

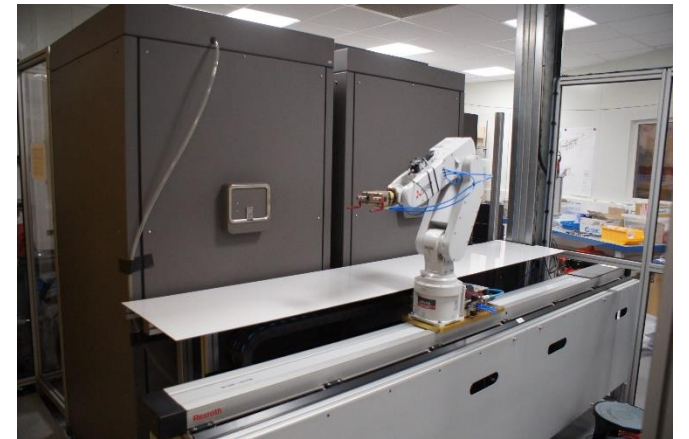
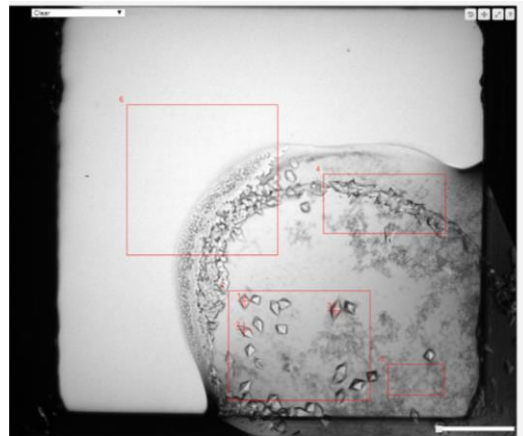
VMXi the only fully *in-situ* fully remote beamline

What the beamline does and how it could benefit your work

Juan Sanchez-Weatherby
James Sandy
Halina Mikolajek

What is VMXi?

- *In-situ*
- Fully automated
- Fully remote



This beamline will be most useful for...

- Projects with small crystals
- Samples that do not cryo-protect well
- Data collection with no manual handling
- Speeds up the early crystal optimisation cycles
- Rapidly solve multiple ligand structures

Current beamline status

- Fully automated handling of plates (*in-situ* plates and films)
- 20 °C soon 4 °C
- $\sim 10 \times 10 \text{ } \mu\text{m}^2$ beam size
- DMM monochromator $> 10^{14}$ phs/s (extremely high flux)
- Eiger2X 4M detector (500 Hz)
- Grid scans 500 Hz (100% beam)
- Omega scans -30° to 30° 560Hz (2-5% beam)
- Lab facility for crystallisation
- Synchweb web interface

Harwell Campus Structural Biology Partnership Crystallisation Facility

- Facility is situated in Research Complex at Harwell
- Integrated with Membrane Protein Laboratory
- Crystallisation can be set up at 4 °C and 20 °C
- Greiner CrystalQuick™X
- Mitegen In Situ-1™
- Batch film



Current status of VMXi

Crystallisation plates arrive at the beamline

Beamline images crystallisation plates

User reviews results and selects point for DC

Beamline loads samples

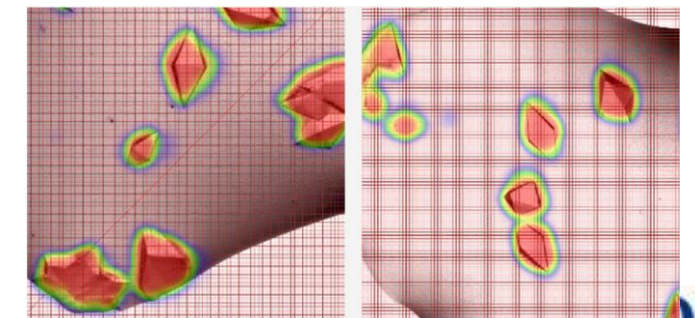
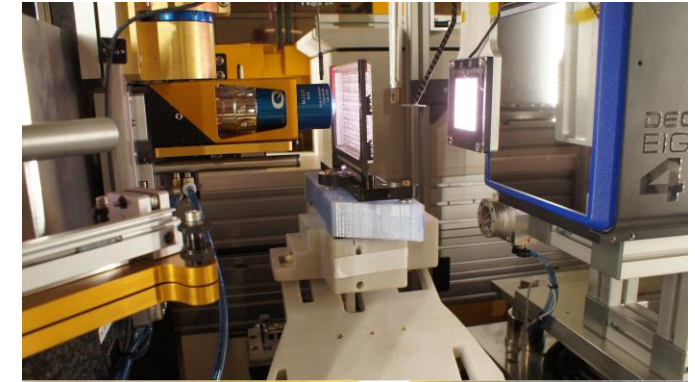
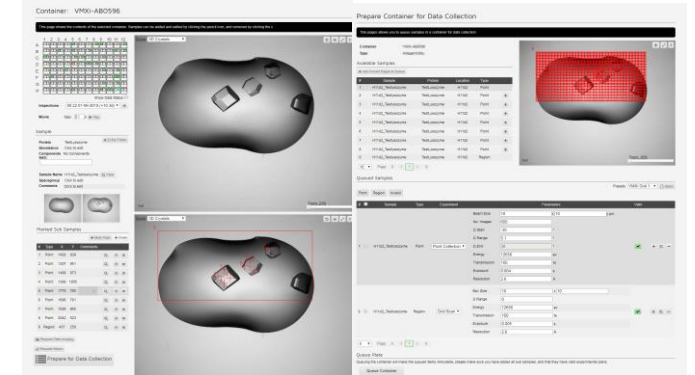
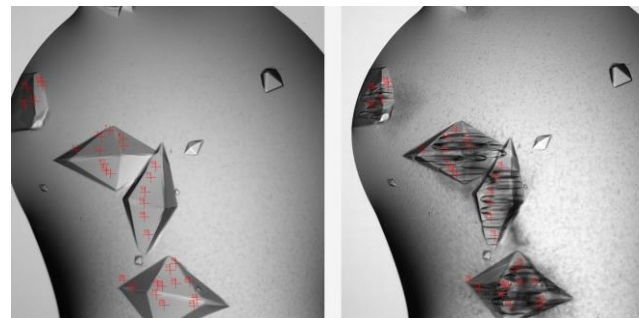
Beamline defines where users wants to collect data

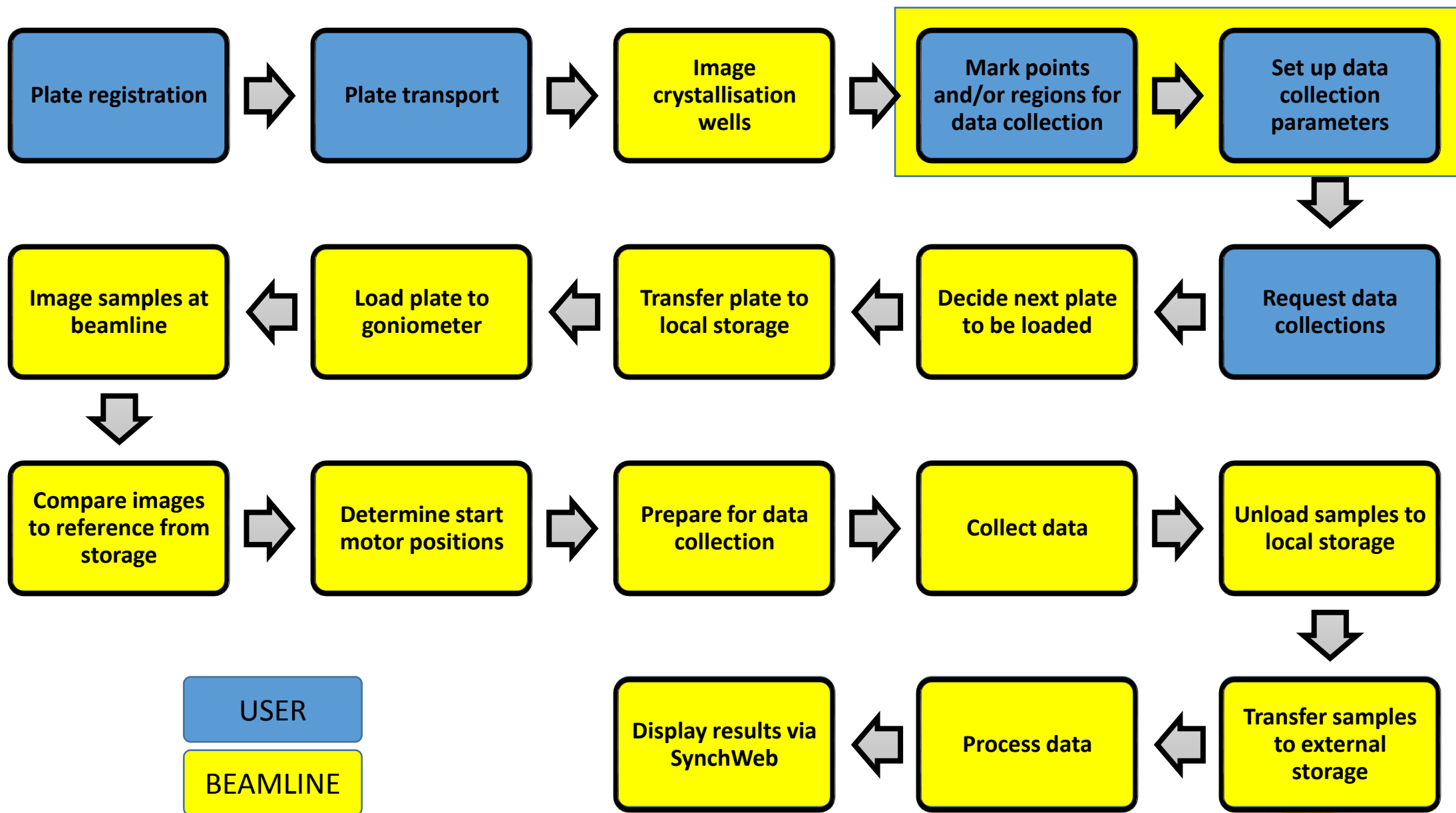
Beamline sets correct DC parameters

Beamline collects data

Beamline unloads samples

Beamline automatically processes data





Paste from Spreadsheet

Shipment

Dewar

Container Type

Container Name

Barcode

Owner

This user will be emailed with container updates. Check your email is up to date!

Comments

Comment for the container

Requested Imager

Imager this container should go into

Imaging Schedule

Requested imaging schedule

Crystallisation Screen

Crystallisation screen that was used for this container

Sample

Protein

Abundance

Sample Name

Spacegroup

Comments

Components

Add:

CCP4_TEST

Dewar1

CrystalQuickX

CCP4_TEST

JUAN_TES_001

Juan Sanchez-Weatherby [You]

Q View

VMXi 20c

Fibonacci

Q View

Ax-CP-CUSTOM-101

+ Plate

+ Column

+ Row

x Plate

x Column

x Row

x

+ Extra Fields

JEWGDH

NONSENS

No Components

	1	2	3	4	5	6	7	8	9	10	11	12
A	1	3	5	7	9	11	13	15	17	19	21	23
B	26	27	29	31	33	35	37	39	41	43	45	47
C	49	51	53	55	57	59	61	63	65	67	69	71
D	73	75	77	79	81	83	85	87	89	91	93	95
E	97	99	101	103	105	107	109	111	113	115	117	119
F	121	123	125	127	129	131	133	135	137	139	141	143
G	145	147	149	151	153	155	157	159	161	163	165	167
H	169	171	173	175	177	179	181	183	185	187	189	191

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

	1	2	3	4	5	6	7	8	9	10	11	12
A	1 2	5 6	9 10	13 14	17 18	21 22	25 26	29 30	33 34	37 38	41 42	45 46
B	49 50	53 54	57 58	61 62	65 66	69 70	73 74	77 78	81 82	85 86	89 90	93 94
C	97 98	101 102	105 106	109 110	113 114	117 118	121 122	125 126	129 130	133 134	137 138	141 142
D	149 150	153 154	157 158	161 162	165 166	169 170	173 174	177 178	181 182	185 186	189 190	193 194
E	197 198	201 202	205 206	209 210	213 214	217 218	221 222	225 226	229 230	233 234	237 238	241 242
F	249 250	253 254	257 258	261 262	265 266	269 270	273 274	277 278	281 282	285 286	289 290	293 294
G	297 298	301 302	305 306	309 310	313 314	317 318	321 322	325 326	329 330	333 334	337 338	341 342
H	349 350	353 354	357 358	361 362	365 366	369 370	373 374	377 378	381 382	385 386	389 390	393 394

Show Data Status ☐ | Loaded 135 out of 192 images

Inspections

13:29 15-12-2017 (+0.0d) [Manual] [+](#)

Movie

Gap: 0.1 s [▶ Play](#)

Sample

Protein

TestThaumatococcus

[+ Extra Fields](#)

Abundance

[Click to edit](#)

Components

No Components

Add:

Sample Name

C2d1_Thaum_Again [Q View](#)

Spacegroup

[Click to edit](#)

Comments

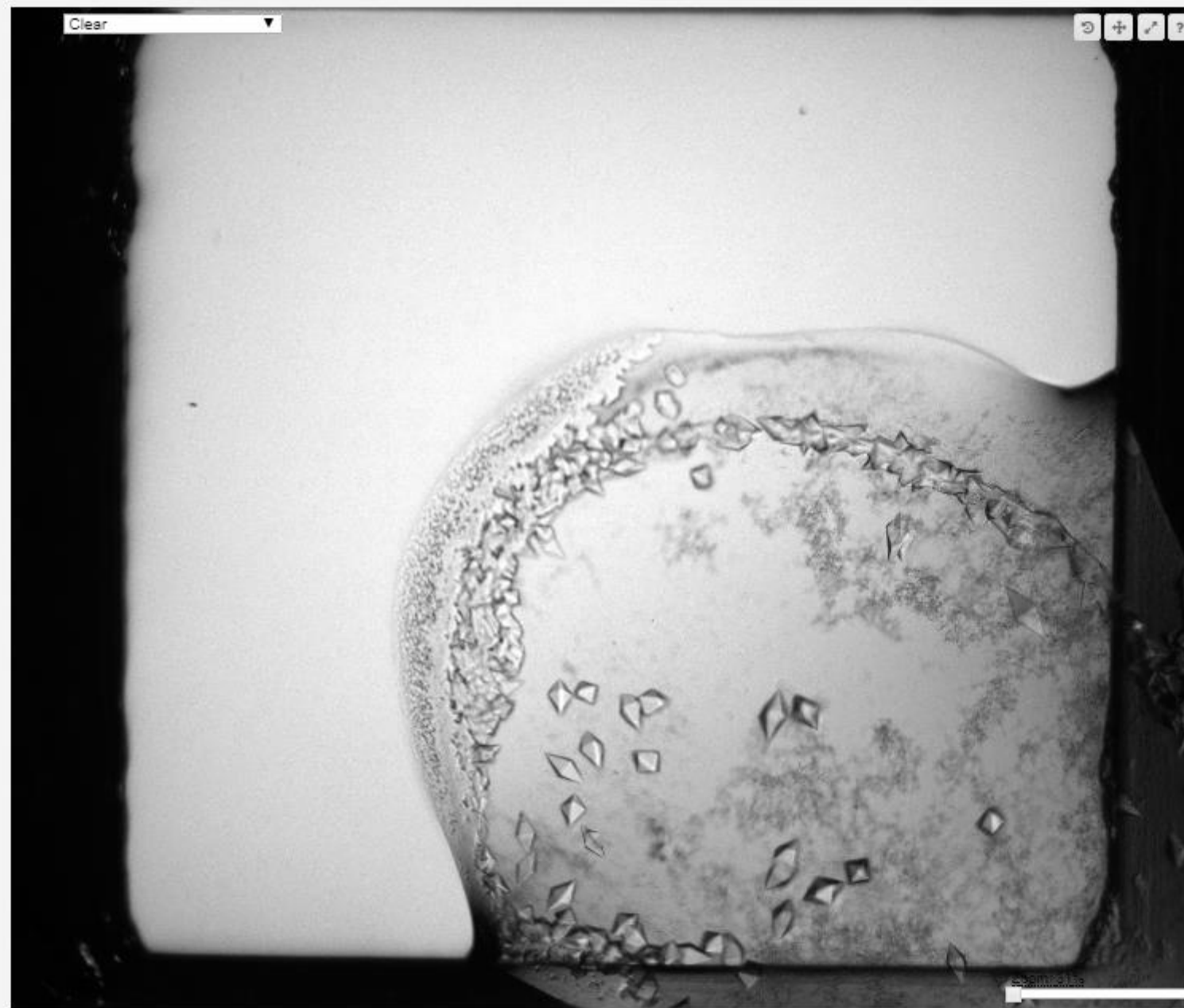
[Click to edit](#)



+0.0d

Marked Sub Samples

[+ Mark Point](#) [+ Mark Region](#)



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

	1	2	3	4	5	6	7	8	9	10	11	12
A	1.12	5.13	5.13	7.13	9.13	10.13	15.13	17.13	17.17	17.17	20.17	22.17
B	24.28	24.28	24.28	31.32	32.32	32.32	35.32	35.37	37.37	37.37	41.37	41.37
C	64.53	51.54	51.54	54.55	57.55	57.55	61.54	62.54	64.55	64.55	67.57	71.57
D	74.74	74.75	74.75	74.75	81.75	83.74	84.75	87.75	87.75	87.75	91.74	95.74
E	95.75	95.75	101.75	101.75	101.75	101.75	101.75	101.75	101.75	101.75	101.75	101.75
F	121.75	121.75	121.75	121.75	121.75	121.75	121.75	121.75	121.75	121.75	121.75	121.75
G	141.75	141.75	141.75	141.75	141.75	141.75	141.75	141.75	141.75	141.75	141.75	141.75
H	161.75	171.74	171.74	171.74	171.74	171.74	171.74	171.74	171.74	171.74	171.74	171.74

Show Data Status ☐ | Loaded 185 out of 192 images

Inspections

13:29 15-12-2017 (+0.0d) [Manual]

Movie

Gap: 0.1 s

Sample

Protein

TestThaumatococcus

Abundance

Click to edit

Components

No Components

Add:

Sample Name

C2d1_Thaum_Again

Spacegroup

Click to edit

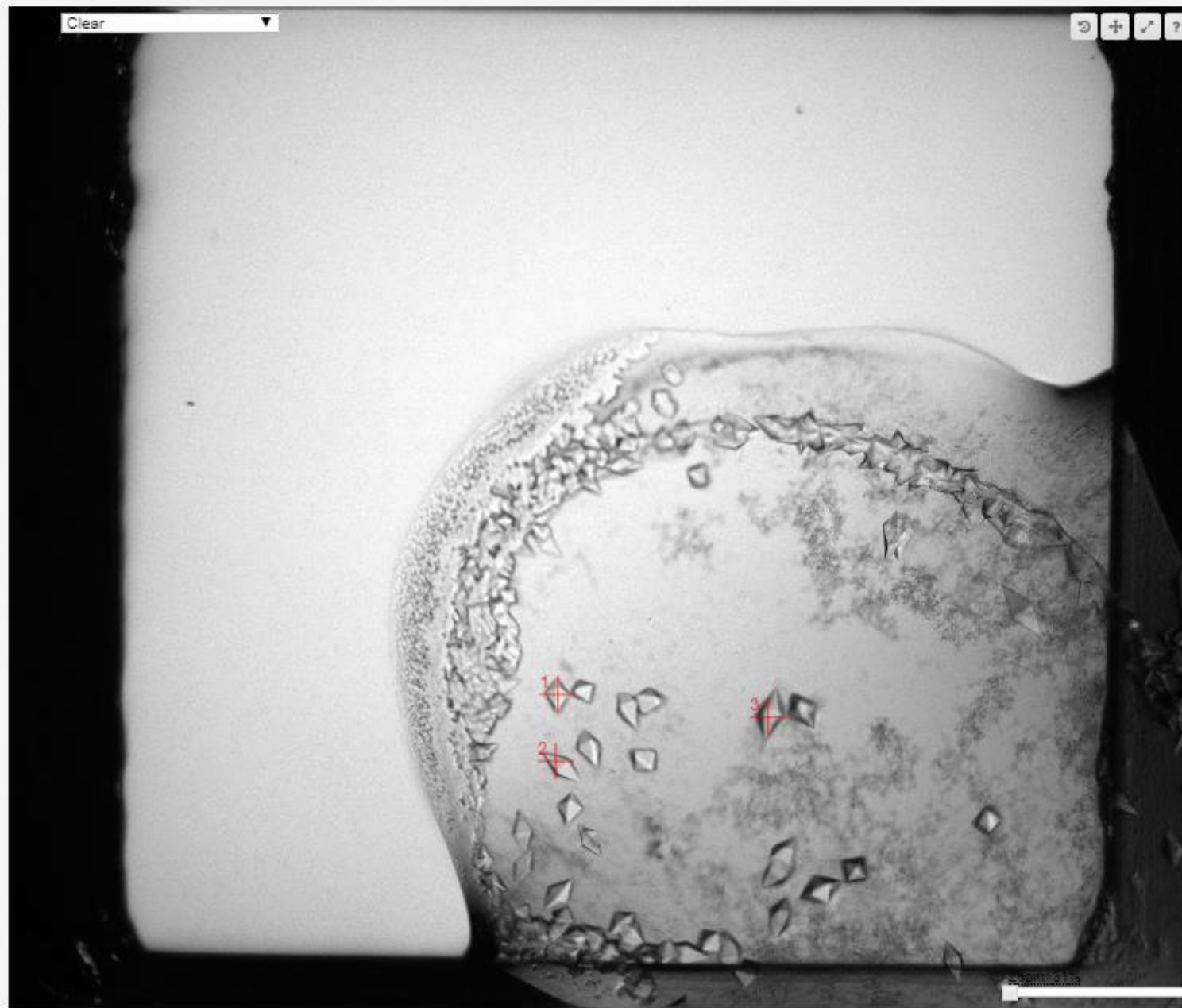
Comments

Click to edit



+0.0d

Marked Sub Samples



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

	1	2	3	4	5	6	7	8	9	10	11	12
A	1.12	5.13	5.13	7.13	9.13	10.13	15.13	17.13	17.17	20.17	20.17	22.17
B	24.28	24.28	24.28	31.32	32.32	32.32	35.32	35.32	41.32	41.32	41.32	41.32
C	64.58	51.58	51.58	54.58	57.58	57.58	61.58	61.58	64.58	64.58	64.58	64.58
D	74.74	74.74	74.74	74.74	81.74	81.74	81.74	81.74	81.74	81.74	81.74	81.74
E	91.98	91.98	91.98	91.98	91.98	91.98	91.98	91.98	91.98	91.98	91.98	91.98
F	124.12	124.12	124.12	124.12	124.12	124.12	124.12	124.12	124.12	124.12	124.12	124.12
G	141.18	141.18	141.18	141.18	141.18	141.18	141.18	141.18	141.18	141.18	141.18	141.18
H	161.11	161.11	161.11	161.11	161.11	161.11	161.11	161.11	161.11	161.11	161.11	161.11

Show Data Status ☐

Inspections 13:29 15-12-2017 (+0.0d) [Manual]

Movie Gap: 0.1 s

Sample

Protein TestThaumatin

Abundance Click to edit

Components No Components

Add:

Sample Name C2d1_Thaum_Again

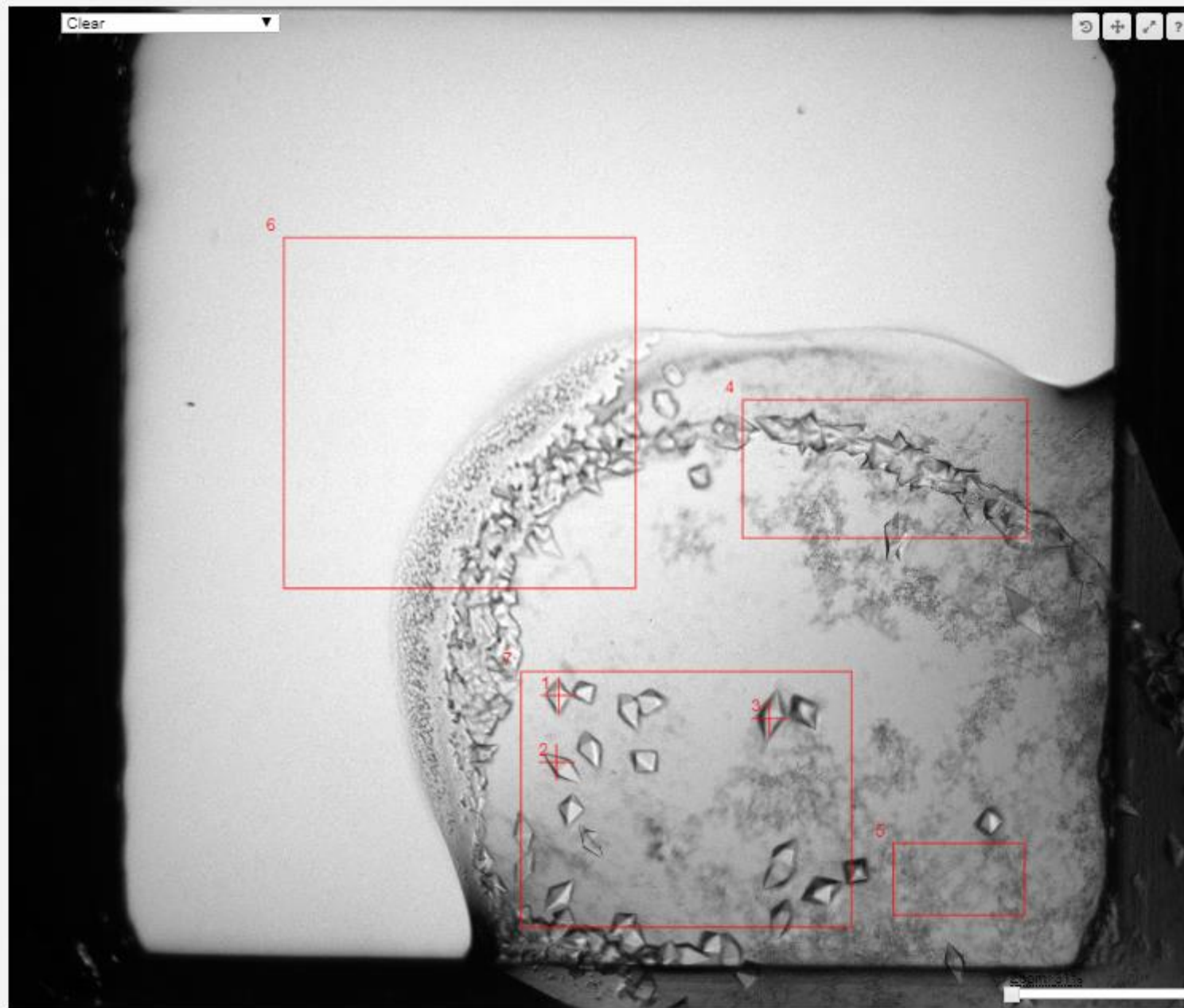
Spacegroup Click to edit

Comments Click to edit



+0.0d

Marked Sub Samples



#	Sample	Protein	Location	Type
51	A8d1_bob	TestThaumatococcus	A8d1	Region
52	A8d1_bob	TestThaumatococcus	A8d1	Region
53	F10d1_bob	TestThaumatococcus	F10d1	Region
54	A1d1_bob	TestThaumatococcus	A1d1	Region
55	A1d1_bob	TestThaumatococcus	A1d1	Region

5 ▾ Page < < 6 > >

Queued Samples

Point Region Invalid

#	Sample	Type
---	--------	------

51	☐	A8d1_bob	Region
----	--------------------------	----------	--------

55	☐	A1d1_bob	Point
----	--------------------------	----------	-------

Grid Scan ▾

Box Size 10 x 10

Ω Range 0

Energy 12658 ev

Transmission 20 %

Exposure 0.002 s

Resolution 2.8 Å

Beam Size 10 x 10

No. Images 600

Ω Start -30 °

Ω Range 0.1 °

Ω End 30 °

Energy 12658 ev

Transmission 100 %

Exposure 0.0014 s

Resolution 2.8 Å

Point Collection ▾

Point Collection ▾

Ω Start -30 °

Ω Range 0.1 °

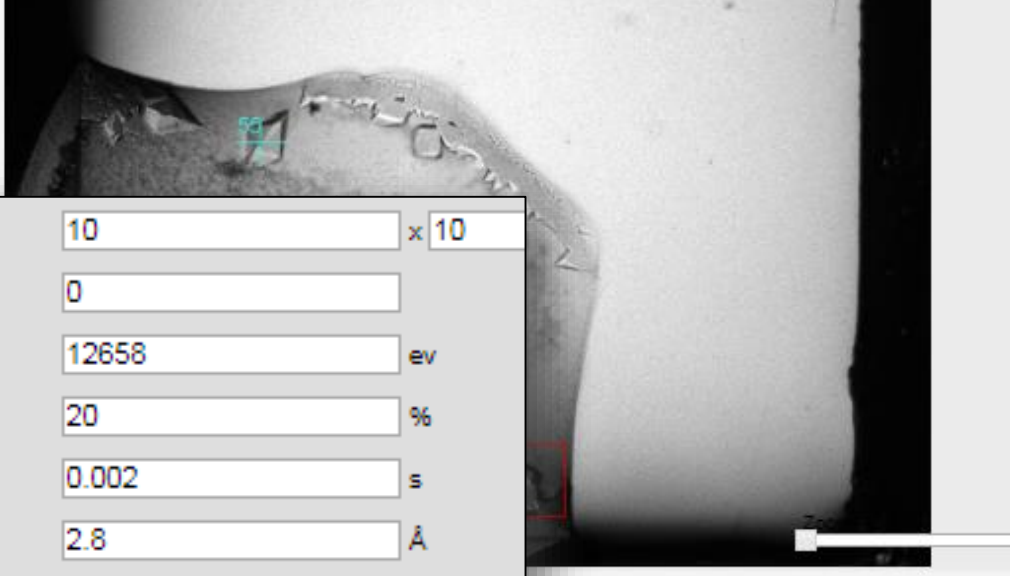
Ω End 30 °

Energy 12658 ev

Transmission 100 %

Exposure 0.0014 s

Resolution 2.8 Å

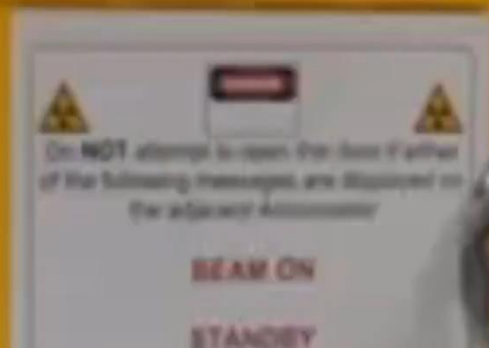
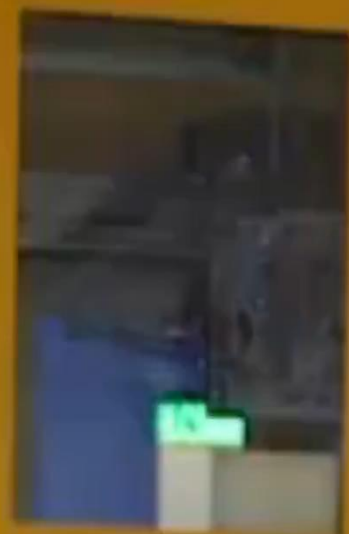


Presets: Point1 ▾

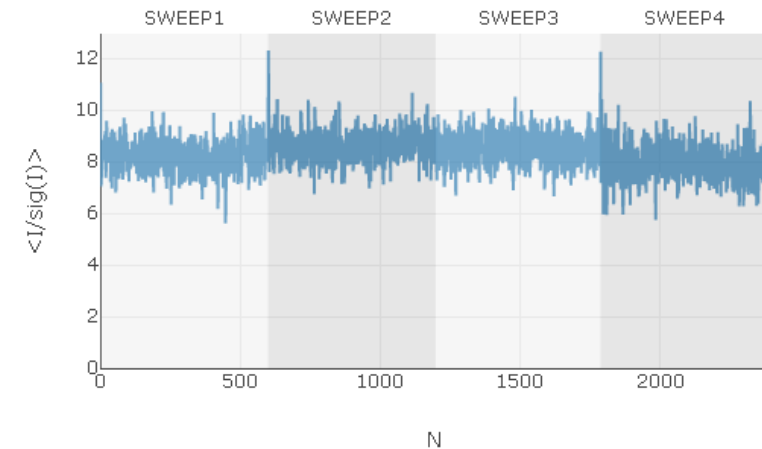
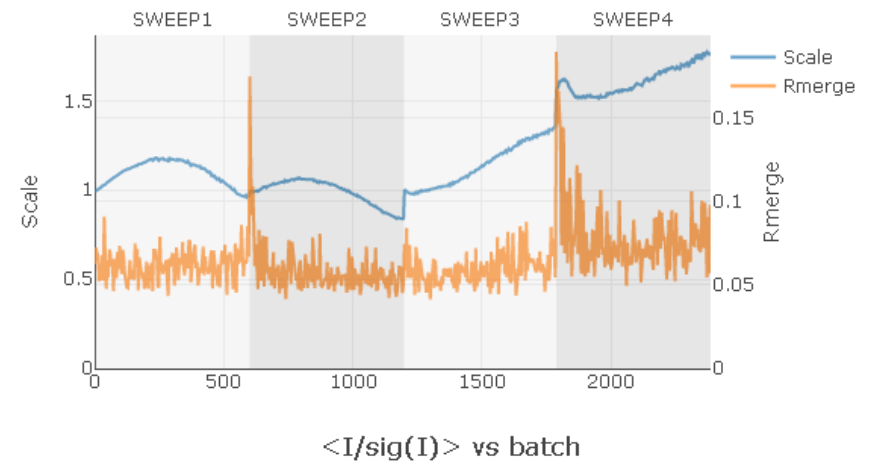
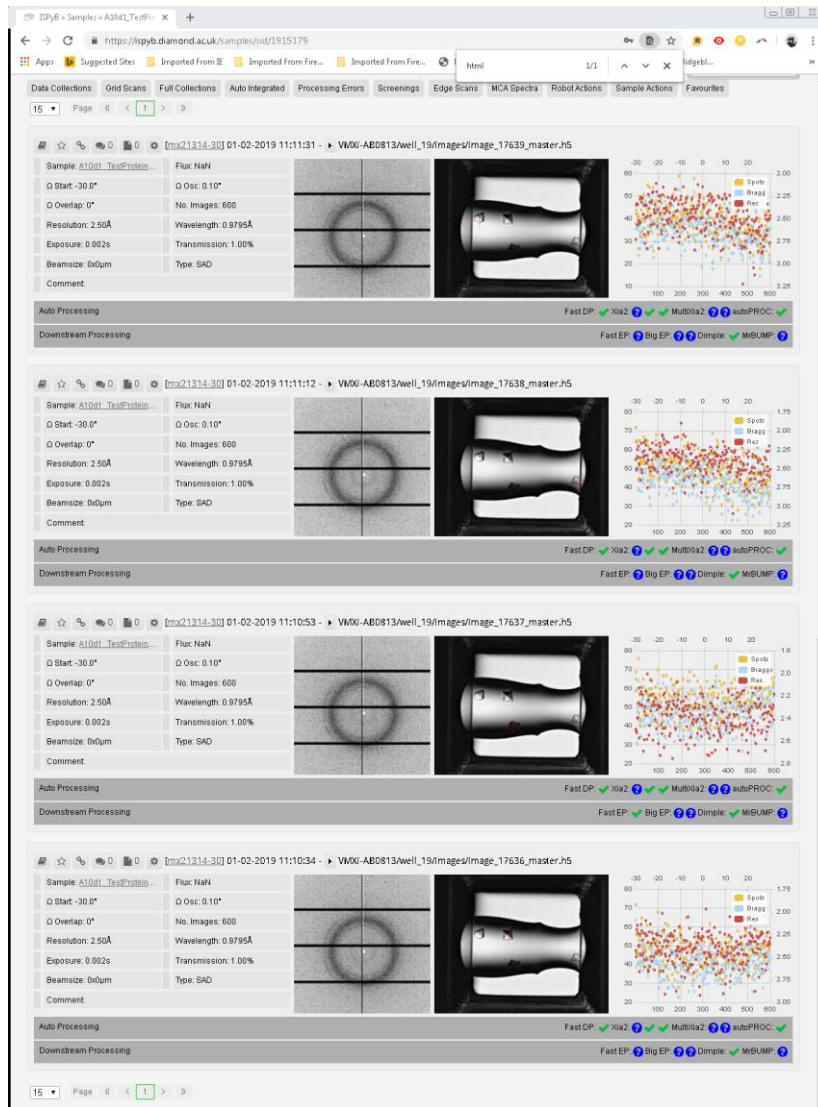
Valid

✓ + -

✓ + -

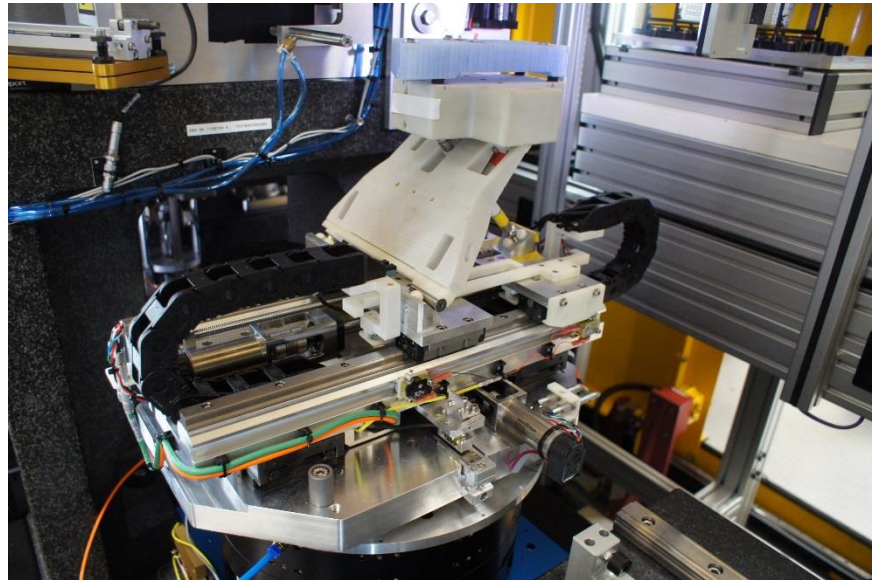


Multiple oscillation datasets



Future updates (Goniometer)

Present



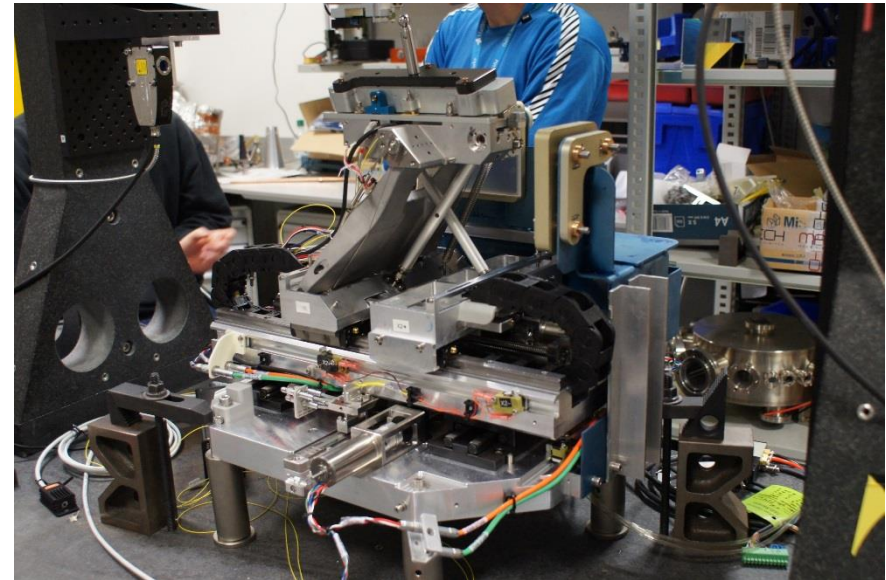
Fast (up to 100mm/s for global positioning)
Accurate with dynamic grid scans up to 1mm/s
Repeatable

~10 microns across the plate
>2 micron within a well

No tilt

No safety sensors

Future



Fast (up to 100mm/s for global positioning)
Expected good accuracy with grid scans up to 5-10mm/s
Expected to be repeatable

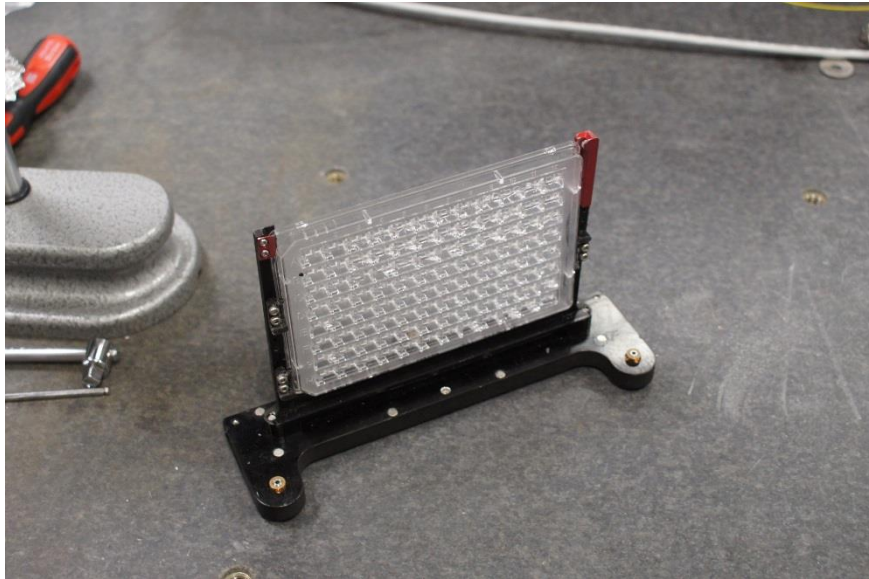
~1 microns across the plate
>0.5 micron within a well

30 degree tilt

Safety sensors to prevent collisions during sample loading

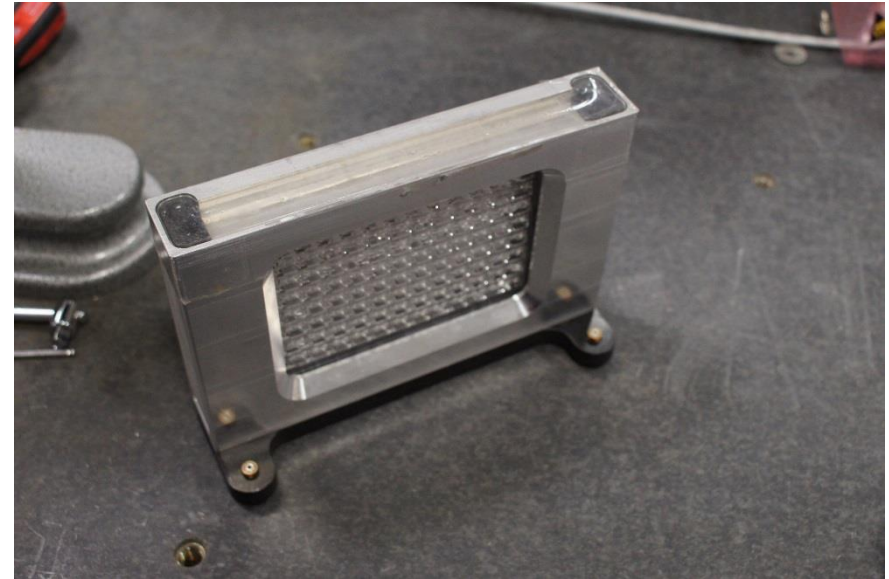
Future updates (4C plate handling)

Present 20°C



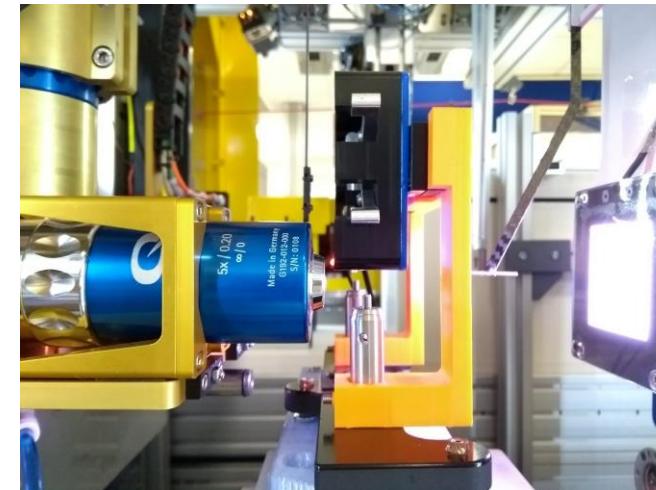
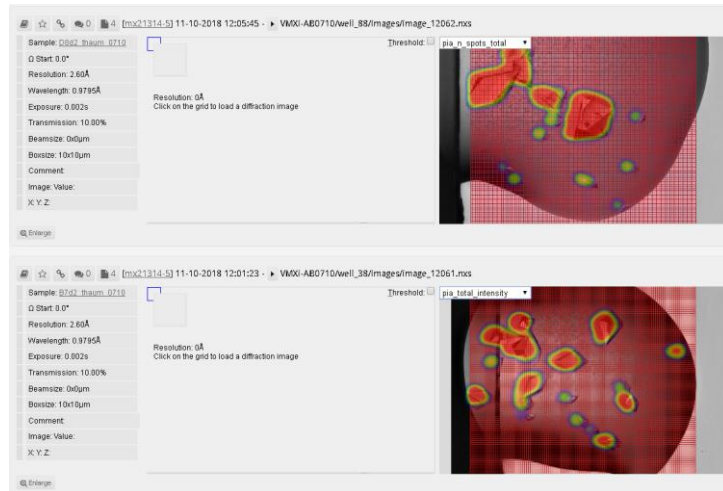
Tested substantially and working reliably

Future 4°C

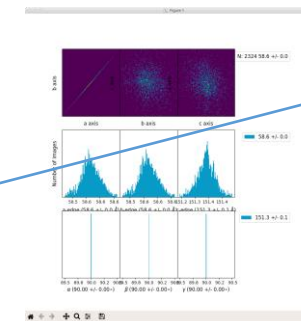
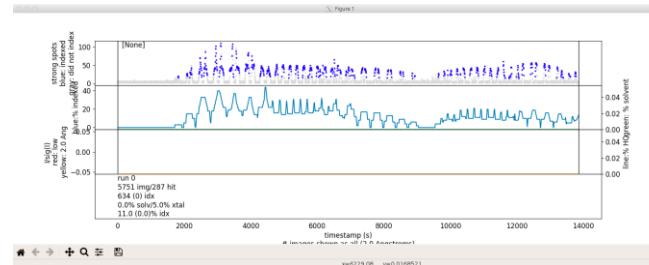


Based on passive cooling using water
Should maintain a plate ~4C for 20-30 minutes
Requires major software improvements and testing

Currently implementing Serial MX at VMXi



Multi grid data processing
LCP jets
Acoustic droplet ejection
Single shot (DMM) data collection



	Thaumatin – Grid scan
Resolution (Å)	54.63 – 2.5 (2.543-2.5)
Space group	P 4 ₁ 2 ₁ 2
Unit cell a,b,c (Å)	58.58, 58.58, 151.34
Unit cell alpha, beta, gamma (°)	90.0, 90.0, 90.0
CC _{1/2} (%)	53.8 (28.3)
Completeness (%)	95.85 (75.00)
I/sigma	25.34 (5.72)
Multiplicity	70.37 (12.25)
Number of integrated images	10617
R _{split}	44.5 (81.4)
Total reflections	695771 (5830)
Unique reflections	9478 (357)

VMXi the “best” beamline
you’ll never want to go to.



Juan Sanchez-Weatherby
James Sandy
Halina Mikolajek