

# eBIC@Diamond – Update/remote

Instruct workshop  
16/10/18

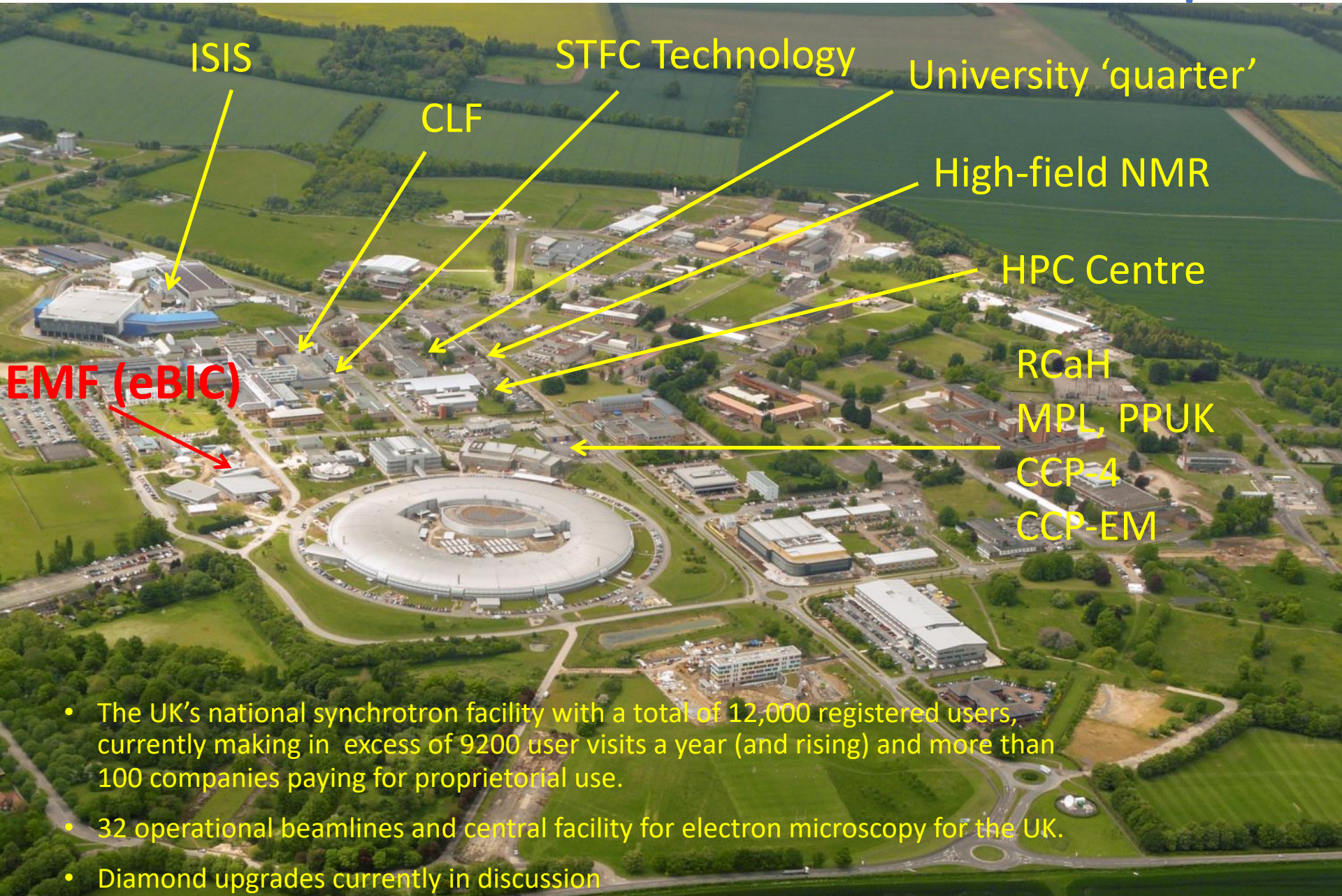
Daniel Clare



Science & Technology  
Facilities Council



# Diamond & Harwell Research Campus



ISIS

STFC Technology

University 'quarter'

CLF

High-field NMR

HPC Centre

EMF (eBIC)

RCaH

MPL, PPUK

CCP-4

CCP-EM

- The UK's national synchrotron facility with a total of 12,000 registered users, currently making in excess of 9200 user visits a year (and rising) and more than 100 companies paying for proprietorial use.
- 32 operational beamlines and central facility for electron microscopy for the UK.
- Diamond upgrades currently in discussion

# eBIC Aims

- The UK National Centre for cryo-EM:
  - Free-at-the-point-of-access to state-of-the art facilities.
  - Peer reviewed application process.
  - Beamline-like 24/7 operation supported by expert staff to facilitate intensive external user program.
- Cutting-edge in-house research program under eBIC director - Peijun Zhang.
- Foster the development of integrated structural biology in the UK, linking with other developments, including CCP-EM, EMDB and iNEXT.
- Training courses to bring in structural and cell biologists:
  - “Advanced Data Collection For High Resolution Cryo-EM” – Sept. 2016
  - 1<sup>st</sup> iNEXT FEI sponsored “Sample Preparation For Cryo-EM” - Jan. 2017
  - 2<sup>nd</sup> “Sample Preparation For Cryo-EM” – October 2017
  - 3<sup>rd</sup> Sample Preparation For Cryo-EM” – October 2018



# User Access (80% of Microscope Time)

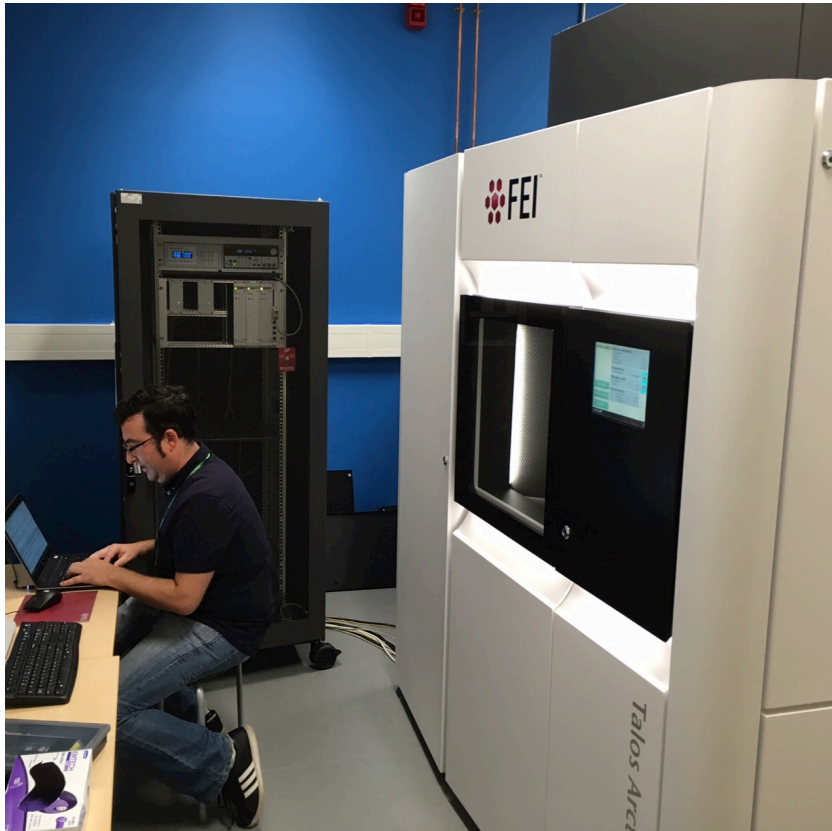
- **1) Rapid access:** 48 hr allocation **now reviewed by beamline staff**
- **2) Block Allocation Group (BAG) access:** Multiple sessions to research group consortia.
  - Deadline every 6 months for a 2 year time period (PRP assess every 6 months).
  - Currently 12 BAGs - 115 days/6 months *i.e.* 55% of total time allocated over 4 Krios.
  - BAGs vary from 5-15 PIs.
  - **Super-user training program to increase flexibility for BAG's**
- **3) eBIC for Industry:** Krios 5 is a collaboration with Thermofisher, dedicated to industrial users
- **Acceptance criteria:** Based on scientific excellence, subject to standard Diamond T&Cs, notably that the work should be published.
- **Travel and subsistence:** Covered for UK users (normally 1-2 people per visit).
- **iNEXT** (EU H2020 I3 type grant) provides funded access to European users.

# eBIC Facility

- Sample preparation, loading and general labs. + multiple rooms for smaller microscopes
- Initially constructed with two large rooms for two Titan Krios
- Now remodelled to house four Krios as of September it is now full!



# Microscopes: Talos Arctica and Scios FIB-SEM



- Falcon III & Ceta camera
- Volta phase plate
- Used for Training and in-house research and MicroED

- Prototype MPI Martinsried cryo stage
- Platinum GIS
- Quorum sample loading system → Themo
- First commissioning visit with external users start this month

# eBIC Control Room



- Krios 1-4 and the Talos controlled operated using the Thermofisher fibre remote control
- No noticeable lag ~ Krios 1 is 400 meters away
- Support PC located by the microscope ~ UI can be accessed when loading
- Disruption to microscope room environment minimised
- Health and Safety concerns minimised ~ Users now remote from the microscope
- Workstations next to microscope controls ~ On-the-fly processing

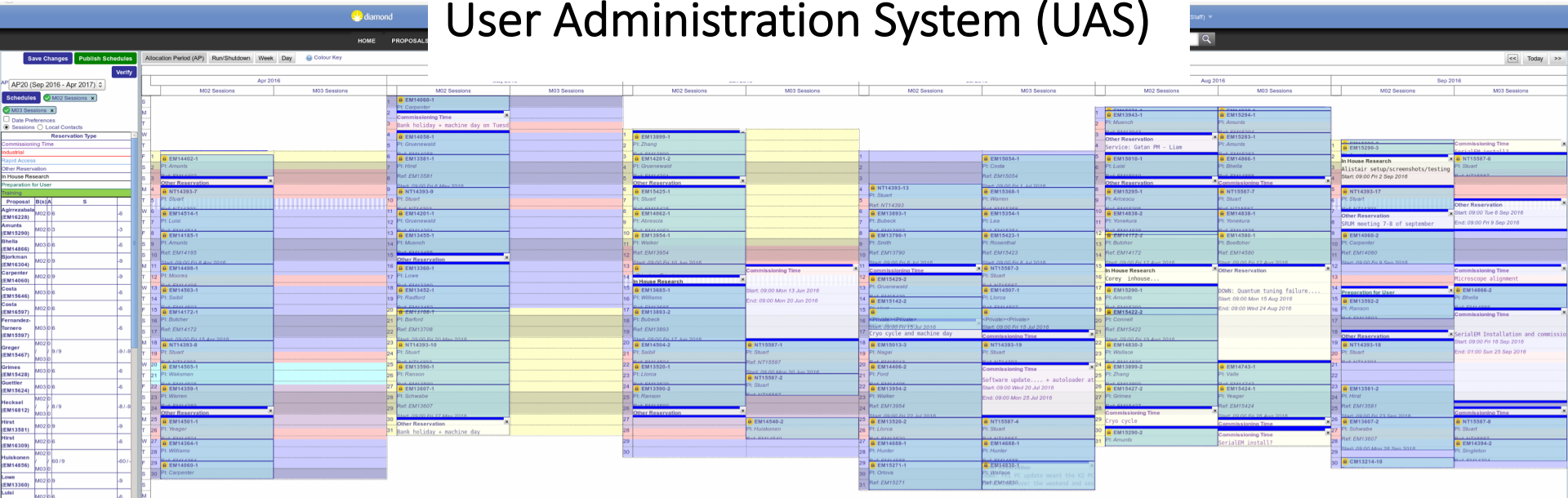
# Remote User Control

## How eBIC can learn from MX



# Infrastructure Required for External Users and Remote User Control

## User Administration System (UAS)



- Schedule visits based on the main synchrotron operational calendar
- Users can submit preferred dates for their visits
- Assignment of local contact for visits
- Once scheduled dedicated user office staff can arrange accommodation, access, subsistence *etc.*
- Automatic, secure data directory structures and archiving!



# UAS – Visit Details

HOME PROPOSALS **SESSIONS** CALENDAR SCHEDULING

NR21005-39: 10:00 Wed 10 Oct 2018 - 09:00 Thu 11 Oct 2018 on M04  
EM In house for internal staff only Principal Investigator Prof Peijun Zhang, University of Oxford  
First Local Contact Dr Zhengyi Yang (01235778648)  
Responsible Administrator Mrs Wendy Collier (01235 778571)  
Email Session Participants Grade Sheet

Investigators: **BOOKED**  
ERA: **VALIDATED**  
Risk Rating: **Low**  
Grant Funded: No  
Access Route: In House

Cancel Changes Save Changes Emergency Instrument Move Change Instrument Withdraw & Edit Session ERA

- Investigators
- ERA
- Samples
- Equipment
- Experimental Methods
- Lab Access
- ERA Summary
- Notes

The arrangements have been booked by Diamond User Office. Please ensure you read all the information carefully, and contact us if you have any questions.

Changes to remote participants and contact details may still be made until the session starts.  
Changes to investigators requiring data access only may continue to be made indefinitely.  
If additional on-site investigators are to be added, they must be registered with Diamond before contacting the User Office.  
Investigators who are not already registered with Diamond should be invited to register.  
The Principal Investigator or Team Leader must contact the User Office once this has been undertaken to add the on-site.  
For further assistance, please contact Diamond User Office by email or phone on +44 (0) 1235 77 8571

- Investigators tab controls not only site access but also data access!

ALL PARTICIPATING TEAM MEMBERS BOTH ON-SITE AND REMOTE - PLUS OTHERS REQUIRING DATA ACCESS ONLY

Email Investigators without Safety Test Add Remote Investigator

Name	Team Role	Remote	Subsistence Request	Arrival	Transport	Access Card Pickup	All Nights	9 Oct	10 Oct
Dr Zhengyi Yang, Diamond Light Source	Leader	<input type="checkbox"/>	User pays	10:00 Wed 10 Oct 2018	Car	User	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>

Taxi requests  
None

eBIC Experiment Type  
 Single Particle  Tomography

eBIC Detector  
 K2  Falcon III Counting  Falcon III Linear

eBIC Software  
 EPU  TOMO4  SerialEM

Phase Plate  
 No  Yes

- Experiment and detector choice (eBIC specific)

Samples to be used on the instrument and in preparation for the instrument

Create New Sample Add From Proposal Add All From Proposal Remove All From Session

Sample	State		
E.coli	Validated	Copy Sample	Remove Sample

- Sample containment level verified by SHE group

Experimental methods to be used for this experiment

Create New Experimental Method Add From Proposal Add All From Proposal Remove All From Session

Experimental Method	State		
CryoEM	Validated	Copy Experimental Method	Remove Experimental Method

# ISPyB – Dewar Shipping

**Select Shipments**

**Tick the dewars you want to send**

**Click Use Facility Account, then Accept the Terms and Conditions**

**Check the details are correct**

**Click Create Airway Bill, this will book the shipment with DHL**

Create Airway Bill: To Facility

Shipment Details

Shipment: NR16818-33\_06092017

Dewars:  DLS-MX-1235  DLS-MX-1234

Weight: 36 Kg

DHL Account Number:

Declared Value:  GBP

Package Description:

Contact Details

Contact: Elizabeth Windsor

Contact Phone Number: 0303 123 7300

Contact Email: lz@royal.uk

Laboratory Details

Laboratory Name: Buckingham Palace

Laboratory Address (excluding post code): The Mall Westminster

Laboratory City: London

Laboratory Postcode: SW1A 1AA

Laboratory Country: United Kingdom [Free For: United Kingdom]

Pickup Details

Package Location: Location where shipment can be picked up from: Stores

Shipping Date: 11-07-2017

Ready By: Time shipment will be ready for pickup: 09:00

Close Time: Time after which shipment cannot be picked up: 17:00

Terms & Conditions

I understand that use of DHL's services is entirely at my own risk and that Diamond makes no representations or warranties of any kind (express or implied) about the reliability or availability of the DHL service. Any reliance that I place on the DHL service is strictly at my own risk. It is my responsibility to ensure that samples arrive at Diamond in advance of any beartime that Diamond may have awarded me and I hereby indemnify and hold Diamond harmless for any loss or damage arising out of my use of DHL's services.

- Dewars can now be shipped to diamond from anywhere within the EU using
- Shipment tracking and email notification

\*Cat2 samples can not be shipped using IspyB\*

[https://www.diamond.ac.uk/Instruments/Mx/Common/Common-Manual/Shipping-Samples/Shipping\\_to\\_Diamond/UK.html](https://www.diamond.ac.uk/Instruments/Mx/Common/Common-Manual/Shipping-Samples/Shipping_to_Diamond/UK.html)

# ISPyB – MX Sample registration

## Shipment Contents

Select a dewar by clicking on the row in the table below. Dewar details are then shown below. Click the + icon to add a container to the selected dewar

+ Add Dewar

Name	Barcode	Facility Code	First Experiment	Tracking # to	Tracking # from	Status	Location	Containers
DLS-01-0001	cm4950-0003872	Click to edit	Click to edit	Click to edit	Click to edit	opened		0
Dewar1	cm4950-1-i03-0003870	Click to edit	cm4950-1	Click to edit	Click to edit	opened		Click to add a container +

## Add Container

This page allows you to add containers to the selected dewar and shipment. If the protein you want to use isn't listed type in a new name and press tab. This will create a new protein

Paste from Spreadsheet

Shipment

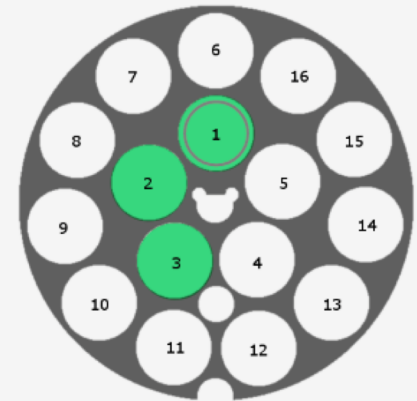
test

Dewar

Dewar1

Puck Name

test



Location	Protein Acronym	Sample Name	Spacegroup	Barcode	Comment
1	lys	lys1			
2	lys	lys2			
3	lys	lys3			

- Diamond labels used to identify dewars in ISPyB – Unique barcode
- Pucks must be clearly labelled – MX have barcodes
- Allows local contact to load pucks into automated sample loader

# Remote connection to MX

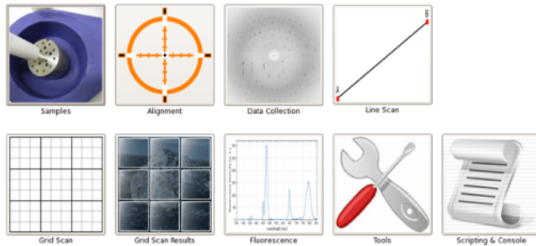
- One or two 1900 x 1200 (or 1900 x 1020) monitors attached to a fast modern PC
- The latest NoMachine Enterprise Client for your OS (runs on all platforms).
- A good connection (at least 10Mb/s) - you can test your connection to Diamond.

How to remotely connect to a  
beamline or Diamond cluster

# Remote User control to MX



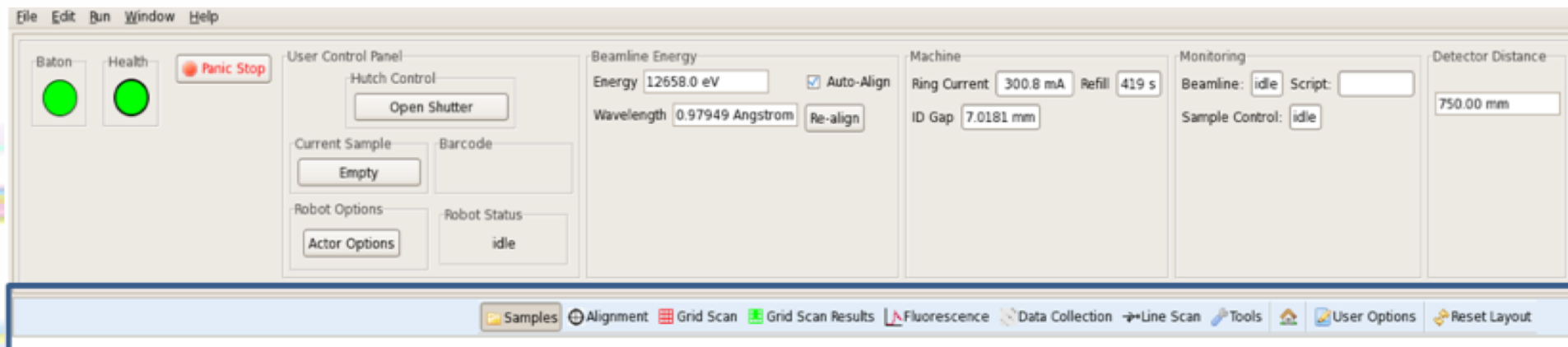
- Main control panel allows access to the different perspectives



- Sample loading control panel

Locn	Container (Puck/Plate)	Position	Sample Name	Barcode	Protein Acronym	Comment
1	No container assigned					
2	No container assigned					
3	No container assigned					
4	cm5925-3:20130620-135013		Expand row to view samples			
4		1	test_1		ferritin	
4		2	test_2		ferritin	
4		3	test_3		ferritin	
4		4	test_4		ferritin	
4		6	test_6		ferritin	
4		7	test_7		ferritin	
4		8	sam_3		ferritin	
4		9	test_9		ferritin	
4		10	test_10		ferritin	
4		11	test_11		ferritin	
4		12	test_12		ferritin	
4		13	test_13		ferritin	
4		14	test_14		ferritin	
4		15	test_15		ferritin	
4		16	test_16		ferritin	
5	No container assigned					

- Baton control panel – who is in control?



# Remote User control to MX

- Crystal Alignment controls



- Data collection parameters

**Data Collection Settings** 2 errors detected

**Scan Control**

**Sample**

Not defined

Barcode

Holder

Position

**Files**

Visit directory

Folder

Prefix

Automatic run number

Run number

Number of passes

Comment

**Omega**

Start  °

Oscillation  °

Total oscillation  °

Delta  °

**Image**

Number of images

Exposure time  s

Total exposure time  s

First image number

**Beam and Detector**

Maximum resolution  Å

Detector distance  mm

Wavelength  Å

Energy  eV

Use current energy

Transmission  %

**Aperture and Beamstop**

Aperture

Beamstop

Queue - waiting

Aperture  Beam Scale  Focal Spot  Slit Gap

**Camera Control**

Zoom

**Beam Visualisation**

**Rotation**

Omega

**Translation**

Readbacks

X

Y

Z

**Nudge**

Size

# Remote Access for eBIC



# What we currently have at eBIC

- UAS registration – Yes
- UAS visit detail – Yes
- ISPyB dewar shipping – Yes
- Sample registration – No
- Remote connection and beamline control for staff – yes
- Remote connection for beamline control by users - No

# ISPyB – MX Sample registration

## Shipment Contents



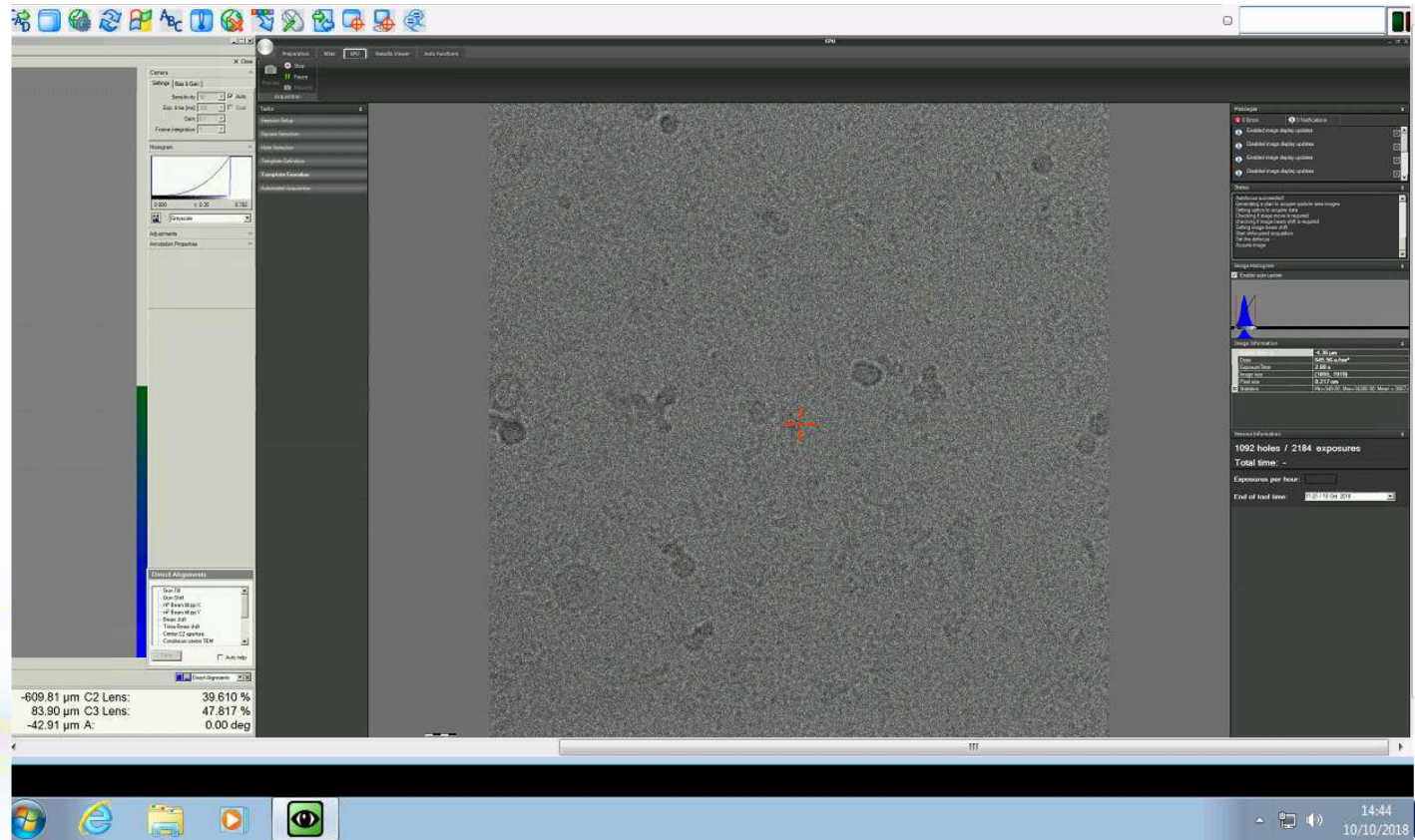
- Diamond labels used to identify dewars in ISPyB – Unique barcode
- We are getting transport canes and pucks which we can distribute to our BAG's
- Need to modify ISPyB MX sample pages to facilitate this style of puck

# Remote connection and beamline control for staff

- Access to microscope support PC with FedID and NoMachine
- Full Access to the Microscope and Detector PC's
- Full access to microscope controls - virtual hand panels + microscope alignment

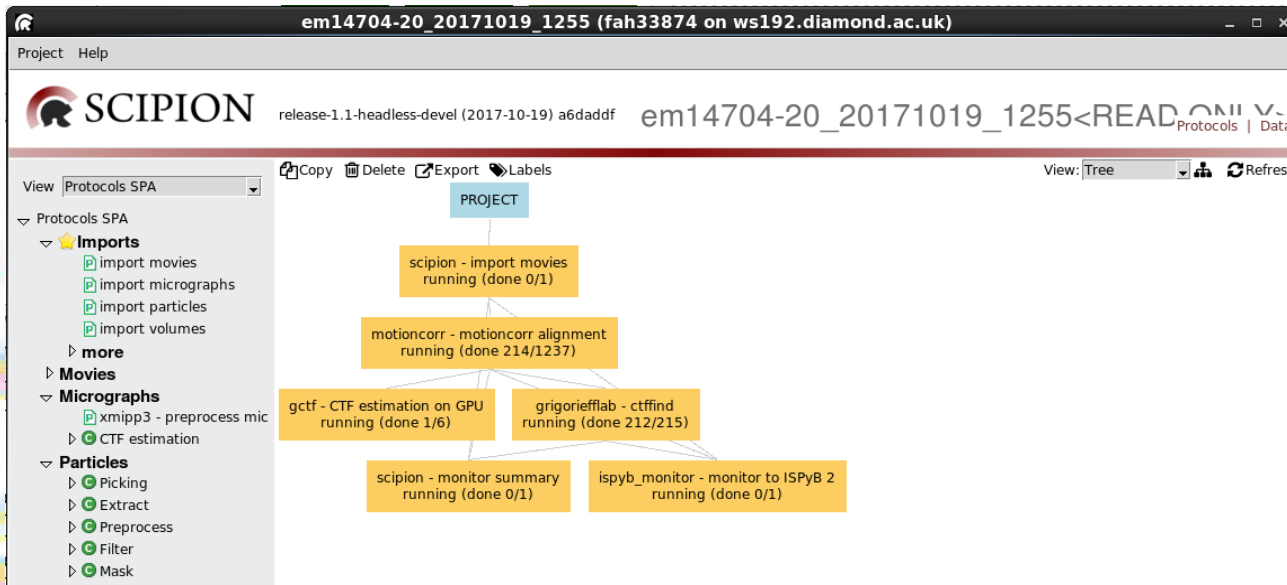
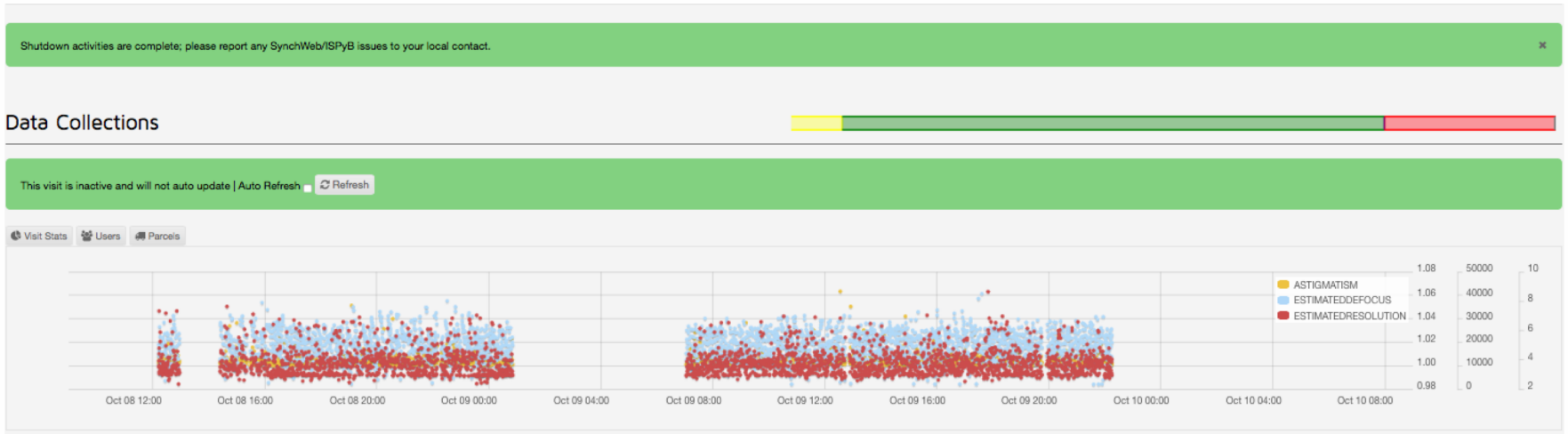


Create a new RDP virtual desktop



# Remote connection for user (now)

- ISPyB monitoring of the visit, alternatively the Scipion project can be viewed using NoMachine (User instructions on eBIC webpage)



- Used to monitor and asses data collection

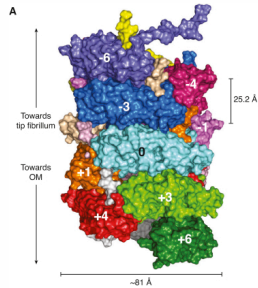


# Remote connection for user (future)

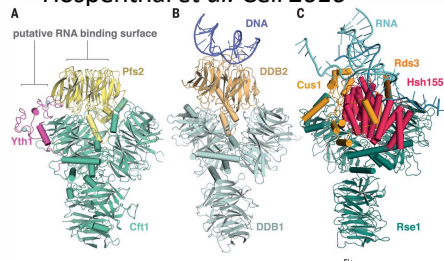
- Controlled access using FedID and visit schedule via NoMachine
  - Copy MX
- A Baton control system to identify current user - TBD
- Staff override of VNC connection - Yes
- Individualized microscope controls – Microscope user accounts
- Data collection software must be able to exchange sample - coming with EPU 2
- Data collection software must be able to do microscope alignments - coming with EPU 2
- Or SerialEM...

Conclusion - Remote user control will happen at diamond based on the existing system in place on other beamlines and eBIC's trained super-users

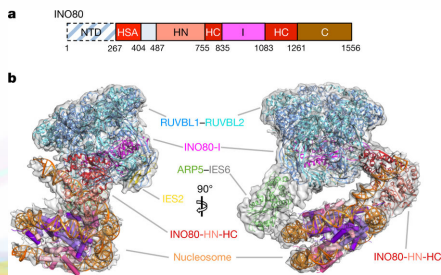
# User Research Highlights



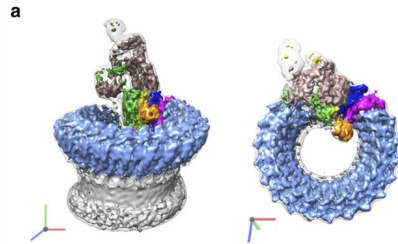
Hospenthal *et al.* Cell 2016



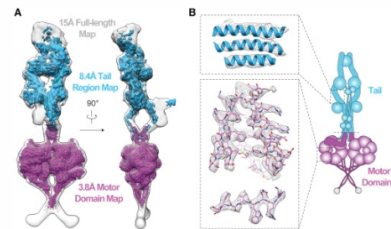
Casañal *et al.* Science 2017



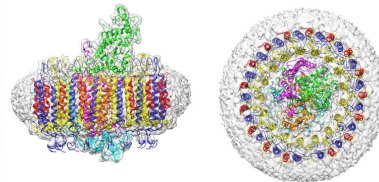
Ayala *et al.* Nature 2018



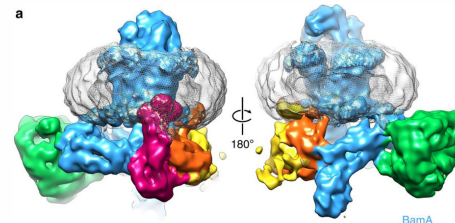
Serna *et al.* Nat. Comms. 2016



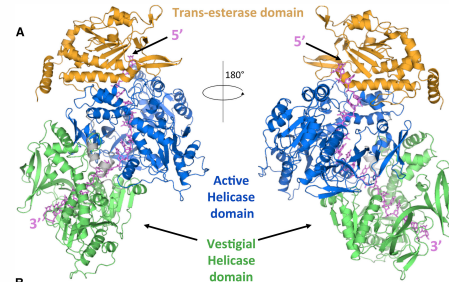
Zhang *et al.* Cell 2017



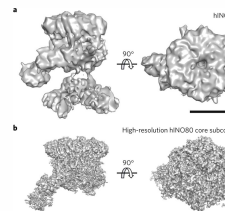
Qian *et al.* Nature 2018



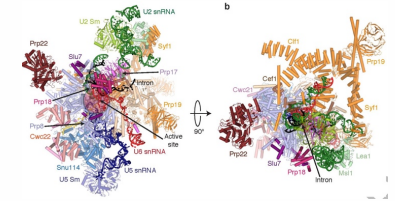
Ladanza *et al.* Nat. Comms. 2016



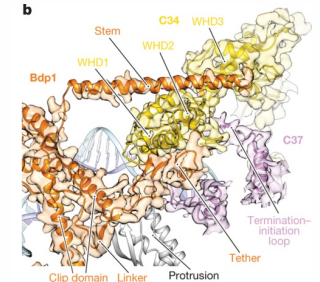
Llangovan *et al.* Cell 2017



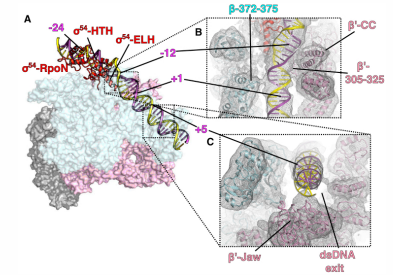
Aramayo *et al.* NSMB 2018



Fica *et al.* Nature 2017



Abascal-Palacios *et al.* Nature 2018



Glyde *et al.* Mol Cell 2018

# Team eBIC

Peijun



Alistair



Me



Jason



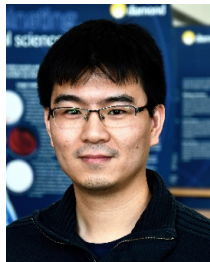
Josh



Katie



Zhenyi



Adriana



James



Yuriy



Andy



Former members

Corey



Kyle



## Executive Committee

Dave Stuart, Helen Saibil, Kay Grunewald  
Martin Walsh, Peijun Zhang

Diamond Light Source staff: Jean Lane, Alun Ashton, Michelle Bennett, Alison Roblin, the EHC team *et al.*

Scipion: JM Carrazo, Roberto Marabini, Carlos Sorzano, Jose Miguel de la Rosa Trevin, Diamond: Alun Ashton, Kevin Savage, Mark Basham, Josh Lobo)

