

How is SynchWeb used for MX at DLS?

Dave Hall



User log book



Logistics



Auto-processing results



Data re-processing



User tools



Staff tools

User Logbook

I03

I04

I04-1

I24

I23

VMXi

VMXm

I19 – small molecule

Home Calendar Logout

Proposals Visits for mx18598

mx18598 v

Proposals Projects Unit Cell Search Feedback Help

Please report any SynchWeb/ISPyB issues to your local contact.

Visit List

This page lists the visits available to the currently selected proposal

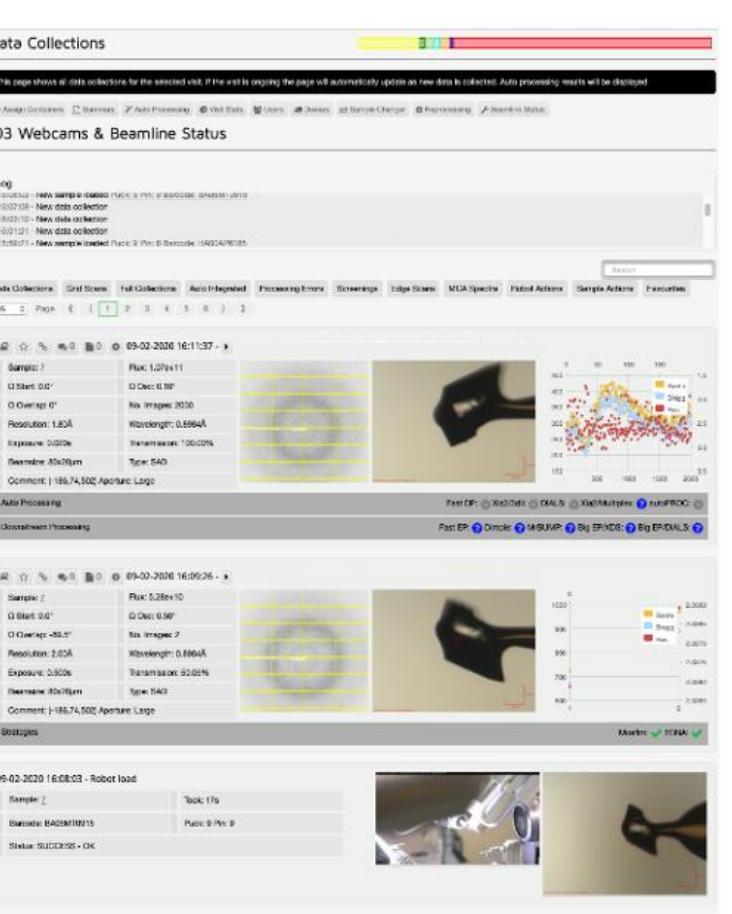
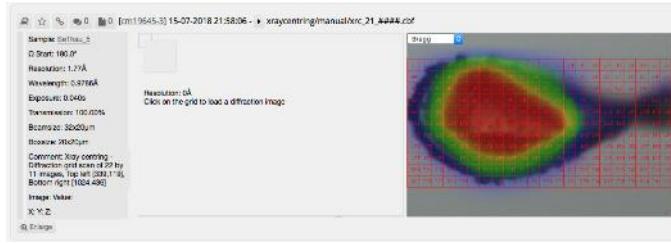
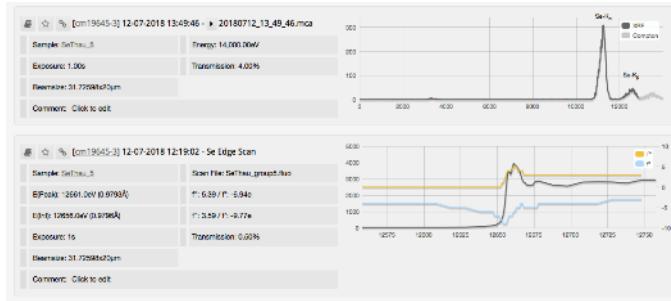
Start	End	Number	Beamline	Local Contact	Comments	Data Collections	Type
17:00 20-02-2020	09:00 21-02-2020	58	i04			0	
10:00 14-02-2020	17:00 14-02-2020	57	i24			0	
10:00 09-02-2020	09:00 10-02-2020	56	i03			138	
12:00 01-02-2020	19:00 01-02-2020	55	i04-1			153	Compulsorily Remote
20:00 22-01-2020	23:00 22-01-2020	68	i04			107	Compulsorily Remote
12:00 18-01-2020	19:00 18-01-2020	54	i04			97	Compulsorily Remote
12:00 15-12-2019	19:00 15-12-2019	67	i24			111	Compulsorily Remote
10:00 15-12-2019	09:00 16-12-2019	53	i04-1			212	
02:00 08-12-2019	09:00 08-12-2019	52	i24			139	Compulsorily Remote
10:00 06-12-2019	18:00 06-12-2019	66	i23			24	

10 Page 1 2 3 4 5 6 7 > >>

SynchWeb? What is This?

Diamond Light Source ©2013-2020

Event driven



Data collection events – view at visit and proposal level

This page shows all data collections for the selected visit. If the visit is ongoing the page will automatically update as new data is collected. Auto processing results will be displayed

[Assign Containers](#) [Summary](#) [Auto Processing](#) [Visit Stats](#) [Users](#) [Dewars](#) [Sample Changer](#) [Reprocessing](#) [Beamline Status](#)

i03 Webcams & Beamline Status

Log

- 14:57:19 - New data collection
- 14:06:09 - New data collection
- 14:03:36 - New data collection
- 14:02:32 - New data collection

Data Collections **Grid Scans** **Full Collections** **Auto Integrated** **Processing Errors** **Screenings** **Edge Scans** **MCA Spectra** **Robot Actions** **Sample Actions** **Favourites**

15 Page (1) }

ellie (highlighted with a red box)

09-02-2020 14:57:19 - ellie/

Sample: 4	Flux: 5.97e+12
Q Start: 0.0°	Q Osc: 0.10°
Q Overlap: 0°	No. Images: 3600
Resolution: 2.00 Å	Wavelength: 1.3513 Å
Exposure: 0.010s	Transmission: 100.00%
Beamsize: 80x20 μm	Type: SAD
Comment: (404, 122, -235) Aperture: Large	

Auto Processing

Fast DP: Xia2/3dli: DIALS: Xia2/Multiplex: autoPROC:

Downstream Processing

Fast EP: Dimple: MrBUMP: Big EP/XDS: Big EP/DIALS:

09-02-2020 14:06:09 - ellie/

Sample: 7	Flux: 1.03e+11
Q Start: 0.0°	Q Osc: 0.10°
Q Overlap: 0°	No. Images: 2000
Resolution: 2.80 Å	Wavelength: 0.8984 Å
Exposure: 0.010s	Transmission: 100.00%
Beamsize: 80x20 μm	Type: SAD

User filterable

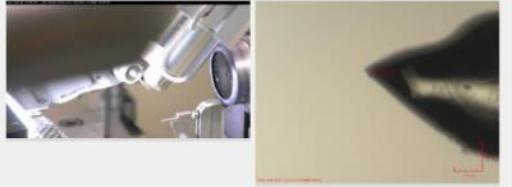
09-02-2020 16:08:03 - Robot load

Sample: 7	Took: 17s
Barcode: BA05MT0915	Puck: 9 Pin: 9
Status: SUCCESS - OK	



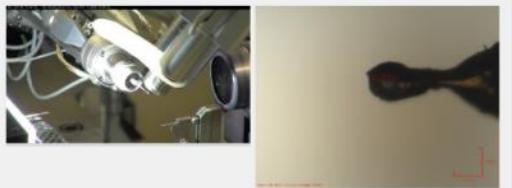
09-02-2020 15:59:21 - Robot load

Sample: 6	Took: 17s
Barcode: HA00AP6185	Puck: 9 Pin: 8
Status: SUCCESS - OK	



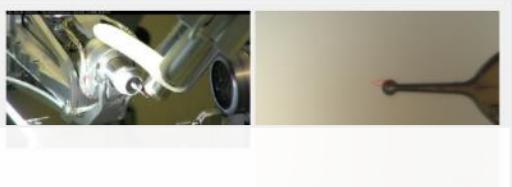
09-02-2020 15:55:49 - Robot load

Sample: 5	Took: 17s
Barcode: BA05MT0916	Puck: 9 Pin: 7
Status: SUCCESS - OK	



09-02-2020 15:54:15 - Robot load

Sample: 4	Took: 17s
Barcode: BA05MT0013	Puck: 9 Pin: 6
Status: SUCCESS - OK	



Defined filters

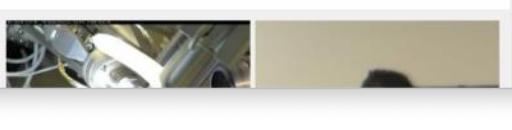
09-02-2020 15:50:01 - Robot load

Sample: 3	Took: 16s
Barcode: BA05MT0012	Puck: 9 Pin: 5
Status: SUCCESS - OK	

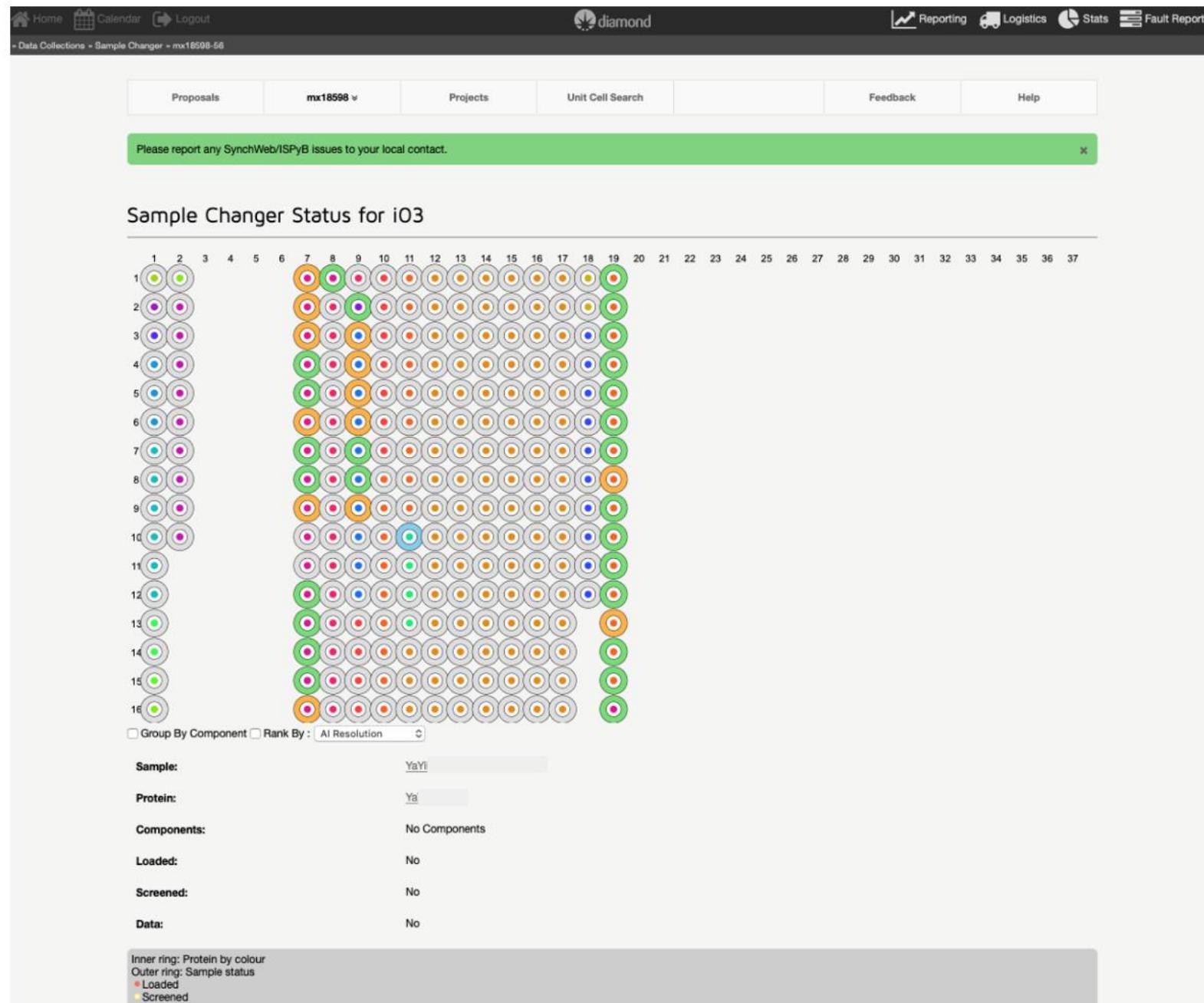


09-02-2020 15:46:59 - Robot load

Sample: 2	Took: 16s
-----------	-----------



Sample changer status



VMXi – fully automated, user free, *in situ* data collection

Container: Z12368764

This page shows the contents of the selected container. Samples can be added and edited by clicking the pencil icon, and removed by clicking the x

1	2	3	4	5	6	7	8	9	10	11	12
A											
B											
C											
D											
E											
F											
G											
H											

Inspections 08:47 09-10-2015 (+d) [Adhoc]

Movie Gap: 0.5 s

Sample

Protein pl_prot1
Sample Name A1d1_X1
Spacegroup Click to edit
Comments a1d1



Screen Components

Component	Concentration	pH
No components for this group		

Manage Beamline Presets



Reporting Imaging Logistics Stats Fault Reports

Proposals cm14559 v Projects Unit Cell Search

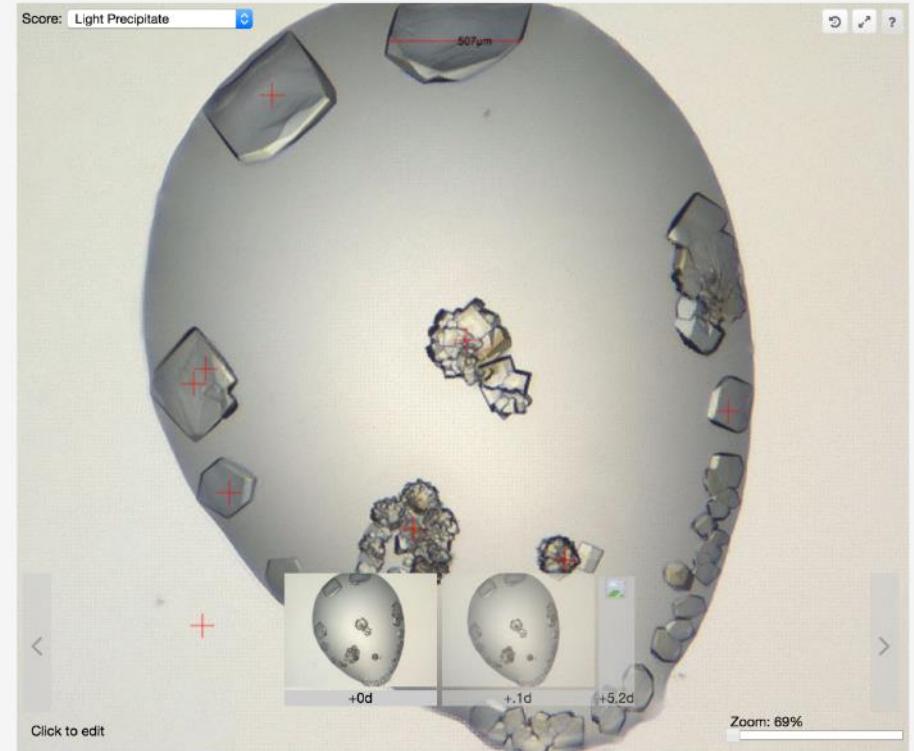
Shutdown activities are complete; please report any SynchWeb/SyPyR issues to your local contact.

Dashboard Imaging Schedules Crystallisation Screens Global Presets Define Parameters

Global Presets

Global presets are currently being saved into "cm14559"

Beamline	Name	Exp. Type	Parameters
i02-2	VMXi Grid 1	Grid Scan	Beam Size <input type="text" value="10"/> $\times 10$ μm D Range <input type="text" value="0"/> Energy <input type="text" value="12658"/> eV Transmission <input type="text" value="100"/> % Exposure <input type="text" value="0.00134"/> s Resolution <input type="text" value="2.6"/> \AA Beam Size <input type="text" value="10"/> $\times 10$ μm No. Images <input type="text" value="600"/> D Start <input type="text" value="-30"/>



Click to edit

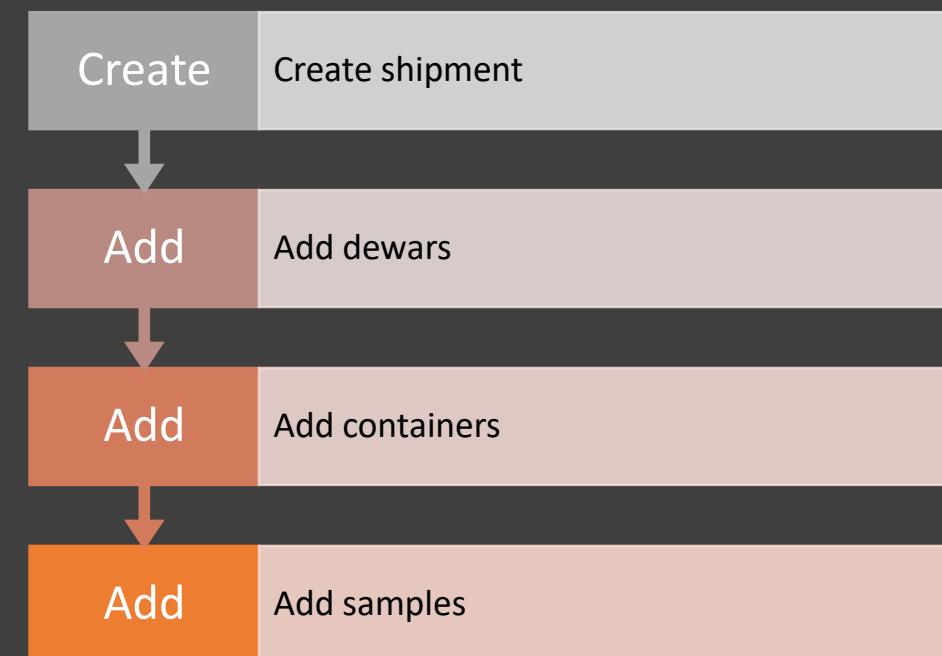
Zoom: 69%

Logistics





Tracking of samples, dewars
& sample information
essential for users and staff
across MX beamlines



Creating a shipment

The screenshot shows two overlapping browser windows. The left window is titled 'ISPyB » Data Collections » i04-1' and displays the 'Data Collections' page. The right window is titled 'ISPyB » Shipments' and displays the 'Shipments' page.

Data Collections Page (Left):

- Header: Home, Calendar, Logout
- Breadcrumbs: » Data Collections » i04-1 » mx24722-3
- Proposals: mx24722
- Visits: Please note that all dewars must now be registered before creating a shipment. This visit is ongoing.
- Assign Containers
- Shipments: (circled in red)
- Registered Dewars
- Registered Containers
- Containers
- Samples
- Proteins
- Lab Contacts
- Statistics
- Migrate

Shipments Page (Right):

- Header: Home, Calendar, Logout, diamond logo, Logistics, Stats, Fault Reports
- Breadcrumbs: » Shipments
- Proposals: mx24722
- Project: mx24722-3
- Message: Please note that all dewars must now be registered before creating a shipment. Please note that all dewars must now be registered before creating a shipment. P
- Add Shipment: (circled in red)
- Shipments: This page shows a list of shipments associated with the currently selected proposal. In order to register your samples you need to create a shipment. Shipments contain dewars, dewar contain containers, and containers individual samples. These can be created sequentially by viewing a particular shipment.
- Table: Shows a list of shipments.

Name	Creation Date	Outgoing Contact	Return Contact	Status	# Comp	Comments
neil_1	03-07-2019	Neil	Neil	opened	1	
Default Shipping mx24722-5						
- Buttons: + Add Shipment, Page, <, >, >>
- Search: Search

Page Footer: SynchWeb? What is This?

Creating a shipment

ISPyB » Shipments » test x + - □ X

← → ⌂ 🔒 https://ispyb.diamond.ac.uk/shipments/sid/29952 ☆ ○ A ⋮

This page shows details and contents of the selected shipment. Most parameters can be edited by simply clicking on them.

Shipments need to have an outgoing and return home lab contact before shipment labels can be printed

You can now book your shipment with DHL using "Create Airway Bill" below

Mark as Sent Create Airway Bill Print Shipment Labels Print Contents

Created	05-07-2019
Status	opened
Outgoing Lab Contact	bl
Return Lab Contact	bl
Safety Level	Green
Courier	Click to edit
Courier Account No.	Click to edit
Shipping Date	00-00-00
Shipping Airway Bill	Click to edit
Shipping Pickup Location	Click to edit
Shipping Ready By	Click to edit
Shipping Close Time	Click to edit
Estimated Delivery Date	00-00-00
Comments	Click to edit

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	Weight (Kg)	First Experiment	Tracking # to	Tracking # from	Status	Location	Containers
Dewar1	cm23005-3-i04-1-0034326	Click to edit	18	cm23005-3	Click to edit	Click to edit	opened	0	+ + + + +

Dewar Details: Dewar1

+ Add Container

No Containers for this dewar

15 Page < < 1 > >>

Date	Status	Location
No history available		

15 Page < < 1 > >>

Origin	N/A
Destination	N/A

Date Status Location Signatory

No tracking available

Add New Container

Assign Containers

Paste from Spreadsheet

Shipment

Ktest

Dewar

DLS-MX-1234

Container Type

Puck

Container Name



Registered Container

✓ Please select one

-
- CPS-2562
- DLS-0001
- DLS-537
- DLS-625
- DLS-627
- DLS-632
- DLS-653

You] View

Automated Collection

Owner

This user will be emailed with container updates. Check your email is up to date!

Comments

Comment for the container

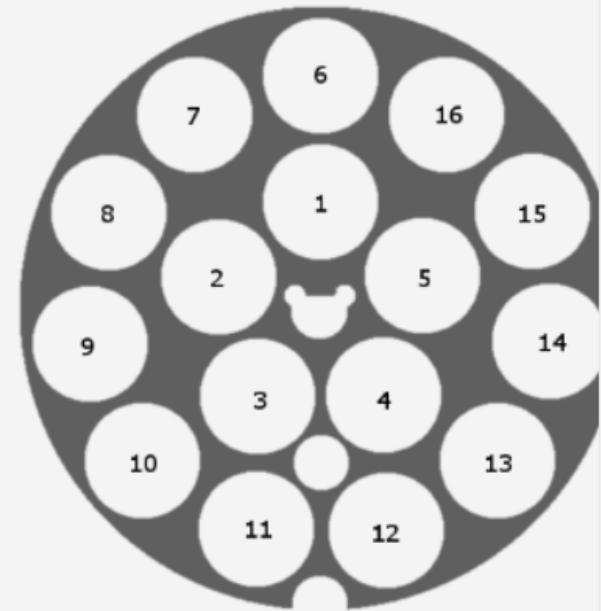
Clone from First Sample

Clear Puck

Extra Fields

Location	Protein Acronym	Abundance
1		
2		
3		

Components	Name	Spacegroup	Barcode	Comment	Centring Method	Experiment Kind		



View Protein

Name	Thaum
Acronym	Thaum
Molecular Mass	Click to edit
Sequence	<pre>ATFEIVNRCSYTVWAAASKGDAALDAGGRQLNSGESWTINVEPGTNGGKIWARTDCYFDD SGSGICKTGDCGGLRCKRFGRPPTLAEFSLNQYGKDYIDI SNIKGFNVPMNFSPTTRG CRGVRCAADIVQCOPAKLKAPGGCNDACTVFQTSEYCCTTGKCGPTEYSRFFKRLCPDA FSYVLDKPTTVTCPGSSNYRVT FCPTA</pre>
Component Type	Protein
Concentration Unit	Click to edit
Global	No
Associated PDB Files	+ Add PDB File
	1rqw [CODE] ×

Tracking sample information

Protein information can include sequence or PDB files or codes

Used by downstream processing pipelines. Presence of

Sequence triggers MrBUMP and is used in BigEP for model building

PDB file or code triggers DIMPLE

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

Shipment	test
Dewar	Dewar1
Puck Name	test

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

Sample Details

This page shows details and history for the selected sample

Name	Se_Thau_15												
Protein Acronym	Thaumatin <input type="button" value="View All"/>												
Abundance	<input type="button" value="Click to edit"/>												
Components	Add: <input type="text"/> <input type="button" value="Add"/> <div style="background-color: #f0f0f0; padding: 5px; border-radius: 5px; margin-top: 5px;"> No Components </div>												
Volume	<input type="button" value="Click to edit"/>												
Spacegroup	<input type="button" value="Click to edit"/>												
Unit Cell	<table border="1" style="margin-left: auto; margin-right: auto;"> <tr> <td>A</td> <td>B</td> <td>C</td> <td>α</td> <td>β</td> <td>γ</td> </tr> <tr> <td><input type="button" value="Click to edit"/></td> </tr> </table>	A	B	C	α	β	γ	<input type="button" value="Click to edit"/>					
A	B	C	α	β	γ								
<input type="button" value="Click to edit"/>	<input type="button" value="Click to edit"/>	<input type="button" value="Click to edit"/>	<input type="button" value="Click to edit"/>	<input type="button" value="Click to edit"/>	<input type="button" value="Click to edit"/>								
Anomalous Scatterer	Se												
Required Resolution	2.0												
Comment	<input type="button" value="Click to edit"/>												
Barcode	<input type="button" value="Click to edit"/>												
Container	cm19645-4_sept2018-DLS0137												
Dewar	Default Dewar:cm19645-4												
Shipment	Default Shipping:cm19645-4												
Snapshots													

Tracking sample information

Sample information added when creating containers

UK/EU academic users book shipping with DHL API

Create Airway Bill: To Facility

Shipment Details

Shipment NR16818-33_06092017
Dewars DLS-MX-1235 DLS-MX-1234

← Tick the dewars you want to send

Weight 36 Kg

DHL Account Number [Click to edit](#) Use Facility Account

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

Declared Value 100 GBP

Package Description Dry shipper - not restricted as per IATA special provision A152

Contact Details

Contact Elizabeth Windsor

Contact Phone Number 0303 123 7300

← Check the details are correct

Contact Email liz@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 beamtime 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.

[Create Airway Bill](#)

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

DHL info
available to users
and staff

Dewar transfer
or shipment
home requested
from here

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

Name	Barcode	Facility Code	Weight (Kg)	First Experiment	Tracking # to	Tracking # from	Status	Location	Containers	Actions
DLS-MX-0950	I03-0039429	DLS-MX-0950	18	mx24447-10	7626191893	Click to edit	at facility	tray-2c	11	
DLS-MX-0806	I03-0039426	DLS-MX-0806	18	mx24447-10	7626191893	Click to edit	at facility	tray-2b	0	

Dewar Details: DLS-MX-0950

This section shows contents and history for the selected dewar. Click the spyglass icon to view the contents of the container

DLS-0033 (16 samples)	
DLS-0030 (16 samples)	
CPS-3080 (16 samples)	
DLS-0032 (16 samples)	
DLS-0035 (16 samples)	
DLS-404 (16 samples)	
DLS-257 (16 samples)	
CPS-3078 (16 samples)	
DLS-258 (16 samples)	
CPS-3075 (16 samples)	
DLS-400 (16 samples)	

Date	Status	Location
09-02-2020 09:34	at facility	tray-2c
08-02-2020 09:16	processing	i03
08-02-2020 09:16	processing	i03
08-02-2020 09:16	processing	i03
08-02-2020 09:15	processing	i03
08-02-2020 09:15	processing	i03
08-02-2020 09:14	processing	i03
08-02-2020 09:14	processing	i03
08-02-2020 09:13	processing	i03
08-02-2020 09:13	processing	i03
08-02-2020 09:13	processing	i03
07-02-2020 16:58	at facility	i03
06-02-2020 13:11	at facility	tray-2c
06-02-2020 11:07	at facility	stores-in

15 Page < (1 2) >

Origin MANCHESTER-GBR
Destination OXFORD-GBR

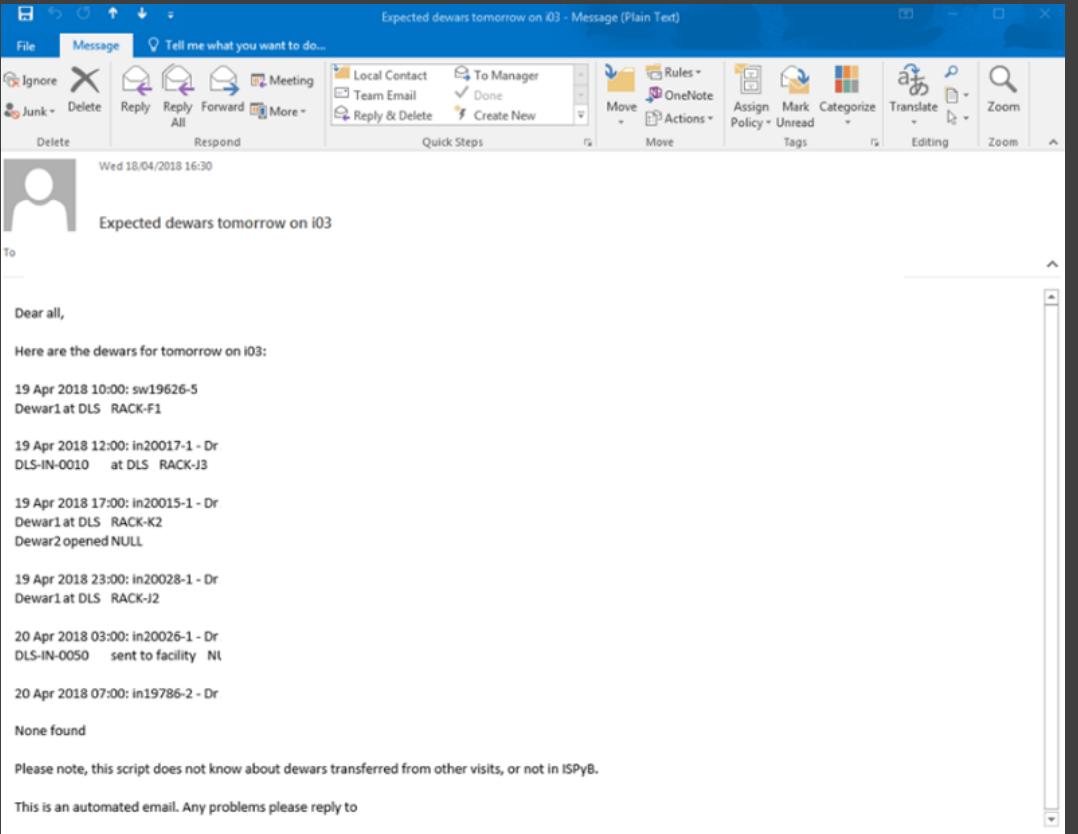
Date	Status	Location	Signatory
2020-02-05 10:23:53	Shipment pick up	MANC	
2020-02-05 21:13:16	Processed at location	MANC	
2020-02-05 21:13:58	Depart facility	MANC	
2020-02-05 23:06:27	Arrived facility	EAST M	
2020-02-05 23:37:03	Processed at location	EAST M	
2020-02-06 00:27:07	Depart facility	EAST M	R
2020-02-06 02:46:35	Arrived facility	LONDON-	R
2020-02-06 03:39:42	Processed at location	LONDON-	R
2020-02-06 04:54:04	Depart facility	LONDON-	R
2020-02-06 06:23:05	Arrival in delivery facility	OXI	
2020-02-06 10:10:45	With delivering courier	OXI	
2020-02-06 10:58:06	Delivery	OXI	



Dewar store



3 x 3 x 7.75 m, > 100 dewars
Centrally sited between I23, I24 and I03, I04, I04-1



Scan Dewar and Rack

Barcode or FacilityCode
Scan the long barcode from the dewar case

Location
Scan the location e.g. RACK-A1

Submit **Cancel**

Find a Dewar

Barcode or FacilityCode
e.g. DLS-MX-####

Search **Cancel**

RACK-A1: mx18565-36-i03-0031989 Sun, 28 Apr 2019 DLS-MX-0016	RACK-A2: mx18565-36-i03-0032319 Mon, 29 Apr 2019 DLS-MX-0013	RACK-A3: in23393-1-i03-0032277 Fri, 26 Apr 2019	RACK-A4: in22897-10-i04-0032016 Fri, 26 Apr 2019 DLS-IN-0228
RACK-B1: mx19946-38-i03-0032400 Mon, 29 Apr 2019 DLS-MX-0567	RACK-B2: mx19946-38-i03-0032397 Mon, 29 Apr 2019 DLS-MX-0566	RACK-B3: mx20221-17-i04-1-0031836 Fri, 19 Apr 2019 dispatch-requested	RACK-B4: mx19800-14-i04-1-0030815 Tue, 30 Apr 2019 DLS-MX-0187
RACK-C1: in23277-1-i24-0032355	RACK-C2: mx17293-8-i24-0032280	RACK-C3: cm23003-5-i03-0031551	RACK-C4: mx19844-13-i03-0032247

(Dewars in need of dispatch - clear once removed from rack)

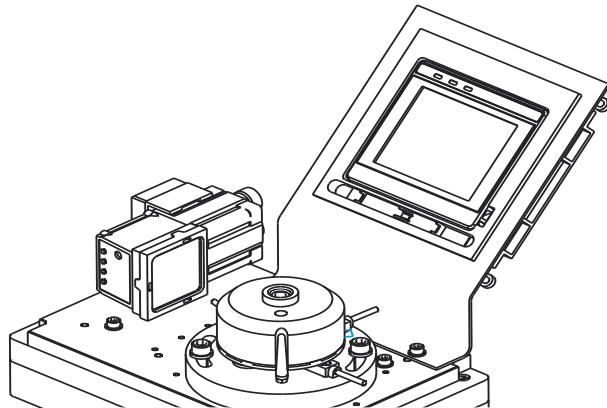
Dewar storage

- Improved tracking of dewars in storage area, interface shows:
 - Location of dewars on-site
 - Which dewars need to be refilled with LN2 or dispatched
 - Which dewars need to be returned to users
- Email to LCs listing dewars needed for next day expts

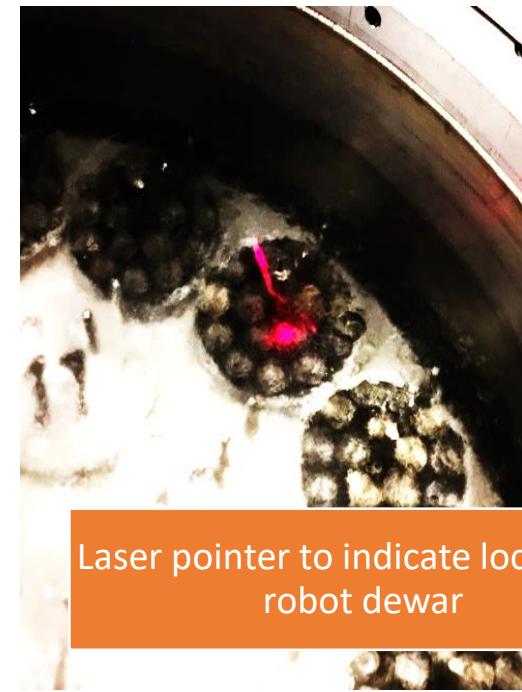
Puck barcodes are read when (un)loading robot



Omron system to read barcodes



Barcode reading station with puck sensor/trigger. Success sound.



Laser pointer to indicate location in robot dewar

Scanned
pucks are
auto-
assigned in
ISPyB ready
for users in
GDA

Container Allocation for cm16788-3 on i24 at 09:00 26-05-2017

This page allows you to allocate samples from ISPyB to the beamline sample changer. Drag and drop containers on to the locations on the beamline. Shipments and Dewars can be expanded by clicking on their titles

[Q Data Collections](#)

Assigned Containers: Sample Changer

1 [DLS-0001]	2 [DLS-0002]	3 [CPS-0012]	4 [LMB-123]	5
DLS-0001	DLS-0002	CPS-0012	LMB-123	
6	7	8	9 [Loaded]	10 cm16788-2_140956
				Q
11	12 cm16788-2_163136	13	14	15
	Q			
16 pierre	17	18	19	20
	Q			
21	22	23	24	25
26	27	28	29	30
31	32	33	34	35
36 cm16788-2_125447	37 test			
	Q	Q		

Locn	Container (Puck/Plate)	Position	Sample Name	Barcode	Protein Acronym	Comr
▼ 1	cm16791-2_123821		Expand row to view samples	DLS-123		
1		1	test_1		test	
1		2	test_2		test	
1		3	test_3		test	
1		4	test_4		test	

Autoprocessing results

Screening for data collection strategies

Sample: Se_Thau_15 Flux: 2.47e+11

Ω Start: 0.0° Ω Osc: 0.15°

Ω Overlap: -44.85° No. Images: 6

ϕ : 310.98001° x: 24.303° Resolution: 1.59 Å

Wavelength: 0.9795 Å Exposure: 0.040s

Transmission: 100.00% Beamsize: 43x30 μm

Type: SAD

Comment: (-98,-256,98) (-133,-274,-5) (-75,-483,146) Aperture: LargeAperture: LargeAperture: Large

Strategies

xia2.strategy

Space Group	A	B	C	α	β	γ
P 4	57.92	57.92	150.54	90.00	90.00	90.00

Strategy Description Ω Start Ω Osc Res (Å) Ranking Res (Å) Rel Trn (%) Abs Trn (%) Exposure (s) No. Images

anomalous Wedge1	Standard Anomalous Dataset Multiplicity=3 I/sig=2 Maxifespan=200s	63	0.10	1.63	1.35	3.4	3.4	0.040	2700
gentle Wedge1	Gentle: Target Multiplicity=2 I/sig=2 Maxifespan=20s	84	0.10	1.63	1.47	6.6	6.6	0.040	1150
high multiplicity Wedge1	Strategy with target multiplicity=16 I/sig=2 200s	0	0.10	1.63	1.98	3.4	3.4	0.040	3600
native Wedge1	Standard Native Dataset Multiplicity=3 I/sig=2 Maxifespan=200s	87	0.10	1.63	1.29	3.4	3.4	0.040	920

dials.align_crystal

Axes	Kappa	Chi	Phi
c* (4-fold)	24.41	310.89999	

EDNA MXV1

Space Group	A	B	C	α	β	γ
P4	57.95	57.95	150.10	90.00	90.00	90.00

Strategy Description Ω Start Ω Osc Res (Å) Ranking Res (Å) Rel Trn (%) Abs Trn (%) Exposure (s) No. Images

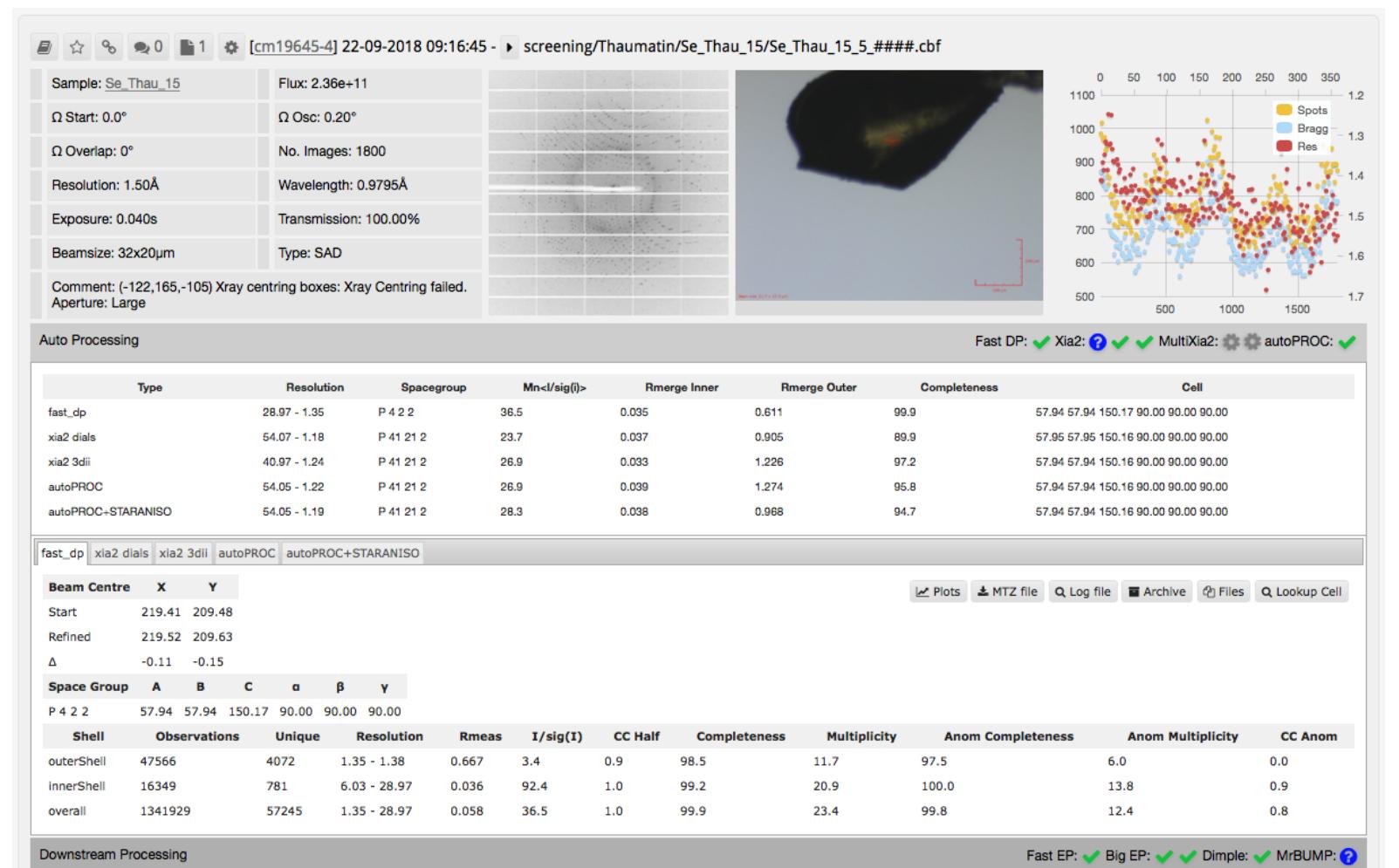
Strategy1 Wedge1	Standard Native Dataset Multiplicity=3 I/sig=2 Maxifespan=200 s	167	0.10	1.61	1.34	10.4	10.4	0.040	760
Strategy2 Wedge1	Standard Anomalous Dataset Multiplicity=3 I/sig=2 Maxifespan=200 s	6	0.10	1.61	1.38	11.6	11.6	0.040	1340
Strategy3 Wedge1	strategy with target multiplicity=16, target I/sig=2 Maxifespan=200 s	0	0.10	1.61	1.34	2.3	2.3	0.040	3600
Strategy4 Wedge1	Gentle: Target Multiplicity=2 and target I/Sig 2 and Maxifespan=20 s	167	0.10	1.61	1.47	10.4	10.4	0.040	760
Strategy5 Wedge1	UnderDEV Anomalous Dataset, RadDamage of standard protein	6	0.10	1.61	1.38	11.6	11.6	0.040	1340

mosflm

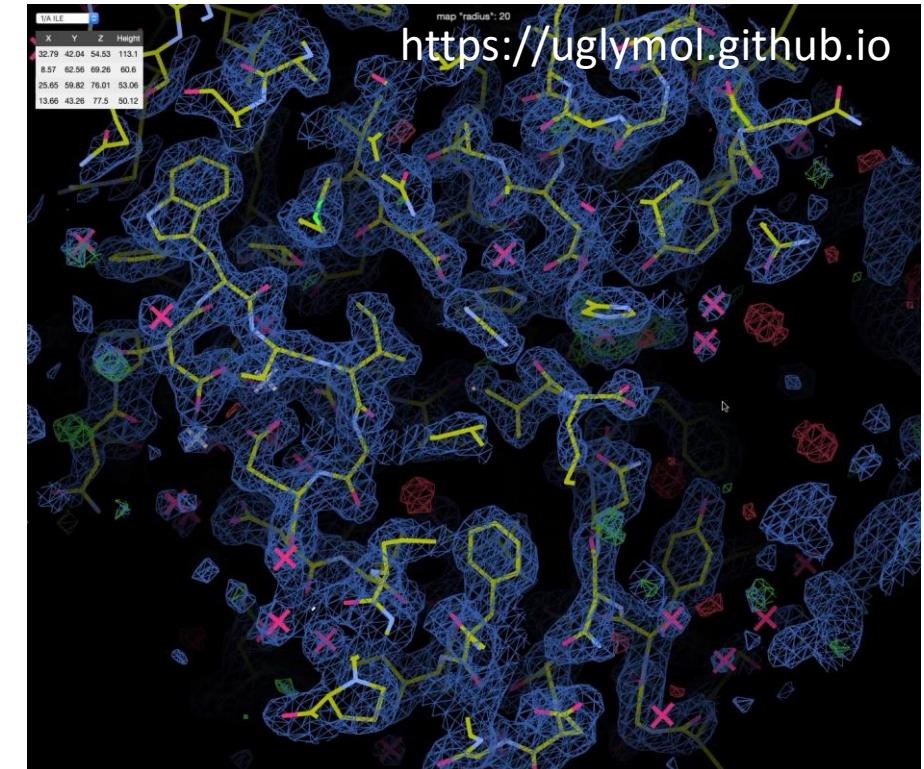
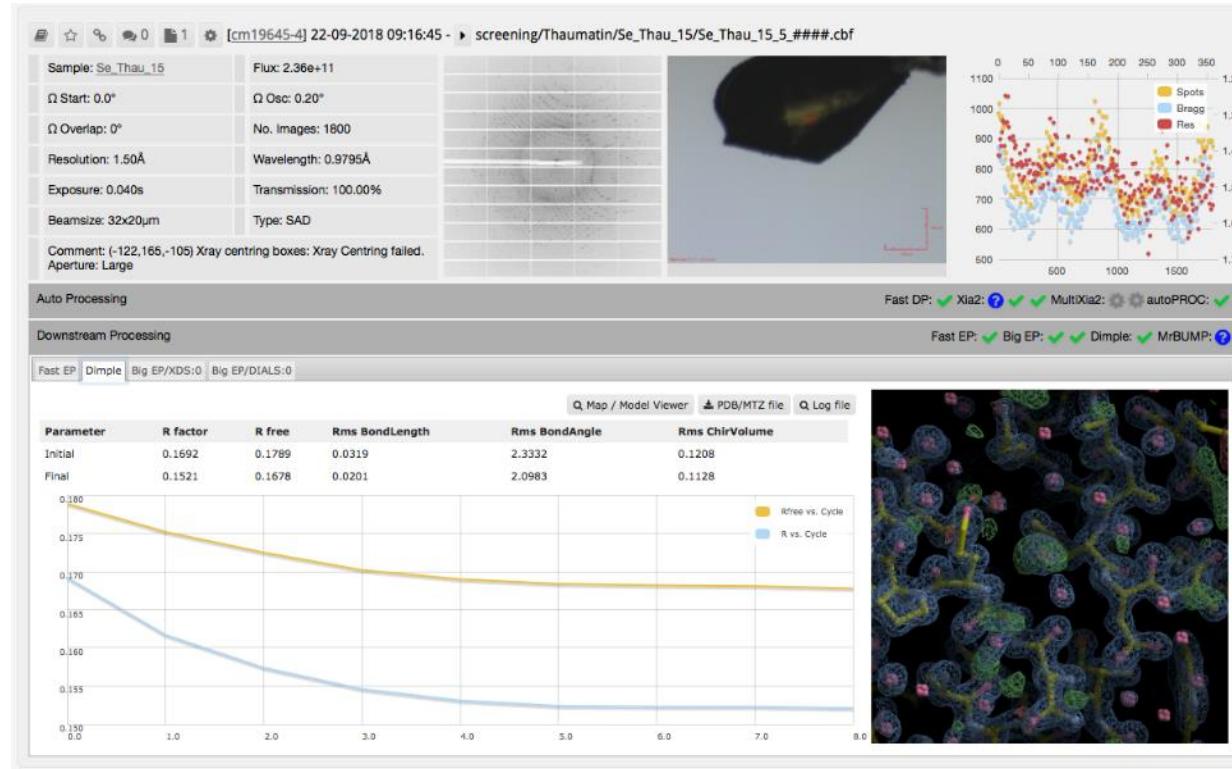
Space Group	A	B	C	α	β	γ
P4	57.97	57.97	150.77	90.00	90.00	90.00

Figure showing a 2D class averages image of a protein crystal with several spots highlighted in red, and a corresponding 1D intensity distribution plot.

Data Collections



Difference Maps - DIMPLE



Phasing and Model Building – BigEP

The image shows the BigEP software interface, which includes a main control panel and a detailed 3D model building view.

Main Control Panel:

- Sample: Se_Thau_15
- Flux: 2.36e+11
- Ω Start: 0.0°
- Ω Osc: 0.20°
- Ω Overlap: 0°
- No. Images: 1800
- Resolution: 1.50 Å
- Wavelength: 0.9795 Å
- Exposure: 0.040s
- Transmission: 100.00%
- Beamsize: 32x20 μm
- Type: SAD
- Comment: (-122,165,-105) Xray centring boxes: Xray Centring failed.
- Aperture: Large

Auto Processing: Fast DP: ✓ Xia2: ? ✓ MultXia2: ? autoPROC: ✓

Downstream Processing: Fast EP: ✓ Big EP: ✓ Dimple: ✓ MrBUMP: ?

Processed: DIALS Anom. scatterer: Se Space group: P41212 Num. scatterers: 6 Dataset type: infl Compound: Protein Sequence: >polysac

Fast EP | Dimple | Big EP/XDS:0 | Big EP/DIALS:0

Settings:

Processed	Anom. scatterer	Space group	Num. scatterers	Dataset type	Compound	Sequence
DIALS	Se	P41212	6	infl	Protein	>polysac AAAAAA

DIALS:

Graph showing CC(1/2) vs Time (min). The yellow line represents < $d^*/\delta g$ > and the blue line represents CC(1/2). Both curves start at approximately 5.0 and decrease rapidly, leveling off around 0.5 after 2.5 minutes.

Pipeline	Resid. / Frag. / Max. Frag.	Best MapCC (Resol.)
AUTOSHARP	195 / 3 / 120	0.67 (1.20)
AUTOBUILD	206 / 1 / 206	0.67 (1.25)
CRANK2	198 / 4 / 110	0.58 (1.20)

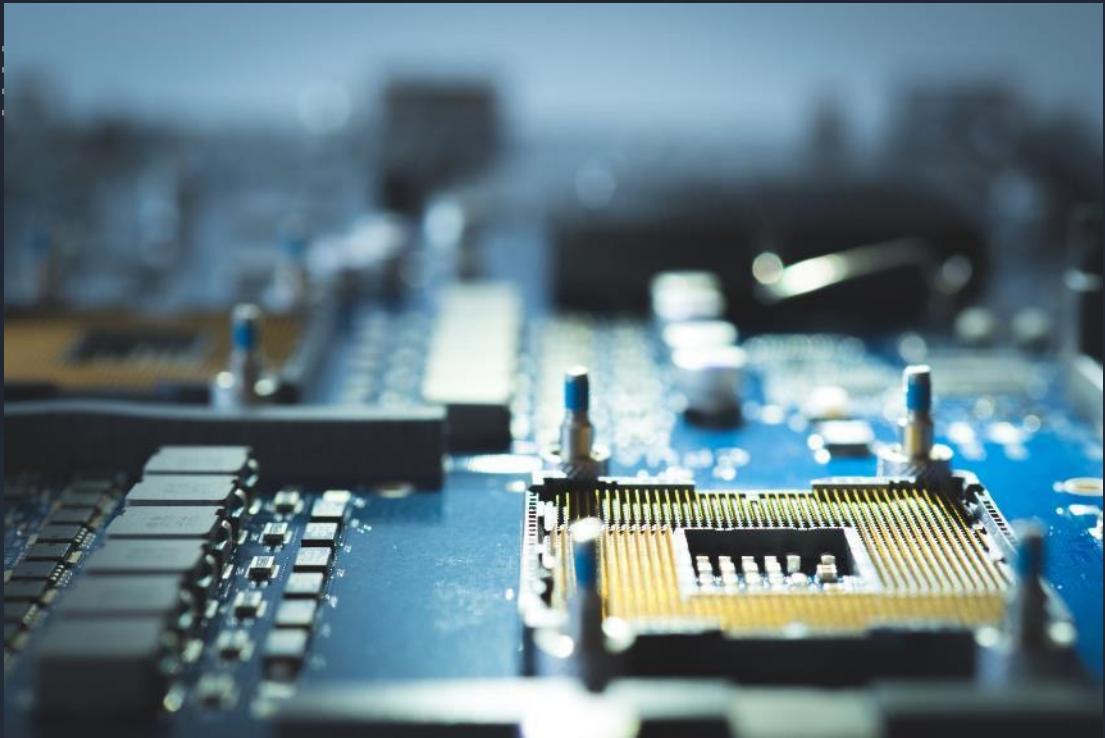
Buttons: Q Map / Model Viewer PDB/MTZ file, Q Log file

3D Model Building View:

A 3D ribbon model of a protein structure. Yellow sticks are placed along the backbone and side chains, indicating specific conformations or restraints used in the model building process. A legend in the top right corner identifies the symbols: yellow for Spots, light blue for Bragg, red for Res, and yellow for Spots.

Auto-processing summary

Prefix	Sample	Date	Fast DP	Xia2/3d	Xia2/3dii	DIALS	MultiXia2/XDS	MultiXia2/DIALS	autoPROC	Fast EP	Big EP/XDS	Big EP/DIALS	Dimple	MrBUMP	
ms-208-lamo-H3-x14_1_master.h5	ms-208-lamo-H3-x14	09-04-2019 05:05:02	✓	?	✓	✓	?	?	✓	?	?	?	✓	?	⚙️ ➔
ms-208-tamo-x9_2_master.h5	ms-208-tamo-x9	09-04-2019 04:45:09	✓	?	✓	✓	?	?	✓	?	?	?	✓	?	⚙️ ➔
ms-208-tamo-x9_1_master.h5	ms-208-tamo-x9	09-04-2019 04:43:10	✓	?	✓	✓	?	?	✓	?	?	?	✓	?	⚙️ ➔
ms-208-tamo-x8_2_master.h5	ms-208-tamo-x8	09-04-2019 04:35:43	✗	?	✓	✓	?	?	✓	?	?	?	?	?	⚙️ ➔
ms-208-tamo-x8_1_master.h5	ms-208-tamo-x8	09-04-2019 04:34:10	✗	?	✓	✓	?	?	✓	?	?	?	?	?	⚙️ ➔
ms-208-apo-D6-x16_1_master.h5	ms-208-apo-D6-x16	09-04-2019 04:28:50	✓	?	✓	✓	?	?	✓	?	✗	⚙️	✗	?	⚙️ ➔
ms-208-apo-C8-x15_1_master.h5	ms-208-apo-C8-x15	09-04-2019 04:24:02	✓	?	✓	✓	?	?	✗	?	?	?	✓	?	⚙️ ➔
ms-208-apo-C7-x13_2_master.h5	ms-208-apo-C7-x13	09-04-2019 04:17:24	✓	?	✓	✓	?	?	✗	?	?	?	✓	?	⚙️ ➔
ms-208-apo-C7-x13_1_master.h5	ms-208-apo-C7-x13	09-04-2019 04:11:15	✓	?	✓	✓	?	?	✓	?	?	?	✓	?	⚙️ ➔
ms-208-apo-C7-x12_1_master.h5	ms-208-apo-C7-x12	09-04-2019 04:08:44	✓	?	✓	✓	?	?	✓	?	?	?	✓	?	⚙️ ➔
ms-wt-tamo-H7-x11_1_master.h5	ms-wt-tamo-H7-x11	09-04-2019 04:02:37	✓	?	✗	✓	?	?	✓	?	?	?	✓	?	⚙️ ➔
ms-wt-tamo-H7-x10_1_master.h5	ms-wt-tamo-H7-x10	09-04-2019 03:59:16	✓	?	✓	✓	?	?	✓	?	?	?	✓	?	⚙️ ➔
ms-wt-tamo-D6-x9_1_master.h5	ms-wt-tamo-D6-x9	09-04-2019 03:53:03	✓	?	✓	✓	?	?	✓	?	?	?	✓	?	⚙️ ➔
ms-wt-tamo-C7-x8_1_master.h5	ms-wt-tamo-C7-x8	09-04-2019 03:46:53	✓	?	✓	✓	?	?	✓	?	?	?	✓	?	⚙️ ➔
ms-wt-tamo-B7-x5_1_master.h5	ms-wt-tamo-B7-x5	09-04-2019 03:34:28	✓	?	✓	✓	?	?	✓	?	?	?	✓	?	⚙️ ➔



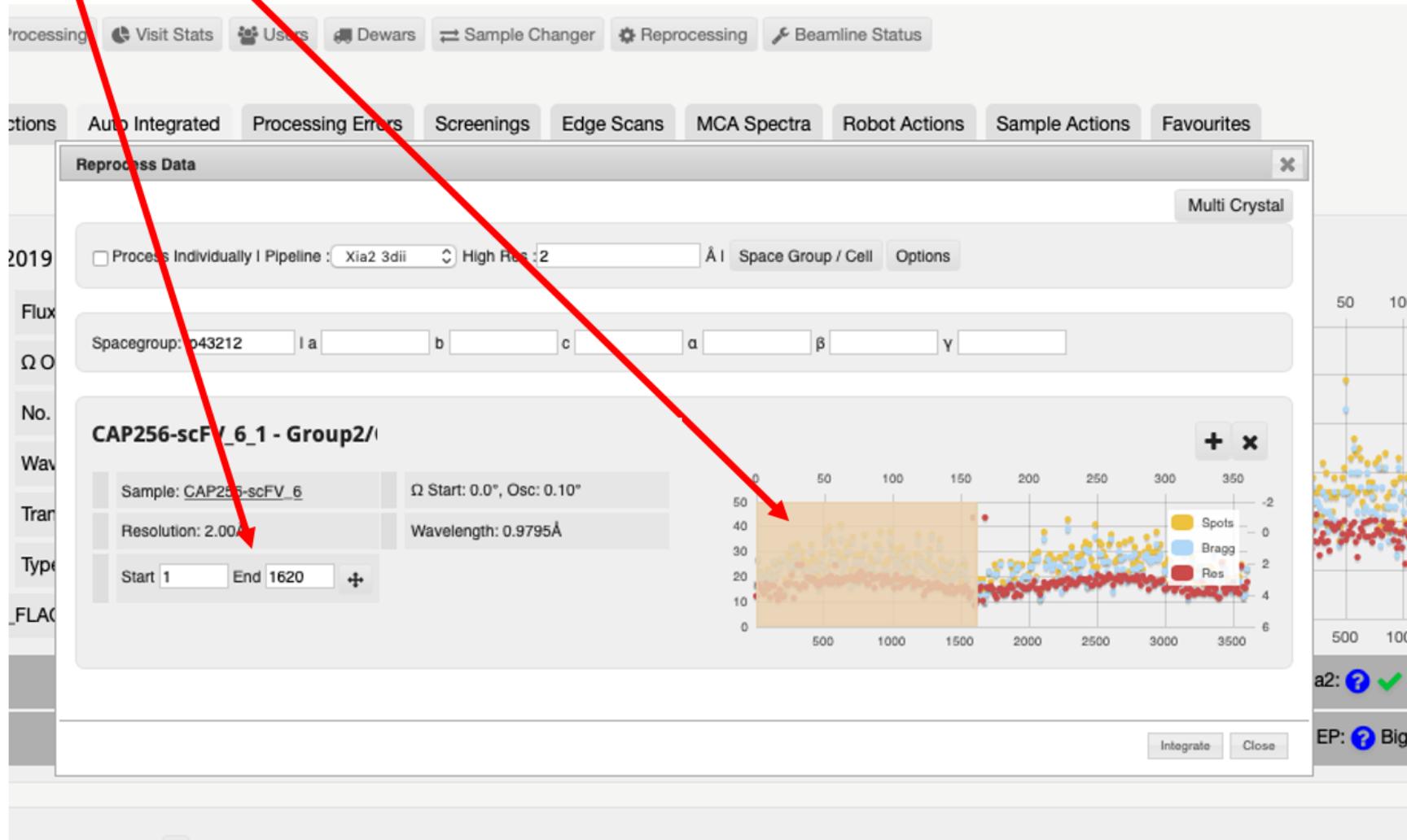
Data Re-processing

Define reprocessing requirements

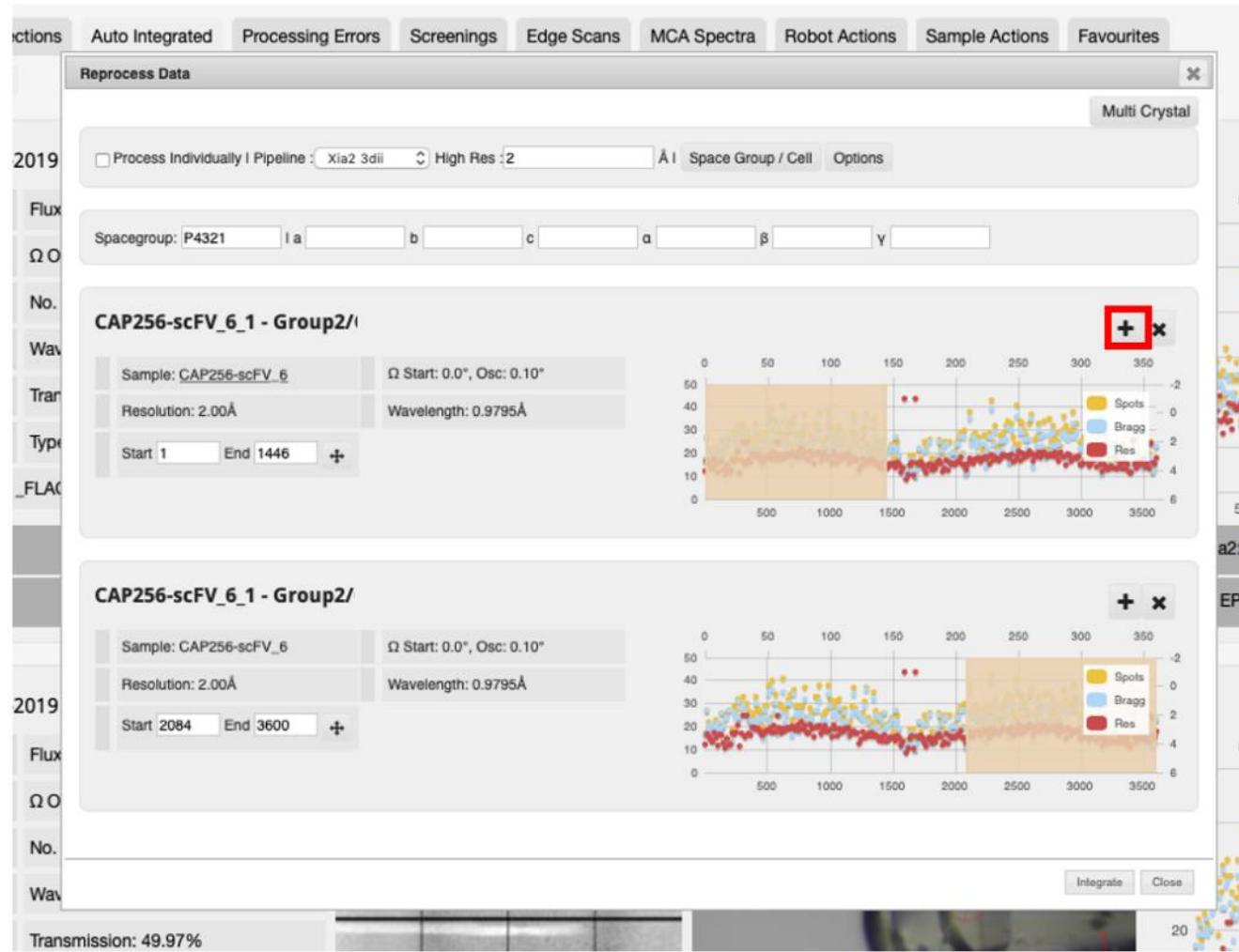
The screenshot shows the iSPYB Diamond software interface. At the top, there's a navigation bar with links for Home, Calendar, Logout, and collections (mx2003-6). Below the navigation bar is a header with tabs for Proposals, mx2003, Projects, Unit Cell Search, Feedback, and Help. A green banner at the top of the main content area says: "Please note that all dewars must now be registered before creating a shipment. Please see the updated help pages for details of the new process." The main content area has a tab bar with Auto Integrated, Processing Errors, Screenings, Edge Scans, MCA Spectra, Robot Actions, Sample Actions, and Favourites. A sub-dialog box titled "Reprocess Data" is open. It contains fields for "Process Individually" (unchecked), "Pipeline" (set to "Xia2 3dii"), "High Res" (set to "2"), "Space Group / Cell" (highlighted with a purple border), and "Options". Below these fields is a "Spacegroup" input field with "p43212" and sliders for "a", "b", "c", "α", "β", and "γ". A section titled "CAP256-scFV_6_1 - Group2/" displays sample information: "Sample: CAP256-scFV_6", "Ω Start: 0.0°, Osc: 0.10°", "Resolution: 2.00 Å", "Wavelength: 0.9795 Å", and controls for "Start", "End", and "Integrate". To the right of this section is a 2D intensity plot showing spots, Bragg reflections, and residuals. At the bottom of the "Reprocess Data" dialog are buttons for "Integrate" and "Close". The footer of the main window shows the date and time "2019 15:50:08" and sections for "Auto Processing" and "Downstream Processing".

- Select pipeline
- Provide high res cut-off if required
- Provide space group if wish to constrain pipeline

Select images

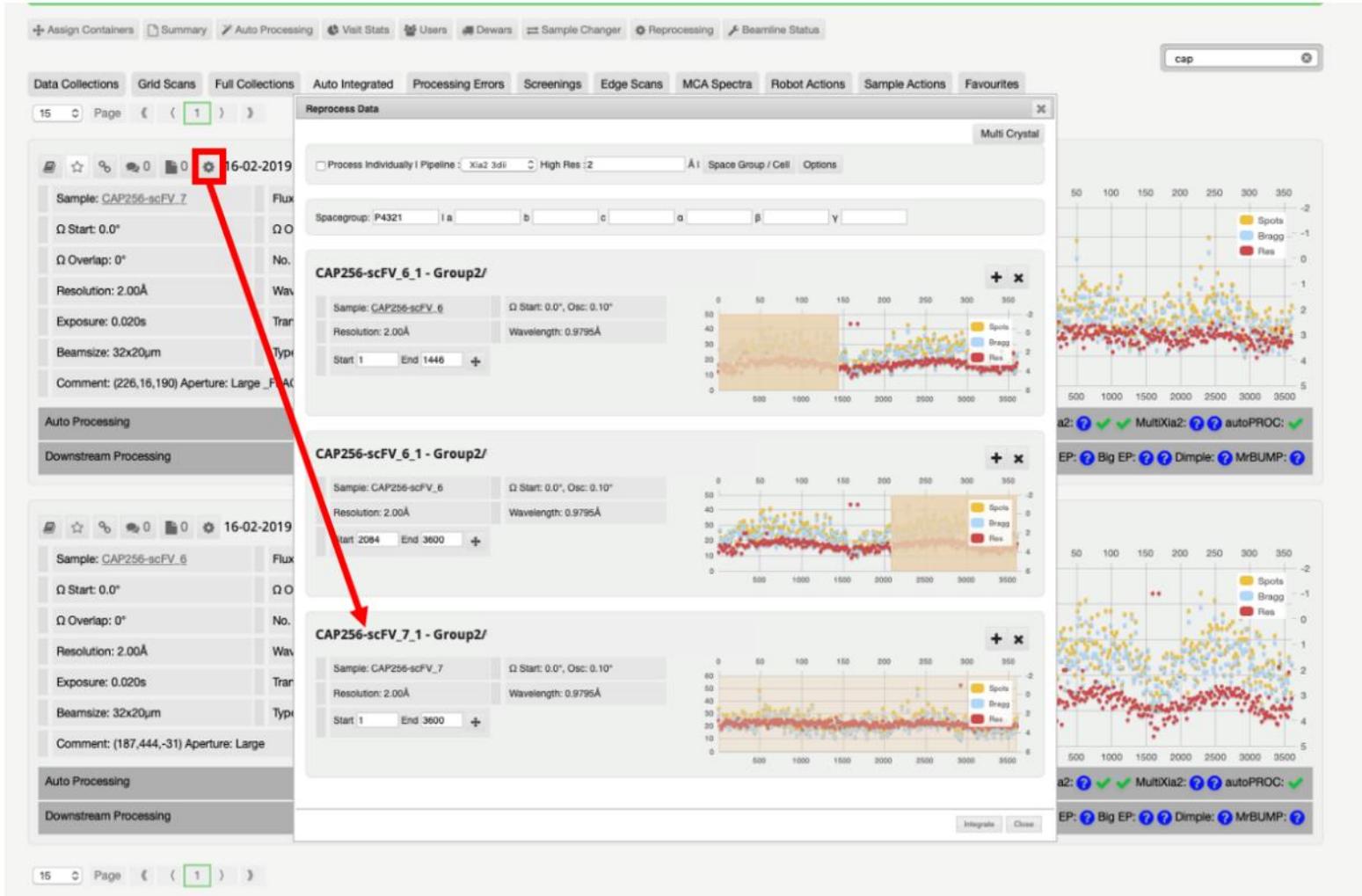


Can process multiple ranges from data set



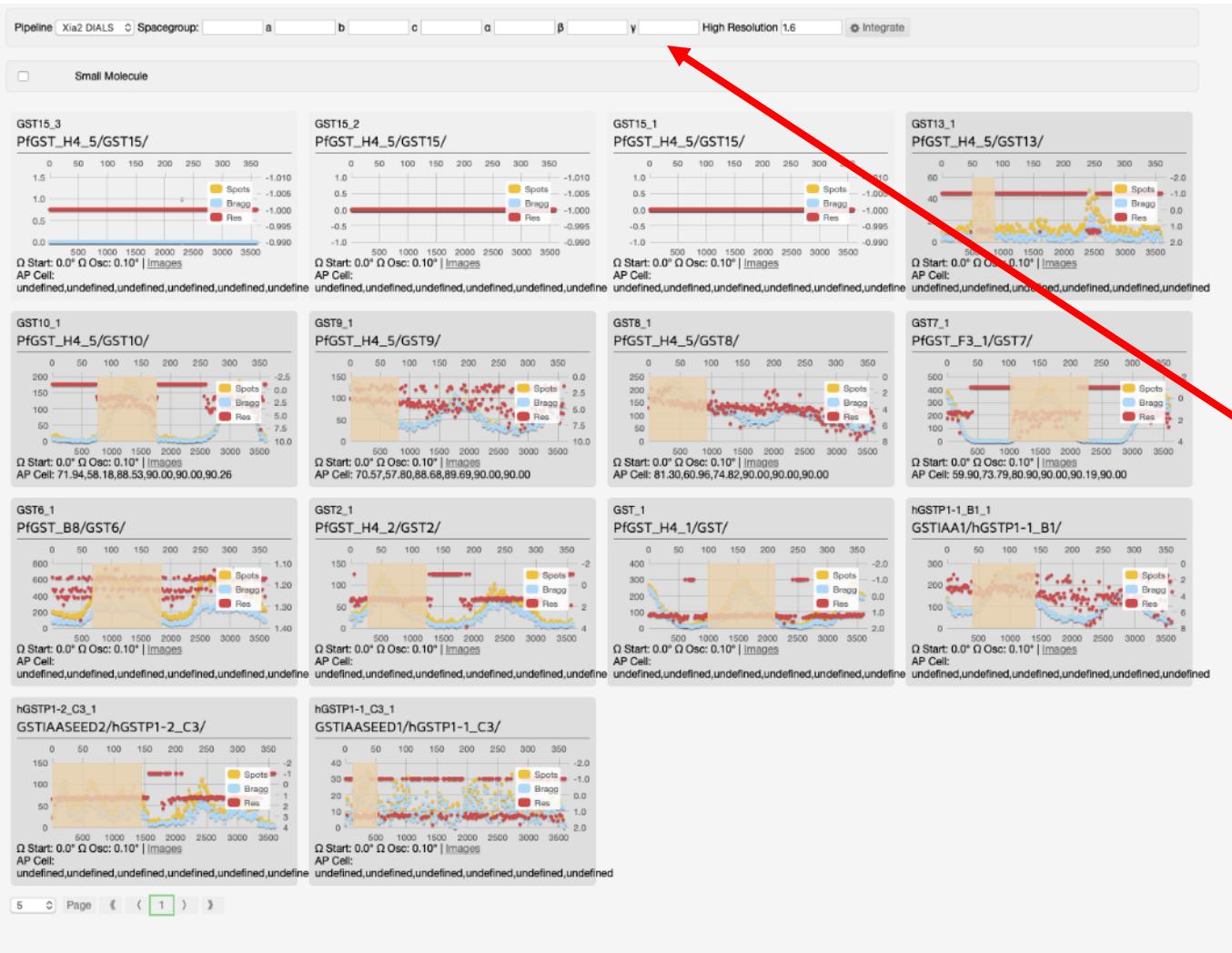
- Click + to add more from same data collection

Can add more data sets



- Click reprocess button on relevant data collection
- Clicking Integrate will combine all 3 together with 1 set of constraints

Many collections reprocessing



- Filter using search field for protein interested in (this time “gst”)
- Scroll down page
- Define parameters for integration
- Select images
- Integrate

Reprocessing results

must be registered before creating a shipment. Please see the updated help pages for details of the new process.

Reprocessing

Status	Sample	DC	Process	Comments	Last Updated	Last Message	Arguments										
✓	TFcore52_14 - TFcore52	TFcore52_14	Xia2 3dli		02-07-2019 12:21	processing successful	<table border="1"><tr><th>Key</th><th>Value</th></tr><tr><td>spacegroup</td><td>P1</td></tr><tr><td>Files</td><td>Image #</td></tr><tr><td colspan="2">/TFcore52/TFcore52_14/TFcore52_14_1 1 - 3600</td></tr></table>	Key	Value	spacegroup	P1	Files	Image #	/TFcore52/TFcore52_14/TFcore52_14_1 1 - 3600			
Key	Value																
spacegroup	P1																
Files	Image #																
/TFcore52/TFcore52_14/TFcore52_14_1 1 - 3600																	
✓	TFcore52_14 - TFcore52	TFcore52_14	Xia2 3dli		02-07-2019 11:20	processing successful	<table border="1"><tr><th>Key</th><th>Value</th></tr><tr><td>spacegroup</td><td>P1</td></tr><tr><td>Files</td><td>Image #</td></tr><tr><td colspan="2">/TFcore52/TFcore52_14/TFcore52_14_1 1 - 3600</td></tr></table>	Key	Value	spacegroup	P1	Files	Image #	/TFcore52/TFcore52_14/TFcore52_14_1 1 - 3600			
Key	Value																
spacegroup	P1																
Files	Image #																
/TFcore52/TFcore52_14/TFcore52_14_1 1 - 3600																	
✓	TFcore52_14 - TFcore52	TFcore52_14	Xia2 3dli		02-07-2019 11:17	processing successful	<table border="1"><tr><th>Key</th><th>Value</th></tr><tr><td>spacegroup</td><td>P1</td></tr><tr><td>Files</td><td>Image #</td></tr><tr><td colspan="2">/TFcore52/TFcore52_14/TFcore52_14_1 1 - 3600</td></tr></table>	Key	Value	spacegroup	P1	Files	Image #	/TFcore52/TFcore52_14/TFcore52_14_1 1 - 3600			
Key	Value																
spacegroup	P1																
Files	Image #																
/TFcore52/TFcore52_14/TFcore52_14_1 1 - 3600																	
✗	CB_GST_75b - PRGST	CB_GST_75b	Xia2 DIALS		26-06-2019 14:33	processing failure	<table border="1"><tr><th>Key</th><th>Value</th></tr><tr><td>d_min</td><td>1.5</td></tr><tr><td>Files</td><td>Image #</td></tr><tr><td colspan="2">/PRGST/CB_GST_75b/CB_GST_75b_1 1 - 750</td></tr><tr><td colspan="2">/PRGST/CB_GST_75b/CB_GST_75b_1 1900 - 2600</td></tr></table>	Key	Value	d_min	1.5	Files	Image #	/PRGST/CB_GST_75b/CB_GST_75b_1 1 - 750		/PRGST/CB_GST_75b/CB_GST_75b_1 1900 - 2600	
Key	Value																
d_min	1.5																
Files	Image #																
/PRGST/CB_GST_75b/CB_GST_75b_1 1 - 750																	
/PRGST/CB_GST_75b/CB_GST_75b_1 1900 - 2600																	
✗	CB_GST_75b - PRGST	CB_GST_75b	Xia2 DIALS		26-06-2019 14:33	processing failure	<table border="1"><tr><th>Key</th><th>Value</th></tr><tr><td>d_min</td><td>1.5</td></tr><tr><td>Files</td><td>Image #</td></tr><tr><td colspan="2">/PRGST/CB_GST_75b/CB_GST_75b_1 1 - 750</td></tr><tr><td colspan="2">/PRGST/CB_GST_75b/CB_GST_75b_1 1900 - 2600</td></tr></table>	Key	Value	d_min	1.5	Files	Image #	/PRGST/CB_GST_75b/CB_GST_75b_1 1 - 750		/PRGST/CB_GST_75b/CB_GST_75b_1 1900 - 2600	
Key	Value																
d_min	1.5																
Files	Image #																
/PRGST/CB_GST_75b/CB_GST_75b_1 1 - 750																	
/PRGST/CB_GST_75b/CB_GST_75b_1 1900 - 2600																	

Close

Fast EP: ? Big EP: ? ?

- Can see status of submitted jobs
- Access results from links to Files on right
- Takes you to the standard analysis results where reprocessed jobs will be added

User Tools

Webcams

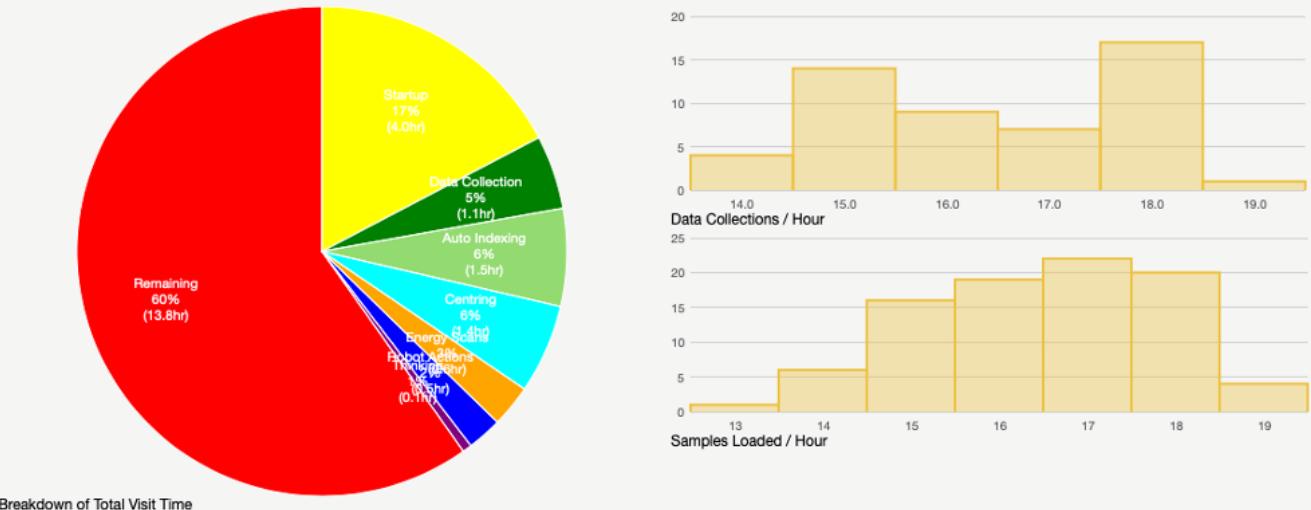
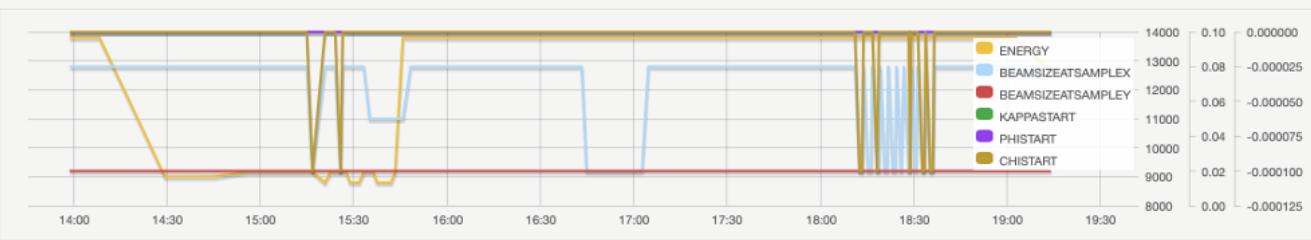
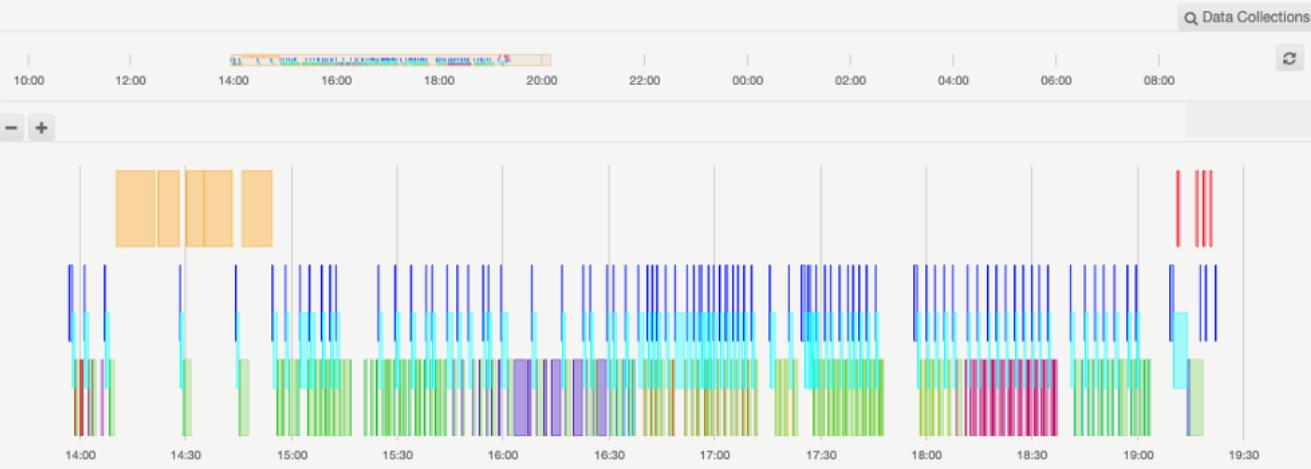


OAV

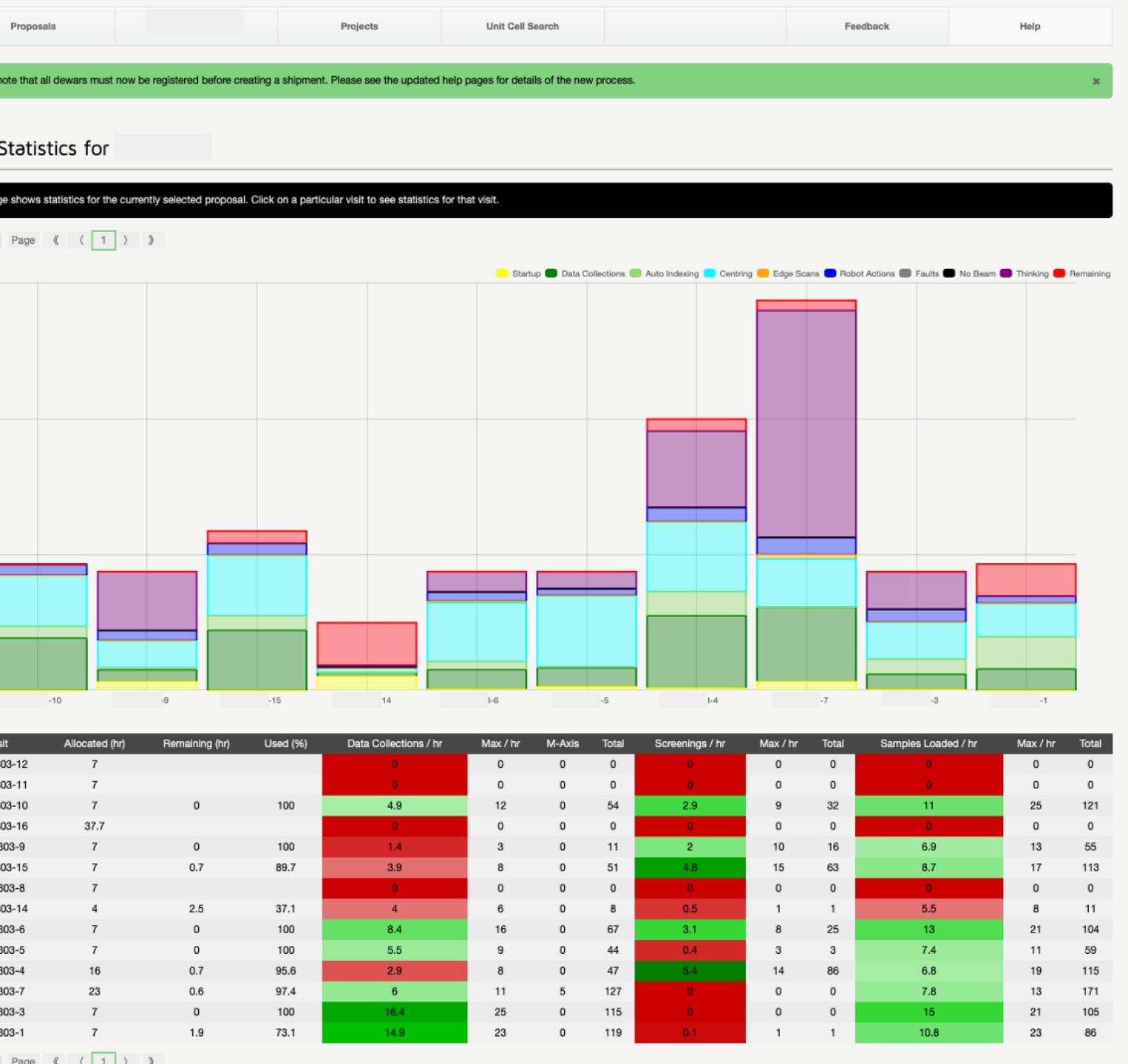


Webcams

Visit Stats



Proposal Stats



Staff Tools

Beamline staff login screen

Proposals No Proposal 

Please report any SynchWeb/ISPyB issues to your local contact. 

Time at Diamond is: Fri Feb 07 2020 16:19:09 (GMT+0000)

Current & Next Visits

i02-1. nr23571-54 Start: 10:00 18-01-2020 End: 00:00 31-03-2020	i03. nr23571-52 Start: 10:00 18-01-2020 End: 00:00 31-03-2020	i04. nr23571-53 Start: 10:00 18-01-2020 End: 00:00 31-03-2020	i04-1. nr23571-57 Start: 10:00 18-01-2020 End: 00:00 31-03-2020	i23. nr23571-55 Start: 10:00 18-01-2020 End: 00:00 31-03-2020
i24-1 nr23571-56 Start: 10:00 18-01-2020 End: 00:00 31-03-2020				

Last Visits

i02. mx19f Start: 09:00 01-12-2017 End: 17:00 20-12-2017	i02-1. nr23570-44 Start: 09:00 23-10-2019 End: 09:00 25-10-2019	i02-2. nr23570-39 Start: 10:00 14-10-2019 End: 09:00 19-10-2019	i03. nr23570-83 Start: 10:00 06-02-2020 End: 17:00 06-02-2020	i04. swf Start: 12:00 07-02-2020 End: 13:00 07-02-2020
i04-1. mx23i Start: 17:45 03-02-2020 End: 09:00 04-02-2020 Compulsorily Remote	i23. mx26288-4 Start: 10:00 12-12-2019 End: 17:00 12-12-2019	i24. mrc Start: 17:00 06-02-2020 End: 09:00 07-02-2020		

Commissioning Visits

i02 cm16768-5 Start: 09:00 27-10-2017 End: 09:00 31-12-2017	i02-1. cm26440-1 Start: 09:00 01-01-2020 End: 09:00 06-03-2020	i02-2. cm26443-1 Start: 09:00 01-01-2020 End: 09:00 06-03-2020	i03. cm26458-1 Start: 09:00 01-01-2020 End: 09:00 06-03-2020	i04-1 cm26459-1 Start: 09:00 01-01-2020 End: 09:00 06-03-2020
i04-1 cm26460-1 Start: 09:00 01-01-2020 End: 09:00 06-03-2020	i23. cm26461-1 Start: 09:00 01-01-2020 End: 09:00 06-03-2020	i24. cm26462-1 Start: 09:00 01-01-2020 End: 09:00 06-03-2020		

Ring Current 298.165	Refill 64.7264	Hutch Locked	Port Shutter Open	Expt Shutter Open	Fast Shutter ---	Wavelength 0.8984	Transmission 100
-------------------------	-------------------	-----------------	----------------------	----------------------	---------------------	----------------------	---------------------

Webcams



OAV

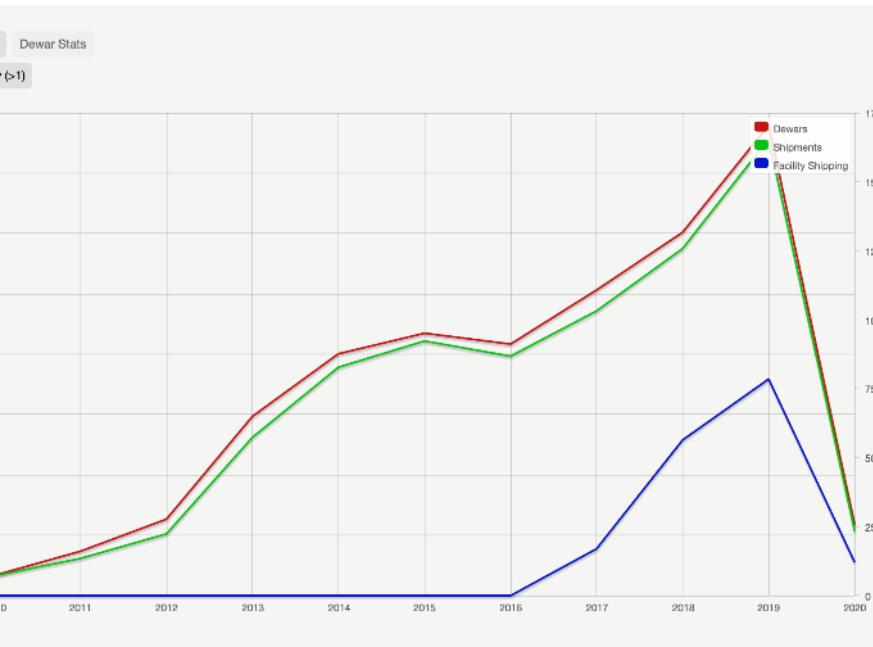
EPICS Screens

Sample Environment
Goniometer
Robot Interface

GDA Log

```
2020-02-09 16:08:25,984 DEBUG [objectserver/1059@i03-control.diamond.ac.uk] gda.px.smargon.SmarGonController - Now executing a move of Z
2020-02-09 16:08:25,984 DEBUG [objectserver/1059@i03-control.diamond.ac.uk] gda.px.smargon.SmarGonController - Move was not pending for Z (but now is)
2020-02-09 16:08:25,984 DEBUG [objectserver/1059@i03-control.diamond.ac.uk] gda.px.smargon.SmarGonScannableMotor - Current thread &quot;jythonCommandRunnerCommand_28885002
2020-02-09 16:08:25,983 INFO [objectserver/1059@i03-control.diamond.ac.uk] gdascripts.messages.handle_messages - autoCentre:Move samz to 400.0021
2020-02-09 16:08:25,620 DEBUG [objectserver/1059@i03-control.diamond.ac.uk] gda.px.smargon.SmarGonController - OMEGA is no longer moving
2020-02-09 16:08:25,520 DEBUG [objectserver/1059@i03-control.diamond.ac.uk] gda.px.smargon.SmarGonController - Waiting for a move of OMEGA to finish
2020-02-09 16:08:25,520 DEBUG [objectserver/1059@i03-control.diamond.ac.uk] gda.px.smargon.SmarGonScannableMotor - Current thread &quot;pool-3-thread-1&quot; is executing a move for
2020-02-09 16:08:25,520 DEBUG [objectserver/1059@i03-control.diamond.ac.uk] gda.px.smargon.SmarGonController - Now executing a move of OMEGA
2020-02-09 16:08:25,520 DEBUG [objectserver/1059@i03-control.diamond.ac.uk] gda.px.smargon.SmarGonController - Move was not pending for OMEGA (but now is)
2020-02-09 16:08:25,520 DEBUG [objectserver/1059@i03-control.diamond.ac.uk] gda.px.smargon.SmarGonScannableMotor - Current thread &quot;jythonCommandRunnerCommand_28885002
2020-02-09 16:08:25,519 INFO [objectserver/1059@i03-control.diamond.ac.uk] gdascripts.messages.handle_messages - autoCentre:Attempt 1
2020-02-09 16:08:25,518 INFO [objectserver/1059@i03-control.diamond.ac.uk] gdascripts.messages.handle_messages - KeyencePositions:startX: 820.451 startY: 754.5
2020-02-09 16:08:25,518 INFO [objectserver/1059@i03-control.diamond.ac.uk] gdascripts.messages.handle_messages - KeyencePositions:requiredX: 869.321 requiredY: 654.5
```

Beamline status



Dewar Overview

This page shows all dewars for all current visits

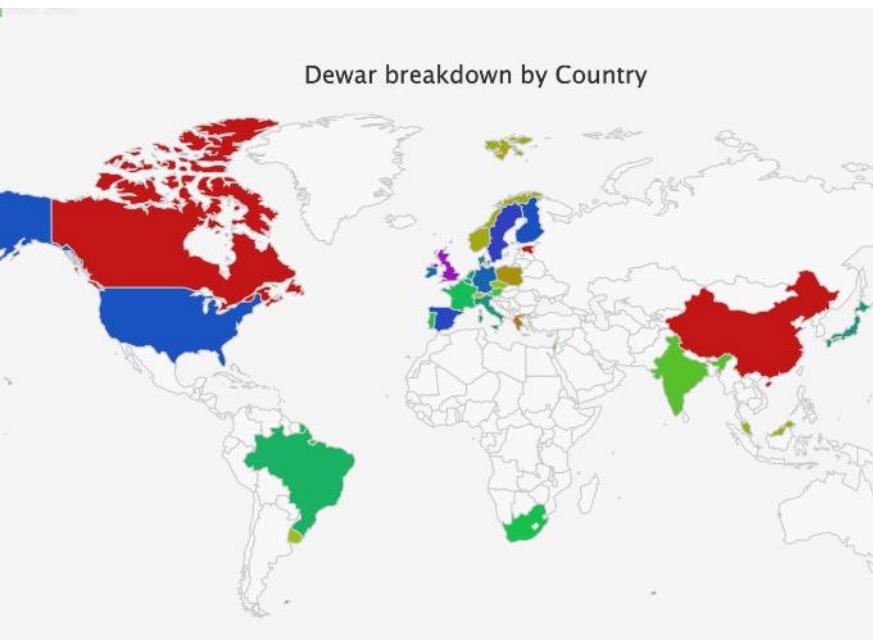
i02 i02-2 i03 i04 i04-1 i23 i24

Imager Requested

First Experiment:

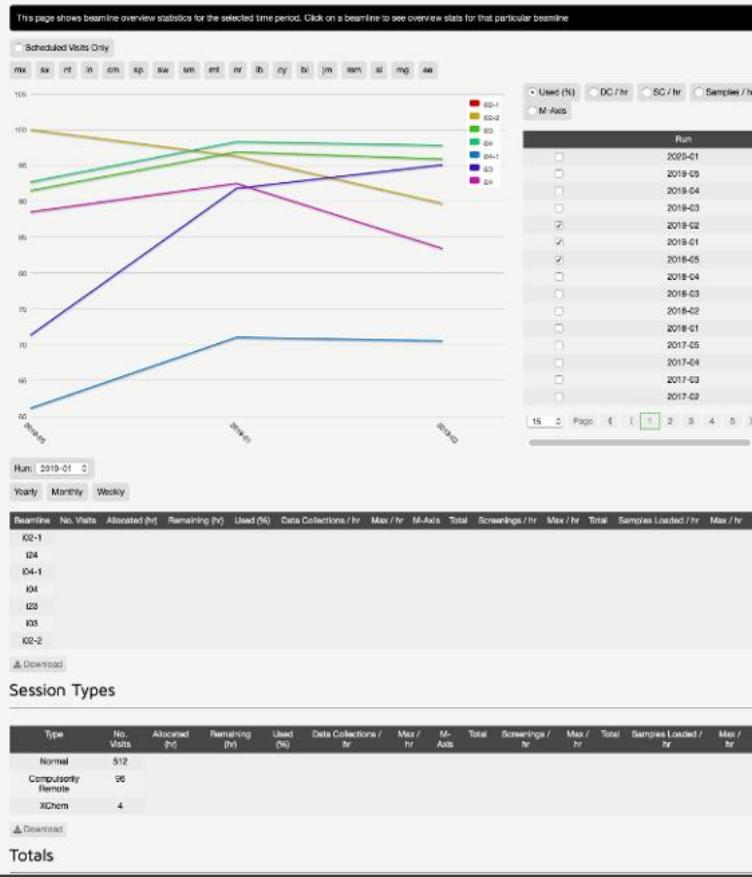
Search

Start Date	Visit	Beamline	Local Contact	Shipment	Dewar Name	Dewar Code	Containers	Courier	Track # to	Status	Location	Tracking
09:00 26-10-2018	cm19647-5	i02-2		cm19647-5_Shipment1	cm19647-5_Dewar1					processing		
10:00 04-08-2018		i04-1			DLS-MX-0663	DLS-MX-0663		DHL		at facility	stores-out	Delivery: OXFORD-GBR
10:00 16-07-2018		i24			BackupDisk			Fedex		opened		
10:00 07-07-2018		i04			Dewar1			YSDS		at DLS	RACK-X2	
10:00 06-07-2018		i24			Dewar1			banana		opened		
09:00 20-06-2018		i03		9_Shipment1	nr19737-9_Dewar					at DLS		

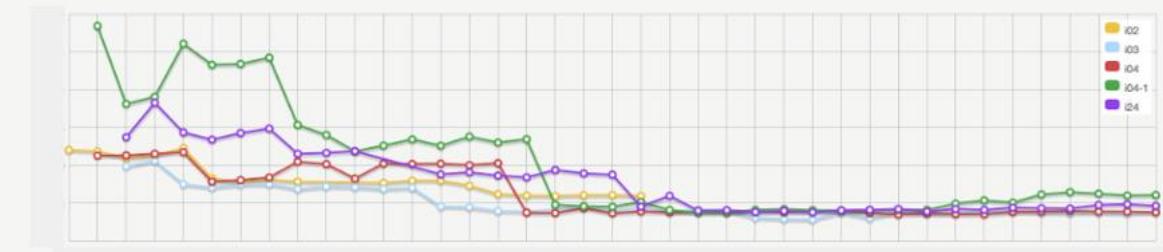


Dewar overview in SynchWeb

Beamlines



Robot Averages



[Download](#)

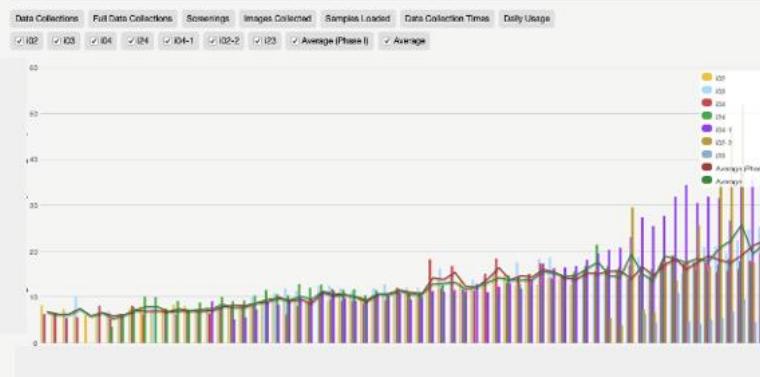
Robot Errors

Time	Beamline	Visit	Action	Duration	Puck	Sample	Barcode	Status	Message
09-02-2020 14:57:25	i04		LOAD	21.0	13	12	null	ERROR	
09-02-2020 14:55:50	i04		LOAD	23.0	13	11	null	ERROR	
09-02-2020 14:05:08	i04		LOAD	23.0	19	8	null	ERROR	
09-02-2020 12:53:28	i04		LOAD	22.0	17	14	null	ERROR	
08-02-2020 22:28:37	i24		UNLOAD	0.0	0	0	null	ERROR	
08-02-2020 20:40:39	i24		LOAD	54.0	20	16	null	ERROR	
08-02-2020 20:29:01	i24		LOAD	56.0	20	16	null	ERROR	
08-02-2020 20:02:48	i24		UNLOAD	0.0	20	8	null	ERROR	
08-02-2020 20:01:51	i24		UNLOAD	0.0	20	8	null	ERROR	

6

Robot Stats Logon Stats Online Stats Beamline Stats Pipeline Stats PDB Stats Reprocessing Stats

Beamline Statistics



Statistics for staff

Faults

[+ Add Fault Report](#)

Beamline: i03

System: -

Component: -

Subcomponent: -

x

Search

Title	Time	Beamline	Visit	System	Component	Resolved	Beamtime Lost	Reporter
User couldn't find correct puck information in GDA	04-03-2019 22:30	i03		User	Other	Yes	No	
Detector in error state, no images collected	23-02-2019 20:40	i03		Detector	Software	Yes	No	
bsz not responding	18-02-2019 18:30	i03		EPICS	Sample Environment	Yes	Yes	
OAV stopped working	10-02-2019 09:30	i03		EPICS	OAV Zoom and Keyence	Yes	No	
Detector didn't arm, IOC reboot necessary	27-01-2019 14:15	i03		Detector	Software	Yes	Yes	
Zoom unit frozen	27-01-2019 06:00	i03		EPICS	OAV Zoom and Keyence	Yes	Yes	
Fzoom unit not working	26-01-2019 23:17	i03		EPICS	OAV Zoom and Keyence	Yes	No	
Futura zoom unit failed	24-01-2019 22:00	i03		EPICS	OAV Zoom and Keyence	Partial	Yes	

Fault database

Summary

- Users
 - From preparing and shipping
 - Providing information for unattended collections and downstream pipelines
 - Following data collections and outcomes of processing
 - Interrogating usage
 - Long term log book
 - Future
 - Improved interfaces for unattended data collection, interface & results
 - VMXi improvements for data collection and results presentation
 - VMXm including SEM
 - SSX interfaces
 - Shipping improvements – 31st Dec 2020 deadline
 -
- Staff
 - Preparing for upcoming expts
 - Finding samples/dewars
 - Following user expts
 - Beamline and user statistics
 - Fault logging and solving