

Typical distances within a regular alpha helix:

hn(i) - hn(i+1)	2.8 Å
ha(i) - hn(i+1)	3.4 Å
hb(i) - hn(i+1)	3.2 Å
hn(i) - hn(i+3)	3.5 Å
o(i) - hn(i+4)	2.1 Å
ha(i) - hn(i+3)	3.4 Å
ha(i) - hb(i+3)	3.4 Å

Typical torsion angles within a regular alpha helix:

phi: c ^o (i-1) - n(i) - c(i) - c ^o (i)	-60 deg
psi: n(i) - c(i) - c ^o (i) - n(i+1)	-60 deg

In X-PLOR notation these 2 torsion angles are:

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assign (resid 1 and name o) (resid 2 and name n)
      (resid 2 and name ca) (resid 2 and name o ) 1.0 -60.0 10.0 2

assign (resid 2 and name n) (resid 2 and name ca)
      (resid 2 and name c) (resid 3 and name n ) 1.0 -60.0 10.0 2
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Typical distances within a regular beta strand:

hn(i) - hn(i+1)	4.2 Å
ha(i) - hn(i+1)	2.2 Å
hb(i) - hn(i+1)	3.5 Å
ha(i) - ha(j)	2.2 Å
hn(i+1) - o(j-1)	2.2 Å
o(i+1) - hn(j-1)	2.2 Å
ha(i+2) - ha(j-2)	2.2 Å
ca(i) - ca(i+1)	3.8 Å
ca(i) - ca(i+2)	6.3 Å
ca(i) - ca(i+3)	9.7 Å
ca(i) - ca(i+4)	12.6 Å

Typical torsion angles within a regular beta strand:

phi: c ^o (i-1) - n(i) - c(i) - c ^o (i)	-120 deg
psi: n(i) - c(i) - c ^o (i) - n(i+1)	+150 deg

beta strand side chain:

hn(i) - n(i) - c(i) - c(i)	-60 deg
o(i) - c ^o (i) - c(i) - c(i)	+60 deg

In X-PLOR notation these 4 beta strand torsion angles are:

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assign (resid 1 and name o) (resid 2 and name n)
      (resid 2 and name ca) (resid 2 and name o ) 1.0 -120.0 10.0 2

assign (resid 2 and name n) (resid 2 and name ca)
      (resid 2 and name c) (resid 3 and name n ) 1.0 150.0 10.0 2

assign (resid 2 and name hn) (resid 2 and name n)
      (resid 2 and name ca) (resid 2 and name cb) 1.0 -60.0 10.0 2

assign (resid 2 and name o) (resid 2 and name c)
      (resid 2 and name ca) (resid 2 and name cb) 1.0 60.0 10.0 2
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