

18th Feb 54

Model Building. - 2 chain helices.

all residues trans.

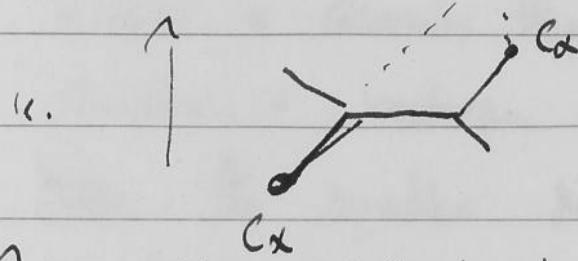
one residue in asymmetric unit.

1 models with both chains running in the same direction.

TRAP Consider first a single chain : the angle of rotation is per residue is $180 - \theta$, where θ is the projection angle of the transhelical Cx angle.
 Thus θ must be less than 110° .
 $\therefore 180 - \theta \dots$ greater than $180 - 110^\circ = 70^\circ$

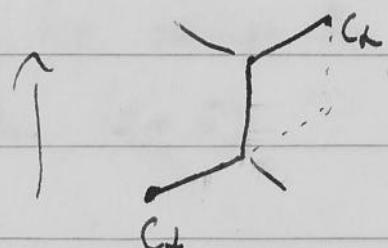
Thus maximum number of residues per chain (for a single chain) is $\frac{360}{70} \approx 5.2$

By inspection of models it looks impossible to get up to a reasonable pitch ^{distance} per turn from the α family, because the stingers of the peptide bond ope reduce the translation per residue.



This could probably be shown very easily analytically.

This decided to by the γ family, which has this sort of arrangement.



i.e. C-N distance increases
↓ vertical translation.

Had no difficulty of ~~in~~ making a single chain of pitch around 10 Å (about 4 residues per turn)

Found that the ~~hydrogen bond~~ C=O and N-H directions were necessarily far from the vertical (see sketch on last page). [Note that this sort of model building (carried out more carefully) would prove that ~~the~~ the polypeptides cannot have high I.R. \uparrow dichroism and have two chains, independent of other evidence.]

Bent helix with $\overset{\text{so}}{\text{C}}-\text{N}$ end roughly vertical.

Bent scroll helix (related by \uparrow twist to the first)

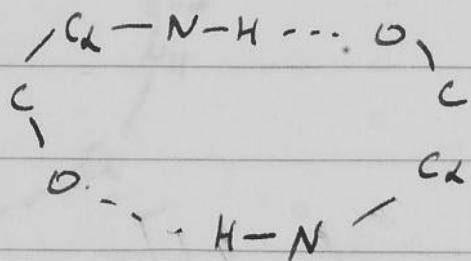
1. A Formed up with hydrogen bonds:

Decided to describe these helices as follows.

Consider a hydrogen bond: also its turn related to the dihedral.

Make the smallest possible ring ~~other~~ ~~not~~, by running along main chain, containing these two ends. This defines helix.

In my first attempt this was all this (2×5)



Characteristics of (2x5) helix

hydrogen bond poor.

N-H direction not nor far from \perp to C=O

$\text{N}-\text{H}-\text{C}=\text{O}$ angle poor (perhaps 25° ; depends on how much).

distance between turns $\approx 2 \times 6.5$ or 2×7.5 Å (very variable)

prob. difficult to reduce this.

residues per turn (of one helix) $\approx 5\frac{1}{2}$ or 6.

turn length per residue $\approx 3.75 \pm 0.25$ Å

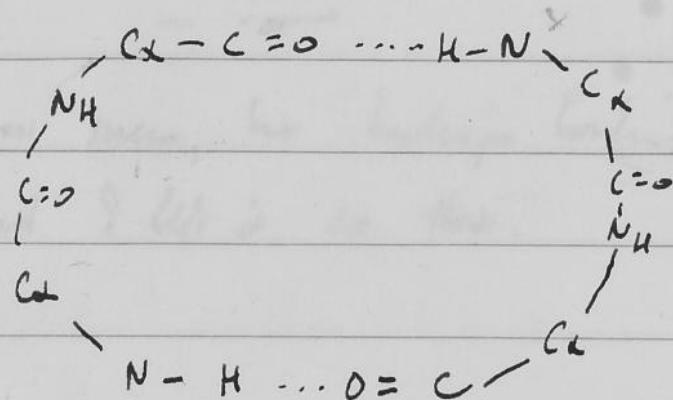
Van der Waals contacts all reasonable

& no hole in centre.

i. B.

Altered hydrogen bonding to build the new, more open helix.

Defining ring is now:



(e. (2x8)

hydrogen bonding were satisfactory, but show now a hole in the middle.

$$\left. \begin{array}{l} \text{avg} \\ \text{approx} \end{array} \right\} \begin{array}{l} \text{pitch distance } \approx 2 \times 6 \text{ \AA} \\ \text{residues / rung of one chain } \approx 5^{\frac{1}{2}} \\ \text{translational / residue } \approx 2^{\frac{1}{2}} \text{ \AA} \end{array}$$

NH hets Θ were nearly head-on (or very 45° off)
and NH roughly vertical or 0

For this reason structure can be defined as hydrogen
bonded, no net cavity possibly defined.

Average distance over several atoms across helix $\approx 5 \text{ \AA}$
(i.e. a hole).

Tried more hydrogen bonds, but hydrogen bonding
looked so far bad I left it at that.

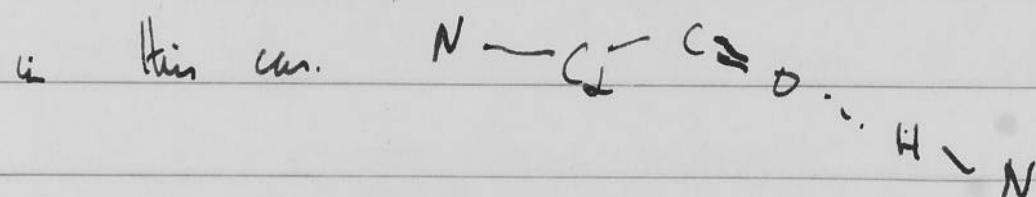
I.C. While working back to the bare structure had changed over half the hydrogen bond + found I had a new structure!

This has two chains related by a screw, not a rotation axis. Thus from the diagram point of view there is a primitive "helix" consisting of a turn of alternating from the two chains.

Thus we have a new family of helices.

Description of helix

define as follows : start at one turn of N: go along the hydrogen bond : then go the step (in the same sense) to the next N related by the primitive helix. (in the direction of the vertical comp. of its NH).



Thus (5×2)

P.S. Here's sketch of this really defines it.

approx. radius /nm for one chain ≈ 5 .

approx pitch distance /nm of one chain $\approx 6.6 \text{ \AA} \times 2$

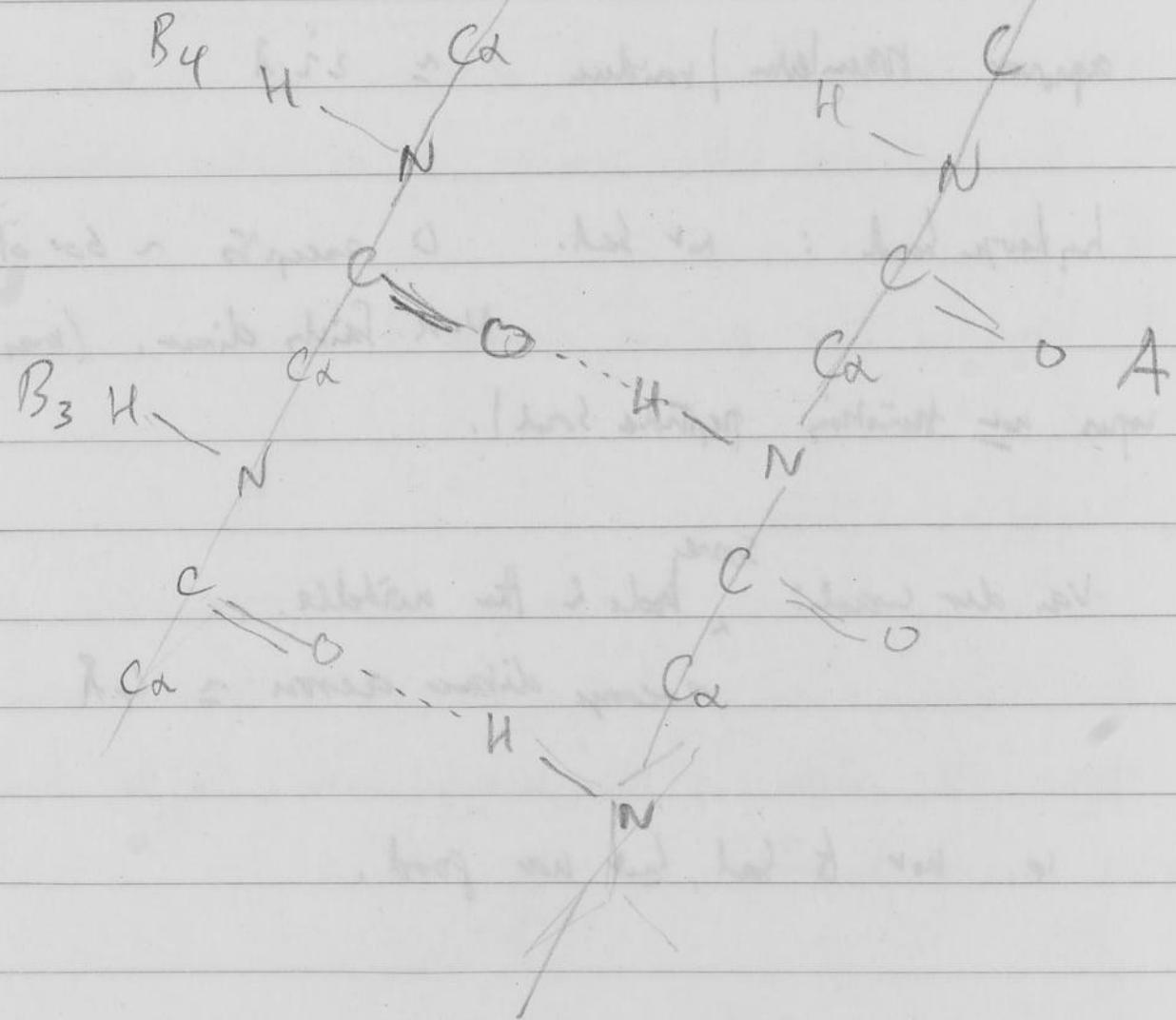
approx width / nm $\approx 2.2 \text{ \AA}$

hydrophobic : not bad. O accepts $\sim 6\text{\AA}$ oft.
N-H fairly direct. (was depend
upon one tripeptide bond).

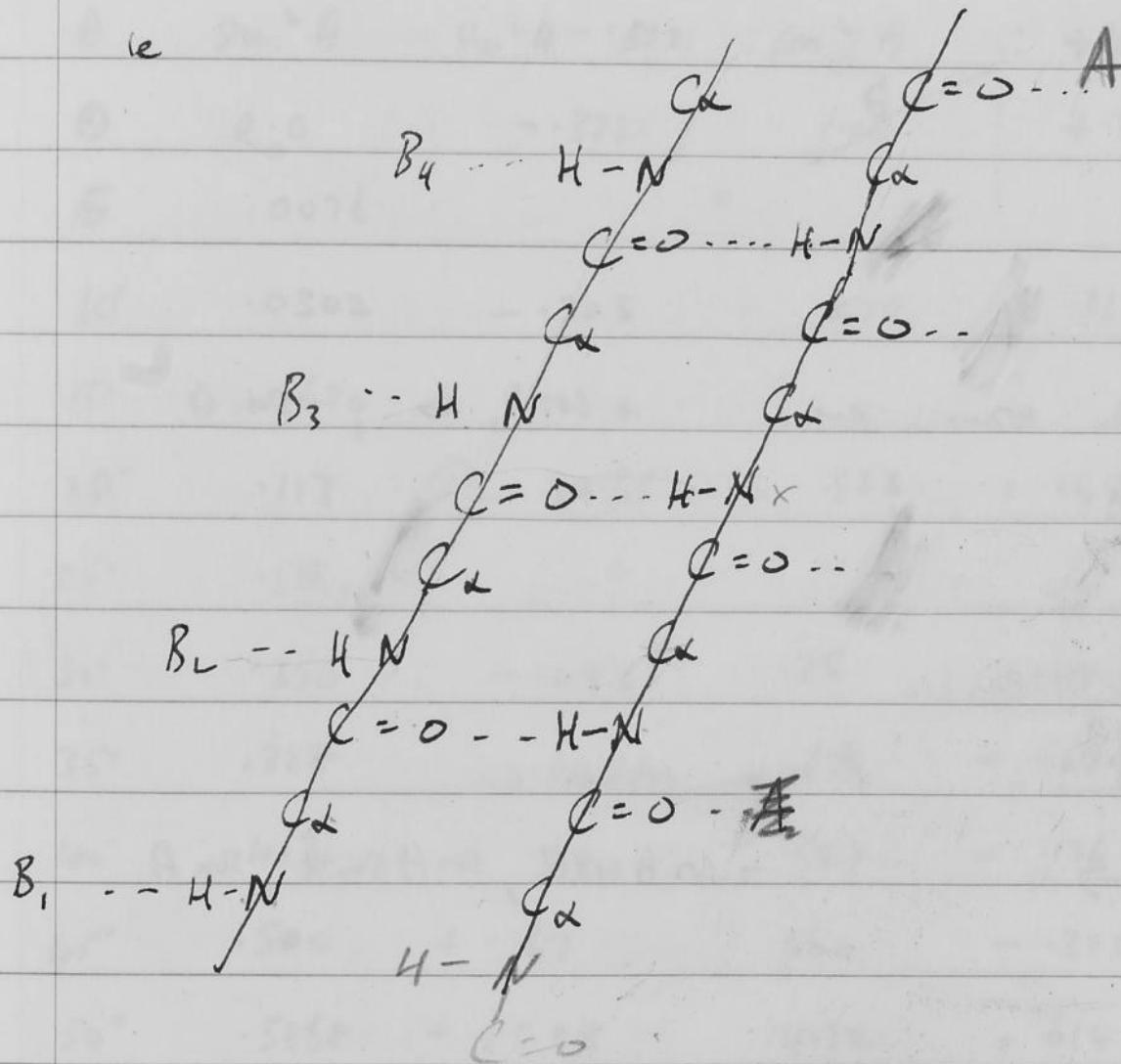
Van der Waals: ^{some} hole in the middle.

accept distance across $\approx 4 \text{ \AA}$

O. not so bad, but not good.



Decided that a different systematic method of description might be more informative. This is the sheet-folded-round method.

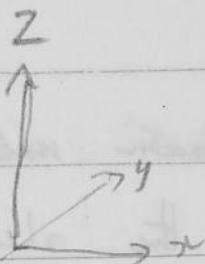


Whatever the connection or the above scheme may be part of it (for chain running in the same direction). Thus we get distance stichments depending upon whether A joins to B_1 , B_2 , B_3 or B_4 .

$\rightarrow B_2$ or the $A-B_1$ is our (2×8)

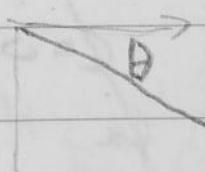
I think $A-B_2$ is the screw one (10.5×2)

$A-B_3$ is our (2×5)

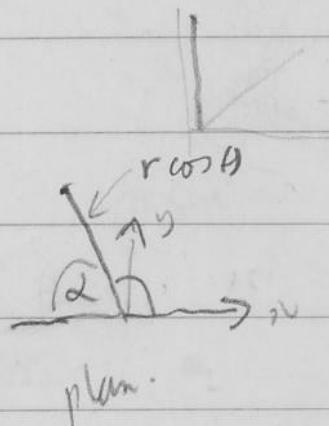


we want \hat{d} in a

function of ψ ($= 110^\circ$) and θ



Then direction cosines are $+ \cos \theta, 0, -\sin \theta$



direction cosines are

$- \cos \theta \cos \alpha, \cos \theta \sin \alpha, \sin \theta$

plan.

$$\text{Then } \cos \psi = - \cos^2 \theta \cos \alpha - \sin^2 \theta$$

$$\text{Then } - \cos \alpha = \frac{\cos \psi + \sin^2 \theta}{\cos^2 \theta}$$

$$-\cos \alpha = \cos \phi + \sin^2 A$$

$$\cos^2 A$$

$$\cos \phi = \cos 109^\circ 45' = - .333$$

θ	$\sin^2 A$	$\sin^2 A - .333$	$\cos^2 A$	$\therefore +\cos \alpha$	$\therefore \alpha$	$\frac{360}{\alpha}$
0	0.0	- .333	1.00	+ .333	$71^\circ 33'$	5.0
5	.0076					
10°	.0302	- .303	- .970	+ .313	71.7°	5.0
15°	.0670					
20°	.117	- .2163	- .883	+ .245	75.8°	4.75
25°	.1785					
30°	.250	- .083	.75	+ .111	83.6°	4.3
35°	.328	- .0053	.671	+ .0079	89.5°	4.01
40°	.413	+ .08	.587	- .136	97.2°	3.70
45°	.500	+ .167	.500	- .333	109.2°	3.29
50°	.5868	+ .2538	.4132	- .614	127.9°	2.81
54.75°						
55°	.6708	+ .3375	.329	> 1.		2.0

$$\text{translata per residue} \approx 3.8 \sin(\theta - 22^\circ) \text{ \AA}$$

θ $\theta - 22^\circ$ $\sin(\theta - 22^\circ)$ trans. pitch

30	80°	.139	0.528	2.2,
35	130°	.225	0.852	3.4,
40	180°	.309	1.17	4.3,
45	230°	.391	1.48	4.8,
50	280°	.469	1.78	5.0

i.e. we fold because amorphous overwheled

by amorphous formula. i.e. $3.8 \sin(\theta - 180^\circ) \text{ \AA}$

~~4.13 \AA~~

θ $\theta - 18^\circ$ $\sin(\theta - 18^\circ)$ trans. pitch.

30	12	.208	0.29	3.4
35	17	.292	1.1,	4.4,
40	22	.375	1.43	5.3
45	27	.454	1.72	5.6,
50	32	.530	2.0,	5.7
$54\frac{1}{2}^\circ$	$36\frac{1}{2}^\circ$.60	2.28	5.5,

actually the 3 fold helix works our about 6

Thus these calculations show that the pitch of a helix (mass, one residue/anymer unit) having the α arrangement (ie , not β) cannot have

a pitch (irrespective of hydrogen bonding) next to even of 6\AA , because of the limitation of the rehelical angle. Thus one cannot form ~~too~~ simple two-chain helices this way.

for other family, we have.

$$\text{translation / residue} \approx 3.8 \sin(A + 18^\circ)$$

A	$A + 18^\circ$	$\sin(A + 18^\circ)$	<u>mm</u>	$\therefore \text{mtl}$	
0	18	.309	1.17	5.9	
10	28	.469	1.78	8.9	
20	38	.616	2.34	11.1	<u>v. approx</u>
30	48	.743	2.82	12.1	only
40	58	.848	3.22	11.9	
50	68	.927	3.52	9.9	

Ans

This work calculation shows (as already found by model)
that the other family ($\sqrt{}$) does give better with
pitch above 10-12 R over a fairly reasonable range.