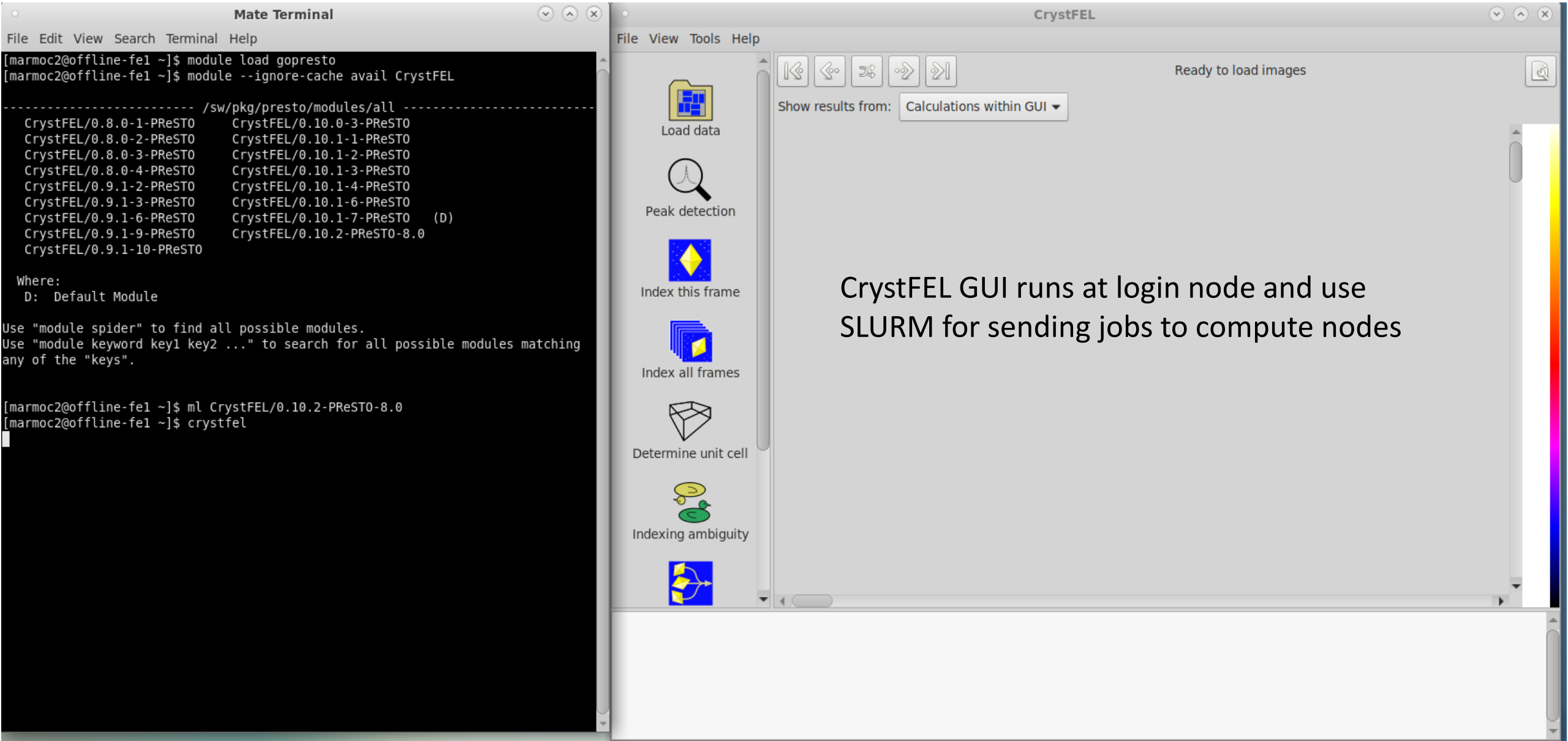
Test CrystFEL GUI version 0.10.2

MAX IV cluster April 2023

Check CrystFEL versions available and start CrystFEL GUI



Test data, 20 master-files, 400 containers

```
[marmoc2@offline-fe1 Lyz-HEC_1]$ pwd
/data/visitors/biomax/20190586/20221208/raw/Lyz/Lyz-HEC_1
[marmoc2@offline-fe1 Lyz-HEC_1]$ ls
Lyz-HEC_1_10_001_data_000001.h5  Lyz-HEC_1_11_001_data_000019.h5  Lyz-HEC_1_14_001_data_000016.h5  Lyz-HEC_1_17_001_data_000013.h5  Lyz-HEC_1_20_001_data_000010.h5  Lyz-HEC_1_4_001_data_000007.h5  Lyz-HEC_1_7_001_data_000004.h5
Lyz-HEC_1_10_001_data_000002.h5  Lyz-HEC_1_11_001_data_000020.h5  Lyz-HEC_1_14_001_data_000017.h5  Lyz-HEC_1_17_001_data_000014.h5  Lyz-HEC_1_20_001_data_000011.h5  Lyz-HEC_1_4_001_data_000008.h5  Lyz-HEC_1_7_001_data_000005.h5
Lyz-HEC_1_10_001_data_000003.h5  Lyz-HEC_1_11_001_master.h5      Lyz-HEC_1_14_001_data_000018.h5  Lyz-HEC_1_17_001_data_000015.h5  Lyz-HEC_1_20_001_data_000012.h5  Lyz-HEC_1_4_001_data_000009.h5  Lyz-HEC_1_7_001_data_000006.h5
Lyz-HEC_1_10_001_data_000004.h5  Lyz-HEC_1_12_001_data_000001.h5  Lyz-HEC_1_14_001_data_000019.h5  Lyz-HEC_1_17_001_data_000016.h5  Lyz-HEC_1_20_001_data_000013.h5  Lyz-HEC_1_4_001_data_000010.h5  Lyz-HEC_1_7_001_data_000007.h5
Lyz-HEC_1_10_001_data_000005.h5  Lyz-HEC_1_12_001_data_000002.h5  Lyz-HEC_1_14_001_data_000020.h5  Lyz-HEC_1_17_001_data_000017.h5  Lyz-HEC_1_20_001_data_000014.h5  Lyz-HEC_1_4_001_data_000011.h5  Lyz-HEC_1_7_001_data_000008.h5
Lyz-HEC_1_10_001_data_000006.h5  Lyz-HEC_1_12_001_data_000003.h5  Lyz-HEC_1_14_001_master.h5       Lyz-HEC_1_17_001_data_000018.h5  Lyz-HEC_1_20_001_data_000015.h5  Lyz-HEC_1_4_001_data_000012.h5  Lyz-HEC_1_7_001_data_000009.h5
Lyz-HEC_1_10_001_data_000007.h5  Lyz-HEC_1_12_001_data_000004.h5  Lyz-HEC_1_15_001_data_000001.h5  Lyz-HEC_1_17_001_data_000019.h5  Lyz-HEC_1_20_001_data_000016.h5  Lyz-HEC_1_4_001_data_000013.h5  Lyz-HEC_1_7_001_data_000010.h5
Lyz-HEC_1_10_001_data_000008.h5  Lyz-HEC_1_12_001_data_000005.h5  Lyz-HEC_1_15_001_data_000002.h5  Lyz-HEC_1_17_001_data_000020.h5  Lyz-HEC_1_20_001_data_000017.h5  Lyz-HEC_1_4_001_data_000014.h5  Lyz-HEC_1_7_001_data_000011.h5
Lyz-HEC_1_10_001_data_000009.h5  Lyz-HEC_1_12_001_data_000006.h5  Lyz-HEC_1_15_001_data_000003.h5  Lyz-HEC_1_17_001_master.h5       Lyz-HEC_1_20_001_data_000018.h5  Lyz-HEC_1_4_001_data_000015.h5  Lyz-HEC_1_7_001_data_000012.h5
Lyz-HEC_1_10_001_data_000010.h5  Lyz-HEC_1_12_001_data_000007.h5  Lyz-HEC_1_15_001_data_000004.h5  Lyz-HEC_1_18_001_data_000001.h5  Lyz-HEC_1_20_001_data_000019.h5  Lyz-HEC_1_4_001_data_000016.h5  Lyz-HEC_1_7_001_data_000013.h5
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Lyz-HEC_1_11_001_data_000013.h5  Lyz-HEC_1_14_001_data_000010.h5  Lyz-HEC_1_17_001_data_000007.h5  Lyz-HEC_1_20_001_data_000004.h5  Lyz-HEC_1_5_001_data_000001.h5   Lyz-HEC_1_6_001_data_000019.h5  Lyz-HEC_1_9_001_data_000016.h5
Lyz-HEC_1_11_001_data_000014.h5  Lyz-HEC_1_14_001_data_000011.h5  Lyz-HEC_1_17_001_data_000008.h5  Lyz-HEC_1_20_001_data_000005.h5  Lyz-HEC_1_5_001_data_000002.h5   Lyz-HEC_1_6_001_data_000020.h5  Lyz-HEC_1_9_001_data_000017.h5
Lyz-HEC_1_11_001_data_000015.h5  Lyz-HEC_1_14_001_data_000012.h5  Lyz-HEC_1_17_001_data_000009.h5  Lyz-HEC_1_20_001_data_000006.h5  Lyz-HEC_1_5_001_data_000003.h5   Lyz-HEC_1_6_001_master.h5       Lyz-HEC_1_9_001_data_000018.h5
Lyz-HEC_1_11_001_data_000016.h5  Lyz-HEC_1_14_001_data_000013.h5  Lyz-HEC_1_17_001_data_000010.h5  Lyz-HEC_1_20_001_data_000007.h5  Lyz-HEC_1_5_001_data_000004.h5   Lyz-HEC_1_7_001_data_000001.h5  Lyz-HEC_1_9_001_data_000019.h5
Lyz-HEC_1_11_001_data_000017.h5  Lyz-HEC_1_14_001_data_000014.h5  Lyz-HEC_1_17_001_data_000011.h5  Lyz-HEC_1_20_001_data_000008.h5  Lyz-HEC_1_5_001_data_000005.h5   Lyz-HEC_1_7_001_data_000002.h5  Lyz-HEC_1_9_001_data_000020.h5
Lyz-HEC_1_11_001_data_000018.h5  Lyz-HEC_1_14_001_data_000015.h5  Lyz-HEC_1_17_001_data_000012.h5  Lyz-HEC_1_20_001_data_000009.h5  Lyz-HEC_1_5_001_data_000006.h5   Lyz-HEC_1_7_001_data_000003.h5  Lyz-HEC_1_9_001_master.h5
[marmoc2@offline-fe1 Lyz-HEC_1]$
```
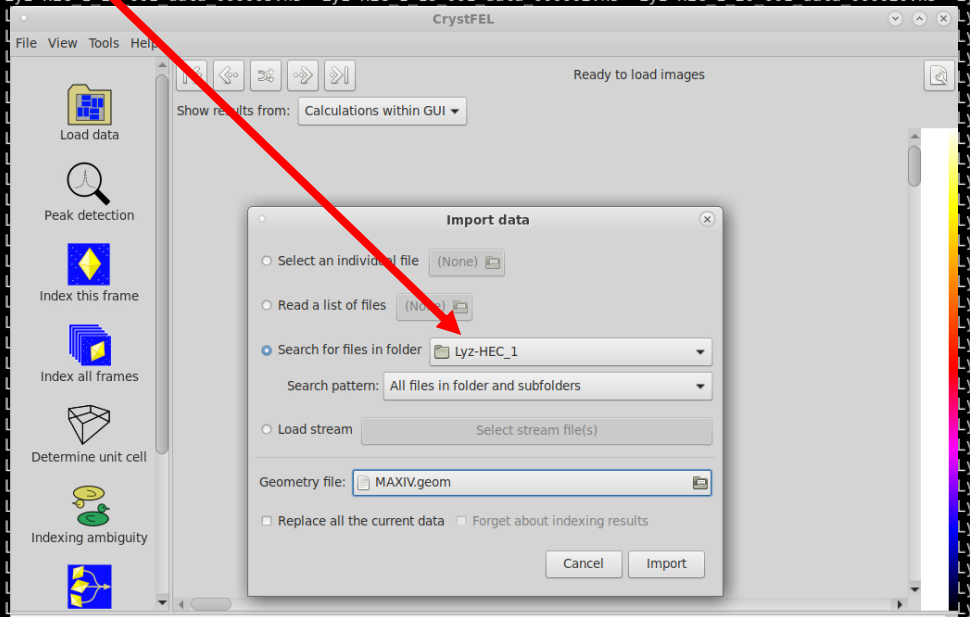
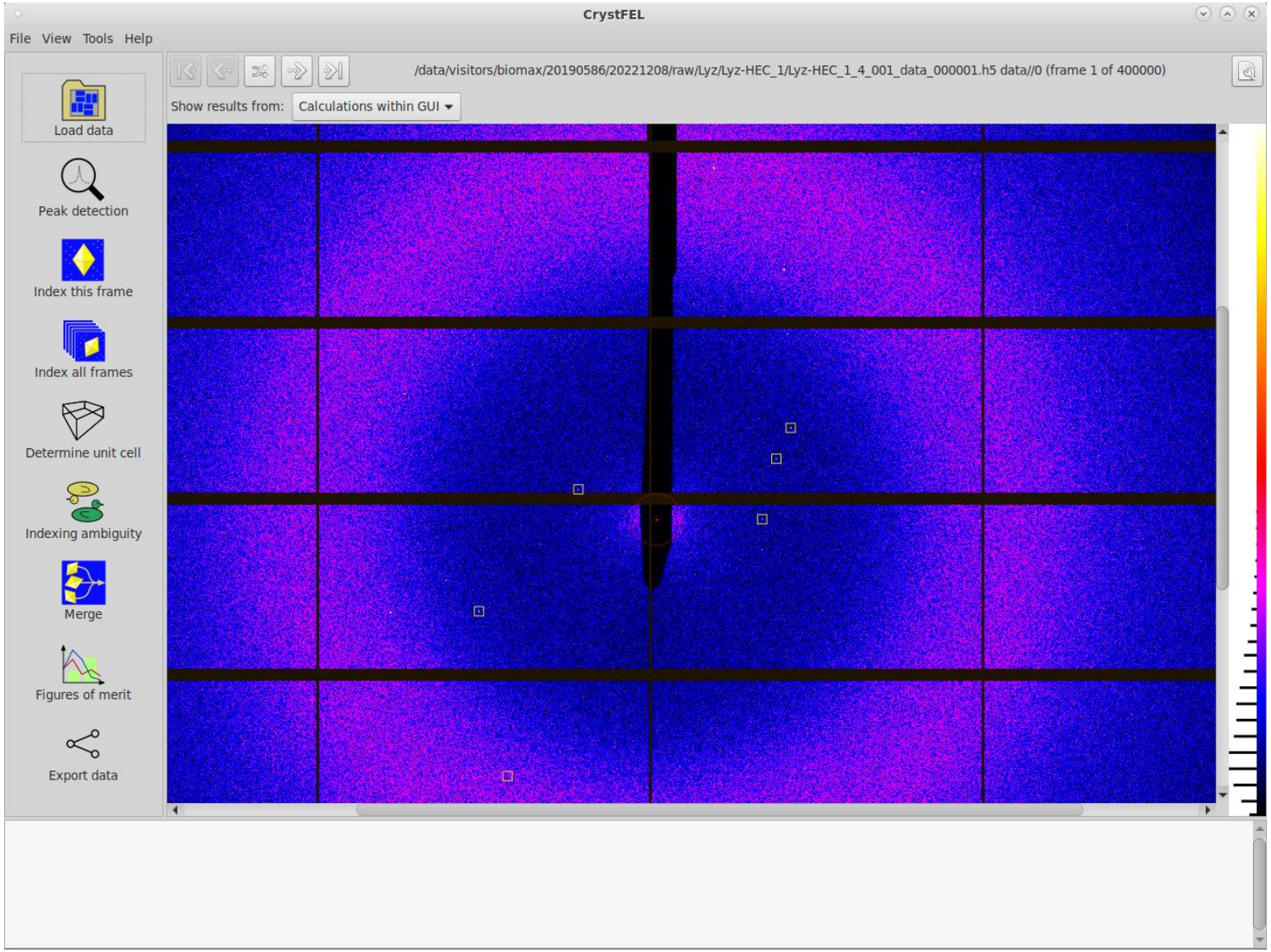
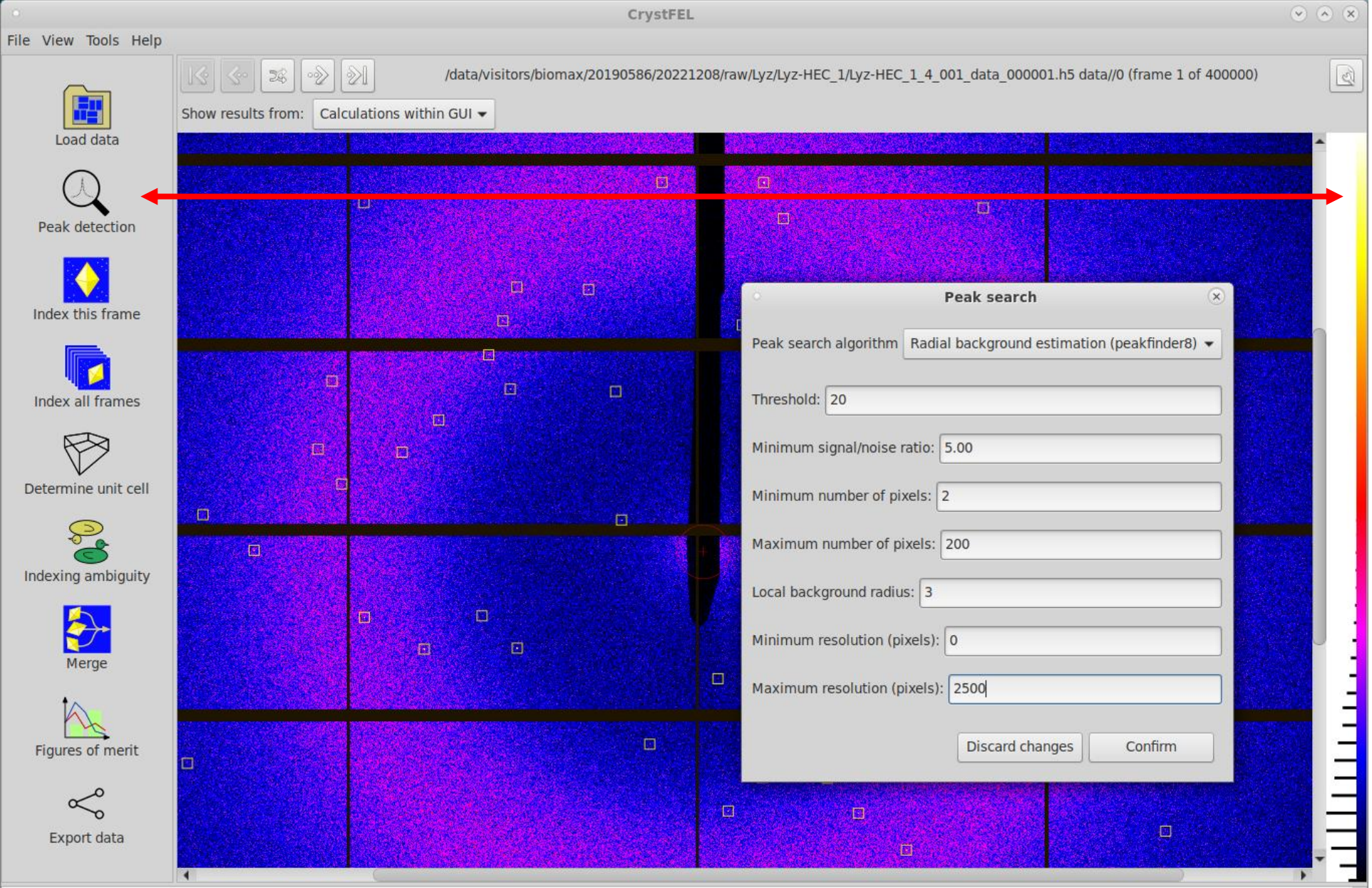



1. Use "*Search for files in folder*" option
2. Geometry file, *MAXIV.geom*, from MAX IV staff

Data is loaded, takes a minute or so…





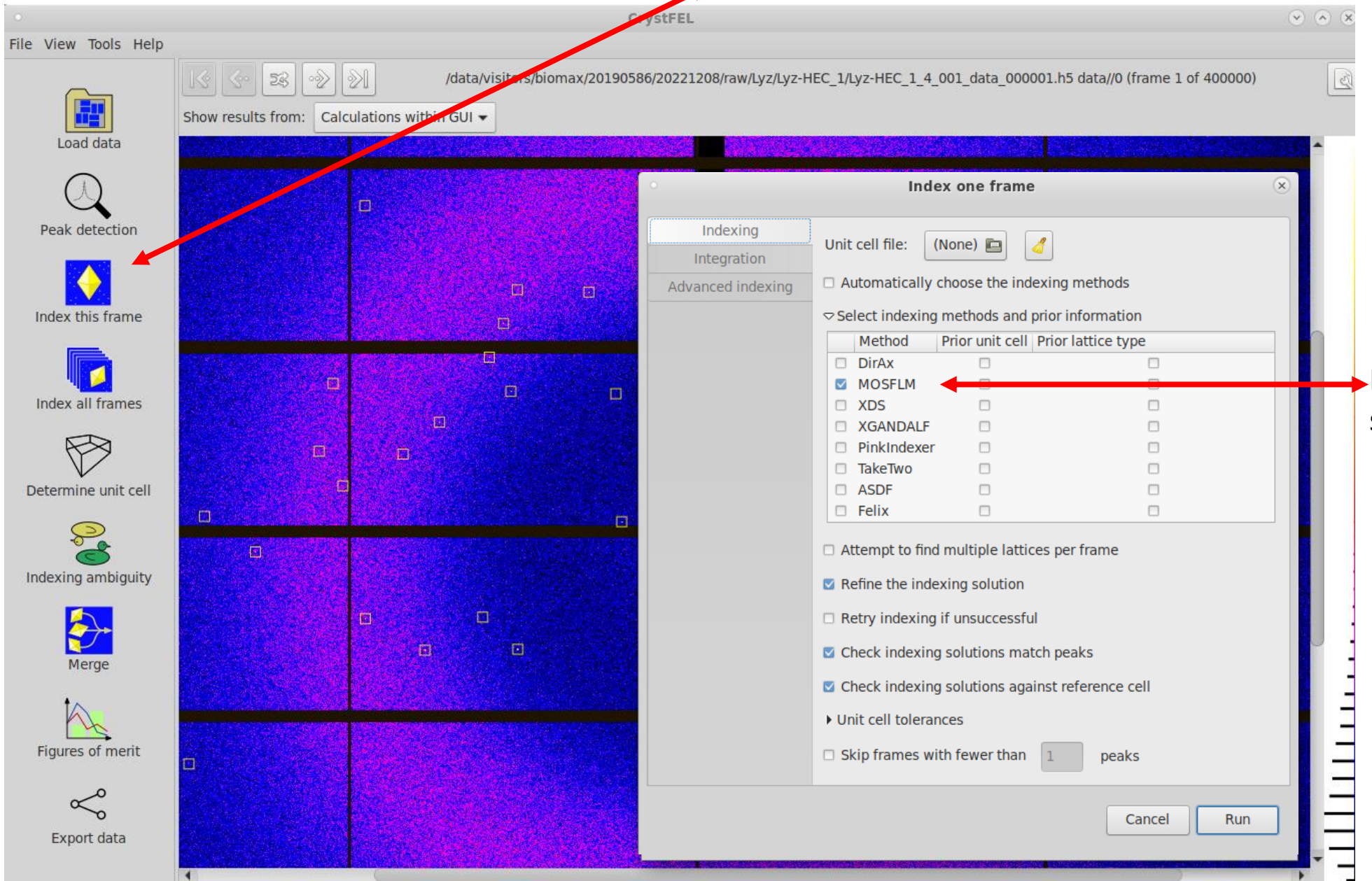
Peak detection

Peak search parameters are dataset specific so these test data parameters are ok for this dataset

We now have more peaks on frame1, compared to previous slide

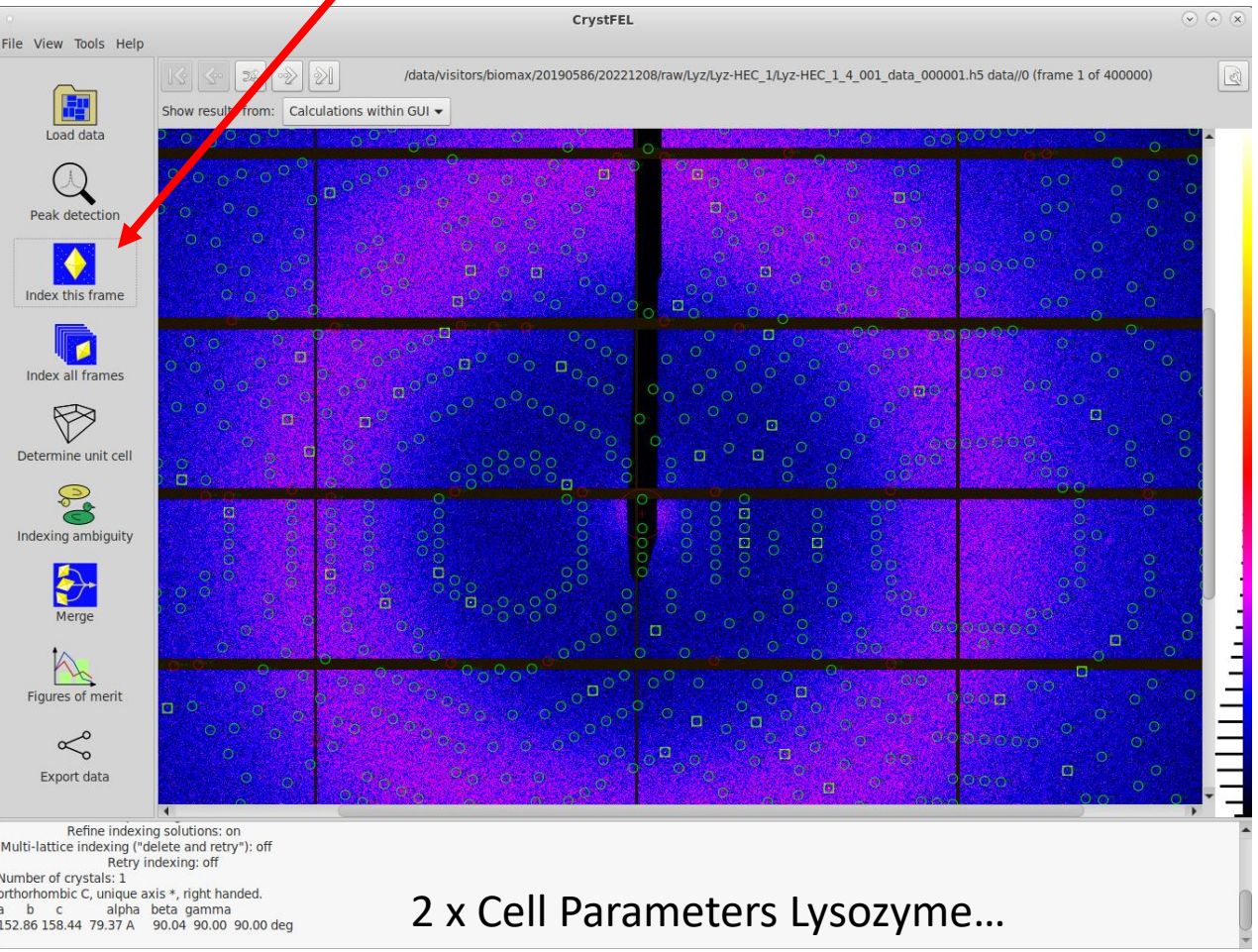
3. Set ”Peak search” parameters, dataset specific

Index this frame

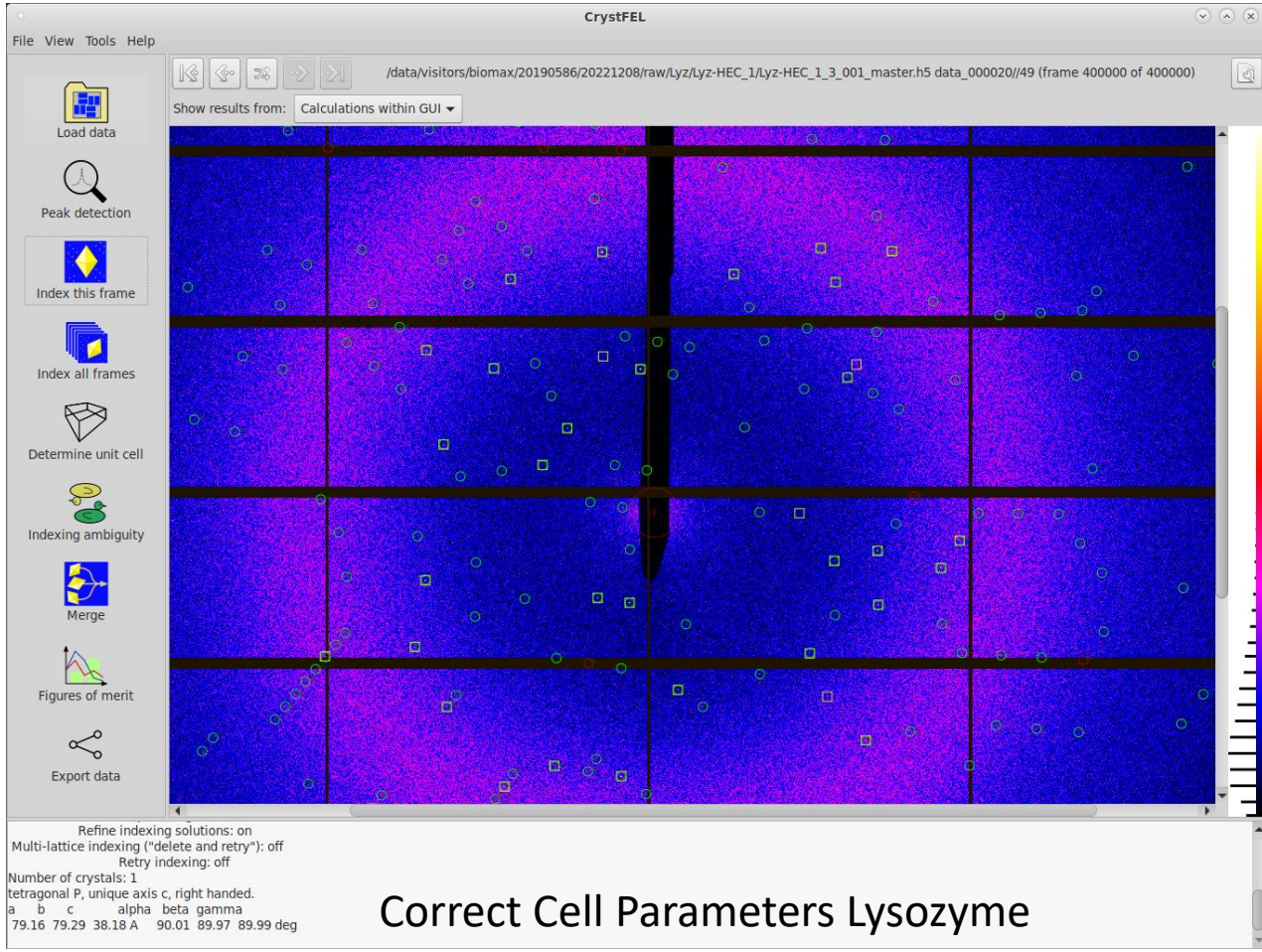


MOSFLM option selected

Index this frame, frame1 (left) frame 400000 (right)

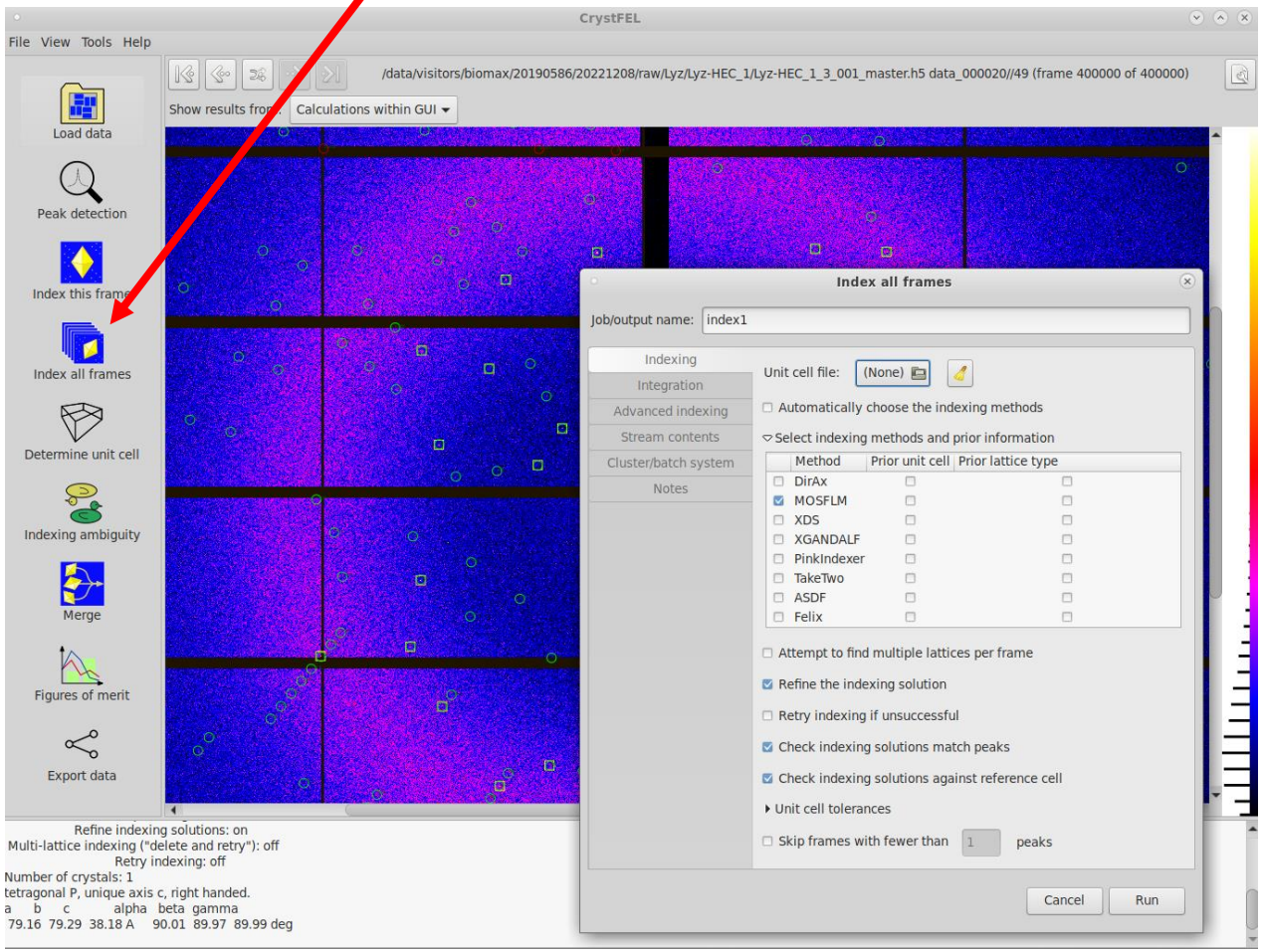


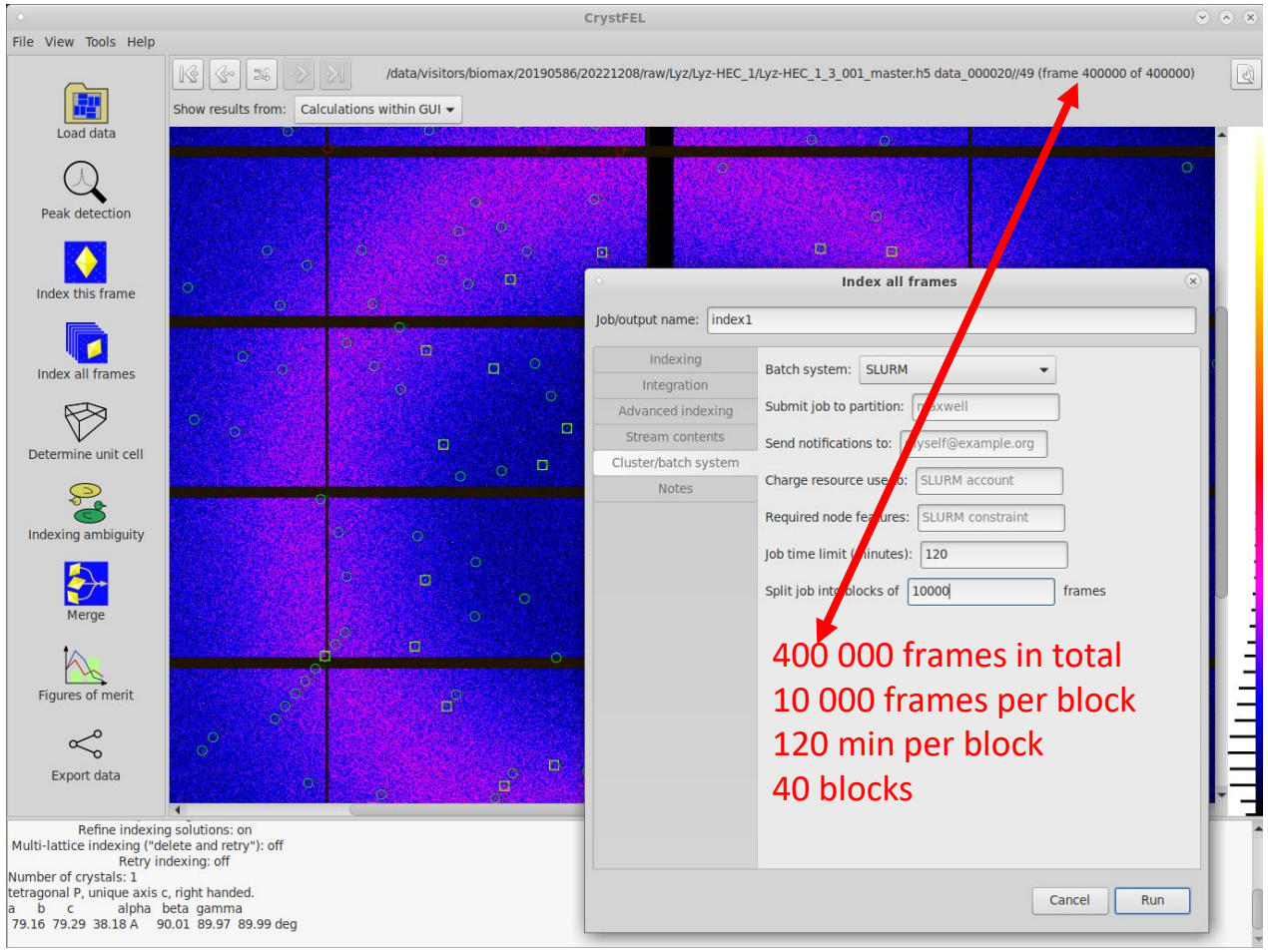
2 x Cell Parameters Lysozyme…



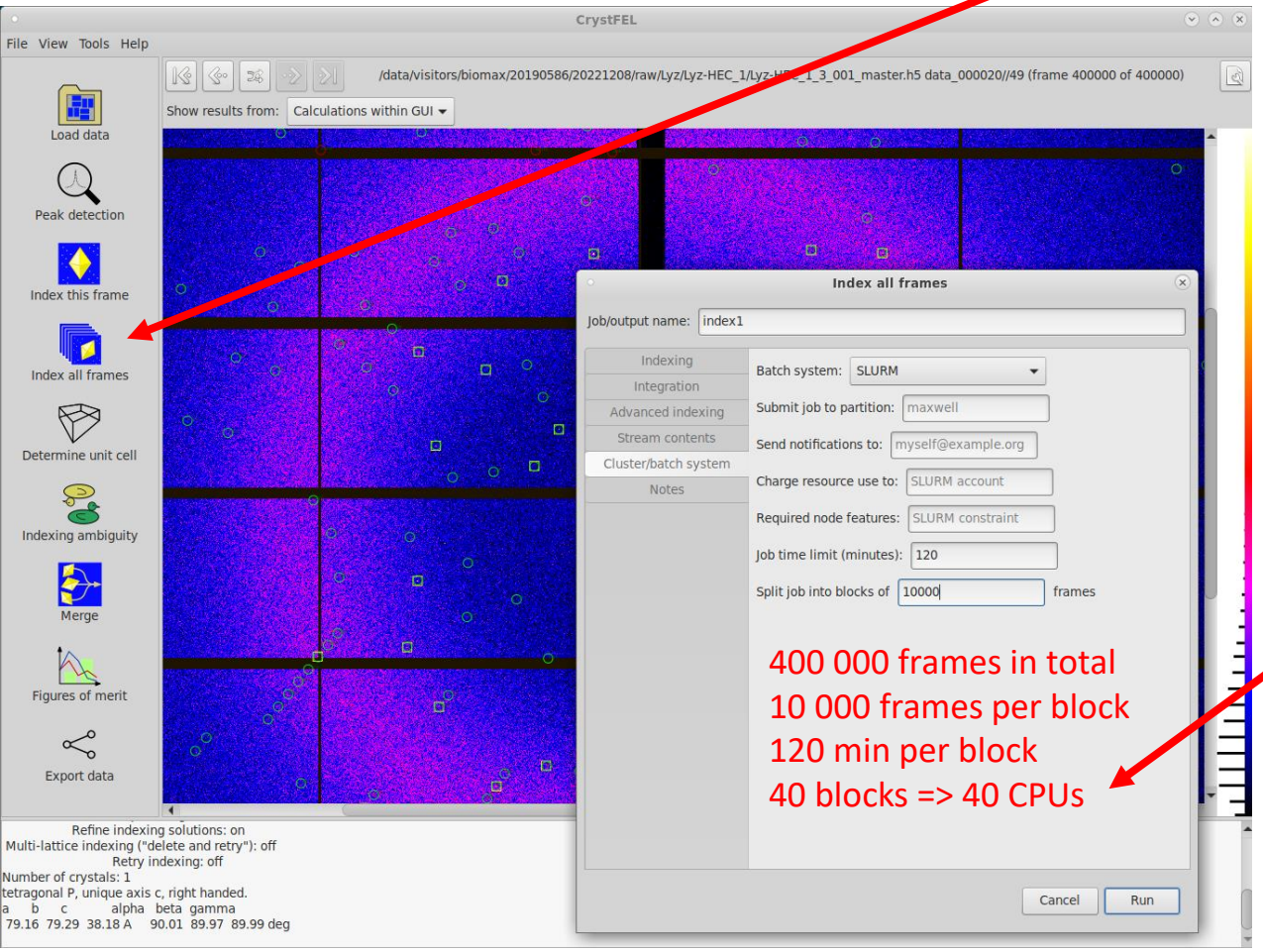
Correct Cell Parameters Lysozyme

Index all frames, indexing and cluster/batch SLURM settings at MAX IV



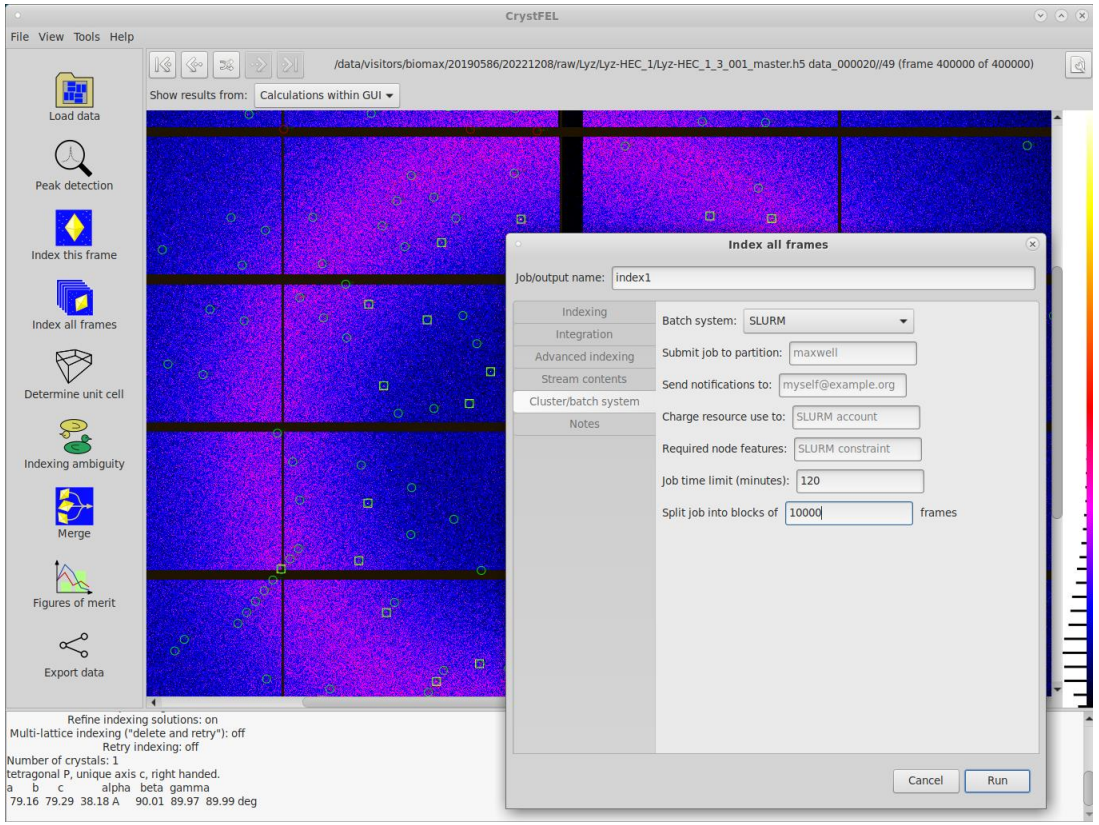


Index all frames - running




```
[marmoc2@offline-fe1 demo]$ squeue -u marmoc2
             JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
         237626_0       all   index1  marmoc2  R       0:43      1 offline-cn11
         237626_1       all   index1  marmoc2  R       0:43      1 offline-cn11
         237626_2       all   index1  marmoc2  R       0:43      1 offline-cn11
         237626_3       all   index1  marmoc2  R       0:43      1 offline-cn11
         237626_4       all   index1  marmoc2  R       0:43      1 offline-cn11
         237626_5       all   index1  marmoc2  R       0:43      1 offline-cn11
         237626_6       all   index1  marmoc2  R       0:43      1 offline-cn11
         237626_7       all   index1  marmoc2  R       0:43      1 offline-cn11
         237626_8       all   index1  marmoc2  R       0:43      1 offline-cn11
         237626_9       all   index1  marmoc2  R       0:43      1 offline-cn11
        237626_10       all   index1  marmoc2  R       0:43      1 offline-cn11
        237626_11       all   index1  marmoc2  R       0:43      1 offline-cn11
        237626_12       all   index1  marmoc2  R       0:43      1 offline-cn8
        237626_13       all   index1  marmoc2  R       0:43      1 offline-cn8
        237626_14       all   index1  marmoc2  R       0:43      1 offline-cn8
        237626_15       all   index1  marmoc2  R       0:43      1 offline-cn8
        237626_16       all   index1  marmoc2  R       0:43      1 offline-cn8
        237626_17       all   index1  marmoc2  R       0:43      1 offline-cn8
        237626_18       all   index1  marmoc2  R       0:43      1 offline-cn8
        237626_19       all   index1  marmoc2  R       0:43      1 offline-cn8
        237626_20       all   index1  marmoc2  R       0:43      1 offline-cn8
        237626_21       all   index1  marmoc2  R       0:43      1 offline-cn8
        237626_22       all   index1  marmoc2  R       0:43      1 offline-cn8
        237626_23       all   index1  marmoc2  R       0:43      1 offline-cn8
        237626_24       all   index1  marmoc2  R       0:43      1 offline-cn8
        237626_25       all   index1  marmoc2  R       0:43      1 offline-cn5
        237626_26       all   index1  marmoc2  R       0:43      1 offline-cn2
        237626_27       all   index1  marmoc2  R       0:43      1 offline-cn2
        237626_28       all   index1  marmoc2  R       0:43      1 offline-cn2
        237626_29       all   index1  marmoc2  R       0:43      1 offline-cn2
        237626_30       all   index1  marmoc2  R       0:43      1 offline-cn2
        237626_31       all   index1  marmoc2  R       0:43      1 offline-cn2
        237626_32       all   index1  marmoc2  R       0:43      1 offline-cn2
        237626_33       all   index1  marmoc2  R       0:43      1 offline-cn2
        237626_34       all   index1  marmoc2  R       0:43      1 offline-cn2
        237626_35       all   index1  marmoc2  R       0:43      1 offline-cn2
        237626_36       all   index1  marmoc2  R       0:43      1 offline-cn2
        237626_37       all   index1  marmoc2  R       0:43      1 offline-cn2
        237626_38       all   index1  marmoc2  R       0:43      1 offline-cn2
        237626_39       all   index1  marmoc2  R       0:43      1 offline-cn2
[marmoc2@offline-fe1 demo]$
```

Index all frames did not finish – index1

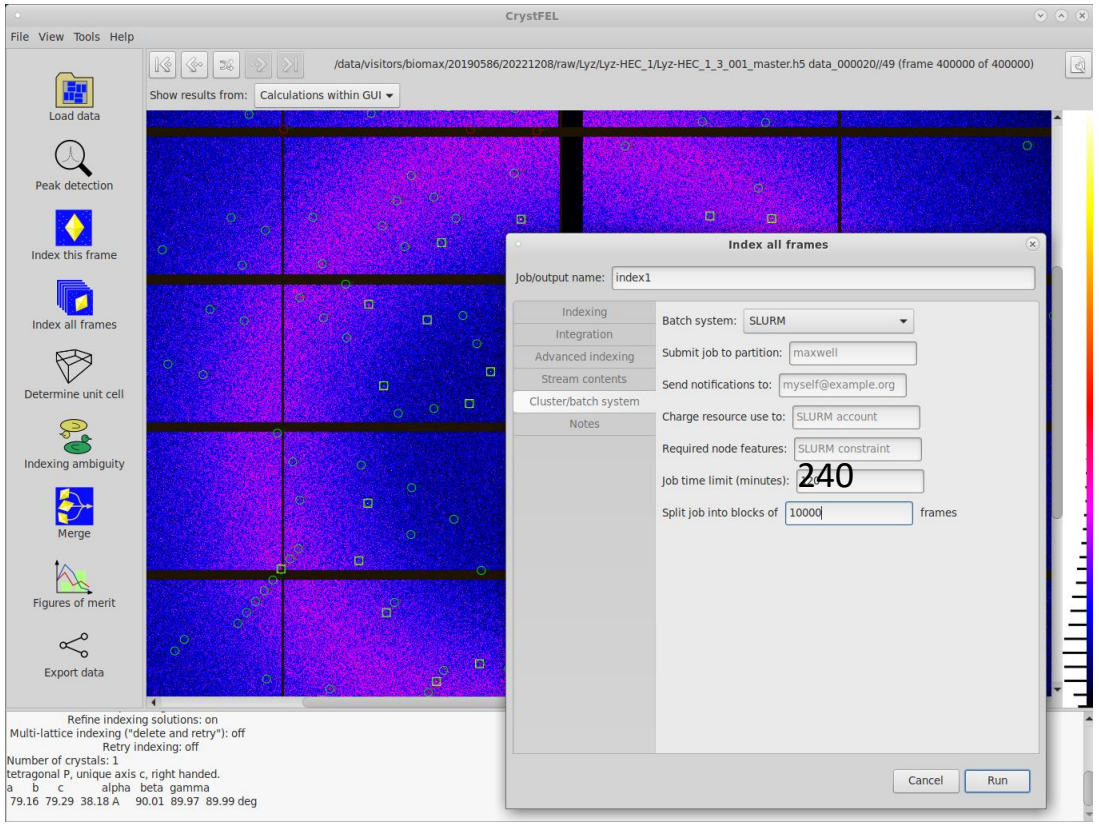



```
[marmoc2@offline-fe1 index1]$ pwd
/home/marmoc2/demo/crystfel-lyz5/index1
[marmoc2@offline-fe1 index1]$ tail -10 stderr-10.log
5090 images processed, 5090 hits (100.0%), 2659 indexable (52.2% of hits, 52.2% overall), 2659 crystals, 0.6 images/sec.
WARNING: 1 implausibly negative reflection in /data/visitors/biomax/20190586/20221208/raw/Lyz/Lyz-HEC_1/Lyz-HEC_1_9_001_data_000011.h5 data//91
5094 images processed, 5094 hits (100.0%), 2663 indexable (52.3% of hits, 52.3% overall), 2663 crystals, 0.8 images/sec.
5098 images processed, 5098 hits (100.0%), 2664 indexable (52.3% of hits, 52.3% overall), 2664 crystals, 0.7 images/sec.
5101 images processed, 5101 hits (100.0%), 2666 indexable (52.3% of hits, 52.3% overall), 2666 crystals, 0.6 images/sec.
5105 images processed, 5105 hits (100.0%), 2668 indexable (52.3% of hits, 52.3% overall), 2668 crystals, 0.7 images/sec.
5110 images processed, 5110 hits (100.0%), 2672 indexable (52.3% of hits, 52.3% overall), 2672 crystals, 0.7 images/sec.
5113 images processed, 5113 hits (100.0%), 2673 indexable (52.3% of hits, 52.3% overall), 2673 crystals, 0.6 images/sec.
5117 images processed, 5117 hits (100.0%), 2674 indexable (52.3% of hits, 52.3% overall), 2674 crystals, 0.8 images/sec.
slurmstepd: error: *** JOB 237637 ON offline-cn11 CANCELLED AT 2023-04-28T13:55:44 DUE TO TIME LIMIT ***
[marmoc2@offline-fe1 index1]$
```

Index1 failed!

- Job time 120 min too short

Index2 did not finish, but it was close…

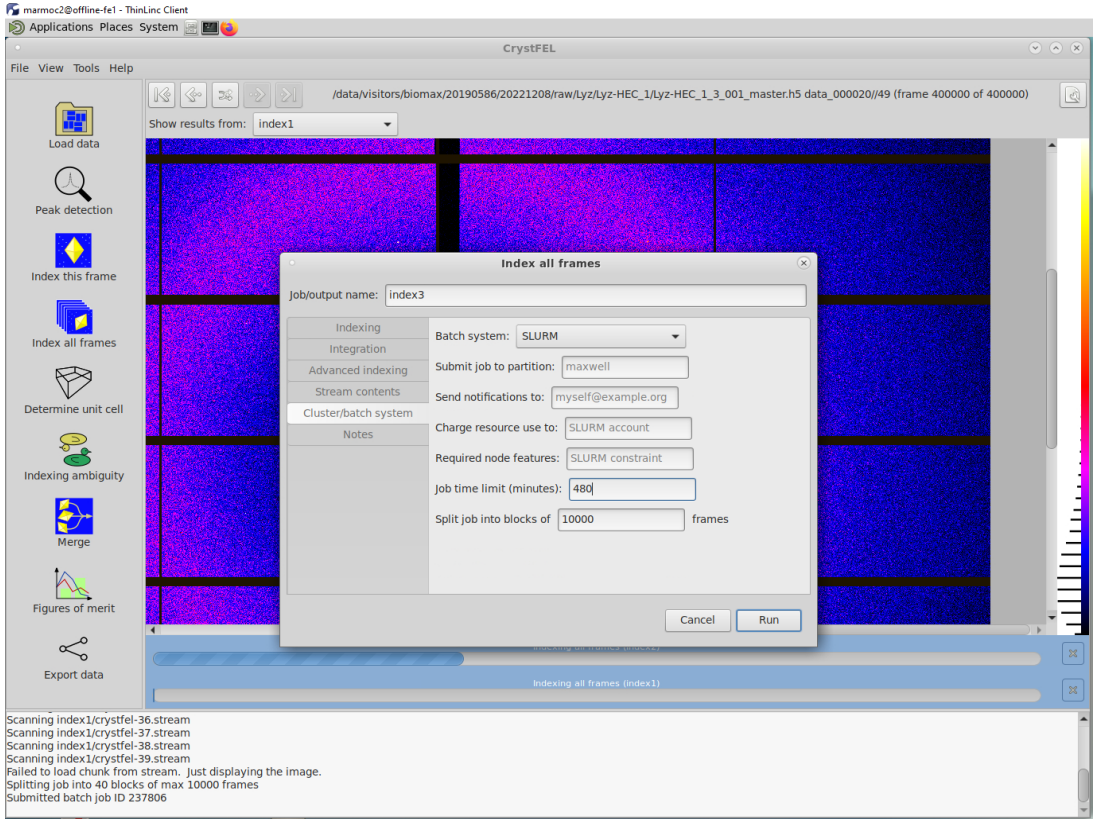



```
[marmoc2@offline-fe1 index2]$ pwd
/home/marmoc2/demo/crystfel-lyz5/index2
[marmoc2@offline-fe1 index2]$ tail -10 stderr-22.log
9969 images processed, 9969 hits (100.0%), 4765 indexable (47.8% of hits, 47.8% overall), 4765 crystals, 0.8 images/sec.
9974 images processed, 9974 hits (100.0%), 4769 indexable (47.8% of hits, 47.8% overall), 4769 crystals, 0.9 images/sec.
9978 images processed, 9978 hits (100.0%), 4773 indexable (47.8% of hits, 47.8% overall), 4773 crystals, 0.8 images/sec.
9981 images processed, 9981 hits (100.0%), 4775 indexable (47.8% of hits, 47.8% overall), 4775 crystals, 0.6 images/sec.
9985 images processed, 9985 hits (100.0%), 4776 indexable (47.8% of hits, 47.8% overall), 4776 crystals, 0.8 images/sec.
9989 images processed, 9989 hits (100.0%), 4776 indexable (47.8% of hits, 47.8% overall), 4776 crystals, 0.8 images/sec.
9993 images processed, 9993 hits (100.0%), 4776 indexable (47.8% of hits, 47.8% overall), 4776 crystals, 0.8 images/sec.
9996 images processed, 9996 hits (100.0%), 4776 indexable (47.8% of hits, 47.8% overall), 4776 crystals, 0.6 images/sec.
Waiting for the last patterns to be processed...
slurmstepd: error: *** JOB 237829 ON offline-cn2 CANCELLED AT 2023-04-28T18:00:16 DUE TO TIME LIMIT ***
[marmoc2@offline-fe1 index2]$
```

Index2 failed!

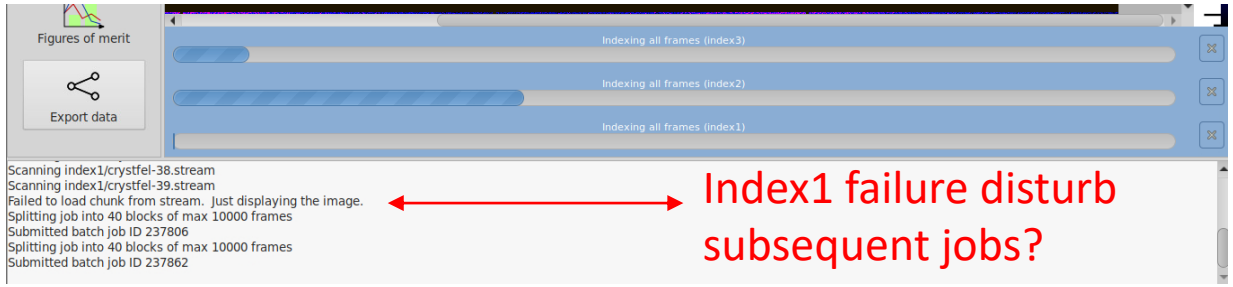
- 240 min slightly too short
- 9 996 of 10 000 images processed!

Index3 finished but what happen then?




```
[marmoc2@offline-fe1 index3]$ pwd
/home/marmoc2/demo/crystfel-lyz5/index3
[marmoc2@offline-fe1 index3]$ grep Final *.log
stderr-0.log:Final: 10000 images processed, 10000 hits (100.0%), 4930 indexable (49.3% of hits, 49.3% overall), 4930 crystals.
stderr-10.log:Final: 10000 images processed, 10000 hits (100.0%), 5026 indexable (50.3% of hits, 50.3% overall), 5026 crystals.
stderr-11.log:Final: 10000 images processed, 10000 hits (100.0%), 4847 indexable (48.5% of hits, 48.5% overall), 4847 crystals.
stderr-12.log:Final: 10000 images processed, 10000 hits (100.0%), 4966 indexable (49.7% of hits, 49.7% overall), 4966 crystals.
stderr-13.log:Final: 10000 images processed, 10000 hits (100.0%), 5092 indexable (50.9% of hits, 50.9% overall), 5092 crystals.
stderr-14.log:Final: 10000 images processed, 10000 hits (100.0%), 4949 indexable (49.5% of hits, 49.5% overall), 4949 crystals.
stderr-15.log:Final: 10000 images processed, 10000 hits (100.0%), 4383 indexable (43.8% of hits, 43.8% overall), 4383 crystals.
stderr-16.log:Final: 10000 images processed, 10000 hits (100.0%), 4973 indexable (49.7% of hits, 49.7% overall), 4973 crystals.
stderr-17.log:Final: 10000 images processed, 10000 hits (100.0%), 5026 indexable (50.3% of hits, 50.3% overall), 5026 crystals.
```

Index3 completed but what went wrong..?



Index1 failure disturb subsequent jobs?
Restart CrystFEL GUI
Right-click to save logfile…

crystfel.project

- Check crystfel.project saved from GUI
- Very many lines in crystfel.project– problem?
- All ExitCodes are 0 for index3

```
[marmoc2@offline-fe1 crystfel-lyz5]$ pwd
/home/marmoc2/demo/crystfel-lyz5
[marmoc2@offline-fe1 crystfel-lyz5]$ more crystfel.project
geom /home/marmoc2/demo/crystfel-lyz5/MAXIV.geom
data_folder /data/visitors/biomax/20190586/20221208/raw/Lyz/Lyz-HEC_1
search_pattern everything
peak_search_params.method peakfinder8
peak_search_params.threshold 20.000000
peak_search_params.min_sq_gradient 100000.000000
peak_search_params.min_snr 5.000000
peak_search_params.min_pix_count 2
peak_search_params.max_pix_count 200
peak_search_params.local_bg_radius 3
```

```
[marmoc2@offline-fe1 crystfel-lyz5]$ cat crystfel.project | wc -l
400217
[marmoc2@offline-fe1 crystfel-lyz5]$
```

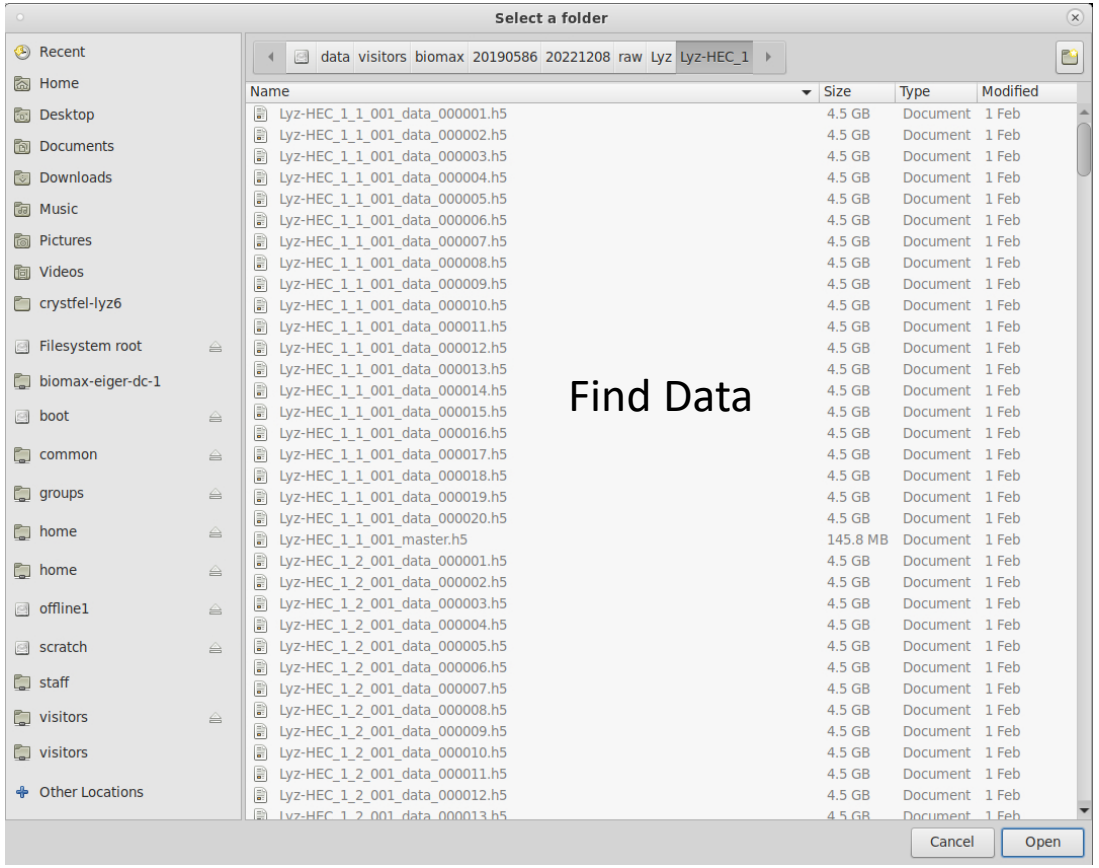
```
[marmoc2@offline-fe1 crystfel-lyz5]$ sacct -j 237862 --format=JobID,JobName,Start,End,MaxRSS,MaxVMSize,ExitCode
JobID           JobName                Start                  End     MaxRSS  MaxVMSize ExitCode
------------ ---------- ------------------- ------------------- ---------- ---------- --------
237862_0         index3 2023-05-02T15:26:38 2023-05-02T18:22:34                           0:0
237862_0.ba+      batch 2023-05-02T15:26:38 2023-05-02T18:22:34    832524K   3374368K      0:0
237862_0.ex+     extern 2023-05-02T15:26:38 2023-05-02T18:22:34      1028K    143604K      0:0
237862_1         index3 2023-05-02T15:26:38 2023-05-02T18:20:42                           0:0
237862_1.ba+      batch 2023-05-02T15:26:38 2023-05-02T18:20:42    816668K   3357600K      0:0
237862_1.ex+     extern 2023-05-02T15:26:38 2023-05-02T18:20:42      1048K    143604K      0:0
237862_2         index3 2023-05-02T15:26:38 2023-05-02T18:49:20                           0:0
```

For index1, exit codes is 15
15 means terminated by SIGTERM
237626 – index1
237862 – index3

```
[marmoc2@offline-fe1 crystfel-lyz5]$ sacct -j 237626 --format=JobID,JobName,Start,End,MaxRSS,MaxVMSize,ExitCode
JobID           JobName                Start                  End     MaxRSS  MaxVMSize ExitCode
------------ ---------- ------------------- ------------------- ---------- ---------- --------
237626_0         index1 2023-04-28T11:55:36 2023-04-28T13:55:44                           0:0
237626_0.ba+      batch 2023-04-28T11:55:36 2023-04-28T13:55:46    811612K   3360420K     0:15
237626_0.ex+     extern 2023-04-28T11:55:36 2023-04-28T13:55:44       352K    108056K      0:0
237626_1         index1 2023-04-28T11:55:36 2023-04-28T13:55:44                           0:0
237626_1.ba+      batch 2023-04-28T11:55:36 2023-04-28T13:55:45    995628K   3378456K     0:15
237626_1.ex+     extern 2023-04-28T11:55:36 2023-04-28T13:55:44      1044K    143604K      0:0
237626_2         index1 2023-04-28T11:55:36 2023-04-28T13:55:44                           0:0
237626_2.ba+      batch 2023-04-28T11:55:36 2023-04-28T13:55:46    833688K   3378072K     0:15
```

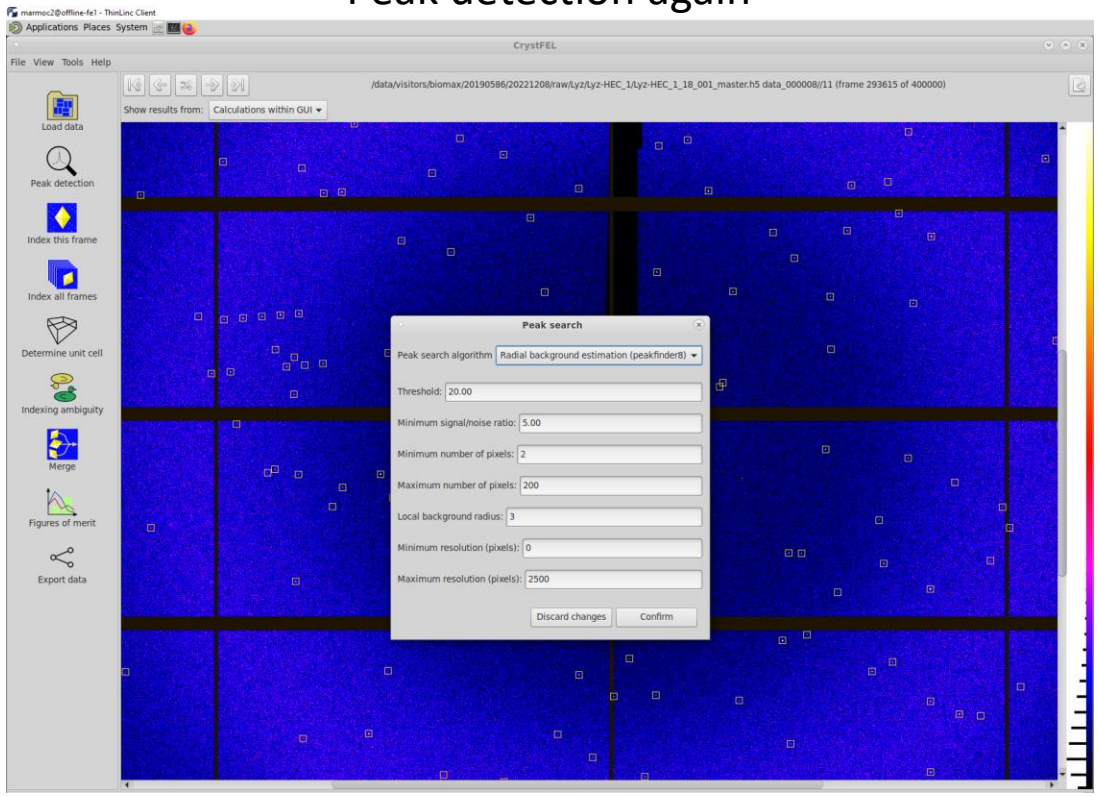
Restart crystfel from scratch in new directory

/home/marmoc2/demo/crystfel-lyz6

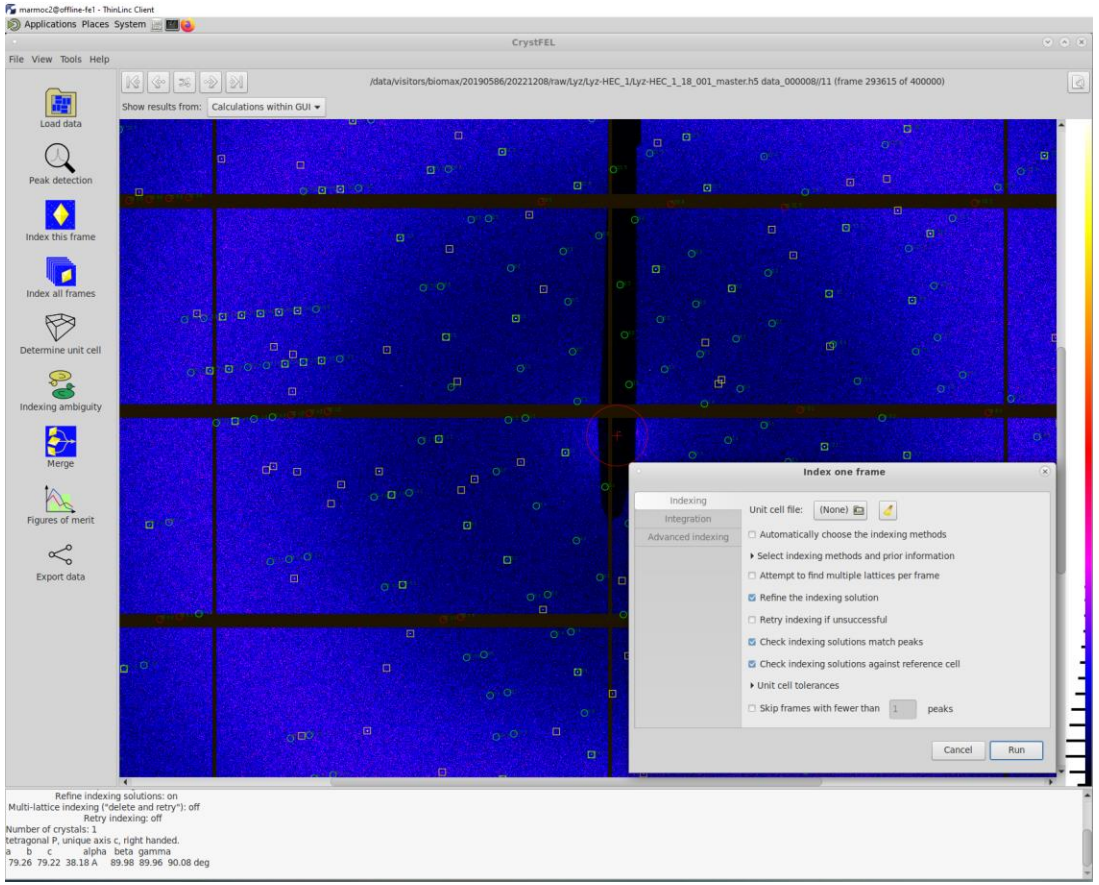


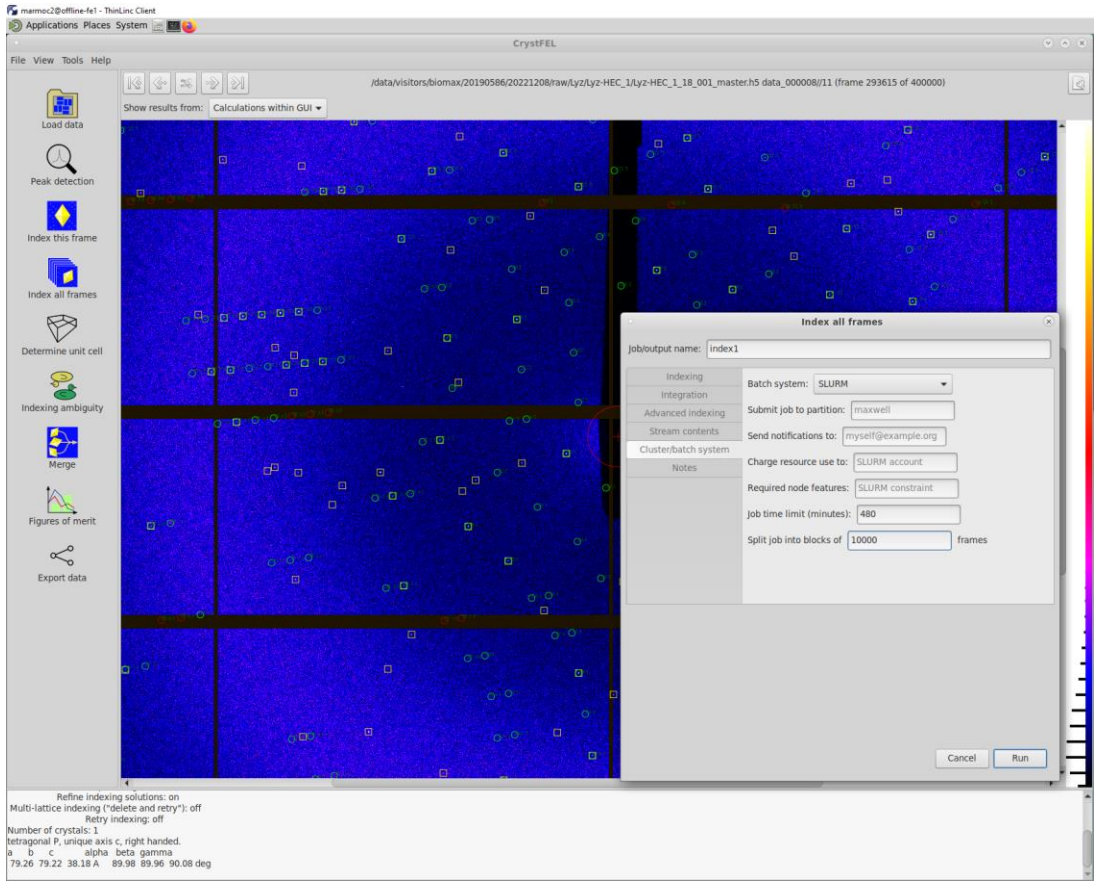
Find Data

Peak detection again



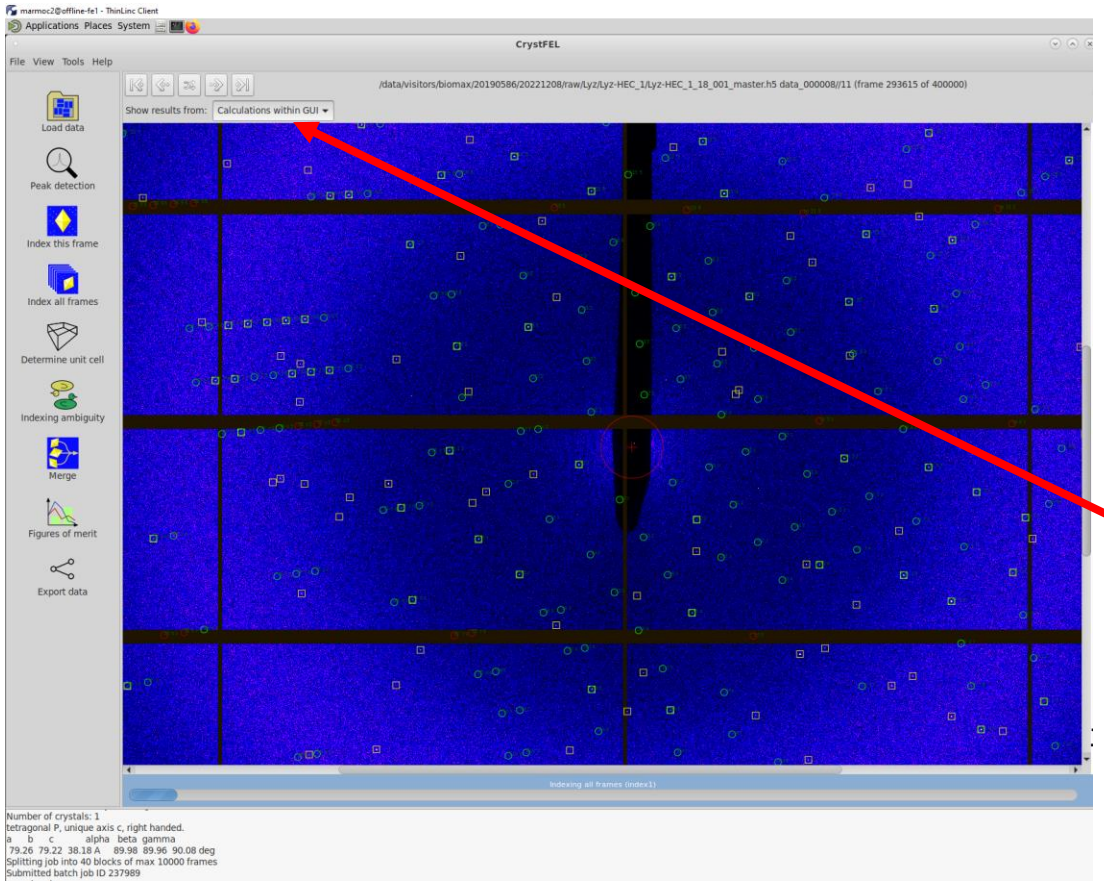
Index one frame (left) and all frames (right)

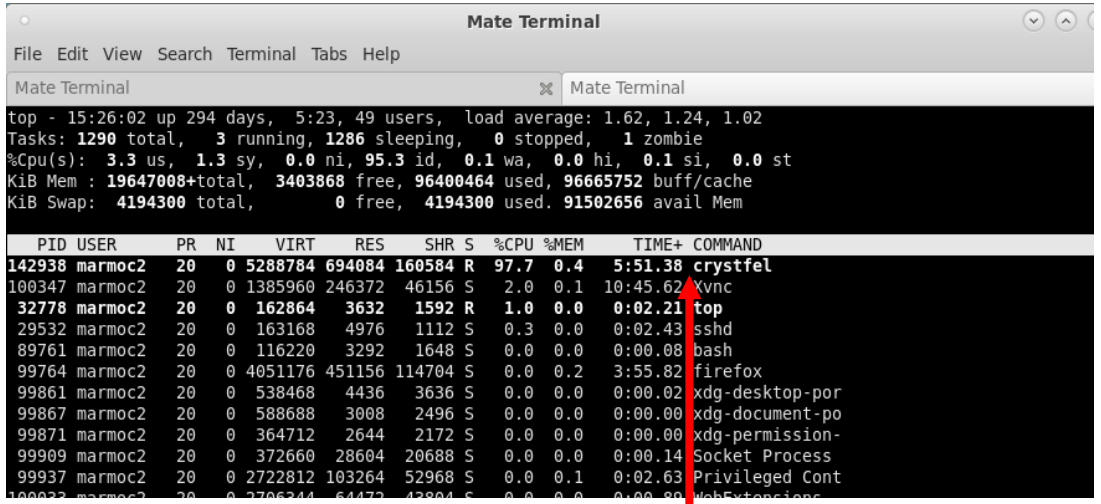




Job time 480 min - so that job will finish…

Wake up CrystFEL after Index1

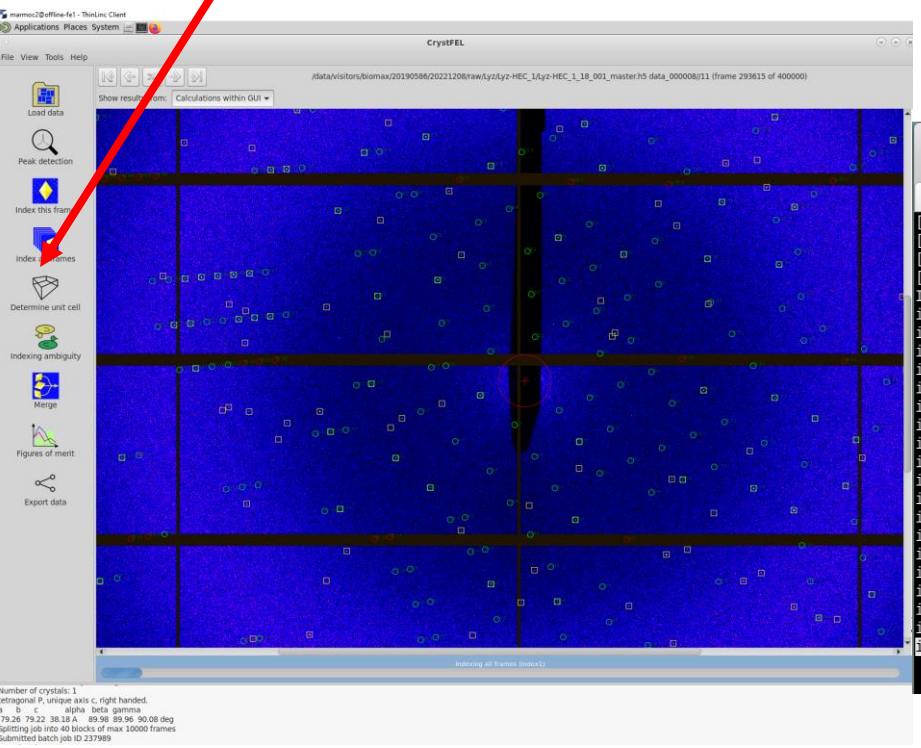


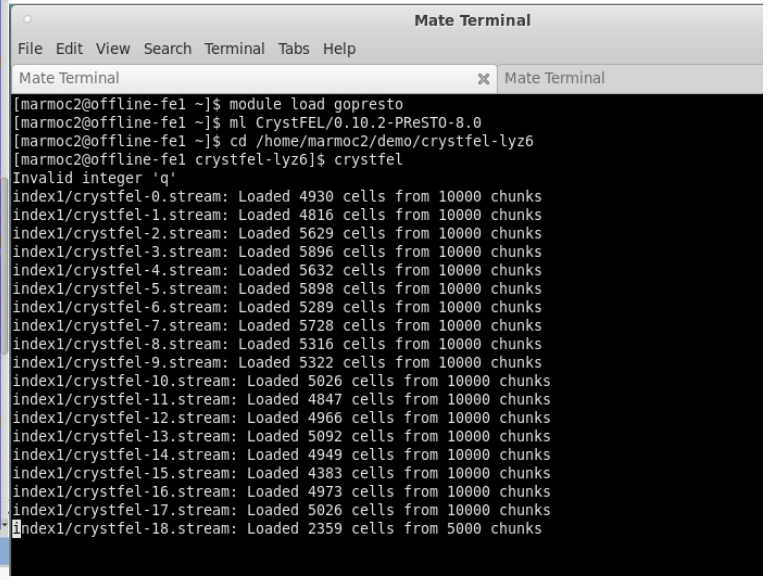


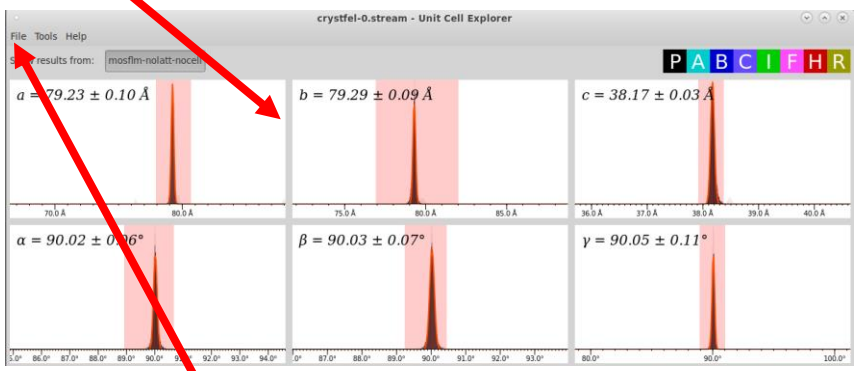
By clicking in the GUI I could wake-up CrystFEL

”Determine unit cell” opens cell explorer and triggers reading of streams

- Celll Explorer commands:
  - Move in diagram by mouse
  - ”+” sets binning
  - Select peak by shift-mouse drag
  - Zoom by scroll wheel



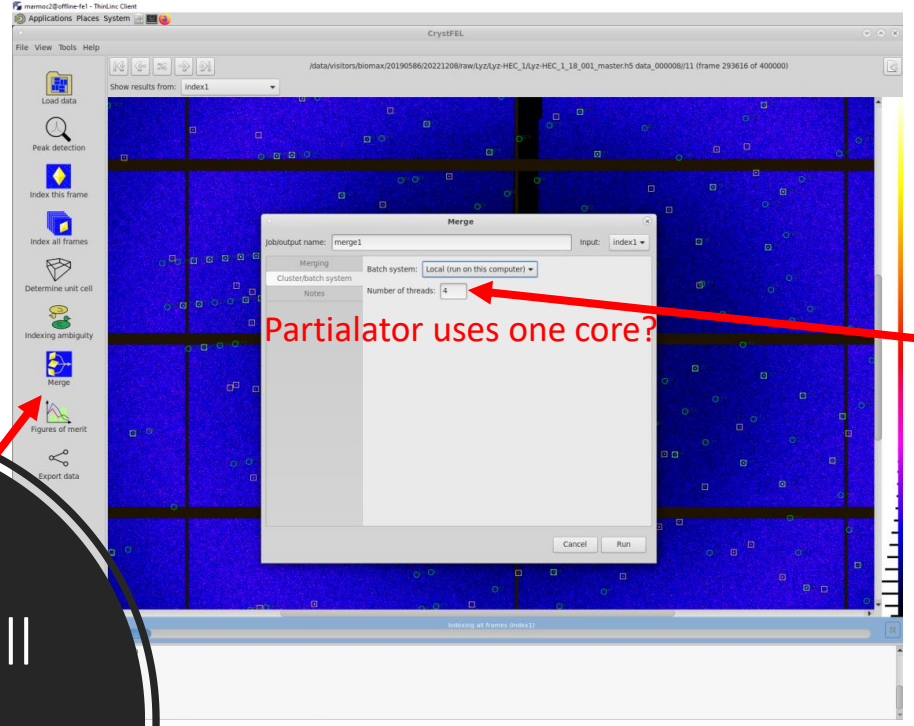


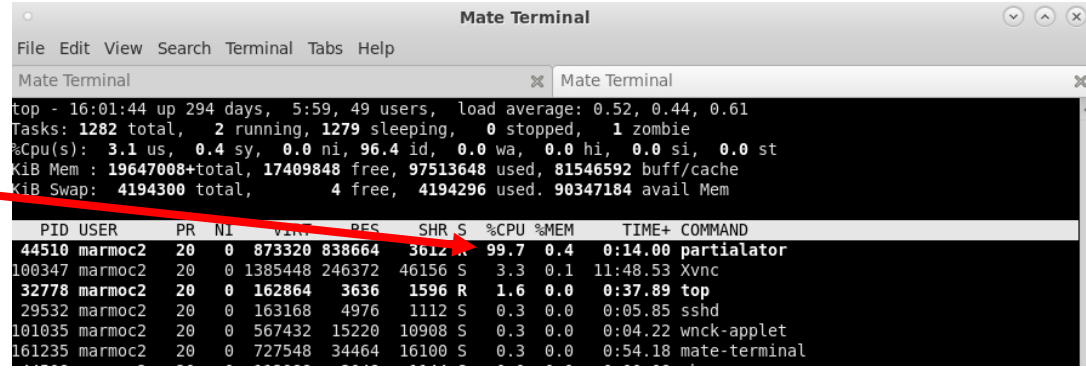


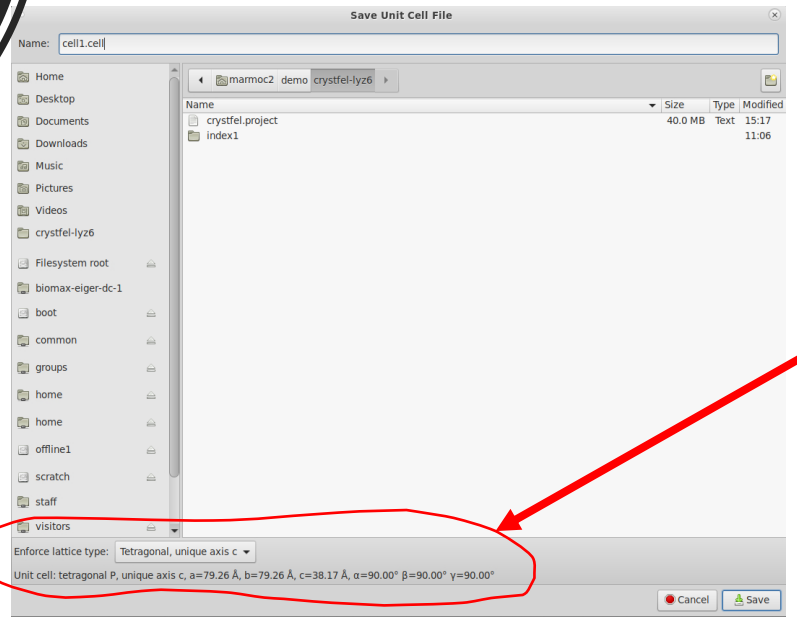
File - Save unit cell as cell1.cell

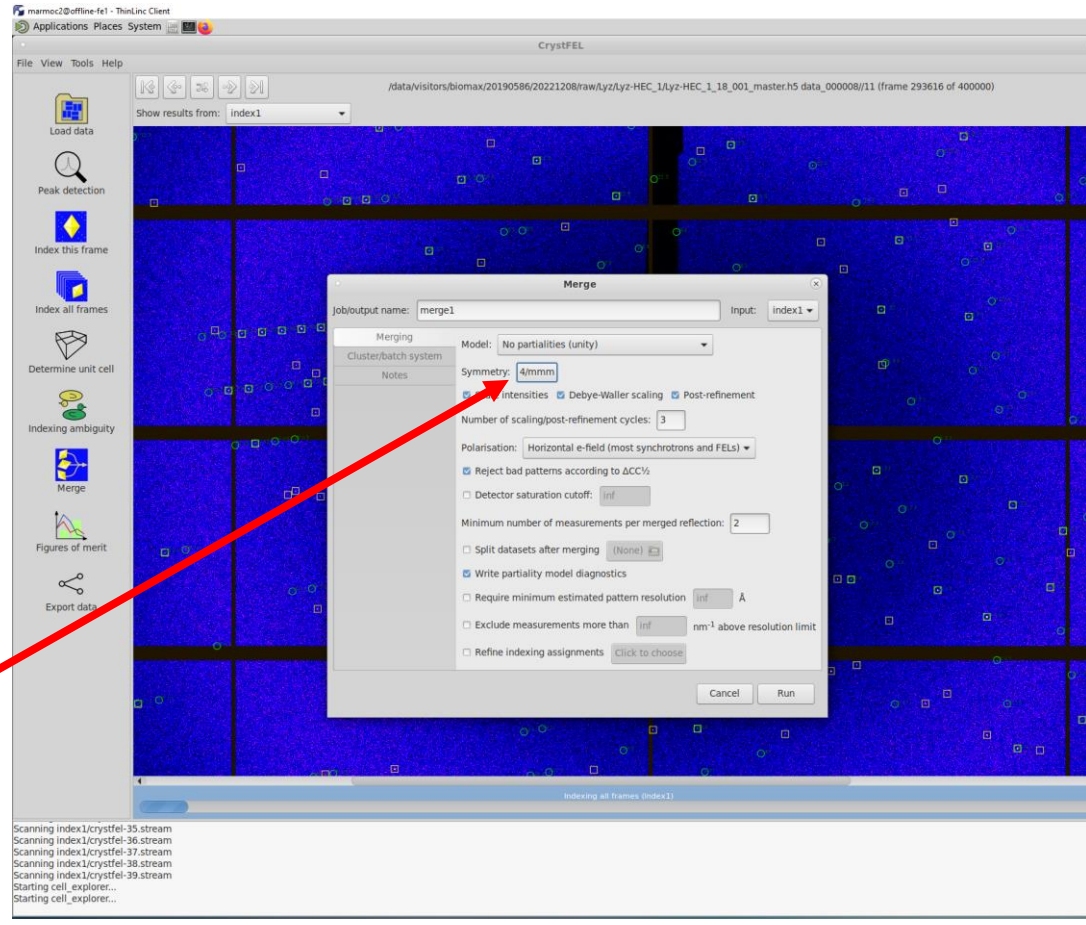
Reading streams takes 1-2 min

Save unit cell and merge data

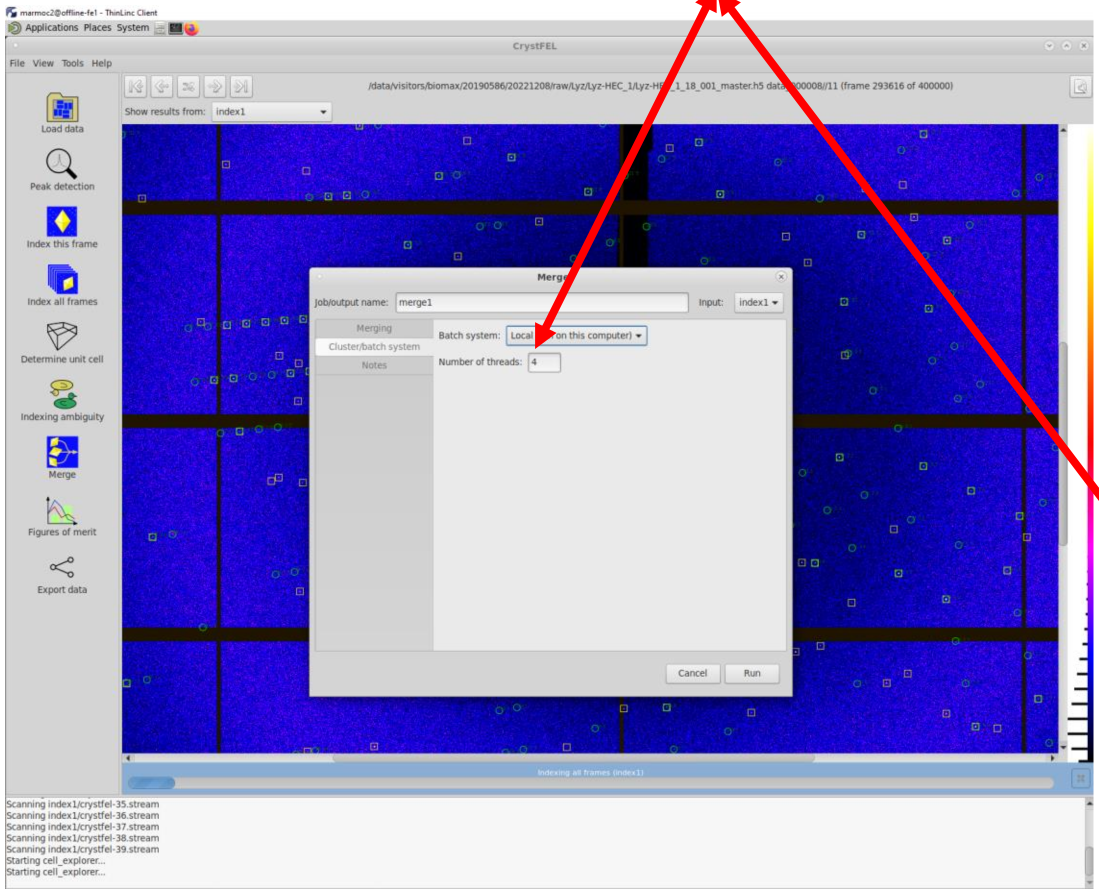


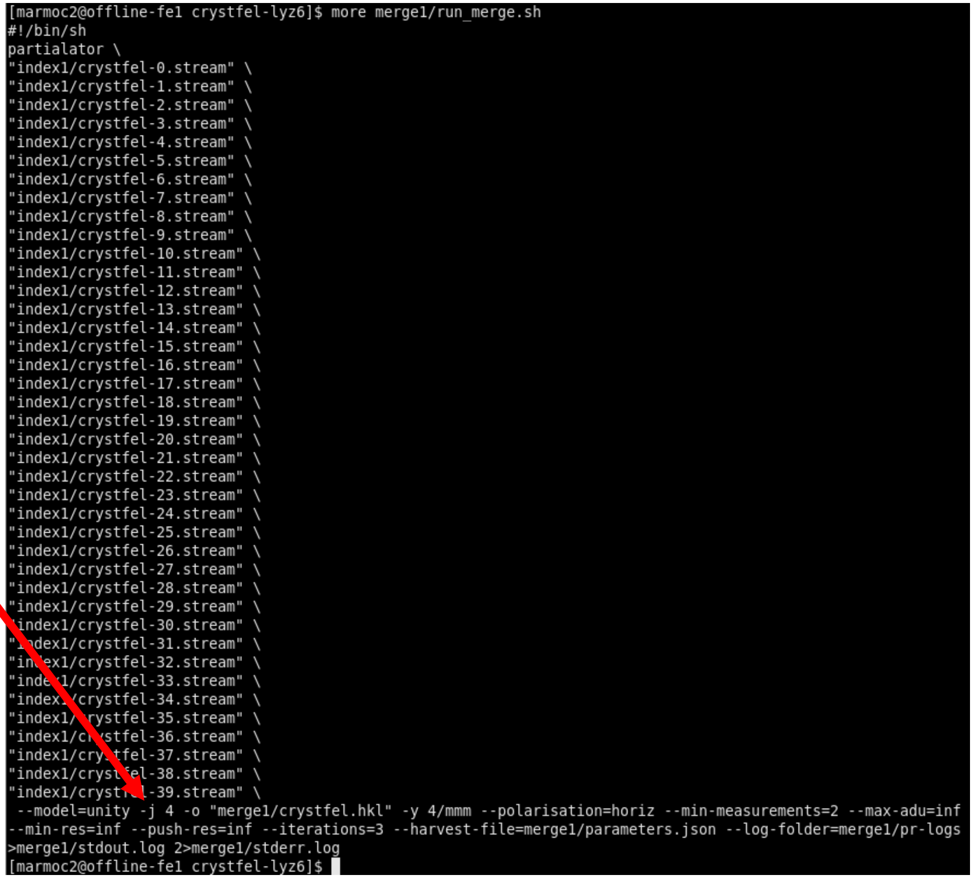






merge1 - I ask for 4 threads but did I get it?





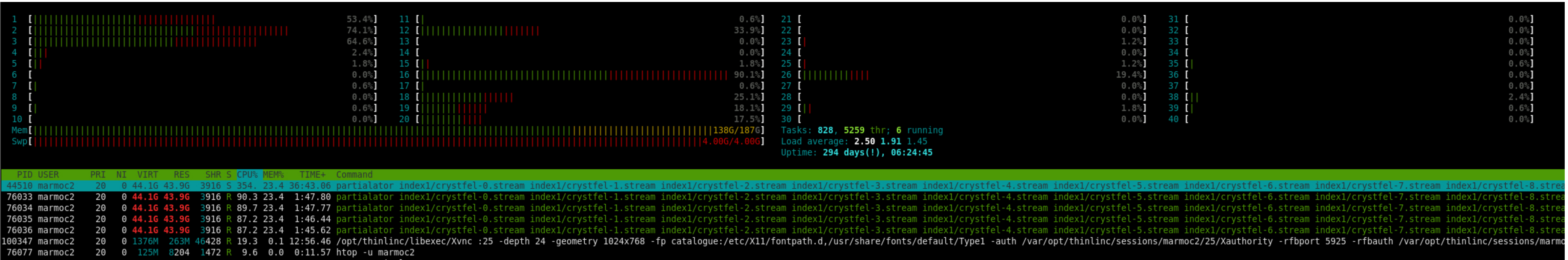
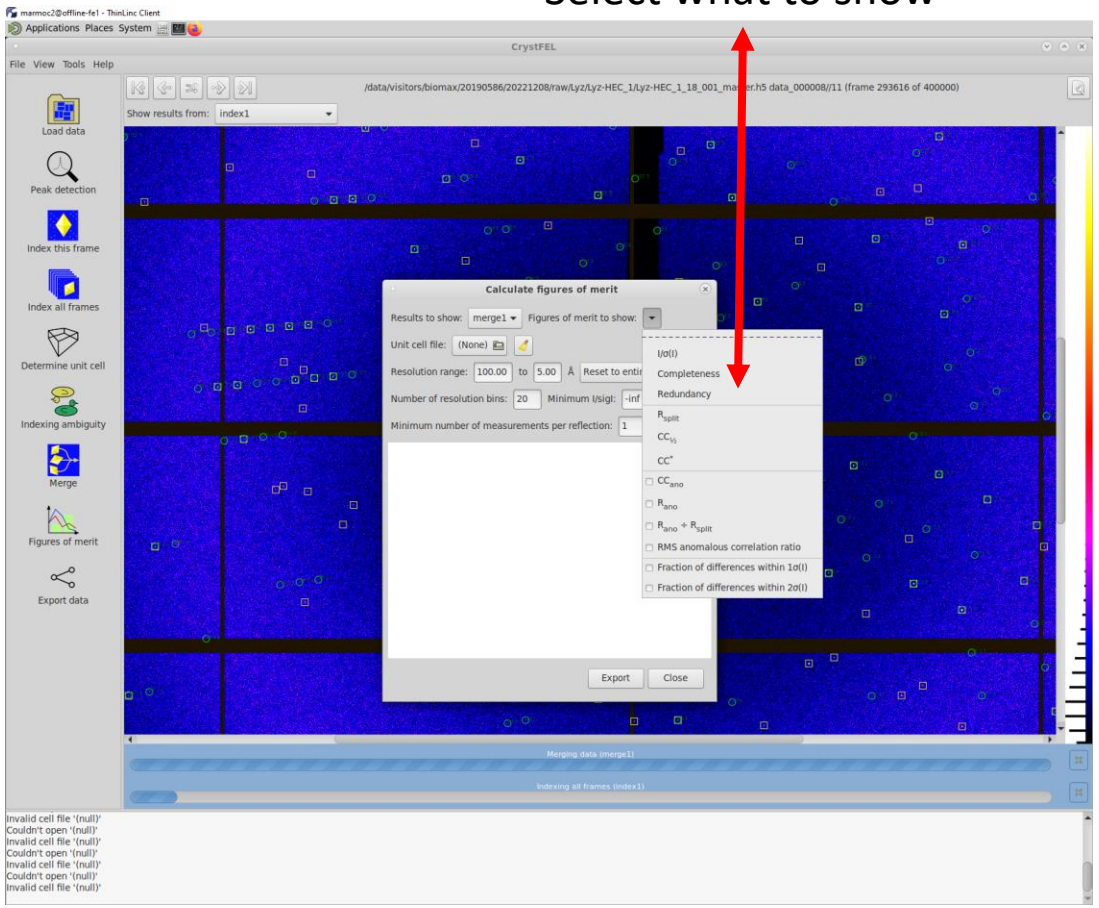
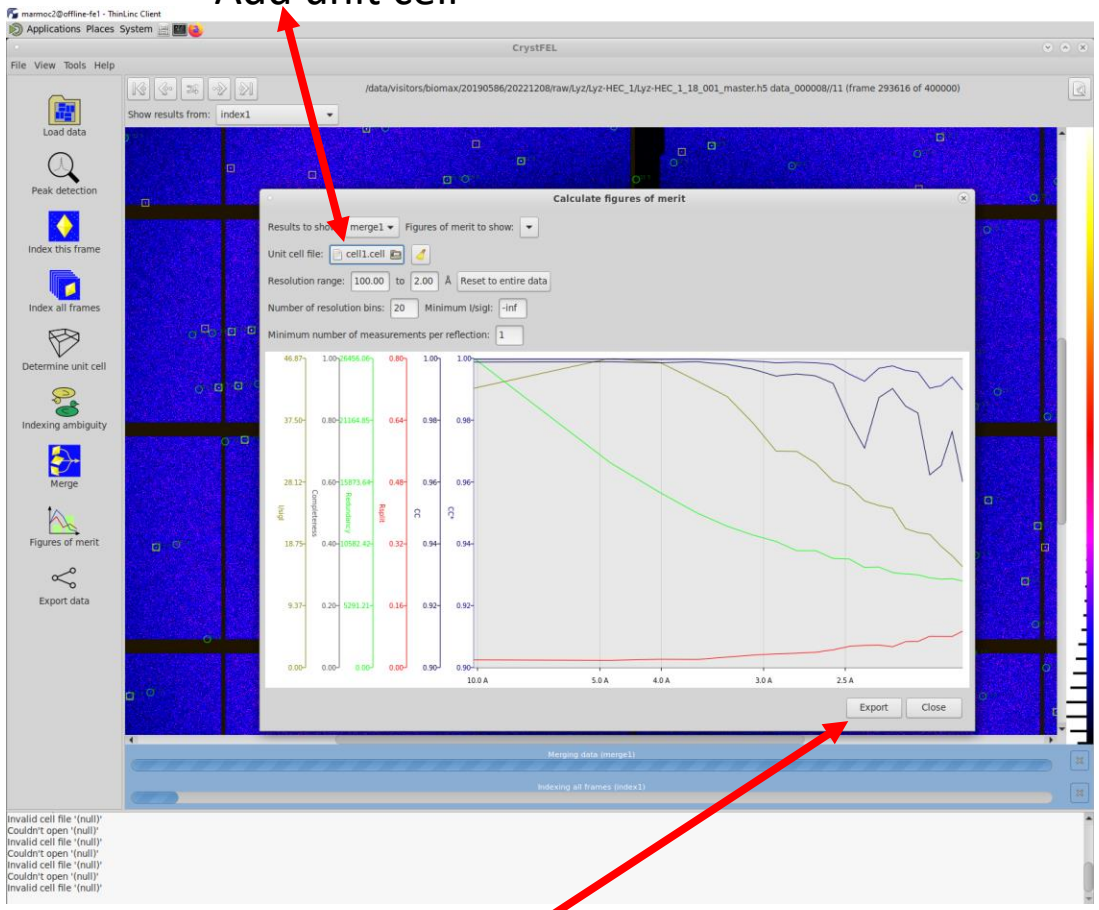


Figure of Merit – merge1

Select what to show

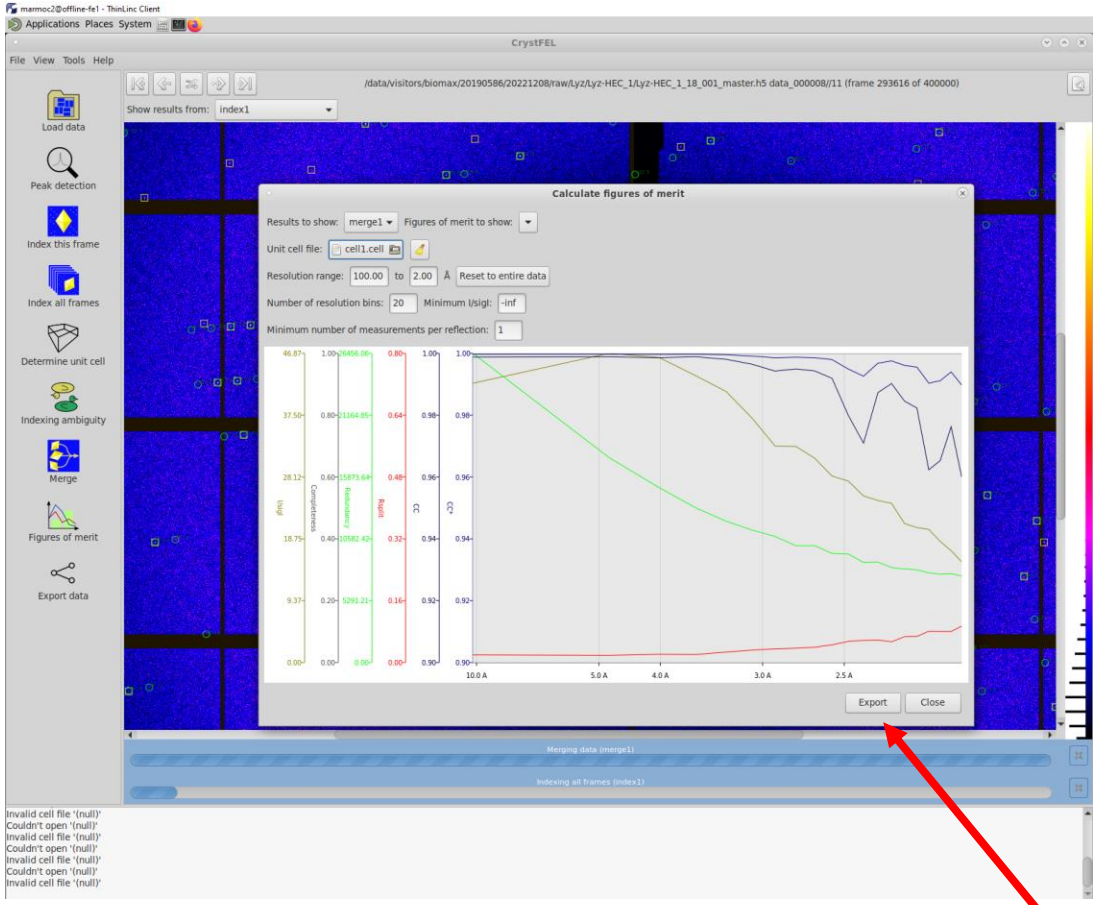


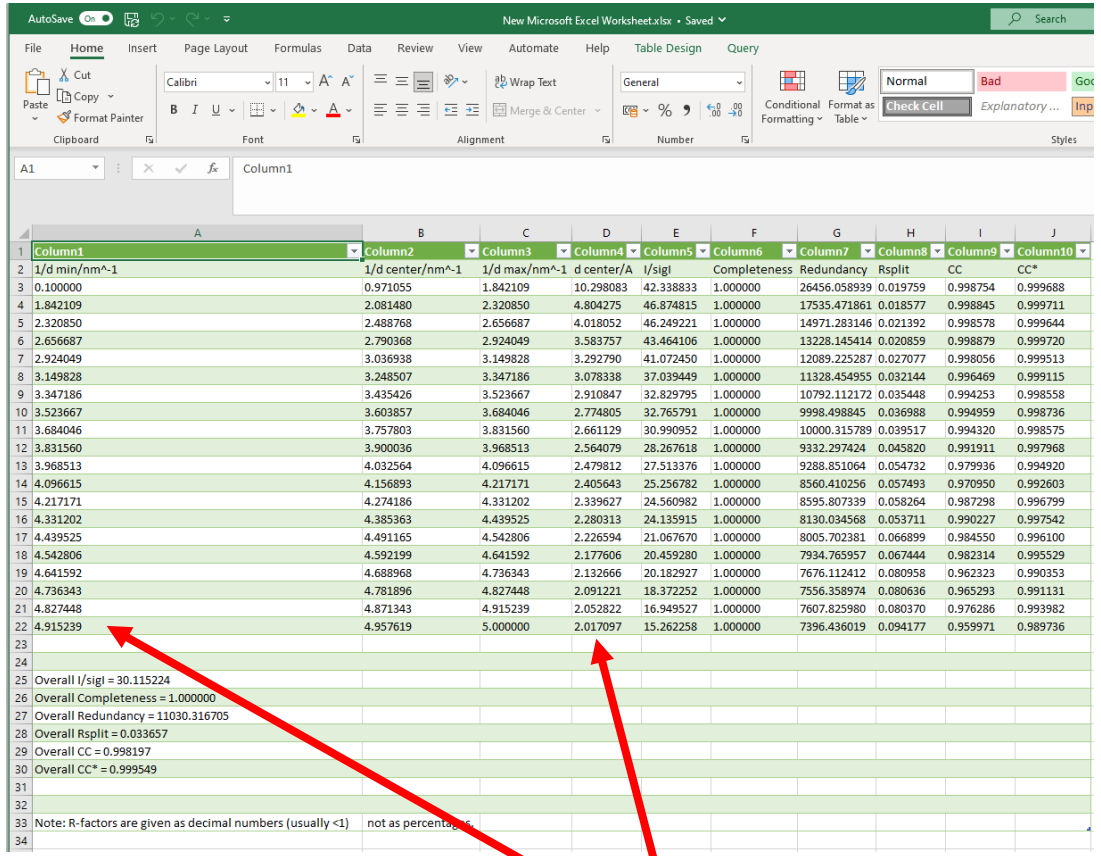
Add unit cell



All Figure of Merit data be exported as .csv file open as text in Excel

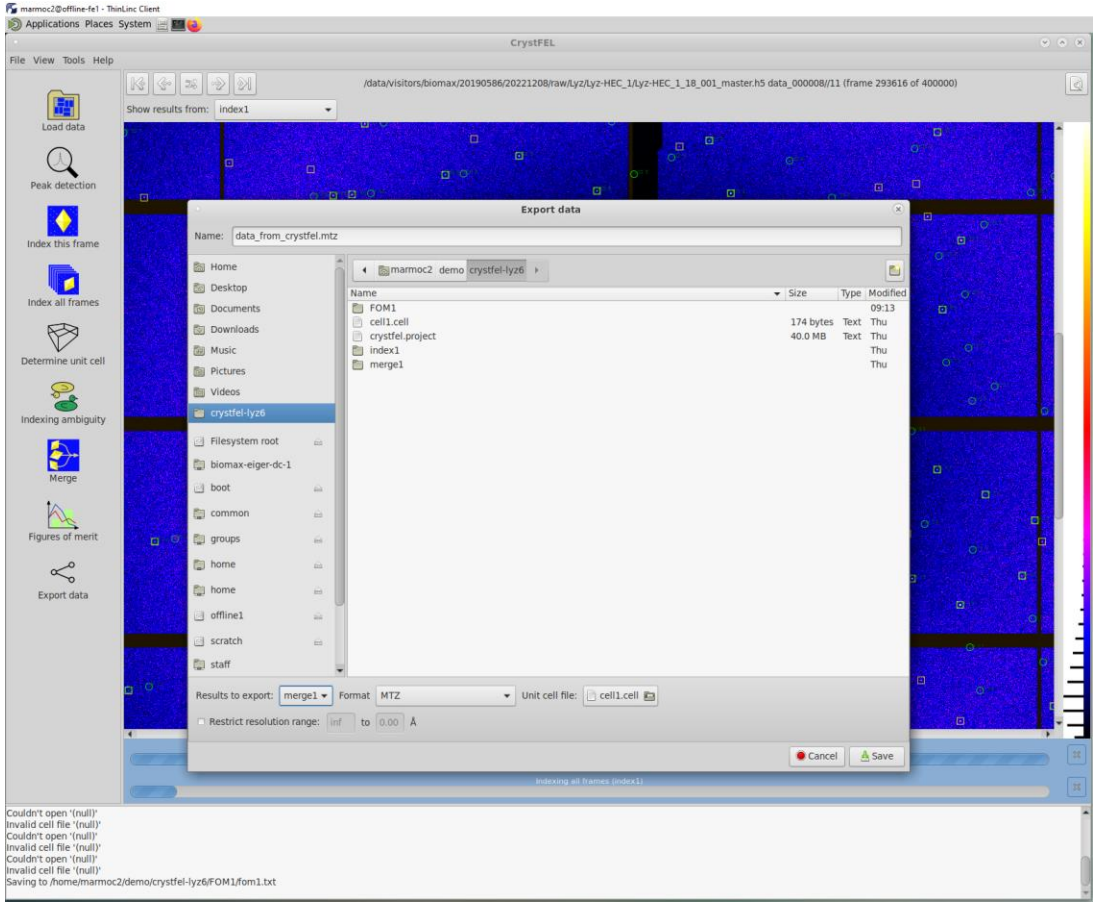
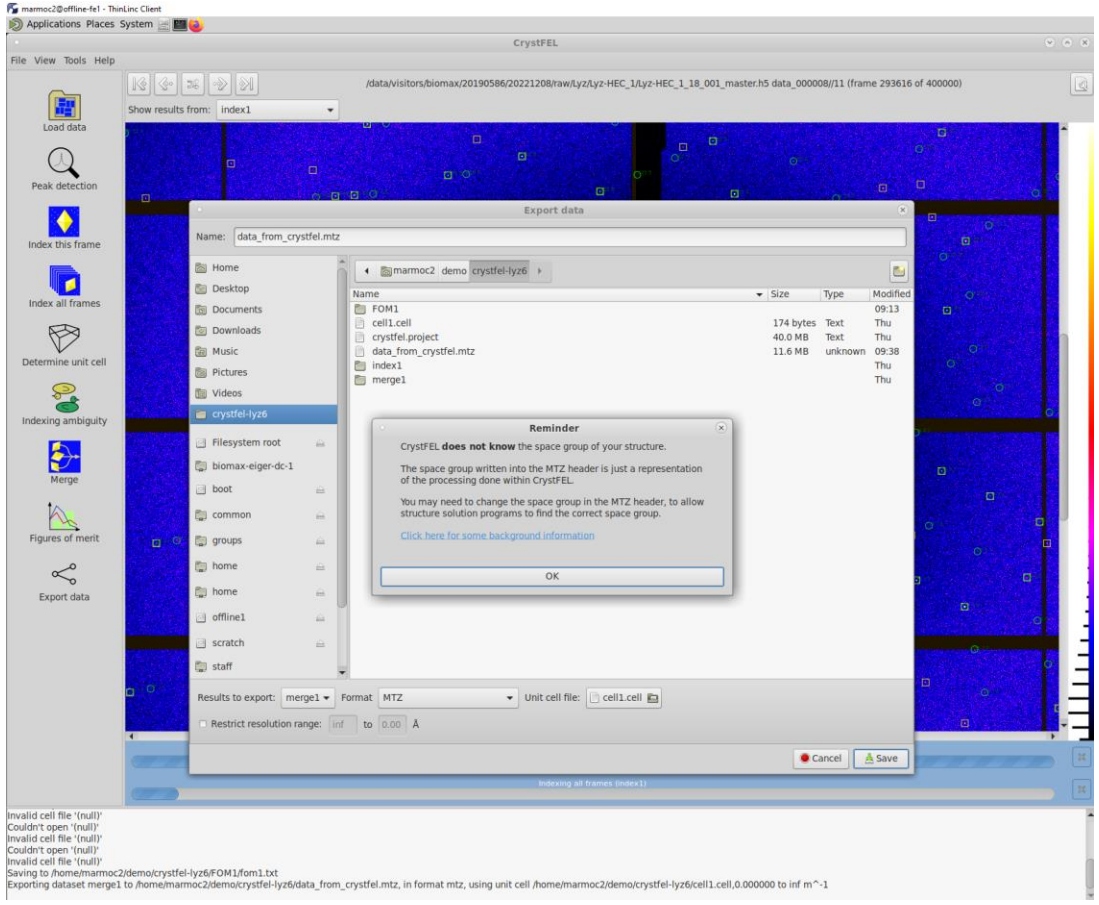
Figure of Merit – exported and open in Excel





Column1	Column2	Column3	Column4	Column5	Column6	Column7	Column8	Column9	Column10
1/d min/nm^-1	1/d center/nm^-1	1/d max/nm^-1	d center/A	I/sigI	Completeness	Redundancy	Rsplit	CC	CC*
0.100000	0.971055	1.842109	10.298083	42.338833	1.000000	26456.058939	0.019759	0.998754	0.999688
1.842109	2.081480	2.320850	4.804275	46.874815	1.000000	17535.471861	0.018577	0.998845	0.999711
2.320850	2.488768	2.656687	4.018052	46.249221	1.000000	14971.283146	0.021392	0.998578	0.999644
2.656687	2.790368	2.924049	3.583757	43.464106	1.000000	13228.145414	0.020859	0.998879	0.999720
2.924049	3.036938	3.149828	3.292790	41.072450	1.000000	12089.225287	0.027077	0.998056	0.999513
3.149828	3.248507	3.347186	3.078338	37.039449	1.000000	11328.454955	0.032144	0.996469	0.999115
3.347186	3.435426	3.523667	2.910847	32.829795	1.000000	10792.112172	0.035448	0.994253	0.998558
3.523667	3.603857	3.684046	2.774805	32.765791	1.000000	9998.498845	0.036988	0.994959	0.998736
3.684046	3.757803	3.831560	2.661129	30.990952	1.000000	10000.315789	0.039517	0.994320	0.998575
3.831560	3.900036	3.968513	2.564079	28.267618	1.000000	9332.297424	0.045820	0.991911	0.997968
3.968513	4.032564	4.096615	2.479812	27.513376	1.000000	9288.851064	0.054732	0.979936	0.994920
4.096615	4.156893	4.217171	2.405643	25.256782	1.000000	8560.410256	0.057493	0.970950	0.992603
4.217171	4.274186	4.331202	2.339627	24.560982	1.000000	8595.807339	0.058264	0.987298	0.996799
4.331202	4.385363	4.439525	2.280313	24.135915	1.000000	8130.034568	0.053711	0.990227	0.997542
4.439525	4.491165	4.542806	2.226594	21.067670	1.000000	8005.702381	0.066899	0.984550	0.996100
4.542806	4.592199	4.641592	2.177606	20.459280	1.000000	7934.765957	0.067444	0.982314	0.995529
4.641592	4.688968	4.736343	2.132666	20.182927	1.000000	7676.112412	0.080958	0.962323	0.990353
4.736343	4.781896	4.827448	2.091221	18.372252	1.000000	7556.358974	0.080636	0.965293	0.991131
4.827448	4.871343	4.915239	2.052822	16.949527	1.000000	7607.825980	0.080370	0.976286	0.993982
4.915239	4.957619	5.000000	2.017097	15.262258	1.000000	7396.436019	0.094177	0.959971	0.989736
Overall I/sigI = 30.115224									
Overall Completeness = 1.000000									
Overall Redundancy = 11030.316705									
Overall Rsplit = 0.033657									
Overall CC = 0.998197									
Overall CC* = 0.999549									
Note: R-factors are given as decimal numbers (usually <1)	not as percentages								

Save as *filename.csv* and open in Excel

2Å = 0.2nm, 1/0.2 = 5
Data better than 2Å!

Export as mtz - preliminary space group reminder