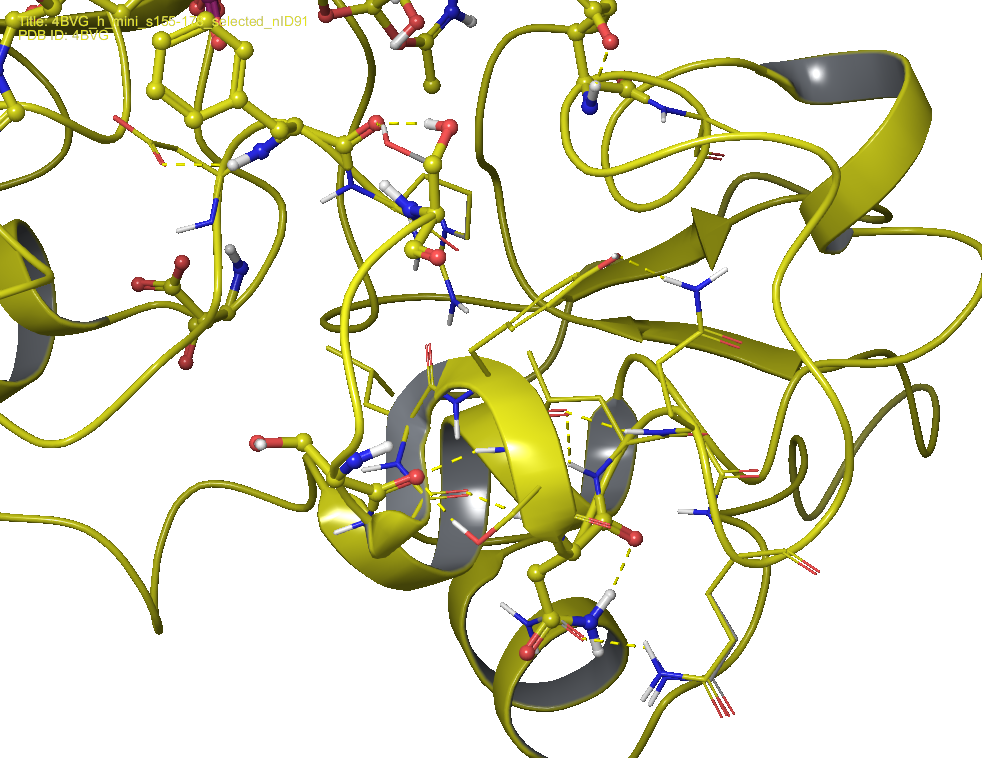
Sidechain prediction for 4BVG with sidechain replacement on residue 155-178 from 4FVT

From the previous calculations on 4BVG, we found that sidechain predictions on structures without heavy atom relaxation from crystal structure leads to energy contributions from not just the sidechain conformational change, therefore we start out with the structure with prime minimization run on selected residues that will be further investigated by sidechain prediction.

Single sidechain prediction suggested little or no changes on the most of its sidechains upon prediction, and for some predicted sidechains that are different than the original; predictions on SER159 and ASN167 lead to lower energy, but predictions on SER162, GLU177 and ASP231 end up in slightly higher energy. (More details can be found in 4BVG-s155-178-sp-set1\_DATA.xlsx.)

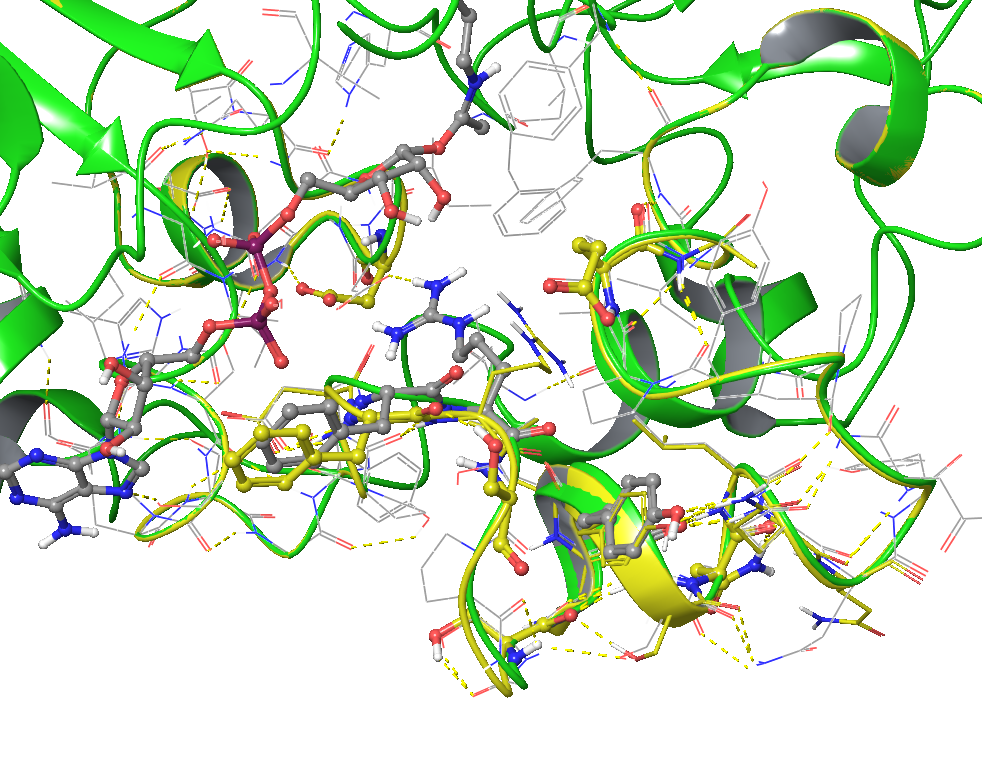


ASN167

SER159

Further sidechain prediction shows that the modification of sidechains of SER159 and ASN167 provides the lower energy but do not have any significantly change in the number of hydrogen bonding, but small adjustment instead. The figure above shows the sidechain prediction on the five residues mentioned above, and only SER159 and ASN167 are found changed (xtal structure in yellow, predicted in grey). The sidechain prediction using sidechain of larger set (155-180,227-234) actually lead to not-so-perfect results as it fails to locate lower energy configuration.

Sidechain prediction using Monte Carlo method (MC) on residue set 155-180, 227-234 lead to significantly lower energy, and two significant changes were identified between ARG158-ASP231, ASN167-GLN170, where we see strengthening of hydrogen bond or increase in the number of hydrogen bonds.



ASN167-GLN170 pair

ARG158-ASP231 pair

The above sidechain predictions do not involve significant backbone changes.

When sidechain prediction using a larger selection of residues (res 144-180, 195, 199, 204, 207, 210, 227-234, 248, 251, 291, 294, 324), some noticeable change is observed in the backbone, leading to significant re-positioning of some residues such as PHE157, and shifting on some residues. (see the figure below)

