

**Table 3. Scale factors  $s$  for the charges of ionic groups in the reservoir region for the active-site step**

residue	$s$	residue	$s$
Glu6	0.0372	Lys8	0.0126
Arg9	0.1049	Asp13	0.0357
Lys18	0.0535	Glu21	0.0959
Glu25	0.0117	Lys36	0.0649
Asp42	0.0153	Glu45	0.0132
Glu57	0.0124	Glu74	0.0251
Glu77	0.0679	Glu78	0.0123
Glu92	0.0517	Arg96	0.0538
Lys101	0.0581	Lys104	0.0243
Lys107	0.0466	Lys125	0.0623
Cyt2	0.0143	Cyt3	0.0209
Ade4	0.0893	Gua11	0.1260
Thy12	0.0404	Ade13	0.0233
Ade18	0.1255	Gua19	0.0765
Cyt20	0.0817	Cyt26	0.0523
Sod1	0.0128	Sod2	0.0127
Sod3	0.0313	Sod10	0.0262
Sod11	0.0127	Sod12	0.0125
Sod16	0.0511	Sod17	0.0155
Sod18	0.0138	Sod19	0.0176
Sod20	0.0213	Sod21	0.1335
Sod22	0.1190	Sod24	0.0130

The origin was taken to be the midpoint between the amide hydrogen atom and  $C_{\beta}$  of Asn157.