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Mixed Helices - A General Folding Pattern in Homologous Peptides?

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Table S1: Backbone torsion angles[a] of the mixed helix $\mathbf{H_{14/16}}$ and the 3_{10}-helix ($\mathbf{H_{10}}$) in hexamers of α-peptides at the HF/6-31G* and DFT/B3LYP/6-31G* level of ab initio MO theory

Type[b]	HF/6-31G*		B3LYP/6-31G*	
	φ	ψ	φ	ψ
$\mathbf{H_{14/16}}$	85.5	–75.2	81.4	–72.1
	–73.6	131.1	–73.6	129.9
	81.1	–66.6	78.6	–67.6
	–80.8	84.5	–76.7	80.2
	121.7	–73.2	123.7	–78.1
	–81.4	82.2	–76.6	78.4
$\mathbf{H_{10}}$[c]	–67.1	–25.5	–65.6	–25.2
	–62.9	–19.5	–59.6	–19.9
	–63.0	–20.1	–60.6	–20.0
	–64.4	–18.3	–61.6	–18.7
	–68.6	–12.9	–67.2	–10.7
	–94.5	–4.8	–100.2	11.3

[a] Angles in degrees. [b] $\mathbf{H_{x/y}}$ denotes mixed helices with alternating rings with x and y atoms, respectively, closed by hydrogen bonds. $\mathbf{H_x}$ denotes periodic helices with rings of x atoms. [c] 3_{10}-helix.

Table S2: Backbone torsion angles[a] of mixed and periodic helices in hexamers of β-peptides at the HF/6-31G* and DFT/B3LYP/6-31G* level of ab initio MO theory

Type[b]	HF/6-31G*			B3LYP/6-31G*		
	φ	θ	ψ	φ	θ	ψ
$\mathbf{H}^{\mathbf{I}}_{\mathbf{12/10}}$	–97.7	56.6	96.8	–97.6	54.7	96.1
	85.7	65.5	–111.1	87.0	64.7	–109.4
	–101.8	61.4	88.9	–103.0	58.7	88.0
	89.6	66.1	–111.0	92.4	64.8	–107.8
	–101.1	63.0	93.7	–104.2	61.8	93.5
	85.0	61.1	–132.8	85.2	61.8	–124.3
$\mathbf{H}^{\mathbf{II}}_{\mathbf{10/12}}$	79.7	58.6	–103.1	80.8	58.9	–97.6
	–16.2	–54.6	165.2	–21.3	–52.4	160.4
	87.4	60.8	–96.2	90.8	59.1	–94.1
	–27.2	–49.6	160.0	–30.0	–47.8	155.0
	82.1	67.6	–93.8	84.7	66.6	–94.2
	–73.3	–60.7	–86.7	–73.6	–59.8	–85.8
$\mathbf{H}^{\mathbf{III}}_{\mathbf{10/12}}$	–85.8	–58.5	–67.2	–94.0	–56.6	–57.7
	–93.0	56.1	80.6	–94.8	54.2	77.4
	178.9	–61.8	–20.8	–178.5	–60.6	–22.1
	–92.7	50.6	87.0	–93.3	49.1	84.5
	177.2	–60.7	–23.4	179.3	–59.2	–26.0
	–90.7	52.0	90.8	–90.5	51.4	87.5
$\mathbf{H}^{\mathbf{I}}_{\mathbf{20/18}}$	75.7	57.4	–162.3	75.8	53.1	–158.5
	–81.6	–79.3	137.8	–81.8	–81.8	136.1
	90.7	66.4	171.1	97.6	65.2	166.1
	–78.5	–56.8	148.6	–78.5	–49.3	145.9
	71.0	74.6	173.9	69.1	79.4	164.5
	–86.4	–60.4	165.1	–83.9	–56.4	162.2
$\mathbf{H}^{\mathbf{II}}_{\mathbf{20/18}}$	76.7	61.3	–168.2	76.1	59.1	–170.5
	–173.4	67.5	4.9	–170.9	67.7	–3.5
	98.8	66.8	172.7	110.5	66.7	163.9
	–150.2	56.6	47.3	–138.1	55.5	49.3
	69.6	69.6	–157.2	68.5	73.6	–155.9
	178.3	57.4	91.1	–179.9	53.8	105.2
$\mathbf{H}^{\mathbf{III}}_{\mathbf{20/18}}$	80.5	–176.7	143.2	81.5	–172.6	114.3
	62.2	43.6	–106.6	57.7	43.6	–103.1
	152.5	162.4	69.1	141.3	166.1	70.7
	72.9	51.7	–143.9	73.6	51.0	–145.4
	168.9	159.4	76.7	169.7	159.3	74.4
	77.0	54.1	–145.7	80.0	50.9	–144.8
$\mathbf{H}^{\mathbf{IV}}_{\mathbf{18/20}}$	77.1	159.5	86.9	80.1	159.4	75.7
	101.7	–54.7	–85.3	105.1	–56.6	84.0
	79.3	–170.7	99.7	77.0	–168.1	102.0
	109.6	–47.5	–43.0	105.7	–49.8	–35.0
	84.0	170.8	73.3	83.9	169.3	75.9
	111.6	–56.7	–32.3	107.3	–57.6	–28.8

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Table S2 continued:

Type[b]	HF/6-31G*			B3LYP/6-31G*		
	φ	θ	ψ	φ	θ	ψ
$\mathbf{H_{14}}$	–146.6	62.6	–119.4	–136.3	62.7	–119.5
	–156.2	62.3	–127.1	–152.1	63.4	–129.8
	–148.3	60.7	–137.5	–144.9	61.6	–137.4
	–135.3	60.1	–143.2	–133.7	61.3	–143.6
	–130.9	58.3	–138.5	–129.9	58.5	–138.2
	–135.3	64.5	–160.3	–132.9	63.7	–154.3
$\mathbf{H_{12}}$	–97.2	80.2	–106.8	–92.5	81.7	–111.7
	–80.4	93.6	–118.2	–90.0	95.6	–117.5
	–86.9	92.1	–108.5	–90.7	93.9	–99.8
	–87.2	91.0	–107.9	–91.8	89.0	–99.1
	–87.3	92.0	–108.9	–90.0	91.2	–102.3
	–83.8	88.6	–107.9	–84.4	86.5	–103.7

[a] Angles in degrees. [b] $\mathbf{H_{x/y}}$ denotes mixed helices with alternating rings with x and y atoms, respectively, closed by hydrogen bonds. $\mathbf{H_x}$ denotes periodic helices with rings of x atoms.

Table S3: Backbone torsion angles[a] of mixed and periodic helices in hexamers of γ-peptides at the HF/6-31G* and DFT/B3LYP/6-31G* level of ab initio MO theory

Type[b]	HF/6-31G*				B3LYP/6-31G*			
	φ	θ	ζ	ψ	φ	θ	ζ	ψ
$\mathbf{H}^{\mathrm{I}}_{\mathbf{14/12}}$	–92.8	78.2	–74.4	162.4	–96.9	78.0	–70.7	154.9
	95.8	81.0	–74.5	–29.9	105.1	76.7	–78.4	–24.5
	–91.1	79.4	–79.5	161.5	–94.1	80.3	–76.1	154.0
	94.4	84.4	–72.8	–29.2	101.1	82.4	–75.0	–26.9
	–96.2	81.4	–79.7	164.7	–101.2	82.9	–76.4	158.2
	85.3	76.9	–53.7	–87.5	89.2	73.6	–55.5	–92.1
$\mathbf{H}^{\mathrm{II}}_{\mathbf{14/12}}$	77.1	58.4	–84.3	–79.2	78.4	61.1	–77.0	–90.9
	–71.2	–36.2	–56.4	142.6	–66.6	–31.1	–56.8	144.5
	65.4	56.2	–125.6	–53.1	59.7	54.8	–130.5	–48.0
	–63.8	–37.0	–60.5	142.5	–60.8	–37.7	–59.6	139.4
	68.4	55.6	–121.9	–58.5	67.3	54.9	–122.8	–55.2
	–65.6	–34.8	–52.5	157.0	–63.8	–37.1	–51.0	152.6
$\mathbf{H}^{\mathrm{I}}_{\mathbf{24/22}}$	108.9	–172.5	–169.1	–153.4	104.9	–173.8	–168.2	–154.5
	–101.7	63.5	–94.4	122.2	–98.6	65.1	–93.4	117.7
	74.2	–176.5	–79.7	–167.7	75.2	–174.8	–76.6	–169.8
	–125.1	61.8	–77.2	154.3	–123.6	61.3	–74.7	154.4
	115.5	–176.9	–177.3	–138.0	114.9	–171.7	–177.3	–137.3
	–160.0	66.9	–74.9	152.9	–158.7	66.5	–72.9	155.3
$\mathbf{H}^{\mathrm{II}}_{\mathbf{24/22}}$	79.3	66.6	–66.3	–80.3	83.4	61.5	–65.6	–79.8
	84.3	69.4	74.8	9.7	85.2	66.3	75.5	7.3
	93.6	79.3	–65.5	–102.1	102.1	74.7	–66.1	–105.4
	122.9	64.4	66.2	16.2	129.3	65.3	66.5	16.0
	74.5	74.4	–73.8	–76.6	71.7	73.9	–72.3	–84.3
	75.2	83.9	65.9	70.5	73.2	84.2	64.5	80.6
$\mathbf{H}^{\mathrm{III}}_{\mathbf{24/22}}$	128.9	–64.9	–178.8	104.8	120.4	–65.9	179.4	97.8
	–75.1	–63.0	80.5	29.3	–68.0	–62.6	83.0	17.6
	116.7	–68.4	–173.7	127.5	128.9	–69.7	–174.9	128.9
	–89.1	–71.9	82.8	57.7	–93.9	–68.2	85.8	52.3
	103.6	–65.7	–173.2	124.3	104.8	–64.1	–171.8	127.2
	–80.4	–74.0	58.5	87.2	–81.6	–72.4	58.3	97.4
$\mathbf{H}_{\mathbf{14}}$	106.1	–62.6	–67.5	165.6	106.1	–62.6	–67.5	165.6
	136.5	–63.2	–68.2	138.3	136.5	–63.2	–68.2	138.3
	138.0	–60.1	–65.1	141.4	138.0	–60.1	–65.1	141.4
	132.9	–61.0	–66.0	144.4	132.9	–61.0	–66.0	144.4
	135.3	–63.4	–66.7	143.0	135.3	–63.4	–66.7	143.0
	138.3	–61.0	–64.1	139.7	138.3	–61.0	–64.1	139.7

[a] Angles in degrees. [b] $\mathbf{H}_{\mathbf{x/y}}$ denotes mixed helices with alternating rings with x and y atoms, respectively, closed by hydrogen bonds. $\mathbf{H}_{\mathbf{x}}$ denotes periodic helices with rings of x atoms.

Table S4: Backbone torsion angles[a] of mixed and periodic helices in hexamers of δ-peptides at the HF/6-31G* and DFT/B3LYP/6-31G* level of ab initio MO theory

	HF/6-31G*					B3LYP/6-31G*				
Type	φ	θ	ζ	ρ	ψ	φ	θ	ζ	ρ	ψ
$\mathbf{H}^{I}_{14/16}$	–80.2	152.4	–74.0	–69.8	118.0	–80.8	154.6	–70.2	–69.0	112.9
	80.8	73.5	–165.9	70.6	–107.9	81.6	74.9	–162.7	70.6	–107.6
	–171.7	159.1	–77.3	–68.1	130.5	–172.2	158.8	–76.5	–69.3	132.4
	75.9	68.6	–167.5	82.1	–125.8	76.9	67.3	–166.8	81.6	–126.7
	–145.8	89.0	–70.9	–69.6	162.7	–141.8	87.6	–68.8	–70.0	167.9
	70.7	63.1	–165.3	71.9	–121.2	67.5	61.6	–160.1	71.0	–111.3
$\mathbf{H}^{II}_{16/14}$	111.7	–46.4	–59.6	152.0	151.4	108.9	–45.3	–58.5	151.3	147.0
	–120.5	83.9	–66.9	–65.0	161.8	–117.3	85.1	–65.2	–65.0	163.0
	113.4	–53.8	–62.3	167.4	158.7	111.8	–53.6	–59.8	169.9	153.5
	–125.9	82.3	–65.9	–67.4	164.4	–122.1	82.9	–64.3	–67.7	164.1
	113.3	–52.6	–63.3	164.6	157.8	112.7	–52.4	–59.9	167.4	150.8
	–12.1	–153.3	101.1	–5.7	–80.9	–6.0	–153.9	101.2	–5.5	–81.2
$\mathbf{H}_{10}$	97.3	–62.8	–68.2	169.2	–86.1	96.9	–61.2	–67.0	166.9	–84.8
	97.9	–62.6	–68.3	168.6	–84.7	97.9	–61.3	–67.0	166.5	–84.1
	98.1	–62.4	–68.4	168.5	–84.5	98.0	–60.9	–67.4	166.2	–83.6
	98.2	–62.4	–68.4	168.4	–84.4	98.3	–61.0	–67.3	166.1	–83.9
	98.3	–62.4	–68.4	168.7	–84.5	98.2	–61.1	–67.7	166.3	–83.0
	99.0	–62.6	–68.8	168.7	–87.1	98.8	–61.2	–67.8	167.1	–85.5
$\mathbf{H}_{8}$	–178.8	66.5	–143.5	69.1	–171.2	–178.4	64.5	–139.6	68.5	–171.5
	–179.0	66.4	–142.5	69.2	–172.7	–179.1	64.2	–138.6	68.4	–172.5
	–179.5	66.4	–142.2	69.1	–172.5	–179.3	64.2	–138.1	68.3	–172.1
	–179.3	66.4	–142.2	69.2	–172.9	–178.7	64.2	–138.0	69.0	–173.1
	–179.4	66.4	–142.5	69.3	–173.1	–179.2	64.6	–138.8	68.4	–172.9
	–178.7	66.6	–143.9	69.7	–173.8	–178.4	64.7	–140.0	69.0	–173.9

[a] Angles in degrees. [b] $\mathbf{H}_{x/y}$ denotes mixed helices with alternating rings with x and y atoms, respectively, closed by hydrogen bonds. $\mathbf{H}_{x}$ denotes periodic helices with rings of x atoms.

Table S5: Total energies[a] of periodic helices used as references for the calculations of stabilisation energies at the HF/6-31G*, DFT/B3LYP/6-31G* and PCM//HF/6-31G* level of ab initio MO theory

Type	E_T		
	HF/6-31G*	B3LYP/6-31G*	PCM//HF/6-31G*
		α-Peptides	
$\mathbf{H_{10}}$	–1487.918103	–1496.607967	–1487.945670
		β-Peptides	
$\mathbf{H_{14}}$	–1722.127594	–1732.493651	–1722.147167
$\mathbf{H_{12}}$	–1722.132691	–1732.503571	–1722.138542
		γ-Peptides	
$\mathbf{H_{14}}$	–1956.361656	–1968.407950	–1956.340687
		δ-Peptides	
$\mathbf{H_{10}}$	–2190.562661	–2204.282712	–2190.528328
$\mathbf{H_{8}}$	–2190.555385	–2204.271987	–2190.543623

[a] In a.u.