Supplementary Material

ASP1			ASP2		
atom name	atom type	charge	atom name	atom type	charge
CB	CT2	-0.18	CB	CT2	-0.18
HB1	HA	0.09	HB1	HA	0.09
HB2	HA	0.09	HB2	HA	0.09
CG	CD	0.61	CG	CD	0.51
OD1	OB	-0.51	OD1	OB	-0.51
P	P	1.50	P	P	1.10
OD2	ON2	-0.62	OD2	ON2	-0.40
H2	HN4	0.34			
OP1	ON3	-0.82	OP1	ON3	-0.90
OP2	ON4	-0.68	OP2	ON3	-0.90
OP3	ON3	-0.82	OP3	ON3	-0.90
bond terms	k_b	b_0			
ON2 CD	230.000	1.4000			
angle terms	k_θ	θ_0	k_{UB}	S_0	
CD ON2 P	20.0	120.0	35.	2.33	
ON2 CD CT2	55.000	110.5000			
ON2 CD CT3	55.000	110.5000			
ON2 CD OB	50.000	123.00	210.00	2.26200	
dihedral terms	k_χ	n	δ		
X CD ON2 X	10.0	1	180.0		
X CD ON2 X	2.25	2	180.00		
X CD ON2 X	1.36	3	180.00		
CD ON2 P ON3	0.1	3	0.00		

Table 1: Parameters for ASP1 and ASP2 compatible with the combined protein and nucleic acid CHARMM27 parameter and topology files.

atom	chrg	epsi	sigm	radi
ASP2				
CB	-0.10	0.118	3.905	1.952
HB1	0.05	0.000	0.000	1.200
HB2	0.05	0.000	0.000	1.200
CG	0.70	0.105	3.750	1.875
OD1	-0.55	0.210	2.960	1.480
P	1.10	0.200	3.74	1.870
OD2	-0.55	0.210	2.960	1.480
OP1	-0.9	0.210	2.96	1.480
OP2	-0.9	0.210	2.96	1.480
OP3	-0.9	0.210	2.96	1.480
N	-0.40	0.170	3.250	1.625
HN	0.25	0.000	0.000	1.200
CA	0.05	0.080	3.800	1.900
HA	0.05	0.000	0.000	1.200
C	0.60	0.105	3.750	1.875
O	-0.55	0.210	2.960	1.480
ASP1				
CB	-0.10	0.118	3.905	1.952
HB1	0.05	0.000	0.000	1.200
HB2	0.05	0.000	0.000	1.200
CG	0.70	0.105	3.750	1.875
OD1	-0.55	0.210	2.960	1.480
P	1.50	0.200	3.74	1.870
OD2	-0.63	0.210	2.960	1.480
H2	0.33	0.000	0.000	1.200
OP1	-0.83	0.210	2.96	1.480
OP2	-0.69	0.210	2.96	1.480
OP3	-0.83	0.210	2.96	1.480
N	-0.40	0.170	3.250	1.625
HN	0.25	0.000	0.000	1.200
CA	0.05	0.080	3.800	1.900
HA	0.05	0.000	0.000	1.200
C	0.60	0.105	3.750	1.875
O	-0.55	0.210	2.960	1.480

Table 2: Parameters for ASP1 and ASP2 used in file pkaS.dat for Poisson-Boltzmann calculations.