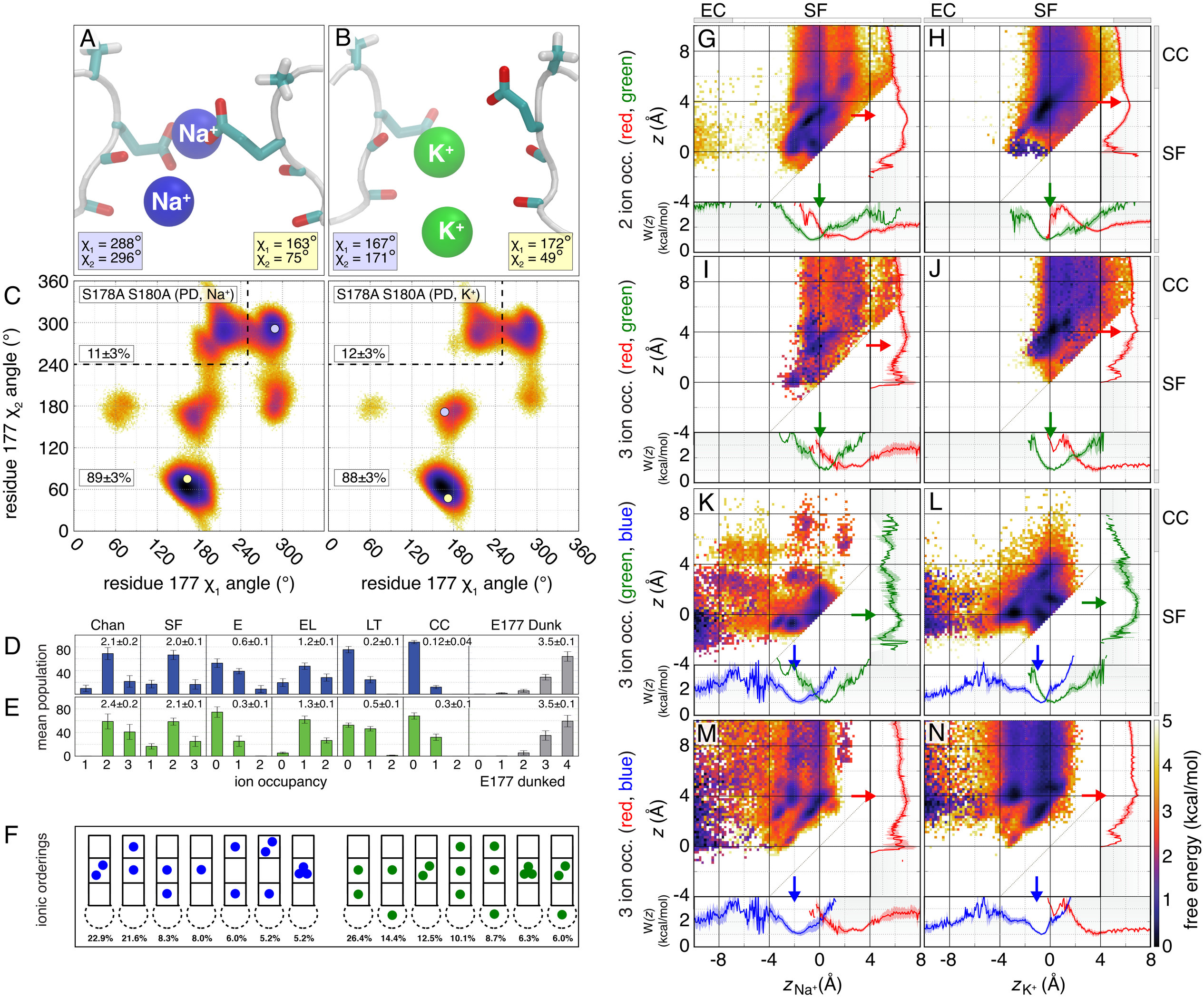
A
Na+
Na+
χ1 = 288°
χ2 = 296°
χ1 = 163°
χ2 = 75°
B
K+
K+
χ1 = 167°
χ2 = 171°
χ1 = 172°
χ2 = 49°
C
S178A S180A (PD, Na+)
S178A S180A (PD, K+)
11±3%
89±3%
12±3%
88±3%
residue 177 χ2 angle (°)
residue 177 χ1 angle (°)
D
E
Chan
SF
E
EL
LT
CC
E177 Dunk
mean population
ion occupancy
E177 dunked
F
ionic orderings
22.9%
21.6%
8.3%
8.0%
6.0%
5.2%
5.2%
26.4%
14.4%
12.5%
10.1%
8.7%
6.3%
6.0%
EC
SF
CC
2 ion occ. (red, green)
3 ion occ. (red, green)
3 ion occ. (green, blue)
3 ion occ. (red, blue)
z (Å)
W(z) (kcal/mol)
free energy (kcal/mol)
z_Na+ (Å)
z_K+ (Å)