Supplementary material

Is It Reliable to Take the Molecular Docking Top Scoring Position as the Best Solution without Considering Available Structural Data?

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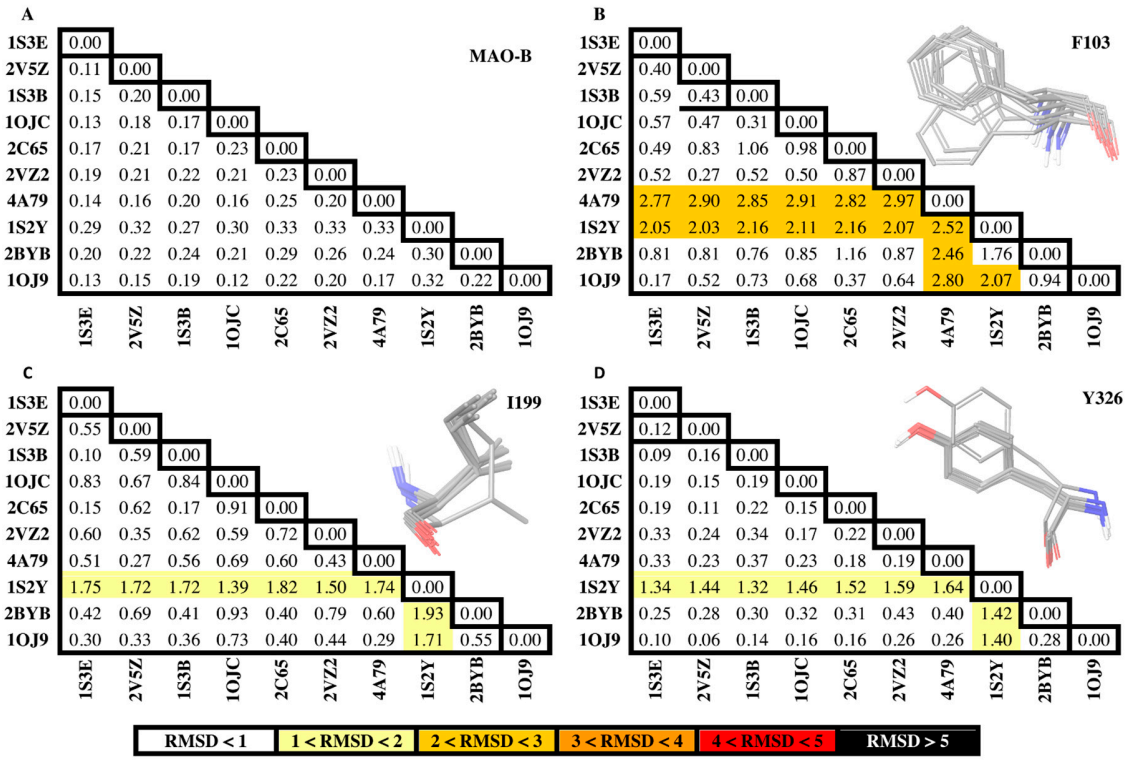

Figure S1. RMSD values (in Å) of different MAO-B crystallographic structures (A), and of their residues F103 (B), I199 (C) and Y326 (D). Conformations of residues are represented to the right.

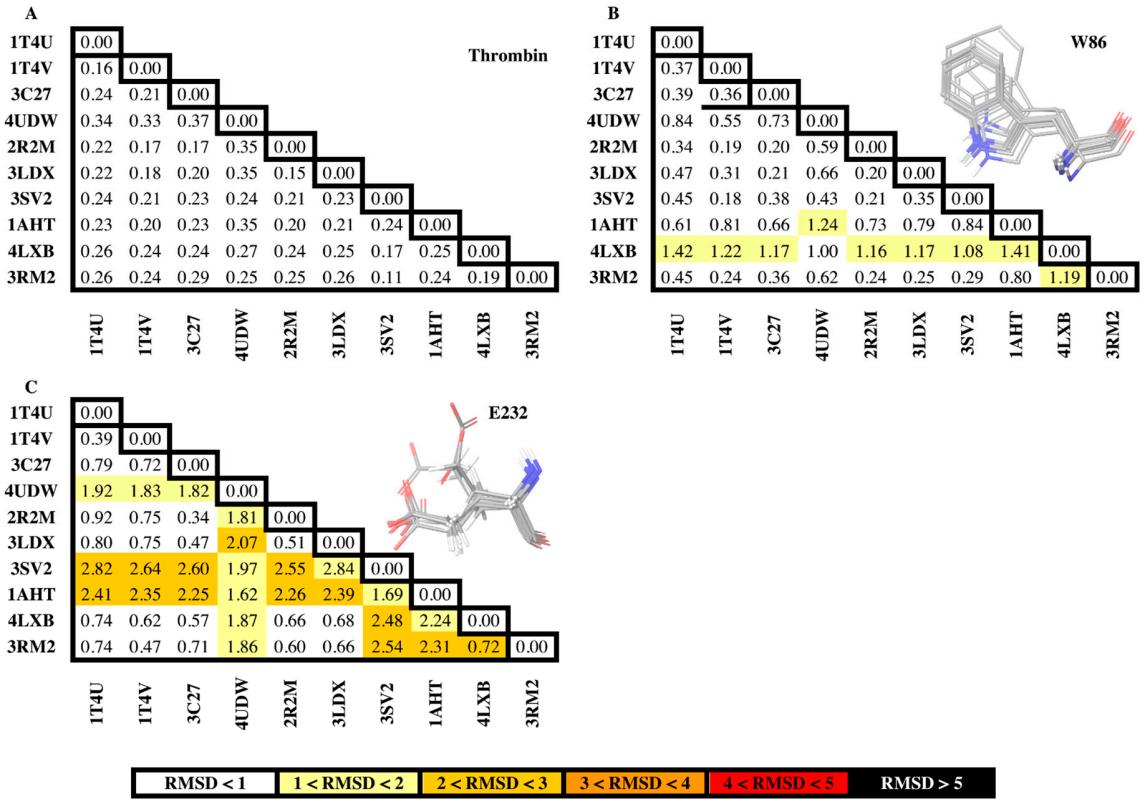

Figure S2. RMSD values (in Å) of different thrombin crystallographic structures (A), and of their residues W86 (B) and E232 (D). Conformations of residues are represented to the right.

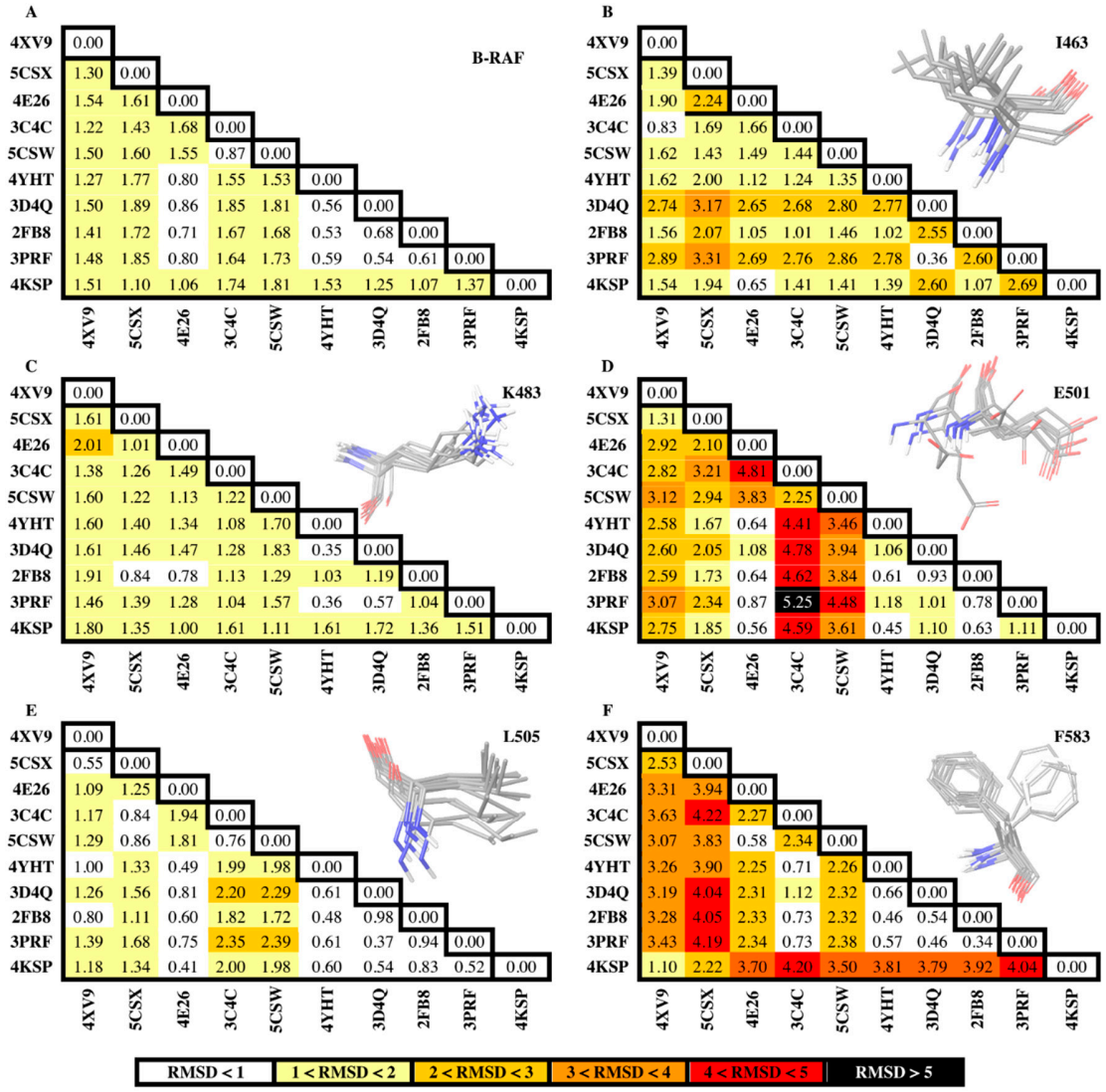

Figure S3. RMSD values (in Å) of different B-RAF crystallographic structures (A), and of their residues I463 (B), K483 (C), E501 (D), L505 (E) and F583 (F). Conformations of residues are represented to the right.