

# Fewer Dimensions, More Structures for Improved Discrete Models of Dynamics of Free Versus Antigen-Bound Antibody

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## Deviation of Structures from Initial/Starting Structures for the Free Antibody System

We demonstrate how far the 160,000 MD-generated structures (collected over all 12 MD trajectories) deviate from each of the 12 initial/seed structures. For each generated structure, we calculate its backbone RMSDs from a given starting structure, and show the backbone RMSDs in the plots below. We also record the maximum backbone RMSD achieved in each plot.

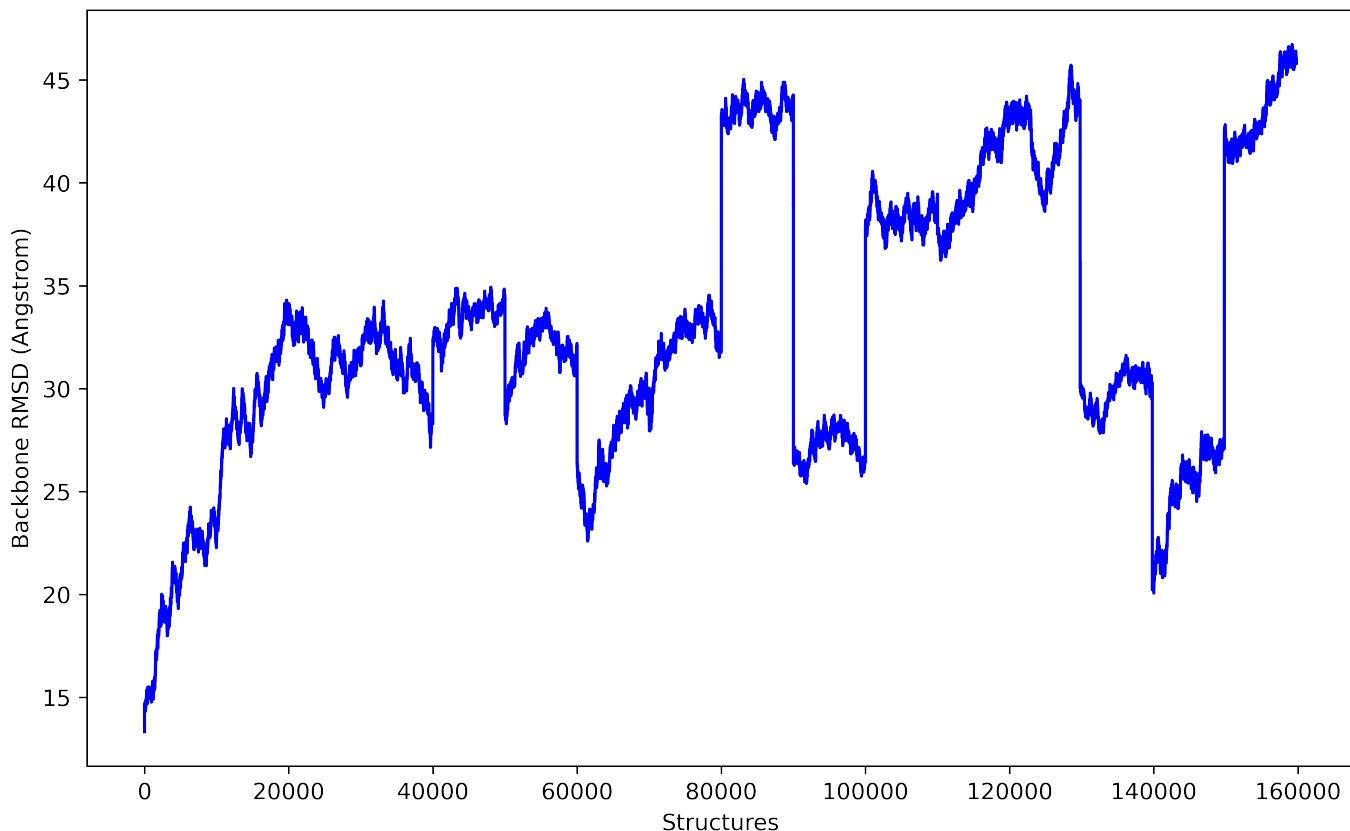


Figure S1: We draw the backbone RMSDs of the 160,000 MD-generated structures from the structure seeding MD trajectory 1/12. The maximum RMSD of 46.725Å is recorded at the 159,191<sup>th</sup> frame.

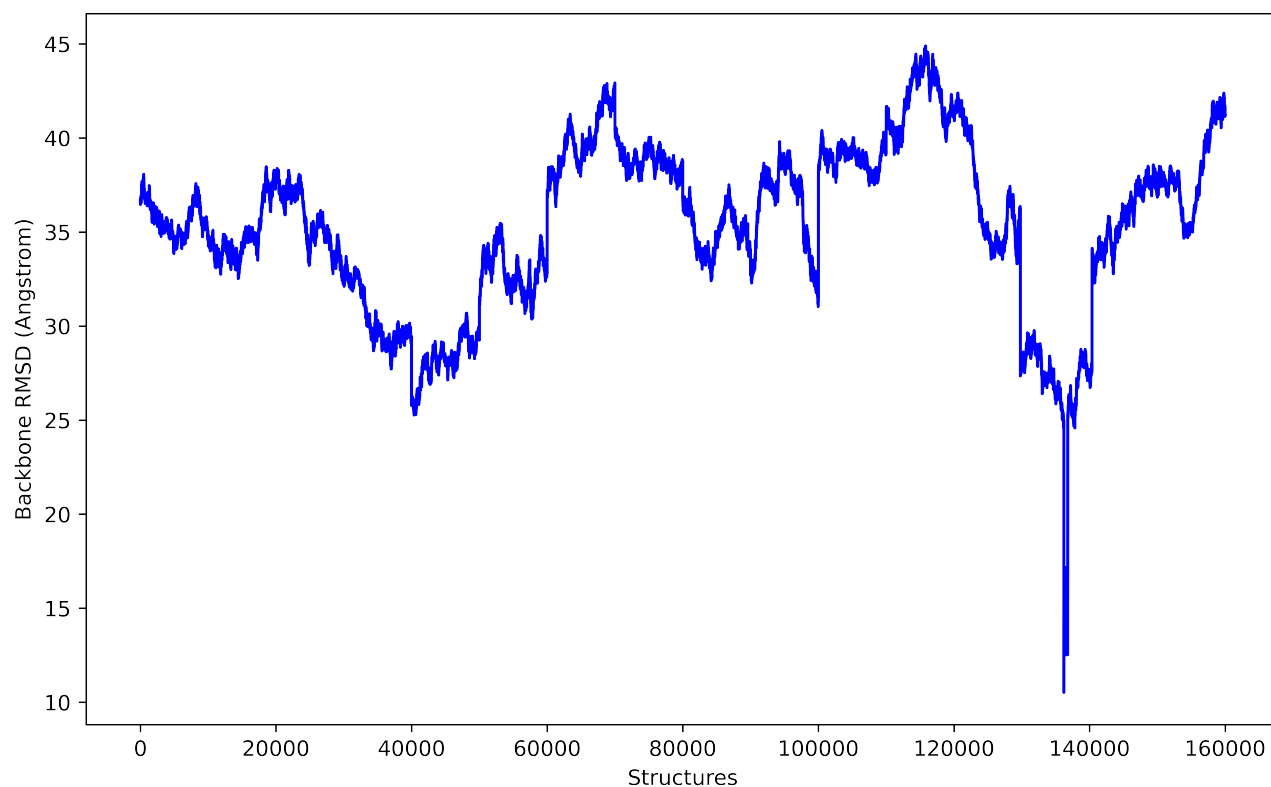


Figure S2: We draw the backbone RMSDs of the 160,000 MD-generated structures from the structure seeding MD trajectory 2/12. The maximum RMSD of  $44.886\text{\AA}$  is recorded at the  $115,808^{th}$  frame.

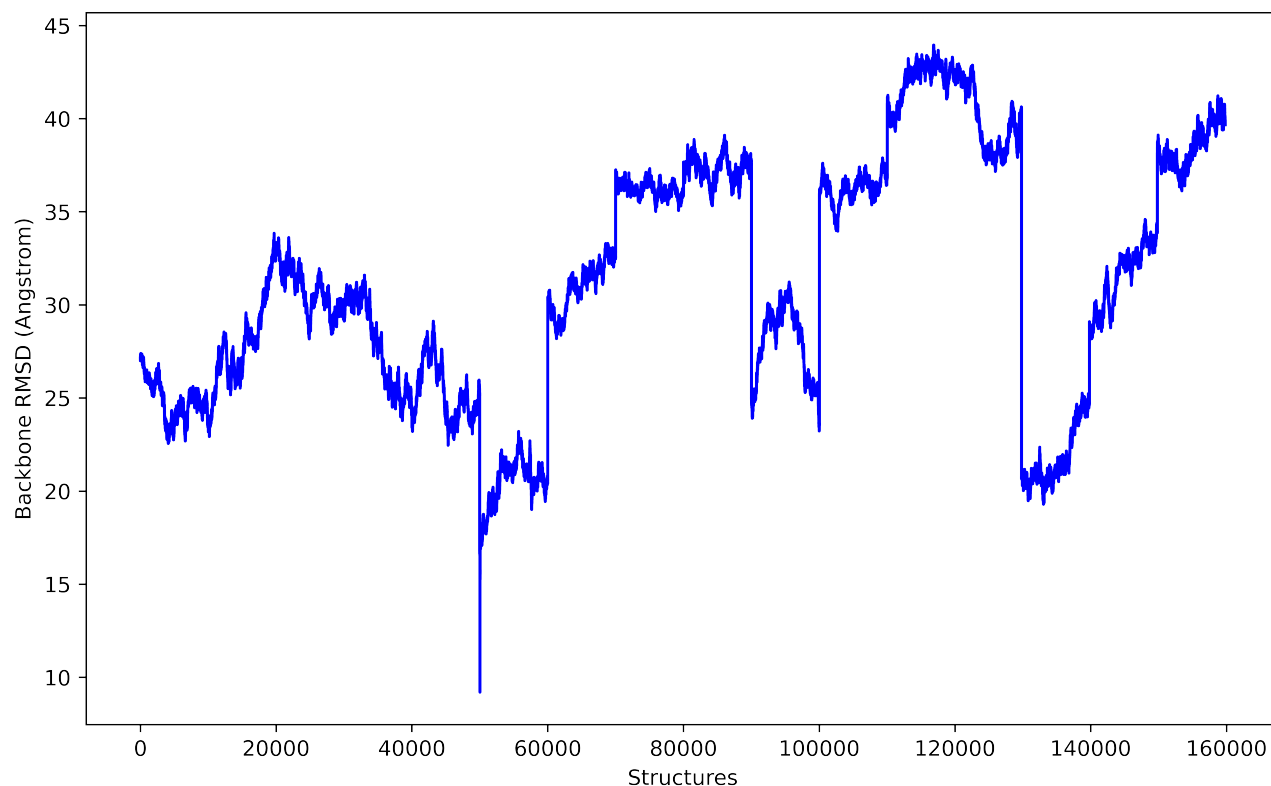


Figure S3: We draw the backbone RMSDs of the 160,000 MD-generated structures from the structure seeding MD trajectory 3/12. The maximum RMSD of  $43.954\text{\AA}$  is recorded at the  $116,861^{th}$  frame.

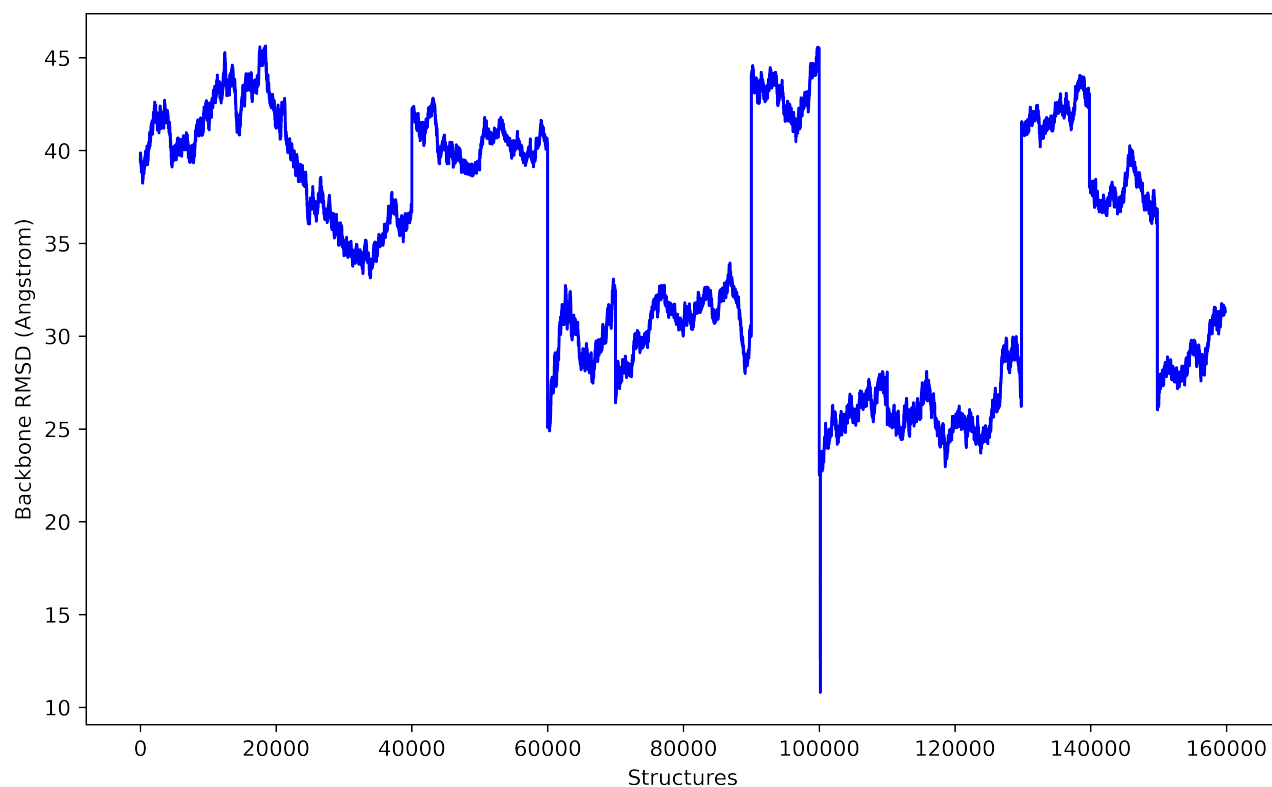


Figure S4: We draw the backbone RMSDs of the 160,000 MD-generated structures from the structure seeding MD trajectory 4/12. The maximum RMSD of 45.633Å is recorded at the 18,453<sup>th</sup> frame.

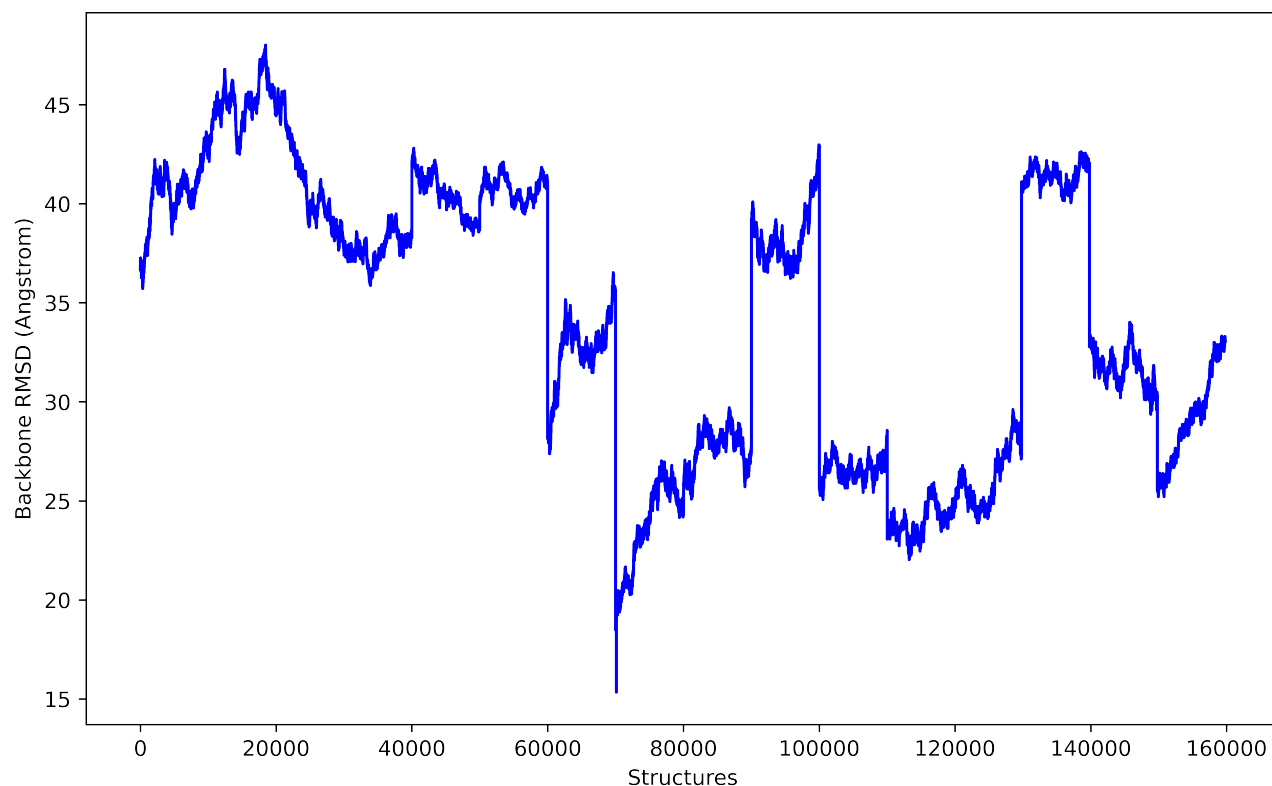


Figure S5: We draw the backbone RMSDs of the 160,000 MD-generated structures from the structure seeding MD trajectory 5/12. The maximum RMSD of 48.016Å is recorded at the 18,453<sup>th</sup> frame.

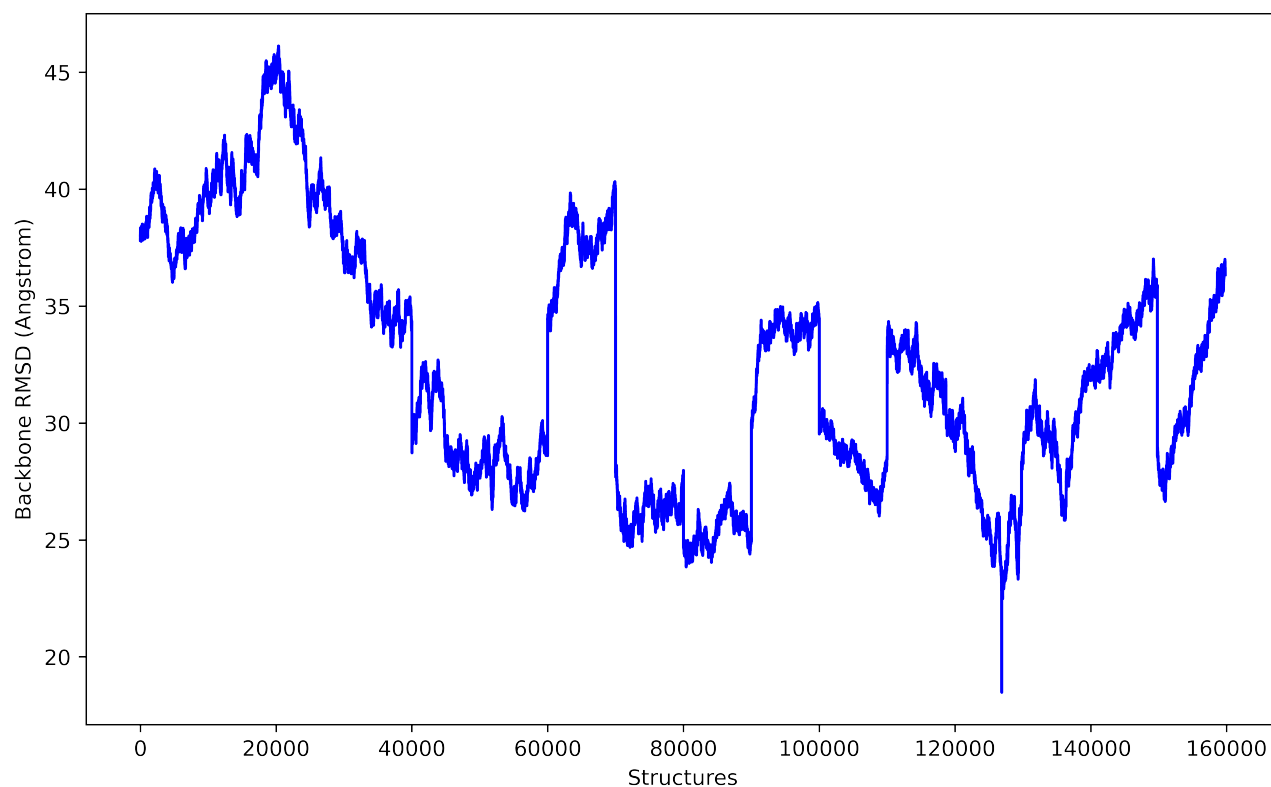


Figure S6: We draw the backbone RMSDs of the 160,000 MD-generated structures from the structure seeding MD trajectory 6/12. The maximum RMSD of 46.124Å is recorded at the 20,357<sup>th</sup> frame.

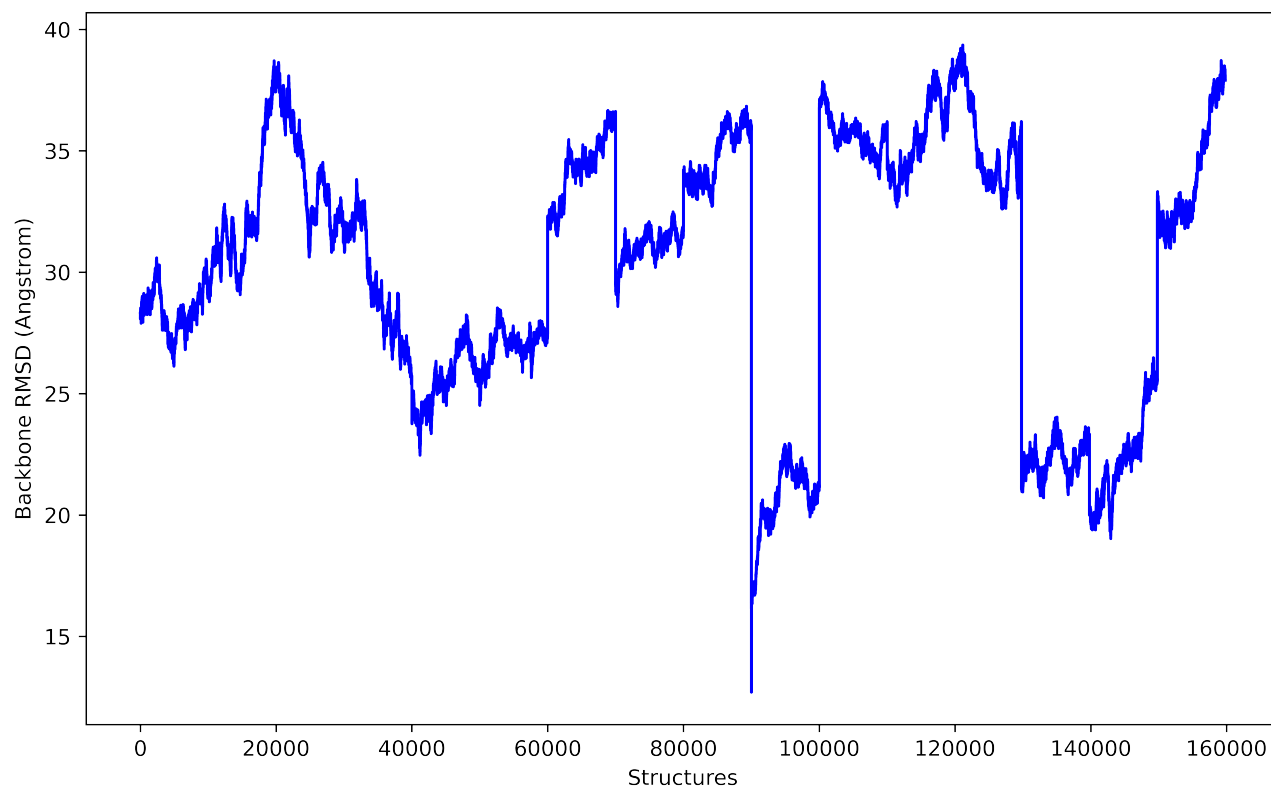


Figure S7: We draw the backbone RMSDs of the 160,000 MD-generated structures from the structure seeding MD trajectory 7/12. The maximum RMSD of 39.357Å is recorded at the 12,1145<sup>th</sup> frame.



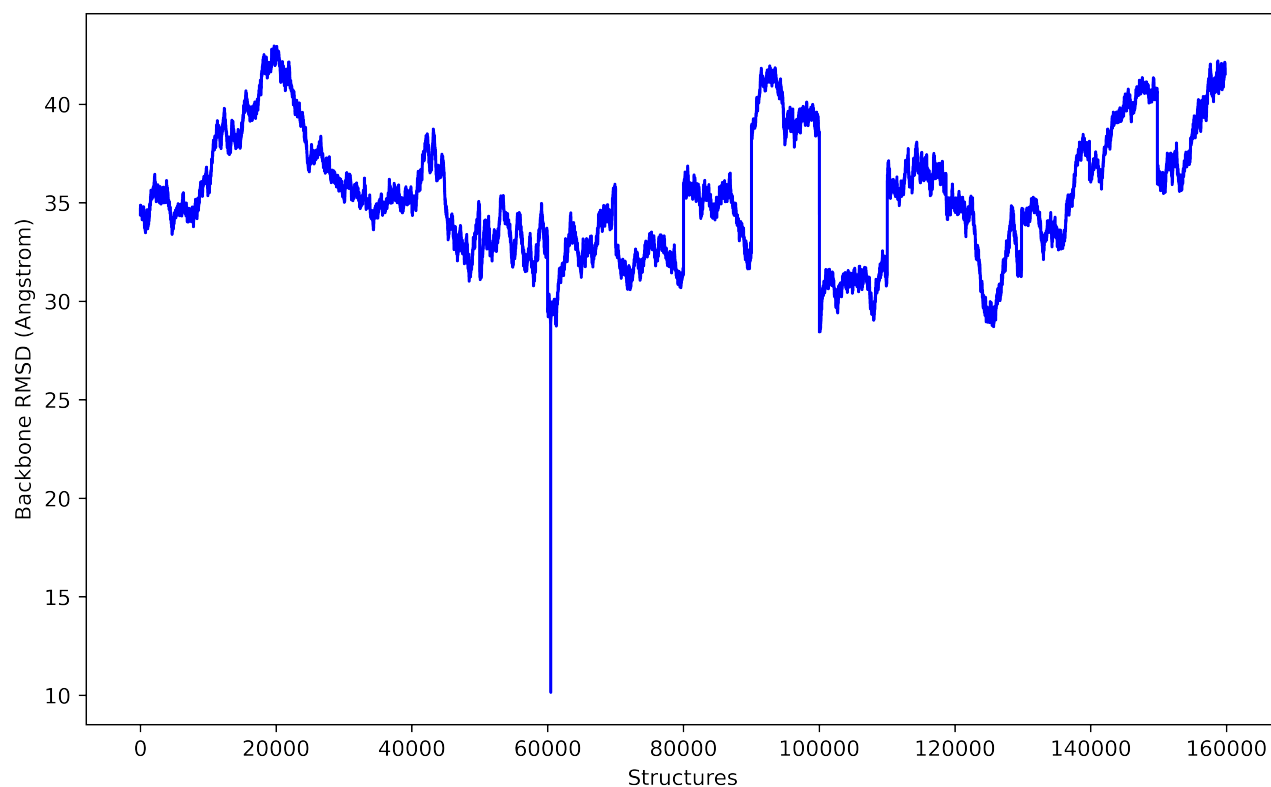


Figure S8: We draw the backbone RMSDs of the 160,000 MD-generated structures from the structure seeding MD trajectory 8/12. The maximum RMSD of 42.962Å is recorded at the 19,711<sup>th</sup> frame.

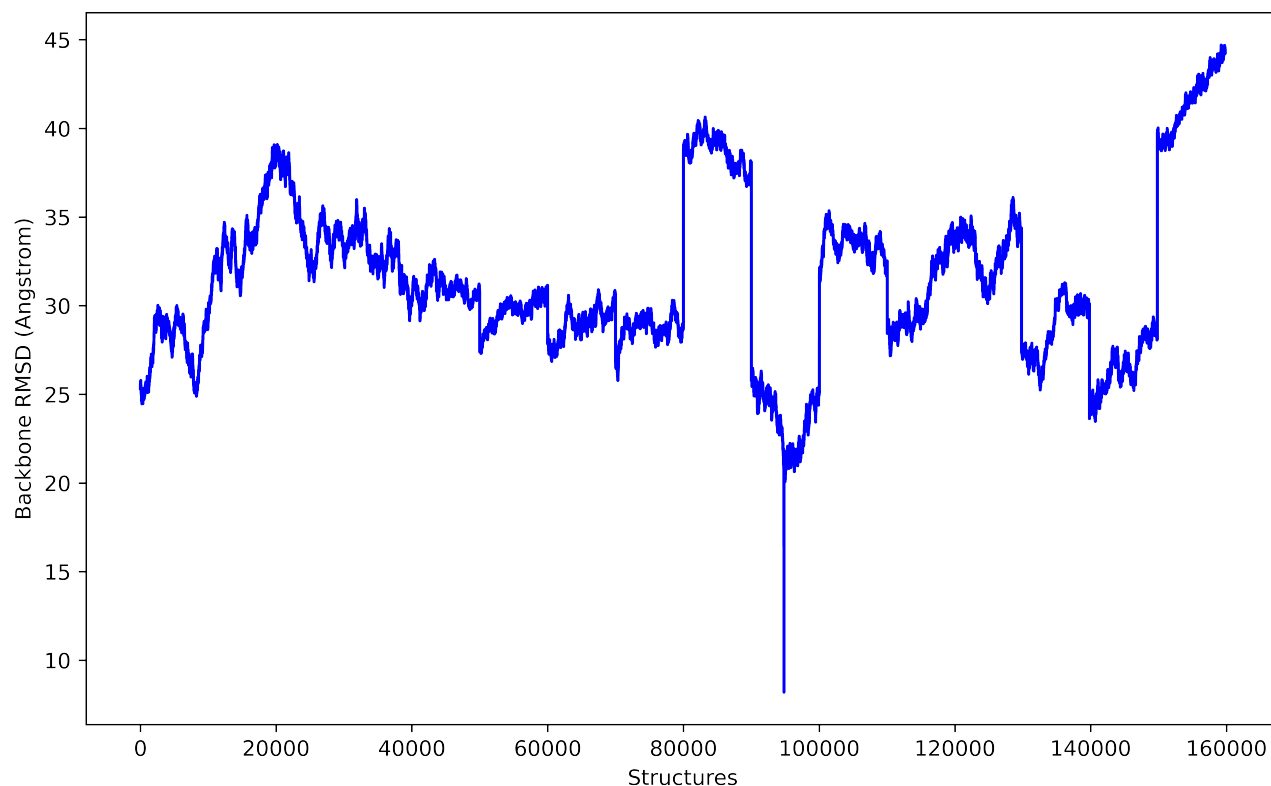


Figure S9: We draw the backbone RMSDs of the 160,000 MD-generated structures from the structure seeding MD trajectory 9/12. The maximum RMSD of 44.701Å is recorded at the 159,207<sup>th</sup> frame.

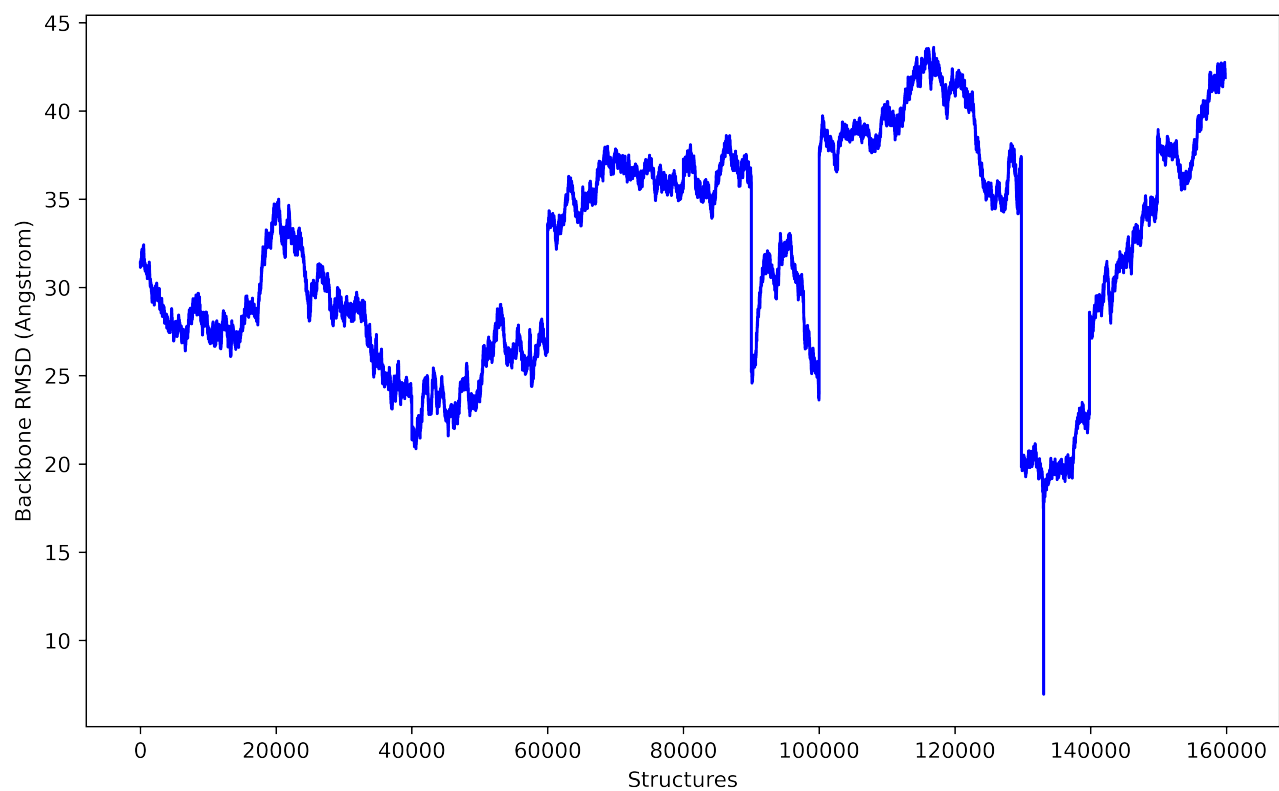


Figure S10: We draw the backbone RMSDs of the 160,000 MD-generated structures from the structure seeding MD trajectory 10/12. The maximum RMSD of 43.603Å is recorded at the 116,871<sup>th</sup> frame.

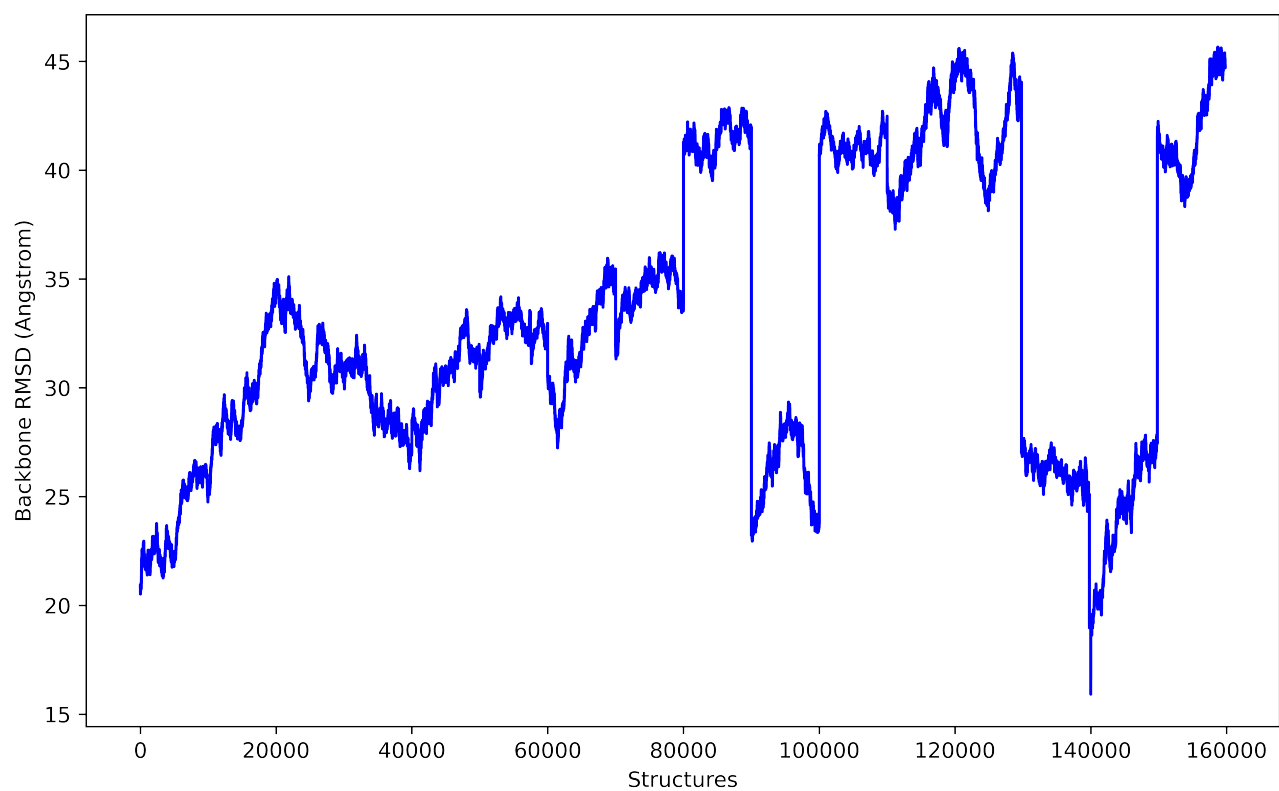


Figure S11: We draw the backbone RMSDs of the 160,000 MD-generated structures from the structure seeding MD trajectory 11/12. The maximum RMSD of 45.66Å is recorded at the 158,710<sup>th</sup> frame.

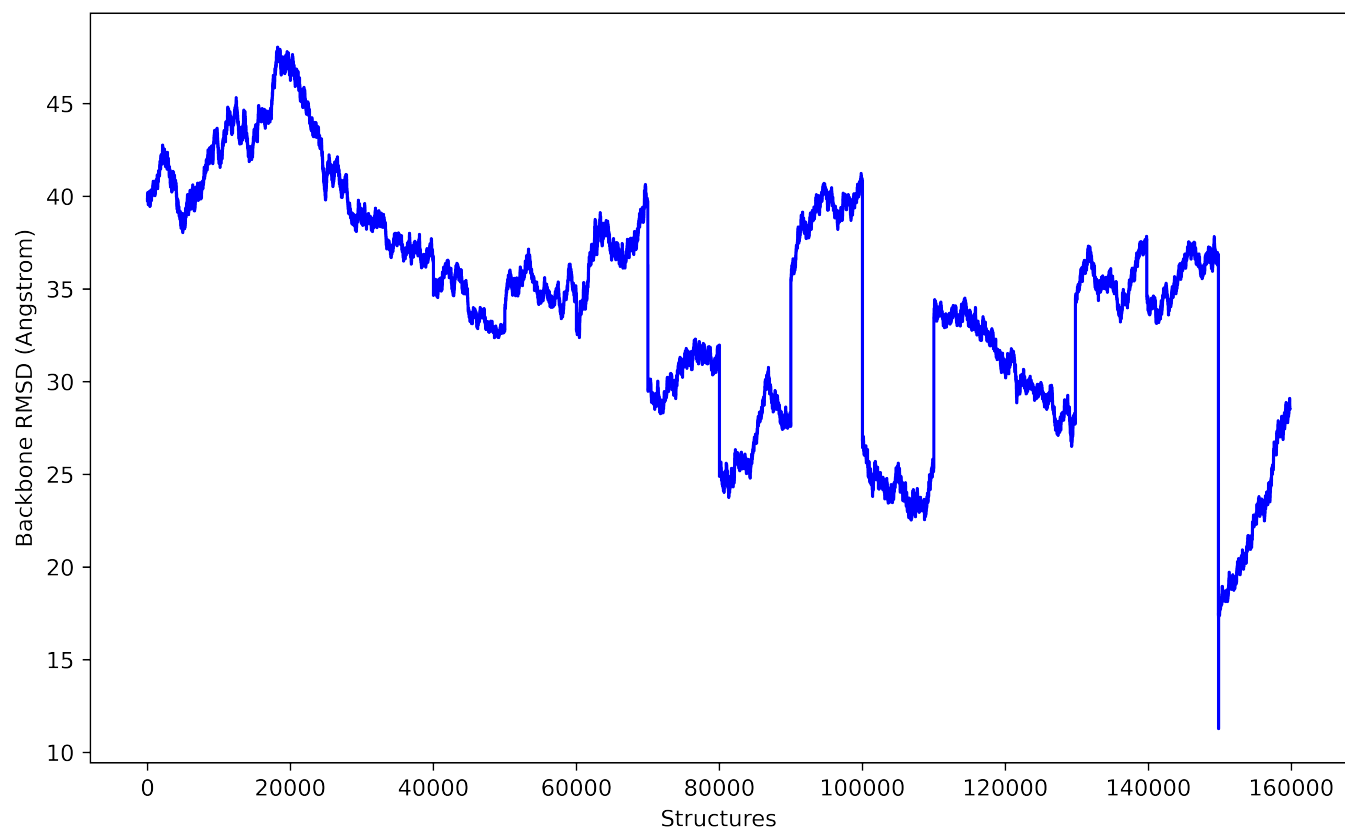


Figure S12: We draw the backbone RMSDs of the 160,000 MD-generated structures from the structure seeding MD trajectory 12/12. The maximum RMSD of 48.04Å is recorded at the 18,222<sup>th</sup> frame.

# MSM Evaluation via the CK Test

## Free Antibody MSM Evaluation via the CK Test

Fig. S13- S15 relate the results obtained from conducting the CK test over the MSM models obtained respectively from Settings A-C for the free antibody. Specifically, these figures visualize the outcome for the five states identified in each setting that have the highest self-transition probabilities. The plots show deviations between the estimated and the predicted model in Settings A-C. These are largest under Setting-A and gradually reduce over Setting-B and Setting-C; the deviations are negligible for Setting-C. In good agreement with the convergence analysis test related in the main manuscript, the CK test additionally confirms that the MSM model obtained from Setting-C is the best, as it stands best to both of these statistical tests.

## Antigen-bound Antibody MSM Evaluation via the CK Test

Fig. S16-S18 relate the results obtained from conducting the CK test over the MSM models obtained respectively from Settings A-C for the antigen-bound antibody. As for the antigen-bound antibody, the figures visualize the outcome for the five states identified in each setting that have the highest self-transition probabilities. The plots show deviations between the estimated and the predicted model in Settings A-C. They show that these are largest under Setting-A and gradually reduce over Setting-B and Setting-C. Again, the deviations are negligible for Setting-C, as for the free antibody. In good agreement with the convergence analysis test related above, the CK test additionally confirms that the MSM model obtained for the antigen-bound antibody from Setting-C stands best to both of the statistical tests (convergence analysis and CK-test).

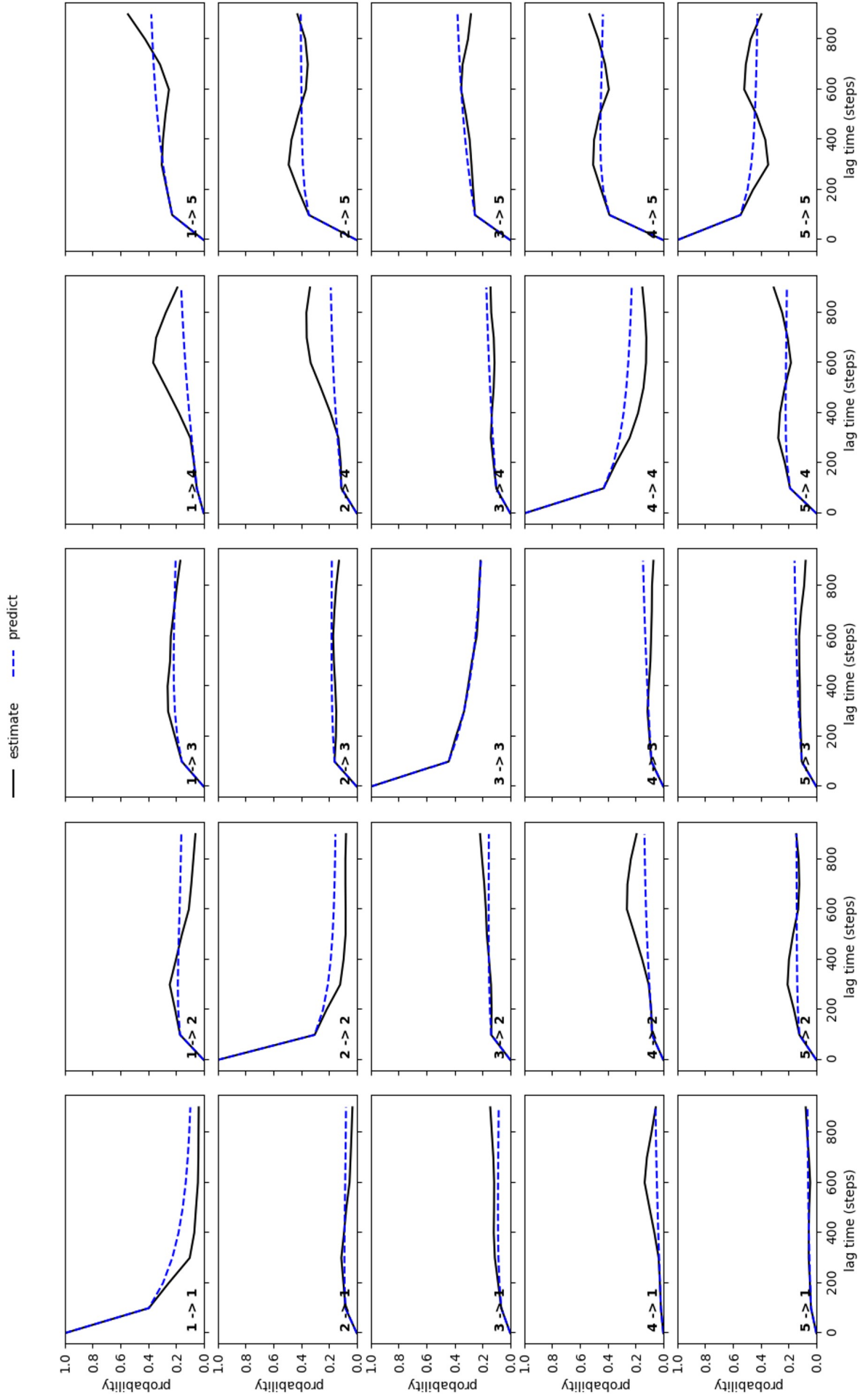


Figure S13: The CK test is carried out on the free antibody MSM model obtained from Setting-A. Deviations between the estimated and the predicted model are large in Setting-A

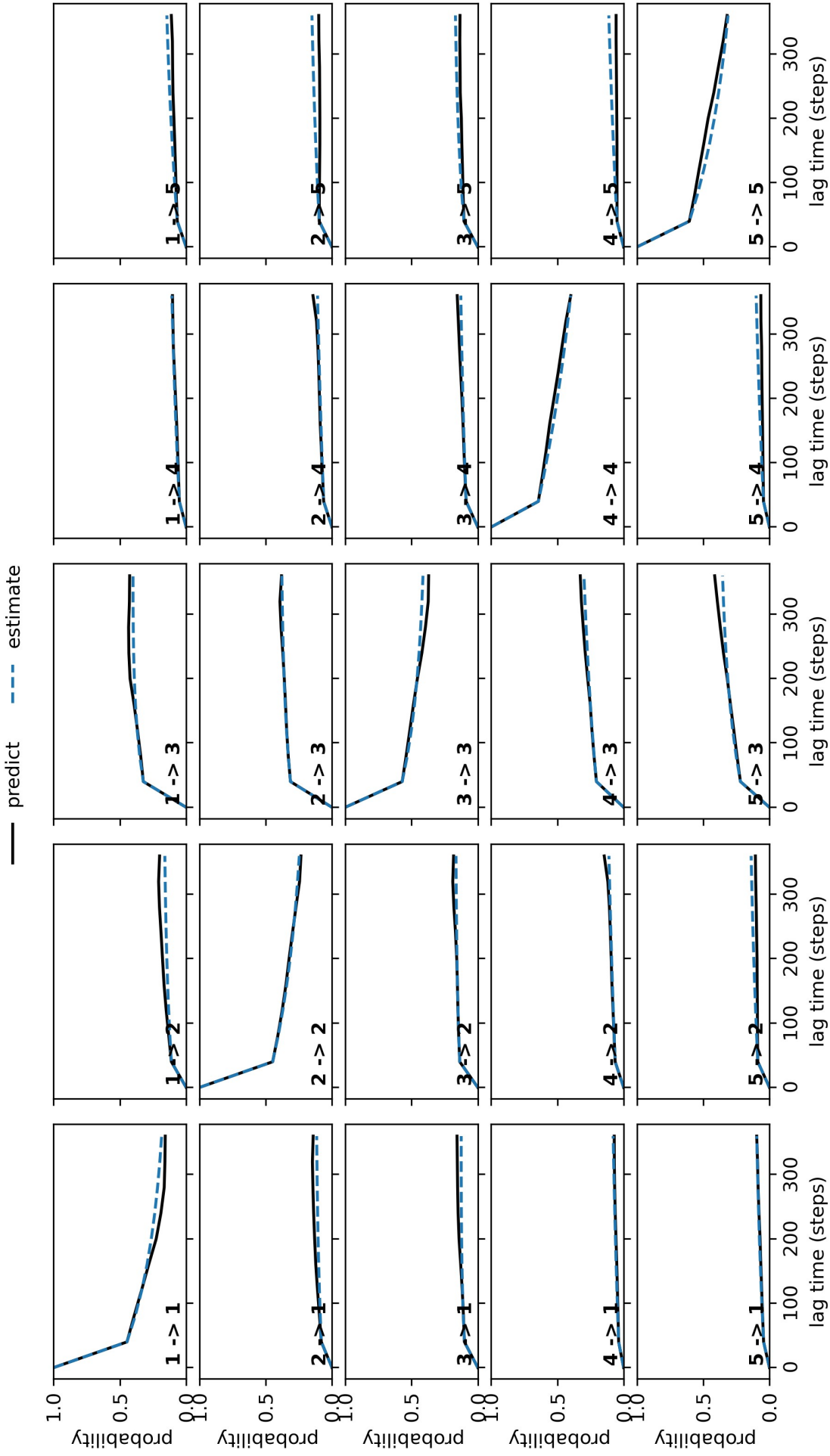


Figure S14: The CK test is carried out on the free antibody MSM model obtained from Setting-B. Deviations between the estimated and the predicted model are less than setting-A

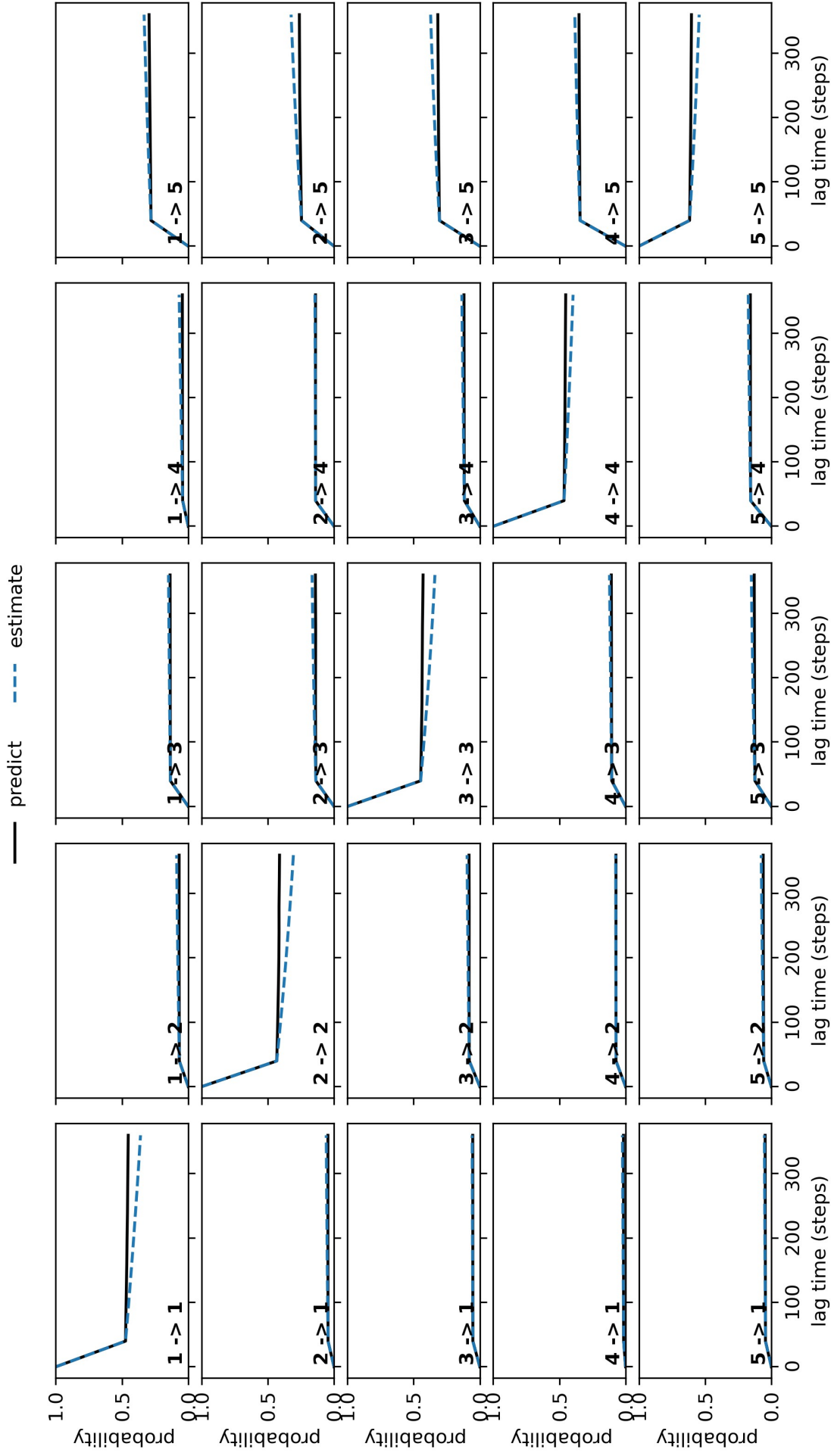


Figure S15: The CK test is carried out on the free antibody MSM model obtained from Setting-C. Deviations between the estimated and the predicted model are negligible



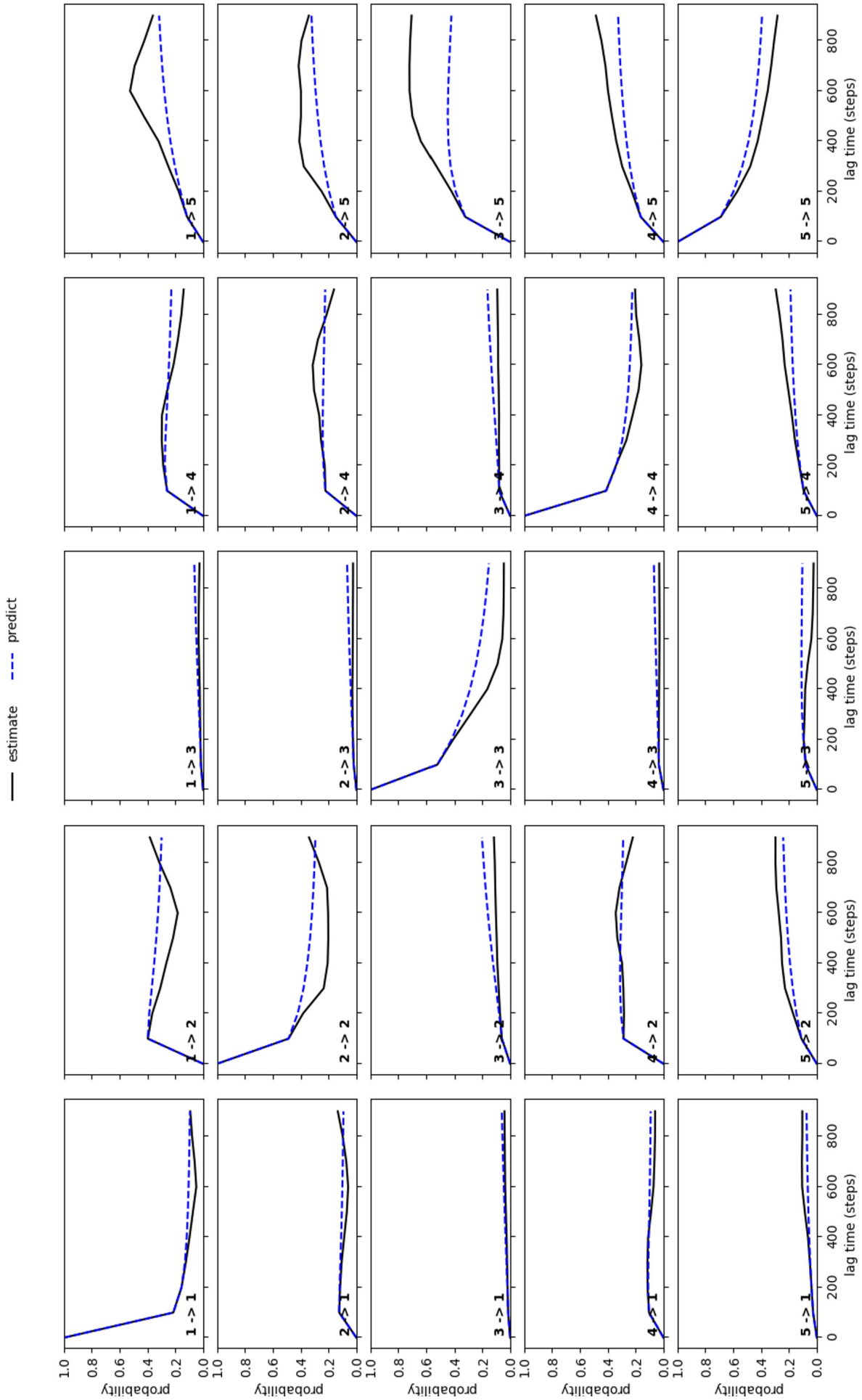


Figure S16: The CK test is carried out on the antigen-antibody complex MSM model obtained from Setting-A. Deviations between the estimated and the predicted model are large in Setting-A

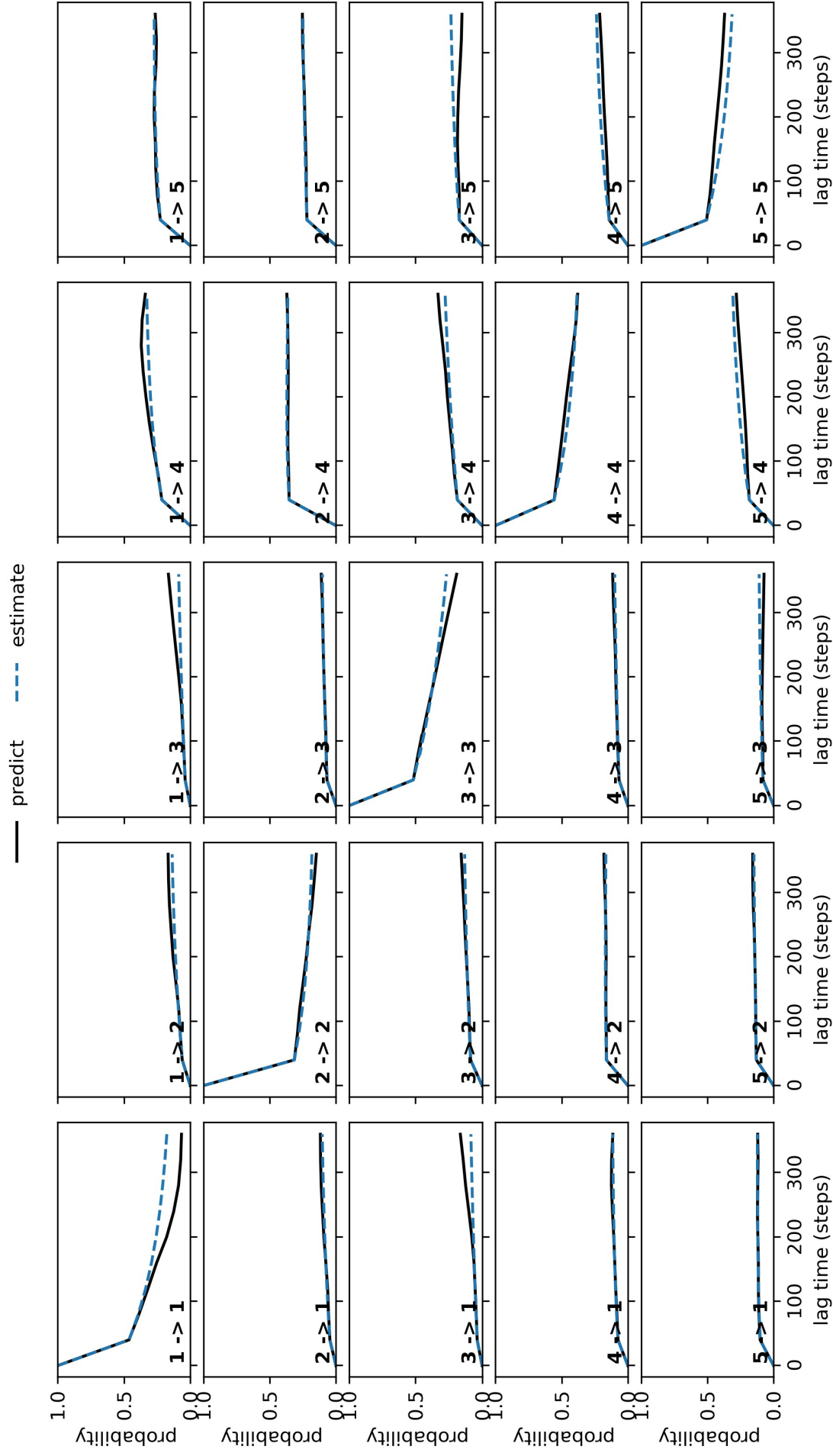


Figure S17: The CK test is carried out on the antigen-antibody complex MSM model obtained from Setting-B. Deviations between the estimated and the predicted model are less than setting-A

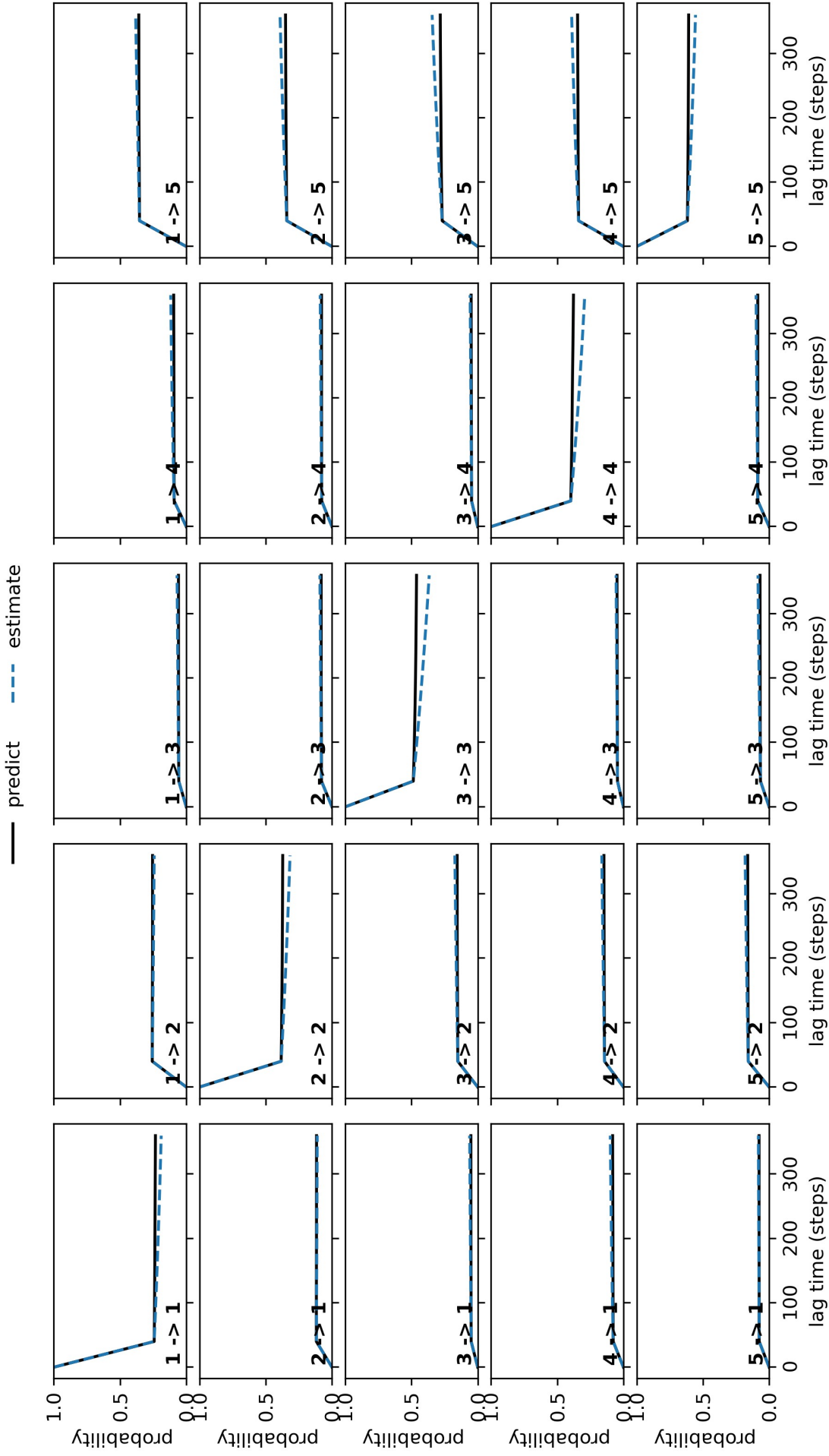


Figure S18: The CK test is carried out on the antigen-antibody complex MSM model obtained from Setting-C. Deviations between the estimated and the predicted model are negligible