



| The European Synchrotron

ID30B news

EMBL

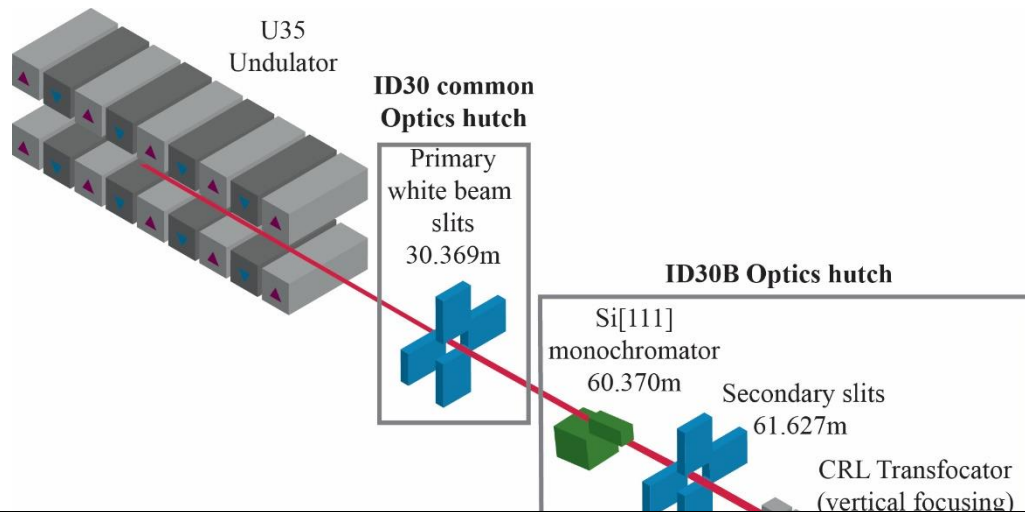


Andrew McCarthy

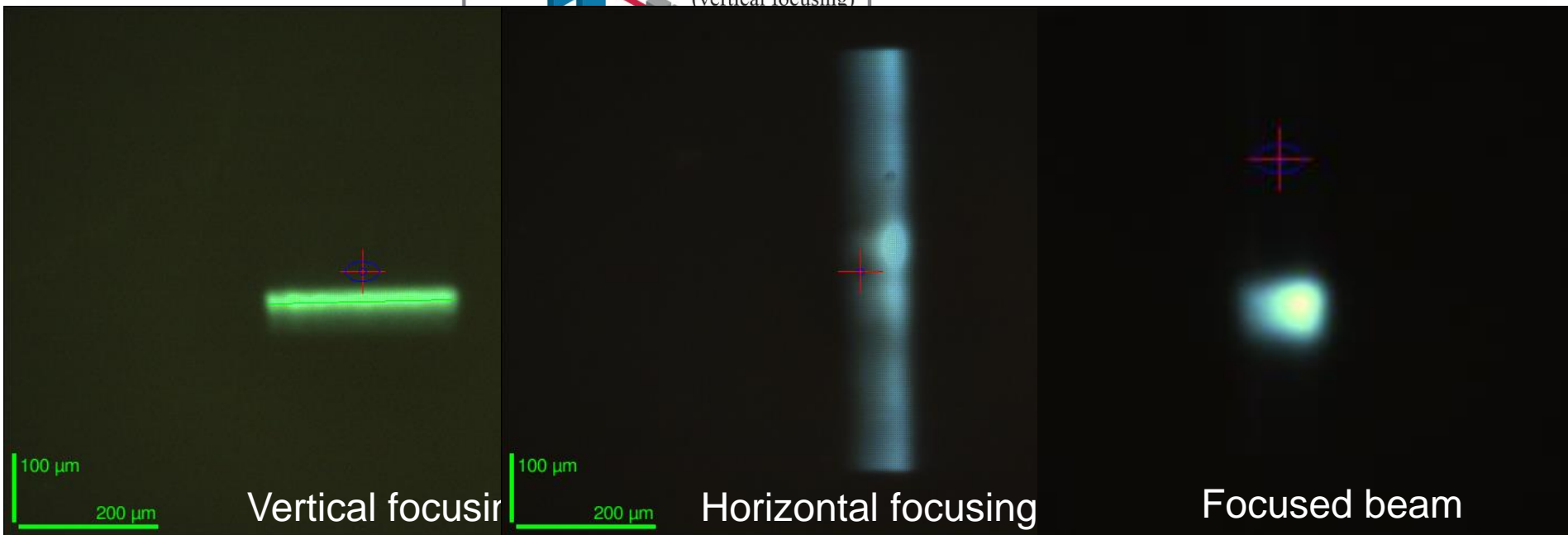
Christoph Mueller-Dieckmann



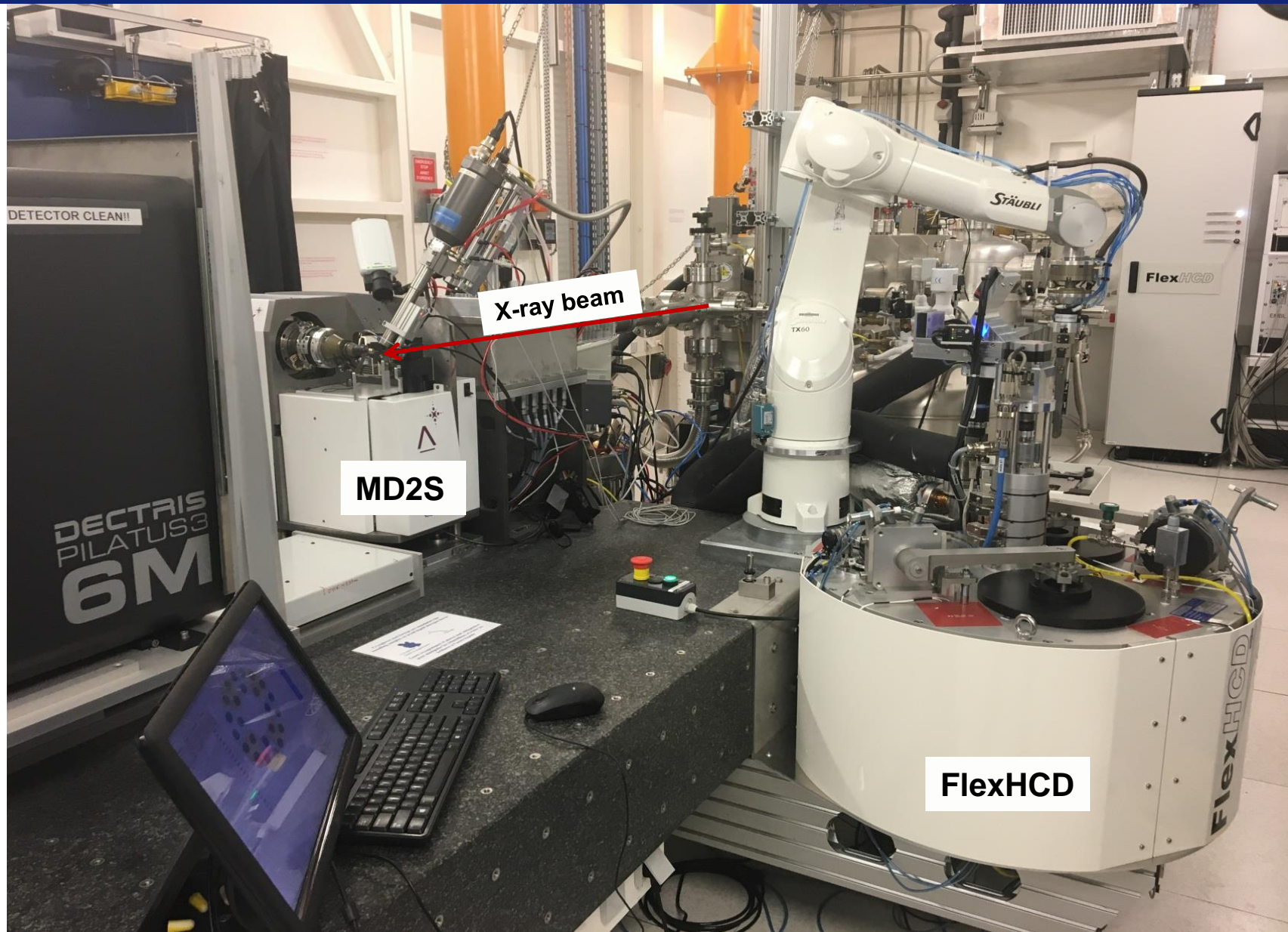
ID30B – OVERVIEW



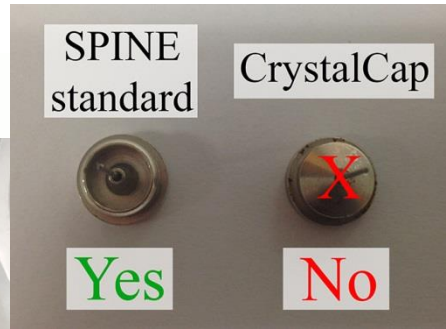
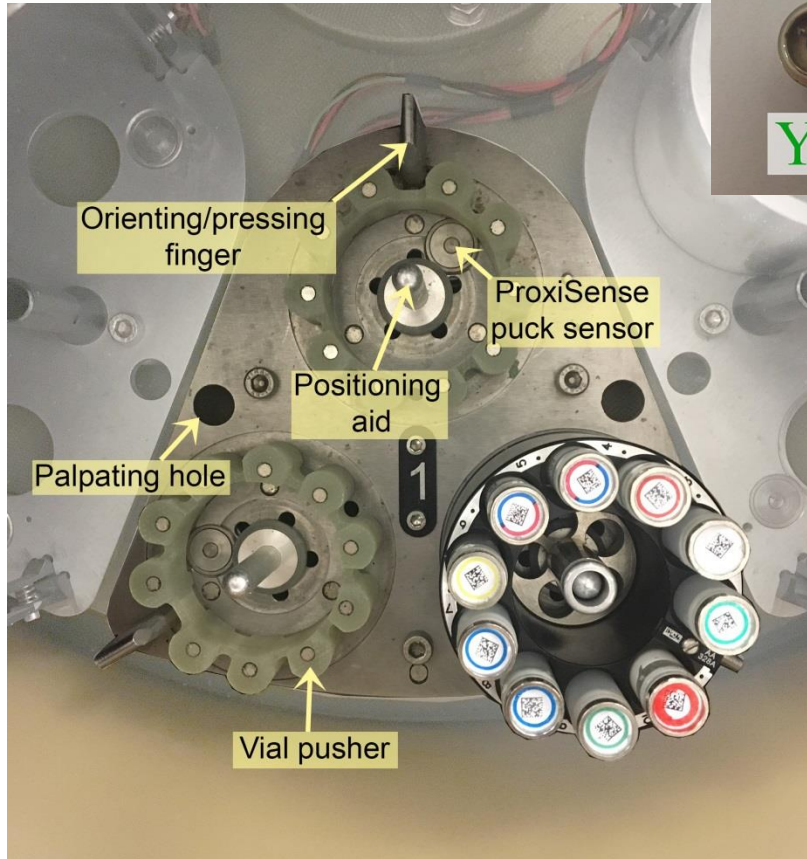
6 – 20 keV
flux: 5×10^{12} ph/s
beam size @ sample:
~ 40 μm (50; 30; 20; 10)



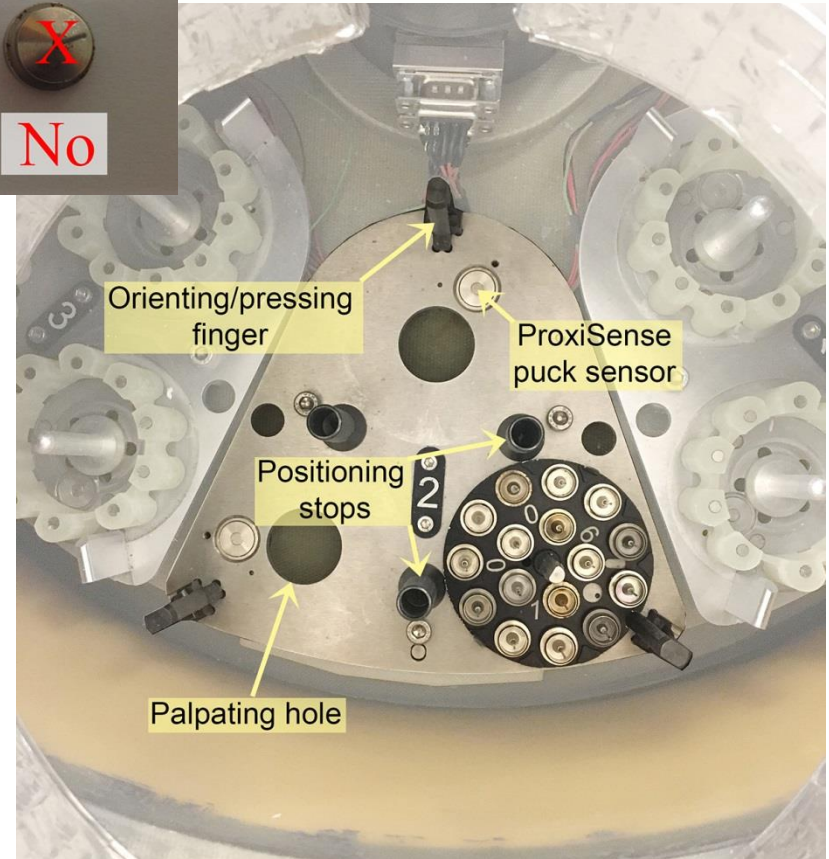
ID30B – EXPERIMENTAL HUTCH



SC3 type pucks (x12)



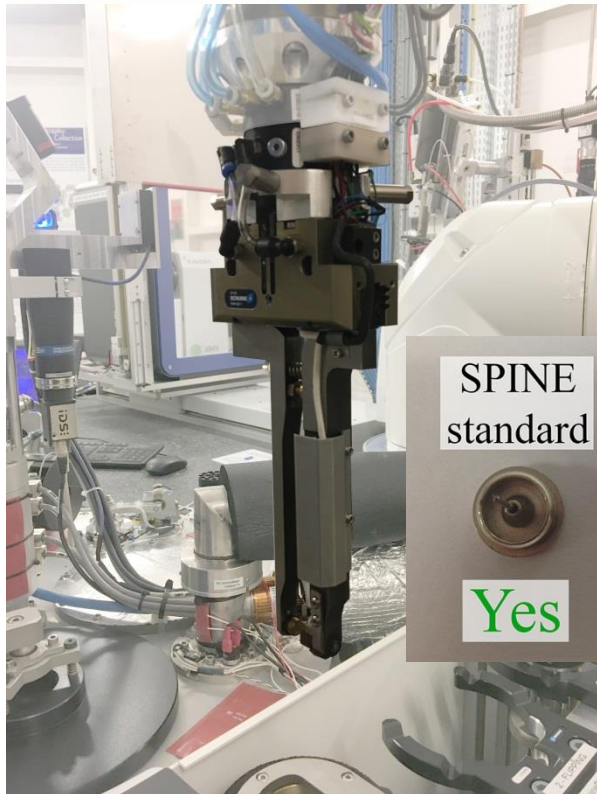
Uni-puck (x11)



13,166 samples in 2017
<0.05 % user intervention

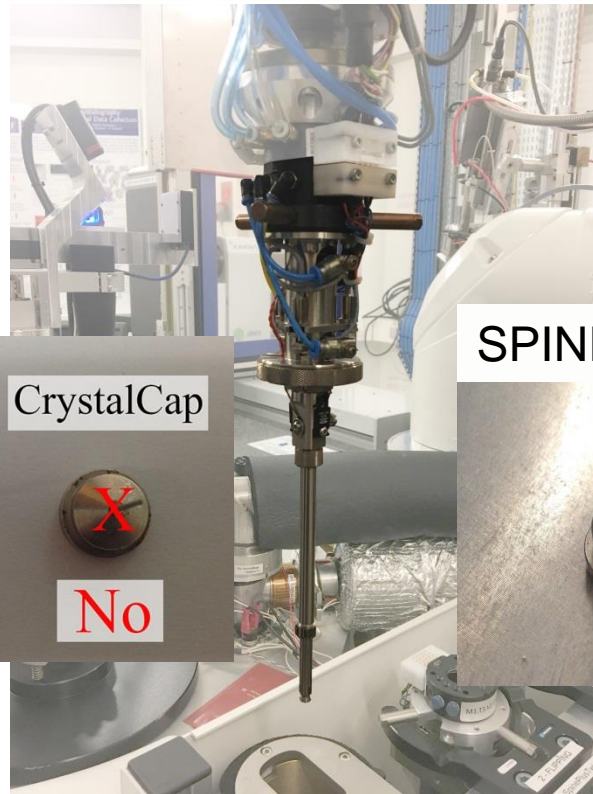
3,253 samples in 2017
<1% user intervention

Flipping gripper (vials)



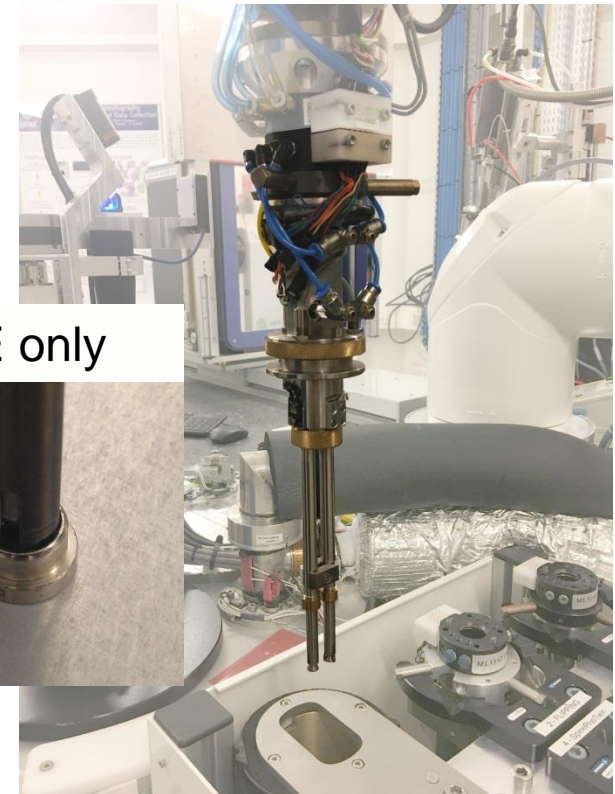
~20s exchange (x2)
~60s sample to sample

Unipuck - Single





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

Unipuck - Double



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

SPINE standard	CrystalCap
	
Yes	No



ID30B – MXPRESS WORKFLOWS

The screenshot displays the MXpress workflow interface. On the left, there's a 'Sample list' with pucks 1 through 5. The main area shows 'Sample centring' controls for Omega, Kappa, and Phi, along with 'Sample position' (Holder length) and 'Sample video' (Back Light, Focus, Front Light, Zoom). A 'Collection method' dropdown is set to 'X-ray Centring'. On the right, a 'Machine current' panel shows 160.6 mA and 04:09. Below the main interface, a browser window shows the 'ExiMX Extended ISPyB for MXBeta' website, displaying a summary of a workflow run. The summary includes parameters like Res. (corner), En. (Wave), Omega range, and a table of P 21 21 21 data. The workflow is identified as MXPressE for protein XDF10, sample BPA23-01, with a resolution of 1.95 Å. The browser also shows a second workflow run with a resolution of 2.71 Å.

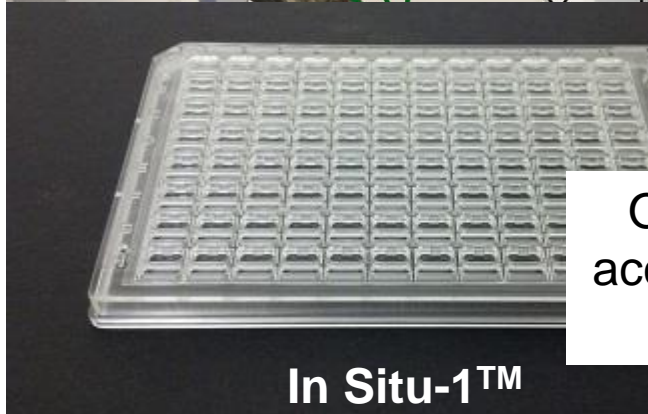
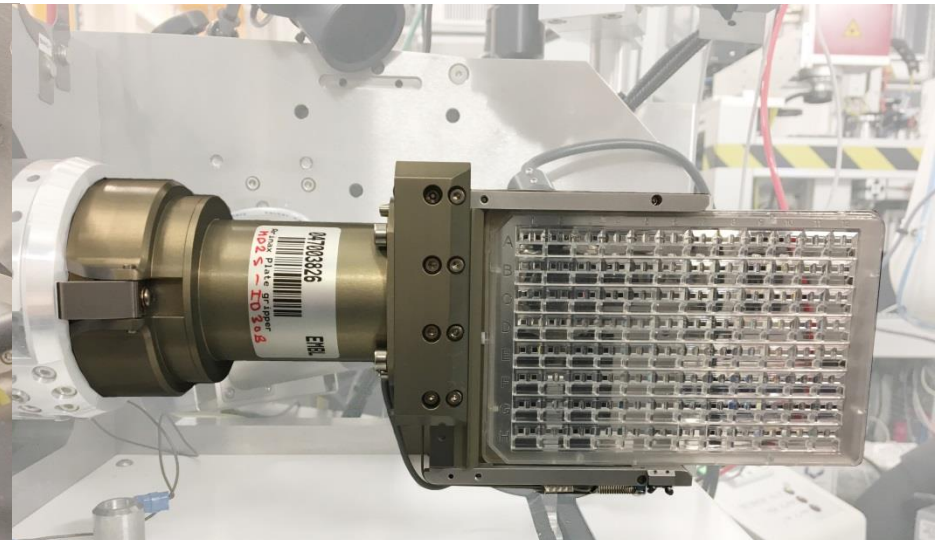
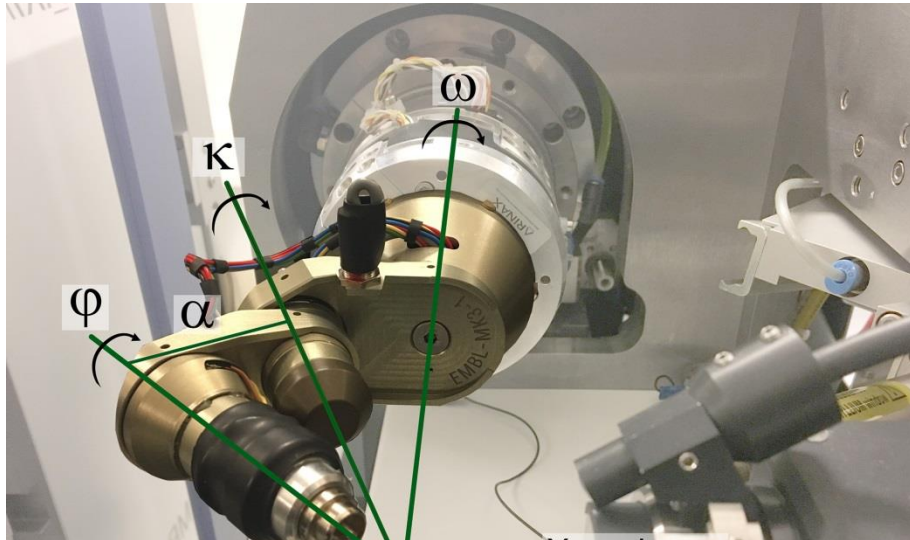
- MXPress v**
- FlexHCL
 - Fast me (points)
 - Currently

[2015-11-10 16:46:33] Centring in progress. Please
 [2015-11-10 16:47:13] Microdiff is not ready, will n
 [2015-11-10 16:48:31] Centring saved

ID30B – VERSATILE SAMPLE ENVIRONMENT

Mini-kappa goniometer head
(Re-orientation)

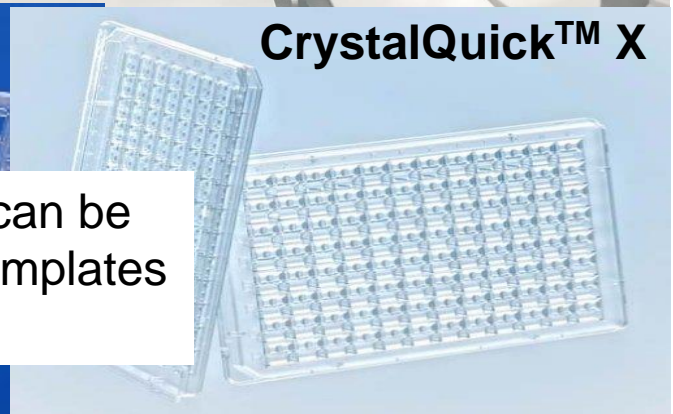
In situ Plate screening



In Situ-1™



Crystal Direct™



CrystalQuick™ X

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

ID30B – IN SITU DATA COLLECTION

mxcube (mx-1743) Expert mode

File Instrumentation Help

Collect System Feedback Chat

User: mx-1743 Group: [] Set Logout

Sample list
Mode: Plate Show SC-details
Centring: No Centring Synch ISPyB

Sample centring
Sample position
Omega: 316.36 Kappa: 0.00 Phi: 0.00
Holder length: 32.500

Sample video
Back Light: 0.60 Focus: -0.729 Front Light: 0.0 Zoom: 5
Aperture diameter: 50

Collection method
Standard Collection
Acquisition
Oscillation range: 0.1 First image: 1
Oscillation start: 316.36 Number of images: 10
Kappa: 0.0 Phi: 0.0
Detector mode: []
Exposure time (s): 0.037
Energy (keV): 12.7 MAD []
Resolution (Å): 1.997
Transmission (%): 100.0
Inverse beam Subwedge size: []
Shutterless

Data location
Folder: /data/visitor/mx1743/id30b/20151104/RAW_DATA
XlyA/A3-2
File name: xyla_23_###.cbf Browse
Prefix: xyla
Run number: 23
Processing
N.o. residues: 200 Space group: []
Unit cell:
a: 0 b: 0 c: 0
α: 0 β: 0 γ: 0
Characterisation
Helical Collection
Energy Scan
XRF Spectrum
Advanced

Machine current: 185.4 mA uniform multibunch 08:57
Flux: +0.00 ph/s
Energy
Current: 12.7000 keV 0.976 A
Move to: [] keV
Resolution
Current: 1.997 Å 391.52 mm
Move to: [] Å
Transmission
Current: 100.00%
Set to: [] Filters

Safety shutter: closed
Fast shutter: closed
Beamstop: in
Capillary: unknown
Current users
Selecting gives control
Allow timeout control
Ask for control
My name: bacon

[2015-11-04 11:49:00] Asking for input files writing
[2015-11-04 11:49:00] Preparing acquisition, start=314.730000, wedge size=10
[2015-11-04 11:49:04] Collection completed

ID30B – IN SITU DATA COLLECTION

Thaumatococcus, 12.7 keV

Run #4 OSC Sep 9, 2016 5:16:44 PM

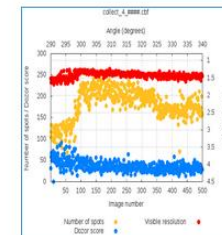
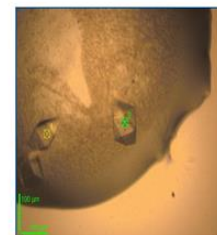
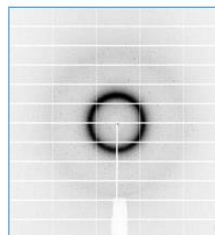
/data/id30b/inhouse/opid30b/20160909/RAW_DATA/Thaumatococcus/D7_1

Summary Beamline Parameters Data Collections 1 Sample Results 8 Workflow

Workflow	Type	OSC
Protein	Res. (corner)	1.5 Å (1.18 Å)
Sample	Wavelength	0.977 Å
Prefix	Phi range	0.1 °
Images	Phi start (total)	340° (50°)
Transmission	Exposure Time	0.02 s
Flux start	Flux end	3.39e+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 4 2 1 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

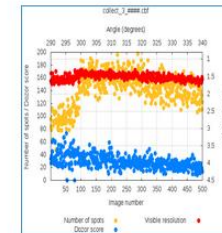
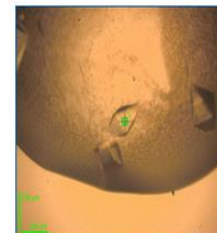
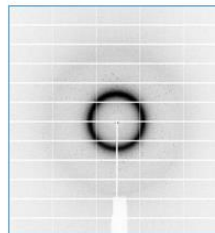
/data/id30b/inhouse/opid30b/20160909/RAW_DATA/Thaumatococcus/D7_1

Summary Beamline Parameters Data Collections 1 Sample Results 15 Workflow

Workflow	Type	OSC
Protein	Res. (corner)	1.5 Å (1.18 Å)
Sample	Wavelength	0.977 Å
Prefix	Phi range	0.1 °
Images	Phi start (total)	340° (50°)
Transmission	Exposure Time	0.02 s
Flux start	Flux end	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	3.51e+10 ph/sec

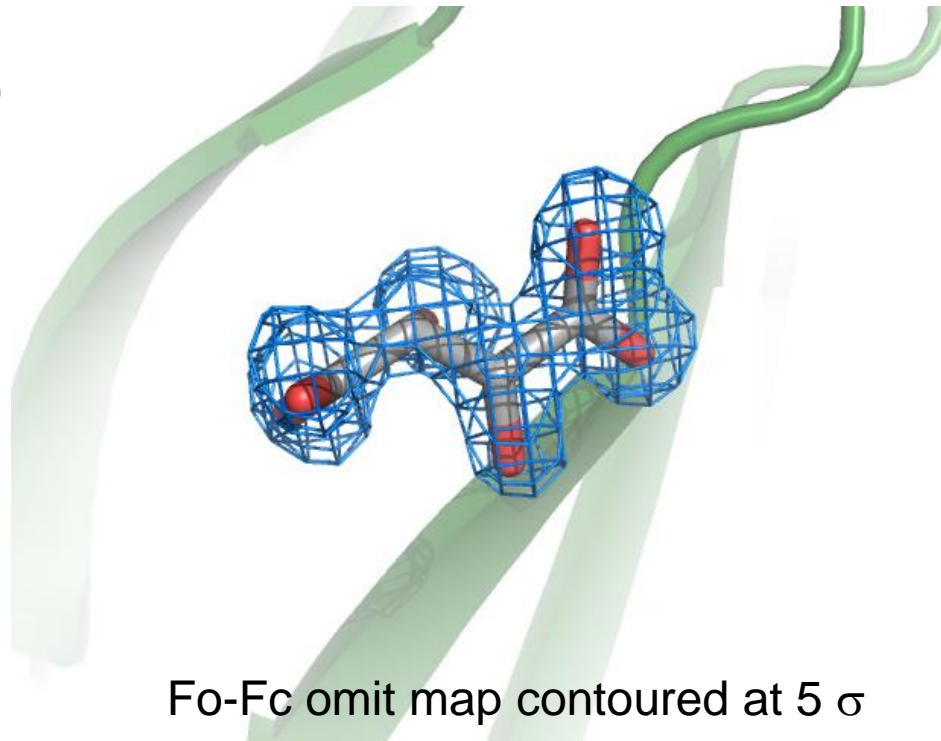
P 4 2 1 2	Completeness	Res.	Rmerge
Inner	93%	4.2	0.1
Outer	99%	1.6	0.8
Overall	99%	1.6	0.1
cell A	cell B	cell C	
58.5727	58.5727	151.579	
Alpha	Beta	Gamma	
90	90	90	



ID30B – *IN SITU* DATA COLLECTION

Data collection statistics

Wavelength (Å)	0.9763	0.7085
Phs/sec (Single bunch 4x10 mA and 20 μm aperture)	3.5×10^{10}	9.3×10^{10}
Exposure time (s)	0.02	0.02
Oscillation range (degrees)		
Total dose (MGy) – <i>flux2dose (Sasha)</i>		
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)		
<l/σ(l)> (final shell)		
<u>Model quality indicators</u>		
R _{cryst} (%) / R _{free} (%)		
rms deviations, bonds (Å)/angles (°)		



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) + MxCuBE³
- 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)

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Thank you for your attention.