Supplementary information

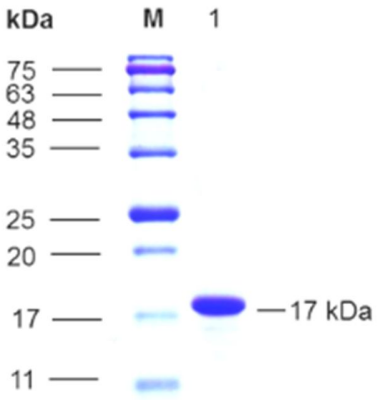

Fig. S1 Purification of HBcAg. SDS-PAGE of concentrated HBcAg particles purified by size exclusion chromatography. Lane M is protein markers in kDa, lane 1 is the purified HBcAg monomer with molecular mass about 17 kDa.

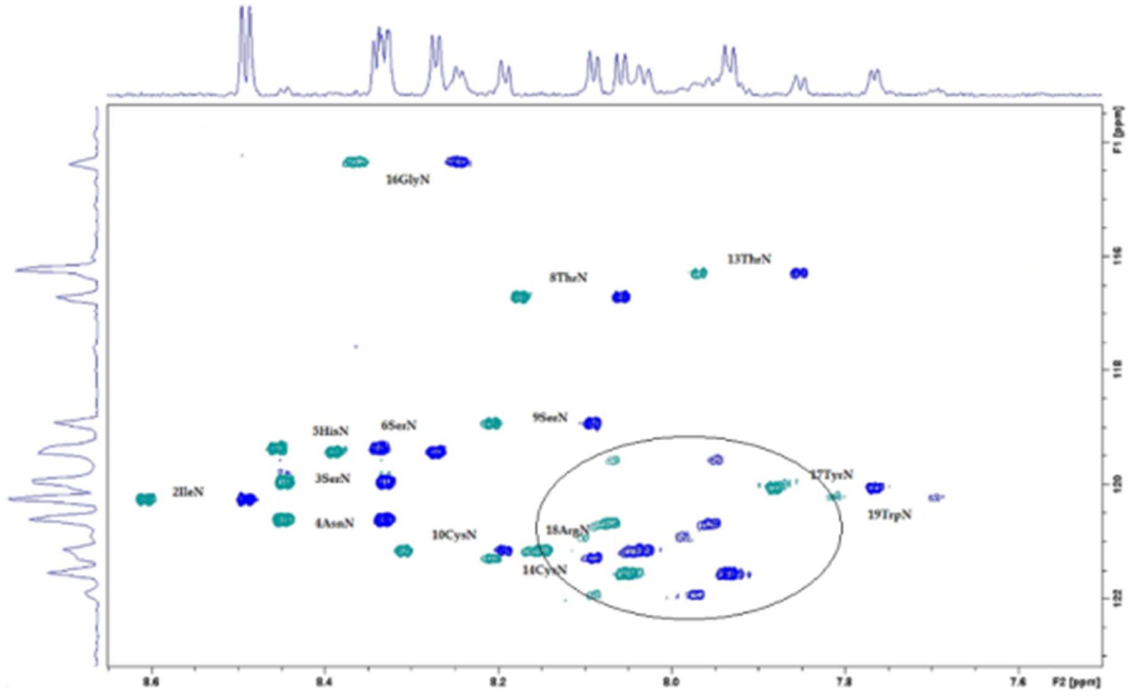

Fig. S2 Non-refocused 2D ^{1}H-^{15}N-HSQC spectra of peptide S. The cross peaks have antiphase structure with respect to the $^{1}J_{NH}$; green and blue colors represent positive and negative peaks, respectively. The assigned resonances are labeled, cross peaks of the five C-terminal amino acids with very similar ^{1}H chemical shifts are circled.

Table S1. Peptide preS chemical shifts at pH 4.

	H	N	Cα	Hα	Cβ	Hβa,b	Cγ	Hγa,b	Cδ	Hδa,b	Cε, Cζ, Cη	Hε, ζ, η
1Arg	-	132.05 (Ɛ)	55.37	3.99	30.76	1.83	26.12	1.58, 1.54	43.17	3.13		7.12 (Ɛ)
2Gln	8.81	122.29, 116.20(Ɛ)	53.92	4.60	28.77	1.90, 2.05	33.35	2.36				7.50 (Ɛ)
3Pro	-	-	63.05	4.40	32.07	2.22	27.38	1.95, 1.82	51.08	3.61, 3.77		6.84 (Ɛ)
4Thr	8.25	118.83	59.91	4.49	69.77	4.06	21.43	1.19				
5Pro	-	-	63.35	4.32	32.18	2.20	27.31	1.81, 1.90	50.72	3.77		
6Leu	8.28	121.32	55.12	4.25	42.38	1.54	26.98	1.49	24.81, 23.46	0.85, 0.80		
7Ser	8.18	119.10	56.30	4.66	63.20	3.78, 3.68						
8Pro	-	-	61.72	4.57	30.81	2.25	27.31	1.92, 1.97	50.63	3.59, 3.73		
9Pro	-	-	62.89	4.33	31.89	2.19	27.35	1.78, 1.93	50.39	3.72, 3.54		
10Leu	8.22	121.21	55.21	4.23	42.42	1.48	27.02	1.56	24.72, 23.61	0.84, 0.80		
11Arg	8.32	121.08, 132.37(Ɛ)	55.96	4.33	30.77	1.51, 1.56	27.08	1.69, 1.77	43.32	3.10		7.10 (Ɛ)
12Thr	8.07	117.65	61.54	4.32	69.73	4.11	21.36	1.07				
13Thr	8.04	117.89	61.62	4.22	69.83	4.07	21.62	1.06				
14His	8.38	120.31	53.23	4.91	28.63	3.13			120.30	7.18	136.30 (Ɛ)	8.46 (Ɛ)
15Pro	-	-	63.07	4.32	32.11	2.21	27.36	1.82, 1.91	50.68	3.51, 3.64		
16Gln	8.49	120.52, 116.21(Ɛ)	55.93	4.20	29.52	1.89, 2.00	33.76	2.30				7.44, 6.79 (Ɛ)
17Ala	8.24	122.50	52.42	4.18	19.20	1.27						
18Met	8.14	119.62	55.34	4.24	32.81	1.75, 1.74	31.93	2.33				1.92 (Ɛ)
19His	8.30	119.57	54.98	4.58	28.87	3.10, 3.02			119.98	7.10	136.21 (Ɛ)	8.46 (Ɛ)
20Trp	8.14	121.32, 124.71(Ɛ)	57.40	4.55	29.72	3.11, 3.18			127.20, 126.97	7.13	120.85 (Ɛ), 114.64 (**ζ**), 122.02 (ζ), 124.62 (η)	10.02, 7.50 (Ɛ); 7.39, 7.04 (ζ); 7.14 (η)
21Asn	8.20	120.36, 116.39(δ)	53.00	4.55	38.87	2.53, 2.57				6.77, 7.42		
22Ser	8.04	117.92	58.43	4.29	63.73	3.79, 3.71						
23Thr	8.10	117.67	61.93	4.30	69.66	4.12	21.58	1.05				
24Thr	7.94	118.10	61.67	4.21	69.86	4.06	21.41	1.03				
25Phe	7.80	123.09	58.52	4.41	39.97	2.89, 3.06			131.96	7.12	131.23 (Ɛ), 129.53 (**ζ**)	7.22 (Ɛ); 7.17 (ζ)

Table S2. Peptide S chemical shifts at pH 4.

	H	N	Cα	Hα	Cβ	Hβa,b	Cγ	Hγa,b	Cδ	Hδa,b	Cε, ζ, η	Hε, ζ, η
1Pro	-	-	62.27	4.34	32.59	2.37	26.40	1.96,1.94	49.40	3.35,3.30		
2Ile	8.55	120.29	61.56	4.14	38.78	1.77	17.39	1.12,0.84	12.91	0.79		
3Ser	8.39	119.96	57.92	4.39	63.89	3.71,3.74	27.32	1.40				
4Asn	8.39	120.65, 116.24(δ)	53.13	4.61	38.82	2.69				7.50,6.81		
5His	8.40	119.40	55.08	4.65	29.01	3.19,3.06			120.08	7.19	136.36 (ε)	8.51**(ε)**
6Ser	8.33	119.46	56.68	4.67	63.17	3.80,3.77						
7Pro	-	-	63.53	4.45	32.11	2.25	27.36	1.90,1.96	50.79	3.66,3.74		
8Thr	8.12	116.72	61.80	4.28	69.71	4.18	21.61	1.13				
9Ser	8.15	118.96	58.19	4.41	63.87	3.78						
10Cys	8.25	121.18	56.39	4.65	27.59	2.69,2.80						
11Pro	-	-	61.67	4.58	30.88	2.24	27.31	1.78,1.89	50.78	3.57,3.67		
12Pro	-	-	63.07	4.26	31.96	2.14	27.30	1.89,1.80	50.38	3.67,3.52		
13Thr	7.91	116.31	61.65	4.17	69.72	4.10	21.72	1.08				
14Cys	8.15	121.32	56.20	4.72	27.62	2.81,2.78						
15Pro	-	-	63.80	4.30	31.98	2.17	27.38	1.88,1.93	50.80	3.64,3.72		
16Gly	8.31	114.38	45.35	3.77,3.83								
17Tyr	7.82	120.08	58.58	4.34	38.76	2.76,2.85			133.21	6.92	118.22(ε)	6.69**(ε)**
18Arg	8.05	121.18	56.70	4.06	30.46	1.52	26.85	1.29	43.29	2.98		7.00(η)
19Trp	7.76	120.25	57.56	4.52	29.32	3.21,3.15			127.28	7.17	120.83 (ε), 114.69,122.08 (ζ), 124.66 (η)	7.47,10.04(ε) 7.34,7.04(ζ) 7.11(η)
20Met	a	a	55.96	4.23	31.81	1.89,1.80	32.84	2.27,2.23			16.86(ε)	1.94(ε)
21Cys	8.01	a	58.73	4.27	27.67	2.74						
22Leu	8.04	a	55.33	4.24	42.39	1.48	26.98	1.54	23.38,24.93	0.81,0.76		
23Arg	8.02	a	55.92	4.15	30.78	1.58,1.63	26.97	1.38,1.43	43.27	2.99		7.01(η)
24Arg	8.10	a	55.88	4.18	30.99	1.54,1.64	26.98	1.39,1.44	43.27	3.02		7.02(η)
25Phe	7.96	a	57.54	4.48	39.69	3.11,2.90			131.96	7.15	131.24(ε), 129.58 (ζ)	7.24**(ε)**, 7.18(ζ)

Table S3. ^{3}J(HN-Hα) coupling constant, calculated φ and simulated φ angle of peptides preS.

Residue	^{3}J(HN-Hα) Hz	Calculated φ (°)	Most Populated Cluster Structure φ (°)
Gln2	6.48	31.6, 88.4, -77.7, -162.3	-95.3
Pro3	-	-	-116.9
Thr4	7.31	40.1, 79.9, -82.2, -157.8	-78.1
Pro5	-	-	-68.5
Leu6	6.80	34.2, 85.8, -78.6, -171.4	-114.5
Ser7	6.90	35.5, 84.5, -79.5, -160.5	-113.1
Pro8	-	-	-66.3
Pro9	-	-	-108.4
Leu10	6.56	32.9, 87.1, -77.7, -162.3	-61.6
Arg11	7.20	38.4, 81.6, -81.3, -158.7	-149.0
Thr12	7.70	43.7, 76.3, -84.1, -155.9	-57.6
Thr13	7.12	36.9, 83.1, -81.3, -158.7	-151.4
His14	7.92	45.9, 74.1, -85.1, -154.92	-110.6
Pro15	-	-	-88.0
Gln16	6.88	35.5, 84.5, -79.5, -160.5	-152.4
Ala17	5.84	27.1, 92.9, -73.6, -166.4	-167.4
Met18	7.12	36.9, 83.1, -81.3, -158.7	-130.5
His19	7.60	41.8, 78.2, -84.1, -155.9	-81.6
Trp20	6.55	-	-44.4
Asn21	7.60	41.8, 78.2, -84.1, -155.9	-154.3
Ser22	-	-	-134.8
Thr23	8.30	51.9, 68.1, -87.1, -152.9	-92.6
Thr24	8.60	-89.3, -150.7	-58.3
Phe25	7.80	43.7, 76.3, -85.1, -154.9	-112.0

Table S4. ^{3}J(HN-Hα) coupling constant, calculated φ and simulated φ angle of peptides S.

Residue	^{3}J(HN-Hα) Hz	Calculated φ (°)	Most Populated Cluster Structure φ (°)
Ile2	7.36	40.1, 79.9, -82.2, -157.8	-121.9
Ser3	7.19	38.4, 81.6, -81.3, -158.7	-75.6
Asn4	7.62	41.8, 78.2, -84.1, -155.9	-158.6
His5	8.08	48.5, 71.5, -86.1, -153.9	-152.9
Ser6	6.44	31.6, 88.4, -76.9, -163.1	-148.3
Pro7	-	-	-84.4
Thr8	7.52	41.8, 78.2, -83.1, -156.9	-147.2
Ser9	7.32	40.1, 79.9, -82.2, -157.8	-61.4
Cys10	7.20	38.4, 81.6, -81.3, -158.7	-146.9
Pro11	-	-	-68.8
Pro12	-	-	-31.3
Thr13	7.64	43.7, 76.3, -84.1, -155.9	-145.6
Cys14	7.16	38.4, 81.6, -81.3, -158.7	-137.4
Pro15	-	-	25.5
Gly16	-	-	-170.7
Tyr17	6.30	30.5, 89.5, -76.1, -163.9	-137.1
Arg18	8.95	-91.6, -148.4	-69.1
Trp19	-	-	-55.3
Met20	-	-	-132.7
Cys21	-	-	-62.2
Leu22	-	-	-143.6
Arg23	-	-	-149.8
Arg24	-	-	-156.9
Phe25	-	-	-90.9

Table S5. Distance restraints used for structure calculations of peptide preS.

Atom 1			Atom 2			Distance (Å)
Intra-residue restraints						
1	ARG	HG2	1	ARG	HB3	3.97
1	ARG	HG3	1	ARG	HB3	3.80
2	GLN	H	2	GLN	HB3	5.27
2	GLN	H	2	GLN	HB2	5.94
2	GLN	H	2	GLN	HA	5.47
2	GLN	HB2	2	GLN	HA	6.10
2	GLN	HB3	2	GLN	HG3	4.29
2	GLN	HB2	2	GLN	HG3	4.60
2	GLN	HE21	2	GLN	HE22	2.77
2	GLN	HB3	2	GLN	HB2	3.25
3	PRO	HA	3	PRO	HB3	4.95
3	PRO	HB3	3	PRO	HG3	3.41
3	PRO	HD2	3	PRO	HD3	3.19
3	PRO	HD2	3	PRO	HG2	3.60
3	PRO	HG2	3	PRO	HG3	3.54
3	PRO	HD2	3	PRO	HB3	5.62
4	THR	QG2	4	THR	HB	4.25
4	THR	QG2	4	THR	H	5.46
4	THR	HB	4	THR	H	4.77
4	THR	HA	4	THR	H	4.89
4	THR	HA	4	THR	HB	5.35
4	THR	HA	4	THR	QG2	4.73
5	PRO	HD3	5	PRO	HG2	3.96
5	PRO	HG3	5	PRO	HB3	3.84
6	LEU	HA	6	LEU	QD1	4.93
6	LEU	QD1	6	LEU	HG	5.27
6	LEU	QD2	6	LEU	HG	4.98
6	LEU	QD1	6	LEU	QD2	3.19
6	LEU	HB2	6	LEU	HG	2.73
6	LEU	HA	6	LEU	HB2	6.01
6	LEU	HA	6	LEU	H	4.52
6	LEU	QD1	6	LEU	H	6.41
6	LEU	HG	6	LEU	H	5.27
6	LEU	HB2	6	LEU	H	4.75
6	LEU	HA	6	LEU	HG	4.76
6	LEU	HB2	6	LEU	QD1	4.68
6	LEU	HB2	6	LEU	QD2	4.46
7	SER	H	7	SER	HB2	4.80
7	SER	H	7	SER	HB3	5.21
7	SER	H	7	SER	HA	4.81
7	SER	HB2	7	SER	HA	4.71
7	SER	HB3	7	SER	HA	4.57
7	SER	HB2	7	SER	HB3	2.58
8	PRO	HB3	8	PRO	HA	4.78
8	PRO	HD2	8	PRO	HB3	5.80
8	PRO	HD2	8	PRO	HD3	3.18
9	PRO	HB3	9	PRO	HG3	3.98
9	PRO	HD2	9	PRO	HD3	3.15
9	PRO	HB3	9	PRO	HD2	6.03
10	LEU	HG	10	LEU	HB2	2.89
10	LEU	QD1	10	LEU	QD2	3.23
10	LEU	HG	10	LEU	HA	4.67
10	LEU	HB2	10	LEU	HA	4.85
10	LEU	QD2	10	LEU	H	6.15
10	LEU	QD1	10	LEU	H	6.13
10	LEU	HG	10	LEU	H	4.14
10	LEU	HA	10	LEU	H	4.48
10	LEU	HB2	10	LEU	H	5.04
10	LEU	HB2	10	LEU	QD2	4.75
10	LEU	HB2	10	LEU	QD1	4.56
11	ARG	HG3	11	ARG	HA	4.45
11	ARG	HA	11	ARG	HB2	5.32
11	ARG	HA	11	ARG	HB3	5.62
11	ARG	HG3	11	ARG	HB3	4.15
11	ARG	HB2	11	ARG	HB3	2.85
11	ARG	HG2	11	ARG	HG3	3.31
11	ARG	HA	11	ARG	HD2	6.03
11	ARG	HG2	11	ARG	H	5.19
11	ARG	HB3	11	ARG	H	5.89
11	ARG	HB2	11	ARG	H	5.30
11	ARG	HG3	11	ARG	H	4.82
11	ARG	HA	11	ARG	H	4.40
11	ARG	HG2	11	ARG	HA	4.47
11	ARG	HG2	11	ARG	HB3	4.26
11	ARG	HG3	11	ARG	HB2	3.99
11	ARG	HG2	11	ARG	HB2	4.21
11	ARG	HG3	11	ARG	HD2	5.57
11	ARG	HG2	11	ARG	HD2	5.69
11	ARG	HB3	11	ARG	HD2	5.10
12	THR	HA	12	THR	QG2	4.00
12	THR	QG2	12	THR	H	4.59
12	THR	H	12	THR	HB	4.78
12	THR	HA	12	THR	H	3.60
12	THR	HA	12	THR	HB	3.93
12	THR	QG2	12	THR	HB	3.66
13	THR	HA	13	THR	QG2	3.94
13	THR	QG2	13	THR	H	4.46
13	THR	HB	13	THR	H	4.90
13	THR	HA	13	THR	H	4.65
13	THR	HA	13	THR	HB	3.54
13	THR	QG2	13	THR	HB	3.74
13	THR	HA	13	THR	QG2	4.09
14	HIS	HB2	14	HIS	HA	4.88

Atom 1			Atom 2			Distance (Å)
14	HIS	HB3	14	HIS	H	5.01
14	HIS	HB2	14	HIS	H	4.80
14	HIS	HA	14	HIS	H	4.74
14	HIS	HB3	14	HIS	HD2	5.03
14	HIS	HB2	14	HIS	HD2	4.85
14	HIS	HB3	14	HIS	HA	4.24
14	HIS	HB2	14	HIS	HB3	2.93
15	PRO	HD3	15	PRO	HB3	5.74
15	PRO	HA	15	PRO	HD3	5.62
15	PRO	HA	15	PRO	HD2	6.21
15	PRO	HA	15	PRO	HB3	3.90
15	PRO	HA	15	PRO	HG3	4.71
15	PRO	HD3	15	PRO	HD2	3.05
15	PRO	HD3	15	PRO	HG3	5.49
15	PRO	HD2	15	PRO	HG3	5.44
15	PRO	HA	15	PRO	HG2	5.18
15	PRO	HD3	15	PRO	HG2	4.04
15	PRO	HD2	15	PRO	HG2	4.07
16	GLN	H	16	GLN	HA	4.48
16	GLN	HA	16	GLN	HB2	6.05
16	GLN	HG3	16	GLN	HB3	3.88
16	GLN	HA	16	GLN	HG3	4.97
16	GLN	HE21	16	GLN	HE22	2.52
16	GLN	HA	16	GLN	HB3	4.26
16	GLN	H	16	GLN	HB2	5.14
16	GLN	H	16	GLN	HG3	4.99
16	GLN	H	16	GLN	HA	4.59
16	GLN	HG3	16	GLN	HB2	3.86
16	GLN	H	16	GLN	HB3	4.52
16	GLN	HB2	16	GLN	HB3	3.10
17	ALA	H	17	ALA	HA	4.32
17	ALA	H	17	ALA	QB	3.78
17	ALA	HA	17	ALA	QB	3.78
18	MET	HB3	18	MET	H	4.87
18	MET	HB2	18	MET	H	4.67
18	MET	HB3	18	MET	HB2	2.88
18	MET	QG	18	MET	QB	3.80
18	MET	QG	18	MET	H	5.88
18	MET	HA	18	MET	H	4.65
18	MET	HB2	18	MET	HA	4.48
18	MET	HB3	18	MET	HA	4.98
18	MET	QB	18	MET	HA	5.15
18	MET	QG	18	MET	HA	5.34
18	MET	HG2	18	MET	HG3	2.64
19	HIS	HB3	19	HIS	HB2	2.75
19	HIS	HB2	19	HIS	HD2	5.07

Atom 1			Atom 2			Distance (Å)
19	HIS	HB3	19	HIS	HD2	5.38
19	HIS	HB3	19	HIS	H	4.93
19	HIS	HB2	19	HIS	H	4.78
19	HIS	HA	19	HIS	H	4.47
19	HIS	HB3	19	HIS	HA	3.83
19	HIS	HB2	19	HIS	HA	4.15
20	TRP	HB2	20	TRP	HA	4.27
20	TRP	HB3	20	TRP	HA	5.31
20	TRP	HB3	20	TRP	HB2	2.97
20	TRP	H	20	TRP	HA	4.54
20	TRP	H	20	TRP	HB2	4.32
20	TRP	H	20	TRP	HH2	5.29
20	TRP	HH2	20	TRP	HE1	3.54
20	TRP	HE1	20	TRP	HZ2	4.74
20	TRP	H	20	TRP	HE3	6.19
20	TRP	HE3	20	TRP	HZ3	3.67
20	TRP	HH2	20	TRP	HZ2	3.45
20	TRP	HZ2	20	TRP	HZ3	4.70
20	TRP	H	20	TRP	HB3	5.08
20	TRP	HA	20	TRP	HE3	4.9
20	TRP	HB3	20	TRP	HH2	4.59
20	TRP	HB2	20	TRP	HH2	4.55
20	TRP	HB3	20	TRP	HE3	5.07
20	TRP	HB2	20	TRP	HE3	5.09
21	ASN	HB3	21	ASN	HA	5.54
21	ASN	QB	21	ASN	H	5.64
21	ASN	HB3	21	ASN	HD21	5.52
21	ASN	HB2	21	ASN	HD21	5.75
21	ASN	HB3	21	ASN	H	4.96
21	ASN	HB2	21	ASN	H	4.98
21	ASN	HA	21	ASN	H	3.61
21	ASN	HD21	21	ASN	HD22	2.32
21	ASN	HB2	21	ASN	HA	4.22
21	ASN	HB2	21	ASN	HB3	2.63
22	SER	HA	22	SER	HB2	4.30
22	SER	HA	22	SER	HB3	4.38
22	SER	HB2	22	SER	H	5.20
22	SER	HB2	22	SER	H	5.05
22	SER	HB3	22	SER	H	5.15
22	SER	HB2	22	SER	HB3	2.58
22	SER	HA	22	SER	H	4.45
23	THR	HA	23	THR	HB	3.49
23	THR	HA	23	THR	QG2	4.63
23	THR	QG2	23	THR	HB	3.89
23	THR	H	23	THR	QG2	5.36
23	THR	QG2	23	THR	HB	4.03

Atom 1			Atom 2			Distance (Å)
23	THR	H	23	THR	HA	4.42
23	THR	H	23	THR	QG2	5.21
23	THR	H	23	THR	HB	5.17
24	THR	QG2	24	THR	HA	5.34
24	THR	QG2	24	THR	H	6.18
24	THR	H	24	THR	HB	5.66
24	THR	HA	24	THR	H	4.35
24	THR	HA	24	THR	HB	3.39
24	THR	QG2	24	THR	HB	3.91
25	PHE	HB2	25	PHE	HB3	2.77
25	PHE	HA	25	PHE	H	4.35
25	PHE	HA	25	PHE	HB2	5.01
25	PHE	HB2	25	PHE	H	5.90
25	PHE	QE	25	PHE	HZ	2.72
	Inter-residue restraints					
2	GLN	H	1	ARG	HA	4.04
2	GLN	HA	3	PRO	HD2	4.46
2	GLN	HA	3	PRO	HD3	4.58
2	GLN	HB2	3	PRO	HD3	5.92
4	THR	QG2	3	PRO	HD2	6.10
4	THR	H	3	PRO	HA	3.75
4	THR	HB	3	PRO	HD3	5.45
4	THR	QG2	3	PRO	HD3	5.57
4	THR	HA	3	PRO	HD2	4.15
4	THR	HA	3	PRO	HD3	4.16
6	LEU	H	5	PRO	HG3	6.09
6	LEU	H	5	PRO	HA	3.60
7	SER	H	5	PRO	HA	5.11
6	LEU	HA	7	SER	H	3.72*(3.10)
6	LEU	H	7	SER	H	4.76#(3.98)
6	LEU	H	10	LEU	HG	4.89
8	PRO	HD2	7	SER	HA	4.09
8	PRO	HD3	7	SER	HA	4.15
9	PRO	HD3	8	PRO	HB3	6.00
9	PRO	HD2	8	PRO	HA	4.08
9	PRO	HD3	8	PRO	HA	4.14
10	LEU	H	9	PRO	HA	3.47
10	LEU	H	9	PRO	HG3	5.59
10	LEU	H	9	PRO	HB3	6.13
10	LEU	HG	11	ARG	HD2	4.81
12	THR	QG2	9	PRO	HD3	5.47
12	THR	H	9	PRO	HA	3.66*(3.04)
11	ARG	H	10	LEU	HB2	5.43
11	ARG	H	10	LEU	HG	5.23
11	ARG	HB2	10	LEU	QD2	4.72
11	ARG	HB2	10	LEU	QD1	4.93
11	ARG	H	10	LEU	H	4.82

*beta-turn H^A-H^N (actual NOE distance)

Atom 1			Atom 2			Distance (Å)
11	ARG	H	10	LEU	HA	3.62
11	ARG	HA	12	THR	H	3.59*(2.99)
11	ARG	H	12	THR	HA	5.52
11	ARG	HG2	12	THR	H	5.74
11	ARG	H	12	THR	H	5.10#(4.25)
11	ARG	HG3	12	THR	H	6.16
12	THR	HA	13	THR	QG2	4.06
12	THR	HA	13	THR	H	3.60*(2.99)
13	THR	QG2	12	THR	HB	3.67
13	THR	H	12	THR	HB	4.99
13	THR	HA	12	THR	H	5.71
13	THR	H	12	THR	H	3.69#(3.07)
13	THR	QG2	14	HIS	H	5.01
13	THR	HB	14	HIS	H	4.92
14	HIS	HB3	11	ARG	HB2	5.47
14	HIS	H	13	THR	H	4.62
13	THR	HA	14	HIS	H	3.56
14	HIS	HB3	15	PRO	HD2	5.45
14	HIS	HB2	15	PRO	HD2	5.84
14	HIS	HA	15	PRO	HD3	4.13
14	HIS	HA	15	PRO	HD2	4.17
15	PRO	HD3	14	HIS	H	5.87
15	PRO	HA	14	HIS	H	5.74
16	GLN	HB3	15	PRO	HD3	3.89
16	GLN	H	15	PRO	HG3	5.45
16	GLN	HB3	15	PRO	HD2	4.13
16	GLN	H	15	PRO	HG2	5.22
16	GLN	H	15	PRO	HA	3.42
16	GLN	H	15	PRO	HD2	6.51
16	GLN	HA	14	HIS	H	5.73
16	GLN	HA	17	ALA	H	3.60
16	GLN	HG3	17	ALA	H	6.15
16	GLN	HB2	17	ALA	H	5.53
16	GLN	H	17	ALA	H	4.71
16	GLN	H	15	PRO	HB3	5.69
18	MET	HB3	20	TRP	H	4.89
18	MET	H	17	ALA	QB	4.64
17	ALA	H	18	MET	H	4.99
17	ALA	HA	18	MET	H	3.71
17	ALA	HA	21	ASN	H	5.47
18	MET	H	17	ALA	QB	4.54
18	MET	HA	19	HIS	H	3.69
18	MET	H	19	HIS	H	4.52
17	ALA	H	18	MET	H	4.36
18	MET	HB2	19	HIS	H	5.83
18	MET	HB3	19	HIS	H	5.65
19	HIS	HB3	18	MET	H	4.67
18	MET	HB2	20	TRP	H	4.67

beta-turn H^N-H^N (actual NOE distance)

Atom 1			Atom 2			Distance (Å)
19	HIS	H	17	ALA	QB	5.84
18	MET	H	20	TRP	HA	4.36
19	HIS	HA	18	MET	H	3.83
18	MET	H	19	HIS	H	4.20
19	HIS	HA	20	TRP	H	3.83
20	TRP	HA	21	ASN	H	5.64
21	ASN	HB3	20	TRP	HA	5.40
20	TRP	H	19	HIS	H	4.18
20	TRP	HA	22	SER	H	4.08
22	SER	HA	23	THR	HB	3.51
20	TRP	HA	21	ASN	H	3.57
20	TRP	H	20	TRP	HH2	4.83
20	TRP	H	21	ASN	H	3.99
22	SER	H	21	ASN	H	4.77
20	TRP	HB2	21	ASN	H	5.49
20	TRP	HB3	21	ASN	H	5.44
21	ASN	HB2	22	SER	H	5.66
21	ASN	HB3	22	SER	H	5.93
21	ASN	HA	22	SER	H	4.06
21	ASN	HB3	22	SER	H	5.71
23	THR	H	22	SER	HA	3.84*(3.20)
24	THR	HA	22	SER	H	4.53
23	THR	H	22	SER	HB2	6.31
23	THR	H	22	SER	HB3	6.23
23	THR	H	22	SER	H	4.11#(3.40)
23	THR	HA	22	SER	H	3.59
23	THR	HA	24	THR	H	4.31*(3.59)
23	THR	H	24	THR	H	4.62#(3.80)
24	THR	H	25	PHE	H	5.12
24	THR	HA	25	PHE	H	4.43
24	THR	H	23	THR	HB	5.77
24	THR	HB	25	PHE	H	6.07
24	THR	H	23	THR	HB	5.48

*beta-turn H^A-H^N (actual NOE distance)
beta-turn H^N-H^N (actual NOE distance)

Table S6. Distance restraints used for structure calculations of peptide S.

Atom 1			Atom 2			Distance (Å)
	Intra-residue restraints					
1	PRO	HB2	1	PRO	HA	5.50
1	PRO	HD2	1	PRO	HD3	2.46
1	PRO	HB2	1	PRO	HD2	5.83
1	PRO	HB2	1	PRO	HD3	5.83
1	PRO	HD2	1	PRO	HG2	4.85
1	PRO	HD2	1	PRO	HG3	4.12
1	PRO	HD3	1	PRO	HG2	4.39
1	PRO	HD3	1	PRO	HG3	5.41
1	PRO	HB2	1	PRO	HG2	4.56
1	PRO	HB2	1	PRO	HG3	4.03
1	PRO	HA	1	PRO	HG2	5.45
1	PRO	HA	1	PRO	HG3	5.35
2	ILE	HN	2	ILE	HA	4.13
2	ILE	HB	2	ILE	QG2	4.52
2	ILE	HG13	2	ILE	QD1	3.90
2	ILE	HG12	2	ILE	HG13	3.61
2	ILE	HG12	2	ILE	QD1	3.62
2	ILE	HA	2	ILE	HB	5.30
2	ILE	HN	2	ILE	HB	5.19
3	SER	HN	3	SER	HB3	4.88
3	SER	HB3	3	SER	HA	6.74
3	SER	HN	3	SER	HB2	4.83
3	SER	HN	3	SER	HA	3.57
3	SER	HB2	3	SER	HA	4.88
4	ASN	HB3	4	ASN	HN	4.02
4	ASN	HN	4	ASN	HA	3.74
4	ASN	HB3	4	ASN	HA	4.04
4	ASN	HD22	4	ASN	HD21	2.23
4	ASN	HD22	4	ASN	HB3	5.31
5	HIS	HN	5	HIS	HB2	5.01
5	HIS	HN	5	HIS	HB3	4.70
5	HIS	HB2	5	HIS	HB3	2.62
5	HIS	HB3	5	HIS	HD2	5.18
5	HIS	HB2	5	HIS	HD2	5.37
5	HIS	HN	5	HIS	HA	4.83
5	HIS	HB3	5	HIS	HA	4.64
6	SER	HN	6	SER	HB3	4.44
6	SER	HN	6	SER	HB2	4.45
6	SER	HB2	6	SER	HA	4.55
6	SER	HB3	6	SER	HA	3.99
7	PRO	HB2	7	PRO	HG2	3.99
7	PRO	HB2	7	PRO	HG3	3.54
7	PRO	HD2	7	PRO	HB2	5.17
7	PRO	HD3	7	PRO	HA	5.74
7	PRO	HD2	7	PRO	HD3	2.85
7	PRO	HG2	7	PRO	HG3	2.75
7	PRO	HD2	7	PRO	HG2	4.29
7	PRO	HD3	7	PRO	HB2	5.88
7	PRO	HD2	7	PRO	HG3	3.87
7	PRO	HD3	7	PRO	HG3	5.07
7	PRO	HD3	7	PRO	HG2	4.13
7	PRO	HB2	7	PRO	HA	4.52
7	PRO	HA	7	PRO	HG2	5.29
7	PRO	HA	7	PRO	HG3	4.93
8	THR	QG2	8	THR	HA	4.00
8	THR	QG2	8	THR	HB	3.68
8	THR	HB	8	THR	HA	3.47
8	THR	QG2	8	THR	HN	4.51
8	THR	HA	8	THR	HN	4.24
9	SER	HN	9	SER	HA	4.46
9	SER	HB3	9	SER	HN	4.09
9	SER	HB3	9	SER	HA	4.03
10	CYS	HN	10	CYS	HB2	4.82
10	CYS	HN	10	CYS	HB3	5.03
10	CYS	HN	10	CYS	HA	5.11
10	CYS	HB3	10	CYS	HB2	3.00
10	CYS	HA	10	CYS	HB3	4.68
10	CYS	HA	10	CYS	HB2	5.02
11	PRO	HD2	11	PRO	HA	3.69
11	PRO	HD2	11	PRO	HG3	4.83
11	PRO	HD3	11	PRO	HA	5.60
11	PRO	HD3	11	PRO	HD2	3.32
11	PRO	HD3	11	PRO	HG3	5.46
11	PRO	HG3	11	PRO	HG2	3.23
11	PRO	HG3	11	PRO	HB2	3.55
11	PRO	HD3	11	PRO	HG2	5.05
11	PRO	HA	11	PRO	HB2	4.37
11	PRO	HA	11	PRO	HG2	5.12
11	PRO	HA	11	PRO	HG3	4.87
12	PRO	HD2	12	PRO	HB2	5.68
12	PRO	HB2	12	PRO	HG2	3.55
12	PRO	HB2	12	PRO	HG3	3.90
12	PRO	HD2	12	PRO	HA	6.46
12	PRO	HD2	12	PRO	HD3	3.03
12	PRO	HD3	12	PRO	HB2	6.10
12	PRO	HA	12	PRO	HB2	4.39
12	PRO	HA	12	PRO	HG2	4.72
12	PRO	HA	12	PRO	HG3	4.91
12	PRO	HD2	12	PRO	HG2	5.33
12	PRO	HD2	12	PRO	HG3	3.76
12	PRO	HG2	12	PRO	HG3	2.83
12	PRO	HD3	12	PRO	HG3	4.11
12	PRO	HD3	12	PRO	HG2	4.92

Atom 1			Atom 2			Distance (Å)
13	THR	HA	13	THR	QG2	3.78
13	THR	HB	13	THR	QG2	3.69
13	THR	HN	13	THR	HB	4.99
13	THR	HA	13	THR	HB	3.39
13	THR	HN	13	THR	QG2	4.72
13	THR	HA	13	THR	HN	4.46
14	CYS	HN	14	CYS	HB2	4.76
14	CYS	HN	14	CYS	HB3	4.71
14	CYS	HA	14	CYS	HB2	4.78
14	CYS	HA	14	CYS	HB3	4.93
15	PRO	HD3	15	PRO	HD2	2.81
15	PRO	HD2	15	PRO	HB2	5.81
15	PRO	HA	15	PRO	HG2	4.80
15	PRO	HD3	15	PRO	HG3	4.21
15	PRO	HD2	15	PRO	HG2	4.11
15	PRO	HD2	15	PRO	HG3	4.10
15	PRO	HB2	15	PRO	HG2	5.08
15	PRO	HG2	15	PRO	HG3	2.49
15	PRO	HD3	15	PRO	HG2	4.50
15	PRO	HA	15	PRO	HG3	4.88
15	PRO	HA	15	PRO	HB2	3.98
15	PRO	HD3	15	PRO	HB2	5.50
15	PRO	HD3	15	PRO	HA	5.31
15	PRO	HD2	15	PRO	HA	5.60
15	PRO	HB2	15	PRO	HG3	3.89
16	GLY	HN	16	GLY	HA3	3.89
16	GLY	HN	16	GLY	HA2	3.92
16	GLY	HA3	16	GLY	HA2	2.77
17	TYR	HN	17	TYR	HA	4.47
17	TYR	QE	17	TYR	QD	2.69
17	TYR	QE	17	TYR	HB3	5.13
17	TYR	HA	17	TYR	HB3	4.59
17	TYR	HA	17	TYR	HB2	4.66
17	TYR	HB3	17	TYR	HB2	3.13
17	TYR	HN	17	TYR	HB3	4.29
17	TYR	HN	17	TYR	HB2	4.22
17	TYR	QD	17	TYR	HB3	3.95
17	TYR	QD	17	TYR	HB2	4.29
17	TYR	HA	17	TYR	QD	4.55
17	TYR	HA	17	TYR	QE	5.82
17	TYR	HN	17	TYR	QD	4.54
18	ARG	HN	18	ARG	HA	5.05
18	ARG	NH1	18	ARG	HG2	4.95
18	ARG	HA	18	ARG	HB2	4.53
18	ARG	HA	18	ARG	HG2	4.88
18	ARG	HG2	18	ARG	HD2	3.95
18	ARG	HG2	18	ARG	HD2	4.07
18	ARG	HB2	18	ARG	HD2	4.51
18	ARG	HB2	18	ARG	HG2	3.59
18	ARG	HN	18	ARG	HG2	5.35

Atom 1			Atom 2			Distance (Å)
18	ARG	NH1	18	ARG	HD2	4.15
18	ARG	HB2	18	ARG	NH1	5.49
18	ARG	HN	18	ARG	HB2	4.47
18	ARG	HA	18	ARG	HD2	5.37
19	TRP	HN	19	TRP	HA	5.20
19	TRP	HE3	19	TRP	HZ2	5.58
19	TRP	HE1	19	TRP	HD1	3.38
19	TRP	HZ3	19	TRP	HZ2	4.50
19	TRP	HZ2	19	TRP	HH2	3.13
19	TRP	HN	19	TRP	HD1	4.71
19	TRP	HA	19	TRP	HE3	4.61
19	TRP	HE3	19	TRP	HB3	4.38
19	TRP	HE3	19	TRP	HB2	4.64
19	TRP	HA	19	TRP	HD1	4.69
19	TRP	HD1	19	TRP	HB3	4.07
19	TRP	HD1	19	TRP	HB2	4.04
19	TRP	HN	19	TRP	HE3	6.02
19	TRP	HZ2	19	TRP	HE1	4.34
19	TRP	HA	19	TRP	HB3	4.20
19	TRP	HA	19	TRP	HB2	4.38
19	TRP	HN	19	TRP	HB3	4.74
19	TRP	HN	19	TRP	HB2	4.71
19	TRP	HB3	19	TRP	HB2	2.81
19	TRP	HZ3	19	TRP	HH2	2.97
19	TRP	HE3	19	TRP	HH2	4.76
19	TRP	HE3	19	TRP	HZ3	3.47
20	MET	HB2	20	MET	HN	5.17
20	MET	HB3	20	MET	HN	5.49
20	MET	HA	20	MET	HB2	5.10
20	MET	HA	20	MET	HG2	5.40
20	MET	HA	20	MET	HG3	5.92
20	MET	HG2	20	MET	HG3	2.65
20	MET	HB2	20	MET	HB3	2.78
20	MET	HB2	20	MET	HG3	4.41
20	MET	HB2	20	MET	HG2	3.90
20	MET	HB3	20	MET	HG3	4.36
20	MET	HB3	20	MET	HG2	3.83
20	MET	HA	20	MET	HB3	4.70
20	MET	HG2	20	MET	QE	4.20
21	CYS	HA	21	CYS	HB3	4.45
21	CYS	HN	21	CYS	HB3	5.01
21	CYS	HN	21	CYS	HA	4.66
22	LEU	HA	22	LEU	HG	4.62
22	LEU	HA	22	LEU	HB2	4.48
22	LEU	QD2	22	LEU	HG	4.39
22	LEU	QD2	22	LEU	HB2	4.31
22	LEU	QD1	22	LEU	HG	4.39
22	LEU	QD1	22	LEU	HB2	4.34
22	LEU	HA	22	LEU	QD1	4.08
22	LEU	HA	22	LEU	QD2	5.23

Atom 1			Atom 2			Distance (Å)
22	LEU	HN	22	LEU	QD2	5.91
22	LEU	HN	22	LEU	QD1	5.74
23	ARG	HN	23	ARG	HG3	5.79
23	ARG	HN	23	ARG	HB2	4.73
23	ARG	HN	23	ARG	HB3	4.93
23	ARG	NH1	23	ARG	HD2	4.30
23	ARG	HA	23	ARG	HB2	4.09
23	ARG	HD2	23	ARG	HG3	4.40
23	ARG	HD2	23	ARG	HG2	4.47
23	ARG	HN	23	ARG	HA	4.39
23	ARG	HB3	23	ARG	HD2	4.97
23	ARG	HN	23	ARG	HG2	5.62
23	ARG	NH1	23	ARG	HG3	5.85
23	ARG	HB2	23	ARG	NH1	5.92
23	ARG	NH1	23	ARG	HG2	5.71
23	ARG	HB3	23	ARG	NH1	5.87
23	ARG	HA	23	ARG	HB3	4.86
23	ARG	HA	23	ARG	HD2	5.33
23	ARG	HA	23	ARG	HG3	4.98
23	ARG	HA	24	ARG	HG2	4.87
24	ARG	HA	24	ARG	HD2	5.45
24	ARG	NH1	24	ARG	HD2	4.56
24	ARG	HB2	24	ARG	HD2	5.10
24	ARG	HN	24	ARG	HA	4.26
24	ARG	HN	24	ARG	HB2	4.78
24	ARG	HN	24	ARG	HB3	4.53
24	ARG	HN	24	ARG	HG2	5.42
24	ARG	HN	24	ARG	HG3	5.48
24	ARG	HA	24	ARG	HB2	4.15
24	ARG	HD2	24	ARG	HG3	4.87
24	ARG	HD2	24	ARG	HG2	4.65
24	ARG	HB3	24	ARG	HD2	5.09
24	ARG	HB2	24	ARG	HD2	5.14
24	ARG	HB3	24	ARG	HG3	3.35
24	ARG	NH1	24	ARG	HD2	4.72
24	ARG	HA	24	ARG	HG2	5.09
24	ARG	HA	24	ARG	HG3	5.09
24	ARG	HG3	24	ARG	HG2	2.58
25	PHE	HN	25	PHE	HB2	5.50
25	PHE	HN	25	PHE	HA	4.97
25	PHE	HB3	25	PHE	HB2	2.81
25	PHE	QD	25	PHE	HB3	4.86
25	PHE	QD	25	PHE	HB2	4.85
25	PHE	HA	25	PHE	HB2	4.82
25	PHE	QD	25	PHE	HA	5.67
25	PHE	HA	25	PHE	HB3	4.83
25	PHE	HN	25	PHE	HB3	4.98

Atom 1			Atom 2			Distance (Å)
	Inter-residue restraints					
1	PRO	HA	2	ILE	HN	4.23
2	ILE	HA	3	SER	HN	3.50
3	SER	HN	2	ILE	HB	5.92
2	ILE	HN	3	SER	HN	5.13
2	ILE	HN	4	ASN	HN	5.15
6	SER	HN	2	ILE	HB	5.30
3	SER	HA	4	ASN	HN	4.24*(3.50)
3	SER	HN	4	ASN	HB3	4.04
5	HIS	HN	3	SER	HA	3.74*(3.11)
4	ASN	HN	5	HIS	HA	4.26
5	HIS	HN	4	ASN	HA	3.83*(3.20)
6	SER	HN	4	ASN	HA	5.15
5	HIS	HN	6	SER	HB2	5.51
6	SER	HN	5	HIS	HA	3.68
5	HIS	HN	6	SER	HB2	5.52
5	HIS	HB3	6	SER	HN	5.62
5	HIS	HN	6	SER	HN	3.87
5	HIS	HB3	6	SER	HN	5.61
5	HIS	HB2	6	SER	HN	5.52
7	PRO	HD3	6	SER	HA	3.87
7	PRO	HA	6	SER	HN	5.66
7	PRO	HG3	8	THR	HN	5.54
7	PRO	HG3	9	SER	HN	5.84
7	PRO	HG2	8	THR	HN	5.97
7	PRO	HB2	8	THR	HN	5.95
7	PRO	HD2	8	THR	HN	5.83
7	PRO	HA	8	THR	HN	3.58
7	PRO	HD3	9	SER	HA	5.21
9	SER	HN	8	THR	HN	3.32
9	SER	HN	8	THR	QG2	5.07
9	SER	HN	8	THR	HA	3.57
10	CYS	HN	9	SER	HA	3.56
10	CYS	HN	9	SER	HB3	4.47
10	CYS	HN	9	SER	HN	4.43
10	CYS	HN	8	THR	HA	5.00
10	CYS	HN	8	THR	HB	4.83
11	PRO	HG2	9	SER	HN	6.01
11	PRO	HD2	10	CYS	HB2	5.68
11	PRO	HD3	10	CYS	HB2	5.80
11	PRO	HD2	10	CYS	HA	3.87
11	PRO	HA	10	CYS	HB2	3.95
11	PRO	HD3	10	CYS	HB3	5.56
11	PRO	HD3	10	CYS	HA	4.36
11	PRO	HB2	12	PRO	HD3	5.37
11	PRO	HG3	12	PRO	HA	4.57
11	PRO	HA	12	PRO	HD3	3.91

*beta-turn H^A-H^N (actual NOE distance)

Atom 1			Atom 2			Distance (Å)
11	PRO	HD3	13	THR	QG2	4.06
11	PRO	HG2	12	PRO	HB2	3.88
11	PRO	HG3	12	PRO	HB2	3.40
12	PRO	HG2	13	THR	HN	5.15
12	PRO	HA	13	THR	HN	3.71
12	PRO	HG3	13	THR	HN	5.80
14	CYS	HN	13	THR	HA	3.50
14	CYS	HN	13	THR	HB	4.8
14	CYS	HN	13	THR	HN	4.54
14	CYS	HN	13	THR	QG2	5.19
14	CYS	HN	13	THR	HA	3.55
15	PRO	HA	11	PRO	HG3	4.38
15	PRO	HB2	12	PRO	HG2	3.44
15	PRO	HD2	14	CYS	HB2	4.91
15	PRO	HD2	14	CYS	HB3	5.02
15	PRO	HD3	14	CYS	HB2	5.65
15	PRO	HD3	14	CYS	HB3	5.74
15	PRO	HD3	14	CYS	HA	4.33
15	PRO	HD2	14	CYS	HA	4.52
15	PRO	HA	16	GLY	HN	3.44
15	PRO	HD3	16	GLY	HA3	4.82
15	PRO	HB2	16	GLY	HN	5.51
15	PRO	HD2	16	GLY	HN	5.67
15	PRO	HA	16	GLY	HA3	5.76
17	TYR	HN	15	PRO	HA	5.31
17	TYR	HN	16	GLY	HN	4.31
17	TYR	HN	16	GLY	HA3	4.22
17	TYR	HN	16	GLY	HA2	4.29
18	ARG	HA	13	THR	QG2	5.45
18	ARG	HN	16	GLY	HN	5.64
18	ARG	HN	17	TYR	HB3	5.07

Atom 1			Atom 2			Distance (Å)
18	ARG	HN	17	TYR	QD	5.95
18	ARG	HN	17	TYR	HN	4.86
18	ARG	HN	17	TYR	HA	4.36
18	ARG	HA	17	TYR	QD	5.89
18	ARG	HA	19	TRP	HN	4.46
18	ARG	HN	19	TRP	HN	5.43
18	ARG	HN	19	TRP	HA	6.19
18	ARG	HB2	19	TRP	HN	5.71
19	TRP	HA	20	MET	HN	5.28
19	TRP	HE3	20	MET	HA	5.79
19	TRP	HB3	20	MET	HN	6.07
21	CYS	HA	22	LEU	HN	4.28
21	CYS	HN	22	LEU	HN	2.86
21	CYS	HN	20	MET	HB3	5.74
21	CYS	HN	20	MET	HB2	5.86
21	CYS	HN	20	MET	HN	4.71
20	MET	HB3	23	ARG	HN	5.76
22	LEU	HN	21	CYS	HB3	4.94
22	LEU	HN	25	PHE	HA	6.12
23	ARG	HN	21	CYS	HB3	5.00
23	ARG	HN	22	LEU	HA	3.67
23	ARG	HA	24	ARG	HN	3.71
23	ARG	HB3	24	ARG	HG3	3.69
23	ARG	HB3	24	ARG	HG2	3.41
24	ARG	HB3	22	LEU	HN	4.31
24	ARG	HN	23	ARG	HB3	4.80
24	ARG	HB3	23	ARG	HB3	2.97
24	ARG	HA	25	PHE	HN	3.96
24	ARG	HB3	25	PHE	HN	5.89
24	ARG	HN	25	PHE	HN	5.00
24	ARG	HB2	25	PHE	HN	5.58