Supplementary Material

Disulfide-mediated beta strand dimers: hyperstable beta sheets lacking tertiary interactions and turns

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Figure S1: Normalized CD melts for peptides of the form `KWRWRTR(linker)RKIKRWY`. (Melting of the exciton couplet maxima, at 228nm, is followed.)

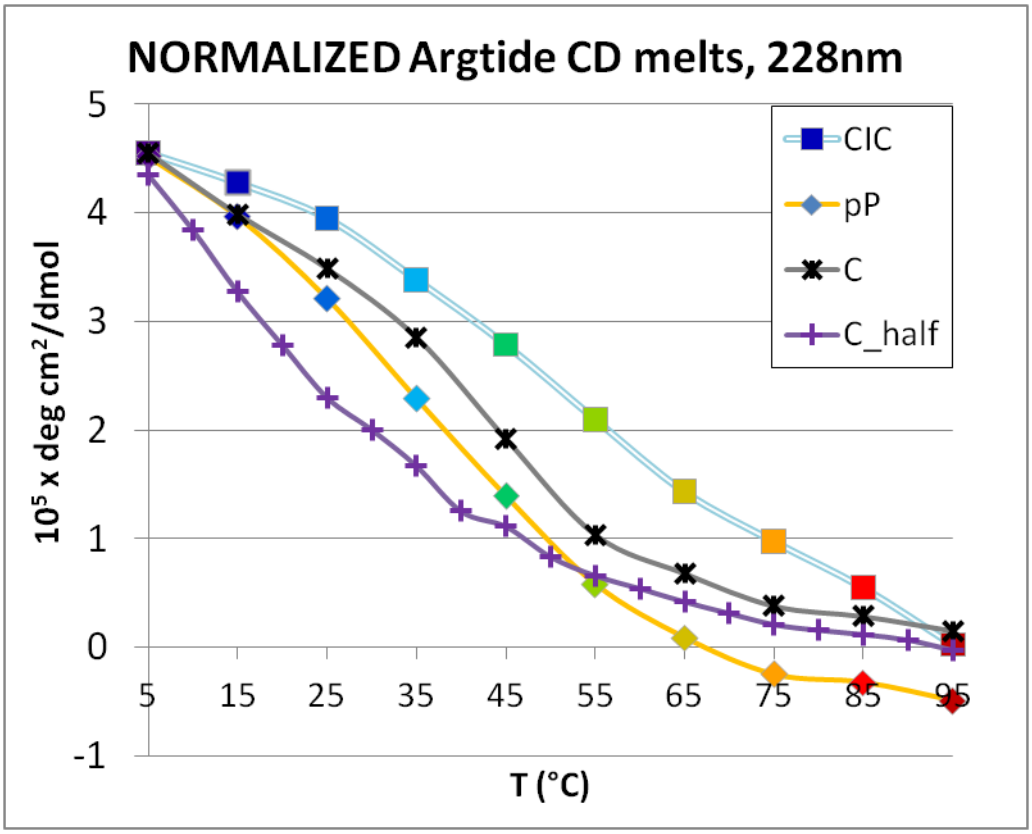
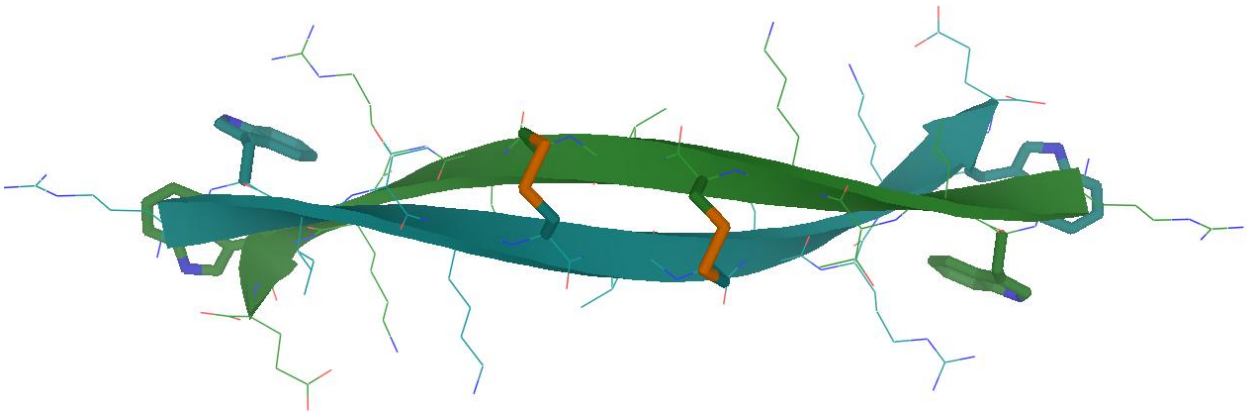
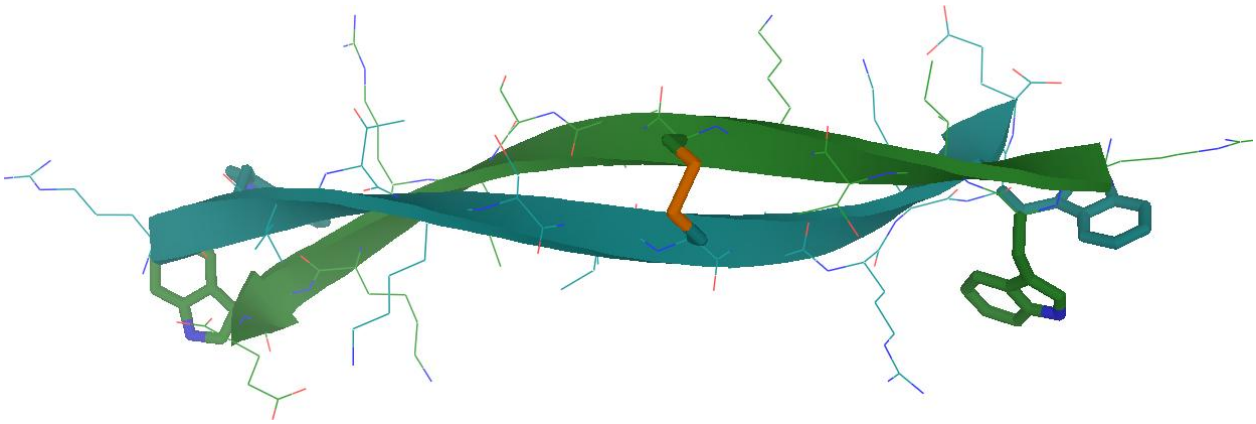


Figure S2: NOE-validated models of disulfide-bearing beta sheet dimers:

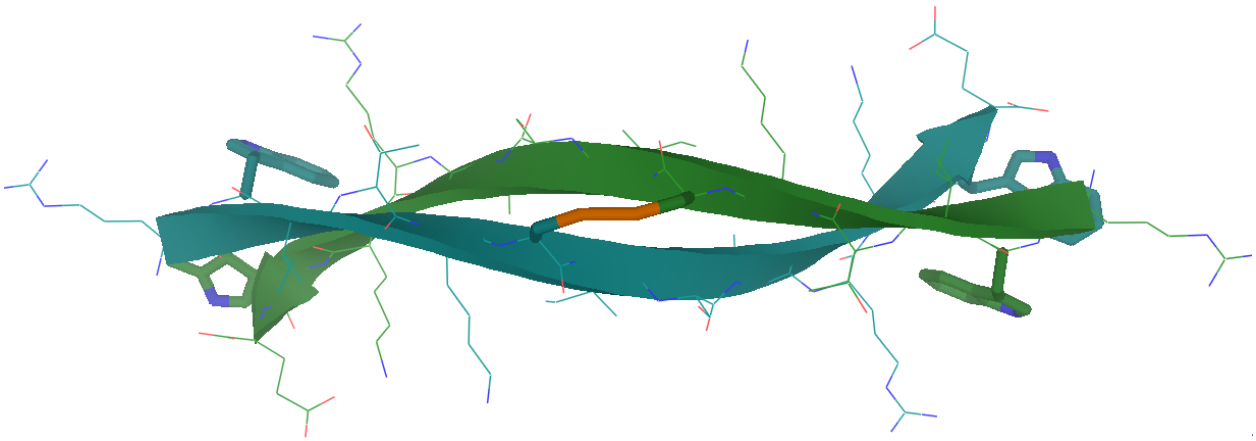
S2a (below): The all-cysteine (bis-disulfide) homodimer. Sequence R**W**ITK**C**I**C**IRK**W**E.



S2b (below): The C6/C8 heterodimer. Sequence R**W**ITK**C**I**S**IRK**W**E + R**W**ITK**S**I**C**IRK**W**E.



S2c (below): The C6 homodimer, or "good" diagonal disulfide. Sequence (R**W**ITK**C**I**S**IRK**W**E)$_2$



S2d (below): The C8 homodimer (the "bad" diagonal disulfide, sequence (R**W**ITK**S**I**C**IRK**W**E)$_2$). Note: this model is ***NOT*** NOE-validated; this is the closest potential fit to the NOEs for the dimer. A dimer of dimers (or other oligomer) is required to explain folding of this peptide at NMR concentrations. Note the distorted / bulged sheets and the strained disulfide.

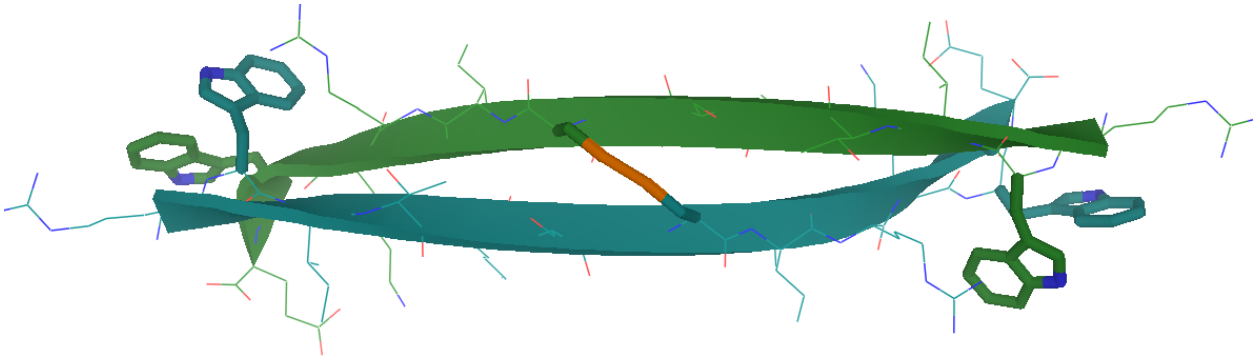


Figure S3 (below): Proposed folding landscape for long loop peptides with a central disulfide (as the oxidized homodimer); the blue chain is labeled AB (A at Nterm, B at Cterm) and the identical green chain is A'B'. By NMR, we observed only the two equivalent fully-folded states (and perhaps a percent or so of the partly-unfolded states) for peptide (R**W**ITVTIGGGG**C**GGGGKKIRV**W**E)$_2$ at 280K. The reduced species (chain AB alone; no A'B') can only access one of the two equivalent folded states and only one of the four equivalent folding pathways (the pathway on the far left). Thus, despite what are almost assuredly identical energies (per chain) for the folded state, its melting point is decreased by circa 8 degrees.

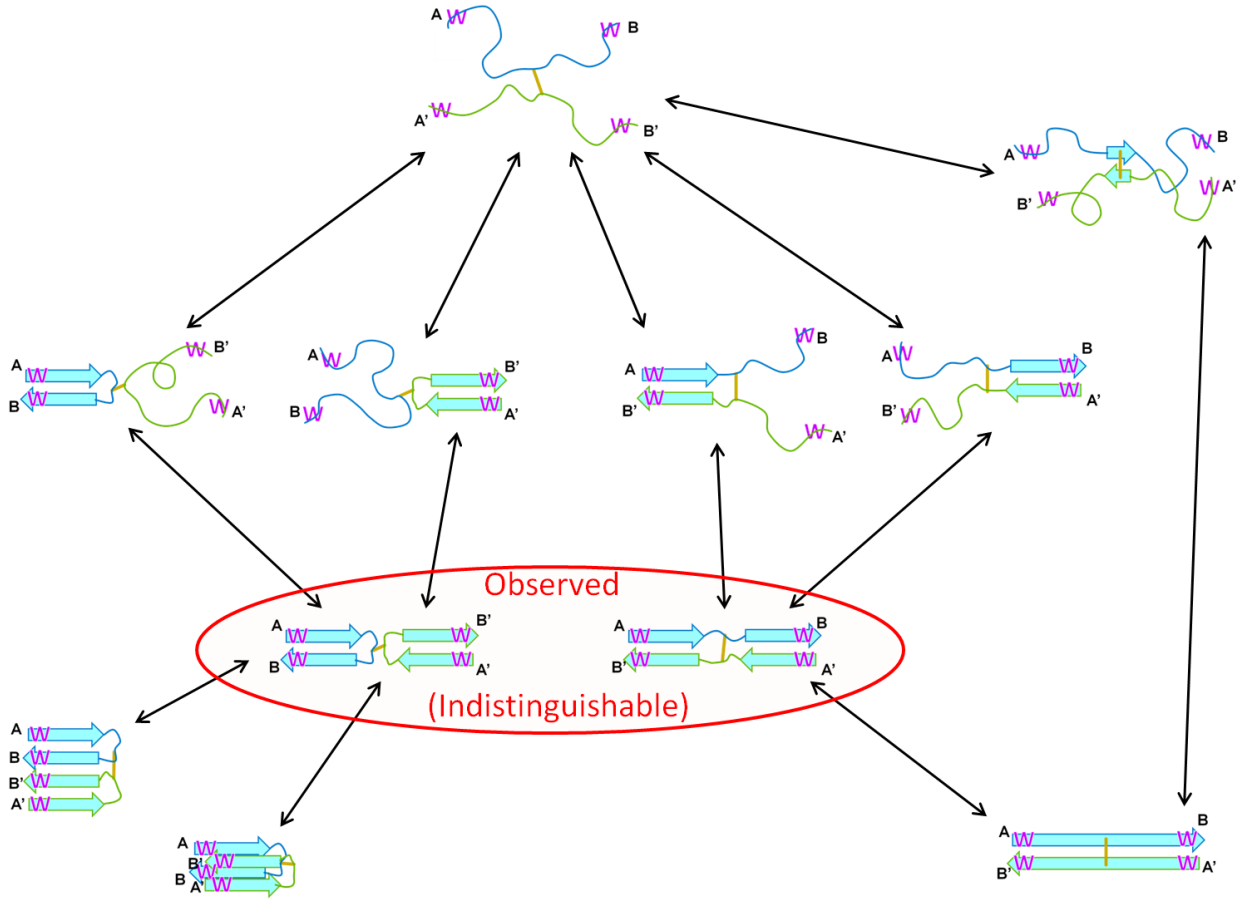


Figure S4: Circular Dichroism melts (as the 228 nm exciton couplet resulting from the Trp/Trp interaction(s)) for peptide RWITVTIGGGGCGGGGKKIRVWE, oxidized (dimerized) and reduced (monomeric). Concentration of 30 micromolar of peptide chain was used. (Total concentration of 15 micromolar of oxidized dimer.)

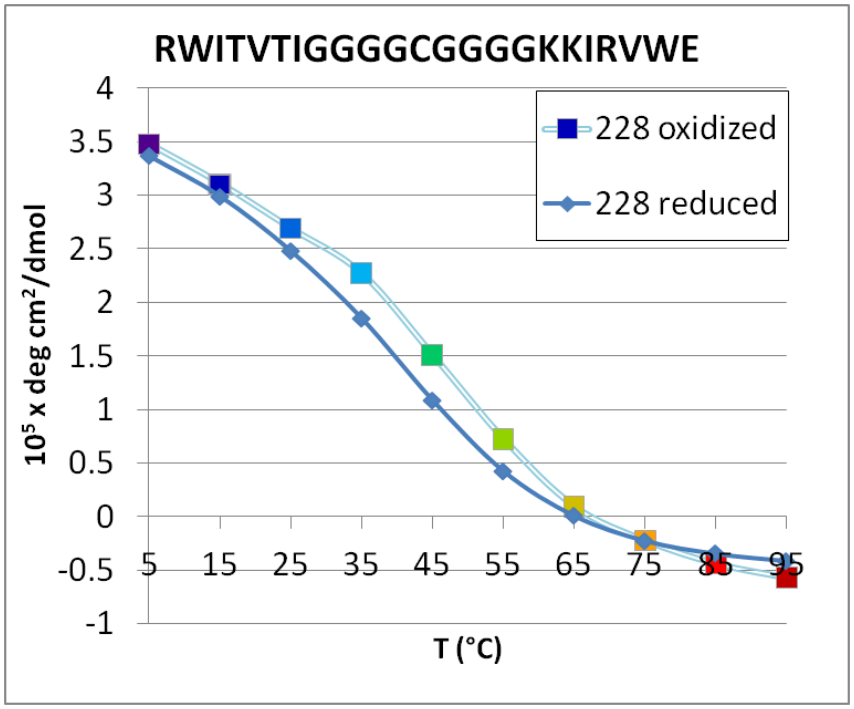
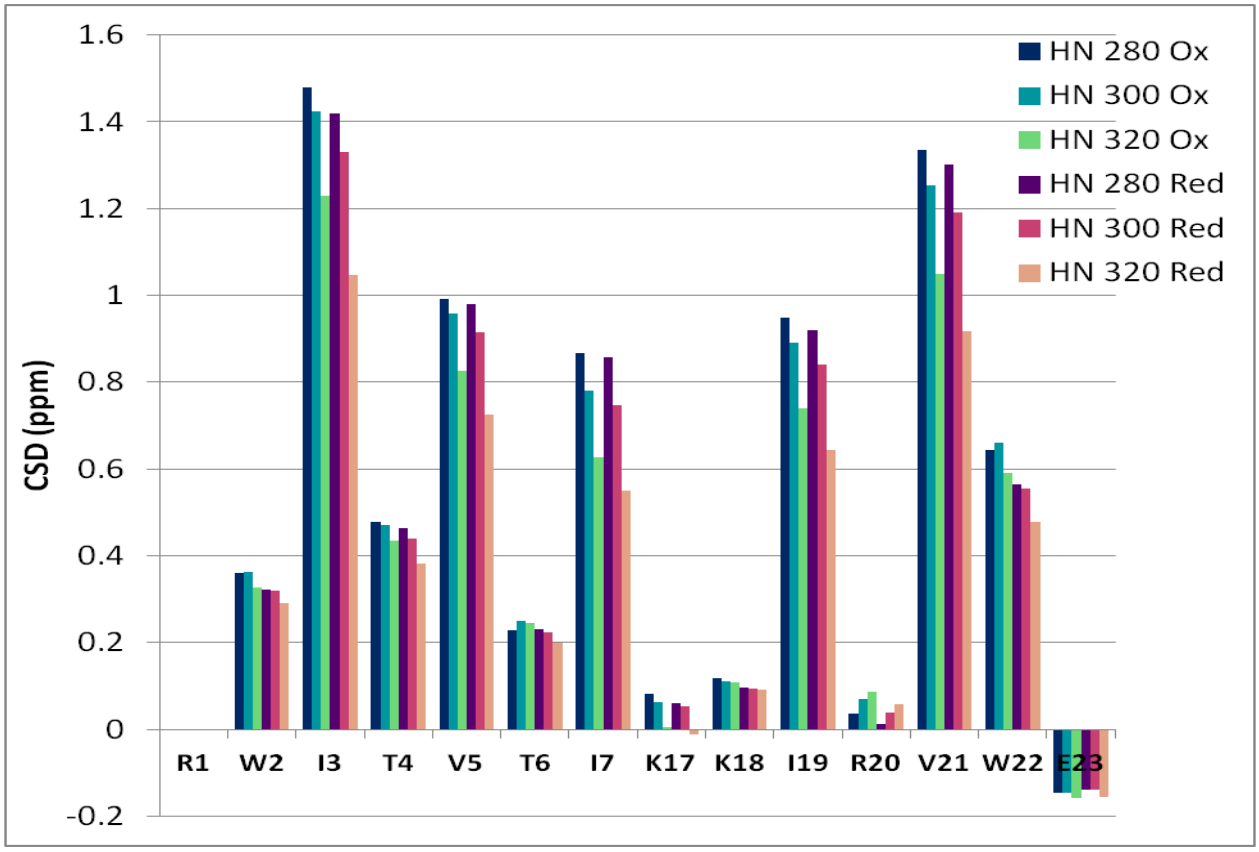


Figure S5 (below): H_N and Hα CSD comparison for peptides of the form (RWITVTIGGGGCGGGGKKIRVWE)$_n$



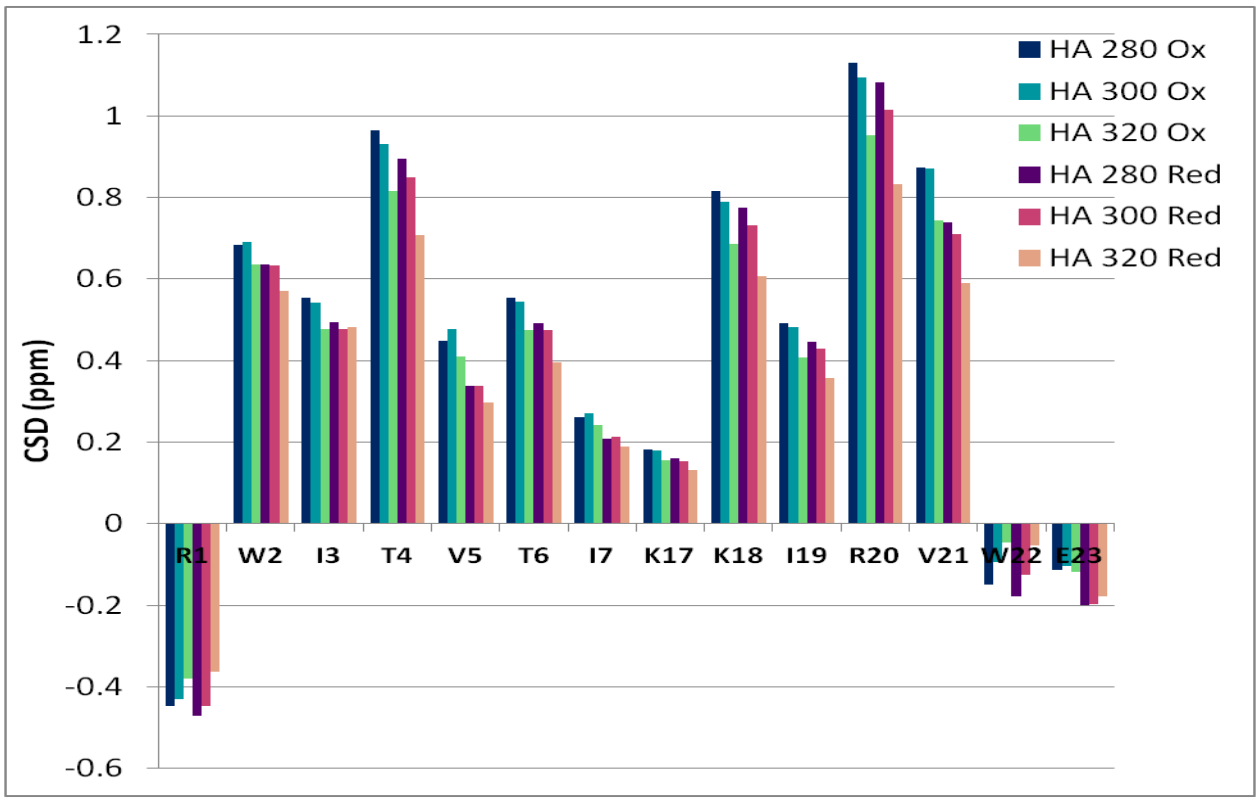
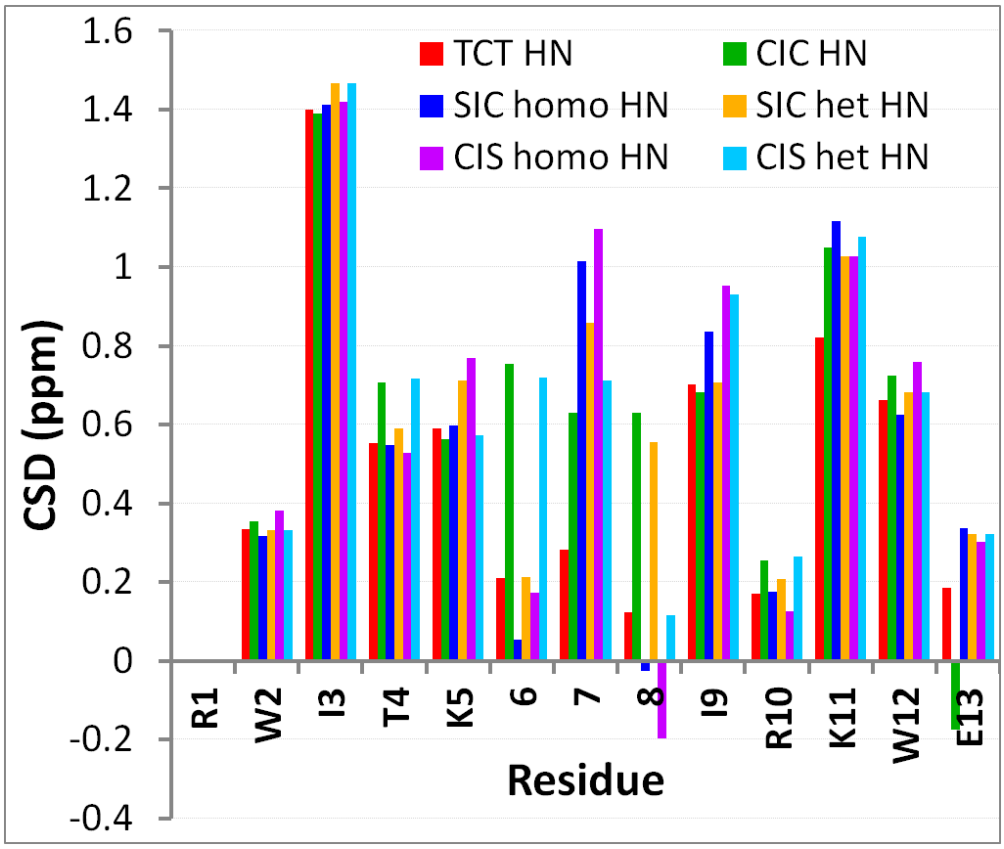


Figure S6, below: Chemical shift deviations for oxidized peptides of the form RWITK**XXX**IRK**W**E. (280K, pH 6)



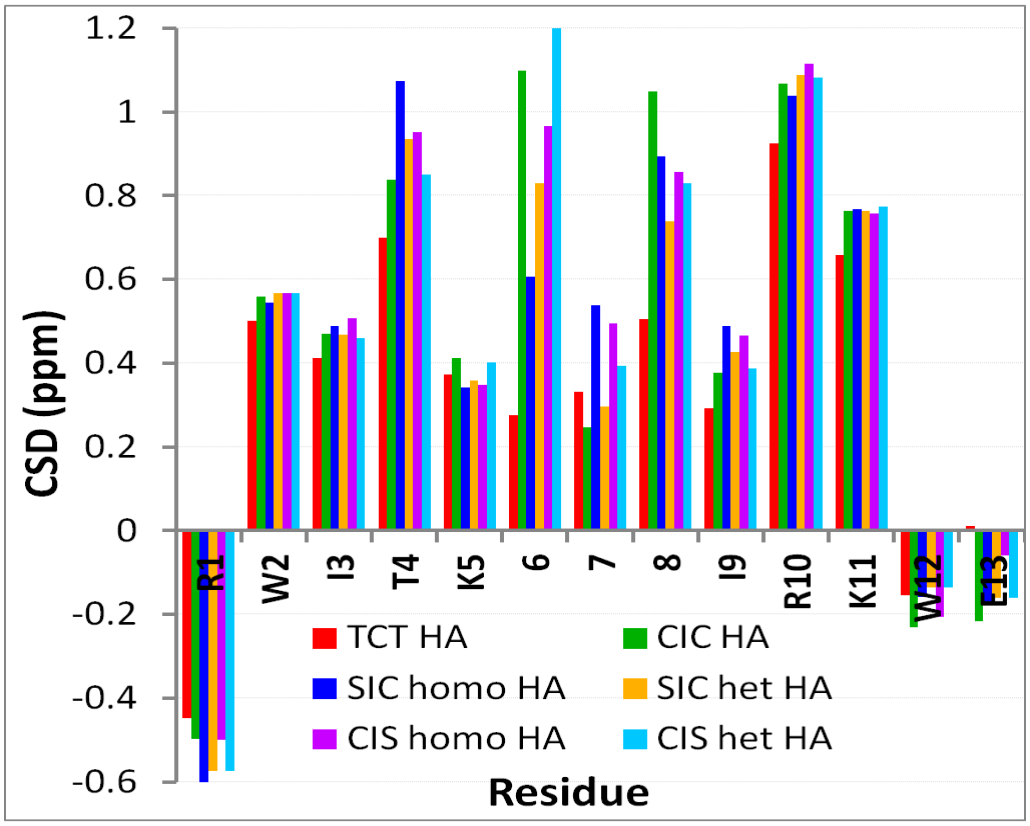
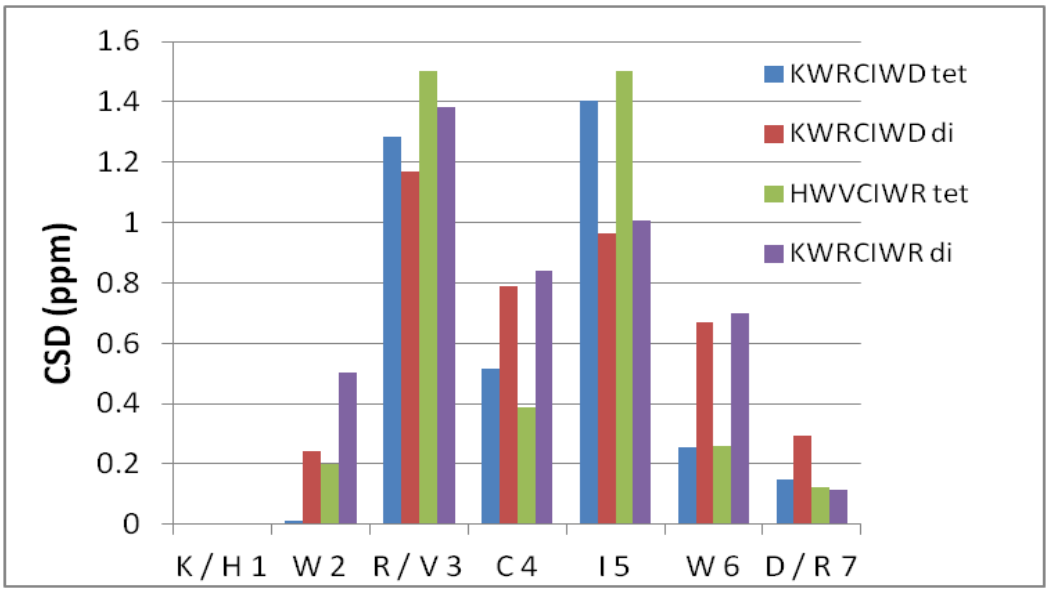


Figure S7: Backbone chemical shift deviations (CSDs) for $(XWXCXWX)_n$ peptides. (Raw data appears in table S1.)

S7a (below): H_N CSDs



S7b (below): Hα CSDs.

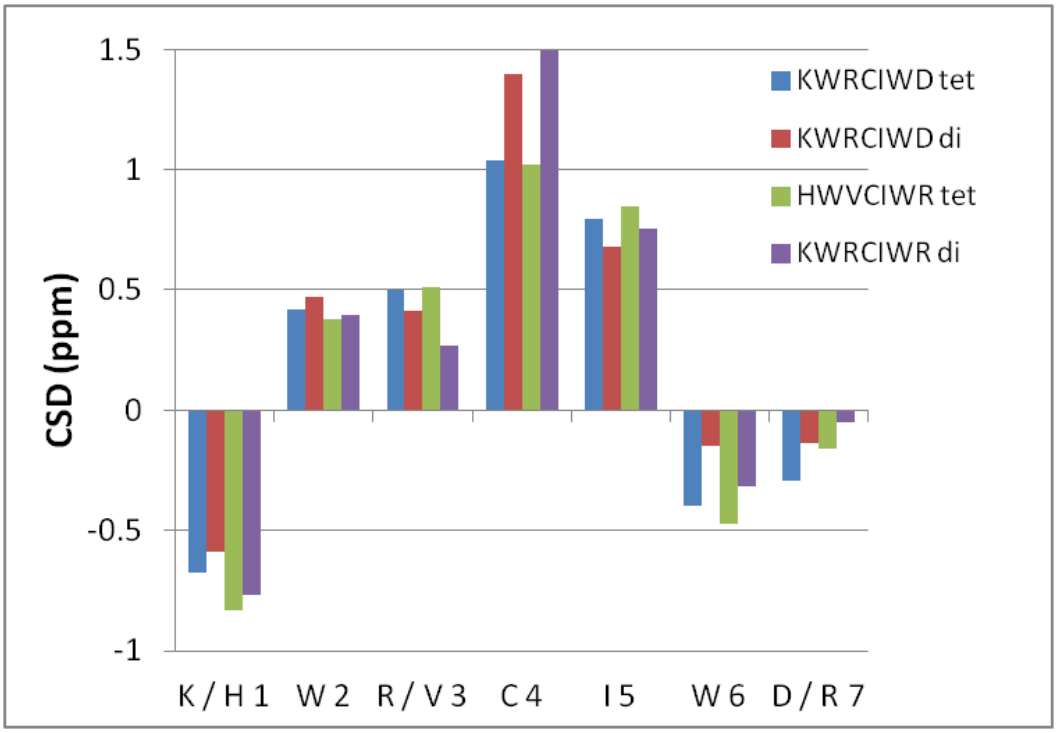


Figure S8: CD Melt (228nm) of KWRCIWD. (Note that dimers and tetramers cannot be distinguished here, and are expected to yield similar CD spectra. However, the concentration used for CD is circa 2 orders of magnitude lower than that for NMR; thus the predominance of dimer is expected. This is especially true since dimer and tetramer exist in roughly equal proportions at 280K, 1 mM, as measured by NMR peak integrals.)

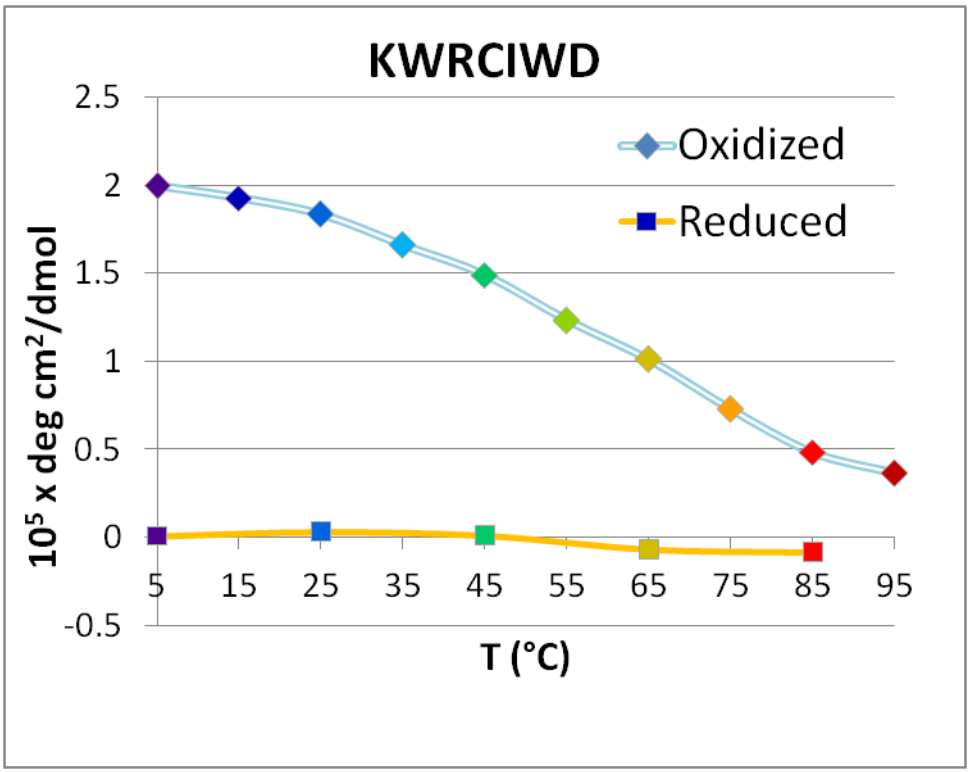


Figure S9a: Dilution data for peptide $(RWRCIWY)_2$. A 25-fold dilution of a 3mM sample results in much cleaner lineshapes, and the disappearance of the 2nd set of peaks. Complete assignments determined by 2D NMR. Note that the relative intensity, or even the existence, of a 2nd set of peaks at high concentration (~3-5 mM) varies for peptides of the form $(XWXCXWX)_2$. Since our best-guess structure for a tetramer places all "X" residues on the exterior, they should theoretically have little impact on the propensity for higher-order association, but we have shown that their impact is non-negligible. In decreasing order from "more higher-order assembly" to "mostly/only dimer": $(KWRCIWD)_2$ = $(HWVCIWR)_2$ > $(RWRCIWY)_2$ > $(HWHCIWD)_2$. A distinct, second set of peaks was never observed for longer beta ribbons, reduced species, or peptides of the form $(Ac\text{-}WXCXWTGP\ldots)_n$. (Ac=Acetyl, or also Propanoyl.)

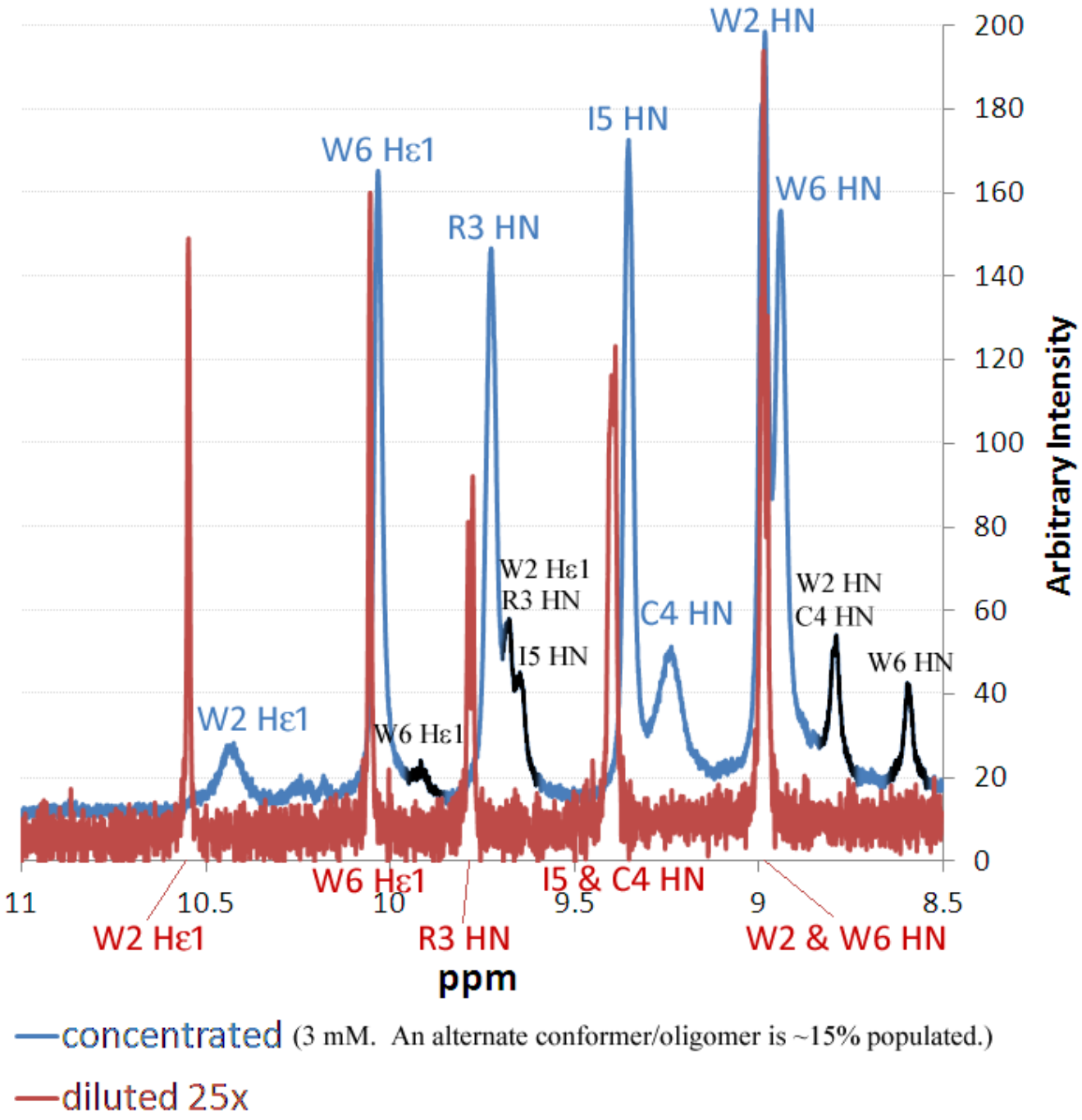


Figure S9b: Higher temperatures resulted in sharper lineshapes for all peaks, and a slight decrease in the relative intensity of the 2nd set of peaks. This is suggestive of two equilibrium processes: rapid docking and undocking of the dominant C2 dimer, and slower disulfide-swapping exchange (proposed mechanism in figure S10).

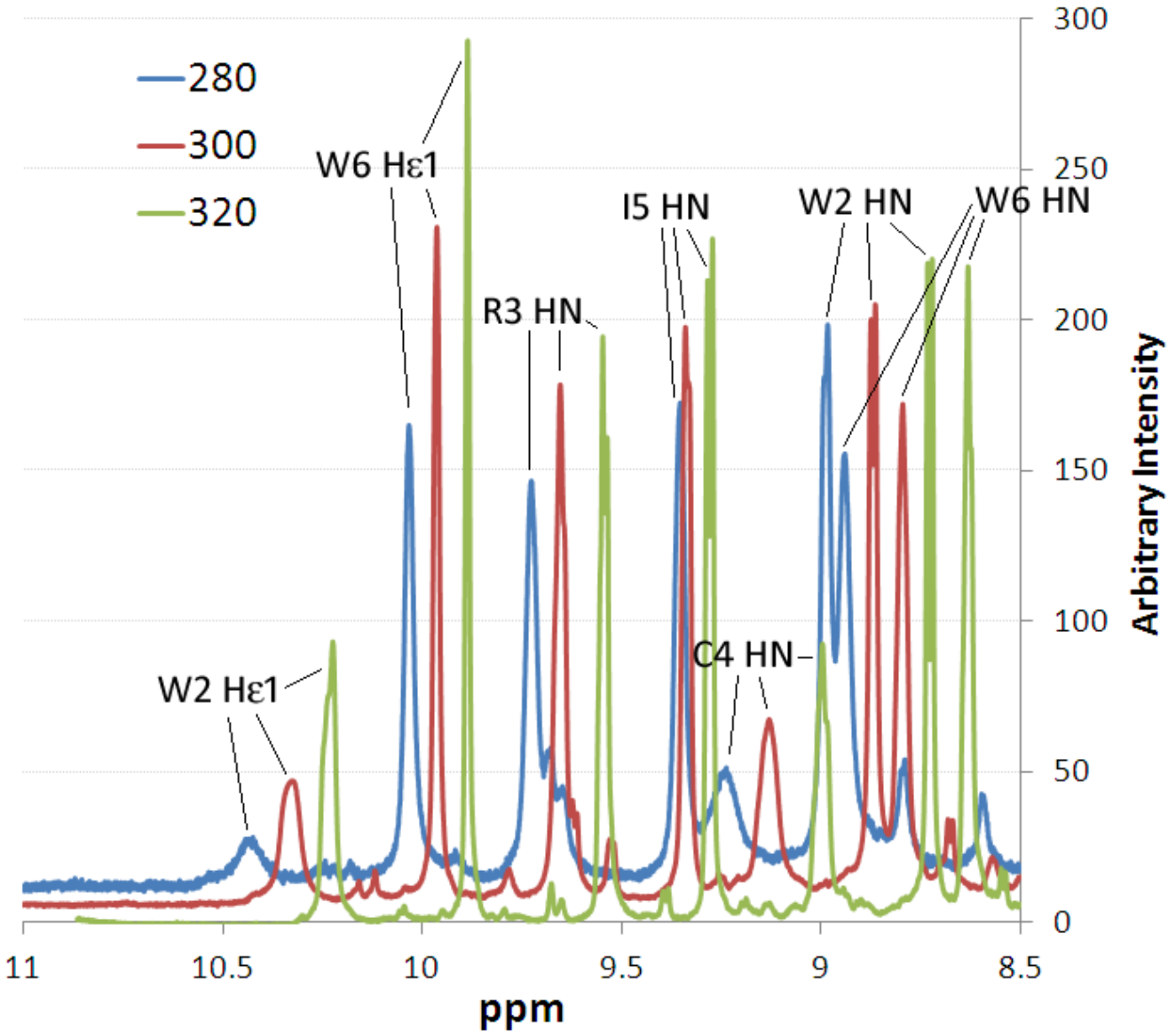


Figure S10: Proposed mechanism for the higher-order assembly of oxidized beta sheet peptides of the form $(XWXCXWX)_2$. The lowest-energy conformation for a tetrameric species involves face-to-face disulfide bonds; these impose less strain on the beta sheets vs. cross-strand edge-to-edge disulfides, and allow for more efficient packing of the hydrophobic W.C.W faces. Broadened lineshapes of the dimer peaks at high concentration suggest a less-efficient tetramerization (or other oligomerization) event with moderately fast interconversion, while the appearance of an entirely new set of peaks suggests a slowly-interconverting species with different disulfide connectivity. To convert between the two tetramers, the peptide must first unfold, then reassemble/refold. The structure shown for the "swapped" tetramer (bottom right) is our best guess from available data, but will require crystallographic methods to explicitly derive.

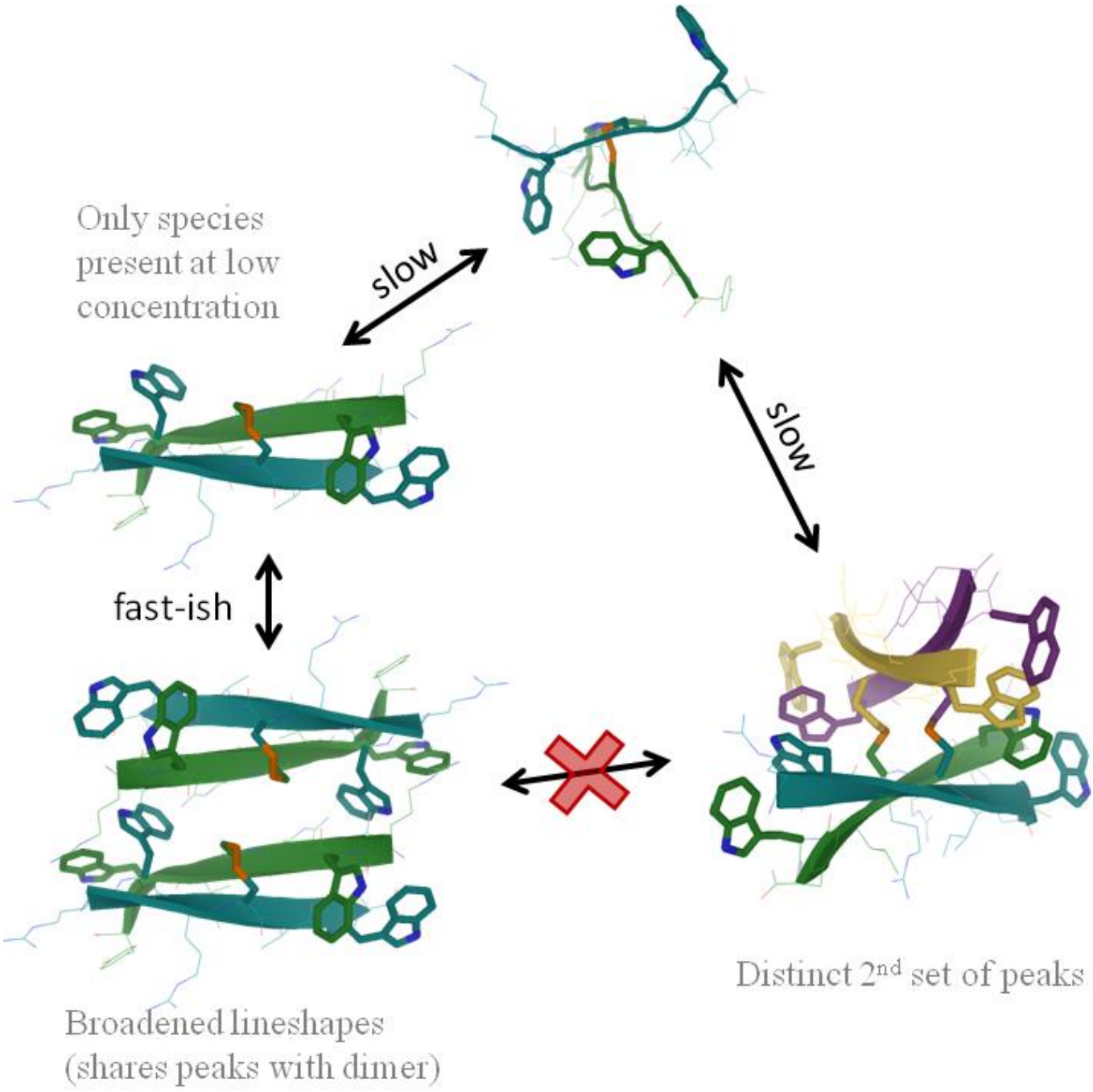


Figure S11: Structural data for double-hairpin peptide (RWICRWDEKSGRWITKKID)$_2$ **a**) Designed structure; validated by 2D NMR NOEs & CSDs. Selected, structurally diagnostic NOEs are marked as orange lines (intrachain) and purple lines (interchain). **b)** A slice of the NOESY spectra showing the structurally-diagnostic contacts highlighted in the upper panel, here as raw NOEs. (Complete NOEs are given in table S11.)

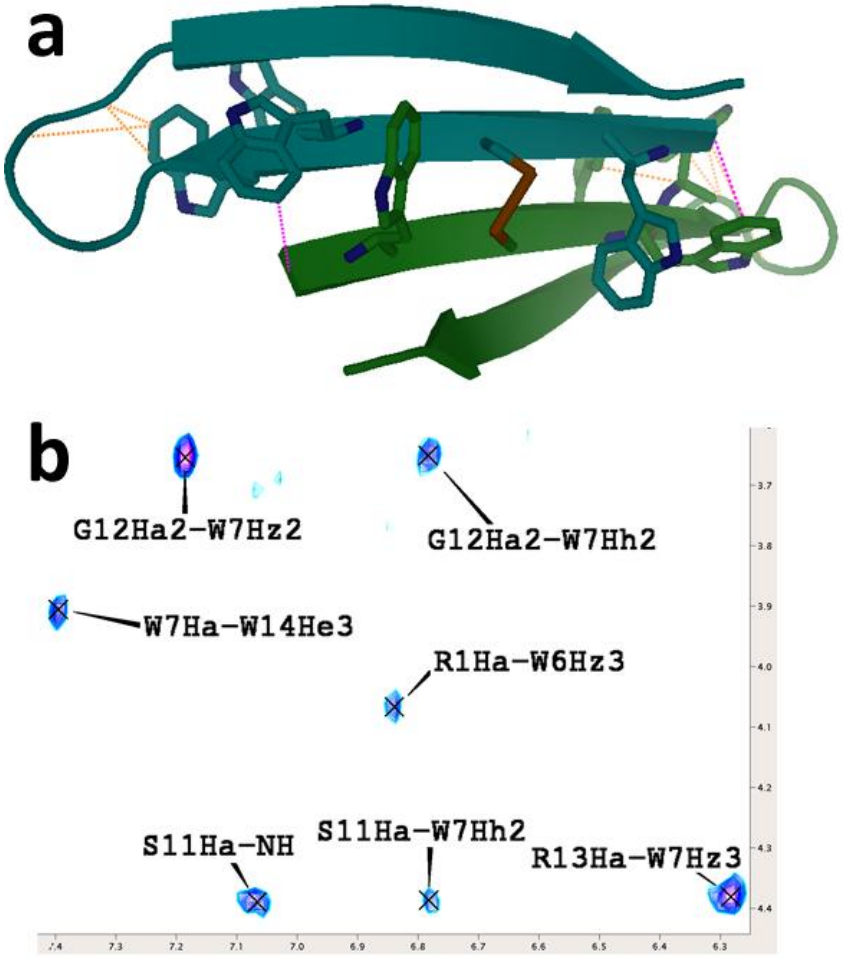


Table S1a: backbone chemical shift deviations for pP: (KWRWRTRpPRKIKRWY)$_2$

Chemical shift deviations highlighted in bold were used to calculate fold population. (100% values defined as the very-well-folded CIC peptide @ 280K, plus 2%.)

	HN 280	HA 280	HN 300	HA 300	HN 320	HA 320
K1		**-0.556**		**-0.52**		**-0.491**
W2	-0.054	**0.704**		**0.647**		**0.501**
R3	**1.005**	**0.479**	**0.928**	**0.431**	**0.769**	**0.381**
W4	**0.954**	**0.704**	**0.887**	**0.712**	**0.688**	**0.637**
R5	**1.367**	**0.534**	**1.323**	**0.513**	**1.13**	**0.442**
T6	**0.824**	**0.63**	**0.765**	**0.639**	**0.654**	**0.593**
R7	**0.708**	0.285	**0.675**	0.273	**0.574**	0.255
dPro	-----	0.068		0.068		0.065
Pro	-----	0.121		0.127		0.125
R*10*	-0.631	0.253	-0.557	0.23	-0.396	0.181
K*11*	0.121	**0.813**	0.138	**0.76**	0.144	**0.626**
I*12*	**0.977**	**0.558**	**0.943**	**0.521**	**0.785**	**0.44**
K*13*	0.189	0.124	0.204	0.135	0.185	0.12
R*14*	**0.698**	**0.587**	**0.635**	**0.533**	**0.439**	**0.402**
W*15*	**0.632**	0.056	**0.588**	0.064	**0.444**	0.071
Y*16*	0.411	-0.153	0.407	-0.122	0.395	-0.076

Table S1b: backbone chemical shift deviations for C: (KWRWRTRCRKIKRWY)$_2$

	HN 280	HA 280	HN 300	HA 300	HN 320	HA 320
K1		**-0.584**		**-0.543**		**-0.473**
W2	-0.047	**0.72**	-0.053	**0.685**		**0.563**
R3	**1.029**	**0.517**	**0.984**	**0.473**	**0.821**	**0.397**
W4	**0.994**	**0.775**	**0.95**	**0.783**	**0.765**	**0.698**
R5	**1.267**	**0.531**	**1.283**	**0.521**	**1.134**	**0.442**
T6	**0.918**	**0.629**	**0.881**	**0.66**	**0.752**	**0.622**
R7	**0.781**	0.447	**0.767**	0.447	**0.655**	0.395
C8	0.891	1.123	0.866	1.11	*0.81*	1.005
R*9*	0.484	0.395	0.523	0.386	0.479	0.339
K*10*	0.34	**0.823**	0.362	**0.816**	0.35	**0.705**
I*11*	**1.128**	**0.597**	**1.119**	**0.578**	**0.933**	**0.494**
K*12*	0.131	0.139	0.173	0.154	0.173	0.144

R*13*	**0.713**	**0.601**	**0.675**	**0.571**	**0.5**	**0.46**
W*14*	**0.666**	0.044	**0.647**	0.055	**0.511**	0.062
Y*15*	0.397	-0.166	0.416	-0.135	0.336	-0.091

Table S1c: backbone chemical shift deviations for CIC: $(KWRWRTRCICRKIKRWY)_2$

	HN 280	HA 280	HN 300	HA 300	HN 320	HA 320
Lys1		**-0.592**		**-0.549**		**-0.494**
Trp2	-0.052	**0.732**	-0.049	**0.705**	-0.049	**0.646**
Arg3	**1.03**	**0.527**	**1.004**	**0.481**	**0.917**	**0.45**
Trp4	**0.993**	**0.788**	**0.964**	**0.806**	**0.881**	**0.793**
Arg5	**1.25**	**0.534**	**1.279**	**0.53**	**1.257**	**0.51**
Thr6	**0.869**	**0.63**	**0.846**	**0.655**	**0.806**	**0.674**
Arg7	**0.773**	0.442	**0.782**	0.432	**0.763**	0.428
Cys8	0.89	1.028	0.888	1.061	0.866	1.085
Ile9	0.566	0.256	0.637	0.275	0.716	0.293
Cys10	0.827	1.093	0.787	1.103	0.749	1.094
Arg11	0.413	0.404	0.455	0.398	0.486	0.388
Lys12	0.327	**0.79**	0.352	**0.795**	0.372	**0.766**
Ile13	**1.127**	**0.594**	**1.133**	**0.597**	**1.086**	**0.561**
Lys14	0.116	0.151	0.158	0.172	0.19	0.185
Arg15	**0.707**	**0.614**	**0.684**	**0.592**	**0.611**	**0.542**
Trp16	**0.69**	0.06	**0.681**	0.065	**0.63**	0.07
Tyr17	0.393	-0.157	0.415	-0.133	0.394	-0.103

Table S1d: backbone chemical shift deviations for Half: KWRWRTRCR + RCRKIKRWY. (Note: due to poor lineshapes resulting from moderately slow folding rate and intermediate fold populations, not all positions could be definitively assigned.)

	HN 280	HA 280	HN 300	HA 300	HN 320	HA 320
K1		**-0.498**		**-0.423**		**-0.329**
W2	-0.026	**0.623**	-0.052	**0.458**		**0.203**
R3		**0.422**		***0.32***		
W4		**0.651**		**0.515**		**0.341**
R5	**1.121**	**0.449**	**0.895**	**0.333**		
T6	**0.836**	**0.537**	**0.653**	**0.45**		**0.272**
R7	**0.703**	0.363	**0.538**	0.303		
C8	0.79	0.675		0.536		0.295
R9	0.168	0.074	0.202	0.058	0.215	0.051
R*1*						
C*2*		0.728		0.58		0.336
R*3*	0.278	0.298	0.251	0.237		
K*4*	0.298	**0.666**	0.269	**0.512**		
I*5*	**0.966**	**0.514**	**0.719**	**0.391**	**0.375**	**0.196**

K*6*	0.137	0.127	0.129	0.099		0.138
R*7*	**0.642**	**0.507**	**0.42**	**0.367**		
W*8*	**0.534**	0.063	**0.36**	0.068	**0.075**	0.077
Y*9*	0.31	-0.132	0.294	-0.079	0.166	-0.008

Table S1e: Key C-term Trp (the shifted "edge" Trp of the edge-to-face interaction) chemical shift deviations for peptides of the form: KWRWRTR(X)RKIKR**W**Y

	Hβ3 280	Hβ3 300	Hβ3 320	Hε3 280	Hε3 300	Hε3 320	Hζ3 280	Hζ3 300	Hζ3 320
pP	**-0.733**	**-0.685**	**-0.553**	**-1.881**	**-1.646**	**-1.184**	**-0.559**	**-0.503**	**-0.376**
C	**-0.748**	**-0.714**	**-0.596**	**-2.015**	**-1.805**	**-1.384**	**-0.592**	**-0.547**	**-0.443**
ClC	**-0.72**	**-0.704**	**-0.654**	**-2.025**	**-1.857**	**-1.629**	**-0.601**	**-0.567**	**-0.518**
C_half	**-0.671**	**-0.512**	**-0.265**	**-1.703**			**-0.477**	**-0.333**	**-0.131**

Table S2a: 280K backbone chemical shift ***deviations*** for Oxidized $(KWRCIWD)_n$ and $(HWVCIWR)_n$ peptides.

	KWRCIWD Tet		KWRCIWD Di		HWVCIWR Tet		HWVCIWR Di	
	HN	Hα	HN	Hα	HN	Hα	HN	Hα
K / H		-0.678		-0.591		-0.834		-0.77
W	0.011	0.419	0.243	0.47	0.199	0.377	0.504	0.397
R / V	1.283	0.499	1.17	0.412	1.503	0.509	1.383	0.27
C	0.517	1.036	0.787	1.399	0.387	1.022	0.84	1.493
I	1.405	0.796	0.966	0.678	1.504	0.849	1.005	0.755
W	0.255	-0.399	0.669	-0.149	0.258	-0.47	0.699	-0.316
D / R	0.148	-0.291	0.293	-0.137	0.122	-0.16	0.112	-0.053

Table S2b: 280K backbone chemical shift**s** for Oxidized $(KWRCIWD)_n$ and $(HWVCIWR)_n$ peptides.

	KWRCIWD Tet		KWRCIWD Di		HWVCIWR Tet		HWVCIWR Di	
	HN	Hα	HN	Hα	HN	Hα	HN	Hα
K / H		3.337		3.424		3.589		3.653
W	8.759	5.072	8.991	5.123	8.987	5.03	9.292	5.05
R / V	9.63	4.804	9.517	4.717	9.7	4.588	9.58	4.349
C	8.875	5.465	9.145	5.828	8.745	5.451	9.198	5.922
I	9.622	4.915	9.183	4.797	9.721	4.968	9.222	4.874
W	8.543	4.254	8.957	4.504	8.546	4.183	8.987	4.337
D / R	8.036	4.142	8.181	4.296	7.91	3.975	7.9	4.082

Table S2c: 280K Trp sidechain chemical shifts for Oxidized $(KWRCIWD)_n$ and $(HWVCIWR)_n$ peptides.

	KWRCIWD 1	KWRCIWD 2	HWVCIWR 1	KWRCIWR 2
W2 Hβ3	-0.531	-0.126	-0.562	-0.125
W2 Hδ1	-0.463	0.259	-0.619	0.355
W2 Hε1	-0.651	0.167	-0.583	0.288
W2 Hε3	-0.479	-0.329		-0.303
W5 Hβ2	-0.65	-0.377	-0.651	-0.445
W5 Hβ3	-1.713	-1.11	-1.619	-1.193
W5 Hδ1	-0.397	-0.272	-0.389	-0.312
W5 Hε1	-0.204	-0.136	-0.126	-0.075
W5 Hε3	-2.559	-2.288	-2.657	-2.517
W5 Hζ2	-0.092	-0.064	-0.084	-0.042
W5 Hζ3	-0.516	-0.619	-0.545	-0.638
W5 Hη3	-0.117	-0.124	-0.134	-0.098

Intra-residue cross-indole NOEs (impossible for the monomer and dimer; not tetramer) were observed between W2 Hδ1 and W2 Hζ3. Additionally, some tetramer peaks (esp. those on W2) exhibited significant lineshape broadening, presumably due to the effects of slower motions associated with noncovalent assembly and/or disulfide exchange.

Table S3: Chemical shift deviations for oxidized and reduced RWITVTIGGGGCGGGGKKIRVWE (see figure S3 for proposed folding pathways and figure S4 for CD spectra.)

Reduced Form:

Red/ Mono pH3	HN 280	HA 280	HN 300	HA 300	HN 320	HA 320
R1		-0.47		-0.446		-0.362
W2	0.322	0.636	0.32	0.633	0.291	0.571
I3	1.42	0.494	1.331	0.478	1.048	0.482
T4	0.463	0.896	0.439	0.849	0.381	0.707
V5	0.981	0.338	0.914	0.338	0.725	0.297
T6	0.231	0.492	0.224	0.476	0.199	0.395
I7	0.857	0.209	0.747	0.214	0.549	0.189
C12	0.186	-0.093	0.076	-0.072	0.08	-0.042
K17	0.061	0.161	0.052	0.154	-0.011	0.131
K18	0.096	0.774	0.093	0.733	0.092	0.606
I19	0.92	0.446	0.841	0.429	0.643	0.357
R20	0.013	1.082	0.038	1.016	0.059	0.833
V21	1.301	0.74	1.19	0.711	0.918	0.591
W22	0.565	-0.179	0.556	-0.126	0.479	-0.053
E23	-0.139	-0.2	-0.14	-0.198	-0.156	-0.178

Oxidized form:

Ox /di pH3	HN 280	HA 280	HN 300	HA 300	HN 320	HA 320
R1		-0.448		-0.431		-0.379
W2	0.36	0.683	0.362	0.69	0.328	0.636
I3	1.479	0.554	1.423	0.541	1.229	0.477
T4	0.478	0.965	0.47	0.93	0.435	0.815
V5	0.991	0.449	0.958	0.478	0.825	0.411
T6	0.229	0.554	0.25	0.545	0.245	0.474
I7	0.868	0.262	0.781	0.271	0.628	0.243
C12	0.192	0.113	0.155	0.127	0.148	0.133
K17	0.081	0.183	0.063	0.18	0.006	0.156
K18	0.117	0.816	0.112	0.789	0.108	0.687
I19	0.949	0.491	0.89	0.483	0.74	0.408
R20	0.037	1.13	0.069	1.095	0.086	0.953
V21	1.336	0.874	1.254	0.871	1.05	0.745
W22	0.644	-0.149	0.661	-0.093	0.592	-0.047
E23	-0.147	-0.113	-0.146	-0.104	-0.158	-0.118

Trp 22 diagnostic sidechain CSDs

	Ox 280	Ox 300	Ox 320	Red 280	Red 300	Red 320
W22 Hb3	-1.253	-1.161	-0.986	-1.223	-1.109	-0.89
W22 He3	-2.433	-2.249	-1.896	-2.445	-2.202	-1.716
W22 Hz3	-0.52	-0.522	-0.487	-0.56	-0.54	-0.454

Table S4: Ration of the oxidized Cys H_N chemical shift deviation vs. the average H_N chemical shift deviation of its two neighbors. Large H_N CSDs in beta sheets are typically a result of amide protons pointing inward and H-bonding to a cross-strand backbone carbonyl. Since the Cys is at a non-H-bonding site, it is expected to have a lower downfield chemical shift than the H-bonding, inwardly-directed H_Ns of its immediate neighbors, and the ratio is expected to range between 0.4 and 0.7 (a reasonable range for NHB/HB H_N CSD ratios in most beta sheets). However, deviations (values greater than 1) are observed, especially when beta sheets are long and/or contain more than one cross-strand disulfide. This suggests some atypical twisting or buckling of the beta sheet in these cases. NOEs cannot confirm significant distortion, partly because they are at symmetric positions in most cases (and therefore ambiguous / blended).

Bulky beta branched residues help prevent inward buckling of the beta sheets and maintain lower C/neighbors H_N CSD ratios, as expected of beta sheets. (This could also be explained by larger CSDs on folding, due to better protection of cross-strand H-bonds.)

When there are multiple disulfides, or a single disulfide corresponding to different positions on heterodimeric strands, the position farthest toward the C-terminus has the lowest, most "sheet-like" value. (This suggests more distortion toward the N-terminus. The trend is also evident in the ratios of i-1 to i+1; the C-term H_N CSDs are almost always smaller in general.)

	Cys H_N / average of i+1, i-1 H_N
KKTCTTT	*1.66*
KKVCITT	0.93
PWVCKHT	1.17
KWRCIWD *conf.1*	0.74
KWRCIWD *conf.2*	0.38
HWVCIWR *conf.1*	0.70
HWVCIWR *conf.2*	0.26
KWRTVCIRTWE	0.79
RWTTHCHRKWE pH 2	2.97
RWTTHCHRKWE pH 5	2.98
RWTTHCHRKWE pH 8	0.95
KWRTIKVCITKRTWE	0.83
Pr-WVCKWTGPK-NH_2	0.89
WVCKWTGPK-NH_2	*13.2*
Pr-WTTVCIRTWTGP-NH_2	0.81
WTTVCIRTWTGP-NH_2	0.72
Bz-WHTHCIRKWTGP-NH_2 *pH 3*	1.52
Bz-WITKCIRKWTGKK	1.21
RWITKCI**S**IRKWE *homo*	0.18
RWITKCI**S**IRKWE *hetero*	1.12
RWITK**S**ICIRKWE *homo*	-.03
RWITK**S**ICIRKWE *hetero*	0.71
RWITKCICIRKWE *C6*	1.27
RWITKCICIRKWE *C8*	0.96
RWITK**T**C**T**IRKWE *	*1.68*
KWRWRTRCRKIKRWY	1.41
KWRWRTRCICRKIKRWY *C8*	1.33

KWRWTRCICRKIKRWY *C10* 1.19
KWRWTRCR *1.81*
RWKCKCKCKWE *C4* 1.50
RWKCKCKCKWE *C6* 2.37
RWKCKCKCKWE *C8* 1.28
RWITVTIGGGGCGGGGKKIRVWE *2.78*

* Cys in this peptide is at an H-bonding site, so a high ratio is expected.

Table S5: Backbone chemical shift deviations for attempted 4-stranded sheet peptides.

Table S5a: Backbone CSDs for peptide $(KRTTKRDGWVCIWT)_2$ (central beta strand with floppy tails extending from N-terminal end of the structured region. Floppy N-terminal region was unassignable due to poor lineshape and overlapped peaks.)

	H_N CSD	Hα CSD
K1		
R2		
T3		
T4		
K5		
R6		
D7		
G8		
W9	1.2	0.437
V10	1.426	0.375
C11	0.773	1.486
I12	1.038	0.73
W13	0.539	-0.335
T14	0.17	0.083

Table S5b: Backbone CSDs for peptide $(KWVCIWDGRKTTRT)_2$ (central beta strand with floppy tails extending from C-terminal end of the structured region)

	H_N CSD	Hα CSD
K1		-0.421
W2	0.504	0.388
V3	1.264	0.284
C4	0.871	1.481
I5	1.012	0.729
W6	0.843	-0.399
D7	-0.243	-0.036
G8	0.041	-0.051

R9	-0.139	-0.074
K10	0.263	0.026
T11	0.043	0.024
T12	0.265	
R13		
T14		

Table S5c: Backbone CSDs for peptide (RWICRWWDEKSGRWITKKID)$_2$ (complete 4-stranded sheet, with some C-terminal fraying)

	H_N CSD	Hα CSD
R1		0.032
W2	0.581	0.804
I3	1.464	0.567
C4	1.303	1.558
R5	0.911	1.532
W6	1.286	0.3
W7	0.063	-0.717
D8	-0.456	-0.705
E9	-0.074	-0.772
K10	-0.474	-0.359
S11	-1.472	-0.099
G12	-0.66	-0.721
R13	-1.889	0.067
W14	0.314	0.382
I15	1.546	0.46
T16	0.668	0.79
K17	0.497	0.256
K18	0.21	0.31
I19	0.145	0.06
D20	-0.119	-0.15

Table S6: Backbone CSDs for peptides of the form (KWTTHCHRKXX)$_n$.

Table S6a: Backbone CSDs for peptide (KWTTHCHRKWA)$_2$ (This is the almost-fully-folded oxidized species; compare with fully unfolded reduced species.)

KWTTHCHRKWA dimer	280 HN	280 HA
K1		-0.426
W2	0.782	0.657
T3	1.24	0.307

T4	0.711	0.621
H5	0.63	0.228
C6	*0.68*	1.17
H7	0.583	0.404
R8	0.5	1.123
K9	1.014	0.77
W10	0.859	-0.126
A11	0.113	-0.17

Table S6b: Backbone CSDs for peptide KWTTHCHRKWA (monomer; reduced. Entirely unstructured.)

KWTTHCHRKWA mono	280 HN	280 HA
K1		-0.2
W2		0.089
T3	-0.005	-0.03
T4	-0.015	0.055
H5	-0.107	0.035
C6	-0.174	0.019
H7	-0.154	0.036
R8	-0.056	-0.137
K9	0.013	-0.042
W10	-0.008	0.022
A11	0.107	-0.055

Table S6c: Backbone CSDs for peptide $(KWTTHCHRKWT)_2$ (This is the fully-folded oxidized species with a properly-aligned beta cap; compare with almost entirely unfolded isomer with the T and W residues swapped, resulting in a misaligned / nonviable beta cap.)

KWTTHCHRKWT	280 HN	280 HA
K1		-0.527
W2	0.715	0.719
T3	1.239	0.253
T4	0.772	0.607
H5	0.678	0.19
C6	*0.7*	1.226
H7	0.626	0.408
R8	0.459	1.168
K9	1.071	0.821
W10	0.887	-0.004
T11	0.316	0.782

Table S6d: Backbone CSDs for peptide $(KWTTHCHRKTW)_2$ (This peptide has a misaligned/nonviable beta cap due to the switched positions of the two C-terminal residues. Almost no evidence for folding exists, even as the oxidized dimer.)

KWTTHCHRKTW	280 HN	280 HA
K1		-0.141
W2		0.149
T3	0.133	0.007
TT4	0.032	0.002
H5	-0.108	0.07
C6		0.164
H7	0.071	0.089
R8	-0.028	-0.047
K9	0.082	-0.152
T10	-0.377	0.019
W11	-0.07	0.02

Table S7: Raw NOEs for beta ribbon peptide $(KWRTIKVCITKRTWE)_2$, a simple disulfide-mediated beta strand dimer with exceptional stability and sharp lineshapes. Inter-chain NOEs are highlighted in light blue; ambiguous (inter or intra?) highlighted in gray. (Distance is in residues, not a formal distance calculation.)

Atoms	Intensity	Distance
K1Ha-Hb2	medium-faint	0
K1Ha-W2Hd1	faint	1
K1Ha-W2NH	very strong	1
K1Ha-W14Hh3	very faint	13
K1Ha-W14Hz3	faint	13
K1Hb2-W14NH	medium-faint	13
W2Ha-Hb2	faint	0
W2Ha-Hb3	faint	0
W2Ha-Hd1	faint	0
W2Ha-He3	medium-strong	0
W2Ha-NH	medium-faint	0
W2Ha-R3NH	very strong	1
W2Ha-T13NH	very faint	11
W2Ha-E15NH	very faint	13
W2Hb2-Hd1	strong	0
W2Hb2-He1	very faint	0
W2Hb2-He3	faint	0
W2Hb2-NH	medium-strong	0
W2Hb2-R3NH	very faint	1
W2Hb3-Hb2	very strong	0
W2Hb3-Hd1	medium-strong	0
W2Hb3-He3	medium-faint	0

W2Hb3-NH	medium-strong	0
W2Hb3-R3NH	faint	1
W2Hb3-R12He	faint	10
W2He1-Hd1	very strong	0
W2He1-Hz2	strong	0
W2He1-W14Hz3	faint	12
W2Hz2-He3	medium-faint	0
W2Hz3-Hh3	very strong	0
W2NH-Hd1	medium-strong	0
W2NH-He3	faint	0
W2NH-Hz3	faint	0
W2NH-W14Hd1	faint	12
W2NH-E15NH	very faint	13
R3Ha-NH	medium-faint	0
R3Ha-T4NH	very strong	1
R3Ha-T13NH	very faint	10
R3Hb2-NH	faint	0
R3Hb2-T4NH	faint	1
R3Hb3-NH	faint	0
R3Hb3-T4NH	faint	1
R3Hd2-He	strong	0
R3Hg2-T4NH	very faint	1
R3Hg2-T13NH	faint	10
R3Hg3-T4NH	very faint	1
R3Hh21-Hh22	medium-strong	0
R3NH-W2He3	medium-faint	1
R3NH-W14NH	very faint	11
T4Ha-Hg2	strong	0
T4Ha-NH	medium-faint	0
T4Ha-I5NH	very strong	1
T4Ha-R12Ha	very faint	8
T4Ha-T13NH	faint	9
T4Hb-Hg2	very strong	0
T4Hb-NH	medium-strong	0
T4Hb-V7NH	faint	3
T4Hg2-NH	faint	0
T4Hg2-I5NH	medium-strong	1
I5Ha-Hb	medium-strong	0
I5Ha-Hg2	strong	0
I5Ha-NH	medium-strong	0
I5Ha-K6NH	very strong	1
I5Hb-Hg12	faint	0
I5Hb-Hg13	medium-faint	0
I5Hb-NH	faint	0
I5Hb-T10NH	medium-strong	5

I5Hg12-Hb	medium-faint	0
I5Hg12-V7NH	medium-faint	2
I5Hg13-Hb	medium-faint	0
I5Hg2-K6NH	medium-faint	1
I5NH-K11NH	medium-strong	6
K6Ha-Hg3	faint	0
K6Ha-NH	medium-strong	0
K6Ha-V7NH	very strong	1
K6Ha-K11NH	very strong	5
K6Hb2-NH	medium-strong	0
K6Hb2-V7NH	faint	1
K6Hb3-NH	medium-strong	0
K6Hb3-V7NH	faint	1
K6Hg2-NH	very faint	0
K6Hg3-T10NH	faint	4
V7Ha-Hb	faint	0
V7Ha-Hg2	very strong	0
V7Ha-NH	medium-faint	0
V7Ha-C8NH	very strong	1
V7Hb-NH	medium-strong	0
V7Hb-C8NH	faint	1
V7Hg1-NH	strong	0
C8Ha-V7Hg2	faint	1
C8Ha-Hb2	very faint	0
C8Ha-Hb3	medium-faint	0
C8Ha-NH	faint	0
C8Ha-I9NH	very strong	1
C8Hb2-V7NH	faint	1
C8Hb2-NH	medium-strong	0
C8Hb3-K6Hg3	faint	2
C8Hb3-Hb2	very strong	0
C8Hb3-NH	faint	0
C8Hb3-I9NH	medium-faint	1
I9Ha-Hb	medium-strong	0
I9Ha-Hd1	faint	0
I9Ha-Hg2	medium-strong	0
I9Ha-NH	medium-strong	0
I9Ha-T10NH	very strong	1
I9Hb-K6NH	medium-strong	3
I9Hb-C8NH	faint	1
I9Hb-Hg13	faint	0
I9Hb-NH	medium-faint	0
I9Hg13-Hb	medium-faint	0
I9Hg13-Hg12	strong	0
I9Hg2-C8NH	very faint	1

I9Hg2-NH	medium-faint	0
I9Hg2-T10NH	medium-faint	1
I9NH-T10NH	medium-faint	1
T10Ha-V7Hg2	faint	3
T10Ha-I9Hg2	faint	1
T10Ha-Hg2	strong	0
T10Ha-NH	medium-strong	0
T10Ha-K11NH	very strong	1
T10Hb-Hg2	very strong	0
T10Hb-NH	medium-strong	0
T10Hb-K11NH	faint	1
T10Hg2-V7NH	medium-strong	3
T10Hg2-C8NH	medium-faint	2
T10Hg2-NH	medium-faint	0
K11Ha-Hb2	medium-faint	0
K11Ha-Hg3	faint	0
K11Ha-NH	medium-faint	0
K11Ha-R12NH	very strong	1
K11Hb2-NH	faint	0
K11Hb2-R12NH	faint	1
K11Hg3-NH	faint	0
K11Hg3-R12NH	faint	1
K11NH-T10NH	faint	1
R12Ha-W2He3	very faint	10
R12Ha-R3NH	very faint	9
R12Ha-T4Hg2	faint	8
R12Ha-I5NH	faint	7
R12Ha-Hb2	medium-faint	0
R12Ha-Hg3	faint	0
R12Ha-NH	medium-faint	0
R12Ha-T13NH	very strong	1
R12Hb-NH	medium-faint	0
R12Hb-T13NH	faint	1
R12Hb2-W2He3	medium-faint	10
R12Hd2-He	medium-faint	0
R12Hd2-Hg3	faint	0
R12Hd3-He	medium-faint	0
R12Hd3-Hg2	faint	0
R12Hg3-W2He3	medium-faint	10
R12Hg3-He	faint	0
R12Hg3-NH	faint	0
R12Hh21-Hh22	faint	0
R12NH-K11NH	very faint	1
T13Ha-Hg2	medium-strong	0
T13Ha-NH	faint	0

T13Ha-W14NH	very strong	1
T13Hb-I5Hd1	very faint	8
T13Hb-Hg2	very strong	0
T13Hb-NH	faint	0
T13Hb-W14NH	medium-faint	1
T13Hg2-NH	faint	0
T13Hg2-W14NH	faint	1
T13NH-W2He3	faint	11
T13NH-R3NH	medium-faint	10
T13NH-R12NH	very faint	1
T13NH-W14NH	very faint	1
W14Ha-W2He3	faint	12
W14Ha-W2Hz3	very faint	12
W14Ha-R3NH	faint	11
W14Ha-Hb2	faint	0
W14Ha-Hb3	faint	0
W14Ha-Hd1	very faint	0
W14Ha-NH	medium-faint	0
W14Ha-E15NH	very strong	1
W14Hb2-W2Hz3	faint	12
W14Hb2-Hd1	strong	0
W14Hb2-He1	very faint	0
W14Hb2-NH	medium-strong	0
W14Hb3-W2He3	faint	12
W14Hb3-W2Hz3	medium-faint	12
W14Hb3-Hb2	very strong	0
W14Hb3-Hd1	medium-strong	0
W14Hb3-NH	medium-strong	0
W14He1-Hd1	very strong	0
W14He1-Hz2	medium-strong	0
W14He3-W2He3	faint	12
W14He3-W2Hz3	very faint	12
W14He3-Hh3	faint	0
W14He3-Hz3	strong	0
W14Hz3-W2Hd1	medium-strong	12
W14Hz3-W2He1	medium-faint	12
W14Hz3-W2Hz2	medium-faint	12
W14Hz3-Hh3	very strong	0
W14Hz3-NH	very faint	0
W14NH-Hz3	very faint	0
E15Ha-W14Hd1	faint	1
E15Ha-Hb2	faint	0
E15Ha-Hb3	medium-faint	0
E15Ha-Hg2	faint	0
E15Ha-Hg3	faint	0

E15Ha-NH	medium-strong	0
E15Hb2-NH	very faint	0
E15Hg2-NH	faint	0

Table S8: Raw NOEs for beta ribbon peptide $(KWRTVCIRTWE)_2$, a simple disulfide-mediated beta strand dimer with exceptional stability and sharp lineshapes. Inter-chain NOEs are highlighted in light blue; ambiguous (inter or intra?) highlighted in gray. (Distance is in residues, not a formal distance calculation.)

Assignment	Intensity	Distance
K1Ha-Hb2	medium-faint	0
K1Ha-Hg3	very faint	0
K1Ha-W2Hd1	faint	1
K1Ha-W2Hz2	very faint	1
K1Ha-W2NH	very strong	1
K1Ha-W10Hh2	faint	9
K1Ha-W10Hz3	faint	9
K1Hb2-W2NH	medium-strong	1
K1He3-Hd2	medium-strong	0
K1He3-Hg2	very faint	0
K1He3-Hz	very faint	0
K1Hg2-W2NH	very faint	1
W2Ha-K1Ha	very faint	1
W2Ha-Hb2	faint	0
W2Ha-Hb3	medium-strong	0
W2Ha-Hd1	faint	0
W2Ha-He3	medium-strong	0
W2Ha-Hz3	very faint	0
W2Ha-NH	medium-faint	0
W2Ha-R3NH	very strong	1
W2Ha-T9NH	faint	7
W2Ha-W10Ha	very faint	8
W2Ha-E11NH	faint	9
W2Hb2-Hd1	strong	0
W2Hb2-He1	very faint	0
W2Hb2-He3	faint	0
W2Hb2-NH	strong	0
W2Hb2-R3NH	very faint	1
W2Hb2-R8He	very faint	6
W2Hb3-Hd1	medium-strong	0
W2Hb3-He3	medium-faint	0
W2Hb3-NH	medium-strong	0
W2Hb3-R3NH	medium-faint	1
W2Hb3-R8Hd2	very faint	6
W2Hb3-R8He	very faint	6

W2Hb3-E11Hg3	very faint	9
W2Hb3-E11NH	very faint	9
W2Hd1-NH	medium-faint	0
W2He1-Hd1	very strong	0
W2He1-Hh2	very faint	0
W2He1-Hz2	medium-strong	0
W2He1-W10Hd1	very faint	8
W2He1-W10Hh2	very faint	8
W2He1-W10Hz2	very faint	8
W2He1-W10Hz3	faint	8
W2He3-NH	very faint	0
W2He3-R3NH	medium-faint	1
W2He3-T9NH	faint	7
W2He3-W10NH	very faint	8
W2He3-E11NH	very faint	9
W2Hh2-W10NH	very faint	8
W2Hz2-R8He	very faint	6
W2Hz3-W10NH	medium-faint	8
W2NH-R3NH	very faint	1
R3Ha-Hb2	medium-faint	0
R3Ha-Hb3	medium-faint	0
R3Ha-Hd2	medium-faint	0
R3Ha-Hg2	medium-faint	0
R3Ha-Hg3	faint	0
R3Ha-NH	medium-faint	0
R3Ha-T4Hb	very faint	1
R3Ha-T4NH	very strong	1
R3Hb2-He	very faint	0
R3Hb2-NH	medium-faint	0
R3Hb2-T4NH	faint	1
R3Hb3-He	very faint	0
R3Hb3-NH	medium-faint	0
R3Hb3-T4NH	faint	1
R3Hb3-T9NH	very faint	6
R3Hd2-Hb2	faint	0
R3Hd2-Hb3	faint	0
R3Hd2-He	medium-strong	0
R3Hd2-Hg3	faint	0
R3Hd2-T4NH	very faint	1
R3Hd2-V5Hg2	medium-faint	2
R3Hg2-He	faint	0
R3Hg2-NH	faint	0
R3Hg2-T4NH	faint	1
R3Hg2-T9NH	faint	6
R3Hg3-He	faint	0

R3Hg3-NH	very faint	0
R3Hg3-T4NH	faint	1
R3Hh22-He	very faint	0
R3NH-T9NH	medium-strong	6
T4Ha-Hb	faint	0
T4Ha-Hg2	strong	0
T4Ha-NH	medium-strong	0
T4Ha-NH	very strong	0
T4Ha-V5Hg2	faint	1
T4Ha-V5NH	very strong	1
T4Ha-T9NH	faint	5
T4Hb-Hg2	very strong	0
T4Hb-NH	strong	0
T4Hb-V5NH	very faint	1
T4Hg2-NH	medium-faint	0
T4Hg2-V5NH	medium-strong	1
T4Hg2-C6NH	very faint	2
T4Hg2-I7NH	medium-faint	3
V5Ha-T4Hg2	very faint	1
V5Ha-Hb	faint	0
V5Ha-Hg2	very strong	0
V5Ha-NH	medium-faint	0
V5Ha-C6Hb2	very faint	1
V5Ha-C6NH	very strong	1
V5Ha-I7NH	medium-faint	2
V5Hb-NH	medium-strong	0
V5Hb-C6NH	very faint	1
V5Hg2-R3Hd2	faint	2
V5Hg2-R3He	faint	2
V5Hg2-Hb	very strong	0
V5Hg2-NH	strong	0
V5Hg2-C6NH	medium-strong	1
V5Hg2-T9Hg2	strong	4
C6Ha-T4Hg2	faint	2
C6Ha-V5NH	very faint	1
C6Ha-Hb2	faint	0
C6Ha-Hb3	medium-strong	0
C6Ha-NH	medium-strong	0
C6Ha-I7Hb	very faint	1
C6Ha-I7Hg2	faint	1
C6Ha-I7NH	very strong	1
C6Hb2-T4Hg2	medium-faint	2
C6Hb2-NH	medium-strong	0
C6Hb2-I7NH	faint	1
C6Hb3-T4Hg2	strong	2

C6Hb3-V5NH	very faint	1
C6Hb3-Hb2	very strong	0
C6Hb3-NH	medium-faint	0
C6Hb3-I7NH	medium-faint	1
I7Ha-Hb	medium-faint	0
I7Ha-Hd1	faint	0
I7Ha-Hg12	very faint	0
I7Ha-Hg13	faint	0
I7Ha-Hg2	strong	0
I7Ha-NH	medium-faint	0
I7Ha-R8Hb2	very faint	1
I7Ha-R8Hb3	very faint	1
I7Ha-R8Hg3	very faint	1
I7Ha-R8NH	very strong	1
I7Hb-NH	medium-faint	0
I7Hb-R8NH	medium-strong	1
I7Hd1-V5NH	very faint	2
I7Hd1-C6NH	very faint	1
I7Hd1-NH	very faint	0
I7Hd1-T9Hg2	medium-faint	2
I7Hg12-NH	faint	0
I7Hg12-R8NH	faint	1
I7Hg13-Hb	medium-faint	0
I7Hg13-NH	faint	0
I7Hg13-R8NH	very faint	1
I7Hg2-NH	medium-strong	0
I7NH-V5NH	medium-strong	2
R8Ha-W2He3	very faint	6
R8Ha-R3NH	very faint	5
R8Ha-T4Hg2	faint	4
R8Ha-T4NH	very faint	4
R8Ha-I7Hg2	very faint	1
R8Ha-Hb2	faint	0
R8Ha-Hb3	faint	0
R8Ha-Hd2	very faint	0
R8Ha-Hg3	medium-faint	0
R8Ha-NH	medium-strong	0
R8Ha-T9Hg2	very faint	1
R8Ha-T9NH	very strong	1
R8Hb2-W2He3	faint	6
R8Hb2-W2Hz3	very faint	6
R8Hb2-He	very faint	0
R8Hb2-NH	medium-strong	0
R8Hb2-T9NH	very faint	1
R8Hb3-W2He3	faint	6

R8Hb3-He	very faint	0
R8Hb3-NH	medium-faint	0
R8Hb3-T9NH	very faint	1
R8Hd2-W2Hb2	very faint	6
R8Hd2-W2He3	very faint	6
R8Hd2-Hb2	faint	0
R8Hd2-He	medium-strong	0
R8Hd2-NH	very faint	0
R8Hg2-W2Hz3	faint	6
R8Hg2-W2NH	very faint	6
R8Hg2-NH	medium-faint	0
R8Hg2-T9NH	faint	1
R8Hg3-W2He3	medium-faint	6
R8Hg3-He	faint	0
R8Hh21-Hd2	very faint	0
R8Hh21-He	very faint	0
R8Hh22-Hd2	very faint	0
R8Hh22-He	very faint	0
R8NH-T9NH	faint	1
T9Ha-W2Hz3	faint	7
T9Ha-Hg2	medium-strong	0
T9Ha-NH	medium-faint	0
T9Ha-W10Hb2	very faint	1
T9Hb-R3NH	very faint	6
T9Hb-V5Hg2	medium-faint	4
T9Hb-Hg2	very strong	0
T9Hb-NH	medium-faint	0
T9Hb-W10NH	medium-faint	1
T9Hg2-R3He	very faint	6
T9Hg2-R3NH	very faint	6
T9Hg2-R8NH	very faint	1
T9Hg2-NH	medium-faint	0
T9Hg2-W10NH	medium-faint	1
T9Hg2-E11Hg3	very faint	2
W10Ha-W2He3	medium-faint	8
W10Ha-W2Hz3	very faint	8
W10Ha-R3NH	faint	7
W10Ha-Hb2	faint	0
W10Ha-Hb3	medium-strong	0
W10Ha-Hd1	very faint	0
W10Ha-NH	medium-faint	0
W10Ha-E11NH	very strong	1
W10Hb2-W2He3	very faint	8
W10Hb2-W2Hh2	very faint	8
W10Hb2-W2Hz3	very faint	8

W10Hb2-Hd1	medium-strong	0
W10Hb2-He1	very faint	0
W10Hb2-NH	strong	0
W10Hb2-E11NH	very faint	1
W10Hb3-W2He3	very faint	8
W10Hb3-W2Hh2	faint	8
W10Hb3-W2Hz3	medium-faint	8
W10Hb3-Hd1	medium-faint	0
W10Hb3-He1	very faint	0
W10Hb3-NH	medium-strong	0
W10Hb3-E11NH	very faint	1
W10Hd1-NH	very faint	0
W10Hd1-E11NH	very faint	1
W10He1-Hd1	very strong	0
W10He1-Hh2	very faint	0
W10He1-Hz2	medium-strong	0
W10He3-K1Ha	very faint	9
W10He3-W2Hd1	faint	8
W10He3-W2He1	faint	8
W10He3-W2He3	faint	8
W10He3-W2Hh2	very faint	8
W10He3-W2Hz2	medium-faint	8
W10He3-W2Hz3	very faint	8
W10He3-W2NH	very faint	8
W10He3-R3NH	very faint	7
W10He3-Ha	very faint	0
W10He3-Hb2	very faint	0
W10He3-Hb3	medium-faint	0
W10He3-Hh2	faint	0
W10He3-Hz3	very strong	0
W10He3-NH	very faint	0
W10He3-E11NH	faint	1
W10Hh2-W2NH	very faint	8
W10Hz2-Hh2	very faint	0
W10Hz3-W2Hd1	medium-strong	8
W10Hz3-W2NH	faint	8
W10Hz3-Hh2	very strong	0
W10NH-R3NH	very faint	7
W10NH-T9NH	very faint	1
E11Ha-W10Hd1	very faint	1
E11Ha-Hb2	very faint	0
E11Ha-Hb3	medium-faint	0
E11Ha-Hg3	faint	0
E11Ha-NH	medium-strong	0
E11Hb2-T9NH	very faint	2

E11Hb2-NH	faint	0
E11Hb3-T9NH	faint	2
E11Hb3-NH	faint	0
E11Hg2-R3NH	very faint	8
E11Hg2-NH	faint	0
E11NH-R3NH	very faint	8
E11NH-W10He1	very faint	1
E11NH-W10NH	very faint	1

Table S9: Raw NOEs for beta ribbon peptide $(KWRCIWD)_2$, a disulfide-mediated beta strand dimer which can also exist (in this case, in the same sample) as a higher-order oligomer. (Likely a tetramer.) Data for the two separate conformers are highlighted in orange and purple; orange represents the presumed tetramer, and purple represents the presumed dimer. Inter-chain NOEs are highlighted in light blue, "impossible" intra-indole NOEs that can only be explained by higher-order assembly (e.g., as the proposed tetramer) are in orange, and ambiguous NOEs appear in gray. Sample concentration was 3.5 mM (per chain; 1.75 mM of dimer). (Distance is in residues, not a formal distance calculation.)

Atoms	Intensity	Distance
K1Ha-Hb2	medium-strong	0
K1Ha-Hg2	faint	0
K1Ha-W2Hd1	very faint	1
K1Ha-W2NH	very strong	1
K1Ha-W6Hh2	faint	5
K1Ha-W6Hz3	medium-faint	5
K1Hb2-W2NH	medium-strong	1
K1Hb2-W6Hz3	very faint	5
K1Hb2-D7NH	very faint	6
K1He2-Hd2	strong	0
K1He2-Hg2	faint	0
K1Hg2-W2NH	faint	1
K1'Ha-Hb2	medium-faint	0
K1'Ha-W2'Hd1	very faint	1
K1'Ha-W2'NH	strong	1
K1'Ha-W6Hh2	very faint	5
K1'Ha-W6'Hz3	faint	5
K1'Ha-D7'NH	very faint	6
K1'Hb2-W2'NH	medium-faint	1
K1'Hg2-W2'NH	very faint	1
K1'Hg2-D7'NH	very faint	6
W2Ha-Hb2	faint	0
W2Ha-He3	medium-faint	0
W2Ha-NH	faint	0
W2Ha-R3Hb2	very faint	1
W2Ha-R3NH	very strong	1

W2Ha-W6Ha	very faint	4
W2Ha-D7NH	faint	5
W2Hb2-Hd1	very faint	0
W2Hb2-He3	faint	0
W2Hb2-NH	faint	0
W2Hb2-R3NH	faint	1
W2Hb3-Hd1	faint	0
W2Hb3-He3	faint	0
W2Hb3-NH	medium-strong	0
W2Hb3-R3NH	very faint	1
W2He1-Hd1	medium-faint	0
W2He1-He3	faint	0
W2He1-Hh2	very faint	0
W2He1-Hz2	medium-strong	0
W2He1-W6Hd1	very faint	4
W2He1-W6Hz3	faint	4
W2He3-Hd1	very faint	0
W2He3-D7NH	very faint	5
W2Hh2-Hd1	very faint	0
W2Hz2-Hd1	very faint	0
W2NH-Hd1	faint	0
W2NH-He3	very faint	0
W2NH-R3NH	very faint	1
W2NH-W6Hz3	faint	4
W2'Ha-K1'Ha	very faint	1
W2'Ha-Hb2	medium-strong	0
W2'Ha-Hd1	very faint	0
W2'Ha-He3	medium-strong	0
W2'Ha-NH	faint	0
W2'Ha-R3'NH	very strong	1
W2'Ha-I5'NH	very faint	3
W2'Ha-D7'NH	faint	5
W2'Hb2-Hd1	strong	0
W2'Hb2-He1	very faint	0
W2'Hb2-He3	medium-strong	0
W2'Hb2-NH	strong	0
W2'Hb2-R3'NH	faint	1
W2'Hb2-W6'Hz3	very faint	4
W2'Hd1-NH	faint	0
W2'Hd1-W6'Hh2	faint	4
W2'He1-Hd1	very strong	0
W2'He1-Hh2	very faint	0
W2'He1-Hz2	medium-faint	0
W2'He1-W6'Hz3	very faint	4
W2'He3-NH	very faint	0

W2'He3-R3'NH	faint	1
W2'He3-I5'NH	very faint	3
W2'He3-W6'NH	very faint	4
W2'He3-D7'NH	very faint	5
W2'Hh2-Hz2	very strong	0
W2'Hh2-W6'NH	very faint	4
W2'Hz3-He3	very strong	0
W2'Hz3-Hh2	very strong	0
W2'Hz3-I5'NH	very faint	3
W2'Hz3-W6'NH	faint	4
R3Ha-W2NH	very faint	1
R3Ha-Hb2	medium-strong	0
R3Ha-Hg2	medium-faint	0
R3Ha-NH	medium-faint	0
R3Ha-C4NH	very strong	1
R3Ha-I5Hg2	medium-faint	2
R3Hb2-He	faint	0
R3Hb2-NH	medium-faint	0
R3Hb2-C4NH	medium-faint	1
R3Hb2-I5Hd1	faint	2
R3Hb2-I5Hg2	faint	2
R3Hb2-D7NH	very faint	4
R3Hd2-He	medium-strong	0
R3Hd2-NH	very faint	0
R3Hd2-I5Hd1	very faint	2
R3Hd2-I5Hg2	faint	2
R3Hg2-He	medium-faint	0
R3Hg2-NH	medium-faint	0
R3Hg2-C4NH	very faint	1
R3NH-W2He3	medium-faint	1
R3NH-W2Hz3	very faint	1
R3'Ha-NH	medium-faint	0
R3'Ha-C4'NH	very strong	1
R3'Hb2-NH	faint	0
R3'Hb2-C4'NH	very faint	1
R3'Hb3-NH	faint	0
R3'Hb3-C4'NH	very faint	1
R3'Hg2-He	very faint	0
R3'Hg2-NH	very faint	0
R3'Hg2-C4'NH	very faint	1
R3'Hg3-NH	very faint	0
R3'Hg3-C4'NH	very faint	1
R3'NH-W2'He3	faint	1
R3'NH-W2'NH	very faint	1
R3'NH-I5'NH	faint	2

C4Ha-Hb2	faint	0
C4Ha-Hb3	medium-faint	0
C4Ha-NH	faint	0
C4Ha-I5Hb	very faint	1
C4Ha-I5Hg2	very faint	1
C4Ha-I5NH	very strong	1
C4Hb2-W2He3	faint	2
C4Hb2-W2Hz3	very faint	2
C4Hb2-NH	medium-strong	0
C4Hb2-I5NH	faint	1
C4Hb3-W2He3	medium-faint	2
C4Hb3-W2Hz3	very faint	2
C4Hb3-NH	medium-faint	0
C4Hb3-I5NH	faint	1
C4NH-R3NH	very faint	1
C4NH-I5NH	very faint	1
C4'Ha-W2'Hb2	very faint	2
C4'Ha-W2'He3	very faint	2
C4'Ha-R3'NH	very faint	1
C4'Ha-Hb2	faint	0
C4'Ha-Hb3	medium-faint	0
C4'Ha-NH	medium-faint	0
C4'Ha-I5'Hg13	very faint	1
C4'Ha-I5'Hg2	very faint	1
C4'Ha-I5'NH	very strong	1
C4'Hb2-W2'He3	faint	2
C4'Hb2-W2'Hz3	very faint	2
C4'Hb2-NH	medium-faint	0
C4'Hb2-I5'NH	very faint	1
C4'Hb2-W6'He1	very faint	2
C4'Hb3-W2'He3	medium-strong	2
C4'Hb3-W2'Hz3	very faint	2
C4'Hb3-R3'NH	very faint	1
C4'Hb3-NH	very faint	0
C4'Hb3-I5'NH	faint	1
I5Ha-W2He3	medium-faint	3
I5Ha-W2Hz2	faint	3
I5Ha-W2Hz3	medium-strong	3
I5Ha-Hb	medium-strong	0
I5Ha-Hd1	medium-faint	0
I5Ha-Hg12	faint	0
I5Ha-Hg13	very faint	0
I5Ha-Hg2	strong	0
I5Ha-NH	medium-faint	0
I5Ha-W6NH	very strong	1

I5Hb-W2Hz3	very faint	3
I5Hb-R3He	very faint	2
I5Hb-Hd1	medium-strong	0
I5Hb-Hg12	medium-strong	0
I5Hb-Hg13	medium-faint	0
I5Hb-Hg2	very strong	0
I5Hb-NH	faint	0
I5Hb-W6NH	medium-strong	1
I5Hd1-R3He	very faint	2
I5Hd1-NH	faint	0
I5Hd1-W6NH	very faint	1
I5Hd1-D7NH	very faint	2
I5Hg12-NH	medium-faint	0
I5Hg12-W6NH	faint	1
I5Hg12-D7NH	very faint	2
I5Hg13-NH	medium-faint	0
I5Hg13-W6NH	very faint	1
I5Hg2-W2Hz3	very faint	3
I5Hg2-R3He	very faint	2
I5Hg2-C4NH	very faint	1
I5Hg2-NH	medium-strong	0
I5Hg2-W6NH	medium-faint	1
I5Hg2-D7NH	very faint	2
I5'Ha-W2'He3	faint	3
I5'Ha-W2'Hz3	faint	3
I5'Ha-NH	medium-faint	0
I5'Ha-W6'Hb3	very faint	1
I5'Ha-W6'NH	very strong	1
I5'Hb-NH	faint	0
I5'Hb-W6'NH	medium-faint	1
I5'Hd1-NH	very faint	0
I5'Hd1-W6'NH	very faint	1
I5'Hg12-NH	very faint	0
I5'Hg12-W6'NH	very faint	1
I5'Hg13-NH	very faint	0
I5'Hg13-W6'NH	very faint	1
I5'Hg2-R3'NH	very faint	2
I5'Hg2-NH	very faint	0
I5'Hg2-W6'NH	faint	1
I5'Hg2-D7'NH	very faint	2
W6Ha-W2He3	very faint	4
W6Ha-W2Hz3	very faint	4
W6Ha-R3NH	faint	3
W6Ha-I5Hb	very faint	1
W6Ha-Hb2	faint	0

W6Ha-Hb3	faint	0
W6Ha-Hd1	very faint	0
W6Ha-Hz3	very faint	0
W6Ha-NH	faint	0
W6Ha-D7Hb3	very faint	1
W6Ha-D7NH	very strong	1
W6Hb2-W2Hh2	very faint	4
W6Hb2-W2Hz2	very faint	4
W6Hb2-Hd1	strong	0
W6Hb2-He1	very faint	0
W6Hb2-NH	medium-strong	0
W6Hb3-W2Hz2	faint	4
W6Hb3-W2Hz3	very faint	4
W6Hb3-Hd1	medium-faint	0
W6Hb3-NH	medium-faint	0
W6Hb3-D7NH	very faint	1
W6Hd1-D7NH	very faint	1
W6He1-Hd1	very strong	0
W6He1-Hh2	very faint	0
W6He1-Hz2	medium-strong	0
W6He3-W2Hd1	very faint	4
W6He3-Hb2	very faint	0
W6He3-Hb3	faint	0
W6He3-Hz3	strong	0
W6Hh2-Hz2	medium-strong	0
W6Hz3-W2Hd1	faint	4
W6Hz3-Hh2	strong	0
W6Hz3-Hz2	medium-faint	0
W6NH-W2He3	very faint	4
W6NH-W2Hz3	faint	4
W6NH-I5NH	very faint	1
W6NH-Hd1	faint	0
W6'Ha-W2'He3	faint	4
W6'Ha-W2'Hz3	very faint	4
W6'Ha-R3'NH	very faint	3
W6'Ha-Hb2	faint	0
W6'Ha-Hb3	medium-faint	0
W6'Ha-Hd1	very faint	0
W6'Ha-NH	faint	0
W6'Ha-D7'NH	very strong	1
W6'Hb2-Hd1	strong	0
W6'Hb2-NH	medium-strong	0
W6'Hb2-D7'NH	very faint	1
W6'Hb3-W2'He3	very faint	4
W6'Hb3-W2'Hh2	very faint	4

W6'Hb3-W2'Hz2	very faint	4
W6'Hb3-W2'Hz3	faint	4
W6'Hb3-Hd1	medium-faint	0
W6'Hb3-NH	medium-faint	0
W6'Hb3-D7'NH	very faint	1
W6'Hd1-NH	very faint	0
W6'He1-Hd1	very strong	0
W6'He1-Hh2	very faint	0
W6'He1-Hz2	medium-strong	0
W6'He3-K1'Ha	very faint	5
W6'He3-W2'Hb2	very faint	4
W6'He3-W2'Hd1	very faint	4
W6'He3-W2'He1	very faint	4
W6'He3-W2'He3	very faint	4
W6'He3-W2'Hz2	very faint	4
W6'He3-W2'NH	very faint	4
W6'He3-Hb2	very faint	0
W6'He3-Hb3	faint	0
W6'He3-Hz3	medium-strong	0
W6'He3-D7'NH	very faint	1
W6'Hz3-W2'Hd1	medium-faint	4
W6'Hz3-W2'NH	very faint	4
W6'Hz3-Hh2	very strong	0
W6'Hz3-Hz2	faint	0
D7Ha-I5Hd1	very faint	2
D7Ha-W6Hd1	medium-faint	1
D7Ha-W6He1	very faint	1
D7Ha-Hb2	faint	0
D7Ha-Hb3	medium-faint	0
D7Ha-NH	medium-strong	0
D7Hb2-I5Hd1	very faint	2
D7Hb2-NH	faint	0
D7Hb3-I5Hd1	faint	2
D7Hb3-W6Hd1	very faint	1
D7Hb3-NH	faint	0
D7NH-W2NH	very faint	5
D7NH-R3NH	very faint	4
D7NH-W6NH	very faint	1
D7'Ha-Hb2	faint	0
D7'Ha-Hb3	medium-faint	0
D7'Ha-NH	medium-strong	0
D7'Hb2-NH	very faint	0
D7'Hb3-NH	very faint	0
D7'NH-R3'NH	very faint	4
D7'NH-W6'NH	very faint	1

Table S10: Raw NOEs for "disulfide zipper" peptide $(RWKCKCKCKWE)_2$, an amphiphilic beta-strand dimer with superfluous disulfide crosslinks. The oligomerization state (e.g., simple dimer, dimer of dimers, or mix of higher-order assemblies) cannot be determined. Lineshapes in the middle of the chain are poor (presumably due to medium-slow exchange between oligomeric states) which makes precise structure determination impossible. (For example, the sheet is likely to be highly buckled and/or twisted in this region, due to the three consecutive tight disulfide constraints, but confirmation of the precise nature of this distortion is impossible with the current data.)

Distances (in residues) are highlighted in blue if the corresponding NOEs are inter-chain (e.g., consistent with confirmed interchain NOEs seen in related structures, and only explainable by contacts at a dimer interface), and in gray if they are ambiguous.

Atoms	Intensity	Distance
R1Ha-Hb2	medium-strong	0
R1Ha-Hb3	medium-strong	0
R1Ha-Hg2	very faint	0
R1Ha-Hg3	very faint	0
R1Ha-W2NH	faint	1
R1Ha-W10Hh2	very faint	9
R1Ha-W10Hz3	very faint	9
R1Hd2-Hb2	medium-strong	0
R1Hd2-Hg2	strong	0
R1Hd3-Hg3	medium-strong	0
W2Ha-Hd1	very faint	0
W2Ha-NH	very faint	0
W2Ha-K3NH	faint	1
W2Ha-W10Ha	very faint	8
W2Hb2-NH	faint	0
W2Hb3-Hd1	medium-faint	0
W2NH-Hd1	very faint	0
K3Ha-W2Hd1	very faint	1
K3Ha-Hb3	strong	0
K3Ha-Hg2	medium-strong	0
K3Ha-Hg3	medium-faint	0
K3Ha-NH	very strong	0
K3Ha-C4NH	very strong	1
K3Hb2-C4NH	medium-faint	1
K3Hb3-NH	medium-faint	0
K3Hb3-C4NH	medium-faint	1
K3He2-Hg2	medium-faint	0
K3He3-Hd3	strong	0
K3He3-Hg3	medium-faint	0

K3NH-W2Hz3	faint	1
K3NH-K9NH	faint	6
K3NH-E11NH	very faint	8
C4Ha-NH	faint	0
C4Ha-K5NH	very strong	1
C4Hb2-NH	medium-faint	0
C4Hb2-K5NH	medium-faint	1
C4Hb3-NH	faint	0
C4Hb3-K5NH	medium-strong	1
K5Ha-C4Ha	medium-strong	1
K5Ha-NH	strong	0
K5Ha-C6NH	very strong	1
K5Ha-K9NH	very faint	4
K5Hb2-NH	medium-strong	0
K5Hb2-C6NH	faint	1
K5Hb3-NH	strong	0
K5Hg2-NH	faint	0
K5Hg3-NH	faint	0
C6Ha-K5Hb2	medium-faint	1
C6Ha-K5Hb3	medium-faint	1
C6Ha-NH	medium-faint	0
C6Ha-K7NH	very strong	1
C6Hb2-NH	medium-strong	0
C6Hb2-K7NH	medium-strong	1
C6Hb3-NH	medium-faint	0
C6Hb3-K7NH	strong	1
C6NH-K5NH	faint	1
C6NH-K7NH	faint	1
K7Ha-C6Ha	medium-strong	1
K7Ha-NH	strong	0
K7Ha-C8NH	medium-faint	1
K7Hb2-NH	strong	0
K7Hb3-NH	strong	0
K7Hg2-NH	medium-faint	0
K7Hg3-NH	faint	0
C8Ha-W2Hz3	very faint	6
C8Ha-K7Hb2	medium-faint	1
C8Ha-K7Hb3	medium-faint	1
C8Ha-K7Hg3	very faint	1
C8Ha-NH	very faint	0
C8Ha-K9NH	strong	1
K9Ha-W2Hz3	faint	7
K9Ha-K3NH	very faint	6
K9Ha-Hb2	medium-strong	0
K9Ha-Hb3	medium-strong	0

K9Ha-Hd3	faint	0
K9Ha-Hg2	faint	0
K9Ha-Hg3	faint	0
K9Ha-NH	faint	0
K9Ha-W10NH	faint	1
K9Hb2-NH	faint	0
K9Hb3-NH	faint	0
K9Hg2-NH	faint	0
K9Hg3-NH	very faint	0
K9NH-W2Hz3	faint	7
W10Ha-W2Hz3	faint	8
W10Ha-K3NH	very faint	7
W10Ha-Hb2	faint	0
W10Ha-Hd1	faint	0
W10Ha-E11NH	very strong	1
W10Hb2-Hd1	strong	0
W10Hb2-E11NH	very faint	1
W10Hb3-Hb2	medium-strong	0
W10Hb3-Hd1	medium-faint	0
W10He1-Hd1	very strong	0
W10He3-Hh2	very faint	0
W10He3-Hz3	very faint	0
W10Hz3-Hh2	medium-strong	0
W10NH-Hd1	faint	0
E11Ha-W10Hd1	medium-faint	1
E11Ha-NH	medium-strong	0
E11Hb2-NH	faint	0
E11Hb3-NH	medium-faint	0
E11Hg2-NH	faint	0
E11Hg3-NH	faint	0

Table S11: Raw NOEs for peptide $(RWICRWDEKSGRWITKKID)_2$, a hairpin that dimerizes (via a disulfide-centered sheet) to a four-stranded sheet. (The outer strands appear frayed at the ends, and lineshape broadening in the inner strands has hampered the calculation of consistenty-calibrated distance constraints.)

Distances (in residues) are highlighted in blue if the corresponding NOEs are inter-chain (e.g., consistent with confirmed interchain NOEs seen in related structures, and only explainable by contacts at a dimer interface), and in gray if they are ambiguous.

Atoms	intensity	distance
R1Ha-Hb2	medium-faint	0
R1Ha-Hb3	faint	0
R1Ha-Hg3	faint	0
R1Ha-W2NH	strong	1
R1Ha-W6Hz3	faint	5

R1Hd2-Hg2	strong	0
W2Ha-Hb2	faint	0
W2Ha-Hd1	faint	0
W2Ha-NH	very faint	0
W2Ha-I3NH	medium	1
W2Ha-W14Hh2	faint	12
W2Hb2-Hd1	strong	0
W2Hb3-NH	medium	0
W2He1-Hd1	strong	0
W2He1-Hz2	medium	0
W2Hh2-Hz2	strong	0
W2Hz3-He3	very strong	0
W2Hz3-Hz2	very strong	0
I3Ha-NH	medium	0
I3Ha-C4NH	medium	1
I3Hb-Hd1	medium	0
I3Hb-Hg2	very strong	0
I3Hb-NH	faint	0
I3Hb-C4NH	very faint	1
I3Hb-W6NH	faint	3
I3Hd1-W14Hh2	faint	11
I3Hd1-W14Hz2	very faint	11
I3Hd1-W14Hz3	faint	11
I3Hg12-Hd1	strong	0
I3Hg13-Hd1	strong	0
I3Hg2-NH	very faint	0
I3Hg2-C4NH	very faint	1
I3Hg2-W14Hh2	faint	11
I3Hg2-W14Hz3	faint	11
C4Ha-NH	very faint	0
C4Ha-R5NH	medium	1
C4Hb2-W2Hd1	medium	2
C4Hb2-NH	very faint	0
C4Hb2-R5NH	very faint	1
C4Hb3-W2He3	strong	2
C4Hb3-NH	very faint	0
C4Hb3-R5NH	very faint	1
R5Ha-W2Hh2	faint	3
R5Ha-Hb2	faint	0
R5Ha-NH	very faint	0
R5Ha-W6NH	medium	1
R5Ha-K17NH	very faint	12
R5Hb2-W6NH	faint	1
R5Hb3-W6NH	very faint	1
R5Hg3-NH	very faint	0

W6Ha-W2Ha	faint	4
W6Ha-Hb2	very faint	0
W6Ha-Hb3	very faint	0
W6Ha-Hd1	very faint	0
W6Ha-NH	faint	0
W6Ha-W7NH	faint	1
W6Ha-W14Hh2	faint	8
W6Hb2-Hb3	faint	0
W6Hb2-Hd1	very faint	0
W6Hb2-NH	faint	0
W6He1-Hd1	medium	0
W6He1-Hz2	strong	0
W6He3-Hz3	strong	0
W6Hz3-Hh2	very strong	0
W6Hz3-Hz2	medium	0
W6NH-W2Hh2	faint	4
W6NH-W2Hz3	very faint	4
W7Ha-NH	very faint	0
W7Ha-D8NH	medium	1
W7Ha-W14He3	faint	7
W7Hb2-Hd1	medium	0
W7Hb2-NH	very faint	0
W7Hb3-Hb2	medium	0
W7Hb3-Hd1	faint	0
W7Hb3-NH	very faint	0
W7Hd1-E9NH	very faint	2
W7He1-Hd1	very strong	0
W7He1-Hz2	strong	0
W7Hh2-Hz2	very strong	0
W7Hz3-Hh2	very strong	0
W7Hz3-W14Hd1	medium	7
W7Hz3-W14NH	very faint	7
W7NH-W14Hh2	faint	7
D8Ha-W6He1	very faint	2
D8Ha-NH	faint	0
D8Ha-E9NH	very strong	1
D8Hb2-NH	medium	0
D8Hb2-G12NH	faint	4
D8Hb3-NH	faint	0
E9Ha-W7Hd1	faint	2
E9Ha-W7He1	strong	2
E9Ha-W7Hz2	faint	2
E9Ha-NH	medium	0
E9Ha-K10NH	very faint	1
E9Ha-G12NH	faint	3

E9Hb2-W7Hd1	faint	2
E9Hb2-NH	strong	0
E9Hb3-W7Hd1	faint	2
E9Hb3-NH	strong	0
E9Hb3-K10NH	faint	1
E9Hg2-NH	very faint	0
E9Hg3-NH	faint	0
E9NH-W7Hd1	very faint	2
K10Ha-W6Hz3	very faint	4
K10Ha-E9NH	strong	1
K10Ha-Hb2	very strong	0
K10Ha-Hd2	faint	0
K10Ha-Hg2	faint	0
K10Ha-Hg3	faint	0
K10Ha-NH	strong	0
K10Hb2-NH	very strong	0
K10Hg2-NH	very faint	0
K10NH-E9NH	medium	1
S11Ha-W7Hh2	very faint	4
S11Ha-NH	faint	0
S11Ha-G12NH	faint	1
S11Hb2-G12NH	faint	1
S11Hb3-G12NH	faint	1
S11NH-G12NH	medium	1
G12Ha2-W7Hh2	faint	5
G12Ha2-W7Hz2	medium	5
G12Ha2-NH	medium	0
G12Ha3-W7Hh2	faint	5
G12Ha3-W7Hz2	medium	5
G12Ha3-NH	strong	0
G12NH-R13NH	very faint	1
R13Ha-W7Hz3	faint	6
R13Ha-W14Hd1	faint	1
R13Ha-W14NH	very strong	1
R13Hb3-W14NH	medium	1
R13Hg2-W14NH	faint	1
W14Ha-NH	very faint	0
W14Hb2-Hd1	strong	0
W14Hb2-He3	faint	0
W14Hb2-NH	medium	0
W14Hb2-I15NH	very faint	1
W14Hb3-Hd1	medium	0
W14Hb3-He3	medium	0
W14Hb3-NH	faint	0
W14Hb3-I15NH	very faint	1

W14He1-W7Hz3	faint	7
W14He1-Hd1	very strong	0
W14He1-Hz2	strong	0
W14Hh2-Hz2	very strong	0
W14Hz3-He3	faint	0
W14Hz3-Hz2	very strong	0
W14NH-W7Hz3	very faint	7
W14NH-Hd1	medium	0
I15Ha-Hd1	medium	0
I15Ha-Hg2	strong	0
I15Ha-NH	very faint	0
I15Ha-T16NH	strong	1
I15Hb-Hd1	medium	0
I15Hb-Hg2	strong	0
I15Hb-NH	very faint	0
I15Hb-T16NH	very faint	1
I15Hd1-W6Hd1	very faint	9
I15Hd1-W6Hz3	very faint	9
I15Hd1-T16NH	very faint	1
I15Hg12-NH	very faint	0
I15Hg13-W6Hz3	very faint	9
I15Hg13-NH	very faint	0
I15Hg2-NH	very faint	0
I15Hg2-T16NH	faint	1
T16Ha-Hg2	faint	0
T16Ha-NH	medium	0
T16Ha-K17NH	faint	1
T16Hb-Hg2	very strong	0
T16Hb-NH	medium	0
T16Hg2-NH	medium	0
K17Ha-NH	faint	0
K17Ha-K18NH	very strong	1
K17Hb2-NH	very faint	0
K17Hb2-K18NH	medium	1
K17Hb3-NH	very faint	0
K17Hb3-K18NH	faint	1
K17He2-Hg3	medium	0
K17He3-Hg3	faint	0
K17Hg3-NH	faint	0
K18Ha-NH	medium	0
K18Ha-I19NH	very strong	1
K18Hb2-NH	medium	0
K18Hb3-NH	strong	0
K18Hg3-W2Hz3	medium	16
K18Hg3-NH	faint	0

I19Ha-NH	medium	0
I19Ha-D20NH	very strong	1
I19Hb-Hd1	medium	0
I19Hb-NH	strong	0
I19Hb-D20NH	medium	1
I19Hg12-NH	faint	0
I19Hg13-NH	faint	0
I19Hg2-W6Hz2	faint	13
I19Hg2-NH	faint	0
I19Hg2-D20NH	medium	1
D20Ha-NH	strong	0
D20Hb2-NH	faint	0
D20Hb3-NH	medium	0