

## Supplementary Information

### Structural and dynamic insights into $Mn_4Ca$ cluster-depleted Photosystem II

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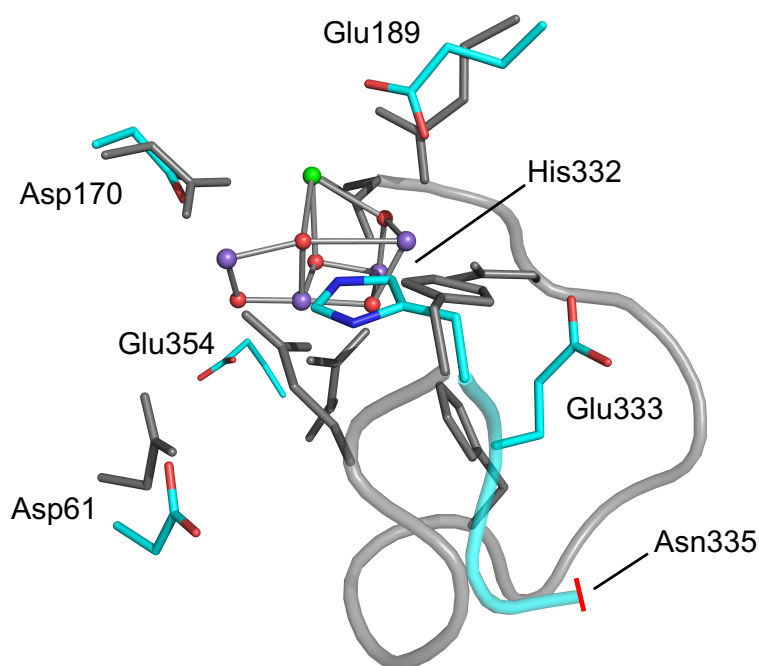


Figure 1: **Cluster cavity in the Cryo-EM structure of *apo*-PSII** Protein residues in the cluster cavity of the cryo-EM structure of *apo*-PSII (PDB ID: 6WJ6 [1]) are reported in sticks representation with carbon atoms coloured cyan. Protein residues and the manganese cluster in the cavity of the native PSII in the S1 state (PDB ID: 6W1O8 [2]) are also reported (with protein residues coloured gray). The C-terminal part of the D1 domain (from His332 to Ala344 in the native PSII and from His332 to Asn335 in the cryo-EM structure, coloured gray and cyan respectively) is shown in cartoon representation.

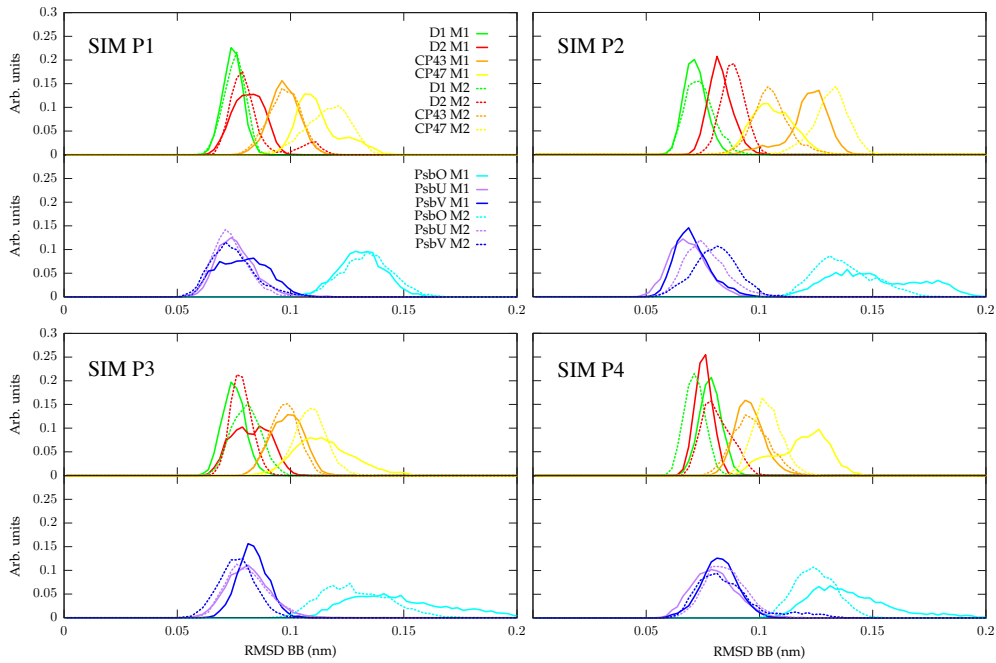


Figure 2: **RMSD of selected chains** Distribution along the four simulated trajectories of the RMSD values calculated on the protein backbone of D1, D2, CP43, and CP47 domains with respect to the starting structure in both monomers.

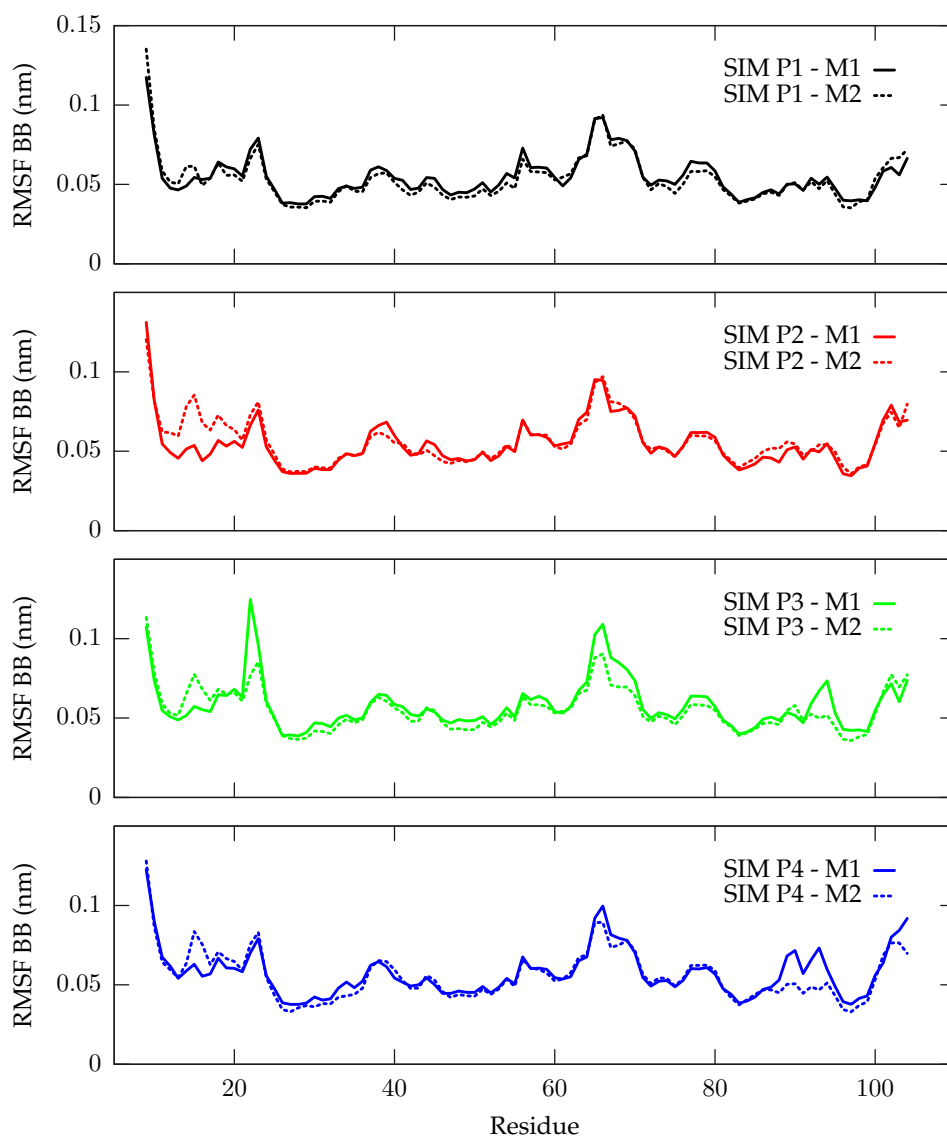


Figure 3: **RMSF of PsbU domain** Root-mean-square fluctuations of the PsbU domain calculated on the protein backbone of both monomers in the four simulated systems. The the first 50 ns of simulation have been neglected in the RMSF calculation.

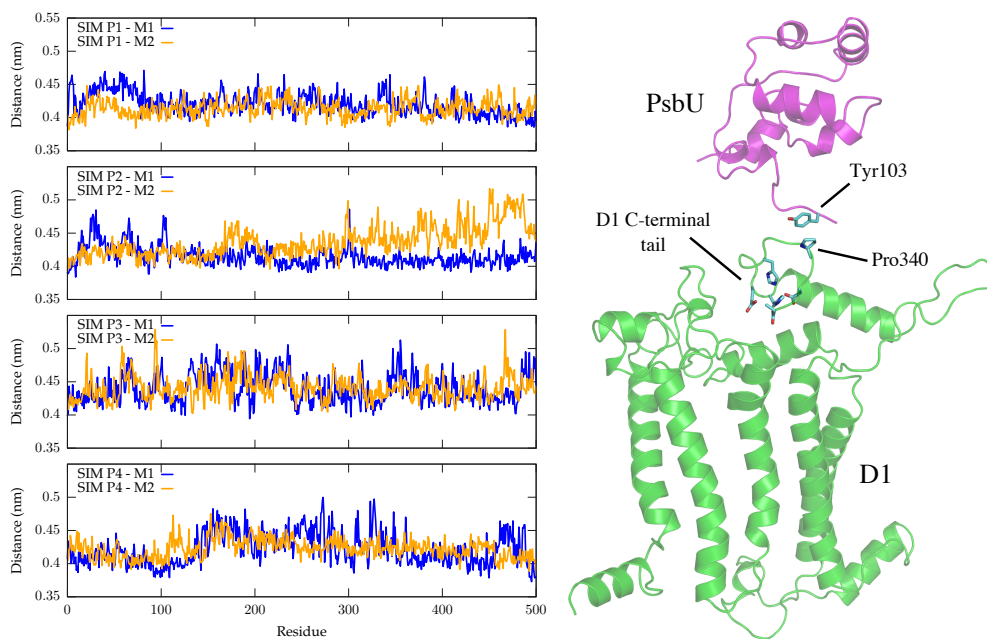


Figure 4: **Tyr103-Pro340 distance** The distance between the center of mass of the PbsU-Tyr103 side chain and the center of mass of the D1-Pro340 side chain is reported as function of time for both monomers in the four simulated systems. On the right, the domains D1 (green) and PbsU (magenta) are shown in cartoon representation. PbsU-Tyr103 and D1-Pro340 are explicitly shown in sticks representation.

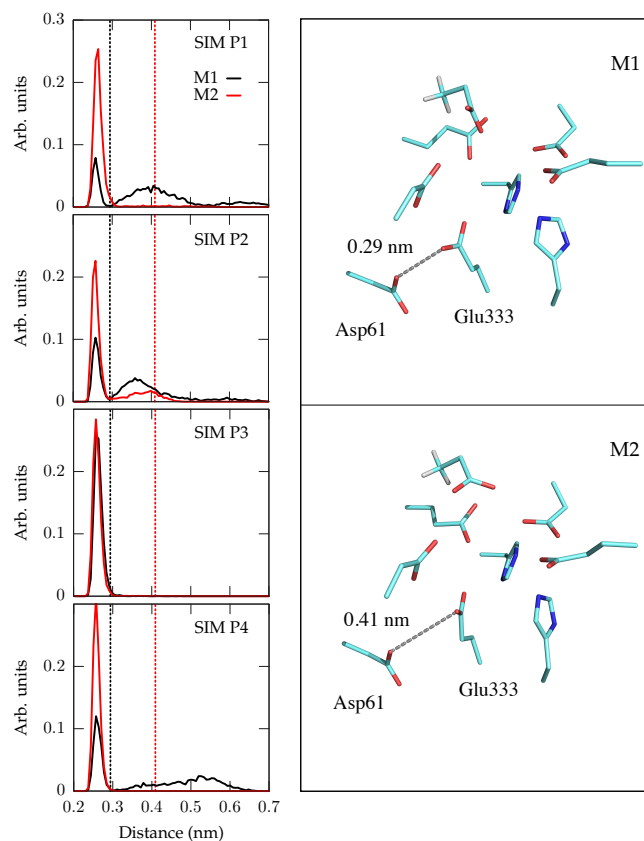


Figure 5: **Asp61-Glu333 distance** On the left, the distribution of the minimum distance between the carboxyl groups of Asp61 and Glu333 sampled along the four simulations is shown for both monomers. Dashed lines indicate the respective x-ray values. On the right, key-residues around the cluster cavity in the positions reported in the x-ray structure (PDB ID: 5MX2) are shown in sticks representation for both monomers. The minimum distance between the carboxyl groups of Asp61 and Glu333 determined in the x-ray structure is also reported.

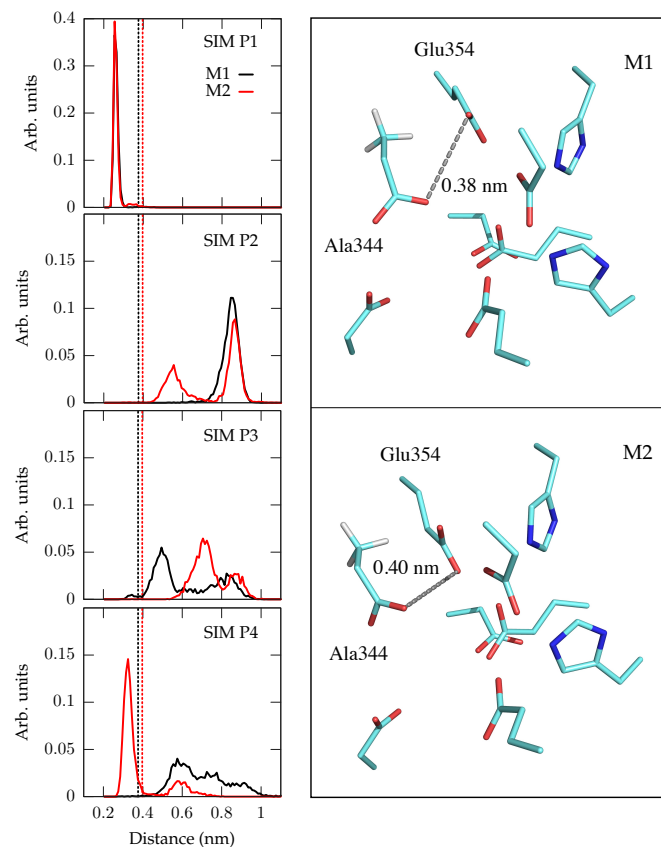


Figure 6: **Ala344-Glu354 distance** On the left, the distribution of the minimum distance between the carboxyl groups of D1-Ala344 and CP43-Glu354 sampled along the four simulations is shown for both monomers. Dashed lines indicate the respective x-ray values. On the right, key-residues around the cluster cavity in the positions reported in the x-ray structure (PDB ID: 5MX2) are shown in sticks representation for both monomers. The minimum distance between the carboxyl groups of D1-Ala344 and CP43-Glu354 determined in the x-ray structure is also reported.

## References

- [1] C. J. Gisriel, K. Zhou, H.-L. Huang, R. J. Debus, Y. Xiong, and G. W. Brudvig. Cryo-EM Structure of Monomeric Photosystem II from *Synechocystis* sp. PCC 6803 Lacking the Water-Oxidation Complex. *Joule*, 4:2131–2148, 2020.
- [2] M. Ibrahim, T. Fransson, R. Chatterjee, M. H. Cheah, R. Hussein, L. Lassalle, K. D. Sutherlin, I. D. Young, F. D. Fuller, S. Gul, I.-S. Kim, P. S. Simon, C. de Lichtenberg, P. Chernev, I. Bogacz, C. C. Pham, A. M. Orville, N. Saichek, T. Northen,

A. Batyuk, S. Carbajo, R. Alonso-Mori, K. Tono, S. Owada, A. Bhowmick, R. Bolo-tovsky, D. Mendez, N. W. Moriarty, J. M. Holton, H. Dobbek, A. S. Brewster, P. D. Adams, N. K. Sauter, U. Bergmann, A. Zouni, J. Messinger, J. Kern, V. K. Yachan-dra, and J. Yano. Untangling the sequence of events during the S2  $\rightarrow$  S3 transition in photosystem II and implications for the water oxidation mechanism. *Proc. Natl. Acad. Sci. USA*, 117(23):12624–12635, 2020.