

Supplementary Text 3

Amber 16 SANDER

2016

| Run on 08/13/2017 at 00:51:42

| Executable path: /usr/local/amber16/bin/sander

| Working directory: /Users/Swati

| Hostname: Unknown

| [-O]verwriting output

File Assignments:

| MDIN: minimization_file_2.in

| MDOUT: 3WY9_min3_2.out

| INPCRD: 3WY9_min3_1.rst

| PARM: /Users/Swati/3WY9_files/3WY9.prmtop

| RESTRT: 3WY9_min3_2.rst

| REFC: refc

| MDVEL: mdvel

| MDFRC: mdfrc

| MDEN: mden

| MDCRD: mdcrd

| MDINFO: mdinfo

| MTMD: mtmd

| INPDIP: inpdip

| RSTDIP: rstcip

| INPTRA: inptraj

Here is the input file:

PROT: minimization_2

&cntrl

imin = 1,

maxcyc = 5000,

ncyc = 10000,

igb = 0,

ntpr = 100,

ntp = 0

cut = 12

&end

1. RESOURCE USE:

| Flags:

| getting box info from netcdf restart file

| NetCDF restart box info found

| Largest sphere to fit in unit cell has radius = 43.021

| New format PARM file being parsed.

| Version = 1.000 Date = 08/08/17 Time = 03:26:06

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NATOM = 108958 NTYPES = 17 NBOH = 104467 MBONA = 4615
NTHETH = 9760 MTHETA = 6270 NPHIH = 20223 MPHIA = 19473
NHPARM = 0 NPARM = 0 NNB = 182012 NRES = 33963
NBONA = 4615 NTHETA = 6270 NPHIA = 19473 NUMBND = 67
NUMANG = 152 NPTRA = 191 NATYP = 36 NPHB = 1
IFBOX = 1 NMXRS = 24 IFCAP = 0 NEXTRA = 0
NCOPY = 0
    
```

```

| Memory Use      Allocated
| Real            8586309
| Hollerith       360839
| Integer         4397980
| Max Pairs       99660250
| nblastReal      1307496
| nblast Int      3585143
| Total           499186 kbytes
    
```

| Note: 1-4 EEL scale factors are being read from the topology file.

| Note: 1-4 VDW scale factors are being read from the topology file.

| Duplicated 0 dihedrals

| Duplicated 0 dihedrals

BOX TYPE: RECTILINEAR

2. CONTROL DATA FOR THE RUN

default_name

General flags:

imin = 1, nmropt = 0

Nature and format of input:

ntx = 1, irest = 0, ntrx = 1

Nature and format of output:

ntxo = 2, ntp = 100, ntrx = 1, ntwr = 1
iwrap = 0, ntwx = 0, ntwv = 0, ntwe = 0
ioutfm = 1, ntwprt = 0, idecomp = 0, rbornstat = 0

Potential function:

ntf = 1, ntb = 1, igb = 0, nsnb = 25
ipol = 0, gbsa = 0, iesp = 0
dielc = 1.00000, cut = 12.00000, intdiel = 1.00000

Frozen or restrained atoms:

ibelly = 0, ntr = 0

Energy minimization:

maxcyc = 5000, ncyc = 10000, ntmin = 1
dx0 = 0.01000, drms = 0.00010

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Ewald parameters:

```
verbose =      0, ew_type =      0, nbflag =      1, use_pme =      1
vdwmeth =      1, eedmeth =      1, netfrnc =      0
Box X = 123.894   Box Y =  86.041   Box Z = 120.804
Alpha =  90.000   Beta  =  90.000   Gamma =  90.000
NFFT1 = 128      NFFT2 =  90      NFFT3 = 120
Cutoff= 12.000   Tol   =0.100E-04
Ewald Coefficient = 0.22664
Interpolation order = 4
```

| INFO: Old style inpcrd file read

3. ATOMIC COORDINATES AND VELOCITIES

default_name

begin time read from input coords = 0.000 ps

Number of triangulated 3-point waters found: 33386

Sum of charges from parm topology file = -0.00000039
Forcing neutrality...

4. RESULTS

APPROXIMATING switch and d/dx switch using CUBIC SPLINE INTERPOLATION
using 5000.0 points per unit in tabled values

TESTING RELATIVE ERROR over r ranging from 0.0 to cutoff

| CHECK switch(x): max rel err = 0.2738E-14 at 2.422500

| CHECK d/dx switch(x): max rel err = 0.7967E-11 at 2.716640

| Local SIZE OF NONBOND LIST = 54068725

| TOTAL SIZE OF NONBOND LIST = 54068725

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
1	-4.0743E+05	3.9773E+00	2.5249E+02	OE2	2287
BOND	= 32679.6549	ANGLE	= 3821.6131	DIHED	= 6769.6726
VDWAALS	= 79544.4577	EEL	= -560075.0788	HBOND	= 0.0000
1-4 VDW	= 3206.3674	1-4 EEL	= 26623.1514	RESTRAINT	= 0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
100	-4.1967E+05	4.3273E-01	3.5870E+01	C	7578
BOND	= 31212.6883	ANGLE	= 1635.0353	DIHED	= 6674.1253
VDWAALS	= 73765.4432	EEL	= -561298.5479	HBOND	= 0.0000
1-4 VDW	= 2242.9987	1-4 EEL	= 26093.3367	RESTRAINT	= 0.0000

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NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
200	-4.2130E+05	5.9209E-01	7.9308E+01	C	7276
BOND =	31291.4606	ANGLE =	1387.4006	DIHED =	6635.4671
VDWAALS =	73779.5780	EEL =	-562451.5931	HBOND =	0.0000
1-4 VDW =	2070.3073	1-4 EEL =	25983.7068	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
300	-4.2227E+05	4.9068E-01	6.7758E+01	CE1	7690
BOND =	31366.6586	ANGLE =	1304.5645	DIHED =	6615.0445
VDWAALS =	74004.2024	EEL =	-563497.4347	HBOND =	0.0000
1-4 VDW =	2001.7591	1-4 EEL =	25938.0316	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
400	-4.2300E+05	4.5303E-01	6.4055E+01	CE1	7690
BOND =	31450.7686	ANGLE =	1261.3643	DIHED =	6594.4938
VDWAALS =	74289.8862	EEL =	-564472.8335	HBOND =	0.0000
1-4 VDW =	1964.4071	1-4 EEL =	25910.4399	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
500	-4.2363E+05	3.7313E-01	5.3893E+01	CE1	7690
BOND =	31533.0108	ANGLE =	1235.5423	DIHED =	6575.3517
VDWAALS =	74610.7520	EEL =	-565413.6388	HBOND =	0.0000
1-4 VDW =	1940.6597	1-4 EEL =	25892.6224	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
600	-4.2416E+05	1.5208E-01	9.0968E+00	CE1	7690
BOND =	31608.1921	ANGLE =	1217.9322	DIHED =	6559.3107
VDWAALS =	74935.1691	EEL =	-566282.2412	HBOND =	0.0000
1-4 VDW =	1923.8000	1-4 EEL =	25878.0264	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
700	-4.2465E+05	1.4002E-01	6.2203E+00	CE1	7690
BOND =	31687.5293	ANGLE =	1207.4636	DIHED =	6543.6779
VDWAALS =	75268.1089	EEL =	-567133.1244	HBOND =	0.0000
1-4 VDW =	1910.5107	1-4 EEL =	25864.7429	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
800	-4.2510E+05	1.3456E-01	6.8662E+00	CE1	7690
BOND =	31764.3137	ANGLE =	1201.0680	DIHED =	6532.2066

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VDWAALS = 75600.9159 EEL = -567949.6462 HBOND = 0.0000
 1-4 VDW = 1900.5196 1-4 EEL = 25852.4024 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 900 -4.2550E+05 5.1118E-01 8.7368E+01 CG 3213

BOND = 31848.9242 ANGLE = 1197.3435 DIHED = 6523.4301
 VDWAALS = 75925.7816 EEL = -568730.5844 HBOND = 0.0000
 1-4 VDW = 1892.5964 1-4 EEL = 25840.2627 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 1000 -4.2589E+05 4.1303E-01 6.6538E+01 CE1 7690

BOND = 31914.9715 ANGLE = 1193.4261 DIHED = 6517.4167
 VDWAALS = 76232.8797 EEL = -569465.1475 HBOND = 0.0000
 1-4 VDW = 1886.1382 1-4 EEL = 25830.2818 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 1100 -4.2625E+05 3.5107E-01 5.5756E+01 CE1 7690

BOND = 31978.8488 ANGLE = 1190.8181 DIHED = 6514.2283
 VDWAALS = 76531.7913 EEL = -570170.3587 HBOND = 0.0000
 1-4 VDW = 1880.4536 1-4 EEL = 25821.5084 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 1200 -4.2660E+05 3.2079E-01 5.0003E+01 CE1 7690

BOND = 32042.4468 ANGLE = 1188.3056 DIHED = 6512.3061
 VDWAALS = 76824.6566 EEL = -570852.3589 HBOND = 0.0000
 1-4 VDW = 1875.6007 1-4 EEL = 25813.8819 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 1300 -4.2691E+05 1.7631E-01 2.3461E+01 CE1 7690

BOND = 32099.0501 ANGLE = 1186.1113 DIHED = 6510.8869
 VDWAALS = 77101.2724 EEL = -571489.0280 HBOND = 0.0000
 1-4 VDW = 1871.2346 1-4 EEL = 25806.8266 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 1400 -4.2721E+05 1.1860E-01 8.1646E+00 CE1 7690

BOND = 32154.5483 ANGLE = 1184.6806 DIHED = 6508.9184
 VDWAALS = 77362.1524 EEL = -572087.1550 HBOND = 0.0000
 1-4 VDW = 1867.1360 1-4 EEL = 25800.4805 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 1500 -4.2749E+05 1.1479E-01 8.5025E+00 CE1 7690

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BOND	=	32209.0346	ANGLE	=	1183.4895	DIHED	=	6506.9186
VDWAALS	=	77614.4593	EEL	=	-572666.9289	HBOND	=	0.0000
1-4 VDW	=	1863.1560	1-4 EEL	=	25795.0427	RESTRAINT	=	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
1600	-4.2776E+05	4.0384E-01	6.2315E+01	CE1	7690

BOND	=	32269.0950	ANGLE	=	1182.8509	DIHED	=	6505.4034
VDWAALS	=	77855.7131	EEL	=	-573226.1031	HBOND	=	0.0000
1-4 VDW	=	1859.4422	1-4 EEL	=	25790.2108	RESTRAINT	=	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
1700	-4.2803E+05	1.0762E-01	6.9342E+00	CE1	7690

BOND	=	32311.4581	ANGLE	=	1181.0826	DIHED	=	6503.8729
VDWAALS	=	78083.4515	EEL	=	-573755.1554	HBOND	=	0.0000
1-4 VDW	=	1856.2124	1-4 EEL	=	25785.6835	RESTRAINT	=	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
1800	-4.2829E+05	2.8655E-01	4.5459E+01	CE1	7690

BOND	=	32364.4811	ANGLE	=	1180.3382	DIHED	=	6502.2780
VDWAALS	=	78307.2847	EEL	=	-574275.4507	HBOND	=	0.0000
1-4 VDW	=	1853.1415	1-4 EEL	=	25781.3818	RESTRAINT	=	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
1900	-4.2854E+05	1.4462E-01	1.7709E+01	CE1	7690

BOND	=	32408.6965	ANGLE	=	1178.8896	DIHED	=	6500.5513
VDWAALS	=	78517.8045	EEL	=	-574771.0444	HBOND	=	0.0000
1-4 VDW	=	1850.5270	1-4 EEL	=	25777.5257	RESTRAINT	=	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
2000	-4.2878E+05	1.0300E-01	6.1988E+00	CE1	7690

BOND	=	32453.6414	ANGLE	=	1177.4678	DIHED	=	6499.1494
VDWAALS	=	78720.5513	EEL	=	-575252.4661	HBOND	=	0.0000
1-4 VDW	=	1848.1772	1-4 EEL	=	25773.9781	RESTRAINT	=	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
2100	-4.2902E+05	1.0659E-01	7.8688E+00	CE1	7690

BOND	=	32498.4418	ANGLE	=	1176.0866	DIHED	=	6498.1178
VDWAALS	=	78920.8095	EEL	=	-575729.2338	HBOND	=	0.0000
1-4 VDW	=	1846.1438	1-4 EEL	=	25770.5828	RESTRAINT	=	0.0000

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NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
2200	-4.2925E+05	1.1979E-01	1.2721E+01	CE1	7690

BOND =	32541.5566	ANGLE =	1175.0323	DIHED =	6497.0650
VDWAALS =	79111.7229	EEL =	-576186.0845	HBOND =	0.0000
1-4 VDW =	1844.2957	1-4 EEL =	25767.2633	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
2300	-4.2947E+05	3.3339E-01	5.1576E+01	CE1	7690

BOND =	32588.0814	ANGLE =	1174.5852	DIHED =	6496.1196
VDWAALS =	79296.2536	EEL =	-576628.6575	HBOND =	0.0000
1-4 VDW =	1842.5833	1-4 EEL =	25764.1456	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
2400	-4.2969E+05	2.7617E-01	4.3559E+01	CE1	7690

BOND =	32627.8686	ANGLE =	1173.7630	DIHED =	6495.2764
VDWAALS =	79479.0684	EEL =	-577067.7093	HBOND =	0.0000
1-4 VDW =	1841.1437	1-4 EEL =	25760.9855	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
2500	-4.2991E+05	2.4414E-01	3.3957E+01	CE1	7690

BOND =	32668.1947	ANGLE =	1172.9840	DIHED =	6494.3507
VDWAALS =	79656.8698	EEL =	-577499.4681	HBOND =	0.0000
1-4 VDW =	1839.6328	1-4 EEL =	25757.8188	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
2600	-4.3012E+05	1.3717E-01	1.6617E+01	CE1	7690

BOND =	32705.3280	ANGLE =	1172.2101	DIHED =	6493.0949
VDWAALS =	79822.3487	EEL =	-577907.6119	HBOND =	0.0000
1-4 VDW =	1838.3512	1-4 EEL =	25754.8170	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
2700	-4.3033E+05	1.0044E-01	7.6430E+00	CE1	7690

BOND =	32743.0278	ANGLE =	1171.6378	DIHED =	6491.7219
VDWAALS =	79980.1719	EEL =	-578303.3298	HBOND =	0.0000
1-4 VDW =	1837.0237	1-4 EEL =	25752.0809	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
2800	-4.3053E+05	3.8553E-01	7.7209E+01	CG	3213

BOND =	32788.1055	ANGLE =	1171.6400	DIHED =	6490.2029
VDWAALS =	80136.0177	EEL =	-578699.0928	HBOND =	0.0000
1-4 VDW =	1835.5900	1-4 EEL =	25749.6499	RESTRAINT =	0.0000

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NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
2900	-4.3073E+05	3.2051E-01	4.9022E+01	CE1	7690
BOND =	32823.3959	ANGLE =	1171.0376	DIHED =	6488.4719
VDWAALS =	80284.2560	EEL =	-579079.1115	HBOND =	0.0000
1-4 VDW =	1834.3608	1-4 EEL =	25747.2164	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
3000	-4.3093E+05	2.6854E-01	4.2445E+01	CE1	7690
BOND =	32857.7391	ANGLE =	1170.5752	DIHED =	6486.7037
VDWAALS =	80424.2435	EEL =	-579442.7223	HBOND =	0.0000
1-4 VDW =	1833.0532	1-4 EEL =	25744.9564	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
3100	-4.3112E+05	2.4035E-01	3.7521E+01	CE1	7690
BOND =	32893.1967	ANGLE =	1169.6927	DIHED =	6485.2343
VDWAALS =	80561.7306	EEL =	-579806.3702	HBOND =	0.0000
1-4 VDW =	1831.8022	1-4 EEL =	25743.5336	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
3200	-4.3132E+05	1.4333E-01	1.8055E+01	CE1	7690
BOND =	32927.3349	ANGLE =	1168.2806	DIHED =	6484.6351
VDWAALS =	80697.6263	EEL =	-580167.9301	HBOND =	0.0000
1-4 VDW =	1830.6338	1-4 EEL =	25742.4137	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
3300	-4.3151E+05	9.7663E-02	7.8731E+00	CE1	7690
BOND =	32962.0136	ANGLE =	1167.3962	DIHED =	6483.6509
VDWAALS =	80830.0793	EEL =	-580519.2542	HBOND =	0.0000
1-4 VDW =	1829.7813	1-4 EEL =	25741.3101	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
3400	-4.3169E+05	1.0844E-01	1.1271E+01	CE1	7690
BOND =	32998.2332	ANGLE =	1166.8887	DIHED =	6481.9417
VDWAALS =	80966.9609	EEL =	-580876.7537	HBOND =	0.0000
1-4 VDW =	1829.0472	1-4 EEL =	25740.2841	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
3500	-4.3188E+05	9.6518E-02	7.8744E+00	CE1	7690
BOND =	33034.5426	ANGLE =	1166.4964	DIHED =	6480.1533

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VDWAALS = 81107.6123 EEL = -581234.8831 HBOND = 0.0000
 1-4 VDW = 1828.4030 1-4 EEL = 25739.4789 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 3600 -4.3205E+05 2.5875E-01 3.8888E+01 CE1 7690

BOND = 33073.7323 ANGLE = 1166.4610 DIHED = 6478.7013
 VDWAALS = 81249.5737 EEL = -581587.8405 HBOND = 0.0000
 1-4 VDW = 1827.7786 1-4 EEL = 25738.8230 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 3700 -4.3223E+05 2.3593E-01 3.5061E+01 CE1 7690

BOND = 33109.2388 ANGLE = 1166.3445 DIHED = 6477.7481
 VDWAALS = 81391.6173 EEL = -581936.8626 HBOND = 0.0000
 1-4 VDW = 1827.1398 1-4 EEL = 25737.9213 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 3800 -4.3240E+05 1.4182E-01 1.7990E+01 CE1 7690

BOND = 33142.9129 ANGLE = 1166.2205 DIHED = 6477.1349
 VDWAALS = 81532.0803 EEL = -582277.2856 HBOND = 0.0000
 1-4 VDW = 1826.5301 1-4 EEL = 25737.2001 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 3900 -4.3256E+05 1.5320E-01 2.0595E+01 CE1 7690

BOND = 33177.9969 ANGLE = 1166.5085 DIHED = 6476.7605
 VDWAALS = 81672.2008 EEL = -582612.6009 HBOND = 0.0000
 1-4 VDW = 1825.8607 1-4 EEL = 25736.2611 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 4000 -4.3271E+05 7.9563E-02 3.3188E+00 CE1 7690

BOND = 33211.0011 ANGLE = 1166.6319 DIHED = 6476.3850
 VDWAALS = 81808.8036 EEL = -582936.2866 HBOND = 0.0000
 1-4 VDW = 1825.2025 1-4 EEL = 25735.3734 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 4100 -4.3286E+05 3.3584E-01 1.0048E+02 CG 3213

BOND = 33249.1173 ANGLE = 1167.2749 DIHED = 6476.0080
 VDWAALS = 81944.1824 EEL = -583255.5236 HBOND = 0.0000
 1-4 VDW = 1824.4520 1-4 EEL = 25734.6292 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 4200 -4.3301E+05 2.3594E-01 3.2671E+01 CE1 7690

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BOND	=	33278.9146	ANGLE	=	1167.5729	DIHED	=	6475.7748
VDWAALS	=	82075.6547	EEL	=	-583562.5531	HBOND	=	0.0000
1-4 VDW	=	1823.8053	1-4 EEL	=	25733.3468	RESTRAINT	=	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
4300	-4.3315E+05	2.3575E-01	3.3055E+01	CG	3213

BOND	=	33310.3633	ANGLE	=	1167.7409	DIHED	=	6475.6843
VDWAALS	=	82205.2476	EEL	=	-583864.5727	HBOND	=	0.0000
1-4 VDW	=	1823.2308	1-4 EEL	=	25732.3246	RESTRAINT	=	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
4400	-4.3329E+05	1.8235E-01	2.2265E+01	CE1	7690

BOND	=	33340.1505	ANGLE	=	1168.1683	DIHED	=	6475.7611
VDWAALS	=	82332.4773	EEL	=	-584160.2654	HBOND	=	0.0000
1-4 VDW	=	1822.5187	1-4 EEL	=	25731.0794	RESTRAINT	=	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
4500	-4.3342E+05	1.5117E-01	1.7610E+01	CE1	7690

BOND	=	33369.3467	ANGLE	=	1168.1790	DIHED	=	6475.8601
VDWAALS	=	82455.7767	EEL	=	-584445.3600	HBOND	=	0.0000
1-4 VDW	=	1821.9624	1-4 EEL	=	25729.7881	RESTRAINT	=	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
4600	-4.3356E+05	7.6819E-02	3.8025E+00	CG	3213

BOND	=	33397.2927	ANGLE	=	1168.3381	DIHED	=	6475.7621
VDWAALS	=	82575.6560	EEL	=	-584723.2739	HBOND	=	0.0000
1-4 VDW	=	1821.3715	1-4 EEL	=	25728.1632	RESTRAINT	=	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
4700	-4.3369E+05	8.8181E-02	7.0531E+00	NE2	8655

BOND	=	33425.2658	ANGLE	=	1168.4641	DIHED	=	6474.2225
VDWAALS	=	82691.2285	EEL	=	-584992.9022	HBOND	=	0.0000
1-4 VDW	=	1820.8578	1-4 EEL	=	25726.4283	RESTRAINT	=	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
4800	-4.3381E+05	7.5012E-02	3.6977E+00	NE2	8655

BOND	=	33452.1764	ANGLE	=	1168.6809	DIHED	=	6472.8166
VDWAALS	=	82802.4675	EEL	=	-585254.9780	HBOND	=	0.0000
1-4 VDW	=	1820.3536	1-4 EEL	=	25724.6591	RESTRAINT	=	0.0000

Supplementary Text 3

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
4900	-4.3394E+05	2.0032E-01	2.6049E+01	NE2	8655
BOND =	33480.3896	ANGLE =	1169.2780	DIHED =	6472.1110
VDWAALS =	82910.9901	EEL =	-585514.6411	HBOND =	0.0000
1-4 VDW =	1819.8707	1-4 EEL =	25722.8852	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
5000	-4.3407E+05	1.7436E-01	2.3542E+01	NE2	8655
BOND =	33506.0853	ANGLE =	1169.2249	DIHED =	6471.6103
VDWAALS =	83017.0209	EEL =	-585770.2257	HBOND =	0.0000
1-4 VDW =	1819.4910	1-4 EEL =	25721.3021	RESTRAINT =	0.0000

Maximum number of minimization cycles reached.

FINAL RESULTS

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
5000	-4.3407E+05	1.7436E-01	2.3542E+01	NE2	8655
BOND =	33506.0853	ANGLE =	1169.2249	DIHED =	6471.6103
VDWAALS =	83017.0209	EEL =	-585770.2257	HBOND =	0.0000
1-4 VDW =	1819.4910	1-4 EEL =	25721.3021	RESTRAINT =	0.0000

5. TIMINGS

Build the list	22.81 (88.24% of List)
Other	3.04 (11.76% of List)
List time	25.85 (0.25% of Nonbo)
Short_ene time	9466.54 (99.66% of Direc)
Other	31.99 (0.34% of Direc)
Direct Ewald time	9498.53 (91.70% of Ewald)
Adjust Ewald time	35.33 (0.34% of Ewald)
Fill Bspline coeffs	27.74 (3.39% of Recip)
Fill charge grid	120.27 (14.71% of Recip)
Scalar sum	155.67 (19.04% of Recip)
Grad sum	205.51 (25.14% of Recip)
FFT time	308.22 (37.71% of Recip)
Recip Ewald time	817.42 (7.89% of Ewald)
Virial junk	2.34 (0.02% of Ewald)
Other	5.12 (0.05% of Ewald)
Ewald time	10358.76 (99.75% of Nonbo)
Nonbond force	10384.62 (99.51% of Force)
Bond/Angle/Dihedral	50.22 (0.48% of Force)
Other	1.38 (0.01% of Force)
Force time	10436.22 (100.0% of Runmd)

Supplementary Text 3

```
| Runmd Time          10436.22 (99.71% of Total)
| Other                30.36 ( 0.29% of Total)
| Total time          10466.62 (100.0% of ALL )
```

```
| Number of list builds :          14
```

```
| Highest rstack allocated: 5837340
| Highest ystack allocated: 108958
|           Job began at 00:51:42.048 on 08/13/2017
|           Setup done at 00:51:43.000 on 08/13/2017
|           Run done at 03:46:08.665 on 08/13/2017
| wallclock() was called 190076 times
```

Amber 16 SANDER

2016

```
| Run on 08/14/2017 at 01:34:10
```

```
| Executable path: /usr/local/amber16/bin/sander
| Working directory: /Users/Swati
| Hostname: Unknown
| [-O]verwriting output
```

File Assignments:

```
| MDIN: minimization_file_2.in
| MDOUT: LJP6_min3_2.out
| INPCRD: LJP6_min3_1.rst
| PARM: /Users/Swati/LJP6_files/LJP6.prmtop
| RESTRT: LJP6_min3_2.rst
| REFC: refc
| MDVEL: mdvel
| MDFRC: mdfrc
| MDEN: mden
| MDCRD: mdcrd
| MDINFO: mdinfo
| MTMD: mtmd
| INPDIP: inp dip
| RSTDIP: rst dip
| INPTRAJ: inp traj
```

Here is the input file:

```
PROT: minimization_2
&cntrl
imin = 1,
maxcyc = 5000,
ncyc = 10000,
igb = 0,
ntpr = 100,
ntp = 0
cut = 12
&end
```

Supplementary Text 3

1. RESOURCE USE:

| Flags:
| getting box info from netcdf restart file
| NetCDF restart box info found
| Largest sphere to fit in unit cell has radius = 44.819
| New format PARM file being parsed.
| Version = 1.000 Date = 08/06/17 Time = 07:17:45
| NATOM = 107805 NTYPES = 17 NBONH = 103425 MBONA = 4491
| NTHETH = 9523 MTHETA = 6101 NPHIH = 19785 MPHIA = 18920
| NHPARM = 0 NPARM = 0 NNB = 179511 NRES = 33643
| NBONA = 4491 NTHETA = 6101 NPHIA = 18920 NUMBND = 67
| NUMANG = 152 NPTRA = 191 NATYP = 36 NPHB = 1
| IFBOX = 1 NMXRS = 24 IFCAP = 0 NEXTRA = 0
| NCOPY = 0

Memory Use	Allocated
Real	8496271
Hollerith	357060
Integer	4323872
Max Pairs	98605640
nblastReal	1293660
nblast Int	3573335
Total	493905 kbytes

| Note: 1-4 EEL scale factors are being read from the topology file.

| Note: 1-4 VDW scale factors are being read from the topology file.

| Duplicated 0 dihedrals
| Duplicated 0 dihedrals

BOX TYPE: RECTILINEAR

2. CONTROL DATA FOR THE RUN

default_name

General flags:

imin = 1, nmropt = 0

Nature and format of input:

ntx = 1, irest = 0, ntrx = 1

Nature and format of output:

ntxo = 2, ntrp = 100, ntrx = 1, ntwr = 1
iwrap = 0, ntwx = 0, ntwv = 0, ntwe = 0
ioutfm = 1, ntwprt = 0, idecomp = 0, rbornstat= 0

Supplementary Text 3

Potential function:

```
ntf      =      1, ntb      =      1, igb      =      0, nsnb      =      25
ipol     =      0, gbsa     =      0, iesp     =      0
dielc    =  1.00000, cut     = 12.00000, intdiel =  1.00000
```

Frozen or restrained atoms:

```
ibelly   =      0, ntr     =      0
```

Energy minimization:

```
maxcyc   =  5000, ncyd    = 10000, ntmin    =      1
dx0      =  0.01000, drms  =  0.00010
```

Ewald parameters:

```
verbose  =      0, ew_type =      0, nbflag   =      1, use_pme  =      1
vdwmeth  =      1, eedmeth =      1, netfrd   =      0
Box X    = 117.910  Box Y    =  89.637  Box Z    = 121.218
Alpha    =  90.000  Beta    =  90.000  Gamma    =  90.000
NFFT1    = 120     NFFT2    =  90     NFFT3    = 125
Cutoff   = 12.000  Tol     =0.100E-04
Ewald Coefficient =  0.22664
Interpolation order =  4
```

| INFO: Old style inpcrd file read

3. ATOMIC COORDINATES AND VELOCITIES

default_name

```
begin time read from input coords =  0.000 ps
```

```
Number of triangulated 3-point waters found:  33071
```

```
Sum of charges from parm topology file = -0.00000035
Forcing neutrality...
```

4. RESULTS

```
-----
APPROXIMATING switch and d/dx switch using CUBIC SPLINE INTERPOLATION
using 5000.0 points per unit in tabled values
TESTING RELATIVE ERROR over r ranging from 0.0 to cutoff
| CHECK switch(x): max rel err =  0.2738E-14  at  2.422500
| CHECK d/dx switch(x): max rel err =  0.7967E-11  at  2.716640
-----
```

```
| Local SIZE OF NONBOND LIST =  53314213
| TOTAL SIZE OF NONBOND LIST =  53314213
```

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
1	-4.0036E+05	4.7605E+00	7.0995E+02	C	3792

Supplementary Text 3

BOND	=	40159.1664	ANGLE	=	4173.9815	DIHED	=	6614.0321
VDWAALS	=	78057.3200	EEL	=	-556195.6061	HBOND	=	0.0000
1-4 VDW	=	2790.3026	1-4 EEL	=	24042.2383	RESTRAINT	=	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
100	-4.1752E+05	4.2203E-01	7.5970E+01	N	3794

BOND	=	32073.8265	ANGLE	=	1993.4333	DIHED	=	6519.7751
VDWAALS	=	73667.5498	EEL	=	-557327.3895	HBOND	=	0.0000
1-4 VDW	=	2081.6286	1-4 EEL	=	23468.1826	RESTRAINT	=	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
200	-4.1948E+05	5.9705E-01	1.3145E+02	C	3812

BOND	=	31640.3039	ANGLE	=	1666.7976	DIHED	=	6482.3217
VDWAALS	=	73787.2375	EEL	=	-558374.2134	HBOND	=	0.0000
1-4 VDW	=	1947.5960	1-4 EEL	=	23368.2252	RESTRAINT	=	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
300	-4.2058E+05	5.2360E-01	9.5490E+01	C	3812

BOND	=	31530.7177	ANGLE	=	1521.5410	DIHED	=	6459.1489
VDWAALS	=	74055.1402	EEL	=	-559374.4469	HBOND	=	0.0000
1-4 VDW	=	1890.2184	1-4 EEL	=	23335.6818	RESTRAINT	=	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
400	-4.2135E+05	4.2680E-01	9.1233E+01	C	3812

BOND	=	31501.2383	ANGLE	=	1447.0847	DIHED	=	6442.6834
VDWAALS	=	74359.0674	EEL	=	-560290.1587	HBOND	=	0.0000
1-4 VDW	=	1860.7054	1-4 EEL	=	23326.2782	RESTRAINT	=	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
500	-4.2196E+05	2.8243E-01	4.8215E+01	CD	3230

BOND	=	31526.1727	ANGLE	=	1388.3608	DIHED	=	6431.1022
VDWAALS	=	74667.2365	EEL	=	-561135.3787	HBOND	=	0.0000
1-4 VDW	=	1842.8537	1-4 EEL	=	23320.2571	RESTRAINT	=	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
600	-4.2247E+05	2.2774E-01	4.4242E+01	C	3812

BOND	=	31561.8449	ANGLE	=	1356.3709	DIHED	=	6423.0452
VDWAALS	=	74973.5376	EEL	=	-561927.1480	HBOND	=	0.0000
1-4 VDW	=	1830.9076	1-4 EEL	=	23316.3241	RESTRAINT	=	0.0000

Supplementary Text 3

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
700	-4.2290E+05	1.4834E-01	1.5758E+01	C	3812
BOND =	31611.3304	ANGLE =	1331.0660	DIHED =	6415.5626
VDWAALS =	75269.2559	EEL =	-562665.9996	HBOND =	0.0000
1-4 VDW =	1821.9016	1-4 EEL =	23313.2512	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
800	-4.2330E+05	1.3579E-01	1.2911E+01	C	3812
BOND =	31663.3559	ANGLE =	1315.7513	DIHED =	6409.5776
VDWAALS =	75566.3926	EEL =	-563384.5002	HBOND =	0.0000
1-4 VDW =	1814.9841	1-4 EEL =	23309.8510	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
900	-4.2367E+05	4.8981E-01	8.8835E+01	C	3812
BOND =	31726.4121	ANGLE =	1307.2666	DIHED =	6403.8369
VDWAALS =	75869.7140	EEL =	-564093.4667	HBOND =	0.0000
1-4 VDW =	1809.5157	1-4 EEL =	23307.7011	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
1000	-4.2401E+05	4.4153E-01	9.6354E+01	CD	3230
BOND =	31785.5620	ANGLE =	1292.2703	DIHED =	6398.9747
VDWAALS =	76158.5055	EEL =	-564755.3911	HBOND =	0.0000
1-4 VDW =	1805.6116	1-4 EEL =	23307.8694	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
1100	-4.2431E+05	3.4125E-01	6.4933E+01	C	3812
BOND =	31832.1085	ANGLE =	1283.9429	DIHED =	6397.6308
VDWAALS =	76428.8077	EEL =	-565368.5764	HBOND =	0.0000
1-4 VDW =	1802.1439	1-4 EEL =	23309.2388	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
1200	-4.2462E+05	3.0420E-01	4.9586E+01	CZ	3806
BOND =	31889.3631	ANGLE =	1225.7687	DIHED =	6411.5608
VDWAALS =	76685.4536	EEL =	-565954.2588	HBOND =	0.0000
1-4 VDW =	1799.1220	1-4 EEL =	23319.3490	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
1300	-4.2491E+05	1.9717E-01	3.1292E+01	CE2	3808
BOND =	31937.1838	ANGLE =	1204.2795	DIHED =	6405.0534
VDWAALS =	76933.9375	EEL =	-566512.3338	HBOND =	0.0000
1-4 VDW =	1796.2227	1-4 EEL =	23321.8231	RESTRAINT =	0.0000

Supplementary Text 3

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
1400	-4.2518E+05	1.5912E-01	2.3584E+01	CZ	3806
BOND =	31984.2500	ANGLE =	1198.7269	DIHED =	6391.9452
VDWAALS =	77164.6413	EEL =	-567033.0362	HBOND =	0.0000
1-4 VDW =	1793.8397	1-4 EEL =	23322.0726	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
1500	-4.2542E+05	1.0919E-01	1.1430E+01	CE2	3808
BOND =	32029.0480	ANGLE =	1195.3299	DIHED =	6386.8404
VDWAALS =	77380.7945	EEL =	-567529.3288	HBOND =	0.0000
1-4 VDW =	1791.7565	1-4 EEL =	23323.5169	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
1600	-4.2565E+05	4.2111E-01	7.8000E+01	CD	3230
BOND =	32081.0993	ANGLE =	1193.8988	DIHED =	6381.9940
VDWAALS =	77586.3012	EEL =	-568011.7539	HBOND =	0.0000
1-4 VDW =	1789.5505	1-4 EEL =	23326.0576	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
1700	-4.2588E+05	3.4467E-01	6.7153E+01	CZ	3806
BOND =	32121.3542	ANGLE =	1191.5326	DIHED =	6377.1254
VDWAALS =	77779.5714	EEL =	-568467.5694	HBOND =	0.0000
1-4 VDW =	1787.7827	1-4 EEL =	23328.0820	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
1800	-4.2610E+05	3.1399E-01	7.2533E+01	CD	3230
BOND =	32160.9932	ANGLE =	1189.7351	DIHED =	6372.6317
VDWAALS =	77964.8542	EEL =	-568905.3069	HBOND =	0.0000
1-4 VDW =	1786.1920	1-4 EEL =	23329.3929	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
1900	-4.2631E+05	2.7061E-01	4.9665E+01	CE2	3808
BOND =	32200.7163	ANGLE =	1188.0689	DIHED =	6368.8913
VDWAALS =	78140.7665	EEL =	-569325.1557	HBOND =	0.0000
1-4 VDW =	1784.5532	1-4 EEL =	23330.1925	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
2000	-4.2652E+05	1.5137E-01	2.5248E+01	CE2	3808
BOND =	32237.8330	ANGLE =	1186.8015	DIHED =	6366.0304

Supplementary Text 3

VDWAALS = 78312.2094 EEL = -569734.2486 HBOND = 0.0000
 1-4 VDW = 1783.1387 1-4 EEL = 23330.6318 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 2100 -4.2672E+05 9.5443E-02 7.1025E+00 CZ 3806

BOND = 32277.0022 ANGLE = 1185.7779 DIHED = 6363.7445
 VDWAALS = 78483.7133 EEL = -570139.4495 HBOND = 0.0000
 1-4 VDW = 1781.8925 1-4 EEL = 23330.9989 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 2200 -4.2691E+05 9.6173E-02 9.0962E+00 CE2 3808

BOND = 32317.5350 ANGLE = 1184.9615 DIHED = 6361.7807
 VDWAALS = 78658.5543 EEL = -570548.0313 HBOND = 0.0000
 1-4 VDW = 1780.7519 1-4 EEL = 23331.4051 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 2300 -4.2710E+05 3.5344E-01 7.2085E+01 CD 3230

BOND = 32363.4110 ANGLE = 1184.7582 DIHED = 6360.2636
 VDWAALS = 78833.4293 EEL = -570955.2340 HBOND = 0.0000
 1-4 VDW = 1779.7350 1-4 EEL = 23331.8598 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 2400 -4.2729E+05 2.8641E-01 5.3787E+01 CD 3230

BOND = 32400.7073 ANGLE = 1183.6718 DIHED = 6359.3655
 VDWAALS = 79001.4905 EEL = -571348.3138 HBOND = 0.0000
 1-4 VDW = 1778.6566 1-4 EEL = 23332.4375 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 2500 -4.2748E+05 2.5626E-01 5.1406E+01 CE2 3808

BOND = 32439.3989 ANGLE = 1183.2020 DIHED = 6355.1172
 VDWAALS = 79169.7727 EEL = -571742.3009 HBOND = 0.0000
 1-4 VDW = 1777.4784 1-4 EEL = 23332.9304 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 2600 -4.2767E+05 1.5318E-01 2.3446E+01 CE2 3808

BOND = 32476.5295 ANGLE = 1182.5608 DIHED = 6352.6728
 VDWAALS = 79338.0036 EEL = -572127.9059 HBOND = 0.0000
 1-4 VDW = 1776.5026 1-4 EEL = 23333.2685 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 2700 -4.2784E+05 1.1493E-01 1.5842E+01 CE2 3808

Supplementary Text 3

BOND	=	32512.6890	ANGLE	=	1181.8367	DIHED	=	6350.0138
VDWAALS	=	79495.5559	EEL	=	-572488.5002	HBOND	=	0.0000
1-4 VDW	=	1775.7392	1-4 EEL	=	23333.5700	RESTRAINT	=	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
2800	-4.2800E+05	8.7812E-02	7.1043E+00	CD1	3802

BOND	=	32548.0015	ANGLE	=	1180.9310	DIHED	=	6347.5716
VDWAALS	=	79647.3427	EEL	=	-572835.4372	HBOND	=	0.0000
1-4 VDW	=	1775.2324	1-4 EEL	=	23333.6533	RESTRAINT	=	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
2900	-4.2816E+05	1.0100E-01	1.3537E+01	CE2	3808

BOND	=	32583.2789	ANGLE	=	1180.1377	DIHED	=	6345.4171
VDWAALS	=	79796.9423	EEL	=	-573176.8380	HBOND	=	0.0000
1-4 VDW	=	1774.7179	1-4 EEL	=	23333.2584	RESTRAINT	=	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
3000	-4.2832E+05	2.8262E-01	5.0628E+01	CE2	3808

BOND	=	32621.9654	ANGLE	=	1179.5955	DIHED	=	6343.3918
VDWAALS	=	79948.1785	EEL	=	-573520.3245	HBOND	=	0.0000
1-4 VDW	=	1774.0978	1-4 EEL	=	23332.5471	RESTRAINT	=	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
3100	-4.2848E+05	2.3012E-01	4.4178E+01	CE2	3808

BOND	=	32655.6422	ANGLE	=	1178.6979	DIHED	=	6341.3892
VDWAALS	=	80097.8365	EEL	=	-573857.3012	HBOND	=	0.0000
1-4 VDW	=	1773.4839	1-4 EEL	=	23331.6245	RESTRAINT	=	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
3200	-4.2863E+05	2.1479E-01	3.6635E+01	CD	3230

BOND	=	32689.5754	ANGLE	=	1178.1486	DIHED	=	6338.9210
VDWAALS	=	80246.8669	EEL	=	-574190.0170	HBOND	=	0.0000
1-4 VDW	=	1772.8807	1-4 EEL	=	23330.6770	RESTRAINT	=	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
3300	-4.2878E+05	1.7219E-01	3.1147E+01	CE2	3808

BOND	=	32721.9198	ANGLE	=	1177.3450	DIHED	=	6336.8914
VDWAALS	=	80391.8714	EEL	=	-574510.0997	HBOND	=	0.0000
1-4 VDW	=	1772.3983	1-4 EEL	=	23329.9326	RESTRAINT	=	0.0000

Supplementary Text 3

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
3400	-4.2893E+05	8.1284E-02	6.7763E+00	CE2	3808
BOND =	32753.9897	ANGLE =	1176.7510	DIHED =	6335.5354
VDWAALS =	80538.5270	EEL =	-574831.7005	HBOND =	0.0000
1-4 VDW =	1771.9497	1-4 EEL =	23329.1356	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
3500	-4.2907E+05	9.4228E-02	1.2073E+01	CE2	3808
BOND =	32787.0335	ANGLE =	1176.3653	DIHED =	6334.4890
VDWAALS =	80683.7861	EEL =	-575150.4336	HBOND =	0.0000
1-4 VDW =	1771.5115	1-4 EEL =	23328.3161	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
3600	-4.2921E+05	2.7081E-01	4.8061E+01	CE2	3808
BOND =	32822.8357	ANGLE =	1176.3322	DIHED =	6333.6054
VDWAALS =	80827.5624	EEL =	-575466.9056	HBOND =	0.0000
1-4 VDW =	1771.0916	1-4 EEL =	23327.4922	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
3700	-4.2935E+05	2.2450E-01	4.2361E+01	CE2	3808
BOND =	32853.8954	ANGLE =	1176.0403	DIHED =	6332.8344
VDWAALS =	80967.9834	EEL =	-575777.9413	HBOND =	0.0000
1-4 VDW =	1770.6226	1-4 EEL =	23326.6463	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
3800	-4.2949E+05	1.9314E-01	3.4823E+01	CE2	3808
BOND =	32884.3866	ANGLE =	1175.5451	DIHED =	6332.2109
VDWAALS =	81103.3377	EEL =	-576078.2902	HBOND =	0.0000
1-4 VDW =	1770.1893	1-4 EEL =	23325.7696	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
3900	-4.2963E+05	1.2553E-01	2.1301E+01	CE2	3808
BOND =	32915.3777	ANGLE =	1175.1394	DIHED =	6331.6896
VDWAALS =	81242.9836	EEL =	-576386.0594	HBOND =	0.0000
1-4 VDW =	1769.7879	1-4 EEL =	23324.7174	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
4000	-4.2976E+05	7.7552E-02	6.0963E+00	CE2	3808
BOND =	32945.4667	ANGLE =	1174.7274	DIHED =	6331.2640
VDWAALS =	81376.7889	EEL =	-576679.1745	HBOND =	0.0000
1-4 VDW =	1769.3567	1-4 EEL =	23323.6069	RESTRAINT =	0.0000

Supplementary Text 3

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
4100	-4.2989E+05	3.0480E-01	5.8444E+01	CE2	3808
BOND =	32980.3989	ANGLE =	1174.7729	DIHED =	6330.2750
VDWAALS =	81511.4227	EEL =	-576974.6184	HBOND =	0.0000
1-4 VDW =	1768.8466	1-4 EEL =	23322.2750	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
4200	-4.3002E+05	7.6980E-02	6.2645E+00	CE2	3808
BOND =	33005.3701	ANGLE =	1174.3094	DIHED =	6327.9855
VDWAALS =	81638.7793	EEL =	-577254.6966	HBOND =	0.0000
1-4 VDW =	1768.2723	1-4 EEL =	23320.6105	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
4300	-4.3014E+05	2.1207E-01	4.1527E+01	CE2	3808
BOND =	33036.4328	ANGLE =	1174.3391	DIHED =	6326.5923
VDWAALS =	81766.4419	EEL =	-577534.9707	HBOND =	0.0000
1-4 VDW =	1767.6381	1-4 EEL =	23318.8112	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
4400	-4.3027E+05	1.9147E-01	3.6979E+01	CE2	3808
BOND =	33064.7771	ANGLE =	1174.3908	DIHED =	6325.7401
VDWAALS =	81892.4315	EEL =	-577811.7660	HBOND =	0.0000
1-4 VDW =	1766.9091	1-4 EEL =	23317.1267	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
4500	-4.3040E+05	1.1142E-01	1.6974E+01	CE2	3808
BOND =	33091.7530	ANGLE =	1174.4080	DIHED =	6324.6254
VDWAALS =	82016.1806	EEL =	-578084.0010	HBOND =	0.0000
1-4 VDW =	1766.1100	1-4 EEL =	23315.3999	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
4600	-4.3052E+05	7.8601E-02	8.2571E+00	CE2	3808
BOND =	33119.5318	ANGLE =	1174.4184	DIHED =	6323.6888
VDWAALS =	82138.9335	EEL =	-578354.1368	HBOND =	0.0000
1-4 VDW =	1765.4470	1-4 EEL =	23313.3861	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
4700	-4.3064E+05	8.7948E-02	1.1624E+01	CE2	3808
BOND =	33147.5502	ANGLE =	1174.3965	DIHED =	6323.4818

Supplementary Text 3

VDWAALS = 82261.6476 EEL = -578623.5613 HBOND = 0.0000
 1-4 VDW = 1764.9577 1-4 EEL = 23311.5059 RESTRAINT = 0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
4800	-4.3075E+05	7.6503E-02	7.9890E+00	CE2	3808

BOND = 33173.5461 ANGLE = 1174.4503 DIHED = 6323.5292
 VDWAALS = 82376.7281 EEL = -578874.9382 HBOND = 0.0000
 1-4 VDW = 1764.4728 1-4 EEL = 23309.8243 RESTRAINT = 0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
4900	-4.3086E+05	2.0427E-01	4.0076E+01	CE2	3808

BOND = 33200.9619 ANGLE = 1174.7099 DIHED = 6323.6537
 VDWAALS = 82490.0201 EEL = -579123.0490 HBOND = 0.0000
 1-4 VDW = 1763.9750 1-4 EEL = 23308.1793 RESTRAINT = 0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
5000	-4.3097E+05	1.9520E-01	3.5763E+01	CD	3230

BOND = 33225.7442 ANGLE = 1174.7834 DIHED = 6323.8304
 VDWAALS = 82601.6250 EEL = -579367.2882 HBOND = 0.0000
 1-4 VDW = 1763.4604 1-4 EEL = 23306.5890 RESTRAINT = 0.0000

Maximum number of minimization cycles reached.

FINAL RESULTS

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
5000	-4.3097E+05	1.9520E-01	3.5763E+01	CD	3230

BOND = 33225.7442 ANGLE = 1174.7834 DIHED = 6323.8304
 VDWAALS = 82601.6250 EEL = -579367.2882 HBOND = 0.0000
 1-4 VDW = 1763.4604 1-4 EEL = 23306.5890 RESTRAINT = 0.0000

 5. TIMINGS

	Build the list	28.42 (90.70% of List)
	Other	2.91 (9.30% of List)
	List time	31.34 (0.31% of Nonbo)
	Short_ene time	9311.51 (99.67% of Direc)
	Other	30.61 (0.33% of Direc)
	Direct Ewald time	9342.11 (91.54% of Ewald)
	Adjust Ewald time	34.72 (0.34% of Ewald)
	Fill Bspline coeffs	27.11 (3.30% of Recip)

Supplementary Text 3

		Fill charge grid	118.67 (14.44% of Recip)
		Scalar sum	155.71 (18.95% of Recip)
		Grad sum	206.43 (25.13% of Recip)
		FFT time	313.68 (38.18% of Recip)
		Recip Ewald time	821.60 (8.05% of Ewald)
		Virial junk	2.36 (0.02% of Ewald)
		Other	4.97 (0.05% of Ewald)
		Ewald time	10205.78 (99.69% of Nonbo)
		Nonbond force	10237.13 (99.51% of Force)
		Bond/Angle/Dihedral	48.98 (0.48% of Force)
		Other	1.34 (0.01% of Force)
		Force time	10287.45 (100.0% of Runmd)
		Runmd Time	10287.45 (99.71% of Total)
		Other	29.56 (0.29% of Total)
	Total time		10317.04 (100.0% of ALL)

| Number of list builds : 18

| Highest rstack allocated: 5732293
 | Highest istack allocated: 107805
 | Job began at 01:34:10.635 on 08/14/2017
 | Setup done at 01:34:11.587 on 08/14/2017
 | Run done at 04:26:07.673 on 08/14/2017
 | wallclock() was called 190084 times

 Amber 16 SANDER 2016

| Run on 08/13/2017 at 14:53:00

| Executable path: /usr/local/amber16/bin/sander
 | Working directory: /Users/Swati
 | Hostname: Unknown
 | [-O]verwriting output

File Assignments:

| MDIN: minimization_file_2.in
 | MDOU: NAT0_min3_2.out
 | INPCRD: NAT0_min3_1.rst
 | PARM: /Users/Swati/NAT0_files/NAT0.prmtop
 | RESTRT: NAT0_min3_2.rst
 | REFC: refc
 | MDVEL: mdvel
 | MDFRC: mdfrc
 | MDEN: mden
 | MDCRD: mdcrd
 | MDINFO: mdinfo
 | MTMD: mtmd
 | INPDIP: inp dip
 | RSTDIP: rst dip
 | INPTRAJ: inp traj

Supplementary Text 3

Here is the input file:

```
PROT: minimization_2
&cntrl
imin = 1,
maxcyc = 5000,
ncyc = 10000,
igb = 0,
ntpr = 100,
ntp = 0
cut = 12
&end
```

1. RESOURCE USE:

```
| Flags:
| getting box info from netcdf restart file
| NetCDF restart box info found
| Largest sphere to fit in unit cell has radius = 43.290
| New format PARM file being parsed.
| Version = 1.000 Date = 08/03/17 Time = 07:15:59
| NATOM = 108587 NTYPES = 17 NBNH = 104265 MBONA = 4427
| NTHETH = 9210 MTHETA = 6011 NPHIH = 19189 MPHIA = 18495
| NHPARM = 0 NPARM = 0 NNB = 179552 NRES = 33974
| NBONA = 4427 NTHETA = 6011 NPHIA = 18495 NUMBND = 67
| NUMANG = 152 NPTRA = 191 NATYP = 36 NPHB = 1
| IFBOX = 1 NMXRS = 24 IFCAP = 0 NEXTRA = 0
| NCOPY = 0
```

```
| Memory Use Allocated
| Real 8557276
| Hollerith 359737
| Integer 4292225
| Max Pairs 99320909
| nblastReal 1303044
| nblast Int 3569367
| Total 497120 kbytes
```

```
| Note: 1-4 EEL scale factors are being read from the topology file.
```

```
| Note: 1-4 VDW scale factors are being read from the topology file.
| Duplicated 0 dihedrals
| Duplicated 0 dihedrals
```

BOX TYPE: RECTILINEAR

2. CONTROL DATA FOR THE RUN

Supplementary Text 3

default_name

General flags:

imin = 1, nmropt = 0

Nature and format of input:

ntx = 1, irest = 0, ntrx = 1

Nature and format of output:

ntxo = 2, ntpr = 100, ntrx = 1, ntwr = 1
iwrap = 0, ntwx = 0, ntwv = 0, ntwe = 0
ioutfm = 1, ntwprt = 0, idecomp = 0, rbornstat= 0

Potential function:

ntf = 1, ntb = 1, igb = 0, nsnb = 25
ipol = 0, gbsa = 0, iesp = 0
dielc = 1.00000, cut = 12.00000, intdiel = 1.00000

Frozen or restrained atoms:

ibelly = 0, ntr = 0

Energy minimization:

maxcyc = 5000, ncyc = 10000, ntmin = 1
dx0 = 0.01000, drms = 0.00010

Ewald parameters:

verbose = 0, ew_type = 0, nbflag = 1, use_pme = 1
vdwmeth = 1, eedmeth = 1, netfrnc = 0
Box X = 122.784 Box Y = 86.581 Box Z = 120.454
Alpha = 90.000 Beta = 90.000 Gamma = 90.000
NFFT1 = 128 NFFT2 = 90 NFFT3 = 120
Cutoff= 12.000 Tol =0.100E-04
Ewald Coefficient = 0.22664
Interpolation order = 4

| INFO: Old style inpcrd file read

3. ATOMIC COORDINATES AND VELOCITIES

default_name

begin time read from input coords = 0.000 ps

Number of triangulated 3-point waters found: 33397

Sum of charges from parm topology file = -0.00000039
Forcing neutrality...

4. RESULTS

Supplementary Text 3

APPROXIMATING switch and d/dx switch using CUBIC SPLINE INTERPOLATION

using 5000.0 points per unit in tabled values

TESTING RELATIVE ERROR over r ranging from 0.0 to cutoff

| CHECK switch(x): max rel err = 0.2738E-14 at 2.422500

| CHECK d/dx switch(x): max rel err = 0.7967E-11 at 2.716640

| Local SIZE OF NONBOND LIST = 53975629

| TOTAL SIZE OF NONBOND LIST = 53975629

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
1	-4.1424E+05	3.4604E+00	3.0891E+02	NE2	3896
BOND =	32215.3288	ANGLE =	2894.2659	DIHED =	6372.8222
VDWAALS =	79840.8552	EEL =	-562877.3862	HBOND =	0.0000
1-4 VDW =	2848.5805	1-4 EEL =	24464.4772	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
100	-4.2360E+05	4.6601E-01	3.8919E+01	C	3051
BOND =	31462.1947	ANGLE =	1483.8942	DIHED =	6296.7741
VDWAALS =	75217.6031	EEL =	-563905.1139	HBOND =	0.0000
1-4 VDW =	2065.4770	1-4 EEL =	23777.4973	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
200	-4.2494E+05	6.4777E-01	1.0087E+02	CG	3137
BOND =	31532.3712	ANGLE =	1356.7681	DIHED =	6270.7246
VDWAALS =	75233.6698	EEL =	-564884.3727	HBOND =	0.0000
1-4 VDW =	1909.7719	1-4 EEL =	23638.7817	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
300	-4.2571E+05	5.0321E-01	5.7089E+01	CZ	3037
BOND =	31595.4569	ANGLE =	1317.2490	DIHED =	6254.6531
VDWAALS =	75441.2149	EEL =	-565764.5486	HBOND =	0.0000
1-4 VDW =	1853.2864	1-4 EEL =	23590.3327	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
400	-4.2629E+05	4.2191E-01	4.9299E+01	CG	3032
BOND =	31665.5164	ANGLE =	1299.8061	DIHED =	6239.8487
VDWAALS =	75698.1963	EEL =	-566585.4903	HBOND =	0.0000
1-4 VDW =	1823.0413	1-4 EEL =	23564.8713	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
500	-4.2680E+05	3.9923E-01	5.4231E+01	CG	3137
BOND =	31737.6234	ANGLE =	1290.4650	DIHED =	6228.5845

Supplementary Text 3

VDWAALS = 75978.8880 EEL = -567391.7847 HBOND = 0.0000
 1-4 VDW = 1803.2996 1-4 EEL = 23550.0282 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 600 -4.2726E+05 3.1711E-01 3.2933E+01 CZ 3037

BOND = 31807.2875 ANGLE = 1285.3807 DIHED = 6217.9236
 VDWAALS = 76266.5985 EEL = -568165.5869 HBOND = 0.0000
 1-4 VDW = 1789.5714 1-4 EEL = 23540.4694 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 700 -4.2766E+05 1.9674E-01 1.9753E+01 NE2 7140

BOND = 31872.9707 ANGLE = 1282.6293 DIHED = 6211.5126
 VDWAALS = 76557.4354 EEL = -568897.6467 HBOND = 0.0000
 1-4 VDW = 1779.8237 1-4 EEL = 23533.4694 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 800 -4.2802E+05 2.0922E-01 2.3429E+01 NE2 7140

BOND = 31938.5833 ANGLE = 1280.8466 DIHED = 6206.8355
 VDWAALS = 76842.1489 EEL = -569589.7889 HBOND = 0.0000
 1-4 VDW = 1772.4628 1-4 EEL = 23526.6868 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 900 -4.2835E+05 1.6197E-01 1.6809E+01 NE2 7140

BOND = 31998.7934 ANGLE = 1279.8446 DIHED = 6202.1679
 VDWAALS = 77113.6431 EEL = -570233.6566 HBOND = 0.0000
 1-4 VDW = 1766.4317 1-4 EEL = 23520.2712 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 1000 -4.2865E+05 4.1924E-01 5.6945E+01 NE2 7140

BOND = 32063.6454 ANGLE = 1280.3819 DIHED = 6197.2454
 VDWAALS = 77375.5533 EEL = -570844.5022 HBOND = 0.0000
 1-4 VDW = 1761.6476 1-4 EEL = 23514.9436 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 1100 -4.2895E+05 3.4879E-01 5.0483E+01 NE2 7140

BOND = 32119.2376 ANGLE = 1278.7164 DIHED = 6192.7311
 VDWAALS = 77636.1601 EEL = -571448.4473 HBOND = 0.0000
 1-4 VDW = 1757.6165 1-4 EEL = 23510.3279 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 1200 -4.2923E+05 2.9712E-01 4.7271E+01 NE2 7140

Supplementary Text 3

BOND	=	32171.5264	ANGLE	=	1276.8961	DIHED	=	6189.0290
VDWAALS	=	77877.6734	EEL	=	-572008.9744	HBOND	=	0.0000
1-4 VDW	=	1754.3479	1-4 EEL	=	23506.7514	RESTRAINT	=	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
1300	-4.2951E+05	2.7565E-01	4.7598E+01	CG	3137

BOND	=	32223.2166	ANGLE	=	1274.9125	DIHED	=	6185.9165
VDWAALS	=	78113.3365	EEL	=	-572557.1914	HBOND	=	0.0000
1-4 VDW	=	1751.4393	1-4 EEL	=	23502.3356	RESTRAINT	=	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
1400	-4.2977E+05	1.5633E-01	1.8948E+01	CG	3137

BOND	=	32272.6721	ANGLE	=	1271.8728	DIHED	=	6182.8827
VDWAALS	=	78344.4628	EEL	=	-573090.5664	HBOND	=	0.0000
1-4 VDW	=	1748.4986	1-4 EEL	=	23497.5877	RESTRAINT	=	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
1500	-4.3003E+05	1.0600E-01	7.1559E+00	NE2	7140

BOND	=	32321.8997	ANGLE	=	1269.4524	DIHED	=	6179.5991
VDWAALS	=	78570.4784	EEL	=	-573607.4335	HBOND	=	0.0000
1-4 VDW	=	1745.7704	1-4 EEL	=	23491.7154	RESTRAINT	=	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
1600	-4.3026E+05	4.0342E-01	6.6590E+01	NE2	7140

BOND	=	32377.0753	ANGLE	=	1269.1114	DIHED	=	6176.1376
VDWAALS	=	78786.7166	EEL	=	-574102.9114	HBOND	=	0.0000
1-4 VDW	=	1743.2674	1-4 EEL	=	23485.6133	RESTRAINT	=	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
1700	-4.3051E+05	1.0492E-01	8.0790E+00	NE2	7140

BOND	=	32416.4014	ANGLE	=	1266.5719	DIHED	=	6173.3124
VDWAALS	=	78991.4158	EEL	=	-574576.7080	HBOND	=	0.0000
1-4 VDW	=	1741.2259	1-4 EEL	=	23480.1534	RESTRAINT	=	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
1800	-4.3074E+05	2.9284E-01	4.6794E+01	NE2	7140

BOND	=	32465.9944	ANGLE	=	1266.7569	DIHED	=	6171.2672
VDWAALS	=	79194.9067	EEL	=	-575050.0222	HBOND	=	0.0000
1-4 VDW	=	1739.5925	1-4 EEL	=	23475.5912	RESTRAINT	=	0.0000

Supplementary Text 3

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
1900	-4.3096E+05	2.6122E-01	4.4354E+01	NE2	7140

BOND =	32510.8017	ANGLE =	1266.0380	DIHED =	6169.5879
VDWAALS =	79388.1708	EEL =	-575504.3753	HBOND =	0.0000
1-4 VDW =	1738.0779	1-4 EEL =	23472.3048	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
2000	-4.3118E+05	1.7050E-01	2.4660E+01	NE2	7140

BOND =	32552.8917	ANGLE =	1265.9018	DIHED =	6168.1082
VDWAALS =	79574.3759	EEL =	-575945.0717	HBOND =	0.0000
1-4 VDW =	1736.6586	1-4 EEL =	23468.9426	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
2100	-4.3139E+05	9.5601E-02	5.4156E+00	NE2	7140

BOND =	32595.7410	ANGLE =	1265.7782	DIHED =	6166.6003
VDWAALS =	79759.5186	EEL =	-576381.2745	HBOND =	0.0000
1-4 VDW =	1735.3018	1-4 EEL =	23466.3394	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
2200	-4.3160E+05	9.4262E-02	5.8576E+00	NE2	7140

BOND =	32638.4719	ANGLE =	1266.0138	DIHED =	6165.1645
VDWAALS =	79940.1316	EEL =	-576805.2965	HBOND =	0.0000
1-4 VDW =	1734.0954	1-4 EEL =	23463.7908	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
2300	-4.3180E+05	1.0345E-01	1.0220E+01	NE2	7140

BOND =	32681.1538	ANGLE =	1266.1527	DIHED =	6164.2512
VDWAALS =	80118.0348	EEL =	-577224.8403	HBOND =	0.0000
1-4 VDW =	1733.0109	1-4 EEL =	23461.3600	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
2400	-4.3199E+05	2.8504E-01	4.4932E+01	NE2	7140

BOND =	32725.1000	ANGLE =	1266.9005	DIHED =	6163.8345
VDWAALS =	80288.1953	EEL =	-577628.4506	HBOND =	0.0000
1-4 VDW =	1732.0082	1-4 EEL =	23459.2293	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
2500	-4.3218E+05	2.6260E-01	4.3027E+01	NE2	7140

BOND =	32764.2839	ANGLE =	1267.7179	DIHED =	6163.5901
VDWAALS =	80452.8748	EEL =	-578020.8732	HBOND =	0.0000
1-4 VDW =	1731.0144	1-4 EEL =	23457.0857	RESTRAINT =	0.0000

Supplementary Text 3

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
2600	-4.3237E+05	2.0783E-01	3.5330E+01	NE2	7140
BOND =	32803.2099	ANGLE =	1267.5864	DIHED =	6163.3478
VDWAALS =	80615.7341	EEL =	-578406.8008	HBOND =	0.0000
1-4 VDW =	1730.1443	1-4 EEL =	23455.5345	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
2700	-4.3256E+05	1.6313E-01	2.6744E+01	NE2	7140
BOND =	32841.9413	ANGLE =	1267.8450	DIHED =	6163.1898
VDWAALS =	80779.3081	EEL =	-578790.3037	HBOND =	0.0000
1-4 VDW =	1729.4671	1-4 EEL =	23453.5036	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
2800	-4.3273E+05	9.0926E-02	7.5705E+00	NE2	7140
BOND =	32879.3537	ANGLE =	1267.7315	DIHED =	6163.0599
VDWAALS =	80936.9516	EEL =	-579159.0330	HBOND =	0.0000
1-4 VDW =	1728.8327	1-4 EEL =	23451.7186	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
2900	-4.3291E+05	9.8809E-02	1.0693E+01	NE2	7140
BOND =	32917.0133	ANGLE =	1268.0488	DIHED =	6162.9778
VDWAALS =	81090.4213	EEL =	-579521.7713	HBOND =	0.0000
1-4 VDW =	1728.2001	1-4 EEL =	23449.8094	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
3000	-4.3307E+05	2.6055E-01	4.5377E+01	NE2	7140
BOND =	32956.3690	ANGLE =	1269.0371	DIHED =	6162.9778
VDWAALS =	81238.8175	EEL =	-579875.2491	HBOND =	0.0000
1-4 VDW =	1727.6017	1-4 EEL =	23447.9570	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
3100	-4.3324E+05	2.5457E-01	4.1911E+01	NE2	7140
BOND =	32992.5337	ANGLE =	1268.9003	DIHED =	6163.0790
VDWAALS =	81383.2390	EEL =	-580220.6466	HBOND =	0.0000
1-4 VDW =	1727.0014	1-4 EEL =	23446.5979	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
3200	-4.3341E+05	1.9830E-01	3.3901E+01	NE2	7140
BOND =	33027.4064	ANGLE =	1269.0671	DIHED =	6163.3758

Supplementary Text 3

VDWAALS = 81528.3702 EEL = -580565.6261 HBOND = 0.0000
 1-4 VDW = 1726.4232 1-4 EEL = 23444.9010 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 3300 -4.3357E+05 1.1338E-01 1.3958E+01 NE2 7140

BOND = 33061.6049 ANGLE = 1268.6299 DIHED = 6163.7865
 VDWAALS = 81670.5939 EEL = -580902.2260 HBOND = 0.0000
 1-4 VDW = 1725.9052 1-4 EEL = 23443.7261 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 3400 -4.3373E+05 8.5630E-02 5.5514E+00 NE2 7140

BOND = 33096.7097 ANGLE = 1268.5578 DIHED = 6164.3304
 VDWAALS = 81814.6162 EEL = -581243.3917 HBOND = 0.0000
 1-4 VDW = 1725.4052 1-4 EEL = 23442.4903 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 3500 -4.3390E+05 8.8931E-02 8.6417E+00 NE2 7140

BOND = 33132.1194 ANGLE = 1268.5123 DIHED = 6164.7963
 VDWAALS = 81958.6953 EEL = -581586.6995 HBOND = 0.0000
 1-4 VDW = 1724.8761 1-4 EEL = 23441.4169 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 3600 -4.3405E+05 2.4537E-01 4.8160E+01 NE2 7140

BOND = 33169.3626 ANGLE = 1268.9965 DIHED = 6165.0873
 VDWAALS = 82099.5677 EEL = -581921.0069 HBOND = 0.0000
 1-4 VDW = 1724.2484 1-4 EEL = 23440.4662 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 3700 -4.3421E+05 2.4109E-01 4.3220E+01 NE2 7140

BOND = 33203.3045 ANGLE = 1269.2048 DIHED = 6165.2235
 VDWAALS = 82237.9050 EEL = -582247.7279 HBOND = 0.0000
 1-4 VDW = 1723.6580 1-4 EEL = 23439.2129 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 3800 -4.3436E+05 1.4181E-01 2.0819E+01 NE2 7140

BOND = 33234.9833 ANGLE = 1268.4792 DIHED = 6165.2444
 VDWAALS = 82372.7976 EEL = -582562.1995 HBOND = 0.0000
 1-4 VDW = 1723.0838 1-4 EEL = 23438.6211 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 3900 -4.3450E+05 1.6010E-01 2.6267E+01 NE2 7140

Supplementary Text 3

BOND	=	33267.3689	ANGLE	=	1268.4968	DIHED	=	6165.1575
VDWAALS	=	82506.2003	EEL	=	-582868.6389	HBOND	=	0.0000
1-4 VDW	=	1722.5826	1-4 EEL	=	23437.8981	RESTRAINT	=	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
4000	-4.3464E+05	8.1295E-02	6.7586E+00	NE2	7140

BOND	=	33298.8828	ANGLE	=	1267.8028	DIHED	=	6164.9211
VDWAALS	=	82638.9229	EEL	=	-583173.5440	HBOND	=	0.0000
1-4 VDW	=	1722.1221	1-4 EEL	=	23437.7997	RESTRAINT	=	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
4100	-4.3478E+05	3.0435E-01	5.2191E+01	NE2	7140

BOND	=	33334.8794	ANGLE	=	1268.1942	DIHED	=	6164.5638
VDWAALS	=	82771.1504	EEL	=	-583479.4189	HBOND	=	0.0000
1-4 VDW	=	1721.7529	1-4 EEL	=	23438.2165	RESTRAINT	=	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
4200	-4.3492E+05	7.9363E-02	6.4143E+00	NE2	7140

BOND	=	33361.6533	ANGLE	=	1267.6805	DIHED	=	6164.1038
VDWAALS	=	82896.8825	EEL	=	-583771.0315	HBOND	=	0.0000
1-4 VDW	=	1721.4096	1-4 EEL	=	23438.2654	RESTRAINT	=	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
4300	-4.3506E+05	2.0912E-01	3.8895E+01	NE2	7140

BOND	=	33394.6399	ANGLE	=	1268.2725	DIHED	=	6163.6830
VDWAALS	=	83025.1295	EEL	=	-584068.4569	HBOND	=	0.0000
1-4 VDW	=	1720.9317	1-4 EEL	=	23437.9518	RESTRAINT	=	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
4400	-4.3519E+05	1.3127E-01	2.0152E+01	CG	6196

BOND	=	33422.7927	ANGLE	=	1267.6905	DIHED	=	6163.6447
VDWAALS	=	83145.8726	EEL	=	-584346.1183	HBOND	=	0.0000
1-4 VDW	=	1720.4557	1-4 EEL	=	23437.0078	RESTRAINT	=	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
4500	-4.3532E+05	1.0463E-01	1.4210E+01	NE2	7140

BOND	=	33451.5082	ANGLE	=	1266.9235	DIHED	=	6163.7132
VDWAALS	=	83264.6678	EEL	=	-584619.4069	HBOND	=	0.0000
1-4 VDW	=	1720.0763	1-4 EEL	=	23436.5790	RESTRAINT	=	0.0000

Supplementary Text 3

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
4600	-4.3544E+05	7.6402E-02	6.2995E+00	NE2	7140

BOND =	33478.6505	ANGLE =	1266.5204	DIHED =	6163.8230
VDWAALS =	83378.4579	EEL =	-584882.5755	HBOND =	0.0000
1-4 VDW =	1719.7523	1-4 EEL =	23436.2583	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
4700	-4.3556E+05	2.8284E-01	5.4720E+01	NE2	7140

BOND =	33508.5333	ANGLE =	1267.1370	DIHED =	6163.9533
VDWAALS =	83490.5650	EEL =	-585142.9004	HBOND =	0.0000
1-4 VDW =	1719.4453	1-4 EEL =	23436.0074	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
4800	-4.3569E+05	7.6255E-02	6.8137E+00	NE2	7140

BOND =	33533.0487	ANGLE =	1265.7543	DIHED =	6164.0501
VDWAALS =	83606.4810	EEL =	-585411.3571	HBOND =	0.0000
1-4 VDW =	1719.1226	1-4 EEL =	23436.1273	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
4900	-4.3581E+05	2.4034E-01	5.2165E+01	CG	6196

BOND =	33562.4024	ANGLE =	1266.0615	DIHED =	6164.1697
VDWAALS =	83723.1315	EEL =	-585676.5399	HBOND =	0.0000
1-4 VDW =	1718.8605	1-4 EEL =	23436.1895	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
5000	-4.3592E+05	1.6471E-01	3.0625E+01	NE2	7140

BOND =	33588.0177	ANGLE =	1265.1992	DIHED =	6164.2564
VDWAALS =	83838.5396	EEL =	-585934.3952	HBOND =	0.0000
1-4 VDW =	1718.5470	1-4 EEL =	23436.4684	RESTRAINT =	0.0000

Maximum number of minimization cycles reached.

FINAL RESULTS

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
5000	-4.3592E+05	1.6471E-01	3.0625E+01	NE2	7140

BOND =	33588.0177	ANGLE =	1265.1992	DIHED =	6164.2564
VDWAALS =	83838.5396	EEL =	-585934.3952	HBOND =	0.0000
1-4 VDW =	1718.5470	1-4 EEL =	23436.4684	RESTRAINT =	0.0000

Supplementary Text 3

5. TIMINGS

```

|           Build the list           22.48 (88.60% of List )
|           Other                    2.89 (11.40% of List )
| List time                          25.37 ( 0.25% of Nonbo)
|           Short_ene time          9366.05 (99.67% of Direc)
|           Other                   30.80 ( 0.33% of Direc)
| Direct Ewald time                  9396.85 (91.67% of Ewald)
| Adjust Ewald time                 34.49 ( 0.34% of Ewald)
|           Fill Bspline coeffs     27.03 ( 3.33% of Recip)
|           Fill charge grid        118.11 (14.54% of Recip)
|           Scalar sum              155.25 (19.11% of Recip)
|           Grad sum                208.52 (25.67% of Recip)
|           FFT time                 303.53 (37.36% of Recip)
| Recip Ewald time                   812.46 ( 7.93% of Ewald)
| Virial junk                        2.26 ( 0.02% of Ewald)
| Other                              4.82 ( 0.05% of Ewald)
|           Ewald time              10250.89 (99.75% of Nonbo)
| Nonbond force                     10276.27 (99.52% of Force)
| Bond/Angle/Dihedral               47.80 ( 0.46% of Force)
| Other                              1.32 ( 0.01% of Force)
| Force time                        10325.39 (100.0% of Runmd)
| Runmd Time                        10325.39 (99.72% of Total)
| Other                              29.19 ( 0.28% of Total)
| Total time                        10354.60 (100.0% of ALL )

```

| Number of list builds : 14

```

| Highest rstack allocated: 5827323
| Highest ystack allocated: 108587
| Job began at 14:53:00.793 on 08/13/2017
| Setup done at 14:53:01.768 on 08/13/2017
| Run done at 17:45:35.434 on 08/13/2017
| wallclock() was called 190076 times

```

Amber 16 SANDER

2016

| Run on 08/13/2017 at 07:02:43

```

| Executable path: /usr/local/amber16/bin/sander
| Working directory: /Users/Swati
| Hostname: Unknown
| [-0]verwriting output

```

File Assignments:

```

| MDIN: minimization_file_2.in
| MDOUT: ZSP9_min3_2.out
| INPCRD: ZSP9_min3_1.rst
| PARM: /Users/Swati/ZSP9_files/ZSP9.prmtop
| RESTR: ZSP9_min3_2.rst

```

Supplementary Text 3

```
| REFC: refc
| MDVEL: mdvel
| MDFRC: mdfrc
| MDEN: mden
| MDCRD: mdcrd
| MDINFO: mdinfo
| MTMD: mtmd
| INPDIP: inpdip
| RSTDIP: rstdip
| INPTRA: inptraj
```

Here is the input file:

```
PROT: minimization_2
&cntrl
imin = 1,
maxcyc = 5000,
ncyc = 10000,
igb = 0,
ntpr = 100,
ntp = 0
cut = 12
&end
```

1. RESOURCE USE:

```
| Flags:
| getting box info from netcdf restart file
| NetCDF restart box info found
| Largest sphere to fit in unit cell has radius = 42.894
| New format PARM file being parsed.
| Version = 1.000 Date = 08/07/17 Time = 06:43:25
| NATOM = 107718 NTYPES = 17 NBOH = 103122 MBONA = 4716
| NTHETH = 9972 MTHETA = 6416 NPHIH = 20783 MPHIA = 19788
| NHPARM = 0 NPARM = 0 NNB = 181165 NRES = 33503
| NBOH = 4716 NTHETA = 6416 NPHIA = 19788 NUMBND = 67
| NUMANG = 152 NPTRA = 191 NATYP = 36 NPHB = 1
| IFBOX = 1 NMXRS = 24 IFCAP = 0 NEXTRA = 0
| NCOPY = 0
```

```
| Memory Use Allocated
| Real 8489530
| Hollerith 356659
| Integer 4411905
| Max Pairs 98526064
| nblastReal 1292616
| nblast Int 3561915
| Total 493831 kbytes
```

Supplementary Text 3

| Note: 1-4 EEL scale factors are being read from the topology file.

| Note: 1-4 VDW scale factors are being read from the topology file.

| Duplicated 0 dihedrals

| Duplicated 0 dihedrals

BOX TYPE: RECTILINEAR

2. CONTROL DATA FOR THE RUN

default_name

General flags:

imin = 1, nmropt = 0

Nature and format of input:

ntx = 1, irest = 0, ntrx = 1

Nature and format of output:

ntxo = 2, ntp = 100, ntrx = 1, ntwr = 1
iwrap = 0, ntwx = 0, ntwv = 0, ntwe = 0
ioutfm = 1, ntwprt = 0, idecomp = 0, rbornstat = 0

Potential function:

ntf = 1, ntb = 1, igb = 0, nsnb = 25
ipol = 0, gbsa = 0, iesp = 0
dielc = 1.00000, cut = 12.00000, intdiel = 1.00000

Frozen or restrained atoms:

ibelly = 0, ntr = 0

Energy minimization:

maxcyc = 5000, ncyc = 10000, ntmin = 1
dx0 = 0.01000, drms = 0.00010

Ewald parameters:

verbose = 0, ew_type = 0, nbflag = 1, use_pme = 1
vdwmeth = 1, eedmeth = 1, netfric = 0
Box X = 119.635 Box Y = 85.788 Box Z = 124.094
Alpha = 90.000 Beta = 90.000 Gamma = 90.000
NFFT1 = 120 NFFT2 = 90 NFFT3 = 125
Cutoff = 12.000 Tol = 0.100E-04
Ewald Coefficient = 0.22664
Interpolation order = 4

| INFO: Old style inpcrd file read

3. ATOMIC COORDINATES AND VELOCITIES

default_name

Supplementary Text 3

begin time read from input coords = 0.000 ps

Number of triangulated 3-point waters found: 32903

Sum of charges from parm topology file = -0.00000034
 Forcing neutrality...

 4. RESULTS

 APPROXIMATING switch and d/dx switch using CUBIC SPLINE INTERPOLATION
 using 5000.0 points per unit in tabled values
 TESTING RELATIVE ERROR over r ranging from 0.0 to cutoff

| CHECK switch(x): max rel err = 0.2738E-14 at 2.422500
CHECK d/dx switch(x): max rel err = 0.7967E-11 at 2.716640

| Local SIZE OF NONBOND LIST = 53421490
 | TOTAL SIZE OF NONBOND LIST = 53421490

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
1	-3.9968E+05	4.4082E+00	3.2481E+02	CE1	5221
BOND =	32433.8734	ANGLE =	4402.9534	DIHED =	7075.4076
VDWAALS =	78355.6999	EEL =	-549978.1784	HBOND =	0.0000
1-4 VDW =	3444.5249	1-4 EEL =	24584.7867	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
100	-4.1405E+05	7.2624E-01	5.7842E+01	CZ	8770
BOND =	30580.8131	ANGLE =	1750.2106	DIHED =	6867.4645
VDWAALS =	71793.1882	EEL =	-551249.0705	HBOND =	0.0000
1-4 VDW =	2303.2207	1-4 EEL =	23904.3005	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
200	-4.1581E+05	5.7657E-01	9.8645E+01	CZ	8770
BOND =	30636.4204	ANGLE =	1493.6331	DIHED =	6803.0545
VDWAALS =	71887.9490	EEL =	-552522.0640	HBOND =	0.0000
1-4 VDW =	2118.9609	1-4 EEL =	23776.7070	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
300	-4.1684E+05	5.5339E-01	9.8778E+01	CG	3232
BOND =	30734.2105	ANGLE =	1392.4934	DIHED =	6771.3743
VDWAALS =	72213.9485	EEL =	-553720.4885	HBOND =	0.0000
1-4 VDW =	2044.2571	1-4 EEL =	23719.8506	RESTRAINT =	0.0000

Supplementary Text 3

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
400	-4.1761E+05	4.6208E-01	9.9316E+01	CG	3232

BOND	=	30827.3013	ANGLE	=	1343.4935	DIHED	=	6749.2181
VDWAALS	=	72582.4226	EEL	=	-554807.1539	HBOND	=	0.0000
1-4 VDW	=	2004.4568	1-4 EEL	=	23685.4693	RESTRAINT	=	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
500	-4.1827E+05	3.7544E-01	7.0650E+01	CZ	8770

BOND	=	30917.9788	ANGLE	=	1315.6533	DIHED	=	6730.8288
VDWAALS	=	72964.3157	EEL	=	-555835.1679	HBOND	=	0.0000
1-4 VDW	=	1979.1137	1-4 EEL	=	23660.1041	RESTRAINT	=	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
600	-4.1884E+05	3.1620E-01	5.6210E+01	CZ	8770

BOND	=	31006.3388	ANGLE	=	1297.8864	DIHED	=	6712.6602
VDWAALS	=	73336.7723	EEL	=	-556793.5465	HBOND	=	0.0000
1-4 VDW	=	1960.7565	1-4 EEL	=	23641.8617	RESTRAINT	=	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
700	-4.1934E+05	1.5491E-01	1.5797E+01	CZ	8770

BOND	=	31086.9947	ANGLE	=	1285.6745	DIHED	=	6698.6341
VDWAALS	=	73701.3199	EEL	=	-557688.8535	HBOND	=	0.0000
1-4 VDW	=	1946.6607	1-4 EEL	=	23627.1187	RESTRAINT	=	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
800	-4.1979E+05	5.7790E-01	1.0820E+02	CZ	8770

BOND	=	31181.7987	ANGLE	=	1279.0035	DIHED	=	6684.3977
VDWAALS	=	74054.8172	EEL	=	-558537.0950	HBOND	=	0.0000
1-4 VDW	=	1935.4130	1-4 EEL	=	23613.7034	RESTRAINT	=	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
900	-4.2021E+05	5.6034E-01	1.5607E+02	CG	3232

BOND	=	31255.1347	ANGLE	=	1273.8222	DIHED	=	6672.4587
VDWAALS	=	74387.0763	EEL	=	-559325.1971	HBOND	=	0.0000
1-4 VDW	=	1926.4883	1-4 EEL	=	23600.8920	RESTRAINT	=	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
1000	-4.2060E+05	1.3018E-01	1.0063E+01	CZ	8770

BOND	=	31315.0988	ANGLE	=	1269.3347	DIHED	=	6663.9999
VDWAALS	=	74702.1636	EEL	=	-560063.8571	HBOND	=	0.0000
1-4 VDW	=	1919.1231	1-4 EEL	=	23589.5280	RESTRAINT	=	0.0000

Supplementary Text 3

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
1100	-4.2096E+05	3.4872E-01	6.9535E+01	CZ	8770
BOND =	31389.1657	ANGLE =	1267.8813	DIHED =	6657.4656
VDWAALS =	75005.5362	EEL =	-560769.4472	HBOND =	0.0000
1-4 VDW =	1912.8305	1-4 EEL =	23579.5959	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
1200	-4.2130E+05	3.2014E-01	6.3435E+01	CZ	8770
BOND =	31454.8264	ANGLE =	1266.5995	DIHED =	6651.7771
VDWAALS =	75297.8929	EEL =	-561452.5029	HBOND =	0.0000
1-4 VDW =	1907.1498	1-4 EEL =	23571.2336	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
1300	-4.2163E+05	2.0882E-01	3.5305E+01	CZ	8770
BOND =	31513.6706	ANGLE =	1265.7256	DIHED =	6646.9245
VDWAALS =	75565.8721	EEL =	-562084.2102	HBOND =	0.0000
1-4 VDW =	1902.3406	1-4 EEL =	23564.0265	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
1400	-4.2194E+05	1.9980E-01	3.5723E+01	CZ	8770
BOND =	31573.0022	ANGLE =	1265.5867	DIHED =	6642.4846
VDWAALS =	75825.9113	EEL =	-562699.3791	HBOND =	0.0000
1-4 VDW =	1898.1290	1-4 EEL =	23557.2946	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
1500	-4.2224E+05	1.1496E-01	7.9267E+00	CZ	8770
BOND =	31629.6175	ANGLE =	1265.4450	DIHED =	6638.3776
VDWAALS =	76076.3709	EEL =	-563294.9112	HBOND =	0.0000
1-4 VDW =	1894.3553	1-4 EEL =	23551.3741	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
1600	-4.2252E+05	4.1203E-01	7.5173E+01	CZ	8770
BOND =	31693.5323	ANGLE =	1266.3129	DIHED =	6635.1195
VDWAALS =	76317.9240	EEL =	-563870.8327	HBOND =	0.0000
1-4 VDW =	1891.0067	1-4 EEL =	23546.8349	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
1700	-4.2280E+05	3.4146E-01	6.2231E+01	CZ	8770
BOND =	31745.8074	ANGLE =	1266.4467	DIHED =	6632.3513

Supplementary Text 3

VDWAALS = 76559.1520 EEL = -564437.7905 HBOND = 0.0000
 1-4 VDW = 1888.1556 1-4 EEL = 23542.9638 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 1800 -4.2307E+05 2.9358E-01 5.4976E+01 CZ 8770

BOND = 31797.0727 ANGLE = 1266.3760 DIHED = 6629.6371
 VDWAALS = 76793.5209 EEL = -564983.5788 HBOND = 0.0000
 1-4 VDW = 1885.7719 1-4 EEL = 23539.6328 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 1900 -4.2333E+05 2.6644E-01 4.4735E+01 CZ 8770

BOND = 31847.8514 ANGLE = 1265.9773 DIHED = 6627.1711
 VDWAALS = 77017.5452 EEL = -565508.9095 HBOND = 0.0000
 1-4 VDW = 1883.5268 1-4 EEL = 23537.2525 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 2000 -4.2358E+05 1.5134E-01 2.2192E+01 CZ 8770

BOND = 31894.1486 ANGLE = 1265.6912 DIHED = 6625.4577
 VDWAALS = 77230.4850 EEL = -566013.2263 HBOND = 0.0000
 1-4 VDW = 1881.6298 1-4 EEL = 23534.8619 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 2100 -4.2382E+05 1.0003E-01 6.0654E+00 CZ 8770

BOND = 31941.1326 ANGLE = 1265.1742 DIHED = 6624.2051
 VDWAALS = 77435.9029 EEL = -566502.6719 HBOND = 0.0000
 1-4 VDW = 1879.9426 1-4 EEL = 23532.8216 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 2200 -4.2406E+05 1.2015E-01 1.6229E+01 CZ 8770

BOND = 31987.6150 ANGLE = 1264.6596 DIHED = 6622.8719
 VDWAALS = 77632.6149 EEL = -566977.3769 HBOND = 0.0000
 1-4 VDW = 1878.4129 1-4 EEL = 23530.3655 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 2300 -4.2428E+05 1.0258E-01 9.5560E+00 CZ 8770

BOND = 32030.2945 ANGLE = 1264.2582 DIHED = 6621.4300
 VDWAALS = 77811.5446 EEL = -567416.0252 HBOND = 0.0000
 1-4 VDW = 1876.9808 1-4 EEL = 23527.8248 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 2400 -4.2450E+05 3.0176E-01 6.5946E+01 CG 3232

Supplementary Text 3

BOND	=	32075.4729	ANGLE	=	1264.2987	DIHED	=	6620.0146
VDWAALS	=	77983.1149	EEL	=	-567843.1782	HBOND	=	0.0000
1-4 VDW	=	1875.6714	1-4 EEL	=	23525.0918	RESTRAINT	=	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
2500	-4.2472E+05	2.4011E-01	4.7700E+01	CZ	8770

BOND	=	32115.6095	ANGLE	=	1263.7981	DIHED	=	6618.7517
VDWAALS	=	78146.8588	EEL	=	-568258.1858	HBOND	=	0.0000
1-4 VDW	=	1874.2964	1-4 EEL	=	23522.6782	RESTRAINT	=	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
2600	-4.2493E+05	1.3877E-01	2.1257E+01	CZ	8770

BOND	=	32154.0198	ANGLE	=	1263.3594	DIHED	=	6617.6831
VDWAALS	=	78307.0140	EEL	=	-568666.1240	HBOND	=	0.0000
1-4 VDW	=	1873.0558	1-4 EEL	=	23520.0227	RESTRAINT	=	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
2700	-4.2513E+05	1.6024E-01	2.9621E+01	CZ	8770

BOND	=	32193.0622	ANGLE	=	1263.1761	DIHED	=	6616.9484
VDWAALS	=	78459.9217	EEL	=	-569054.4248	HBOND	=	0.0000
1-4 VDW	=	1871.9028	1-4 EEL	=	23517.3045	RESTRAINT	=	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
2800	-4.2533E+05	1.1155E-01	1.5362E+01	CZ	8770

BOND	=	32230.1978	ANGLE	=	1262.9511	DIHED	=	6616.4419
VDWAALS	=	78606.8973	EEL	=	-569428.7949	HBOND	=	0.0000
1-4 VDW	=	1870.7755	1-4 EEL	=	23514.5940	RESTRAINT	=	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
2900	-4.2551E+05	3.1444E-01	6.7749E+01	CZ	8770

BOND	=	32271.4215	ANGLE	=	1263.2161	DIHED	=	6616.1796
VDWAALS	=	78747.6580	EEL	=	-569791.9180	HBOND	=	0.0000
1-4 VDW	=	1869.6984	1-4 EEL	=	23511.7658	RESTRAINT	=	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
3000	-4.2570E+05	2.8699E-01	5.7515E+01	CG	3232

BOND	=	32307.0646	ANGLE	=	1263.2544	DIHED	=	6616.1606
VDWAALS	=	78885.0426	EEL	=	-570153.6433	HBOND	=	0.0000
1-4 VDW	=	1868.6803	1-4 EEL	=	23508.7907	RESTRAINT	=	0.0000

Supplementary Text 3

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
3100	-4.2589E+05	2.4908E-01	4.9826E+01	CZ	8770

BOND =	32341.2695	ANGLE =	1263.2754	DIHED =	6616.2173
VDWAALS =	79011.7911	EEL =	-570494.0503	HBOND =	0.0000
1-4 VDW =	1867.6754	1-4 EEL =	23506.1864	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
3200	-4.2607E+05	1.9836E-01	4.0496E+01	CZ	8770

BOND =	32375.4351	ANGLE =	1263.4432	DIHED =	6616.4433
VDWAALS =	79137.6124	EEL =	-570837.3433	HBOND =	0.0000
1-4 VDW =	1866.7113	1-4 EEL =	23503.5005	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
3300	-4.2625E+05	1.5616E-01	2.9536E+01	CZ	8770

BOND =	32408.5616	ANGLE =	1263.6488	DIHED =	6616.5889
VDWAALS =	79258.6925	EEL =	-571169.0227	HBOND =	0.0000
1-4 VDW =	1865.8489	1-4 EEL =	23500.8772	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
3400	-4.2643E+05	3.6594E-01	6.9534E+01	CZ	8770

BOND =	32447.5500	ANGLE =	1264.2796	DIHED =	6616.5170
VDWAALS =	79378.7844	EEL =	-571499.0024	HBOND =	0.0000
1-4 VDW =	1865.0241	1-4 EEL =	23498.4710	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
3500	-4.2661E+05	3.0422E-01	6.4807E+01	CZ	8770

BOND =	32478.4387	ANGLE =	1264.4189	DIHED =	6616.1881
VDWAALS =	79495.7339	EEL =	-571820.0529	HBOND =	0.0000
1-4 VDW =	1864.3610	1-4 EEL =	23495.8511	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
3600	-4.2678E+05	2.7596E-01	6.3445E+01	CG	3232

BOND =	32510.2506	ANGLE =	1264.5700	DIHED =	6615.4842
VDWAALS =	79612.4280	EEL =	-572140.8481	HBOND =	0.0000
1-4 VDW =	1863.6485	1-4 EEL =	23493.4272	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
3700	-4.2695E+05	2.4080E-01	4.7797E+01	CZ	8770

BOND =	32541.6134	ANGLE =	1264.8384	DIHED =	6614.6970
VDWAALS =	79724.4035	EEL =	-572450.0645	HBOND =	0.0000
1-4 VDW =	1862.8613	1-4 EEL =	23491.2777	RESTRAINT =	0.0000

Supplementary Text 3

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
3800	-4.2712E+05	1.5149E-01	2.9079E+01	CZ	8770
BOND =	32571.7818	ANGLE =	1265.0748	DIHED =	6613.7944
VDWAALS =	79836.4213	EEL =	-572757.0903	HBOND =	0.0000
1-4 VDW =	1862.0373	1-4 EEL =	23489.1915	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
3900	-4.2729E+05	1.5089E-01	2.8782E+01	CZ	8770
BOND =	32603.9725	ANGLE =	1265.5565	DIHED =	6612.8637
VDWAALS =	79951.8510	EEL =	-573069.3684	HBOND =	0.0000
1-4 VDW =	1861.2330	1-4 EEL =	23487.0234	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
4000	-4.2745E+05	8.3240E-02	5.8736E+00	CZ	8770
BOND =	32633.3962	ANGLE =	1265.8517	DIHED =	6611.8438
VDWAALS =	80062.0119	EEL =	-573364.3710	HBOND =	0.0000
1-4 VDW =	1860.5512	1-4 EEL =	23485.0477	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
4100	-4.2760E+05	3.3192E-01	9.2775E+01	CG	3232
BOND =	32668.8279	ANGLE =	1266.6559	DIHED =	6610.5334
VDWAALS =	80176.2413	EEL =	-573664.9225	HBOND =	0.0000
1-4 VDW =	1859.8365	1-4 EEL =	23483.3216	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
4200	-4.2775E+05	2.4405E-01	4.8546E+01	CZ	8770
BOND =	32696.0130	ANGLE =	1267.0561	DIHED =	6608.8537
VDWAALS =	80287.1886	EEL =	-573953.4938	HBOND =	0.0000
1-4 VDW =	1859.3439	1-4 EEL =	23481.2563	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
4300	-4.2790E+05	2.3221E-01	4.5121E+01	CZ	8770
BOND =	32724.7778	ANGLE =	1267.3376	DIHED =	6606.5795
VDWAALS =	80395.4680	EEL =	-574235.9642	HBOND =	0.0000
1-4 VDW =	1858.6716	1-4 EEL =	23479.9656	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
4400	-4.2806E+05	1.4525E-01	2.7806E+01	CZ	8770
BOND =	32751.9228	ANGLE =	1266.7909	DIHED =	6604.9175

Supplementary Text 3

VDWAALS = 80503.7824 EEL = -574521.7083 HBOND = 0.0000
 1-4 VDW = 1858.0279 1-4 EEL = 23479.0393 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 4500 -4.2821E+05 1.4245E-01 2.6434E+01 CZ 8770

BOND = 32780.8036 ANGLE = 1265.9738 DIHED = 6604.2400
 VDWAALS = 80611.6085 EEL = -574809.5537 HBOND = 0.0000
 1-4 VDW = 1857.4086 1-4 EEL = 23478.3815 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 4600 -4.2836E+05 1.0197E-01 1.5087E+01 CZ 8770

BOND = 32808.6095 ANGLE = 1265.5495 DIHED = 6603.8858
 VDWAALS = 80717.7924 EEL = -575092.5015 HBOND = 0.0000
 1-4 VDW = 1856.8678 1-4 EEL = 23477.6491 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 4700 -4.2851E+05 8.7249E-02 9.6396E+00 CZ 8770

BOND = 32836.9438 ANGLE = 1265.3513 DIHED = 6603.4892
 VDWAALS = 80827.2761 EEL = -575377.9045 HBOND = 0.0000
 1-4 VDW = 1856.3565 1-4 EEL = 23476.8394 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 4800 -4.2865E+05 2.3059E-01 4.8289E+01 CZ 8770

BOND = 32867.2165 ANGLE = 1265.4592 DIHED = 6602.9873
 VDWAALS = 80938.2322 EEL = -575659.6539 HBOND = 0.0000
 1-4 VDW = 1855.9070 1-4 EEL = 23475.9226 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 4900 -4.2880E+05 2.2264E-01 4.2970E+01 CZ 8770

BOND = 32894.8902 ANGLE = 1265.5494 DIHED = 6602.4111
 VDWAALS = 81051.7878 EEL = -575943.0636 HBOND = 0.0000
 1-4 VDW = 1855.4865 1-4 EEL = 23474.8693 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 5000 -4.2894E+05 1.7728E-01 3.5294E+01 CZ 8770

BOND = 32921.1156 ANGLE = 1265.3979 DIHED = 6601.7029
 VDWAALS = 81161.7586 EEL = -576215.3173 HBOND = 0.0000
 1-4 VDW = 1855.0540 1-4 EEL = 23473.9436 RESTRAINT = 0.0000

Maximum number of minimization cycles reached.

Supplementary Text 3

FINAL RESULTS

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
5000	-4.2894E+05	1.7728E-01	3.5294E+01	CZ	8770
BOND =	32921.1156	ANGLE =	1265.3979	DIHED =	6601.7029
VDWAALS =	81161.7586	EEL =	-576215.3173	HBOND =	0.0000
1-4 VDW =	1855.0540	1-4 EEL =	23473.9436	RESTRAINT =	0.0000

 5. TIMINGS

	Build the list	21.09 (87.47% of List)
	Other	3.02 (12.53% of List)
	List time	24.11 (0.23% of Nonbo)
	Short_ene time	9420.14 (99.67% of Direc)
	Other	30.85 (0.33% of Direc)
	Direct Ewald time	9450.99 (91.62% of Ewald)
	Adjust Ewald time	35.53 (0.34% of Ewald)
	Fill Bspline coeffs	27.13 (3.30% of Recip)
	Fill charge grid	119.99 (14.61% of Recip)
	Scalar sum	156.59 (19.06% of Recip)
	Grad sum	202.58 (24.66% of Recip)
	FFT time	315.14 (38.36% of Recip)
	Recip Ewald time	821.46 (7.96% of Ewald)
	Virial junk	2.33 (0.02% of Ewald)
	Other	5.27 (0.05% of Ewald)
	Ewald time	10315.60 (99.77% of Nonbo)
	Nonbond force	10339.72 (99.49% of Force)
	Bond/Angle/Dihedral	51.30 (0.49% of Force)
	Other	1.36 (0.01% of Force)
	Force time	10392.37 (100.0% of Runmd)
	Runmd Time	10392.37 (99.69% of Total)
	Other	32.01 (0.31% of Total)
	Total time	10424.41 (100.0% of ALL)

| Number of list builds : 13

| Highest rstack allocated: 5729944
 | Highest istack allocated: 107718
 | Job began at 07:02:43.142 on 08/13/2017
 | Setup done at 07:02:44.005 on 08/13/2017
 | Run done at 09:56:27.585 on 08/13/2017
 | wallclock() was called 190074 times

 Amber 16 SANDER

2016

| Run on 02/21/2019 at 04:29:15

Supplementary Text 3

```
| Executable path: /usr/local/amber16/bin/sander  
| Working directory: /Users/Swati  
| Hostname: Unknown  
| [-O]verwriting output
```

File Assignments:

```
| MDIN: /Users/Swati/minimization_file_2.in  
| MDOUT: /Users/Swati/3WY9_files_2/truncated_3WY9_min3_2.out  
| INPCRD: /Users/Swati/3WY9_files_2/truncated_3WY9_min3_1.rst  
| PARM: /Users/Swati/3WY9_files_2/3WY9.prmtop  
| RESTRT: /Users/Swati/3WY9_files_2/truncated_3WY9_min3_2.rst  
| REFC: refc  
| MDVEL: mdvel  
| MDFRC: mdfrc  
| MDEN: mden  
| MDCRD: mdcrd  
| MDINFO: mdinfo  
| MTMD: mtmd  
| INPDIP: inpdip  
| RSTDIP: rstcip  
| INPTRA: inptraj
```

Here is the input file:

```
PROT: minimization_2  
&cntrl  
imin = 1,  
maxcyc = 5000,  
ncyc = 10000,  
igb = 0,  
ntpr = 100,  
ntp = 0  
cut = 12  
&end
```

1. RESOURCE USE:

```
| Flags:  
| getting box info from netcdf restart file  
| NetCDF restart box info found  
| Largest sphere to fit in unit cell has radius = 43.417  
| New format PARM file being parsed.  
| Version = 1.000 Date = 08/09/17 Time = 18:38:06  
NATOM = 89944 NTYPES = 17 NBONH = 86305 MBONA = 3731  
NTHETH = 7791 MTHETA = 5069 NPHIH = 16227 MPHIA = 15704  
NHPARM = 0 NPARM = 0 NNB = 149382 NRES = 28096  
NBONA = 3731 NTHETA = 5069 NPHIA = 15704 NUMBND = 67  
NUMANG = 152 NPTRA = 191 NATYP = 36 NPHB = 1  
IFBOX = 1 NMXRS = 24 IFCAP = 0 NEXTRA = 0
```

Supplementary Text 3

NCOPY = 0

Memory Use	Allocated
Real	7102941
Hollerith	297930
Integer	3593065
Max Pairs	82268778
nblastReal	1079328
nblast Int	2979057
Total	412122 kbytes

| Note: 1-4 EEL scale factors are being read from the topology file.

| Note: 1-4 VDW scale factors are being read from the topology file.

| Duplicated 0 dihedrals

| Duplicated 0 dihedrals

BOX TYPE: RECTILINEAR

 2. CONTROL DATA FOR THE RUN

default_name

General flags:

imin = 1, nmropt = 0

Nature and format of input:

ntx = 1, irest = 0, ntrx = 1

Nature and format of output:

ntxo = 2, ntrp = 100, ntrx = 1, ntwr = 1
 iwrap = 0, ntwx = 0, ntwv = 0, ntwe = 0
 ioutfm = 1, ntwprt = 0, idecomp = 0, rbornstat = 0

Potential function:

ntf = 1, ntb = 1, igb = 0, nsnb = 25
 ipol = 0, gbsa = 0, iesp = 0
 dielc = 1.00000, cut = 12.00000, intdiel = 1.00000

Frozen or restrained atoms:

ibelly = 0, ntr = 0

Energy minimization:

maxcyc = 5000, ncyc = 10000, ntmin = 1
 dx0 = 0.01000, drms = 0.00010

Ewald parameters:

verbose = 0, ew_type = 0, nbflag = 1, use_pme = 1
 vdwmeth = 1, eedmeth = 1, netfric = 0
 Box X = 117.210 Box Y = 86.834 Box Z = 105.320
 Alpha = 90.000 Beta = 90.000 Gamma = 90.000

Supplementary Text 3

NFFT1 = 120 NFFT2 = 90 NFFT3 = 108
 Cutoff= 12.000 Tol = 0.100E-04
 Ewald Coefficient = 0.22664
 Interpolation order = 4

| INFO: Old style inpcrd file read

 3. ATOMIC COORDINATES AND VELOCITIES

default_name

begin time read from input coords = 0.000 ps

Number of triangulated 3-point waters found: 27622

Sum of charges from parm topology file = -0.00000030
 Forcing neutrality...

 4. RESULTS

 APPROXIMATING switch and d/dx switch using CUBIC SPLINE INTERPOLATION
 using 5000.0 points per unit in tabled values

TESTING RELATIVE ERROR over r ranging from 0.0 to cutoff

| CHECK switch(x): max rel err = 0.2738E-14 at 2.422500

| CHECK d/dx switch(x): max rel err = 0.7967E-11 at 2.716640

| Local SIZE OF NONBOND LIST = 44435104

| TOTAL SIZE OF NONBOND LIST = 44435104

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
1	-3.3570E+05	4.4705E+00	7.3544E+02	C	3773
BOND =	36377.0014	ANGLE =	2650.3300	DIHED =	5381.3421
VDWAALS =	65807.3845	EEL =	-469077.7931	HBOND =	0.0000
1-4 VDW =	2197.8628	1-4 EEL =	20962.0641	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
100	-3.5025E+05	6.9449E-01	1.2712E+02	N	3789
BOND =	27031.5879	ANGLE =	1516.8236	DIHED =	5402.5154
VDWAALS =	63530.8221	EEL =	-469847.9188	HBOND =	0.0000
1-4 VDW =	1690.4601	1-4 EEL =	20426.3791	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
200	-3.5175E+05	6.1494E-01	9.4068E+01	C	3787
BOND =	26640.0580	ANGLE =	1283.0204	DIHED =	5371.9422

Supplementary Text 3

VDWAALS = 63592.7272 EEL = -470584.0847 HBOND = 0.0000
 1-4 VDW = 1589.9694 1-4 EEL = 20353.6026 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 300 -3.5250E+05 5.8636E-01 1.2914E+02 CD 3234

BOND = 26552.7552 ANGLE = 1204.3470 DIHED = 5347.5305
 VDWAALS = 63746.9670 EEL = -471238.9004 HBOND = 0.0000
 1-4 VDW = 1555.3613 1-4 EEL = 20335.4100 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 400 -3.5302E+05 4.7726E-01 7.9582E+01 CD 3234

BOND = 26545.3261 ANGLE = 1145.6396 DIHED = 5333.5248
 VDWAALS = 63922.7691 EEL = -471837.0130 HBOND = 0.0000
 1-4 VDW = 1534.5648 1-4 EEL = 20333.0602 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 500 -3.5346E+05 4.2275E-01 6.4251E+01 C 3787

BOND = 26566.4500 ANGLE = 1082.2853 DIHED = 5324.1443
 VDWAALS = 64111.0034 EEL = -472400.4148 HBOND = 0.0000
 1-4 VDW = 1521.8673 1-4 EEL = 20338.5228 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 600 -3.5384E+05 3.5467E-01 6.1094E+01 N 3789

BOND = 26593.6258 ANGLE = 1019.4151 DIHED = 5320.7823
 VDWAALS = 64310.9792 EEL = -472942.4822 HBOND = 0.0000
 1-4 VDW = 1511.0032 1-4 EEL = 20342.3286 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 700 -3.5418E+05 2.8741E-01 4.7548E+01 C 3787

BOND = 26626.0208 ANGLE = 990.4963 DIHED = 5315.1192
 VDWAALS = 64503.3558 EEL = -473465.7901 HBOND = 0.0000
 1-4 VDW = 1502.9418 1-4 EEL = 20345.6433 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 800 -3.5447E+05 1.2379E-01 8.5597E+00 C 3787

BOND = 26657.1895 ANGLE = 977.7999 DIHED = 5310.7030
 VDWAALS = 64694.8466 EEL = -473961.6221 HBOND = 0.0000
 1-4 VDW = 1498.4252 1-4 EEL = 20348.4099 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 900 -3.5474E+05 1.2717E-01 1.1239E+01 N 3789

Supplementary Text 3

BOND	=	26696.4335	ANGLE	=	968.5064	DIHED	=	5308.0440
VDWAALS	=	64889.9751	EEL	=	-474452.5659	HBOND	=	0.0000
1-4 VDW	=	1494.9843	1-4 EEL	=	20350.5116	RESTRAINT	=	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
1000	-3.5498E+05	4.5368E-01	6.7079E+01	N	3789

BOND	=	26745.0513	ANGLE	=	963.1718	DIHED	=	5306.3550
VDWAALS	=	65082.6645	EEL	=	-474925.2180	HBOND	=	0.0000
1-4 VDW	=	1491.8941	1-4 EEL	=	20351.5484	RESTRAINT	=	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
1100	-3.5522E+05	3.8712E-01	5.2983E+01	C	3787

BOND	=	26780.8717	ANGLE	=	961.2304	DIHED	=	5305.6539
VDWAALS	=	65273.0402	EEL	=	-475381.6141	HBOND	=	0.0000
1-4 VDW	=	1489.3339	1-4 EEL	=	20353.0157	RESTRAINT	=	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
1200	-3.5544E+05	4.0197E-01	6.6361E+01	CD	3234

BOND	=	26824.4265	ANGLE	=	955.4600	DIHED	=	5306.7788
VDWAALS	=	65459.9214	EEL	=	-475824.7086	HBOND	=	0.0000
1-4 VDW	=	1486.8931	1-4 EEL	=	20353.5044	RESTRAINT	=	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
1300	-3.5565E+05	3.0666E-01	3.8369E+01	C	3787

BOND	=	26858.8046	ANGLE	=	954.2594	DIHED	=	5303.4012
VDWAALS	=	65636.7127	EEL	=	-476245.2930	HBOND	=	0.0000
1-4 VDW	=	1484.6364	1-4 EEL	=	20355.1162	RESTRAINT	=	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
1400	-3.5585E+05	2.4090E-01	3.1480E+01	C	3787

BOND	=	26898.5396	ANGLE	=	950.7193	DIHED	=	5301.7393
VDWAALS	=	65810.8529	EEL	=	-476650.4426	HBOND	=	0.0000
1-4 VDW	=	1482.4716	1-4 EEL	=	20356.0021	RESTRAINT	=	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
1500	-3.5604E+05	1.2237E-01	1.1506E+01	C	3802

BOND	=	26934.9643	ANGLE	=	949.7724	DIHED	=	5300.1586
VDWAALS	=	65979.5224	EEL	=	-477046.6295	HBOND	=	0.0000
1-4 VDW	=	1480.7263	1-4 EEL	=	20357.7625	RESTRAINT	=	0.0000

Supplementary Text 3

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
1600	-3.5623E+05	1.0447E-01	6.5359E+00	C	3787

BOND =	26973.5337	ANGLE =	948.3894	DIHED =	5298.8699
VDWAALS =	66143.2977	EEL =	-477433.7001	HBOND =	0.0000
1-4 VDW =	1479.1077	1-4 EEL =	20359.4025	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
1700	-3.5641E+05	3.5904E-01	4.9246E+01	C	3787

BOND =	27016.3501	ANGLE =	947.6783	DIHED =	5297.6234
VDWAALS =	66304.1595	EEL =	-477813.7997	HBOND =	0.0000
1-4 VDW =	1477.7307	1-4 EEL =	20360.9338	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
1800	-3.5659E+05	3.0895E-01	4.3408E+01	CG	3219

BOND =	27051.3977	ANGLE =	946.7535	DIHED =	5295.9649
VDWAALS =	66459.2936	EEL =	-478186.0448	HBOND =	0.0000
1-4 VDW =	1476.5156	1-4 EEL =	20362.9189	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
1900	-3.5677E+05	2.6565E-01	3.0004E+01	C	3787

BOND =	27088.3226	ANGLE =	943.6513	DIHED =	5295.6954
VDWAALS =	66604.8802	EEL =	-478540.7310	HBOND =	0.0000
1-4 VDW =	1475.4424	1-4 EEL =	20363.6225	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
2000	-3.5695E+05	2.3324E-01	2.8154E+01	CG	3219

BOND =	27123.8935	ANGLE =	942.8663	DIHED =	5294.8963
VDWAALS =	66750.9726	EEL =	-478897.0472	HBOND =	0.0000
1-4 VDW =	1474.5281	1-4 EEL =	20364.7091	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
2100	-3.5711E+05	1.2024E-01	1.0887E+01	C	3756

BOND =	27159.1501	ANGLE =	940.8324	DIHED =	5294.8052
VDWAALS =	66892.3006	EEL =	-479240.0677	HBOND =	0.0000
1-4 VDW =	1473.5660	1-4 EEL =	20365.2272	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
2200	-3.5728E+05	1.0093E-01	6.8957E+00	C	3756

BOND =	27194.4651	ANGLE =	940.0978	DIHED =	5294.2600
VDWAALS =	67031.2324	EEL =	-479575.1310	HBOND =	0.0000
1-4 VDW =	1472.7296	1-4 EEL =	20365.8945	RESTRAINT =	0.0000

Supplementary Text 3

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
2300	-3.5743E+05	3.5229E-01	4.5395E+01	C	3756
BOND =	27233.9260	ANGLE =	940.7672	DIHED =	5293.4005
VDWAALS =	67170.3450	EEL =	-479910.3779	HBOND =	0.0000
1-4 VDW =	1472.1051	1-4 EEL =	20366.5537	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
2400	-3.5759E+05	3.4363E-01	7.7904E+01	CG	3219
BOND =	27269.6344	ANGLE =	938.4750	DIHED =	5293.1087
VDWAALS =	67304.5438	EEL =	-480235.5482	HBOND =	0.0000
1-4 VDW =	1471.5003	1-4 EEL =	20366.9713	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
2500	-3.5774E+05	2.4859E-01	3.2101E+01	C	3756
BOND =	27300.1420	ANGLE =	938.0541	DIHED =	5292.2229
VDWAALS =	67434.7792	EEL =	-480548.9865	HBOND =	0.0000
1-4 VDW =	1470.9216	1-4 EEL =	20368.1478	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
2600	-3.5789E+05	2.4858E-01	4.3231E+01	CG	3219
BOND =	27333.6367	ANGLE =	936.5515	DIHED =	5292.0147
VDWAALS =	67561.9958	EEL =	-480854.3612	HBOND =	0.0000
1-4 VDW =	1470.3106	1-4 EEL =	20368.6210	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
2700	-3.5804E+05	1.8594E-01	2.2011E+01	C	3756
BOND =	27363.4995	ANGLE =	936.2022	DIHED =	5291.3768
VDWAALS =	67685.7290	EEL =	-481151.1435	HBOND =	0.0000
1-4 VDW =	1469.6473	1-4 EEL =	20369.5776	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
2800	-3.5817E+05	1.2001E-01	1.1859E+01	C	3756
BOND =	27393.5415	ANGLE =	935.1194	DIHED =	5291.2036
VDWAALS =	67803.2085	EEL =	-481436.7262	HBOND =	0.0000
1-4 VDW =	1468.9505	1-4 EEL =	20370.0416	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
2900	-3.5831E+05	1.0956E-01	8.9988E+00	C	3745
BOND =	27422.4813	ANGLE =	934.8567	DIHED =	5290.8932

Supplementary Text 3

VDWAALS = 67915.6454 EEL = -481712.6968 HBOND = 0.0000
 1-4 VDW = 1468.3352 1-4 EEL = 20370.5190 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 3000 -3.5844E+05 3.5022E-01 9.0234E+01 CG 3219

BOND = 27453.8586 ANGLE = 934.9934 DIHED = 5290.8182
 VDWAALS = 68023.0113 EEL = -481979.6135 HBOND = 0.0000
 1-4 VDW = 1467.7146 1-4 EEL = 20371.2099 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 3100 -3.5857E+05 2.4742E-01 3.2119E+01 CG 3219

BOND = 27480.4746 ANGLE = 934.2605 DIHED = 5290.9548
 VDWAALS = 68128.4966 EEL = -482245.9187 HBOND = 0.0000
 1-4 VDW = 1467.1954 1-4 EEL = 20371.4153 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 3200 -3.5871E+05 2.2581E-01 1.9924E+01 NE2 2687

BOND = 27506.5788 ANGLE = 934.3734 DIHED = 5290.8974
 VDWAALS = 68230.6592 EEL = -482506.2406 HBOND = 0.0000
 1-4 VDW = 1466.8148 1-4 EEL = 20371.8743 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 3300 -3.5884E+05 1.8625E-01 1.8575E+01 NE2 2687

BOND = 27533.0392 ANGLE = 933.4891 DIHED = 5291.1381
 VDWAALS = 68331.2722 EEL = -482763.5724 HBOND = 0.0000
 1-4 VDW = 1466.3332 1-4 EEL = 20372.2477 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 3400 -3.5897E+05 8.5762E-02 4.4971E+00 NE2 2687

BOND = 27557.7019 ANGLE = 933.1223 DIHED = 5291.3123
 VDWAALS = 68430.8792 EEL = -483016.7188 HBOND = 0.0000
 1-4 VDW = 1465.9792 1-4 EEL = 20372.6957 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 3500 -3.5909E+05 8.1721E-02 3.5374E+00 NE2 2687

BOND = 27583.3052 ANGLE = 932.6942 DIHED = 5291.6138
 VDWAALS = 68530.8927 EEL = -483270.1362 HBOND = 0.0000
 1-4 VDW = 1465.6215 1-4 EEL = 20373.1603 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 3600 -3.5921E+05 2.9391E-01 4.1567E+01 CG 3219

Supplementary Text 3

BOND	=	27610.4751	ANGLE	=	932.7623	DIHED	=	5292.0204
VDWAALS	=	68626.6159	EEL	=	-483512.8218	HBOND	=	0.0000
1-4 VDW	=	1465.2609	1-4 EEL	=	20373.7782	RESTRAINT	=	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
3700	-3.5933E+05	2.5350E-01	4.9543E+01	CG	3219

BOND	=	27633.1467	ANGLE	=	932.4384	DIHED	=	5292.4257
VDWAALS	=	68720.6220	EEL	=	-483750.9871	HBOND	=	0.0000
1-4 VDW	=	1464.9873	1-4 EEL	=	20374.3681	RESTRAINT	=	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
3800	-3.5945E+05	2.2008E-01	2.6801E+01	NE2	2687

BOND	=	27656.5848	ANGLE	=	931.8160	DIHED	=	5292.8884
VDWAALS	=	68815.3417	EEL	=	-483986.0734	HBOND	=	0.0000
1-4 VDW	=	1464.6792	1-4 EEL	=	20374.8191	RESTRAINT	=	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
3900	-3.5957E+05	1.0382E-01	9.9506E+00	NE2	2687

BOND	=	27678.8134	ANGLE	=	931.2730	DIHED	=	5293.2151
VDWAALS	=	68912.7542	EEL	=	-484221.9820	HBOND	=	0.0000
1-4 VDW	=	1464.4012	1-4 EEL	=	20375.4670	RESTRAINT	=	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
4000	-3.5967E+05	1.5135E-01	1.7563E+01	NE2	2687

BOND	=	27701.9718	ANGLE	=	930.8378	DIHED	=	5293.1598
VDWAALS	=	69006.7114	EEL	=	-484445.1331	HBOND	=	0.0000
1-4 VDW	=	1464.0853	1-4 EEL	=	20376.1478	RESTRAINT	=	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
4100	-3.5977E+05	7.4426E-02	3.5786E+00	NE2	2687

BOND	=	27723.3847	ANGLE	=	930.4472	DIHED	=	5292.9322
VDWAALS	=	69098.4270	EEL	=	-484660.4658	HBOND	=	0.0000
1-4 VDW	=	1463.8385	1-4 EEL	=	20376.8030	RESTRAINT	=	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
4200	-3.5987E+05	2.8711E-01	3.3497E+01	NE2	2687

BOND	=	27748.2469	ANGLE	=	930.9931	DIHED	=	5292.9934
VDWAALS	=	69191.8753	EEL	=	-484877.0549	HBOND	=	0.0000
1-4 VDW	=	1463.6234	1-4 EEL	=	20377.5125	RESTRAINT	=	0.0000

Supplementary Text 3

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
4300	-3.5997E+05	7.3571E-02	4.2971E+00	NE2	2687

BOND =	27766.8385	ANGLE =	929.8444	DIHED =	5293.2808
VDWAALS =	69283.0656	EEL =	-485084.9309	HBOND =	0.0000
1-4 VDW =	1463.3472	1-4 EEL =	20378.3734	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
4400	-3.6006E+05	2.1425E-01	3.4098E+01	CD	3234

BOND =	27790.2077	ANGLE =	930.0020	DIHED =	5293.4777
VDWAALS =	69377.4692	EEL =	-485298.0072	HBOND =	0.0000
1-4 VDW =	1463.1633	1-4 EEL =	20379.1465	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
4500	-3.6016E+05	1.7655E-01	2.2437E+01	NE2	2687

BOND =	27810.8422	ANGLE =	929.4957	DIHED =	5293.5194
VDWAALS =	69468.2680	EEL =	-485502.9157	HBOND =	0.0000
1-4 VDW =	1463.0261	1-4 EEL =	20379.6328	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
4600	-3.6025E+05	9.2804E-02	8.5069E+00	NE2	2687

BOND =	27830.5447	ANGLE =	929.0364	DIHED =	5293.5466
VDWAALS =	69556.9879	EEL =	-485703.9807	HBOND =	0.0000
1-4 VDW =	1462.9877	1-4 EEL =	20380.0500	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
4700	-3.6034E+05	7.3819E-02	5.0223E+00	NE2	2687

BOND =	27850.0203	ANGLE =	928.7309	DIHED =	5293.7118
VDWAALS =	69642.4630	EEL =	-485897.1561	HBOND =	0.0000
1-4 VDW =	1462.8310	1-4 EEL =	20380.3379	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
4800	-3.6043E+05	7.9689E-02	6.7168E+00	NE2	2687

BOND =	27869.5112	ANGLE =	928.5959	DIHED =	5293.9324
VDWAALS =	69728.2261	EEL =	-486090.7836	HBOND =	0.0000
1-4 VDW =	1462.6960	1-4 EEL =	20380.6114	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
4900	-3.6051E+05	2.2971E-01	2.8571E+01	NE2	2687

BOND =	27890.1278	ANGLE =	928.8873	DIHED =	5294.1834
VDWAALS =	69812.6451	EEL =	-486279.9148	HBOND =	0.0000
1-4 VDW =	1462.6257	1-4 EEL =	20380.8848	RESTRAINT =	0.0000

Supplementary Text 3

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
5000	-3.6059E+05	1.9451E-01	2.4554E+01	NE2	2687
BOND =	27908.1261	ANGLE =	928.1343	DIHED =	5294.5330
VDWAALS =	69895.8320	EEL =	-486464.6504	HBOND =	0.0000
1-4 VDW =	1462.5575	1-4 EEL =	20381.2479	RESTRAINT =	0.0000

Maximum number of minimization cycles reached.

FINAL RESULTS

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
5000	-3.6059E+05	1.9451E-01	2.4554E+01	NE2	2687
BOND =	27908.1261	ANGLE =	928.1343	DIHED =	5294.5330
VDWAALS =	69895.8320	EEL =	-486464.6504	HBOND =	0.0000
1-4 VDW =	1462.5575	1-4 EEL =	20381.2479	RESTRAINT =	0.0000

5. TIMINGS

Build the list	26.24 (91.22% of List)
Other	2.53 (8.78% of List)
List time	28.77 (0.17% of Nonbo)
Short_ene time	8205.70 (99.68% of Direc)
Other	26.35 (0.32% of Direc)
Direct Ewald time	8232.05 (47.70% of Ewald)
Adjust Ewald time	30.72 (0.18% of Ewald)
Fill Bspline coeffs	24.31 (0.27% of Recip)
Fill charge grid	102.29 (1.14% of Recip)
Scalar sum	140.77 (1.57% of Recip)
Grad sum	8437.62 (93.87% of Recip)
FFT time	283.53 (3.15% of Recip)
Recip Ewald time	8988.53 (52.08% of Ewald)
Virial junk	1.87 (0.01% of Ewald)
Other	4.33 (0.03% of Ewald)
Ewald time	17257.52 (99.83% of Nonbo)
Nonbond force	17286.30 (99.75% of Force)
Bond/Angle/Dihedral	42.12 (0.24% of Force)
Other	1.04 (0.01% of Force)
Force time	17329.46 (100.0% of Runmd)
Runmd Time	17329.46 (99.85% of Total)
Other	26.33 (0.15% of Total)
Total time	17355.86 (100.0% of ALL)

| Number of list builds : 19

Supplementary Text 3

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| Highest rstack allocated: 4877674
| Highest irstack allocated: 89944
|           Job began at 04:29:15.661 on 02/21/2019
|           Setup done at 04:29:16.533 on 02/21/2019
|           Run done at 09:18:31.519 on 02/21/2019
| wallclock() was called 190086 times
```

```
-----
Amber 16 SANDER                               2016
-----
```

| Run on 02/21/2019 at 12:02:52

```
| Executable path: /usr/local/amber16/bin/sander
| Working directory: /Users/Swati
|           Hostname: Unknown
| [-O]verwriting output
```

File Assignments:

```
| MDIN: /Users/Swati/minimization_file_2.in
| MDOUT: /Users/Swati/LJP6_files_2/truncated_LJP6_min3_2.out
| INPCRD: /Users/Swati/LJP6_files_2/truncated_LJP6_min3_1.rst
| PARM: /Users/Swati/LJP6_files_2/LJP6.prmtop
| RESTRT: /Users/Swati/LJP6_files_2/truncated_LJP6_min3_2.rst
| REFC: refc
| MDVEL: mdvel
| MDFRC: mdfrc
| MDEN: mden
| MDCRD: mdcrd
| MDINFO: mdinfo
| MTMD: mtmd
| INPDIP: inpdip
| RSTDIP: rstcip
| INPTRAJ: inptraj
```

Here is the input file:

```
PROT: minimization_2
&cntrl
imin = 1,
maxcyc = 5000,
ncyc = 10000,
igb = 0,
ntpr = 100,
ntp = 0
cut = 12
&end
```

```
-----
1. RESOURCE USE:
-----
```

Supplementary Text 3

```
| Flags:
| getting box info from netcdf restart file
| NetCDF restart box info found
| Largest sphere to fit in unit cell has radius = 42.185
| New format PARM file being parsed.
| Version = 1.000 Date = 08/09/17 Time = 04:08:03
| NATOM = 87372 NTYPES = 17 NBONH = 83756 MBONA = 3718
| NTHETH = 7789 MTHETA = 5057 NPHIH = 16221 MPHIA = 15711
| NHPARM = 0 NPARM = 0 NNB = 145906 NRES = 27236
| NBONA = 3718 NTHETA = 5057 NPHIA = 15711 NUMBND = 67
| NUMANG = 152 NPTRA = 191 NATYP = 36 NPHB = 1
| IFBOX = 1 NMXRS = 24 IFCAP = 0 NEXTRA = 0
| NCOPY = 0
```

```
| Memory Use Allocated
| Real 6902375
| Hollerith 289354
| Integer 3534516
| Max Pairs 79916256
| nblastReal 1048464
| nblast Int 2924001
| Total 400647 kbytes
```

| Note: 1-4 EEL scale factors are being read from the topology file.

| Note: 1-4 VDW scale factors are being read from the topology file.

| Duplicated 0 dihedrals

| Duplicated 0 dihedrals

BOX TYPE: RECTILINEAR

2. CONTROL DATA FOR THE RUN

default_name

General flags:

imin = 1, nmropt = 0

Nature and format of input:

ntx = 1, irest = 0, ntrx = 1

Nature and format of output:

ntxo = 2, ntp = 100, ntrx = 1, ntwr = 1
iwrap = 0, ntwx = 0, ntwv = 0, ntwe = 0
ioutfm = 1, ntwprt = 0, idecomp = 0, rbornstat = 0

Potential function:

ntf = 1, ntb = 1, igb = 0, nsnb = 25
ipol = 0, gbsa = 0, iesp = 0
dielc = 1.00000, cut = 12.00000, intdiel = 1.00000

Supplementary Text 3

Frozen or restrained atoms:

ibelly = 0, ntr = 0

Energy minimization:

maxcyc = 5000, ncyc = 10000, ntmin = 1
 dx0 = 0.01000, drms = 0.00010

Ewald parameters:

verbose = 0, ew_type = 0, nbflag = 1, use_pme = 1
 vdwmeth = 1, eedmeth = 1, netfrnc = 0
 Box X = 117.910 Box Y = 84.370 Box Z = 105.320
 Alpha = 90.000 Beta = 90.000 Gamma = 90.000
 NFFT1 = 120 NFFT2 = 90 NFFT3 = 108
 Cutoff= 12.000 Tol = 0.100E-04
 Ewald Coefficient = 0.22664
 Interpolation order = 4

| INFO: Old style inpcrd file read

 3. ATOMIC COORDINATES AND VELOCITIES

default_name

begin time read from input coords = 0.000 ps

Number of triangulated 3-point waters found: 26771

Sum of charges from parm topology file = -0.00000030
 Forcing neutrality...

 4. RESULTS

 APPROXIMATING switch and d/dx switch using CUBIC SPLINE INTERPOLATION
 using 5000.0 points per unit in tabled values
 TESTING RELATIVE ERROR over r ranging from 0.0 to cutoff

| CHECK switch(x): max rel err = 0.2738E-14 at 2.422500
 | CHECK d/dx switch(x): max rel err = 0.7967E-11 at 2.716640

| Local SIZE OF NONBOND LIST = 42990561
 | TOTAL SIZE OF NONBOND LIST = 42990561

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
1	-3.2648E+05	4.4620E+00	7.3662E+02	C	3764
BOND =	36149.0277	ANGLE =	2659.3115	DIHED =	5394.6458
VDWAALS =	66891.9642	EEL =	-459857.9824	HBOND =	0.0000
1-4 VDW =	2117.0330	1-4 EEL =	20167.4574	RESTRAINT =	0.0000

Supplementary Text 3

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
100	-3.4060E+05	6.2106E-01	1.3272E+02	CD	3231

BOND =	26923.6423	ANGLE =	1568.8696	DIHED =	5408.8239
VDWAALS =	64557.1993	EEL =	-460414.3375	HBOND =	0.0000
1-4 VDW =	1698.2596	1-4 EEL =	19660.0467	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
200	-3.4200E+05	7.7236E-01	2.1460E+02	CD	3231

BOND =	26497.6987	ANGLE =	1352.0073	DIHED =	5349.4163
VDWAALS =	64510.0292	EEL =	-460926.7872	HBOND =	0.0000
1-4 VDW =	1605.2364	1-4 EEL =	19614.0185	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
300	-3.4271E+05	6.8305E-01	1.6928E+02	CD	3231

BOND =	26395.6662	ANGLE =	1232.6552	DIHED =	5329.3898
VDWAALS =	64569.7896	EEL =	-461403.9473	HBOND =	0.0000
1-4 VDW =	1564.1965	1-4 EEL =	19604.0078	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
400	-3.4320E+05	5.8303E-01	1.0341E+02	CD	2309

BOND =	26363.0651	ANGLE =	1147.6336	DIHED =	5319.7943
VDWAALS =	64671.5429	EEL =	-461845.3620	HBOND =	0.0000
1-4 VDW =	1539.1826	1-4 EEL =	19605.4762	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
500	-3.4359E+05	1.4666E-01	1.2756E+01	CD	2309

BOND =	26352.1294	ANGLE =	1087.3992	DIHED =	5311.7066
VDWAALS =	64788.8793	EEL =	-462265.5709	HBOND =	0.0000
1-4 VDW =	1521.9374	1-4 EEL =	19611.5782	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
600	-3.4392E+05	3.7980E-01	3.8033E+01	C	3778

BOND =	26367.8209	ANGLE =	1052.6143	DIHED =	5304.2604
VDWAALS =	64918.2934	EEL =	-462689.8453	HBOND =	0.0000
1-4 VDW =	1510.4032	1-4 EEL =	19618.0880	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
700	-3.4422E+05	3.2621E-01	5.7659E+01	C	3778

BOND =	26382.9183	ANGLE =	1033.6388	DIHED =	5297.1536
VDWAALS =	65062.0022	EEL =	-463116.9104	HBOND =	0.0000
1-4 VDW =	1502.4715	1-4 EEL =	19622.0635	RESTRAINT =	0.0000

Supplementary Text 3

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
800	-3.4448E+05	2.8480E-01	4.7931E+01	C	3778
BOND =	26409.3702	ANGLE =	1017.7793	DIHED =	5290.2470
VDWAALS =	65204.5772	EEL =	-463519.3186	HBOND =	0.0000
1-4 VDW =	1496.7465	1-4 EEL =	19625.1903	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
900	-3.4471E+05	1.0826E-01	6.4968E+00	C	3764
BOND =	26431.1516	ANGLE =	1009.4331	DIHED =	5284.9138
VDWAALS =	65344.0906	EEL =	-463895.7200	HBOND =	0.0000
1-4 VDW =	1493.1978	1-4 EEL =	19626.4434	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
1000	-3.4492E+05	1.6565E-01	2.3569E+01	CE3	3293
BOND =	26460.0928	ANGLE =	1002.5586	DIHED =	5281.1643
VDWAALS =	65482.6495	EEL =	-464261.7446	HBOND =	0.0000
1-4 VDW =	1490.4363	1-4 EEL =	19627.4617	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
1100	-3.4511E+05	1.2459E-01	1.3834E+01	CE3	3293
BOND =	26486.7742	ANGLE =	998.1471	DIHED =	5278.3816
VDWAALS =	65611.5460	EEL =	-464597.9856	HBOND =	0.0000
1-4 VDW =	1488.1282	1-4 EEL =	19627.7368	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
1200	-3.4528E+05	3.4377E-01	4.2185E+01	CE3	3293
BOND =	26518.0861	ANGLE =	995.0684	DIHED =	5276.5006
VDWAALS =	65736.9188	EEL =	-464923.8084	HBOND =	0.0000
1-4 VDW =	1486.1351	1-4 EEL =	19627.4402	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
1300	-3.4545E+05	3.0200E-01	5.4765E+01	CD	3231
BOND =	26544.7795	ANGLE =	991.0255	DIHED =	5275.3691
VDWAALS =	65854.4218	EEL =	-465231.0297	HBOND =	0.0000
1-4 VDW =	1484.6102	1-4 EEL =	19626.8976	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
1400	-3.4562E+05	2.8895E-01	5.1999E+01	CD	3231
BOND =	26571.3771	ANGLE =	988.7225	DIHED =	5274.1737

Supplementary Text 3

VDWAALS = 65972.2163 EEL = -465537.4058 HBOND = 0.0000
 1-4 VDW = 1483.2770 1-4 EEL = 19625.7474 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 1500 -3.4579E+05 1.6689E-01 1.6758E+01 CG 1665

BOND = 26596.9559 ANGLE = 985.7913 DIHED = 5273.0063
 VDWAALS = 66085.0737 EEL = -465831.9439 HBOND = 0.0000
 1-4 VDW = 1482.3057 1-4 EEL = 19623.7843 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 1600 -3.4594E+05 1.2292E-01 1.1621E+01 CD 3231

BOND = 26622.8836 ANGLE = 983.6852 DIHED = 5271.8127
 VDWAALS = 66196.0323 EEL = -466116.7374 HBOND = 0.0000
 1-4 VDW = 1481.4584 1-4 EEL = 19621.2646 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 1700 -3.4609E+05 9.3302E-02 4.7774E+00 CZ 1670

BOND = 26648.7818 ANGLE = 981.7191 DIHED = 5270.7631
 VDWAALS = 66303.5196 EEL = -466392.7296 HBOND = 0.0000
 1-4 VDW = 1480.6247 1-4 EEL = 19618.8036 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 1800 -3.4623E+05 3.6171E-01 7.6343E+01 CD 3231

BOND = 26679.2044 ANGLE = 980.2070 DIHED = 5270.1468
 VDWAALS = 66408.6158 EEL = -466664.8559 HBOND = 0.0000
 1-4 VDW = 1479.8266 1-4 EEL = 19616.3067 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 1900 -3.4638E+05 9.1529E-02 4.2000E+00 CZ 1670

BOND = 26699.7213 ANGLE = 978.4234 DIHED = 5269.5707
 VDWAALS = 66510.7294 EEL = -466929.3312 HBOND = 0.0000
 1-4 VDW = 1479.0883 1-4 EEL = 19613.8837 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 2000 -3.4651E+05 2.3658E-01 2.2007E+01 CG 1665

BOND = 26726.2894 ANGLE = 977.0274 DIHED = 5268.5579
 VDWAALS = 66611.0936 EEL = -467187.6254 HBOND = 0.0000
 1-4 VDW = 1478.3391 1-4 EEL = 19611.9851 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 2100 -3.4665E+05 2.0572E-01 1.7530E+01 NE2 4277

Supplementary Text 3

BOND	=	26749.4764	ANGLE	=	975.7397	DIHED	=	5267.5818
VDWAALS	=	66711.0546	EEL	=	-467442.3161	HBOND	=	0.0000
1-4 VDW	=	1477.5832	1-4 EEL	=	19610.6054	RESTRAINT	=	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
2200	-3.4678E+05	1.2300E-01	1.3916E+01	CD	3231

BOND	=	26771.4785	ANGLE	=	974.3260	DIHED	=	5266.9597
VDWAALS	=	66806.6277	EEL	=	-467683.7994	HBOND	=	0.0000
1-4 VDW	=	1476.8559	1-4 EEL	=	19609.7682	RESTRAINT	=	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
2300	-3.4690E+05	8.8033E-02	4.0194E+00	CE1	3805

BOND	=	26793.8936	ANGLE	=	973.2777	DIHED	=	5266.7557
VDWAALS	=	66903.1107	EEL	=	-467925.5079	HBOND	=	0.0000
1-4 VDW	=	1476.0618	1-4 EEL	=	19609.0067	RESTRAINT	=	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
2400	-3.4703E+05	9.9168E-02	6.3925E+00	NE2	4277

BOND	=	26816.7042	ANGLE	=	972.3388	DIHED	=	5267.1167
VDWAALS	=	66999.3025	EEL	=	-468166.7445	HBOND	=	0.0000
1-4 VDW	=	1475.2995	1-4 EEL	=	19608.4316	RESTRAINT	=	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
2500	-3.4715E+05	2.7355E-01	2.4149E+01	CE1	3805

BOND	=	26841.0923	ANGLE	=	971.8678	DIHED	=	5268.2662
VDWAALS	=	67091.7688	EEL	=	-468400.7551	HBOND	=	0.0000
1-4 VDW	=	1474.5809	1-4 EEL	=	19608.0848	RESTRAINT	=	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
2600	-3.4726E+05	2.4630E-01	4.3352E+01	CD	3231

BOND	=	26861.4176	ANGLE	=	971.4684	DIHED	=	5269.5810
VDWAALS	=	67183.9304	EEL	=	-468630.2856	HBOND	=	0.0000
1-4 VDW	=	1473.9361	1-4 EEL	=	19606.9981	RESTRAINT	=	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
2700	-3.4738E+05	2.0281E-01	1.8575E+01	CE1	3805

BOND	=	26882.3431	ANGLE	=	970.7817	DIHED	=	5270.3541
VDWAALS	=	67274.2643	EEL	=	-468857.4501	HBOND	=	0.0000
1-4 VDW	=	1473.3011	1-4 EEL	=	19606.4151	RESTRAINT	=	0.0000

Supplementary Text 3

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
2800	-3.4750E+05	1.2340E-01	1.0326E+01	CG	3216
BOND =	26902.3913	ANGLE =	970.4593	DIHED =	5268.0970
VDWAALS =	67365.1851	EEL =	-469084.1496	HBOND =	0.0000
1-4 VDW =	1472.4758	1-4 EEL =	19605.8274	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
2900	-3.4761E+05	1.3480E-01	1.2941E+01	NE2	4277
BOND =	26923.4534	ANGLE =	969.9944	DIHED =	5267.7358
VDWAALS =	67454.3995	EEL =	-469300.8215	HBOND =	0.0000
1-4 VDW =	1471.8941	1-4 EEL =	19605.5292	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
3000	-3.4771E+05	7.4287E-02	3.1739E+00	NE2	4277
BOND =	26942.9708	ANGLE =	969.7152	DIHED =	5267.4567
VDWAALS =	67541.6150	EEL =	-469510.7864	HBOND =	0.0000
1-4 VDW =	1471.4196	1-4 EEL =	19605.1413	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
3100	-3.4781E+05	2.5958E-01	3.0057E+01	NE2	4277
BOND =	26964.7716	ANGLE =	969.8831	DIHED =	5267.0999
VDWAALS =	67626.5072	EEL =	-469713.9406	HBOND =	0.0000
1-4 VDW =	1471.0129	1-4 EEL =	19604.7974	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
3200	-3.4791E+05	2.2658E-01	3.6526E+01	CD	3231
BOND =	26984.1144	ANGLE =	968.9749	DIHED =	5266.6164
VDWAALS =	67709.5848	EEL =	-469913.4681	HBOND =	0.0000
1-4 VDW =	1470.6812	1-4 EEL =	19604.7350	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
3300	-3.4800E+05	2.0546E-01	2.2739E+01	NE2	4277
BOND =	27002.1510	ANGLE =	968.9363	DIHED =	5266.1040
VDWAALS =	67788.4473	EEL =	-470104.9372	HBOND =	0.0000
1-4 VDW =	1470.3544	1-4 EEL =	19604.6139	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
3400	-3.4810E+05	1.3043E-01	1.3502E+01	NE2	4277
BOND =	27020.4102	ANGLE =	968.2175	DIHED =	5265.5456
VDWAALS =	67866.0296	EEL =	-470295.0620	HBOND =	0.0000
1-4 VDW =	1470.0864	1-4 EEL =	19604.8411	RESTRAINT =	0.0000

Supplementary Text 3

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
3500	-3.4819E+05	6.9864E-02	2.7520E+00	NE2	4277
BOND =	27038.5407	ANGLE =	967.9475	DIHED =	5264.8434
VDWAALS =	67941.9742	EEL =	-470481.1142	HBOND =	0.0000
1-4 VDW =	1469.8078	1-4 EEL =	19604.7990	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
3600	-3.4829E+05	7.0653E-02	2.8802E+00	NE2	4277
BOND =	27057.2044	ANGLE =	967.6987	DIHED =	5264.1806
VDWAALS =	68016.8331	EEL =	-470665.9241	HBOND =	0.0000
1-4 VDW =	1469.4970	1-4 EEL =	19604.6754	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
3700	-3.4837E+05	2.5765E-01	3.8031E+01	CD	3231
BOND =	27077.9999	ANGLE =	967.7479	DIHED =	5263.6106
VDWAALS =	68090.4415	EEL =	-470848.0506	HBOND =	0.0000
1-4 VDW =	1469.1901	1-4 EEL =	19604.5269	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
3800	-3.4847E+05	2.2048E-01	3.1478E+01	CD	3231
BOND =	27094.9451	ANGLE =	967.8412	DIHED =	5263.1438
VDWAALS =	68162.2888	EEL =	-471026.4877	HBOND =	0.0000
1-4 VDW =	1468.8254	1-4 EEL =	19604.1827	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
3900	-3.4855E+05	1.8172E-01	1.7269E+01	CD	3231
BOND =	27112.9626	ANGLE =	967.5811	DIHED =	5262.7221
VDWAALS =	68235.8586	EEL =	-471206.2842	HBOND =	0.0000
1-4 VDW =	1468.5240	1-4 EEL =	19604.0975	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
4000	-3.4864E+05	1.0695E-01	9.6503E+00	NE2	4277
BOND =	27130.2050	ANGLE =	967.7138	DIHED =	5262.3512
VDWAALS =	68310.2895	EEL =	-471384.8043	HBOND =	0.0000
1-4 VDW =	1468.1709	1-4 EEL =	19603.9577	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
4100	-3.4873E+05	1.2404E-01	1.2289E+01	NE2	4277
BOND =	27148.4205	ANGLE =	967.5636	DIHED =	5262.0253

Supplementary Text 3

VDWAALS = 68383.0841 EEL = -471559.1192 HBOND = 0.0000
 1-4 VDW = 1467.9159 1-4 EEL = 19604.0203 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 4200 -3.4881E+05 9.6300E-02 9.0546E+00 NE2 4277

BOND = 27165.1744 ANGLE = 967.6734 DIHED = 5261.8014
 VDWAALS = 68452.7510 EEL = -471726.1793 HBOND = 0.0000
 1-4 VDW = 1467.7097 1-4 EEL = 19603.9879 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 4300 -3.4888E+05 2.5289E-01 3.7627E+01 CD 3231

BOND = 27183.7208 ANGLE = 967.9507 DIHED = 5261.6963
 VDWAALS = 68520.3363 EEL = -471889.0819 HBOND = 0.0000
 1-4 VDW = 1467.5138 1-4 EEL = 19603.9510 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 4400 -3.4896E+05 6.5908E-02 3.0517E+00 NE2 4277

BOND = 27197.8904 ANGLE = 967.5960 DIHED = 5261.7182
 VDWAALS = 68587.2483 EEL = -472048.7466 HBOND = 0.0000
 1-4 VDW = 1467.3635 1-4 EEL = 19603.9363 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 4500 -3.4904E+05 1.8788E-01 1.9282E+01 CE1 3805

BOND = 27214.7405 ANGLE = 967.9593 DIHED = 5261.9303
 VDWAALS = 68652.7409 EEL = -472204.3973 HBOND = 0.0000
 1-4 VDW = 1467.1902 1-4 EEL = 19603.7123 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 4600 -3.4911E+05 1.4908E-01 1.5097E+01 NE2 4277

BOND = 27229.8672 ANGLE = 967.7202 DIHED = 5262.3635
 VDWAALS = 68715.6209 EEL = -472355.8674 HBOND = 0.0000
 1-4 VDW = 1467.0266 1-4 EEL = 19603.4986 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 4700 -3.4918E+05 6.2037E-02 2.5142E+00 H2 50427

BOND = 27243.9090 ANGLE = 967.9383 DIHED = 5262.9719
 VDWAALS = 68777.0871 EEL = -472505.3085 HBOND = 0.0000
 1-4 VDW = 1466.8564 1-4 EEL = 19603.0514 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 4800 -3.4926E+05 6.3348E-02 2.9948E+00 NE2 4277

Supplementary Text 3

```

BOND      = 27258.7432  ANGLE   = 967.9374  DIHED     = 5263.4251
VDWAALS   = 68838.9422  EEL     = -472654.0098  HBOND     = 0.0000
1-4 VDW   = 1466.7231  1-4 EEL = 19602.7008  RESTRAINT = 0.0000
  
```

```

NSTEP      ENERGY          RMS           GMAX          NAME      NUMBER
4900      -3.4932E+05      2.2864E-01    2.7341E+01    NE2       4277
  
```

```

BOND      = 27275.5046  ANGLE   = 967.8371  DIHED     = 5263.5070
VDWAALS   = 68900.5214  EEL     = -472800.6770  HBOND     = 0.0000
1-4 VDW   = 1466.6135  1-4 EEL = 19602.5027  RESTRAINT = 0.0000
  
```

```

NSTEP      ENERGY          RMS           GMAX          NAME      NUMBER
5000      -3.4939E+05      1.8539E-01    2.3386E+01    NE2       4277
  
```

```

BOND      = 27288.8469  ANGLE   = 968.1360  DIHED     = 5263.3696
VDWAALS   = 68961.7778  EEL     = -472945.1878  HBOND     = 0.0000
1-4 VDW   = 1466.5092  1-4 EEL = 19602.1465  RESTRAINT = 0.0000
  
```

Maximum number of minimization cycles reached.

FINAL RESULTS

```

NSTEP      ENERGY          RMS           GMAX          NAME      NUMBER
5000      -3.4939E+05      1.8539E-01    2.3386E+01    NE2       4277
  
```

```

BOND      = 27288.8469  ANGLE   = 968.1360  DIHED     = 5263.3696
VDWAALS   = 68961.7778  EEL     = -472945.1878  HBOND     = 0.0000
1-4 VDW   = 1466.5092  1-4 EEL = 19602.1465  RESTRAINT = 0.0000
  
```

5. TIMINGS

```

|          Build the list          27.75 (92.22% of List )
|          Other                   2.34 ( 7.78% of List )
| List time                       30.09 ( 0.32% of Nonbo)
|   Short_ene time                 8417.60 (99.68% of Direc)
|   Other                          26.69 ( 0.32% of Direc)
| Direct Ewald time                8444.29 (91.34% of Ewald)
| Adjust Ewald time                32.43 ( 0.35% of Ewald)
|   Fill Bspline coeffs           26.41 ( 3.47% of Recip)
|   Fill charge grid              104.54 (13.72% of Recip)
|   Scalar sum                    148.86 (19.54% of Recip)
|   Grad sum                      184.30 (24.19% of Recip)
|   FFT time                      297.80 (39.08% of Recip)
| Recip Ewald time                 761.93 ( 8.24% of Ewald)
| Virial junk                      1.92 ( 0.02% of Ewald)
  
```

Supplementary Text 3

	Other	4.58 (0.05% of Ewald)
	Ewald time	9245.17 (99.68% of Nonbo)
	Nonbond force	9275.27 (99.52% of Force)
	Bond/Angle/Dihedral	43.86 (0.47% of Force)
	Other	1.00 (0.01% of Force)
	Force time	9320.14 (100.0% of Runmd)
	Runmd Time	9320.14 (99.72% of Total)
	Other	26.07 (0.28% of Total)
	Total time	9346.23 (100.0% of ALL)

| Number of list builds : 20

| Highest rstack allocated: 4808230
 | Highest istack allocated: 87372
 | Job began at 12:02:52.833 on 02/21/2019
 | Setup done at 12:02:53.500 on 02/21/2019
 | Run done at 14:38:39.064 on 02/21/2019
 | wallclock() was called 190088 times

 Amber 16 SANDER

2016

| Run on 02/21/2019 at 17:36:44

| Executable path: /usr/local/amber16/bin/sander
 | Working directory: /Users/Swati
 | Hostname: Unknown
 | [-O]verwriting output

File Assignments:

| MDIN: /Users/Swati/minimization_file_2.in
 | MDOUT: /Users/Swati/NAT0_files_2/truncated_NAT0_min3_2.out
 | INPCRD: /Users/Swati/NAT0_files_2/truncated_NAT0_min3_1.rst
 | PARM: /Users/Swati/NAT0_files_2/NAT0.prmtop
 | RESTR: /Users/Swati/NAT0_files_2/truncated_NAT0_min3_2.rst
 | REFC: refc
 | MDVEL: mdvel
 | MDFRC: mdfrc
 | MDEN: mden
 | MDCRD: mdcrd
 | MDINFO: mdinfo
 | MTMD: mtmd
 | INPDIP: inpdip
 | RSTDIP: rstcip
 | INPTRA: inptraj

Here is the input file:

PROT: minimization_2
 &cntrl
 imin = 1,
 maxcyc = 5000,

Supplementary Text 3

```
ncyc = 10000,  
igb = 0,  
ntpr = 100,  
ntp = 0  
cut = 12  
&end
```

1. RESOURCE USE:

```
| Flags:  
| getting box info from netcdf restart file  
| NetCDF restart box info found  
| Largest sphere to fit in unit cell has radius = 44.861  
| New format PARM file being parsed.  
| Version = 1.000 Date = 08/09/17 Time = 07:09:32  
| NATOM = 65080 NTYPES = 17 NBONH = 61577 MBONA = 3583  
| NTHETH = 7353 MTHETA = 4865 NPHIH = 15405 MPHIA = 14966  
| NHPARM = 0 NPARM = 0 NNB = 114677 NRES = 19909  
| NBONA = 3583 NTHETA = 4865 NPHIA = 14966 NUMBND = 67  
| NUMANG = 151 NPTRA = 191 NATYP = 36 NPHB = 1  
| IFBOX = 1 NMXRS = 24 IFCAP = 0 NEXTRA = 0  
| NCOPY = 0
```

```
| Memory Use Allocated  
| Real 5163211  
| Hollerith 215151  
| Integer 2953777  
| Max Pairs 59526506  
| nblastReal 780960  
| nblast Int 2187281  
| Total 299886 kbytes
```

```
| Note: 1-4 EEL scale factors are being read from the topology file.
```

```
| Note: 1-4 VDW scale factors are being read from the topology file.
```

```
| Duplicated 0 dihedrals
```

```
| Duplicated 0 dihedrals
```

BOX TYPE: RECTILINEAR

2. CONTROL DATA FOR THE RUN

default_name

General flags:

```
imin = 1, nmropt = 0
```

Nature and format of input:

Supplementary Text 3

ntx = 1, irest = 0, ntrx = 1

Nature and format of output:

ntxo = 2, ntrp = 100, ntrx = 1, ntwr = 1
 iwrap = 0, ntwx = 0, ntwv = 0, ntwe = 0
 ioutfm = 1, ntwprt = 0, idecomp = 0, rbornstat= 0

Potential function:

ntf = 1, ntb = 1, igb = 0, nsnb = 25
 ipol = 0, gbsa = 0, iesp = 0
 dielc = 1.00000, cut = 12.00000, intdiel = 1.00000

Frozen or restrained atoms:

ibelly = 0, ntr = 0

Energy minimization:

maxcyc = 5000, ncyc = 10000, ntmin = 1
 dx0 = 0.01000, drms = 0.00010

Ewald parameters:

verbose = 0, ew_type = 0, nbflag = 1, use_pme = 1
 vdwmeth = 1, eedmeth = 1, netfrc = 0
 Box X = 97.446 Box Y = 89.722 Box Z = 90.199
 Alpha = 90.000 Beta = 90.000 Gamma = 90.000
 NFFT1 = 100 NFFT2 = 90 NFFT3 = 90
 Cutoff= 12.000 Tol =0.100E-04
 Ewald Coefficient = 0.22664
 Interpolation order = 4

| INFO: Old style inpcrd file read

 3. ATOMIC COORDINATES AND VELOCITIES

default_name

begin time read from input coords = 0.000 ps

Number of triangulated 3-point waters found: 19440

Sum of charges from parm topology file = -0.00000033

Forcing neutrality...

 4. RESULTS

 APPROXIMATING switch and d/dx switch using CUBIC SPLINE INTERPOLATION

using 5000.0 points per unit in tabled values

TESTING RELATIVE ERROR over r ranging from 0.0 to cutoff

| CHECK switch(x): max rel err = 0.2738E-14 at 2.422500

CHECK d/dx switch(x): max rel err = 0.7967E-11 at 2.716640

Supplementary Text 3

| Local SIZE OF NONBOND LIST = 31615604
 | TOTAL SIZE OF NONBOND LIST = 31615604

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
1	-2.3729E+05	5.0938E+00	7.4715E+02	C	3693
BOND =	28585.6938	ANGLE =	2442.4317	DIHED =	4978.7907
VDWAALS =	47953.8265	EEL =	-342825.6076	HBOND =	0.0000
1-4 VDW =	2043.3985	1-4 EEL =	19532.0386	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
100	-2.5048E+05	4.5926E-01	3.5916E+01	C	3693
BOND =	19947.3321	ANGLE =	1548.1980	DIHED =	5039.9904
VDWAALS =	45641.8821	EEL =	-343221.3344	HBOND =	0.0000
1-4 VDW =	1622.3101	1-4 EEL =	18938.1554	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
200	-2.5210E+05	7.5401E-01	1.1553E+02	C	3693
BOND =	19341.2335	ANGLE =	1278.7278	DIHED =	5025.6976
VDWAALS =	45582.9834	EEL =	-343690.6421	HBOND =	0.0000
1-4 VDW =	1516.2520	1-4 EEL =	18848.3444	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
300	-2.5281E+05	2.0389E-01	1.5748E+01	C	3693
BOND =	19180.7572	ANGLE =	1176.6028	DIHED =	5009.2266
VDWAALS =	45630.1284	EEL =	-344104.9118	HBOND =	0.0000
1-4 VDW =	1478.9464	1-4 EEL =	18820.9000	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
400	-2.5324E+05	1.7517E-01	1.4872E+01	C	3693
BOND =	19133.7180	ANGLE =	1121.6991	DIHED =	4997.7892
VDWAALS =	45701.8446	EEL =	-344461.4214	HBOND =	0.0000
1-4 VDW =	1459.8386	1-4 EEL =	18808.5995	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
500	-2.5355E+05	4.7329E-01	7.2942E+01	C	3693
BOND =	19128.0608	ANGLE =	1088.6742	DIHED =	4993.6844
VDWAALS =	45786.1896	EEL =	-344799.4563	HBOND =	0.0000
1-4 VDW =	1447.9195	1-4 EEL =	18801.6533	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
600	-2.5382E+05	3.9844E-01	5.4750E+01	C	3693

Supplementary Text 3

BOND = 19126.5551 ANGLE = 1070.1137 DIHED = 4990.8832
 VDWAALS = 45875.1357 EEL = -345117.7008 HBOND = 0.0000
 1-4 VDW = 1439.4902 1-4 EEL = 18795.7758 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 700 -2.5405E+05 3.7197E-01 5.1310E+01 C 3693

BOND = 19139.6031 ANGLE = 1054.0001 DIHED = 4987.3849
 VDWAALS = 45965.5959 EEL = -345425.9048 HBOND = 0.0000
 1-4 VDW = 1432.7050 1-4 EEL = 18792.7068 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 800 -2.5426E+05 3.0274E-01 3.8816E+01 C 3693

BOND = 19151.1553 ANGLE = 1044.8119 DIHED = 4988.4247
 VDWAALS = 46057.9873 EEL = -345722.8119 HBOND = 0.0000
 1-4 VDW = 1427.2656 1-4 EEL = 18790.0595 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 900 -2.5446E+05 2.0526E-01 2.2304E+01 CA 3697

BOND = 19168.1819 ANGLE = 1036.7133 DIHED = 4987.6238
 VDWAALS = 46148.3345 EEL = -346010.0011 HBOND = 0.0000
 1-4 VDW = 1422.9260 1-4 EEL = 18788.2307 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 1000 -2.5464E+05 1.1422E-01 5.8816E+00 C 3707

BOND = 19185.3412 ANGLE = 1031.1800 DIHED = 4985.2251
 VDWAALS = 46237.2713 EEL = -346284.0687 HBOND = 0.0000
 1-4 VDW = 1419.5525 1-4 EEL = 18785.8113 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 1100 -2.5481E+05 1.0674E-01 4.6692E+00 N 3695

BOND = 19204.4187 ANGLE = 1026.4402 DIHED = 4983.5029
 VDWAALS = 46323.8608 EEL = -346544.6668 HBOND = 0.0000
 1-4 VDW = 1417.1359 1-4 EEL = 18783.6136 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 1200 -2.5496E+05 4.3881E-01 8.3362E+01 CD 3153

BOND = 19229.2372 ANGLE = 1023.2889 DIHED = 4983.4150
 VDWAALS = 46411.2339 EEL = -346802.2012 HBOND = 0.0000
 1-4 VDW = 1415.4418 1-4 EEL = 18781.7179 RESTRAINT = 0.0000

Supplementary Text 3

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
1300	-2.5511E+05	3.2445E-01	3.9888E+01	CA	3697

BOND =	19246.4908	ANGLE =	1020.4848	DIHED =	4982.4567
VDWAALS =	46498.8281	EEL =	-347054.0654	HBOND =	0.0000
1-4 VDW =	1413.9343	1-4 EEL =	18779.6000	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
1400	-2.5526E+05	2.8238E-01	3.7812E+01	CA	3697

BOND =	19267.7220	ANGLE =	1017.7156	DIHED =	4979.3180
VDWAALS =	46586.3043	EEL =	-347302.0486	HBOND =	0.0000
1-4 VDW =	1412.3957	1-4 EEL =	18778.7959	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
1500	-2.5540E+05	2.7796E-01	3.6376E+01	CD	3153

BOND =	19286.8217	ANGLE =	1016.5958	DIHED =	4976.5127
VDWAALS =	46671.3788	EEL =	-347535.2549	HBOND =	0.0000
1-4 VDW =	1410.8885	1-4 EEL =	18776.9996	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
1600	-2.5553E+05	1.5224E-01	1.7244E+01	CA	3697

BOND =	19306.3614	ANGLE =	1014.7036	DIHED =	4973.6169
VDWAALS =	46752.1717	EEL =	-347757.3156	HBOND =	0.0000
1-4 VDW =	1409.4291	1-4 EEL =	18775.7831	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
1700	-2.5565E+05	9.9662E-02	6.1878E+00	C	3707

BOND =	19324.9297	ANGLE =	1013.5467	DIHED =	4972.4166
VDWAALS =	46827.9712	EEL =	-347968.0408	HBOND =	0.0000
1-4 VDW =	1408.3049	1-4 EEL =	18774.2395	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
1800	-2.5577E+05	1.1762E-01	1.1245E+01	C	3707

BOND =	19344.7276	ANGLE =	1012.5963	DIHED =	4971.7632
VDWAALS =	46903.5360	EEL =	-348179.3329	HBOND =	0.0000
1-4 VDW =	1407.3290	1-4 EEL =	18773.0393	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
1900	-2.5587E+05	3.9047E-01	9.1599E+01	CD	3153

BOND =	19367.4021	ANGLE =	1011.8896	DIHED =	4970.7499
VDWAALS =	46976.9559	EEL =	-348379.6915	HBOND =	0.0000
1-4 VDW =	1406.5087	1-4 EEL =	18771.9684	RESTRAINT =	0.0000

Supplementary Text 3

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
2000	-2.5598E+05	2.8806E-01	4.1529E+01	CD	3153
BOND =	19383.8279	ANGLE =	1011.3198	DIHED =	4969.4916
VDWAALS =	47050.7344	EEL =	-348574.9661	HBOND =	0.0000
1-4 VDW =	1405.7827	1-4 EEL =	18770.7187	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
2100	-2.5609E+05	2.5927E-01	3.8279E+01	CD	3153
BOND =	19402.7588	ANGLE =	1010.5311	DIHED =	4967.2599
VDWAALS =	47123.3933	EEL =	-348768.7741	HBOND =	0.0000
1-4 VDW =	1405.0345	1-4 EEL =	18770.3972	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
2200	-2.5619E+05	2.0463E-01	1.9622E+01	CE1	3736
BOND =	19419.6568	ANGLE =	1009.5154	DIHED =	4964.6032
VDWAALS =	47194.1160	EEL =	-348954.8121	HBOND =	0.0000
1-4 VDW =	1404.4610	1-4 EEL =	18769.9712	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
2300	-2.5629E+05	1.2962E-01	1.3693E+01	CE1	3736
BOND =	19437.0025	ANGLE =	1008.2553	DIHED =	4963.0635
VDWAALS =	47263.4346	EEL =	-349137.2948	HBOND =	0.0000
1-4 VDW =	1403.9515	1-4 EEL =	18770.3257	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
2400	-2.5639E+05	8.7337E-02	5.1149E+00	CE1	3736
BOND =	19453.9932	ANGLE =	1007.3400	DIHED =	4961.9996
VDWAALS =	47332.4261	EEL =	-349316.3724	HBOND =	0.0000
1-4 VDW =	1403.4338	1-4 EEL =	18770.3249	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
2500	-2.5648E+05	9.8944E-02	8.6679E+00	CE1	3736
BOND =	19470.8559	ANGLE =	1006.4447	DIHED =	4959.9416
VDWAALS =	47398.2040	EEL =	-349489.6870	HBOND =	0.0000
1-4 VDW =	1403.0594	1-4 EEL =	18770.0532	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
2600	-2.5657E+05	8.3405E-02	4.7471E+00	CE1	3736
BOND =	19486.9804	ANGLE =	1005.7509	DIHED =	4958.1882

Supplementary Text 3

VDWAALS = 47462.1862 EEL = -349658.1287 HBOND = 0.0000
 1-4 VDW = 1402.5573 1-4 EEL = 18770.7885 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 2700 -2.5666E+05 2.4412E-01 3.9325E+01 CD 3153

BOND = 19504.8897 ANGLE = 1005.3800 DIHED = 4957.1746
 VDWAALS = 47527.9992 EEL = -349828.5323 HBOND = 0.0000
 1-4 VDW = 1402.1534 1-4 EEL = 18771.5747 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 2800 -2.5675E+05 1.4581E-01 1.6354E+01 CD 1360

BOND = 19520.6758 ANGLE = 1004.6567 DIHED = 4956.2857
 VDWAALS = 47593.9899 EEL = -349999.0338 HBOND = 0.0000
 1-4 VDW = 1401.7628 1-4 EEL = 18772.4518 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 2900 -2.5683E+05 1.2988E-01 1.4694E+01 CE1 3736

BOND = 19536.4943 ANGLE = 1004.2739 DIHED = 4955.2191
 VDWAALS = 47655.9546 EEL = -350160.1285 HBOND = 0.0000
 1-4 VDW = 1401.4328 1-4 EEL = 18773.3257 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 3000 -2.5691E+05 1.3161E-01 1.5703E+01 CE1 3736

BOND = 19552.5116 ANGLE = 1003.8994 DIHED = 4954.4691
 VDWAALS = 47719.7273 EEL = -350318.5405 HBOND = 0.0000
 1-4 VDW = 1401.1979 1-4 EEL = 18773.7737 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 3100 -2.5699E+05 7.3400E-02 3.1449E+00 CE1 3736

BOND = 19567.5627 ANGLE = 1003.5576 DIHED = 4953.9054
 VDWAALS = 47783.6941 EEL = -350472.4012 HBOND = 0.0000
 1-4 VDW = 1400.9552 1-4 EEL = 18773.5300 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 3200 -2.5706E+05 2.7807E-01 4.7568E+01 CD 1360

BOND = 19584.9666 ANGLE = 1003.5340 DIHED = 4953.4875
 VDWAALS = 47847.5830 EEL = -350625.8682 HBOND = 0.0000
 1-4 VDW = 1400.7372 1-4 EEL = 18773.0712 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 3300 -2.5714E+05 2.3348E-01 4.5663E+01 CD 1360

Supplementary Text 3

BOND	=	19598.8921	ANGLE	=	1003.2048	DIHED	=	4953.2211
VDWAALS	=	47908.1524	EEL	=	-350771.9947	HBOND	=	0.0000
1-4 VDW	=	1400.5471	1-4 EEL	=	18772.6409	RESTRAINT	=	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
3400	-2.5721E+05	2.0717E-01	3.0334E+01	CD	1360

BOND	=	19612.3822	ANGLE	=	1002.7484	DIHED	=	4953.0651
VDWAALS	=	47967.9718	EEL	=	-350915.6156	HBOND	=	0.0000
1-4 VDW	=	1400.3012	1-4 EEL	=	18772.1066	RESTRAINT	=	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
3500	-2.5728E+05	1.6313E-01	1.9731E+01	CE1	3736

BOND	=	19626.5341	ANGLE	=	1002.4136	DIHED	=	4952.9153
VDWAALS	=	48028.2555	EEL	=	-351058.2297	HBOND	=	0.0000
1-4 VDW	=	1400.0877	1-4 EEL	=	18771.6304	RESTRAINT	=	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
3600	-2.5734E+05	9.9984E-02	1.0084E+01	CE1	3736

BOND	=	19639.7743	ANGLE	=	1001.9611	DIHED	=	4952.6233
VDWAALS	=	48088.0464	EEL	=	-351195.8917	HBOND	=	0.0000
1-4 VDW	=	1399.8750	1-4 EEL	=	18771.3380	RESTRAINT	=	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
3700	-2.5741E+05	6.7959E-02	2.9889E+00	CE1	3736

BOND	=	19652.9327	ANGLE	=	1001.6696	DIHED	=	4952.2857
VDWAALS	=	48145.3015	EEL	=	-351329.5753	HBOND	=	0.0000
1-4 VDW	=	1399.6939	1-4 EEL	=	18771.3666	RESTRAINT	=	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
3800	-2.5747E+05	2.8797E-01	6.5180E+01	CD	1360

BOND	=	19668.0652	ANGLE	=	1001.7359	DIHED	=	4952.0943
VDWAALS	=	48199.8708	EEL	=	-351460.1990	HBOND	=	0.0000
1-4 VDW	=	1399.5403	1-4 EEL	=	18771.6102	RESTRAINT	=	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
3900	-2.5753E+05	6.9890E-02	3.7067E+00	CE1	3736

BOND	=	19678.3132	ANGLE	=	1001.2382	DIHED	=	4952.1442
VDWAALS	=	48254.4272	EEL	=	-351590.8492	HBOND	=	0.0000
1-4 VDW	=	1399.3669	1-4 EEL	=	18772.1790	RESTRAINT	=	0.0000

Supplementary Text 3

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
4000	-2.5760E+05	1.7862E-01	2.0855E+01	CE1	3736
BOND =	19691.7732	ANGLE =	1001.1391	DIHED =	4952.1422
VDWAALS =	48310.0288	EEL =	-351722.8566	HBOND =	0.0000
1-4 VDW =	1399.1573	1-4 EEL =	18772.9077	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
4100	-2.5766E+05	1.6401E-01	2.4464E+01	CD	1360
BOND =	19703.8431	ANGLE =	1000.8625	DIHED =	4951.9531
VDWAALS =	48363.6775	EEL =	-351848.6962	HBOND =	0.0000
1-4 VDW =	1398.9136	1-4 EEL =	18773.3828	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
4200	-2.5772E+05	1.3145E-01	1.4750E+01	CE1	3736
BOND =	19715.5384	ANGLE =	1000.6629	DIHED =	4951.7359
VDWAALS =	48416.7486	EEL =	-351972.3506	HBOND =	0.0000
1-4 VDW =	1398.6927	1-4 EEL =	18773.8971	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
4300	-2.5777E+05	6.7613E-02	3.9060E+00	CE1	3736
BOND =	19726.7826	ANGLE =	1000.4054	DIHED =	4951.5450
VDWAALS =	48467.8076	EEL =	-352090.8392	HBOND =	0.0000
1-4 VDW =	1398.4779	1-4 EEL =	18774.2564	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
4400	-2.5783E+05	2.3647E-01	2.9786E+01	CE1	3736
BOND =	19739.9542	ANGLE =	1000.3457	DIHED =	4951.3716
VDWAALS =	48519.7107	EEL =	-352211.9185	HBOND =	0.0000
1-4 VDW =	1398.2677	1-4 EEL =	18774.5800	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
4500	-2.5789E+05	6.5272E-02	3.1731E+00	CE1	3736
BOND =	19749.9589	ANGLE =	999.9141	DIHED =	4951.1892
VDWAALS =	48569.2097	EEL =	-352328.6791	HBOND =	0.0000
1-4 VDW =	1398.1150	1-4 EEL =	18774.9336	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
4600	-2.5794E+05	1.8523E-01	2.2717E+01	CE1	3736
BOND =	19761.9385	ANGLE =	999.6354	DIHED =	4950.9861
VDWAALS =	48617.9748	EEL =	-352443.8519	HBOND =	0.0000
1-4 VDW =	1397.9960	1-4 EEL =	18775.2182	RESTRAINT =	0.0000

Supplementary Text 3

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
4700	-2.5800E+05	8.4924E-02	7.7125E+00	CE1	3736
BOND =	19772.3444	ANGLE =	999.1556	DIHED =	4950.7728
VDWAALS =	48666.2314	EEL =	-352558.9612	HBOND =	0.0000
1-4 VDW =	1397.9158	1-4 EEL =	18775.5280	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
4800	-2.5805E+05	1.2121E-01	1.2972E+01	CE1	3736
BOND =	19783.5534	ANGLE =	998.6850	DIHED =	4950.5749
VDWAALS =	48714.4218	EEL =	-352674.0511	HBOND =	0.0000
1-4 VDW =	1397.8214	1-4 EEL =	18775.6940	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
4900	-2.5811E+05	2.6278E-01	3.0804E+01	CE1	3736
BOND =	19795.9177	ANGLE =	998.4538	DIHED =	4950.3923
VDWAALS =	48761.7961	EEL =	-352787.2207	HBOND =	0.0000
1-4 VDW =	1397.7154	1-4 EEL =	18775.7614	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
5000	-2.5816E+05	7.1486E-02	4.6857E+00	CE1	3736
BOND =	19804.7813	ANGLE =	997.8405	DIHED =	4950.2105
VDWAALS =	48807.9069	EEL =	-352897.2595	HBOND =	0.0000
1-4 VDW =	1397.5974	1-4 EEL =	18775.8161	RESTRAINT =	0.0000

Maximum number of minimization cycles reached.

FINAL RESULTS

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
5000	-2.5816E+05	7.1486E-02	4.6857E+00	CE1	3736
BOND =	19804.7813	ANGLE =	997.8405	DIHED =	4950.2105
VDWAALS =	48807.9069	EEL =	-352897.2595	HBOND =	0.0000
1-4 VDW =	1397.5974	1-4 EEL =	18775.8161	RESTRAINT =	0.0000

5. TIMINGS

	Build the list	18.37 (91.58% of List)
	Other	1.69 (8.42% of List)

Supplementary Text 3

```

|      List time                20.05 ( 0.29% of Nonbo)
|      Short_ene time           6236.74 (99.68% of Direc)
|      Other                     19.96 ( 0.32% of Direc)
|      Direct Ewald time         6256.70 (91.62% of Ewald)
|      Adjust Ewald time         25.77 ( 0.38% of Ewald)
|      Fill Bspline coeffs       18.76 ( 3.47% of Recip)
|      Fill charge grid          75.46 (13.95% of Recip)
|      Scalar sum                103.82 (19.19% of Recip)
|      Grad sum                  129.38 (23.91% of Recip)
|      FFT time                  213.62 (39.48% of Recip)
|      Recip Ewald time          541.06 ( 7.92% of Ewald)
|      Virial junk                1.42 ( 0.02% of Ewald)
|      Other                     4.37 ( 0.06% of Ewald)
|      Ewald time                6829.33 (99.71% of Nonbo)
|      Nonbond force             6849.39 (99.41% of Force)
|      Bond/Angle/Dihedral       40.05 ( 0.58% of Force)
|      Other                     0.66 ( 0.01% of Force)
|      Force time                6890.10 (100.0% of Runmd)
|      Runmd Time                6890.10 (99.72% of Total)
|      Other                     19.65 ( 0.28% of Total)
| Total time                    6909.77 (100.0% of ALL )

```

| Number of list builds : 18

```

| Highest rstack allocated: 3470642
| Highest irstack allocated: 65080
|   Job began at 17:36:44.410 on 02/21/2019
|   Setup done at 17:36:44.947 on 02/21/2019
|   Run done at 19:31:54.181 on 02/21/2019
| wallclock() was called 190084 times

```

Amber 16 SANDER 2016

| Run on 02/20/2019 at 17:17:31

```

| Executable path: /usr/local/amber16/bin/sander
| Working directory: /Users/Swati
| Hostname: Unknown
| [-O]verwriting output

```

File Assignments:

```

| MDIN: /Users/Swati/minimization_file_2.in
| MDOUT: /Users/Swati/ZSP9_files_2/truncated_ZSP9_min3_2.out
| INPCRD: /Users/Swati/ZSP9_files_2/truncated_ZSP9_min3_1.rst
| PARM: /Users/Swati/ZSP9_files_2/ZSP9.prmtop
| RESTRT: /Users/Swati/ZSP9_files_2/truncated_ZSP9_min3_2.rst
| REFC: refc
| MDVEL: mdvel
| MDFRC: mdfrc
| MDEN: mden
| MDCRD: mdcrd
| MDINFO: mdinfo

```

Supplementary Text 3

```
| MTMD: mtmd
| INPDIP: inpdip
| RSTDIP: rstdip
| INPTRA: inptraj
```

Here is the input file:

```
PROT: minimization_2
&cntrl
imin = 1,
maxcyc = 5000,
ncyc = 10000,
igb = 0,
ntpr = 100,
ntp = 0
cut = 12
&end
```

1. RESOURCE USE:

```
| Flags:
| getting box info from netcdf restart file
| NetCDF restart box info found
| Largest sphere to fit in unit cell has radius = 43.290
| New format PARM file being parsed.
| Version = 1.000 Date = 08/10/17 Time = 02:13:56
| NATOM = 92322 NTYPES = 17 NBONH = 88587 MBONA = 3843
| NTHETH = 8001 MTHETA = 5230 NPHIH = 16775 MPHIA = 16079
| NHPARM = 0 NPARM = 0 NNB = 153390 NRES = 28827
| NBONA = 3843 NTHETA = 5230 NPHIA = 16079 NUMBND = 67
| NUMANG = 152 NPTRA = 191 NATYP = 36 NPHB = 1
| IFBOX = 1 NMXRS = 24 IFCAP = 0 NEXTRA = 0
| NCOPY = 0
```

```
| Memory Use Allocated
| Real 7288505
| Hollerith 305795
| Integer 3691274
| Max Pairs 84443856
| nblastReal 1107864
| nblast Int 3033137
| Total 422917 kbytes
```

| Note: 1-4 EEL scale factors are being read from the topology file.

```
| Note: 1-4 VDW scale factors are being read from the topology file.
| Duplicated 0 dihedrals
| Duplicated 0 dihedrals
```


Supplementary Text 3

BOX TYPE: RECTILINEAR

2. CONTROL DATA FOR THE RUN

default_name

General flags:

imin = 1, nmropt = 0

Nature and format of input:

ntx = 1, irest = 0, ntrx = 1

Nature and format of output:

ntxo = 2, ntp = 100, ntr = 1, ntw = 1
iwrap = 0, ntwx = 0, ntwv = 0, ntwe = 0
ioutfm = 1, ntwprt = 0, idecomp = 0, rbornstat = 0

Potential function:

ntf = 1, ntb = 1, igb = 0, nsnb = 25
ipol = 0, gbsa = 0, iesp = 0
dielc = 1.00000, cut = 12.00000, intdiel = 1.00000

Frozen or restrained atoms:

ibelly = 0, ntr = 0

Energy minimization:

maxcyc = 5000, ncyc = 10000, ntmin = 1
dx0 = 0.01000, drms = 0.00010

Ewald parameters:

verbose = 0, ew_type = 0, nbflag = 1, use_pme = 1
vdwmeth = 1, eedmeth = 1, netfr = 0
Box X = 118.606 Box Y = 86.581 Box Z = 106.952
Alpha = 90.000 Beta = 90.000 Gamma = 90.000
NFFT1 = 120 NFFT2 = 90 NFFT3 = 108
Cutoff = 12.000 Tol = 0.100E-04
Ewald Coefficient = 0.22664
Interpolation order = 4

| INFO: Old style inpcrd file read

3. ATOMIC COORDINATES AND VELOCITIES

default_name

begin time read from input coords = 0.000 ps

Number of triangulated 3-point waters found: 28349

Sum of charges from parm topology file = -0.00000026

Forcing neutrality...

Supplementary Text 3

4. RESULTS

 APPROXIMATING switch and d/dx switch using CUBIC SPLINE INTERPOLATION
 using 5000.0 points per unit in tabled values
 TESTING RELATIVE ERROR over r ranging from 0.0 to cutoff
 | CHECK switch(x): max rel err = 0.2738E-14 at 2.422500
CHECK d/dx switch(x): max rel err = 0.7967E-11 at 2.716640

| Local SIZE OF NONBOND LIST = 45680654
 | TOTAL SIZE OF NONBOND LIST = 45680654

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
1	-3.4663E+05	4.4204E+00	7.3532E+02	C	3786
BOND =	37478.5623	ANGLE =	2727.8166	DIHED =	5547.3663
VDWAALS =	69428.2816	EEL =	-483213.4724	HBOND =	0.0000
1-4 VDW =	2150.0887	1-4 EEL =	19251.9883	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
100	-3.6114E+05	7.0015E-01	1.3230E+02	C	3800
BOND =	28167.2649	ANGLE =	1601.1037	DIHED =	5565.4396
VDWAALS =	67040.0381	EEL =	-483880.1840	HBOND =	0.0000
1-4 VDW =	1705.8561	1-4 EEL =	18658.3330	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
200	-3.6261E+05	7.4260E-01	9.7903E+01	C	3800
BOND =	27790.1455	ANGLE =	1359.9399	DIHED =	5530.1852
VDWAALS =	67051.7976	EEL =	-484551.8178	HBOND =	0.0000
1-4 VDW =	1613.4361	1-4 EEL =	18600.9306	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
300	-3.6334E+05	1.8066E-01	1.4320E+01	C	3800
BOND =	27685.3367	ANGLE =	1275.8406	DIHED =	5507.8262
VDWAALS =	67168.2024	EEL =	-485147.3485	HBOND =	0.0000
1-4 VDW =	1582.0614	1-4 EEL =	18592.2689	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
400	-3.6383E+05	1.5222E-01	1.1507E+01	N	3802
BOND =	27674.7094	ANGLE =	1227.5164	DIHED =	5492.1901
VDWAALS =	67309.2572	EEL =	-485690.7491	HBOND =	0.0000
1-4 VDW =	1565.2225	1-4 EEL =	18595.3366	RESTRAINT =	0.0000

Supplementary Text 3

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
500	-3.6421E+05	3.9962E-01	6.3379E+01	CD	3248
BOND =	27696.1168	ANGLE =	1182.9635	DIHED =	5486.9177
VDWAALS =	67459.1429	EEL =	-486192.2990	HBOND =	0.0000
1-4 VDW =	1554.0706	1-4 EEL =	18599.8108	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
600	-3.6458E+05	4.0079E-01	8.8124E+01	CD	3248
BOND =	27722.9446	ANGLE =	1124.0107	DIHED =	5482.9957
VDWAALS =	67615.6574	EEL =	-486669.9080	HBOND =	0.0000
1-4 VDW =	1541.0633	1-4 EEL =	18606.7278	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
700	-3.6488E+05	2.9902E-01	4.8884E+01	C	3800
BOND =	27747.6299	ANGLE =	1104.1064	DIHED =	5477.3560
VDWAALS =	67769.6794	EEL =	-487120.3763	HBOND =	0.0000
1-4 VDW =	1535.2137	1-4 EEL =	18611.2458	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
800	-3.6514E+05	1.9460E-01	3.2227E+01	C	3800
BOND =	27773.3351	ANGLE =	1094.2684	DIHED =	5471.4371
VDWAALS =	67921.0933	EEL =	-487545.6466	HBOND =	0.0000
1-4 VDW =	1531.3028	1-4 EEL =	18613.1607	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
900	-3.6539E+05	1.1548E-01	8.6733E+00	C	3800
BOND =	27805.0273	ANGLE =	1084.4201	DIHED =	5466.8761
VDWAALS =	68073.5225	EEL =	-487959.4723	HBOND =	0.0000
1-4 VDW =	1527.8796	1-4 EEL =	18614.1880	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
1000	-3.6561E+05	1.1159E-01	9.6165E+00	C	3800
BOND =	27835.8712	ANGLE =	1078.2597	DIHED =	5464.7244
VDWAALS =	68221.5710	EEL =	-488351.6049	HBOND =	0.0000
1-4 VDW =	1525.0294	1-4 EEL =	18615.0592	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
1100	-3.6582E+05	1.2129E-01	1.1991E+01	C	3800
BOND =	27867.1875	ANGLE =	1072.0871	DIHED =	5462.3794

Supplementary Text 3

VDWAALS = 68362.3188 EEL = -488720.9874 HBOND = 0.0000
 1-4 VDW = 1522.4596 1-4 EEL = 18615.8866 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 1200 -3.6601E+05 1.0463E-01 8.0162E+00 C 3800

BOND = 27895.9711 ANGLE = 1067.5870 DIHED = 5459.0860
 VDWAALS = 68494.3449 EEL = -489067.2985 HBOND = 0.0000
 1-4 VDW = 1520.2909 1-4 EEL = 18617.1296 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 1300 -3.6620E+05 2.7121E-01 4.1542E+01 C 3786

BOND = 27926.4790 ANGLE = 1064.5321 DIHED = 5456.1348
 VDWAALS = 68620.4396 EEL = -489400.6047 HBOND = 0.0000
 1-4 VDW = 1518.5528 1-4 EEL = 18618.4072 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 1400 -3.6638E+05 2.7349E-01 5.5638E+01 CD 3248

BOND = 27957.4091 ANGLE = 1058.2656 DIHED = 5454.1160
 VDWAALS = 68741.3593 EEL = -489721.9453 HBOND = 0.0000
 1-4 VDW = 1516.9460 1-4 EEL = 18618.8287 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 1500 -3.6655E+05 2.0681E-01 2.8565E+01 C 3786

BOND = 27983.4766 ANGLE = 1055.7493 DIHED = 5450.7975
 VDWAALS = 68859.0686 EEL = -490033.8112 HBOND = 0.0000
 1-4 VDW = 1515.5989 1-4 EEL = 18618.8380 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 1600 -3.6672E+05 1.5971E-01 2.0657E+01 C 3786

BOND = 28012.8247 ANGLE = 1050.9059 DIHED = 5448.9518
 VDWAALS = 68974.4986 EEL = -490337.3630 HBOND = 0.0000
 1-4 VDW = 1514.3189 1-4 EEL = 18618.2802 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 1700 -3.6688E+05 1.2484E-01 1.2174E+01 C 3786

BOND = 28039.7998 ANGLE = 1048.4214 DIHED = 5447.3351
 VDWAALS = 69089.1193 EEL = -490633.8849 HBOND = 0.0000
 1-4 VDW = 1513.1617 1-4 EEL = 18618.0611 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 1800 -3.6703E+05 3.6876E-01 9.4931E+01 CD 3248

Supplementary Text 3

BOND	=	28072.2979	ANGLE	=	1045.9289	DIHED	=	5446.5784
VDWAALS	=	69204.5488	EEL	=	-490927.5841	HBOND	=	0.0000
1-4 VDW	=	1512.0119	1-4 EEL	=	18618.0587	RESTRAINT	=	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
1900	-3.6718E+05	2.7025E-01	4.1302E+01	CD	3248

BOND	=	28098.7350	ANGLE	=	1043.0701	DIHED	=	5446.5324
VDWAALS	=	69321.2035	EEL	=	-491218.0143	HBOND	=	0.0000
1-4 VDW	=	1510.9964	1-4 EEL	=	18618.3152	RESTRAINT	=	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
2000	-3.6733E+05	2.3184E-01	3.6436E+01	CE1	4295

BOND	=	28125.6654	ANGLE	=	1041.0862	DIHED	=	5445.9318
VDWAALS	=	69437.8749	EEL	=	-491506.1993	HBOND	=	0.0000
1-4 VDW	=	1510.0575	1-4 EEL	=	18618.2840	RESTRAINT	=	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
2100	-3.6747E+05	1.9943E-01	3.1100E+01	CE1	4295

BOND	=	28152.6367	ANGLE	=	1039.0362	DIHED	=	5444.8202
VDWAALS	=	69551.4856	EEL	=	-491784.9647	HBOND	=	0.0000
1-4 VDW	=	1509.2391	1-4 EEL	=	18618.6103	RESTRAINT	=	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
2200	-3.6761E+05	8.1550E-02	4.3438E+00	CE1	4295

BOND	=	28178.0119	ANGLE	=	1037.6783	DIHED	=	5443.7066
VDWAALS	=	69663.8008	EEL	=	-492058.0224	HBOND	=	0.0000
1-4 VDW	=	1508.5560	1-4 EEL	=	18619.3298	RESTRAINT	=	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
2300	-3.6774E+05	8.6683E-02	6.9881E+00	CE1	4295

BOND	=	28203.9160	ANGLE	=	1036.5201	DIHED	=	5442.5775
VDWAALS	=	69772.4943	EEL	=	-492319.6287	HBOND	=	0.0000
1-4 VDW	=	1508.0854	1-4 EEL	=	18620.1604	RESTRAINT	=	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
2400	-3.6786E+05	9.6730E-02	1.0718E+01	CE1	4295

BOND	=	28229.0495	ANGLE	=	1035.3760	DIHED	=	5441.6269
VDWAALS	=	69879.1572	EEL	=	-492572.5971	HBOND	=	0.0000
1-4 VDW	=	1507.7375	1-4 EEL	=	18621.1848	RESTRAINT	=	0.0000

Supplementary Text 3

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
2500	-3.6797E+05	2.6478E-01	4.2194E+01	CE1	4295

BOND =	28255.9595	ANGLE =	1034.3797	DIHED =	5440.7486
VDWAALS =	69983.7137	EEL =	-492818.0215	HBOND =	0.0000
1-4 VDW =	1507.4789	1-4 EEL =	18622.2806	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
2600	-3.6809E+05	2.6669E-01	4.7175E+01	CD	3248

BOND =	28279.2279	ANGLE =	1033.4382	DIHED =	5439.8894
VDWAALS =	70085.3300	EEL =	-493056.5576	HBOND =	0.0000
1-4 VDW =	1507.2935	1-4 EEL =	18623.3776	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
2700	-3.6820E+05	1.9430E-01	2.8482E+01	CE1	4295

BOND =	28300.3820	ANGLE =	1032.0697	DIHED =	5439.0808
VDWAALS =	70180.1453	EEL =	-493281.5462	HBOND =	0.0000
1-4 VDW =	1507.0786	1-4 EEL =	18624.3268	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
2800	-3.6831E+05	1.2155E-01	1.5814E+01	CE1	4295

BOND =	28321.5353	ANGLE =	1031.1002	DIHED =	5438.3562
VDWAALS =	70273.5559	EEL =	-493504.6618	HBOND =	0.0000
1-4 VDW =	1506.9063	1-4 EEL =	18625.2379	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
2900	-3.6841E+05	1.2971E-01	1.8693E+01	CE1	4295

BOND =	28343.5533	ANGLE =	1030.1451	DIHED =	5437.7478
VDWAALS =	70364.3602	EEL =	-493722.7234	HBOND =	0.0000
1-4 VDW =	1506.7125	1-4 EEL =	18626.0308	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
3000	-3.6852E+05	7.2695E-02	4.1749E+00	CE1	4295

BOND =	28363.9884	ANGLE =	1029.3344	DIHED =	5437.2615
VDWAALS =	70450.3790	EEL =	-493930.3167	HBOND =	0.0000
1-4 VDW =	1506.5222	1-4 EEL =	18626.6680	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
3100	-3.6861E+05	2.5753E-01	3.8613E+01	CE1	4295

BOND =	28386.7906	ANGLE =	1028.9284	DIHED =	5436.8264
VDWAALS =	70533.5734	EEL =	-494130.9366	HBOND =	0.0000
1-4 VDW =	1506.3472	1-4 EEL =	18627.1935	RESTRAINT =	0.0000

Supplementary Text 3

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
3200	-3.6871E+05	2.2447E-01	3.2015E+01	CD	3248
BOND =	28406.3276	ANGLE =	1028.1899	DIHED =	5436.4316
VDWAALS =	70615.5617	EEL =	-494329.6855	HBOND =	0.0000
1-4 VDW =	1506.1184	1-4 EEL =	18627.6294	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
3300	-3.6881E+05	1.9700E-01	2.9960E+01	CE1	4295
BOND =	28425.4591	ANGLE =	1027.7356	DIHED =	5436.1076
VDWAALS =	70694.5066	EEL =	-494523.2472	HBOND =	0.0000
1-4 VDW =	1505.8997	1-4 EEL =	18628.0232	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
3400	-3.6890E+05	1.1264E-01	1.5029E+01	CE1	4295
BOND =	28443.6111	ANGLE =	1027.0876	DIHED =	5435.8257
VDWAALS =	70771.1237	EEL =	-494713.3948	HBOND =	0.0000
1-4 VDW =	1505.6911	1-4 EEL =	18628.3762	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
3500	-3.6900E+05	6.8921E-02	3.2235E+00	CE1	4295
BOND =	28462.2049	ANGLE =	1026.5364	DIHED =	5435.4973
VDWAALS =	70845.4748	EEL =	-494901.3085	HBOND =	0.0000
1-4 VDW =	1505.5177	1-4 EEL =	18628.7444	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
3600	-3.6909E+05	6.9897E-02	3.7045E+00	CE1	4295
BOND =	28481.0985	ANGLE =	1026.0004	DIHED =	5435.1262
VDWAALS =	70918.3720	EEL =	-495088.2440	HBOND =	0.0000
1-4 VDW =	1505.3579	1-4 EEL =	18629.1116	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
3700	-3.6919E+05	2.4359E-01	3.8109E+01	CE1	4295
BOND =	28502.6700	ANGLE =	1025.6823	DIHED =	5434.7467
VDWAALS =	70992.5797	EEL =	-495278.0821	HBOND =	0.0000
1-4 VDW =	1505.2094	1-4 EEL =	18629.3990	RESTRAINT =	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
3800	-3.6928E+05	1.9925E-01	3.1286E+01	CE1	4295
BOND =	28520.6148	ANGLE =	1025.2592	DIHED =	5434.3808

Supplementary Text 3

VDWAALS = 71065.1410 EEL = -495460.7795 HBOND = 0.0000
 1-4 VDW = 1505.0690 1-4 EEL = 18629.5592 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 3900 -3.6937E+05 1.9398E-01 2.8176E+01 CE1 4295

BOND = 28539.1807 ANGLE = 1024.8723 DIHED = 5434.0431
 VDWAALS = 71137.9021 EEL = -495641.1939 HBOND = 0.0000
 1-4 VDW = 1504.9204 1-4 EEL = 18629.6226 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 4000 -3.6946E+05 1.1106E-01 1.4786E+01 CE1 4295

BOND = 28556.2450 ANGLE = 1024.4932 DIHED = 5433.7193
 VDWAALS = 71209.0657 EEL = -495816.1178 HBOND = 0.0000
 1-4 VDW = 1504.7553 1-4 EEL = 18629.6141 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 4100 -3.6954E+05 8.9660E-02 9.7689E+00 CE1 4295

BOND = 28574.1840 ANGLE = 1024.1973 DIHED = 5433.4208
 VDWAALS = 71281.4450 EEL = -495991.7591 HBOND = 0.0000
 1-4 VDW = 1504.5755 1-4 EEL = 18629.5400 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 4200 -3.6963E+05 9.1967E-02 1.1361E+01 CE1 4295

BOND = 28592.2865 ANGLE = 1024.0040 DIHED = 5433.1436
 VDWAALS = 71354.8166 EEL = -496166.2822 HBOND = 0.0000
 1-4 VDW = 1504.4007 1-4 EEL = 18629.4276 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 4300 -3.6971E+05 2.3073E-01 3.7107E+01 CE1 4295

BOND = 28613.0665 ANGLE = 1023.9930 DIHED = 5432.8856
 VDWAALS = 71431.9416 EEL = -496347.3792 HBOND = 0.0000
 1-4 VDW = 1504.2191 1-4 EEL = 18629.2536 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 4400 -3.6980E+05 6.5940E-02 4.1776E+00 CE1 4295

BOND = 28629.5197 ANGLE = 1023.6695 DIHED = 5432.6823
 VDWAALS = 71508.2030 EEL = -496523.9302 HBOND = 0.0000
 1-4 VDW = 1504.0178 1-4 EEL = 18629.0171 RESTRAINT = 0.0000

NSTEP ENERGY RMS GMAX NAME NUMBER
 4500 -3.6988E+05 1.8210E-01 2.8073E+01 CE1 4295

Supplementary Text 3

BOND	=	28649.3638	ANGLE	=	1023.6940	DIHED	=	5432.5193
VDWAALS	=	71586.1405	EEL	=	-496700.2771	HBOND	=	0.0000
1-4 VDW	=	1503.8322	1-4 EEL	=	18628.7284	RESTRAINT	=	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
4600	-3.6995E+05	1.4625E-01	2.2198E+01	CE1	4295

BOND	=	28667.1274	ANGLE	=	1023.5582	DIHED	=	5432.4164
VDWAALS	=	71663.9946	EEL	=	-496872.8122	HBOND	=	0.0000
1-4 VDW	=	1503.6264	1-4 EEL	=	18628.3877	RESTRAINT	=	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
4700	-3.7003E+05	1.1834E-01	1.6957E+01	CE1	4295

BOND	=	28684.6762	ANGLE	=	1023.5645	DIHED	=	5432.3493
VDWAALS	=	71742.1966	EEL	=	-497043.9552	HBOND	=	0.0000
1-4 VDW	=	1503.4356	1-4 EEL	=	18628.0332	RESTRAINT	=	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
4800	-3.7010E+05	8.9065E-02	1.1228E+01	CE1	4295

BOND	=	28701.7054	ANGLE	=	1023.5616	DIHED	=	5432.3279
VDWAALS	=	71818.2087	EEL	=	-497209.9717	HBOND	=	0.0000
1-4 VDW	=	1503.2390	1-4 EEL	=	18627.6473	RESTRAINT	=	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
4900	-3.7018E+05	2.2767E-01	3.5888E+01	CE1	4295

BOND	=	28721.0842	ANGLE	=	1023.7886	DIHED	=	5432.3323
VDWAALS	=	71895.7751	EEL	=	-497379.6785	HBOND	=	0.0000
1-4 VDW	=	1503.0453	1-4 EEL	=	18627.2209	RESTRAINT	=	0.0000

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
5000	-3.7025E+05	6.2254E-02	4.2246E+00	CE1	4295

BOND	=	28735.8677	ANGLE	=	1023.7488	DIHED	=	5432.3510
VDWAALS	=	71970.5825	EEL	=	-497542.7263	HBOND	=	0.0000
1-4 VDW	=	1502.8557	1-4 EEL	=	18626.7793	RESTRAINT	=	0.0000

Maximum number of minimization cycles reached.

FINAL RESULTS

NSTEP	ENERGY	RMS	GMAX	NAME	NUMBER
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Supplementary Text 3

5000	-3.7025E+05	6.2254E-02	4.2246E+00	CE1	4295
BOND	=	28735.8677	ANGLE	=	1023.7488
VDWAALS	=	71970.5825	EEL	=	-497542.7263
1-4 VDW	=	1502.8557	1-4 EEL	=	18626.7793
			DIHED	=	5432.3510
			HBOND	=	0.0000
			RESTRAINT	=	0.0000

5. TIMINGS

Build the list	26.60 (91.36% of List)
Other	2.52 (8.64% of List)
List time	29.12 (0.30% of Nonbo)
Short_ene time	8705.69 (99.69% of Direc)
Other	27.42 (0.31% of Direc)
Direct Ewald time	8733.11 (91.72% of Ewald)
Adjust Ewald time	32.32 (0.34% of Ewald)
Fill Bspline coeffs	24.45 (3.26% of Recip)
Fill charge grid	106.50 (14.21% of Recip)
Scalar sum	143.78 (19.19% of Recip)
Grad sum	186.72 (24.92% of Recip)
FFT time	287.87 (38.42% of Recip)
Recip Ewald time	749.33 (7.87% of Ewald)
Virial junk	2.02 (0.02% of Ewald)
Other	4.56 (0.05% of Ewald)
Ewald time	9521.36 (99.70% of Nonbo)
Nonbond force	9550.48 (99.53% of Force)
Bond/Angle/Dihedral	44.35 (0.46% of Force)
Other	1.10 (0.01% of Force)
Force time	9595.94 (100.0% of Runmd)
Runmd Time	9595.94 (99.72% of Total)
Other	26.75 (0.28% of Total)
Total time	9622.71 (100.0% of ALL)

Number of list builds : 18

Highest rstack allocated: 4941880
Highest istack allocated: 92322
Job began at 17:17:31.941 on 02/20/2019
Setup done at 17:17:32.739 on 02/20/2019
Run done at 19:57:54.656 on 02/20/2019
wallclock() was called 190084 times