Optimising the Diamond experience from a user's perspective

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John Innes Centre

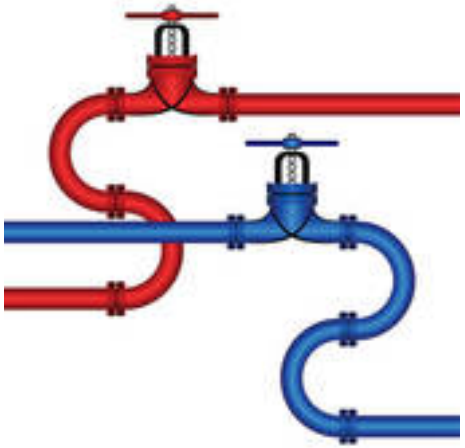
Unlocking Nature's Diversity

UKRI Biotechnology and Biological Sciences Research Council

Strategy

Tools

Pipelines



Remote

- Maximizing efficiency
- Minimizing time commitment
- Managing your data
- How to ~~collect~~ data

“Routine” data collection:

- on non-hazardous samples
- at cryogenic temperatures
- on pre-cooled crystals in pucks
- at conventional wavelengths

Primary goals (data quantity **AND** quality…)

- To collect as much data as possible…
- To collect the best possible data…
- To collect the data that will enable me to:
  - Solve my structure
  - Extend the resolution of my structure
  - Show that my ligand is bound

Secondary goal (make your life easier!)

Primary goals (data quantity **AND** quality…)

- To collect as much data as possible…
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- To collect the data that will enable me to:
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Secondary goal (make your life easier!)

- Try to answer these questions **during** your beamtime:
  - Can I solve my structure?
  - Can I extend the resolution of my structure?
  - Is my ligand bound?
- Make best use of time and minimise the amount of follow-up work…

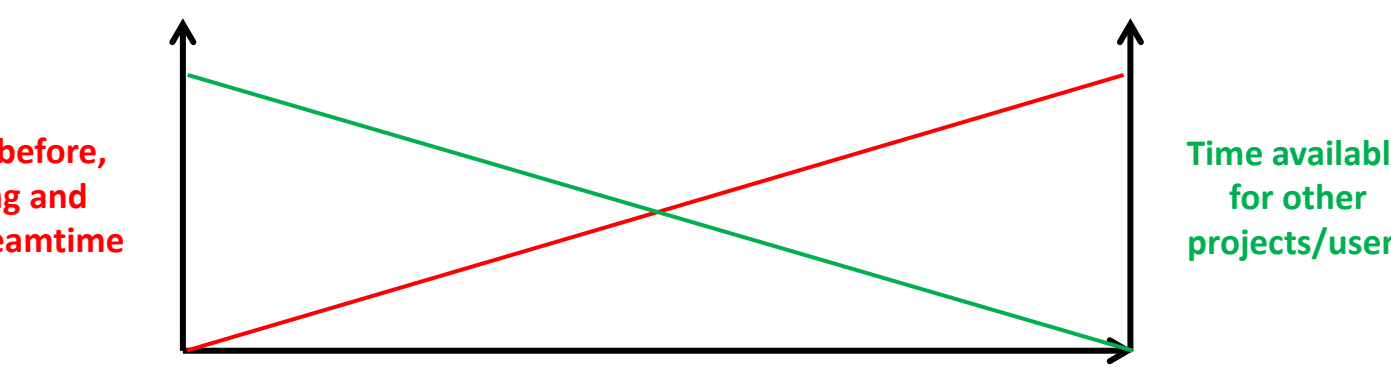
How many samples to prepare per project…

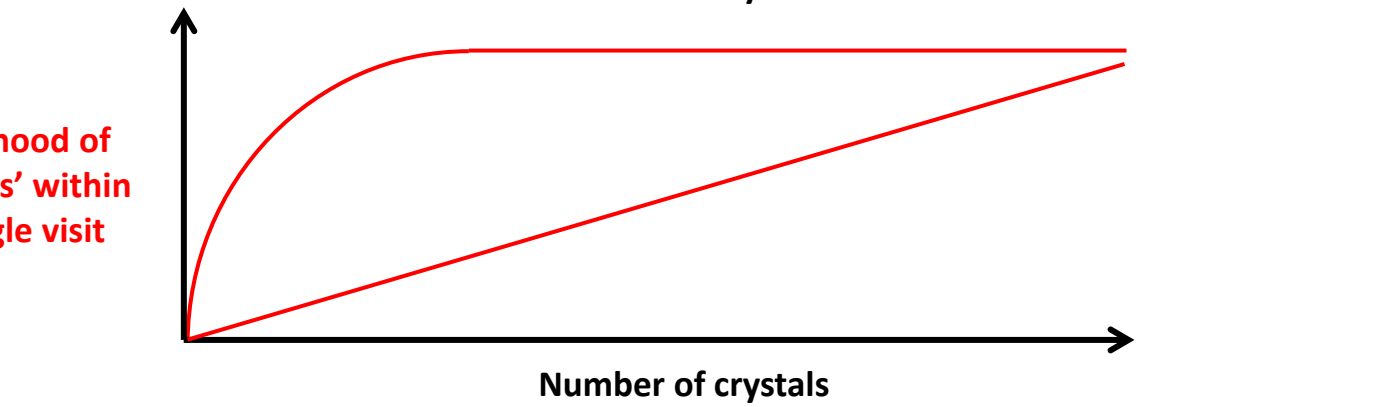
One crystal

High visit frequency

Low visit frequency

A dewar full of crystals (112)





Data collection is always a compromise…

How much data do I need?

What resolution do I need?

What are the data for?

How much time do I have?

How many crystals do I have?

Be prepared!

Think about this **before** your beamtime!

Planning phase:
- estimate feasibility
- cost/benefit analysis
- homology model sufficient?

Target selection

- Experimental data
- Bioinformatics

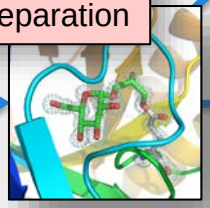
RCSB PDB PROTEIN DATA BANK

Deposition

Alter protein:
- choose ortholog
- truncate
- mutate

Cloning

Figure preparation



Validation & interpretation

+ "other" data

Publication

Alternative expression system?

Expression & purification?

Model building & refinement

Structure solution?

?

Modify protocols (refold?)

Is sample:
- soluble?
- stable?
- pure?

Solve structure by molecular replacement?

Heavy atom soaks?

X-ray data collection?

?

Modify conditions:
- change conc.
- change temp.
- add ligands
- etc...

Hits from crystal trials?

Optimised crystals?

Template structure?

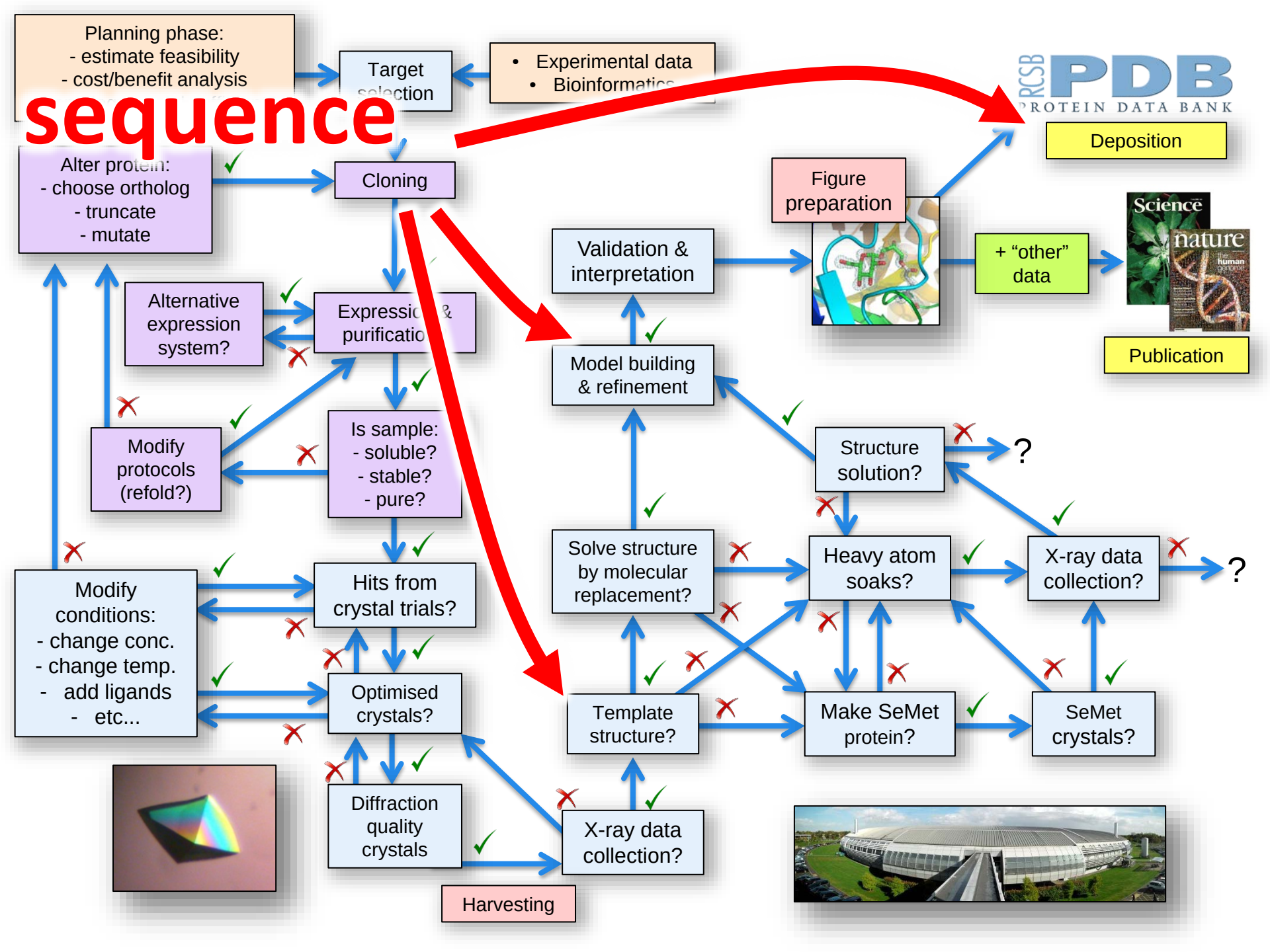
Make SeMet protein?

SeMet crystals?

Diffraction quality crystals

X-ray data collection?

Harvesting


Planning phase:
- estimate feasibility
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Target selection
• Experimental data
• Bioinformatics
sequence
RCSB PDB
PROTEIN DATA BANK
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Science
nature
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Hits from crystal tri...?

- chang...ic.
- change temp.
- add ligands
- etc...

Optimised crystals?

Diffraction quality crystals

Harvesting

X-ray data collection?

Validation & interpretation

Model building & refinement

S...e structure molecular ...placement?

Template structure?

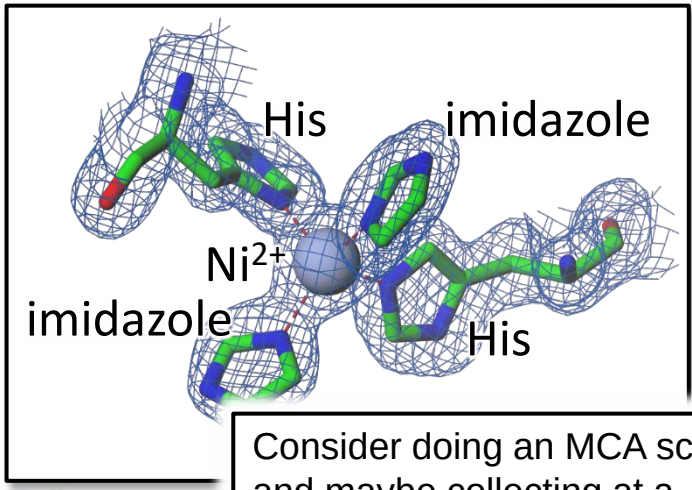
Heavy a... soaks?

Make SeMet protein?

Struct... solutio...

collection?

SeMet crystals?



Consider doing an MCA scan and maybe collecting at a different wavelength – could help with:
- phasing
- map interpretation

potential ligands

Methods

Planning phase:
- estimate feasibility
- cost/benefit analysis
- homology model sufficient?

Target selection

- Experimental data
- Bioinformatics

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+ "other"

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- add ligands
- etc...

Hits from crystal trials?

Optimise crystals?

Template structure?

Make SeMet protein?

Se crystals?

Diffraction quality crystals

X-ray data collection?

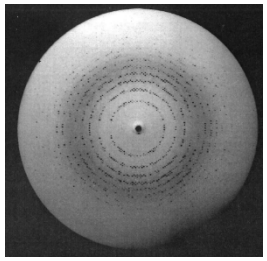
Harvesting

Detector types

hours

readout time

1 ms



Film

Image plate

CCD (charge-coupled device)

360° data sets possible in <10 s!

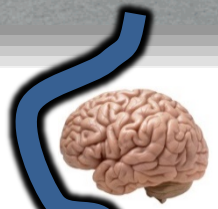
HPC (hybrid photon counting)

1990 2000 2010 2020

MX data collection has become faster…

20th century data collection

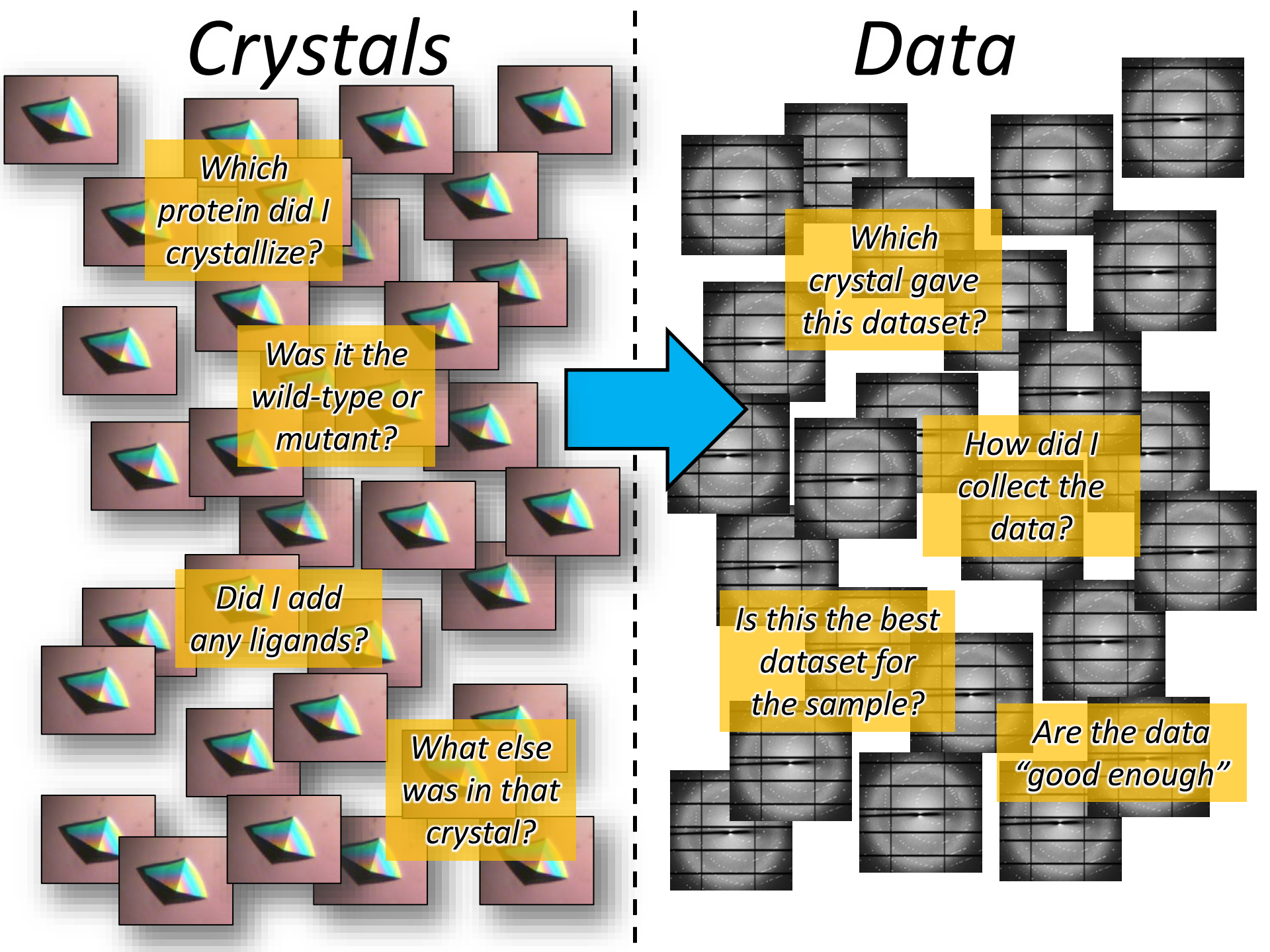
21st century data collection



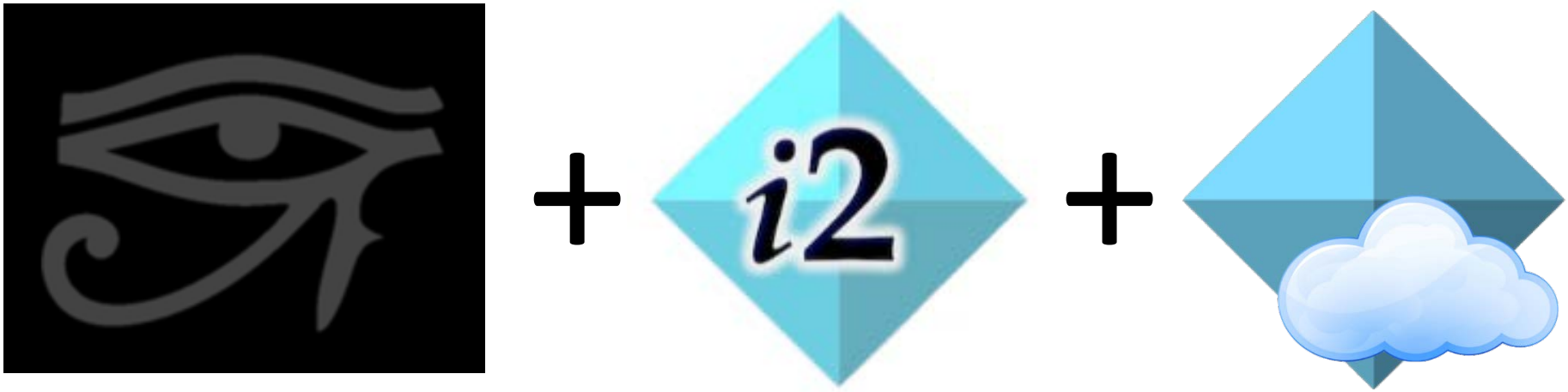
MX data collection has become much faster…

- In principle, could collect one dataset every 5 mins

  (mounting/aligning + evaluating test images + collection)
- In practice, 4 “useful” data sets per hour is good
  - includes screening for “best” crystal
  - …and thinking!
- But - beamtime is still in high demand
  - users are generating crystals more rapidly
  - can get away with “marginal” samples
- Each session is often split between several groups
  - therefore need to be efficient and organised...

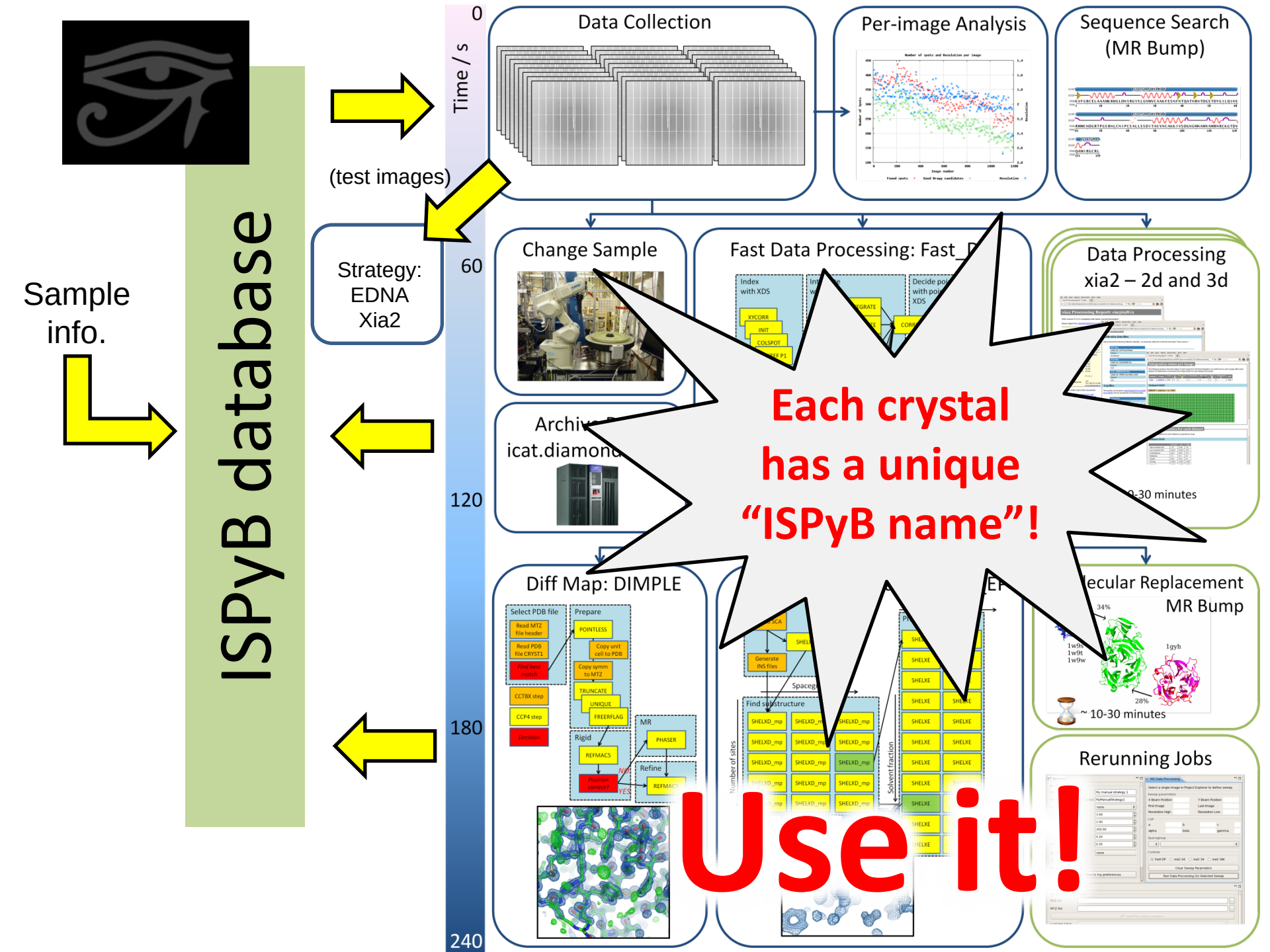

Crystals
Data
Which protein did I crystallize?
Was it the wild-type or mutant?
Did I add any ligands?
What else was in that crystal?
Which crystal gave this dataset?
How did I collect the data?
Is this the best dataset for the sample?
Are the data "good enough"

Taking back control...



ISPyB *CCP4i2* *CCP4 Cloud*

F·R·I·E·N·D·S


Sample info.
ISPyB database
(test images)
Strategy: EDNA Xia2
Time / s
0
60
120
180
240
Data Collection
Per-image Analysis
Sequence Search (MR Bump)
Change Sample
Fast Data Processing: Fast_
Data Processing xia2 – 2d and 3d
Archiv
icat.diamond
Diff Map: DIMPLE
Select PDB file
Prepare
Rigid
MR
Refine
Find substructure
Generate INS files
Rerunning Jobs
Each crystal has a unique "ISPyB name"!
Use it!

Planning phase:
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RCSB PDB PROTEIN DATA BANK

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- mutate

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Figure preparation

Validation & interpretation

+ "other" data

Science

nature

Publication

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- etc...

Hits from crystal trials?

Solve structure by molecular replacement?

Heavy atom soaks?

X-ray data collection?

?

assign

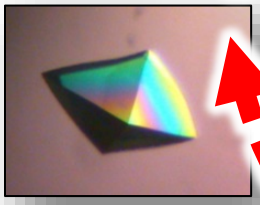
Optimised crystals

Template structure?

Make SeMet protein?

SeMet crystals?

ISPyB



Diffraction quality crystal

X-ray data collection?

name

Harvesting


Date: 29-JUL-2017
Beamline: i03 Diamond
Visit ID: mx13467-41
Protein acronym: NmADH9
ISPyB name: NmADH9_23
Dataset name: NmADH9_23_1
100 µm
100 µm
Beam size: 50.0 × 20.0 µm

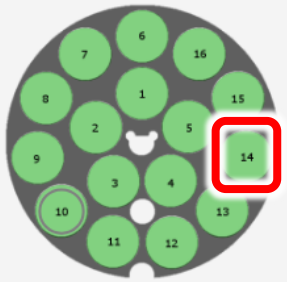
Harvest your crystals and enter sample info into ISPyB

Container: DLS-442

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

This container is currently assigned and in use on a beamline sample changer. Unassign it to make it editable

Shipment	JIC_260717_I03
Dewar	DLS-MX-0002
Container Type	Puck
Registered Container	DLS-442 [View]
Barcode	Click to edit
Automated Collection	+ Queue this container for Auto Collect
Comments	Click to edit



Location History

Date	Status	Location	Beamline
08-09-2017 10:49	at facility		
04-08-2017 15:58	at DLS		
29-07-2017 11:26	processing	7	i03
21-07-2017 12:04	at DLS		

10 ▾ Page « ‹ 1 › »

this is **UNIQUE**

+ Extra Fields

Location	Protein Acronym	Abundance	Components	Name	Spacegroup	Barcode	Comment	Status
9	NmADH9			NmADH9_18				
10	NmADH9			NmADH9_19				
11	NmADH9			NmADH9_20				
12	NmADH9			NmADH9_21				
13	NmADH9			NmADH9_2				
14	NmADH9			NmADH9_23				
15	NmADH9			NmADH9_24				
16	NmADH9			NmADH9_25				

Comment	Anomalous	Required Res	Status
	Zn	1.5	Auto Integrated
	Zn	1.5	Auto Integrated

turns on EP pipelines

Required for UDC

Use a spreadsheet…

crystals_MX13467-41_i03_29-July-2017

Puck number – DLS442

Position	Person	Protein name	IspyB_name	Plate	Well	Conditions	Soak/cryo	Space group	Test	Resolution	Comments
9	Benjy	NmADH9	NmADH9_18	MCBL0004	A11.1	"	Cis cis nepetalactol+ 20%EG				10mM soak for approx 1 h
10	Benjy	NmADH9	NmADH9_19	MCBL0004	A11.1	"	8 oxogeranial+ 20%EG				10mM soak for approx 1 h
11	Benjy	NmADH9	NmADH9_20	MCBL0004	A11.1	"	8 oxogeranial+ 20%EG				10mM soak for approx 1 h
12	Benjy	NmADH9	NmADH9_21	HD01	B6	PEG 4k 29%, 0.1M Mes pH 6.5, 1 mM NAD	8-oxocitronellal+ 20%EG				5mM soak for approx 1.5 h
13	Benjy	NmADH9	NmADH9_22	HD01	B4	"	8-oxocitronellal+ 20%EG				5mM soak for approx 1.5 h
14	Benjy	NmADH9	NmADH9_23	HD01	B3	"	Cis cis nepetalactone+ 20%EG				5mM soak for approx 1.5 h
15	Benjy	NmADH9	NmADH9_24	HD01	B2	"	Cis cis nepetalactol+ 20%EG				5mM soak for approx 1.5 h
16	Benjy	NmADH9	NmADH9_25	HD01	B1	"	8 hydroxygeraniol+ 20%EG				5mM soak for approx 1 h

annotate hardcopy during data collection – helps decision making

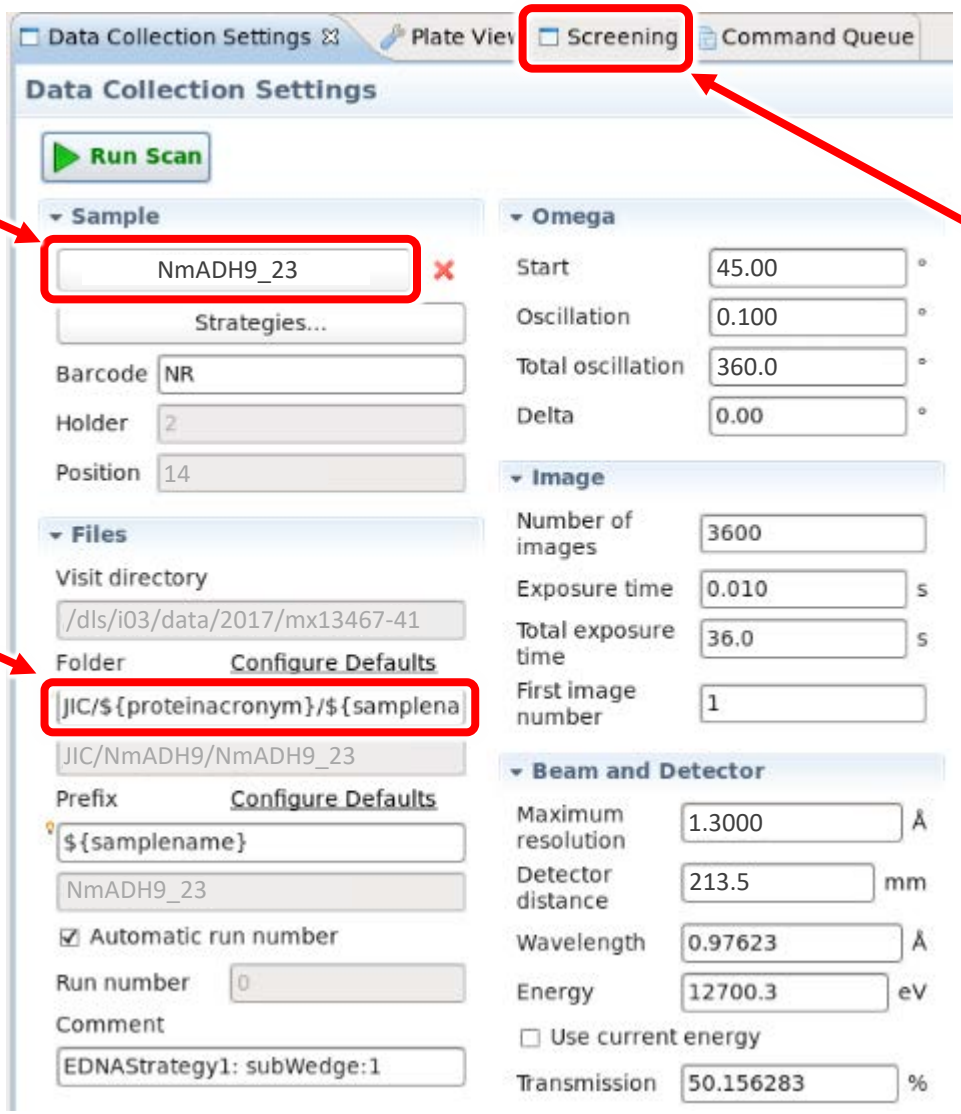
Data collection setup in GDA

Select required sample from drop-down menu:

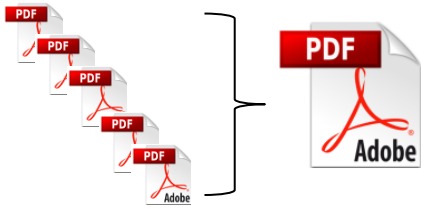
- no need to enter sample information or specify sample location
- less likely to get the wrong sample

Put your data into your own directory....

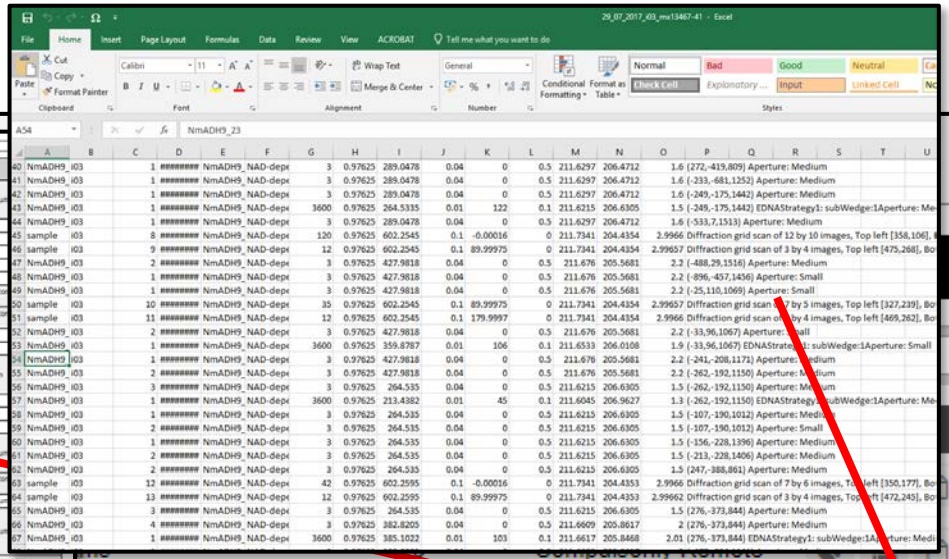
...especially important if there are multiple users from several institutions – simplifies backing up too....



use the "screening" tab for test images – keeps them separate from datasets



⇦ simple to search this for an ISPyB name

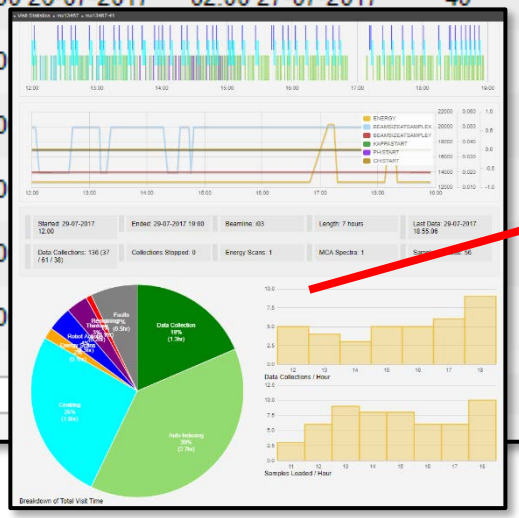


Visit List

This page lists the

Start						
19:00 15-09-2017						
02:00 11-09-2017						
10:00 05-08-2017					395	
12:00 29-07-2017	19:00 29-07-2017	41	i03	Dr Katherine McAuley	136	Compulsorily Remote
19:00 26-07-2017	02:00 27-07-2017	40	i03	Mr Mark Williams	71	Compulsorily Remote
02:0			i03	Dr Neil Paterson	38	Compulsorily Remote
17:0			i03	Dr Neil Paterson	76	
19:0			i04	Dr Melanie Vollmar	69	Compulsorily Remote
12:0			i04	Dr Dave Hall	106	Compulsorily Remote
02:0			i03	Dr Neil Paterson	82	Compulsorily Remote

10 5 6 7 › »



What you did...

(1) ISPyB interface

(2) Visit PDF (combine with others...)

mx13467-41 on i03 at 29-07-2017 12:00

Sample	Images	Res	λ	Ω Osc	Spacegroup	Unit Cell	Processed Resolution	Rmeas	Completeness	Comments
NmADH9_23	3600	1.3	0.9763	0.10	P 1 2 1	63.92, 107.75, 69.36 90.00, 104.27, 90.00	29.77 - 1.5 29.77 - 6.7 1.54 - 1.5	0.085 0.036 0.824	98.8 98.7 96.6	(-262,-192,1150) EDNAStrategy1: subWedge:1Aperture: Medium

(3) Visit Excel sheet (annotate...)

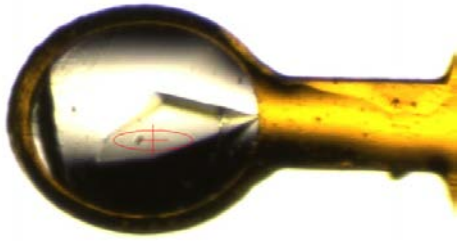
	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T	
1		mx13467-41_i03_29-JUL-2017 - 7 hr - Pilatus3 6M detector (100 Hz)																			
2																					
3	data	Image prefix	Run	Sta	Sam	Prot	# imag	Wavele	Dista	Exp.	Phi st	Phi ra	Xbea	Ybea	Dete	auto/m	resoln	space gr	cell	twinnin	comments
54		NmADH9_23	2	##	NmA	NAD	3	0.9763	428	0.04	0	0.5	212	206	2.2						
55		NmADH9_23	3	##	NmA	NAD	3	0.9763	265	0.04	0	0.5	212	207	1.5						
56	12	NmADH9_23	1	##	NmA	NAD	3600	0.9763	213	0.01	45	0.1	212	207	1.3	a/3dii	1.37	P21	64 108 69 / 90 104 90	2.09	Binary complex with NAD - best data so far
57		NmADH9_24	1	##	NmA	NAD	3	0.9763	265	0.04	0	0.5	212	207	1.5						
58		NmADH9_24	2	##	NmA	NAD	3	0.9763	265	0.04	0	0.5	212	207	1.5						

Ideal scenario during session:

- Load first sample
- Collect test images
- Based on these, decide:
  - to collect...
  - not to collect...
  - to revisit later...
- For a “suitable” sample:
  - devise a data collection strategy
  - collect data set
- Analyse data as they are collected
- Based on this analysis, revise plans if appropriate
- Move onto next sample…

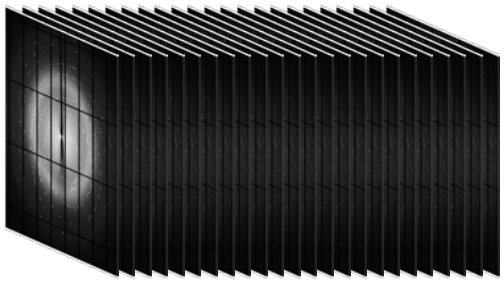
– not practical without automation

robotic sample exchange



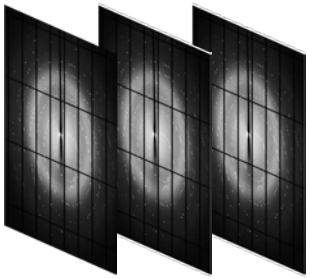
align crystal in X-ray beam

analyse data on-the-fly



typically 3,600 x 0.1° images

collect dataset



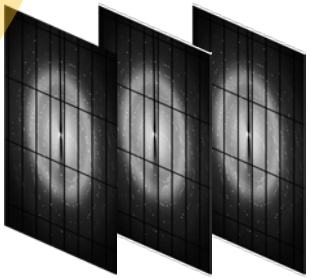
collect test images

devise data collection strategy based on test images (and what you want to use the data for)

Don't forget to think!

robotic sample exchange

align crystal in X-ray beam

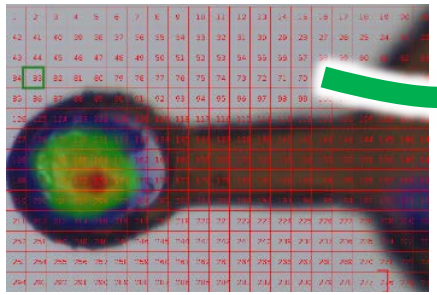


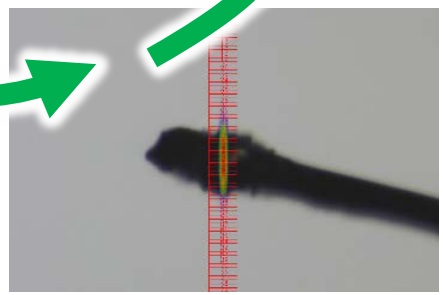
collect test images

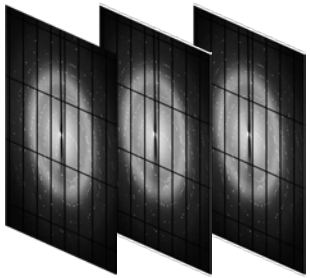
More efficient to screen your samples in batches,

then decide what to do…

- do this automatically with X-ray centring
- also an opportunity to grab a coffee!

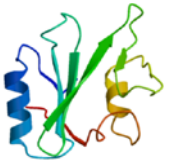






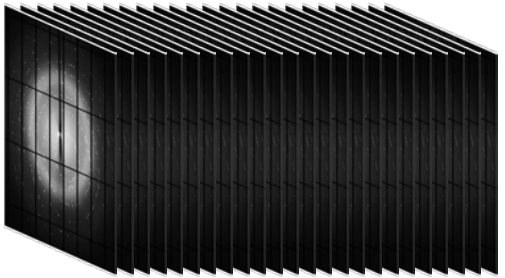
test images

before session...



template

sequence



dataset

< 1 min

Strategies:
Mosflm
EDNA
Xia2

ISPyB

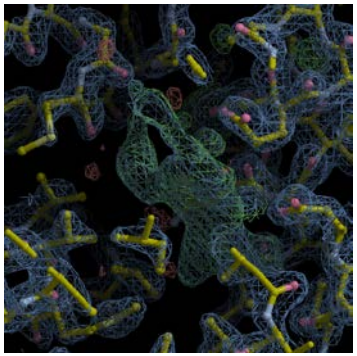
< 2 min

Fast DP

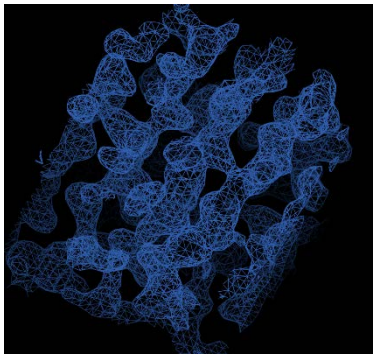
h	k	l	Iplus	SIGIplus	Iminus	SIGIminus
-45	0	4	-1.00	1.20	-1.00	1.20
-45	0	5	-0.03	1.82	-0.03	1.82
-45	0	6	2.17	2.01	2.17	2.01
-45	0	7	-0.22	1.24	-0.22	1.24
-45	0	8	0.63	1.33	0.63	1.33
-45	0	9	1.46	1.40	1.46	1.40
-45	0	10	0.11	1.34	0.11	1.34
-45	0	11	2.02	1.41	2.02	1.41

< 5 min

Quick feedback

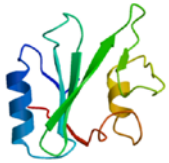


Dimple

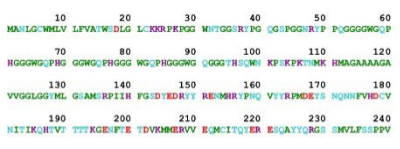


Fast EP

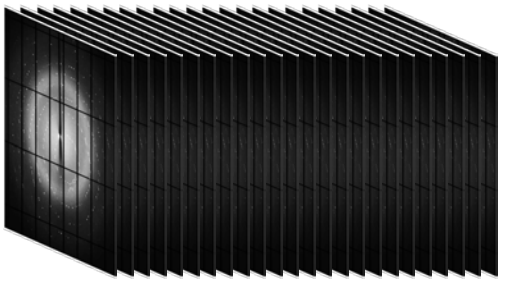
before session...



template



sequence



dataset

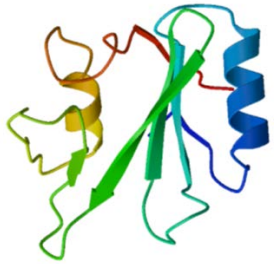
ISPyB

20-30 min

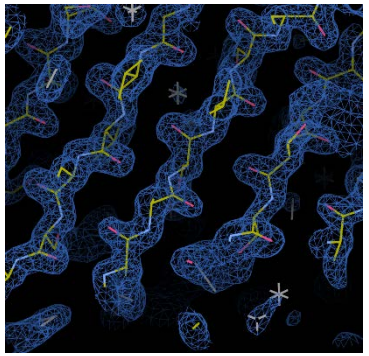
Xia2
DIALS
MultiXia2
autoPROC

h	k	l	Iplus	SIGIplus	Iminus	SIGIminus
-45	0	4	-1.00	1.20	-1.00	1.20
-45	0	5	-0.03	1.82	-0.03	1.82
-45	0	6	2.17	2.01	2.17	2.01
-45	0	7	-0.22	1.24	-0.22	1.24
-45	0	8	0.63	1.33	0.63	1.33
-45	0	9	1.46	1.40	1.46	1.40
-45	0	10	0.11	1.34	0.11	1.34
-45	0	11	2.02	1.41	2.02	1.41

hours



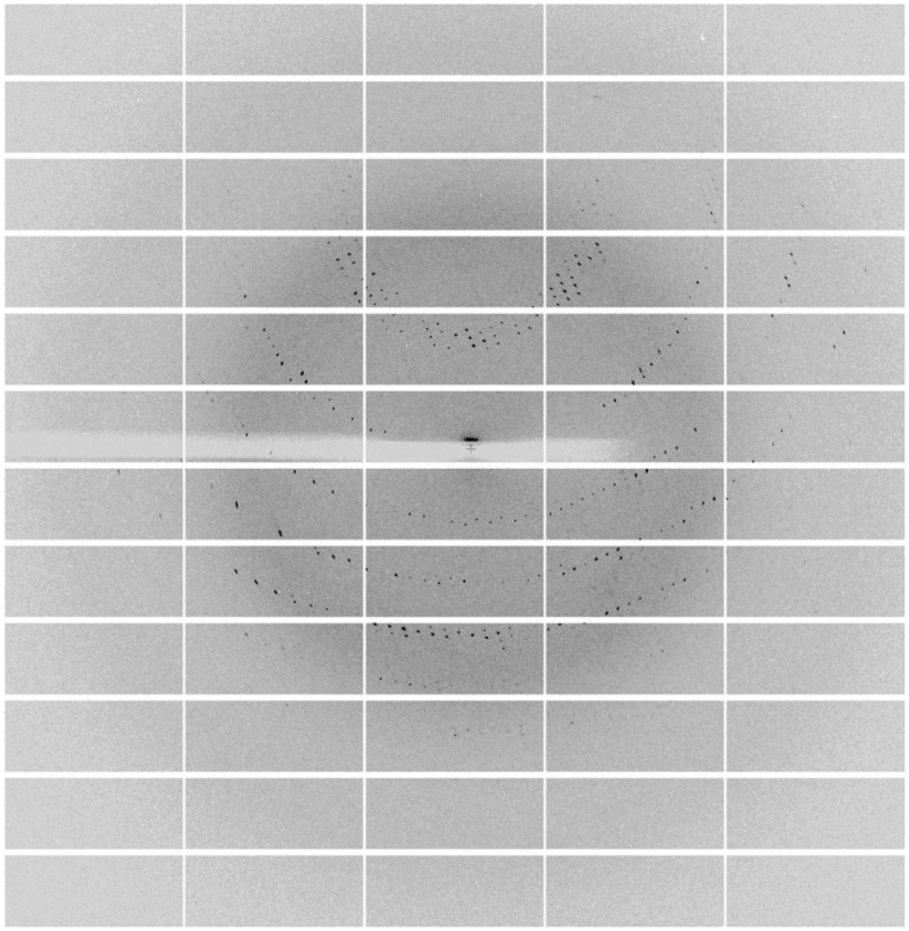
MrBUMP

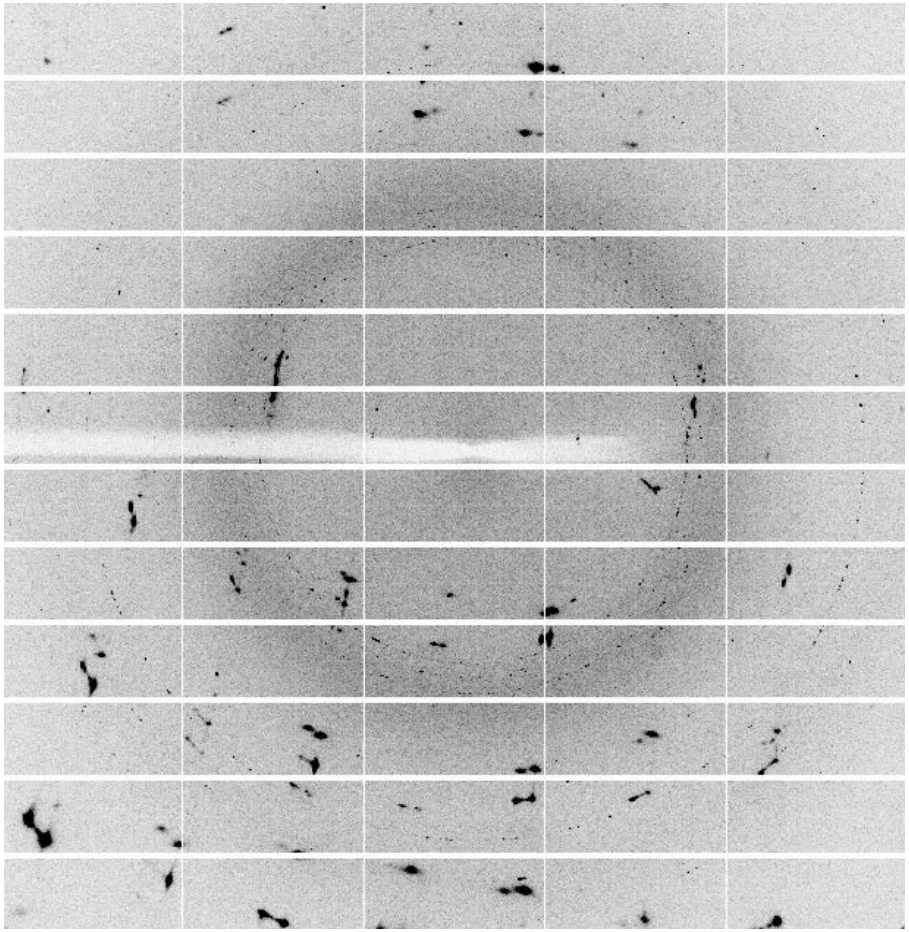


Big EP

Slower feedback

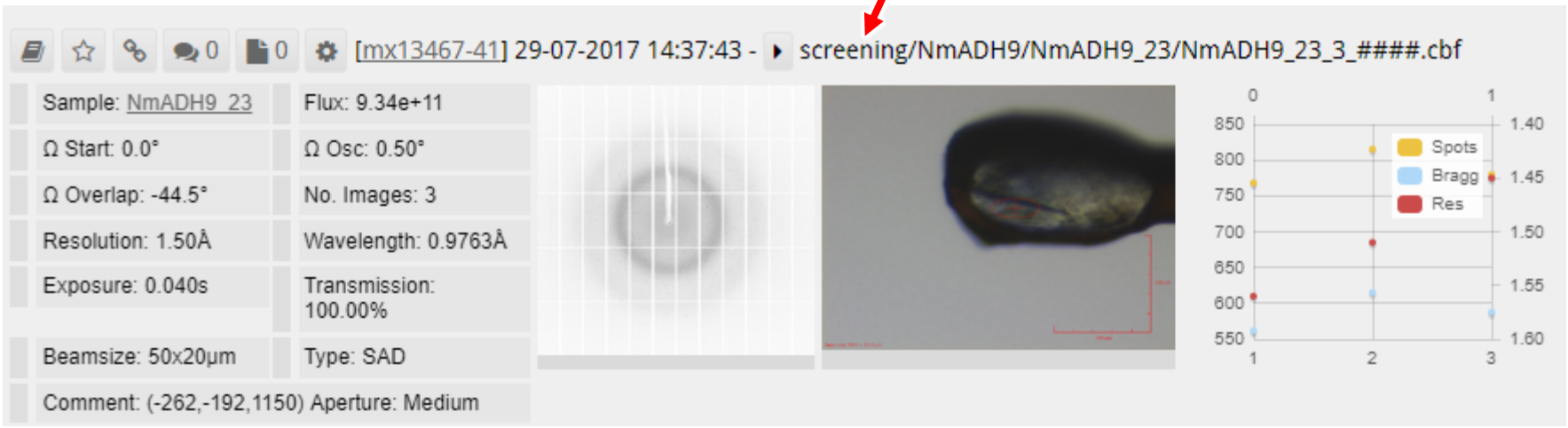
LOOK at your images!!!!



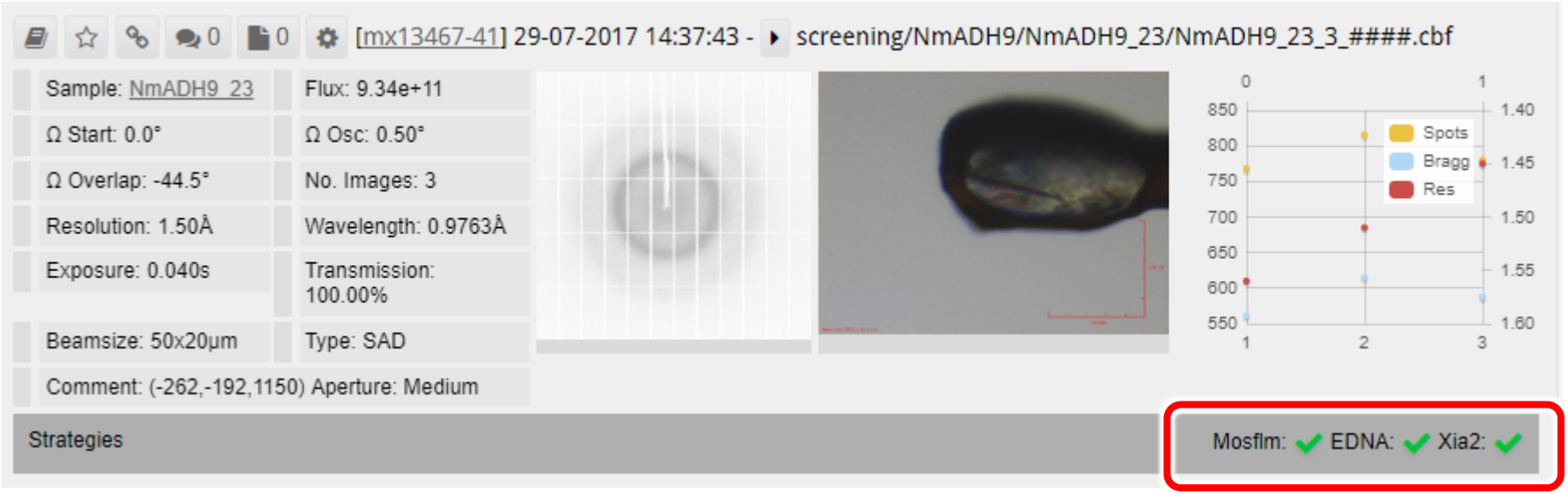


Screening…

(using the “screening” tab...)



Screening…


0
0
[mx13467-41] 29-07-2017 14:37:43 - screening/NmADH9/NmADH9_23/NmADH9_23_3_####.cbf
Sample: NmADH9_23
Flux: 9.34e+11
Ω Start: 0.0°
Ω Osc: 0.50°
Ω Overlap: -44.5°
No. Images: 3
Resolution: 1.50Å
Wavelength: 0.9763Å
Exposure: 0.040s
Transmission: 100.00%
Beamsize: 50x20µm
Type: SAD
Comment: (-262,-192,1150) Aperture: Medium
0
1
850
800
750
700
650
600
550
1.40
1.45
1.50
1.55
1.60
1
2
3
Spots
Bragg
Res
Strategies
Mosflm:
EDNA:
Xia2:

Screening…

Have I seen this crystal form before?

Strategies — Mosflm: ✔ EDNA: ✔ Xia2: ✔

xia2.strategy

Space Group	A	B	C	α	β	γ
P 1 2 1	63.87	107.69	69.31	90.00	104.25	90.00

Lookup Cell

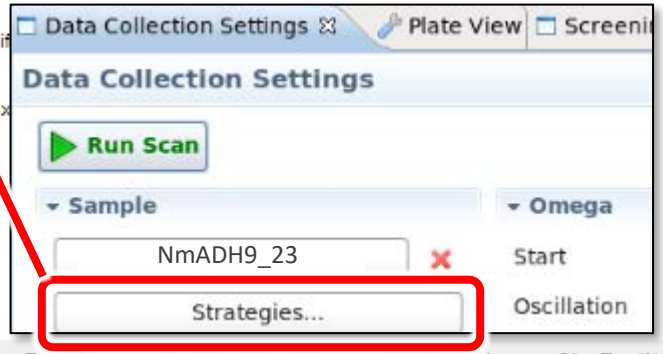
Strategy	Description	Ω Start	Ω Osc	Res (Å)	Ranking Res	Rel Trn (%)	Abs Trn (%)	Exposure (s)	No. Images
anomalous Wedge1	Standard Anomalous Dataset Multiplicity=3 I/sig=2 202s	0	0.15	1.51	1.1	4.0	4	0.010	2214
gentle Wedge1	Gentle: Target Multiplicity=2 I/sig=2 Maxlifespan=20s	6	0.15	1.51	1.2	4.0	4	0.010	2000
high multiplicity Wedge1	Strategy with target multiplicity=16 I/sig=2 202s	0	0.15	1.51	1.1	4.1	4.1	0.010	2400
native Wedge1	Standard Native Dataset Multiplicity=3 I/sig=2 Maxlifespan=202s	162	0.15	1.51	1.2	2.2	2.2	0.010	1947

EDNA MXv1

Space Group	A	B	C	α	β	γ
P2	63.99	107.49	69.28	90.00	104.37	90.00

Lookup Cell

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 Maxlifespan=202 s	45	0.10	1.51	1.21	11.0	11	0.010	1630
Strategy2 Wedge1	Standard Anomalous Dataset Multiplicity=3 I/sig=2 Maxlifespan=202 s	78	0.10	1.51	1.24	12.4	12.4	0.010	2740
Strategy3 Wedge1	strategy with target multiplicity=16, target I/sig=2 Maxlifespan=202 s						5.1	0.010	3600
Strategy4 Wedge1	Gentle: Target Multiplicity=2 and target I/Sig 2 and Maxlifespan=202 s						14.8	0.010	1110
Strategy5 Wedge1	UnderDEV Anomalous Dataset, RadDamage of standard						12.4	0.010	2740



mosflm

Space Group	A	B	C	α	β	γ
P2	63.80	107.65	69.44	90.00	104.13	90.00

Lookup Cell

Strategy	Description	Ω Start	Ω Osc	Res (Å)	Ranking Res (Å)	Rel Trn (%)	Abs Trn (%)	Exposure (s)	No. Images
anomalous Wedge1		196	0.20	1.46	0.00	0.0	0	0.000	525
native Wedge1		211	0.20	1.46	0.00	0.0	0	0.000	525

Notes about strategies…

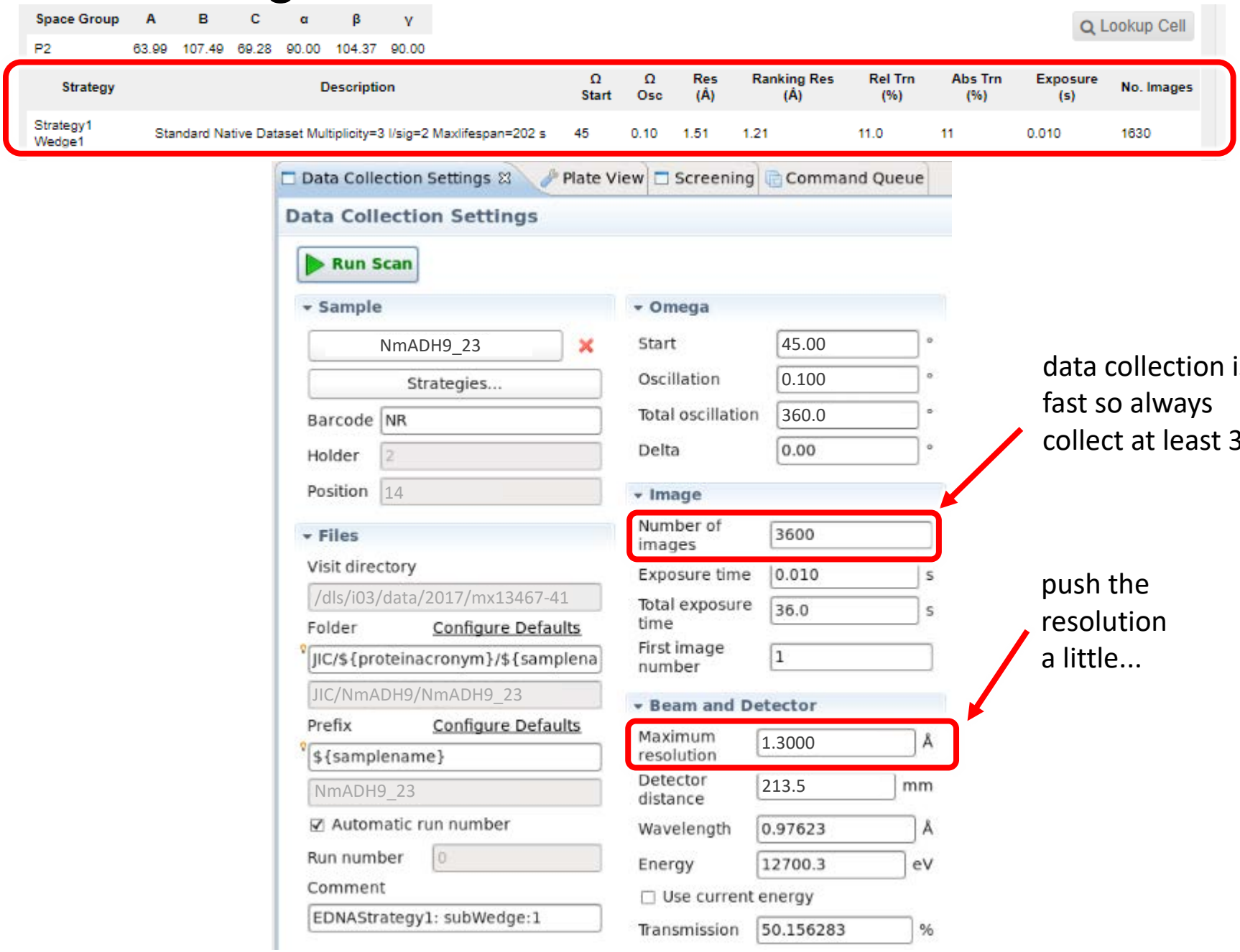
Despite what the strategy programs may suggest (or your supervisor/colleague!)…

- always collect a minimum of 360° (unless you have a very good reason not to)
- consider multiple 360° passes if you have low symmetry (ideally rotating around a different axis for each – see data collection talks…)

If you can't get a sensible strategy and the crystal is diffracting reasonably well…

- collect a data set anyway – it might be useful!
  - inspect screening images in ADXV (may need to sum several adjacent images)
  - look for highest resolution spots (NOT ice or salt spots!)
  - subtract 0.5 from this resolution value. E.g. spots at 2.5 Å → collect to 2.0 Å
  - collect 3600 x 0.1° images with a total dose of 1-2 MGy

Collecting a dataset…



data collection is fast so always collect at least 360°

push the resolution a little...

Checking the results…

Checking the results…

Auto Processing — Fast DP: ✔ Xia2: ✔ ✔ ✔ MultiXia2: ? ? autoPROC: ✔

Type	Resolution	Spacegroup	Mn<I/sig(I)>	Rmeas Inner	Rmeas Outer	Completeness	Cell	Status
fast_dp	29.77 - 1.50	P 1 2 1	15.2	0.036	0.824	98.8	63.92 107.75 69.36 90.00 104.27 90.00	
xia2 3d	28.52 - 1.37	P 1 21 1	10.9	0.038	1.688	98.4	63.92 107.75 69.36 90.00 104.27 90.00	
xia2 3dii	42.04 - 1.37	P 1 21 1	10.8	0.038	1.685	98.5	63.92 107.75 69.36 90.00 104.27 90.00	
xia2 dials	107.77 - 1.30	P 1 21 1	8.9	0.039	1.753	98.2	63.94 107.77 69.37 90.00 104.26 90.00	
autoPROC 1.0.5 (see: http://www.globalphasing.com/autoproc/)	107.76 - 1.50	P 1 21 1	13.3	0.038	0.877	98.8	63.93 107.76 69.37 90.00 104.26 90.00	

fast_dp | xia2 3d | xia2 3dii | xia2 dials | autoPROC 1.0.5 (see: http://www.globalphasing.com/autoproc/)

Plots | Archive | Logs & Files | Lookup Cell

Beam Centre	X	Y
Start	211.60	206.96
Refined	211.50	206.92
Δ	0.10	0.04

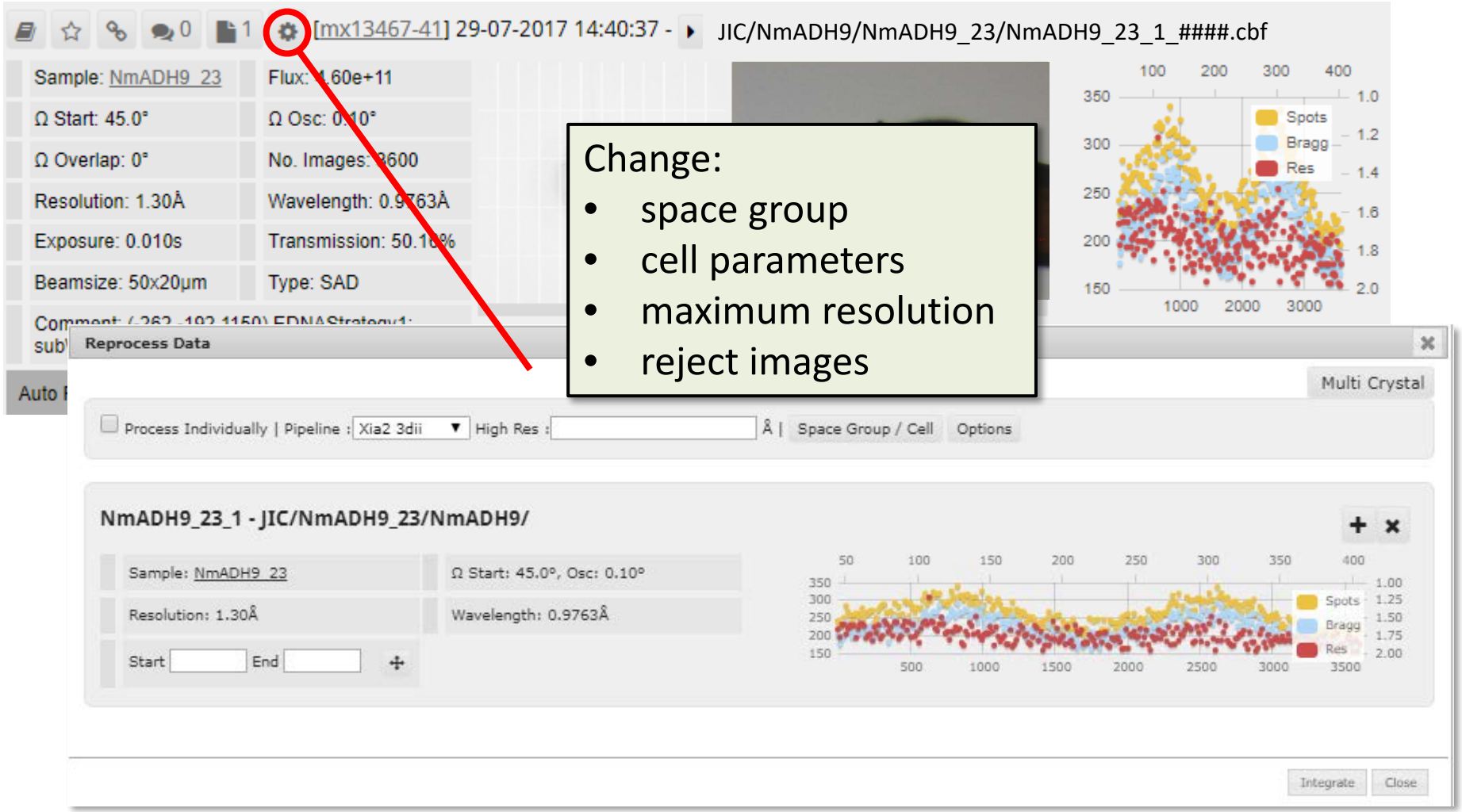
Space Group	A	B	C	α	β	γ
P 1 21 1	63.92	107.75	69.36	90.00	104.27	90.00

Shell	Observations	Unique	Resolution	Rmeas	I/sig(I)	CC Half	Completeness	Multiplicity	Anom Completeness	Anom Multiplicity	CC Anom
outerShell	64205	9220	1.37 - 1.39	1.685	1.1	0.5	96.7	7.0	96.0	3.5	0.0
innerShell	64845	9660	3.72 - 42.06	0.038	44.2	1.0	99.9	6.7	98.6	3.5	0.1
overall	1285570	187412	1.37 - 42.04	0.099	10.8	1.0	98.5	6.9	98.0	3.5	0.1

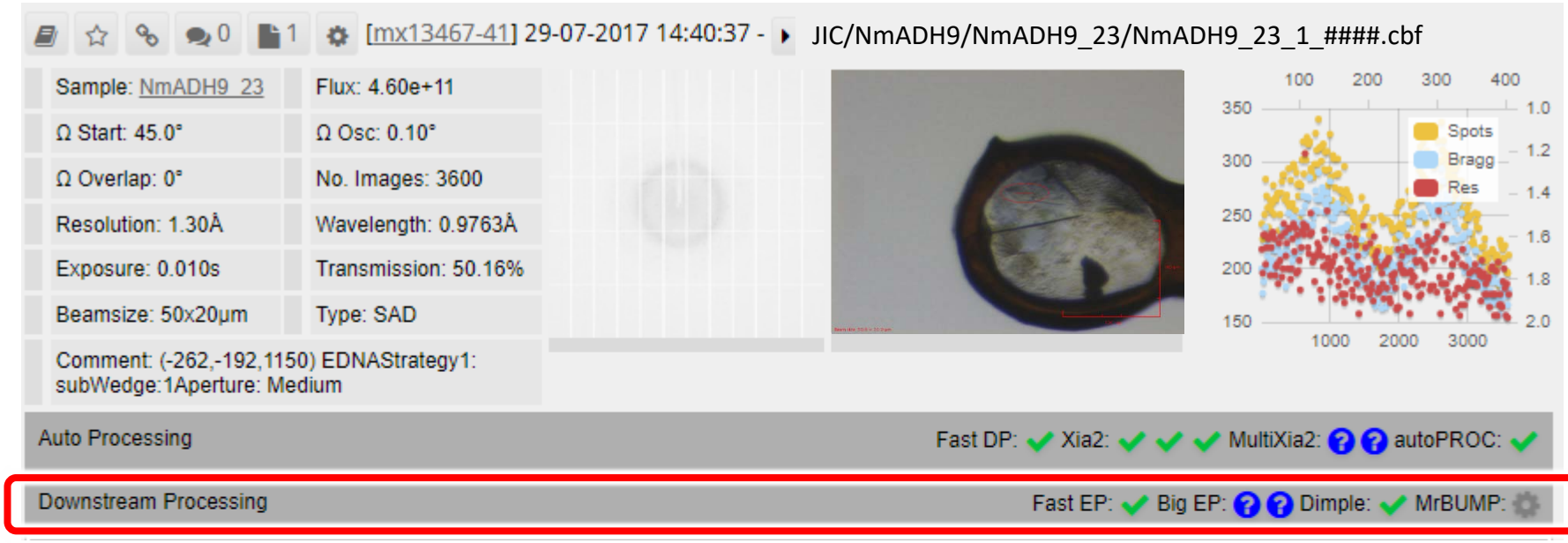
N.B. space group is only a hypothesis at this stage! – see talk(s) about data processing

Re-running jobs:

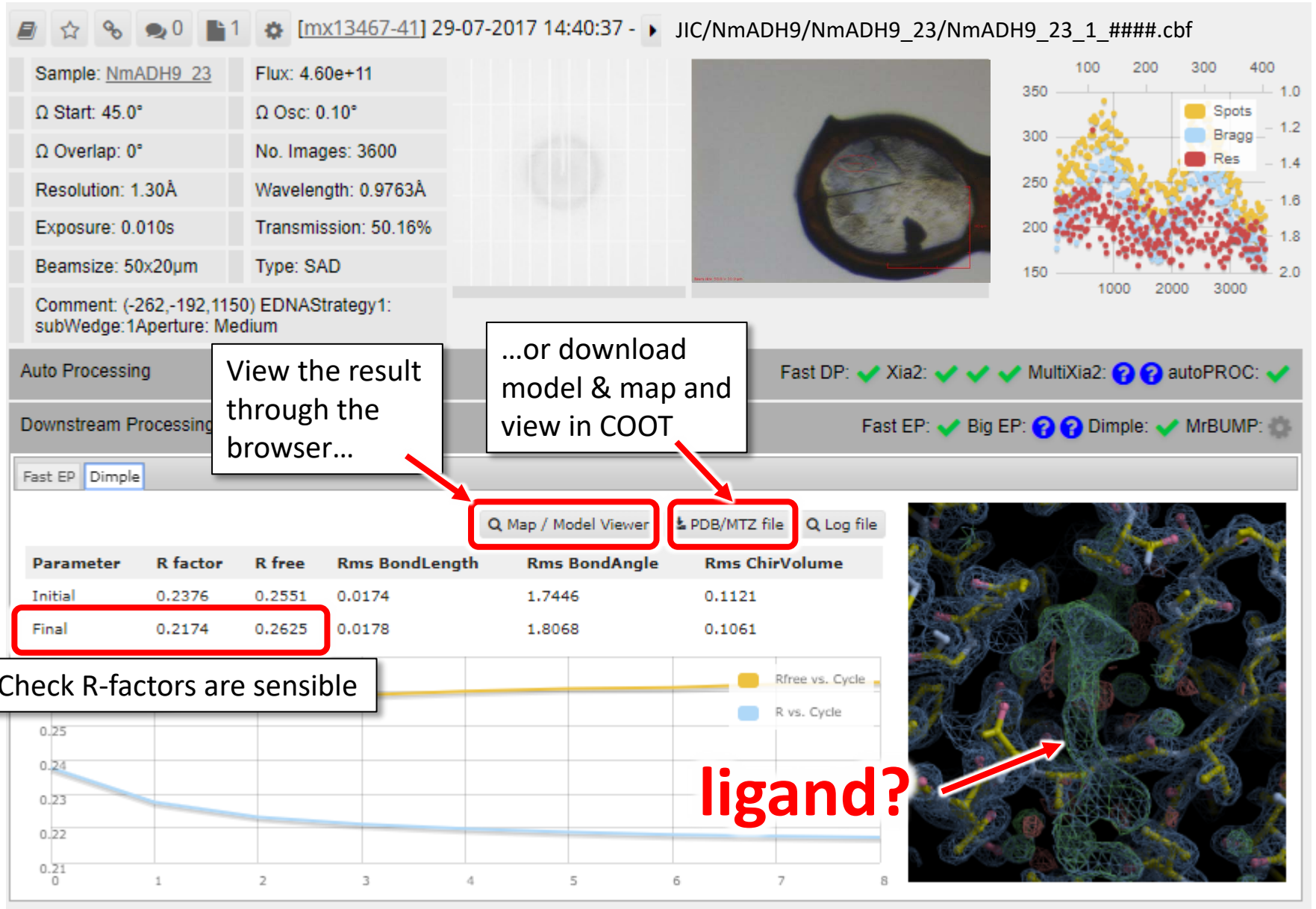
- Most pipelines will run from the command line (Terminal window)
- Also through ISPyB interface...



Checking the results…



Checking the results…



View the result through the browser…

…or download model & map and view in COOT

Check R-factors are sensible

Ideal scenario after session:

- Each data set characterised as:
  - useful/may be useful/not useful
- Some datasets processed to your satisfaction
- You may have interpretable experimental maps
- You may have preliminary structures
- You **will** have less follow-up work to do!

What to do with all the data...

Raw data (images)
- removed from disk after 40 days – still available through TopCAT (tape archive)

"Meta" data – all the other "stuff" – removed from disk after 40 days – not backed up

>90% of useful datasets derived from **Meta data** rather than going back to **Raw data**

...just be thankful it's not cryo-EM!

Getting your data home…

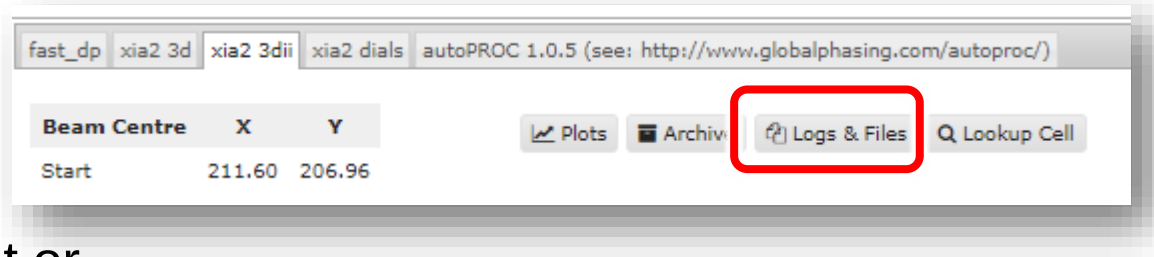
- FTP data home (use an App or a script)

Quite slow...

globus

Faster...

In the meantime:

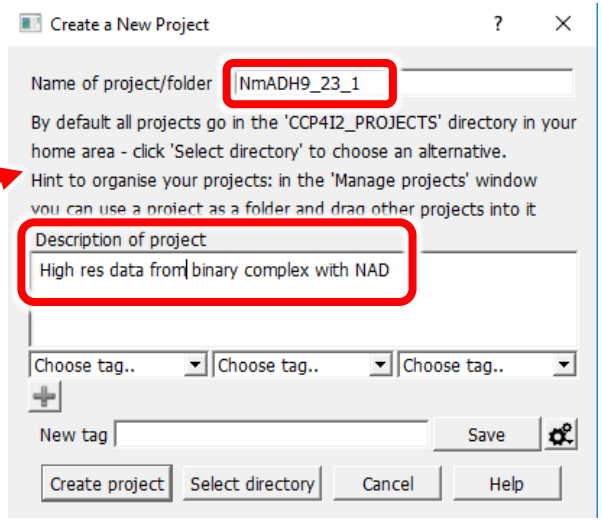


- use autoprocessing output or...
- (re)process data remotely on DLS computers and transfer output only
- copy and archive raw data later

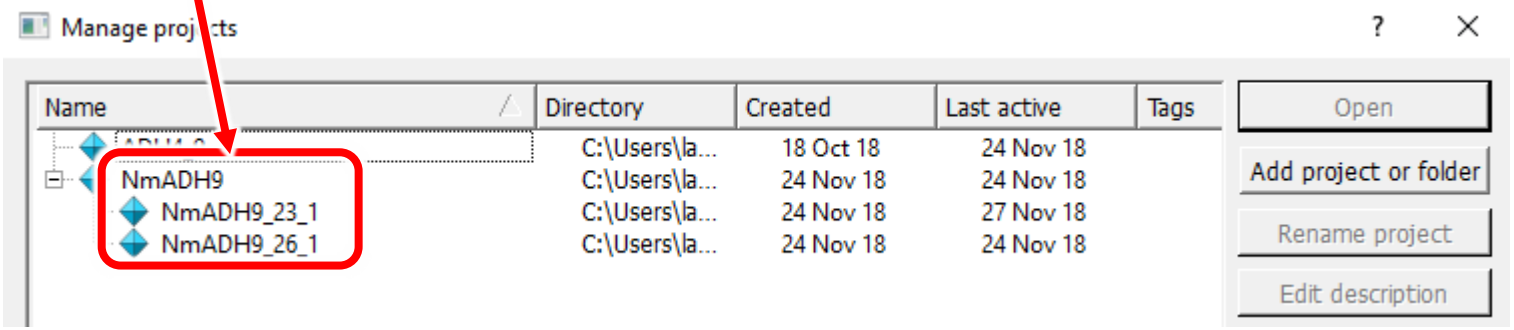
Retain ISPyB name in CCP4i2...

CCP4i2

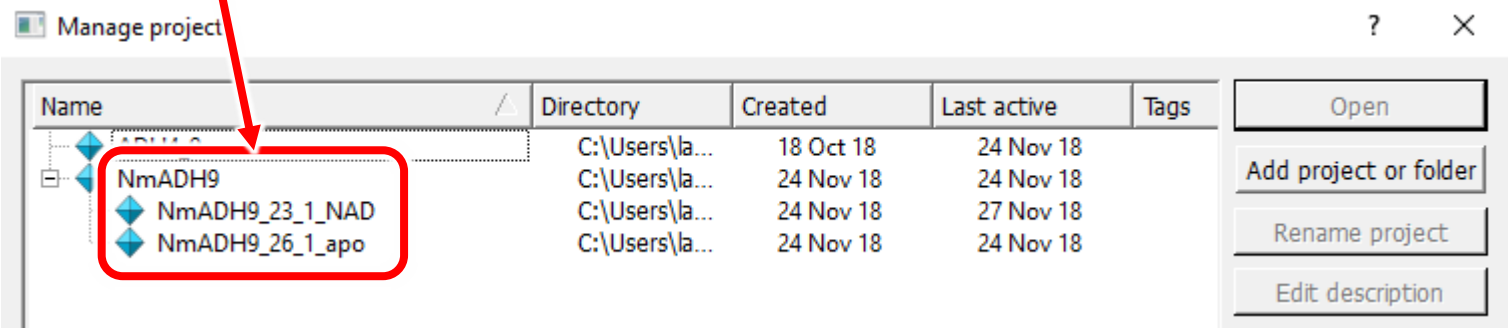
Create a separate "project" for each dataset



If you have more than one dataset for a given protein – create a separate "dummy project" and group the "dataset projects" under this:



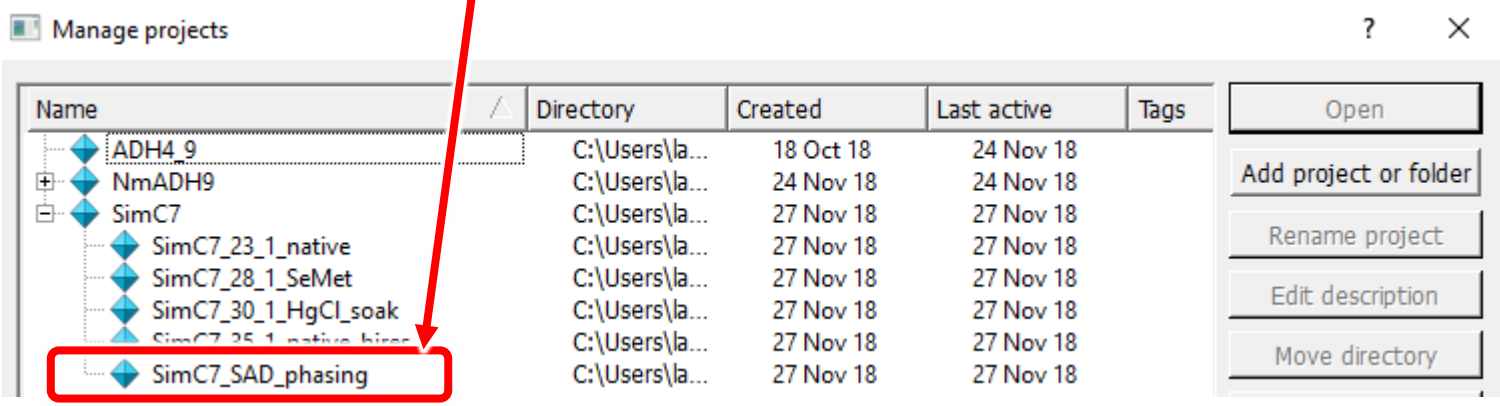
Can rename "projects" later... (when you know more...)*



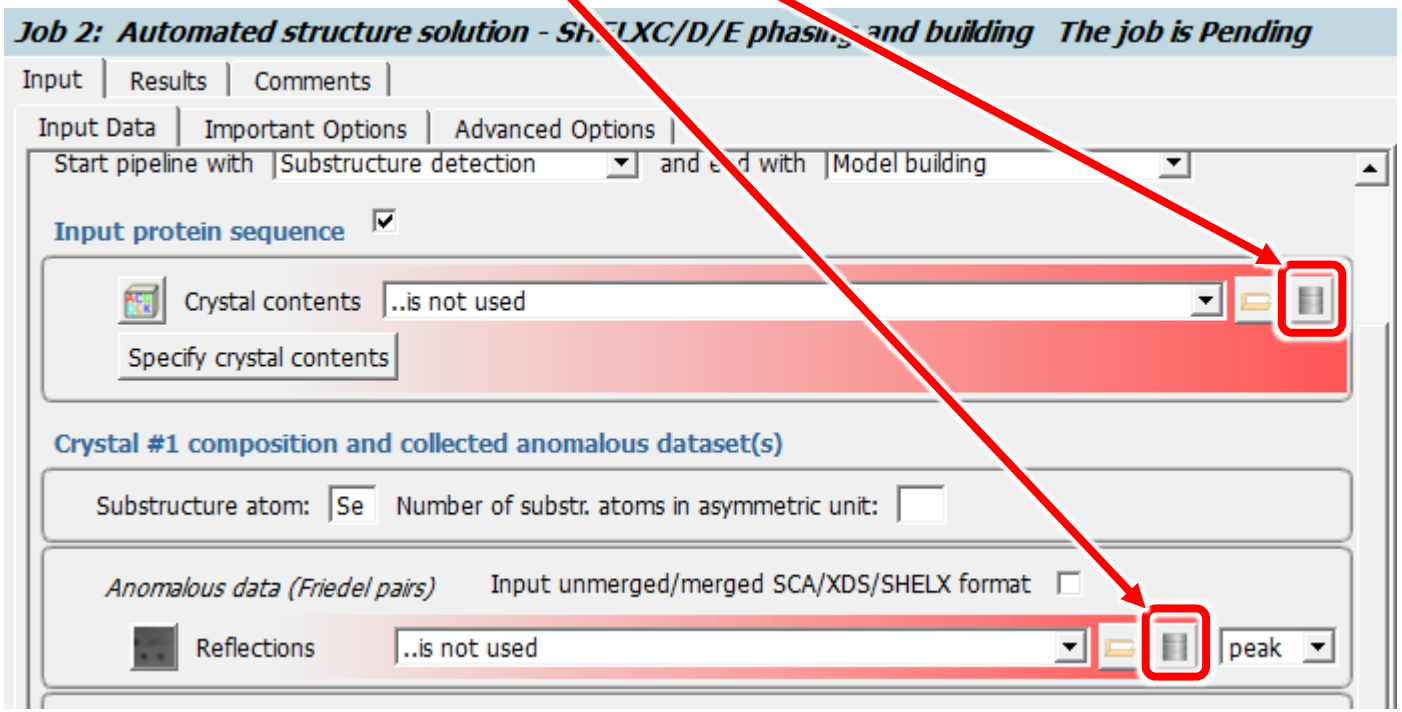
*but directory names remain the same

CCP4i2

Could create “non-dataset projects” for specific activities such as phasing...

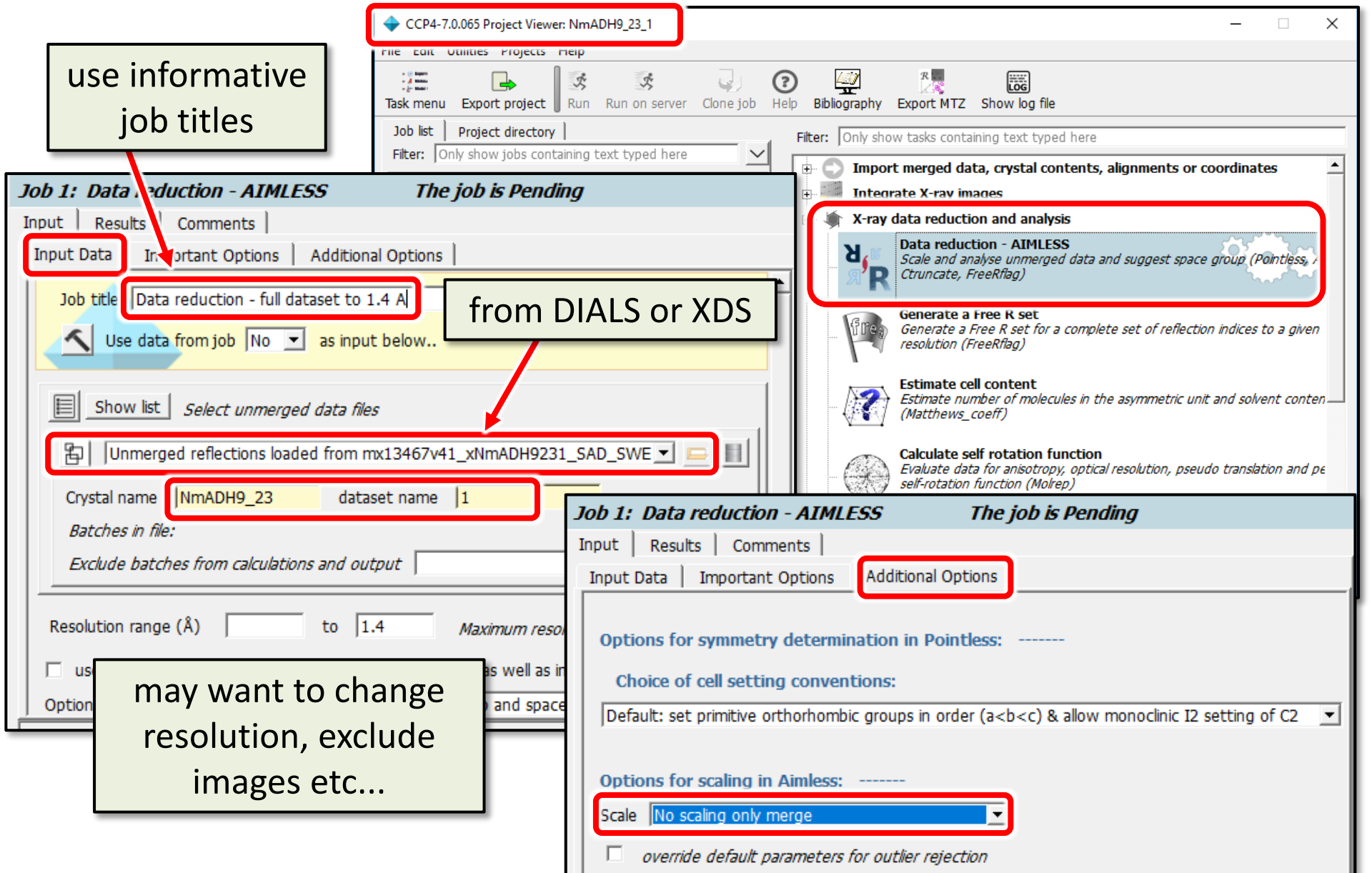


...then “borrow” files from other projects...



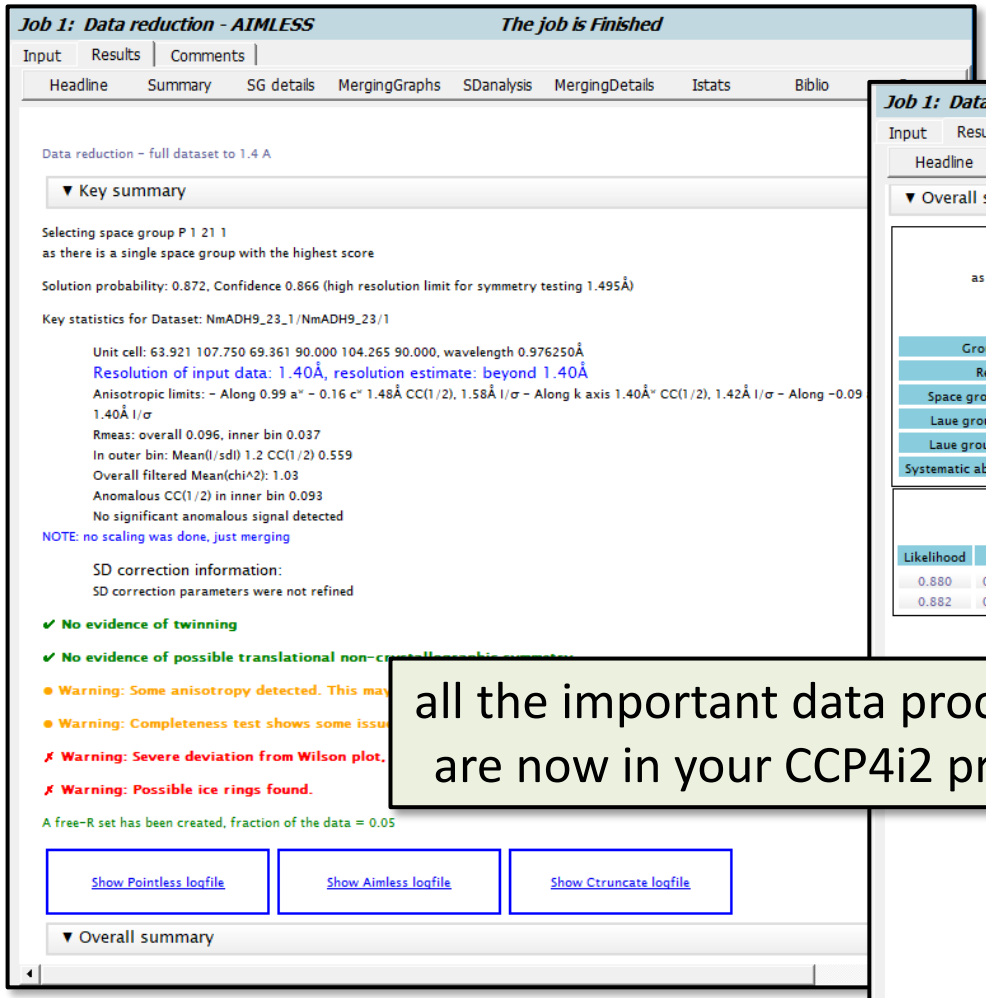
My preferred option for processing...

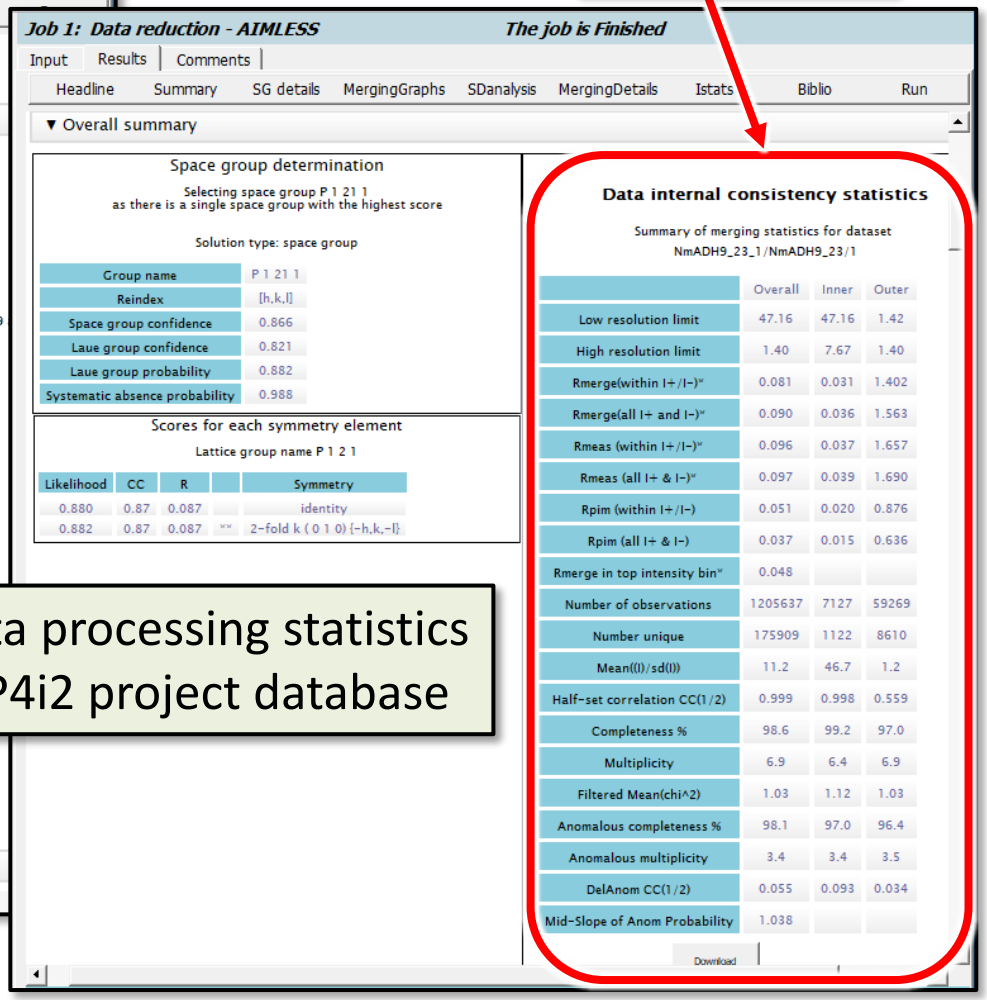
- where the pipelines have done a good job – take part-processed dataset (from the "Meta" data) and re-run the merging step in CCP4i2



Gives lots of output – useful for troubleshooting...

for your paper/thesis





all the important data processing statistics are now in your CCP4i2 project database

...or reprocess from scratch using DIALS or XDS…

Summary - why use ISPyB & pipelines?

- Faster sample changing (select by ISPyB name)
  - essential for remote…
- Informs the decision making process
  - make decisions sooner
  - revise strategy on the fly
    - (e.g. recollect dataset x... no more data required for project y...)
  - make better overall use of beamtime
- Reduces amount of post-beamtime follow-up work
- Simple to keep track of your samples and data

Remote data collection

not going to cover unattended data collection (UDC)…

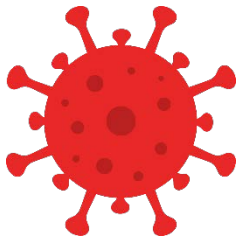
During the lockdowns…
remote data collection?
it's a no-brainer!

remote users
since 2010…

On-site data collection can be a big time commitment…

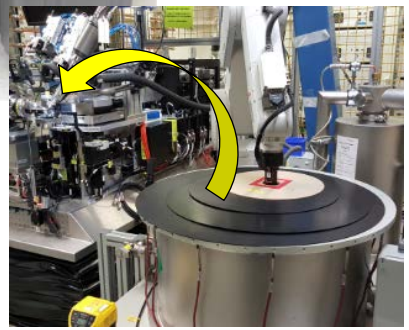
Remote data collection saves you time…

…and the planet



…and is covid-secure

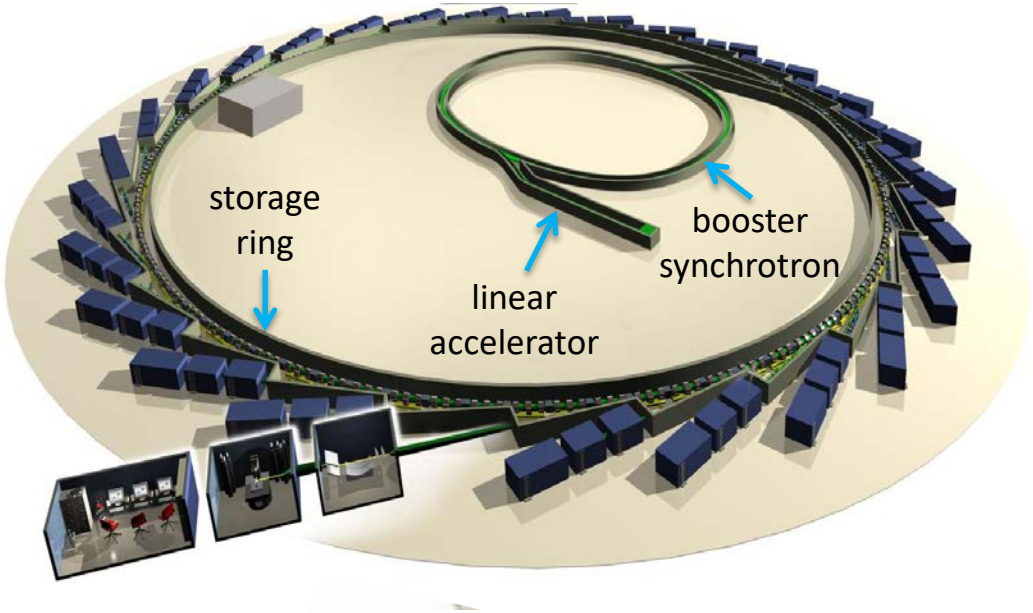
For routine data collection at 100 K:

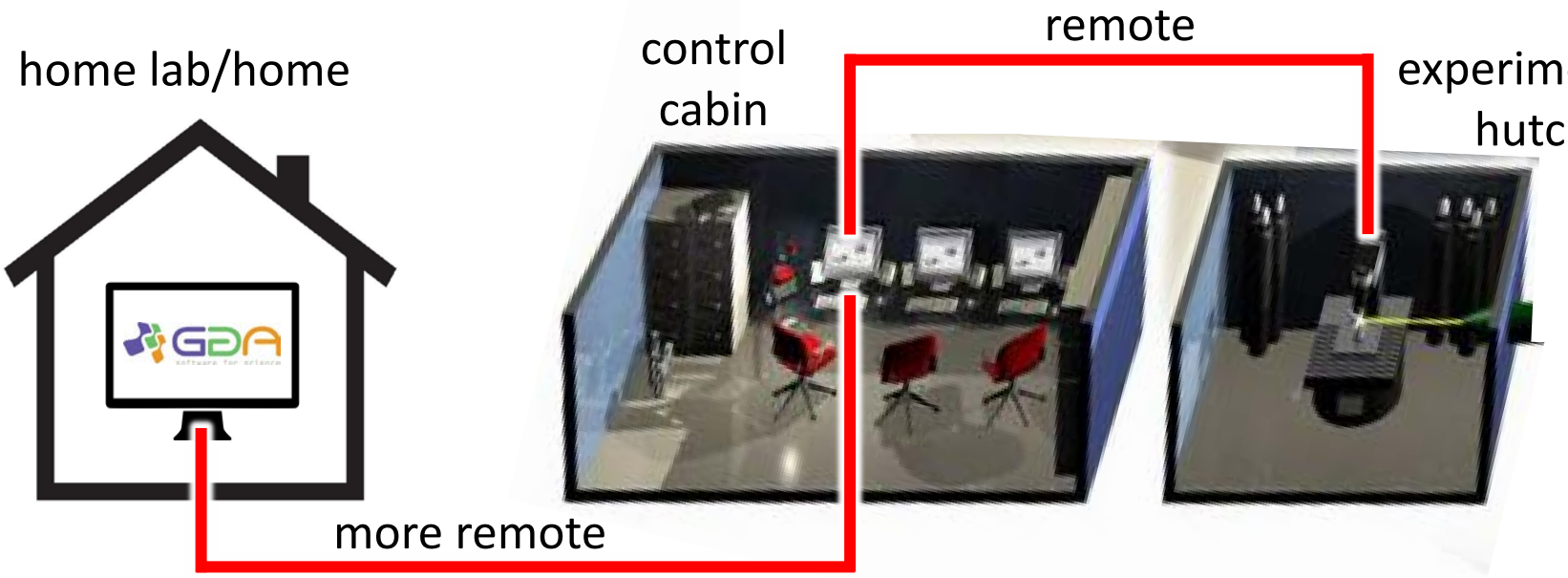


- Samples prepared and cryo-cooled in home lab
- Sample information entered into ISPyB database
- Transported to Diamond in dry shipping dewars
- Samples mounted robotically
- Data collection controlled through GDA interface
- Only manual operation at DLS: loading/unloading pucks
  - Up to 592 samples can be loaded at once
- Everything else computer driven…

Therefore you don’t need to be there!

What is remote data collection?

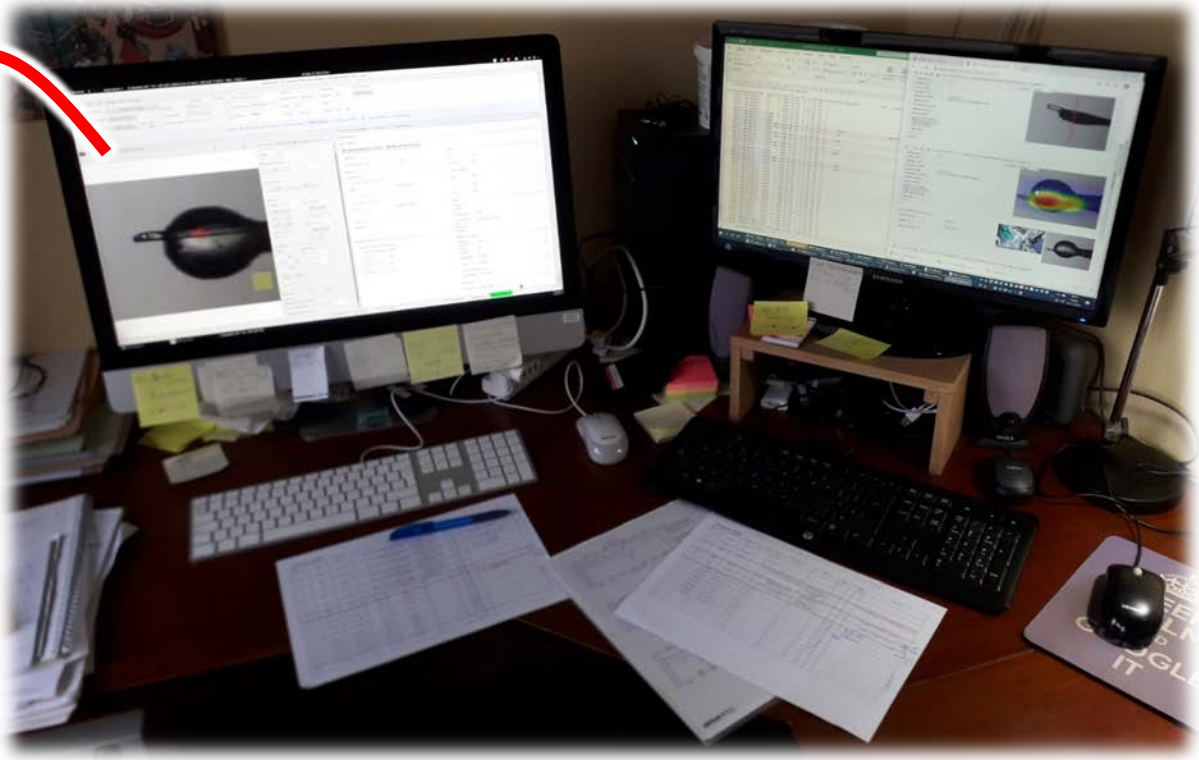




Remote data collection lockdown style!

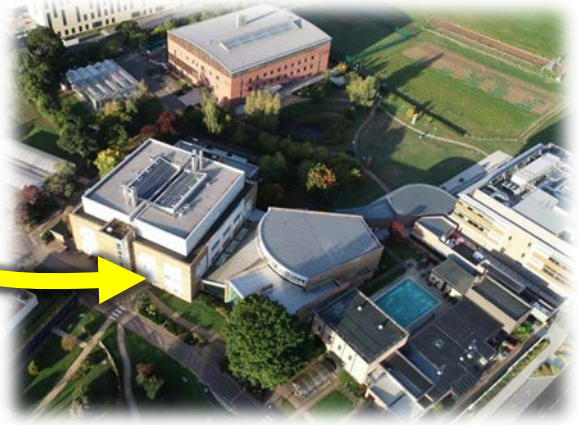
…from here

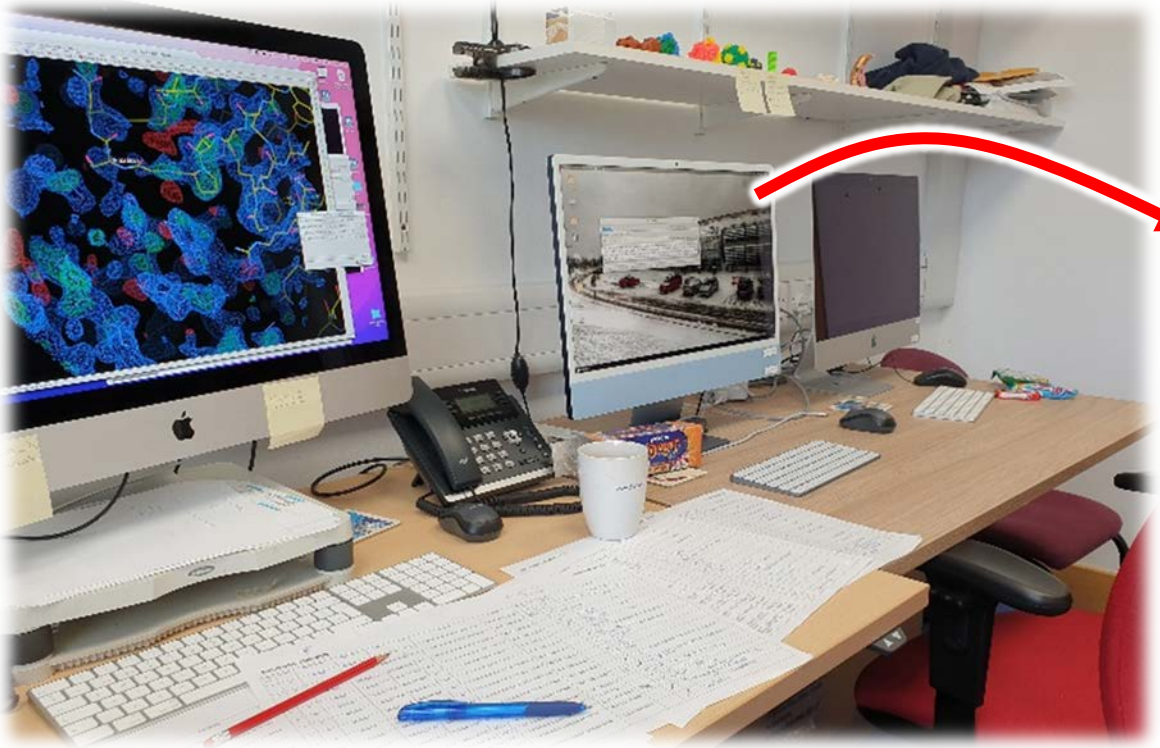
share screen
with others



Remote data collection – normality resumed

…from here



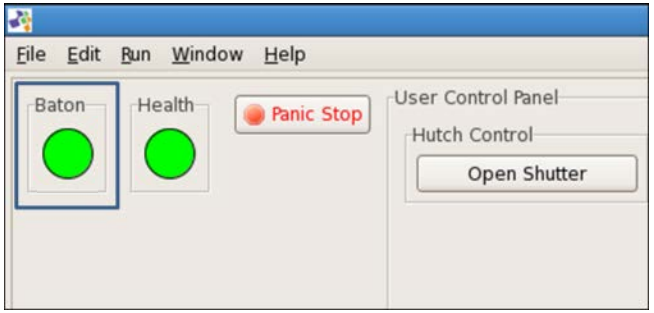


share screen
with others

Timeline for fully remote data collection

Sometime prior to shift:

- LC loads pucks into beamline dewar and enters puck positions into ISPyB database

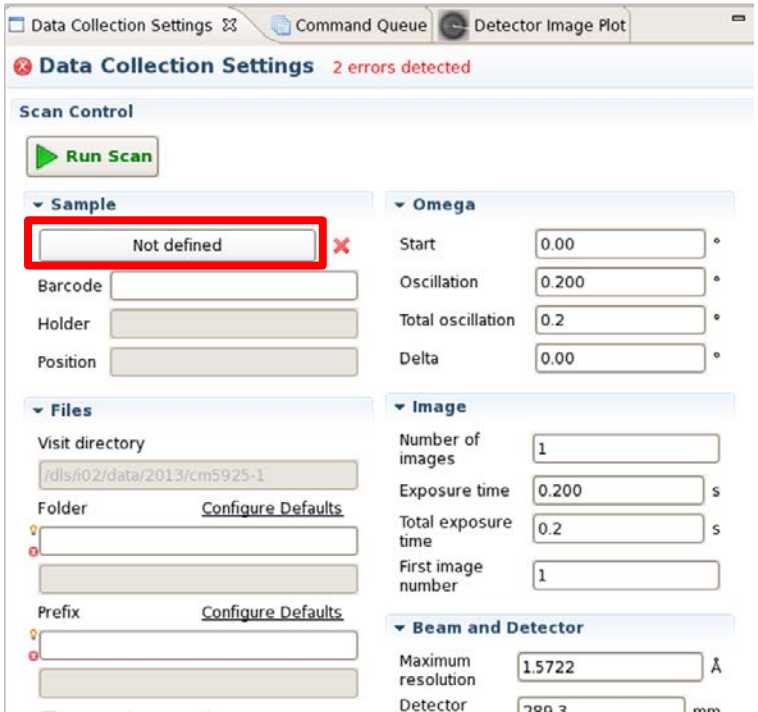


Shortly before start of shift (or slot in running order):

- connect to beamline computer using NX client
- start GDA

Zero hour:

- take the baton, select sample from menu, collect data!



When things go wrong…

Can **you** fix things?

- probably not!

On-site user:

- During normal working hours – call local contact
- Out of hours – call EHC

Remote user:

- During normal working hours – call local contact
- Out of hours – call EHC

Therefore you don’t need to be there!

Check the webcams!

If you suspect a problem – call the EHC!

If you see no diffraction – 3 main causes:

…could be all 3 😖

(1) there is a problem (any number of things…)

(2) you are doing something wrong/stupid

(3) your sample is rubbish!

Pop a couple of test crystals into one of your pucks (something you know will diffract e.g. lysozyme)

Advantages of remote data collection:

- Beamtime is fully used
- Users collect data on their own crystals
- Users stay at home labs (or at home)
  - time commitment is low
  - your boss/collaborator can observe data collection
  - useful for training non-experts
- Time can be used flexibly
- Less stressful
- Difficult to “break” the beamline

Are there any disadvantages of remote data collection?

- miss the “wow factor” of being at a synchrotron
- lose face-to-face interactions with Diamond staff
  - do BAG training
  - go to User meeting
  - get in touch online

Take home messages

- make full use of ISPyB (use ISPyB name!)
- exploit the MX software tools/pipelines (collect 360°!)
- use remote data collection for routine experiments
- think before and during data collection
- this is may be your last experiment – don’t mess it up!

Acknowledgements

- Access to MX beamlines at Diamond
- Excellent support from:
  - Beamline staff
  - EHC/Control Room staff
  - User Office
- Software developers
- BBSRC

John Innes Centre

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