

		Size of dimensions (x, y, z)	Energy (pre-minimization, kJ/mol)	Energy (post-minimization, kJ/mol)	Number of atoms
		100.167755, 100.167755, 127.064628 (original size from charmmgui)	-1180126.872	-1472590.016	118459
		100.167755, 100.167755, 130.064628	-1157669.21	-1470485.67	118459
		100, 100, 128	-1165534.667	-1473427.743	118459
		100, 100, 100	5.48E+19	-1503256.659	118459
		90, 90, 90	5.64E+23	-1182843.844	118459
		85, 85, 85	1.01E+24	-162892.4205	118459
		83, 83, 83	3.65E+20	685031.1176	118459