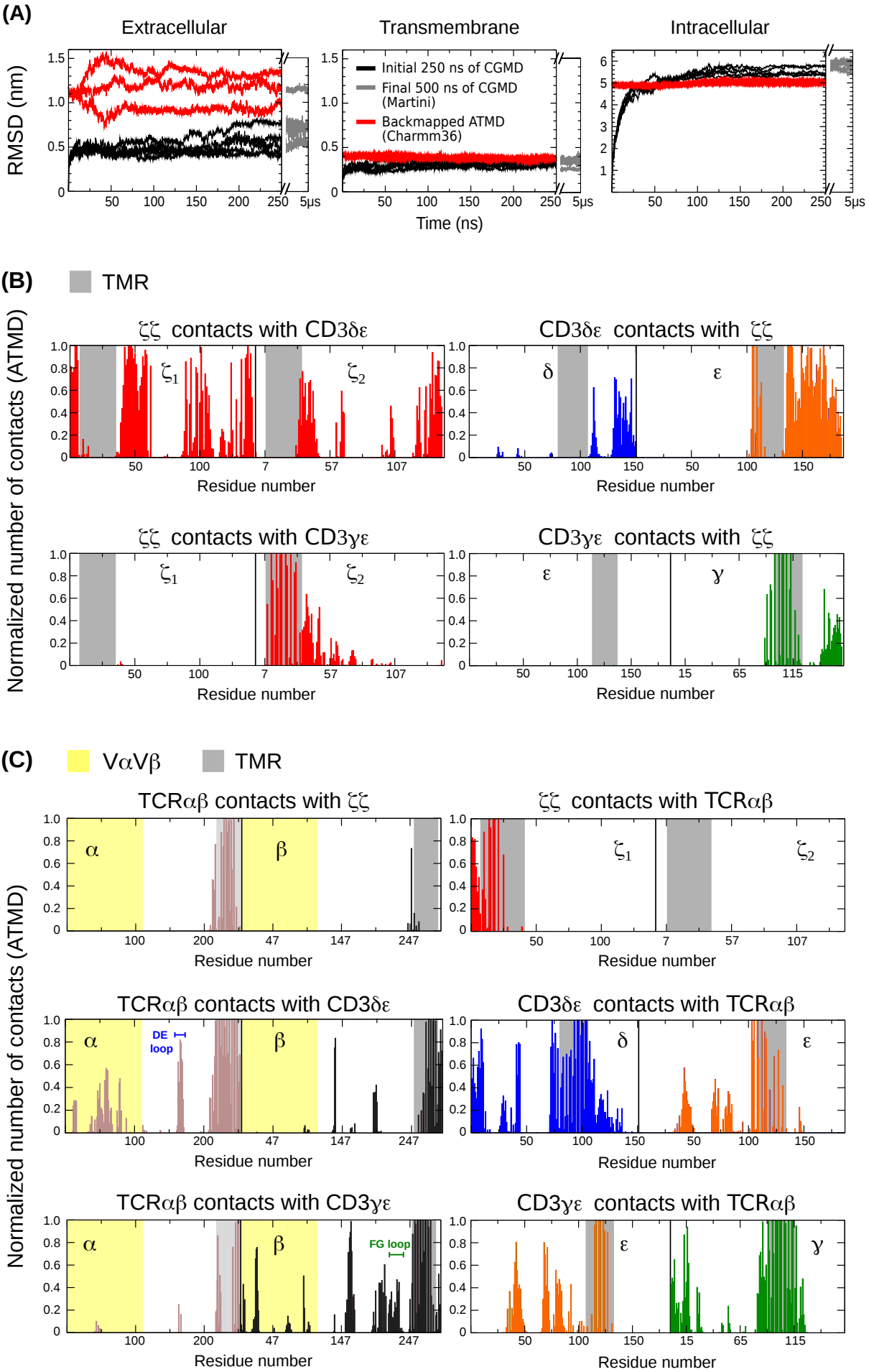
(A)
Extracellular
Transmembrane
Intracellular
RMSD (nm)
Initial 250 ns of CGMD
Final 500 ns of CGMD (Martini)
Backmapped ATMD (Charmm36)
Time (ns)
5μs
(B)
TMR
Normalized number of contacts (ATMD)
ζζ contacts with CD3δε
CD3δε contacts with ζζ
ζζ contacts with CD3γε
CD3γε contacts with ζζ
ζ1
ζ2
δ
ε
γ
Residue number
(C)
VαVβ
TMR
TCRαβ contacts with ζζ
ζζ contacts with TCRαβ
TCRαβ contacts with CD3δε
CD3δε contacts with TCRαβ
TCRαβ contacts with CD3γε
CD3γε contacts with TCRαβ
α
β
DE loop
FG loop