

**SUPPORTING MATERIAL****TABLE S1:** Chemical shifts (ppm)

Residue	NH	$\alpha$ H	$\beta$ H	Others
1. Asp	-	4.06	2.41, 2.56	
2. Val	8.50	4.28	1.92	$\gamma$ CH <sub>3</sub> 0.75*, 0.82*
3. Pro	-	4.11	1.48, 1.97	$\gamma$ CH <sub>2</sub> 1.78* $\delta$ CH <sub>2</sub> 3.49, 3.64
4. Cys	8.19	4.24	2.77, 2.85	
5. Phe	8.31	4.38	2.75, 2.92	$\delta$ CH 7.05 $\epsilon$ CH 7.15 $\xi$ CH 7.09
6. Gly	8.24	3.34, 3.86		
7. Trp	8.35	4.47	3.14, 3.02	$\delta$ CH 7.06 $\epsilon^1$ NH 10.09 $\epsilon^3$ CH 7.46 $\xi^2$ CH 7.28 $\xi^3$ CH 6.95 $\eta$ CH 7.018
8. Cys	8.05	4.32	2.73, 2.96	
9. Gln	8.04	4.00	1.65*	$\gamma$ CH <sub>2</sub> 1.84, 1.77 $\epsilon$ NH <sub>2</sub> 6.70, 7.41
10. Asp	8.25	4.40	2.43, 2.58	
11. Ala	7.70	3.92	1.13*	

\* Chemical shifts representing peaks of degenerated protons.

**TABLE S2:** NOE constraints

Atom1		Atom2		Upper limit (Å)
1. Asp	$\alpha$ H	2. Val	NH	3.5
2. Val	NH		$\beta$ H	3.5
			$\gamma$ H	3.5
	$\alpha$ H		$\gamma$ H	3.5
		3. Pro	$\delta$ H	3.5
3. Pro	$\alpha$ H	4. Cys	NH	2.8
	$\beta$ H	3. Pro	$\delta$ H	3.5
		4. Cys	NH	5.0
	$\gamma$ H	3. Pro	$\delta$ H	3.5
4. Cys	NH	8. Cys	NH	3.5
		4. Cys	$\beta$ H	3.5
	$\alpha$ H	5. Phe	NH	2.8
5. Phe	NH		$\beta$ H	3.5
	$\alpha$ H		$\delta$ H	3.5
		6. Gly	NH	5.0
	$\beta$ H	5. Phe	$\delta$ H	3.5
			$\epsilon$ H	5.0
		6. Gly	NH	3.5
	$\delta$ H	6. Gly	NH	5.0
		7. Trp	NH	3.5
		8. Cys	NH	5.0
6. Gly	NH	9. Gln	$\beta$ H	5.0
			$\gamma$ H	5.0
	$\alpha$ H	7. Trp	NH	2.8
			$\beta$ H	3.5
7. Trp	NH	7. Trp	$\beta$ H	3.5
			$\delta$ H	5.0

			$\epsilon^3\text{H}$	5.0
		8. Cys	NH	3.5
	$\alpha\text{H}$		NH	3.5
	$\beta\text{H}$	7. Trp	$\epsilon^3\text{H}$	3.5
			$\delta\text{H}$	3.5
		8. Cys	NH	5.0
	$\epsilon^1\text{H}$	7. Trp	$\xi^2\text{H}$	3.5
	$\epsilon^3\text{H}$	7. Trp	$\eta\text{H}$	3.5
			$\xi^2\text{H}$	3.5
		8. Cys	NH	3.5
	$\eta\text{H}$	9. Gln	$\epsilon^2\text{H}$	5.0
8. Cys	NH	8. Cys	$\alpha\text{H}$	5.0
			$\beta\text{H}$	3.5
9. Gln	NH	9. Gln	$\beta\text{H}$	3.5
			$\gamma\text{H}$	3.5
		10. Asp	NH	3.5
	$\alpha\text{H}$	9. Gln	$\beta\text{H}$	5.0
			$\gamma\text{H}$	3.5
		10. Asp	NH	2.8
	$\epsilon^{21}\text{H}$	9. Gln	$\epsilon^{22}\text{H}$	2.8
10. Asp	NH	10. Asp	$\beta\text{H}$	3.5
		11. Ala	NH	5.0
	$\alpha\text{H}$		NH	3.5
11. Ala	NH		$\beta\text{H}$	5.0

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