LJ8: learned CV = func(NN(sort(cnum)))

Set A: func < 0.1, contains min 2;   set B: func > 0.9, contains min 1

BETA = 10.0

FFS:

$k_{AB} = 0.722$, $\text{std}(k_{AB}) = 0.024$
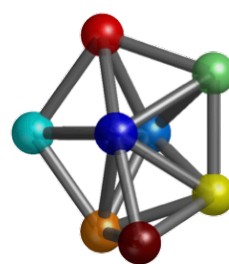
CPU time = 23 min (1400 seconds)

Brute Force:

$k_{AB} = 0.739$, $\text{std}(k_{AB}) = 0.010$

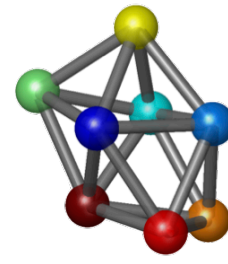$k_{BA} = 0.117$, $\text{std}(k_{BA}) = 0.005$

$\rho_A = 0.137$, $\text{std}(\rho_A) = 0.005$

$\rho_B = 0.863$, $\text{std}(\rho_B) = 0.005$

CPU time = 5 hours (18302 seconds)

Minimum 1   Minimum 2