Home > cistem vs relion maps for model building in coot - different real space ref weights

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Fri, 04/20/2018 - 10:36   #1

Jonas

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Hi all,

For model building in coot with relion maps, I usually use map2map to get ccp4 maps, then phenix.map_to_structure_factors go get the mtz file.

This works also for the cistem maps but for some reason, the refinement weight I have to use in coot to get decent geometry values with "real space refine zone" is drastically different. With the standard coot value of 60, realspace refine zone results in good geometry values with the relion map but horrible values using the cistem map (same well resolved area realspacerefined, see attached pdf). I have to reduce the weight to 1 to get decent values with cistem map.

I also tried mapmask and sfall to generate mtz without success.

What is the recomended procedure for mrc to mtz conversion of cistem maps?

Thanks a lot for the input.

Best

J

File:
📄 realspaceref.pdf

timgrant

Hi,

The restraints (in coot for sure, but possibly other programs) are based on the absolute value of the map. This means that normalising to different values (i.e. multiplying by some constant) will change how the weights work. Whereas in EM we tend to think of multiplying by a constant as being more or less arbritrary and not really changing the map. I am not sure what is the correct value to normalise the map to, but I have been told that running the following command in the chimera command line :-

"vop scale *vol-spec* rms 0.03"

Where vol-spec is the number of your model (e.g. #0 if there is only one model), and then saving the scaled result, results in a map with ok scaling.

Thanks!

Tim

Jonas

Hi Tim,

Thanks a lot for the quick response.

Best

Jonas

Fri, 04/20/2018 - 11:07 <u>(Reply to #3)</u>

alexis

Estimate

Hi Jonas,

I have had decent luck just opening the map directly (without going via mtz) and then using coot's built in "Estimate" function to guess an appropriate weight.

Cheers,
Alexis

timgrant

Is this from a sharpened map?

Is this from a sharpened map? Can you let me know if the 0.03 normalised map works well for you? If so, I will change cisTEM to automatically normalise to 0.03 during the sharpening.

Thanks,

Tim

Jonas

This was from a sharpened map

This was from a sharpened map. The 0.03 normalized map works well.

Thanks a lot,

Jonas

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