

**Table 2. Scale factors  $s$  for the charges of ionic groups in the reservoir region for the unstacking step**

residue	$s$	residue	$s$
Glu6	0.0508	Lys8	0.0135
Arg9	0.1053	Asp13	0.0176
Lys18	0.0202	Glu21	0.0688
Glu25	0.0129	Lys36	0.0165
Asp42	0.0124	Glu45	0.0117
Glu57	0.0136	Glu74	0.0182
Glu77	0.1664	Glu78	0.0127
Arg175	0.0637	Cyt2	0.0601
Cyt3	0.0505	Ade4	0.1337
Thy12	0.0502	Ade13	0.0178
Ade15	0.0862	Cyt16	0.0939
Thy17	0.1098	Ade18	0.0938
Gua19	0.1453	Cyt26	0.0639
Sod1	0.0175	Sod2	0.0126
Sod3	0.0554	Sod10	0.0274
Sod11	0.0172	Sod12	0.0125
Sod14	0.0876	Sod16	0.0127
Sod17	0.0299	Sod18	0.0125
Sod24	0.1079		

Each scale factor is the ratio of the potential at the origin from a specific residue in vacuum ( $\epsilon = 1$ ) and that in aqueous solution ( $\epsilon = 1$  for the protein and  $\epsilon = 80$  for the solution). The origin was taken to be the  $C_\alpha$  atom of Gly131.