Supporting Material

Insights into unfolded proteins from the intrinsic ϕ/ψ propensities of the AAXAA host-guest series

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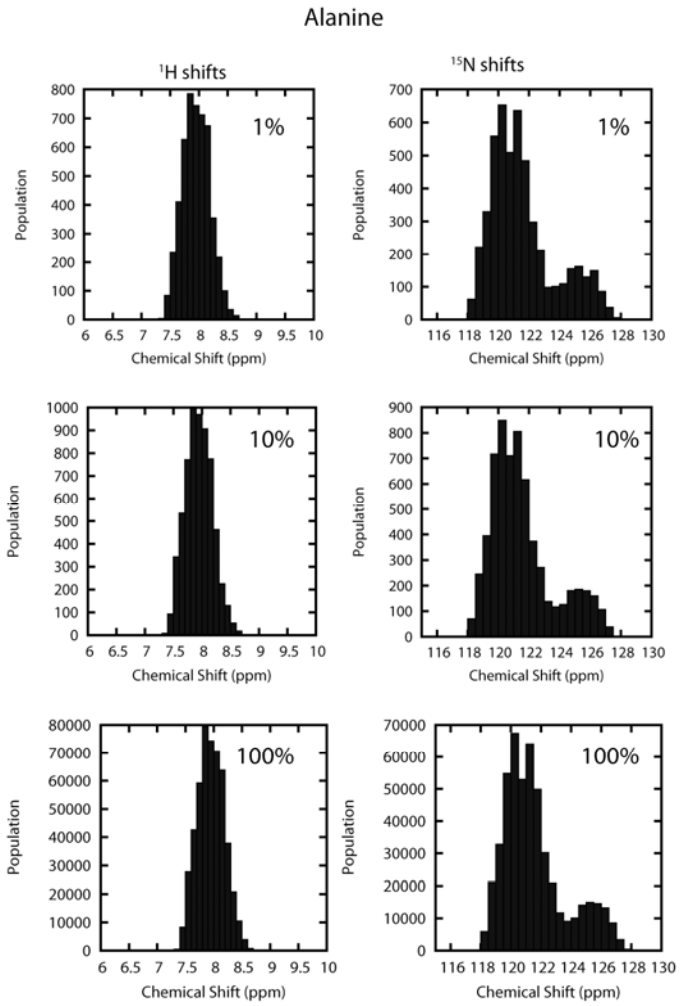
Supporting Material Figure Legends

Figure S1. Ensemble averaged chemical shifts calculated for the full, 10% and 1% portions of the alanine and valine production trajectories in 8M urea demonstrating 1% of trajectory to be representative of the full ensembles. Histograms show the change in distribution of $^{1}H_N$ and $^{15}N_H$ chemical shifts for the different ensembles used in the calculations. The mean chemical shifts for the $^{1}H_N$ and $^{15}N_H$ nuclei are tabulated with the standard deviations given in brackets.

Figure S2. Convergence of conformational sampling of AAAAA in water. (A) Comparison of the fractional population of the 64 states sampled over different sections of the trajectory for run #1 of AAAAA at 298 K. (B) Correlation coefficient for run #1 of AAAAA at 298 K. (C) Comparison of the fractional populations sampled between each pair of the three 298 K AAAAA simulations. (D) Comparison of the fractional populations of the 64 states over different sections of each of the three 498 K AAAAA simulations. (E) Comparisons of the fractional populations sampled between each pair of the three AAAAA 498 K simulations.

Figure S3. Convergence of conformational sampling of AAGAA and AAWAA in 8M urea at 298 K. Comparison of fractional population of the 64 states within individual simulations, (A) AAGAA and (C) AAWAA, and over different sections of the trajectories for run #1, (B) AAGAA and (D) AAWAA.



	% of MD ensemble	Mean chemical shift (ppm) ¹H	¹⁵N
Ala	1	7.95 (0.23)	121.60 (2.13)
Ala	10	7.95 (0.23)	121.56 (2.07)
Ala	100	7.95 (0.24)	121.57 (2.09)
Val	1	7.87 (0.30)	117.94 (3.04)
Val	10	7.87 (0.30)	117.94 (3.04)
Val	100	7.87 (0.30)	117.96 (3.06)

Figure S1

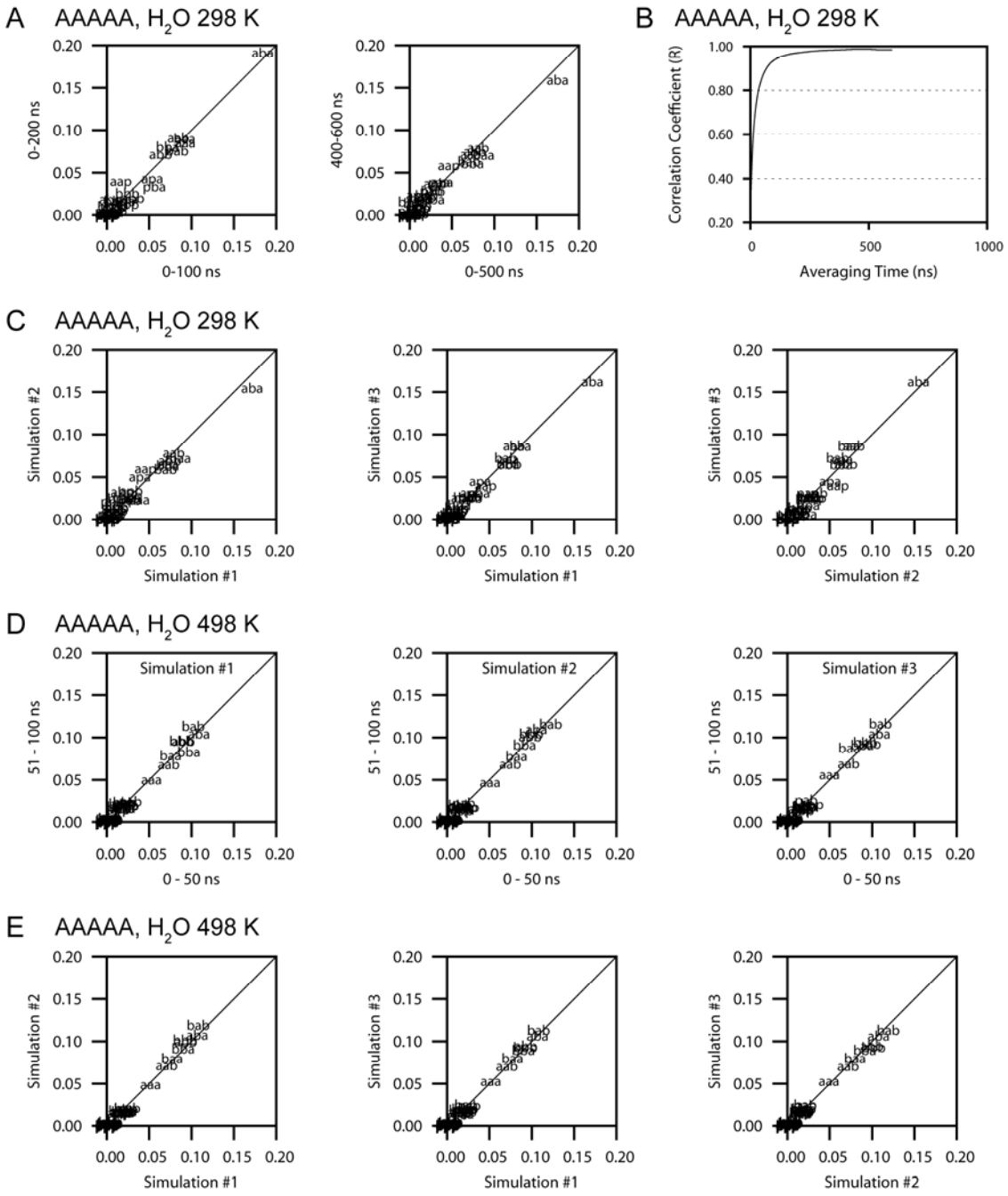

A AAAAA, H2O 298 K
0-200 ns
0-100 ns
400-600 ns
0-500 ns
B AAAAA, H2O 298 K
Correlation Coefficient (R)
Averaging Time (ns)
C AAAAA, H2O 298 K
Simulation #2
Simulation #1
Simulation #3
Simulation #1
Simulation #3
Simulation #2
D AAAAA, H2O 498 K
Simulation #1
Simulation #2
Simulation #3
51 - 100 ns
0 - 50 ns
E AAAAA, H2O 498 K
Simulation #2
Simulation #1
Simulation #3
Simulation #1
Simulation #3
Simulation #2

Figure S2

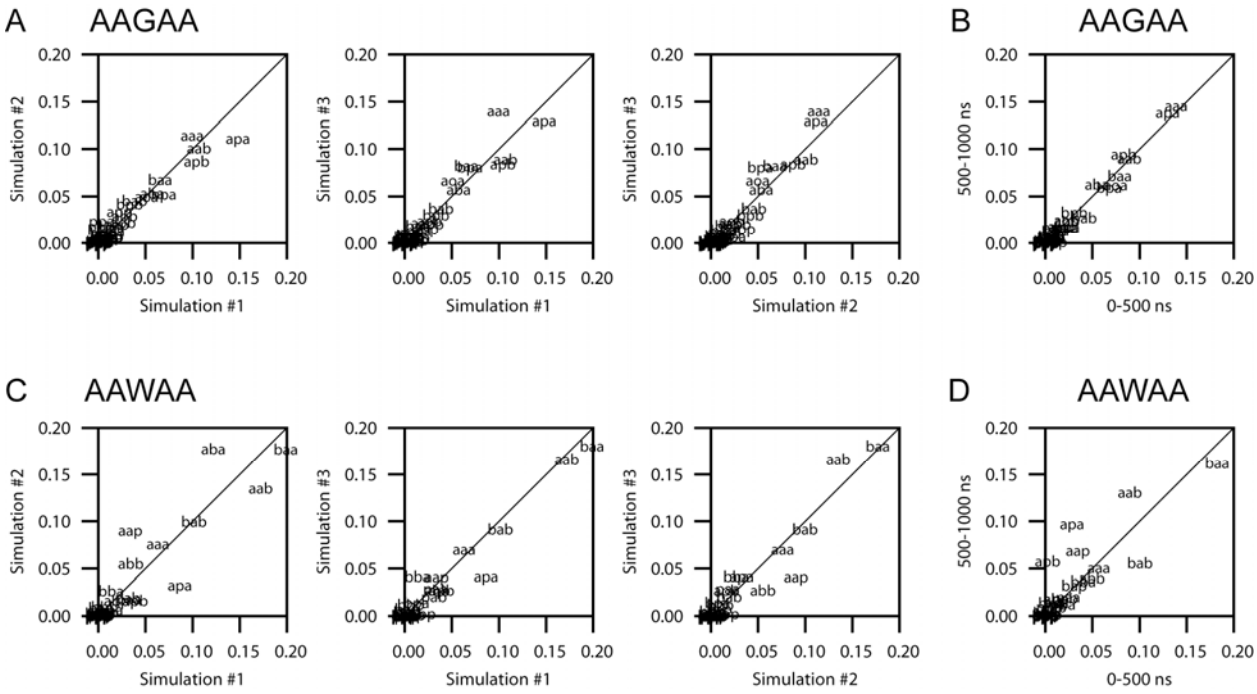

A
AAGAA
B
AAGAA
C
AAWAA
D
AAWAA
Simulation #1
Simulation #2
Simulation #3
500-1000 ns
0-500 ns
0.00
0.05
0.10
0.15
0.20

Figure S3

Table S1. Chemical shifts determined for random samples of conformations taken from different portions of the AAXAA MD simulations. Values given are the ensemble averages for a 1% random sample of 500 ns of dynamics; standard deviations are given in parentheses.

		First 500 ns Portion									Latter 500 ns Portion								
Res	#	H_N	N_H	Hα	Hβ1	Hβ2	$Hβ_3$	C’	Cα	Cβ	H_N	N_H	Hα	$Hβ_1$	$Hβ_2$	$Hβ_3$	C’	Cα	Cβ
Ala	1	7.92 (0.24)	121.59 (2.00)	4.40 (0.10)	1.39 (0.05)	1.72 (0.04)	1.64 (0.05)	177.17 (0.65)	52.50 (0.82)	19.64 (0.86)	7.95 (0.24)	121.55 (2.09)	4.41 (0.10)	1.39 (0.05)	1.72 (0.04)	1.64 (0.05)	177.17 (0.65)	52.64 (0.83)	19.63 (0.85)
Ala	2	7.95 (0.24)	121.86 (2.17)	4.40 (0.10)	1.39 (0.05)	1.72 (0.04)	1.64 (0.05)	177.22 (0.64)	52.66 (0.87)	19.63 (0.81)	7.99 (0.24)	121.90 (2.23)	4.39 (0.10)	1.39 (0.05)	1.72 (0.04)	1.64 (0.05)	177.20 (0.67)	52.75 (0.84)	19.56 (0.87)
Ala	3	7.97 (0.24)	121.92 (2.14)	4.40 (0.10)	1.39 (0.05)	1.72 (0.04)	1.64 (0.05)	177.19 (0.65)	52.69 (0.84)	19.56 (0.90)	7.97 (0.24)	121.78 (2.11)	4.39 (0.11)	1.39 (0.05)	1.72 (0.04)	1.64 (0.05)	177.2 (0.63)	52.66 (0.83)	19.48 (0.93)
Arg	1	8.01 (0.25)	118.81 (2.20)	4.38 (0.15)	-	1.82 (0.07)	1.89 (0.06)	175.90 (0.52)	56.49 (0.90)	30.98 (1.13)	8.02 (0.25)	118.96 (2.39)	4.39 (0.14)	-	1.81 (0.06)	1.89 (0.05)	175.93 (0.92)	56.57 (0.92)	31.15 (0.95)
Asp	1	8.10 (0.19)	119.04 (2.55)	4.66 (0.10)	-	2.74 (0.04)	2.76 (0.04)	175.73 (0.69)	54.85 (0.80)	41.50 (0.72)	8.12 (0.20)	119.06 (2.72)	4.67 (0.10)	-	2.74 (0.04)	2.76 (0.05)	175.73 (0.71)	54.92 (0.79)	41.60 (0.64)
Ash	1	8.14 (0.23)	119.84 (2.65)	4.65 (0.11)	-	2.75 (0.04)	2.76 (0.05)	175.88 (0.64)	55.22 (0.85)	41.54 (0.64)	8.09 (0.24)	119.56 (2.48)	4.64 (0.11)	-	2.75 (0.05)	2.77 (0.05)	175.85 (0.64)	54.97 (0.91)	41.40 (0.72)
Asn	1	8.18 (0.24)	117.43 (2.55)	4.74 (0.11)	-	2.84 (0.05)	2.79 (0.07)	174.92 (0.60)	54.12 (0.87)	39.39 (0.63)	8.10 (0.23)	116.72 (2.16)	4.74 (0.11)	-	2.84 (0.05)	2.79 (0.07)	174.80 (0.63)	53.81 (0.88)	39.29 (0.74)
Cys	1	8.14 (0.29)	116.61 (2.36)	4.66 (0.13)	-	2.96 (0.09)	2.88 (0.07)	174.20 (0.49)	58.88 (1.10)	28.58 (0.88)	8.09 (0.28)	116.04 (2.06)	4.66 (0.13)	-	2.96 (0.09)	2.87 (0.07)	174.16 (0.49)	58.68 (1.06)	28.59 (0.87)
Glu	1	8.18 (0.28)	119.27 (2.27)	4.36 (0.17)	-	2.06 (0.06)	2.09 (0.07)	176.25 (0.53)	56.83 (0.86)	30.20 (1.17)	8.14 (0.28)	119.53 (2.34)	4.38 (0.15)	-	2.05 (0.04)	2.07 (0.07)	176.29 (0.51)	56.94 (0.93)	30.54 (0.82)
Glh	1	8.15 (0.28)	119.11 (2.28)	4.41 (0.15)	-	2.04 (0.05)	2.07 (0.07)	176.26 (0.56)	56.94 (0.97)	30.66 (0.88)	8.17 (0.29)	119.36 (2.31)	4.38 (0.17)	-	2.05 (0.06)	2.08 (0.07)	176.22 (0.56)	56.92 (0.89)	30.31 (1.19)
Gln	1	8.07 (0.28)	118.88 (2.18)	4.36 (0.16)	-	2.06 (0.06)	2.08 (0.07)	175.65 (0.54)	56.28 (0.85)	29.49 (1.28)	8.08 (0.27)	118.79 (2.37)	4.39 (0.15)	-	2.05 (0.05)	2.08 (0.07)	175.74 (0.53)	56.44 (0.92)	29.82 (1.02)
Gly	1	8.12 (0.25)	107.40 (1.86)	4.00 (0.10)	-	-	-	174.23 (0.54)	45.66 (0.60)	-	8.12 (0.25)	107.39 (1.78)	4.00 (0.09)	-	-		174.20 (0.57)	45.63 (0.59)	-
Gly	2	8.12 (0.25)	107.38 (1.81)	4.00 (0.09)	-	-	-	174.20 (0.55)	45.61 (0.58)	-	8.13 (0.25)	107.49 (1.87)	4.00 (0.09)	-	-		174.17 (0.57)	45.62 (0.58)	-
Gly	3	8.14 (0.25)	107.47 (1.87)	3.99 (0.09)	-	-	-	174.19 (0.57)	45.64 (0.61)	-	8.13 (0.25)	107.41 (1.84)	4.00 (0.09)	-	-		174.21 (0.55)	45.62 (0.58)	-
Hid	1	8.13 (0.27)	117.59 (2.63)	4.73 (0.13)	-	3.22 (0.06)	3.22 (0.05)	174.31 (0.57)	56.08 (0.82)	30.37 (0.79)	8.19 (0.28)	117.85 (2.79)	4.73 (0.14)	-	3.24 (0.06)	3.22 (0.05)	174.29 (0.55)	56.22 (0.80)	30.35 (0.88)
Hie	1	8.10 (0.27)	117.31 (2.37)	4.68 (0.17)	-	3.23 (0.07)	3.23 (0.06)	174.36 (0.58)	56.10 (0.83)	30.01 (1.17)	8.08 (0.28)	116.59 (2.37)	4.71 (0.14)	-	3.22 (0.07)	3.22 (0.05)	174.31 (0.57)	55.91 (0.83)	30.25 (0.89)

		First 500 ns Portion									Latter 500 ns Portion								
Res	#	H_N	N_H	Hα	Hβ1	Hβ2	$Hβ_3$	C’	Cα	Cβ	H_N	N_H	Hα	$Hβ_1$	$Hβ_2$	$Hβ_3$	C’	Cα	Cβ
Hip	1	8.15 (0.26)	117.65 (2.34)	4.66 (0.20)	-	3.24 (0.07)	3.22 (0.06)	174.19 (0.55)	56.10 (0.68)	29.68 (1.62)	8.18 (0.24)	117.44 (2.58)	4.70 (0.18)	-	3.24 (0.06)	3.22 (0.05)	174.17 (0.54)	56.10 (0.62)	30.03 (1.46)
Ile	1	7.79 (0.28)	117.12 (3.15)	4.28 (0.13)	1.87 (0.06)	-	-	175.88 (0.53)	60.89 (1.02)	39.19 (0.74)	7.75 (0.27)	116.80 (2.87)	4.28 (0.13)	1.87 (0.05)	-	-	175.88 (0.51)	60.70 (0.95)	39.15 (0.84)
Leu	1	7.92 (0.28)	120.57 (2.50)	4.41 (0.14)	-	1.68 (0.05)	1.56 (0.07)	177.07 (0.47)	55.61 (0.99)	42.75 (0.80)	7.92 (0.27)	120.42 (2.50)	4.40 (0.14)	-	1.69 (0.05)	1.57 (0.07)	177.06 (0.50)	55.63 (0.98)	42.69 (0.84)
Lys	1	8.04 (0.26)	118.83 (2.19)	4.38 (0.14)	-	1.82 (0.06)	1.89 (0.05)	176.25 (0.53)	56.68 (0.90)	33.35 (0.95)	8.03 (0.27)	119.10 (2.32)	4.37 (0.14)	-	1.87 (0.06)	1.88 (0.05)	176.26 (0.52)	56.73 (0.90)	33.34 (0.94)
Met	1	8.03 (0.25)	118.24 (2.33)	4.52 (0.14)	-	2.04 (0.05)	2.08 (0.06)	175.89 (0.51)	55.96 (0.95)	33.14 (1.03)	8.04 (0.26)	118.87 (2.54)	4.54 (0.13)	-	2.03 (0.05)	2.07 (0.06)	175.90 (0.52)	56.06 (0.99)	33.37 (0.83)
Phe	1	8.05 (0.38)	118.58 (2.75)	4.65 (0.18)	-	3.08 (0.09)	2.99 (0.11)	175.38 (0.60)	58.55 (1.02)	40.15 (0.90)	8.04 (0.39)	118.62 (2.73)	4.66 (0.17)	-	3.07 (0.08)	2.99 (0.11)	175.37 (0.62)	58.40 (1.06)	40.17 (0.83)
Pro	1	-	-	4.47 (0.05)	-	2.16 (0.06)	2.15 (0.06)	176.85 (0.44)	63.01 (0.45)	32.23 (0.40)	-	-	4.46 (0.06)	-	2.16 (0.06)	2.15 (0.07)	176.87 (0.41)	63.07 (0.48)	32.22 (0.40)
Ser	1	8.00 (0.25)	114.91 (2.05)	4.49 (0.12)	-	3.95 (0.07)	4.04 (0.08)	174.32 (0.43)	58.49 (0.84)	63.90 (0.68)	8.05 (0.25)	115.05 (2.10)	4.48 (0.13)	-	3.95 (0.07)	4.03 (0.08)	174.38 (0.44)	58.83 (0.95)	63.91 (0.70)
Thr	1	7.98 (0.25)	113.67 (2.73)	4.35 (0.13)	4.27 (0.14)	-	-	174.53 (0.43)	62.56 (1.06)	69.95 (0.60)	8.03 (0.25)	113.98 (2.77)	4.35 (0.14)	4.24 (0.13)	-	-	174.49 (0.43)	62.76 (1.00)	69.98 (0.56)
Trp	1	7.97 (0.41)	119.77 (2.73)	4.72 (0.18)	-	3.23 (0.07)	3.21 (0.07)	175.65 (0.64)	57.95 (1.00)	30.15 (1.21)	7.98 (0.39)	119.88 (2.80)	4.71 (0.18)	-	3.24 (0.07)	3.22 (0.07)	175.70 (0.62)	58.15 (0.96)	30.14 (1.34)
Trp	2	8.06 (0.39)	119.96 (2.85)	4.72 (0.17)	-	3.22 (0.06)	3.21 (0.07)	175.69 (0.67)	58.16 (1.00)	30.40 (0.90)	7.99 (0.40)	119.75 (2.81)	4.73 (0.17)	-	3.23 (0.06)	3.21 (0.07)	175.70 (0.63)	58.07 (1.04)	30.31 (1.10)
Trp	3	7.98 (0.41)	119.94 (2.75)	4.69 (0.19)	-	3.24 (0.07)	3.22 (0.08)	175.68 (0.62)	58.09 (0.98)	29.94 (1.43)	7.98 (0.43)	119.91 (2.75)	4.71 (0.18)	-	3.23 (0.07)	3.22 (0.07)	175.74 (0.61)	58.07 (1.07)	30.20 (1.18)
Tyr	1	7.97 (0.35)	117.88 (2.54)	4.62 (0.16)	-	2.99 (0.08)	2.82 (0.09)	175.43 (0.59)	58.59 (0.97)	39.41 (0.80)	8.04 (0.36)	119.06 (2.98)	4.63 (0.16)	-	3.00 (0.07)	2.82 (0.09)	175.51 (0.57)	58.78 (0.98)	39.50 (0.68)
Val	1	7.83 (0.28)	116.99 (2.86)	4.19 (0.13)	2.08 (0.08)	-	-	175.80 (0.49)	62.25 (1.22)	33.13 (0.70)	7.88 (0.30)	117.97 (3.01)	4.19 (0.14)	2.07 (0.07)	-	-	175.80 (0.49)	62.37 (1.19)	33.12 (0.74)
							Pearson Correlation between Datasets:			**0.93**	**0.99**	**1.00**	**1.00**	**1.00**	**1.00**	**1.00**	**1.00**	**1.00**

Table S2. Correlation coefficients (R) between initial and latter portions of the trajectories for the 64 conformational states populated by the three central residues.

X	Water* 298 K	8M Urea† 298 K	Water§ 498 K
Ala-1	0.99	0.98	1.00
Ala-2	0.98	0.95	1.00
Ala-3	0.99	0.98	0.99
Arg	0.96	0.95	0.99
Asp	0.97	0.98	0.99
Ash	0.95	0.90	1.00
Asn	0.93	0.88	0.99
Cyh	0.98	0.94	0.99
Gln	0.97	0.94	1.00
Glu	0.98	0.91	0.99
Glh	0.96	0.95	0.99
Gly-1	0.98	0.97	0.99
Gly-2	-	0.98	-
Gly-3	-	0.97	-
Hid	0.96	0.92	0.99
Hie	0.94	0.82	1.00
Hip	0.72	0.92	1.00
Ile	0.95	0.97	1.00
Leu	0.90	0.97	0.99
Lys	0.95	0.94	0.99
Met	0.92	0.92	0.99
Phe	0.95	0.95	1.00
Pro	0.99	0.97	1.00
Ser	0.96	0.87	1.00
Thr	0.95	0.87	1.00
Trp-1	0.97	0.89	0.99
Trp-2	-	0.94	-
Trp-3	-	0.93	-
Tyr	0.91	0.84	0.99
Val	0.88	0.92	0.99
Average	0.95	0.93	0.99

The latter portions were that part of the trajectory (production dynamics) used for analysis. The start position and length of the production dynamics for each set of simulations was defined by the convergence behavior as exhibited in Figures 1, S2 – S3. *last 300 ns, †last 500 ns, §last 50 ns

Table S3. Conformational propensities of the guest residues (X) in water at 298 K.

	Population Frequency (%)													
	By quadrant				By specific conformational region								Total α-basin	Total β-basin
X	Q_α	Q_β	$Q_{\alpha L}$	Q_o	α_R	Near α_R	α_L	β	Non-P β	P_{IIL}	P_{IR}	Other	($\alpha + n\alpha_R$)	($nP\beta + P_{IIL} + P_{IR}$)
Ala-1	46.2	39.8	13.6	0.4	20.3	18.1	11.6	28.9	12.8	13.7	6.6	16.9	38.4	33.1
Ala-2	41.7	41.8	16.2	0.4	17.7	16.1	14.0	32.2	14.4	15.4	6.1	16.2	33.8	35.9
Ala-3	45.6	41.7	12.4	0.3	20.3	17.3	10.4	31.3	13.7	15.2	6.5	16.6	37.6	35.4
Arg	55.6	33.8	10.3	0.2	26.6	21.7	9.2	28.0	12.0	14.5	3.4	12.6	48.3	29.9
Asn	59.2	33.4	7.3	0.1	34.0	21.6	6.3	27.7	16.0	8.7	4.9	8.5	55.6	29.6
Asp	67.8	21.8	10.3	0.1	29.2	36.2	9.7	6.9	4.6	0.4	6.5	13.5	65.4	11.5
Ash	65.4	24.5	10.0	0.1	36.5	25.4	9.1	20.0	12.3	5.4	3.9	7.5	61.9	21.6
Cys	48.2	41.4	10.0	0.4	20.8	20.3	8.8	33.2	14.3	17.3	4.3	14.3	41.1	35.9
Gln	48.2	32.2	19.4	0.2	22.9	18.8	17.7	26.4	11.0	14.1	3.2	12.2	41.7	28.3
Glu	50.6	36.8	12.4	0.2	25.9	18.1	11.4	28.9	12.7	14.5	4.2	13.2	44.0	31.4
Glh	51.4	33.9	14.6	0.1	22.7	22.2	13.3	26.4	11.7	13.0	4.2	12.9	44.9	28.9
Gly	41.2	9.2	39.4	10.2	14.2	3.2	11.5	8.0	3.7	3.9	1.2	62.4	17.4	8.8
Hid	62.3	29.6	8.0	0.1	27.3	28.3	7.2	23.1	11.8	9.5	4.0	11.9	55.6	25.3
Hie	54.6	35.1	10.2	0.1	27.9	20.0	8.9	29.5	13.1	14.9	3.0	12.2	47.9	31.0
Hip	42.3	27.1	30.1	0.5	8.8	28.2	24.7	16.6	10.3	3.2	8.2	16.6	37.0	21.7
Ile	39.6	55.7	4.7	«0.1	15.5	17.0	4.4	46.1	14.2	31.4	1.8	15.7	32.5	47.4
Leu	61.1	21.0	17.6	0.3	33.7	21.2	15.8	18.0	6.9	10.4	1.3	10.7	54.9	18.6
Lys	55.2	32.1	12.5	0.2	27.2	21.1	11.3	26.3	10.9	14.0	3.3	12.2	48.3	28.2
Met	51.0	28.7	20.0	0.3	25.3	19.7	18.0	23.0	10.0	11.7	2.8	12.4	45.0	24.5
Phe	56.8	25.8	17.2	0.2	26.4	25.1	15.5	20.4	10.5	8.3	3.2	10.9	51.5	22.0
Pro	5.1	94.9	-	-	3.1	-	-	89.4	11.2	78.2	-	7.6	3.1	89.4
Ser	45.0	49.9	5.0	0.1	24.0	10.2	4.5	44.6	12.7	31.3	1.7	15.5	34.2	45.7
Thr	55.0	44.3	0.7	<0.1	35.7	14.2	0.7	38.1	12.1	25.5	1.2	10.5	49.9	38.8
Trp	62.3	26.0	11.6	0.2	28.6	28.0	10.5	20.5	10.8	8.1	3.2	10.8	56.6	22.1
Tyr	54.0	25.7	20.0	0.3	24.0	24.4	18.0	20.1	10.9	7.5	3.7	11.6	48.4	22.1
Val	42.3	56.5	1.2	«0.1	16.8	19.0	1.1	49.4	17.0	31.4	2.3	12.3	35.8	50.7

Table S4. Conformational propensities of the 'guest' residues (X) in 8M urea at 298 K.

	Population Frequency (%)													
	By quadrant				By specific conformational region								Total α-basin	Total β-basin
X	Q_α	Q_β	$Q_{\alpha L}$	Q_o	α_R	Near α_R	α_L	β	Non-P β	P_{IIL}	P_{IR}	Other	$(\alpha + n\alpha_R)$	$(nP\beta + P_{IIL} + P_{IR})$
Ala-1	45.1	48.1	6.7	0.2	13.1	23.6	5.3	39.7	18.2	17.6	8.1	14.0	36.7	43.9
Ala-2	50.4	40.4	8.8	0.3	16.2	26.3	7.0	32.7	13.8	16.3	5.9	14.6	42.5	36.0
Ala-3	40.6	48.5	10.6	0.3	13.6	19.3	8.9	39.0	16.5	19.0	8.3	14.4	32.9	43.8
Arg	55.8	37.9	6.2	0.1	19.2	29.7	5.7	33.2	14.6	16.8	3.6	10.4	48.9	35.0
Asn	50.9	44.7	4.3	<0.1	20.1	27.2	3.7	37.8	20.9	12.5	7.2	8.3	47.3	40.6
Asp	81.7	15.8	2.4	<0.1	23.7	55.5	2.2	5.4	3.4	0.3	4.7	10.3	79.2	8.4
Ash	57.7	34.5	7.7	0.1	25.0	29.7	6.8	28.0	16.5	5.8	8.9	7.2	54.7	31.2
Cys	44.2	50.7	5.0	0.1	13.0	22.7	4.2	44.4	19.7	21.9	6.1	12.4	35.7	47.7
Gln	58.6	32.8	8.5	0.1	21.9	29.5	7.5	28.8	12.2	15.0	3.3	10.7	51.4	30.5
Glu	53.6	42.9	3.4	0.1	22.0	23.7	3.0	38.6	15.6	21.3	3.4	11.1	45.7	40.3
Glh	48.1	36.3	15.4	0.2	15.9	25.2	13.5	31.2	13.5	15.6	4.5	11.9	41.1	33.6
Gly-1	35.2	12.1	39.1	13.5	8.5	3.7	9.8	11.3	5.4	5.0	1.9	65.7	12.2	12.3
Gly-2	37.9	12.3	38.4	11.4	9.5	4.7	8.9	11.5	5.3	5.5	1.6	64.6	14.2	12.4
Gly-3	39.5	11.0	37.0	12.5	9.3	4.6	8.7	10.4	5.1	4.5	1.9	66.0	13.9	11.5
Hid	75.9	19.8	4.1	0.2	25.1	44.2	3.5	15.4	8.1	6.1	2.6	10.4	69.3	16.8
Hie	53.8	41.9	4.2	<0.1	16.9	29.1	3.5	37.4	17.4	17.6	4.3	11.1	46.0	39.3
Hip	63.3	14.7	21.5	0.5	10.0	47.7	16.6	8.6	4.7	2.1	4.4	14.5	57.7	11.2
Ile	29.5	67.7	2.9	<0.1	6.8	15.6	2.6	64.2	23.5	39.8	1.7	10.0	22.4	65.0
Leu	55.1	36.8	7.8	0.3	22.9	25.7	6.9	33.3	13.5	18.2	3.1	9.8	48.6	34.8
Lys	53.4	39.9	6.7	<0.1	19.2	27.2	6.0	35.3	14.5	18.7	4.3	10.1	46.4	37.5
Met	60.8	34.7	4.5	0.1	21.9	31.5	4.0	30.4	12.6	16.1	3.5	10.4	53.4	32.2
Phe	60.1	35.9	3.9	<0.1	20.2	34.5	3.4	30.2	16.3	10.4	6.2	9.0	54.7	32.9
Pro	7.1	92.9	-	-	5.0	-	-	86.9	10.3	76.6	-	8.1	5.0	86.9
Ser	48.8	45.2	5.7	0.3	23.5	15.4	4.9	41.8	10.3	31.2	0.9	13.7	38.9	42.4
Thr	71.3	28.6	0.1	<0.1	42.1	24.2	0.1	24.9	7.1	17.6	0.6	8.4	66.3	25.3
Trp-1	64.2	20.5	15.0	0.3	19.4	38.9	13.1	16.7	9.3	5.9	2.9	10.5	58.3	18.1
Trp-2	63.2	30.0	6.6	0.2	22.0	35.0	5.6	25.3	14.3	8.6	4.5	10.0	57.0	27.4
Trp-3	61.0	29.8	9.1	0.2	22.0	33.3	7.9	25.3	13.3	9.4	4.6	9.4	55.3	27.3
Tyr	76.5	22.6	0.9	<0.1	25.8	44.2	0.8	18.0	10.4	5.7	3.9	9.2	70.0	20.0
Val	51.5	46.6	1.8	<0.1	16.1	29.3	1.7	42.4	16.8	24.7	1.8	9.6	45.4	43.3

Table S5. Conformational propensities of the 'guest' residues (X) in water at 498 K.

	Population Frequency (%)													
	By quadrant					By specific conformational region							Total α-basin	Total β-basin
X	Q_α	Q_β	$Q_{\alpha L}$	Q_o	α_R	Near α_R	α_L	β	Non-P β	P_{IIL}	P_{IR}	Other	$(\alpha + n\alpha_R)$	$(nP\beta + P_{IIL} + P_{IR})$
Ala-1	39.8	48.8	9.5	1.9	15.4	12.9	5.9	33.6	20.6	10.1	7.4	27.8	28.3	38.1
Ala-2	40.1	49.6	8.6	1.8	14.9	13.5	5.1	33.5	20.6	9.9	7.5	28.5	28.4	38.0
Ala-3	39.4	50.1	8.3	2.2	15.0	13.0	5.0	34.7	21.0	10.8	7.2	28.2	28.0	39.0
Arg	44.2	48.9	6.0	0.9	19.4	15.7	4.6	34.4	19.9	12.1	5.5	22.7	35.1	37.5
Asn	45.0	47.0	7.3	0.7	21.5	15.9	5.0	36.6	22.5	11.1	5.5	18.4	37.4	39.1
Asp	48.5	37.1	13.3	1.1	20.4	23.0	10.3	15.1	9.8	2.4	8.2	25.9	43.4	20.4
Ash	49.0	40.9	9.0	1.1	23.0	19.5	6.5	29.2	19.3	6.1	7.2	18.5	42.5	32.6
Cys	43.2	51.2	5.1	0.6	18.4	14.4	3.5	36.1	20.6	13.3	5.1	24.6	32.8	39.0
Gln	44.6	46.1	8.5	0.8	20.1	15.4	6.4	32.3	18.7	11.3	5.1	22.9	35.5	35.1
Glu	40.8	50.7	8.0	0.5	19.3	12.4	6.4	35.8	20.1	13.4	5.4	23.1	31.7	38.9
Glh	43.2	48.9	7.2	0.7	17.7	16.2	5.4	33.4	20.0	10.7	6.4	23.6	33.9	37.1
Gly	31.5	17.1	32.0	19.4	9.2	4.2	6.0	11.5	7.2	3.3	2.7	67.4	13.4	13.2
Hid	42.4	47.2	9.4	1.0	17.4	16.4	6.9	33.0	20.0	10.2	6.0	23.2	33.8	36.2
Hie	47.4	47.7	4.2	0.8	22.4	13.5	3.0	36.1	19.2	15.4	3.3	23.3	35.9	37.9
Hip	47.2	46.6	5.6	0.5	14.5	23.0	3.7	28.4	19.4	4.9	9.6	24.8	37.5	33.9
Ile	39.2	59.7	1.0	0.1	17.3	13.2	0.8	45.0	21.9	21.9	2.9	22.0	30.5	46.7
Leu	52.2	39.9	6.8	1.1	26.0	16.7	5.1	29.9	16.7	11.3	3.8	20.3	42.7	31.8
Lys	47.1	45.5	6.6	0.9	21.4	16.0	5.0	32.2	18.6	11.3	4.9	22.7	37.4	34.8
Met	47.6	44.4	6.7	1.3	22.0	16.0	5.1	31.3	17.9	11.4	4.7	22.9	38.0	34.0
Phe	45.0	49.0	5.5	0.5	19.9	16.5	4.1	36.5	21.3	12.8	5.0	20.5	36.4	39.1
Pro	23.5	76.5	<0.1	-	19.1	«0.1	-	67.1	18.7	48.5	«0.1	13.7	19.1	67.2
Ser	43.9	51.2	4.2	0.8	21.8	10.0	3.2	37.0	17.9	17.5	3.8	25.7	31.8	39.2
Thr	48.6	50.2	1.1	0.1	28.1	11.1	0.9	37.3	17.6	18.8	2.4	21.2	39.2	38.8
Trp	44.4	47.9	6.9	0.8	20.2	15.2	5.3	35.3	20.0	13.4	4.1	21.9	35.4	37.5
Tyr	48.7	43.2	7.1	1.0	22.3	17.8	5.4	30.9	18.0	10.7	4.5	21.2	40.1	33.2
Val	33.9	63.1	3.0	<0.1	15.4	11.2	2.5	49.9	24.8	23.5	3.5	19.1	26.6	51.8

Table S6. Similarity correlation matrices for the sampling of ϕ/ψ space by the AAXAA guest residues in water at 298 K. Correlations below 0.5 are shaded grey, correlations below 0.7 are emphasized in bold italic.

Water 298 K

ARG	ASH	ASN	ASP	CYS	GLH	GLN	GLU	GLY	HID	HIE	HIP	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL	
0.95	0.87	0.88	0.80	0.96	0.96	0.96	0.96	***0.38***	0.92	0.96	0.73	0.73	0.92	0.95	0.95	0.93	***0.30***	0.81	0.84	0.93	0.93	0.79	**ALA**
	0.91	0.92	0.83	0.98	0.98	0.96	0.98	***0.35***	0.98	0.99	***0.67***	0.73	0.97	0.99	0.97	0.97	***0.19***	0.78	0.87	0.98	0.96	0.81	**ARG**
		0.99	0.78	0.85	0.89	0.86	0.91	***0.33***	0.93	0.93	***0.59***	***0.48***	0.94	0.92	0.89	0.94	***0.08***	***0.63***	0.82	0.94	0.91	***0.58***	**ASH**
			0.76	0.87	0.89	0.87	0.93	***0.33***	0.94	0.95	***0.57***	***0.52***	0.93	0.93	0.89	0.93	***0.13***	***0.67***	0.85	0.94	0.90	***0.63***	**ASN**
				0.83	0.83	0.79	0.78	***0.20***	0.86	0.81	***0.68***	***0.52***	0.80	0.81	0.80	0.84	***-0.02***	***0.54***	***0.69***	0.88	0.84	***0.59***	**ASP**
					0.97	0.95	0.96	***0.31***	0.94	0.97	***0.68***	0.80	0.92	0.97	0.94	0.93	***0.29***	0.84	0.88	0.94	0.93	0.86	**CYS**
						0.99	0.98	***0.37***	0.96	0.97	0.77	0.70	0.96	0.99	0.98	0.98	***0.18***	0.74	0.81	0.97	0.98	0.77	**GLH**
							0.97	***0.40***	0.92	0.95	0.75	***0.69***	0.96	0.97	0.99	0.97	***0.20***	0.75	0.80	0.94	0.97	0.75	**GLN**
								0.40	0.95	0.98	***0.67***	***0.69***	0.96	0.99	0.97	0.96	***0.22***	0.77	0.87	0.95	0.95	0.76	**GLU**
									0.31	***0.37***	***0.38***	***0.18***	***0.41***	***0.37***	***0.40***	***0.36***	***0.06***	***0.30***	***0.30***	***0.33***	***0.37***	***0.18***	**GLY**
										0.96	***0.69***	***0.64***	0.95	0.97	0.94	0.97	***0.10***	***0.68***	0.81	0.99	0.96	0.73	**HID**
											0.64	0.72	0.97	0.99	0.96	0.96	***0.25***	0.81	0.91	0.97	0.94	0.80	**HIE**
												0.40	***0.65***	***0.67***	0.74	0.75	***-0.01***	***0.34***	***0.36***	0.71	0.79	***0.43***	**HIP**
													0.61	0.70	***0.64***	***0.60***	***0.49***	0.86	0.75	***0.62***	***0.59***	0.98	**ILE**
														0.98	0.98	0.98	***0.12***	0.71	0.83	0.97	0.97	***0.68***	**LEU**
															0.98	0.98	***0.19***	0.77	0.86	0.98	0.96	0.78	**LYS**
																0.98	***0.15***	0.71	0.79	0.96	0.98	0.70	**MET**
																	0.09	***0.66***	0.78	0.99	0.99	***0.67***	**PHE**
																		0.61	***0.42***	***0.09***	***0.07***	***0.48***	**PRO**
																			0.90	***0.67***	***0.63***	0.88	**SER**
																				0.80	0.74	0.82	**THR**
																					0.98	0.71	**TRP**
																						0.66	**TYR**

Water 298 K

Table S7. Similarity correlation matrices for the sampling of ϕ/ψ space by the AAXAA guest residues in water at 498 K. Correlations below 0.5 are shaded grey, correlations below 0.7 are emphasized in bold italic.

Water 498 K

ARG	ASH	ASN	ASP	CYS	GLH	GLN	GLU	GLY	HID	HIE	HIP	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL	
0.92	0.88	0.92	0.82	0.93	0.93	0.92	0.92	***0.39***	0.93	0.90	0.87	0.81	0.88	0.91	0.91	0.92	***0.33***	0.87	0.83	0.92	0.91	0.81	**ALA**
	0.90	0.95	0.83	0.96	0.97	0.97	0.96	***0.36***	0.96	0.94	0.88	0.87	0.95	0.97	0.97	0.97	***0.32***	0.90	0.90	0.97	0.97	0.87	**ARG**
		0.95	0.86	0.87	0.90	0.91	0.88	***0.39***	0.92	0.85	0.88	***0.68***	0.93	0.92	0.92	0.92	***0.25***	0.79	0.80	0.90	0.93	***0.68***	**ASH**
			0.80	0.93	0.94	0.95	0.94	***0.38***	0.95	0.92	0.86	0.80	0.95	0.95	0.95	0.96	***0.36***	0.87	0.88	0.95	0.96	0.81	**ASN**
				0.82	0.84	0.84	0.79	***0.35***	0.86	0.78	0.87	***0.66***	0.81	0.84	0.84	0.82	***0.10***	0.72	0.72	0.82	0.87	***0.61***	**ASP**
					0.96	0.95	0.95	***0.34***	0.95	0.96	0.86	0.91	0.92	0.95	0.95	0.96	***0.37***	0.93	0.92	0.97	0.95	0.90	**CYS**
						0.97	0.95	***0.37***	0.97	0.92	0.91	0.85	0.94	0.97	0.96	0.96	***0.29***	0.88	0.87	0.96	0.96	0.85	**GLH**
							0.96	***0.39***	0.97	0.94	0.88	0.85	0.96	0.97	0.97	0.97	***0.32***	0.90	0.90	0.97	0.97	0.85	**GLN**
								0.38	0.95	0.94	0.82	0.87	0.94	0.96	0.95	0.96	***0.43***	0.93	0.92	0.96	0.94	0.88	**GLU**
									0.37	***0.37***	***0.30***	***0.24***	***0.41***	***0.39***	***0.40***	***0.36***	***0.11***	***0.35***	***0.35***	***0.37***	***0.38***	***0.23***	**GLY**
										0.92	0.91	0.84	0.94	0.96	0.96	0.96	***0.28***	0.87	0.85	0.96	0.96	0.83	**HID**
											0.79	0.91	0.93	0.94	0.95	0.95	***0.45***	0.96	0.96	0.96	0.94	0.90	**HIE**
												0.71	0.83	0.87	0.87	0.87	***0.10***	0.71	***0.69***	0.85	0.88	***0.68***	**HIP**
													0.81	0.85	0.85	0.87	***0.44***	0.91	0.90	0.89	0.84	0.96	**ILE**
														0.97	0.97	0.96	***0.31***	0.88	0.90	0.95	0.97	0.80	**LEU**
															0.98	0.97	***0.31***	0.90	0.90	0.97	0.97	0.84	**LYS**
																0.97	***0.31***	0.90	0.90	0.97	0.97	0.84	**MET**
																	0.35	0.90	0.91	0.97	0.97	0.87	**PHE**
																		0.55	***0.51***	***0.38***	***0.30***	***0.51***	**PRO**
																			0.96	0.93	0.89	0.91	**SER**
																				0.92	0.90	0.89	**THR**
																					0.97	0.88	**TRP**
																						0.83	**TYR**

Water 498 K

Table S8. Similarity correlation matrices for the sampling of ϕ/ψ space by the AAXAA guest residues in 8M urea at 298 K.

8M Urea 298 K

ARG	ASH	ASN	ASP	CYS	GLH	GLN	GLU	GLY	HID	HIE	HIP	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL	
0.94	0.86	0.88	0.76	0.96	0.93	0.92	0.93	***0.25***	0.86	0.96	0.76	***0.67***	0.91	0.94	0.91	0.91	***0.34***	0.83	0.78	0.87	0.85	0.89	**ALA**
	0.90	0.90	0.81	0.94	0.97	0.99	0.97	***0.24***	0.95	0.99	0.77	***0.58***	0.98	0.99	0.99	0.98	***0.19***	0.80	0.85	0.95	0.95	0.92	**ARG**
		0.97	0.78	0.78	0.86	0.91	0.87	***0.22***	0.92	0.89	0.74	***0.29***	0.90	0.89	0.90	0.94	***0.08***	***0.67***	0.85	0.91	0.92	0.73	**ASH**
			0.73	0.81	0.86	0.91	0.90	***0.21***	0.88	0.92	0.71	***0.37***	0.90	0.90	0.90	0.93	***0.21***	0.71	0.82	0.86	0.88	0.76	**ASN**
				0.74	0.76	0.80	0.72	***0.10***	0.88	0.82	0.84	***0.33***	0.74	0.78	0.81	0.86	***-0.02***	***0.54***	0.72	0.88	0.89	0.75	**ASP**
					0.93	0.91	0.94	***0.22***	0.83	0.95	***0.69***	0.78	0.91	0.95	0.92	0.89	***0.30***	0.85	0.77	0.83	0.83	0.95	**CYS**
						0.97	0.93	***0.32***	0.90	0.95	0.80	***0.60***	0.95	0.97	0.95	0.93	***0.18***	0.78	0.78	0.94	0.89	0.88	**GLH**
							0.96	***0.28***	0.96	0.97	0.77	***0.54***	0.99	0.99	0.99	0.97	***0.18***	0.79	0.87	0.96	0.95	0.89	**GLN**
								0.28	0.89	0.96	***0.66***	***0.65***	0.97	0.98	0.96	0.92	***0.29***	0.87	0.90	0.86	0.88	0.91	**GLU**
									0.21	***0.23***	***0.25***	***0.14***	***0.28***	***0.26***	***0.24***	***0.20***	***0.09***	***0.30***	***0.25***	***0.25***	***0.19***	***0.18***	**GLY**
										0.93	0.84	***0.38***	0.92	0.93	0.96	0.98	***0.03***	***0.66***	0.82	0.97	0.99	0.83	**HID**
											0.77	***0.61***	0.96	0.98	0.97	0.97	***0.24***	0.80	0.84	0.92	0.93	0.92	**HIE**
												0.31	***0.68***	0.73	0.74	0.80	***-0.01***	***0.44***	***0.52***	0.87	0.81	***0.65***	**HIP**
													0.56	***0.61***	***0.54***	***0.46***	***0.49***	0.75	***0.46***	***0.40***	***0.39***	0.80	**ILE**
														0.99	0.99	0.95	***0.19***	0.82	0.89	0.92	0.92	0.89	**LEU**
															0.99	0.96	***0.20***	0.82	0.86	0.93	0.93	0.92	**LYS**
																0.98	***0.15***	0.78	0.87	0.94	0.96	0.91	**MET**
																	0.10	0.71	0.84	0.96	0.98	0.87	**PHE**
																		0.59	***0.24***	***0.03***	***0.01***	***0.31***	**PRO**
																			0.84	***0.65***	***0.65***	0.84	**SER**
																				0.78	0.83	0.80	**THR**
																					0.96	0.82	**TRP**
																						0.84	**TYR**

8M Urea 298 K

Table S9. Water Residence Times by Conformational Region and Transitions for AAXAA in pure water at 298 K.

	Conformational Region							Transitions	
Residue	**α_R**	**nα_R**	**β**	**P_{IIL}**	**P_{IR}**	**α_L**	**other**	**N**	**N>10ps**
Ala-1	75	43	37	42	31	213	129	111887	3619
Ala-2	86	40	35	47	26	170	104	110214	3689
Ala-3	66	28	33	50	22	183	211	113097	3501
Arg	99	42	57	51	25	269	131	107562	3976
Ash	217	54	57	34	23	160	37	105056	4148
Asn	143	43	81	39	26	230	86	111435	3729
Asp	132	70	29	11	45	300	38	96370	4502
Cys	106	44	52	42	22	218	436	114198	3442
Glh	93	42	49	57	23	288	90	29864	69
Gln	79	46	45	47	16	330	121	106150	3901
Glu	125	47	63	75	33	248	610	100146	4154
Gly	70	15	17	33	14	25	534	86520	4669
Hie	90	40	65	50	21	233	88	108859	3887
Hip	58	63	51	53	37	340	260	93323	5217
Hid	118	43	71	44	47	183	122	113031	3633
Ile	74	62	38	65	23	234	55	108005	4313
Leu	110	33	23	41	21	306	201	99028	4274
Lys	101	53	56	49	29	252	376	105275	3985
Met	67	44	66	45	25	283	233	102725	3842
Phe	181	51	58	37	22	332	97	104088	3913
Pro	218	1	21	76	1	1	11	80754	6958
Ser	85	38	28	47	30	370	80	109253	4079
Thr	157	44	34	50	17	155	44	102235	4754
Trp	157	45	86	41	32	356	137	106353	3785
Tyr	178	48	71	45	27	436	334	102222	3838
Val	75	51	31	82	25	176	41	114415	3986

Table S10. Experimental and Calculated Chemical Shifts used for validating the AAXAA peptide system.

	Experimental AAXAA[1] (ppm)		Experimental GGXGG[2] (ppm)				MD Calculated AAXAA (ppm)					
Res	$^{1}H_N$	$^{15}N_H$	$^{1}H\alpha$	Cα	Cβ	C'	$^{1}H_N$	$^{15}N_H$	$^{1}H\alpha$	Cα	Cβ	C'
*Ala	8.29 (H_2O: 8.38)[3]	123.2 (H_2O: 124.2)	4.35 (H_2O: 4.29)	52.8 (H_2O: 52.3)	19.3 (H_2O: 19.3)	178.5 (H_2O: 177.3)	7.97 (H_2O: 8.01)	121.7 (H_2O: 122.0)	4.40 (H_2O: 4.37)	52.7 (H_2O: 52.8)	19.6 (H_2O: 19.3)	177.2 (H_2O: 177.2)
Arg	8.32	120.4	4.38	56.5	30.9	177.1	8.02	119.0	4.39	56.6	31.1	175.9
Asn	8.36	117.4	4.79	53.3	39.1	176.1	8.10	116.7	4.74	53.8	39.3	174.8
Asp	8.38	117.4	4.82	53.0	38.3	175.9	8.09	119.6	4.64	55.0	41.4	175.9
Cys	8.33	117.4	4.59	58.6	28.3	175.3	8.09	116.0	4.66	58.7	28.6	174.2
Gln	8.32	119.2	4.38	56.2	29.5	176.8	8.08	118.8	4.39	56.4	29.8	175.7
Glu	8.27	119.0	4.42	56.1	29.9	176.8	8.17	119.4	4.38	56.9	30.3	176.2
*Gly	8.32	107.8	4.02	45.4	-	174.9	8.13	107.4	4.00	45.6	-	174.2
Hip	8.51	117.3	4.79	55.4	29.1	175.1	8.18	117.4	4.70	56.1	30.0	174.2
Ile	8.10	120.4	4.21	61.6	38.9	177.1	7.75	116.8	4.28	60.7	39.2	175.9
Leu	8.17	121.4	4.38	55.5	42.5	178.2	7.92	120.4	4.40	55.6	42.7	177.1
Met	8.33	119.4	4.52	55.8	32.9	177.1	8.04	118.9	4.54	56.1	33.4	175.9
Phe	8.09	118.8	4.65	58.1	39.8	176.6	8.04	118.6	4.66	58.4	40.2	175.4
Pro	-	-	4.45	63.7	32.2	177.8	-	-	4.46	63.1	32.2	176.9
Ser	8.27	114.1	4.51	58.7	64.1	175.4	8.05	115.0	4.48	58.8	63.9	174.4
Thr	8.06	112.3	4.43	62.0	70.0	175.6	8.03	114.0	4.34	62.8	70.0	174.5
Trp	7.95	119.2	4.70	57.6	29.8	177.1	7.98	119.8	4.72	58.1	30.2	175.7
*Tyr	8.04	118.9	4.58	58.3	38.9	176.7	8.04	119.1	4.63	58.8	39.5	175.5
Val	8.10	119.1	4.16	62.6	31.8	177.0	7.88	118.0	4.19	62.4	33.1	175.8

[1]Prestegard JH *et al.* (2013) Chemical shift prediction for denatured proteins. *J Biomol NMR* 55(2):201–209 (AAXAA, 8M urea at pH 2.5), [2]Schwarzinger S *et al.* (2000) Random coil chemical shifts in acidic 8 M urea: Implementation of random coil shift data in NMRView. *J Biomol NMR* 18:43-48 (GGXGG, 8M urea at 293 K, pH 2.3), [3]Graf J *et al.* (2007) Structure and dynamics of the homologous series of alanine peptides: a joint molecular dynamics/NMR study. *J Am Chem Soc* 129(5):1179–1189 (AAAAA, H_2O at 300 K, pH 2).

*average values calculated over the triplicate simulations for this residue.

Table S11: Backbone propensity library based on the modal ϕ/ψ angles for the central 'X' residue when inhabiting defined regions within a Ramachandran plot.

	Modal Dihedral Angles within Conformational Regions (°)													
	α_R		Near α_R		α_L		nPβ		P_{IIL}		P_{IR}		Global Mode	
'X'	ϕ	ψ	ϕ	ψ	ϕ	ψ	ϕ	ψ	ϕ	ψ	ϕ	ψ	ϕ	ψ
Ala	-93.1	-39.7	-104.8	-38.1	52.6	64.6	-79.4	-176.0	-72.0	149.9	-151.6	61.4	-93.1	-39.7
Arg	-92.4	-41.5	-104.8	-37.9	52.6	69.2	-88.1	-176.1	-78.1	162.2	-119.7	86.3	-92.4	-41.5
Asn	-83.6	-44.0	-104.8	-40.4	52.2	71.1	-76.8	115.7	-68.0	125.1	-119.6	95.5	-83.6	-44.0
Asp	-94.9	-32.6	-104.6	-31.5	52.4	67.9	-91.3	84.9	-77.7	123.5	-147.2	62.7	-94.9	-32.6
Ash	-86.4	-43.0	-104.4	-40.0	52.6	83.8	-71.6	114.8	-70.6	124.3	-152.2	95.5	-86.4	-43.0
Cys	-95.3	-37.9	-104.7	-35.6	52.8	67.2	-73.9	115.7	-74.4	156.4	-131.3	66.1	-97.5	-37.9
Gln	-92.3	-41.0	-104.7	-39.9	53.1	67.7	-77.2	115.6	-74.6	156.7	-119.7	83.2	-92.3	-41.0
Glu	-87.3	-43.8	-104.6	-38.2	52.3	66.8	-81.3	115.9	-78.0	151.3	-126.2	76.3	-87.3	-43.8
Glh	-95.0	-41.0	-111.2	-37.4	54.4	68.9	-79.5	115.1	-77.9	157.3	-125.4	78.0	-95.6	-41.0
Gly	-67.7	-68.6	-104.0	-43.9	68.2	67.2	-75.2	-174.9	-80.7	175.8	-173.1	77.6	76.4	58.2
Hid	-95.2	-39.0	-104.7	-40.2	53.0	71.6	-78.3	115.7	-81.2	147.2	-123.5	82.1	-102.0	-40.2
Hie	-87.7	-41.9	-104.7	-38.8	54.4	68.5	-73.7	115.8	-73.8	157.4	-119.6	92.0	-104.4	-58.5
Hip	-95.7	-38.5	-131.8	-35.3	60.3	64.0	-138.1	104.5	-87.9	162.5	-141.3	67.8	60.3	64.0
Ile	-92.2	-43.1	-118.2	-14.2	53.5	82.1	-114.6	161.3	-72.0	158.6	-130.2	54.2	-72.0	158.6
Leu	-92.8	-41.6	-104.5	-39.5	53.0	68.8	-85.5	116.2	-74.4	153.6	-119.8	94.7	-92.8	-41.6
Lys	-95.0	-39.2	-104.7	-38.3	52.1	69.4	-72.8	116.0	-77.7	161.4	-119.7	87.5	-96.4	-39.2
Met	-94.4	-41.6	-104.7	-38.6	52.3	68.5	-75.3	115.6	-76.6	156.6	-122.6	80.2	-94.4	-41.6
Phe	-92.5	-41.2	-104.9	-39.4	52.5	70.9	-69.4	115.8	-72.2	131.4	-119.7	83.7	-92.5	-41.2
Pro	-60.9	-55.1	-	-	-	-	-64.1	116.2	-63.2	149.1	-	-	-63.2	149.1
Ser	-81.9	-41.6	-104.3	-36.0	51.7	70.2	-77.9	-176.1	-69.7	156.7	-118.6	75.8	-69.7	156.7
Thr	-79.5	-42.7	-104.6	-34.6	46.9	77.8	-71.7	116.1	-70.5	144.2	-118.8	95.7	-79.5	-42.7
Trp	-95.1	-39.9	-104.8	-38.5	53.2	71.5	-75.1	115.5	-72.3	142.2	-119.6	85.2	-100.1	-38.5
Tyr	-95.3	-39.3	-105.0	-38.6	53.2	69.4	-77.7	115.9	-78.9	125.0	-119.6	92.5	-98.7	-39.3
Val	-92.7	-41.3	-104.7	-38.4	52.6	83.6	-114.7	162.7	-73.8	160.1	-119.4	95.7	-73.8	160.1
Mean	-89.2	-42.4	-104.2	-35.7	51.6	68.6	-82.2	127.9	-74.8	149.6	-126.3	78.8		
(±SD)	(8.7)	(6.5)	(19.5)	(9.0)	(11.0)	(14.4)	(16.2)	(27.9)	(4.9)	(13.8)	(25.1)	(19.0)		