ISPYB / MX CUBE JANUARY 2018

PRESENTATION OF PROCESSING AND REPROCESSING RESULTS AT DLS

OVERVIEW

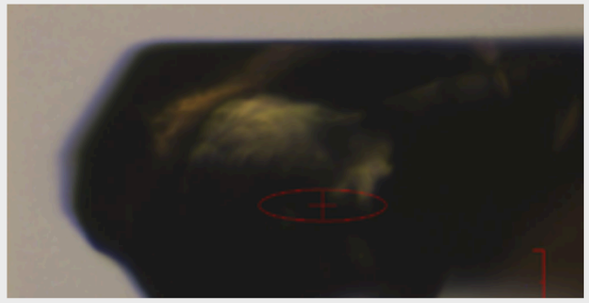
- Interactions of user with SynchWeb
- Auto-processing results
- Reprocessing - creating job, submission, results

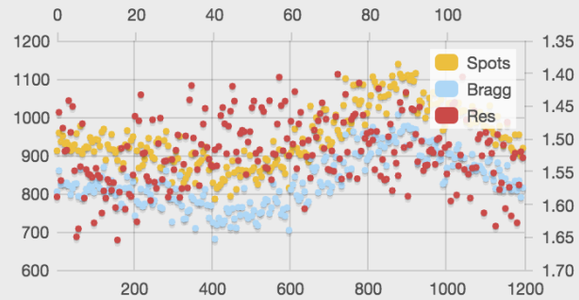
AUTO PROCESSING - REPORT

0 1 17-01-2018 12:59:52 - 2018_01_17/rot_calib/thau/thau_1/thau_1_3_####.cbf

Sample: thau_1	Flux: 1.49e+11
Ω Start: 0.0°	Ω Osc: 0.10°
Ω Overlap: 0°	No. Images: 1200
ϕ: 45° χ: 45°	Resolution: 1.80Å
Wavelength: 0.9762Å	Exposure: 0.050s
Transmission: 9.99%	Beamsize: 80x20µm
Type: SAD	

Comment: (-354,-1827,-391) (-67,-162,-272) Aperture: Large dials.align_crystalAperture: Large





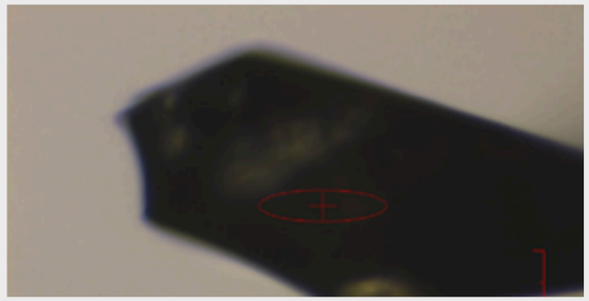
Auto Processing — Fast DP: ✔ Xia2: ✔ ✔ ✔ MultiXia2: ✔ ✔ autoPROC: ✔

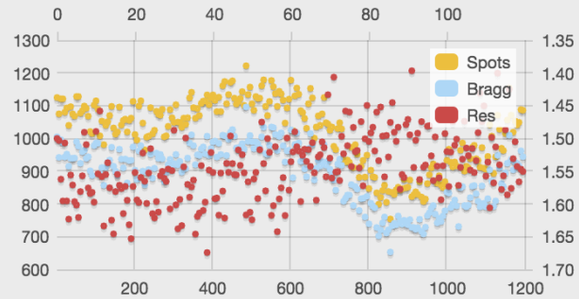
Downstream Processing — Fast EP: ✔ Big EP: ? ? Dimple: ? MrBUMP: ✘

0 1 17-01-2018 12:57:58 - 2018_01_17/rot_calib/thau/thau_1/thau_1_2_####.cbf

Sample: thau_1	Flux: 1.50e+11
Ω Start: 0.0°	Ω Osc: 0.10°
Ω Overlap: 0°	No. Images: 1200
ϕ: 0° χ: 45°	Resolution: 1.80Å
Wavelength: 0.9762Å	Exposure: 0.050s
Transmission: 9.99%	Beamsize: 80x20µm
Type: SAD	

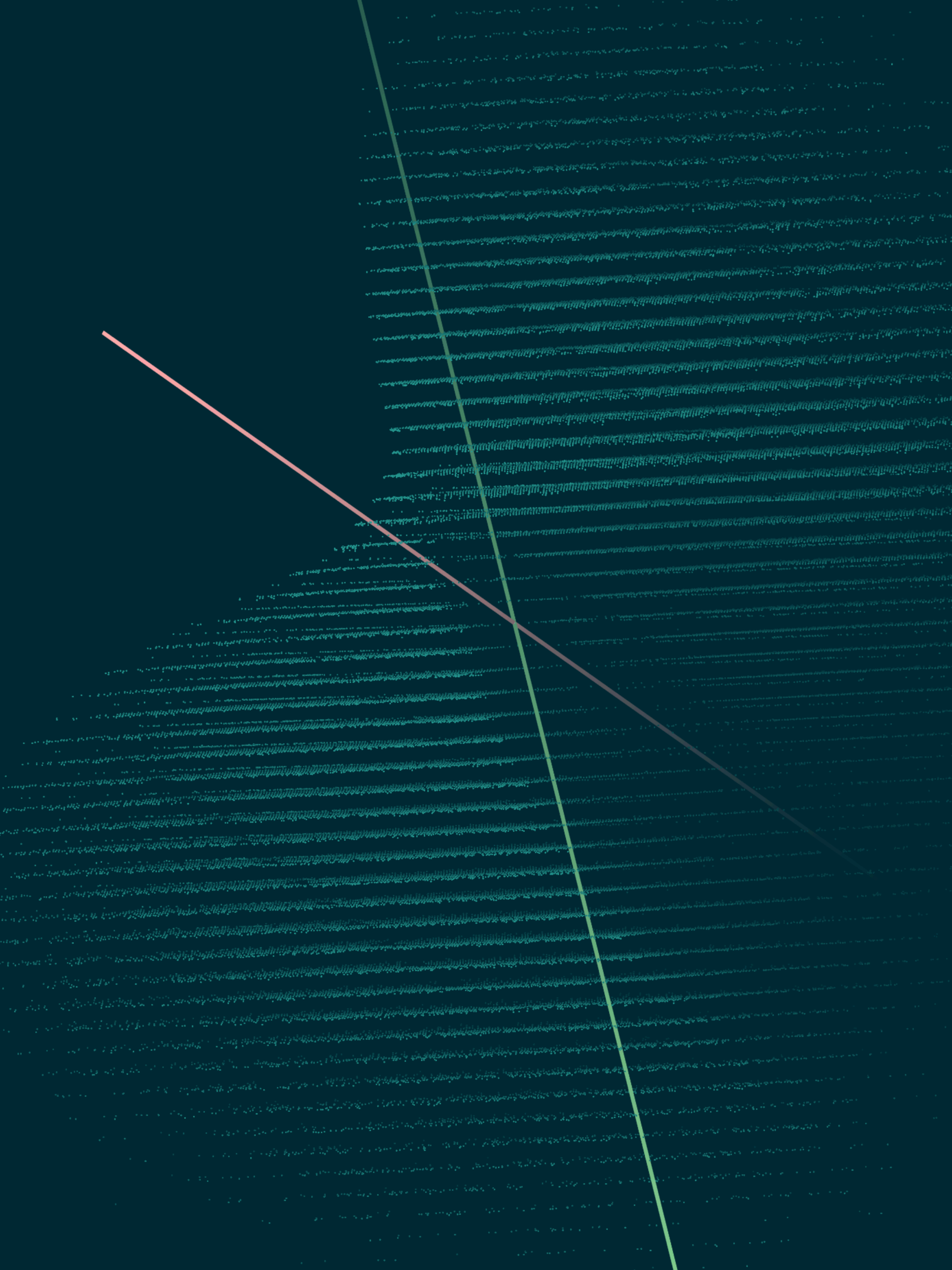
Comment: (-606,-1604,-483) (-67,-162,-272) Aperture: Large dials.align_crystalAperture: Large





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

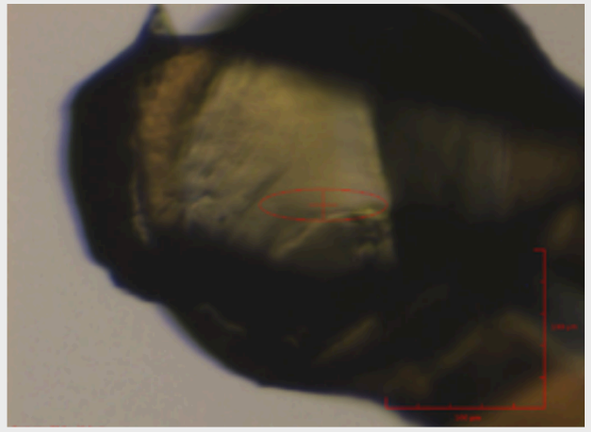
Downstream Processing — Fast EP: ✔ Big EP: ? ? Dimple: ? MrBUMP: ✘

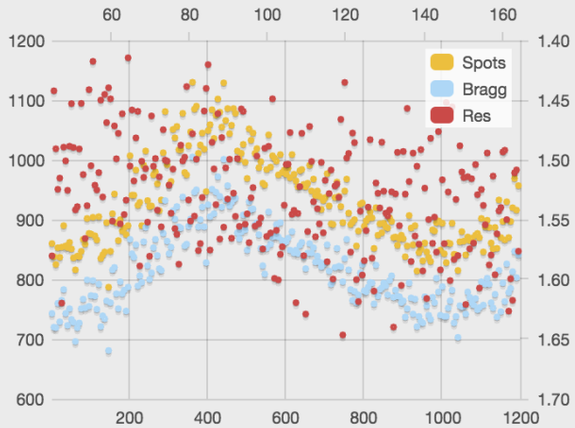


DETAILS

0 1 17-01-2018 13:01:27 - 2018_01_17/rot_calib/thau/thau_1/thau_1_4_####.cbf

Sample: thau_1	Flux: 1.51e+11
Ω Start: 45.0°	Ω Osc: 0.10°
Ω Overlap: 0°	No. Images: 1200
ϕ: 45° χ: 45°	Resolution: 1.80Å
Wavelength: 0.9762Å	Exposure: 0.050s
Transmission: 9.99%	Beamsize: 80x20μm
Type: SAD	
Comment: (-354,-1827,-391) (-67,-162,-272) Aperture: Large dials.align_crystalAperture: Large	





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

Fast DP | XIA2 3d | XIA2 3dii | XIA2 DIALS | autoPROC | XIA2 DIALS | XIA2 3dii

Plots | MTZ file | Log file | Archive | Lookup Cell

Beam Centre	X	Y
Start	211.42	206.11
Refined	211.40	206.05
Δ	0.02	0.06

Space Group	A	B	C	α	β	γ
P 41 21 2	57.80	57.80	150.37	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	1030	671	1.35 - 1.38	0.315	1.5	0.9	24.2	1.5	3.5	1.4	0.0
innerShell	94944	3146	3.68 - 57.85	0.043	63.1	1.0	100.0	30.2	100.0	17.8	-0.0
overall	1147174	51350	1.35 - 57.80	0.069	26.0	1.0	91.0	22.3	86.1	12.2	-0.1

Downstream Processing — Fast EP: ✔ Big EP: ? ? Dimple: ? MrBUMP: ✘

DETAILS

0 1 17-01-2018

Sample: thau_1

Ω Start: 45.0°

Ω Overlap: 0°

ϕ: 45° χ: 45°

Wavelength: 0.9762Å

Transmission: 9.99%

Type: SAD

Comment: (-354,-1827,-391) (-67,-162,-272) A
Large

Auto Processing

Fast DP | XIA2 3d | XIA2 3dii | XIA2 DIALS | autoPROC

Beam Centre	X	Y
Start	211.42	206.11
Refined	211.40	206.05
Δ	0.02	0.06

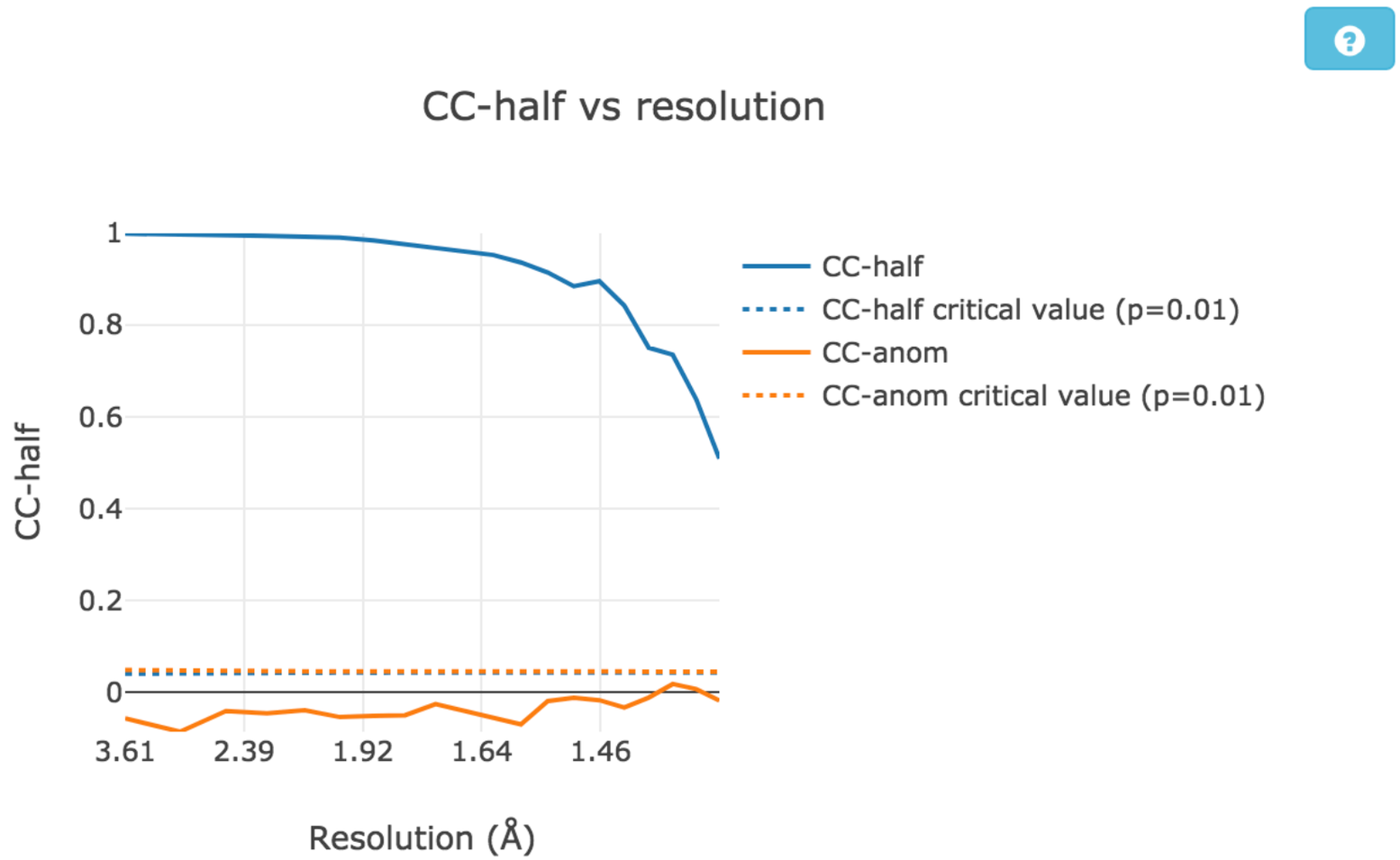
Space Group	A	B	C	α	
P 41 21 2	57.80	57.80	150.37	90.00	9

Shell	Observations	
outerShell	1030	6
innerShell	94944	3
overall	1147174	5

Downstream Processing

Analysis plots

Analysis by resolution



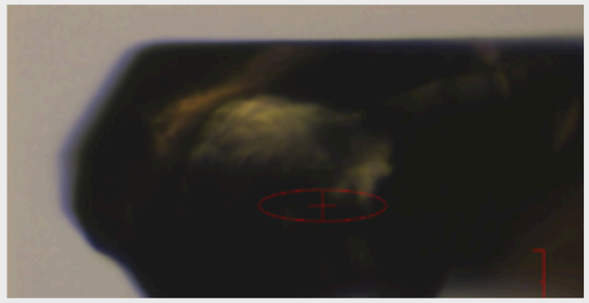
<I/sig(I)> vs resolution

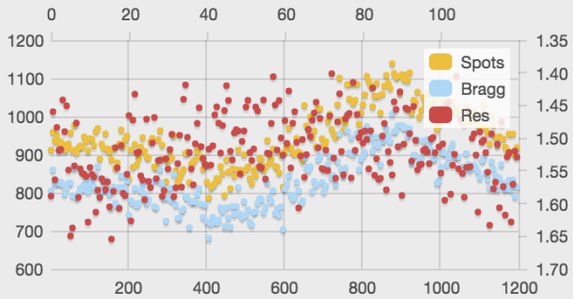
REPROCESSING

0 1 17-01-2018 12:59:52 - 2018_01_17/rot_calib/thau/thau_1/thau_1_3_####.cbf

Sample: thau_1	Flux: 1.49e+11
Ω Start: 0.0°	Ω Osc: 0.10°
Ω Overlap: 0°	No. Images: 1200
ϕ: 45° χ: 45°	Resolution: 1.80Å
Wavelength: 0.9762Å	Exposure: 0.050s
Transmission: 9.99%	Beamsize: 80x20μm
Type: SAD	

Comment: (-354,-1827,-391) (-67,-162,-272) Aperture: Large dials.align_crystalAperture: Large





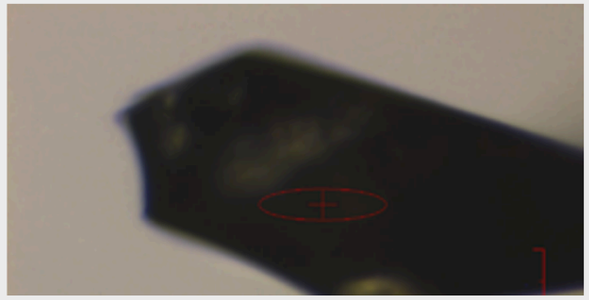
Auto Processing — Fast DP: ✔ Xia2: ✔ ✔ ✔ MultiXia2: ✔ ✔ autoPROC: ✔

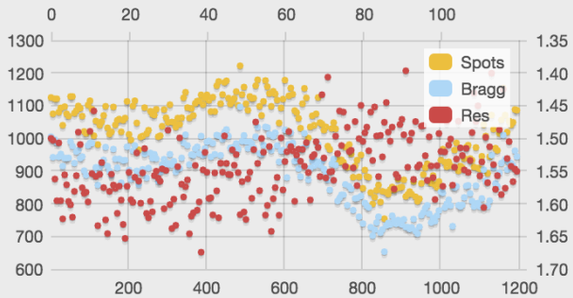
Downstream Processing — Fast EP: ✔ Big EP: ? ? Dimple: ? MrBUMP: ✘

0 1 17-01-2018 12:57:58 - 2018_01_17/rot_calib/thau/thau_1/thau_1_2_####.cbf

Sample: thau_1	Flux: 1.50e+11
Ω Start: 0.0°	Ω Osc: 0.10°
Ω Overlap: 0°	No. Images: 1200
ϕ: 0° χ: 45°	Resolution: 1.80Å
Wavelength: 0.9762Å	Exposure: 0.050s
Transmission: 9.99%	Beamsize: 80x20μm
Type: SAD	

Comment: (-606,-1604,-483) (-67,-162,-272) Aperture: Large dials.align_crystalAperture: Large

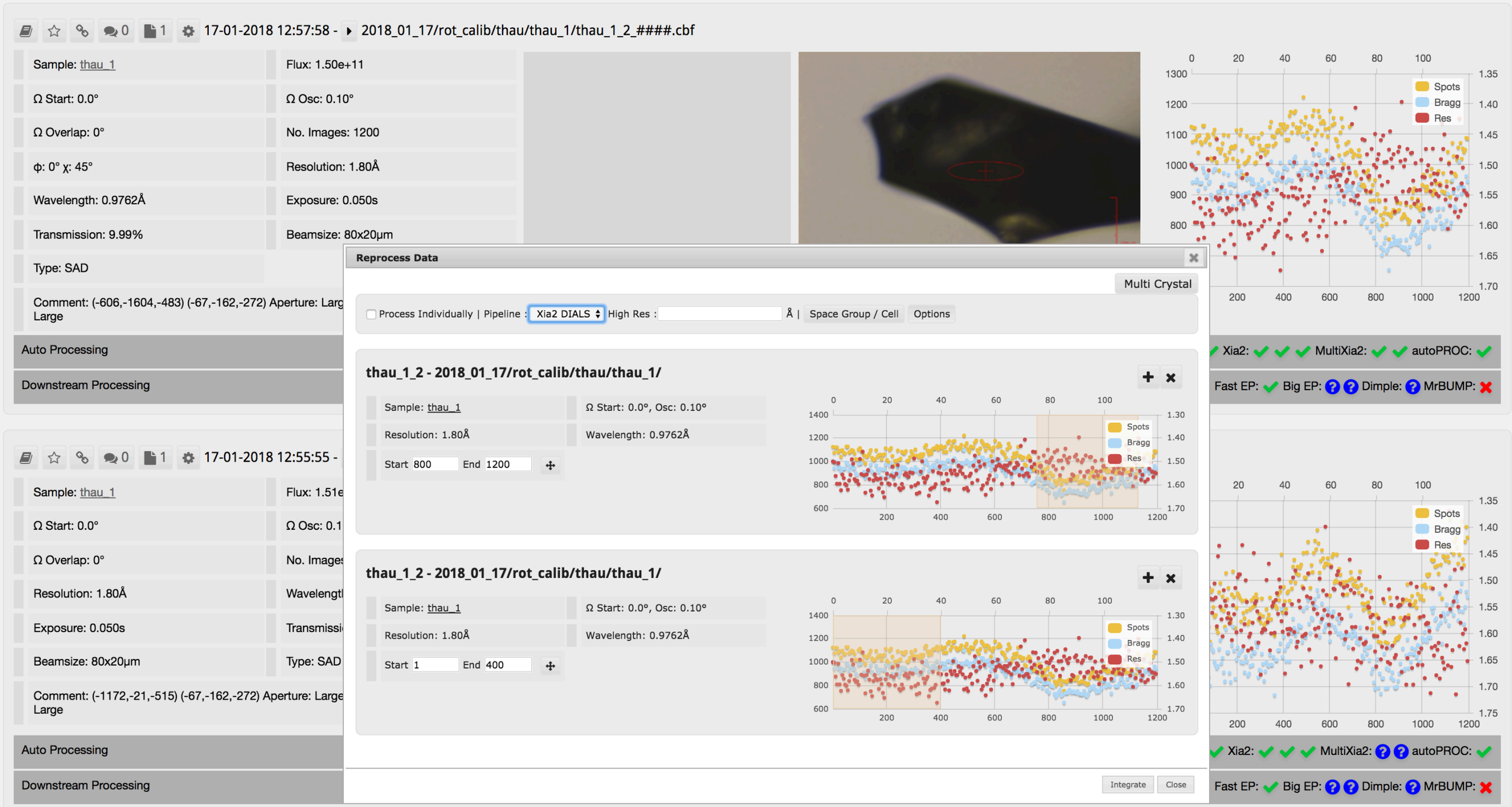




Auto Processing — Fast DP: ✔ Xia2: ✔ ✔ ✔ MultiXia2: ✔ ✔ autoPROC: ✔

Downstream Processing — Fast EP: ✔ Big EP: ? ? Dimple: ? MrBUMP: ✘

REPROCESSING



Reprocess Data

Multi Crystal

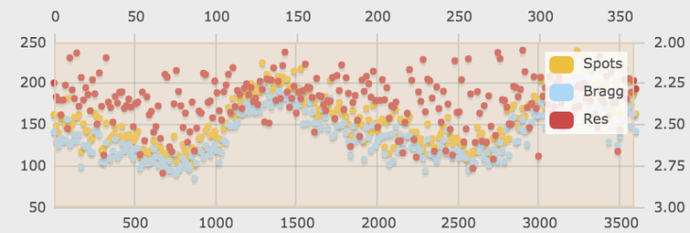
☐ Process Individually | Pipeline : Xia2 DIALS High Res : Å | Space Group / Cell Options

thau_1_8 - 2018_01_17/screen/thau/thau_1/

Sample: thau_1 | Ω Start: 0.0°, Osc: 0.10°

Resolution: 2.17Å | Wavelength: 1.7712Å

Start 1 End 3600

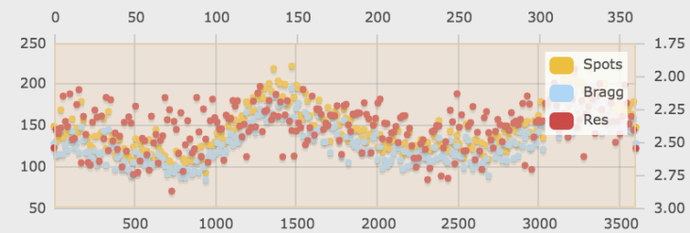


thau_1_7 - 2018_01_17/screen/thau/thau_1/

Sample: thau_1 | Ω Start: 0.0°, Osc: 0.10°

Resolution: 2.17Å | Wavelength: 1.7712Å

Start 1 End 3600

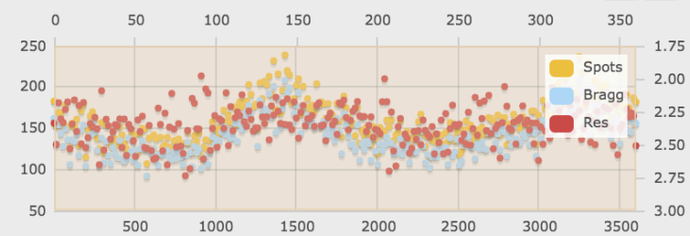


thau_1_6 - 2018_01_17/screen/thau/thau_1/

Sample: thau_1 | Ω Start: 0.0°, Osc: 0.10°

Resolution: 2.17Å | Wavelength: 1.7712Å

Start 1 End 3602

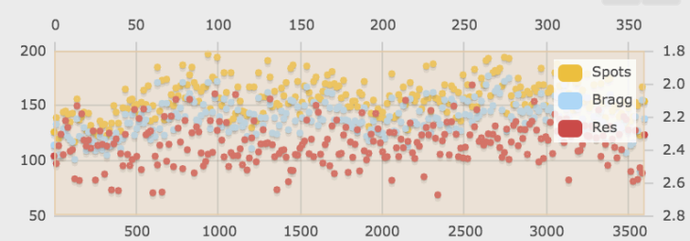


thau_1_5 - 2018_01_17/screen/thau/thau_1/

Sample: thau_1 | Ω Start: 0.0°, Osc: 0.10°

Resolution: 2.17Å | Wavelength: 1.7712Å

Start 1 End 3601

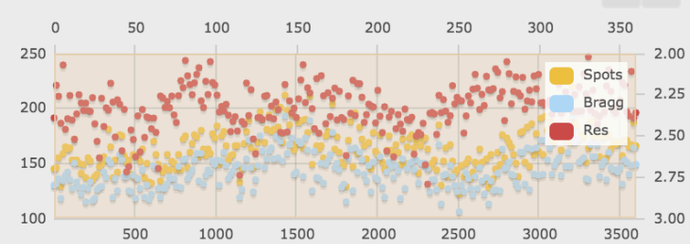


thau_1_4 - 2018_01_17/screen/thau/thau_1/

Sample: thau_1 | Ω Start: 0.0°, Osc: 0.10°

Resolution: 2.17Å | Wavelength: 1.7712Å

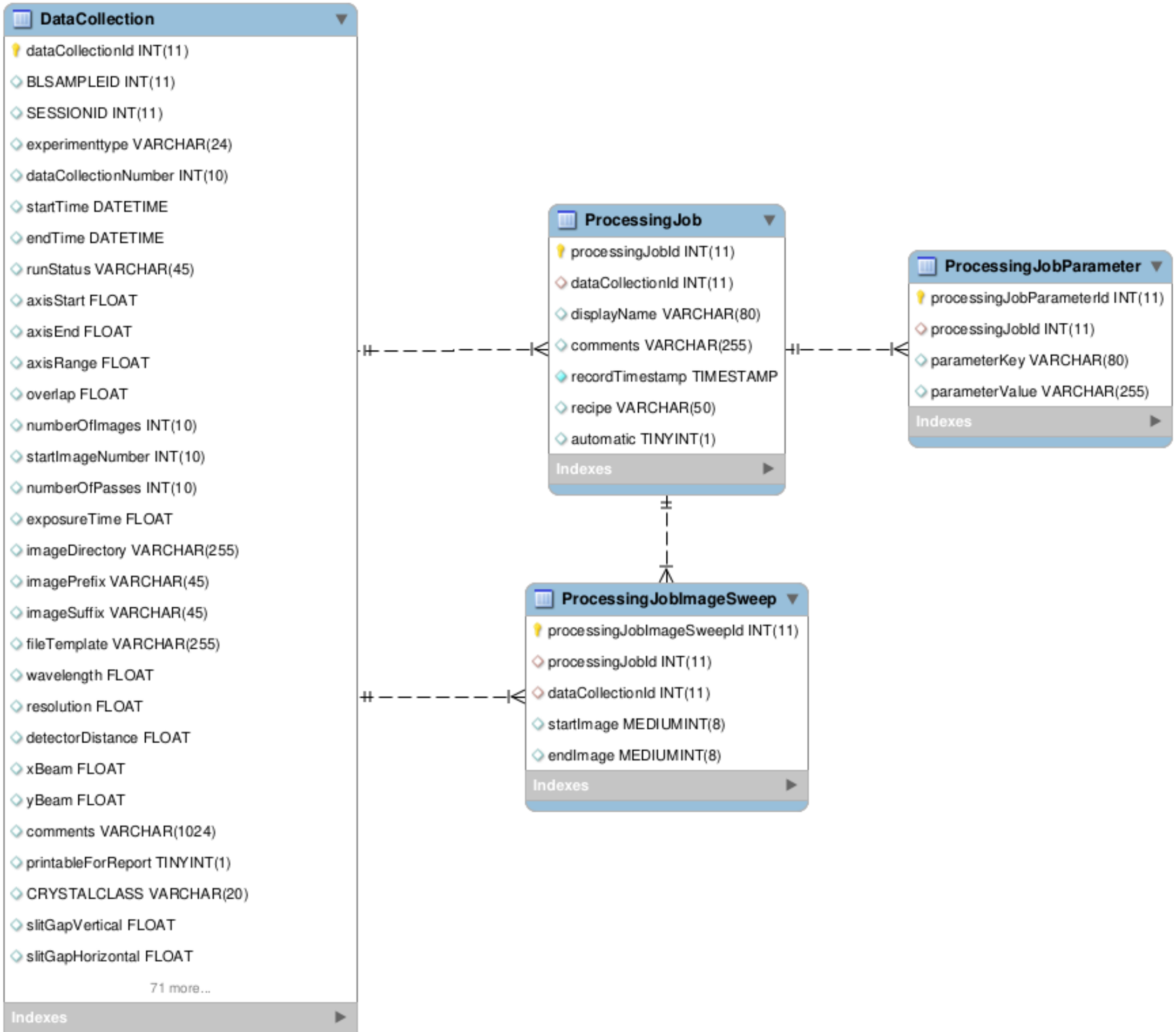
Start 1 End 3602



CREATE REPROCESSING JOB

- 1 entry in ProcessingJob (describing the job)
- 1 or more entries in ProcessingJobImageSweep (selecting data to be used for the job)
- 0 or more entries in ProcessingJobParameter (arbitrary key/value pairs)

in the database, plus sending a trigger message to ActiveMQ which references the ProcessingJob row.


DataCollection
dataCollectionId INT(11)
BLSAMPLEID INT(11)
SESSIONID INT(11)
experimenttype VARCHAR(24)
dataCollectionNumber INT(10)
startTime DATETIME
endTime DATETIME
runStatus VARCHAR(45)
axisStart FLOAT
axisEnd FLOAT
axisRange FLOAT
overlap FLOAT
numberOfImages INT(10)
startImageNumber INT(10)
numberOfPasses INT(10)
exposureTime FLOAT
imageDirectory VARCHAR(255)
imagePrefix VARCHAR(45)
imageSuffix VARCHAR(45)
fileTemplate VARCHAR(255)
wavelength FLOAT
resolution FLOAT
detectorDistance FLOAT
xBeam FLOAT
yBeam FLOAT
comments VARCHAR(1024)
printableForReport TINYINT(1)
CRYSTALCLASS VARCHAR(20)
slitGapVertical FLOAT
slitGapHorizontal FLOAT
71 more...
Indexes
ProcessingJob
processingJobId INT(11)
dataCollectionId INT(11)
displayName VARCHAR(80)
comments VARCHAR(255)
recordTimestamp TIMESTAMP
recipe VARCHAR(50)
automatic TINYINT(1)
Indexes
ProcessingJobParameter
processingJobParameterId INT(11)
processingJobId INT(11)
parameterKey VARCHAR(80)
parameterValue VARCHAR(255)
Indexes
ProcessingJobImageSweep
processingJobImageSweepId INT(11)
processingJobId INT(11)
dataCollectionId INT(11)
startImage MEDIUMINT(8)
endImage MEDIUMINT(8)
Indexes

TABLES

```
ProcessingJobImageSweep
  processingJobImageSweepId - Autoincrementing unique ID
  processingJobId - Job this entry belongs to
  dataCollectionId - because although a ProcessingJob is
                     already connected to one DCID, data
                     may come from other DCIDs as well
  startImage
  endImage

ProcessingJobParameter
  processingJobParameterId - Autoincrementing unique ID
  processingJobId - Job this entry belongs to
  parameterKey
  parameterValue
```

ISPyB database connector
GDA
DLS SciSoft status screen
File monitoring service
Live processing status viewer
Per-image-analysis
ActiveMQ Messaging Server
Live reciprocal lattice viewer
Spot finding service
Live diffraction image viewer
Indexing service
Process monitoring service
Data reduction service
Structure solution service

{
 "environment": {
   "ID": "38c1219c-8ae9-4b22-8e62-8fd5e1594194",
   "ispyb_autoprocprogram_id": 68626954
 },
 "recipe": {
   "1": {
     "output": [
       2
     ],
     "parameters": {
       "cmdline": "xia2 via zocalo",
       "environment": {},
       "ispyb_command": "register_processing",
       "program": "xia2-dials",
       "rpid": "4024",
       "store_result": "ispyb_autoprocprogram_id"
     },
     "queue": "ispyb_connector",
     "service": "DLS ISPyB connector"
   },
   "2": {
     "job_parameters": {
       "dcid": "2227029",
       "ispyb_parameters": {},
       "results_directory": "/dls/i03/data/2018/cm19644-1/processed/2018_01_17/
rot_calib/thau/thau_1/thau_1_2_/86449557-7045-44dd-8892-0ccff51815e4/ispyb-xia2-
dials",
       "timeout": null,
       "working_directory": "/dls/i03/data/2018/cm19644-1/tmp/zocalo/2018_01_17/
rot_calib/thau/thau_1/thau_1_2_/86449557-7045-44dd-8892-0ccff51815e4/ispyb-xia2-
dials",

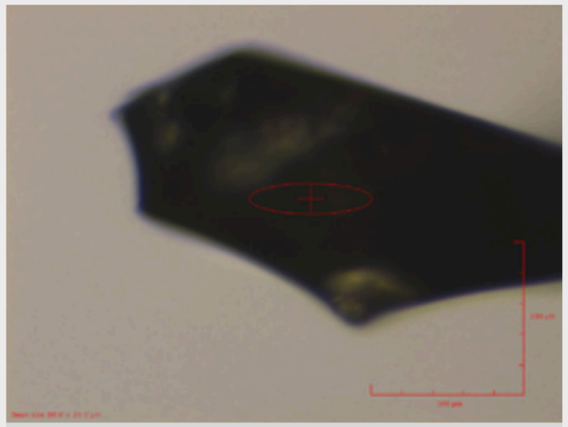
```
xia2 pipeline=dials min_images=3 failover=True \
project=AUTOMATIC crystal=DEFAULT read_all_image_headers=False atom=S \
image=/dls/../rot_calib/thau/thau_1/thau_1_2_0801.cbf:801:1200 \
image=/dls/../rot_calib/thau/thau_1/thau_1_2_0001.cbf:1:400 \
image=/dls/../rot_calib/thau/thau_1/thau_1_2_0401.cbf:401:800
```

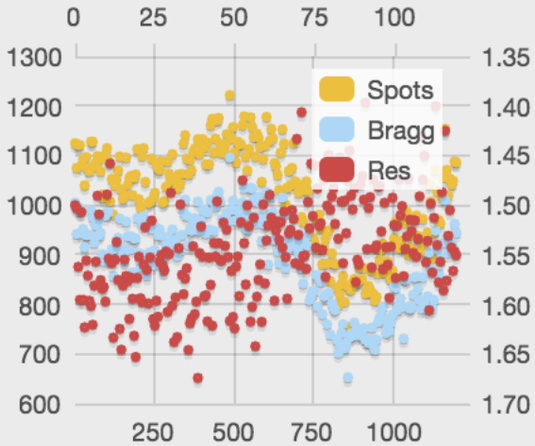
RESULTS

0 1 17-01-2018 12:57:58 - 2018_01_17/rot_calib/thau/thau_1/thau_1_2_####.cbf

Sample: thau_1	Flux: 1.50e+11
Ω Start: 0.0°	Ω Osc: 0.10°
Ω Overlap: 0°	No. Images: 1200
ϕ: 0° χ: 45°	Resolution: 1.80Å
Wavelength: 0.9762Å	Exposure: 0.050s
Transmission: 9.99%	Beamsize: 80x20μm
Type: SAD	

Comment: (-606,-1604,-483) (-67,-162,-272) Aperture: Large dials.align_crystalAperture: Large





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

Fast DP | XIA2 3d | XIA2 DIALS | XIA2 3dii | autoPROC | XIA2 3dii | XIA2 DIALS | xia2 via zocalo

Plots | MTZ file | Log file | Archive | Lookup Cell

Beam Centre	X	Y
Start	211.42	206.11
Refined	211.46	206.04
Δ	-0.04	0.07

Space Group	A	B	C	α	β	γ
P 41 21 2	57.82	57.82	150.55	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	703	512	1.36 - 1.38	0.348	1.4	0.8	18.7	1.4	2.7	1.2	0.0
innerShell	46837	3116	3.69 - 57.87	0.048	38.4	1.0	100.0	15.0	100.0	8.9	-0.2
overall	572636	49004	1.36 - 57.82	0.076	17.2	1.0	87.8	11.7	80.9	6.5	-0.3

Downstream Processing — Fast EP: ✔ Big EP: ? ? Dimple: ? MrBUMP: ✘