challenges importing frealign params

Thu, 01/18/2018 - 11:05   **#1**

sstagg

challenges importing frealign params

Hi all,

I'm having a problem where when I import frealign parameters, cistem is setting the occupancy to 0 for all particles, and there's nothing I can do to recover from that after they are imported. The problem boils down to how cistem interprets if the parameter file has a phase shift column or not. FYI, I have code that is generating the frealign format parameter file, so my guess is that it's just not being parsed properly. Is it being interpreted using white space, or do the columns have to line up exactly?

Thanks,

Scott

niko

When importing a Frealign

When importing a Frealign parameter file, *cis*TEM checks if it is written in an older format that does not contain phase shifts. The test consists of checking the length of the lines in the parameter file. Anything less than 142 characters per line is interpreted as a parameter file that does not contain phase shifts. Also, standard Frealign parameter files have 17 columns (including the phase shifts); old-style parameter files have 16 columns. The final column is not used anymore (it indicated Score changes in the last refinement cycle). However, it is important to include this final column when importing a parameter file into *cis*TEM due to the check of the line length. Values in the final column can be set to 0.0.

sstagg

Thanks. That helps

Source URL: https://cistem.org/challenges-importing-frealign-params?page=0