

**Table 1.** Average constraint force  $\bar{f}$ , taken at MD simulation time 6 ps and 10 ps. Forces are expressed in atomic units; the last column shows the root mean square fluctuation of the constraint force over 10 ps.

$\text{\AA}$	$\bar{f}$ at 6 ps	$\bar{f}$ at 10 ps	difference	RMS fluctuation
3.8	0.00034	0.00046	1.2e-4	1.5e-4
4.0	-0.00048	-0.00083	3.5e-4	1.5e-4
4.2	-0.00102	-0.00100	0.2e-4	1.7e-4
4.4	-0.00103	-0.00089	1.4e-4	1.6e-4
4.8	-0.00017	-0.00005	-1.2e-4	1.5e-4
5.0	-0.00064	-0.00099	-3.5e-4	1.8e-4
5.2	-0.00112	-0.00159	-4.7e-4	2.2e-4
5.4	-0.00140	-0.00136	0.4e-4	1.7e-4
5.6	-0.00182	-0.00181	0.1e-4	2.1e-4
5.8	-0.00094	-0.00104	-0.9e-4	1.6e-4