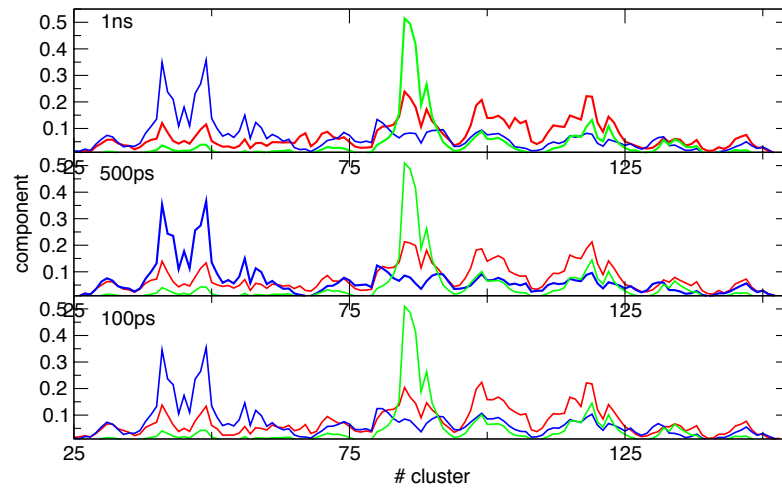


Supplementary Information

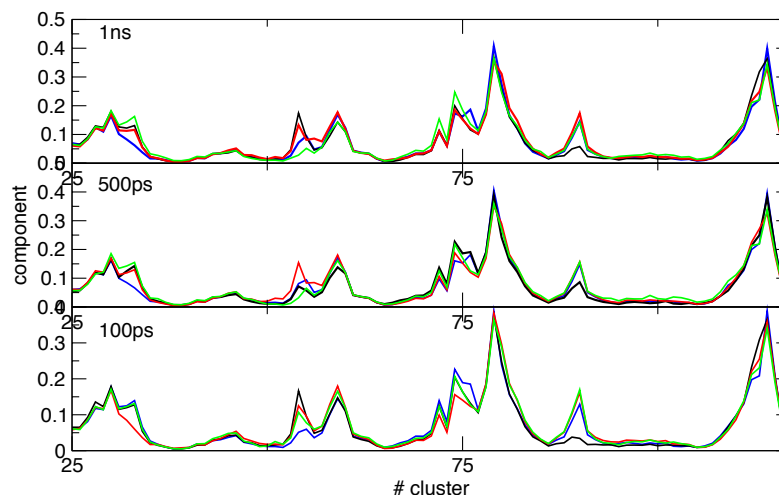
Figure S1

Cluster representatives resulting from the clustering of different time series of energy profiles, obtained with striding 1ns, 500ps and 100ps respectively. The three systems are shown.

FGF



PDZ



HSP90

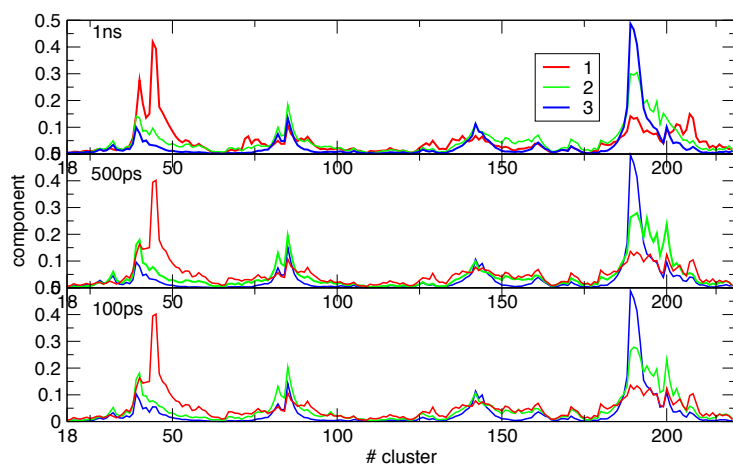
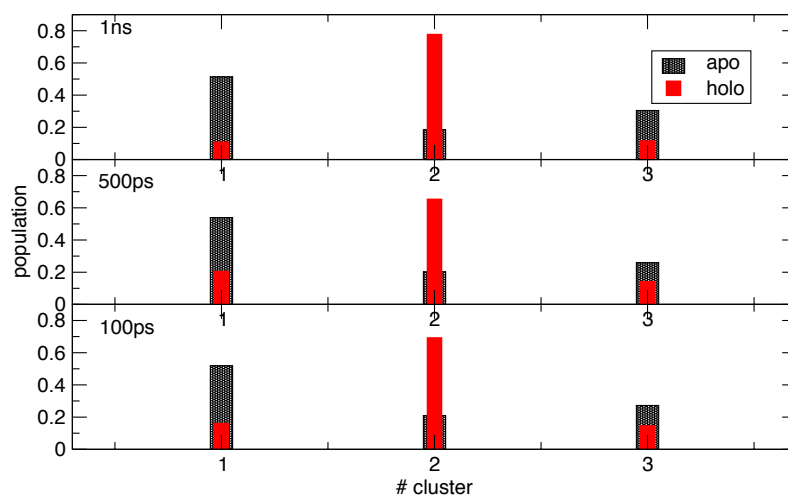


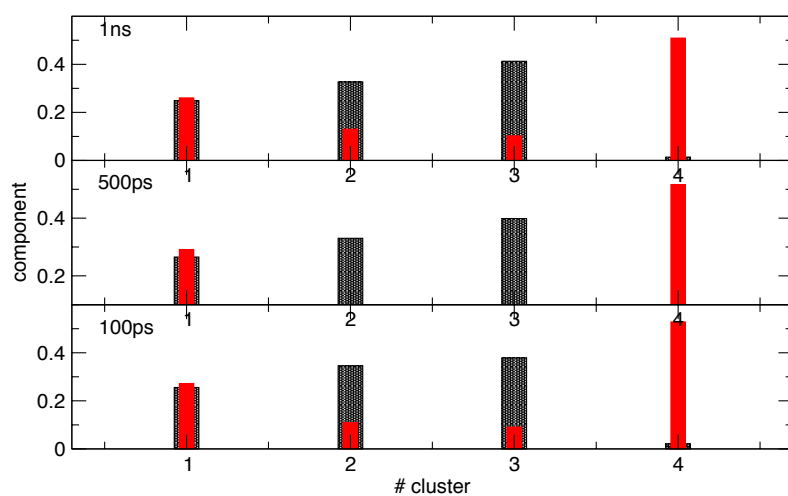
Figure S2

Population of the above represented clusters obtained with striding 1ns, 500ps and 100ps for the three systems.

FGF



PDZ



HSP90

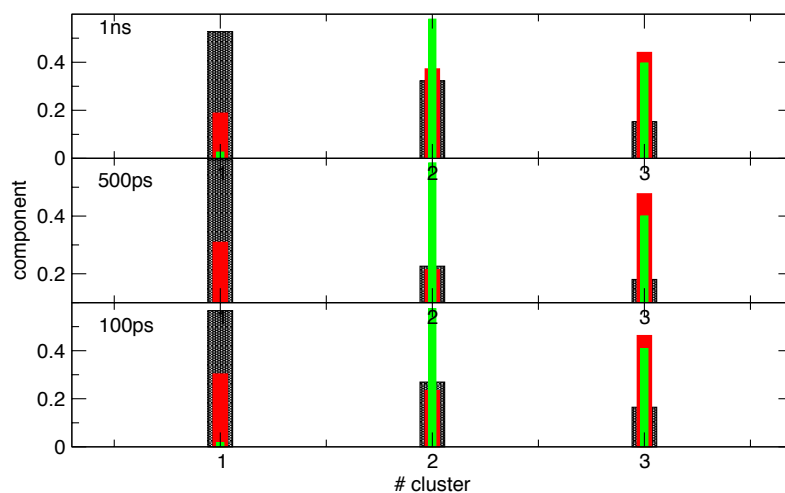


Figure S3

Population of each energy cluster plotted against the persistence of the same cluster

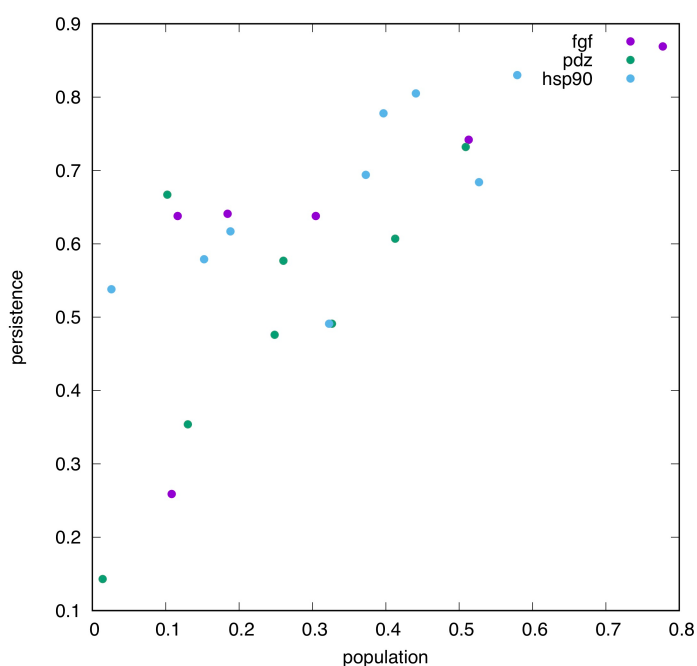


Table S1. Transition matrices between energy clusters in FGF

FGF

APO	1	2	3
1	0.74	0.07	0.19
2	0.28	0.65	0.07
3	0.27	0.09	0.64

Sm27	1	2	3
1	0.25	0.66	0.09
2	0.10	0.86	0.04
3	0.07	0.29	0.64

Figure S4. RMSD clusters in FGF. Left, cluster 1; Right, cluster 2

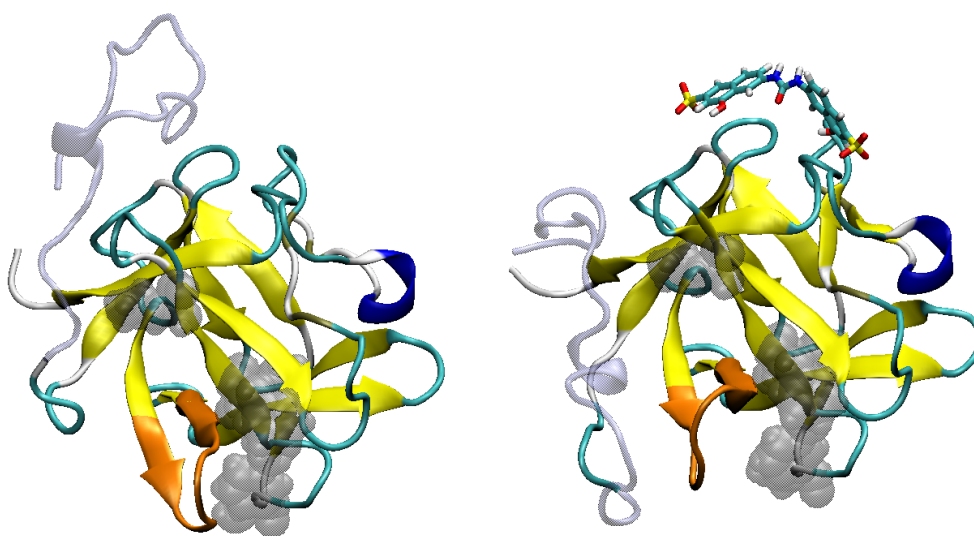
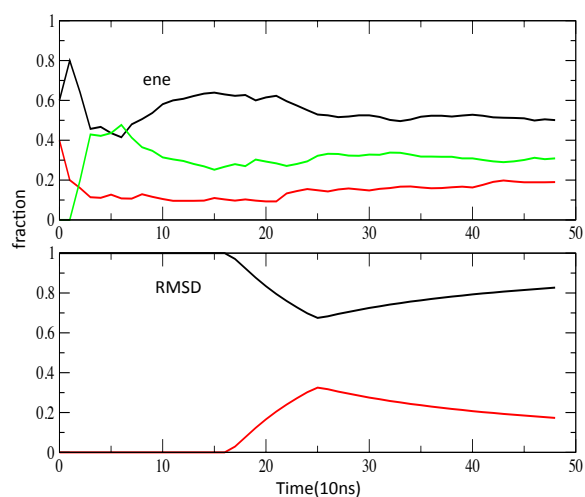


Figure S5. Timeline of population of energy and RMSD clusters in the APO (top) and sm27 FGF bound system.

Convergence profile clustering decomposition FGF APO



Convergence profile clustering decomposition FGF sm27

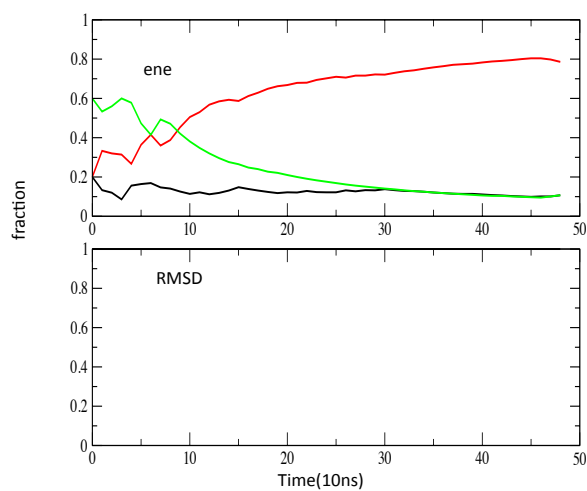


Table S2. Transition matrices between energy clusters in PDZ

APO	1	2	3	4
1	0.48	0.27	0.23	0.02
2	0.19	0.49	0.31	0.01
3	0.15	0.23	0.61	0.01
4	0.43	0.29	0.14	0.14

RA	1	2	3	4
1	0.58	0.11	0.06	0.25
2	0.22	0.36	0.03	0.39
3	0.10	0.04	0.67	0.19
4	0.14	0.10	0.03	0.73

Figure S6. RMSD clusters in PDZ. Left, cluster 1; Right, cluster 2

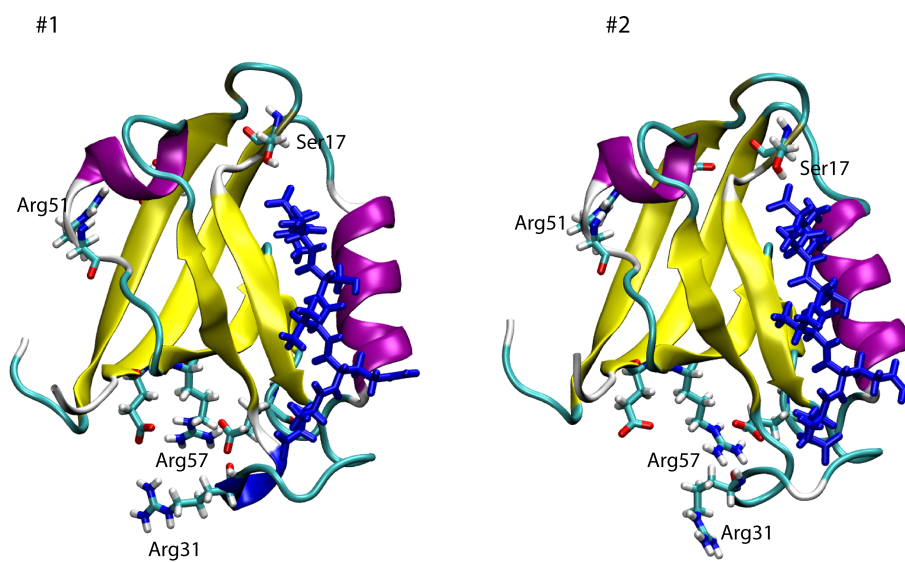


Figure S7 Energy clusters in PDZ.

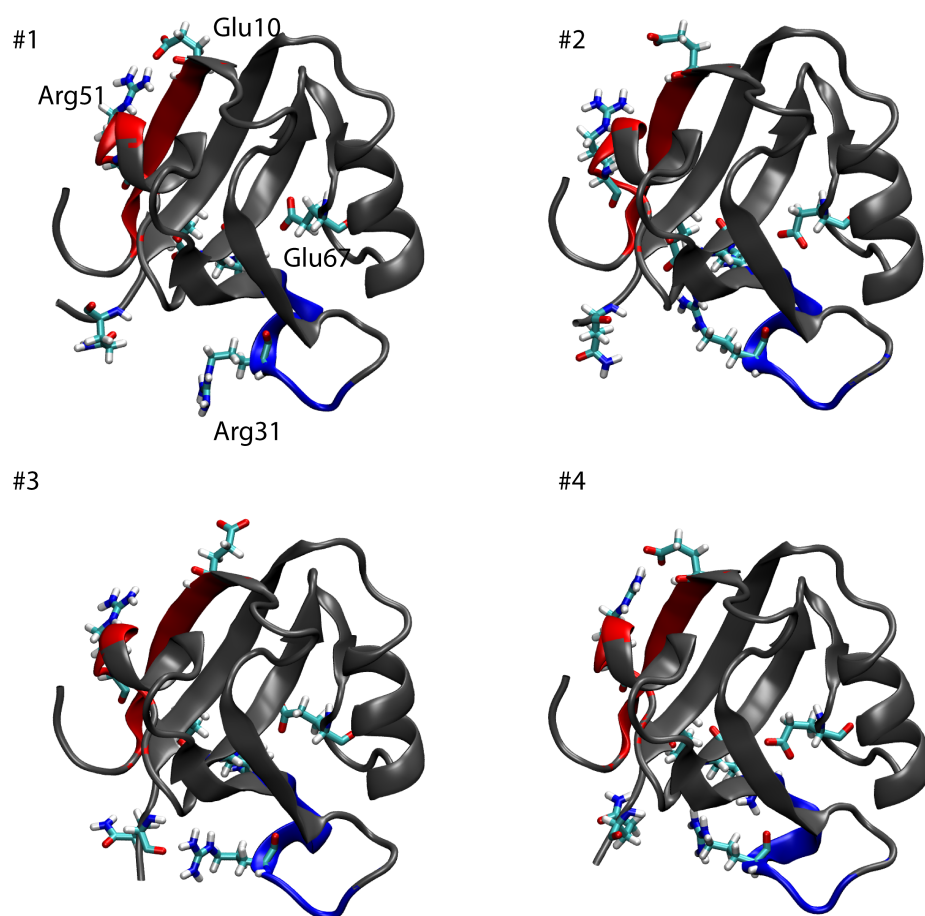


Figure S8. Timeline of population of energy (top) and RMSD (bottom) clusters in the APO (left) and RAF-G2 PDZ2 bound system (right).

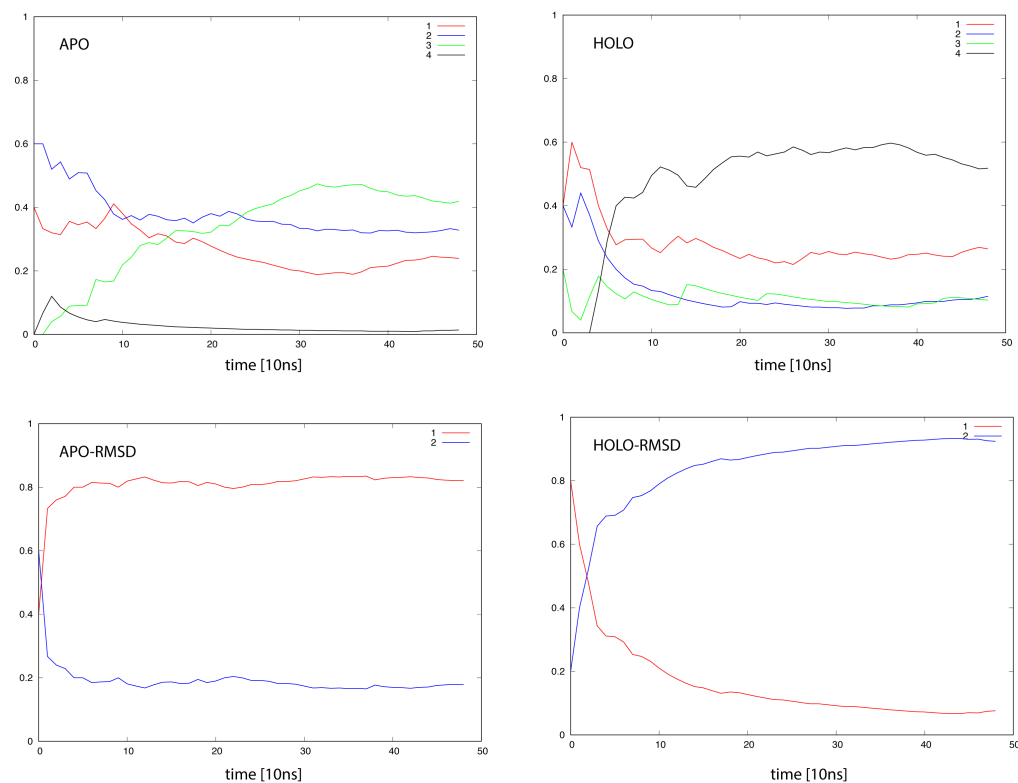


Table S3. Transition matrices between energy clusters in Hsp90

APO	1	2	3
1	0.68	0.26	0.06
2	0.40	0.49	0.10
3	0.24	0.18	0.58

ADP	1	2	3
1	0.50	0.46	0.04
2	0.02	0.83	0.15
3	0.01	0.22	0.77

ATP	1	2	3
1	0.61	0.25	0.14
2	0.15	0.69	0.16
3	0.04	0.15	0.81

Figure S9. RMSD clusters in the N terminal domain of Hsp90.

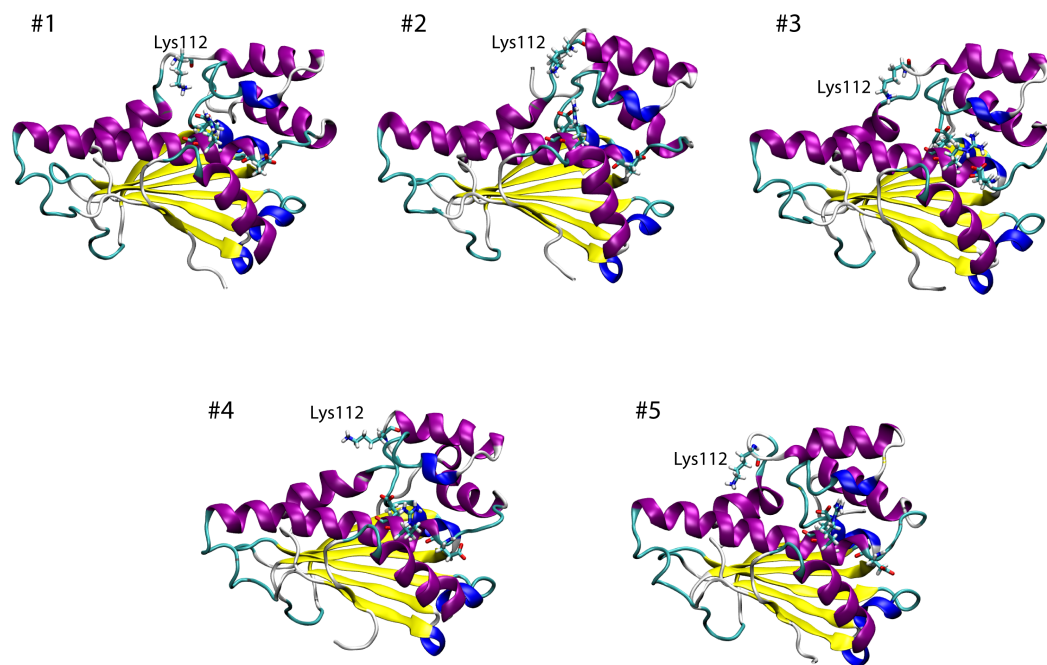


Figure S10. Timeline of population of energy and RMSD clusters in the APO (top) ADP bound (middle) and ATP bound (bottom) system.

