|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Compound | Energy | V-S-ASP-452 | V-S-TYR-455 | V-S-ARG-553 | V-S-ASP-623 | V-S-ARG-624 | V-S-ASP-760 |  |  |  |  |  |  |  |  |  |  |
| 6nur-GissitorviffirnaTM2.....-0.pdb | -75.3 | -552.846 | -148.044 | -954.718 | -112.557 | -682.854 | -826.477 |  |  |  |  |  |  |  |  |  |  |
| Compound | Energy | V-M-ASN-330 | V-M-ALA-331 | V-M-THR-332 | V-S-THR-332 | V-S-LYS-333 | V-S-TRP-423 | V-S-ILE-428 | V-S-ARG-495 | V-M-LYS-333 | V-S-LYS-333 | V-M-ILE-428 | V-M-ASP-429 | V-S-ASN-435 | V-M-ASN-437 | V-S-ASN-437 | V-S-TYR-438 |
| 2ghv-GissitorviffirnaTM2.....-0.pdb | -93.8 | -719.179 | -635.389 | -990.665 | -645.926 | -689.001 | -545.936 | -505.747 | -880.065 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 2ghv-GissitorviffirnaTM1....-0.pdb | -83.6 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -401.959 | -116.821 | -550.052 | -621.887 | -600.567 | -452.625 | -11.821 | -148.798 |
| Compound | Energy | V-M-TYR-3 | V-S-TYR-3 | V-M-HIS-4 | V-S-TYR-5 | V-M-ASN-28 | V-S-ASN-28 | V-S-THR-44 | V-M-SER-45 | V-M-THR-46 | V-S-THR-46 | V-S-HIS-47 | V-S-THR-59 | V-S-GLN-61 |  |  |  |
| 1xak-GissitorviffirnaTM1....-0.pdb | -74.9 | 0 | 0 | 0 | 0 | -489.748 | -925.783 | -445.556 | -124.852 | -100.815 | -870.546 | -796.912 | 0 | -226.724 |  |  |  |
| 1xak-GissitorviffirnaTM2.....-0.pdb | -71.2 | -850.976 | -194.761 | -584.652 | -445.764 | 0 | 0 | 0 | 0 | 0 | 0 | -835.425 | -846.354 | -82.281 |  |  |  |