map quality decays after refinement

Mon, 03/25/2019 - 10:20
#1

rddey80

map quality decays after refinement

Dear Members,

I always see the quality of map decays after auto-refinement from ab-initio 3D model. Please check the attached file. During the creation of refinement package I gave 3 for number of classes (for 3D ref). While starting autorefinement, under starting reference, I see three volulems all with same name as 'Volume From Startup #1 - class#2'. But, under the directory of Assets/Volumes/ I see, startup_volume_1_1.mrc, startup_volume_1_2.mrc, startup_volume_1_3.mrc

Could you please explain the 3 volumes with same name shown under starting reference?

Please also advise how I can improve the map quality after autorefinement. I have done map sharpening, but it did not help.

Thanks for your time,

Raj

File:
📄 startupVol-and-Ref-from pp-data3.14.2019.docx

timgrant

Hi Raj,

The volume after ab-inito is likely overfit - as nothing is done to prevent overfitting in ab-inito, so the higher resolution features you are seeing are probably wrong. The autorefinement is much more careful, and so should not overfit so much.

The last number in the filename is the class number, so startup_volume_1_1/2/3.mrc are the 3 classes. Autorefinement takes one initial model and classifies into the number of classes you specify.

Cheers,

Tim

Mon, 03/25/2019 - 16:01 <u>(Reply to #2)</u>

rddey80

Hi Tim,

Thanks for your reply. Could you please tell how I can avoid overfitting during the ab-inition model building?

Thanks,

Raj

guochj

Same problem

Hi Raj,

I have met the same thing just like yours. But I think we met this problem because the amount of our particles is too little. How many partilce have you used in auto-refinement?

Mon, 03/25/2019 - 22:30 <u>(Reply to #4)</u>

rddey80

Hi Guochj,

30k particles. But, I can get good map using sample data (about 20K particles) from tutorial.

Thanks,

Raj

Mon, 03/25/2019 - 22:55 <u>(Reply to #5)</u>

guochj

Hi Raj

Ok, sample data has an O symmetry. So, I think you can try to add some data and try again. We just use around 10k particles with C2 symmetry. And we are trying to get extra data.

Thanks,

Chj

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