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**Supporting information for article:**

# Molecular-dynamics simulation methods for macromolecular crystallography

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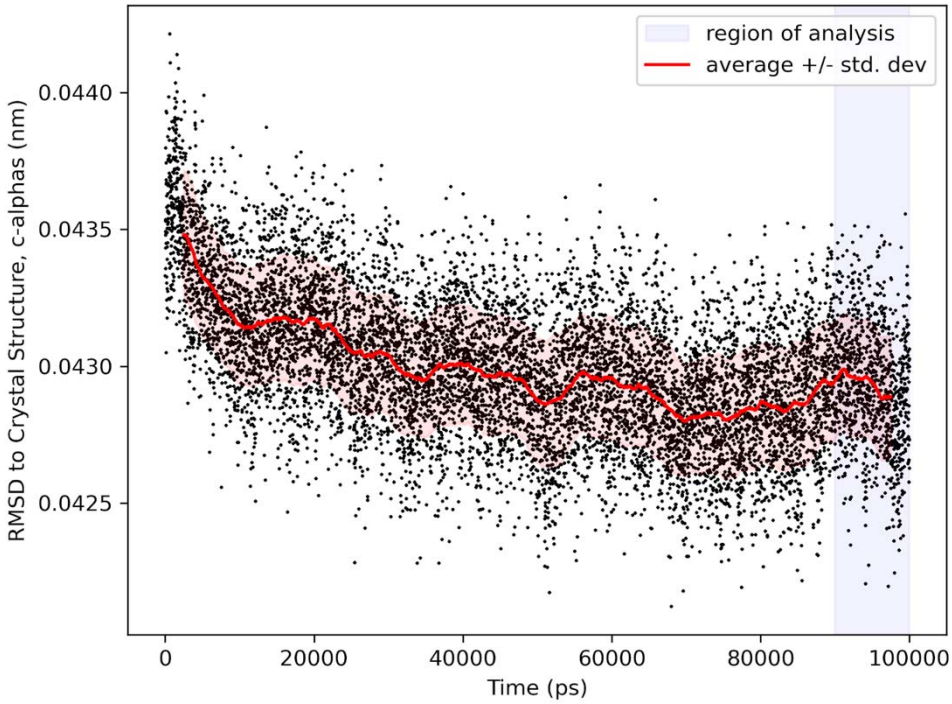


**Figure S1** The c-alpha RMSD (nm) between the coordinates from the initial MD ensemble and the coordinates from production simulation. The moving average (red line) +/- standard deviation (transparent red envelope) is plotted with a window size of 5 ns (500 frames). The portion of the trajectory in which frames were processed to calculate structure factors and densities (the "region of analysis") is marked in blue.

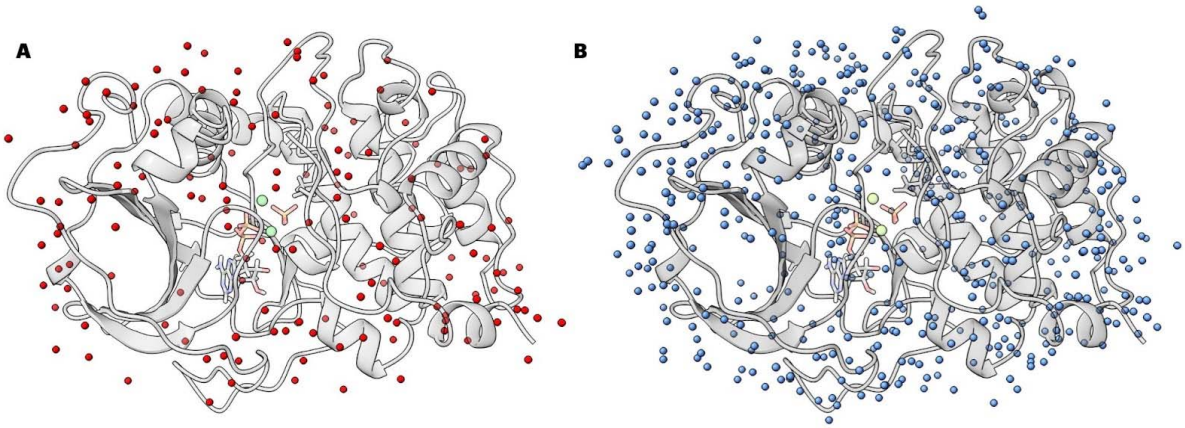


**Figure S2** A comparison of the ordered water model from (A) the initial crystal structure model, *S* with 148 waters (red spheres), and (B) the MD-revised model $R_f$ with 494 waters (blue spheres). Many of the additional waters in $R_f$ appear in the first and second hydration layers.