[1/1] ML_AB_normalmass (CsPbBr3 Cubic MLFF 400 K)

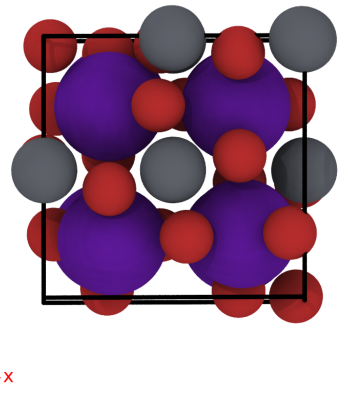
file

name	ML_AB_normalmass
structure groups	1
total structures	722

overview

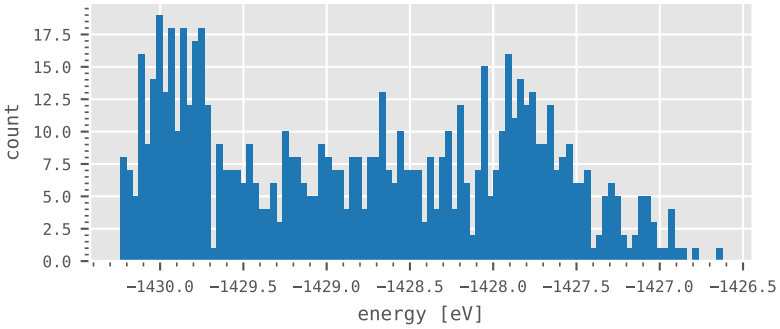
energy	-1428.8 ± 0.95	eV
volume	1653.3 ± 34.79	ang^3
lattice vector a	11.8 ± 0.15	ang
lattice vector b	11.8 ± 0.14	ang
lattice vector c	11.8 ± 0.16	ang
non-periodic radius	5.7 (min. for group)	ang

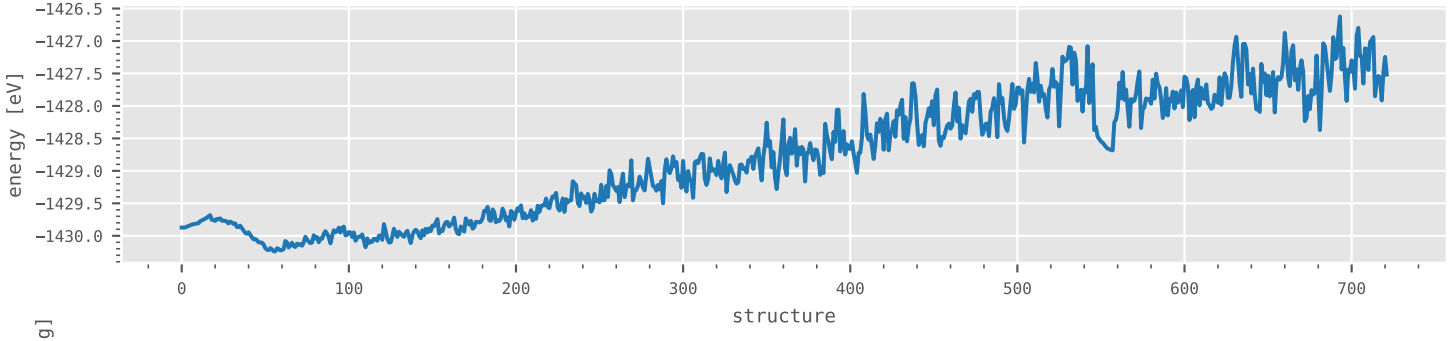
min energy configuration

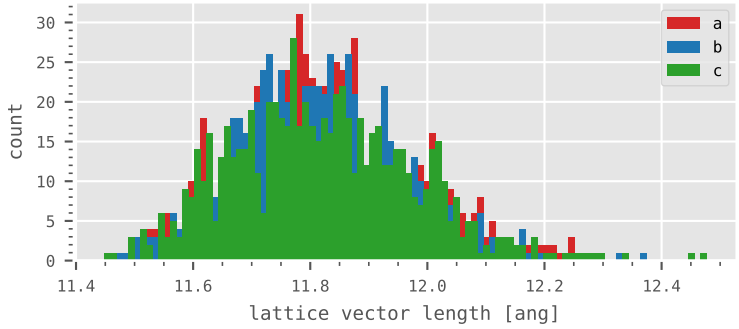


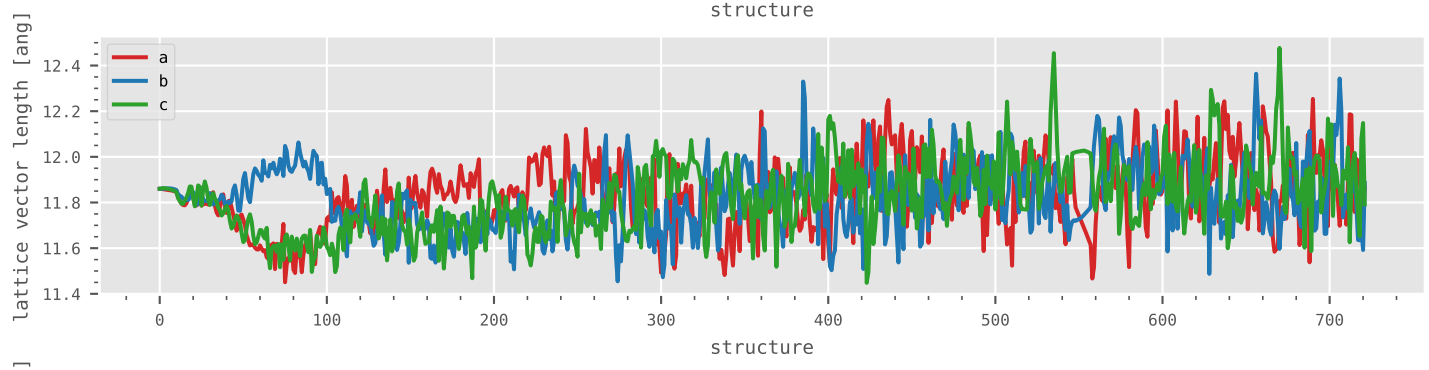
current structure group

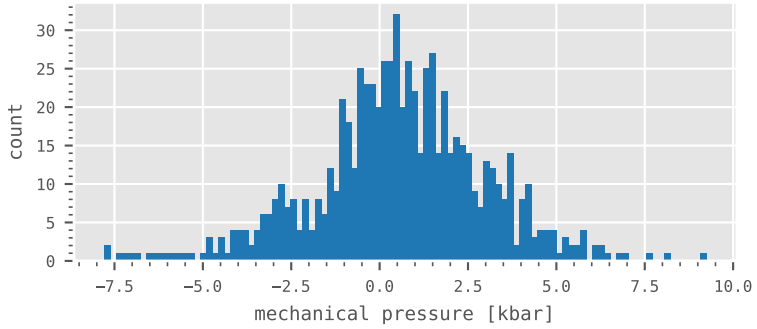
name	CsPbBr3 Cubic MLFF 400 K
structure group	1 (of 1 in file)
structures	722 (of 722 in file)
atoms	Pb (8), Br (24), Cs (8)
	40 total

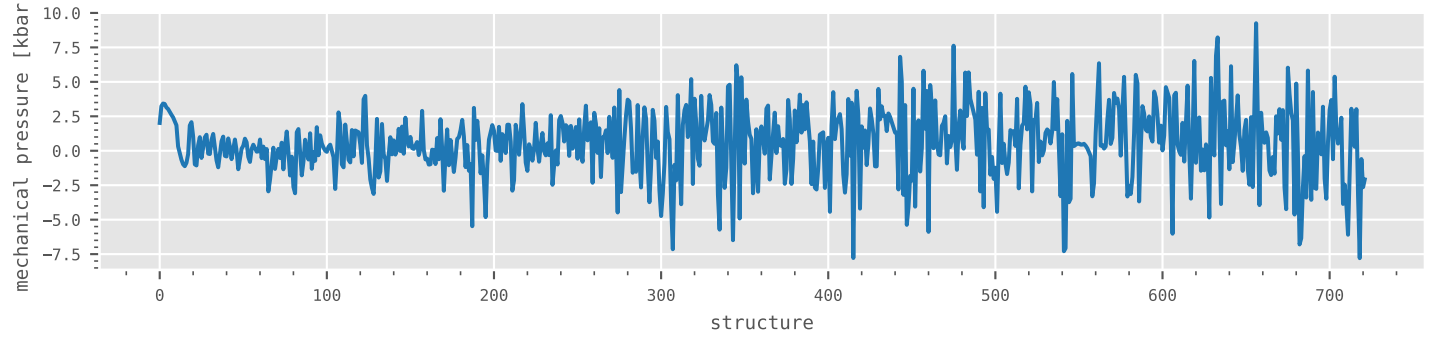




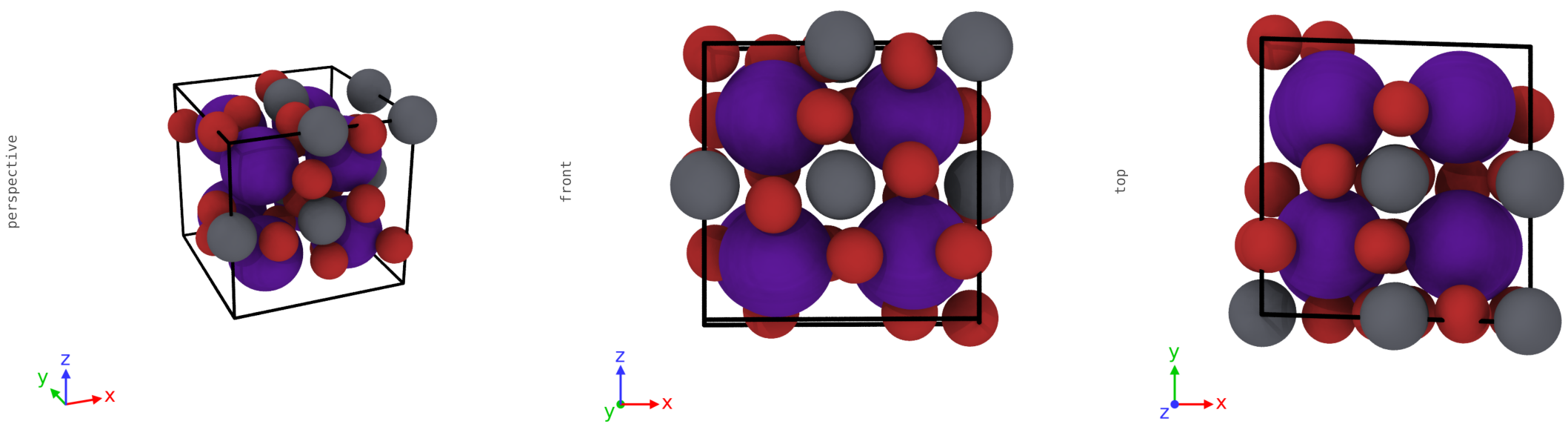




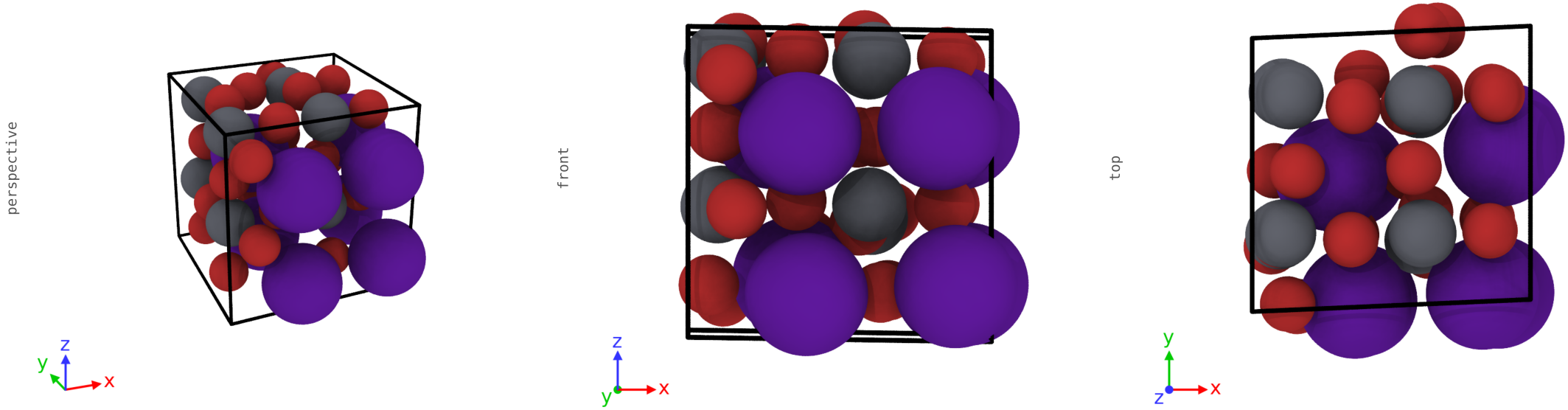


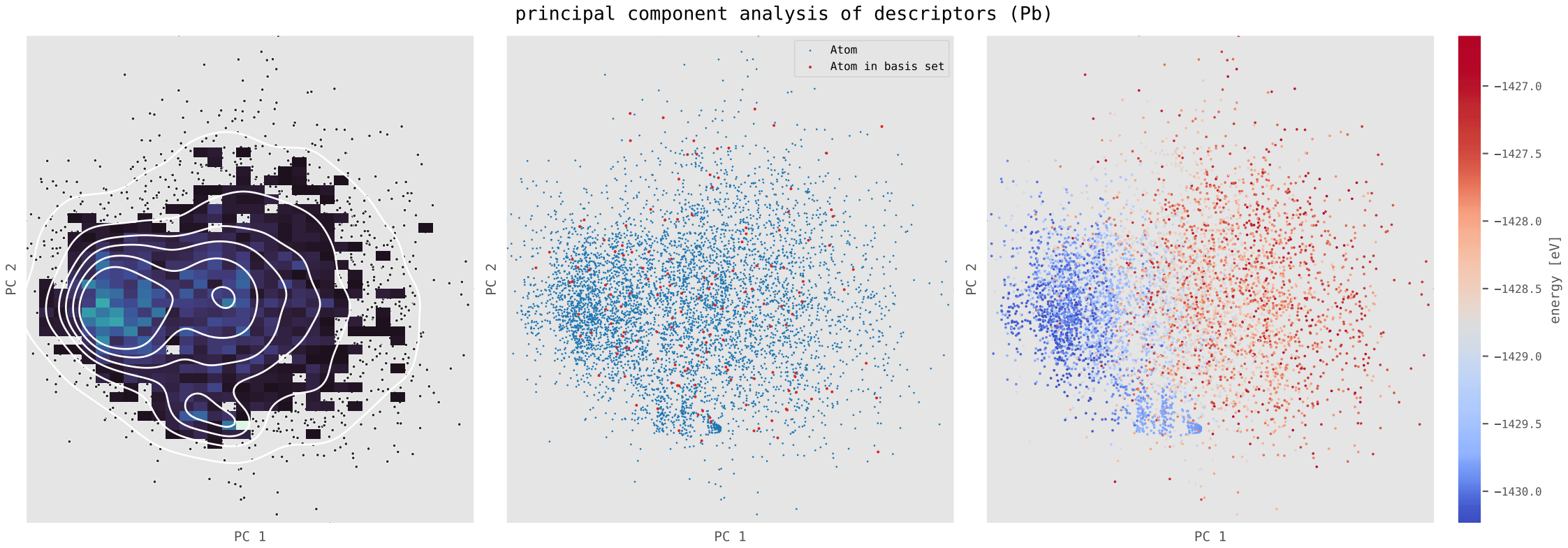


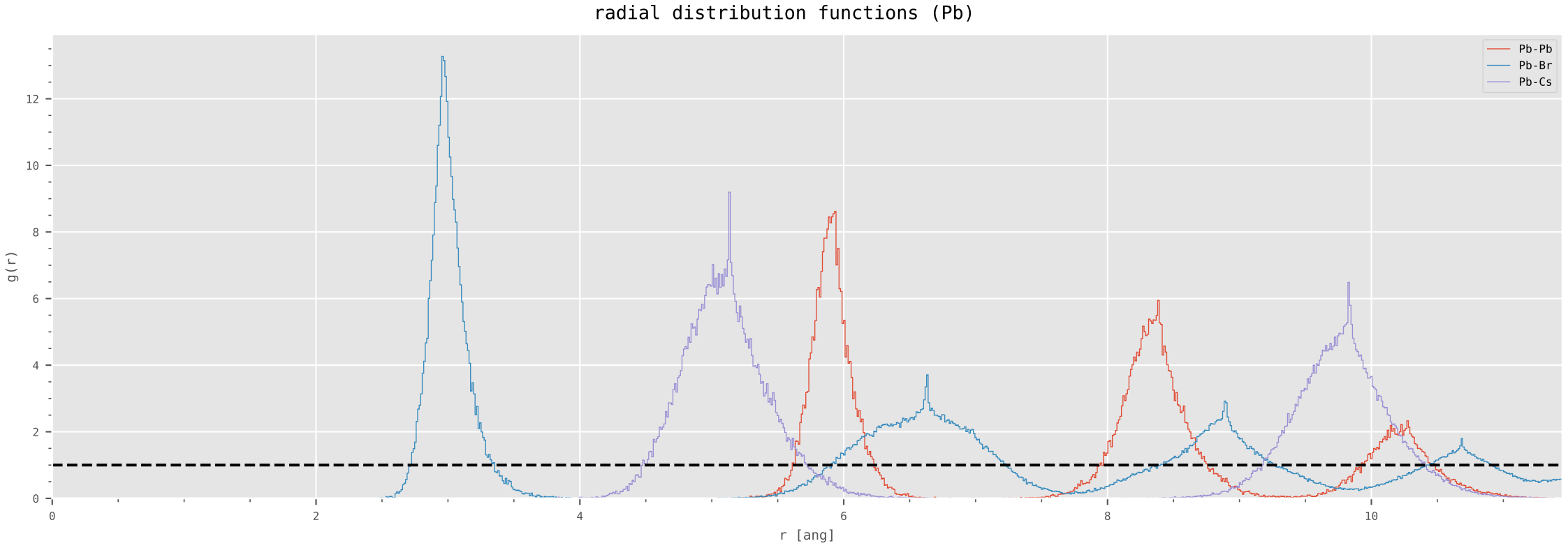
minimum energy configuration (structure 57)



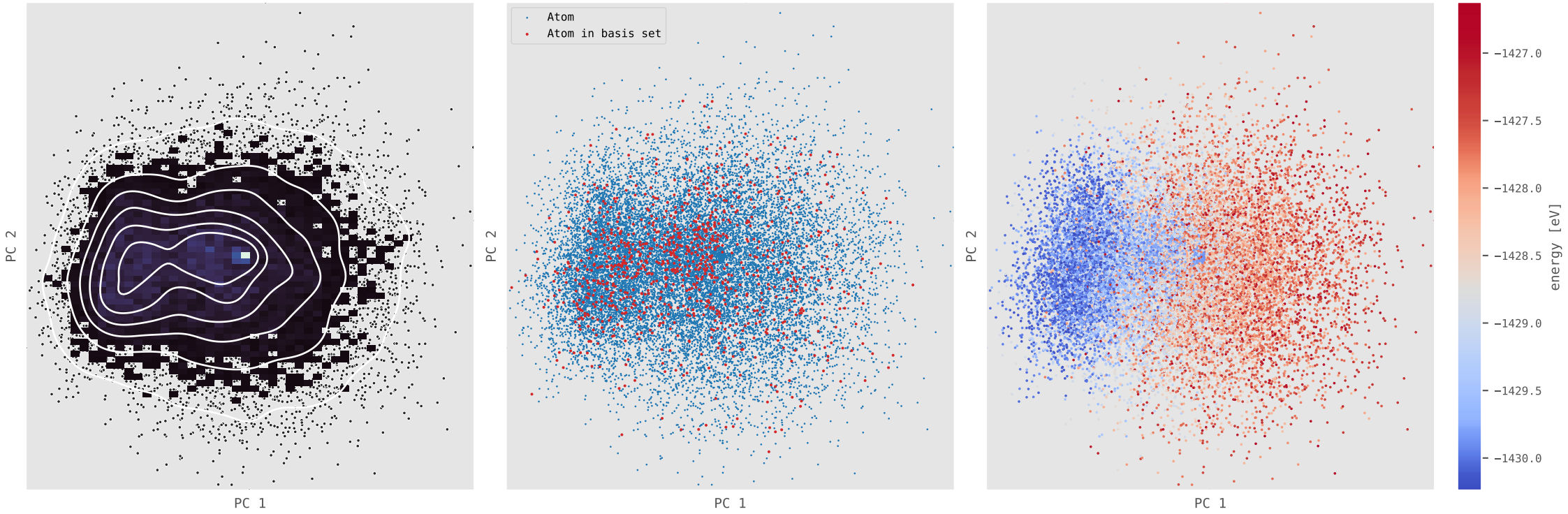
maximum energy configuration (structure 694)



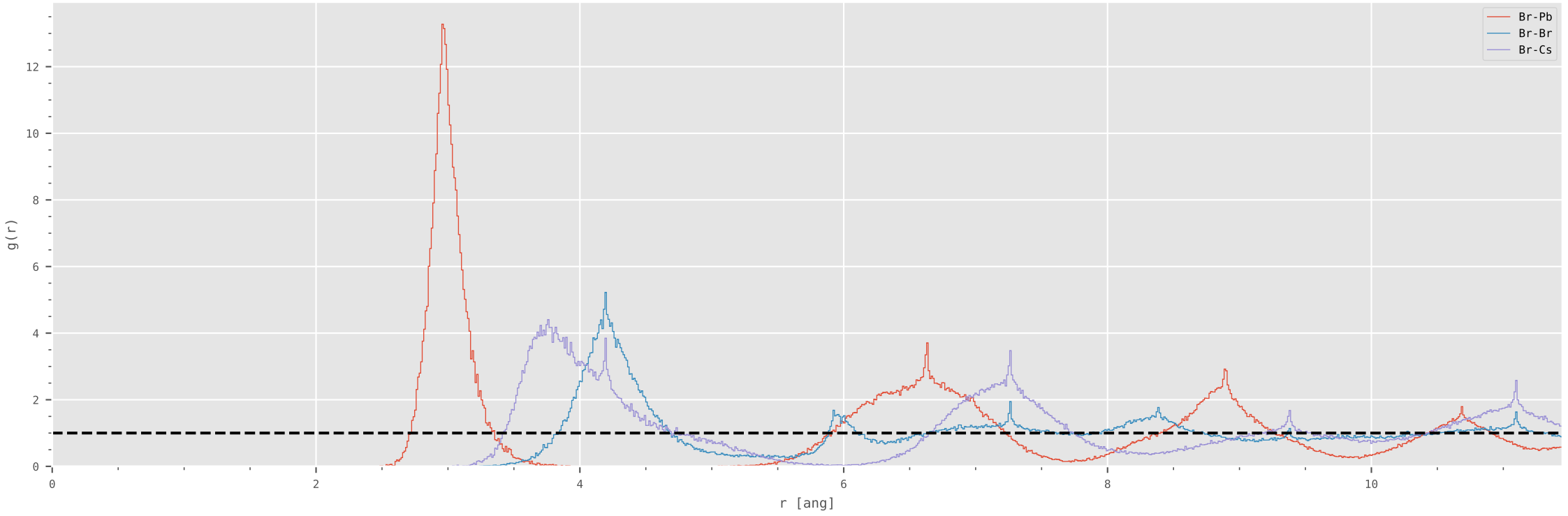

principal component analysis of descriptors (Pb)
PC 2
PC 1
Atom
Atom in basis set
PC 2
PC 1
PC 2
PC 1
−1427.0
−1427.5
−1428.0
−1428.5
−1429.0
−1429.5
−1430.0
energy [eV]

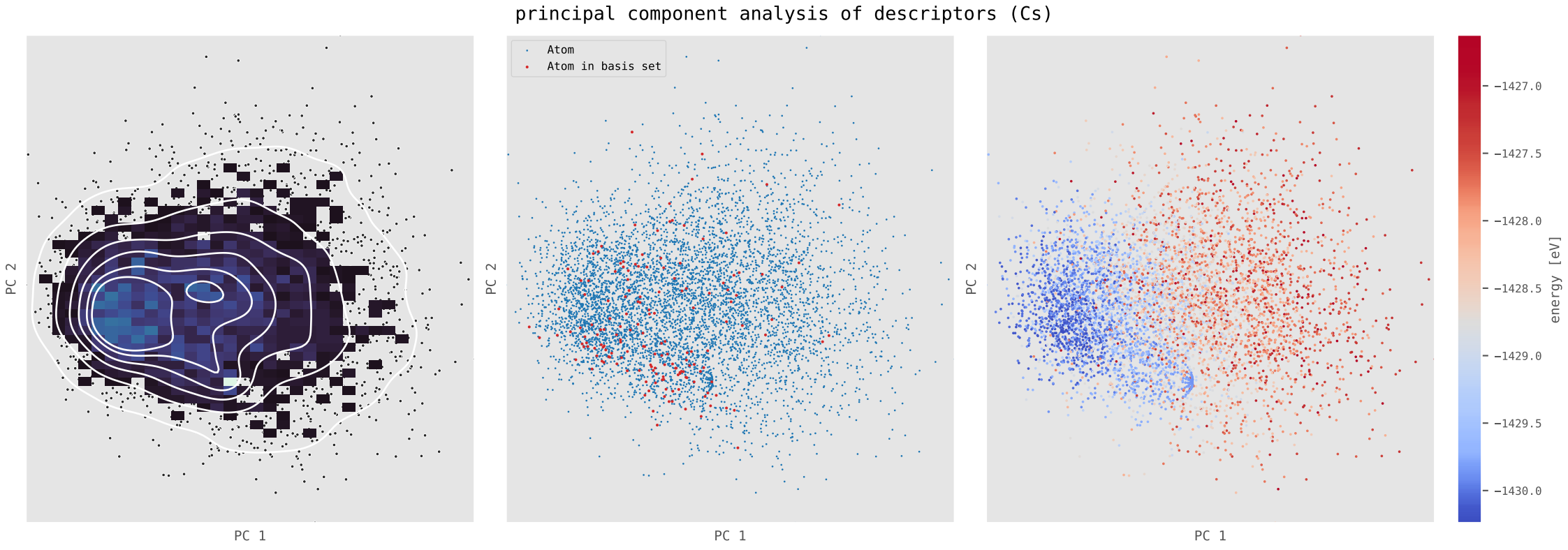

radial distribution functions (Pb)
Pb-Pb
Pb-Br
Pb-Cs
g(r)
0
2
4
6
8
10
12
r [ang]

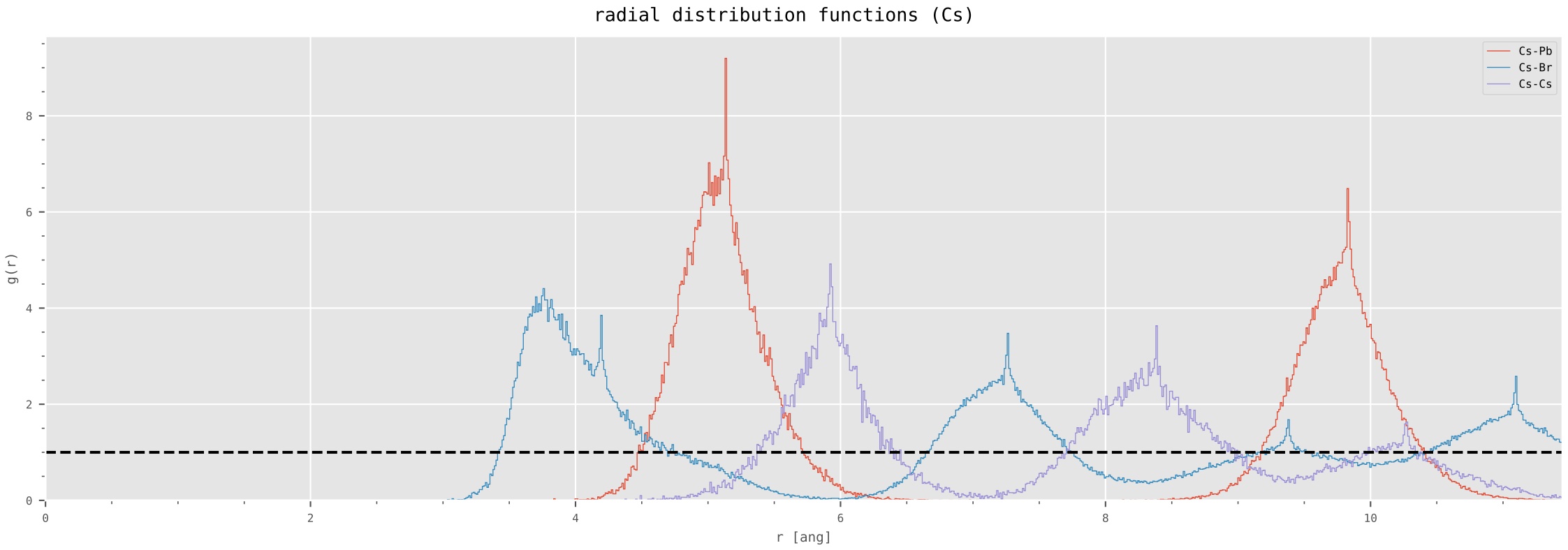
principal component analysis of descriptors (Br)



radial distribution functions (Br)




principal component analysis of descriptors (Cs)
PC 2
PC 1
Atom
Atom in basis set
PC 2
PC 1
PC 2
PC 1
energy [eV]
−1427.0
−1427.5
−1428.0
−1428.5
−1429.0
−1429.5
−1430.0


radial distribution functions (Cs)
Cs-Pb
Cs-Br
Cs-Cs
g(r)
r [ang]
0
2
4
6
8
10