

# Tiltgroup\_wrangler.py Instructions

2023-03-04

# Go to Summary



[Home][Logout ricew01][ricew01 Profile] [summary] [user results] [processing] [make jpgs] [report]

Test (1) 22dec15b - mApof Krios 165k  
Select all projects -all microscopes

#images :9209

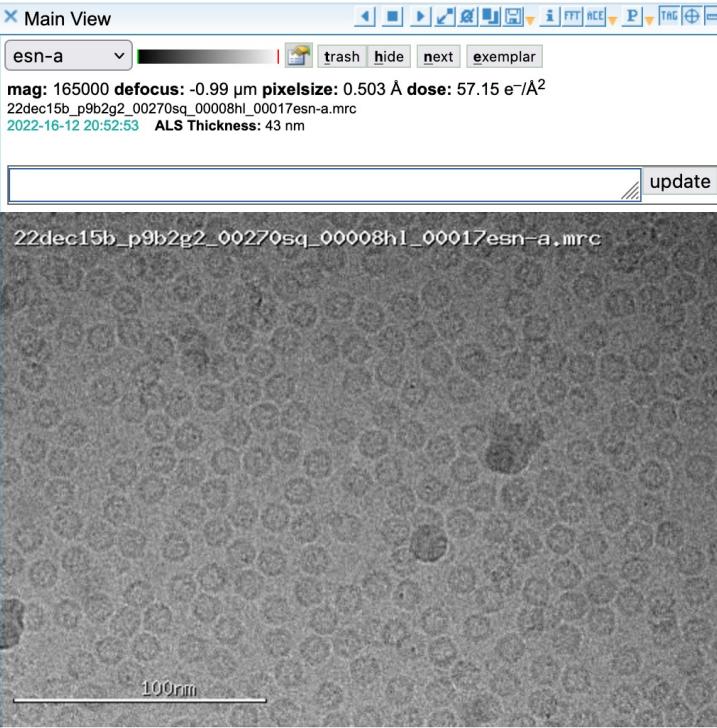
p9b2g2\_270sq\_8hl\_17esn-a  
p9b2g2\_270sq\_8hl\_16esn-a  
p9b2g2\_270sq\_8hl\_15esn-a  
p9b2g2\_270sq\_8hl\_14esn-a  
p9b2g2\_270sq\_8hl\_13esn-a  
p9b2g2\_270sq\_8hl\_12esn-a  
p9b2g2\_270sq\_8hl\_11esn-a  
p9b2g2\_270sq\_8hl\_10esn-a  
p9b2g2\_270sq\_8hl\_9esn-a  
p9b2g2\_270sq\_8hl\_8esn-a  
p9b2g2\_270sq\_8hl\_7esn-a  
p9b2g2\_270sq\_8hl\_6esn-a  
p9b2g2\_270sq\_8hl\_5esn-a  
p9b2g2\_270sq\_8hl\_4esn-a  
p9b2g2\_270sq\_8hl\_3esn-a  
p9b2g2\_270sq\_8hl\_2esn-a  
p9b2g2\_270sq\_7hl\_16esn-a  
p9b2g2\_270sq\_7hl\_15esn-a  
p9b2g2\_270sq\_7hl\_14esn-a  
p9b2g2\_270sq\_7hl\_13esn-a  
p9b2g2\_270sq\_7hl\_12esn-a  
p9b2g2\_270sq\_7hl\_11esn-a  
p9b2g2\_270sq\_7hl\_10esn-a  
p9b2g2\_270sq\_7hl\_9esn-a  
p9b2g2\_270sq\_7hl\_8esn-a  
p9b2g2\_270sq\_7hl\_7esn-a  
p9b2g2\_270sq\_7hl\_6esn-a

Main View esn-a trash hide next exemplar  
mag: 165000 defocus: -0.99 µm pixelsize: 0.503 Å dose: 57.15 e-/Å<sup>2</sup>  
22dec15b\_p9b2g2\_00270sq\_00008hl\_00017esn-a.mrc  
2022-16-12 20:52:53 ALS Thickness: 43 nm

update

22dec15b\_p9b2g2\_00270sq\_00008hl\_00017esn-a.mrc

100nm



# Scroll down to CTF information, click report

CTF

report »

maximum allowed CTF appion resolution (Å) for phase shift graph:

Phase shift by phase plate

Final mean for preset af

Too much information to display in summary

Click here to see the single graph

[data]

See summary in report »

Particles

report »

Imaging Summary

Preset label	Mag (X)	Dose (e <sup>-</sup> /Å <sup>2</sup> )	Pixel size (Å)	Dimensions	Binning	Image count
gr	82		4,426.4	1008x1008	8	28
sq	740		476.0	1440x1023	8	137
hl	3600		101.7	1440x1023	8	675
esn	165000	57.153	0.252	11520x8184	1	9209
esn-a	165000	57.153	0.503	5760x4092	2	9209
esn-a-DW	165000	57.153	0.503	5760x4092	2	9209

# Scroll down CTF report , click to download star file with beam tilt

Generate Histogram

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esn-a Preset  
Select Run: all Ctf Run  
Update Preset/Run Selection

→ [download star file for RELION 1.4](#)  
[download star file for Relion 3 without beam tilt values](#)  
[download star file with expected beam tilt for Relion 3.0](#)  
[download best ctf data](#)  
[download best ctf EMX file](#)

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**Relion star file with beam tilt group**

The number of tilt groups: 50 Relion version: 3.1 Download

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If you only want the Relion star file, choose number of groups and download star file directly

Generate Histogram

---

esn-a Preset  
Select Run: all Ctf Run  
Update Preset/Run Selection

download star file for RELION 1.4  
download star file for Relion 3 without beam tilt values  
download star file with expected beam tilt for Relion 3.0  
download best ctf data  
download best ctf EMX file

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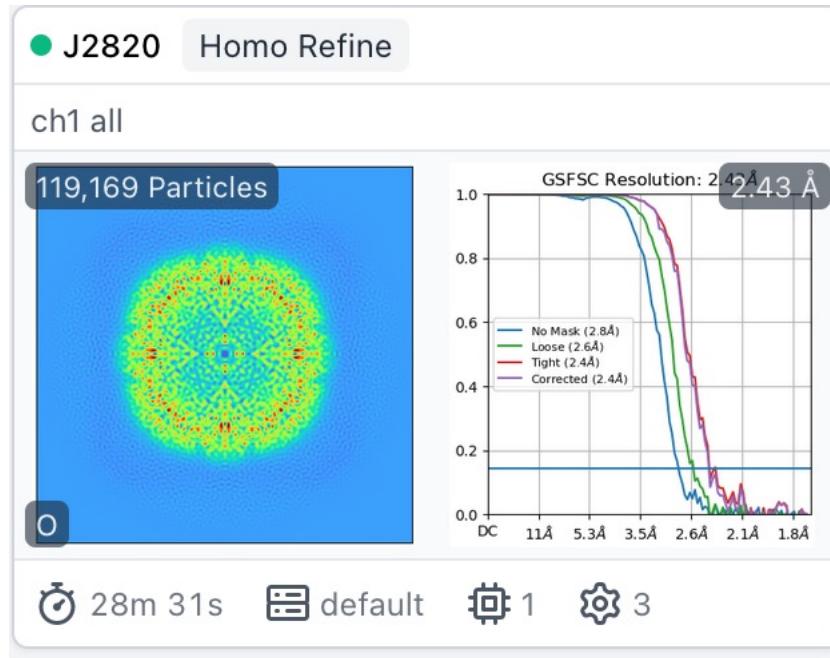
Relion star file with beam tilt group



The number of tilt groups: 50 Relion version: 3.1 Download

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# Copy over the required files from a refinement

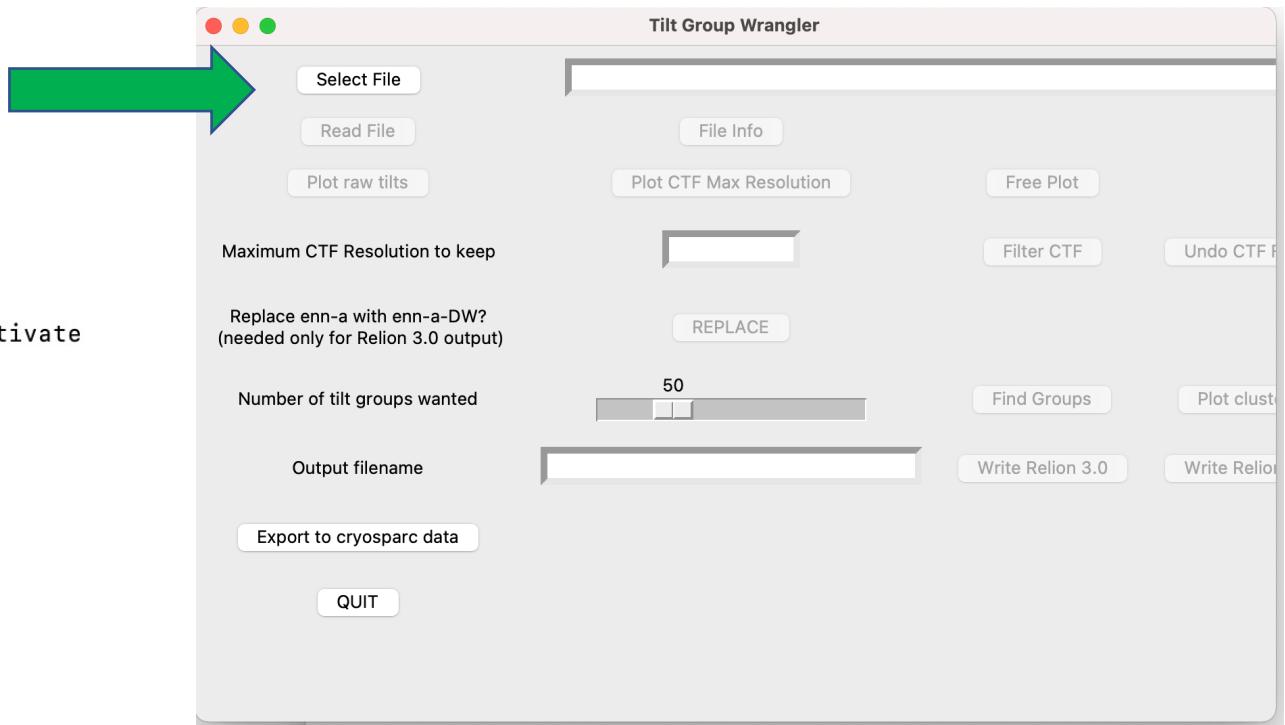


```
cryosparc_user@cryosparcpc-skirball:/mnt/raid5_2/cryosparc_user/P2/J2820$ ls -lh
total 547M
-rw-rw-r-- 1 cryosparc_user cryosparc_user 133K Mar 3 14:00 events.bson
drwxrwxr-x 2 cryosparc_user cryosparc_user 4.0K Mar 3 08:45 gridfs_data
-rw-rw-r-- 1 cryosparc_user cryosparc_user 40M Mar 3 08:45 J2820_011_particles.cs
-rw-rw-r-- 1 cryosparc_user cryosparc_user 247 Mar 3 08:45 J2820_011_volume_map.cs
-rw-rw-r-- 1 cryosparc_user cryosparc_user 254 Mar 3 08:45 J2820_011_volume_map_half_A.cs
-rw-rw-r-- 1 cryosparc_user cryosparc_user 65M Mar 3 08:45 J2820_011_volume_map_half_A.mrc
-rw-rw-r-- 1 cryosparc_user cryosparc_user 254 Mar 3 08:45 J2820_011_volume_map_half_B.cs
-rw-rw-r-- 1 cryosparc_user cryosparc_user 65M Mar 3 08:45 J2820_011_volume_map_half_B.mrc
-rw-rw-r-- 1 cryosparc_user cryosparc_user 65M Mar 3 08:45 J2820_011_volume_map.mrc
-rw-rw-r-- 1 cryosparc_user cryosparc_user 253 Mar 3 08:45 J2820_011_volume_map_sharp.cs
-rw-rw-r-- 1 cryosparc_user cryosparc_user 65M Mar 3 08:45 J2820_011_volume_map_sharp.mrc
-rw-rw-r-- 1 cryosparc_user cryosparc_user 257 Mar 3 08:45 J2820_011_volume_mask_fsc_auto.cs
-rw-rw-r-- 1 cryosparc_user cryosparc_user 65M Mar 3 08:45 J2820_011_volume_mask_fsc_auto.mrc
-rw-rw-r-- 1 cryosparc_user cryosparc_user 252 Mar 3 08:45 J2820_011_volume_mask_fsc.cs
-rw-rw-r-- 1 cryosparc_user cryosparc_user 65M Mar 3 08:45 J2820_011_volume_mask_fsc.mrc
-rw-rw-r-- 1 cryosparc_user cryosparc_user 255 Mar 3 08:45 J2820_011_volume_mask_refine.cs
-rw-rw-r-- 1 cryosparc_user cryosparc_user 65M Mar 3 08:45 J2820_011_volume_mask_refine.mrc
-rw-rw-r-- 1 cryosparc_user cryosparc_user 253 Mar 3 08:45 J2820_011_volume_precision.cs
-rw-rw-r-- 1 cryosparc_user cryosparc_user 33M Mar 3 08:45 J2820_011_volume_precision.mrc
-rw-rw-r-- 1 cryosparc_user cryosparc_user 257 Mar 3 14:00 J2820_mask.csg
-rw-rw-r-- 1 cryosparc_user cryosparc_user 619 Mar 3 14:00 J2820_particles.cs
-rw-rw-r-- 1 cryosparc_user cryosparc_user 27M Mar 3 08:45 J2820_passthrough_particles.cs
-rw-rw-r-- 1 cryosparc_user cryosparc_user 934 Mar 3 14:00 J2820_volume.csg
-rw-rw-r-- 1 cryosparc_user cryosparc_user 1.2M Mar 3 14:00 job.json
-rw-rw-r-- 1 cryosparc_user cryosparc_user 31K Mar 3 08:45 job.log
cryosparc_user@cryosparcpc-skirball:/mnt/raid5_2/cryosparc_user/P2/J2820$
```

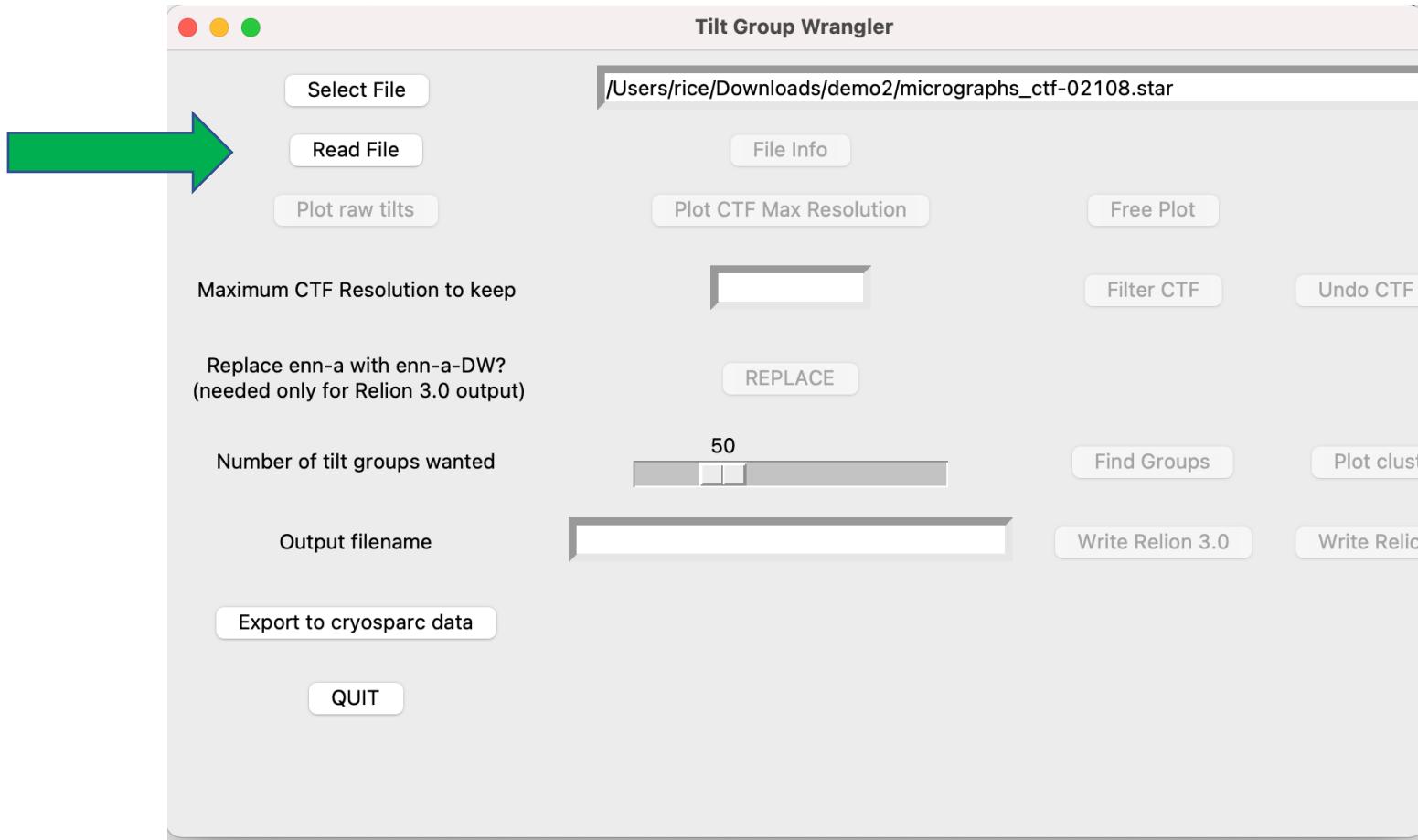
Files highlighted in blue

# Start tiltgroup\_wrangler.py

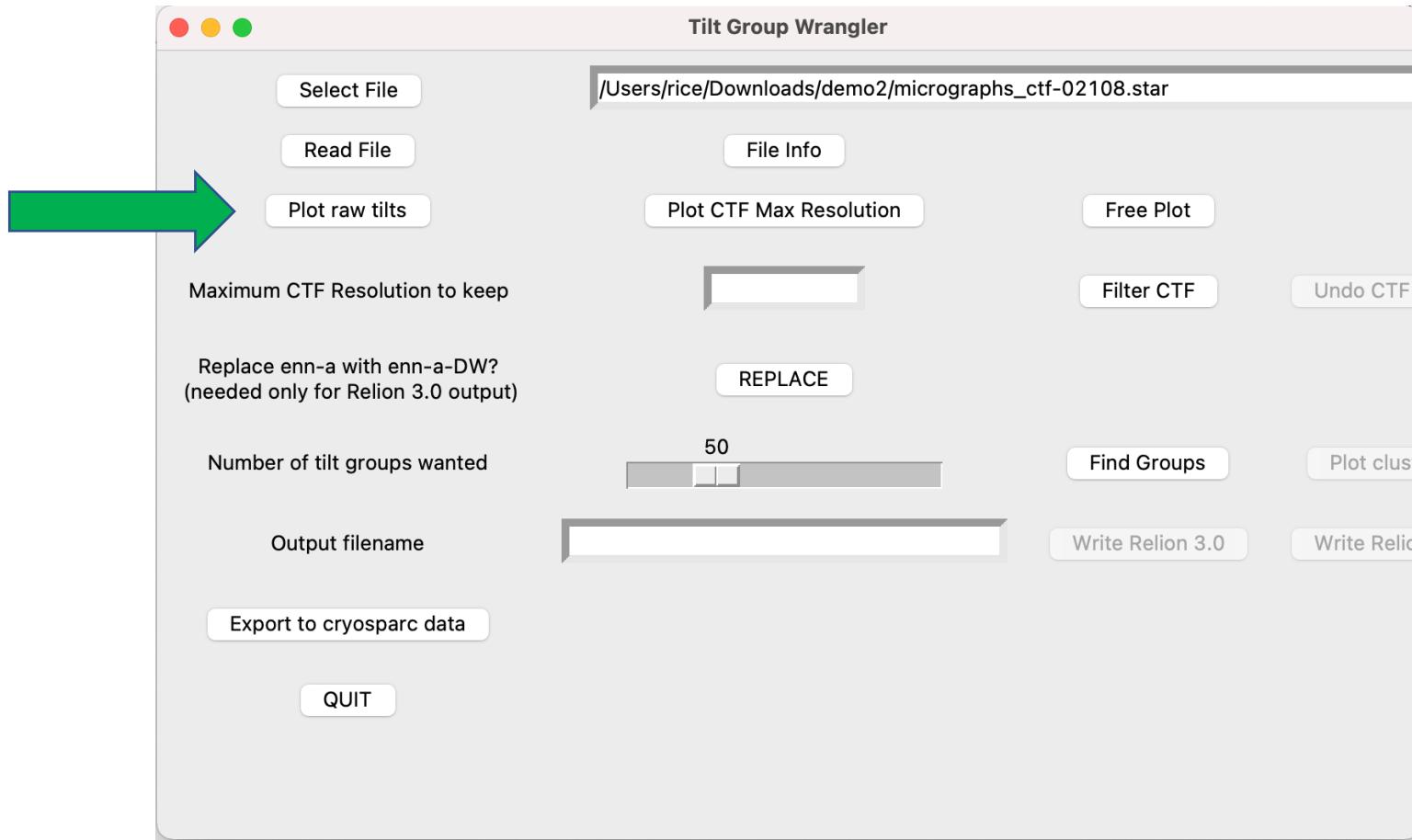
```
[rice@RICEW01-MBP15T demo2 % source ~/eman2-sphire-spark/bin/activate  
[base) rice@RICEW01-MBP15T demo2 % ./tiltgroup_wrangler.py
```



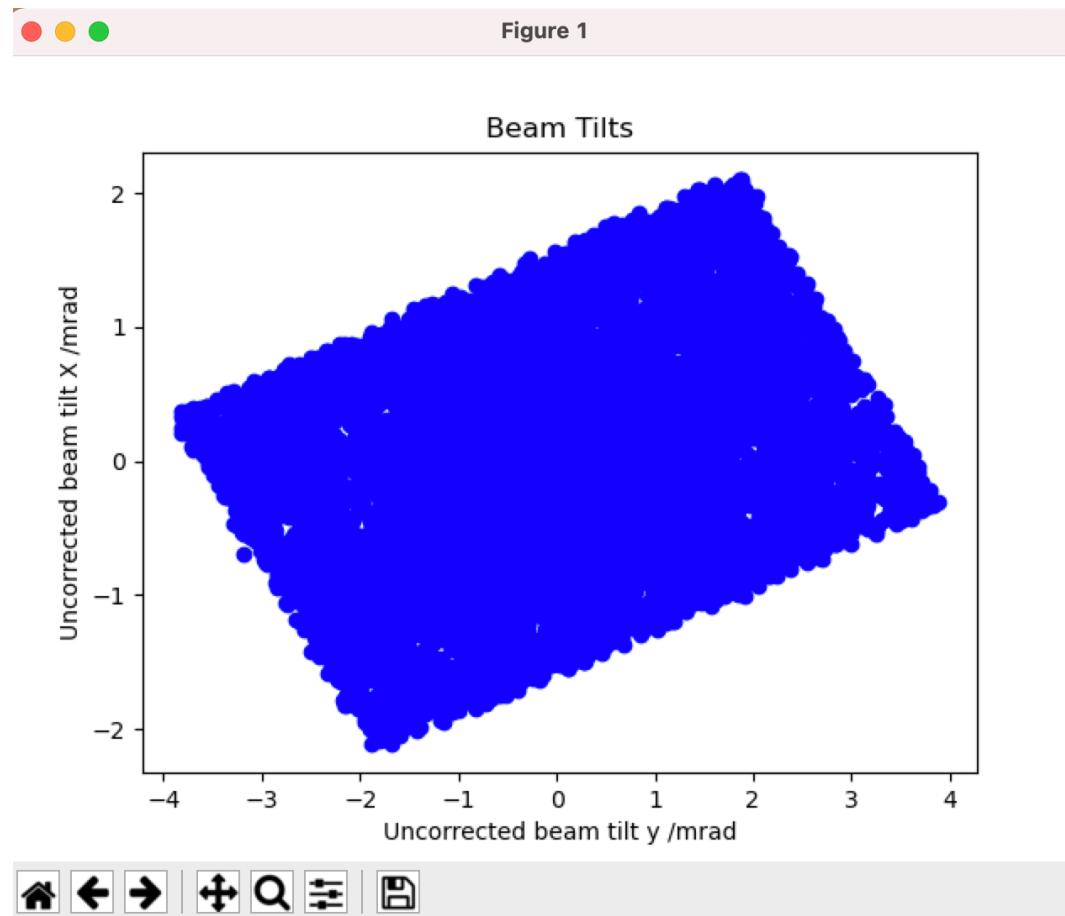
# Select downloaded CTF file as input



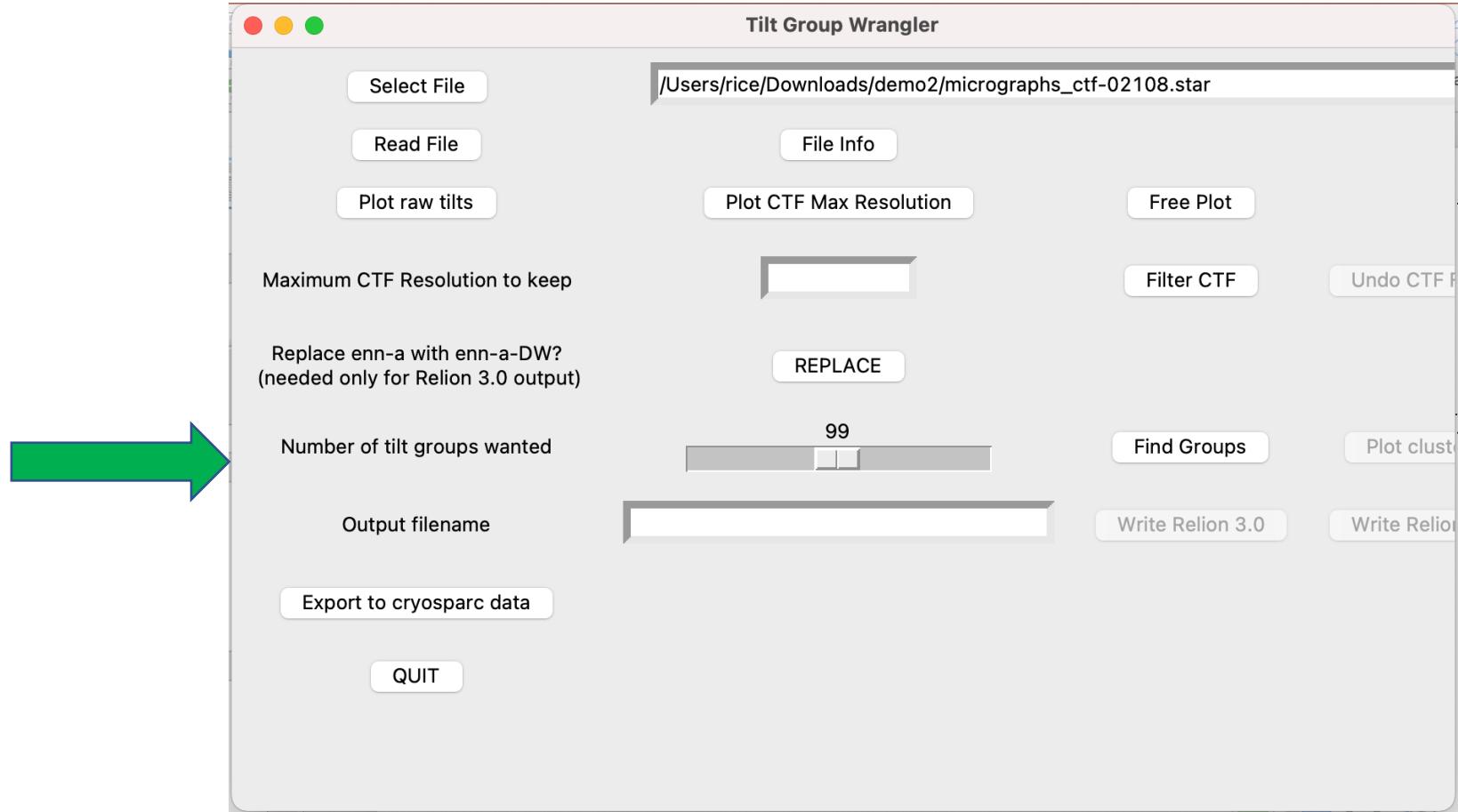
# After clicking Read file, plot raw tilts



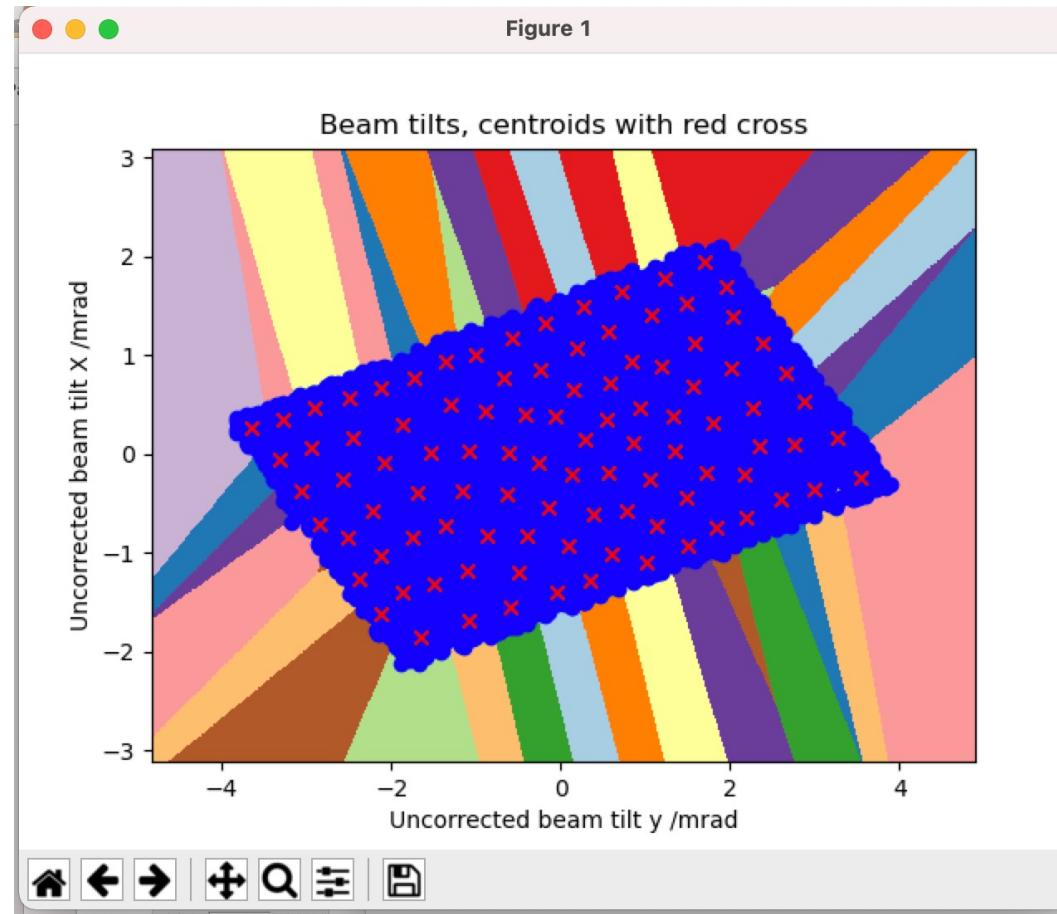
# Raw tilts



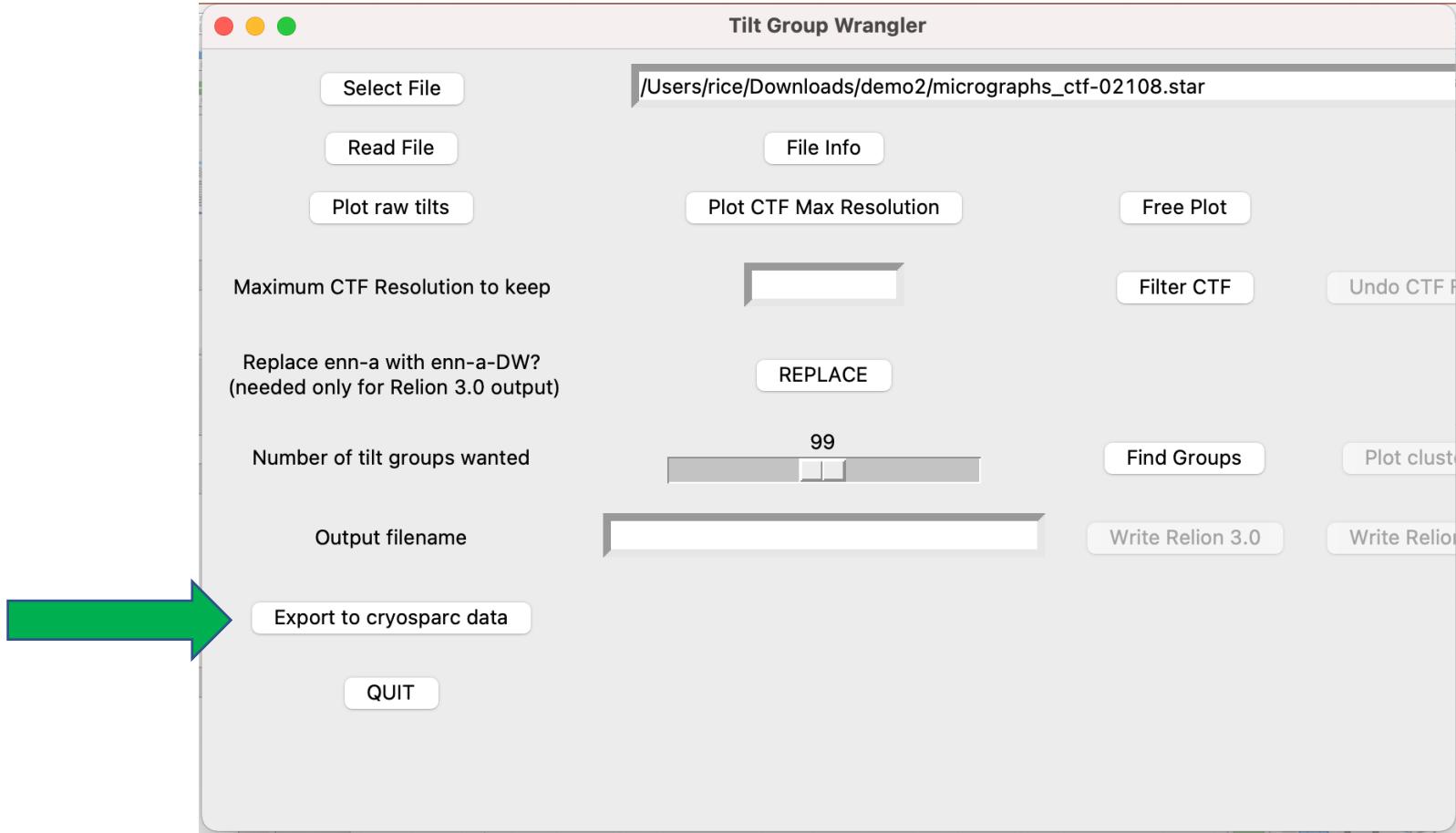
Use slider to select number of groups,  
Click Find Groups



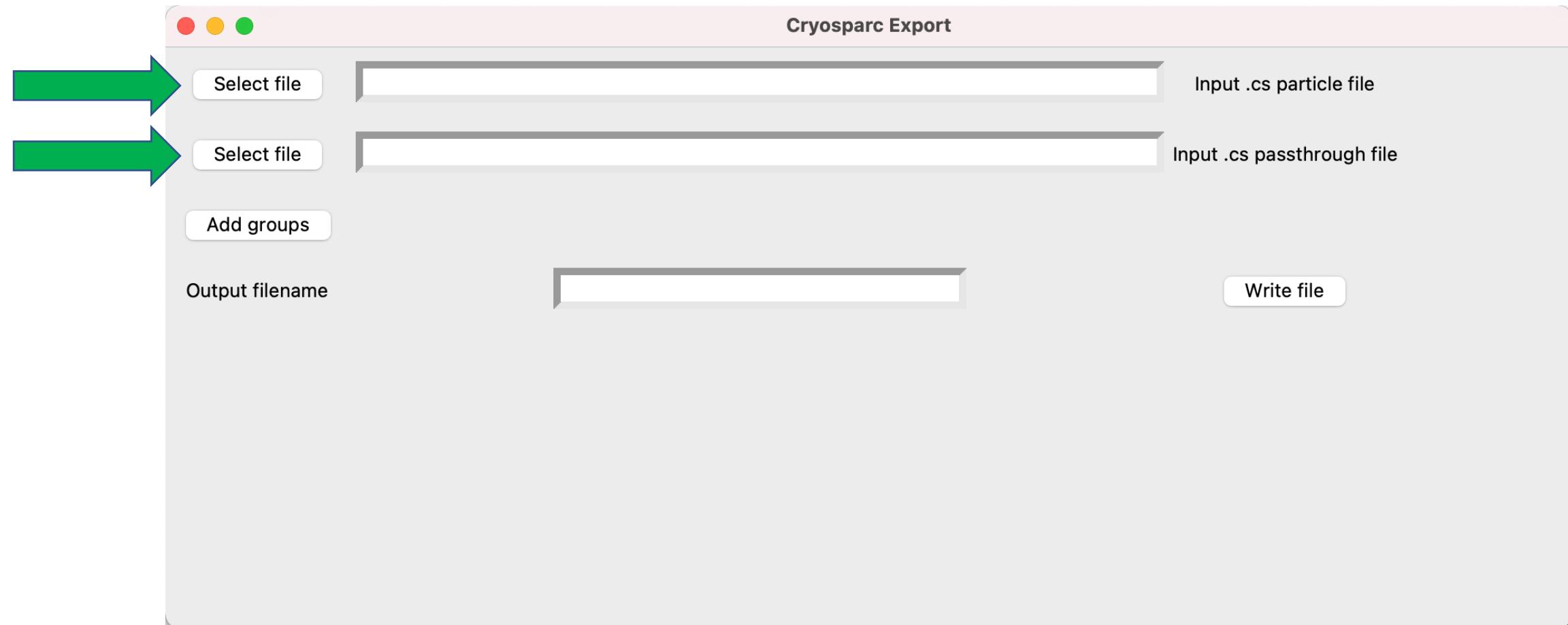
Plot of grouped data. Points within same color are in the same group



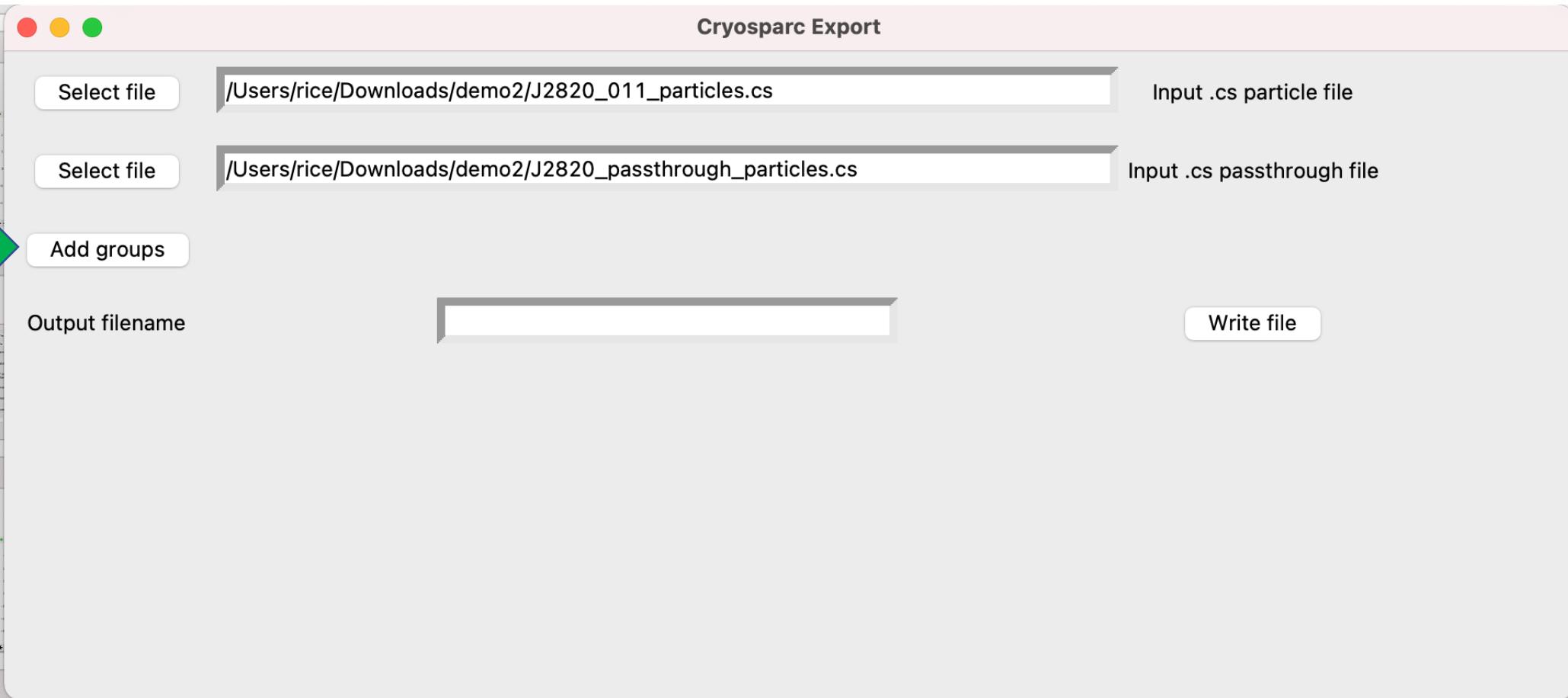
# Click Export to cryosparc data



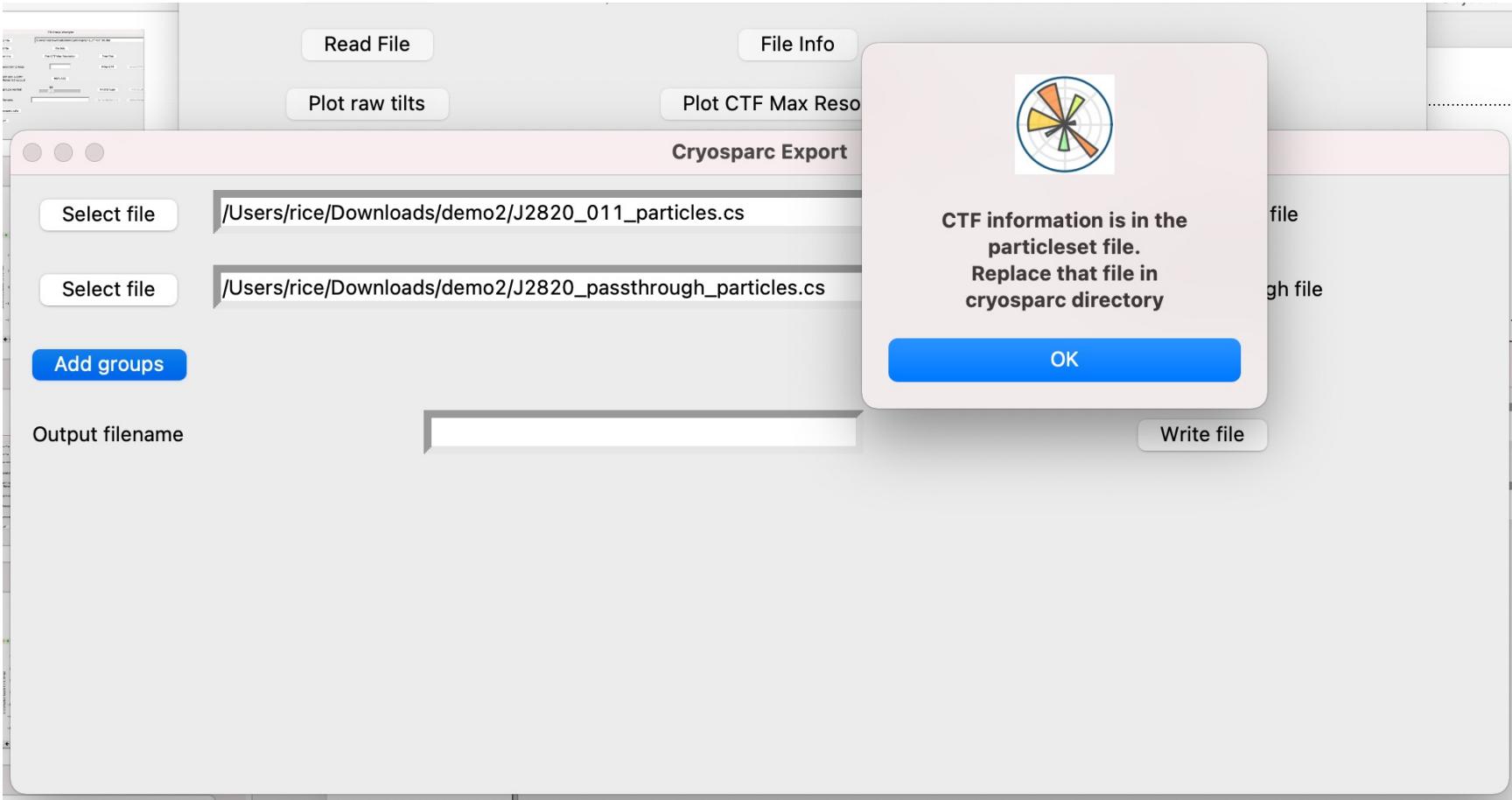
# Click Select file to browse to cryoSPARC files



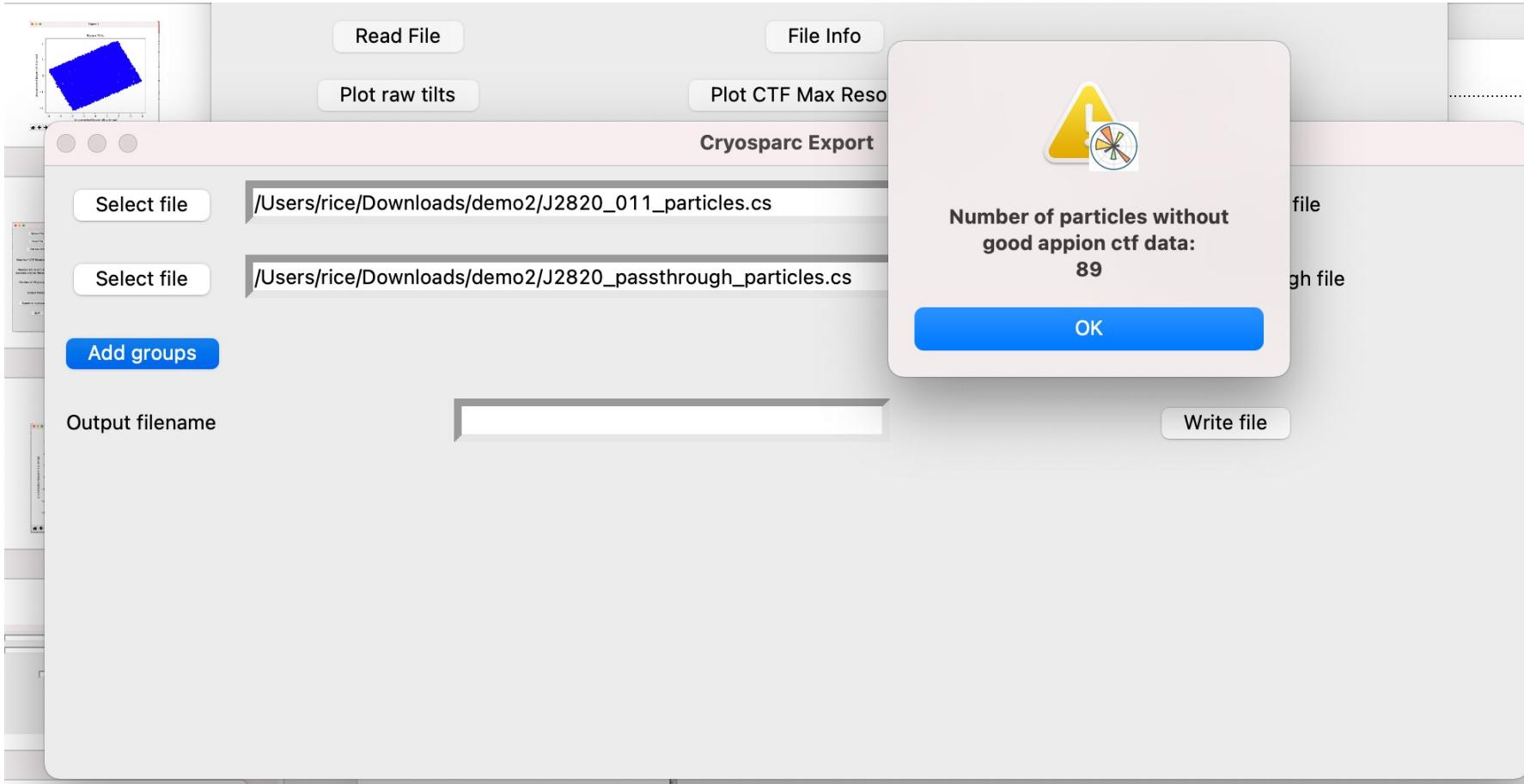
# Click Add groups



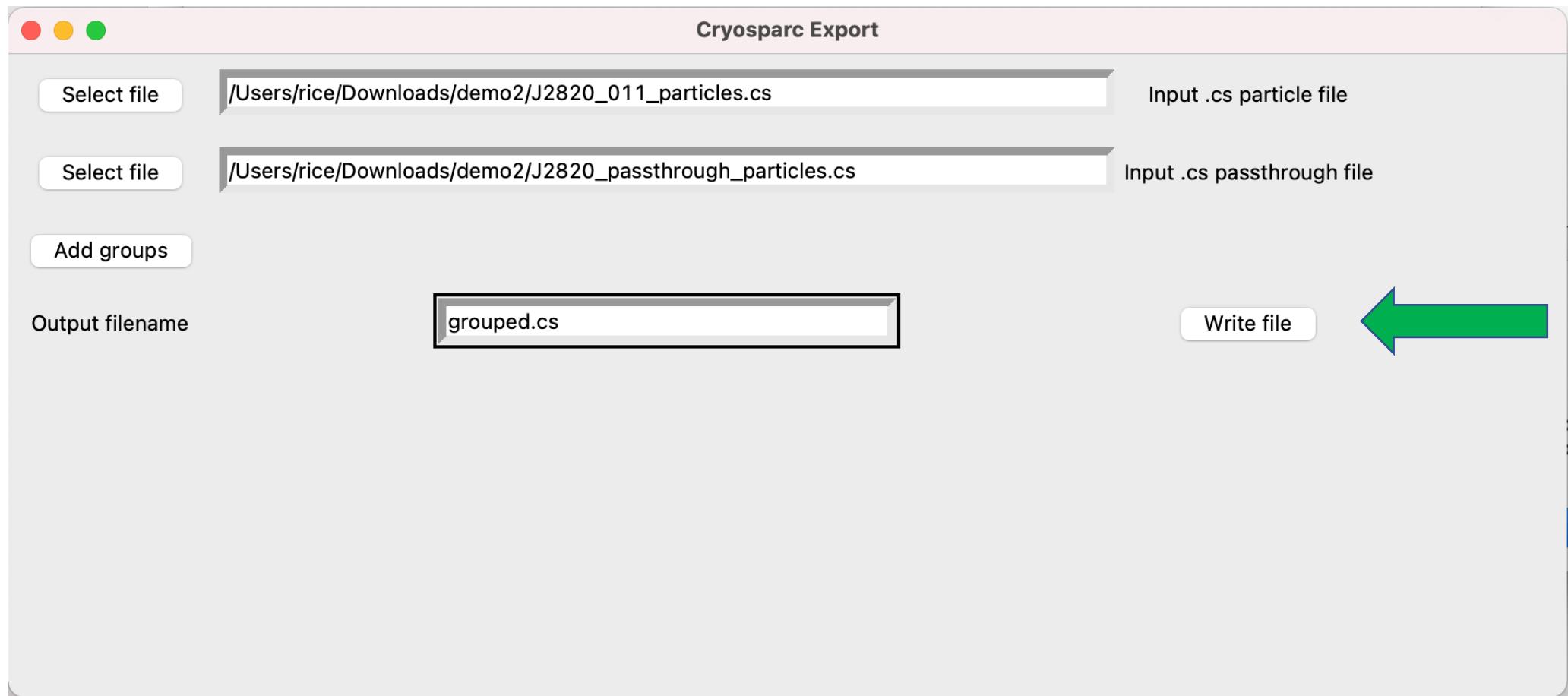
Window pops up telling you which file has the CTF information. This is the file which needs to be replaced



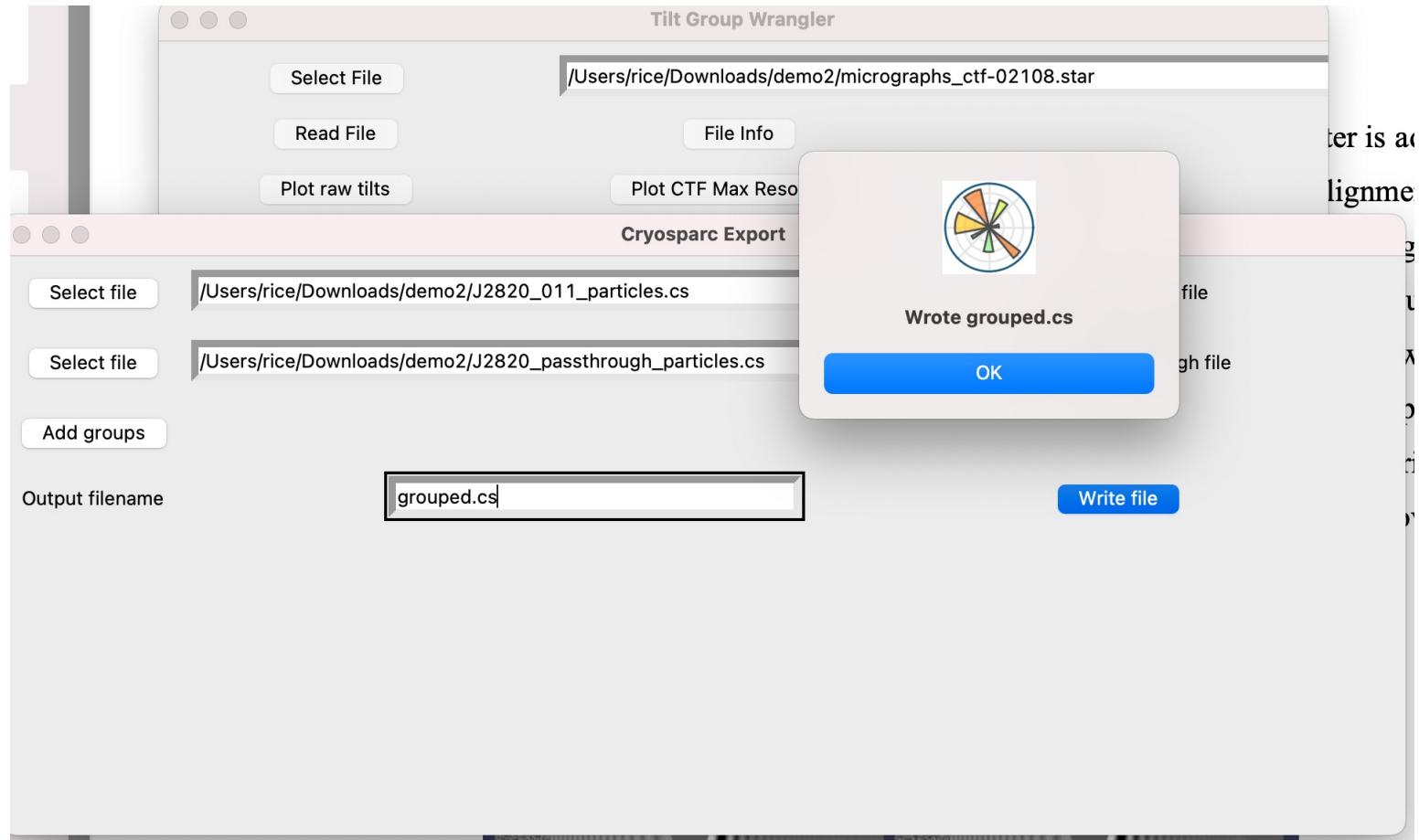
If any particles are missing CTF data, these will go into their own group



# Enter the output filename and click Write file



# Should get confirmation. Quit program



Copy the grouped.cs file to the cryosparc job folder  
Rename the original particles file.  
Link grouped.cs to the particles file

```
-rw-rw-r-- 1 cryosparc_user cryosparc_user 133K Mar  3 14:00 events.bson
drwxrwxr-x 2 cryosparc_user cryosparc_user 4.0K Mar  3 08:45 gridfs_data
-rw-rw-r-- 1 cryosparc_user cryosparc_user 40M Mar  3 08:45 J2820_011_particles.cs
-rw-rw-r-- 1 cryosparc_user cryosparc_user 247 Mar  3 08:45 J2820_011_volume_map.cs
-rw-rw-r-- 1 cryosparc_user cryosparc_user 254 Mar  3 08:45 J2820_011_volume_map_half_A.cs
-rw-rw-r-- 1 cryosparc_user cryosparc_user 65M Mar  3 08:45 J2820_011_volume_map_half_A.mrc
-rw-rw-r-- 1 cryosparc_user cryosparc_user 254 Mar  3 08:45 J2820_011_volume_map_half_B.cs
-rw-rw-r-- 1 cryosparc_user cryosparc_user 65M Mar  3 08:45 J2820_011_volume_map_half_B.mrc
-rw-rw-r-- 1 cryosparc_user cryosparc_user 65M Mar  3 08:45 J2820_011_volume_map.mrc
-rw-rw-r-- 1 cryosparc_user cryosparc_user 253 Mar  3 08:45 J2820_011_volume_map_sharp.cs
-rw-rw-r-- 1 cryosparc_user cryosparc_user 65M Mar  3 08:45 J2820_011_volume_map_sharp.mrc
-rw-rw-r-- 1 cryosparc_user cryosparc_user 257 Mar  3 08:45 J2820_011_volume_mask_fsc_auto.cs
-rw-rw-r-- 1 cryosparc_user cryosparc_user 65M Mar  3 08:45 J2820_011_volume_mask_fsc_auto.mrc
-rw-rw-r-- 1 cryosparc_user cryosparc_user 252 Mar  3 08:45 J2820_011_volume_mask_fsc.cs
-rw-rw-r-- 1 cryosparc_user cryosparc_user 65M Mar  3 08:45 J2820_011_volume_mask_fsc.mrc
-rw-rw-r-- 1 cryosparc_user cryosparc_user 255 Mar  3 08:45 J2820_011_volume_mask_refine.cs
-rw-rw-r-- 1 cryosparc_user cryosparc_user 65M Mar  3 08:45 J2820_011_volume_mask_refine.mrc
-rw-rw-r-- 1 cryosparc_user cryosparc_user 253 Mar  3 08:45 J2820_011_volume_precision.cs
-rw-rw-r-- 1 cryosparc_user cryosparc_user 33M Mar  3 08:45 J2820_011_volume_precision.mrc
-rw-rw-r-- 1 cryosparc_user cryosparc_user 257 Mar  3 14:00 J2820_mask.csg
-rw-rw-r-- 1 cryosparc_user cryosparc_user 619 Mar  3 14:00 J2820_particles.csg
-rw-rw-r-- 1 cryosparc_user cryosparc_user 27M Mar  3 08:45 J2820_passthrough_particles.cs
-rw-rw-r-- 1 cryosparc_user cryosparc_user 934 Mar  3 14:00 J2820_volume.csg
-rw-rw-r-- 1 cryosparc_user cryosparc_user 1.2M Mar  3 14:00 job.json
-rw-rw-r-- 1 cryosparc_user cryosparc_user 31K Mar  3 08:45 job.log
[cryosparc_user@cryosparcpc-skirball:/mnt/raid5_2/cryosparc_user/P2/J2820$ mv J2820_011_particles.cs J2820_011_particles.cs.orig
[cryosparc_user@cryosparcpc-skirball:/mnt/raid5_2/cryosparc_user/P2/J2820$ mv ..../grouped.cs .
[cryosparc_user@cryosparcpc-skirball:/mnt/raid5_2/cryosparc_user/P2/J2820$ ln -s grouped.cs J2820_011_particles.cs
[cryosparc_user@cryosparcpc-skirball:/mnt/raid5_2/cryosparc_user/P2/J2820$ ls -lh
total 587M
-rw-rw-r-- 1 cryosparc_user cryosparc_user 133K Mar  3 14:00 events.bson
drwxrwxr-x 2 cryosparc_user cryosparc_user 4.0K Mar  3 08:45 gridfs_data
-rwxrwxr-- 1 cryosparc_user cryosparc_user 40M Mar  3 13:48 grouped.cs
lrwxrwxrwx 1 cryosparc_user cryosparc_user 10 Mar  4 18:55 J2820_011_particles.cs -> grouped.cs
-rw-rw-r-- 1 cryosparc_user cryosparc_user 40M Mar  3 08:45 J2820_011_particles.cs.orig
-rw-rw-r-- 1 cryosparc_user cryosparc_user 247 Mar  3 08:45 J2820_011_volume_map.cs
-rw-rw-r-- 1 cryosparc_user cryosparc_user 254 Mar  3 08:45 J2820_011_volume_map_half_A.cs
-rw-rw-r-- 1 cryosparc_user cryosparc_user 65M Mar  3 08:45 J2820_011_volume_map_half_A.mrc
-rw-rw-r-- 1 cryosparc_user cryosparc_user 254 Mar  3 08:45 J2820_011_volume_map_half_B.cs
-rw-rw-r-- 1 cryosparc_user cryosparc_user 65M Mar  3 08:45 J2820_011_volume_map_half_B.mrc
-rw-rw-r-- 1 cryosparc_user cryosparc_user 65M Mar  3 08:45 J2820_011_volume_map.mrc
-rw-rw-r-- 1 cryosparc_user cryosparc_user 253 Mar  3 08:45 J2820_011_volume_map_sharp.cs
-rw-rw-r-- 1 cryosparc_user cryosparc_user 65M Mar  3 08:45 J2820_011_volume_map_sharp.mrc
-rw-rw-r-- 1 cryosparc_user cryosparc_user 257 Mar  3 08:45 J2820_011_volume_mask_fsc_auto.cs
-rw-rw-r-- 1 cryosparc_user cryosparc_user 65M Mar  3 08:45 J2820_011_volume_mask_fsc_auto.mrc
-rw-rw-r-- 1 cryosparc_user cryosparc_user 252 Mar  3 08:45 J2820_011_volume_mask_fsc.cs
-rw-rw-r-- 1 cryosparc_user cryosparc_user 65M Mar  3 08:45 J2820_011_volume_mask_fsc.mrc
-rw-rw-r-- 1 cryosparc_user cryosparc_user 255 Mar  3 08:45 J2820_011_volume_mask_refine.cs
-rw-rw-r-- 1 cryosparc_user cryosparc_user 65M Mar  3 08:45 J2820_011_volume_mask_refine.mrc
-rw-rw-r-- 1 cryosparc_user cryosparc_user 253 Mar  3 08:45 J2820_011_volume_precision.cs
-rw-rw-r-- 1 cryosparc_user cryosparc_user 33M Mar  3 08:45 J2820_011_volume_precision.mrc
-rw-rw-r-- 1 cryosparc_user cryosparc_user 257 Mar  3 14:00 J2820_mask.csg
-rw-rw-r-- 1 cryosparc_user cryosparc_user 619 Mar  3 14:00 J2820_particles.csg
-rw-rw-r-- 1 cryosparc_user cryosparc_user 27M Mar  3 08:45 J2820_passthrough_particles.cs
-rw-rw-r-- 1 cryosparc_user cryosparc_user 934 Mar  3 14:00 J2820_volume.csg
-rw-rw-r-- 1 cryosparc_user cryosparc_user 1.2M Mar  3 14:00 job.json
-rw-rw-r-- 1 cryosparc_user cryosparc_user 31K Mar  3 08:45 job.log
```

# As test, do a global CTF refinement with aligned particle set as input



## Inputs

### Particle stacks

Type: particle Name: particles

#### J2820.particles

##### blob

J2820.particles.blob.F

##### ctf

J2820.particles.ctf.F

##### alignments3D

J2820.particles.alignments3D.F

##### Passthrough

J2820.particles.alignments2D.F

### Input volume

Type: volume Name: volume

#### J2820.volume

# Results should show the number of groups requested

