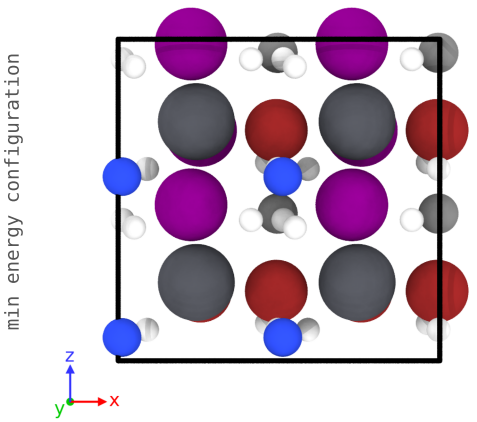
[1/2] ML_ABCAR-MAPbI1.5Br1.5 (Cubic-(SSHS-MAPbIBr-4-4))

file

name	ML_ABCAR-MAPbI1.5Br1.5
structure groups	2
total structures	3267

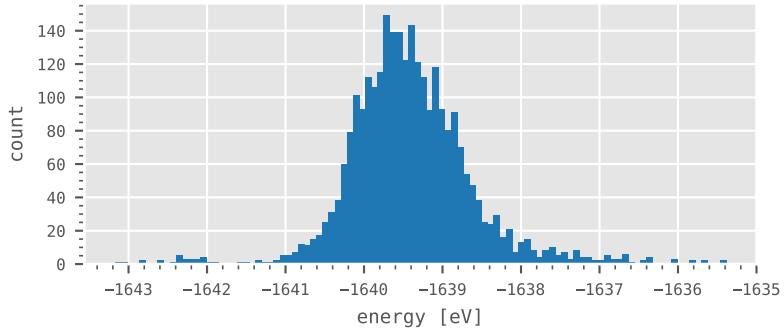
overview

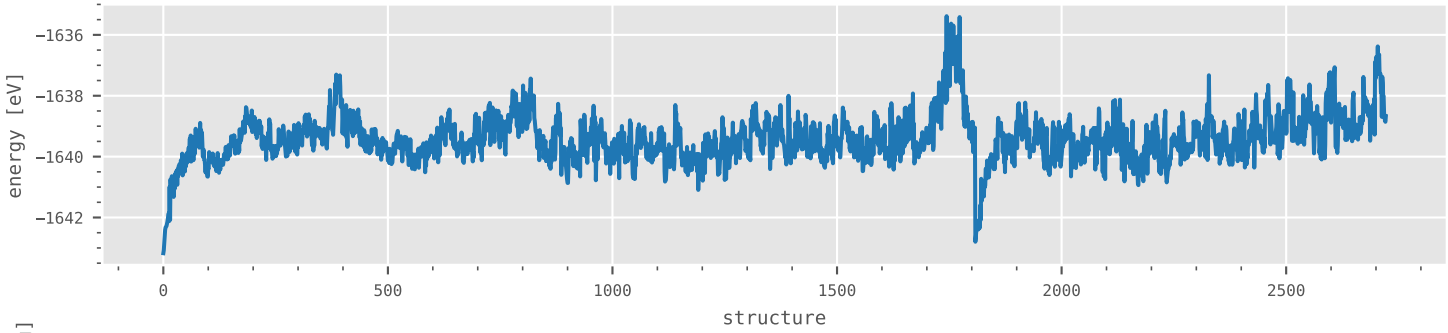
energy	-1639.4 ± 0.79	eV
volume	1881.4 ± 35.34	ang^3
lattice vector a	12.1 ± 0.24	ang
lattice vector b	12.4 ± 0.20	ang
lattice vector c	12.6 ± 0.22	ang
non-periodic radius	5.7 (min. for group)	ang

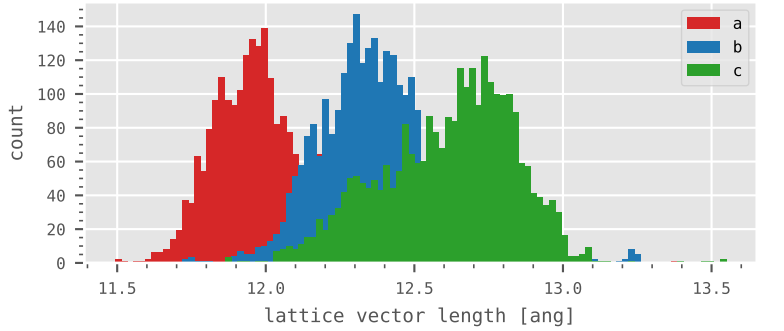


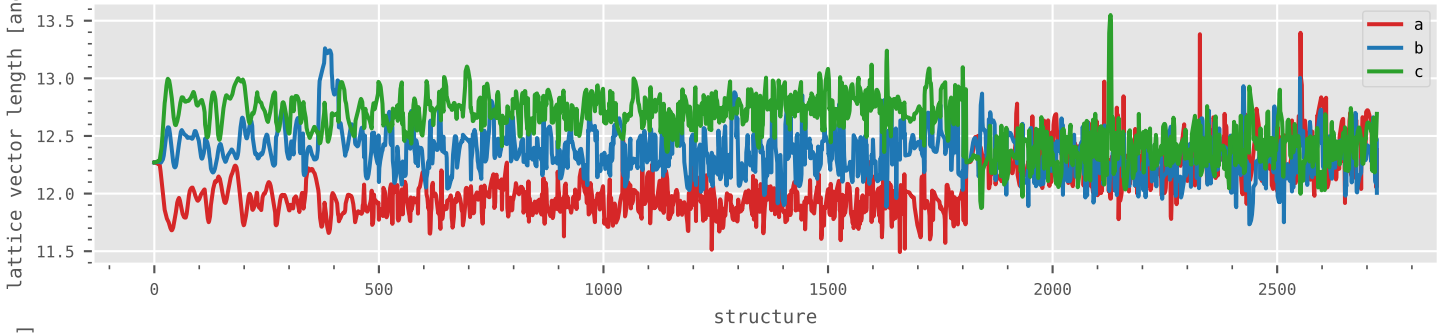
current structure group

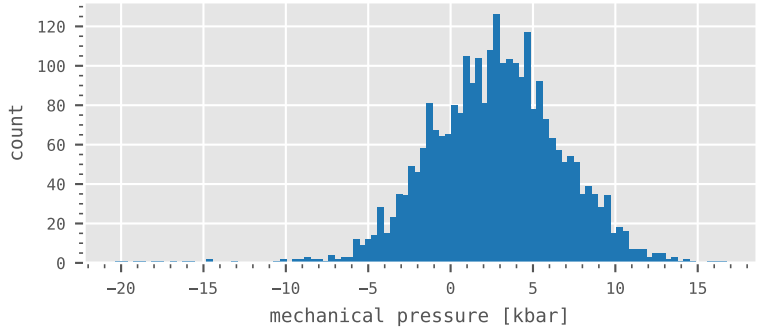
name	Cubic-(SSHS-MAPbIBr-4-4)
structure group	1 (of 2 in file)
structures	2723 (of 3267 in file)
atoms	Pb (8), I (12), Br (12), C (8), N (8), H (48)
	96 total

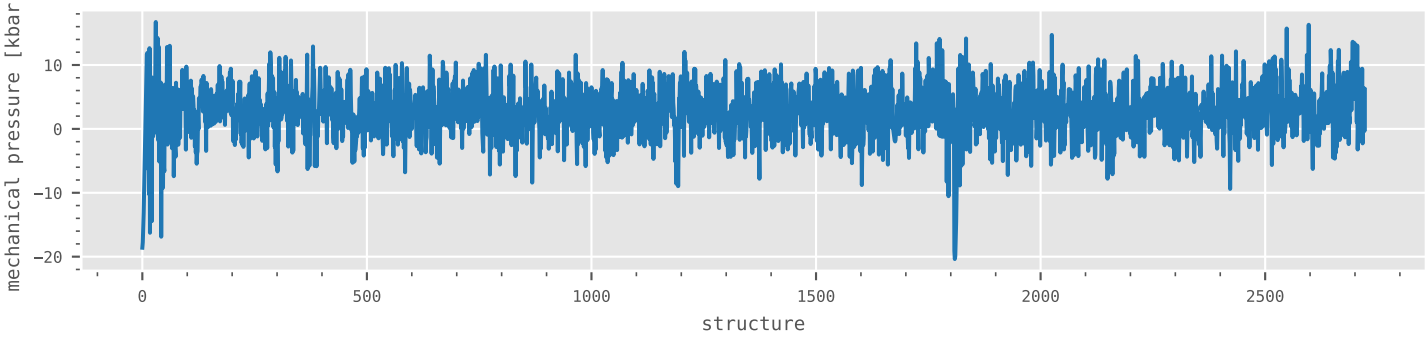




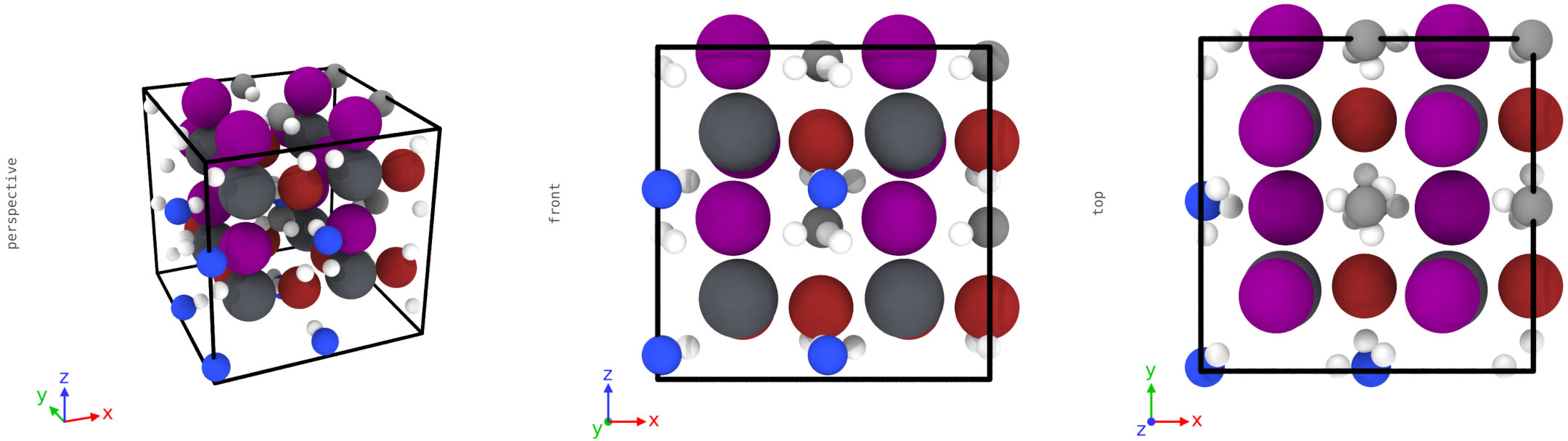




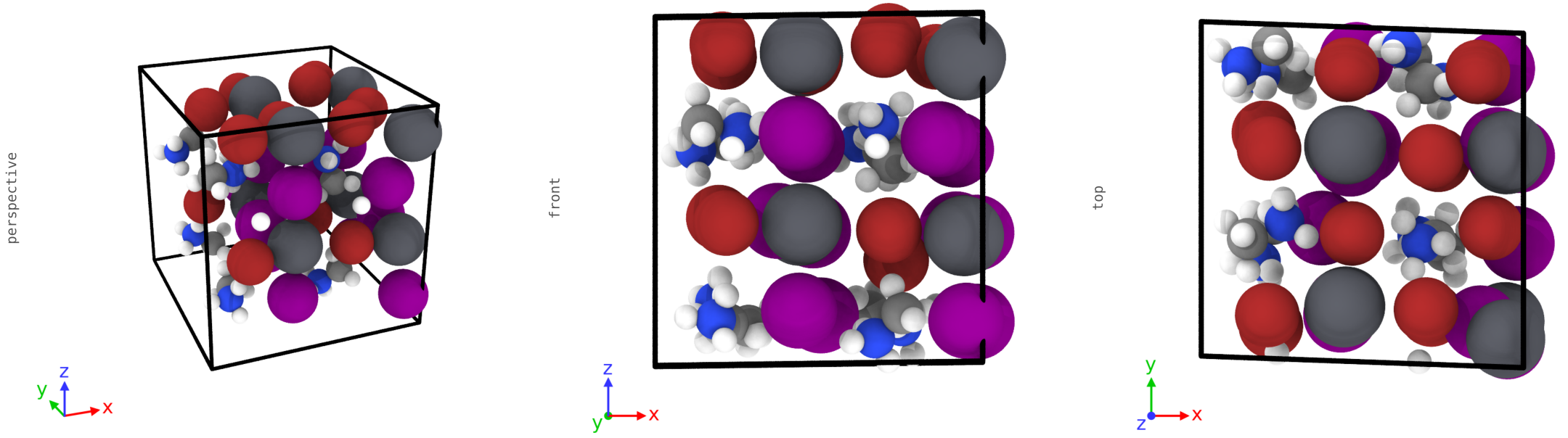




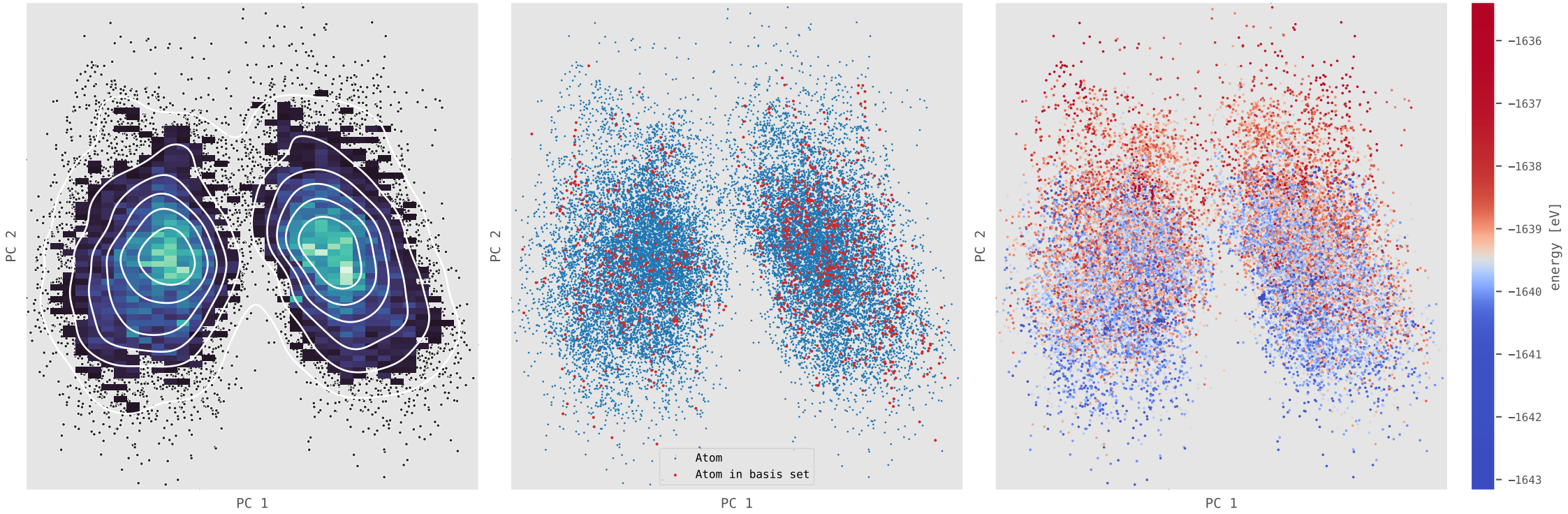
minimum energy configuration (structure 1)



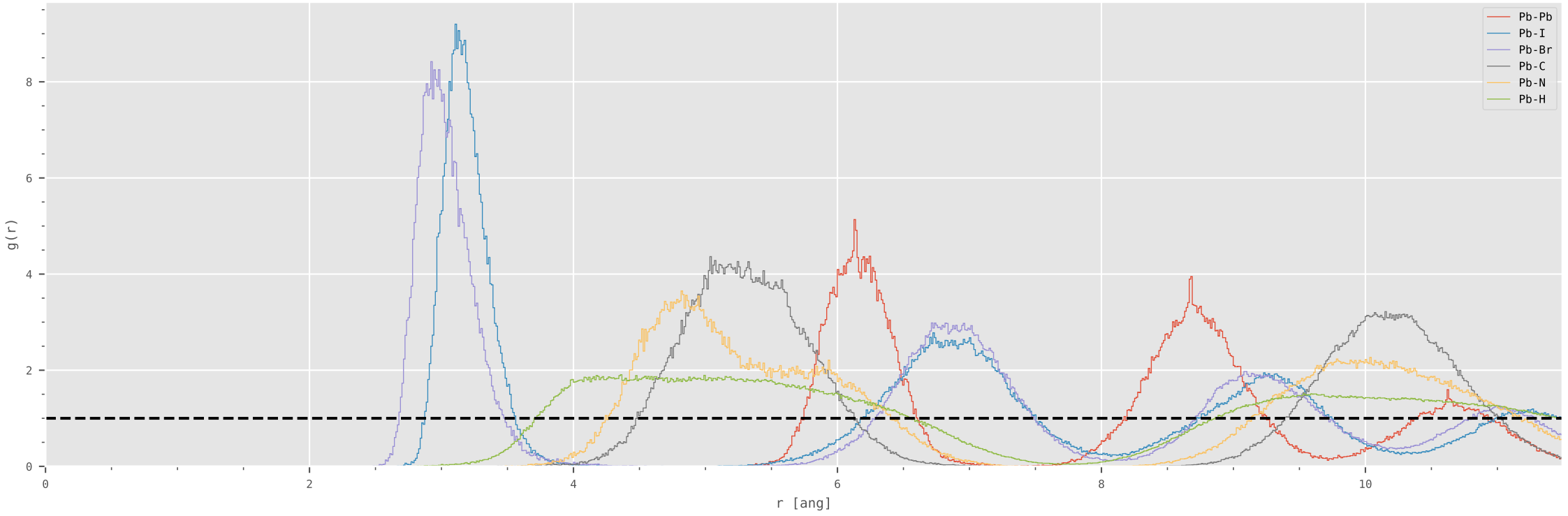
maximum energy configuration (structure 1745)



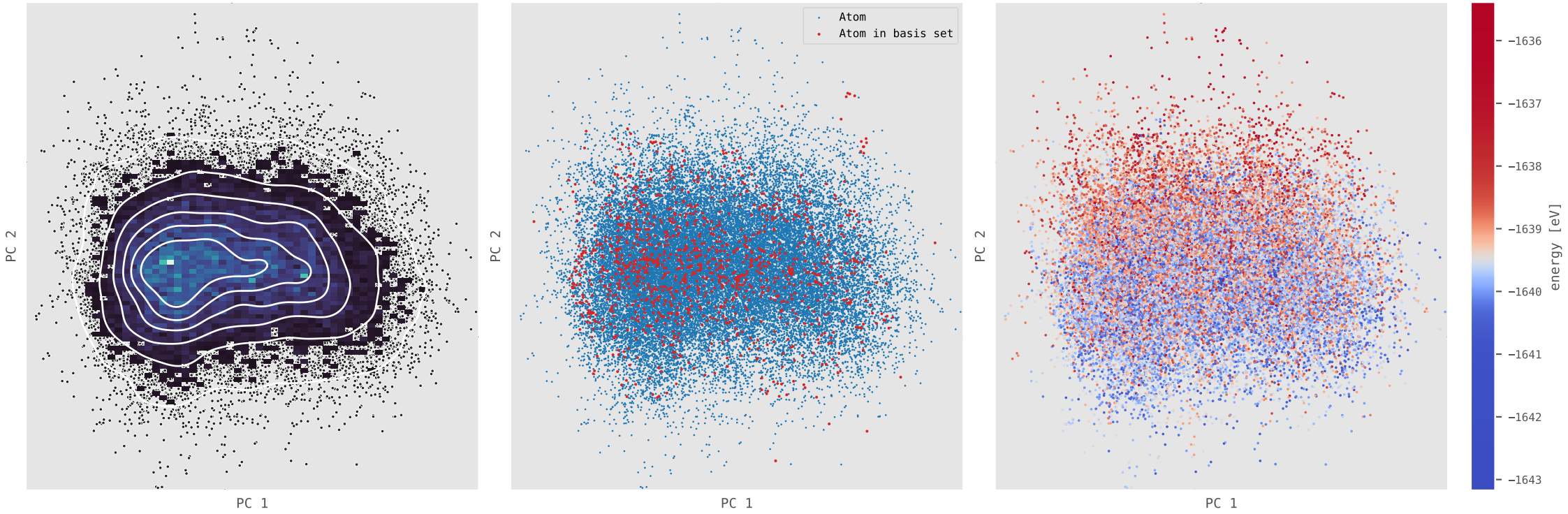
principal component analysis of descriptors (Pb)



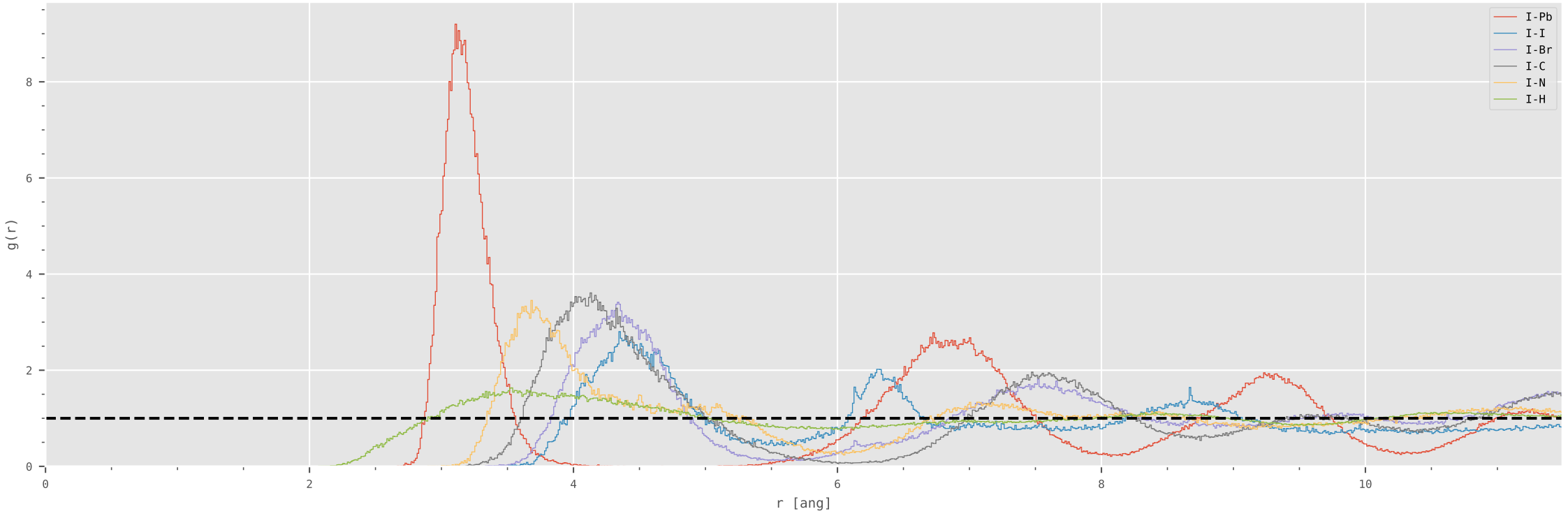
radial distribution functions (Pb)



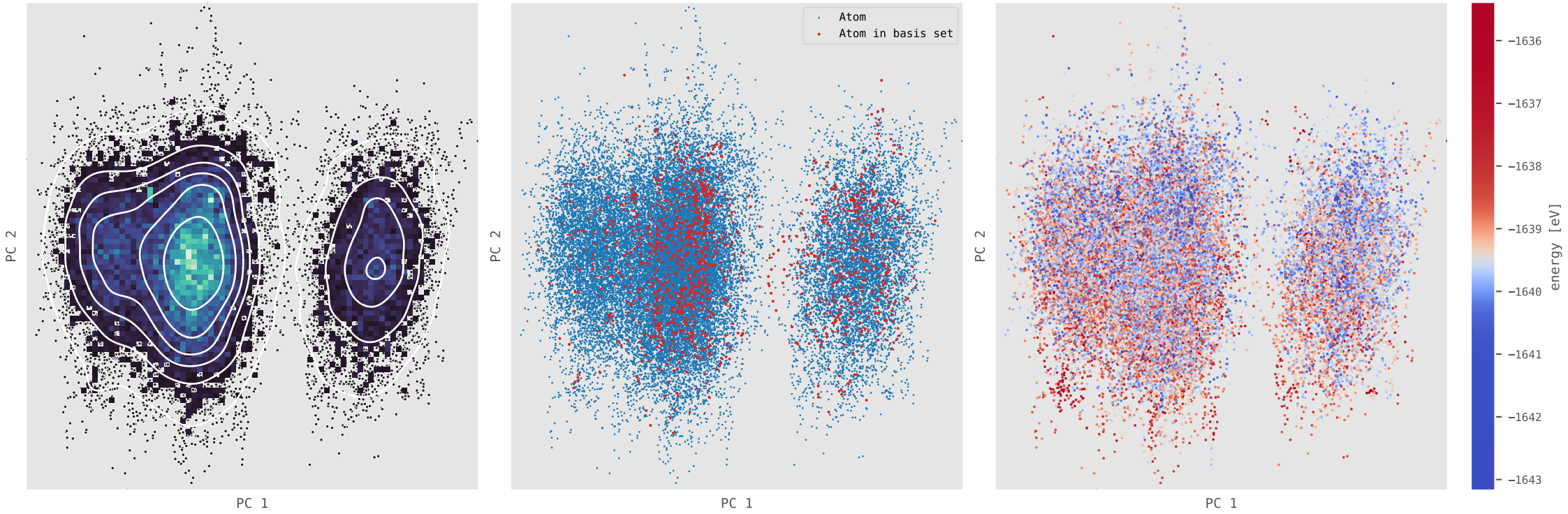
principal component analysis of descriptors (I)



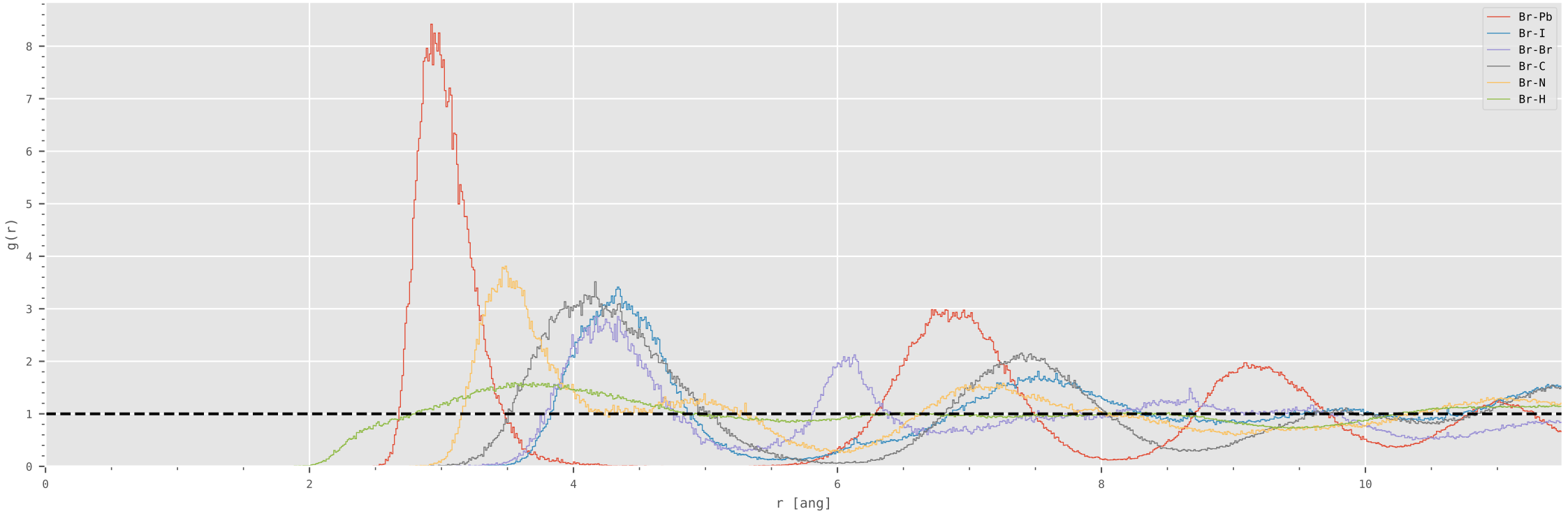
radial distribution functions (I)

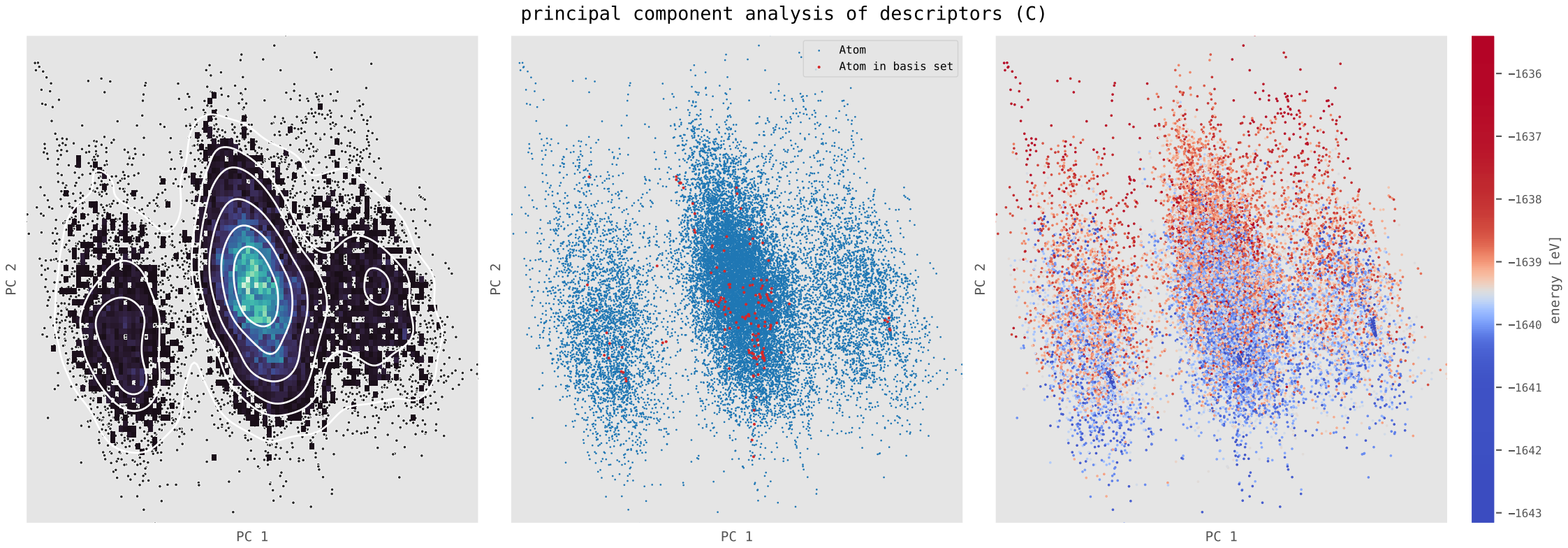


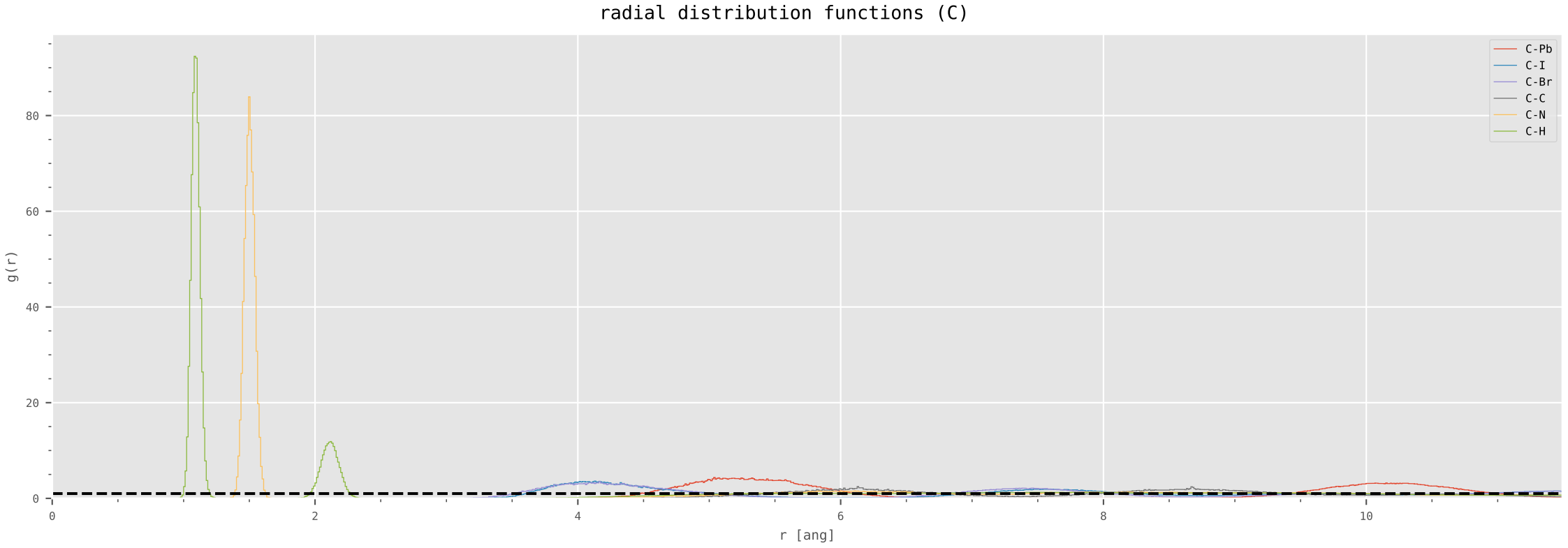
principal component analysis of descriptors (Br)

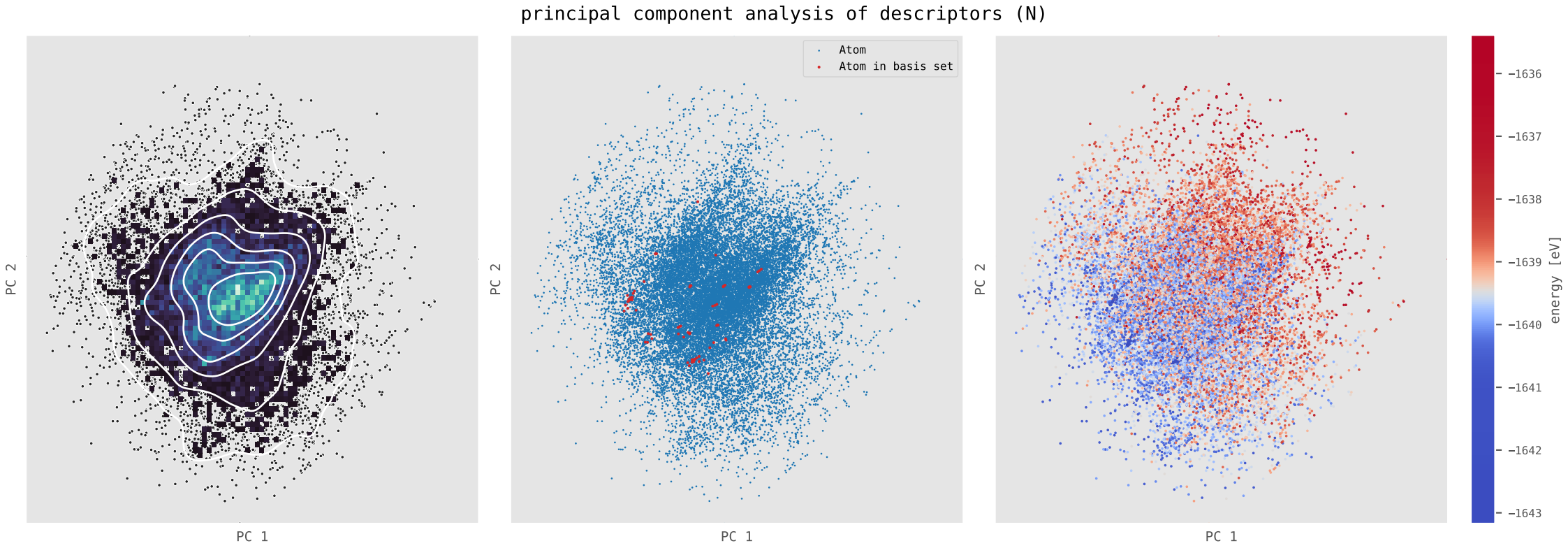


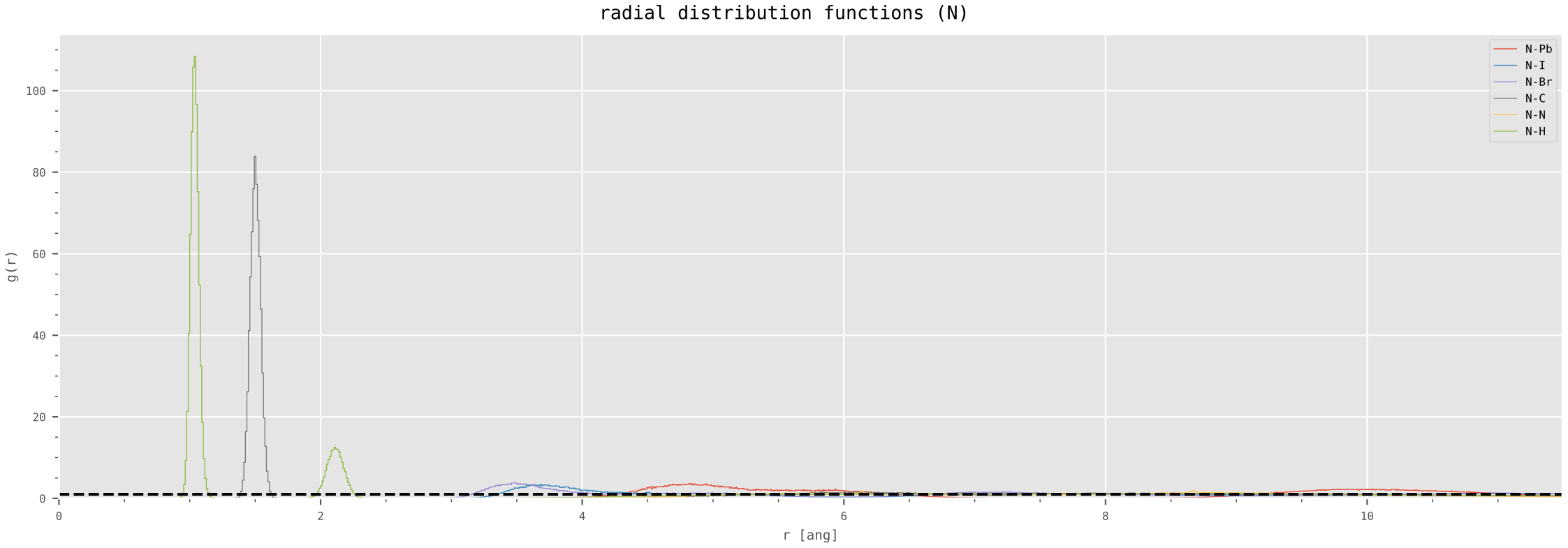
radial distribution functions (Br)

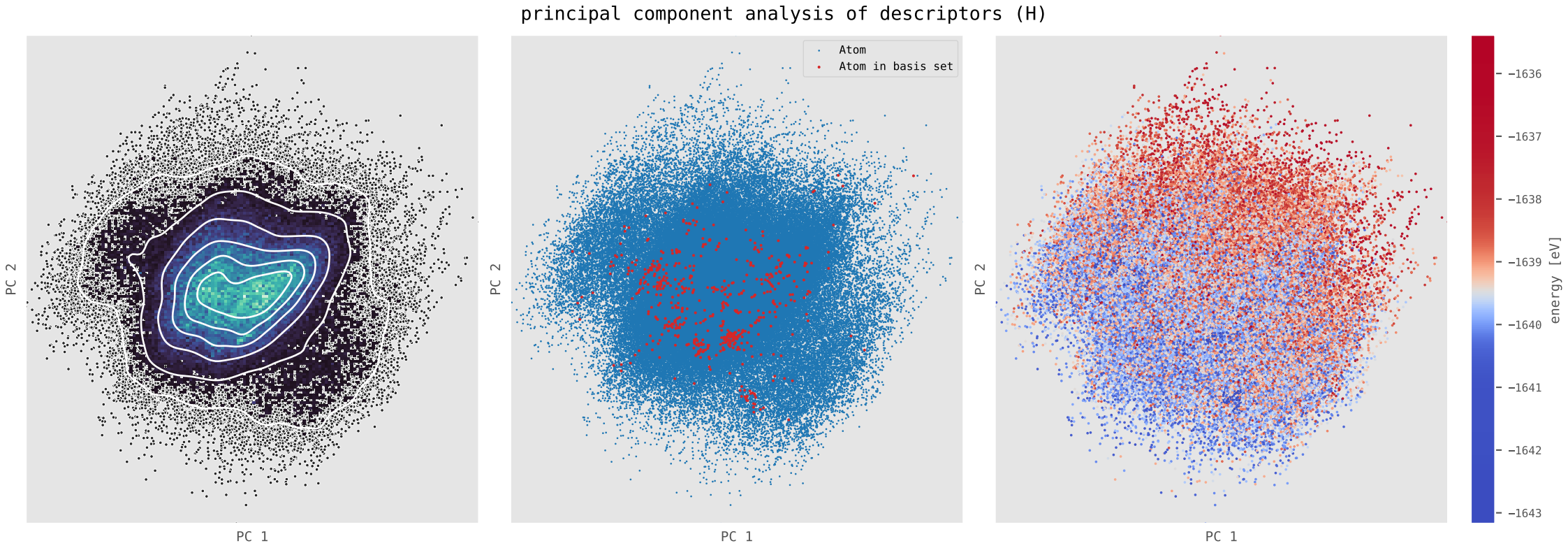


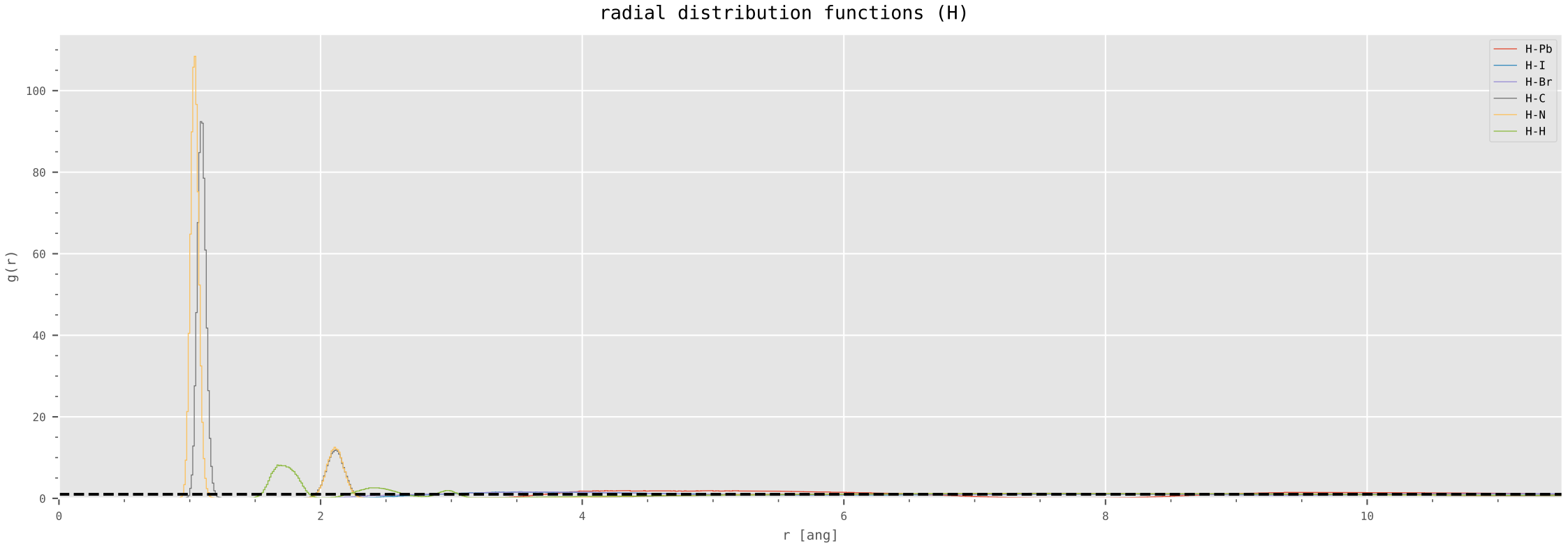

principal component analysis of descriptors (C)
PC 2
PC 1
Atom
Atom in basis set
PC 2
PC 1
PC 2
PC 1
−1636
−1637
−1638
−1639
−1640
−1641
−1642
−1643
energy [eV]


radial distribution functions (C)
C-Pb
C-I
C-Br
C-C
C-N
C-H
g(r)
0
20
40
60
80
0
2
4
6
8
10
r [ang]


principal component analysis of descriptors (N)
PC 2
PC 1
Atom
Atom in basis set
PC 2
PC 1
PC 2
PC 1
−1636
−1637
−1638
−1639
−1640
−1641
−1642
−1643
energy [eV]


radial distribution functions (N)
N-Pb
N-I
N-Br
N-C
N-N
N-H
g(r)
0
20
40
60
80
100
0
2
4
6
8
10
r [ang]


principal component analysis of descriptors (H)
PC 2
PC 1
Atom
Atom in basis set
PC 2
PC 1
PC 2
PC 1
−1636
−1637
−1638
−1639
−1640
−1641
−1642
−1643
energy [eV]


radial distribution functions (H)
H-Pb
H-I
H-Br
H-C
H-N
H-H
g(r)
r [ang]
0
20
40
60
80
100
0
2
4
6
8
10

[2/2] ML_ABCAR-MAPbI1.5Br1.5 (MAPbBr3)

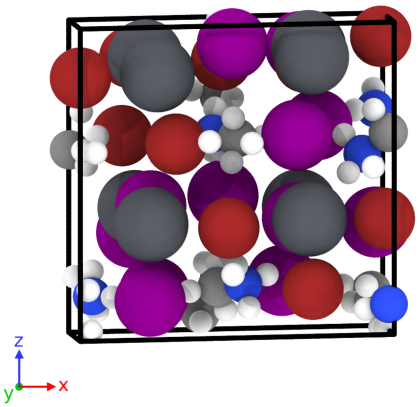
file

name	ML_ABCAR-MAPbI1.5Br1.5
structure groups	2
total structures	3267

overview

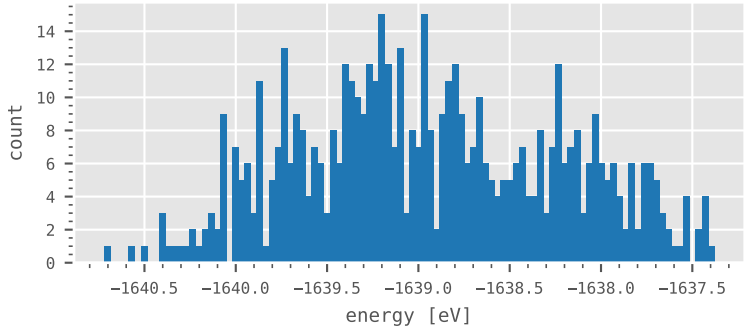
energy	-1638.9 ± 0.72	eV
volume	1887.2 ± 32.39	ang^3
lattice vector a	12.4 ± 0.19	ang
lattice vector b	12.4 ± 0.18	ang
lattice vector c	12.3 ± 0.13	ang
non-periodic radius	5.9 (min. for group)	ang

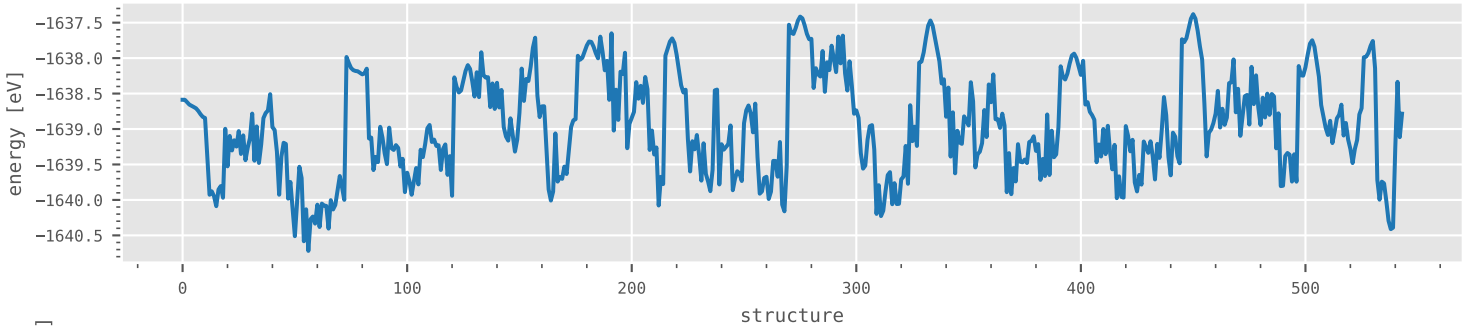
min energy configuration

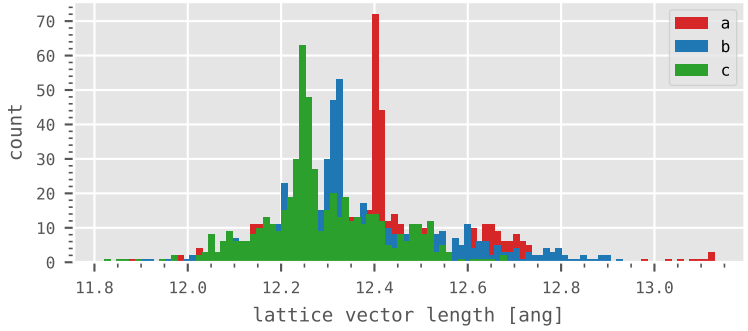


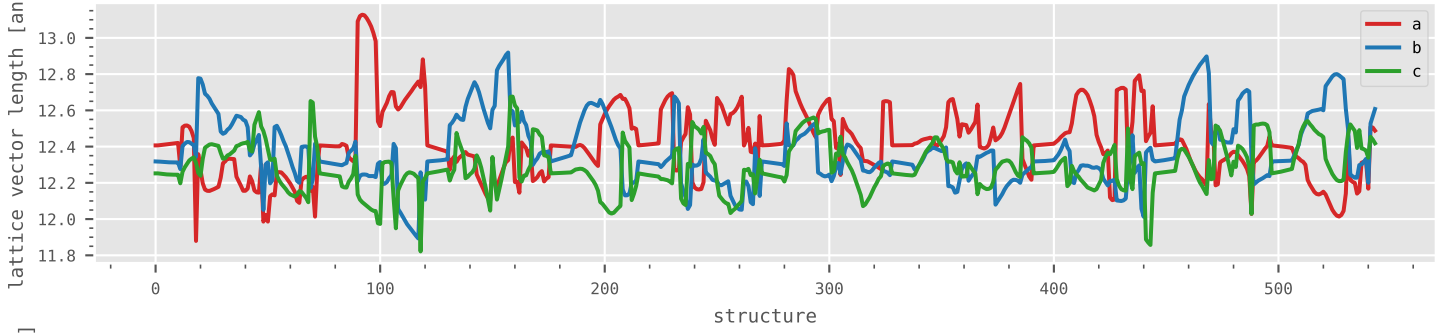
current structure group

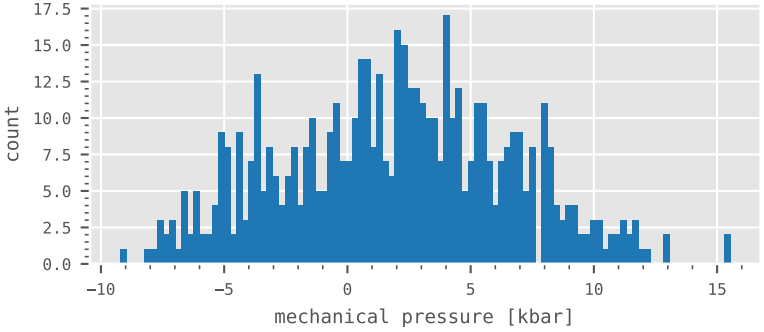
name	MAPbBr3
structure group	2 (of 2 in file)
structures	544 (of 3267 in file)
atoms	Pb (8), I (12), Br (12), C (8), N (8), H (48)
	96 total

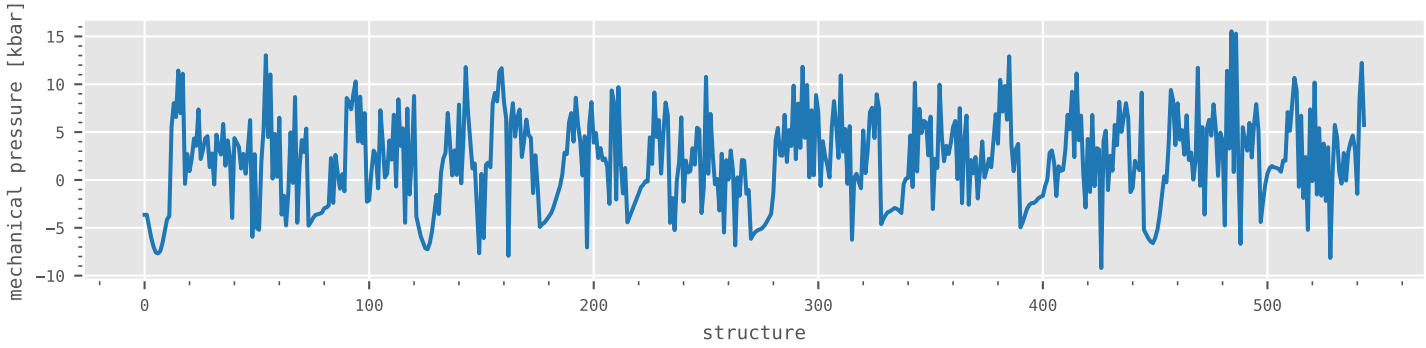




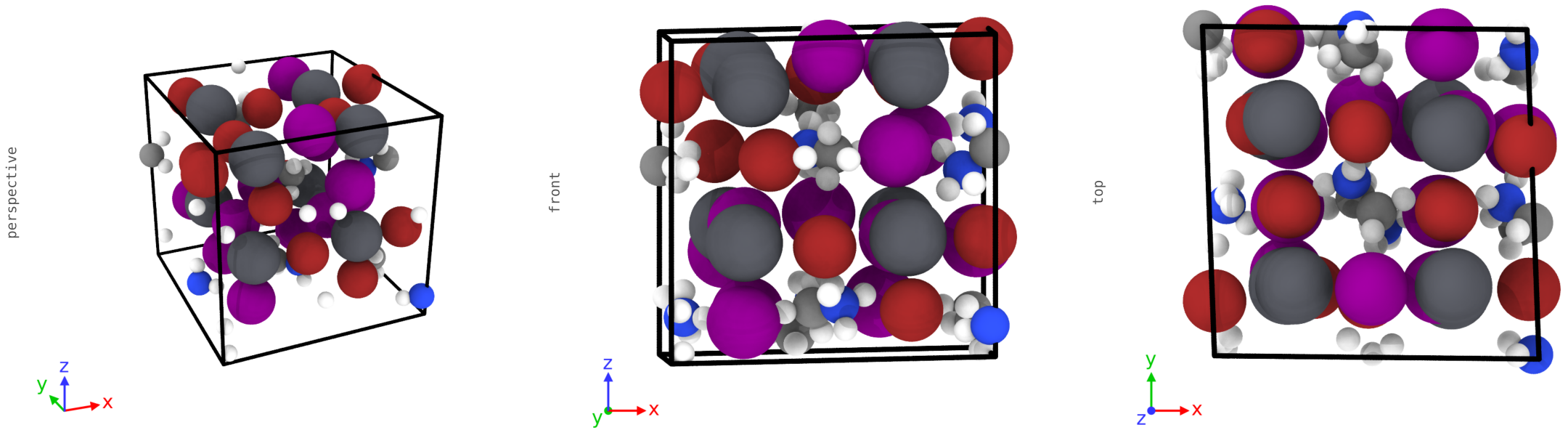




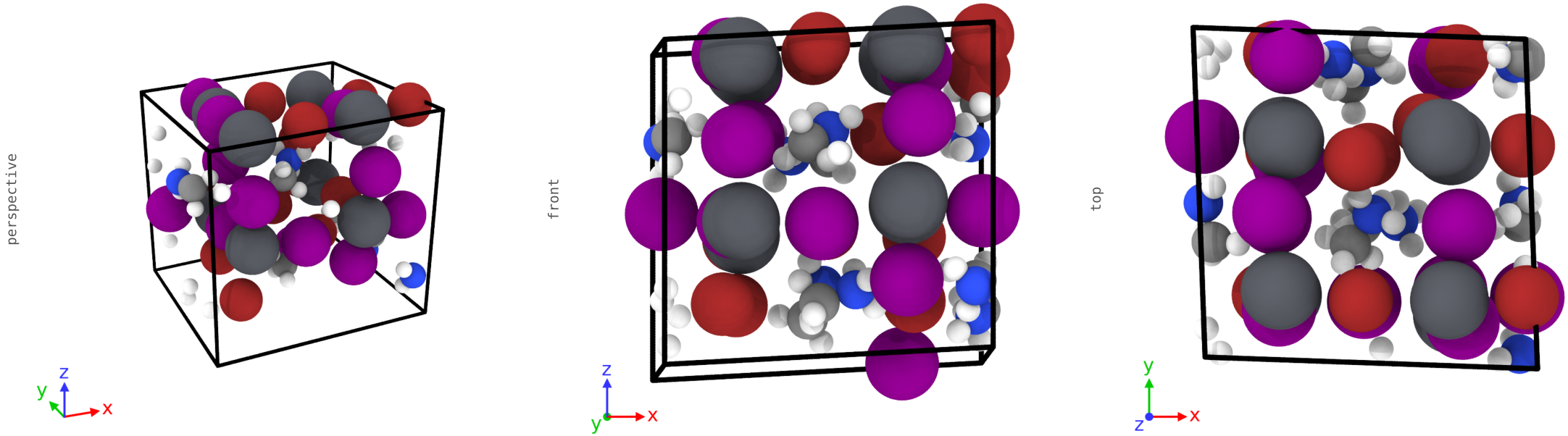


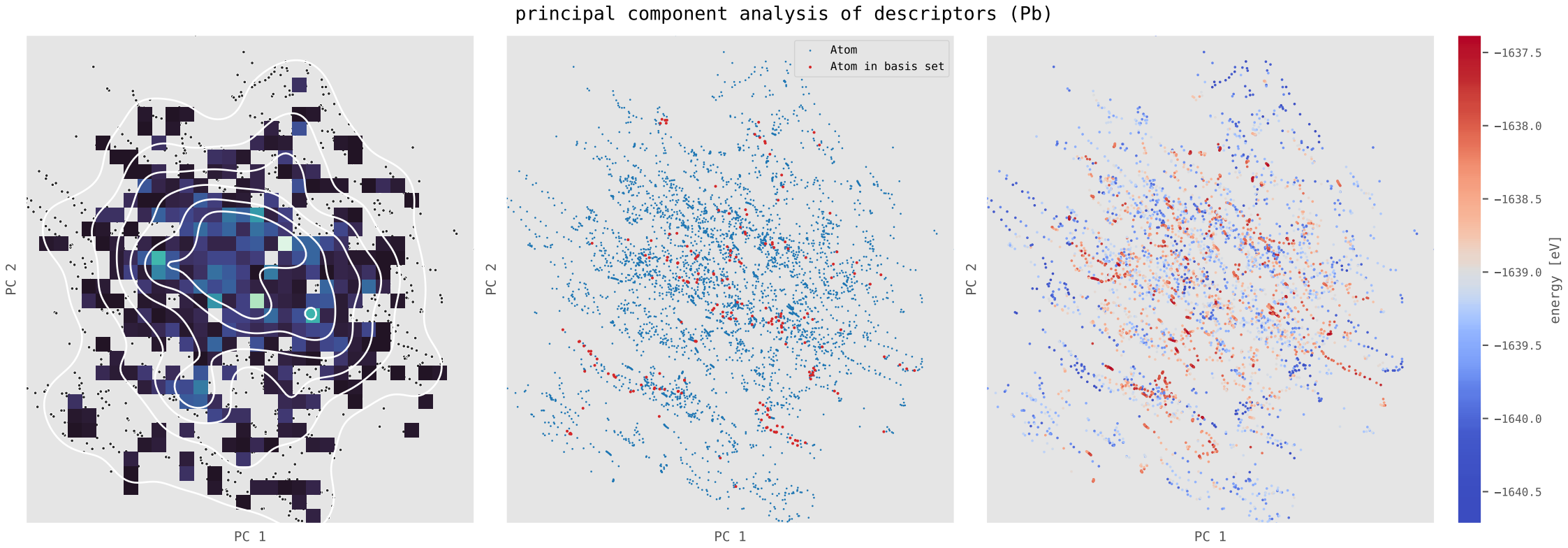


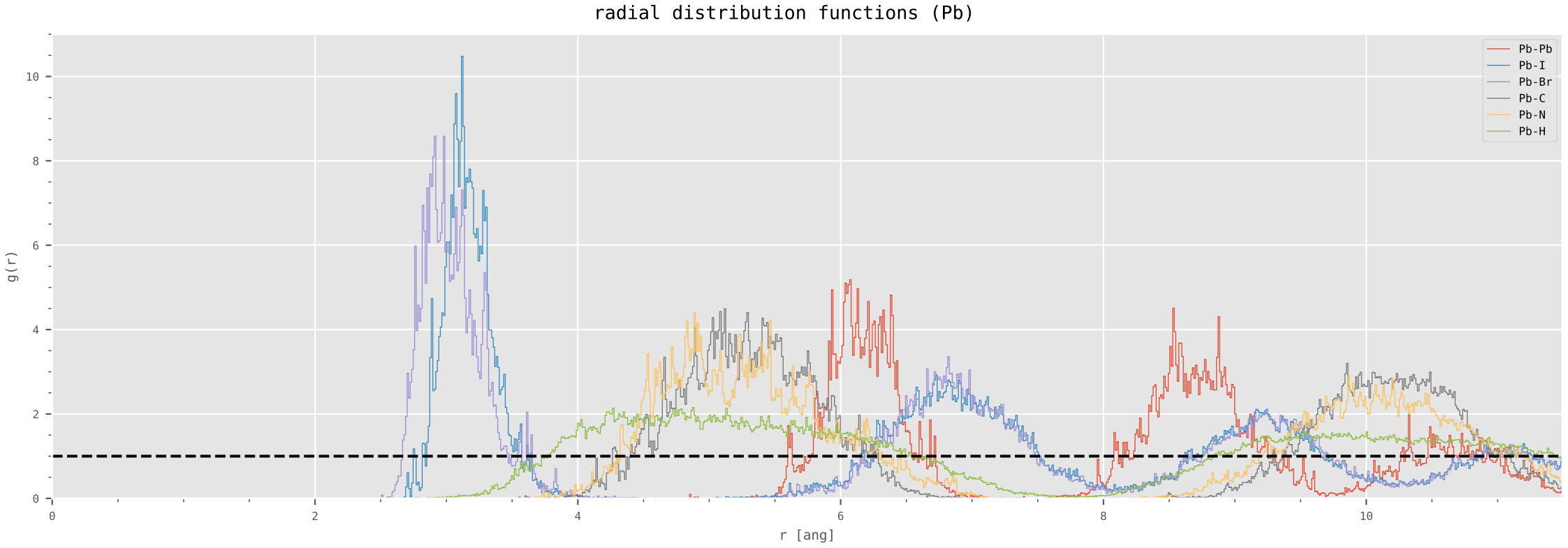
minimum energy configuration (structure 57)

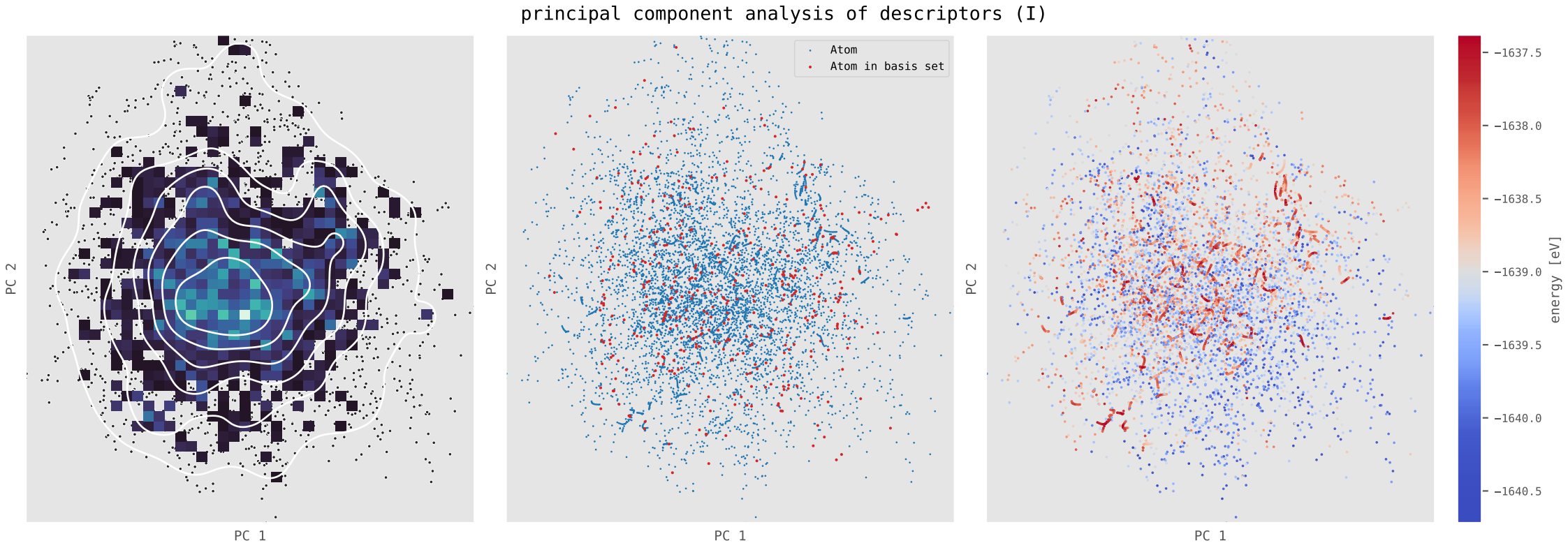


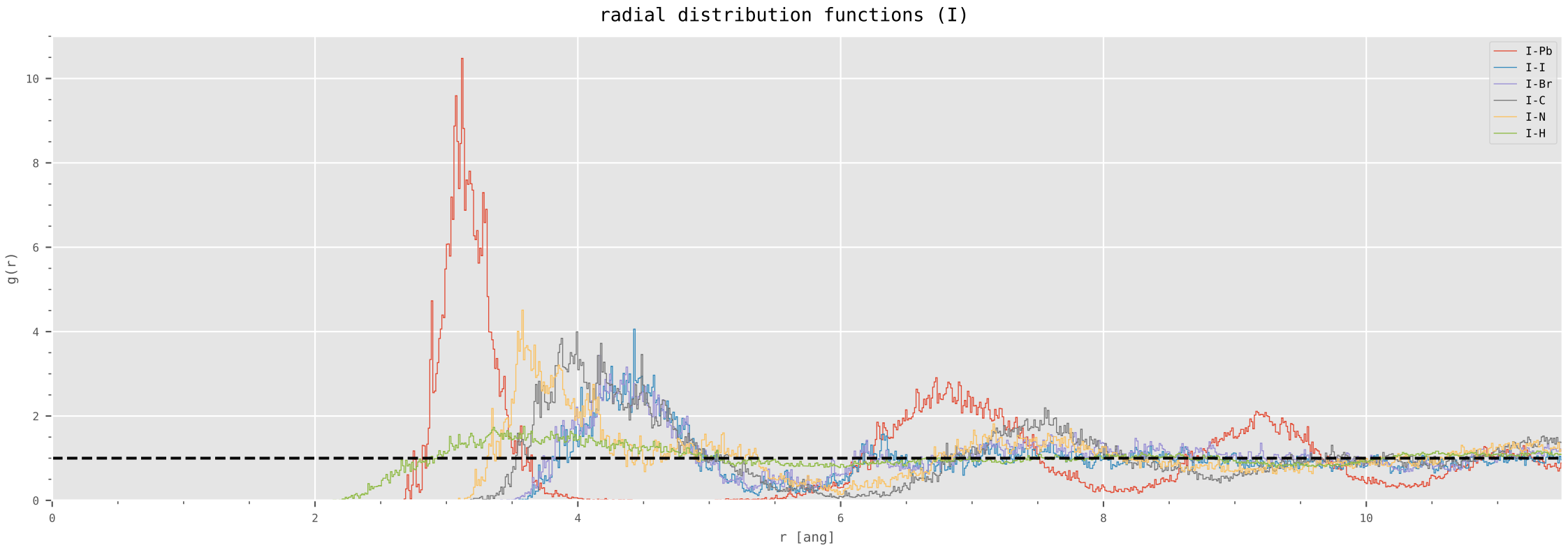
maximum energy configuration (structure 451)

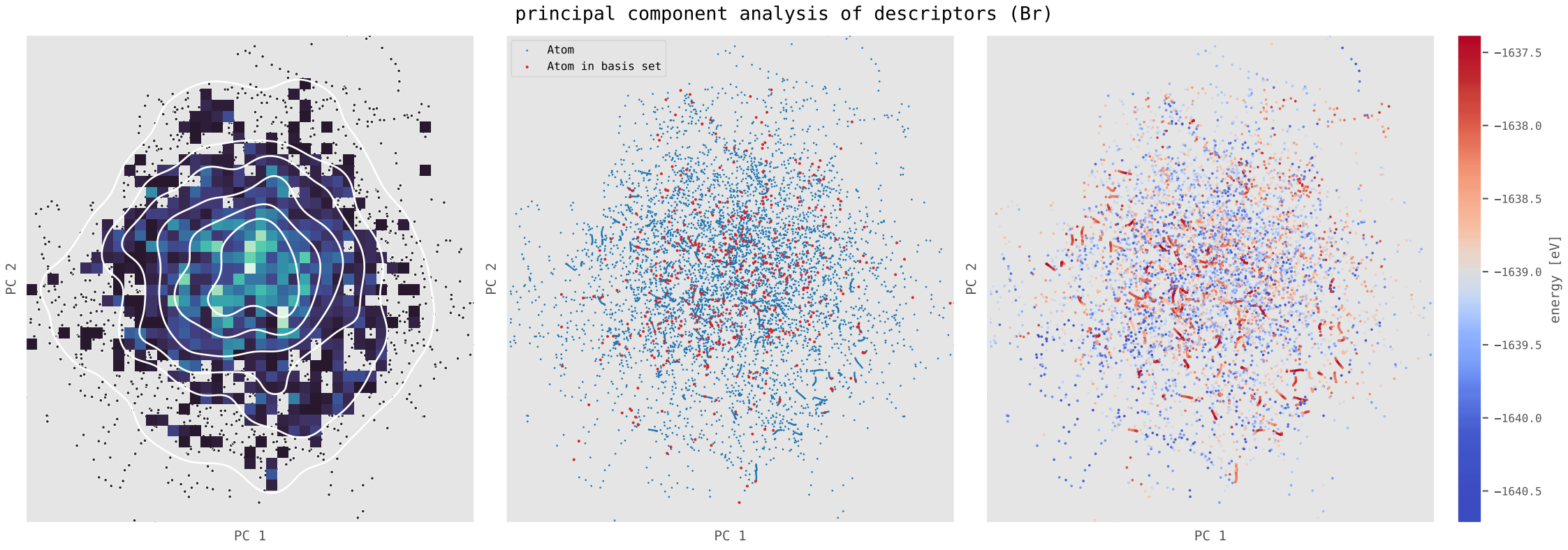


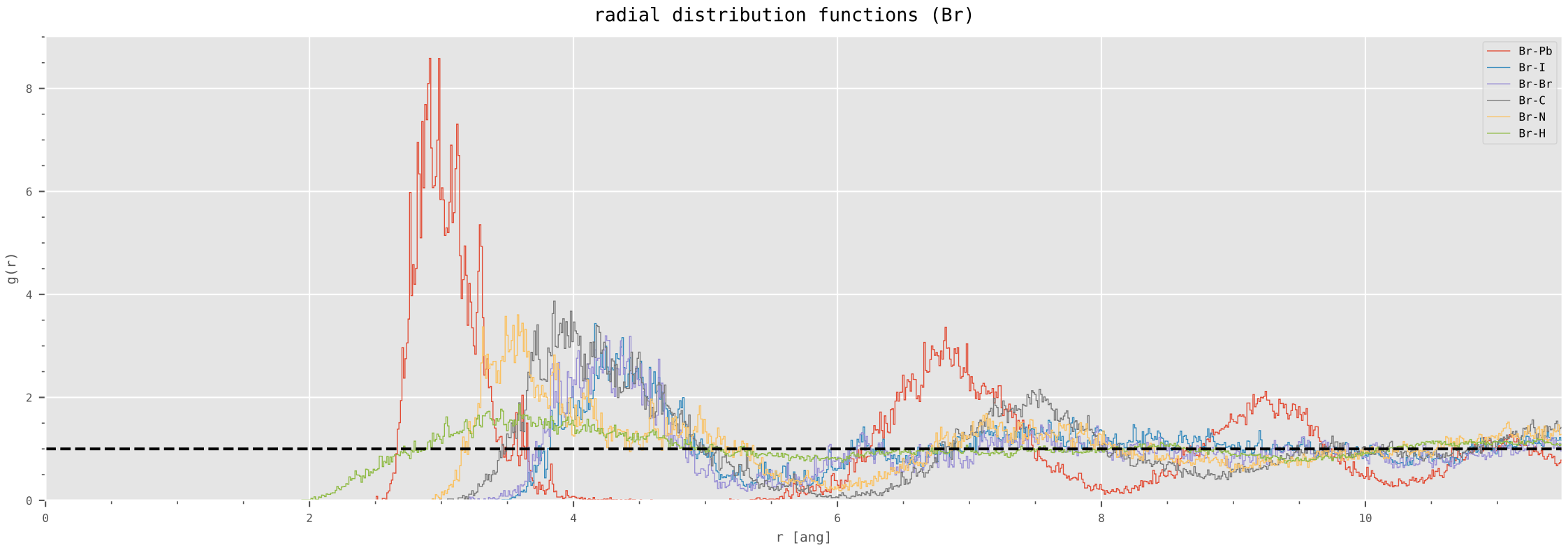

principal component analysis of descriptors (Pb)
PC 2
PC 1
Atom
Atom in basis set
PC 2
PC 1
PC 2
PC 1
−1637.5
−1638.0
−1638.5
−1639.0
−1639.5
−1640.0
−1640.5
energy [eV]

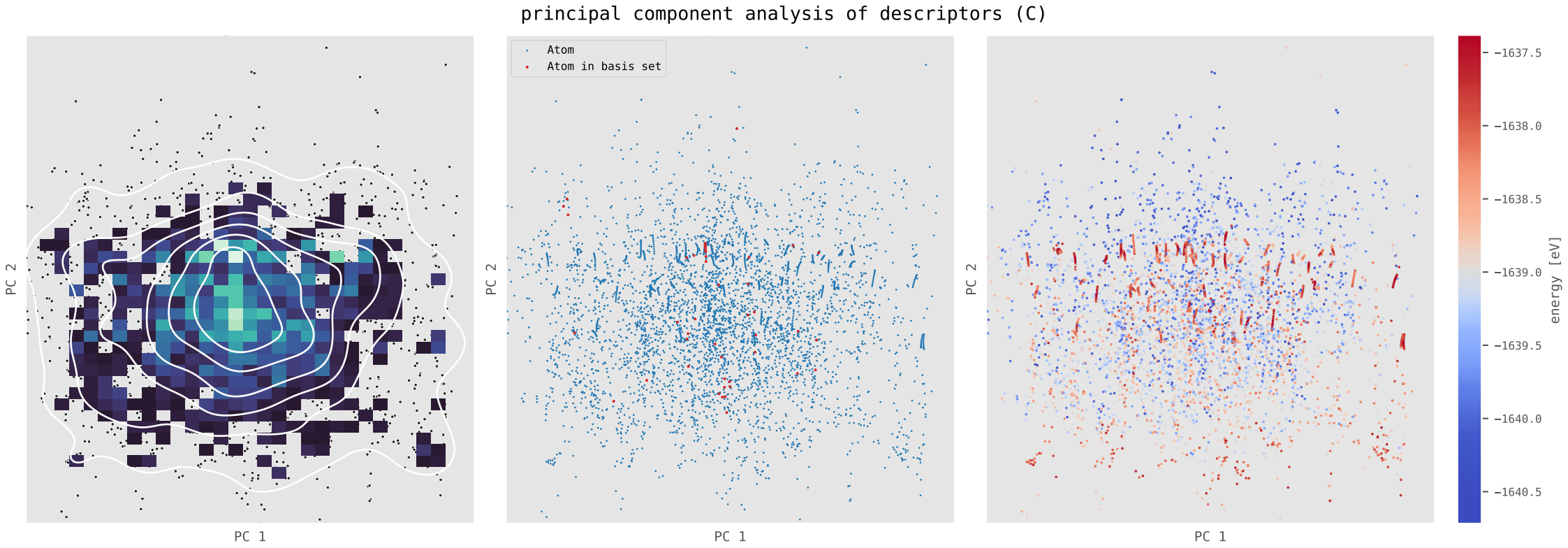

radial distribution functions (Pb)
Pb-Pb
Pb-I
Pb-Br
Pb-C
Pb-N
Pb-H
g(r)
r [ang]
0
2
4
6
8
10

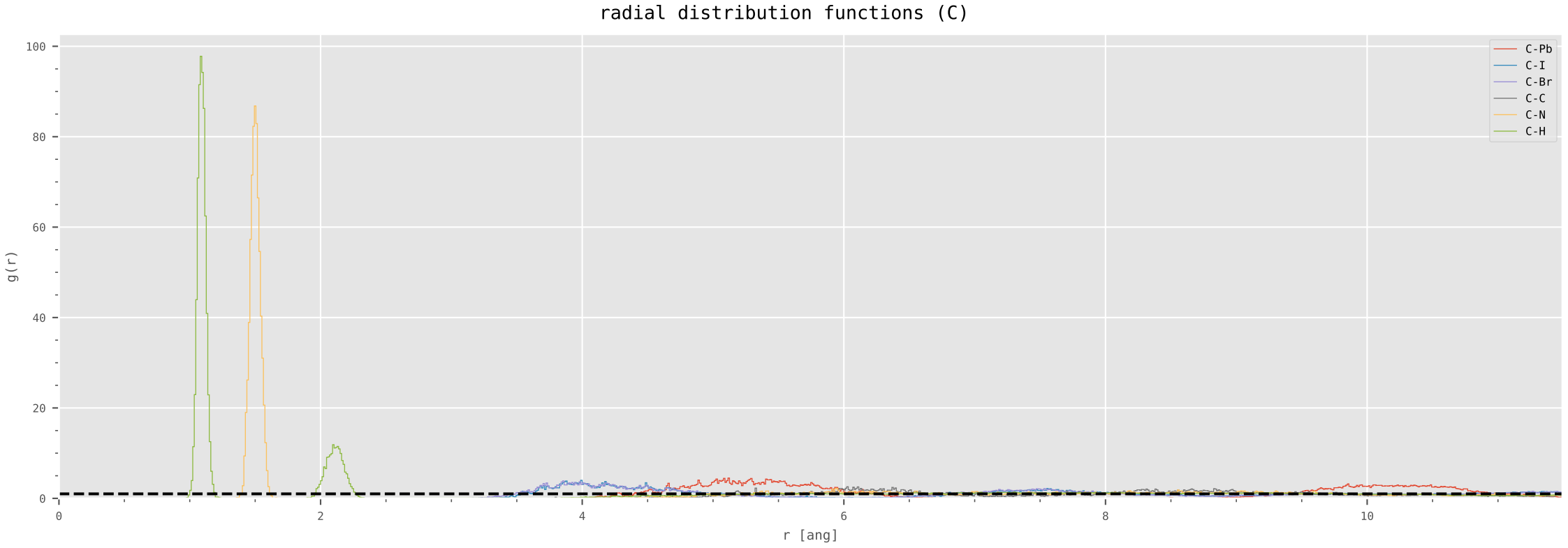

principal component analysis of descriptors (I)
PC 2
PC 1
Atom
Atom in basis set
PC 2
PC 1
PC 2
PC 1
energy [eV]
−1637.5
−1638.0
−1638.5
−1639.0
−1639.5
−1640.0
−1640.5

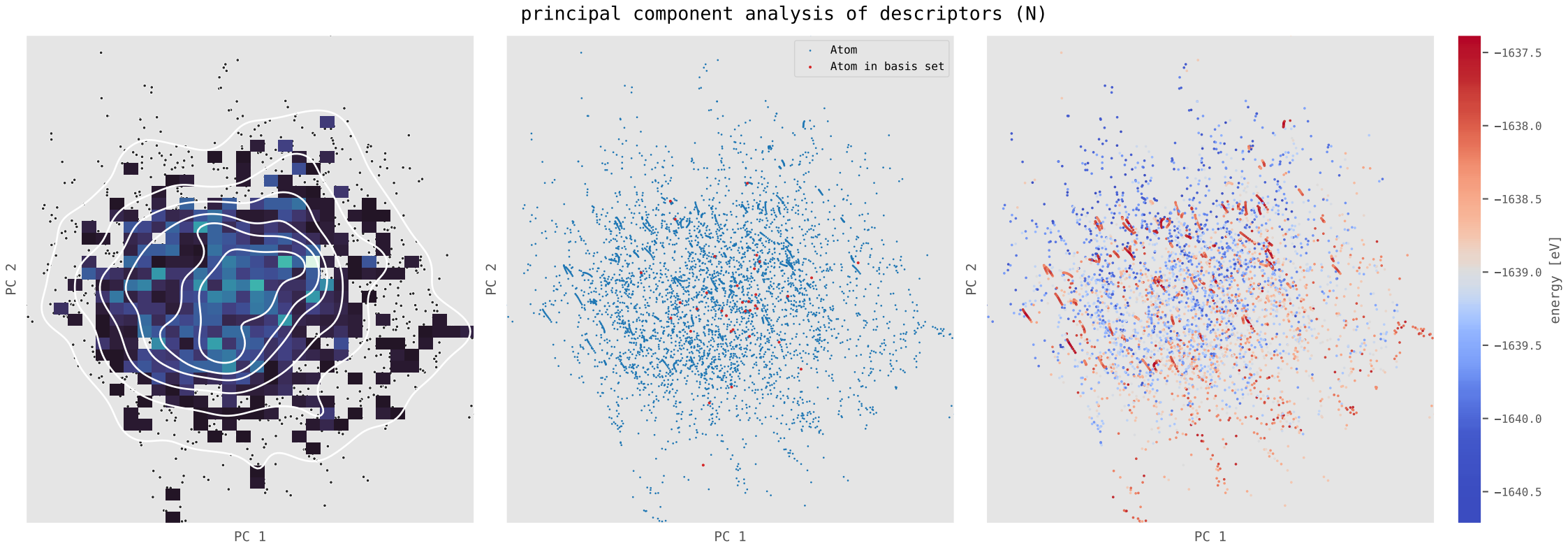

radial distribution functions (I)
I-Pb
I-I
I-Br
I-C
I-N
I-H
g(r)
r [ang]
0
2
4
6
8
10

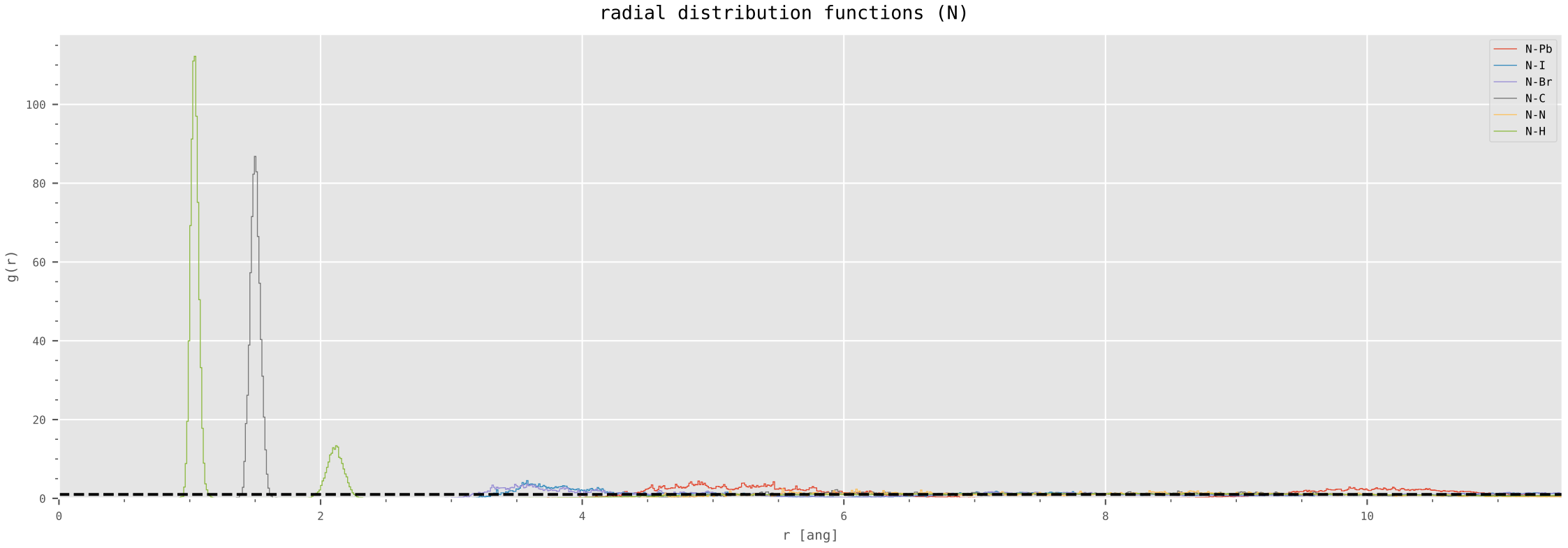

principal component analysis of descriptors (Br)
PC 2
PC 1
Atom
Atom in basis set
PC 2
PC 1
PC 2
PC 1
−1637.5
−1638.0
−1638.5
−1639.0
−1639.5
−1640.0
−1640.5
energy [eV]

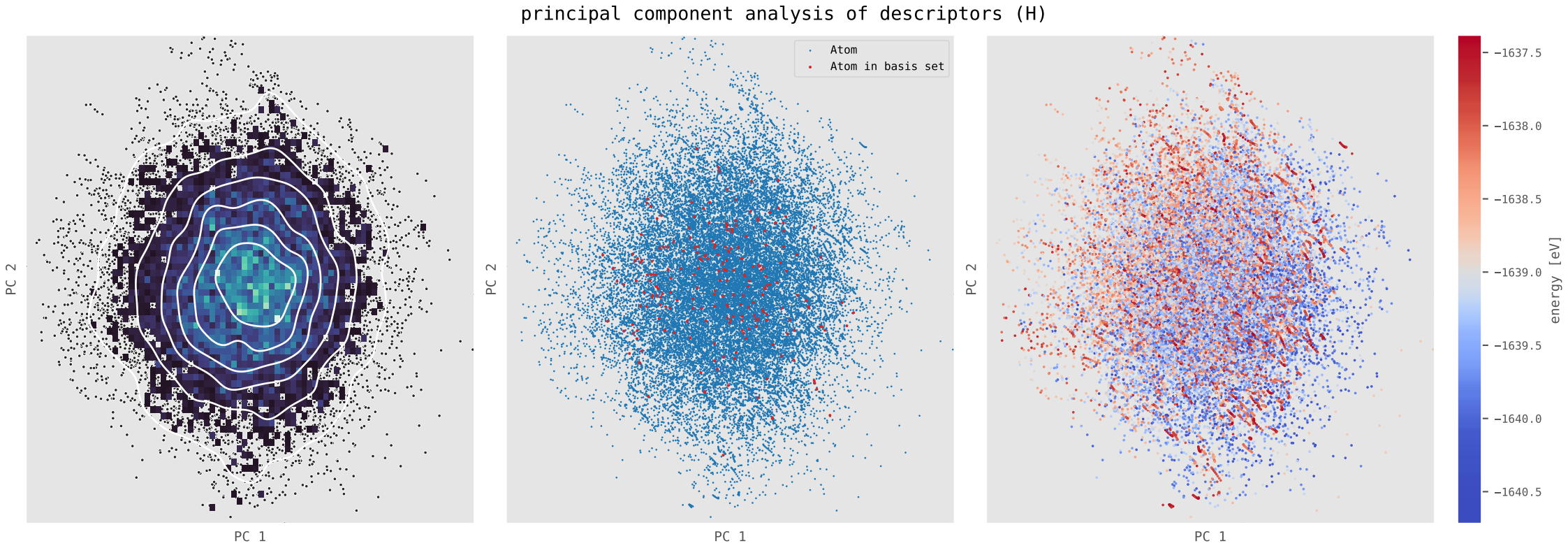

radial distribution functions (Br)
Br-Pb
Br-I
Br-Br
Br-C
Br-N
Br-H
g(r)
0
2
4
6
8
r [ang]
0
2
4
6
8
10

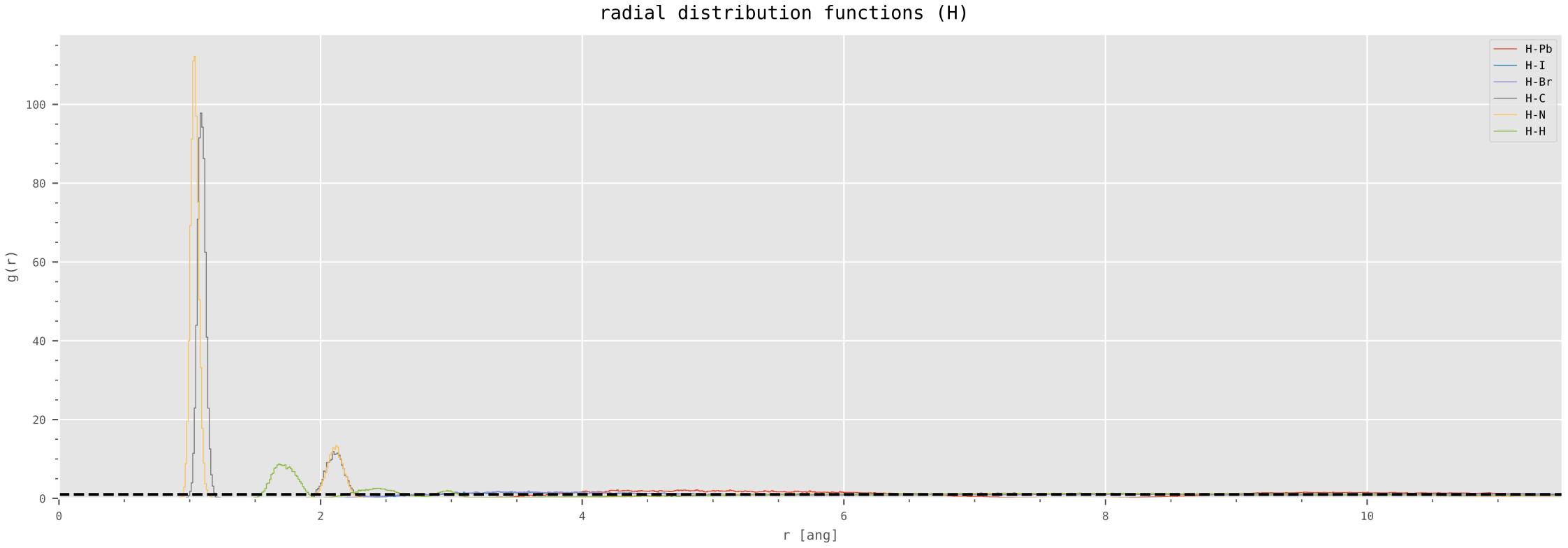

principal component analysis of descriptors (C)
PC 2
PC 1
Atom
Atom in basis set
PC 2
PC 1
PC 2
PC 1
−1637.5
−1638.0
−1638.5
−1639.0
−1639.5
−1640.0
−1640.5
energy [eV]


radial distribution functions (C)
C-Pb
C-I
C-Br
C-C
C-N
C-H
g(r)
r [ang]
0
20
40
60
80
100
0
2
4
6
8
10


principal component analysis of descriptors (N)
PC 2
PC 1
Atom
Atom in basis set
PC 2
PC 1
PC 2
PC 1
−1637.5
−1638.0
−1638.5
−1639.0
−1639.5
−1640.0
−1640.5
energy [eV]


radial distribution functions (N)
N-Pb
N-I
N-Br
N-C
N-N
N-H
g(r)
0
20
40
60
80
100
0
2
4
6
8
10
r [ang]


principal component analysis of descriptors (H)
PC 2
PC 1
Atom
Atom in basis set
energy [eV]
−1637.5
−1638.0
−1638.5
−1639.0
−1639.5
−1640.0
−1640.5


radial distribution functions (H)
H-Pb
H-I
H-Br
H-C
H-N
H-H
g(r)
r [ang]
0
20
40
60
80
100
0
2
4
6
8
10