Dose driven data collection to optimise your experiments

Better (starting) collection parameters

Towards the best data in a world of less experienced beamline users

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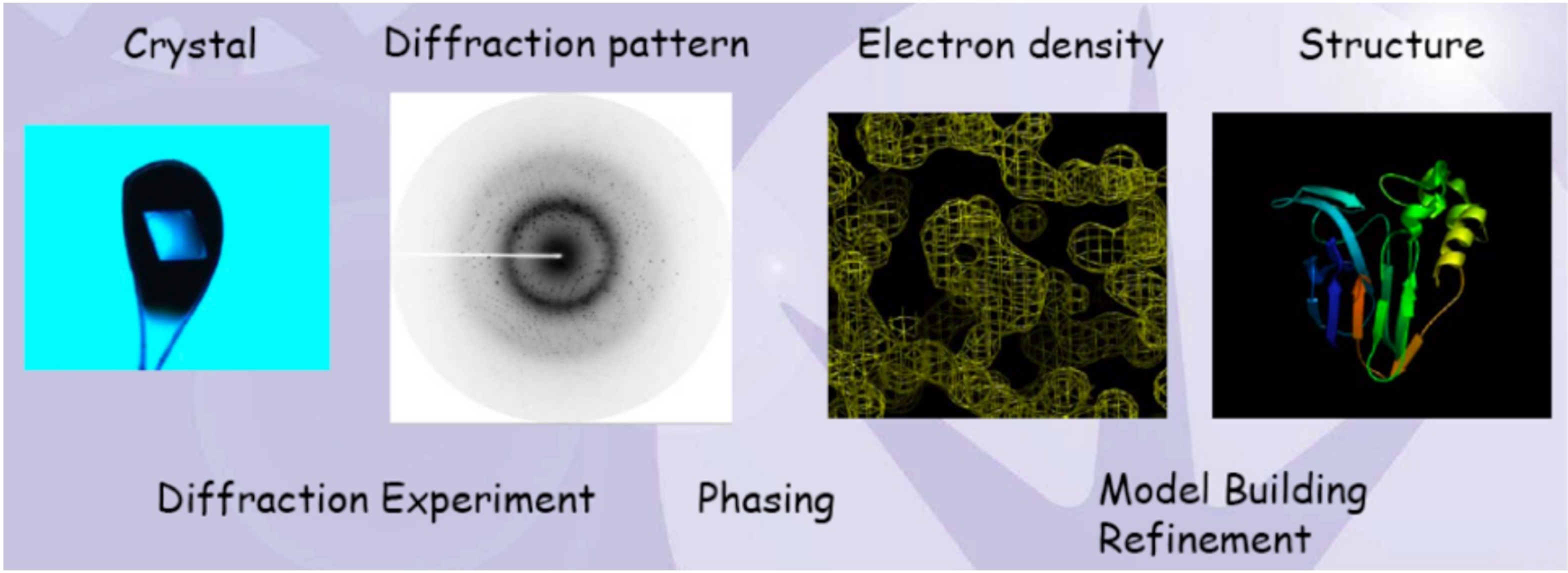
Thanks to
Neil Paterson
Gwyndaf Evans
Ralf Flaig
Daniela Stock
Murray Stuart
Meitian Wang
Tom Caradoc-Davies
[redacted] Andreas Förster <3
for slides & ideas

diamond

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



Crystal

Diffraction pattern

Electron density

Structure

Diffraction Experiment

Phasing

Model Building
Refinement

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

REC TC: 00:00:00:00

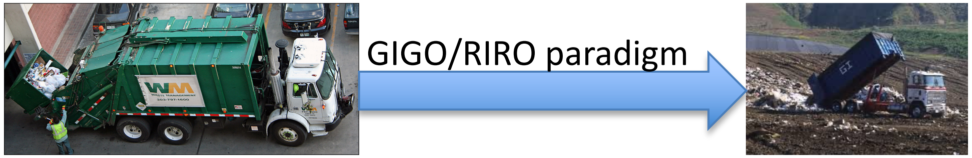
Data collection is important!

<ins>This is the last experimental step</ins>

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

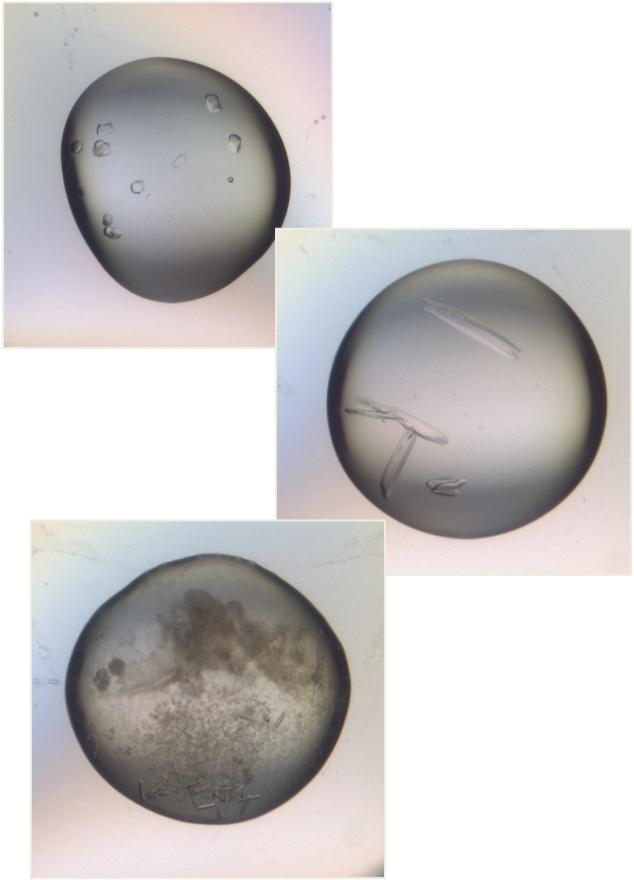
"One good friend is better than a thousand poor ones." Indian Proverb

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

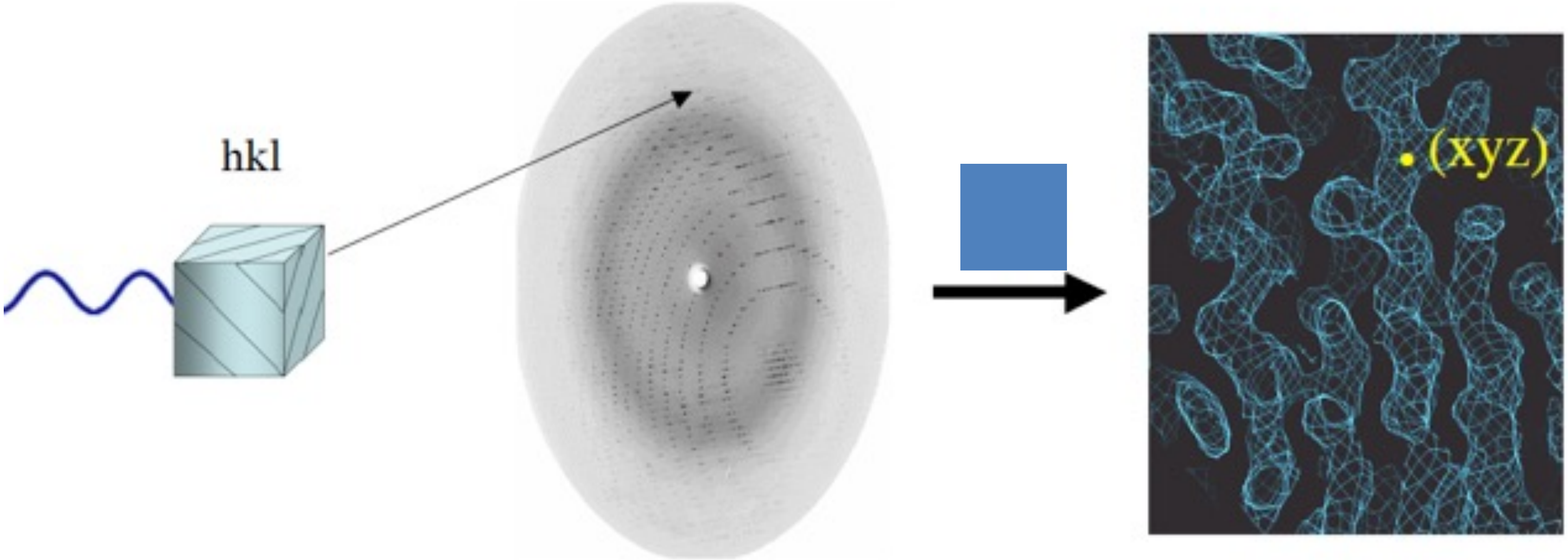


GIGO/RIRO paradigm

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

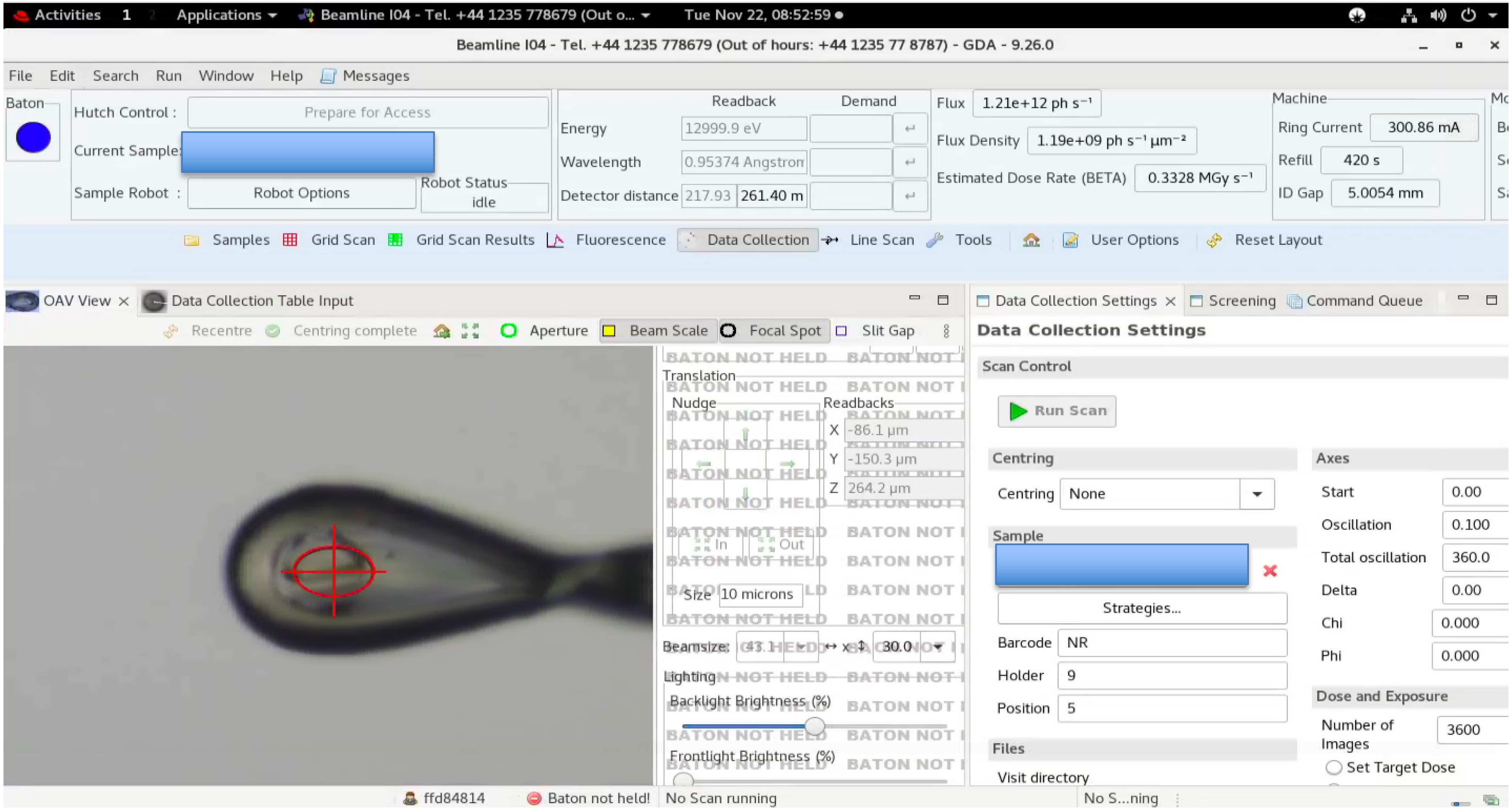


Data collection: the goal



- 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



Beamline I04 - Tel. +44 1235 778679 (Out of hours: +44 1235 77 8787) - GDA - 9.26.0

Tue Nov 22, 08:52:59

Hutch Control :

Current Sample:

Sample Robot :

Robot Status idle

	Readback	Demand
Energy	12999.9 eV	
Wavelength	0.95374 Angstrom	
Detector distance	217.93	261.40 m

Flux 1.21e+12 ph s^{-1}

Flux Density 1.19e+09 ph s^{-1} µm^{-2}

Estimated Dose Rate (BETA) 0.3328 MGy s^{-1}

Ring Current 300.86 mA

Refill 420 s

ID Gap 5.0054 mm

Translation

X -86.1 µm

Y -150.3 µm

Z 264.2 µm

Size 10 microns

Beamsize: 43.1 ↔ x ↕ 30.0

Data Collection Settings

Centring None

Barcode NR

Holder 9

Position 5

Start 0.00

Oscillation 0.100

Total oscillation 360.0

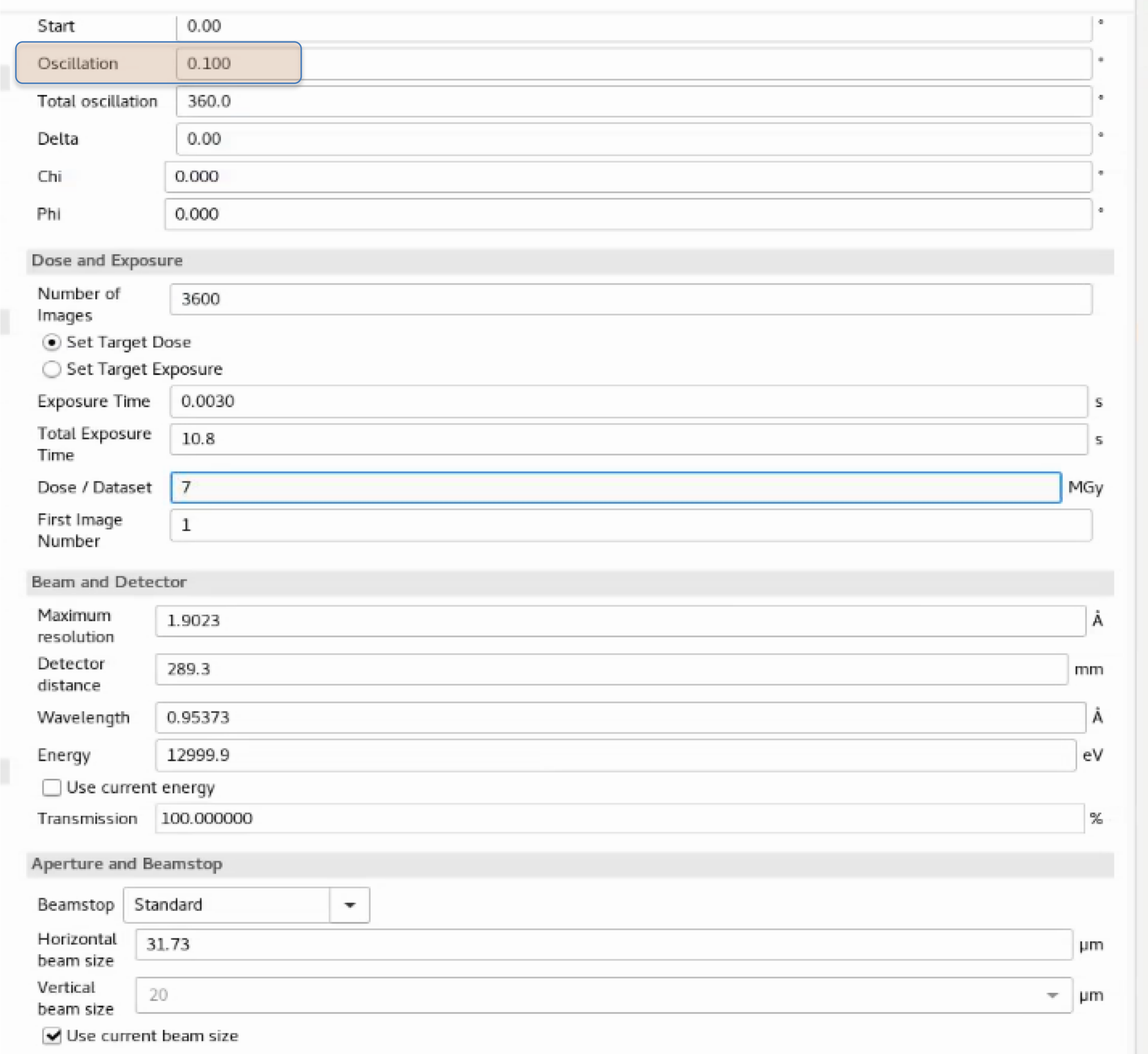
Delta 0.00

Chi 0.000

Phi 0.000

Number of Images 3600

ffd84814 Baton not held! No Scan running No S...ning



Start 0.00 °

Oscillation 0.100 °

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Chi 0.000 °

Phi 0.000 °

Dose and Exposure

Number of Images 3600

● Set Target Dose

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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

☐ Use current energy

Transmission 100.000000 %

Aperture and Beamstop

Beamstop Standard

Horizontal beam size 31.73 µm

Vertical beam size 20 µm

☑ Use current beam size

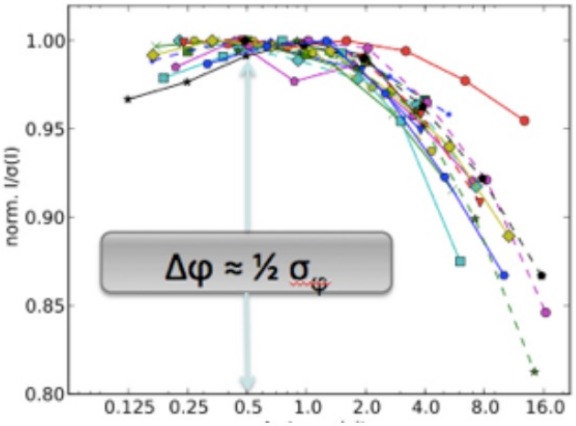
Random errors, counting statistics

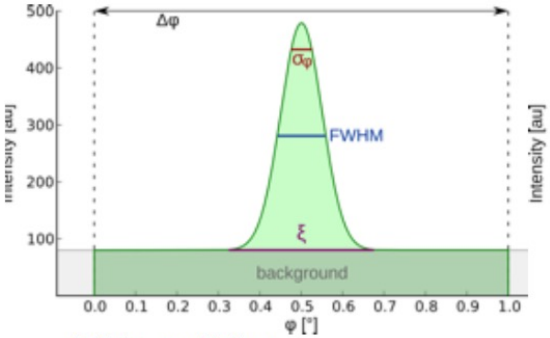
$\sigma_{count} = N^{1/2}$

$I = N_p - N_b$ **Signal is the difference**

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

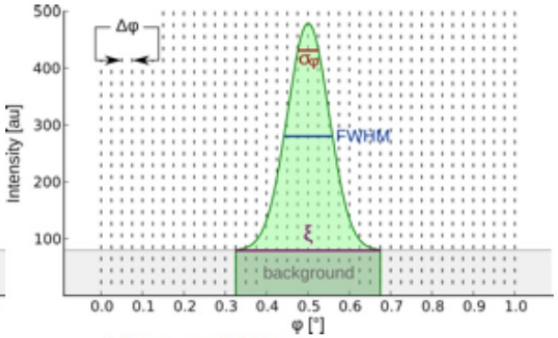
$\sigma_I = (N_p + N_b)^{1/2}$ **Uncertainty is the sum**





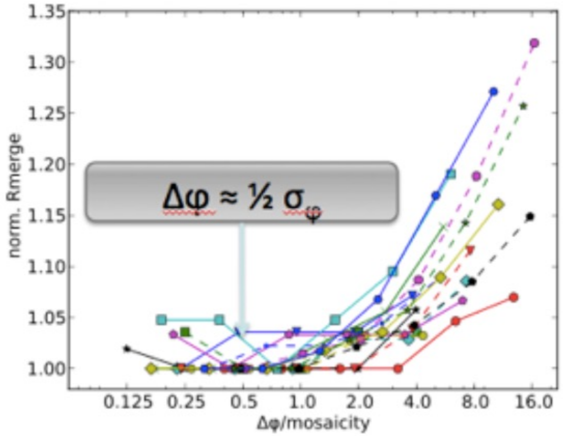
Wide φ-slicing

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



Fine φ-slicing

- Small $\Delta\varphi$ ($\Delta\varphi << \xi$)
- Minimal overlap of reflections and background along φ
- Many images



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

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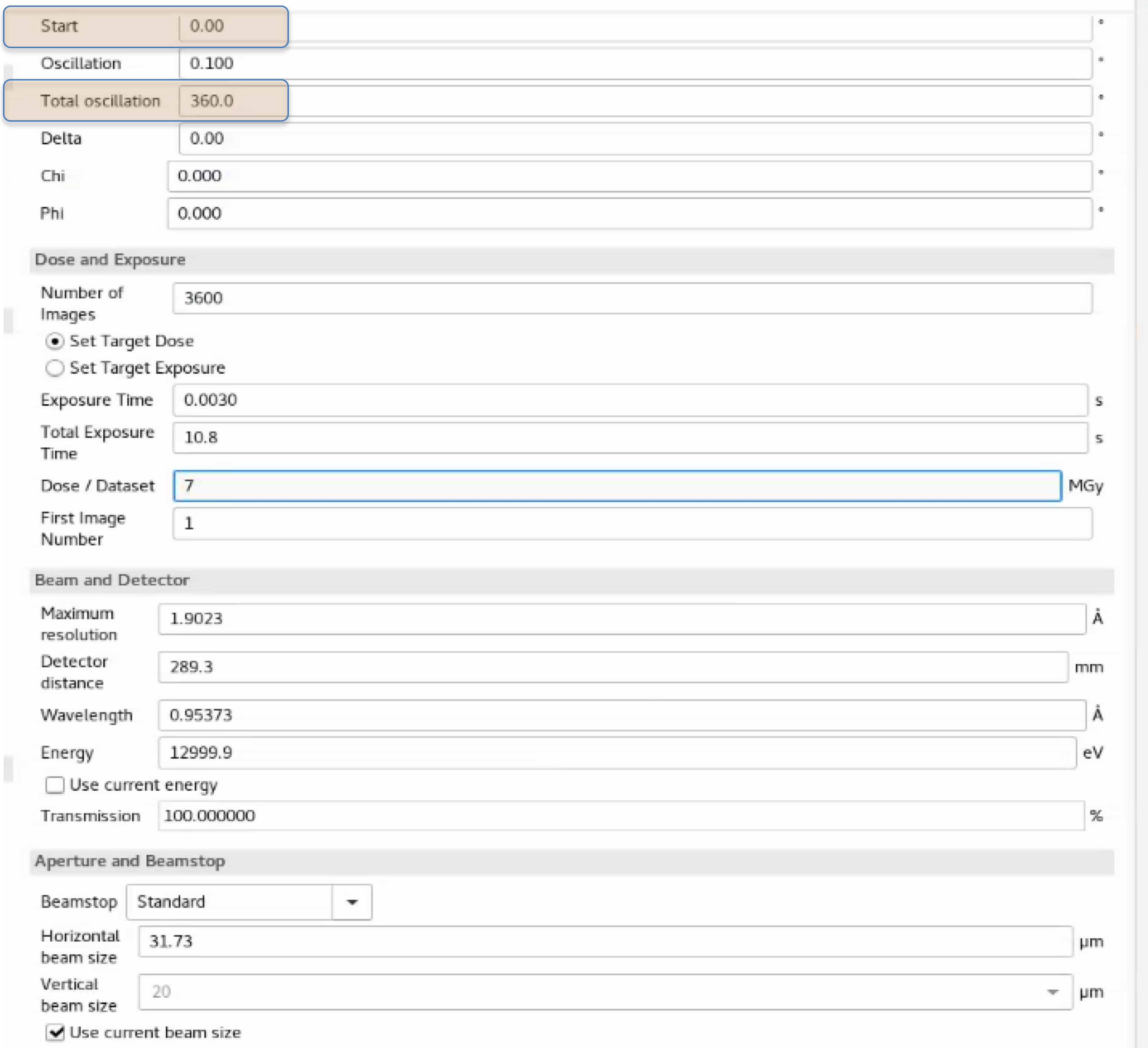
Mueller, *et al*, *Acta Cryst*. **D68**, 42 (2012)



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Wavelength 0.95373 Å

Energy 12999.9 eV

☐ Use current energy

Transmission 100.000000 %

Beamstop Standard

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Vertical beam size 20 µm

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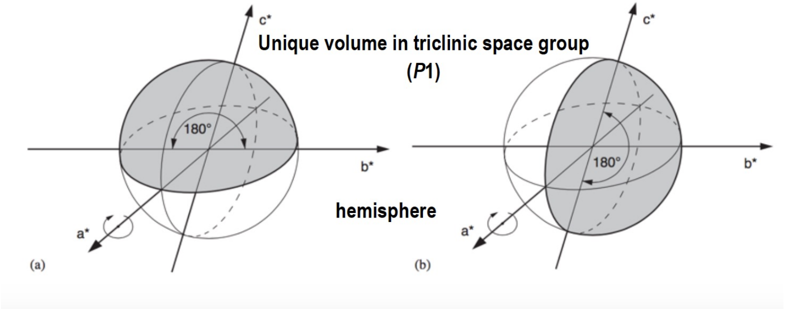
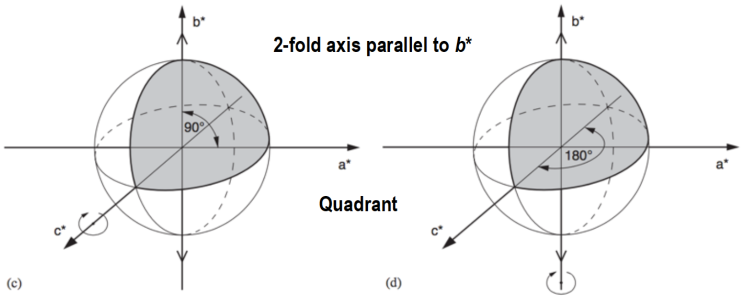
Completeness - crystal symmetry

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

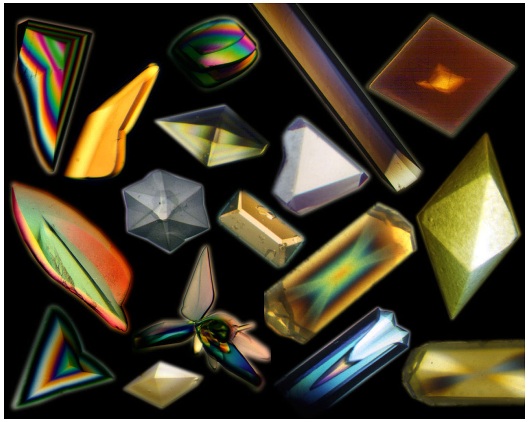
thus even for P1 only 180º are needed to obtain complete data set of unique reflections - unless there is anomalous scattering



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

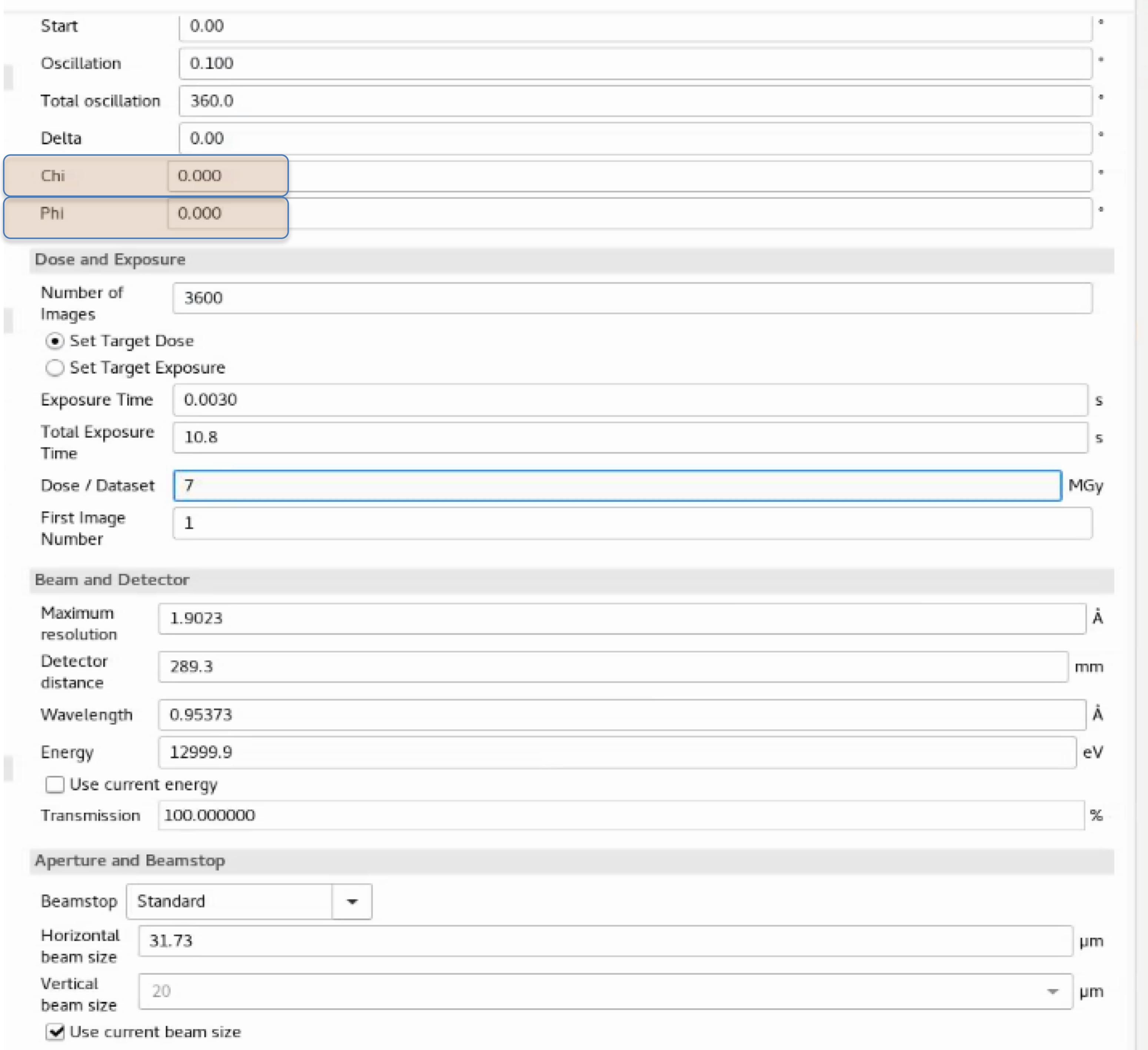


“Introduction to space groups” this morning by Andrey Lebedev



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

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



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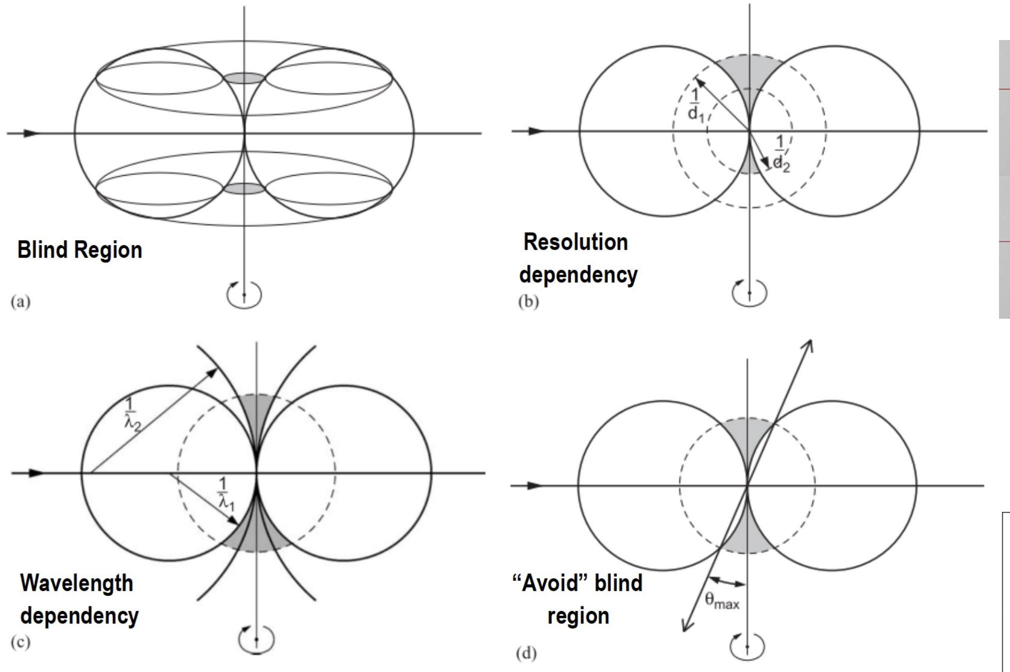
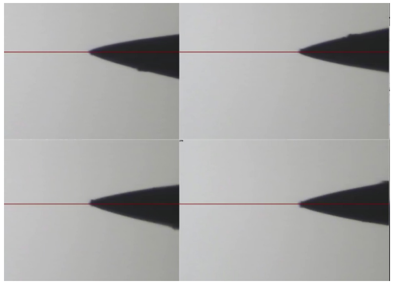
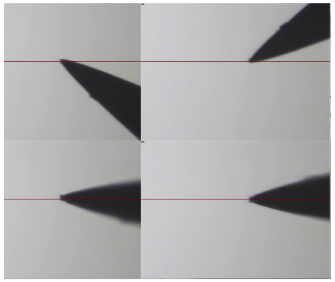


Dauter, *Prog. Biophys Mol. Bio.* **89**, 153 (2005)

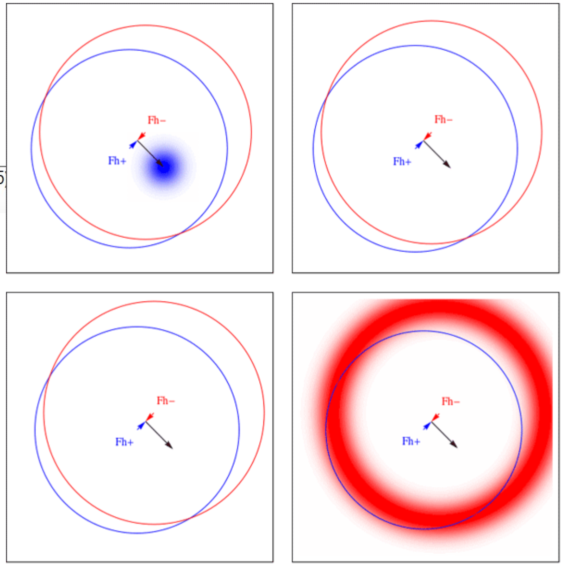


Chi=0 deg

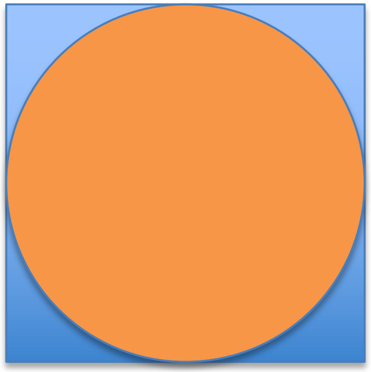


Chi=30 deg

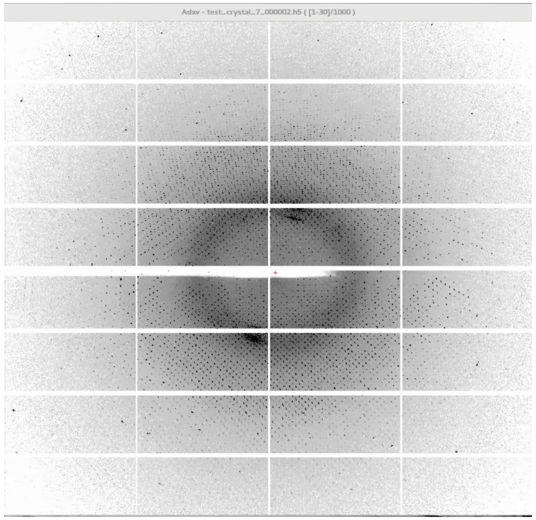
Experimental Phasing



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

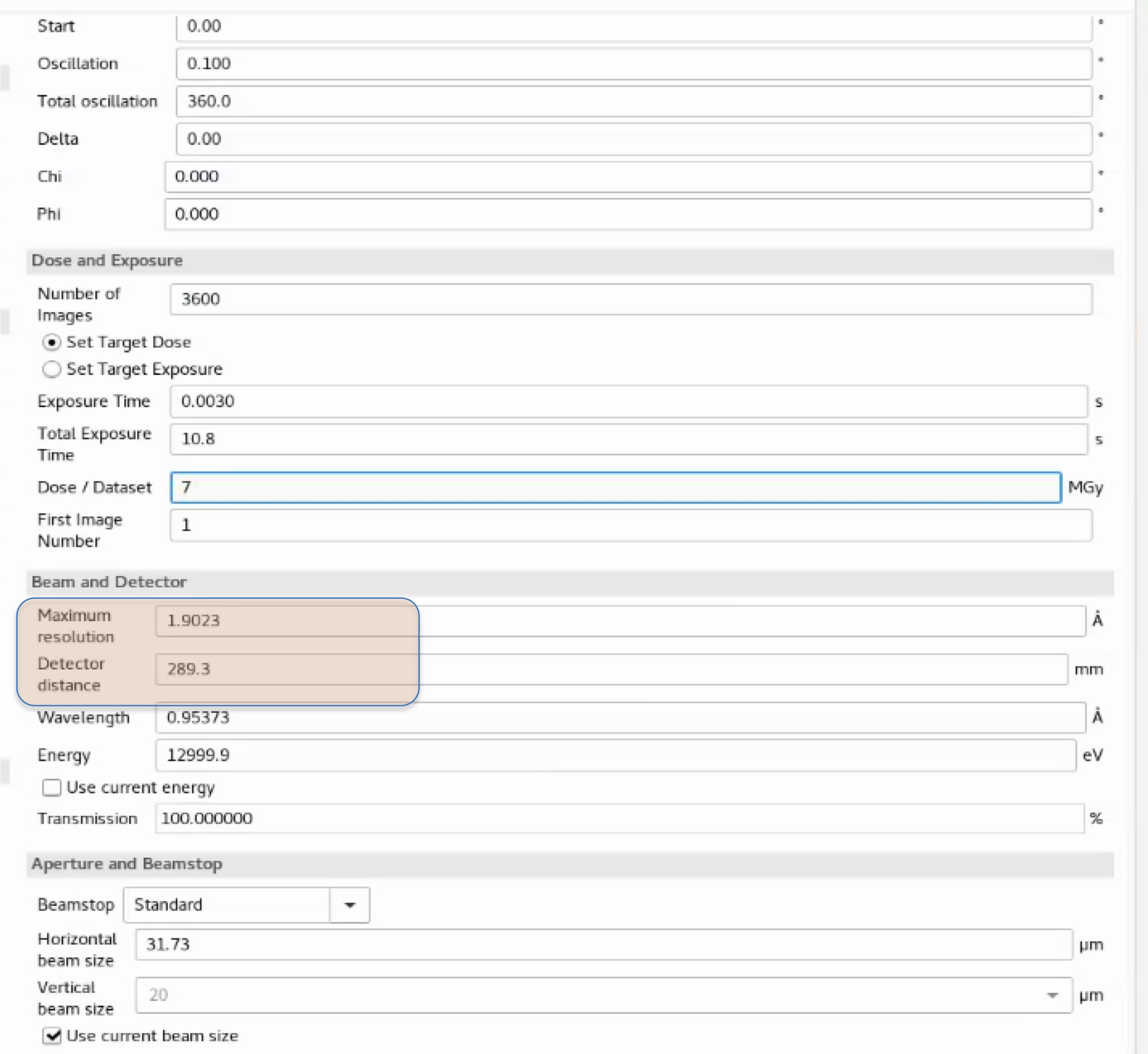


Corner vs Edge



Systematic error reduction
Detector module gaps

Wed 24th Nov
The phase problem, Ed Lowe
Experimental Phasing, Ed Lowe



Start 0.00 °

Oscillation 0.100 °

Total oscillation 360.0 °

Delta 0.00 °

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Dose and Exposure

Number of Images 3600

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Dose / Dataset 7 MGy

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Transmission 100.000000 %

Aperture and Beamstop

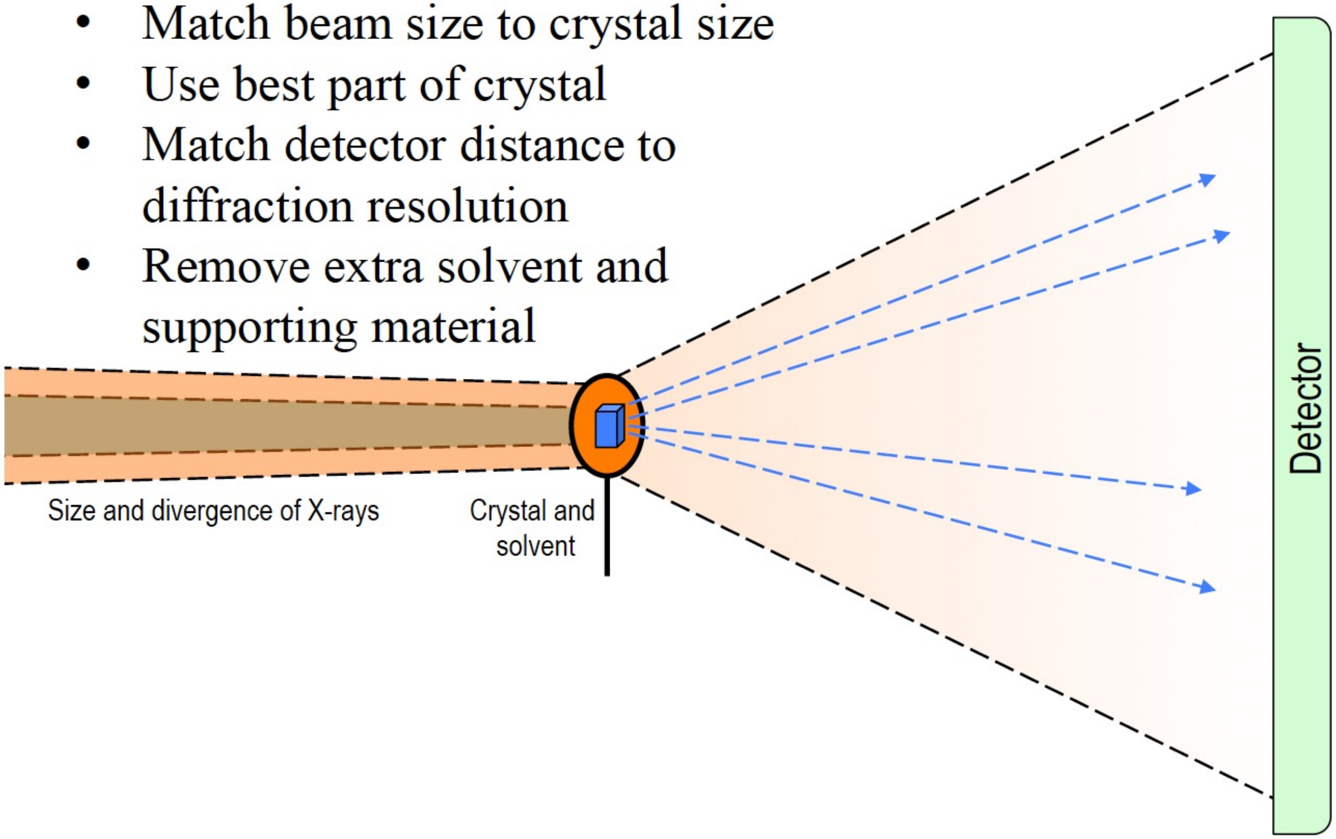
Beamstop Standard

Horizontal beam size 31.73 µm

Vertical beam size 20 µm

☑ Use current beam size

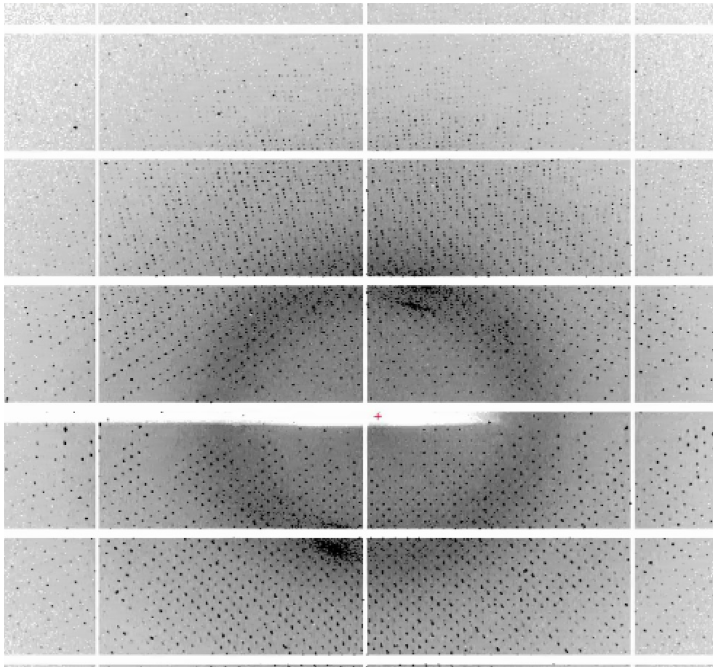
- Match beam size to crystal size
- Use best part of crystal
- Match detector distance to diffraction resolution
- Remove extra solvent and supporting material



Screening and analysis

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

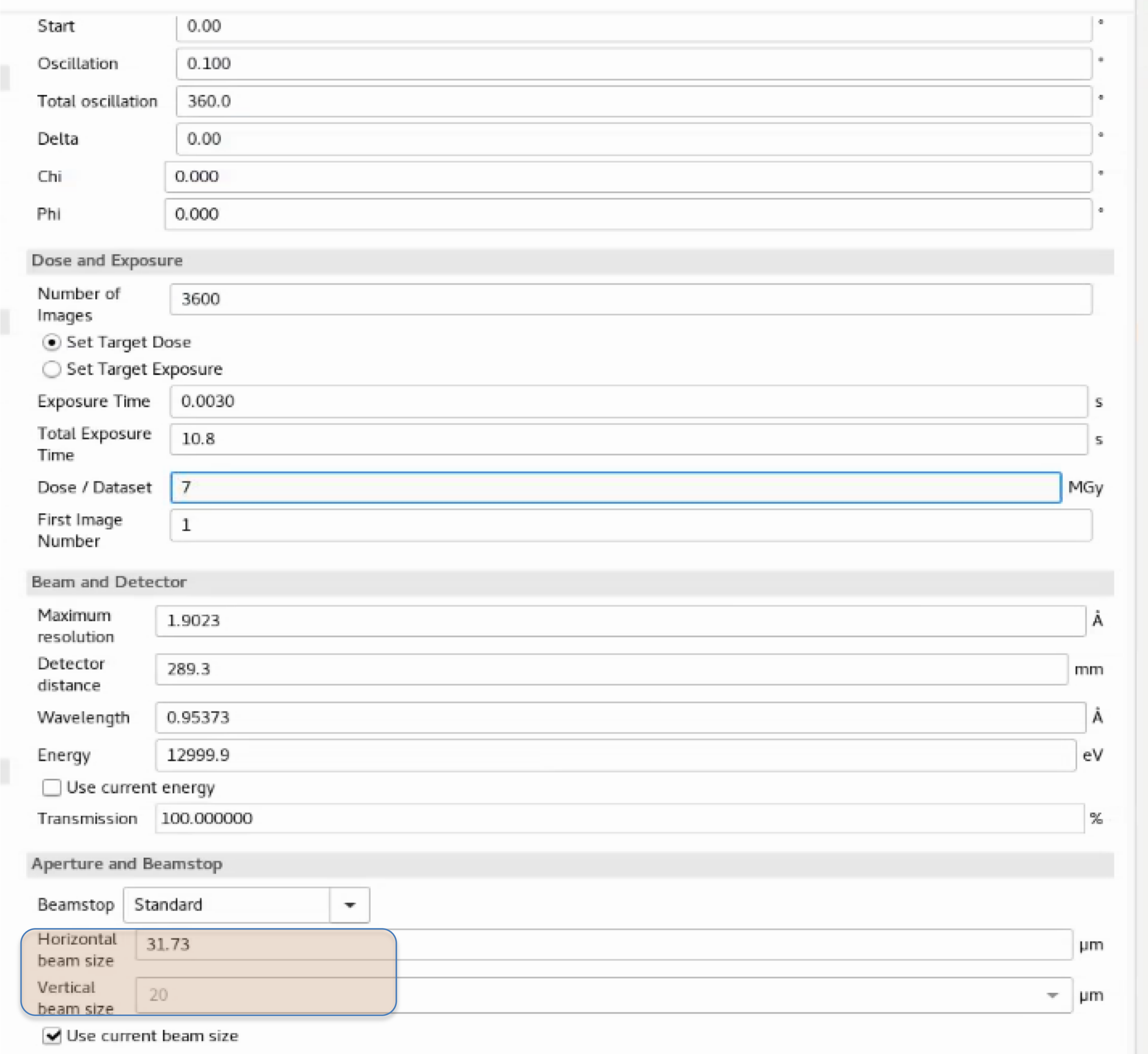
Usually by collecting a small wedge of 15-20 degrees ideally at the thickest part of the crystal (or the old method of 3 images 45 degrees away from each other)



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 then looking at fine sliced images. Max res: best to rely on data reduction programs and apply a buffer (e.g 0.5 A)



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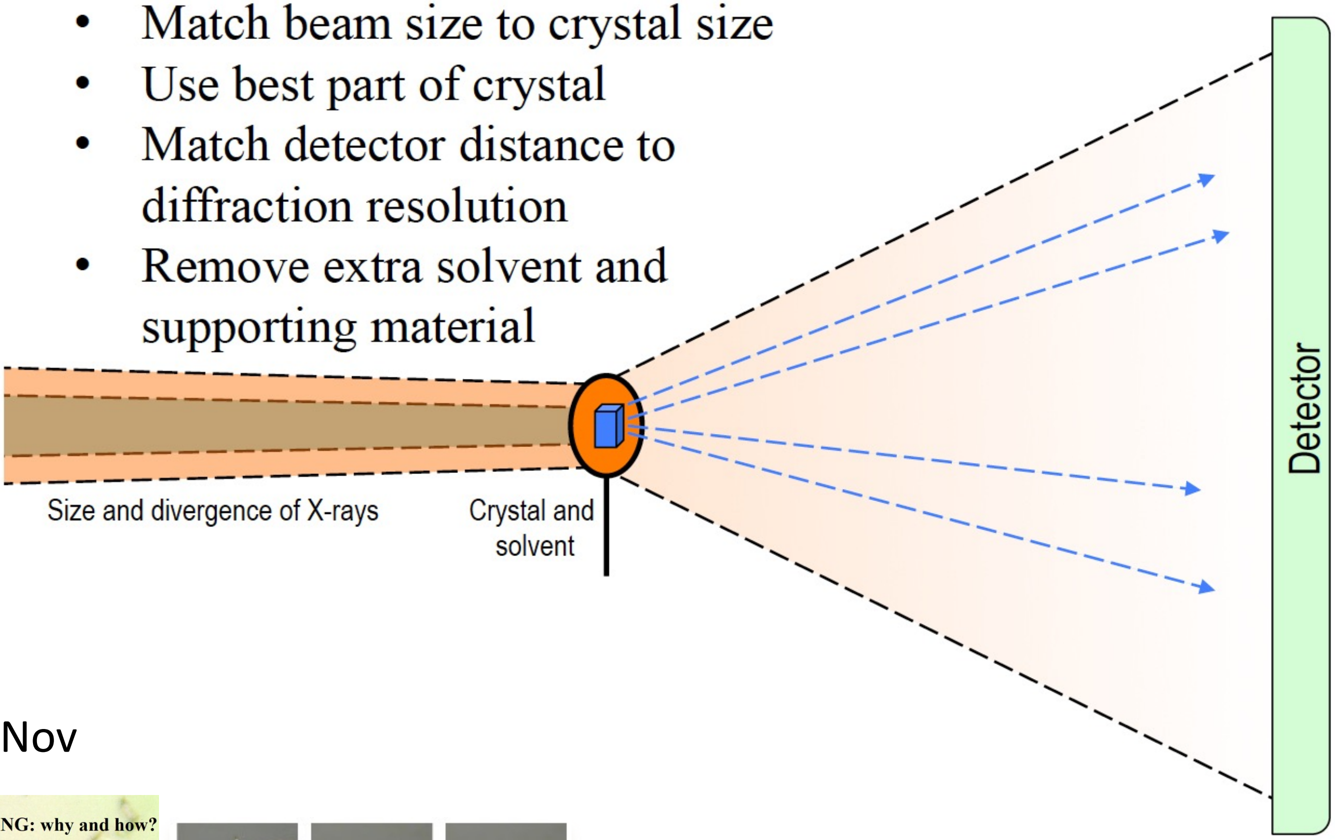
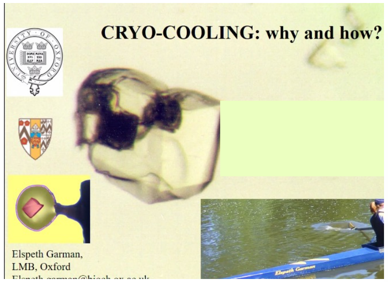
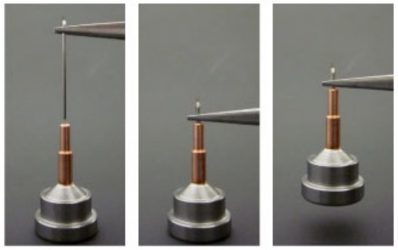


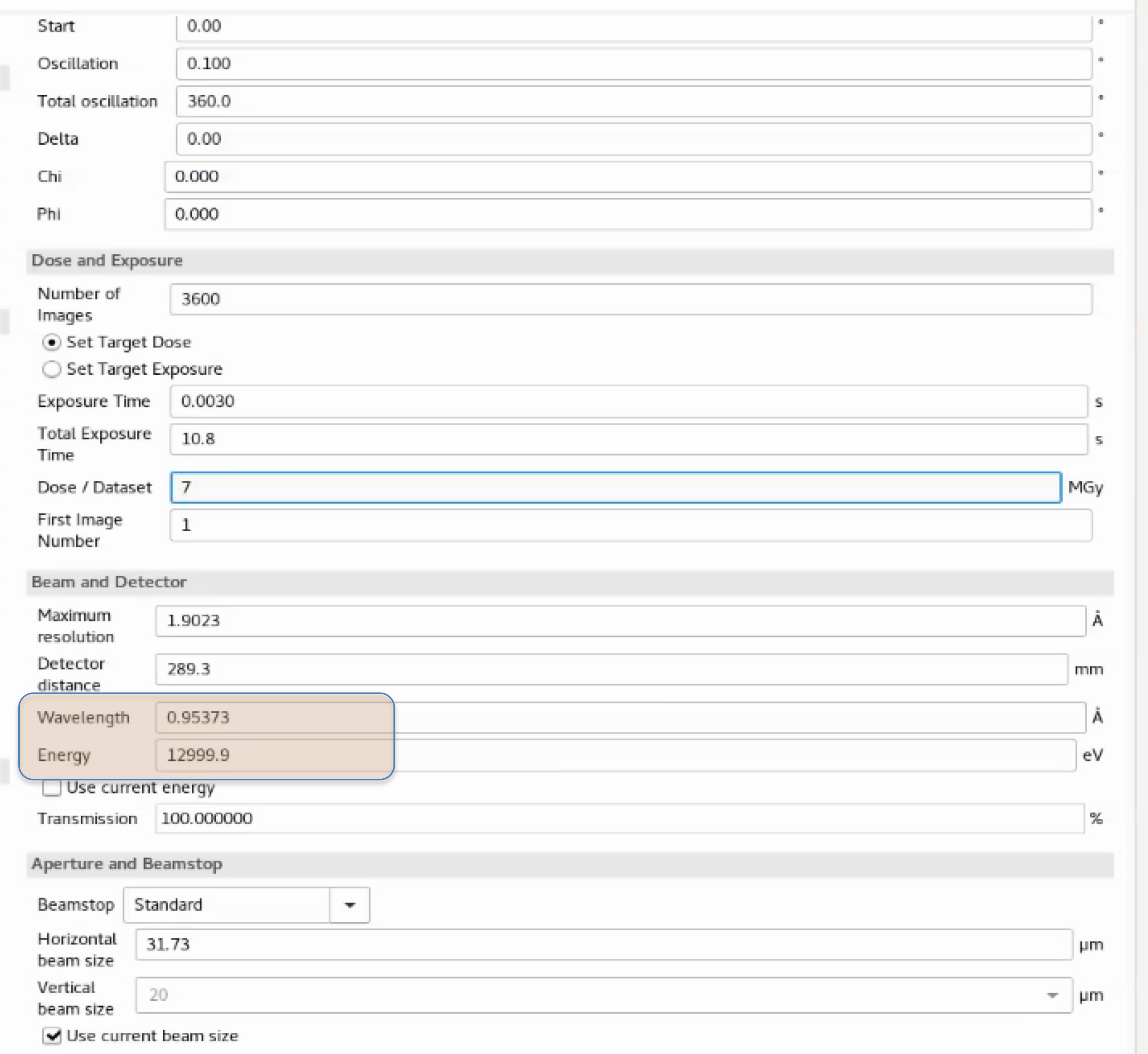
Mon, 17th Nov



CRYO-COOLING: why and how?

Elspeth Garman,
LMB, Oxford
Elspeth.garman@bioch.ox.ac.uk





Start 0.00 °

Oscillation 0.100 °

Total oscillation 360.0 °

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Aperture and Beamstop

Beamstop Standard

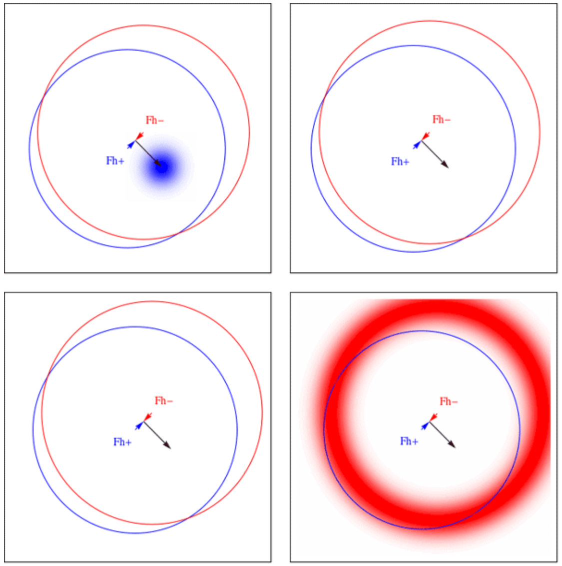
Horizontal beam size 31.73 µm

Vertical beam size 20 µm

☑ Use current beam size

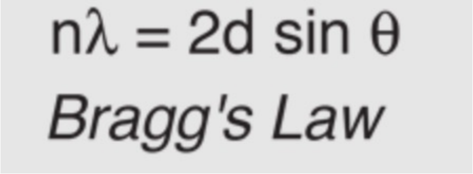
Energy selection

Experimental Phasing



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

High resolution



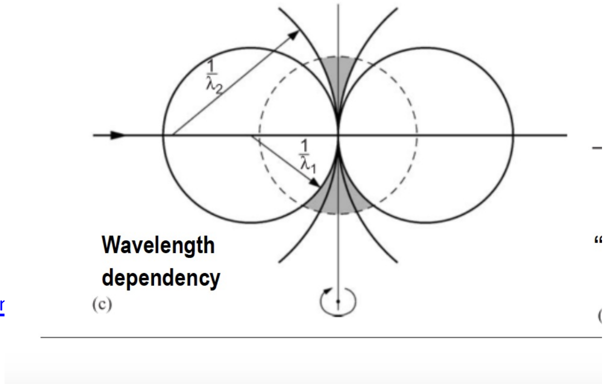
$n\lambda = 2d \sin \theta$

Bragg's Law

https://www.diamond.ac.uk/Instruments/Mx/Common/Calculators.htr

(search for "useful calculators diamond")

Blind region / Cuspid



Basic Diffraction Theory, Kamel El Omari

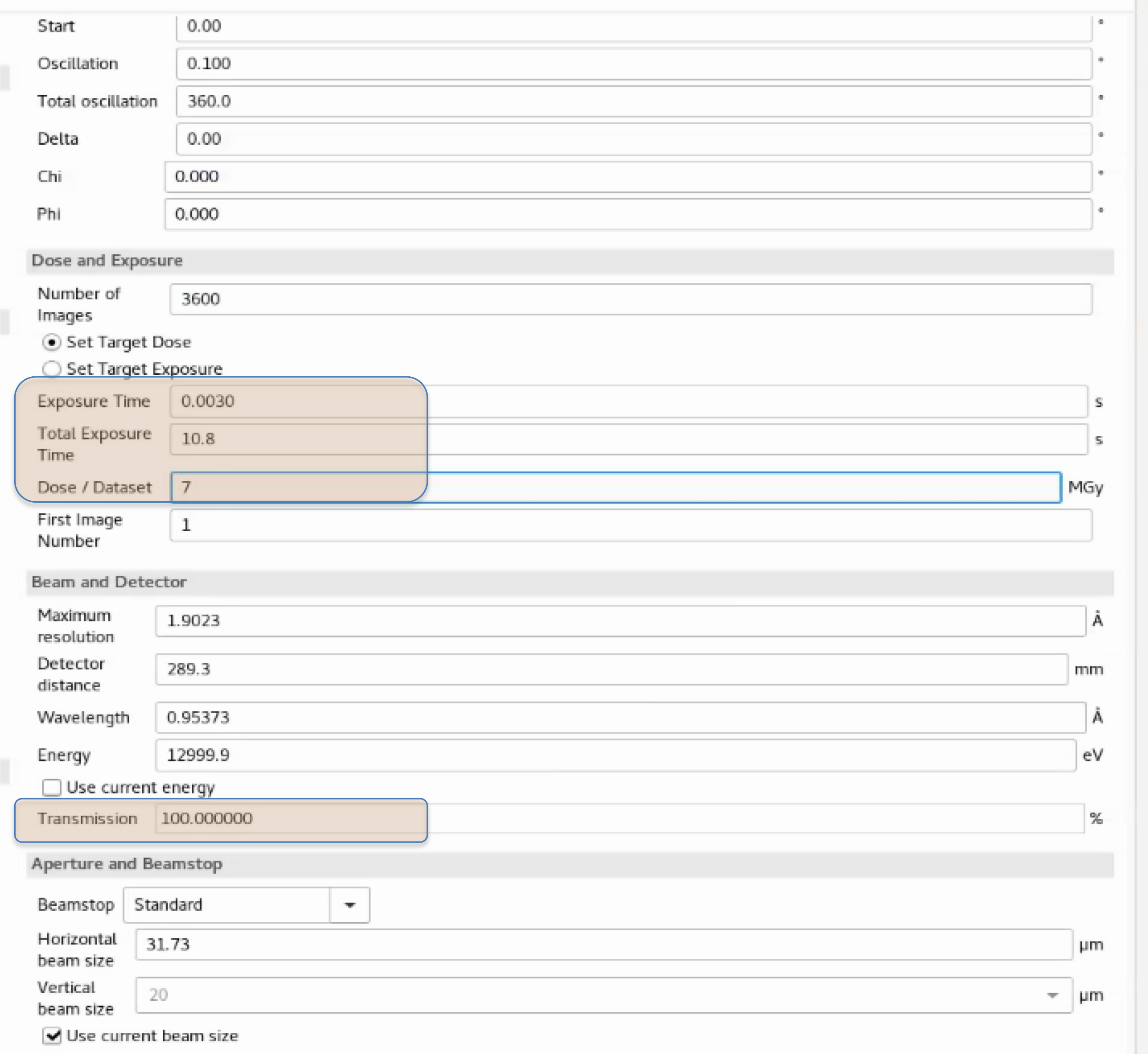
Crystal life time / Radiation damage for small crystals

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

Selina L. S. Storm,[a‡] Danny Axford[a] and Robin L. Owen[a*]

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 °

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Total oscillation: 360.0 °

Delta: 0.00 °

Chi: 0.000 °

Phi: 0.000 °

Dose and Exposure

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Detector distance: 289.3 mm

Wavelength: 0.95373 Å

Energy: 12999.9 eV

☐ Use current energy

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Aperture and Beamstop

Beamstop: Standard

Horizontal beam size: 31.73 µm

Vertical beam size: 20 µm

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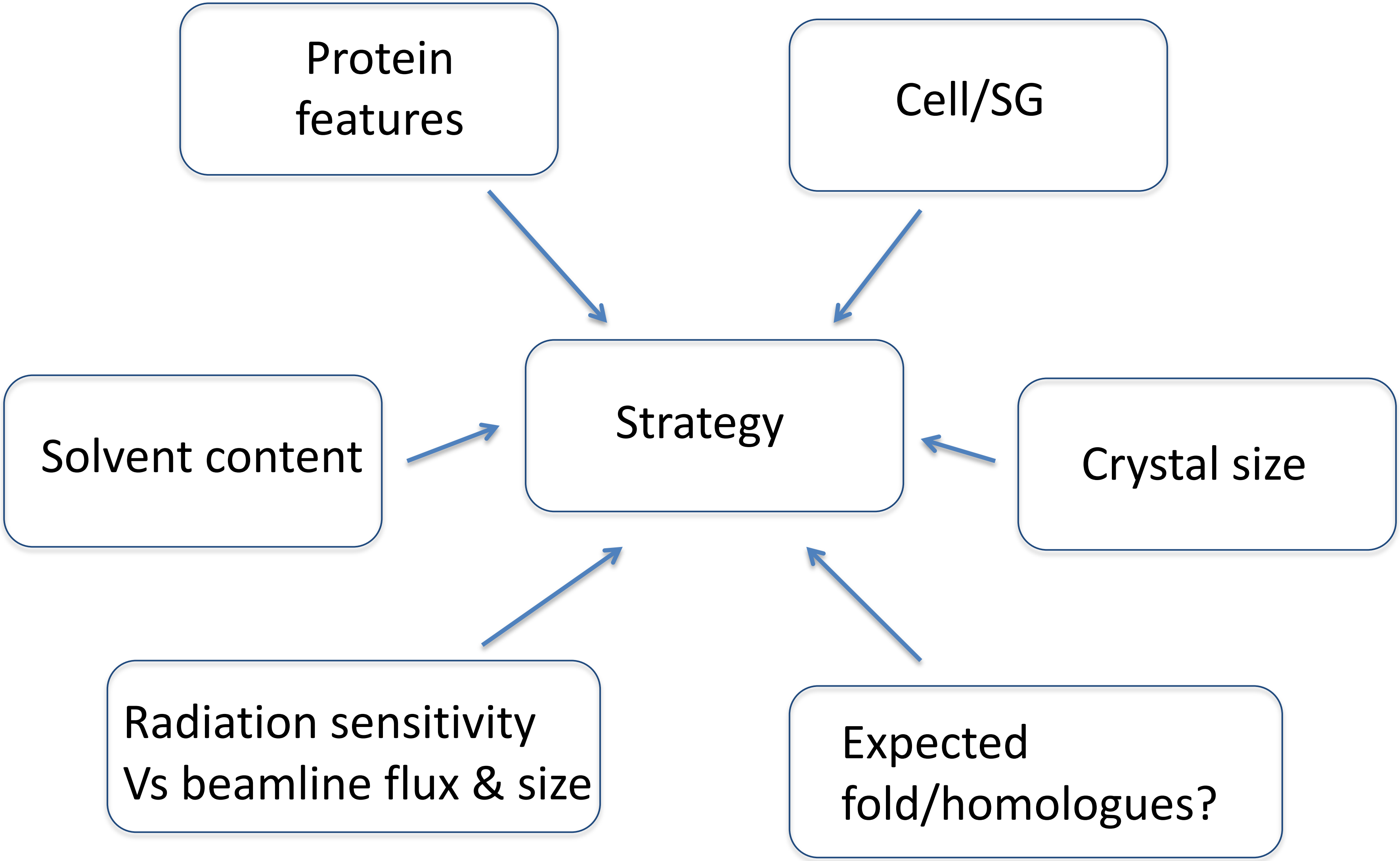
Preparation - Prior knowledge



Protein features

Cell/SG

Solvent content

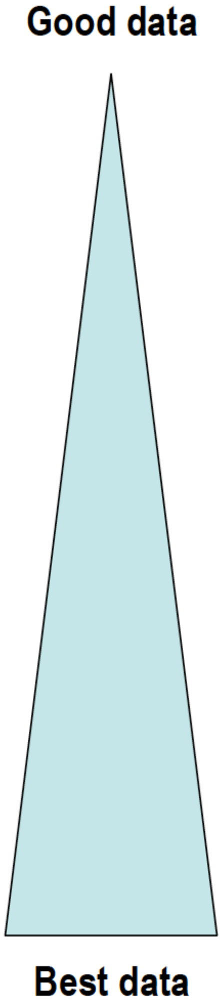
Strategy

Crystal size

Radiation sensitivity
Vs beamline flux & size

Expected fold/homologues?

- 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)
Native data collection	High resolution (e.g < 1.8 A) 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 A), complete data. High throughput (FAST)	High redundancy	10 - 20 MGy (*)

Trying to collect everything at once will usually result in failure

(*)For a ~3A resolution dataset per Diamond UDC recipe

expected crystal lifetime calculator
https://bl831.als.lbl.gov/xtallife.html

Raddose 3D
https://github.com/GarmanGroup/RADDOSE-3D

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

Assumptions:
Beamline energy at 0.9537 A / 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

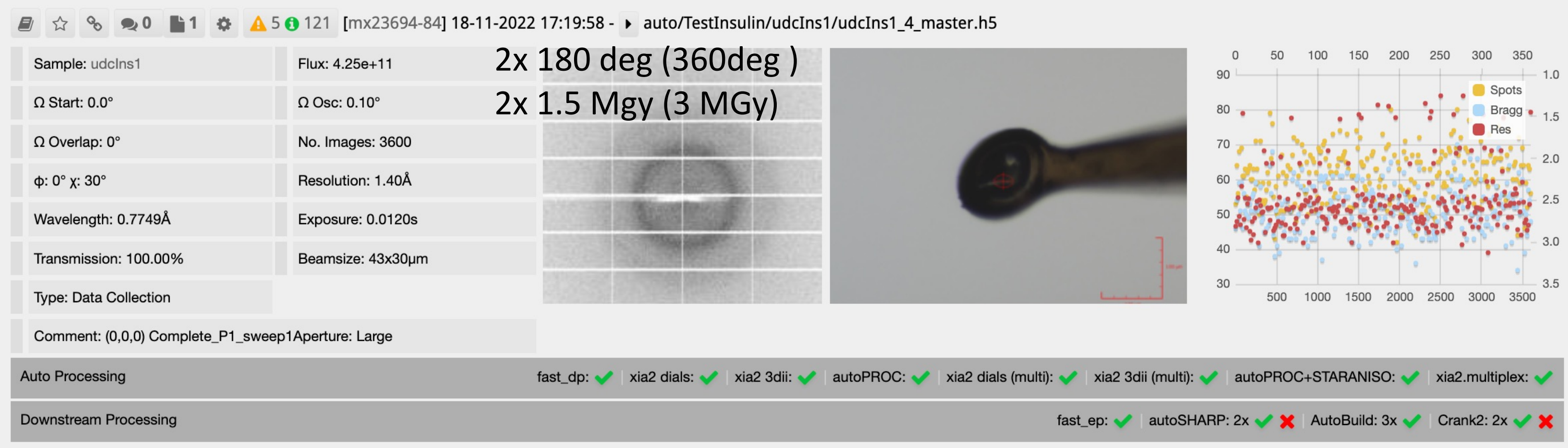
Be mindful of how the beamline generates a small beam size. Focusing (I04 +I24) can increase the flux density massively compared to apertures (I03)

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

E.g. 50x50 μm^2 beam will deliver around 45x less dose than 9x6 μm^2 beam on I24

So match beam to crystal, but attenuate when required

Example with Phasing UDC



0 1 ⚠ 5 ℹ 121 [mx23694-84] 18-11-2022 17:19:58 - ▸ auto/TestInsulin/udcIns1/udcIns1_4_master.h5

Sample: udcIns1

Ω Start: 0.0°

Ω Overlap: 0°

ϕ: 0° χ: 30°

Wavelength: 0.7749Å

Transmission: 100.00%

Type: Data Collection

Comment: (0,0,0) Complete_P1_sweep1Aperture: Large

Flux: 4.25e+11

Ω Osc: 0.10°

No. Images: 3600

Resolution: 1.40Å

Exposure: 0.0120s

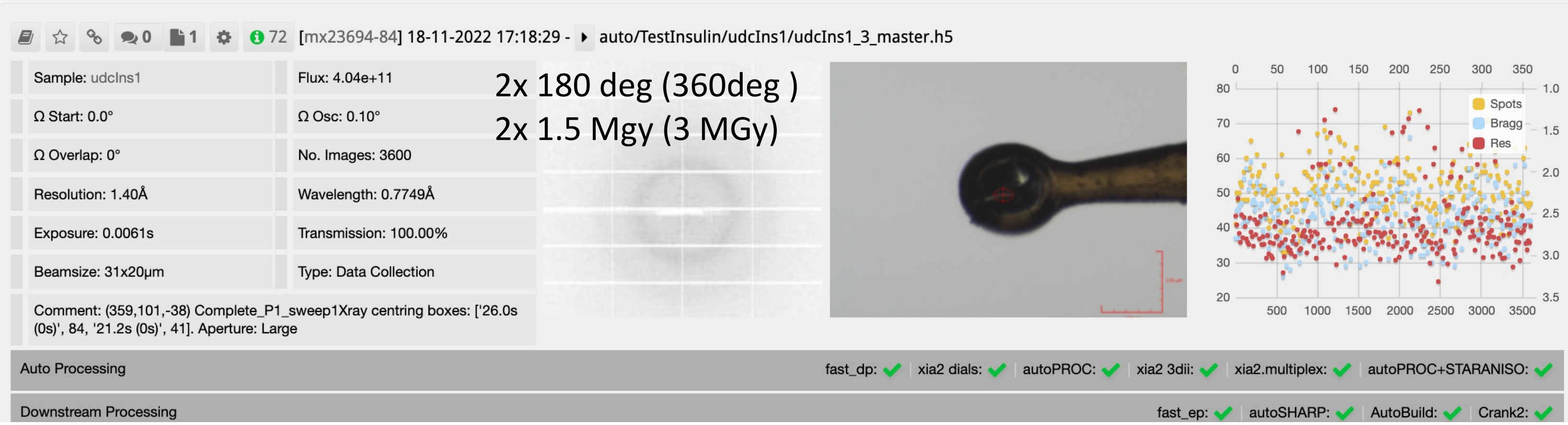
Beamsize: 43x30μm

2x 180 deg (360deg)

2x 1.5 Mgy (3 MGy)

Auto Processing: fast_dp: ✓ xia2 dials: ✓ xia2 3dii: ✓ autoPROC: ✓ xia2 dials (multi): ✓ xia2 3dii (multi): ✓ autoPROC+STARANISO: ✓ xia2.multiplex: ✓

Downstream Processing: fast_ep: ✓ autoSHARP: 2x ✓ ✗ AutoBuild: 3x ✓ Crank2: 2x ✓ ✗



0 1 ℹ 72 [mx23694-84] 18-11-2022 17:18:29 - ▸ auto/TestInsulin/udcIns1/udcIns1_3_master.h5

Sample: udcIns1

Ω Start: 0.0°

Ω Overlap: 0°

Resolution: 1.40Å

Exposure: 0.0061s

Beamsize: 31x20μm

Comment: (359,101,-38) Complete_P1_sweep1Xray centring boxes: ['26.0s (0s)', 84, '21.2s (0s)', 41]. Aperture: Large

Flux: 4.04e+11

Ω Osc: 0.10°

No. Images: 3600

Wavelength: 0.7749Å

Transmission: 100.00%

Type: Data Collection

2x 180 deg (360deg)

2x 1.5 Mgy (3 MGy)

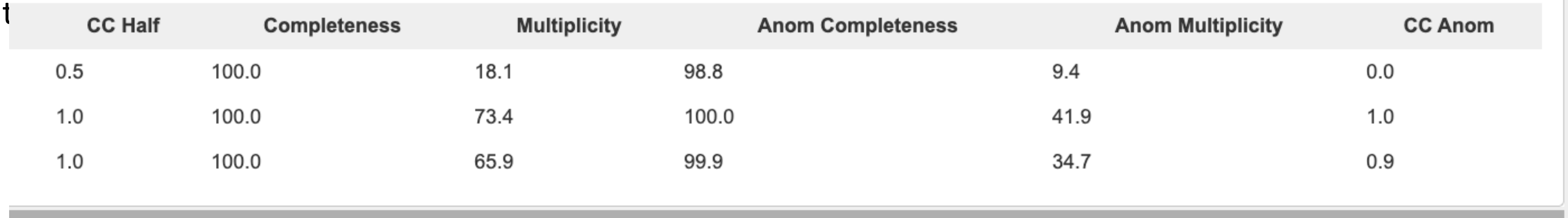
Auto Processing: fast_dp: ✓ xia2 dials: ✓ autoPROC: ✓ xia2 3dii: ✓ xia2.multiplex: ✓ autoPROC+STARANISO: ✓

Downstream Processing: fast_ep: ✓ autoSHARP: ✓ AutoBuild: ✓ Crank2: ✓

720 degrees with 2x 360 deg at two different Chi angles

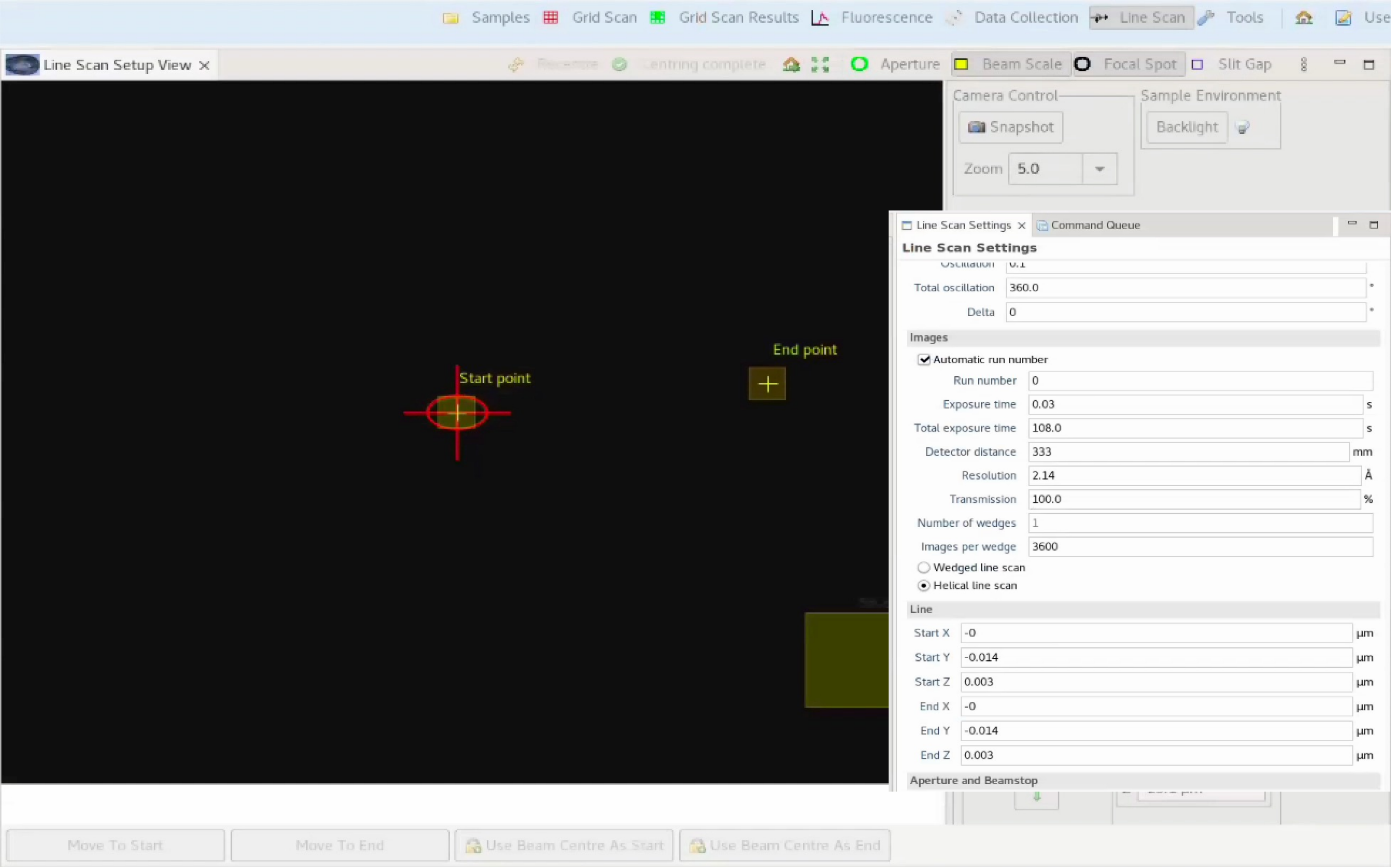
6 Mgy for a 1.4 A max diffraction

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



Zoom 5.0

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

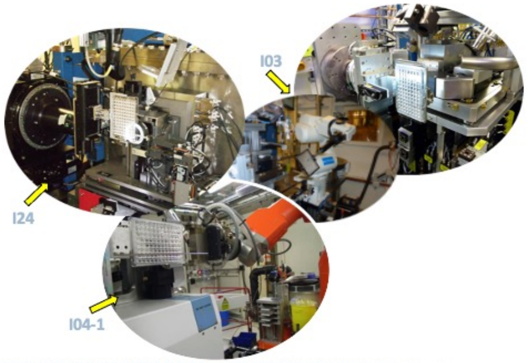
● Helical line scan

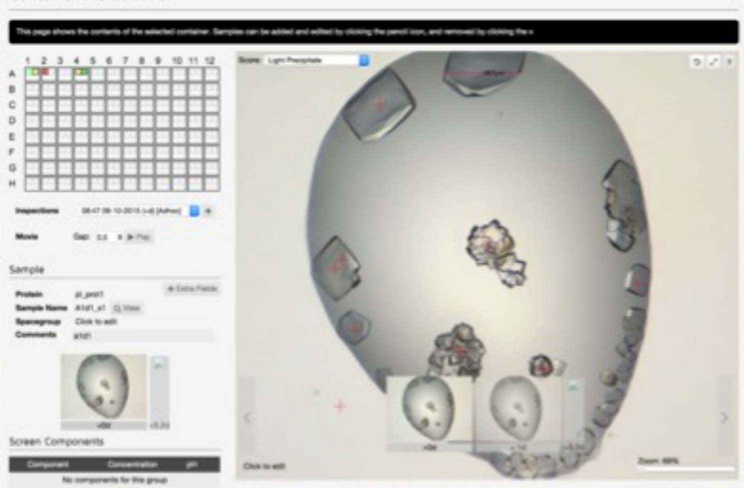
Line

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

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




Container: Z12368764

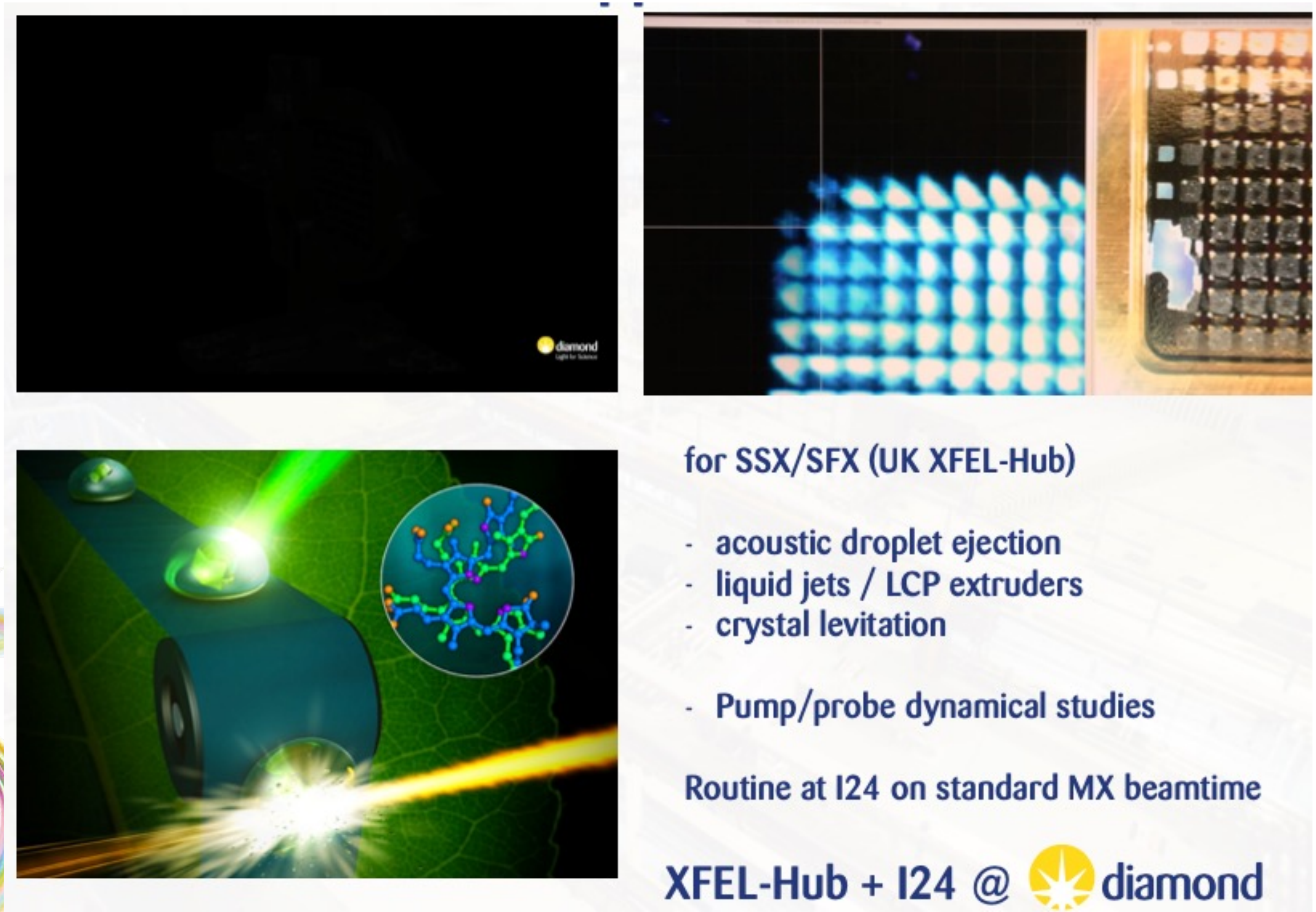
Sample

Screen Components


Global Presets

VMXi @ diamond

Serial Crystallography



for SSX/SFX (UK XFEL-Hub)

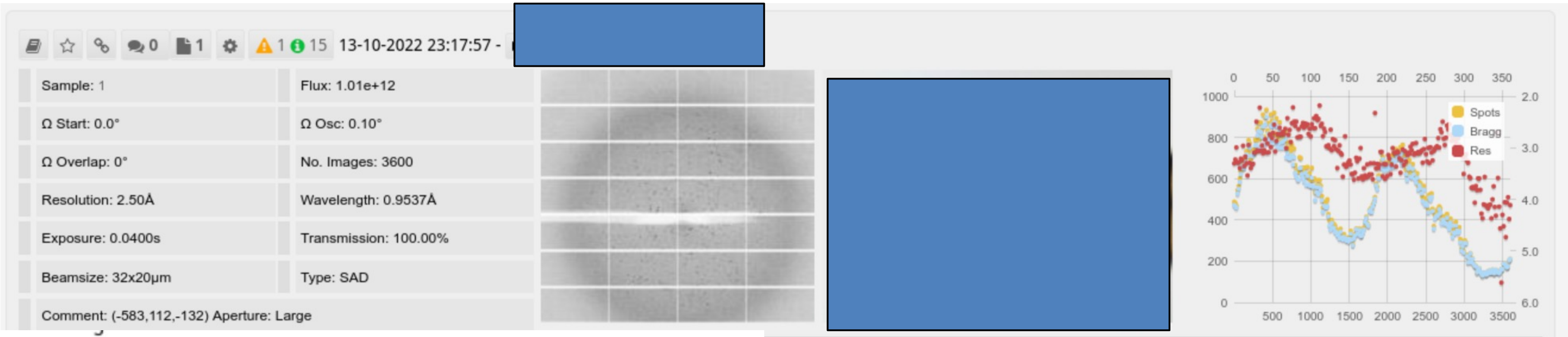
- acoustic droplet ejection
- liquid jets / LCP extruders
- crystal levitation

- 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?



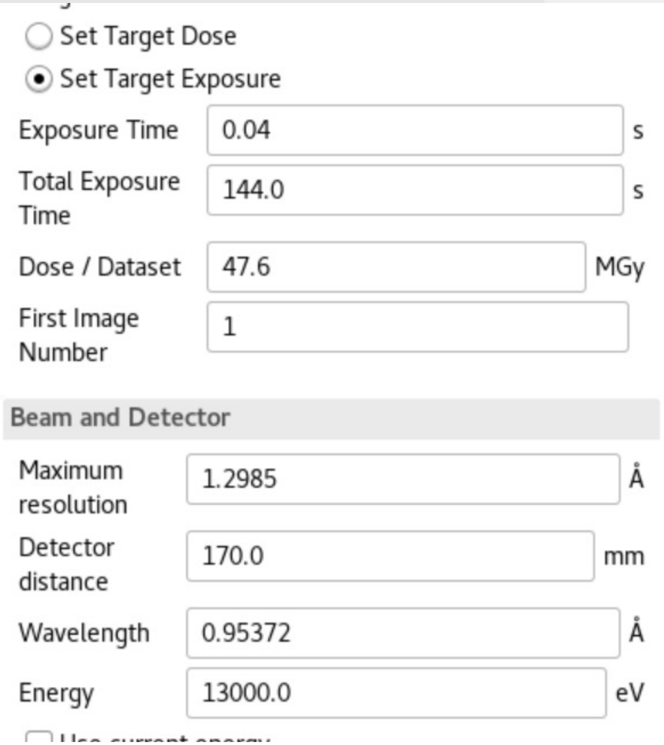
0 1 1 15 13-10-2022 23:17:57 - [redacted]

Sample: 1	Flux: 1.01e+12
Ω Start: 0.0°	Ω Osc: 0.10°
Ω Overlap: 0°	No. Images: 3600
Resolution: 2.50Å	Wavelength: 0.9537Å
Exposure: 0.0400s	Transmission: 100.00%
Beamsize: 32x20µm	Type: SAD
Comment: (-583,112,-132) Aperture: Large	

[redacted]

fast_dp: ✗ xia2 dials: ✓ xia2 3dii: ✗ autoPROC: ✓ xia2.multiplex: ✓ autoPROC+STARANISO: ✓

No processing results



○ Set Target Dose

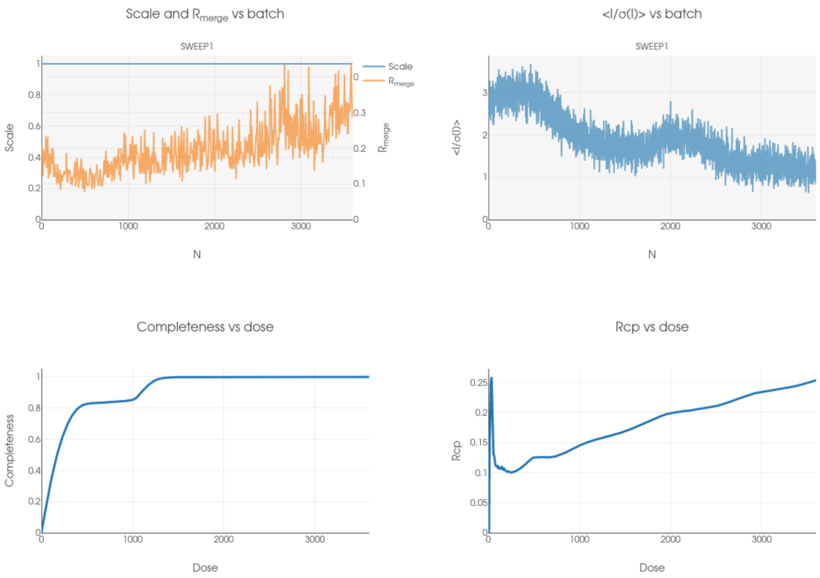
● Set Target Exposure

Exposure Time	0.04	s
Total Exposure Time	144.0	s
Dose / Dataset	47.6	MGy
First Image Number	1	

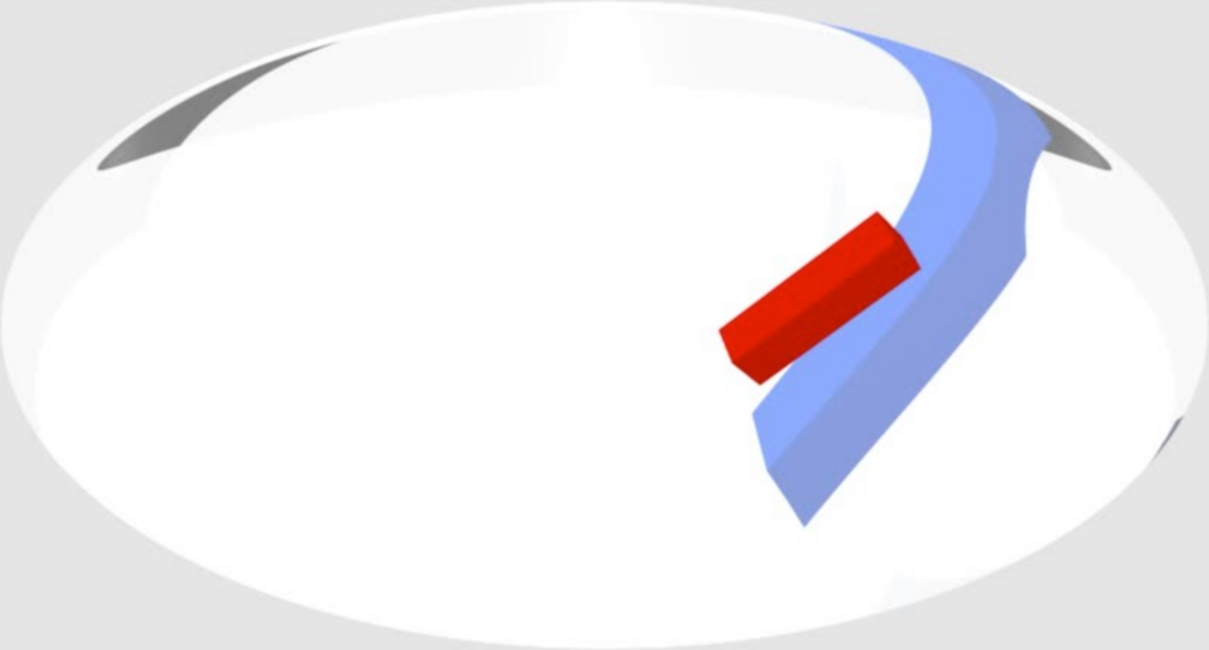
Beam and Detector

Maximum resolution	1.2985	Å
Detector distance	170.0	mm
Wavelength	0.95372	Å
Energy	13000.0	eV

☐ Use current energy



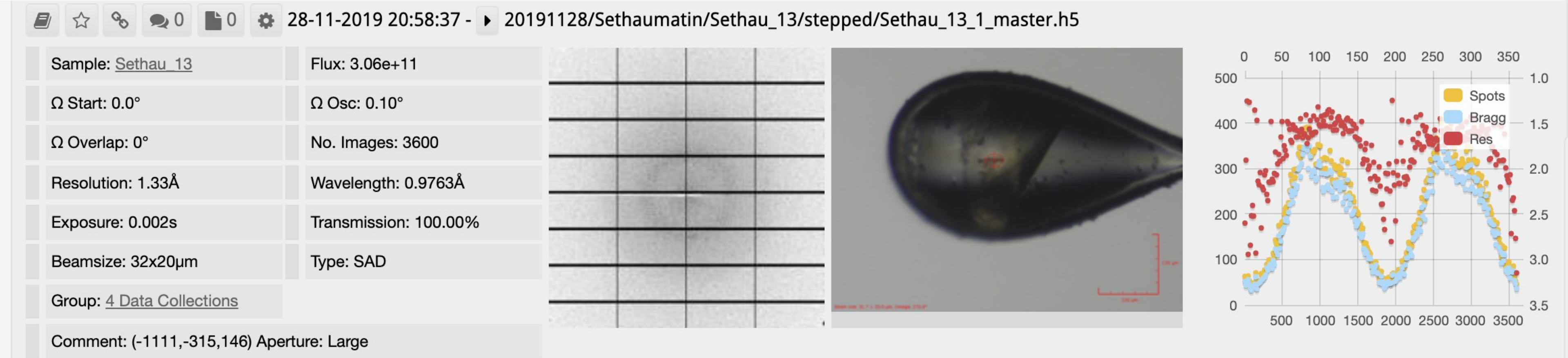
Good alignment is crucial



28-11-2019 21:05:04 - 20191128/Sethaumatin/Sethau_14/stepped/Sethau_14_1_master.h5

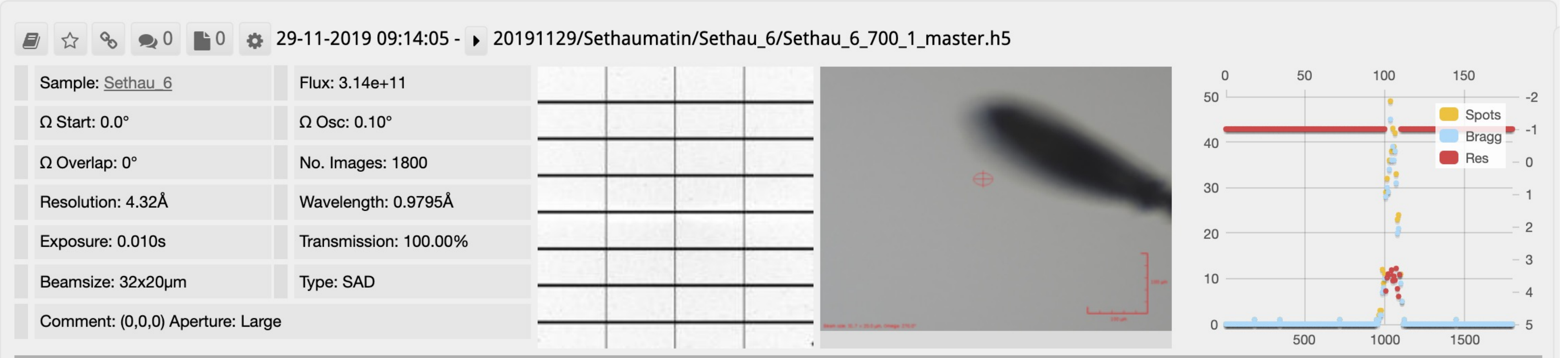
Sample: Sethau_14
Flux: 3.04e+11
Ω Start: 0.0°
Ω Osc: 0.10°
Ω Overlap: 0°
No. Images: 3600
Resolution: 1.33Å
Wavelength: 0.9763Å
Exposure: 0.002s
Transmission: 100.00%
Beamsize: 32x20µm
Type: SAD
Group: 4 Data Collections
Comment: (34,-126,78) Aperture: Large

Strategy2 Wedge1 Standard Anomalous Dataset Multiplicity=3 I/sig=2 Maxlifespan=200 s 105 0.05 1.16 1.04 24.9 24.9 0.010 3600



28-11-2019 20:58:37 - 20191128/Sethaumatin/Sethau_13/stepped/Sethau_13_1_master.h5

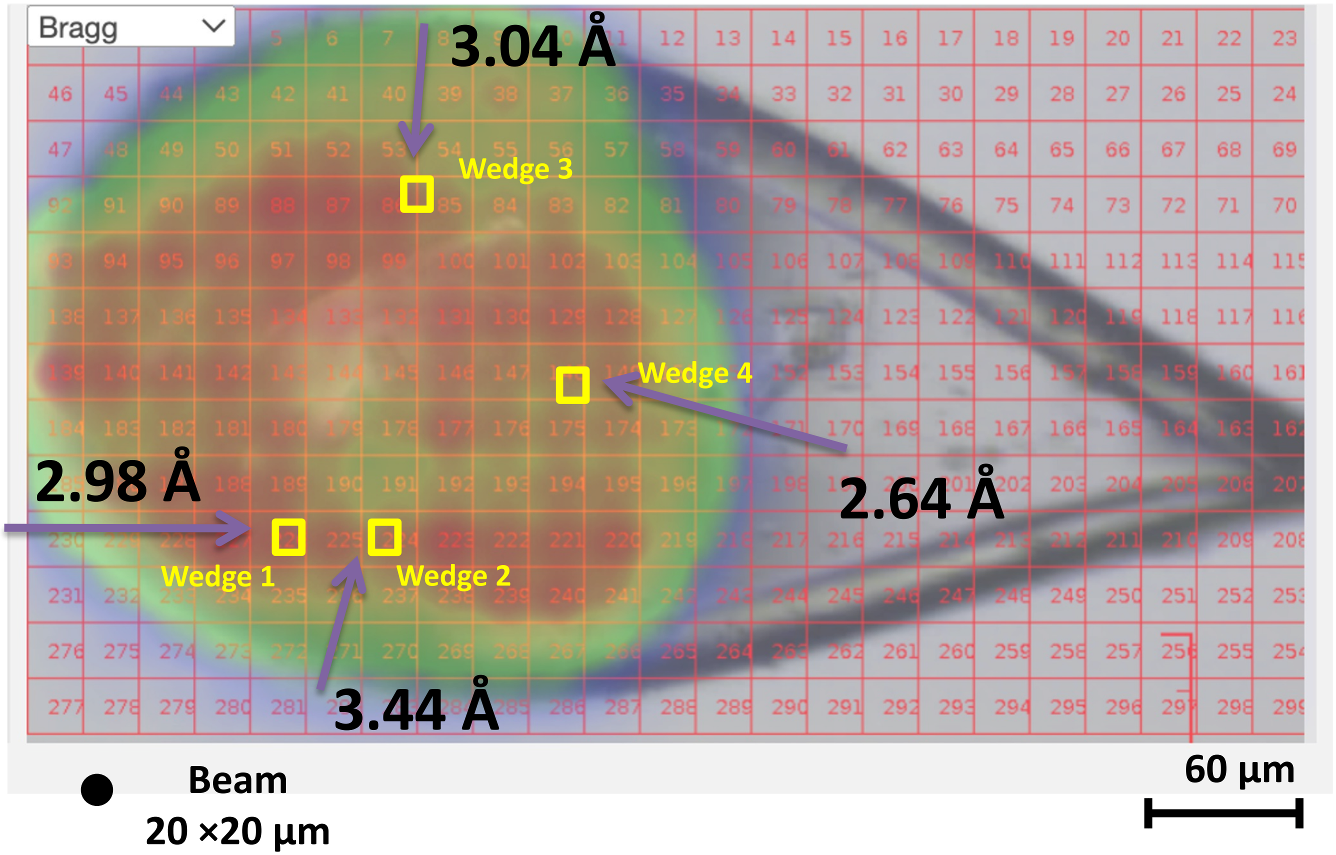
Sample: Sethau_13
Flux: 3.06e+11
Ω Start: 0.0°
Ω Osc: 0.10°
Ω Overlap: 0°
No. Images: 3600
Resolution: 1.33Å
Wavelength: 0.9763Å
Exposure: 0.002s
Transmission: 100.00%
Beamsize: 32x20µm
Type: SAD
Group: 4 Data Collections
Comment: (-1111,-315,146) Aperture: Large



29-11-2019 09:14:05 - 20191129/Sethaumatin/Sethau_6/Sethau_6_700_1_master.h5

Sample: Sethau_6
Flux: 3.14e+11
Ω Start: 0.0°
Ω Osc: 0.10°
Ω 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!

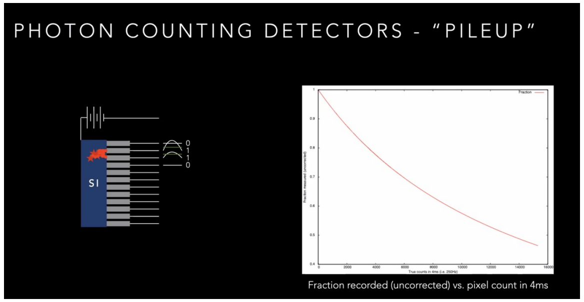
Decision time

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



PHOTON COUNTING DETECTORS - “PILEUP”

Fraction recorded (uncorrected) vs. pixel count in 4ms

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.

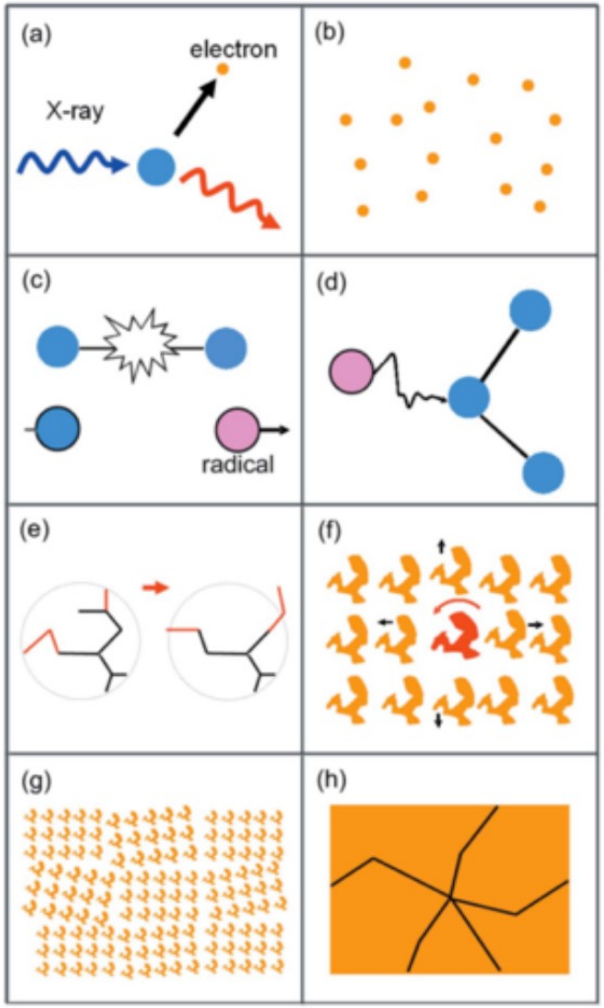
I worse issue is also that some highly count rate corrected peaks won’t show easy to see visible pathology.

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 ~3A resolution dataset**
Native data collection	High resolution (e.g < 1.8 A) 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 but 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 A), 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

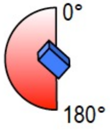
- Resolution dependency of 10 MGy / Å, Howells *et al. J. El. Spect. & Rel. Phen.* **170**, 4 (2009)
- Does estimation, Holton, *J. Synchrotron Rad.* **16**, 133 (2009)

$$Dose = (t_{expo} \times flux) / (k_{dose} \times \mathrm{I}_{\text{H-beam}} \times \mathrm{I}_{\text{B-beam}})$$

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

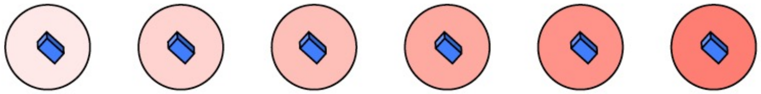
Traditional high-dose coarse-phi slicing strategy

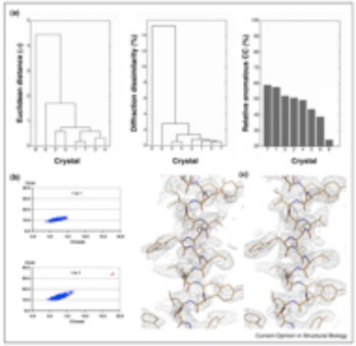
- 0.5-1° per image,180°, 4-fold redundancy, and 10 MGy
- CCD detector

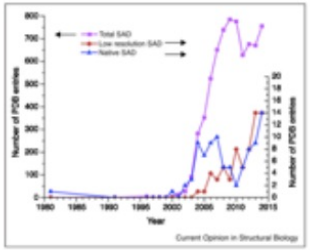


low dose, fine-phi slicing, high redundancy strategy

- ½ mosaicity slicing, *n* × 360° 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

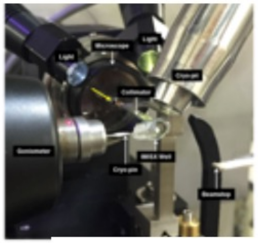


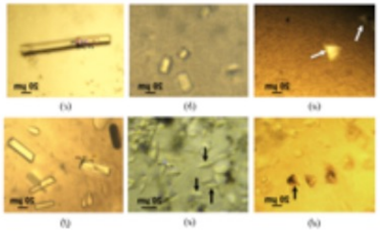




Multi-orientation and multi-crystal strategy

- 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)

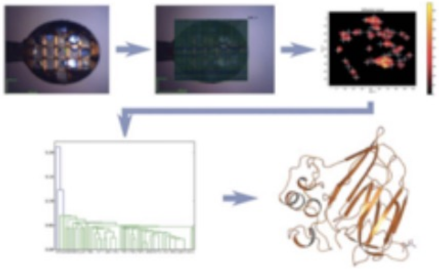




Micro-crystallography

- 10-20° data per crystal × *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*J. 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. Sync. 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. Sync. Rad.* **9**, 347-354.

500 kGy for Br-RNA:

Olieric V, Ennifar E, Meents A, Fleurant M, Besnard C, Pattison P, Schiltz M, Schulze-Briese 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:

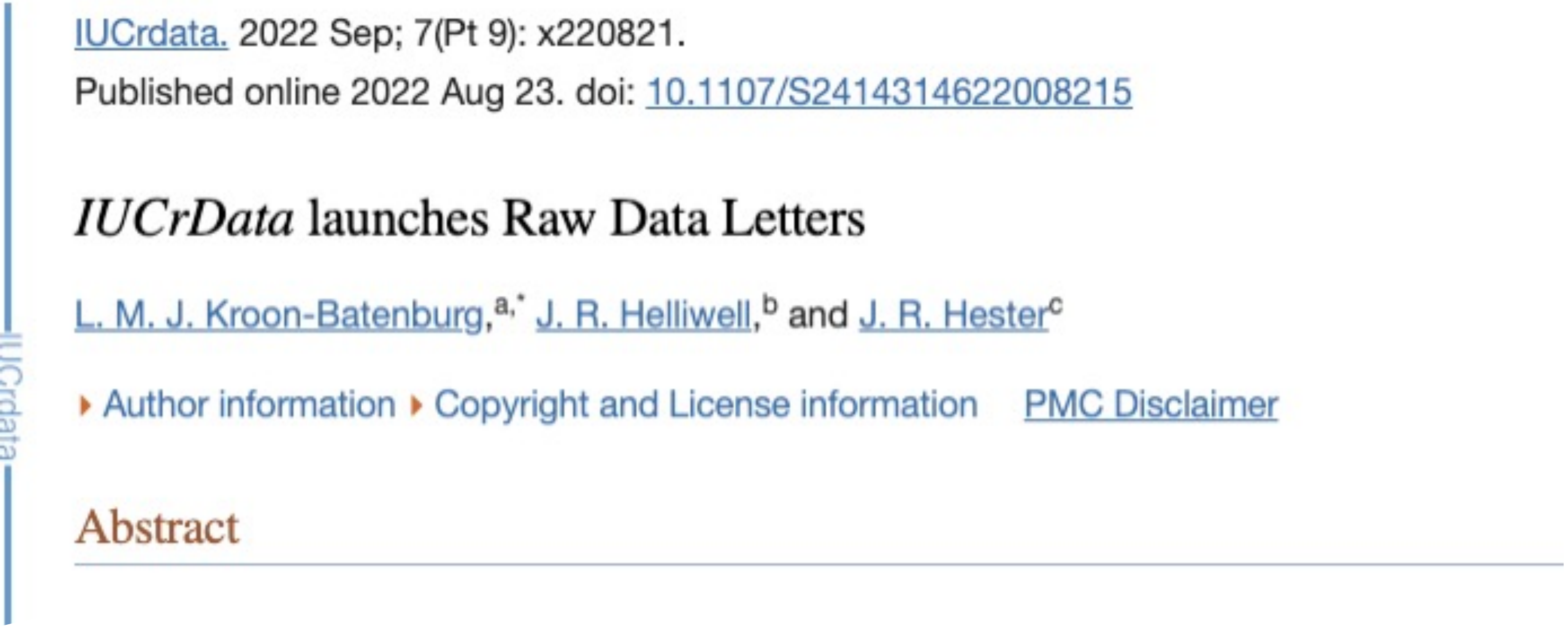
Radiat Phys Chem Oxf Engl 1993 **76**, 714-721.

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.



IUCrdata. 2022 Sep; 7(Pt 9): x220821.
Published online 2022 Aug 23. doi: 10.1107/S2414314622008215

IUCrData launches Raw Data Letters

L. M. J. Kroon-Batenburg,[a,*] J. R. Helliwell,[b] and J. R. Hester[c]

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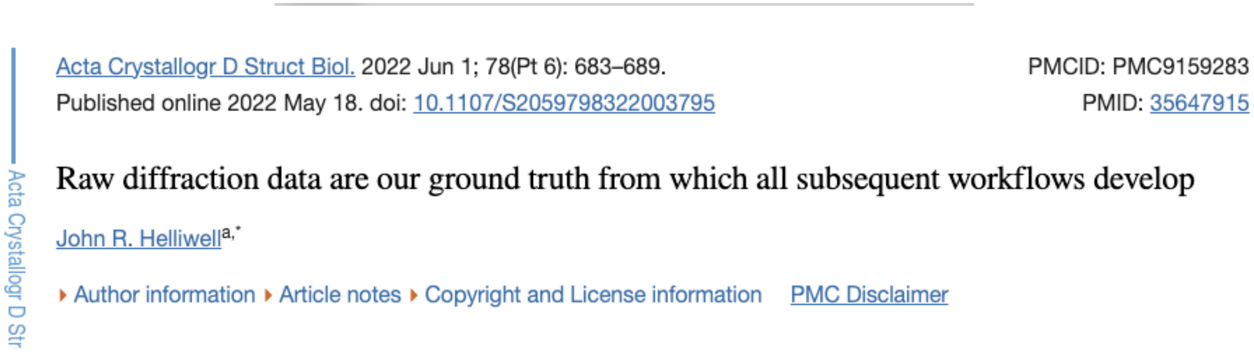
Abstract

FAIR data are data which meet principles of findability, accessibility, interoperability, and reusability

- Zenodo? others

Consider making your raw data public!



Acta Crystallogr D Struct Biol. 2022 Jun 1; 78(Pt 6): 683–689. PMCID: PMC9159283
Published online 2022 May 18. doi: 10.1107/S2059798322003795 PMID: 35647915

Raw diffraction data are our ground truth from which all subsequent workflows develop

John R. Helliwell[a,*]

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