S2 Fig. The salt bridge between the N1 atom of SB269652 and Asp $^{3.32}$  remains stable in all conditions. Distributions of the minimum distances between the N1 nitrogen atom of SB269652 and carboxyl oxygen atoms of Asp $^{3.32}$  for each MS of the indicated conditions are shown. The MSs for each condition are colored according to Fig 1.

