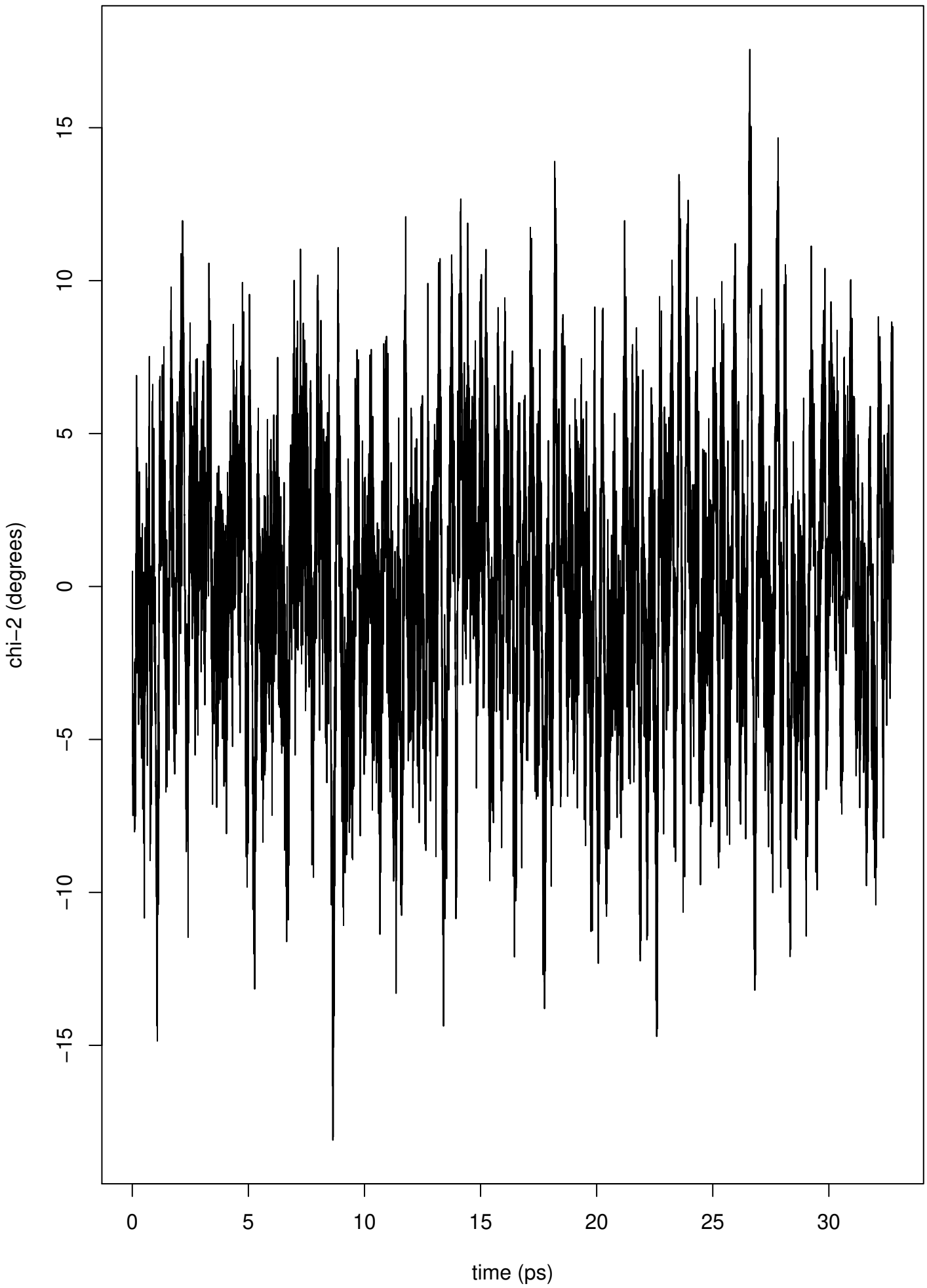
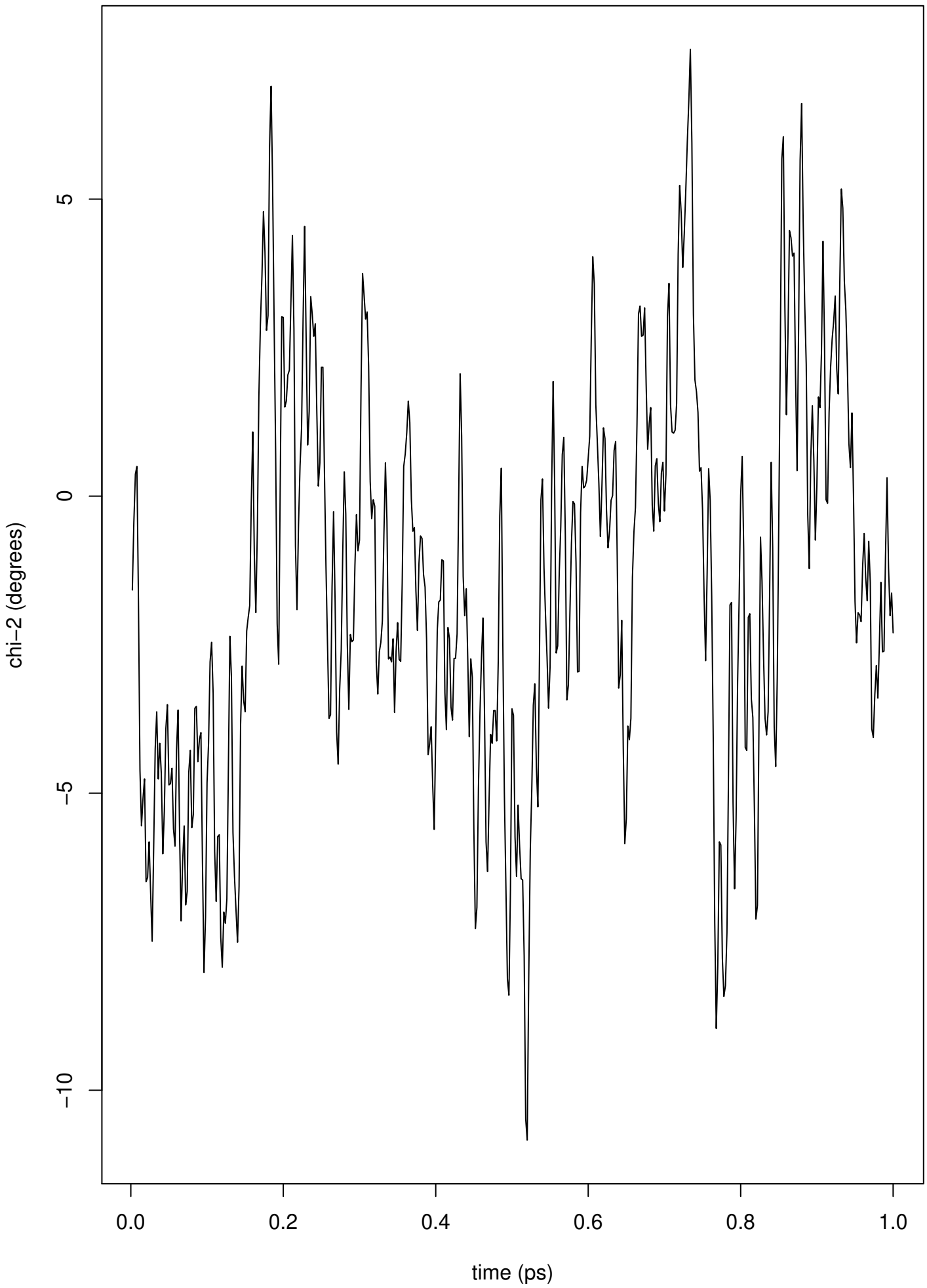
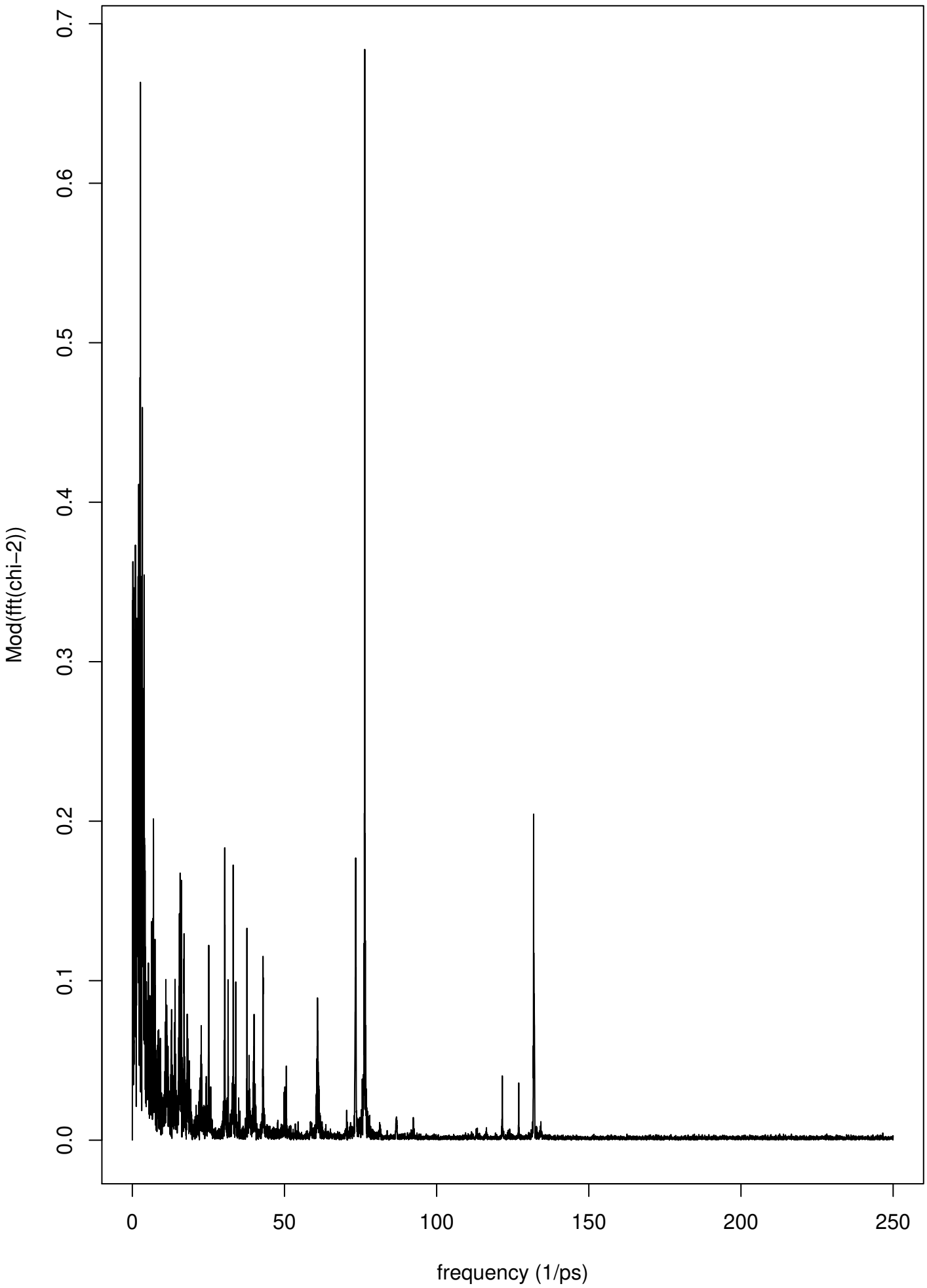
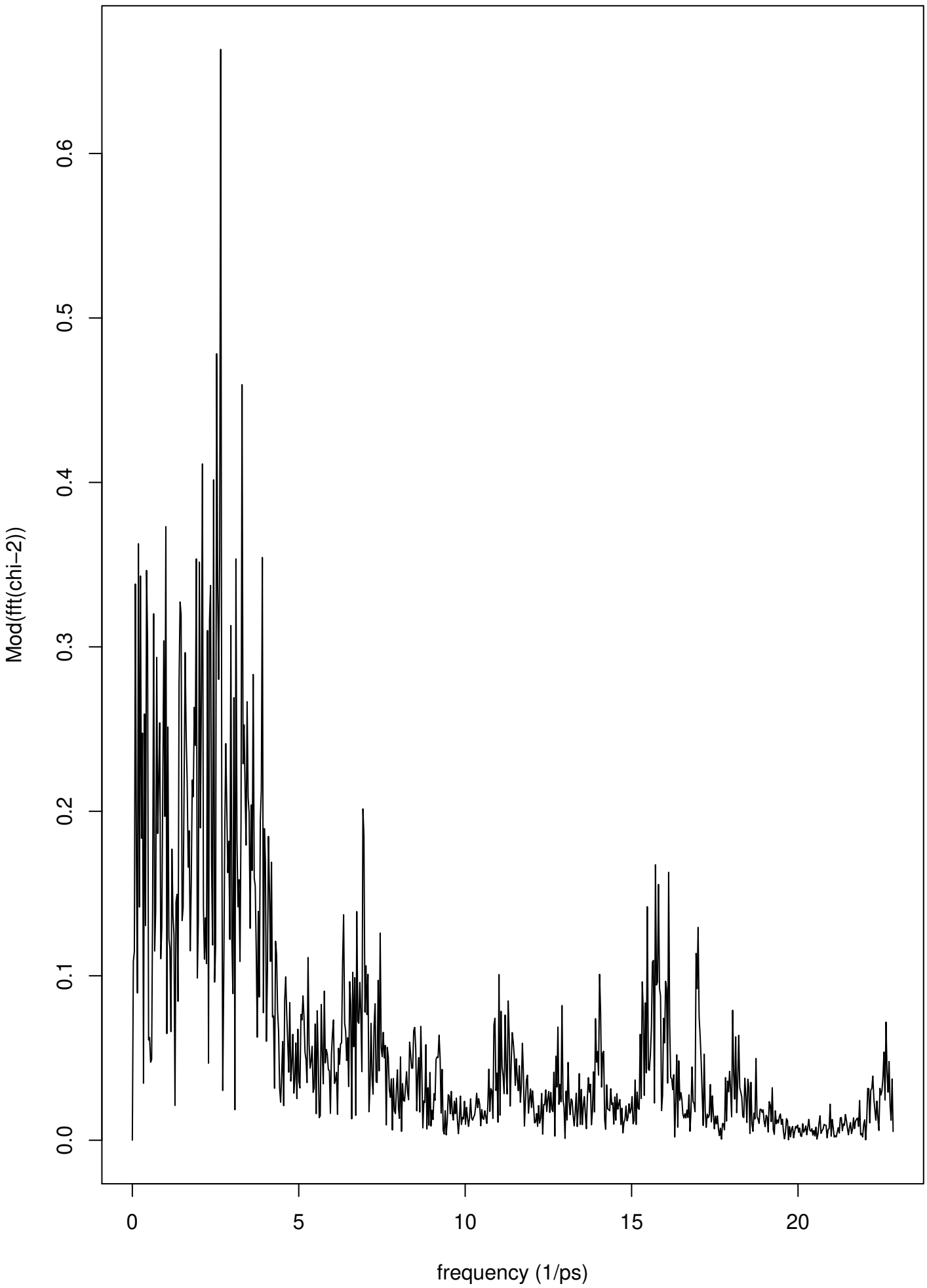
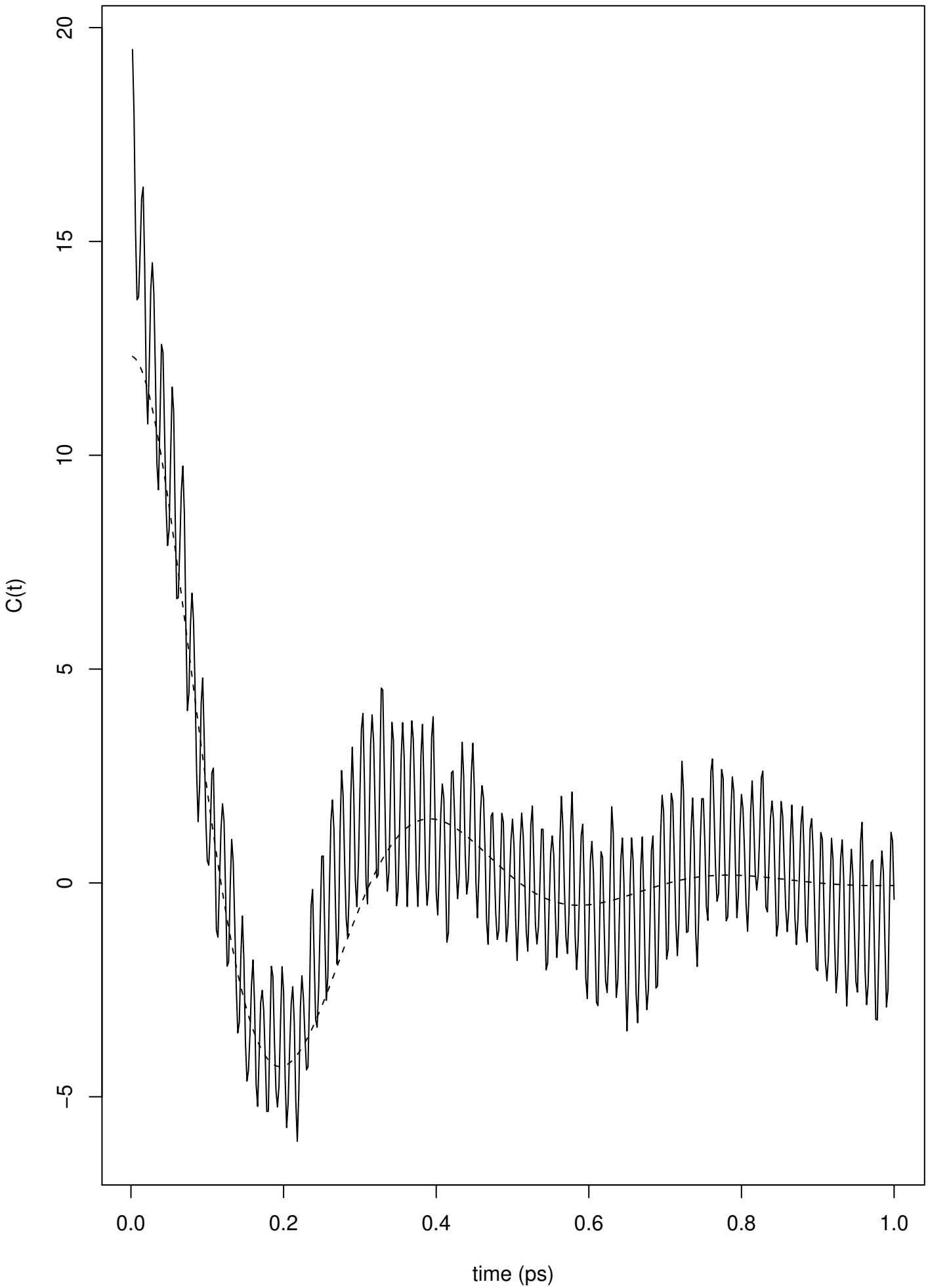

Trajectory of chi−2 of Tyr−35, from 32 ps MD simulation
chi−2 (degrees)
15
10
5
0
−5
−10
−15
0
5
10
15
20
25
30
time (ps)


Trajectory of chi−2 of Tyr−35, from 32 ps MD simulation
chi−2 (degrees)
5
0
−5
−10
0.0
0.2
0.4
0.6
0.8
1.0
time (ps)


Fourier transform of trajectory of chi−2 of Tyr−35
Mod(fft(chi−2))
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0
50
100
150
200
250
frequency (1/ps)


Fourier transform of trajectory of chi−2 of Tyr−35
Mod(fft(chi−2))
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0
5
10
15
20
frequency (1/ps)


Correlation func. C(t) for trajectory of chi−2 of Tyr−35
(dashed line, fitted values from Brownian relaxation model)
C(t)
20
15
10
5
0
−5
0.0
0.2
0.4
0.6
0.8
1.0
time (ps)