crystals

Supplementary File

Crystal Packing of Protomers Provides a Valuable Structural Insight into Protein Structure

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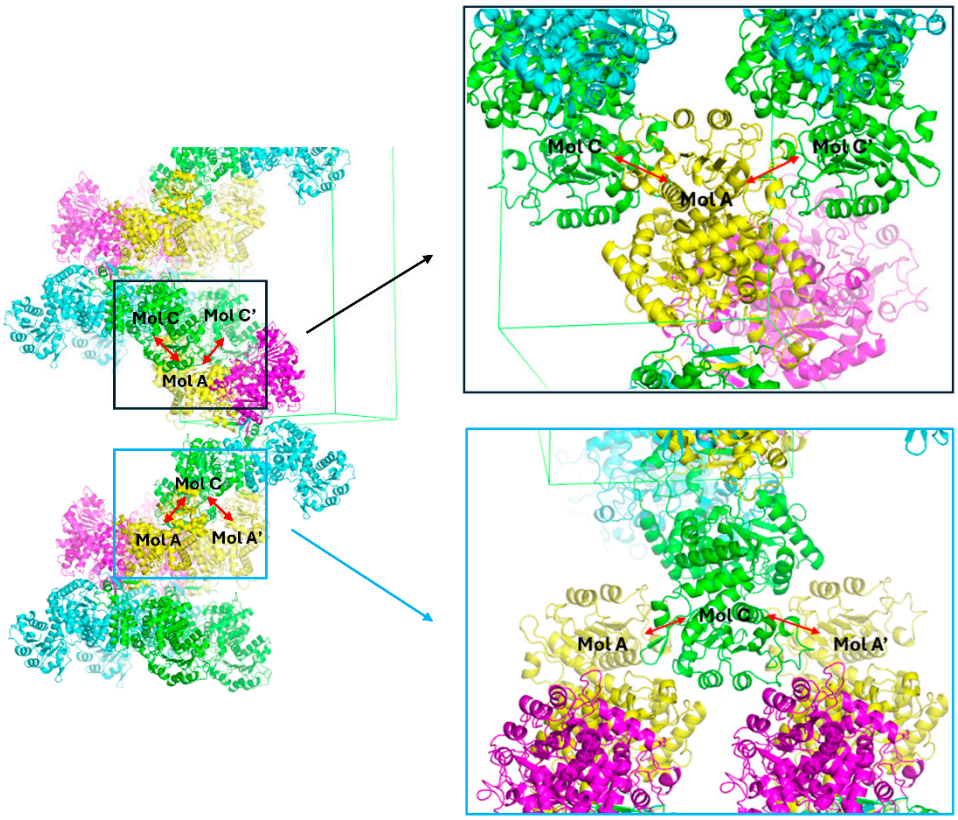


Figure S1. Vertical interactions between protomers along the P2$_1$ screw axis. The vertical interactions between protomer Mol A and Mol C along the P2$_1$ axis are represented. Each protomer of Mol A is bound by two protomers of Mol C, and each protomer of Mol C by two protomers of Mol A.

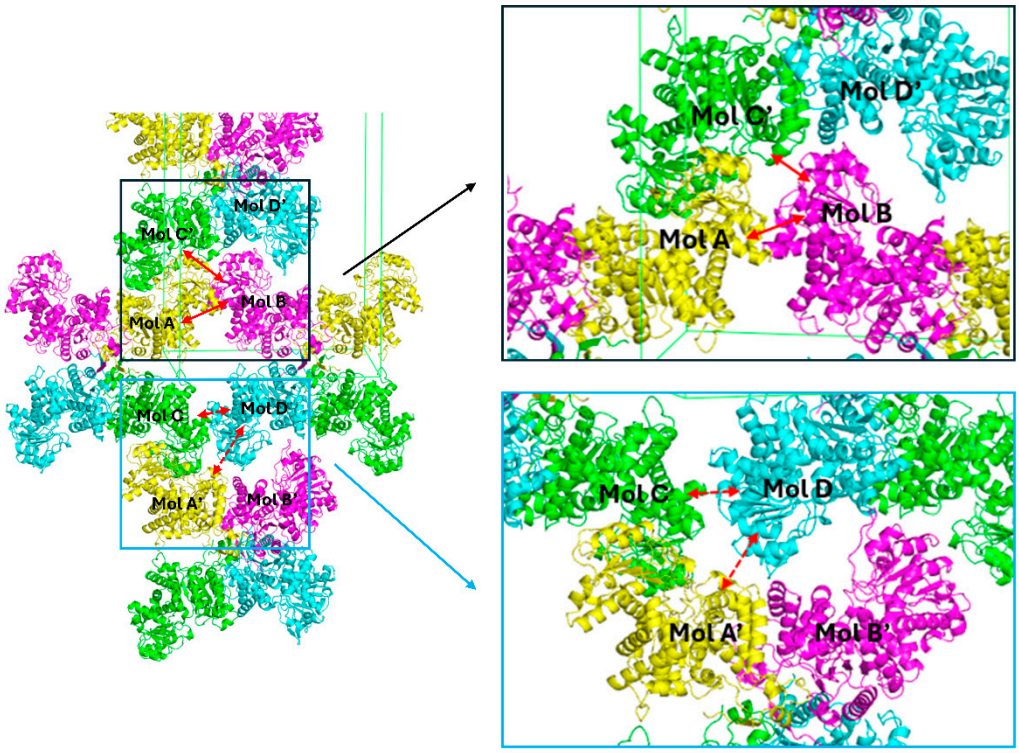


Figure S2. Horizontal interactions between protomers perpendicular to the $P2_1$ screw axis. The horizontal interactions between protomer Mol A and Mol B are represented. A protomer of Mol B is bound by two protomers of Mol A and C, and a protomer of Mol D is bound by two protomers of Mol A and C. The interactions of Mol B are stronger than those of Mol D.

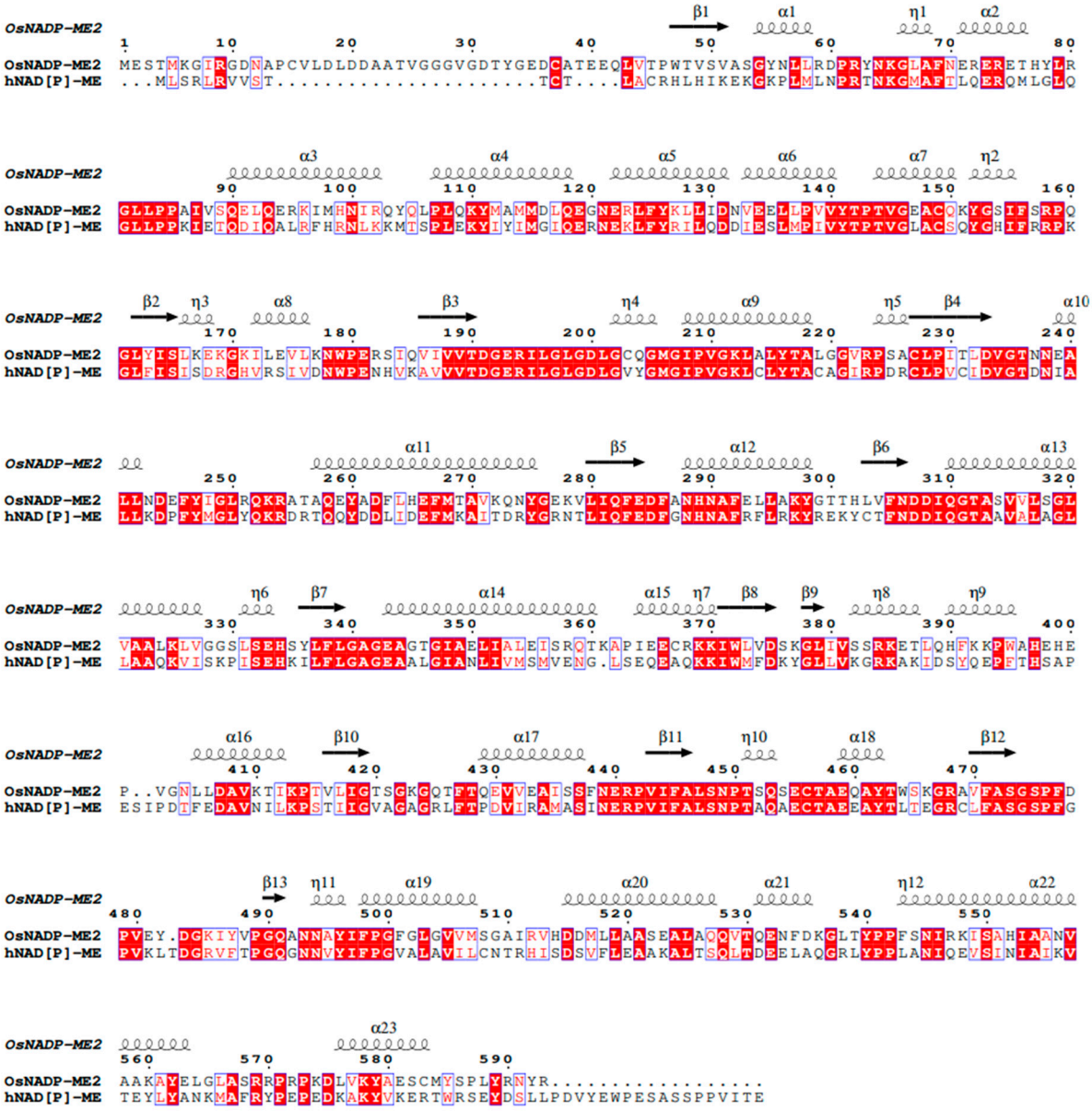


Figure S3. Sequence alignment of OsNADP-ME2 and human NAD(P)-ME. The amino acid sequences of OsNADP-ME2 (gene ID: LOC_Os01g52500.3) and human NAD(P)-ME (gene ID: NP_002387.1) are aligned with the secondary structures of OsNADP-ME2.

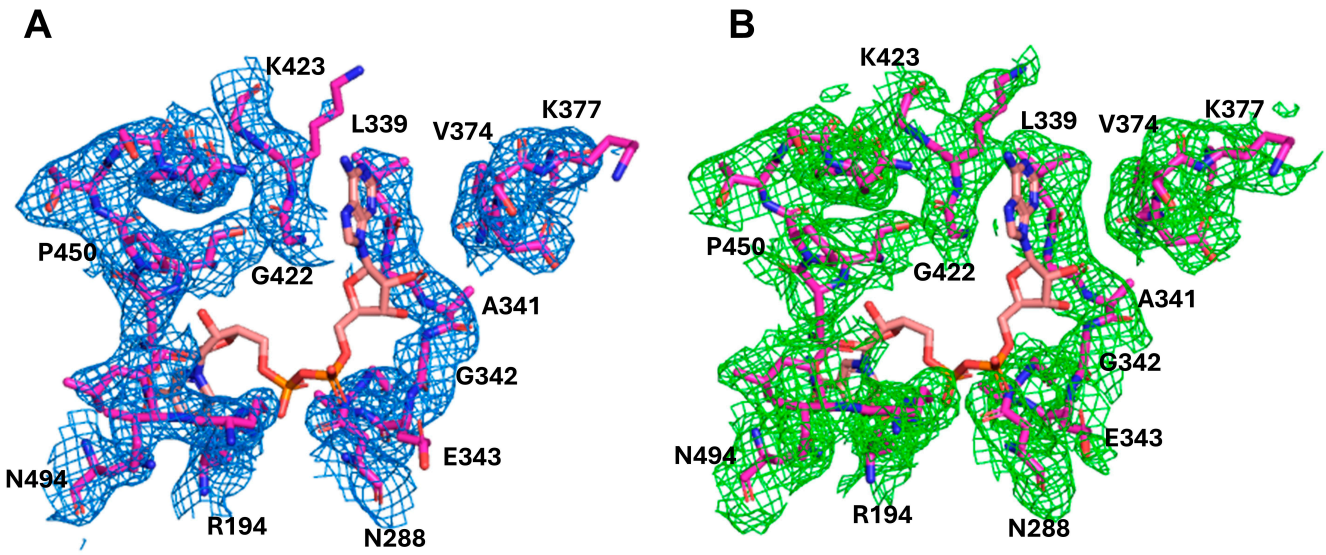


Figure S4. The electron density map of the NADP-binding site of OsNADP-ME2. (A) The refined electron density map of the NADP-binding site of the OsNADP-ME2 structure (purple color). The 2Fo-Fc electron density map (contoured at 1.0 σ, blue mesh) is shown with the NAD ligand (orange color) superimposed from the human NAD(P)-ME structure (PDB ID: 1PJ2). (B) The unbiased Fo-Fc map of the same residues in the NADP-binding site of the OsNADP-ME2 structure is shown as a green mesh.

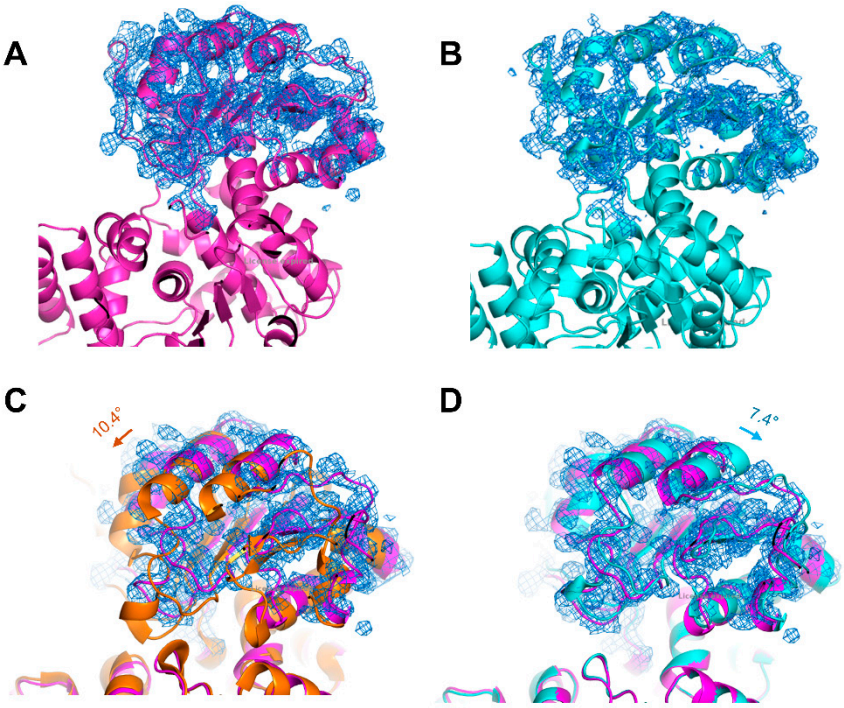


Figure S5. The electron density map of the mobile NADP-binding domain of OsNADP-ME2. (A) The structure of OsNADP-ME2 Mol B with the 2Fo-Fc electron density map of the mobile NADP-binding domain. (B) The structure of OsNADP-ME2 Mol D with the 2Fo-Fc electron density map of the mobile NADP-binding domain. (C) The superimposed structures of OsNADP-ME2 (Mol B, purple) and NAD-bound human NAD(P)-ME (shown in orange) with the electron density map of OsNADP-ME2 Mol B. (D) The superimposed structures of OsNADP-ME2 Mol B (shown in purple) and Mol D (cyan) with the electron density map of OsNADP-ME2 Mol B.

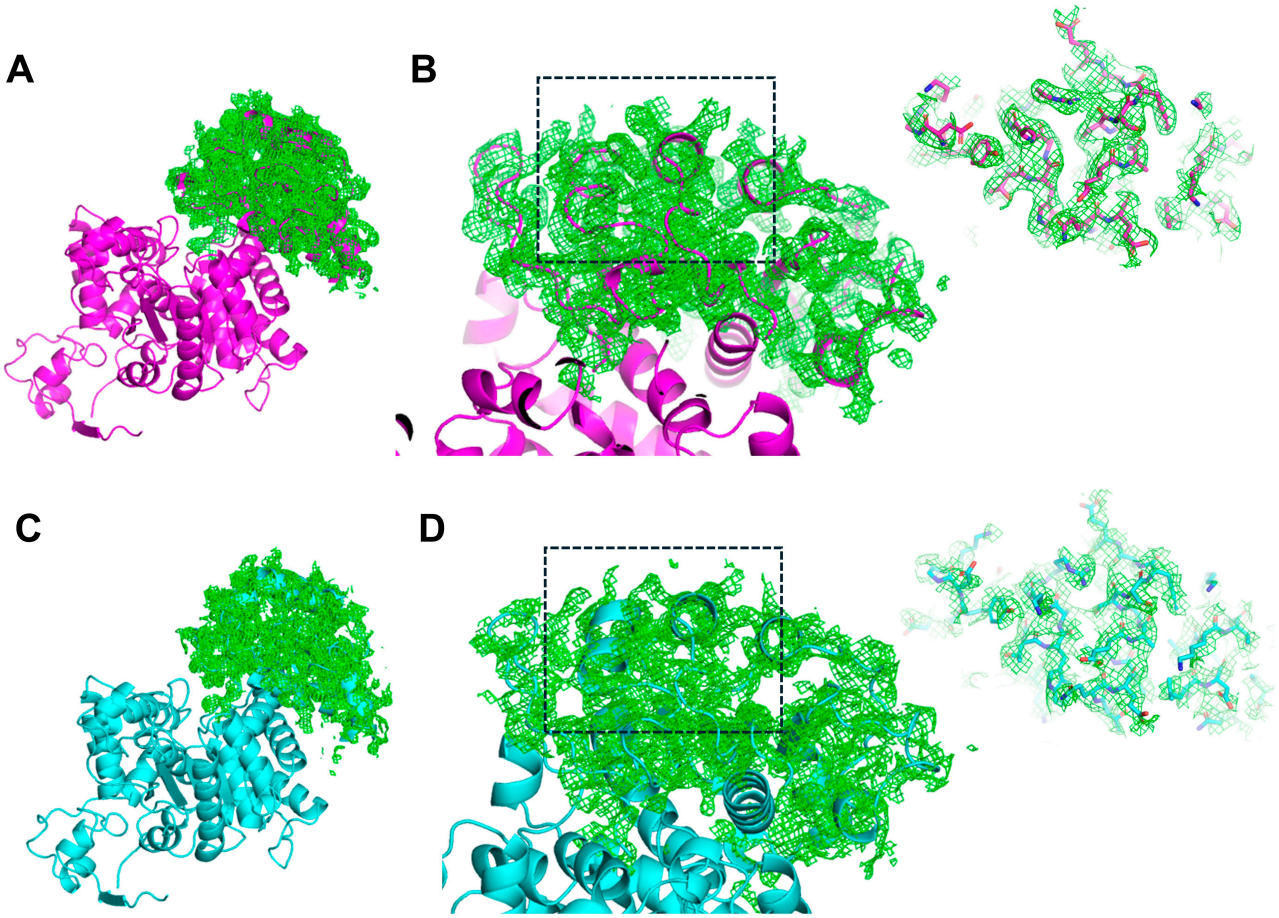


Figure S6. The unbiased Fo-Fc map of the mobile NADP-binding domain of OsNADP-ME2. (A) The structure of OsNADP-ME2 Mol B with the unbiased Fo-Fc electron density map of the mobile NADP-binding domain. (B) The enlarged structure of the mobile NADP-binding domain in Mol B with the same unbiased Fo-Fc electron density map. The residues in the black dashed square are additionally shown in the upright position. (C) The structure of OsNADP-ME2 Mol D with the unbiased Fo-Fc electron density map of the mobile NADP-binding domain. (D) The enlarged structure of the mobile NADP-binding domain in Mol D with the same unbiased Fo-Fc electron density map. The residues in the black dashed square are additionally shown in the upright position.