| #Ligand | TotalEnergy | VDW | |
|---|---|---|---|
| 6m2q-Roccustyrna_fr1-0.pdb | | -896.465 | -896.465 |
| 6m2q-Roccustyrna_fr2-0.pdb | | -798.627 | -798.627 |
| 6m2q-Roccustyrna_fr3-0.pdb | | 168.424 | 168.424 |
| 6m2q-Roccustyrna_fr4-0.pdb | | -785.438 | -785.438 |
| 6m2q-Roccustyrna_fr5-0.pdb | | 348.743 | 348.743 |
| 6m2q-Roccustyrna_fr6-0.pdb | | -904.774 | -904.774 |
| 6m2q-Roccustyrna_fr7-0.pdb | | -846.778 | -846.778 |
| 6m2q-Zanamivir_CID_60855-0.pdb | | -613.535 | -613.535 |
| 6m2q-Vidarabine_CID_21704-0.pdb | | -661.163 | -661.163 |
| 6m2q-Valganciclovir_CID_135413535-0.pdb | | 198.156 | 198.156 |
| 6m2q-Tenofovir_CID_464205-0.pdb | | -638.549 | -638.549 |
| 6m2q-Taribavirin_CID_451448-0.pdb | | -606.346 | -606.346 |
| 6m2q-Sorivudine_CID_5282192-0.pdb | | 820.449 | 820.449 |
| 6m2q-Sofosbuvir_CID_45375808-0.pdb | | 296.684 | 296.684 |
| 6m2q-Ritonavir_CID_392622-0.pdb | | 155.543 | 155.543 |
| 6m2q-Penciclovir_CID_135398748-0.pdb | | -69.663 | -69.663 |
| 6m2q-Nelfinavir_CID_64143-0.pdb | | 487.507 | 487.507 |
| 6m2q-Merimepodib_CID_153241-0.pdb | | -821.219 | -821.219 |
| 6m2q-Maribavir_CID_471161-0.pdb | | -720.599 | -720.599 |
| 6m2q-Lopinavir_CID_92727-0.pdb | | 353.779 | 353.779 |
| 6m2q-Indinavir_CID_5362440-0.pdb | | -920.937 | -920.937 |
| 6m2q-Inarigivir_CID_6912016-0.pdb | | -904.684 | -904.684 |
| 6m2q-Galidesivir_CID_10445549-0.pdb | | -700.417 | -700.417 |
| 6m2q-Famciclovir_CID_3324-0.pdb | | 484.732 | 484.732 |
| 6m2q-Faldaprevir_CID_42601552-0.pdb | | 196.047 | 196.047 |
| 6m2q-Darunavir_CID_213039-0.pdb | | -811.094 | -811.094 |
| 6m2q-Cytarabine_CID_6253-0.pdb | | -590.168 | -590.168 |
| 6m2q-Boceprevir_CID_10324367-0.pdb | | 242.807 | 242.807 |
| 6m2q-Atazanavir_CID_148192-0.pdb | 290.66 | 290.66 | |
| 6m2q-Asunaprevir_CID_16076883-0.pdb | | -797.693 | -797.693 |
| 6m2q-Amprenavir_CID_65016-0.pdb | | -813.987 | -813.987 |
| 6m2q-GissitorviffirnaTM1-0.pdb | | -70.081 | -70.081 |
| 6m2q-GissitorviffirnaTM4-0.pdb | -69.95 | -69.95 | |
| 6m2q-GissitorviffirnaTM6-0.pdb | | 166.473 | 166.473 |
| 6m2q-GissitorviffirnaTM7-0.pdb | | -790.107 | -790.107 |
| 6m2q-GissitorviffirnaTM8-0.pdb | | -731.542 | -731.542 |
| 6m2q-GissitorviffirnaTM9-0.pdb | | -842.045 | -842.045 |
| 6m2q-Roccustyrna_gs1-0.pdb | | 261.182 | 261.182 |
| 6m2q-Roccustyrna_gs2-0.pdb | | -690.297 | -690.297 |
| 6m2q-Roccustyrna_gs3-0.pdb | | 204.639 | 204.639 |
| 6m2q-Roccustyrna_gs4-0.pdb | | -334.177 | -334.177 |
| 6m2q-Roccustyrna_gs5-0.pdb | | 100.983 | 100.983 |
| 6m2q-Roccustyrna_gs6-0.pdb | | -635.585 | -635.585 |
| 6m2q-Roccustyrna_gs8-0.pdb | | 306.373 | 306.373 |

AverConPair
10.058
165.152
134.359
151.111
794.118
173.421
210.286
166.522
230.526
22.84
215.789
222.353
18.05
188.056
8.8
251.111
25.95
160.606
204.167
178.261
184.889
144.359
221.579
217.391
150.175
134.211
223.529
15
193.137
133.529
162.571
216.818
22.8
140.256
135.789
154.737
187.353
138.043
235.263
182.766
898.039
10.5
24
12.74