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Magn. Reson. Discuss., referee comment RC3
https://doi.org/10.5194/mr-2021-28-RC3, 2021

Comment on mr-2021-28

Anonymous Referee #3

Referee comment on "Bootstrap aggregation for model selection in the model-free formalism" by Timothy Crawley and Arthur G. Palmer III, Magn. Reson. Discuss., https://doi.org/10.5194/mr-2021-28-RC3, 2021

Excellent manuscript that brings new approaches to the problem of model selection in the analysis of model-free dynamics data. It has been recognized for a long time the problem of selecting the model that most robustly fits the analysis, and then the issue of selecting a single model that is marginally "better". This manuscript uses bootstrap aggregation, from machine learning approaches to improve the possibilities of what is (are) the best model(s) and how that adds to our knowledge of the influsence of dynamics on structure/function - the purpose of doing the work. I particularly liked the Arg examples given - especially Arg11 and also Arg26, the idea that the dynamics reflects its position at the juncture of the coiled-coil and basic regions. More conventional analyses may miss this insight.

Like the other reviewers, discussion needs to address the issues of using two or three fields. Data at two fields are the most commonly acquired and so would this method be inapproriate or do the authors have alternate approaches/ideas.

The paper is well-written and accessible to most in the field. A good balance of theory, method and application. I agree that the tables need better notes - for example the description of the colour scheme in Figure 1 has to be repeated in Fig 2 and 3; better decriptive footnotes in Table 2,3,4 (and actually I think this could be put into a single table with residue first column and clear breaks); possibly the same for Tables 5,6,7.

Very few errrors found. Including the detected typos line 199 "highlighted"