

Large-scale application of free energy perturbation calculations for antibody design

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The Supplementary Information includes the following files:

- [m396+Cov2.pdb](#): Equilibrated simulation system for the complex of m396 Fab and the Sars-Cov-2 RBD
- [SingleMutation.csv](#): All computational results regarding the single mutations on m396
- [Multipoint.csv](#): All computational results for 221 multi-point mutants of m396, some of which also have experimental melting temperatures