

[1/1] ML_ABN (03 Ru Sr)

file

name ML_ABN
structure groups 1
total structures 675

overview

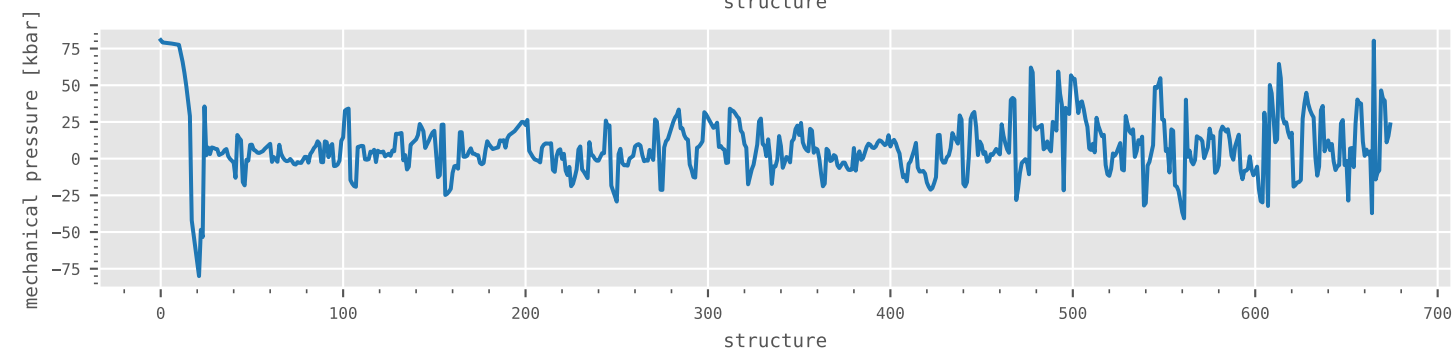
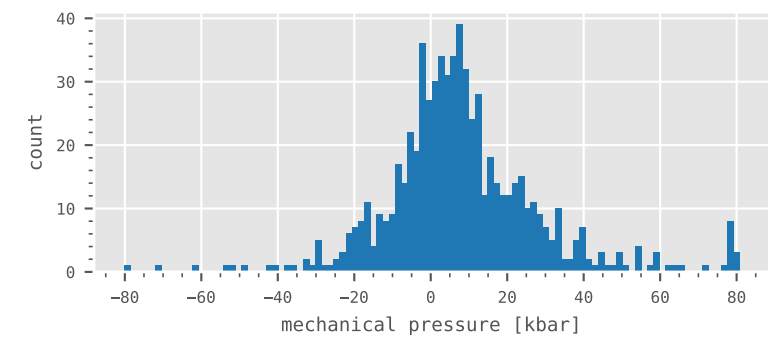
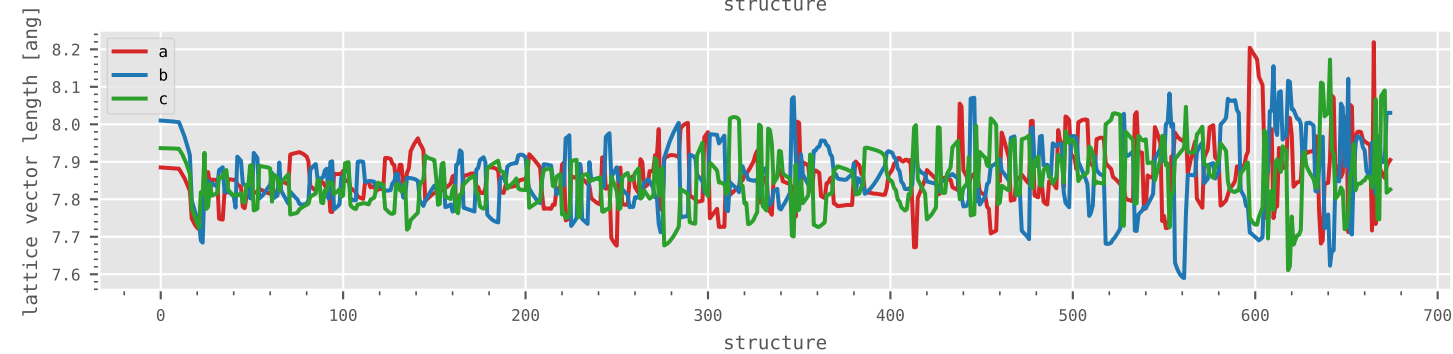
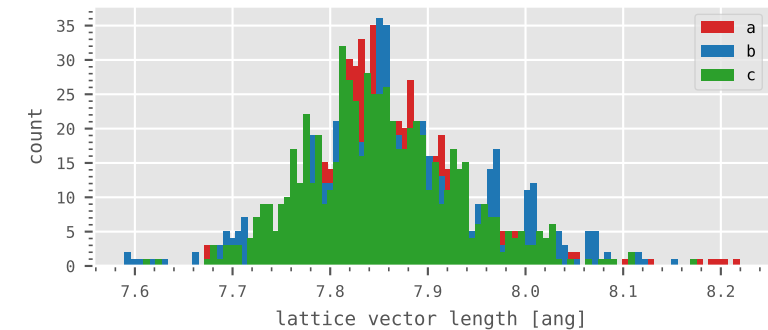
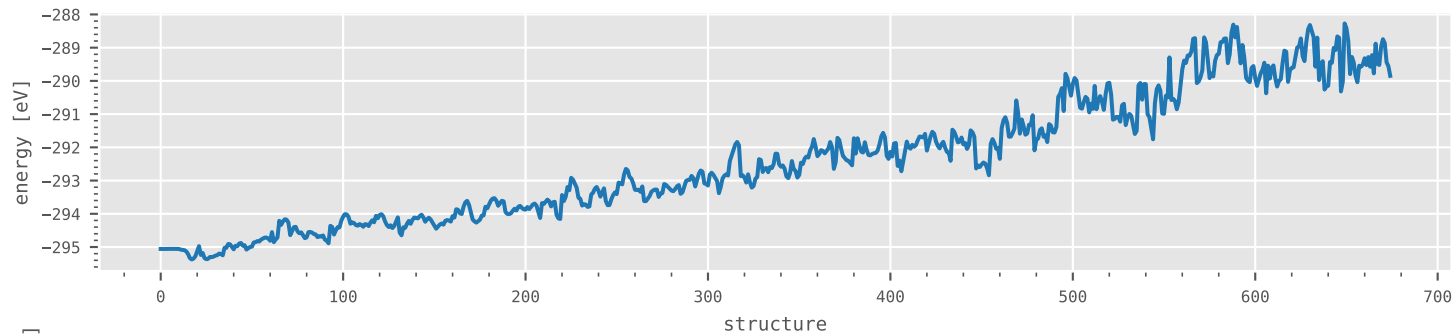
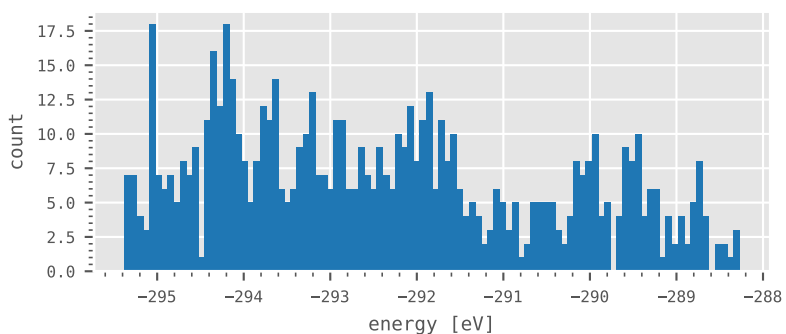
energy -292.4 ± 1.88 eV
volume 485.4 ± 6.63 ang³
lattice vector a 7.9 ± 0.08 ang
lattice vector b 7.9 ± 0.09 ang
lattice vector c 7.9 ± 0.08 ang
non-periodic radius 3.8 (min. for group) ang

min energy configuration



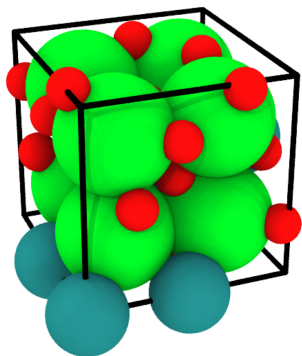
current structure group

name 03 Ru Sr
structure group 1 (of 1 in file)
structures 675 (of 675 in file)
atoms Sr (8), Ru (8), O (24)
40 total

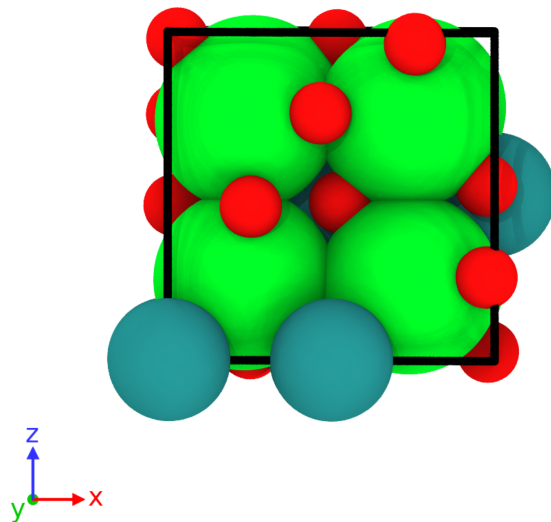


minimum energy configuration (structure 18)

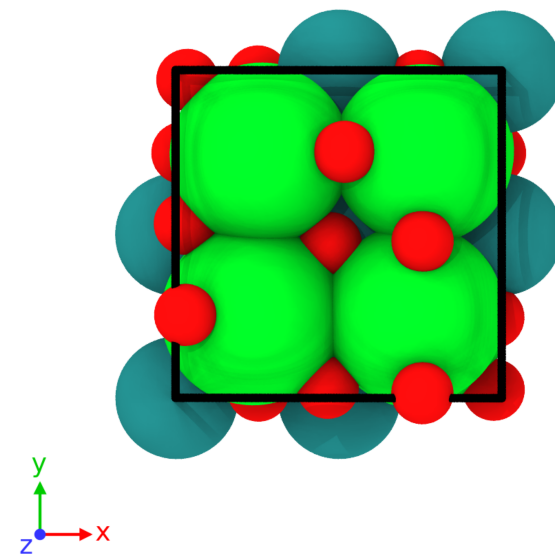
perspective



front

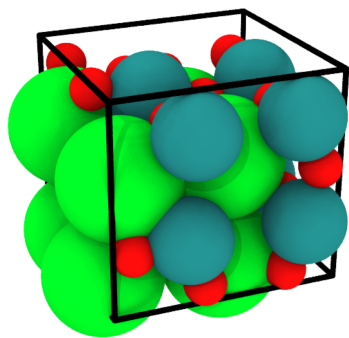


top

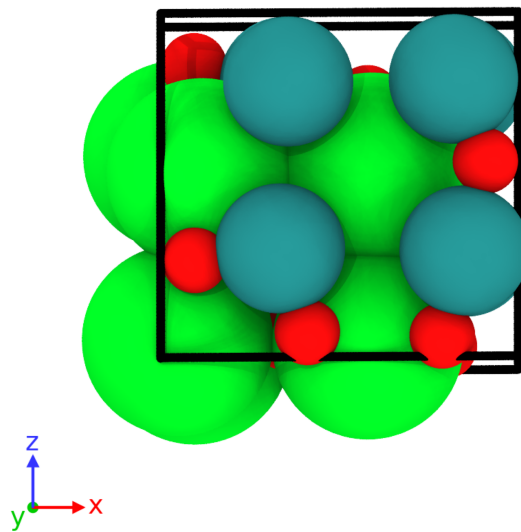


maximum energy configuration (structure 650)

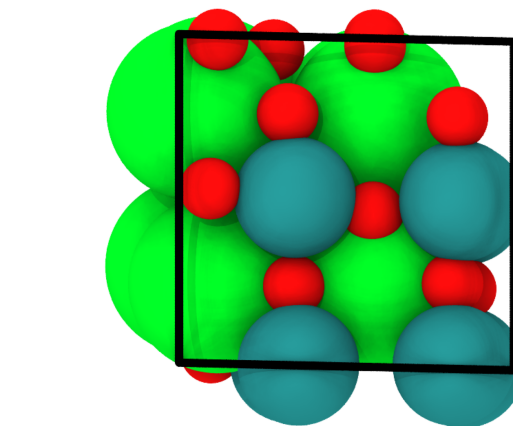
perspective



front



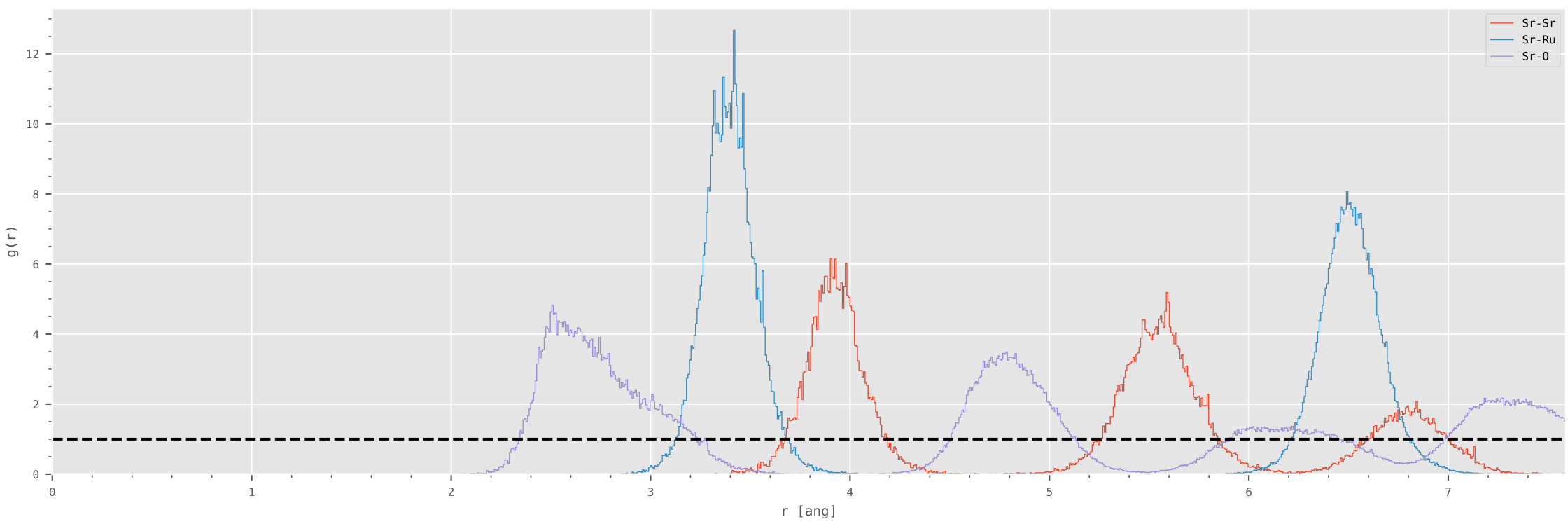
top



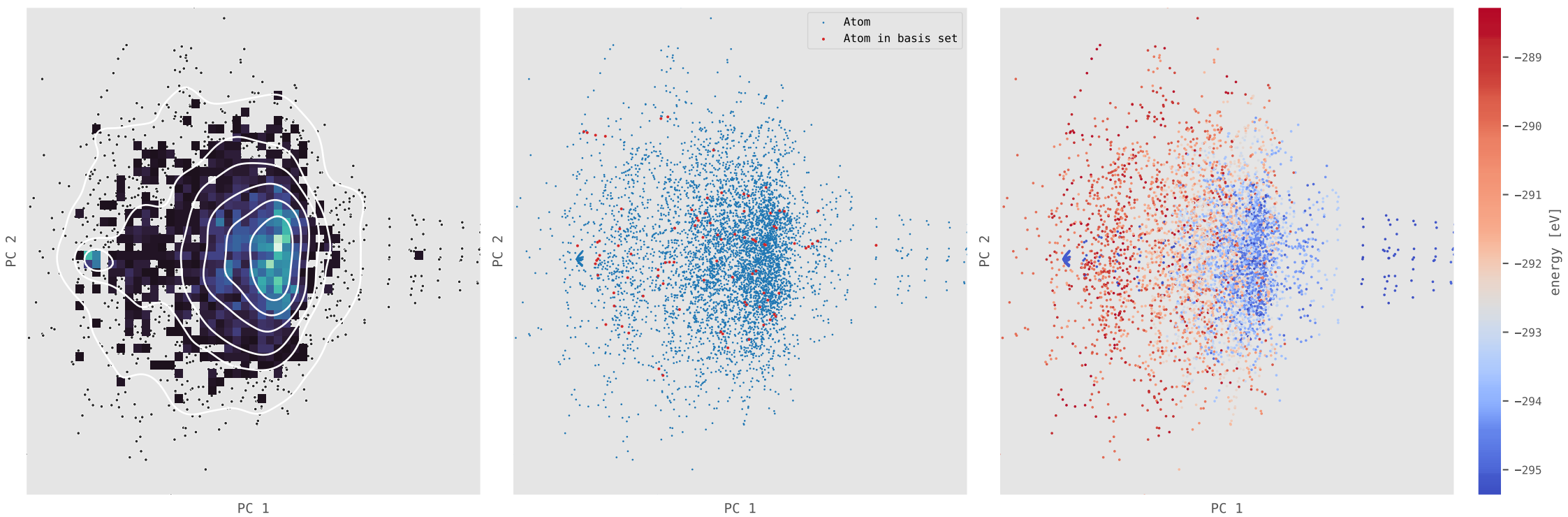
principal component analysis of descriptors (Sr)



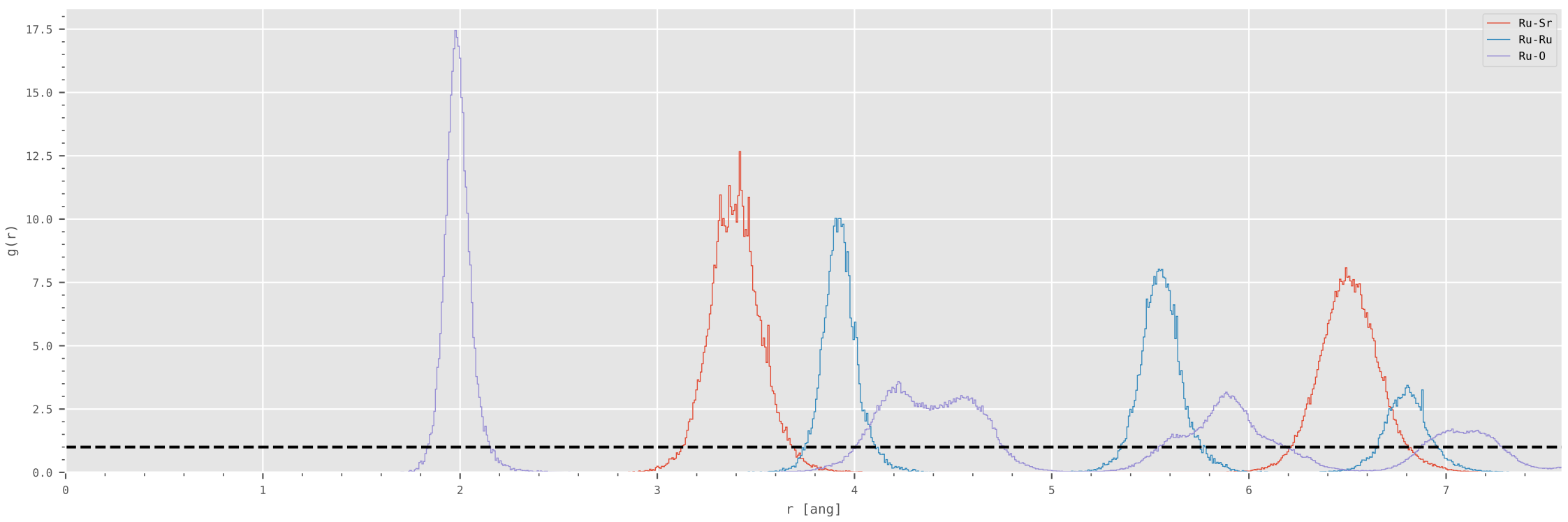
radial distribution functions (Sr)



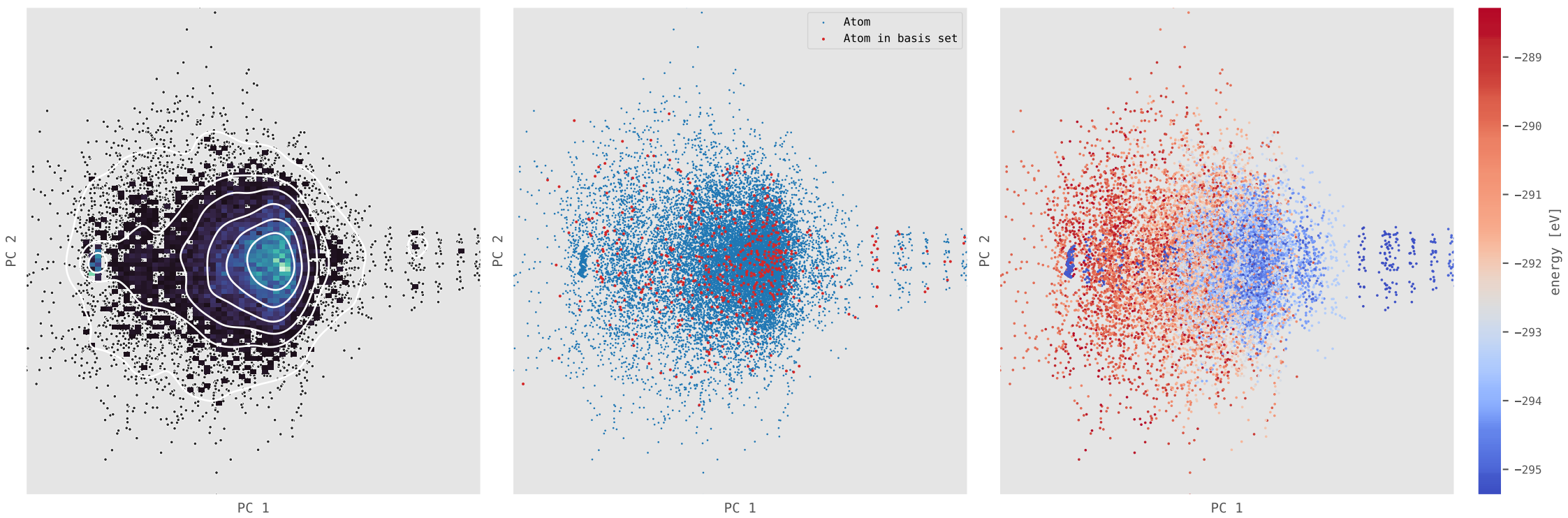
principal component analysis of descriptors (Ru)



radial distribution functions (Ru)



principal component analysis of descriptors (0)



radial distribution functions (0)

