Supporting information: A coil-to-globule transition capable coarse-grained model for poly(N-isopropylacrylamide)

H. A. Pérez-Ramírez and G. Odriozola*
Área de Física de Procesos Irreversibles, División de Ciencias Básicas e Ingeniería,
Universidad Autónoma Metropolitana-Azcapotzalco,
Av. San Pablo 180, 02200 Ciudad de México, Mexico
(Dated: July 20, 2020)

This file contents the comparison of the radial distribution functions (RDFs) and probability density functions (PDFs) obtained from coarse-grained and atomistic simulations. Also, in the second section we are including the topology files needed to simulate a 35-mer with the Gromacs package. These files include definitions of the bonded and non-bonded parameters and must be linked to the corresponding *topology.top* file.

I. RADIAL DISTRIBUTION AND PROBABILITY DENSITY FUNCTIONS

Each figure compares the outcomes from the coarse-grained (dashed lines) and the atomistic (continuous lines) models. Blue lines correspond to T =288 K and red lines to T =328 K, each one being below and above T_c = (302.1 ± 1.6) K, respectively. The insets show in highlighted colors the reference bead types. For all cases, to make the RDFs and PDFs comparable, we are considering the center of mass of the AA groups in correspondence to the centers of the CG beads. All data from CG simulations are obtained through 10 μs trajectories and discarding the first 8 μs.

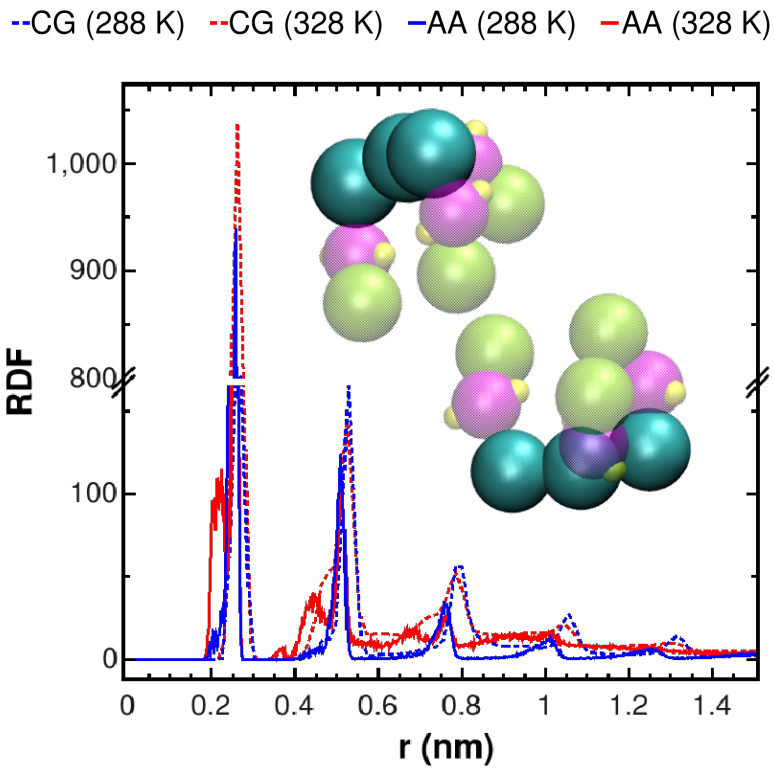

FIG. S1: Radial distribution function for the SC1-SC1 (backbone-backbone) pair.

* godriozo@azc.uam.mx

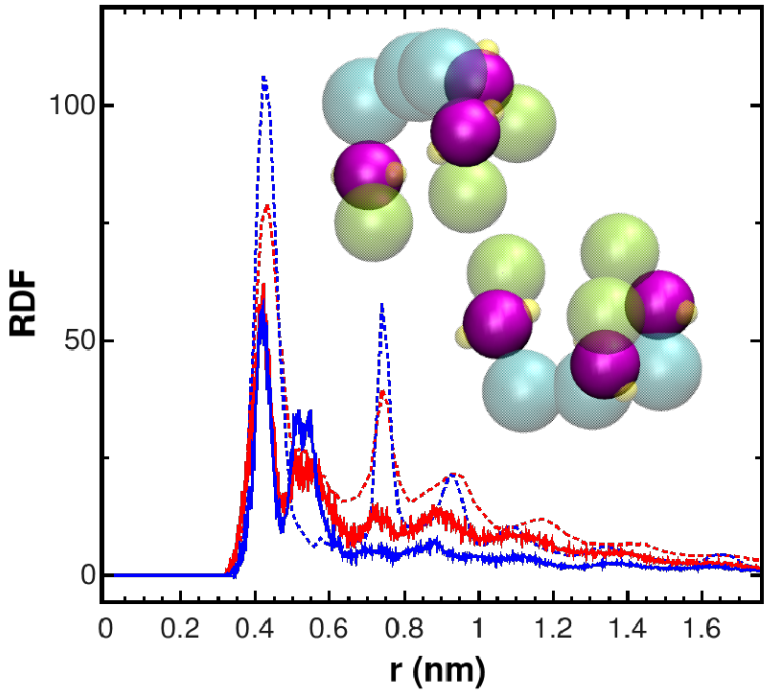

FIG. S2: Radial distribution function for the SNda-SNda (amide-amide) pair.

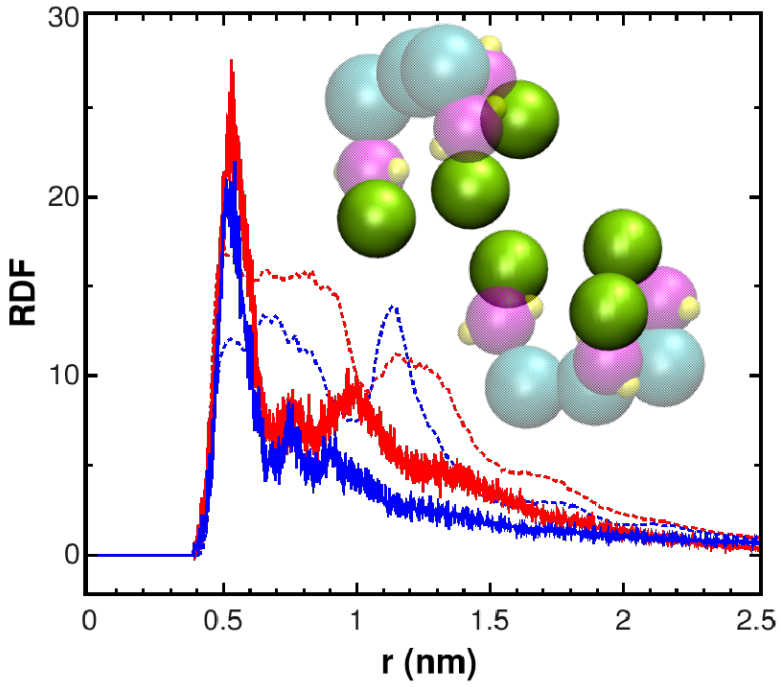

FIG. S3: Radial distribution function for the SC3-SC3 (isopropyl-isopropyl) pair.

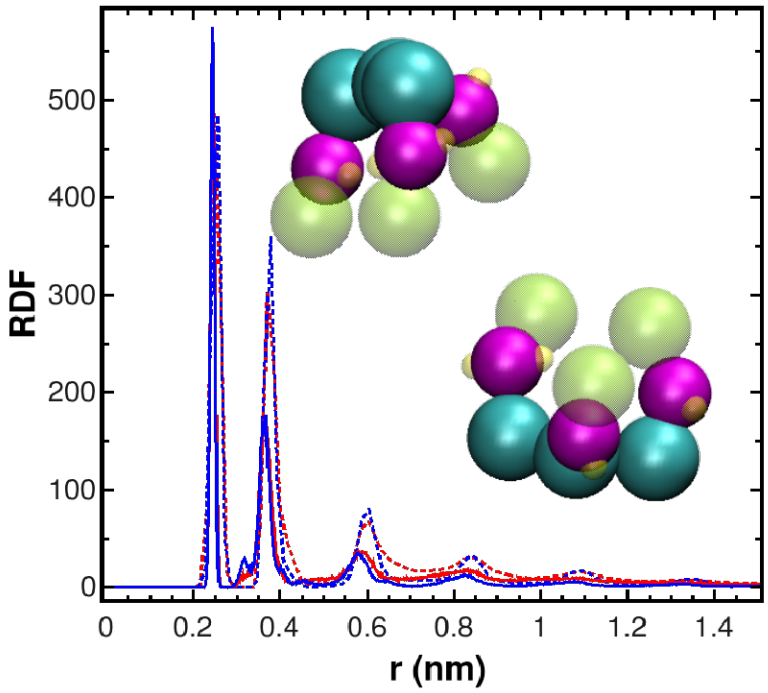

FIG. S4: Radial distribution function for the SC1-SNda (backbone-amide) pair.

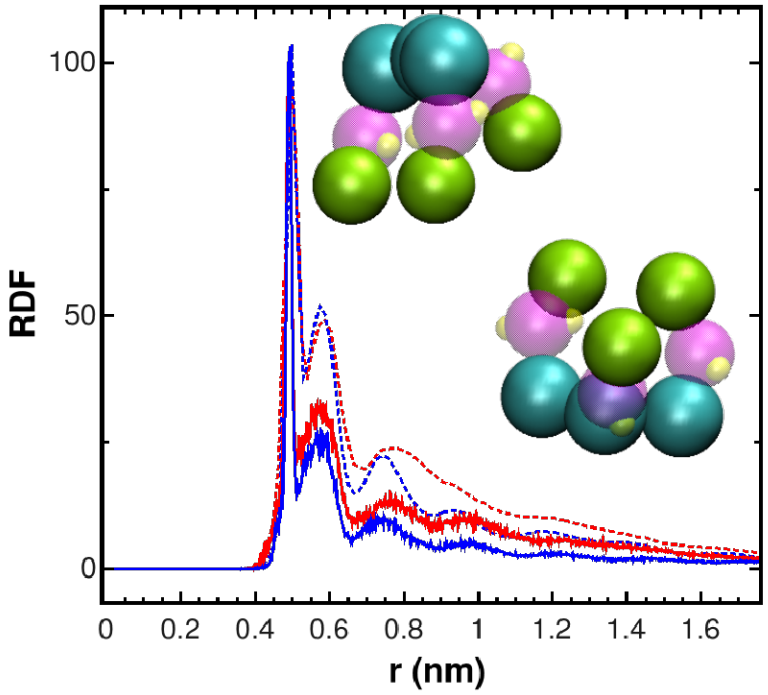

FIG. S5: Radial distribution function for the SC1-SC3 (backbone-isopropyl) pair.

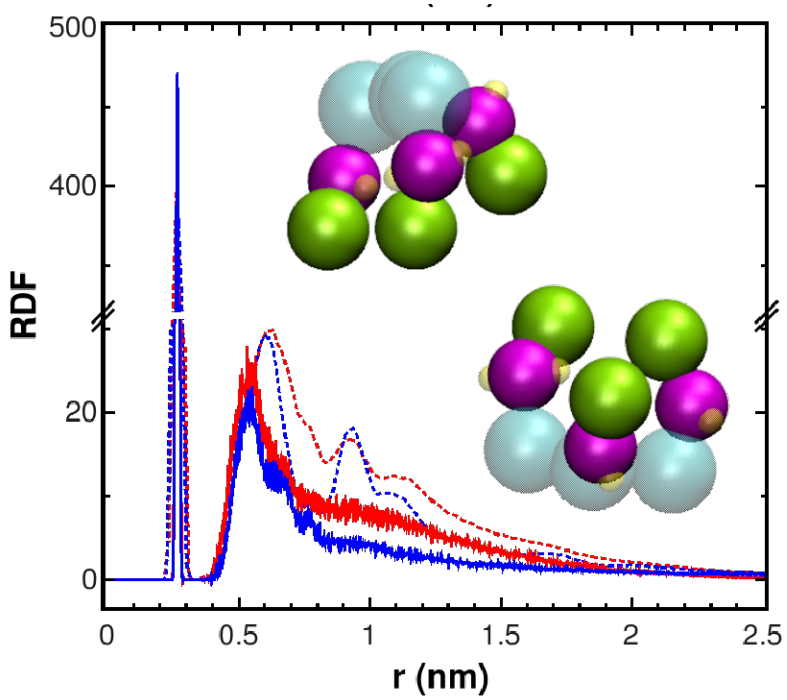

FIG. S6: Radial distribution function for the SNda-SC3 (amide-isopropyl) pair.

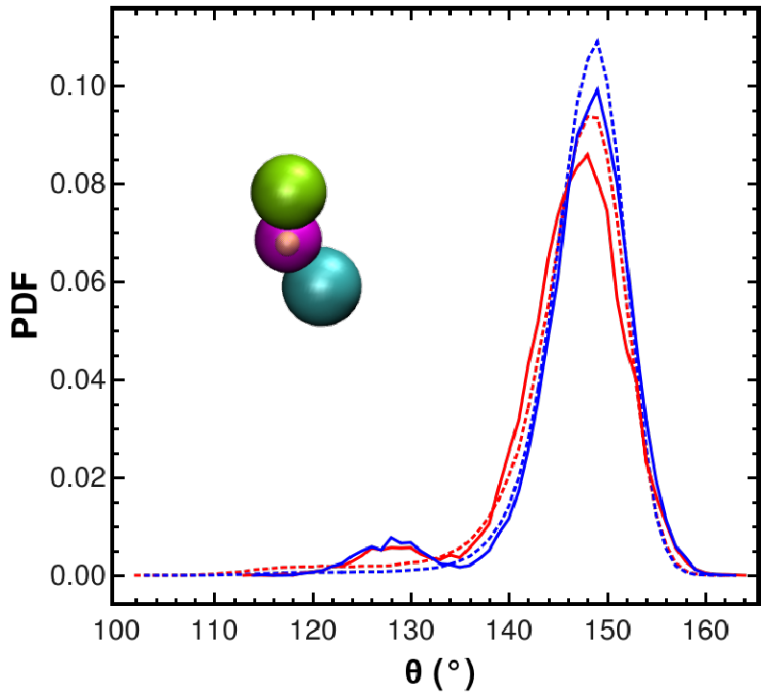

FIG. S7: Probability density function for the angle formed by the bonded particles SC3-SNda-SC1 (isopropyl-amide-backbone).

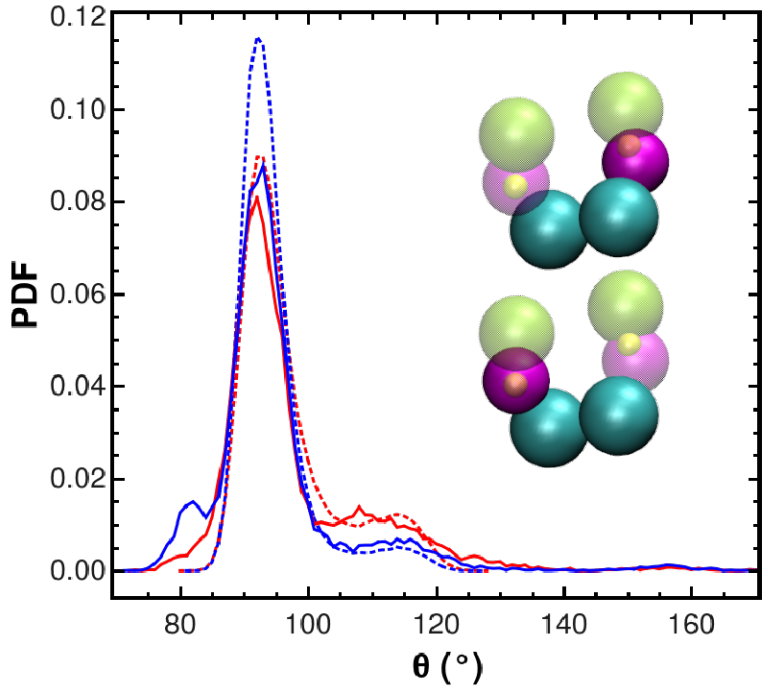

FIG. S8: Probability density function for the angle formed by the bonded particles SNda-SC1-SC1 (amide-backbone-backbone).

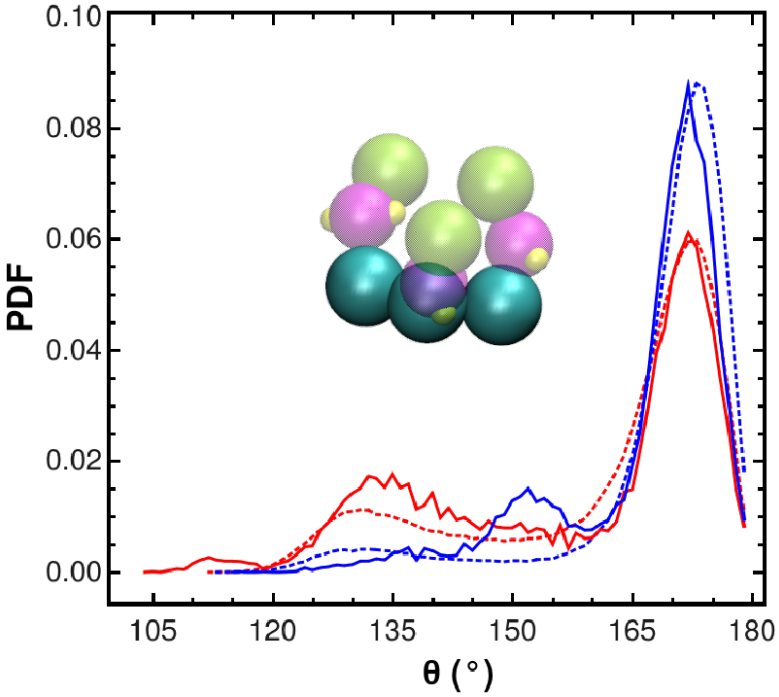

FIG. S9: Probability density function for the angle formed by the bonded particles SC1-SC1-SC1 (backbone-backbone-backbone).

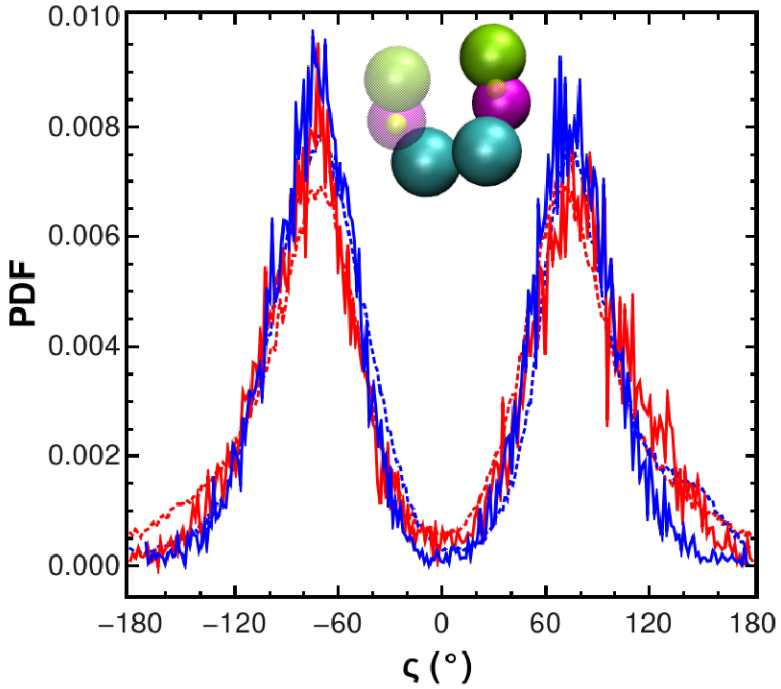

FIG. S10: Probability density function for the proper dihedral angle formed by the bonded particles SC3-SNda-SC1-SC1 (isopropyl-amide-backbone-backbone). It is important that this dihedral can jump from one configuration to the other. This allows the dipole moment of the SNda bead to align according to the local electrical field.

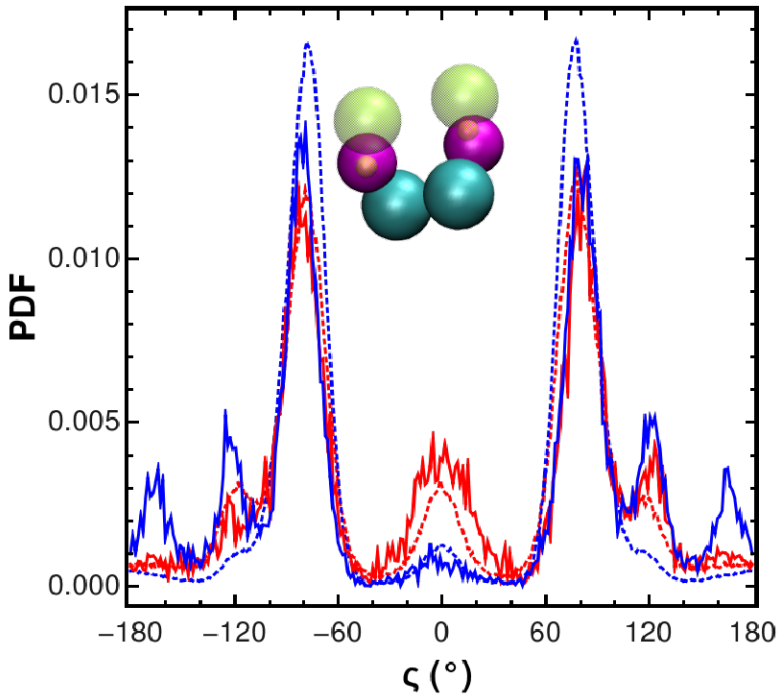

FIG. S11: Probability density function of the proper dihedral angle formed by the bonded particles SNda-SC1-SC1-SNda (amide-backbone-backbone-amide).

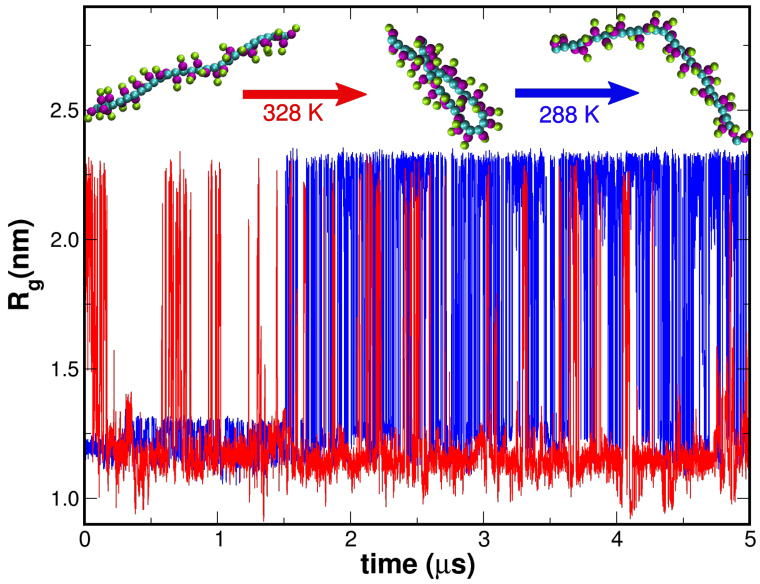

FIG. S12: Time evolution of the radius of gyration depicting the coil-to-globule reversibility. The red curve corresponds to 328 K when starting from a set of identical coil configurations. The blue curve corresponds to 288 K when starting from the final state of the red curve (a set of identical globule configurations). Both curves are obtained through REMD simulations.

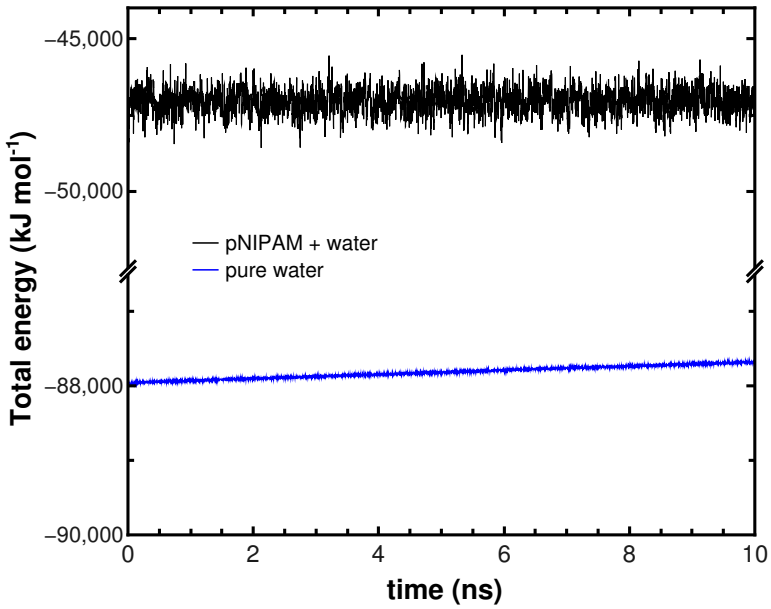

FIG. S13: Time evolution of the total energy at the microcanonical ensemble (298 K) for pure water (blue) and a single 30−mer in water (black). In both cases, the systems were firstly equilibrated employing the NPT ensemble.

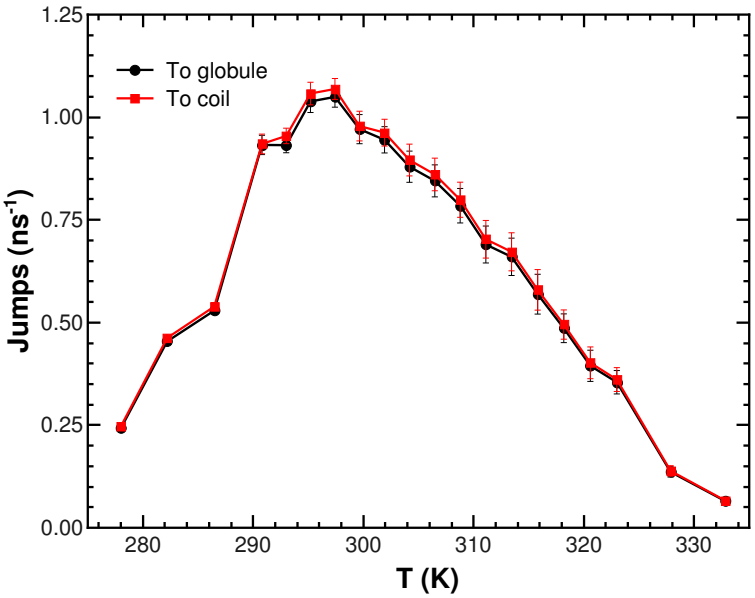

FIG. S14: Number of coil-to-globule (black) and globule-to-coil (red) jumps per ns detected along the REMD simulations as a function of temperature. Note that both curves are very similar at each temperature. Equilibrium of the whole set of replicas implyies that the overall number of coil-to-globule jumps must be equal to the overall number of globule-to-coil ones. However, we observe equilibrium at all temperatures. Note that the curve peaks relatively close to the transition temperature.

II. TOPOLOGY FILES

The following topology files can be used to simulate a 35-mer of a CG pNIPAM. This *pnipam.itp* file must be attached to the corresponding *topology.top* file.

pnipam.itp

```
[ moleculetype ]
; molname nrexcl
PNIPA 1

[ atoms ]
;id type resnr residu atom chgrp charge mass
1 SC3   1   PNIPA   SC3   1 0 43
2 SNda 1   PNIPA   SNda 2 0 0
3 D     1   PNIPA   D     3 0.48 21.5
4 D     1   PNIPA   D     4 -0.48 21.5
5 SC1   1   PNIPA   SC1   5 0 43
6 SC3   2   PNIPA   SC3   1 0 43
7 SNda 2   PNIPA   SNda 2 0 0
8 D     2   PNIPA   D     3 0.48 21.5
9 D     2   PNIPA   D     4 -0.48 21.5
10 SC1   2   PNIPA   SC1   5 0 43
11 SC3   3   PNIPA   SC3   1 0 43
12 SNda 3   PNIPA   SNda 2 0 0
13 D     3   PNIPA   D     3 0.48 21.5
14 D     3   PNIPA   D     4 -0.48 21.5
15 SC1   3   PNIPA   SC1   5 0 43
16 SC3   4   PNIPA   SC3   1 0 43
17 SNda 4   PNIPA   SNda 2 0 0
18 D     4   PNIPA   D     3 0.48 21.5
```

```
19 D      4    PNIPA   D      4 -0.48 21.5
20 SC1    4    PNIPA   SC1    5 0 43
21 SC3    5    PNIPA   SC3    1 0 43
22 SNda 5    PNIPA   SNda 2 0 0
23 D      5    PNIPA   D      3 0.48 21.5
24 D      5    PNIPA   D      4 -0.48 21.5
25 SC1    5    PNIPA   SC1    5 0 43
26 SC3    6    PNIPA   SC3    1 0 43
27 SNda 6    PNIPA   SNda 2 0 0
28 D      6    PNIPA   D      3 0.48 21.5
29 D      6    PNIPA   D      4 -0.48 21.5
30 SC1    6    PNIPA   SC1    5 0 43
31 SC3    7    PNIPA   SC3    1 0 43
32 SNda 7    PNIPA   SNda 2 0 0
33 D      7    PNIPA   D      3 0.48 21.5
34 D      7    PNIPA   D      4 -0.48 21.5
35 SC1    7    PNIPA   SC1    5 0 43
36 SC3    8    PNIPA   SC3    1 0 43
37 SNda 8    PNIPA   SNda 2 0 0
38 D      8    PNIPA   D      3 0.48 21.5
39 D      8    PNIPA   D      4 -0.48 21.5
40 SC1    8    PNIPA   SC1    5 0 43
41 SC3    9    PNIPA   SC3    1 0 43
42 SNda 9    PNIPA   SNda 2 0 0
43 D      9    PNIPA   D      3 0.48 21.5
44 D      9    PNIPA   D      4 -0.48 21.5
45 SC1    9    PNIPA   SC1    5 0 43
46 SC3    10   PNIPA   SC3    1 0 43
47 SNda 10   PNIPA   SNda 2 0 0
48 D      10   PNIPA   D      3 0.48 21.5
49 D      10   PNIPA   D      4 -0.48 21.5
50 SC1    10   PNIPA   SC1    5 0 43
51 SC3    11   PNIPA   SC3    1 0 43
52 SNda 11   PNIPA   SNda 2 0 0
53 D      11   PNIPA   D      3 0.48 21.5
54 D      11   PNIPA   D      4 -0.48 21.5
55 SC1    11   PNIPA   SC1    5 0 43
56 SC3    12   PNIPA   SC3    1 0 43
57 SNda 12   PNIPA   SNda 2 0 0
58 D      12   PNIPA   D      3 0.48 21.5
59 D      12   PNIPA   D      4 -0.48 21.5
60 SC1    12   PNIPA   SC1    5 0 43
61 SC3    13   PNIPA   SC3    1 0 43
62 SNda 13   PNIPA   SNda 2 0 0
63 D      13   PNIPA   D      3 0.48 21.5
64 D      13   PNIPA   D      4 -0.48 21.5
65 SC1    13   PNIPA   SC1    5 0 43
66 SC3    14   PNIPA   SC3    1 0 43
67 SNda 14   PNIPA   SNda 2 0 0
68 D      14   PNIPA   D      3 0.48 21.5
69 D      14   PNIPA   D      4 -0.48 21.5
70 SC1    14   PNIPA   SC1    5 0 43
71 SC3    15   PNIPA   SC3    1 0 43
72 SNda 15   PNIPA   SNda 2 0 0
73 D      15   PNIPA   D      3 0.48 21.5
74 D      15   PNIPA   D      4 -0.48 21.5
75 SC1    15   PNIPA   SC1    5 0 43
```

```
76 SC3   16   PNIPA   SC3   1 0 43
77 SNda 16   PNIPA   SNda 2 0 0
78 D      16   PNIPA   D      3 0.48 21.5
79 D      16   PNIPA   D      4 -0.48 21.5
80 SC1   16   PNIPA   SC1   5 0 43
81 SC3   17   PNIPA   SC3   1 0 43
82 SNda 17   PNIPA   SNda 2 0 0
83 D      17   PNIPA   D      3 0.48 21.5
84 D      17   PNIPA   D      4 -0.48 21.5
85 SC1   17   PNIPA   SC1   5 0 43
86 SC3   18   PNIPA   SC3   1 0 43
87 SNda 18   PNIPA   SNda 2 0 0
88 D      18   PNIPA   D      3 0.48 21.5
89 D      18   PNIPA   D      4 -0.48 21.5
90 SC1   18   PNIPA   SC1   5 0 43
91 SC3   19   PNIPA   SC3   1 0 43
92 SNda 19   PNIPA   SNda 2 0 0
93 D      19   PNIPA   D      3 0.48 21.5
94 D      19   PNIPA   D      4 -0.48 21.5
95 SC1   19   PNIPA   SC1   5 0 43
96 SC3   20   PNIPA   SC3   1 0 43
97 SNda 20   PNIPA   SNda 2 0 0
98 D      20   PNIPA   D      3 0.48 21.5
99 D      20   PNIPA   D      4 -0.48 21.5
100 SC1   20   PNIPA   SC1   5 0 43
101 SC3   21   PNIPA   SC3   1 0 43
102 SNda 21   PNIPA   SNda 2 0 0
103 D      21   PNIPA   D      3 0.48 21.5
104 D      21   PNIPA   D      4 -0.48 21.5
105 SC1   21   PNIPA   SC1   5 0 43
106 SC3   22   PNIPA   SC3   1 0 43
107 SNda 22   PNIPA   SNda 2 0 0
108 D      22   PNIPA   D      3 0.48 21.5
109 D      22   PNIPA   D      4 -0.48 21.5
110 SC1   22   PNIPA   SC1   5 0 43
111 SC3   23   PNIPA   SC3   1 0 43
112 SNda 23   PNIPA   SNda 2 0 0
113 D      23   PNIPA   D      3 0.48 21.5
114 D      23   PNIPA   D      4 -0.48 21.5
115 SC1   23   PNIPA   SC1   5 0 43
116 SC3   24   PNIPA   SC3   1 0 43
117 SNda 24   PNIPA   SNda 2 0 0
118 D      24   PNIPA   D      3 0.48 21.5
119 D      24   PNIPA   D      4 -0.48 21.5
120 SC1   24   PNIPA   SC1   5 0 43
121 SC3   25   PNIPA   SC3   1 0 43
122 SNda 25   PNIPA   SNda 2 0 0
123 D      25   PNIPA   D      3 0.48 21.5
124 D      25   PNIPA   D      4 -0.48 21.5
125 SC1   25   PNIPA   SC1   5 0 43
126 SC3   26   PNIPA   SC3   1 0 43
127 SNda 26   PNIPA   SNda 2 0 0
128 D      26   PNIPA   D      3 0.48 21.5
129 D      26   PNIPA   D      4 -0.48 21.5
130 SC1   26   PNIPA   SC1   5 0 43
131 SC3   27   PNIPA   SC3   1 0 43
132 SNda 27   PNIPA   SNda 2 0 0
```

```
133 D      27    PNIPA   D      3 0.48 21.5
134 D      27    PNIPA   D      4 -0.48 21.5
135 SC1    27    PNIPA   SC1    5 0 43
136 SC3    28    PNIPA   SC3    1 0 43
137 SNda 28    PNIPA   SNda 2 0 0
138 D      28    PNIPA   D      3 0.48 21.5
139 D      28    PNIPA   D      4 -0.48 21.5
140 SC1    28    PNIPA   SC1    5 0 43
141 SC3    29    PNIPA   SC3    1 0 43
142 SNda 29    PNIPA   SNda 2 0 0
143 D      29    PNIPA   D      3 0.48 21.5
144 D      29    PNIPA   D      4 -0.48 21.5
145 SC1    29    PNIPA   SC1    5 0 43
146 SC3    30    PNIPA   SC3    1 0 43
147 SNda 30    PNIPA   SNda 2 0 0
148 D      30    PNIPA   D      3 0.48 21.5
149 D      30    PNIPA   D      4 -0.48 21.5
150 SC1    30    PNIPA   SC1    5 0 43
151 SC3    31    PNIPA   SC3    1 0 43
152 SNda 31    PNIPA   SNda 2 0 0
153 D      31    PNIPA   D      3 0.48 21.5
154 D      31    PNIPA   D      4 -0.48 21.5
155 SC1    31    PNIPA   SC1    5 0 43
156 SC3    32    PNIPA   SC3    1 0 43
157 SNda 32    PNIPA   SNda 2 0 0
158 D      32    PNIPA   D      3 0.48 21.5
159 D      32    PNIPA   D      4 -0.48 21.5
160 SC1    32    PNIPA   SC1    5 0 43
161 SC3    33    PNIPA   SC3    1 0 43
162 SNda 33    PNIPA   SNda 2 0 0
163 D      33    PNIPA   D      3 0.48 21.5
164 D      33    PNIPA   D      4 -0.48 21.5
165 SC1    33    PNIPA   SC1    5 0 43
166 SC3    34    PNIPA   SC3    1 0 43
167 SNda 34    PNIPA   SNda 2 0 0
168 D      34    PNIPA   D      3 0.48 21.5
169 D      34    PNIPA   D      4 -0.48 21.5
170 SC1    34    PNIPA   SC1    5 0 43
171 SC3    35    PNIPA   SC3    1 0 43
172 SNda 35    PNIPA   SNda 2 0 0
173 D      35    PNIPA   D      3 0.48 21.5
174 D      35    PNIPA   D      4 -0.48 21.5
175 SC1    35    PNIPA   SC1    5 0 43

[ virtual_sites2 ]
;Site from funct a
2   3   4 1 0.5
7   8   9 1 0.5
12 13 14 1 0.5
17 18 19 1 0.5
22 23 24 1 0.5
27 28 29 1 0.5
32 33 34 1 0.5
37 38 39 1 0.5
42 43 44 1 0.5
47 48 49 1 0.5
52 53 54 1 0.5
```

```
57 58 59 1 0.5
62 63 64 1 0.5
67 68 69 1 0.5
72 73 74 1 0.5
77 78 79 1 0.5
82 83 84 1 0.5
87 88 89 1 0.5
92 93 94 1 0.5
97 98 99 1 0.5
102 103 104 1 0.5
107 108 109 1 0.5
112 113 114 1 0.5
117 118 119 1 0.5
122 123 124 1 0.5
127 128 129 1 0.5
132 133 134 1 0.5
137 138 139 1 0.5
142 143 144 1 0.5
147 148 149 1 0.5
152 153 154 1 0.5
157 158 159 1 0.5
162 163 164 1 0.5
167 168 169 1 0.5
172 173 174 1 0.5

[ bonds ]
; i j funct length force
1 2 1 0.268 20500
2 5 1 0.242 25000
5 10 1 0.254 20000
6 7 1 0.268 20500
7 10 1 0.242 25000
10 15 1 0.254 20000
11 12 1 0.268 20500
12 15 1 0.242 25000
15 20 1 0.254 20000
16 17 1 0.268 20500
17 20 1 0.242 25000
20 25 1 0.254 20000
21 22 1 0.268 20500
22 25 1 0.242 25000
25 30 1 0.254 20000
26 27 1 0.268 20500
27 30 1 0.242 25000
30 35 1 0.254 20000
31 32 1 0.268 20500
32 35 1 0.242 25000
35 40 1 0.254 20000
36 37 1 0.268 20500
37 40 1 0.242 25000
40 45 1 0.254 20000
41 42 1 0.268 20500
42 45 1 0.242 25000
45 50 1 0.254 20000
46 47 1 0.268 20500
47 50 1 0.242 25000
50 55 1 0.254 20000
```

```
51 52 1 0.268 20500
52 55 1 0.242 25000
55 60 1 0.254 20000
56 57 1 0.268 20500
57 60 1 0.242 25000
60 65 1 0.254 20000
61 62 1 0.268 20500
62 65 1 0.242 25000
65 70 1 0.254 20000
66 67 1 0.268 20500
67 70 1 0.242 25000
70 75 1 0.254 20000
71 72 1 0.268 20500
72 75 1 0.242 25000
75 80 1 0.254 20000
76 77 1 0.268 20500
77 80 1 0.242 25000
80 85 1 0.254 20000
81 82 1 0.268 20500
82 85 1 0.242 25000
85 90 1 0.254 20000
86 87 1 0.268 20500
87 90 1 0.242 25000
90 95 1 0.254 20000
91 92 1 0.268 20500
92 95 1 0.242 25000
95 100 1 0.254 20000
96 97 1 0.268 20500
97 100 1 0.242 25000
100 105 1 0.254 20000
101 102 1 0.268 20500
102 105 1 0.242 25000
105 110 1 0.254 20000
106 107 1 0.268 20500
107 110 1 0.242 25000
110 115 1 0.254 20000
111 112 1 0.268 20500
112 115 1 0.242 25000
115 120 1 0.254 20000
116 117 1 0.268 20500
117 120 1 0.242 25000
120 125 1 0.254 20000
121 122 1 0.268 20500
122 125 1 0.242 25000
125 130 1 0.254 20000
126 127 1 0.268 20500
127 130 1 0.242 25000
130 135 1 0.254 20000
131 132 1 0.268 20500
132 135 1 0.242 25000
135 140 1 0.254 20000
136 137 1 0.268 20500
137 140 1 0.242 25000
140 145 1 0.254 20000
141 142 1 0.268 20500
142 145 1 0.242 25000
145 150 1 0.254 20000
```

```
146 147 1 0.268 20500
147 150 1 0.242 25000
150 155 1 0.254 20000
151 152 1 0.268 20500
152 155 1 0.242 25000
155 160 1 0.254 20000
156 157 1 0.268 20500
157 160 1 0.242 25000
160 165 1 0.254 20000
161 162 1 0.268 20500
162 165 1 0.242 25000
165 170 1 0.254 20000
166 167 1 0.268 20500
167 170 1 0.242 25000
170 175 1 0.254 20000
171 172 1 0.268 20500
172 175 1 0.242 25000

[ angles ]
; ai aj ak funct angle fc
1 2 5 6 138.52 3.63 -29.06 -32.86 350.6 650.93
1 2 3 2 61.00 200.00
1 2 4 2 119.00 150.00
3 2 4 2 161.00 150.00
3 2 5 2 90.00 150.00
4 2 5 2 90.00 150.00
2 5 10 6 98.09 3.95 37.9 -38.2 -575.7 1400.7
5 10 7 6 98.09 3.95 37.9 -38.2 -575.7 1400.7
5 10 15 6 166.158 6.718 -40.527 -1 176.41 179.444
6 7 10 6 138.52 3.63 -29.06 -32.86 350.6 650.93
6 7 8 2 61.00 200.00
6 7 9 2 119.00 150.00
8 7 9 2 161.00 150.00
8 7 10 2 90.00 150.00
9 7 10 2 90.00 150.00
7 10 15 6 98.09 3.95 37.9 -38.2 -575.7 1400.7
10 15 12 6 98.09 3.95 37.9 -38.2 -575.7 1400.7
10 15 20 6 166.158 6.718 -40.527 -1 176.41 179.444
11 12 15 6 138.52 3.63 -29.06 -32.86 350.6 650.93
11 12 13 2 61.00 200.00
11 12 14 2 119.00 150.00
13 12 14 2 161.00 150.00
13 12 15 2 90.00 150.00
14 12 15 2 90.00 150.00
12 15 20 6 98.09 3.95 37.9 -38.2 -575.7 1400.7
15 20 17 6 98.09 3.95 37.9 -38.2 -575.7 1400.7
15 20 25 6 166.158 6.718 -40.527 -1 176.41 179.444
16 17 20 6 138.52 3.63 -29.06 -32.86 350.6 650.93
16 17 18 2 61.00 200.00
16 17 19 2 119.00 150.00
18 17 19 2 161.00 150.00
18 17 20 2 90.00 150.00
19 17 20 2 90.00 150.00
17 20 25 6 98.09 3.95 37.9 -38.2 -575.7 1400.7
20 25 22 6 98.09 3.95 37.9 -38.2 -575.7 1400.7
20 25 30 6 166.158 6.718 -40.527 -1 176.41 179.444
21 22 25 6 138.52 3.63 -29.06 -32.86 350.6 650.93
```

```
21 22 23 2 61.00 200.00
21 22 24 2 119.00 150.00
23 22 24 2 161.00 150.00
23 22 25 2 90.00 150.00
24 22 25 2 90.00 150.00
22 25 30 6 98.09 3.95 37.9 -38.2 -575.7 1400.7
25 30 27 6 98.09 3.95 37.9 -38.2 -575.7 1400.7
25 30 35 6 166.158 6.718 -40.527 -1 176.41 179.444
26 27 30 6 138.52 3.63 -29.06 -32.86 350.6 650.93
26 27 28 2 61.00 200.00
26 27 29 2 119.00 150.00
28 27 29 2 161.00 150.00
28 27 30 2 90.00 150.00
29 27 30 2 90.00 150.00
27 30 35 6 98.09 3.95 37.9 -38.2 -575.7 1400.7
30 35 32 6 98.09 3.95 37.9 -38.2 -575.7 1400.7
30 35 40 6 166.158 6.718 -40.527 -1 176.41 179.444
31 32 35 6 138.52 3.63 -29.06 -32.86 350.6 650.93
31 32 33 2 61.00 200.00
31 32 34 2 119.00 150.00
33 32 34 2 161.00 150.00
33 32 35 2 90.00 150.00
34 32 35 2 90.00 150.00
32 35 40 6 98.09 3.95 37.9 -38.2 -575.7 1400.7
35 40 37 6 98.09 3.95 37.9 -38.2 -575.7 1400.7
35 40 45 6 166.158 6.718 -40.527 -1 176.41 179.444
36 37 40 6 138.52 3.63 -29.06 -32.86 350.6 650.93
36 37 38 2 61.00 200.00
36 37 39 2 119.00 150.00
38 37 39 2 161.00 150.00
38 37 40 2 90.00 150.00
39 37 40 2 90.00 150.00
37 40 45 6 98.09 3.95 37.9 -38.2 -575.7 1400.7
40 45 42 6 98.09 3.95 37.9 -38.2 -575.7 1400.7
40 45 50 6 166.158 6.718 -40.527 -1 176.41 179.444
41 42 45 6 138.52 3.63 -29.06 -32.86 350.6 650.93
41 42 43 2 61.00 200.00
41 42 44 2 119.00 150.00
43 42 44 2 161.00 150.00
43 42 45 2 90.00 150.00
44 42 45 2 90.00 150.00
42 45 50 6 98.09 3.95 37.9 -38.2 -575.7 1400.7
45 50 47 6 98.09 3.95 37.9 -38.2 -575.7 1400.7
45 50 55 6 166.158 6.718 -40.527 -1 176.41 179.444
46 47 50 6 138.52 3.63 -29.06 -32.86 350.6 650.93
46 47 48 2 61.00 200.00
46 47 49 2 119.00 150.00
48 47 49 2 161.00 150.00
48 47 50 2 90.00 150.00
49 47 50 2 90.00 150.00
47 50 55 6 98.09 3.95 37.9 -38.2 -575.7 1400.7
50 55 52 6 98.09 3.95 37.9 -38.2 -575.7 1400.7
50 55 60 6 166.158 6.718 -40.527 -1 176.41 179.444
51 52 55 6 138.52 3.63 -29.06 -32.86 350.6 650.93
51 52 53 2 61.00 200.00
51 52 54 2 119.00 150.00
53 52 54 2 161.00 150.00
```

```
53 52 55 2 90.00 150.00
54 52 55 2 90.00 150.00
52 55 60 6 98.09 3.95 37.9 -38.2 -575.7 1400.7
55 60 57 6 98.09 3.95 37.9 -38.2 -575.7 1400.7
55 60 65 6 166.158 6.718 -40.527 -1 176.41 179.444
56 57 60 6 138.52 3.63 -29.06 -32.86 350.6 650.93
56 57 58 2 61.00 200.00
56 57 59 2 119.00 150.00
58 57 59 2 161.00 150.00
58 57 60 2 90.00 150.00
59 57 60 2 90.00 150.00
57 60 65 6 98.09 3.95 37.9 -38.2 -575.7 1400.7
60 65 62 6 98.09 3.95 37.9 -38.2 -575.7 1400.7
60 65 70 6 166.158 6.718 -40.527 -1 176.41 179.444
61 62 65 6 138.52 3.63 -29.06 -32.86 350.6 650.93
61 62 63 2 61.00 200.00
61 62 64 2 119.00 150.00
63 62 64 2 161.00 150.00
63 62 65 2 90.00 150.00
64 62 65 2 90.00 150.00
62 65 70 6 98.09 3.95 37.9 -38.2 -575.7 1400.7
65 70 67 6 98.09 3.95 37.9 -38.2 -575.7 1400.7
65 70 75 6 166.158 6.718 -40.527 -1 176.41 179.444
66 67 70 6 138.52 3.63 -29.06 -32.86 350.6 650.93
66 67 68 2 61.00 200.00
66 67 69 2 119.00 150.00
68 67 69 2 161.00 150.00
68 67 70 2 90.00 150.00
69 67 70 2 90.00 150.00
67 70 75 6 98.09 3.95 37.9 -38.2 -575.7 1400.7
70 75 72 6 98.09 3.95 37.9 -38.2 -575.7 1400.7
70 75 80 6 166.158 6.718 -40.527 -1 176.41 179.444
71 72 75 6 138.52 3.63 -29.06 -32.86 350.6 650.93
71 72 73 2 61.00 200.00
71 72 74 2 119.00 150.00
73 72 74 2 161.00 150.00
73 72 75 2 90.00 150.00
74 72 75 2 90.00 150.00
72 75 80 6 98.09 3.95 37.9 -38.2 -575.7 1400.7
75 80 77 6 98.09 3.95 37.9 -38.2 -575.7 1400.7
75 80 85 6 166.158 6.718 -40.527 -1 176.41 179.444
76 77 80 6 138.52 3.63 -29.06 -32.86 350.6 650.93
76 77 78 2 61.00 200.00
76 77 79 2 119.00 150.00
78 77 79 2 161.00 150.00
78 77 80 2 90.00 150.00
79 77 80 2 90.00 150.00
77 80 85 6 98.09 3.95 37.9 -38.2 -575.7 1400.7
80 85 82 6 98.09 3.95 37.9 -38.2 -575.7 1400.7
80 85 90 6 166.158 6.718 -40.527 -1 176.41 179.444
81 82 85 6 138.52 3.63 -29.06 -32.86 350.6 650.93
81 82 83 2 61.00 200.00
81 82 84 2 119.00 150.00
83 82 84 2 161.00 150.00
83 82 85 2 90.00 150.00
84 82 85 2 90.00 150.00
82 85 90 6 98.09 3.95 37.9 -38.2 -575.7 1400.7
```

```
85 90 87 6 98.09 3.95 37.9 -38.2 -575.7 1400.7
85 90 95 6 166.158 6.718 -40.527 -1 176.41 179.444
86 87 90 6 138.52 3.63 -29.06 -32.86 350.6 650.93
86 87 88 2 61.00 200.00
86 87 89 2 119.00 150.00
88 87 89 2 161.00 150.00
88 87 90 2 90.00 150.00
89 87 90 2 90.00 150.00
87 90 95 6 98.09 3.95 37.9 -38.2 -575.7 1400.7
90 95 92 6 98.09 3.95 37.9 -38.2 -575.7 1400.7
90 95 100 6 166.158 6.718 -40.527 -1 176.41 179.444
91 92 95 6 138.52 3.63 -29.06 -32.86 350.6 650.93
91 92 93 2 61.00 200.00
91 92 94 2 119.00 150.00
93 92 94 2 161.00 150.00
93 92 95 2 90.00 150.00
94 92 95 2 90.00 150.00
92 95 100 6 98.09 3.95 37.9 -38.2 -575.7 1400.7
95 100 97 6 98.09 3.95 37.9 -38.2 -575.7 1400.7
95 100 105 6 166.158 6.718 -40.527 -1 176.41 179.444
96 97 100 6 138.52 3.63 -29.06 -32.86 350.6 650.93
96 97 98 2 61.00 200.00
96 97 99 2 119.00 150.00
98 97 99 2 161.00 150.00
98 97 100 2 90.00 150.00
99 97 100 2 90.00 150.00
97 100 105 6 98.09 3.95 37.9 -38.2 -575.7 1400.7
100 105 102 6 98.09 3.95 37.9 -38.2 -575.7 1400.7
100 105 110 6 166.158 6.718 -40.527 -1 176.41 179.444
101 102 105 6 138.52 3.63 -29.06 -32.86 350.6 650.93
101 102 103 2 61.00 200.00
101 102 104 2 119.00 150.00
103 102 104 2 161.00 150.00
103 102 105 2 90.00 150.00
104 102 105 2 90.00 150.00
102 105 110 6 98.09 3.95 37.9 -38.2 -575.7 1400.7
105 110 107 6 98.09 3.95 37.9 -38.2 -575.7 1400.7
105 110 115 6 166.158 6.718 -40.527 -1 176.41 179.444
106 107 110 6 138.52 3.63 -29.06 -32.86 350.6 650.93
106 107 108 2 61.00 200.00
106 107 109 2 119.00 150.00
108 107 109 2 161.00 150.00
108 107 110 2 90.00 150.00
109 107 110 2 90.00 150.00
107 110 115 6 98.09 3.95 37.9 -38.2 -575.7 1400.7
110 115 112 6 98.09 3.95 37.9 -38.2 -575.7 1400.7
110 115 120 6 166.158 6.718 -40.527 -1 176.41 179.444
111 112 115 6 138.52 3.63 -29.06 -32.86 350.6 650.93
111 112 113 2 61.00 200.00
111 112 114 2 119.00 150.00
113 112 114 2 161.00 150.00
113 112 115 2 90.00 150.00
114 112 115 2 90.00 150.00
112 115 120 6 98.09 3.95 37.9 -38.2 -575.7 1400.7
115 120 117 6 98.09 3.95 37.9 -38.2 -575.7 1400.7
115 120 125 6 166.158 6.718 -40.527 -1 176.41 179.444
116 117 120 6 138.52 3.63 -29.06 -32.86 350.6 650.93
```

```
116 117 118 2 61.00 200.00
116 117 119 2 119.00 150.00
118 117 119 2 161.00 150.00
118 117 120 2 90.00 150.00
119 117 120 2 90.00 150.00
117 120 125 6 98.09 3.95 37.9 -38.2 -575.7 1400.7
120 125 122 6 98.09 3.95 37.9 -38.2 -575.7 1400.7
120 125 130 6 166.158 6.718 -40.527 -1 176.41 179.444
121 122 125 6 138.52 3.63 -29.06 -32.86 350.6 650.93
121 122 123 2 61.00 200.00
121 122 124 2 119.00 150.00
123 122 124 2 161.00 150.00
123 122 125 2 90.00 150.00
124 122 125 2 90.00 150.00
122 125 130 6 98.09 3.95 37.9 -38.2 -575.7 1400.7
125 130 127 6 98.09 3.95 37.9 -38.2 -575.7 1400.7
125 130 135 6 166.158 6.718 -40.527 -1 176.41 179.444
126 127 130 6 138.52 3.63 -29.06 -32.86 350.6 650.93
126 127 128 2 61.00 200.00
126 127 129 2 119.00 150.00
128 127 129 2 161.00 150.00
128 127 130 2 90.00 150.00
129 127 130 2 90.00 150.00
127 130 135 6 98.09 3.95 37.9 -38.2 -575.7 1400.7
130 135 132 6 98.09 3.95 37.9 -38.2 -575.7 1400.7
130 135 140 6 166.158 6.718 -40.527 -1 176.41 179.444
131 132 135 6 138.52 3.63 -29.06 -32.86 350.6 650.93
131 132 133 2 61.00 200.00
131 132 134 2 119.00 150.00
133 132 134 2 161.00 150.00
133 132 135 2 90.00 150.00
134 132 135 2 90.00 150.00
132 135 140 6 98.09 3.95 37.9 -38.2 -575.7 1400.7
135 140 137 6 98.09 3.95 37.9 -38.2 -575.7 1400.7
135 140 145 6 166.158 6.718 -40.527 -1 176.41 179.444
136 137 140 6 138.52 3.63 -29.06 -32.86 350.6 650.93
136 137 138 2 61.00 200.00
136 137 139 2 119.00 150.00
138 137 139 2 161.00 150.00
138 137 140 2 90.00 150.00
139 137 140 2 90.00 150.00
137 140 145 6 98.09 3.95 37.9 -38.2 -575.7 1400.7
140 145 142 6 98.09 3.95 37.9 -38.2 -575.7 1400.7
140 145 150 6 166.158 6.718 -40.527 -1 176.41 179.444
141 142 145 6 138.52 3.63 -29.06 -32.86 350.6 650.93
141 142 143 2 61.00 200.00
141 142 144 2 119.00 150.00
143 142 144 2 161.00 150.00
143 142 145 2 90.00 150.00
144 142 145 2 90.00 150.00
142 145 150 6 98.09 3.95 37.9 -38.2 -575.7 1400.7
145 150 147 6 98.09 3.95 37.9 -38.2 -575.7 1400.7
145 150 155 6 166.158 6.718 -40.527 -1 176.41 179.444
146 147 150 6 138.52 3.63 -29.06 -32.86 350.6 650.93
146 147 148 2 61.00 200.00
146 147 149 2 119.00 150.00
148 147 149 2 161.00 150.00
```

```
148 147 150 2 90.00 150.00
149 147 150 2 90.00 150.00
147 150 155 6 98.09 3.95 37.9 -38.2 -575.7 1400.7
150 155 152 6 98.09 3.95 37.9 -38.2 -575.7 1400.7
150 155 160 6 166.158 6.718 -40.527 -1 176.41 179.444
151 152 155 6 138.52 3.63 -29.06 -32.86 350.6 650.93
151 152 153 2 61.00 200.00
151 152 154 2 119.00 150.00
153 152 154 2 161.00 150.00
153 152 155 2 90.00 150.00
154 152 155 2 90.00 150.00
152 155 160 6 98.09 3.95 37.9 -38.2 -575.7 1400.7
155 160 157 6 98.09 3.95 37.9 -38.2 -575.7 1400.7
155 160 165 6 166.158 6.718 -40.527 -1 176.41 179.444
156 157 160 6 138.52 3.63 -29.06 -32.86 350.6 650.93
156 157 158 2 61.00 200.00
156 157 159 2 119.00 150.00
158 157 159 2 161.00 150.00
158 157 160 2 90.00 150.00
159 157 160 2 90.00 150.00
157 160 165 6 98.09 3.95 37.9 -38.2 -575.7 1400.7
160 165 162 6 98.09 3.95 37.9 -38.2 -575.7 1400.7
160 165 170 6 166.158 6.718 -40.527 -1 176.41 179.444
161 162 165 6 138.52 3.63 -29.06 -32.86 350.6 650.93
161 162 163 2 61.00 200.00
161 162 164 2 119.00 150.00
163 162 164 2 161.00 150.00
163 162 165 2 90.00 150.00
164 162 165 2 90.00 150.00
162 165 170 6 98.09 3.95 37.9 -38.2 -575.7 1400.7
165 170 167 6 98.09 3.95 37.9 -38.2 -575.7 1400.7
165 170 175 6 166.158 6.718 -40.527 -1 176.41 179.444
166 167 170 6 138.52 3.63 -29.06 -32.86 350.6 650.93
166 167 168 2 61.00 200.00
166 167 169 2 119.00 150.00
168 167 169 2 161.00 150.00
168 167 170 2 90.00 150.00
169 167 170 2 90.00 150.00
167 170 175 6 98.09 3.95 37.9 -38.2 -575.7 1400.7
170 175 172 6 98.09 3.95 37.9 -38.2 -575.7 1400.7
171 172 175 6 138.52 3.63 -29.06 -32.86 350.6 650.93
171 172 173 2 61.00 200.00
171 172 174 2 119.00 150.00
173 172 174 2 161.00 150.00
173 172 175 2 90.00 150.00
174 172 175 2 90.00 150.00

[ dihedrals ] ; ai aj ak funct C0 C1 C2 C3 C4 C5 1 2 5 10 3 1.35 4.30 1.3 -5.8 1.30 1.60
2 5 10 7 3 -1.20 8.5 17.7 -27.7 -17.1 25.5
6 7 10 15 3 1.35 4.30 1.3 -5.8 1.30 1.60
7 10 15 12 3 -1.20 8.5 17.7 -27.7 -17.1 25.5
11 12 15 20 3 1.35 4.30 1.3 -5.8 1.30 1.60
12 15 20 17 3 -1.20 8.5 17.7 -27.7 -17.1 25.5
16 17 20 25 3 1.35 4.30 1.3 -5.8 1.30 1.60
17 20 25 22 3 -1.20 8.5 17.7 -27.7 -17.1 25.5
21 22 25 30 3 1.35 4.30 1.3 -5.8 1.30 1.60
22 25 30 27 3 -1.20 8.5 17.7 -27.7 -17.1 25.5
```

```
26 27 30 35 3 1.35 4.30 1.3 -5.8 1.30 1.60
27 30 35 32 3 -1.20 8.5 17.7 -27.7 -17.1 25.5
31 32 35 40 3 1.35 4.30 1.3 -5.8 1.30 1.60
32 35 40 37 3 -1.20 8.5 17.7 -27.7 -17.1 25.5
36 37 40 45 3 1.35 4.30 1.3 -5.8 1.30 1.60
37 40 45 42 3 -1.20 8.5 17.7 -27.7 -17.1 25.5
41 42 45 50 3 1.35 4.30 1.3 -5.8 1.30 1.60
42 45 50 47 3 -1.20 8.5 17.7 -27.7 -17.1 25.5
46 47 50 55 3 1.35 4.30 1.3 -5.8 1.30 1.60
47 50 55 52 3 -1.20 8.5 17.7 -27.7 -17.1 25.5
51 52 55 60 3 1.35 4.30 1.3 -5.8 1.30 1.60
52 55 60 57 3 -1.20 8.5 17.7 -27.7 -17.1 25.5
56 57 60 65 3 1.35 4.30 1.3 -5.8 1.30 1.60
57 60 65 62 3 -1.20 8.5 17.7 -27.7 -17.1 25.5
61 62 65 70 3 1.35 4.30 1.3 -5.8 1.30 1.60
62 65 70 67 3 -1.20 8.5 17.7 -27.7 -17.1 25.5
66 67 70 75 3 1.35 4.30 1.3 -5.8 1.30 1.60
67 70 75 72 3 -1.20 8.5 17.7 -27.7 -17.1 25.5
71 72 75 80 3 1.35 4.30 1.3 -5.8 1.30 1.60
72 75 80 77 3 -1.20 8.5 17.7 -27.7 -17.1 25.5
76 77 80 85 3 1.35 4.30 1.3 -5.8 1.30 1.60
77 80 85 82 3 -1.20 8.5 17.7 -27.7 -17.1 25.5
81 82 85 90 3 1.35 4.30 1.3 -5.8 1.30 1.60
82 85 90 87 3 -1.20 8.5 17.7 -27.7 -17.1 25.5
86 87 90 95 3 1.35 4.30 1.3 -5.8 1.30 1.60
87 90 95 92 3 -1.20 8.5 17.7 -27.7 -17.1 25.5
91 92 95 100 3 1.35 4.30 1.3 -5.8 1.30 1.60
92 95 100 97 3 -1.20 8.5 17.7 -27.7 -17.1 25.5
96 97 100 105 3 1.35 4.30 1.3 -5.8 1.30 1.60
97 100 105 102 3 -1.20 8.5 17.7 -27.7 -17.1 25.5
101 102 105 110 3 1.35 4.30 1.3 -5.8 1.30 1.60
102 105 110 107 3 -1.20 8.5 17.7 -27.7 -17.1 25.5
106 107 110 115 3 1.35 4.30 1.3 -5.8 1.30 1.60
107 110 115 112 3 -1.20 8.5 17.7 -27.7 -17.1 25.5
111 112 115 120 3 1.35 4.30 1.3 -5.8 1.30 1.60
112 115 120 117 3 -1.20 8.5 17.7 -27.7 -17.1 25.5
116 117 120 125 3 1.35 4.30 1.3 -5.8 1.30 1.60
117 120 125 122 3 -1.20 8.5 17.7 -27.7 -17.1 25.5
121 122 125 130 3 1.35 4.30 1.3 -5.8 1.30 1.60
122 125 130 127 3 -1.20 8.5 17.7 -27.7 -17.1 25.5
126 127 130 135 3 1.35 4.30 1.3 -5.8 1.30 1.60
127 130 135 132 3 -1.20 8.5 17.7 -27.7 -17.1 25.5
131 132 135 140 3 1.35 4.30 1.3 -5.8 1.30 1.60
132 135 140 137 3 -1.20 8.5 17.7 -27.7 -17.1 25.5
136 137 140 145 3 1.35 4.30 1.3 -5.8 1.30 1.60
137 140 145 142 3 -1.20 8.5 17.7 -27.7 -17.1 25.5
141 142 145 150 3 1.35 4.30 1.3 -5.8 1.30 1.60
142 145 150 147 3 -1.20 8.5 17.7 -27.7 -17.1 25.5
146 147 150 155 3 1.35 4.30 1.3 -5.8 1.30 1.60
147 150 155 152 3 -1.20 8.5 17.7 -27.7 -17.1 25.5
151 152 155 160 3 1.35 4.30 1.3 -5.8 1.30 1.60
152 155 160 157 3 -1.20 8.5 17.7 -27.7 -17.1 25.5
156 157 160 165 3 1.35 4.30 1.3 -5.8 1.30 1.60
157 160 165 162 3 -1.20 8.5 17.7 -27.7 -17.1 25.5
161 162 165 170 3 1.35 4.30 1.3 -5.8 1.30 1.60
162 165 170 167 3 -1.20 8.5 17.7 -27.7 -17.1 25.5
166 167 170 175 3 1.35 4.30 1.3 -5.8 1.30 1.60
```

```
167 170 175 172 3 -1.20 8.5 17.7 -27.7 -17.1 25.5

[ constraints ]
; i j funct length
3 4 1 0.226
8 9 1 0.226
13 14 1 0.226
18 19 1 0.226
23 24 1 0.226
28 29 1 0.226
33 34 1 0.226
38 39 1 0.226
43 44 1 0.226
48 49 1 0.226
53 54 1 0.226
58 59 1 0.226
63 64 1 0.226
68 69 1 0.226
73 74 1 0.226
78 79 1 0.226
83 84 1 0.226
88 89 1 0.226
93 94 1 0.226
98 99 1 0.226
103 104 1 0.226
108 109 1 0.226
113 114 1 0.226
118 119 1 0.226
123 124 1 0.226
128 129 1 0.226
133 134 1 0.226
138 139 1 0.226
143 144 1 0.226
148 149 1 0.226
153 154 1 0.226
158 159 1 0.226
163 164 1 0.226
168 169 1 0.226
173 174 1 0.226
```

The following [**nonbond_params**] must replace the corresponding lines of the original Martini force field file. martini.itp

```
[ nonbond_params ]

;;; self terms
; i j f c6 c12
SNda SNda 1 0.30788E-01 0.78995E-04
SC3 SC3 1 0.73073E-01 0.60678E-03
SC1 SC1 1 0.60685E-01 0.38361E-03

;;; cross terms
; i j f c6 c12
SNda SC3 1 0.43179E-01 0.35855E-03
SNda SC1 1 0.19660E-01 0.80530E-04
SC3 SC1 1 0.58156E-01 0.36762E-03
```

```
;;; water cross terms
POL SNda 1 0.57344E-01 0.23488E-03
POL SC3 1 0.32768E-01 0.13421E-03
POL SC1 1 0.28149E-01 0.99052E-04
;;;
```