

bond

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0.030	19.84700
0.040	19.79600
0.050	19.74500
0.060	19.69400
0.070	19.64300
0.080	19.59200
0.090	19.54100
0.100	19.49000
0.110	19.43900
0.120	19.38800
0.130	19.33700
0.140	19.28600
0.150	19.23500
0.160	19.18400
0.170	19.13300
0.180	19.08200
0.190	19.03100
0.200	18.98000
0.210	18.92900
0.220	18.87800
0.230	18.82700
0.240	18.77600
0.250	18.72500
0.260	18.67400
0.270	18.62300
0.280	18.57200
0.290	18.52100
0.300	18.47000
0.310	18.41900
0.320	18.36800
0.330	18.31700
0.340	18.26600
0.350	18.21500
0.360	18.16400
0.370	18.11300
0.380	18.06200
0.390	18.01100
0.400	17.96000
0.410	17.90900
0.420	17.85800
0.430	17.80700
0.440	17.75600
0.450	17.70500
0.460	17.65400
0.470	17.60300
0.480	17.55200
0.490	17.50100
0.500	17.45000
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0.530	17.29700
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0.560	17.14400
0.570	17.09300
0.580	17.04200

0.590	16.99100
0.600	16.94000
0.610	16.88900
0.620	16.83800
0.630	16.78700
0.640	16.73600
0.650	16.68500
0.660	16.63400
0.670	16.58300
0.680	16.53200
0.690	16.48100
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0.710	16.37900
0.720	16.32800
0.730	16.27700
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0.750	16.17500
0.760	16.12400
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0.830	15.76700
0.840	15.71600
0.850	15.66500
0.860	15.61400
0.870	15.56300
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0.900	15.41000
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4.180 0.52683

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5.990 8.04900
6.000 8.10000

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nonbonded AA

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0.540	23.20100
0.550	23.18250
0.560	23.16400
0.570	23.14550
0.580	23.12700
0.590	23.10850
0.600	23.09000
0.610	23.07150
0.620	23.05300
0.630	23.03450
0.640	23.01600
0.650	22.99750
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0.670	22.96050
0.680	22.94200
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0.780	22.75700
0.790	22.73850
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0.810	22.70150
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0.860	22.60900
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0.880	22.57200
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0.900	22.53500
0.910	22.51650
0.920	22.49800
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0.940	22.46100
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1.110	22.14650

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1.860	20.75900
1.870	20.74050
1.880	20.72200
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1.900	20.68500
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nonbonded AB

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