18th Jan 54

Model Building. – 2 chain helices.

all residues trans.

one residue in asymetric unit.

! models with both chains running in the same direction.

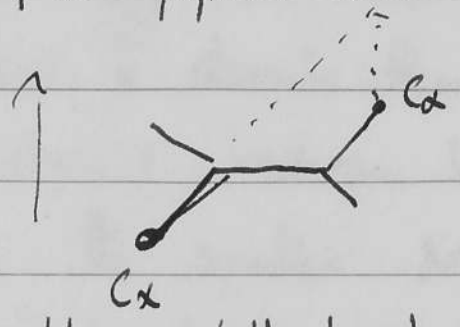
Consider first a single chain: the angle of rotation per residue is $180-\theta$, where θ is the projection angle of the tetrahedral C_α angle.

Thus θ must be less than 110°

$\therefore$ $180-\theta$ - - - greater than $180-110° = 70°$

Thus maximum number of residues per chain (for a single chain) is $\frac{360}{70} \triangleq 5{\cdot}2$

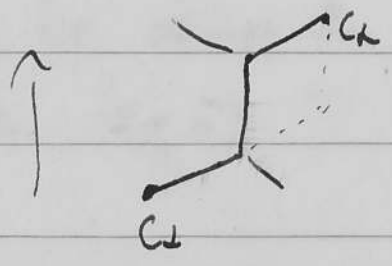
By inspection of models it looks impossible to get up to a reasonable pitch/residue per turn from the α family. Because the shape of the peptide bond tends reduces the translation per residue



i.e.

This could probably be shown very easily analytically.

Thus classified by the β family, which has this sort of arrangement.



i.e. C–N distance increases

α restricted translation.

Had no difficulty of making a right chain of pitch around to A (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 polypeptides cannot have high I.R. ↑ dichroism and have two chains, independent of other evidence.]

Built helix with C–N ~~and~~ nearly vertical.

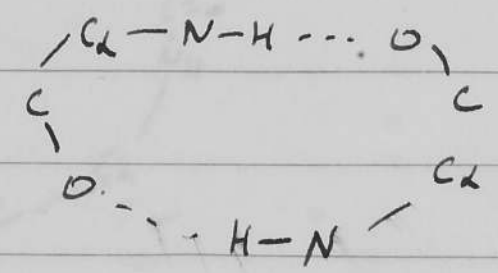
Built second helix (related by ↑ diad to the first)

1 A Joined up with hydrogen bonds:

Decided to describe these helices as follows.

Consider a hydrogen bond: also its mate related by the diad.

Make the smallest possible ring ~~attached~~ by running along main chain, containing these two bonds. This defines helix.



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

Characteristics of (2×5) helix

hydrogen bond poor.

N-H direction not far from ⊥ to C=O

N-H - - - O ← angle poor (perhaps 25°; depends on how radial.

distance between turns ≃ 2 × 6·5 or 2 × 7·5 Å (very variable)

prob. difficult to reduce this.

residues per turn (of one helix) : 5½ or 6.

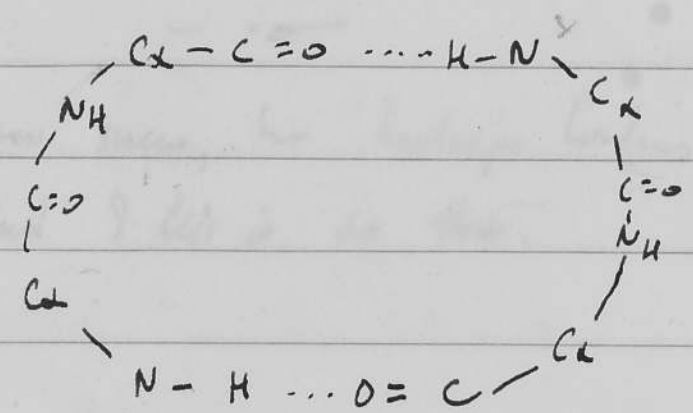
translation per residue ≃ 3 Å. 2·8 Å

Van der Waals contacts all reasonable

+ no hole in centre.

1. B. Altered hydrogen bonding to build the newer, more open helix.

Defining ring is new.



12. (2×8)

hydrogen bonding more satisfactory, but there now a hole in the middle.

very approx. { pitch distance ≃ 2 × 6 Å
residues/turn of one chain ≃ 5½
translation/residue ≃ 2½ Å }

NH bonds ⊙ more nearly head-on (say 40° off)
and NH roughly pointing at O

For these reasons structure can be deformed as hydrogen bond, so not easily precisely defined.

average distance between atoms across helix ≃ 5 Å
i.e. a hole.

—·o—

Tried more tightly screw, but hydrogen bonding looked so bad I left it at that.

1 C. While translating back to the true structure had changed over half the hydrogen bonds + found 9 had a new structure!

This has two chain related by a screw, not a rotation axis. Thus in the diffraction point of view there is a pointless "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 ~~Ha of~~ N: go along the hydrogen bond: then go ~~Ha abo~~ (in the same sense / to the next N) related by the pointless helix. (in the direction of the vector comp. of the NH).

in this case. $N-C_{\alpha}-C=O\cdots H-N$

Thus (5×2,)

P.S. Have doubt of this really defines it.

approx. residues / turn for one chain ≙ 5.

approx pitch distance / turn of one chain ≙ 6 - 6.5 Å × 2

approx translation / residue ≃ 2 ± Å

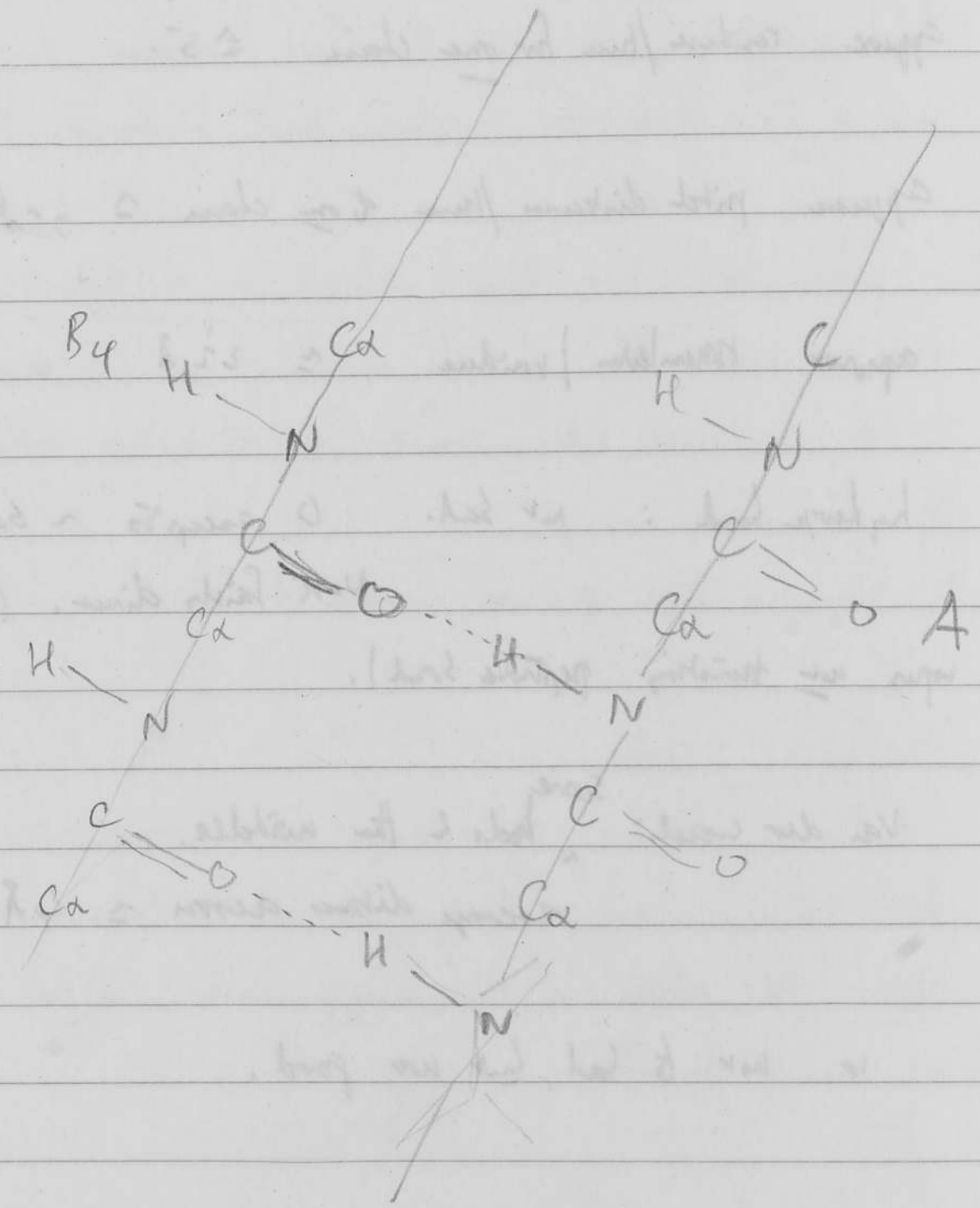
hydrogen bonds: not bad. 0 acceptors ~ 60% oft.

Not fairly direct. (may depend upon non twisting peptide bond).

Van der Waals: some holes in the middle.

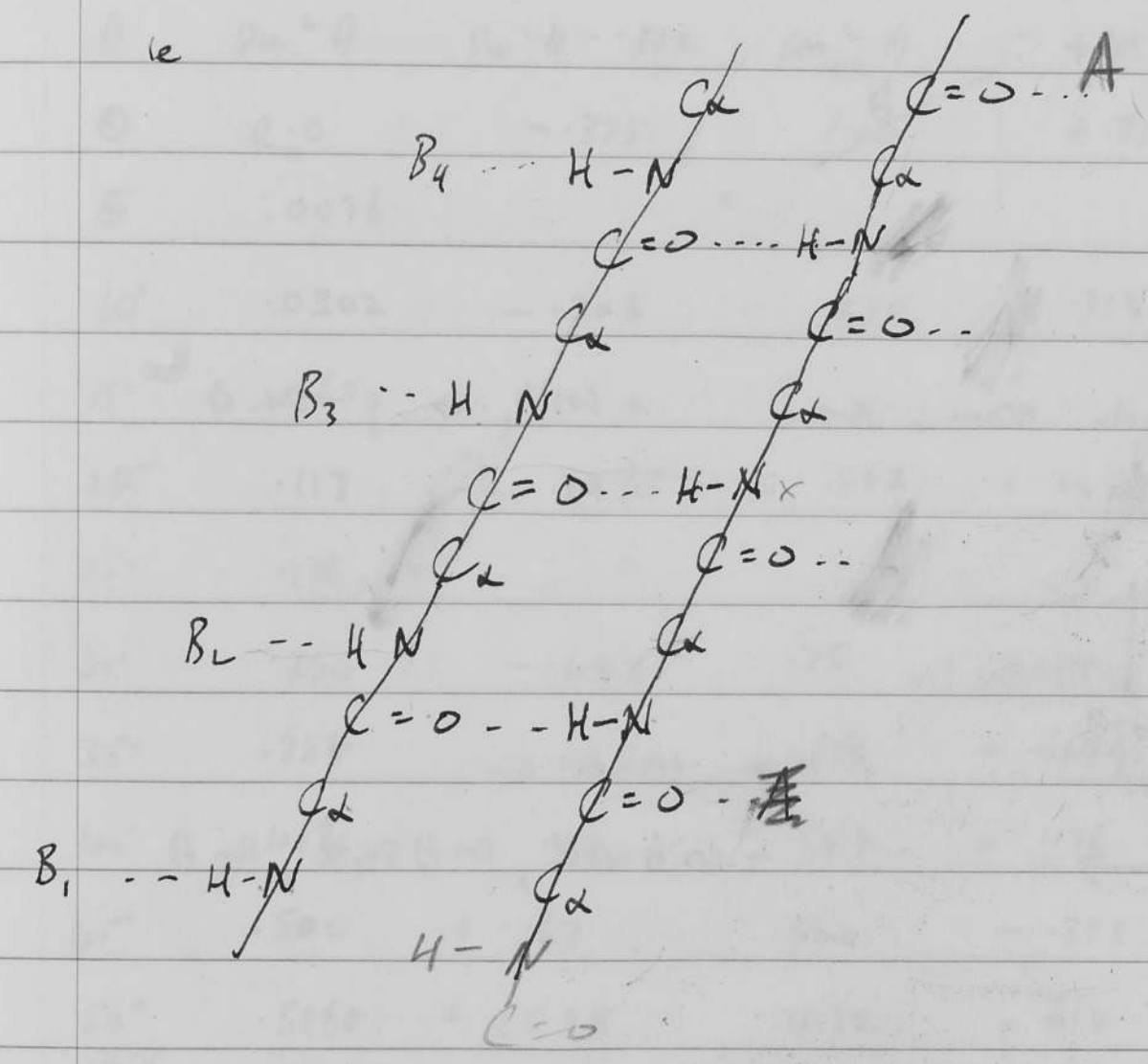
average distance across ≃ 4 Å

ie. not to bad, but not good.


B_4
H
N
C_α
C
O
H
N
C_α
C
O
A
B_3
H
N
C_α
C
O
H
N
C_α
C
O

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

ie

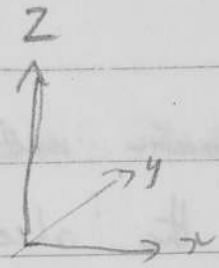


Whatever the connection at the above scheme must be part of it (for chain running in the same direction). Thus we get different structures depending upon whether A joins to B_1, B_2, B_3 or B_4.

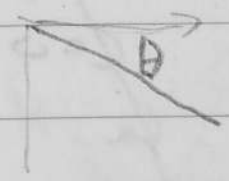
+ ~~B_2 is the~~ A-B_1 is one (2×8)

I think A-B_2 is the screw one [ie 5×2,]

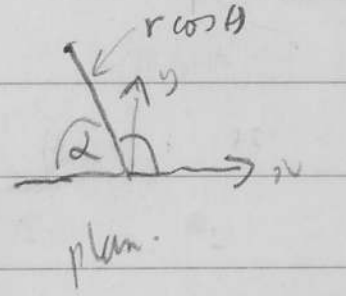
A-B_3 is one (2×5)



we want α in terms of ψ ($=110°$) and θ



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



direction cosines are

$-\cos\beta\cos\alpha,\ \cos\beta\sin\alpha,\ \sin\beta$

Then $\cos\psi = -\cos^2\theta\cos\alpha \ \& - \sin^2\theta$

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

$$-\cos\alpha = \frac{\cos\psi + \sin^2 A}{\cos^2 A} \qquad \cos\psi = \cos 109°45' = -\cdot 333$$

θ	$\sin^2 A$	$\sin^2 A - \cdot 333$,	$\cos^2 A$	$\therefore +\cos\alpha$	$\therefore \alpha$	$\frac{360}{\alpha}$
0	0·0	−·3733	1·00	+·333	71°33′	5·0₂
5	·0076					
10°	·0302	−·303	·970	+·313	71·7₅°	5·0₁
15°	·0670					
20°	·117	−·2163	·883	+·245	75·8°	4·7₅
25°	·178₅					
30°	·250	−·083	·75	+·111	83·6°	4·3₁
35°	·328	−·0053	·671	+·0079	89·5₅°	4·01
40°	·413	+·08	·587	−·136	97·2°	3·70
45°	·500	+·167	·500	−·333	109½°	3·29
50°	·5868	+·2538	·4132	−·614	127·9°	2·81
54·75						2·0
55°	·6708	+·3375	·329	>1·	—	

Translation per revolution $\triangleq$ $3.8 \sin(\theta - 22°)$ Å

θ	$\theta - 22°$	$\sin(\theta - 22°)$	$\therefore$ trans	$\therefore$ pitch
30	8°	.139	0.52₈	2.2₇
35	13°	.225	0.8₅₅	3.4₂
40	18°	.309	1.17	4.3₇
45	23°	.391	1.48	4.8₁
50	28°	.469	1.78	5.0

i.e. not good because assumptions oversimplified.

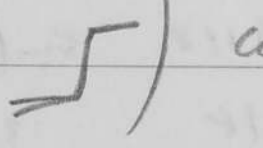
try compromise formula. ie. $3.8 \sin(\theta - 18°)$ Å

~~$\theta + 4°$~~

θ	$\theta - 18$	$\sin \theta - 18°$	trans.	pitch.
30	12	.208	0.79	3.4
35	17	.292	1.1₁	4.4₇
40	22	.375	1.4₃	5.3
45	27	.454	1.7₂	5.6₅
50	32	.530	2.0₂	5.7
54½°	36¾	.60	2.28	5.5₆

actually the 3 fold helix works out about 6

Thus these calculations show that the pitch of a helix (trans, one residue/asymmetric unit) having the α arrangement (ie 

, not ) cannot have a pitch (irrespective of hydrogen bonding) much in excess of 6 Å, because of the limitation of the ramachandran angle. Thus one cannot have simple two-chain helices this way.

For other Family, we have.

translation/vertical $\simeq 3.8 \sin(A+18)$

A	A+18°	sin(A+18°)	trans	∴ pitch
0	18	.309	1.17	5.9
10	28	.469	1.78	8.9
20	38	.616	2.34	11.1
30	48	.743	2.82	12.1
40	58	.848	3.22	11.9
50	68	.927	3.52	9.9

v. approx only

This rough calculation shows (as already found by model)
← that the other family (⎽⎺) does give helices with
pitch about 10–12 Å over a fairly reasonable range.