

Supporting Information for:

Enzyme microheterogeneous hydration and stabilization in supercritical carbon dioxide

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Content: Supplemental figures S1 and S2:

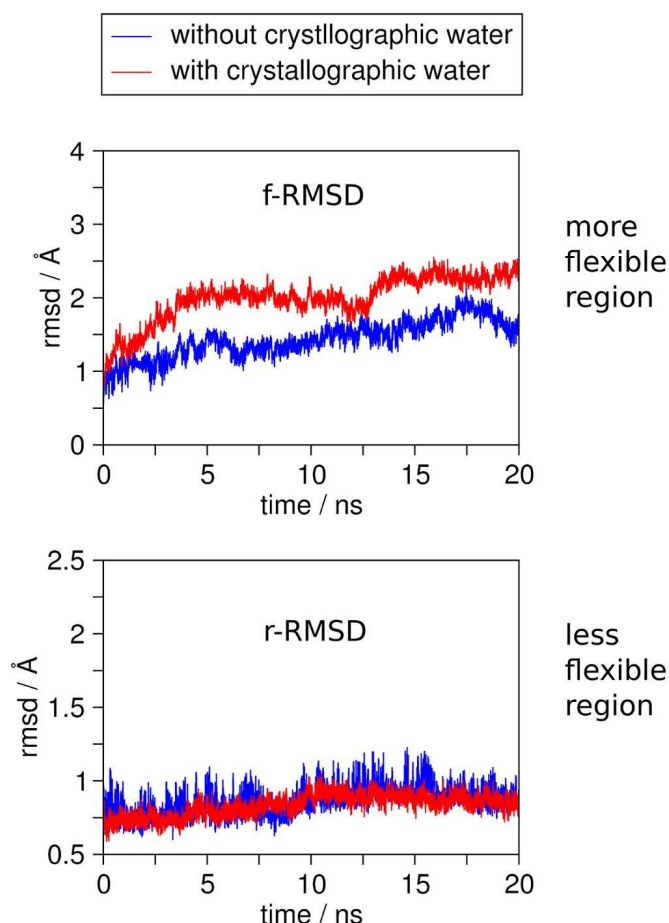


Figure S1: RMSD of CALB immersed in water at 328.15 K and 100 bar. Results are shown for r-RMSD and f-RMSD (see main text for definition) for simulations with and without the crystallographic water molecules in the initial configuration. The result shows that the deviations are modest and similar, suggesting that the high structure deviations observed in pure scCO₂ (main text, Figs. 2 and 3) do not result from removal of structural waters only.

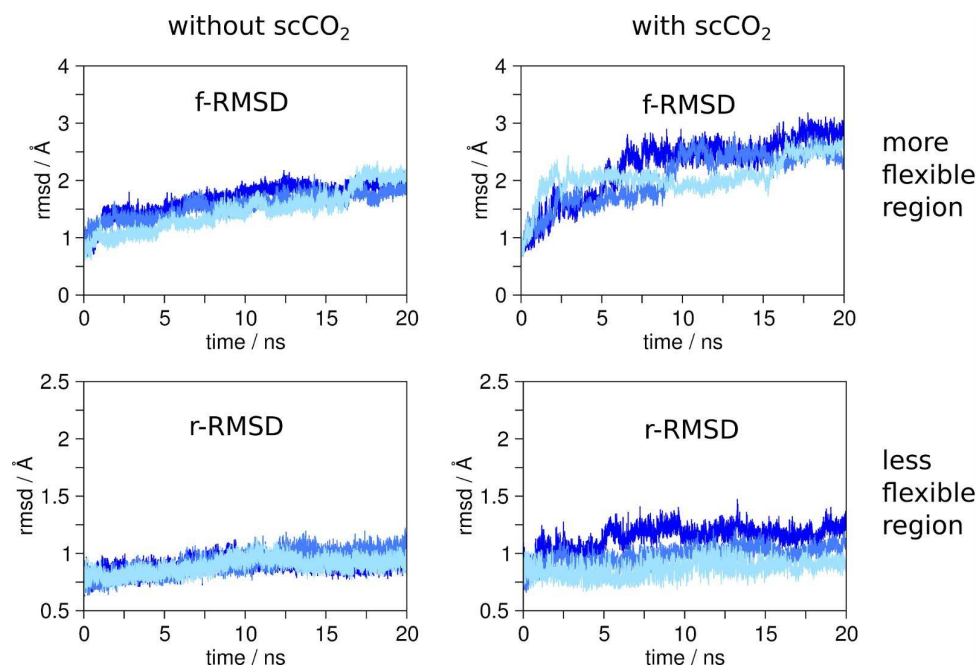


Figure S2: RMSD of CALB plus crystallographic water in vacuum and immersed in scCO₂ at 328.15 K and 100 bar. Results are shown for r-RMSD and f-RMSD (see main text for definition) for simulations with and without the crystallographic water molecules in the initial configuration. The result shows that the presence of scCO₂ enhances the flexibility of the more flexible parts of the protein, whereas no significant effect is noticed in the less flexible regions.