supplementary
Supporting information for manuscript JA020429L-3-a-78

"Studying Enzyme Binding Specificity in Acetylcholinesterase using a Combined Molecular Dynamics and Multiple Docking Approach"

Jeremy Kua, Yingkai Zhang, and J. Andrew McCammon

Figure Captions:

Figure S01. C-O distance of acetyl carbonyl carbon to Ser203-O along 1ns MD ACh-AChE trajectory.

Figure S02. O-N distance of Ser203-O to G121-N along 1ns MD ACh-AChE trajectory.

Figure S03. O-N distance of Ser203-O to G122-N along 1ns MD ACh-AChE trajectory.

Figure S04. O-N distance of Ser203-O to A204-N along 1ns MD ACh-AChE trajectory.

Figure S05. Angle alpha along 1ns MD ACh-AChE trajectory.

Figure S06. N+ distance to W86 ring center along 1ns MD ACh-AChE trajectory.

Figure S07. N+ distance to Y337 ring center along 1ns MD ACh-AChE trajectory.

Figure S08. N+ distance to Y337 phenol-O along 1ns MD ACh-AChE trajectory.

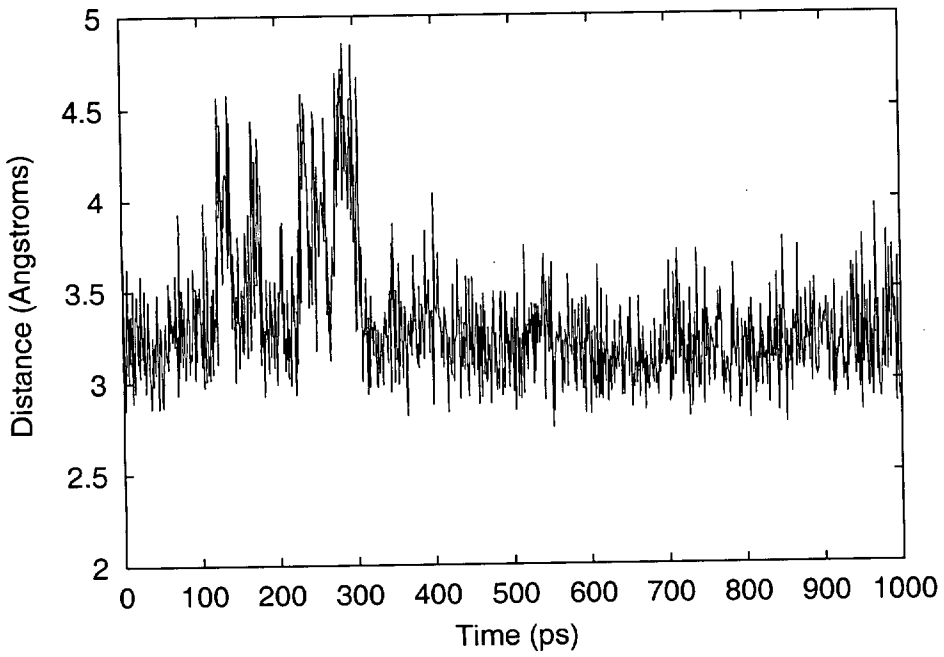
Figure S09. N+ distance to E202-O2 along 1ns MD ACh-AChE trajectory.

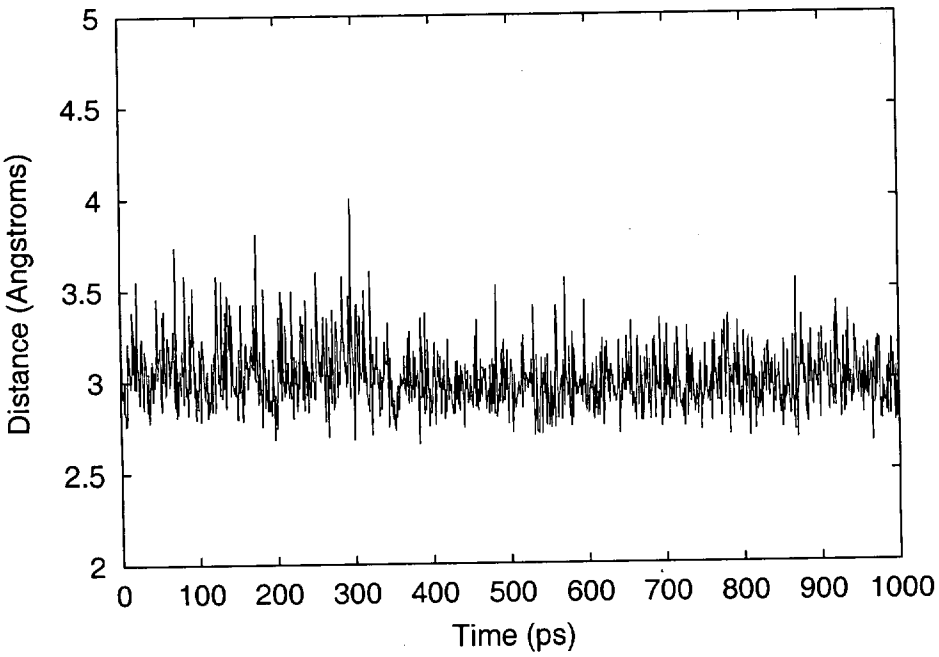
Figure S10. N+ distance to E202-O1 along 1ns MD ACh-AChE trajectory.

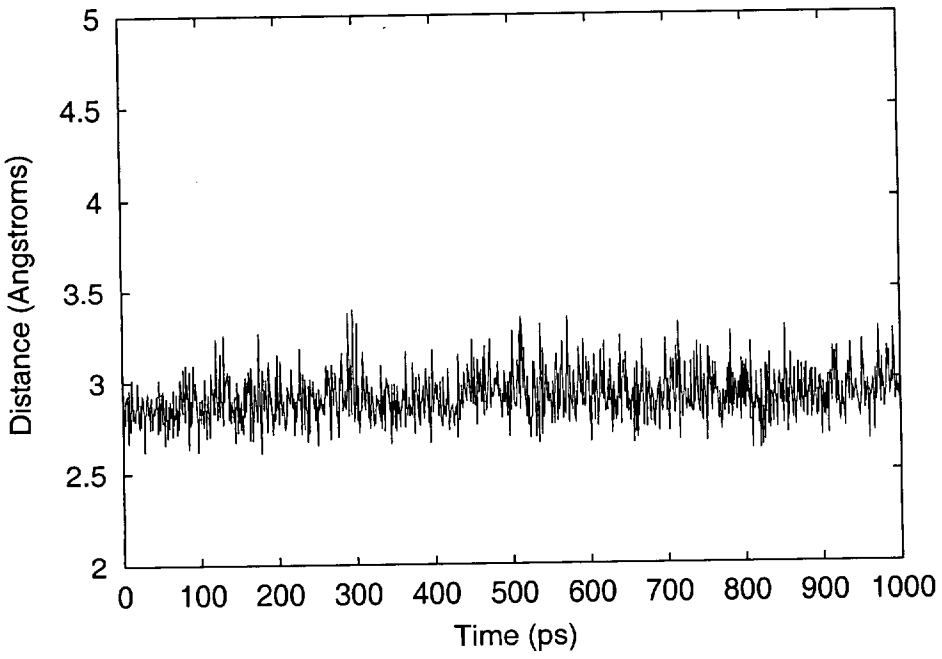
Figure S11. Angle beta along 1ns MD ACh-AChE trajectory.

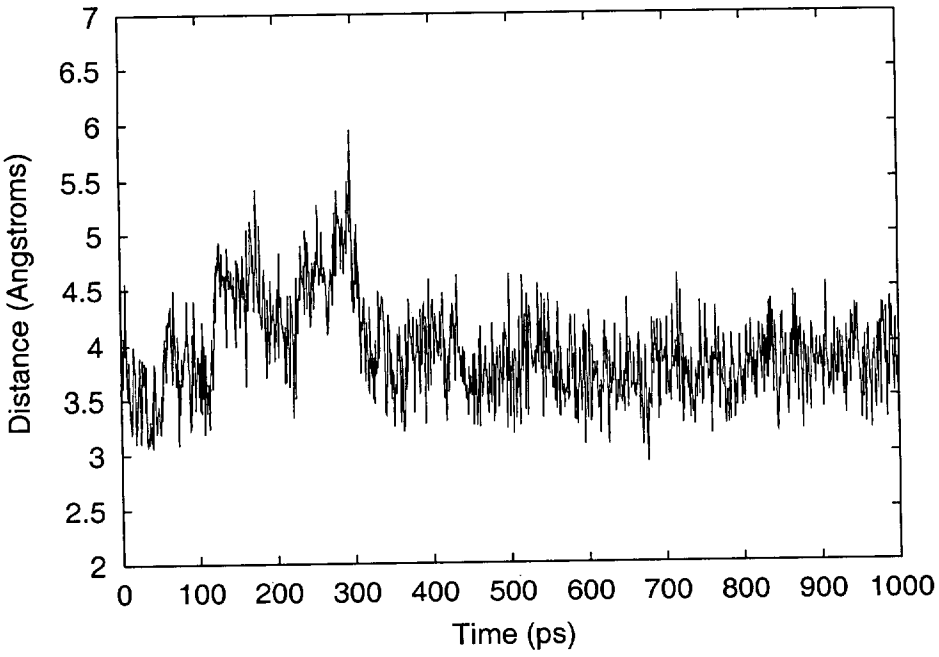
Figure S12. Angle gamma along 1ns MD ACh-AChE trajectory.

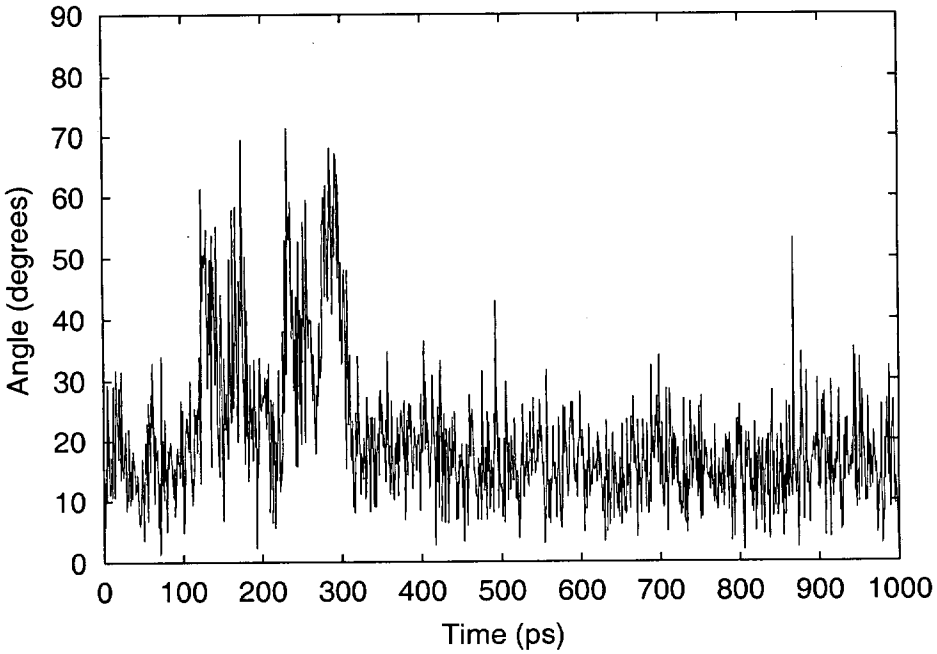
Corresponding eps files are FigS01.eps through FigS12.eps

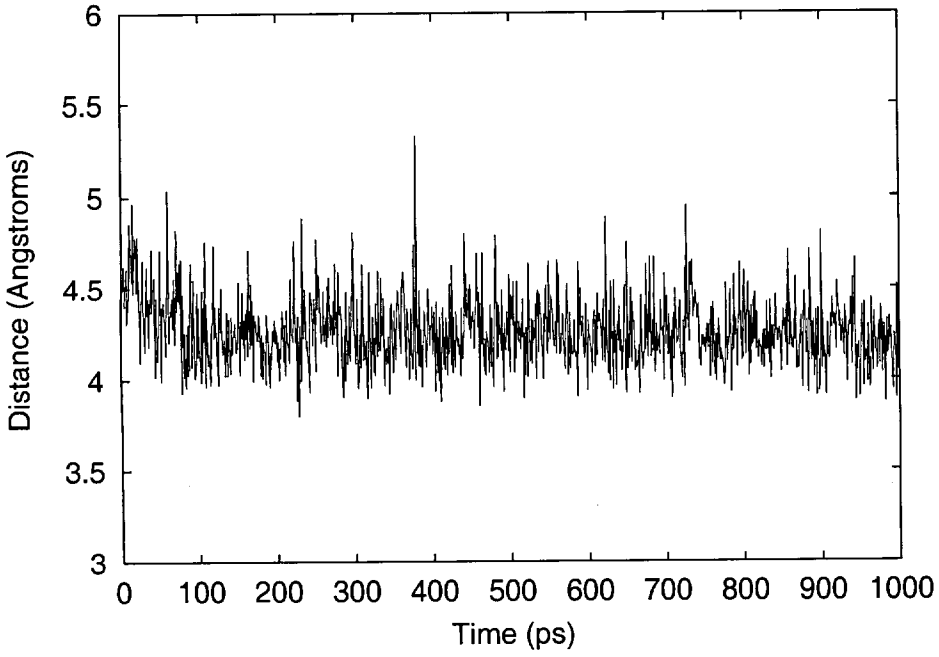

Distance (Angstroms)
5
4.5
4
3.5
3
2.5
2
0
100
200
300
400
500
600
700
800
900
1000
Time (ps)

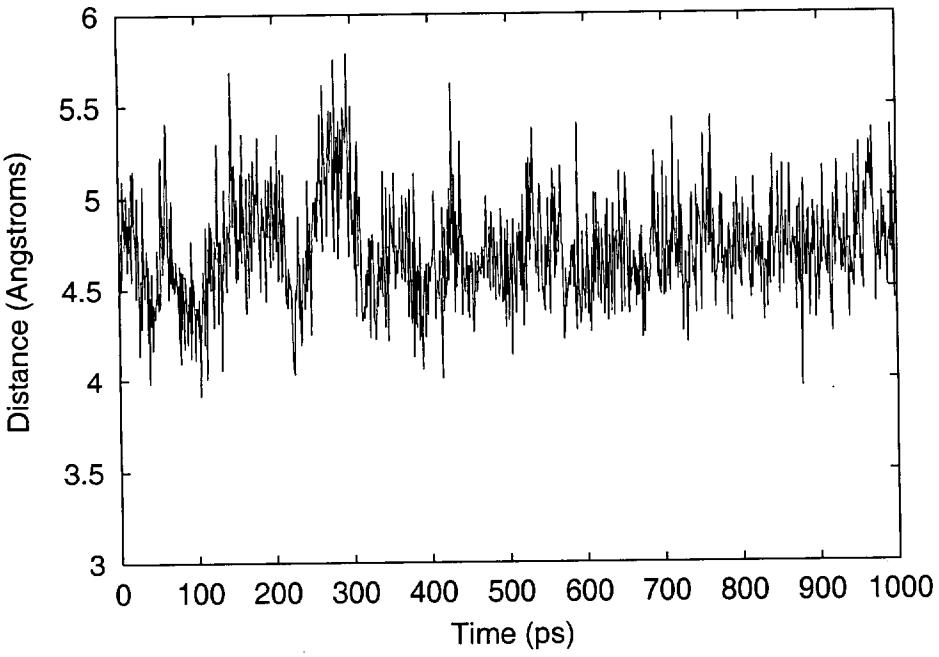

Distance (Angstroms)
5
4.5
4
3.5
3
2.5
2
0
100
200
300
400
500
600
700
800
900
1000
Time (ps)

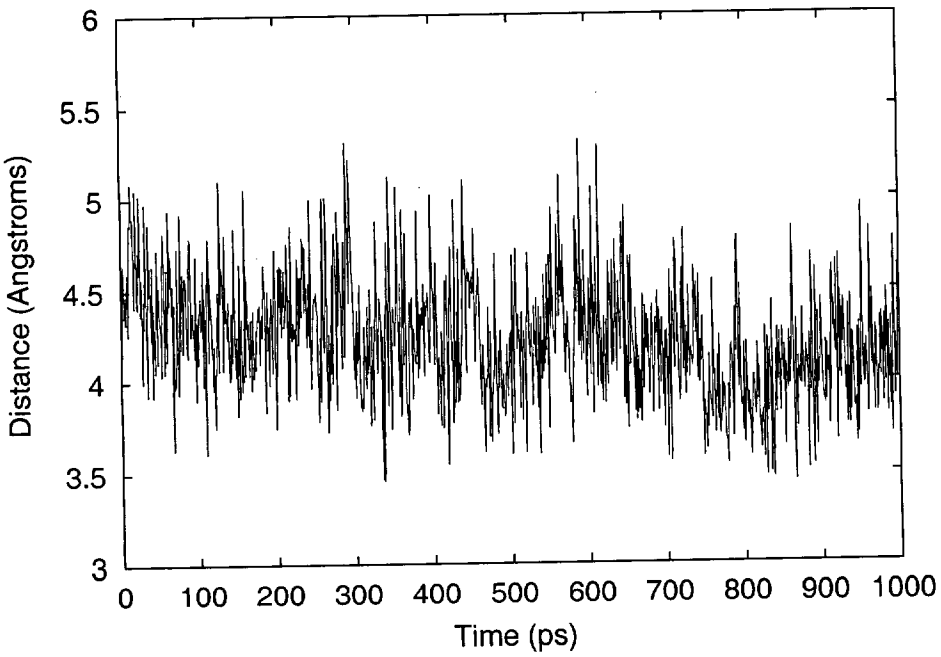

Distance (Angstroms)
5
4.5
4
3.5
3
2.5
2
0
100
200
300
400
500
600
700
800
900
1000
Time (ps)

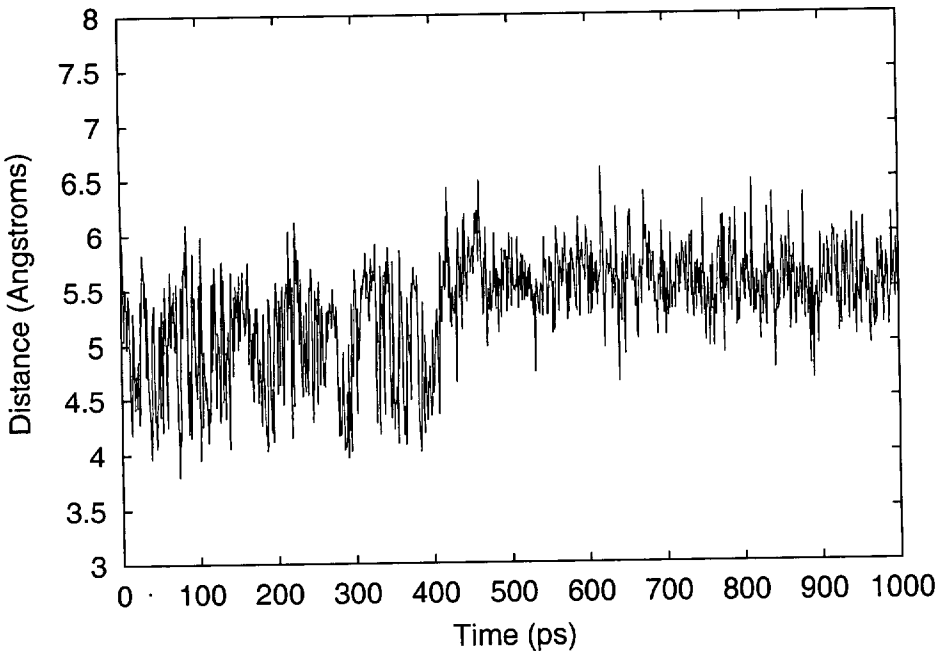

Distance (Angstroms)
Time (ps)
7
6.5
6
5.5
5
4.5
4
3.5
3
2.5
2
0
100
200
300
400
500
600
700
800
900
1000

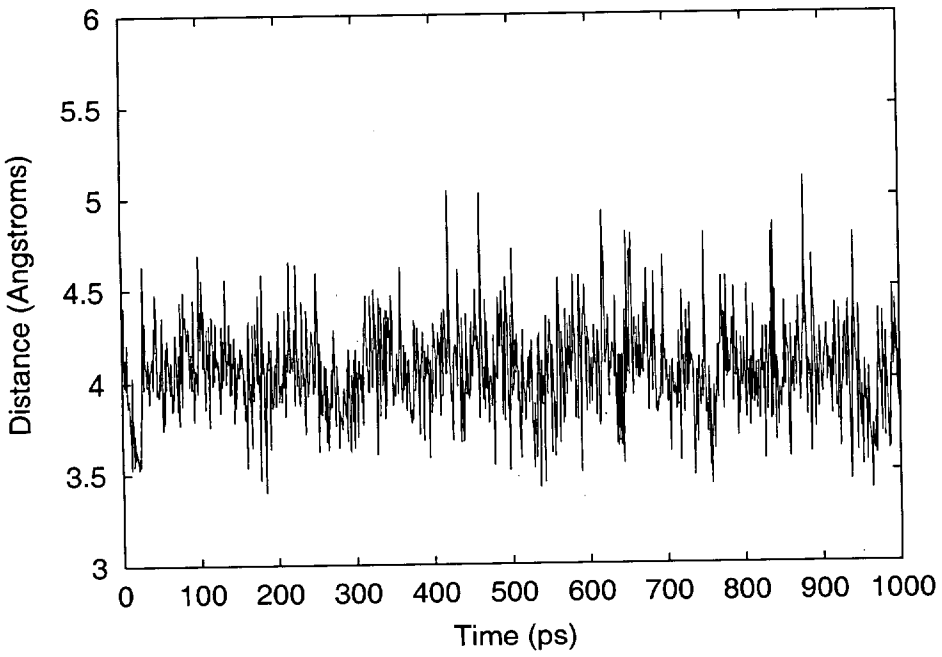

90
80
70
60
50
40
30
20
10
0
Angle (degrees)
0
100
200
300
400
500
600
700
800
900
1000
Time (ps)

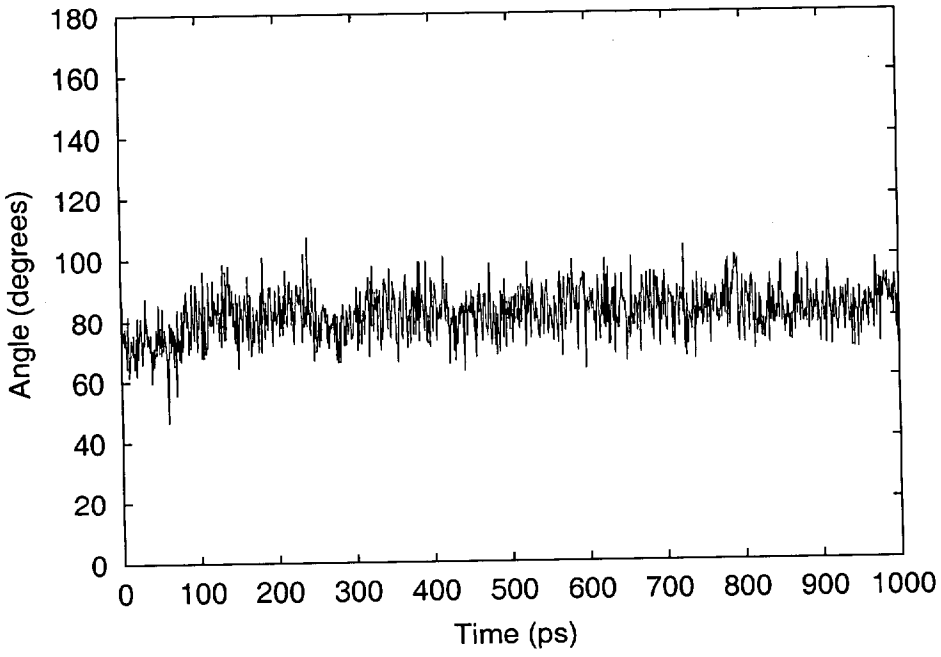

Distance (Angstroms)
6
5.5
5
4.5
4
3.5
3
0
100
200
300
400
500
600
700
800
900
1000
Time (ps)

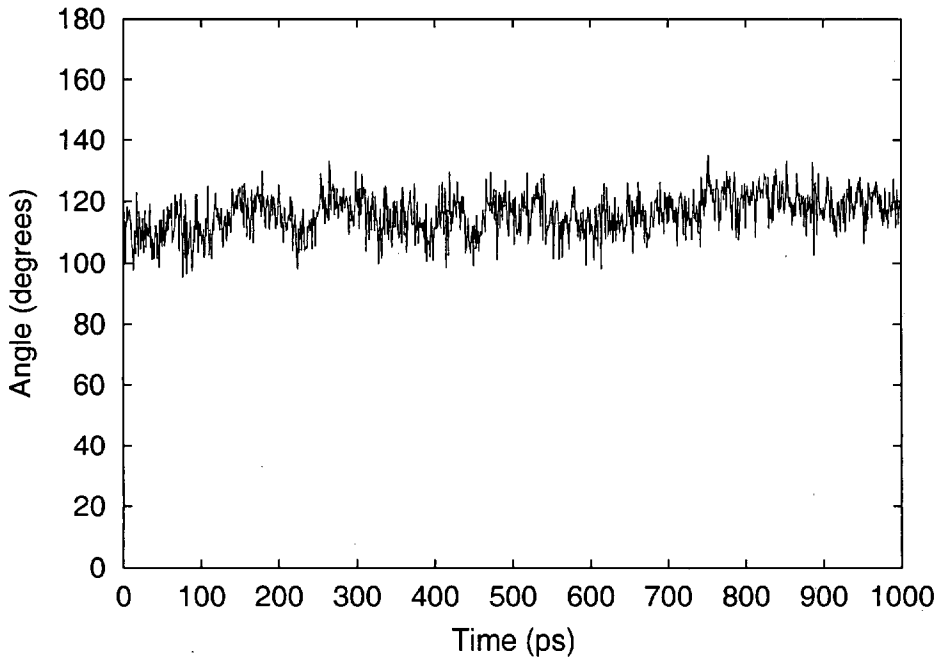

Distance (Angstroms)
6
5.5
5
4.5
4
3.5
3
0
100
200
300
400
500
600
700
800
900
1000
Time (ps)


Distance (Angstroms)
Time (ps)
6
5.5
5
4.5
4
3.5
3
0
100
200
300
400
500
600
700
800
900
1000


Distance (Angstroms)
8
7.5
7
6.5
6
5.5
5
4.5
4
3.5
3
0
100
200
300
400
500
600
700
800
900
1000
Time (ps)


Distance (Angstroms)
Time (ps)
6
5.5
5
4.5
4
3.5
3
0
100
200
300
400
500
600
700
800
900
1000


180
160
140
120
100
80
60
40
20
0
Angle (degrees)
0
100
200
300
400
500
600
700
800
900
1000
Time (ps)


180
160
140
120
100
80
60
40
20
0
Angle (degrees)
0
100
200
300
400
500
600
700
800
900
1000
Time (ps)