

Macromolecular Crystallography at Diamond

Dave Hall



Macromolecular
Crystallography



Soft Condensed
Matter



Imaging and
Microscopy



Biological
Cryo-Imaging



Magnetic
Materials



Structures and
Surfaces



Crystallography



Spectroscopy



MX
Beamlines +
XChem Lab

eBIC

CCP4



Crystallisation
Facility

MX Team

dls.mx @Diamond_MX



Group Support

Felicity Bertram
Marco Mazzorana
Elliot Nelson

ILO

Isabel Barker
Christofer Bjorkelid
Alex Dias
Anna Kroner
Ailsa Powell
Jitka Waterman

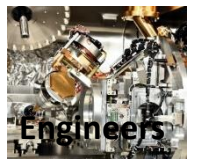
Software



Controls



Technicians

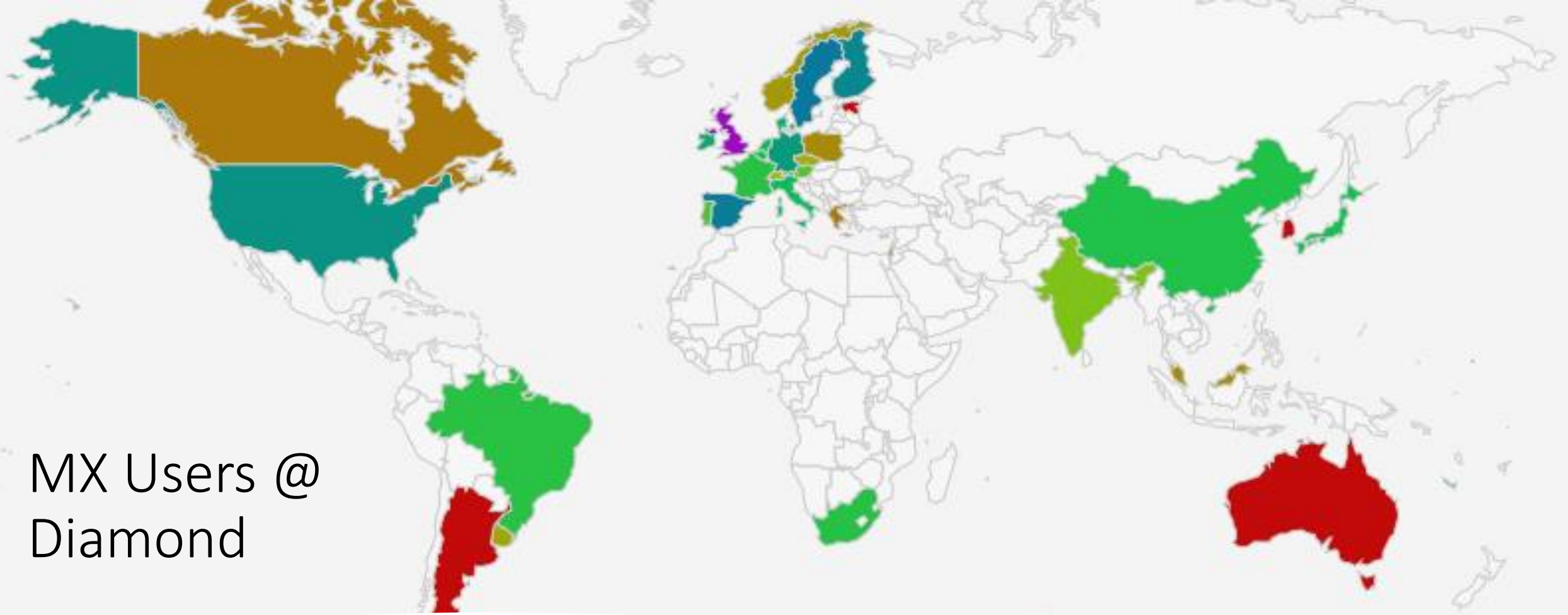


mx-usersupport@diamond.ac.uk



MX Users @ Diamond

- Large proportion of Diamond academic users are from the MX community
 - <https://www.diamond.ac.uk/Users.html>
- Large industrial user base
 - <https://www.diamond.ac.uk/industry.html>
- International reach
 - ~20% from outside UK



APS Access, BAG or Rapid Proposal, Standard Proposal, Commissioning Proposal



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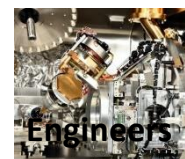
Software



Controls

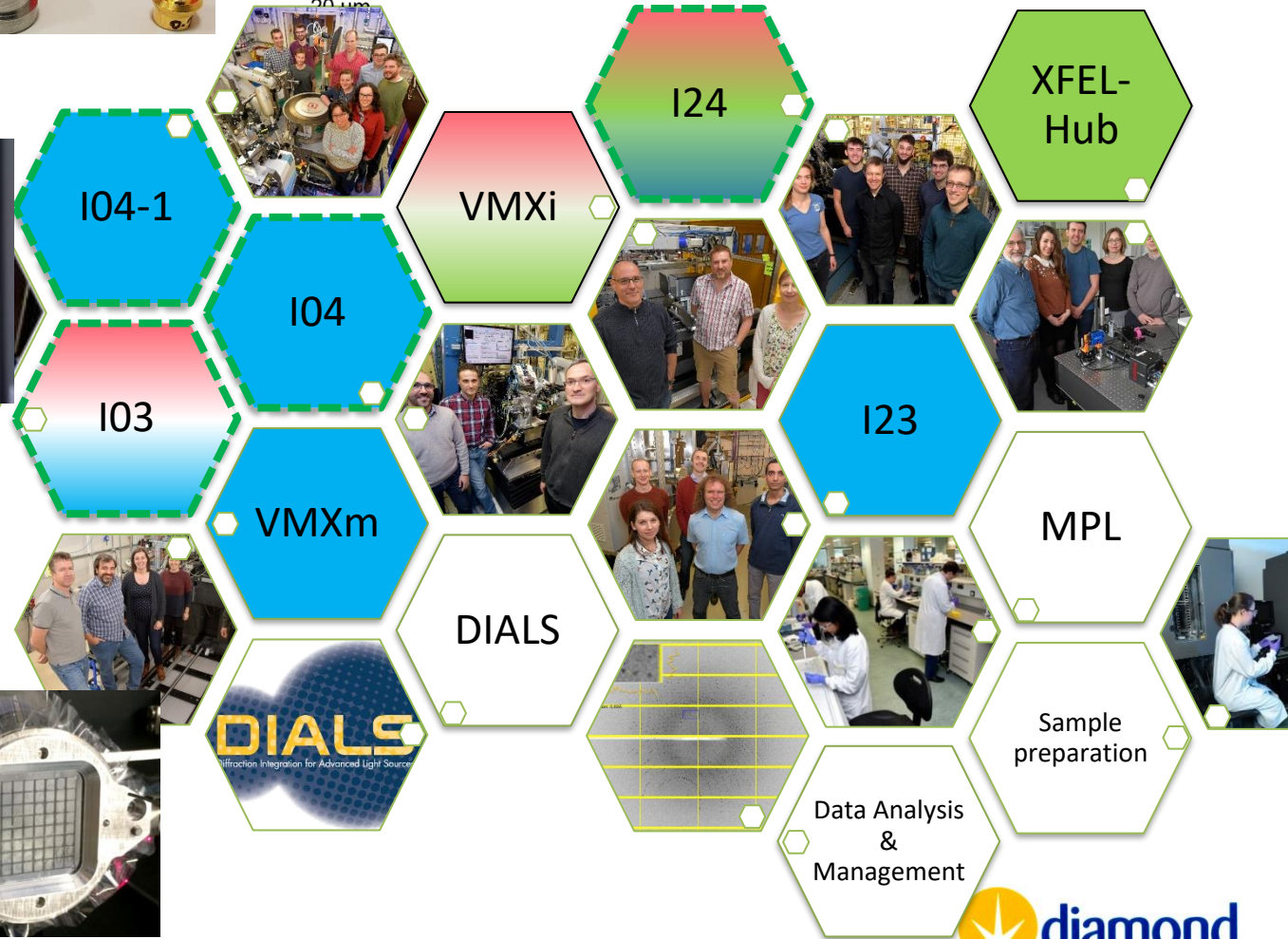
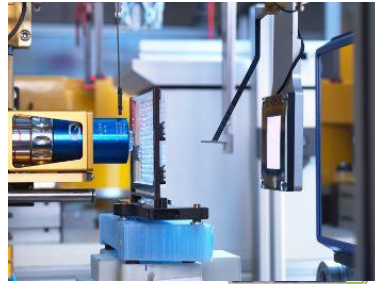
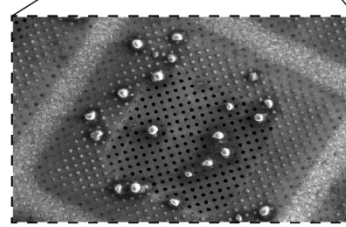


Technicians



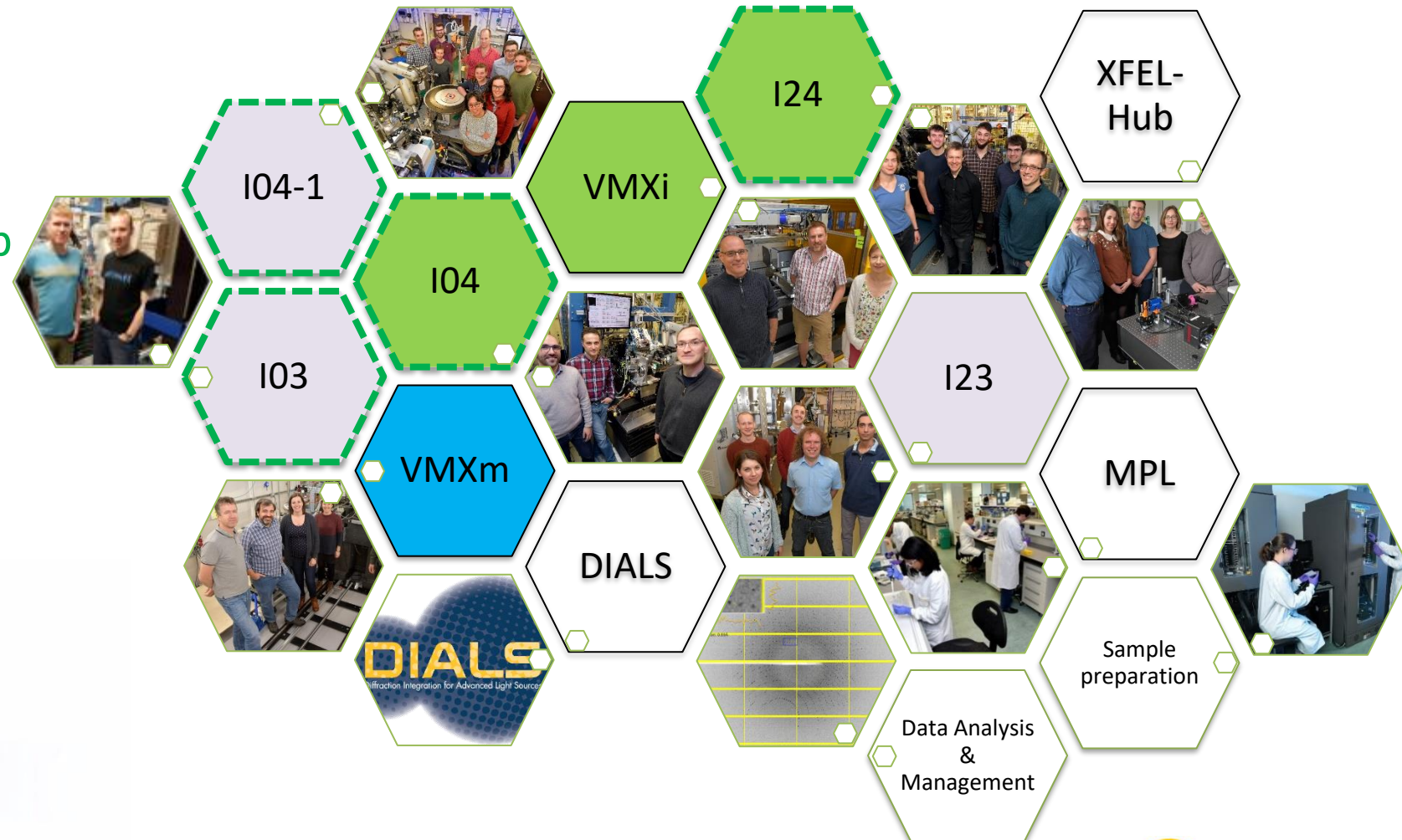
Cryo, Room Temperature & SSX

- Cryo
 - standard SPINE pins
 - I23 specific holders
 - VMXm – EM grids
- Room temperature *in-situ*:
 - VMXi dedicated beamline
 - I03 for biological containment
- SSX at I24, VMXi and XFEL Hub
 - Extruders
 - Fixed targets
 - Thin films
 - Acoustic drop ejection
 - Tape drives (in dev)



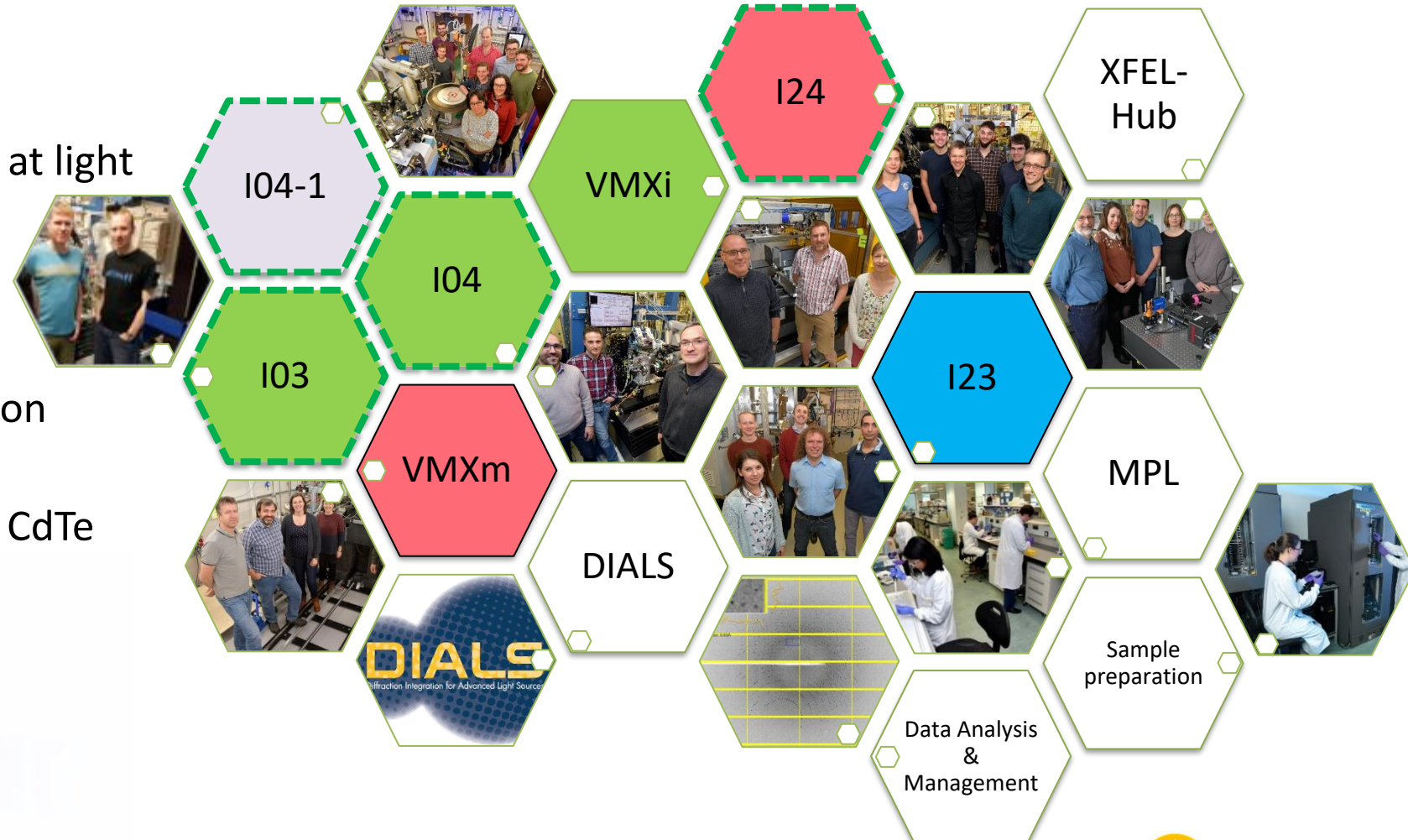
Microfocus and beyond – 0.4 to 100 μm coverage over suite

- Flexible beam size range available across beamlines
- I03, I04-1 – 20 μm and up
- I04, I24 and VMXi – 5 μm and up
- VMXm 0.4 – 10 μm
- Equipped with fast rastering



Energy Extremes – Low (2.1keV) to High (26 keV)

- All tuneable (except I04-1)
- High resolution data
- Metal identification
 - I23 uniquely equipped to look at light elements such as Na, K, Cl
 - Assist model building (S, P)
- Phasing
- High energies – minimising radiation damage
 - I24 and VMXm equipped with CdTe Eiger2 9M detectors



Automated Data Analysis and Management

- Multiple automated pipelines
- Data reduction
 - Fast_dp
 - Xia2 DIALs & XDS
 - Autoproc
 - Multiplex
- Structure solution
 - DIMPLE
 - MrBUMP
 - BigEP phasing – Solve, Autosharp, Crank2
 - Alphafold2 for MR based on your sequence
- Reprocessing
- Accessible via ISPyB
- All data archived on tape



Summary of Beamline Specs available through APS call

Beamline	I03	I04	I04-1	I24
Wavelength range (Å)	0.6 - 2.3	0.69 - 2.07	0.92 (fixed)	0.62 - 2.0
Energy range (keV)	5.5 - 25	6.0 - 18.0	13.5 (fixed)	6.4 - 23.0
Default settings (Å/keV)	0.98 / 12.7	0.95 / 13.0	0.92 / 13.53	0.62 / 20.0
Flux (ph/s) in full beam at default energy at 300 mA	1.0×10^{13}	1.2×10^{12}	3.8×10^{12}	2.0×10^{12}
Default beamsize (μm)	80 x 20	30 x 20	60 x 50	7 x 7
Full beam size at sample (μm)	80 x 20	10 x 5 --> 110 x 100	60 x 50	7 x 7 --> 50 x 50
Available apertures (μm)	20, 50, 100		10, 20, 30, 50 and 70	
Detector	Eiger2 XE 16M (500 Hz)	Eiger2 XE 16M (500 Hz)	Eiger2 XE 9M (500Hz)	P3-6M (100 Hz) EIGER2 X CdTe 9M (250Hz)
Multi-Axis Goniometry	Yes	Yes	No	No
Number of unipucks / SPINE pins	37 / 592	37 / 592	37 / 592	37 / 592
Maximum samples / hour	32	32	35	30
Typical samples / hour	15 - 25	15 - 25	15 - 35	15 - 25
Minimum Detector Distance (mm)	140	170	166	200

<https://dls.mx>

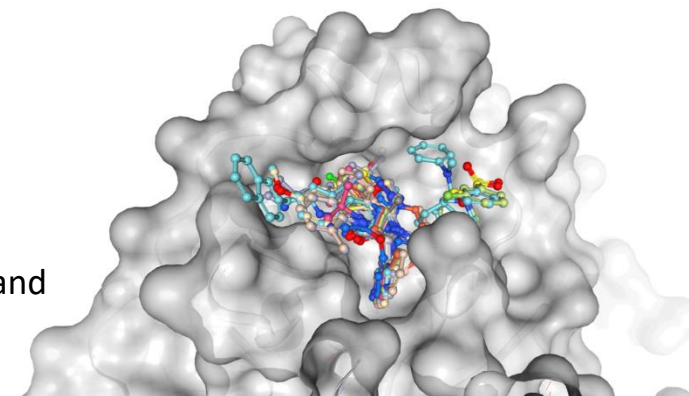
Beyond the beamlines



XChem Facility

Lab linked to I04-1 for efficient soaking, harvesting, automatic data collection and data analysis of fragment screening libraries at large scale

Available to both academia and industry



XFEL Hub: tools and strategies to enable dynamic structural biology facilitating

- ✓ (time-resolved) serial structural biology experiments via sample preparation, delivery, data collection, and processing
- ✓ the transfer of methods between XFEL, synchrotron, and/or cryo-EM sources
- ✓ access to, and data collection from complementary facilities (DLS, CLF, eBIC)



Crystallisation Facility @ Harwell

A high throughput platform open to academic groups and industry that provides users with an easy route into the VMXi beamline, the fully automated *in situ* and serial crystallography beamline at Diamond Light Source, UK.



Diamond MX – Key Software Interfaces

The screenshot shows the Diamond MX User Administration System (UAS) homepage. At the top, there is a navigation bar with 'HOME', 'PROPOSALS', and 'SESSIONS' tabs. A prominent red banner contains important notices about proposal submission deadlines and session arrangements. Below the banner, there are sections for 'Useful Links' (including 'Create New Proposal', 'Update Registration Details', 'Online User Claims', 'Publications Database', and 'Safety Video and Test'), 'Diamond Safety Test' (with a video player and instructions), and 'Contact Details' (listing various support teams and their contact information). A '31 outstanding actions' section is visible, listing tasks like 'Submit Report' and 'Submit Feedback' with their respective due dates.

UAS

User Administration System

<https://uas.diamond.ac.uk/>

The screenshot shows the Diamond MX ISPyB login page. At the top, there is a navigation bar with 'Home' and 'Login' tabs. A green banner contains a message: 'Please report any SynchWeb / ISPyB issues to your local contact. (Release 2023-R1.3)'. Below the banner, there is a 'Login' section with input fields for 'Username (Fedi)' and 'Password', and a 'Login' button. At the bottom, there is a section for 'SynchWeb? What is This?' and the Diamond Light Source logo.

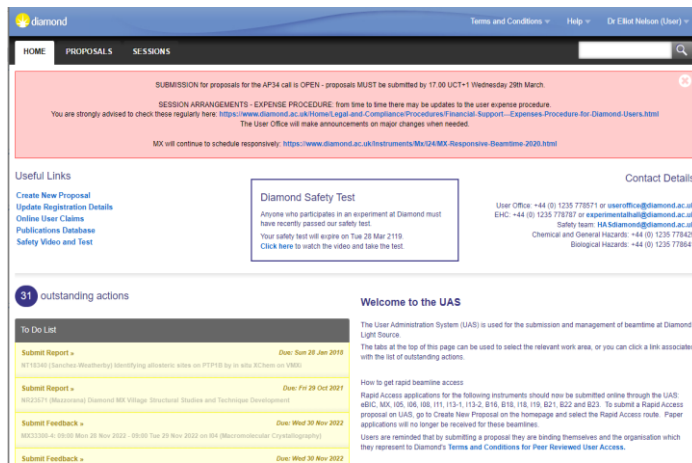
ISPyB

<https://ispyb.diamond.ac.uk/>

Shipment to Processed Data

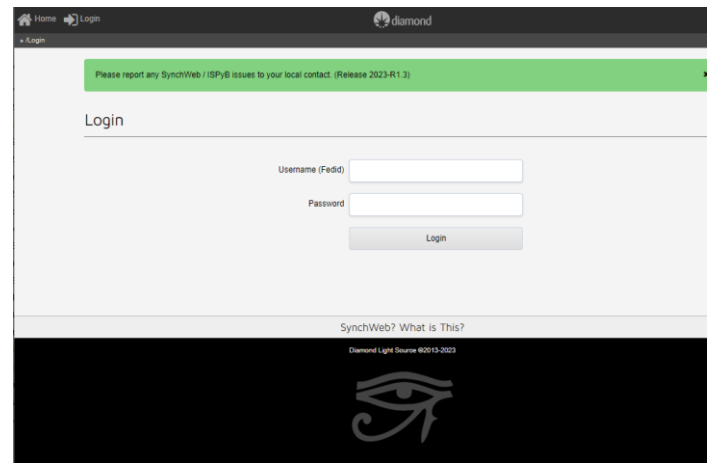
Unattended Data Collection

Diamond MX – Key Software Interfaces



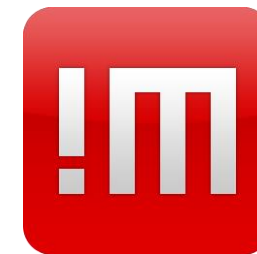
UAS

User Administration System
<https://uas.diamond.ac.uk/>

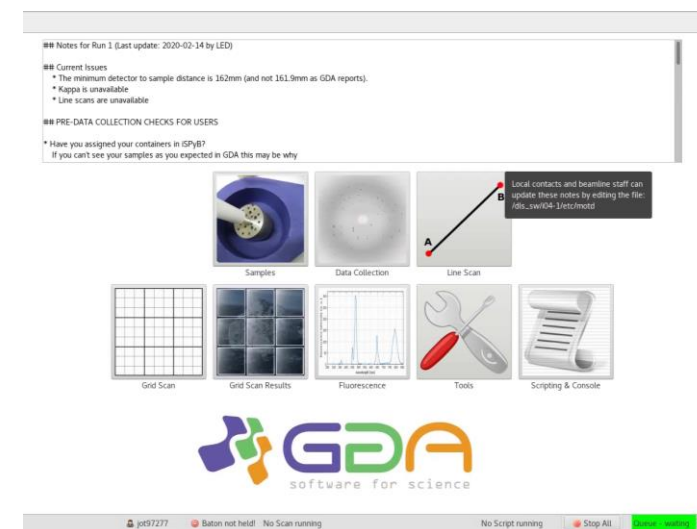


ISPyB

<https://ispyb.diamond.ac.uk/>
Shipment to Processed Data



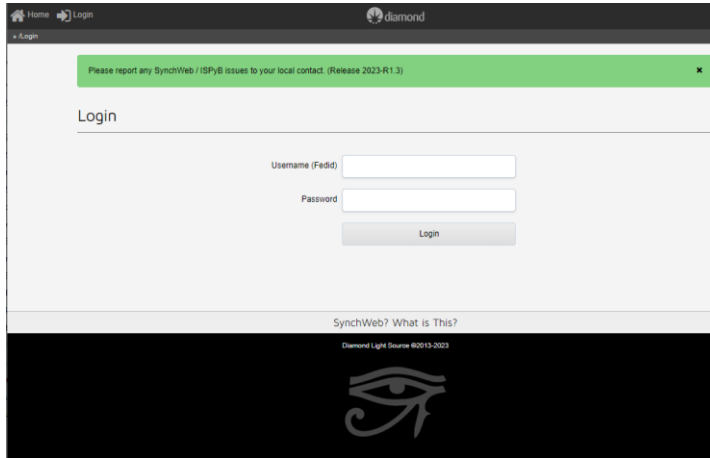
No Machine – Remote Access
nx.diamond.ac.uk



GDA – Data Collection

Remote Data Collection

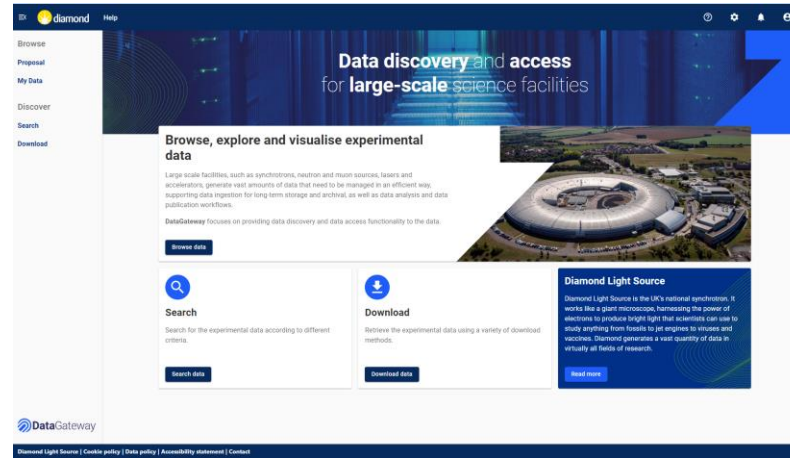
Diamond MX – Key Software Interfaces



ISPyB

<https://ispyb.diamond.ac.uk/>

Processed Data Files



Data Gateway

<https://icat.diamond.ac.uk/>

Archived Raw Data



Globus

<http://www.globus.org/>

Live Data – Raw & Processed

- Sign in with your organisation login, or personal Globus ID.

Data Retrieval

Data held on file system for 40 days

1 copy archived to tape – access through icat.diamond.ac.uk

<https://www.diamond.ac.uk/Users/Experiment-at-Diamond/IT-User-Guide/Not-at-DLS/Retrieve-data.html>