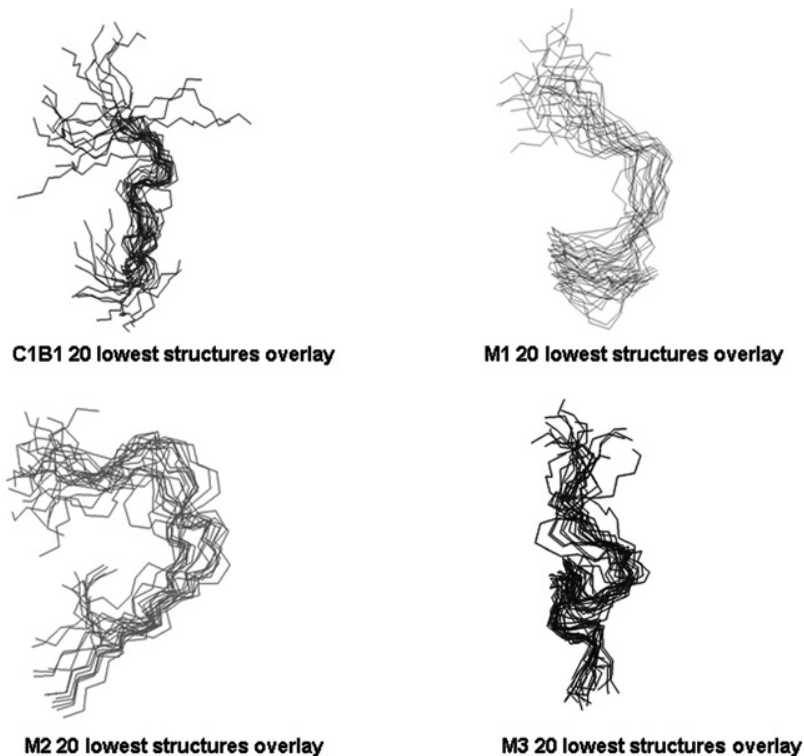


SUPPLEMENTARY MATERIAL

**Figure S1.** Overlay of the 20 lowest energy structures for each peptide. RMSDs can be seen in Table 1.**Table S1.** Proton Chemical Shifts (ppm) for C1B1 in TFE:H₂O (50:50) at 10° C

	NH	C α H	C β H	C γ H	C δ H	C ϵ H	C ζ H
H1	-	4.254	3.266	-	7.113	8.521	-
K2	8.723	4.371	1.649, 1.744	1.352	1.403	2.948	7.604
F3	8.354	4.633	3.026, 3.057	-	-	7.292	7.239
R4	8.133	4.321	1.672, 1.771	1.545	3.136	7.157	-
L5	8.05	4.233	1.525	1.48	0.8611, .9095	-	-
H6	8.268	4.628	3.109, 3.16	-	7.152	8.49	-
S7	8.22	4.404	3.751, 3.816	-	-	-	-
Y8	8.169	4.586	2.975, 3.059	-	7.106	6.79	-
S9	8.003	4.46	3.79	-	-	-	-
S10	8.087	4.761	3.86	-	-	-	-
P11	-	4.524	2.283	2.019	3.784	-	-
T12	7.962	4.421	4.359	1.173	-	-	-

Table S2. Proton Chemical Shifts (ppm) for Mutant 1 in TFE: H₂O (50:50) at 10° C.

	NH	C α H	C β H	C γ H	C δ H	C ϵ H	C ζ H
H1	-	4.272	3.282	-	7.127	8.527	-
K2	8.729	4.387	1.668, 1.761	1.367	1.426	2.963	7.613

(Table S2) contd....

	NH	C α H	C β H	C γ H	C δ H	C ϵ H	C ζ H
F3	8.342	4.649	3.044, 3.066	-	7.25	7.131, 7.3	-
R4	8.123	4.334	1.686, 1.784	1.561	3.151	7.175	-
L5	8.027	4.242	1.551	1.501	0.8751, .9227	-	-
H6	8.223	4.635	3.122, 3.176	-	7.128	8.469	-
S7	8.205	4.408	3.758, 3.821	-	-	-	-
F8	8.209	4.659	3.051	-	7.26	-	-
S9	8.049	-	3.8, 3.835	-	-	-	-
S10	8.063	4.485	3.873	-	-	-	-
P11	-	4.536	2.286	2.031	3.786	-	-
T12	7.929	4.424	4.366	1.183	-	-	-

Table S3. Proton Chemical Shifts (ppm) for Mutant 2 in TFE: H₂O (50:50) at 10° C

	NH	C α H	C β H	C γ H	C δ H	C ϵ H	C ζ H
H1	-	4.253	3.267	-	7.117	8.525	-
K2	8.724	4.373	1.654,1,749	1.357	1.407	2.949	7.606
F3	8.357	4.636	3.027, 3.055	-	-	7.114, 7.238	7.151
R4	8.141	4.322	1.676, 1.772	1.55	3.14	7.162	7.291
L5	8.056	4.237	1.526,9105	1.485	0.863	-	-
H6	8.271	4.624	3.116, 3.156	-	7.152	8.485	-
S7	8.198	4.402	3.745, 3.81	-	-	-	-
Y8	8.099	4.535	2.936, 3.052	-	7.103	6.792	-
A9	7.993	4.33	1.309	-	-	-	-
S10	8	-	3.845	-	-	-	-
P11	-	4.526	2.282	2.019	3.778	-	-
T12	7.958	4.42	4.362	1.178	-	-	-

Table S4. Proton Chemical Shifts (ppm) for Mutant 3 in TFE:H₂O (50:50) at 10° C

	NH	C α H	C β H	C γ H	C δ H	C ϵ H	C ζ H
H1	-	4.204	3.221	-	7.097	8.477	-
K2	8.686	4.322	1.594,1.69	1.299	1.353	2.896	7.545
F3	8.334	4.572	2.986	-	7.16	7.231	-
R4	8.025	4.207	1.585, 1.641	1.428	3.038	7.048	-
L5	7.817	4.152	1.375	1.324	0.7554, .812	-	-
F6	7.816	4.365	2.899, 3.012	-	7.102	7.171	-
S7	8.039	4.693	3.799, 3.802	-	-	-	-

(Table S4) contd....

	NH	CαH	CβH	CγH	CδH	CϵH	CζH
Y8	7.939	4.502	2.906, 3.005	-	7.048	6.746	-
S9	7.903	4.332	3.655	-	-	-	-
S10	7.916	4.405	3.729	-	-	-	-
P11	-	4.462	2.217	1.959	3.717	-	-
T12	7.909	4.348	4.296	1.123	-	-	-