Supporting Information

Table S1: Partial atomic charges of Asp

	Asp		
atom	protonated Amber99sb	protonated, OD2 tautomer, three states model	deprotonated, three states model/ Amber99sb
N	-0.41570	-0.5163	-0.5163
H	0.27190	0.2936	0.2936
CA	0.03410	0.0381	0.0381
HA	0.08640	0.088	0.088
C	0.59730	0.5366	0.5366
O	-0.56790	-0.5819	-0.5819
CB	-0.03160	-0.0105	-0.0303
HB1	0.04880	0.0699	-0.0122
HB2	0.04880	0.0699	-0.0122
CG	0.64620	0.6676	0.7994
OD1	-0.55540	-0.5343	-0.8014
HD1	-	0.0	0.0/-
OD2	-0.63760	-0.6165	-0.8014
HD2	0.47470	0.4958	0.0/-

Table S2: Partial atomic charges of Glu

	Glu		
atom	protonated Amber99sb	protonated, OE2 tautomer, three states model	deprotonated, three states model/ Amber99sb
N	-0.41570	-0.5163	-0.5163
H	0.27190	0.2936	0.2936
CA	0.01450	0.0397	0.0397
HA	0.07790	0.1105	0.1105
C	0.59730	0.5366	0.5366
O	-0.56790	-0.5819	-0.5819
CB	-0.00710	0.00248	0.056
HB1	0.02560	0.03518	-0.0173
HB2	0.02560	0.03518	-0.0173
CG	-0.01740	-0.00782	0.0136
HG1	0.04300	0.05258	-0.0425
HG2	0.04300	0.05258	-0.0425
CD	0.68010	0.68968	0.8054
OE1	-0.58380	-0.57422	-0.8188
HE1	-	0.0	0.0/-
OE2	-0.65110	-0.64152	-0.8188
HE2	0.46410	0.47368	0.0/-

Table S3: Partial atomic charges of His

	His NE2 tautomer		
atom	protonated, three states model/ Amber99sb	deprotonated NE2 tautomer Amber99sb	deprotonated NE2 tautomer three states model
N	-0.3479	-0.41570	-0.3479
H	0.2747	0.27190	0.2747
CA	-0.1354	-0.05810	-0.1354
HA	0.1212	0.13600	0.1212
C	0.7341	0.59730	0.7341
O	-0.5894	-0.56790	-0.5894
CB	-0.0414	-0.00740	-0.0159
HB1	0.081	0.03670	0.0282
HB2	0.081	0.03670	0.0282
CG	-0.0012	0.18680	0.1783
ND1	-0.1513	-0.54320	-0.5520
HD1	0.3866	-	0.0
CE1	-0.017	0.16350	0.1550
HE1	0.2681	0.14350	0.1350
NE2	-0.1718	-0.27950	-0.2880
HE2	0.3911	0.33390	0.3254
CD2	-0.1141	-0.22070	-0.2292
HD2	0.2317	0.18620	0.1777

Table S4: Partial atomic charges of His

	His ND1 tautomer		
atom	protonated, three states model/ Amber99sb	deprotonated ND1 tautomer Amber99sb	deprotonated ND1 tautomer three states model
N	-0.3479	-0.41570	-0.3479
H	0.2747	0.27190	0.2747
CA	-0.1354	0.01880	-0.1354
HA	0.1212	0.08810	0.1212
C	0.7341	0.59730	0.7341
O	-0.5894	-0.56790	-0.5894
CB	-0.0414	-0.04620	-0.0521
HB1	0.081	0.04020	0.0343
HB2	0.081	0.04020	0.0343
CG	-0.0012	-0.02660	-0.0325
ND1	-0.1513	-0.38110	-0.3870
HD1	0.3866	0.36490	0.3591
CE1	-0.017	0.20570	0.1998
HE1	0.2681	0.13920	0.1333
NE2	-0.1718	-0.57270	-0.5786
HE2	0.3911	-	0.0
CD2	-0.1141	0.12920	0.1233
HD2	0.2317	0.11470	0.1088