3D initial model in RELION 2.1

If you do not have the selected particles after 2D Classification, copy them from the precalculated results to the working directory:

#>cp -r PrecalculatedResults/Select/job015 Select/job015

	RELION-2.1.0: /ssd/reliontuto/relion21_tutorial/bet	tagal 🔶 🗕 🗙
File Jobs Autorun	I/O CTF SGD Sampling Compute Running	
Import Motion correction CTF estimation Manual picking Auto-picking Particle extraction Particle sorting Subset selection 2D classification 3D classification 3D auto-refine Movie refinement Particle polishing Mask creation Join star files Particle subtraction Post-processing Local resolution	Input images STAR file: Select/j Continue from here:	ob015/particles.star 🦻 Browse
Job actions Current	Frint co ; job: Give_alias_here Display	nmand Schedule Run now!
Finished jobs	Running jobs	Input to this job
PostProcess/job023/ MaskCreate/job022/ Refine3D/job011/ Class3D/job013/ Class3D/job018/ InitialModel/job017/ InitialModel/job016/ Select/job015/ Class2D/job014/ Extract/allmics_autopicked/ AutoPick/job011/ Select/job011/ Select/job011/ Select/job011/ Select/job011/ Select/job011/	Scheduled jobs	Dutput from this job
stdout will go here; double-c	lick this window to open stdout in a separate window	
stderr will go here; double-c	lick this window to open stderr in a separate window	

CIF tab:

I/O CTF SGD Sampling Compute Running

Do CTF-correction?	Yes	\$?)
Have data been phase-flipped?	No		
Ignore CTFs until first peak?	No	\$?	

SGD tab:

I/O CTF SGD Sampling Compute Running					
Mask diameter (A):	200 ?				
Symmetry:	D2 ?				
Number of iterations:	3 7				
SGD subset size:	200 -0 - 7				
Write-out frequency subsets:	10 7				
Limit resolution SGD to (A):	20				
SGD increased noise variance half-life:	-1 ()				
Sampling tab:					
I/O CTF SGD Sampling Compute Running					
Angular sampling interval*	15 degrees				
Offset search range (pix):					
Offset search step (pix):	2				
Compute tab:					
1/U CIF SGD Sampling Compute Running					
Use parallel disc I/0?	Yes 🗢 ?				
Number of pooled particles:	3?				
Pre-read all particles into RAM?	Yes 🔷				
Copy particles to scratch directory:					
Combine iterations through disc?	No 🔷 ?				
Use GPU acceleration?	No 🔷 ?				
Which GPUs to use:	2				
Running tab:					
I/O CTF SGD Sampling Compute Running					
Number of MPI procs:	1 2				
Number of threads:	1 0 7				
Submit to queue?	No 🔷 ?				
Queue name:	openmpi ?				
Queue submit command:	qsub ?				
Standard submission script:	64-linux/vlion/none/bin/qsub.csh ? Browse				
Minimum dedicated cores per node:	1 7				
Additional arguments:	2				

If your run takes too long you can copy the precalculated run to the running directory and use these results:

#>cp -r PrecalculatedResults/InitialModel/job016 InitialModel/job016
#>cp -r PrecalculatedResults/InitialModel/job017 InitialModel/job017

Visual inspection of the correspondence between 2D projections and the experimental images.

#>cd InitialModel/symC1 (or cd InitialModel/job016)
#>mkdir Projections
#>relion_project --i run_it003_class001.mrc --o Projections/proj --nr_uniform 50
#>relion_display --i Projections/proj.star

Or alternatively (with bsoft):

#>bproject -origin 50,50,50 -random 50 run_it003_class001.mrc #>Projections/prjs.mrc #>relion_display --i Projections/prjs.mrc --gui



If you repeat the initial model creation process by changing only the symmetry to C1 in the SGD tab:

I/0	CTF	SGD	Sampling	Compute	Running		
Mask diameter (A): 200							
Symmetry:				Symmet	ry: C1 ?		
				Number of	iteratio	ns: 3 2	
				SGD	subset si	ze: 200 7	
			Write-c	ut freque	ncy subse	.ts: 10 ?	
			Limit re	solution	SGD to (A): 20 ?	
	SGD	incr	eased nois	e varianc	e half-li	fe: -1 () ?	

you should get a different (better) result:



Now, let's use Chimera to align the apparent symmetry axes parallel to the XYZ axes.

#>chimera InitialModel/job017/run_it003_class001.mrc;

Use the duplicate option under the File menu of the Volume viewer.

Deactivate map #1 on the Model Panel;

Rotate map #0 to have it's symmetry axis parallel to the XYZ axes;

Save this model as InitialModel/symC1/inimodel.mrc

Check the result of the alignment by imposing D2 symmetry on the resulting map:

#>relion_image_handler --i inimodel.mrc --o inimodel_symD2.mrc --sym D2

The output map should be similar to the input map:

#>chimera inimodel.mrc inimodel_symD2.mrc