

Look between the “stars”

- What was the pixel size we used to collect the data?
- Did we use the right value when we imported?
- Have we merged data in this pipeline?
- Which micrograph has the worst case of beam-induced motion?
- What is the box size used?
- Did my particles get extracted?

MOTIONCORR .STAR FILE

```
File Edit View Terminal Tabs Help
# version 50001

data_optics

loop
_rlnOpticsGroupName #1
_rlnOpticsGroup #2
_rlnMicrographOriginalPixelSize #3
_rlnVoltage #4
_rlnSphericalAberration #5
_rlnAmplitudeContrast #6
_rlnMicrographPixelSize #7
opticsGroup1 1 0.299500 300.000000 2.700000 0.100000 0.599000

# version 50001

data_micrographs

loop
_rlnCtfPowerSpectrum #1
_rlnMicrographName #2
_rlnMicrographMetadata #3
_rlnOpticsGroup #4
_rlnAccumMotionTotal #5
_rlnAccumMotionEarly #6
_rlnAccumMotionLate #7
MotionCorr/job003/data/22feb18a_c_00024gr_00006sq_v01_00007hl_00004ex_frames_mrc_PS.mrc MotionCorr/job003/data/22feb18a_c_00024gr_00006sq_v01_00007hl_00004ex_frames_mrc.mrc MotionCorr/job003
/data/22feb18a_c_00024gr_00006sq_v01_00007hl_00004ex_frames_mrc.star I 87.656830 10.490118 77.166712
MotionCorr/job003/data/22feb18a_c_00024gr_00006sq_v01_00007hl_00006ex_frames_mrc_PS.mrc MotionCorr/job003/data/22feb18a_c_00024gr_00006sq_v01_00007hl_00006ex_frames_mrc.mrc MotionCorr/job003
/data/22feb18a_c_00024gr_00006sq_v01_00007hl_00006ex_frames_mrc.star I 98.970564 9.439957 89.530607
MotionCorr/job003/data/22feb18a_c_00024gr_00006sq_v01_00007hl_00007ex_frames_mrc_PS.mrc MotionCorr/job003/data/22feb18a_c_00024gr_00006sq_v01_00007hl_00007ex_frames_mrc.mrc MotionCorr/job003
/data/22feb18a_c_00024gr_00006sq_v01_00007hl_00007ex_frames_mrc.star I 102.986207 10.696708 92.289499
MotionCorr/job003/data/22feb18a_c_00024gr_00006sq_v01_00007hl_00009ex_frames_mrc_PS.mrc MotionCorr/job003/data/22feb18a_c_00024gr_00006sq_v01_00007hl_00009ex_frames_mrc.mrc MotionCorr/job003
/data/22feb18a_c_00024gr_00006sq_v01_00007hl_00009ex_frames_mrc.star I 118.037664 9.307539 108.730125
MotionCorr/job003/data/22feb18a_c_00024gr_00006sq_v01_00007hl_00010ex_frames_mrc_PS.mrc MotionCorr/job003/data/22feb18a_c_00024gr_00006sq_v01_00007hl_00010ex_frames_mrc.mrc MotionCorr/job003
/data/22feb18a_c_00024gr_00006sq_v01_00007hl_00010ex_frames_mrc.star I 101.748843 9.774639 91.974204
MotionCorr/job003/data/22feb18a_c_00024gr_00006sq_v01_00007hl_00012ex_frames_mrc_PS.mrc MotionCorr/job003/data/22feb18a_c_00024gr_00006sq_v01_00007hl_00012ex_frames_mrc.mrc MotionCorr/job003
/data/22feb18a_c_00024gr_00006sq_v01_00007hl_00012ex_frames_mrc.star I 127.192950 6.356208 120.836743
MotionCorr/job003/data/22feb18a_c_00024gr_00006sq_v01_00008hl_00006ex_frames_mrc_PS.mrc MotionCorr/job003/data/22feb18a_c_00024gr_00006sq_v01_00008hl_00006ex_frames_mrc.mrc MotionCorr/job003
/data/22feb18a_c_00024gr_00006sq_v01_00008hl_00006ex_frames_mrc.star I 100.124575 8.387675 91.736900
@@@
```

CTFFIND .STAR FILE

```
File Edit View Terminal Tabs Help
# version 50001

data_optics

loop
_rlnOpticsGroupName #1
_rlnOpticsGroup #2
_rlnMicrographOriginalPixelSize #3
_rlnVoltage #4
_rlnSphericalAberration #5
_rlnAmplitudeContrast #6
_rlnMicrographPixelSize #7
opticsGroup1 1 0.299500 300.000000 2.700000 0.100000 0.599000

# version 50001

data_micrographs

loop
_rlnMicrographName #1
_rlnOpticsGroup #2
_rlnCtfImage #3
_rlnDefocusU #4
_rlnDefocusV #5
_rlnCtfAstigmatism #6
_rlnDefocusAngle #7
_rlnCtfFigureOfMerit #8
_rlnCtfMaxResolution #9
_rlnCtfIceRingDensity #10
MotionCorr/job003/data/22feb18a_c_00024gr_00006sq_v01_00007hl_00004ex_frames_mrc.mrc 1 CtfFind/job004/data/22feb18a_c_00024gr_00006sq_v01_00007hl_00004ex_frames_mrc_PS.ctf:mrc 115
57.298828 11002.017578 555.281250 -30.88050 0.141870 3.183070 0.801670
MotionCorr/job003/data/22feb18a_c_00024gr_00006sq_v01_00007hl_00006ex_frames_mrc.mrc 1 CtfFind/job004/data/22feb18a_c_00024gr_00006sq_v01_00007hl_00006ex_frames_mrc_PS.ctf:mrc 86
19.941406 8291.441406 328.500000 -16.56563 0.115045 3.850488 1.399660
MotionCorr/job003/data/22feb18a_c_00024gr_00006sq_v01_00007hl_00007ex_frames_mrc.mrc 1 CtfFind/job004/data/22feb18a_c_00024gr_00006sq_v01_00007hl_00007ex_frames_mrc_PS.ctf:mrc 76
76.532715 7367.039062 309.493652 -15.98214 0.125570 3.060644 2.580320
MotionCorr/job003/data/22feb18a_c_00024gr_00006sq_v01_00007hl_00009ex_frames_mrc.mrc 1 CtfFind/job004/data/22feb18a_c_00024gr_00006sq_v01_00007hl_00009ex_frames_mrc_PS.ctf:mrc 100
17.360352 9588.654297 428.706055 -26.29451 0.110285 3.410432 2.739880
MotionCorr/job003/data/22feb18a_c_00024gr_00006sq_v01_00007hl_00010ex_frames_mrc.mrc 1 CtfFind/job004/data/22feb18a_c_00024gr_00006sq_v01_00007hl_00010ex_frames_mrc_PS.ctf:mrc 119
45.680664 11511.793945 433.886719 -16.62733 0.116208 3.226084 1.652540
MotionCorr/job003/data/22feb18a_c_00024gr_00006sq_v01_00007hl_00012ex_frames_mrc.mrc 1 CtfFind/job004/data/22feb18a_c_00024gr_00006sq_v01_00007hl_00012ex_frames_mrc_PS.ctf:mrc 50
15.837402 4423.685547 592.151855 -27.06781 0.109507 3.394269 2.118720
```


AUTOPICK .STAR FILE

```
File Edit View Terminal Tabs Help
# version 50001
data_coordinate_files
loop
_rlnMicrographName #1
_rlnMicrographCoordinates #2
Mics-ln/19jan04d_Mix13gr2_00004gr_00034sq_v02_00007hln_00003enn-a-DW.mrc AutoPick/job004/Mics-ln/19jan04d_Mix13gr2_00004gr_00034sq_v02_00007hln_00003enn-a-DW_autopick.star
Mics-ln/19jan04d_Mix13gr2_00007gr_00023sq_v02_00008hln_00005enn-a-DW.mrc AutoPick/job004/Mics-ln/19jan04d_Mix13gr2_00007gr_00023sq_v02_00008hln_00005enn-a-DW_autopick.star
Mics-ln/19jan04d_Mix13gr2_00003gr_00004sq_v02_00002hln_00007enn-a-DW.mrc AutoPick/job004/Mics-ln/19jan04d_Mix13gr2_00003gr_00004sq_v02_00002hln_00007enn-a-DW_autopick.star
Mics-ln/19jan04d_Mix13gr2_00003gr_00010sq_v02_00006hln_00005enn-a-DW.mrc AutoPick/job004/Mics-ln/19jan04d_Mix13gr2_00003gr_00010sq_v02_00006hln_00005enn-a-DW_autopick.star
Mics-ln/19jan04d_Mix13gr2_00006gr_00028sq_v02_00010hln_00004enn-a-DW.mrc AutoPick/job004/Mics-ln/19jan04d_Mix13gr2_00006gr_00028sq_v02_00010hln_00004enn-a-DW_autopick.star
Mics-ln/19jan04d_Mix13gr2_00002gr_00014sq_v02_00005hln_00002enn-a-DW.mrc AutoPick/job004/Mics-ln/19jan04d_Mix13gr2_00002gr_00014sq_v02_00005hln_00002enn-a-DW_autopick.star
Mics-ln/19jan04d_Mix13gr2_00004gr_00033sq_v02_00003hln_00006enn-a-DW.mrc AutoPick/job004/Mics-ln/19jan04d_Mix13gr2_00004gr_00033sq_v02_00003hln_00006enn-a-DW_autopick.star
Mics-ln/19jan04d_Mix13gr2_00006gr_00030sq_v02_00002hln_00004enn-a-DW.mrc AutoPick/job004/Mics-ln/19jan04d_Mix13gr2_00006gr_00030sq_v02_00002hln_00004enn-a-DW_autopick.star
Mics-ln/19jan04d_Mix13gr2_00006gr_00049sq_v02_00006hln_00002enn-a-DW.mrc AutoPick/job004/Mics-ln/19jan04d_Mix13gr2_00006gr_00049sq_v02_00006hln_00002enn-a-DW_autopick.star
Mics-ln/19jan04d_Mix13gr2_00007gr_00019sq_v02_00002hln_00010enn-a-DW.mrc AutoPick/job004/Mics-ln/19jan04d_Mix13gr2_00007gr_00019sq_v02_00002hln_00010enn-a-DW_autopick.star
Mics-ln/19jan04d_Mix13gr2_00004gr_00034sq_v02_00003hln_00007enn-a-DW.mrc AutoPick/job004/Mics-ln/19jan04d_Mix13gr2_00004gr_00034sq_v02_00003hln_00007enn-a-DW_autopick.star
Mics-ln/19jan04d_Mix13gr2_00005gr_00037sq_v02_00004hln_00005enn-a-DW.mrc AutoPick/job004/Mics-ln/19jan04d_Mix13gr2_00005gr_00037sq_v02_00004hln_00005enn-a-DW_autopick.star
Mics-ln/19jan04d_Mix13gr2_00002gr_00013sq_v02_00009hln_00004enn-a-DW.mrc AutoPick/job004/Mics-ln/19jan04d_Mix13gr2_00002gr_00013sq_v02_00009hln_00004enn-a-DW_autopick.star
Mics-ln/19jan04d_Mix13gr2_00007gr_00019sq_v02_00005hln_00008enn-a-DW.mrc AutoPick/job004/Mics-ln/19jan04d_Mix13gr2_00007gr_00019sq_v02_00005hln_00008enn-a-DW_autopick.star
Mics-ln/19jan04d_Mix13gr2_00006gr_00002sq_v02_00006hln_v01_00007enn-a-DW.mrc AutoPick/job004/Mics-ln/19jan04d_Mix13gr2_00006gr_00002sq_v02_00006hln_v01_00007enn-a-DW_autopick.star
Mics-ln/19jan04d_Mix13gr2_00005gr_00039sq_v02_00009hln_00002enn-a-DW.mrc AutoPick/job004/Mics-ln/19jan04d_Mix13gr2_00005gr_00039sq_v02_00009hln_00002enn-a-DW_autopick.star
Mics-ln/19jan04d_Mix13gr2_00006gr_00029sq_v02_00003hln_00003enn-a-DW.mrc AutoPick/job004/Mics-ln/19jan04d_Mix13gr2_00006gr_00029sq_v02_00003hln_00003enn-a-DW_autopick.star
Mics-ln/19jan04d_Mix13gr2_00014gr_00044sq_v02_00008hln_00003enn-a-DW.mrc AutoPick/job004/Mics-ln/19jan04d_Mix13gr2_00014gr_00044sq_v02_00008hln_00003enn-a-DW_autopick.star
Mics-ln/19jan04d_Mix13gr2_00005gr_00039sq_v02_00002hln_00003enn-a-DW.mrc AutoPick/job004/Mics-ln/19jan04d_Mix13gr2_00005gr_00039sq_v02_00002hln_00003enn-a-DW_autopick.star
Mics-ln/19jan04d_Mix13gr2_00005gr_00036sq_v02_00002hln_00004enn-a-DW.mrc AutoPick/job004/Mics-ln/19jan04d_Mix13gr2_00005gr_00036sq_v02_00002hln_00004enn-a-DW_autopick.star
```

EXTRACT PARTICLES .STAR FILE

```
File Edit View Terminal Tabs Help
_rlnCtfDataAreCtfPremultiplied #10
opticsGroup1      1      1.096000      300.000000      2.700000      0.100000      1.096000      360      2      0

# version 50001

data_particles

loop
_rlnCoordinateX #1
_rlnCoordinateY #2
_rlnAutopickFigureOfMerit #3
_rlnClassNumber #4
_rlnAnglePsi #5
_rlnImageName #6
_rlnMicrographName #7
_rlnOpticsGroup #8
_rlnCtfMaxResolution #9
_rlnCtfFigureOfMerit #10
_rlnDefocusU #11
_rlnDefocusV #12
_rlnDefocusAngle #13
_rlnCtfBfactor #14
_rlnCtfScalefactor #15
_rlnPhaseShift #16
1460.000000 1236.000000 4.851944 0 0.000000 000001@Extract/job014/Mics-ln/19jan04d_Mix13gr2_00004gr_00034sq_v02_00007hln_00003enn-a-DW.mrcs Mics-ln/19jan04d_Mix13gr2_000
04gr_00034sq_v02_00007hln_00003enn-a-DW.mrc 1 4.479900 0.119948 19400.328125 19360.400391 -37.49638 0.000000 1.000000 0.000000
2348.000000 1100.000000 4.256220 0 0.000000 000002@Extract/job014/Mics-ln/19jan04d_Mix13gr2_00004gr_00034sq_v02_00007hln_00003enn-a-DW.mrcs Mics-ln/19jan04d_Mix13gr2_000
04gr_00034sq_v02_00007hln_00003enn-a-DW.mrc 1 4.479900 0.119948 19400.328125 19360.400391 -37.49638 0.000000 1.000000 0.000000
1076.000000 1600.000000 3.656661 0 0.000000 000003@Extract/job014/Mics-ln/19jan04d_Mix13gr2_00004gr_00034sq_v02_00007hln_00003enn-a-DW.mrcs Mics-ln/19jan04d_Mix13gr2_000
04gr_00034sq_v02_00007hln_00003enn-a-DW.mrc 1 4.479900 0.119948 19400.328125 19360.400391 -37.49638 0.000000 1.000000 0.000000
624.000000 1036.000000 3.331323 0 0.000000 000004@Extract/job014/Mics-ln/19jan04d_Mix13gr2_00004gr_00034sq_v02_00007hln_00003enn-a-DW.mrcs Mics-ln/19jan04d_Mix13gr2_000
04gr_00034sq_v02_00007hln_00003enn-a-DW.mrc 1 4.479900 0.119948 19400.328125 19360.400391 -37.49638 0.000000 1.000000 0.000000
2396.000000 1580.000000 3.088531 0 0.000000 000005@Extract/job014/Mics-ln/19jan04d_Mix13gr2_00004gr_00034sq_v02_00007hln_00003enn-a-DW.mrcs Mics-ln/19jan04d_Mix13gr2_000
04gr_00034sq_v02_00007hln_00003enn-a-DW.mrc 1 4.479900 0.119948 19400.328125 19360.400391 -37.49638 0.000000 1.000000 0.000000
2876.000000 652.000000 2.887012 0 0.000000 000006@Extract/job014/Mics-ln/19jan04d_Mix13gr2_00004gr_00034sq_v02_00007hln_00003enn-a-DW.mrcs Mics-ln/19jan04d_Mix13gr2_000
04gr_00034sq_v02_00007hln_00003enn-a-DW.mrc 1 4.479900 0.119948 19400.328125 19360.400391 -37.49638 0.000000 1.000000 0.000000
588.000000 1760.000000 2.553856 0 0.000000 000007@Extract/job014/Mics-ln/19jan04d_Mix13gr2_00004gr_00034sq_v02_00007hln_00003enn-a-DW.mrcs Mics-ln/19jan04d_Mix13gr2_000
04gr_00034sq_v02_00007hln_00003enn-a-DW.mrc 1 4.479900 0.119948 19400.328125 19360.400391 -37.49638 0.000000 1.000000 0.000000
2456.000000 368.000000 2.396864 0 0.000000 000008@Extract/job014/Mics-ln/19jan04d_Mix13gr2_00004gr_00034sq_v02_00007hln_00003enn-a-DW.mrcs Mics-ln/19jan04d_Mix13gr2_000
04gr_00034sq_v02_00007hln_00003enn-a-DW.mrc 1 4.479900 0.119948 19400.328125 19360.400391 -37.49638 0.000000 1.000000 0.000000
1672.000000 1456.000000 2.369285 0 0.000000 000009@Extract/job014/Mics-ln/19jan04d_Mix13gr2_00004gr_00034sq_v02_00007hln_00003enn-a-DW.mrcs Mics-ln/19jan04d_Mix13gr2_000
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JOB .STAR FILE

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File Edit View Terminal Tabs Help

# version 50001

data_job

_rlnJobTypeLabel          relion.extract
_rlnJobIsContinue         0
_rlnJobIsTomo             0

# version 50001

data_joboptions_values

loop
_rlnJobOptionVariable #1
_rlnJobOptionValue #2
bg_diameter              -1
black_dust               -1
coords_suffix            AutoPick/job013/autopick.star
do_cut_into_segments    Yes
do_extract_helical_tubes Yes
do_extract_helix        No
do_float16              No
do_fom_threshold        No
do_invert               Yes
do_norm                 Yes
do_queue                No
do_recenter             No
do_reextract            No
do_rescale              No
do_reset_offsets        No
extract_size            360
fndata_reextract        ""
helical_bimodal_angular_priors Yes
helical_nr_asu          1
helical_rise            1
helical_tube_outer_diameter 200
min_dedicated           1
minimum_pick_fom        0
nr_mpi                  1
other_args               ""
qsub                    sbatch
```

https://relion.readthedocs.io/en/release-5.0/SPA_tutorial/Preprocessing.html