Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supplementary information

for

Energetics of β-turn formation in a mutant peptide YPGDV from Influenza Hemagglutinin: An MD simulation study

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Table S1 Lists the β-turn forming percentages in the YPYDV and YP**G**DV simulations at 293 K using the distance criteria for β-turn formation i.e. D5:H-Y2:O distance <= 0.26 nm

Peptide systems	**Percentage of β-turn conformations**
Ac- ^{2}YPYDV^{6} -NMe	1.3 %
Ac- ^{2}YP**G**DV^{6} -NMe	26.7 %

Table S2 Lists the equilibrium constant (**K_{eq}**) and change in free energy of folding (**$\Delta A_{folding}$**) for the simulations of YP**G**DV peptide at 10 different temperatures calculated using D5:H-Y2:O distance <=0.26 nm

Temperature (K)	**K_{eq} (fraction folded/fraction unfolded)**	**$\Delta A_{folding}$ (J/mol)**
280	0.41	2058
290	0.34	2568
293	0.36	2462
300	0.41	2167
310	0.30	3066
320	0.33	2899
330	0.35	2812
340	0.31	3252
350	0.30	3410
360	0.24	4164

Table S3 Lists the atom depth values and standard deviations for the amide protons of the residues in the simulation of YP**G**DV peptide at 280 K and 360 K for the folded and unfolded ensembles.

	Atom depth values (nm)			
	280 K		360 K	
Amide proton	**Unfolded**	**Folded**	**Unfolded**	**Folded**
Y2	0.23 ± 0.04	0.26 ± 0.06	0.24 ± 0.05	0.27 ± 0.06
P3	---------	---------	---------	---------
G4	0.22 ± 0.04	0.22 ± 0.04	0.24 ± 0.05	0.23 ± 0.05
D5	0.24 ± 0.05	**0.31 ± 0.06**	0.24 ± 0.05	**0.31 ± 0.06**
V6	0.24 ± 0.04	0.25 ± 0.06	0.25 ± 0.05	0.26 ± 0.06

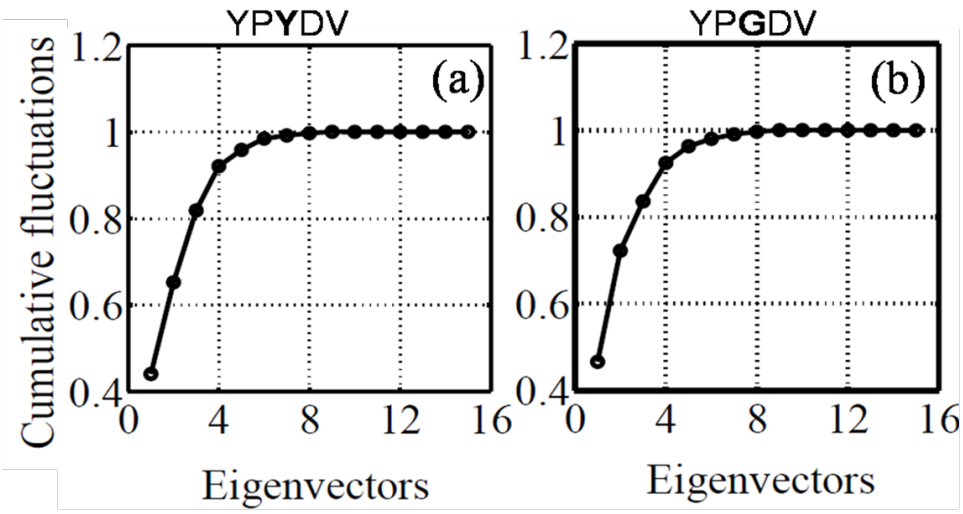

Figure S1 Relative cumulative contribution of the 15 eigenvectors to the overall dynamics of the YPYDV peptide is shown in (a) and for YP**G**DV peptide in (b) for the 293 K simulations.

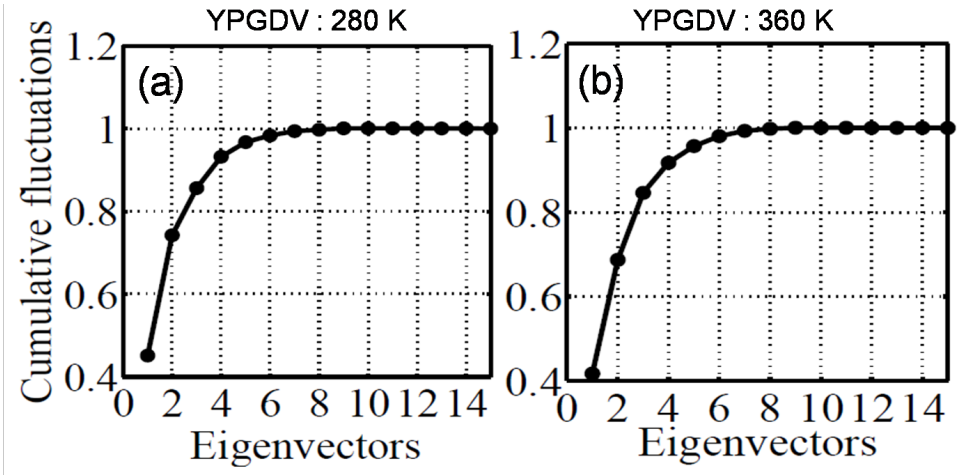

Figure S2 Relative cumulative contribution of the 15 eigenvectors to the overall dynamics of the YP**G**DV peptide is shown in (a) for 280 K simulation and in (b) for the 360 K simulation.

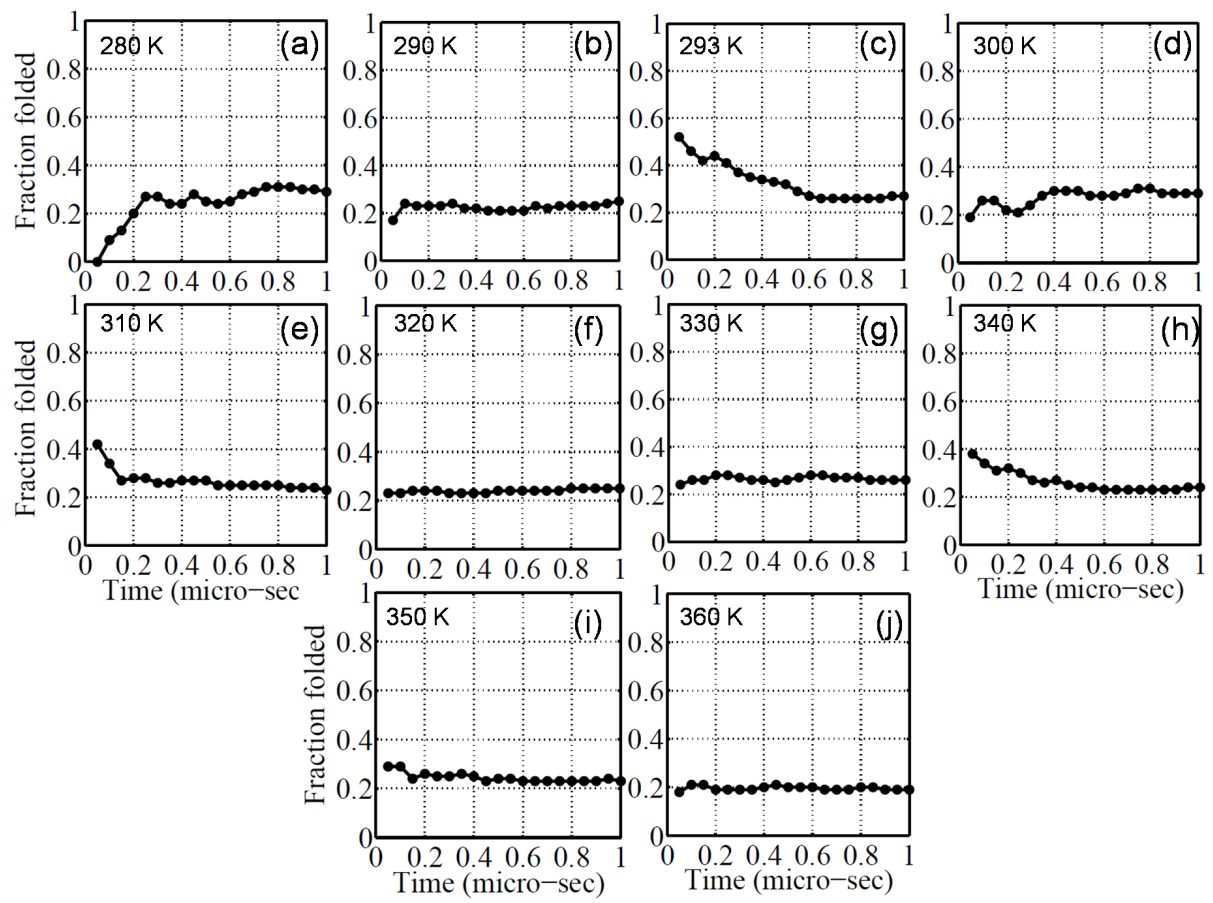

Figure S3 Variation of fraction folded, calculated using criteria D5:H-Y2:O distance <= 0.26 nm, with respect to simulation time in YP**G**DV peptide simulations at 280 K is shown in (a), at 290 K in (b), at 293 K in (c), at 300 K in (d), at 310 K in (e), at 320 K in (f), at 330 K in (g), at 340 K in (h), at 350 K in (i) and at 360 K in (j).

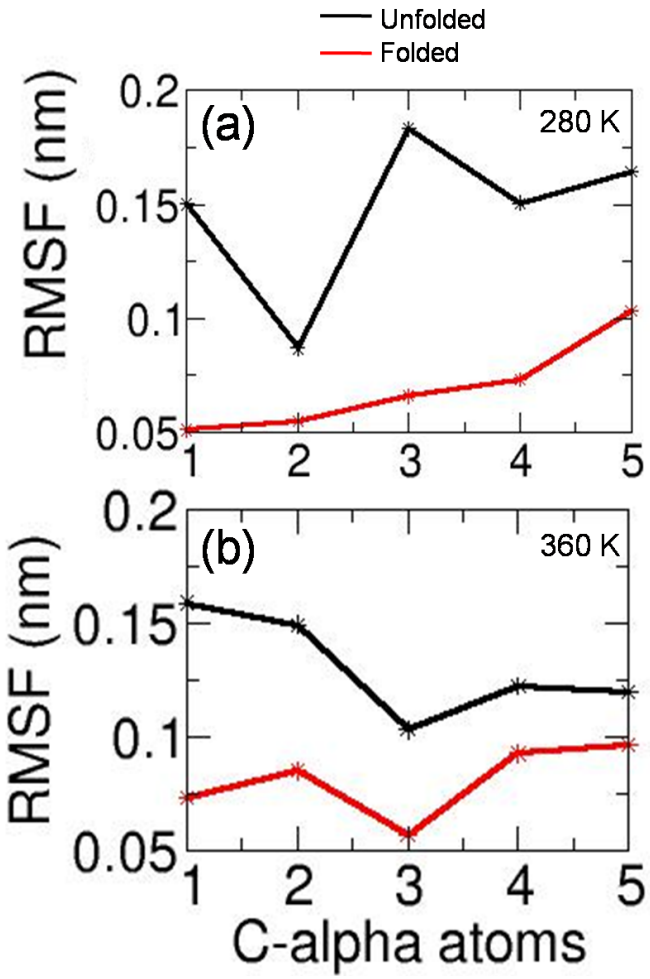

Figure S4 Root mean square fluctuations (RMSF) for C-α atoms of YP**G**DV peptide is shown for the unfolded (black) and folded (red) ensembles for the 280 K simulation in (a) and for 360 K simulation in (b).

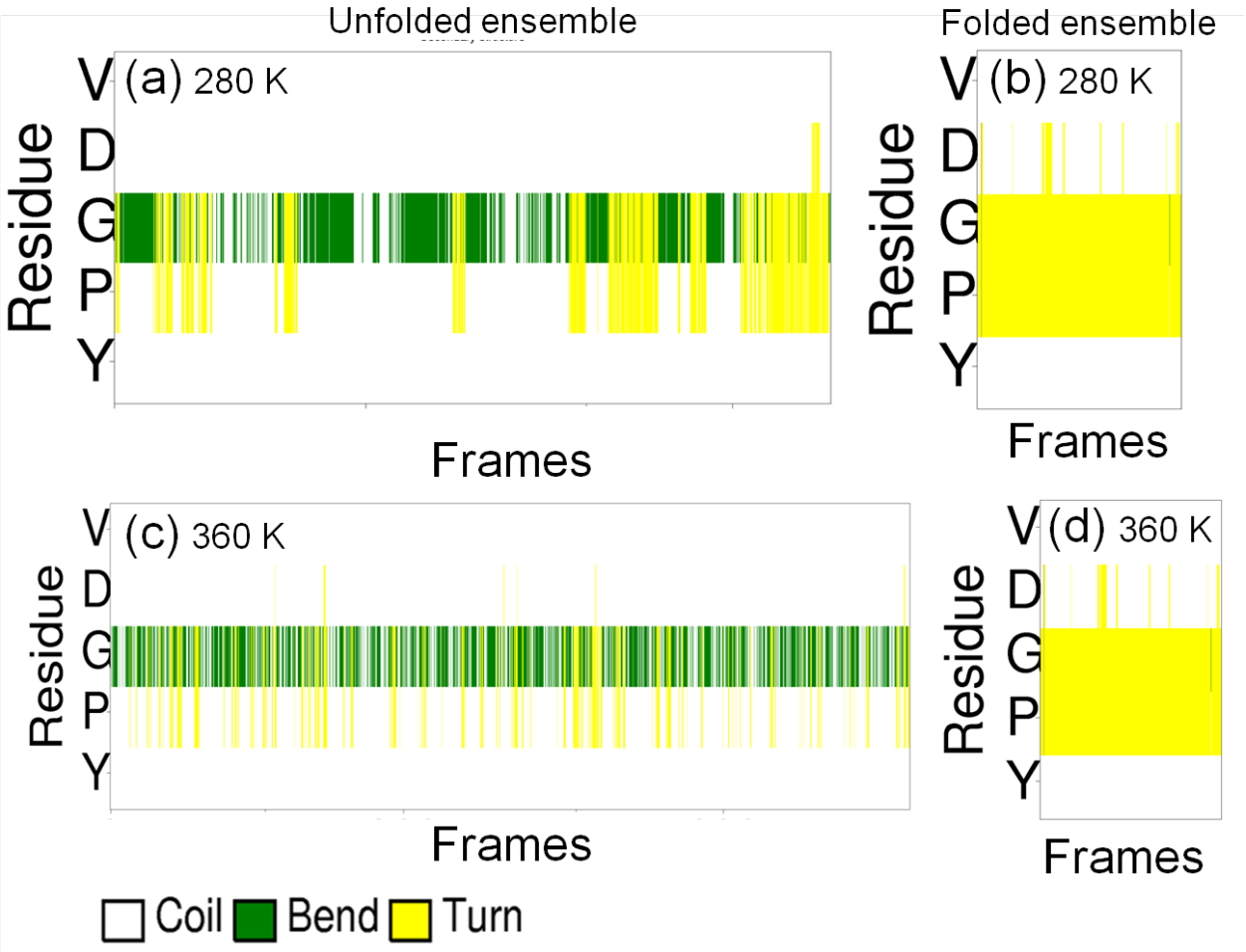

Figure S5 Variation of secondary structure with respect to unfolded frames of YP**G**DV peptide at 280 K and 360 K is shown in (a) and (c) respectively and the secondary structure variation for the folded frames of YP**G**DV peptide at 280 K and 360 K is shown in (b) and (d) respectively. The different colour codes for the secondary structural elements are shown at the bottom of the figure.

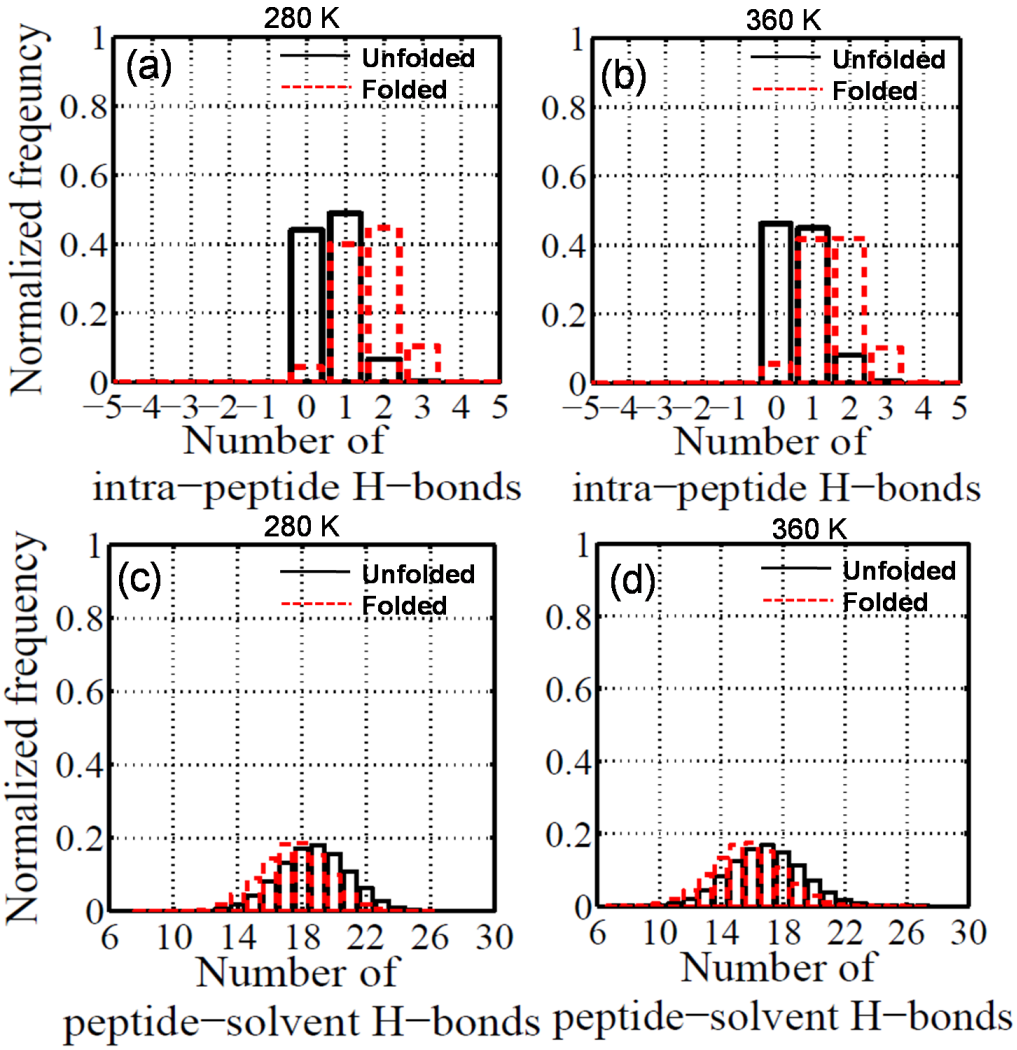

Figure S6 Comparison of the normalized frequency distributions of the number of intra-peptide hydrogen bonds between the unfolded and folded ensembles is shown for YP**G**DV simulations at 280 K in (a) and at 360 K in (b). Similarly, a comparison of the normalized frequency distributions of the number of peptide-solvent hydrogen bonds between the unfolded and folded ensembles is shown for YP**G**DV simulations at 280 K in (c) and at 360 K in (d).

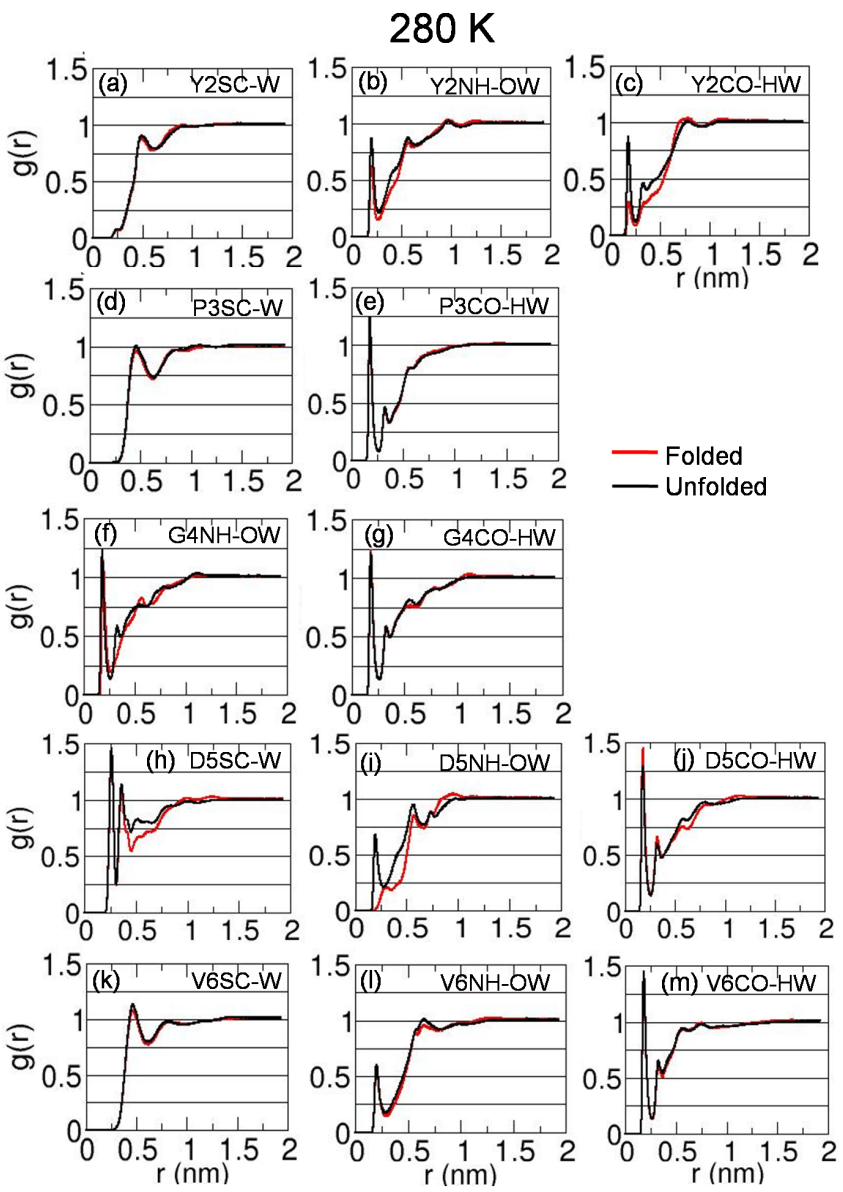

Figure S7 Radial distribution function (RDF) of water molecules (W) around the side chains of Y2, P3, D5 and V6 residues is shown for the unfolded and folded ensembles in (a), (d), (h) and (k) respectively. RDF of water oxygen atoms (OW) around the main chain amide protons of Y2, G4, D5 and V6 residues is shown in (b), (g), (i) and (l) respectively and RDF of water hydrogen atoms (HW) around the main chain carbonyl oxygen of Y2, P3, G4, D5 and V6 residues is shown in (c), (e), (g), (j) and (m) respectively. All the graphs are from 280 K simulation of YP**G**DV peptide.

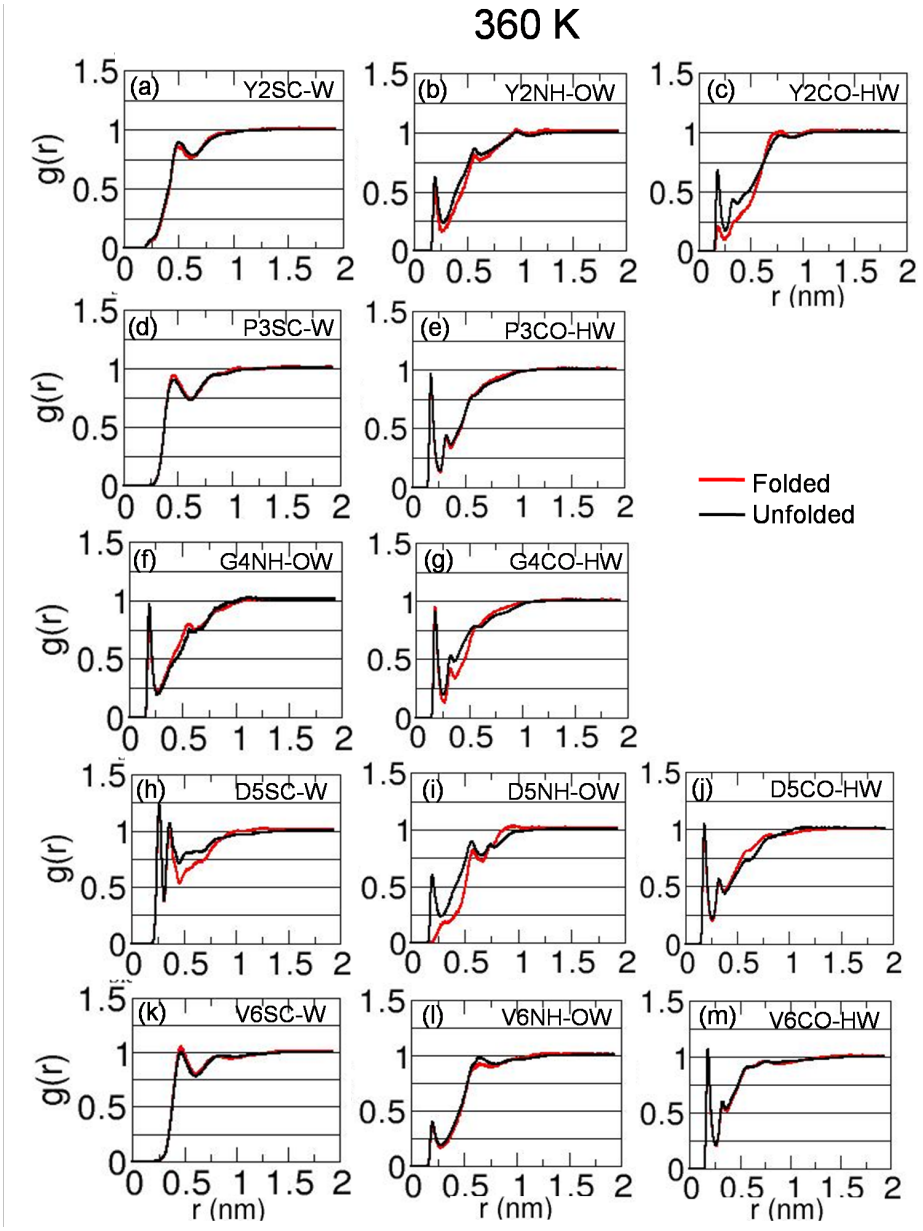

Figure S8 Radial distribution function (RDF) of water molecules (W) around the side chains of Y2, P3, D5 and V6 residues is shown for the unfolded and folded ensembles in (a), (d), (h) and (k) respectively. RDF of water oxygen atoms (OW) around the main chain amide protons of Y2, G4, D5 and V6 residues is shown in (b), (g), (i) and (l) respectively and RDF of water hydrogen atoms (HW) around the main chain carbonyl oxygen of Y2, P3, G4, D5 and V6 residues is shown in (c), (e), (g), (j) and (m) respectively. All the graphs are from 360 K simulation of YP**G**DV peptide.