Mechanisms of protein-ligand association and its modulation by protein mutations

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Supplement

Calculated Association Rates

Mutant	Net Charge [e]	k_{on} [$10^8 M^{-1}s^{-1}$]	k_{on} [$10^8 M^{-1}s^{-1}$] Huang and Briggs [Biopolymers, 63, 2002]
wt (modeled)	0	27.9	28.3
A197W	0	26.4	25.0
D56N	+1	73.9	80.1
D137T	+1	77.8	105.4
T141D	-1	1.6	7.6
R135Q	-1	5.9	1.6
K43M	-1	11.3	7.6
K43Q	-1	11.4	5.7
R134Q	-1	12.4	12.5
3mut	-3	2.5	1.7
6mut	0	9.3	8.8
PBP:P_i	-2	3.0	

Table 1: Net charge and computed bimolecular association rates of considered mutant structures at ionic strength of $0mM$.

Association Free Energy Profiles, First Hitting Densities, Association Pathways, Mutation Sites
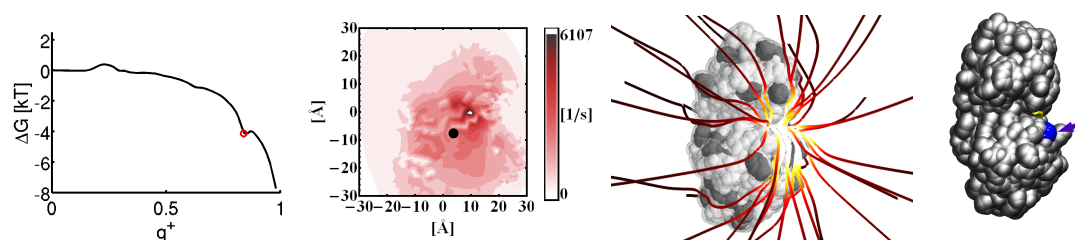

Figure 2: Mutant D137T - Committor Free Energy Profile, First Hitting Density, Association Pathways, Mutation Site
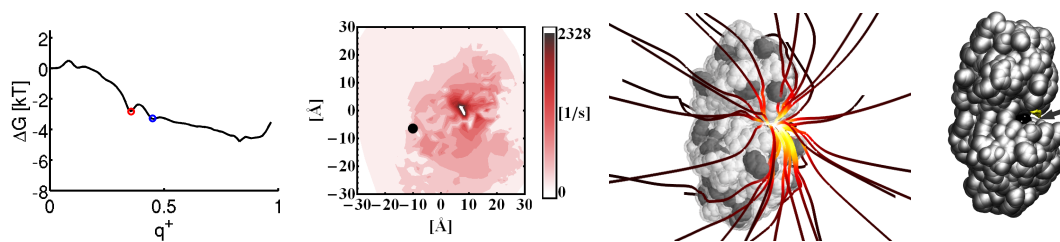
Figure 1: Mutant A197W - Committor Free Energy Profile, First Hitting Density, Association Pathways, Mutation Site
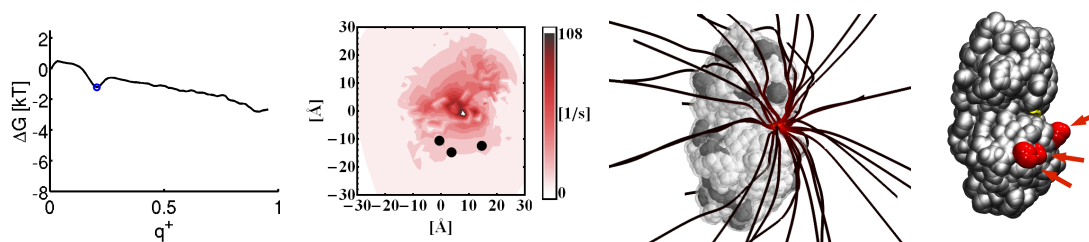

Figure 3: Mutant 3 mut. - Committor Free Energy Profile, First Hitting Density, Association Pathways, Mutation Site
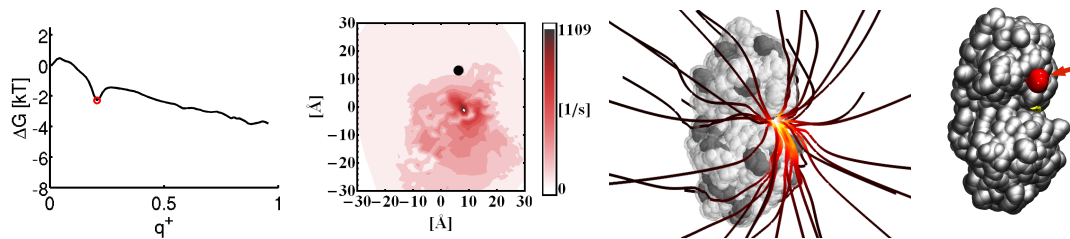

Figure 4: Mutant K43Q. - Committor Free Energy Profile, First Hitting Density, Association Pathways, Mutation Site
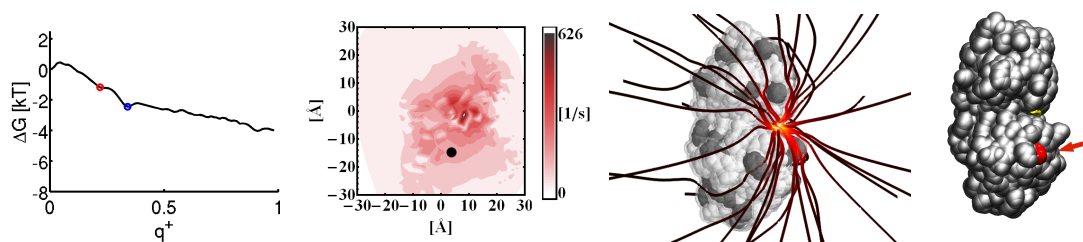
Figure 5: Mutant R134Q. - Committor Free Energy Profile, First Hitting Density, Association Pathways, Mutation Site
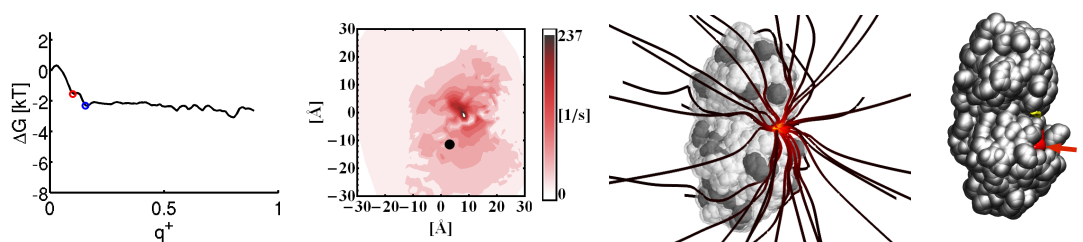

Figure 6: Mutant R135Q. - Committor Free Energy Profile, First Hitting Density, Association Pathways, Mutation Site