

Table 7. Mean numbers of hydrogen bonds formed by the MgADP at binding site 2 with individual SUR1 residues in the four different simulations

	wt ADP+ Pi	R1380L ADP+ Pi	wt ADP no Pi	R1380L no Pi
H816	0.21	0.10		
Q819		0.16		
E824		0.21	0.05	
N828		0.10	0.47	0.60
L829		0.16		
S830		0.31	1.02	0.92
G831	0.55	0.76	0.05	0.04
G832	0.65	0.03		
Q833			1.06	2.14
R834	0.47	0.49		
S1357	0.23			
T1381	0.88	1.00		
G1382	1.35	0.45		
S1383	0.57			0.24
G1384	0.18	0.91		
K1385	0.33	0.09	0.81	0.89
S1386	0.74		0.86	0.90
S1387			1.11	1.00
H1538			0.05	0.35
TOTAL	6.16	4.77	5.48	7.08