Supporting Information for Enthalpic Breakdown of Water Structure on Protein Active-Site Surfaces

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Table S1: Standard deviations of the average quantities shown in Table 2 in main text for different hydration site categories.

	Number	E_{sw}	E_{ww}	E_{tot}	$\bar{E}_{ww}^{nbr}$	N^{nbr}	f_{enc}	N_{sw}^{HB}	N_{ww}^{HB}	f_{ww}^{HB}	$N_{ww,lost}^{HB}$
A.En.F	32	1.03	1.00	0.47	0.18	0.45	0.07	0.01	0.23	5.27	0.28
A.En.U	17	0.84	1.00	0.32	0.22	0.53	0.10	0.02	0.28	6.56	0.34
A.Fr.F	2	0.84	1.13	0.29	0.03	0.07	0.01	0.07	0.20	3.31	0.02
A.Fr.U	5	0.87	1.37	0.51	0.04	0.80	0.12	0.04	0.43	2.36	0.53
P.En.F	45	1.55	1.24	0.61	0.18	0.77	0.14	0.49	0.45	6.88	0.27
P.En.U	30	1.12	1.24	0.54	0.30	0.85	0.16	0.44	0.49	9.13	0.45
P.Fr.F	17	2.70	2.27	0.63	0.20	0.53	0.09	0.42	0.42	5.97	0.27
P.Fr.U	11	1.59	1.63	0.35	0.11	0.86	0.15	0.28	0.48	5.33	0.49
C.En.F	18	2.38	1.80	0.89	0.22	0.77	0.15	0.57	0.57	7.03	0.35
C.En.F	42	2.52	2.17	0.74	0.36	1.08	0.19	0.56	0.64	12.54	0.42
Displaced sites	104	2.60	2.12	1.00	0.39	0.79	0.14	0.67	0.58	11.50	0.09
Undisplaced sites	114	2.73	2.29	0.76	0.38	1.02	0.18	0.65	0.70	11.16	0.12

Figure S1: Normalized probability distribution plots of the interaction energy of water molecules with their first shell neighbors, corresponding to the number density distribution plots shown in the main text (shown in Figure 3, 5, 6 and 7). The normalized distribution plots differ from the number density distribution plots in that integrating over the former gives unity whereas integrating over the later gives the average number of neighbors in the first shell.