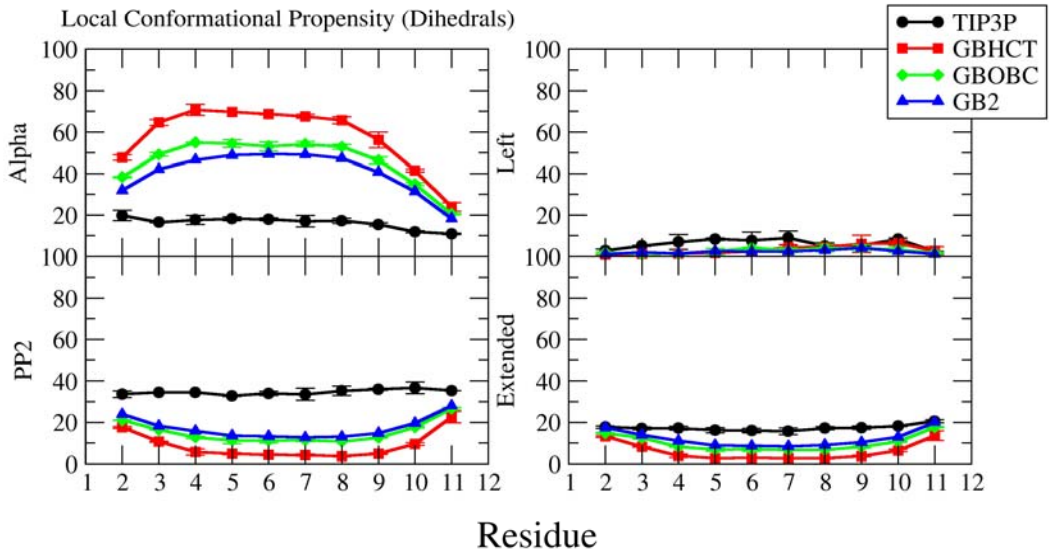

Figure S1. Local conformational propensities for each residue of Ala10 from unrestrained REMD simulations using various solvent models at 300.0 K. Residues 1 and 12 are the acetyl and amide N- and C-caps respectively. GB2 refers to GBOBC simulations with alternative α, β, and γ parameters (see Methods for details).

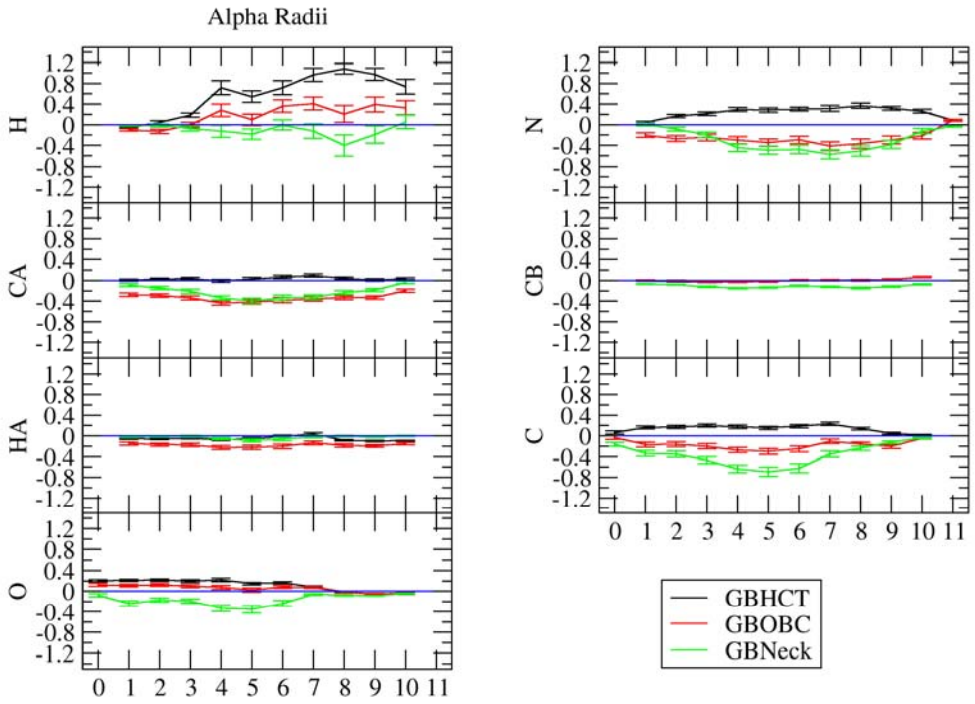

Figure S2. Average difference (over all structures used in analysis shown in Tables 4-6) of effective radii for the Alpha conformation calculated with either GBHCT, GBOBC, or GBNeck from perfect radii calculated with PE for several atom types (H=Amide Hydrogen, CA=Alpha Carbon, HA=Alpha Hydrogen, O=Carboxyl Oxygen, N=Amide Nitrogen, CB=Beta Carbon, C=Carboxyl Carbon) across all residues of Ala10. Residues 0 and 11 correspond to N-acetyl and C-amide capping groups respectively. Error bars are ± 1 standard deviation.

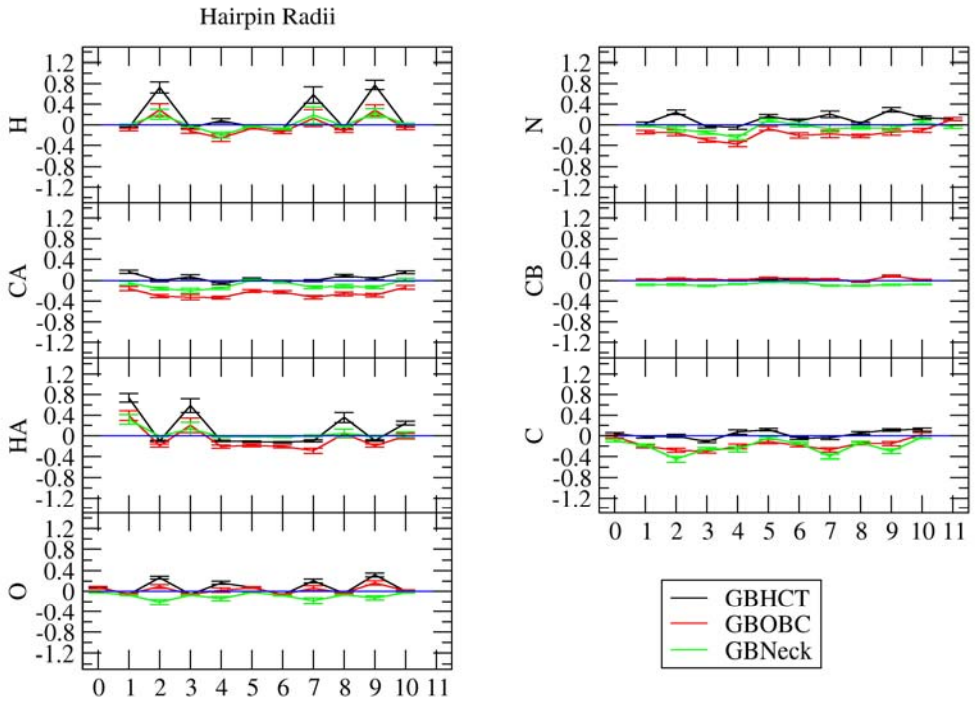

Figure S3. Average difference (over all structures used in analysis shown in Tables 4-6) of effective radii for the Hairpin conformation calculated with either GBHCT, GBOBC, or GBNeck from perfect radii calculated with PE for several atom types (H=Amide Hydrogen, CA=Alpha Carbon, HA=Alpha Hydrogen, O=Carboxyl Oxygen, N=Amide Nitrogen, CB=Beta Carbon, C=Carboxyl Carbon) across all residues of Ala10. Residues 0 and 11 correspond to N-acetyl and C-amide capping groups respectively. Error bars are ± 1 standard deviation.

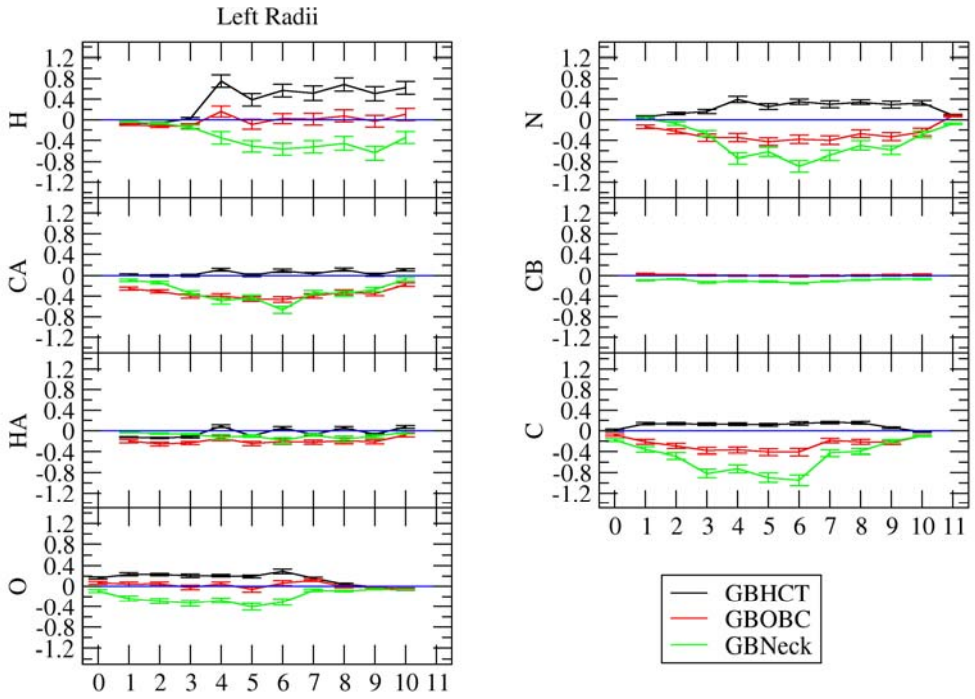

Figure S4. Average difference (over all structures used in analysis shown in Tables 4-6) of effective radii for the Left conformation calculated with either GBHCT, GBOBC, or GBNeck from perfect radii calculated with PE for several atom types (H=Amide Hydrogen, CA=Alpha Carbon, HA=Alpha Hydrogen, O=Carboxyl Oxygen, N=Amide Nitrogen, CB=Beta Carbon, C=Carboxyl Carbon) across all residues of Ala10. Residues 0 and 11 correspond to N-acetyl and C-amide capping groups respectively. Error bars are ± 1 standard deviation.

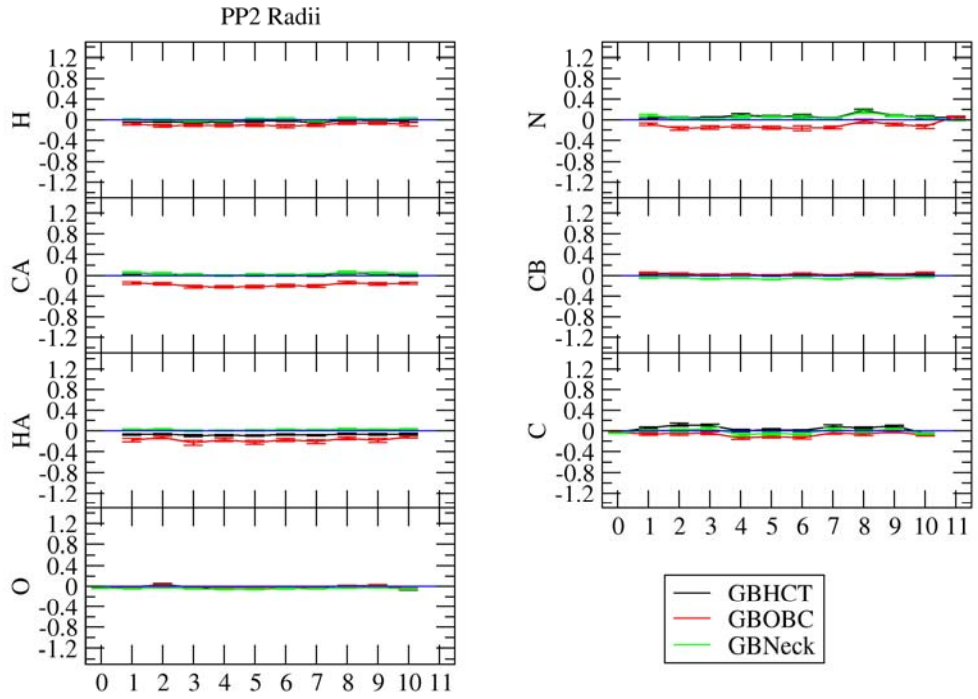

Figure S5. Average difference (over all structures used in analysis shown in Tables 4-6) of effective radii for the PP2 conformation calculated with either GBHCT, GBOBC, or GBNeck from perfect radii calculated with PE for several atom types (H=Amide Hydrogen, CA=Alpha Carbon, HA=Alpha Hydrogen, O=Carboxyl Oxygen, N=Amide Nitrogen, CB=Beta Carbon, C=Carboxyl Carbon) across all residues of Ala10. Residues 0 and 11 correspond to N-acetyl and C-amide capping groups respectively. Error bars are ± 1 standard deviation.

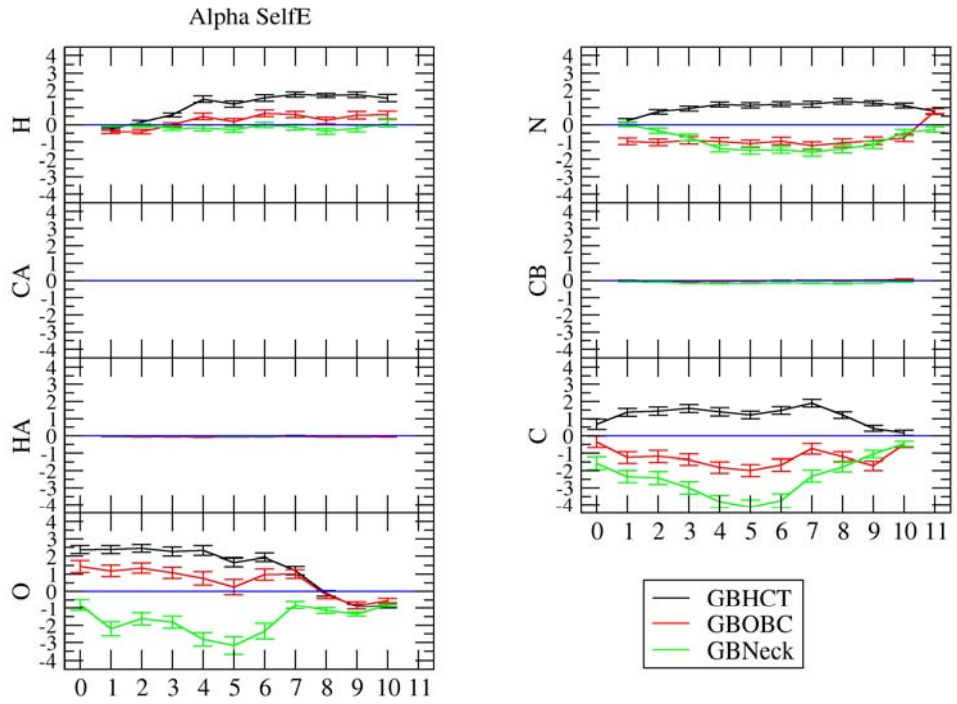

Figure S6. Average difference (over all structures used in analysis shown in Tables 4-6) of Self solvation energy for the Alpha conformation calculated with either GBHCT, GBOBC, or GBNeck from Self solvation energy calculated with PE for several atom types (H=Amide Hydrogen, CA=Alpha Carbon, HA=Alpha Hydrogen, O=Carboxyl Oxygen, N=Amide Nitrogen, CB=Beta Carbon, C=Carboxyl Carbon) across all residues of Ala10. Residues 0 and 11 correspond to N-acetyl and C-amide capping groups respectively. Error bars are ± 1 standard deviation.

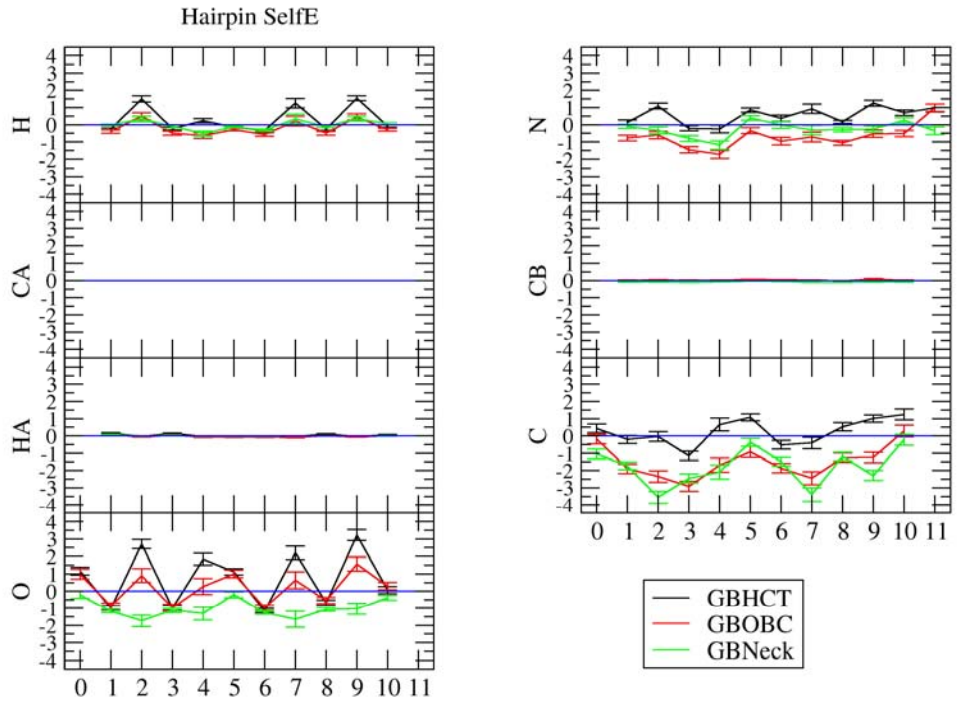

Figure S7. Average difference (over all structures used in analysis shown in Tables 4-6) of Self solvation energy for the Hairpin conformation calculated with either GBHCT, GBOBC, or GBNeck from Self solvation energy calculated with PE for several atom types (H=Amide Hydrogen, CA=Alpha Carbon, HA=Alpha Hydrogen, O=Carboxyl Oxygen, N=Amide Nitrogen, CB=Beta Carbon, C=Carboxyl Carbon) across all residues of Ala10. Residues 0 and 11 correspond to N-acetyl and C-amide capping groups respectively. Error bars are ± 1 standard deviation.

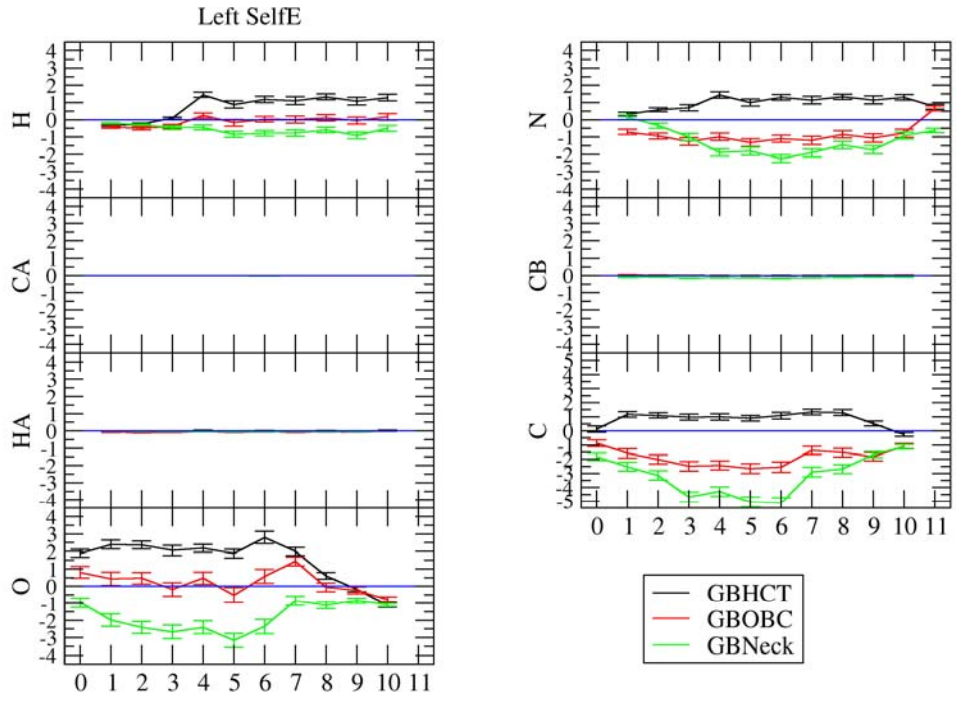

Figure S8. Average difference (over all structures used in analysis shown in Tables 4-6) of Self solvation energy for the Left conformation calculated with either GBHCT, GBOBC, or GBNeck from Self solvation energy calculated with PE for several atom types (H=Amide Hydrogen, CA=Alpha Carbon, HA=Alpha Hydrogen, O=Carboxyl Oxygen, N=Amide Nitrogen, CB=Beta Carbon, C=Carboxyl Carbon) across all residues of Ala10. Residues 0 and 11 correspond to N-acetyl and C-amide capping groups respectively. Error bars are ± 1 standard deviation.

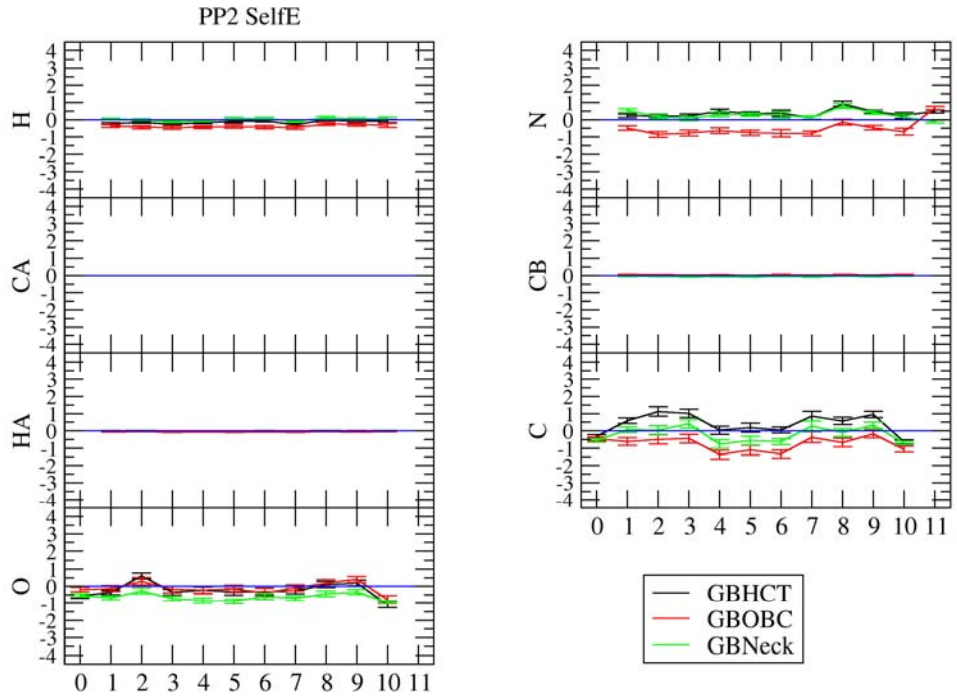

Figure S9. Average difference (over all structures used in analysis shown in Tables 4-6) of Self solvation energy for the PP2 conformation calculated with either GBHCT, GBOBC, or GBNeck from Self solvation energy calculated with PE for several atom types (H=Amide Hydrogen, CA=Alpha Carbon, HA=Alpha Hydrogen, O=Carboxyl Oxygen, N=Amide Nitrogen, CB=Beta Carbon, C=Carboxyl Carbon) across all residues of Ala10. Residues 0 and 11 correspond to N-acetyl and C-amide capping groups respectively. Error bars are ± 1 standard deviation.