Model Building: 2 chain helix.  All residues trans.

One residue in asymmetric unit.

1 models with both chains running in the same direction.

For space group hcr-1: a single chain: the angle of rotation A per residue is 180 - B, where B is the projection angle of the tetrahedral Ca angle. Thus B must be less than 110°.

\[ 180 - B > 180 - 110 = 70° \]

Thus maximum number of residues per chain (for a single chain)

\[ \frac{360°}{70°} \approx 5.2 \]

By inspection of models it looks impossible to see up to a reasonable part per turn from the 2 family, because the change of the peptide bond makes reduces the protrusion per residue.

This could probably be shown very easily, analytically. This is limited to the 2 family, which has thin twist arrangement.

\[ \text{i.e. C-N distance increases and twisted molecule.} \]
Had no difficulty of making a single chain of pitch around 15A (about 4 residues per turn)

Found that the hydrogen C=O and N-H direction were necessary for the correct (see model on last page). [Note that the use of model building (carried out more carefully) would prove this too. The polypeptides cannot have high IR. + dichroism and have two chains, independent of other evidence]

Bend helix with $\leftarrow$-N bond nearly vertical

Bend second helix (related by $\leftarrow$-link to the first)

1 A

Joined up with hydrogen bonds:

Needed to describe these helices as follows.

Consider a hydrogen bond: also its vice versa related by the chord.

Make the smallest possible ring attached by running along monomer chain, colouring their two ends. This defines helix.

\[
\begin{array}{c}
\text{C} - \text{N} - \text{H} \cdots \text{O} \\
\end{array}
\]

In my first attempt the area $\leftarrow$-N bond with

call them (2 $\times$ 5)
Character of (2x5) helix
hydrogen bond poor.
N-H distance too far from C=O
N-H...< angle poor (perhaps 25°; depends on bond).

Distance between turns 2x6.5 or 2x7.5 Å (very wide)

prob. difficult to reduce this.
residues per turn (6 one helix) 5/2 or 6.
tunnel per residue ≈ 3 Å max; 2.8 Å

Van der Waals contacts all reasonable
+ no hole in centre.

I.B.

Altered hydrogen bonds to build the new, more open helix.
Defining ring is new.

\[
\begin{align*}
C_6 - C = O & \quad \cdots \quad H - N \\
\text{NH} & \\
C = O & \\
\text{C} & \\
N - H \cdots O = C & \quad \text{(2x8)}
\end{align*}
\]
hydroxy binding was satisfactory, but there was a hole in the middle.

\[ \text{with distance } \approx 2 \times 6 \text{ ft} \]

\[ \text{residue from } \text{one side } \approx 5 \frac{1}{2} \]

\[ \text{translation/residue } \approx 2 \frac{1}{8} \]

The hole is more nearly head-on (say, 45°-off) and the roughly position at 0

for this range much can be achieved as before

but no we only precisely defined.

average distance from center atom across hole \( \geq 5 \text{ ft} \)

\(\text{i.e. a hole.}\)

Tried more tighter screw but hydroxy binding

looked so the kind 3 left it at that.
In

While tunneling back to the first machine head
clamped over half the hydrogen bond I found I had
a new structure.

This has two chains related by a screw, not a
rotaxane axis. Then in the direction point of view there
is a primitive helix consisting of a residue alternately from
the two chains.

Thus we have a new family of helices.

Description of helix

define as follows: start at one.

The hydrogen bond then go the one in the same sense / the
residue N related by the primitive helix. (in the direction of the
next arm of the NH).


\[ \text{This can: } N \xrightarrow{C} O \xrightarrow{H} N \]

Q.S. What about of this really define it.
approx. residues/mm for one chain ≤ 5.

approx. pitch distance/mm for chain ≤ $6 \times 6 \times 3 \times 2$

approx. molecular radius = 2\AA

hydrogen bond: not bad. 0 except ≤ 6X off.

Nick finds direct. (may depend upon not breaking peptide bond).

Van der Waals: best in the middle.

dimer across = 4X

e. not bad, but not good.
Decided that a different symmetric method of description might be more informative. This is the cheetah folded round method.

\[ \text{Diagram:} \]

\[ B_4 \rightarrow H - N \rightarrow C = 0 \rightarrow H - N \rightarrow \]

\[ B_3 \rightarrow H - N \rightarrow C = 0 \rightarrow H - N \rightarrow \]

\[ B_2 \rightarrow H - N \rightarrow C = 0 \rightarrow H - N \rightarrow \]

\[ B_1 \rightarrow H - N \rightarrow C = 0 \rightarrow H - N \rightarrow \]

Whenever the connections of the above scheme must be part of it (for chains running in the same direction). Then we get different structures depending on whether A joins B, B_1, B_2, B_3, or B_4.

To B_2, A-B_1 is our \((2 \times 8)\)

I think A-B_1 in the screw one \((2 \times 5)\)\)

A-B_3 in our \((2 \times 5)\)
we want c = c

-110° and \( \theta \)

\[ \cos \theta \cos \phi, \cos \phi \sin \theta, \sin \theta \]

direction cosines of

\[ \cos \theta \cos \phi, \cos \phi \sin \theta, \sin \theta \]

plan:

\[ \cos^2 \phi (\cos^2 \theta - \sin^2 \phi) = \cos^2 \phi - \sin^2 \phi \]

\[ \cos \phi = \frac{\cos \psi + \sin^2 \phi}{\cos^2 \phi} \]
\[ \cos d = \cos \phi + \sin \phi \sin \alpha \]

\[ \cos \psi = \cos \log \cos \nu = -0.333 \]

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<th>( \cos \alpha )</th>
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</table>
\[
\text{Fractional per revolution} = 3.8 \sin (\theta - 22^\circ) \quad \AA
\]

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<tr>
<th>(\theta)</th>
<th>(8^\circ)</th>
<th>(\sin (\theta - 22^\circ))</th>
<th>(\text{mm} / \text{pitch})</th>
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<td>50</td>
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</table>

*Note: The pitch is measured.*

\[
\text{Fractional per revolution} = 3.8 \sin (\theta - 180^\circ) \quad \AA
\]

<table>
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<tr>
<th>(\theta)</th>
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<th>(\sin (\theta - 180^\circ))</th>
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Actually, the 3-fold helix works, our choice is 6.
Thus these calculations show that the pitch of a helix (even, one vector/anywhere unit, having the same period, say, \( \frac{\sqrt{5}}{2} \)) cannot have a pitch (independent of helix size) next to any \( 6 \frac{2}{3} \), because of the limitations of the helical angle. Thus one cannot have a two-screw helix this way.
For other family, we have

\[ \text{transl. vertical} = 3.8 \sin (A + 18) \]

<table>
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<tr>
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<th>( A + 18 )</th>
<th>( \sin (A + 18) )</th>
<th>( \text{Transl. vertical} )</th>
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<td>68</td>
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</table>
This rough calculation shows (as already found in model) that the other family (S) does some better work, pitch about 10-12 & over a fairly reasonable range.