SUPPORTING INFORMATION

Exploring with Molecular Dynamics the Structural Fate of PLGA Oligomers in Various Solvents

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S1. Parameter Files for the GAFF Force Field

GAFF force field parameters including the RESP atomic charges for the ethyl acetate solvent and each of the seven PLGA oligomers considered are given in the accompanying topology (.top) files. Names of the latter are:

- 22-PLGA_A.top
- 22-PLGA_B.top
- 22-PLGA_C.top
- 10-PLGA_I.top
- 10-PLGA_J.top

- 10-PLGA_K.top
- 4-PLGA.top
- Ethyl_Acetate.top

Figure S1 gives the structure of the seven PLGA oligomers used for the calculation of the RESP charges and indicates the sequence of lactic acid monomers (L) and glycolic acid monomers (G) random organization within each model. Figure S2 gives the distribution of the calculated charges/monomer along the oligomers chains according to their sequence of lactic acid and glycolic acid monomers given in Table 1 of the main paper.

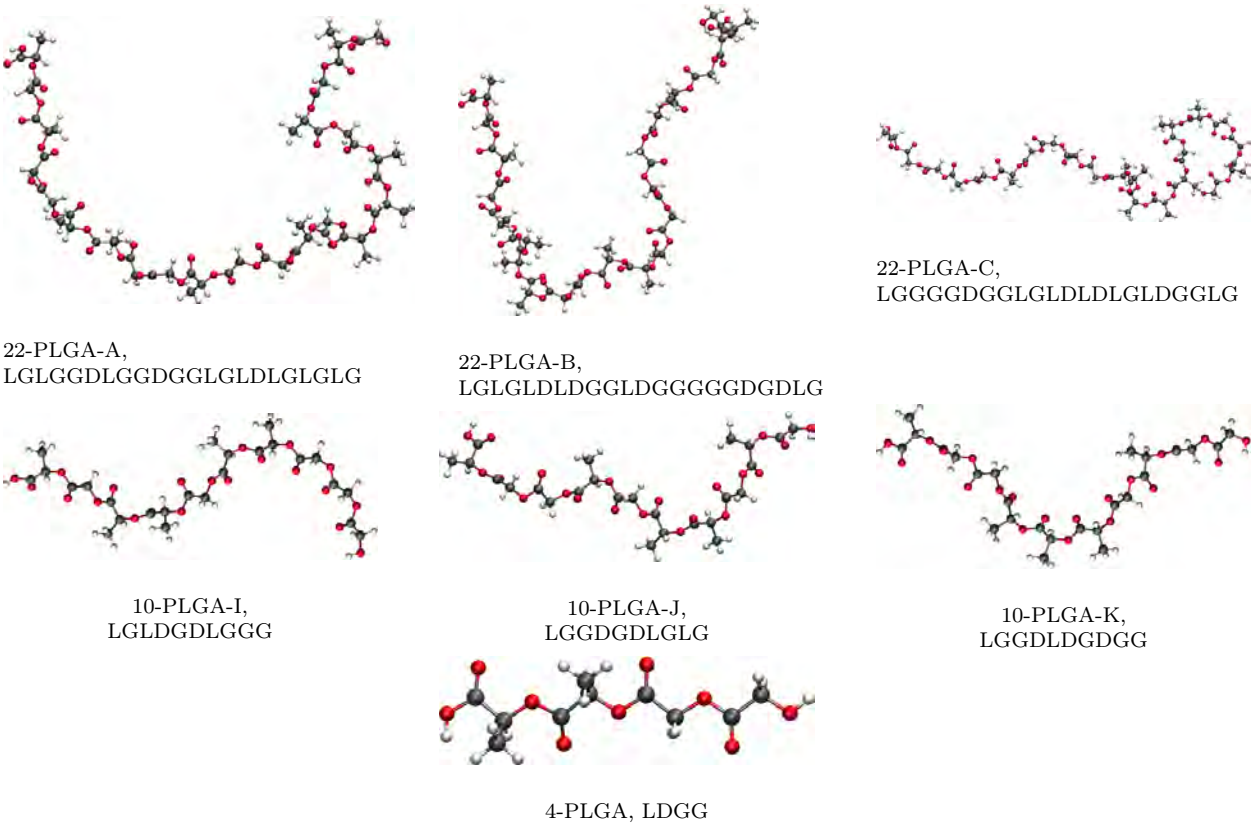

Figure S1: Geometry of the seven PLGA oligomers used for the BCC and RESP atomic charge calculations of each PLGA model.

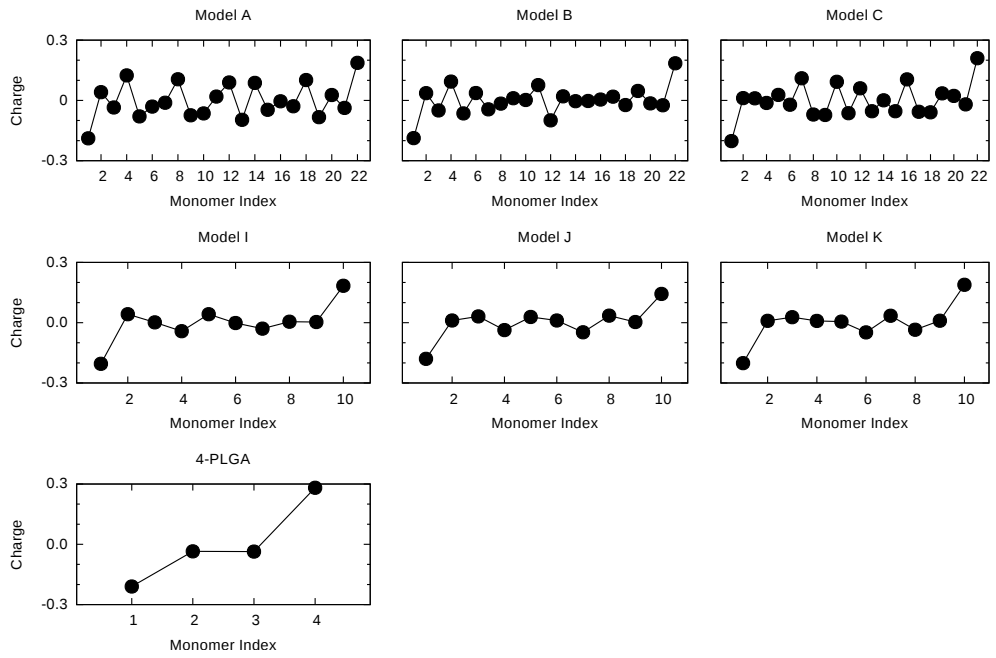

Figure S2: Distribution of RESP charges summed on each monomer along the length of each PLGA oligomer.

S2. System Size

Each model was solvated in a system proportional to their size. Table S1 shows the molecule and atom count for each solvent for each PLGA oligomer size.

Table S1: Number of molecules and atoms for each model length and solvent system.

		MIX		EA		Water	
		Molecules	Atoms	Molecules	Atoms	Molecules	Atoms
22-PLGA	PLGA	1	168	1	168	1	168
	EA	603	8442	1204	16856		
	WAT	5454	16362			5908	17724
	Total		24972		17024		17892
10-PLGA	PLGA	1	78	1	78	1	78
	EA	279	3906	557	7798		
	WAT	2519	7557			2729	8187
	Total		11541		7876		8265
4-PLGA	PLGA	1	33	1	33	1	33
	EA	116	1624	232	3248		
	WAT	932	2796			1134	3402
	Total		4453		3281		3435

S3. Time Evolution

Molecular Dynamics simulations were done for the seven different PLGA oligomers shown in Fig. S1 solvated in ethyl acetate (EA), TIP3P water, SPC/E water, and mixtures of EA with each type of water. Figures S3 through S26 show the time evolution of the PLGA potential energy per monomer, their interaction energy with their respective solvents, the PLGA radius of gyration, and the ratio of the PLGA third and first moments of inertia (I_C/I_A)

S3.a. PLGA Solvated in Ethyl Acetate

For each PLGA oligomer solvated in ethyl acetate (EA), simulations using both the GAFF-BCC and GAFF-RESP cases are provided in Fig. S3 through Fig. S10.

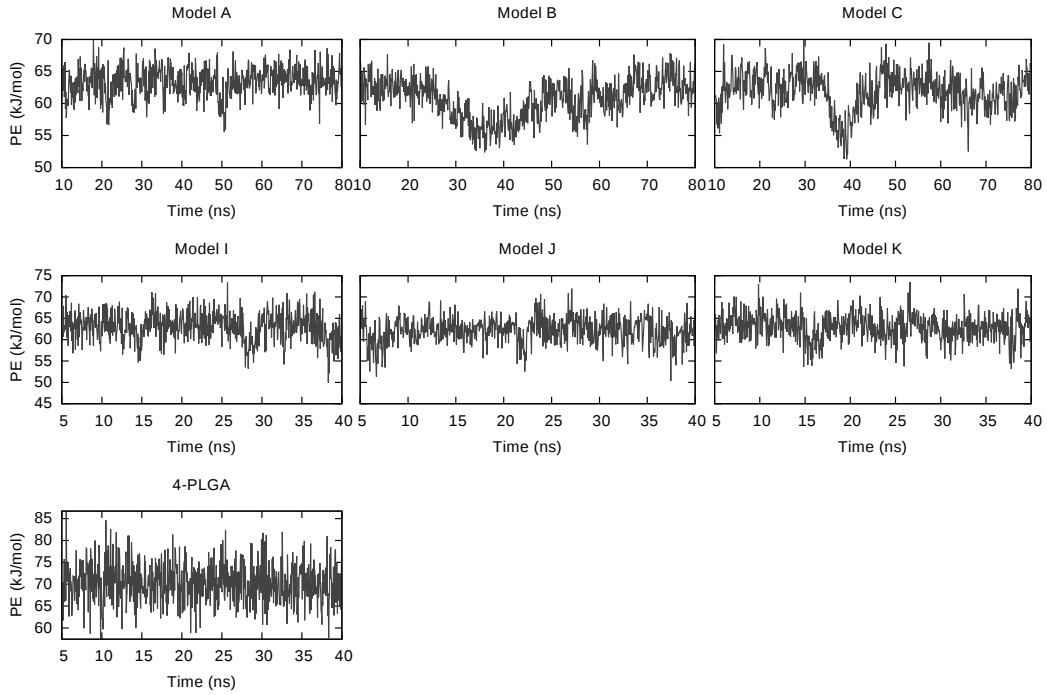

Figure S3: Potential energy of PLGA oligomers in ethyl acetate solvent with AM1-BCC charges during NVE production stage of MD for the 7 oligomers considered.

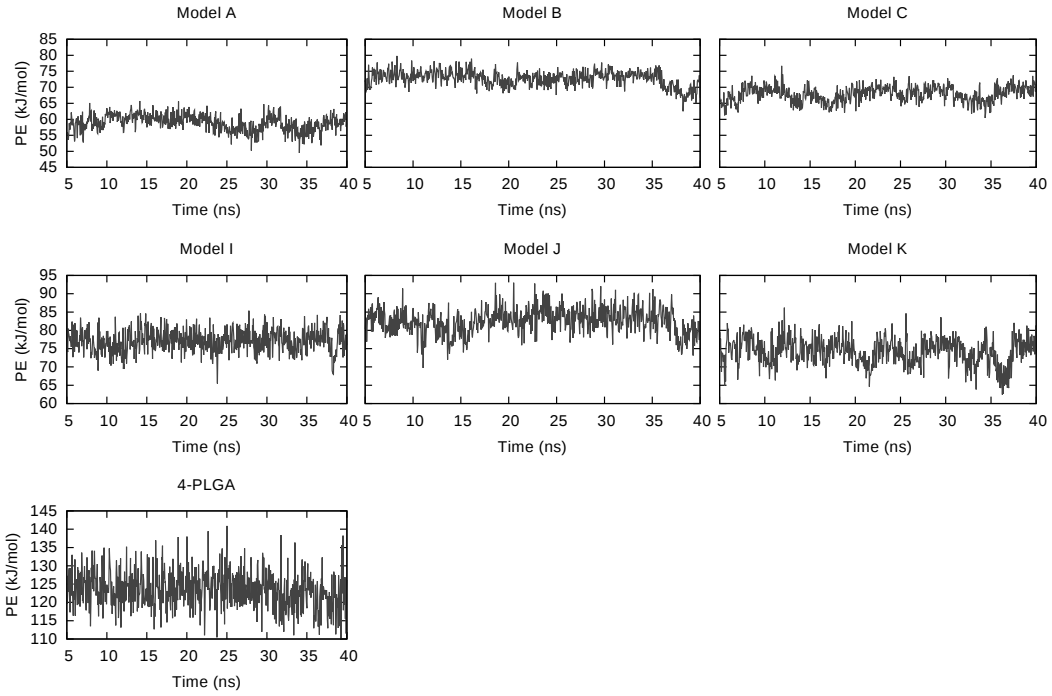

Figure S4: Potential energy/monomer of PLGA oligomer in ethyl acetate solvent with RESP charges during NVE production stage of MD for the 7 PLGA oligomers studied.

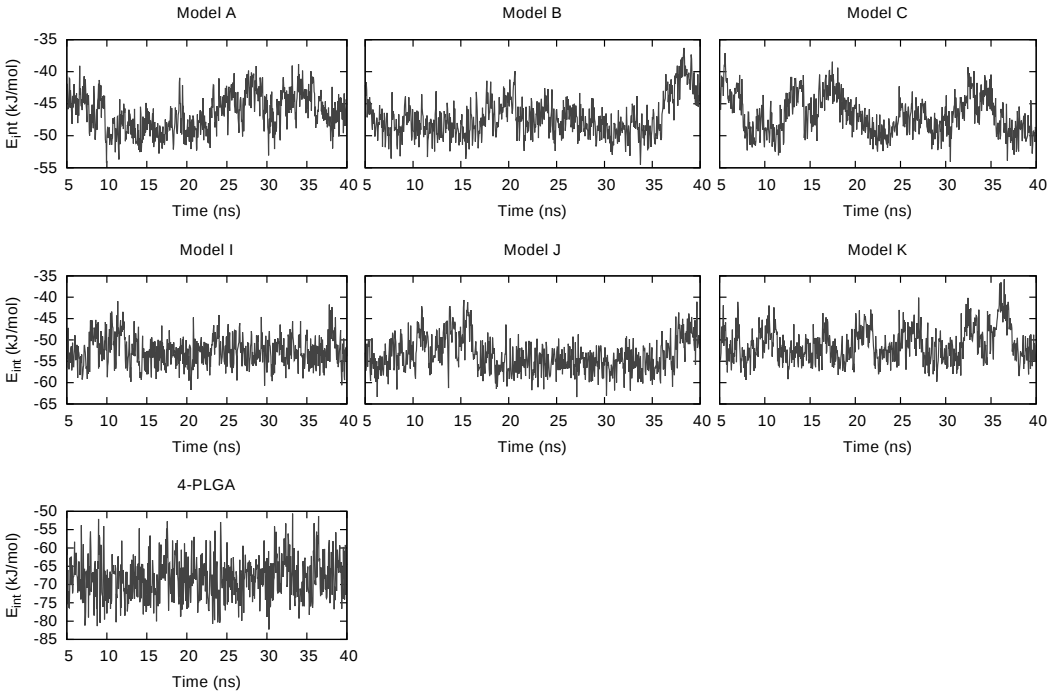

Figure S5: Interaction energy between PLGA polymer and ethyl acetate solvent with RESP charges during NVE production stage of MD for each simulated model.

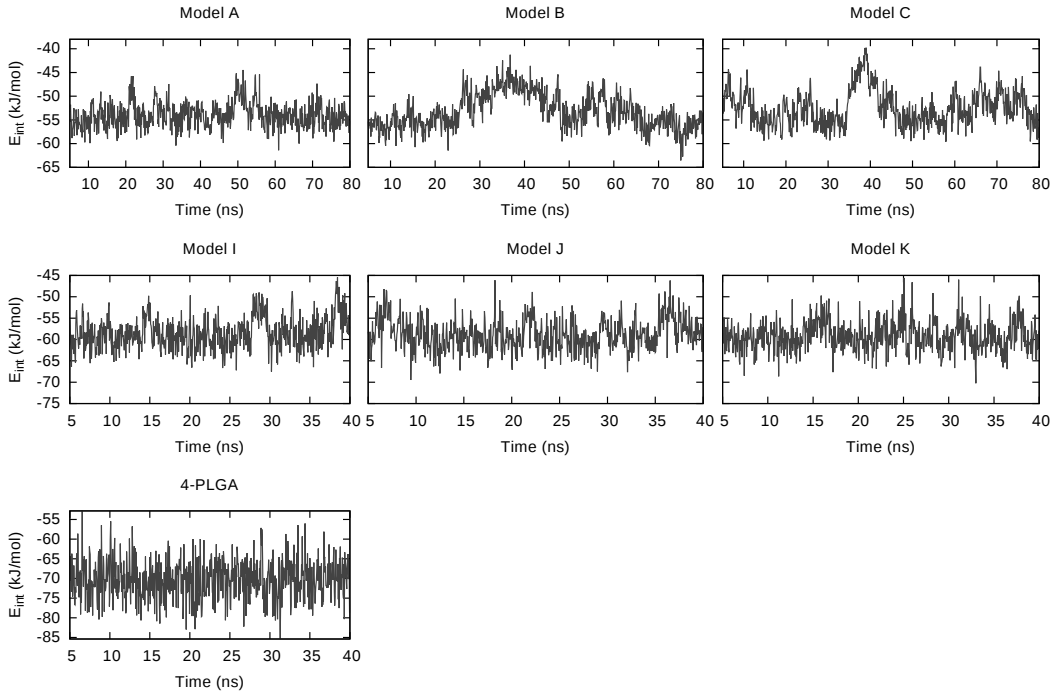

Figure S6: Interaction energy between PLGA polymer and ethyl acetate solvent with AM1-BCC charges during NVE production stage of MD for each simulated model.

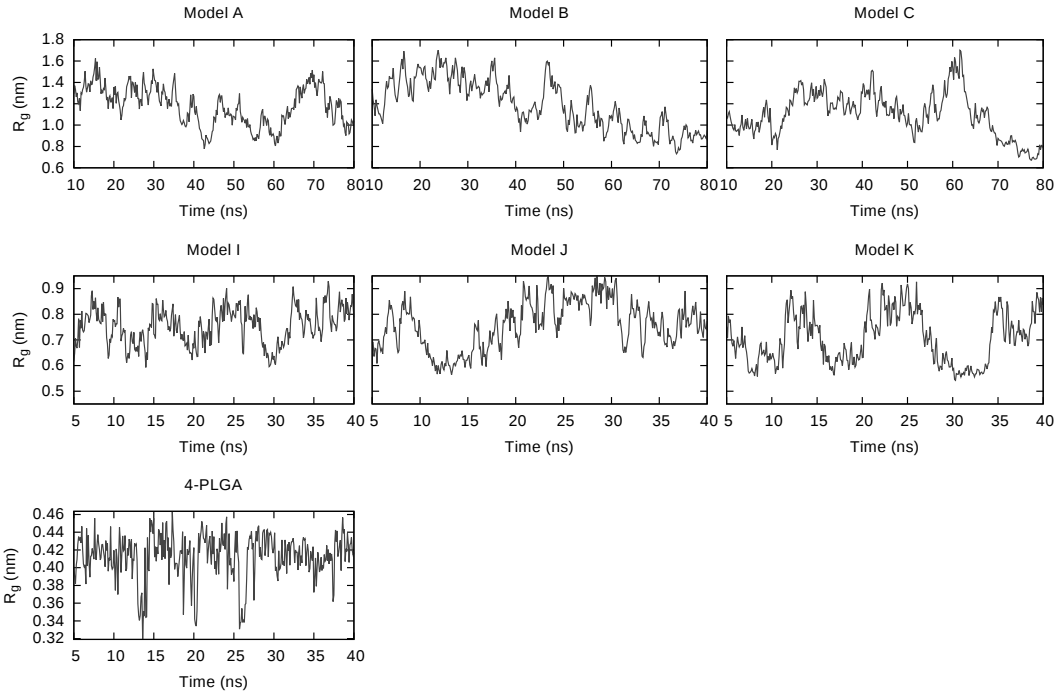

Figure S7: PLGA polymer radius of gyration during NVE production stage of MD for each simulated PLGA model in ethyl acetate solvent with AM1-BCC charges.

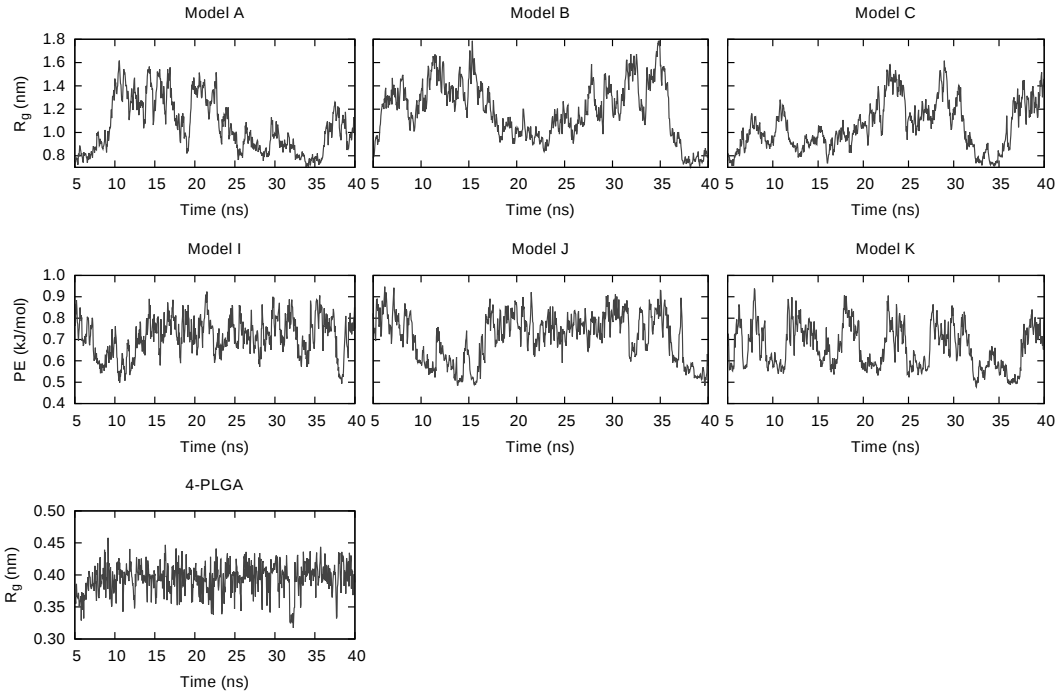

Figure S8: PLGA polymer radius of gyration during NVE production stage of MD for each simulated model in ethyl acetate solvent with RESP charges.

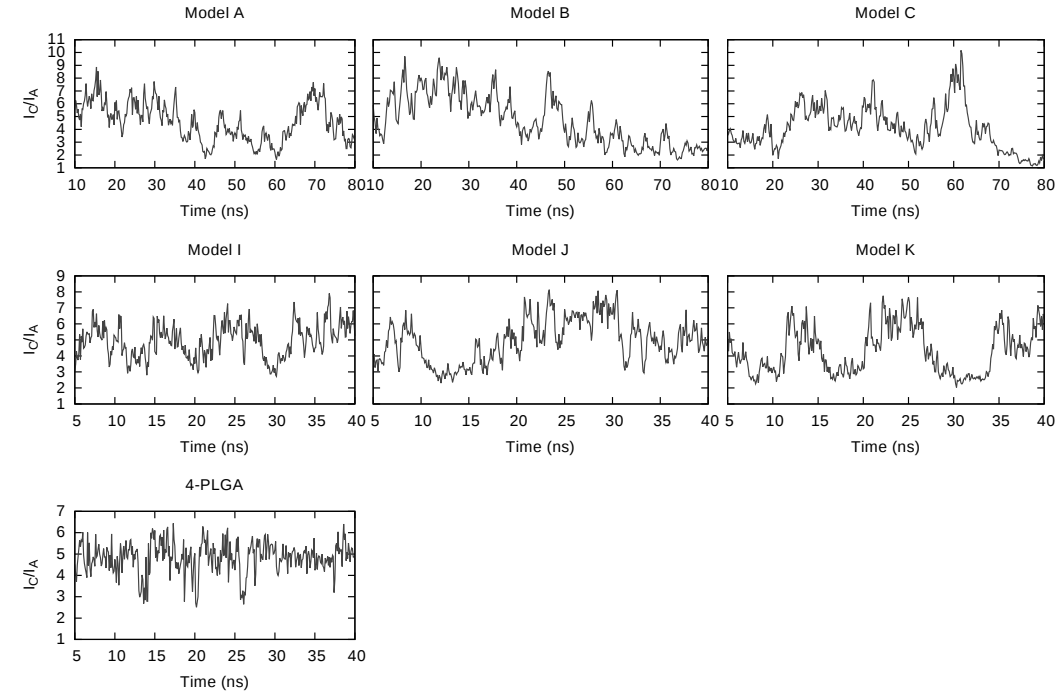

Figure S9: PLGA polymer I_C principal moment of inertia relative to I_A in ethyl acetate solvent during NVE production stage of MD simulation with AM1-BCC charges.

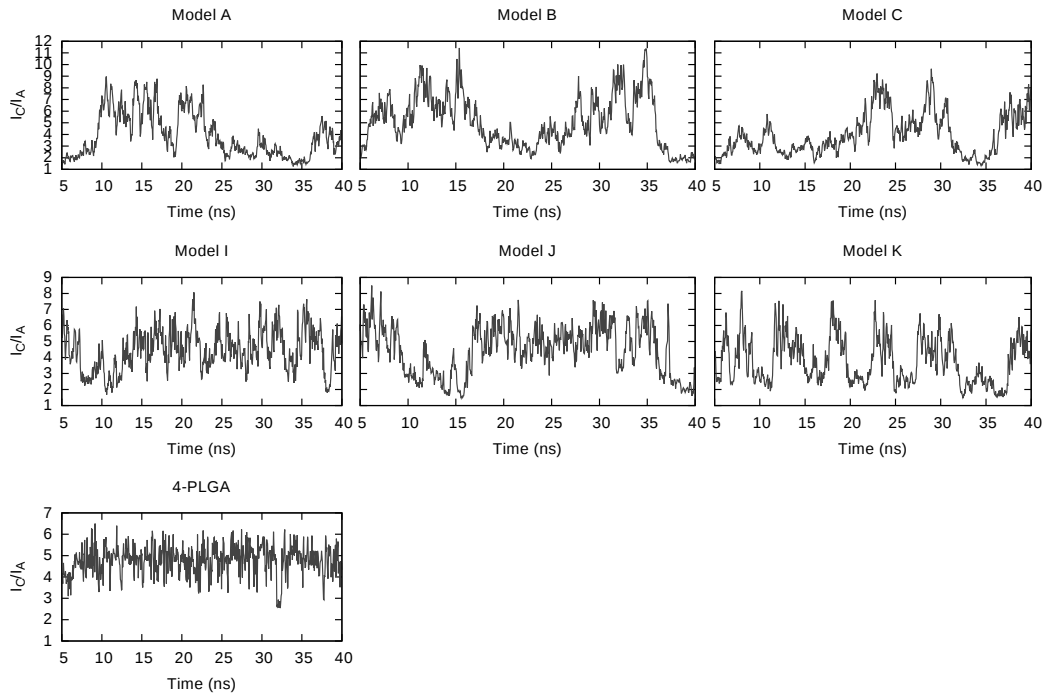

Figure S10: PLGA polymer I_C principal moment of inertia relative to I_A in ethyl acetate solvent during NVE production stage of MD simulation with RESP charges.

S3.b PLGA Solvated in Water Modeled with TIP3P and SPC/E

containing water, two water models were simulated, the TIP3P and the SPC/E. Each system underwent 40 ns of NVE production runs where data were collected. Figures S11 through S18 show the time evolution of the potential energy per monomer and the interaction energy. Figures S19 through S26 show the time evolution of the radius of gyration of each model.

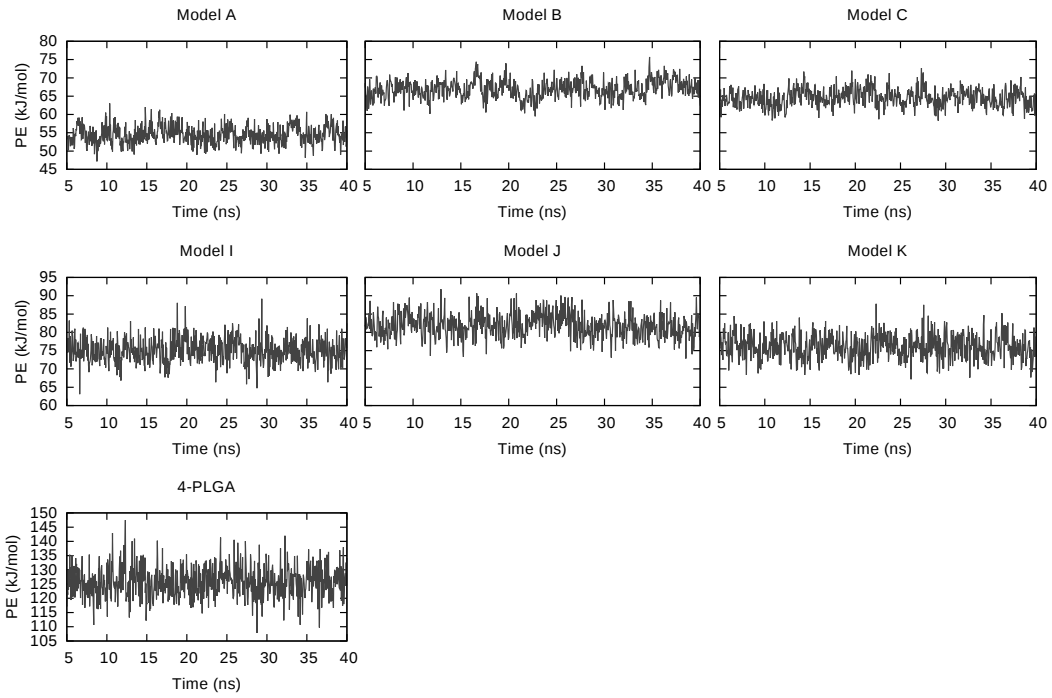

Figure S11: Potential energy of PLGA polymer in TIP3P water solvent with RESP charges during NVE production stage of MD for each simulated model.

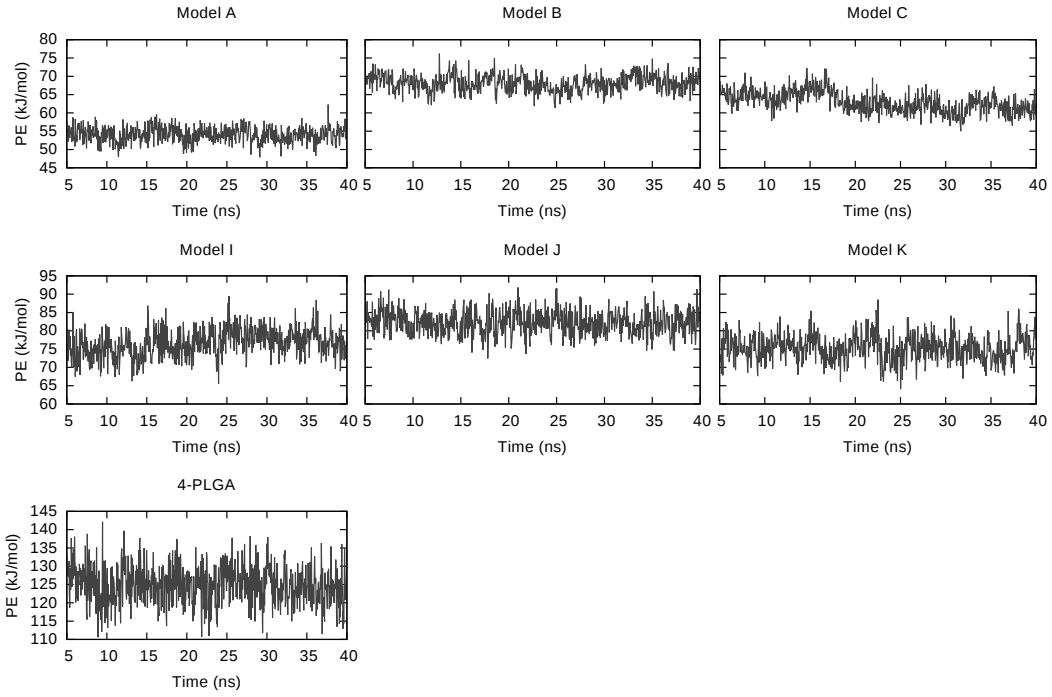

Figure S12: Potential energy of PLGA polymer in SPC/E water solvent with RESP charges during NVE production stage of MD for each simulated model.

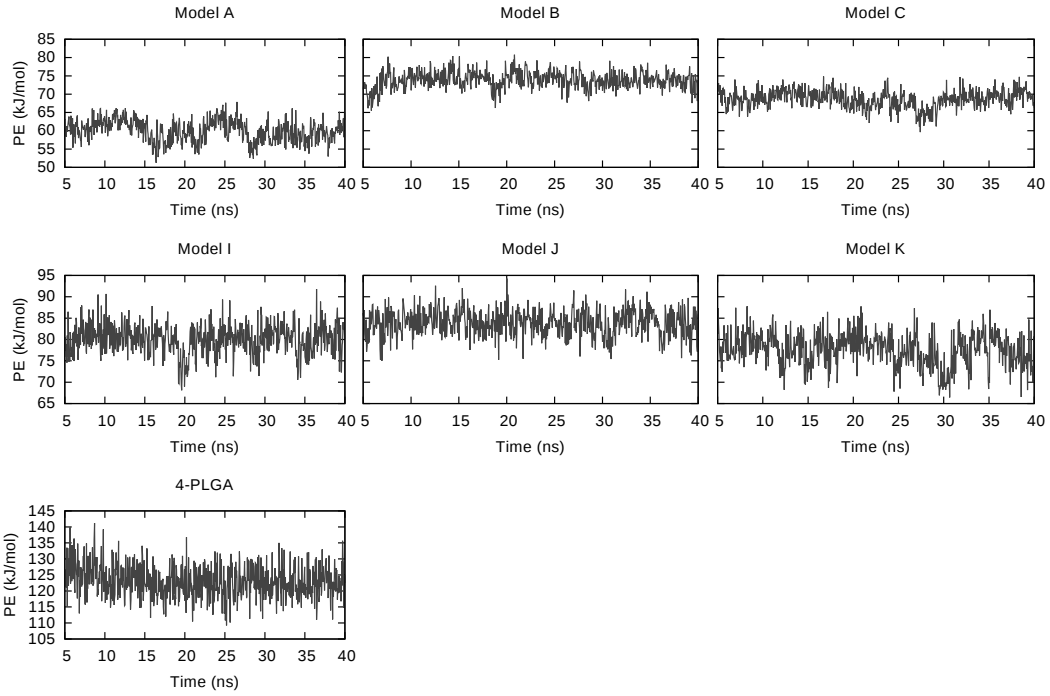

Figure S13: Potential energy of PLGA polymer in ethyl acetate and TIP3P water mixed solvent with RESP charges during NVE production stage of MD for each simulated model.

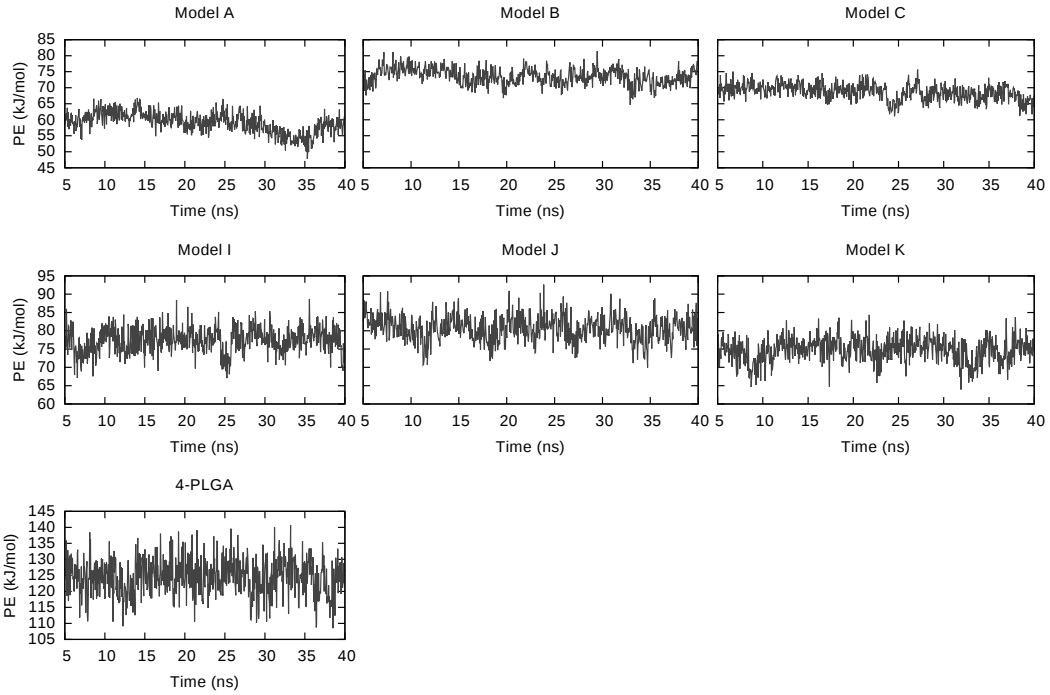

Figure S14: Potential energy of PLGA polymer in ethyl acetate and SPC/E water mixed solvent with RESP charges during NVE production stage of MD for each simulated model.

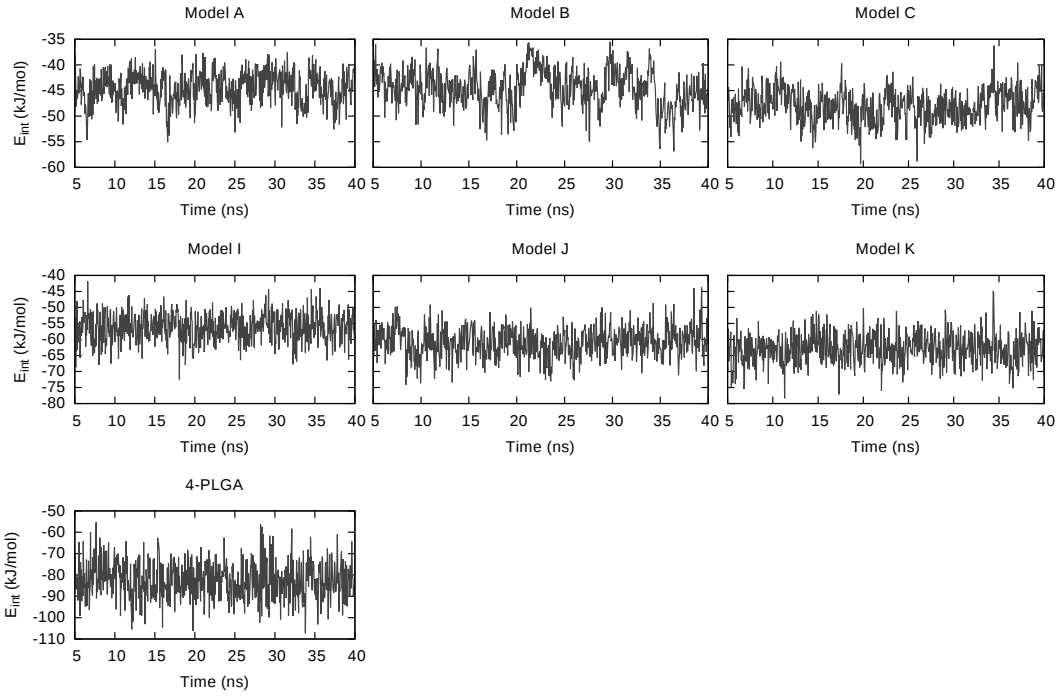

Figure S15: Interaction energy between PLGA polymer and TIP3P water solvent with RESP charges during NVE production stage of MD for each simulated model.

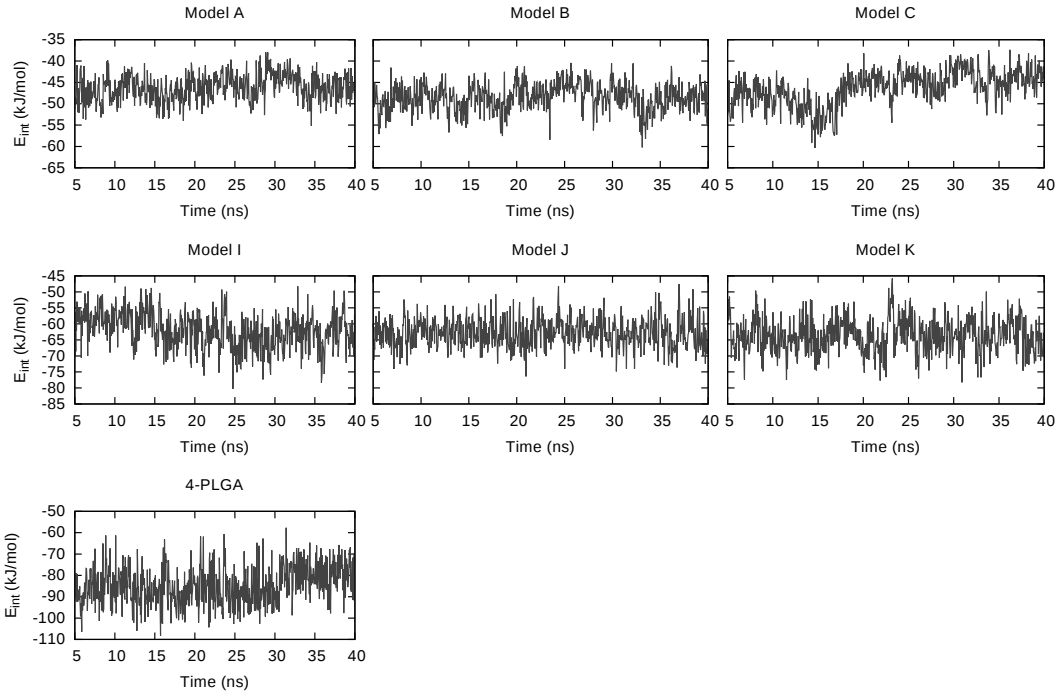

Figure S16: Interaction energy between PLGA polymer and SPC/E water solvent with RESP charges during NVE production stage of MD for each simulated model.

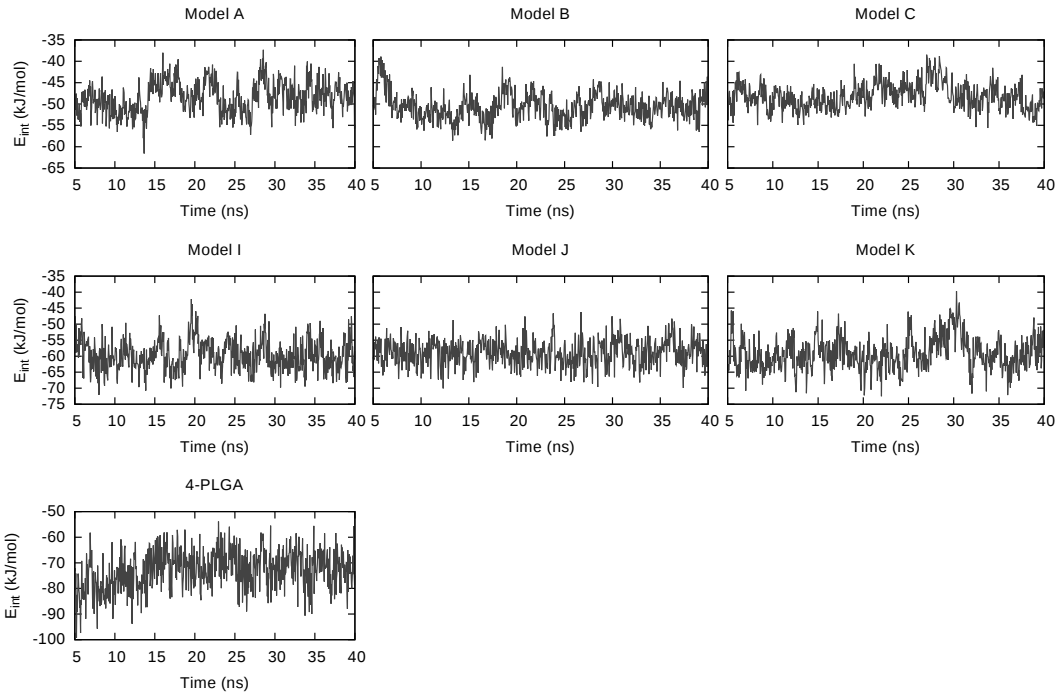

Figure S17: Interaction energy between PLGA polymer and ethyl acetate and TIP3P water mixed solvent with RESP charges during NVE production stage of MD for each simulated model.

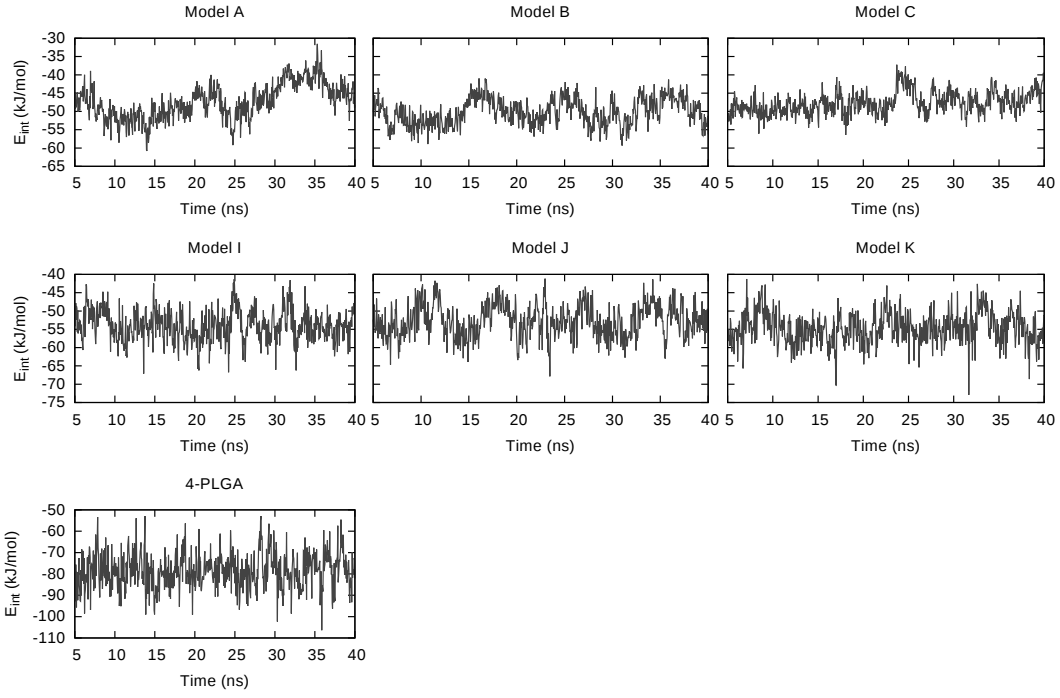

Figure S18: Interaction energy between PLGA polymer and ethyl acetate and SPC/E water mixed solvent with RESP charges during NVE production stage of MD for each simulated model.

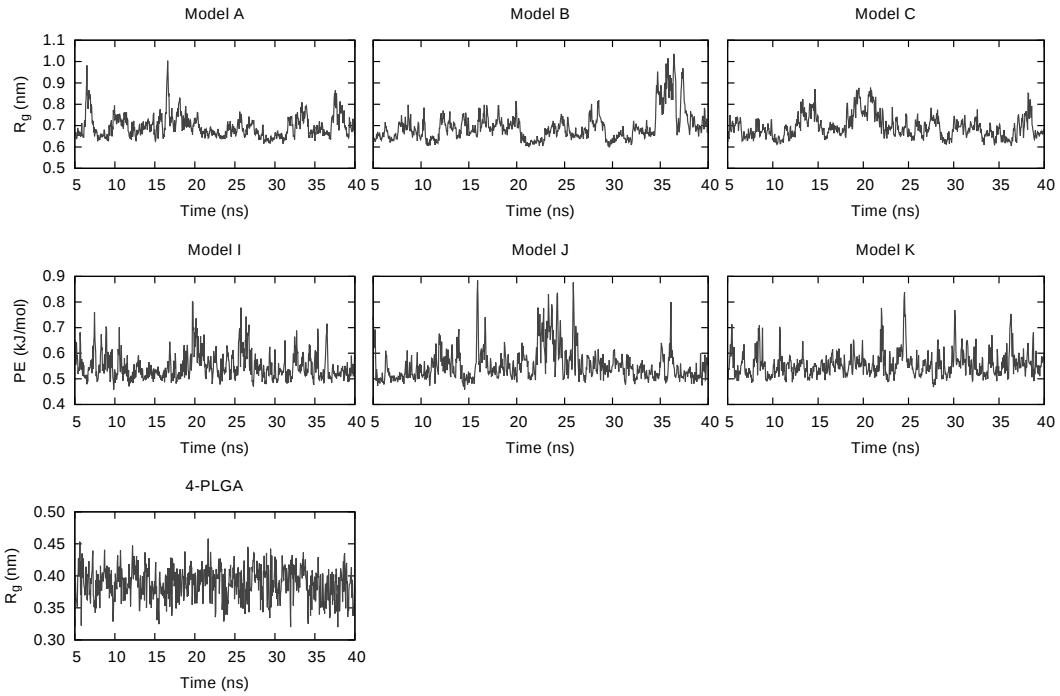

Figure S19: PLGA polymer radius of gyration during NVE production stage of MD for each simulated model in TIP3P water solvent with RESP charges.

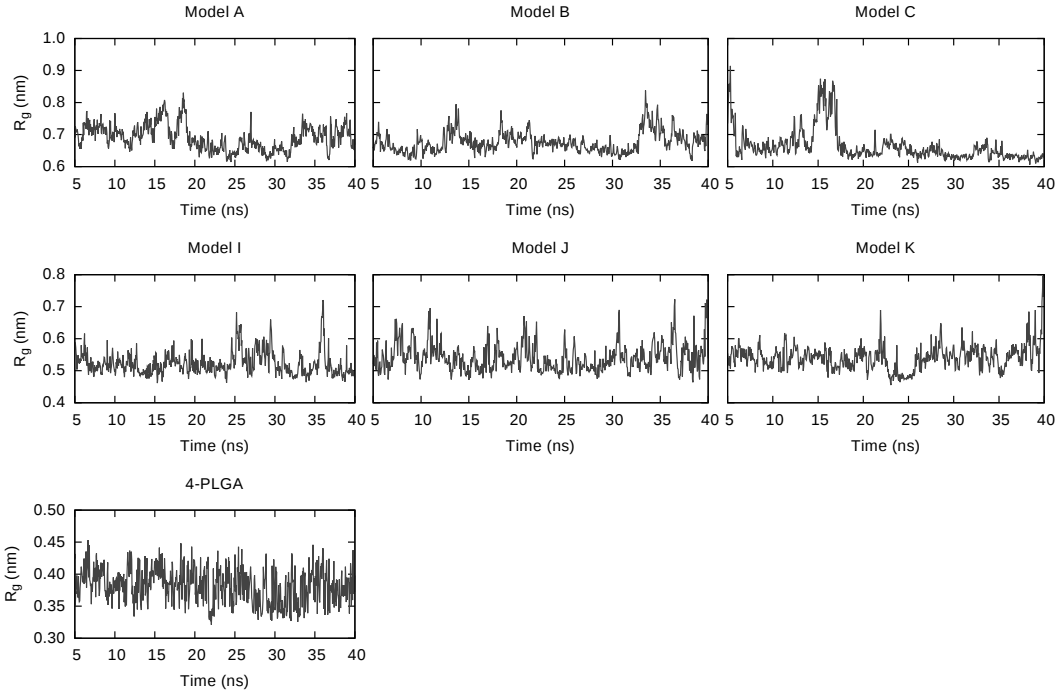

Figure S20: PLGA polymer radius of gyration during NVE production stage of MD for each simulated model in SPC/E water solvent with RESP charges.

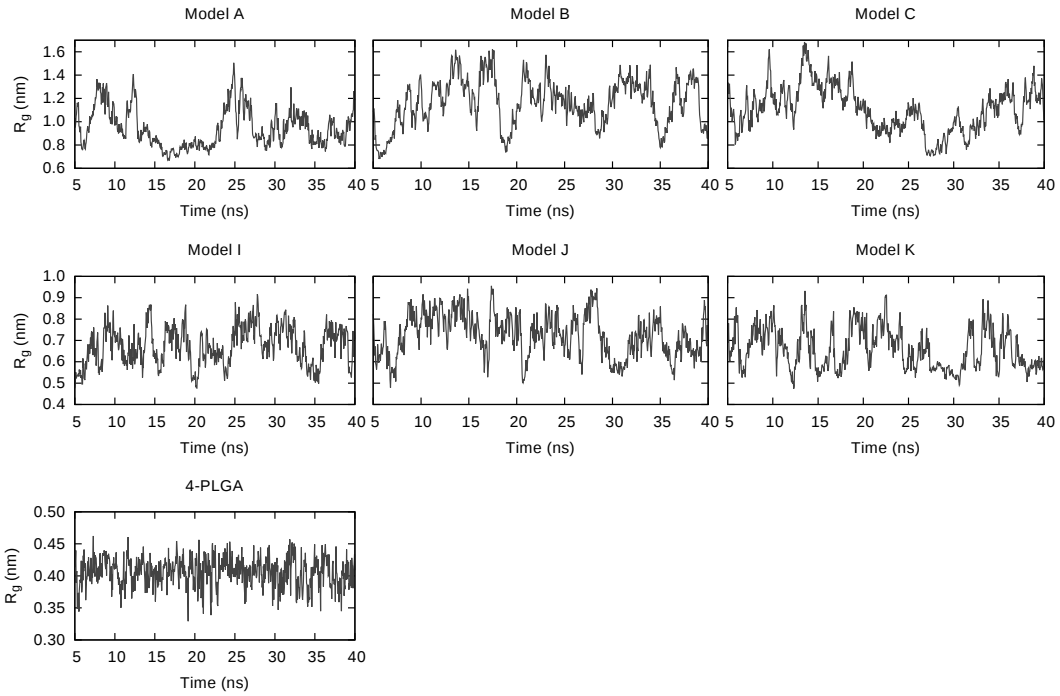

Figure S21: PLGA polymer radius of gyration during NVE production stage of MD for each simulated model in ethyl acetate and TIP3P water mixed solvent with RESP charges.

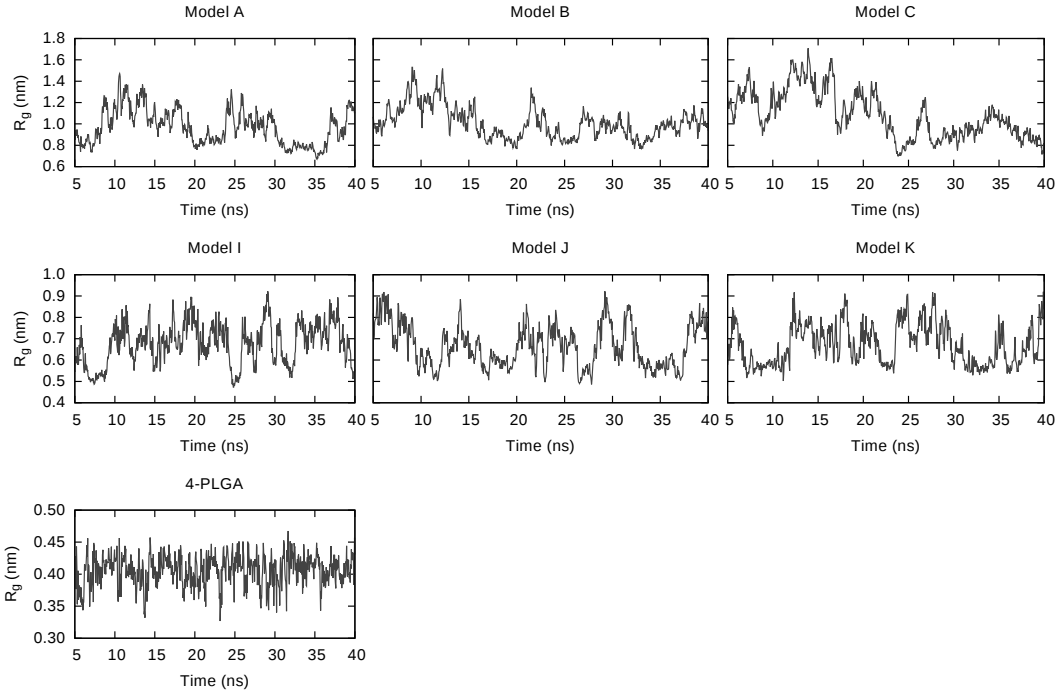

Figure S22: PLGA polymer radius of gyration during NVE production stage of MD for each simulated model in ethyl acetate and SPC/E water mixed solvent with RESP charges.

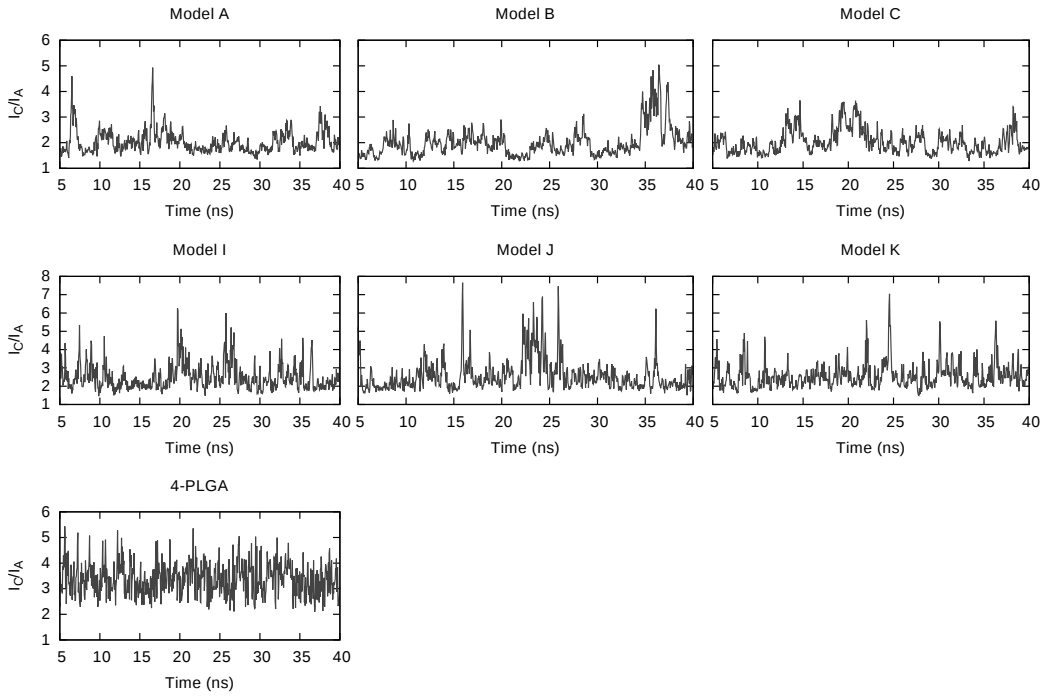

Figure S23: PLGA polymer I_C principal moment of inertia relative to I_A in TIP3P water solvent during NVE production stage of MD simulation with RESP charges.

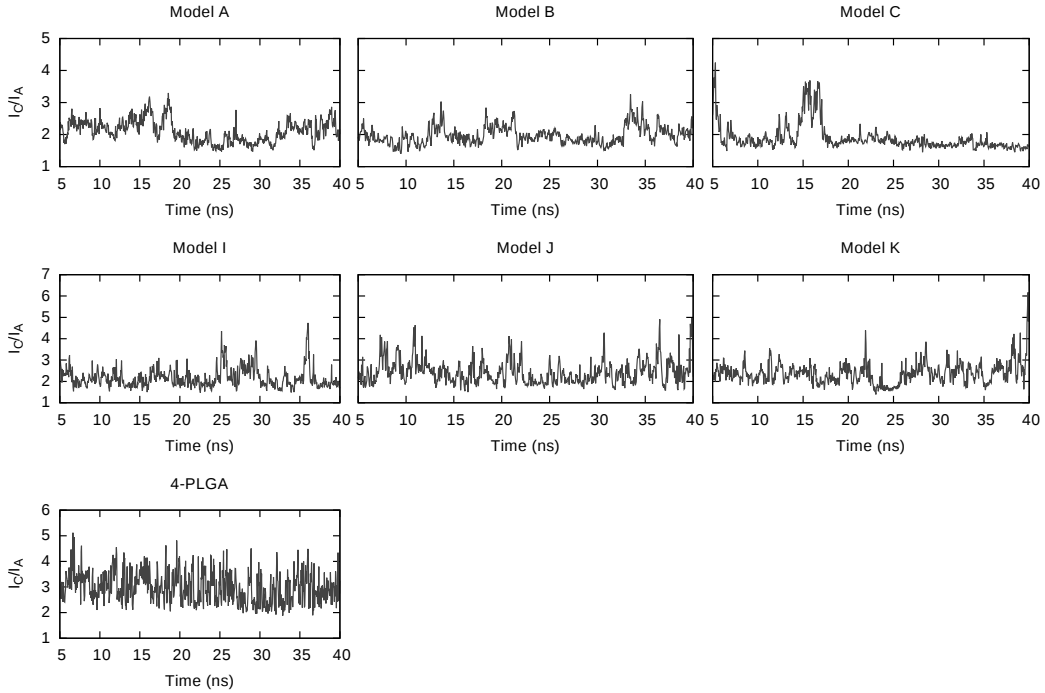

Figure S24: PLGA polymer I_C principal moment of inertia relative to I_A in SPC/E water solvent during NVE production stage of MD simulation with RESP charges.

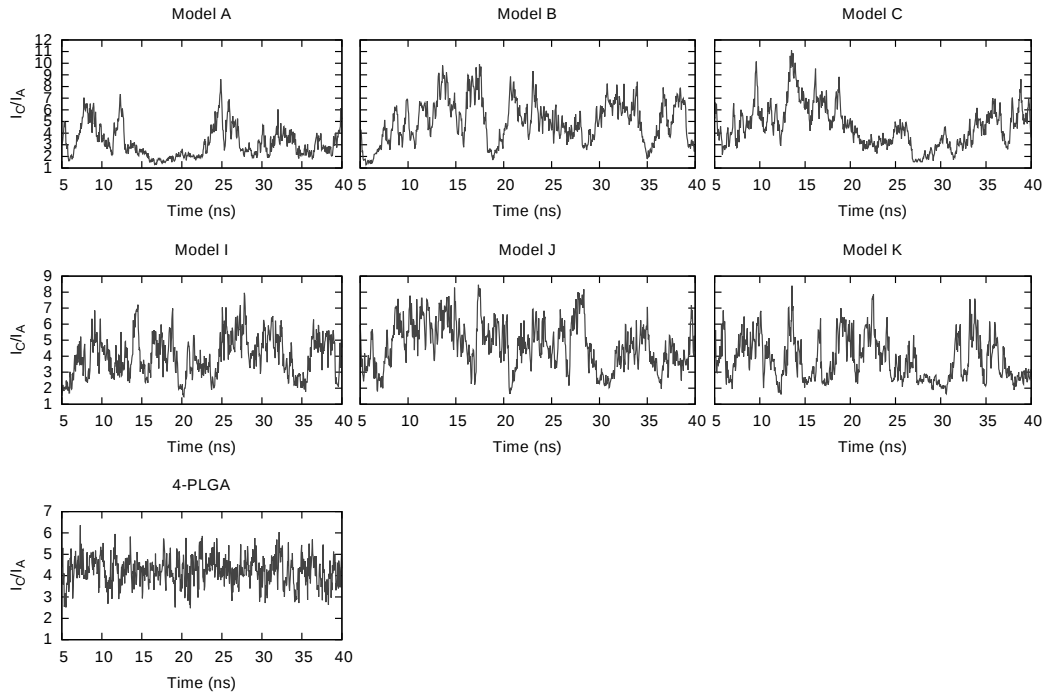

Figure S25: PLGA polymer I_C principal moment of inertia relative to I_A in ethyl acetate and TIP3P water mixed solvent with RESP charges during NVE production stage of MD simulation.

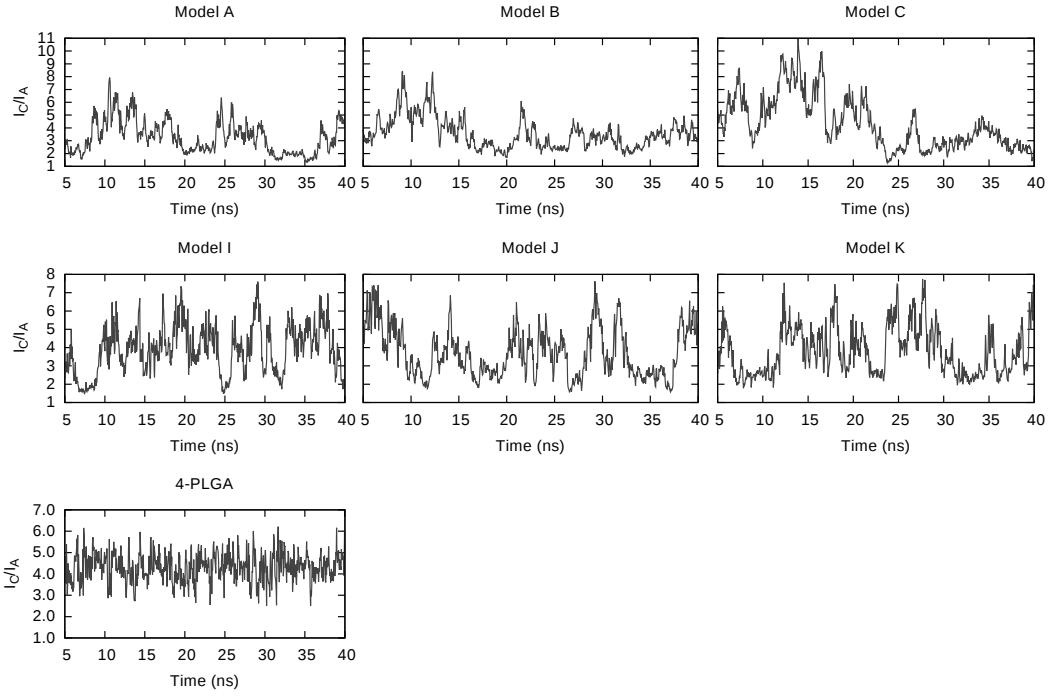

Figure S26: PLGA polymer I_C principal moment of inertia relative to I_A in ethyl acetate and SPC/E water mixed solvent with RESP charges during NVE production stage of MD simulation.

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;   Created by:
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      27     33     1
      28     30     1
      28     31     1
      30     33     1
      31     33     1

[ angles ]
;    ai     aj     ak funct         c0         c1
c2         c3
       2      3      4     1   122.1000523 635.131200
       2      3      5     1   112.7300484 572.371200
       3      5      7     1   109.2100466 569.024000
       3      5      8     1   111.0400475 529.694400
       4      3      5     1   123.2000528 564.003200
       5      7     12     1   115.9800495 529.694400
       7      5      8     1   107.9700462 569.024000
       7     12     13     1   123.2500525 630.110400
       7     12     14     1   110.7200477 576.555200
      12     14     16     1   109.2100466 569.024000
      12     14     17     1   111.0400475 529.694400
      13     12     14     1   123.2000528 564.003200
      14     16     21     1   115.9800495 529.694400
      16     14     17     1   107.9700462 569.024000
      16     21     22     1   123.2500525 630.110400
      16     21     23     1   110.7200477 576.555200
      21     23     26     1   109.2100466 569.024000
      22     21     23     1   123.2000528 564.003200
      23     26     27     1   115.9800495 529.694400
      26     27     28     1   123.2500525 630.110400
      26     27     29     1   110.7200477 576.555200
      27     29     32     1   108.7900468 571.534400
      28     27     29     1   123.2000528 564.003200
```

```
     1      2      3     1   106.5500460 417.563200
     3      5      6     1   108.2200466 393.296000
     5      8      9     1   109.8000471 387.438400
     5      8     10     1   109.8000471 387.438400
     5      8     11     1   109.8000471 387.438400
     6      5      7     1   109.7800468 425.094400
     6      5      8     1   109.5600471 388.275200
     9      8     10     1   107.5800459 329.699200
     9      8     11     1   107.5800459 329.699200
    10      8     11     1   107.5800459 329.699200
    12     14     15     1   108.2200466 393.296000
    14     17     18     1   109.8000471 387.438400
    14     17     19     1   109.8000471 387.438400
    14     17     20     1   109.8000471 387.438400
    15     14     16     1   109.7800468 425.094400
    15     14     17     1   109.5600471 388.275200
    18     17     19     1   107.5800459 329.699200
    18     17     20     1   107.5800459 329.699200
    19     17     20     1   107.5800459 329.699200
    21     23     24     1   108.2200466 393.296000
    21     23     25     1   108.2200466 393.296000
    24     23     25     1   108.4600466 328.025600
    24     23     26     1   109.7800468 425.094400
    25     23     26     1   109.7800468 425.094400
    27     29     30     1   108.2200466 393.296000
    27     29     31     1   108.2200466 393.296000
    29     32     33     1   107.2600461 396.643200
    30     29     31     1   108.4600466 328.025600
    30     29     32     1   110.2600474 425.931200
    31     29     32     1   110.2600474 425.931200

[ dihedrals ]
;    ai     aj     ak     al funct         c0
c1         c2         c3         c4         c5
      2      3      5      7     1  180.0000771
0.0000000  2
      2      3      5      8     1  180.0000771
0.0000000  2
      3      5      7     12     1  0.0000000
1.6038667  3
      4      3      5      7     1  180.0000771
```

```
0.0000000  2
      4      3      5      8      1  180.0000771
0.0000000  2
      5      7     12     13      1  180.0000771
5.8576000  1
      5      7     12     13      1  180.0000771
11.2968000  2
      5      7     12     14      1  0.0000000
0.0000000  1
      5      7     12     14      1  180.0000771
11.2968000  2
      5      7     12     14      1  0.0000000
4.8116000  3
      7     12     14     16      1  180.0000771
0.0000000  2
      7     12     14     17      1  180.0000771
0.0000000  2
      8      5      7     12      1  180.0000771
3.3472000  1
      8      5      7     12      1  0.0000000
1.6024720  3
     12     14     16     21      1  0.0000000
1.6038667  3
     13     12     14     16      1  180.0000771
0.0000000  2
     13     12     14     17      1  180.0000771
0.0000000  2
     14     16     21     22      1  180.0000771
5.8576000  1
     14     16     21     22      1  180.0000771
11.2968000  2
     14     16     21     23      1  0.0000000
0.0000000  1
     14     16     21     23      1  180.0000771
11.2968000  2
     14     16     21     23      1  0.0000000
4.8116000  3
     16     21     23     26      1  180.0000771
0.0000000  2
     17     14     16     21      1  180.0000771
3.3472000  1
```

```
     17     14     16     21     1  0.0000000
1.6024720  3
     21     23     26     27     1  0.0000000
1.6038667  3
     22     21     23     26     1  180.0000771
0.0000000  2
     23     26     27     28     1  180.0000771
5.8576000  1
     23     26     27     28     1  180.0000771
11.2968000  2
     23     26     27     29     1  0.0000000
0.0000000  1
     23     26     27     29     1  180.0000771
11.2968000  2
     23     26     27     29     1  0.0000000
4.8116000  3
     26     27     29     32     1  180.0000771
0.0000000  2
     28     27     29     32     1  180.0000771
0.0000000  2
      5      4      3      2     4  180.0000771
4.6024000  2
     14     13     12      7     4  180.0000771
43.9320000  2
     23     22     21     16     4  180.0000771
43.9320000  2
     29     28     27     26     4  180.0000771
43.9320000  2
      1      2      3      4     1  0.0000000
7.9496000  1
      1      2      3      4     1  180.0000771
9.6232000  2
      1      2      3      5     1  180.0000771
9.6232000  2
      2      3      5      6     1  180.0000771
0.0000000  2
      3      5      8      9     1  0.0000000
0.6508444  3
      3      5      8     10     1  0.0000000
0.6508444  3
      3      5      8     11     1  0.0000000
```

```
0.6508444  3
      4      3      5      6      1  0.0000000
3.3472000  1
      4      3      5      6      1  0.0000000
0.0000000  2
      4      3      5      6      1  180.0000771
0.3347200  3
      6      5      7     12      1  0.0000000
1.6038667  3
      6      5      8      9      1  0.0000000
0.6508444  3
      6      5      8     10      1  0.0000000
0.6508444  3
      6      5      8     11      1  0.0000000
0.6508444  3
      7      5      8      9      1  0.0000000
1.0460000  1
      7      5      8      9      1  0.0000000
0.0000000  3
      7      5      8     10      1  0.0000000
1.0460000  1
      7      5      8     10      1  0.0000000
0.0000000  3
      7      5      8     11      1  0.0000000
1.0460000  1
      7      5      8     11      1  0.0000000
0.0000000  3
      7     12     14     15      1  180.0000771
0.0000000  2
     12     14     17     18      1  0.0000000
0.6508444  3
     12     14     17     19      1  0.0000000
0.6508444  3
     12     14     17     20      1  0.0000000
0.6508444  3
     13     12     14     15      1  0.0000000
3.3472000  1
     13     12     14     15      1  0.0000000
0.0000000  2
     13     12     14     15      1  180.0000771
0.3347200  3
```

```
     15     14     16     21     1  0.0000000
1.6038667  3
     15     14     17     18     1  0.0000000
0.6508444  3
     15     14     17     19     1  0.0000000
0.6508444  3
     15     14     17     20     1  0.0000000
0.6508444  3
     16     14     17     18     1  0.0000000
1.0460000  1
     16     14     17     18     1  0.0000000
0.0000000  3
     16     14     17     19     1  0.0000000
1.0460000  1
     16     14     17     19     1  0.0000000
0.0000000  3
     16     14     17     20     1  0.0000000
1.0460000  1
     16     14     17     20     1  0.0000000
0.0000000  3
     16     21     23     24     1  180.0000771
0.0000000  2
     16     21     23     25     1  180.0000771
0.0000000  2
     22     21     23     24     1  0.0000000
3.3472000  1
     22     21     23     24     1  0.0000000
0.0000000  2
     22     21     23     24     1  180.0000771
0.3347200  3
     22     21     23     25     1  0.0000000
3.3472000  1
     22     21     23     25     1  0.0000000
0.0000000  2
     22     21     23     25     1  180.0000771
0.3347200  3
     24     23     26     27     1  0.0000000
1.6038667  3
     25     23     26     27     1  0.0000000
1.6038667  3
     26     27     29     30     1  180.0000771
```

```
0.0000000  2
     26     27     29     31     1  180.0000771
0.0000000  2
     27     29     32     33     1  0.0000000
0.6973333  3
     28     27     29     30     1  0.0000000
3.3472000  1
     28     27     29     30     1  0.0000000
0.0000000  2
     28     27     29     30     1  180.0000771
0.3347200  3
     28     27     29     31     1  0.0000000
3.3472000  1
     28     27     29     31     1  0.0000000
0.0000000  2
     28     27     29     31     1  180.0000771
0.3347200  3
     30     29     32     33     1  0.0000000
0.6973333  3
     31     29     32     33     1  0.0000000
0.6973333  3

[ system ]
; Name
Generic title

[ molecules ]
; Compound       #mols
MOL                 1
```

```
;
;   File EEE.top  was generated
;   By user: james (1000)
;   On host: cmasc2
;   At date: Wed. October  3 18:40:53 2019
;
;   This is a standalone topology file
;
;   Created by:
;   ParmEd:       amber2gmx.py, VERSION 3.0.3
;   Executable:   amber2gmx.py
;   Library dir:  /usr/local/gromacs/share/gromacs/top
;   Command line:
;     amber2gmx.py
;

[ defaults ]
; nbfunc        comb-rule       gen-pairs       fudgeLJ
fudgeQQ
1               2               yes             0.5
0.83333333

[ atomtypes ]
; name    at.num    mass    charge ptype  sigma
epsilon
hc              1   1.008000  0.00000000  A
0.26495328      0.0656888
c3              6  12.010000  0.00000000  A
0.33996695      0.4577296
o               8  16.000000  0.00000000  A
0.29599219         0.87864
c               6  12.010000  0.00000000  A
0.33996695        0.359824
os              8  16.000000  0.00000000  A
0.30000123         0.71128
h1              1   1.008000  0.00000000  A
0.2471353       0.0656888


[ moleculetype ]
; Name            nrexcl
```

```
EEE          3

[ atoms ]
;   nr       type  resnr residue  atom   cgnr    charge
mass  typeB    chargeB      massB
; residue    1 MOL rtp MOL q 0.0
    1         hc      1    MOL     H1      1 0.15392200
1.008000   ; qtot 0.153922
    2         hc      1    MOL     H2      2 0.15392200
1.008000   ; qtot 0.307844
    3         hc      1    MOL     H3      3 0.15392200
1.008000   ; qtot 0.461766
    4         c3      1    MOL     C1      4
-0.56191600  12.010000   ; qtot -0.100150
    5          o      1    MOL     O1      5
-0.55649000  16.000000   ; qtot -0.656640
    6          c      1    MOL     C2      6 0.82336500
12.010000   ; qtot 0.166725
    7         os      1    MOL     O2      7
-0.46661400  16.000000   ; qtot -0.299889
    8         c3      1    MOL     C3      8 0.38941800
12.010000   ; qtot 0.089529
    9         h1      1    MOL     H4      9
-0.01524900   1.008000   ; qtot 0.074280
   10         h1      1    MOL     H5     10
-0.01524900   1.008000   ; qtot 0.059031
   11         hc      1    MOL     H6     11 0.09268200
1.008000   ; qtot 0.151713
   12         hc      1    MOL     H7     12 0.09268200
1.008000   ; qtot 0.244395
   13         c3      1    MOL     C4     13
-0.33707700  12.010000   ; qtot -0.092682
   14         hc      1    MOL     H8     14 0.09268200
1.008000   ; qtot 0.000000

[ bonds ]
;    ai     aj funct         c0         c1         c2
c3
      4      6     1   0.15241 261918.400000
      5      6     1   0.12183 533627.360000
      6      7     1   0.13584 327021.440000
```

```
      7      8     1   0.14316 258236.480000
      8     13     1   0.15375 251793.120000
      1      4     1   0.10969 276646.080000
      2      4     1   0.10969 276646.080000
      3      4     1   0.10969 276646.080000
      8      9     1   0.10969 276646.080000
      8     10     1   0.10969 276646.080000
     11     13     1   0.10969 276646.080000
     12     13     1   0.10969 276646.080000
     13     14     1   0.10969 276646.080000

[ pairs ]
;    ai     aj funct         c0         c1         c2
c3
      4      8     1
      5      8     1
      6     13     1
      1      5     1
      1      7     1
      2      5     1
      2      7     1
      3      5     1
      3      7     1
      6      9     1
      6     10     1
      7     11     1
      7     12     1
      7     14     1
      9     11     1
      9     12     1
      9     14     1
     10     11     1
     10     12     1
     10     14     1

[ angles ]
;    ai     aj     ak funct         c0         c1
c2         c3
      4      6      5     1   123.2000528 564.003200
      4      6      7     1   110.7200477 576.471520
      5      6      7     1   123.2500525 630.277760
```

```
     6      7      8     1   115.9800495 529.527040
     7      8     13     1   107.9700462 569.024000
     1      4      2     1   107.5800459 329.699200
     1      4      3     1   107.5800459 329.699200
     1      4      6     1   108.7700466 392.710240
     2      4      3     1   107.5800459 329.699200
     2      4      6     1   108.7700466 392.710240
     3      4      6     1   108.7700466 392.710240
     7      8      9     1   109.7800468 425.094400
     7      8     10     1   109.7800468 425.094400
     8     13     11     1   109.8000471 387.773120
     8     13     12     1   109.8000471 387.773120
     8     13     14     1   109.8000471 387.773120
     9      8     10     1   108.4600466 328.360320
     9      8     13     1   109.5600471 388.191520
    10      8     13     1   109.5600471 388.191520
    11     13     12     1   107.5800459 329.699200
    11     13     14     1   107.5800459 329.699200
    12     13     14     1   107.5800459 329.699200

[ dihedrals ]
;    ai     aj     ak     al funct         c0
c1         c2         c3         c4         c5
     4      6      7      8     1  0.0000000
0.0000000  1
     4      6      7      8     1  180.0000771
11.2968000  2
     4      6      7      8     1  0.0000000
4.8116000  3
     5      6      7      8     1  180.0000771
5.8576000  1
     5      6      7      8     1  180.0000771
11.2968000  2
     6      7      8     13     1  180.0000771
3.3472000  1
     6      7      8     13     1  0.0000000
1.6024720  3
     4      5      6      7     4  180.0000771
43.9320000  2
     1      4      6      5     1  0.0000000
3.3472000  1
```

```
      1      4      6      5      1  0.0000000
0.0000000  2
      1      4      6      5      1  180.0000771
0.3347200  3
      1      4      6      7      1  180.0000771
0.0000000  2
      2      4      6      5      1  0.0000000
3.3472000  1
      2      4      6      5      1  0.0000000
0.0000000  2
      2      4      6      5      1  180.0000771
0.3347200  3
      2      4      6      7      1  180.0000771
0.0000000  2
      3      4      6      5      1  0.0000000
3.3472000  1
      3      4      6      5      1  0.0000000
0.0000000  2
      3      4      6      5      1  180.0000771
0.3347200  3
      3      4      6      7      1  180.0000771
0.0000000  2
      6      7      8      9      1  0.0000000
1.6038667  3
      6      7      8     10      1  0.0000000
1.6038667  3
      7      8     13     11      1  0.0000000
1.0460000  1
      7      8     13     11      1  0.0000000
0.0000000  3
      7      8     13     12      1  0.0000000
1.0460000  1
      7      8     13     12      1  0.0000000
0.0000000  3
      7      8     13     14      1  0.0000000
1.0460000  1
      7      8     13     14      1  0.0000000
0.0000000  3
      9      8     13     11      1  0.0000000
0.6508444  3
      9      8     13     12      1  0.0000000
```

```
0.6508444  3
      9      8     13     14     1  0.0000000
0.6508444  3
     10      8     13     11     1  0.0000000
0.6508444  3
     10      8     13     12     1  0.0000000
0.6508444  3
     10      8     13     14     1  0.0000000
0.6508444  3

[ system ]
; Name
Generic title

[ molecules ]
; Compound       #mols
EEE                 1
```