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Thu, 11/08/2018 - 18:45

#1

ivo lu

Validation for models

Hi all,

I am new to cisTEM. I am wondering that since I already constructed several models of a protein, what is the standard method in cisTEM to validate these models?

Thank you all in advance!

Best regards,

Ivo

timgrant

Hi Ivo,

Hi Ivo,

Do you mean validate the resulting maps, or validating molecular models built into them? In the former case, you mainly want to make sure that the highest resolution used in refinement is considerably lower than your estimated resolution, and that the map "looks" ok. In the latter case, it shouldn't be any different from any other case.

Thanks!

Tim

Fri, 11/16/2018 - 23:29 (Reply to #2)

ivo lu

Hi Tim,

Hi Tim,

Sorry I didn't make my question clearer. What I really want to figure out is how particle pool changes between each iteration of refinement in auto-refine.

Another question I want to ask is that if one auto-refine is not enough, should I gradually decrease high-resolution limit within multiple auto-refines?

Best,

Ivo

timgrant

Hi Ivo,

Hi Ivo,

I basically always do an auto-refine, then if the resolution is decent (fair bit better than 8Å), I do another auto-refine starting at 8Å. that should probably be enough in most cases.

You can get access to the parameters by going to the results->refinement panel, then clicking on the icon above the angular plot that looks like a document with a plus. You can save these parameters to a file from different rounds and compare them to see how things are moving.

Cheers,

Tim

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