

# My Questions

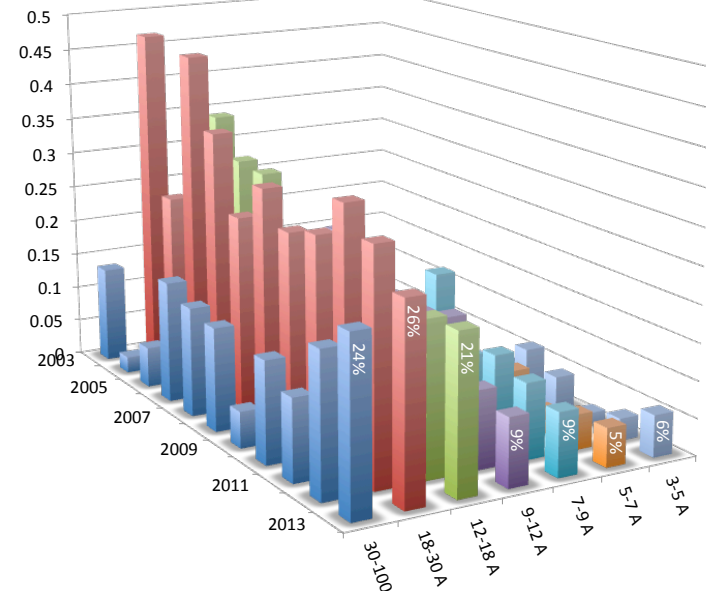
- Tools for routine/robust single particle work:
  - Are we there yet?
  - Should any lab be able to do this without being embedded in the community for years?
  - Do we need centralized resources?
  - Can a standard lab gather the necessary resources?
- New classification algorithms
- Inter-software comparison as a validation

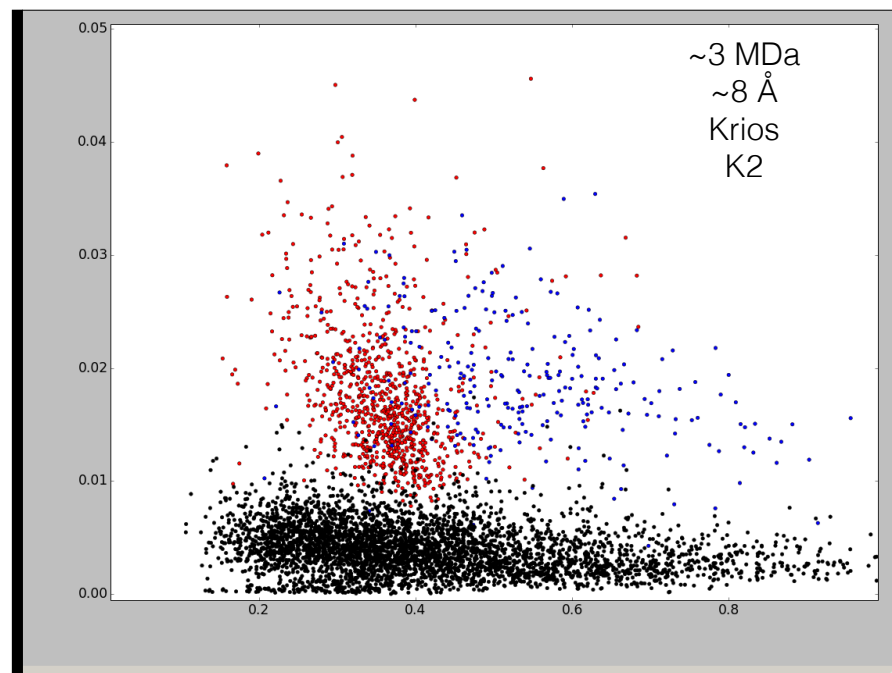
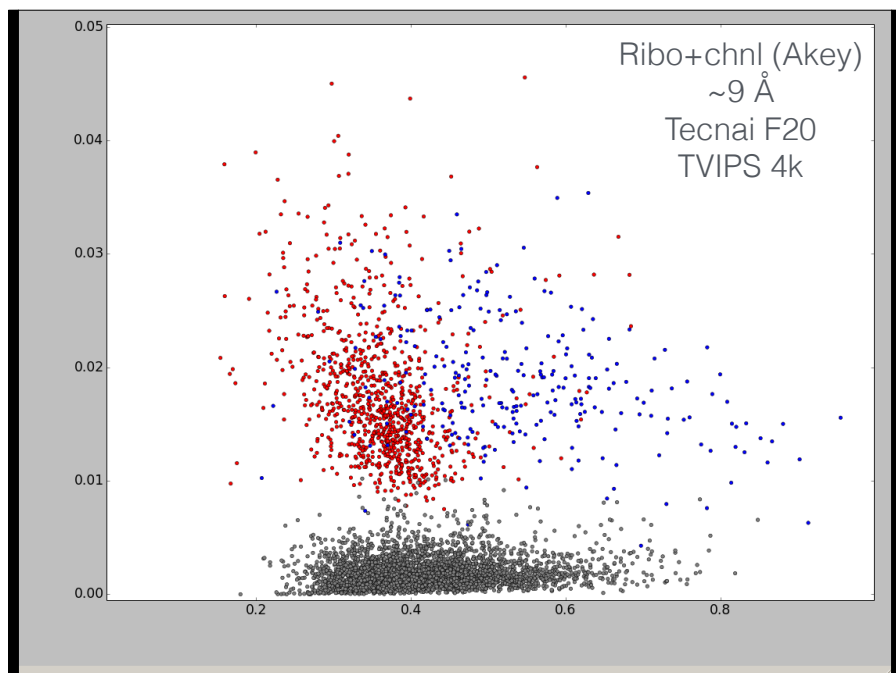
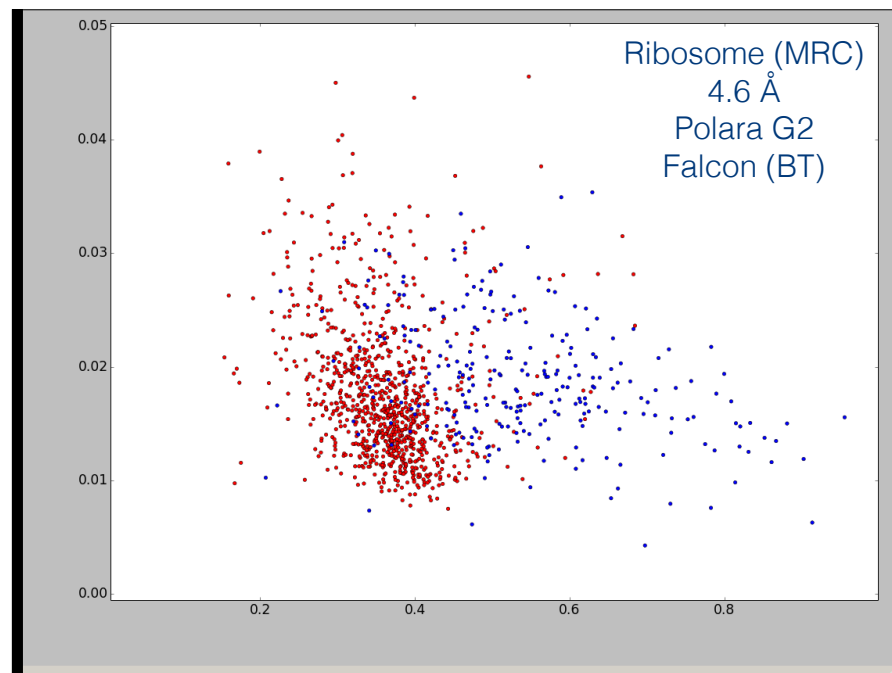
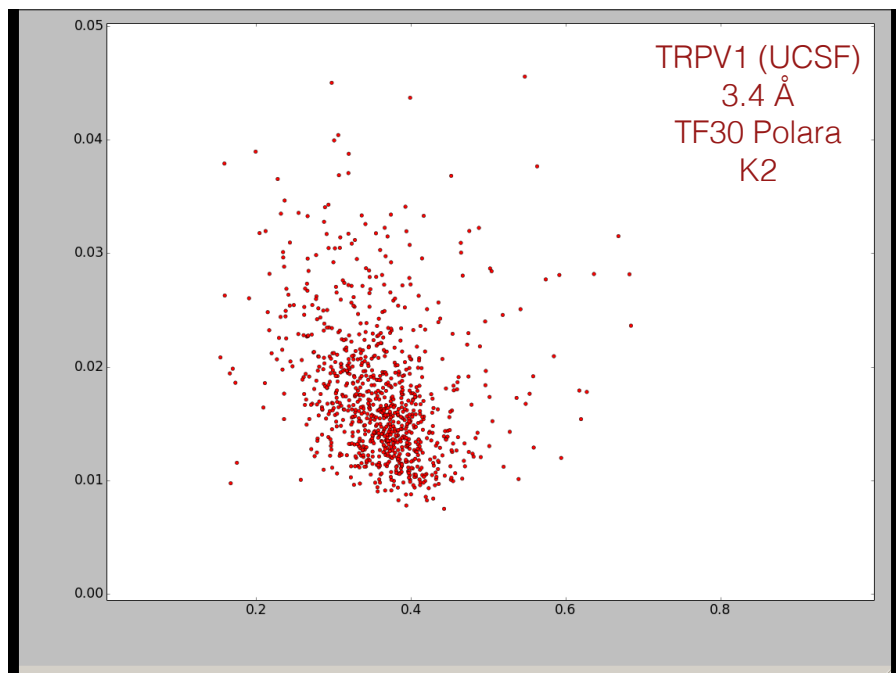
# My Questions

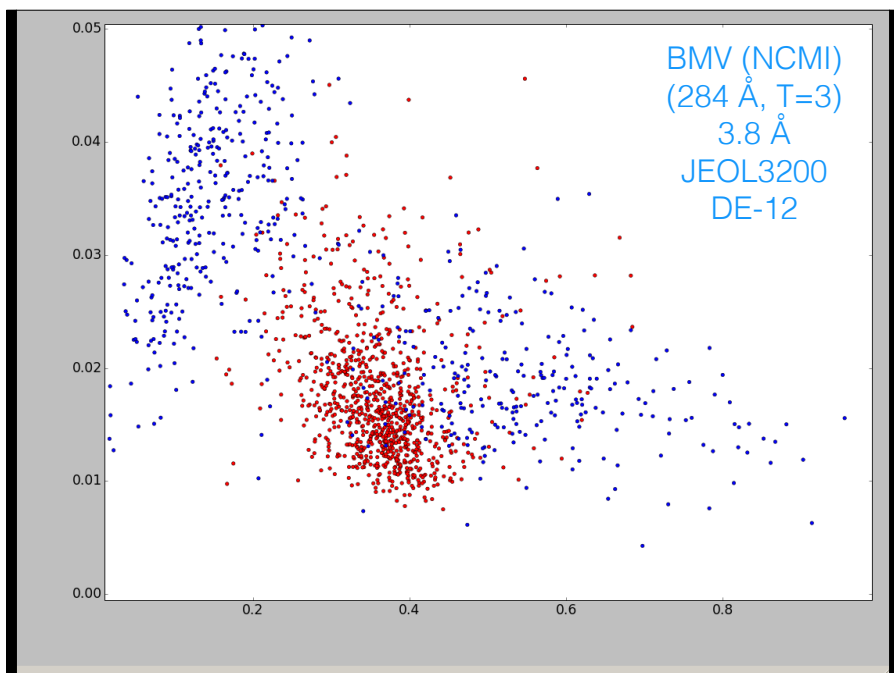
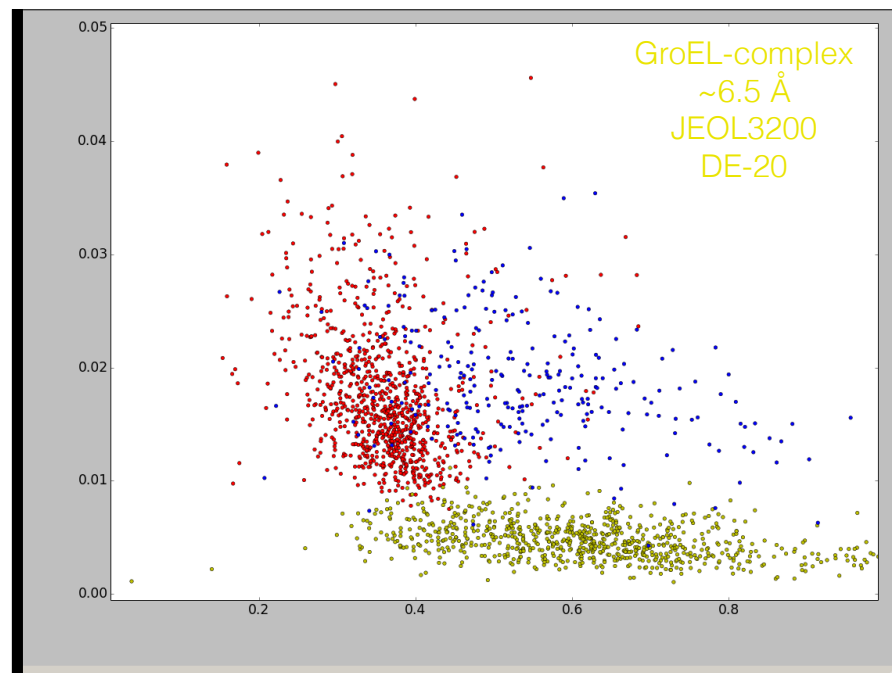
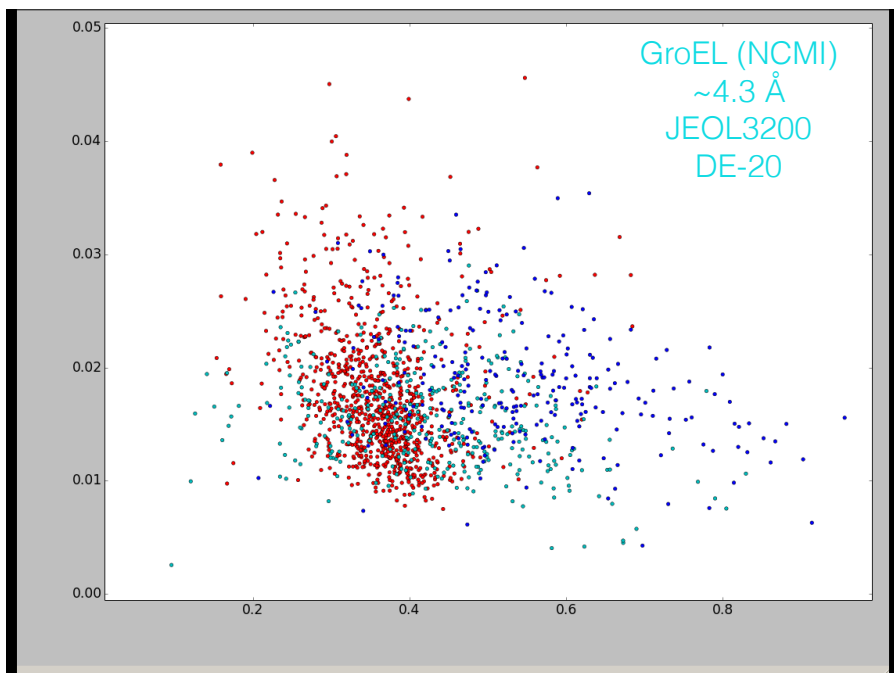
- Tools for routine/robust single particle work:
  - Are we there yet?
  - Should any lab be able to do this without being embedded in the community for years?
  - Do we need centralized resources?
  - Can a standard lab gather the necessary resources?
- ~~New classification algorithms~~
- Inter-software comparison as a validation

# My Questions

- Tools for routine/robust single particle work:
  - Are we there yet?
  - Should any lab be able to do this without being embedded in the community for years?
  - Do we need centralized resources?
  - Can a standard lab gather the necessary resources?
- **Can we tell the difference between good data and bad data without doing a reconstruction?**
- Inter-software comparison as a validation

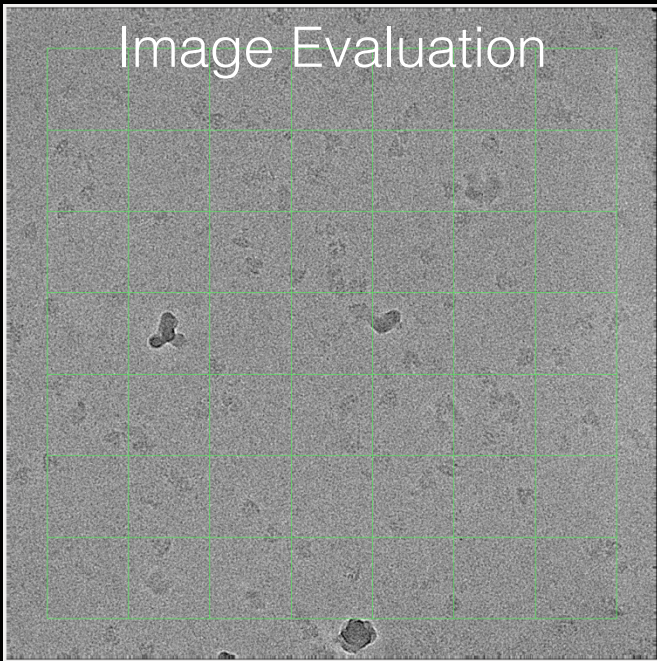




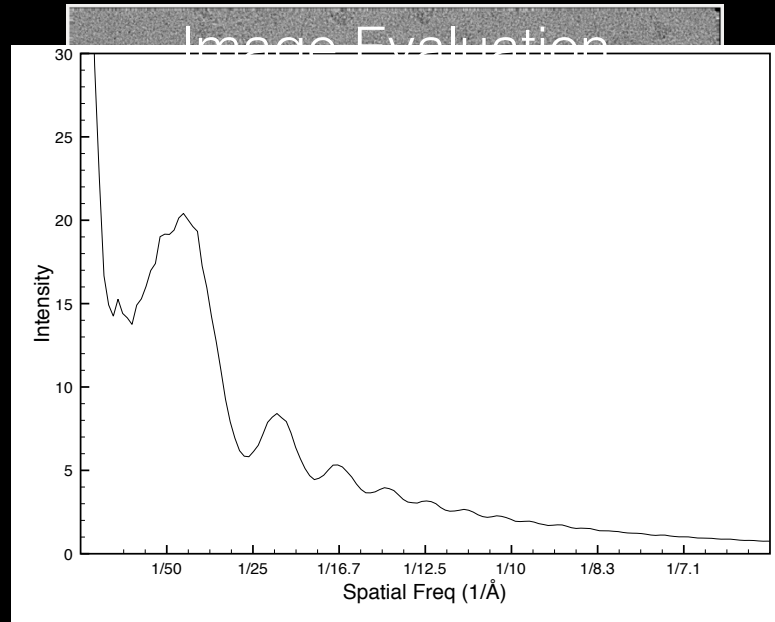


Particle-based quality  
assessment

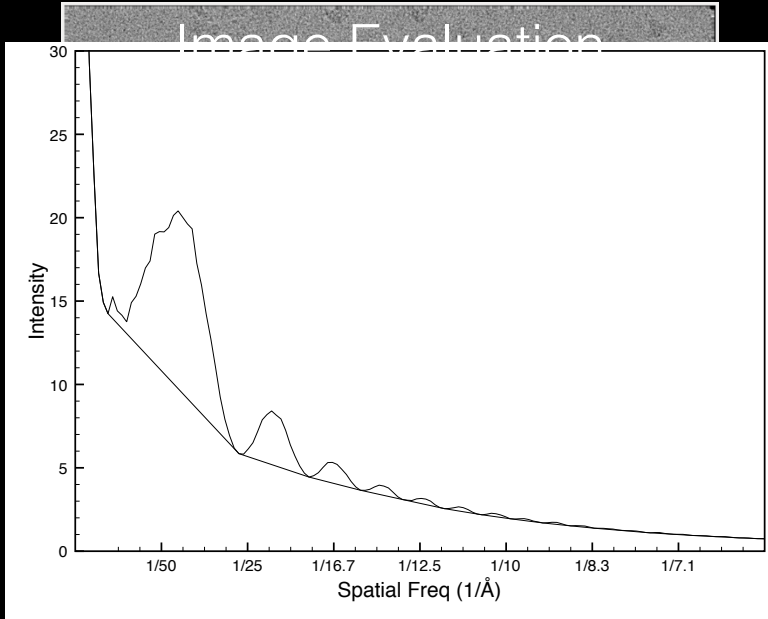
# Image Evaluation



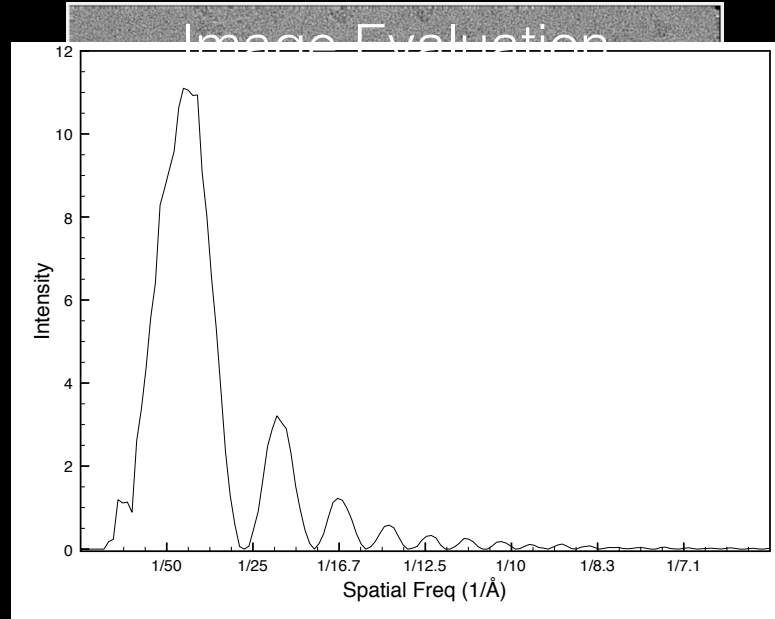
# Image Evaluation



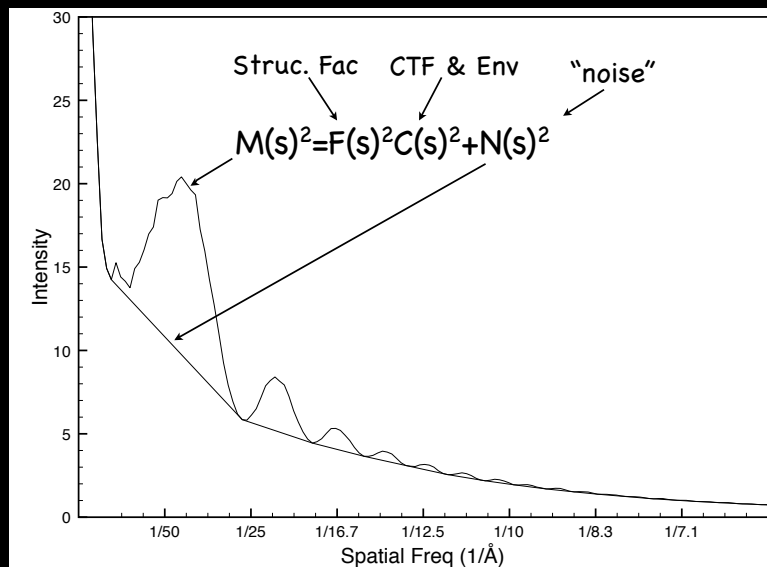
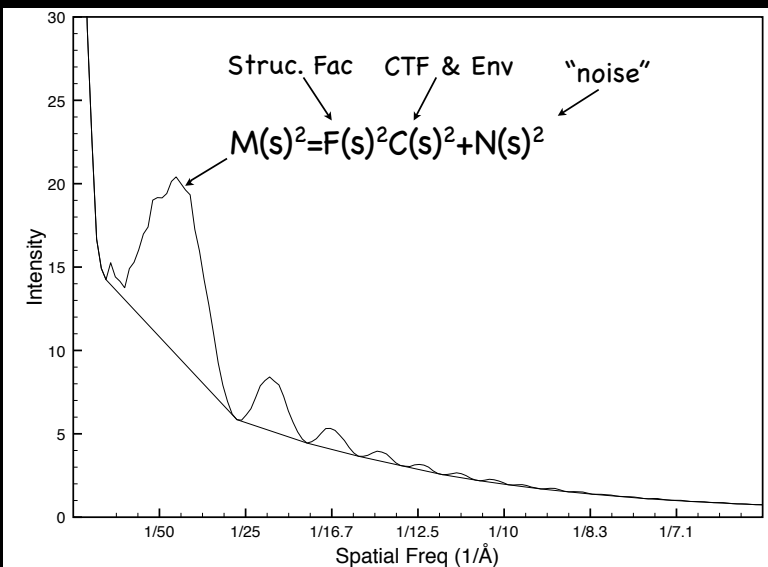
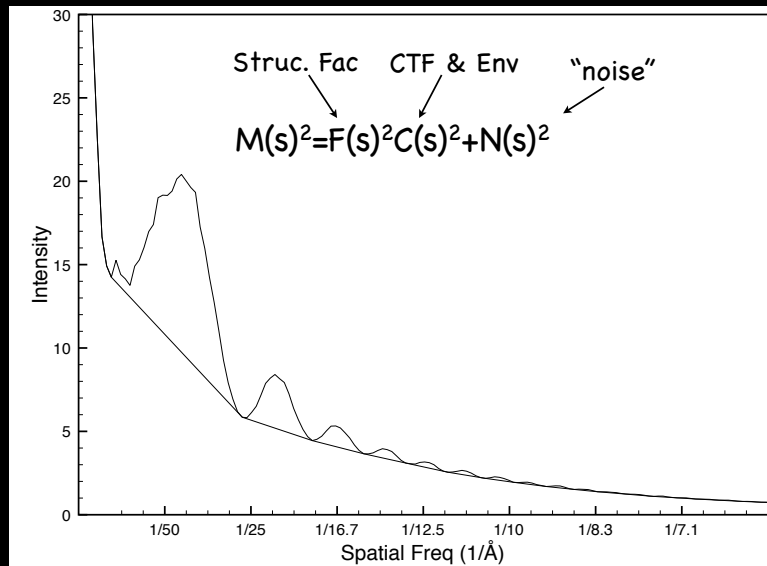
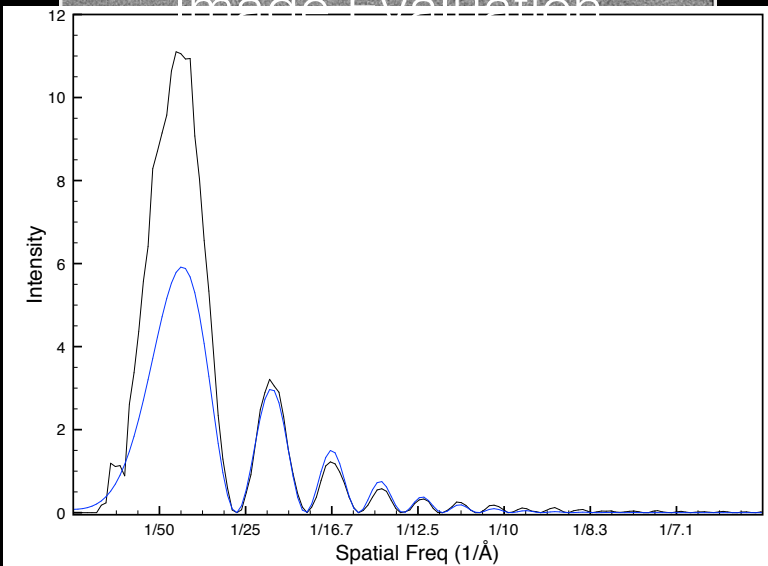
# Image Evaluation

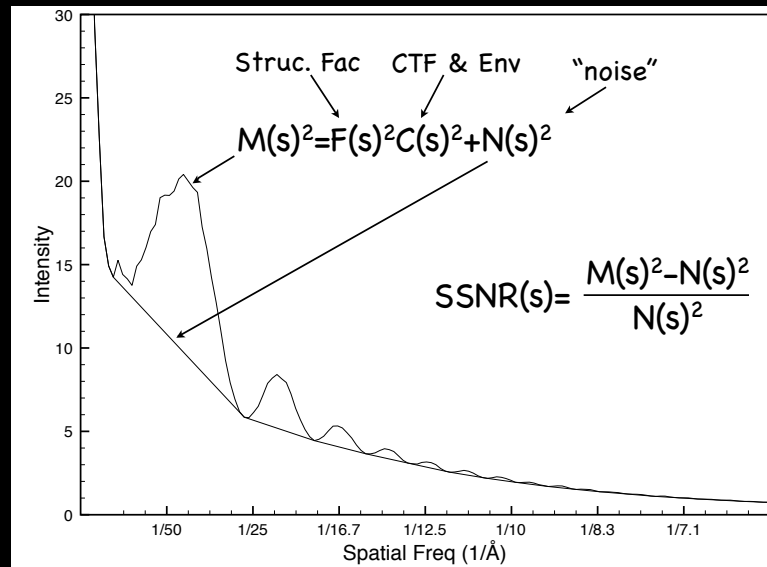
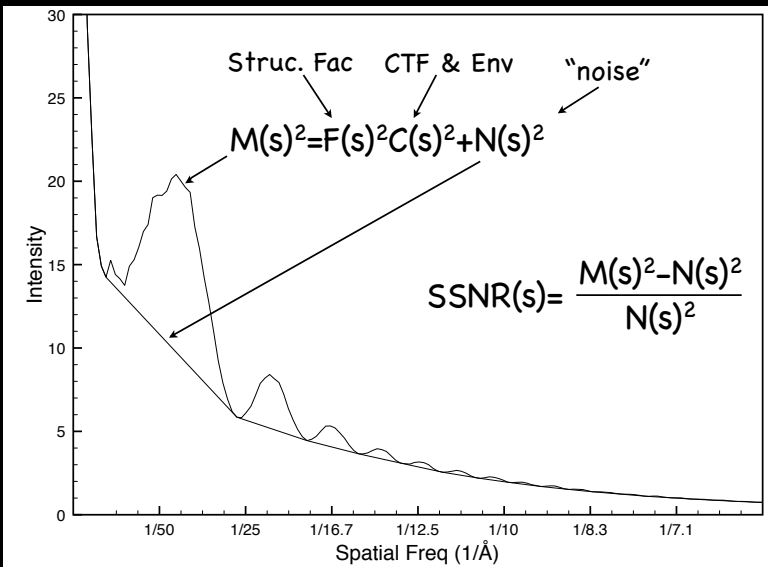


# Image Evaluation

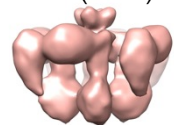


# Image Evaluation

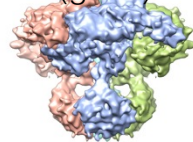




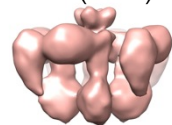
2002 (bad)



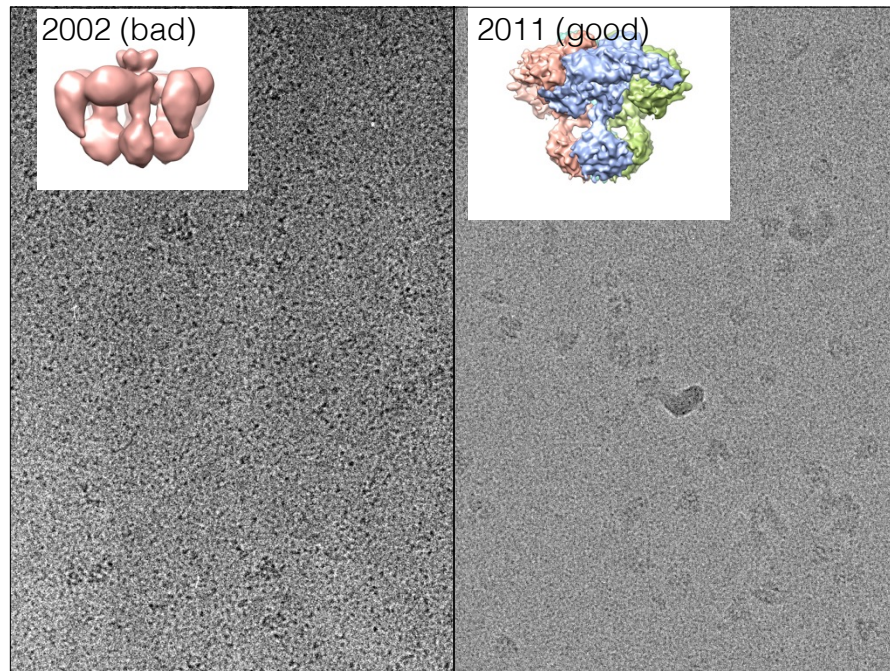
2011 (good)

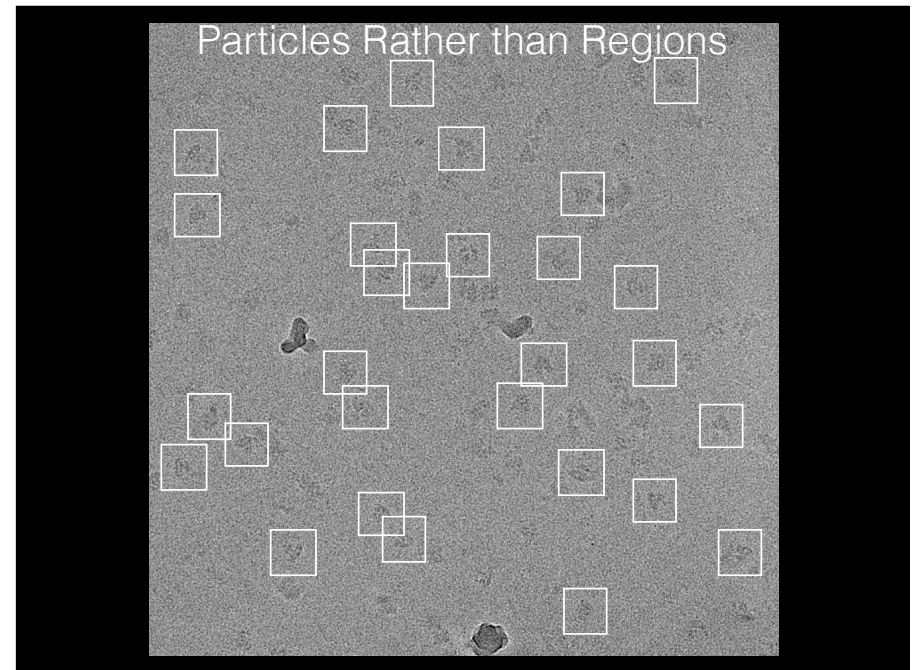
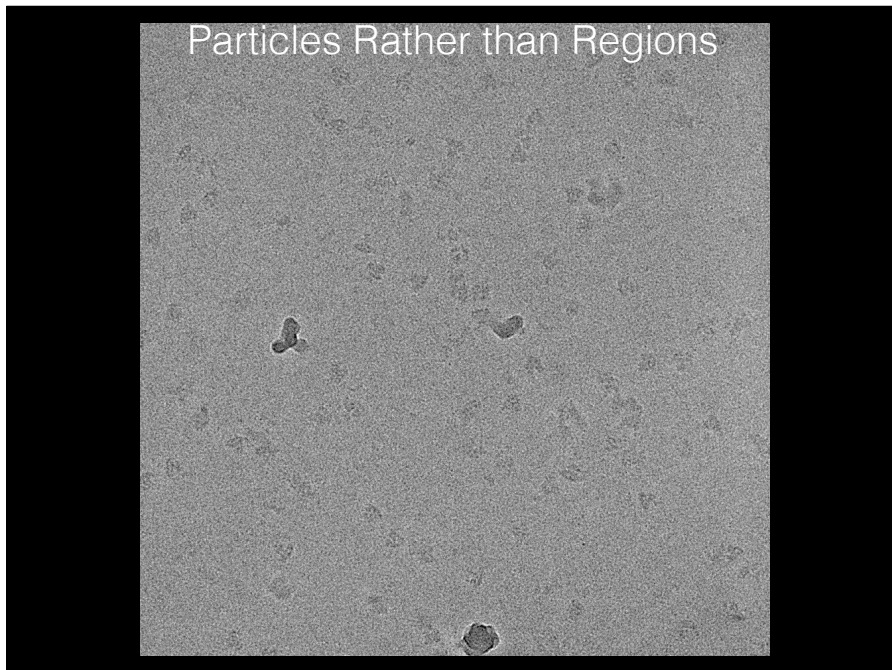
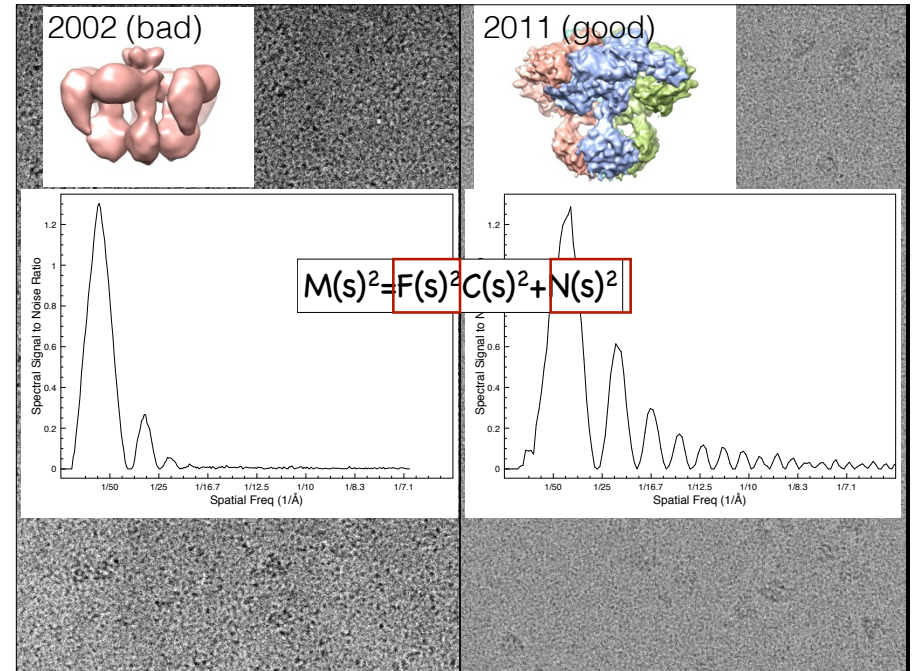
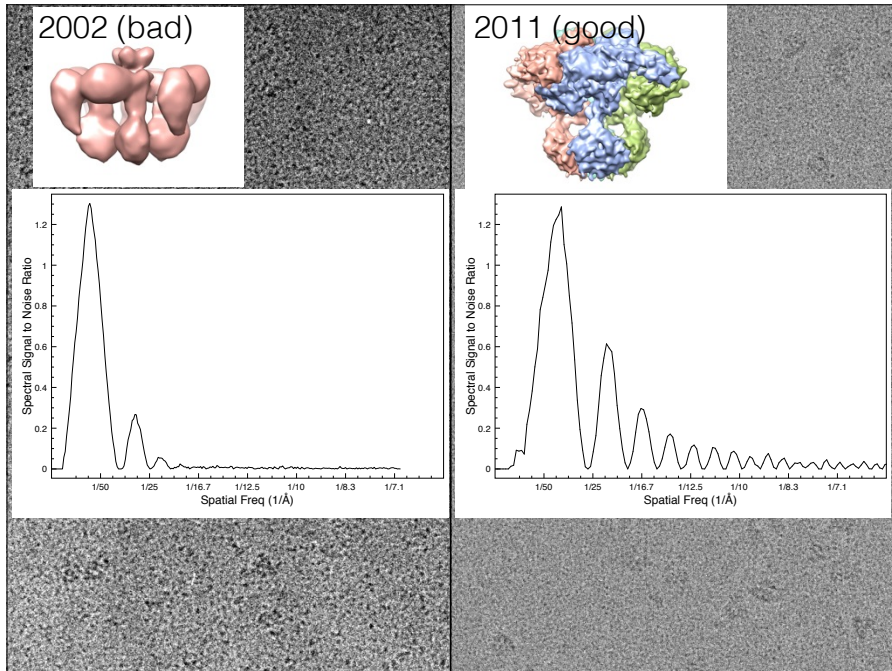


2002 (bad)

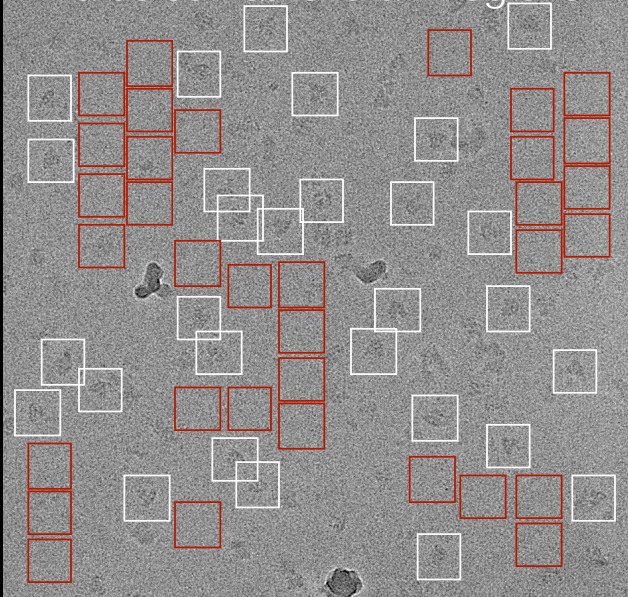


2011 (good)





Particles Rather than Regions



Density Problems

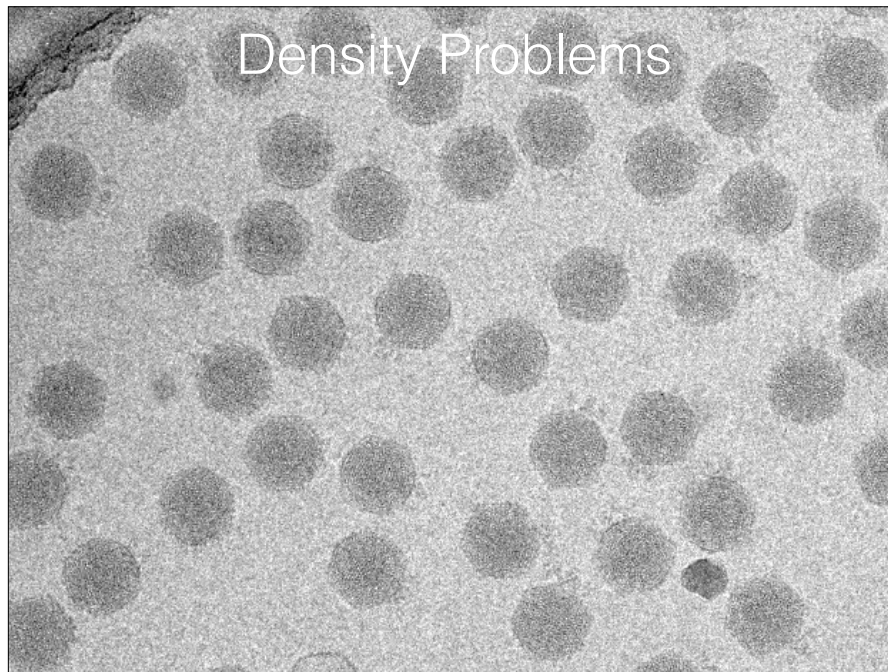


Image Evaluation

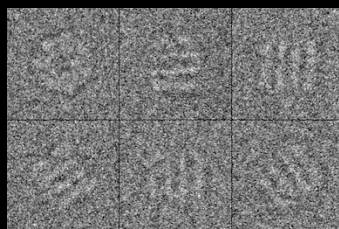
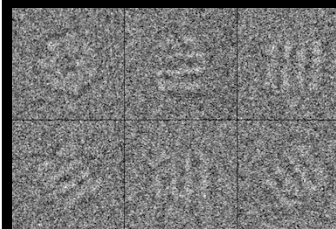
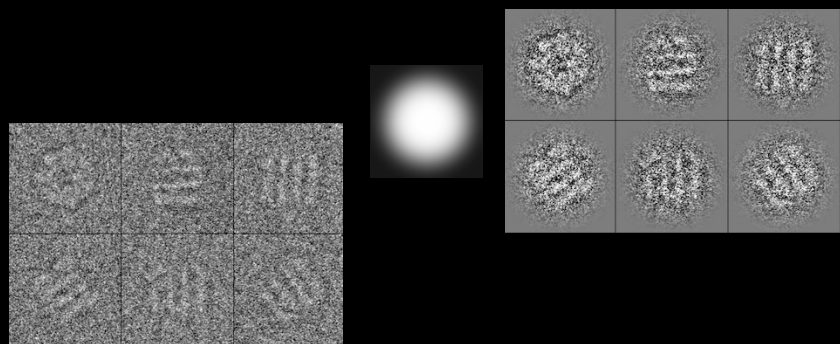


Image Evaluation

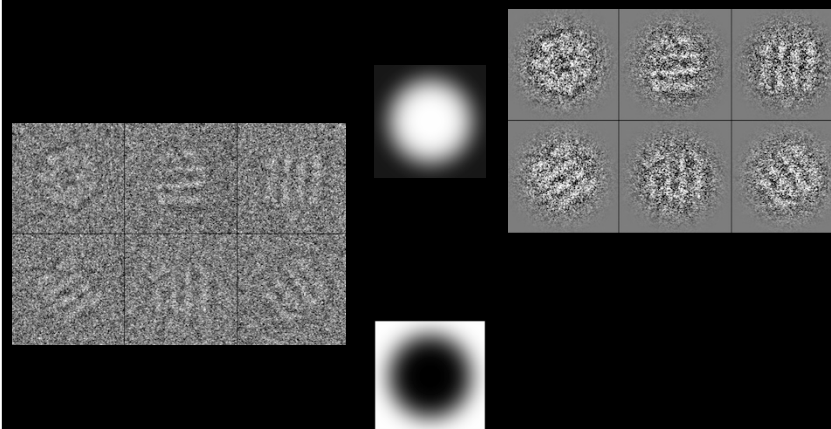




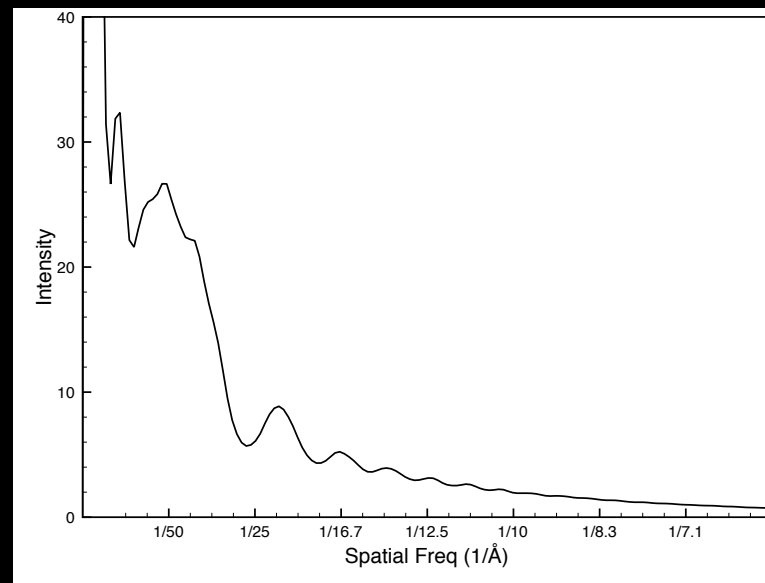
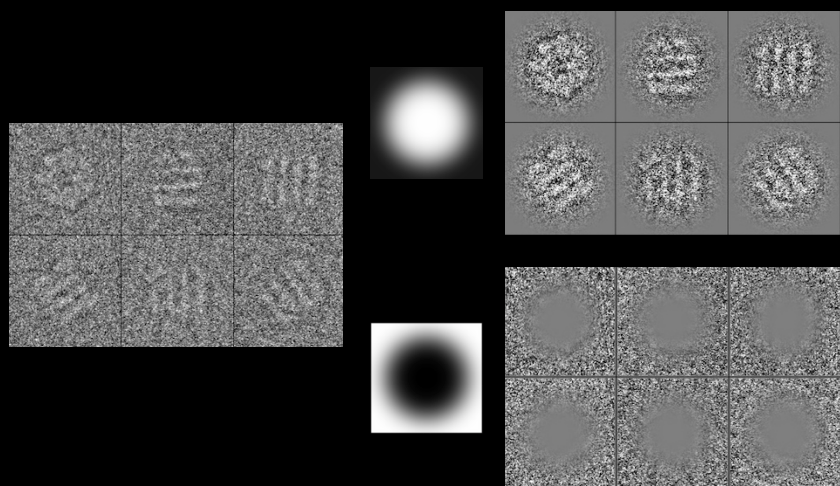
# Image Evaluation

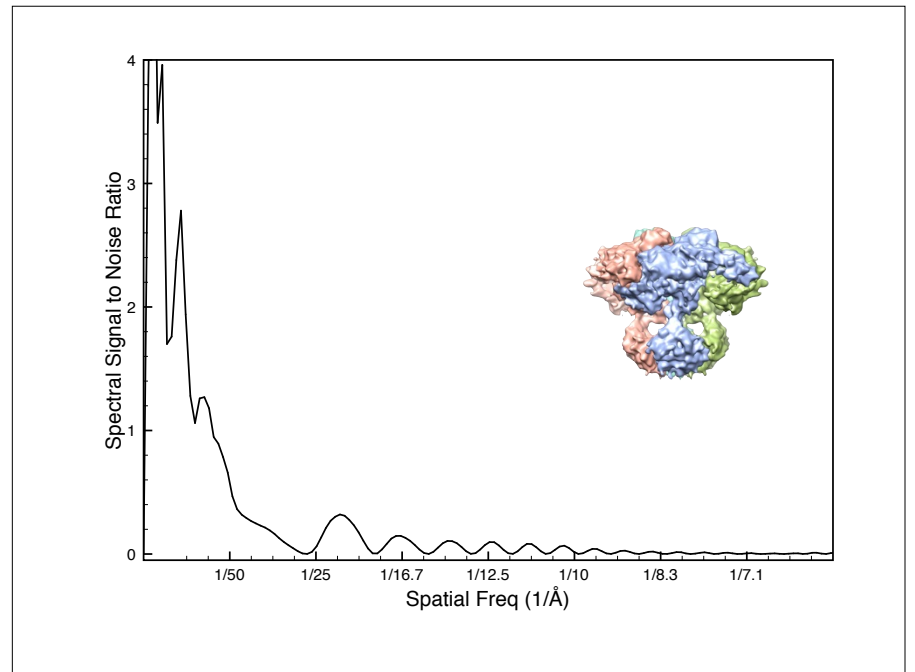
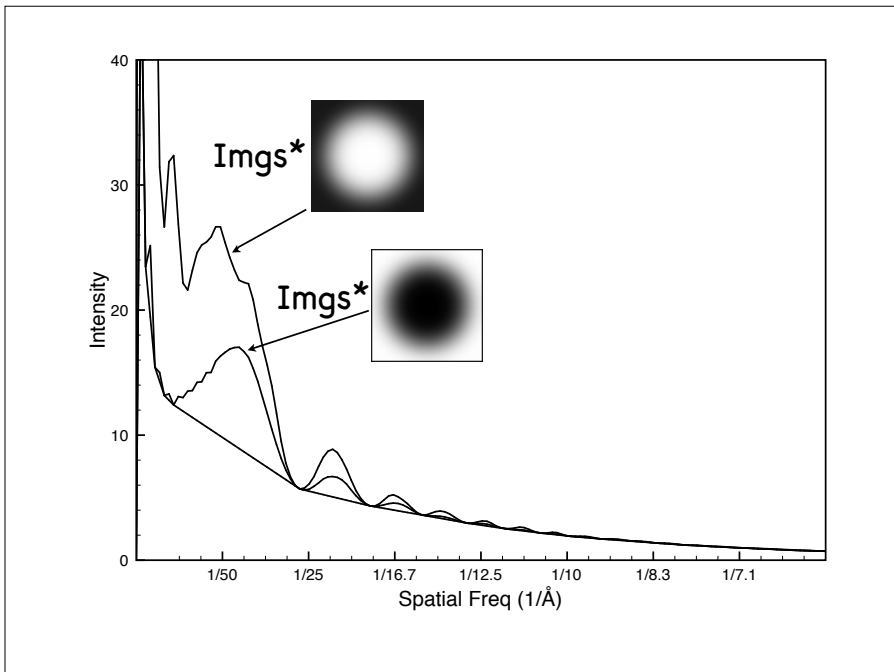
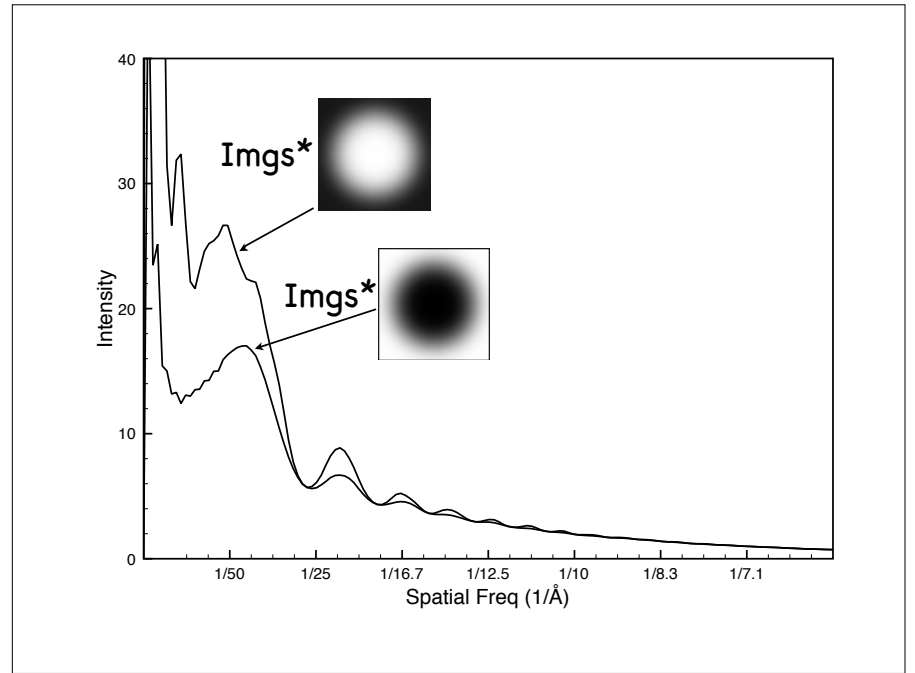
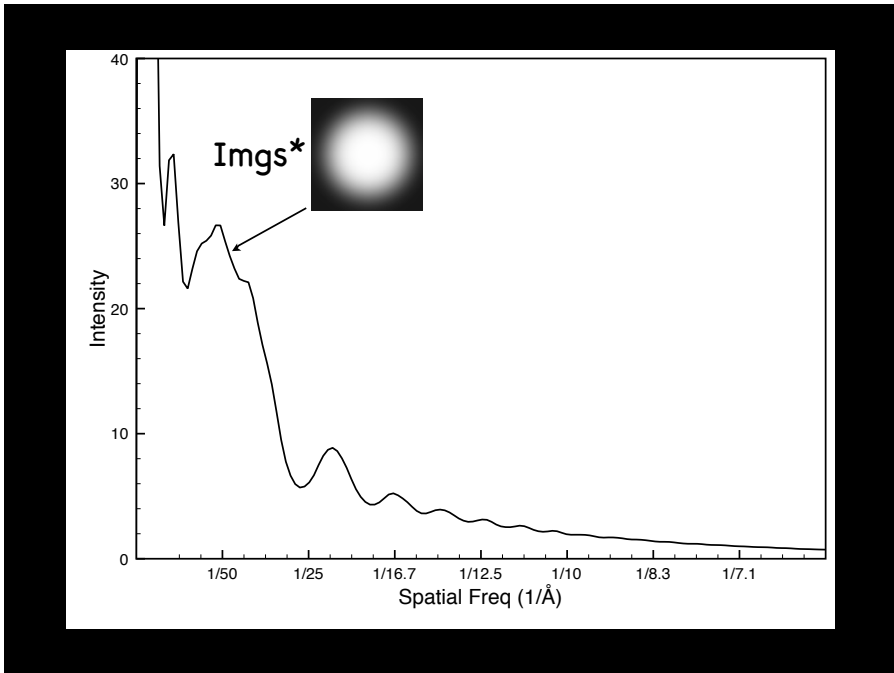


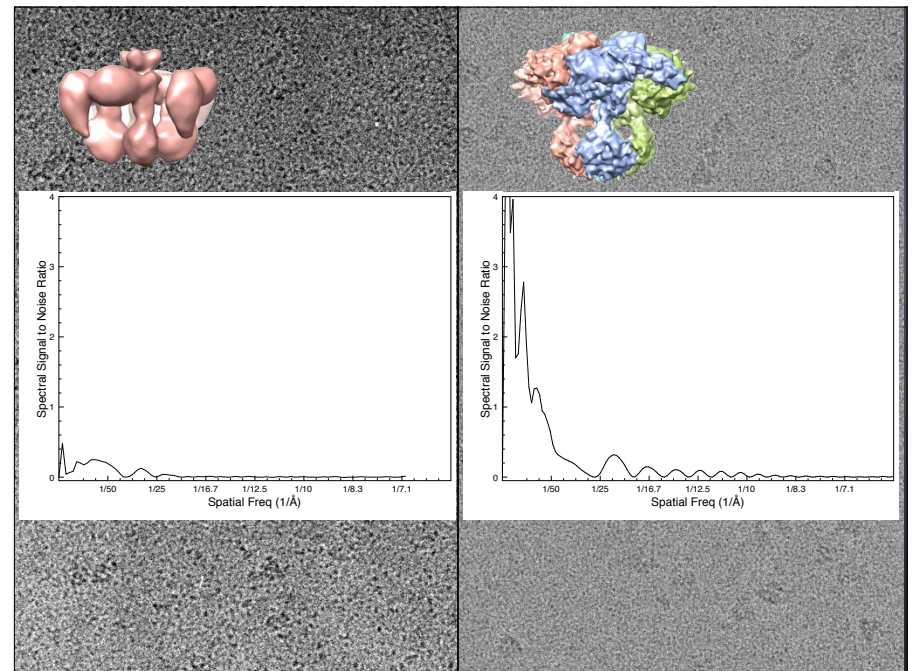
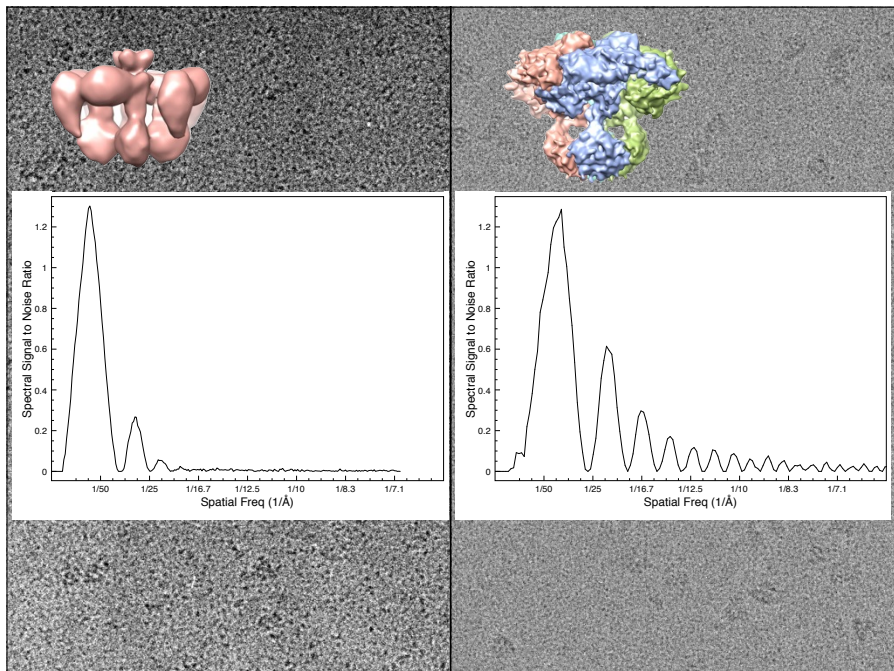
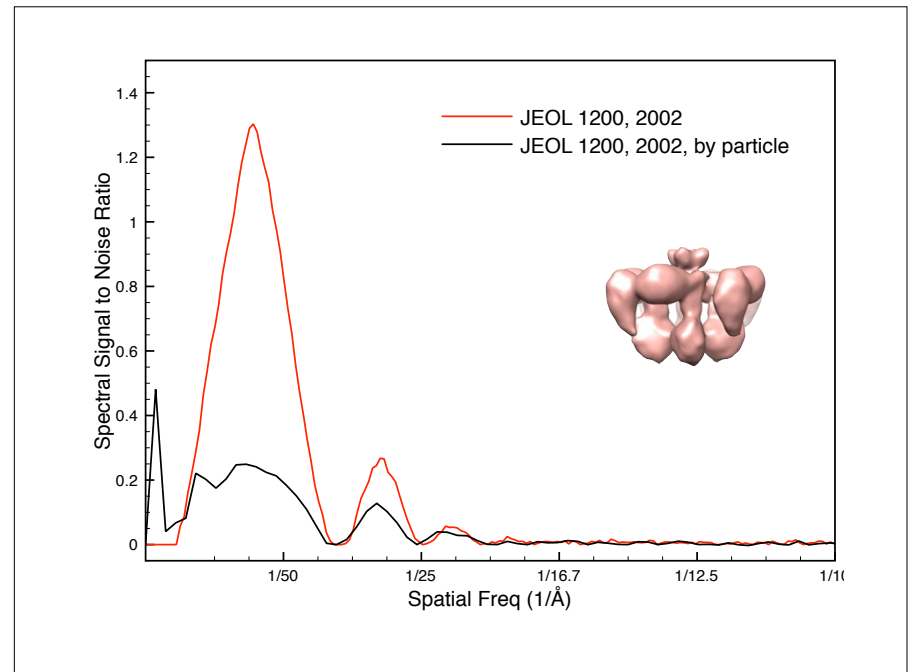
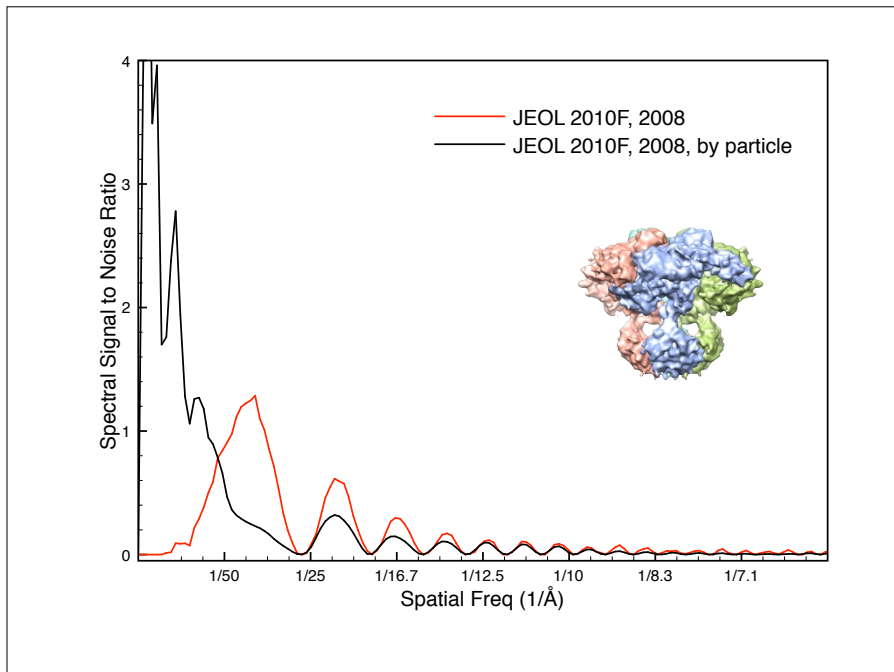
# Image Evaluation

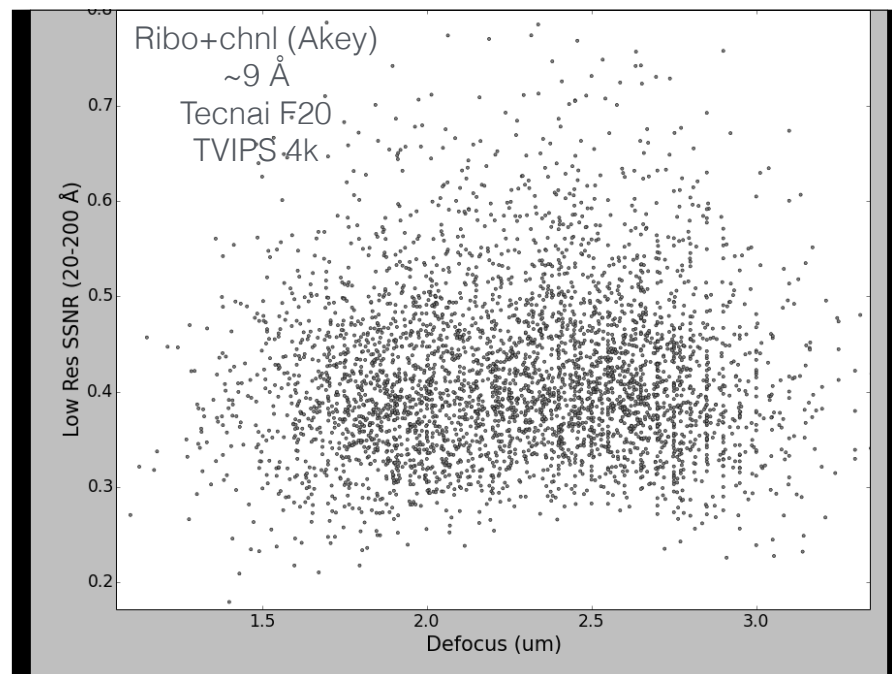
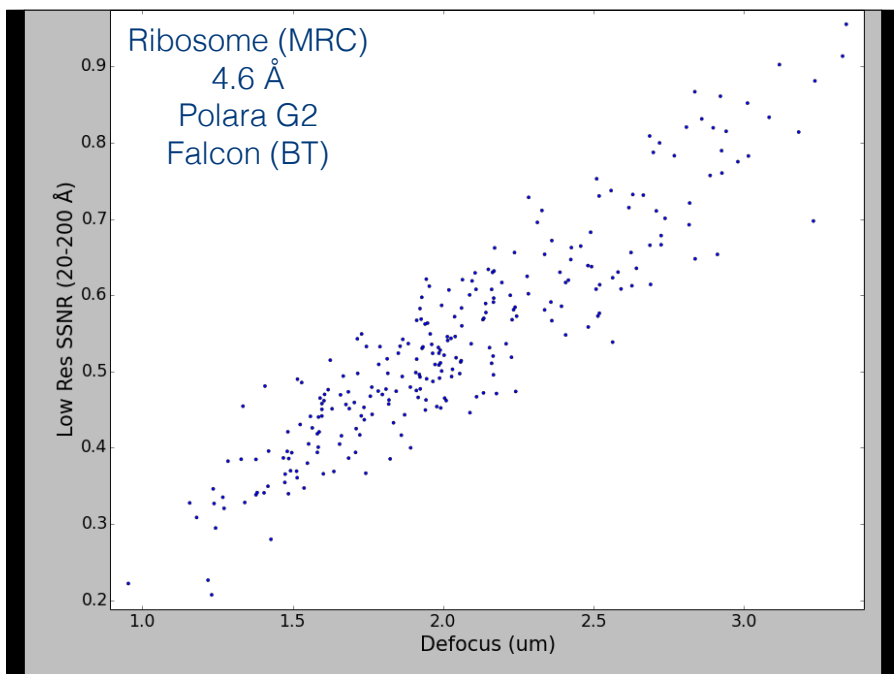
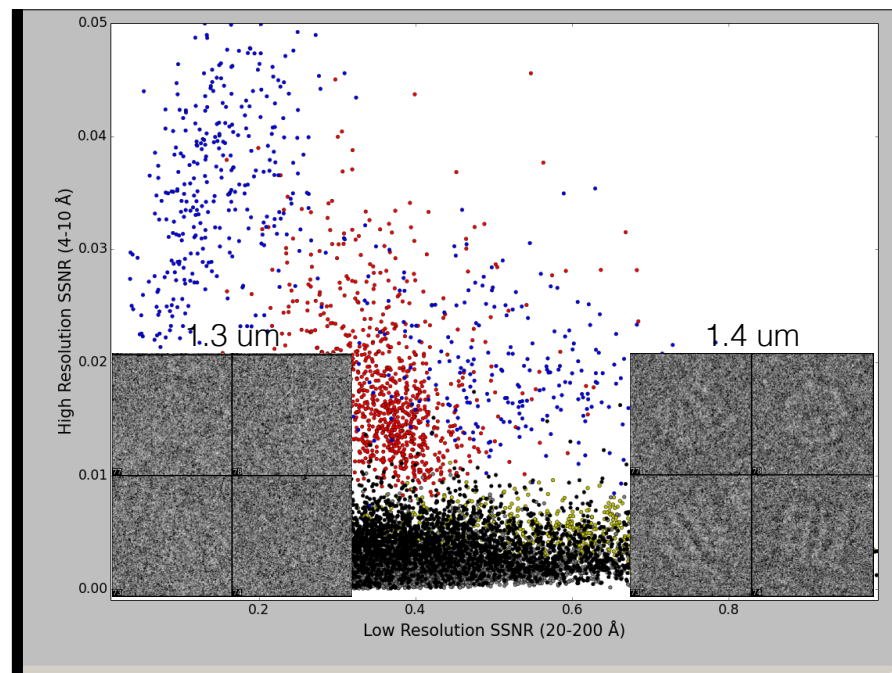
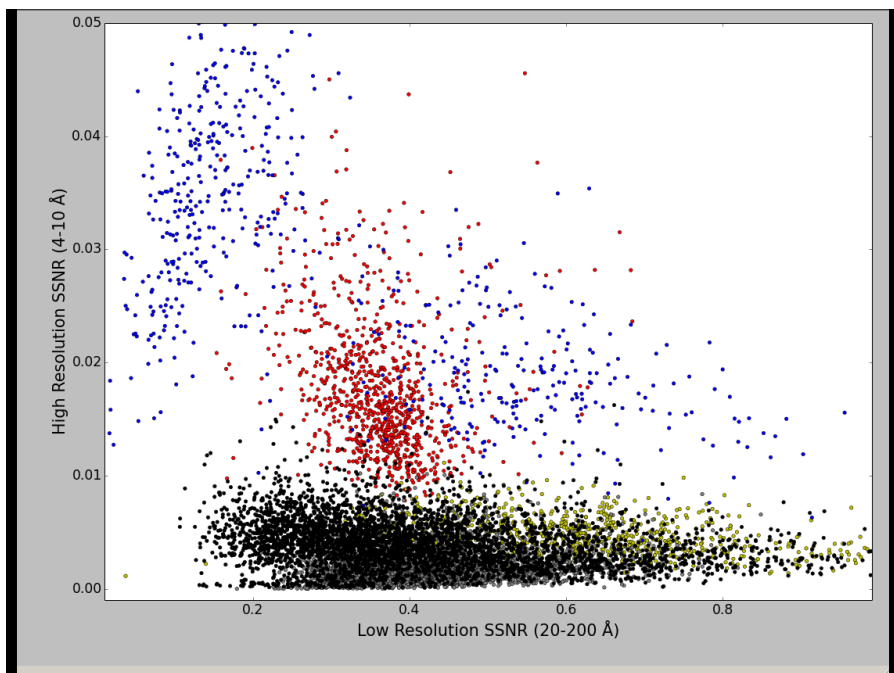


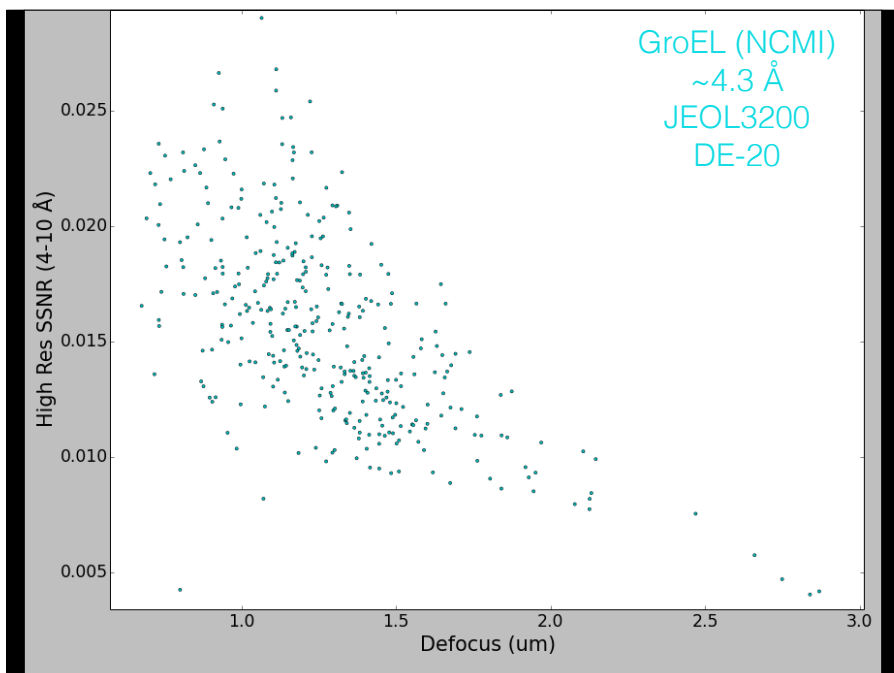
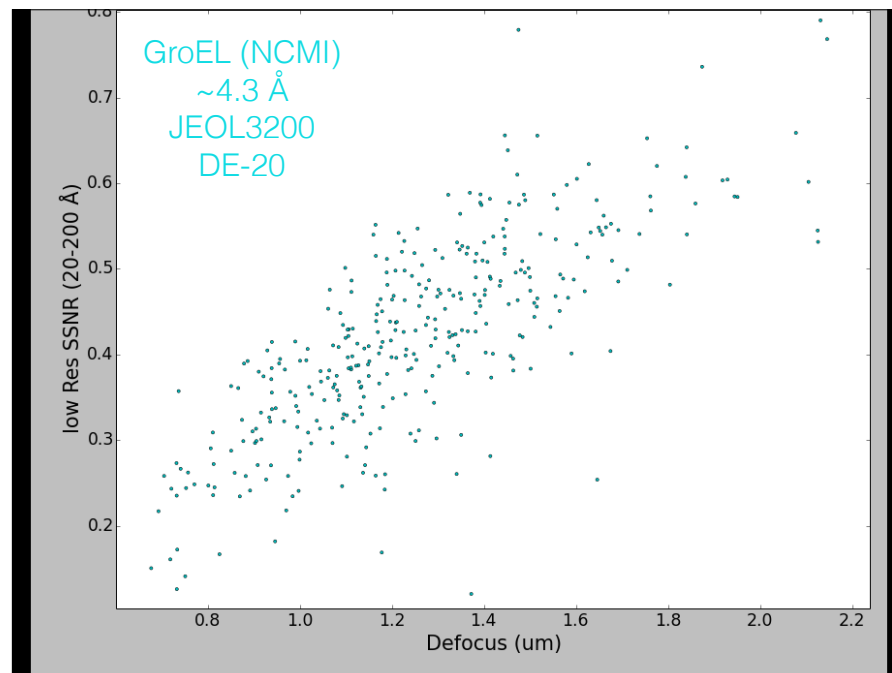
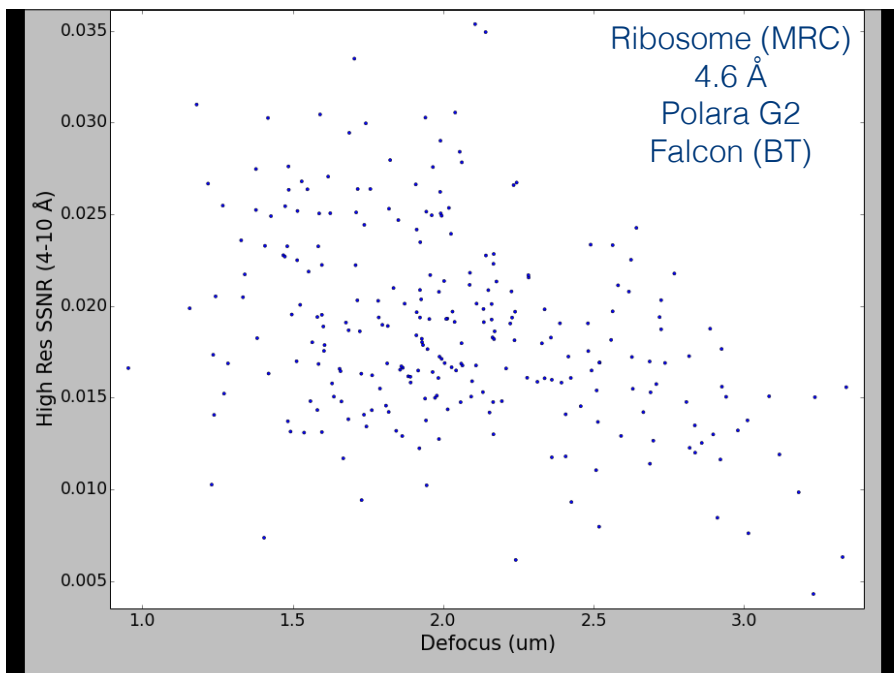
# Image Evaluation





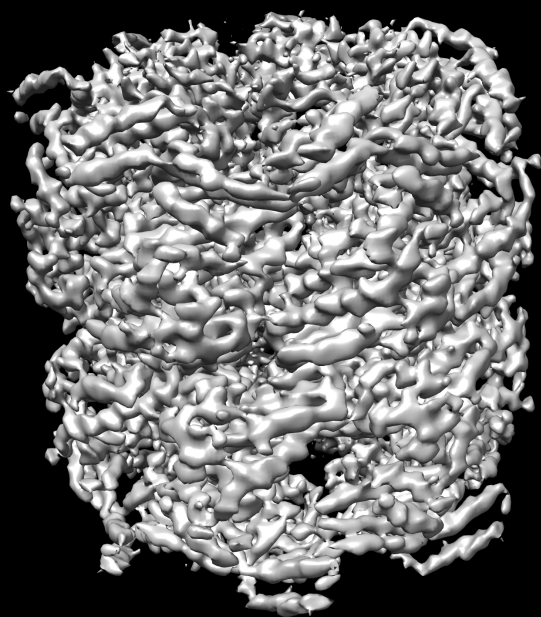




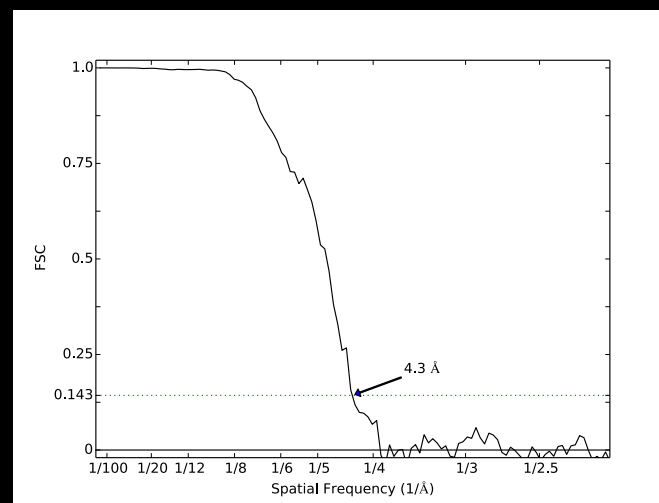


## Particle SSNR Based Assessment

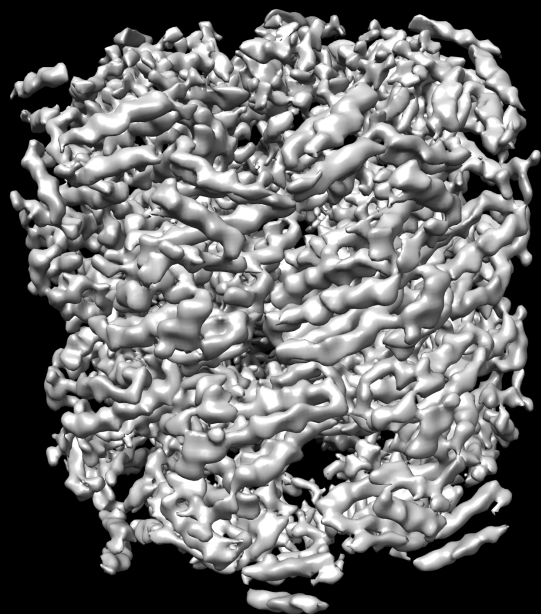
- Fairly robust assessment, immune to most confounders
- No reconstruction or model required
- Particles must be boxed, but not well
- Very high particle density can cause problems



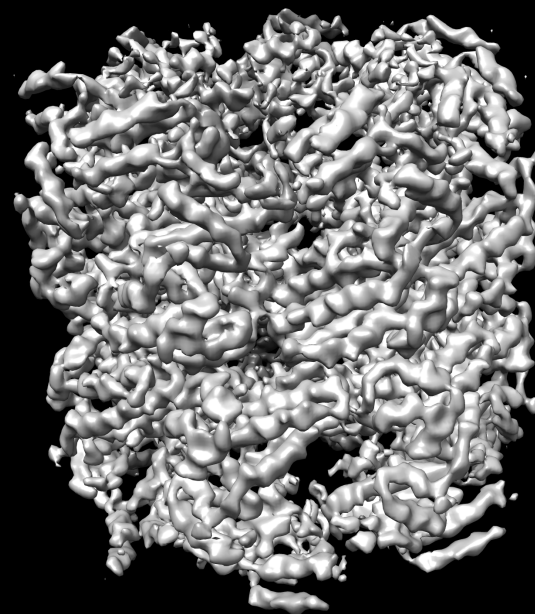
GroEL  
JEOL3200  
DE20  
85k ptcl  
4.3 Å  
EMAN2.1



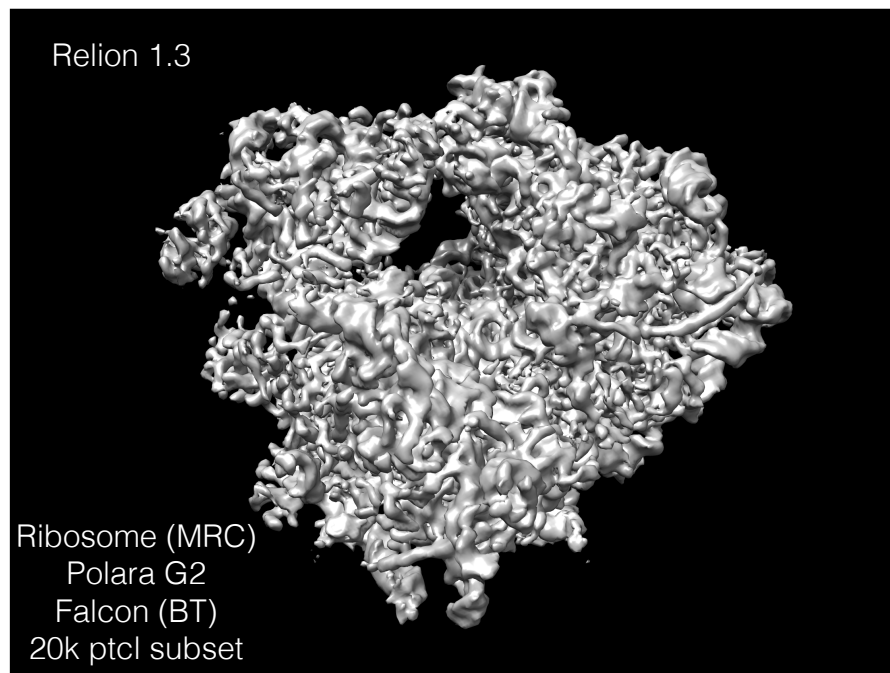
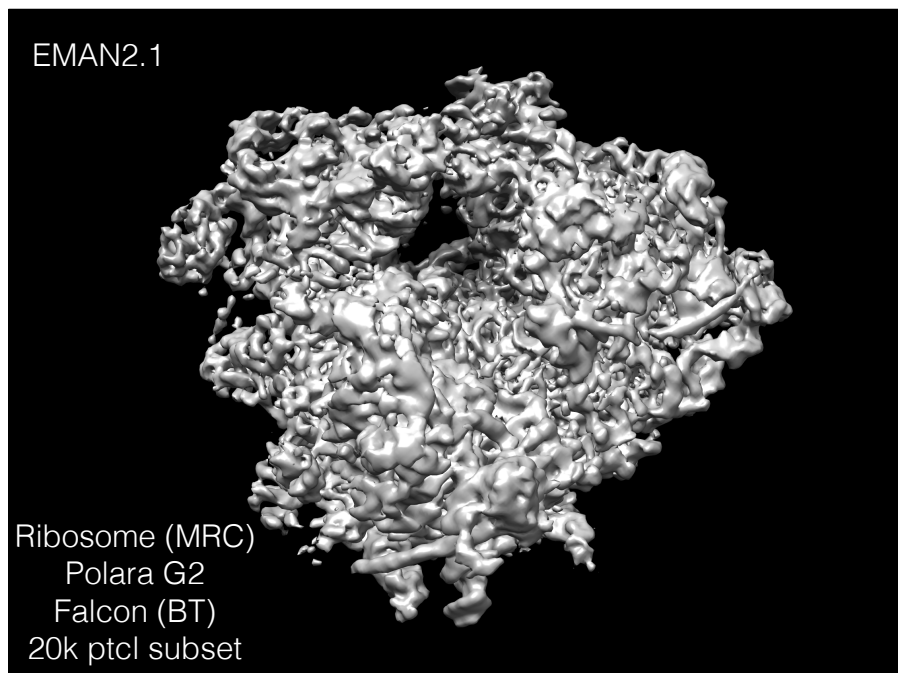
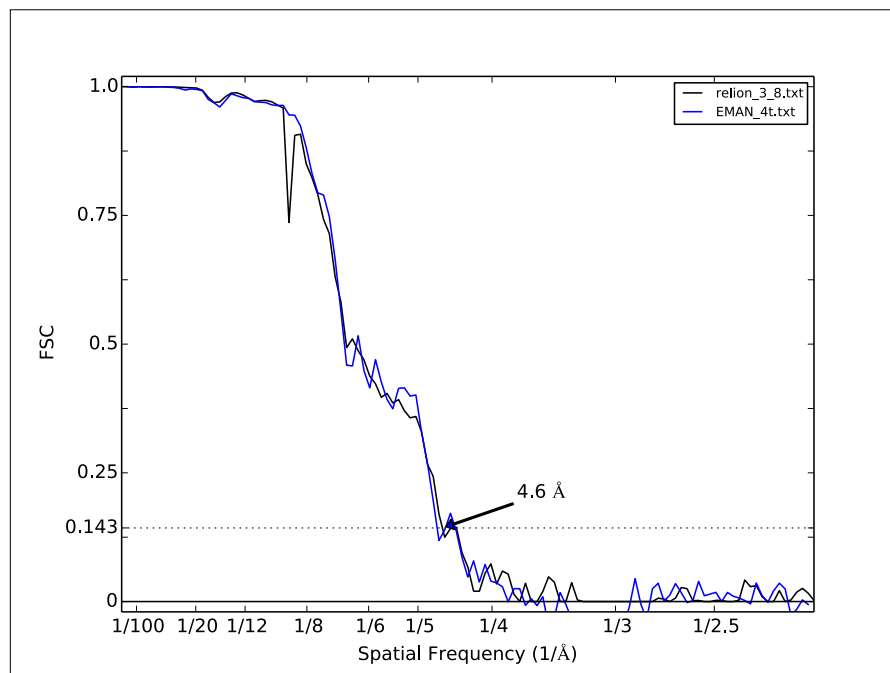
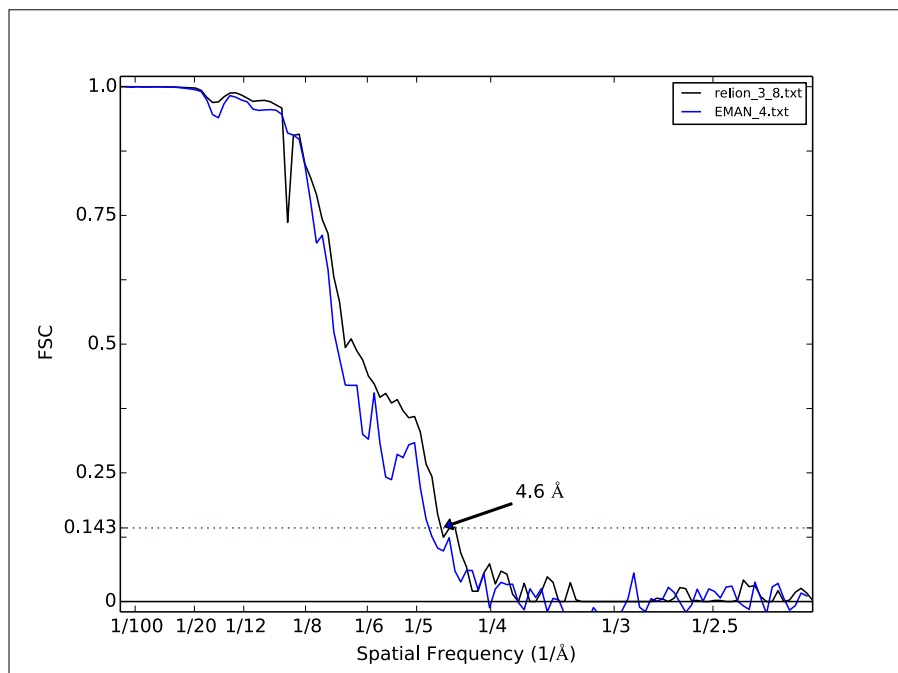
GroEL  
JEOL3200  
DE20  
85k ptcl  
4.3 Å  
EMAN2.1

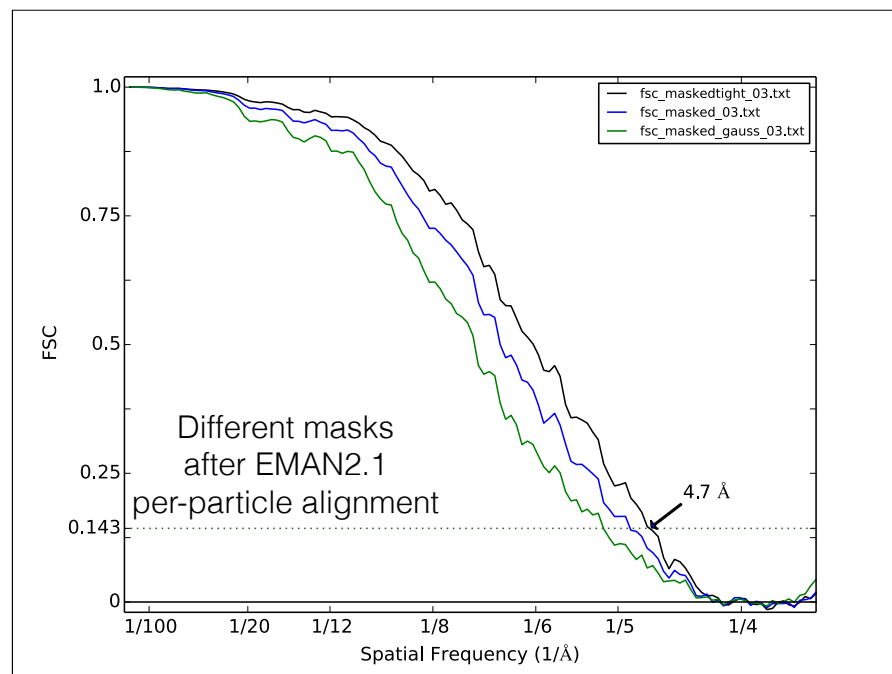
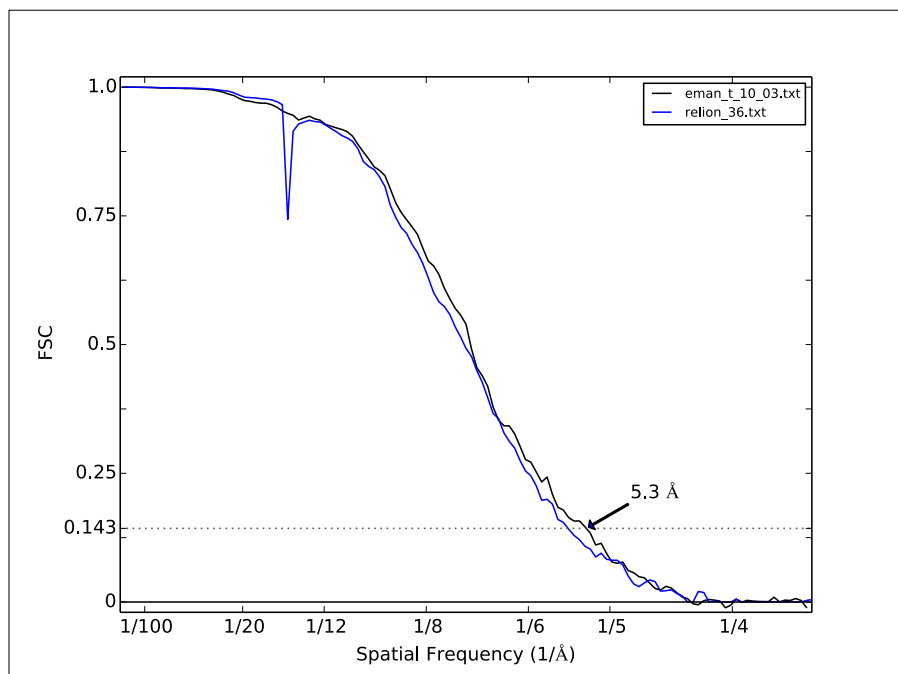
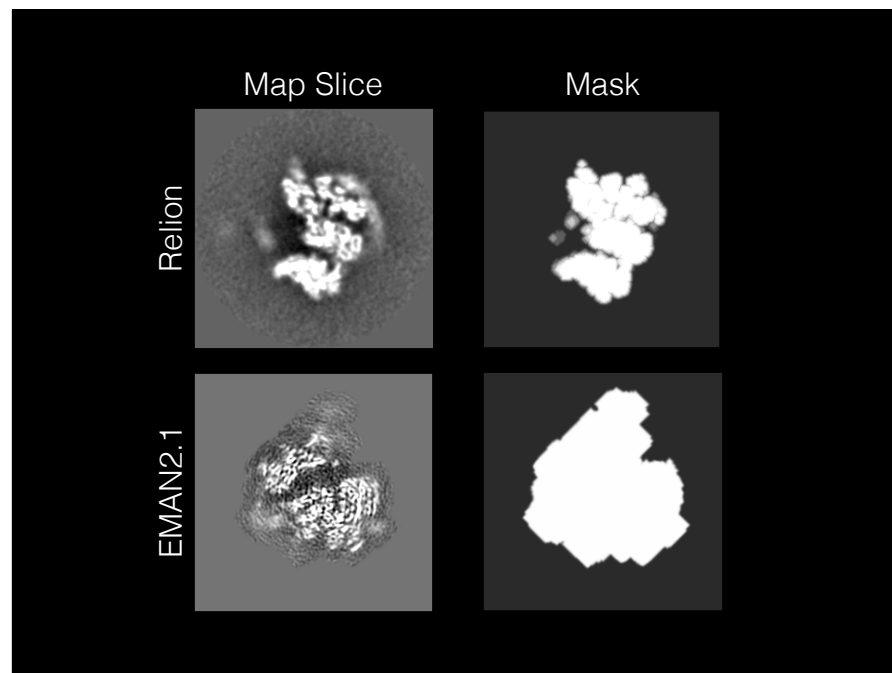
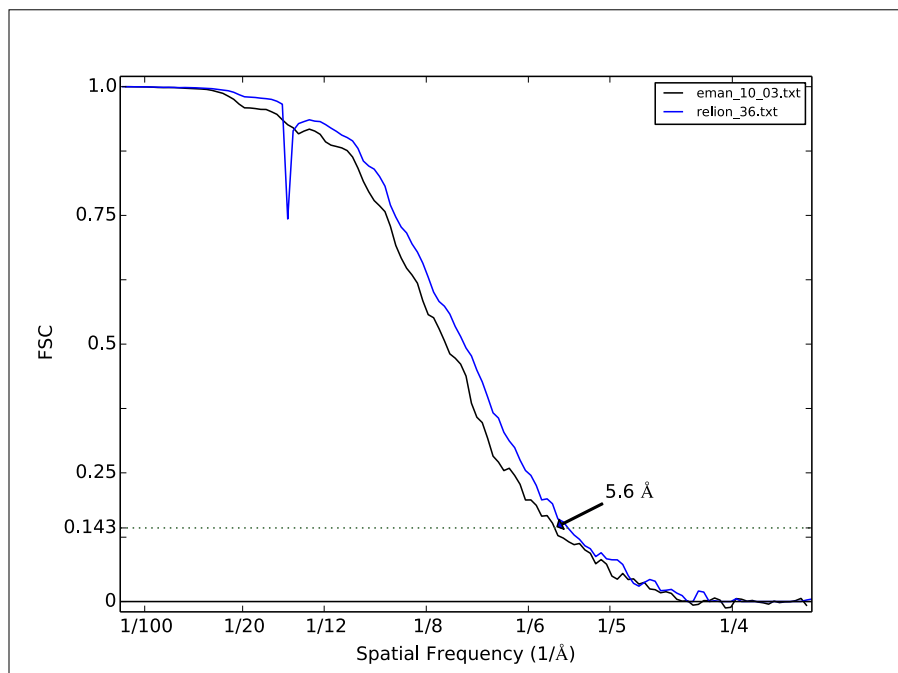


GroEL  
JEOL3200  
DE20  
5k ptcl  
EMAN2.1  
1 CPU-day



GroEL  
JEOL3200  
DE20  
5k ptcl  
Relion  
10 CPU-days







## EMAN 2.1/SPARX Released!

- Gold Standard Refinement
  - Heuristic parameters
  - Refinement report
  - Automatic filtration
- Multi-model 3D classification
- Full suite for subtomogram averaging
- BDB is no longer used!
  - (HDF & human readable text files)
- Typ. 10-20x faster than Relion, similar maps
- Tilt validation
- Interconversion Relion, Frealign, CTFFIND3, EMX

## EMAN2.0 vs. EMAN2.1

```
e2refine.py --input=bdb:sets#set-all_phase_flipped-hp --parallel=dc:localhost:9990
--mass=800.0 --apix=2.12 --automask3d=2,21,1,1,21 --iter=6 --sym=d7
--model=bdb:/refine/refine/workshop/eman2/groel-done/refine_01#threed_filt_04
--path=refine_badang --orientgen=eman:delta=5:inc_mirror=0 --projector=standard
--simcmp=frc:zeromask=1:snrweight=1 --simalign=rotate_translate_flip
--simaligncmp=frc:zeromask=1:snrweight=1 --simralign=refine
--simraligncmp=frc:zeromask=1:snrweight=1 --twostage=2
--classcmp=frc:snrweight=1:zeromask=1 --classalign=rotate_translate_flip
--classaligncmp=frc:zeromask=1:snrweight=1 --classralign=refine
--classraligncmp=frc:zeromask=1:snrweight=1 --classiter=1 --classkeep=1.5
--classnormproc=normalize.edgemean --classaverager=ctf.auto --sep=5
--m3diter=2 --m3dkeep=1.5 --recon=fourier --m3dpreprocess=normalize.edgemean
--m3dpostprocess=filter.lowpass.gauss:cutoff_freq=.125 --pad=192
--classkeepsig --classrefsf --m3dkeepsig --m3dsetsf
```

## EMAN2.0 vs. EMAN2.1

```
e2refine_easy.py --startfrom=refine_02 --targetres=7.0 --sym=d7
--iter=2 --mass=800.0 --apix=2.1 --parallel=thread:16
```

## Training

- <http://blake.bcm.edu/emanwiki/EMAN2>
- <https://groups.google.com/forum/#!forum/eman2>
- Google Hangouts on Air (sludtke42)
  - bi-weekly sessions (when I'm in town)
  - Archived on the Wiki
- Wiki
  - Written tutorials
  - Video Tutorials
  - Documentation ... gradually improving

# My Questions

- Tools for routine/robust single particle work:
  - Are we there yet?
  - Should any lab be able to do this without being embedded in the community for years?
  - Do we need centralized resources?
  - Can a standard lab gather the necessary resources?

# Acknowledgements

**Comparisons**

**Stephen Murray**

**GroEL**

**Chiu Lab**

**Soung-Hun Roh**

**IP3R Project**

**UTHSC**

**Medical School**

**Serysheva Lab**

**Olga Popova**

**Thao Tran**

**Tri Le**

**Que Ngo**

**Wah Chiu**

**Mike Schmid**

**Ludtke Lab**

**Stephen Murray**

**John Flanagan**

Research under support of the NIH/National Institute of General Medical Sciences and The National Institute of Arthritis and Musculoskeletal and Skin Diseases

