



Residue	$\Delta H \text{ (kJ.mol}^{-1}\text{)}$		
	Coul	LJ	Total
K64	-38.4	-3.3	-41.7
W65	-28.0	-38.4	-66.4
N67	-19.1	-6.6	-25.7
R69	-6.1	-4.6	-10.7
N70	-6.9	-18.0	-24.8
Y72	-6.4	-33.4	-39.8
F74	-3.3	-31.8	-35.1
D83	-22.6	-3.1	-25.6
F85	-3.0	-35.9	-38.9
H87	-12.0	-23.8	-35.8
Q88	-4.8	-2.2	-7.0
E117	0.9	-4.0	-3.0
K118	-62.0	-26.1	-88.1
G119	-7.6	-5.8	-13.4
A120	-1.6	-4.9	-6.4
E121	-35.8	-4.5	-40.3
Total	-256.9	-251.7	-508.6

