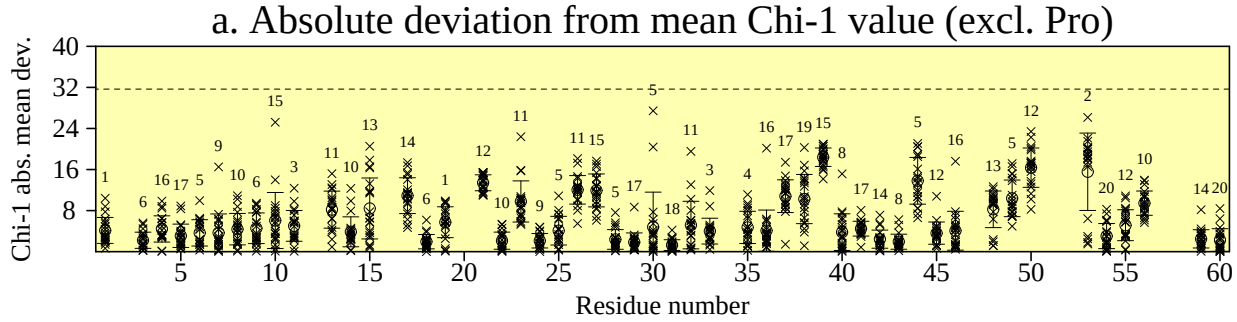
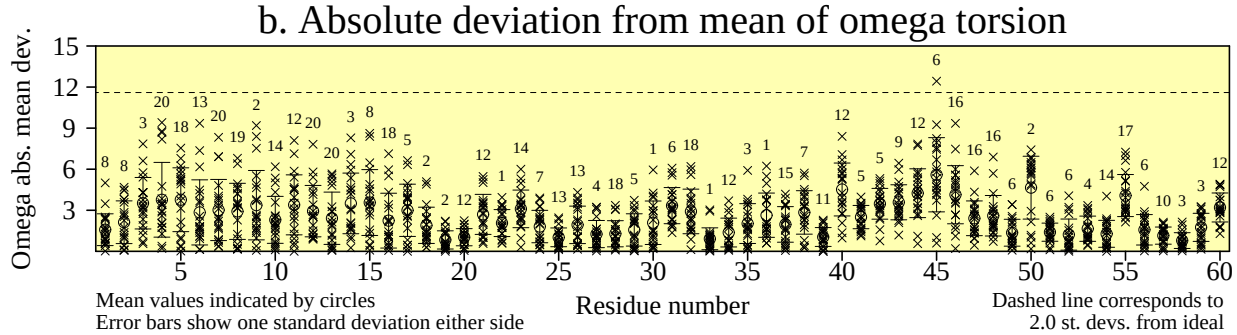
Residue properties

ensemble_refined (20 models)

a. Absolute deviation from mean Chi-1 value (excl. Pro)



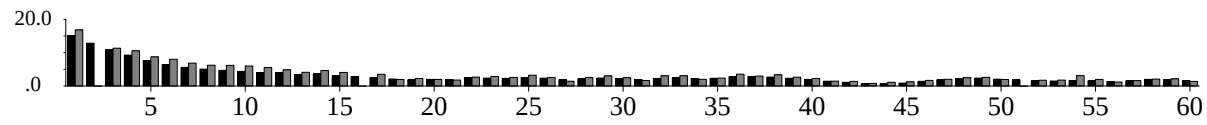
b. Absolute deviation from mean of omega torsion



Mean values indicated by circles
Error bars show one standard deviation either side

Dashed line corresponds to
2.0 st. devs. from ideal
Numbers indicate models with highest deviation

c. RMS devs from mean coords: main-chain (black) and side-chain (grey)



d. Secondary structure & average estimated accessibility

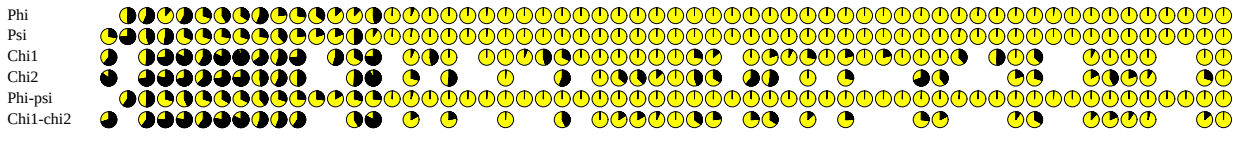
Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

e. Sequence & average estimated accessibilities

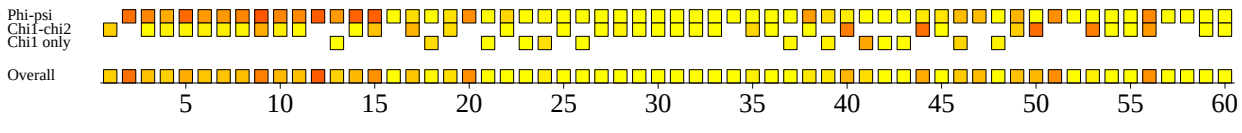
Accessible Buried

M G H H H H H H L E M A S E E G Q V I A C H T V E T W N E Q L Q K A N E S K T L V V V D F T A S W C G P C R F I A P F F

f. Circular variances



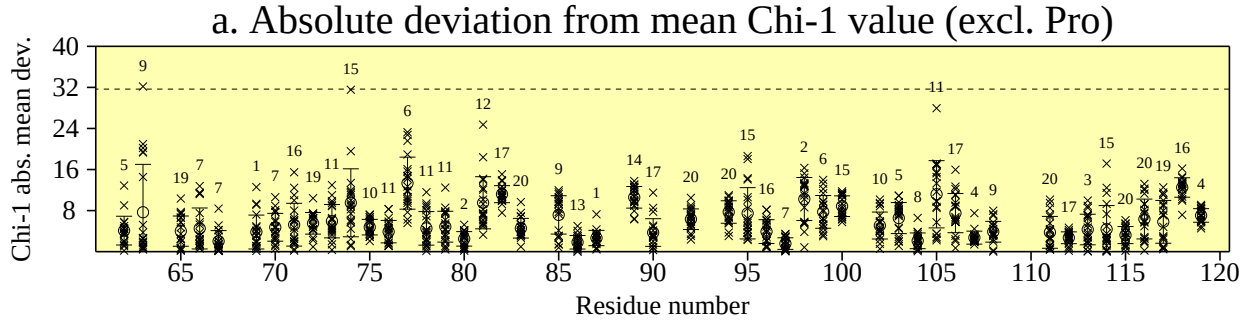
g. G-factors



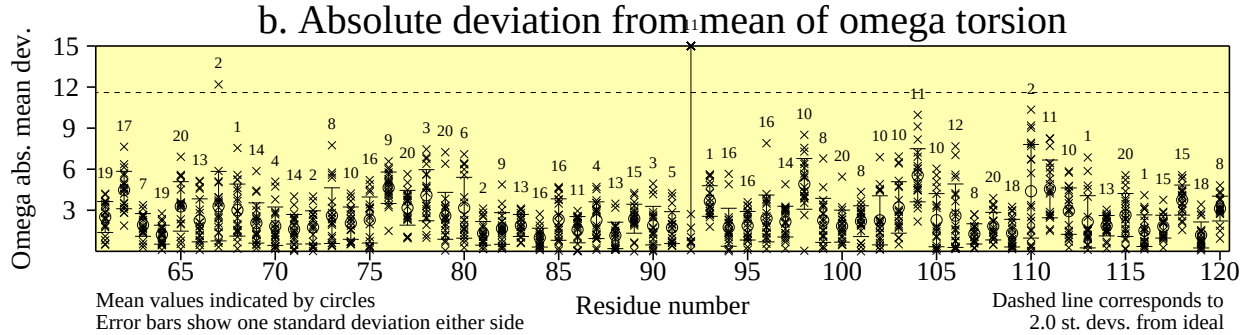
Residue properties

ensemble_refined (20 models)

a. Absolute deviation from mean Chi-1 value (excl. Pro)



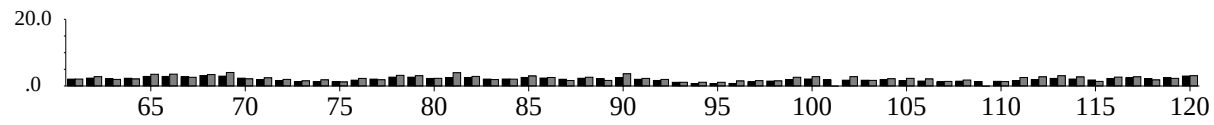
b. Absolute deviation from mean of omega torsion



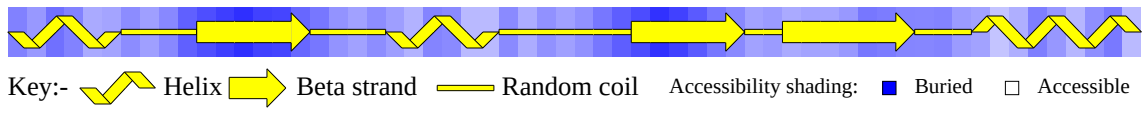
Mean values indicated by circles
Error bars show one standard deviation either side

Dashed line corresponds to
2.0 st. devs. from ideal
Numbers indicate models with highest deviation

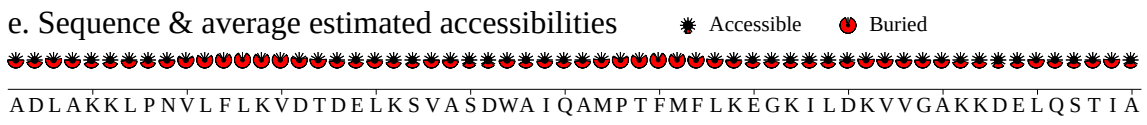
c. RMS devs from mean coords: main-chain (black) and side-chain (grey)



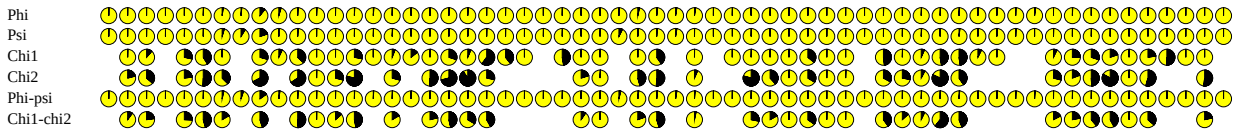
d. Secondary structure & average estimated accessibility



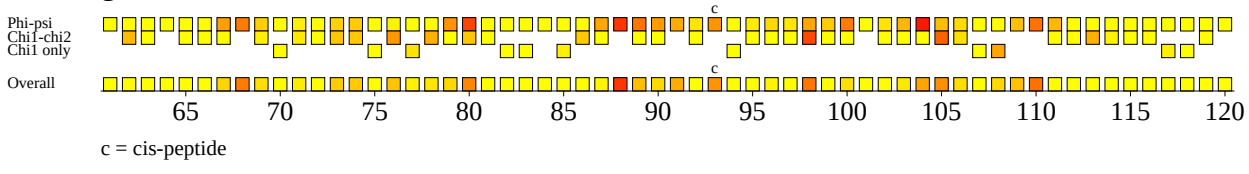
e. Sequence & average estimated accessibilities



f. Circular variances



g. G-factors

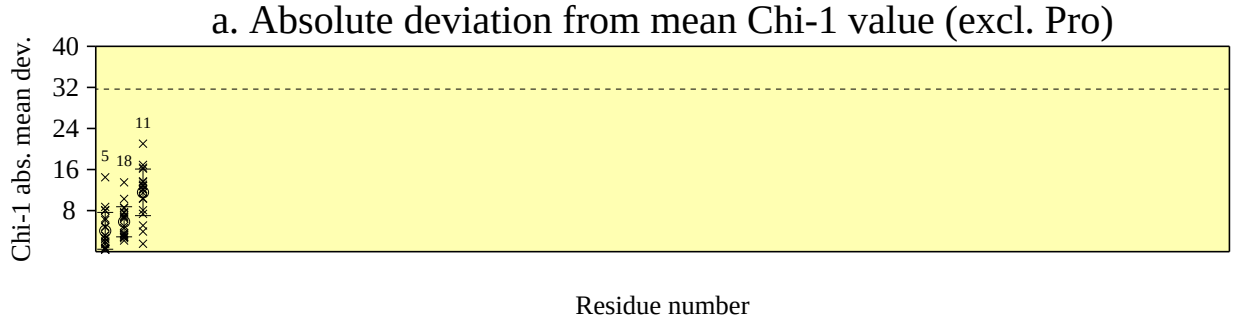


c = cis-peptide

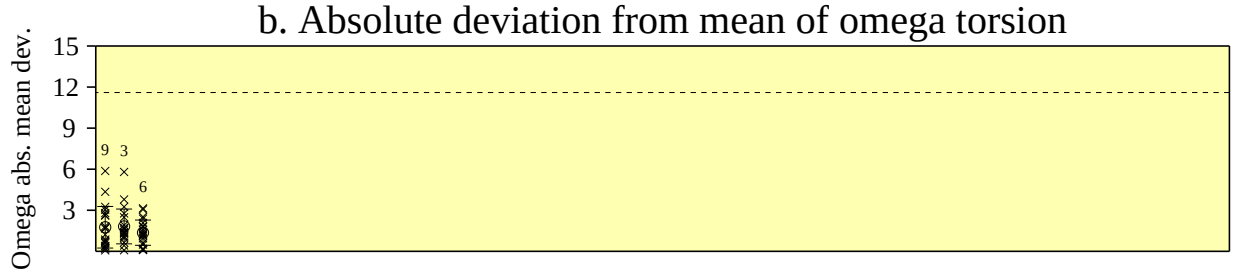
Residue properties

ensemble_refined (20 models)

a. Absolute deviation from mean Chi-1 value (excl. Pro)



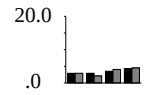
b. Absolute deviation from mean of omega torsion



Mean values indicated by circles
Error bars show one standard deviation either side

Dashed line corresponds to
2.0 st. devs. from ideal
Numbers indicate models with highest deviation

c. RMS devs from mean coords: main-chain (black) and side-chain (grey)



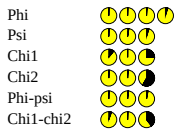
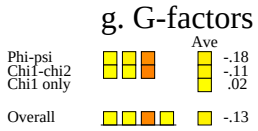
d. Secondary structure & average estimated accessibility

Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

e. Sequence & average estimated accessibilities Accessible Buried

K H L A

f. Circular variances



g. G-factors