Supplementary Data

For

Nature versus Design: The Conformational Propensities of D-amino acids and the Importance of Side Chain Chirality

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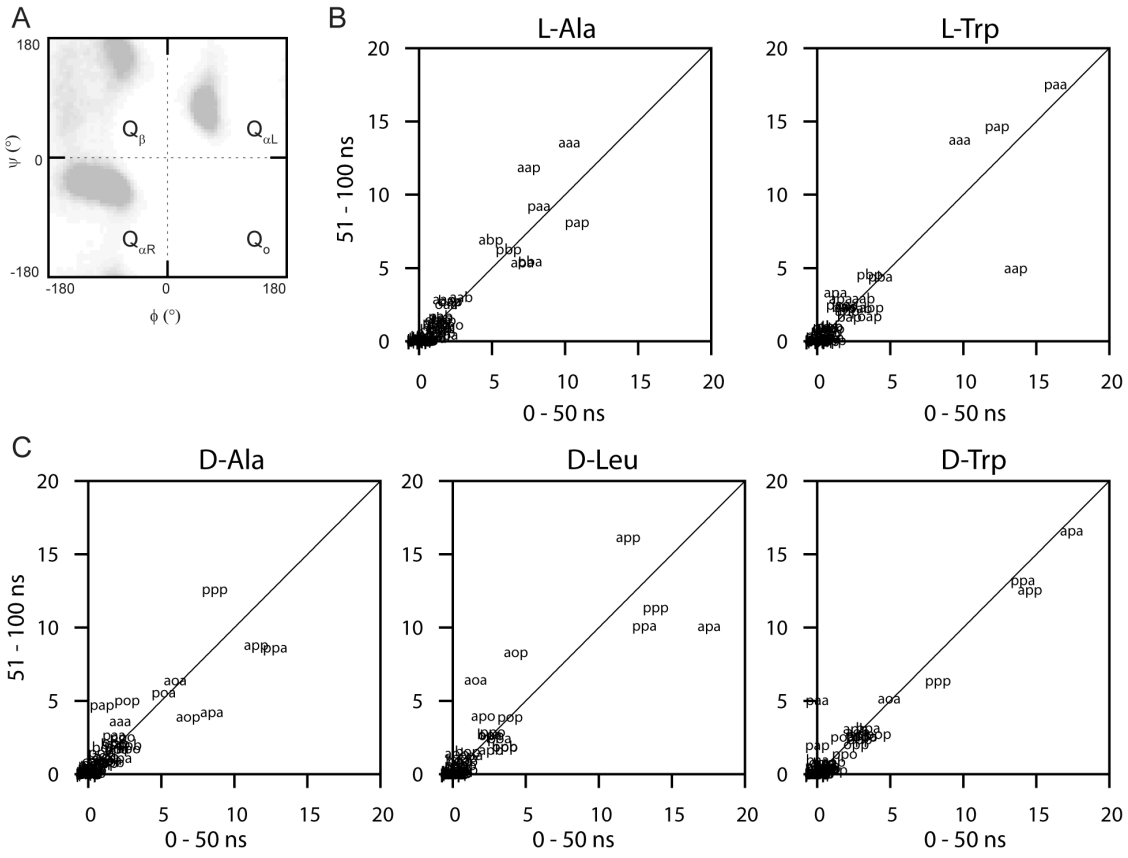

Figure S1. (A) Quadrants of the Ramachandran plot used to assess convergence. (B) Plots of conformational populations of the 64 states in the first and latter portions of the Ala and Trp trajectories. (C) Plots of conformational population of the 64 states in the first and latter portions of pentapeptides containing the D-isomers of Ala, Leu, and Trp. In (B) and (C) the datapoint

labels correspond to the four quadrants in (A) as follows: $Q\alpha_R$ labeled a, $Q\beta$ labeled b, $Q\alpha_L$ labeled p and Q_o labeled o.

Table S1. Correlation coefficients (R) between initial and latter portions of the trajectories for the 64 conformational states populated by the three central residues.

Guest X Residue	L-isomer	D-isomer
Ala-1	0.94	0.89
Ala-2	0.98	0.93
Ala-3	0.93	0.95
Arg-1	0.92	0.93
Arg-2	0.95	-
Asp-1	0.95	0.94
Asp-2	0.98	-
Ash	0.91	0.96
Asn-1	0.92	0.92
Asn-2	0.96	-
Cys-1	0.96	0.99
Cys-2	0.98	-
Gln-1	0.92	0.94
Gln-2	0.75	-
Glu-1	0.94	0.96
Glu-2	0.88	-
Glh	0.88	0.90
Gly-1	0.96	
Gly-2	0.97	
Gly-3	0.96	
Hid-1	0.88	0.90
Hid-2	0.93	-
Hie	0.93	0.95
Hip	0.86	0.92
Ile-1	0.93	0.99
Ile-2	0.88	-
allo-Ile	-	0.91
Leu-1	0.98	0.90
Leu-2	0.91	-
Lys-1	0.93	0.94
Lys-2	0.86	-
Met	0.83	0.97
Phe	0.88	0.93
Pro	0.94	0.98
Ser	0.87	0.95
Thr	0.97	0.94
allo-Thr	-	0.93
Trp	0.91	0.97
Tyr	0.94	0.86
Val	0.90	0.91

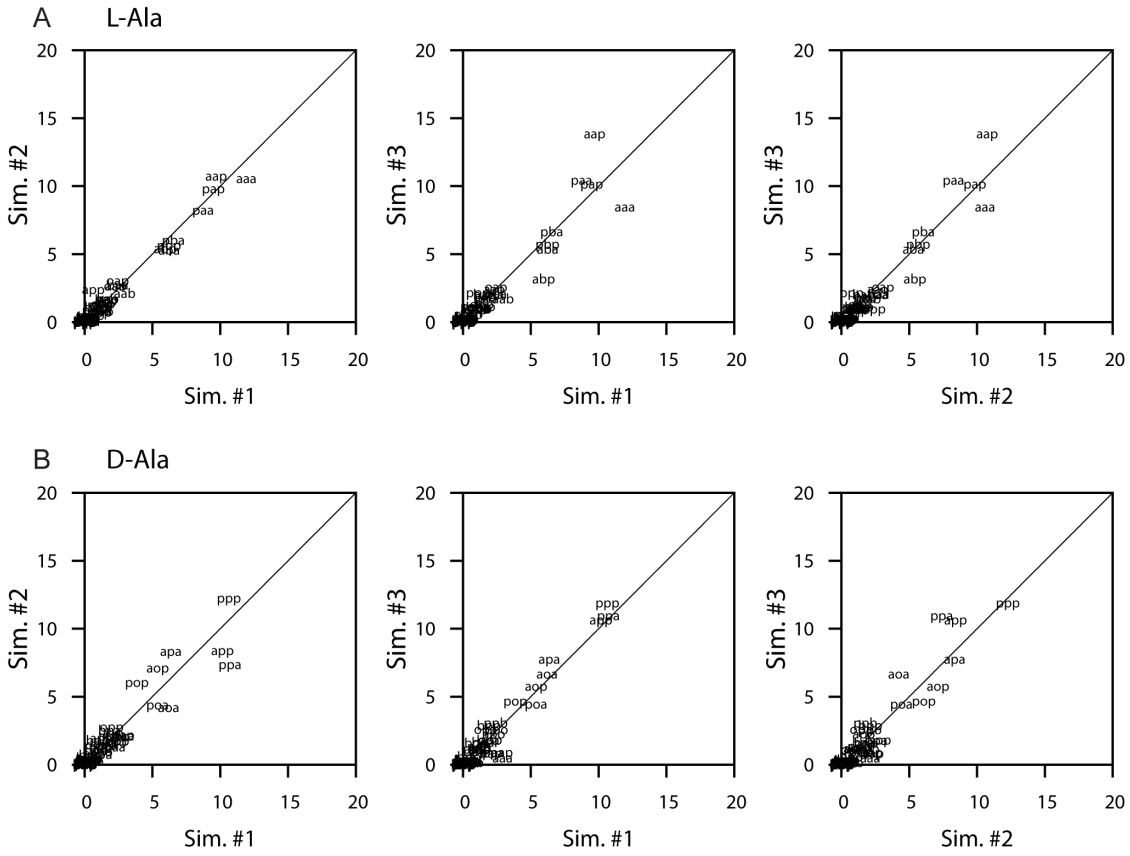

Figure S2. (A) Plots of conformational populations of the 64 states between simulations of L-Ala. (B) Plots of conformational population of the 64 states between simulations of D-Ala. Again, the datapoint labels correspond to one of the four quadrants shown in Fig. S1A as follows: $Q\alpha_R$ labeled a, $Q\beta$ labeled b, $Q\alpha_L$ labeled p and Q_o labeled o.

Table S2. Correlation coefficients (R) between production trajectories from multiple simulations of the same central 'guest' residue.

Guest X Residue	Simulation #1 vs. Simulation #2	Simulation #1 vs. Simulation #3	Simulation #2 vs. Simulation #3
L-Ala	0.99	0.95	0.97
D-Ala	0.95	0.98	0.95
L-Arg	0.98	-	-
L-Asp	0.96	-	-
L-Asn	0.97	-	-
L-Cys	0.96	-	-
L-Gln	0.97	-	-
L-Glu	0.96	-	-
Gly	0.98	0.97	0.94
L-Hid	0.97	-	-
L-Ile	0.89	-	-
L-Leu	0.98	-	-
L-Lys	0.94	-	-

Table S3. Population of the four quadrants of the Ramchandran plot

Guest 'X' Residue	Population Frequency (%)							
	L-amino acids				D-amino acids			
	Q_α	Q_β	$Q_{\alpha L}$	Q_o	Q_α	Q_β	$Q_{\alpha L}$	Q_o
Ala-1	58.5	35.5	5.6	0.4	14.0	0.5	55.0	30.5
Ala-2	59.5	32.9	7.1	0.5	11.9	0.5	54.5	33.1
Ala-3	61.2	30.5	8.0	0.4	5.3	0.3	61.3	33.0
Arg	65.7	26.3	8.0	0.1	8.3	0.1	67.6	24.1
Asn	80.0	18.0	1.9	0.1	4.7	0.1	79.7	15.5
Asp	76.4	17.6	5.9	0.1	12.5	0.1	64.4	22.9
Ash	84.3	12.0	3.5	0.3	11.0	0.2	71.6	17.2
Cys	67.7	25.6	6.5	0.2	13.4	0.2	55.5	30.9
Gln	59.0	26.0	14.8	0.2	7.1	0.1	64.4	28.4
Glu	62.6	30.4	6.3	0.7	3.4	0.1	64.6	31.9
Glh	59.8	27.7	12.5	0.1	6.1	0.1	68.8	25.0
Gly	43.0	9.4	37.4	10.1	-	-	-	-
Hid	64.9	25.7	9.3	0.1	12.0	0.2	63.2	24.5
Hie	68.6	25.9	5.4	0.1	7.5	0.1	62.9	29.6
Hip	63.8	29.7	6.4	0.1	0.1	0.0	66.4	33.4
Ile	54.8	45.1	0.0	0.0	0.4	0.1	61.1	38.3
allo-Ile	-	-	-	-	0.9	0.0	65.2	33.8
Leu	70.7	24.0	5.2	0.1	2.4	0.0	73.7	23.9
Lys	74.1	21.1	4.6	0.1	4.2	0.0	71.3	24.4
Met	66.2	22.6	11.1	0.1	1.5	0.0	69.31	29.19
Phe	71.0	27.5	1.5	0.0	6.7	0.1	71.2	21.9
Pro	19.1	80.9	-	-	-	-	6.8	93.2
Ser	54.2	41.1	4.5	0.2	2.5	0.0	53.0	44.5
Thr	67.9	30.4	1.7	-	0.1	-	74.7	25.1
allo-Thr	-	-	-	-	0.0	-	53.3	46.7
Trp	72.3	20.2	7.3	0.2	5.4	0.1	75.2	19.3
Tyr	63.8	25.9	10.0	0.3	5.7	0.2	74.1	20.0
Val	56.4	39.6	4.0	-	0.3	0.0	47.8	51.9

Table S4. Population of conformational regions by the L- and D-amino acids.

Guest 'X' Residue	Population Frequency (%)													
	L-amino acids							D-amino acids						
	α_R	Near α_R	α_L	nPβ	P_{IIL}	P_{IR}	Other	$D\alpha_R$	Near $D\alpha_R$	$D\alpha_L$	DnPβ	DP_{IIL}	DP_{IR}	Other
Ala-1	23.6	26.2	4.4	10.9	9.1	6.4	19.4	22.4	24.9	11.7	9.1	7.3	6.0	18.7
Ala-2	23.5	27.4	5.7	9.3	7.5	6.7	19.9	22.8	23.8	9.9	9.2	8.9	5.9	19.6
Ala-3	25.0	27.6	6.6	8.5	7.4	5.9	19.0	24.7	28.3	4.1	8.7	7.3	7.0	19.9
Arg	28.1	29.8	7.1	8.3	9.1	3.0	14.5	29.5	30.2	7.4	7.9	8.7	2.4	13.9
Asn	40.2	34.6	1.6	7.6	4.7	2.6	8.5	39.7	34.9	4.1	7.0	3.3	2.7	8.3
Asp	30.6	42.2	5.5	2.4	0.2	4.9	14.2	26.0	35.4	11.9	4.7	0.4	6.4	15.2
Ash	40.0	39.6	3.1	5.4	1.8	2.4	7.7	36.9	31.1	9.9	8.4	3.3	2.8	7.6
Cys	28.6	33.3	5.8	8.5	7.0	3.8	12.9	22.6	26.3	12.1	9.9	10.5	3.6	15.1
Gln	26.7	25.5	13.5	8.6	9.1	2.8	13.8	28.9	28.0	6.5	9.1	10.5	3.2	14.0
Glu	31.8	23.7	5.8	10.0	11.6	2.8	14.4	33.1	24.6	3.0	10.6	11.9	3.0	13.9
Glh	28.2	24.8	11.3	9.4	9.1	3.6	13.6	26.9	33.9	5.5	7.6	6.1	4.2	15.9
Gly	16.7	5.5	9.8	3.4	3.3	1.5	59.9	-	-	-	-	-	-	-
Hid	24.6	33.1	8.1	9.2	7.2	3.6	14.1	24.9	31.8	10.5	9.3	7.2	2.8	13.5
Hie	30.9	30.4	4.7	8.2	10.7	1.8	13.3	29.2	26.7	6.7	10.0	12.3	2.3	12.8
Hip	15.3	41.0	5.4	8.9	2.6	8.4	18.4	12.4	45.6	0.0	9.9	1.8	10.3	20.0
Ile	16.3	29.4	0.0	11.1	19.6	1.6	21.9	15.8	40.7	0.2	13.2	15.3	2.1	12.7
allo-Ile	-	-	-	-	-	-	-	32.7	26.1	0.9	10.9	16.4	1.3	11.7
Leu	35.9	27.4	4.3	8.3	10.5	1.6	11.9	38.2	28.0	2.1	8.1	10.7	1.7	11.2
Lys	32.8	32.8	4.2	7.0	7.0	2.1	14.1	31.7	31.4	3.8	7.9	8.2	2.7	14.3
Met	31.0	27.8	10.2	7.4	7.9	2.6	13.0	31.4	29.5	1.3	10.2	10.7	3.2	13.6
Phe	29.0	35.5	1.3	10.3	9.8	2.8	11.4	29.8	35.1	5.9	7.9	6.8	2.4	12.1
Pro	17.4	-	-	15.8	59.2	-	7.6	4.9	-	-	16.3	70.3	-	8.4
Ser	28.3	17.0	4.0	12.1	21.0	2.1	15.5	27.4	16.0	2.2	12.3	23.8	2.2	16.0
Thr	41.5	21.7	1.6	9.1	14.2	0.9	11.1	47.1	24.0	0.2	6.8	10.9	0.6	10.4
allo-Thr	-	-	-	-	-	-	-	19.0	26.2	0.0	10.9	24.0	2.0	17.9
Trp	30.7	35.2	6.4	6.7	6.0	2.2	12.7	29.9	38.0	4.9	7.3	6.3	1.8	11.8
Tyr	25.3	32.5	8.7	9.7	7.8	2.9	13.2	31.0	36.6	5.2	7.2	6.5	2.1	11.5
Val	21.7	28.3	3.8	11.4	18.6	1.8	14.5	17.2	23.7	0.2	15.4	27.1	1.9	14.5

Table S5. Simulation-to-simulation variability and maximum population differences for replicate simulations of the pentapeptides.

Guest 'X' Residue	Population Frequency (%)					Population Frequency (%)							
	Q_α	Q_β	$Q_{\alpha L}$	Q_o	Max. Δ (%)	α_R	Near α_R	α_L	nPβ	P_{IIL}	P_{IR}	other	Max. Δ (%)
Ala-1	58.50	35.52	5.61	0.37		23.59	26.19	4.42	10.87	9.10	6.42	19.41	
Ala-2	59.55	32.93	7.07	0.45	5.03	23.46	27.44	5.68	9.34	7.50	6.68	19.90	2.34
Ala-3	61.18	30.49	7.95	0.38		24.99	27.56	6.57	8.53	7.45	5.94	18.96	
Arg-1	65.66	26.34	7.95	0.06	5.51	28.11	29.82	7.10	8.35	9.11	3.03	14.48	1.82
Arg-2	69.37	20.83	9.65	0.16		29.66	31.26	8.75	6.70	7.29	2.26	14.07	
Asn-1	79.99	17.99	1.90	0.13	3.24	40.23	34.65	1.62	7.61	4.74	2.62	8.53	1.53
Asn-2	81.76	14.75	3.35	0.14		41.35	34.99	2.95	6.29	3.21	2.62	8.59	
Asp-1	76.36	17.60	5.92	0.13	1.76	30.65	42.24	5.48	2.39	0.18	4.86	14.21	1.62
Asp-2	74.59	18.21	7.05	0.14		30.91	40.62	6.56	3.31	0.31	4.27	14.02	
Cys-1	67.74	25.60	6.49	0.17	4.38	28.63	33.26	5.84	8.49	7.04	3.81	12.93	2.94
Cys-2	72.12	24.28	3.41	0.18		31.10	34.86	2.90	8.65	6.41	3.60	12.48	
Gln-1	59.01	26.01	14.81	0.16	8.65	26.70	25.53	13.52	8.59	9.08	2.82	13.77	4.96
Gln-2	67.66	22.92	9.33	0.09		29.29	30.49	8.60	7.67	6.95	2.66	14.34	
Glu-1	62.61	30.41	6.25	0.73	4.17	31.77	23.68	5.77	9.96	11.60	2.79	14.45	2.91
Glu-2	58.44	32.10	9.32	0.14		29.88	21.67	8.68	11.37	11.87	2.85	13.69	
Gly-1	43.01	9.44	37.43	10.13		16.66	5.51	9.81	3.35	3.32	1.46	59.91	
Gly-2	46.30	9.08	35.62	9.01	9.87	18.19	6.69	9.24	3.07	2.84	1.53	58.44	4.73
Gly-3	36.43	9.80	44.31	9.46		13.46	5.12	12.73	3.54	3.34	1.49	60.33	
Hid-1	64.91	25.66	9.32	0.11	3.18	24.62	33.11	8.12	9.25	7.19	3.58	14.14	2.71
Hid-2	61.78	25.50	12.50	0.22		23.59	31.72	10.83	9.71	6.97	3.34	13.84	
Ile-1	54.85	45.12	0.04	0.00	4.29	16.28	29.42	0.03	11.12	19.58	1.64	21.94	6.15
Ile-2	50.55	48.12	1.32	0.00		18.00	23.58	1.22	12.64	25.73	1.43	17.41	
Leu-1	70.67	24.02	5.16	0.15	2.74	35.94	27.39	4.33	8.33	10.50	1.62	11.90	1.74
Leu-2	73.08	21.28	5.56	0.08		36.81	29.13	5.03	7.56	9.24	1.41	10.84	
Lys-1	74.14	21.13	4.62	0.12	6.14	32.79	32.80	4.24	6.97	7.04	2.10	14.07	2.92
Lys-2	68.01	24.87	6.96	0.17		30.36	29.88	6.18	8.54	8.81	2.60	13.63	
D-Ala-1	14.02	0.49	54.95	30.54		22.42	24.86	11.72	9.06	7.30	5.98	18.67	
D-Ala-2	11.94	0.46	54.47	33.13	8.70	22.75	23.82	9.87	9.21	8.85	5.94	19.56	7.63
D-Ala-3	5.33	0.32	61.32	33.03		24.75	28.26	4.09	8.75	7.27	6.98	19.91	

Table S6. Effect Size Analysis of the ϕ/ψ distributions within defined conformational regions for the guest residues in replicate simulations.

	Difference between Means		Pooled Standard Deviations		Effect Size	
Sim #1/Sim #2	**ϕ**	**ψ**	**ϕ**	**ψ**	**ϕ**	**ψ**
Ala-1/Ala-2 α_L	0.25	0.62	11.85	19.38	0.02	0.03
Ala-1/Ala-2 α_R	0.29	0.03	13.06	15.27	0.02	0.00
Ala-1/Ala-2 β	0.17	2.51	32.24	27.41	0.01	0.09
Ala-1/Ala-2 nα_R	0.27	0.05	19.02	12.65	0.01	0.00
Ala-1/Ala-2 o	2.61	0.73	40.56	60.42	0.06	0.01
Ala-1/Ala-2 P_{IIL}	0.40	0.17	14.15	15.34	0.03	0.01
Ala-1/Ala-2 P_{IR}	0.22	0.47	15.85	13.95	0.01	0.03
Ala-1/Ala-3 α_L	0.14	0.73	12.61	20.60	0.01	0.04
Ala-1/Ala-3 α_R	0.10	0.76	13.27	15.39	0.01	0.05
Ala-1/Ala-3 β	2.34	1.15	31.45	27.38	0.07	0.04
Ala-1/Ala-3 nα_R	0.22	0.02	18.90	12.64	0.01	0.00
Ala-1/Ala-3 o	1.32	3.10	40.71	60.21	0.03	0.05
Ala-1/Ala-3 P_{IIL}	0.57	1.53	14.08	15.23	0.04	0.10
Ala-1/Ala-3 P_{IR}	0.47	0.18	15.46	13.58	0.03	0.01
Ala-2/Ala-3 α_L	0.11	0.11	11.62	18.96	0.01	0.01
Ala-2/Ala-3 α_R	0.20	0.73	13.26	15.54	0.01	0.05
Ala-2/Ala-3 β	2.17	3.66	32.93	27.97	0.07	0.13
Ala-2/Ala-3 nα_R	0.49	0.02	18.77	12.55	0.03	0.00
Ala-2/Ala-3 o	1.29	2.37	40.69	58.96	0.03	0.04
Ala-2/Ala-3 P_{IIL}	0.18	1.36	14.70	15.93	0.01	0.09
Ala-2/Ala-3 P_{IR}	0.25	0.29	15.17	13.37	0.02	0.02
Arg-1/Arg-2 α_L	0.20	0.42	11.47	18.91	0.02	0.02
Arg-1/Arg-2 α_R	0.23	0.81	12.45	14.88	0.02	0.05
Arg-1/Arg-2 β	1.30	2.54	25.96	27.32	0.05	0.09
Arg-1/Arg-2 nα_R	0.40	0.26	14.27	12.44	0.03	0.02
Arg-1/Arg-2 o	0.25	13.83	37.98	59.97	0.01	0.23
Arg-1/Arg-2 P_{IIL}	0.75	1.21	14.03	14.83	0.05	0.08
Arg-1/Arg-2 P_{IR}	0.78	0.74	12.31	13.28	0.06	0.06
Asn-1/Asn-2 α_L	2.09	5.87	13.64	21.51	0.15	0.27
Asn-1/Asn-2 α_R	0.23	0.45	12.71	12.69	0.02	0.04
Asn-1/Asn-2 β	0.34	0.17	31.23	18.44	0.01	0.01
Asn-1/Asn-2 nα_R	0.27	0.29	17.63	11.19	0.02	0.03
Asn-1/Asn-2 o	2.80	5.04	35.86	54.94	0.08	0.09
Asn-1/Asn-2 P_{IIL}	1.81	0.85	13.66	13.71	0.13	0.06
Asn-1/Asn-2 P_{IR}	0.40	0.92	15.87	13.84	0.02	0.07
Asp-1/Asp-2 α_L	0.00	0.62	11.65	16.64	0.00	0.04
Asp-1/Asp-2 α_R	0.19	0.26	11.52	12.42	0.02	0.02

	Difference between Means		Pooled Standard Deviations		Effect Size	
Sim #1/Sim #2	**ϕ**	**ψ**	**ϕ**	**ψ**	**ϕ**	**ψ**
Asp-1/Asp-2 β	3.22	0.49	30.62	13.67	0.11	0.04
Asp-1/Asp-2 $n\alpha_R$	0.38	0.22	17.65	11.23	0.02	0.02
Asp-1/Asp-2 o	3.11	2.96	30.56	29.77	0.10	0.10
Asp-1/Asp-2 P_{IIL}	0.70	0.56	16.71	8.87	0.04	0.06
Asp-1/Asp-2 P_{IR}	2.30	0.80	15.11	12.88	0.15	0.06
Cys-1/Cys-2 α_L	0.63	7.98	9.83	15.57	0.06	0.51
Cys-1/Cys-2 α_R	0.02	0.32	12.96	13.96	0.00	0.02
Cys-1/Cys-2 β	3.19	2.23	31.83	26.50	0.10	0.08
Cys-1/Cys-2 $n\alpha_R$	0.45	0.03	17.70	12.22	0.03	0.00
Cys-1/Cys-2 o	0.67	6.18	36.22	54.16	0.02	0.11
Cys-1/Cys-2 P_{IIL}	0.80	1.08	14.74	15.51	0.05	0.07
Cys-1/Cys-2 P_{IR}	0.64	0.77	15.36	14.02	0.04	0.05
Gln-1/Gln-2 α_L	0.02	1.57	9.84	16.33	0.00	0.10
Gln-1/Gln-2 α_R	0.28	0.43	12.90	15.21	0.02	0.03
Gln-1/Gln-2 β	3.91	3.86	25.67	26.62	0.15	0.15
Gln-1/Gln-2 $n\alpha_R$	0.39	0.15	14.86	12.80	0.03	0.01
Gln-1/Gln-2 o	2.89	9.20	40.57	61.30	0.07	0.15
Gln-1/Gln-2 P_{IIL}	0.58	0.54	13.75	14.75	0.04	0.04
Gln-1/Gln-2 P_{IR}	0.75	0.34	12.40	13.81	0.06	0.02
Glu-1/Glu-2 α_L	0.91	1.89	12.38	19.40	0.07	0.10
Glu-1/Glu-2 α_R	0.18	0.73	12.25	15.00	0.02	0.05
Glu-1/Glu-2 β	0.82	1.38	28.02	28.18	0.03	0.05
Glu-1/Glu-2 $n\alpha_R$	0.14	0.25	13.85	12.11	0.01	0.02
Glu-1/Glu-2 o	0.29	10.30	38.84	62.07	0.01	0.17
Glu-1/Glu-2 P_{IIL}	0.81	0.59	14.43	15.74	0.06	0.04
Glu-1/Glu-2 P_{IR}	0.42	1.25	12.82	14.02	0.03	0.09
Gly-1/Gly-2 α_L	0.07	0.77	8.82	19.18	0.01	0.04
Gly-1/Gly-2 α_R	0.08	0.36	13.85	15.48	0.01	0.02
Gly-1/Gly-2 β	0.58	0.33	36.34	34.16	0.02	0.01
Gly-1/Gly-2 $n\alpha_R$	0.21	0.29	22.68	13.59	0.01	0.02
Gly-1/Gly-2 o	11.55	31.29	67.86	78.80	0.17	0.40
Gly-1/Gly-2 P_{IIL}	0.44	0.30	13.64	16.24	0.03	0.02
Gly-1/Gly-2 P_{IR}	0.12	1.03	17.36	14.21	0.01	0.07
Gly-1/Gly-3 α_L	0.19	0.89	9.66	20.95	0.02	0.04
Gly-1/Gly-3 α_R	0.09	1.05	12.90	14.52	0.01	0.07
Gly-1/Gly-3 β	0.38	0.17	37.45	35.22	0.01	0.00
Gly-1/Gly-3 $n\alpha_R$	0.39	0.38	21.18	12.69	0.02	0.03
*Gly-1/Gly-3 o	8.52	161.75	66.22	78.82	0.13	2.05
Gly-1/Gly-3 P_{IIL}	0.15	0.42	14.06	17.01	0.01	0.02
Gly-1/Gly-3 P_{IR}	0.43	1.75	17.14	14.29	0.03	0.12

	Difference between Means		Pooled Standard Deviations		Effect Size	
Sim #1/Sim #2	**ϕ**	**ψ**	**ϕ**	**ψ**	**ϕ**	**ψ**
Gly-2/Gly-3 α_L	0.12	0.12	8.40	18.09	0.01	0.01
Gly-2/Gly-3 α_R	0.01	0.70	14.80	16.67	0.00	0.04
Gly-2/Gly-3 β	0.95	0.15	36.09	33.70	0.03	0.00
Gly-2/Gly-3 nα_R	0.18	0.08	23.21	13.84	0.01	0.01
*Gly-2/Gly-3 o	20.07	130.46	65.81	77.70	0.30	1.68
Gly-2/Gly-3 P_{IIL}	0.30	0.12	13.59	16.35	0.02	0.01
Gly-2/Gly-3 P_{IR}	0.32	0.71	16.98	14.10	0.02	0.05
Hid-1/Hid-2 α_L	0.15	1.50	11.47	20.40	0.01	0.07
Hid-1/Hid-2 α_R	0.02	0.45	11.96	14.06	0.00	0.03
Hid-1/Hid-2 β	2.26	5.23	29.06	25.56	0.08	0.20
Hid-1/Hid-2 nα_R	0.06	0.50	15.71	12.09	0.00	0.04
Hid-1/Hid-2 o	1.48	3.55	44.45	61.39	0.03	0.06
Hid-1/Hid-2 P_{IIL}	2.56	4.34	15.00	15.64	0.17	0.28
Hid-1/Hid-2 P_{IR}	0.40	1.26	14.49	14.00	0.03	0.09
Ile-1/Ile-2 α_L	24.28	8.23	50.90	65.25	0.48	0.13
Ile-1/Ile-2 α_R	0.57	3.25	11.29	16.01	0.05	0.20
Ile-1/Ile-2 β	1.24	4.23	22.48	27.21	0.06	0.16
Ile-1/Ile-2 nα_R	1.83	2.58	12.05	12.07	0.15	0.21
Ile-1/Ile-2 o	2.52	0.97	22.07	41.87	0.11	0.02
Ile-1/Ile-2 P_{IIL}	0.98	1.36	16.00	14.79	0.06	0.09
Ile-1/Ile-2 P_{IR}	0.13	0.70	10.43	13.59	0.01	0.05
Leu-1/Leu-2 α_L	0.54	5.55	11.46	18.44	0.05	0.30
Leu-1/Leu-2 α_R	0.32	0.69	12.67	14.40	0.03	0.05
Leu-1/Leu-2 β	1.84	3.00	25.03	25.98	0.07	0.12
Leu-1/Leu-2 nα_R	0.36	0.36	14.06	12.04	0.03	0.03
Leu-1/Leu-2 o	0.87	3.72	37.09	61.02	0.02	0.06
Leu-1/Leu-2 P_{IIL}	0.53	0.95	14.14	15.34	0.04	0.06
Leu-1/Leu-2 P_{IR}	0.30	0.17	12.81	13.83	0.02	0.01
Lys-1/Lys-2 α_L	0.07	2.13	12.19	20.01	0.01	0.11
Lys-1/Lys-2 α_R	0.23	0.13	12.12	14.45	0.02	0.01
Lys-1/Lys-2 β	2.49	2.17	28.30	29.75	0.09	0.07
Lys-1/Lys-2 nα_R	0.54	0.24	13.49	11.88	0.04	0.02
Lys-1/Lys-2 o	0.60	4.58	34.38	58.40	0.02	0.08
Lys-1/Lys-2 P_{IIL}	0.69	0.15	15.67	16.64	0.04	0.01
Lys-1/Lys-2 P_{IR}	0.74	0.89	13.14	15.00	0.06	0.06

*o pertains to anywhere on the Ramachandran plot (the "other" region) that does not fall within well-defined conformational regions. Hence, due to the large area and multimodal natures of these distributions, the effect size is misleading. As the interest is in determining the size of an

effect between the sampling of the defined conformational regions, these were excluded from defining a threshold value.

Table S7. Effect Size Analysis of the L versus D ϕ/ψ distributions within defined conformational regions of the Ramachandran plot for the pentapeptide guest residues.

	L-amino acids				D-amino acids				Difference between Means		Pooled Standard Deviations		Effect Size	
	Mean		Standard Deviation		Mean		Standard Deviation							
State	ϕ	ψ	ϕ	ψ	ϕ	ψ	ϕ	ψ	ϕ	ψ	ϕ	ψ	ϕ	ψ
Ala-1 α_L	52.8	75.2	11.2	18.4	-52.3	-73.9	11.3	18.7	0.4	1.2	11.3	18.6	0.04	0.07
Ala-1 α_R	-79.8	-45.1	13.1	15.2	79.9	45.2	13.0	15.3	0.2	0.2	13.0	15.2	0.01	0.01
Ala-1 β	-117.6	128.3	33.1	28.8	113.9	-124.8	33.8	28.2	3.7	3.5	33.4	28.5	0.11	0.12
Ala-1 nα_R	-129.0	-32.1	18.7	12.5	128.8	31.8	18.6	12.4	0.2	0.3	18.7	12.4	0.01	0.03
Ala-1 o	-126.5	1.1	40.1	60.9	129.9	-5.7	49.2	62.6	3.4	4.7	44.8	61.8	0.08	0.08
Ala-1 P_{IIL}	-77.9	148.4	14.8	16.1	77.3	-147.5	14.8	16.1	0.5	0.8	14.8	16.1	0.04	0.05
Ala-1 P_{IR}	-148.7	72.7	15.8	13.9	149.1	-72.7	15.7	13.9	0.4	0.0	15.8	13.9	0.02	0.00
Arg-1 α_L	52.5	77.6	10.9	18.1	-52.2	-77.3	11.1	17.7	0.3	0.2	11.0	17.9	0.03	0.01
Arg-1 α_R	-82.2	-45.6	12.2	14.7	81.9	45.9	12.3	14.8	0.3	0.3	12.3	14.7	0.02	0.02
Arg-1 β	-109.7	125.2	27.3	28.1	110.8	-128.4	26.8	29.2	1.1	3.2	27.1	28.6	0.04	0.11
Arg-1 nα_R	-120.8	-33.0	13.9	12.3	120.8	33.4	13.9	12.2	0.0	0.4	13.9	12.2	0.00	0.03
Arg-1 o	-114.3	-14.2	37.6	60.2	113.1	20.0	38.1	60.7	1.3	5.8	37.8	60.4	0.03	0.10
Arg-1 P_{IIL}	-79.5	148.5	14.9	15.6	79.9	-149.1	14.8	15.6	0.5	0.6	14.9	15.6	0.03	0.04
Arg-1 P_{IR}	-136.1	74.1	13.4	14.2	134.4	-74.2	12.6	14.0	1.7	0.1	13.0	14.1	0.13	0.01
Ash-1 α_L	53.4	83.9	11.5	17.6	-52.7	-82.4	11.5	18.1	0.6	1.6	11.5	18.0	0.05	0.09
Ash-1 α_R	-80.5	-44.3	12.5	12.2	79.0	43.3	13.1	12.5	1.5	1.1	12.8	12.3	0.12	0.09
Ash-1 β	-106.7	109.6	33.6	13.0	107.3	-111.3	34.5	13.6	0.6	1.7	34.2	13.4	0.02	0.13
Ash-1 nα_R	-127.2	-35.5	18.5	10.9	126.6	35.2	18.3	11.1	0.6	0.3	18.4	11.0	0.03	0.03
Ash-1 o	-129.8	-29.2	37.4	51.2	125.1	5.2	52.4	62.9	4.6	24.0	45.4	57.3	0.10	0.42
Ash-1 P_{IIL}	-76.1	130.9	14.7	9.3	75.7	-131.8	14.6	9.8	0.4	0.9	14.6	9.6	0.03	0.09
Ash-1 P_{IR}	-146.9	78.9	15.5	13.6	147.0	-80.5	16.0	13.5	0.0	1.6	15.7	13.6	0.00	0.12
Asn-1 α_L	50.5	76.2	11.8	19.4	-53.2	-80.6	11.2	18.3	2.6	4.5	11.4	18.6	0.23	0.24
Asn-1 α_R	-80.4	-44.9	12.6	12.7	80.0	45.5	12.7	12.4	0.3	0.6	12.6	12.6	0.03	0.05
Asn-1 β	-106.9	113.8	32.4	19.0	104.4	-112.0	32.4	17.1	2.5	1.9	32.4	18.1	0.08	0.10
Asn-1 nα_R	-125.0	-35.5	17.5	11.2	125.9	35.7	17.8	11.1	1.0	0.2	17.7	11.2	0.06	0.01
Asn-1 o	-120.5	-26.2	35.4	55.8	123.1	29.6	40.2	56.2	2.6	3.4	37.9	56.0	0.07	0.06
Asn-1 P_{IIL}	-76.5	139.0	14.9	14.6	77.3	-138.2	14.7	14.5	0.8	0.8	14.8	14.6	0.05	0.05
Asn-1 P_{IR}	-145.9	78.8	15.9	13.8	146.7	-78.5	15.8	13.7	0.7	0.3	15.9	13.7	0.04	0.03
Asp-1 α_L	51.8	72.6	11.1	15.7	-51.5	-72.8	11.2	15.9	0.3	0.1	11.2	15.8	0.03	0.01
Asp-1 α_R	-83.0	-34.5	11.6	12.4	83.0	34.0	11.4	12.4	0.0	0.5	11.5	12.4	0.00	0.04
Asp-1 β	-98.6	101.4	29.1	12.3	94.3	-101.0	27.5	11.8	4.2	0.3	28.0	12.0	0.15	0.03
Asp-1 nα_R	-126.2	-27.5	17.8	11.4	126.6	27.3	18.0	11.4	0.3	0.2	17.9	11.4	0.02	0.02
Asp-1 o	-129.1	17.3	29.8	29.2	129.0	-23.4	33.4	30.6	0.2	6.1	31.7	29.9	0.01	0.20
Asp-1 P_{IIL}	-77.4	128.2	14.1	7.1	78.1	-128.3	14.6	7.2	0.7	0.0	14.4	7.2	0.05	0.01
Asp-1 P_{IR}	-147.5	70.9	15.4	13.1	145.7	-71.1	15.5	13.3	1.8	0.2	15.5	13.2	0.11	0.01
Cys-1 α_L	51.9	70.5	11.3	18.3	-51.9	-73.1	11.1	18.3	0.0	2.6	11.2	18.3	0.00	0.14

	L-amino acids				D-amino acids				Difference between Means		Pooled Standard Deviations		Effect Size	
	Mean		Standard Deviation		Mean		Standard Deviation							
State	ϕ	ψ	ϕ	ψ	ϕ	ψ	ϕ	ψ	ϕ	ψ	ϕ	ψ	ϕ	ψ
Cys-1 α_R	-80.8	-43.9	12.8	13.8	81.8	42.9	12.5	14.9	1.0	1.1	12.6	14.3	0.08	0.07
Cys-1 β	-116.6	125.0	31.8	26.7	111.2	-128.6	28.8	29.0	5.4	3.6	30.2	28.0	0.18	0.13
Cys-1 nα_R	-126.1	-33.0	17.3	12.1	123.2	31.0	15.6	12.4	2.9	2.1	16.6	12.2	0.18	0.17
Cys-1 o	-124.6	-1.5	37.8	54.9	118.5	-7.8	43.3	60.5	6.1	9.3	40.9	58.0	0.15	0.16
Cys-1 P_{IIL}	-78.0	147.6	15.1	15.8	79.6	-149.2	14.9	15.8	1.6	1.7	15.0	15.8	0.11	0.10
Cys-1 P_{IR}	-144.1	74.2	15.6	14.2	140.1	-73.3	14.9	14.2	4.0	0.9	15.2	14.2	0.26	0.06
Glh-1 α_L	53.1	75.9	10.5	18.4	-53.6	-74.0	10.6	18.0	0.5	1.9	10.5	18.3	0.05	0.10
Glh-1 α_R	-81.0	-46.4	12.4	14.6	82.0	45.5	12.3	14.9	1.0	0.9	12.4	14.7	0.08	0.06
Glh-1 β	-107.2	122.7	26.5	26.5	113.5	-124.9	27.7	27.5	6.3	2.2	27.0	26.9	0.23	0.08
Glh-1 nα_R	-121.2	-33.1	14.0	12.4	122.8	32.4	14.4	12.4	1.6	0.7	14.2	12.4	0.11	0.05
Glh-1 o	-117.3	-8.8	42.2	60.8	119.0	11.6	33.2	55.3	1.7	2.8	37.6	57.9	0.05	0.05
Glh-1 P_{IIL}	-81.3	146.2	14.6	15.7	80.3	-147.8	14.8	15.6	1.0	1.7	14.7	15.7	0.07	0.11
Glh-1 P_{IR}	-137.3	73.3	13.1	14.2	137.0	-73.4	12.8	14.1	0.2	0.0	12.9	14.2	0.02	0.00
Gln-1 α_L	52.6	73.8	10.8	18.4	-52.4	-75.0	10.8	17.7	0.2	1.2	10.8	18.2	0.02	0.07
Gln-1 α_R	-81.1	-45.3	12.6	15.0	81.4	45.6	12.5	14.8	0.4	0.3	12.6	14.9	0.03	0.02
Gln-1 β	-104.9	120.3	25.7	26.7	106.4	-124.0	26.4	28.2	1.6	3.7	26.1	27.4	0.06	0.14
Gln-1 nα_R	-121.2	-33.1	14.1	12.3	120.9	33.0	13.9	12.2	0.3	0.1	14.0	12.3	0.02	0.01
Gln-1 o	-111.9	-9.2	44.0	62.6	112.3	12.8	35.0	60.7	0.3	3.6	39.8	61.7	0.01	0.06
Gln-1 P_{IIL}	-80.0	147.0	14.5	15.6	80.0	-148.5	14.6	15.7	0.0	1.5	14.6	15.7	0.00	0.10
Gln-1 P_{IR}	-135.2	74.9	12.4	13.9	135.4	-74.7	12.7	14.1	0.2	0.2	12.6	14.0	0.02	0.01
Glu-1 α_L	52.3	75.9	10.8	16.9	-52.1	-76.7	11.1	17.7	0.2	0.7	10.9	17.2	0.02	0.04
Glu-1 α_R	-80.3	-46.1	12.5	15.1	80.6	45.5	12.4	15.2	0.3	0.6	12.4	15.2	0.03	0.04
Glu-1 β	-103.3	121.4	27.9	27.6	98.9	-118.0	26.0	26.1	4.4	3.4	26.1	26.8	0.16	0.13
Glu-1 nα_R	-120.8	-32.3	14.0	12.4	120.8	32.4	14.3	12.3	0.0	0.1	14.2	12.4	0.00	0.01
Glu-1 o	-108.4	-16.7	41.6	62.6	108.7	7.2	33.3	61.1	0.3	9.5	37.8	61.9	0.01	0.15
Glu-1 P_{IIL}	-78.6	147.2	14.2	15.8	78.8	-146.9	14.3	15.6	0.1	0.3	14.3	15.7	0.01	0.02
Glu-1 P_{IR}	-134.9	74.0	12.5	14.0	135.4	-74.4	13.0	14.1	0.5	0.4	12.7	14.0	0.04	0.03
Hid-1 α_L	53.7	77.0	10.5	18.6	-52.8	-77.9	11.0	18.1	0.9	0.9	10.7	18.4	0.08	0.05
Hid-1 α_R	-82.6	-44.5	12.1	14.4	80.6	44.6	12.7	14.7	2.0	0.1	12.5	14.6	0.16	0.01
Hid-1 β	-114.1	125.1	27.7	26.8	109.9	-127.1	29.9	28.1	4.2	2.0	28.9	27.5	0.14	0.07
Hid-1 nα_R	-123.7	-32.7	15.9	12.3	123.2	32.7	16.3	12.3	0.5	0.0	16.1	12.3	0.03	0.00
Hid-1 o	-120.4	-9.0	41.0	59.6	112.3	11.2	40.9	64.3	8.0	2.2	41.0	61.8	0.20	0.03
Hid-1 P_{IIL}	-82.5	146.7	15.0	16.2	78.3	-147.8	14.8	15.7	4.1	1.1	14.9	15.9	0.28	0.07
Hid-1 P_{IR}	-139.2	75.1	14.5	14.2	139.0	-75.8	14.8	14.5	0.2	0.7	14.6	14.3	0.01	0.05
Hie-1 α_L	52.9	78.7	11.2	19.0	-53.2	-78.0	10.8	18.4	0.4	0.7	10.9	18.6	0.04	0.04
Hie-1 α_R	-81.1	-44.4	12.4	14.7	82.6	44.7	12.2	14.3	1.5	0.4	12.3	14.5	0.12	0.03
Hie-1 β	-111.4	128.0	30.4	28.1	110.6	-122.0	30.3	24.8	0.8	6.0	30.4	26.4	0.03	0.23
Hie-1 nα_R	-124.0	-31.8	16.6	12.5	123.8	33.1	15.9	12.1	0.3	1.3	16.3	12.3	0.02	0.11
Hie-1 o	-115.2	-13.9	39.3	60.3	119.5	9.3	46.9	62.7	4.2	4.6	43.3	61.5	0.10	0.08

	L-amino acids				D-amino acids				Difference between Means		Pooled Standard Deviations		Effect Size	
	Mean		Standard Deviation		Mean		Standard Deviation							
State	ϕ	ψ	ϕ	ψ	ϕ	ψ	ϕ	ψ	ϕ	ψ	ϕ	ψ	ϕ	ψ
Hie-1 P_{IIL}	-78.4	148.8	14.6	15.6	80.2	-142.9	15.2	15.6	1.8	5.9	14.8	15.6	0.12	0.38
Hie-1 P_{IR}	-140.6	75.9	15.5	14.3	140.7	-75.3	15.5	14.6	0.0	0.5	15.5	14.5	0.00	0.04
Hip-1 α_L	49.3	78.1	12.5	17.6	-	-	-		-	-	-	-	-	-
Hip-1 α_R	-82.8	-41.8	11.9	14.2	83.8	42.4	12.0	14.2	1.0	0.6	11.9	14.2	0.08	0.04
Hip-1 β	-132.5	131.9	23.5	25.3	133.1	-130.6	22.4	25.0	0.6	1.3	22.9	25.2	0.03	0.05
Hip-1 nα_R	-130.5	-32.0	15.5	12.4	130.7	31.8	15.2	12.4	0.2	0.2	15.4	12.4	0.02	0.02
Hip-1 o	-134.2	1.1	30.1	49.3	134.1	1.0	18.4	45.5	0.1	2.1	24.7	47.4	0.00	0.04
Hip-1 P_{IIL}	-83.2	147.9	15.4	16.2	86.2	-145.8	14.7	16.1	3.0	2.0	15.1	16.2	0.20	0.13
Hip-1 P_{IR}	-143.3	72.7	12.5	13.9	142.0	-72.8	12.2	14.0	1.3	0.1	12.4	14.0	0.10	0.01
Leu-1 α_L	52.5	82.6	11.1	17.9	-53.1	-79.4	11.0	18.1	0.6	3.2	11.0	18.0	0.06	0.18
Leu-1 α_R	-80.7	-45.9	12.6	14.4	80.9	46.3	12.5	14.2	0.2	0.4	12.5	14.3	0.02	0.03
Leu-1 β	-101.6	121.6	25.2	27.5	103.7	-120.6	26.3	26.1	2.2	1.1	25.8	26.8	0.08	0.04
Leu-1 nα_R	-119.2	-34.5	14.0	11.9	118.9	34.6	13.9	11.9	0.2	0.1	14.0	11.9	0.02	0.01
Leu-1 o	-107.3	-33.9	40.0	64.7	107.3	38.3	31.1	59.8	0.0	4.4	36.0	62.4	0.00	0.07
Leu-1 P_{IIL}	-80.4	147.2	14.7	15.9	80.2	-147.2	14.7	15.7	0.2	0.0	14.7	15.8	0.01	0.00
Leu-1 P_{IR}	-133.4	76.3	12.8	14.3	136.1	-77.1	14.3	14.4	2.7	0.8	13.6	14.3	0.20	0.05
Lys-1 α_L	52.6	75.6	11.0	18.5	-52.6	-79.4	11.1	17.8	0.0	3.8	11.0	18.1	0.00	0.21
Lys-1 α_R	-81.7	-46.0	12.3	14.7	81.4	45.5	12.5	14.6	0.2	0.5	12.4	14.7	0.02	0.03
Lys-1 β	-110.3	127.1	26.8	28.5	107.5	-124.6	26.0	28.3	2.8	2.5	26.4	28.4	0.10	0.09
Lys-1 nα_R	-120.8	-33.7	13.9	12.1	121.0	33.4	14.2	12.2	0.2	0.2	14.0	12.2	0.01	0.02
Lys-1 o	-113.2	-28.0	31.2	56.8	114.1	20.0	31.7	58.5	0.9	8.0	31.5	57.6	0.03	0.14
Lys-1 P_{IIL}	-80.6	148.2	14.8	15.6	80.5	-148.1	14.8	15.9	0.2	0.1	14.8	15.8	0.01	0.01
Lys-1 P_{IR}	-134.1	73.9	12.3	14.3	135.0	-74.1	13.2	14.3	0.9	0.2	12.8	14.3	0.07	0.02
Met-1 α_L	52.4	74.0	10.8	17.6	-52.4	-78.7	11.1	17.5	0.0	4.7	10.8	17.6	0.00	0.27
Met-1 α_R	-81.2	-46.2	12.6	14.7	82.0	46.1	12.2	14.6	0.8	0.1	12.4	14.6	0.07	0.01
Met-1 β	-104.8	120.9	25.6	27.1	108.5	-124.7	26.4	28.1	3.7	3.8	26.0	27.7	0.14	0.14
Met-1 nα_R	-120.2	-33.5	14.0	12.2	120.1	33.6	13.9	12.1	0.1	0.2	14.0	12.2	0.01	0.02
Met-1 o	-112.2	-22.3	38.8	60.3	112.3	26.0	27.3	59.0	0.0	3.8	33.4	59.6	0.00	0.06
Met-1 P_{IIL}	-80.8	147.2	14.6	15.9	81.0	-147.9	14.7	15.7	0.3	0.6	14.7	15.8	0.02	0.04
Met-1 P_{IR}	-135.1	74.6	12.9	14.2	134.7	-74.8	12.9	14.2	0.4	0.2	12.9	14.2	0.03	0.01
Phe-1 α_L	51.5	75.4	11.7	18.0	-52.6	-78.6	10.5	17.8	1.1	3.2	10.8	17.9	0.10	0.18
Phe-1 α_R	-82.3	-43.6	12.2	13.9	82.8	43.9	11.9	13.7	0.5	0.3	12.0	13.8	0.04	0.02
Phe-1 β	-114.4	126.0	28.8	26.0	111.9	-123.6	30.4	25.2	2.5	2.4	29.5	25.7	0.09	0.09
Phe-1 nα_R	-123.5	-33.0	16.0	12.0	122.9	33.2	15.8	12.0	0.6	0.2	15.9	12.0	0.04	0.02
Phe-1 o	-117.1	-15.4	29.9	56.3	119.0	13.6	40.0	58.9	1.8	1.8	35.4	57.7	0.05	0.03
Phe-1 P_{IIL}	-81.0	146.8	15.0	15.9	79.6	-144.3	15.0	15.4	1.4	2.4	15.0	15.7	0.10	0.16
Phe-1 P_{IR}	-140.3	76.8	15.2	14.4	138.9	-74.8	14.5	14.6	1.4	2.0	14.9	14.5	0.09	0.14
Pro-1 α_R	-63.0	-49.6	8.9	13.4	63.0	48.5	9.1	13.7	0.1	1.1	9.0	13.5	0.01	0.08
Pro-1 β	-67.2	113.7	9.0	19.8	67.2	-114.8	9.1	21.6	0.0	1.1	9.0	20.7	0.00	0.05

	L-amino acids				D-amino acids				Difference between Means		Pooled Standard Deviations		Effect Size	
	Mean		Standard Deviation		Mean		Standard Deviation							
State	ϕ	ψ	ϕ	ψ	ϕ	ψ	ϕ	ψ	ϕ	ψ	ϕ	ψ	ϕ	ψ
Pro-1 o	-47.9	139.6	9.7	32.9	47.4	-140.0	9.0	26.5	0.5	0.4	9.3	29.7	0.05	0.01
Pro-1 P_{IIL}	-65.0	146.0	8.5	15.2	65.1	-147.1	8.4	15.1	0.1	1.1	8.4	15.2	0.01	0.07
Ser-1 α_L	51.6	74.6	11.4	18.1	-52.0	-73.9	11.1	18.3	0.3	0.8	11.3	18.2	0.03	0.04
Ser-1 α_R	-79.2	-42.7	13.1	15.3	79.2	42.3	13.1	15.6	0.0	0.4	13.1	15.4	0.00	0.02
Ser-1 β	-94.3	128.6	26.6	33.1	96.5	-132.5	27.7	33.7	2.2	3.9	27.1	33.4	0.08	0.12
Ser-1 nα_R	-119.4	-30.6	14.3	12.4	119.4	30.4	14.4	12.5	0.0	0.2	14.3	12.5	0.00	0.01
Ser-1 o	-96.2	24.7	37.3	74.0	96.9	-21.6	33.6	73.7	0.7	3.1	35.5	73.8	0.02	0.04
Ser-1 P_{IIL}	-75.8	150.9	14.2	16.2	75.8	-151.3	14.0	15.9	0.0	0.3	14.1	16.0	0.00	0.02
Ser-1 P_{IR}	-137.1	73.4	14.2	14.0	138.0	-73.1	14.9	14.2	0.9	0.4	14.6	14.1	0.06	0.03
Trp-1 α_L	52.5	79.3	10.8	18.0	-52.2	-77.9	10.7	18.1	0.3	1.3	10.8	18.1	0.03	0.07
Trp-1 α_R	-82.1	-44.1	12.3	13.8	83.1	44.8	11.9	13.8	0.9	0.7	12.1	13.8	0.08	0.05
Trp-1 β	-113.5	124.9	29.0	26.4	113.3	-127.9	28.9	27.4	0.2	3.0	29.0	26.9	0.01	0.11
Trp-1 nα_R	-123.6	-32.7	16.4	12.1	123.3	33.1	16.0	12.0	0.3	0.4	16.2	12.0	0.02	0.04
Trp-1 o	-121.1	-9.7	41.1	58.0	118.6	26.9	35.0	56.5	2.5	17.2	38.3	57.3	0.07	0.30
Trp-1 P_{IIL}	-80.8	145.9	15.0	15.6	80.9	-146.5	15.1	15.8	0.1	0.6	15.0	15.7	0.01	0.04
Trp-1 P_{IR}	-138.0	74.6	14.5	14.4	139.0	-75.0	15.0	14.7	1.1	0.4	14.7	14.5	0.07	0.03
Tyr-1 α_L	52.4	77.8	10.9	18.2	-52.6	-75.6	10.7	18.6	0.1	2.1	10.8	18.4	0.01	0.12
Tyr-1 α_R	-82.8	-44.1	12.0	13.9	82.5	44.1	12.2	13.6	0.2	0.0	12.1	13.7	0.02	0.00
Tyr-1 β	-115.0	124.3	30.0	25.5	110.8	-122.8	29.4	25.5	4.2	1.5	29.7	25.5	0.14	0.06
Tyr-1 nα_R	-124.4	-32.6	16.4	12.2	123.6	32.9	16.5	12.1	0.8	0.2	16.4	12.1	0.05	0.02
Tyr-1 o	-120.8	-4.6	46.8	61.0	119.6	20.0	36.9	56.3	1.2	15.4	42.5	58.9	0.03	0.26
Tyr-1 P_{IIL}	-80.7	144.9	15.1	15.7	79.9	-144.5	14.8	15.7	-0.8	0.4	14.9	15.7	0.05	0.03
Tyr-1 P_{IR}	-141.2	77.0	15.1	14.3	138.7	-76.7	14.4	14.3	2.5	0.4	14.8	14.3	0.17	0.03
Val-1 α_L	52.7	83.2	11.2	16.3	-48.0	-84.9	15.0	16.0	4.7	1.7	11.5	16.3	0.41	0.10
Val-1 α_R	-83.6	-43.3	11.4	14.4	84.1	41.7	11.1	15.1	0.6	1.6	11.3	14.7	0.05	0.11
Val-1 β	-112.4	141.3	23.3	28.8	112.0	-141.9	23.1	28.9	0.4	0.6	23.2	28.9	0.02	0.02
Val-1 nα_R	-120.1	-28.0	12.6	13.4	120.1	27.3	12.7	13.4	0.0	0.7	12.7	13.4	0.00	0.05
Val-1 o	-116.2	8.8	29.2	49.0	113.6	-11.3	28.5	51.1	2.6	2.5	28.8	50.0	0.09	0.05
Val-1 P_{IIL}	-79.4	152.7	15.0	14.9	79.9	-153.2	14.9	14.8	0.4	0.5	14.9	14.9	0.03	0.03
Val-1 P_{IR}	-132.9	72.7	11.1	14.6	131.9	-74.8	10.8	14.9	0.9	2.1	10.9	14.7	0.09	0.14

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