

Figure S1.

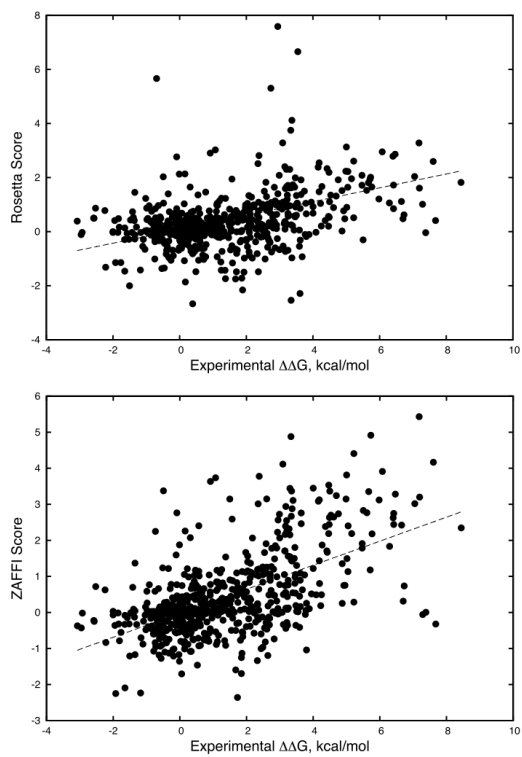
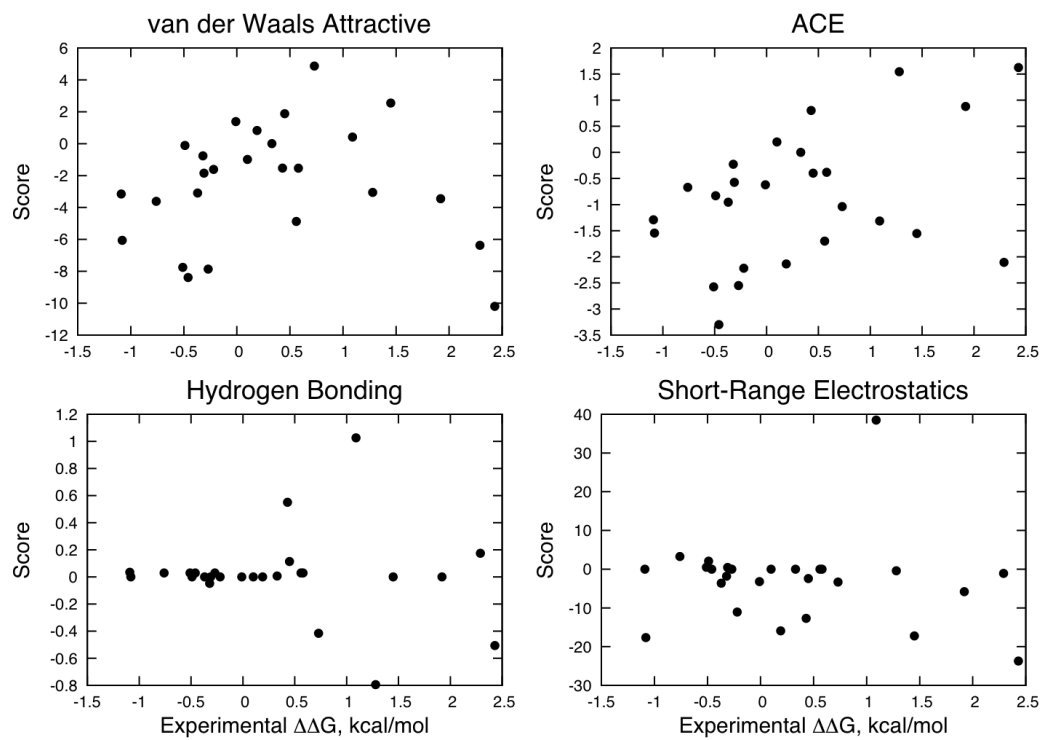


Figure S2.



**Figure S3.**

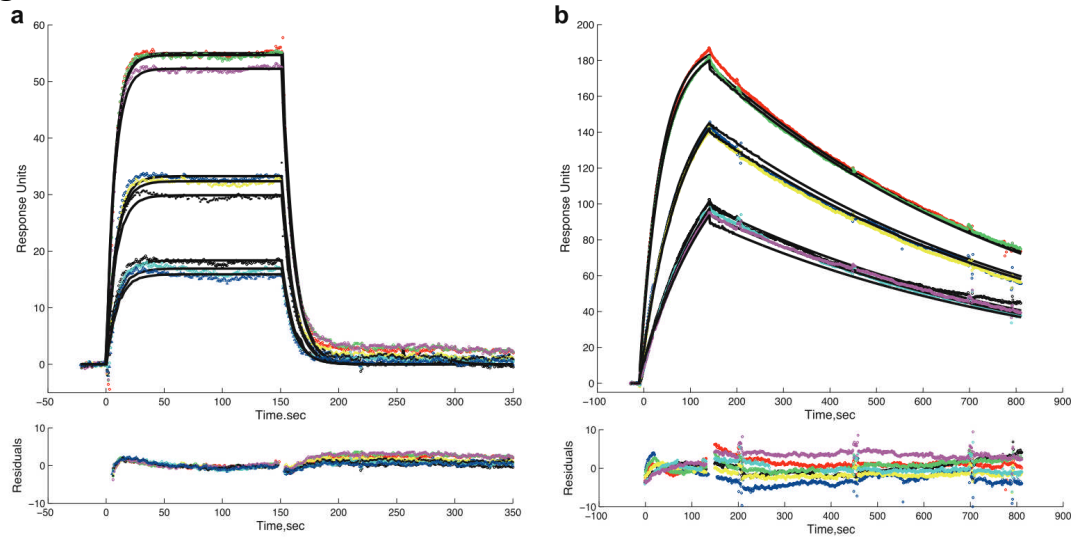


Table S1.

<b>Mutation</b>	<b>vdW_atr</b>	<b>vdW_rep</b>	<b>Solv</b>	<b>Intra</b>	<b>ACE</b>	<b>Total</b>	<b><math>\Delta\Delta G</math></b>
D26M	0.20	0.00	-0.03	0.04	-0.70	-0.49	0.19
D26V	0.61	0.01	-0.22	0.00	-0.51	-0.11	1.45
D26W	-1.44	0.22	0.40	0.28	-0.50	-1.05	-1.08
R27F	-0.38	0.02	-0.14	-0.05	-0.72	-1.28	-0.22
G28A	-0.37	0.01	0.02	0.00	-0.12	-0.46	0.58
G28I	-1.87	0.59	0.17	1.06	-0.83	-0.89	-0.27
G28L	-2.00	2.47	0.12	0.05	-1.07	-0.43	-0.46
G28M	-1.85	0.17	0.65	-0.01	-0.84	-1.88	-0.51
G28R	-2.43	0.72	2.38	0.45	0.53	1.65	2.43
G28T	-0.86	0.06	0.05	0.00	-0.22	-0.97	-0.76
G28V	-1.16	0.41	0.10	1.72	-0.55	0.52	0.56
S29A	0.00	0.00	0.00	0.00	0.00	0.00	0.33
Q30N	1.16	0.00	-0.72	0.00	-0.34	0.10	0.73
Q30E	-0.36	0.01	-0.32	-0.01	0.26	-0.42	0.43
S51M	-0.74	0.01	0.13	0.00	-0.31	-0.90	-0.37
K68H	0.10	0.00	-0.48	-0.01	-0.43	-0.83	1.09
S100A	0.33	-0.01	-0.32	0.00	-0.20	-0.19	-0.01
S100N	-0.82	0.00	1.08	0.04	0.29	0.58	1.92
S100T	-0.03	0.00	-0.16	0.00	-0.27	-0.46	-0.49
S100Y	-1.52	1.43	0.85	0.17	-0.68	0.26	2.29
I54R	-0.73	0.00	0.76	0.00	0.50	0.54	1.28
A99M	-0.44	0.00	-0.19	0.09	-0.19	-0.72	-0.31
A99K	-0.24	0.00	0.03	0.00	0.06	-0.14	0.10
G100S	-0.18	0.00	0.00	0.00	-0.07	-0.25	-0.32
G101A	-0.75	0.09	0.09	0.00	-0.42	-1.00	-1.09
R102Q	0.45	-0.02	-0.32	0.00	-0.13	-0.03	0.45