

[1/1] ML_ABN (LaMnO3:)

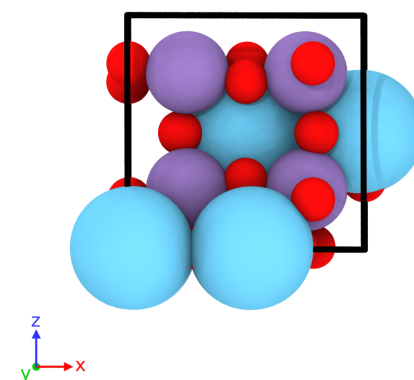
file

name	ML_ABN
structure groups	1
total structures	571

overview

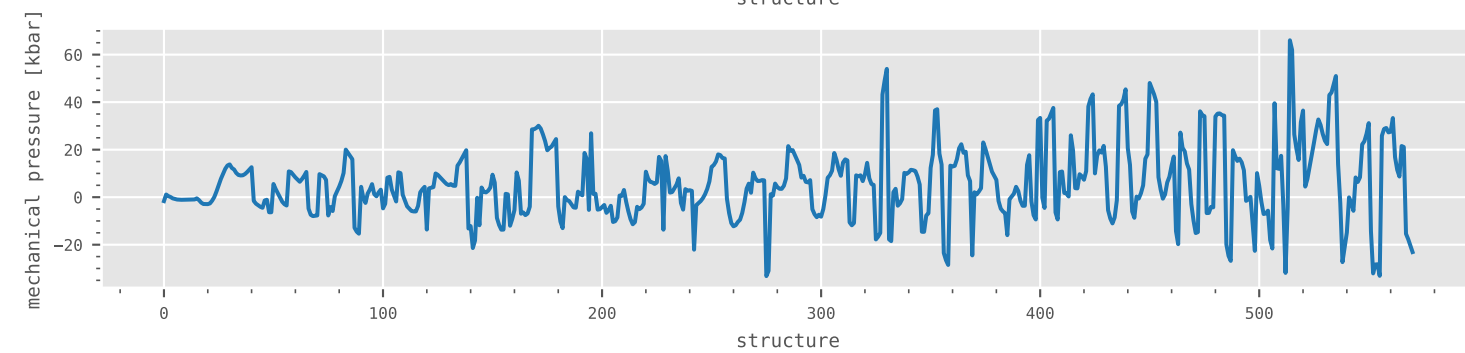
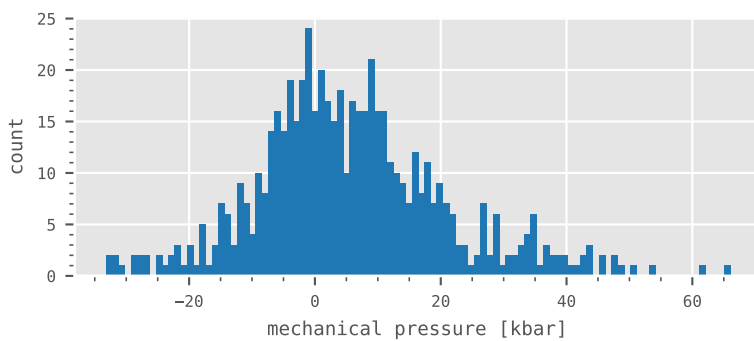
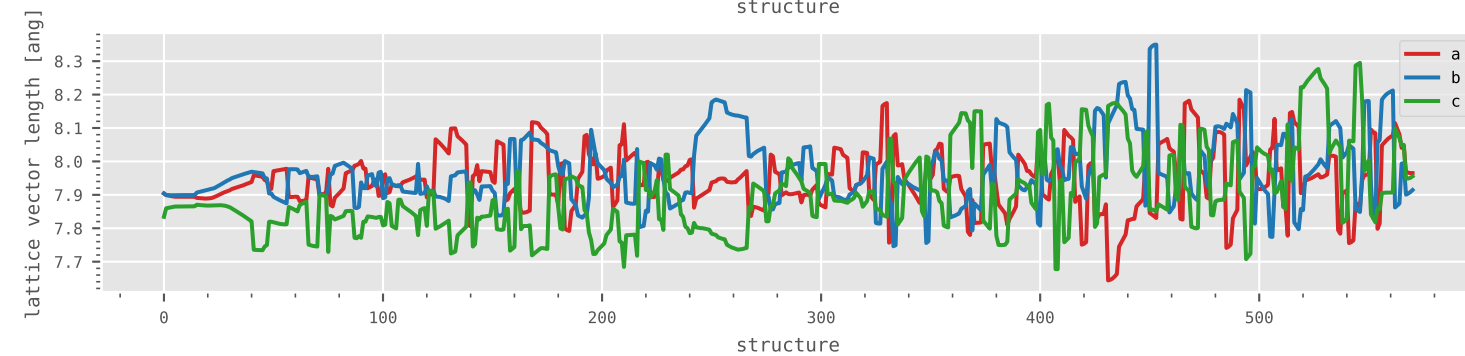
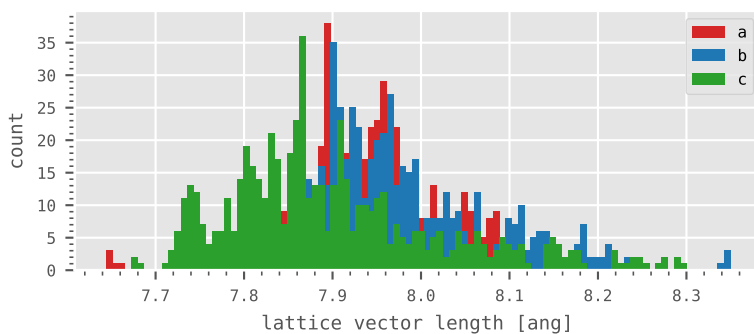
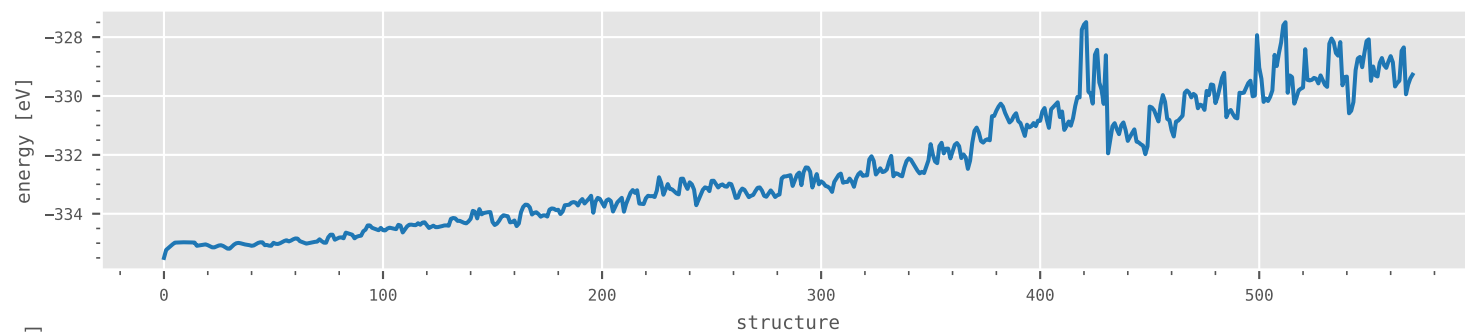
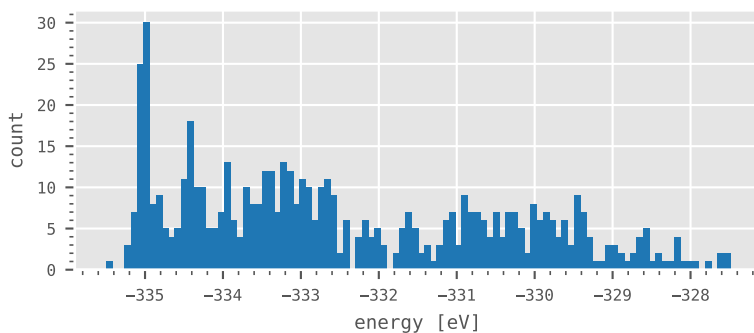
energy	-332.4 ± 2.04	eV
volume	500.3 ± 8.76	ang ³
lattice vector a	7.9 ± 0.09	ang
lattice vector b	8.0 ± 0.10	ang
lattice vector c	7.9 ± 0.12	ang
non-periodic radius	3.8 (min. for group)	ang

min energy configuration



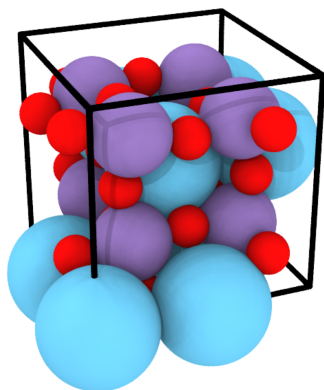
current structure group

name	LaMnO3:
structure group	1 (of 1 in file)
structures	571 (of 571 in file)
atoms	La (8), Mn (8), O (24)
	40 total

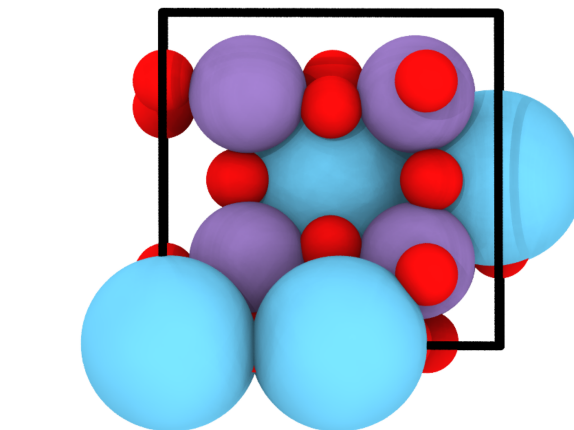


minimum energy configuration (structure 1)

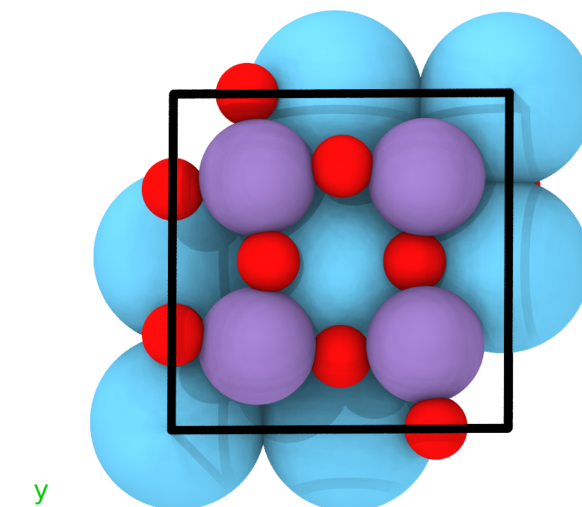
perspective



front

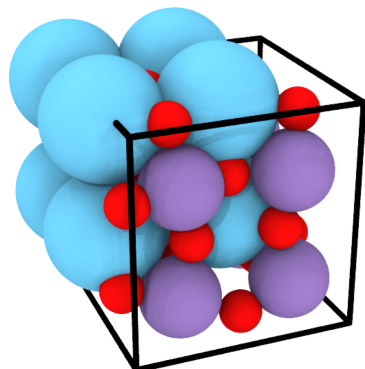


top

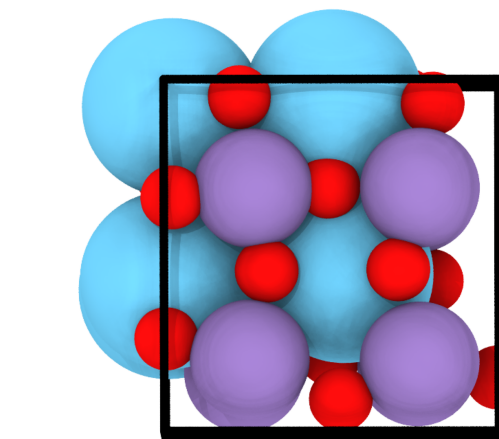


maximum energy configuration (structure 422)

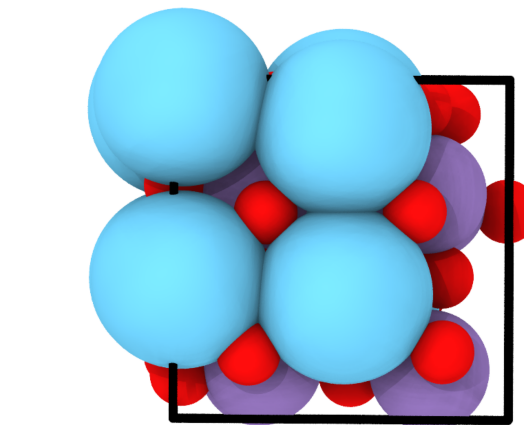
perspective



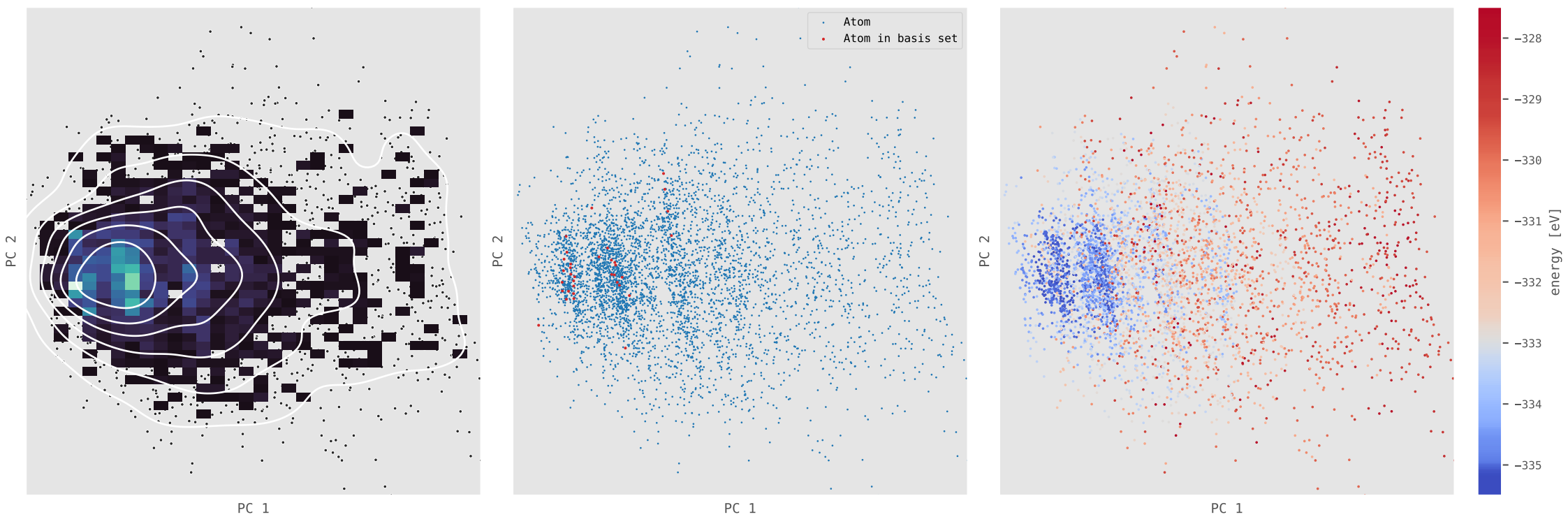
front



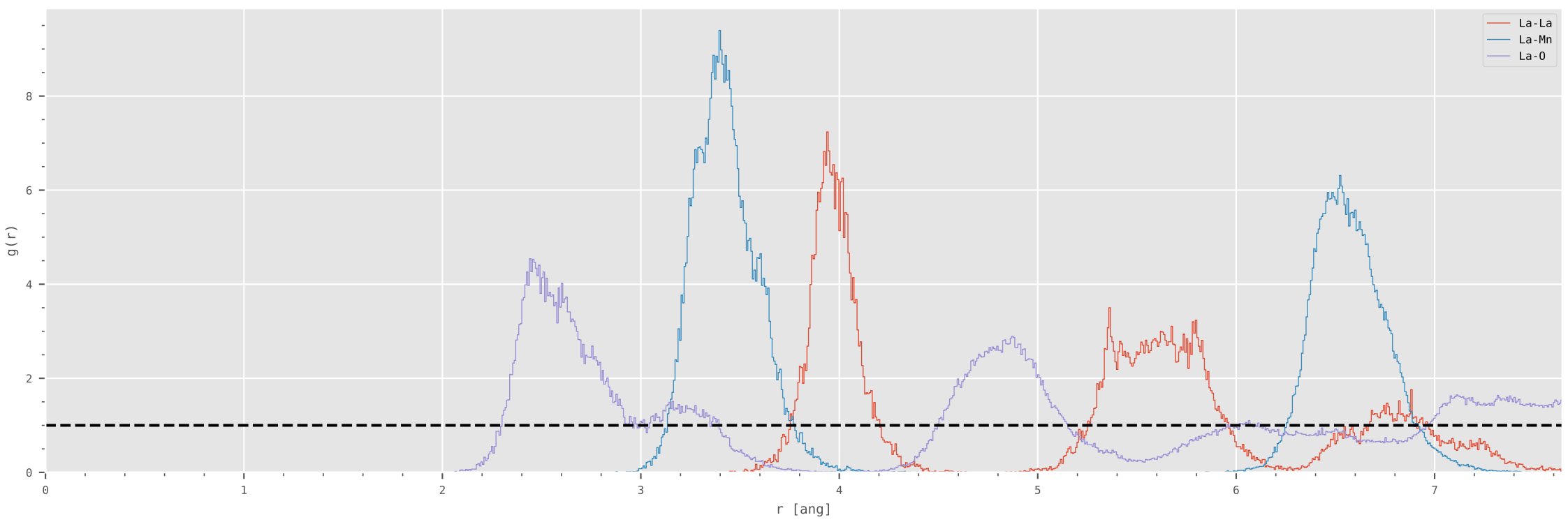
top



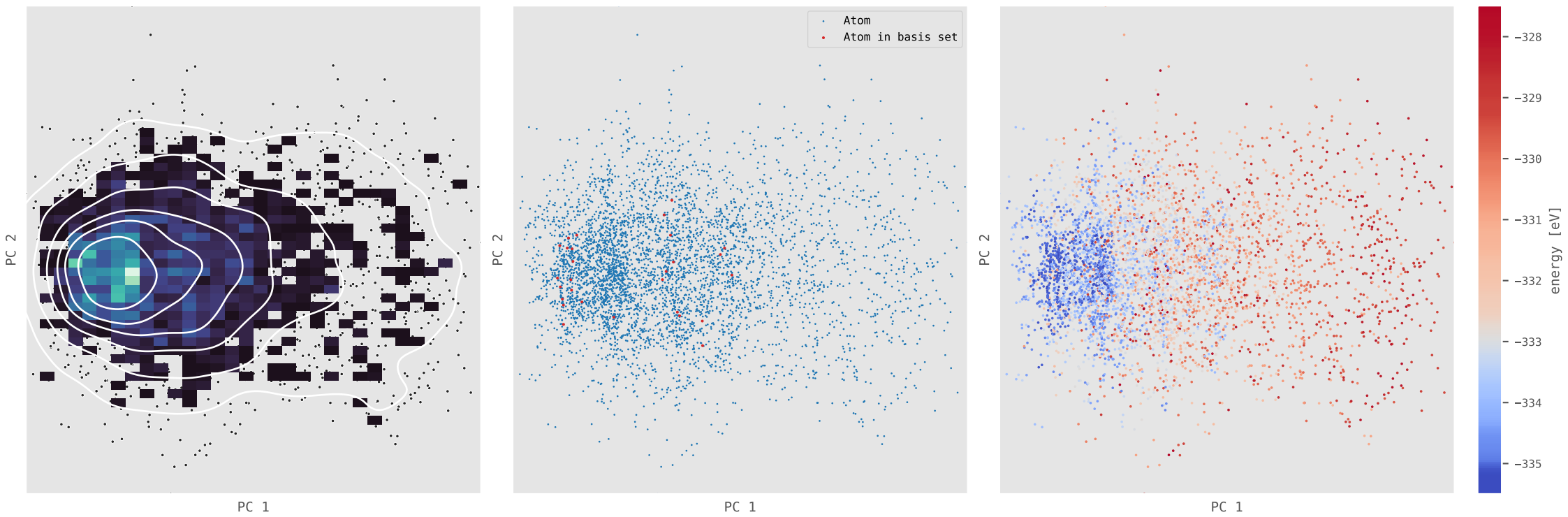
principal component analysis of descriptors (La)



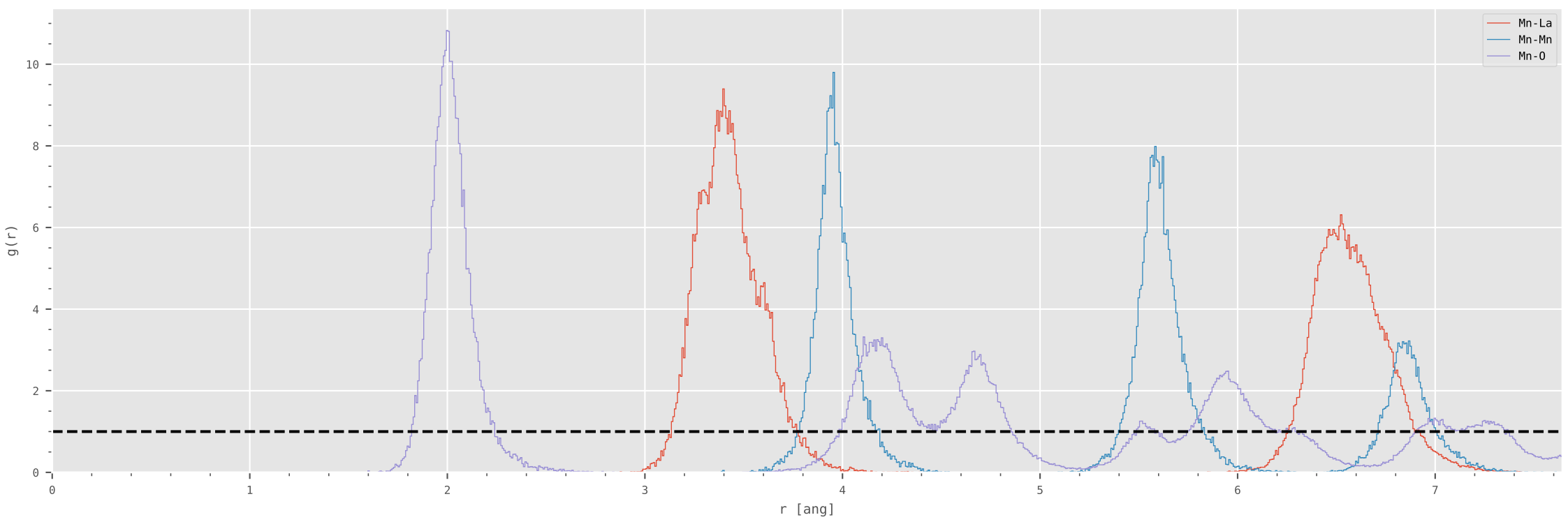
radial distribution functions (La)



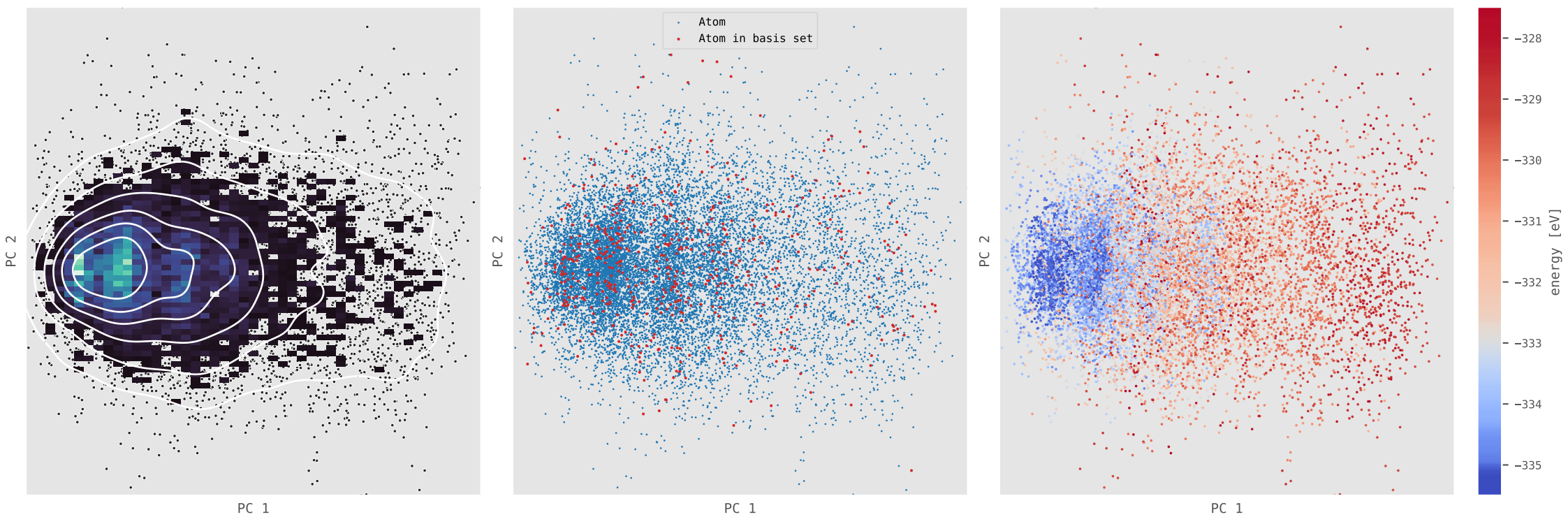
principal component analysis of descriptors (Mn)



radial distribution functions (Mn)



principal component analysis of descriptors (0)



radial distribution functions (0)

