biases

colvars

components

harmonic restraint:
$$\frac{1}{2} K \left[(d-d_0(t))^2/w_d^2 + (c-c_0(t))^2/w_c^2 \right]$$

histogram:
(alpha, c)

colvar "d"
$(d_1 - d_2)$

colvar "c"
(coord)

colvar "alpha"
(alpha)

distance "d_1":
atoms [1, 2] [3-5]
($C = 1.0$, $p = 1$)

distance "d_2":
atoms [7] [8-10]
($C = -1.0$, $p = 1$)

coord. num. "coord":
atoms [1-10] [11-20]
radius 6 Å

alpha helix "alpha":
residues [1-10]