Supplementary Information

Accelerated molecular dynamics study of interaction mechanism between small molecule inhibitors and phosphoglycerate mutantase 1

Yanqi Sun,[a] Chaoyue Jia,[a] Shaolong Zhang,[a] Qinggang Zhang,[a] Jianzhong Chen*[b] and Xinguo Liu*[a]

[a] School of Physics and Electronics, Shandong Normal University, Jinan, China 250358. E-mail: liuxinguo@sdnu.edu.cn

[b] School of Science, Shandong Jiaotong University, Jinan, China 250357. E-mail: jzchen@sdjtu.edu.cn, chenjianzhong1970@163.com

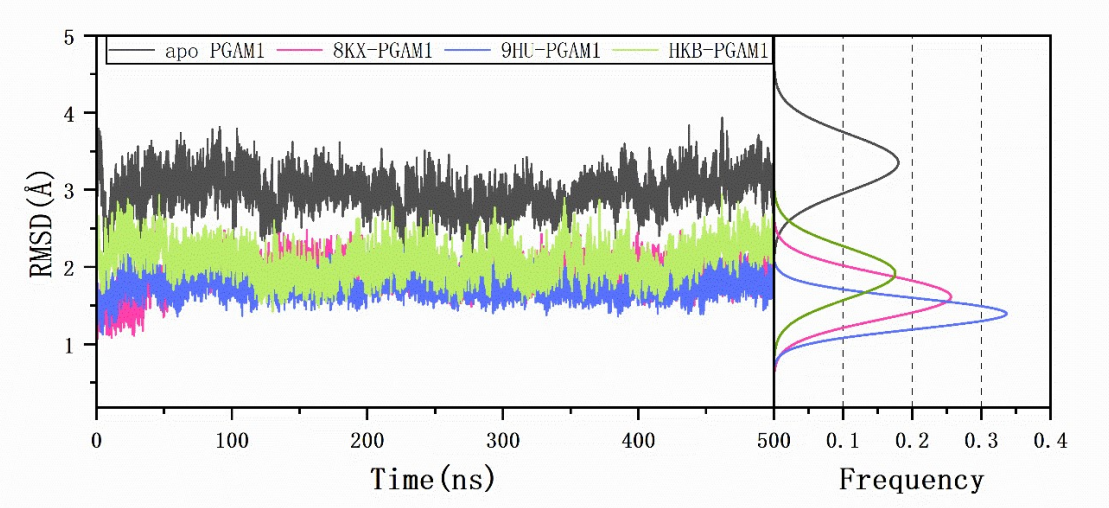

Fig. S1 The root-mean-square deviations of the backbone atoms relative to the initial optimized structure (RMSDs).

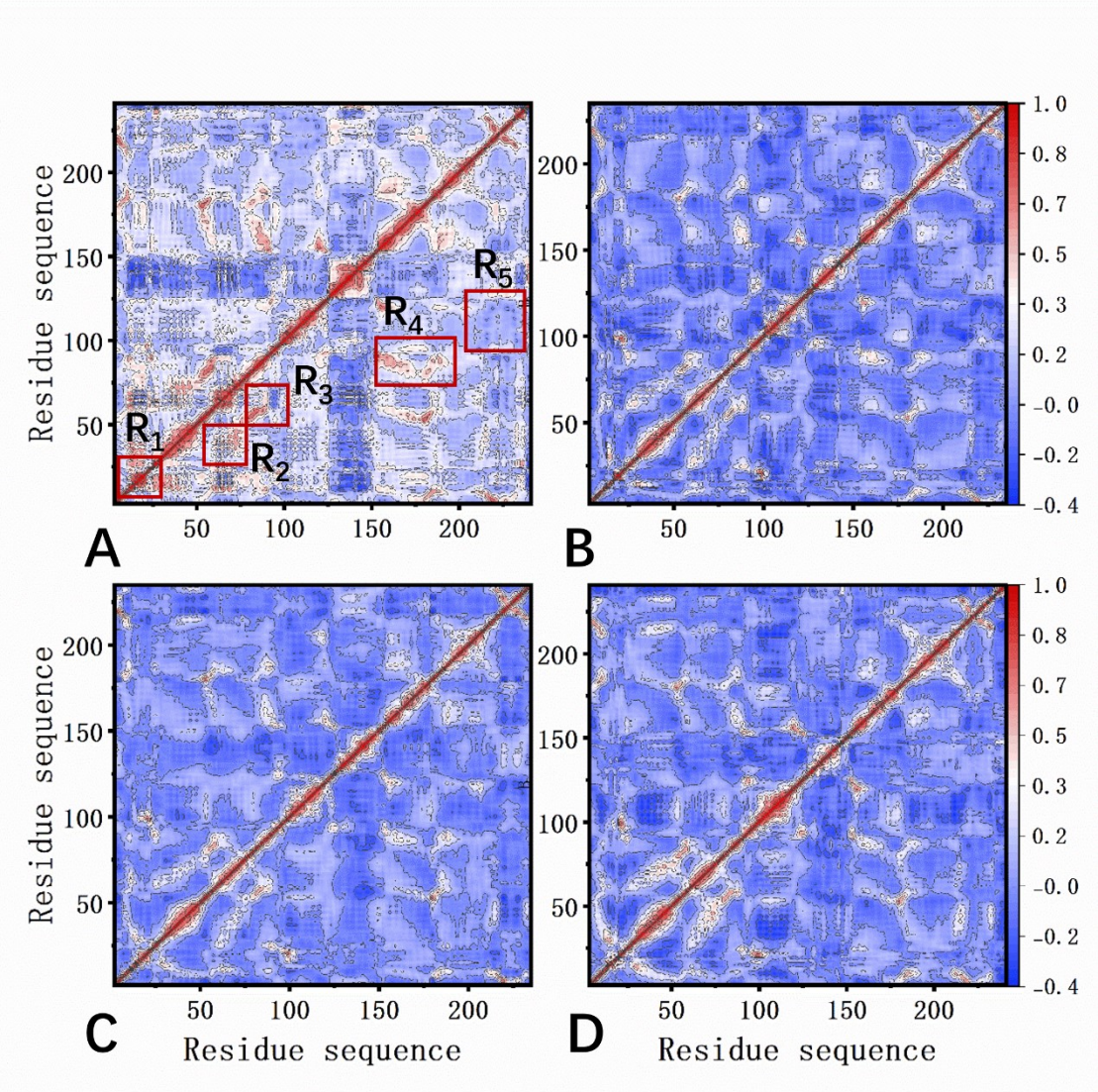

Fig. S2 The dynamic cross correlation maps calculated using the coordinates of the C_α atoms in the aMD trajectory: (A) the *apo* PGAM1, (B) the 8KX-bound PGAM1, (C) the 9HU-bound PGAM1, and (D) the HKB-bound PGAM1. Inhibitor binding affects the movement pattern of the PGAM1, and the red box indicates areas where the movement pattern is highly variable.

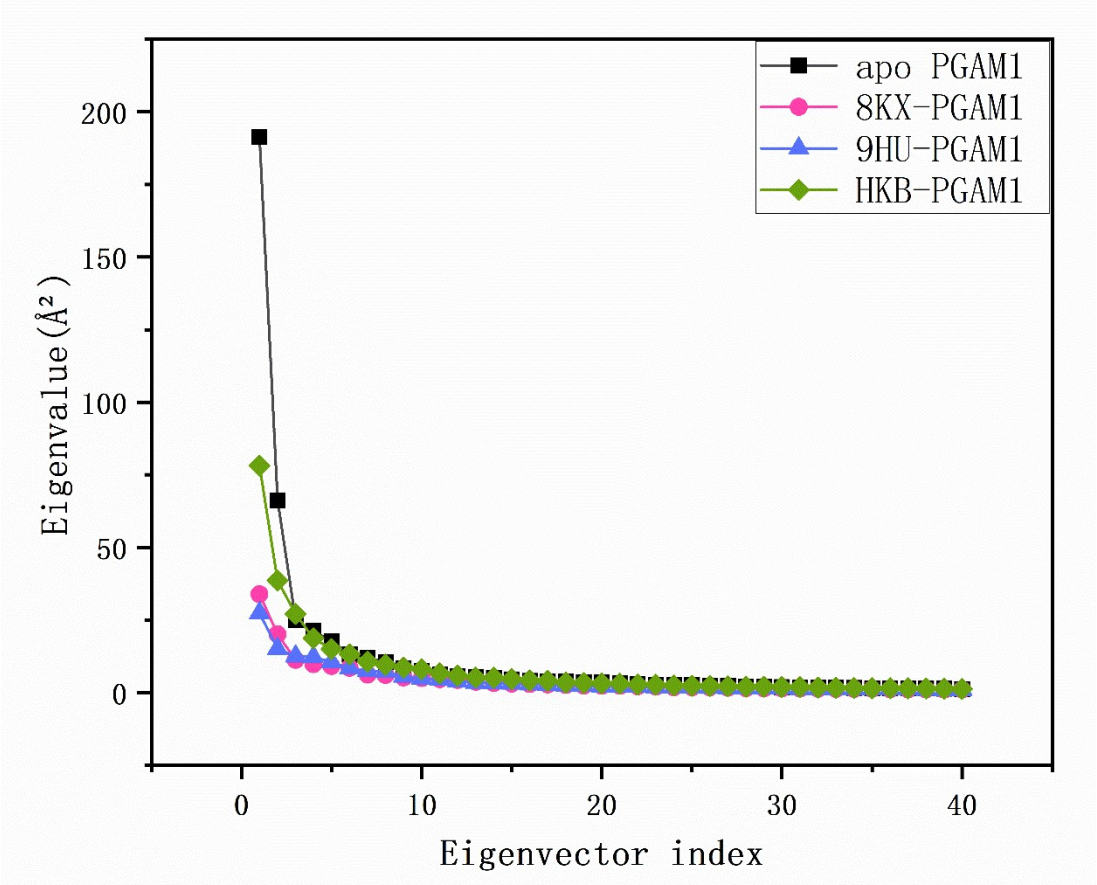

Fig. S3 Relationship between eigenvalues and eigenvector index of the *apo* PGAM1 and inhibitor-bound PGAM1.

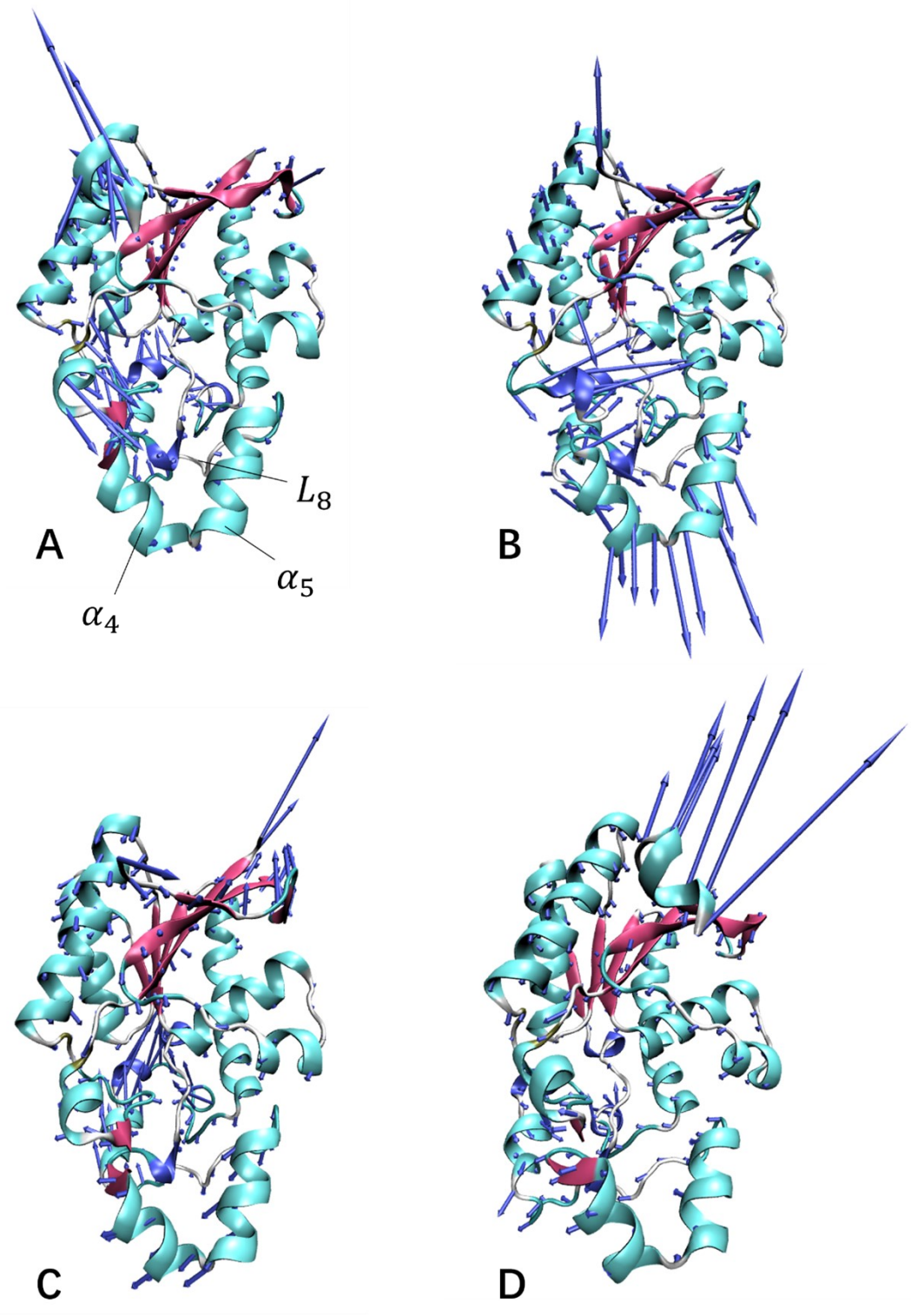

Fig. S4 Collective motion of structural domain in the PGAM1 along the first eigenvector derived from the PCA: (A) the *apo* PGAM1, (B) the 8KX-bound PGAM1, (C) the 9HU-bound PGAM1, (D) the HKB-bound PGAM1. The direction and length of the arrows in the figure reflect the direction and intensity of movement in the PGAM1 region, respectively. The binding of 8KX, 9HU, and HKB has a significant effect on the movement of α-helixs α_4, α_5 and loop L_8 in the PGAM1.

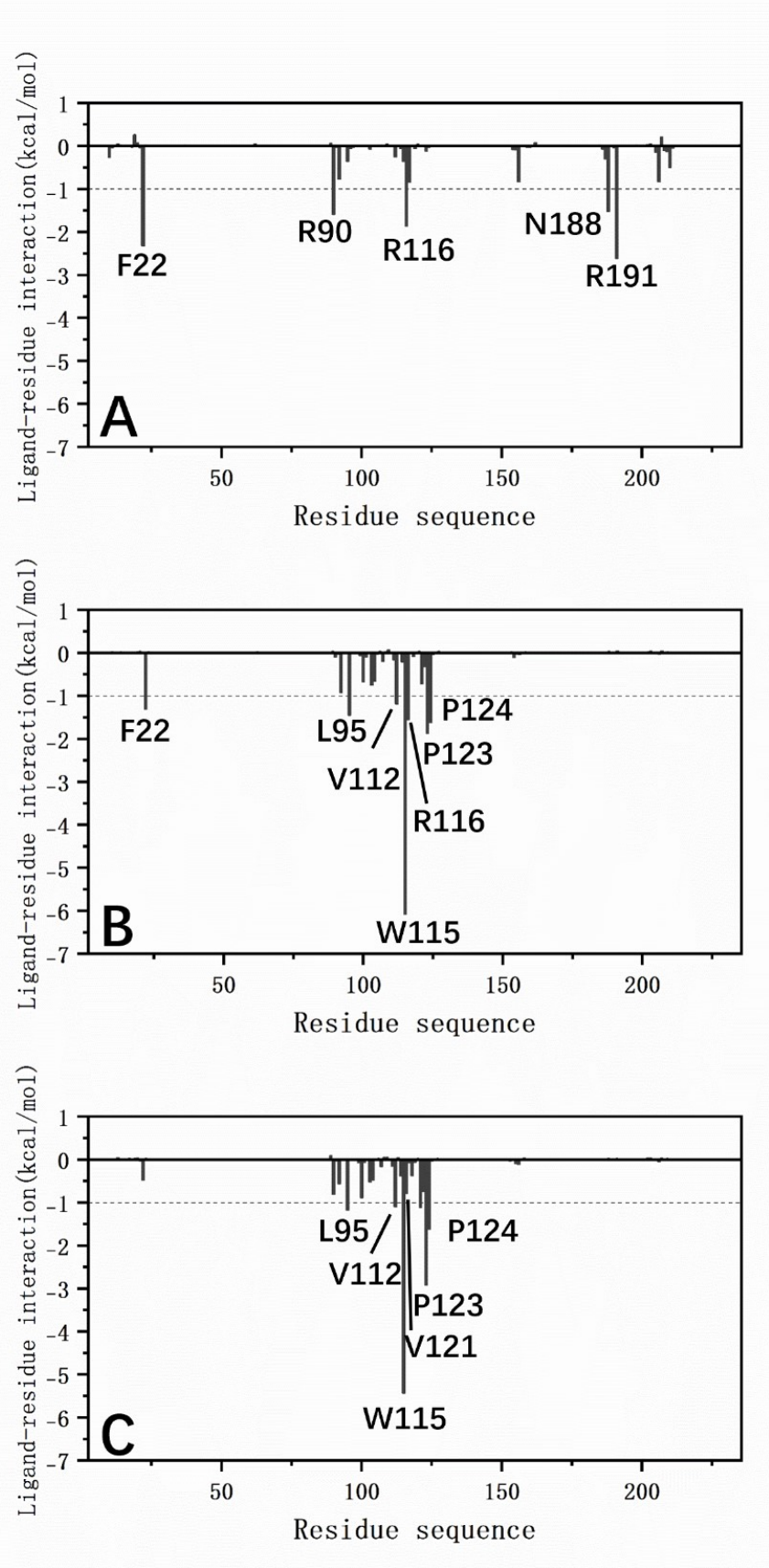

Fig. S5 Interaction energies of the residues of the PGAM1 with the inhibitors: (A) 8KX–PGAM1, (B) 9HU–PGAM1, and (C) HKB–PGAM1.

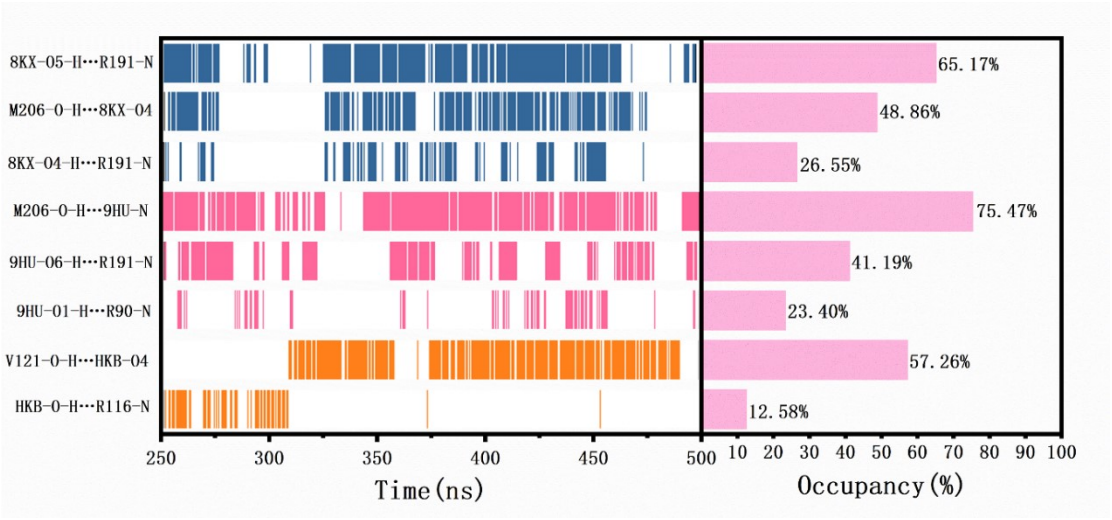

Fig. S6 Evolution and occupancy of specific hydrogen bonds formed by inhibitor-receptor proteins over simulated time.