(a)
Atomistic pvpH (Target)
Fourier Fit (4 terms)
U (Dihedral)
H-B-B′-H′ Dihedral [Degree]
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
0
60
120
180
240
300
360
(b)
Atomistic pvpY (Target)
Fourier Fit (4 terms)
U (Dihedral)
B-B′-B″-B‴ Dihedral [Degree]
1.5
1.0
0.5
0.0
-0.5
0
60
120
180
240
300
360