Binding Mode and Induced Fit Predictions for Prospective Computational Drug Design

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Supporting Information

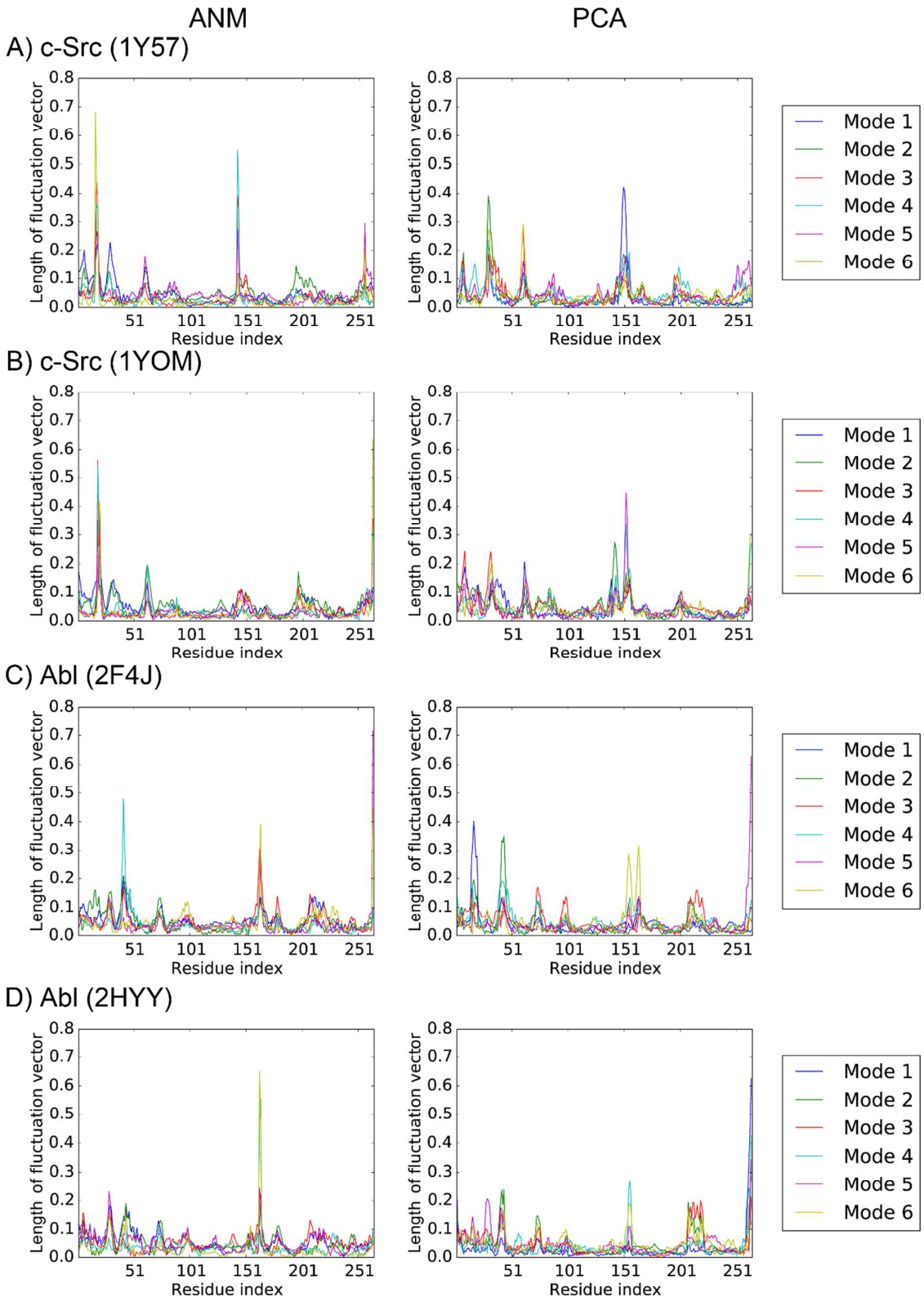

Figure S1 First six normal modes from ANM and the first six principal components from PCA of the MD simulations for c-Src and Abl kinase.

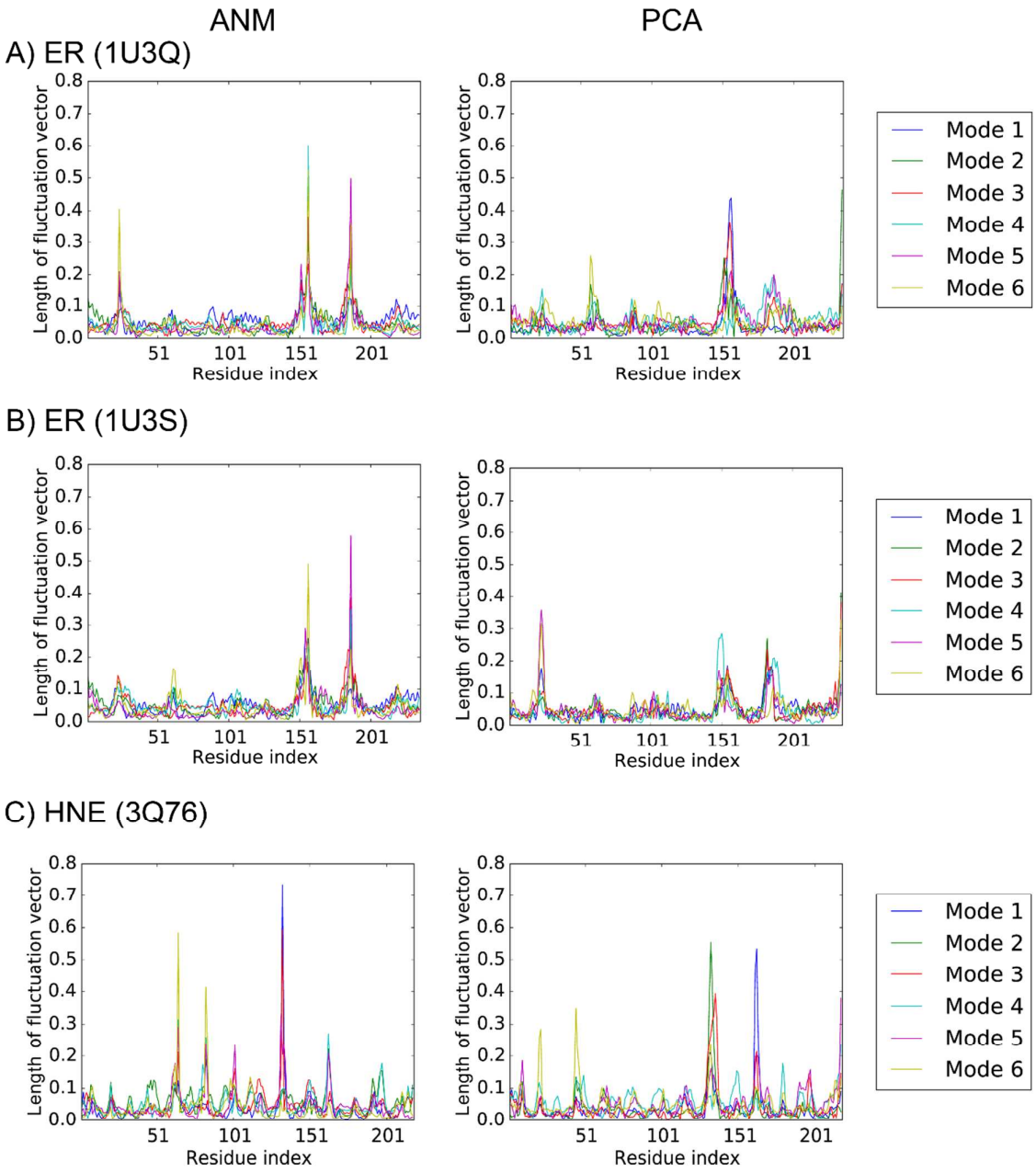

Figure S2 First six normal modes from ANM and the first six principal components from PCA of the MD simulations for ER and HNE.

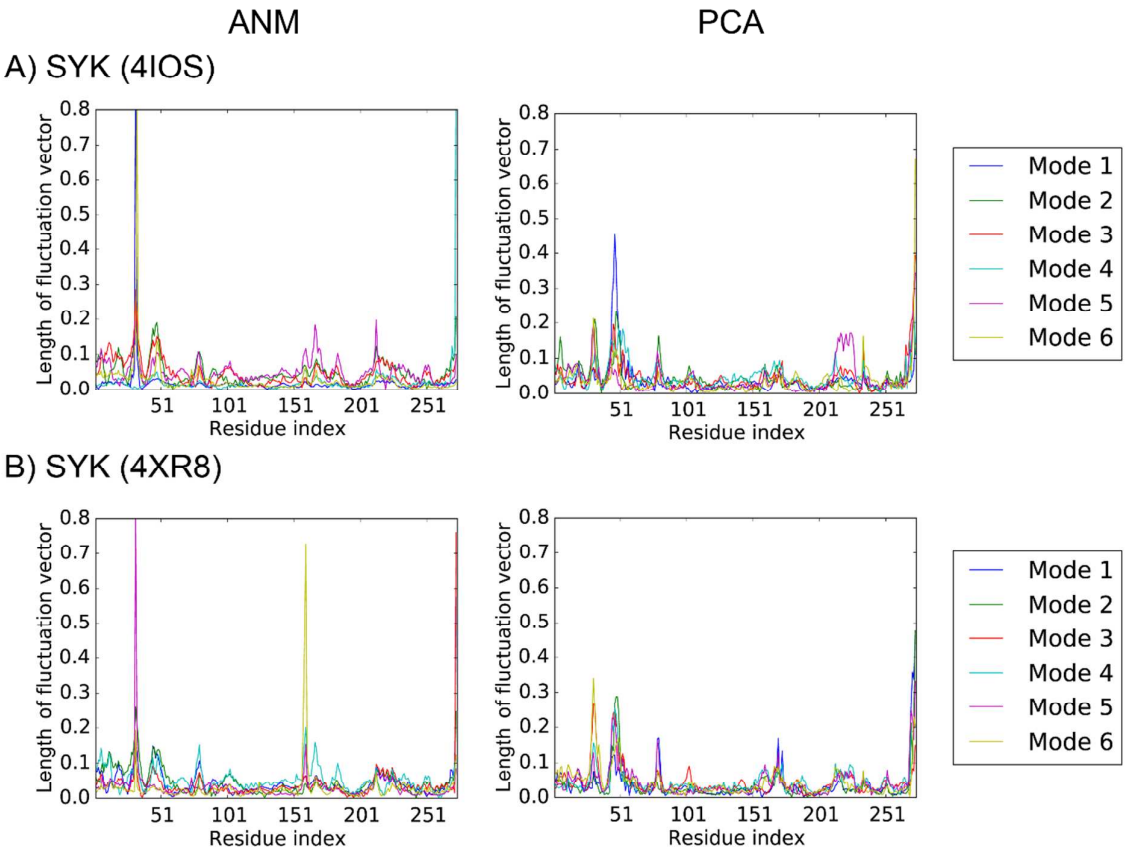

Figure S3 First six normal modes from ANM and the first six principal components from PCA of the MD simulations for the SYK kinase.

HNE

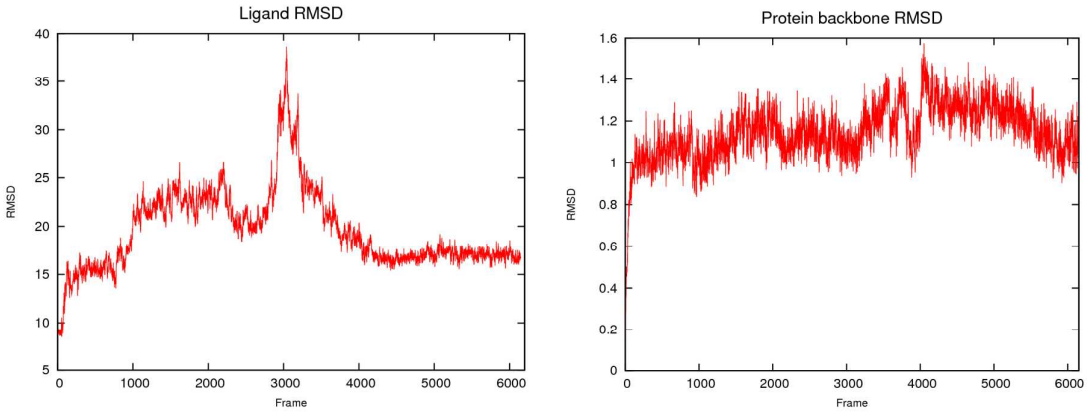

Figure S4 LRMSD and backbone RMSD of 3Q77 during MD simulation.

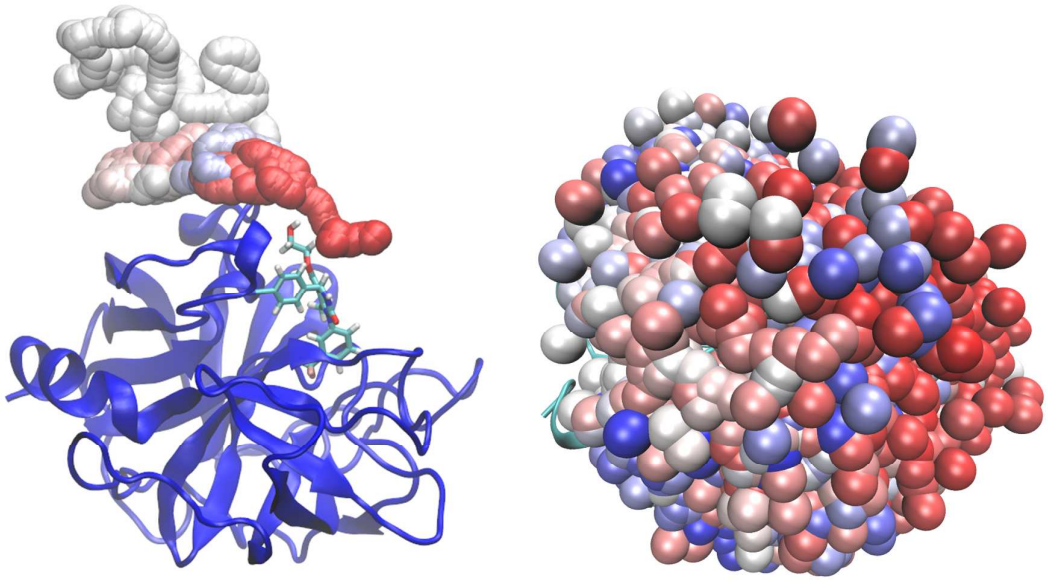

Figure S5 Ligand positions during the MD (left) and the PELE (right) simulation for 3Q77. The central atom of the ligand is indicated by a sphere colored due to its simulation step (red to blue).

ER
1U3Q

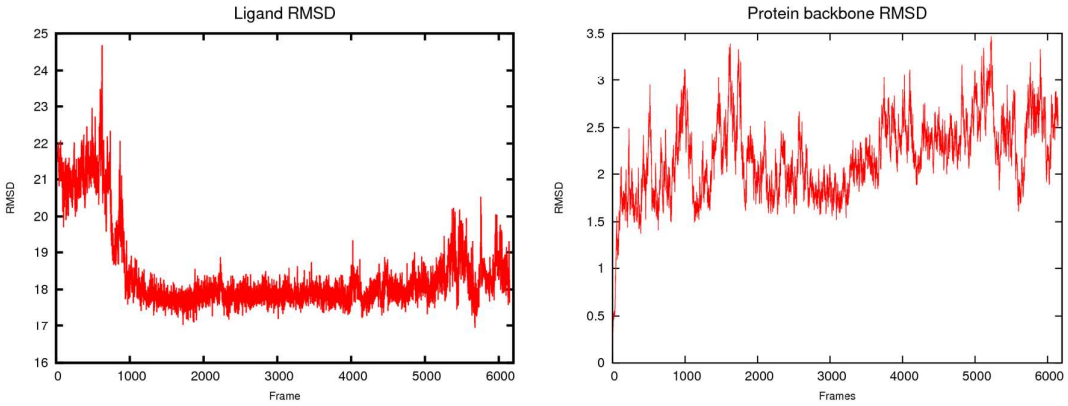

Figure S6 LRMSD and backbone RMSD of 1U3Q during MD simulation.

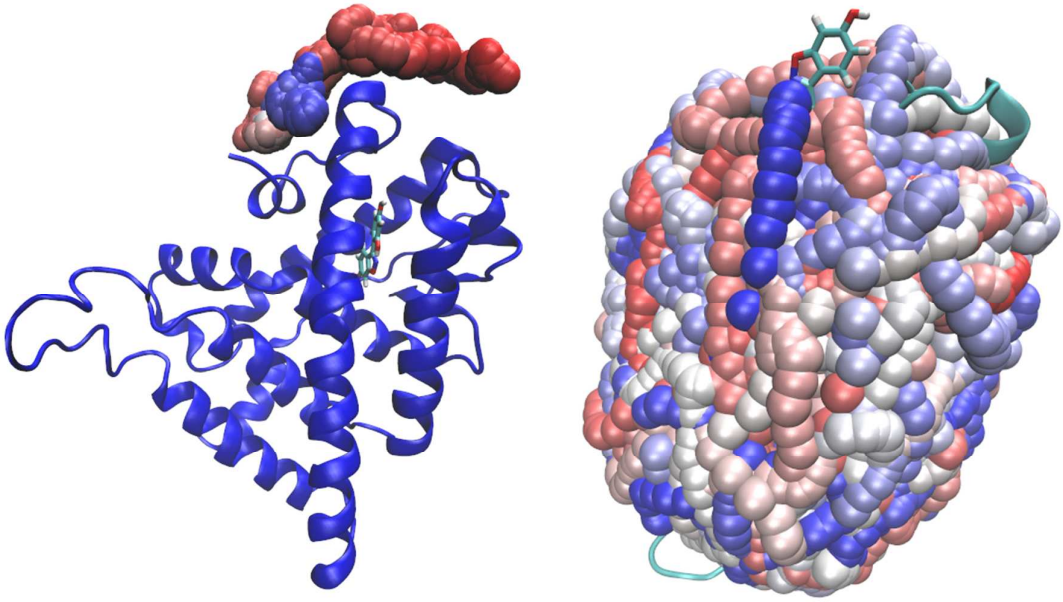

Figure S7 Ligand positions during the MD (left) and the PELE (right) simulation for 1U3Q. The central atom of the ligand is indicated by a sphere colored due to its simulation step (red to blue).

1U3S

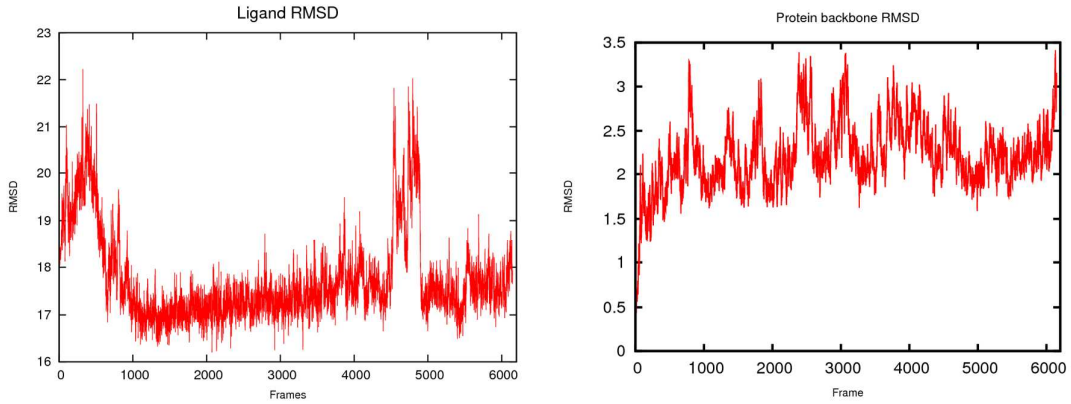

Figure S8 LRMSD and backbone RMSD of 1U3S during MD simulation.

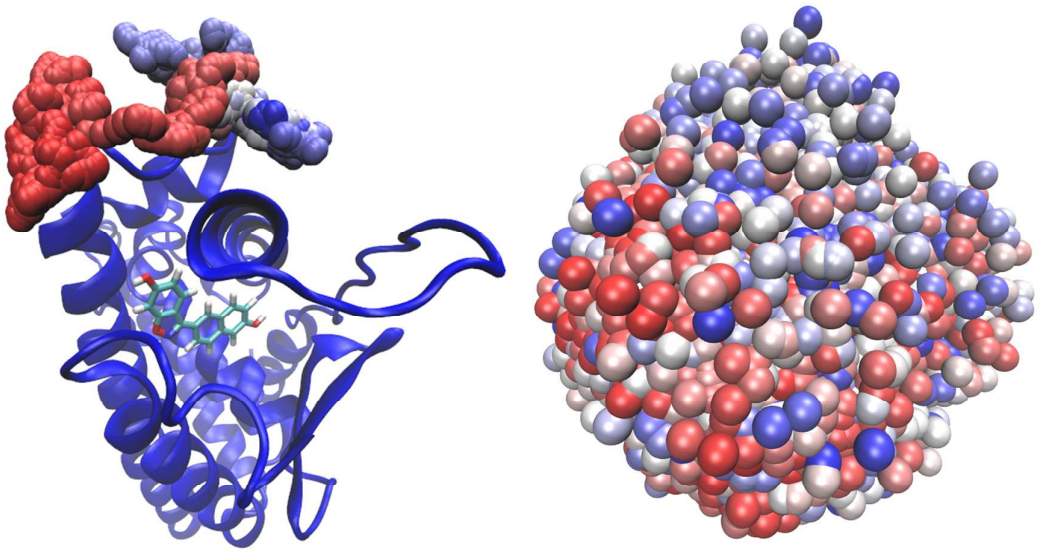

Figure S9 Ligand positions during the MD (left) and the PELE (right) simulation for 1U3S. The central atom of the ligand is indicated by a sphere colored due to its simulation step (red to blue).

SYK
4IOS

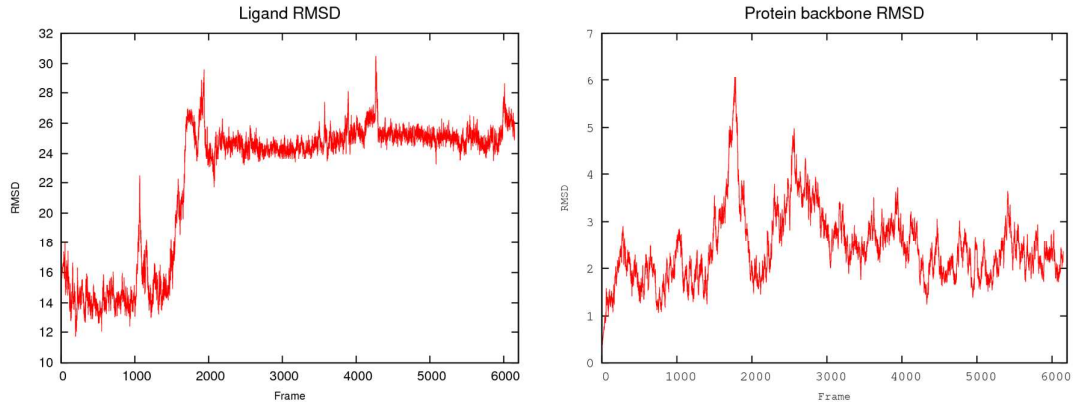

Figure S10 LRMSD and backbone RMSD of 4IOS during MD simulation.

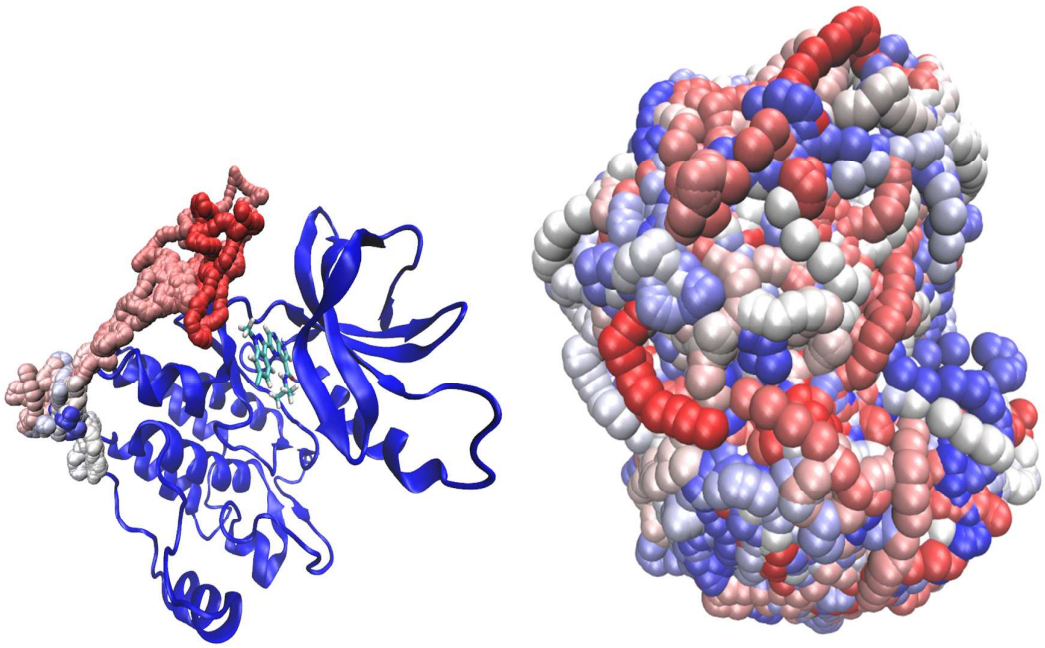

Figure S11 Ligand positions during the MD (left) and the PELE (right) simulation for 4IOS. The central atom of the ligand is indicated by a sphere colored due to its simulation step (red to blue).

4XR8

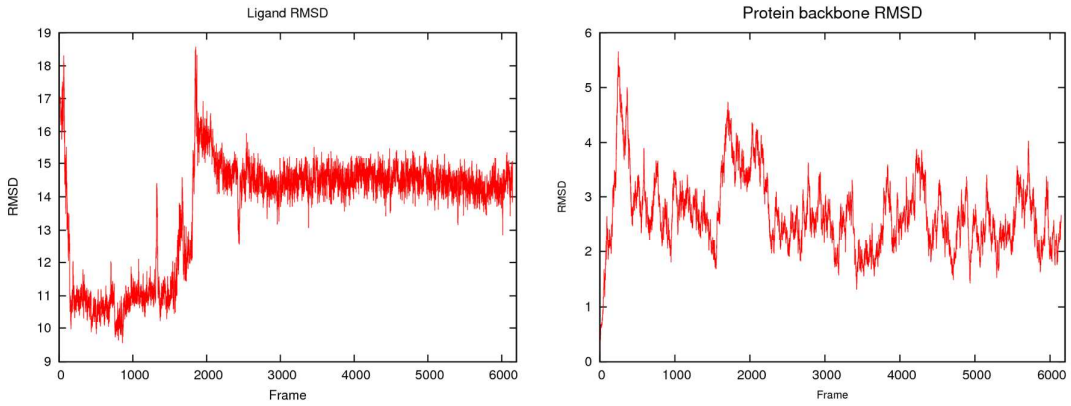

Figure S12 LRMSD and backbone RMSD of 4XR8 during MD simulation.

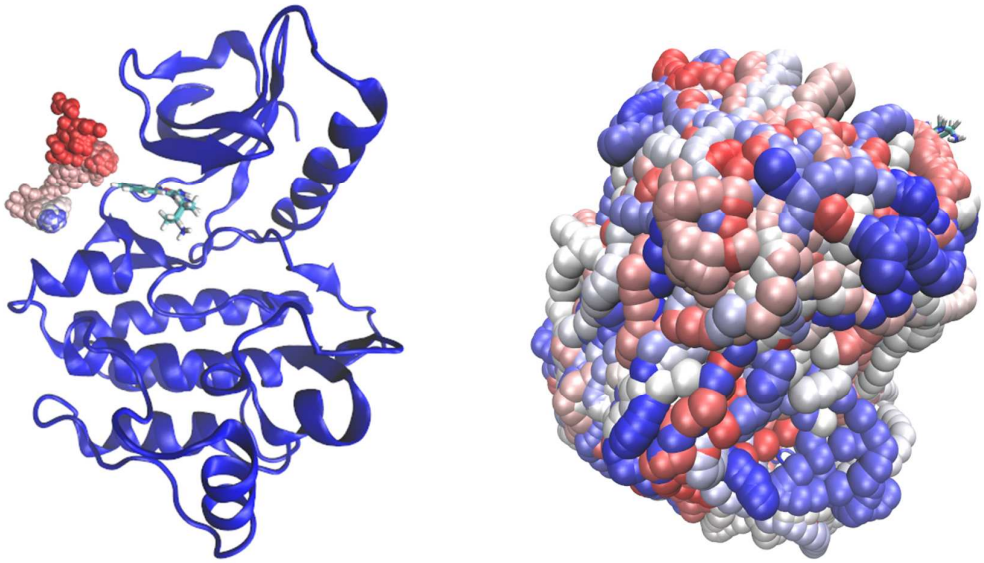

Figure S13 Ligand positions during the MD (left) and the PELE (right) simulation for 4XR8. The central atom of the ligand is indicated by a sphere colored due to its simulation step (red to blue).

Abl

2HYY

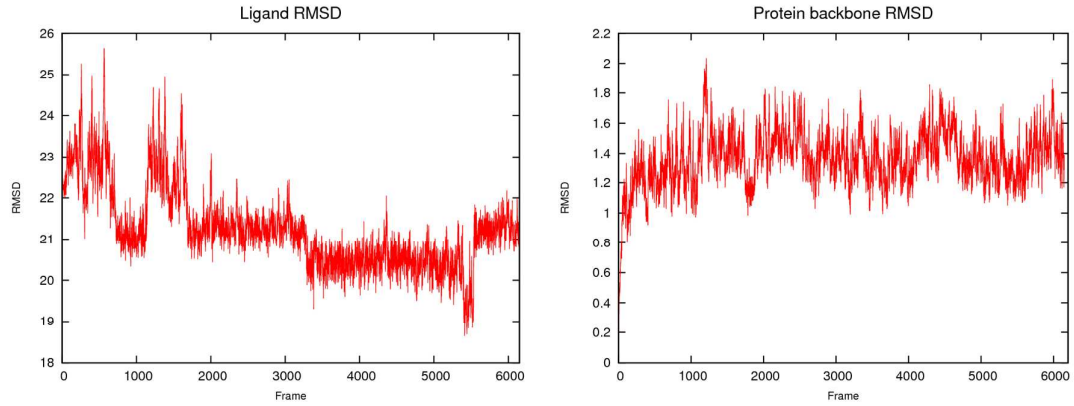

Figure S14 LRMSD and backbone RMSD of 2HYY during MD simulation.

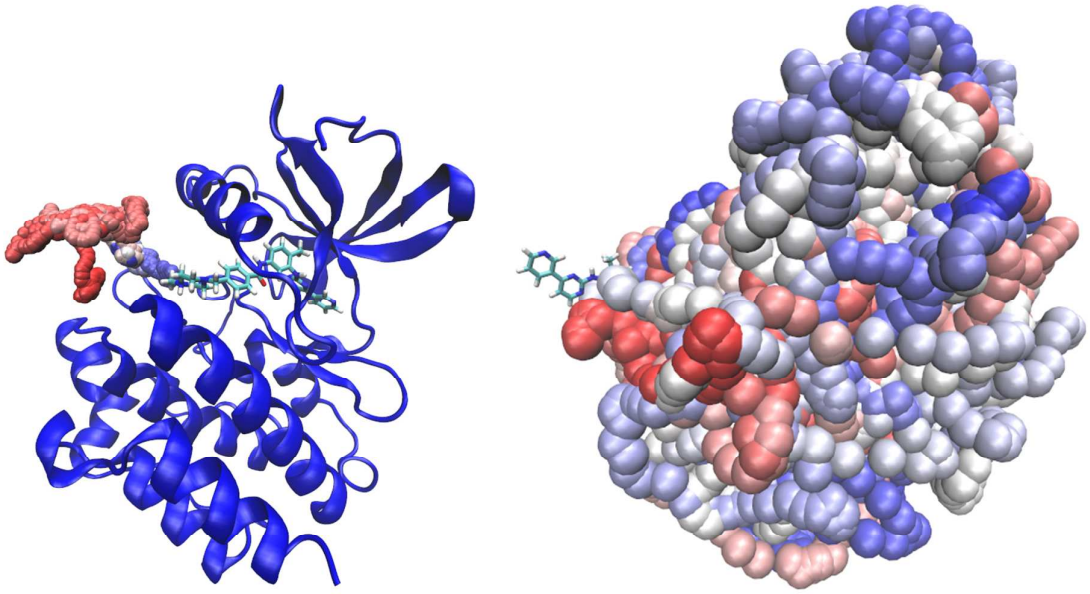

Figure S15 Ligand positions during the MD (left) and the PELE (right) simulation for 2HYY. The central atom of the ligand is indicated by a sphere colored due to its simulation step (red to blue).

2F4J

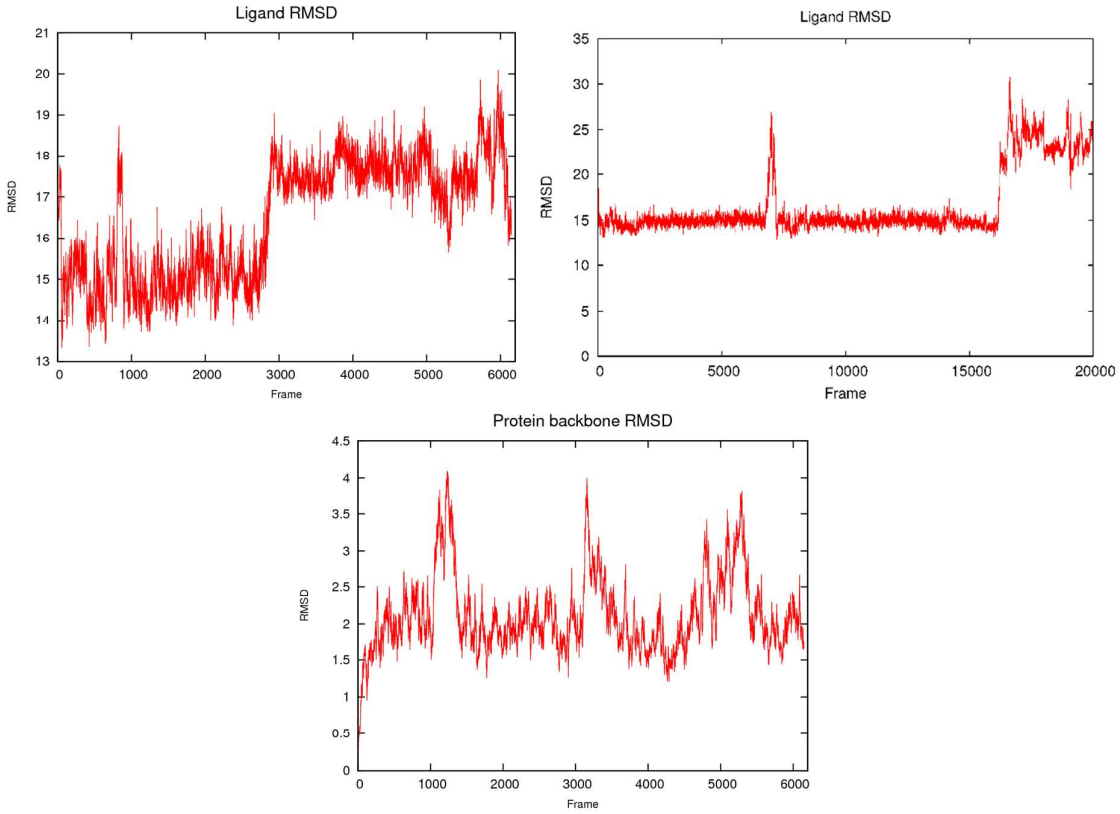

Figure S16 LRMSD (for 60ns and 200ns) and backbone RMSD of 2F4J during MD simulation.

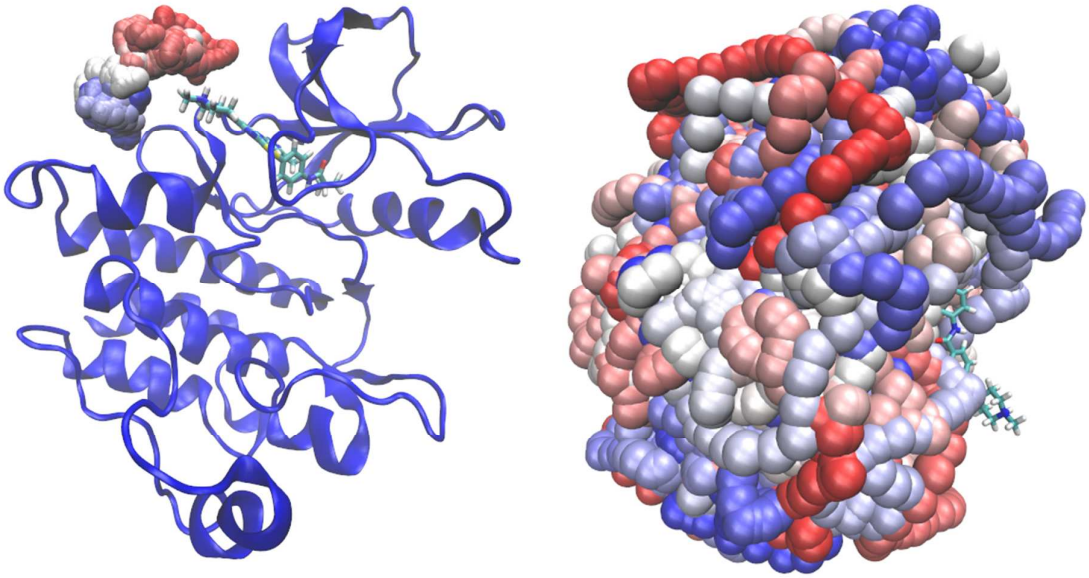

Figure S17 Ligand positions during the MD (left) and the PELE (right) simulation for 2F4J. The central atom of the ligand is indicated by a sphere colored due to its simulation step (red to blue).

c-Src
1Y57

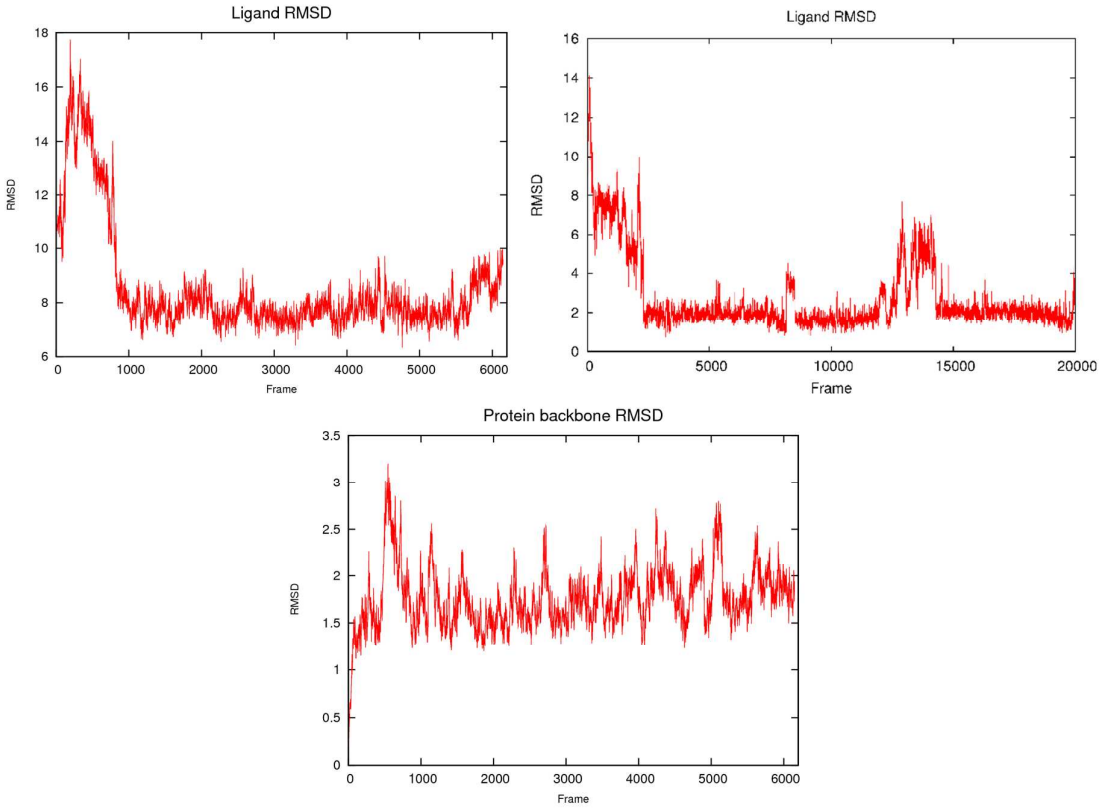

Figure S18 LRMSD (for 60ns and 200ns) and backbone RMSD of 1Y57 during MD simulation.

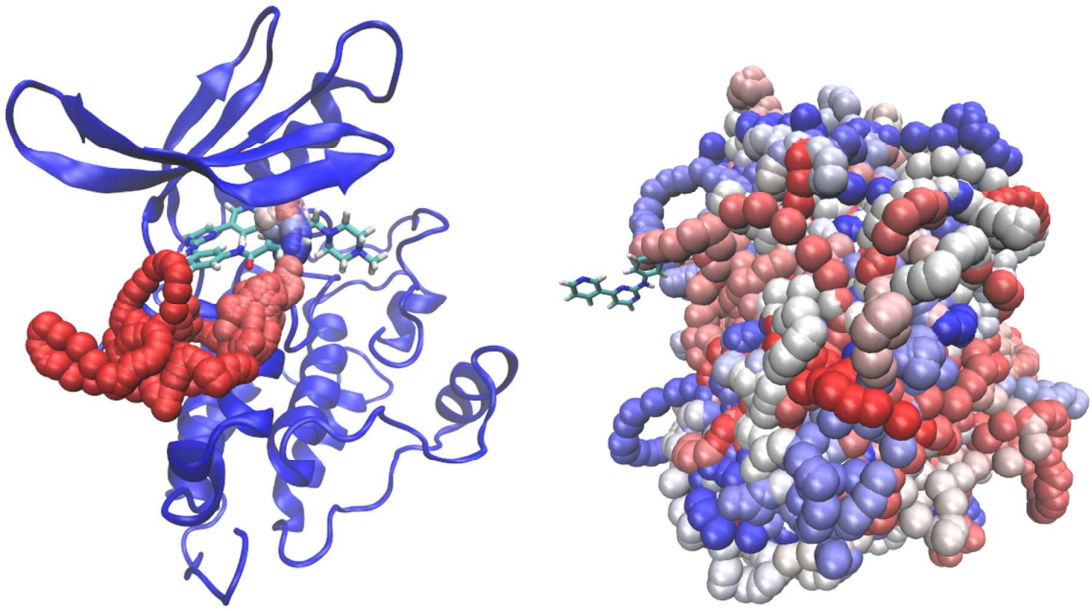

Figure S19 Ligand positions during the MD (left) and the PELE (right) simulation for 1Y57. The central atom of the ligand is indicated by a sphere colored due to its simulation step (red to blue).

1YOM

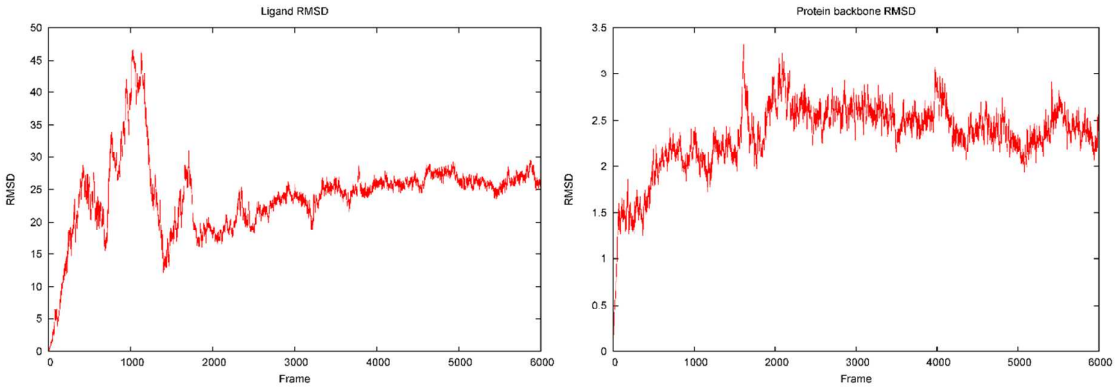

Figure S20 LRMSD and backbone RMSD of 1YOM during MD simulation.

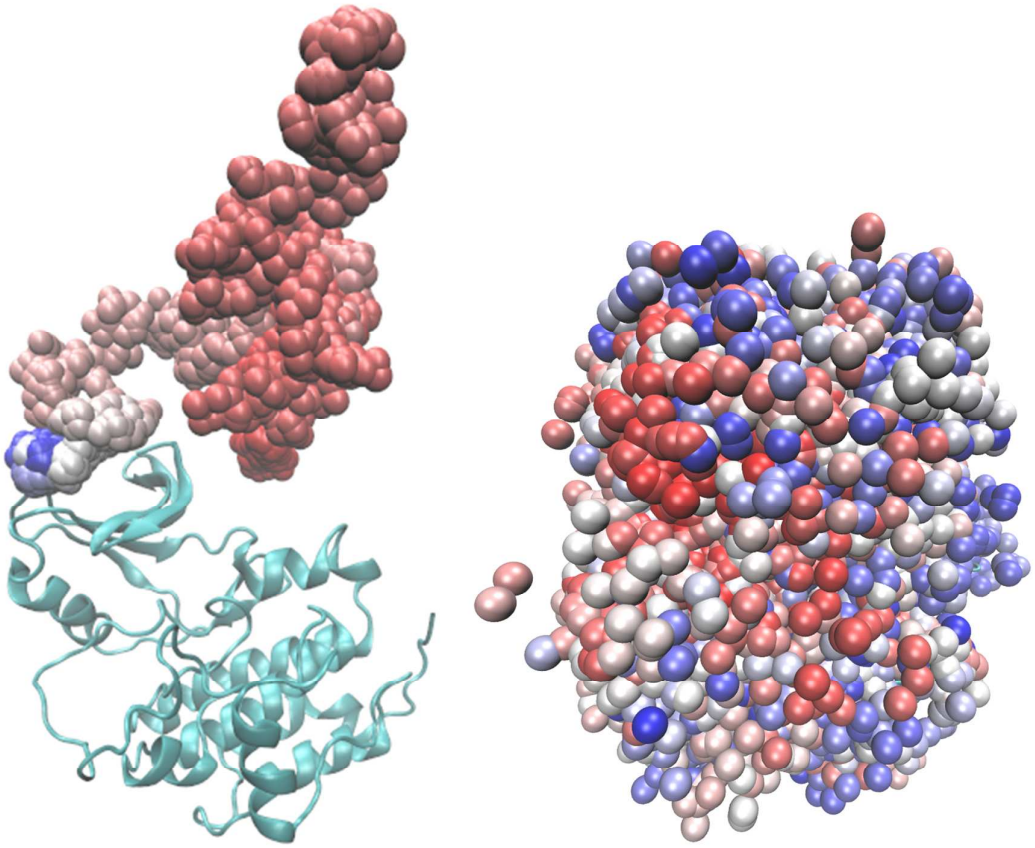

Figure S21 Ligand positions during the MD (left) and the PELE (right) simulation for 1YOM. The central atom of the ligand is indicated by a sphere colored due to its simulation step (red to blue).