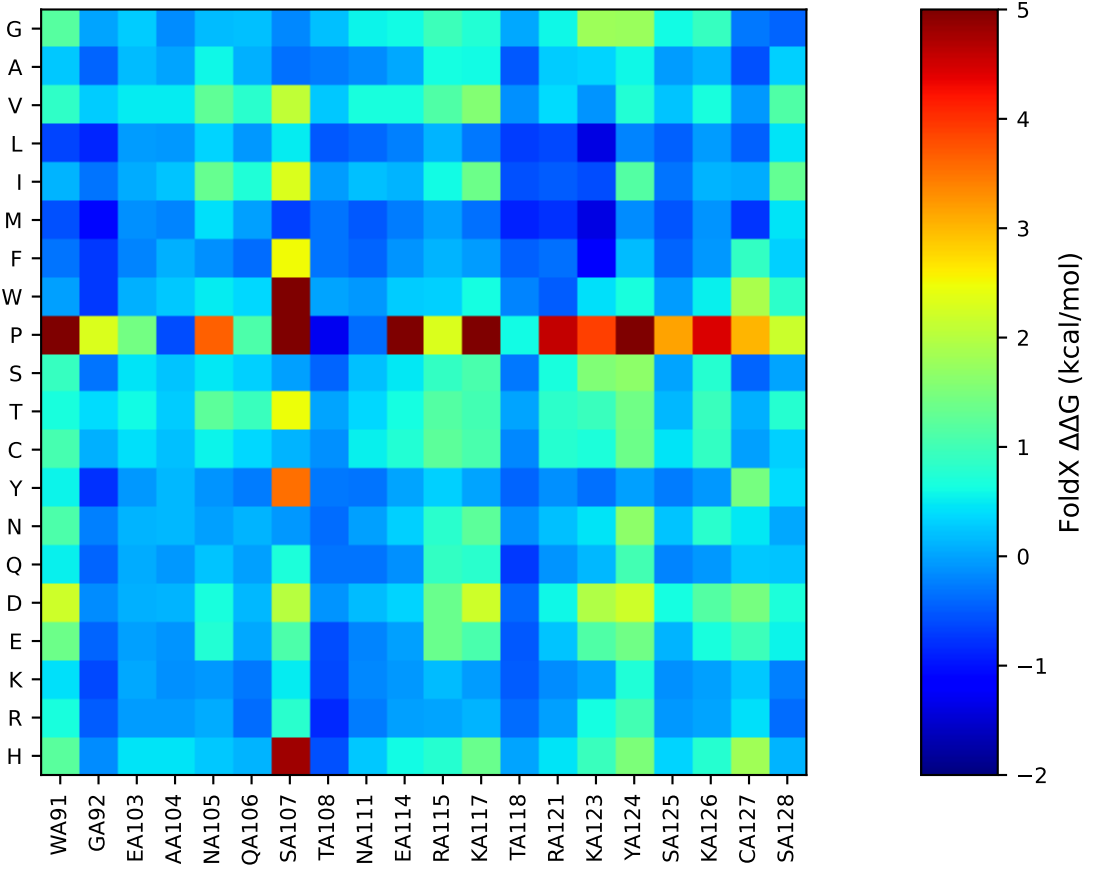
G
A
V
L
I
M
F
W
P
S
T
C
Y
N
Q
D
E
K
R
H
WA91
GA92
EA103
AA104
NA105
QA106
SA107
TA108
NA111
EA114
RA115
KA117
TA118
RA121
KA123
YA124
SA125
KA126
CA127
SA128
5
4
3
2
1
0
−1
−2
FoldX ΔΔG (kcal/mol)