#Ligand	TotalEnerg	VDW	AverConPair
6m2q-cav3fqq_GOL-Roccustyrna-0-0.pdb	-985.174	-985.174	206.571
6m2q-2ghv-Roccustyrna_fr3-1-0.pdb	-982.866	-982.866	192.051
6m2q-1xak-Roccustyrna_gs8-1-0.pdb	-964.658	-964.658	14.74
6m2q-1xak-Roccustyrna_gs4-1-0.pdb	-962.523	-962.523	136.863
6m2q-7bv2-Roccustyrna_gs4-1-0.pdb	-958.548	-958.548	130.588
6m2q-cav6w63_X77-Roccustyrna_fr2-0-0.pdb	-947.003	-947.003	193.939
6m2q-7bv2-Roccustyrna_fr2-0-0.pdb	-946.782	-946.782	194.545
6m2q-1xak-Roccustyrna_fr1-1-0.pdb	-940.667	-940.667	131.014
6m2q-6m2q-Roccustyrna_fr6-0-0.pdb	-940.278	-940.278	170.263
6m2q-1xak-Roccustyrna_fr1-0-0.pdb	-940.173	-940.173	13.087
6m2q-1xak-Roccustyrna_fr4-1-0.pdb	-926.256	-926.256	17.5
6m2q-7khp-Roccustyrna_fr4-0-0.pdb	-925.595	-925.595	174.444
6m2q-cav6wzu_GOL-roccustyrnareywarrior-1-0.pdb	-915.976	-915.976	963.636
6m2q-2ghv-Roccustyrna_fr6-0-0.pdb	-914.226	-914.226	178.158
6m2q-7khp-Roccustyrna_fr6-0-0.pdb	-904.862	-904.862	171.842
6m2q-2ghv-Roccustyrna_fr5-1-0.pdb	-903.985	-903.985	131.569
6m2q-2ghv-Roccustyrna_fr6-1-0.pdb	-903.793	-903.793	174.737
6m2q-6w9c-Roccustyrna-0-0.pdb	-901.507	-901.507	206.857
6m2q-cav7b3o_NAG-Roccustyrna_fr1-0-0.pdb	-898.142	-898.142	138.986
6m2q-2ghv-Roccustyrna_fr1-1-0.pdb	-896.877	-896.877	101.159
6m2q-7bv2-Roccustyrna_fr1-1-0.pdb	-894.018	-894.018	101.594
6m2q-1xak-Roccustyrna_fr6-0-0.pdb	-890.917	-890.917	163.947
6m2q-7bv2-Roccustyrna_gs5-1-0.pdb	-889.186	-889.186	113.281
6m2q-1xak-Roccustyrna_gs1-1-0.pdb	-882.498	-882.498	136.957
6m2q-1xak-Roccustyrna_fr3-1-0.pdb	-880.818	-880.818	161.026
6m2q-7bv2-Roccustyrna_gs8-1-0.pdb	-875.473	-875.473	15.14
6m2q-7khp-Roccustyrna_fr2-0-0.pdb	-872.488	-872.488	198.182
6m2q-7bv2-Roccustyrna_fr7-1-0.pdb	-864.661	-864.661	169.429
6m2q-7khp-Roccustyrna_fr1-0-0.pdb	-862.559	-862.559	250.725
6m2q-1xak-Roccustyrna_fr6-1-0.pdb	-857.911	-857.911	156.053
6m2q-cav6wzu_GOL-Roccustyrna_less_admet_-0-0.pdb	-850.699	-850.699	148.857
6m2q-7bv2-Roccustyrna_fr3-1-0.pdb	-845.405	-845.405	165.385
6m2q-1xak-Roccustyrna_fr7-0-0.pdb	-844.969	-844.969	209.143
6m2q-1xak-Roccustyrna_fr2-1-0.pdb	-843.812	-843.812	184.545
6m2q-7bv2-Roccustyrna_gs1-1-0.pdb	-834.156	-834.156	140.217
6m2q-1xak-Roccustyrna_gs5-1-0.pdb	-832.894	-832.894	103.594
6m2q-6m2q-Roccustyrna_fr7-0-0.pdb	-830.036	-830.036	171.429
6m2q-7bv2-Roccustyrna_fr5-1-0.pdb	-829.931	-829.931	12.902
6m2q-cav6w63_X77-Roccustyrna_fr4-0-0.pdb	-829.818	-829.818	156.667
6m2q-cav7b3o_NAG-Roccustyrna_fr2-0-0.pdb	-828.712	-828.712	169.394
6m2q-1xak-Roccustyrna_gs3-1-0.pdb	-828.541	-828.541	13
6m2q-2ghv-Roccustyrna_fr7-0-0.pdb	-826.718	-826.718	151.429
6m2q-cav6lu7_02J-Roccustyrna_fr2-0-0.pdb	-826.349	-826.349	197.576
6m2q-1xak-Roccustyrna_fr7-1-0.pdb	-819.744	-819.744	146.286
6m2q-7bv2-Roccustyrna_fr1-0-0.pdb	-812.041	-812.041	836.232
6m2q-2ghv-Roccustyrna_fr2-0-0.pdb	-808.844	-808.844	171.818
6m2q-2g9t-Roccustyrna-0-0.pdb	-807.535	-807.535	18.6
6m2q-7bv2-Roccustyrna_fr7-0-0.pdb	-803.217	-803.217	15.4
6m2q-cav6w63_X77-Roccustyrna_fr7-0-0.pdb	-801.576	-801.576	180.571

6m2q-1xak-Roccustyrna_fr4-0-0.pdb	-801.143	-801.143	155.278
6m2q-7bv2-Roccustyrna_gs3-1-0.pdb	-796.733	-796.733	129.149
6m2q-7bv2-Roccustyrna_fr2-1-0.pdb	-792.078	-792.078	152.424
6m2q-cav6wzu_GOL-Roccustyrna_less_admet_-1-0.pdb	-791.451	-791.451	143.714
6m2q-1xak-Roccustyrna_fr5-1-0.pdb	-789.498	-789.498	129.804
6m2q-2ghv-Roccustyrna_fr4-0-0.pdb	-785.868	-785.868	151.667
6m2q-cav6lu7_02J-Roccustyrna_fr7-0-0.pdb	-780.107	-780.107	147.429
6m2q-6m2q-Roccustyrna_fr4-0-0.pdb	-778.889	-778.889	179.722
6m2q-2ghv-Roccustyrna_fr2-1-0.pdb	-778.206	-778.206	155.758
6m2q-7bv2-Roccustyrna_fr4-0-0.pdb	-776.914	-776.914	162.778
6m2q-1xak-Roccustyrna_fr2-0-0.pdb	-774.953	-774.953	164.242
6m2q-cav6woj_APR-Roccustyrna_fr2-0-0.pdb	-771.752	-771.752	152.727
6m2q-6m2q-Roccustyrna_fr2-0-0.pdb	-769.096	-769.096	164.545
6m2q-7bv2-Roccustyrna_fr4-1-0.pdb	-768.219	-768.219	145.556
6m2q-cav6woj_APR-Roccustyrna_fr6-0-0.pdb	-764.606	-764.606	172.632
6m2q-7bv2-Roccustyrna_fr6-0-0.pdb	-764.145	-764.145	145.526
6m2q-cav6lu7_02J-Roccustyrna_fr6-0-0.pdb	-760.653	-760.653	159.211
6m2q-cav6wzu_GOL-Roccustyrna_fr4-0-0.pdb	-758.692	-758.692	137.778
6m2q-cav7b3o_NAG-Roccustyrna_fr4-0-0.pdb	-754.486	-754.486	143.056
6m2q-cav6lu7_02J-Roccustyrna_fr4-0-0.pdb	-754.243	-754.243	142.778
6m2q-2ghv-Roccustyrna_fr4-1-0.pdb	-745.954	-745.954	139.722
6m2q-cav6w63_X77-Roccustyrna_fr6-0-0.pdb	-738.086	-738.086	136.316
6m2q-6xs6-Roccustyrna-0-0.pdb	-727.245	-727.245	202.286
6m2q-6m2q-Roccustyrna_fr3-0-0.pdb	-727.033	-727.033	866.667
6m2q-2ghv-Roccustyrna_fr7-1-0.pdb	-724.376	-724.376	14.4
6m2q-7khp-Roccustyrna_fr7-0-0.pdb	-718.966	-718.966	132.857
6m2q-cav6wzu_GOL-Roccustyrna_fr7-0-0.pdb	-717.846	-717.846	142.857
6m2q-cav6woj_APR-Roccustyrna_fr4-0-0.pdb	-716.406	-716.406	13.75
6m2q-cav6wzu_GOL-Roccustyrna_gs2-0-0.pdb	-681.496	-681.496	227.368
6m2q-cav6w63_X77-Roccustyrna_gs2-0-0.pdb	-672.525	-672.525	251.579
6m2q-cav6wzu_GOL-Roccustyrna_fr2-0-0.pdb	-672.054	-672.054	146.667
6m2q-1xak-Roccustyrna_gs2-0-0.pdb	-671.804	-671.804	248.421
6m2q-cav6lu7_02J-Roccustyrna_gs6-0-0.pdb	-670.564	-670.564	21.95
6m2q-cav6woj_APR-Roccustyrna_gs6-0-0.pdb	-670.416	-670.416	21.9
6m2q-7khp-Roccustyrna_gs6-0-0.pdb	-669.617	-669.617	21.75
6m2q-7bv2-Roccustyrna_gs2-0-0.pdb	-664.127	-664.127	229.474
6m2q-cav6wzu_GOL-Roccustyrna_gs6-0-0.pdb	-659.585	-659.585	20.75
6m2q-7khp-Roccustyrna_gs2-0-0.pdb	-655.249	-655.249	215.789
6m2q-cav6woj_APR-Roccustyrna_gs2-0-0.pdb	-654.573	-654.573	216.842
6m2q-7bv2-Roccustyrna_gs2-1-0.pdb	-652.705	-652.705	35
6m2q-1xak-Roccustyrna_gs2-1-0.pdb	-647.197	-647.197	236.842
6m2q-cav6lu7_02J-Roccustyrna_gs2-0-0.pdb	-641.806	-641.806	237.895
6m2q-6m2q-Roccustyrna_gs2-0-0.pdb	-637.308	-637.308	244.211
6m2q-6m2q-Roccustyrna_gs6-0-0.pdb	-616.215	-616.215	21.55
6m2q-1xak-Roccustyrna_gs6-0-0.pdb	-613.245	-613.245	20.95
6m2q-1xak-Roccustyrna_gs6-1-0.pdb	-610.579	-610.579	19.3
6m2q-7bv2-Roccustyrna_gs6-1-0.pdb	-607.647	-607.647	21.55
6m2q-cav6w63_X77-Roccustyrna_gs6-0-0.pdb	-605.187	-605.187	20.2
6m2q-cav6lu7_02J-Roccustyrna_gs1-0-0.pdb	-503.128	-503.128	647.826
6m2q-cav6wzu_GOL-Roccustyrna_fr3-0-0.pdb	-377.249	-377.249	104.872

6m2q-1xak-Roccustyrna_fr3-0-0.pdb	-366.947	-366.947	746.154
6m2q-cav6lu7_02J-Roccustyrna_fr1-0-0.pdb	-314.175	-314.175	611.594
6m2q-7bv2-Roccustyrna_gs5-0-0.pdb	-267.127	-267.127	607.813
6m2q-cav6woj_APR-Roccustyrna_fr1-0-0.pdb	-260.501	-260.501	469.565
6m2q-cav6wzu_GOL-Roccustyrna_gs5-0-0.pdb	-193.143	-193.143	39.375
6m2q-cav6wzu_GOL-Roccustyrna_fr1-0-0.pdb	-154.288	-154.288	450.725
6m2q-cav6woj_APR-Roccustyrna_gs5-0-0.pdb	-149.376	-149.376	192.188
6m2q-cav2zu5_ZU5-Roccustyrna-0-0.pdb	-112.883	-802.291	199.143
6m2q-2ghv-Roccustyrna-0-0.pdb	-103.524	-762.791	174.286
6m2q-7bv2-Roccustyrna_fr6-1-0.pdb	-90.358	-90.358	170.526
6m2q-cav6woj_APR-Roccustyrna_fr7-0-0.pdb	-80.296	-80.296	15.4
6m2q-cav6wzu_GOL-Roccustyrna_fr6-0-0.pdb	-75.464	-75.464	158.947
6m2q-7bv2-Roccustyrna_gs6-0-0.pdb	-63.204	-63.204	20.75
6m2q-cav6wzu_GOL-Roccustyrna-0-0.pdb	0	0	0
6m2q-cav6w63_X77-Roccustyrna_gs4-0-0.pdb	60.682	60.682	984.314
6m2q-cav6lu7_02J-Roccustyrna_gs8-0-0.pdb	100.707	100.707	10.42
6m2q-7bv2-Roccustyrna_fr5-0-0.pdb	101.258	101.258	998.039
6m2q-cav6w63_X77-Roccustyrna_fr3-0-0.pdb	106.924	106.924	115.897
6m2q-cav6woj_APR-Roccustyrna_gs4-0-0.pdb	108.074	108.074	823.529
6m2q-cav6wzu_GOL-Roccustyrna_gs4-0-0.pdb	110.503	110.503	580.392
6m2q-1xak-Roccustyrna_gs4-0-0.pdb	111.545	111.545	578.431
6m2q-cav6woj_APR-Roccustyrna_fr3-0-0.pdb	114.364	114.364	14.359
6m2q-cav7b3o_NAG-Roccustyrna_fr3-0-0.pdb	119.792	119.792	129.487
6m2q-7khp-Roccustyrna_gs4-0-0.pdb	125.763	125.763	652.941
6m2q-6m2q-Roccustyrna_gs4-0-0.pdb	126.235	126.235	114.118
6m2q-7bv2-Roccustyrna_gs4-0-0.pdb	126.975	126.975	114.902
6m2q-cav6lu7_02J-Roccustyrna_gs4-0-0.pdb	128.987	128.987	161.765
6m2q-cav6woj_APR-Roccustyrna_gs8-0-0.pdb	142.721	142.721	16.14
6m2q-7bv2-Roccustyrna_gs1-0-0.pdb	156.136	156.136	153.478
6m2q-cav6w63_X77-Roccustyrna_gs5-0-0.pdb	169.566	169.566	392.188
6m2q-cav6wzu_GOL-Roccustyrna_gs1-0-0.pdb	173.085	173.085	108.261
6m2q-cav6w63_X77-Roccustyrna_fr5-0-0.pdb	187.472	187.472	95.098
6m2q-2ghv-Roccustyrna_fr3-0-0.pdb	192.385	192.385	186.923
6m2q-cav6wzu_GOL-Roccustyrna_fr5-0-0.pdb	196.624	196.624	138.039
6m2q-6m2q-Roccustyrna_gs1-0-0.pdb	210.638	210.638	125.217
6m2q-7khp-Roccustyrna_gs1-0-0.pdb	223.389	223.389	130.652
6m2q-cav6wzu_GOL-Roccustyrna_gs3-0-0.pdb	231.856	231.856	182.128
6m2q-1xak-Roccustyrna_gs8-0-0.pdb	255.086	255.086	14.86
6m2q-6m2q-Roccustyrna_fr5-0-0.pdb	272.766	272.766	588.235
6m2q-cav6w63_X77-Roccustyrna_gs1-0-0.pdb	281.252	281.252	122.609
6m2q-cav6wzu_GOL-Roccustyrna_gs8-0-0.pdb	306.273	306.273	20.52
6m2q-2g9t-Roccustyrna_fr1-0-0.pdb	306.914	306.914	942.029
6m2q-7khp-Roccustyrna_fr3-0-0.pdb	321.237	321.237	117.179
6m2q-cav6woj_APR-Roccustyrna_gs3-0-0.pdb	328.756	328.756	142.979
6m2q-7khp-Roccustyrna_fr5-0-0.pdb	349.906	349.906	621.569
6m2q-6m2q-Roccustyrna_fr1-0-0.pdb	353.322	353.322	112.464
6m2q-1xak-Roccustyrna_gs1-0-0.pdb	399.541	399.541	110.435
6m2q-7bv2-Roccustyrna_fr3-0-0.pdb	401.714	401.714	794.872
6m2q-6m2q-Roccustyrna_gs8-0-0.pdb	412.943	412.943	20.06
6m2q-7khp-Roccustyrna_gs5-0-0.pdb	415.998	415.998	495.313

6m2q-cav6w63_X77-Roccustyrna_gs8-0-0.pdb	506.105	506.105	10.5	
6m2q-cav6lu7_02J-Roccustyrna_fr3-0-0.pdb	515.916	515.916		961.538
6m2q-cav6wzu_GOL-roccustyrnareywarrior-0-0.pdb	562.482	562.482		127.273
6m2q-7khp-Roccustyrna_gs8-0-0.pdb	570.409	570.409	19.38	
6m2q-1xak-Roccustyrna_gs5-0-0.pdb	574.623	574.623		795.313
6m2q-cav6w63_X77-Roccustyrna_gs3-0-0.pdb	657.519	657.519		255.745
6m2q-6zgg-Roccustyrna_fr1-0-0.pdb	700.271	700.271		166.232
6m2q-6m2q-Roccustyrna_gs3-0-0.pdb	739.682	739.682		243.617
6m2q-cav6lu7_02J-Roccustyrna_gs3-0-0.pdb	743.566	743.566		271.064
6m2q-cav6woj_APR-Roccustyrna_gs1-0-0.pdb	750.401	750.401		110.217
6m2q-7khp-Roccustyrna_gs3-0-0.pdb	754.418	754.418		289.574
6m2q-cav6lu7_02J-Roccustyrna_gs5-0-0.pdb	770.489	770.489		74.375
6m2q-cav6woj_APR-Roccustyrna_fr5-0-0.pdb	795.981	795.981		990.196
6m2q-1xak-Roccustyrna_fr5-0-0.pdb	836.569	836.569		907.843
6m2q-cav6w63_X77-Roccustyrna_fr1-0-0.pdb	886.964	886.964		314.493
6m2q-7bv2-Roccustyrna_gs8-0-0.pdb	915.307	915.307	23.2	
6m2q-2ghv-Roccustyrna_fr1-0-0.pdb	933.156	933.156		226.957
6m2q-cav6lu7_02J-Roccustyrna_fr5-0-0.pdb	952.142	952.142		637.255
6m2q-6m2q-Roccustyrna_gs5-0-0.pdb	995.124	995.124		61.875
6m2q-7bv2-Roccustyrna_gs3-0-0.pdb	1024.91	1024.91		322.553
6m2q-2ghv-Roccustyrna_fr5-0-0.pdb	158.21	158.21		122.941
6m2q-1xak-Roccustyrna_gs3-0-0.pdb	172.63	172.63		151.064
6m2q-6xs6 (1)-Roccustyrna_fr1-0-0.pdb	793.78	793.78		266.812