

Domain standardization in the IgSF and MhcSF superfamilies: the IMGT integrated approach for genetics, genomics and 3D structures

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Université Montpellier, CNRS
Institut Universitaire de France

ESF Myelin Structure and its role in Autoimmunity II
MARIE Network, May 6, 2005, Potenza, Italy



The international ImMunoGeneTics information system®
Coordinator: M.-P. Lefranc, Montpellier, France <http://imgt.cines.fr>



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Created in 1989 (Université Montpellier II and CNRS)

1) IMGT domains of research:

Immunogenetics -Immunoinformatics

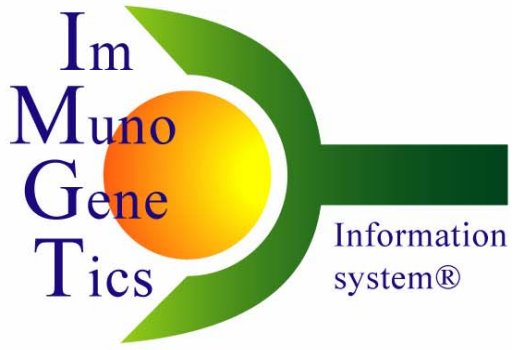
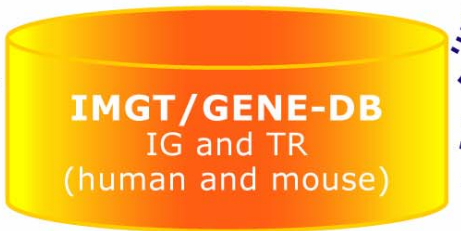
- * *Immunoglobulins (IG), T cell receptors (TR), major histocompatibility complex (MHC) of human and other vertebrates,*
- * *Immunoglobulin superfamily IgSF and MhcSF,*
- * *Related proteins of the immune system (RPI)*

2) IMGT-ONTOLOGY concepts

3) IMGT-Choreography: *Dynamic knowledge management*

IMGT databases and tools

Sequences



<http://imgt.cines.fr>

Genome



2D and 3D structures

IMGT® Web Resources

IMGT Repertoire **8,000 HTML pages**
Chromosomal localizations
Locus representations, ...

IMGT Bloc-notes
Interesting links
The IMGT Immunoinformatics page
(databases, tools, resources, ...)

IMGT Education
Tutorials, IMGT Lexique, ...

Structural domains

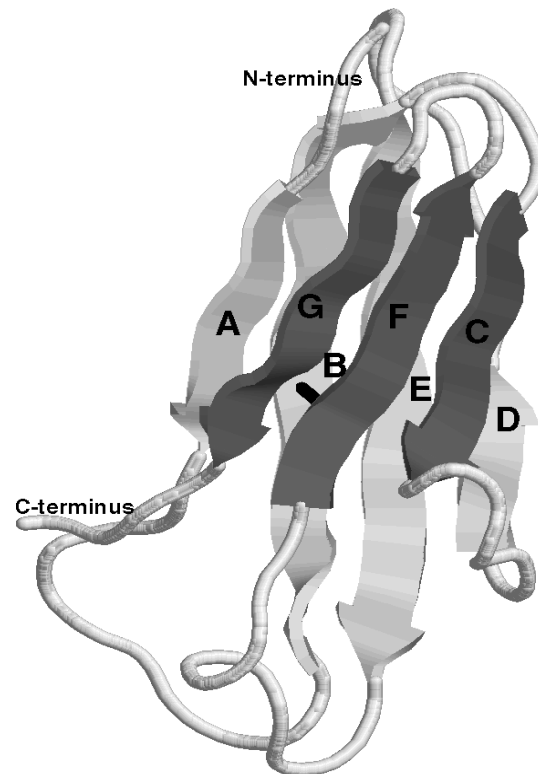
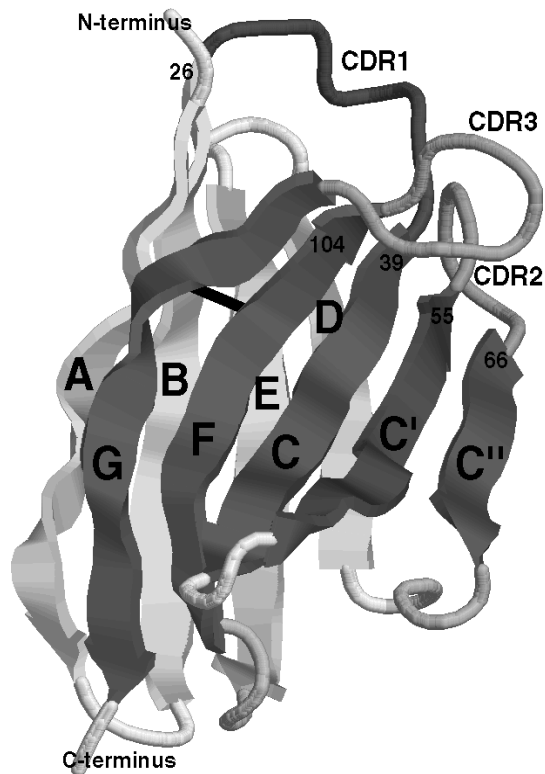
IG and TR

MHC

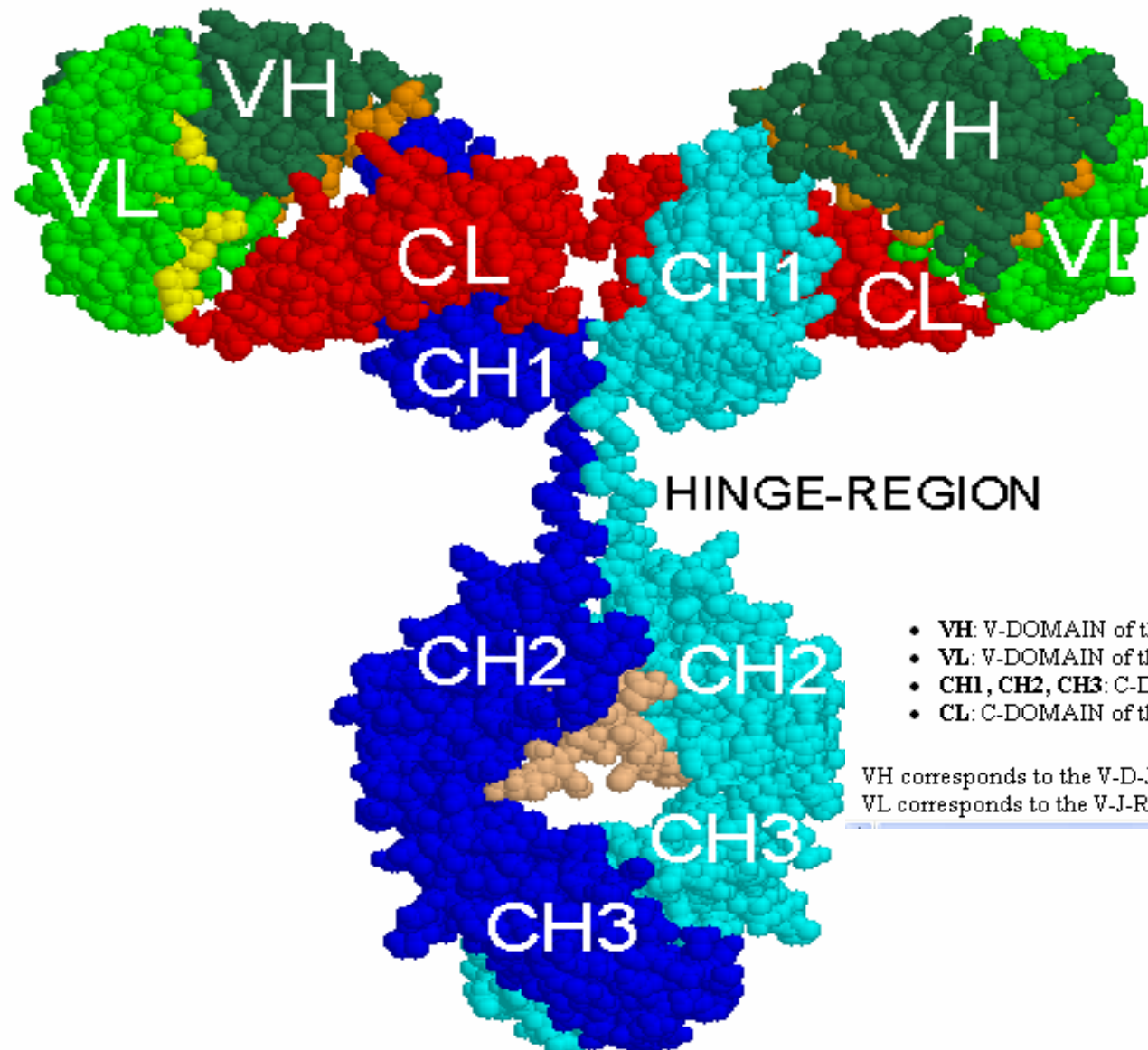
V-DOMAIN

C-DOMAIN

G-DOMAINS



Spacefill 3D representation of an IgG immunoglobulin

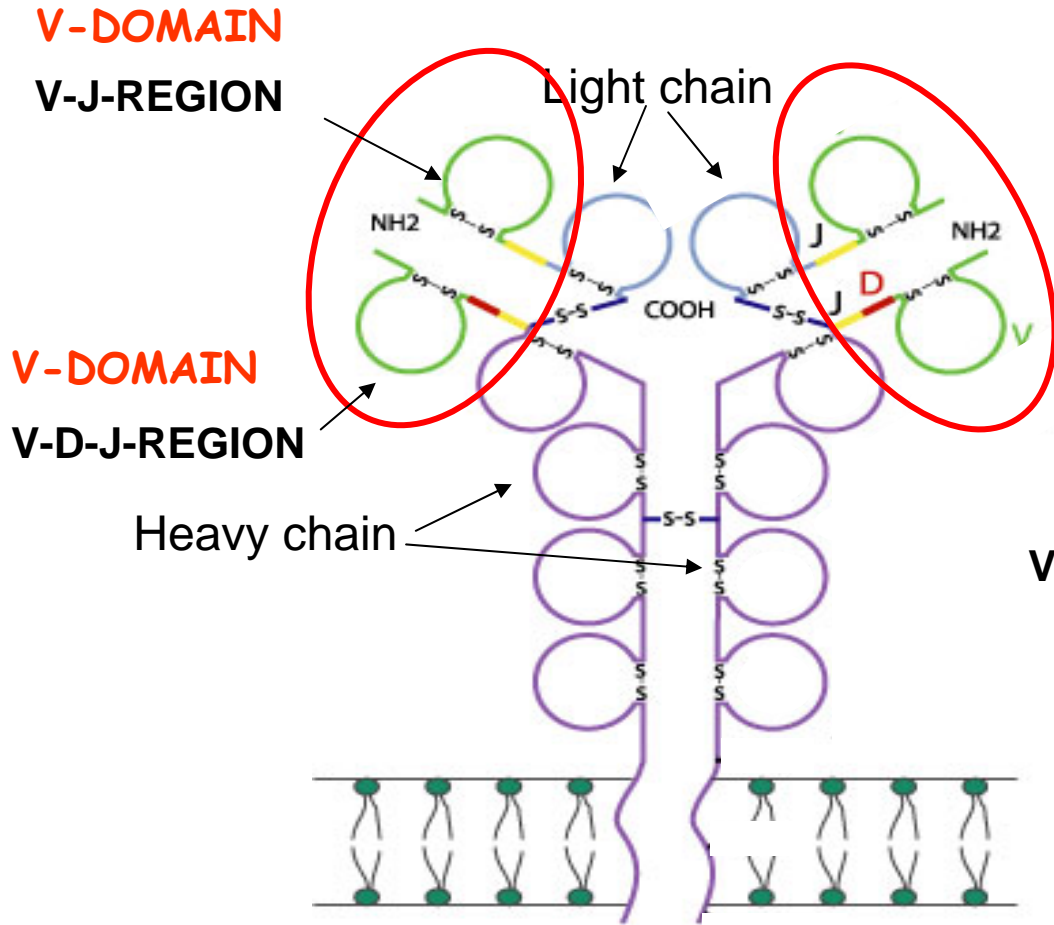


- **VH:** V-DOMAIN of the immunoglobulin heavy chain
- **VL:** V-DOMAIN of the immunoglobulin light chain
- **CH1, CH2, CH3:** C-DOMAIN of the immunoglobulin heavy chain
- **CL:** C-DOMAIN of the immunoglobulin light chain

VH corresponds to the V-D-J-REGION (in green (V), orange (DJ)) of the heavy chain.
VL corresponds to the V-J-REGION (in green (V) and yellow (J)) of the light chain.

Immunoglobulin (IG)

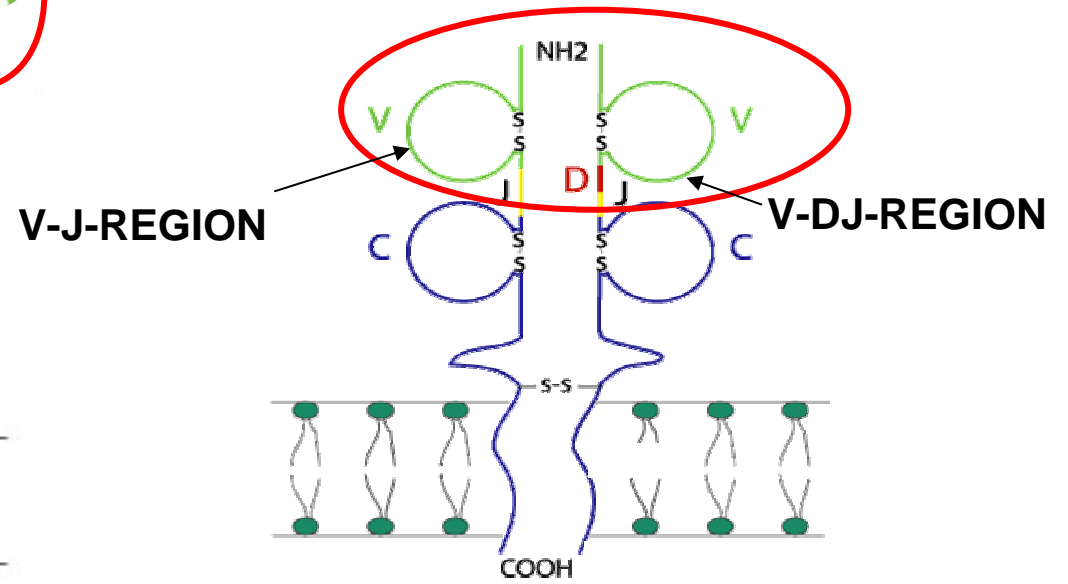
T cell receptor (TR)



Membrane IgM

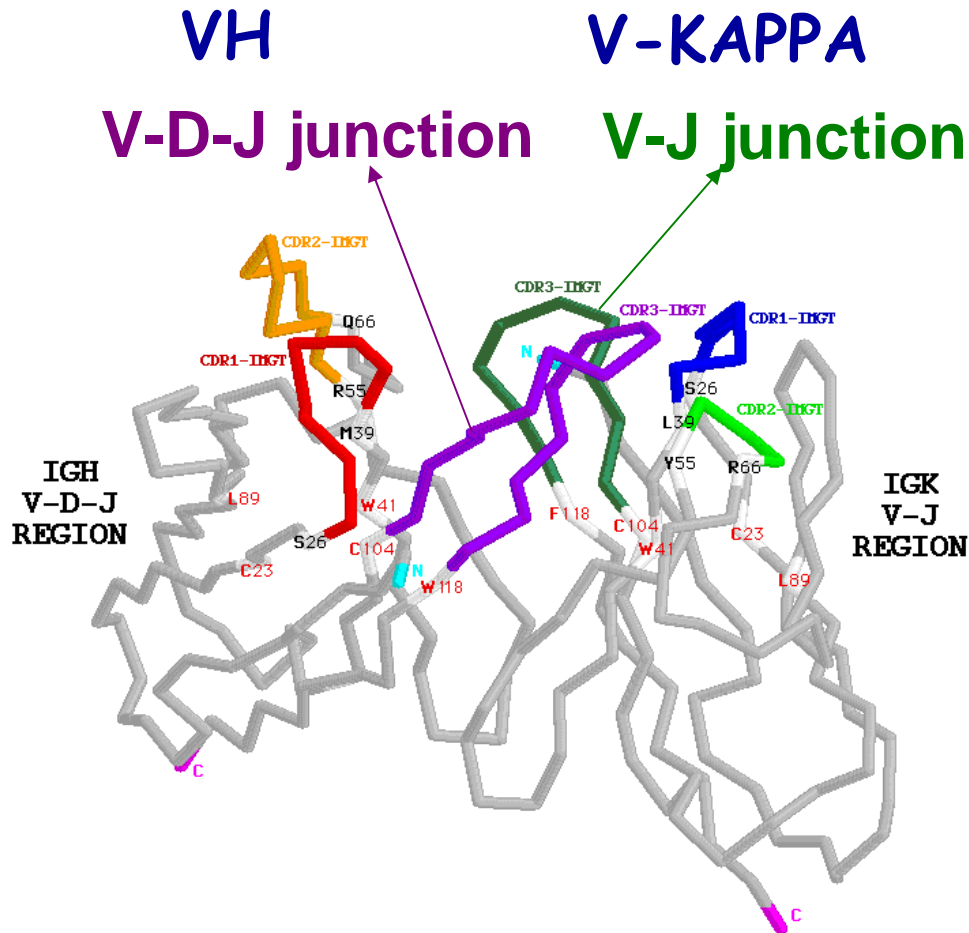
Contribution of the 2 V-DOMAINS to the antigen binding site

Alpha - Beta
Gamma - Delta

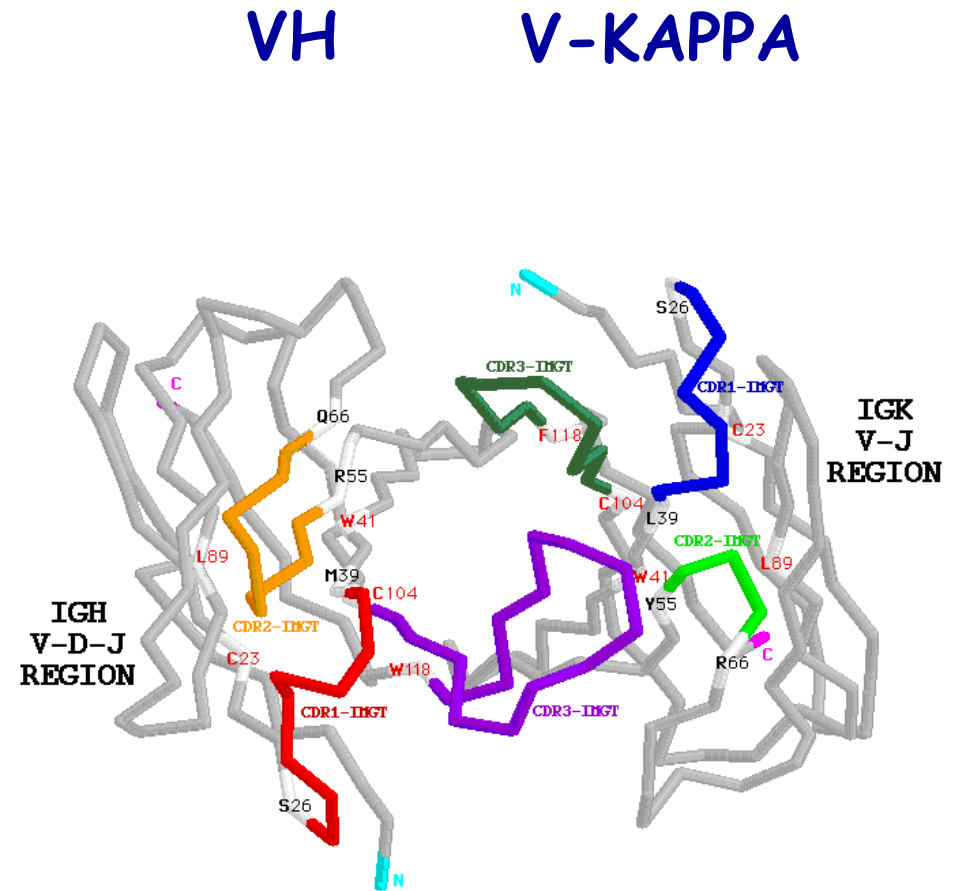


T cell receptor

V-DOMAINS: VH and V-KAPPA



Side view of the V-DOMAINS



View from above the CDRs

Mouse (*Mus musculus*) E5.2Fv

CDR3-IMGT= Complementarity determining region (105-117)
V-J junction (104-118)
V-D-J junction (104-118)



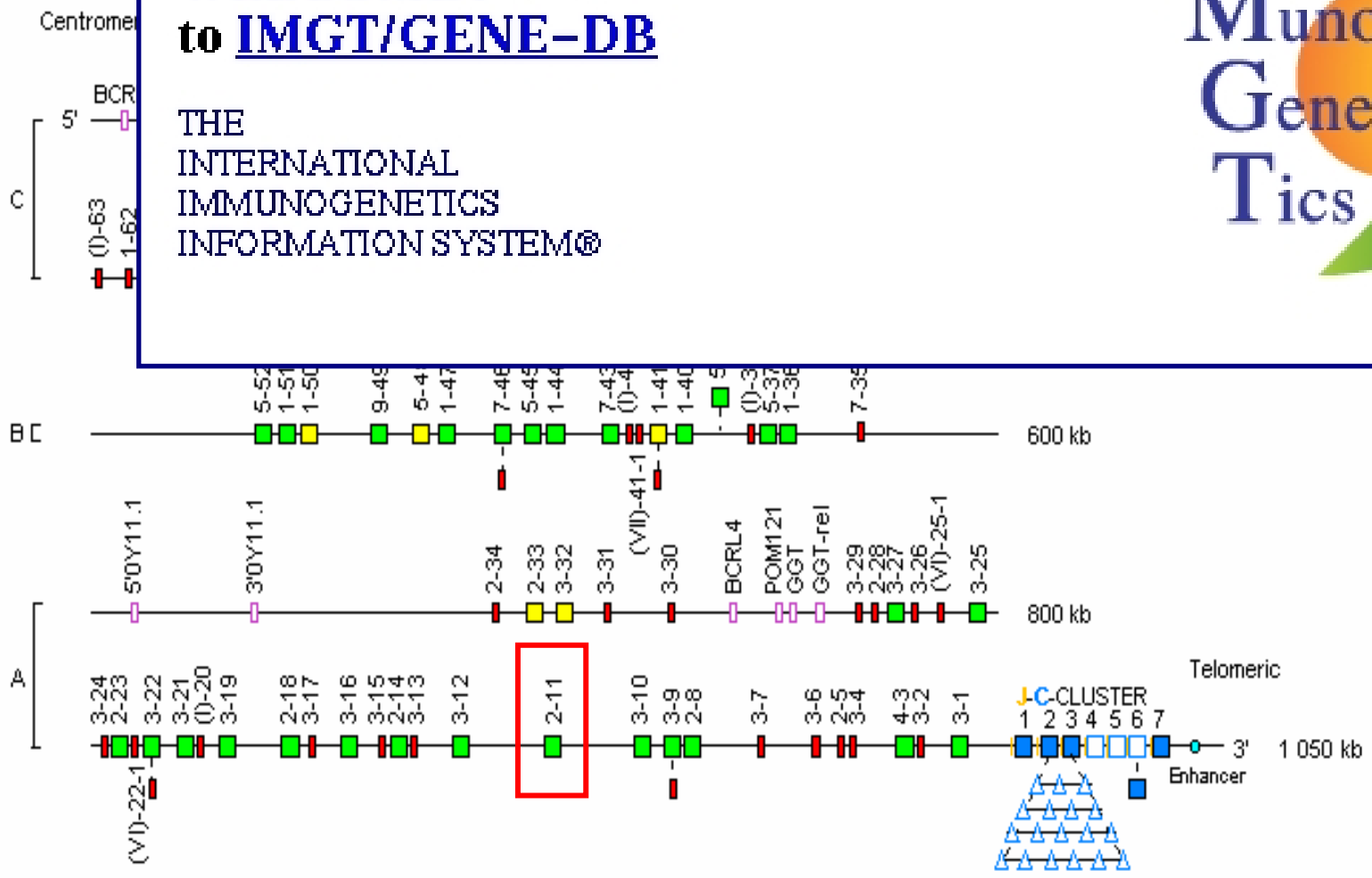
Locus representation: Human IGL

Human IGL 2

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IMGT/LIGM-DB Consultation module v3 - Netscape
 Fichier Edition Affcher Aller Communicator Aide
 Signets Adresse : <http://ligm.igh.cnrs.fr:8104/cgi-bin/IMGTlect.jv> Infos connexes

FT	V-GENE	<1..297>
FT		(partial)
FT		
FT		
FT		
FT		
FT		
FT		
FT	V-REGION	
FT		
FT		
FT		
FT		
FT	FR1-IMGT	
FT		
FT		
FT	1st-CYS	
FT	CDR1-IMGT	
FT		
FT		
FT	FR2-IMGT	103..153
FT		/AA_IMGT="39 to 55"
FT		/translation="VSWYQQHPGKAPKLMIIY"
FT	CONSERVED-TRP	109..111
FT	CDR2-IMGT	154..162
FT		/AA_IMGT="56 to 58"
FT		/translation="DVS"
FT	FR3-IMGT	163..270
FT		/AA_IMGT="66 to 104, AA 73, 81, 82 missing"
FT		/translation="KRPSGVPPDRFSGSKSGNTASLTISGLQAEDEADYYC"
FT	2nd-CYS	268..270
FT	CDR3-IMGT	271..297
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XX		
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		tcctcactc gaaccaccac tcatattgat attataact atctctcctc ataccaacac 120

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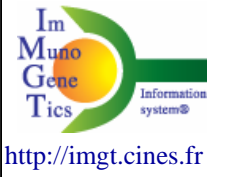
IMGT/LIGM-DB ON LINE, HERE YOU ARE !

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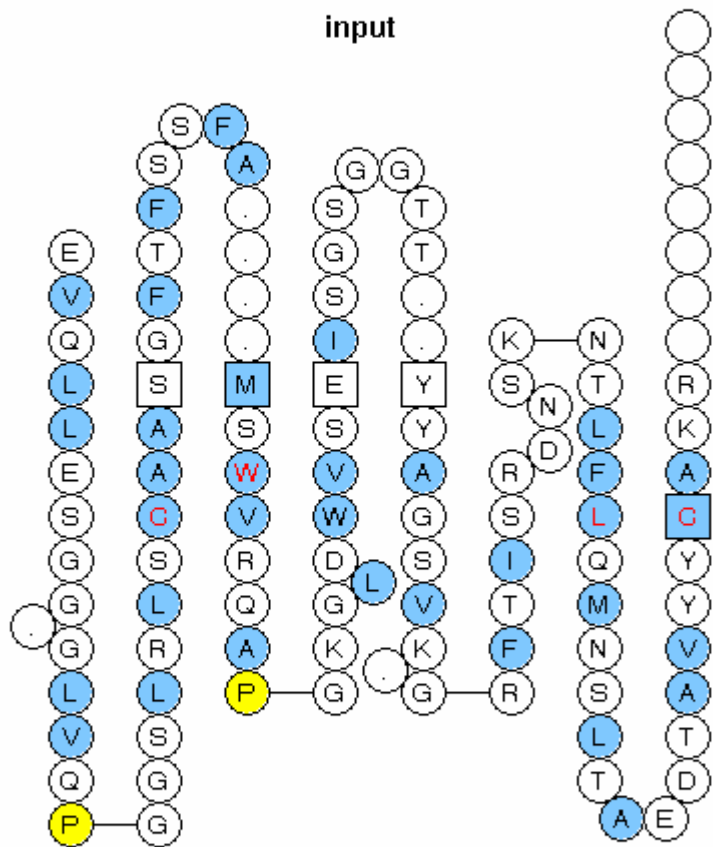
Catalogue

accession number, mnemonic, definition, creation date, length, [annotation level](#)





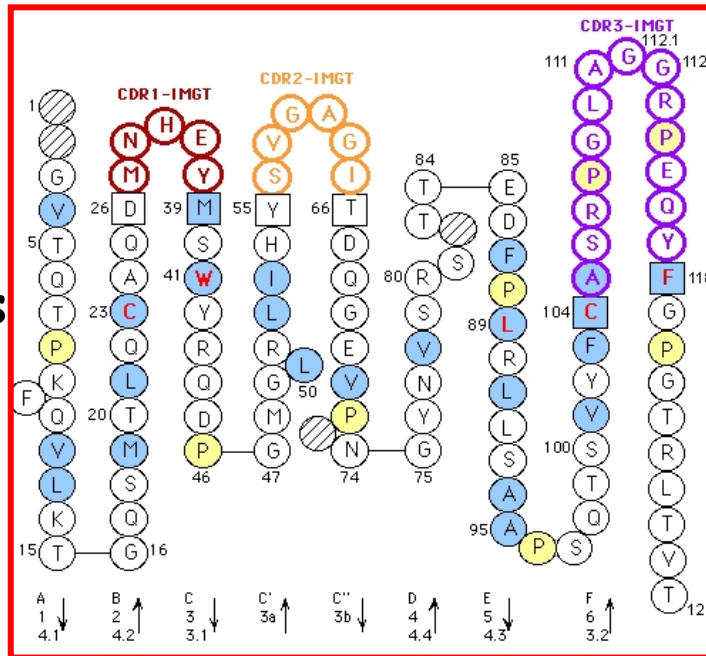
Collier de Perles



A	B	C	C'	C''	D	E	F
1	2	3	3a	3b	4	5	6
↓	↑	↓	↑	↓	↑	↓	↑
4.1	4.2	3.1			4.4	4.3	3.2

"NUMEROTATION" concept

Collier de Perles



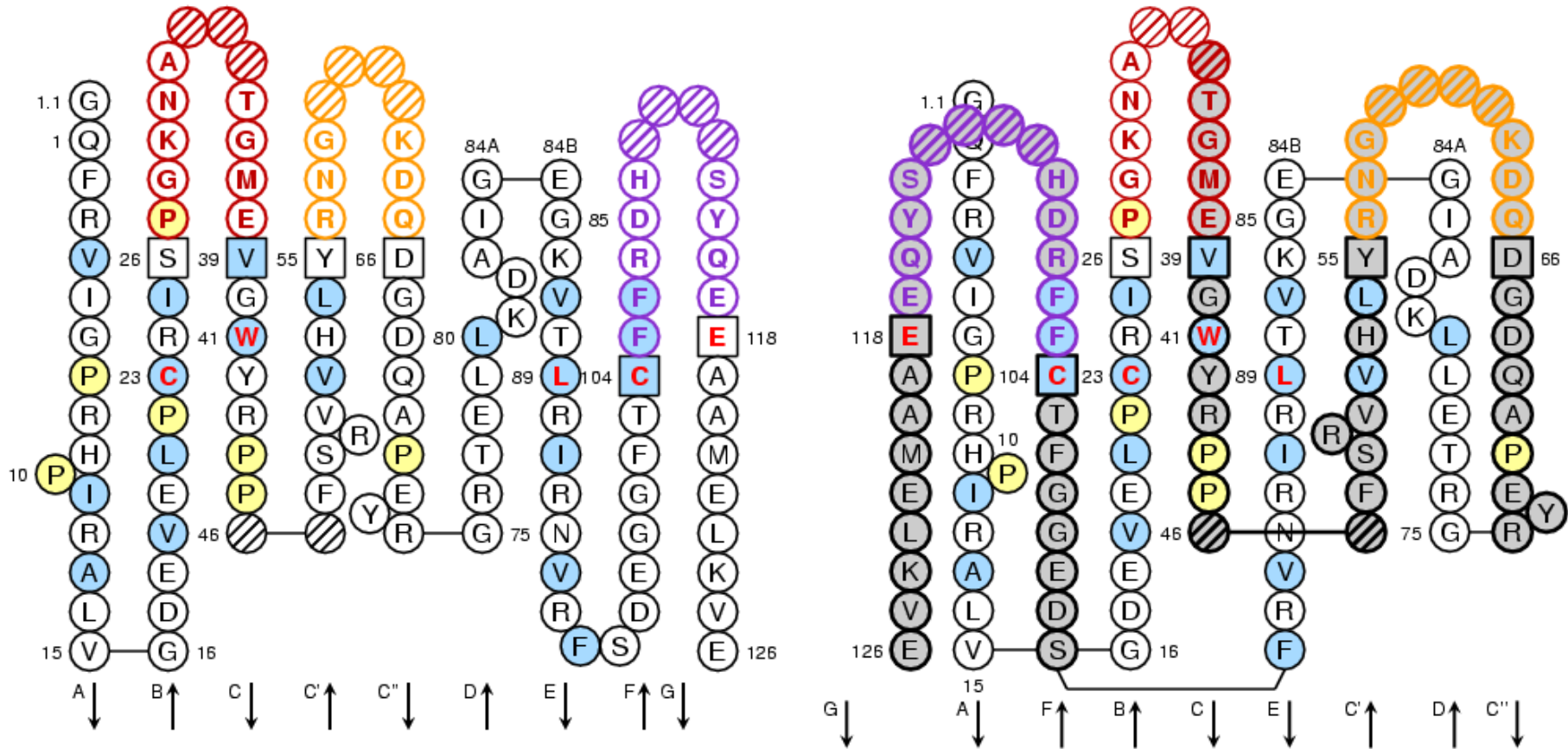
Sequence	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	
X02850 ,TRAV8-6*01	A	Q	S	V	T	Q	L	D	S	Q	V	F	F	E	E	R	F	V	E		
AE000659 ,TRAV8-6*02	GCC	CAG	TCT	GTG	ACC	CAG	CTT	GAC	AGC	CRA	GTC	CCT	ETC	TTT	GAA	GAA	GCC	CCT	GTG	GAG	
M86361 ,TRAV8-6*02	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---
X02850 ,TRAV8-6*01	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---
AE000659 ,TRAV8-6*02	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---
M86361 ,TRAV8-6*02	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---
X02850 ,TRAV8-6*01	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---
AE000659 ,TRAV8-6*02	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---
M86361 ,TRAV8-6*02	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---
X02850 ,TRAV8-6*01	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---
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M86361 ,TRAV8-6*02	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---
X02850 ,TRAV8-6*01	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---
AE000659 ,TRAV8-6*02	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---
M86361 ,TRAV8-6*02	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---
X02850 ,TRAV8-6*01	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---
AE000659 ,TRAV8-6*02	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---
M86361 ,TRAV8-6*02	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---
X02850 ,TRAV8-6*01	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---
AE000659 ,TRAV8-6*02	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---
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X02850 ,TRAV8-6*01	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---
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X02850 ,TRAV8-6*01	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---
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M86361 ,TRAV8-6*02	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---
X02850 ,TRAV8-6*01	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---
AE000659 ,TRAV8-6*02	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---
M86361 ,TRAV8-6*02	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---
X02850 ,TRAV8-6*01	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---
AE000659 ,TRAV8-6*02	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---
M86361 ,TRAV8-6*02	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---
X02850 ,TRAV8-6*01	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---
AE000659 ,TRAV8-6*02	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---
M86361 ,TRAV8-6*02	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---
X02850 ,TRAV8-6*01	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---
AE000659 ,TRAV8-6*02	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---
M86361 ,TRAV8-6*02	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---
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AE000659 ,TRAV8-6*02	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---
M86361 ,TRAV8-6*02	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---
X02850 ,TRAV8-6*01	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---
AE000659 ,TRAV8-6*02	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---
M86361 ,TRAV8-6*02	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---
X02850 ,TRAV8-6*01	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---
AE000659 ,TRAV8-6*02	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---
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Alignment of alleles

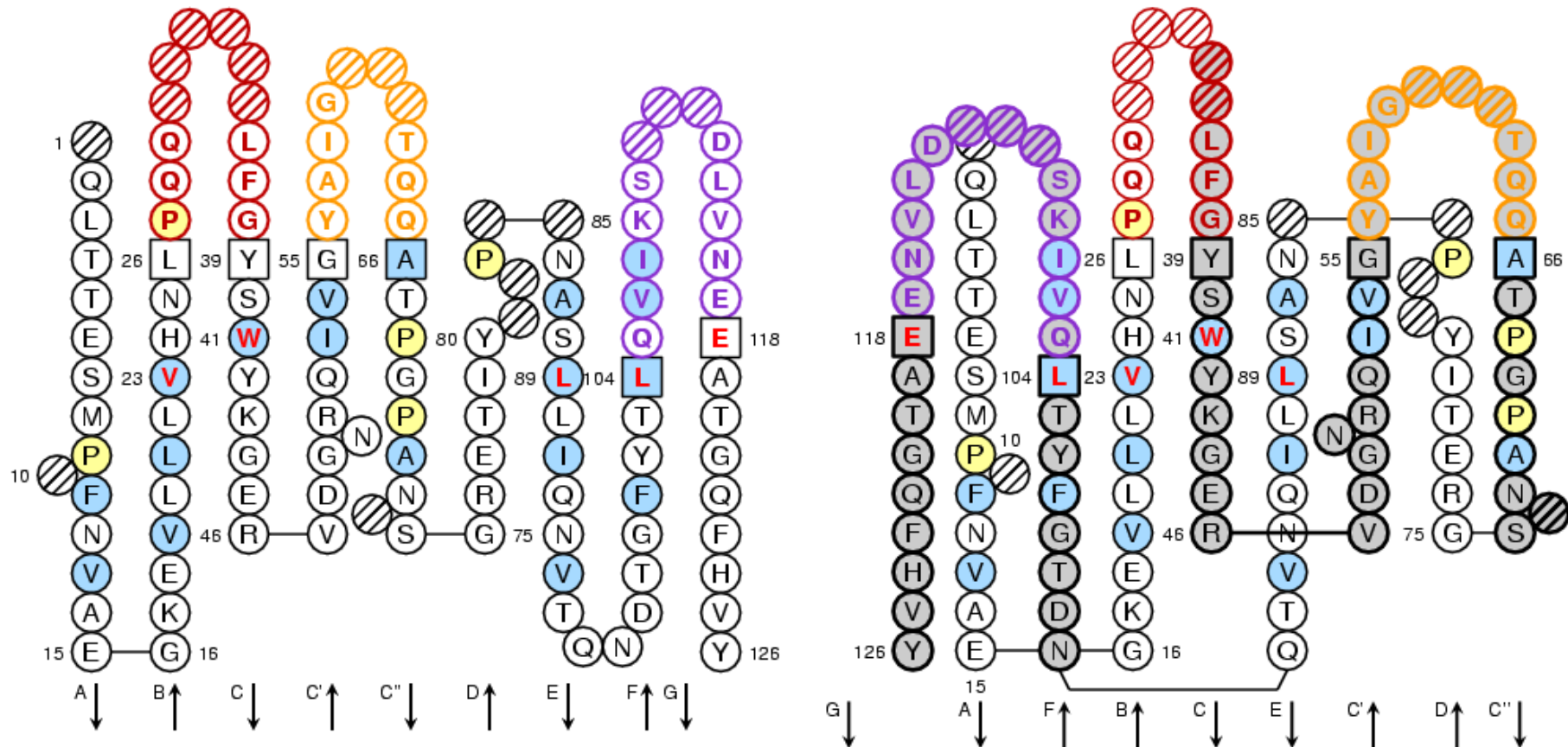
Protein Display

TRAV gene	FR1-IMGT (1-26)	CDR1-IMGT (27-38)	FR2-IMGT (39-55)	CDR2-IMGT (56-65)	FR3-IMGT (66-104)	CDR3-IMGT (105-115)					
AE000658, TRAV1-1	GQSLEQ	PSEVTAVEGAI	VQINCTYQ	TSGFYG	LSWYQQHDGGAP	TFLSY NALDGL	LEETG	RFSSFLSRSDSYGYLLQLQMKDSASYFC	AVR		
AE000658, TRAV1-2	GQNIDQ	PTEMTATEGAI	VQINCTYQ	TSGFNG	LFWYQQHAGEAPT	FLSY NVLDGL	LEEKG	RFSSFLSRSKGYSYLLKELQMKDSASYLC	AVR		
AE000658, TRAV2	KDQVFQ	PSTVASSEGAVVE	IFCNHS	VSNAVY	FFWYLRHHPGCAP	RLLVK GSK	PSQQG	RYNMTYER	FSSLLILQVREDAAVYYC	AVE	
AE000658, TRAV3	AQSVAQPEDQVNV	AEAGNPLT	VKCTYS	VSGNPY	LFWYVQYPNRLG	QFLLK YITGDNL	VKGSY	GFEAEFNKSTSPHLKPKSALVSDSALYFC	AVRD		
AE000658, TRAV4	LAKITQ	PISMSDYE	QGEVNI	TCSHN	NIATNDY	ITWYQQPPSQG	PRFIIQ GYKT	KVINE	VASLFIPADRKSSTLSLPRVSLSDTAVYYC	LVGD	
AE000659, TRAV5	GEDVEQS	LFLSVREGDSS	VINCTY	DSSSTY	LYWYKQEPGAGL	QLLTY IFSNMD	MKQDQ	RLTVLLNKKDKHL	SLRIADTQTGDSAIYFC	AES	
AE000659, TRAV6	SQKIEQNSEAL	NIQEGKTAT	LTLCNYT	NYSPAY	LQWYRQDPGRGP	VFLLL IRENEK	EKRKE	RLKVTFDITL	KQSLFHITASQPADSATYLC	ALD	
AE000659, TRAV7	LNQVHEHSPH	FLGPQGDV	ASMSCTYS	VSRFNN	LQWYRQNTGM	GPKHLLS MYSAGY	EKQKG	RLNAILLK	NGSSLYITAVQPEDSATYFC	AVD	
AE000659, TRAV8-1	AQSVSQHNHH	VILSEAA	SELGCNYS	YGGTVN	LFWYVQYPGQHL	QLLLK YFSGDPL	VKGIK	GFEAEF	IKSKFSPNLRKPSVQWSDTAEYFC	AVN	
AE000659, TRAV8-2	AQSVTQLD	SHSVS	VEGTPV	LLRCNYS	SSYSPS	LFWYVQHPNKG	LQLLLK YTSAATL	VKGIN	GFEAEFKKSETSPHLTKPSAHMSDAAEYFC	VVS	
AE000659, TRAV8-3	AQSVTQPD	IHIITV	SEGASLE	LRNYS	YGATPY	LFWYVQSPGQGL	QLLLK YFSGDTL	VQGIK	GFEAEFKRSQSSFNLRKPSVHWSDAEYFC	AVG	
AE000659, TRAV8-4	AQSVTQLG	SHSVS	VEGALV	LLRCNYS	SSVPPY	LFWYVQYPNQGL	QLLLK YTSAATL	VKGIN	GFEAEFKKSETSPHLTKPSAHMSDAAEYFC	AVS	
X02850, TRAV8-6	AQSVTQLDS	QVPV	FEAPV	ELRCNYS	SSVSVY	LFWYVQYPNQGL	QLLLK YLSGDTL	YESIN	GFEAEFNKSTSPHLRKP	SVHISDTAEYFC	AVS
AE000660, TRAV8-7	TQSVTQLD	GHIITV	SEEA	PLELKC	NYS	YSGVPS	LFWYVQYSSQSL	QLLLK DLTEATQ	VKGIK	GFEAEFKKSETSPYLRKPSVHWSDAEYFC	AVGDR
AE000659, TRAV9-1	GSVWQTEG	QWVLS	FEGR	SLIVN	CSYF	TTQVPS	LFWYVQYVGRG	PDHLK AMKAND	KGRNK	GFEAMVYKETTSPHLFKDSVQVSDSAVYFC	ALS

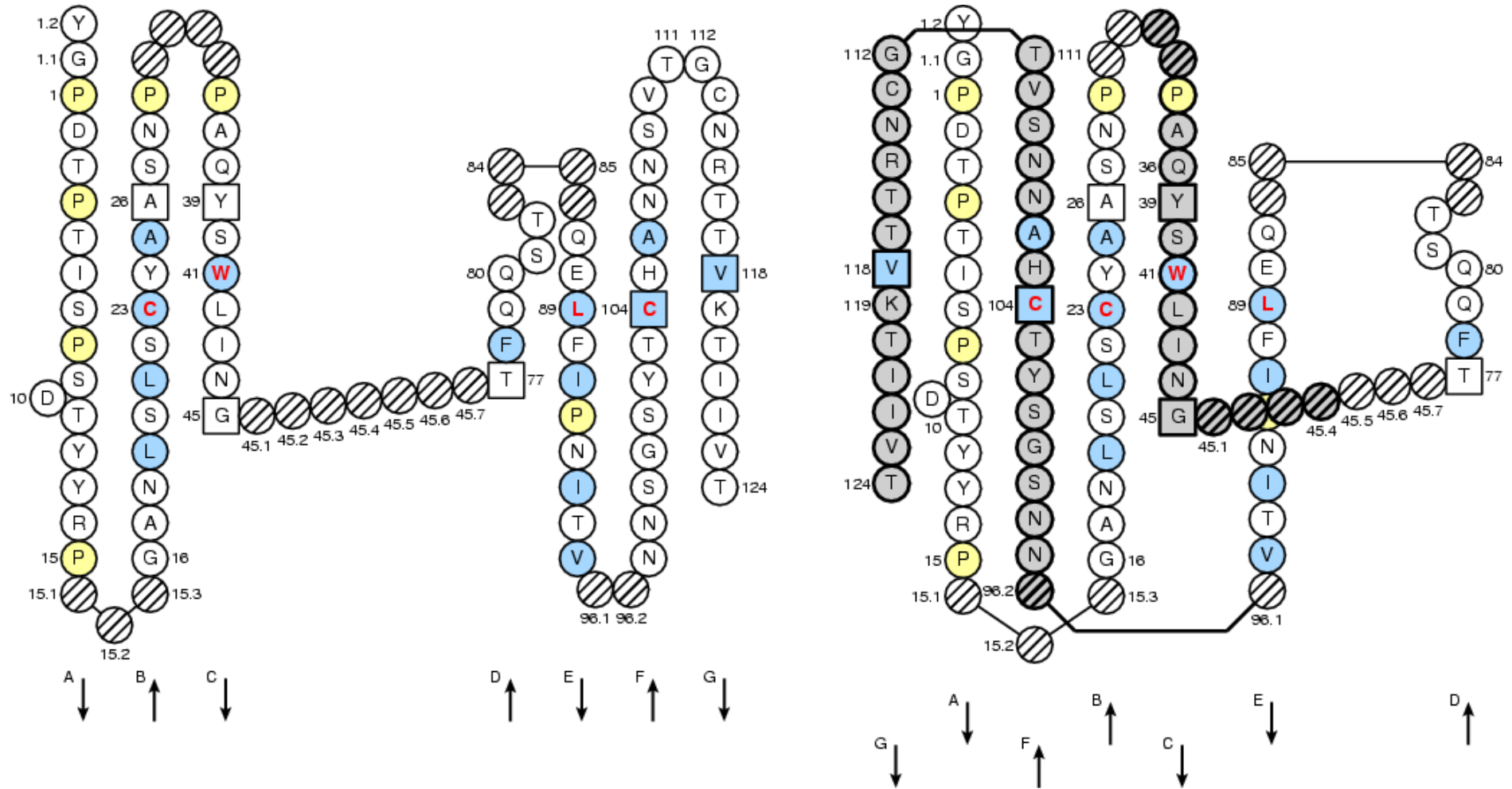
Homo sapiens MOG [D] V-LIKE-DOMAIN



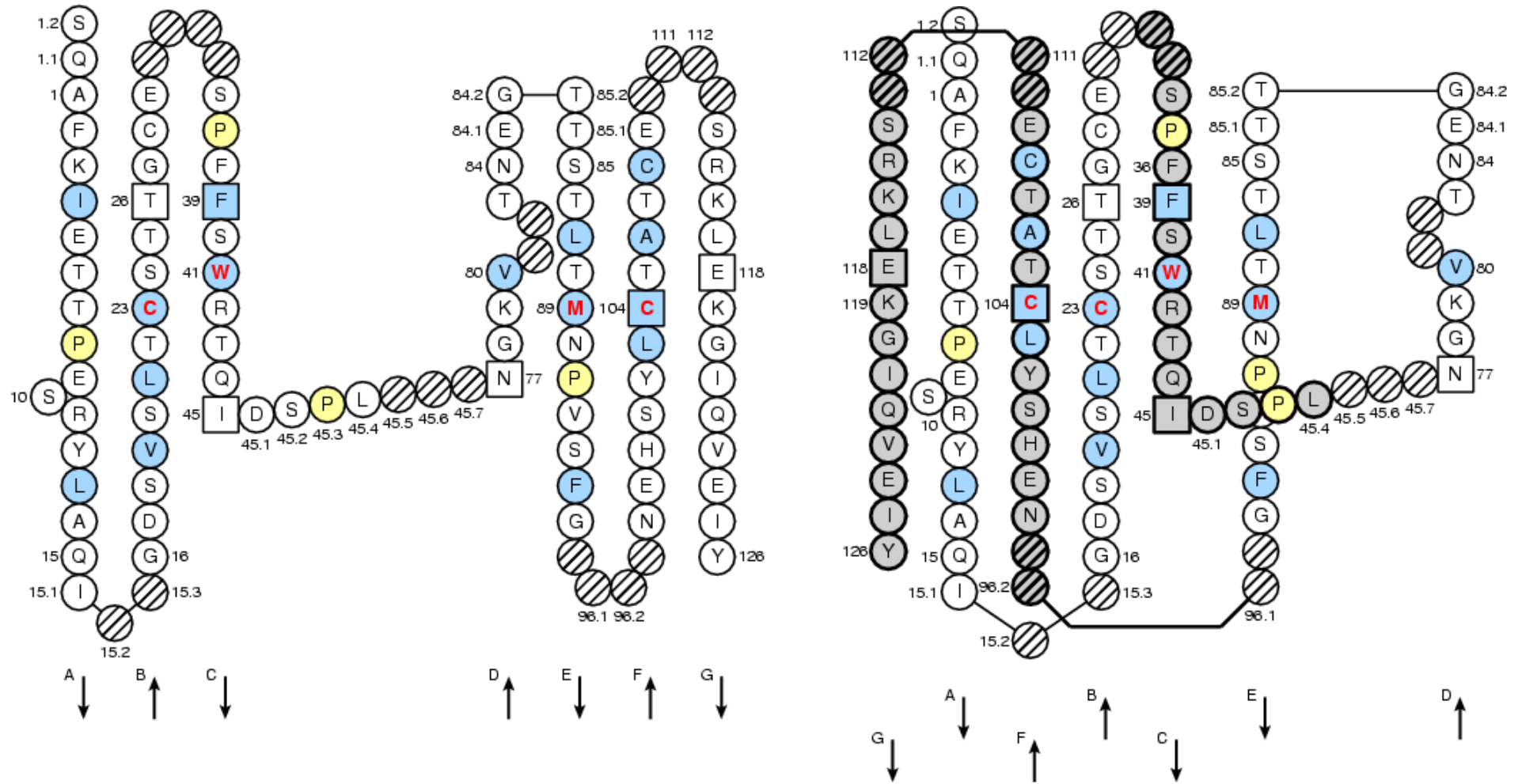
Homo sapiens CEACAM1 [D1] V-LIKE-DOMAIN



Homo sapiens CEACAM1 [D3] C-LIKE-DOMAIN

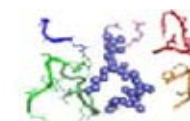


Homo sapiens VCAM1 [D1] C-LIKE-DOMAIN



IMGT/3Dstructure-DB and IMGT/StructuralQuery

IMGT/3Dstructure-DB card for : 1u8k



IMGT protein name	IMGT receptor description	Type	Ligand(s)	Species	CC	Chain ID
2F5	FAB-GAMMA-3_KAPPA	IG		<i>Homo sapiens</i> (Human)	1	[1u8k_A 1u8k_B]
	Peptide		GP41		1	[1u8k_C]

Experimental technique X-ray diffraction Resolution 2.24 PDB release date 05-OCT-04

Chain ID	1u8k_B	
IMGT chain description	VH-CH1	
Chain amino acid sequence	<pre>[IGHV_1 RI TLKESGPPLVKPTQTLTLTCSFSGFSLSDFGVGVGWIRQPPGKALEWLAI I YSDDDKRYSPSINTRLTI TKDTSKNQVVLVMTRVSPV] [D] [IGHJ_1] [IG DTATYFC_AHRRGPTTLFGVPIARGPVNAMDVWGQGI TVTI SSTSTKGPSVFPLAPCS RSTAGGTAALGCLVKDYFPEPVTVSWNSGALTS HC_1] GVHTFPAVLQSSGLYSLSSVVTVPSSSLGTQTYTCNVNHKPSNTKVDKRVPEPKS</pre>	
V-DOMAIN	IMGT domain description	VH
	IGHV gene and allele name	IGHV2-5*05 (85.00%), IGHV2-5*06 (85.00%), Alignment details
	IGHJ gene and allele name	IGHJ6*01 (83.33%), IGHJ6*02 (83.33%), Alignment details
	2D representation	Collier de Perles or Collier de Perles on 2 layers
	CDR-IMGT lengths	[10.7.24]
	Sheet composition	[A B D E] [C C' C' F G]
	<pre>[CDR1] [CDR2] RI TLKESGP . PLVKPTQTLTLTCSFSGFSLSDFGVG . . VGWIRQPPGKALEWLAI I YSDDDK . . . RYSPSIN . TRLTI TKDTSKNQVVLV [CDR3] MTRVSPVDTATYFC_AHRRGPTTLFGVPIARGPVNAMDVWGQGI TVTI</pre>	
IMGT domain		

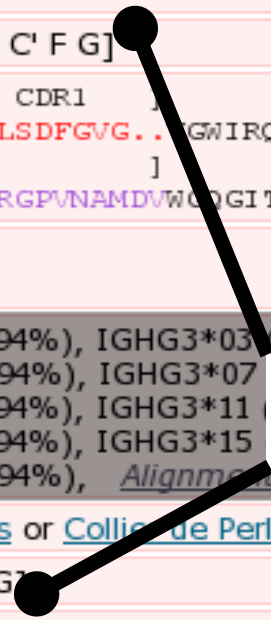
Chain ID	1u8k_B	
IMGT chain description	VH-CH1	
Chain amino acid sequence	<pre> [IGHV_1 RI TLKESGPPLVKPTQTLTLTCSFSGFSLSDFGVGVGWIRQPPGKALEWLAI I YSDDDKRYSPSINTRLTI TKDTSKNQVVLVMTRVSPV] [D] [IGHJ_1] [IG DTATYFCAHRRGPTTLFGVPIARGPVNAMDVWQGI TVTI SSTSTKGPSVFPLAPCSKSTAGGTAALGCLVKDYFPEPVTVSWNSGALTS HC_1 GVHTFPAVLQSSGLYSLSSVVTVPSSSLGTQTYTQNVNHKPSNTKVDKRVPEPKS </pre>	

V-DOMAIN	IMGT domain description	VH
	IGHV gene and allele name	IGHV2-5*05 (85.00%), IGHV2-5*06 (85.00%), Alignment details
	IGHJ gene and allele name	IGHJ6*01 (83.33%), IGHJ6*02 (83.33%), Alignment details
	2D representation	Collier de Perles or Collier de Perles on 2 layers
	CDR-IMGT lengths	[10.7.24]
	Sheet composition	[A B D E] [C C' C' F G]
	<pre> [CDR1] [CDR2] RI TLKESGP . PLVKPTQTLTLTCSFSGFSLSDFGVGVGWIRQPPGKALEWLAI I YSDDDKRYSPSIN . TRLTI TKDTSKNQVVLV [CDR3] MTRVSPVDTATYFCAHRRGPTTLFGVPIARGPVNAMDVWQGI TVTI </pre>	

IMGT Colliers de Perles

C-DOMAIN	IMGT domain description	CH1
	IGHC gene and allele name	IGHG3*01 (97.94%), IGHG3*03 (97.94%), IGHG3*04 (97.94%), IGHG3*05 (97.94%), IGHG3*06 (97.94%), IGHG3*07 (97.94%), IGHG3*08 (97.94%), IGHG3*09 (97.94%), IGHG3*10 (97.94%), IGHG3*11 (97.94%), IGHG3*12 (97.94%), IGHG3*13 (97.94%), IGHG3*14 (97.94%), IGHG3*15 (97.94%), IGHG3*16 (97.94%), IGHG3*17 (97.94%), IGHG3*18 (97.94%), IGHG3*19 (97.94%), IGHG3*20 (97.94%), Alignment details
	2D representation	Collier de Perles or Collier de Perles on 2 layers
	Sheet composition	[A B D E] [C F G]
	<pre>STKGPSVFPLAPCSKSTA...GGTAALGCLVKDYFP...EPVTVSWNSGALTS....GVHTFPAVLQSS.....GLYSLSSVVTV PSSSL...GTQTYTQNVNHK...SNTKVDKRV </pre>	

IG domain sheet composition (hydrogen bond networks)



Chain ID	1u8k_B		
IMGT chain description	VH-CH1		
Chain amino acid sequence	[RI TLKESGPPLVKPTQTL...RLTI TKDTSINQVVLVMTRVSPV...IG...SALTS		
V-DOMAIN	<p>IMGT renumbered coordinate file</p> <pre> REMARK 410 IMGT/3Dstructure-DB analysis: REMARK 410 HELP PROT (protein number) NAME (protein name) REMARK 410 HELP PROT (protein number) RECEP (receptor description) REMARK 410 HELP PROT (protein number) CHAIN (protein chain codes) REMARK 410 HELP DOM (protein number) (chain code) (domain number) (domain type) REMARK 410 HELP (start residue number)(insertion code) (last residue REMARK 410 HELP number)(insertion code) REMARK 410 HELP DOM (protein number) (chain code) (domain number) CDR (CDR1 REMARK 410 HELP length) (CDR2 length) (CDR3 length) REMARK 410 HELP REG (protein number) (chain code) (domain number) (region REMARK 410 HELP number) (start residue number)(insertion code) (last REMARK 410 HELP residue number) (genes and alleles) REMARK 410 PROT 0 NAME ANTIBODY 2F5 (LIGHT CHAIN) REMARK 410 PROT 0 CHAIN A,B REMARK 410 DOM 0 A 1 V 1 127 REMARK 410 DOM 0 A 1 CDR 6 3 9 REMARK 410 REG 0 A 1 1 1 115 IGKV1-13*02 REMARK 410 REG 0 A 1 3 117 127 IGKJ4*02,IGKJ4*01 REMARK 410 DOM 0 A 2 C 1001D 1126 REMARK 410 REG 0 A 2 1 1001D 1126 IGKC*01 REMARK 410 DOM 0 B 1 V 1 126 REMARK 410 DOM 0 B 1 CDR 10 7 24 REMARK 410 REG 0 B 1 1 1 107 IGHV2-5*06,IGHV2-5*05 REMARK 410 REG 0 B 1 2 108 114 D-REGION REMARK 410 REG 0 B 1 3 115 126 IGHJ6*02,IGHJ6*01 REMARK 410 DOM 0 B 2 C 2001C 2121 REMARK 410 REG 0 B 2 1 2001C 2121 IGHG3*10,IGHG3*11,IGHG3*12,IGHG3*13,IGHG3 REMARK 410 REG 0 B 2 1 2001C 2121 *14,IGHG3*15,IGHG3*16,IGHG3*17,IGHG3*04,I REMARK 410 REG 0 B 2 1 2001C 2121 GHG3*05,IGHG3*20,IGHG3*07,IGHG3*08,IGHG3* REMARK 410 REG 0 B 2 1 2001C 2121 01,IGHG3*03,IGHG3*06,IGHG3*09 </pre>		
	C-DOMAIN	<pre> PSSSL...GTQTYTQNVNHKP...SNTKVDKRV </pre>	

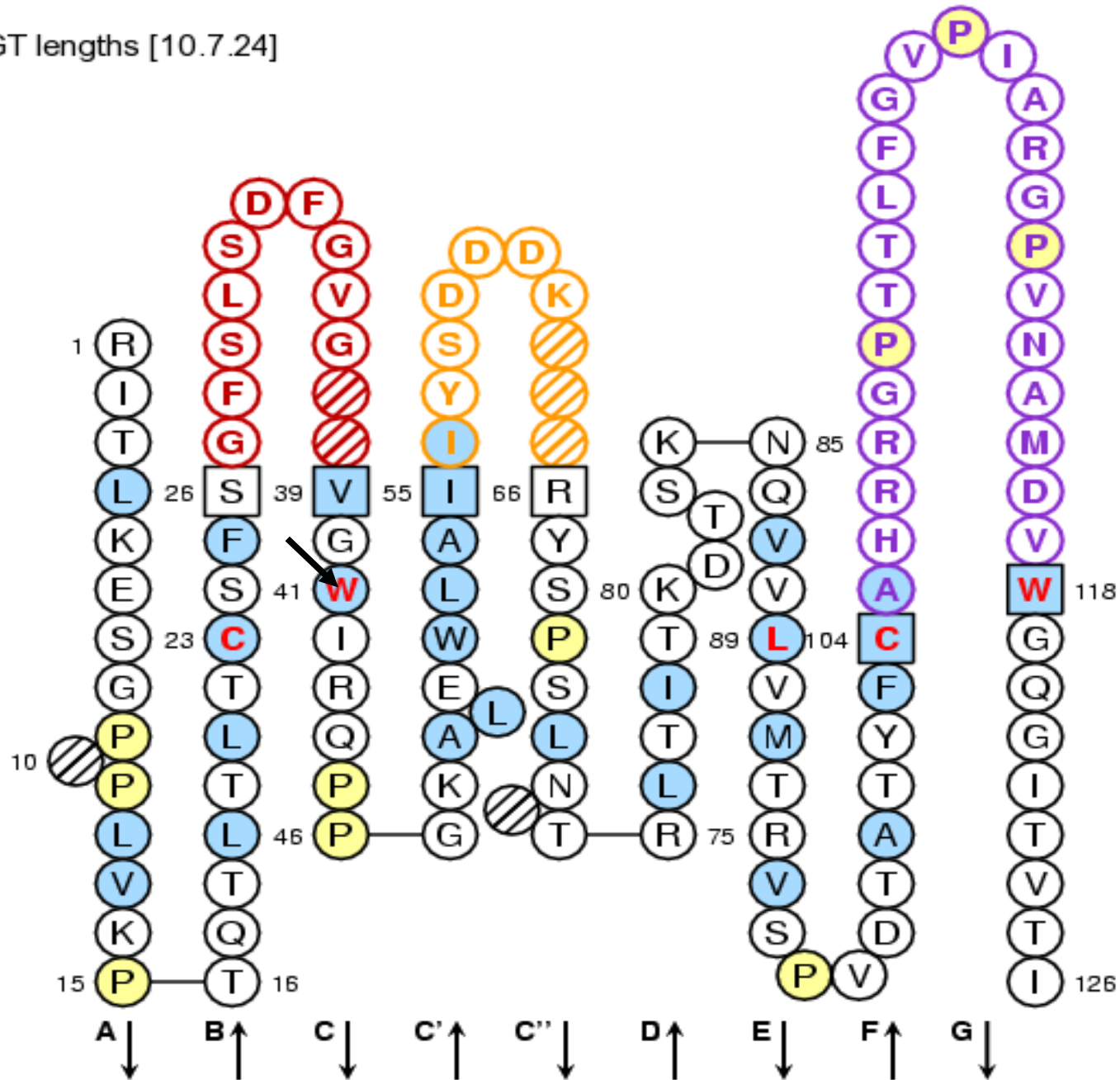
Domain

CDR-IMGT lengths

IMGT gene and allele

IMGT Collier de Perles : *Homo sapiens* (Human) IGHV_1 V-DOMAIN from 2F5 (PDB: 1u8k_B)

CDR-IMGT lengths [10.7.24]



From IMGT Colliers de Perles or from domain/chain sequence

41V - TRP (W)

chain : 1u8k_B

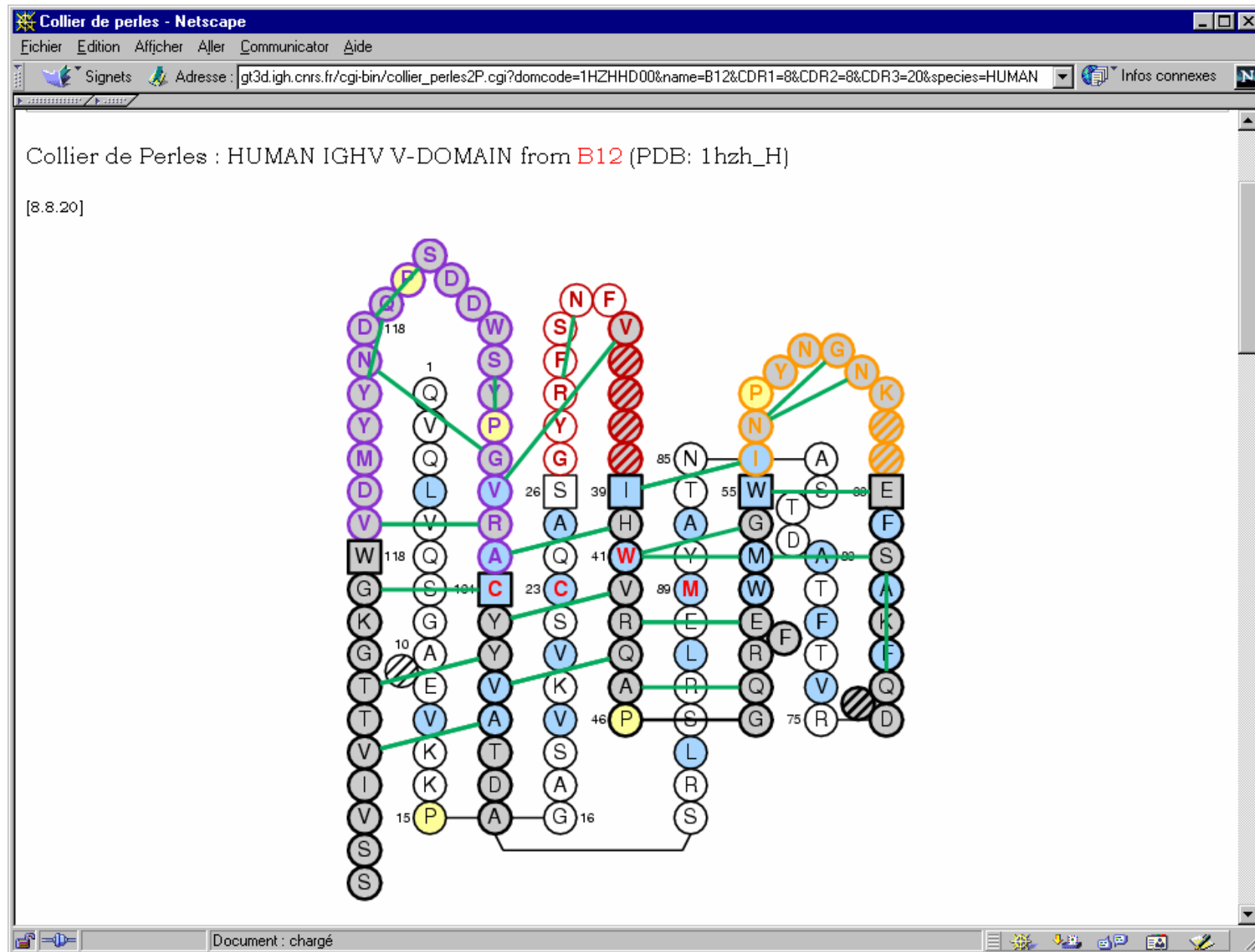
Secondary structure	Extended conformation
Phi	-122.64
Psi	137.12
ASA	0.0

Residue local structure

IMGT Num	Code 1C	Code 3C	Chain	Domain	Tot	NCov	Pol	HB	NPol	Cov	SS
Info	6V1	E	GLU	1u8k_B VH	6	6	0	0	6	0	0
Info	21V1	L	LEU	1u8k_B VH	17	17	0	0	17	0	0
Info	22V1	T	THR	1u8k_B VH	8	8	0	0	8	0	0
Info	23V1	C	CYS	1u8k_B VH	10	10	0	0	10	0	0
Info	39V1	V	VAL	1u8k_B VH	2	2	1	0	1	0	0
Info	43V1	R	ARG	1u8k_B VH	2	2	1	0	1	0	0
Info	51V1	E	GLU	1u8k_B VH	2	2	1	0	1	0	0
Info	52V1	W	TRP	1u8k_B VH	11	11	3	0	8	0	0
Info	53V1	L	LEU	1u8k_B VH	15	15	1	1	14	0	0
Info	54V1	A	ALA	1u8k_B VH	18	18	4	2	14	0	0
Info	55V1	I	ILE	1u8k_B VH	2	2	1	0	1	0	0
Info	78V1	I	ILE	1u8k_B VH	5	5	0	0	5	0	0
Info	87V1	V	VAL	1u8k_B VH	11	11	1	0	10	0	0
Info	88V1	V	VAL	1u8k_B VH	6	6	2	0	4	0	0
Info	89V1	L	LEU	1u8k_B VH	33	33	1	0	32	0	0
Info	102V1	Y	TYR	1u8k_B VH	5	5	0	0	5	0	0
Info	103V1	F	PHE	1u8k_B VH	18	18	2	0	16	0	0
Info	104V1	C	CYS	1u8k_B VH	26	26	0	0	26	0	0
Info	105V1	A	ALA	1u8k_B VH	1	1	1	0	0	0	0

Tot	Total number of atomic pair contacts
NCo	Number of non covalent atomic pair contacts
Pol	Number of polar atomic pair contacts
HB	Number of hydrogen bonds
NPol	Number of non polar atomic pair contacts
Cov	Number of covalent links (other than chain covalent links)
SS	Number of disulfide bridges

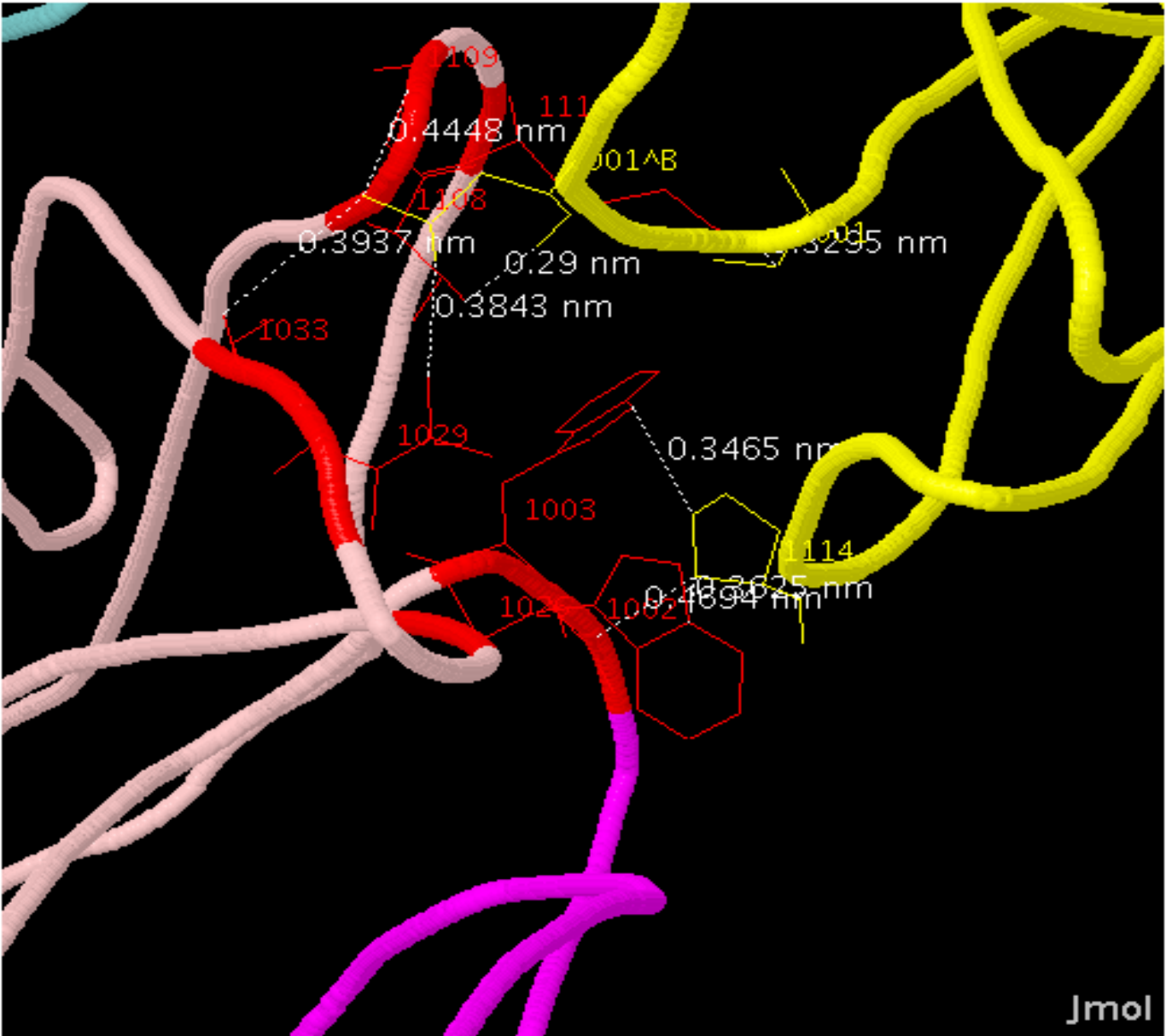
IMGT Collier de Perles



(1e4k)

IGHG1
(FC-GAMMA1)

CH2



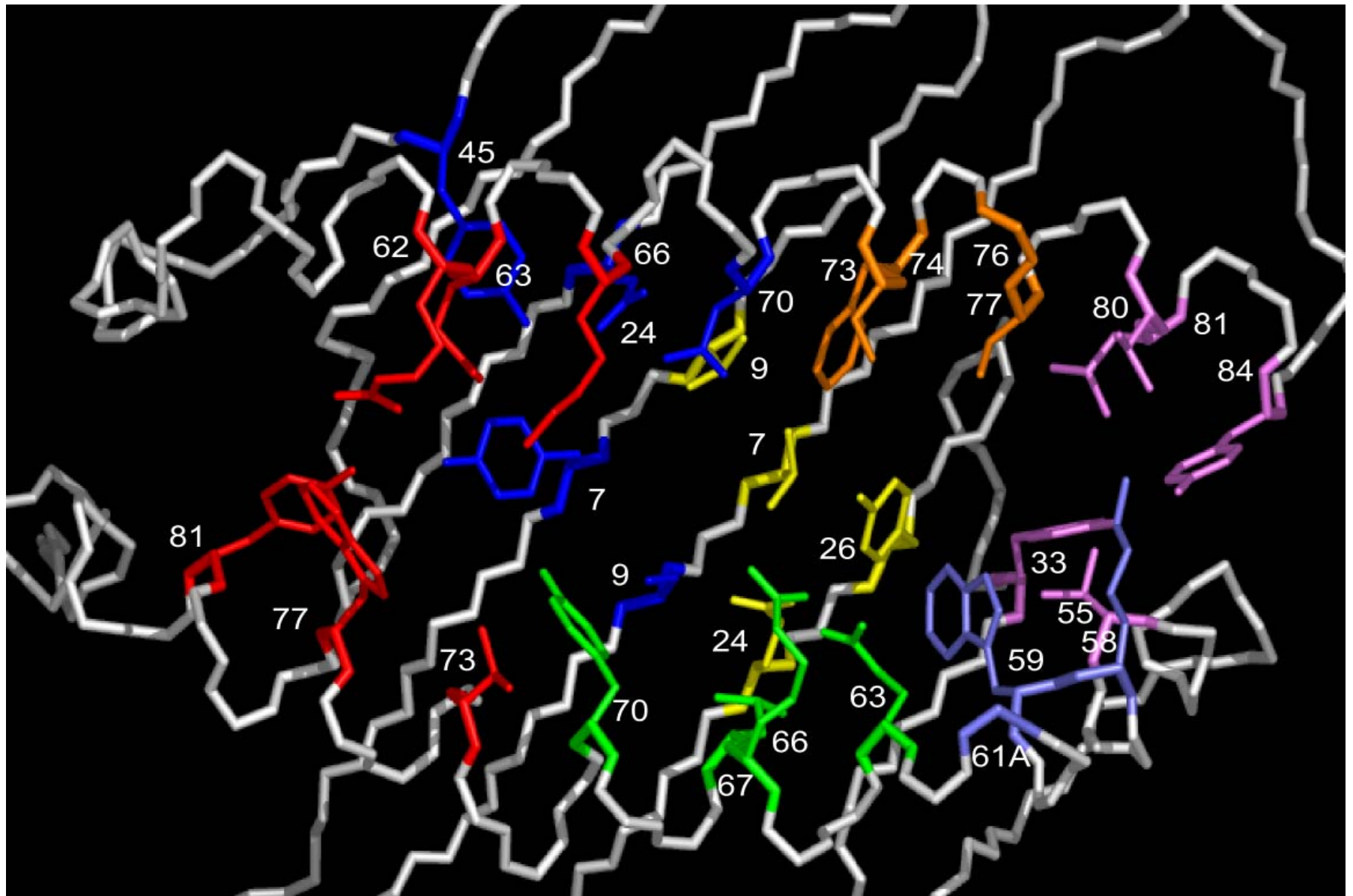
[D2]

FCGR3B

[D1]

MHC class I IMGT contact sites

C1	1 E
C2	--
C3	2 Q
C4	3 Y
C5	(4 K)
C6	5 F
C7	--
C8	--
C9	6 Y
C10	7 S
C11	8 V



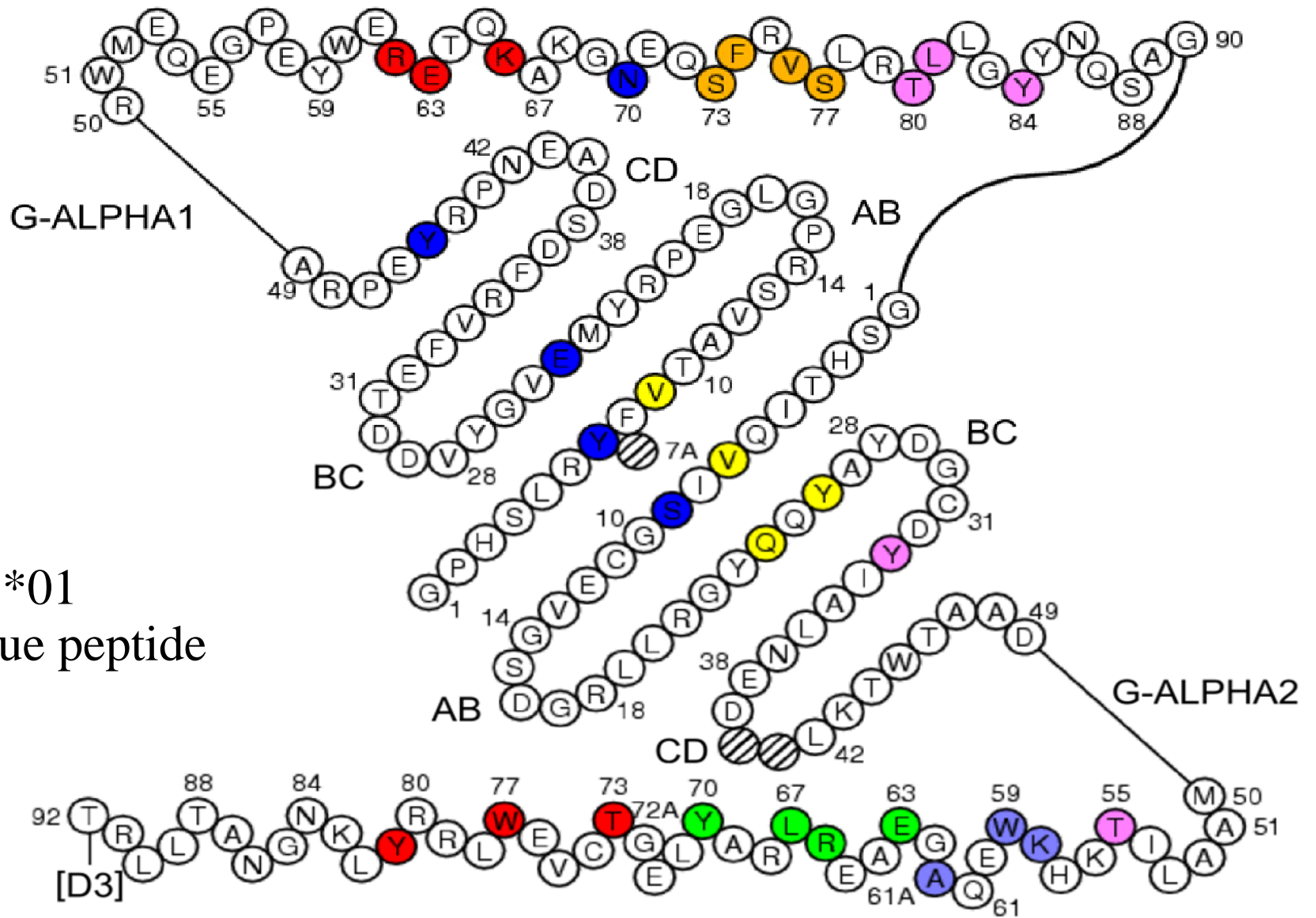
H2-K1*01

8 residue peptide

(code 1jtr)

MHC class I IMGT contact sites

C1	■	1 E
C2	■	--
C3	■	2 Q
C4	■	3 Y
C5	■	(4 K)
C6	■	5 F
C7	■	--
C8	■	--
C9	■	6 Y
C10	■	7 S
C11	■	8 V



H2-K1*01
8 residue peptide

The eleven IMGT amino acid classes according to the physico-chemical properties

(Pommié et al. *J. Mol Recogn.* 17:17-32, 2004)

'Volume' classes		'Hydropathy' classes						
	in Å ³	Hydrophobic		Neutral		Hydrophilic		
Very large	189-228	F		W	Y			
Large	162-174	I	L	M		H	K R	
Medium	138-154	V					E Q	
Small	108-117			C	P		D N	
Very small	60-90	A			G			
		Aliphatic		Sulfur	Hydroxyl	Basic	Acidic	Amide
		Nonpolar			Uncharged	Charged	Uncharged	
					Polar			

JUNCTION alignments

Click on mutated (underscored) amino acid to see the original one:

	104	105	106	107	108	109	110	111	111.1	111.2	111.3	111.4	112.5	112.4	112.3	112.2	112.1	112	113	114	115	116	117	118	Frame	CDR3-IMGT Length	Molecular mass			
#1 Z70256	C	<u>V</u>	R	V	V	Q	<u>R</u>	L	V									P	K	Y	H	F	D	<u>H</u>	W	+	15	2,438.76		
#2 Z70257	C	A	R	D	G	S	<u>S</u>	Y	A								R	P	Y	W	Y	F	D	L	W	+	16	2,256.49		
#3 Z70606	C	A	R	A	T	T	H												Y	A	F	D	V	W	+	11	1,604.77			
#4 Z70608	C	A	R	V	T	I	F	G	V	V								I	P	R	G	N	A	F	D	I	W	+	18	2,426.78
#5 Z70610	C	A	R	V	G	S	D	F	W	S	G							Y	S	R	H	D	A	F	D	I	W	+	19	2,539.73
#6 Z70611	C	A	R	H	G	<u>N</u>	Y	N	A									G	V	D	W	F	D	P	W	+	15	2,072.21		
#7 Z70613	C	A	R	A	A	A	G												T	S	L	F	D	Y	W	+	12	1,531.71		
#8 Z70614	C	A	R	H	Y	N	<u>S</u>	G											<u>I</u>	Y	P	L	D	Y	W	+	13	1,846.01		
#9 Z70615	C	A	R	G	L	V	<u>K</u>	<u>R</u>	V									S	E	Y	W	Y	F	D	L	W	+	16	2,419.75	
#10 Z70616	C	A	R	A	G	L	G												S	H	W	F	D	P	W	+	12	1,602.8		
#11 Z70620	C	A	R	D	R	G	<u>G</u>	M											<u>V</u>	R	D	A	F	D	I	W	+	14	1,932.17	
#12 Z70621	C	A	R	H	H	D	L	W	F										G	E	F	D	P	L	D	Y	W	+	16	2,307.53
	C	A	R	D	C	P	A	P	A	K	M	Y	Y	Y	G	S	G	I	C	T	F	D	Y	W						

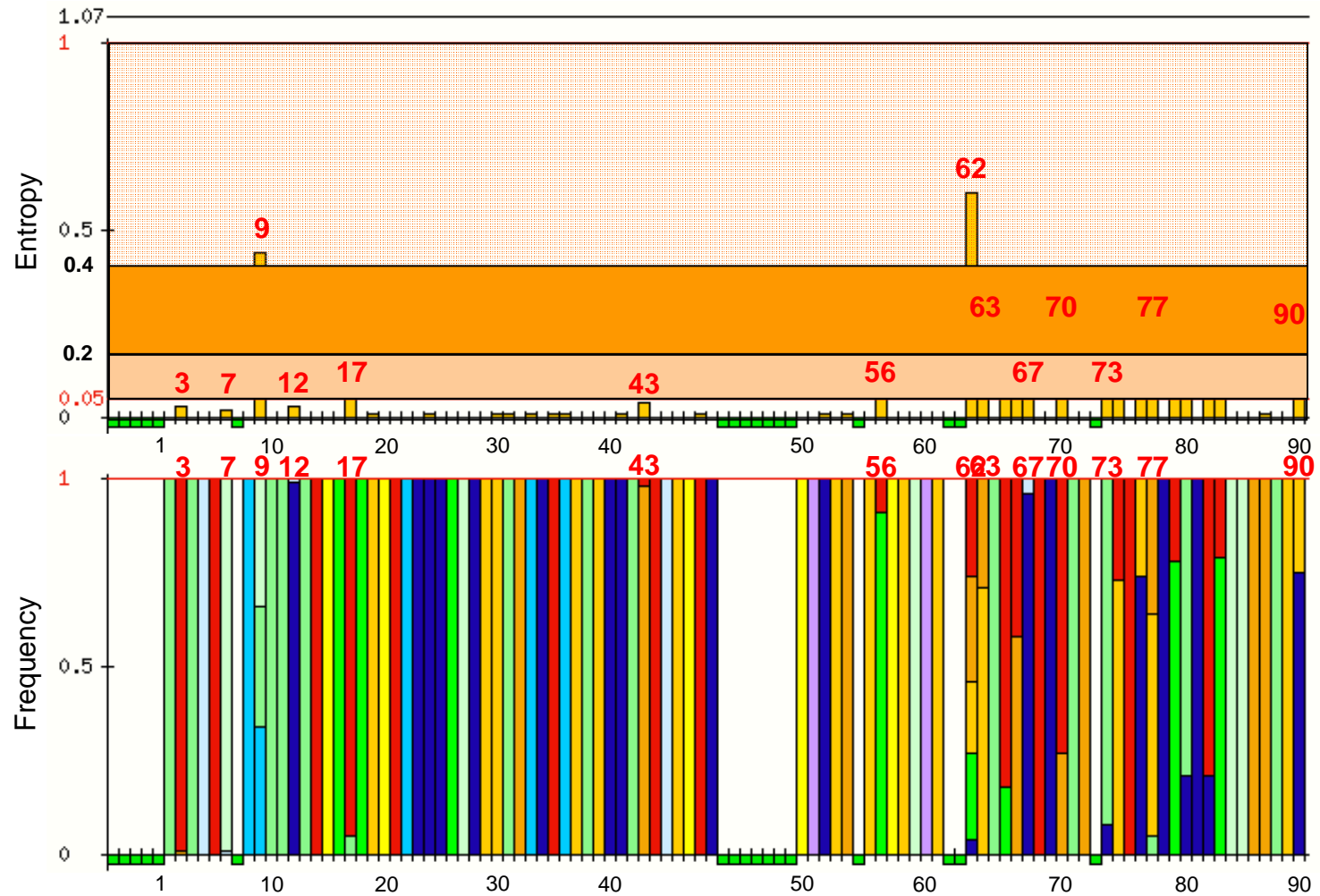
HLA-A sequence polymorphism according to the IMGT unique numbering

G-ALPHA1 [D1] domain

The eleven IMGT amino acid classes

- Basic (H,K,R)
- Amide (N,Q)
- Acidic (D,E)
- Proline (P)
- Tyrosine (Y)
- Tryptophan (W)
- Hydroxyl (S,T)
- Glycine (G)
- Sulfur (C,M)
- Phenylalanine (F)
- Aliphatic (A,V,I,L)

HLA-A gene:
212 alleles



V-DOMAIN 3D representation (TR A6, 1ao7)

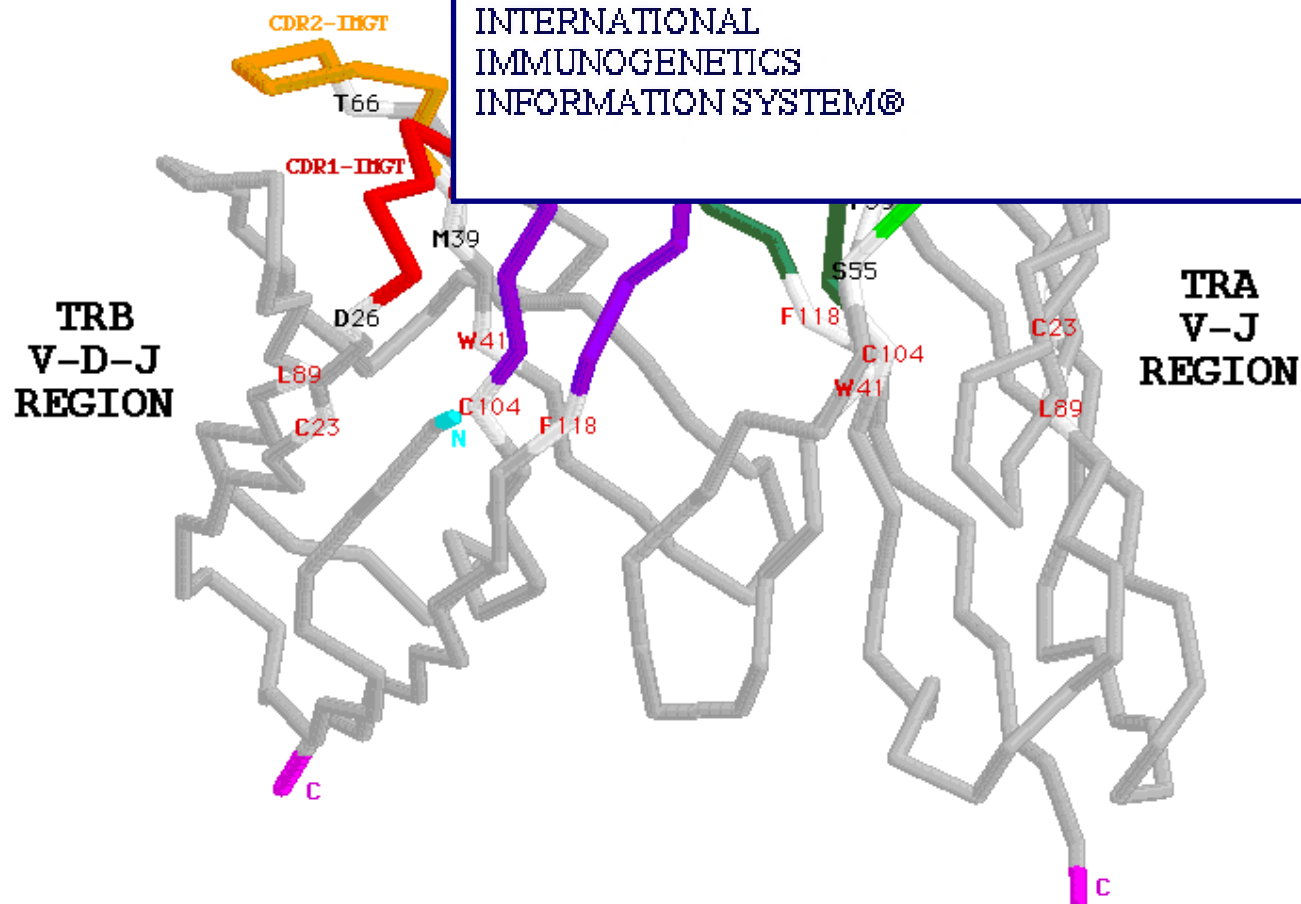
WELCOME !

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The IMGT team at Montpellier, France



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