

Optimising the Diamond experience from a user's perspective

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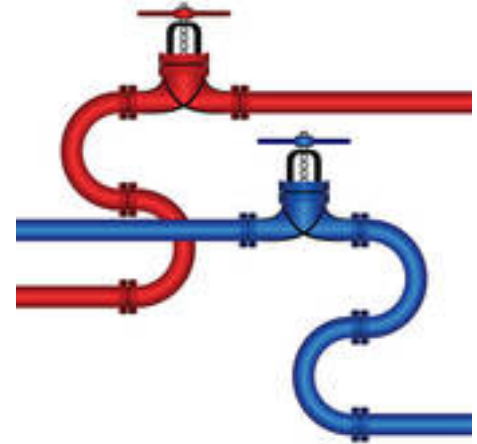
Strategy



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 (get a life!)

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 (get a life!)

- 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!

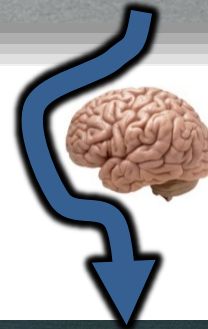
Do as much of this thinking **before** your beamtime as possible!

MX data collection has become faster...

20th century data collection



21st century data collection

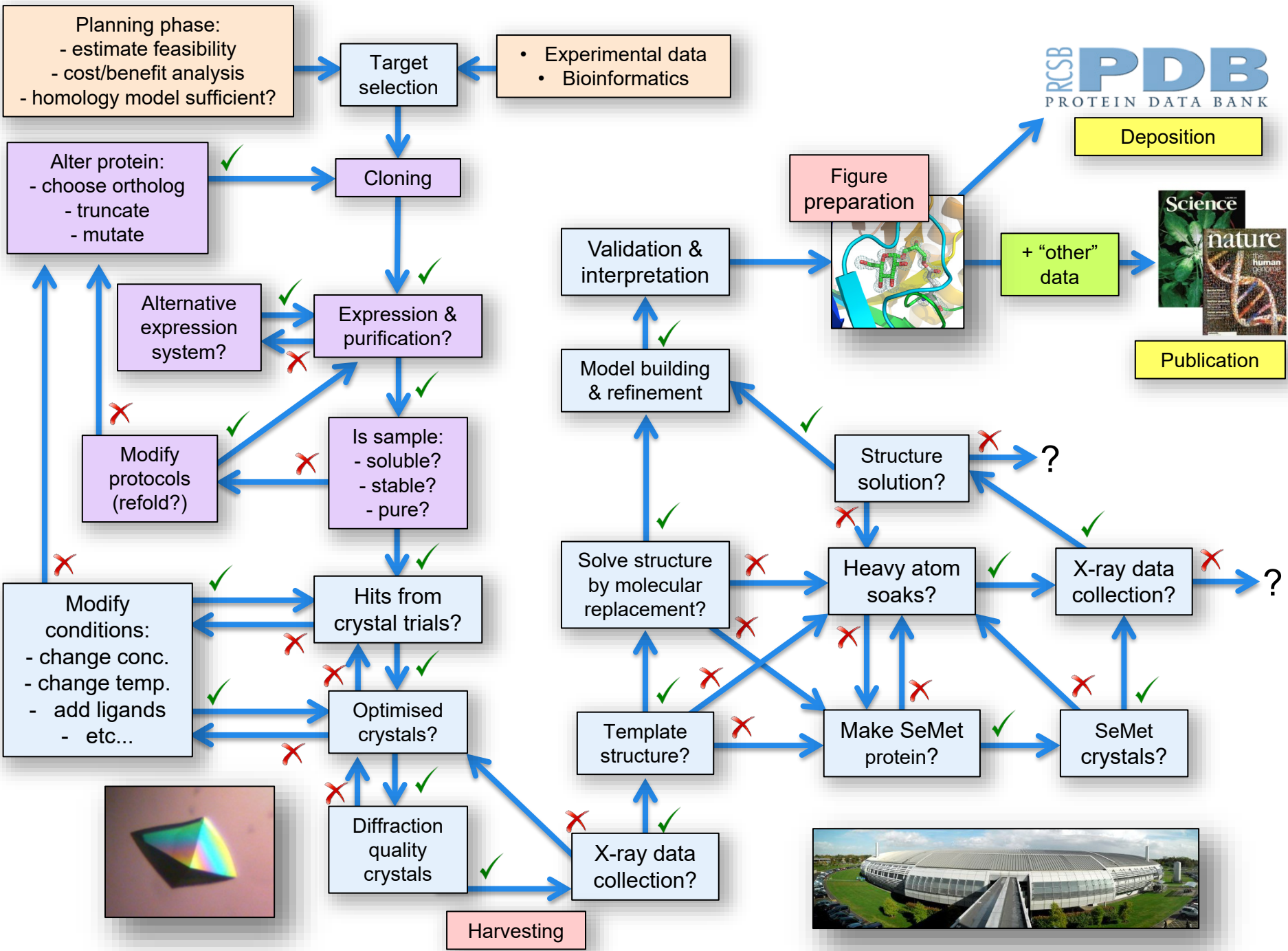


MX data collection has become much faster...

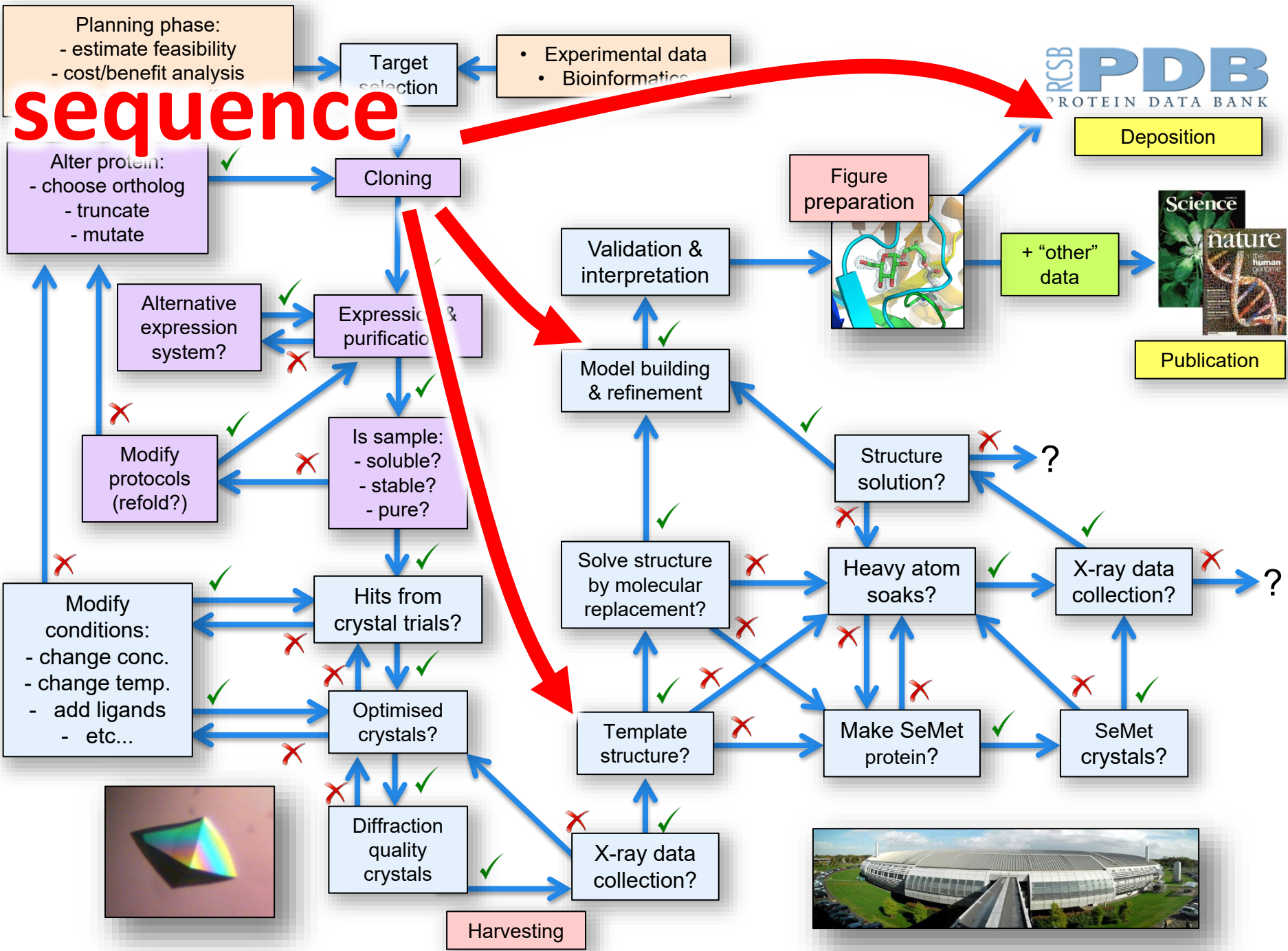
- In theory, could collect one dataset every 5 mins
(mounting + alignment + collection)
- In practice, 4 “useful” data sets per hour is good
 - includes screening for “best” crystal
 - ...and thinking!
- But - beamtime is still in high demand
 - users are generating crystals more rapidly
 - can get away with “marginal” samples
- Each session is often split between several groups
 - therefore need to be efficient and organised...

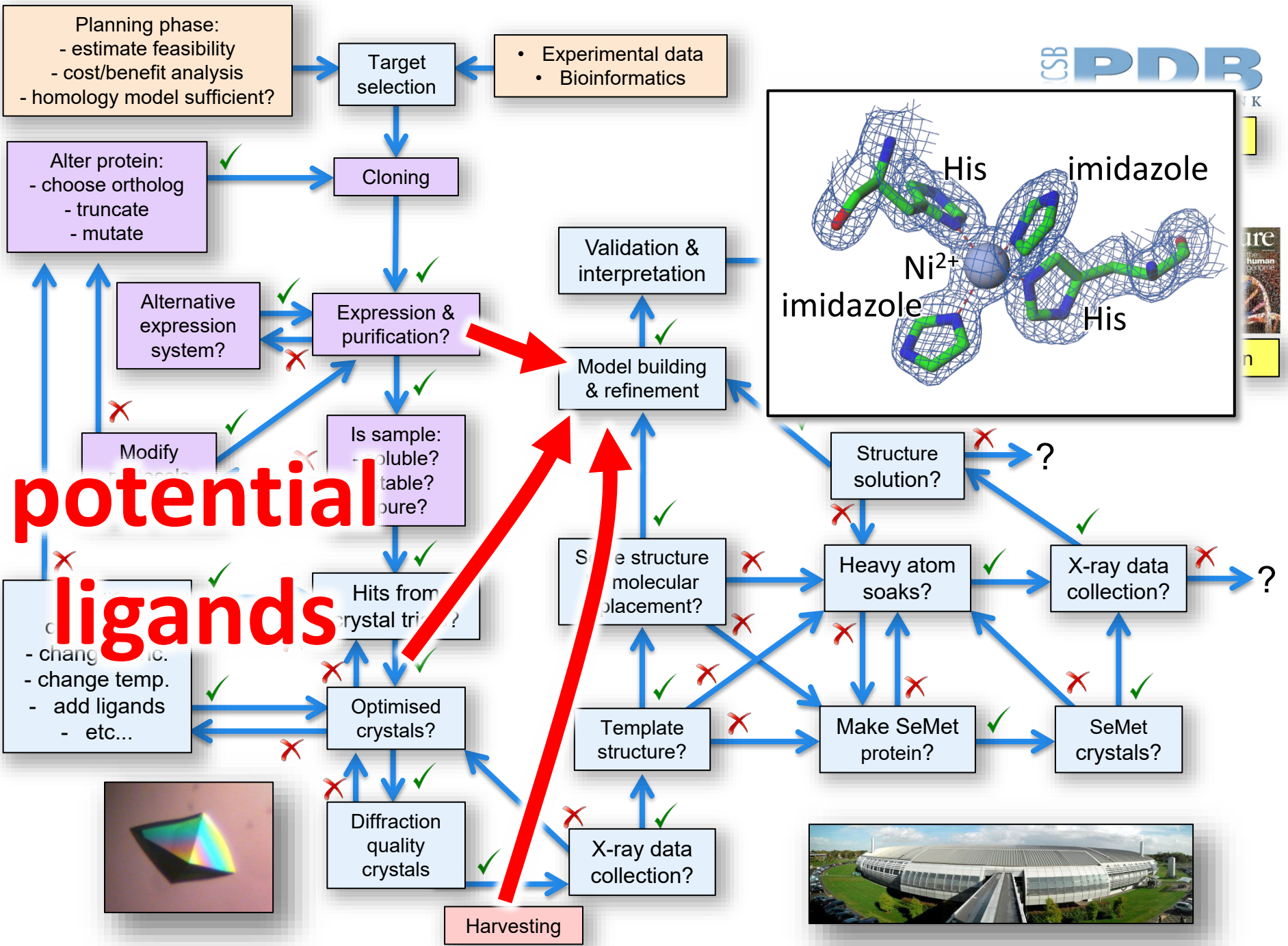


“Take back control”

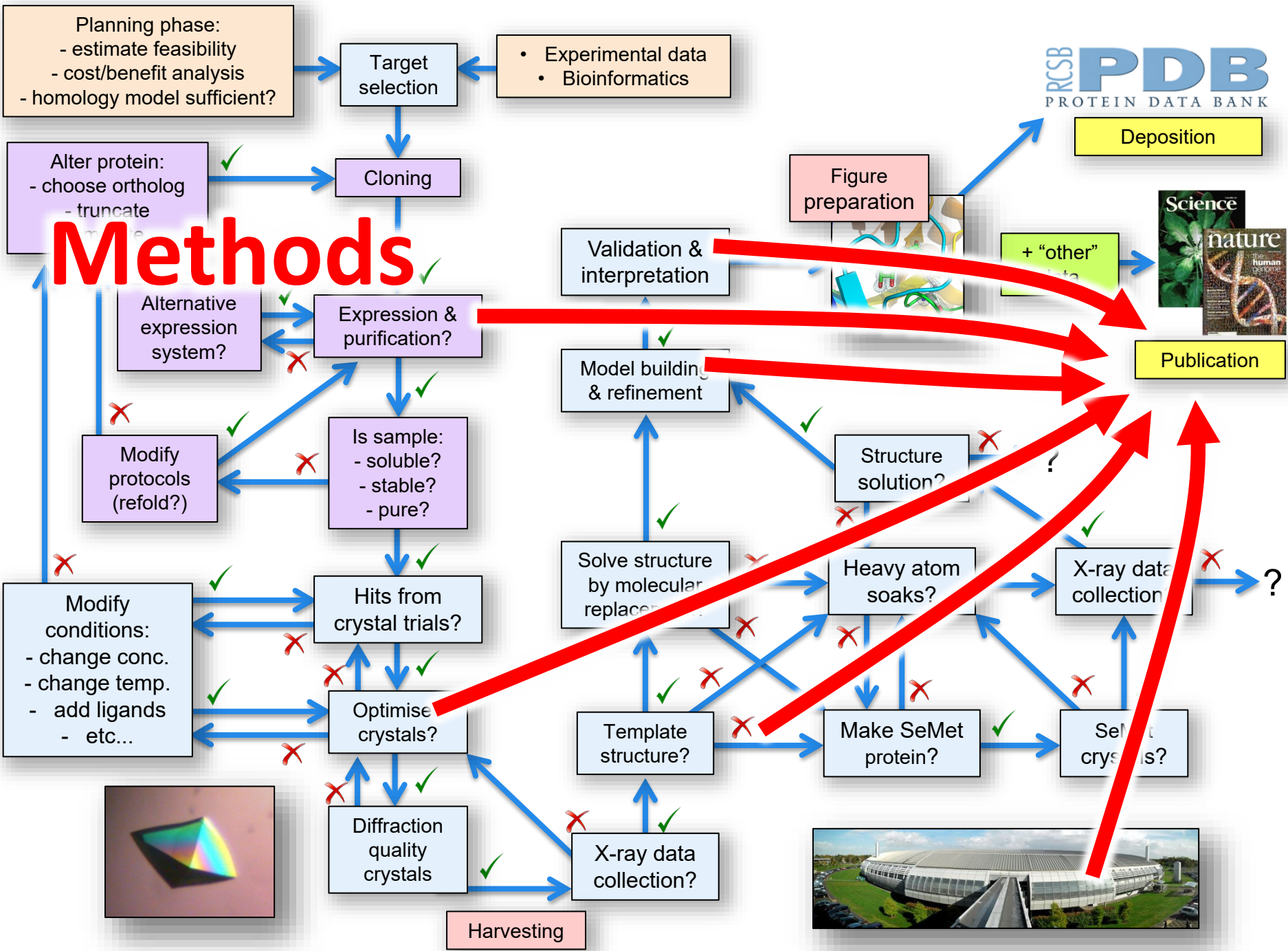


sequence





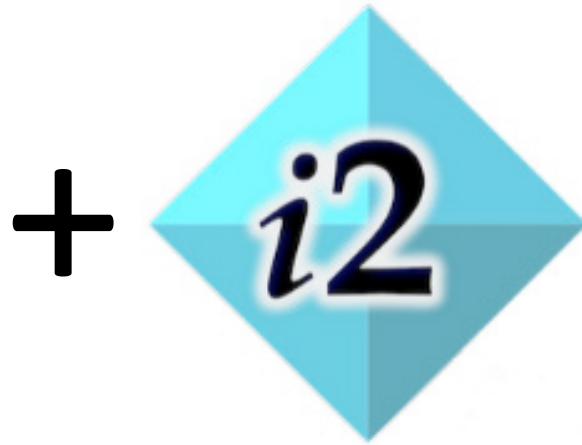
Methods



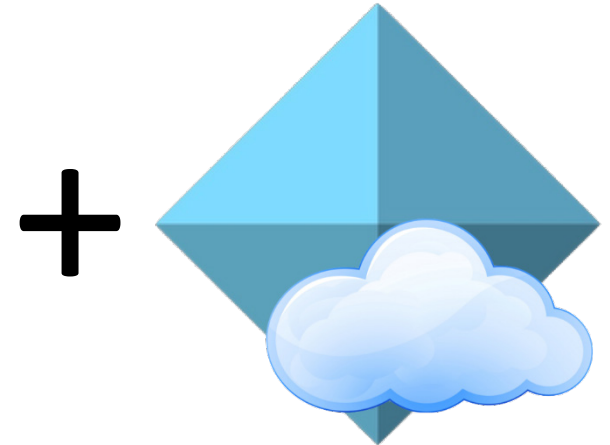
Taking back control...



ISPyB



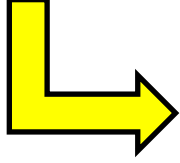
CCP4i2



CCP4 Cloud

F•R•I•E•N•D•S

Sample
info.



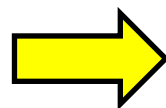
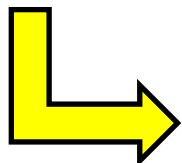
ISPyB database





ISPyB database

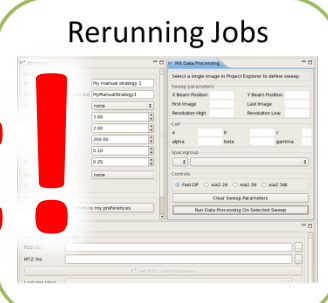
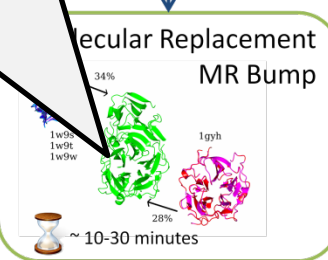
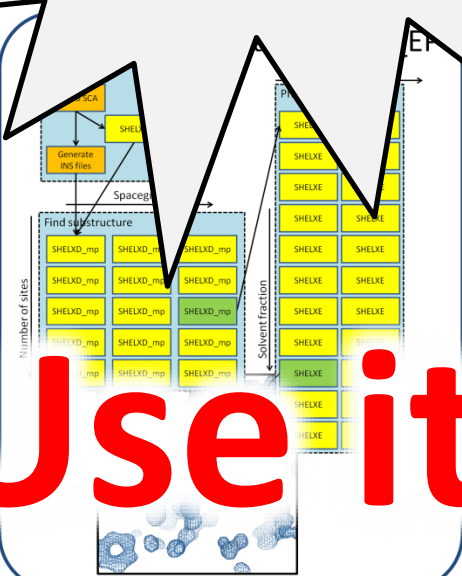
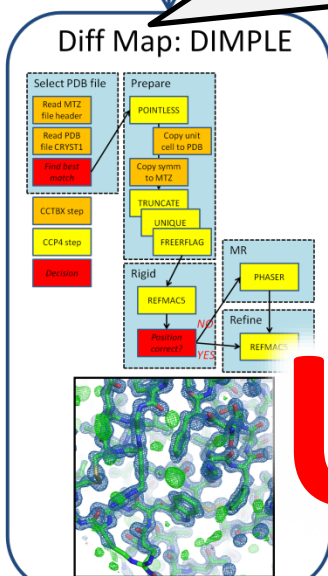
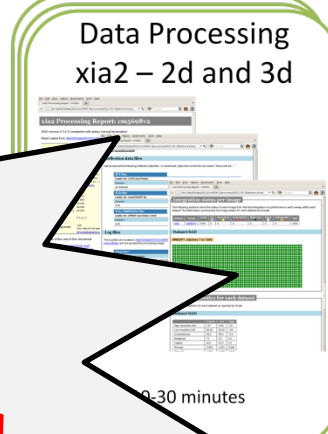
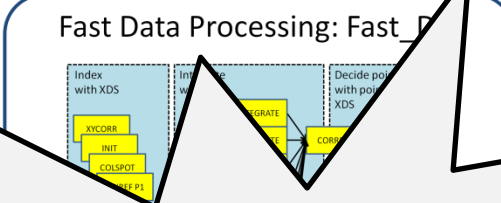
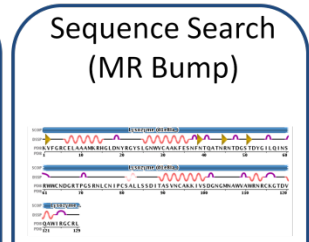
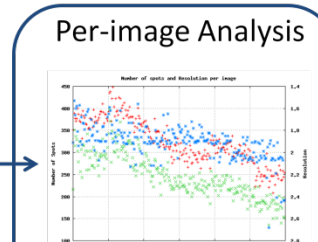
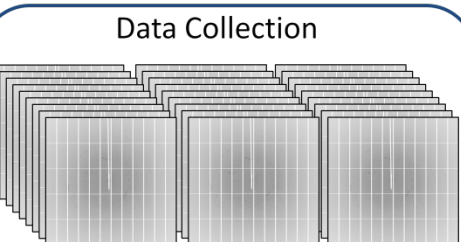
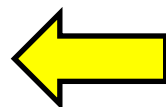
Sample info.



(test images)



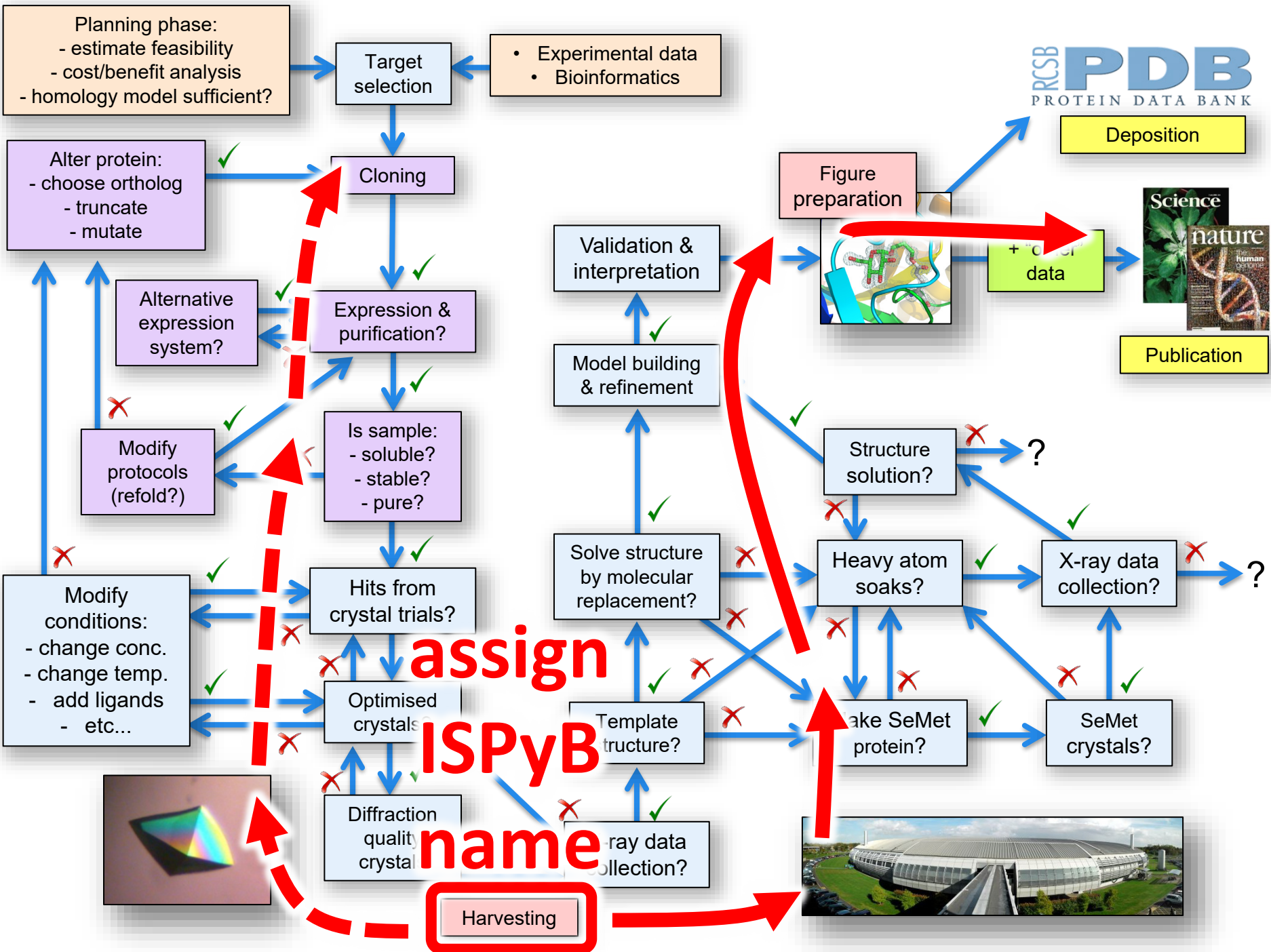
Strategy:
EDNA
Xia2



Each crystal has a unique "ISPyB name"!

Use it!

240



Date: 29-JUL-2017

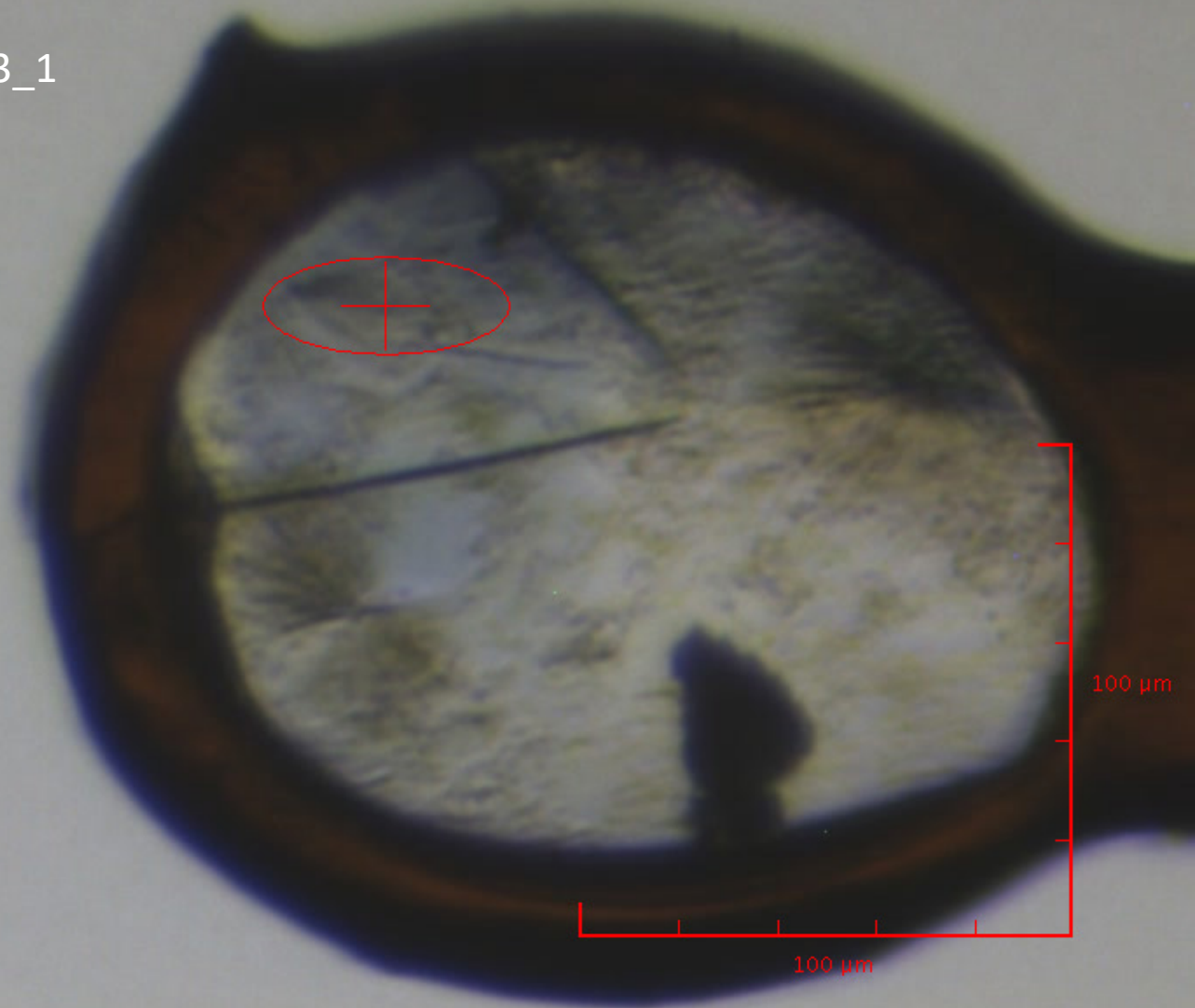
Beamline: i03 Diamond

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

Container: DLS-442

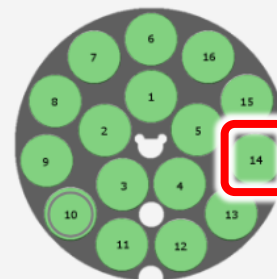
This page shows the contents of the selected container. Samples can be added and edited by clicking the pencil icon, and removed by clicking the x

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		

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this is **UNIQUE**

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_22				
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

Puck number – DLS442

Position	Person	Protein name	IsprB_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 oxogeralial+ 20%EG				10mM soak for approx 1 h
11	Benjy	NmADH9	NmADH9_20	MCBL0004	A11.1	"	8 oxogeralial+ 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
							8-oxogeralial+ 20%EG				5mM soak for approx 1 h

MX13467-41 7 hrs I03 from 12:00 Sat 29 Jul 2017 to 19:00 Sat 29 Jul 2017

First Local Contact: Dr Katherine McAuley (01235 778405)

Beamline I03: 01235 778707

Experimental Hall Coordinator: 01235 778787

Institution	JIC	Group(s)	Lawson
Contact name(s) and number(s)	Dave Lawson: 01603 123456 / 07778 123456		
Approx. timings	12:00 – 15:00	On-site/remote?	Remote
Dewar ID	Puck ID (# samples)	Users and comments	
DLS-MX-0002	DLS0086 (16 samples)	Sue	
	DLS0087 (12 samples)	JC	
	DLS0090 (12 samples)	Sue	
	DLS442 (16 samples)	Benjy	
Anomalous elements:	Zn		
Other requirements:	MCA scans		
Comments/ questions:			

annotate during data collection – helps decision making

Decide on a running order for users and samples – share your plans with LC and EHC

Institution	UEA	Group(s)	Hemmings
Contact name(s) and number(s)	Andrew Hemmings: 01603 123456/07799 123456		
Approx. timings	15:00 – 19:00	On-site/remote?	Remote
Dewar ID	Puck ID (# samples)	Users and comments	

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....

Data Collection Settings

☐ Data Collection Settings ☒ Plate View ☒ **Screening** ☐ Command Queue

Run Scan

Sample

NmADH9_23

Strategies...

Barcode NR

Holder 2

Position 14

Files

Visit directory
/dls/i03/data/2017/mx13467-41

Folder **Configure Defaults**
JIC/\${proteinacronym}/\${samplename}

Prefix **Configure Defaults**
\${samplename}

☒ Automatic run number

Run number 0

Comment
EDNAStrategy1: subWedge:1

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

Beam and Detector

Maximum resolution 1.3000 Å

Detector distance 213.5 mm

Wavelength 0.97623 Å

Energy 12700.3 eV

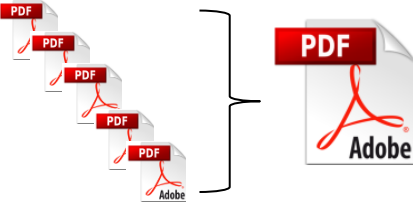
☐ Use current energy

Transmission 50.156283 %

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

Gives: /dls/{beamline}/data/{year}/{visit-ID}/{your-name}/{proteinacronym}/{samplename}/{samplename}_{run_no.}_{image_no.}.cbf

e.g.: /dls/i03/data/2017/mx13467-41/JIC/NmADH9/NmADH9_23/NmADH9_23_1_3600.cbf



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

12:00 29-07-2017

Sample	Images	Res	λ	Q Osc	Spacegroup	Unit Cell	Processed Resolution	Rmeas	Completeness	Comments
NmADH9_23	3600	1.5	0.9763	0.10	P 1 2 1	63.84, 107.75, 90.00, 104.25, 90.00	29.77 - 1.5, 29.77 - 6.7, 1.54 - 1.5	0.085, 98.8, 0.036, 98.7, 0.024, 96.9		(-262, -192, 1150) EDNAStrategy1: subWedge:1Aperture: Medium
NmADH9_24	3	1.5	0.9763	0.50						(-107, -190, 1012) Aperture: Medium
NmADH9_24	3	1.5	0.9763	0.50						(-107, -190, 1012) Aperture: Small
NmADH9_25	3	1.5	0.9763	0.50						(-156, -228, 1396) Aperture: Medium
NmADH9_25	3	1.5	0.9763	0.50						(-156, -228, 1396) Aperture: Small
NmADH9_15	3	1.5	0.9763	0.50						(-247, -388, 861) Aperture: Medium
NmADH9_15	42	3.0	0.9763	0.00						Diffraction grid scan of 7 by 6 images, Top left (350,177), Bottom right (576,463)
NmADH9_15	12	3.0	0.9763	0.00						Diffraction grid scan of 3 by 4 images, Top left (472,245), Bottom right (576,463)
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, 107.76, 71.76, 90.00, 105.05, 90.00	30.02 - 3.04, 29.02 - 3.16, 3.12 - 3.04	0.167, 99.4, 0.040, 99.0, 0.033, 93.3		(-276, -373, 844) EDNAStrategy1: subWedge:1Aperture: Medium
NmADH9_11	3	2.0	0.9763	0.50						(-477, -294, 1143) Aperture: Medium
NmADH9_12	3	2.0	0.9763	0.50						(-696, -216, 1130) Aperture: Medium
NmADH9_12	3	1.6	0.9763	0.50						(-696, -216, 1130) Aperture: Small
NmADH9_12	3600	1.6	0.9763	0.10	P 1 2 1	63.84, 108.11, 69.29, 90.00, 104.25, 90.00	29.74 - 1.69, 29.74 - 6.38, 1.73 - 1.69	0.085, 98.8, 0.036, 98.7, 0.024, 96.9		(-496, -216, 1130) EDNAStrategy1: subWedge:1Aperture: Medium
TAPHY_27_1	4	3.0	0.9763	0.00						Diffraction grid scan of 1 by 4 images, Top left (540,265), Bottom right (576,463)
TAPHY_27_1	3	1.8	0.9763	0.50						(-109, -296, 1303) EDNAStrategy1: subWedge:1Aperture: Medium
TAPHY_27_1	1200	1.5	0.9763	0.10	H 3	126.66, 126.66, 1207.16, 90.00, 90.00, 120.00	29.27 - 1.92, 29.27 - 6.38, 1.97 - 1.92	0.078, 99.0, 0.036, 96.6, 0.094, 95.9		(-109, -296, 1303) EDNAStrategy1: subWedge:1Aperture: Medium
TAPHY_27_2	5	3.0	0.9763	0.00						Diffraction grid scan of 1 by 5 images, Top left (534,251), Bottom right (576,463)
TAPHY_27_2	3	1.5	0.9763	0.50						(-136, -104, 1462) EDNAStrategy1: subWedge:1Aperture: Medium

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29.07.2017_03_rml1367-41 - Excel										
File Home Insert Page Layout Formulas Data Review View ACROBAT Tell me what you want to do										
Clipboard Font Alignment Number Conditional Format as Formatting Table- Check Cell Bad Explanatory... Input Neutral Cell Ca										
Styles										
AS4										
NmADH9_23										
A	B	C	D	E	F	G	H	I	J	K
40	NmADH9_103	1	0.97625	289.0478	0.04	0	0.5	211.6297	206.4712	1.6 (272,-419,809) Aperture: Medium
41	NmADH9_103	1	0.97625	289.0478	0.04	0	0.5	211.6297	206.4712	1.6 (-231,-681,1252) Aperture: Medium
42	NmADH9_103	3	0.97625	289.0478	0.04	0	0.5	211.6297	206.4712	1.6 (-249,-175,1442) Aperture: Medium
43	NmADH9_103	1	0.97625	289.0478	0.04	0	0.5	211.6297	206.4712	1.6 (-249,-175,1442) EDNAStrategy1: subWedge:1Aperture: Medium
44	NmADH9_103	8	0.97625	289.0478	0.04	0	0.5	211.6297	206.4712	1.6 (-533,7,1513) Aperture: Medium
45	sample 103	8	0.97625	602.2545	0.1	-0.00016	0	0.5	211.7341	204.4354
46	sample 103	9	0.97625	602.2545	0.1	89.99975	0	0.5	211.7341	204.4354
47	NmADH9_103	2	0.97625	427.9818	0.04	0	0.5	211.676	205.5681	2.2 (-488,25,1516) Aperture: Medium
48	NmADH9_103	1	0.97625	427.9818	0.04	0	0.5	211.676	205.5681	2.2 (-496,457,1456) Aperture: Small
49	NmADH9_103	3	0.97625	427.9818	0.04	0	0.5	211.676	205.5681	2.2 (-25,110,1069) Aperture: Small
50	sample 103	10	0.97625	602.2545	0.1	89.99975	0	211.7341	204.4354	2.9967 Diffraction grid scan of 7 by 5 images, Top left (327,239), Bottom right (576,463)
51	sample 103	11	0.97625	602.2545	0.1	179.9997	0	211.7341	204.4354	2.9966 Diffraction grid scan of 7 by 4 images, Top left (469,262), Bottom right (576,463)
52	NmADH9_103	2	0.97625	427.9818	0.04	0	0.5	211.676	205.5681	2.2 (-33,96,1067) Aperture: Small
53	NmADH9_103	1	0.97625	359.8787	0.01	106	0	0.5	211.6533	206.0108
54	NmADH9_103	1	0.97625	427.9818	0.04	0	0.5	211.676	205.5681	2.2 (-241,-208,1371) Aperture: Medium
55	NmADH9_103	2	0.97625	427.9818	0.04	0	0.5	211.676	205.5681	2.2 (-262,-192,1150) Aperture: Medium
56	NmADH9_103	3	0.97625	264.5335	0.04	0	0.5	211.6215	206.6305	1.5 (-262,-192,1150) Aperture: Medium
57	NmADH9_103	1	0.97625	213.4382	0.01	45	0	0.5	211.6045	206.9627
58	NmADH9_103	1	0.97625	264.5335	0.04	0	0.5	211.6215	206.6305	1.5 (-107,-190,1012) Aperture: Medium
59	NmADH9_103	2	0.97625	264.5335	0.04	0	0.5	211.6215	206.6305	1.5 (-107,-190,1012) Aperture: Small
60	NmADH9_103	1	0.97625	264.5335	0.04	0	0.5	211.6215	206.6305	1.5 (-156,-228,1396) Aperture: Medium
61	NmADH9_103	2	0.97625	264.5335	0.04	0	0.5	211.6215	206.6305	1.5 (-213,-228,1406) Aperture: Medium
62	NmADH9_103	2	0.97625	264.5335	0.04	0	0.5	211.6215	206.6305	1.5 (-247,-388,861) Aperture: Medium
63	sample 103	4	0.97625	385.1022	0.01	-0.00016	0	211.7341	204.4353	2.9966 Diffraction grid scan of 7 by 6 images, Top left (350,177), Bottom right (576,463)
64	sample 103	13	0.97625	602.2595	0.1	89.99975	0	211.7341	204.4353	2.99662 Diffraction grid scan of 3 by 4 images, Top left (472,245), Bottom right (576,463)
65	NmADH9_103	3	0.97625	264.5335	0.04	0	0.5	211.6215	206.6305	1.5 (-276,-373,844) Aperture: Medium
66	NmADH9_103	4	0.97625	382.8205	0.04	0	0.5	211.6609	205.8617	2 (276,-373,844) Aperture: Medium
67	NmADH9_103	1	0.97625	385.1022	0.01	103	0	211.6617	205.8468	2.01 (276,-373,844) EDNAStrategy1: subWedge:1Aperture: Medium

19:00 26-07-2017

02:00 27-07-2017

02:00

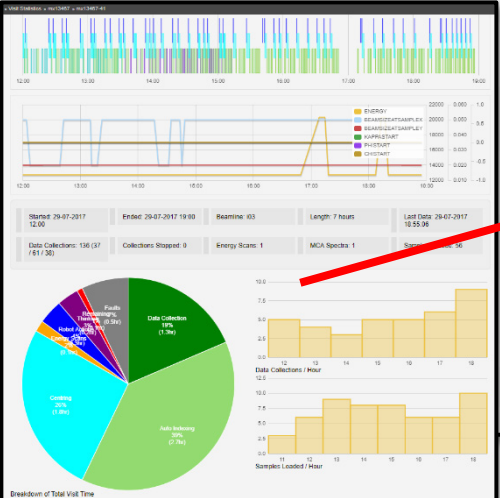
17:00

19:00

12:00

02:00

10



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	Compulsorily Remote
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

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

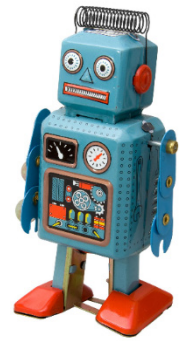
(3) Visit Excel sheet (annotate...)

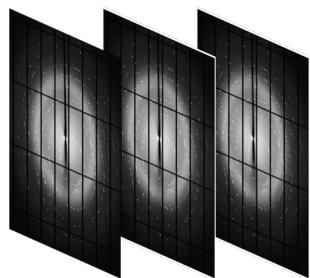
	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T	
1		mx13467-41_i03_29-JUL-2017 - 7 hr - Pilatus3 6M detector (100 Hz)																			
2																					
3		data Image prefix	Run	Sta	Sam	Prot	# imag	Wavele	Dista	Exp.	Phi s	Phi ra	Xbe	Ybe	Det	auto/m	resoln	space gr	cell	twinn	in comments
54		NmADH9_23	2	##	NmADH9	NAI	3	0.9763	428	0.04	0	0.5	212	206	2.2						
55		NmADH9_23	3	##	NmADH9	NAI	3	0.9763	265	0.04	0	0.5	212	207	1.5						
56	12	NmADH9_23	1	##	NmADH9	NAI	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	##	NmADH9	NAI	3	0.9763	265	0.04	0	0.5	212	207	1.5						
58		NmADH9_24	2	##	NmADH9	NAI	3	0.9763	265	0.04	0	0.5	212	207	1.5						

Ideal scenario during session:

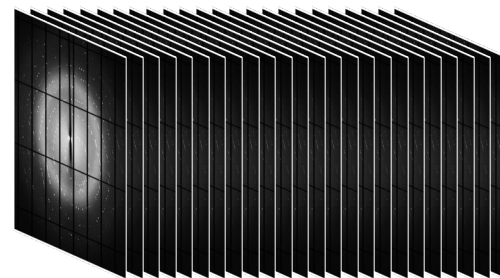
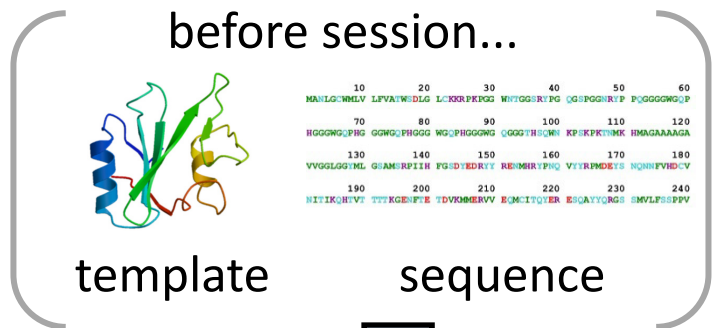
- Load first sample
- Collect test images
- Based on these, decide:
 - to collect...
 - not to collect...
 - to revisit later...
- For a “suitable” sample:
 - devise a data collection strategy
 - collect data set
- Analyse data as they are collected
- Based on this analysis, revise plans if appropriate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

– not practical
without automation

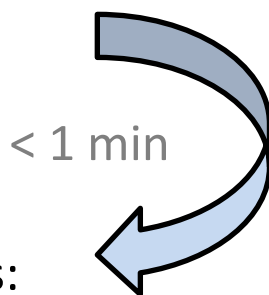




test images



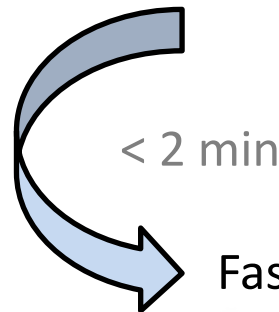
dataset



Strategies:
Mosflm
EDNA
Xia2

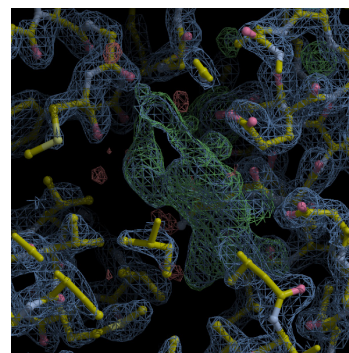


ISPyB

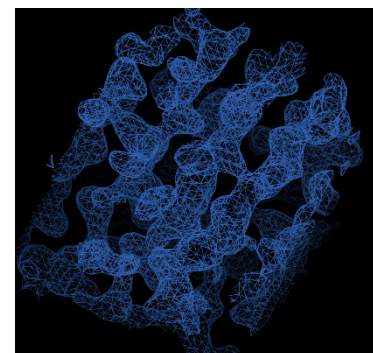


Fast DP

h	k	l	lplus	SIGlplus	lminus	SIGlminus
-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

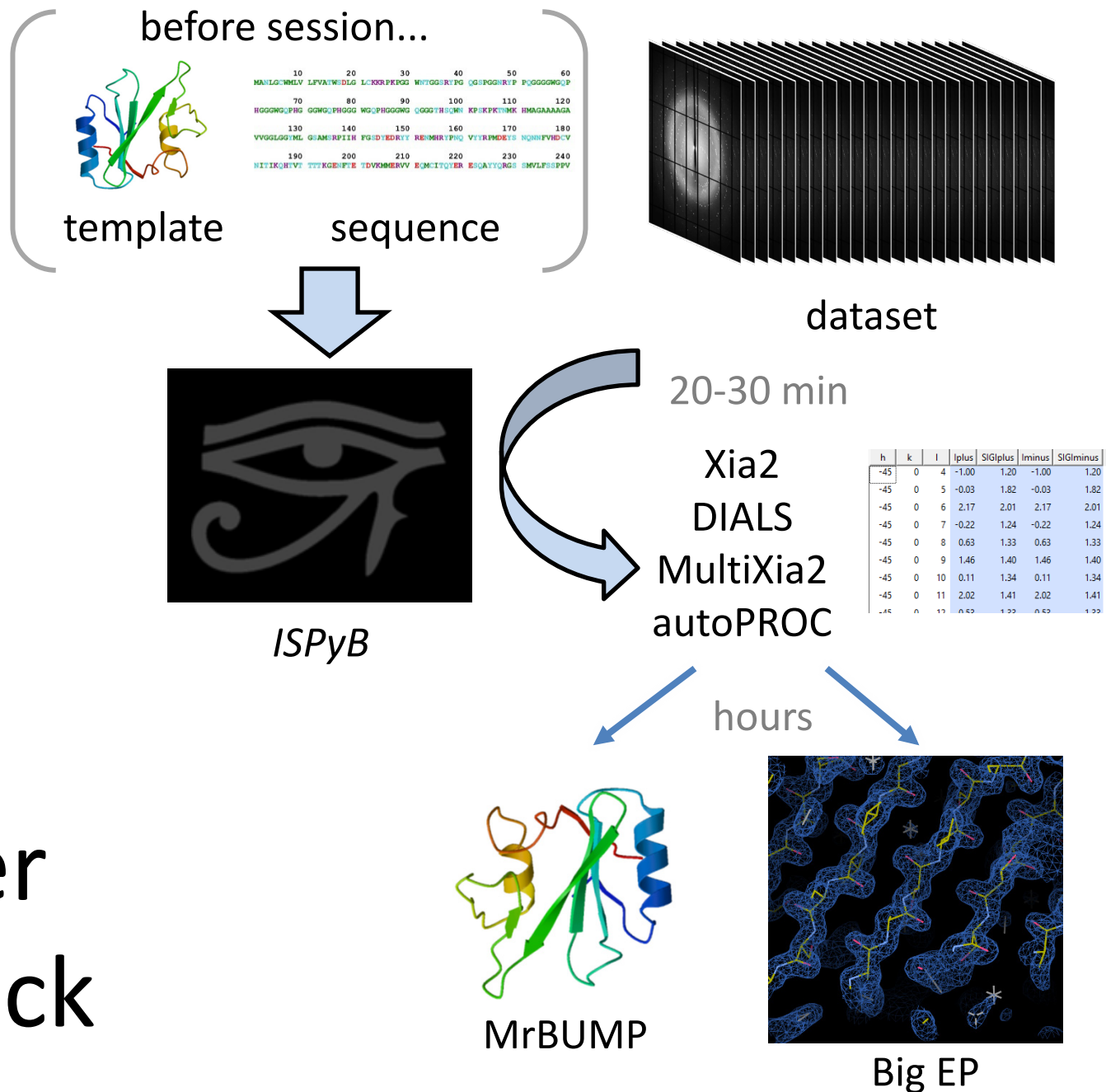


Dimple



Fast EP

Quick
feedback

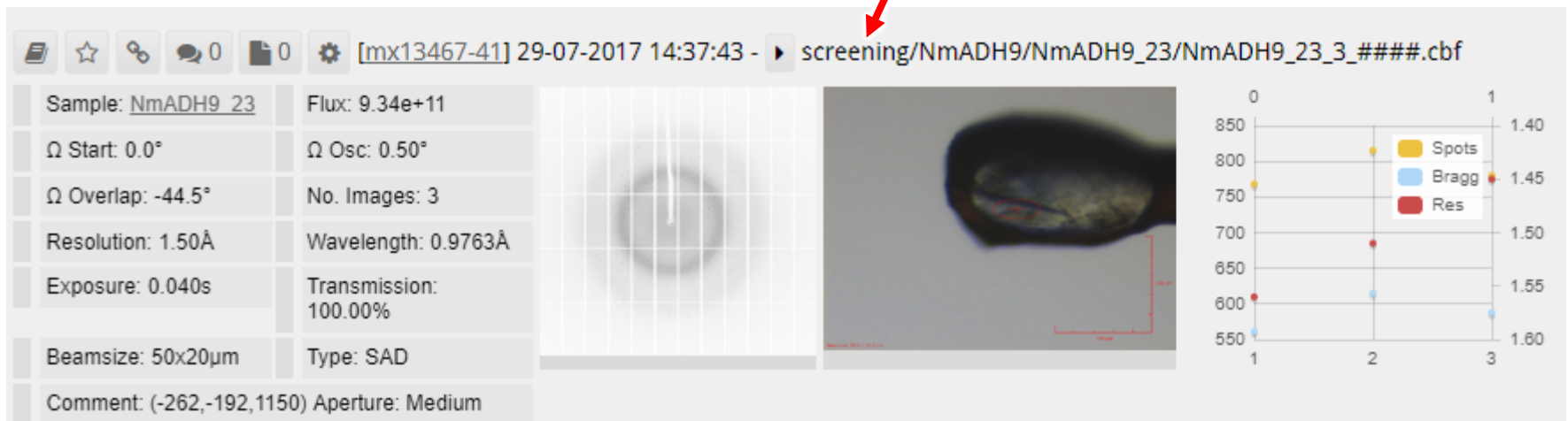


Slower
feedback

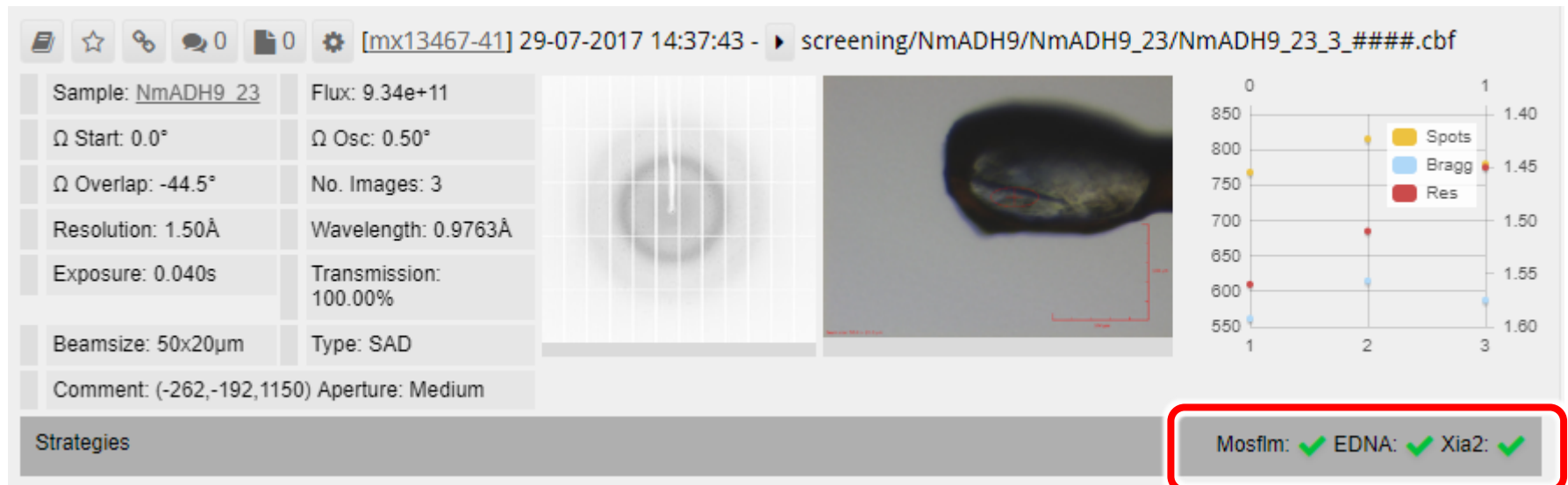
More detail on ISPyB output

Screening...

(using the “screening” tab...)



Screening...



Screening...

Strategies
Mosfilm: ✔ EDNA: ✔ Xia2: ✔

xia2.strategy
Lookup Cell

Space Group	A	B	C	α	β	γ
P 1 2 1	63.87	107.69	69.31	90.00	104.25	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 202s	0	0.15	1.51	1.17	4.0	4	0.010	2214
gentle Wedge1	Gentle: Target Multiplicity=2 I/sig=2 Maxlifespan=20s	6	0.15	1.51	1.29	4.0	4	0.010	2000
high multiplicity Wedge1	Strategy with target multiplicity=16 I/sig=2 202s	0	0.15	1.51	1.17	4.1	4.1	0.010	2400
native Wedge1	Standard Native Dataset Multiplicity=3 I/sig=2 Maxlifespan=202s	162	0.15	1.51	1.14	2.2	2.2	0.010	1947

EDNA MXv1
Lookup Cell

Space Group	A	B	C	α	β	γ
P2	63.99	107.49	69.28	90.00	104.37	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 Maxlifespan=202 s	45	0.10	1.51	1.21	11.0	11	0.010	1630
Strategy2 Wedge1	Standard Anomalous Dataset Multiplicity=16 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 target Maxlifespan=202 s						14.8	0.010	1110
Strategy5 Wedge1	UnderDEV Anomalous Dataset, RadDamage of standard						12.4	0.010	2740

mosfilm
Lookup Cell

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

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

Data Collection Settings
Plate View
Screening

Run Scan

Sample

NmADH9_23

Strategies...

Omega

Start

Oscillation

Collecting a dataset...

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

Q 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	1830

☐ Data Collection Settings ☒ Plate View ☐ Screening ☐ Command Queue

Data Collection Settings

Run Scan

Sample

NmADH9_23 ✖

Strategies...

Barcode NR

Holder 2

Position 14

Files

Visit directory
/dls/i03/data/2017/mx13467-41

Folder [Configure Defaults](#)
JIC/\${proteinacronym}/\${samplena
JIC/NmADH9/NmADH9_23

Prefix [Configure Defaults](#)
\${samplename}
NmADH9_23

☒ Automatic run number

Run number 0

Comment
EDNASTrategy1: subWedge:1

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

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 %

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<l/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 2 1 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 2 1 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 2 1 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 2 1 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/>)

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

Plots

Archive

Logs & Files

Lookup Cell

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

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

Reprocessing:

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

[mx13467-41] 29-07-2017 14:40:37 - JIC/NmADH9/NmADH9_23/NmADH9_23_1_####.cbf

Sample: NmADH9_23	Flux: 1.60e+11
Ω Start: 45.0°	Ω Osc: 0.10°
Ω Overlap: 0°	No. Images: 3600
Resolution: 1.30Å	Wavelength: 0.9763Å
Exposure: 0.010s	Transmission: 50.16%
Beamsize: 50x20µm	Type: SAD

Comment: (262, 102, 1150) EDNA Strategy 1
sub

Reprocess Data

Auto

Multi Crystal

☐ Process Individually | Pipeline : Xia2 3dii | High Res : | Å | Space Group / Cell Options

NmADH9_23_1 - JIC/NmADH9_23/NmADH9/

Sample: NmADH9_23	Ω Start: 45.0°, Osc: 0.10°
Resolution: 1.30Å	Wavelength: 0.9763Å

Start End +

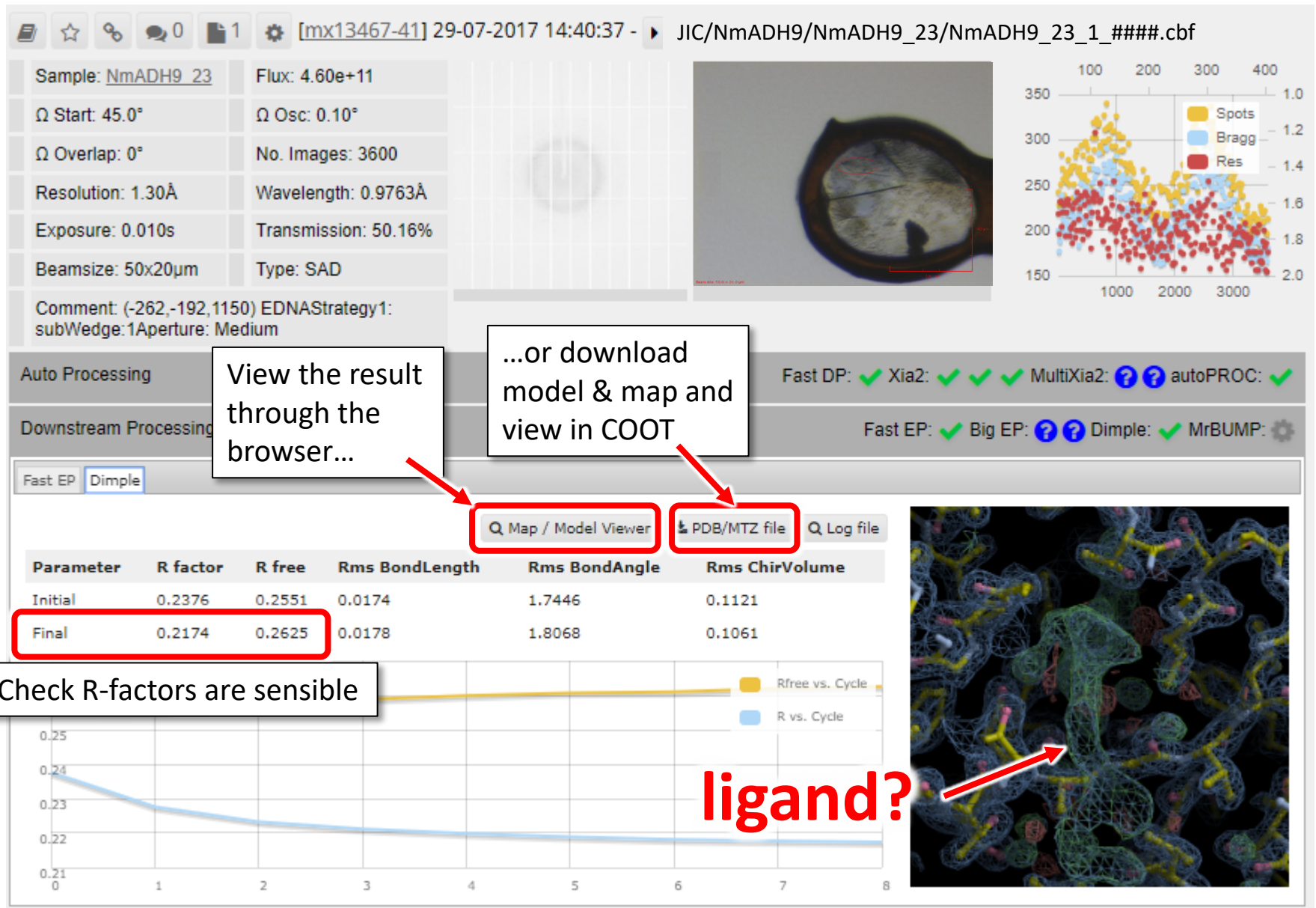
Integrate Close

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

Checking the results...



Checking the results...



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)

- deleted after 40 days
- still available through TopCAT (tape archive)



“Meta” data (all the other “stuff”)

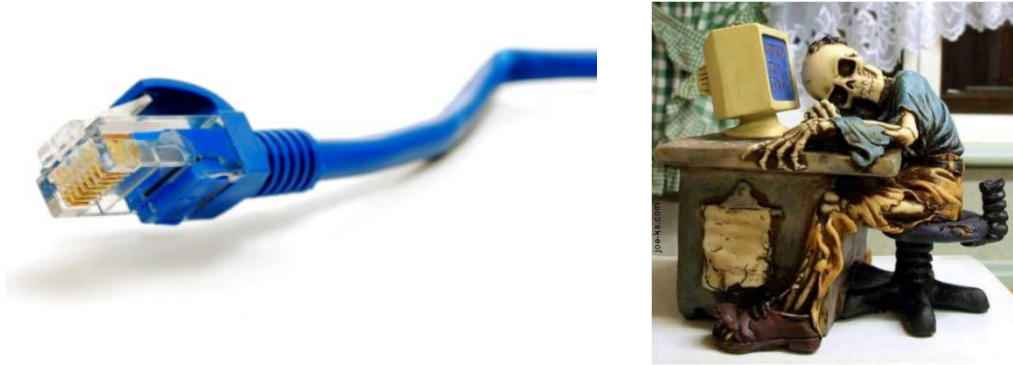
- deleted after 40 days
- not backed up

>90% of useful datasets start 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)



Slow...



Faster?

In the meantime:

- use autoproccessing output or...
- (re)process data remotely on DLS computers and FTP 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:

Create a New Project

Name of project/folder: NmADH9_23_1

By default all projects go in the 'CCP4I2_PROJECTS' directory in your home area - click 'Select directory' to choose an alternative.
Hint to organise your projects: in the 'Manage projects' window you can use a project as a folder and drag other projects into it

Description of project: High res data from binary complex with NAD

Choose tag.. Choose tag.. Choose tag..

New tag

Save

Create project Select directory Cancel Help

Manage projects

Name	Directory	Created	Last active	Tags
NmADH9	C:\Users\la...	18 Oct 18	24 Nov 18	
NmADH9_23_1	C:\Users\la...	24 Nov 18	24 Nov 18	
NmADH9_26_1	C:\Users\la...	24 Nov 18	27 Nov 18	
	C:\Users\la...	24 Nov 18	24 Nov 18	

Open

Add project or folder

Rename project

Edit description

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

Manage project

Name	Directory	Created	Last active	Tags
NmADH9	C:\Users\la...	18 Oct 18	24 Nov 18	
NmADH9_23_1_NAD	C:\Users\la...	24 Nov 18	24 Nov 18	
NmADH9_26_1_apo	C:\Users\la...	24 Nov 18	27 Nov 18	
	C:\Users\la...	24 Nov 18	24 Nov 18	

Open

Add project or folder

Rename project

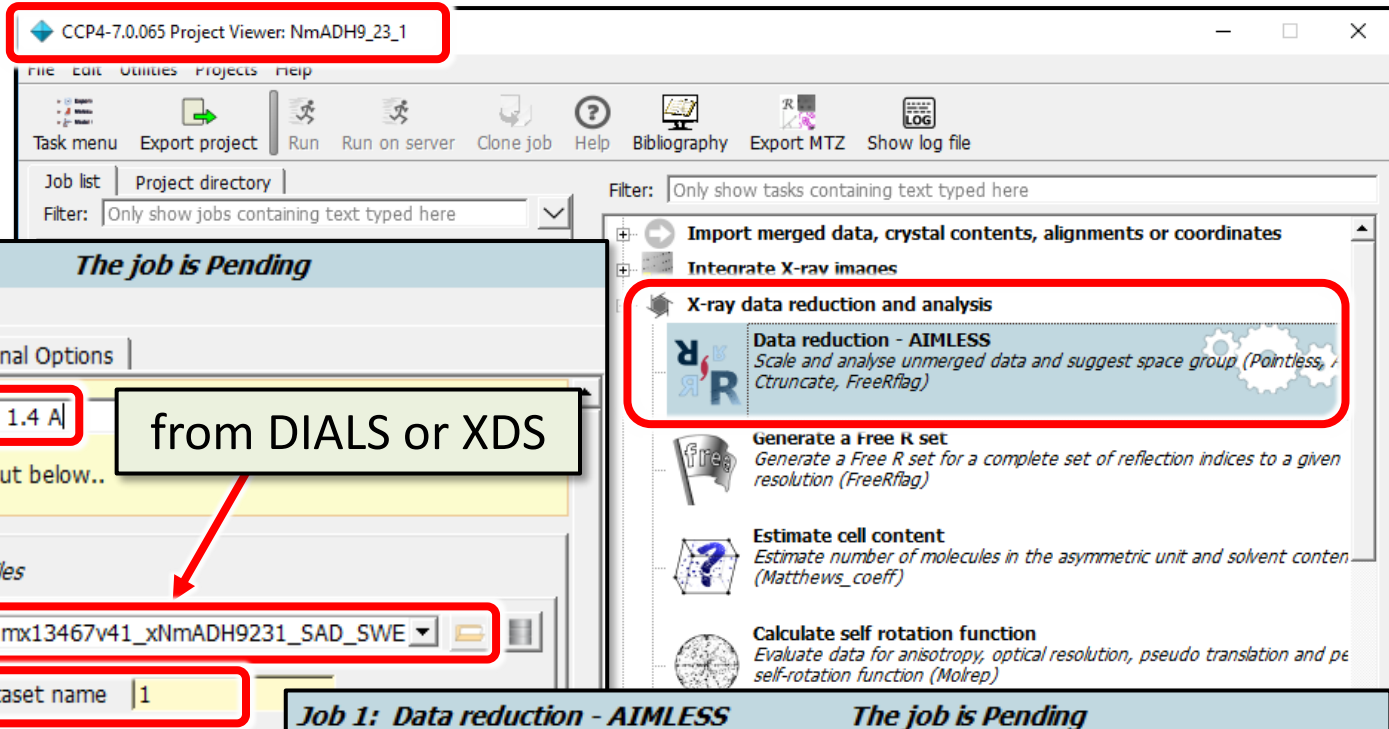
Edit description

*but directory names remain the same

My preferred option for processing...

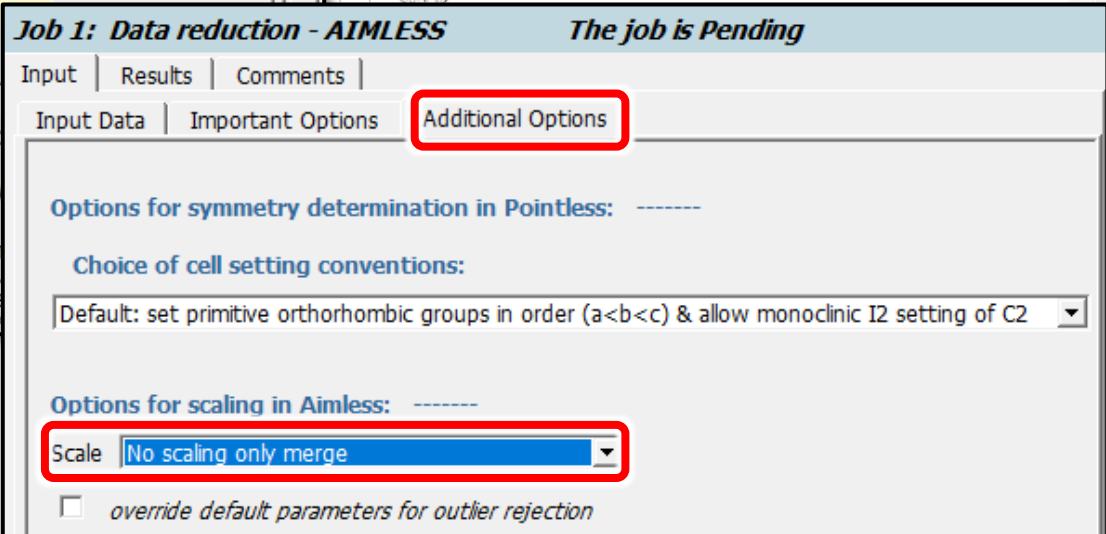
- where the pipelines have done a good job – take part-processed dataset (from the “Meta” data) and re-run the merging step in CCP4i2

use informative
job titles



from DIALS or XDS

may want to change
resolution, exclude
images etc...



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 1.495 Å)

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 0.976250 Å
Resolution of input data: 1.40 Å, resolution estimate: beyond 1.40 Å
Anisotropic limits: - Along 0.99 a° - 0.16 c° 1.48 Å CC(1/2), 1.58 Å I/σ - Along k axis 1.40 Å CC(1/2), 1.42 Å I/σ - Along -0.09 1.40 Å I/σ
Rmeas: overall 0.096, inner bin 0.037
In outer bin: Mean(I)/sd(I) 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 data.

● 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 21 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(I)/sd(I)	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 the Dials User Interface



Integrate images with Dials
Launch DUI and capture output

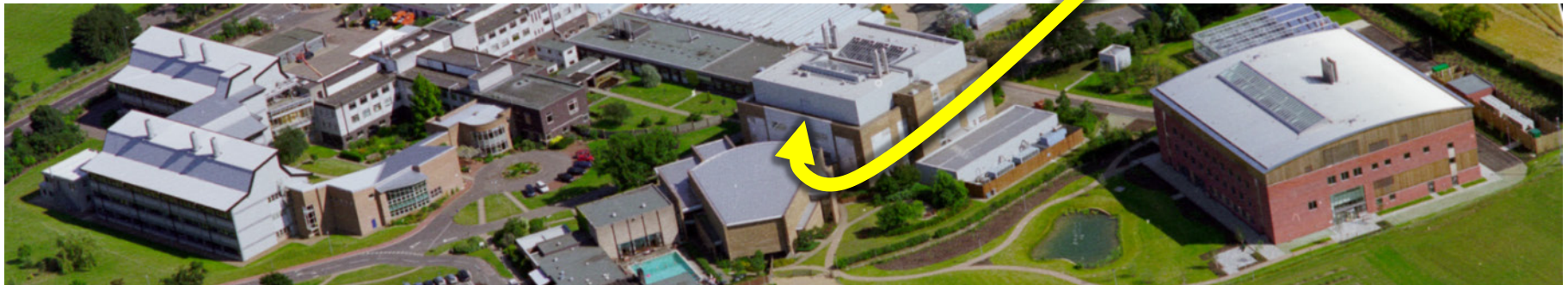
see DIALS talk...

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

...from here



it's 2020...
remote data collection?
it's a no-brainer!

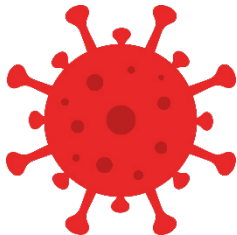
On-site data collection can be a big time commitment...



Remote data collection saves you time...



...and the planet

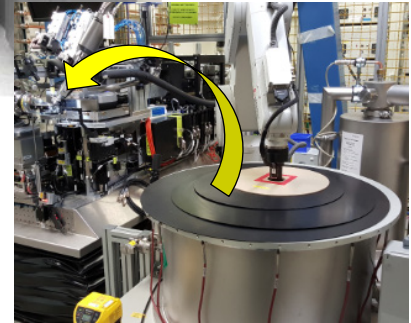
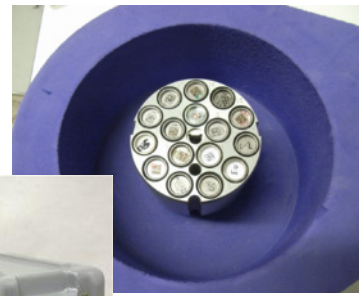


...and is covid-secure



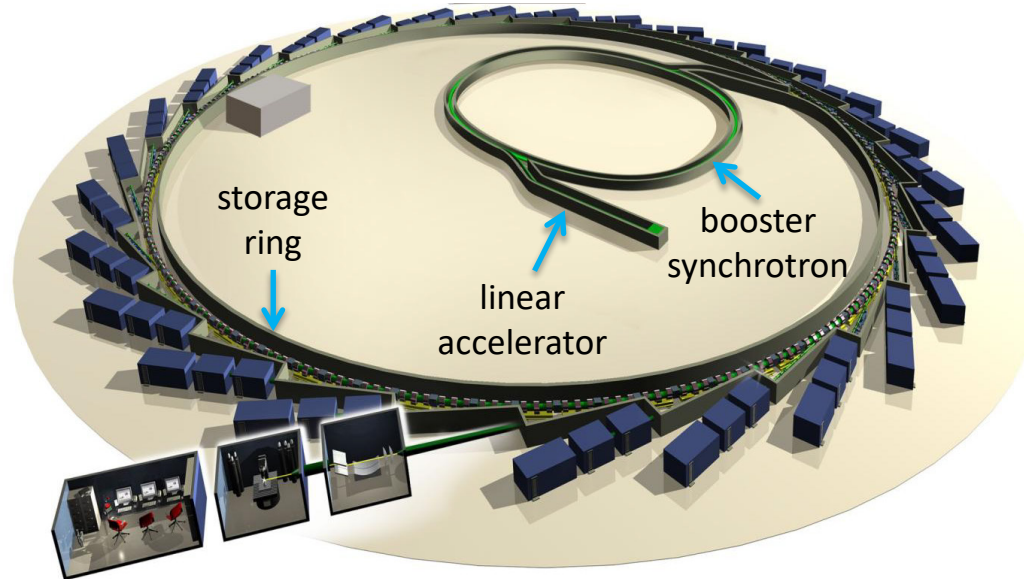
For routine data collection at 100 K:

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



Therefore you don't need to be there!

What is remote data collection?



home lab/home



more remote

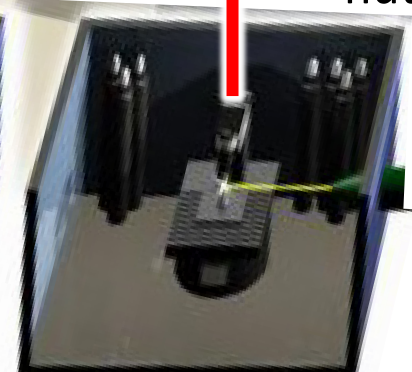
control
cabin



remote



experimental
hutch



iMac with extra
monitor:
(i) data collection
(ii) data evaluation

View
ISPyB

2nd iMac:
(i) data evaluation
(ii) data (re)processing

webcams

GDA
interface

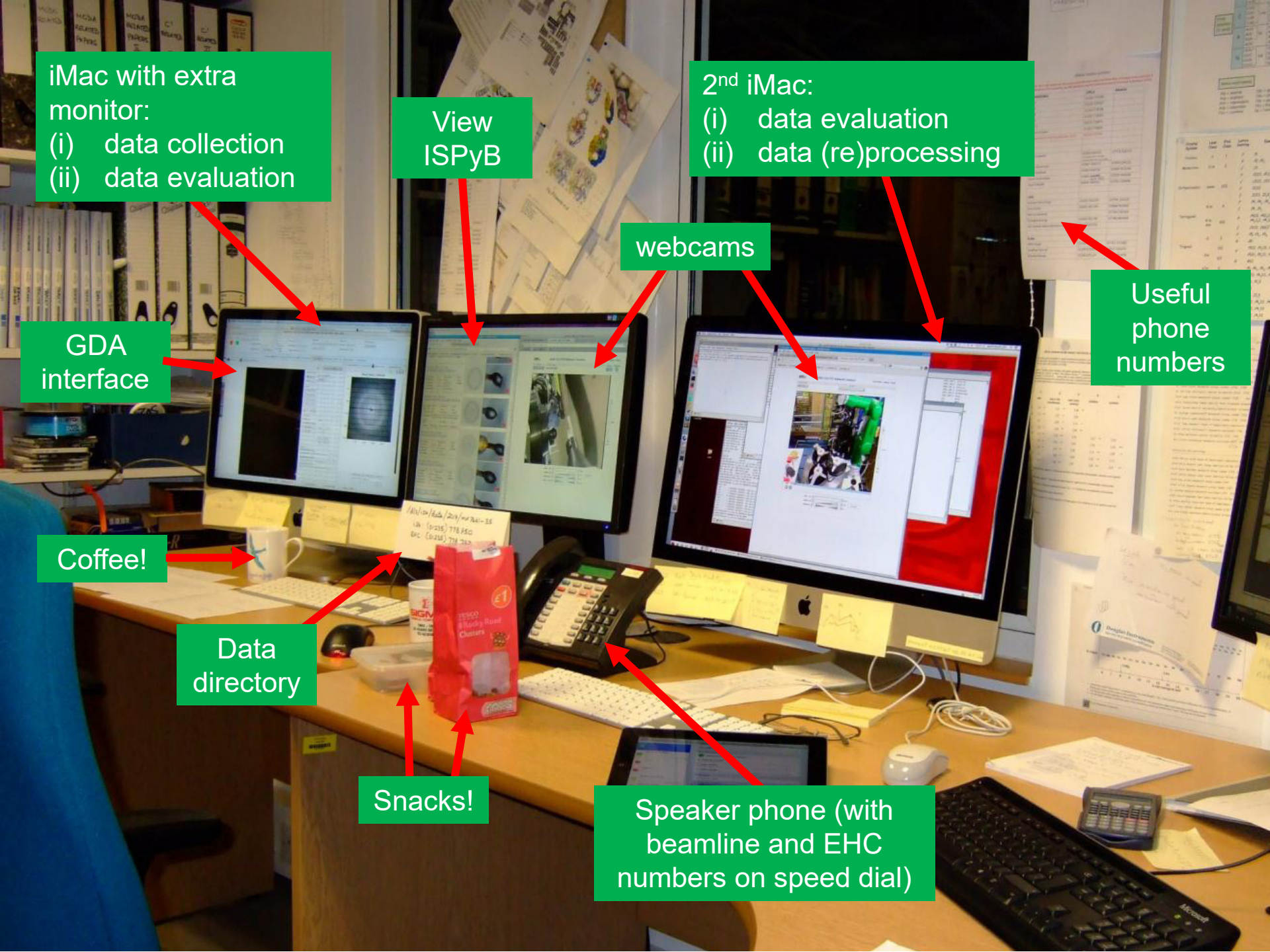
Useful
phone
numbers

Coffee!

Data
directory

Snacks!

Speaker phone (with
beamline and EHC
numbers on speed dial)



Remote data collection

...in 2020



...from here

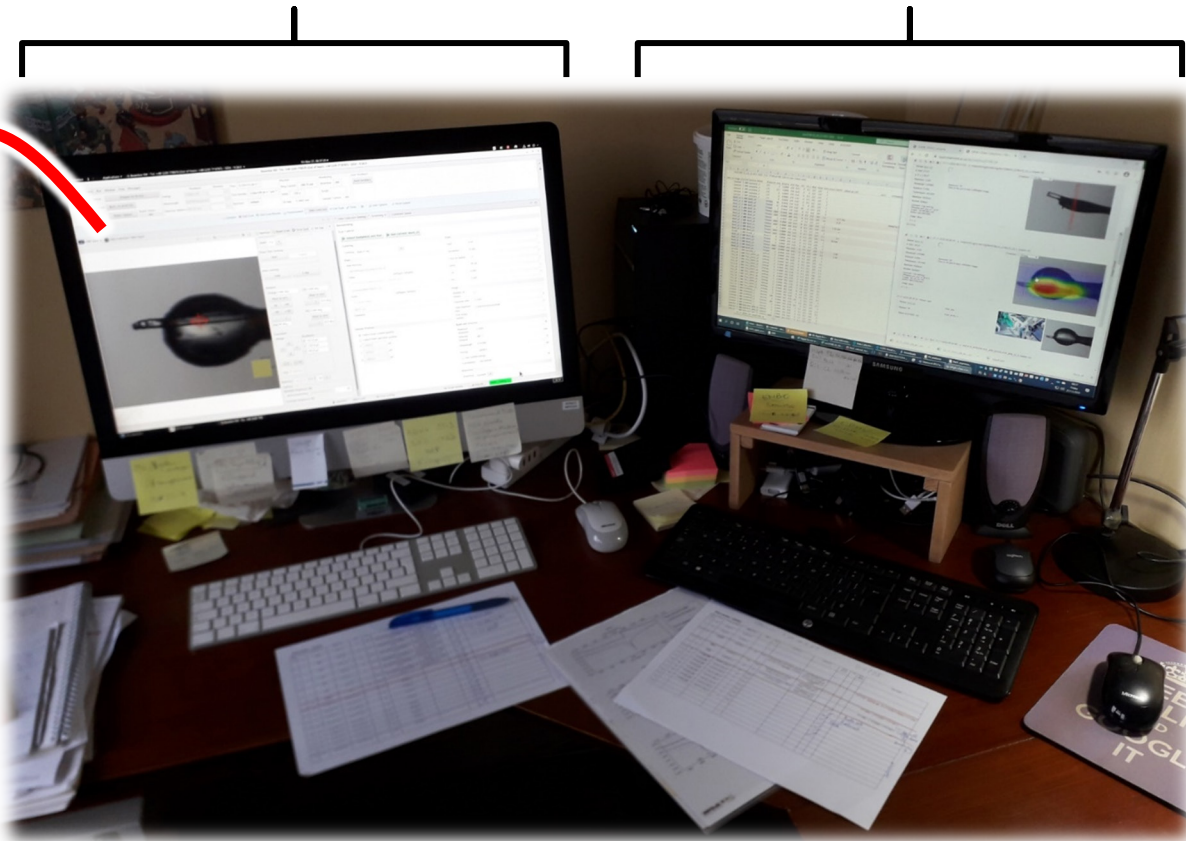
Remote data collection 2020 style!

iMac connected to
beamline computer
via NX client

PC connected to
work PC via VPN



share screen
with others



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

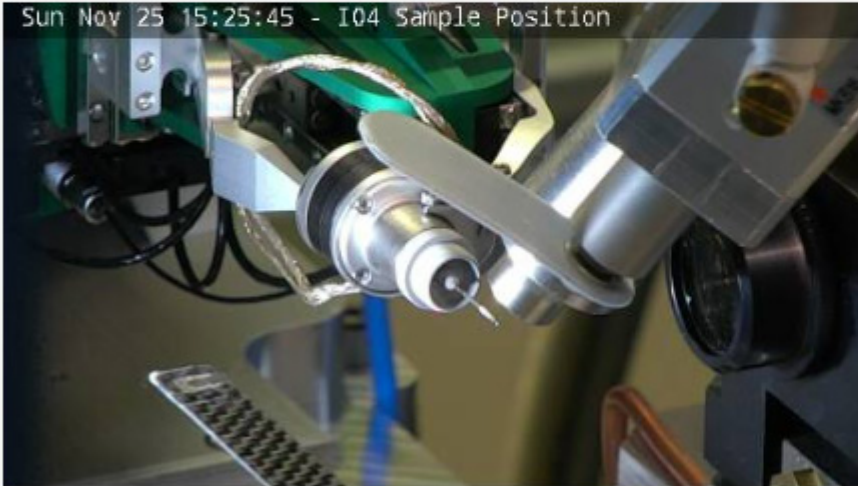
Port Shutter
Open

Expt Shutter
Open

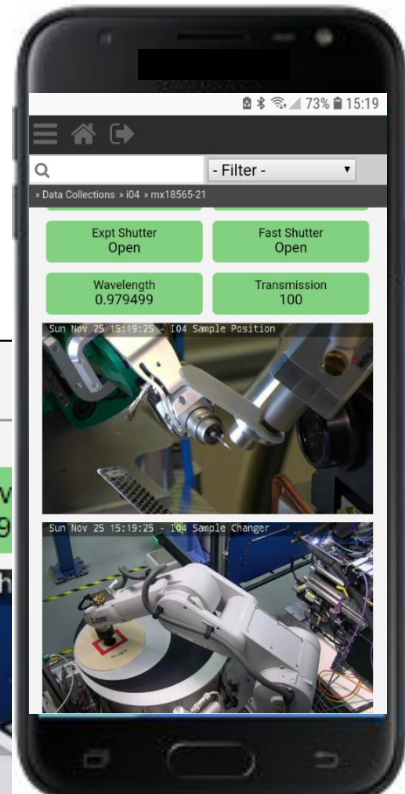
Fast Shutter
Open

Wav
0.9

Sun Nov 25 15:25:45 - I04 Sample Position



Sun Nov 25 15:25:45 - I04 Sample Ch



If you suspect a problem – call the EHC!

If you see no diffraction – 3 main causes:

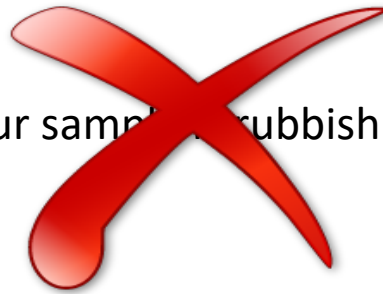
(1) there is a problem (any number of things...)



(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:

- Users collect data on their own crystals
- Users stay at home labs
 - 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

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
- use remote data collection for routine experiments
- think before and during data collection
- this is 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