

H.sapiens 99 K D V Y I V Q D L M E T D L Y K L L K T Q H L S N D H I C Y F L Y Q I L R G L K Y I H S A N V L H 147
R.norvegicus 97 K D V Y I V Q D L M E T D L Y K L L K T Q H L S N D H I C Y F L Y Q I L R G L K Y I H S A N V L H 145

MAPK1 wild-type in complex with pepHePTP

receptor's backbone RMSD

RMSD [Å]

Time [ns]

Rep1 Rep2 Rep3 Rep4 Rep5

MAPK1^{Y126C} in complex with pepHePTP

receptor's backbone RMSD

RMSD [Å]

Time [ns]

Rep1 Rep2 Rep3 Rep4 Rep5

MAPK1 wild-type in complex with pepHePTP

peptide RMSD

RMSD [Å]

Time [ns]

Rep1 Rep2 Rep3 Rep4 Rep5

MAPK1^{Y126C} in complex with pepHePTP

peptide RMSD

RMSD [Å]

Time [ns]

Rep1 Rep2 Rep3 Rep4 Rep5

MAPK1 wild-type in complex with pepHePTP

whole complex RMSF

RMSF [Å]

Rep1 Rep2 Rep3 Rep4 Rep5

Residue

MAPK1^{Y126C} in complex with pepHePTP
whole complex RMSF

RMSF [Å]

Rep1 Rep2 Rep3 Rep4 Rep5

Residue

A bar chart comparing the difference in free energy of binding (ΔG) between wild-type and Y126C variant proteins. The y-axis is labeled "kcal/mol" and ranges from -80 to 0. The x-axis shows two conditions: "wild-type" and "Y126C variant". The wild-type bar is green with a brick pattern, and the Y126C variant bar is grey with a checkerboard pattern. Both bars include error bars. A horizontal line at 0 kcal/mol serves as a reference. A bracket above the bars, marked with four asterisks (****), indicates a statistically significant difference between the two groups.

Condition	ΔG (kcal/mol)
wild-type	-51 ± 17
Y126C variant	-45 ± 19

Figure 10: Free energy of binding (ΔG) of the residues in the wild-type and Y126C variant proteins. The y-axis represents ΔG in kcal/mol, ranging from -4 to 2. The x-axis lists the residues. For each residue, two bars are shown: a green bar for the wild-type and a grey bar for the Y126C variant. Error bars represent standard deviation. A horizontal dotted line is at 0 kcal/mol.

Residue	Wild-type ΔG (kcal/mol)	Y126C variant ΔG (kcal/mol)
Glu 79	-0.4	-0.2
Leu 113	-1.1	-1.0
His 123	-0.8	-0.7
Tyr/Cys 126	-2.1	-0.4
Tyr 129	-0.2	-0.4
Leu 155	-0.4	-0.4
Thr 157	-1.9	-2.0
Thr 158	-2.1	-2.1
Cys 159	-2.1	-1.9
Asp 160	0.4	0.2
Gln 313	-0.4	-1.2
Tyr 314	-1.9	-2.5
Asp 316	-0.4	-0.6
Asp 319	-1.6	-0.3