Helix Formation and Folding in γ-Peptides and their Vinylogues [Supporting Information]

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Dedicated to Prof. Dr. *Dieter Seebach* on the occasion of his 65th birthday

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Table S1. *Backbone Torsion Angles of Conformers of the Blocked* γ*-Peptide Hexamer* ***1*** *with Hydrogen Bonds Formed in Forward Direction Obtained at the B3LYP/6-31G* Level of* ab initio *MO Theory* [a])

Conf.	φ	θ	ζ	ψ	Conf.	φ	θ	ζ	ψ
$\mathbf{H_7}^{\mathbf{I}}$	-171.5	-65.4	90.8	143.7	$\mathbf{H_{17}}^{\mathbf{I}}$	78.3	71.5	-75.8	148.8
	-173.9	-64.3	90.3	143.7		82.6	67.3	-81.0	145.3
	-169.7	-65.1	89.2	141.5		85.5	60.6	-166.3	-170.1
	-173.7	-64.5	89.9	144.0		73.2	64.5	-81.2	150.4
	-169.0	-65.6	89.1	143.1		78.8	57.7	-170.8	-165.3
	-172.9	-65.8	89.8	146.7		79.2	65.7	-71.3	135.9
$\mathbf{H_7}^{\mathbf{II}}$	-97.2	-46.2	-48.6	-104.2	$\mathbf{H_{17}}^{\mathbf{II}}$	114.3	-52.6	71.8	55.4
	-98.8	-45.0	-48.5	-107.3		-160.9	178.2	61.2	57.9
	-102.5	-44.5	-47.8	-108.9		144.9	-65.1	78.9	53.6
	-102.6	-45.4	-47.8	-106.8		164.6	-167.4	74.2	96.8
	-101.7	-45.0	-47.7	-108.1		133.3	-72.3	72.8	68.9
	-100.9	-46.3	-48.1	-106.1		109.1	-178.8	67.3	-162.6
$\mathbf{H_{12}}^{\mathbf{I}}$	80.2	68.2	-76.7	143.3	$\mathbf{H_{22}}^{\mathbf{I}}$	125.1	178.8	-177.0	92.6
	87.9	69.5	-76.5	141.0		95.7	176.7	177.8	84.1
	89.3	69.8	-77.1	142.0		78.6	178.8	179.6	94.0
	89.2	69.3	-77.8	143.9		84.5	178.4	179.9	98.9
	88.7	68.6	-79.2	147.3		76.7	177.7	168.6	109.1
	88.0	65.7	-74.2	134.1		77.3	-172.2	166.6	149.9
$\mathbf{H_{12}}^{\mathbf{II}}$	115.5	-57.6	77.0	58.6	$\mathbf{H_{22}}^{\mathbf{II}}$	109.9	65.9	179.4	-153.5
	148.3	-64.6	79.8	63.6		83.0	63.9	-171.8	-179.4
	149.6	-69.5	75.0	70.8		75.3	61.9	-163.1	-164.9
	147.2	-66.3	76.9	70.1		77.1	60.5	-169.2	-160.8
	143.1	-65.0	79.9	68.5		73.7	59.4	-166.3	-160.3
	137.8	-62.5	81.8	65.4		73.5	65.2	-165.1	-108.3

[a]) Torsion angles in degrees.

Table S2. *Backbone Torsion Angles of Conformers of the Blocked* γ*-Peptide Hexamer* ***1*** *with Hydrogen Bonds Formed in Backward Direction Obtained at the B3LYP/6-31G* Level of* ab initio *MO Theory* [a])

Conf.	φ	θ	ζ	ψ	Conf.	φ	θ	ζ	ψ
$\mathbf{H_9}^{\mathbf{I}}$	97.5	-69.2	-74.4	95.0	$\mathbf{H_{19}}^{\mathbf{I}}$	114.5	-63.1	-69.7	179.8
	96.5	-69.5	-73.8	94.1		163.7	-64.2	-71.7	165.0
	97.2	-68.7	-74.3	93.6		151.0	-64.5	-67.6	153.6
	96.9	-69.1	-74.1	94.5		178.4	-67.7	-69.8	158.4
	97.6	-69.0	-74.3	93.8		150.7	-61.6	-70.9	162.2
	97.7	-70.1	-74.3	95.4		167.8	-63.6	-71.4	162.0
$\mathbf{H_9}^{\mathbf{II}}$	73.8	-158.7	72.6	2.0	$\mathbf{H_{19}}^{\mathbf{II}}$	72.2	64.7	-172.1	143.3
	73.8	-158.8	73.2	1.0		70.3	61.9	-165.7	150.3
	73.5	-158.9	72.2	2.5		72.0	66.0	-168.6	149.9
	73.9	-158.7	73.1	1.0		75.2	64.2	-173.3	140.6
	73.3	-159.5	71.8	3.5		78.8	63.2	-173.2	149.6
	73.9	-160.4	72.1	2.7		86.3	58.2	168.5	147.6
$\mathbf{H_9}^{\mathbf{III}}$	43.4	52.2	-152.0	62.5	$\mathbf{H_{19}}^{\mathbf{III}}$	125.1	-179.5	63.5	90.7
	44.4	51.7	-148.8	57.8		131.7	-172.9	64.4	84.0
	44.0	52.1	-148.8	59.5		124.3	-175.5	62.2	81.6
	44.5	51.4	-149.0	59.5		141.9	-175.4	62.6	80.3
	44.9	51.4	-148.6	59.0		128.1	-173.6	61.8	79.1
	45.2	51.6	-151.0	63.7		135.2	-169.2	63.2	74.8
$\mathbf{H_{14}}^{\mathbf{I}}$	105.9	-61.1	-67.0	165.1	$\mathbf{H_{24}}^{\mathbf{I}}$	-133.4	-177.3	-66.0	-99.3
	135.2	-62.6	-69.4	140.2		-127.4	-174.6	-67.2	-111.0
	134.4	-58.6	-66.4	140.6		-147.7	173.3	-68.9	-108.6
	133.7	-60.4	-66.4	140.8		-99.3	-177.8	-62.1	-99.1
	135.7	-62.1	-66.4	141.9		-171.5	-179.7	-62.4	-65.0
	134.0	-60.7	-63.0	138.8		164.4	177.6	-63.1	-74.6
$\mathbf{H_{14}}^{\mathbf{II}}$	-60.9	-58.7	152.6	-124.8	$\mathbf{H_{24}}^{\mathbf{II}}$	77.5	178.6	172.3	89.4
	-61.9	-57.8	156.6	-122.5		69.2	178.2	166.5	80.1
	-61.8	-57.5	151.5	-120.3		76.0	178.7	179.5	-121.0
	-59.0	-57.3	152.7	-123.5		-89.3	177.2	174.4	89.4
	-66.1	-60.6	159.5	-111.9		80.0	178.2	171.2	66.2
	-73.6	-57.5	176.0	-128.1		82.9	177.8	172.5	63.2
$\mathbf{H_{14}}^{\mathbf{III}}$	97.4	-165.5	63.1	79.4					
	102.0	-163.6	58.3	67.8					
	111.2	-159.6	60.8	63.4					
	110.6	-159.5	60.4	66.4					
	107.9	-161.8	58.3	65.6					
	120.4	-168.2	65.0	45.7					

[a]) Torsion angles in degrees.

Table S3. *Backbone Torsion Angles of Conformers of the Blocked* γ*-Peptide Hexamer* ***1*** *with Hydrogen Bonds Formed in Forward Direction Obtained at the SCRF/HF/6-31G* Level of* ab initio *MO Theory* [a])

Conf.	φ	θ	ζ	ψ	Conf.	φ	θ	ζ	ψ
$\mathbf{H_7}^{\mathbf{I}}$	-169.6	-66.5	90.9	145.2	$\mathbf{H_{17}}^{\mathbf{I}}$	80.8	69.1	-77.4	153.8
	-171.0	-66.4	90.8	143.6		80.5	67.3	-80.4	147.3
	-170.9	-66.1	90.2	144.4		84.5	64.6	-160.8	-175.5
	-169.5	-66.7	89.9	143.8		76.0	65.0	-84.2	150.9
	-171.1	-66.5	90.3	145.3		78.1	62.0	-168.0	-167.5
	-167.1	-68.9	88.6	146.6		77.1	62.6	-77.2	144.5
$\mathbf{H_7}^{\mathbf{II}}$	-101.9	-45.1	-49.7	-112.8	$\mathbf{H_{17}}^{\mathbf{II}}$	127.5	-64.1	68.2	64.4
	-110.9	-46.7	-47.6	-105.6		-168.1	-177.8	63.6	71.6
	-106.8	-45.9	-48.1	-108.7		145.2	-72.2	75.7	58.3
	-108.8	-46.0	-47.8	-108.3		167.1	-169.0	74.4	90.2
	-106.3	-45.5	-48.5	-110.9		148.6	-79.4	68.1	73.1
	-113.7	-46.9	-46.9	-105.1		121.6	176.8	69.3	178.1
$\mathbf{H_{12}}^{\mathbf{I}}$	81.8	66.3	-78.2	148.8	$\mathbf{H_{22}}^{\mathbf{I}}$	96.4	175.5	178.6	97.0
	86.0	68.6	-76.5	145.8		85.5	177.0	178.4	92.5
	88.9	67.0	-77.7	148.2		80.6	179.1	178.8	95.1
	87.5	66.7	-77.5	149.6		81.7	178.4	179.7	94.8
	88.0	66.3	-79.7	156.0		80.0	178.8	175.9	99.6
	84.5	62.8	-77.8	149.6		80.5	178.7	172.5	123.3
$\mathbf{H_{12}}^{\mathbf{II}}$	137.8	-69.2	68.6	69.9	$\mathbf{H_{22}}^{\mathbf{II}}$	88.5	66.1	-175.6	-162.6
	161.6	-76.0	70.4	77.0		80.6	65.3	-167.7	-170.9
	156.7	-77.1	68.7	80.0		77.0	64.1	-164.3	-169.2
	154.7	-77.1	68.7	80.4		78.6	64.6	-158.4	-166.8
	153.3	-75.9	72.7	82.5		75.0	63.5	-165.0	-164.3
	147.0	-78.5	70.6	86.2		76.0	63.3	-170.8	-138.4

[a]) Torsion angles in degrees.

Table S4. *Backbone Torsion Angles of Conformers of the Blocked* γ*-Peptide Hexamer* ***1*** *with Hydrogen Bonds Formed in Backward Direction Obtained at the SCRF/HF/6-31G* Level of* ab initio *MO Theory* [a])

Conf.	φ	θ	ζ	ψ	Conf.	φ	θ	ζ	ψ
$\mathbf{H_9}^{\mathbf{I}}$	99.7	-64.9	-77.2	86.3	$\mathbf{H_{19}}^{\mathbf{I}}$	130.3	-61.7	-68.8	174.3
	97.1	-68.3	-74.5	90.3		165.1	-64.8	-70.2	164.0
	97.6	-66.6	-75.5	87.6		150.2	-64.2	-67.9	161.6
	97.2	-67.7	-74.8	89.8		168.0	-66.9	-69.9	160.3
	97.9	-66.2	-76.3	86.6		154.5	-63.2	-70.2	159.1
	97.7	-70.1	-73.3	92.8		170.7	-64.3	-70.7	159.7
$\mathbf{H_9}^{\mathbf{II}}$	75.9	-156.7	79.3	-8.0	$\mathbf{H_{19}}^{\mathbf{II}}$	69.5	62.7	-165.6	154.8
	74.7	-157.3	76.5	-3.3		70.1	61.7	-162.5	148.5
	74.9	-156.8	78.1	-6.7		72.8	65.0	-166.4	147.6
	74.7	-156.9	76.7	-3.7		73.8	63.4	-168.2	143.9
	74.7	-157.7	77.9	-6.2		75.0	63.7	-167.5	147.6
	74.9	-158.2	77.0	-3.9		78.9	61.8	179.7	157.1
$\mathbf{H_9}^{\mathbf{III}}$	42.7	53.8	-152.6	61.7	$\mathbf{H_{19}}^{\mathbf{III}}$	143.7	-175.9	63.9	76.7
	40.4	54.1	-153.8	63.6		140.6	-171.0	64.2	71.1
	42.7	53.0	-151.0	61.1		139.8	-173.8	61.1	74.7
	41.5	53.6	-152.4	63.5		146.4	-174.7	61.3	68.3
	43.9	52.3	-151.2	59.8		145.2	-172.0	62.7	64.6
	42.1	54.0	-153.4	71.3		160.1	-175.5	65.3	61.3
$\mathbf{H_{14}}^{\mathbf{I}}$	112.9	-56.9	-66.1	159.5	$\mathbf{H_{24}}^{\mathbf{I}}$	-166.1	-179.0	-64.8	-81.0
	135.0	-62.5	-67.6	138.8		-153.0	-179.4	65.4	-87.2
	136.0	-58.8	-64.1	140.6		-153.2	-179.7	-64.7	-87.9
	132.7	-59.2	-65.2	141.8		-150.1	-175.1	-62.6	-77.5
	134.4	-62.2	-65.9	139.5		-168.2	-178.6	-61.7	-69.6
	139.1	-59.2	-60.1	134.0		-171.0	177.3	-63.8	-68.7
$\mathbf{H_{14}}^{\mathbf{II}}$	-61.8	-65.2	131.6	-122.7	$\mathbf{H_{24}}^{\mathbf{II}}$	76.1	177.4	167.2	79.3
	-60.5	-57.2	149.9	-120.2		72.8	178.3	167.1	75.9
	-61.4	-57.0	145.5	-119.5		75.0	174.3	168.8	72.2
	-60.9	-57.1	147.2	-118.3		76.9	175.2	169.2	79.0
	-65.9	-60.5	154.2	-107.6		76.4	176.5	170.8	70.5
	-70.1	-61.7	164.5	-128.3		80.6	177.4	173.8	71.6
$\mathbf{H_{14}}^{\mathbf{III}}$	102.0	-161.1	68.1	72.7					
	100.7	-161.1	61.9	62.9					
	114.7	-156.5	62.9	59.7					
	109.4	-155.4	63.4	62.0					
	112.5	-160.8	59.8	53.5					
	133.8	-164.0	66.1	43.6					

[a]) Torsion angles in degrees.

Table S5. *Backbone Torsion Angles of Conformers of the Blocked Vinylogous* γ*-Peptide Hexamer* ***2*** *with Hydrogen Bonds Formed in Backward and Forward Direction Obtained at the B3LYP/6-31G* Level of* ab initio *MO Theory* [a])

Conf.	φ	θ	ψ	Conf.	φ	θ	ψ
$\mathbf{vH}_{14}$	67.8	18.6	165.7	$\mathbf{vH}_{17}$	-152.6	-131.1	14.0
	65.0	12.9	166.0		81.7	-100.8	35.8
	65.6	15.5	161.8		95.0	-99.3	37.6
	65.5	16.4	162.2		83.2	-97.6	46.3
	68.6	12.3	155.3		85.8	-96.9	42.4
	84.1	-7.1	178.8		82.5	-91.6	44.1
$\mathbf{vH}_{19}$	78.1	7.8	-175.6	$\mathbf{vH}_{22}^{\mathbf{I}}$	122.1	115.8	167.6
	69.3	31.1	174.4		75.8	104.2	159.5
	84.4	12.7	-173.3		64.8	106.0	159.5
	88.7	10.9	179.0		72.3	106.2	160.6
	92.2	12.3	-177.3		70.8	105.0	160.4
	117.7	-3.9	-176.9		72.2	131.2	-175.6
$\mathbf{vH}_{24}$	75.9	-118.9	32.1	$\mathbf{vH}_{22}^{\mathbf{II}}$	114.6	-125.5	28.4
	73.8	-127.7	38.2		103.1	-117.3	33.7
	82.7	-118.3	-35.6		99.4	-108.3	34.3
	104.3	-116.1	29.6		91.2	-104.6	35.1
	95.3	-116.6	-20.9		85.0	-101.9	38.9
	104.3	-129.5	-19.6		88.0	-101.5	38.1

[a]) Torsion angles in degrees.

Table S6. *Backbone Torsion Angles of Conformers of the Blocked Vinylogous* γ*-Peptide Hexamer* ***2*** *with Hydrogen Bonds Formed in Backward and Forward Direction Obtained at the SCRF/HF/6-31G* Level of* ab initio *MO Theory* [a])

Conf.	φ	θ	ψ	Conf.	φ	θ	ψ
$\mathbf{vH_{14}}$	61.4	41.5	157.4	$\mathbf{vH_{17}}$	114.8	-123.4	36.4
	61.1	16.2	161.6		95.1	-107.2	39.7
	60.7	24.8	158.6		96.4	-101.3	39.8
	61.6	22.2	158.0		84.9	-99.6	48.2
	64.0	21.3	150.7		86.0	-101.1	46.0
	72.1	4.5	-177.4		83.1	-96.5	45.4
$\mathbf{vH_{19}}$	72.8	27.3	-173.2	$\mathbf{vH_{22}^{I}}$	91.2	113.9	161.5
	69.5	32.5	-176.0		73.9	108.6	156.5
	74.3	24.3	-174.3		68.2	111.0	157.8
	74.8	28.6	179.7		71.5	109.7	154.7
	77.9	23.9	-177.2		70.8	111.1	157.7
	95.4	7.7	-167.4		73.8	122.2	173.7
$\mathbf{vH_{24}}$	73.8	-132.3	30.3	$\mathbf{vH_{22}^{II}}$	94.7	-124.5	29.2
	75.5	-128.7	32.2		91.8	-113.6	34.5
	85.1	-108.3	-17.1		102.3	-111.8	37.3
	87.6	-119.6	23.4		88.7	-109.2	42.0
	79.5	-122.6	10.5		85.8	-105.4	40.8
	86.1	-129.7	13.8		86.2	-110.2	38.7

[a]) Torsion angles in degrees