#Ligand	TotalEnergy	VDW	AverConPa
6nur-2ghv-Roccustyrna_fr1-1-0.pdb	-989.072	-989.072	106.667
6nur-1xak-Roccustyrna_gs3-1-0.pdb	-964.665	-964.665	139.574
6nur-1xak-Roccustyrna_gs5-1-0.pdb	-945.605	-945.605	109.219
6nur-2ghv-Roccustyrna_fr5-1-0.pdb	-940.938	-940.938	129.608
6nur-1xak-Roccustyrna_fr1-1-0.pdb	-896.056	-896.056	968.116
6nur-1xak-Roccustyrna_fr5-1-0.pdb	-895.178	-895.178	159.804
6nur-2ghv-Roccustyrna_fr2-0-0.pdb	-893.167	-893.167	199.394
6nur-1xak-Roccustyrna_gs1-1-0.pdb	-891.583	-891.583	136.522
6nur-1xak-Roccustyrna_fr1-0-0.pdb	-876.053	-876.053	93.913
6nur-2ghv-Roccustyrna_fr7-1-0.pdb	-875.345	-875.345	180.857
6nur-2ghv-Roccustyrna_fr3-1-0.pdb	-821.522	-821.522	152.564
6nur-1xak-Roccustyrna_fr4-0-0.pdb	-816.363	-816.363	161.111
6nur-1xak-Roccustyrna_fr4-1-0.pdb	-812.804	-812.804	14
6nur-2ghv-Roccustyrna_fr7-0-0.pdb	-812.735	-812.735	194.286
6nur-2ghv-Roccustyrna_fr6-1-0.pdb	-810.878	-810.878	149.474
6nur-1xak-Roccustyrna_fr6-0-0.pdb	-808.214	-808.214	144.211
6nur-1xak-Roccustyrna_fr2-0-0.pdb	-783.792	-783.792	165.152
6nur-1xak-Roccustyrna_fr7-1-0.pdb	-775.423	-775.423	166.857
6nur-2ghv-Roccustyrna_fr6-0-0.pdb	-775.395	-775.395	163.421
6nur-2ghv-Roccustyrna_fr4-1-0.pdb	-752.812	-752.812	185.556
6nur-2ghv-Roccustyrna_fr4-0-0.pdb	-752.756	-752.756	158.611
6nur-1xak-Roccustyrna_fr3-1-0.pdb	-739.619	-739.619	18
6nur-6m2q-Roccustyrna_fr2-0-0.pdb	-736.117	-736.117	157.273
6nur-2g9t-Roccustyrna-0-0.pdb	-733.913	-733.913	191.714
6nur-1xak-Roccustyrna_fr2-1-0.pdb	-730.823	-730.823	165.152
6nur-2ghv-Roccustyrna_fr2-1-0.pdb	-726.746	-726.746	155.758
6nur-1xak-Roccustyrna_gs2-0-0.pdb	-695.097	-695.097	24
6nur-1xak-Roccustyrna_gs6-1-0.pdb	-593.342	-593.342	22.05
6nur-1xak-Roccustyrna_gs6-0-0.pdb	-586.867	-586.867	20.45
6nur-2ghv-Roccustyrna-0-0.pdb	-101.552	-638.832	164.857
6nur-1xak-Roccustyrna_gs8-1-0.pdb	-100.131	-100.131	13.14
6nur-1xak-Roccustyrna_gs4-1-0.pdb	-87.727	-87.727	13.098
6nur-1xak-Roccustyrna_fr6-1-0.pdb	-83.305	-83.305	163.947
6nur-1xak-Roccustyrna_fr7-0-0.pdb	-74.832	-74.832	151.429
6nur-1xak-Roccustyrna_gs2-1-0.pdb	-71.254	-71.254	271.579
6nur-1xak-Roccustyrna_gs5-0-0.pdb	58.011	58.011	742.188
6nur-1xak-Roccustyrna_gs1-0-0.pdb	104.361	104.361	17.413
6nur-1xak-Roccustyrna_gs3-0-0.pdb	182.712	182.712	139.787
6nur-1xak-Roccustyrna_fr5-0-0.pdb	199.347	199.347	138.039
6nur-2ghv-Roccustyrna_fr3-0-0.pdb	341.023	341.023	95.641
6nur-2ghv-Roccustyrna_fr1-0-0.pdb	501.494	501.494	902.899
6nur-1xak-Roccustyrna_fr3-0-0.pdb	504.939	504.939	126.667
6nur-2ghv-Roccustyrna_fr5-0-0.pdb	527.362	527.362	226.078
6nur-1xak-Roccustyrna_gs8-0-0.pdb	658.242	658.242	19.24
6nur-1xak-Roccustyrna_gs4-0-0.pdb	742.563	742.563	986.275
6nur-2g9t-Roccustyrna_fr1-0-0.pdb	764.115	764.115	830.435
6nur-6m2q-Roccustyrna_fr1-0-0.pdb	892.746	892.746	223.043

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