LABORATORY NOTEBOOK

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GENENTECH, INC.

Celltrion v. Genentech
IPR2017-01374
Genentech Exhibit 2002

NOTEBOOK NO. 10823

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ON December 5 19 89

DEPARTMENT BIOMOL. CHEM

RETURNED _____ 19 ____

—SCIENTIFIC NOTEBOOK CO.—
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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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Using Biosym Insight program; all superimposed on 1FB4 VL (output files = *.NEWROT)

1FB4	2RHE	2MCP	3FAB
V18-D24	V18-D24	V19-S25	V18-D24
V32-Q37	V34-Q39	L39-Q44	V32-Q37
R60-S66	R62-S68	R67-~~S73~~ D72	R53-S66
S69-I74	S71-I76	D76-I81	S69-I74
D84-A88	D86-A90	V91-Q95	D84-Q88
RMS NCaC	0.40	0.60	0.53

1FBJ	2HFL	1REI(molA)	(molB)
V19-A25	V19-A25	V19-A25	
L32-Q37	M32-Q37	L33-Q38	
R60-~~S~~D65	R60-D65	R61-D66	
S69-I74	S69-I74	D70-I75	
I84-Q88	E84-Q88	T85-Q89	
0.54	0.48	0.50	0.47

Superimposed on 1FBJ (output files = *.ONFBJ)

	RMS NCaC
2MCP	0.470
2HFL	0.388
1REI(molA)	0.499
(molB)	0.444

To Page No.

Witnessed & Understood by me, Date

Invented by Date 12-15-88

Recorded by Leonard Presta

Project No._____
Book No._____ TITLE Cα-Cα Distance Matches

From Page No.__

From PDB files: 1fb4.test 2mcp.test
Maximum distance cutoff for CA-CA was 2.50
NUMRES molecules 1&2 112 118

1fb4 Res		2mcp Res		Dist
GLU	1	ASP	1	2.31
VAL	3	VAL	3	2.46
LEU	4	MET	4	0.30
THR	5	THR	5	0.62
GLN	6	GLN	6	0.74
PRO	7	SER	7	1.60
PRO	7	PRO	8	2.49
PRO	8	SER	9	0.93
SER	9	SER	10	1.08
ALA	10	LEU	11	1.91
SER	11	SER	12	2.48
GLY	12	VAL	13	1.83
THR	13	SER	14	1.68
PRO	14	ALA	15	1.05
GLY	15	GLY	16	1.06
GLN	16	GLU	17	1.12
ARG	17	ARG	18	0.91
VAL	18	VAL	19	0.40
THR	19	THR	20	0.47
ILE	20	MET	21	0.40
SER	21	SER	22	0.18
CYS	22	CYS	23	0.33
THR	23	LYS	24	1.21
GLY	24	SER	25	0.84
THR	25	SER	26	2.16
THR	25	GLN	27	2.49
GLY	28	SER	28	1.67
THR	31	ASN	37	2.18
THR	31	PHE	38	2.28
VAL	32	LEU	39	1.41
ASN	33	ALA	40	0.73
TRP	34	TRP	41	0.37
TYR	35	TYR	42	0.30
GLN	36	GLN	43	0.35
GLN	37	GLN	44	0.31
ALA	42	PRO	49	0.56
PRO	43	PRO	50	0.33
LYS	44	LYS	51	0.24
LEU	45	LEU	52	0.48
LEU	46	LEU	53	0.76
ILE	47	ILE	54	0.56
TYR	48	TYR	55	0.67
ARG	49	GLY	56	0.79
ASP	50	ALA	57	0.67
ALA	51	SER	58	0.57
MET	52	THR	59	0.59
ARG	53	ARG	60	1.25
PRO	54	GLU	61	1.43
SER	55	SER	62	1.37
GLY	56	GLY	63	1.01
VAL	57	VAL	64	0.25
PRO	58	PRO	65	0.19
THR	59	ASP	66	0.24
ARG	60	ARG	67	0.48
PHE	61	PHE	68	0.22
SER	62	THR	69	0.28
GLY	63	GLY	70	0.51
SER	64	SER	71	0.49
LYS	65	GLY	72	1.14
THR	68	THR	75	1.01
SER	69	ASP	76	0.65
ALA	70	PHE	77	0.35
SER	71	THR	78	0.55
LEU	72	LEU	79	0.44
ALA	73	THR	80	0.64
ILE	74	ILE	81	0.21
SER	75	SER	82	0.21
GLY	76	SER	83	0.72
LEU	77	VAL	84	0.73
GLU	78	GLN	85	0.74
ALA	79	ALA	86	0.88
GLU	80	GLU	87	0.80
ASP	81	ASP	88	0.85
GLU	82	LEU	89	1.15
SER	83	ALA	90	0.70
ASP	84	VAL	91	0.37
TYR	85	TYR	92	0.38
TYR	86	TYR	93	0.28
CYS	87	CYS	94	0.37
ALA	88	GLN	95	0.80
SER	89	ASN	96	1.48
TRP	90	HIS	98	1.73
SER	96	TYR	100	1.26
SER	96	PRO	101	2.29
TYR	97	LEU	102	1.35
VAL	98	THR	103	1.51
PHE	99	PHE	104	0.82
GLY	100	GLY	105	1.38
THR	101	GLY	105	2.48
THR	101	ALA	106	1.56
GLY	102	GLY	107	0.81
THR	103	THR	108	0.66
LYS	104	LYS	109	0.59
VAL	105	LEU	110	0.74
THR	106	GLU	111	0.92
VAL	107	ILE	112	1.26
LEU	108	LYS	113	1.82

From PDB files: 1fb4.test 1fbj.test
Maximum distance cutoff for CA-CA was 2.50
NUMRES molecules 1&2 112 111

1fb4 Res		1fbj Res		Dist
GLU	1	GLU	1	1.53
LEU	4	LEU	4	1.23
THR	5	THR	5	0.93
GLN	6	GLN	6	0.57
PRO	7	SER	7	1.28
PRO	7	PRO	8	2.34
PRO	8	ALA	9	0.68
SER	9	ILE	10	1.37
ALA	10	THR	11	1.91
SER	11	ALA	12	1.43
GLY	12	ALA	13	0.88
THR	13	SER	14	0.44
PRO	14	LEU	15	0.62
GLY	15	GLY	16	0.17
GLN	16	GLN	17	0.30
ARG	17	LYS	18	0.25
VAL	18	VAL	19	0.68
THR	19	THR	20	0.85
ILE	20	ILE	21	0.12
SER	21	THR	22	0.46
CYS	22	CYS	23	0.28
THR	23	SER	24	0.99
GLY	24	ALA	25	0.37
THR	25	SER	26	1.95
THR	25	SER	27	2.33
SER	26	SER	27	1.77
SER	27	SER	28	2.44
ILE	30	SER	30	1.00
THR	31	SER	31	1.47
VAL	32	LEU	32	1.00
ASN	33	HIS	33	0.26
TRP	34	TRP	34	0.47
TYR	35	TYR	35	0.53
GLN	36	GLN	36	0.38
GLN	37	GLN	37	0.41
LEU	38	LYS	38	2.15
LEU	38	SER	39	2.13
MET	41	THR	41	2.21
ALA	42	SER	42	0.50
PRO	43	PRO	43	0.96
LYS	44	LYS	44	0.63
LEU	45	PRO	45	0.83
LEU	46	TRP	46	0.75
ILE	47	ILE	47	0.14
TYR	48	TYR	48	0.51
ARG	49	GLU	49	1.61
ASP	50	ILE	50	1.22
ALA	51	SER	51	0.40
MET	52	LYS	52	0.74
ARG	53	LEU	53	1.02
PRO	54	ALA	54	2.21
PRO	54	SER	55	2.33
SER	55	SER	55	2.19
GLY	56	GLY	56	1.26
VAL	57	VAL	57	1.16
PRO	58	PRO	58	0.92
THR	59	ALA	59	0.52
ARG	60	ARG	60	0.59
PHE	61	PHE	61	0.56
SER	62	SER	62	0.33
GLY	63	GLY	63	0.55
SER	64	SER	64	0.33
LYS	65	GLY	65	0.90
SER	66	SER	66	2.13
THR	68	THR	68	0.85
SER	69	SER	69	0.96
ALA	70	TYR	70	0.31
SER	71	SER	71	0.45
LEU	72	LEU	72	0.25
ALA	73	THR	73	0.45
ILE	74	ILE	74	0.78
SER	75	ASN	75	1.03
GLY	76	THR	76	0.52
LEU	77	MET	77	0.69
GLU	78	GLU	78	0.75
ALA	79	ALA	79	0.95
GLU	80	GLU	80	0.61
ASP	81	ASP	81	1.24
GLU	82	ALA	82	1.40
SER	83	ALA	83	0.35
ASP	84	ILE	84	0.16
TYR	85	TYR	85	0.23
TYR	86	TYR	86	0.54
CYS	87	CYS	87	0.56
ALA	88	GLN	88	0.48
SER	89	GLN	89	0.53
TRP	90	TRP	90	1.58
ASN	95	PRO	93	2.10
SER	96	LEU	94	1.57
TYR	97	ILE	95	0.62
VAL	98	THR	96	0.70
PHE	99	PHE	97	0.64
GLY	100	GLY	98	0.77
THR	101	ALA	99	1.18
GLY	102	GLY	100	0.67
THR	103	THR	101	0.23
LYS	104	LYS	102	0.36
VAL	105	LEU	103	0.67
THR	106	GLU	104	1.08
VAL	107	LEU	105	0.65
LEU	108	LYS	106	0.65
GLY	109	ARG	107	2.30

Using MATCH program

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

Recorded by

From Page No. 2

From PDB files: 1FB4.TEST 1REI MOLECULE A
Maximum distance cutoff for CA-CA was 2.50
NUMRES molecules 1&2 112 107

1FB4 Res		1REI Res		Dist
GLU	1	ASP	1	2.48
LEU	4	MET	4	0.65
THR	5	THR	5	0.57
GLN	6	GLN	6	0.56
PRO	7	SER	7	1.73
PRO	7	PRO	8	2.24
PRO	8	SER	9	0.70
SER	9	SER	10	1.42
ALA	10	LEU	11	2.40
SER	11	SER	12	2.38
GLY	12	ALA	13	1.67
THR	13	SER	14	2.18
PRO	14	VAL	15	1.41
GLY	15	GLY	16	0.43
GLN	16	ASP	17	1.03
ARG	17	ARG	18	0.62
VAL	18	VAL	19	0.45
THR	19	THR	20	0.68
ILE	20	ILE	21	0.48
SER	21	THR	22	0.36
CYS	22	CYS	23	0.34
THR	23	GLN	24	0.75
GLY	24	ALA	25	0.69
THR	25	SER	26	2.29
THR	25	GLN	27	2.19
SER	26	GLN	27	2.34
SER	26	ASP	28	2.04
GLY	28	ASP	28	2.09
THR	31	TYR	32	1.26
VAL	32	LEU	33	0.89
ASN	33	ASN	34	0.68
TRP	34	TRP	35	0.22
TYR	35	TYR	36	0.25
GLN	36	GLN	37	0.34
GLN	37	GLN	38	0.55
LEU	38	THR	39	2.29
ALA	42	ALA	43	0.78
PRO	43	PRO	44	0.39
LYS	44	LYS	45	0.35
LEU	45	LEU	46	0.40
LEU	46	LEU	47	0.61
ILE	47	ILE	48	0.43
TYR	48	TYR	49	0.44
ARG	49	GLU	50	1.04
ASP	50	ALA	51	0.78
ALA	51	SER	52	0.60
MET	52	ASN	53	0.53
ARG	53	LEU	54	0.58
PRO	54	GLN	55	1.13
SER	55	ALA	56	1.64
GLY	56	GLY	57	0.85
VAL	57	VAL	58	0.37
PRO	58	PRO	59	0.26
THR	59	SER	60	0.29
ARG	60	ARG	61	0.17
PHE	61	PHE	62	0.09
SER	62	SER	63	0.22
GLY	63	GLY	64	0.18
SER	64	SER	65	0.38
LYS	65	GLY	66	0.46
GLY	67	GLY	68	2.27
THR	68	THR	69	0.66
SER	69	ASP	70	0.74
ALA	70	TYR	71	0.49
SER	71	THR	72	0.90
LEU	72	PHE	73	0.39
ALA	73	THR	74	0.38
ILE	74	ILE	75	0.22
SER	75	SER	76	0.22
GLY	76	SER	77	0.65
LEU	77	LEU	78	0.96
GLU	78	GLN	79	1.15
ALA	79	PRO	80	1.71
GLU	80	GLU	81	1.20
ASP	81	ASP	82	1.22
GLU	82	ILE	83	1.35
SER	83	ALA	84	0.92
ASP	84	THR	85	0.25
TYR	85	TYR	86	0.25
TYR	86	TYR	87	0.24
CYS	87	CYS	88	0.52
ALA	88	GLN	89	0.74
SER	89	GLN	90	0.97
TRP	90	TYR	91	1.72
SER	96	LEU	94	1.26
SER	96	PRO	95	1.55
TYR	97	TYR	96	0.91
VAL	98	THR	97	1.44
PHE	99	PHE	98	0.78
GLY	100	GLY	99	0.89
THR	101	GLN	100	1.02
GLY	102	GLY	101	1.11
THR	103	THR	102	0.81
LYS	104	LYS	103	0.71
VAL	105	LEU	104	0.95
THR	106	GLN	105	1.40
VAL	107	ILE	106	1.53
LEU	108	THR	107	1.55

From PDB files: 1FB4.TEST 1REI MOLECULE B
Maximum distance cutoff for CA-CA was 2.50
NUMRES molecules 1&2 112 107

1FB4 Res		1REI Res		Dist
GLU	1	ASP	1	2.28
LEU	4	MET	4	0.81
THR	5	THR	5	0.43
GLN	6	GLN	6	0.58
PRO	7	SER	7	1.84
PRO	7	PRO	8	2.13
PRO	8	SER	9	0.65
SER	9	SER	10	1.45
ALA	10	LEU	11	2.08
GLY	12	ALA	13	1.84
THR	13	SER	14	1.54
PRO	14	VAL	15	1.09
GLY	15	GLY	16	0.83
GLN	16	ASP	17	1.11
ARG	17	ARG	18	0.52
VAL	18	VAL	19	0.42
THR	19	THR	20	0.49
ILE	20	ILE	21	0.48
SER	21	THR	22	0.28
CYS	22	CYS	23	0.25
THR	23	GLN	24	0.75
GLY	24	ALA	25	0.58
THR	25	SER	26	1.64
SER	26	GLN	27	2.25
SER	26	ASP	28	2.27
GLY	28	ASP	28	1.82
THR	31	TYR	32	1.41
VAL	32	LEU	33	0.93
ASN	33	ASN	34	0.61
TRP	34	TRP	35	0.29
TYR	35	TYR	36	0.23
GLN	36	GLN	37	0.18
GLN	37	GLN	38	0.48
ALA	42	ALA	43	0.77
PRO	43	PRO	44	0.38
LYS	44	LYS	45	0.42
LEU	45	LEU	46	0.28
LEU	46	LEU	47	0.59
ILE	47	ILE	48	0.56
TYR	48	TYR	49	0.55
ARG	49	GLU	50	1.06
ASP	50	ALA	51	0.88
ALA	51	SER	52	0.81
MET	52	ASN	53	0.81
ARG	53	LEU	54	1.05
PRO	54	GLN	55	1.31
SER	55	ALA	56	1.43
GLY	56	GLY	57	0.91
VAL	57	VAL	58	0.44
PRO	58	PRO	59	0.50
THR	59	SER	60	0.45
ARG	60	ARG	61	0.36
PHE	61	PHE	62	0.22
SER	62	SER	63	0.20
GLY	63	GLY	64	0.25
SER	64	SER	65	0.40
LYS	65	GLY	66	0.43
GLY	67	GLY	68	2.36
THR	68	THR	69	0.30
SER	69	ASP	70	0.60
ALA	70	TYR	71	0.52
SER	71	THR	72	0.69
LEU	72	PHE	73	0.31
ALA	73	THR	74	0.32
ILE	74	ILE	75	0.27
SER	75	SER	76	0.29
GLY	76	SER	77	0.47
LEU	77	LEU	78	0.87
GLU	78	GLN	79	1.21
ALA	79	PRO	80	1.36
GLU	80	GLU	81	1.15
ASP	81	ASP	82	0.93
GLU	82	ILE	83	0.90
SER	83	ALA	84	0.63
ASP	84	THR	85	0.14
TYR	85	TYR	86	0.26
TYR	86	TYR	87	0.21
CYS	87	CYS	88	0.50
ALA	88	GLN	89	0.70
SER	89	GLN	90	0.84
TRP	90	TYR	91	1.73
SER	96	LEU	94	1.25
SER	96	PRO	95	1.54
TYR	97	TYR	96	1.00
VAL	98	THR	97	1.48
PHE	99	PHE	98	0.82
GLY	100	GLY	99	0.87
THR	101	GLN	100	0.99
GLY	102	GLY	101	0.76
THR	103	THR	102	0.54
LYS	104	LYS	103	0.58
VAL	105	LEU	104	0.63
THR	106	GLN	105	1.34
VAL	107	ILE	106	1.73
LEU	108	THR	107	2.45

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Witnessed & Understood by me, Date Invented by Date

Recorded by

From PDB files: 1fb4.test 2rhe.newrot
Maximum distance cutoff for CA-CA was 2.50
NUMRES molecules 1&2 112 114

1fb4 Res		2rhe Res		Dist
VAL	3	VAL	3	1.05
LEU	4	LEU	4	0.37
THR	5	THR	5	0.32
GLN	6	GLN	6	0.14
PRO	7	PRO	7	0.31
PRO	8	PRO	8	0.29
SER	9	SER	9	0.70
ALA	10	ALA	10	0.74
SER	11	SER	11	0.58
GLY	12	GLY	12	0.36
THR	13	THR	13	0.18
PRO	14	PRO	14	0.74
GLY	15	GLY	15	0.64
GLN	16	GLN	16	0.34
ARG	17	ARG	17	0.60
VAL	18	VAL	18	0.52
THR	19	THR	19	0.54
ILE	20	ILE	20	0.07
SER	21	SER	21	0.11
CYS	22	CYS	22	0.06
THR	23	THR	23	0.34
GLY	24	GLY	24	0.22
THR	25	SER	25	0.37
SER	26	ALA	26	0.60
SER	27	THR	27	0.63
ASN	27A	ASP	28	0.38
ILE	27B	ILE	29	0.29
GLY	28	GLY	30	0.40
SER	29	SER	31	0.59
ILE	30	ASN	32	0.50
THR	31	SER	33	0.76
VAL	32	VAL	34	0.28
ASN	33	ILE	35	0.29
TRP	34	TRP	36	0.10
TYR	35	TYR	37	0.49
GLN	36	GLN	38	0.68
GLN	37	GLN	39	1.29
LEU	38	VAL	40	2.15
GLY	40	PRO	41	1.91
MET	41	LYS	43	2.34
ALA	42	LYS	43	2.35
ALA	42	ALA	44	1.96
PRO	43	PRO	45	1.31
LYS	44	LYS	46	0.89
LEU	45	LEU	47	0.77
LEU	46	LEU	48	0.37
ILE	47	ILE	49	0.14
TYR	48	TYR	50	0.07
ARG	49	TYR	51	0.47
ASP	50	ASN	52	0.52
ALA	51	ASP	53	0.44
MET	52	LEU	54	0.46
ARG	53	LEU	55	0.64
PRO	54	PRO	56	0.79
SER	55	SER	57	1.05
GLY	56	GLY	58	0.69
VAL	57	VAL	59	0.50
PRO	58	SER	60	0.33
THR	59	ASP	61	0.29
ARG	60	ARG	62	0.40
PHE	61	PHE	63	0.37
SER	62	SER	64	0.24
GLY	63	ALA	65	0.66
SER	64	SER	66	0.34
LYS	65	LYS	67	0.16
SER	66	SER	68	0.36
GLY	67	GLY	69	0.19
THR	68	THR	70	0.19
SER	69	SER	71	0.25
ALA	70	ALA	72	0.14
SER	71	SER	73	0.33
LEU	72	LEU	74	0.26
ALA	73	ALA	75	0.21
ILE	74	ILE	76	0.24
SER	75	SER	77	0.51
GLY	76	GLY	78	1.01
LEU	77	LEU	79	0.65
GLU	78	GLU	80	0.46
ALA	79	SER	81	0.41
GLU	80	GLU	82	0.54
ASP	81	ASP	83	0.45
GLU	82	GLU	84	0.32
SER	83	ALA	85	0.25
ASP	84	ASP	86	0.23
TYR	85	TYR	87	0.27
TYR	86	TYR	88	0.28
CYS	87	CYS	89	0.33
ALA	88	ALA	90	0.36
SER	89	ALA	91	0.20
TRP	90	TRP	92	0.33
ASN	91	ASN	93	0.80
SER	92	ASP	94	1.37
ASP	94	SER	95	1.86
ASP	94	LEU	96	2.34
ASN	95	ASP	97	0.76
SER	96	GLU	98	1.74
TYR	97	PRO	99	0.50
VAL	98	GLY	100	0.56
PHE	99	PHE	101	0.98
GLY	100	GLY	102	0.77
THR	101	GLY	103	0.96
GLY	102	GLY	104	0.89
THR	103	THR	105	0.25
LYS	104	LYS	106	0.43
VAL	105	LEU	107	0.20
THR	106	THR	108	0.25
VAL	107	VAL	109	0.32
LEU	108	LEU	110	1.45
ILE	74	ILE	74	0.97
SER	75	THR	75	0.94
GLY	76	GLY	76	1.39
LEU	77	LEU	77	1.14
GLU	78	GLN	78	0.36
ALA	79	ALA	79	0.43
GLU	80	GLU	80	0.69
ASP	81	ASP	81	0.51
GLU	82	GLU	82	0.48
SER	83	ALA	83	0.25
ASP	84	ASP	84	0.39
TYR	85	TYR	85	0.18
TYR	86	TYR	86	0.18
CYS	87	CYS	87	0.30
ALA	88	GLN	88	0.27
SER	89	SER	89	0.64
TRP	90	TYR	90	0.95
ASN	91	ASP	91	0.59
SER	92	ARG	92	1.93
SER	96	LEU	94	0.94
TYR	97	ARG	95	0.28
VAL	98	VAL	98	0.71
PHE	99	PHE	99	0.87
GLY	100	GLY	100	0.25
THR	101	GLY	101	2.24
GLY	102	GLY	102	1.65
THR	103	THR	103	0.58
LYS	104	LYS	104	0.41
VAL	105	LEU	105	0.37
THR	106	THR	106	0.33
VAL	107	VAL	107	0.30
LEU	108	LEU	108	0.83
GLY	109	ARG	109	2.46
GLN	110	GLN	110	2.46

From PDB files: 1FB4.TEST 3FAB.TEST
Maximum distance cutoff for CA-CA was 2.50
NUMRES molecules 1&2 112 108

1FB4 Res		3FAB Res		Dist
SER	2	SER	2	1.75
VAL	3	SER	2	2.49
LEU	4	LEU	4	0.72
THR	5	THR	5	0.26
GLN	6	GLN	6	0.41
PRO	7	PRO	7	0.56
PRO	8	PRO	8	0.34
SER	9	SER	9	0.58
ALA	10	VAL	10	0.40
SER	11	SER	11	0.47
GLY	12	GLY	12	0.58
THR	13	ALA	13	0.87
PRO	14	PRO	14	1.08
GLY	15	GLY	15	1.12
GLN	16	GLN	16	1.13
ARG	17	ARG	17	0.88
VAL	18	VAL	18	0.71
THR	19	THR	19	0.79
ILE	20	ILE	20	0.39
SER	21	SER	21	0.47
CYS	22	CYS	22	0.20
THR	23	THR	23	0.63
GLY	24	GLY	24	0.50
THR	25	SER	25	0.59
SER	26	SER	26	0.54
SER	27	SER	27	1.49
ASN	27A	ASN	27A	0.98
ILE	27B	ILE	27B	0.61
GLY	28	GLY	27C	0.84
SER	29	ALA	28	1.67
ILE	30	ASN	30	0.59
THR	31	HIS	31	0.94
VAL	32	VAL	32	0.53
ASN	33	LYS	33	0.49
TRP	34	TRP	34	0.70
TYR	35	TYR	35	0.48
GLN	36	GLN	36	0.69
GLN	37	GLN	37	0.74
LEU	38	LEU	38	1.82
MET	41	THR	41	1.88
ALA	42	ALA	42	1.40
PRO	43	PRO	43	0.80
LYS	44	LYS	44	0.84
LEU	45	LEU	45	0.82
LEU	46	LEU	46	1.04
ARG	53	PHE	48	2.01
THR	59	ALA	52	1.41
ARG	60	ARG	53	0.20
PHE	61	PHE	61	0.17
SER	62	SER	62	0.18
GLY	63	VAL	63	0.60
SER	64	SER	64	0.83
LYS	65	LYS	65	0.73
SER	66	SER	66	0.93
GLY	67	GLY	67	0.78
THR	68	SER	68	0.59
SER	69	SER	69	0.47
ALA	70	ALA	70	0.22
SER	71	THR	71	0.35
LEU	72	LEU	72	0.57
ALA	73	ALA	73	0.36

Witnessed & Understood by me, Date

Invented by Date

Recorded by

From Page No. 4

From PDB files: 1fb4.test 2hfl.test
Maximum distance cutoff for CA-CA was 2.50
NUMRES molecules 1&2 112 110

1fb4 Res		2hfl Res		Dist
LEU	4	LEU	4	0.87
THR	5	THR	5	0.46
GLN	6	GLN	6	0.46
PRO	7	SER	7	2.09
PRO	7	PRO	8	2.02
PRO	8	ALA	9	0.51
SER	9	ILE	10	1.75
ALA	10	MET	11	2.16
SER	11	SER	12	1.79
GLY	12	ALA	13	1.27
THR	13	SER	14	0.96
PRO	14	PRO	15	0.69
GLY	15	GLY	16	0.38
GLN	16	GLU	17	0.99
ARG	17	LYS	18	0.39
VAL	18	VAL	19	0.50
THR	19	THR	20	0.65
ILE	20	MET	21	0.32
SER	21	THR	22	0.40
CYS	22	CYS	23	0.28
THR	23	SER	24	0.43
GLY	24	ALA	25	0.37
THR	25	SER	27	1.91
SER	26	SER	28	2.31
GLY	28	SER	28	1.89
THR	31	TYR	31	1.01
VAL	32	MET	32	0.39
ASN	33	TYR	33	0.39
TRP	34	TRP	34	0.40
TYR	35	TYR	35	0.58
GLN	36	GLN	36	0.43
GLN	37	GLN	37	0.43
LEU	38	LYS	38	1.71
ALA	42	SER	42	0.43
PRO	43	PRO	43	0.37
LYS	44	LYS	44	0.46
LEU	45	ARG	45	0.48
LEU	46	TRP	46	0.57
ILE	47	ILE	47	0.39
TYR	48	TYR	48	0.51
ARG	49	ASP	49	0.31
ASP	50	THR	50	0.30
ALA	51	SER	51	0.16
MET	52	LYS	52	0.28
ARG	53	LEU	53	1.24
PRO	54	ALA	54	2.15
GLY	56	GLY	56	1.19
VAL	57	VAL	57	1.04
PRO	58	PRO	58	0.81
THR	59	VAL	59	0.34
ARG	60	ARG	60	0.42
PHE	61	PHE	61	0.42
SER	62	SER	62	0.59
GLY	63	GLY	63	0.33
SER	64	SER	64	0.34
LYS	65	GLY	65	1.11
SER	66	SER	66	2.08
GLY	67	GLY	67	2.25
THR	68	THR	68	0.62
SER	69	SER	69	0.72
ALA	70	TYR	70	0.36
SER	71	SER	71	0.63
LEU	72	LEU	72	0.31
ALA	73	THR	73	0.42
ILE	74	ILE	74	0.59
SER	75	SER	75	0.89
GLY	76	SER	76	0.42
LEU	77	MET	77	0.44
GLU	78	GLU	78	0.47
ALA	79	THR	79	0.47
GLU	80	GLU	80	0.21
ASP	81	ASP	81	0.80
GLU	82	ALA	82	0.68
SER	83	ALA	83	0.39
ASP	84	GLU	84	0.27
TYR	85	TYR	85	0.20
TYR	86	TYR	86	0.42
CYS	87	CYS	87	0.67
ALA	88	GLN	88	0.56
SER	89	GLN	89	0.68
TRP	90	TRP	90	2.33
TRP	90	GLY	91	2.28
ASN	95	ARG	92	2.32
SER	96	ASN	93	0.38
TYR	97	PRO	94	0.40
VAL	98	THR	95	0.55
PHE	99	PHE	96	0.39
GLY	100	GLY	97	0.85
THR	101	GLY	98	0.91
GLY	102	GLY	99	0.70
THR	103	THR	100	0.41
LYS	104	LYS	101	0.41
VAL	105	LEU	102	0.48
THR	106	GLU	103	1.08
VAL	107	ILE	104	1.32
LEU	108	LYS	105	0.88
GLY	109	ARG	106	1.12

To Page No. 6

From PDB files: 1fbj.test 2mcp.test
Maximum distance cutoff for CA-CA was 2.50
NUMRES molecules 1&2 111 118

1fbj Res		2mcp Res		Dist
GLU	1	ASP	1	1.67
ILE	2	ILE	2	0.48
VAL	3	VAL	3	0.84
LEU	4	MET	4	1.32
THR	5	THR	5	0.61
GLN	6	GLN	6	0.31
SER	7	SER	7	0.50
PRO	8	PRO	8	0.28
ALA	9	SER	9	0.60
ILE	10	SER	10	0.81
THR	11	LEU	11	1.00
ALA	12	SER	12	1.10
ALA	13	VAL	13	1.35
SER	14	SER	14	1.71
LEU	15	ALA	15	1.62
GLY	16	GLY	16	1.13
GLN	17	GLU	17	1.05
LYS	18	ARG	18	1.15
VAL	19	VAL	19	0.52
THR	20	THR	20	0.45
ILE	21	MET	21	0.34
THR	22	SER	22	0.55
CYS	23	CYS	23	0.32
SER	24	LYS	24	0.42
ALA	25	SER	25	0.60
SER	26	SER	26	0.41
SER	27	GLN	27	1.57
SER	28	SER	28	1.94
VAL	29	LEU	29	0.75
SER	31	PHE	38	1.43
LEU	32	LEU	39	0.67
HIS	33	ALA	40	0.71
TRP	34	TRP	41	0.30
TYR	35	TYR	42	0.38
GLN	36	GLN	43	0.48
GLN	37	GLN	44	0.54
LYS	38	LYS	45	0.66
SER	39	PRO	46	2.07
GLY	40	GLY	47	0.52
THR	41	GLN	48	0.74
SER	42	PRO	49	0.36
PRO	43	PRO	50	0.76
LYS	44	LYS	51	0.77
PRO	45	LEU	52	0.73
TRP	46	LEU	53	0.67
ILE	47	ILE	54	0.62
TYR	48	TYR	55	0.89
GLU	49	GLY	56	1.57
ILE	50	ALA	57	0.96
SER	51	SER	58	0.80
LYS	52	THR	59	1.15
LEU	53	ARG	60	1.20
ALA	54	GLU	61	1.34
SER	55	SER	62	1.89
GLY	56	GLY	63	1.17
VAL	57	VAL	64	1.01
PRO	58	PRO	65	1.00
ALA	59	ASP	66	0.60
ARG	60	ARG	67	0.64
PHE	61	PHE	68	0.66
SER	62	THR	69	0.11
GLY	63	GLY	70	0.23
SER	64	SER	71	0.70
GLY	65	GLY	72	0.58
SER	66	SER	73	0.87
GLY	67	GLY	74	0.54
THR	68	THR	75	0.32
SER	69	ASP	76	0.66
TYR	70	PHE	77	0.15
SER	71	THR	78	0.15
LEU	72	LEU	79	0.22
THR	73	THR	80	0.36
ILE	74	ILE	81	0.76
ASN	75	SER	82	1.02
THR	76	SER	83	0.91
MET	77	VAL	84	1.36
GLU	78	GLN	85	1.38
ALA	79	ALA	86	1.83
GLU	80	GLU	87	1.38
ASP	81	ASP	88	0.70
ALA	82	LEU	89	1.87
ALA	83	ALA	90	0.62
ILE	84	VAL	91	0.26
TYR	85	TYR	92	0.39
TYR	86	TYR	93	0.34
CYS	87	CYS	94	0.22
GLN	88	GLN	95	0.40
GLN	89	ASN	96	1.12
TRP	90	ASP	97	1.75
TRP	90	HIS	98	2.05
THR	91	HIS	98	1.90
LEU	94	TYR	100	1.12
ILE	95	LEU	102	1.63
THR	96	THR	103	1.28
PHE	97	PHE	104	1.19
GLY	98	GLY	105	1.57
ALA	99	ALA	106	1.56
GLY	100	GLY	107	0.62
THR	101	THR	108	0.73
LYS	102	LYS	109	0.74
LEU	103	LEU	110	1.00
GLU	104	GLU	111	0.80
LEU	105	ILE	112	1.32
LYS	106	LYS	113	1.25
ARG	107	ARG	114	1.20

From PDB files: 1fbj.test 2hfl.test
Maximum distance cutoff for CA-CA was 2.50
NUMRES molecules 1&2 111 110

1fbj Res		2hfl Res		Dist
GLU	1	ASP	1	1.34
ILE	2	ILE	2	0.24
VAL	3	VAL	3	0.48
LEU	4	LEU	4	0.51
THR	5	THR	5	0.81
GLN	6	GLN	6	0.20
SER	7	SER	7	0.93
PRO	8	PRO	8	0.48
ALA	9	ALA	9	0.19
ILE	10	ILE	10	0.88
THR	11	MET	11	0.41
ALA	12	SER	12	0.48
ALA	13	ALA	13	0.65
SER	14	SER	14	0.74
LEU	15	PRO	15	1.17
GLY	16	GLY	16	0.52
GLN	17	GLU	17	0.93
LYS	18	LYS	18	0.55
VAL	19	VAL	19	0.23
THR	20	THR	20	0.25
ILE	21	MET	21	0.44
THR	22	THR	22	0.55
CYS	23	CYS	23	0.12
SER	24	SER	24	0.88
ALA	25	ALA	25	0.40
SER	26	SER	26	0.72
SER	27	SER	27	0.85
SER	28	SER	28	2.20
VAL	29	VAL	29	1.20
SER	31	TYR	31	2.06
LEU	32	MET	32	0.74
HIS	33	TYR	33	0.26
TRP	34	TRP	34	0.19
TYR	35	TYR	35	0.30
GLN	36	GLN	36	0.08
GLN	37	GLN	37	0.49
LYS	38	LYS	38	0.49
SER	39	SER	39	1.20
GLY	40	GLY	40	0.97
THR	41	THR	41	0.50
SER	42	SER	42	0.37
PRO	43	PRO	43	0.83
LYS	44	LYS	44	0.34
PRO	45	ARG	45	0.50
TRP	46	TRP	46	0.54
ILE	47	ILE	47	0.29
TYR	48	TYR	48	0.08
GLU	49	ASP	49	1.48
ILE	50	THR	50	1.18
SER	51	SER	51	0.33
LYS	52	LYS	52	0.50
LEU	53	LEU	53	0.71
ALA	54	ALA	54	0.78
SER	55	SER	55	0.84
GLY	56	GLY	56	1.23
VAL	57	VAL	57	0.18
PRO	58	PRO	58	0.19
ALA	59	VAL	59	0.74
ARG	60	ARG	60	0.51
PHE	61	PHE	61	0.14
SER	62	SER	62	0.27
GLY	63	GLY	63	0.64
SER	64	SER	64	0.26
GLY	65	GLY	65	0.27
SER	66	SER	66	0.36
GLY	67	GLY	67	0.69
THR	68	THR	68	0.34
SER	69	SER	69	0.40
TYR	70	TYR	70	0.07
SER	71	SER	71	0.43
LEU	72	LEU	72	0.37
THR	73	THR	73	0.05
ILE	74	ILE	74	0.20
ASN	75	SER	75	0.25
THR	76	SER	76	0.19
MET	77	MET	77	0.29
GLU	78	GLU	78	0.26
ALA	79	THR	79	0.52
GLU	80	GLU	80	0.47
ASP	81	ASP	81	0.48
ALA	82	ALA	82	0.78
ALA	83	ALA	83	0.34
ILE	84	GLU	84	0.33
TYR	85	TYR	85	0.15
TYR	86	TYR	86	0.52
CYS	87	CYS	87	0.15
GLN	88	GLN	88	0.28
GLN	89	GLN	89	0.19
TRP	90	TRP	90	1.00
THR	91	GLY	91	1.87
TYR	92	ARG	92	2.33
PRO	93	ARG	92	1.84
LEU	94	ASN	93	1.23
ILE	95	PRO	94	0.45
THR	96	THR	95	0.26
PHE	97	PHE	96	0.33
GLY	98	GLY	97	0.62
ALA	99	GLY	98	0.72
GLY	100	GLY	99	0.16
THR	101	THR	100	0.38
LYS	102	LYS	101	0.43
LEU	103	LEU	102	0.32
GLU	104	GLU	103	0.46
LEU	105	ILE	104	0.97
LYS	106	LYS	105	0.66
ARG	107	ARG	106	1.59

Witnessed & Understood by me, Date

Invented by Date

Recorded by

From Page No. 6

From PDB files: 1fbj.test 1rei.testa
Maximum distance cutoff for CA-CA was 2.50
NUMRES molecules 1&2 111 107

1fbj Res		1rei Res		Dist
GLU	1	ASP	1	2.29
ILE	2	ILE	2	0.44
VAL	3	GLN	3	0.64
LEU	4	MET	4	0.68
THR	5	THR	5	0.48
GLN	6	GLN	6	0.15
SER	7	SER	7	0.69
PRO	8	PRO	8	0.42
ALA	9	SER	9	0.76
ILE	10	SER	10	0.67
THR	11	LEU	11	0.87
ALA	12	SER	12	1.04
ALA	13	ALA	13	1.23
SER	14	SER	14	1.97
LEU	15	VAL	15	1.58
GLY	16	GLY	16	0.51
GLN	17	ASP	17	0.90
LYS	18	ARG	18	0.79
VAL	19	VAL	19	0.98
THR	20	THR	20	0.68
ILE	21	ILE	21	0.41
THR	22	THR	22	0.41
CYS	23	CYS	23	0.45
SER	24	GLN	24	0.66
ALA	25	ALA	25	0.41
SER	26	SER	26	0.43
SER	27	GLN	27	0.70
SER	28	ASP	28	2.20
VAL	29	ILE	29	0.84
SER	31	TYR	32	0.25
LEU	32	LEU	33	0.13
HIS	33	ASN	34	0.68
TRP	34	TRP	35	0.41
TYR	35	TYR	36	0.55
GLN	36	GLN	37	0.37
GLN	37	GLN	38	0.72
LYS	38	THR	39	0.63
SER	39	PRO	40	1.55
GLY	40	GLY	41	0.93
THR	41	LYS	42	0.86
SER	42	ALA	43	1.14
PRO	43	PRO	44	0.99
LYS	44	LYS	45	0.88
PRO	45	LEU	46	0.90
TRP	46	LEU	47	0.66
ILE	47	ILE	48	0.55
TYR	48	TYR	49	0.65
GLU	49	GLU	50	1.36
ILE	50	ALA	51	1.28
SER	51	SER	52	0.96
LYS	52	ASN	53	1.20
LEU	53	LEU	54	1.09
ALA	54	GLN	55	1.54
SER	55	ALA	56	1.37
GLY	56	GLY	57	1.12
VAL	57	VAL	58	1.16
PRO	58	PRO	59	1.11
ALA	59	SER	60	0.33
ARG	60	ARG	61	0.58
PHE	61	PHE	62	0.56
SER	62	SER	63	0.51
GLY	63	GLY	64	0.39
SER	64	SER	65	0.33
GLY	65	GLY	66	0.76
SER	66	SER	67	0.85
GLY	67	GLY	68	0.80
THR	68	THR	69	0.70
SER	69	ASP	70	0.24
TYR	70	TYR	71	0.22
SER	71	THR	72	0.61
LEU	72	PHE	73	0.20
THR	73	THR	74	0.18
ILE	74	ILE	75	0.68
ASN	75	SER	76	0.85
THR	76	SER	77	0.73
MET	77	LEU	78	1.52
GLU	78	LEU	78	2.47
GLU	78	GLN	79	1.61
GLU	80	GLU	81	1.84
ASP	81	ASP	82	0.64
ALA	82	ILE	83	1.82
ALA	83	ALA	84	0.83
ILE	84	THR	85	0.26
TYR	85	TYR	86	0.34
TYR	86	TYR	87	0.47
CYS	87	CYS	88	0.03
GLN	88	GLN	89	0.31
GLN	89	GLN	90	0.50
TRP	90	TYR	91	0.71
THR	91	GLN	92	1.37
THR	91	SER	93	2.46
LEU	94	LEU	94	0.69
ILE	95	TYR	96	1.39
THR	96	THR	97	1.28
PHE	97	PHE	98	1.24
GLY	98	GLY	99	1.39
ALA	99	GLN	100	1.13
GLY	100	GLY	101	0.83
THR	101	THR	102	0.86
LYS	102	LYS	103	0.77
LEU	103	LEU	104	1.29
GLU	104	GLN	105	1.19
LEU	105	ILE	106	1.68
LYS	106	THR	107	0.97

From PDB files: 1fbj.test 1rei.testb
Maximum distance cutoff for CA-CA was 2.50
NUMRES molecules 1&2 111 107

1fbj Res		1rei Res		Dist
GLU	1	ASP	1	2.35
ILE	2	ILE	2	0.49
VAL	3	GLN	3	0.51
LEU	4	MET	4	0.50
THR	5	THR	5	0.87
GLN	6	GLN	6	0.19
SER	7	SER	7	0.69
PRO	8	PRO	8	0.24
ALA	9	SER	9	0.58
ILE	10	SER	10	0.41
THR	11	LEU	11	0.39
ALA	12	SER	12	1.25
ALA	13	ALA	13	1.51
SER	14	SER	14	1.41
LEU	15	VAL	15	1.31
GLY	16	GLY	16	0.95
GLN	17	ASP	17	0.96
LYS	18	ARG	18	0.71
VAL	19	VAL	19	0.88
THR	20	THR	20	0.65
ILE	21	ILE	21	0.42
THR	22	THR	22	0.41
CYS	23	CYS	23	0.26
SER	24	GLN	24	0.56
ALA	25	ALA	25	0.36
SER	26	SER	26	0.32
SER	27	GLN	27	1.04
SER	28	ASP	28	2.36
VAL	29	ILE	29	0.73
SER	31	TYR	32	0.31
LEU	32	LEU	33	0.08
HIS	33	ASN	34	0.57
TRP	34	TRP	35	0.40
TYR	35	TYR	36	0.60
GLN	36	GLN	37	0.38
GLN	37	GLN	38	0.60
LYS	38	THR	39	0.76
SER	39	PRO	40	1.94
GLY	40	GLY	41	0.84
THR	41	LYS	42	0.93
SER	42	ALA	43	0.76
PRO	43	PRO	44	1.16
LYS	44	LYS	45	1.04
PRO	45	LEU	46	0.92
TRP	46	LEU	47	0.75
ILE	47	ILE	48	0.67
TYR	48	TYR	49	0.74
GLU	49	GLU	50	1.28
ILE	50	ALA	51	1.22
SER	51	SER	52	1.18
LYS	52	ASN	53	1.43
LYS	52	LEU	54	2.42
LEU	53	LEU	54	1.51
ALA	54	GLN	55	1.62
SER	55	ALA	56	1.41
GLY	56	GLY	57	1.37
VAL	57	VAL	58	1.12
PRO	58	PRO	59	0.97
ALA	59	SER	60	0.11
ARG	60	ARG	61	0.32
PHE	61	PHE	62	0.36
SER	62	SER	63	0.25
GLY	63	GLY	64	0.33
SER	64	SER	65	0.16
GLY	65	GLY	66	0.63
SER	66	SER	67	0.85
GLY	67	GLY	68	0.61
THR	68	THR	69	0.58
SER	69	ASP	70	0.41
TYR	70	TYR	71	0.23
SER	71	THR	72	0.32
LEU	72	PHE	73	0.16
THR	73	THR	74	0.18
ILE	74	ILE	75	0.71
ASN	75	SER	76	0.78
THR	76	SER	77	0.64
MET	77	LEU	78	1.43
GLU	78	LEU	78	2.48
GLU	78	GLN	79	1.57
ALA	79	PRO	80	2.14
GLU	80	PRO	80	2.44
GLU	80	GLU	81	1.79
ASP	81	ASP	82	0.76
ALA	82	ILE	83	1.68
ALA	83	ALA	84	0.54
ILE	84	THR	85	0.08
TYR	85	TYR	86	0.31
TYR	86	TYR	87	0.47
CYS	87	CYS	88	0.08
GLN	88	GLN	89	0.29
GLN	89	GLN	90	0.38
TRP	90	TYR	91	0.71
THR	91	GLN	92	1.31
LEU	94	LEU	94	0.61
ILE	95	TYR	96	1.47
THR	96	THR	97	1.35
PHE	97	PHE	98	1.20
GLY	98	GLY	99	1.32
ALA	99	GLN	100	1.01
GLY	100	GLY	101	0.67
THR	101	THR	102	0.65
LYS	102	LYS	103	0.52
LEU	103	LEU	104	0.96
GLU	104	GLN	105	1.00
LEU	105	ILE	106	1.62
LYS	106	THR	107	1.90

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Project No.______

Book No.______

TITLE Residues for average Coords

From Page No.__

```
*****************************************************************************
FB4L, 3FAB and RHE are lambda-type  REI, MCPL, FBJL AND 2HFL are kappa-type
*****************************************************************************
a) residues between parentheses are included in beta-sheet based on backbone
          dihedral angles and hydrogen-bonding patterns
b) letter repeats above sequences correspond to beta-sheet strands
c) L1, L2, L3 correspond to hypervariable loops
d) @ first residue is PCA - pyroglutamyl
e) small letter in sequence - Ca-Ca distance between proteins > 1.0 A
*****************************************************************************
              AAAAAAAAAAA   A'A'A'A'A'A'  BBBBBBBBBBBBBBBBB ----------L1----------
FB4L    E S V L T Q   P)P(S A S G T)P)G(Q R V T I S C T G)T)S S N I G
3FAB    @ s v L T Q   P P S V S G A p g q R V T I S C T G S S s N I G a
RHE     e s v L T Q   P)P(S A S G T)P)G(Q(R V T I S C T G)S)A T D I G
REI     d(i(q M T Q s p)S(s l s a s)v)G(d R V T I T C Q A)s q d i i
MCPL   (d i(v M T Q s p)S(s l s v)s a g(e(R V T M S C k S)s q s l l n s g n q
FBJL   (e i(v l T Q s p)A(i t a A S)L)G(Q K V T I T C S A)s s s v
2HFL    d i v L T Q s p A i m s a S P G E K V T M T C S A s s s v
        1            10                 20    23      27 a b  29
*****************************************************************************
      -L1--CCCCCCCCCCCCCCCC   C'C'C'C'C'C'C'C'--L2--C"C"C"C"
FB4L   S(I T(V N W Y Q Q L)P)G(M A(P K L)L(I Y)R D A(M R)P S)G V P
3FAB   g N H V K W Y Q Q l p g t a P K L l i f h n n
RHE    S(N S(V I W Y Q q)v p)g(k a(p K L)L(I Y)Y N D(L L)P S)G V S
REI       k(y L N W Y Q Q t)p)g(k A P(K L)L(I Y)E A S(N L q)a)G V P
MCPL  (k n(f l A W Y Q Q k)p)g(q P(P K L L I Y)G A S(T r e)s)g V P
FBJL      S(s L H W Y Q Q k)s)g(t s(P K P)W(I)Y)e i(S(K l a)s g v P
2HFL      n Y M Y W Y Q Q k s g t S P K R W I Y D T S K l a s g V P
      30       35       40                 50                 59
*****************************************************************************
            DDDDDDDDDDD      EEEEEEEEEEEEE          FFFFFFFFFFFFFFF
FB4L    T R(F S G S K S)G T(S A S L A I S)G L E A E D(E(S D Y Y C A S
3FAB    a R F S V S K S G S S A T L A I T g l Q A E D E A D Y Y C Q S
RHE     D R(F S A S K S)G T(S A S L A I S)G L E S E D(E A D Y Y C A A
REI     S R(F S G S)G s g T(D Y T F T I)S S L q p e d(i(A T Y Y C Q Q)
MCPL    D R(F T G S)g s g t(D F T L T I)S S V Q A E D(l(A V Y Y C Q n)
FBJL    A R(F S G S)G s)g T(S Y S L T I)N T M E A E d(a A I Y Y C Q Q
2HFL    V R F S G S g s g T S Y S L T I S S M E T E D A A E Y Y C Q Q
        60                70                80                  90
*****************************************************************************
        -----L3-----GGGGGGGGG        HHHHHHHHHHH      -J1- LIGHT CONSTANT->
FB4L    W N)S S D N(S Y V F G)T G(T K V T V L)      G Q(P(K A N P T V T
3FAB    Y D       r s L R V F G g g T K L T V L      r q
RHE     W N)d s l D(e P G F G)G G(T K L T V l)      g
REI     y q     (s l p Y(t F G)q g(T K L q i t)
MCPL    d)h     (s y p l(t F g)a G(T K L E i k)      r
FBJL    w t y)      p(l I T F G)a G(T K L E L K)      r
2HFL    w         g r N P T F G G G T K L e i K      r
        91              97     100                      110
*****************************************************************************
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☐ residues included in average Coordinates

allonfbf.avgcrd or KAPLAM.avgcrd

To Page No._____

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

Recorded by

From Page No.

```
*************************************************************************
FB4L, 3FAB and RHE are lambda-type
*************************************************************************
a) residues between parentheses are included in beta-sheet based on backbone
        dihedral angles and hydrogen-bonding patterns
b) letter repeats above sequences correspond to beta-sheet strands
c) L1, L2, L3 correspond to hypervariable loops
d) @ first residue is PCA = pyroglutamyl
e) small letter in sequence = Ca-Ca distance between proteins > 1.0 A
*************************************************************************
          AAAAAAAAA   A'A'A'A'A'A'   BBBBBBBBBBBBBBBBB ---------L1--
FB4L    E S V(L T Q)P)P(S A S G T)P)G(Q R V T I S C T G)T)S S N I G
3FAB    @ s v L T Q P P S V S G A p g q R V T I S C T G S S s N I G a
RHE     e s v(L T Q)P)P(S A S G T)P)G(Q(R V T I S C T G)S)A T D I G
        1                  10                  20    23      27 a b  29
*************************************************************************
   -L1--CCCCCCCCCCCCCCCC C'C'C'C'C'C'C'C'C' --L2--C"C"C"C"
FB4L  S(I T(V N W Y Q Q L)P)G(M A(P K L)L(I Y)R D A(M R)P S)G V P
3FAB  g N H V K W Y Q Q l p g t a P K L l i f h n n
RHE   S(N S(V I W Y Q q v p)g(k a(p K L)L(I Y)Y N D(L L)P S)G V S
      30        35        40                  50                59
*************************************************************************
        DDDDDDDDDD     EEEEEEEEEEEE          FFFFFFFFFFFFFF
FB4L   T R(F S G S K S)G T(S A S L A I S)G L E A E D(E(S D Y Y C A S
3FAB   a R F S V S K S G S S A T L A I T g l Q A E D E A D Y Y C Q S
RHE    D R(F S A S K S)G T(S A S L A I S)G L E S E D(E A D Y Y C A A
       60                70                  80                90
*************************************************************************
     -----L3-----GGGGGGGGG     HHHHHHHHHHH    -J1- LIGHT CONSTANT->
FB4L   W N)S S D N(S Y V F G)T G(T K V T V L)   G Q(P(K A N P T V T
3FAB   Y D    r s L R V F G g g T K L T V L     r q
RHE    W N)d s l D(e P G F G)G G(T K L T V l)   g
       91              97    100                 110
*************************************************************************
```

☐ residues included in average coordinates

LAMBDA.Avgcrd

```
*************************************************************************
REI, MCPL, FBJL AND 2HFL are kappa-type
*************************************************************************
a) residues between parentheses are included in beta-sheet based on backbone
        dihedral angles and hydrogen-bonding patterns
b) letter repeats above sequences correspond to beta-sheet strands
c) L1, L2, L3 correspond to hypervariable loops
d) small letter in sequence = Ca-Ca distance between proteins > 1.0 A
*************************************************************************
          AAAAAAAAAA   A'A'A'A'A'A'   BBBBBBBBBBBBBBBBB ---------L1--------
FBJL  (E I(V L T Q S P)A(I T A A S)L G(Q K V T I T C S A)S S S V
REI     d(I(Q M T Q S P)S(S L s a s)v G(D R V T I T C Q A)S Q d I i
MCPL  (d I(V m T Q S P)S(S L s v)s a g(e(r V T M S C K S)S q s l l n s g n q
2HFL    d I V L T Q S P A I M S A S p G E K V T M T C S A S S s v
        1                  10                  20    23      27 a b c d e f  29
*************************************************************************
      L1--CCCCCCCCCCCCCCCC   C'C'C'C'C'C'C'C'--L2--C"C"C"C"
FBJL    S(S L H W Y Q Q K)S G(T S(P K P)W(I)Y)E I(S(K L A)S G V P
REI     k(Y L N W Y Q Q T)p G(K A P(K L)L(I Y)e a S(n l q)a)g v p
MCPL (k n(f L A W Y Q Q K)p G(Q P(P K L L I Y)g A S(t r e)s)g v P
2HFL    n y M Y W Y Q Q K s G T S P K R W I Y d t S K L A S g V P
     30        35        40                  50
*************************************************************************
        DDDDDDDDDD     EEEEEEEEEEE          FFFFFFFFFFFFFF
FBJL   A R(F S G S)G S)G T(S Y S L T I)N T M E A E D(A A I Y Y C Q Q
REI    S R(F S G S)G S G T(D Y T F T I)S S l q p e D(i(A T Y Y C Q Q)
MCPL   D R(F T G S)G S G T(D F T L T I)S S v q a e D(l(A V Y Y C Q n)
2HFL   V R F S G S G S G T S Y S L T I S S M E T E D A A E Y Y C Q Q
       60                70                  80                90
*************************************************************************
     -----L3-----GGGGGGGGG     HHHHHHHHHHH    -J1- LIGHT CONSTANT->
FBJL   W T Y)     P(l I T F G)A G(T K L E L K)    R
REI    Y q     (s l p y(t f g)q G(T K l q i T)
MCPL   d h     (s y p l(t f g)a G(T K L E i k)    r
2HFL   W       g r n P T F G G G T K L E I K      r
       91              97    100                 110
*************************************************************************
```

☐ residues included in average coordinates

KAPPA.Avgcrd

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

Recorded by

From Page No. 9

AVB 3D #1/20

Bond Lengths & Angles for KAPPA variable light

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-
1.459	1.515	1.208	1.288	1.508	123.5	110.0	120.5	116.6	123.1	110.3	111.4
0.012	0.012	0.062	0.049	0.026	4.2	4.0	1.9	4.0	4.1	2.1	2.4
72	72	72	65	66	65	72	72	65	65	66	66

Bond Lengths & Angles for LAMBDA variable light

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-
1.453	1.514	1.217	1.298	1.522	124.4	111.4	120.1	117.0	122.7	110.4	109.9
0.017	0.018	0.063	0.061	0.031	6.0	2.4	1.9	4.8	4.9	2.7	2.4
97	97	97	92	87	92	97	97	92	92	87	87

Bond Lengths & Angles for KAPPA & LAMBDA variable light

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-
1.452	1.510	1.190	1.288	1.510	124.3	110.7	120.6	117.5	121.9	110.4	110.8
0.014	0.016	0.129	0.081	0.029	6.7	3.1	2.5	7.6	9.6	2.1	2.2
62	62	62	52	60	52	62	62	52	52	60	60

Average germ for average coordinate files

To Page No._____

```
**************************************************************************
FB4L, 3FAB and RHE are lambda-type  REI, MCPL, FBJL AND 2HFL are kappa-type
hll = human lambda light
hkl = human kappa light
**************************************************************************
a) residues between parentheses are included in beta-sheet based on backbone
          dihedral angles and hydrogen-bonding patterns
b) letter repeats above sequences correspond to beta-sheet strands
c) L1, L2, L3 correspond to hypervariable loops
d) @ first residue is PCA = pyroglutamyl
e) small letter in sequence = Ca-Ca distance between proteins > 1.0 A
**************************************************************************
          AAAAAAAAAAA   A'A'A'A'A'A'  BBBBBBBBBBBBBBBBB ---------L1----------
FB4L   E S V(L T Q)  P)P(S A S G T)P)G(Q R V T I S C T G)T)S S N     I G
3FAB   @ s v L T Q   P P S V S G A p g q R V T I S C T G S S s N     I G a
RHE    e s v(L T Q)  P)P(S A S G T)P)G(Q(R V T I S C T G)S)A T D     I G
REI    d(i(q M T Q s p)S(s l s a s)v)G(d R V T I T C Q A)s q d i     i
MCPL  (d i(v M T Q s p)S(s l s v)s a g(e(R V T M S C k S)s q s l l n s g n q
FBJL  (e i(v l T Q s p)A(i t a A S)L)G(Q K V T I T C S A)s s s v
2HFL   d i v L T Q s p A i m s a S P G E K V T M T C S A s s s v
       1              10                  20    23      27 a b      29
con    D I V M T Q S P S S L S V S P G E R V T I S C R A S Q S LLSSV D G
hllI   @ S V L T Q - P P S A S G T P G Q R V T I S C S G S S S NI    I G
hllII  @ S A L T Q - P A S V S G S P G Q S I T I S C T G T S S D V   G G
hllIII S Y E L T Q - P P S V S V S P G Q T A R I T C S G D A         L G
hllVI  N F M L T Q - P H S V S E S P G K T V T I S C T x S x G S D S I A
hklI   D I Q M T Q S P S S L S A S V G D R V T I T C R A S Q S V xxS D I
                                                                   S
hklII  D I V M T Q S P L S L P V T P G E P A S I S C R S S Q SLLHS x D G
hklIII E I V L T Q S P G T L S L S P G E R A T L S C R A S Q S       V S
hklIV  D I V M T Q S P D S L A V S L G E R A T I N C K S S Q SVLYS S N N
**************************************************************************
      -L1--CCCCCCCCCCCCCCCC   C'C'C'C'C'C'C'C'C'--L2--C"C"C"C"C"
FB4L  S(I T(V N W Y Q Q L)P)G(M A(P K L)L(I Y)R D A(M R)P S)G V P
3FAB  g N H V K W Y Q Q l p g t a P K L l i f h n n
RHE   S(N S(V I W Y Q q)v p)g(k a(p K L)L(I Y)Y N D(L L)P S)G V S
REI     k(y L N W Y Q Q t)p)g(k A P(K L)L(I Y)E A S(N L q)a)G V P
MCPL (k n(f l A W Y Q Q k)p)g(q P(P K L L I Y)G A S(T r e)s)g V P
FBJL    S(s L H W Y Q Q k)s)g(t s(P K P)W(I)Y)e i(S(K l a)s g v P
2HFL    n Y M Y W Y Q Q k s g t S P K R W I Y D T S K l a s g V P
    30         35         40                  50                  59
con   S N Y L A W Y Q Q K P G Q S P K L L I Y G A S N L A S G V P
      S
hllI  S N Y V x W Y Q Q L P G T A P K L L I Y S N N Q R P S G V P
hllII Y N Y V S W Y Q Q H P G K A P K L x I Y D V S x R P S G V x
hllIII EK Y V Y W Y Q Q K P G Q A P V L V I Y E D S K R P S G I P
hllVI S x Y V Q W Y Q Q R P G S A P T T V I Y E D N Q R P S G V P
hklI  S S Y L N W Y Q Q K P G K A P K L L I Y x A S S L E S G V P
                A
hklII N N Y L N W Y L Q K P G Q S P Q L L I Y L G S N R A S G V P
      D
hklIII SS Y L A W Y Q Q K P G Q A P R L L I Y G A S S R A T G I P
hklIV K N Y L A W Y Q Q K P G Q P P K L L I Y W A S T R E S G V P
**************************************************************************
```


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

Recorded by

Project No._____
Book No._____ TITLE Sequence Alignments

From Page No. 11

```
                DDDDDDDDDDD     EEEEEEEEEEEEE                FFFFFFFFFFFFFFFF
FB4L   T R(F S G S K S)G T(S A S L A I S)G L E A E D(E(S D Y Y C A S
3FAB   a R F S V S K S G S S A T L A I T g l Q A E D E A D Y Y C Q S
RHE    D R(F S A S K S)G T(S A S L A I S)G L E S E D(E A D Y Y C A A
REI    S R(F S G S)G s g T(D Y T F T I)S S L q p e d(i(A T Y Y C Q Q)
MCPL   D R(F T G S)g s g t(D F T L T I)S S V Q A E D(l(A V Y Y C Q n)
FBJL   A R(F S G S)G s)g T(S Y S L T I)N T M E A E d(a A I Y Y C Q Q
2HFL   V R F S G S g s g T S Y S L T I S S M E T E D A A E Y Y C Q Q
      60                  70                  80                  90
con    A R F S G S G S G T D F T L T I S S V E A E D A A T Y Y C Q Q
hllI   D R F S G S K S G T S A S L A I S G L Q S E D E A D Y Y C A T
hllII  D R F S G S K S G N T A S L T I S G L Q A E D E A D Y Y C S S

hllIII E R F S G S N S G T T A T L T I S G V Q A x D E A D Y Y C Q A
hllVI  D R F S G S S S N S A S L T I S G L K T E D E Q D Y Y C Q S Y
hklI   S R F S G S G S G T D F T L T I S S L Q P E D F A T Y Y C Q Q
hklII  D R F S G S G S G T D F T L K I S R V E A E D V G V Y Y C M Q
hklIII D R F S G S G S G T D F T L T I S R L E P E D F A V Y Y C Q Q
hklIV  D R F S G S G S G T D F T L T I S S L Q A E D V A V Y Y C Q Q
*******************************************************************************
      -----L3-----GGGGGGGGG      HHHHHHHHHHH    -J1- LIGHT CONSTANT->
FB4L   W N)S S D N(S Y V F G)T G(T K V T V L)     G Q(P(K A N P T V T
3FAB   Y D     r s L R V F G g g T K L T V L     r q
RHE    W N)d s l D(e P G F G)G G(T K L T V l)     g
REI    y q    (s l p Y(t F G)q g(T K L q i t)
MCPL   d)h    (s y p l(t F g)a G(T K L E i k)     r
FBJL   w t y)    p(l I T F G)a G(T K L E L K)     r
2HFL   w       g r N P T F G G G T K L e i K      r
      91                97    100                      110
con    W N S N PSGDS W T F G G G T K L E I L      K R P
           S
hllI   W D D S L D G P V F G G G T K x T V L      G Q P
hllII  Y A G S x x x V V F G G G T K L T V L      G Q P
hllIII W D S x T x x V V F G G G T K L T V L      G Q P
hllVI  D S N N x     W V F G G G T K L T V L      G Q P
hklI   Y N S L PxxYD Y T F G Q G T K V E I K      R T
hklII  A L Q x P     Y T F G Q G T K x E I K      R T
hklIII Y G S S P P   Y T F G Q G T K V E I K      R T
hklIV  Y Y S T P     x T F G Q G T K x E I K      R T
*******************************************************************************
```

hllI = human lambda light subgroup I

hkI = human kappa light subgroup I

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Loop 12-15 Superimpose NCaC on KAPPA.aogrd using res 10, 11, 16, 17

	RMC NCaC	
2HFL	0.307	use HFL
1FBJ	0.282	
2MCP	0.283	
1REI(A)	0.201	

Loop 39 res 37, 38, 40, 41 NCaC

	RMS		
2HFL	0.373		
1FBJ	0.209		
2MCP	0.151	(44, 45, 47, 48)	use MCP
1REI(A)	0.171	(38, 39, 41, 42)	

Loop 77-80 res 75, 76, 81, 82 NCaC

	RMS		
1FBJ	0.168	(75, 76, 81, 82)	
2MCP	0.386	(82, 83, 88, 89)	
2HFL	0.334	(75, 76, 81, 82)	
1REI(A)	0.359	(A76, A77, A82, A83)	use REI(A)
1F19	0.486	(76, 77, 82, 83)	

Res 105-110

use REI

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Project No._____
Book No._____ TITLE Building Kappa I

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CDR1 res 25-33 Kabat 24-34 Chothia/Lesk 26-32

res 23, 24, 35, 36 NCaC

	RMS	#AA
1F19	0.317	11
2HFM	0.169	11
1REI(A)	0.123	11
2HFL		10
1FBJ		10

use REI(A)

68/72 Kabat segs. have CDR1 = 11 res for subgroup I human

file: kappa.pdbcdr1

CDR2 res 49-57 Kabat 50-56 Chothia/Lesk 50-52

res 48, 49, 58, 60 NCaC

	RMS	
1FBJ	0.170	47, 48, 58, 59
2HFL	0.209	
1REI(A)	0.238	(A48, A49, A59, A60)
1F19	0.343	(48, 49, 59, 60)
2MCP	0.187	(54, 55, 65, 66)

use HFL

All Kabat segs. human light CDR2 = 7 res

file: kappa.pdbcdr12

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CDR3 res 91-98 Kabat 89-97 Chothia/Lesk 91-96

res ~~89 90, 99, 100~~ 90, 91, 101, 102 NCxC

	RMS		
1F19	0.294	(90, 91, 101, 102)	
1FBJ	0.225	(89, 90, 100, 101)	
2MCP	0.501	(96, 97, 107, 108)	0.242 (96, 107, 108)
3HFM	0.285	(90, 91, 101, 102)	
1REI(A)	0.154	(A90, A91, A101, A102)	use REI(A)
2HFL	0.239	(89, 90, 99, 100)	

file: kappa.pdbcdr123

Human Subgroup	#res in CDR3 (Kabat) 89-97	
I	9	30/32
II	9	7/7
III	9	18/20
IV	9	2/3

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Invented by

Recorded by Leonard Presta

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Project No._____
Book No._____ TITLE Orienting V_L-V_H

From Page No.__

Consensus kappa and V_H

Oriented V_L-V_H domains on those of 1FB4

	1FB4	1FBJ	2HFL	2MCP	3FAB	3HFM	1F19
VH	18-25	SAME	SAME	18-25	18-25	18-25	SAME
	34-39			34-39	34-39	34-39	
	46-52			46-52	46-52	46-52	
	57-61			59-63	56-60	56-60	
	68-71	FB4	FB4	70-73	67-70	67-70	FB4
	78-84			80-86	77-83	77-83	
	92-99			94-101	91-98	91-98	
VL	18-24	19-25	SAME	19-25	18-24	19-25	SAME
	32-37	32-37		39-44	32-37	33-38	
	60-66	60-66		67-73	53-66	61-67	
	69-74	69-74	FBJ	76-81	69-74	70-75	HFM
	84-88	84-88		91-95	84-88	85-89	
RMS Cα		0.729	1.01	0.834	0.944	0.868	1.180

3HFM on 1FB4 VH 135 atoms
Rms 0.72 Å

VL-VH 228 atoms
Rms 0.853

Hfm on Hfl VL-VH 0.87 93
VL 0.47
VH 0.94

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res #s ( ) long distance or poor geom

Kabat #s		FB4	HFL	FBJ	MCP	HFM	FI9	REI	RHE	FAB
Q6 NE2	081 T102	6,103	—	(6,101)	(6,108)	—	—	6,86	6,105	6,103
Q6 NE2	O Y86	6,85	(6,85)	6,85	6,92	6,86	—	6,86	6,87	6,85
R61 Nz	OGx D82	60,81	60,81	60,81	67,88	61,82	61,82	61,82	62,83	—
R61 Nz	OEx E81	60,80	60,80	60,80	67,87	—	—	—	—	—
C88 N	OE1 Q6	87,6	87,6	(87,6)	94,6	—	—	(88,6)	(89,6)	(87,6)
G101 N	OE1 Q6	(102,6)	99,6	100,6	(107,6)	101,6	—	—	(104,6)	—
T102 081	O P8	—	100,8	101,8	108,8	102,8	102,8	102,8	105,7	103,7
S70 8	081 T22		(7,22)		7,22					
T14 081	OE1 Q17	13,16			(14,17)			14,17	13,16	
T20 081	O V19		(20,19)	20,19	20,19			(20,19)		
Y36 OH	OS1 N34	35,33								
Y36 OH	OE1 Q89		35,88			36,89	36,89			
Q38 NE2	O Q42				44,48	38,42			39,43	
K39 Nz	O E81			38,80	45,87	39,81				
R54 NE	O F82	(53,61)			60,68					
E79 N	S8 m78		(78,77)	78,77						
E81 N	081 T80		(80,79)			(81,80)				
@ Y86 Oh	OE1 Q37		85,36	85,36	92,43		86,37			
Y86 Oh	O D82					86,82	(86,82)	86,82	87,83	85,81
* Q37 NE2	Oh Y86	36,85						(39,86)	38,87	36,85
Q89 NE2	Oh Y36			(88,35)	95,42			89,36		89,35
T97 081	OE1 Q90			96,89	103,96	97,90	97,90			
T97 081	O I2				103,2	97,2		97,2		
Q90 NE2	081 T97							90,97		

* kappa only

@ λ only

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<sequence of HuLys, unpublished, Foote and Winter>
DIQMTQSPSSLSASVGDRVTITCRASGNIHNYLAWYQQKPGKAPKLLIYYTTTLADGVPS
RFSGSGSGTDFTFTISSLQPEDIATYYCQHFWSTPRTFGQGTKVEIKR

```
<Fri Feb 16 08:54:28 1990
<first sequence: /va/Biocat/presta/igg/pl.HuLys (length = 108)
<second sequence: /va/Biocat/presta/igg/pl.humki (length = 109)

<90 matches in an overlap of 108: 83.33 percent similarity
<gaps in first sequence: 0, gaps in second sequence: 0
<score: 455 (Dayhoff PAM 250 matrix, gap penalty = 8 + 4 per residue)
<endgaps not penalized

                10        20        30        40        50
HuLys   DIQMTQSPSSLSASVGDRVTITCRASGNIHNYLAWYQQKPGKAPKLLIYY
        ************************** .* .** ***************
humki   DIQMTQSPSSLSASVGDRVTITCRASQDISSYLNWYQQKPGKAPKLLIYA
                10        20        30        40        50

                60        70        80        90       100
HuLys   TTTLADGVPSRFSGSGSGTDFTFTISSLQPEDIATYYCQHFWSTPRTFGQ
        ...*  ****************.*********.******.. * * ****
humki   ASSLESGVPSRFSGSGSGTDFTLTISSLQPEDFATYYCQQYNSLPYTFGQ
                60        70        80        90       100


HuLys   GTKVEIKR
        ********
humki   GTKVEIKRT

50 iterations:
    12    17    27    21    23    13    12    12    21    18
    16    20    12     8    11    16    12    16    14     7
    21     6    31    26    11    19    19    17    26    16
    17    23    24    36    13    32    12    20    18     8
    16    25    14    18    14     9    26    12    18    25
mean = 17.60, std dev = 6.69, z-score = 65.40
```

Residues in KappahumI altered for HuLys

CDR1
- Q27 G
- D28 N — Asn conf 4 −158,3 (1REI)
- S30 H — His conf −69,69
- S31 N
- N34 A

CDR2
- A50 Y — Tyr conf −167, −86 (1F19)
- A51 T — Thr conf −57
- S52 T — " " −169
- S53 T — " " −61

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E55A
S56D — altered conf K45 to hbond to D56
L73F
F83I — Ile conf -55, -174 (1REI)
Q90H
CDR3 Y91F
N92W
L94T
Y96R

Files: HULYS.PDBH1S90 backbone = KappahumI H90
HULYS.PDBGLN90 " " Q90
HULYS.PDBMCPCDR3 CDR3 backbone taken from 2MCP where res 90 is Asn

For purposes of creating a framework human kappa I Vk for general use as a construct for inserting new CDRs, the following HULYS residues should be altered:

D27Q Glx in human kappa subgroups I-IV
F73L Leu " " " "
I83F Phe in human kappa subgroups I & III
Val " " " " II & IV
H90Q Glx in " " " I-IV

A55E
D56S } may not be necessary

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Project No._____
Book No._____ TITLE Building 4D5 VL (kappa)

From Page No.__

Kappahum I. PDB converted to 4D5 VL (kappa)

Residues Changed

	Q	3	V
	P	8	H
	S	9	K
	S	10	F
	L	11	M
	A	13	T
	T	20	S
	R	24	K
	I	29	V
CDR1	S	30	N
	S	31	T
	Y	32	A
	L	33	V
	K	42	H
	A	43	S
	A	50	S
	S	53	F
	L	54	R
	E	55	Y
CDR2	S	56	T
	S	60	D
	S	63	T
	S	65	N
	D	66	R
	L	73	F
	L	78	V
	P	80	A
	F	83	L
	T	85	V
	Y	91	H
	N	92	Y

CDR3	S	93 T
	L	94 T
	Y	96 P
	Q	100 D

HER2.KAP1 R54-P59 from 2MCP (kappa)
R66-F71 from 2FB4 (λ)

HER2.KAP2 R54-P59 from 2MCP (kappa)
R66-F71 from 2FB4 (λ)
CDR1 moved to accomodate R66

HER2.KAP3 • KAP2 + new conf for residues Y49, F53, Y55

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Witnessed & Understood by me, | Date | Invented by | Date 2-19-90
Recorded by Leonard Presta

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In kappa structures 1REI, 2MCP, 1FBJ, 2HFL & 3HFM the peptide bond between S7-P8 is cis. In 1F19 and 4D5 res 8 is T or H (not P). Therefore the backbone of 1F19 from residues 7-19 was taken from 1F19.

Formation of VL-VH dimer

VL file	VH file	filename	Comments
Ner2lv.KAP2	HER2HV.MCP	Dimer.kap2mcp	
HER2lv.KAP2	HER2HV.MCP	Dimer.kap2mcpnew	bbone 7-10 altered
"	"	Dimer.kap2mcpnew2	bbone 7-10 altered & His 91 @ -60°
HER2lv.KAP3	HER2HV.MCP	Dimer.kap3mcp	
HER2lv.KAP2	HER2HV.PRC2	Dimer.kap2prc	
HER2lv.KAP2	HER2HV.model	Dimer.kap2mod	
HER2lv.KAP3	HER2HV.model	Dimer.kap3mod	

⊛ Protonation states of His residues

VL His 8 ⊕ VH His 35 NEH
His 42 ⊕
His 91 NEH

To Page No.

Dennis and Paul,
here are the human consensus sequences and the proposed humanized 4D5 sequences.

```
##########################################################################
VARIABLE LIGHT
HuLys has 83% similarity to human kappa subgroup I even when the
CDR sequences are included. The sequences inside the CDR boxes
(Chothia/Lesk definition) can be taken from HuLys or humkapI --
those outside the boxes should be taken from humkapI.

(Kabat/Wu CDR in capital letters; Chothia/Lesk CDR in boxes)

                1                                   10
humkapI  asp ile gln met thr gln ser pro ser ser leu ser ala ser val gly
HuLys

                        20                                  30
humkapI  asp arg val thr ile thr cys ARG ALA|SER GLN ASP ILE SER SER TYR|
HuLys                                       |    GLY ASN     HIS ASN  |
                                            ------------------------------

                                        40
humkapI  LEU ASN trp tyr gln gln lys pro gly lys ala pro lys leu leu ile
HuLys        ALA

                  |50                                          60
humkapI  tyr      |ALA ALA SER|SER LEU GLU SER gly val pro ser arg phe ser gly
HuLys             |TYR THR THR|THR     ALA ASP
                  -------------

                                70                                      80
humkapI  ser gly ser gly thr asp phe thr leu thr ile ser ser leu gln pro
HuLys                           phe

                                                   90
humkapI  glu asp phe ala thr tyr tyr cys GLN GLN|TYR ASN SER LEU PRO TYR|
HuLys            ile                           HIS|PHE TRP     THR     ARG|
                                                 ------------------------

                        100
humkapI  THR phe gly gln gly thr lys val glu ile lys arg thr
HuLys
##########################################################################
VARIABLE HEAVY
The sequences inside the CDR boxes (Chothia/Lesk definition) can be taken
from KOL or humIII -- those outside the boxes should be taken from humIII.

(Kabat/Wu CDR in capital letters; Chothia/Lesk CDR between bars)

                1                                   10
humiii   glu val gln leu val glu ser gly gly gly leu val gln pro gly gly
kol                          gln                 val                 arg

                        20                                  30
humiii   ser leu arg leu ser cys ala ala ser|GLY PHE THR PHE SER ASP TYR
kol                                 ser ser |     ILE     SER
                                            ------------------------------
         ----------
                                        40
humiii   ALA MET|SER trp val arg gln ala pro gly lys gly leu glu trp val
kol             |TYR
         --------

              50      52|52a  53                                  60
humiii   ala VAL ILE SER|GLU ASN GLY SER|ASP THR TYR TYR ALA ASP SER VAL
kol           ILE     TRP|ASP ASP       |    GLN HIS
                         ---------------
```

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```
                                                    70
humiii   LYS GLY arg phe thr ile ser arg asp asp ser lys asn thr leu tyr
kol                                                 asn                 phe

          80      82 82a 82b 82c  83                                  90
humiii   leu gln met asn ser leu arg ala glu asp thr ala val tyr tyr cys
kol               asp             pro             gly         phe

                                                  100  a   b   c   d   e   f   g   h
humiii   ala arg ASP ARG GLY GLY ALA VAL SER TYR GLY PHE PHE GLY TYR GLY
kol               GLY     HIS GLY PHE CYS SER SER ALA SER CYS PHE GLY

          i   j   k  101                                          110
humiii   GLY PHE PHE ASP VAL trp gly gln gly thr leu val thr val ser ser
kol      PRO --- ---     TYR                 pro

################################################################################
The following are proposed humanized 4D5 sequences; changes in Hum4D5b
and Hum4D5c from Hum4D5a are followed by an asterisk

           1                                        10
humkapI  asp ile gln met thr gln ser pro ser ser leu ser ala ser val gly
Hum4D5a
Hum4D5b
Hum4D5c

                     20                                          30
humkapI  asp arg val thr ile thr cys ARG ALA SER GLN ASP ILE SER SER TYR
Hum4D5a                                                  VAL ASN THR ALA
Hum4D5b                                                  VAL ASN THR ALA
Hum4D5c                                                  VAL ASN THR ALA

                                    40
humkapI  LEU ASN trp tyr gln gln lys pro gly lys ala pro lys leu leu ile
Hum4D5a  VAL ALA
Hum4D5b  VAL ALA
Hum4D5c  VAL ALA

         |  50                                                  60
humkapI  tyr ALA ALA SER SER LEU GLU SER gly val pro ser arg phe ser gly
Hum4D5a  |   SER     PHE
Hum4D5b  |   SER     PHE
Hum4D5c  |   SER     PHE     TYR*

                               70                                        80
humkapI  ser gly ser gly thr asp phe thr leu thr ile ser ser leu gln pro
Hum4D5a      arg
Hum4D5b      gly*
Hum4D5c      arg

                                           90
humkapI  glu asp phe ala thr tyr tyr cys GLN GLN TYR ASN SER LEU PRO TYR
Hum4D5a                                     HIS TYR THR THR     PRO
Hum4D5b                                     HIS TYR THR THR     PRO
Hum4D5c                                     HIS TYR THR THR     PRO

                    100
humkapI  THR phe gly gln gly thr lys val glu ile lys arg thr
Hum4D5a
Hum4D5b
Hum4D5c
```

V_L

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Project No._____
Book No._____ TITLE Humanized 405

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V_H

```
                1                                                  10
humiii   glu val gln leu val glu ser gly gly gly leu val gln pro gly gly
Hum4D5a
Hum4D5b
Hum4D5c

                        20                                                  30
humiii   ser leu arg leu ser cys ala ala ser|GLY PHE THR PHE SER ASP TYR
Hum4D5a                                     |        ASN ILE LYS      THR
Hum4D5b                                     |        ASN ILE LYS      THR
Hum4D5c                                     |        ASN ILE LYS      THR

                                           40
humiii   ALA MET|SER trp val arg gln ala pro gly lys gly leu glu trp val
Hum4D5a  TYR ILE|HIS
Hum4D5b  TYR ILE|HIS
Hum4D5c  TYR ILE|HIS

              50        52|52a  53                                    60
humiii   ala VAL ILE SER|GLU ASN GLY SER|ASP THR TYR TYR ALA ASP SER VAL
Hum4D5a      ARG      TYR|PRO THR ASN GLY|TYR      ARG
Hum4D5b      ARG      TYR|PRO THR ASN GLY|TYR      ARG
Hum4D5c      ARG      TYR|PRO THR ASN GLY|TYR      ARG

                                      70
humiii   LYS GLY arg phe thr ile ser arg asp asp ser lys asn thr leu tyr
Hum4D5a                           ala     thr                   ala
Hum4D5b                           ala     thr                   leu*
Hum4D5c                           ala     thr                   ala

          80       82 82a 82b 82c  83                                  90
humiii   leu gln met asn ser leu arg ala glu asp thr ala val tyr tyr cys
Hum4D5a
Hum4D5b
Hum4D5c

                                        100  a   b   c  101|
humiii   ala arg ASP|ARG GLY GLY ALA VAL SER TYR GLY ASP|VAL trp gly gln
Hum4D5a  ser     TRP|GLY GLY ASP GLY PHE TYR ALA MET ASP|
Hum4D5b  ser     TRP|GLY GLY ASP GLY PHE TYR ALA MET ASP|
Hum4D5c  ser     TRP|GLY GLY ASP GLY PHE TYR ALA MET ASP|TYR*

humiii   gly thr leu val thr val ser ser
Hum4D5a
Hum4D5b
Hum4D5c
```

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Witnessed & Understood by me,

Date

Invented by Leonard Presta

Date 3-5-90

Recorded by Leonard Presta

From Page No. 24

V_L 4D5

(1) Res 66 is Gly in human and mouse kappa sequences but is non-Gly in lambda sequences. Mouse 4D5 has an Arg at 66 though it is otherwise a kappa sequence. The sidechain at 66 should affect the conformations of CDR1, CDR2 and the hairpin turn at 68-69. Since kappa CDR1 should have a different canonical backbone conformation than lambda CDR1, the exact affect of Arg 66 cannot be deduced from available crystal structures. Hence the only difference between Hum 4D5a and Hum 4D5b V_L humanized sequences is Arg 66 versus Gly 66, respectively.

(2) Although res 55 is part of the Kabat/Wu CDR2, it is not included in the Chothia/Lesk CDR2. From model-building, the 4D5 Tyr 55 sidechain may play one of two roles: stabilizing the conformation of V_H CDR3 or providing an interaction in the V_L-V_H interface. The latter function may be dependent on the presence of V_H Typ 102

(3) Note that 4D5 Val 29 & Val 33 are smaller than consensus sequences of human kappa I and mouse kappa V where I 29 & L 33 provide buried interaction. Hence V_L CDR1 in 4D5 may have a CDR1 conformation different from those canonical conformations of Chothia/Lesk.

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V_H

(1) Tyr 102 in 4D5 may function to stabilize V_H CDR3 or provide a V_L-V_H interface interaction in concert with V_L Tyr 55

(2) The conformation of V_H CDR1 is dependent on interactions between CDR1 res 29 and sidechains of res 34, 71, 78 & 94.

	29	34	71	78	94
humIII	F	M	R	L	R
mouseIIc	I	M	A	A	R
4D5	I	I	A	A	R

The presence of Ile at 29 & 34 as well as Ala at res 71 & 78 may affect the structure of CDR1. However in previous studies of Chothia/Lesk res 78 has not been considered. As a test of the importance of this residue on the conformation of V_H CDR1, sequence Hum4D5b differs from Hum4D5a by Leu 78 only (see page 24).

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Model	Energy 6000 cycles	Phe10	CDR3H	R66 NE	R66 Nh1	R66 Nh2
A4D5K2L	-1402	out	modeled	N300'	G680' N300'	T310'
A4D5K2LNEW *	-1379	out	modeled	G680'	G680'	
A4D5K2M	-1404	in	2MCP	G680'	G680' N300'	
A4D5K3M @	-1398	out	2MCP	G680' N300'	G680' N300'	
A4D5K2P	-1381	out	2PRC	G680' N300'	G680' N300'	
A4D5K2MODA	-1413	in	2MCP	S500'	S520'	T310' S500' S500'
A4D5K2MODB	-1420	in	2MCP	T310'	S520'	A510' S520' S500'
A4D5K2MODC	-1419	in	2MCP	S520' S500'	S520'	N300' T310'
A4D5K2MODD	-1420	in	2MCP		T310'	S500' S520' T310'
A4D5K2MODE	-1424	in	2MCP	S500'		N300' T310'

* A4D5K2LNEW = A4D5K2L after 3000 cycles + alter conformation F53-V58, Y49, F60B to restack

@ A4D5K3M = A4D5K2M + new conformation for Y49, F53, Y55

To Page No.____

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by Leonard Presta	4-20-90

[redacted]

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by Leonard Presta	6-20-91

[redacted]

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by Leonard Pecota	6-20-91

[redacted]

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by Leonard Presta	6-20-91

[redacted]

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by Leonard Presta	6-21-91

[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 Leonard Presta	6-24-91

[redacted]

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by Leonard Presta	6-26-91

[redacted]

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by Leonard Presta	7-2-91

[redacted]

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by Leonard Presta	7-10-91

[redacted]

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by Leonard Presta	7-11-91

[redacted]

Witnessed & Understood by me,	Date	Invented by	Date
		Leonard Presta	7-12-91
		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]

[redacted]

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 Presta	8-13-91

[redacted]

Witnessed & Understood by me,

Date

Invented by

Date 8-30-91

Recorded by Leonard Presta

[redacted]

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by Leonard Presta	9-7-91

[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 Leonard Presta	9-10-91

[redacted]

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by Leonard Presta	9-13-91

[redacted]

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by Leonard Testa	9-14-91

[redacted]

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by Leonard Presta	9-23-91

[redacted]

Recorded by Leonard Presta

Date 10-10-91