

REyes – Autonomous Electron Diffraction Software

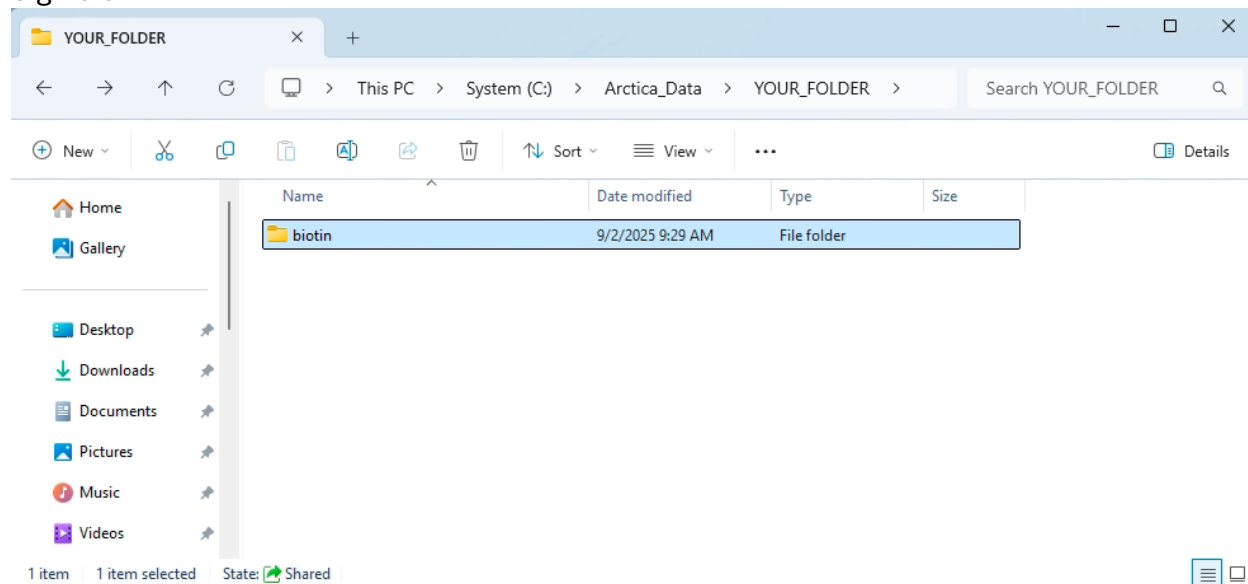
Start setting up REyes on Support PC followed by Scope PC or Apollo PC

I. On Support PC:

a. CETA camera

- In your user directory 'C:\Arctica_Data\{YOUR_FOLDER}' create a folder for the sample you plan to analyze

e.g. 'biotin'



- Open the WSL Ubuntu terminal and change the working directory to your created folder with REyes files

...

```
cd /mnt/c/Arctica_Data/YOUR_FOLDER/biotin
```

...

Activate python environment created upon REyes installation (in particular system we use micromamba for python) and run the command to start REyes, check the software works, and familiarize yourself with the help menu:

...

```
micromamba activate reyes_env
```

```
reyes-monitor -h
```

...

Because AutoProcess 2.0 and AutoSolve are fully integrated into REyes, their arguments are also displayed.

```

root@NPC9955630: /mnt/c/A
(reyes_env) root@NPC9955630: /mnt/c/Arctica_Data/YOUR_FOLDER/biotin# reyes-monitor -h

Thank you for using

=====
RRRRRRRRRR      EEEEEEEEEEE
RR      RR      EE
RR      RR      EE
RRRRRRRRRR      EEEEEEEEEEE yy yy eeeee sssss
RR      RR      EE      yy yy ee ee ss s
RR      RR      EE      yy yy eeeee ss
RR      RR      EE      yy ee ss
RR      RR      EE      yy ee e s ss
RR      RR      EEEEEEEEEEE yy eeeee sssss
=====

usage: reyes-monitor [-h]
                    [--microscope {Arctica-CETA,F200C-Apollo,Arctica-Apollo-SM,Arctica-Apollo-Prot,F30-TVIPS,Spectra-CETA}]
                    [--filtering {default,1,4,9,16,25,36,49,64,81,100,121,144,169,196,96,None}] [--manual-squares]
                    [--camera-length CAMERA_LENGTH] [--top-target-per-category TOP_TARGET_PER_CATEGORY]
                    [--top-target-per-block TOP_TARGET_PER_BLOCK]
                    [--starting-state {WAITING_FOR_MONTAGE,WAITING_FOR_GRID_SQUARES,WAITING_FOR_MANUAL_SQUARES,WAITING_FOR_DIFFRACTION_MAP,GENERATING_TARGETS,GENERATING_FINAL_MAP,WAITING_FOR_MOVIES,RUNNING_AUTOSOLVE,COMPLETED}]
                    [--current-block CURRENT_BLOCK] [--stepscan-only] [--autoprocess]
                    [--microscope-config MICROSCOPE_CONFIG] [--rotation-axis ROTATION_AXIS] [--frame-size FRAME_SIZE]
                    [--signal-pixel SIGNAL_PIXEL] [--min-pixel MIN_PIXEL] [--background-pixel BACKGROUND_PIXEL]
                    [--pixel-size PIXEL_SIZE] [--wavelength WAVELENGTH] [--beam-center-x BEAM_CENTER_X]
                    [--beam-center-y BEAM_CENTER_Y] [--file-extension FILE_EXTENSION] [--autosolve]
                    [--shelx {t,d,td}] [--ntryt NTRYT] [--ntryf NTRYF]

REyes Processing Monitor Settings

options:
  -h, --help            show this help message and exit
  --microscope {Arctica-CETA,F200C-Apollo,Arctica-Apollo-SM,Arctica-Apollo-Prot,F30-TVIPS,Spectra-CETA}
                        Microscope configuration to use

REyes arguments:
  Arguments for REyes processing

  --filtering {default,1,4,9,16,25,36,49,64,81,100,121,144,169,196,96,None}
                        Filtering type to use (default: default)
  --manual-squares      Enable manual squares processing step
  --camera-length CAMERA_LENGTH
                        Optional override for camera length in mm (default: based on microscope config)
  --top-target-per-category TOP_TARGET_PER_CATEGORY
                        Number of top targets to select per category (used by create-final-targets)
  --top-target-per-block TOP_TARGET_PER_BLOCK
                        Number of top targets to select per block (used by create-final-targets)
  --starting-state {WAITING_FOR_MONTAGE,WAITING_FOR_GRID_SQUARES,WAITING_FOR_MANUAL_SQUARES,WAITING_FOR_DIFFRACTION_MAP,GENERATING_TARGETS,GENERATING_FINAL_MAP,WAITING_FOR_MOVIES,RUNNING_AUTOSOLVE,COMPLETED}
                        States:
                          WAITING_FOR_MONTAGE: Wait for montage image acquisition
                          WAITING_FOR_GRID_SQUARES: Wait for grid squares processing and eucentricity
                          WAITING_FOR_MANUAL_SQUARES: Wait for manual grid squares selection
                          WAITING_FOR_DIFFRACTION_MAP: Wait for diffraction mapping
                          GENERATING_TARGETS: Generate target lists
                          GENERATING_FINAL_MAP: Generate final diffraction atlas
                          WAITING_FOR_MOVIES: Wait for movie acquisition
                          RUNNING_AUTOSOLVE: Run AutoSolve for structure solution
                          COMPLETED: Processing completed
  --current-block CURRENT_BLOCK
                        Current block number (for diffraction map state)
  --stepscan-only       Do not collect tilt series movies for targets
  --autoprocess         Run AutoProcess after movie acquisition

Autoprocess arguments:
  Arguments passed to autoprocess.py

  --microscope-config MICROSCOPE_CONFIG

```

- Initiate REyes FSD with preferred settings:

```
...
```

```

reyes-monitor --microscope Arctica-CETA --filtering 9 --top-targets-
per-category 4 --autoprocess --microscope-config Arctica-CETA-mrc-SM
--autosolve --shelx d

```

```
...
```

```

root@NPC9955630: /mnt/c/A  X  +  v
(reyes_env) root@NPC9955630:/mnt/c/Arctica_Data/YOUR_FOLDER/biotin# reyes-monitor --microscope Arctica-CETA --filtering 9
--top-target-per-category 4 --autoprocess --microscope-config Arctica-CETA-mrc-SM --autosolve --shelx d

Thank you for using

=====
RRRRRRRRR  EEEEEEEEE
RR   RR   EE
RR   RR   EE
RRRRRRRRR  EEEEEEEEE  yy  yy  eeee  sssss
RR   RR   EE          yy  yy  ee   ee  ss  s
RR   RR   EE          yy  yy  eeeee  ss
RR   RR   EE          yy  ee   e   ss
RR   RR   EE          yy  ee   e  s  ss
RR   RR  EEEEEEEEEEE  yy  eeeee  sssss
=====

2025-09-02 09:48:49 - Initializing with state: WAITING_FOR_MONTAGE
2025-09-02 09:48:49 - Current block: 1
2025-09-02 09:48:49 - Starting monitoring in working directory: /mnt/c/Arctica_Data/YOUR_FOLDER/biotin

```

Description of arguments:

- `--microscope Arctica-CETA` selects camera-specific diffraction processing parameters for a given microscope;
- `--filtering 9` indicates that 9 grid squares near the stage origin (0, 0) in a square arrangement will be selected for analysis;
- `--top-targets-per-category 4` selects crystal target selection method with set of 4 targets from each of REyes categories: Quality, # of diffraction peaks, and frame intensity;
- `--microscope-config Arctica-CETA-mrc-SM` chooses AutoProcess parameters;
- `--autosolve --shelx d` enables SHELXD-only phasing for the indexed data.

You can adjust settings to expand (or lower) the number of screened grid squares and collect 1 best target from each grid square, as in this example:

```

...
reyes-monitor --microscope Arctica-CETA --filtering 25 --top-targets-per-block 1 --autoprocess --microscope-config Arctica-CETA-mrc-SM
--autosolve --shelx d
...

```

Once launched, REyes will monitor for all necessary files to arrive in the folder and process them as they come. Every step will be carefully logged.

NOTE: You can run REyes without AutoSolve but still collect and index movies by removing `--autosolve --shelx d` arguments.

NOTE: You can run REyes without AutoProcess but still collect movies by removing `--autoprocess --microscope-config Arctica-CETA-mrc-SM` arguments.

NOTE: Alternatively, if you run REyes for diffraction mapping only, add `--stepscan-only` argument.

NOTE: Preferred REyes launch parameters could also be added as an alias to the .bashrc (or any other shell you use) and they can be called by a simplified command such as REyes-CETA. The following command will add the settings demonstrated above and they will be available as REyes-CETA after restarting WSL terminal.

```
```
```

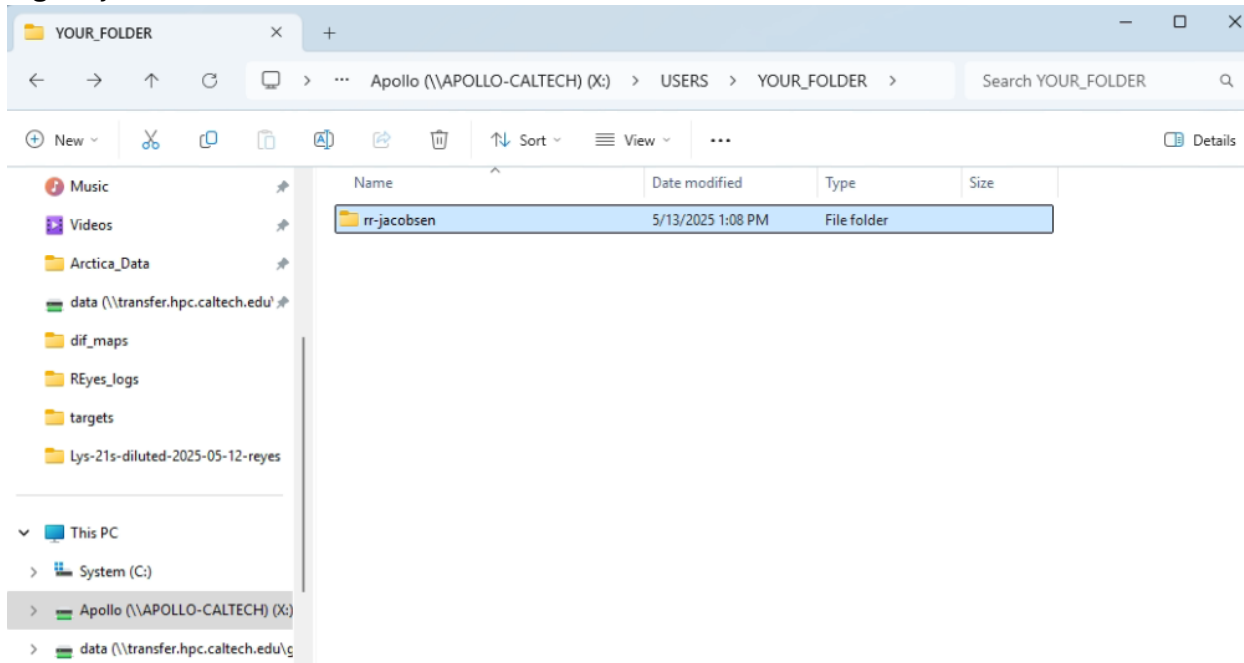
```
echo "alias REyes-CETA='reyes-monitor --microscope Arctica-CETA -
-filtering 25 --top-targets-per-block 1 --autoprocess --
microscope-config Arctica-CETA-mrc-SM --autosolve --shelx d'" >>
~/.bashrc
```

```
```
```

REyes has several other powerful features that are well documented, feel free to reach out to the developer (eremin@caltech.edu)

b. DE Apollo camera

- In your user directory 'X:\USERS\{USER_FOLDER\NAME}' create a folder for the sample you plan to analyze
e.g. 'rr-jacobsen'



- Open the WSL Ubuntu terminal and change the working directory to your created folder with REyes files

```
```
```

```
cd /mnt/x/USERS/YOUR_USER/rr-jacobsen
```

```
```
```

Run the command to start REyes, check the software works, and familiarize yourself with the help menu:

```
```
```

```
micromamba activate reyes_env
```

```
reyes-monitor -h
```

```
```
```

Because AutoProcess 2.0 and AutoSolve are fully integrated into REyes, their arguments are also displayed.

```

root@NPC9955630: /mnt/x/U  X  +  v
(reyes_env) root@NPC9955630:/mnt/x/USERS/YOUR_FOLDER/rr-jacobsen# reyes-monitor -h

Thank you for using

=====
RRRRRRRRRR  EEEEEEEEEEE
RR    RR    EE
RR    RR    EE
RRRRRRRRRR  EEEEEEEEEEE  yy  yy  eeeee  sssss
RR    RR    EE          yy  yy  ee  ee  ss  s
RR    RR    EE          yy  yy  eeeee  ss
RR    RR    EE          yy  ee  ss
RR    RR    EE          yy  ee  e  s  ss
RR    RR    EEEEEEEEEEE  yy  eeeee  sssss
=====

usage: reyes-monitor [-h]
                    [--microscope {Arctica-CETA,F200C-Apollo,Arctica-Apollo-SM,Arctica-Apollo-Prot,F30-TVIPS,Spectra-CETA}]
                    [--filtering {default,1,4,9,16,25,36,49,64,81,100,121,144,169,196,96,None}] [--manual-squares]
                    [--camera-length CAMERA_LENGTH] [--top-target-per-category TOP_TARGET_PER_CATEGORY]
                    [--top-target-per-block TOP_TARGET_PER_BLOCK]
                    [--starting-state {WAITING_FOR_MONTAGE,WAITING_FOR_GRID_SQUARES,WAITING_FOR_MANUAL_SQUARES,WAITING_FOR_DIFFRACTION_MAP,GENERATING_TARGETS,GENERATING_FINAL_MAP,WAITING_FOR_MOVIES,RUNNING_AUTOSOLVE,COMPLETED}]
                    [--current-block CURRENT_BLOCK] [--stepscan-only] [--autoprocess]
                    [--microscope-config MICROSCOPE_CONFIG] [--rotation-axis ROTATION_AXIS] [--frame-size FRAME_SIZE]
                    [--signal-pixel SIGNAL_PIXEL] [--min-pixel MIN_PIXEL] [--background-pixel BACKGROUND_PIXEL]
                    [--pixel-size PIXEL_SIZE] [--wavelength WAVELENGTH] [--beam-center-x BEAM_CENTER_X]
                    [--beam-center-y BEAM_CENTER_Y] [--file-extension FILE_EXTENSION] [--autosolve]
                    [--shelx {t,d,td}] [--ntryt NTRYT] [--ntryf NTRYF]

REyes Processing Monitor Settings

options:
  -h, --help            show this help message and exit
  --microscope {Arctica-CETA,F200C-Apollo,Arctica-Apollo-SM,Arctica-Apollo-Prot,F30-TVIPS,Spectra-CETA}
                        Microscope configuration to use

REyes arguments:
  Arguments for REyes processing

  --filtering {default,1,4,9,16,25,36,49,64,81,100,121,144,169,196,96,None}
                        Filtering type to use (default: default)
  --manual-squares      Enable manual squares processing step
  --camera-length CAMERA_LENGTH
                        Optional override for camera length in mm (default: based on microscope config)
  --top-target-per-category TOP_TARGET_PER_CATEGORY
                        Number of top targets to select per category (used by create-final-targets)
  --top-target-per-block TOP_TARGET_PER_BLOCK
                        Number of top targets to select per block (used by create-final-targets)
  --starting-state {WAITING_FOR_MONTAGE,WAITING_FOR_GRID_SQUARES,WAITING_FOR_MANUAL_SQUARES,WAITING_FOR_DIFFRACTION_MAP,GENERATING_TARGETS,GENERATING_FINAL_MAP,WAITING_FOR_MOVIES,RUNNING_AUTOSOLVE,COMPLETED}
                        States:
                          WAITING_FOR_MONTAGE: Wait for montage image acquisition
                          WAITING_FOR_GRID_SQUARES: Wait for grid squares processing and eucentricity
                          WAITING_FOR_MANUAL_SQUARES: Wait for manual grid squares selection
                          WAITING_FOR_DIFFRACTION_MAP: Wait for diffraction mapping
                          GENERATING_TARGETS: Generate target lists
                          GENERATING_FINAL_MAP: Generate final diffraction atlas
                          WAITING_FOR_MOVIES: Wait for movie acquisition
                          RUNNING_AUTOSOLVE: Run AutoSolve for structure solution
                          COMPLETED: Processing completed
  --current-block CURRENT_BLOCK
                        Current block number (for diffraction map state)
  --stepscan-only       Do not collect tilt series movies for targets
  --autoprocess         Run AutoProcess after movie acquisition

Autoprocess arguments:
  Arguments passed to autoprocess.py

  --microscope-config MICROSCOPE_CONFIG

```

- Initiate REyes FSD with preferred settings:

```

...

```

```

reyes-monitor --microscope Arctica-Apollo --filtering 16
--top-targets-per-category 3 --autoprocess --microscope-config
Talos-Apollo-SM --autosolve --shelx d
...

```

```

root@NPC9955630: /mnt/x/U X + v
(reyes_env) root@NPC9955630: /mnt/x/USERS/YOUR_FOLDER/rr-jacobsen# reyes-monitor --microscope Arctica-Apollo-SM --filtering 16
--top-target-per-category 3 --autoprocess --microscope-config Talos-Apollo-SM --autosolve --shelx d

Thank you for using

=====
RRRRRRRRR  EEEEEEEEEEE
RR   RR   EE
RR   RR   EE
RRRRRRRRR  EEEEEEEEEEE  yy   yy  eeeee  sssss
RR   RR   EE           yy  yy  ee   ee  ss   s
RR   RR   EE           yy  yy  eeeee   ss
RR   RR   EE           yy   ee   e     ss
RR   RR   EE           yy   ee   e  s   ss
RR   RR  EEEEEEEEEEE  yy   eeeee  sssss
=====

2025-09-02 09:59:42 - Initializing with state: WAITING_FOR_MONTAGE
2025-09-02 09:59:42 - Current block: 1
2025-09-02 09:59:42 - Starting monitoring in working directory: /mnt/x/USERS/YOUR_FOLDER/rr-jacobsen

```

Description of arguments:

- `--microscope Arctica-Apollo` selects camera-specific diffraction processing parameters for a given microscope;
- `--filtering 16` indicates that 16 grid squares near the stage origin (0, 0) in a square arrangement will be selected for analysis;
- `--top-targets-per-category 3` selects crystal target selection method with set of 3 targets from each of REyes categories: Quality, # of diffraction peaks, and frame intensity;
- `--microscope-config Talos-Apollo-SM` chooses AutoProcess parameters;
- `--autosolve --shelx d` enables SHELXD-only phasing for the indexed data.

You can adjust settings to lower (or extend) the number of screened grid squares and collect 1 best target from each grid square, as in this example:

```

...
reyes-monitor --microscope Arctica-Apollo --filtering 9 --top-targets-per-block 1 --autoprocess --microscope-config Talos-Apollo-SM
--autosolve --shelx d
...

```

Once launched, REyes will monitor for all necessary files to arrive in the folder and process them as they come. Every step will be carefully logged.

NOTE: You can run REyes without AutoSolve but still collect and index movies by removing `--autosolve --shelx d` arguments.

NOTE: You can run REyes without AutoProcess but still collect movies by removing `--autoprocess --microscope-config Talos-Apollo-SM` arguments.

NOTE: Alternatively, if you run REyes for diffraction mapping only, add `--stepscan-only` argument.

NOTE: Preferred REyes launch parameters could also be added as an alias to the .bashrc (or any other shell you use) and they can be called by a simplified command such as REyes-Apollo. The following command will add the settings demonstrated above and they will be available as REyes-Apollo after restarting WSL terminal.

```
```\n\necho "alias REyes-Apollo='reyes-monitor --microscope Arctica-\nApollo --filtering 25 --top-targets-per-block 1 --autoprocess --\nmicroscope-config Talos-Apollo-SM --autosolve --shelx d'" >>\n~/ .bashrc\n```\n
```

REyes has several other powerful features that are well documented, feel free to reach out to the developer ([eremin@caltech.edu](mailto:eremin@caltech.edu))

*NOTE: AutoSolve is already implemented but still is in testing stage. Package will become public on GitHub later this year. In the meantime, please, email [eremin@caltech.edu](mailto:eremin@caltech.edu) to get a beta version of AutoSolve.*



## II. SerialEM

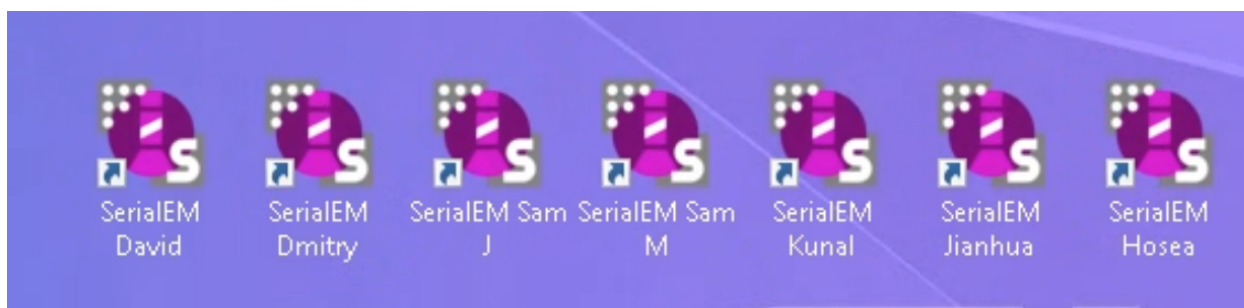
### a. On Scope PC (CETA)

- Load your grid onto the stage
- Open SerialEM by clicking the REYES icon on the right desktop



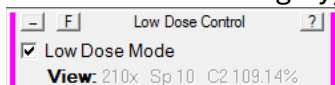
### b. On Apollo PC (DE Apollo)

- Load your grid onto the stage
- Open SerialEM by clicking the your personal icon on the right desktop

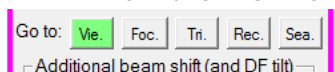


### c. Next steps are identical for both cameras

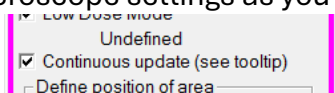
- Turn on Low Dose mode in SerialEM and turn Low Dose off in TFS software (button will become grey):



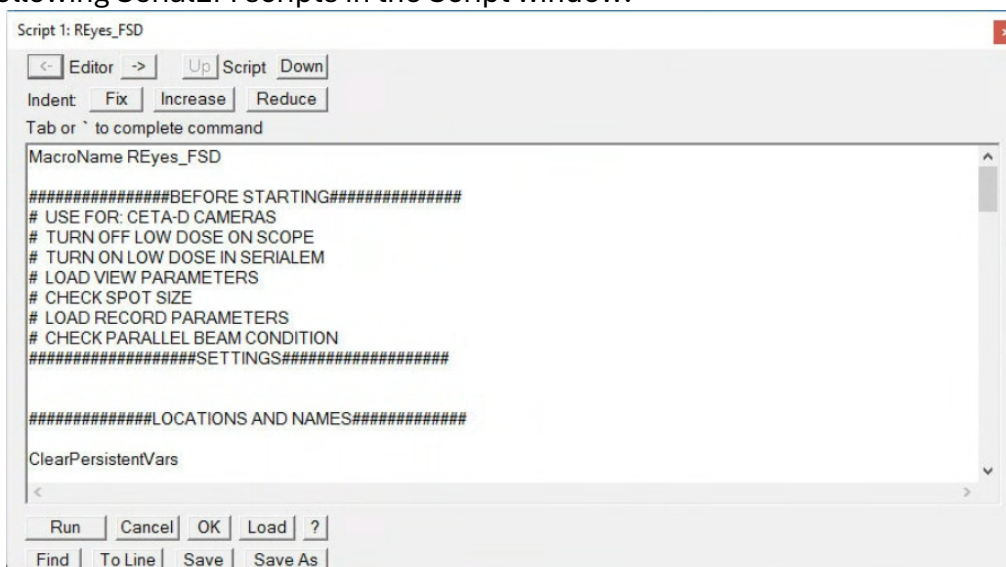
- Activate **View** low dose mode:



- Change condenser 2 aperture of 50  $\mu\text{m}$
- Keep beam stop in
- Open column valves
- Check 'Continuous update' in the low dose section. This will continuously save microscope settings as you set up the microscope.



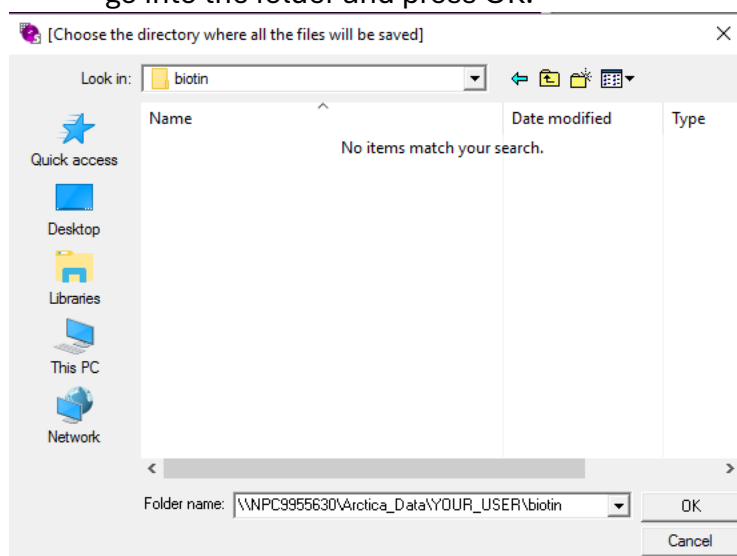
- Adjust beam centering, focus, etc., as needed, if needed. Stick to true focus!
- Move to an empty area and change mode to **Record** in SerialEM
- You can check beam intensity focus in imaging and diffraction mode now. (While 'Continuous update' is checked, all changes you make will be saved.)
- Adjust beam centering if needed.
- CRITICAL STEP! Go back and forth between **View** and **Record 3 – 5 times** and adjust beam centering in **Record** every time. Ensure that the 'Continuous update' is still being checked. You want SerialEM to save adjustments of settings as you make them. With this step, you make sure the beam is stable and does not drift in **Record** mode.
- Uncheck 'Continuous update' in the low dose section.
- Once the beam is stable and you are ready, stay in **View** mode and open one of the following SerialEM scripts in the Script window:



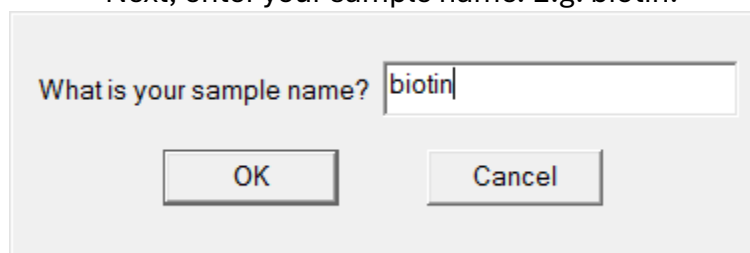
- Script 3: REyes\_Screen
- Script 5: REyes\_FSD
- Script 7: REyes\_Manual-1

(If you choose Manual mode for REyes, consult the developer at [eremin@caltech.edu](mailto:eremin@caltech.edu) for onboarding and additional instructions. A detailed user tutorial will become public soon. Stay tuned.)

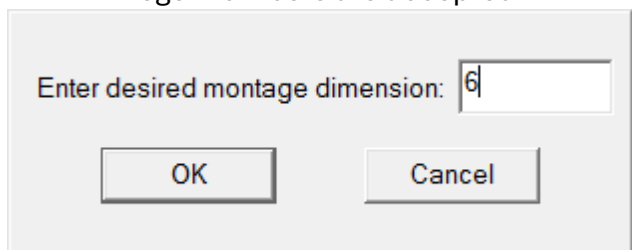
- Press 'Run' for the selected Script and follow the next steps as SerialEM asks you for input information
- In the popped window, choose a folder for the sample you created:
  - CETA: on the mounted Support PC A:\ drive location;
  - Apollo: on the mounted Apollo PC X:\ drive location;go into the folder and press OK:



- Next, enter your sample name. E.g. biotin:

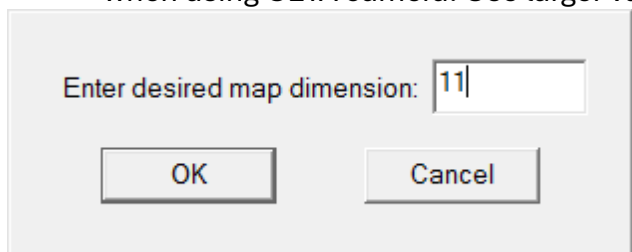


- Next, enter the dimension of the montage you need. E.g. 6 means it will be 6x6; only integer numbers are accepted:



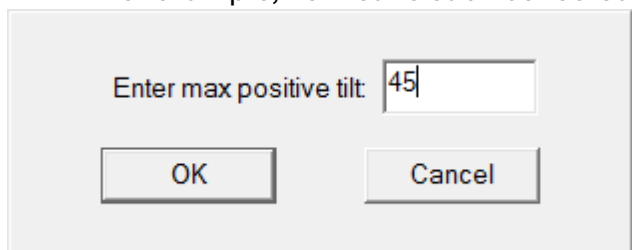
A dialog box with a light gray background. It contains a text label "Enter desired montage dimension:" followed by a text input field containing the number "6". Below the input field are two buttons: "OK" on the left and "Cancel" on the right.

- Next, enter the dimension of the diffraction mapping blocks (only integer numbers are accepted).  
11 is the recommended value for mesh 200 grids. Each grid square will be imaged in diffraction space for an 11x11 area with a 5  $\mu\text{m}$  step. This block will take *ca.* 16 min when using CETA camera. Use larger values for other grid mesh sizes.



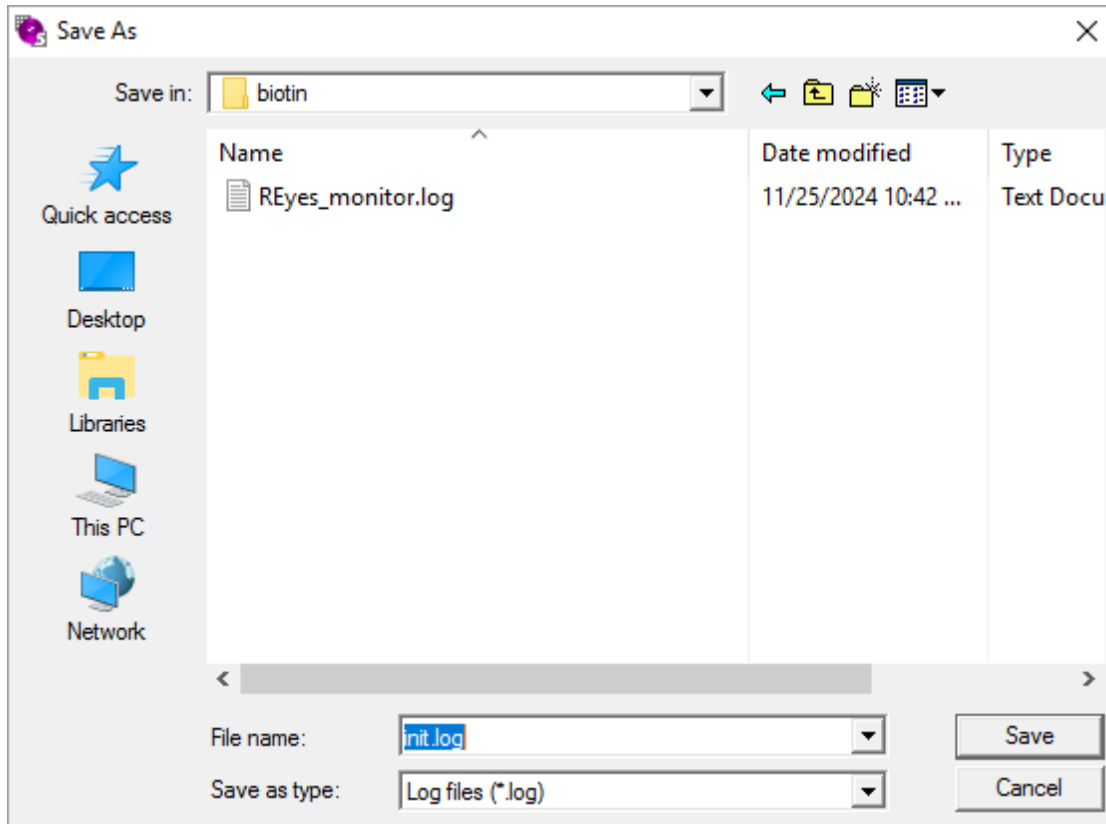
A dialog box with a light gray background. It contains a text label "Enter desired map dimension:" followed by a text input field containing the number "11". Below the input field are two buttons: "OK" on the left and "Cancel" on the right.

- If you run REyes in FSD mode, enter the maximum positive tilt for the tilt series collection next (integer numbers are recommended).  
For example, 45 means each collected movie will be in the +45 to -45 range.



A dialog box with a light gray background. It contains a text label "Enter max positive tilt:" followed by a text input field containing the number "45". Below the input field are two buttons: "OK" on the left and "Cancel" on the right.

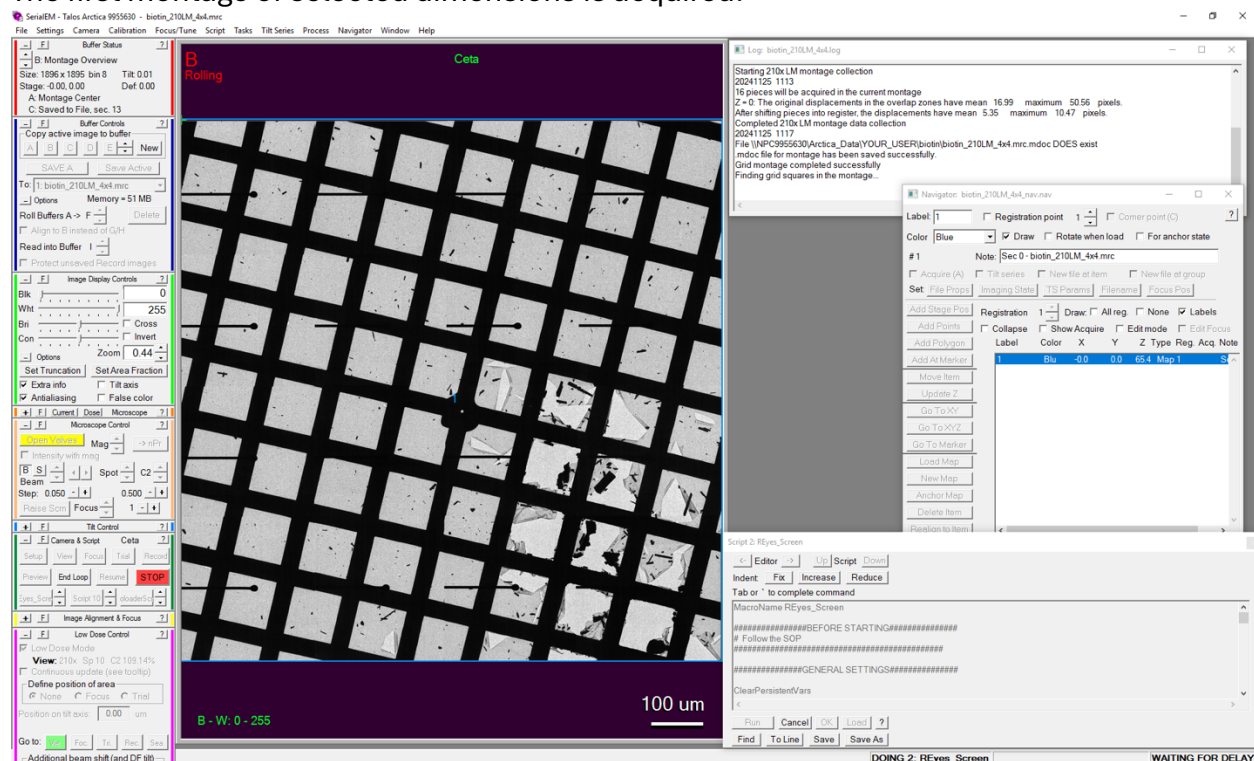
- You will be asked to save the current SerialEM log. It is recommended that you save it into the same folder for your sample as init.log; make sure you choose the correct location to avoid losing it. REyes monitoring log file is already there.



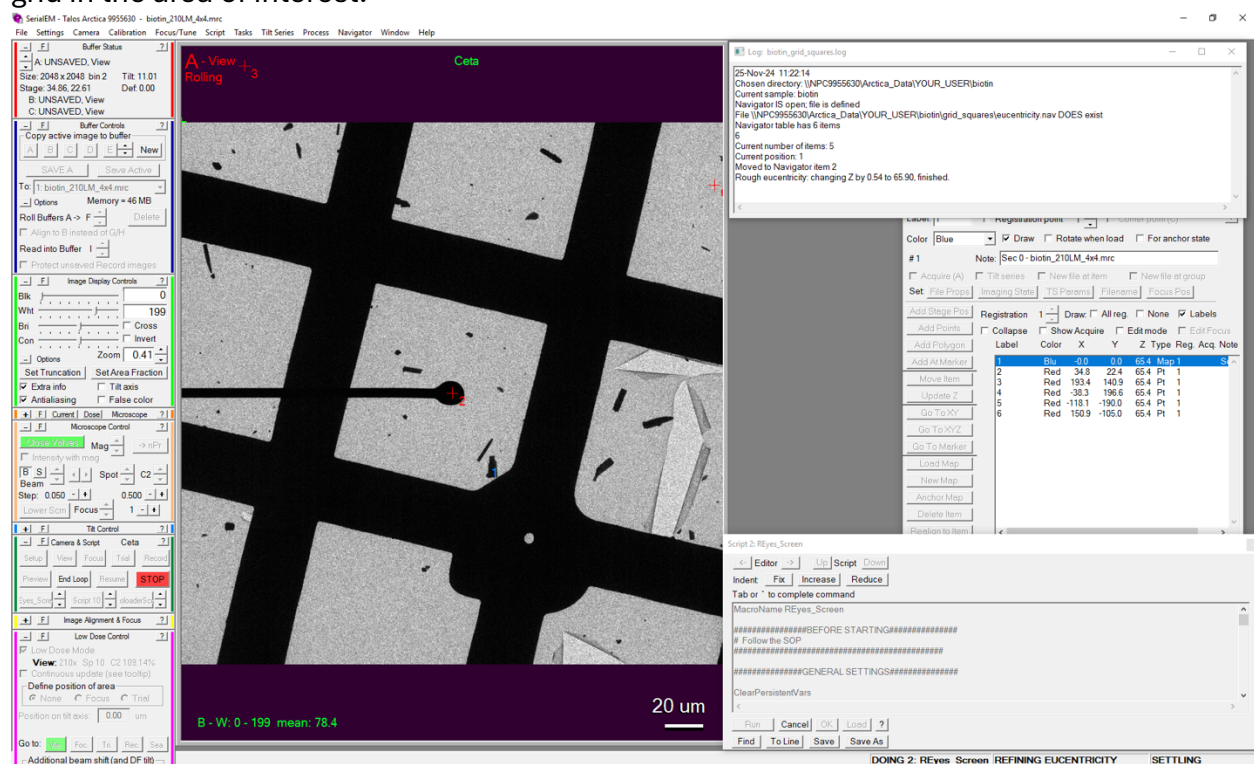
Now, REyes will take care of everything from montage to eucentricity, diffraction screening, and movie collection!

## Workflow details (For REyes in Screen mode).

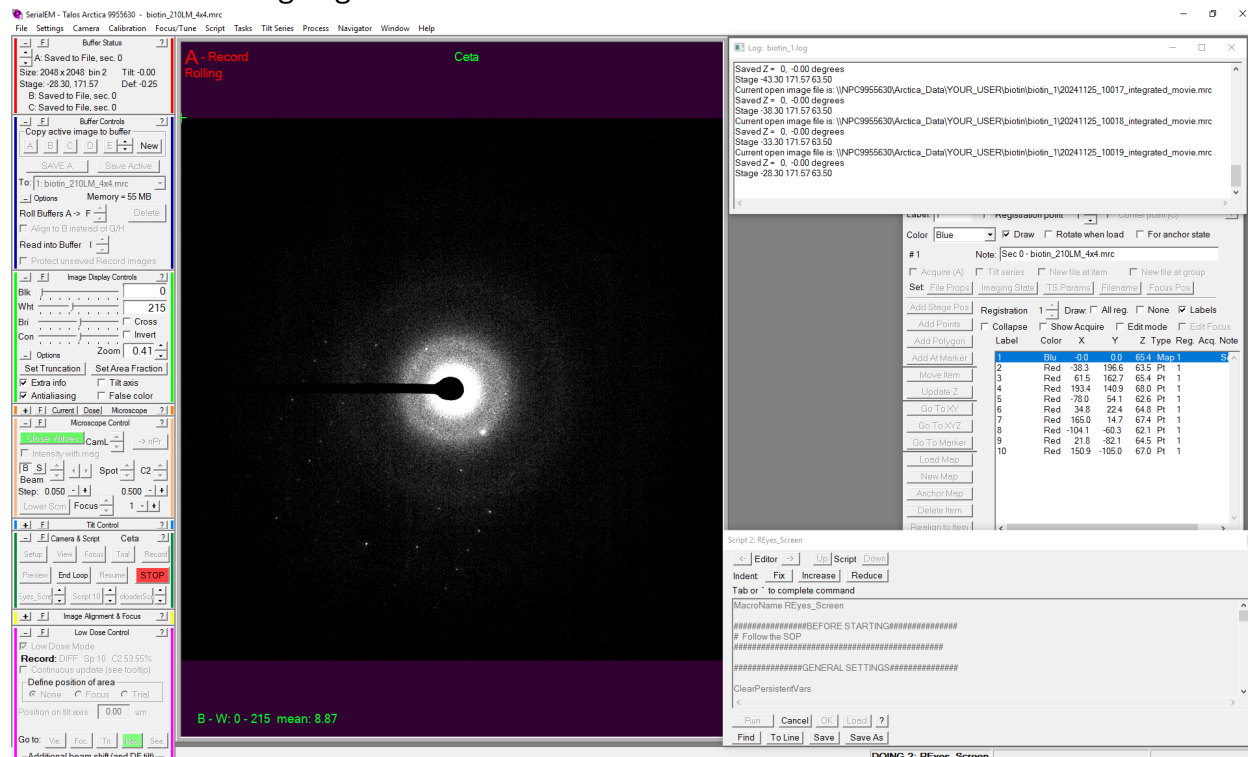
The first montage of selected dimensions is acquired:



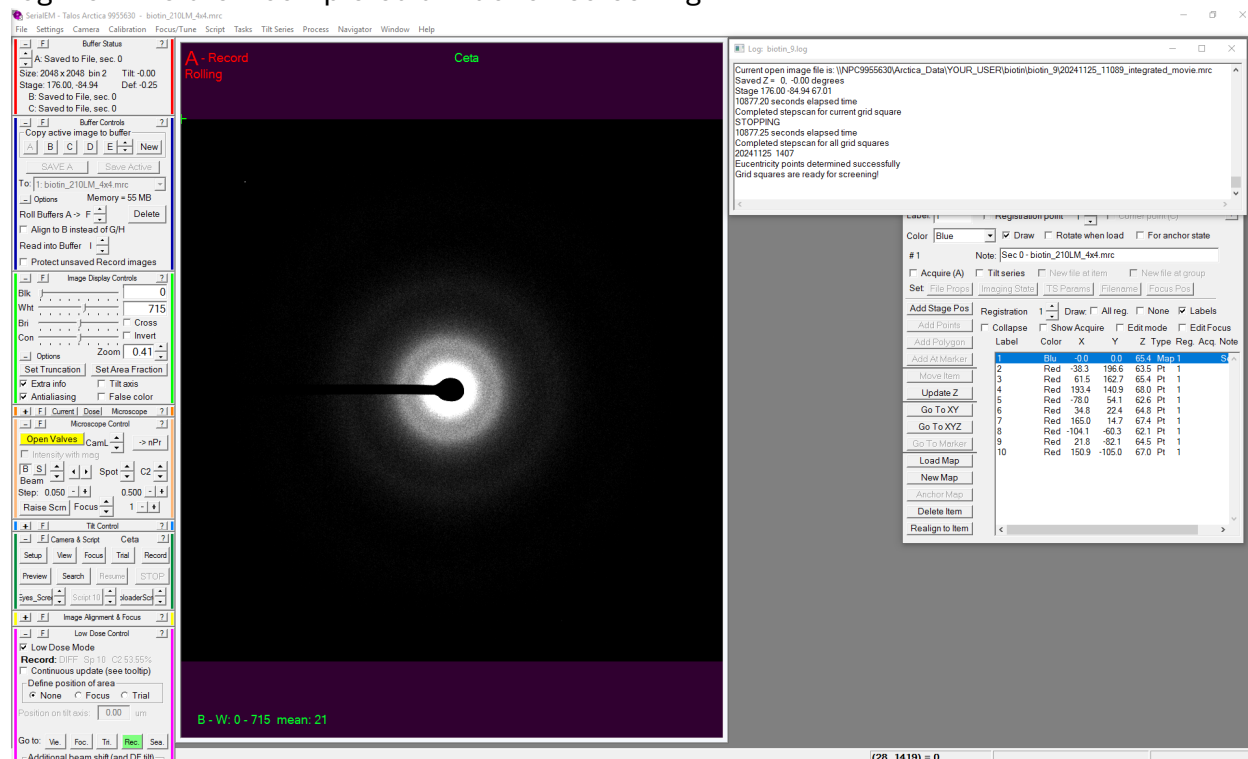
After the montage, the eucentricity plane will be found using 5 geometrical points on the grid in the area of interest:



Once the eucentric plane is obtained, grid squares of interest will be passed along, and diffraction screening begins.



After diffraction screening, column valves will be closed, and the beam will be blanked. A log file will state it completed diffraction screening:





On the Support PC, the REyes monitor will also indicate completion:

```

root@NPC9955630: /mnt/c/A X + v - □ X

Selected item at coordinates (-3.23, -107.16)
Selected 2 items, skipped 4 items
Successfully parsed 36 items from targets_sum.nav
Selected item at coordinates (81.46, 152.67)
Selected item at coordinates (-67.95, 34.04)
Selected 2 items, skipped 3 items
Successfully created targets.nav with 6 items

Processing completed successfully!

2024-11-25 14:12:59 - Successfully executed create final nav script
2024-11-25 14:12:59 - Moving to final map generation state
2024-11-25 14:13:04 - Starting plot diffraction atlas script
2024-11-25 14:13:04 - Executing command: /root/.micromamba/envs/reyes_env/bin/python /mnt/c/Arctica_Data/YOUR_USER/biotin/3-0_mnt_maps_targets.py
2024-11-25 14:14:07 - Process output:
Thank you for using

=====
RRRRRRRRRR EEEEEEEEEEE
RR RR EE
RR RR EE
RRRRRRRRRR EEEEEEEEE yy yy eeeee sssss
RR RR EE yy yy ee ee ss s
RR RR EE yy yy eeeee ss
RR RR EE yy ee ss
RR RR EE yy ee e s ss
RR RR EEEEEEEEEEE yy eeeee sssss
=====

/root/.micromamba/envs/reyes_env/lib/python3.12/site-packages/numpy/_core/getlimits.py:545: UserWarning: Signature b'\x00\xd0\xcc\xcc\xcc\xcc\xcc\xcc\xfb\xbf\x00\x00\x00\x00\x00\x00' for <class 'numpy.longdouble'> does not match any known type: falling back to type probe function.
This warnings indicates broken support for the dtype!
 machar = _get_machar(dtype)

REyes FMP v3.0.2 will plot:
- Montage background
- Diffraction map overlay
- Selected targets

Processing map from /mnt/c/Arctica_Data/YOUR_USER/biotin/dif_map_sums.csv
Using automatic plot limits: x[-163.81, 253.18], y[-170.19, 251.79]
Processing map from /mnt/c/Arctica_Data/YOUR_USER/biotin/dif_map_sums.csv
Using automatic plot limits: x[-163.81, 253.18], y[-170.19, 251.79]
Processing map from /mnt/c/Arctica_Data/YOUR_USER/biotin/dif_map_sums.csv
Using automatic plot limits: x[-163.81, 253.18], y[-170.19, 251.79]
Processing map from /mnt/c/Arctica_Data/YOUR_USER/biotin/dif_map_sums.csv
Using automatic plot limits: x[-163.81, 253.18], y[-170.19, 251.79]
Processing map from /mnt/c/Arctica_Data/YOUR_USER/biotin/dif_map_sums.csv
Using automatic plot limits: x[-163.81, 253.18], y[-170.19, 251.79]

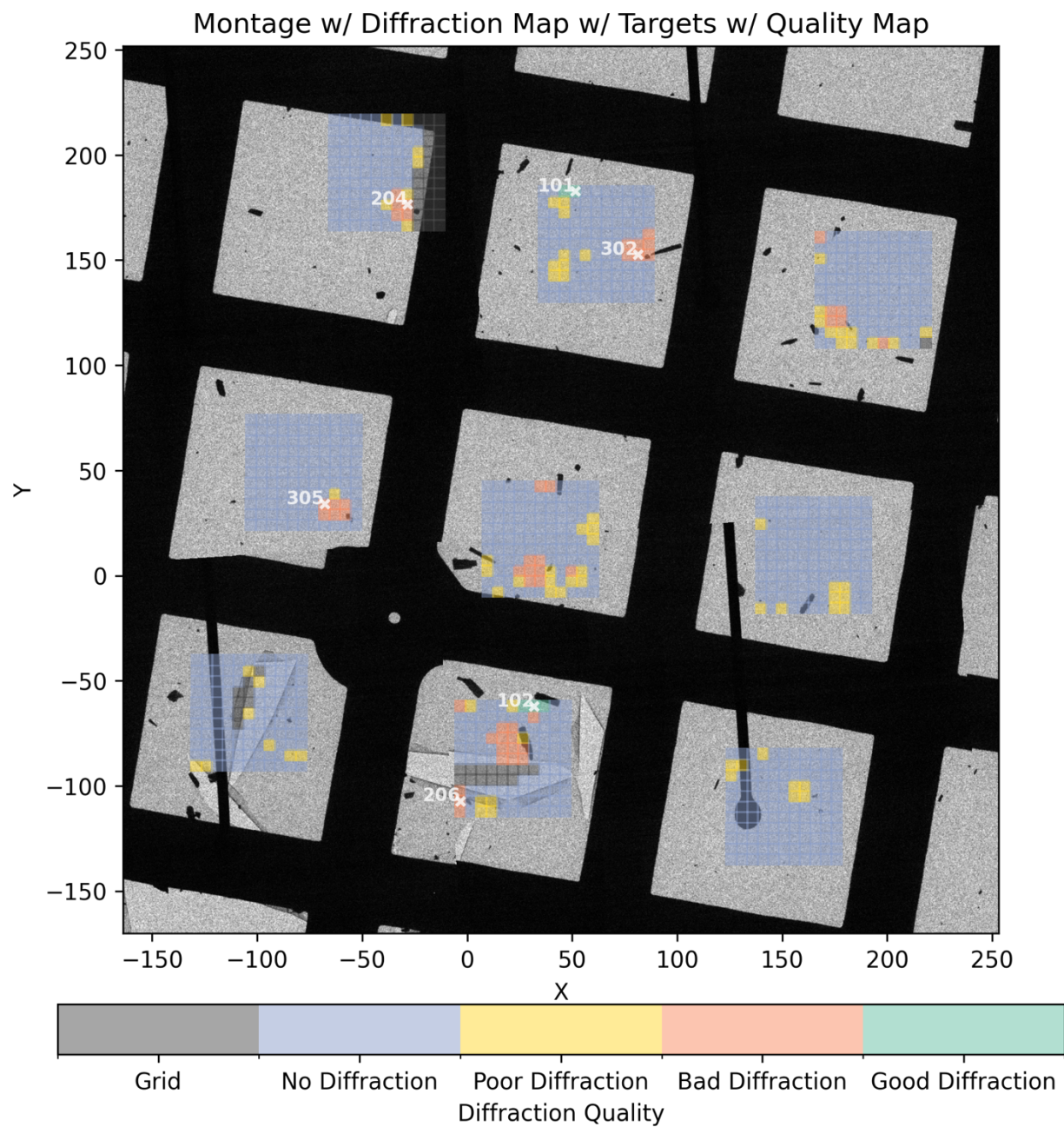
Processing completed successfully!

2024-11-25 14:14:07 - Successfully executed plot diffraction atlas script
2024-11-25 14:14:07 - Processing completed
root@NPC9955630: /mnt/c/Arctica_Data/YOUR_USER/biotin#

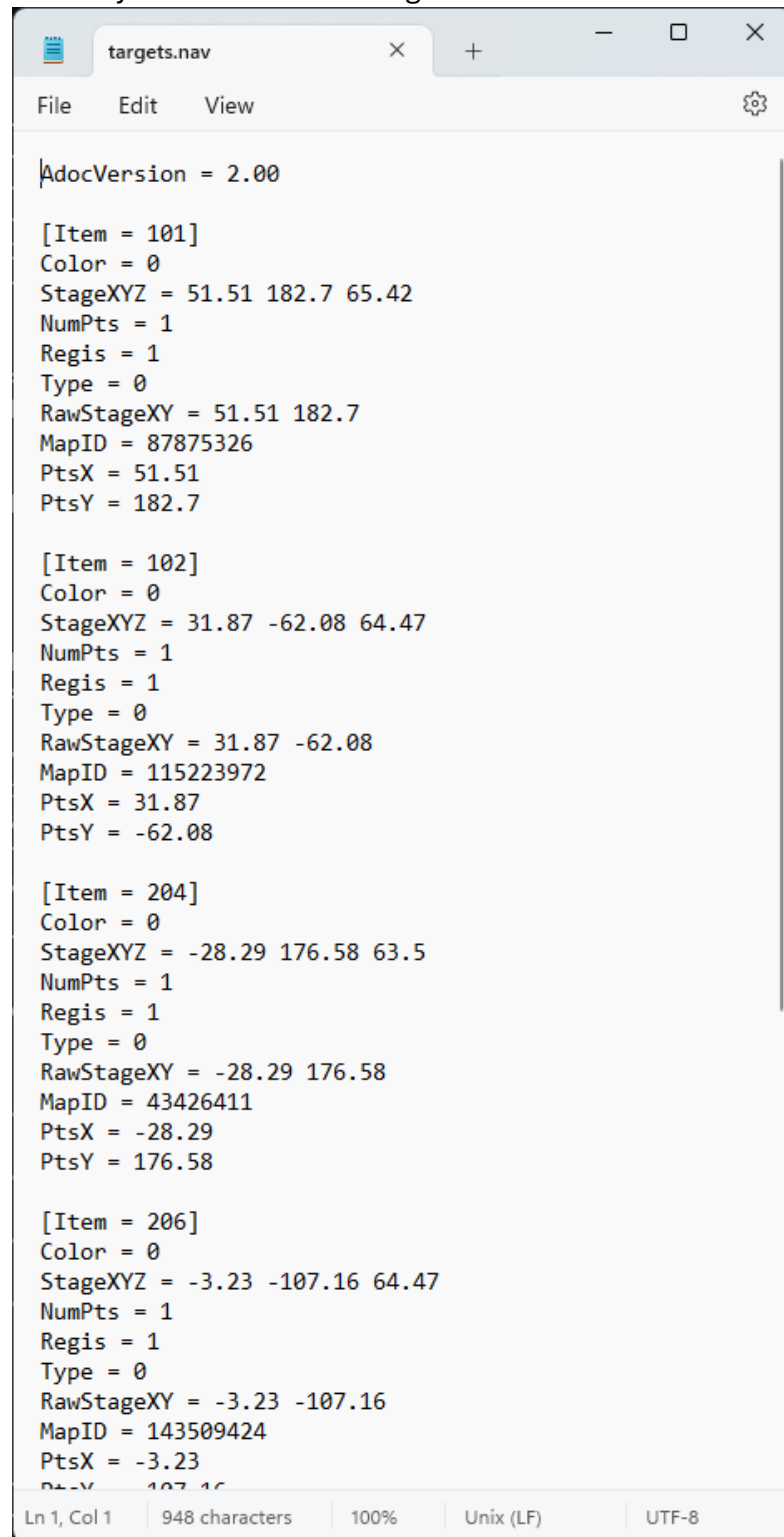
```



Review the generated maps, especially the quality ones:



Best coordinates for targets based on quality, number of diffraction peaks and diffraction intensity are saved to the 'targets.nav' file:



```
AdocVersion = 2.00

[Item = 101]
Color = 0
StageXYZ = 51.51 182.7 65.42
NumPts = 1
Regis = 1
Type = 0
RawStageXY = 51.51 182.7
MapID = 87875326
PtsX = 51.51
PtsY = 182.7

[Item = 102]
Color = 0
StageXYZ = 31.87 -62.08 64.47
NumPts = 1
Regis = 1
Type = 0
RawStageXY = 31.87 -62.08
MapID = 115223972
PtsX = 31.87
PtsY = -62.08

[Item = 204]
Color = 0
StageXYZ = -28.29 176.58 63.5
NumPts = 1
Regis = 1
Type = 0
RawStageXY = -28.29 176.58
MapID = 43426411
PtsX = -28.29
PtsY = 176.58

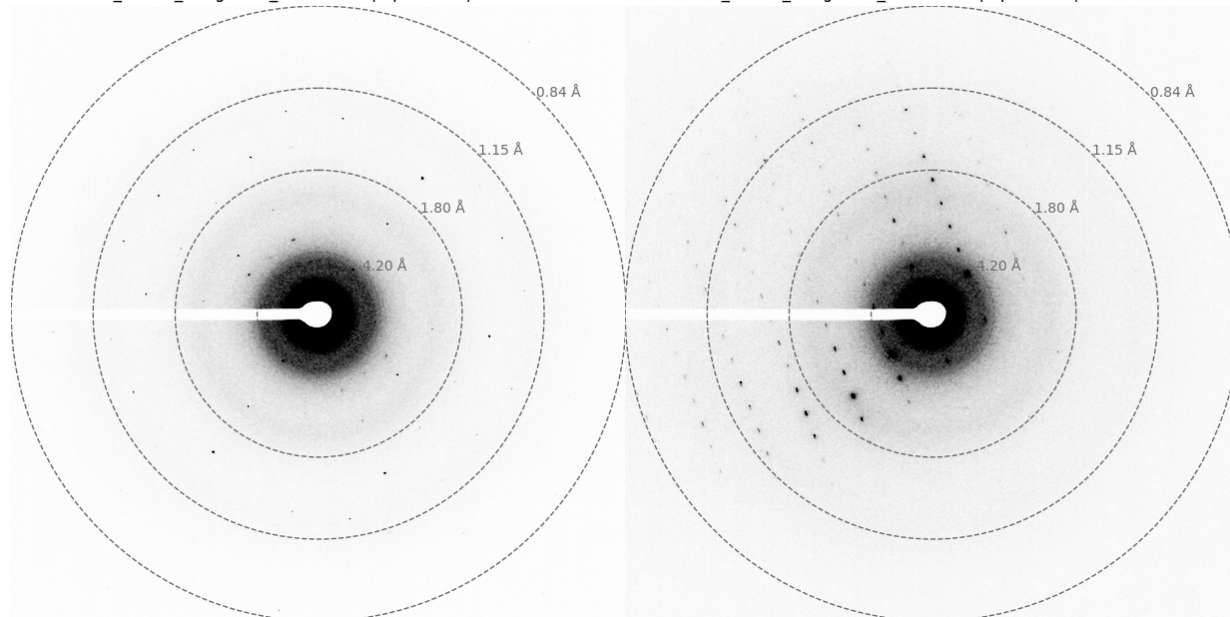
[Item = 206]
Color = 0
StageXYZ = -3.23 -107.16 64.47
NumPts = 1
Regis = 1
Type = 0
RawStageXY = -3.23 -107.16
MapID = 143509424
PtsX = -3.23
PtsY = -107.16
```

Targets in the 100 range are quality-based, 200 – number of diffraction spots, 300 – intensity.

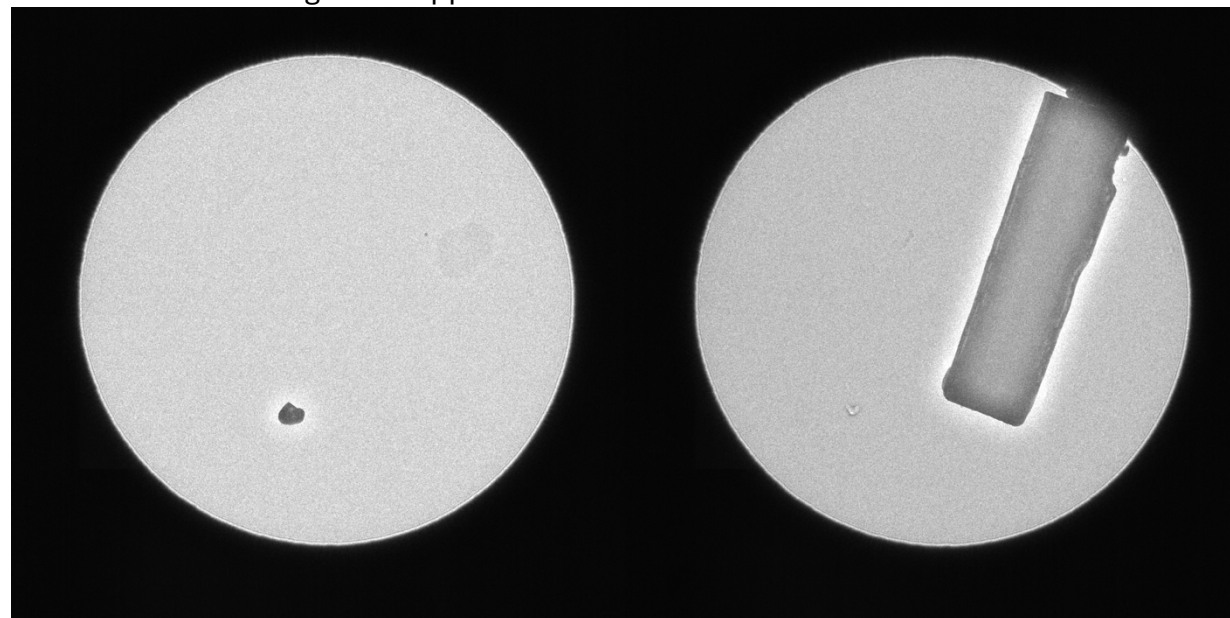
In this example, the two best-found biotin crystals, 101 and 102, were selected based on diffraction:

20241125\_10235\_integrated\_movie.mrc | Spots: 37 | Sum: 87875326

20241125\_10965\_integrated\_movie.mrc | Spots: 53 | Sum: 115223972



And have the following visual appearance:



Note that the stage position in these photos corresponds to the true selected coordinates, and the crystal has not been recentered intentionally.