

Mutation	ΔG , kJ/mol	err, kJ/mol
A2C	16.09	0.16
A2F	31.48	0.27
A2H	-59.28	0.33
A2M	5.73	0.37
A2Q	-289.57	0.46
A2S	-39.55	0.19
A2T	-121.14	0.31
A2W	49.63	0.67
A2Y	-52.09	0.41
D2E	26.99	0.76
F2L	-103.00	0.31
H2N	-296.90	0.41
H2Q	-229.92	0.53
H2S	19.34	0.51
I2A	-12.08	0.22
I2L	-85.44	0.37
I2T	-130.17	0.35
I2V	-84.51	0.16
K2R	-662.70	0.29
L2A	70.54	0.29
L2Q	-217.63	0.29
L2T	-50.81	0.49
L2V	-1.23	0.21
N2A	356.23	0.25
Q2I	301.58	0.40
Q2S	248.85	0.34
T2N	-241.13	0.32
T2Q	-166.23	0.39
T2S	80.64	0.30
T2V	45.17	0.24
V2A	71.84	0.21
Y2F	84.53	0.12
Y2S	11.18	0.55

Table 1: GXG tripeptide ΔG values in the Amber99sb force field (TIP3P water)