|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | sB-WT  | sB-D30N | sB-D30V | sB-V32E | sB-WT-V32E | sC-WT | sC-D30V | sC-V32E |
| Structure Type | crystala | model | model | model | model | model | model | model |
| Ramachandranb | 95.6 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| DOPEc | - | -22662 | -23193 | -21813 | -21745 | -21841 | -21338 | -20957 |
| BEd | -17 | -14.1 | -13.6 | -14.2 | -15.9 | -14.2 | -14.8 | -10.9 |

aCrystal structure of a subtype B protease obtained from the PDB, under the access code 1OHR.

bPercentage (%) of residues in most favoured regions of the Ramachandran Plot.

cModeller DOPE score.

dValue of Binding Energy (BE) for the best docking conformation with Nelfinavir.