

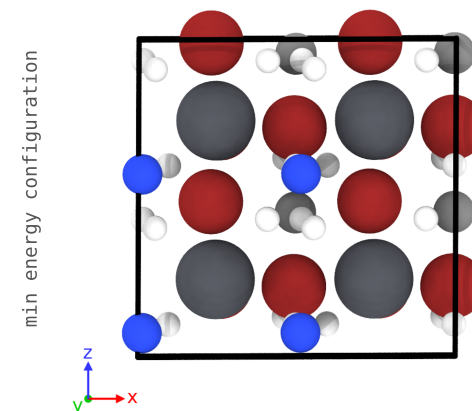
[1/1] ML_ABCAR-MAPbBr3 (Cubic- (SSHS-MAPbBr3))

file

name	ML_ABCAR-MAPbBr3
structure groups	1
total structures	853

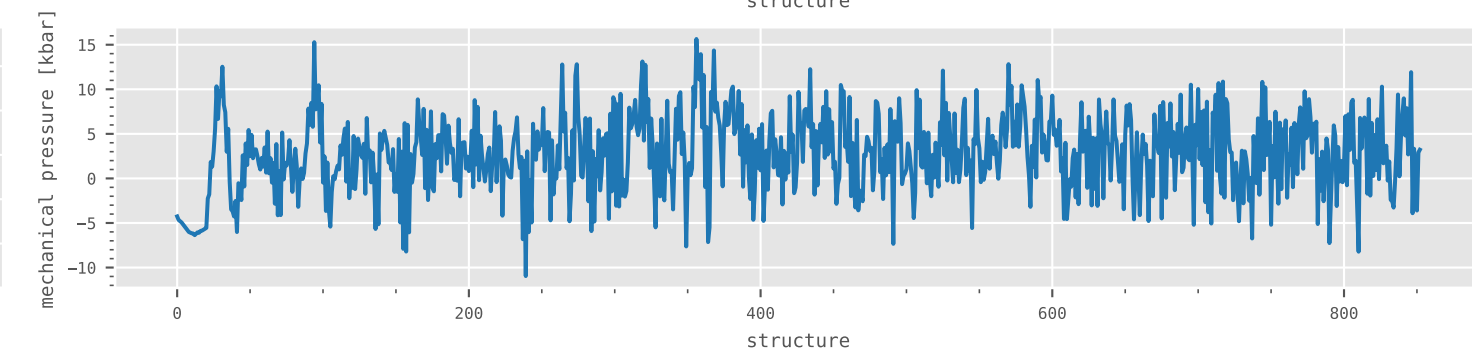
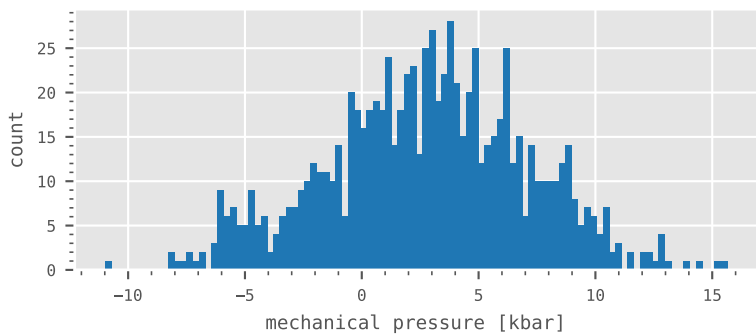
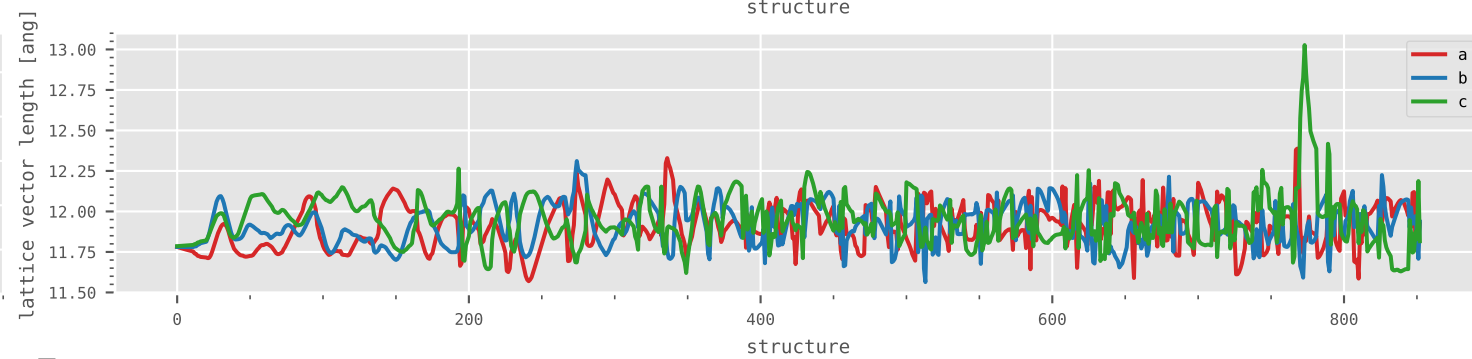
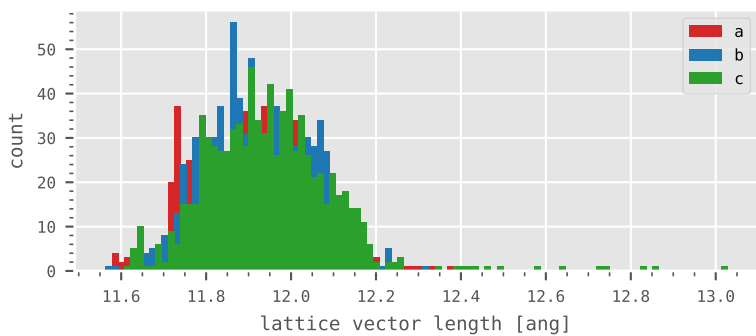
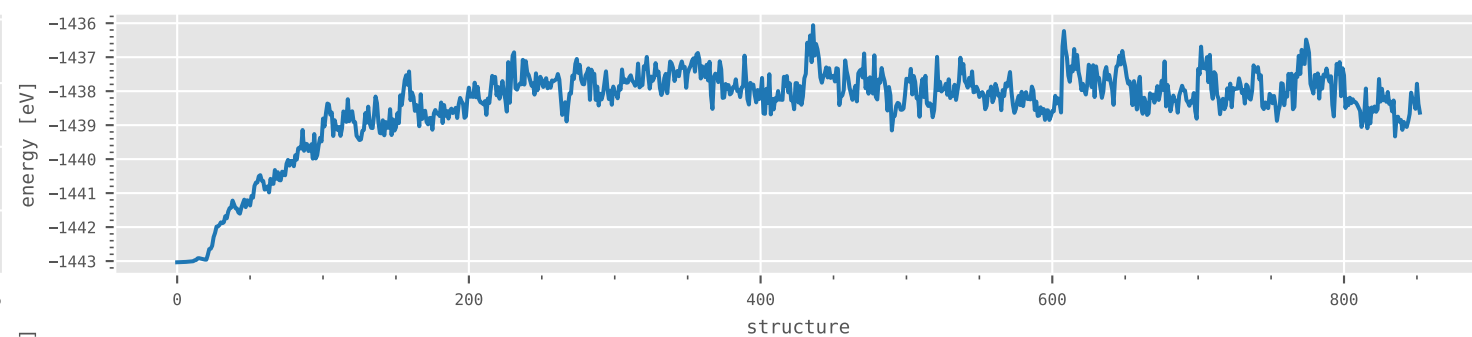
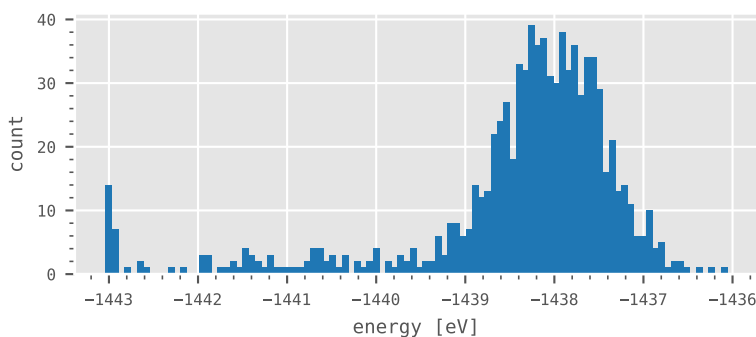
overview

energy	-1438.4 ± 1.24	eV
volume	1696.3 ± 28.10	ang ³
lattice vector a	11.9 ± 0.13	ang
lattice vector b	11.9 ± 0.12	ang
lattice vector c	11.9 ± 0.15	ang
non-periodic radius	5.8 (min. for group)	ang



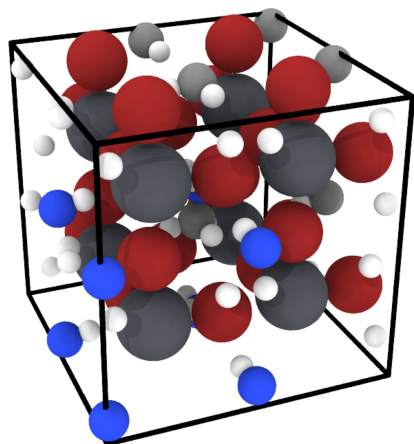
current structure group

name	Cubic- (SSHS-MAPbBr3)
structure group	1 (of 1 in file)
structures	853 (of 853 in file)
atoms	Pb (8), Br (24), C (8), N (8), H (48) 96 total

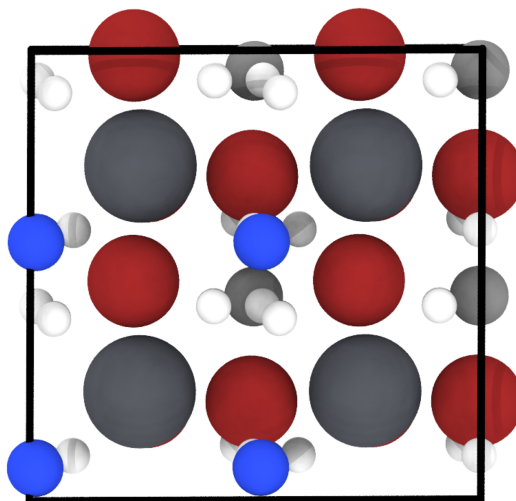
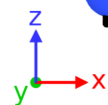


minimum energy configuration (structure 1)

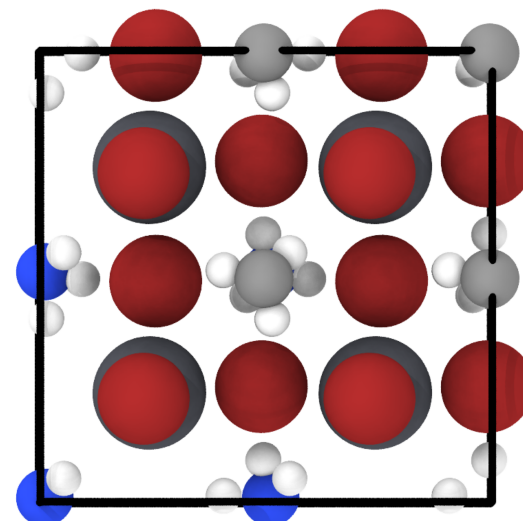
perspective



front

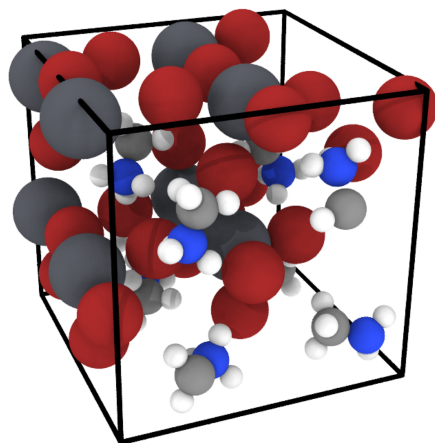


top

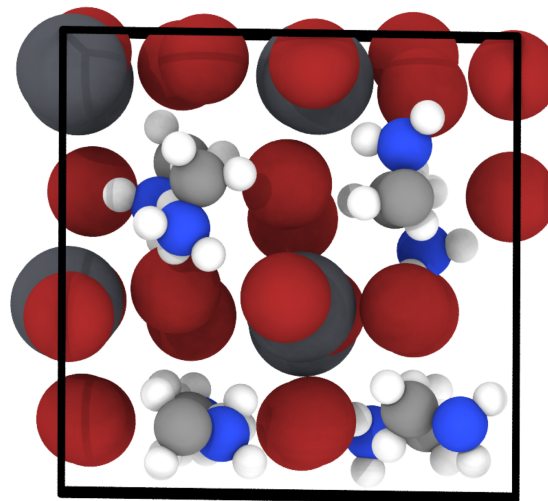
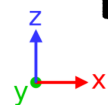


maximum energy configuration (structure 437)

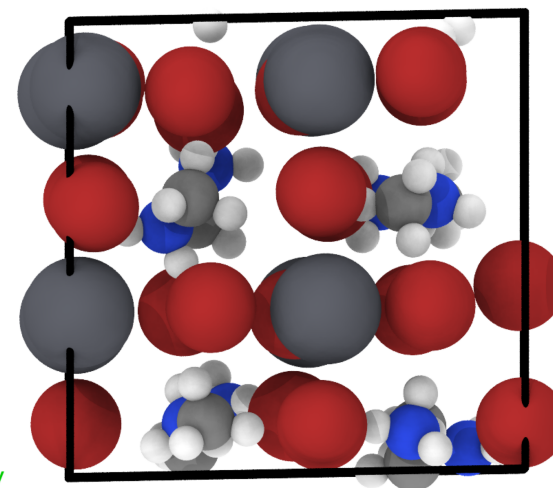
perspective



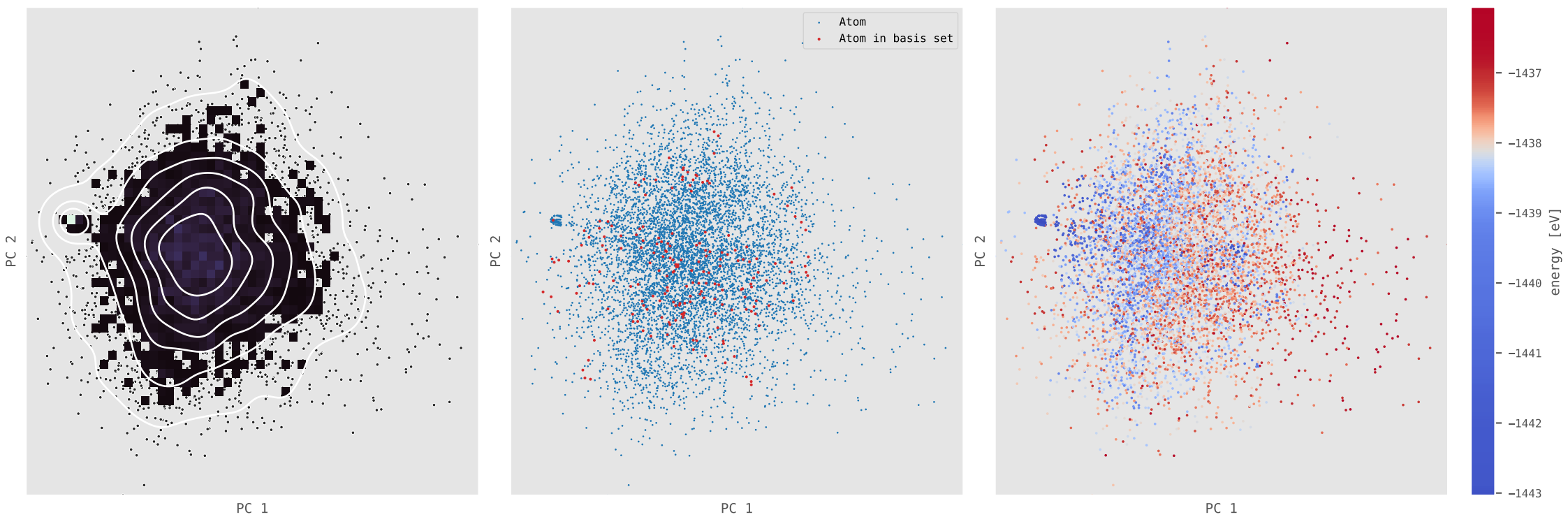
front



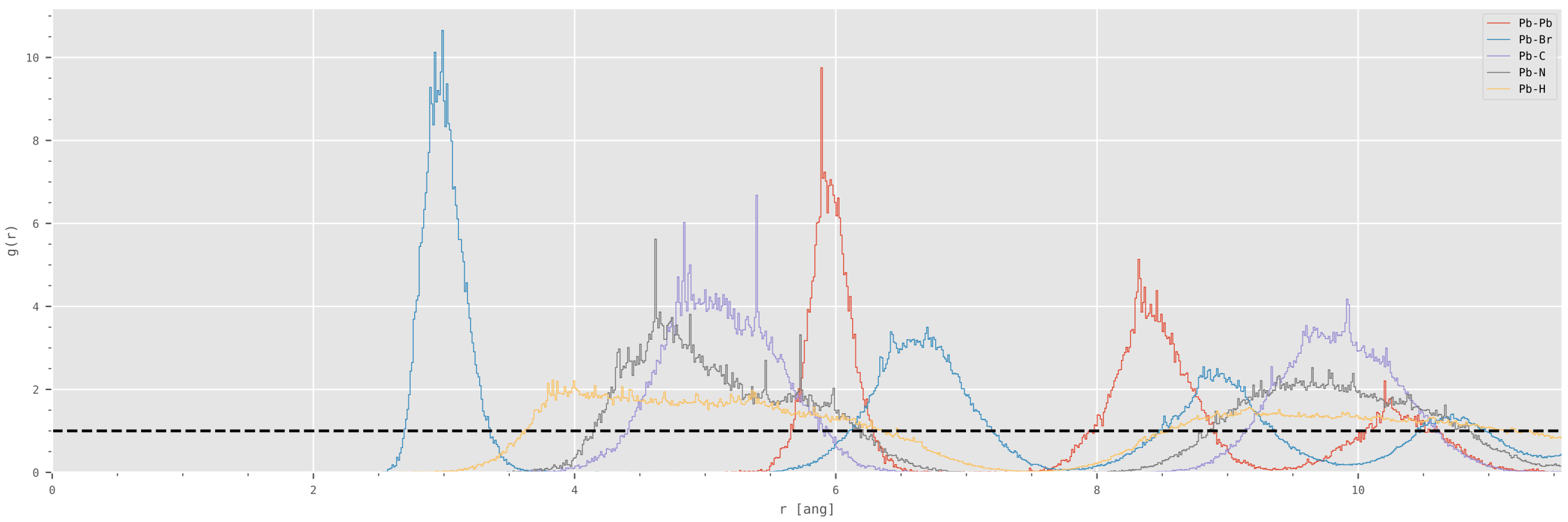
top



principal component analysis of descriptors (Pb)



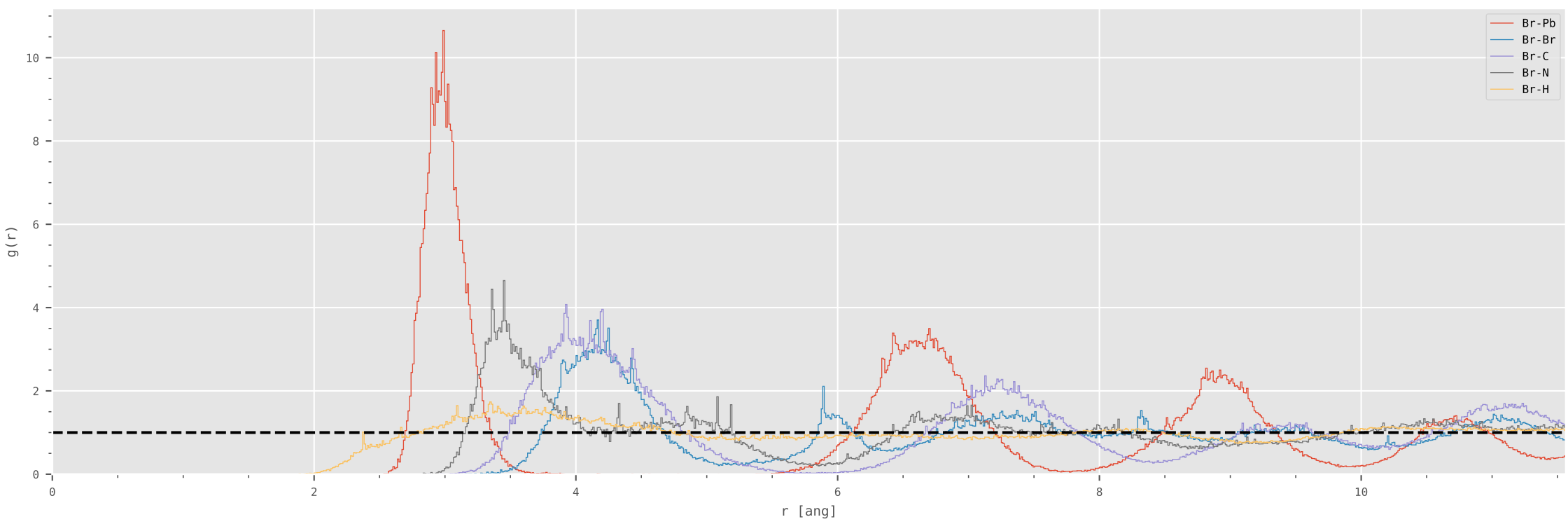
radial distribution functions (Pb)



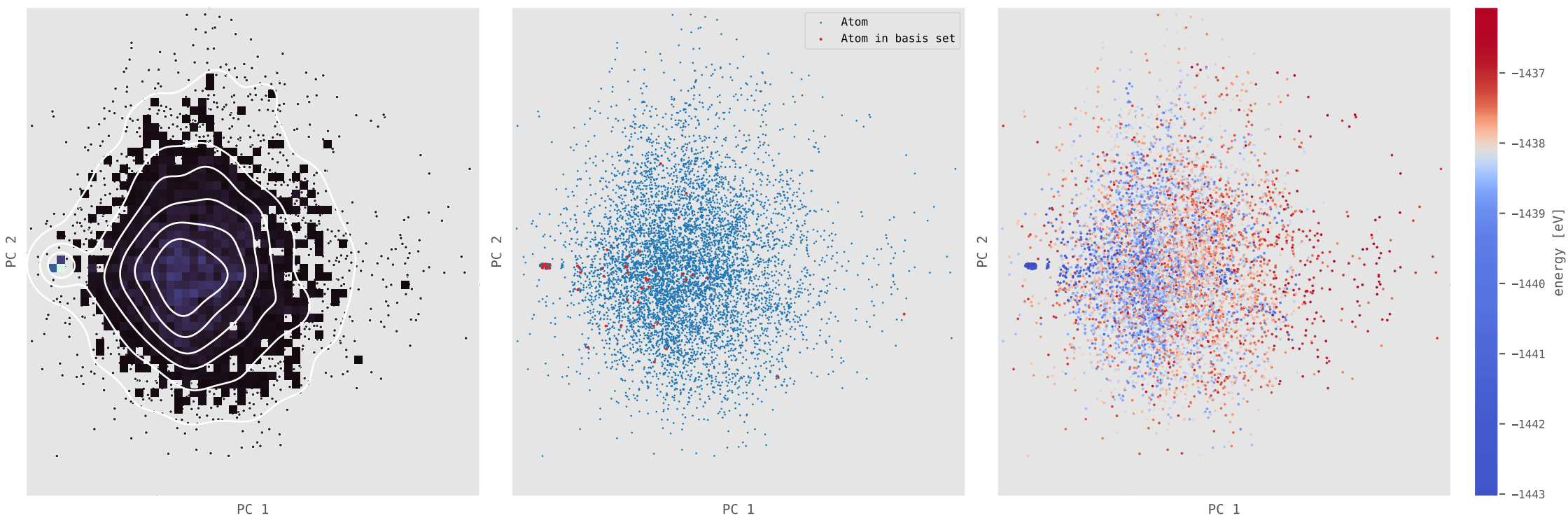
principal component analysis of descriptors (Br)



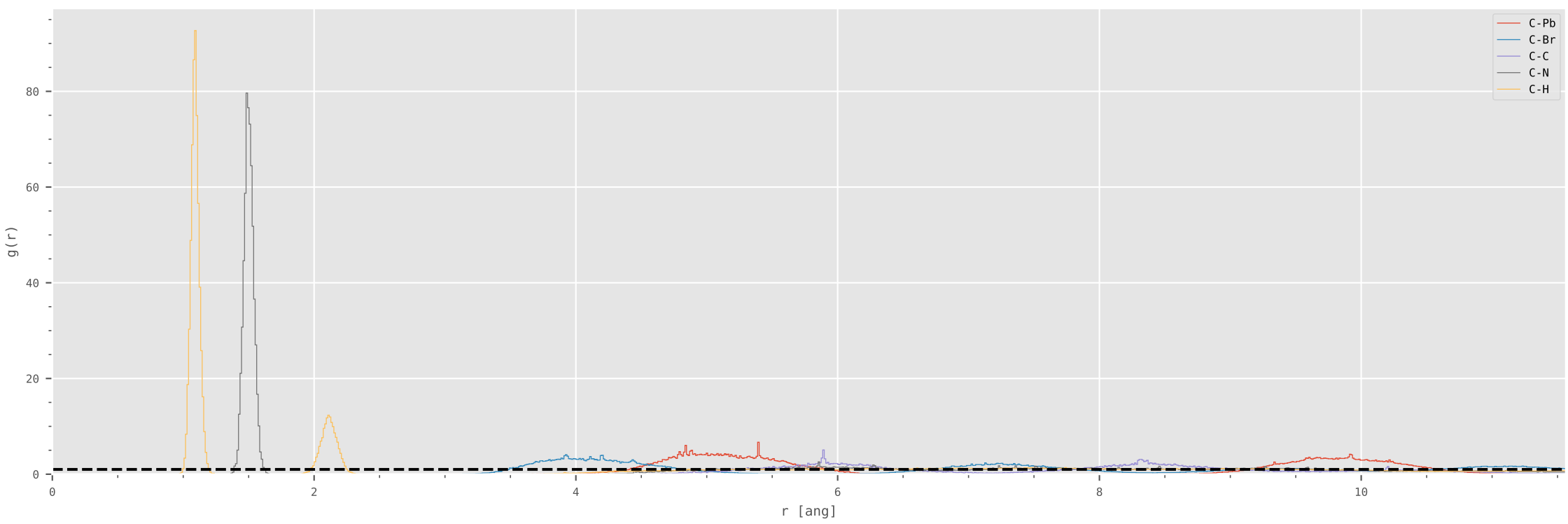
radial distribution functions (Br)



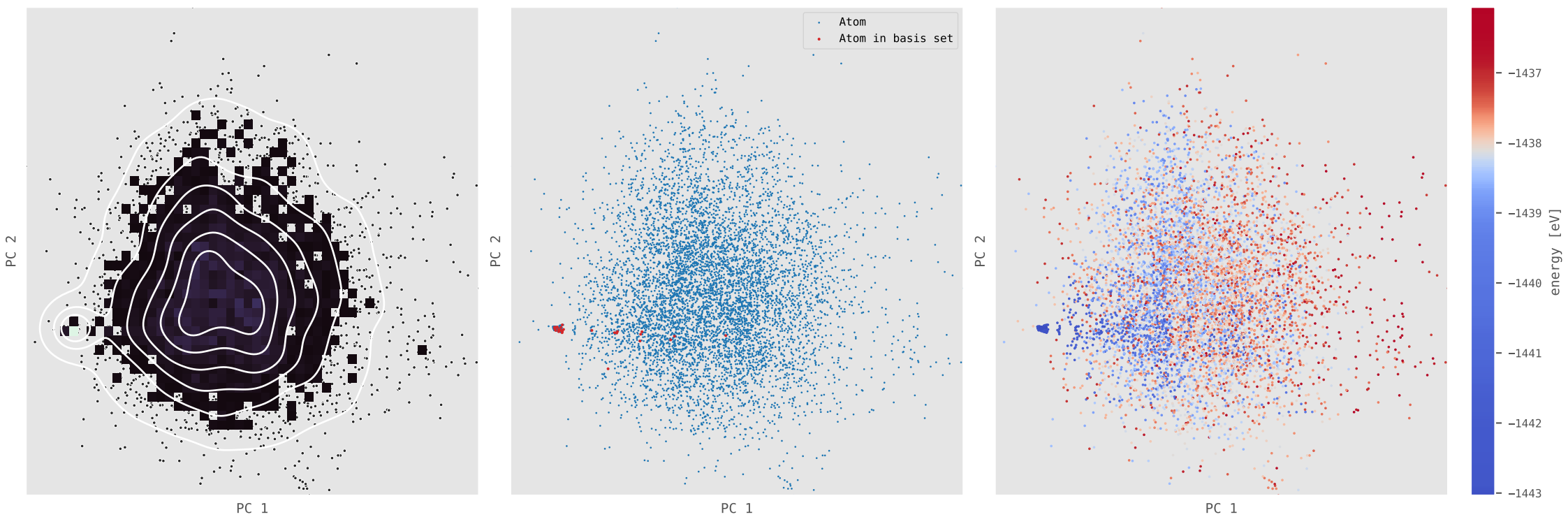
principal component analysis of descriptors (C)



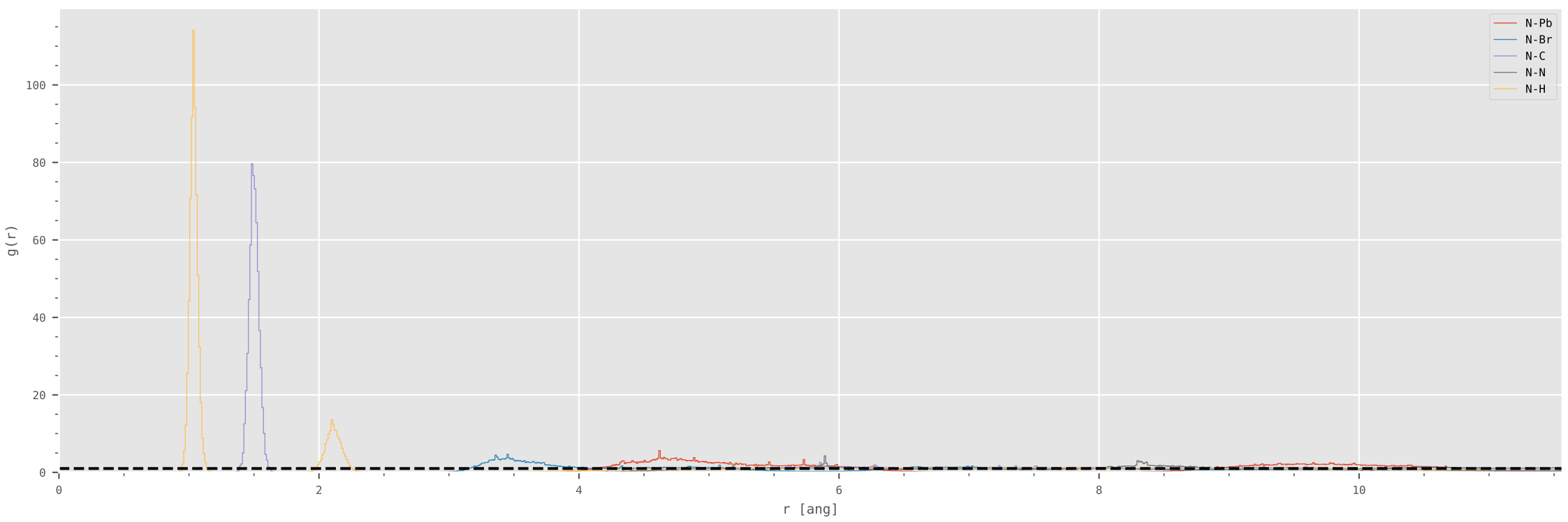
radial distribution functions (C)



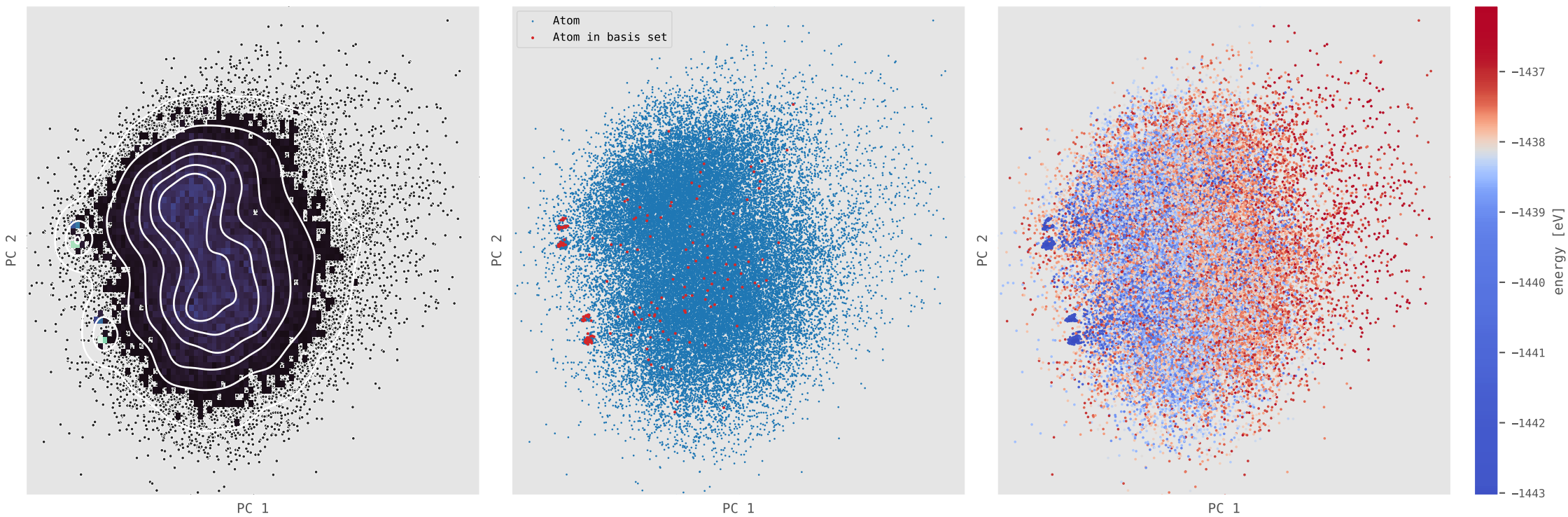
principal component analysis of descriptors (N)



radial distribution functions (N)



principal component analysis of descriptors (H)



radial distribution functions (H)

