Implementation of Eiger2 Detectors at Diamond Light Source

Katherine McAuley

ACA 2019



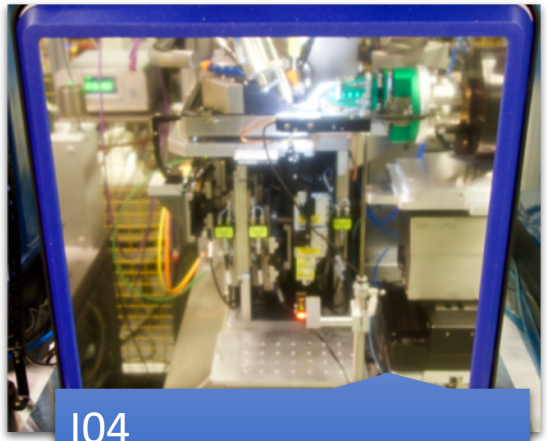
Athena SWAN Bronze Award

diamond

Detectors on the MX beamlines



I03
- Eiger2 X 16M



I04
- Eiger2 X 16M



I04-1
- Pilatus2 6M-F

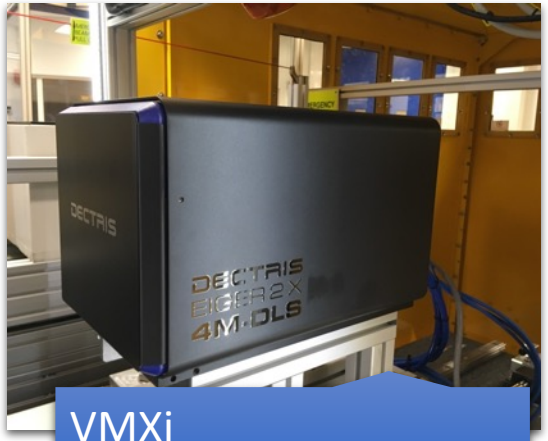


I23
- Pilatus2



CdTe Eiger 9M for 2020

I24
- Pilatus3 6M



VMXi
- Eiger2 X 4M

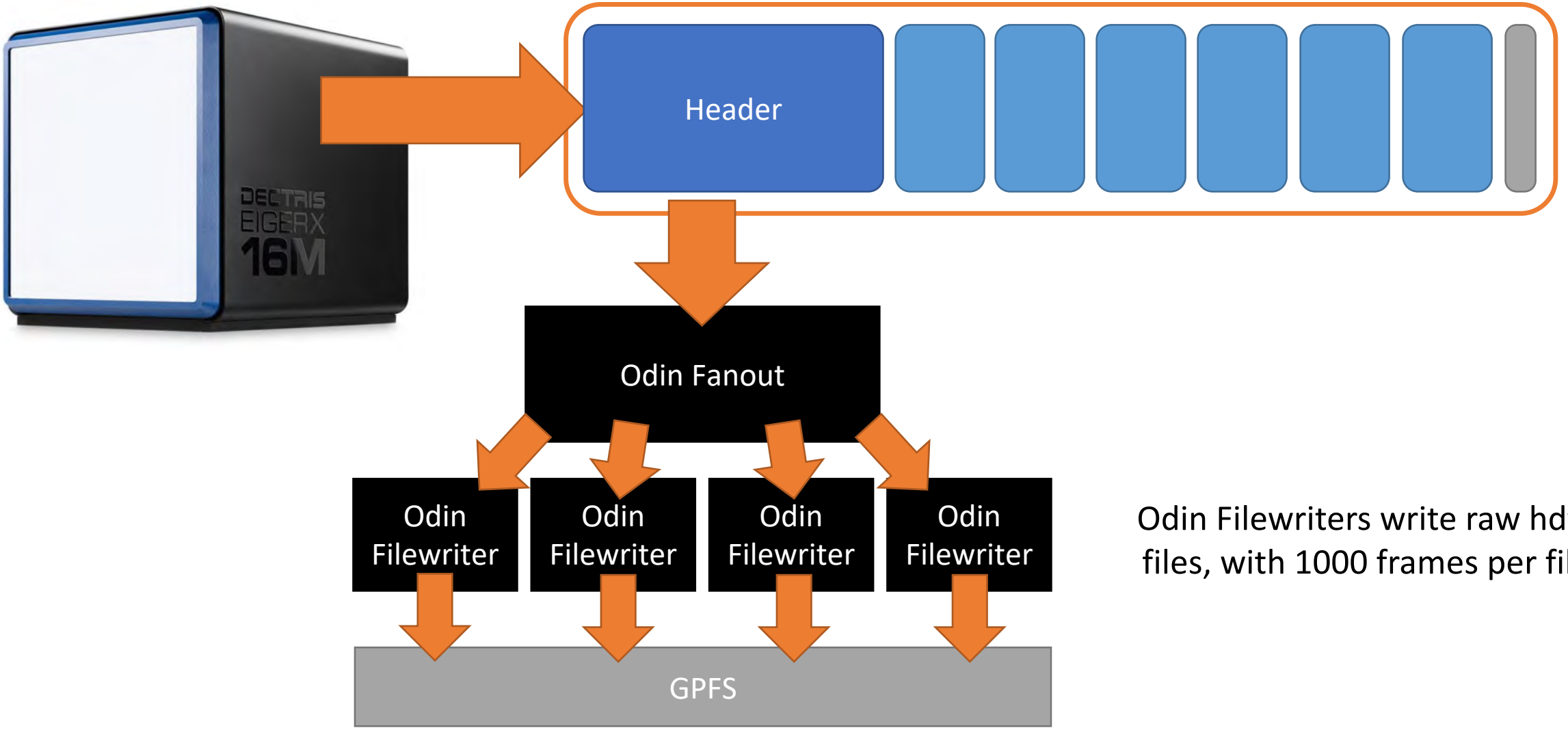


CdTe Eiger 9M for 2020

VMXm
- Pilatus3 6M

Eiger implementation





Odin Filewriters write raw hdf5 files, with 1000 frames per file

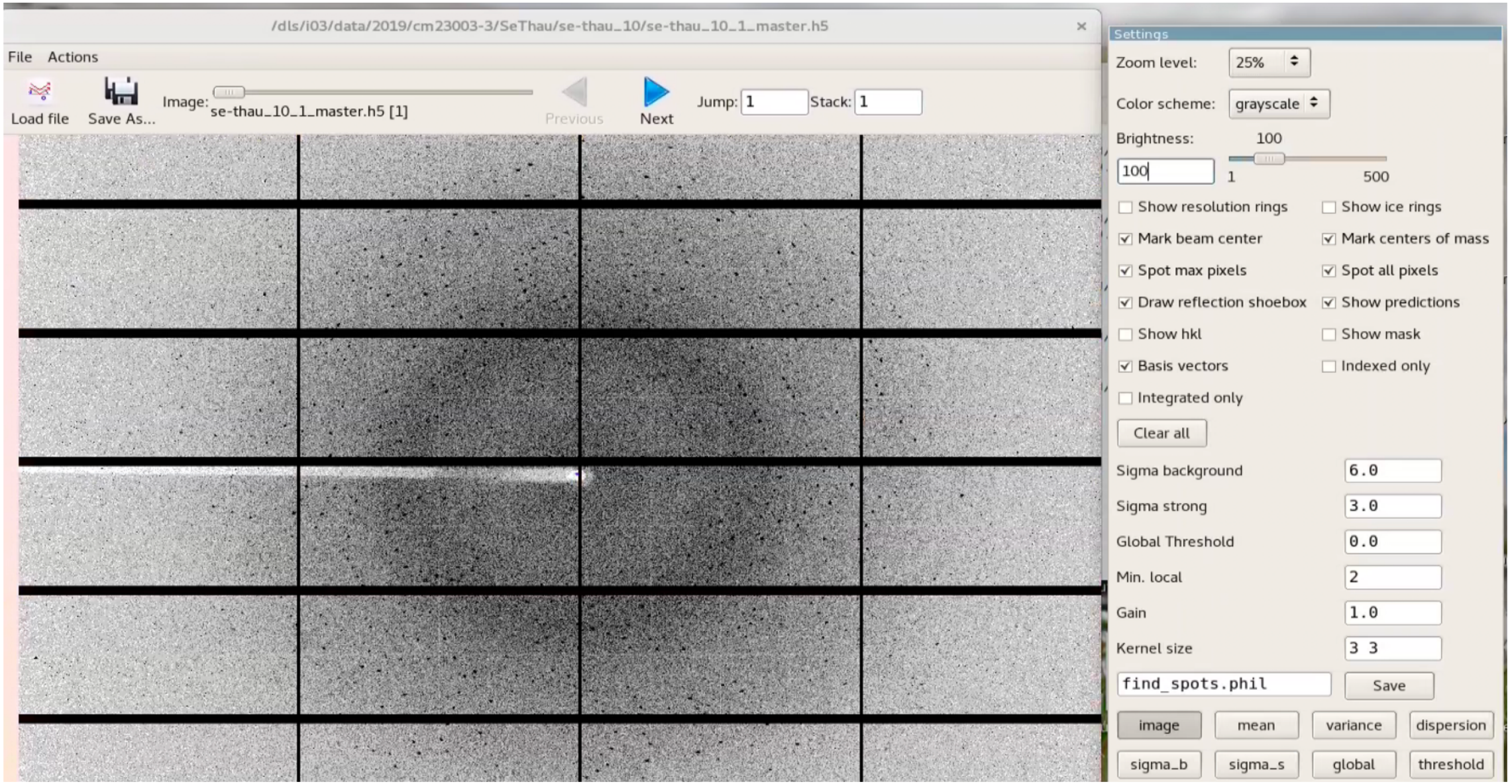
Viewing Eiger images

- For fine sliced data, worth stacking up enough images to get e.g. 1° rotation or similar
- Images can be viewed with ADXV, Dials Image Viewer, Albula etc
  - In ADXV open the *_header.cbf file first and then the h5 file (zoom 100% or use slab)
  - In DIALS or Albula, open the *_master.h5 file

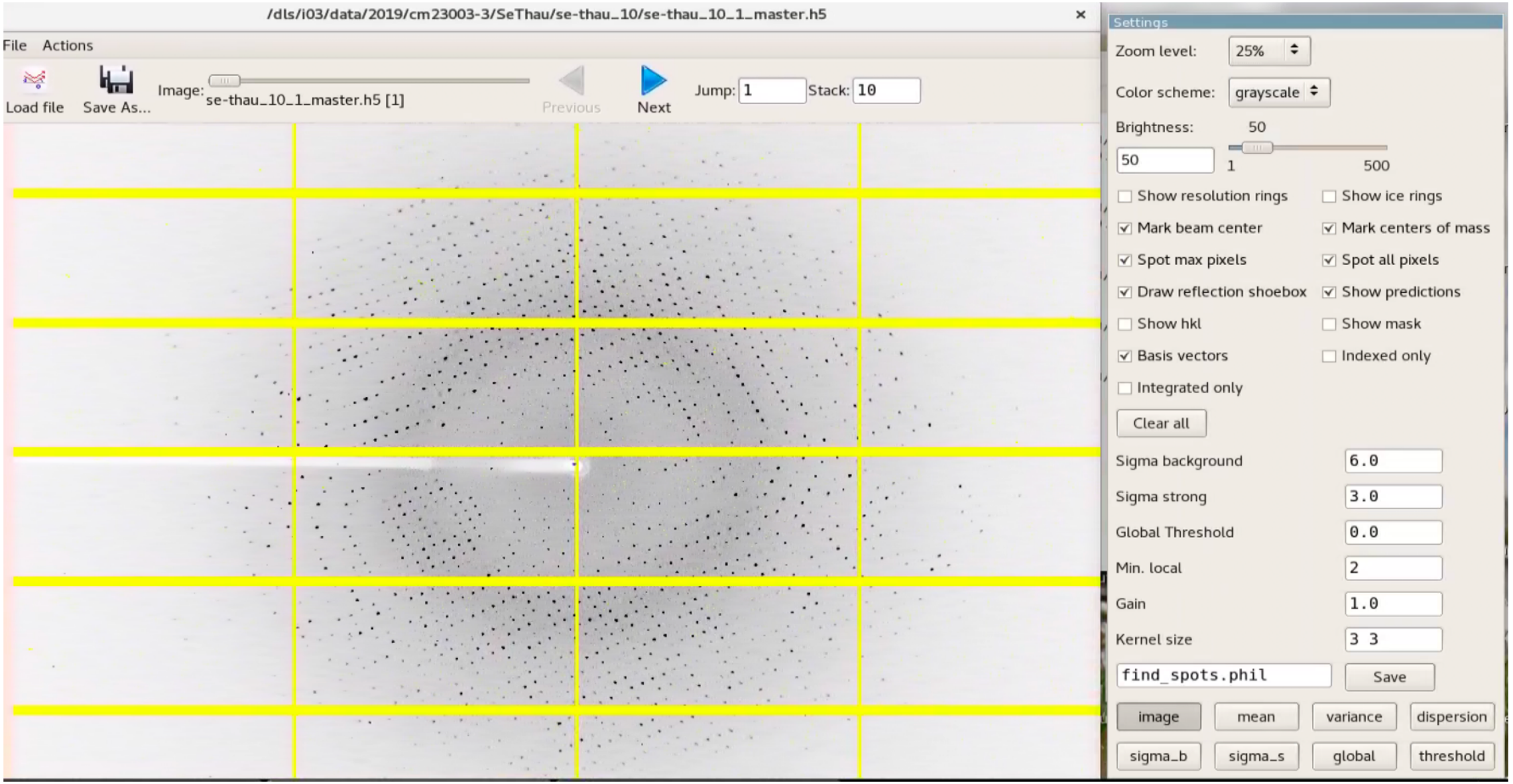
An example of the files produced for a 3600 frame acquisition (Given the ID of thermolysin_xtal1):

thermolysin_xtal1_1.nxs
thermolysin_xtal1_1_header.cbf (header only - to be loaded in ADXV before the h5 frame files)
thermolysin_xtal1_1_master.h5
thermolysin_xtal1_1_000001.h5 (frames 1 - 1000)
thermolysin_xtal1_1_000002.h5 (frames 1001 - 2000)
thermolysin_xtal1_1_000003.h5 (frames 2001 - 3000)
thermolysin_xtal1_1_000004.h5 (frames 3001 - 3600)
thermolysin_xtal1_1_meta.h5

Default setting in Dials image viewer



Same dataset, 10 images stacked



Processing Eiger data from Diamond

- All automated processing pipelines work
- With DIALS - easy though be aware that the detector has 2.5 x as many pixels as Pilatus 6M so processing will take longer.
- If you are using XDS you will need durin: https://github.com/DiamondLightSource/durin/releases/tag/2019v1
- If using xia2, will need hdf5_plugin=durin-plugin.so command-line option.
- For most reprocessing would recommend using SynchWeb reprocessing options.

Advice on how to collect and process Eiger data can be found at:
https://www.diamond.ac.uk/Instruments/Mx/I03/I03-Manual/Eiger2-Detectors.html

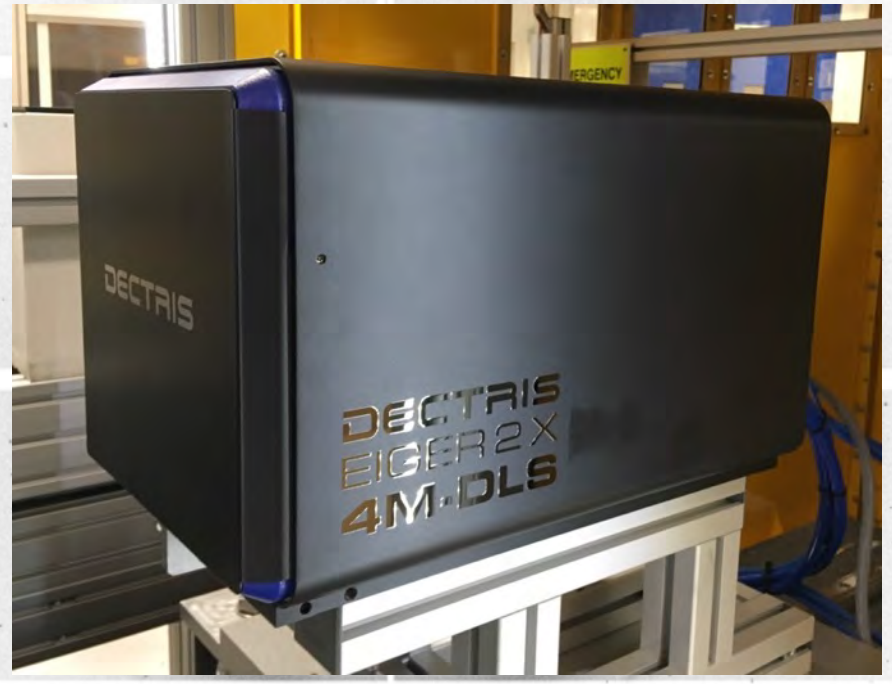
Eigers in use

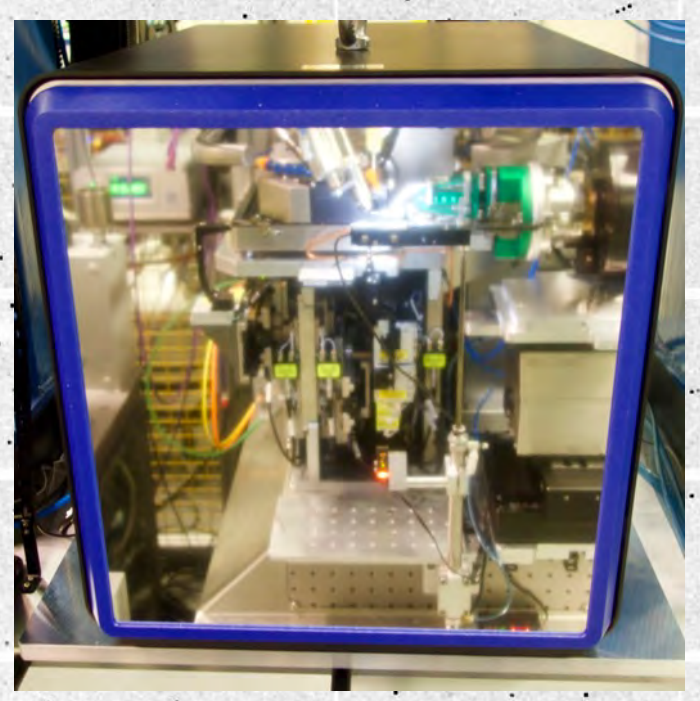


diamond

Latest Detectors for MX – Eiger2

- Keeping Diamond at the forefront of detector technology with first installations of latest generation Dectris pixel array detectors

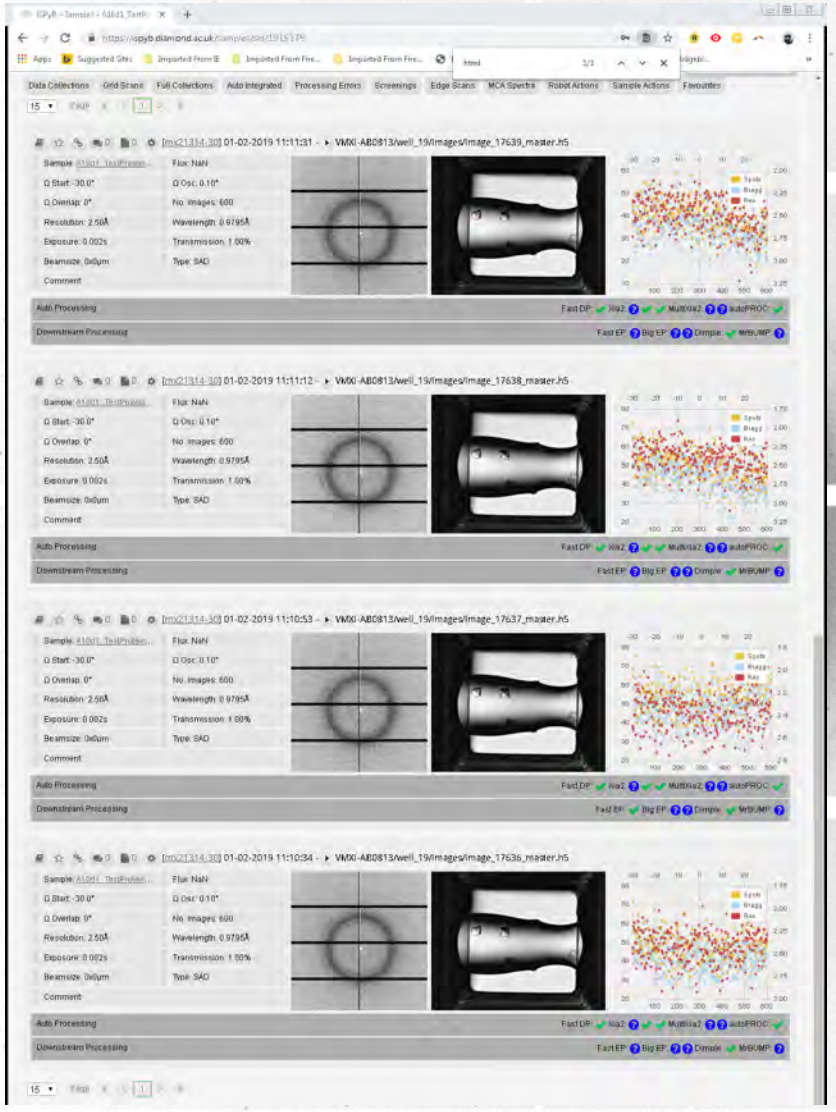


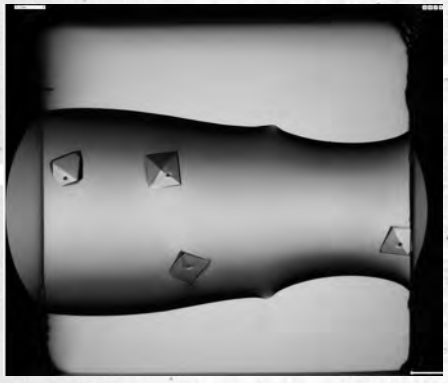


- 4M on VMXi since September 2018
  - 560 Hz

- 16M on I04 since December 2018
- 16M on I03 since April 2019

Rapid data collection rates and structure solution - VMXi





- 4M on VMXi capable of rapidly collecting huge amounts of room temperature data for
  - Crystallogenesis analysis
  - Structure solution
  - Serial synchrotron crystallography

xia2 multi-crystal report

Merging statistics

Filename:
Space group: P 4 2 2 (No. 89)
Unit cell: (68.3739, 68.3739, 103.991, 90, 90, 90)

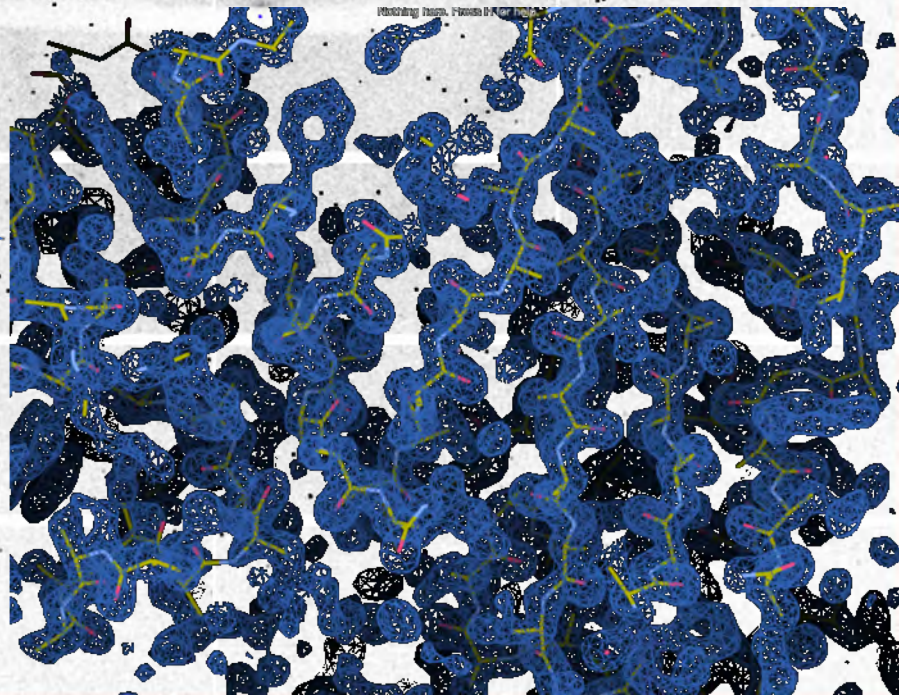
Overall

	Overall	Low resolution	High resolution
Resolution (Å)	68.37 - 1.79	68.42 - 4.86	1.82 - 1.79
Observations	220999	21420	160
Unique reflections	20875	1363	151
Multiplicity	10.6	15.7	1.1
Completeness	86.98%	100.00%	12.89%
Mean I/sigma(I)	20.4	41.0	1.4
Rmerge	0.069	0.044	0.415
Rmeas	0.072	0.045	0.582
Rpim	0.019	0.011	0.407
CC1/2	0.999	0.999	0.386

Rapid data collection rates and structure solution I03 & I04

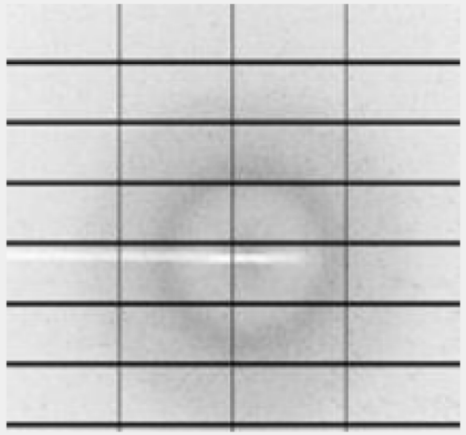
- Early results from I04
  - Rapid collection (eg <30s) of fine phi sliced, highly redundant data
  - Excellent quality statistics
  - Automatically phased and built model from data collected (in 78s) on first full day of use
- Opens up new opportunities for high throughput automated collection

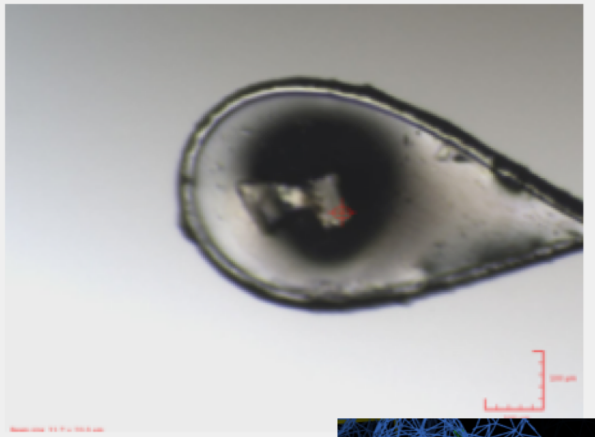
	Overall	Low resolution	High resolution
Resolution (Å)	54.10 - 1.19	54.16 - 3.23	1.21 - 1.19
Observations	1496759	112621	4832
Unique reflections	78083	4561	2137
Multiplicity	19.2	24.7	2.3
Completeness	94.04%	100.00%	52.19%
Mean I/sigma(I)	22.8	96.5	0.8
Rmerge	0.060	0.026	0.614
Rmeas	0.061	0.027	0.771
Rpim	0.012	0.005	0.456
CC1/2	1.000	1.000	0.572

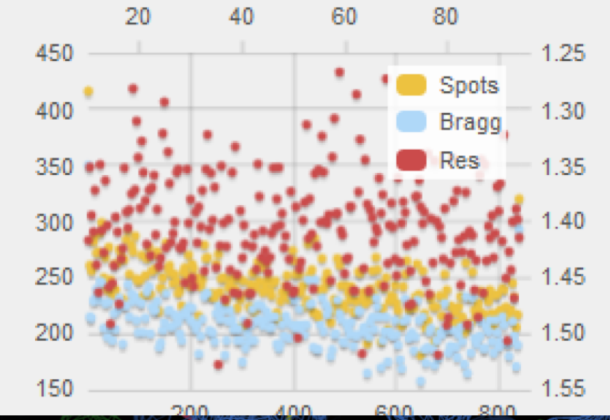


Thaumatin crystal collected on I04

Sample: Thau_14	Flux: 2.69e+11
Ω Start: 10.0°	Ω Osc: 0.10°
Ω Overlap: 0°	No. Images: 840
Resolution: 1.51Å	Wavelength: 0.9795Å
Exposure: 0.008s	Transmission: 100.00%
Beamsize: 32x20µm	Type: SAD
Comment: (-577,-69,-153) Aperture: Large	





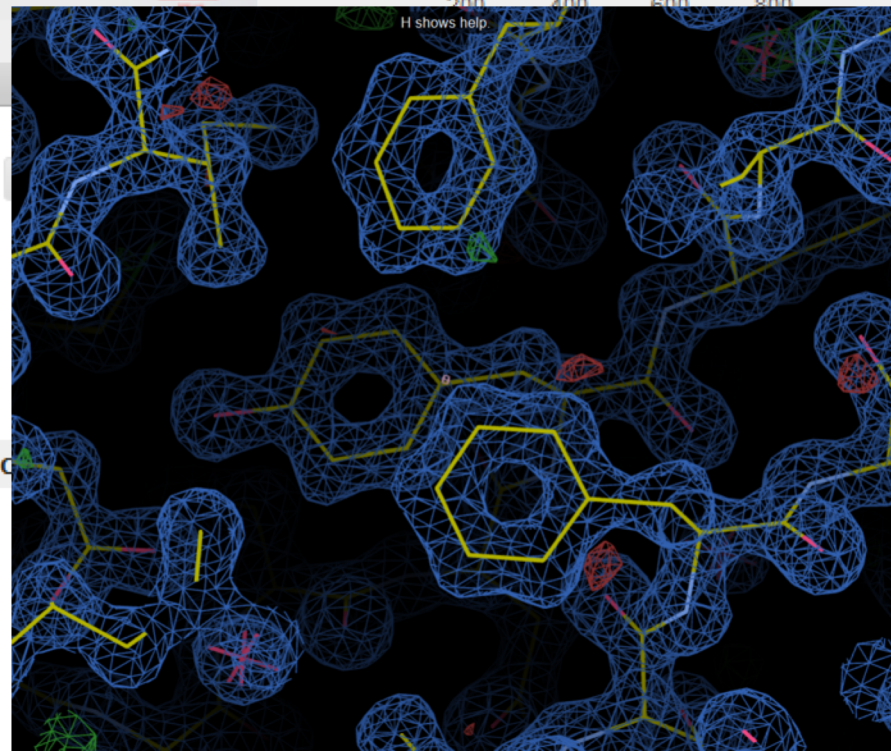


fast_dp | xia2 dials | xia2 3dii | autoPROC | xia2 dials | xia2 3dii | xia2.multiplex | autoPROC+STARANISO

Beam Centre	X	Y
Start	166.13	172.88
Refined	166.11	172.92
Δ	0.02	-0.04

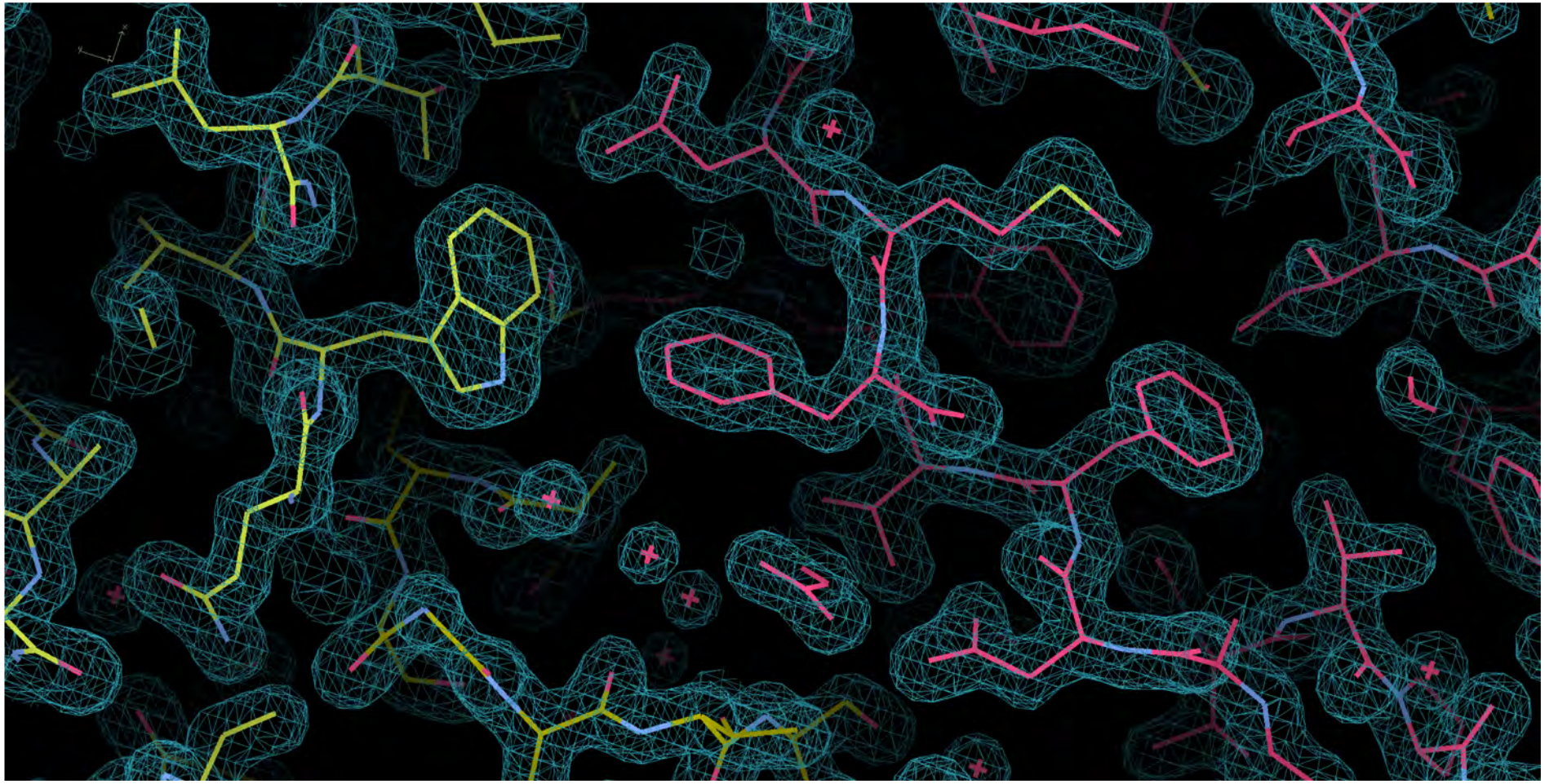
Space Group	A	B	C	α	β	γ
P 41 21 2	57.77	57.77	149.95	90.00	90.00	90.00

Shell	Observations	Unique	Resolution	Rmeas	I/sig(I)	CC Half	Completeness	Multiplicity	Anom C
outerShell	244	230	1.15 - 1.17	0.511	1.4	0.6	5.2	1.1	0.3
innerShell	28644	4956	3.12 - 45.80	0.023	55.1	1.0	100.0	5.8	98.7
overall	345126	71148	1.15 - 45.76	0.040	18.3	1.0	78.4	4.9	67.2



125 frames per second, 7s for data set (flux limited)

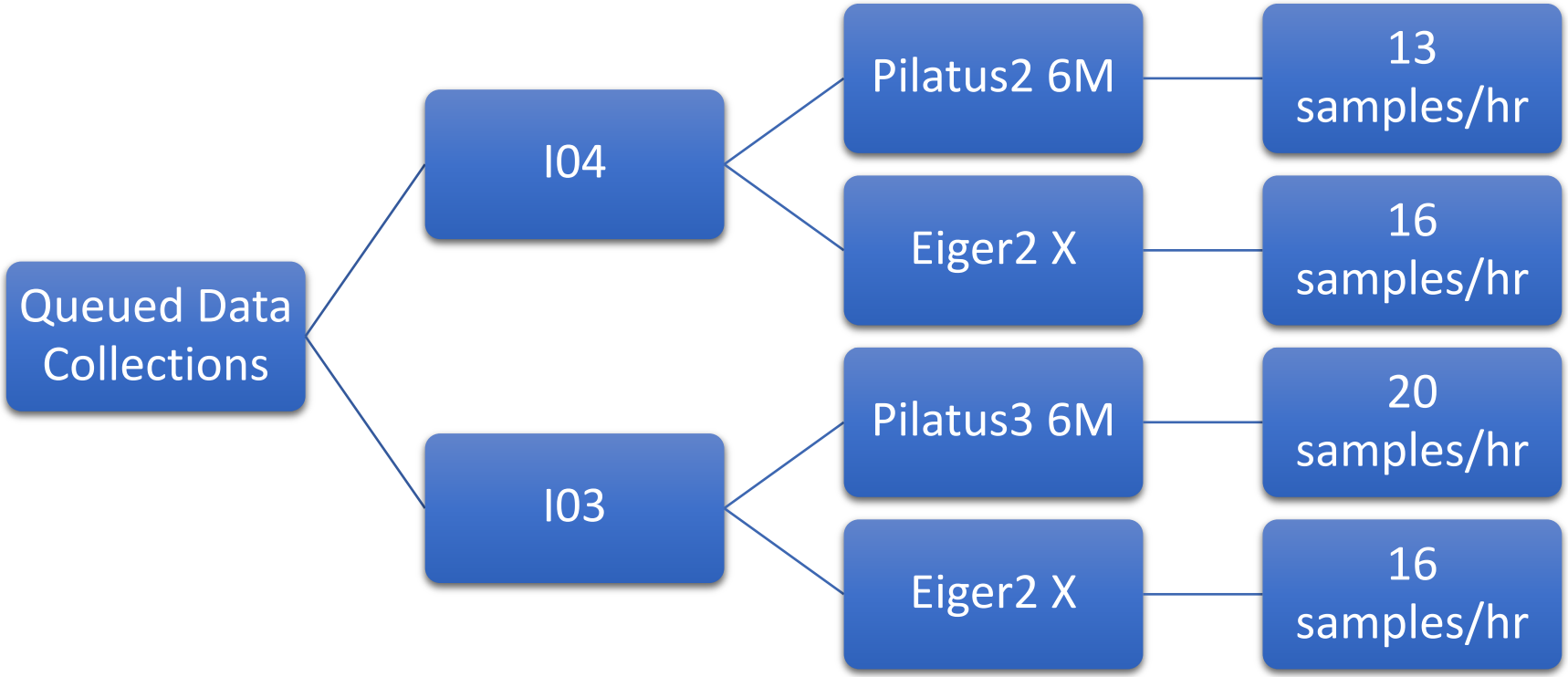
Beamline I03 – a rare example, a virus structure in half a minute



Autocollected. Resolution 1.67 Ang, SG: I222, a= 342.7, b= 348.3, c= 351.6 Ang (Helen Duyvesteyn, Jingshan Ren, Liz Fry, DIS) – hi res clarifies biological puzzle

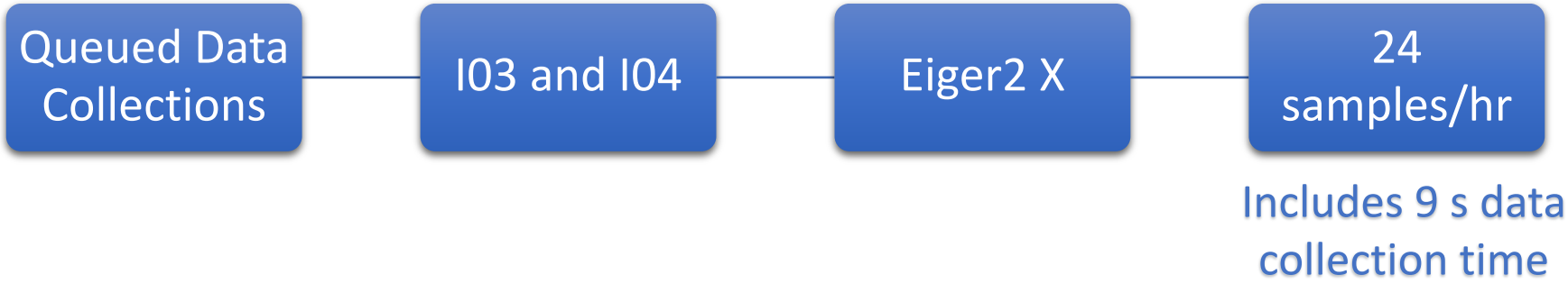
Beamline performance – Eiger vs Pilatus

- Both I03 and I04 offer queued mode that uses X-ray centring
  - Important to maintain or improve performance of queued data collections



Beamline performance – Improving Eiger performance

- Queued data collection mode re-optimized for Eiger detectors
- Use ROI for X-ray centring grid scans at 250 Hz
- Process data before all files written to disk



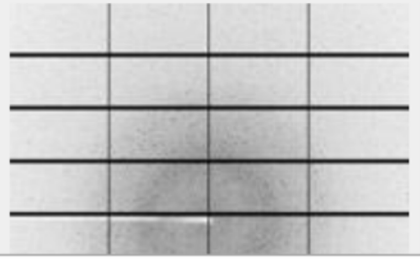
Testing 500 Hz data collections

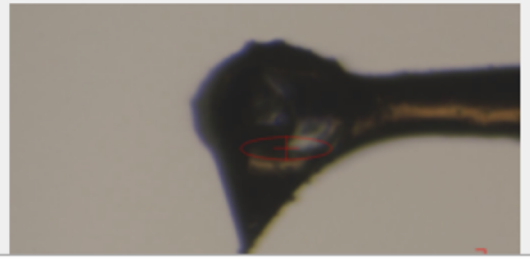


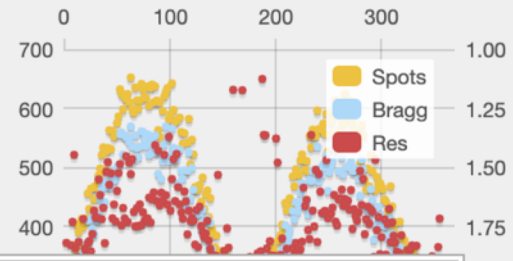
Thaumatin crystal 500 Hz, I03

0 0 20-07-2019 13:21:24 - SeThau/se-thau_10/se-thau_10_1_master.h5

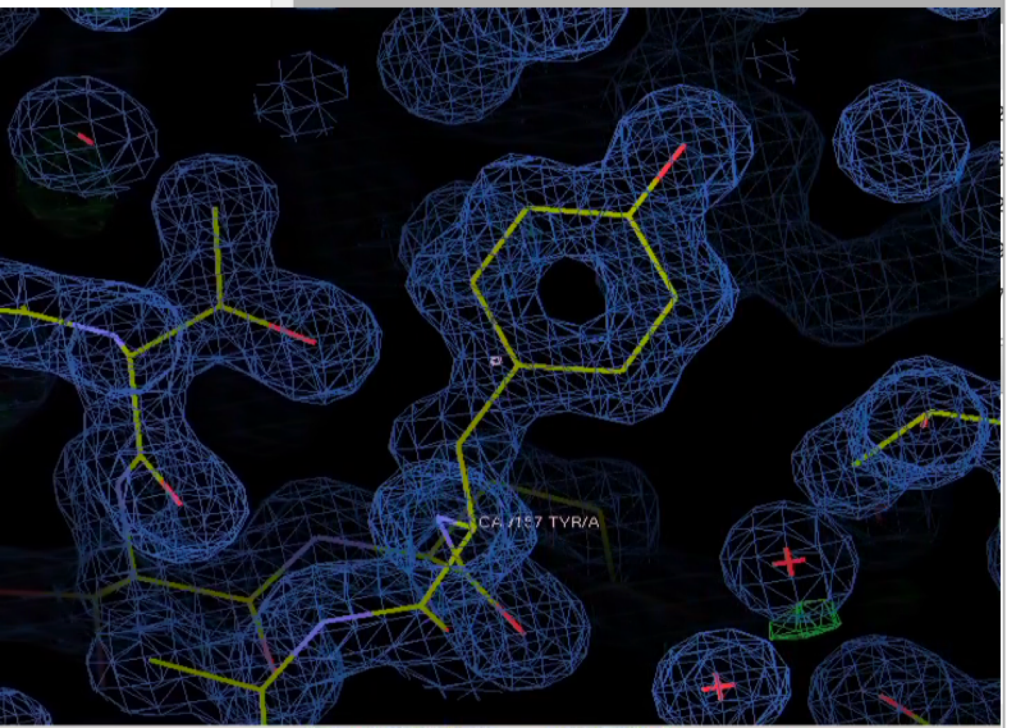
Sample: se-thau_10	Flux: 1.92e+12
Ω Start: 0.0°	Ω Osc: 0.10°
Ω Overlap: 0°	No. Images: 3600
Resolution: 1.38Å	Wavelength: 0.9790Å
Exposure: 0.002s	Transmission: 49.97%
Beamsize: 80x20µm	Type: SAD
Comment: (161,-207,-421) Aperture: Large	







Auto Processing



xia2.txt Log File

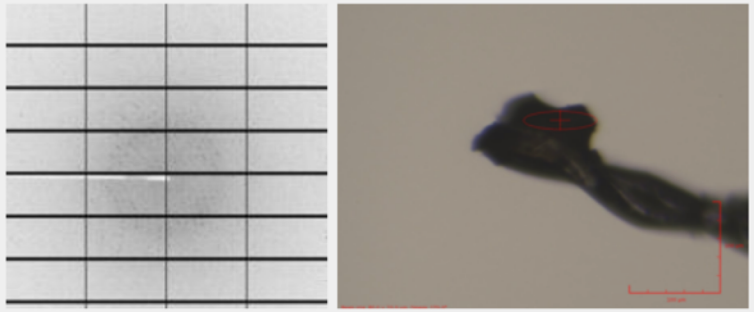
```
Crystal: DEFAULT
Sequence:
Wavelength name: SAD
Wavelength 0.97895
Sweeps:
SWEEP SWEEP1 [WAVELENGTH SAD]
TEMPLATE se-thau_10_1_master.h5
DIRECTORY /dls/i03/data/2019/cm23003-3/SeThau/se-thau_10
IMAGES (USER) 1 to 3600
MTZ file: /dls/i03/data/2019/cm23003-3/tmp/zocalo/SeThau/se-thau_10/se-thau_10_1_/a8e22
```

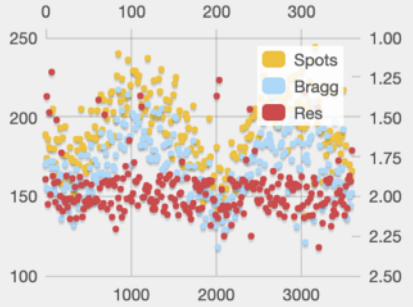
For AUTOMATIC/DEFAULT/SAD	Overall	Low	High
High resolution limit	1.21	3.28	1.21
Low resolution limit	50.06	50.10	1.23
Completeness	99.3	100.0	92.2
Multiplicity	23.1	24.0	9.1
I/sigma	25.2	103.6	1.0
Rmerge(I)	0.056	0.023	1.772
Rmerge(I+/-)	0.055	0.022	1.675
Rmeas(I)	0.058	0.023	1.880
Rmeas(I+/-)	0.057	0.023	1.881
Rpim(I)	0.012	0.005	0.611
Rpim(I+/-)	0.016	0.006	0.840
CC half	1.000	1.000	0.530
Wilson B factor	14.105		
Anomalous completeness	99.2	100.0	92.7
Anomalous multiplicity	12.2	13.9	4.7
Anomalous correlation	0.112	0.166	0.022
Anomalous slope	1.001		

Selenourea soaked lysozyme, 500 Hz

0 0 20-07-2019 11:49:41 - TestLysozyme/se-lys_1/se-lys_1_1_master.h5

Sample: se-lys_1	Flux: 1.89e+12
Ω Start: 0.0°	Ω Osc: 0.10°
Ω Overlap: 0°	No. Images: 3600
Resolution: 1.38Å	Wavelength: 0.9786Å
Exposure: 0.002s	Transmission: 50.12%
Beamsize: 80x20µm	Type: SAD
Comment: (714,131,-533) Aperture: Large	





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

Type	Resolution	Spacegroup	Mn<I/sig(I)>	Rmeas Inner	Rmeas Outer	Completeness	Cell	Status
xia2 dials	39.75 - 1.40	P 41 21 2	12.5	0.062	2.038	100.0	79.50 79.50 37.10 90.00 90.00 90.00	processing successful
xia2 3dii	37.15 - 1.46	P 41 21 2	20.9	0.046	2.602	100.0	79.45 79.45 37.15 90.00 90.00 90.00	processing successful
autoPROC	56.05 - 1.42	P 41 21 2	12.0	0.063	7.150	100.0	79.27 79.27 37.07 90.00 90.00 90.00	processing successful
fast_dp	28.09 - 1.52	P 4 2 2	28.9	0.039	0.817	99.1	79.45 79.45 37.16 90.00 90.00 90.00	processing successful
fast_dp	28.07 - 1.49	P 4 2 2	23.9	0.038	0.866	99.0	79.39 79.39 37.14 90.00 90.00 90.00	processing successful
autoPROC+STARANISO	56.05 - 1.44	P 41 21 2	14.8	0.059	2.315	95.6	79.27 79.27 37.07 90.00 90.00 90.00	processing successful

xia2 dials | xia2 3dii | autoPROC | fast_dp | fast_dp | autoPROC+STARANISO

Plots | Archive | Logs & Files | Lookup Cell

Beam Centre	X	Y
Start	154.86	167.83
Refined	154.83	167.82
Δ	0.03	0.01

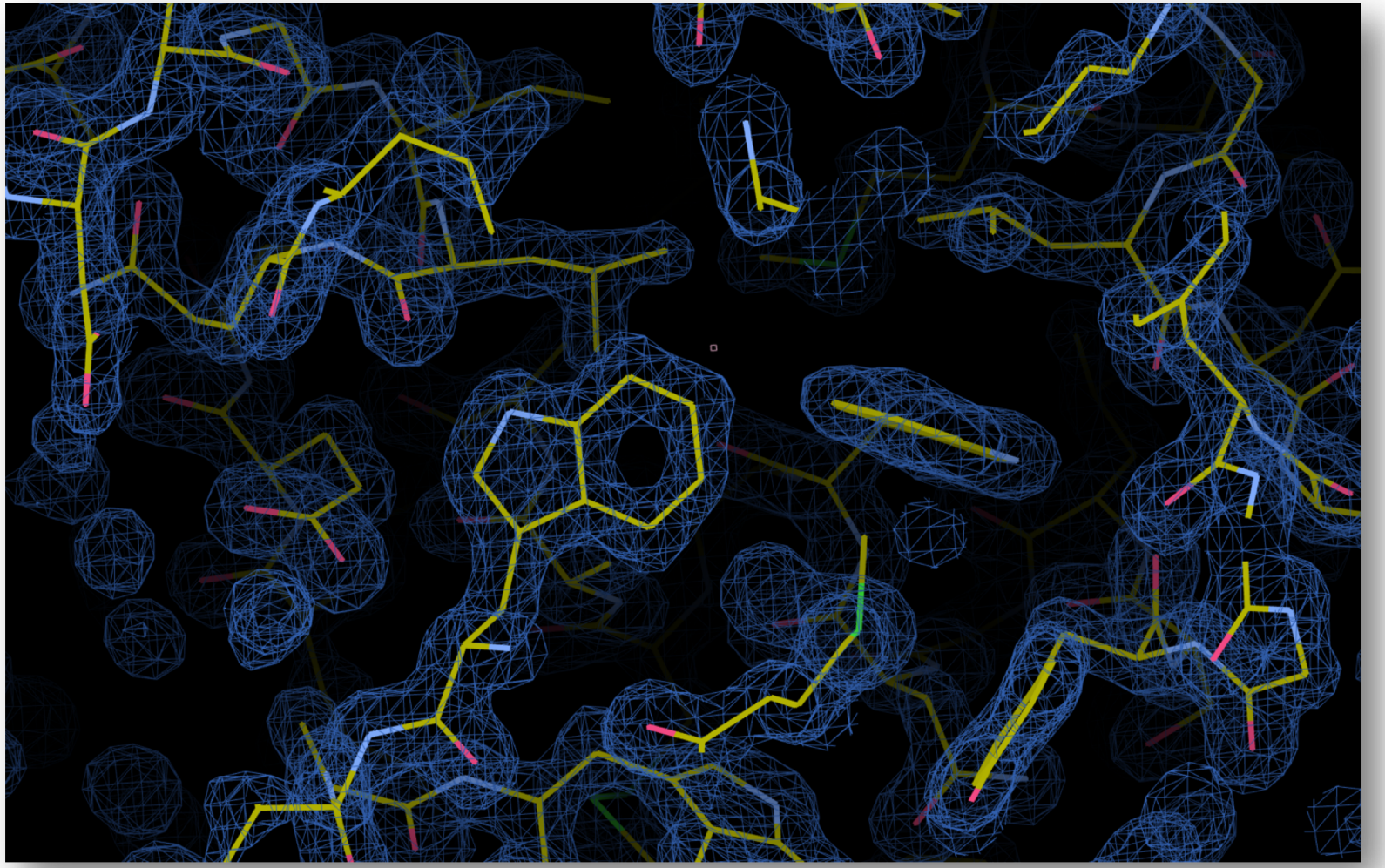
Space Group	A	B	C	α	β	γ
P 41 21 2	79.50	79.50	37.10	90.00	90.00	90.00

Shell	Observations	Unique	Resolution	Rmeas	I/sig(I)	CC Half	Completeness	Multiplicity	Anom Completeness	Anom Multiplicity	CC Anom
outerShell	30430	1166	1.40 - 1.42	2.038	1.5	0.8	97.2	26.1	97.2	13.7	-0.0
innerShell	31744	1350	3.80 - 39.77	0.062	37.7	1.0	100.0	23.5	100.0	14.1	0.4
overall	612348	24092	1.40 - 39.75	0.124	12.5	1.0	100.0	25.4	99.9	13.6	0.1

Selenourea soaked lysozyme, 500 Hz

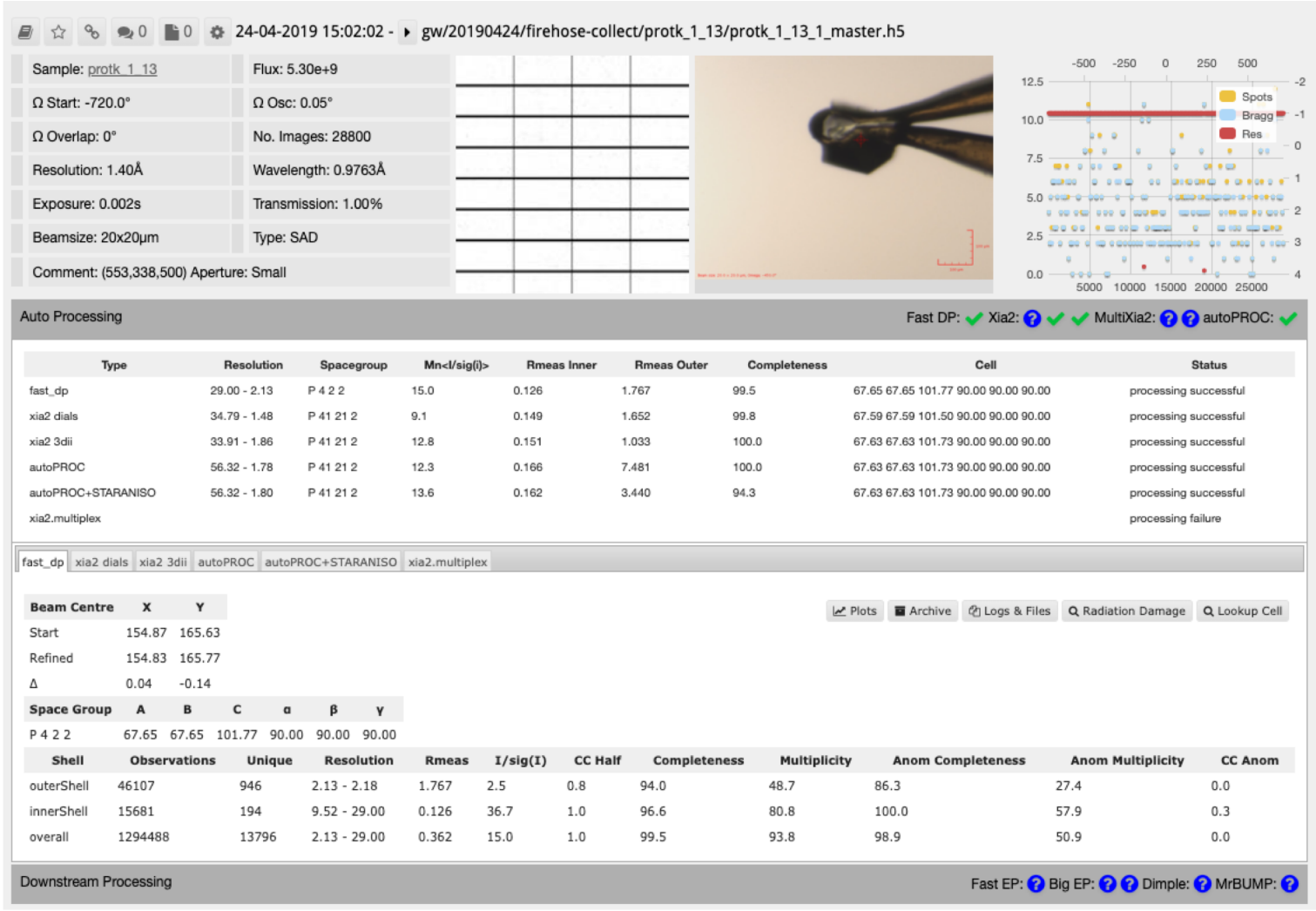
Data auto-processed with Dials

Solved using BigEP with Crank2



And finally....

28 800 images @ 500 Hz, 57.6s, 1% transmission



24-04-2019 15:02:02 - gw/20190424/firehose-collect/protk_1_13/protk_1_13_1_master.h5

Sample: protk_1_13	Flux: 5.30e+9
Ω Start: -720.0°	Ω Osc: 0.05°
Ω Overlap: 0°	No. Images: 28800
Resolution: 1.40Å	Wavelength: 0.9763Å
Exposure: 0.002s	Transmission: 1.00%
Beamsize: 20x20µm	Type: SAD
Comment: (553,338,500) Aperture: Small	

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

Type	Resolution	Spacegroup	Mn<I/sig(i)>	Rmeas Inner	Rmeas Outer	Completeness	Cell	Status
fast_dp	29.00 - 2.13	P 4 2 2	15.0	0.126	1.767	99.5	67.65 67.65 101.77 90.00 90.00 90.00	processing successful
xia2 dials	34.79 - 1.48	P 41 21 2	9.1	0.149	1.652	99.8	67.59 67.59 101.50 90.00 90.00 90.00	processing successful
xia2 3dii	33.91 - 1.86	P 41 21 2	12.8	0.151	1.033	100.0	67.63 67.63 101.73 90.00 90.00 90.00	processing successful
autoPROC	56.32 - 1.78	P 41 21 2	12.3	0.166	7.481	100.0	67.63 67.63 101.73 90.00 90.00 90.00	processing successful
autoPROC+STARANISO	56.32 - 1.80	P 41 21 2	13.6	0.162	3.440	94.3	67.63 67.63 101.73 90.00 90.00 90.00	processing successful
xia2.multiplex								processing failure

fast_dp | xia2 dials | xia2 3dii | autoPROC | autoPROC+STARANISO | xia2.multiplex

Plots | Archive | Logs & Files | Radiation Damage | Lookup Cell

Beam Centre	X	Y
Start	154.87	165.63
Refined	154.83	165.77
Δ	0.04	-0.14

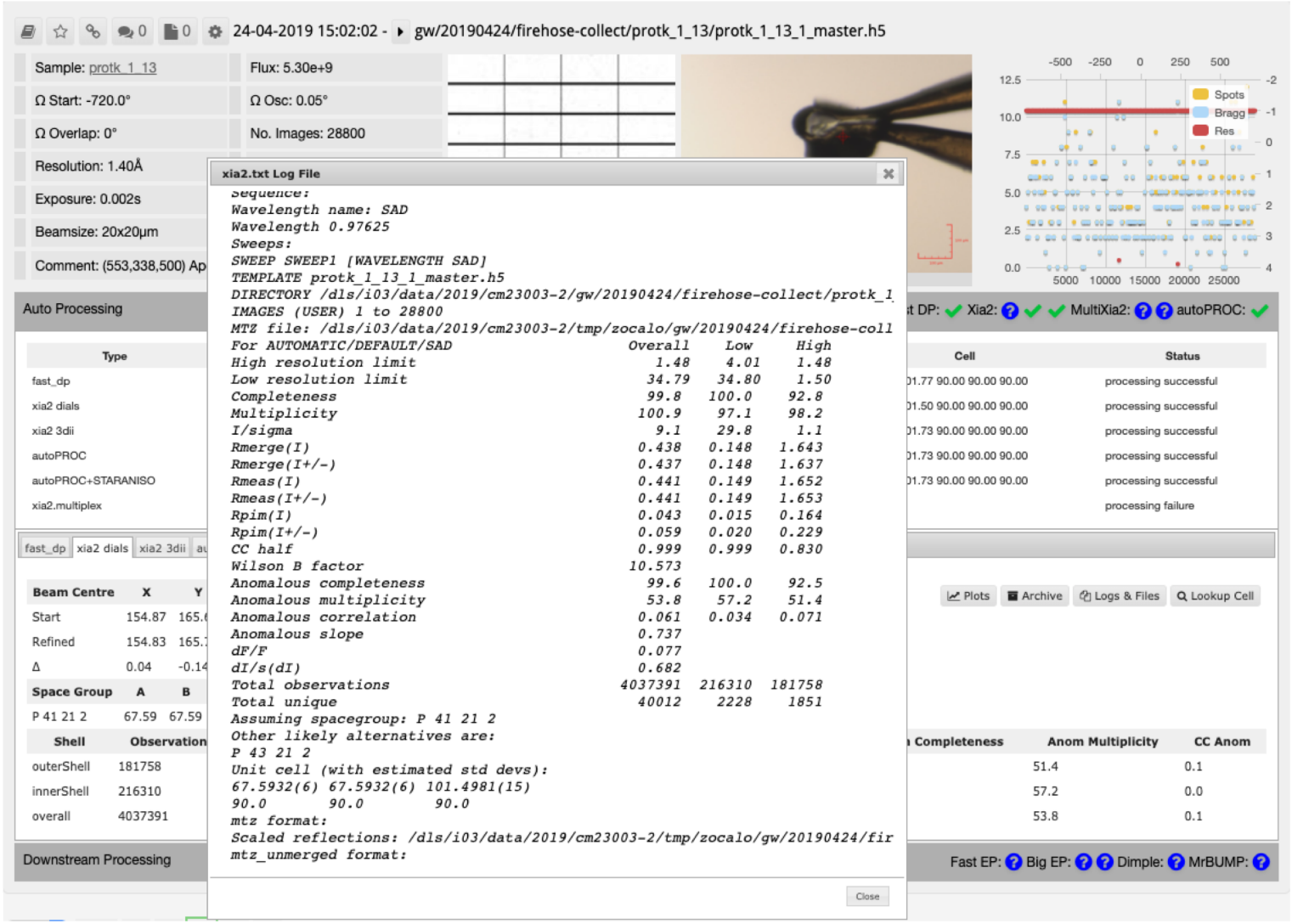
Space Group	A	B	C	α	β	γ
P 4 2 2	67.65	67.65	101.77	90.00	90.00	90.00

Shell	Observations	Unique	Resolution	Rmeas	I/sig(I)	CC Half	Completeness	Multiplicity	Anom Completeness	Anom Multiplicity	CC Anom
outerShell	46107	946	2.13 - 2.18	1.767	2.5	0.8	94.0	48.7	86.3	27.4	0.0
innerShell	15681	194	9.52 - 29.00	0.126	36.7	1.0	96.6	80.8	100.0	57.9	0.3
overall	1294488	13796	2.13 - 29.00	0.362	15.0	1.0	99.5	93.8	98.9	50.9	0.0

Downstream Processing — Fast EP: Big EP: Dimple: MrBUMP:

And finally....

28 800 images @ 500 Hz, 57.6s, 1% transmission



Great team achievement

- Matt Taylor
- Gary Yendell
- Ulrik Pederson
- James O'Hea
- Lee Hudson
- Charles Mita
- Richard Fearn
- Graeme Winter
- Richard Gildea
- Richard Lear
- Markus Gerstel
- Andrew Richards
- Karl Levik
- Dave Butler
- Adam Taylor
- Adam Prescott
- Halina Mikolajek
- Dave Hall
- Neil Smith
- Alun Ashton
- Graham Duller
- Richard Parr
- Richard Littlewood
- Jon Kelly
- Scott Williams
- Graeme Richards
- Nicola Tartoni
- Juan Sanchez-Weatherby
- James Sandy
- Ralf Flaig
- Pierpaolo Romano
- Marco Mazzorana
- Katherine McAuley
- Neil Paterson
- Mark Williams
- Dectris – Stefan Brandstetter, Andy Moesch, Lucas Wagner



