Helices in peptoids of α- and β-peptides

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Table S1. Torsion angles, relative energies in the gas phase and in solution and relative free enthalpies for the trans and cis conformers of the blocked α-peptoid monomer models **Ia** and **Ib** at the DFT/B3LYP/6-31G* level of *ab initio* MO theory[a].

Conformers[b]	ω	φ	ψ	ω_2	ΔE
trans (**Ia**)					
α_D	-172.4	86.9	-177.0	177.4	3.0
$C_{7\beta}$	-174.7	-113.9	98.4	177.3	**0.0**[b]
α	-173.2	-55.6	-46.7	175.1	28.1
cis (**Ib**)					
α_D	-10.8	-80.7	-171.9	-0.1	8.6
$C_{7\beta}$	10.4	-148.9	64.4	7.1	17.7
α	-12.0	61.2	53.4	4.6	22.0

[a] Torsion angles in degrees, energy values in kJ mol^{-1}.

[b] Cf. structure formulae **Ia** and **Ib**.

[c] E_T = -535.146747 au.

Table S2. Torsion angles for the blocked hexamer helices of α-peptoids at the DFT/B3LYP/6-31G* level of *ab initio* MO theory[a].

Hexamer[b]	ω	φ	ψ	Hexamer[b]	ω	φ	ψ
trans (**Ia**, *n* = 6)				cis (**Ib**, *n* = 6)			
α_D	-172.5	89.7	-178.2	α_D	9.0	85.4	-179.4
	-170.3	88.4	-179.5		13.9	80.1	-177.3
	-170.1	86.5	-177.5		17.5	76.1	-177.5
	-171.1	88.2	-178.1		18.8	75.1	179.4
	-169.9	87.0	-178.8		20.3	73.1	173.0
	-170.2	85.8	-179.1		16.7	73.3	165.4
	-180.0				-2.6		
$C_{7\beta}$	173.7	-81.9	169.7	$C_{7\beta}$	13.6	-145.1	65.4
	-175.8	-100.6	116.5		17.7	-159.1	71.9
	-177.4	-124.5	75.0		14.1	-157.2	71.0
	-173.9	-125.1	74.7		14.2	-159.1	73.7
	-173.9	-126.2	69.4		8.6	-156.2	81.7
	-175.9	-107.2	104.6		8.0	-152.6	71.2
	175.9				0.9		
α	-172.4	-57.2	-45.5	α/α_D	-8.9	60.4	42.8
	-173.1	-56.5	-44.6		5.5	77.7	165.9
	-175.6	-53.6	-46.7		-17.8	55.8	53.1
	-174.2	-55	-44.4		14.5	77.9	160.9
	-175.3	-56.4	-45.9		-9.5	61.6	55.4
	-172.5	-54.4	-48.4		13.5	73.9	168.8
	175.5				-3.0		

[a] Torsion angles in degrees.

[b] Derived from the conformers of **Ia** and **Ib** in table S1.

Table S3. Relative energies in the gas phase and in solution and relative free enthalpies for the blocked trans and cis hexamer helices of α-peptoids at the DFT/B3LYP/6-31G* level of *ab initio* MO theory[a].

Hexamer[b]	ΔE	Hexamer[b]	ΔE
trans (**Ia**, $n = 6$)		cis (**Ib**, $n = 6$)	
α_D	**0.0**[c]	α_D	2.1
$C_{7\beta}$	12.8	α/α_D	58.0
α	99.4	$C_{7\beta}$	120.3

[a] Energies in kJ/mol.

[b] Derived from the conformers of **Ia** and **Ib** in table S1.

[c] $E_T = -1771.725336$ au.

Table S4. Torsion angles, relative energies in the gas phase and in solution and relative free enthalpies for the trans and cis conformers of the blocked β-peptoid monomer models **IIa** and **IIb** at the DFT/B3LYP/6-31G* level of *ab initio* MO theory[a].

Conformers[b]	ω	φ	θ	ψ	ω_2	ΔE
trans (**IIa**)						
t-**1**	-175.2	-76.7	-72.2	171.4	178.3	**0.0**[c]
t-**2**	173.0	-94.4	47.0	87.5	-171.5	3.6
t-**3**	-179.9	-80.1	177.8	-84.5	-178.4	4.3
t-**4**	-177.9	-78.4	-172.6	-172.5	-179.6	7.2
t-**5**	-176.2	79.4	66.5	87.9	178.3	15.0
t-**6**	178.9	-85.4	-179.3	85.8	178.7	21.5
t-**7**	-172.7	127.0	-63.2	-177.6	178	23.8
t-**8**	-171.1	9.9	-79.6	-8.1	-174.1	65.8
cis (**IIb**)						
c-**1**	4.0	95.8	-179.4	-179.2	-1.1	8.6
c-**2**	-0.5	119.7	-75.3	161.5	1.0	8.9
c-**3**	-3.8	92.2	82.7	-169.5	-1.5	12.0
c-**4**	-0.9	119.8	-52.1	-79.3	-0.9	20.2
c-**5**	-3.1	-93.4	-69.7	-78.9	-2.7	23.4
c-**6**	5.5	-72.7	-36.5	-81.1	-6.1	28.0

[a] Torsion angles in degrees, energies in kJ mol^{-1}.

[b] Cf. structure formulae **IIa** and **IIb**.

[c] E_T = -574.463126 au.

Table S5. Torsion angles for the blocked hexamer helices of trans β-peptoids at the DFT/B3LYP/6-31G* level of *ab initio* MO theory[a].

Hexamer[b]	ω	φ	θ	ψ	Hexamer[a]	ω	φ	θ	ψ
t-**1**	-172.4	-78.2	-72.4	169.0	t-**4**	-174.9	-78.7	-174.3	-175.1
	-175.7	-79.1	-73.4	170.3		-178.2	-79.9	-175.3	-176.5
	-175.6	-79.0	-72.7	170.0		-178.6	-79.7	-175.4	-175.4
	-175.0	-78.9	-73.3	170.1		-178.4	-79.3	-174.9	-175.3
	-175.8	-79.2	-72.6	168.4		178.7	-78.0	-173.6	-176.5
	-175.0	-78.4	-74.0	171.8		-178.1	-79.0	-173.6	-173.4
	178.1					178.7			
t-**2**	176.8	-98.6	46.9	80.4	t-**5**	-178.3	81.0	67.0	90.6
	-171.3	-121.9	42.7	72.9		-175.1	76.4	57.8	94.0
	-175.7	-106.8	44.9	78.6		-177.1	78.1	59.3	94.7
	-172.0	-118.8	41.5	78.4		-176.8	77.3	57.9	94.7
	179.8	-107.9	46.1	75.4		-177.6	76.8	60.3	96.8
	-175.7	-101.6	48.2	84.5		-173.7	77.2	55.2	91.4
	-172.1					177.2			
t-**3**	-175.1	-79.7	176.2	-88.6	t-**7**	-161.4	122.9	-62.0	151.1
	-178.0	-81.9	176.3	-88.4		-168.3	128.0	-61.9	166.5
	-179.0	-81.3	175.7	-88.9		-167.2	122.2	-61.2	160.0
	-177.6	-82.1	175.8	-87.5		-169.5	123.0	-61.9	164.2
	-179.2	-81.1	176.6	-88.3		-168.5	122.3	-59.5	160.7
	-178.4	-82.0	177.4	-83.7		-170.7	122.3	-64.8	179.4
	-178.5					-179.2			

[a] Torsion angles in degrees.

[b] Derived from the conformers of **IIa** in table S4.

Table S6. Torsion angles for the blocked hexamer helices of cis β-peptoids at the DFT/B3LYP/6-31G* level of *ab initio* MO theory[a].

Hexamer[b]	ω	φ	θ	ψ	Hexamer[b]	ω	φ	θ	ψ
c-**1**	0.7	98.2	-178.4	-175.1	c-**3**	10.1	86.7	71.6	-139.5
	2.4	98.1	179.0	-176.6		-9.1	89.6	78.7	-175.1
	2.4	98.9	-178.8	-174.9		-7.6	102.4	88.2	176.0
	2.1	98.5	-177.5	-176.2		10.8	93.6	78.1	-149.8
	2.7	99.8	-179.0	-174.8		-4.5	89.2	78.9	-164.7
	2.5	98.7	-178.1	-177.0		-4.9	96.1	85.8	-175.2
	-2.9					-0.1			
c-**2**	-1.9	119.4	-77.3	167.3	c-**5**	2.3	-93.3	-70.4	-83.7
	7.7	114.5	-73.7	170.5		-6.6	-89.0	-65.8	-83.5
	8.0	114.3	-73.4	170.1		-8.8	-87.7	-62.4	-83.9
	8.9	113.9	-72.9	169.2		-9.4	-87.1	-62.8	-83.5
	9.1	114.2	-72.7	171.1		-10.4	-86.6	-63.7	-84.1
	8.2	114.3	-73.7	167.3		-9.8	-86.6	-63.8	-80.7
	1.8					-3.7			

[a] Torsion angles in degrees.

[b] Derived from the conformers of **IIb** in table S4.

Table S7. Relative energies in the gas phase and in solution and relative free enthalpies for the blocked hexamer helices of α-peptoids at the DFT/B3LYP/6-31G* level of *ab initio* MO theory[a].

Hexamer[b]	ΔI	Hexamer[b]	ΔE
trans (**IIa**, $n = 6$)		cis (**IIb**, $n = 6$)	
t-**1**	**0.0**[c]	t-**2**	28.6
t-**3**	21.6	t-**1**	47.5
t-**4**	38.1	t-**3**	23.8
t-**5**	31.3	t-**5**	137.8
t-**2**	53.1		
t-**7**	73.7		

[a] Energies in kJ mol^{-1}.

[b] Derived from the conformers of **IIa** and **IIb** in table S4.

[c] $E_T = $ -2007.626697 au.