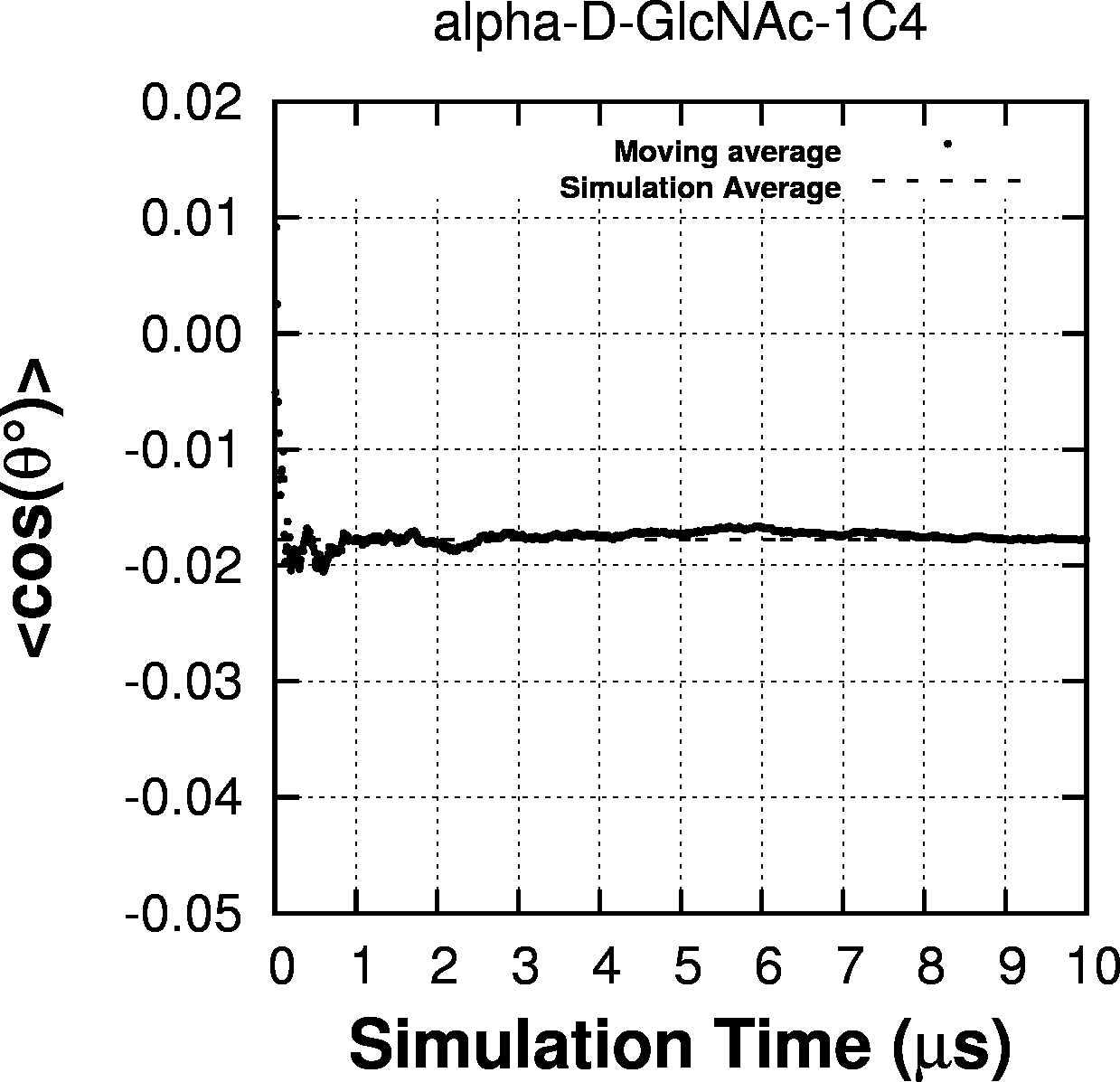
S1: Cremer-Pople analysis for the twenty 10 µs explicit solvent molecular dynamics simulations.

For each simulation, the puckering parameters Q and θ are plotted against simulation time, θ and φ are plotted against each other and $cos\langle\theta\rangle$ is plotted against simulation time (reports convergence of conformation).

Key:
pages 2-41: α-anomers (1-OH), denoted alpha-D-X
pages 42-81: 1-*O*-methyl glycosides
-1C4 postfix: $^{1}C_{4}$-initiated simulations, otherwise $^{4}C_{1}$-


alpha-D-GlcNAc-1C4
Moving average
Simulation Average
0.02
0.01
0.00
-0.01
-0.02
-0.03
-0.04
-0.05
<cos(θ°)>
0
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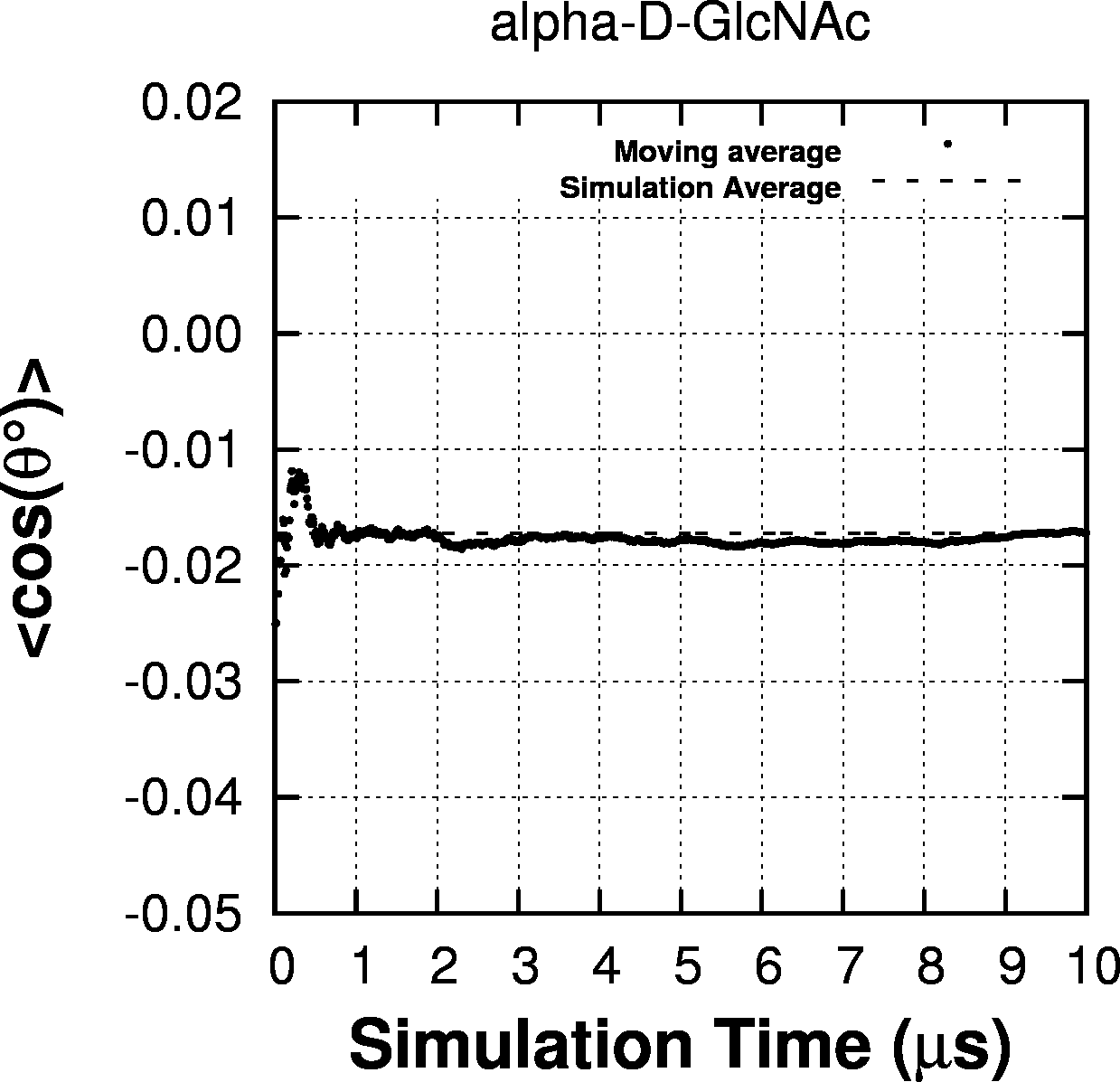
Simulation Time (μs)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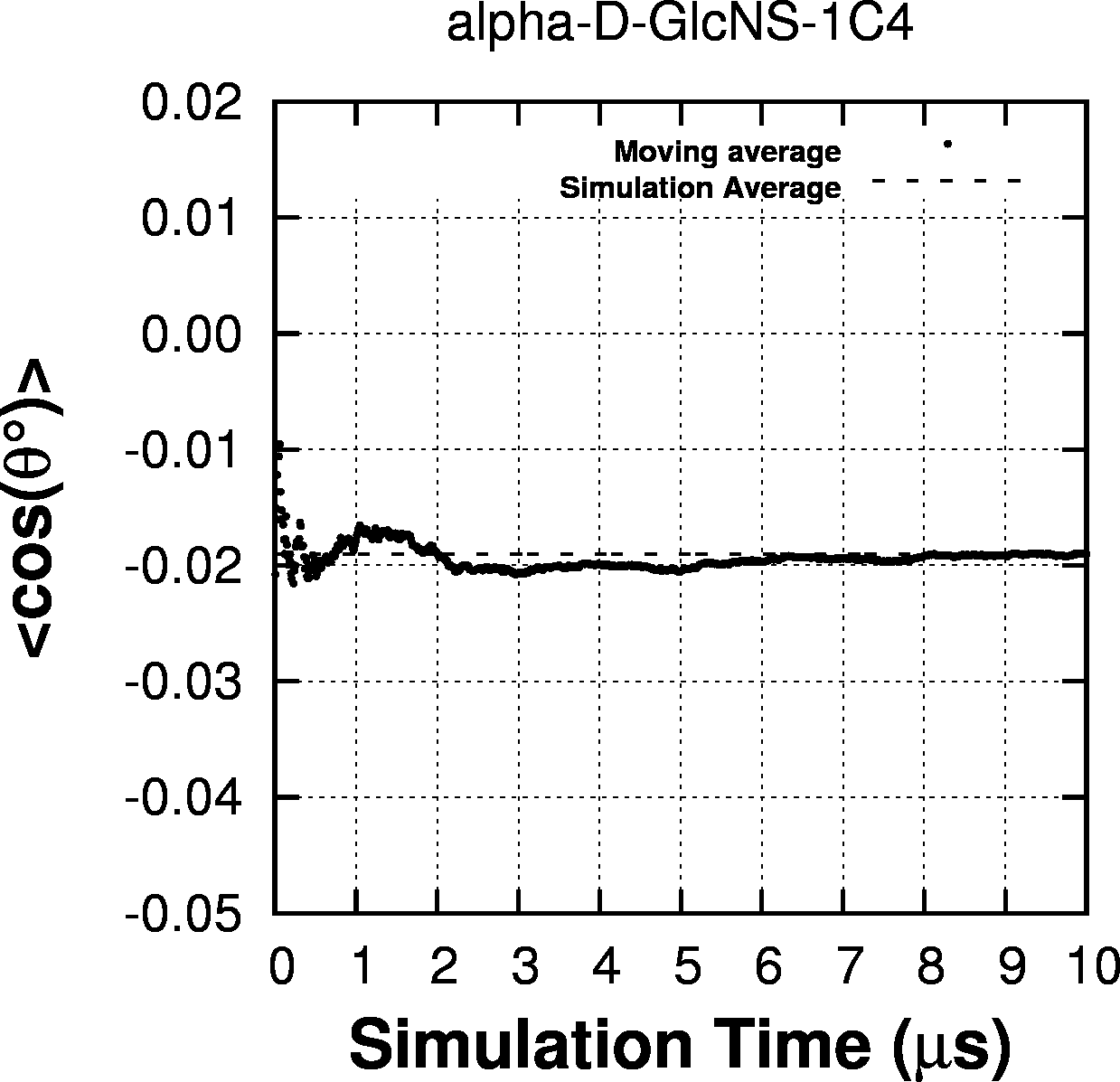
Simulation Time (μs)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Simulation Average
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0.00
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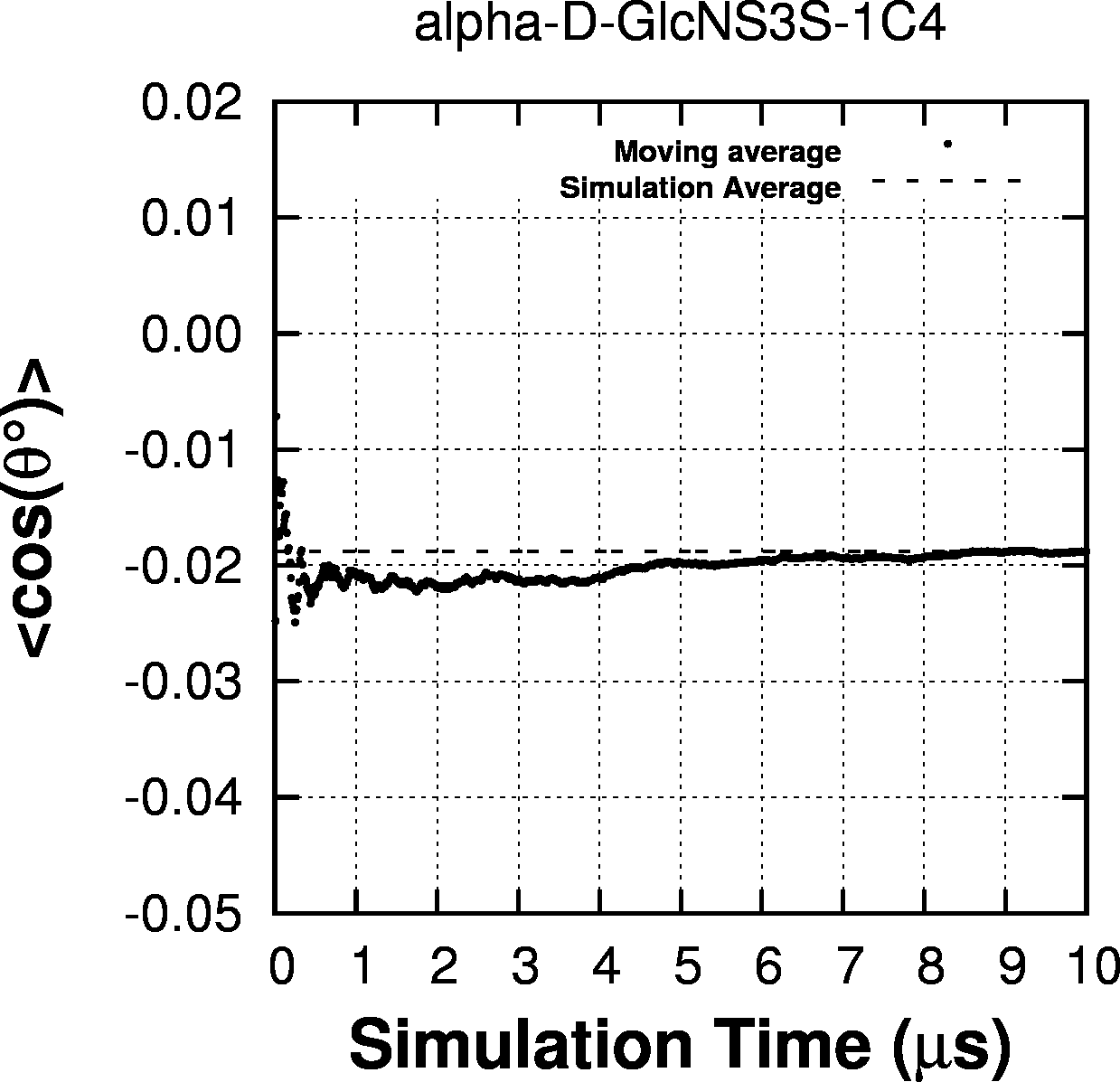
Simulation Time (μs)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Simulation Average
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-0.02
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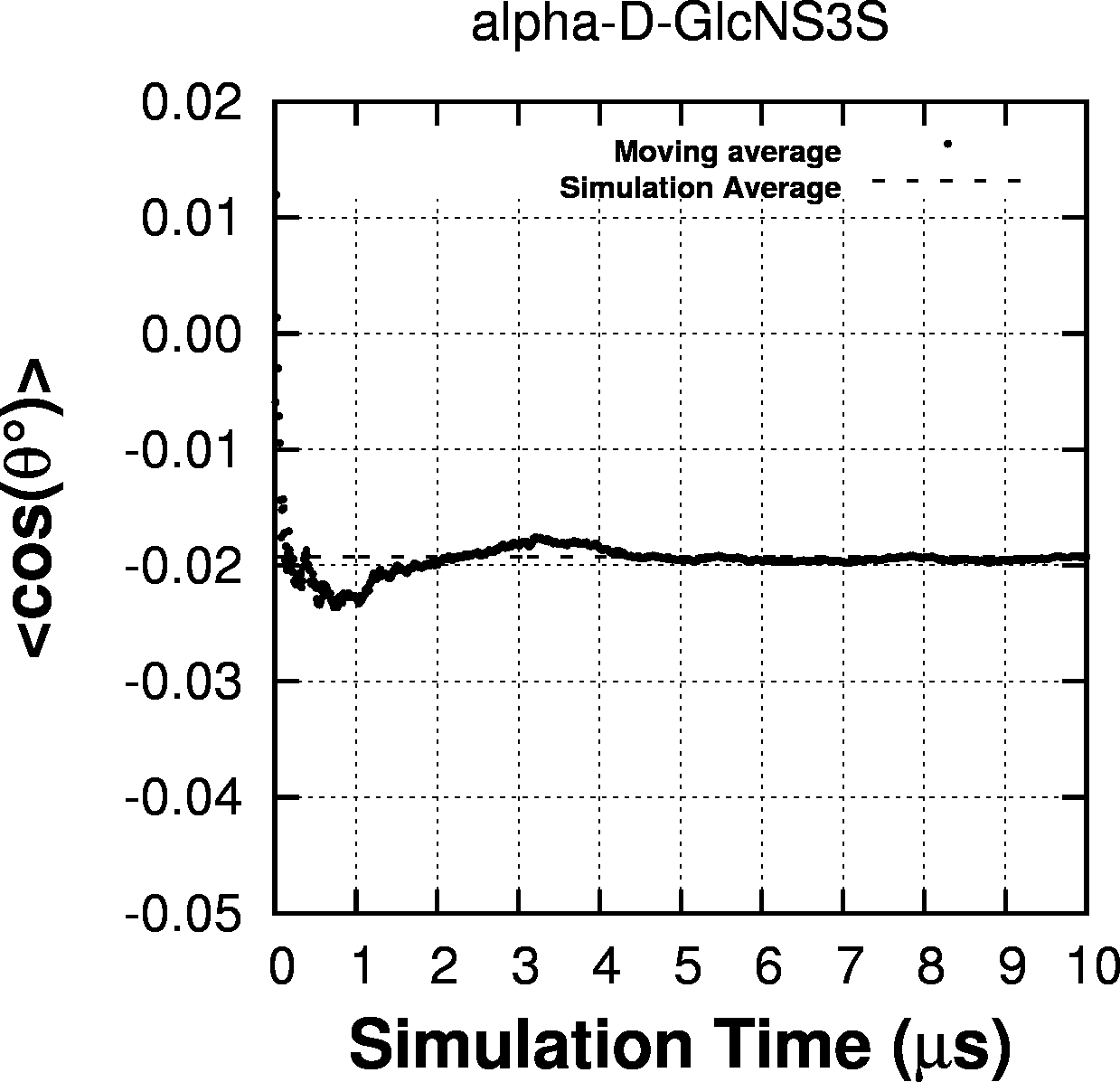
Simulation Time (μs)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Moving average
Simulation Average
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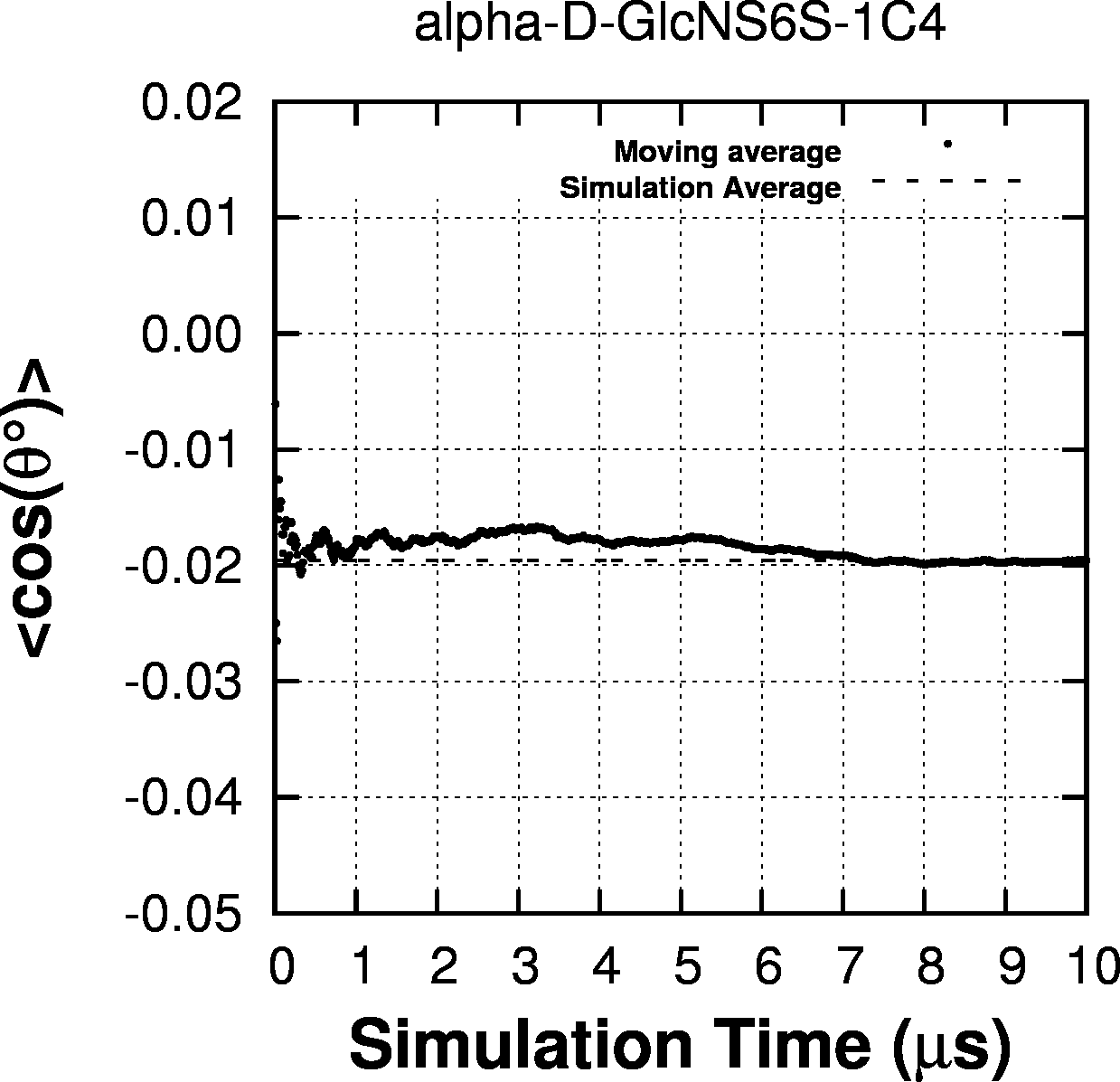
Simulation Time (μs)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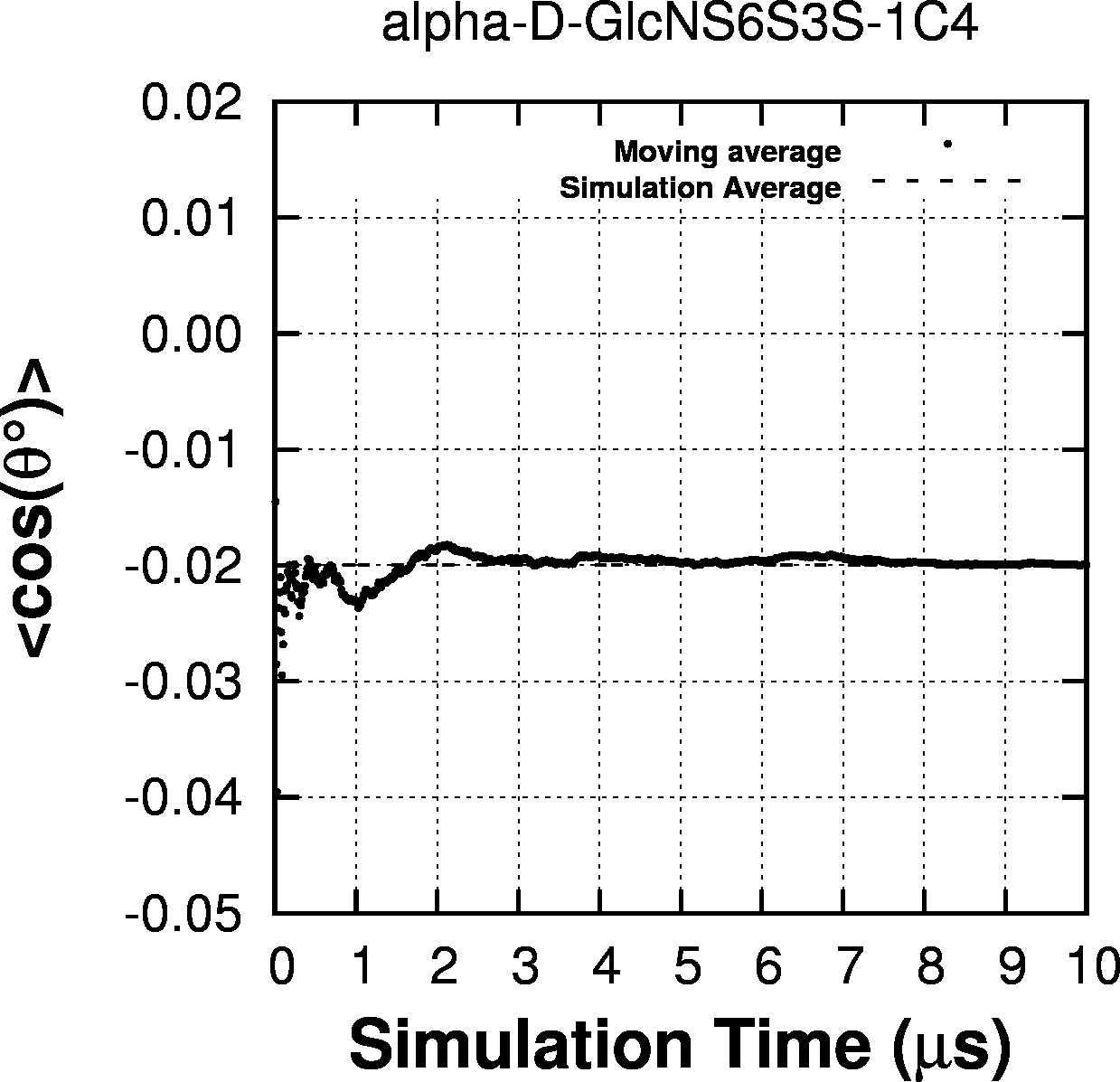
Simulation Time (μs)


alpha-D-GlcNS6S3S-1C4
Moving average
Simulation Average
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-0.02
-0.03
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-0.05
<cos(θ°)>
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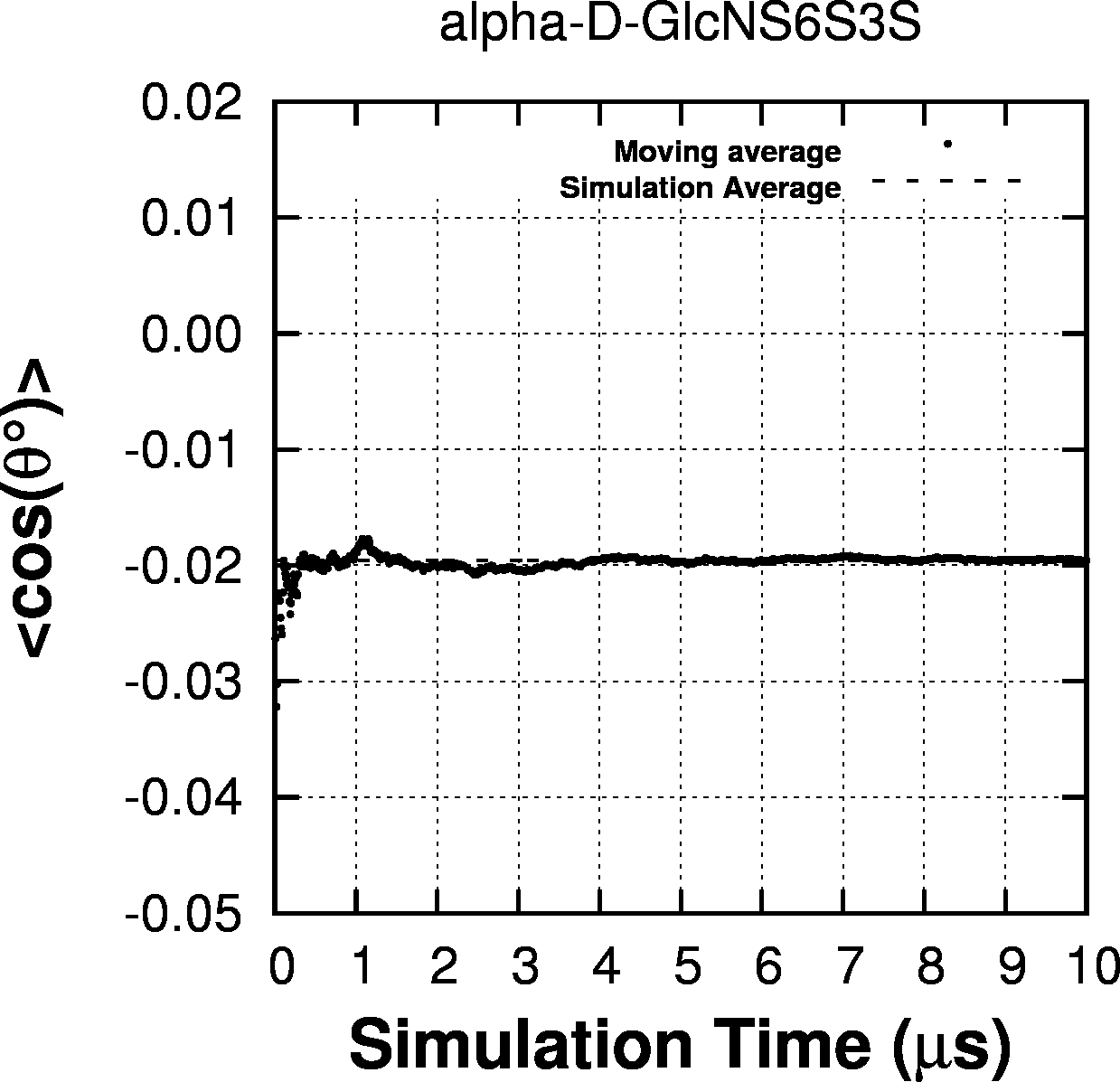
Simulation Time (μs)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Moving average
Simulation Average
<cos(θ°)>
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0.00
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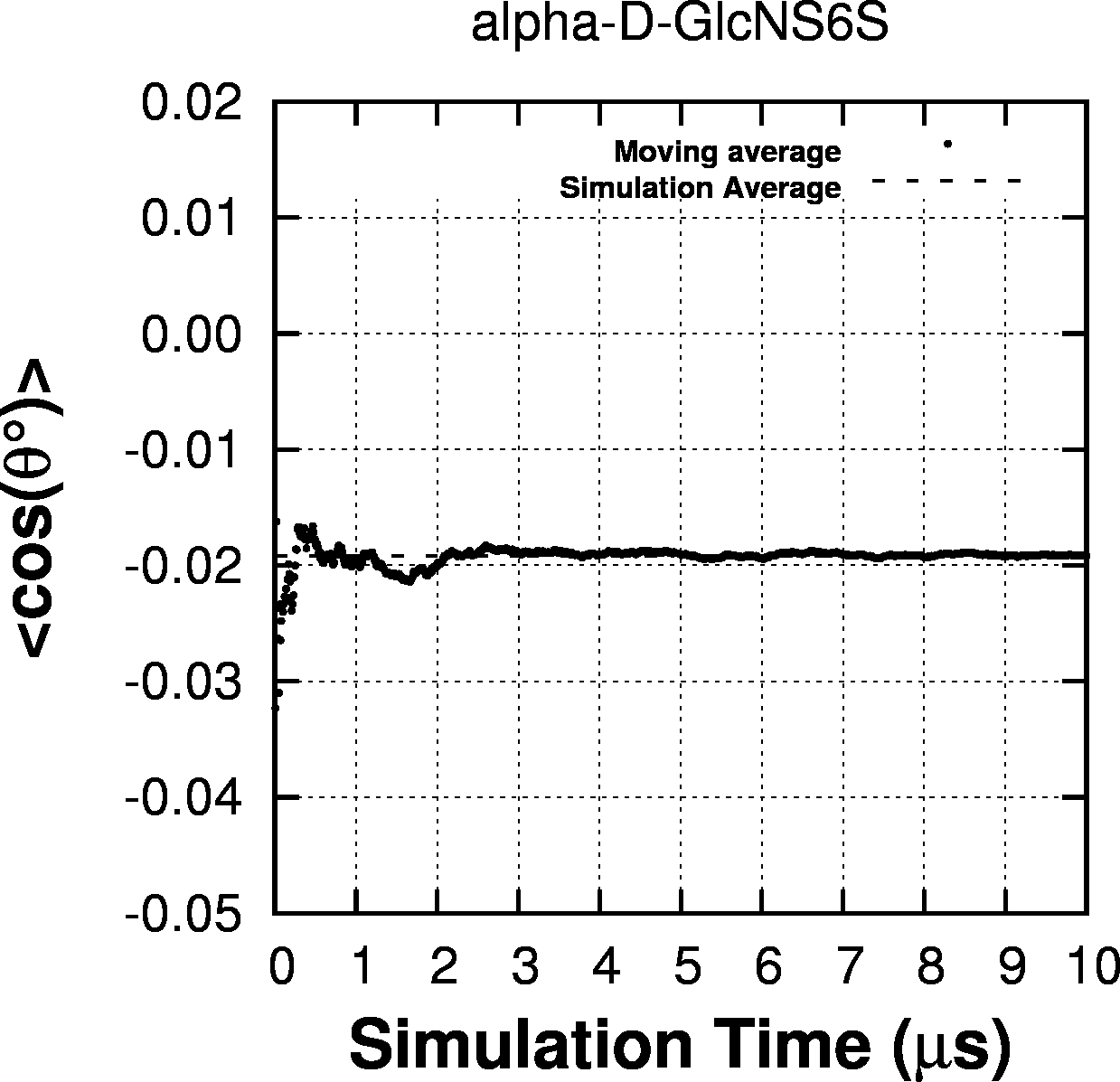
Simulation Time (μs)


alpha-D-GlcNS6S
Moving average
Simulation Average
0.02
0.01
0.00
-0.01
-0.02
-0.03
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-0.05
<cos(θ°)>
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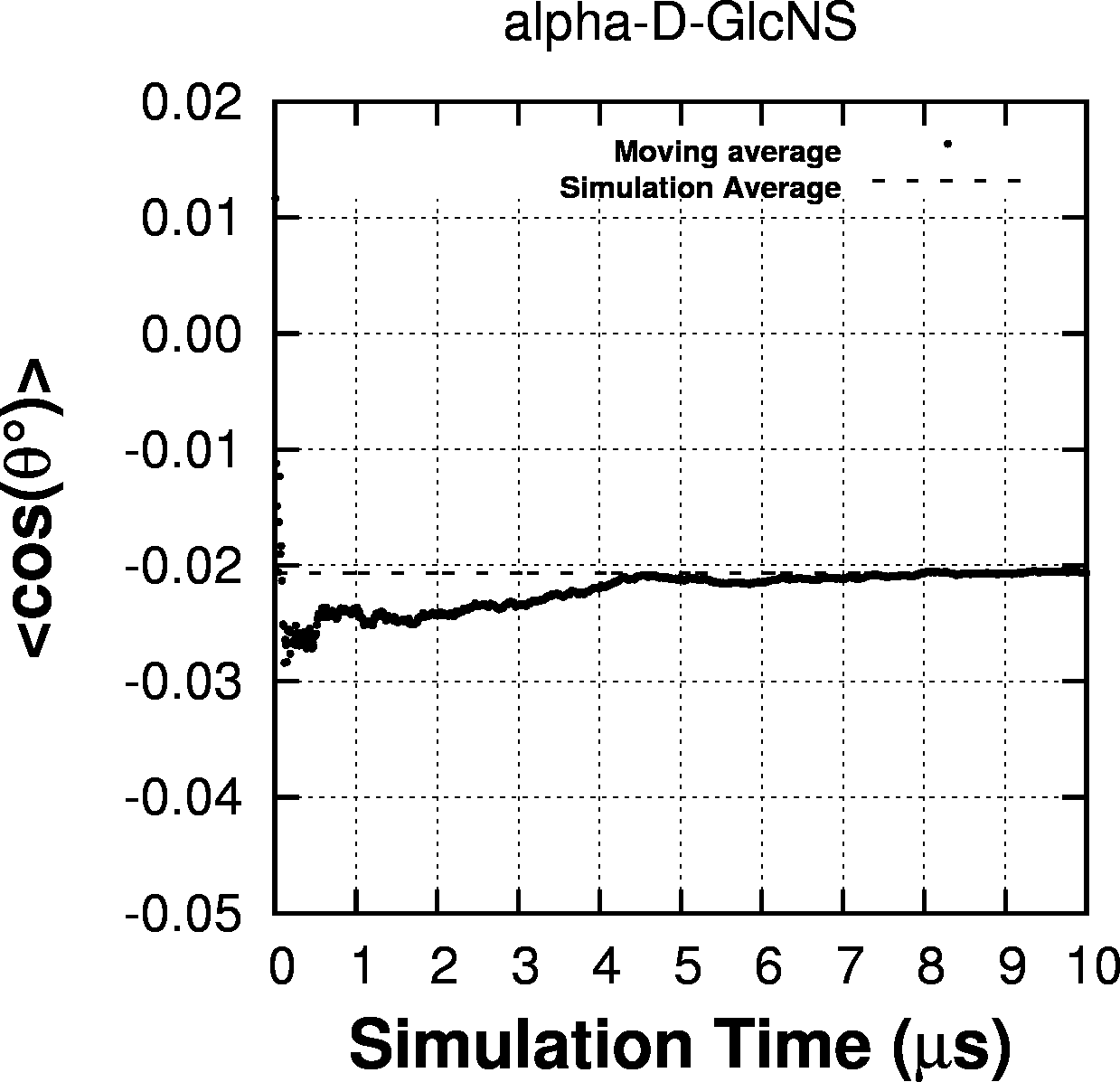
Simulation Time (μs)


alpha-D-GlcNS
Moving average
Simulation Average
<cos(θ°)>
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0.00
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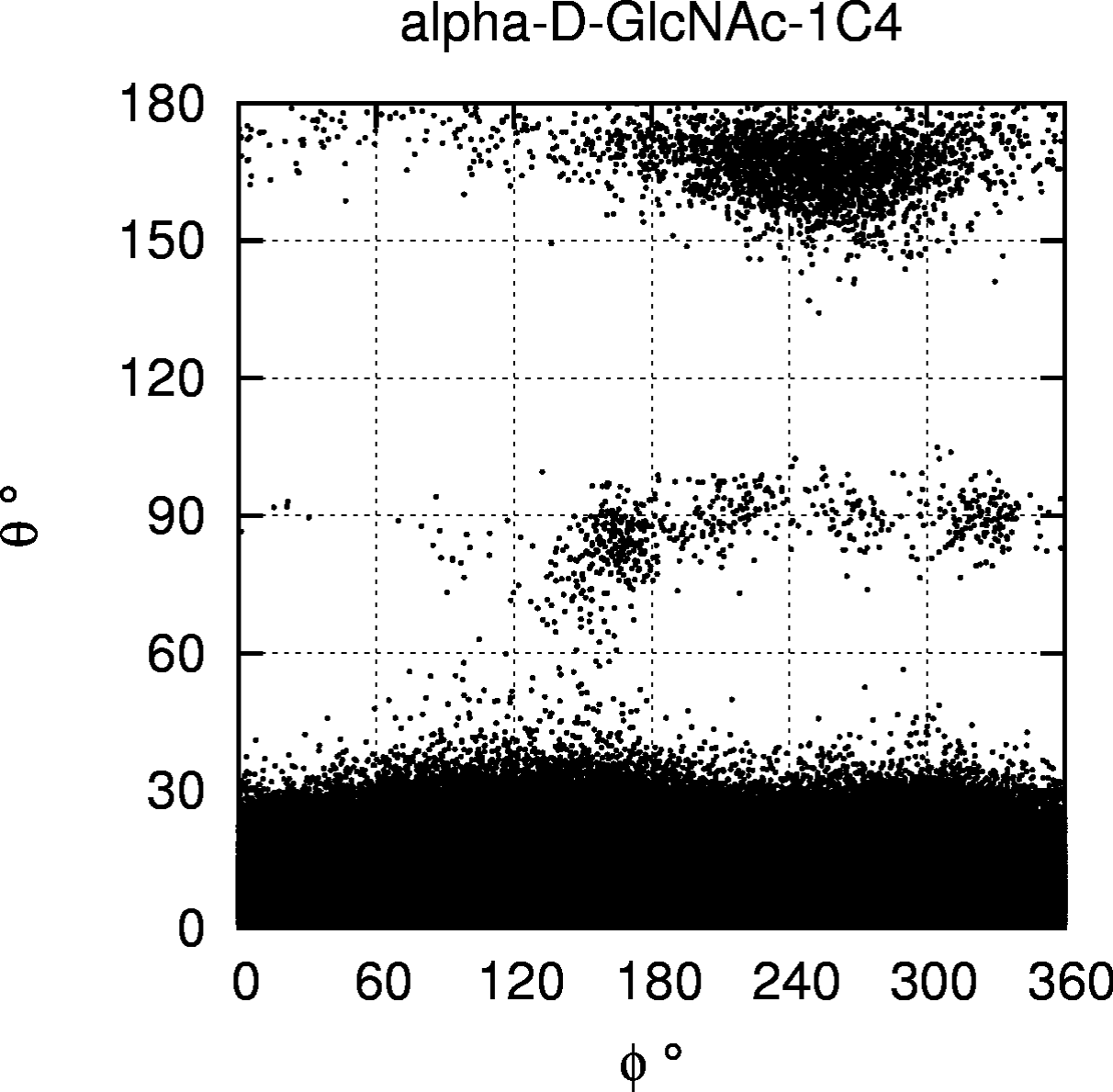
Simulation Time (μs)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180
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θ °
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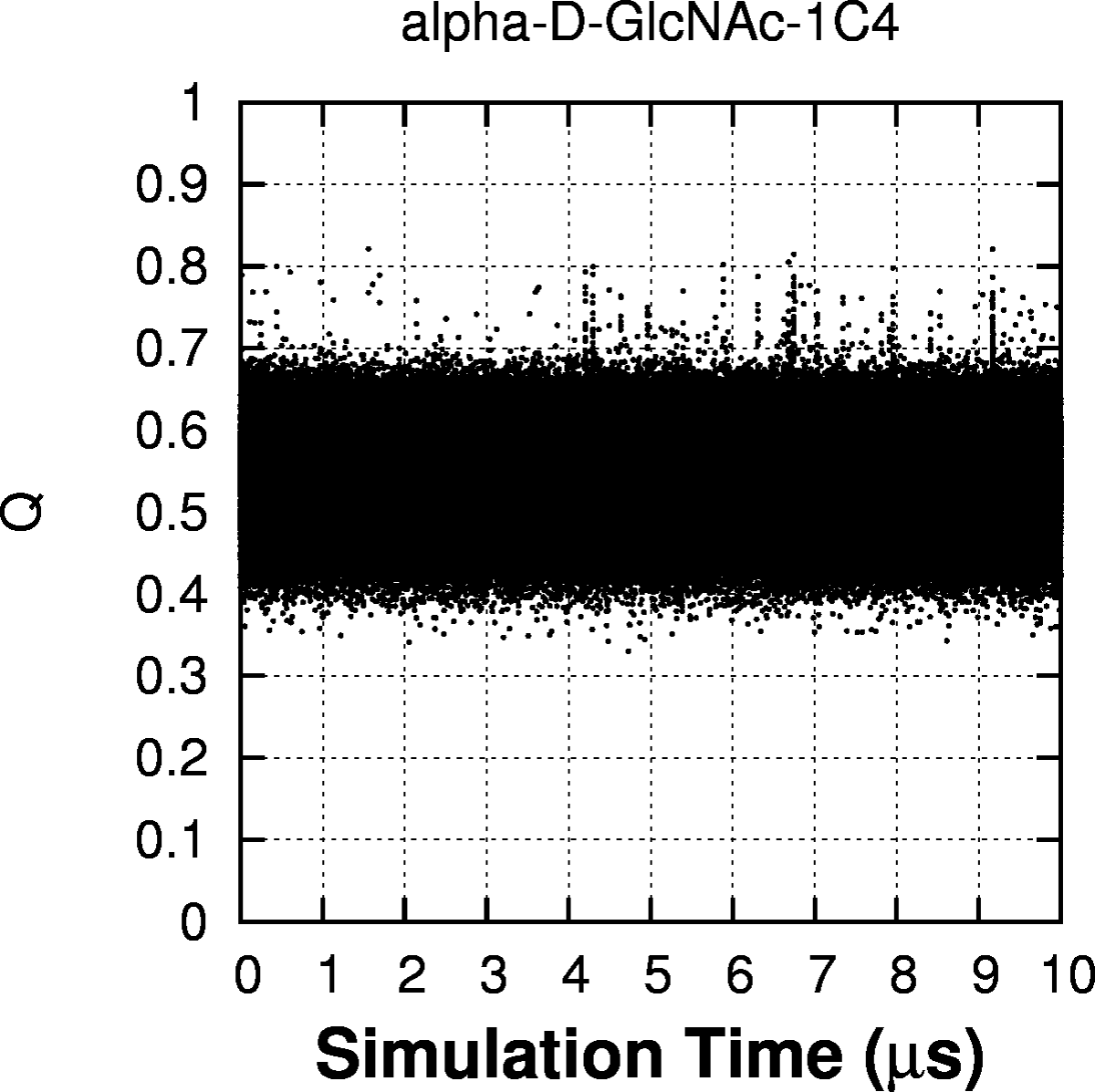
alpha-D-GlcNAc-1C4
Q
1
0.9
0.8
0.7
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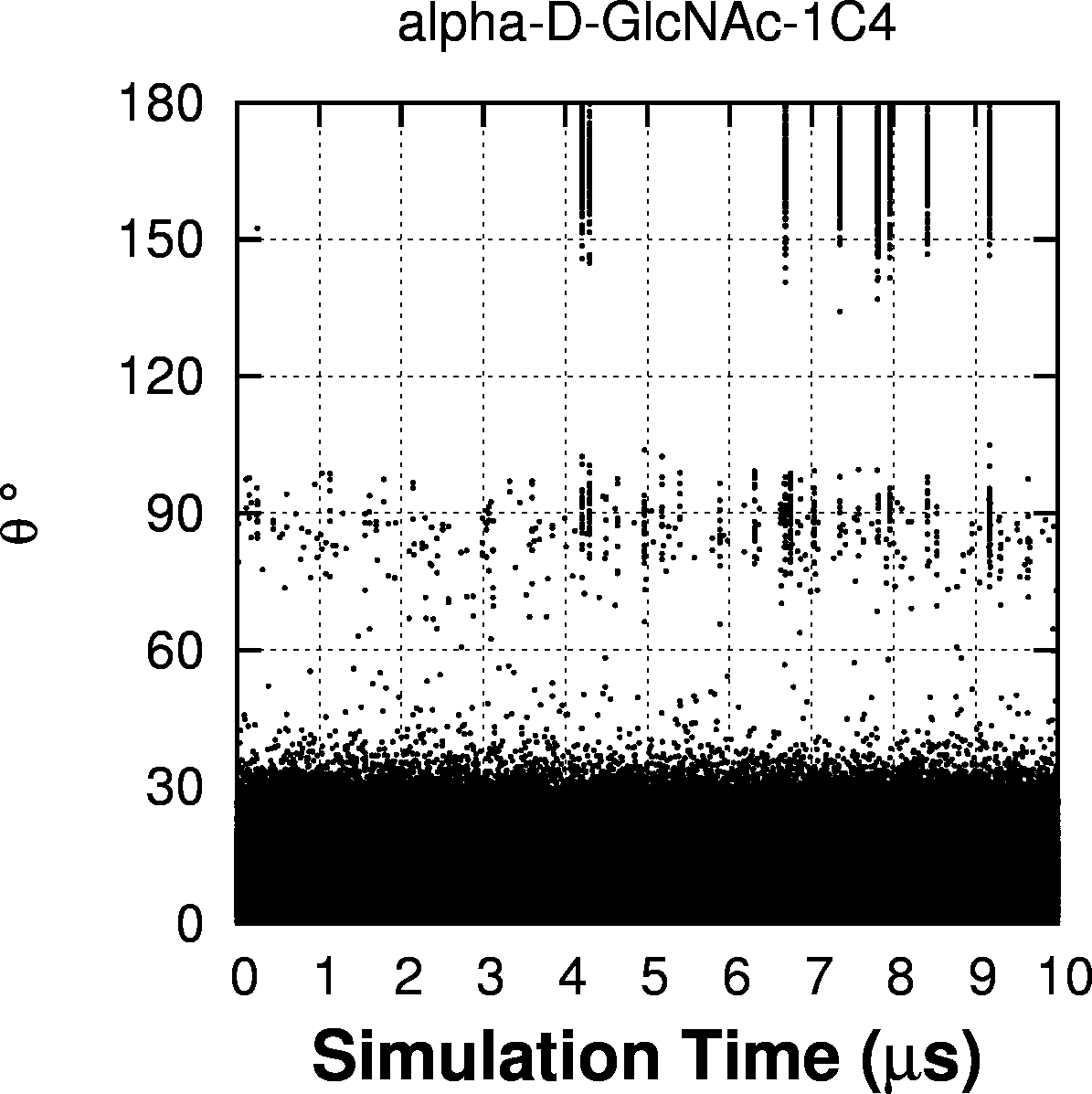
0 1 2 3 4 5 6 7 8 9 10
Simulation Time (μs)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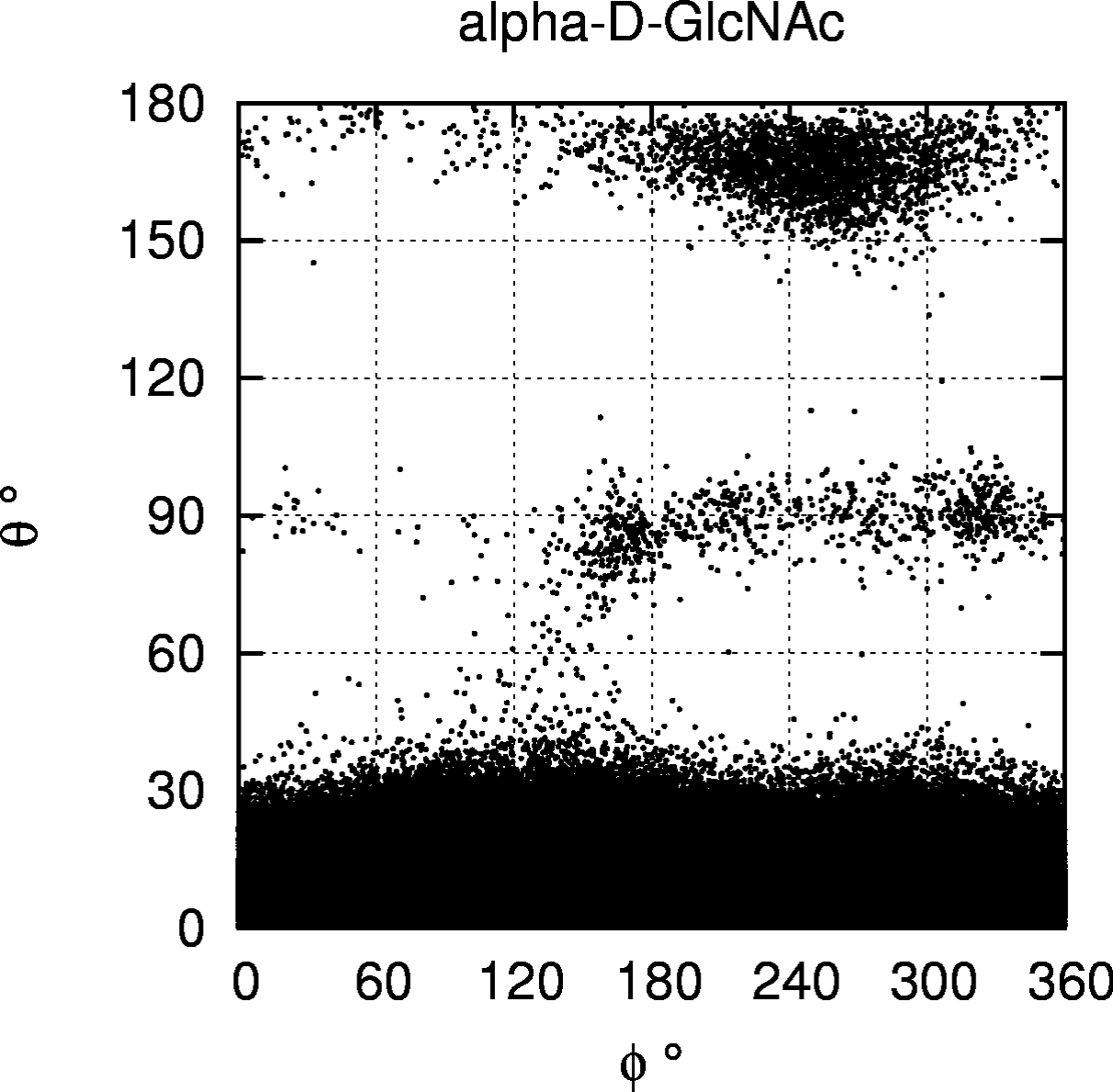
Simulation Time (μs)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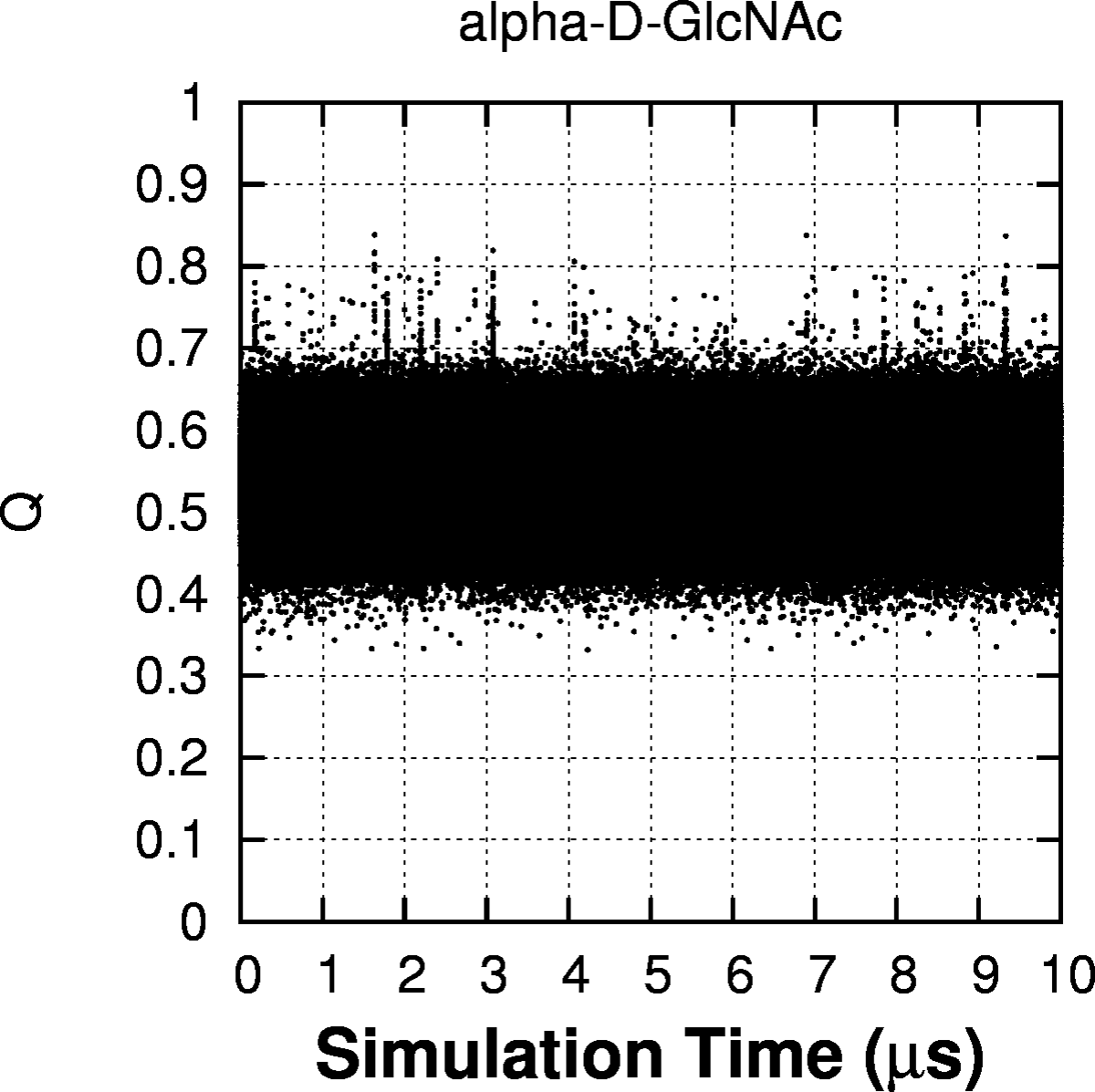
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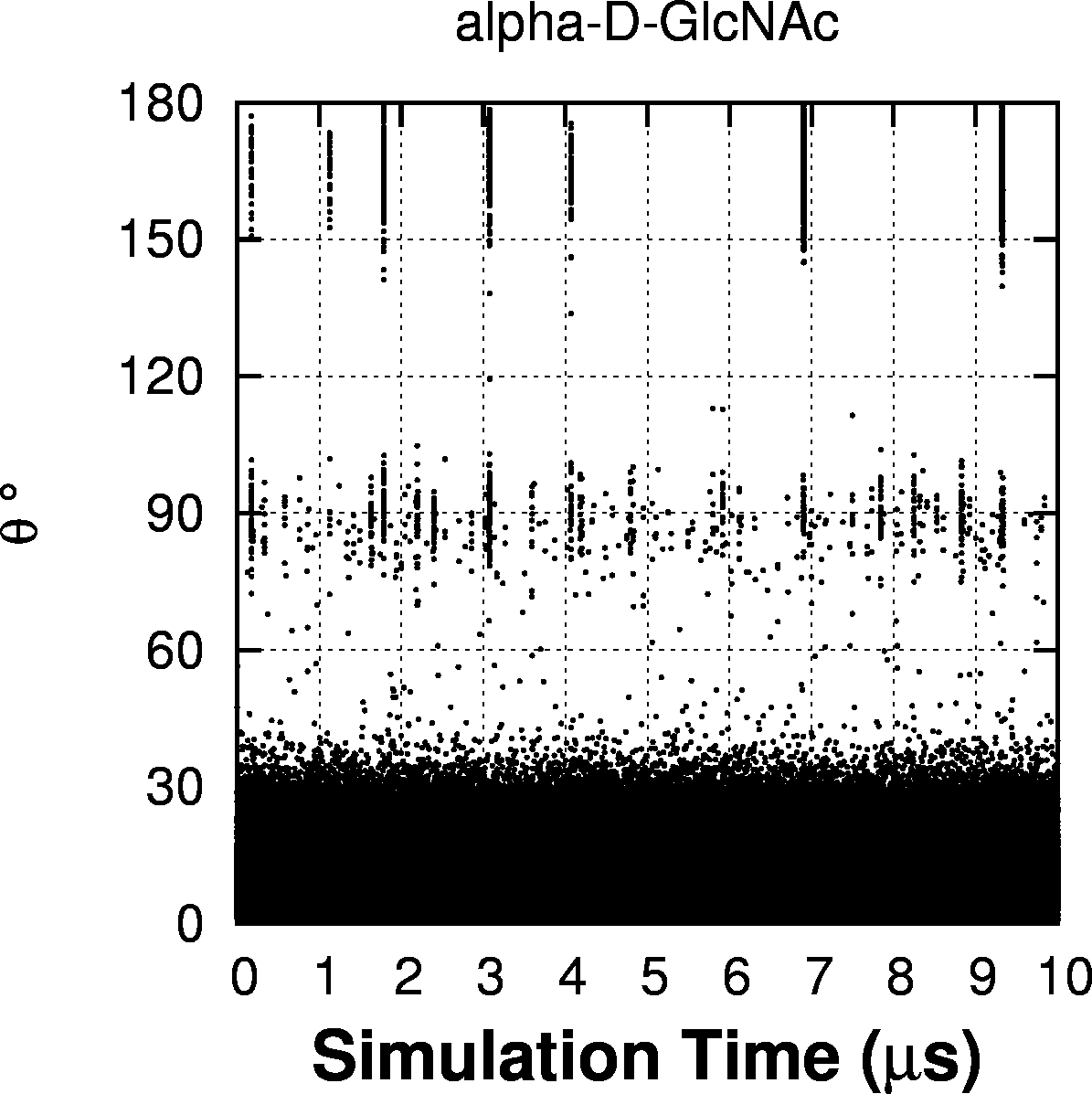
Simulation Time (μs)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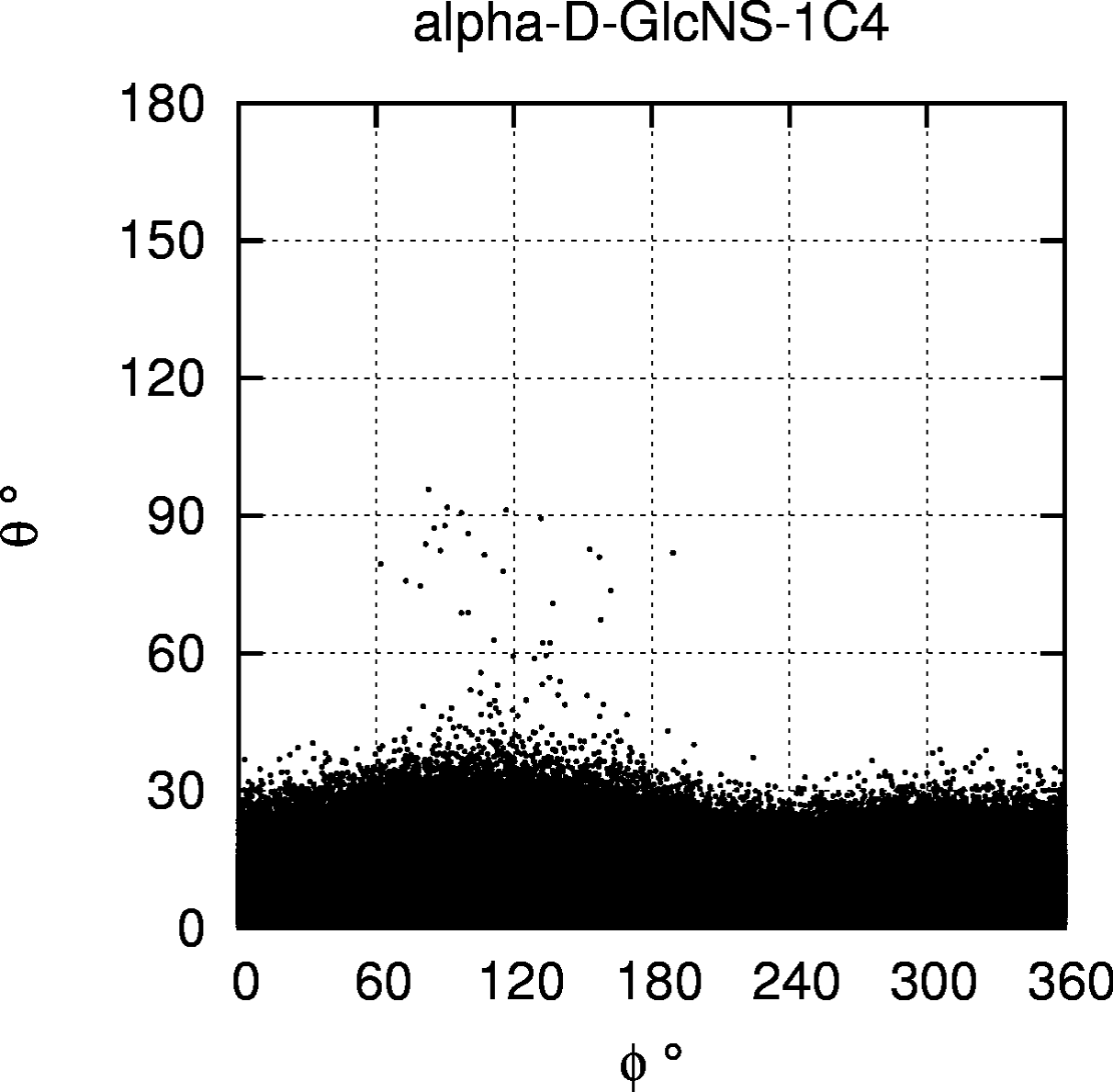
Simulation Time (μs)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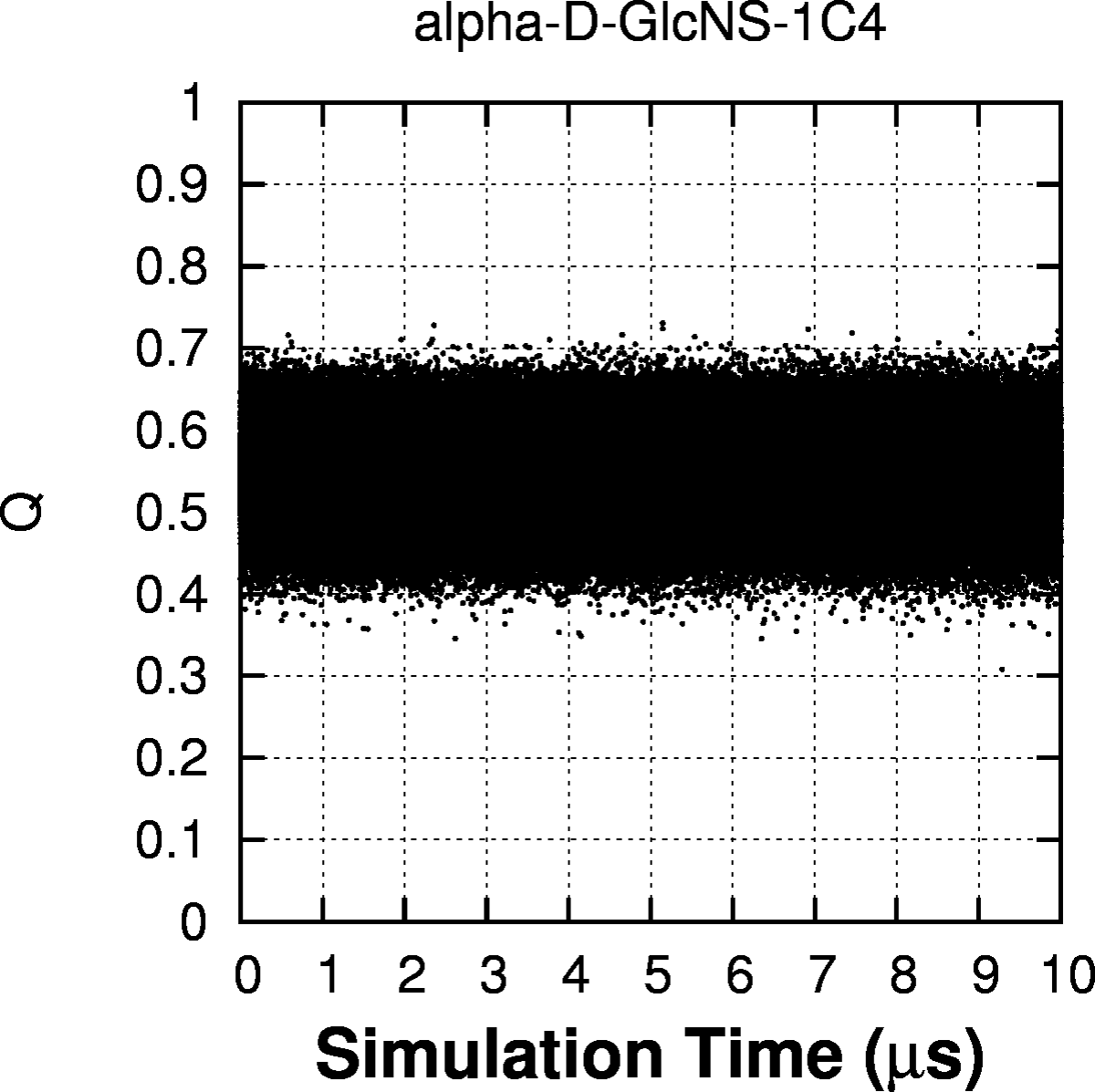
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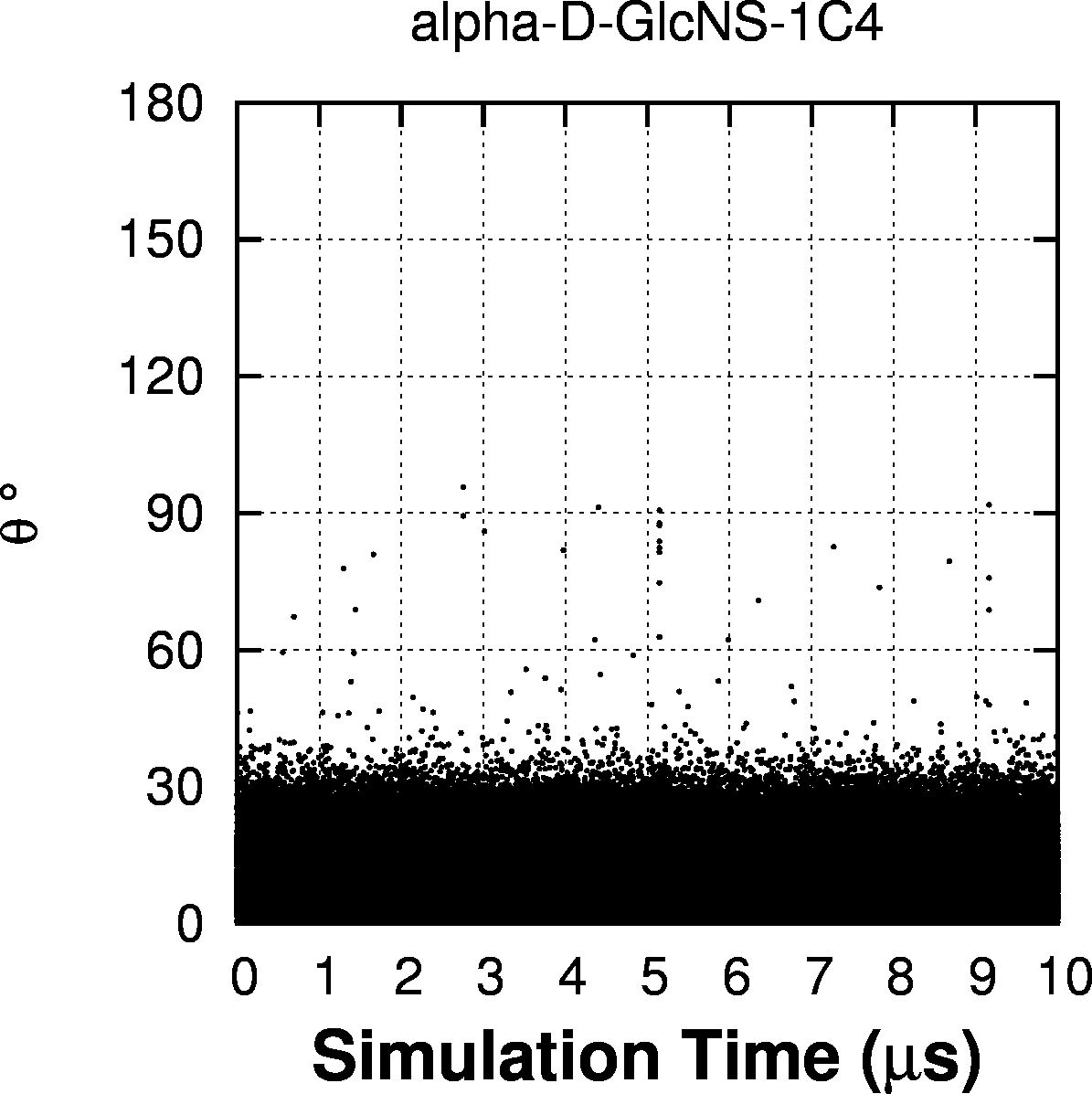
Simulation Time (μs)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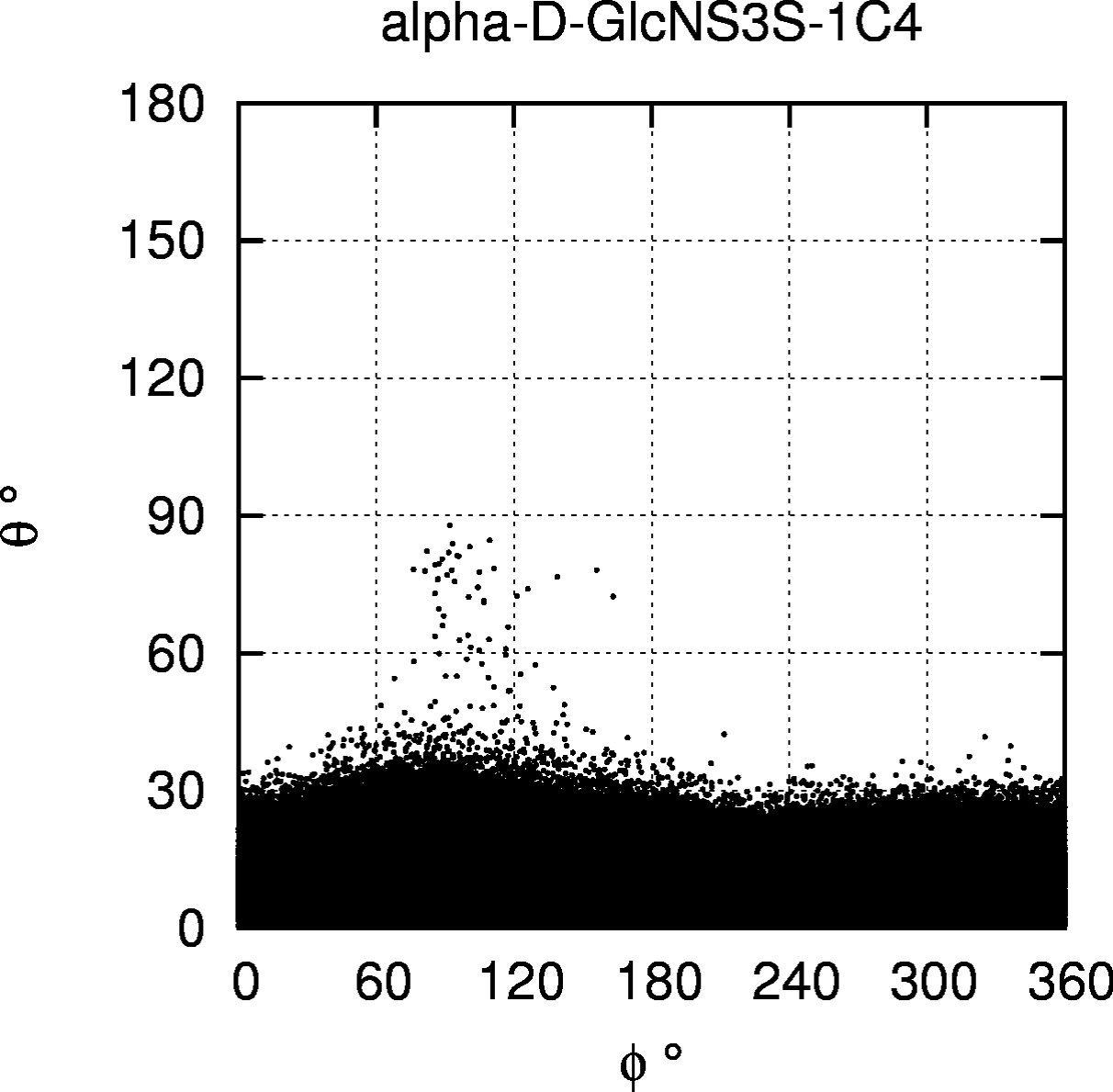
Simulation Time (μs)


alpha-D-GlcNS3S-1C4
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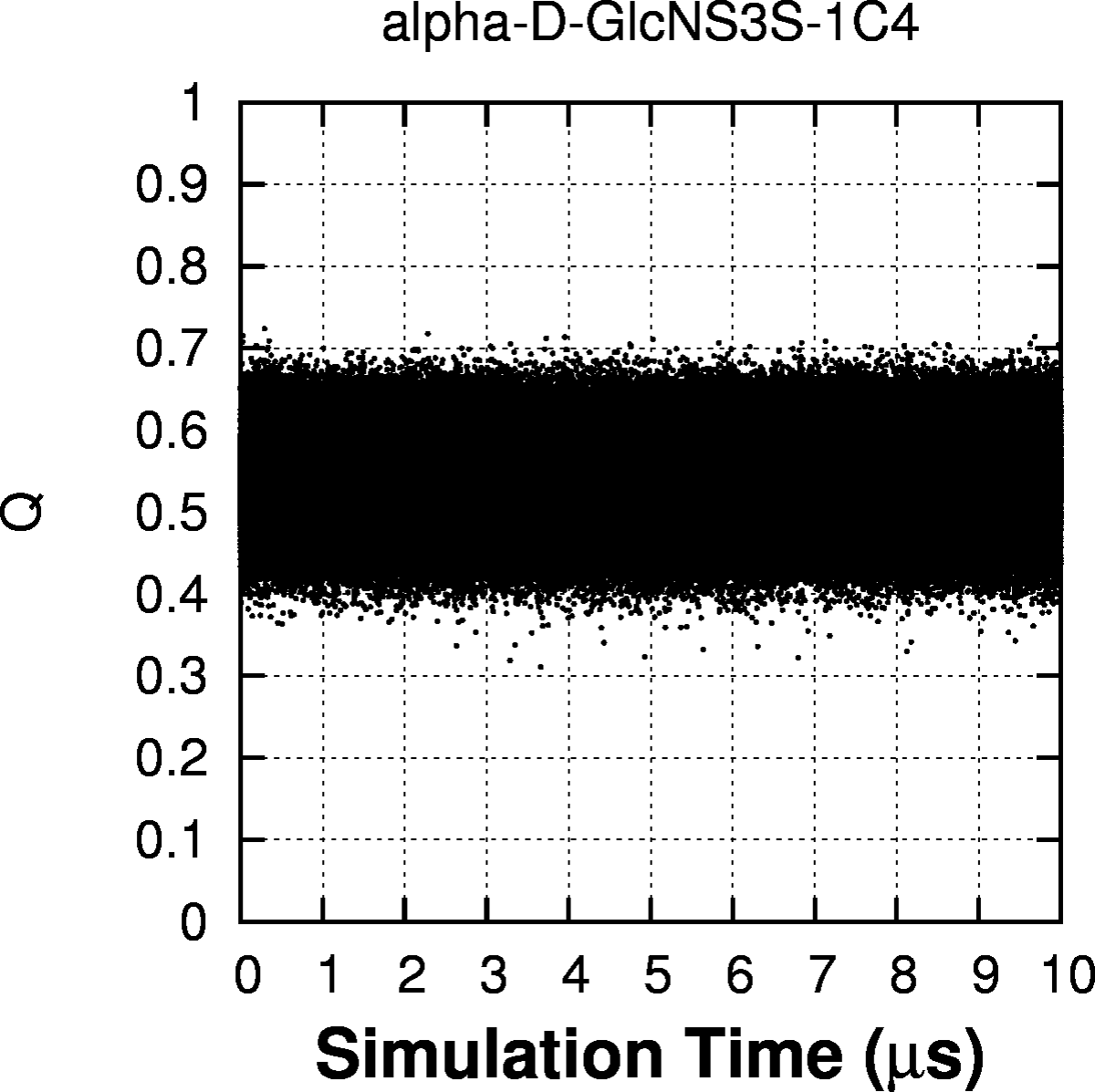
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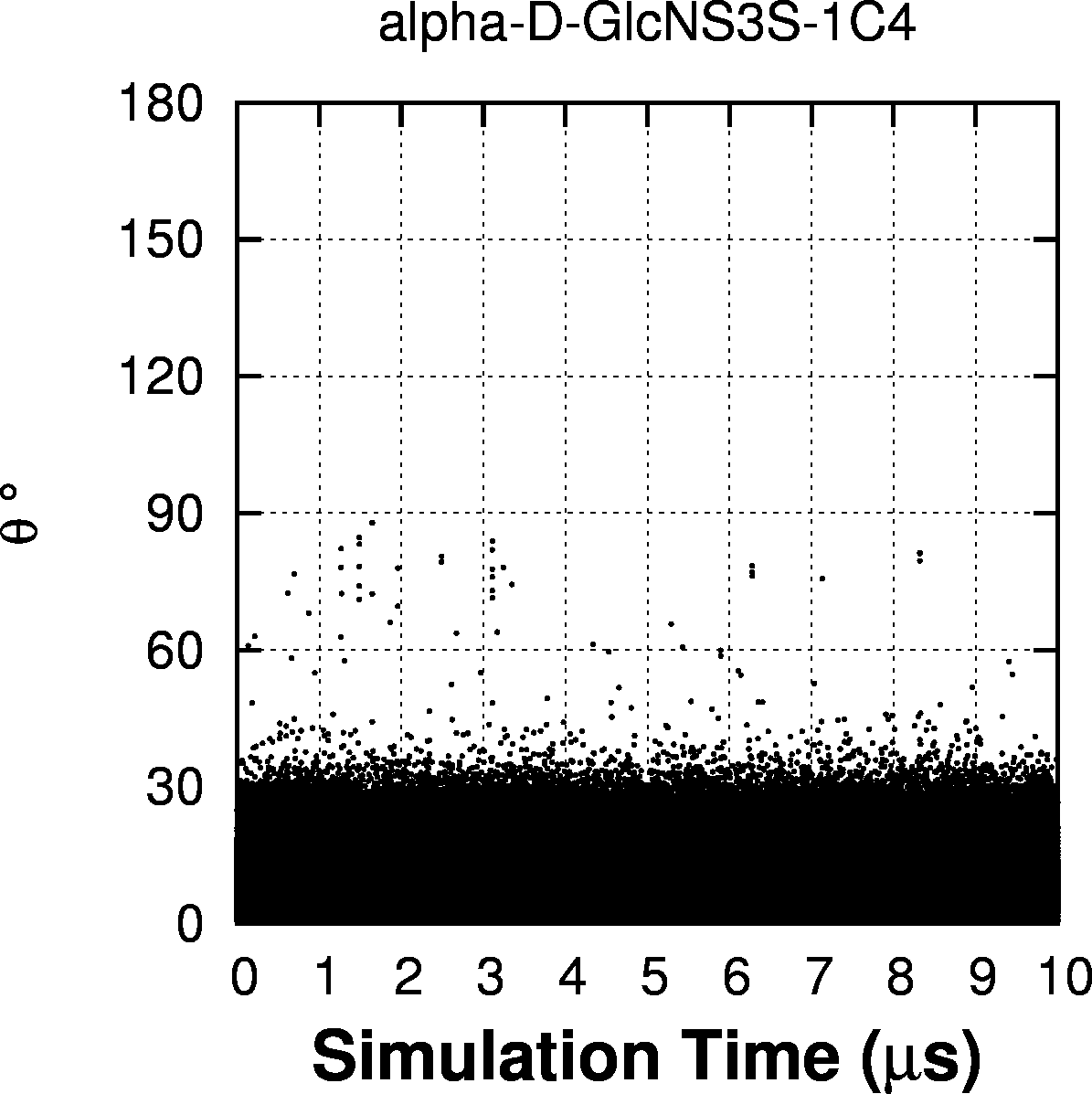
Simulation Time (μs)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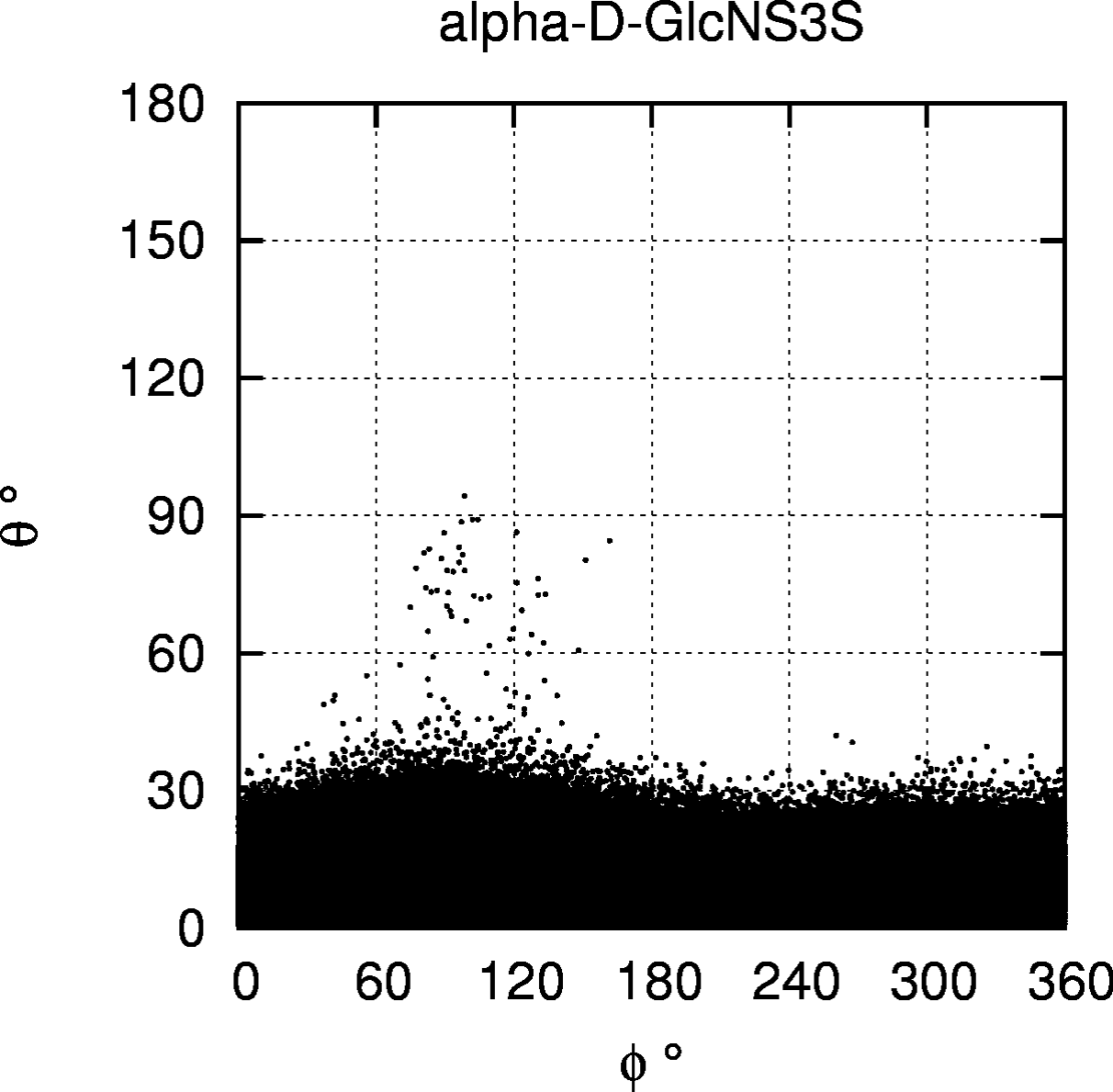
Simulation Time (μs)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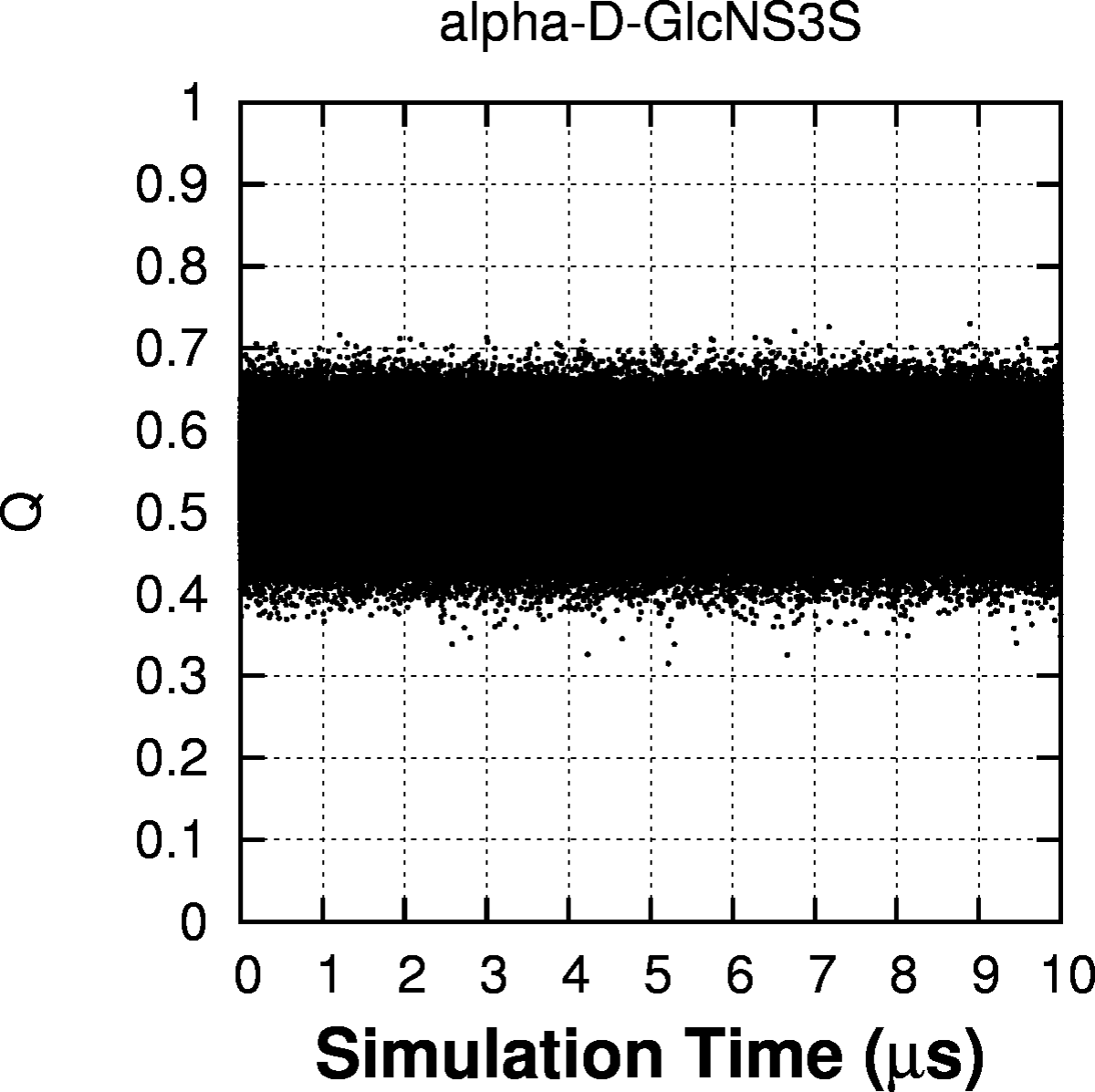
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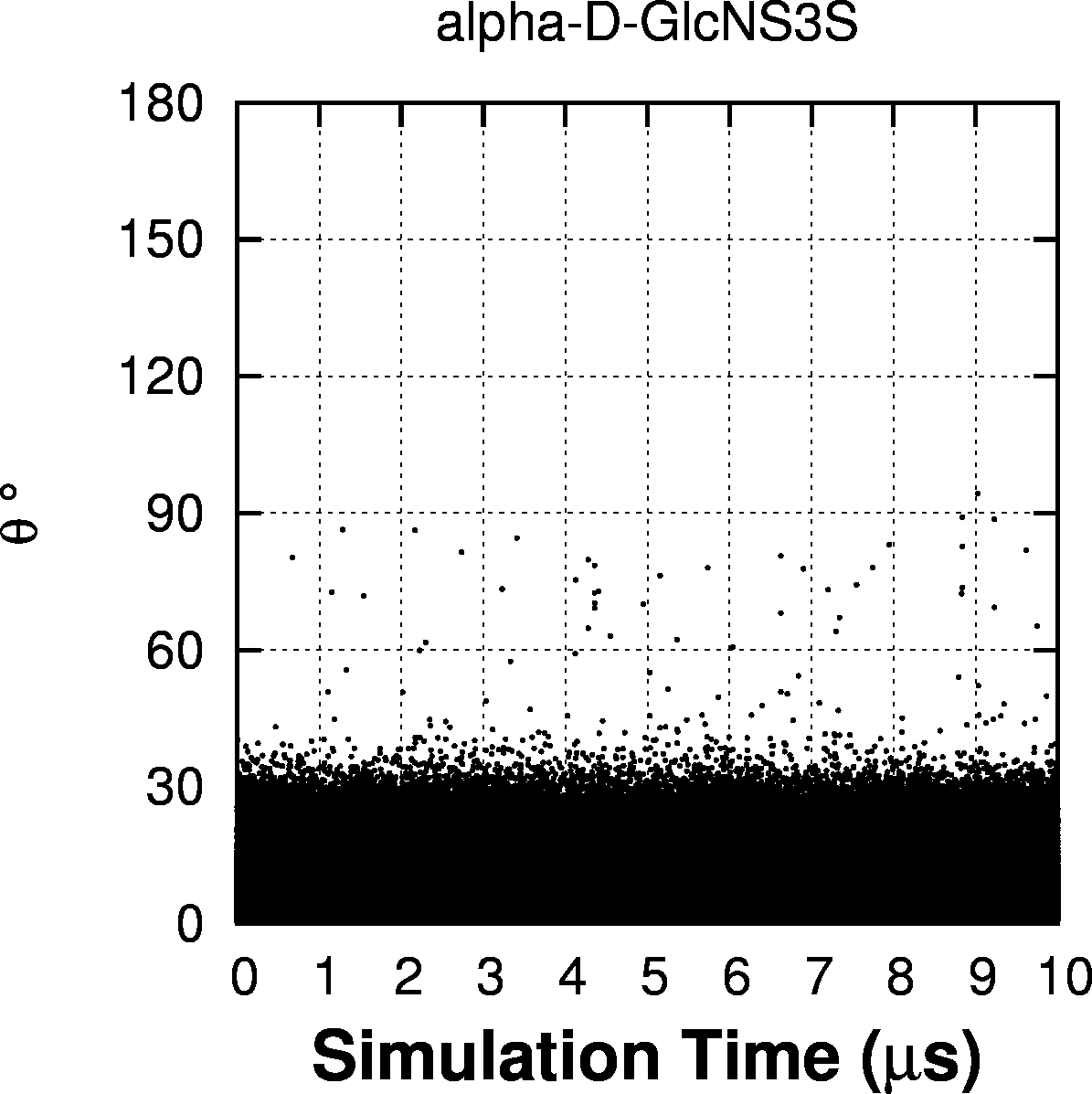
Simulation Time (μs)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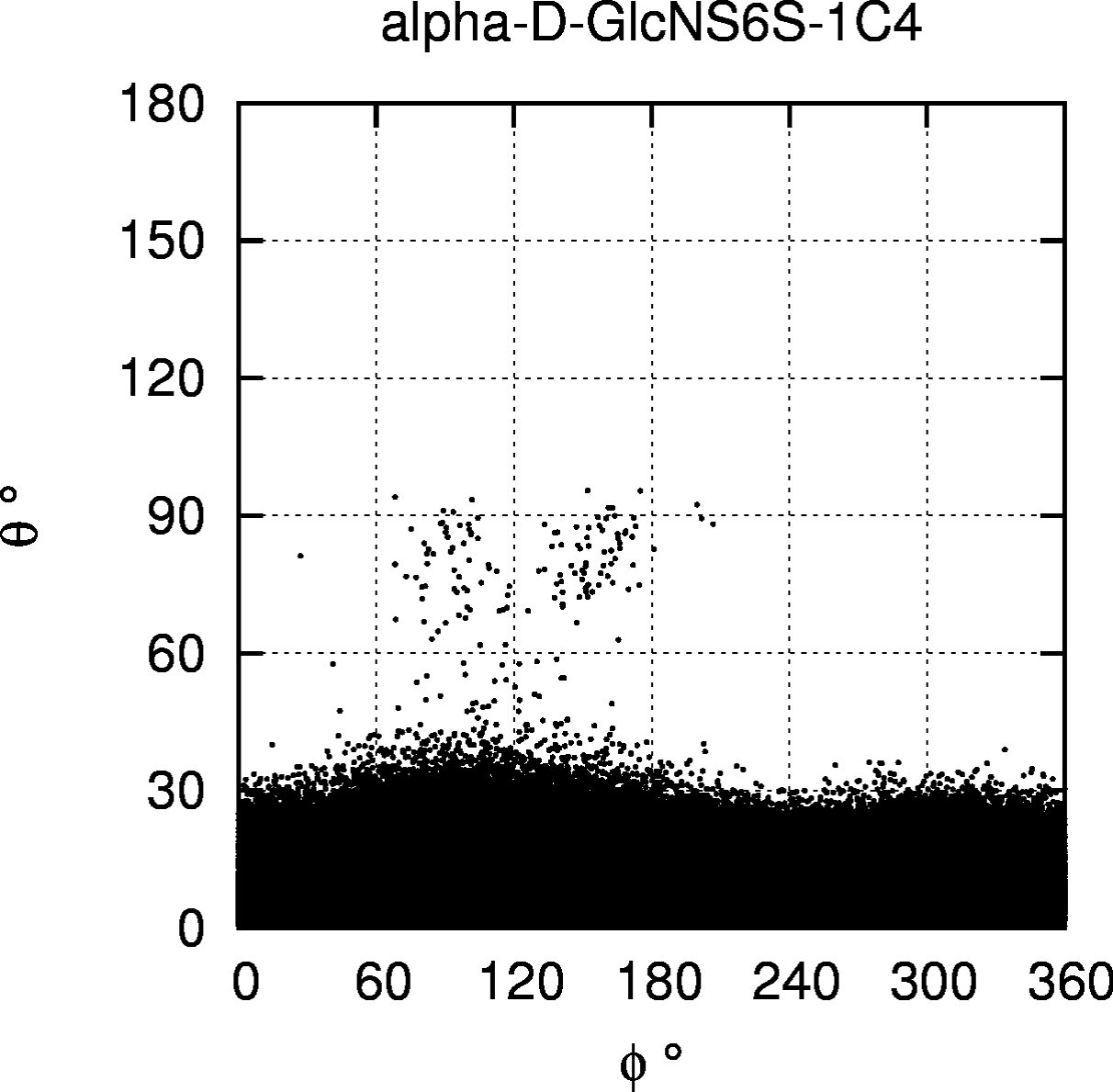
Simulation Time (μs)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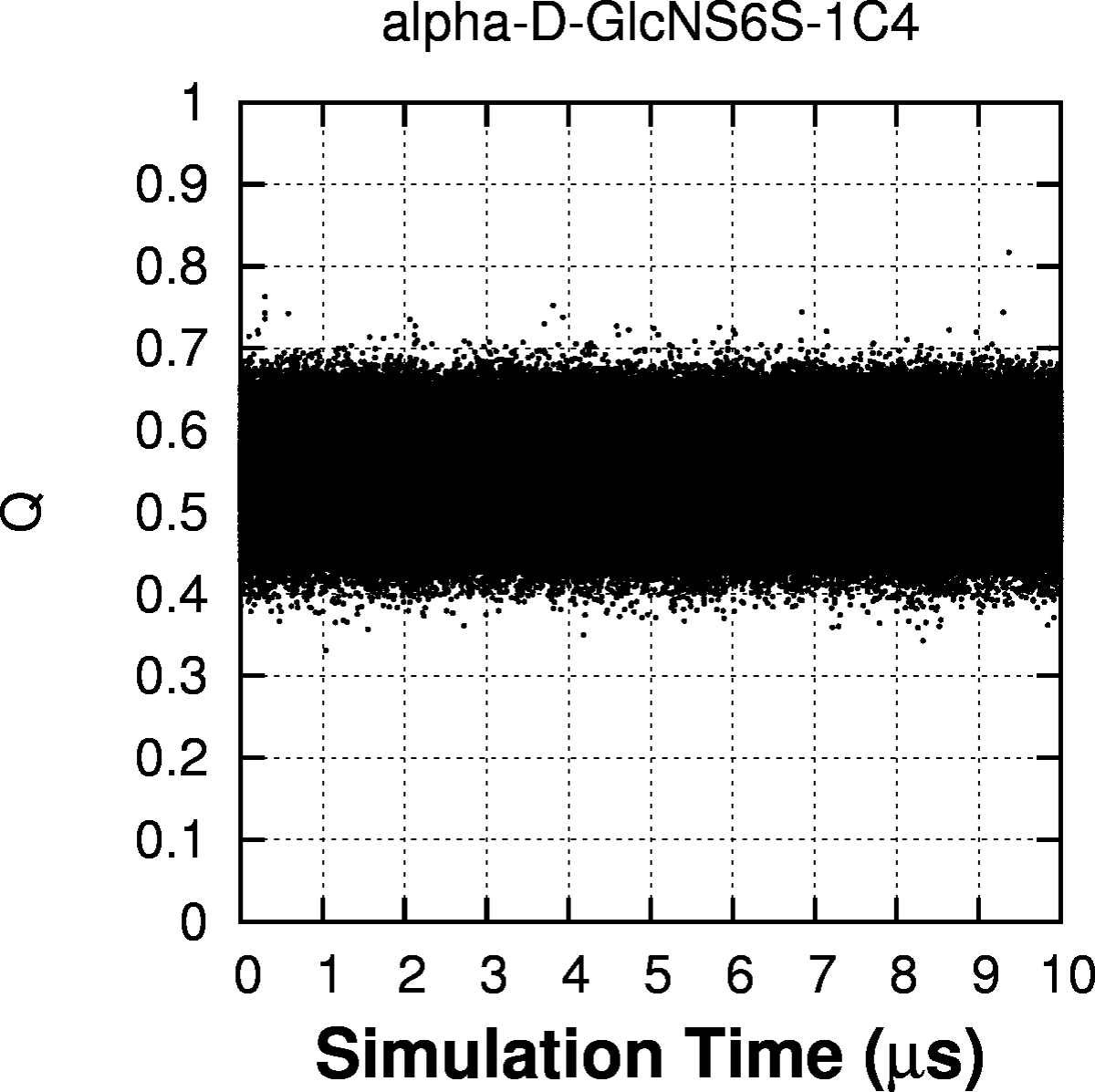
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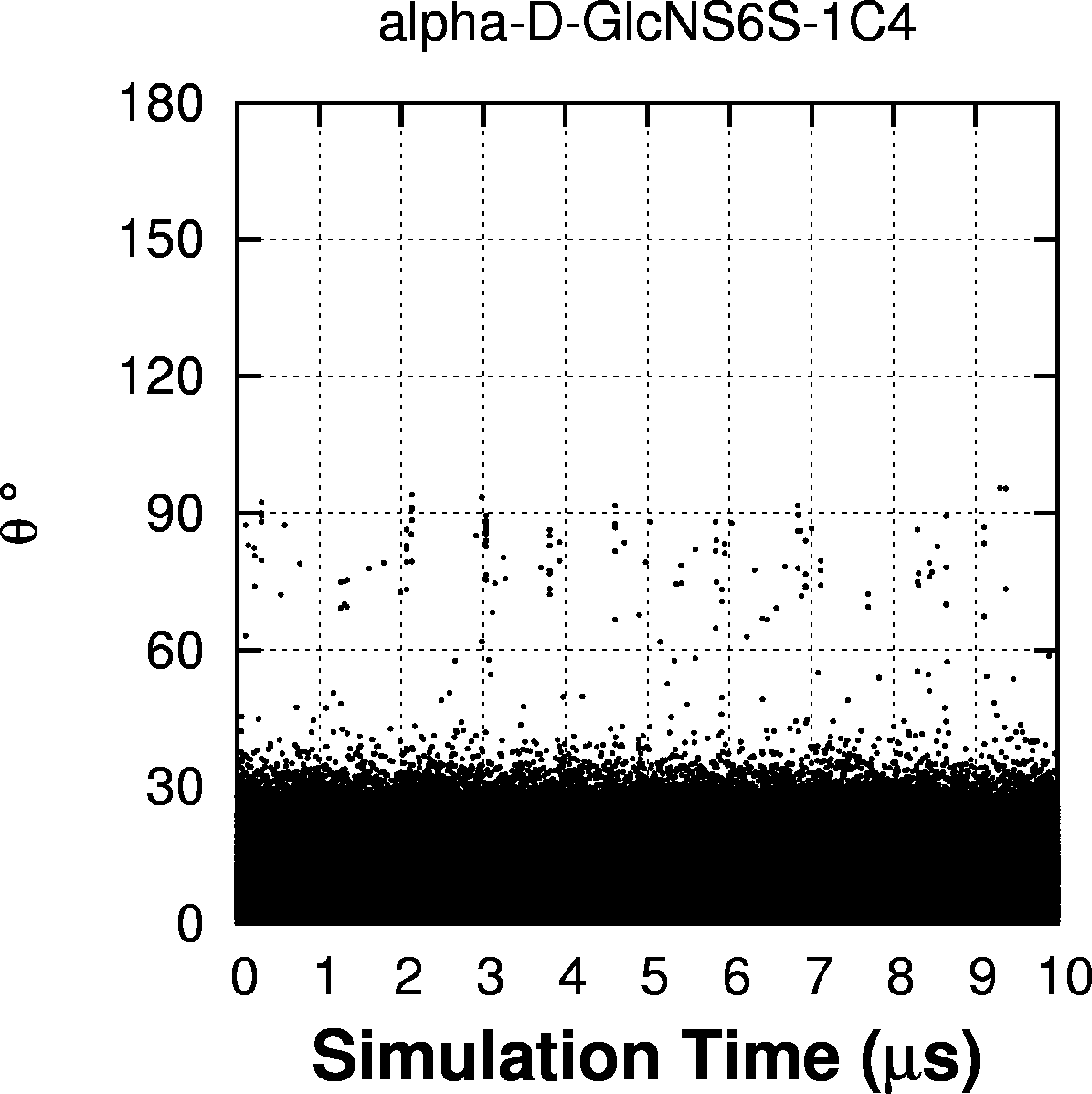
Simulation Time (μs)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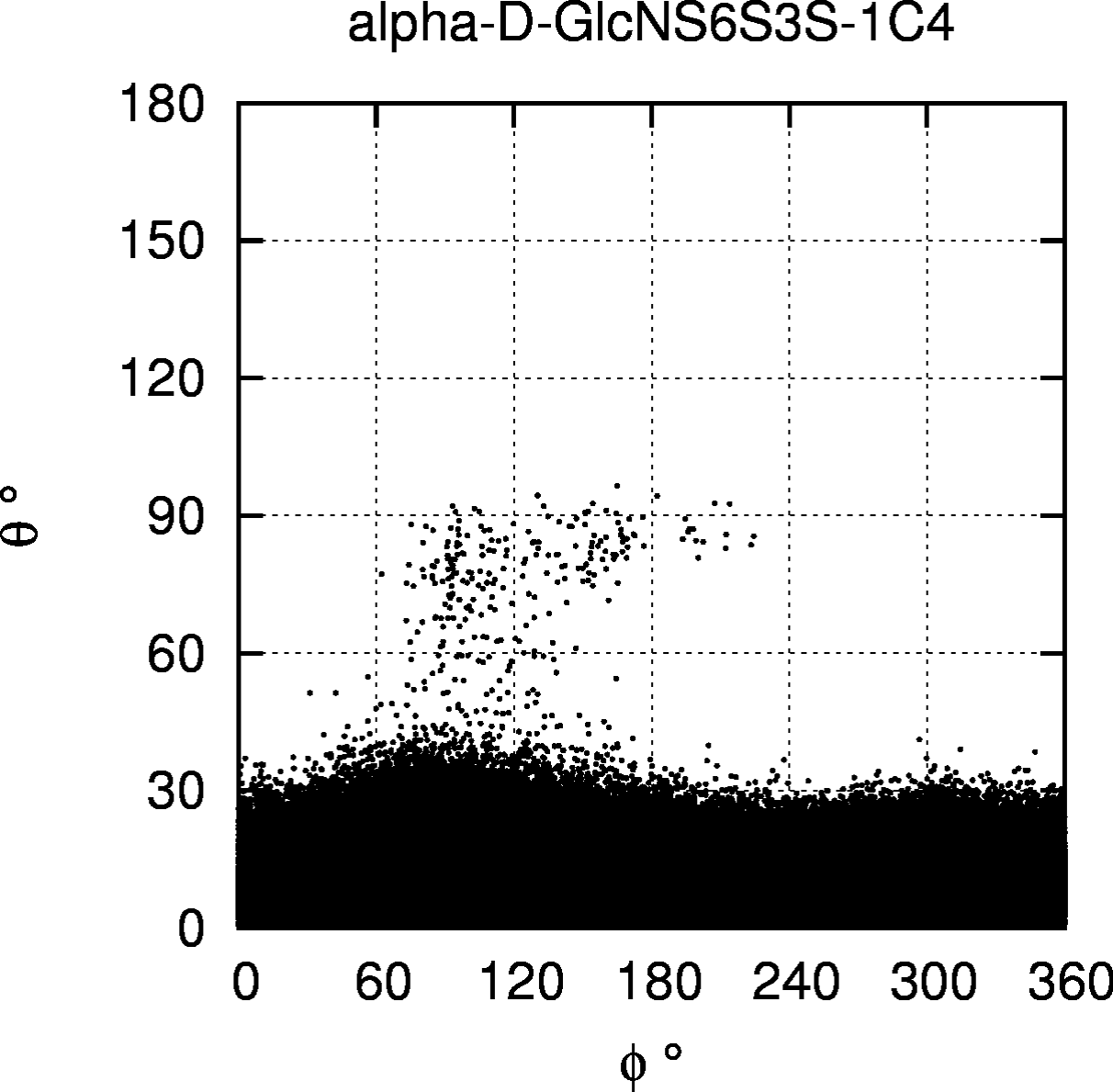
Simulation Time (μs)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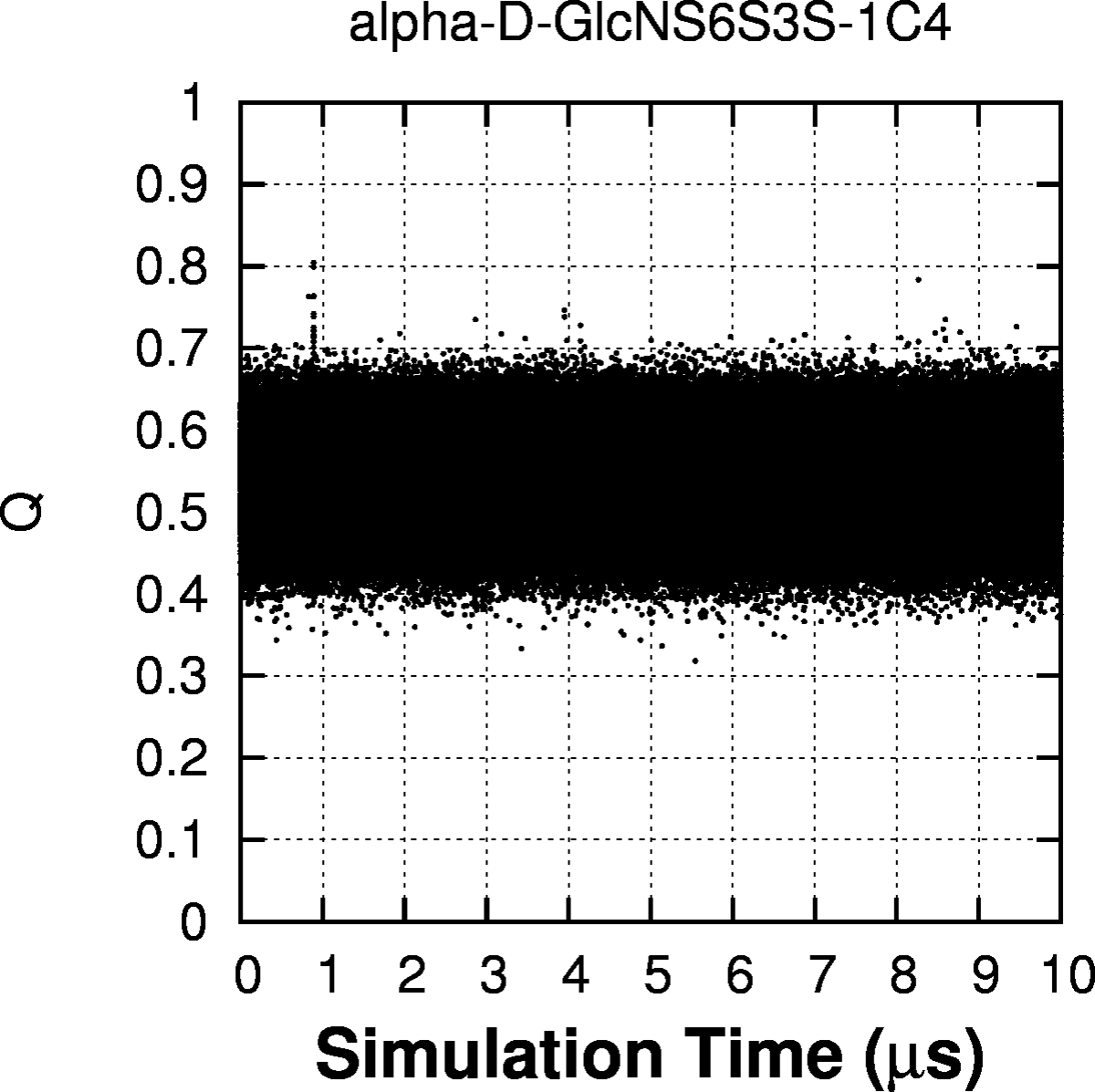
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Q
1
0.9
0.8
0.7
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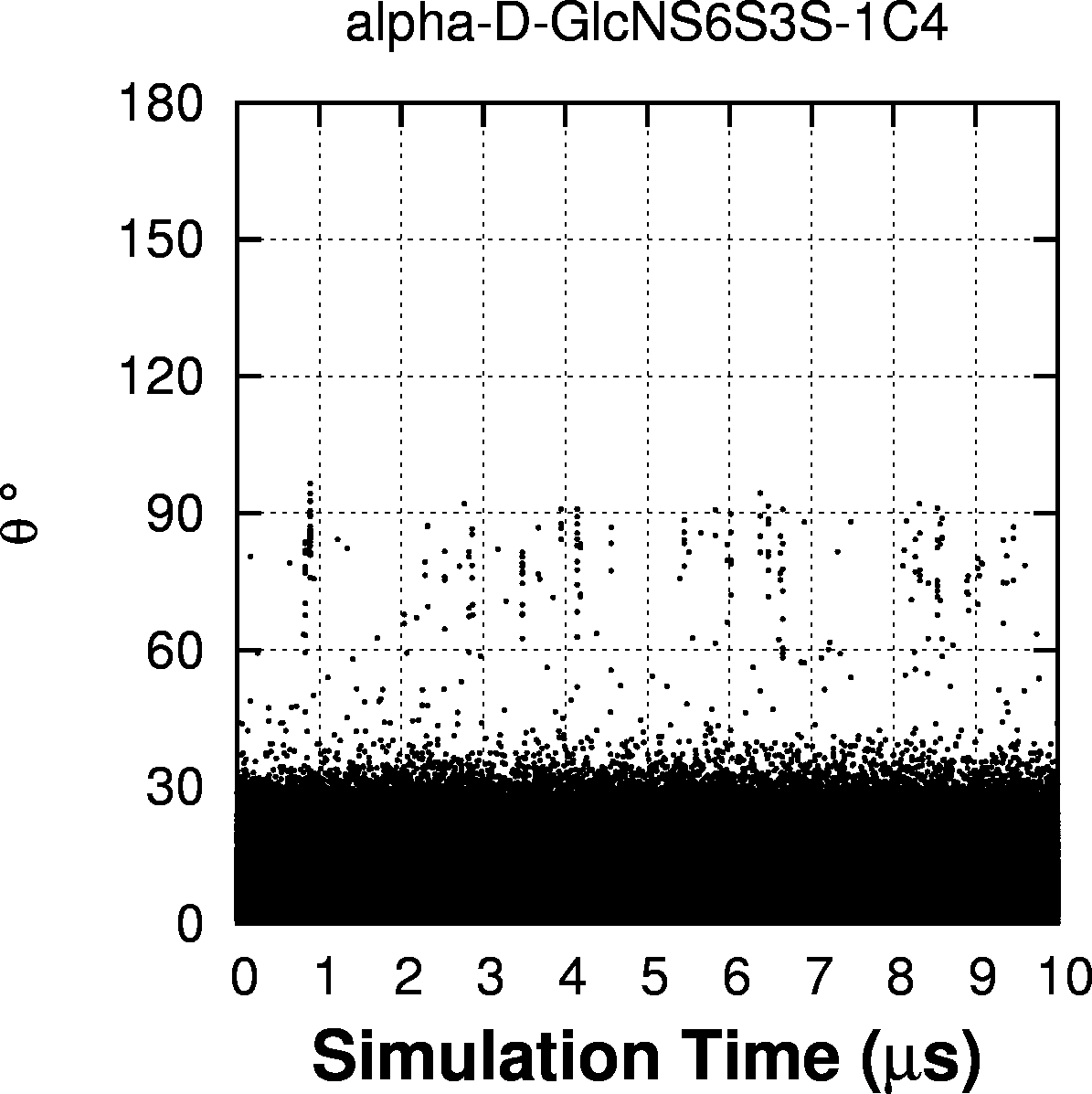
0 1 2 3 4 5 6 7 8 9 10
Simulation Time (μs)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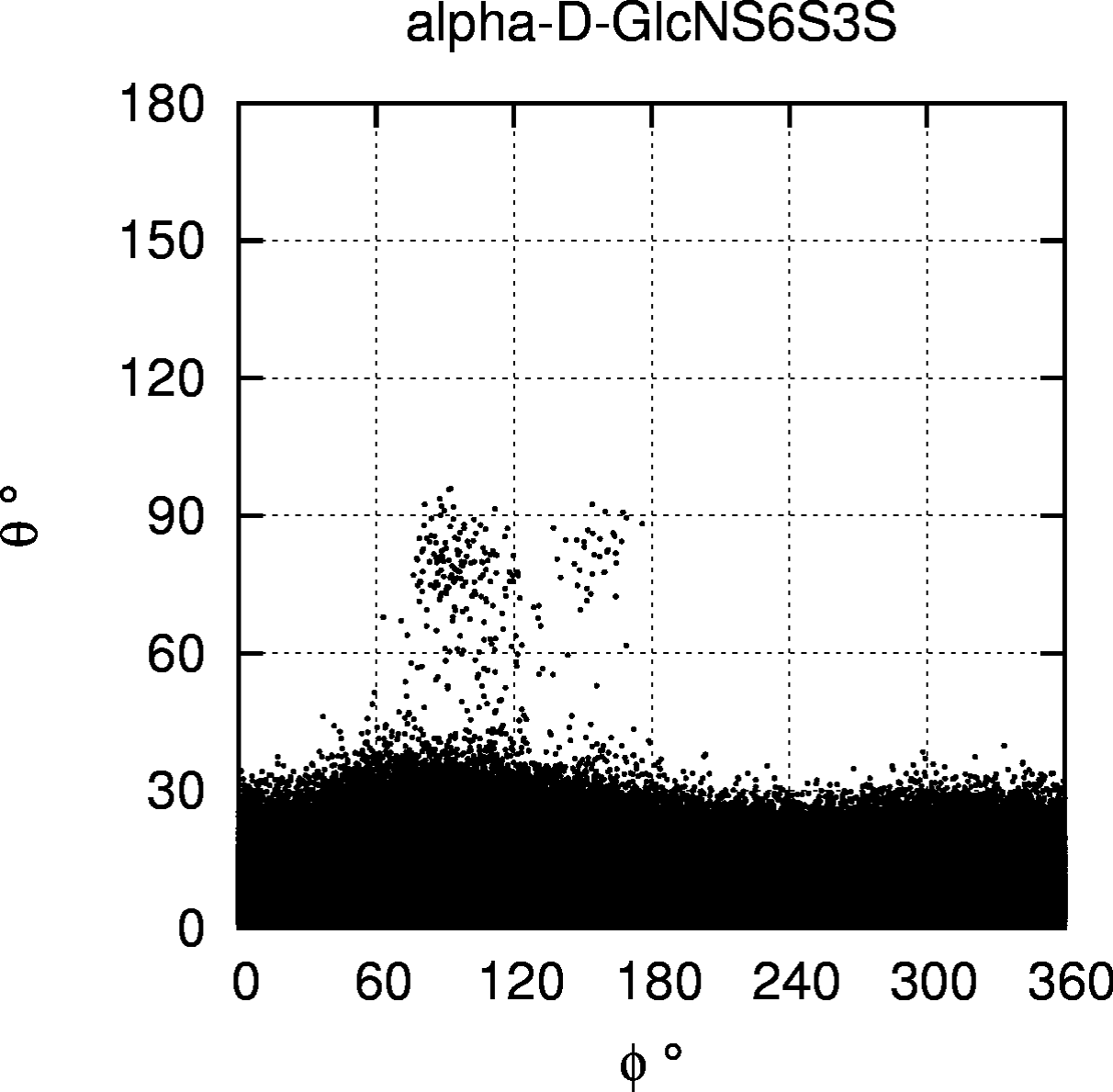
Simulation Time (μs)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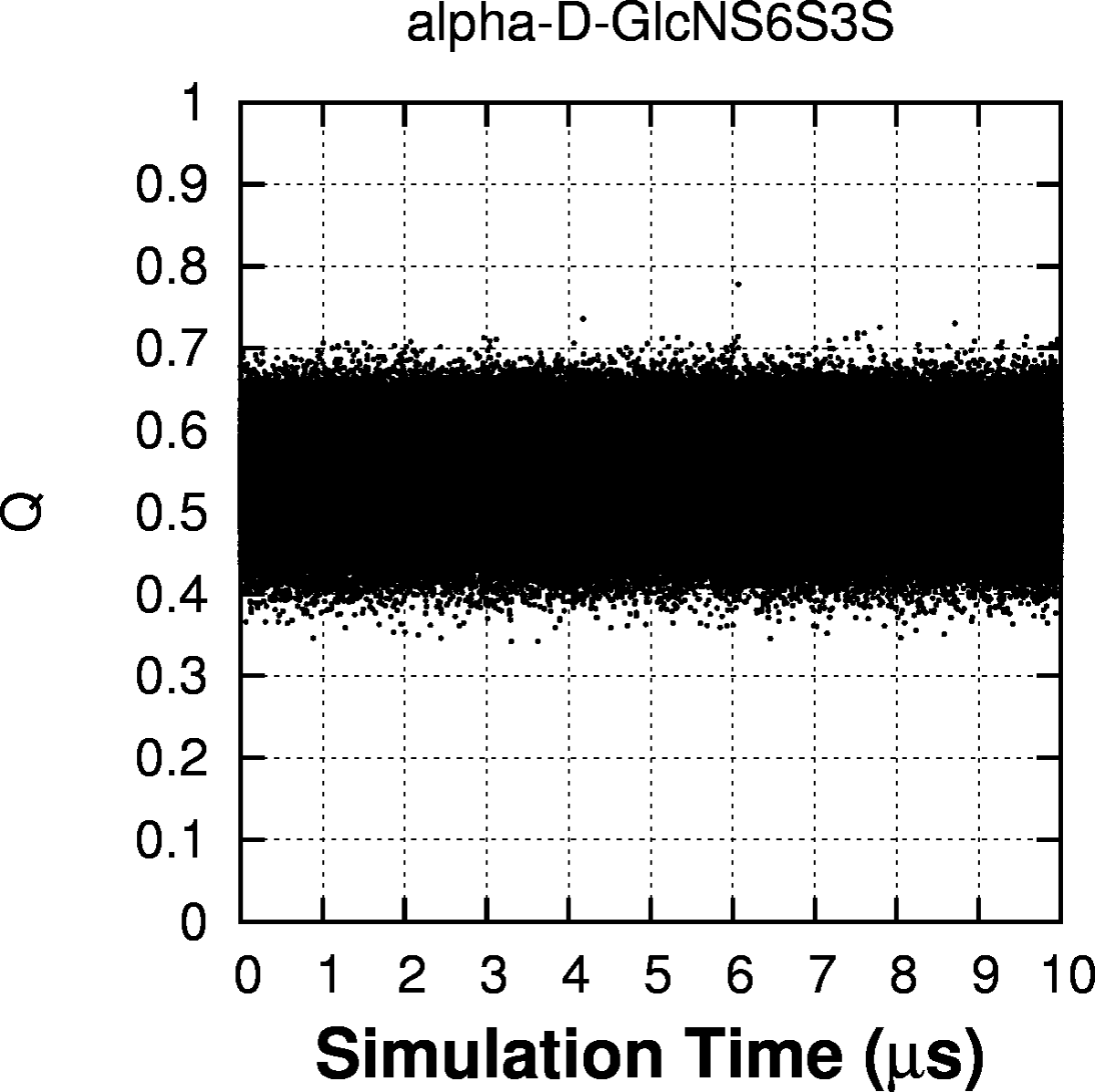
ϕ °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Q
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
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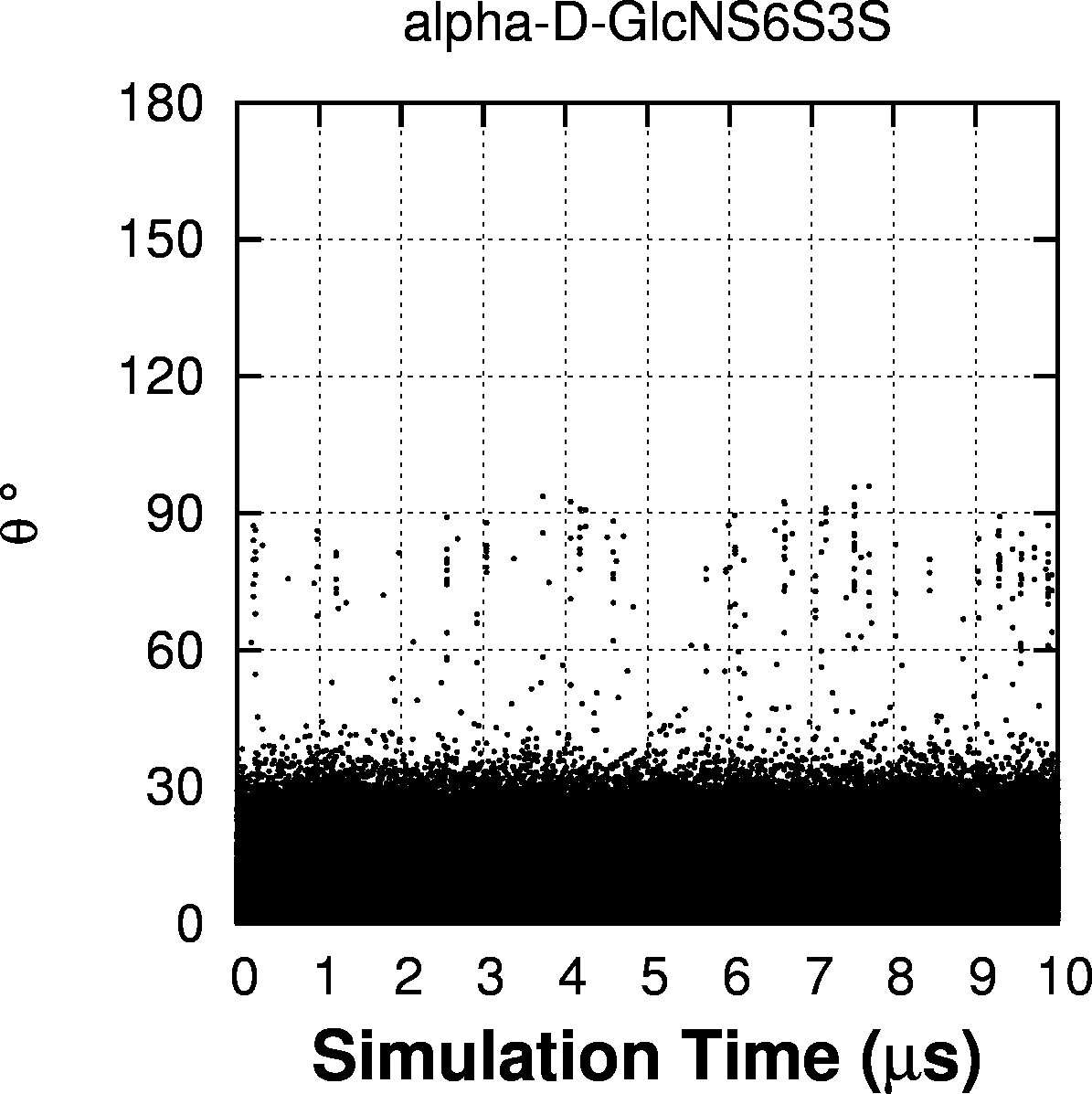
0 1 2 3 4 5 6 7 8 9 10
Simulation Time (μs)


alpha-D-GlcNS6S3S
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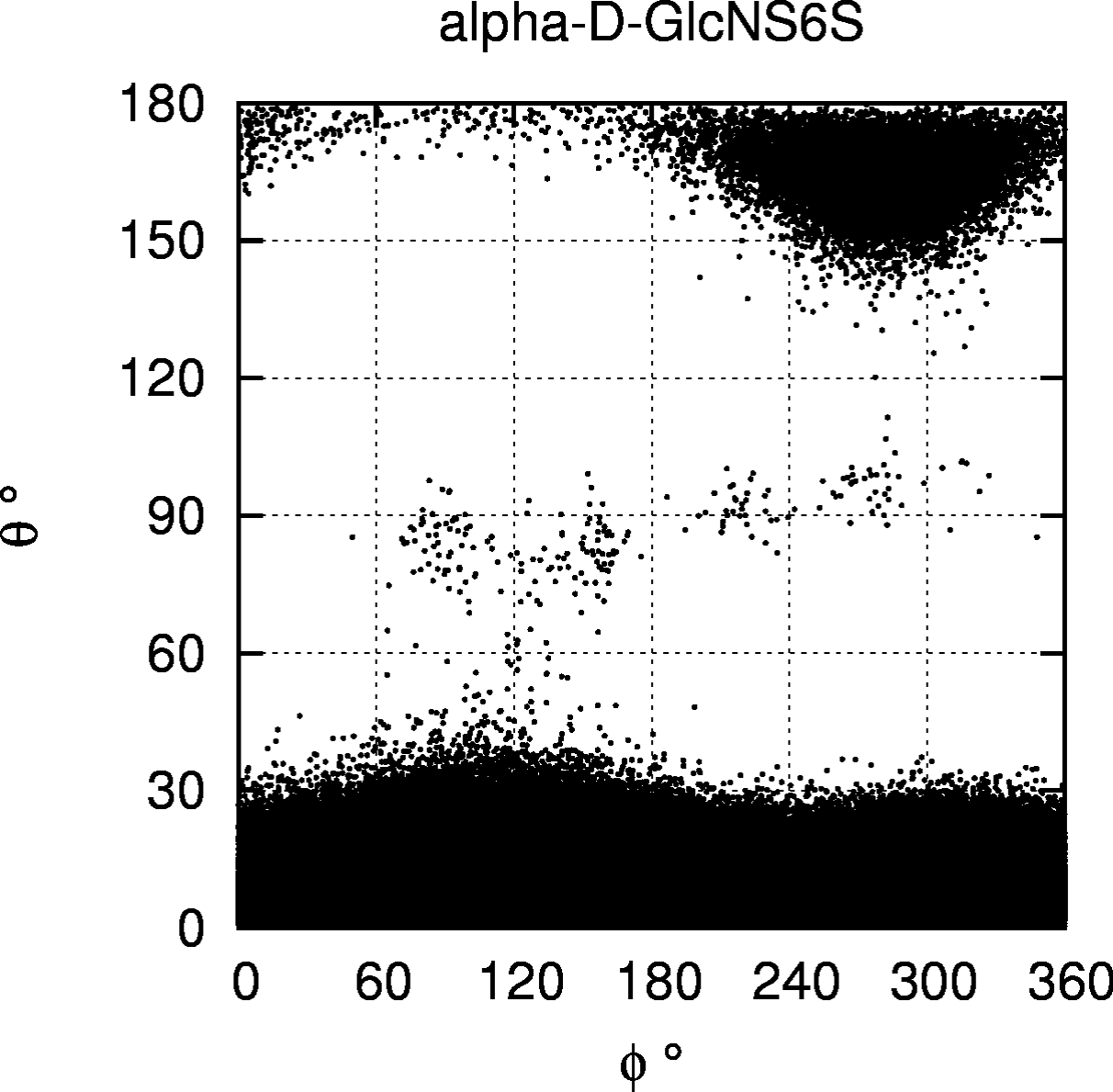
Simulation Time (μs)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θ °
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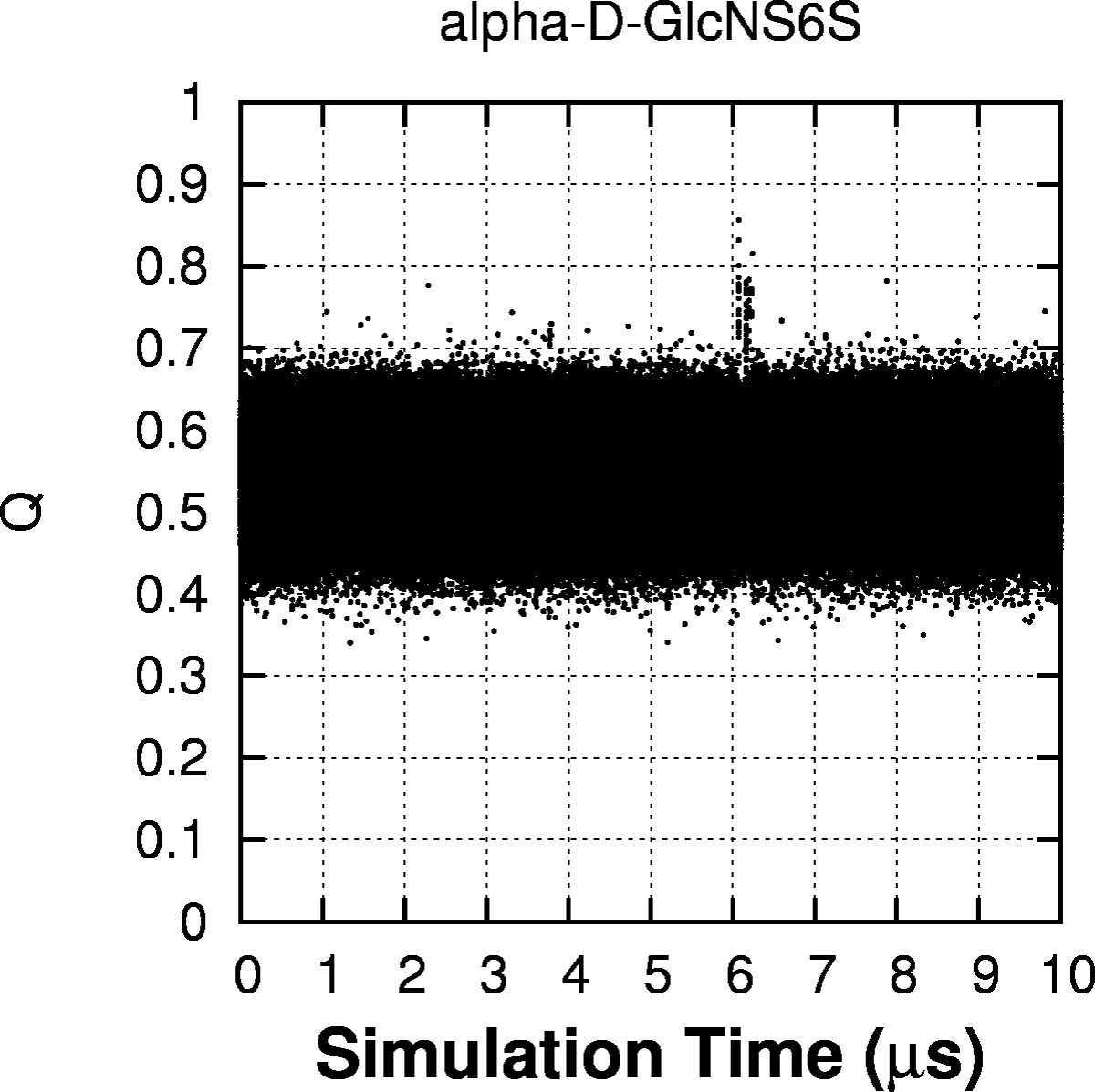
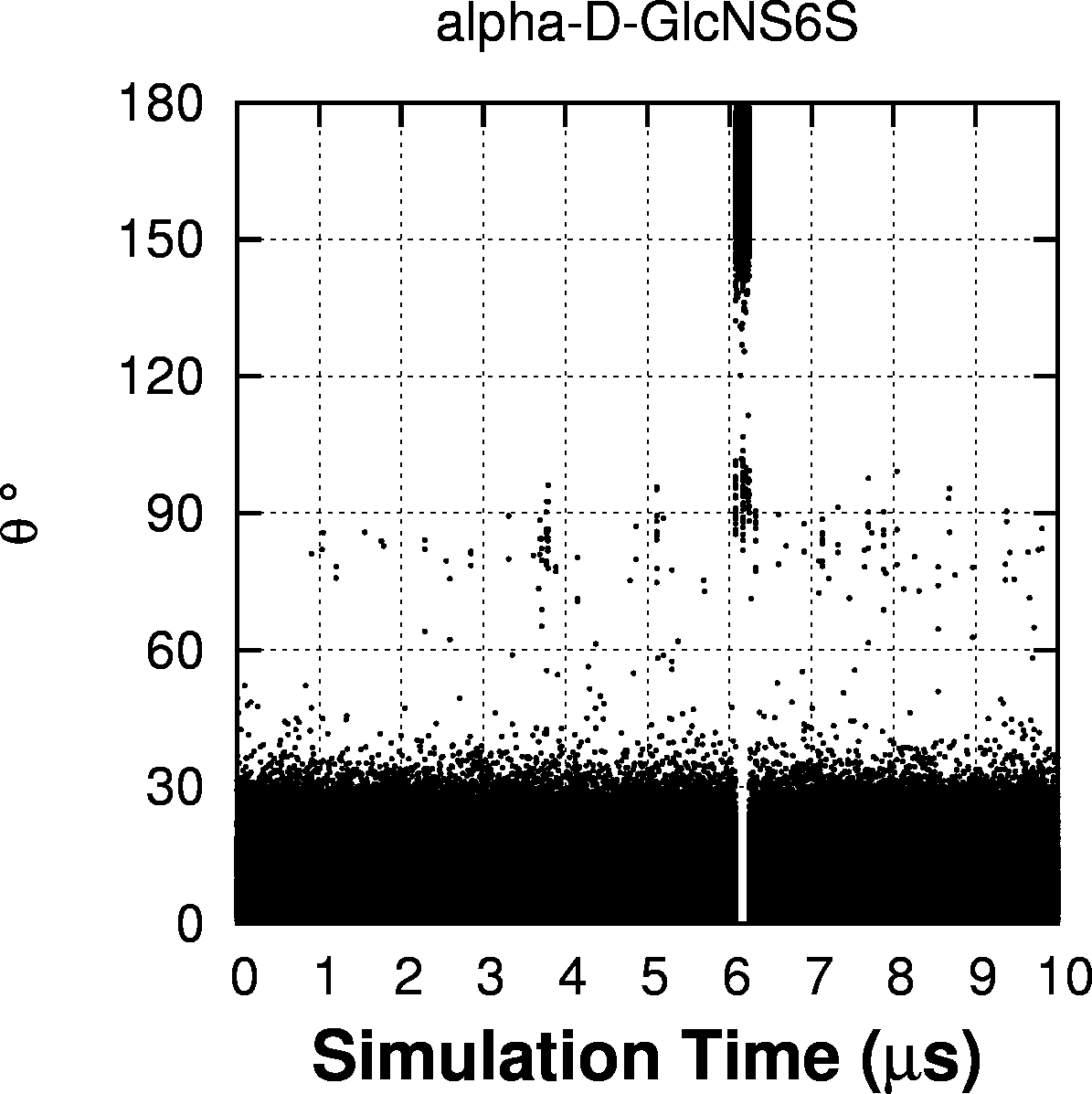
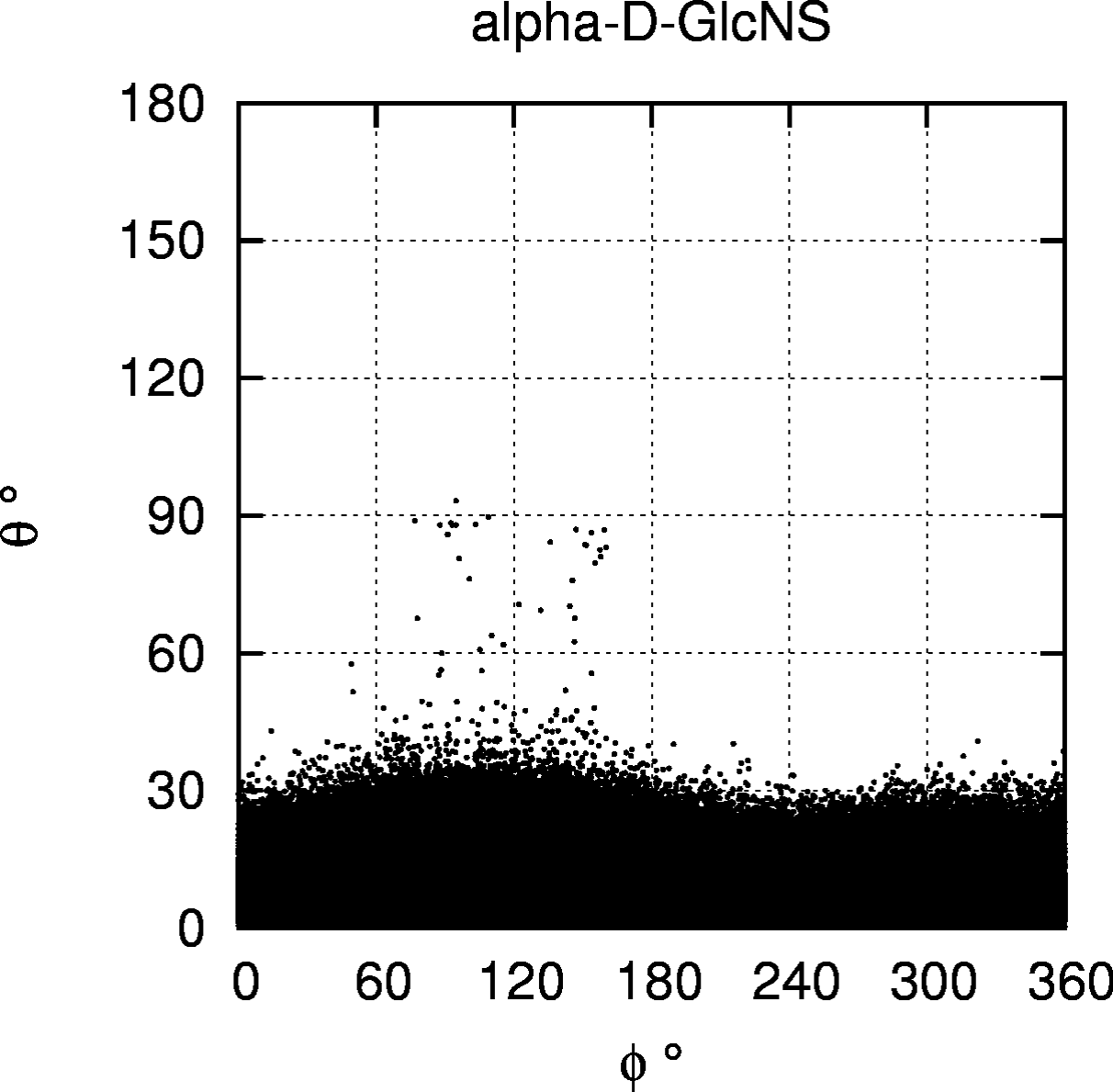
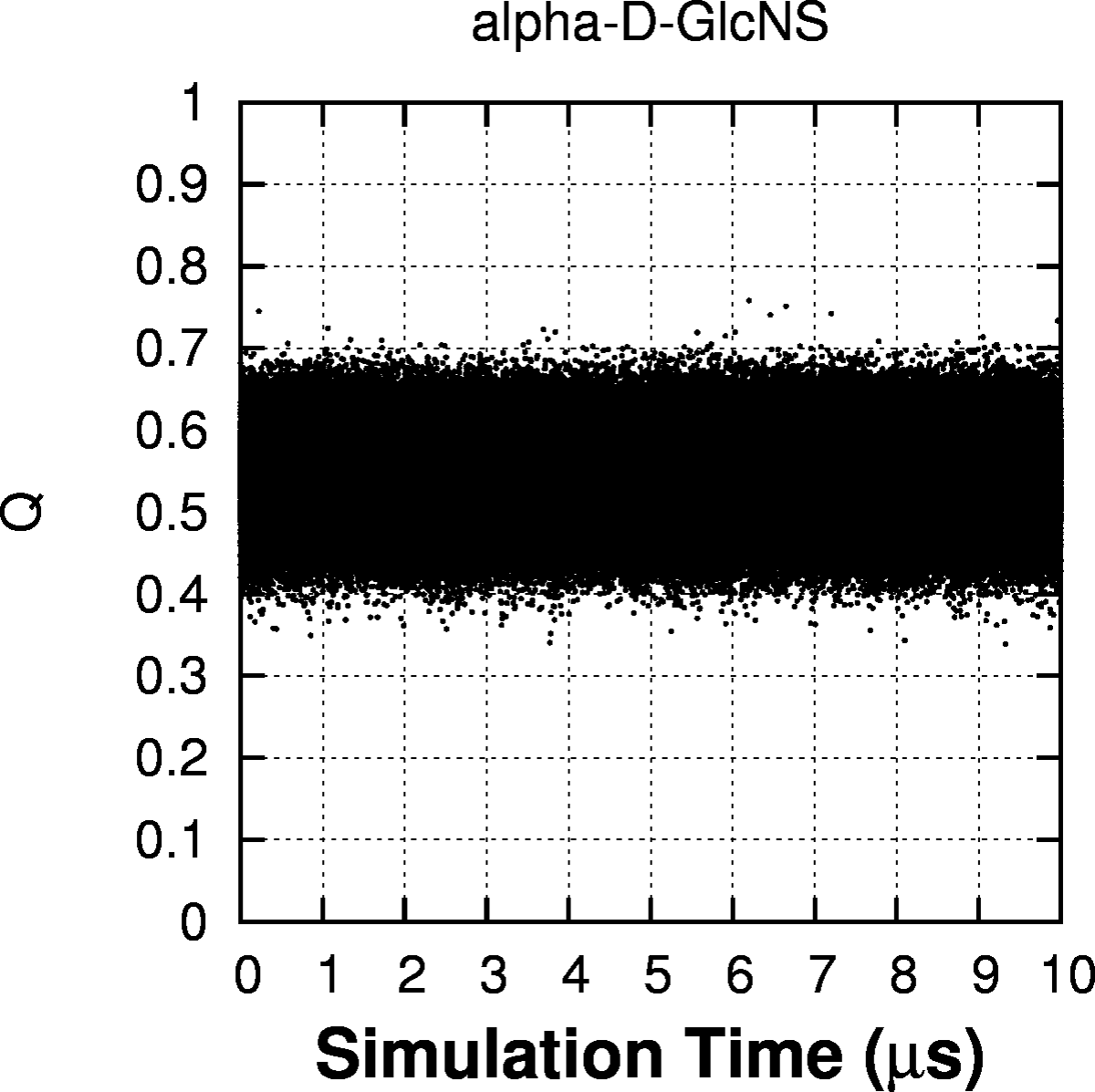
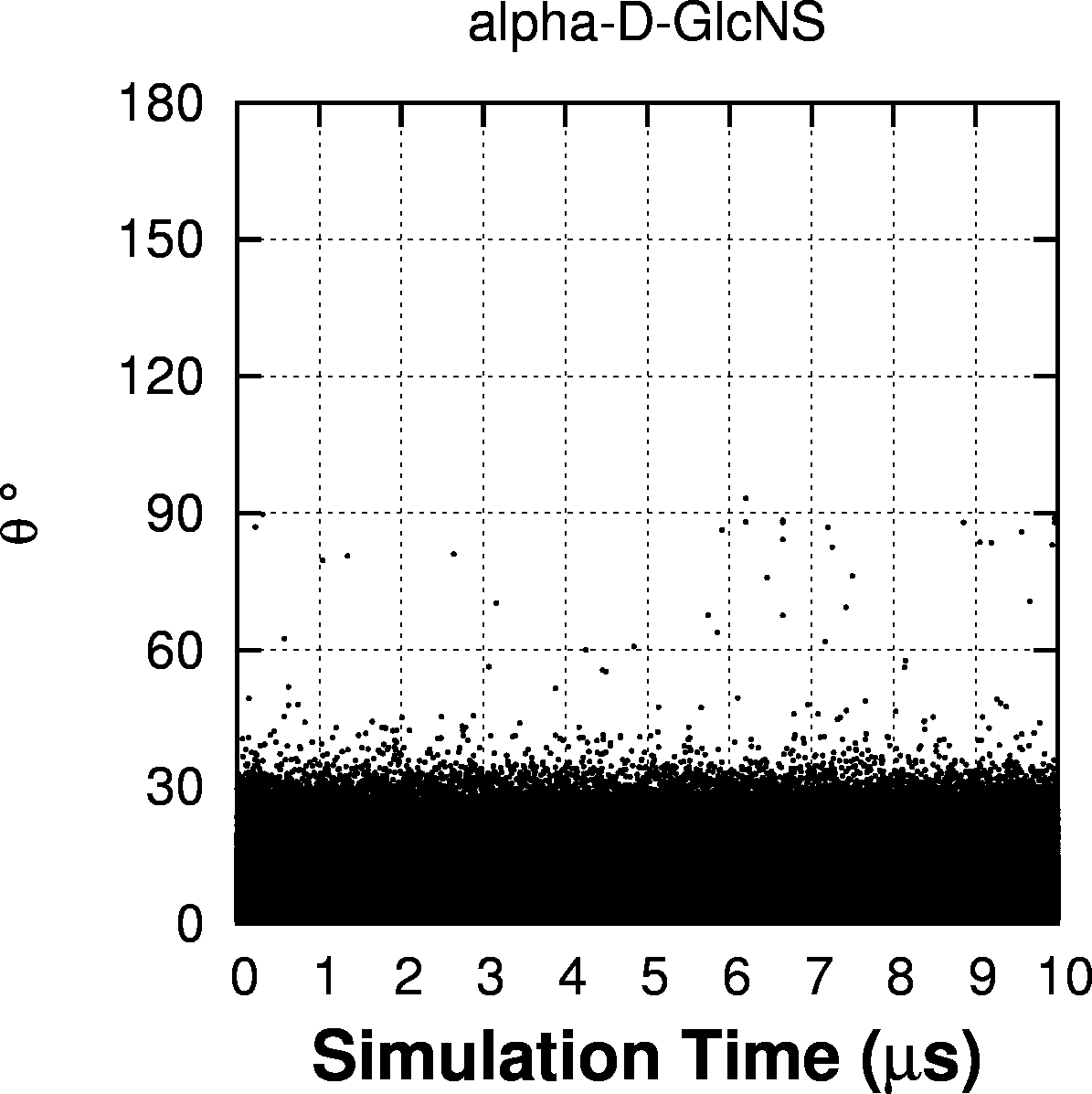
ϕ °

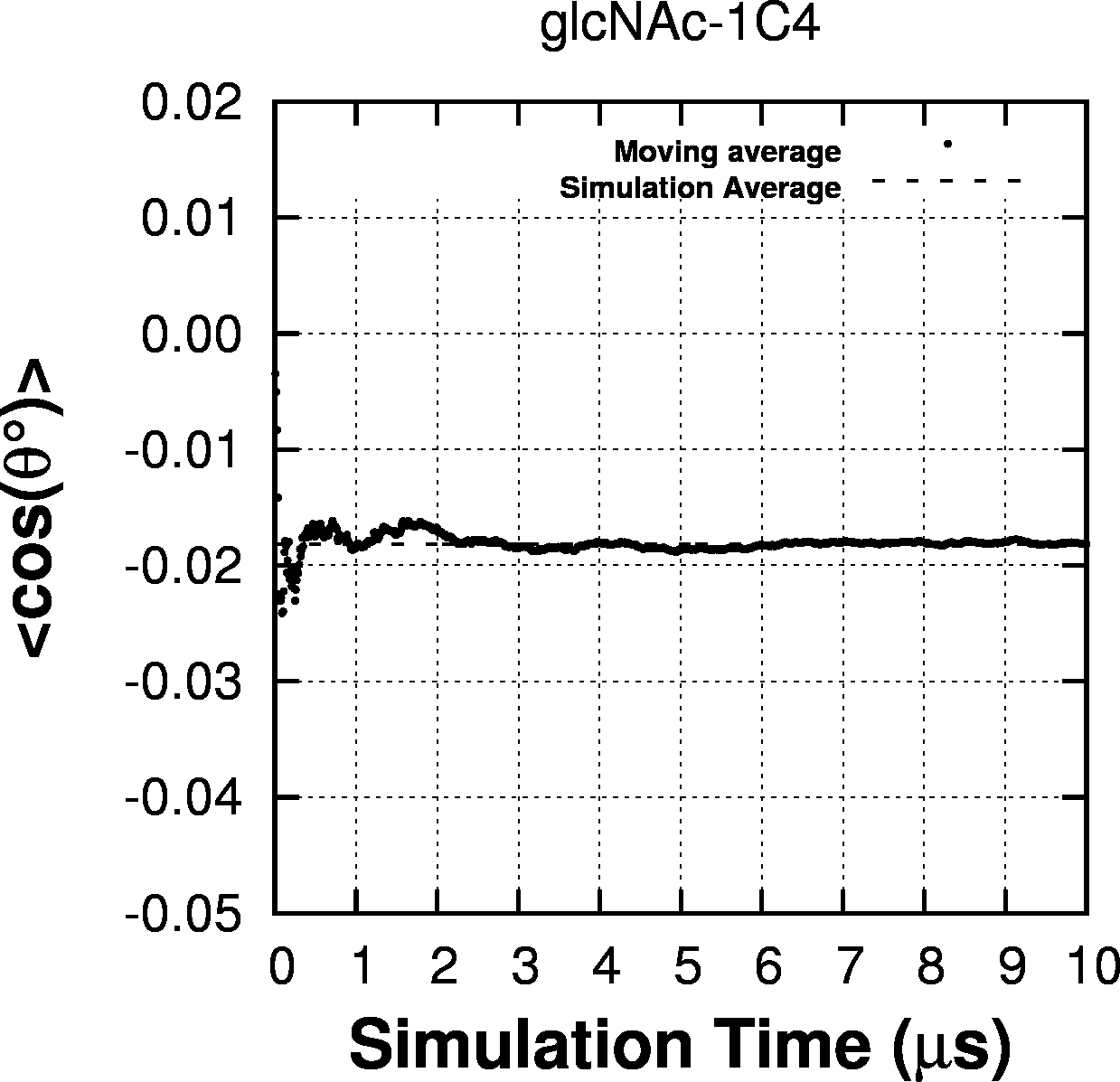

alpha-D-GlcNS6S
Q
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0 1 2 3 4 5 6 7 8 9 10
Simulation Time (μs)

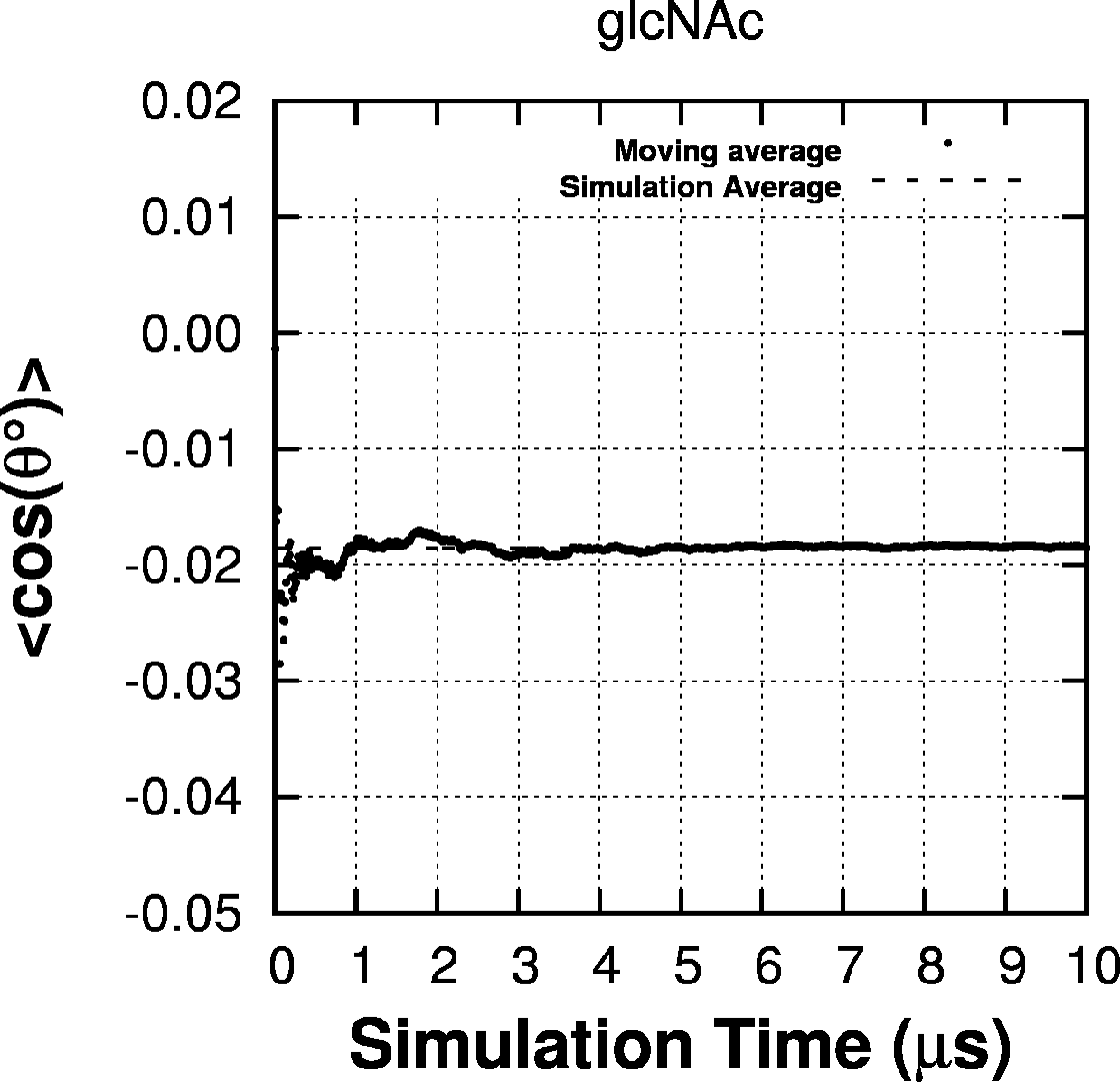

alpha-D-GlcNS6S
180
150
120
90
60
30
0
θ°
0
1
2
3
4
5
6
7
8
9
10
Simulation Time (μs)

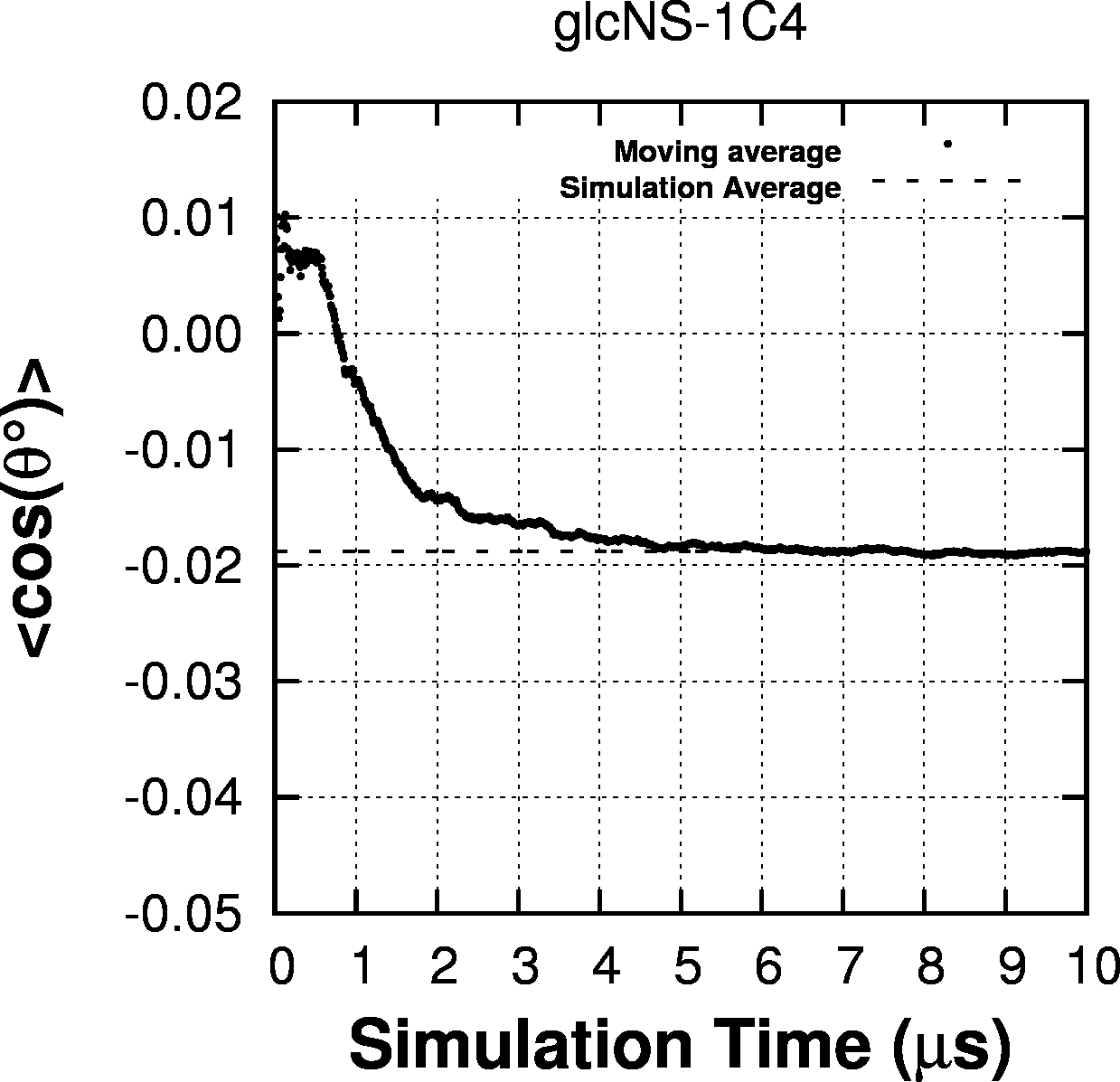

alpha-D-GlcNS
180
150
120
90
60
30
0
θ °
0
60
120
180
240
300
360
ϕ °

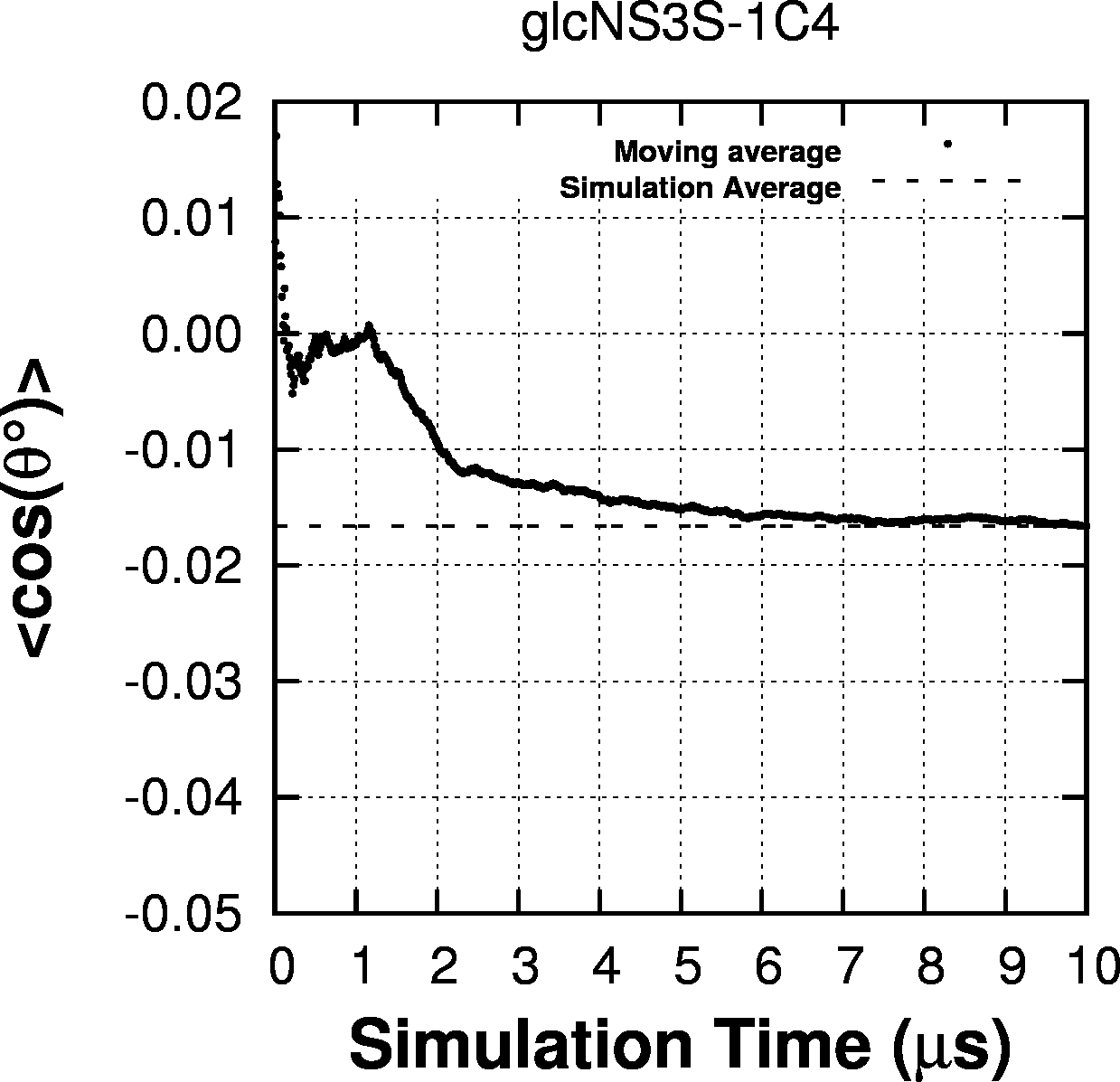

alpha-D-GlcNS
Q
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0 1 2 3 4 5 6 7 8 9 10
Simulation Time (μs)

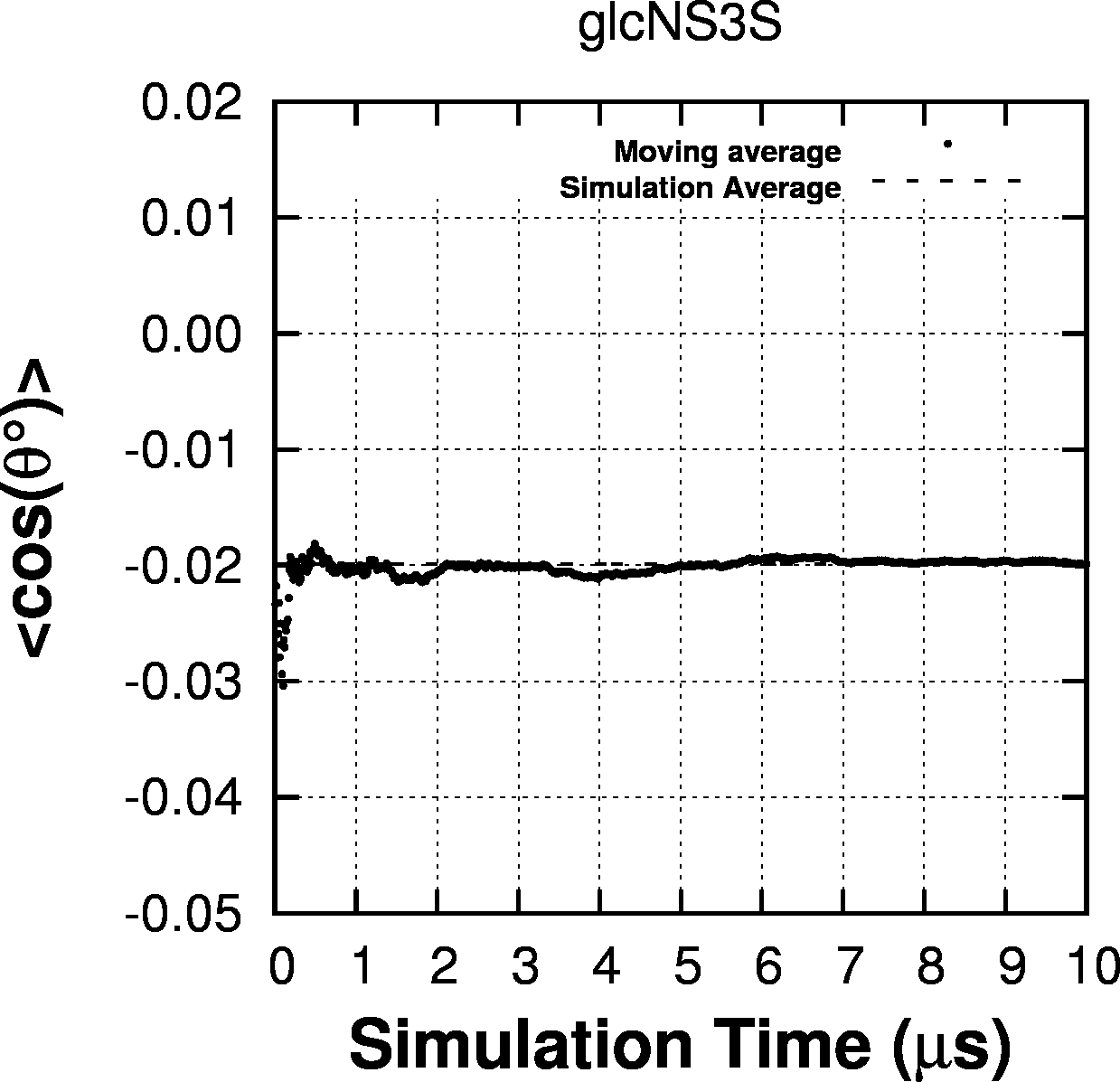

alpha-D-GlcNS
180
150
120
90
60
30
0
θ°
0
1
2
3
4
5
6
7
8
9
10
Simulation Time (μs)

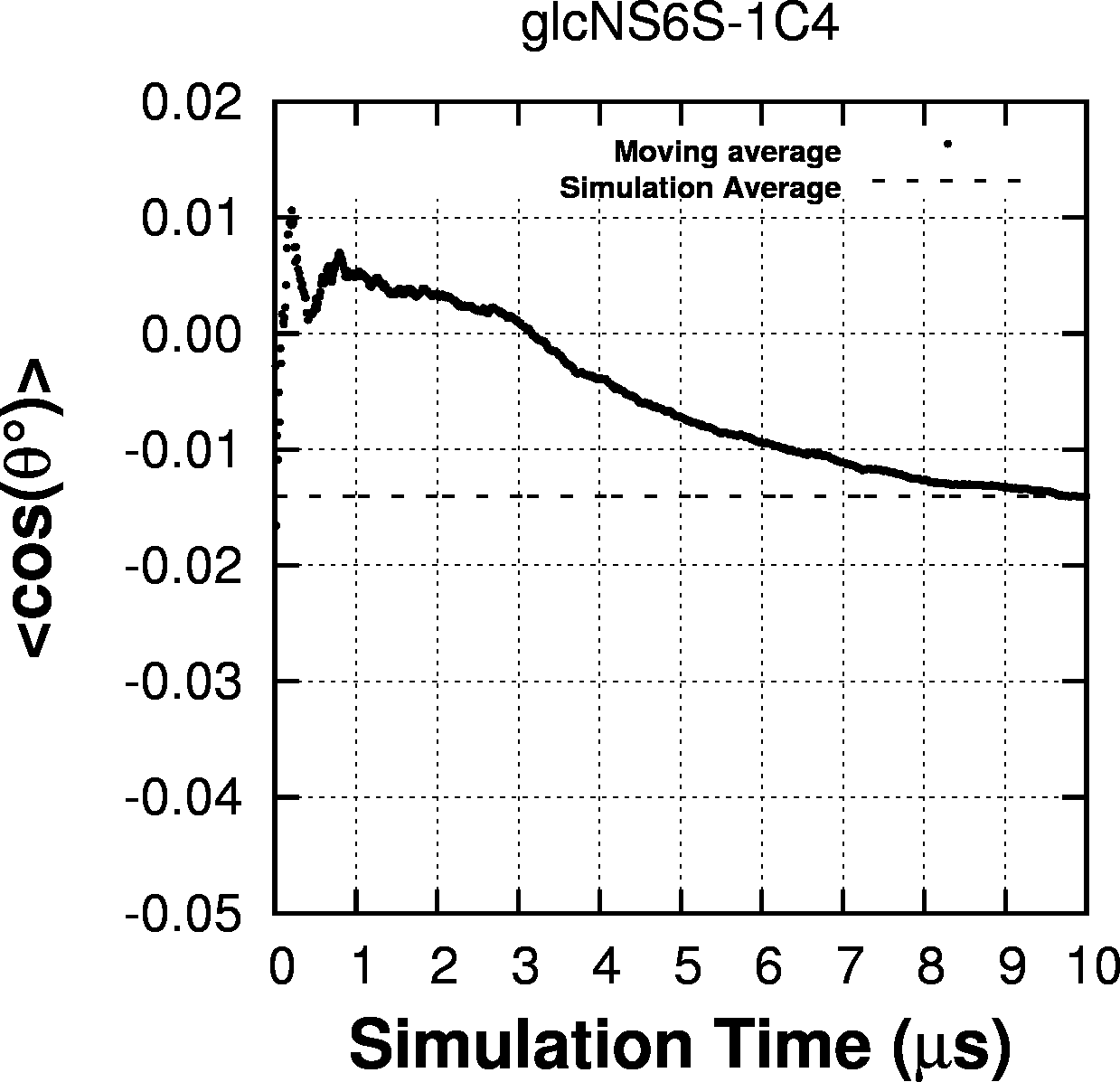

glcNAc-1C4
Moving average
Simulation Average
<cos(θ°)>
0.02
0.01
0.00
-0.01
-0.02
-0.03
-0.04
-0.05
0
1
2
3
4
5
6
7
8
9
10
Simulation Time (μs)

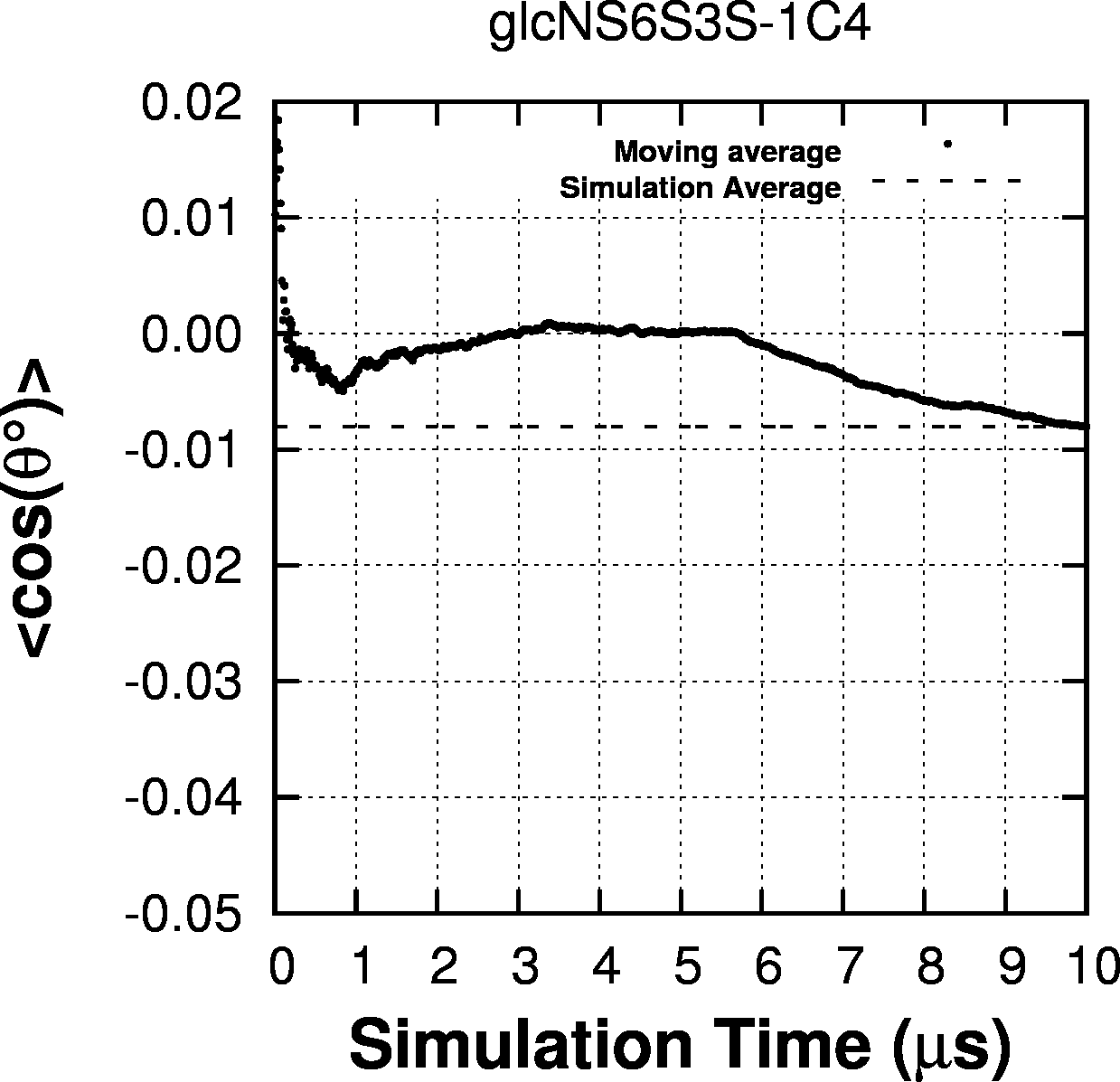

glcNAc
Moving average
Simulation Average
<cos(θ°)>
0.02
0.01
0.00
-0.01
-0.02
-0.03
-0.04
-0.05
0
1
2
3
4
5
6
7
8
9
10
Simulation Time (μs)

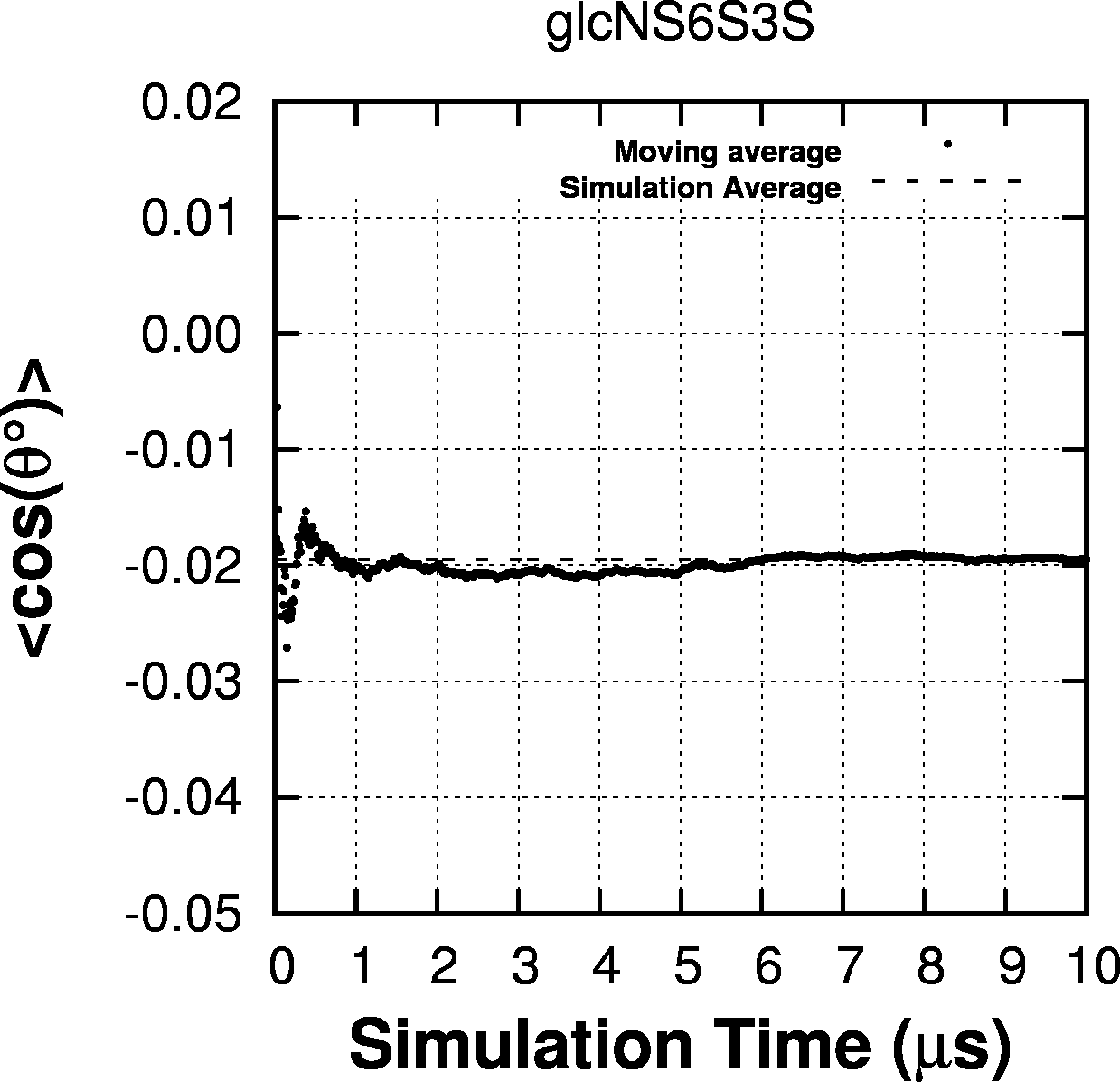

glcNS-1C4
Moving average
Simulation Average
<cos(θ°)>
0.02
0.01
0.00
-0.01
-0.02
-0.03
-0.04
-0.05
0
1
2
3
4
5
6
7
8
9
10
Simulation Time (μs)


glcNS3S-1C4
Moving average
Simulation Average
0.02
0.01
0.00
-0.01
-0.02
-0.03
-0.04
-0.05
0
1
2
3
4
5
6
7
8
9
10
<cos(θ°)>
Simulation Time (μs)


glcNS3S
Moving average
Simulation Average
0.02
0.01
0.00
-0.01
-0.02
-0.03
-0.04
-0.05
<cos(θ°)>
0
1
2
3
4
5
6
7
8
9
10
Simulation Time (μs)


glcNS6S-1C4
Moving average
Simulation Average
0.02
0.01
0.00
-0.01
-0.02
-0.03
-0.04
-0.05
<cos(θ°)>
0
1
2
3
4
5
6
7
8
9
10
Simulation Time (μs)


glcNS6S3S-1C4
Moving average
Simulation Average
0.02
0.01
0.00
-0.01
-0.02
-0.03
-0.04
-0.05
<cos(θ°)>
0
1
2
3
4
5
6
7
8
9
10
Simulation Time (μs)


glcNS6S3S
Moving average
Simulation Average
<cos(θ°)>
0.02
0.01
0.00
-0.01
-0.02
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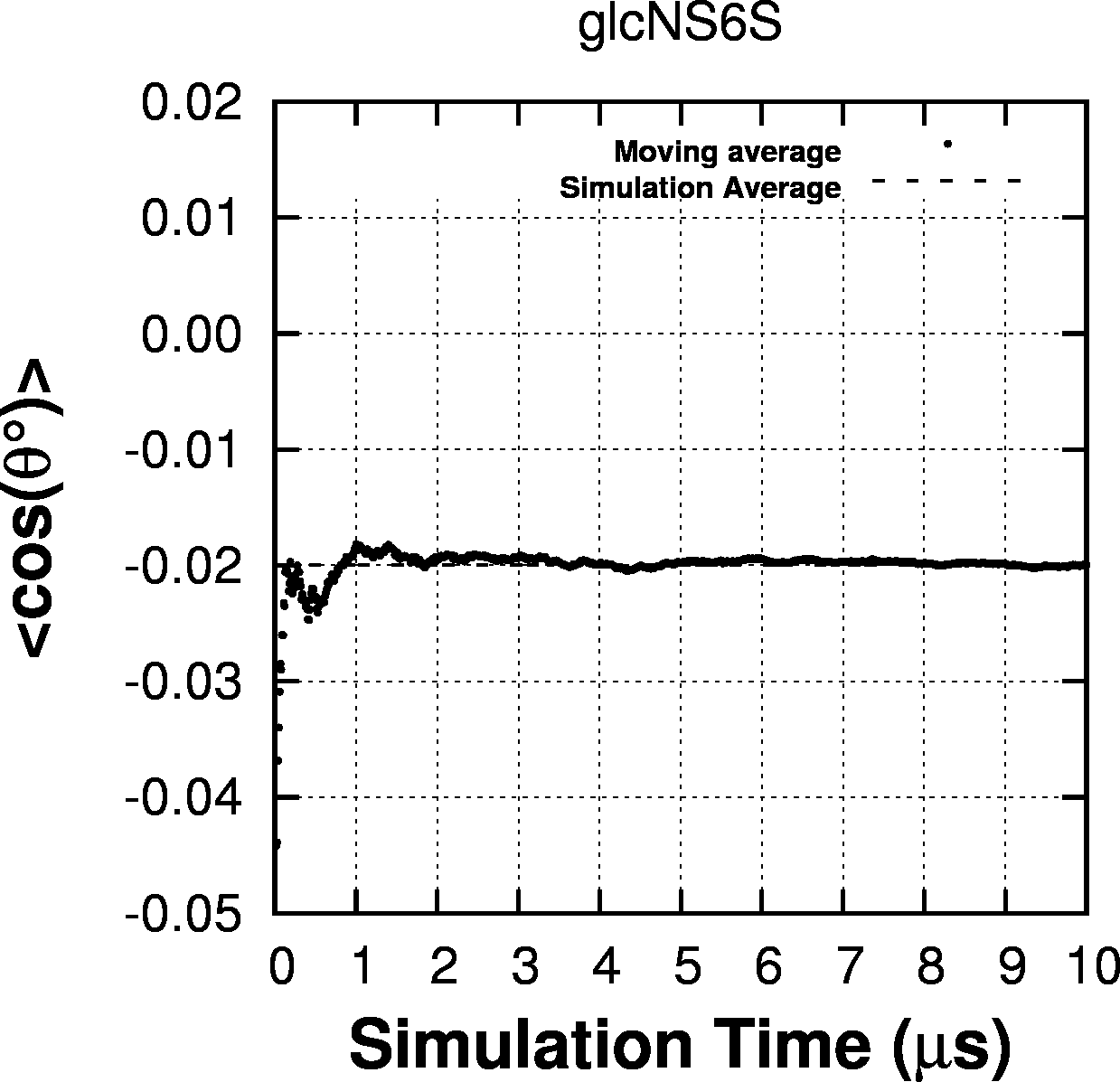
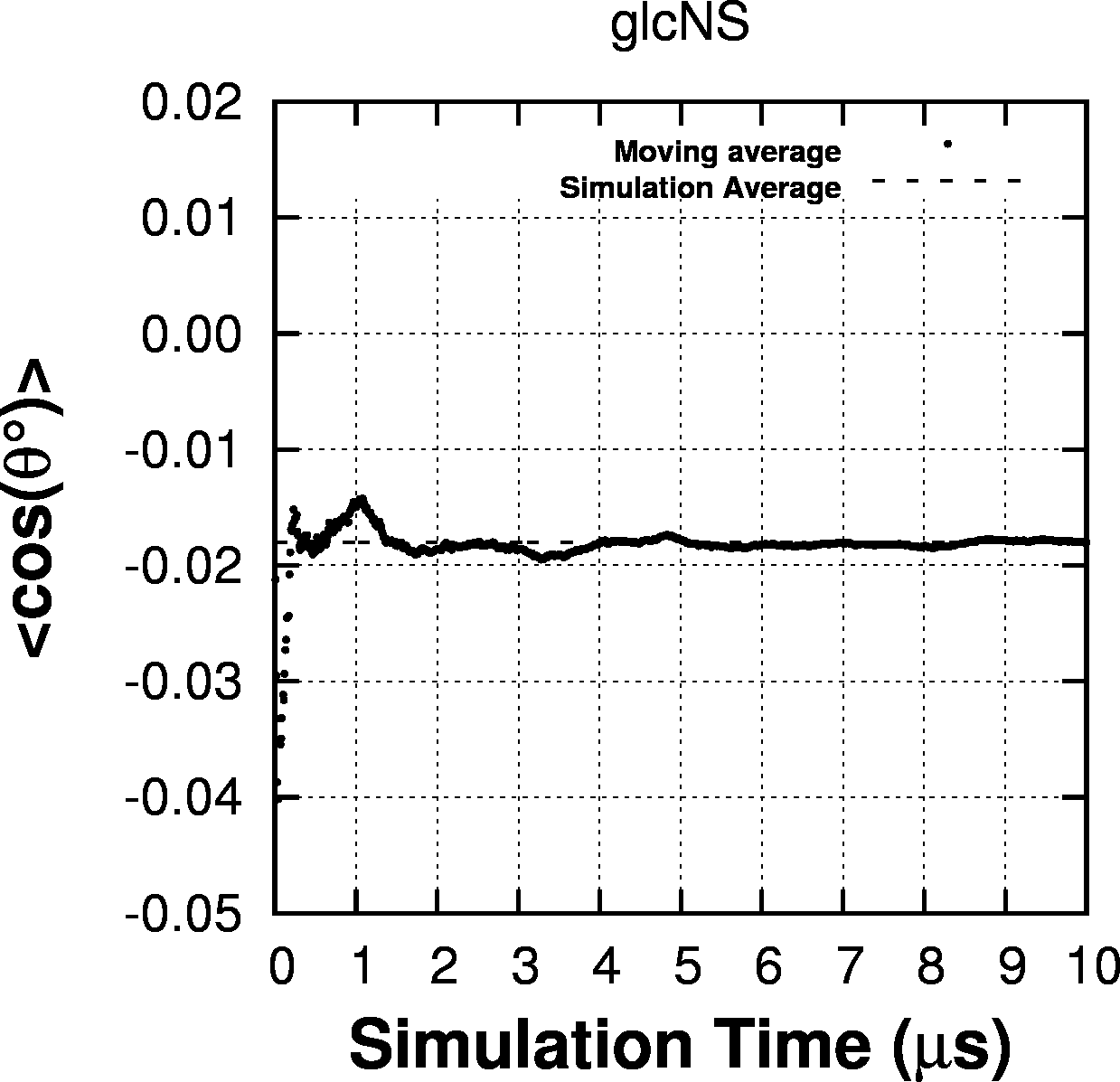
-0.04
-0.05
0
1
2
3
4
5
6
7
8
9
10
Simulation Time (μs)


glcNS6S
Moving average
Simulation Average
<cos(θ°)>
0.02
0.01
0.00
-0.01
-0.02
-0.03
-0.04
-0.05
0
1
2
3
4
5
6
7
8
9
10
Simulation Time (μs)


glcNS
Moving average
Simulation Average
<cos(θ°)>
0.02
0.01
0.00
-0.01
-0.02
-0.03
-0.04
-0.05
0
1
2
3
4
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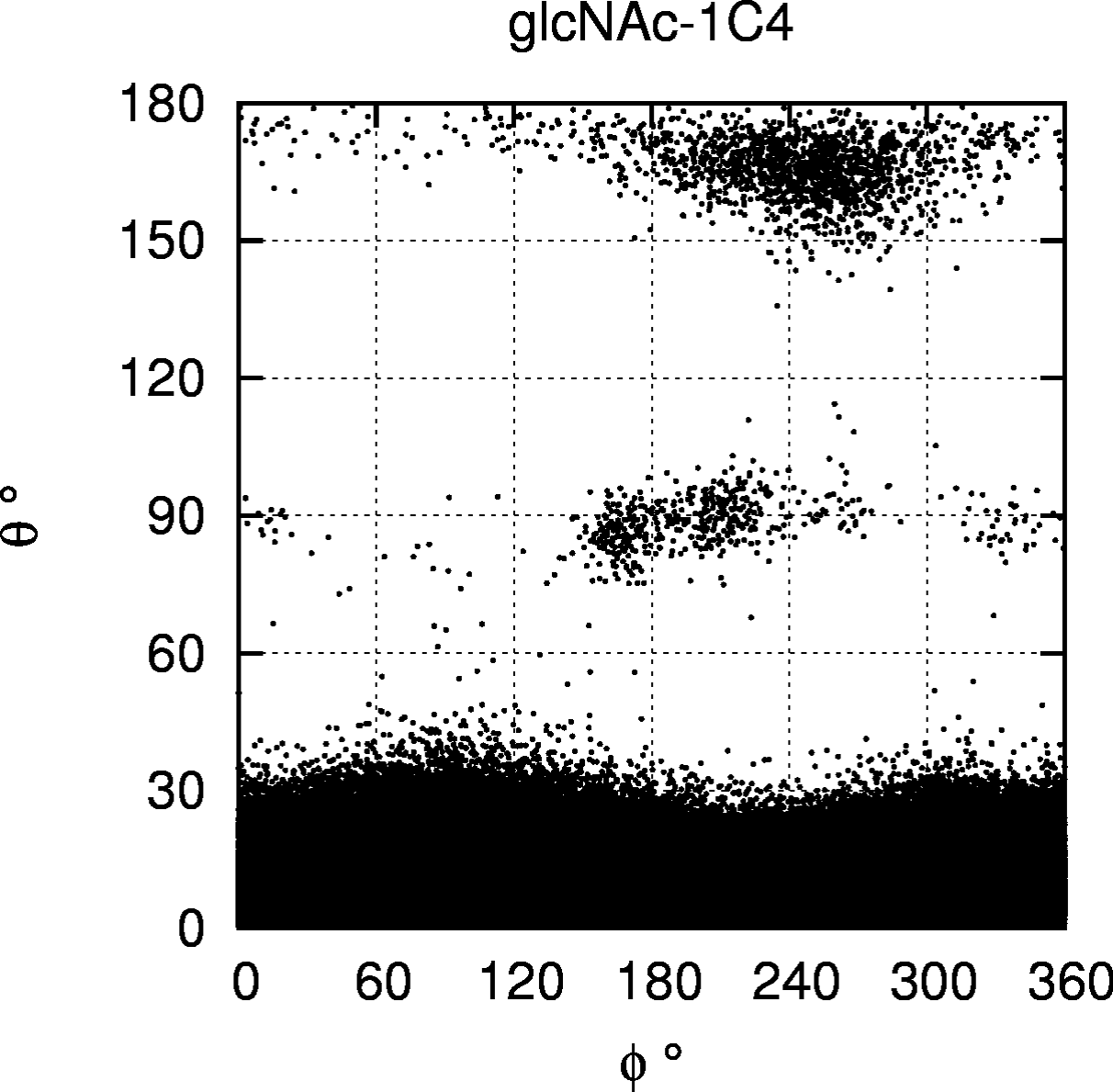
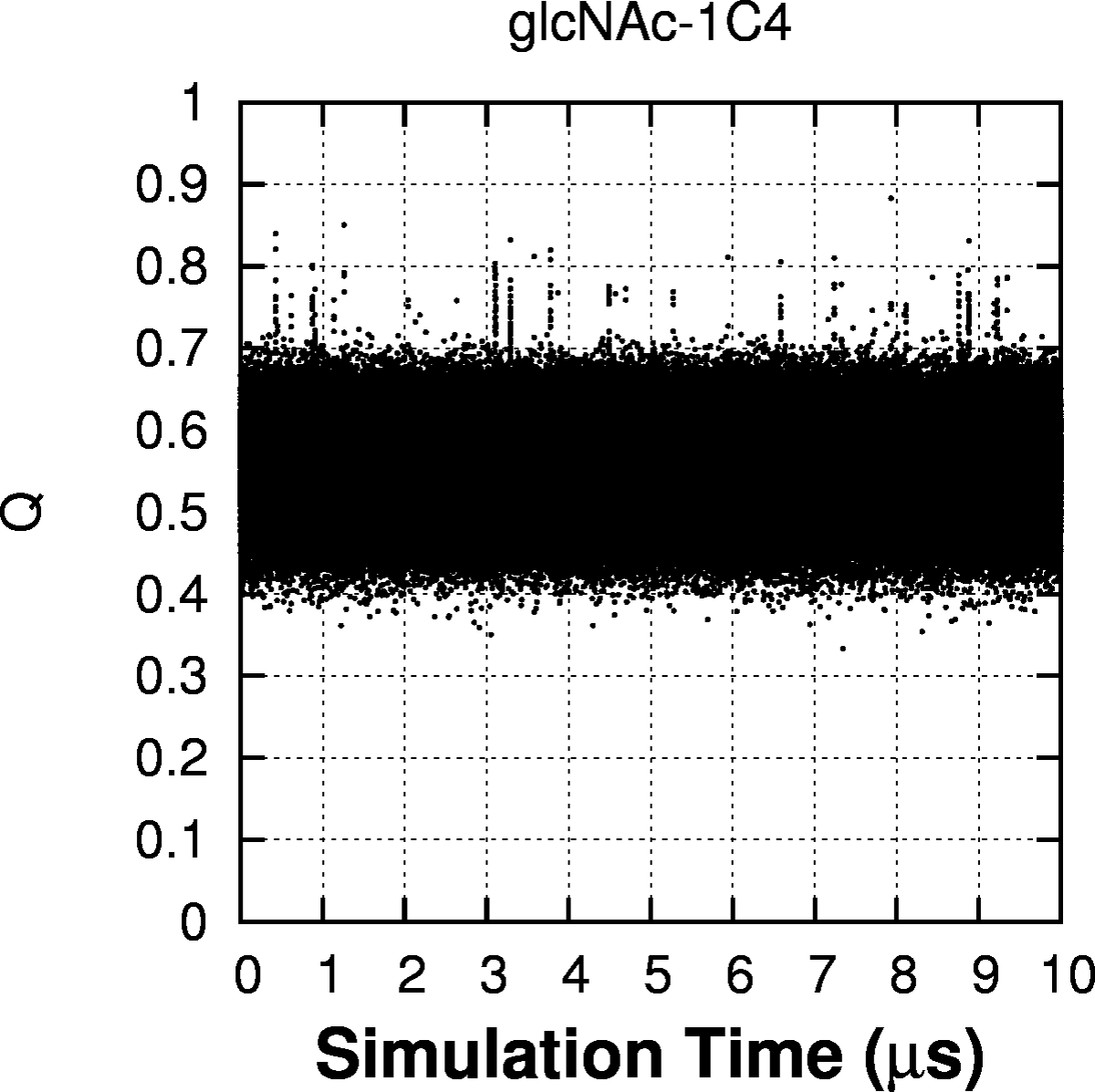
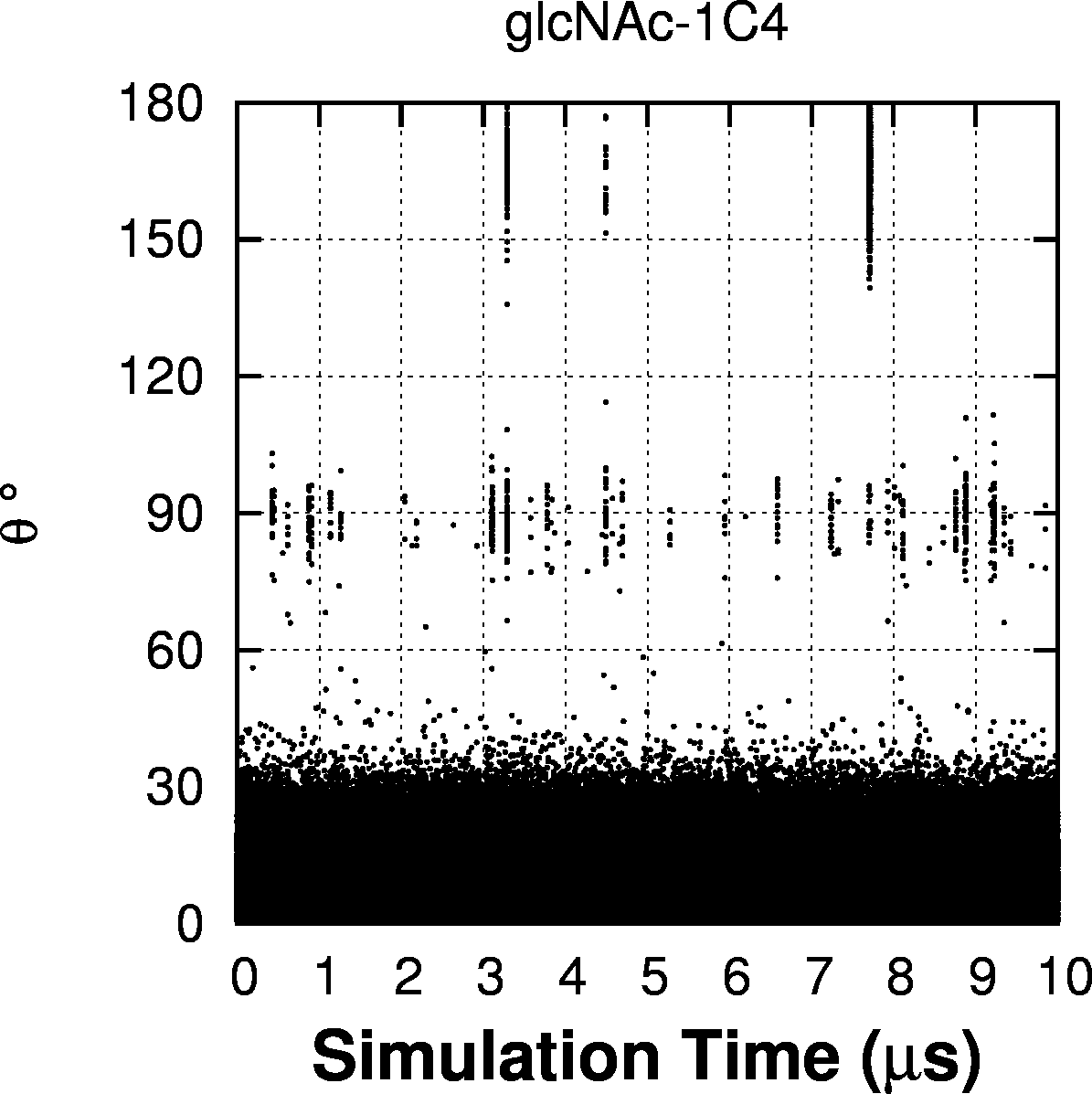
6
7
8
9
10
Simulation Time (μs)


glcNAc-1C4
180
150
120
90
60
30
0
θ °
0
60
120
180
240
300
360
ϕ °


glcNAc-1C4
Q
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0 1 2 3 4 5 6 7 8 9 10
Simulation Time (μs)


glcNAc-1C4
180
150
120
90
60
30
0
θ°
0
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3
4
5
6
7
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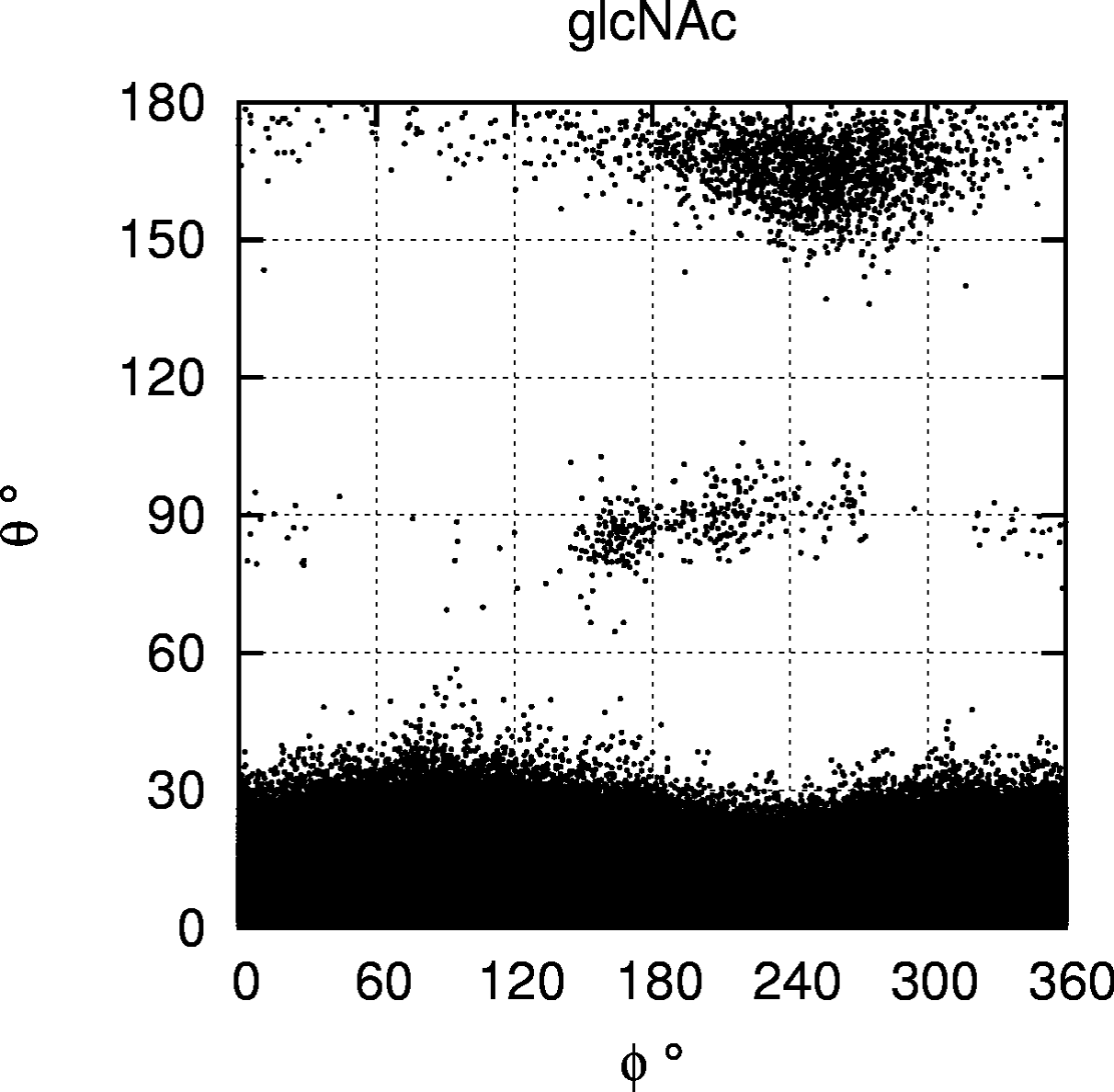
10
Simulation Time (μs)


glcNAc
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120
90
60
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0
θ °
0
60
120
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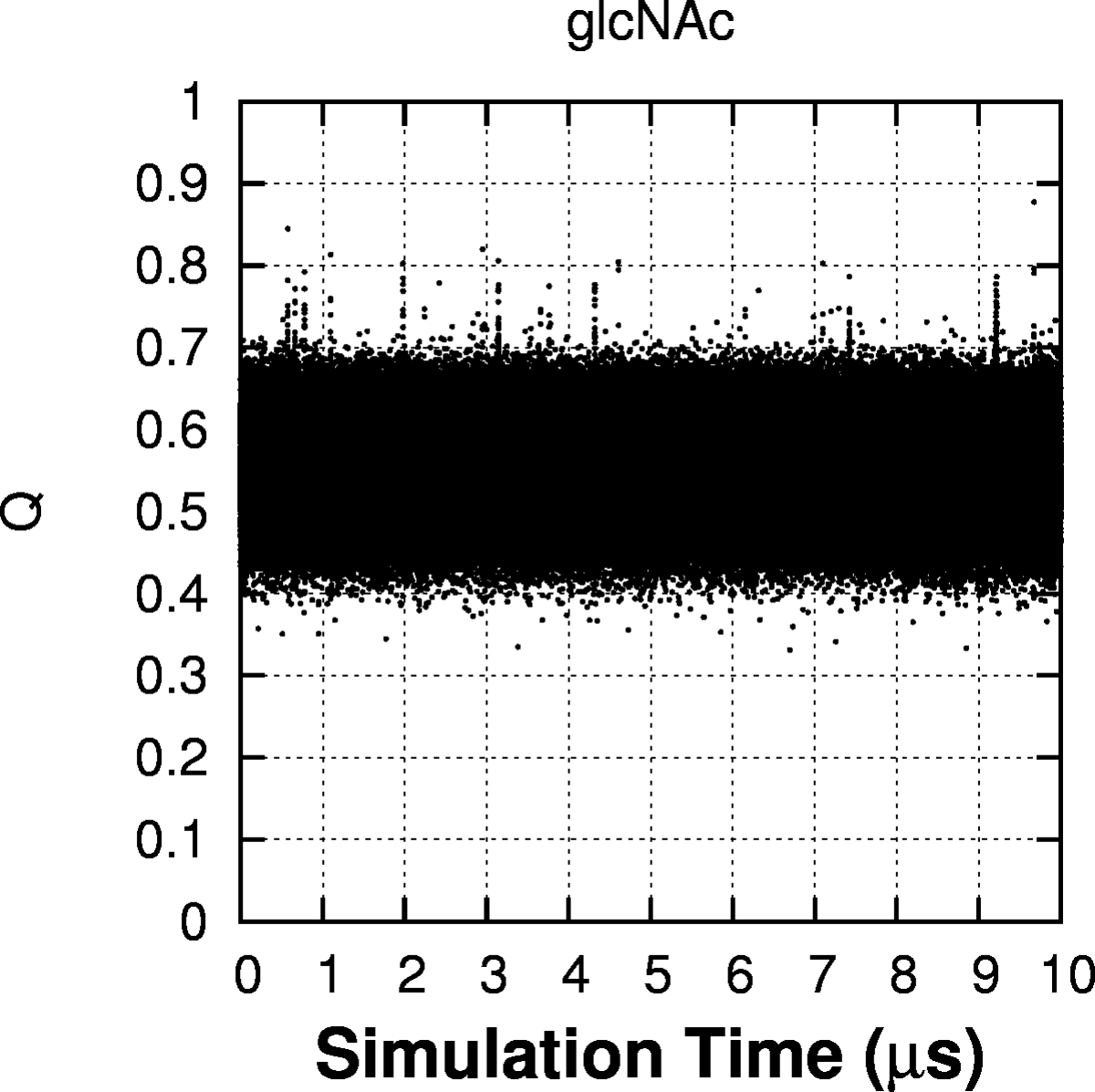
240
300
360
ϕ °


glcNAc
Q
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0.9
0.8
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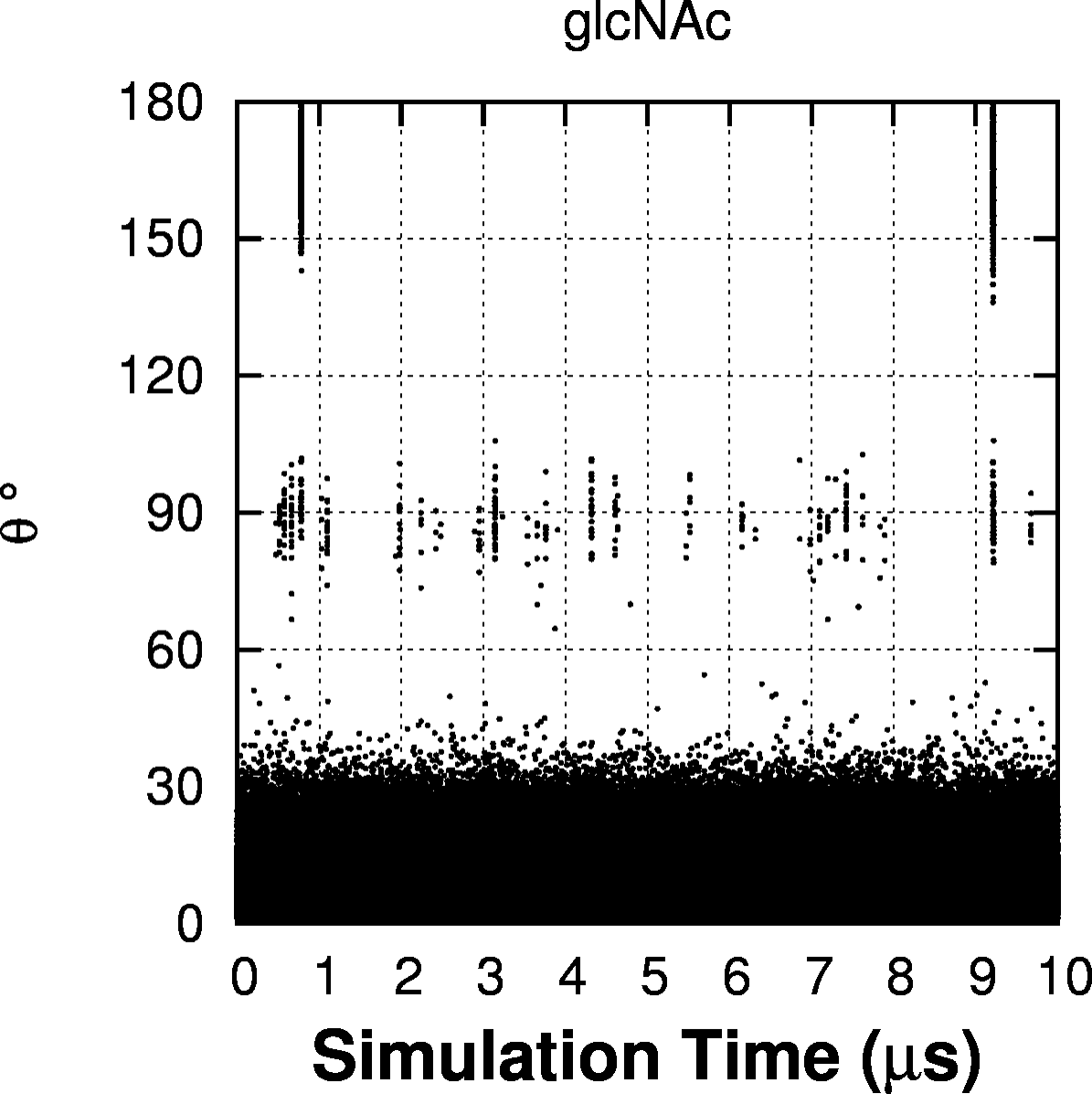
0.4
0.3
0.2
0.1
0
0 1 2 3 4 5 6 7 8 9 10
Simulation Time (μs)


glcNAc
180
150
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90
60
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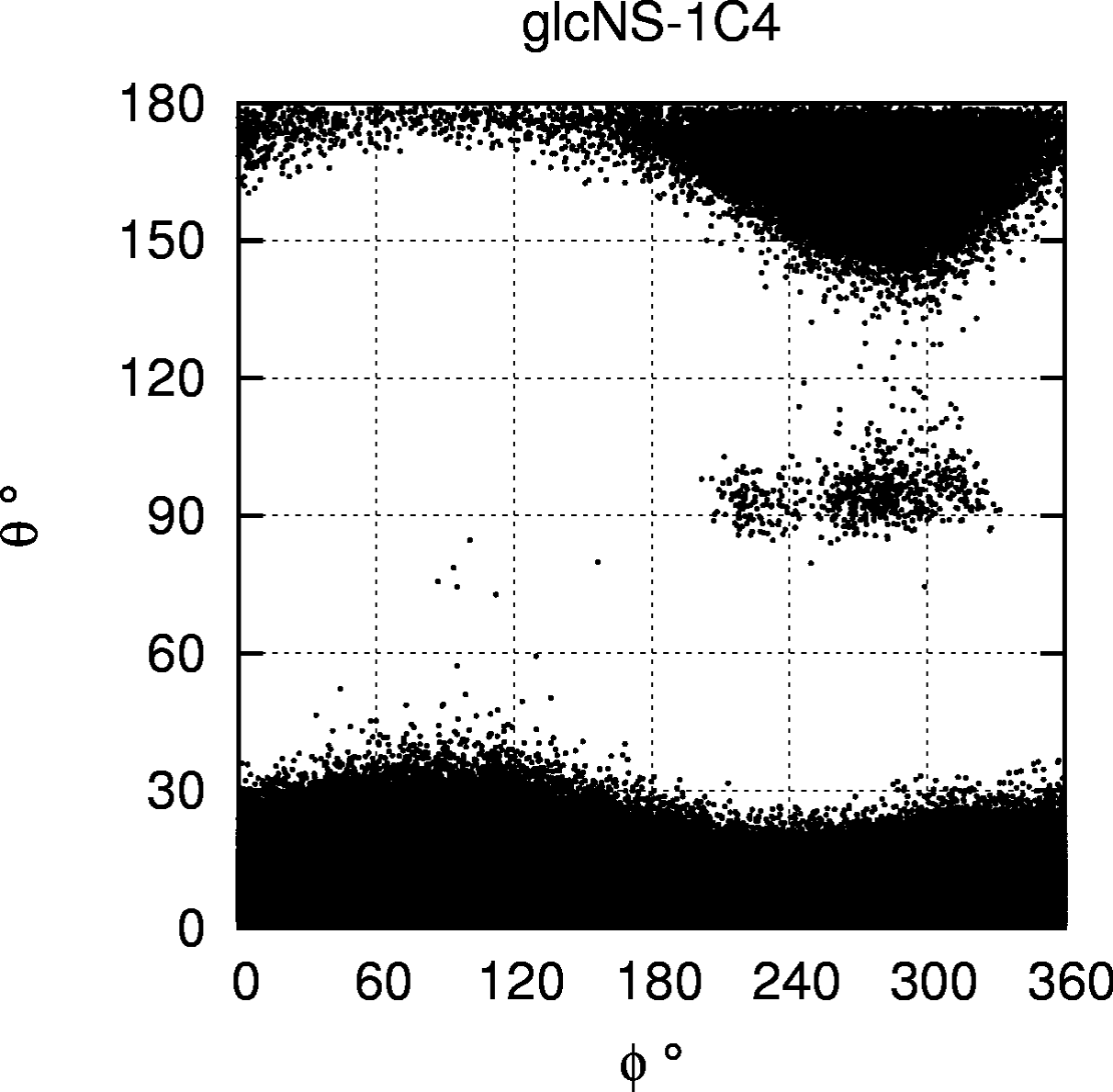
0
θ°
0
1
2
3
4
5
6
7
8
9
10
Simulation Time (μs)


glcNS-1C4
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θ°
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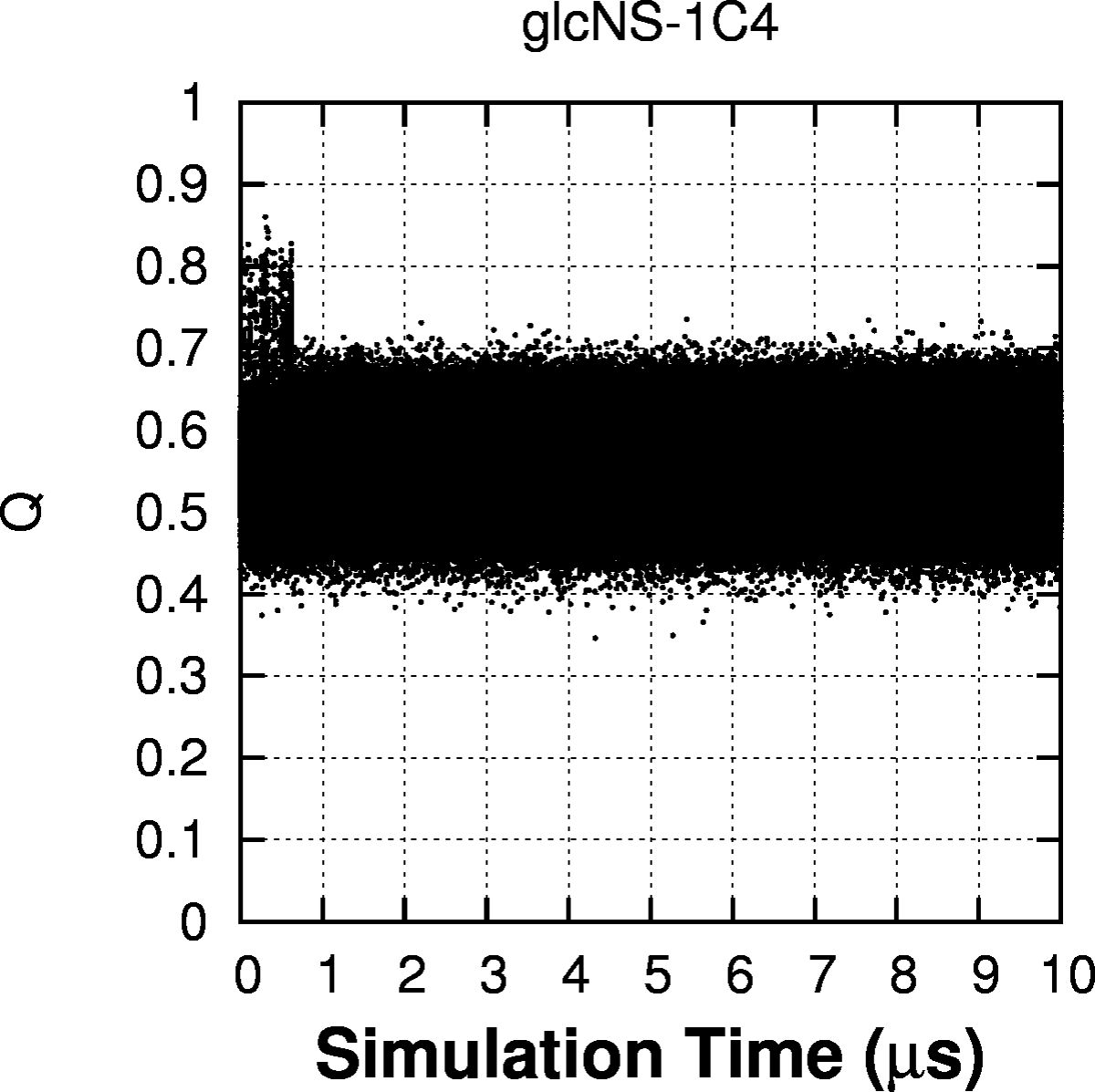
300
360
ϕ °


glcNS-1C4
Q
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0.9
0.8
0.7
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0.5
0.4
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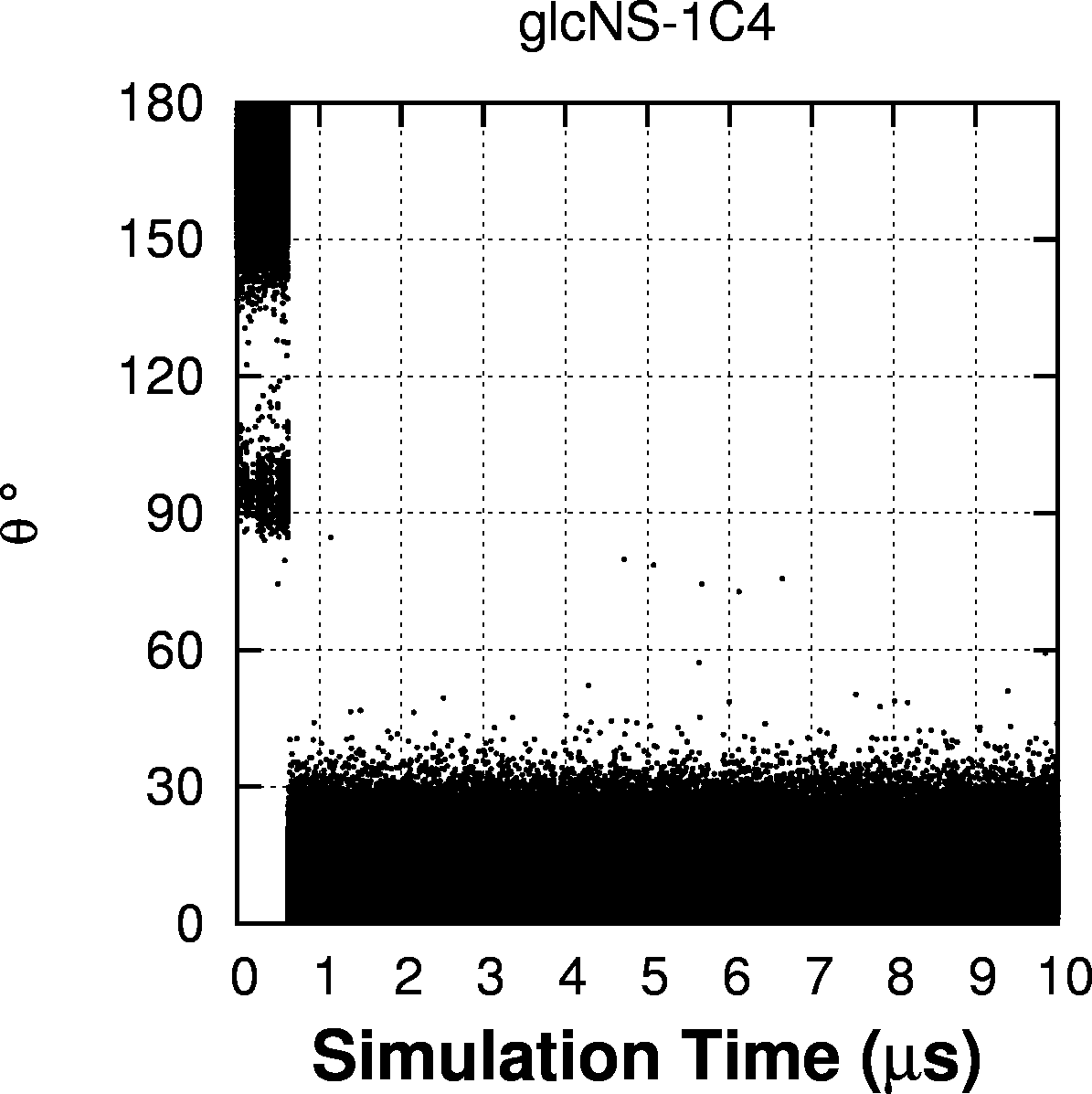
10
Simulation Time (μs)


glcNS-1C4
180
150
120
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60
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0
θ°
0
1
2
3
4
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6
7
8
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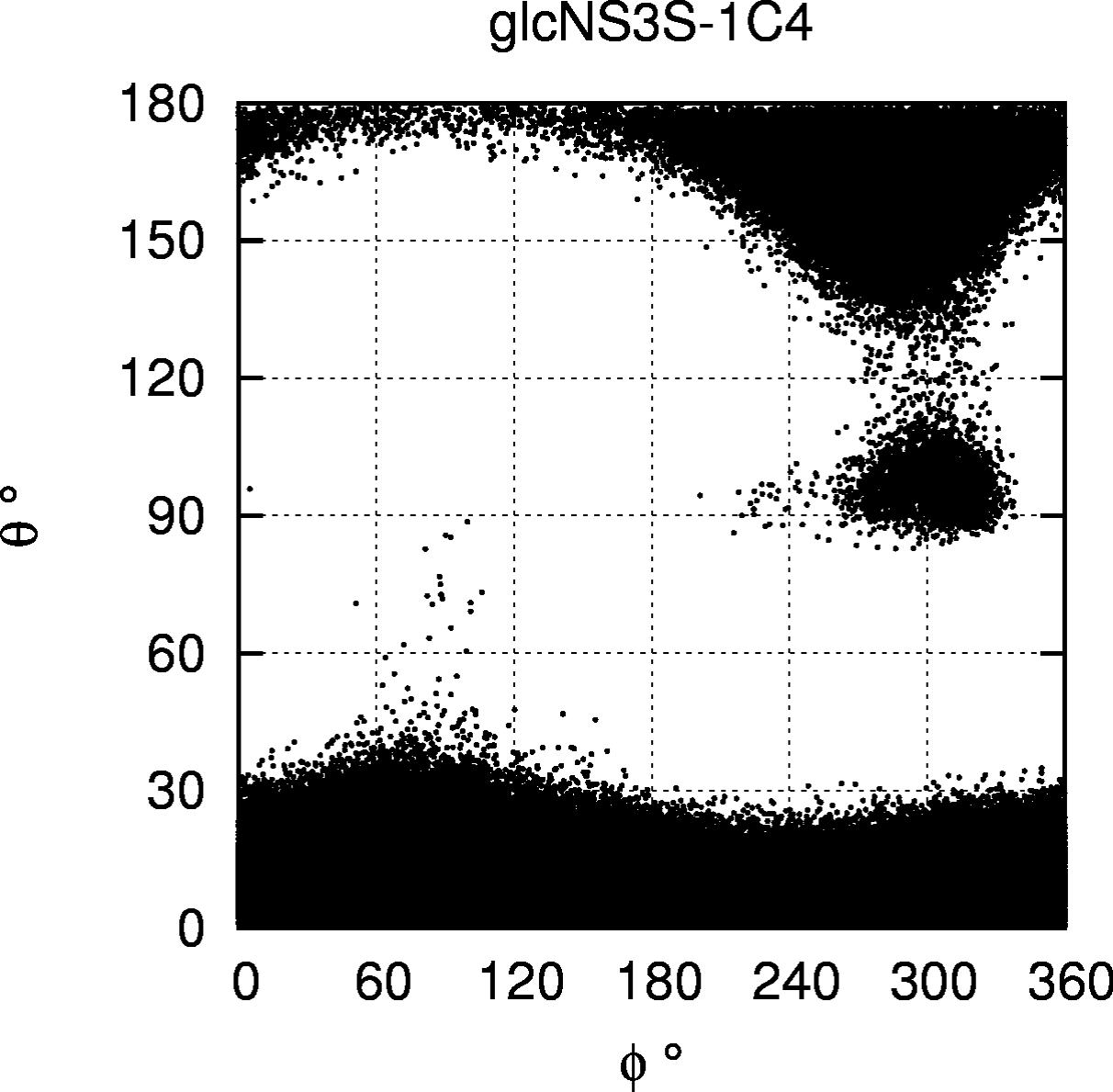
10
Simulation Time (μs)


glcNS3S-1C4
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θ°
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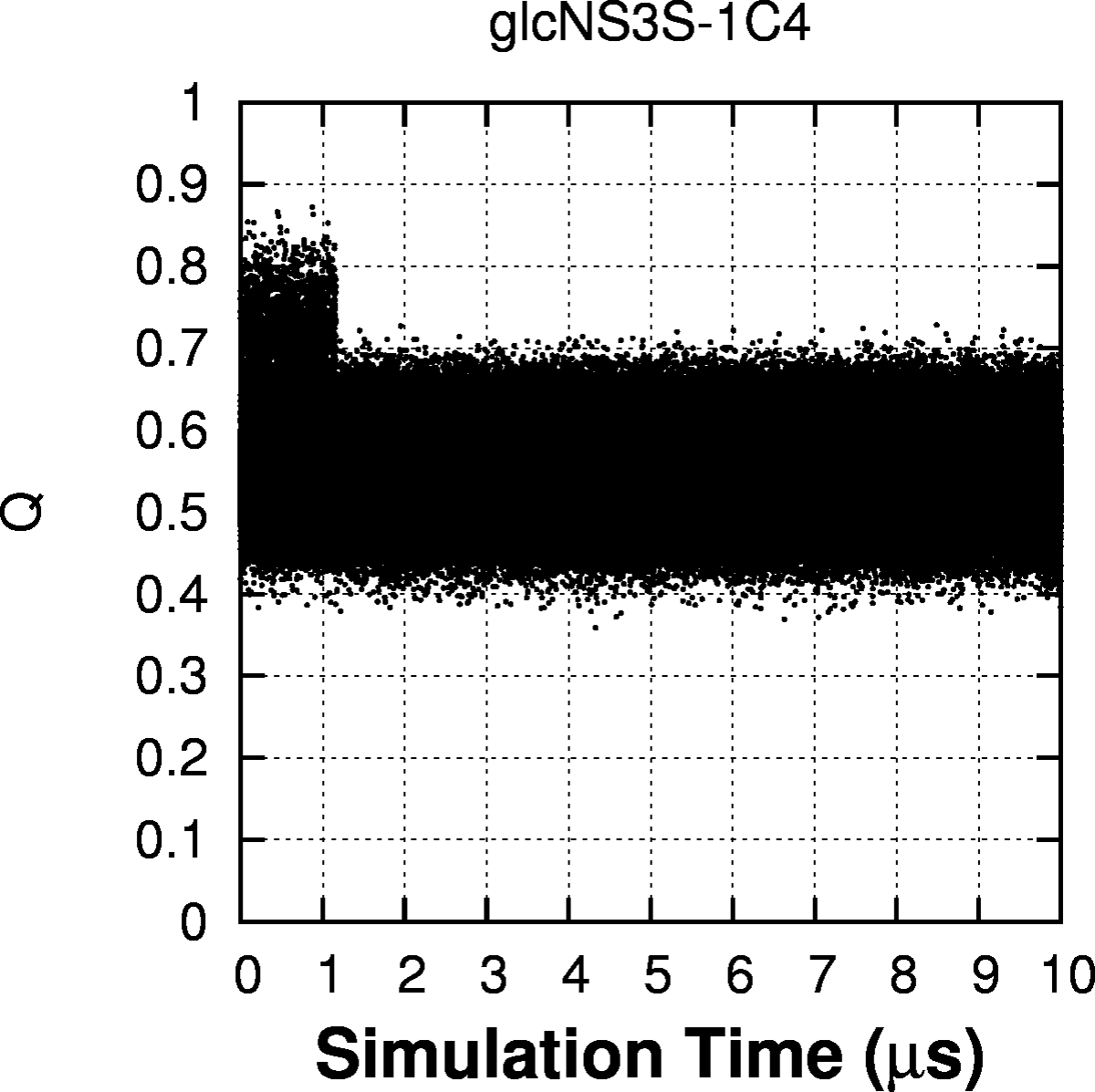
240
300
360
ϕ °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Q
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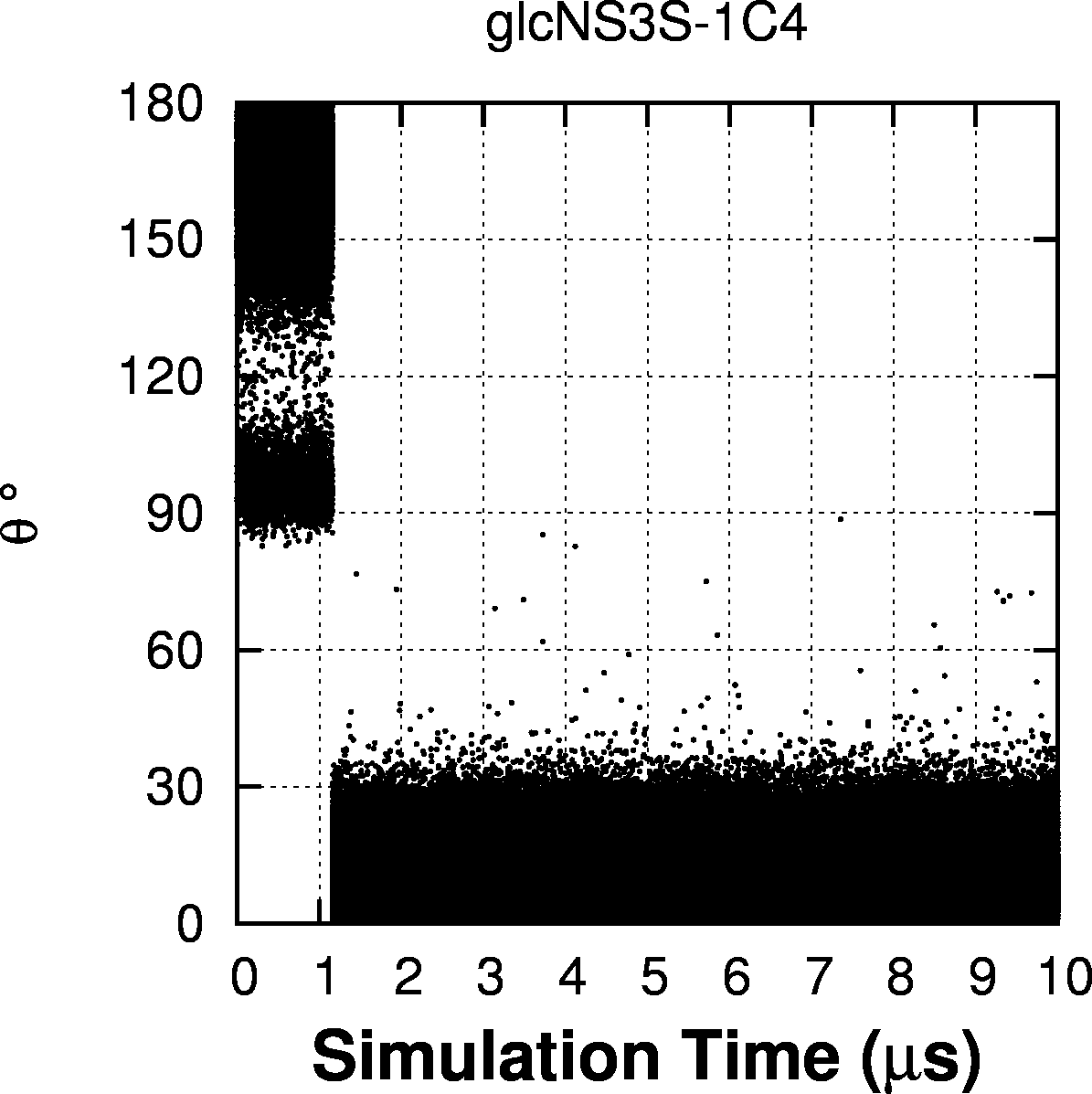
0.6
0.5
0.4
0.3
0.2
0.1
0
0 1 2 3 4 5 6 7 8 9 10
Simulation Time (μs)


glcNS3S-1C4
180
150
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90
60
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0
θ°
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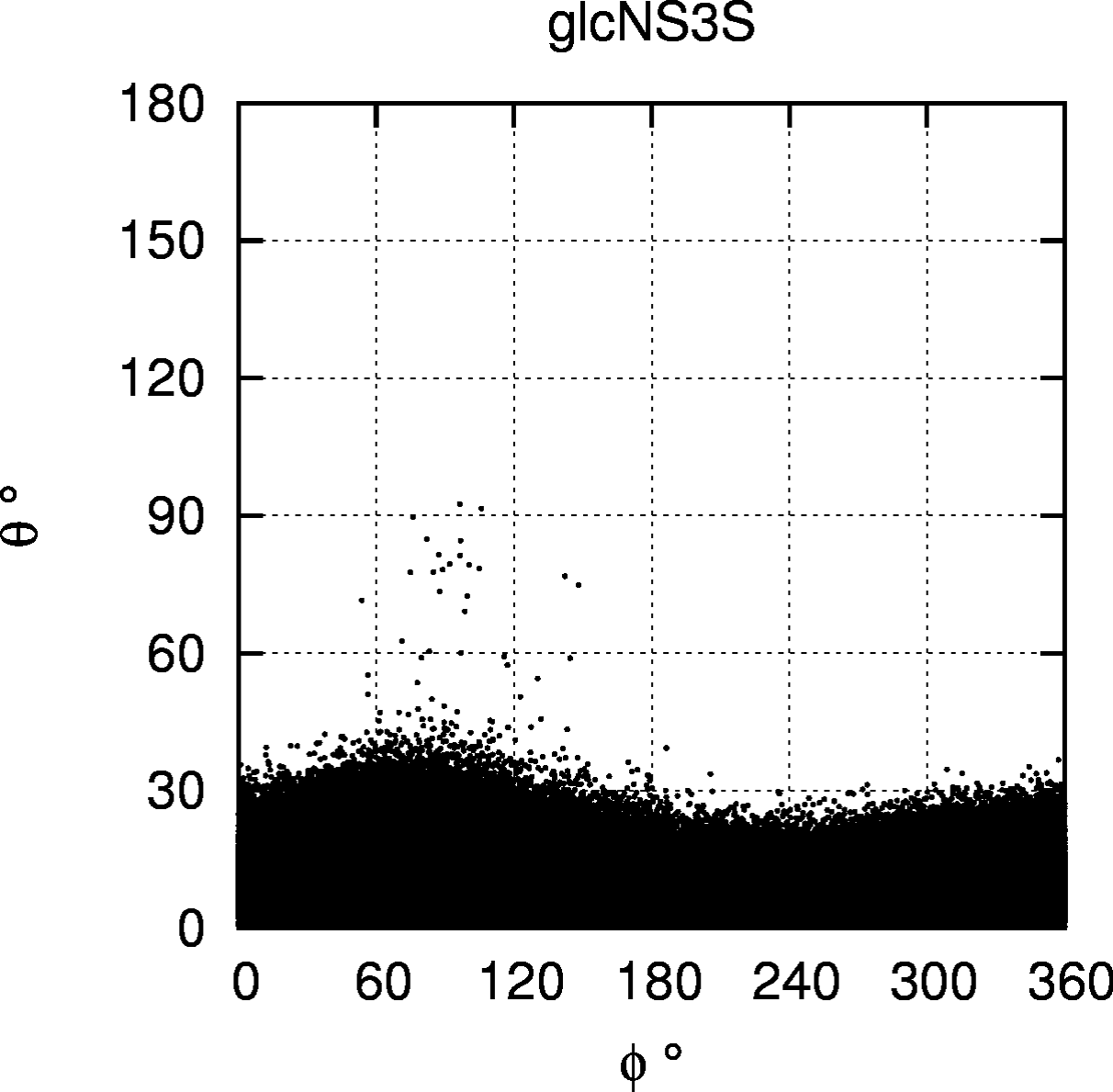
1
2
3
4
5
6
7
8
9
10
Simulation Time (μs)


glcNS3S
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30
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θ °
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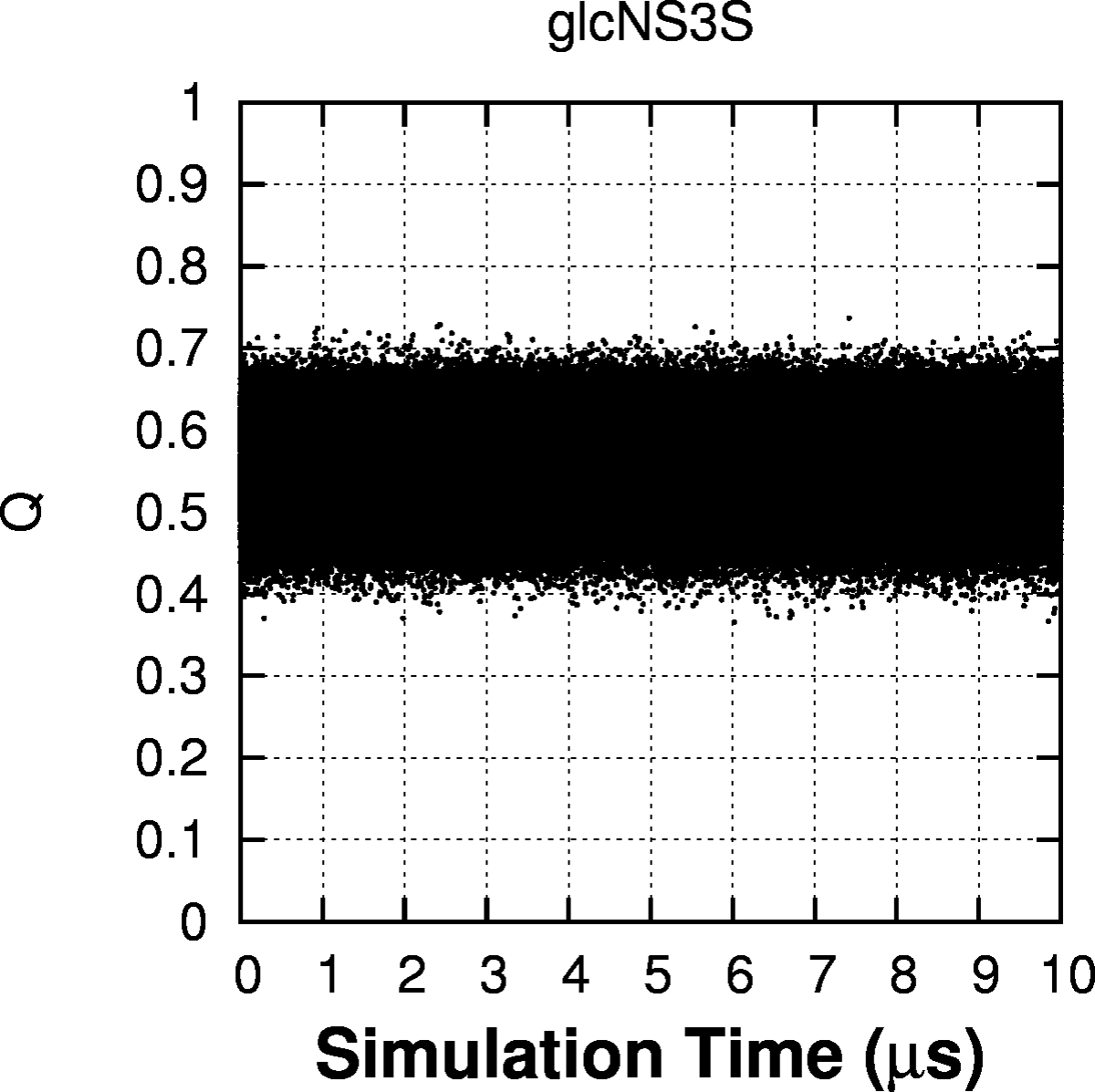
60
120
180
240
300
360
ϕ °


glcNS3S
Q
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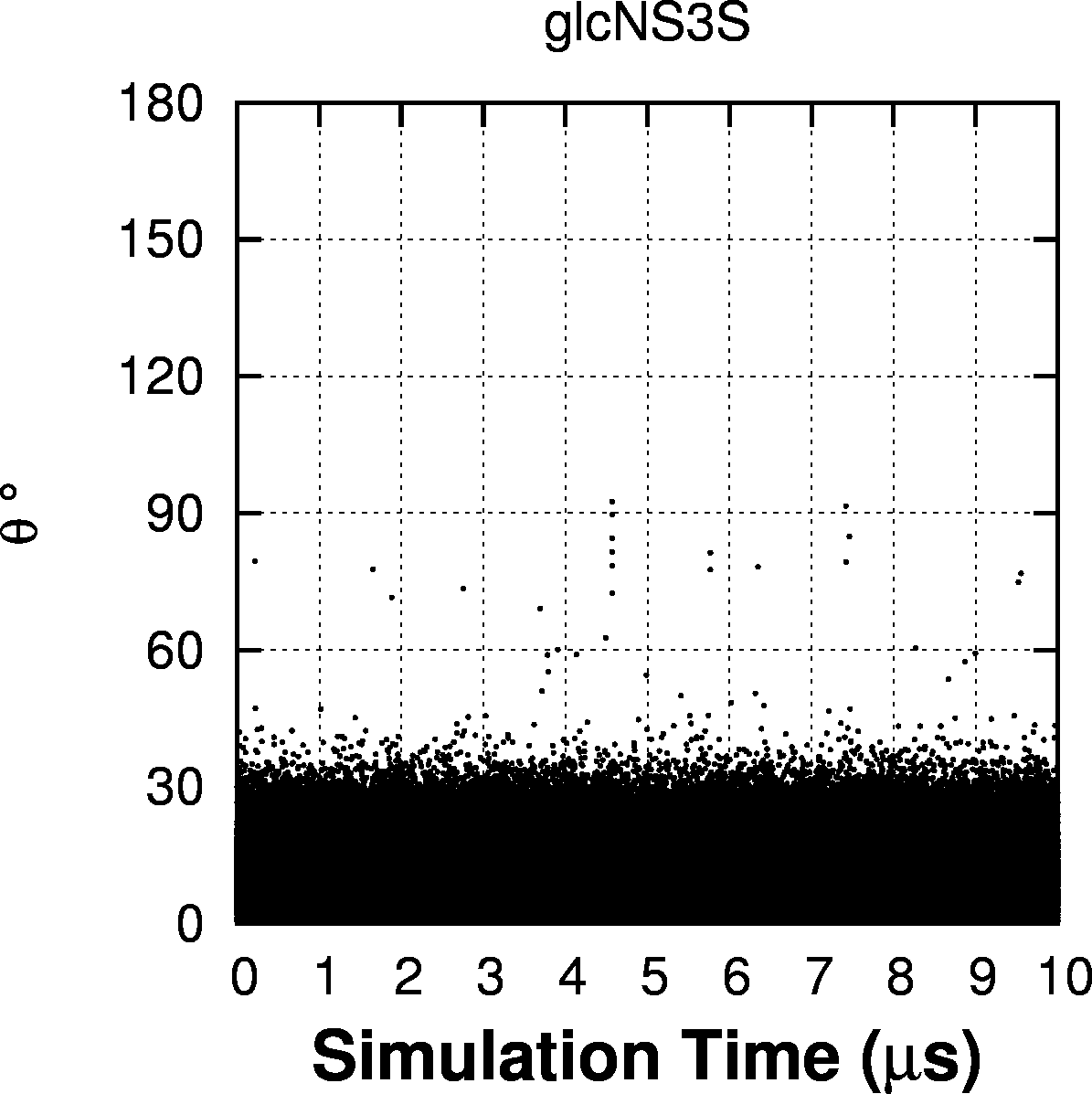
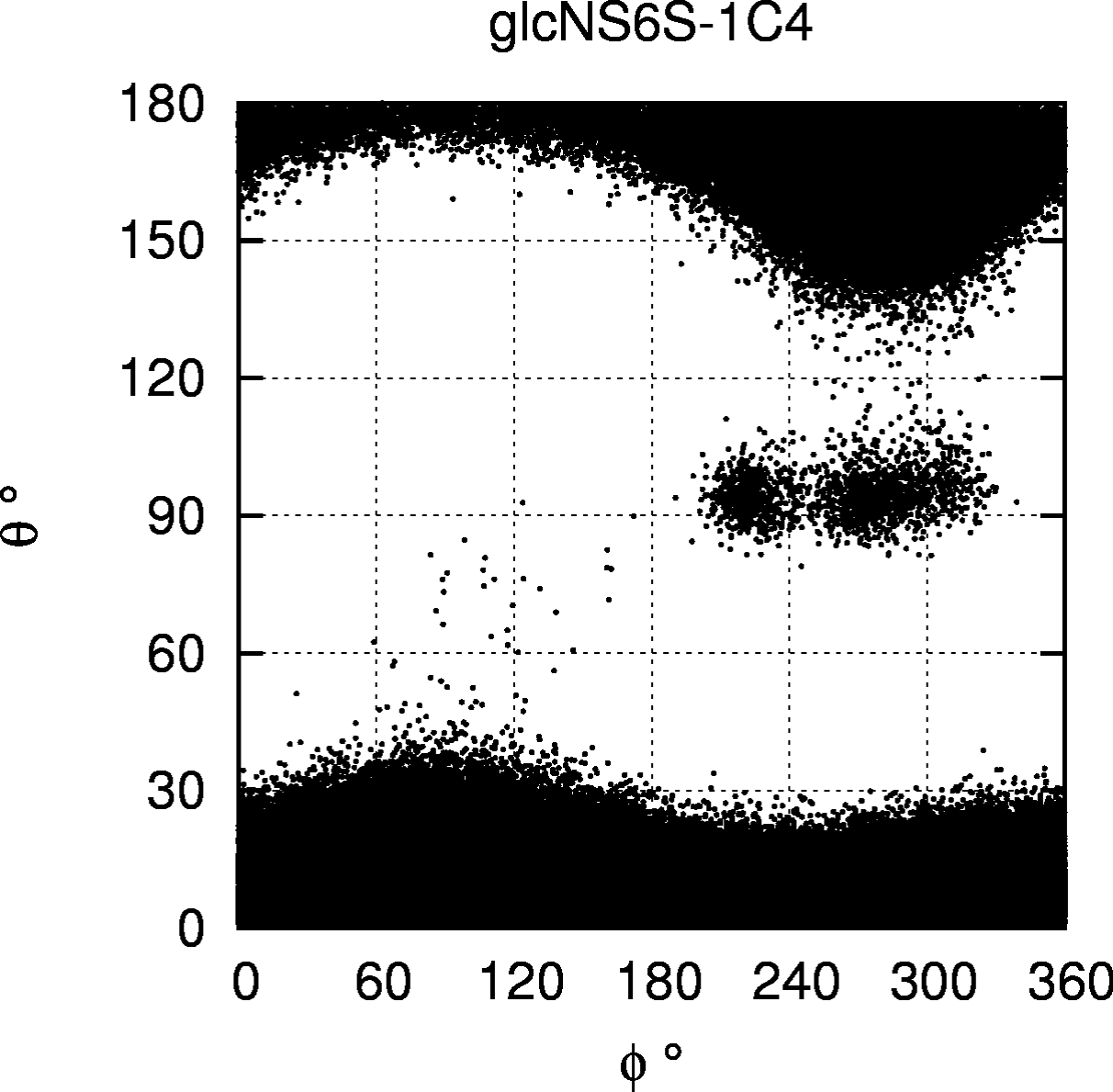
0.6
0.5
0.4
0.3
0.2
0.1
0
0 1 2 3 4 5 6 7 8 9 10
Simulation Time (μs)


glcNS3S
180
150
120
90
60
30
0
θ°
0
1
2
3
4
5
6
7
8
9
10
Simulation Time (μs)


glcNS6S-1C4
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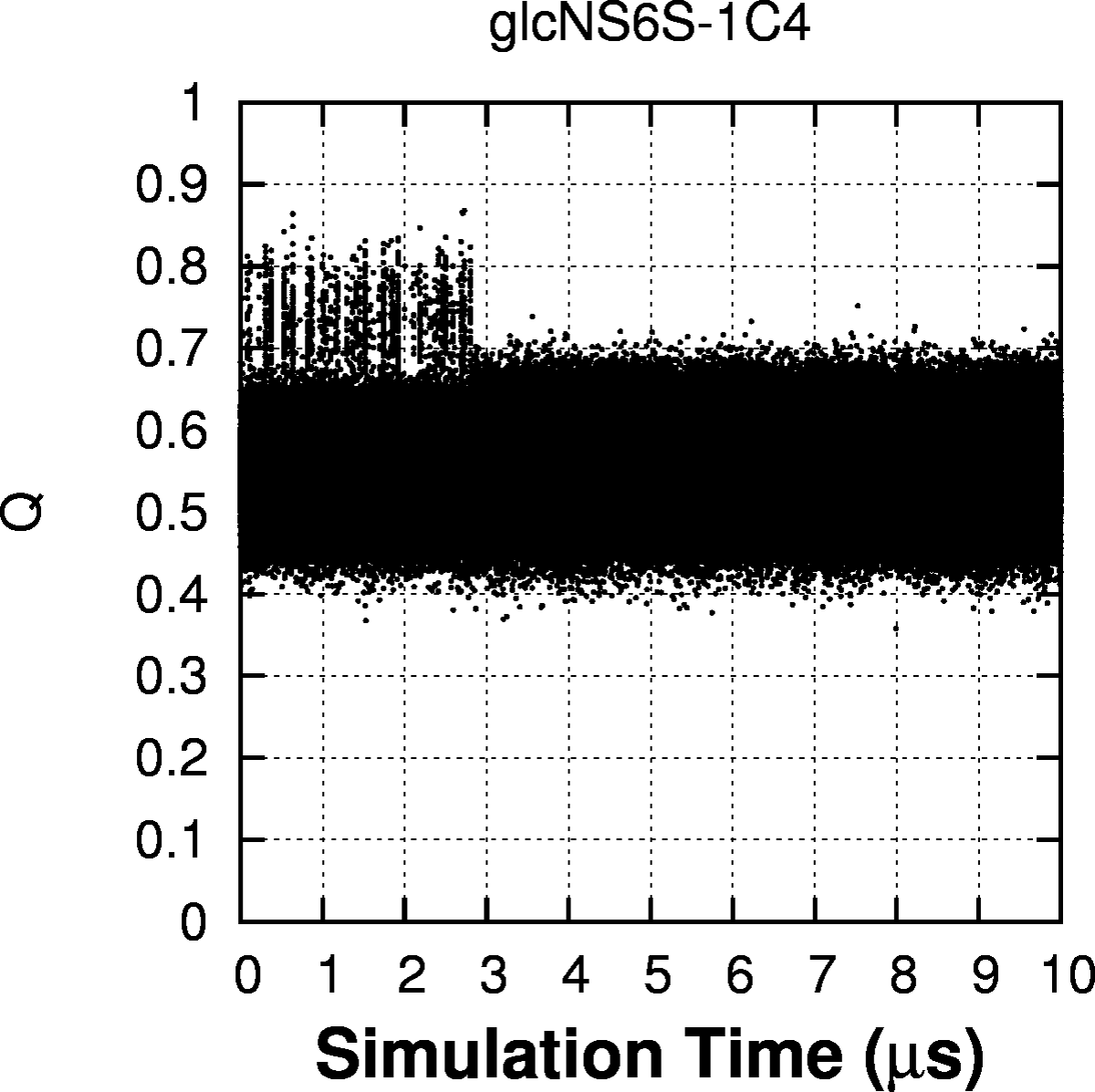
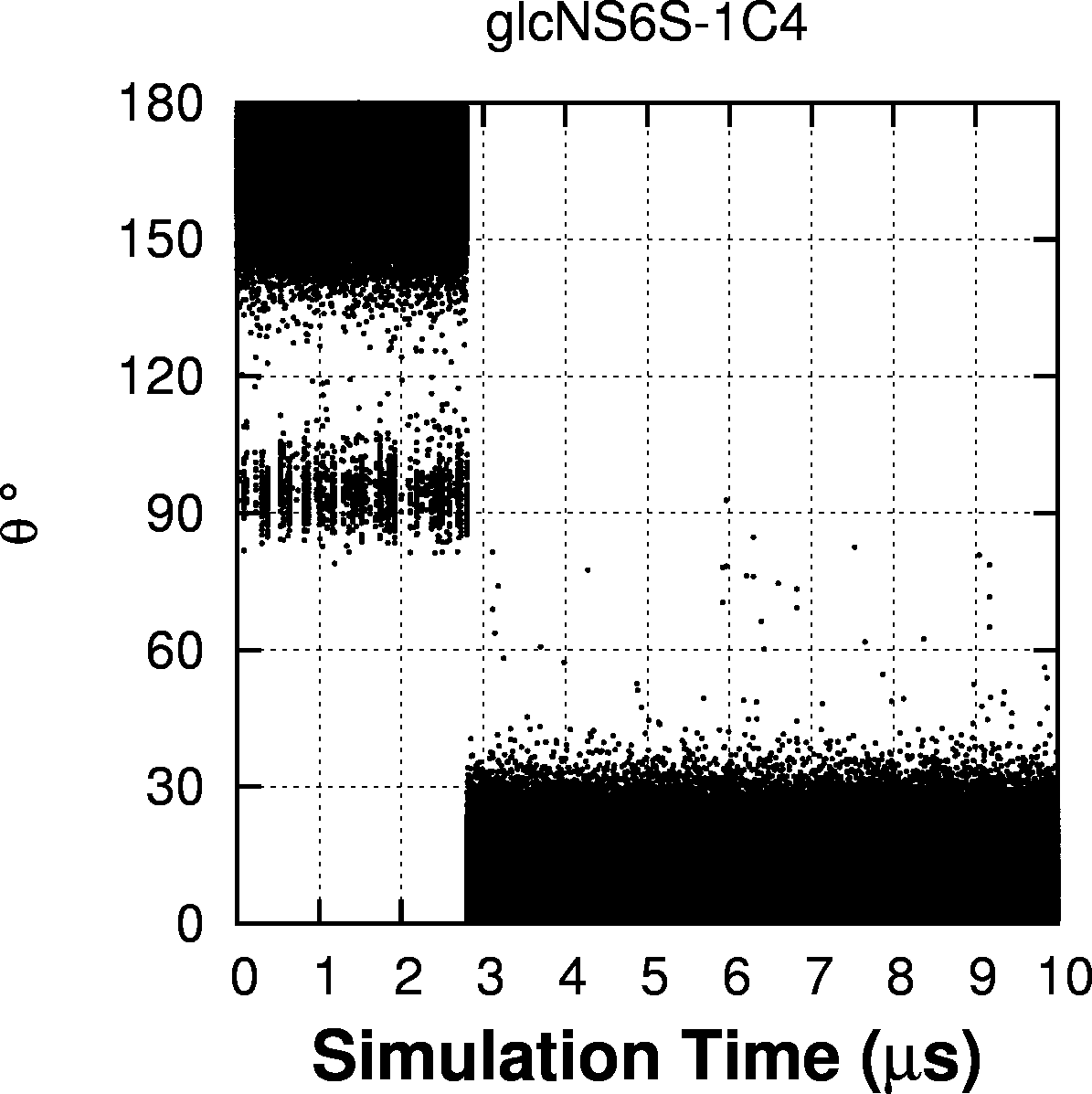
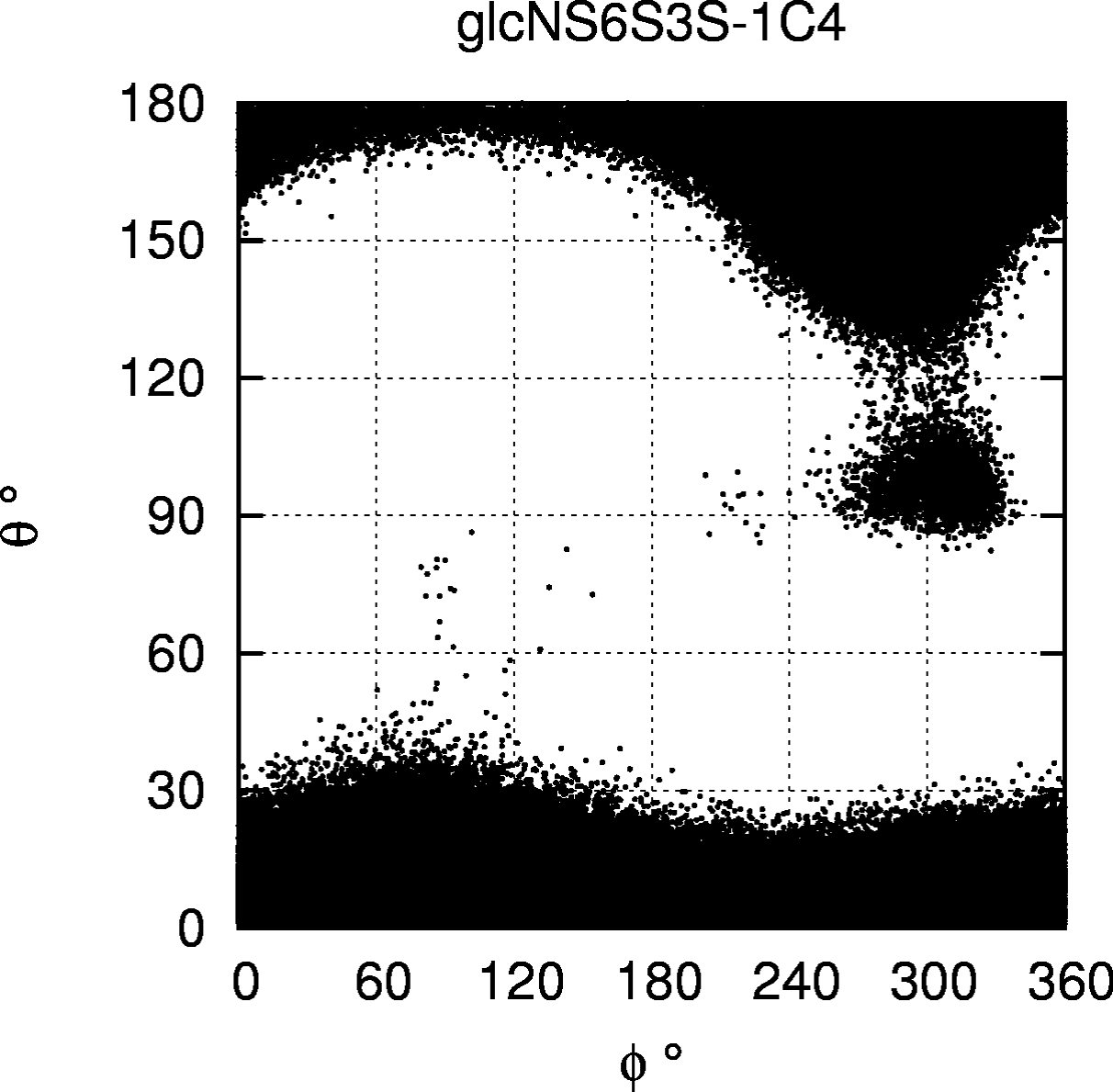
150
120
90
60
30
0
θ °
0
60
120
180
240
300
360
ϕ °


glcNS6S-1C4
Q
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0 1 2 3 4 5 6 7 8 9 10
Simulation Time (μs)


glcNS6S-1C4
180
150
120
90
60
30
0
θ°
0
1
2
3
4
5
6
7
8
9
10
Simulation Time (μs)


glcNS6S3S-1C4
180
150
120
90
60
30
0
θ °
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60
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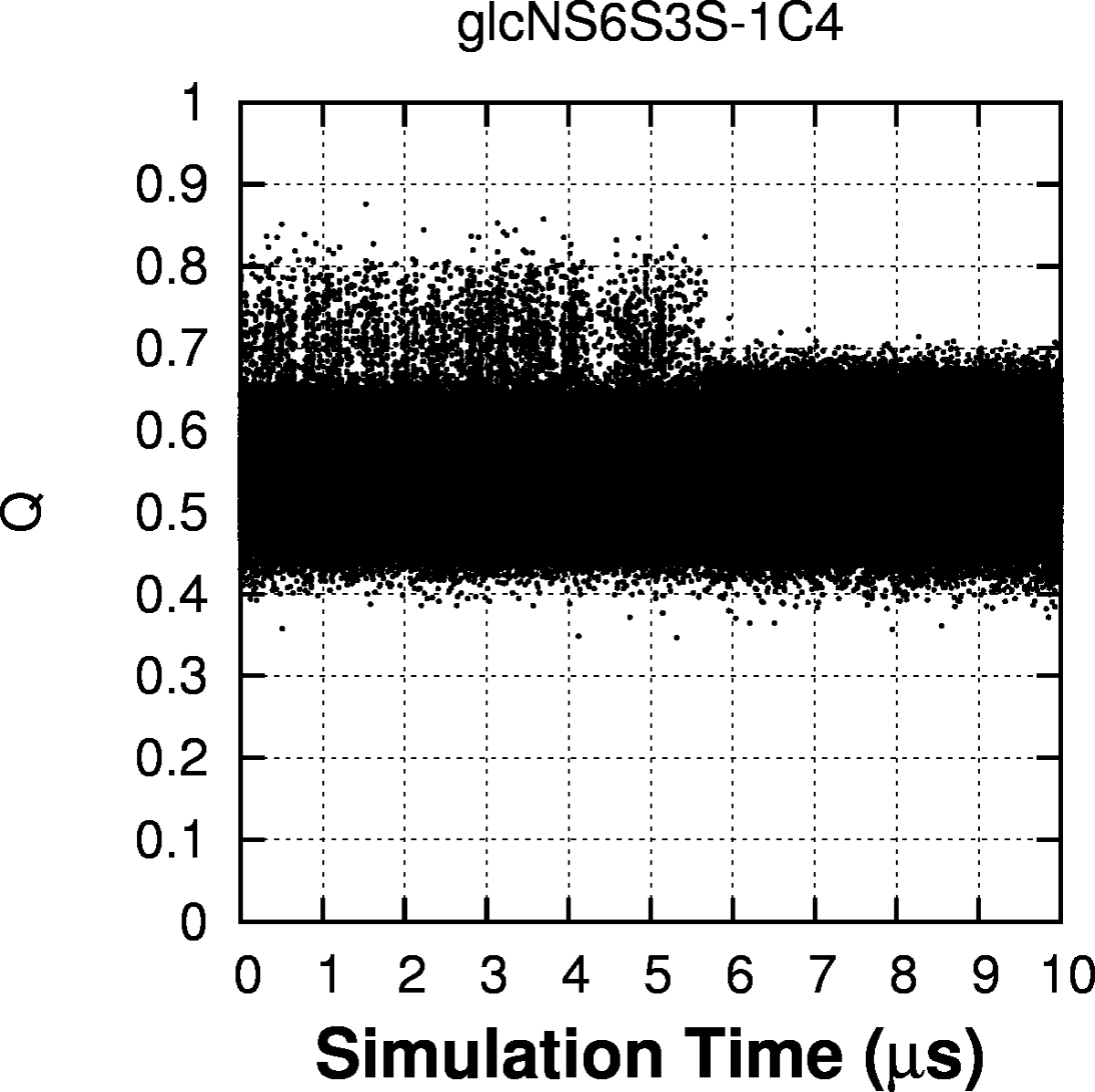
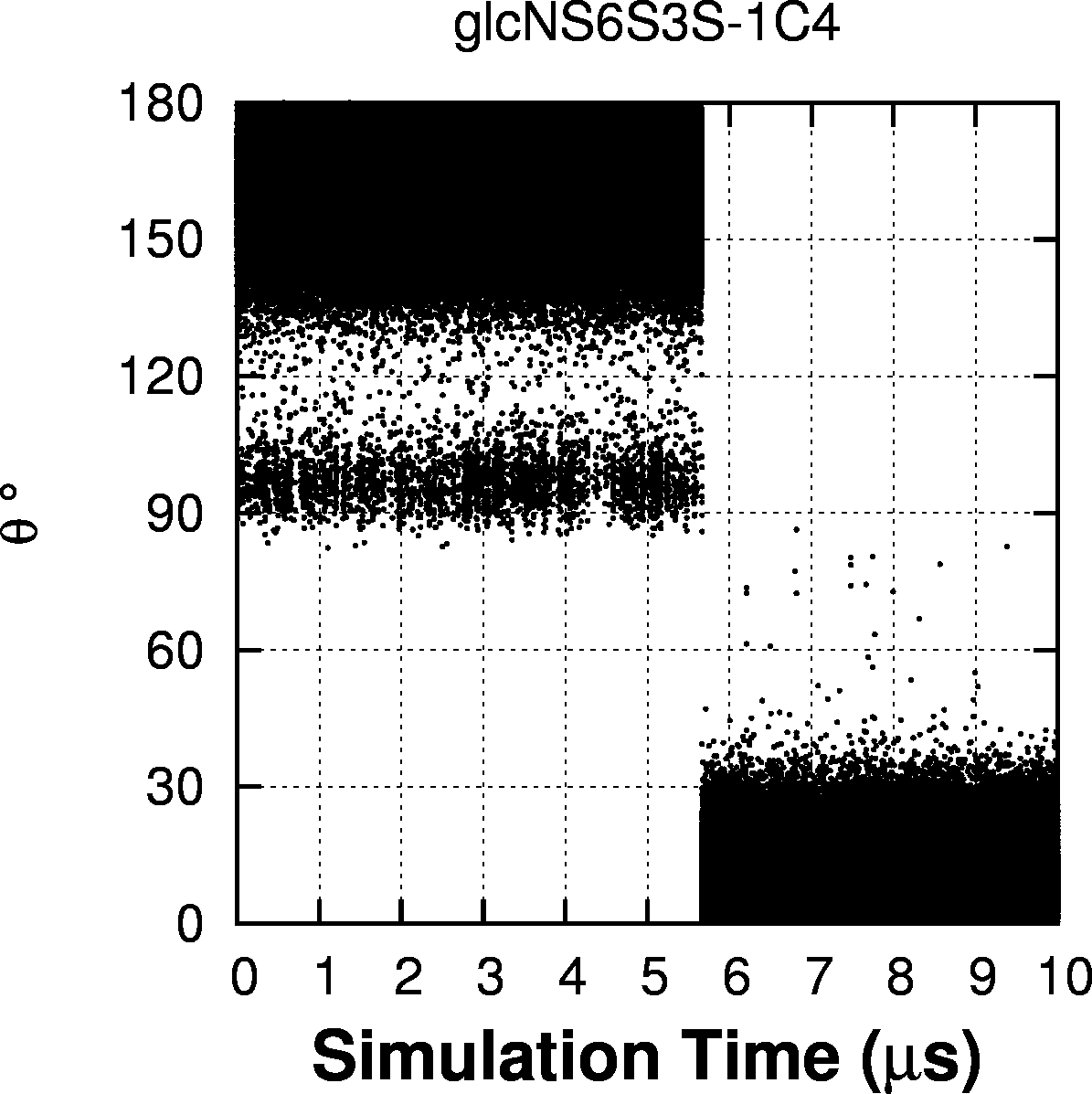
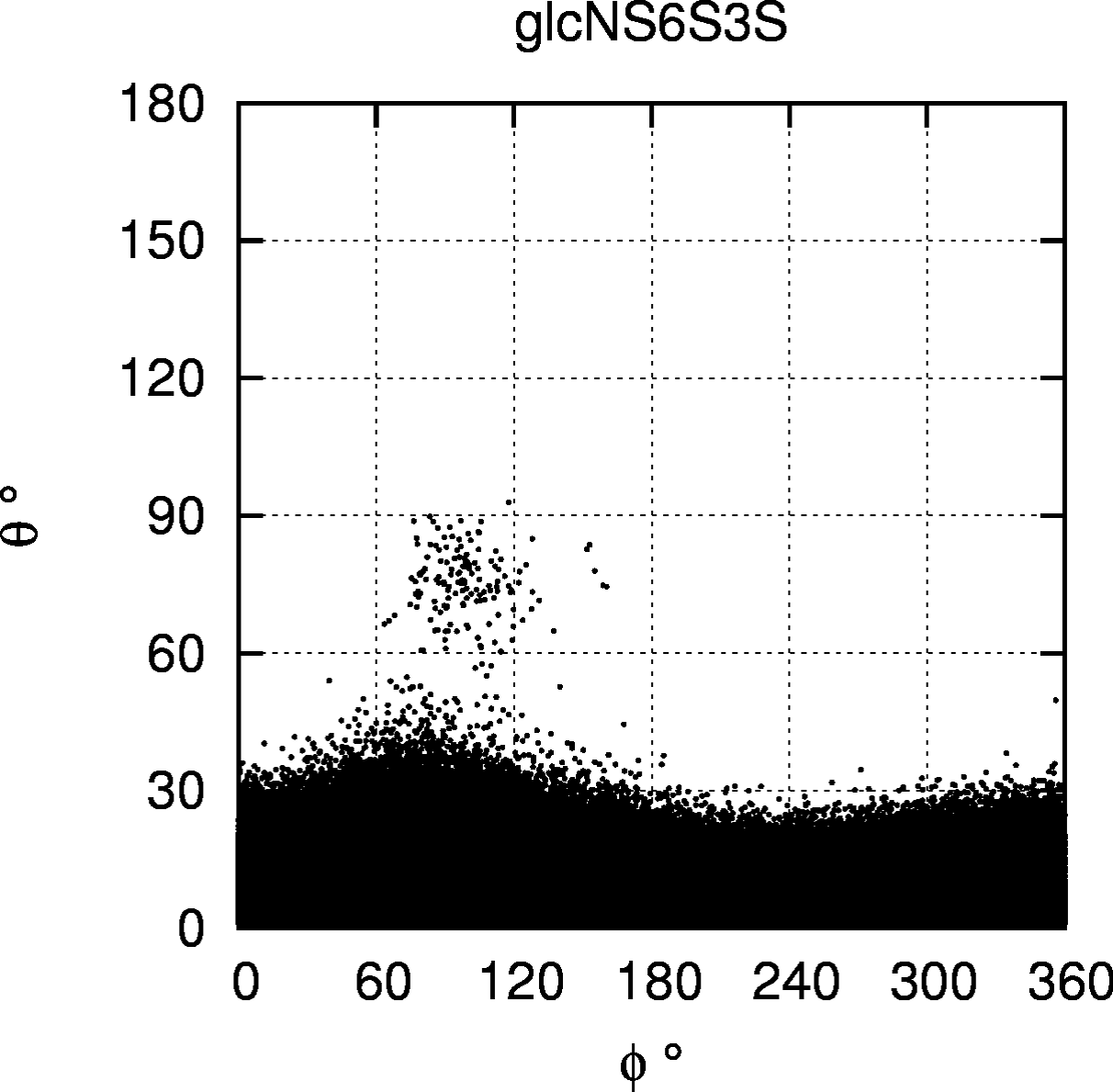
180
240
300
360
ϕ °


glcNS6S3S-1C4
Q
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0 1 2 3 4 5 6 7 8 9 10
Simulation Time (μs)


glcNS6S3S-1C4
180
150
120
90
60
30
0
θ°
0
1
2
3
4
5
6
7
8
9
10
Simulation Time (μs)


glcNS6S3S
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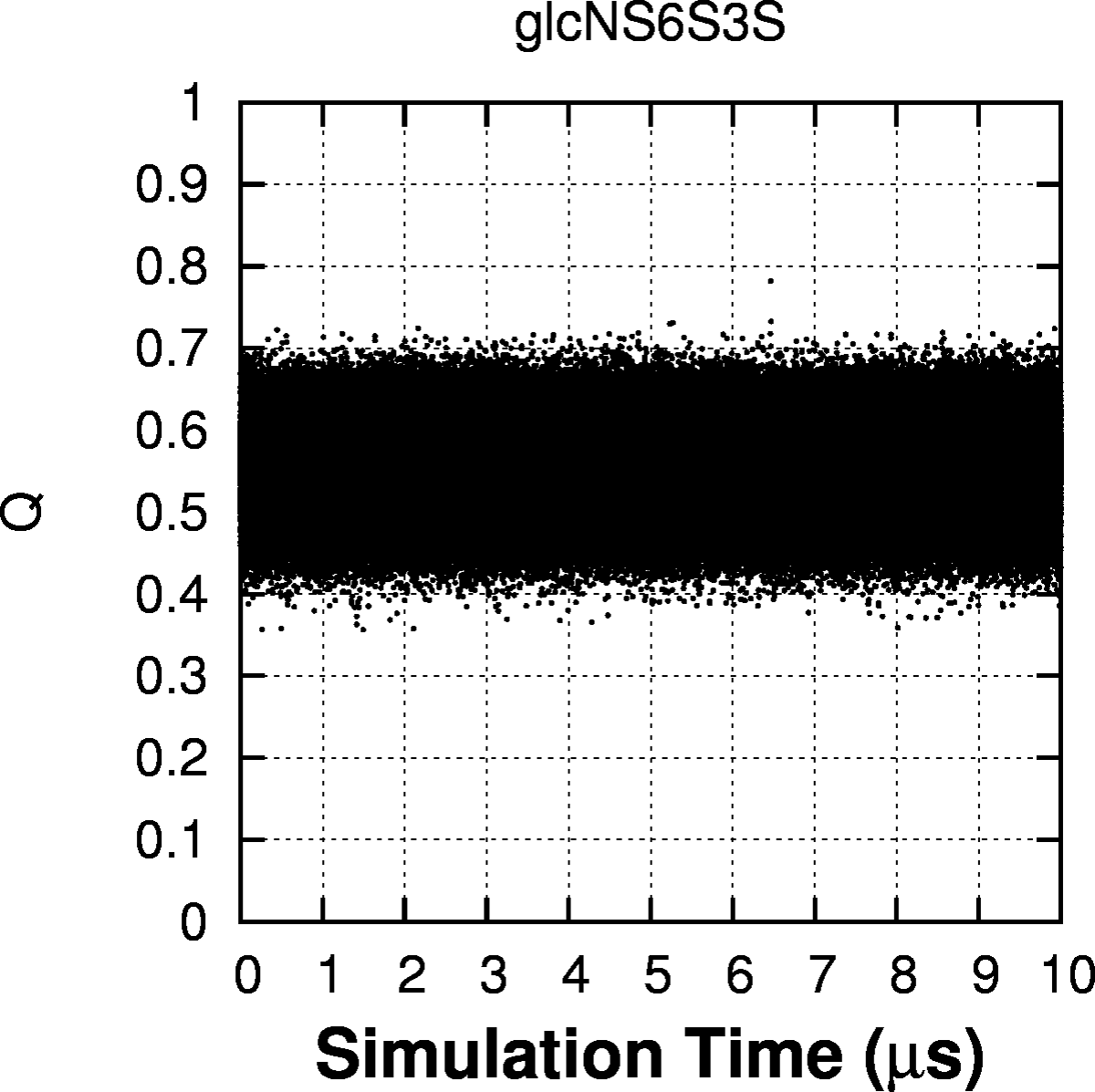
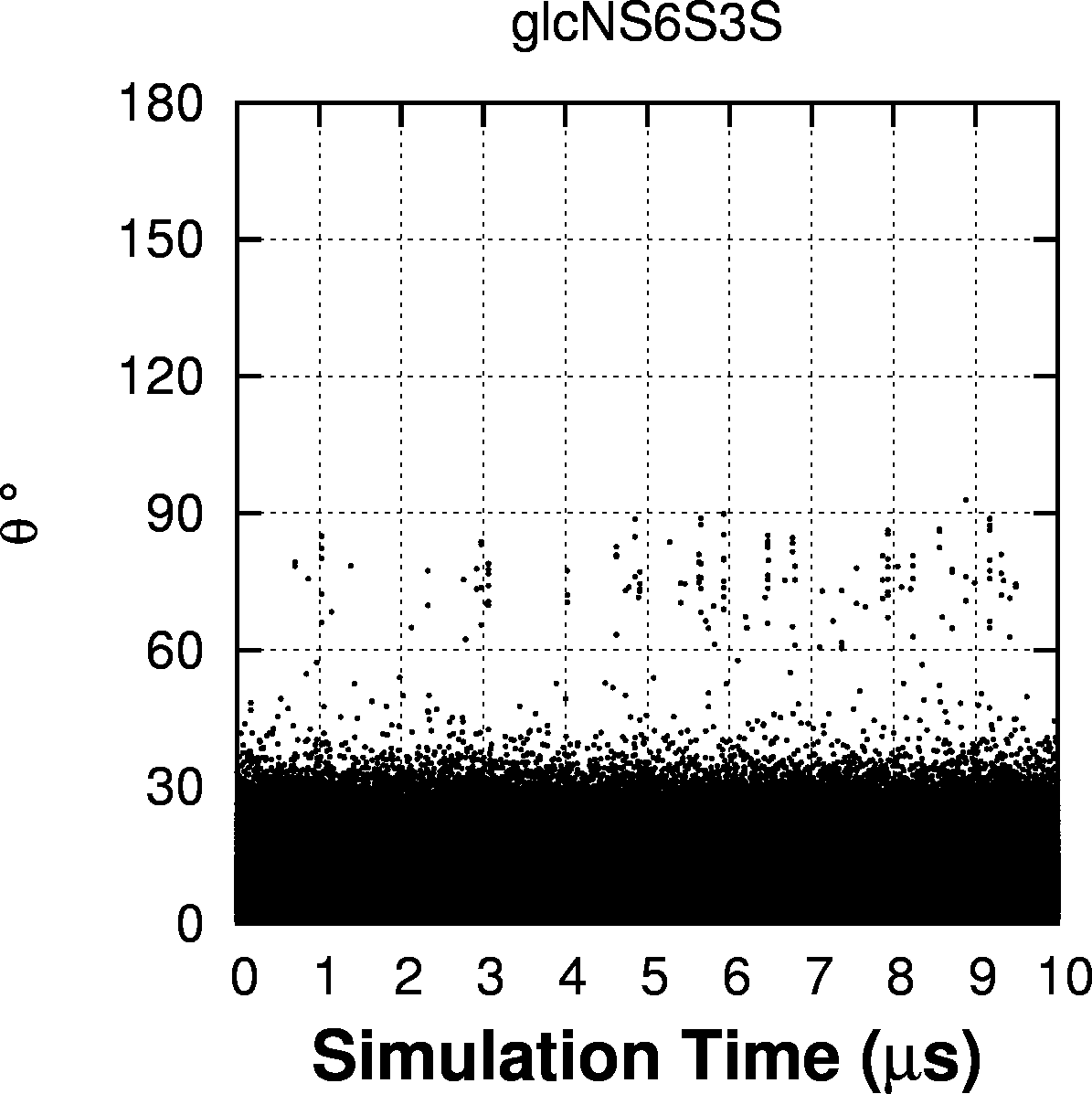
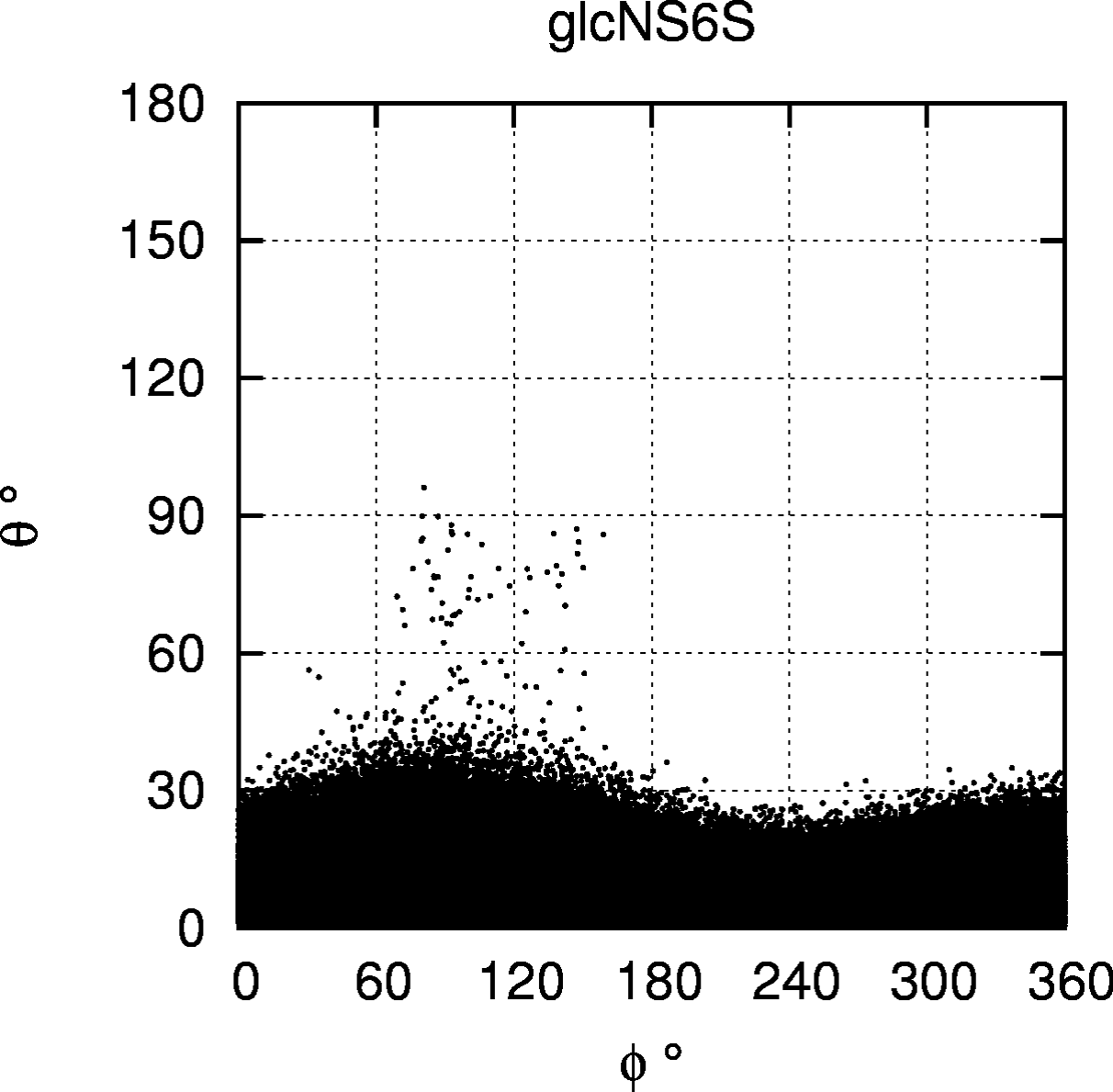
150
120
90
60
30
0
θ°
0
60
120
180
240
300
360
ϕ °


glcNS6S3S
Q
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0
1
2
3
4
5
6
7
8
9
10
Simulation Time (μs)


glcNS6S3S
180
150
120
90
60
30
0
θ°
0
1
2
3
4
5
6
7
8
9
10
Simulation Time (μs)


glcNS6S
180
150
120
90
60
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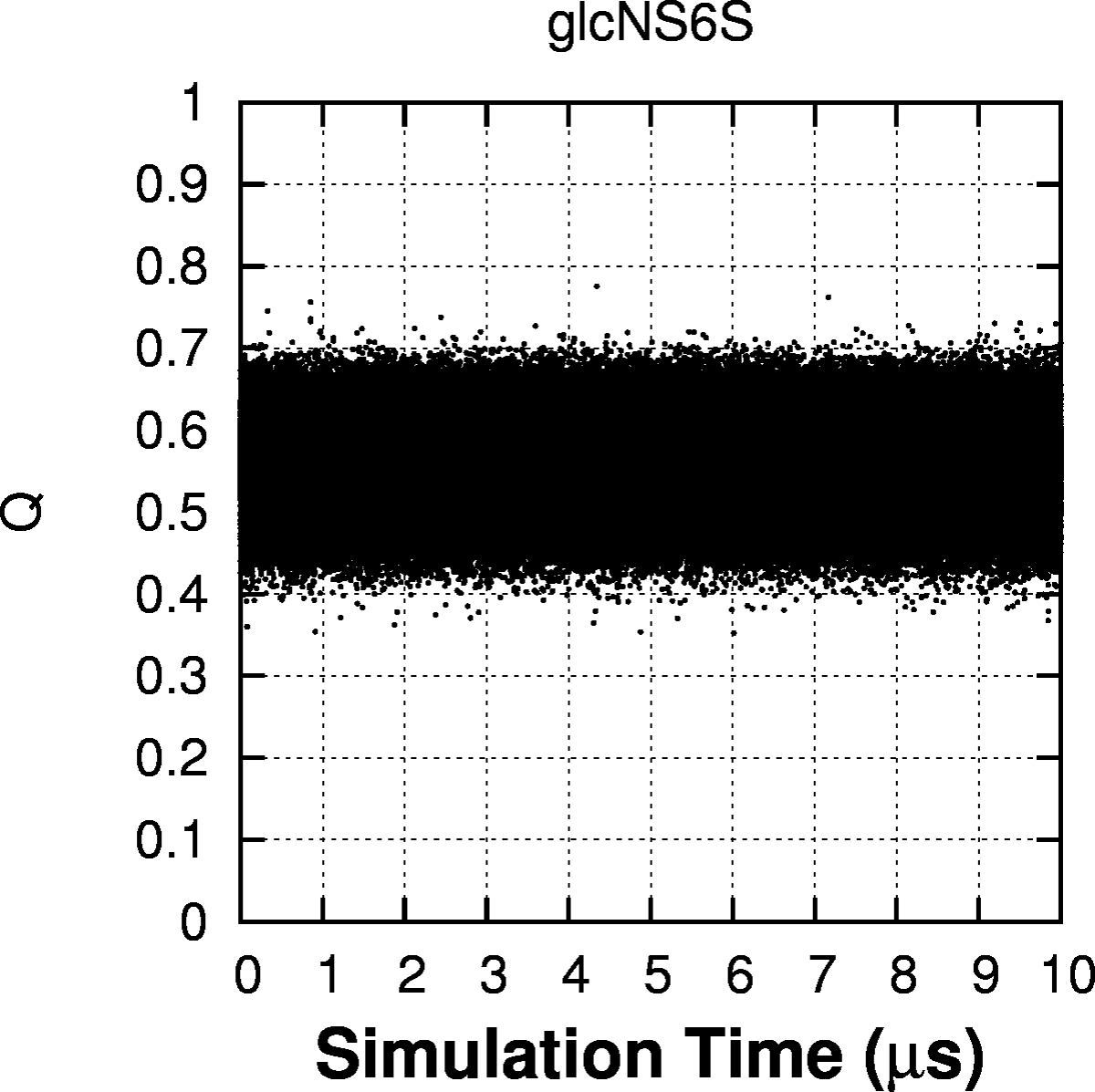
θ °
0
60
120
180
240
300
360
ϕ °


glcNS6S
Q
1
0.9
0.8
0.7
0.6
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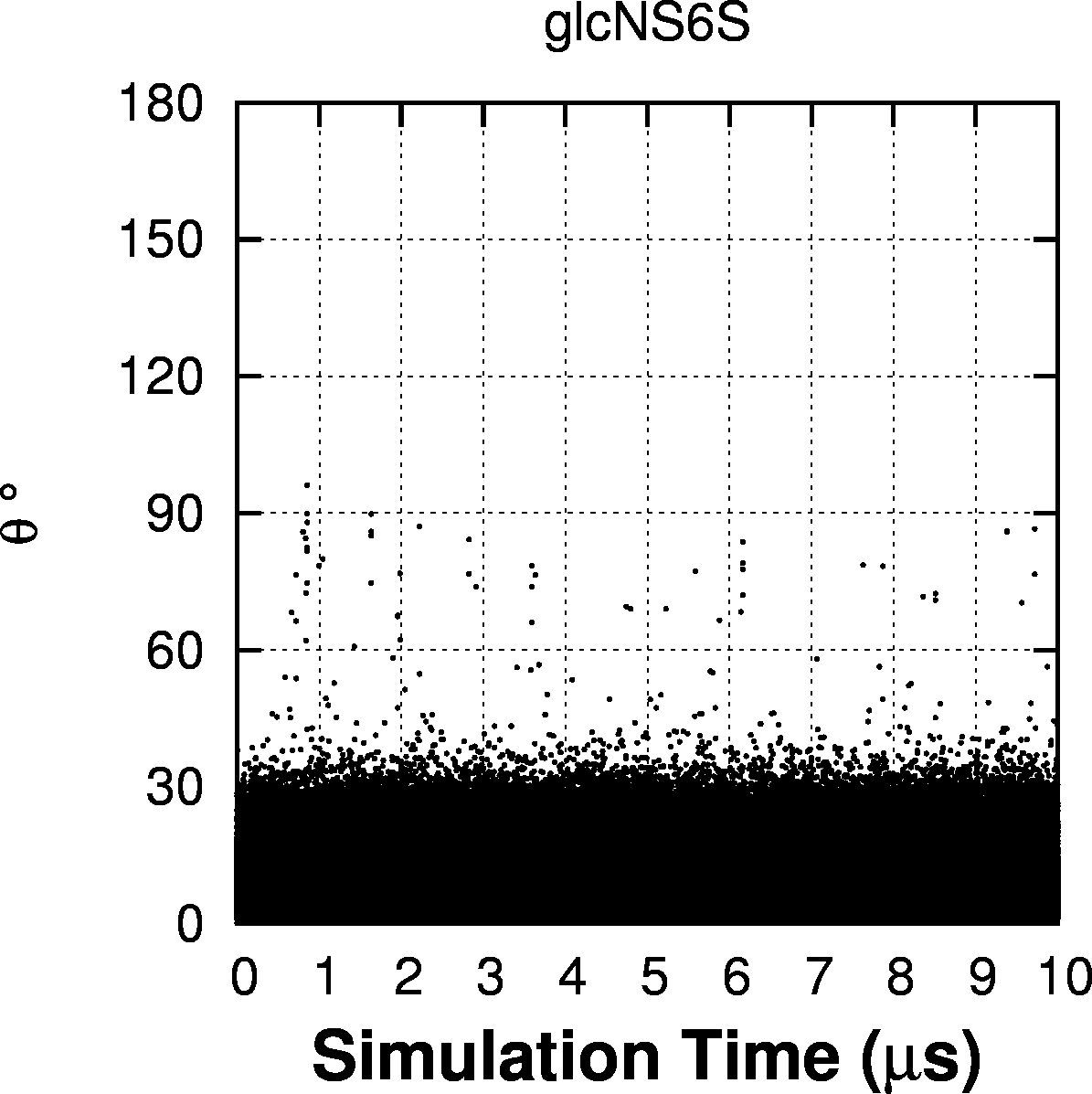
0.2
0.1
0
0 1 2 3 4 5 6 7 8 9 10
Simulation Time (μs)


glcNS6S
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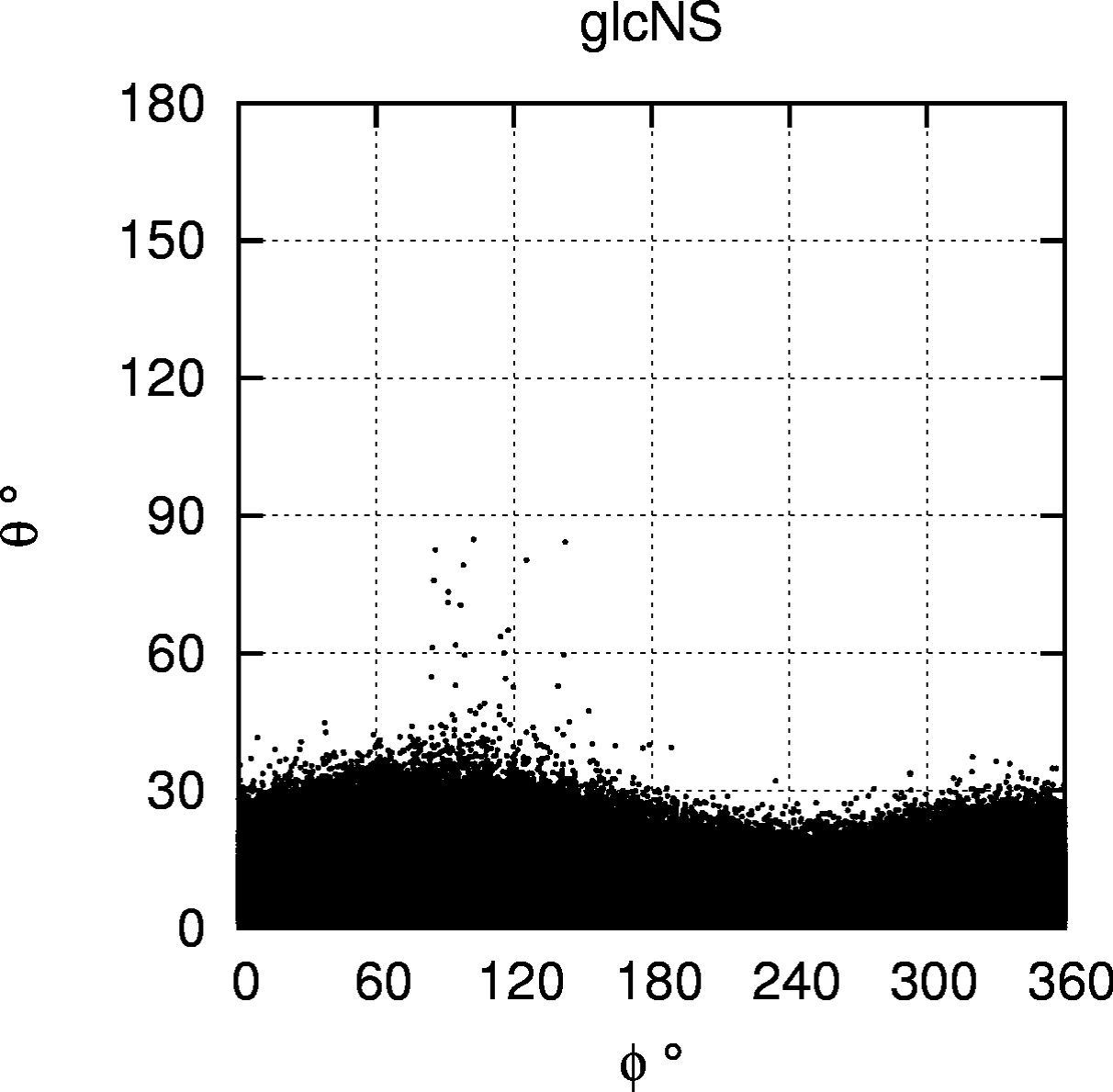
Simulation Time (μs)


glcNS
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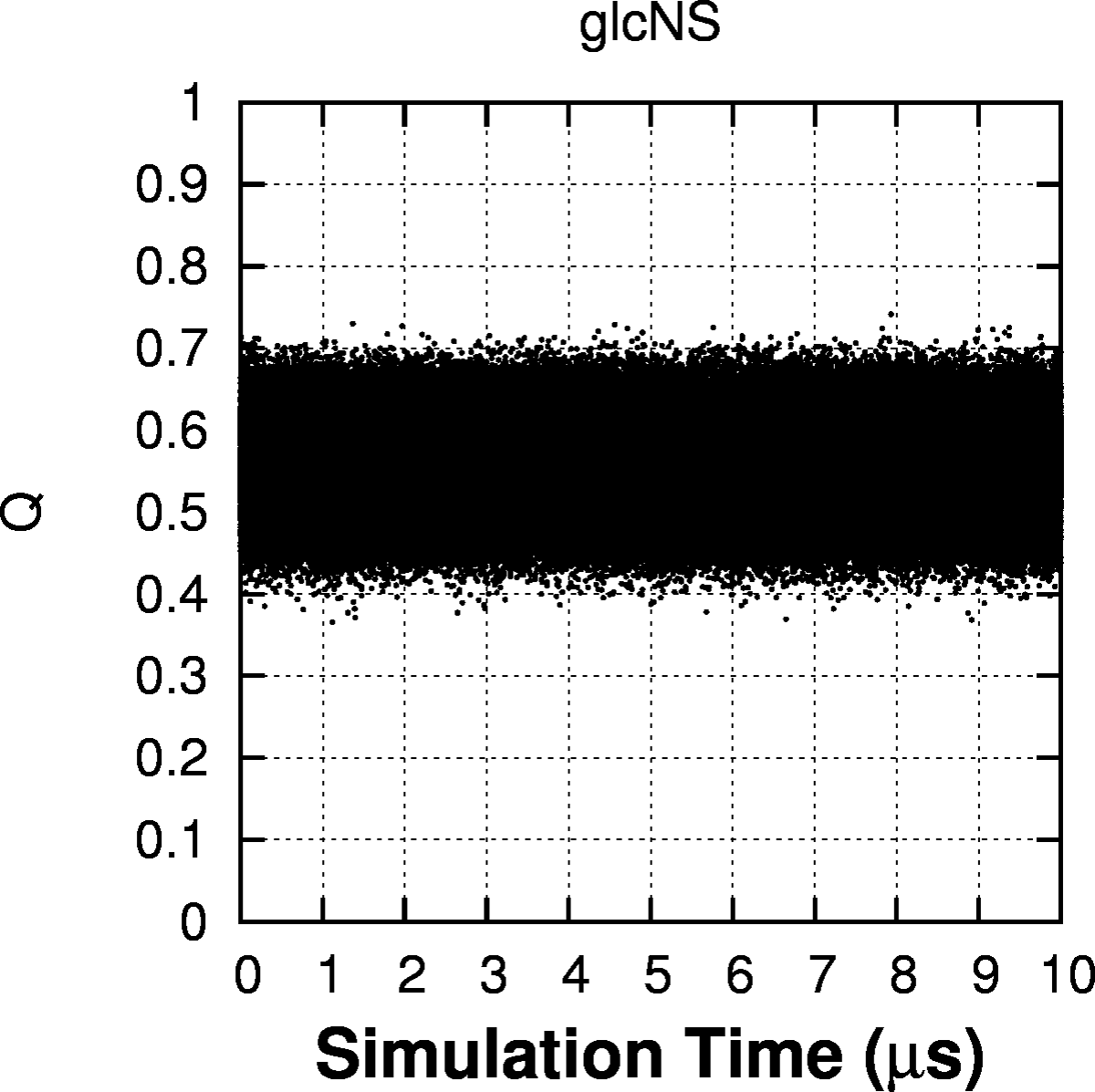
ϕ °


glcNS
Q
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0.3
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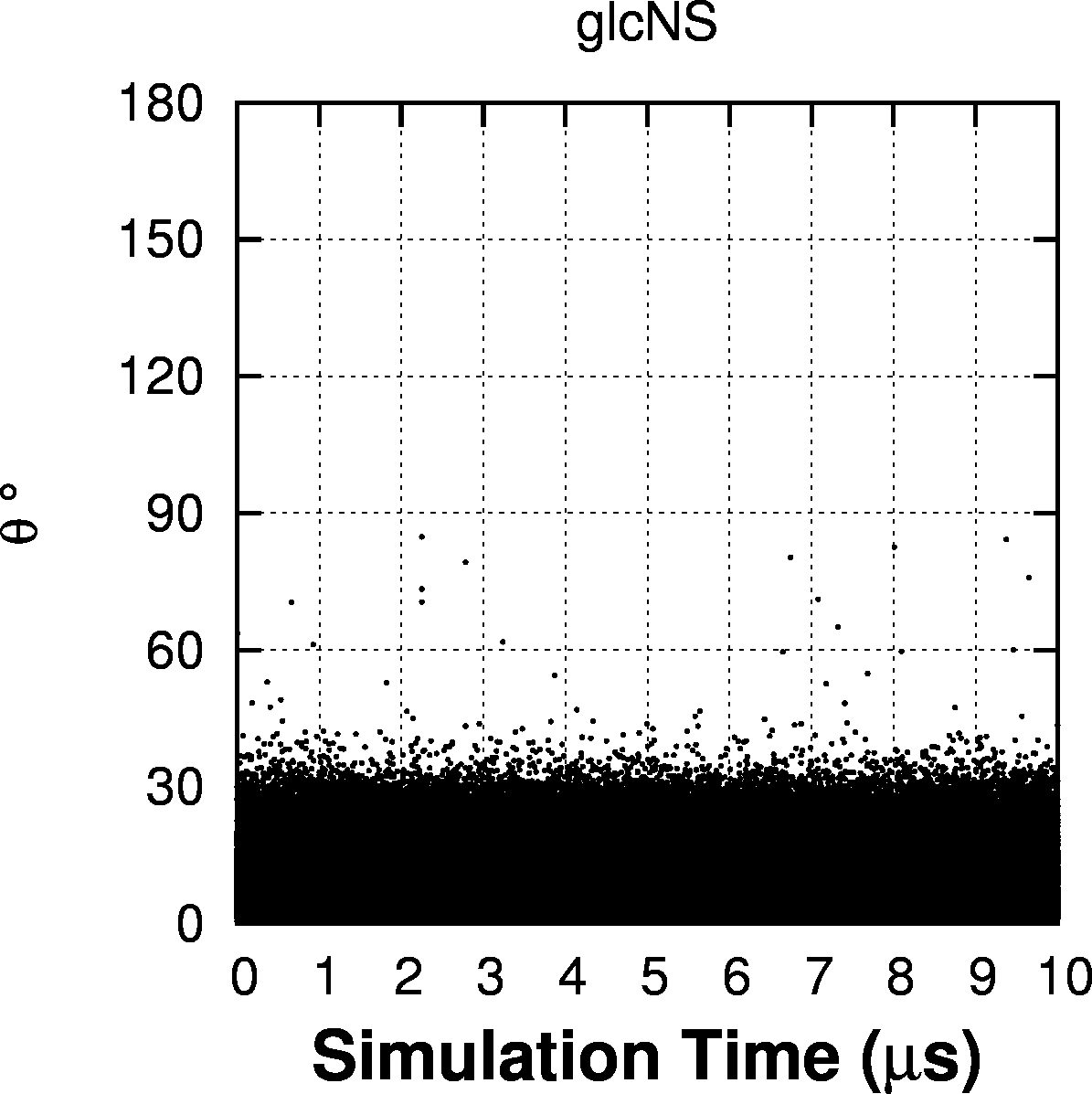
0 1 2 3 4 5 6 7 8 9 10
Simulation Time (μs)


glcNS
180
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θ°
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1
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Simulation Time (μs)