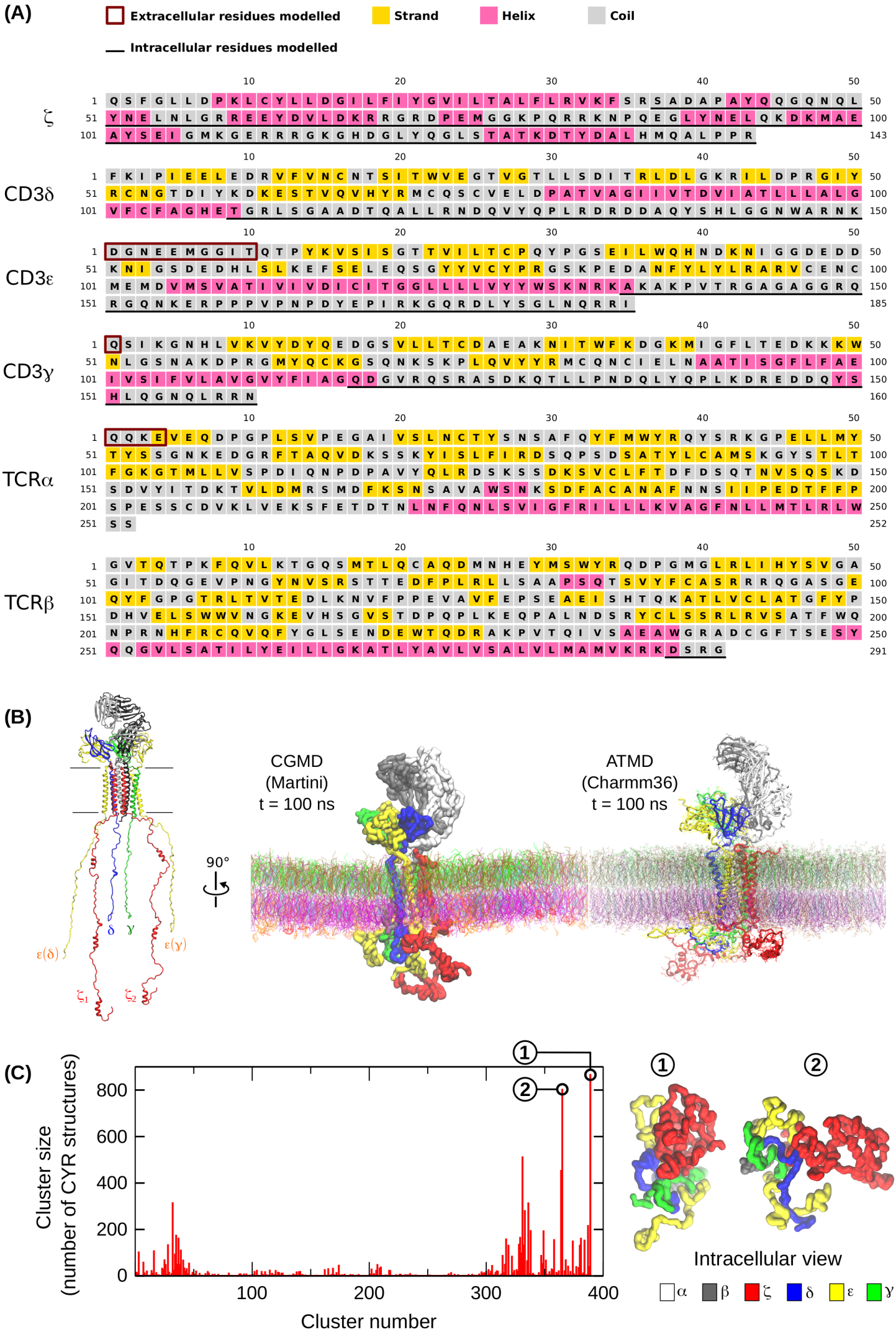
(A)
Extracellular residues modelled
Strand
Helix
Coil
Intracellular residues modelled
ζ
CD3δ
CD3ε
CD3γ
TCRα
TCRβ
(B)
CGMD
(Martini)
t = 100 ns
ATMD
(Charmm36)
t = 100 ns
90°
δ
γ
ε(δ)
ε(γ)
ζ1
ζ2
(C)
Cluster size
(number of CYR structures)
Cluster number
Intracellular view
α
β
ζ
δ
ε
γ