

Implementation of Eiger2 Detectors at Diamond Light Source

Katherine McAuley



Detectors on the MX beamlines



I03

- Eiger2 XE 16M



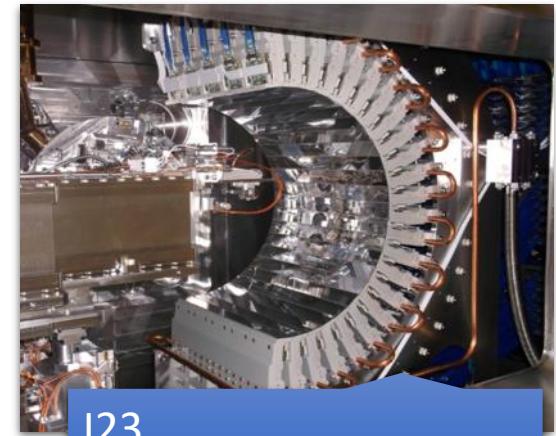
I04

- Eiger2 XE 16M



I04-1

- Pilatus2 6M-F



I23

- Pilatus2



I24

- Pilatus3 6M



VMXi

- Eiger2 X 4M



VMXm

- Pilatus3 6M

Detectors on the MX beamlines



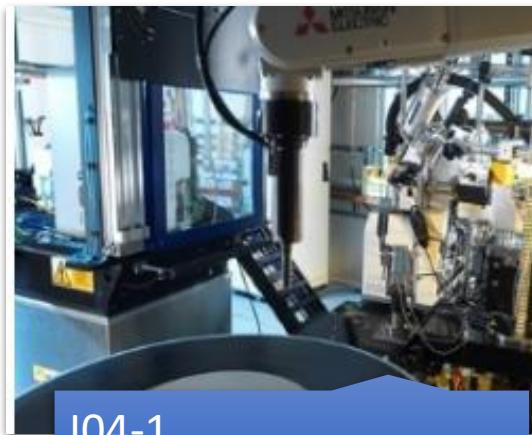
I03

- Eiger2 XE 16M



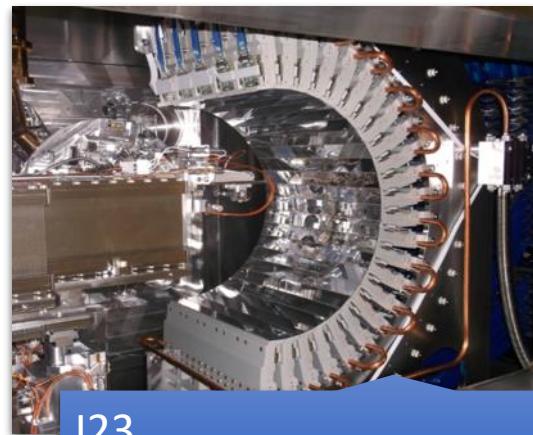
I04

- Eiger2 XE 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

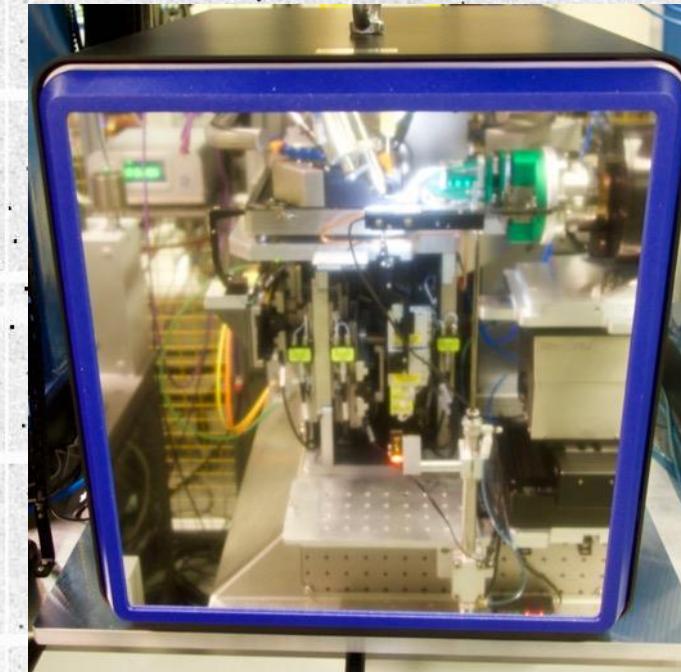
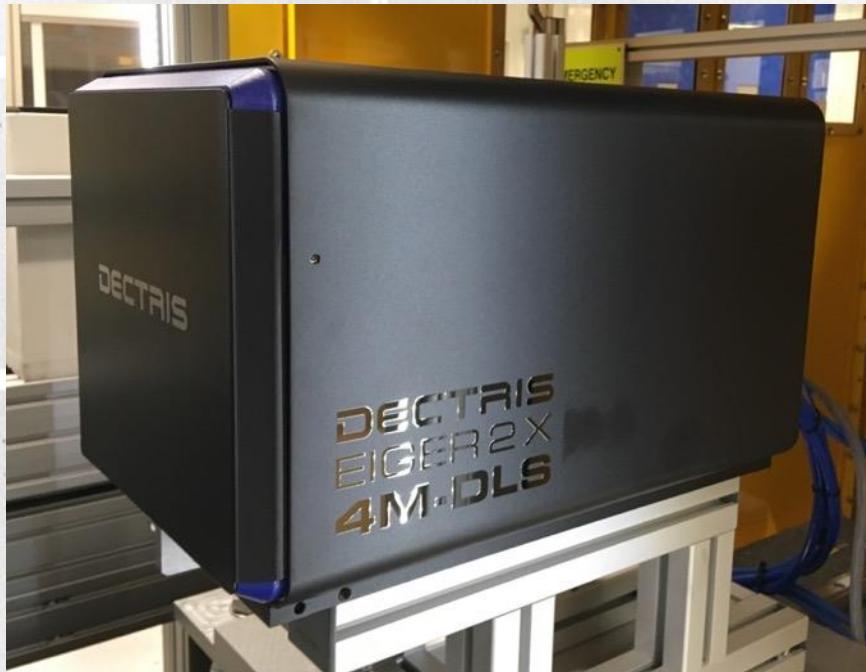
- Pilatus3 6M

Eigers in use



Latest Detectors for MX – Eiger2

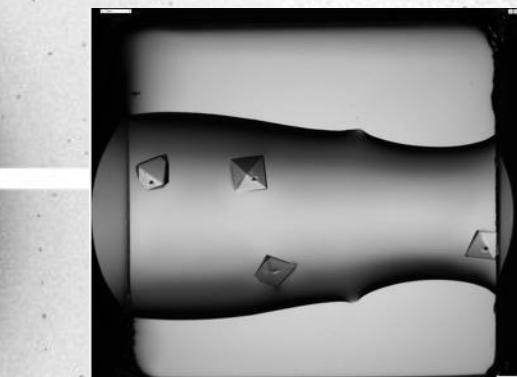
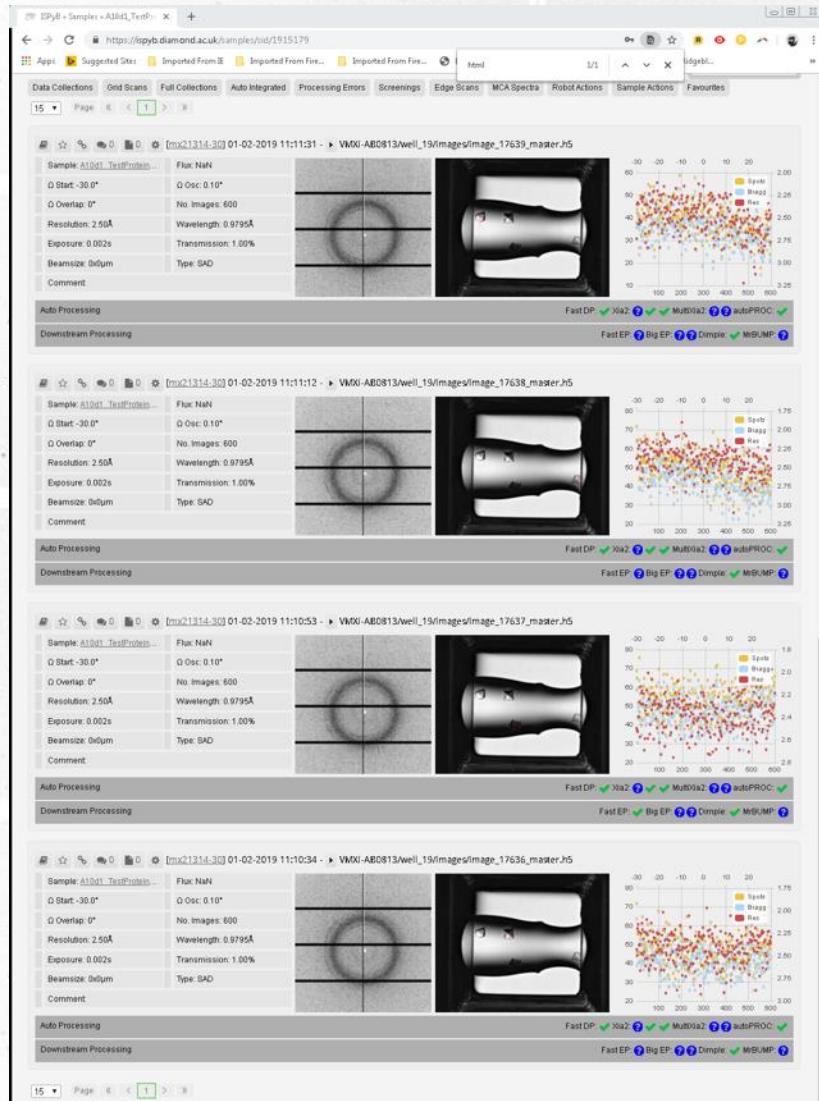
- Keeping Diamond at the forefront of detector technology with first installations of latest generation Dectris pixel array detectors



- 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

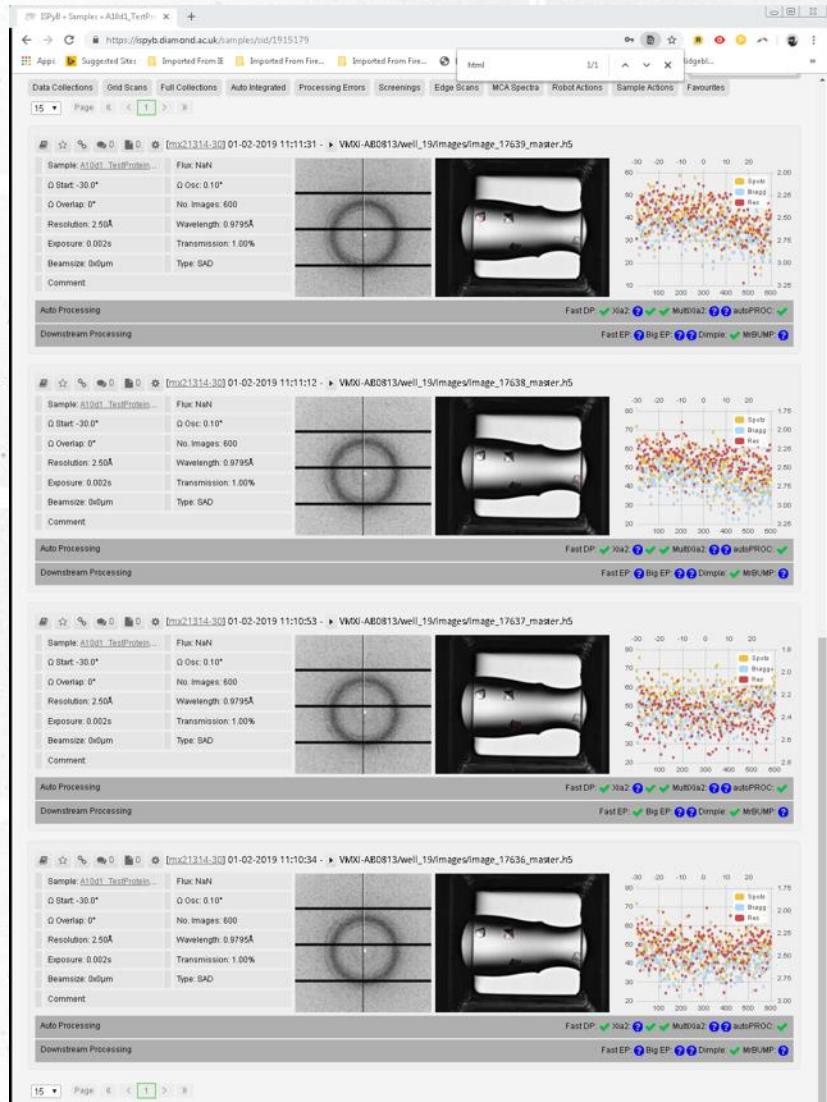
xia2 multi-crystal report

Merging statistics

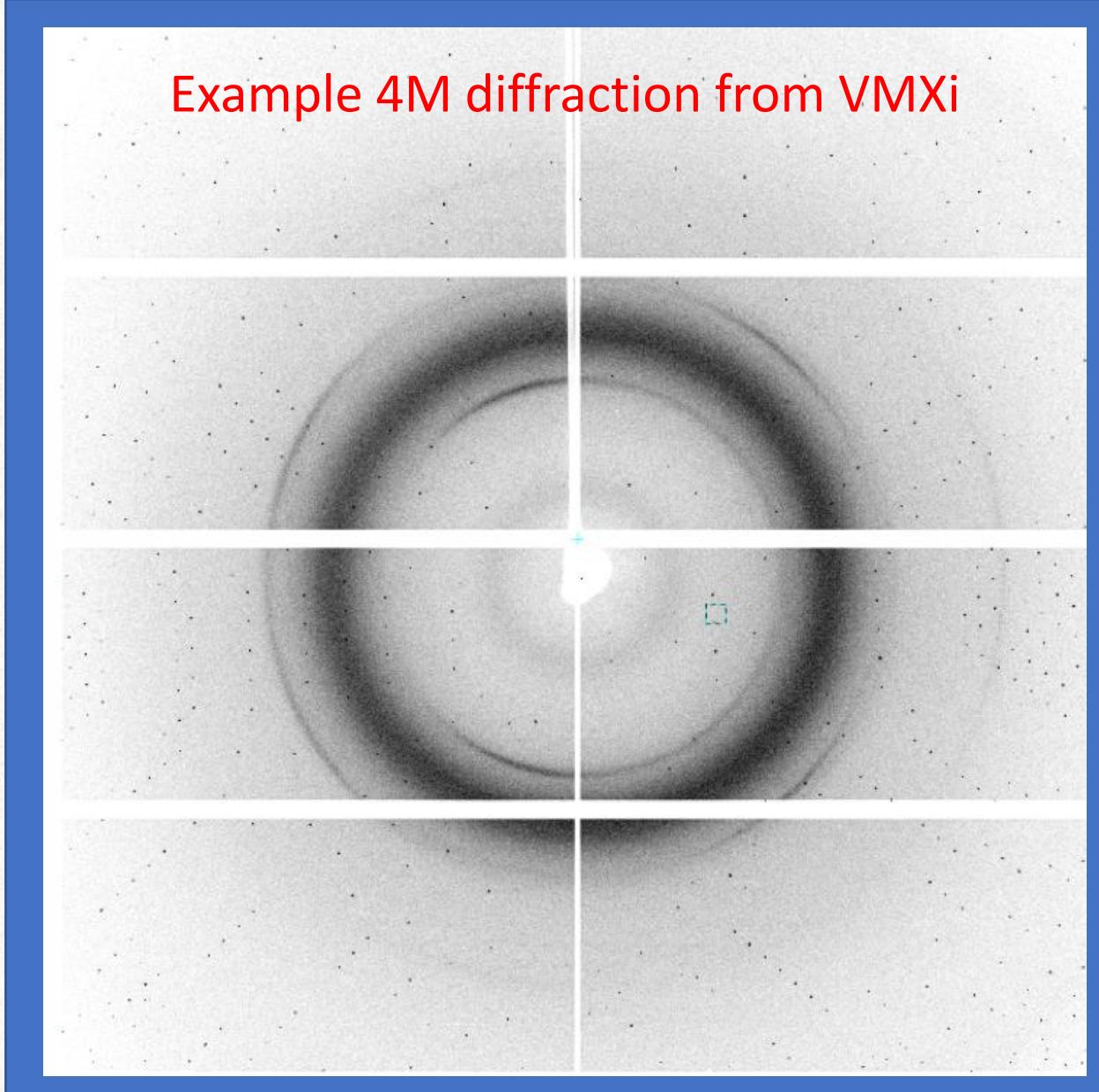
Filename:
Space group: P 4 2 2 (No. 89)
Unit cell: (68.3739, 68.3739, 103.991, 90, 90, 90)

	Overall	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 - VMXi



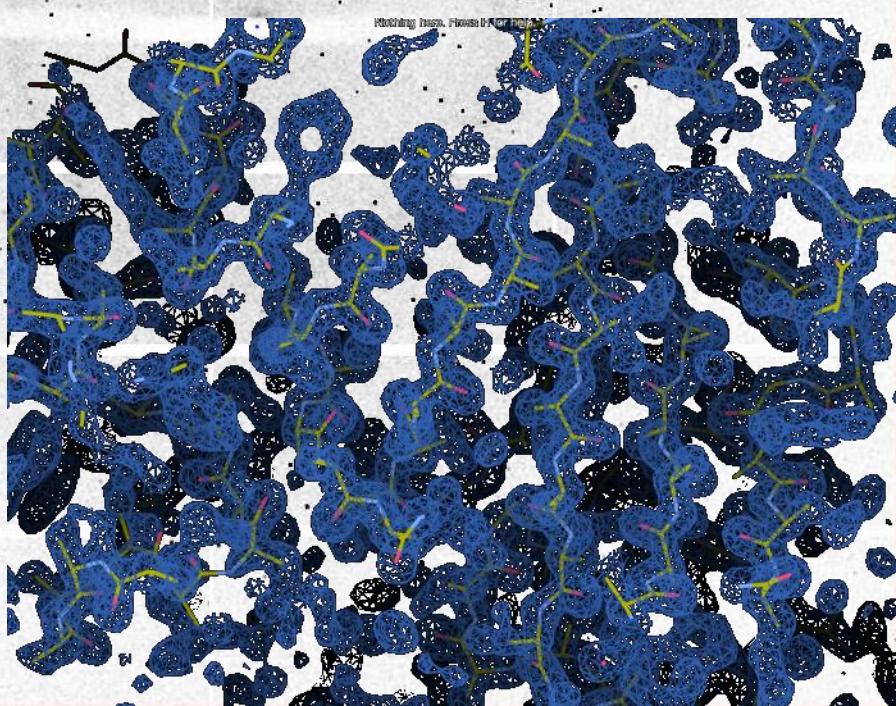
Example 4M diffraction from VMXi



Rapid data collection rates and structure solution I03 & I04

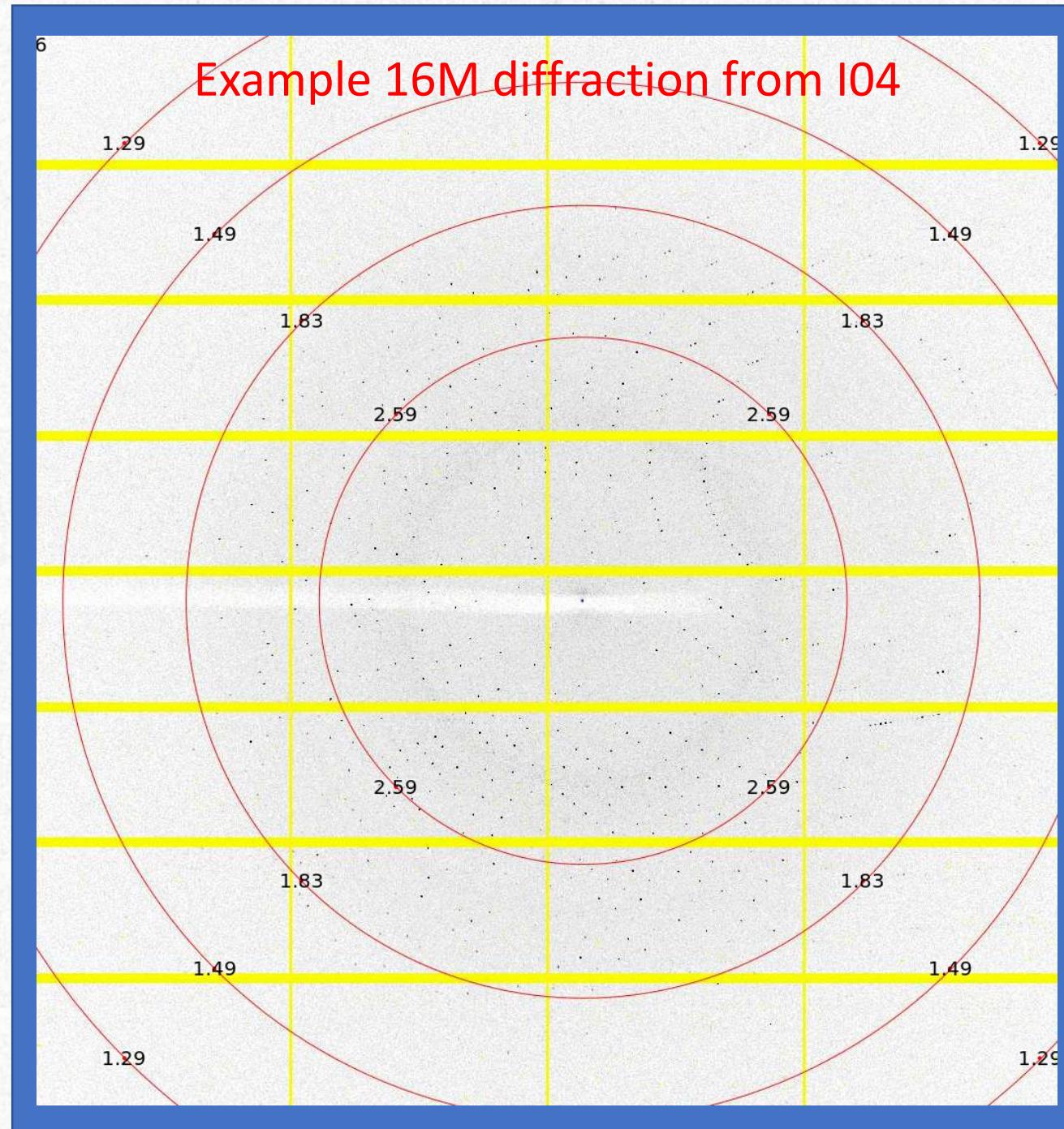
- Early results from I04
 - Rapid collection (eg <30s) of fine phi sliced, highly redundant data
 - Excellent quality statistics
 - Automatically phased and built model from data collected (in 78s) on first full day of use
- Opens up new opportunities for high throughput automated collection

	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
Rfree	0.012	0.005	0.456
CC1/2	1.000	1.000	0.572

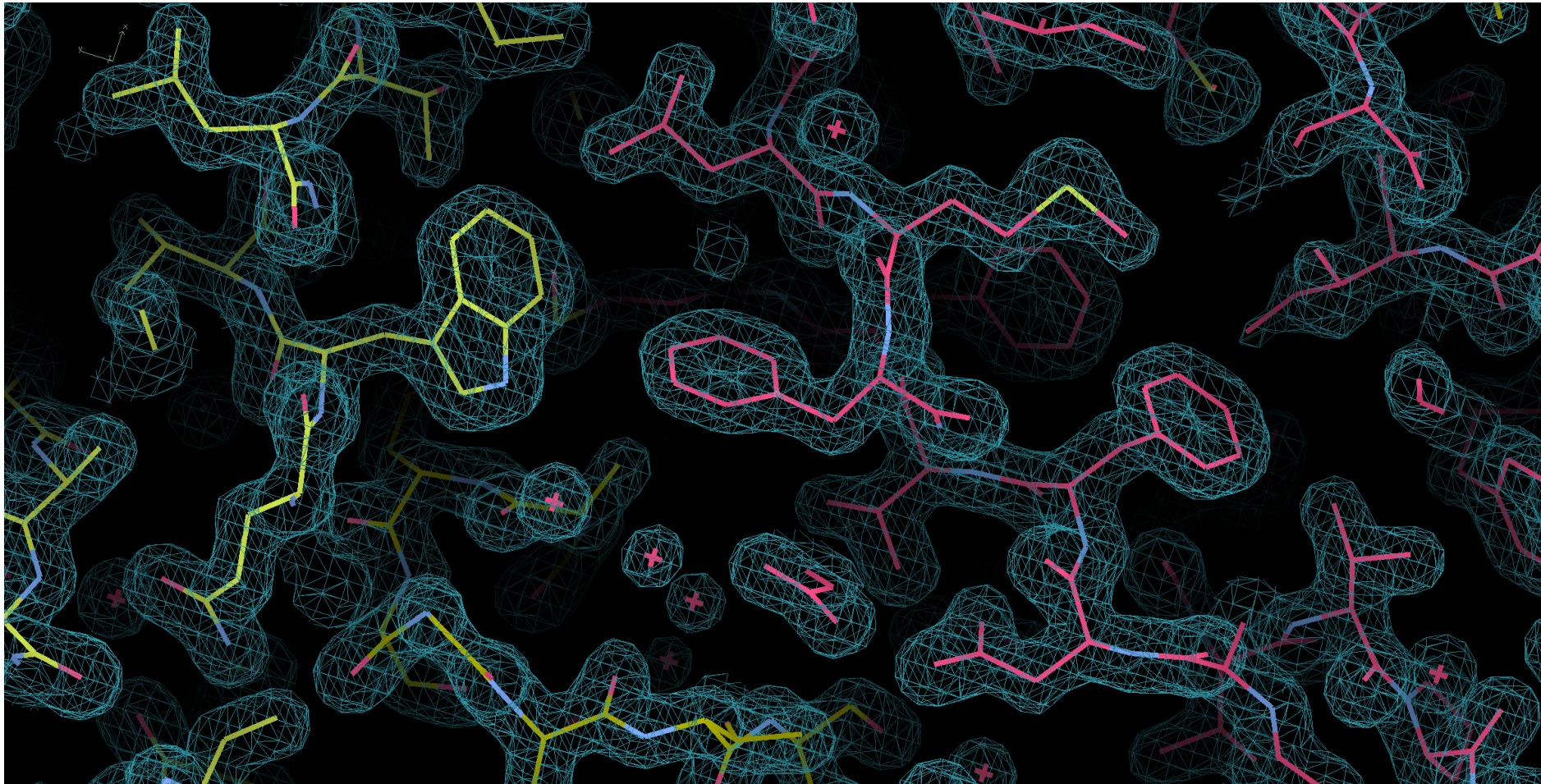


Rapid data collection rates and structure solution I03 & I04

- 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



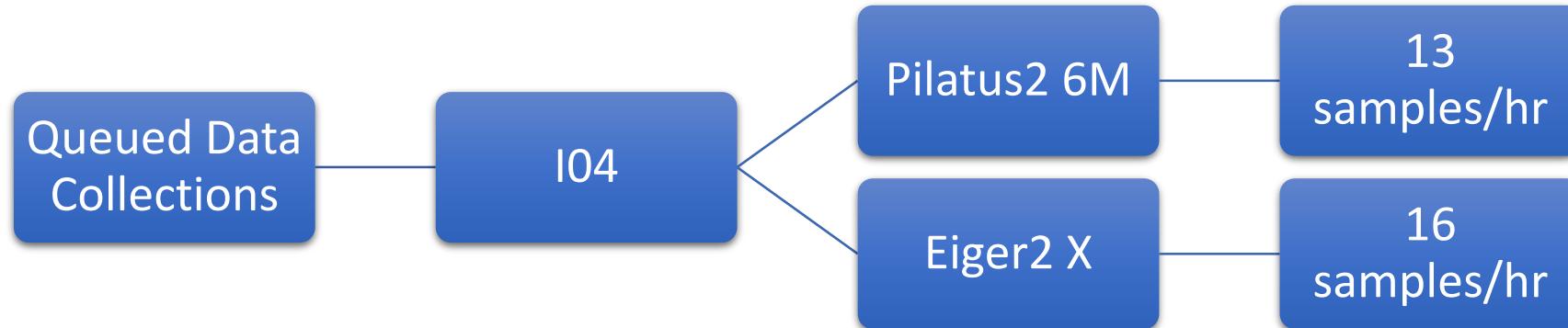
Beamline I03 – a rare example, a virus structure in half a minute



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



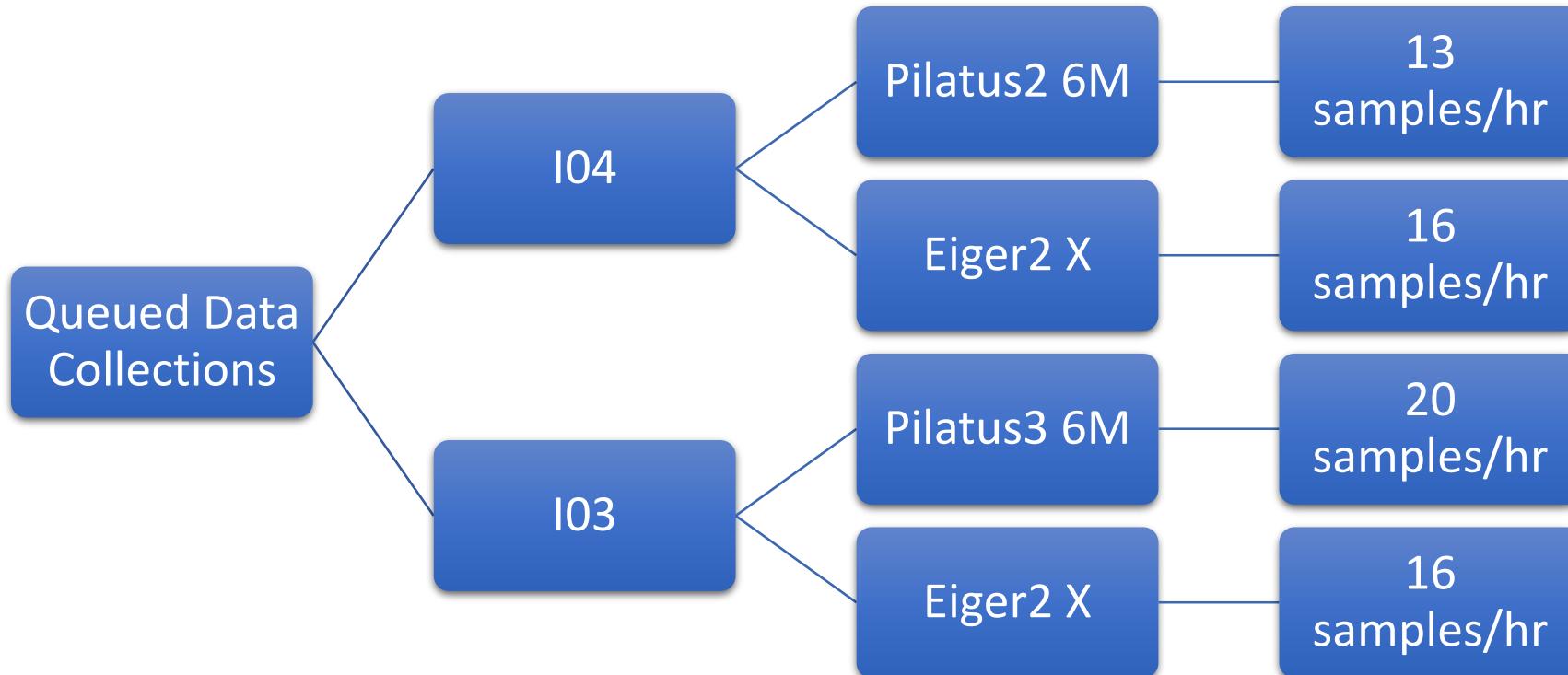
Sample exchange

X-ray Centring (2 grid scans)

180 deg data collection

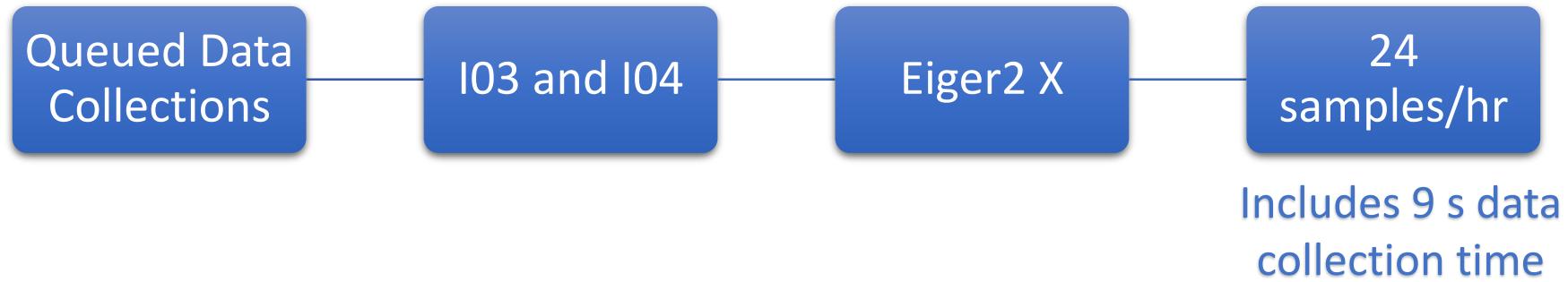
Beamline performance – Eiger vs Pilatus

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



Beamline performance – Eiger vs Pilatus

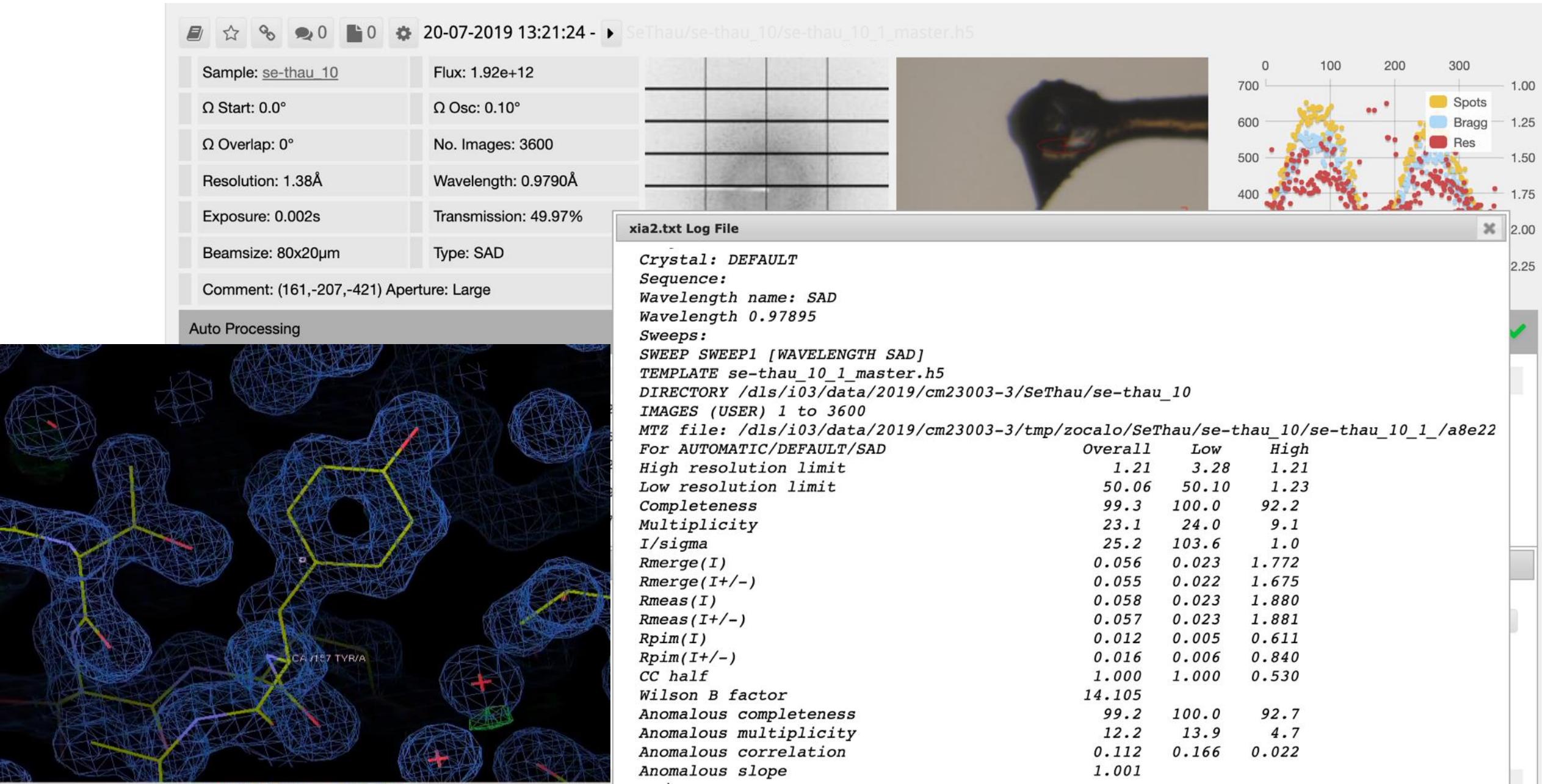
- Data collection is faster but data analysis is slower
- Queued data collection mode re-optimized for Eiger detectors
- Use ROI for X-ray centring grid scans at 250 Hz
- Process data before all files written to disk



Testing 500 Hz data collections



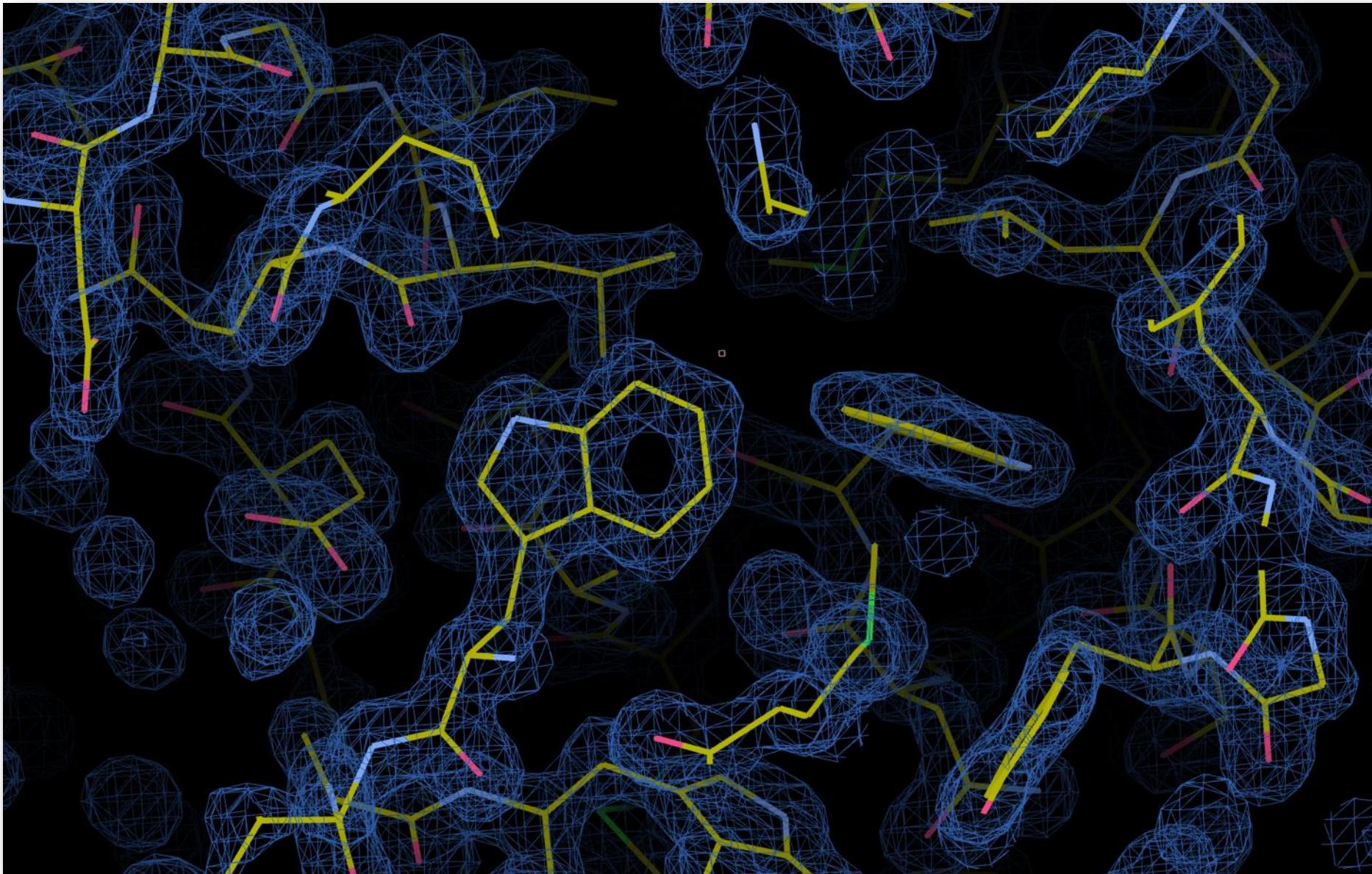
Thaumatin crystal 500 Hz, I03



Selenourea soaked lysozyme, 500 Hz

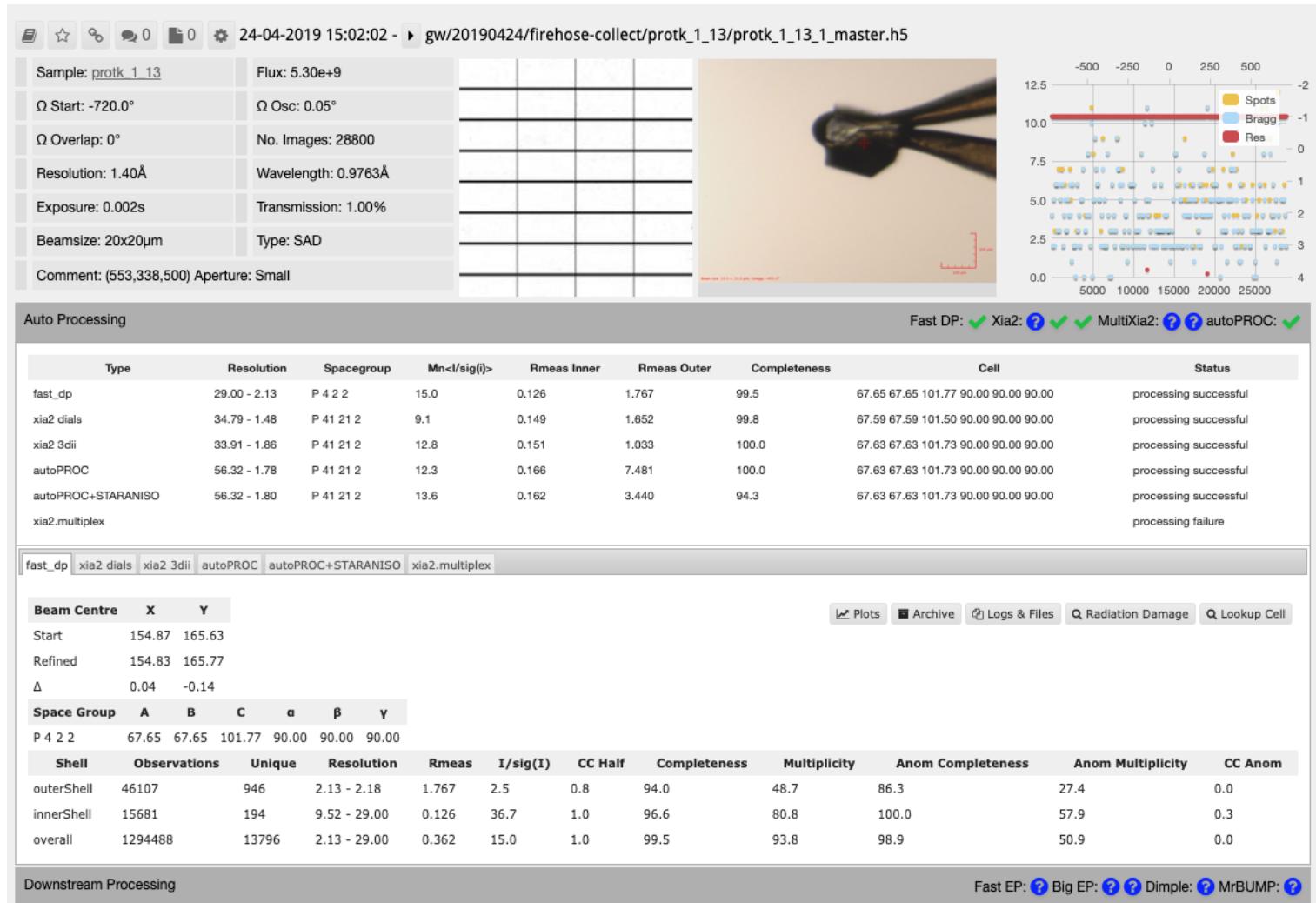


Selenourea soaked lysozyme, 500 Hz



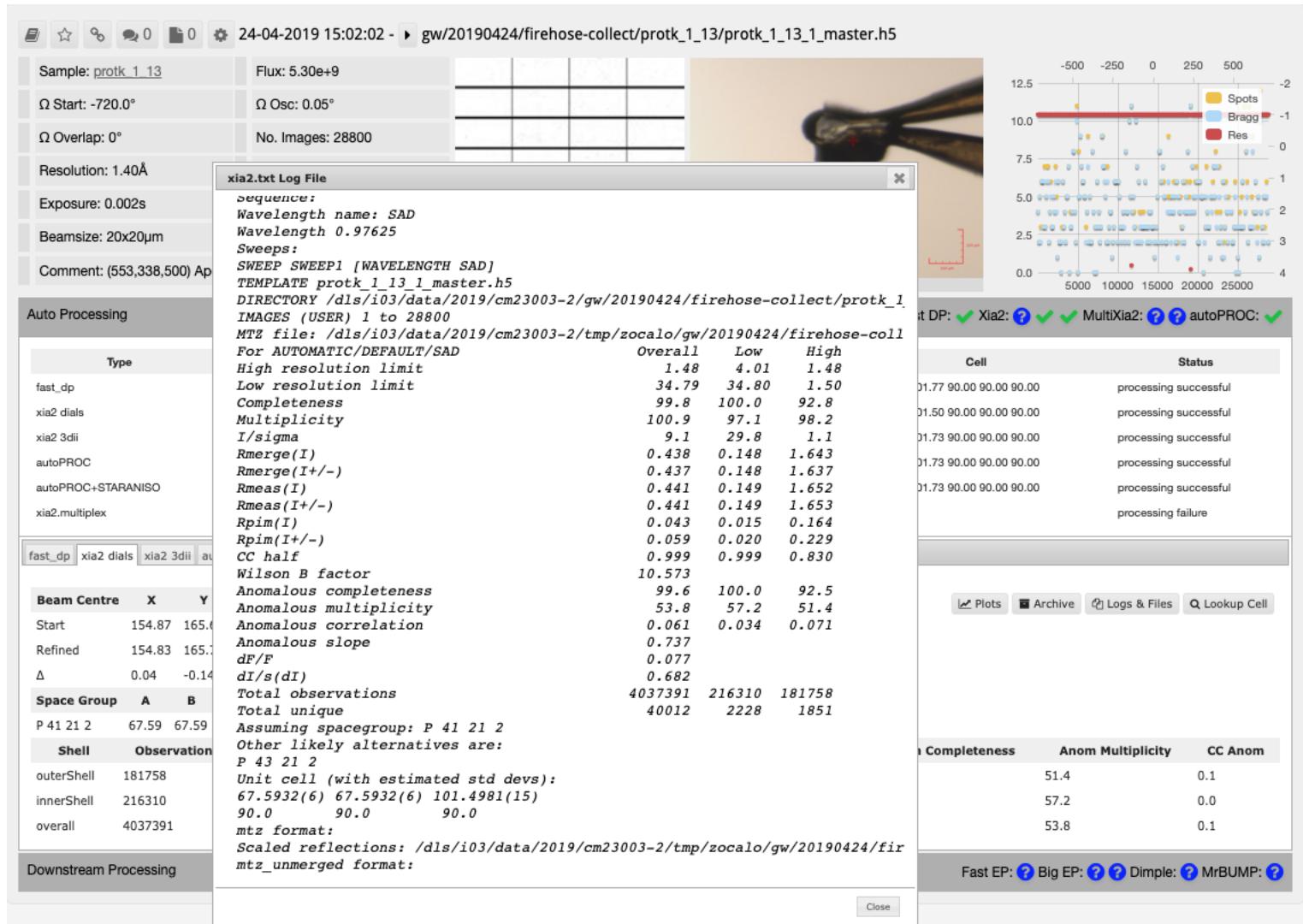
Pushing the limits....

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



Pushing the limits....

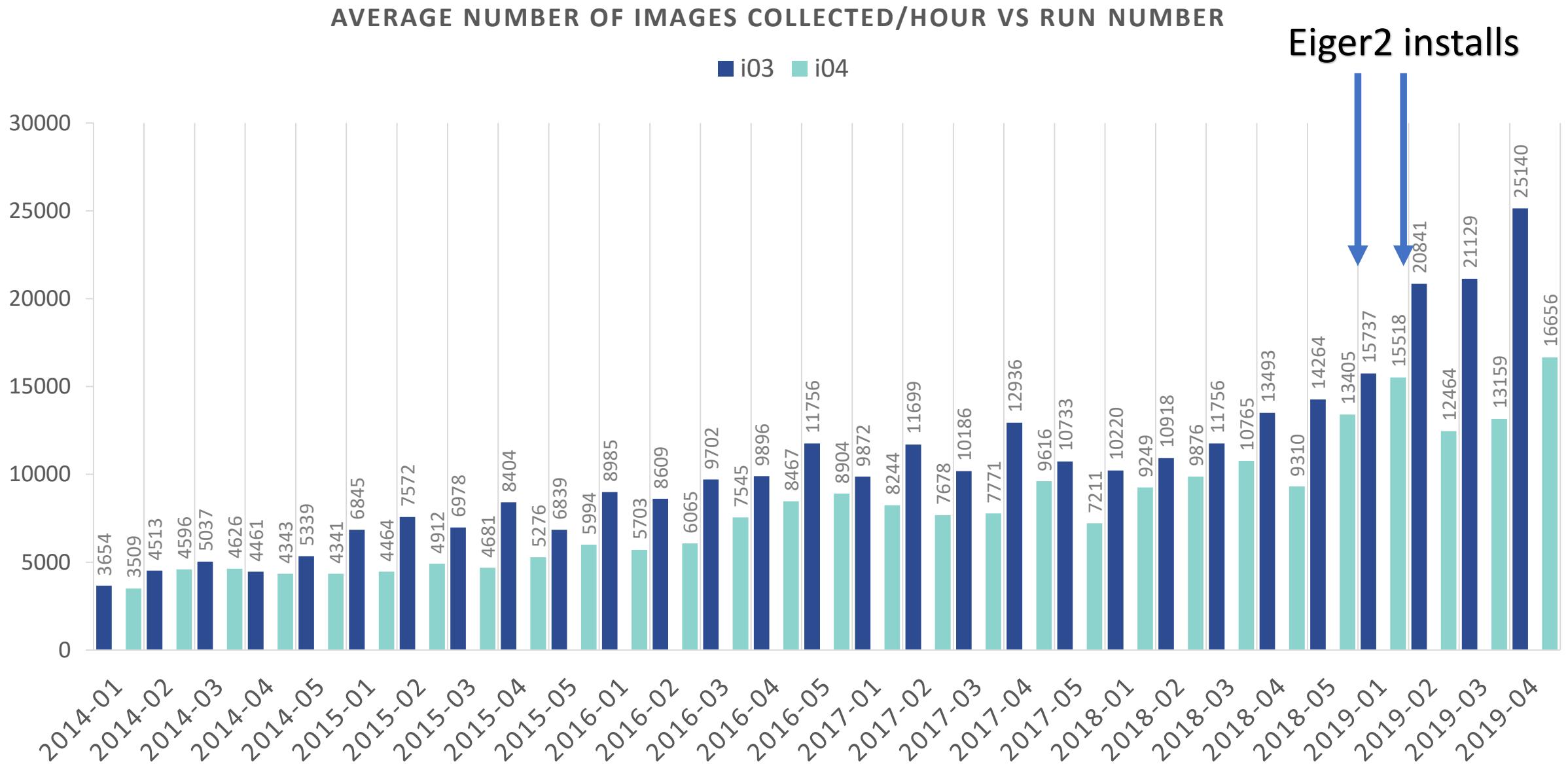
28 800 images @ 500 Hz, 57.6s, 1% transmission



Several months later



Impact of Eiger2 detectors (I03 and I04)



Summary

Currently

- All Eiger detectors in full operation
- User feedback mostly positive but
 - Users would like to see per image analysis plots during data collections
 - Still some comments that data processing is too slow
 - Image viewing could be improved for remote users
- 500 Hz data collections
 - Used routinely by UDC
 - Can be flux limited

Future work

- Improve processing
 - Kafka project to enable on-the-fly processing of data
 - Diffraction image viewing in GDA
 - Upgrade cluster
- Increase flux
 - CPMUs for I24 & I03
 - DMM for I04 being considered
 - Diamond-II

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

