Electronic Supplementary Material for PCCP

Supplementary Information

Figure S1. The ZDOCK/RDOCK predicted ALP-eglin C complex is superimposed with the crystal structure of ALP in complex with peptide boronic acid inhibitor (PDB 1gbk). Atoms of enzymes are used for superimposition. Backbone atoms of eglin C and peptide boronic acid (green) are shown, while atoms of ALP are omitted. The location of the binding interface is indicated.

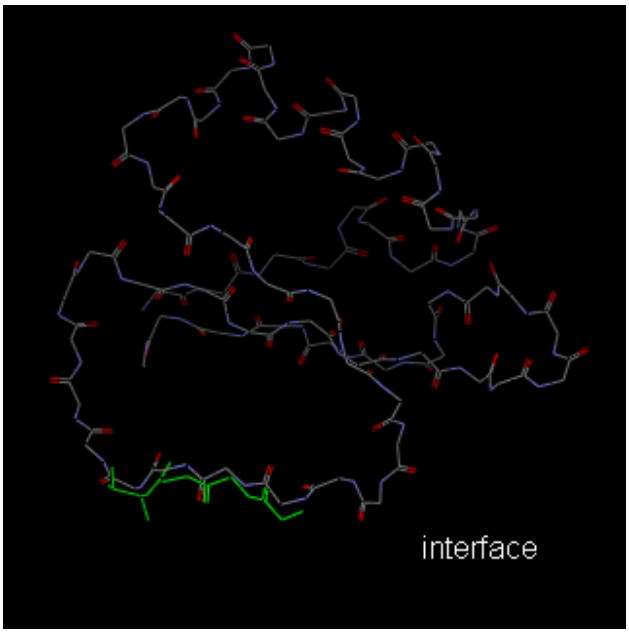
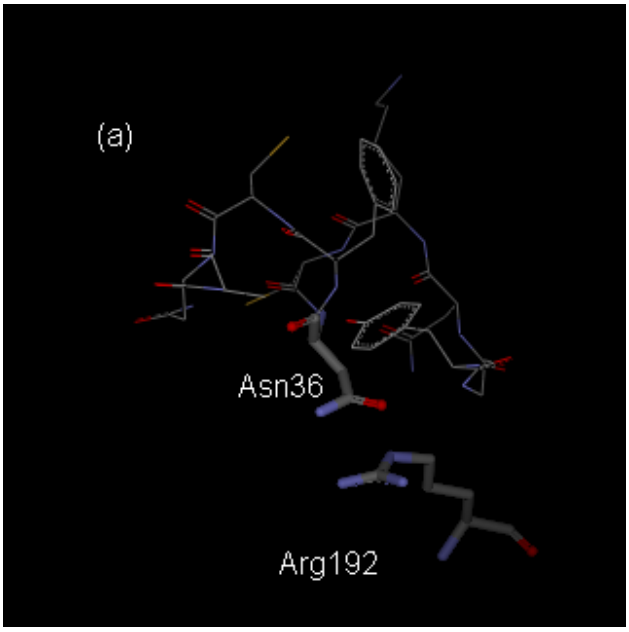


Figure S2. Interaction between Asn36 of wild type OMTKY3 and Arg192 of ALP (shown in (a)) is compared with that between Asp36 of mutant OMTKY3M with Arg192 of ALP (shown in (b)). Both structures are the snapshots at the end of 10 ns MD trajectory of the corresponding complexes.

(a)



(b)

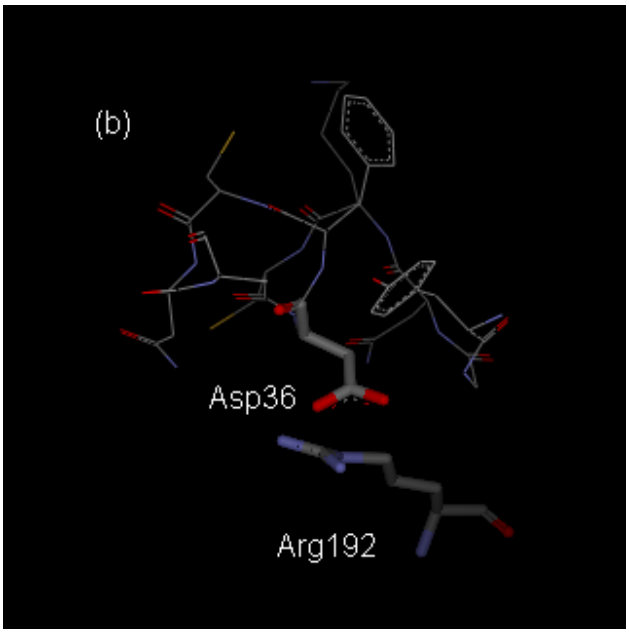
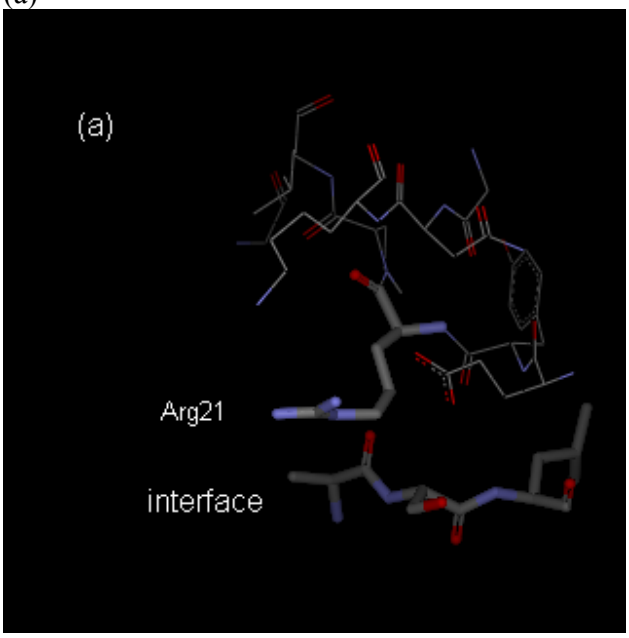


Figure S3. Structural basis for the reduced electrostatic free energy of desolvation associated with Arg21→Thr mutation: Arg21 of wild type OMTKY3 and Thr21 of mutant OMTKY3M in complex with ALP are shown in (a) and (b), respectively. Their nearest neighbors within 4 Å are also shown. Arg21, Thr21 and residues of ALP are represented as stick, while other residues as lines. Structures are the snapshots taken at the end of 10 ns MD trajectory of the corresponding complexes.

(a)



(b)

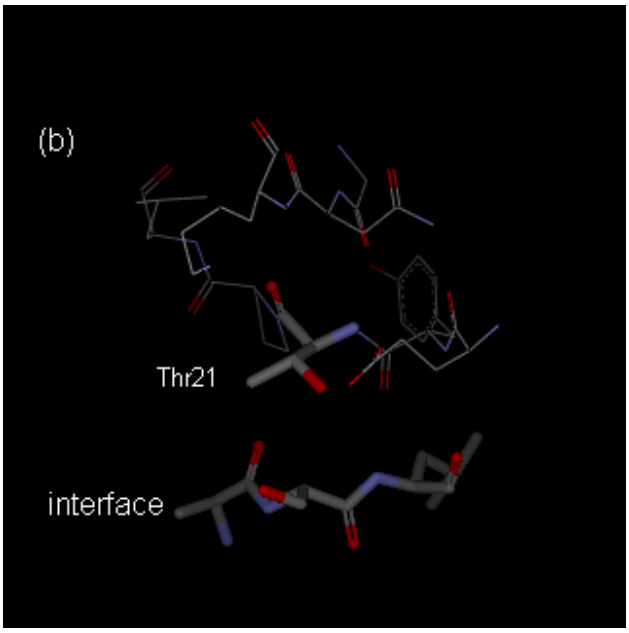
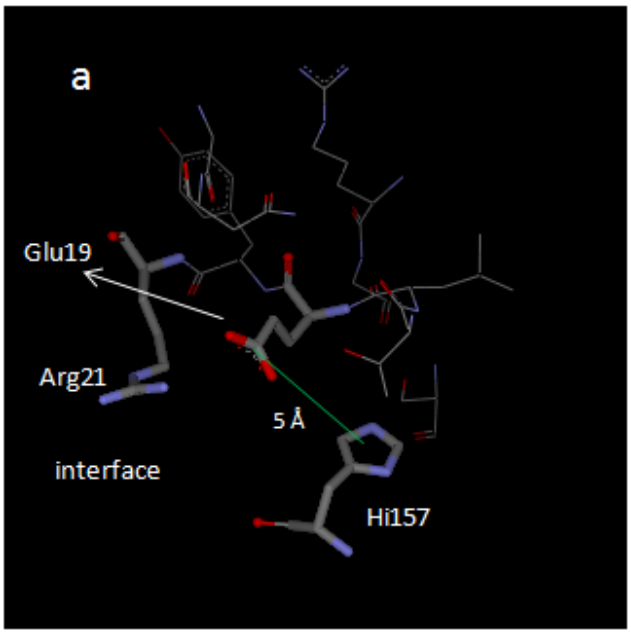


Figure S4. Interaction of Glu19 with its nearest neighbors in (a) ALP-OMTKY3 and (b) ALP-OMTKY3M.

(a)



(b)

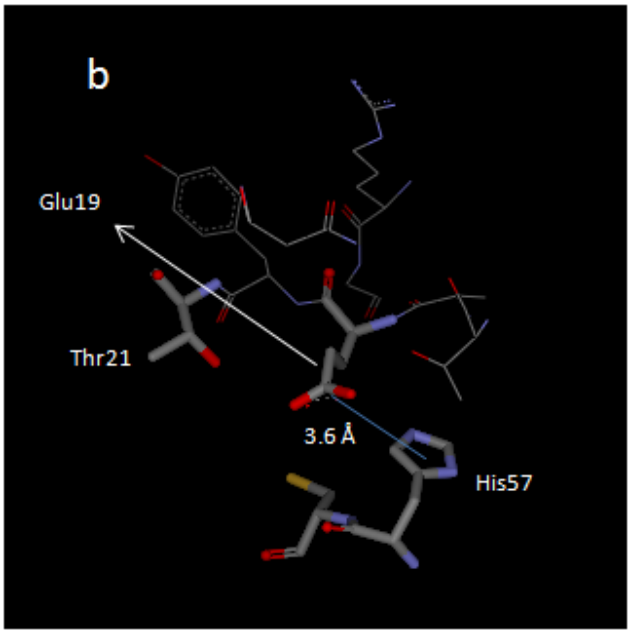


Figure S5. Conformation change in ALP-OMTKY3M (yellow) relative to ALP-OMTKY3 (blue). Leu18 and Ala18 are displayed as ball and stick. Arrow indicates change in the binding loop near the Leu18 mutation site. The structures of ALP-OMTKY3 and ALP-OMTKY3M are superimposed using ALP atoms as references. Both structures are the snapshots taken at the end of 10 ns MD trajectory of the corresponding complexes.

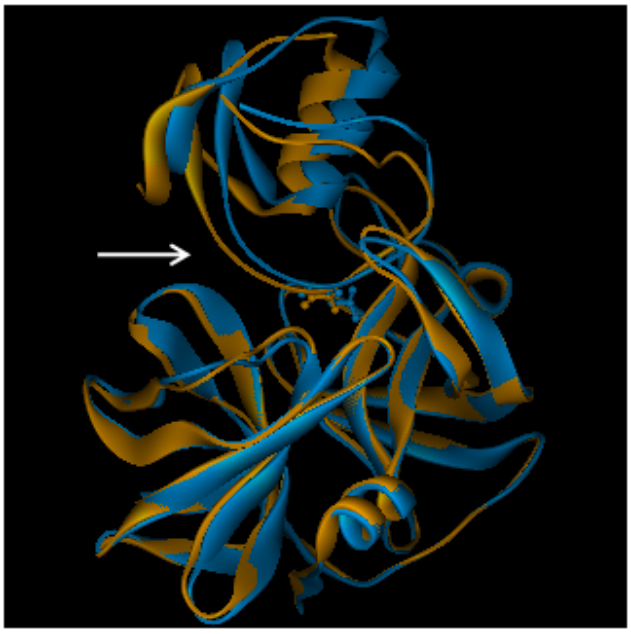
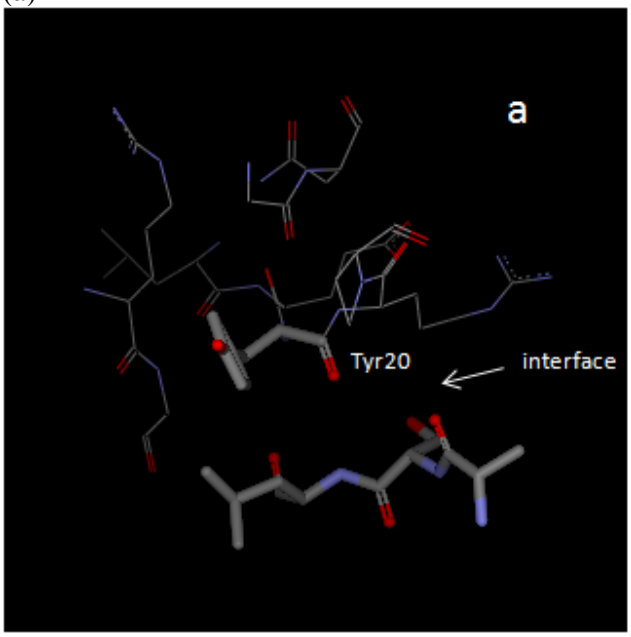


Figure S6 Interaction of Tyr20 with its nearest neighbors in (a) ALP-OMTKY3 and (b) ALP-OMTKY3M. Presence of intermolecular hydrogen bond is indicated by green dotted line.

(a)



(b)

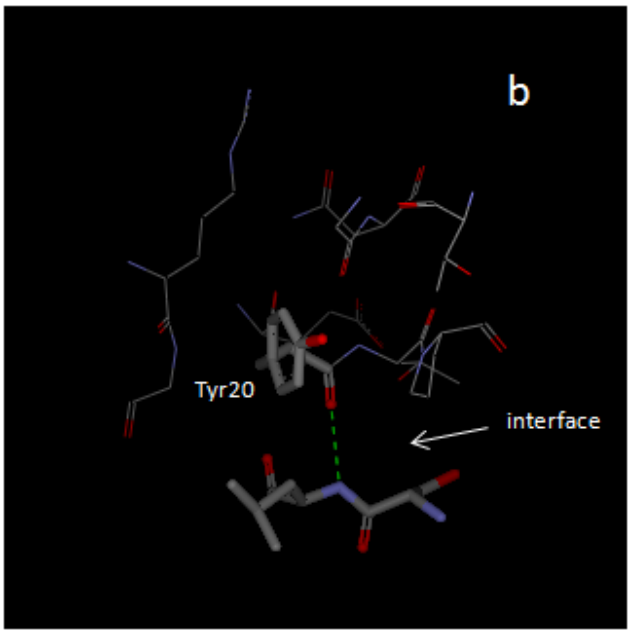
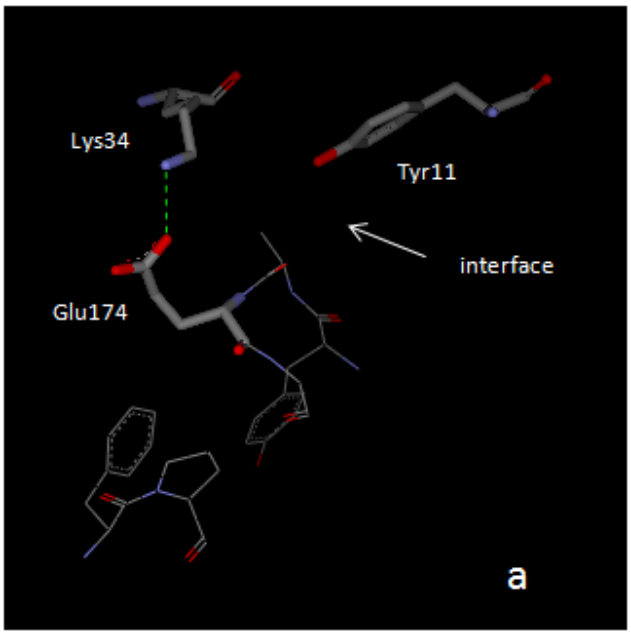


Figure S7. Ionic and hydrogen bonding interactions involving Tyr11, Lys34 and Glu174 of ALP in (a) ALP-OMTKY3 and (b) ALP-OMTKY3M. Presence of intermolecular hydrogen bond is indicated by green dotted line.

(a)



(b)

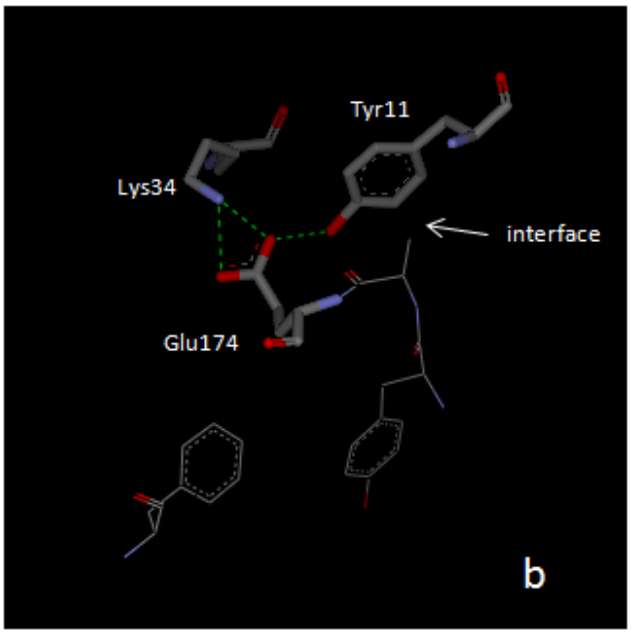


Figure S8. The conformational change that causes Tyr11 to make hydrogen bond with Glu174 of ALP in ALP-OMTKY3M (yellow). Wild-type complex ALP-OMTKY3 is shown in blue.