file

name	ML_ABN
structure groups	1
total structures	1384

overview

energy	-318.7 ± 2.35	eV
volume	513.6 ± 8.69	ang^3
lattice vector a	8.1 ± 0.10	ang
lattice vector b	8.1 ± 0.10	ang
lattice vector c	7.9 ± 0.17	ang
non-periodic radius	3.8 (min. for group)	ang

current structure group

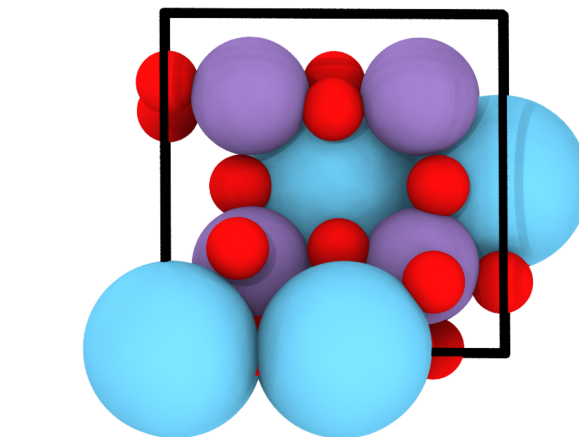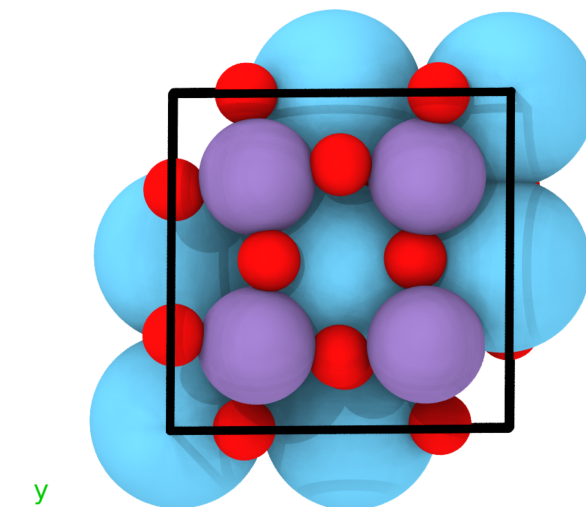|	
name	LaMnO3:
structure group	1 (of 1 in file)
structures	1384 (of 1384 in file)
atoms	La (8), Mn (8), O (24)
	40 total
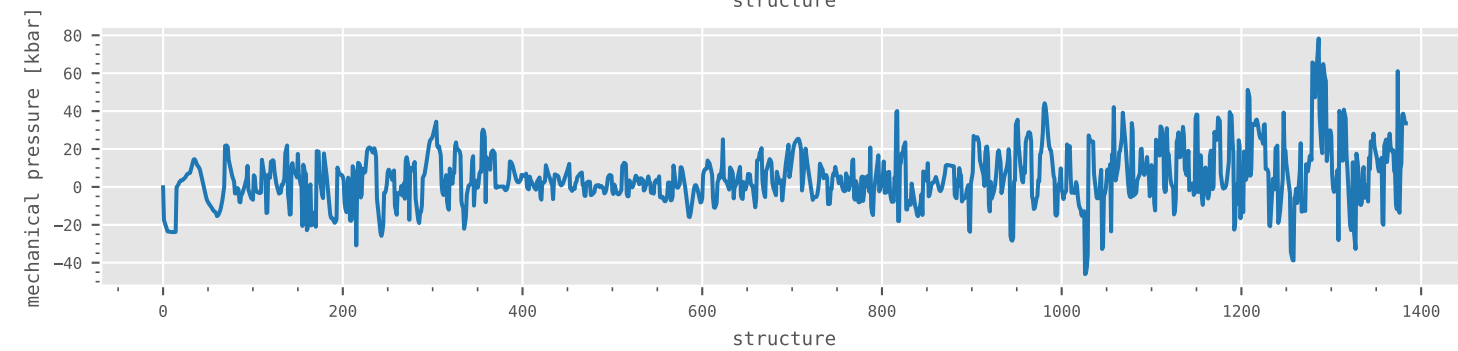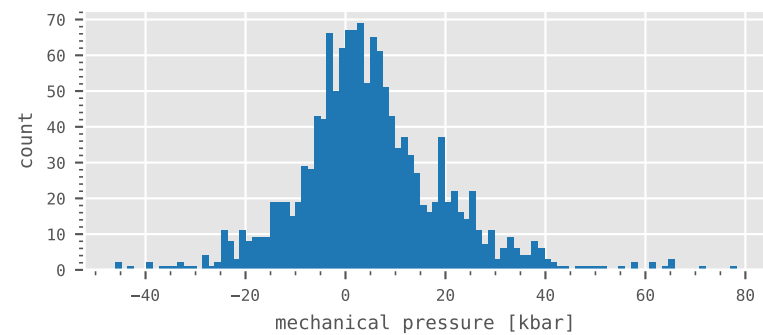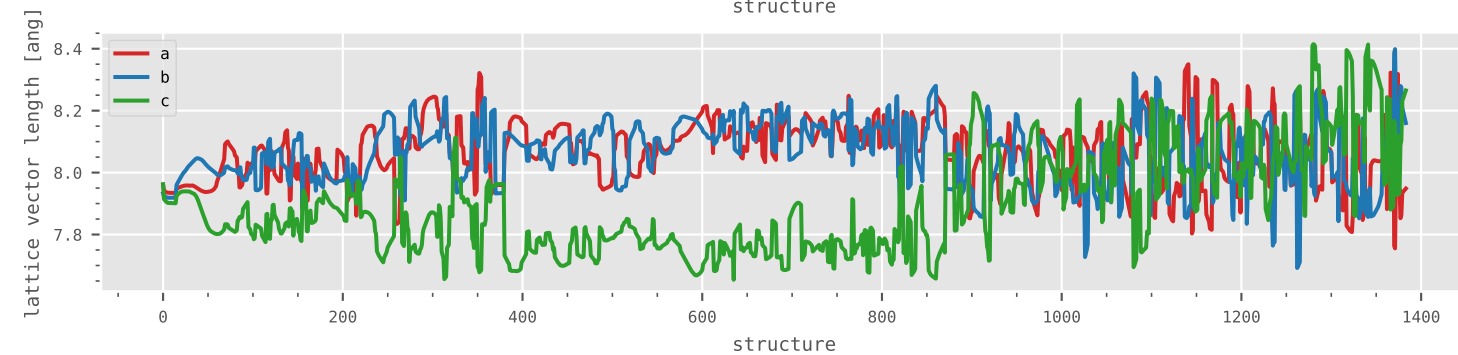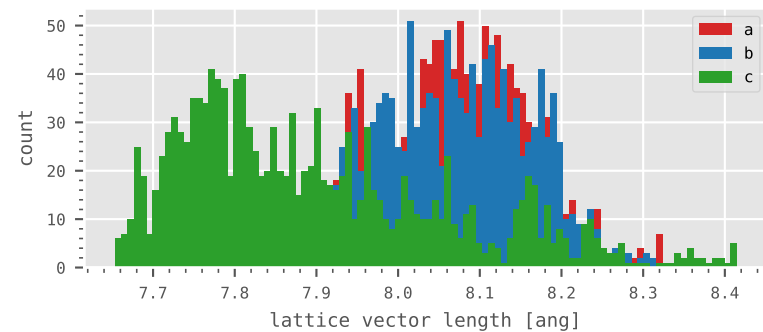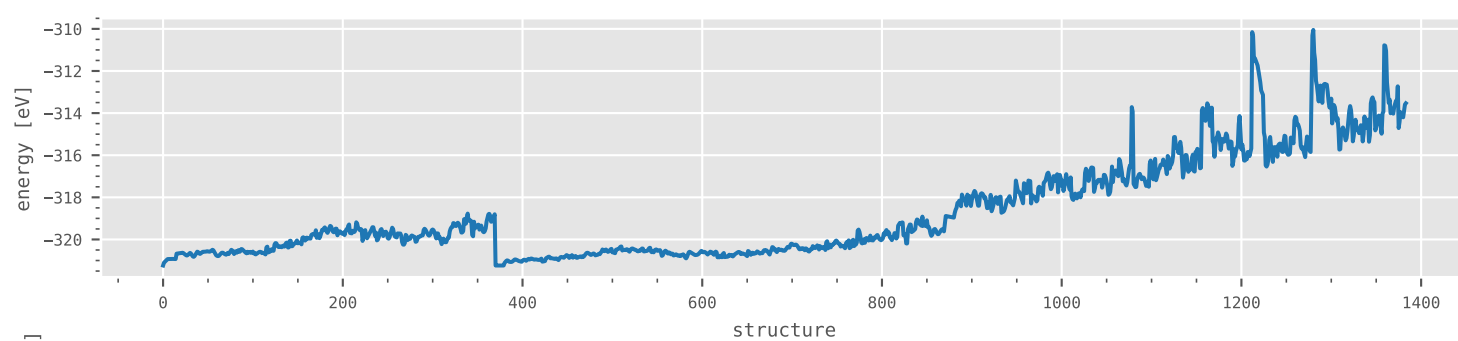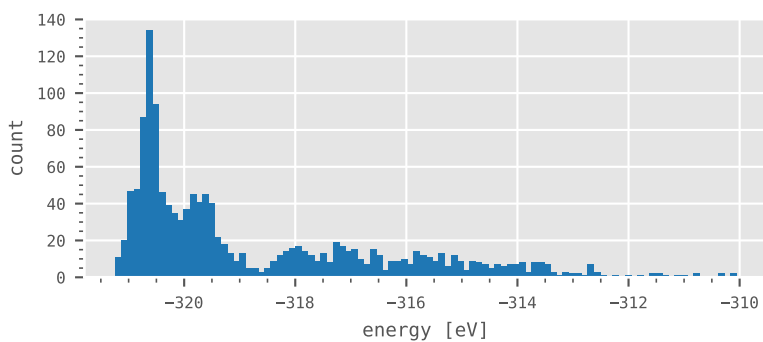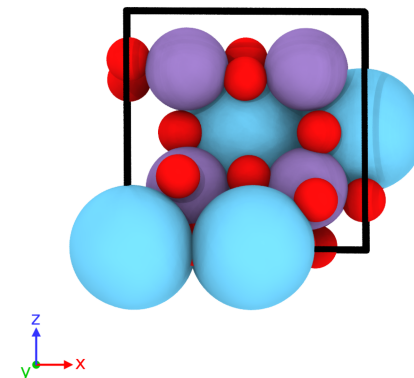
minimum energy configuration (structure 1)
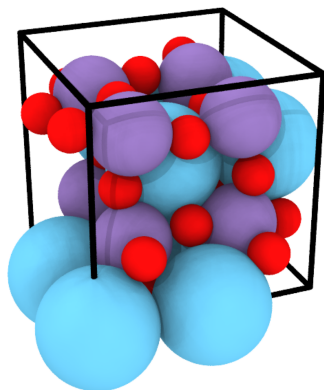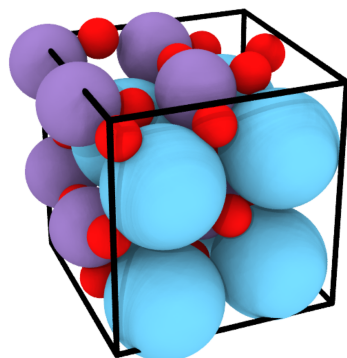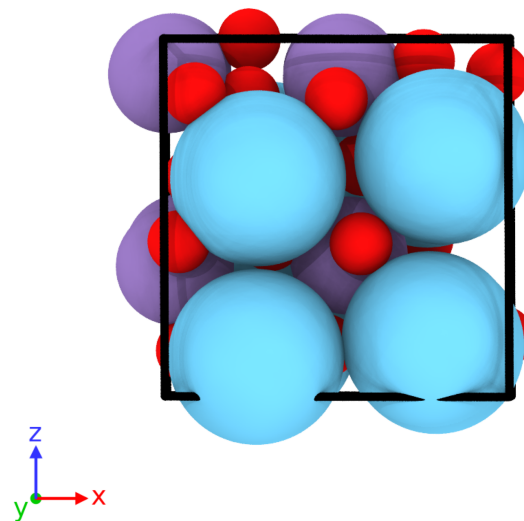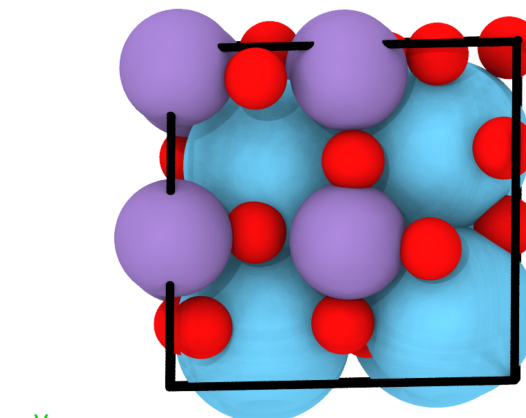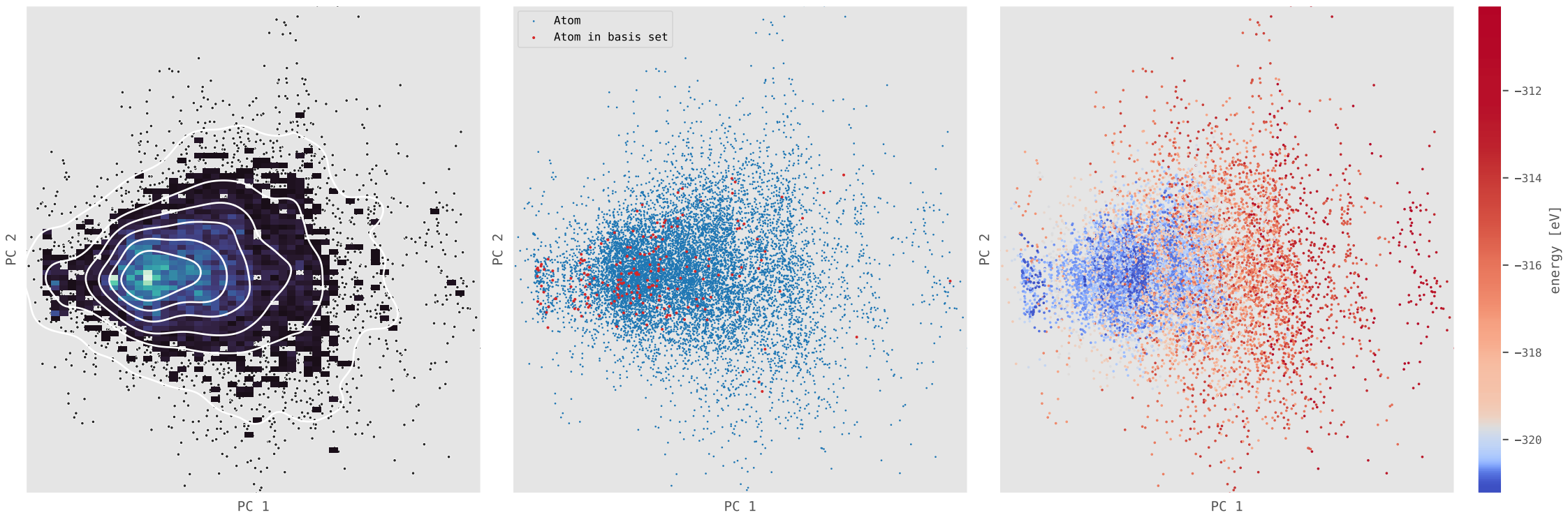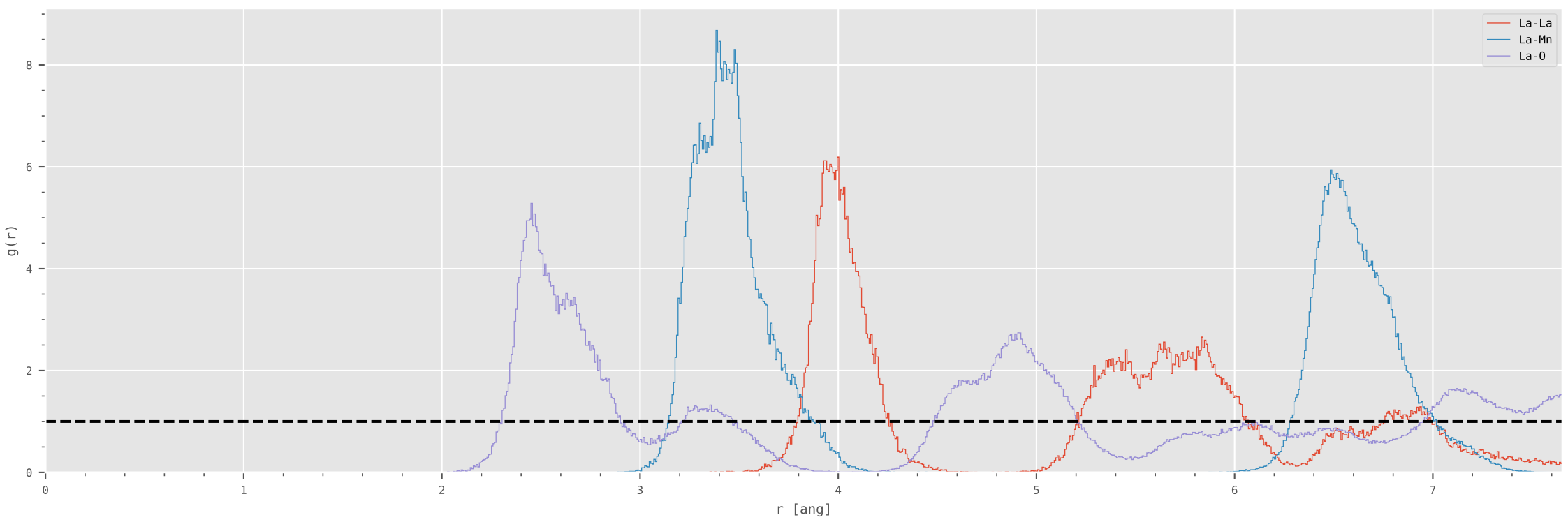
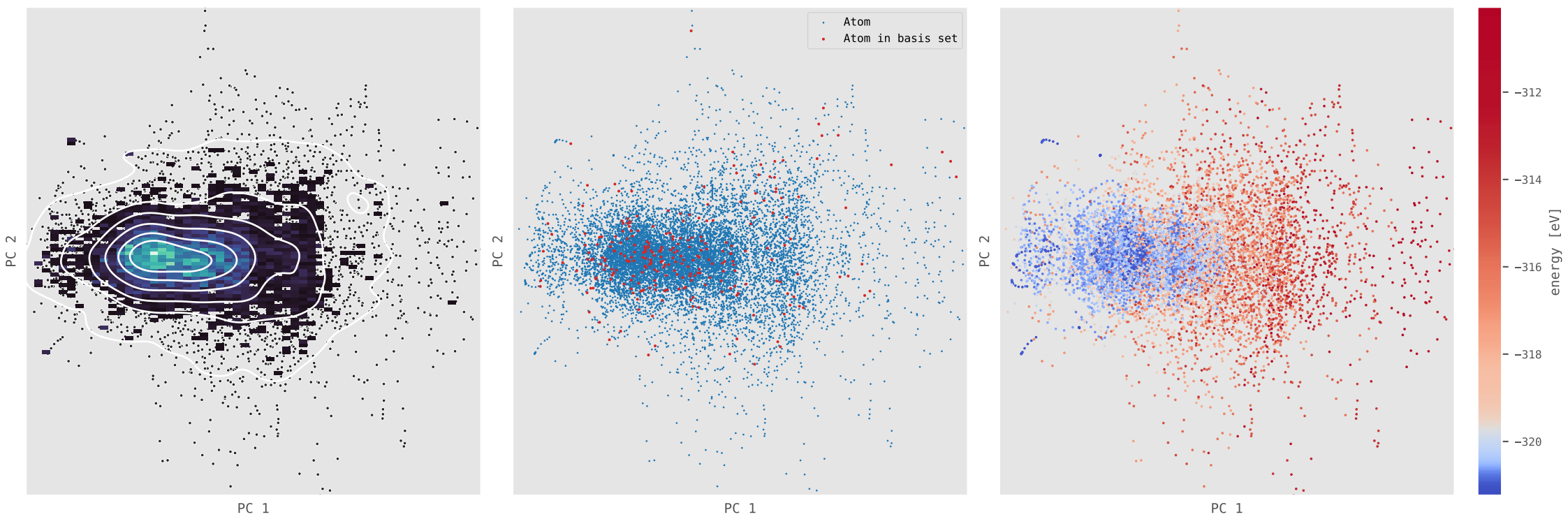maximum energy configuration (structure 1281)

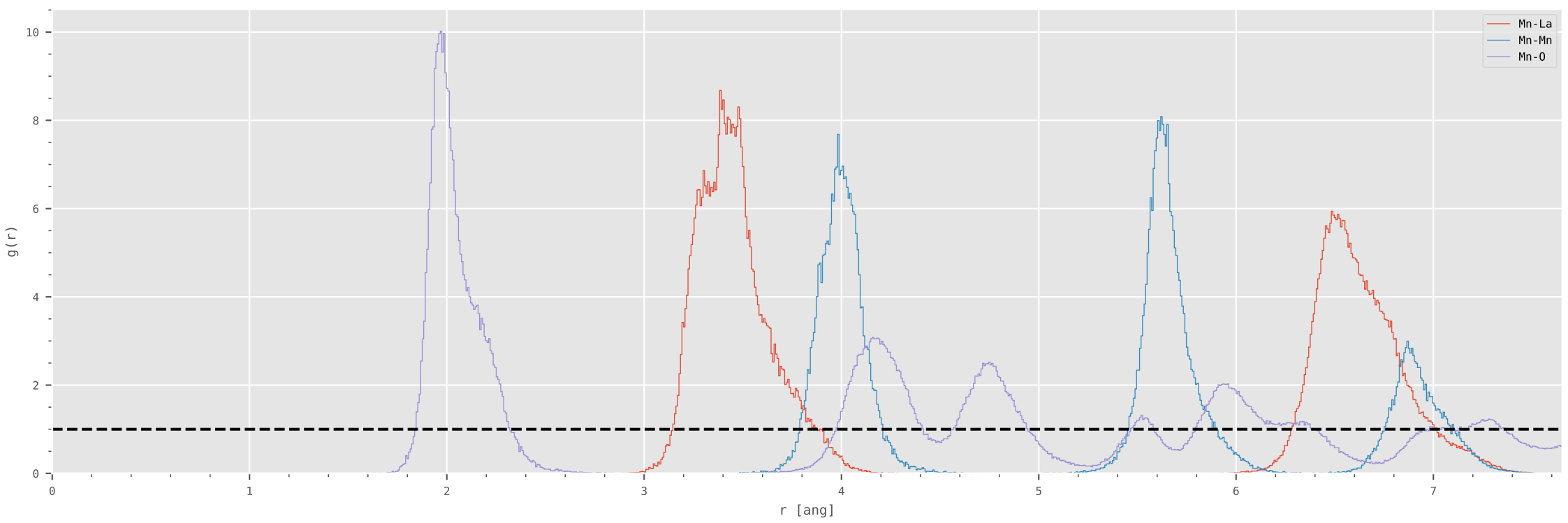principal component analysis of descriptors (La)
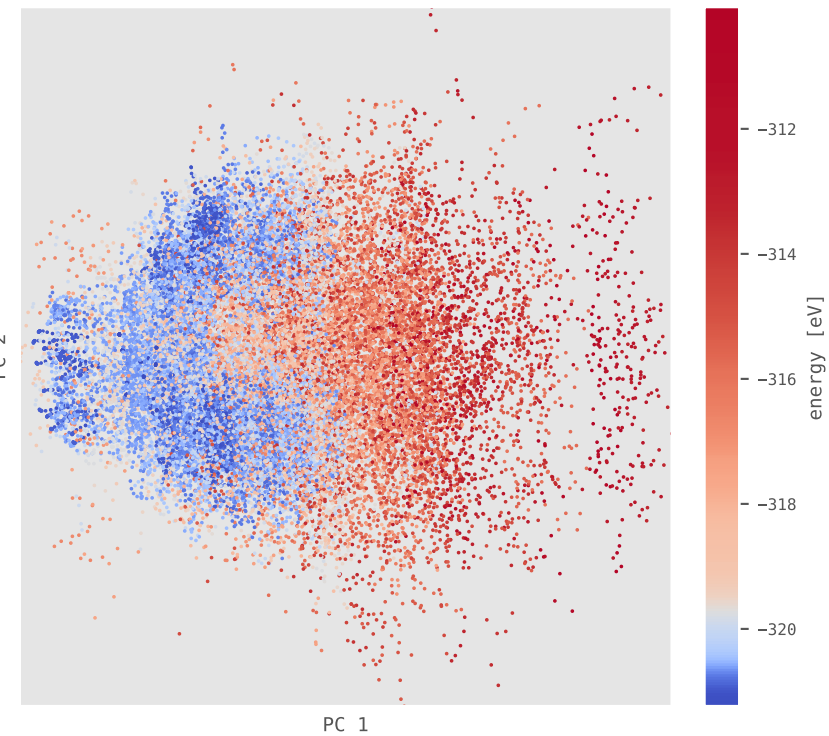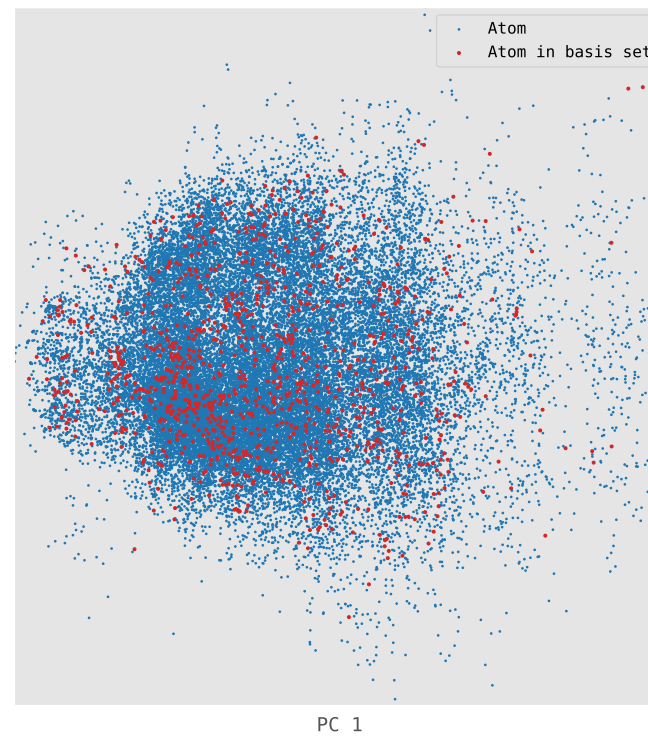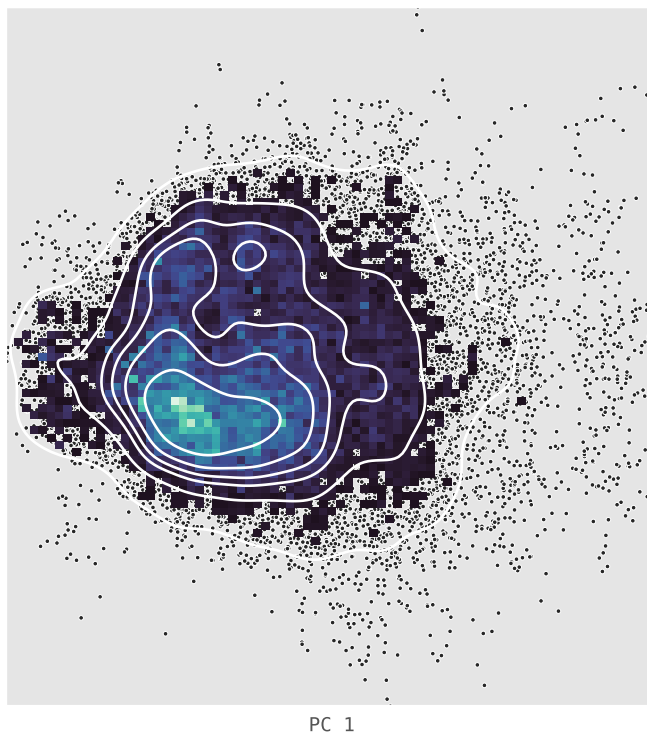
radial distribution functions (La)

principal component analysis of descriptors (Mn)

radial distribution functions (Mn)

principal component analysis of descriptors (O)

radial distribution functions (O)