# Supplementary Content

## Molecular dynamics simulations give insight into D-glucose dioxidation at C2 and C3 by *Agaricus meleagris* pyranose dehydrogenase

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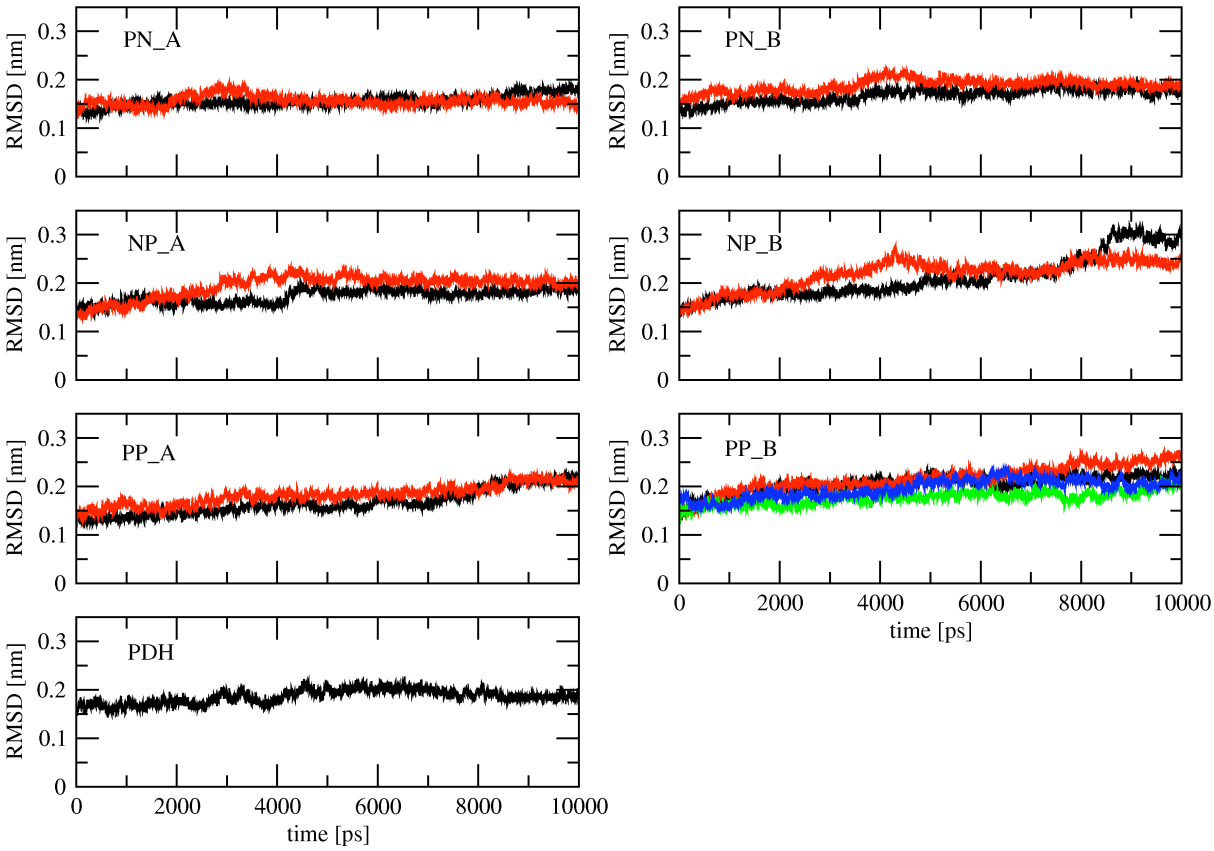
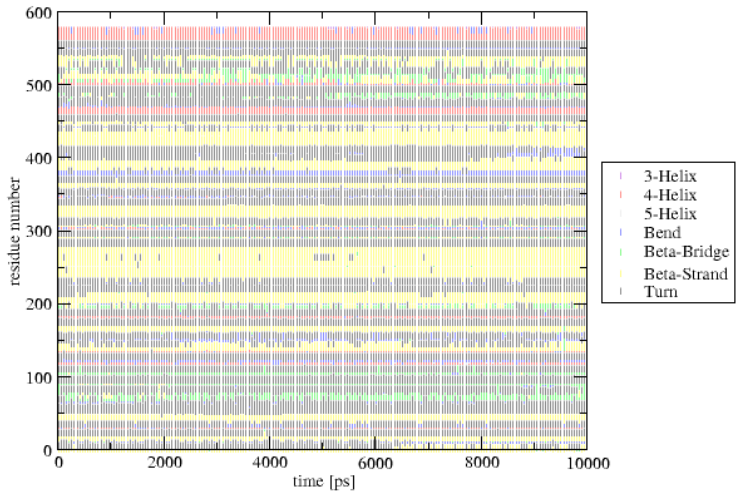
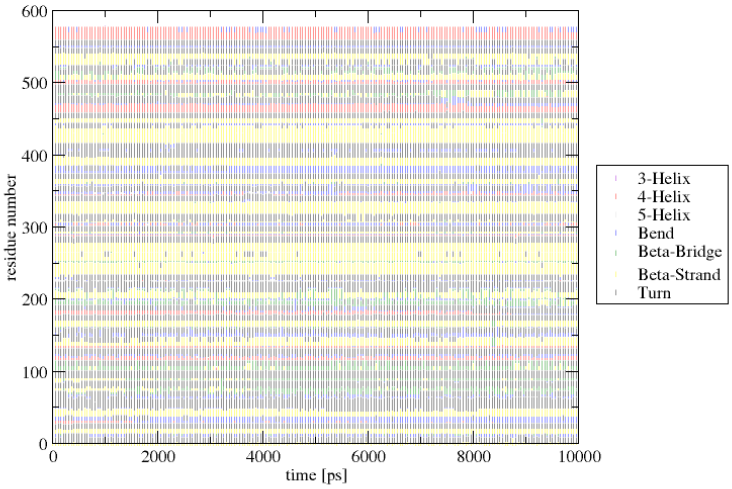
**Supplementary Fig. S1** Root-mean-square deviation (RMSD) of the backbone during the 10 ns MD simulations of systems PN_A, PN_B, NP_A, NP_B, PP_A, PP_B and PDH. Coloring scheme: run 1 (black), run 2 (red), run 3 (green), run 4 (blue).



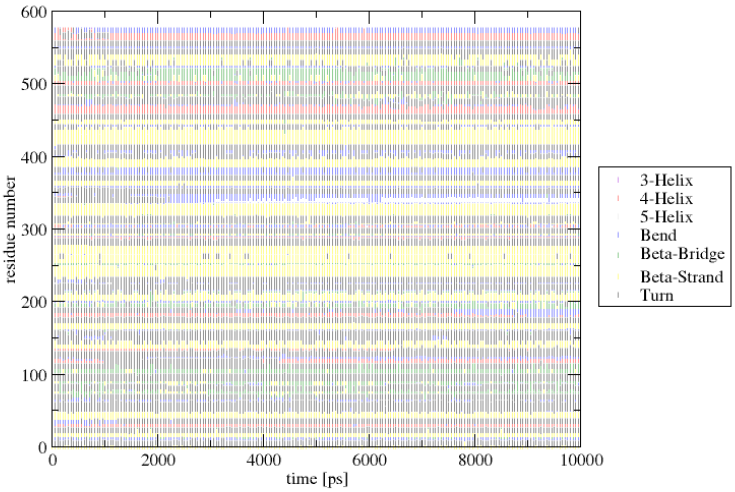
**Supplementary Fig. S2** Secondary structure elements (DSSP) classification as a function of time for selected simulations.




**PDH**

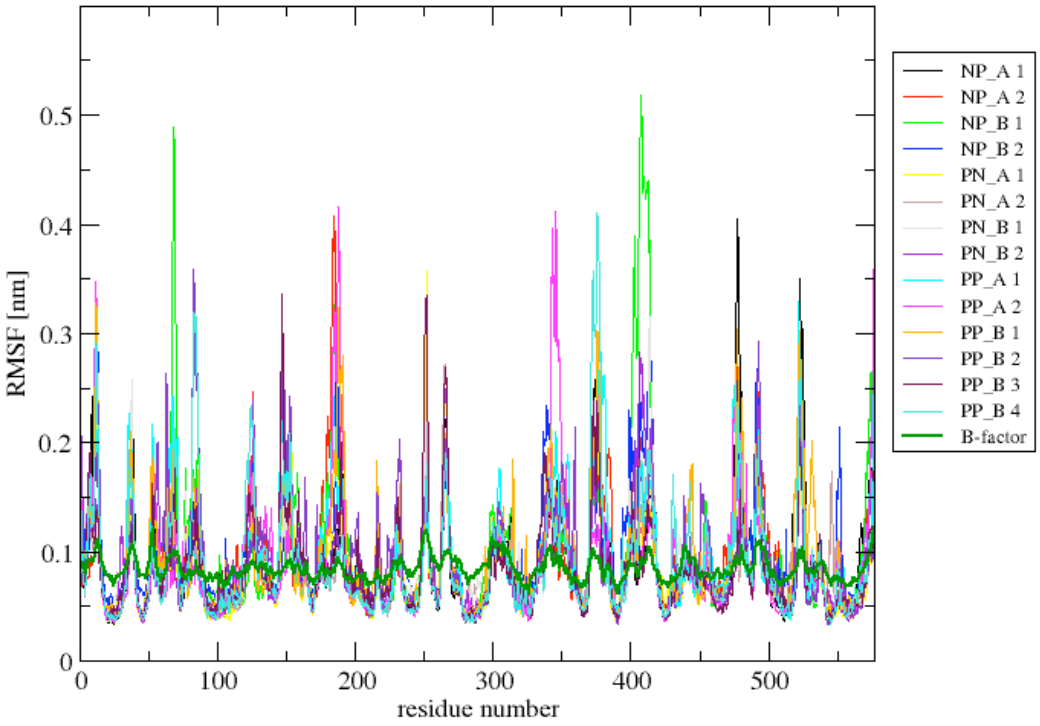



**PP_A**, run 1




**PP_A**, run 2

**Supplementary Fig. S3** Atom-positional root-mean-square fluctuations (RMSF) for the individual simulations. The average of the simulation curves yields the curve in figure 2 of the main manuscript. The RMSF values calculated from the crystal structure B-factor values are indicated with a thicker green curve.



**Supplementary Fig. S4** Normalized distributions of the atom-positional root-mean-square deviation (RMSD) of D-glucose after a roto-translational fit of the protein backbone with respect to the initial structure during the 10 ns MD simulations.