

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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0.440	21.18600
0.450	21.16750
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0.470	21.13050
0.480	21.11200
0.490	21.09350
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0.510	21.05650

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0.540	21.00100
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0.570	20.94550
0.580	20.92700
0.590	20.90850
0.600	20.89000
0.610	20.87150
0.620	20.85300
0.630	20.83450
0.640	20.81600
0.650	20.79750
0.660	20.77900
0.670	20.76050
0.680	20.74200
0.690	20.72350
0.700	20.70500
0.710	20.68650
0.720	20.66800
0.730	20.64950
0.740	20.63100
0.750	20.61250
0.760	20.59400
0.770	20.57550
0.780	20.55700
0.790	20.53850
0.800	20.52000
0.810	20.50150
0.820	20.48300
0.830	20.46450
0.840	20.44600
0.850	20.42750
0.860	20.40900
0.870	20.39050
0.880	20.37200
0.890	20.35350
0.900	20.33500
0.910	20.31650
0.920	20.29800
0.930	20.27950
0.940	20.26100
0.950	20.24250
0.960	20.22400
0.970	20.20550
0.980	20.18700
0.990	20.16850
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1.010	20.13150
1.020	20.11300
1.030	20.09450
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1.060	20.03900
1.070	20.02050
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1.170 19.83550
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1.980	18.33700
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2.450	17.46750
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2.480	17.41200
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nonbonded AB

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nonbonded BB

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