

# Dose driven data collection to optimise your experiments

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Thanks to  
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Gwyndaf Evans  
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for slides & ideas

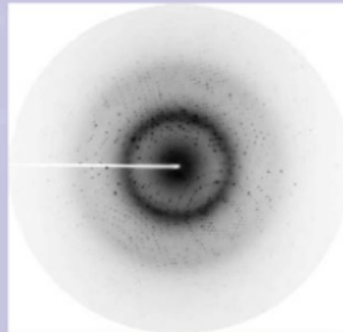


$$\rho(xyz) = \frac{1}{V} \sum_{hkl} F_{hkl} \exp(i\alpha_{hkl}) \exp[2\pi i(hx + ky + lz)]$$

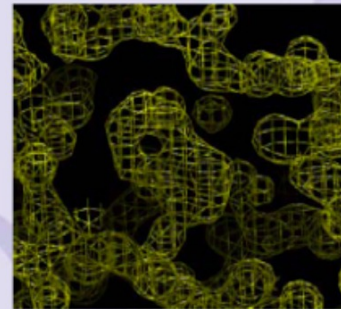
Crystal



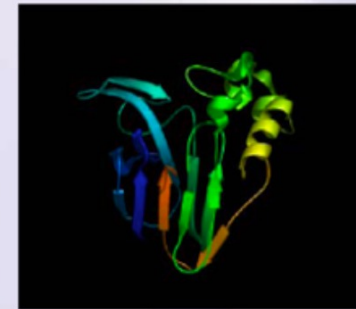
Diffraction pattern



Electron density



Structure



Diffraction Experiment

Phasing

Model Building  
Refinement

$$I(hkl) = I_0 \cdot \frac{\lambda^3}{\omega V_{\text{cell}}^2} \cdot V_{\text{cr}} \cdot L \cdot P \cdot T_r \cdot r_e^2 \cdot |F_{hkl}|^2$$

REC TC: 00:00:00:00

# Data collection is important!

This is the last experimental step

Time taken now to collect the best possible data can prevent pain and possible failure later on.

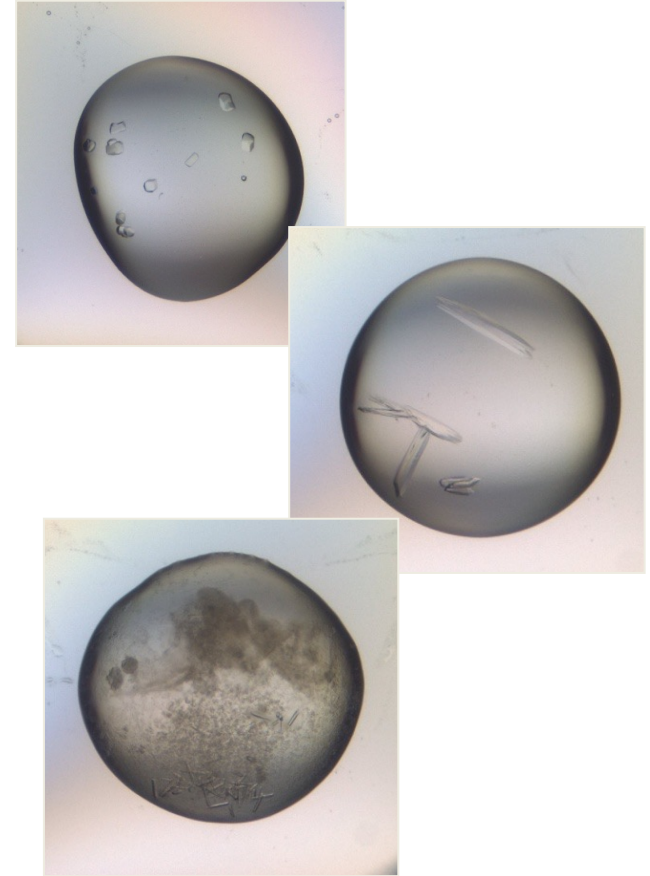
*"One good friend is better than a thousand poor ones." Indian Proverb*

If the original data are poor then not much can be done about it later.



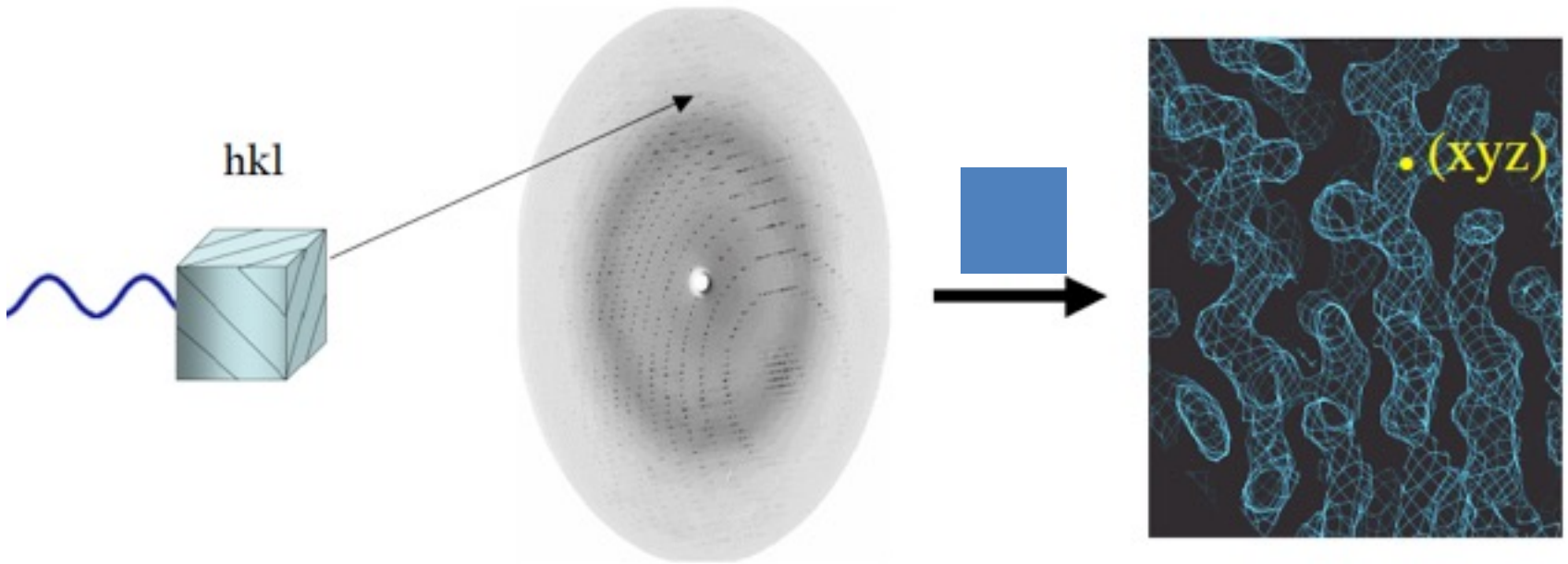
With fast sample changers, goniometers and detectors a lot of data can be collected very fast.

*Quantity  $\neq$  Quality*



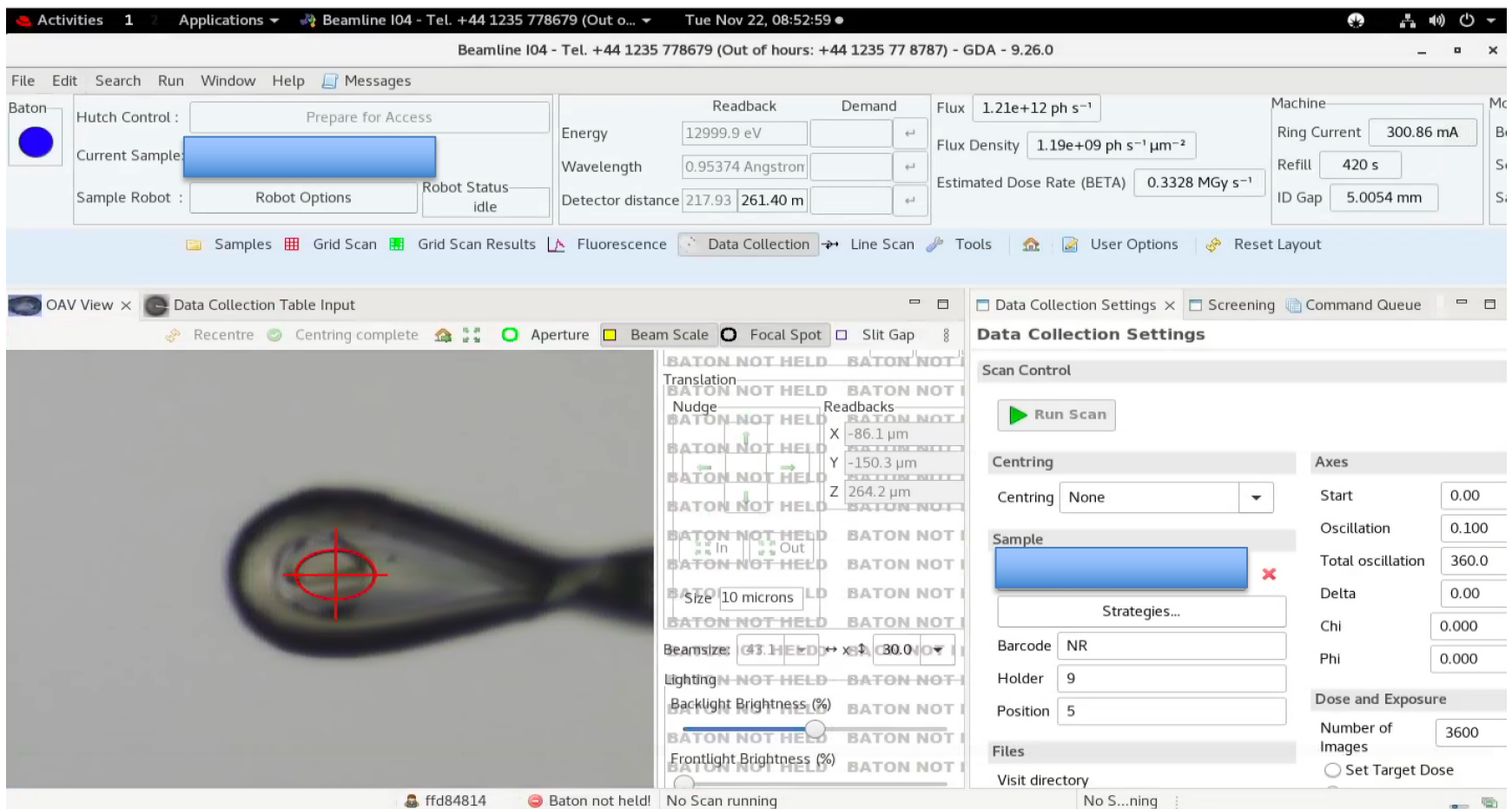


# Data collection: the goal



- record complete set of X-ray diffraction intensities from a crystal
- the better the data (high resolution, high completeness, low noise), the easier the following steps and the better refinement works
- like all previous steps this might need some optimisation and a lot of patience

# Data collection GUI



Start	0.00	*
Oscillation	0.100	*
Total oscillation	360.0	*
Delta	0.00	*
Chi	0.000	*
Phi	0.000	*

#### Dose and Exposure

Number of Images	3600
<input checked="" type="radio"/> Set Target Dose	
<input type="radio"/> Set Target Exposure	
Exposure Time	0.0030 s
Total Exposure Time	10.8 s
Dose / Dataset	7 MGy
First Image Number	1

#### Beam and Detector

Maximum resolution	1.9023 Å
Detector distance	289.3 mm
Wavelength	0.95373 Å
Energy	12999.9 eV
<input type="checkbox"/> Use current energy	
Transmission	100.000000 %

#### Aperture and Beamstop

Beamstop	Standard ▼
Horizontal beam size	31.73 μm
Vertical beam size	20 μm ▼
<input checked="" type="checkbox"/> Use current beam size	

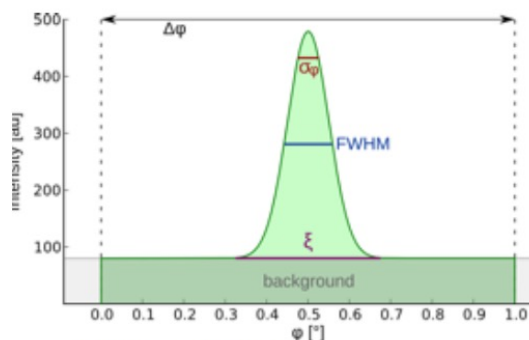
# Random errors, counting statistics

$$\sigma_{count} = N^{1/2}$$

$$I = N_p - N_b \quad \text{Signal is the difference}$$

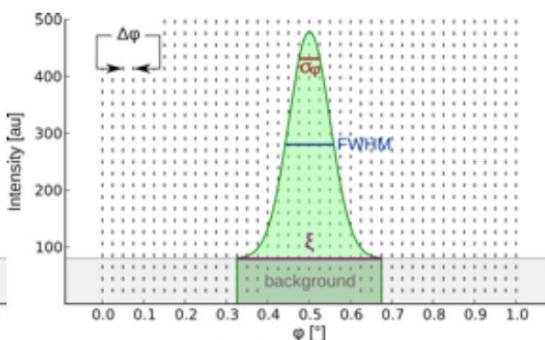
$$\sigma_I = (\sigma_p^2 + \sigma_b^2)^{1/2}$$

$$\sigma_I = (N_p + N_b)^{1/2} \quad \text{Uncertainty is the sum}$$



## Wide $\phi$ -slicing

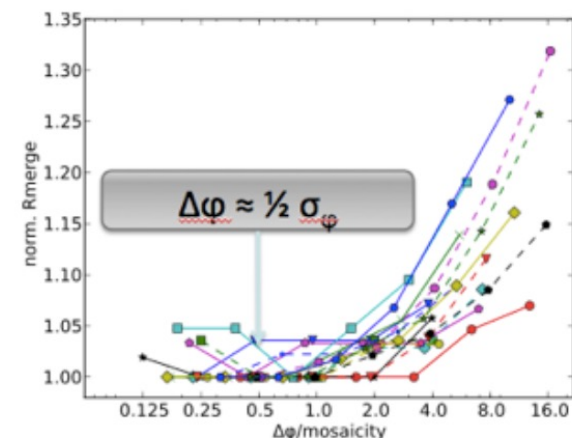
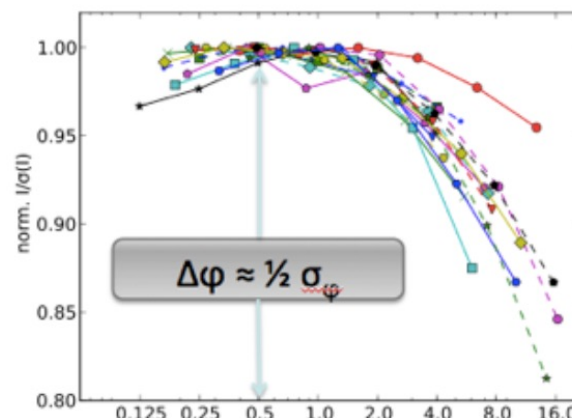
- Large  $\Delta\phi$  ( $\Delta\phi > \xi$ )
- Large overlap of reflections and background along  $\phi$
- Few images



## Fine $\phi$ -slicing

- Small  $\Delta\phi$  ( $\Delta\phi \ll \xi$ )
- Minimal overlap of reflections and background along  $\phi$
- Many images

Fine-phi slicing data collection is enabled by the pixel array detector (PILATUS, EIGER), which has single-photon sensitivity and no readout noise



Start	0.00	*
Oscillation	0.100	*
Total oscillation	360.0	*
Delta	0.00	*
Chi	0.000	*
Phi	0.000	*

#### Dose and Exposure

Number of Images	3600
<input checked="" type="radio"/> Set Target Dose	
<input type="radio"/> Set Target Exposure	
Exposure Time	0.0030 s
Total Exposure Time	10.8 s
Dose / Dataset	7 MGy
First Image Number	1

#### Beam and Detector

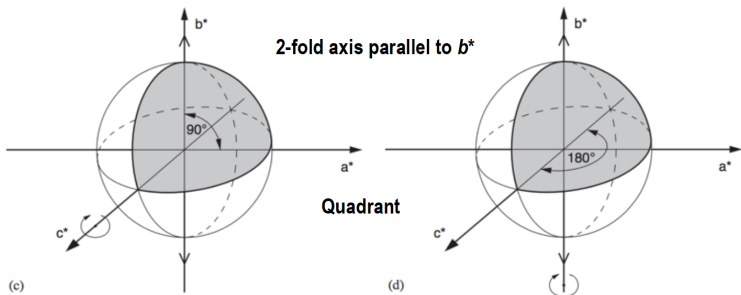
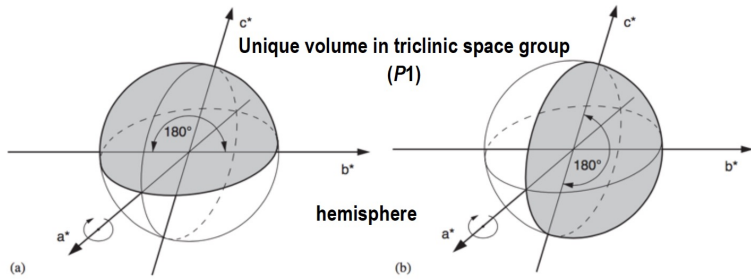
Maximum resolution	1.9023 Å
Detector distance	289.3 mm
Wavelength	0.95373 Å
Energy	12999.9 eV
<input type="checkbox"/> Use current energy	
Transmission	100.000000 %

#### Aperture and Beamstop

Beamstop	Standard ▼
Horizontal beam size	31.73 μm
Vertical beam size	20 μm ▼
<input checked="" type="checkbox"/> Use current beam size	

# Completeness - crystal symmetry

- reciprocal space symmetry = crystal symmetry plus
- Friedel's law :  $I(h\ k\ l) = I(-h\ -k\ -l)$



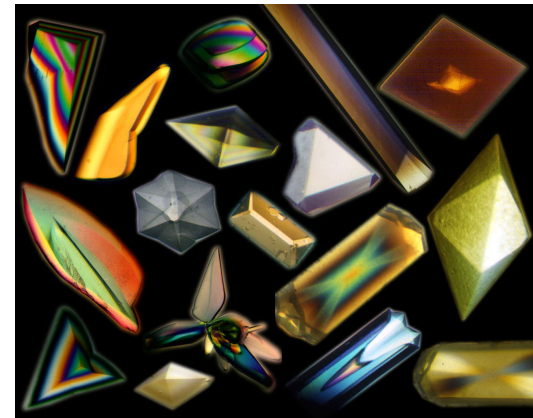
More on Tuesday 29<sup>th</sup> Nov

"Introduction to space groups" by Andrey Lebedev

Give yourself options (Radiation Damage) ← collect same dose in larger range

thus even for P1 only 180° are needed to obtain complete data set of unique reflections - unless there is anomalous scattering

for N-fold symmetry along rotation axis, need 180/N degrees of data to obtain complete data set (assuming Friedel's law holds)



Crystals of proteins grown on the U.S. Space Shuttle or Russian Space Station, Mir.

Start	0.00	*
Oscillation	0.100	*
Total oscillation	360.0	*
Delta	0.00	*
Chi	0.000	*
Phi	0.000	*

#### Dose and Exposure

Number of Images	3600
<input checked="" type="radio"/> Set Target Dose	
<input type="radio"/> Set Target Exposure	
Exposure Time	0.0030 s
Total Exposure Time	10.8 s
Dose / Dataset	7 MGy
First Image Number	1

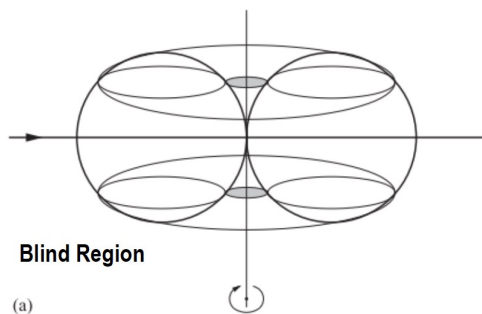
#### Beam and Detector

Maximum resolution	1.9023 Å
Detector distance	289.3 mm
Wavelength	0.95373 Å
Energy	12999.9 eV
<input type="checkbox"/> Use current energy	
Transmission	100.000000 %

#### Aperture and Beamstop

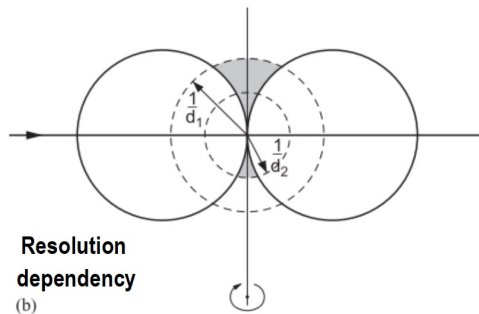
Beamstop	Standard ▼
Horizontal beam size	31.73 μm
Vertical beam size	20 μm ▼
<input checked="" type="checkbox"/> Use current beam size	





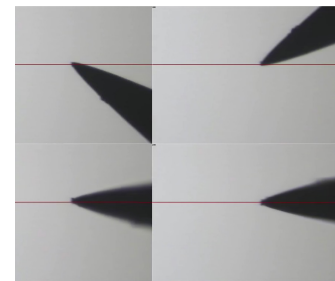
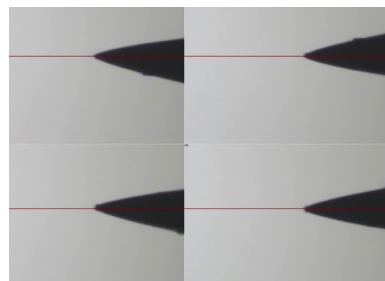
Blind Region

(a)



Resolution dependency

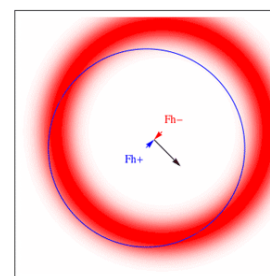
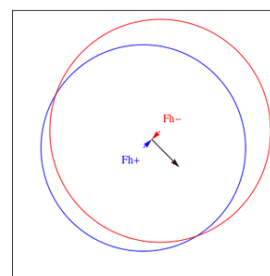
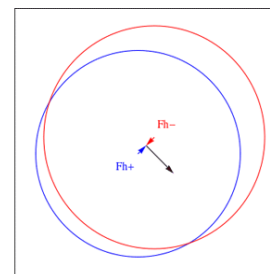
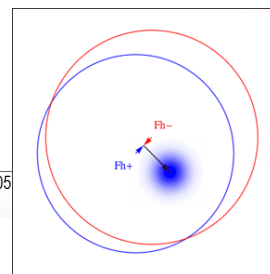
(b)



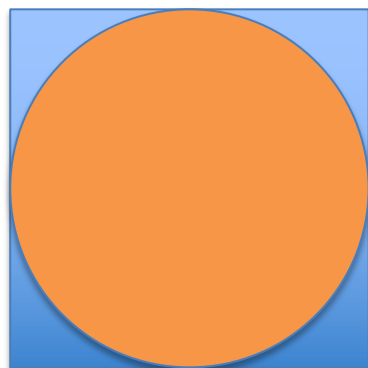
Chi=0 deg

Chi=30 deg

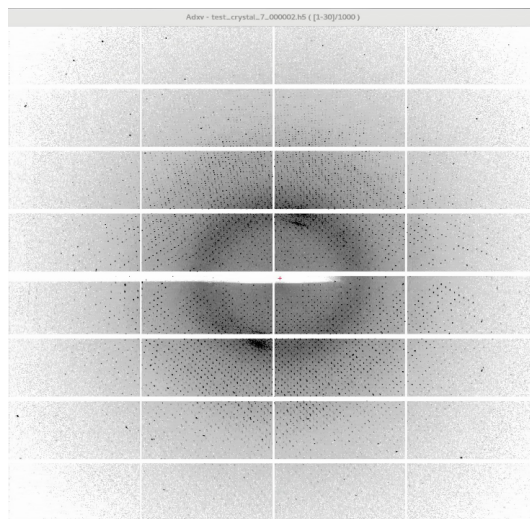
## Experimental Phasing



Picture courtesy of Acta Crystallogr D Biol Crystallogr. 2011 Apr 1; 67:338–344.



Corner vs Edge



Systematic error reduction  
Detector module gaps

Wed 30<sup>th</sup> Nov

The phase problem, Ed Lowe  
Experimental Phasing, Ed Lowe  
EP case studies, Erika Mancini



Start	0.00	*
Oscillation	0.100	*
Total oscillation	360.0	*
Delta	0.00	*
Chi	0.000	*
Phi	0.000	*

#### Dose and Exposure

Number of Images	3600
<input checked="" type="radio"/> Set Target Dose	
<input type="radio"/> Set Target Exposure	
Exposure Time	0.0030 s
Total Exposure Time	10.8 s
Dose / Dataset	7 MGy
First Image Number	1

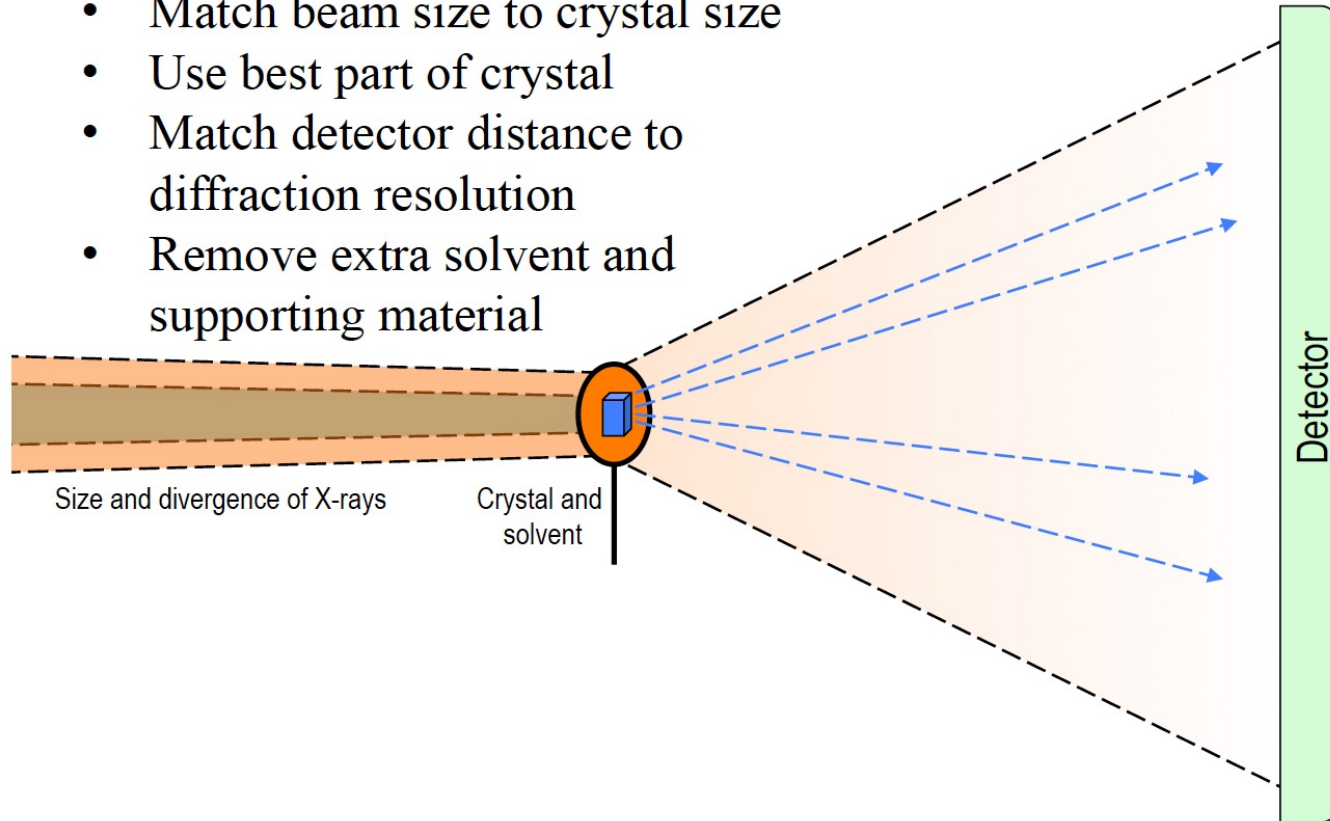
#### Beam and Detector

Maximum resolution	1.9023 Å
Detector distance	289.3 mm
Wavelength	0.95373 Å
Energy	12999.9 eV
<input type="checkbox"/> Use current energy	
Transmission	100.000000 %

#### Aperture and Beamstop

Beamstop	Standard ▼
Horizontal beam size	31.73 μm
Vertical beam size	20 μm ▼
<input checked="" type="checkbox"/> Use current beam size	

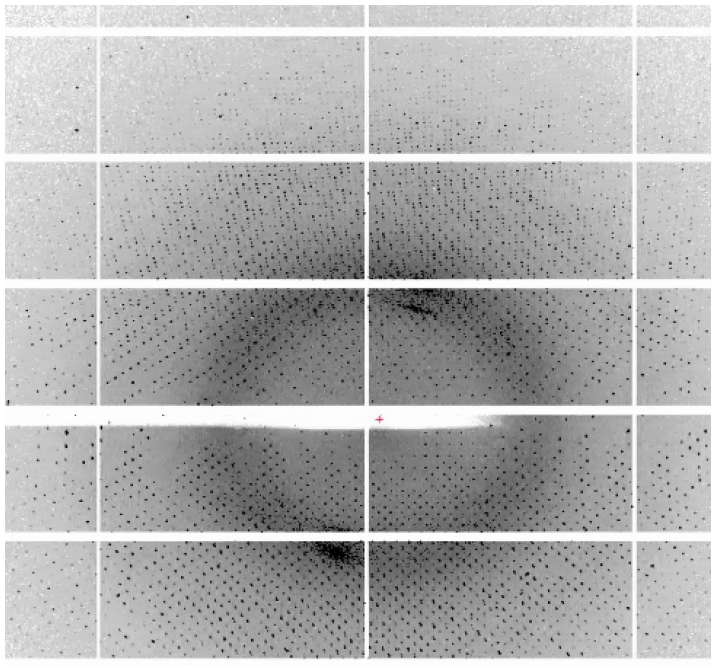
- Match beam size to crystal size
- Use best part of crystal
- Match detector distance to diffraction resolution
- Remove extra solvent and supporting material



# Screening and analysis

Determine crystal diffraction properties, orientation matrix and appropriate settings for data collection

Usually by collecting a small wedge of 15-20 degrees ideally at the thickest part of the crystal (or the old method of 3 images 45 degrees away from each other)



Important to check the images:

- Spot quality – circular, well spaced
- Resolution? Guides on
  - Detector distance
  - Dose/Exposure to deliver
- Autoindexing successful?

If evaluating by eye remember to “join” images to at least 1.0 degree rather than looking at fine sliced images. Max res: best to rely on data reduction programs and apply a buffer (e.g 0.5 Å)

Start	<input type="text" value="0.00"/>	*
Oscillation	<input type="text" value="0.100"/>	*
Total oscillation	<input type="text" value="360.0"/>	*
Delta	<input type="text" value="0.00"/>	*
Chi	<input type="text" value="0.000"/>	*
Phi	<input type="text" value="0.000"/>	*

#### Dose and Exposure

Number of Images	<input type="text" value="3600"/>	
<input checked="" type="radio"/> Set Target Dose <input type="radio"/> Set Target Exposure		
Exposure Time	<input type="text" value="0.0030"/>	s
Total Exposure Time	<input type="text" value="10.8"/>	s
Dose / Dataset	<input type="text" value="7"/>	MGy
First Image Number	<input type="text" value="1"/>	

#### Beam and Detector

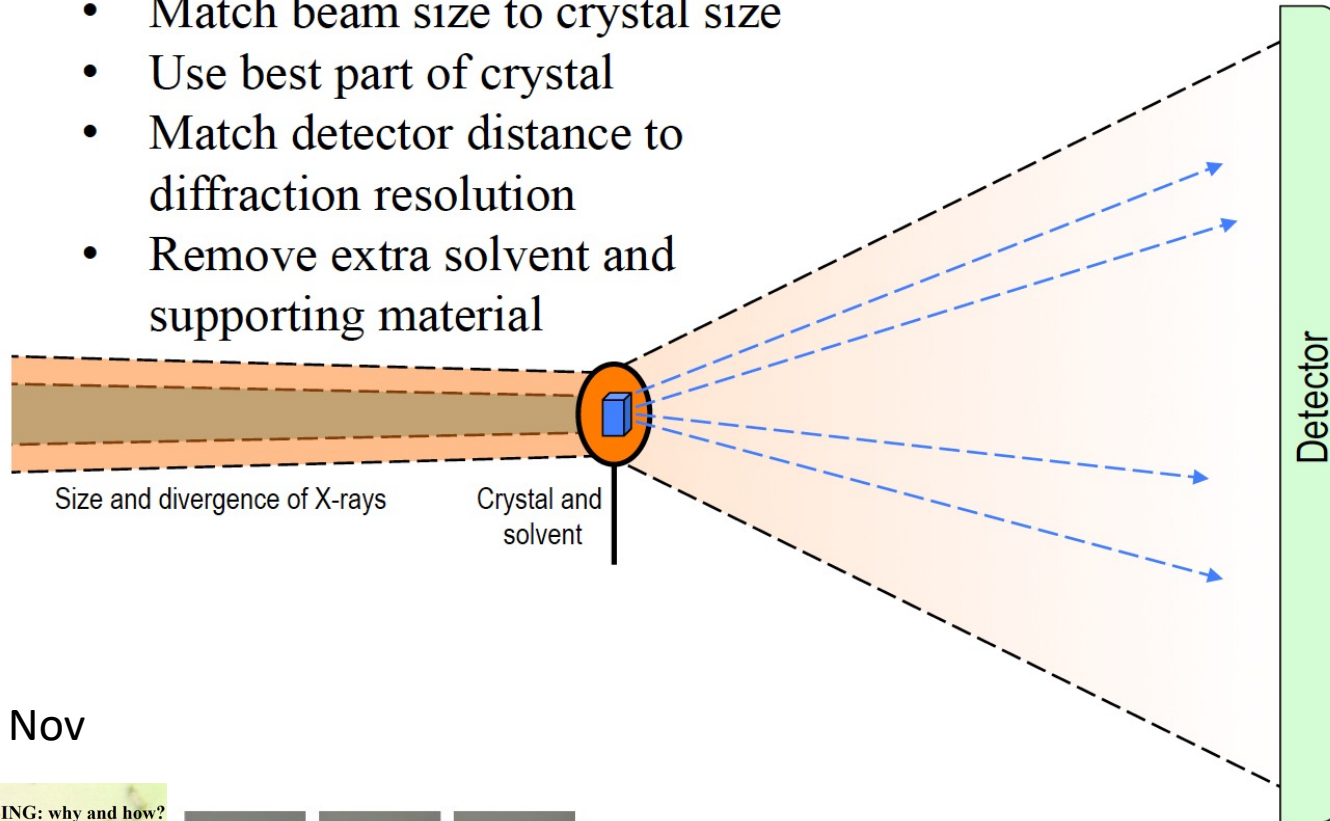
Maximum resolution	<input type="text" value="1.9023"/>	Å
Detector distance	<input type="text" value="289.3"/>	mm
Wavelength	<input type="text" value="0.95373"/>	Å
Energy	<input type="text" value="12999.9"/>	eV
<input type="checkbox"/> Use current energy		
Transmission	<input type="text" value="100.000000"/>	%

#### Aperture and Beamstop

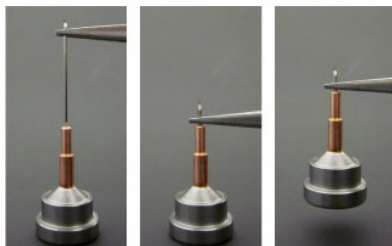
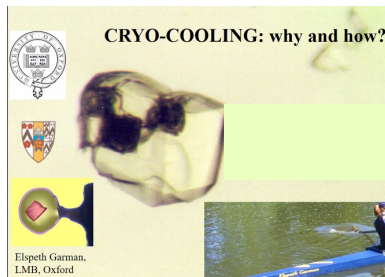
Beamstop	<input type="text" value="Standard"/>	▼
Horizontal beam size	<input type="text" value="31.73"/>	μm
Vertical beam size	<input type="text" value="20"/>	μm ▼

☒ Use current beam size

- Match beam size to crystal size
- Use best part of crystal
- Match detector distance to diffraction resolution
- Remove extra solvent and supporting material



Mon, 17<sup>th</sup> Nov



Start	<input type="text" value="0.00"/>	*
Oscillation	<input type="text" value="0.100"/>	*
Total oscillation	<input type="text" value="360.0"/>	*
Delta	<input type="text" value="0.00"/>	*
Chi	<input type="text" value="0.000"/>	*
Phi	<input type="text" value="0.000"/>	*

#### Dose and Exposure

Number of Images	<input type="text" value="3600"/>	
<input checked="" type="radio"/> Set Target Dose		
<input type="radio"/> Set Target Exposure		
Exposure Time	<input type="text" value="0.0030"/>	s
Total Exposure Time	<input type="text" value="10.8"/>	s
Dose / Dataset	<input type="text" value="7"/>	MGy
First Image Number	<input type="text" value="1"/>	

#### Beam and Detector

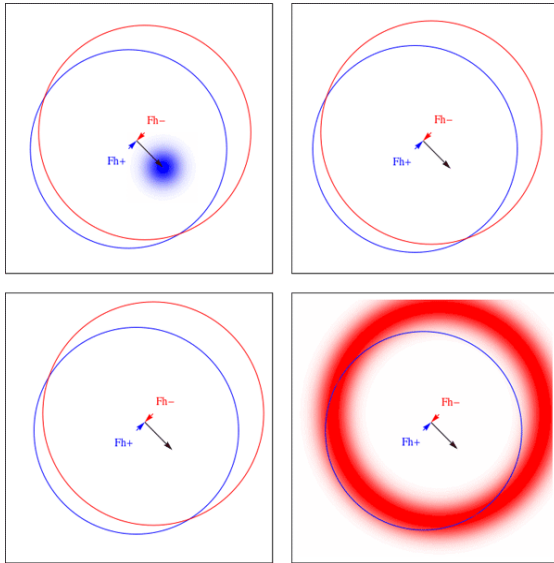
Maximum resolution	<input type="text" value="1.9023"/>	Å
Detector distance	<input type="text" value="289.3"/>	mm
Wavelength	<input type="text" value="0.95373"/>	Å
Energy	<input type="text" value="12999.9"/>	eV
<input type="checkbox"/> Use current energy		
Transmission	<input type="text" value="100.000000"/>	%

#### Aperture and Beamstop

Beamstop	<input type="text" value="Standard"/>	▼
Horizontal beam size	<input type="text" value="31.73"/>	μm
Vertical beam size	<input type="text" value="20"/>	μm
<input checked="" type="checkbox"/> Use current beam size		

# Energy selection

## Experimental Phasing



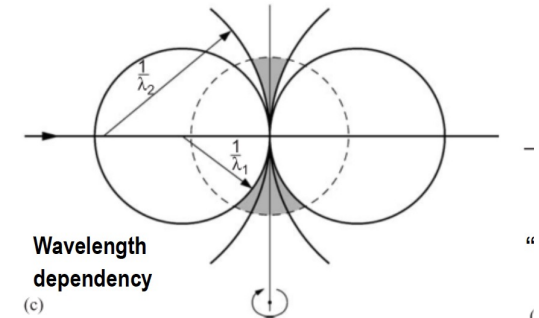
## High resolution

$$n\lambda = 2d \sin \theta$$

*Bragg's Law*

<https://www.diamond.ac.uk/Instruments/Mx/Common/Calculators.htm>  
(search for “useful calculators diamond”)

## Blind region / Cuspid



## Basic Diffraction Theory, Kamel El Omari

## Crystal life time / Radiation damage for small crystals

### Experimental evidence for the benefits of higher X-ray energies for macromolecular crystallography

Selina L. S. Storm,<sup>a\*</sup> Danny Axford<sup>a</sup> and Robin L. Owen<sup>a\*</sup>

IUCrJ 2021 Sep 9;8:896-904.

Most often: use the default energy that the beamline you using has been most optimised for

Start	0.00	*
Oscillation	0.100	*
Total oscillation	360.0	*
Delta	0.00	*
Chi	0.000	*
Phi	0.000	*

#### Dose and Exposure

Number of Images	3600
<input checked="" type="radio"/> Set Target Dose	
<input type="radio"/> Set Target Exposure	
Exposure Time	0.0030 s
Total Exposure Time	10.8 s
Dose / Dataset	7 MGy
First Image Number	1

#### Beam and Detector

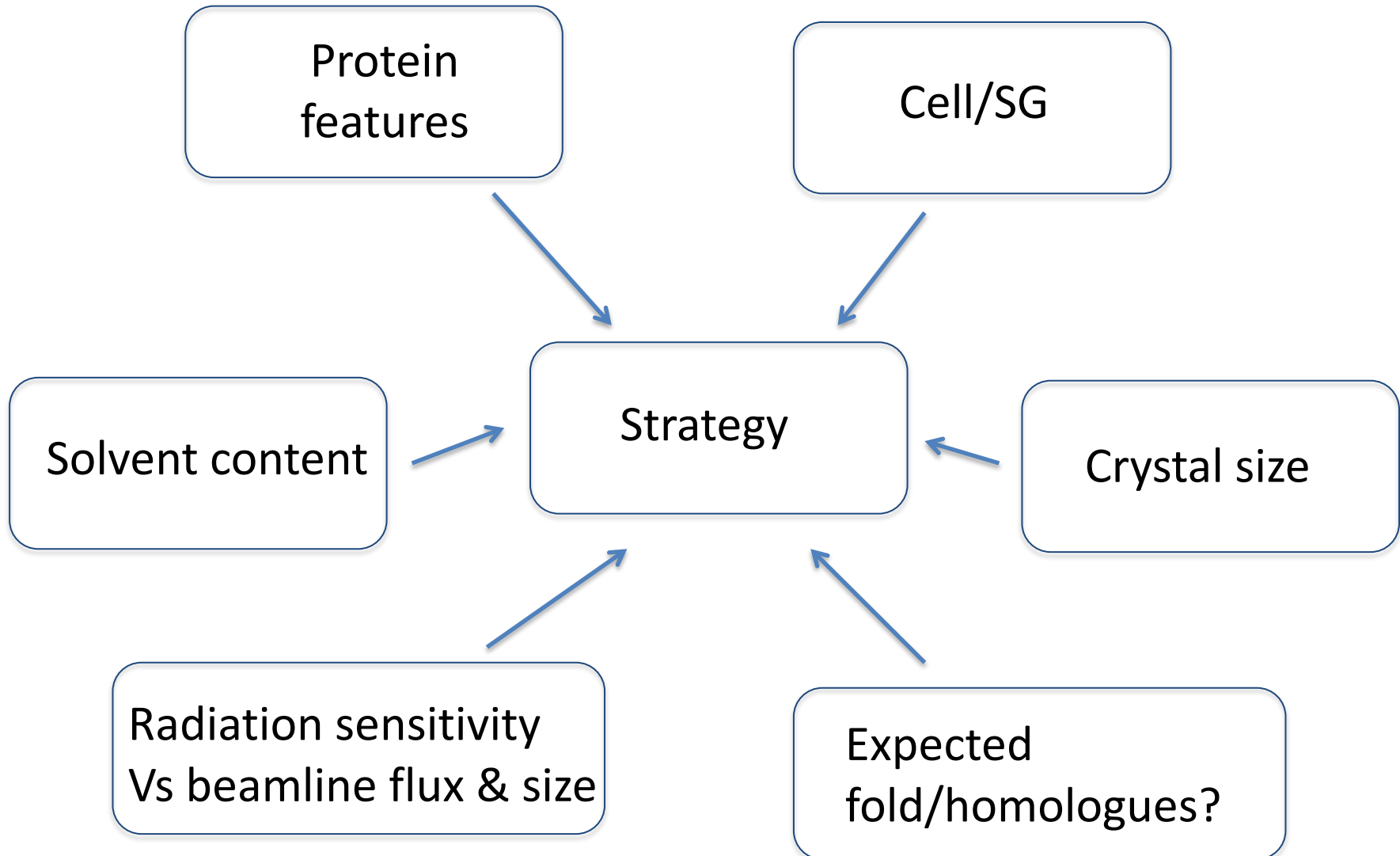
Maximum resolution	1.9023 Å
Detector distance	289.3 mm
Wavelength	0.95373 Å
Energy	12999.9 eV
<input type="checkbox"/> Use current energy	
Transmission	100.000000 %

#### Aperture and Beamstop

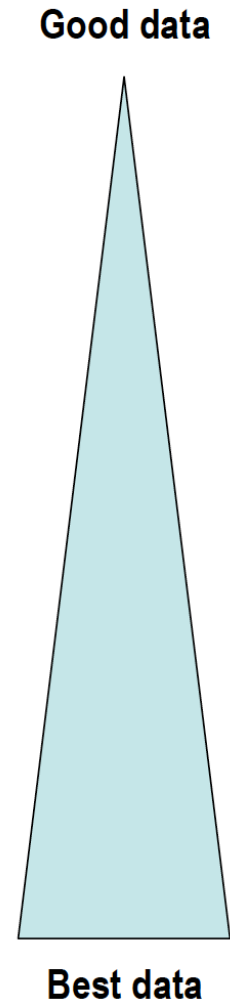
Beamstop	Standard ▼
Horizontal beam size	31.73 μm
Vertical beam size	20 μm ▼
<input checked="" type="checkbox"/> Use current beam size	



# Preparation - Prior knowledge



- Molecular substitution
- Molecular replacement
- Isomorphous replacement (Hg, Pt)
- MAD/SAD phasing
- Native-SAD phasing (Sulfur-SAD)



# What's the goal?

Aim	High priorities	Lower priority	Max Dose per dataset (e.g. per 120, 180 or 360 degrees) For a ~2Å resolution dataset
Native data collection	High resolution (e.g < 1.8 Å) Complete data Minimise radiation damage particular for high resolution data.	High redundancy Speed	~20 MGy
Multi-wavelength anomalous dispersion (MAD) Single Anomalous dispersion (SAD)	Accurate, complete and highly redundant Very little radiation damage Choice of wavelength	High resolution data	1 - 5 MGy (heavy atom will increase dose for same exposure)
Sulphur SAD	As above + extra high redundancy (40- 200fold) if not on I23 beamline		0.3-0.5 MGy
Molecular replacement	Completeness at low resolution (< 3Å) Good quality low resolution	High resolution data High redundancy	~20 MGy
Ligand/mutation	Medium resolution (e.g. 2 Å), complete data. High throughput (FAST)	High redundancy	10 - 20 MGy

**Trying to collect everything at once will usually result in failure**

## expected crystal lifetime calculator

Raddose 3D

<https://bl831.als.lbl.gov/xtallife.html>

<https://github.com/GarmanGroup/RADDOSE-3D>

Beamline settings	Flux (ph/s)	Beam size (um)	Exposure (s)	Dose (MGy)
A	$3.8 \times 10^{12}$	100 x 100	~93	20
B	$1.2 \times 10^{12}$	30x 20	~28	20
C	$1.2 \times 10^{12}$	20x10	~10	20
D	$1.0 \times 10^{13}$	80x15	~8	20
E	$3.0 \times 10^{12}$	8x6	~1	20
F	$3.0 \times 10^{12}$	20x20	~8	20

Assumptions:

Beamline energy at 0.9537 Å / 13.0 KeV

Crystal of the size of the beam

100% transmission

“standard” sample = no heavy metals (e.g. no Se, no As, average amount of S)

# Beam size and flux density

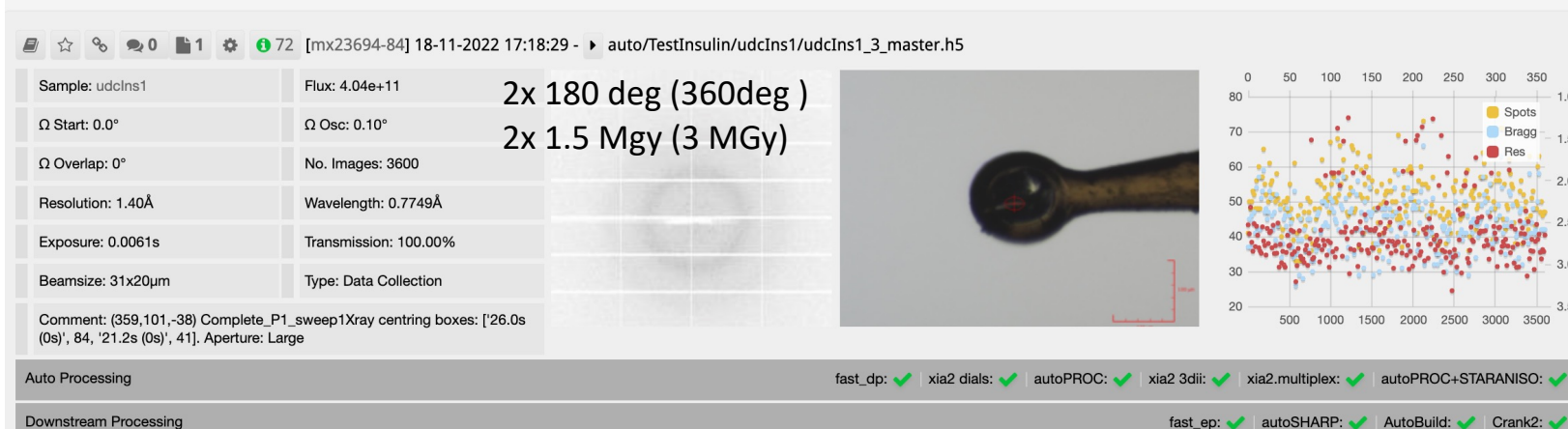
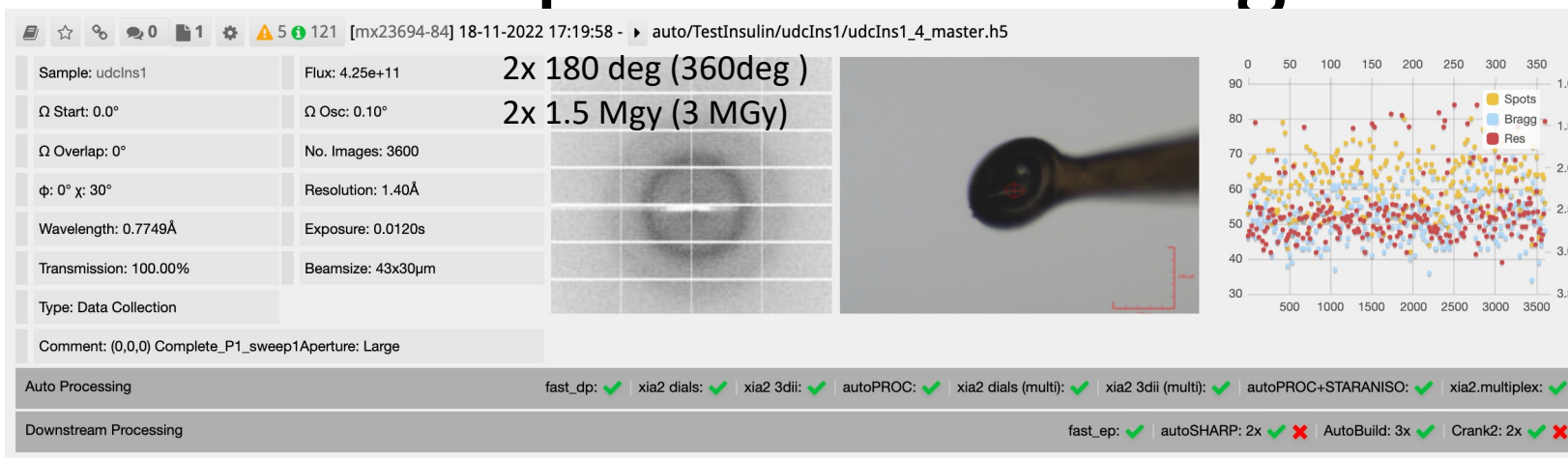
Be mindful of how the beamline generates a small beam size. Focusing (I04 +I24) can increase the flux density massively compared to apertures (I03)

Radiation damage is related to the flux density so small beam sizes on I04/I24 can kill a crystal very quickly.

E.g.  $50 \times 50 \mu\text{m}^2$  beam will deliver around 45x less dose than  $9 \times 6 \mu\text{m}^2$  beam on I24

So match beam to crystal, but attenuate when required

# Example with Phasing UDC



720 degrees with 2x 360 deg at two different Chi angles  
 6 Mgy for a 1.4 Å max diffraction  
 Highly redundant

	CC Half	Completeness	Multiplicity	Anom Completeness	Anom Multiplicity	CC Anom
	0.5	100.0	18.1	98.8	9.4	0.0
	1.0	100.0	73.4	100.0	41.9	1.0
	1.0	100.0	65.9	99.9	34.7	0.9

# Sample with Line scan

Line Scan Setup View

Camera Control: Snapshot, Zoom 5.0

Sample Environment: Backlight

Line Scan Settings

Line Scan Settings

Oscillation: 0.1

Total oscillation: 360.0

Delta: 0

Images

☒ Automatic run number

Run number: 0

Exposure time: 0.03 s

Total exposure time: 108.0 s

Detector distance: 333 mm

Resolution: 2.14 Å

Transmission: 100.0 %

Number of wedges: 1

Images per wedge: 3600

☐ Wedged line scan

☒ Helical line scan

Line

Start X: -0 μm

Start Y: -0.014 μm

Start Z: 0.003 μm

End X: -0 μm

End Y: -0.014 μm

End Z: 0.003 μm

Aperture and Beamstop

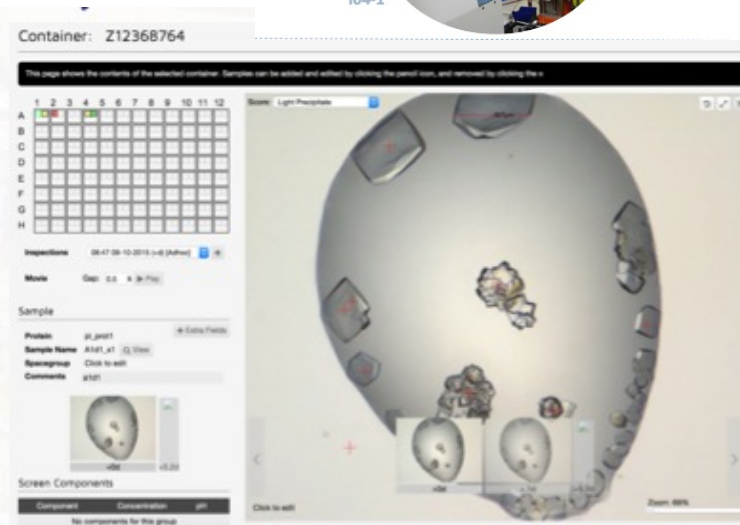
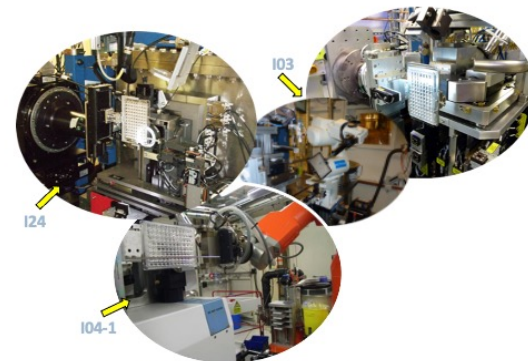
Move To Start

Move To End

Use Beam Centre As Start

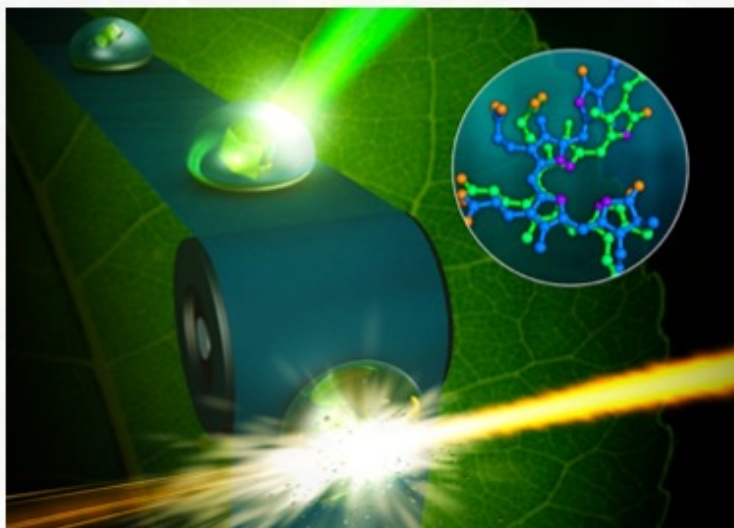
Use Beam Centre As End

Room temperature: VMXi  
fully automated, user free, in situ






# Serial Crystallography



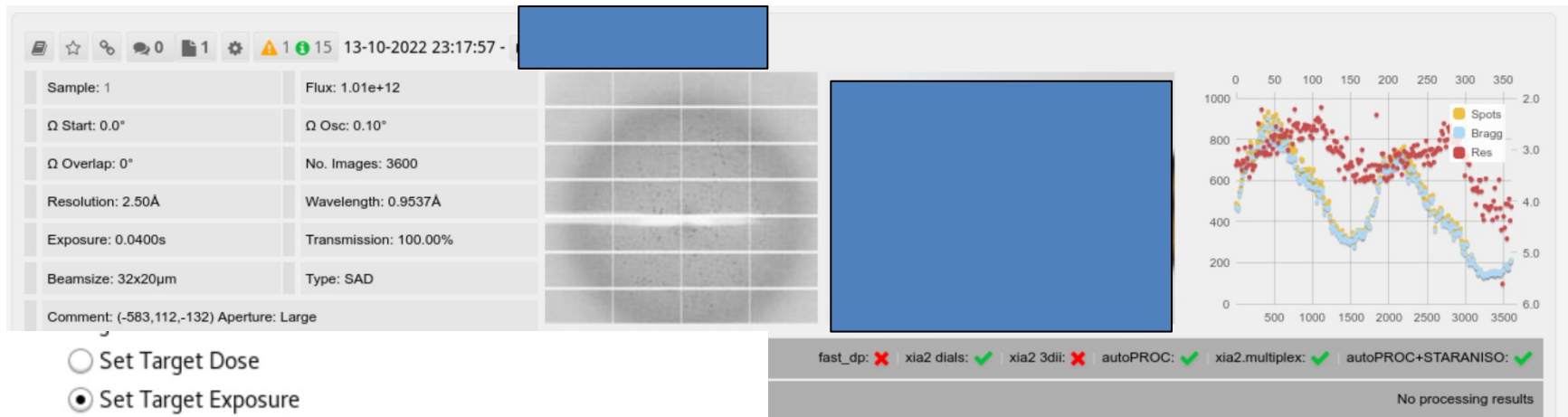
for SSX/SFX (UK XFEL-Hub)

- acoustic droplet ejection
- liquid jets / LCP extruders
- crystal levitation
- Pump/probe dynamical studies

Routine at I24 on standard MX beamtime

XFEL-Hub + I24 @  diamond

# What happens if you don't pay attention to dose?



☐ Set Target Dose

☒ Set Target Exposure

Exposure Time 0.04 s

Total Exposure Time 144.0 s

Dose / Dataset 47.6 MGy

First Image Number 1

## Beam and Detector

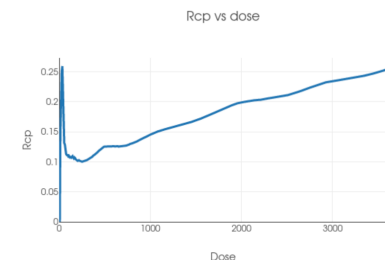
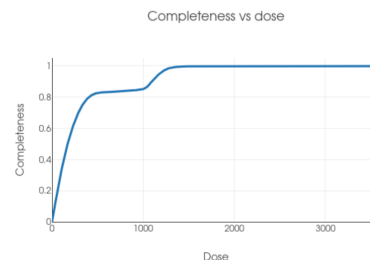
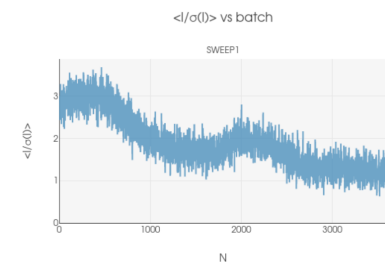
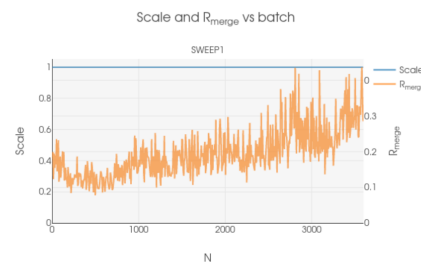
Maximum resolution 1.2985 Å

Detector distance 170.0 mm

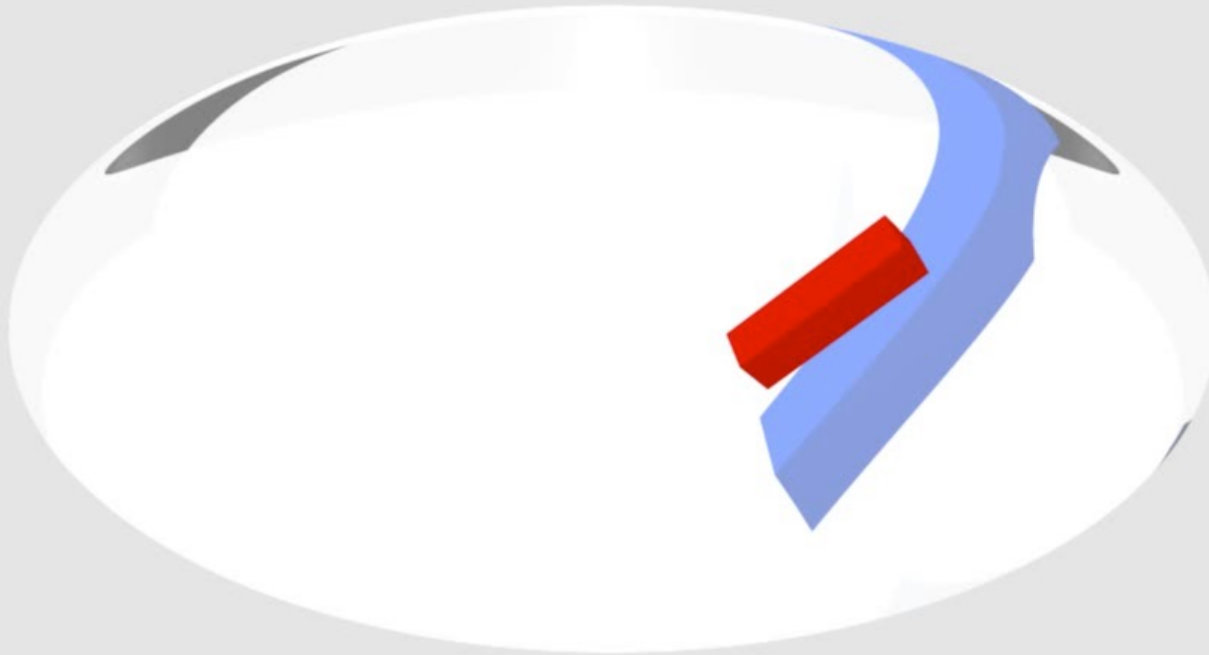
Wavelength 0.95372 Å

Energy 13000.0 eV

☐ Use current energy



# Good alignment is crucial



28-11-2019 21:05:04 - 20191128/Sethaumatina/Sethau\_14/stepped/Sethau\_14\_1\_master.h5

Sample: [Sethau\\_14](#)

Flux: 3.04e+11

$\Omega$  Start: 0.0°

$\Omega$  Osc: 0.10°

$\Omega$  Overlap: 0°

No. Images: 3600

Resolution: 1.33Å

Wavelength: 0.9763Å

Exposure: 0.002s

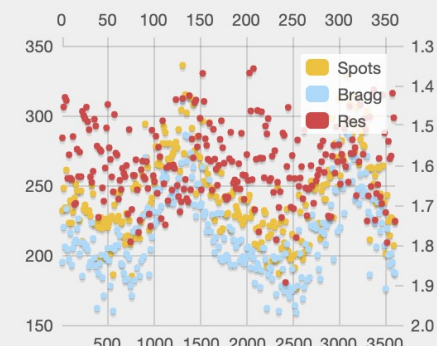
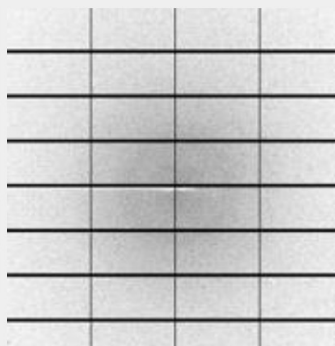
Transmission: 100.00%

Beamsize: 32x20μm

Type: SAD

Group: [4 Data Collections](#)

Comment: (34,-126,78) Aperture: Large



strategy: vedge1 Standard Anomalous Dataset multiplicity=3 / sig=2 maxitespan=200 s

28-11-2019 20:58:37 - 20191128/Sethaumatina/Sethau\_13/stepped/Sethau\_13\_1\_master.h5

Sample: [Sethau\\_13](#)

Flux: 3.06e+11

$\Omega$  Start: 0.0°

$\Omega$  Osc: 0.10°

$\Omega$  Overlap: 0°

No. Images: 3600

Resolution: 1.33Å

Wavelength: 0.9763Å

Exposure: 0.002s

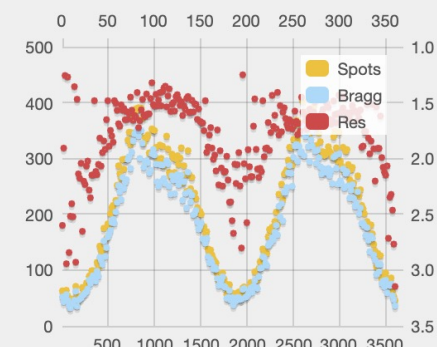
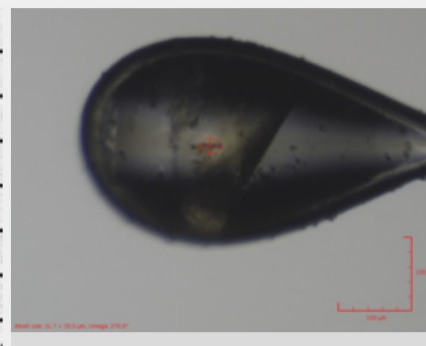
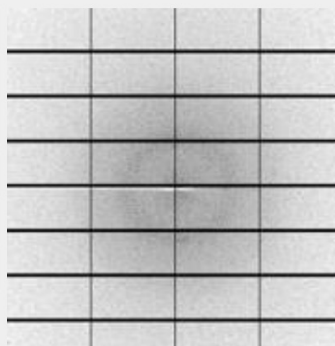
Transmission: 100.00%

Beamsize: 32x20μm

Type: SAD

Group: [4 Data Collections](#)

Comment: (-1111,-315,146) Aperture: Large



29-11-2019 09:14:05 - 20191129/Sethaumatina/Sethau\_6/Sethau\_6\_700\_1\_master.h5

Sample: [Sethau\\_6](#)

Flux: 3.14e+11

$\Omega$  Start: 0.0°

$\Omega$  Osc: 0.10°

$\Omega$  Overlap: 0°

No. Images: 1800

Resolution: 4.32Å

Wavelength: 0.9795Å

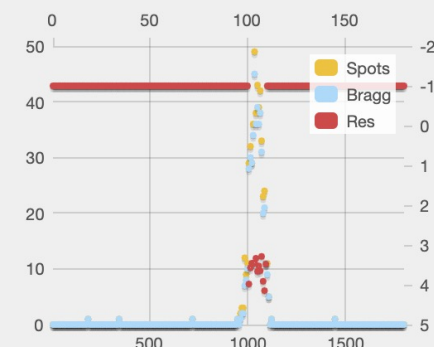
Exposure: 0.010s

Transmission: 100.00%

Beamsize: 32x20μm

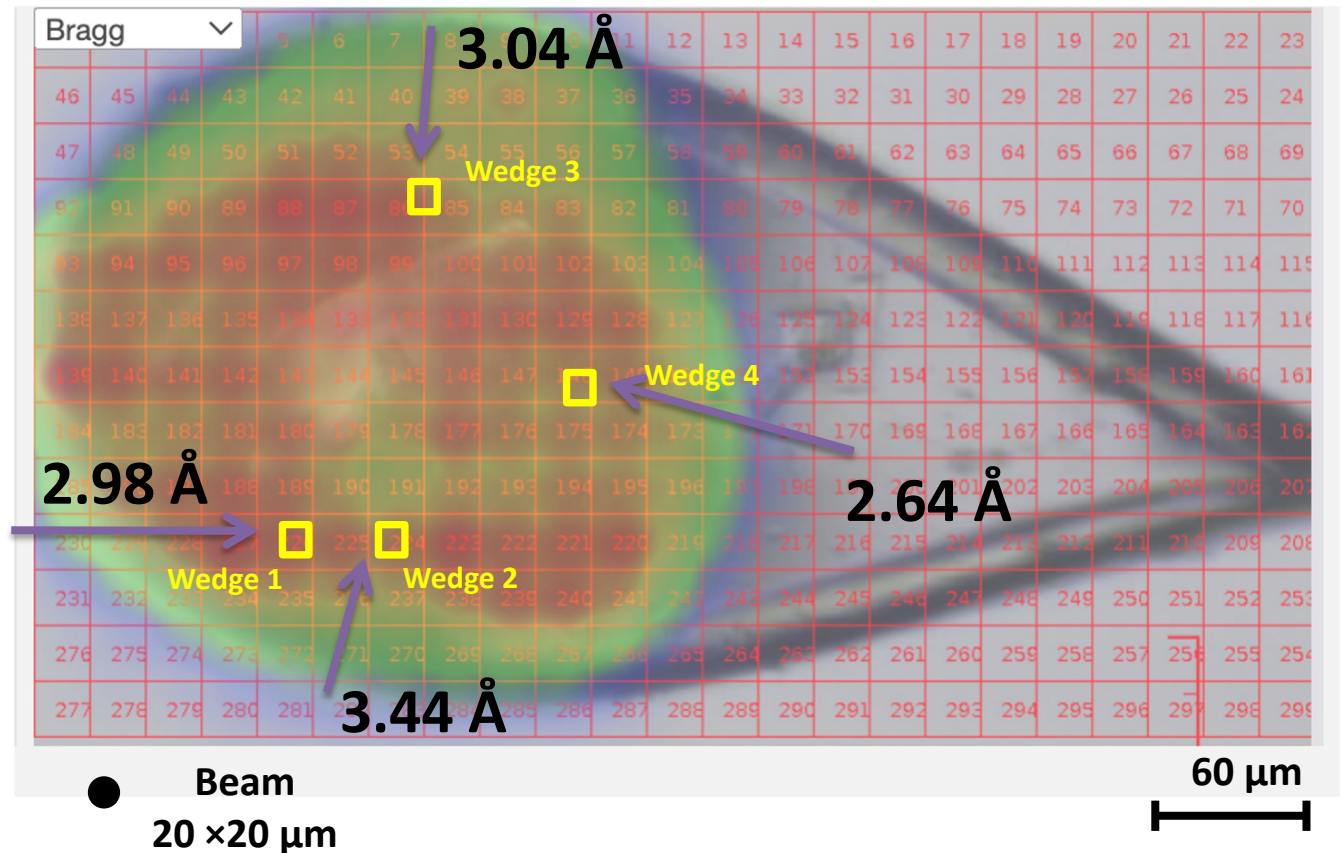
Type: SAD

Comment: (0,0,0) Aperture: Large





Even the same crystal can show a lot of variation...



Sometimes worthwhile, sometimes not. Learn when to move on.

# Data collection - think!



- before starting data collection make sure xtal is properly centered and does not “walk” out of beam
- consider dose (exposure time, attenuation, energy), wedge angle, detector distance... before it is too late!

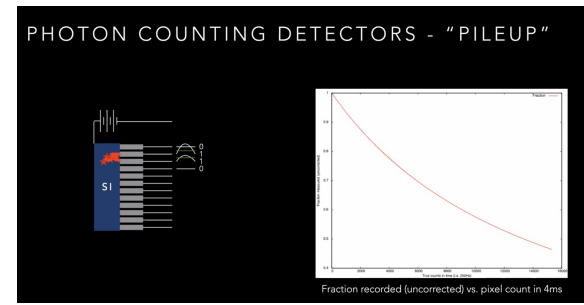
## Decision time

Remember the aim of your experiment – will this sample give you what you need, or get you closer to your goal? If not, move on.

Experimental phasing is the most critical at this point, a trivial case can be made borderline by bad choices. Most common error is overexposing the crystal, next is not collecting enough data.

Remember that low energy = stronger diffraction and faster radiation damage. Transmission of  $<5\%$  not uncommon. If the edge is very different to the screening energy then consider repeating the screening shots.

# Saturated detectors



The Pilatus 6M and Eiger 16M have a large dynamic range.

When the dynamic range is exceeded, the counter starts from zero again. The only indication for this is that when extreme holes may be observed in a few peaks.

I worse issue is also that some highly count rate corrected peaks won't show easy to see visible pathology.

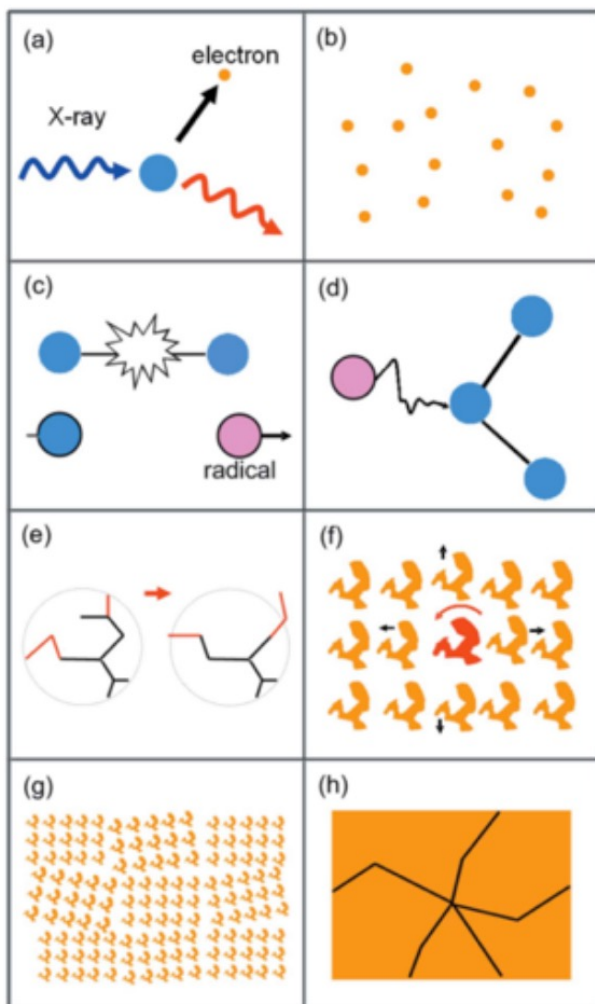
**Conclusion:** Even if there is no radiation damage one might have had "too much photons on our detector" resulting in damaged data – ATTENTION: Flux dependent not exposure dependent, fine slicing helps but not totally fixes it



# What's the goal?

Aim	High priorities	Lower priority	Max Dose per dataset (e.g. per 120, 180 or 360 degrees) For a ~2Å resolution dataset
Native data collection	High resolution (e.g < 1.8 Å) Complete data	High redundancy	Up to 20 Mgy (inverse scale your dose exposure with the diffracting resolution of your crystals)
Multi-wavelength anomalous dispersion (MAD) Single Anomalous dispersion (SAD)	Accurate, complete and highly redundant Very little radiation damage Choice of wavelength	High resolution data	1 - 5 MGy (heavy atom will increase dose for same exposure, routine on most MX beamlines))
Sulphur SAD	As above + extra high redundancy (40-200fold) if not on I23 beamline		0.3-0.5 Mgy (inherently hard experiment not worth a try, if not try i23)
Molecular replacement	Completeness at low resolution (< 3Å) Good quality low resolution	High resolution data High redundancy	Up to 20 Mgy (be careful with count rate correction)
Ligand/mutation	Medium resolution (e.g. 2 Å), complete data. High throughput (FAST)	High redundancy	2 - 20 MGy (speed might be an important consideration)

**Trying to collect everything at once will usually result in failure**



M. Warkentin *et al. J. Synchrotron Rad.* **20**, 7 (2013)

## Room temperature 298 K

(0.1 – 0.5 MGy)

- Owen, *et al. Acta Cryst.* **D68**, 810 (2012)
- Warkentin, *et al. J. Synchrotron Rad.* **20**, 7 (2013)

## Cryo-temperature 100 K

Native data collection (20 MGy)

- Henderson, *Proc. R. Soc. B.* **241**, 6 (1990)
- Owen, *et al. Proc. Natl. Acad. Sci. USA*, **103**, 4912 (2006)

Experimental phasing (< 5 MGy)

- Holton, J. M. *J. Synchrotron Rad.* **14**, 51 (2007)
- Olieric, *et al. Acta Cryst.* **D63**, 759 (2007)

## Rule of thumb

- Resolution dependency of 10 MGy / Å, Howells *et al. J. El. Spect. & Rel. Phen.* **170**, 4 (2009)
- Does estimation, Holton, *J. Synchrotron Rad.* **16**, 133 (2009)

$$Dose = (t_{expo} \times flux) / (k_{dose} \times I_{H-beam} \times I_{B-beam})$$

$$k_{dose} = 2000\lambda^{-2}$$

## Traditional high-dose coarse-phi slicing strategy

- 0.5-1° per image, 180°, 4-fold redundancy, and 10 MGy
- CCD detector

## low dose, fine-phi slicing, high redundancy strategy

- ½ mosaicity slicing,  $n \times 360^\circ$  Mueller, *et al.*, *Acta Cryst.* **D68**, 42 (2012)
- Distribute x-ray dose to multiple data sets. Liu *et al.* *Acta Cryst.* **A67**, 544, (2011)
- PILATUS detector

## Multi-orientation and multi-crystal strategy

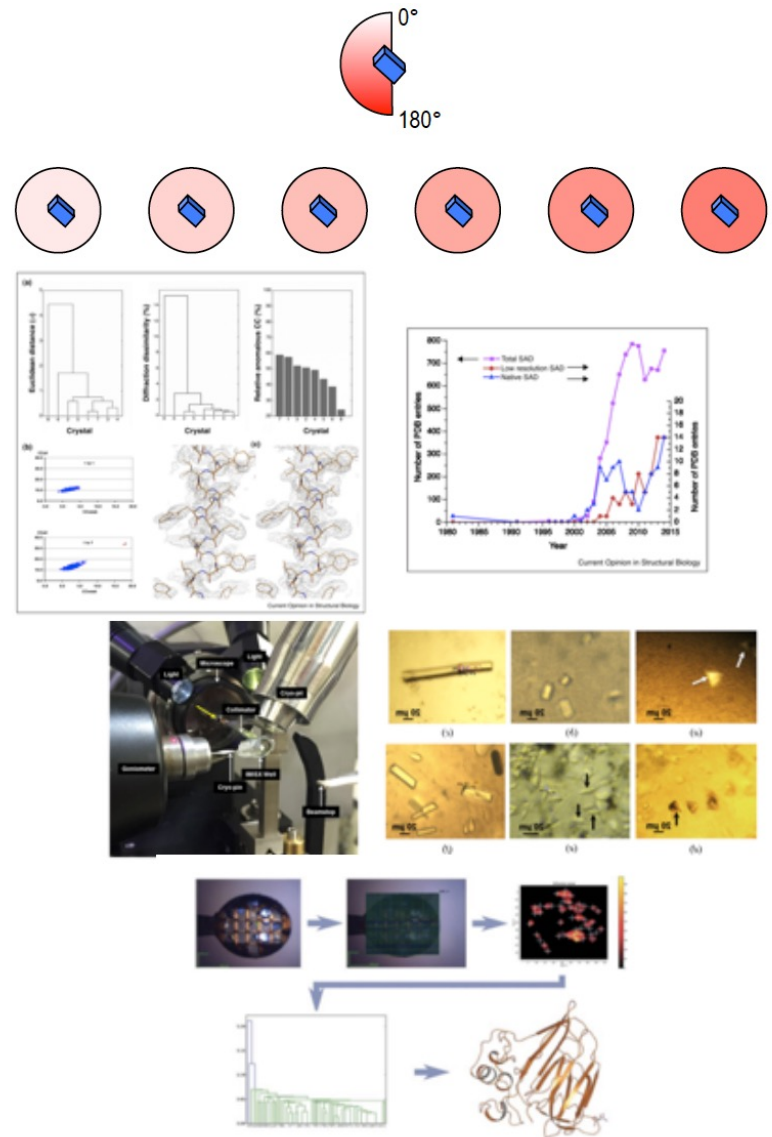
- Distribute x-ray dose to multiple data sets and multiple crystals
- Liu & Hendrickson *Curr. Opin. Struc. Bio.* **34**, 99 (2015)
- Weinert *et al.* *Nature Methods* **12**, 131, (2015)

## Micro-crystallography

- 10-20° data per crystal  $\times n$  crystals
- Smith *et al.* *Curr. Opin. Struc. Bio.* **22**, 602 (2012)

## Serial crystallography

- Injector method. Botha *et al.* *Acta Cryst.* **D71**, 397 (2015), Nogly *et al.* *IUCrJ*, **2**, 168 (2015)
- *In-situ* method. Huang *et al.* *Acta Cryst.* **D71**, 1238 (2015), **D72**, 93 (2016)
- Scanning method. Gati *et al.* *IUCrJ*, **1**, 87 (2014), Zander *et al.*, *Acta Cryst.* **D71**, 2328 (2015)



# References on dose choice

## **10 MGy/A resolution:**

Howells MR, Beetz T, Chapman HN, Cui C, Holton JM, Jacobsen CJ, Kirz J, Lima E, Marchesini S, Miao H, Sayre D, Shapiro DA, Spence JHC & Starodub D (2009). *Electron Spectrosc. Relat. Phenom.* **170**, 4-12.

## **1% non-isomorphism per MGy:**

Banumathi S, Zwart PH, Ramagopal UA, Dauter M & Dauter Z (2004) *Acta Cryst. D* **60**, 1085-1093.

## **200 kGy for Room Temperature:**

Warkentin M, Badeau R, Hopkins JB, Mulichak AM, Keefe LJ & Thorne RE (2012). *Acta Cryst. D* **68**, 124-133.

Barker AI, Southworth-Davies RJ, Paithankar KS, Carmichael I & Garman EF (2009). *J. Synch. Rad.* **16**, 205-216.

Blake CCF & Phillips DC (1962)., pp. 183-191. Vienna: IAEA.

## **5 MGy for Se-Met:**

Holton JM (2007). *J. Synch. Rad.* **14**, 51-72.

## **4 MGy for Hg-Cys:**

Ramagopal UA, Dauter Z, Thirumuruhan R, Fedorov E & Almo SC (2005).", *Acta Cryst. D* **61**, 1289-1298.

## **2 MGy for Cys-Cys:**

Murray JW & Garman EF (2002). *J. Synch. Rad.* **9**, 347-354.

## **500 kGy for Br-RNA:**

Olieric V, Ennifar E, Meents A, Fleurant M, Besnard C, Pattison P, Schiltz M, Schulze-Briesse C & Dumas P (2007, *Acta Cryst. D* **63**, 759-768.

## **500 kGy for Photosystem II:**

Yano J, Kern J, Irrgang K-D, Latimer MJ, Bergmann U, Glatzel P, Pushkar Y, Biesiadka J, Loll B, Sauer K, Messinger J, Zouni A & Yachandra VK (2005). *PNAS USA* **102**, 12047-12052.

## **60 kGy for putidaredoxin:**

Corbett MC, Latimer MJ, Poulos TL, Sevrioukova IF, Hodgson KO & Hedman B (2007, *Acta Cryst. D* **63**, 951-960.

## **60 kGy for bacteriorhodopsin:**

Borshchevskiy V, Round E, Erofeev I, Weik M, Ishchenko A, Gushchin I, Mishin A, Willbold D, Buldt G & Gordeliy V (2014). *Acta Cryst. D* **70**, 2675-2685.

## **20 kGy for Fe reduction in myoglobin:**

*Radiat Phys Chem Oxf Engl* 1993 **76**, 714-721.

## **rough rotisserie factor:**

Holton JM (2009). "A beginner's guide to radiation damage", *J. Synch. Rad.* **16**, 133-142.

## **more accurate rotisserie factor calculations:**

Zeldin OB, Brockhauser S, Bremridge J, Holton JM & Garman EF (2013). *PNAS USA* **110**, 20551-20556.





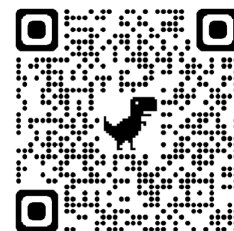
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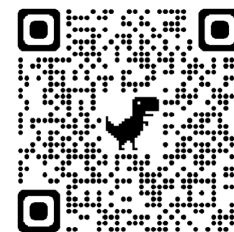






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