



Optimising the Diamond experience from a user's perspective

Structural Biology Platform
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Biotechnology and
Biological Sciences
Research Council

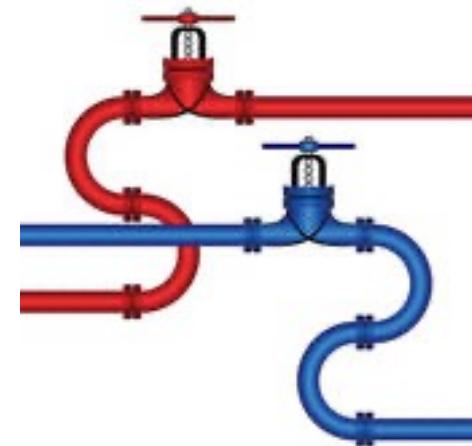
Strategy



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
- not unattended data collection (UDC)

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...
- 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!)

- 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...

Data collection is always a compromise...



*How much
data do I
need?*

*What
resolution
do I need?*

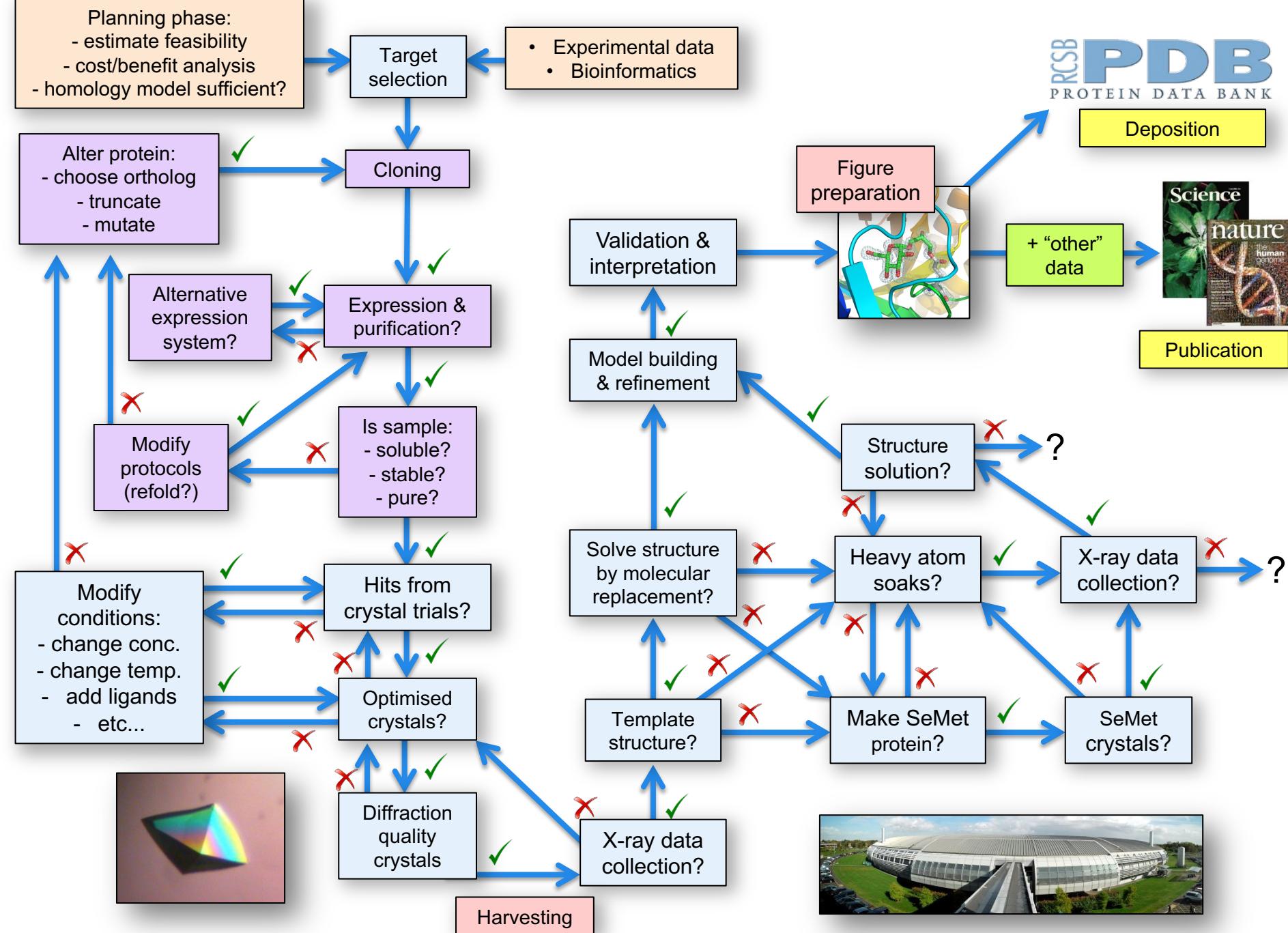
*What are
the data
for?*

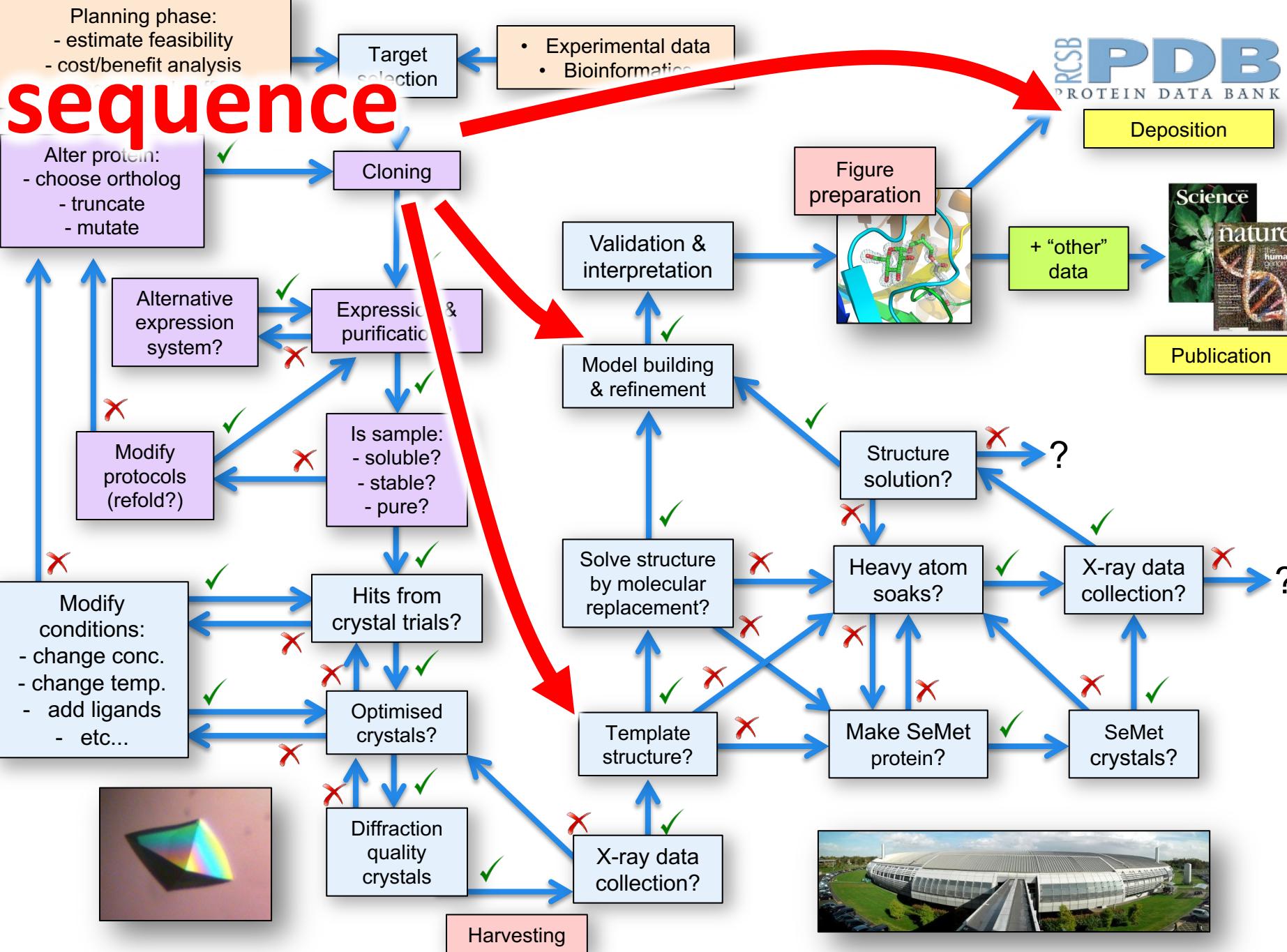
*How much
time do I
have?*

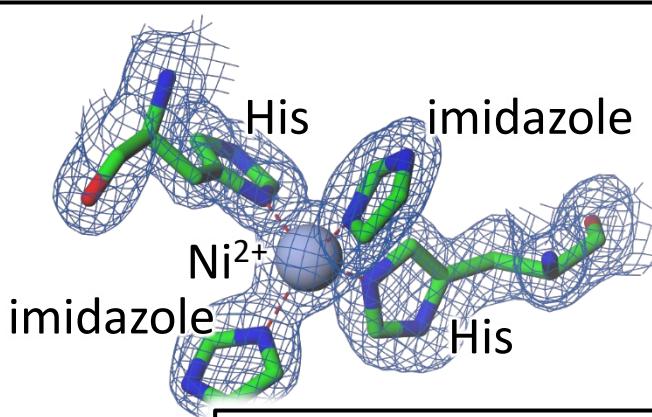
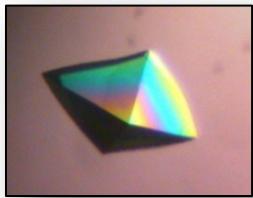
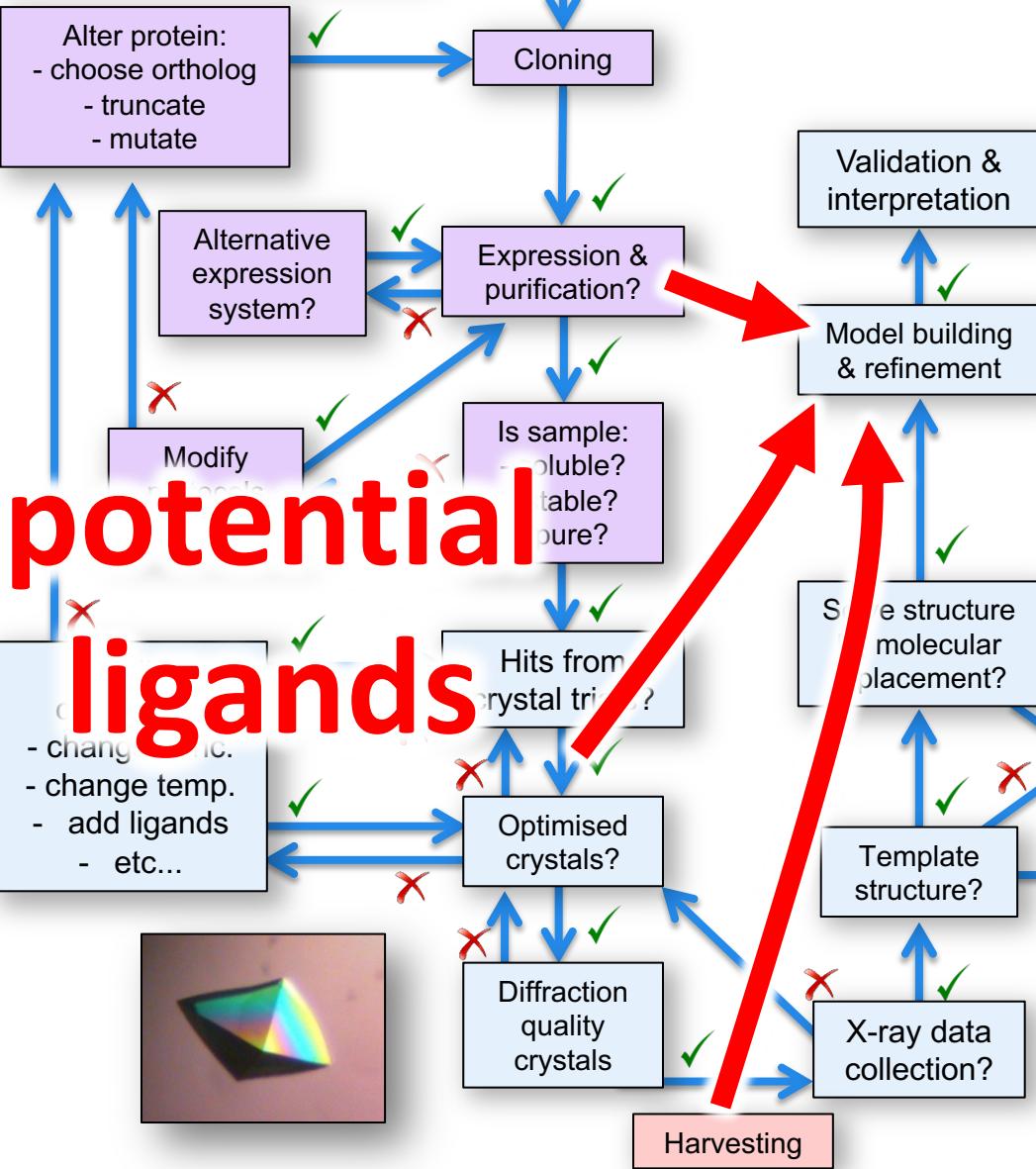
*How many
crystals do
I have?*

Be prepared!

Think about this **before** your beamtime!







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

- phasing
- map interpretation



Harvesting

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

Target selection

- Experimental data
- Bioinformatics

Alter protein:
 - choose ortholog
 - truncate

Cloning

Methods

Alternative expression system?

Expression & purification?

Modify protocols (refold?)

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

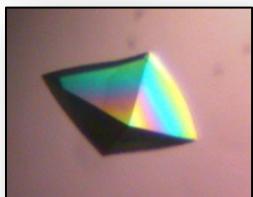
Modify conditions:
 - change conc.
 - change temp.
 - add ligands
 - etc...

Hits from crystal trials?

Optimise crystals?

Diffraction quality crystals

Harvesting



Validation & interpretation

Model building & refinement

Solve structure by molecular replacement

Template structure?

X-ray data collection?

Figure preparation

+ "other"

Science

nature
human genome

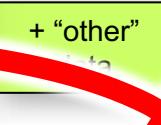
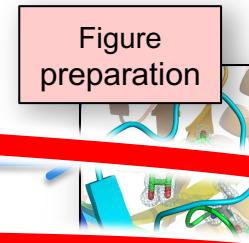
Publication

Heavy atom soaks?

X-ray data collection?

Make SeMet protein?

Select crystals?



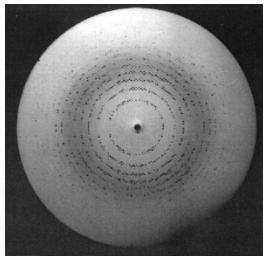
Deposition

Detector types

hours

readout time

1 ms



Film



Image plate



CCD (charge-coupled device)



HPC (hybrid photon counting)

1990

2000

2010

2020

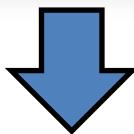
360° data sets possible in <10 s!

MX data collection has become faster...

20th century data collection



21st century data collection



Crystals

Which protein did I crystallize?

Was it the wild-type or mutant?

Did I add any ligands?

What else was in the crystallization?

AAAAAH...



Data

Which crystal gave this dataset?

How did I collect the data?

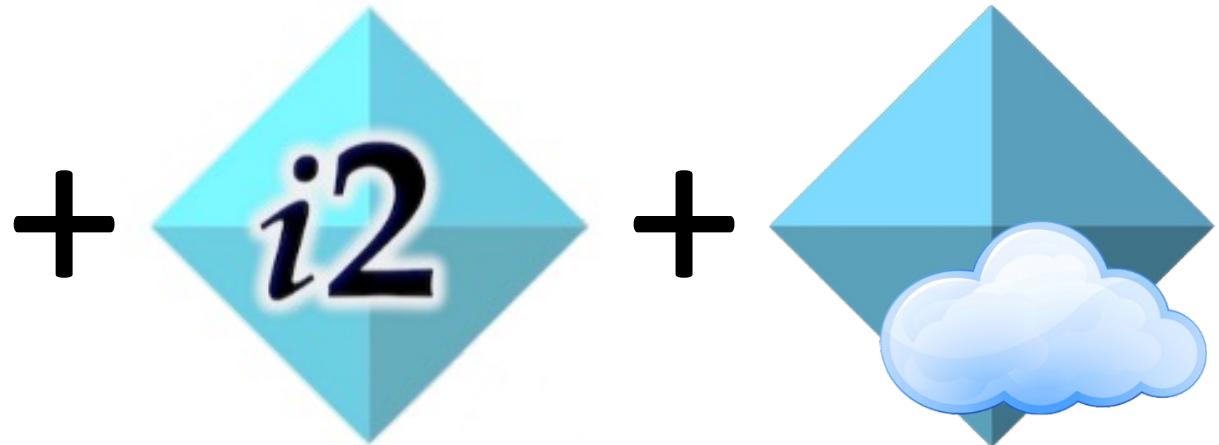
Is this the best dataset for the sample?

Are the data "good enough"

Help is at hand...



ISPyB/SynchWeb



CCP4i2

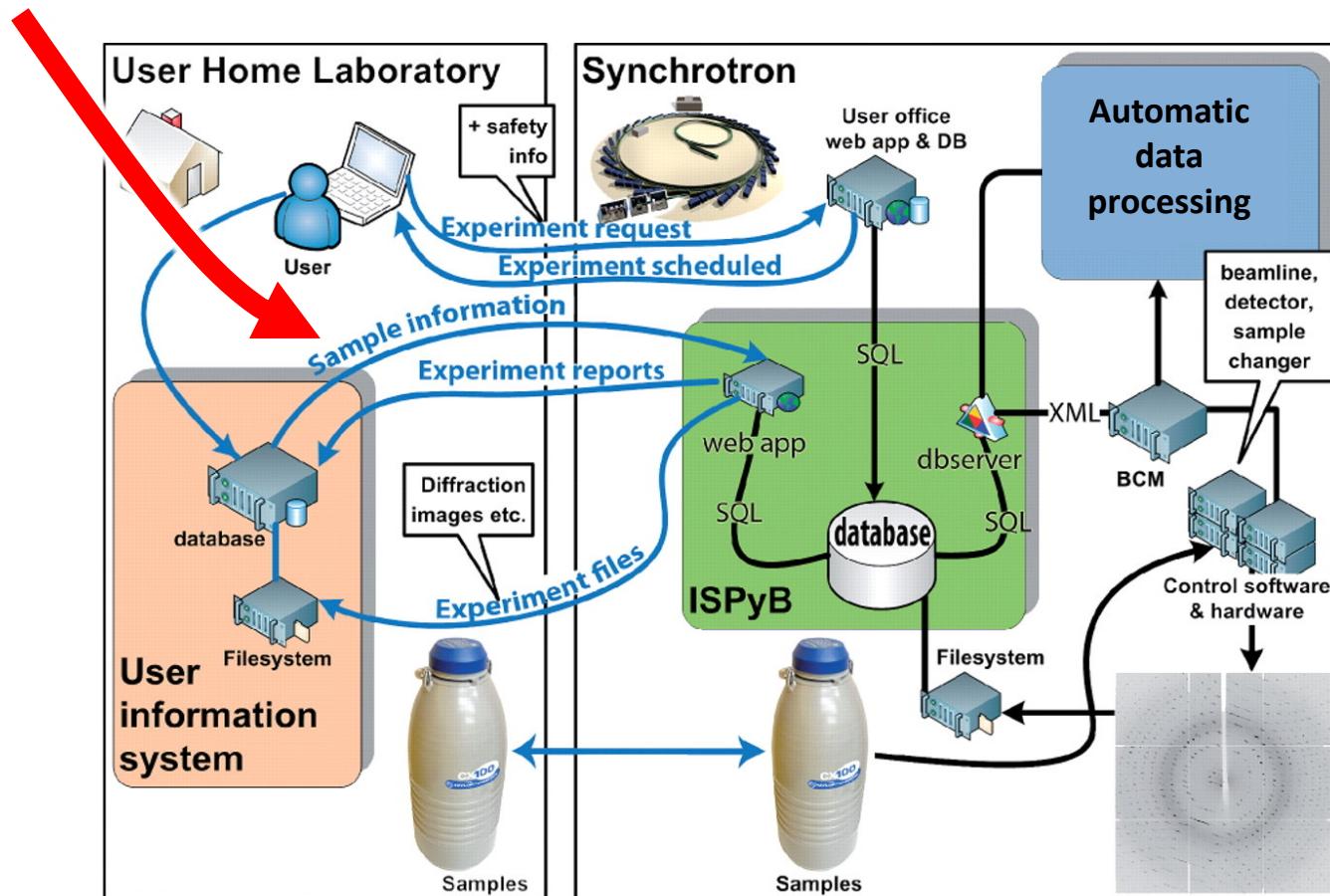


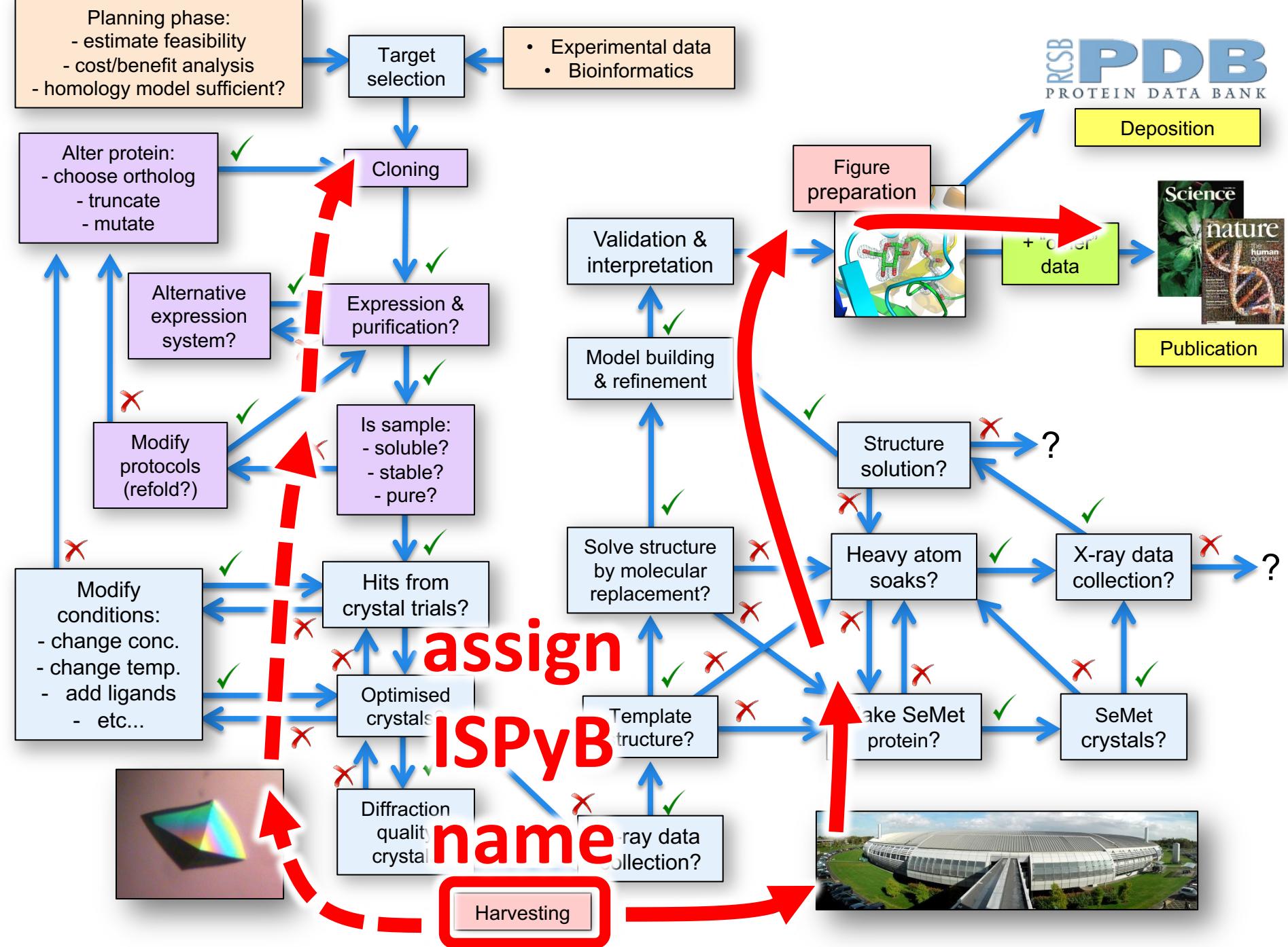
CCP4 Cloud



Each crystal is
assigned a unique
“ISPyB name”!

ISPyB/SynchWeb





Date: 29-JUL-2017

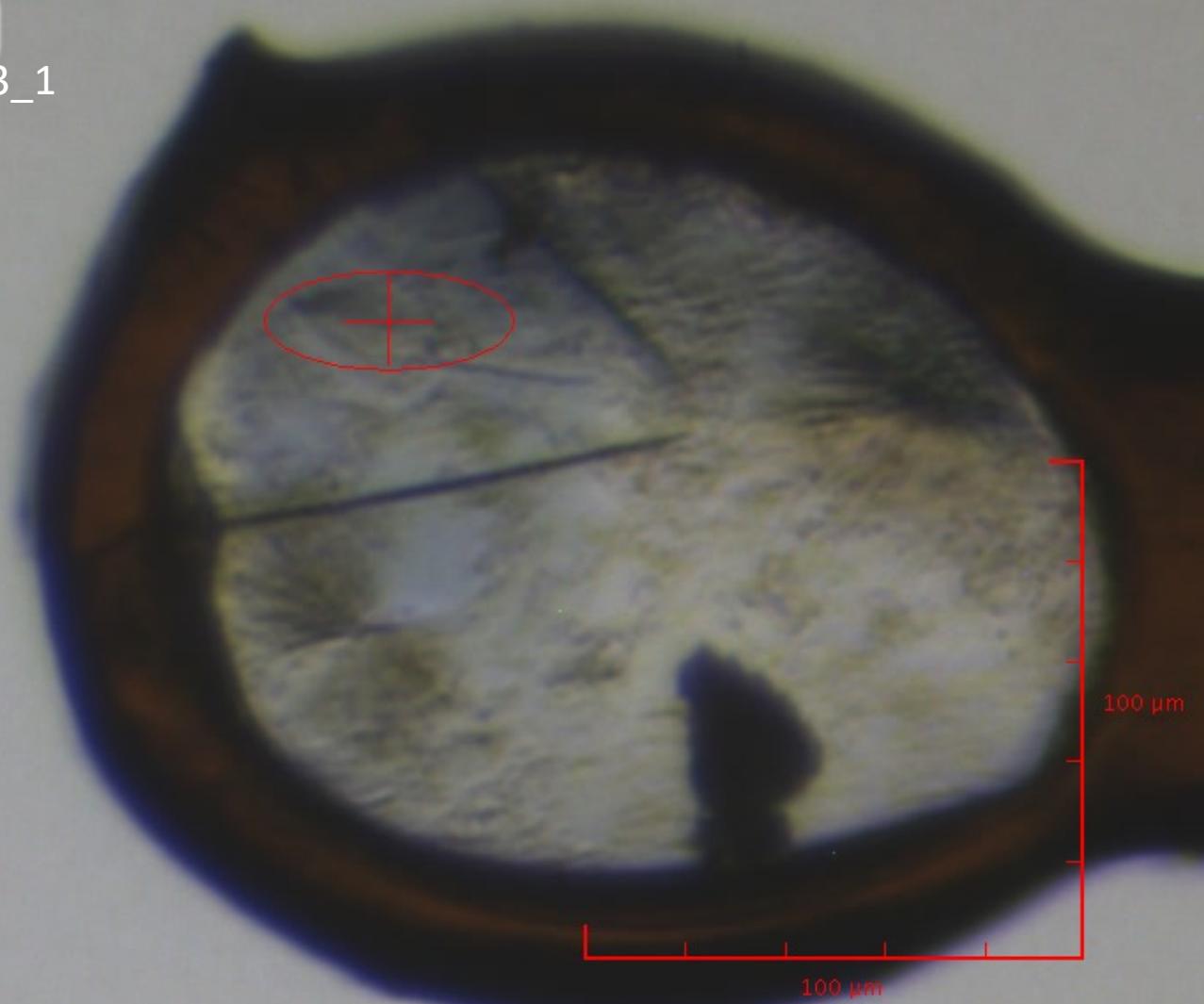
Beamline: i03 Diamond

Visit ID: mx13467-41

Protein acronym: NmADH9

ISPyB name: NmADH9_23

Dataset name: NmADH9_23_1



Beam size: 50.0 × 20.0 µm

Harvest your crystals and enter sample info into ISPyB



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**

Location	Protein Acronym	Abundance	Components	Name	Spacegroup	Barcode	Comment	Status	+ Extra Fields
9	NmADH9			NmADH9_18					
10	NmADH9			NmADH9_19					
11	NmADH9			NmADH9_20					
12	NmADH9			NmADH9_21					
13	NmADH9			NmADH9_2					
14	NmADH9			NmADH9_23					

Loc	Protein Acronym	Name	Sample Group	Anomalous	Barcode	Comment	Status	Basic	Extra Fields	Unattended (UDC)
1	LYS	JIC_LYS_OCT	-							

turns on EP
pipelines

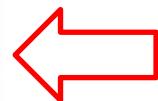
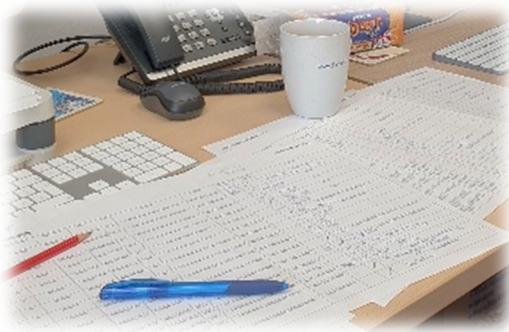
Required
for UDC

Use a spreadsheet...

crystals_MX13467-41_i03_29-July-2017

Puck number – DLS442 [\(+\)](#)

Position	Person	Protein name	I spy B 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 oxogeraniol+ 20%EG				10mM soak for approx 1 h
11	Benjy	NmADH9	NmADH9_20	MCBL0004	A11.1	"	8 oxogeraniol+ 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....

The screenshot shows the 'Data Collection Settings' window in GDA. A red arrow points to the 'Sample' section where 'NmADH9_23' is selected. Another red arrow points to the 'Files' section where the 'Folder' path is set to 'JIC/\${protein acronym}/\${sample name}'. The window includes sections for Omega parameters (Start, Oscillation, Total oscillation, Delta), Image settings (Number of images, Exposure time, Total exposure time, First image number), Beam and Detector settings (Maximum resolution, Detector distance, Wavelength, Energy, Use current energy), and a Command Queue tab.

Sample: NmADH9_23

Barcode: NR

Holder: 2

Position: 14

Omega

- Start: 45.00
- Oscillation: 0.100
- Total oscillation: 360.0
- Delta: 0.00

Image

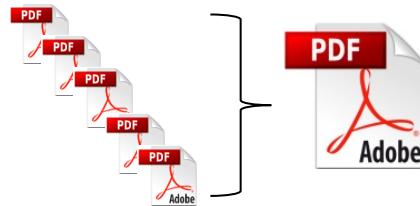
- Number of images: 3600
- Exposure time: 0.010 s
- Total exposure time: 36.0 s
- First image number: 1

Files

- Visit directory: /dls/i03/data/2017/mx13467-41
- Folder: JIC/\${protein acronym}/\${sample name}
- Prefix: \${sample name}
- Comment: EDNAStrategy1: subWedge:1

Beam and Detector

- Maximum resolution: 1.3000 Å
- Detector distance: 213.5 mm
- Wavelength: 0.97623 Å
- Energy: 12700.3 eV
- Use current energy
- Transmission: 50.156283 %



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

mx13467_41 on i03 at 29-07-2017 12:00											
Sample	Images	Res	z	D Osr	Spacegroup	Unit Cell	Processed Resolution	Rmsas	Completeness	Comments	
NmADH9_23	3600	1.3	0.9763	0.10	P 1 2 1	98.00, 98.00, 98.00	107.75, -1.5	0.085	98.8	(-262,-192,1150) EDNAStrategy1: subWedge1Aperture: Medium	
NmADH9_23	3600	1.3	0.9763	0.10	P 1 2 1	98.00, 98.00, 98.00	29.77, -1.5	0.085	98.7	(-262,-192,1150) EDNAStrategy1: subWedge1Aperture: Medium	
NmADH9_23	3600	1.3	0.9763	0.10	P 1 2 1	98.00, 98.00, 98.00	-5.54, -1.5	0.084	98.7	(-262,-192,1150) EDNAStrategy1: subWedge1Aperture: Medium	
NmADH9_24	3	1.5	0.9763	0.50						(-107,-190,1032) Aperture: Medium	
NmADH9_24	3	1.5	0.9763	0.50						(-107,-190,1032) Aperture: Small	
NmADH9_25	3	1.5	0.9763	0.50						(-154,-228,1396) Aperture: Medium	
NmADH9_25	3	1.5	0.9763	0.50						(-213,-228,1406) Aperture: Medium	
NmADH9_15	3	1.5	0.9763	0.50						(247,-388,861) Aperture: Medium	
NmADH9_15	42	3.0	0.9763	0.00						Diffractogram grid scan of 7 by 6 images, Top left [350,177], Bottom right [478,245]	
NmADH9_15	42	3.0	0.9763	0.00						Diffractogram grid scan of 3 by 4 images, Top left [472,245], Bottom right [590,313]	
NmADH9_15	3	1.5	0.9763	0.50						(276,-373,844) Aperture: Medium	
NmADH9_15	3	2.0	0.9763	0.50						(276,-373,844) Aperture: Medium	
NmADH9_15	3600	2.0	0.9763	0.10	P 1 2 1	62.17, 107.70, 99.00, 105.00, 99.00	30.02, -3.04	0.167	99.4	(276,-373,844) EDNAStrategy1: subWedge1Aperture: Medium	
NmADH9_11	3	2.0	0.9763	0.50						(-477,-294,1141) Aperture: Medium	
NmADH9_12	3	2.0	0.9763	0.50						(-499,-740,1396) Aperture: Medium	
NmADH9_12	3	1.6	0.9763	0.50						(-63.84,-106.11), (-69.29,-116.16), (-71.16,-105.01), (-83.93,-97.3)	
TAPHY_27_1	4	3.0	0.9763	0.00						(-496,-216,1130) EDNAStrategy1: subWedge1Aperture: Medium	
TAPHY_27_1	3	1.8	0.9763	0.50						(-109,-296,1303) EDNAStrategy1: subWedge1Aperture: Medium	
TAPHY_27_1	1200	1.5	0.9763	0.10	H 3	126.66, 126.66, 107.16, 107.16, 95.00, 95.00, 90.00, 90.00, 120.00	29.37, -1.92	0.078	99.0	(-109,-296,1303) EDNAStrategy1: subWedge1Aperture: Medium	
TAPHY_27_2	5	3.0	0.9763	0.00						(-576,-463) Diffractogram grid scan of 1 by 1 images, Top left [540,251], Bottom right [576,463]	
TAPHY_27_2	3	1.5	0.9763	0.50						(136,-104,1462) EDNAStrategy1: subWedge1Aperture: Medium	

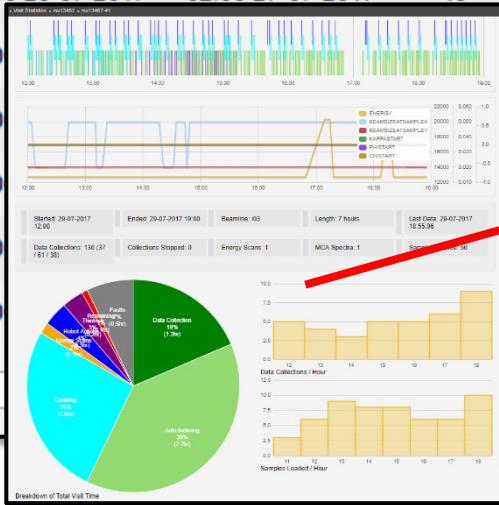
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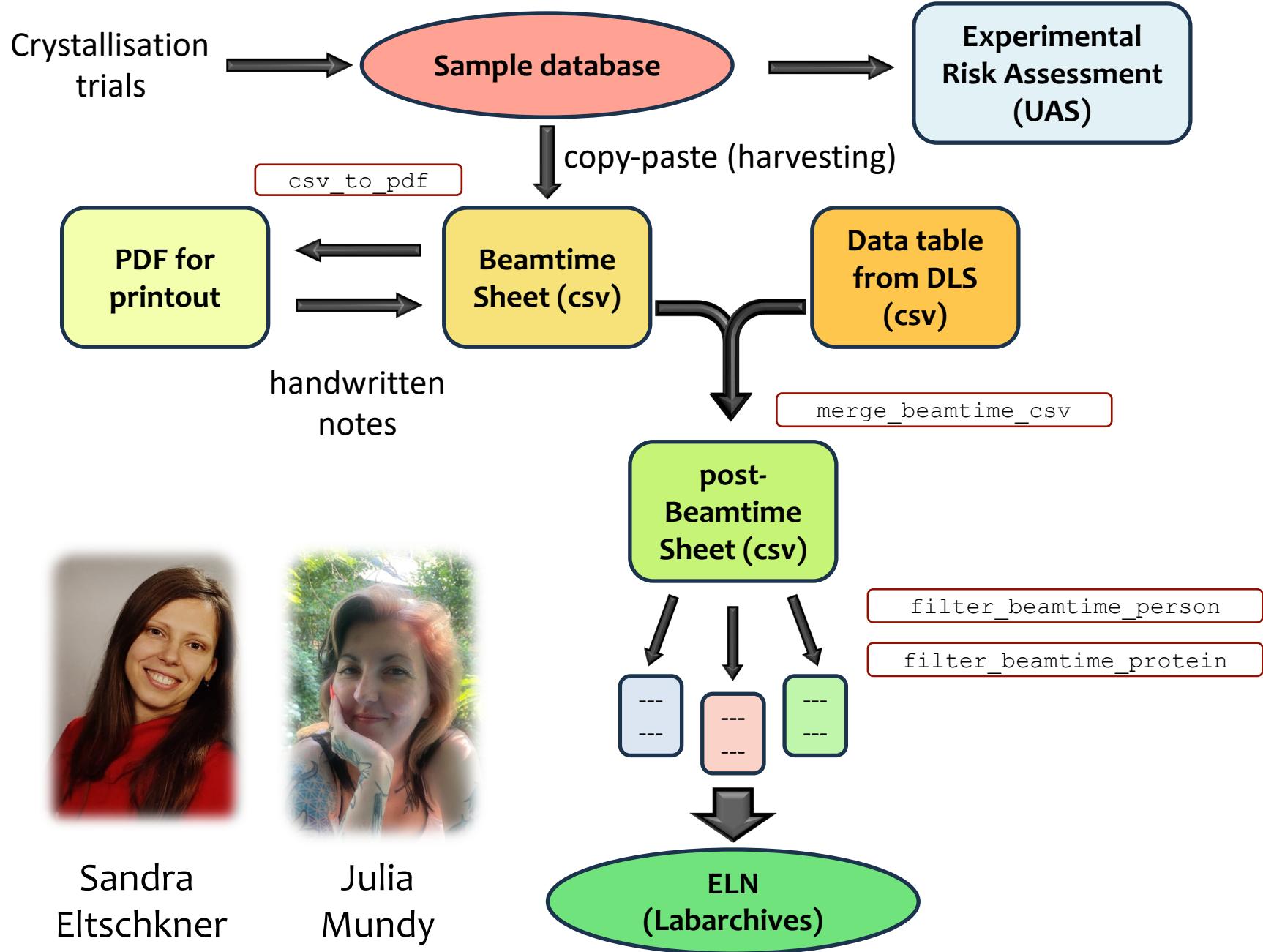
29-07-2017, mx13467_41 on i03																	
File	Home	Insert	Page Layout	Formulas	Data	Review	View	ACROBAT	Tell me what you want to do	Normal	Bad	Good	Neutral	Check Cell	Explanatory...	Input	Linked Cell

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	
02:00			i03	Dr Neil Paterson	38	Compulsorily Remote	
17:00			i03	Dr Neil Paterson	76		
19:00			i04	Dr Melanie Vollmar	69	Compulsorily Remote	
12:00			i04	Dr Dave Hall	106	Compulsorily Remote	
02:00			i03	Dr Neil Paterson	82	Compulsorily Remote	
10:00							

5 6 7 > >>

10

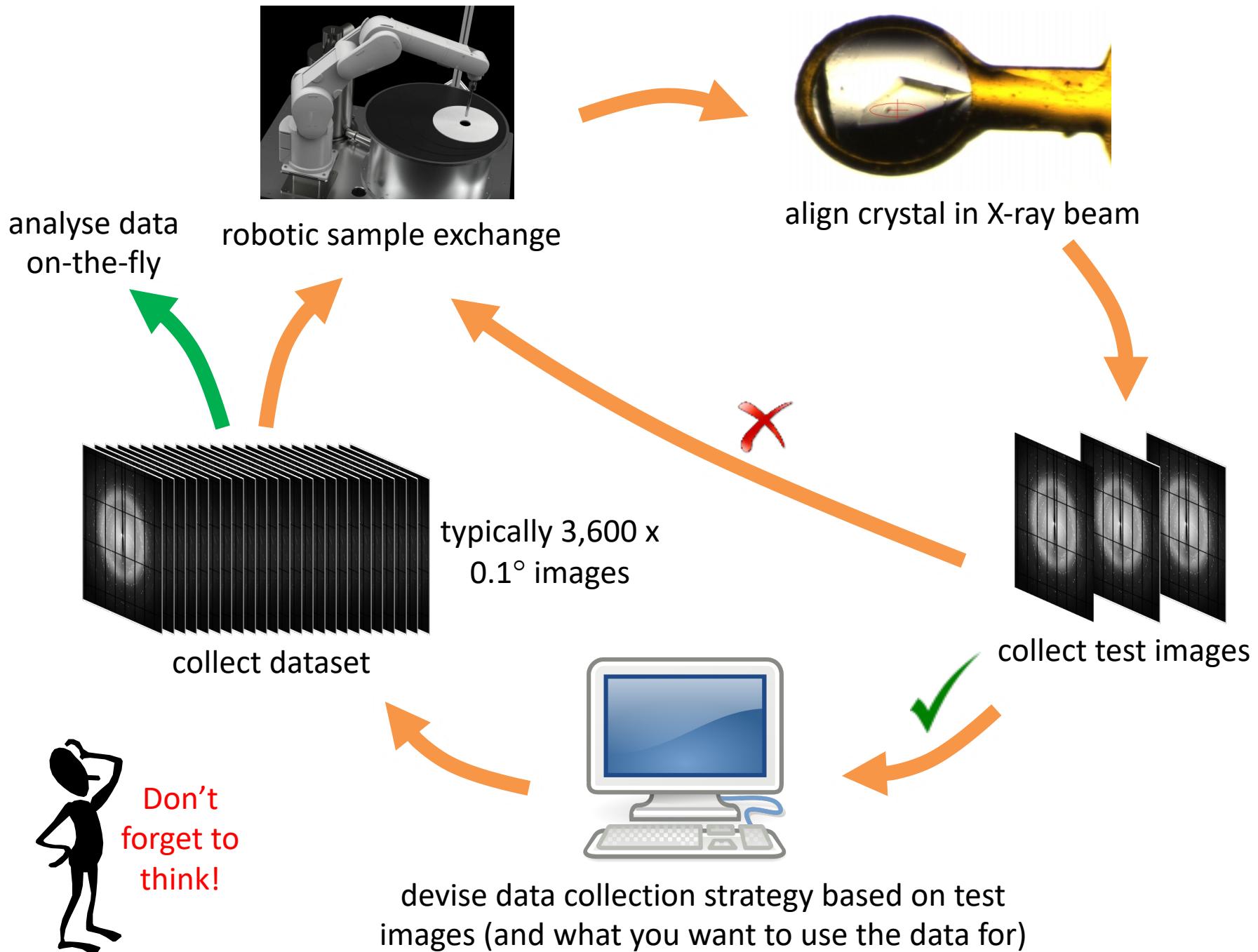




Ideal scenario during session:

- 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 on to next sample...
- not efficient
without automation



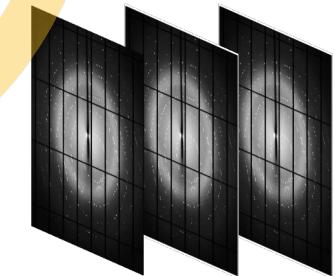
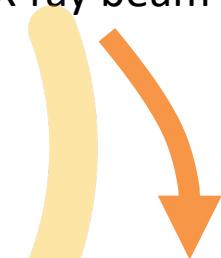




robotic sample exchange



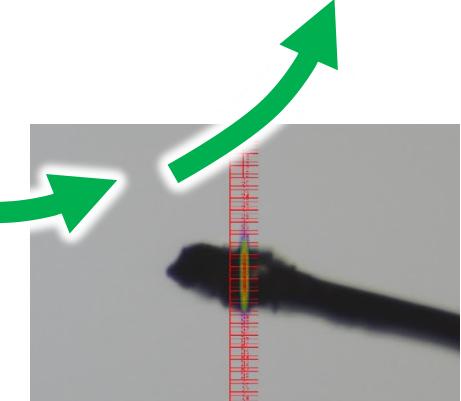
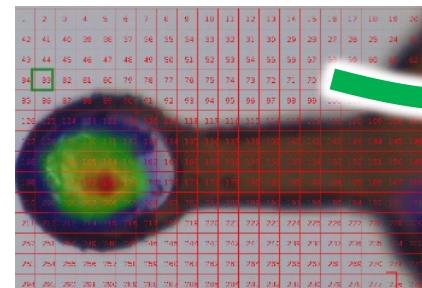
align crystal in X-ray beam

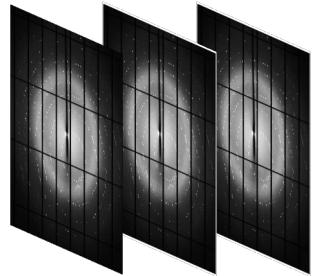


collect test images

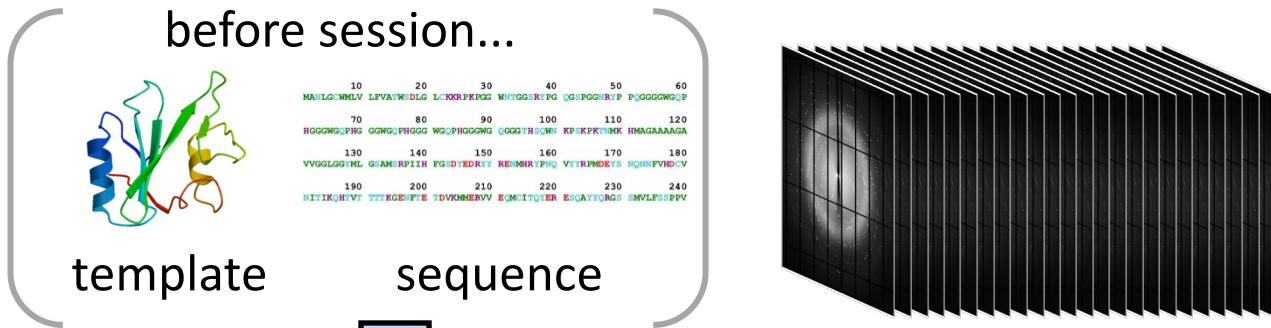
May be more efficient to screen your samples in batches, then decide what to do...

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

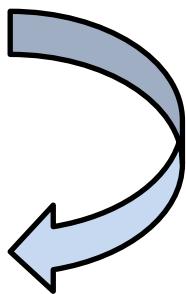




test images

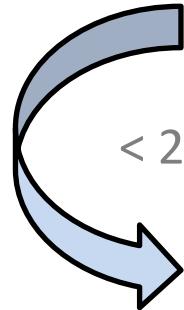


Look at images
(e.g. in ADXV)
- can they be
indexed?



ISPyB

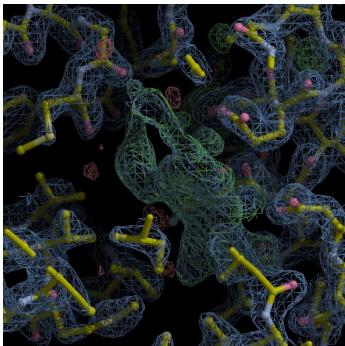
< 2 min



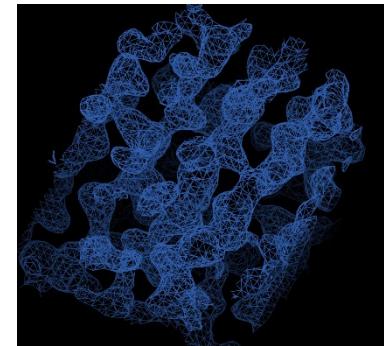
Fast DP

< 5 min

h	k	l	I	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	
-45	0	12	0.63	1.33	0.63	1.33	



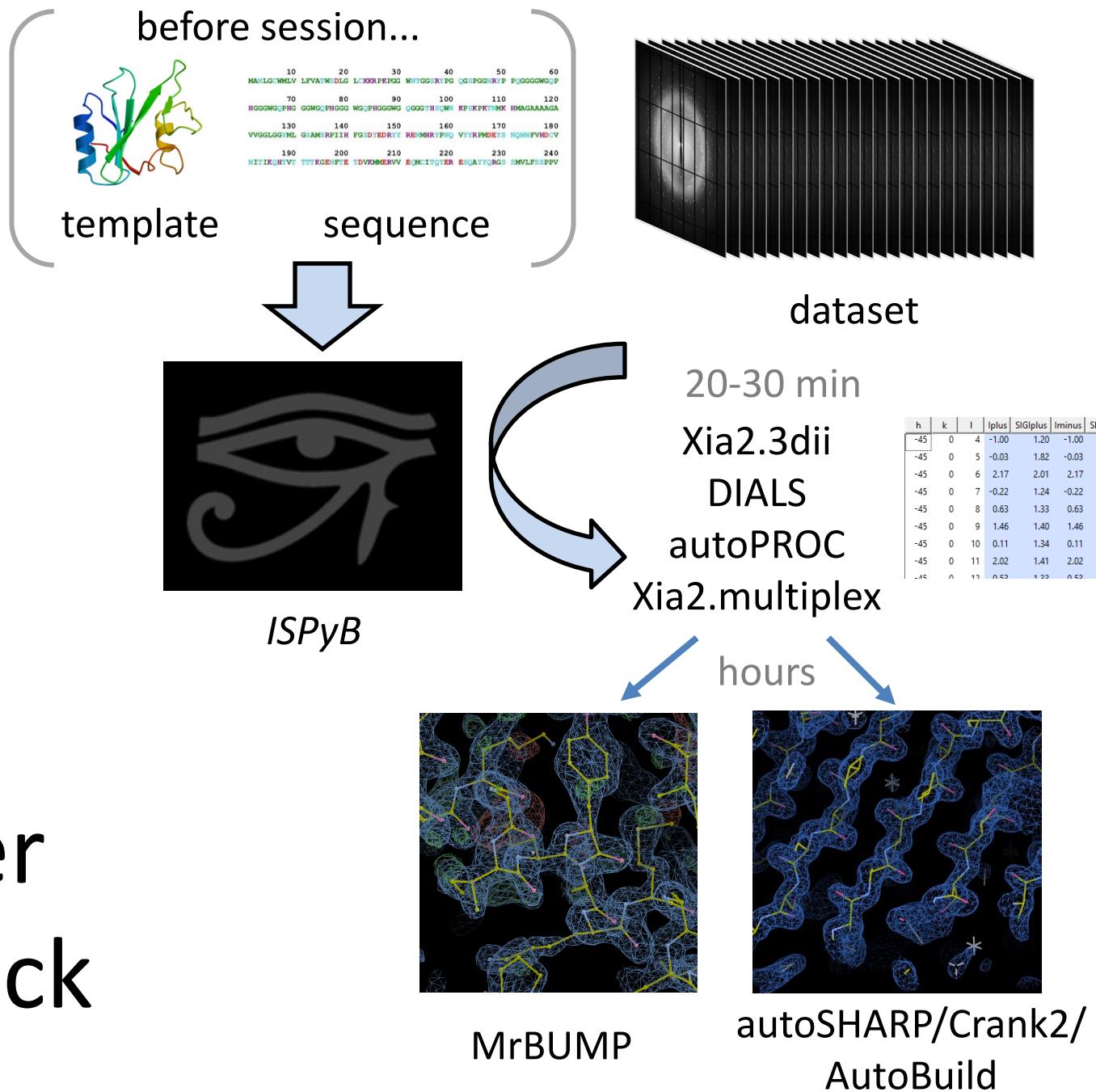
Dimple



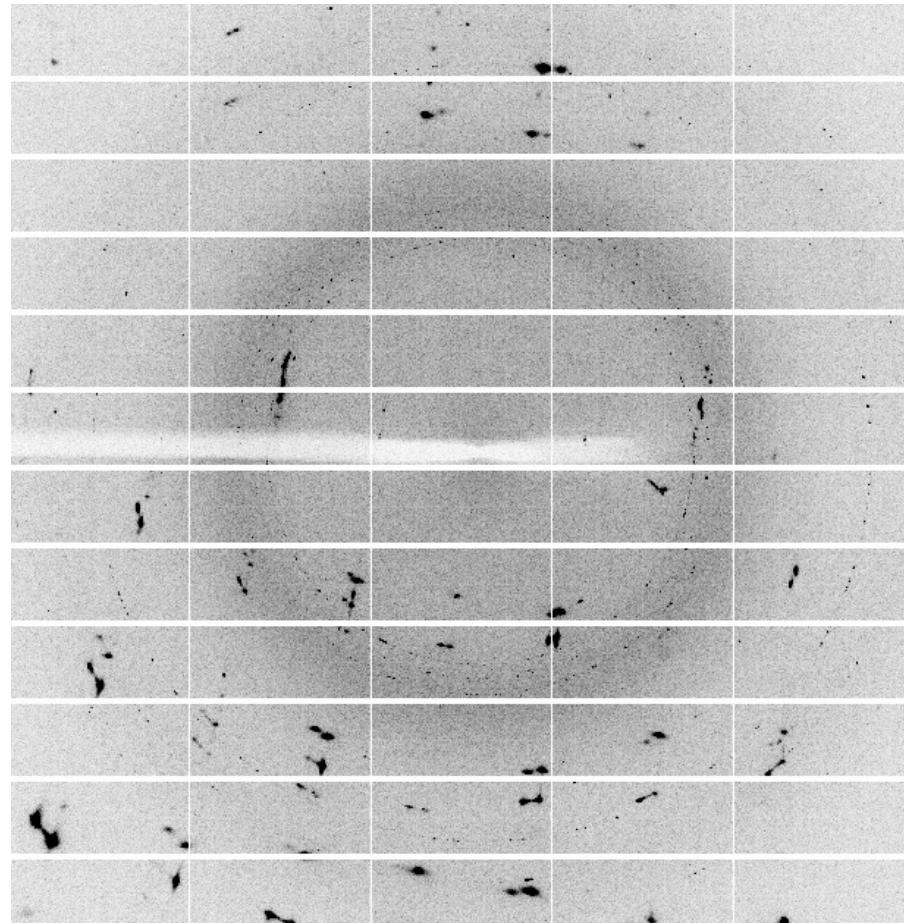
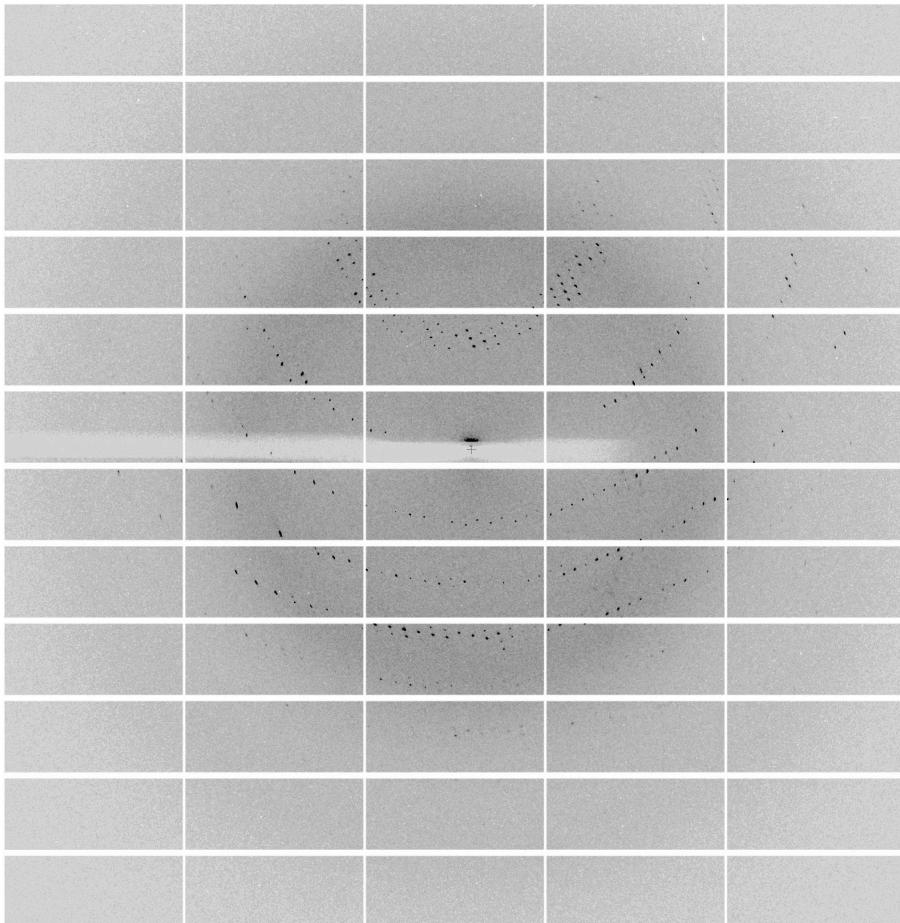
Fast EP

Quick feedback

Slower feedback



LOOK at your images!!!!



Notes about strategies...

Despite what your supervisor or colleague advises...

- 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 your test images don't index, but the crystal is diffracting reasonably well...

- collect a data set anyway – it might be useful (e.g. to establish what you crystallized!)
 - inspect screening images in ADXV
 - look for highest resolution spots (NOT ice or salt spots!)
 - subtract 0.5 from this resolution value. E.g. spots at 2.5 \AA → collect to 2.0 \AA
 - collect $3,600 \times 0.1^\circ$ images

Checking the results...



Checking the results...

Auto Processing		Fast DP: ✓ Xia2: ✓ ✓ MultiXia2: ? ? autoPROC: ✓						
Type	Resolution	Spacegroup	In<l/sig(l)>	Rmeas Inner	Rmeas Outer	Completeness	Cell	Status
fast_dp	29.77 - 1.50	P 1 2 1	5.2	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 2 1 1	0.9	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 2 1 1	0.8	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 2 1 1	.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 2 1 1	3.3	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/>)

Beam Centre	X	Y	Plots	Archive	Logs & Files	Lookup Cell		
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 2 1 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

Consistent indexing gives more confidence in the results...

... but treat space group assignment as only a hypothesis at this stage! (see later talks)



Re-running jobs:

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

The screenshot shows the ISPyB software interface for reprocessing data. The top window displays experimental parameters for a dataset named [mx13467-41] from July 29, 2017, at 14:40:37. A red arrow points to the settings gear icon in the top bar. A callout box highlights changes that can be made:

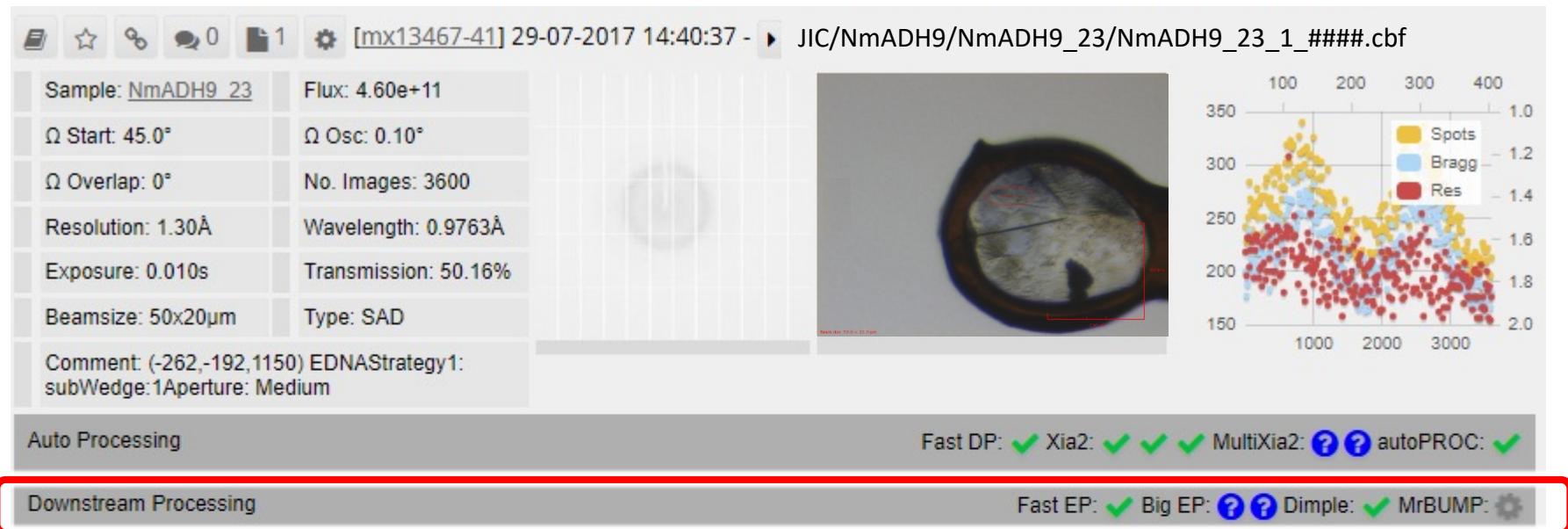
- space group
- cell parameters
- maximum resolution
- reject images

The bottom window shows a summary for the dataset NmADH9_23_1 - JIC/NmADH9_23/NmADH9/. It includes sample information, resolution, wavelength, and processing options. Both windows feature scatter plots of spots, Bragg reflections, and residuals against resolution.

Change:

- space group
- cell parameters
- maximum resolution
- reject images

Checking the results...



Checking the results...

[mx13467-41] 29-07-2017 14:40:37 - JIC/NmADH9/NmADH9_23/NmADH9_23_1 #####.cbf

Sample: NmADH9_23 Flux: 4.60e+11
Ω Start: 45.0° Ω Osc: 0.10°
Ω Overlap: 0° No. Images: 3600
Resolution: 1.30 Å Wavelength: 0.9763 Å
Exposure: 0.010s Transmission: 50.16%
Beamsize: 50x20µm Type: SAD
Comment: (-262,-192,1150) EDNAStrategy1:
subWedge:1Aperture: Medium

Auto Processing

Downstream Processing

Fast EP Dimple

View the result through the browser...

...or download model & map and view in COOT

Fast DP: ✓ Xia2: ✓✓✓ MultiXia2: ?? autoPROC: ✓
Fast EP: ✓ Big EP: ?? Dimple: ✓ MrBUMP: ?

Parameter	R factor	R free	Rms BondLength	Rms BondAngle	Rms ChirVolume
Initial	0.2376	0.2551	0.0174	1.7446	0.1121
Final	0.2174	0.2625	0.0178	1.8068	0.1061

Check R-factors are sensible

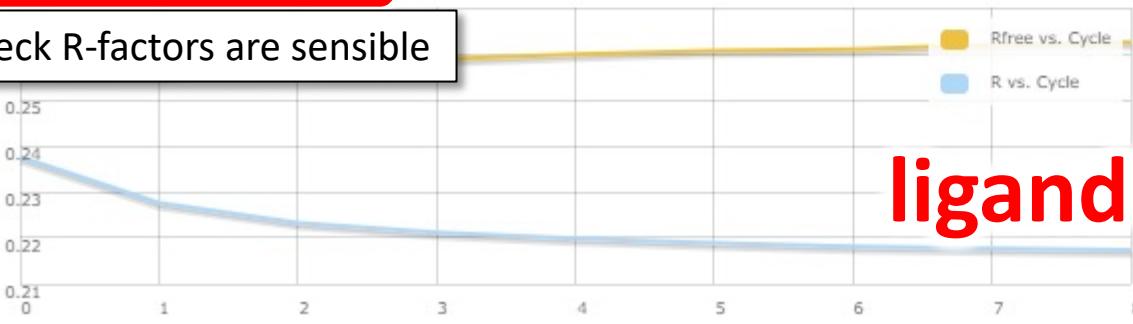
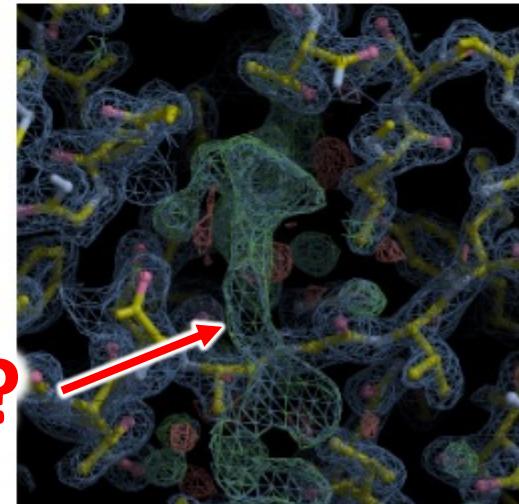
Rfree vs. Cycle

R vs. Cycle

PDB/MTZ file

Log file

ligand?



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!



If you used your only crystals for a project...

- still might be useful for seeding



What to do with all the data...

Raw data (images)

- removed from disk
after 30 days – still
available through
TopCAT (tape archive)



“**Meta**” data – all the other “stuff” – most is removed from disk after 30 days – but important files persist for > 1 year

>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...



Faster...

A screenshot of a software interface with a navigation bar at the top containing buttons for "xia2 dials", "xia2 3dii", "autoPROC", "fast_dp", "autoPROC+STARANISO", "xia2 3dii", "autoPROC", and "autoPROC+STARANISO". Below the bar, a green notification box says "8 check(s) passed". Underneath, there's a table for "Beam Centre X Y" with a single row: "Start" at "158.90 166.46". At the bottom right, there are several buttons: "Processing Log", "Plots", "Archive", "Logs & Files" (which is highlighted with a red box), and "Lookup Cell".

In the meantime:

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

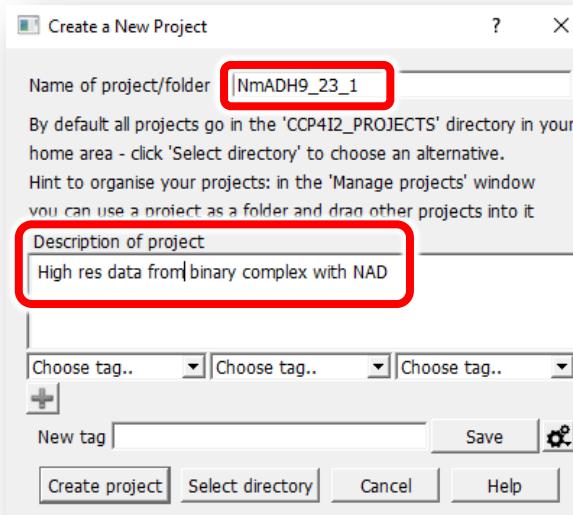
Retain ISPyB name in CCP4 downstream processing

Create a separate “project” for each dataset...

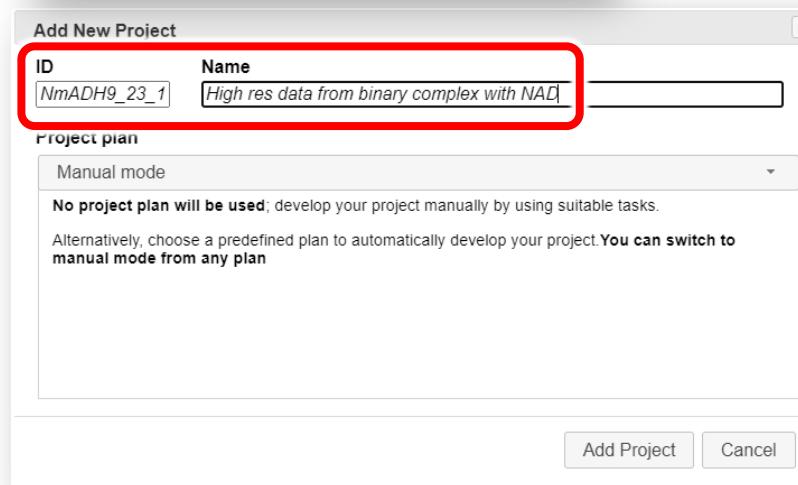
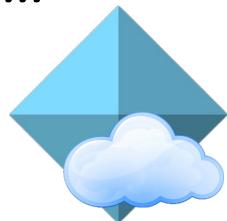
either...



CCP4i2



or...



- where the pipelines have done a good job – take part-processed dataset (download this directly from SyncWeb) and re-run the merging step in CCP4i2/Cloud

Gives lots of output – useful for troubleshooting...

for your
paper/thesis

Job 1: Data reduction - AIMLESS **The job is Finished**

Input Results | Comments |

Headline Summary SG details MergingGraphs SDanalysis MergingDetails Istats Biblio

Data reduction – full dataset to 1.4 Å

▼ Key summary

Selecting space group P 1 21 1 as there is a single space group with the highest score

Solution probability: 0.872, Confidence 0.866 (high resolution limit for symmetry testing 1.495Å)

Key statistics for Dataset: NmADH9_23_1/NmADH9_23/1

Unit cell: 63.921 107.750 69.361 90.000 104.265 90.000, wavelength 0.976250Å

Resolution of input data: 1.40Å, **resolution estimate:** beyond 1.40Å

Anisotropic limits: - Along a^* -0.16 c* 1.48Å CC(1/2), 1.58Å l/σ - Along k axis 1.40Å* CC(1/2), 1.42Å l/σ - Along -0.09 1.40Å l/σ

Rmeas: overall 0.096, inner bin 0.037

In outer bin: Mean(l/sd) 1.2 CC(1/2) 0.559

Overall filtered Mean(chi^2): 1.03

Anomalous CC(1/2) in inner bin 0.093

No significant anomalous signal detected

NOTE: no scaling was done, just merging

SD correction information:
SD correction parameters were not refined

✓ No evidence of twinning

✓ No evidence of possible translational non-crystallographic symmetry

● Warning: Some anisotropy detected. This may affect the quality of the model.

● Warning: Completeness test shows some issues

✗ Warning: Severe deviation from Wilson plot.

✗ Warning: Possible ice rings found.

A free-R set has been created, fraction of the data = 0.05

Show Pointless logfile Show Aimless logfile Show Ctruncate logfile

▼ Overall summary

Job 1: Data reduction - AIMLESS **The job is Finished**

Input Results | Comments |

Headline Summary SG details MergingGraphs SDanalysis MergingDetails Istats Biblio Run

▼ Overall summary

Space group determination

Selecting space group P 1 21 1 as there is a single space group with the highest score

Solution type: space group

Group name	P 1 21 1
Reindex	[h, k, l]
Space group confidence	0.866
Laue group confidence	0.821
Laue group probability	0.882
Systematic absence probability	0.988

Scores for each symmetry element

Lattice group name P 1 2 1

Likelihood	CC	R	Symmetry
0.880	0.87	0.087	identity
0.882	0.87	0.087	2-fold k (0 1 0) {-h, k, -l}

Data internal consistency statistics

Summary of merging statistics for dataset NmADH9_23_1/NmADH9_23/1

	Overall	Inner	Outer
Low resolution limit	47.16	47.16	1.42
High resolution limit	1.40	7.67	1.40
Rmerge(within I+ /I-)*	0.081	0.031	1.402
Rmerge(all I+ and I-)*	0.090	0.036	1.563
Rmeas (within I+ /I-)*	0.096	0.037	1.657
Rmeas (all I+ & I-)*	0.097	0.039	1.690
Rpim (within I+ /I-)	0.051	0.020	0.876
Rpim (all I+ & I-)	0.037	0.015	0.636
Rmerge in top intensity bin*	0.048		
Number of observations	1205637	7127	59269
Number unique	175909	1122	8610
Mean(l/sd))	11.2	46.7	1.2
Half-set correlation CC(1/2)	0.999	0.998	0.559
Completeness %	98.6	99.2	97.0
Multiplicity	6.9	6.4	6.9
Filtered Mean(chi^2)	1.03	1.12	1.03
Anomalous completeness %	98.1	97.0	96.4
Anomalous multiplicity	3.4	3.4	3.5
DelAnom CC(1/2)	0.055	0.093	0.034
Mid-Slope of Anom Probability	1.038		

Download

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)...

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



Remote data collection saves you time...



...and the planet



For routine data collection at 100 K:

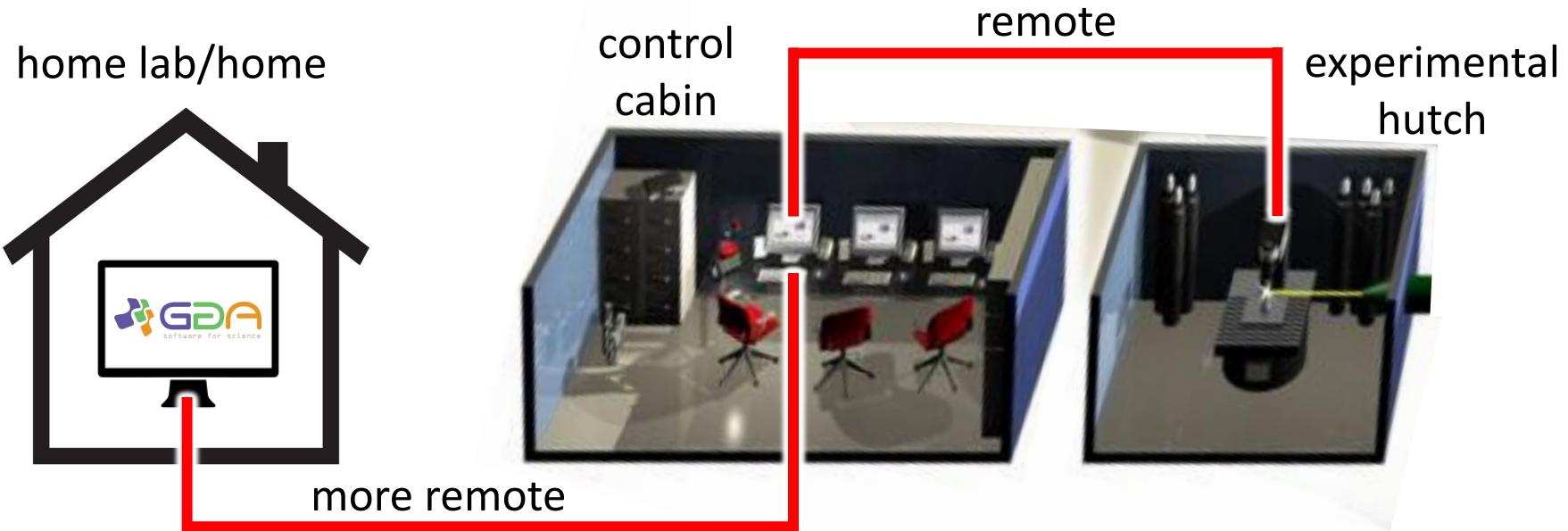
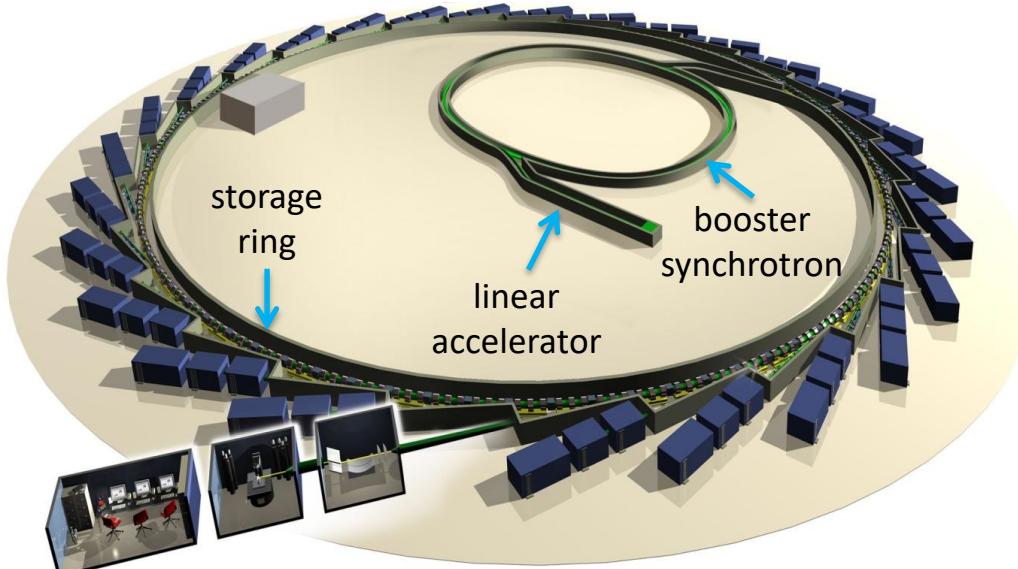
- Samples prepared and cryo-cooled in home lab
- Sample information entered into ISPyB database
- Transported to Diamond in dry shipping dewars
- Samples mounted robotically
- Data collection controlled through GDA interface
- Only manual operation at DLS: loading/unloading pucks
- Everything else computer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



users not permitted
to do this anyway!

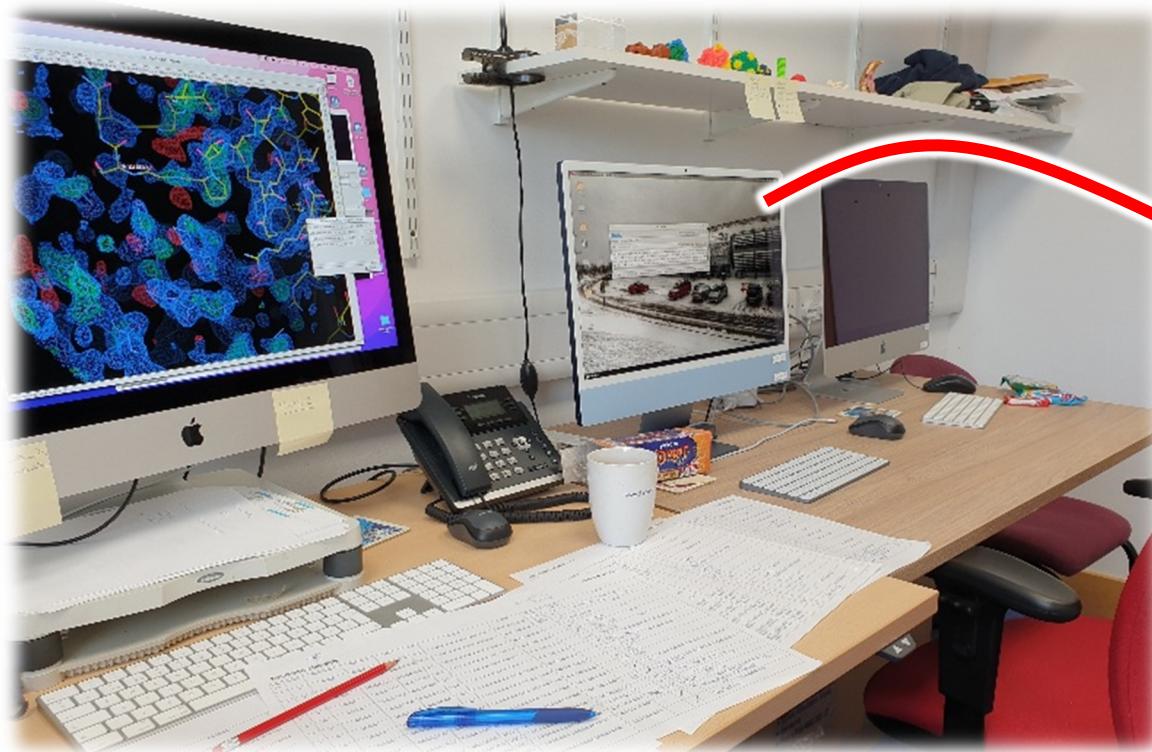
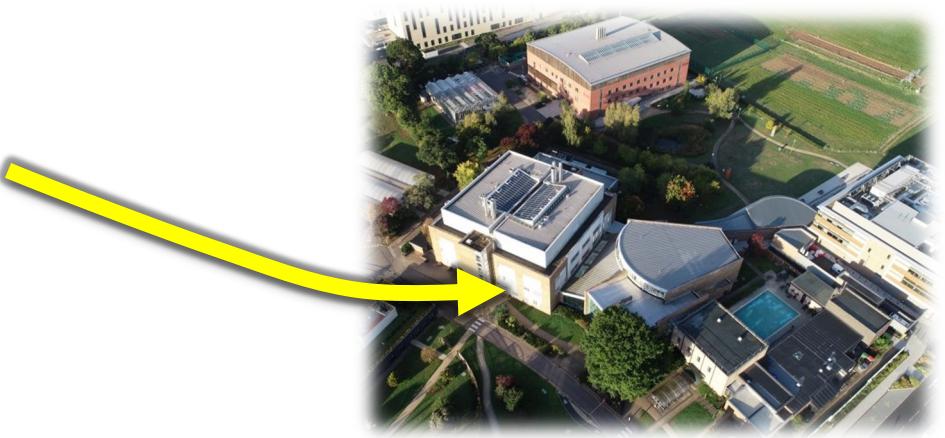
Therefore you don't need to be there!

What is remote data collection?



Remote data collection – in practice

...from here



share screen
with others

Do these 3 things BEFORE your session

1.

Think about the experiments that you want to run

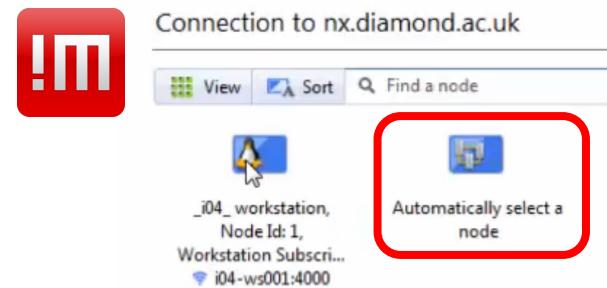
- discuss with your local contact if necessary



2.

Check that your remote NX connection works

- if you are given the option to “automatically select a node”, choose this (unless you are going to collect data)
- if intending to use a 2nd monitor – check it works



3.

While you are connected, read the beamline “message of the day”

- open a Terminal window and type:
- more /dls_sw/<beamline_name>/etc/motd

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!

i04 Webcams & Beamline Status

Ring Current
299.991

Refill
255.758

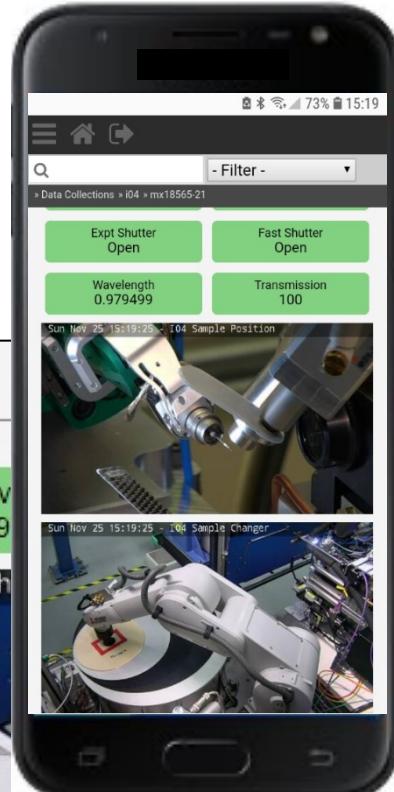
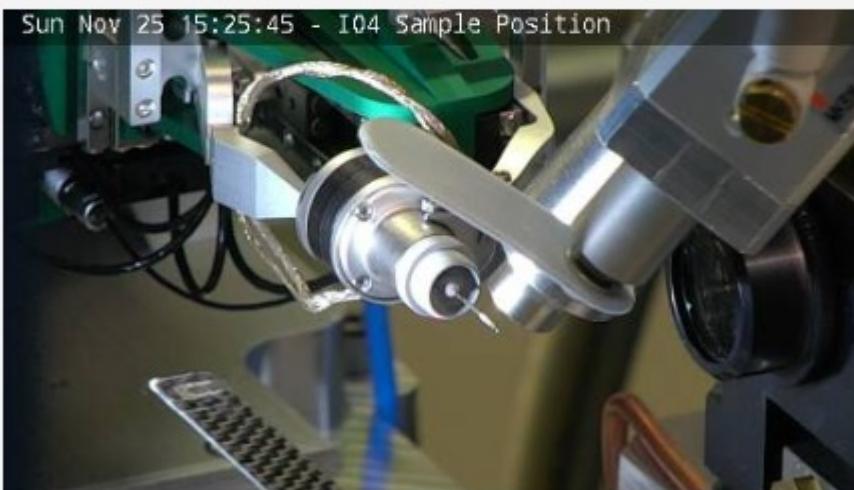
Hutch
Locked

Port Shutter
Open

Expt Shutter
Open

Fast Shutter
Open

Wav
0.9



If you suspect a problem – call the EHC!

If you see no diffraction – 3 main causes:

...could be all 3



"Houston – we have a problem"



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



(2) you are doing something wrong



(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:

- 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
- 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
 - request an on-site session

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