LABORATORY NOTEBOOK

To HEAVY VAR

IGE

GENENTECH, INC.

NOTEBOOK NO. 10098

ISSUED TO LEONARD PRESTA

ON July 10 **19** 89

DEPARTMENT BIOMOLECULAR CHEM.

RETURNED _____ **19** ____

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Genentech Laboratory Notebook Procedures

Important steps for maintenance of your notebooks:

1) **Use dark permanent ink to record all of your work in your notebook on a daily basis. Sign and date each day's entries.**

2) **Permanently affix all attachments without covering any other entries. Please attach copies of any computer data entered into your computer files. These data are considered part of your experimental record.**

3) **Make any changes in data in dark permanent ink and, if appropriate, initial and date in the margin. Ensure that the original entry remains visible. Leave no open areas. When the book is completed line out any unused portion of a page at the end of each experiment.**

4) **Have a witness who understands and is aware of your work, but who is not directly involved in your project, sign and date your notebook entries (not later than one month after you do the work).**

5) **Don't hold back data for later entry and don't keep a "rough draft" notebook.**

6) **Report the quantitative or qualitative results only.** Avoid over broad and potentially inflammatory comments like "failed experiment", "doesn't work", or "toxic compound."

7) **The source and character of starting materials should be described.** Preferably, refer to the notebook pages describing the starting material and its method of preparation.

8) **Be sure your notebook record is understandable.** Omit abbreviations or slang that would not be understood by others working in your field. It is helpful to introduce each experiment with a statement of purpose, and make liberal use of cross-references to related experiments. While sufficient detail should be included to enable reproduction of experiments, it is acceptable to refer to conventional or published procedures. However, record any changes you may make to such procedures.

9) **Record your ideas too, not just experimental data.** This is important to demonstrate when an invention or thought occurred to you, and is an important part of establishing priority in inventorship contests. Don't hesitate to broaden the scope of your ideas; there is no reason to limit them to specific experiments planned for the next few days, although you should include as much detail as possible. Your notebook will not be published and there is no penalty for guessing wrong on notebook *idea* entries, so don't hesitate to let your imagination run.

10) **Try to keep a different notebook for each product and/or project. Please complete the table of contents indicating which product and/or project this work concerns.**

Genentech's success, and with it your own prosperity and research support, depends upon the quality and timing of your work. This may require that we prove what you did and when you did it in the face of a contrary challenge. Such challenges have and will continue to arise in judicial proceedings, in patent validity or infringement or challenge, inventorship priority contests and product liability actions. The key to winning in such cases is the ability to supply appropriate evidence.

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TITLE Secondary Structure Assignment Project No.____ Book No.____ Heavy, Variable

From Page No.___ Based on hydrogen bonding & backbone dihedral angle

1FB4 (V2) Q3-S7
(G9) G10-V12 (Q13)
(S17) L18-S25
A33-A40
(L45) E46-W47
A49-W52
D57-A61
F68-N73
T78-D84
(T91) G92-D99
Y107-G109
T112-S117

3FAB L4-S7(G8)
L11-V12(R13)
(T17) L18-S25
(Y32) Y33-Q39 (P40)
(L45) E46-F52
T56-T59

(V67) T68-V71
F78-L82 (S83)
(T90) A91-N98
(G110) S111-S116

2HFL (L4) Q5-S7
E10-M12 (K13)
(S17) V18-A24 (S25)
(W33) I34-Q39 (R40)
(L45) E46-L52
S57-H61
A68-D73
T78-N84
(S91) G92-H98
G105-S115

2MCP (V2) K3-S7
(G9) G10-V12 (Q13)
G16-S25
Y33-Q39 (P40)
(L45) I46-R52
T59-S63
F70-D75
I80-N86
(T93) A94-Y102 (Y103)
(W107) Y108-F109
T116-S121

1FBJ (L4) L5-S7
(G9) G10-G10(L11)
L18-A23(A24)
M34-Q39
(L45) E46-H52
T57-T61
F68-S71
(S78) L79-S84
(T91) A92-L99
(A106) Y107-G109
T112-T115

res in ( ) are outside h bond pattern, but have β strand backbone dihedral angles

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Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by Leonard Presta	11-20-89

Project No.
Book No.
TITLE Superpositioning

From Page No.

All heavy variable domains superpositioned on 1FB4 HV using Insight (Biosym) program

Res	1FB4	1FBJ	2HFL	2mcP	3FAB
	18-25				
	34-39				
	46-52	Same	Same		
	57-61			59-63	56-60
	68-71			70-73	67-70
	78-84			80-86	77-83
	92-99			94-101	91-98

superpositioning using N, Cα, C atoms (135 atoms)

1FB4 vs.	1FBJ	0.623 Å
	2mcP	0.425
	2HFL	0.913
	3FAB	0.854

Using 1FBJ as template

1FBJ vs	1FB4	0.623 Å
	2mcP	0.690
	2HFL	0.921
	3FAB	1.001

Using 2HFL as template

2HFL vs.	1FB4	0.913
	1FBJ	0.921
	2mcP	0.726
	3FAB	0.771

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Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by Leonard Presta	11-20-89

TITLE Average Coords. 1FB4 template

Project No.

Book No.

3

From Page No.

Cα-Cα distances between analogous residues in the five crystal structures (superpositioned on 1FB4) were used to define a set of residues to comprise the basic VH backbone. For a residue position to qualify, 4 of the 5 must have Cα-Cα distances ≤ 1.0Å (MATCH program). These residues were then used to calculate average coords. for N, Cα, C, O, Cβ atoms using superpositioned coords. of the five crystal structs.

```
*****************************************************************************
1FB4 and 3FAB are lambda-type  2MCP, 1FBJ AND 2HFL are kappa-type

() denotes beta-strand residues

capital letters - Ca < 1.0A from 1FB4 HV
*****************************************************************************

1FB4   E(V Q L V Q S)G G G V V Q)P G R S L R L S C S S S)G F I F S
3FAB   @ v Q(L E Q S G)p g(l v r)p s q(t l)S L T C T v s)G t s f d
1FBJ   e V K(L L E S)G G g l)v q p g g S(L K L S C A A)S G F d F s
2HFL   @ v Q(L q q s)q a(e l m k)p g A(S V K I S C K a s)g y t f s
2MCP   e(V K L V E S)G G g L V q)P G(G S L R L S C A T S)g F T F S

1FB4   S Y(A M Y W V R Q A)P G K G(L E W)V(A I I W)D D G S(D Q H Y A)D S V K
3FAB   d(y y s)T W V R Q P)p g r g(l E W I G Y V f)y h g -(t S D T)D T p l r
1FBJ   k y W(M S W V R Q)A P g k g(L E W I G E I H)p d s g(T I N y t)p s l k
2HFL   d Y(W I E W V K Q R)P G H G(L E W I G E I l)p g s g(s T N Y H)E r f k
2MCP   d F(Y M E W V R Q P)P G K R(L E W I A A S R)N kgnky(T T E Y S)A S V K

1FB4   G R(F T I S R N)D S K N(T L F L Q M D)S L R P E D(T G V Y F C A
3FAB   s R(v T m l V)N t s k N Q(F S L R l S)s v t a a d(t A V Y Y C A
1FBJ   d K(F I I S)R D n A K N(S L Y L Q M s)k v r)s e d(t L Y Y C A
2HFL   g k(A T F T l)d)t s S S(T A Y M Q L n)S l t s e d(s G V Y Y C L
2MCP   G R(F I V S R d)t s Q S(I L Y L Q M N)A L R A E D(T A I Y Y C A

1FB4   R D)GGHGFCSSASCFGPD(Y W G)Q G(T P V T V S)S A S
3FAB   R n)l i a g c i   d(v W l)Q(G S l)v t v s)s a s
1FBJ   R L)h y y g   y n(a Y W G)Q G(T L v t)v s a e s
2HFL   D g n y d f       d(G W G Q G T T L t v s)s a k
2MCP   R N Y y)g s t(wyf)d V W G A G(T T V T V s)s e s
```

2MCP A49→S

1FB4 A49→S
S92→A

2HFL S92→A
S105→A

Circled residues were <u>not</u> used to calculate average coords.

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Witnessed & Understood by me,

Date

Invented by

Date

Recorded by

Project No._____
Book No._____ TITLE Average Coords (1FB4 Template)

From Page No. 3

```
1FB4.PDBASALA                    62 residues and   306 atoms
GAP IN SEQUENCE:    0-   3 in file:1FB4.PDBASALA
GAP IN SEQUENCE:    8-  17 in file:1FB4.PDBASALA
GAP IN SEQUENCE:   23-  33 in file:1FB4.PDBASALA
GAP IN SEQUENCE:   41-  45 in file:1FB4.PDBASALA
GAP IN SEQUENCE:   51-  58 in file:1FB4.PDBASALA
GAP IN SEQUENCE:   62-  67 in file:1FB4.PDBASALA
GAP IN SEQUENCE:   72-  76 in file:1FB4.PDBASALA
GAP IN SEQUENCE:   83-  92 in file:1FB4.PDBASALA
GAP IN SEQUENCE:   98- 107 in file:1FB4.PDBASALA
1FBJ.PDBASALA                    62 residues and   306 atoms
GAP IN SEQUENCE:    0-   3 in file:1FBJ.PDBASALA
GAP IN SEQUENCE:    8-  17 in file:1FBJ.PDBASALA
GAP IN SEQUENCE:   23-  33 in file:1FBJ.PDBASALA
GAP IN SEQUENCE:   41-  45 in file:1FBJ.PDBASALA
GAP IN SEQUENCE:   51-  58 in file:1FBJ.PDBASALA
GAP IN SEQUENCE:   62-  67 in file:1FBJ.PDBASALA
GAP IN SEQUENCE:   72-  76 in file:1FBJ.PDBASALA
GAP IN SEQUENCE:   83-  92 in file:1FBJ.PDBASALA
GAP IN SEQUENCE:   98- 107 in file:1FBJ.PDBASALA
2HFL.PDBASALA                    62 residues and   306 atoms
GAP IN SEQUENCE:    0-   3 in file:2HFL.PDBASALA
GAP IN SEQUENCE:    8-  17 in file:2HFL.PDBASALA
GAP IN SEQUENCE:   23-  33 in file:2HFL.PDBASALA
GAP IN SEQUENCE:   41-  45 in file:2HFL.PDBASALA
GAP IN SEQUENCE:   51-  58 in file:2HFL.PDBASALA
GAP IN SEQUENCE:   62-  67 in file:2HFL.PDBASALA
GAP IN SEQUENCE:   72-  76 in file:2HFL.PDBASALA
GAP IN SEQUENCE:   83-  92 in file:2HFL.PDBASALA
GAP IN SEQUENCE:   98- 105 in file:2HFL.PDBASALA
2MCP.PDBASALA                    62 residues and   306 atoms
GAP IN SEQUENCE:    0-   3 in file:2MCP.PDBASALA
GAP IN SEQUENCE:    8-  17 in file:2MCP.PDBASALA
GAP IN SEQUENCE:   23-  33 in file:2MCP.PDBASALA
GAP IN SEQUENCE:   41-  45 in file:2MCP.PDBASALA
GAP IN SEQUENCE:   51-  60 in file:2MCP.PDBASALA
GAP IN SEQUENCE:   64-  69 in file:2MCP.PDBASALA
GAP IN SEQUENCE:   74-  78 in file:2MCP.PDBASALA
GAP IN SEQUENCE:   85-  94 in file:2MCP.PDBASALA
GAP IN SEQUENCE:  100- 111 in file:2MCP.PDBASALA
3FAB.PDBASALA                    62 residues and   306 atoms
GAP IN SEQUENCE:    0-   3 in file:3FAB.PDBASALA
GAP IN SEQUENCE:    8-  17 in file:3FAB.PDBASALA
GAP IN SEQUENCE:   23-  33 in file:3FAB.PDBASALA
GAP IN SEQUENCE:   41-  45 in file:3FAB.PDBASALA
GAP IN SEQUENCE:   51-  57 in file:3FAB.PDBASALA
GAP IN SEQUENCE:   61-  66 in file:3FAB.PDBASALA
GAP IN SEQUENCE:   71-  75 in file:3FAB.PDBASALA
GAP IN SEQUENCE:   82-  91 in file:3FAB.PDBASALA
GAP IN SEQUENCE:   97- 108 in file:3FAB.PDBASALA
GAP IN SEQUENCE:  108- 107 in file:3FAB.PDBASALA
MAXAT =   306 : MAXRES =    62
B-factor range is:   2.00 to  33.72
B-factor BIN range is:    2 to   34
B-FACTOR STATS DO NOT INCLUDE 3FAB
Bin#     Range      Avg.Dst.  R.M.S.  #values    Dist range
  1   2.00 -  5.20   0.119    0.221     620    0.000 -  1.440
  2   5.20 -  8.40   0.364    0.423     145    0.037 -  1.306
  3   8.40 - 11.60   0.368    0.420     192    0.021 -  1.474
  4  11.60 - 14.80   0.372    0.417     235    0.035 -  1.016
  5  14.80 - 18.00   0.391    0.455     177    0.044 -  1.489
  6  18.00 - 21.20   0.434    0.490     104    0.065 -  1.505
  7  21.20 - 24.40   0.633    0.752      42    0.237 -  2.033
  8  24.40 - 27.60   0.616    0.828       9    0.265 -  1.866
  9  27.60 - 30.80   0.565    0.724       5    0.359 -  1.195
 10  30.80 - 34.00   0.268    0.268       1    0.268 -  0.268
```

Bond Lengths & Angles for HVONFB4HV

N-Ca	Ca-C	C=O	C-N	Ca-Cb	C-N-Ca	N-Ca-C	Ca-C=O	Ca-C-N	O=C-N	N-Ca-Cb	Cb-Ca-C
1.451	1.507	1.160	1.282	1.499	125.3	110.3	120.9	117.6	122.2	110.6	111.2
0.023	0.033	0.177	0.065	0.039	4.6	2.8	7.1	5.2	4.9	2.5	2.2
62	62	62	53	58	53	62	62	53	53	58	58

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Witnessed & Understood by me, | Date | Invented by | Date

Recorded by Leonard Prusta | 11-26-89

TITLE Average Coords (2HFL Template) Project No._____ Book No._____ 5

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Same treatment but using coords. superpositioned on 2HFL (instead of 1FB4)

```
*****************************************************************************
1FB4 and 3FAB are lambda-type  2MCP, 1FBJ AND 2HFL are kappa-type

() denotes beta-strand residues

capital letters = Ca < 1.0A from 2HFL HV
*****************************************************************************

2HFL   @ V Q(L Q Q S)G A(E L M K)P G A(S V K I S C K A S)G Y T F S
1FB4   e(v Q L v q s)g(g g v v q)p g R(S L R L S C S s s)g f i f s
3FAB   @ v Q(L E Q s g)p g(L v r)p s g(t D S L T C T V S)G t s F d
1FBJ   e v K(L L E s)g(g G L)V Q P G G S(L K L S C a a)s g f d F s
2MCP   e(v K L V E s)g(g g l v q)p G G S L R L S C A T s)g F T F S

2HFL   D Y(W I E W V K Q R)P G H G(L E W I G E I L)P G S G(S T N Y H)E R F K
1FB4   s Y(A M Y W V R Q A)P G K G(L E W)V(A I I W)d d g s(d Q H Y A)D s v k
3FAB   d(y Y S T W V R Q P)P g r g(L E W I G Y V F)y - h g(T S D T)D T p l r
1FBJ   k y W(M S W V R Q)A P G K g(L E W I G E I h)p d s g(t I N Y T)D s L K
2MCP   d F(Y M E W V R Q P)P g K R(L E W I A A S r)n kgnky(t T E Y S)A S V K

2HFL   G K(A T F T A D)T S S S(T A Y M Q L N)S L T S E D(S G V Y Y C L
1FB4   g r(F T I S r n)d s K N(T L F L Q M d)S l r p e d(t G V Y F C A
3FAB   s r(V t M L V)n t s K N Q(F S L R L S)s V T A A D(T A V Y Y C A
1FBJ   D k(F I I S)r d n A K N(S L Y L Q m s)K V R)S E D(T A L Y Y C A
2MCP   G r(F I V S R D)T S Q S(I L Y L Q M N)A l r a e d(t A I Y Y C A

2HFL   H)G N Y D F       D(G W G Q G T T L T V S)S A K
1FB4   r d)gghgfcssascfgpd(Y W G)Q G(T P V t v s)s a s
3FAB   R n)l i a g c i   d v G S q G S 1 V T V S)S a s
1FBJ   r l)h y y g   y n(a y W G)q G(T L V T)V S a e s
2MCP   r n y y)g s t(wyf)d V W G A G(T T V t v s)s e s
```

2MCP A49 → G

1FB4 A49 → G
G92 → A

2HFL G92 → A
G105 → A

Bond Lengths & Angles for HVONHFLHV

N-Ca	Ca-C	C=O	C-N	Ca-Cb	C-N-Ca	N-Ca-C	Ca-C-O	Ca-C-N	O-C-N	N-Ca-Cb	Cb-Ca-C
1.456	1.515	1.202	1.293	1.501	124.0	109.7	121.0	115.9	123.8	110.8	111.1
0.020	0.021	0.132	0.035	0.051	2.3	2.7	7.4	1.9	2.1	2.1	2.7
57	57	57	47	54	47	57	57	47	47	54	54

To compare the two average structures use N, Cα, C of res: 3-6, 17-23, 33-41, 45-51, 58-62, 68-71, 76-83, 92-97, 108-109, 111-113

Avg HFL on Avg FB4 = 0.118 Å 165 atoms

Added res 16, 114 from HVONHFLHV.AVSCRD to HVONFB4HV.AVSCRD

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Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by Leonard Presta	11-26-89

Project No._____

Book No._____ TITLE Seq. Alignments with Consensus Sequence

From Page No.__

```
*******************************************************************************
1FB4 and 3FAB are lambda-type  2MCP, 1FBJ AND 2HFL are kappa-type

() denotes beta-strand residues

capital letters = Ca < 1.0A from 1FB4 HV

consensus sequence from Kabat et al., "Sequences of Proteins of Immunological
          Interest", 4th ed., 1987; numbering according to Kabat;
          * marks Kabat variance between 1 - 10, @ variance between 11 - 20
*******************************************************************************

1FB4   E(V Q L V Q S)G(G G V V Q)P G R(S L R L S C S S S)G F I F S
3FAB   @ v q(L E Q S G)p g(l v r)p s q(t l S L T C T v s)G t s f d
1FBJ   e V K(L L E S)G(G g l)v q p g g S(L K L S C A A)S G F d F s
2HFL   @ v Q(L q q s)g a(e l m k)p g A(S V K I S C K a s)g y t f s
2MCP   e(V K L V E S)G(G g L V q)P G(G S L R L S C A T S)g F T F S
       @ @   *   @ * * @   @ @   * @   *     @ @ *   @ * * @   *
con    E V Q L V E S G G G L V Q P G G S L K L S C A A S G F T F S
                               K
       1               10                  20                  30

1FB4   S Y(A M Y W V R Q A)P G K G(L E W)V(A I I W)D D G S(D Q H Y A)D S V K
3FAB   d(y y s T W V R Q P)p g r g(l E W I G Y V f)y h g -(t S D T)D T p l r
1FBJ   k y W(M S W V R Q)A P g k g(L E W I G E I H)p d s g(T I N y t)p s l k
2HFL   d Y(W I E W V K Q R)P G H G(L E W I G E I l)p g s g(s T N Y H)E r f k
2MCP   d F(Y M E W V R Q P)P G K R(L E W I A A S R)N kgnky(T T E Y S)A S V K
         @   @   * *   *   * * @ @ * * * * @   @           @   *       @
con    S Y Y M H W V R Q A P G K G L E W I G Y I N PKANS G S T N Y N E S F K
                 V
              35a       40                  50     abc           60

1FB4   G R(F T I S R N)D S K N(T L F L Q M D)S L R P E D(T G V Y F C A
3FAB   s R(v T m l V)N t s k N Q(F S L R l S)s v t a a d(t A V Y Y C A
1FBJ   d K(F I I S)R D n A K N(S L Y L Q M s)k v r)s e d(t a L Y Y C A
2HFL   g k(A T F T a d)t s S S(T A Y M Q L n)S l t s e d(s G V Y Y C L
2MCP   G R(F I V S R d)t s Q S(I L Y L Q M N)A L R A E D(T A I Y Y C A
       @ * @ @ @ * @ *   @   @ @   @ @ @ @ @         @ * * @ *   * * * *
con    G R F T I S R D T S K S T A Y L Q M N S L T S E D T A V Y Y C A
                70                  80     a b c           90

1FB4   R D)G G H G F CSSAS C F G P D(Y W G)Q G(T P V T V S)S A S
3FAB   R n)l i a g c i             d v W g Q(G S l v t v s)s a s
1FBJ   R L)h y y g             y n(a Y W G)Q G(T L v t)v s a e s
2HFL   h)g n y                 d f d(G W G Q G T T L t v s)s a k
2MCP   R N Y y)  g s t      (w y f)d V W G A G(T T V T V s)s e s
       @                               * * @ * * @ * * * * *
con    R D Y Y Y G S SYY?YYYYW Y F D Y W G Q G T T V T V S S
                 100abcdefghi j k                 110
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		Recorded by Leonard Presta	11-28-89

TITLE Crystal Struct. Backbone Confs.

Project No.

Book No.

From Page No.

	1FB4		3FAB		1FBJ		2HFL		2MCP	
1	1000.0	129.9	1000.0	-131.5	1000.0	110.3	1000.0	-93.0	1000.0	14.5
2	-67.9	121.3	-145.2	-169.3	-77.8	134.3	129.9	-164.9	-86.1	109.7
3	-116.5	135.9	130.2	130.7	-158.2	149.2	81.0	-164.0	-124.2	140.5
4	-123.8	121.1	-107.0	143.4	-126.0	106.1	-122.8	123.3	-131.6	126.8
5	-120.5	110.1	-139.5	125.9	-98.4	110.5	-119.0	89.5	-134.7	116.0
6	-81.0	146.7	-109.3	157.1	-90.8	146.8	-95.7	151.0	-98.1	153.2
7	-152.4	152.6	-156.8	139.6	-140.3	168.6	-149.3	170.9	-151.2	170.1
8	115.4	-12.1	-178.6	-168.4	85.7	1.7	110.2	-98.5	80.0	96.7
9	-62.4	151.9	-82.1	163.4	-93.2	129.2	111.4	150.7	-174.6	145.7
10	-161.9	-171.0	-84.0	-69.2	-165.4	-147.9	-164.6	154.5	165.1	-143.5
11	-107.2	121.9	-93.3	142.3	-87.9	113.8	-109.0	134.5	-69.9	137.6
12	-134.7	163.7	-137.2	140.3	-116.3	-179.7	-155.6	141.1	-154.3	130.1
13	-96.8	159.9	-83.6	140.3	-130.8	139.2	-78.4	138.8	-79.5	144.1
14	-62.8	137.8	-65.1	135.3	-35.1	89.5	-52.8	133.9	-52.6	138.7
15	93.0	-10.3	104.0	-32.3	107.9	67.2	94.3	3.0	92.9	-20.8
16	-90.9	-179.2	-77.5	130.7	-157.7	158.3	-94.5	-149.9	-64.1	-175.2
17	-118.2	158.5	-61.7	146.7	-114.2	154.3	-151.0	169.1	-144.8	160.8
18	-140.8	164.7	-98.4	102.2	-147.6	172.8	-161.6	146.7	-151.0	160.1
19	-132.8	123.7	-90.1	140.3	-149.3	119.1	-124.4	109.7	-136.9	95.9
20	-97.4	148.6	-136.4	150.8	-100.4	139.1	-97.2	135.0	-82.5	148.8
21	-131.2	148.4	-137.5	143.5	-111.6	156.6	-101.6	163.7	-135.0	152.2
22	-131.9	104.9	-133.1	121.3	-147.5	106.3	-153.2	99.5	-126.6	107.5
23	-93.0	137.5	-109.6	120.2	-111.0	116.3	-86.8	124.2	-86.5	108.3
24	-125.0	164.5	-98.0	145.1	-127.2	125.5	-111.0	140.5	-98.4	116.6
25	-161.1	160.5	-159.6	153.2	-94.8	-150.8	-149.2	157.4	-135.1	158.8
26	87.5	13.2	84.2	-23.4	48.6	-12.0	85.8	0.2	85.8	21.3
27	-166.9	158.8	-89.3	141.5	-148.3	-172.9	-147.3	169.9	-169.3	166.6
28	-78.6	88.9	-79.3	107.7	-110.4	132.7	-76.1	94.2	-74.2	83.8
29	-49.0	-45.9	-74.5	47.4	-79.6	83.3	-73.7	-33.8	-48.9	-49.1
30	-65.7	-2.6	-116.7	-84.2	-157.5	-34.1	-64.2	11.8	-54.0	13.3
31	-91.7	-15.9	-43.9	-53.8	-79.3	35.3	-173.3	45.8	-166.0	38.6
32	-119.9	150.0	-60.5	167.9	-48.6	-132.6	-147.5	128.7	-136.8	140.9
33	-72.5	144.1	-159.4	100.2	65.9	91.8	-72.3	152.7	-71.1	131.5
34	-119.0	147.9	-82.0	121.9	-123.3	147.7	-126.8	141.6	-106.0	151.5
35	-110.7	163.3	-95.9	173.1	-153.7	171.0	-124.3	150.8	-138.4	147.0
36	-126.0	131.2	-127.4	80.6	-137.9	120.3	-119.0	120.1	-113.5	129.4
37	-133.5	141.1	-91.3	153.8	-95.2	162.0	-123.0	139.2	-133.6	142.3
38	-123.4	163.2	-131.7	163.5	-146.0	126.1	-113.4	137.9	-125.9	157.5
39	-143.9	108.8	-144.2	102.0	-114.9	91.1	-129.3	111.0	-140.5	95.1
40	-75.1	138.9	-60.7	143.0	-55.9	155.5	-60.0	-179.1	-57.3	162.1
41	-54.9	122.4	-75.5	131.1	-57.1	125.2	-49.2	-71.6	-42.7	-57.5
42	85.6	-4.5	113.0	14.4	75.1	-29.7	-123.9	66.0	-127.7	59.5
43	-114.3	177.9	70.9	147.9	-77.8	-159.3	-146.0	157.9	-147.1	162.5
44	-82.5	179.7	128.5	118.9	-129.8	-170.3	-56.1	174.3	-61.5	169.6
45	-65.3	132.6	-100.7	136.5	-67.4	125.6	-77.7	162.5	-69.1	148.4
46	-129.6	112.3	-140.8	119.5	-127.0	117.5	-147.1	127.6	-134.3	123.6
47	-60.8	135.6	-68.3	143.0	-76.6	125.5	-88.0	134.4	-84.6	137.7
48	-102.6	-58.4	-105.0	-60.9	-90.5	-55.1	-107.3	-69.8	-119.0	-101.5
49	-154.9	164.0	178.2	-173.9	174.1	174.5	-135.9	-164.9	-80.0	176.7
50	-135.0	142.6	-151.1	173.2	-126.5	171.0	-172.5	162.9	-163.6	126.2
51	-128.1	134.1	-151.1	153.0	-153.2	149.6	-162.3	155.3	-104.0	166.4
52	-59.3	158.0	-115.7	153.0	-120.2	159.9	-109.3	98.2	-131.5	161.0
53	-41.2	-48.0	-52.6	-32.1	-83.1	-29.0	-51.8	-70.3	-69.6	149.2
54	-100.0	6.3	-64.8	-20.8	-45.0	-36.6	-30.5	-27.5	-68.7	65.5
55	70.8	15.0	83.5	45.1	-163.4	-22.6	-150.1	66.2	60.7	120.3
56	-70.6	-16.4	0.0	0.0	112.2	40.7	-33.4	67.6	-57.0	54.4
57	-156.6	155.5	-109.5	117.2	-85.9	146.6	-113.5	117.0	-65.5	155.8
58	-145.8	140.6	-126.9	169.9	-126.6	133.8	-102.9	167.4	-122.1	175.5
59	-130.2	145.3	-160.9	110.2	-118.3	153.7	-152.4	127.7	-157.4	141.0
60	-124.2	153.6	-87.1	154.4	-148.8	148.7	-132.3	135.9	-134.0	145.1
61	-65.1	141.0	-54.1	-101.9	-79.4	112.5	-78.6	131.8	-64.5	149.1
62	-46.4	-43.8	-177.2	-71.2	-36.7	-43.0	-9.9	-90.7	-56.1	-37.3
63	-58.9	-13.6	-46.9	-24.8	-65.7	-13.4	-34.9	-5.8	-60.9	-19.8
64	-126.3	-10.1	-84.7	-46.2	-120.0	3.0	-130.3	-49.3	-131.8	-11.3
65	-61.5	123.6	-18.8	107.2	-49.0	-50.0	-25.8	129.4	-52.8	118.6

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66	96.6	-27.1	140.8	-61.4	-74.1	30.1	92.1	-27.6	113.0	-34.7
67	-93.0	-28.5	-107.4	74.5	178.9	16.7	-91.1	-52.4	-103.0	-35.0
68	-106.9	140.6	-158.4	117.0	-145.1	128.8	-89.7	160.9	-94.3	149.5
69	-125.5	122.7	-130.1	131.1	-122.8	119.6	-155.3	116.9	-146.8	124.1
70	-91.5	132.6	-109.5	121.3	-89.0	135.9	-96.7	158.7	-98.5	129.5
71	-151.0	170.6	-104.4	149.5	-127.2	167.4	-156.8	175.8	-138.2	172.9
72	-146.5	159.2	-108.8	-159.8	-139.3	168.3	-157.9	144.5	-143.5	131.1
73	-130.5	86.7	-0.9	-139.3	-166.0	115.3	-121.7	91.9	-91.9	87.0
74	-61.8	-14.9	153.7	8.3	-52.6	1.3	-41.7	-49.7	-56.1	-34.5
75	-74.2	-40.1	118.0	-37.7	-135.7	-48.9	-51.9	-47.2	-65.6	-39.1
76	-105.9	13.1	-138.7	146.2	-73.0	-34.9	-99.6	6.3	-102.1	5.0
77	51.1	41.0	-3.5	120.0	77.3	44.5	45.8	47.0	57.9	45.6
78	-125.8	139.0	157.8	133.0	-127.2	123.7	-121.6	121.3	-119.8	140.9
79	-107.3	133.3	-142.1	149.9	-109.2	137.9	-111.1	136.9	-112.3	121.4
80	-110.7	155.9	-144.9	155.4	-112.8	169.8	-119.8	158.1	-102.4	154.8
81	-136.0	101.2	-116.7	137.0	-157.6	98.0	-125.0	112.6	-140.4	107.5
82	-86.3	115.3	-134.9	90.2	-74.7	147.4	-102.6	107.6	-89.7	114.8
83	-110.9	106.6	-87.2	109.2	-128.4	147.0	-110.2	123.0	-103.8	105.0
84	-105.3	157.9	-71.0	-176.1	-121.2	-144.5	-92.2	151.7	-103.8	143.3
85	41.4	52.4	77.2	-105.2	-46.5	84.1	31.9	76.5	46.1	70.0
86	-60.7	138.3	73.4	135.0	-77.8	121.6	-63.2	141.7	-73.8	154.4
87	-120.7	148.1	-152.9	173.8	-106.1	156.0	-122.9	-169.4	-133.0	171.4
88	-56.5	-25.6	-66.9	-34.0	-49.0	-21.9	-80.6	-38.5	-65.9	-30.9
89	-75.0	-0.4	-69.8	10.2	-91.6	24.3	-48.5	-19.8	-62.5	-17.7
90	-94.7	6.8	-124.5	17.5	-110.9	-1.4	-80.1	-7.7	-76.9	-10.2
91	-71.4	135.4	-91.0	112.6	-55.4	123.1	-70.6	152.3	-67.1	118.4
92	174.8	178.4	-168.4	-162.0	-176.4	-176.7	154.4	-178.4	-176.1	169.2
93	-95.7	129.2	-117.2	135.5	-114.2	126.7	-109.6	113.3	-82.0	128.2
94	-102.8	123.2	-109.2	122.0	-103.8	119.4	-92.2	130.1	-105.4	138.3
95	-105.4	137.8	-103.2	157.1	-106.0	145.5	-118.2	137.8	-126.5	144.7
96	-95.0	155.9	-129.8	85.5	-109.9	131.3	-107.3	128.3	-113.4	139.4
97	-144.0	153.7	-90.6	-167.8	-130.1	174.2	-131.2	-167.7	-135.3	159.6
98	-89.1	139.2	-134.5	107.5	-135.7	119.5	-135.9	138.8	-105.7	122.1
99	-81.3	129.4	-97.1	168.3	-71.1	179.6	-127.5	86.7	-100.0	90.4
100	-82.9	-5.5	-166.7	67.9	-160.0	-173.4	-126.5	79.3	-70.9	-46.8
106	-108.5	-54.2	145.7	76.3	-134.4	-166.8	-106.7	150.3	-127.6	129.0
107	-104.7	145.8	-75.0	-155.7	-174.4	133.0	-109.2	160.8	-111.5	156.4
108	-120.1	158.2	-170.8	176.7	-122.1	163.8	-84.7	179.2	-84.2	-176.1
109	-89.2	-167.2	-169.1	125.7	-101.0	166.2	-67.1	-41.8	-88.1	-24.6
110	-94.2	-19.5	-19.9	142.5	-79.8	-17.8	112.9	153.3	96.1	169.6
111	101.6	146.1	-112.1	160.4	77.4	168.7	-139.5	132.9	-154.0	126.5
112	-132.4	121.9	-101.5	139.4	-139.8	141.5	-91.9	142.1	-84.0	134.5
113	-76.0	136.7	-81.7	112.8	-84.0	147.1	-125.9	121.6	-129.3	114.9
114	-122.6	123.4	-115.3	117.5	-138.0	120.2	-117.4	99.7	-108.8	115.5
115	-120.4	115.2	-118.2	114.4	-119.0	108.5	-93.1	118.3	-100.6	104.1
116	-112.3	114.0	-95.4	122.9	-86.8	109.0	-165.7	145.9	-141.7	146.5
117	-142.4	148.9	-166.1	147.9	-173.3	150.1	-94.6	2.7	-69.0	-36.2
118	-69.9	-20.3	-66.8	-50.3	-101.4	10.5	-81.6	172.8	-59.3	-179.7
119	-65.0	155.7	-42.0	116.8	-78.3	142.9	-135.8	166.2	-137.6	144.9
120	-109.9	167.7	-65.2	148.1	-73.5	142.9	-43.0	122.7	-48.8	140.7
121	-59.0	123.2	-68.3	151.9	-71.0	138.2	-138.1	122.8	-148.9	113.9
122	-127.5	123.8	-153.9	130.9	-131.8	137.6	-74.6	164.7	-70.7	147.8
123	-67.0	155.3	-80.0	150.1	-99.9	146.8	-98.4	158.1	-62.2	1000.0

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Due to averaging procedure, bond lengths & angles of the "average structure" are off from standard values. Therefore the "average structure" was subjected to energy minimization using the AMBER forcefield of the DISCOVER (Biosym) program. Cα atoms were constrained to remain in place with a force constant of 20.0

HVONFB4HV is the unminimized "average structure"

Bond Lengths & Angles for HVONFB4HV

N-Ca	Ca-C	C=O	C-N	Ca-Cb	C-N-Ca	N-Ca-C	Ca-C=O	Ca-C-N	O=C-N	N-Ca-Cb	Cb-Ca-C
1.451	1.507	1.160	1.282	1.499	125.3	110.3	120.9	117.6	122.2	110.6	111.2
0.023	0.033	0.177	0.065	0.039	4.6	2.8	7.1	5.2	4.9	2.5	2.2
62	62	62	53	58	53	62	62	53	53	58	58

mean
sd.
#values

Bond Lengths & Angles for AVERAGE after 50 cycles minimization (.COR)

N-Ca	Ca-C	C=O	C-N	Ca-Cb	C-N-Ca	N-Ca-C	Ca-C=O	Ca-C-N	O=C-N	N-Ca-Cb	Cb-Ca-C
1.450	1.522	1.230	1.334	1.528	123.6	109.4	120.1	116.6	123.3	109.8	111.1
0.005	0.006	0.002	0.005	0.003	1.2	1.9	0.9	1.3	0.6	1.2	1.1
64	64	64	55	60	55	64	64	55	55	60	60

Bond Lengths & Angles for AVERAGE after 100 cycles minimization (.COR2)

N-Ca	Ca-C	C=O	C-N	Ca-Cb	C-N-Ca	N-Ca-C	Ca-C=O	Ca-C-N	O=C-N	N-Ca-Cb	Cb-Ca-C
1.452	1.524	1.231	1.335	1.530	124.0	109.5	120.1	116.6	123.3	109.8	111.1
0.004	0.005	0.003	0.004	0.002	1.1	1.6	0.7	1.0	0.5	0.9	0.8
64	64	64	55	60	55	64	64	55	55	60	60

Bond Lengths & Angles for AVERAGE after 200 cycles minimization (.COR3)

N-Ca	Ca-C	C=O	C-N	Ca-Cb	C-N-Ca	N-Ca-C	Ca-C=O	Ca-C-N	O=C-N	N-Ca-Cb	Cb-Ca-C
1.454	1.526	1.230	1.337	1.530	124.2	109.7	120.2	116.6	123.3	109.8	111.1
0.003	0.003	0.002	0.002	0.001	0.9	1.4	0.6	0.8	0.4	0.6	0.6
64	64	64	55	60	55	64	64	55	55	60	60

Bond Lengths & Angles for AVERAGE (.COR4)
after 300 cycles minimization (100 Ca released)

N-Ca	Ca-C	C=O	C-N	Ca-Cb	C-N-Ca	N-Ca-C	Ca-C=O	Ca-C-N	O=C-N	N-Ca-Cb	Cb-Ca-C
1.454	1.528	1.231	1.338	1.531	124.2	109.9	120.4	116.5	123.1	109.5	111.2
0.002	0.002	0.001	0.001	0.001	0.6	0.9	0.4	0.4	0.2	0.3	0.5
64	64	64	55	60	55	64	64	55	55	60	60

Bond Lengths & Angles for AVERAGE (.COR5)
after 600 cycles minimization (400 Ca released)

N-Ca	Ca-C	C=O	C-N	Ca-Cb	C-N-Ca	N-Ca-C	Ca-C=O	Ca-C-N	O=C-N	N-Ca-Cb	Cb-Ca-C
1.454	1.528	1.230	1.338	1.531	124.1	110.0	120.5	116.5	123.1	109.6	111.3
0.002	0.002	0.001	0.001	0.001	0.6	0.8	0.4	0.4	0.2	0.4	0.6
64	64	64	55	60	55	64	64	55	55	60	60

Bond Lengths & Angles for AVERAGE after 200 cycles minimization with Ca at 20
(.COR3c) 50 cycles with Ca at 10
100 cycles with Ca at 2.5
100 cycles with Ca at 0.5

N-Ca	Ca-C	C=O	C-N	Ca-Cb	C-N-Ca	N-Ca-C	Ca-C=O	Ca-C-N	O=C-N	N-Ca-Cb	Cb-Ca-C
1.455	1.528	1.231	1.338	1.531	124.2	110.0	120.4	116.5	123.1	109.5	111.2
0.002	0.002	0.001	0.001	0.001	0.6	0.8	0.4	0.4	0.2	0.3	0.4
64	64	64	55	60	55	64	64	55	55	60	60

AMBER std.

N-Cα	1.449
Cα-C	1.522
C=O	1.229
C-N	1.335
Cα-Cβ	1.526
C-N-Cα	121.9
N-Cα-C	110.1
Cα-C=O	120.4
Cα-C-N	116.6
O=C-N	122.9
N-Cα-Cβ	109.5
Cβ-Cα-C	111.1

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Dihedral Angles for AVERAGE after 200 cycles minimization

			PHI	PSI	OMEGA
1.	ALA	3	1000.0	152.0	173.6
2.	ALA	4	-123.5	123.4	179.7
3.	ALA	5	-122.1	111.8	176.2
4.	ALA	6	-87.1	151.7	-179.6
5.	ALA	7	-150.5	160.8	177.9
6.	GLY	8	113.5	1000.0	1000.0
7.	ALA	16	1000.0	179.5	-175.3
8.	ALA	17	-128.2	161.6	171.8
9.	ALA	18	-147.0	164.7	174.4
10.	ALA	19	-134.2	112.6	174.1
11.	ALA	20	-90.7	143.4	176.6
12.	ALA	21	-118.2	155.8	179.7
13.	ALA	22	-140.9	104.1	-177.5
14.	ALA	23	-95.8	1000.0	1000.0
15.	ALA	33	1000.0	130.3	174.9
16.	ALA	34	-115.2	144.3	177.6
17.	ALA	35	-123.9	156.9	168.7
18.	ALA	36	-120.1	118.4	172.1
19.	ALA	37	-113.7	150.3	179.7
20.	ALA	38	-128.9	149.3	-178.7
21.	ALA	39	-134.7	100.5	172.5
22.	ALA	40	-58.8	163.1	-173.6
23.	ALA	41	-57.2	1000.0	1000.0
24.	ALA	45	1000.0	138.4	178.3
25.	ALA	46	-130.6	115.3	177.4
26.	ALA	47	-70.1	133.8	178.8
27.	ALA	48	-102.5	-64.9	-179.1
28.	GLY	49	-153.3	175.8	175.3
29.	ALA	50	-146.1	157.2	179.8
30.	ALA	51	-143.7	1000.0	1000.0
31.	ALA	58	1000.0	154.5	174.5
32.	ALA	59	-144.6	135.6	-177.8
33.	ALA	60	-124.0	149.8	173.5
34.	ALA	61	-69.1	155.6	-177.5
35.	ALA	62	-60.1	1000.0	1000.0
36.	ALA	67	1000.0	-19.2	167.7
37.	ALA	68	-99.4	143.1	174.0
38.	ALA	69	-137.6	117.2	177.2
39.	ALA	70	-87.9	139.8	177.3
40.	ALA	71	-140.4	171.1	-172.7
41.	ALA	72	-137.1	1000.0	1000.0
42.	ALA	76	1000.0	5.7	-173.8
43.	ALA	77	49.9	55.9	-174.2
44.	ALA	78	-134.2	129.2	175.4
45.	ALA	79	-112.1	135.8	-177.3
46.	ALA	80	-118.4	157.5	174.7
47.	ALA	81	-134.7	104.6	177.4
48.	ALA	82	-88.4	117.6	-173.7
49.	ALA	83	-109.7	1000.0	1000.0
50.	ALA	92	1000.0	172.2	170.3
51.	ALA	93	-95.6	126.0	-178.5
52.	ALA	94	-102.5	115.9	177.5
53.	ALA	95	-101.0	141.1	167.6
54.	ALA	96	-105.0	129.9	-178.1
55.	ALA	97	-128.6	165.3	-179.6
56.	ALA	98	-112.2	1000.0	1000.0
57.	ALA	107	1000.0	125.2	179.7
58.	ALA	108	-106.2	156.6	169.7
59.	GLY	109	-85.0	174.1	178.8
60.	ALA	110	-74.6	-25.5	-178.3
61.	GLY	111	91.3	154.5	173.9
62.	ALA	112	-133.2	136.4	-175.5
63.	ALA	113	-83.4	139.9	176.2
64.	ALA	114	-127.8	1000.0	1000.0

.COR3

Dihedral Angles for AVERAGE after 600 cycles minimization

			PHI	PSI	OMEGA
1.	ALA	3	1000.0	161.6	173.1
2.	ALA	4	-118.1	88.1	-178.8
3.	ALA	5	-75.3	89.9	178.0
4.	ALA	6	-66.4	146.1	-177.3
5.	ALA	7	-160.4	174.0	-178.9
6.	GLY	8	68.0	1000.0	1000.0
7.	ALA	16	1000.0	163.8	175.6
8.	ALA	17	-117.6	167.3	178.2
9.	ALA	18	-146.4	162.0	179.6
10.	ALA	19	-134.8	91.8	178.0
11.	ALA	20	-77.9	154.5	-175.1
12.	ALA	21	-135.9	155.9	-179.5
13.	ALA	22	-150.1	93.8	-176.4
14.	ALA	23	-82.5	1000.0	1000.0
15.	ALA	33	1000.0	123.4	176.2
16.	ALA	34	-73.0	140.4	175.9
17.	ALA	35	-125.2	157.6	-179.5
18.	ALA	36	-147.0	136.1	-179.2
19.	ALA	37	-147.3	140.8	178.0
20.	ALA	38	-100.6	123.4	175.4
21.	ALA	39	-104.7	99.0	-178.2
22.	ALA	40	-70.3	156.3	177.8
23.	ALA	41	-67.5	1000.0	1000.0
24.	ALA	45	1000.0	163.3	179.3
25.	ALA	46	-135.6	121.6	179.8
26.	ALA	47	-62.8	126.1	179.3
27.	ALA	48	-88.6	-50.5	-179.6
28.	GLY	49	178.1	-172.6	-178.3
29.	ALA	50	-155.3	159.4	-178.1
30.	ALA	51	-160.9	1000.0	1000.0
31.	ALA	58	1000.0	172.5	-178.5
32.	ALA	59	-147.4	152.2	177.8
33.	ALA	60	-148.7	142.3	-178.8
34.	ALA	61	-72.6	158.4	-179.3
35.	ALA	62	-65.7	1000.0	1000.0
36.	ALA	67	1000.0	-49.5	-178.0
37.	ALA	68	-85.8	66.1	-179.8
38.	ALA	69	-74.4	100.7	174.6
39.	ALA	70	-64.8	145.8	-176.4
40.	ALA	71	-156.6	174.7	177.4
41.	ALA	72	-165.6	1000.0	1000.0
42.	ALA	76	1000.0	-43.4	-176.0
43.	ALA	77	57.5	64.5	177.8
44.	ALA	78	-146.2	126.9	172.1
45.	ALA	79	-85.2	166.2	-178.8
46.	ALA	80	-153.6	162.6	177.2
47.	ALA	81	-143.3	102.6	175.3
48.	ALA	82	-79.4	101.1	178.5
49.	ALA	83	-83.5	1000.0	1000.0
50.	ALA	92	1000.0	152.4	174.2
51.	ALA	93	-79.6	103.2	178.2
52.	ALA	94	-73.4	92.7	-175.8
53.	ALA	95	-95.6	110.0	170.8
54.	ALA	96	-79.7	160.3	-178.2
55.	ALA	97	-160.5	170.7	177.3
56.	ALA	98	-74.2	1000.0	1000.0
57.	ALA	107	1000.0	135.2	178.6
58.	ALA	108	-117.4	143.2	-179.5
59.	GLY	109	-82.0	169.7	174.7
60.	ALA	110	-62.7	-41.3	-179.8
61.	GLY	111	88.5	162.0	-178.0
62.	ALA	112	-123.8	129.1	177.6
63.	ALA	113	-66.3	120.0	-177.6
64.	ALA	114	-135.1	1000.0	1000.0

.COR5

RMS	.COR3c on .COR3	.COR5 on .COR3
NCαCOCβ	0.326	0.585
NCαCO	0.329	0.573
NCαC	0.259	0.493

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TITLE Minimization

Project No.

Book No.

From Page No. 10

Dihedral Angles for AVERAGE
after 200 cycles minimization with Ca at 20.0
50 cycles with Ca at 10.0
100 cycles with Ca at 2.5
100 cycles with Ca at 0.5

.COR3C

			PHI	PSI	OMEGA
1.	ALA	3	1000.0	161.6	179.8
2.	ALA	4	-128.9	103.2	-177.6
3.	ALA	5	-96.6	101.0	174.3
4.	ALA	6	-73.2	146.1	-179.5
5.	ALA	7	-155.7	170.8	178.5
6.	GLY	8	69.6	1000.0	1000.0
7.	ALA	16	1000.0	168.8	178.3
8.	ALA	17	-118.7	164.8	177.2
9.	ALA	18	-150.6	157.8	-179.7
10.	ALA	19	-132.6	91.7	175.4
11.	ALA	20	-74.5	142.1	178.6
12.	ALA	21	-116.6	156.3	-179.9
13.	ALA	22	-146.0	97.6	-179.6
14.	ALA	23	-83.1	1000.0	1000.0
15.	ALA	33	1000.0	130.6	177.1
16.	ALA	34	-95.5	144.4	179.5
17.	ALA	35	-133.2	148.1	176.9
18.	ALA	36	-120.8	131.2	178.8
19.	ALA	37	-138.4	138.1	179.6
20.	ALA	38	-107.7	144.5	176.4
21.	ALA	39	-127.4	105.4	179.8
22.	ALA	40	-70.0	164.1	179.0
23.	ALA	41	-65.7	1000.0	1000.0
24.	ALA	45	1000.0	151.8	-179.3
25.	ALA	46	-140.5	112.5	177.8
26.	ALA	47	-62.7	123.9	-179.6
27.	ALA	48	-86.7	-51.8	-179.9
28.	GLY	49	-177.4	-172.0	-179.4
29.	ALA	50	-156.7	162.1	-179.3
30.	ALA	51	-157.5	1000.0	1000.0
31.	ALA	58	1000.0	170.4	178.3
32.	ALA	59	-142.9	153.6	-178.6
33.	ALA	60	-146.6	149.1	177.9
34.	ALA	61	-76.5	162.9	-178.4
35.	ALA	62	-66.1	1000.0	1000.0
36.	ALA	67	1000.0	-54.5	178.2
37.	ALA	68	-78.9	123.6	179.4
38.	ALA	69	-126.0	106.4	176.8
39.	ALA	70	-74.6	149.6	179.4
40.	ALA	71	-153.2	169.8	-179.3
41.	ALA	72	-140.7	1000.0	1000.0
42.	ALA	76	1000.0	-4.5	-176.9
43.	ALA	77	54.3	52.5	-175.1
44.	ALA	78	-134.6	114.8	169.5
45.	ALA	79	-82.3	157.2	-178.6
46.	ALA	80	-144.1	154.0	-178.8
47.	ALA	81	-138.2	96.8	178.3
48.	ALA	82	-80.8	102.0	177.6
49.	ALA	83	-85.8	1000.0	1000.0
50.	ALA	92	1000.0	155.1	175.3
51.	ALA	93	-85.2	105.3	178.8
52.	ALA	94	-83.1	106.5	179.8
53.	ALA	95	-107.4	124.0	169.6
54.	ALA	96	-84.2	152.2	179.5
55.	ALA	97	-151.5	158.9	178.6
56.	ALA	98	-83.8	1000.0	1000.0
57.	ALA	107	1000.0	133.1	178.1
58.	ALA	108	-119.9	141.3	179.9
59.	GLY	109	-81.2	174.7	177.8
60.	ALA	110	-64.6	-44.8	177.9
61.	GLY	111	95.9	168.2	-177.5
62.	ALA	112	-135.3	130.7	179.0
63.	ALA	113	-71.5	138.8	178.5
64.	ALA	114	-141.1	1000.0	1000.0

		AVERAGE.PDB3					AVERAGE.PDB5				
Res#	Res#	Dist	D-A-AA	A-D-DD	A-D<	D-A<	Dist	D-A-AA	A-D-DD	A-D<	D-A<
6	4						2.98	98.0	132.8	32.3	-148.2
5	23	3.00	156.5	118.7	6.4	40.7	2.86	149.3	109.9	-18.2	55.3
23	5	2.98	142.8	119.5	-9.4	73.3	3.01	127.3	117.9	-14.8	72.5
7	21	2.90	147.3	128.1	10.0	-68.1	2.89	139.9	115.6	17.3	-83.6
21	7	2.90	154.0	122.8	-3.1	-61.4	2.94	131.3	113.1	4.9	-96.7
18	83	3.21	143.0	132.3	-5.1	-41.4	3.01	152.5	123.8	2.5	16.2
83	18	2.90	160.6	115.1	-2.5	-80.2	2.84	149.1	107.5	-28.5	-95.4
20	81	3.04	142.1	123.1	-11.6	61.3	2.98	139.9	113.2	-21.3	77.4
81	20	2.89	153.6	125.5	8.2	-49.3	2.94	134.3	124.7	2.9	-75.2
22	79	2.76	166.2	112.4	29.5	30.3	2.89	138.9	113.6	18.7	-89.3
79	22	3.00	143.1	122.9	-0.6	50.0	2.91	142.3	116.1	-22.6	70.9
34	51	2.97	164.4	125.2	-9.5	-42.9	2.84	152.8	110.8	-31.1	-92.8
51	34	2.95	166.3	126.7	7.5	-32.0	2.95	145.0	128.7	0.0	-57.8
35	97	2.89	147.7	120.6	2.4	-72.9	2.91	138.7	109.6	1.7	-92.6
97	35	2.95	143.6	126.7	-3.2	-63.6	2.92	136.0	116.7	17.7	-83.9
36	49	2.91	152.7	123.7	1.5	-75.9	2.93	158.2	108.3	25.4	-102.4
48	36	2.89	156.1	102.0	-0.3	-154.2	2.90	133.8	108.1	-14.3	-137.7
49	36	3.31	143.8	133.7	-10.8	-5.3	3.25	136.6	125.6	-3.2	-56.7
37	95	2.96	159.4	121.0	-15.8	-49.0	2.94	149.5	113.5	13.8	80.9
95	37	2.83	166.5	112.0	-15.6	-88.0	2.82	166.3	103.6	-17.8	101.3
38	46	2.87	150.9	117.6	6.1	68.3	2.87	155.1	120.9	-16.1	65.5
46	38	2.84	170.9	111.0	12.6	15.4	2.97	145.9	112.2	17.9	83.1
39	93	2.94	153.7	123.9	15.2	46.2	3.01	134.0	118.3	2.6	63.6
93	39	3.12	128.4	122.4	-5.4	77.8	2.93	130.3	117.5	-11.0	72.8
48	46						3.34	102.1	123.9	68.6	-159.8
61	48	2.72	170.0	112.7	13.2	-55.9	2.99	141.7	121.4	1.6	-103.9
50	59	2.95@	164.3	128.4	8.6	-23.5	2.97@	134.2	127.3	0.9	-68.7
59	50	3.13@	148.6	127.1	6.3	-60.3	2.91@	148.5	118.8	12.0	-69.7
69	67						3.05	88.1	140.3	11.6	-139.0
70	68						3.09	100.0	135.2	37.7	-150.2
69	82	2.90	154.4	126.1	13.2	20.6	2.92	145.9	108.3	-27.0	79.0
82	69	2.93	148.3	114.1	-7.8	63.7	2.92	143.0	109.6	-21.6	78.1
71	80	3.06	137.2	125.6	1.6	-65.8	2.92	136.1	111.6	13.8	-91.2
80	71	2.94	134.3	122.2	-6.4	-85.4	2.88	131.0	109.7	16.3	-104.2
78	76	3.42	74.1	114.2	90.1	130.4					
83	81						3.23	94.0	134.9	38.8	-143.5
92	114	3.13	153.2	131.7	38.6	-30.9	2.95	128.1	130.3	36.2	-100.1
114	92	2.94	161.8	114.1	12.0	88.7	2.92	150.6	105.9	7.9	94.0
94	92						3.27	94.1	135.2	40.0	-143.1
94	112	2.94	146.9	120.5	-2.6	66.2	2.85	141.6	109.1	-18.5	77.5
112	94	3.14	134.4	129.9	10.1	65.1	3.03	126.5	128.5	4.1	70.6
95	93						3.01	97.7	127.5	40.6	-146.7
109	96	2.80	159.7	107.6	25.9	94.3	2.87	150.8	105.5	0.7	-121.7
98	107	2.92	162.9	126.0	14.3	38.4	2.93	172.0	120.4	5.9	-54.4
114	112						3.29	101.1	123.8	64.0	-154.9

* after dist denotes a possible alpha helix res
@ after dist denotes a possible 3-10 helix res

Hbonds
.COR3(.PDB3) after 200 cycles
.COR5(.PDB5) after 600 cycles

To Page No.

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Recorded by Leonard Presta

Date 11-28-89

Project No.
Book No.
TITLE Frameworks

From Page No.

Framework Model: to be used for generating model of a variable, heavy domain

Archetype model: special version of framework model to be used to generate model of a "consensus" human, variable heavy

Both based on HVONFB4HV after 200 cycles minimization (.COR3)

B-sheet	Framework Res. (1FB4 numbering)	Archetype Res.	Loop to insert
4-7	4-7	1-7 (1-3 FB4, FBJ, MCP)	
			8-15
18-25	16-23	16-23	
			24-33
34-39	34-40	34-40	
			41-44
46-52	45-51	45-51	
			52-57
57-61	58-60	58-62 (61-62 FB4, HFL, MCP)	
			61-67 (framework)
			63-65 (archetype)
68-71	68-72	66-83 (66-67 FB4, HFL, MCP)	
		(73-76 FB4, FBJ, HFL, MCP)	73-76 (framework)
78-84	77-83		
			84-91
92-99	92-98	92-98	
			99-106
	107-108	107-114	
			109-111 (framework)
	112-114		
			115-123

For archetype model, inclusion of res 61, 62, 66, 67 assumes no Pro at 62 or 63 (as in 3FAB or 1FBJ) and Gly at 66 (missing in 3FAB & 1FBJ)

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		Recorded by Leonard Presta	11-29-89

TITLE Renumber

Project No.
Book No.

From Page No.

Renumber Archetype & Consensus according to Kabat et al Sequences of Proteins of Immunological Interest 4th Ed 1987

Kabat	Archetype	Consensus	Kabat
57-61	58-62	58-60	57-59
65-82	66-83	68-72	67-71
88-94	92-98	77-83	76-82
102-109	107-114	92-98	88-94
		107-108	102-103
		112-114	107-109

To Page No.

Witnessed & Understood by me, | Date | Invented by | Date
Recorded by

Project No._____

Book No._____ TITLE Archetype

From Page No.__

Dihedral Angles for ARCHETYPE

			PHI	PSI	OMEGA
1.	ALA	1		150.2	180.0
2.	ALA	2	-77.3	121.4	-180.0
3.	ALA	3	-132.9	141.9	173.6
4.	ALA	4	-123.5	123.4	179.7
5.	ALA	5	-122.1	111.8	176.2
6.	ALA	6	-87.1	151.7	-179.6
7.	ALA	7	-150.5		
8.	ALA	16		179.5	-175.3
9.	ALA	17	-128.2	161.6	171.8
10.	ALA	18	-147.0	164.7	174.4
11.	ALA	19	-134.2	112.6	174.1
12.	ALA	20	-90.7	143.4	176.6
13.	ALA	21	-118.2	155.8	179.7
14.	ALA	22	-140.9	104.1	-177.5
15.	ALA	23	-95.8		
16.	ALA	34		144.3	177.6
17.	ALA	35	-123.9	156.9	168.7
18.	ALA	36	-120.1	118.4	172.1
19.	ALA	37	-113.7	150.3	179.7
20.	ALA	38	-128.9	149.3	-178.7
21.	ALA	39	-134.7	100.5	172.5
22.	ALA	40	-58.8		
23.	ALA	45		138.4	178.3
24.	ALA	46	-130.6	115.3	177.4
25.	ALA	47	-70.1	133.8	178.8
26.	ALA	48	-102.5	-64.9	-179.1
27.	GLY	49	-153.3	175.8	175.3
28.	ALA	50	-146.1	157.2	179.8
29.	ALA	51	-143.7		
30.	ALA	57		154.5	174.5
31.	ALA	58	-144.6	135.6	-177.8
32.	ALA	59	-124.0	149.8	177.4
33.	ALA	60	-74.1	145.6	178.5
34.	ALA	61	-37.9		
35.	GLY	65		-36.1	-180.0
36.	ALA	66	-111.7	-19.2	167.7
37.	ALA	67	-99.4	145.5	174.0
38.	ALA	68	-137.6	117.2	177.2
39.	ALA	69	-87.9	139.8	177.3
40.	ALA	70	-140.4	171.1	-172.7
41.	ALA	71	-137.1	116.2	152.2
42.	ALA	72	-82.7	89.6	-180.0
43.	ALA	73	-52.9	-35.3	175.1
44.	ALA	74	-62.1	-25.5	-180.0
45.	ALA	75	-111.1	5.6	-173.8
46.	ALA	76	49.9	55.9	-174.2
47.	ALA	77	-134.2	129.2	175.4
48.	ALA	78	-112.1	135.8	-177.3
49.	ALA	79	-118.4	157.5	174.7
50.	ALA	80	-134.7	104.6	177.4
51.	ALA	81	-88.4	117.6	-173.7
52.	ALA	82	-109.7		
53.	ALA	88		172.2	170.3
54.	ALA	89	-95.6	126.0	-178.5
55.	ALA	90	-102.5	115.9	177.5
56.	ALA	91	-101.0	141.1	167.6
57.	ALA	92	-105.0	129.9	-178.1
58.	ALA	93	-128.6	165.3	-179.6
59.	ALA	94	-112.2		
60.	ALA	102		125.2	179.7
61.	ALA	103	-106.2	156.6	169.7
62.	GLY	104	-85.0	174.1	178.8
63.	ALA	105	-74.6	-25.5	-178.3
64.	GLY	106	91.3	154.5	173.9
65.	ALA	107	-133.2	136.4	-175.5
66.	ALA	108	-83.4	139.9	176.2
67.	ALA	109	-127.8		

FROM PDB FILE: ARCHETYPE.PDB
Doing residues: 1 to 67

Res	Res#	Atnm	Res	Res#	Atnm	Dist	D-A-AA	A-D-DD	A-D<	D-A<
ALA	5	N	ALA	23	O	3.00	156.5	118.7	6.4	40.7
ALA	23	N	ALA	5	O	2.98	142.8	119.5	-9.4	73.3
ALA	7	N	ALA	21	O	2.90	147.3	128.1	10.0	-68.1
ALA	21	N	ALA	7	O	2.90	154.0	122.8	-3.1	-61.4
ALA	18	N	ALA	82	O	3.21	143.0	132.3	-5.1	-41.4
ALA	82	N	ALA	18	O	2.90	160.6	115.1	-2.5	-80.2
ALA	20	N	ALA	80	O	3.04	142.1	123.1	-11.6	61.3
ALA	80	N	ALA	20	O	2.89	153.6	125.5	8.2	-49.3
ALA	22	N	ALA	78	O	2.76	166.2	112.4	29.5	30.3
ALA	78	N	ALA	22	O	3.00	143.1	122.9	-0.6	50.0
ALA	34	N	ALA	51	O	2.97	164.4	125.2	46.9	-42.9
ALA	51	N	ALA	34	O	2.95	166.3	126.7	7.5	-32.0
ALA	35	N	ALA	93	O	2.89	147.7	120.6	2.4	-72.9
ALA	93	N	ALA	35	O	2.95	143.6	126.7	-3.2	-63.6
ALA	36	N	GLY	49	O	2.91	152.7	123.7	1.5	-75.9
ALA	48	N	ALA	36	O	2.89	156.1	102.0	-0.3	-154.2
GLY	49	N	ALA	36	O	3.31	143.8	133.7	-10.8	-5.3
ALA	37	N	ALA	91	O	2.96	159.4	121.0	-15.8	-49.0
ALA	91	N	ALA	37	O	2.83	166.5	112.0	-15.6	-88.0
ALA	38	N	ALA	46	O	2.87*	150.9	117.6	6.1	68.3
ALA	46	N	ALA	38	O	2.84*	170.9	111.0	12.6	15.4
ALA	39	N	ALA	89	O	2.94	153.7	123.9	15.2	46.2
ALA	89	N	ALA	39	O	3.12	128.4	122.4	-5.4	77.8
ALA	60	N	ALA	48	O	2.72	170.0	111.7	15.9	-55.9
ALA	50	N	ALA	58	O	2.95@	164.3	128.4	8.6	-23.5
ALA	58	N	ALA	50	O	3.13@	148.6	127.1	6.3	-60.3
ALA	68	N	ALA	81	O	2.90	154.4	126.1	13.2	20.6
ALA	81	N	ALA	68	O	2.93	148.3	114.1	-7.8	63.7
ALA	70	N	ALA	79	O	3.06	137.2	125.6	1.6	-65.8
ALA	79	N	ALA	70	O	2.94	134.3	122.2	-6.4	-85.4
ALA	72	N	ALA	77	O	2.82	164.1	117.8	-32.2	-45.4
ALA	74	N	ALA	72	O	3.29	79.4	116.4	-75.1	-131.7
ALA	75	N	ALA	72	O	2.81@	127.9	108.6	-17.2	-101.5
ALA	76	N	ALA	72	O	3.00*	160.6	109.9	44.4	163.5
ALA	77	N	ALA	72	O	3.35	130.5	119.5	14.3	69.0
ALA	75	N	ALA	73	O	3.46	72.8	125.3	-64.7	-128.2
ALA	76	N	ALA	73	O	3.48@	100.3	107.6	-10.9	-90.2
ALA	77	N	ALA	75	O	3.42	74.1	114.2	90.1	130.4
ALA	88	N	ALA	109	O	3.13	153.2	131.7	38.6	-30.9
ALA	109	N	ALA	88	O	2.94	161.8	114.1	12.0	88.7
ALA	90	N	ALA	107	O	2.94	146.9	120.5	-2.6	66.2
ALA	107	N	ALA	90	O	3.14	134.4	129.9	10.1	65.1
GLY	104	N	ALA	92	O	2.80	159.7	107.6	25.9	94.3
ALA	94	N	ALA	102	O	2.92	162.9	126.0	14.3	38.4

* after dist denotes a possible alpha helix res
@ after dist denotes a possible 3-10 helix res

To Page No.____

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TITLE Archetype Sidechains

Project No.

Book No.

From Page No.

Res	Conf
2 Val	175.8°
4 Leu	-73.9, 176.6
16 Gly	
17 Ser	-61.5
20 Leu	-74, 177
21 Ser	54
22 Cys	175
23 Ala	
34 Met	-66, -68, -59
36 Trp	-73, 97
37 Val	164
38 Arg	64, 169, 178, -174
39 Gln	173, 176, 64
40 Ala	
45 Leu	-65, 172
46 Glu	175, -153, 46
47 Trp	179, 78
49 Ala	
~~50 His~~	~~79, -91~~
51 Ile	-161, 178
57 Thr	45
58 ~~Asn~~ TYR	-71, ~~174~~ 90
59 Tyr	-62, -89
65 Gly	
67 Phe	-64, ~~-85~~ 17
68 Thr	-40
70 Ser	-52
72 Asp	-178, 16
75 Lys	-77, 180, 180, 180
77 Thr	~~-8~~ -51
78 Leu	176, 80
80 Tyr	-59, -74
81 Leu	179, 77
82 Gln	178, 65, 56

Res	Conf
19 Arg	-174, 173, -85, 180
82 Met	-67, 179, 72
88 Ala	
89 Val	168
90 TYR	-68, 70
91 Tyr	-55, -79
92 Cys	72
93 Ala	
~~94~~ 103 Trp	-66, 68
104 Gly	
109 Val	173

* from 1FB4

Res	Conf
1 Glu	*52, -66, -69
3 Gln	*-55, -82, -95
5 Val	*-166
6 Glu	*-60, 83, -16 FB4* FB5
7 Ser	56 Nte
18 Leu	*-68, 168
35 ~~His~~ Ser	-65, ~~85 -100~~
48 Val	*176
50 ~~His~~ Val	~~29, 95~~ 79
60 ~~Asn~~ Ala	~~-171, -28~~ 90
61 ~~Glu~~ Asp	-65, ~~180, 99~~
66 Arg	*-45, -169, -74, 111
© 69 Ile	*-167, 168
71 Arg	*60, -170, -60, 148
73 Asp	~~-73~~, -86
74 Ser	180
76 Asn	-47, 171
94 Arg	*-166, 180, 73, 159
102 Tyr	*-69, -88
105 Gln	*-57, 180, -118
107 Thr	180
108 Thr	*-60

File: Archetype.PDBSC

© Sidechain conf of res 69

χ1 ~180 if 49 = ala

~-40 if 49 = Gly

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Date 12-20-89

Project No.
Book No.
TITLE Loop 1 : Res 8-15

From Page No.

Dg's loops superimposed on Archetype

Prot	res	RMS NCaC	file
FB4	6,7,16,17	0.186	
FB4	7,16	0.159	LOOP1.FB4
FBJ	6,7,16,17	0.333	LOOP1.FBJ
HFL	5,6,16,17	0.263	
	6,7,16,17	0.559	LOOP1.HFL
FAB	6,7,16,17	0.525	LOOP1.FAB

file: Archetype.PDBLOOP1

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		Recorded by Leonard Presta	12-20-89

TITLE Loop 3: Res 41-44

Project No.
Book No.

From Page No.

1FB4, 1FBJ have one conf and A40

2MCP, 2HFL have second conf and P40

model based on Human III — a40

Prot	res	RMS NCaC	file
1FB4	40, 45	0.126	LOOP3.FB4
1FBJ	40, 45	0.202	LOOP3.FBJ
2HFL	40, 45	0.195	LOOP3.HFL
2MCP	~~39~~, 40, 45	0.132	LOOP3.MCP

file: Archetype. PDBLPI_3

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Project No.
Book No.
TITLE Loop5: 62-64

From Page No.

Group 1: 1FB4, 2HFL, 2mcP

2: 3fab Pro @62

3: 1FB5 Pro @61

	Prot	res	RMS NCAC	Archetype
use	1FB4	62,66	0.165	61,65
	2mcP	64,68	0.166	
	2HFL	62,66	0.203	

file: Archetype.PDBLP1-4

To Page No.

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TITLE Loop 6: 83-87

Project No.

Book No.

From Page No.

Prot	res	Archetype	RMS NCaC	
1FB4	82,83 92,93	81,82 88,89	0.157	Loop6.FB4
2mcP	84,85 94,95	"	0.206	.mcP
	on Loop6.FB4		0.203	
2HFL	82,83 92,93	"	0.191	.HFL
	on Loop6.FB4		0.486	.HFL2
1FBJ	82,83 92,93	81,82 88,89	0.311	.FBJ
	on Loop6.FB4		0.449	.FBJ2
3fab	81,82 91,92		0.327	.FAB
	on Loop6.FB4		0.588	.FAB2

file: Archetype.PDB1-6

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Date 12-20-89

Project No.
Book No.
TITLE CDR1 Heavy Res 26-35

From Page No. Heavy CDR1: Res 26-32 (Chothia/Lesk JMB 196:901 1987)
Res 31-35 (Kabat 1987)

Prot	Res	Archetype Res	RMS NCaC	file
1FB4	22,23,34,35	22,23,34,35	0.178	LOOPH1.FB4
2MCP	"	"	0.153	.MCP
1FBJ	"	"	0.294	.FBJ
2NFL	"	"	0.312	.Nfl
3FAB	"	"	0.303	.fab

Sidechains within 6Å

Res	1FB4	1FBJ	2NFL	2MCP	3FAB	Hum III (Kabat)
F27	V2	V2		V2		V2
	L4			L4		L4
	S24	A24	A24	T24		A24
	F29	F29	F29	F29		F29
	Y32		Y32	F32		Y32
	M34	M34	I34	M34		M34
	R98	R98	H98	R100		R94
			F103			
F29	S24	A24		T24		A24
	F27	F27	F27	F27		F27
	M34	M34	I34	M34		M34
	R72		A72	R74		R71
	D74		T74	T76		D73
	N77	N77	S77	S79		N76
	L79	L79				L78
		Y32	P53			

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Witnessed & Understood by me, | Date | Invented by | Date
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TITLE CDR1 Heavy Res 26-35

Project No.
Book No.

From Page No. 20

	1FB4	1FBJ	2NFL	2MCP	3FAB	HumIII
M34	F27		F27	F27		F27
	F29	F29	F29	F29		F29
	Y32	Y32				Y32
	I51	I51		S51		I51
	R72			R74		R71
	L79	L79	A79	L81		L78
	R98	R98	H98			R94
	C22	C22	C22	C22		C22
	C96	C96	C96	C98		C92
				R100		
				T24		
				L4		

CDR1 Heavy Res 26-35b (26-32 Chothia/Lesk; 31-35b Kabat)

Lengths HumI 10 HumII 10-12 (10=8; 11=1; 12=7) HumIII 10 (Kabat 1987)

Res	I			II			III			#segs – #AA – # most common then other AAs
*26	G	10-2-9	E	G	12-1-12		G	58-3-56	VA	
*27	Y	10-4-5	GDE	F	11-5-4	GLYS	F	56-2-55	I	
28	T	8-2-6	DE	S	11-3-9	TP	T	51-8-30	SNKIAPL	
*29	F	8-2-7	A	L	10-4-5	IFV	F	53-4-47	IVL	
*30	S	8-5-3	NVIR	S	10-4-7	NTR	S	50-9-39	asx GTPFAR	
31	D	8-7-2	RGSHTL	T	10-5-4	SGNR	DT	47-11-15/11	SARYKPEG	
32	Y	8-2-5	S		10-7	TSDERGY	Y	50-10-21	SNDFATHGV	
33	Y/A	8-6	TKDG	G	10-4-5	YTR	A	46-12-13	YGTSVWNLDEF	
*34	I	8-4-4	MGR	M	10-4-4	YVW	M	50-7-35	VIYLR	
35	H	8-5-3	SILD		10-8	CSRGAWTY	S	46-12-11	HDYNEFKVRT	
35a				V	8-3-6	GW				
35b				G	7-3-4	SA				

General: 26 GFTFSxYxMx

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Project No._____
Book No._____ TITLE CDR2 Heavy Res 50-65

From Page No.__

Prot	Res	Archetype	RMS	NC&C
1FB4	50,51,58,59	50,51,57,58	0.120	
2MCP	50,51,60,61	"	0.246	
2HFL	50,51,58,59	"	0.232	
1FBJ	50,51,58,59		0.275	
3FAB	50,51,57,58		0.194	

Heavy CDR2:
Res 53-55 (Chothia / Lesk)
50-65 (Kabat)

Human Subgroup I

Res	#Segs	#AA	#major	others
50	7	7	1(+)	GSIQWVE
	7	3	5(ILE)	PV
	7	6	2(ASN)	VAPHD
	6	3	4(PRO)	KL
53	7	6	2(SER)	MWRNY
	7	5	2(+)	PSTGD
	7	3	4(GLY)	DN
	7	5	2(+)	PGSRT
	7	4	4(THR)	PFE
	7	6	2(ASN)	QSVD
	7	3	5(TYR)	GK
60	6	4	3(ALA)	VNG
	6	3	3(PRO)	GY
	6	4	2(+)	KRIG
	6	3	3(PHE)	SK
	7	4	4(GLN)	WVK
65	7	5	3(GLY)	EVAS

Human Subgroup II

Res	#Segs	#AA	#major	others
50	10	7	3(ARG)	WFSYGE
	10	4	6(ILE)	VLD
	10	6	3(ASN) : 3(ASP)	YFIL
	2	2	1(+)	Y
53	9	5	4(TRP)	YHL asx
	10	5	5(ASP) : 4(ASP)	NGHT
	10	2	6(ASP)	G
	10	4	5(ASP)	STK
	10	6	4(LYS)	TSIPN
	10	4	6(TYR)	RDN
	10	4	7(TYR)	WFD
60	10	5 : 6	3(+) : 3(SER)	NGTK
	10	3	5(THR)	PA
	10	2	9(SER)	P
	10	1	10(LEU)	
	10	3	4(ARG)	KE
65	10	3	5(SER)	TG

Human Subgroup III

Res				
50	34	12	6 V	WAHYFGRTNIL
51	34	6	23 I	RKVFM
52	33	11	6 S	YGEWVTKLN Gly
52a	30	10	5E/5Y	NGQKD SVW Gly
52b	8*	1		K
52c	8*	2		TS
53	33	12	10 N	asx GSKDT ALERVQ
54	32	6	16 G	SANKV
55	31	8	10 S	G asx YNVKA
56	31	11	[redacted]	SD asx TAN LFIER Gly
57	33	8	15 T	K Gly SQVI
58	32	11	10 Y	HI STFALMV asx
59	33	2	29 Y	F
60	33	6	20 A	GR TVI
61	33	5	19 D	VAEN
62	34	2	32 S	R

* related segs (see Kabat)

63	34	4	31 V	ALF
64	33	4	31 K	NQR
65	33	2	32 G	A

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Recorded by Leonard Presta | 12-22-89

TITLE CDR2 Heavy Res 50-65 Project No. Book No. 23

From Page No. 22

#Res 50-65

Hum I 17
II 17(1); 16(9)
III 17(21); 16(2); 19(8*)

	50	51	52	52a	53	54	55	56	57	58	59	60	61	62	63	64	65
I											Y	(A)	(D)	S	V	K	G

CDR3 Heavy Res 95-102

Hum I 8(1); 10(1); 13(2); 16(1); 19(1)
II 9(2); 10(1); 11(1); 13(1); 15(2); 16(1); 18(2); 19(1)
III 5(1); 7(1); 9(2+8*); 11(2); 12(2); 13(7); 17(2); 19(1)
10(5)

Heavy CDR3: Res 96-101 (Chothia/Lesk) Res 95-102 (Kabat)

3FAB = NEWM Human II

1FB4 = KOL Human III

2MCP = MCPC 603 Mouse III (A)

1FBJ = J539 Mouse III (B)

To Page No.

Witnessed & Understood by me, Date Invented by Date 12-22-89

Recorded by Leonard Presta

Project No.
Book No.
TITLE Building VH

From Page No.

Consensus structure for use in designing antibodies to target protein (lysozyme or bpti)

CDR1 use 2MCP 24-33 T S Ø F T F S D F Y
↓ ↓ ↓
subgrp humIII A Y A

CDR2 use 1FB4 52-57 W D D Ø S D Q
↓ ↓
subgrp humIII S T

CDR3 use 2HFL 94-101 H Ø N Y D F D
↓ ↓ ↓ ↓ ↓ ↓
subgrp humIII R D A A A A D

file: Archetype.PDBCDR123

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Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by Leonard Presta	1-31-90

TITLE B-sheet H-bonds

Project No.

Book No.

From Page No.

β-sheet h-bonds found in crystal structures and Archetype. PDBCDR123 (consensus structure)

Res	FBH	FAB	FBJ	MCP	HFL	Arch dist.
3=25	✓	✓	–	✓	(½)	3.07 3.27*
5=23	✓	✓	✓	✓	✓	3.00 2.98
7=21	✓	(✓)	✓	✓	–	2.90 2.90
18=82	✓	✓	½	✓	✓	3.15* 2.90
20=80	✓	✓	✓	✓	✓	3.04 2.89
22=78	✓	(✓)	✓	✓	✓	3.76 3.00
24→76	✓	–	–	✓	✓	3.21*
82A→66	✓	–	✓	✓	✓	2.91
81=68	✓	✓	✓	✓	✓	2.93 2.90
79=70	✓	✓	½	✓	✓	2.66 3.06
77←72	✓	(✓)	–	✓	✓	2.76
88=109	✓	✓	✓	✓	✓	3.13* 2.94
90=107	✓	✓	✓	✓	✓	2.98 3.14*
92←104	✓	–	✓	✓	✓	2.80
94→102	✓	–	✓	✓	✓	2.84
↖101 or 102	✓	–	–	✓	–	–
39=89	✓	✓	½	✓	✓	2.94 3.12*
37=91	✓	✓	✓	✓	✓	2.96 2.83
35=93	✓	(½)	✓	✓	✓	2.89 2.95
33←95	✓	✓	✓	✓	–	3.29*
38=46	✓	✓	✓	✓	✓	2.87 2.84
36←48	✓	✓	✓	✓	✓	2.89
↘49	✓	✓	✓	✓	✓	2.91
34=51	✓	–	✓	✓	✓	2.97 2.95

Res	FBH	FAB	FBJ	MCP	HFL	Arch
52→56	✓	✓	(✓)	✓	✓	3.11*
50=58	✓	(½)	✓	✓	✓	2.95 3.13*
48←60	✓	✓	(✓)	(✓)	(✓)	2.71
15→82C	✓	–	✓	✓	✓	3.17*
82C→16	✓	–	✓	✓	✓	3.28*
12←112	✓	✓	–	✓	✓	2.94
↘110	✓	(✓)	–	✓	✓	3.20
10↙	✓	(✓)	✓	✓	✓	3.14
↘108	(✓)	–	(✓)	✓	✓	–

( ) = poor geometry

* = long distance in Archetype

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Date

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Date 1-31-90

Recorded by Leonard Presta

Project No.
Book No.
TITLE Conserved V_H Hbonds

From Page No.

res #s ( ) long distance

		HFM	HFL	MCP	F19	FBJ	FB4	FAB
S7 oδ	oδ S21		7,21	7,21	7,21			
S17 oδ	oδ1 N82a	17,83					17,84	
W36 NE1	o F/Y 79	36,79		36,82		36,80	36,80	
R38 NE	oε E46	38,46				38,46	38,46	38,46
Nh1	oh Y90	38,93	(38,94)	(38,96)		38,94	38,94	
Nh1	oδ D86			38,92			38,90	
Nh2	oε E46	38,46		38,46		38,46	38,46	38,46
W47 NE1	o x49			47,49			47,49	
NE1	oε E35		47,35	47,35				
R66 Nh1	oδ D86	66,89		69,92			67,90	66,89
Nh1	o S82b	66,84					67,85	
Nh2	oδ D86	66,89		69,92			67,90	66,89
Nh2	o S62			69,65			67,63	
K66 NZ	oδ D86		67,90		(67,90)			
x69 N	oh Y59	(59,69)	(70,60)	(72,62)		70,60	70,60	
Q81 NE2	o L18			(84,18)		(82,18)	(82,18)	
NE2	oδ D/N82a		(82,84)	84,86			(82,84)	
Y90 oh	o D86	93,89 ~~89,90~~	94,90	96,92	94,90	94,90	94,90	93,89
R94 NE	oδ D101			(100,110)	98,112		98,106	
Nh2	oδ D101			100,110	98,112		98,106	
Q105 N	oε Q6			114,6		(110,6)	110,6	
Q106 N	oε Q6	106,6		115,6		111,6	111,6	

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Recorded by Leonard Presta

From Page No.

Archetype: PDBCDR123 → hvhumiii.pdb
human V_H subgroup III
D52aY Y102V T108L

Building 4D5 VH from Archetype

(1) Conf. of residues 7-15 depends on identity of residues 9,10; in human subgroup III G9, G10 in 4D5 P9, E10; change conf. res 7-15 to (3HFM, 3FAB) conf.

(2) conf. of CDR2 (H2) dependent on position of Gly; in archetype, res 51-57 from 1FB4 -- replace with I51-T57 from 2HFL; conformation of H2 also dependent on res 71 -- when R, H2 folds "out", when A H2 folds "in"; since res 71 is A in 4D5 and 2HFL, H2 taken from 2HFL

	49	50	51	52	52a	b	c	53	54	55	56	71	
3FAB	G	Y	V	F	-	-	-	Y	H	G	T	V	Conf 1
D1.3								G	D	G			
3HFM	G	Y	V	S	-	-	-	Y	S	G	S	R	
2HFL	G	E	I	L	P	-	-	G	S	G	S	A	conf 2
2FB4	A	I	I	W	D	-	-	D	G	S	D	R	conf 3
1FBJ	G	E	I	H	P	-	-	D	S	G	T	R	
2MCP	A	A	S	R	N	K	G	N	K	Y	T	R	conf 4
4D5	G	R	I	Y	P	-	-	T	N	G	Y	A	

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Witnessed & Understood by me, Date Invented by Recorded by Leonard Presta Date 2-20-90

Project No.
Book No.
TITLE Building 4D5

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(3) CDR1: use conf from 2HFL/2MCP

res	24	27	29	34	71	78	94	
2FB4	S	F	F	M	R	L	R	conf1
1FBJ	A	F	F	M	R	L	R	conf1
2MCP	T	F	F	M	R	L	R	conf1
1F19	A	Y	F	V	V	A	R	conf1
2HFL	A	Y	F	I	A	A	R	conf1
3HFM	V	D	I	W	R	Y	N	conf2
3FAB	V	T	F	S	V	F	R	conf2
4D5	A	F	I	I	A	A	R	
hum III	A	F	F	M	R	L	R	
mouse II	A	Y/F	F/I	M	A	A	R	

(4) CDR3:

	94						100										101		103
2FB4	R	D	G	G	H	G	F	C	S	S	A	S	C	F	G	P	D	Y	W
1F19	R	S	F	Y	G	G	S	D	L	A	V	Y	Y	F			D	S	W
3FAB	R	N	L	I	A	G	C	I									D	V	W
1FBJ	R	L	H	Y	Y	G	Y	N									A	Y	W
2HFL	H	G	N	Y	D	F											D	G	W
3HFM	N	W	D	G													D	Y	W
2MCP	R	N	Y	Y	G	S	T	W	Y	F							D	V	W
4D5	R	W	G	G	D	G	F	Y	A	M							D	Y	W

in one model, use H3 from 2MCP

Insight loop search gave one good one:

1PRC resC11-C19 PATTT-QTGFRGLSM-GEVLH

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Recorded by Leonard Presta

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files:

HER2.MCP H3 from 2MCP
.MCP2 altered conf res Y56 (sidechain only) Y100a W95
.PRC H3 from 1PRC
.PRC2 " " " (slightly diff conf)
.MODEL modeled from 1PRC

Residues converted from archetype human III → 4D5

V 5 Q
E 6 Q
G 9 P
G 10 E
Q 13 K
G 16 A
R 19 K
A 23 T
T 28 N
F 29 I
S 30 K
Y 32 T
A 33 Y
M 34 I
S 35 H
R 38 K
A 40 R
G 42 E
K 43 Q
V 48 I
A 49 G

CDR1

V 50 R
S 52 Y
E 52a P
N 53 T
G 54 N
S 55 G
D 56 Y
Y 58 R
A 60 D
D 61 P
S 62 K
V 63 F
K 64 Q
G 65 D
R 66 K
F 67 A
S 70 T
R 71 A
D 73 T
K 75 S
L 78 A

CDR2

M 82 V
N 82a S
S 82b R
R 83 T
A 84 S
A 93 S
D 95 W
R 96 G
A 97 G
A 98 D
A 99 G
100a Y
100b A
100c M
V 100 F
V 102 Y
T 107 A
L 108 S

CDR3

To Page No.

Witnessed & Understood by me, Date Invented by Date 2-20-90
Recorded by Leonard Presta

[redacted]

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by	

[redacted]

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by Leonard Presta	5-1-90

[redacted]

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by Leonard Presto	5-1-80

[redacted]

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by Leonard Presta	3-19-91

[redacted]

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by Leonard Presta	3-19-91

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by Leonard Pretty	3-19-91

[redacted]

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by Leonard Presto	3-19-91

[redacted]

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by Leonard Pruta	3-19-91

[redacted]

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by Leonard Presta	3-19-91

[redacted]

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by Leonard Presta	3-19-91

[redacted]

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by Leonard Presta	3-21-91

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by Leonard Presty	3-22-91

[redacted]

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by Leonard Pretty	3-25-91

[redacted]

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by Leonard Presta	3-25-91

[redacted]

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by Leonard Presta	4-5-91

[redacted]

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by Leonard Presta	4-5-91

[redacted]

To Page No.

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by Leonard Presta	4-10-91

[redacted]

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by Leonard Presta	4-11-91

[redacted]

To Page No.

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by Leonard Presta	4-11-91

[redacted]

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by Leonard Preta	4-15-91

[redacted]

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by Leonard Presta	4-18-91

[redacted]

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by Leonard Presty	4-20-91

[redacted]

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by	

[redacted]

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by Leonard Prestes	4-23-91

[redacted]

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by	

[redacted]

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by	

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by Leonard Presta	5-1-91

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by Leonard Presty	5-1-91

[redacted]

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by Leonard Presta	5-6-91

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by Leonard Presta	5-6-91

[redacted]

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by	

[redacted]

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by Leonard Presta	5-24-91

[redacted]

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by Leonard Presta	5-29-91

[redacted]

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by	

[redacted]

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by	

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by Leonard Presto	7-1-91

[redacted]

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by Leonard Prieto	8-8-91

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by Leonard Presta	8-12-91

[redacted]

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by Leonard Presta	8-13-91

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by Leonard Prestl	8-29-91

[redacted]

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by Leonore Presta	9-3-91

[redacted]

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by Leonard Presta	9-9-91

[redacted]

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by Leonard Presta	9-9-91

[redacted]

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by	

[redacted]

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by	

[redacted]

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by	

[redacted]

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by	

[redacted]

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by	

[redacted]

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by Leonard Prieto	4-21-92