

...file opened, and lambdas: md_00.ene 0.00 1.00

Number of points: 1000

state	EQtot	EQbond	EQang	EQtor	EQimp	EQel	EQvdW
1	-1087.71	-578.19	7.68	0.63	0.00	-541.46	22.70
2	-1145.21	-586.25	31.48	1.16	0.00	-603.21	10.68

state	Eel_qq	EvdW_qq	Eel_qp	EvdW_qp	Eel_qw	EvdW_qw	Eqrstr
1	112.02	0.57	-18.78	-1.97	-634.70	24.10	0.00
2	0.00	-0.30	-5.32	-2.51	-597.89	13.50	0.00

etc...

lambda(1)	dGf	sum(dGf)	dGr	sum(dGr)	<dG>
0.00	0.00	0.00	-5.71	-284.20	0.00
0.01	5.64	5.64	-5.54	-278.49	5.67
0.02	5.63	11.27	-5.45	-272.95	11.26
0.03	5.48	16.74	-5.28	-267.50	16.72
0.04	5.38	22.12	-10.41	-262.22	22.05
0.06	10.37	32.49	-10.07	-251.80	32.44

etc...

Min energy-gap is: -292.238384870069

Max energy-gap is: 330.166319351831

Lambda1	Ibin	Energy	gap	dGa	dGb	dGg	#	pts
0.00	1	-284.46	-31.28	247.20	-47.72		65	
0.00	2	-268.90	-31.28	231.53	-48.50		200	
0.00	3	-253.34	-31.28	216.31	-49.35		231	
0.00	4	-237.78	-31.28	201.25	-50.31		88	
0.01	2	-268.90	-31.40	231.23	-48.73		79	
0.01	3	-253.34	-31.26	216.16	-49.42		303	
0.01	4	-237.78	-31.13	201.59	-50.14		181	
0.01	5	-222.22	-30.99	189.55	-51.00		25	

etc...