

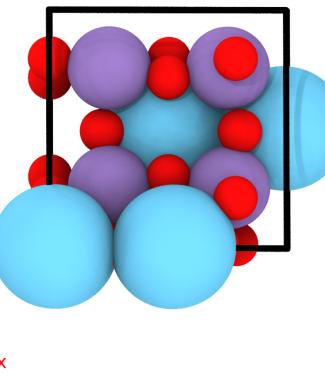
[1/1] ML_ABN (LaMnO₃:

file

name ML_ABN
 structure groups 1
 total structures 577

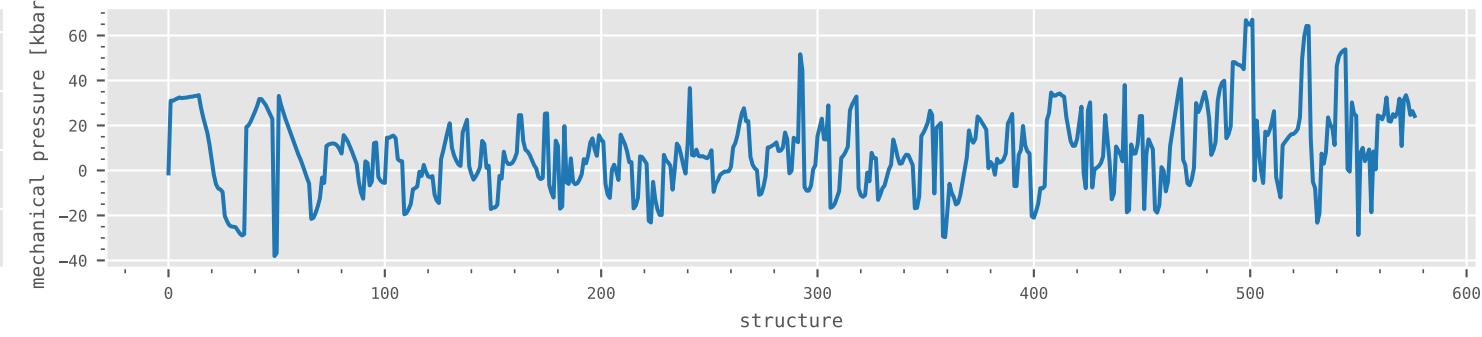
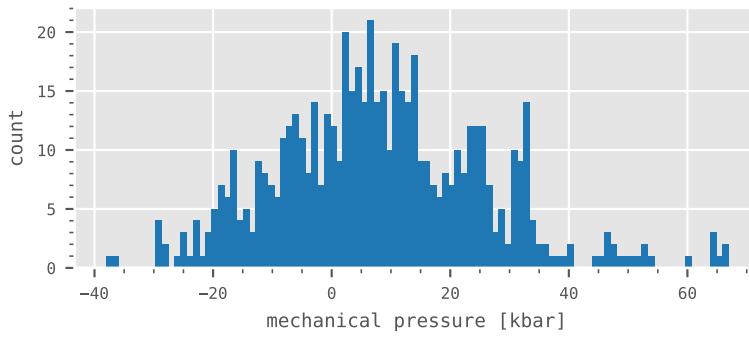
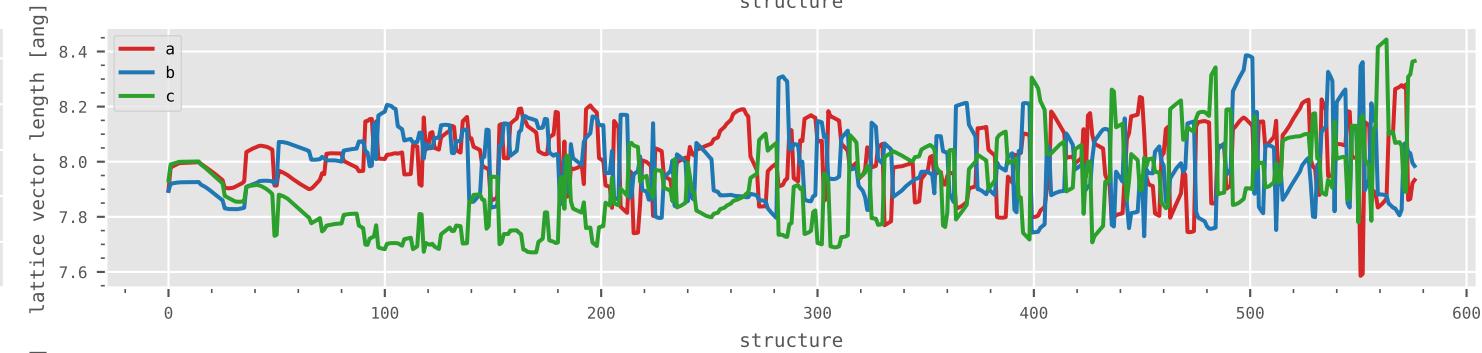
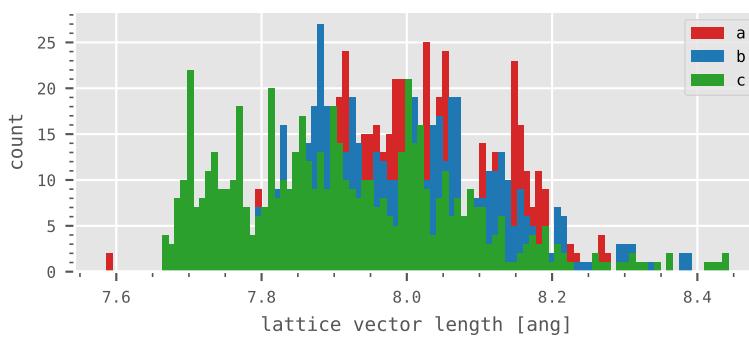
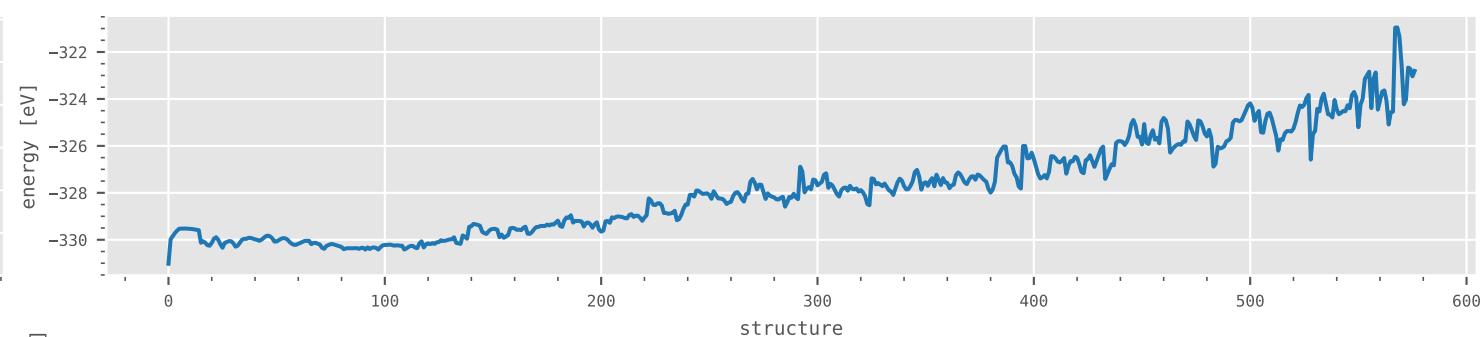
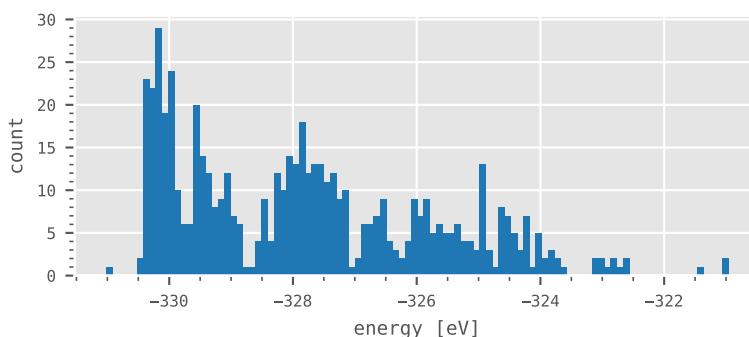
overview

energy	-327.8 ± 2.06	eV
volume	506.7 ± 9.25	ang ³
lattice vector a	8.0 ± 0.12	ang
lattice vector b	8.0 ± 0.13	ang
lattice vector c	7.9 ± 0.16	ang
non-periodic radius	3.8 (min. for group)	ang



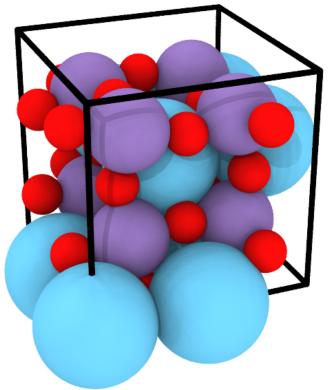
current structure group

name LaMnO₃:
 structure group 1 (of 1 in file)
 structures 577 (of 577 in file)
 atoms La (8), Mn (8), O (24)
 40 total

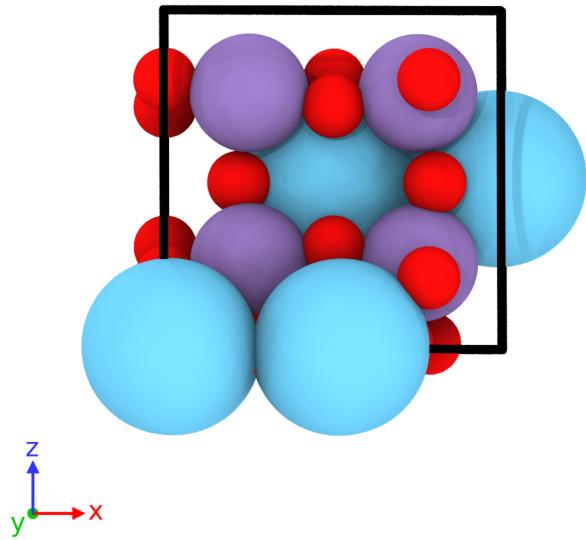


minimum energy configuration (structure 1)

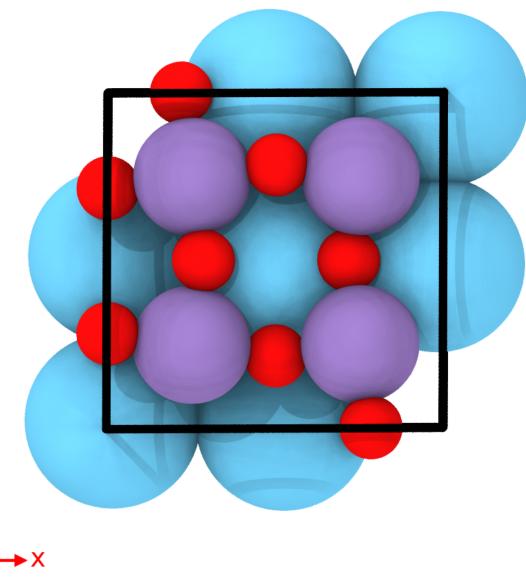
perspective



front

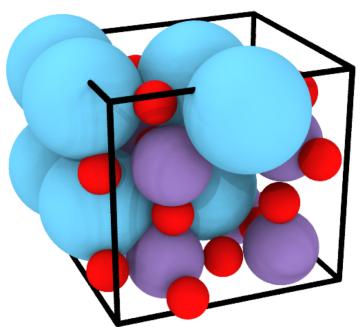


top

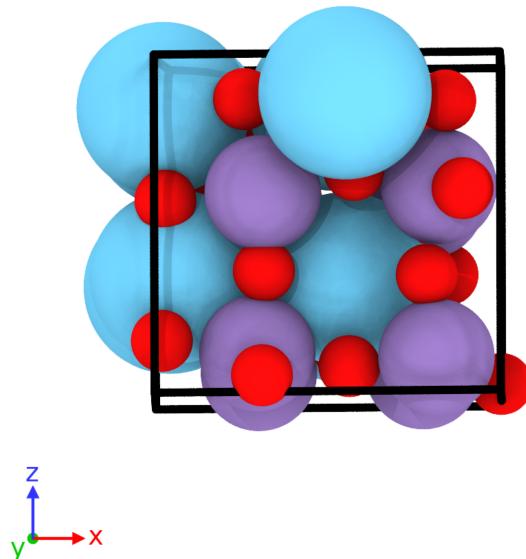


maximum energy configuration (structure 569)

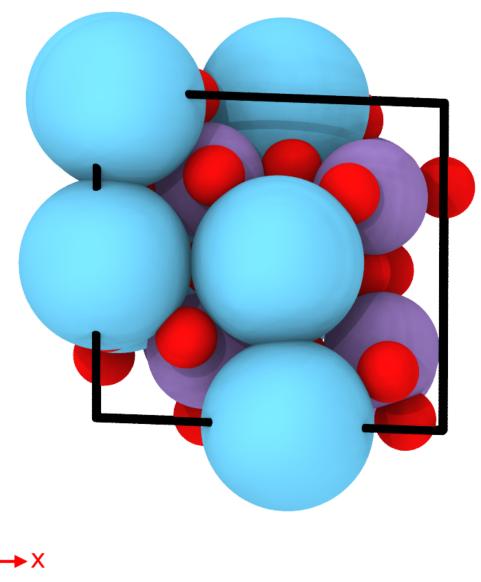
perspective



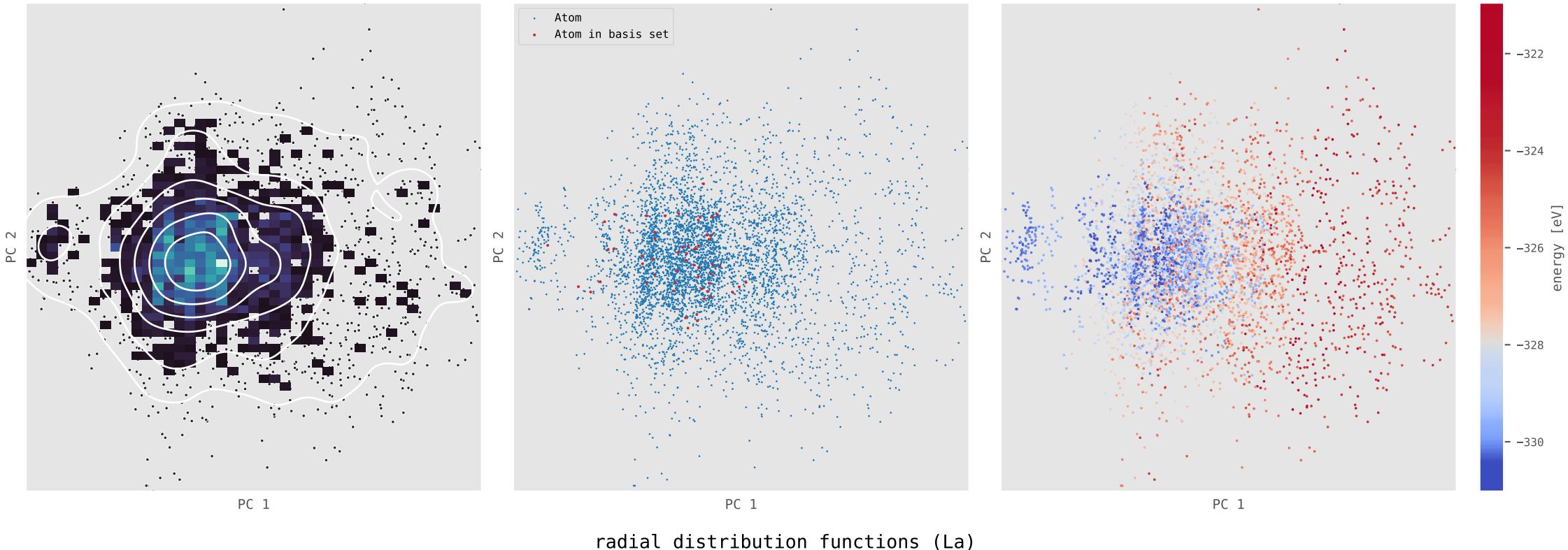
front



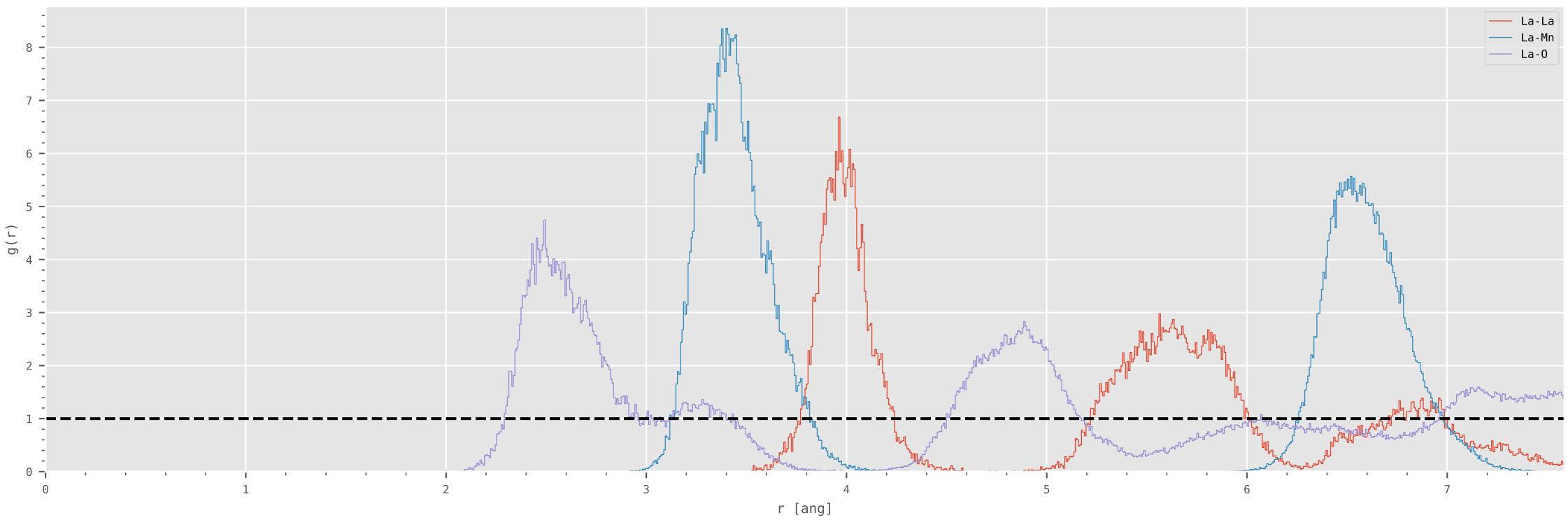
top



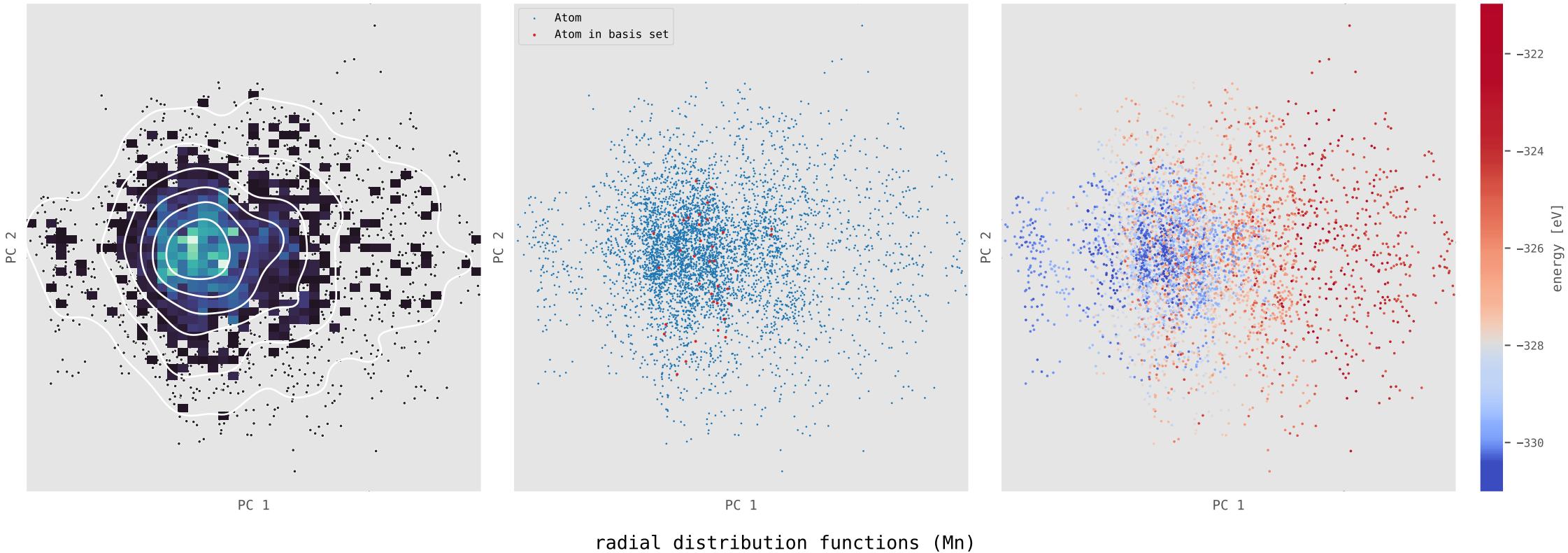
principal component analysis of descriptors (La)



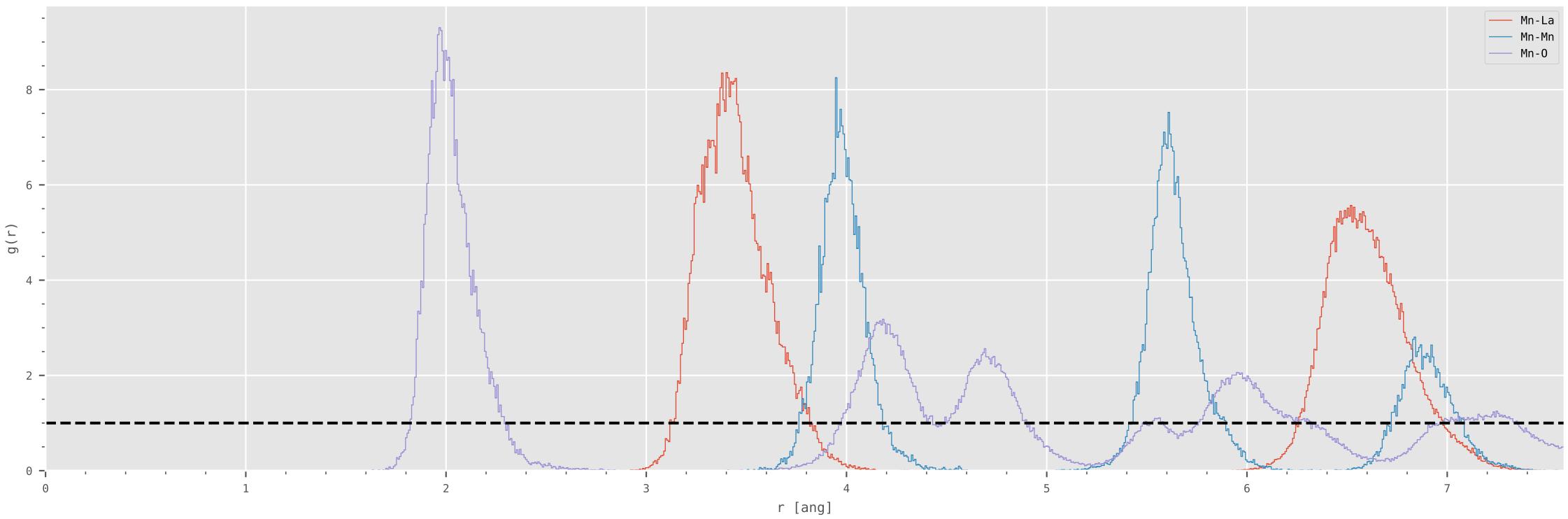
radial distribution functions (La)



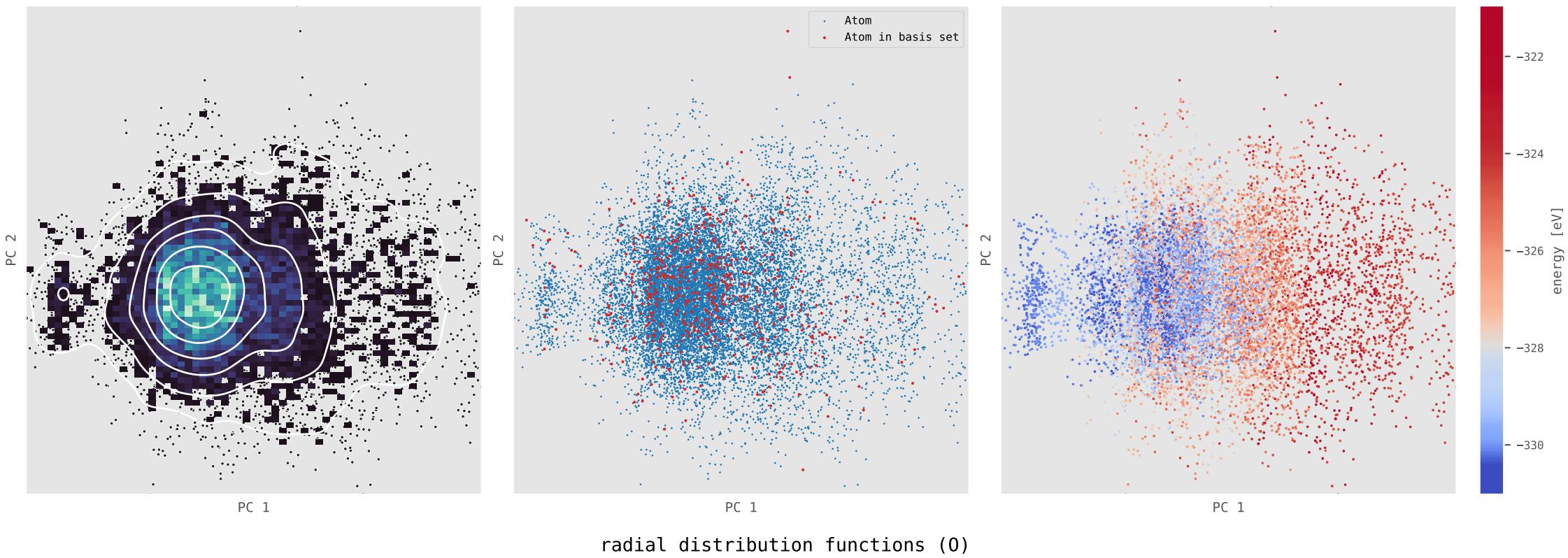
principal component analysis of descriptors (Mn)



radial distribution functions (Mn)



principal component analysis of descriptors (0)



radial distribution functions (0)

