Single sidechain prediction results on 4BVG:

Starting from 4BVG prepared w/ Protein preparation wizard 7 h-opt w/o relaxation on heavy atoms, which has a prime energy of -9614.9 kcal/mol.

|  |  |  |
| --- | --- | --- |
| **Residues** | **Prime Energy** | **Energy Gap** |
| 155 PRO | -9628.0 | -13.1 |
| 156 ASP | -9618.5 | -3.6 |
| 157 PHE | -9616.2 | -1.3 |
| 158 ARG | -9616.8 | -1.9 |
| 159 SER | -9613.2 | 1.7 |
| 160 PRO | -9615.5 | -0.6 |
| 161 GLY |  |  |
| 162 SER | -9617.1 | -2.2 |
| 163 GLY |  |  |
| 164 LEU | -9656.4 | -41.5 |
| 165 TYR | -9619.1 | -4.2 |
| 166 SER | -9617.6 | -2.7 |
| 167 ASN | -9615.2 | -0.3 |
| 168 LEU | -9707.2 | -92.3 |
| 169 GLN | -9619.4 | -4.5 |
| 170 GLN | -9624.9 | -10.0 |
| 171 TYR | -9644.4 | -29.5 |
| 172 ASP | -9622.6 | -7.7 |
| 173 LEU | -9621.0 | -6.1 |
| 174 PRO | -9626.9 | -12.0 |
| 175 TYR | -9617.9 | -3.0 |
| 176 PRO | -9616.1 | -1.2 |
| 177 GLU | -9622.2 | -7.3 |
| 178 ALA |  |  |
| 179 ILE | -9618.3 | -3.4 |
| 195 LEU | -9616.8 | -1.9 |
| 204 TYR | -9618.8 | -3.9 |
| 229 ASN | -9636.4 | -21.5 |
| 233 LEU | -9615.8 | -0.9 |
| 248 HIS | -9618.7 | -3.8 |

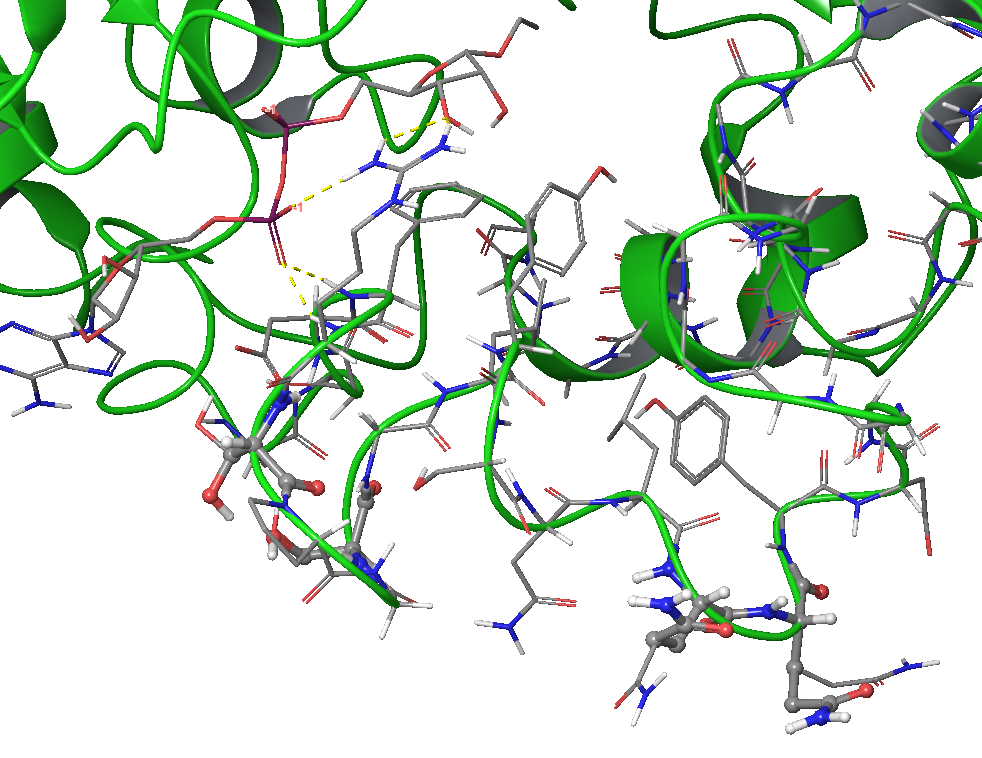
The above starting structure was minimized by Prime on the selected residues, then serves as starting point for single sidechain prediction:

The starting structure has a prime energy of -10301.2 kcal/mol.

|  |  |  |
| --- | --- | --- |
| **Residues** | **Prime Energy** | **Energy Gap** |
| 155 PRO | -10301.2 | 0.0 |
| 156 ASP | -10301.2 | 0.0 |
| 157 PHE | -10301.2 | 0.0 |
| 158 ARG | -10301.2 | 0.0 |
| 159 SER | -10298.5 | 2.7 |
| 160 PRO | -10301.2 | 0.0 |
| 161 GLY |  |  |
| 162 SER | -10300.7 | 0.5 |
| 163 GLY |  |  |
| 164 LEU | -10301.2 | 0.0 |
| 165 TYR | -10301.2 | 0.0 |
| 166 SER | -10301.2 | 0.0 |
| 167 ASN | -10301.2 | 0.0 |
| 168 LEU | -10301.2 | 0.0 |
| 169 GLN | -10304.0 | -2.8 |
| 170 GLN | -10303.8 | -2.6 |
| 171 TYR | -10301.1 | 0.1 |
| 172 ASP | -10301.3 | -0.1 |
| 173 LEU | -10301.2 | 0.0 |
| 174 PRO | -10301.2 | 0.0 |
| 175 TYR | -10301.2 | 0.0 |
| 176 PRO | -10301.2 | 0.0 |
| 177 GLU | -10301.1 | 0.1 |
| 178 ALA |  |  |
| 179 ILE | -10301.2 | 0.0 |
| 195 LEU | -10301.1 | 0.1 |
| 204 TYR | -10301.2 | 0.0 |
| 229 ASN | -10301.2 | 0.0 |
| 233 LEU | -10301.2 | 0.0 |
| 248 HIS | -10301.2 | 0.0 |

The sidechain predictions that lead to rise or decrease of prime energy do not find any residues in direct contact with C pocket (potential NAM).

RMSD data for the each selected residues can be found in the Dropbox\PMC-AT PLIN\4BVG-ssp-DATA.xlsx .



GLN170

GLN169

SER162

SER159

Does it mean there is sampling error in sidechain prediction? The +/- 0.1 kcal/mol that we saw in the table where little/no structural change was observed is the energy error that you have mentioned?