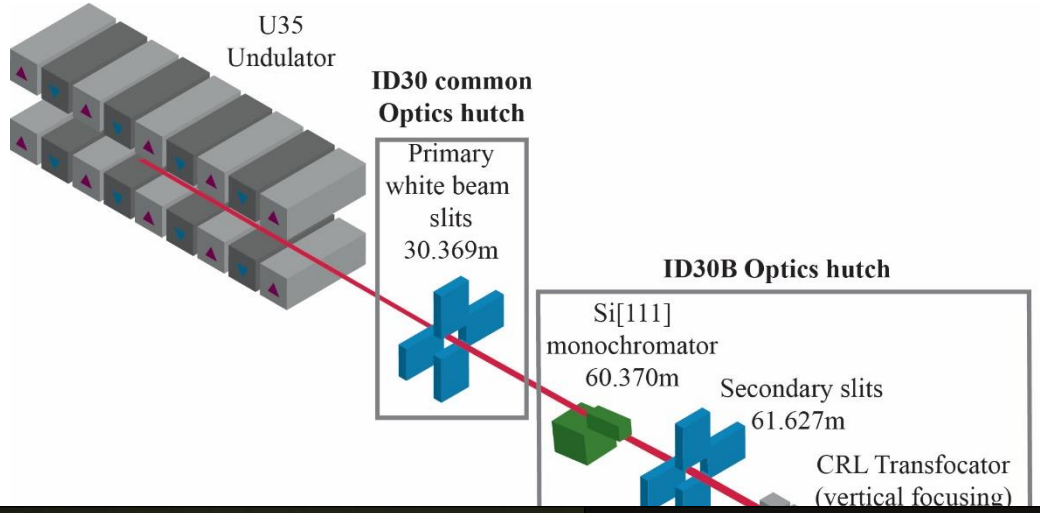
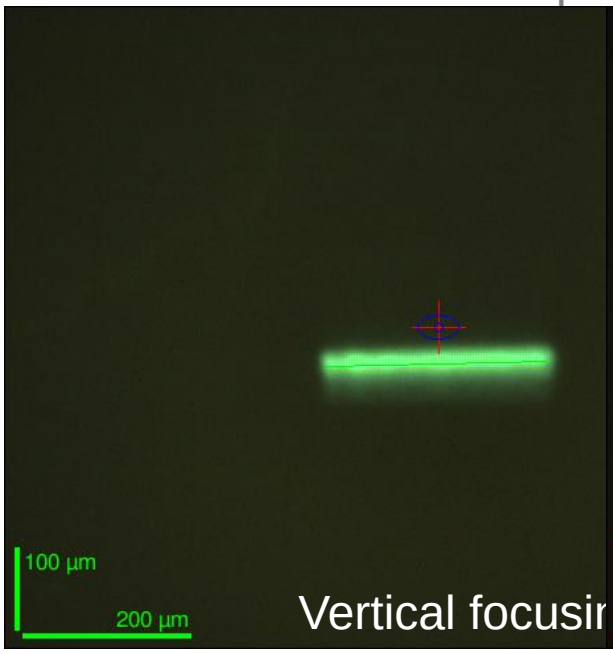

ESRF
The European Synchrotron

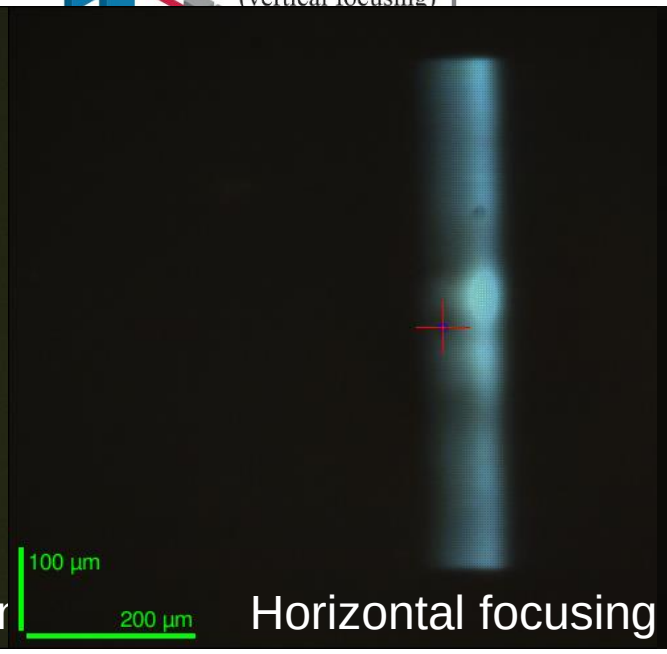

ID30B
news
EMBL
Andrew McCarthy
Christoph Mueller-Dieckmann
ESRF

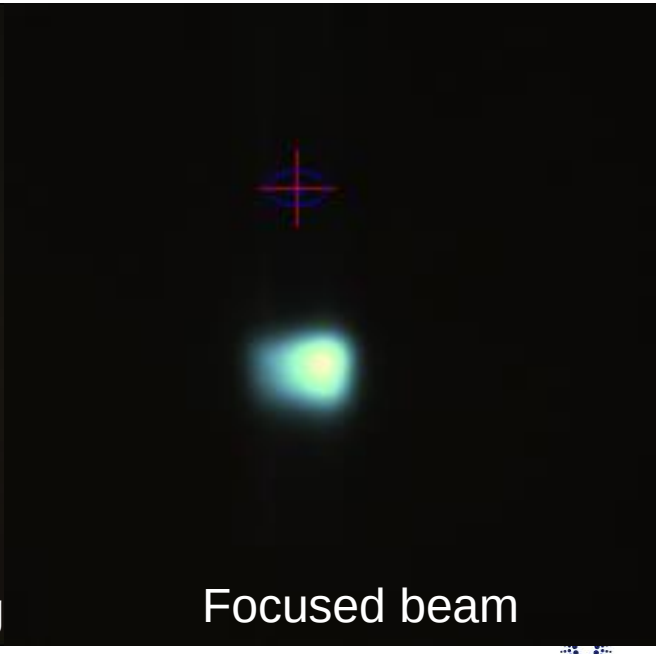
ID30B – OVERVIEW



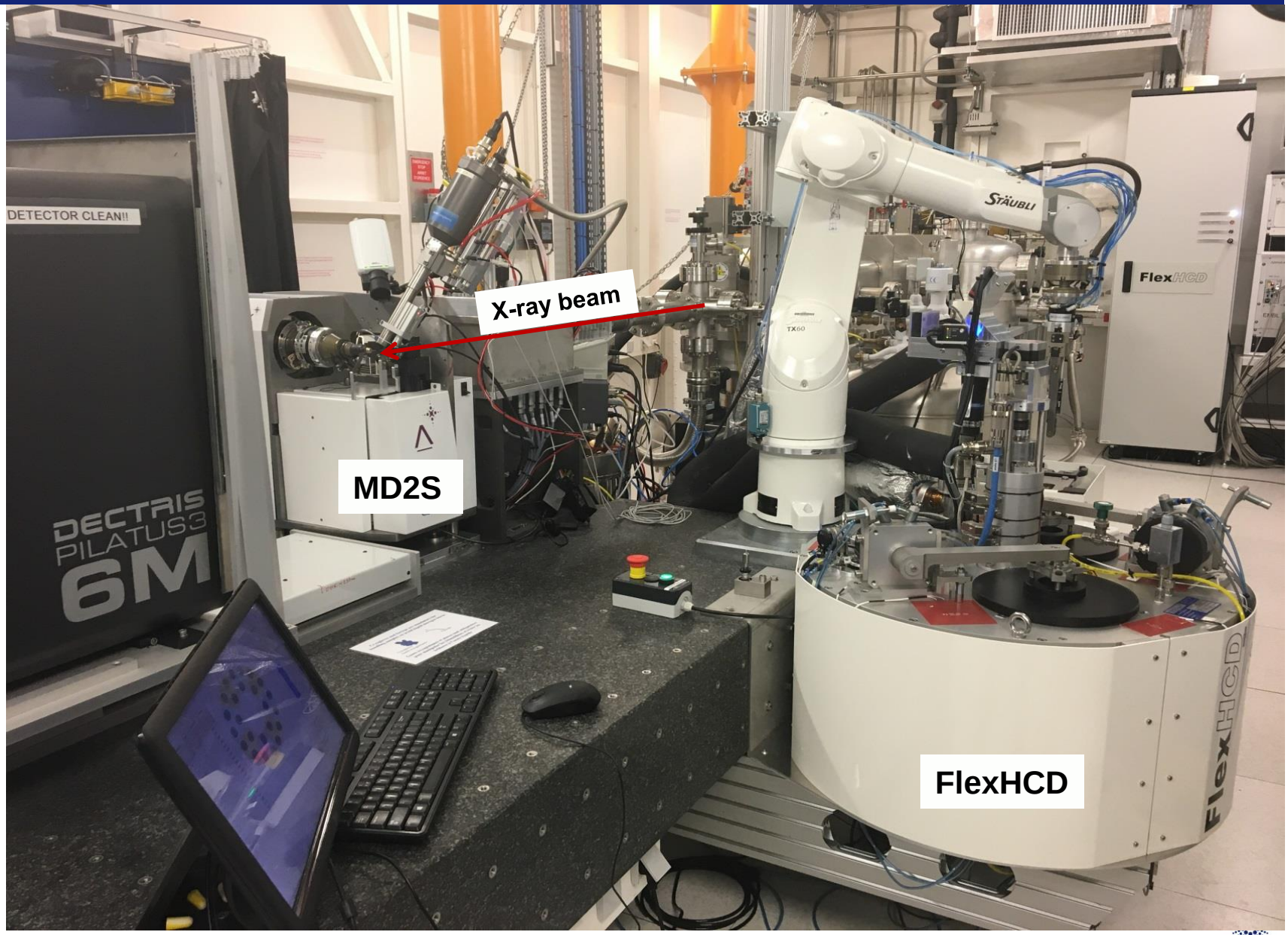
6 – 20 keV
flux: 5 x 10^{12} ph/s
beam size @ samle:
~ 40 μm (50; 30; 20; 10)





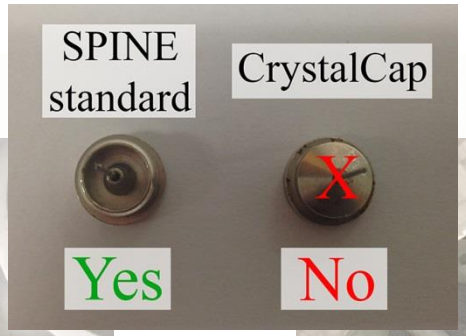


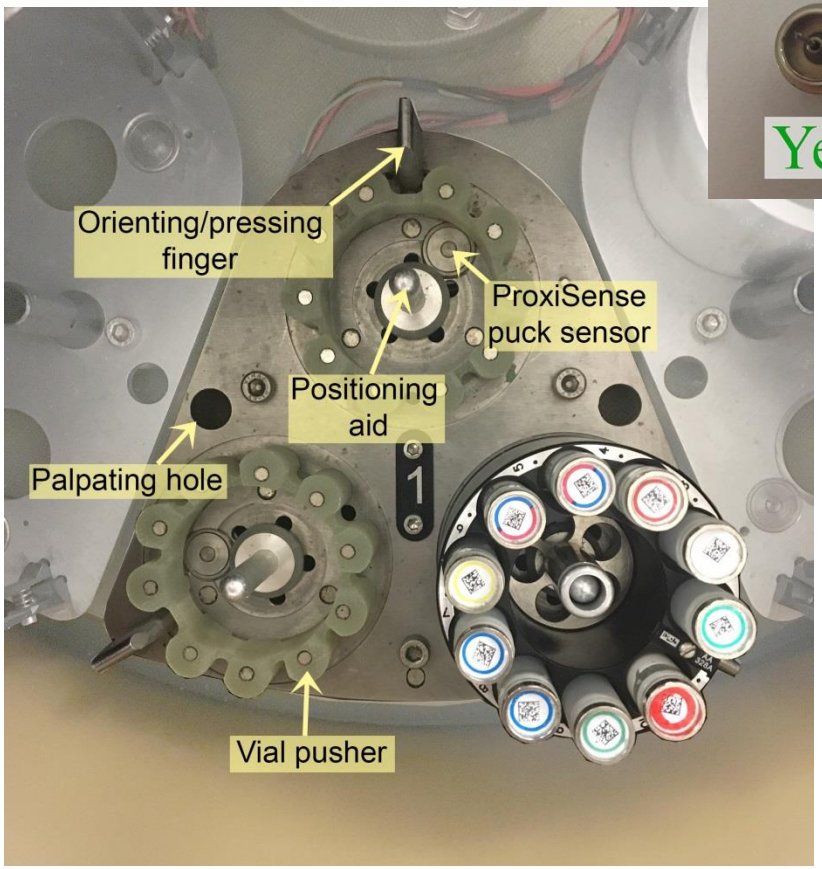
ID30B – EXPERIMENTAL HUTCH



ID30B – FLEXHCD

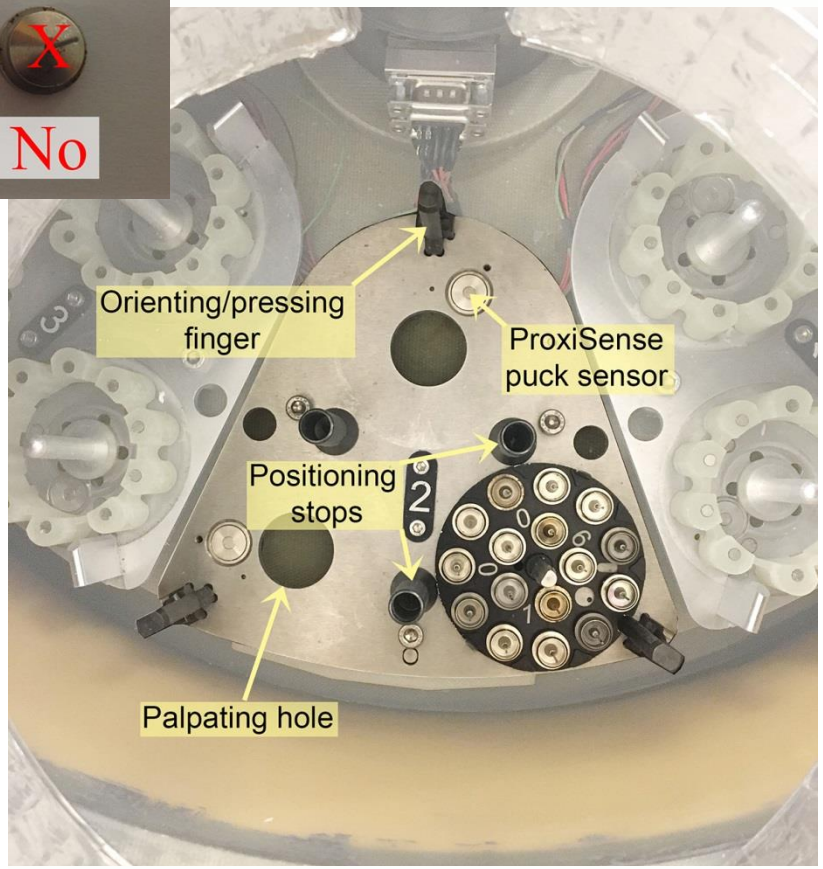
SC3 type pucks (x12)





13,166 samples in 2017
<0.05 % user intervention

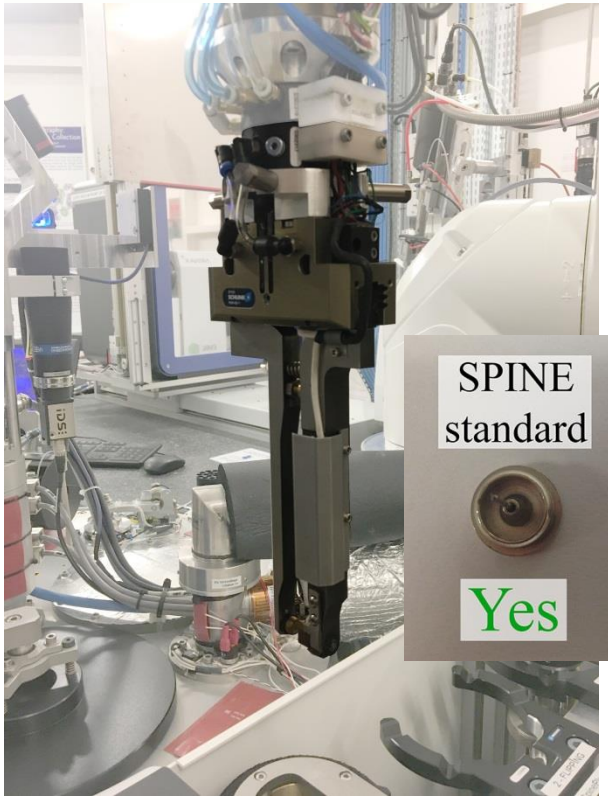
Uni-puck (x11)



3,253 samples in 2017
<1% user intervention

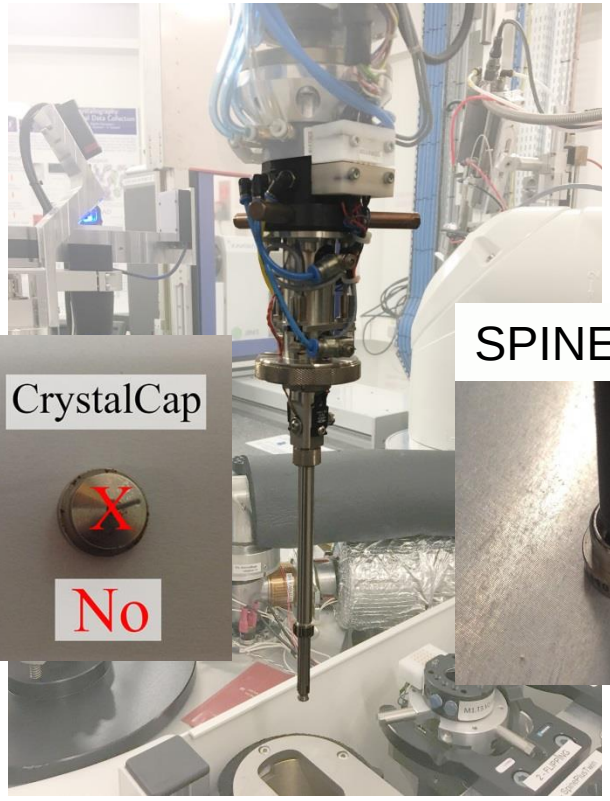
ID30B – FLEXHCD

Flipping gripper (vials)



~20s exchange (x2)
~60s sample to sample

Unipuck - Single

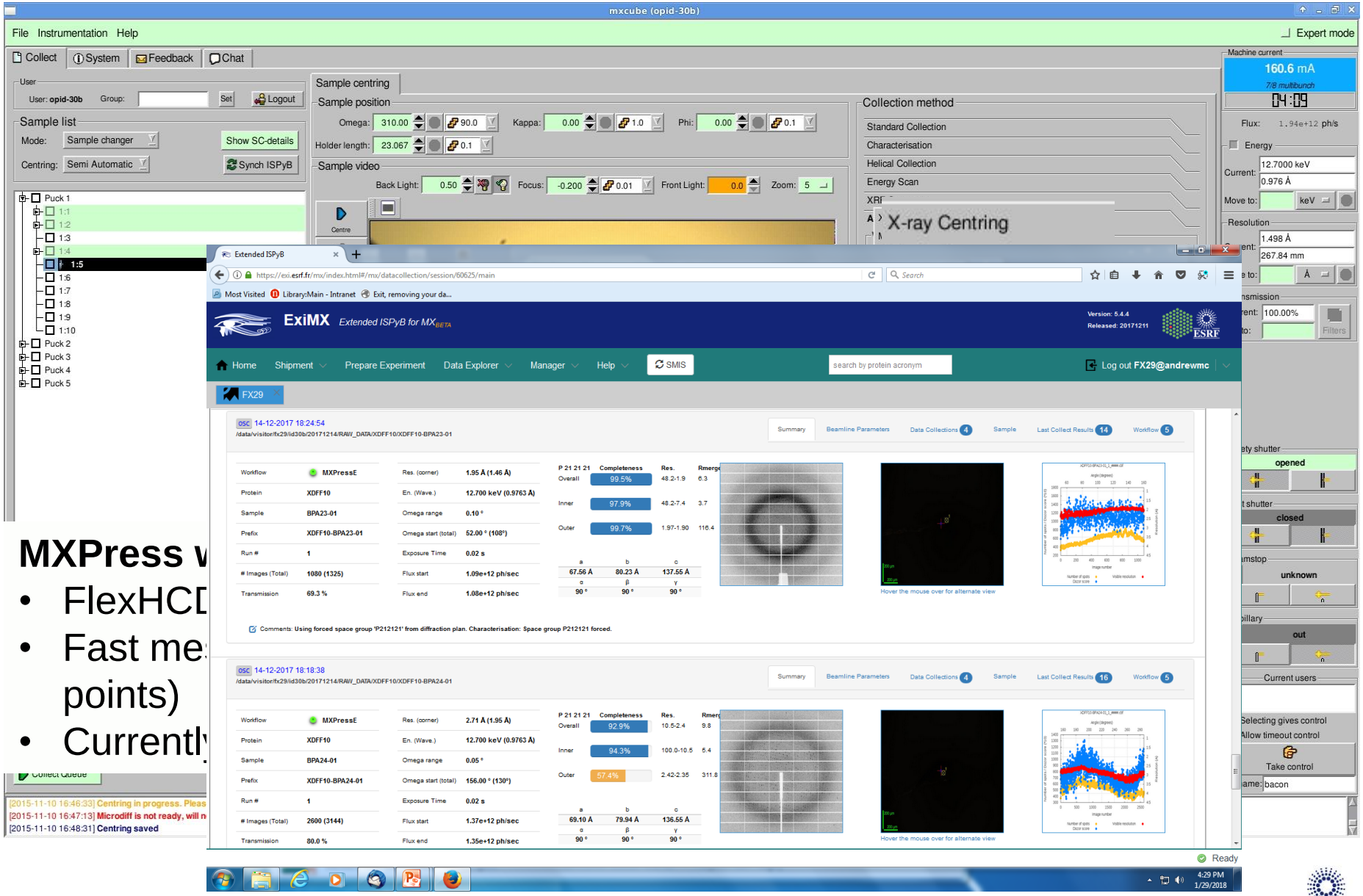


~12s exchange (x2)
~50s sample to sample

Unipuck - Double

~14s exchange (x1)
~40s sample to sample

ID30B – MXPRESS WORKFLOWS



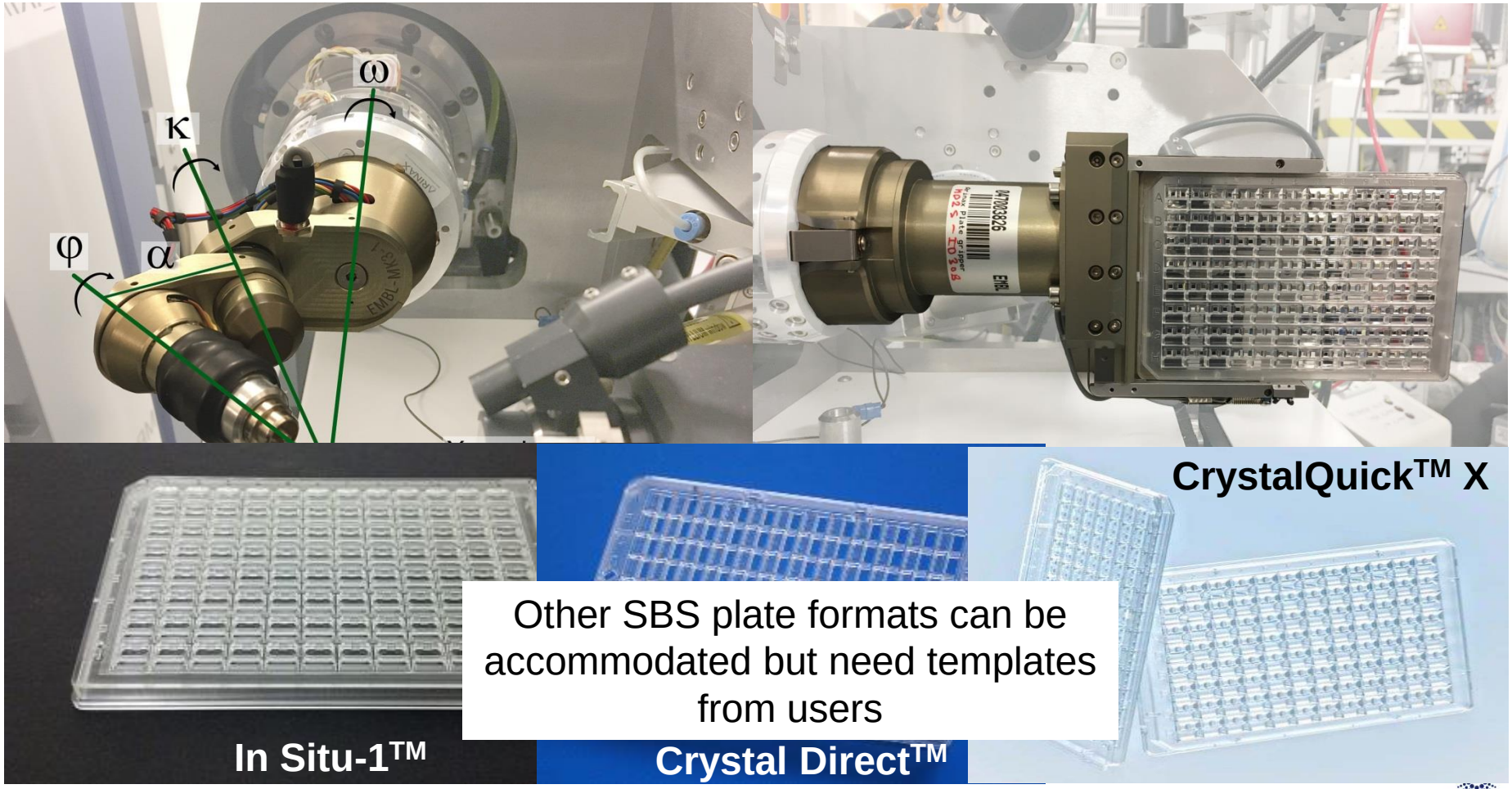
MXPress v

- FlexHCD
- Fast me points)
- Currentl

ID30B – VERSATILE SAMPLE ENVIRONMENT

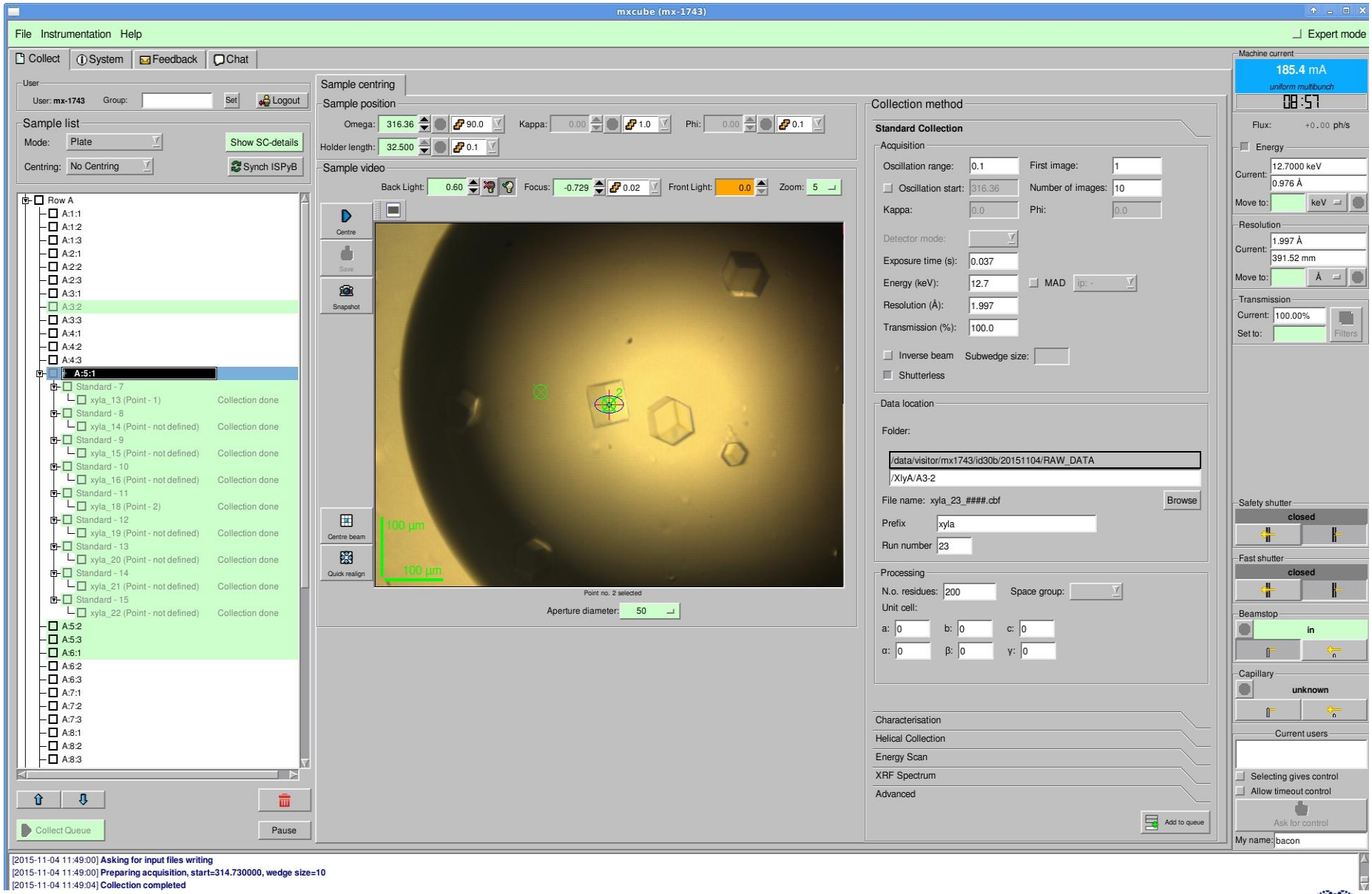
Mini-kappa goniometer head
(Re-orientation)

In situ Plate screening



Other SBS plate formats can be accommodated but need templates from users

ID30B – *IN SITU* DATA COLLECTION



ID30B – *IN SITU* DATA COLLECTION

Thaumatin, 12.7 keV

Extended ISPyB

exi.esrf.fr/mx/#/mx/datacollection/session/54151/main

Most Visited | Library:Main - Intranet | Exit, removing your da...

ExiMX *Extended ISPyB for MX$_{BETA}$*

Version: 0.9.6
Released: 2016/11/15

ESRF

Home | Shipment | Proteins and Crystals | Prepare Experiment | Data Explorer | Offline Data Analysis | Help | search by protein acronym | Log out OPID30b@andrewmc

New Tab

Run #4 OSC Sep 9, 2016 5:16:44 PM
/data/id30b/inhouse/opid30b/20160909/RAW_DATA/Thaumatin/D7_1

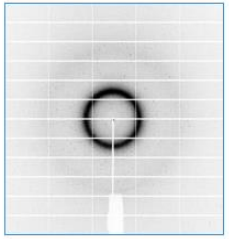
Summary | Beamline Parameters | Data Collections 1 | Sample | Results 8 | Workflow

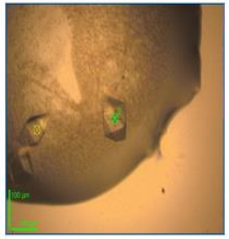
Workflow	
Protein	
Sample	
Prefix	collect
Images	500
Transmission	9.82789
Flux start	3.5e+10 ph/sec

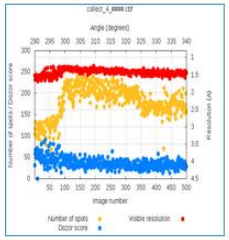
Type	OSC
Res. (corner)	1.5 Å (1.18 Å)
Wavelength	0.977 Å
Phi range	0.1 °
Phi start (total)	340° (50°)
Exposure Time	0.02 s
Flux end	3.39e+10 ph/sec

P 42 21 2	Completeness	Res.	Rmerge
Inner	91%	4.1	0.1
Outer	100%	1.5	0.7
Overall	98%	1.5	0.1

cell A	cell B	cell C
58.5689	58.5689	151.592
Alpha	Beta	Gamma
90	90	90







Run #3 OSC Sep 9, 2016 5:12:05 PM
/data/id30b/inhouse/opid30b/20160909/RAW_DATA/Thaumatin/D7_1

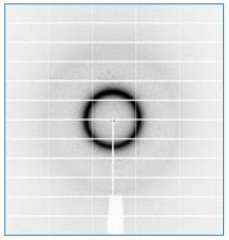
Summary | Beamline Parameters | Data Collections 1 | Sample | Results 15 | Workflow

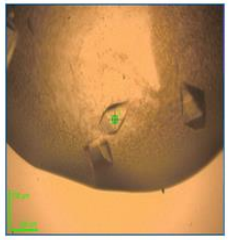
Workflow	
Protein	
Sample	
Prefix	collect
Images	500
Transmission	9.82789
Flux start	3.51e+10 ph/sec

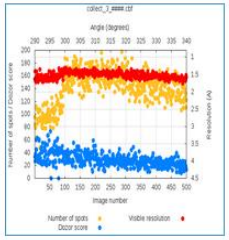
Type	OSC
Res. (corner)	1.5 Å (1.18 Å)
Wavelength	0.977 Å
Phi range	0.1 °
Phi start (total)	340° (50°)
Exposure Time	0.02 s
Flux end	3.52e+10 ph/sec

P 4 21 2	Completeness	Res.	Rmerge
Inner	93%	4.2	0.1
Outer	99%	1.6	0.8
Overall	99%	1.6	0.1

cell A	cell B	cell C
58.5727	58.5727	151.579
Alpha	Beta	Gamma
90	90	90







Ready

3:41 PM
11/22/2016

ID30B – *IN SITU* DATA COLLECTION

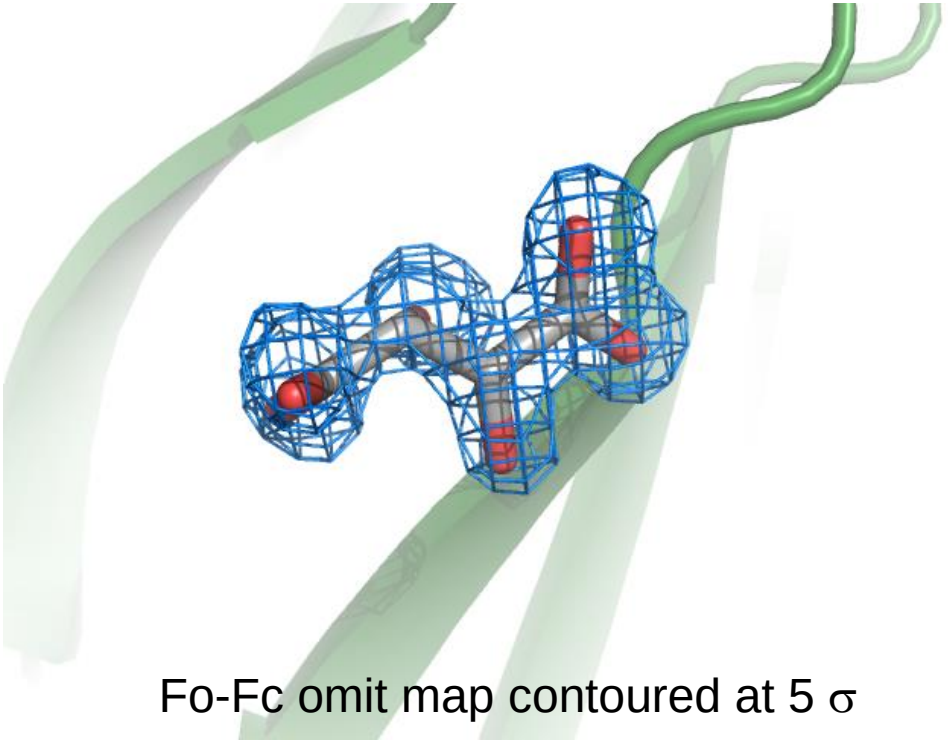
Data collection statistics

Wavelength (Å)	0.9763	0.7085
Phs/sec (Single bunch 4x10 mA and 20 μm aperture)	3.5 x 10^{10}	9.3 x 10^{10}
Exposure time (s)	0.02	0.02
Oscillation range (degrees)		
Total dose (MGy) – *flux2dose (Sasha)*		
Space group		
Cell Dimensions a, b, c (Å)		.5, 90, 90, 90
Resolution (Å) (final shell)		5)
Observed Reflections		)
Unique Reflections		
Completeness (%) (final shell)		
R_{meas} (%) (final shell)		
<I/σ(I)> (final shell)		

Model quality indicators

R_{cryst} (%) / R_{free} (%)

rms deviations, bonds (Å)/angles (°)



Fo-Fc omit map contoured at 5 σ

ID30B – WHAT COMES NEXT?

Immediate future

- Installation of REx nozzle changer for rapid exchange between humidified and cryogenic air streams
- Expand/Improve MXPress automatic data collection WFs

Near future

- New control PC (id30control) + MxCuBE^3
- Develop plate functionalities in ISPyB/Exi
- Add move to Si strip for lower energy ranges

Future

- Improve long term beam stability
- Develop and implement dynamic beam size routines
- Automate data collection from plates (MASSIF style)
- Phase plate commissioning (D. de Sanctis)

ID30B – ACKNOWLEDGEMENT

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Thank you for your attention.