Supplementary Material

Figure Captions

Figure S1: Dependence of average standard deviations of the angle dependent terms on distances. (a) $E(\theta \mid r_{ab})$; (b) $E(\psi \mid r_{ab})$; (c) $E(\chi \mid r_{ab})$. Polar atoms are nitrogen and oxygen atoms in all residue types and the SG in CYS; all other atoms are non-polar.

Figure S2: Examples of the angular dependence of the energy term on angles at given distance: (a) ψ dependence of the disulfide bond at distance of 2.25 Å; (b) ψ dependence of the N atom in the hydrogen bond between ALA N and ALA O at a distance of 2.75 Å; (c) ψ dependence of the CB between ALA CB-ALA O at a distance of 3.25 Å; (d) θ dependence of the CB between ALA CB-ALA CB at a distance 3.75 Å; (e) ψ dependence of the CB between ALA CB-ALA CB at a distance of 3.75 Å; (f) χ dependence of the CB between ALACB-ALACB at a distance of 3.75 Å.

Figure S3: Covariance of angle pairs at different distances in the main-chain for the N-O interaction.

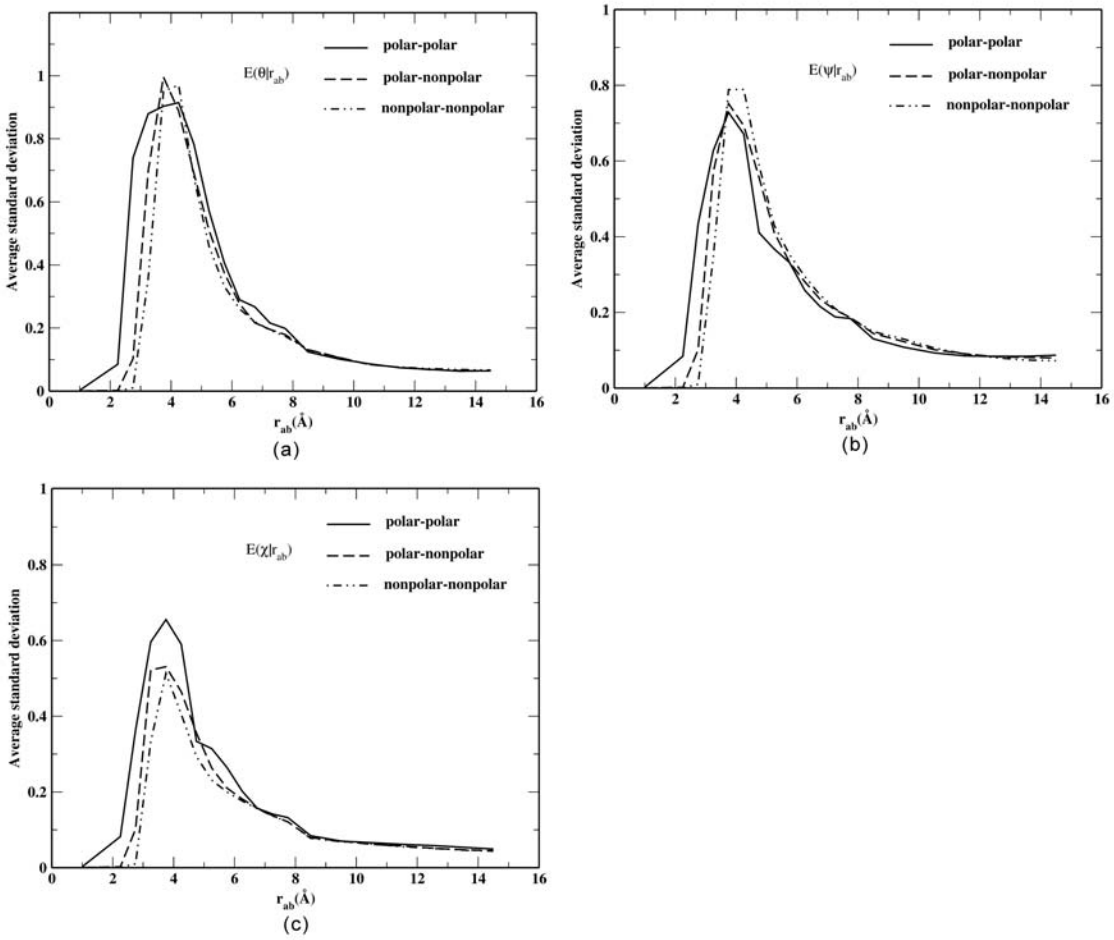
polar-polar
polar-nonpolar
nonpolar-nonpolar
E(θ|r_ab)
E(ψ|r_ab)
E(χ|r_ab)
Average standard deviation
r_ab(Å)
(a)
(b)
(c)

Figure S1

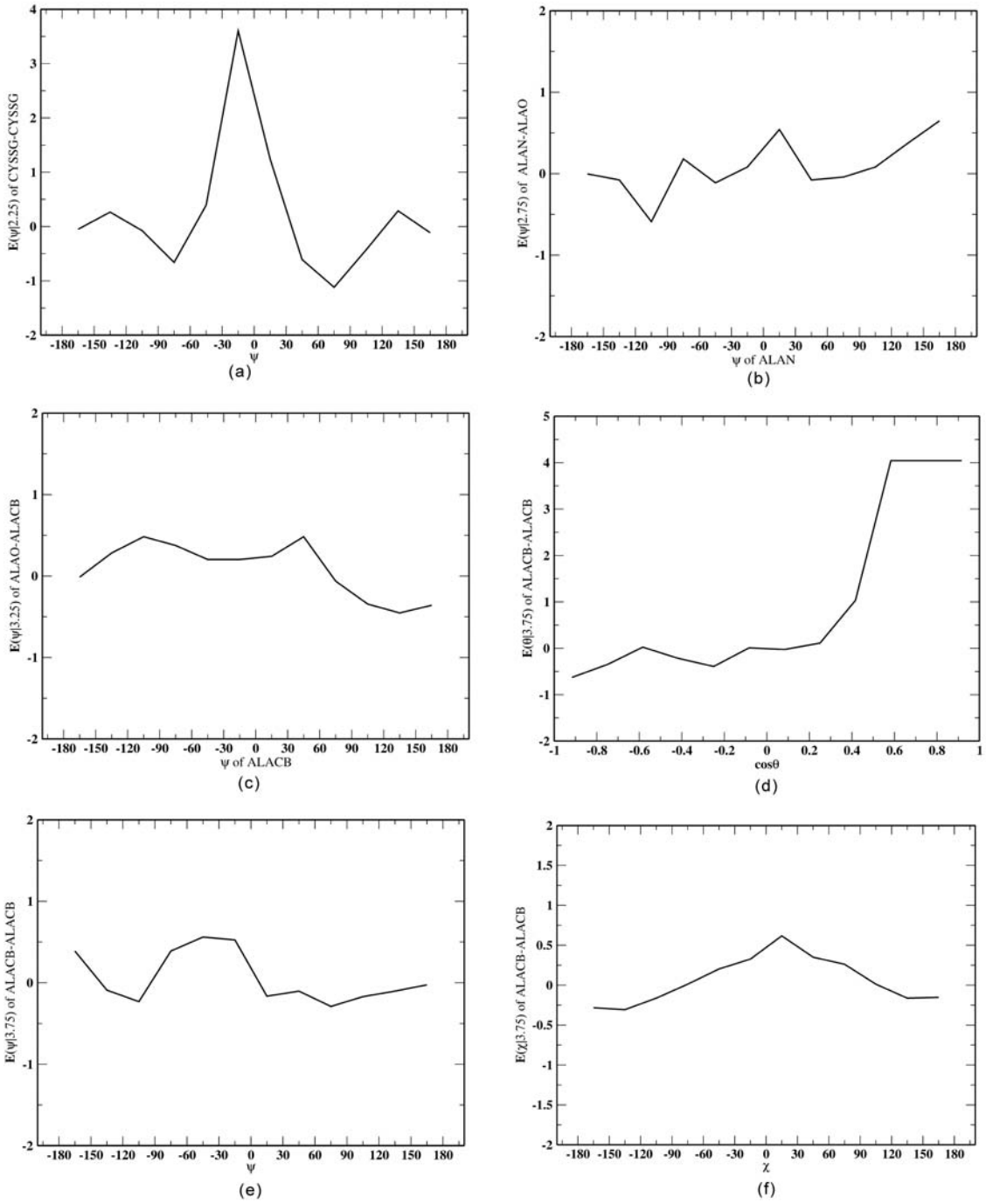
E(ψ|2.25) of CYSSG-CYSSG
ψ
(a)
E(ψ|2.75) of ALAN-ALAO
ψ of ALAN
(b)
E(ψ|3.25) of ALAO-ALACB
ψ of ALACB
(c)
E(θ|3.75) of ALACB-ALACB
cosθ
(d)
E(ψ|3.75) of ALACB-ALACB
ψ
(e)
E(χ|3.75) of ALACB-ALACB
χ
(f)

Figure S2

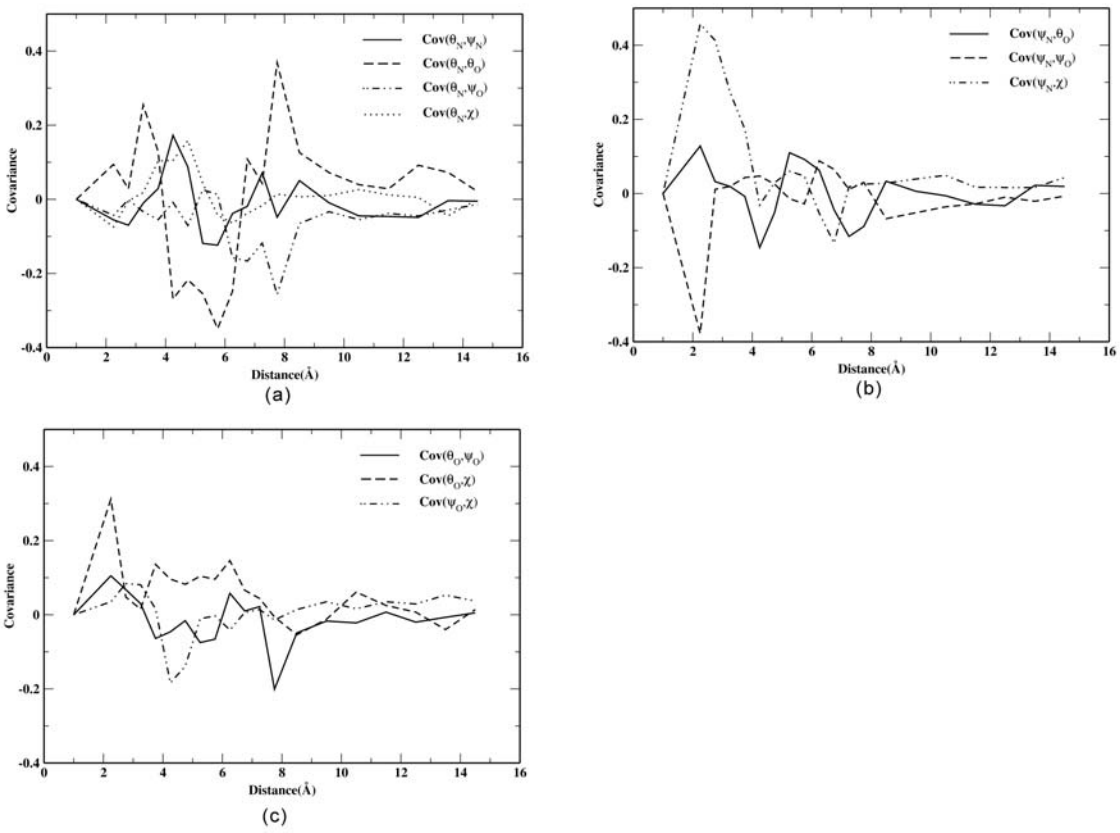
Cov(θN,ΨN)
Cov(θN,θO)
Cov(θN,ΨO)
Cov(θN,χ)
Covariance
Distance(Å)
(a)
Cov(ΨN,θO)
Cov(ΨN,ΨO)
Cov(ΨN,χ)
Covariance
Distance(Å)
(b)
Cov(θO,ΨO)
Cov(θO,χ)
Cov(ΨO,χ)
Covariance
Distance(Å)
(c)

Figure S3