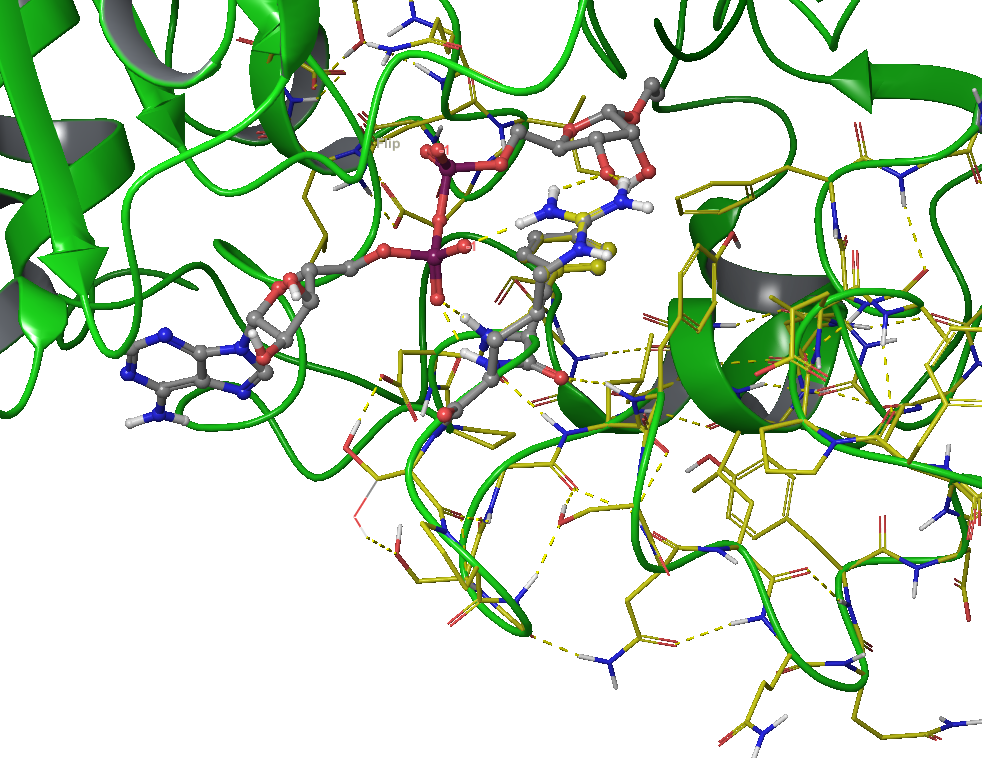
Sidechain prediction & validation using short chains lead to some interesting results:

Associated RMSD and energy information can be found in file 4BVG-sp-set2\_DATA.xlsx

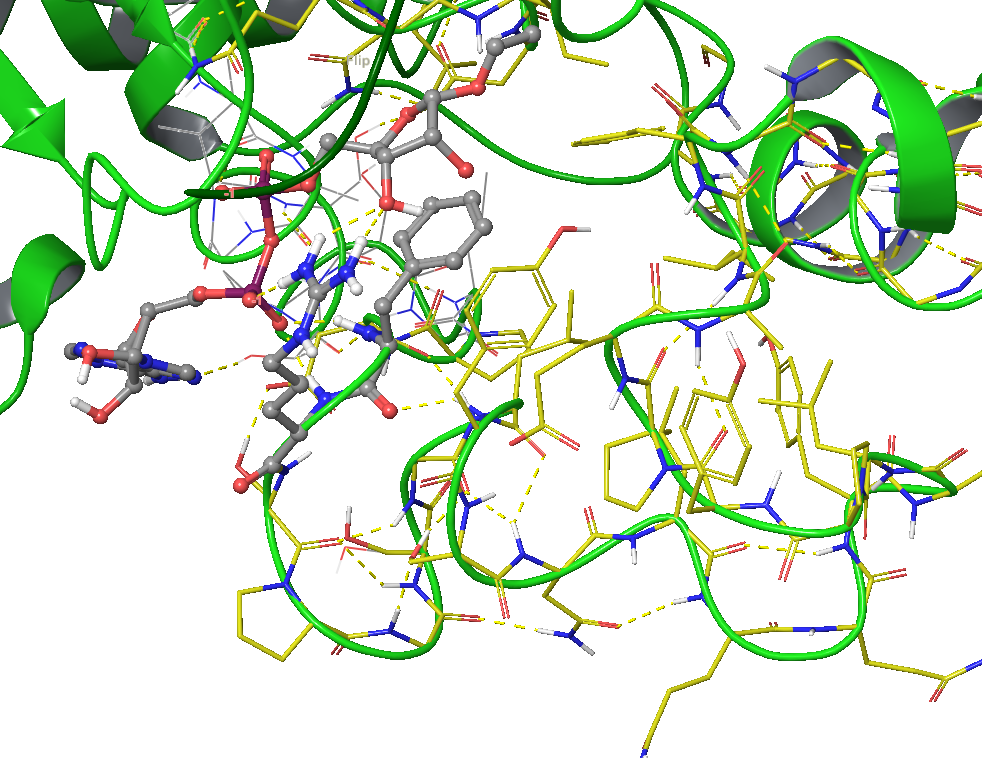
1. In three-residue sidechain prediction, predicted sidechain of SER159 lead to higher energy



SER159

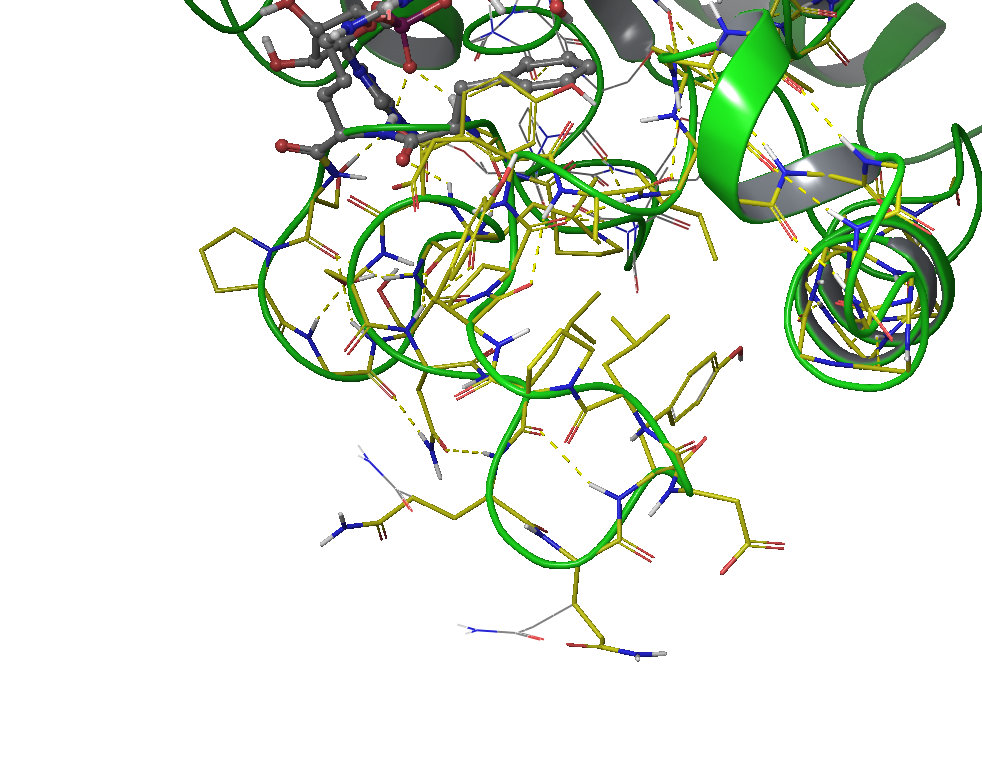
The predicted SER159 prefer forming hydrogen bond with SER162 instead of ASP156 in native structure (native in yellow and stick).

1. In three-residue sidechain prediction, predicted sidechain of SER162 raise the energy slightly



SER162

1. In three-residue sidechain prediction, predicted sidechain of GLN169 and GLN170 lead to lower energy, but no significant change in term of hydrogen bonding. Predicted sidechain of TYR171 doesn’t change, the reported large RMSD is a result of ring-flipping.



TYR171

GLN170

GLN169

1. Using Monte Carlo method in 3-residue sidechain prediction usually lead to slightly lower energies.
2. Five-residue sidechain prediction for residues near SER159, GLN169, GLN170 is consistent with the 3-residue sidechain prediction.
3. Five-residue sidechain prediction for residue 168-172 lead to significant change in loop structure and significant lower energy.

