

IMGT-ONTOLOGY: a must for integrative immunogenetics and immunoinformatics

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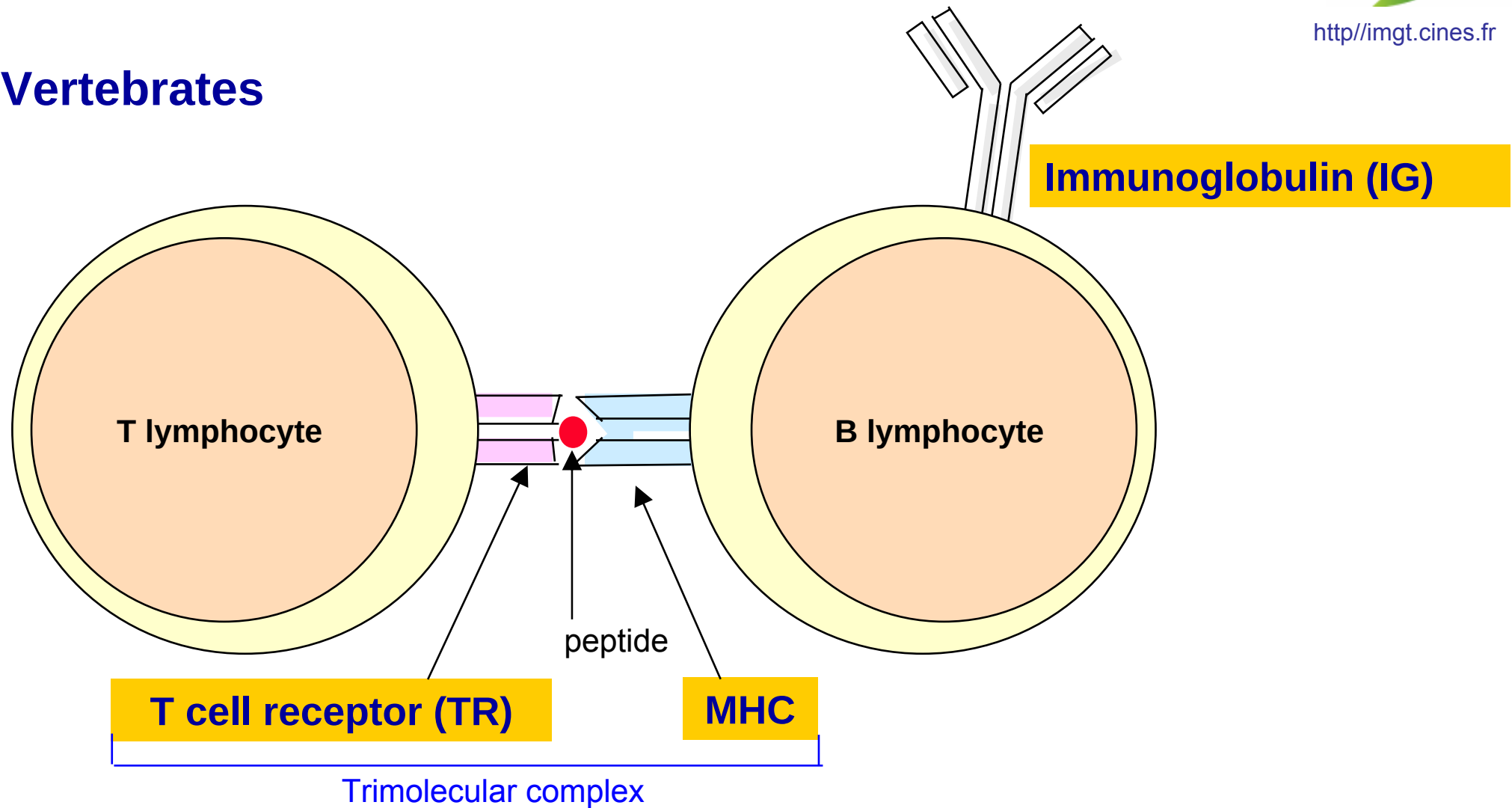
First Immunomics Summer School

Computer modelling, from molecules to clinics

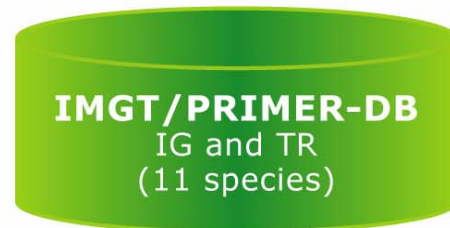
Catania, 24 August-3 September 2007

IMGT®: the adaptive immune response

Vertebrates



Sequences



IMGT/V-QUEST

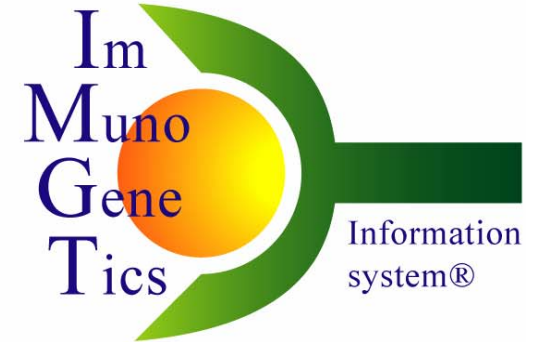
IMGT/JunctionAnalysis

IMGT/Allele-Align

IMGT/PhyloGene

IMGT/GENE-DB
IG and TR
(human and mouse)

IMGT/3Dstructure-DB
IG, TR and MHC



<http://imgt.cines.fr>

Genome

IMGT/GeneInfo

IMGT/LocusView

IMGT/GeneSearch

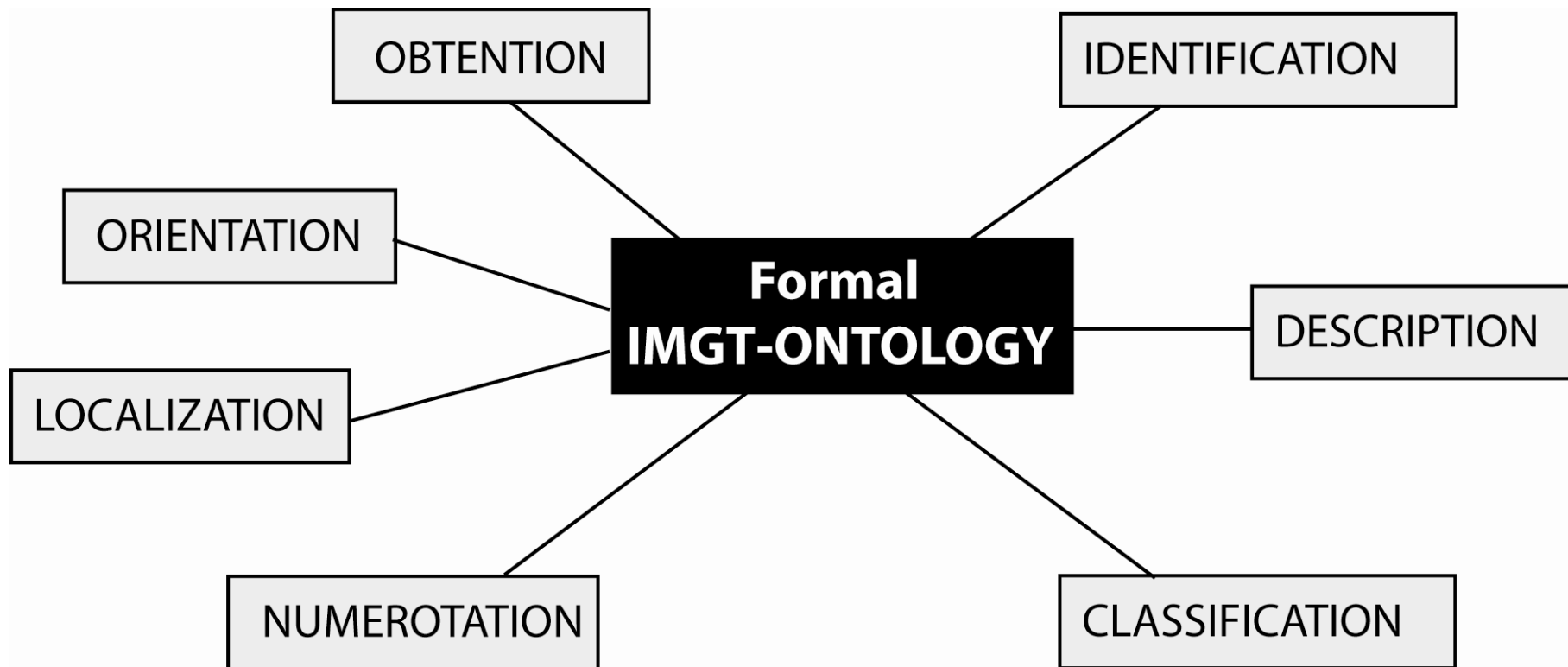
IMGT/GeneView

IMGT/StructuralQuery

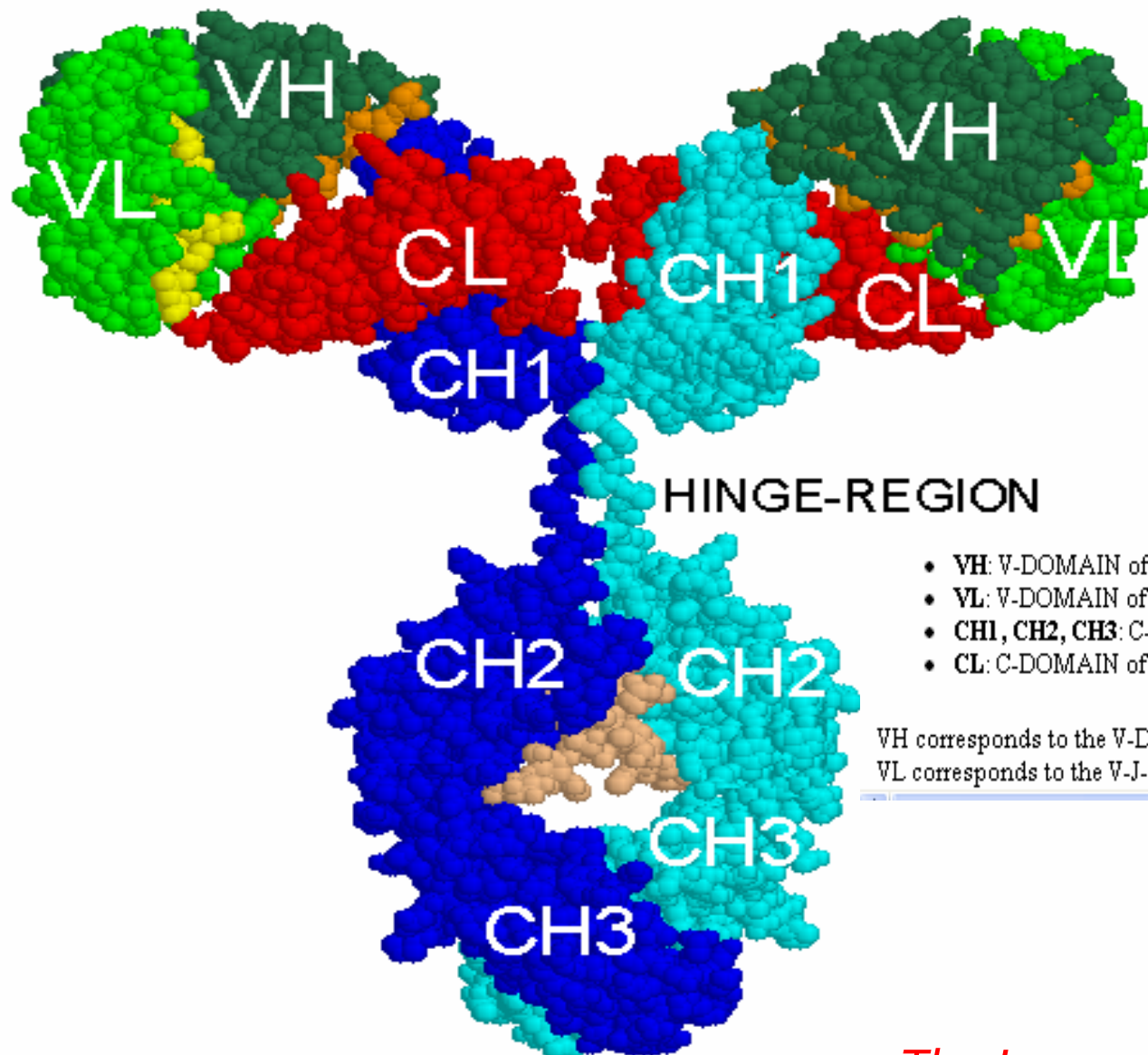
2D and 3D structures

IMGT-ONTOLOGY seven axioms:

To share, reuse and represent knowledge
in Immunogenetics and Life Sciences



1. Immunoglobulin IgG

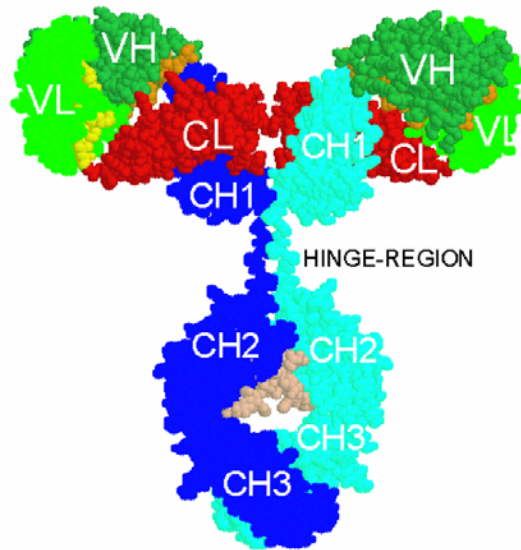


- VH: V-DOMAIN of the immunoglobulin heavy chain
- VL: V-DOMAIN of the immunoglobulin light chain
- CH1, CH2, CH3: C-DOMAIN of the immunoglobulin heavy chain
- CL: C-DOMAIN of the immunoglobulin light chain

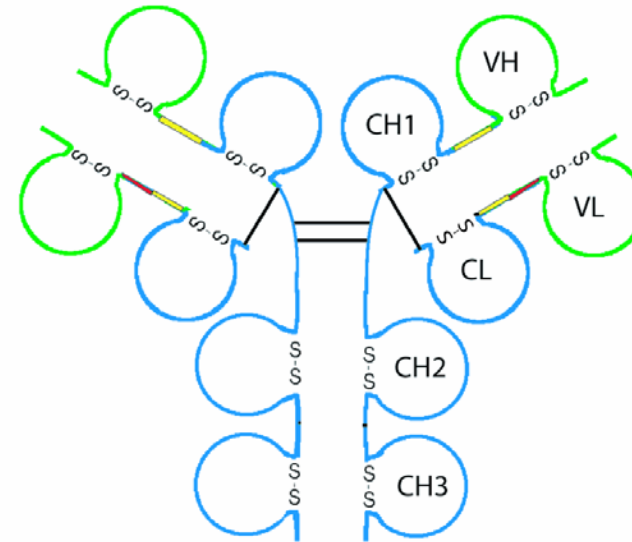
VH corresponds to the V-D-J-REGION (in green (V), orange (DJ)) of the heavy chain.
VL corresponds to the V-J-REGION (in green (V) and yellow (J)) of the light chain.

1. Immunoglobulin IgG

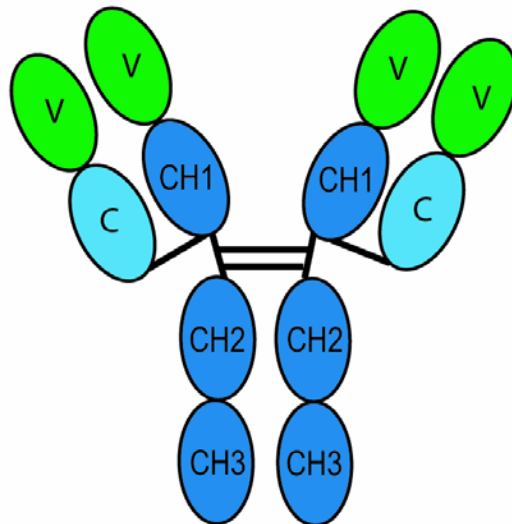
A



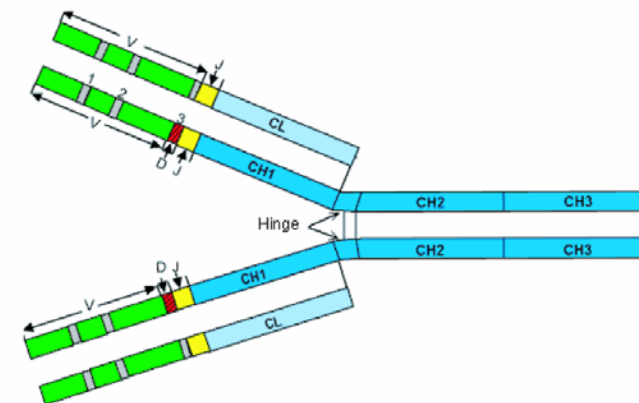
B



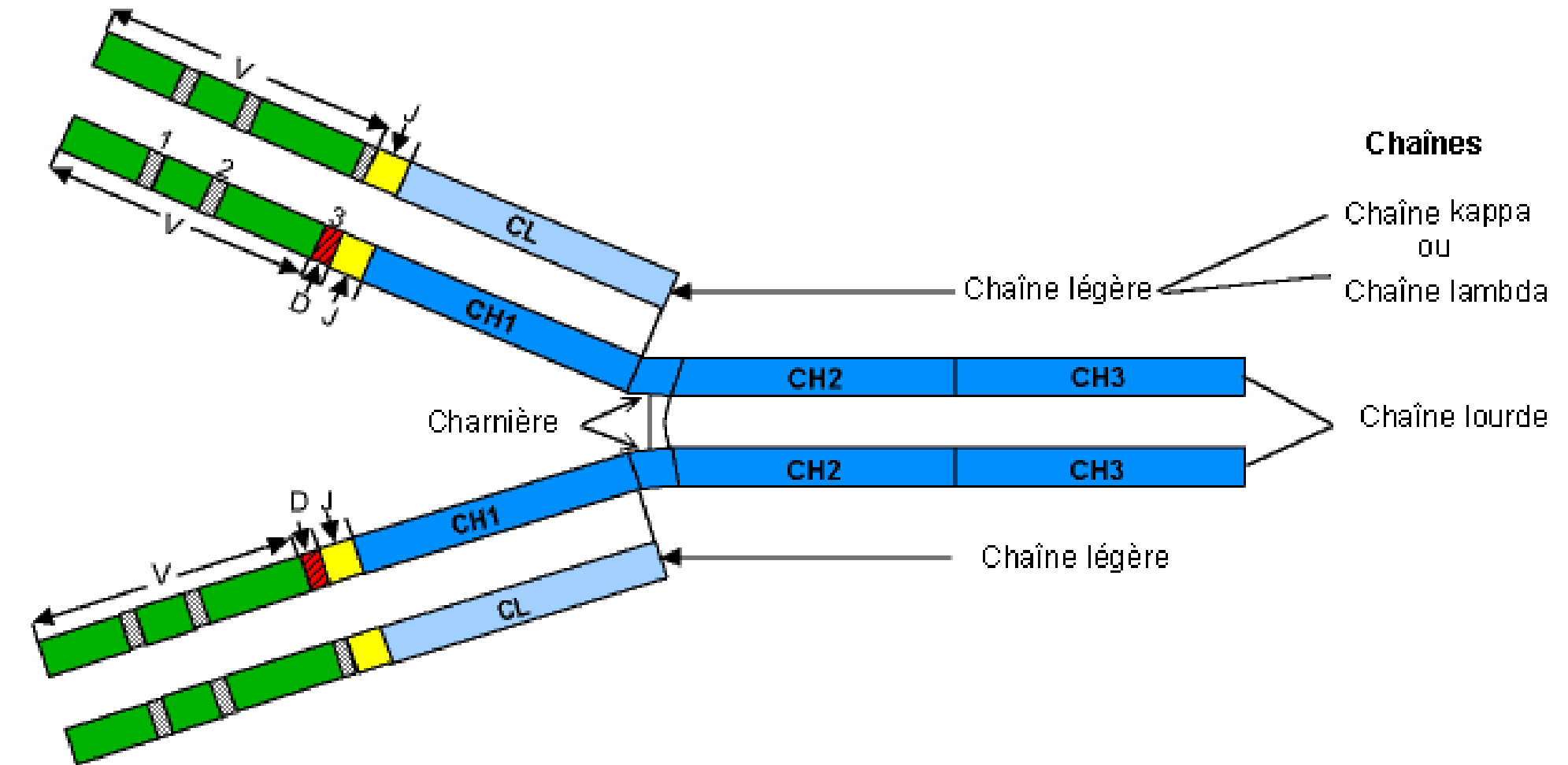
C



D



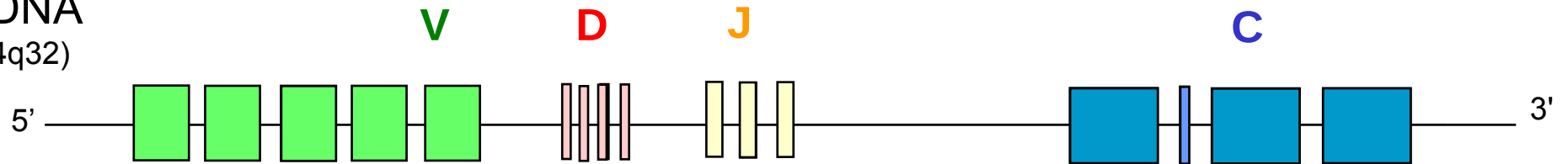
1. Immunoglobulin IgG



1.

Immunoglobulin (IG) synthesis

genomic DNA
(IGH Locus 14q32)

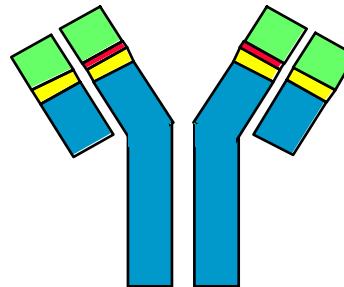


rearranged
DNA



mRNA

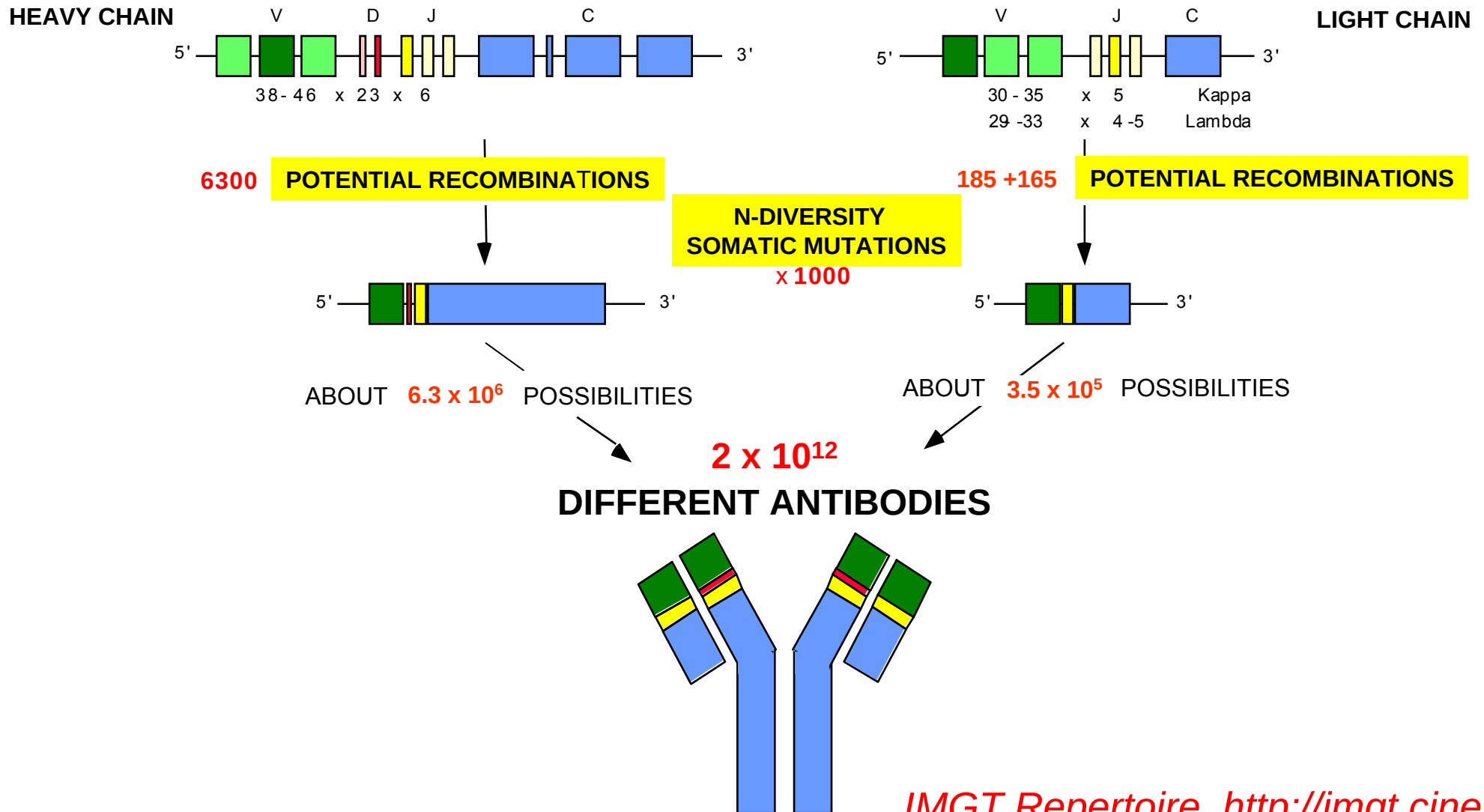
2×10^{12} different IG
per individual



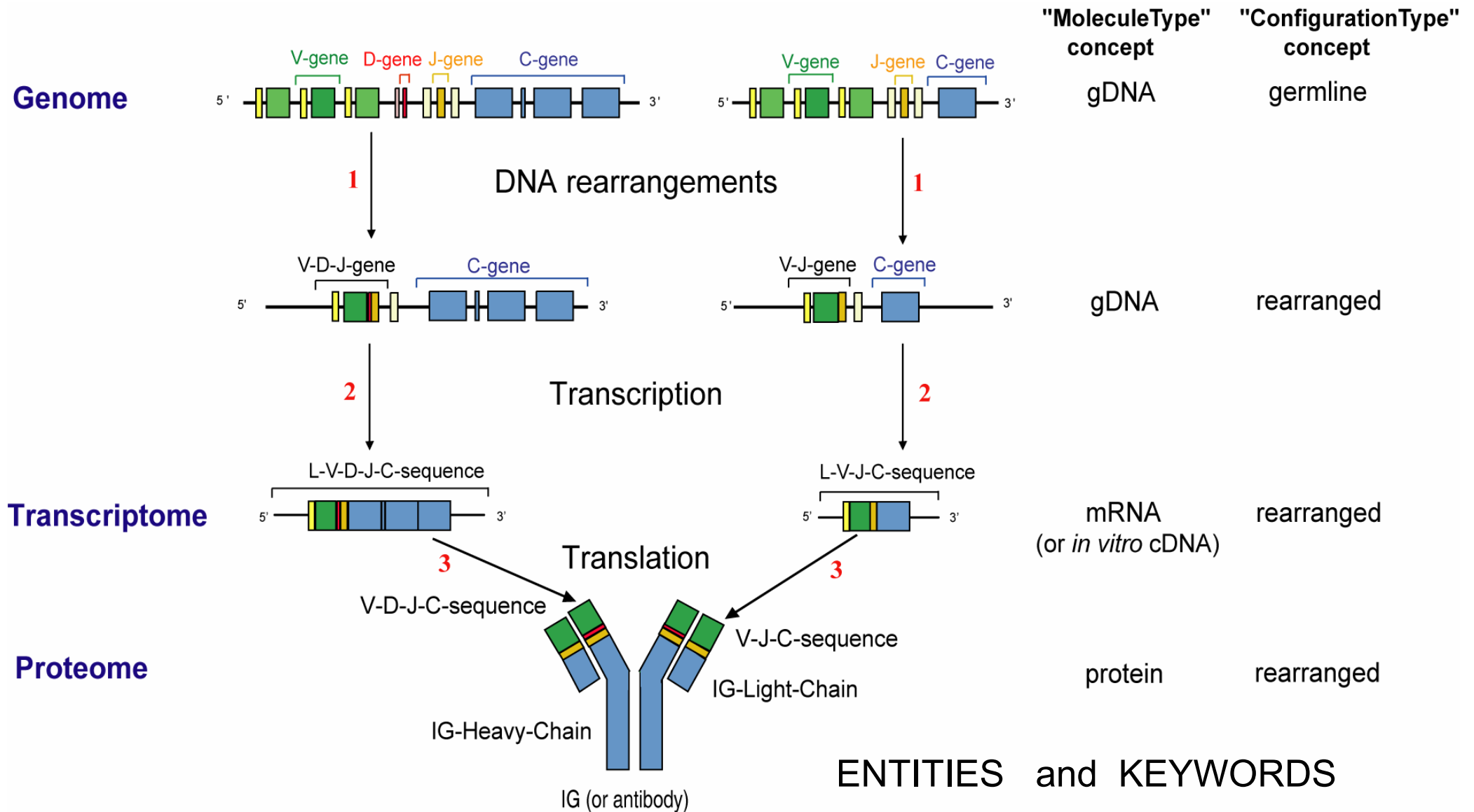
1.

Immunoglobulin (IG) synthesis

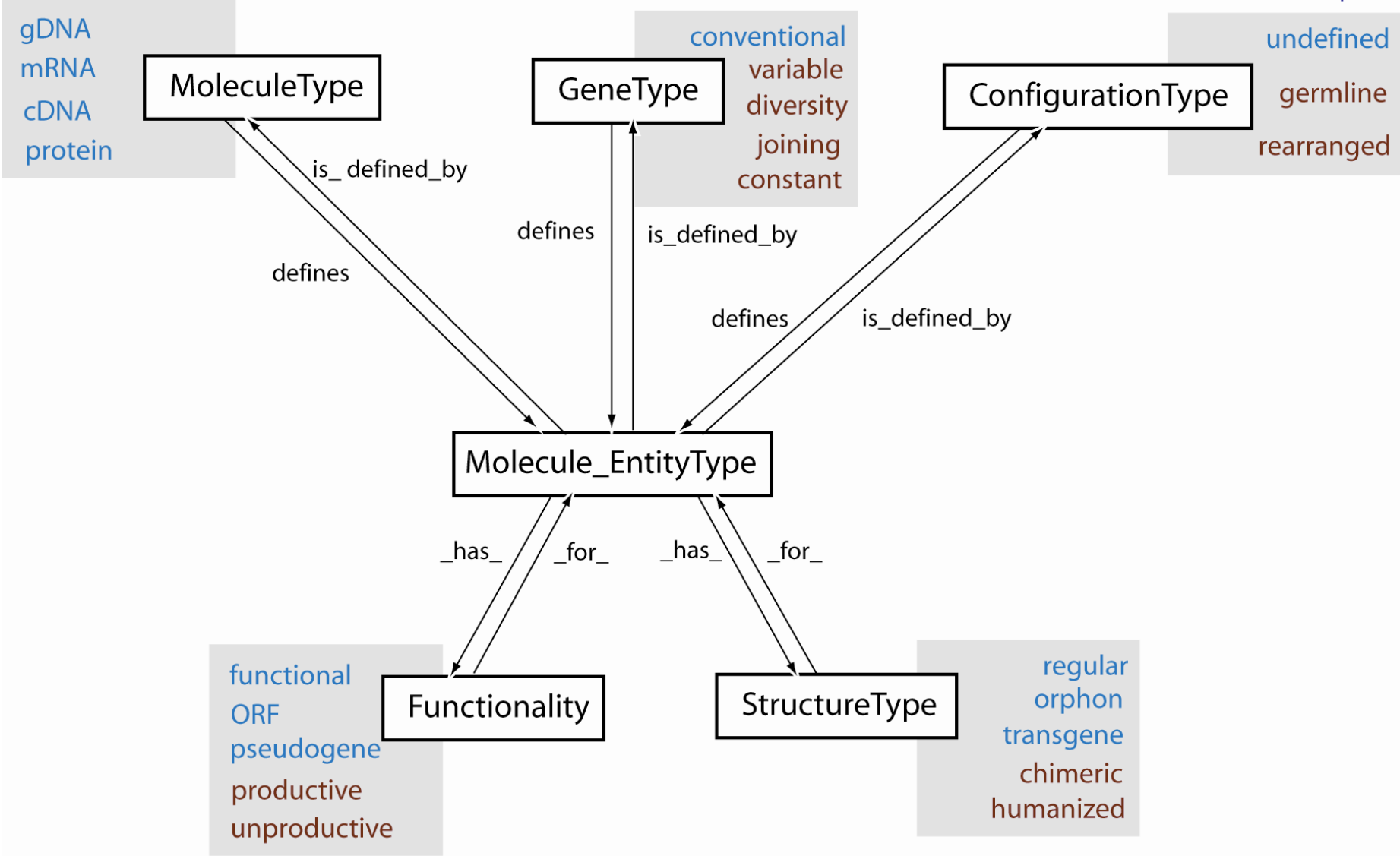
150
FUNCTIONAL IG GENES



1. IDENTIFICATION axiom



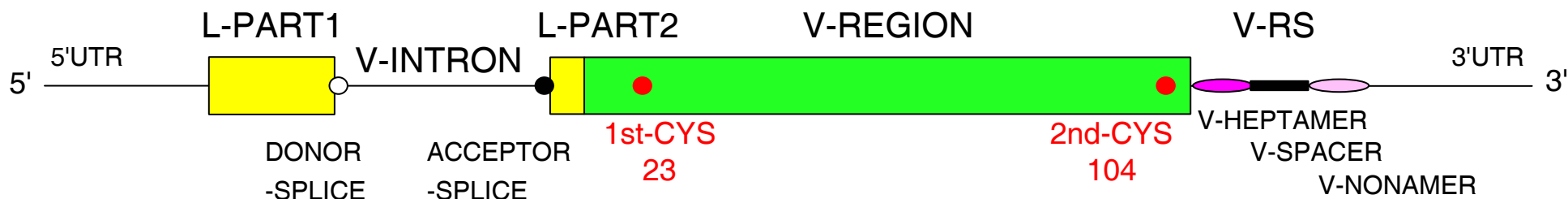
1. IDENTIFICATION axiom



2. Description of a V-GENE

>X62106.0|HSVI2|*Homo sapiens* VI-2 gene for immunoglobulin heavy chain

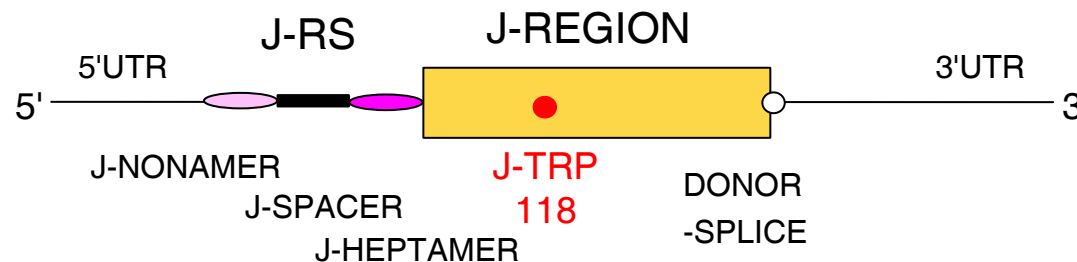
tgagagctcc	gttcctcacc	atggactgga	cctggaggat	cctcttcttg	gtggcagcag	60
ccacagggt	aa gaggctccct	agtcccagtg	atgagaaaga	gattgagtcc	agtccagggg	120
gatctcatcc	acttctgtgt	tctctccaca	ggagcccact	ccaggtgca	gctggtgcag	180
tctggggctg	aggtgaagaa	gcctggggcc	tcagtgaagg	tctcctgcaa	ggcttctgga	240
tacaccttca	ccggctacta	tatgcactgg	gtgcgacagg	cccctggaca	agggcttgag	300
tgatgggat	ggatcaacc	taacagtgg	ggcacaaact	atgcacagaa	gtttcagggc	360
agggtcacca	tgaccaggg	cacgtccatc	agcacagcct	acatggagct	gagcaggctg	420
agatctgacg	acacggccgt	gtattactgt	gcgagagaca	cagtg	tgaaa accc	480
tgaggggtg	tc agaaacc	caa gggaggagg	c ag			



2. Description of a J-GENE

>J00256|IGHJ1*01|*Homo sapiens* J-GENE

accccgggct	gtgggtttct	gtgcccctgg	ctcagggctg	actcaccgtg	gctgaatact	60
tccagcactg	gggccagggc	accctgggtca	ccgtctcctc	aggtagagtct	gctgtactgg	120
ggatagcggg	gagccatgtg	tactggggcca	agcaagggct	ttggcttcag		170



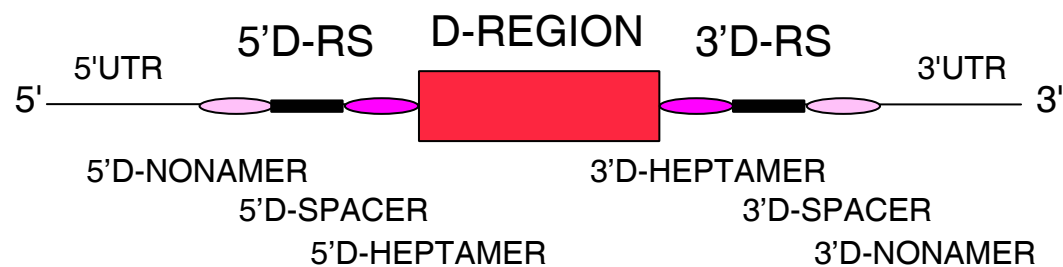
Heavy chain	WGXX (J-TRP)
Light chain	FGXX (J-PHE)

2. Description of a D-GENE

>J00256|IGHD7-27*01|*Homo sapiens* D-GENE

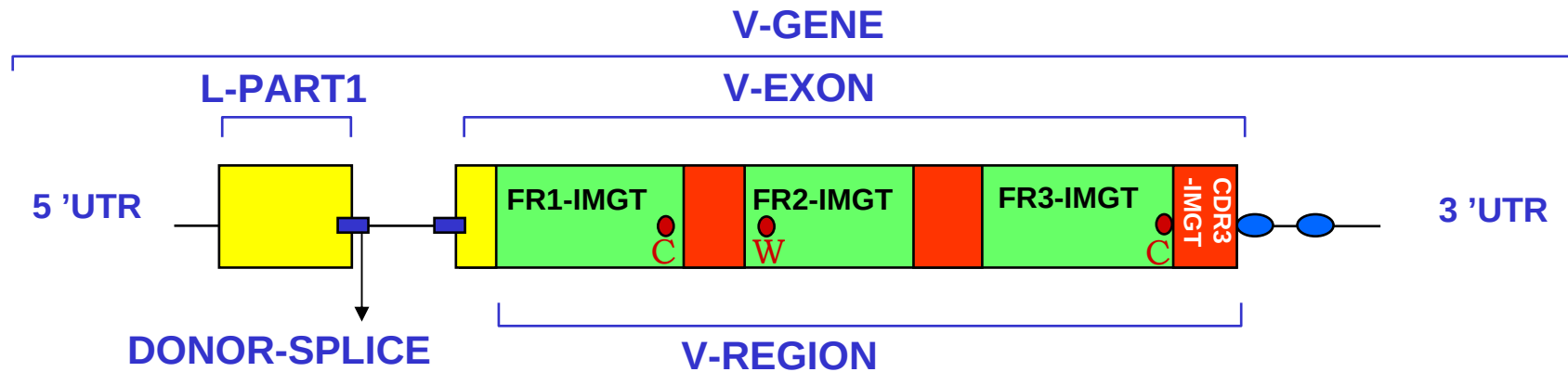
```
ccagccgcag gggtttttggc tgagctgaga accactgtgc taactgggga cacagtgaatt  
ggcagctcta caaaaaccat gctcccccg g
```

60



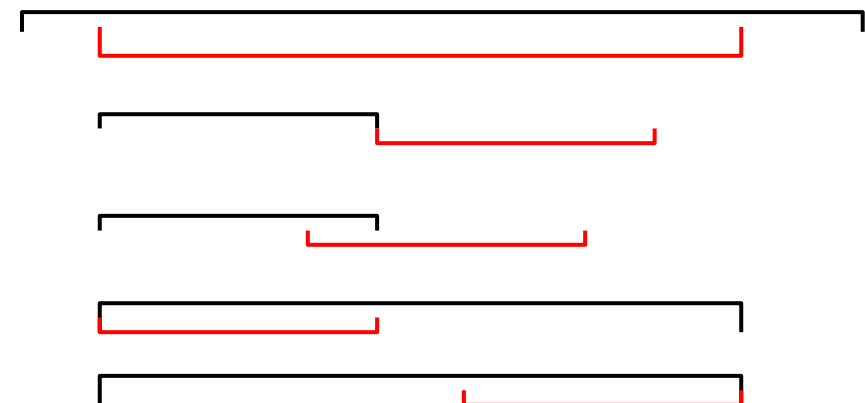
2. DESCRIPTION axiom

PROTOTYPE for a V-GENE



Label 1	Label 2
V-GENE	V-EXON
FR3-IMGT	CDR3-IMGT
L-PART1	DONOR-SPLICE
V-REGION	FR1-IMGT
V-REGION	CDR3-IMGT

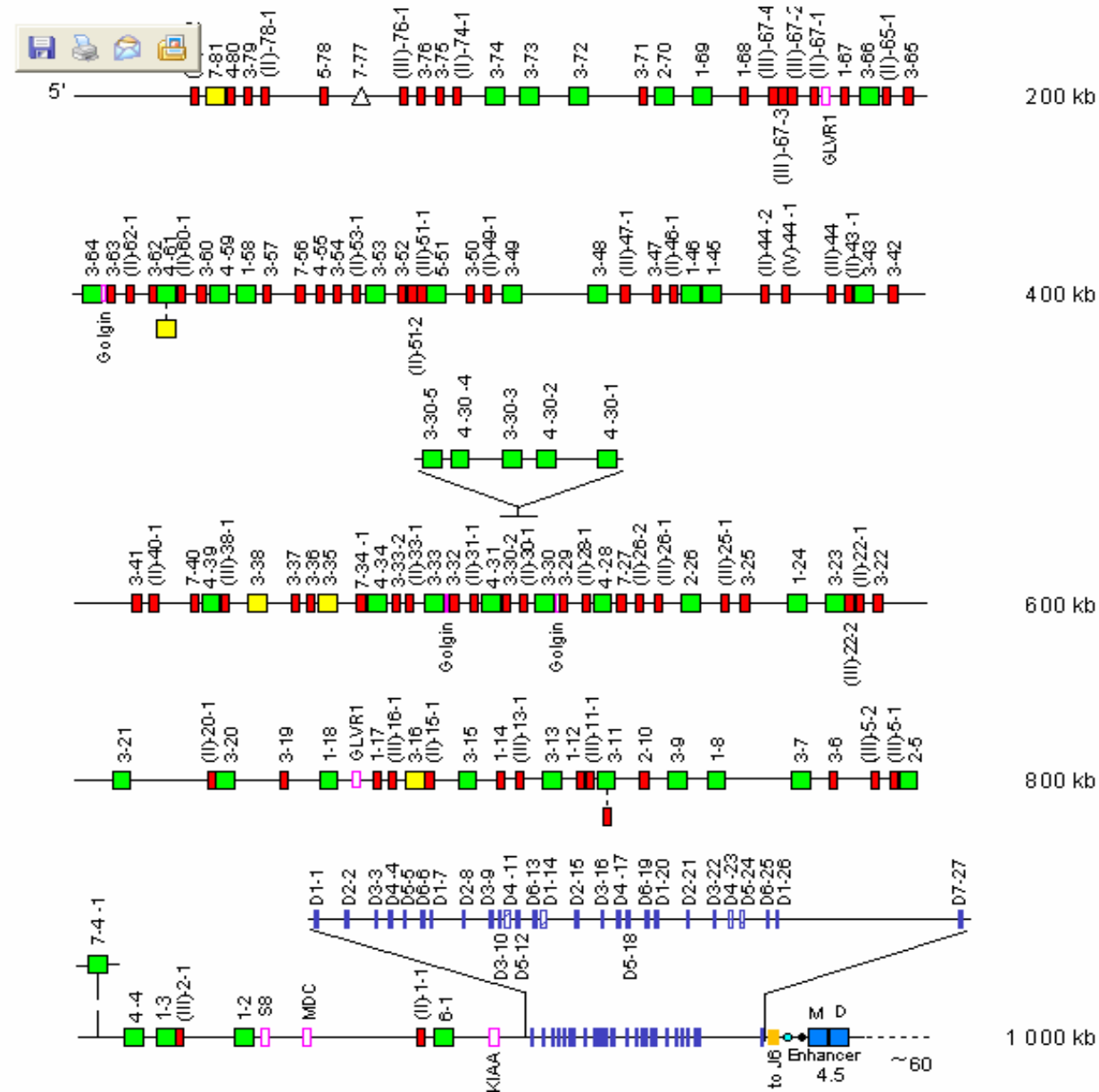
Relations entre Labels



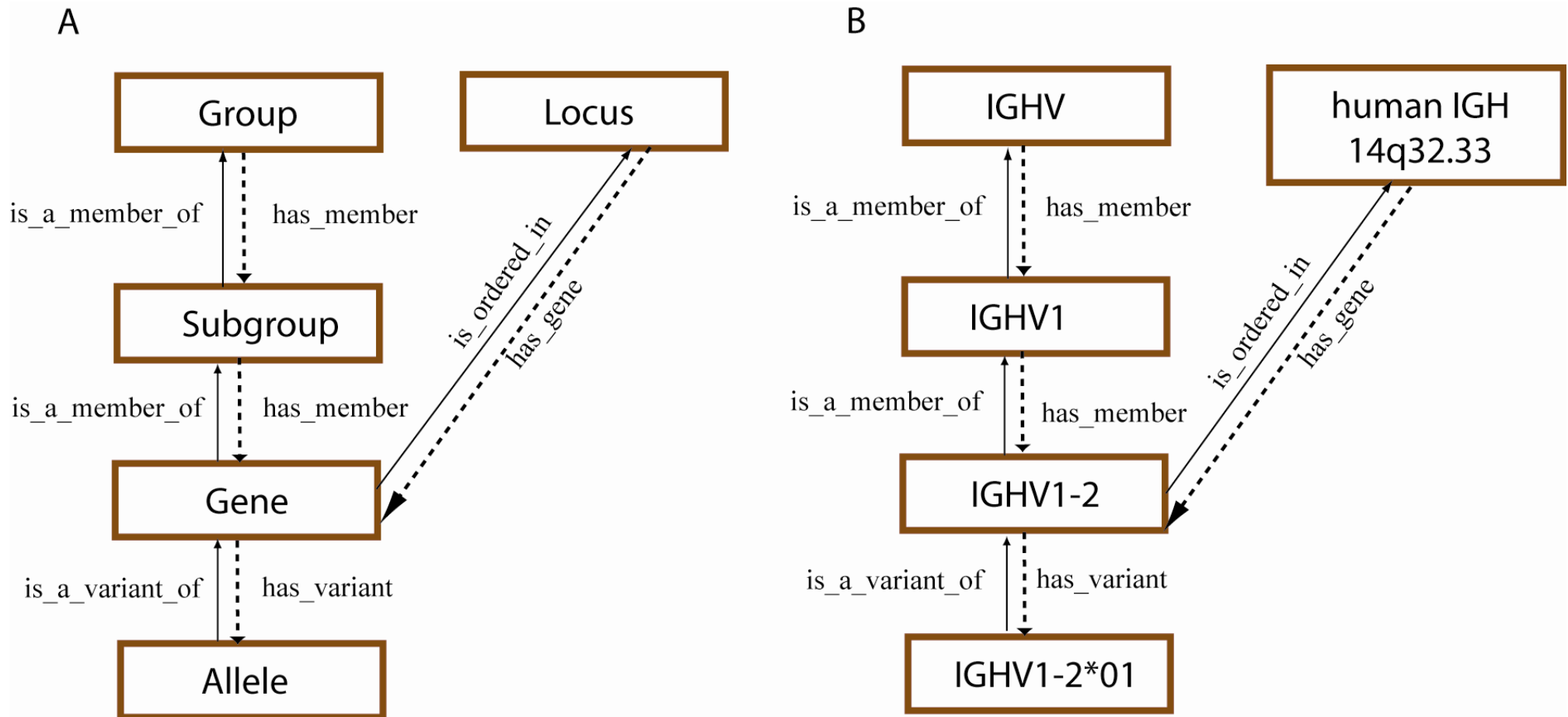
ENTITY PROTOTYPE and LABELS

3.

Chromosome 14q32.33



3. CLASSIFICATION axiom

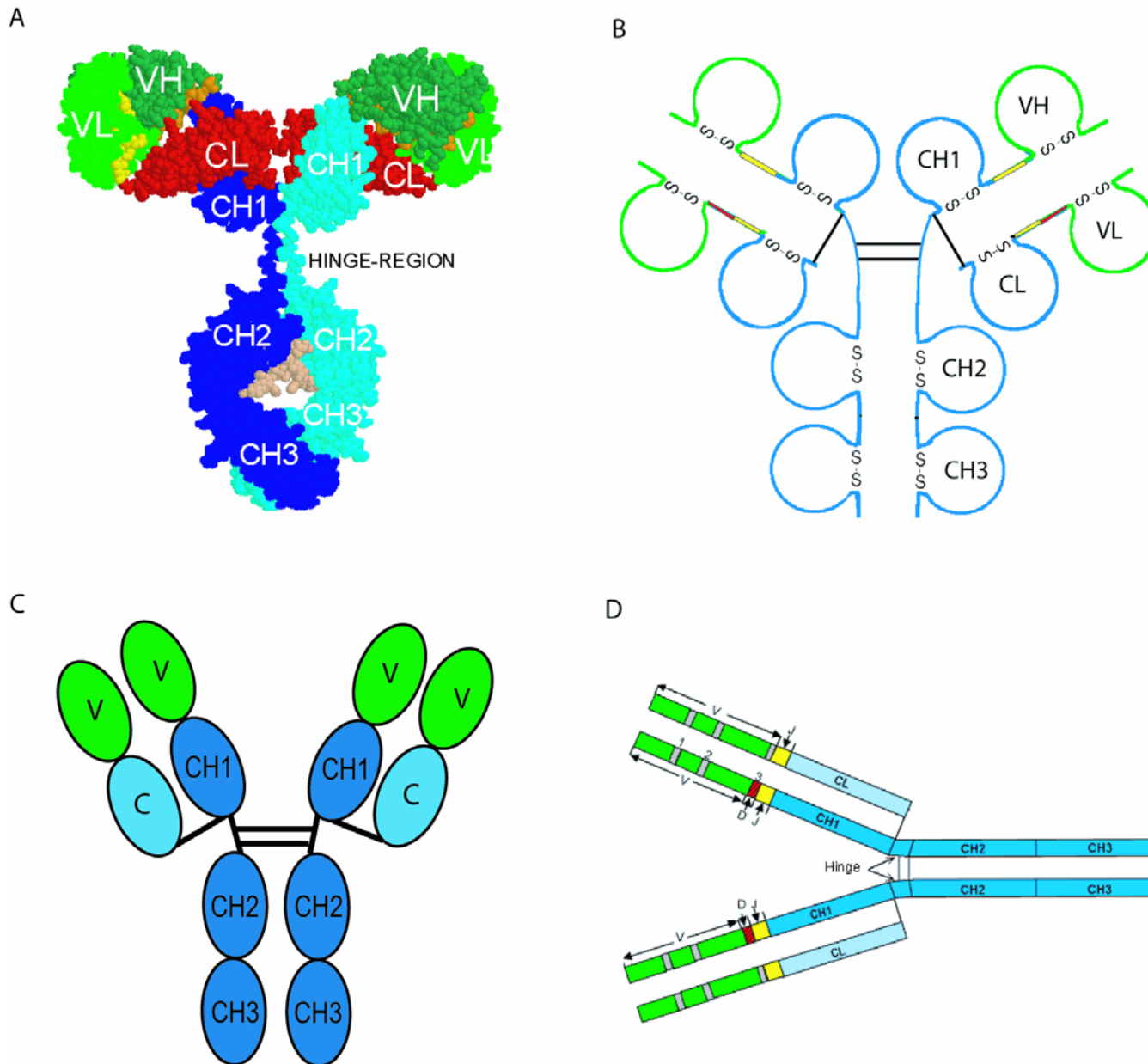


« Concepts »

« Concept instances »

NOMENCLATURE

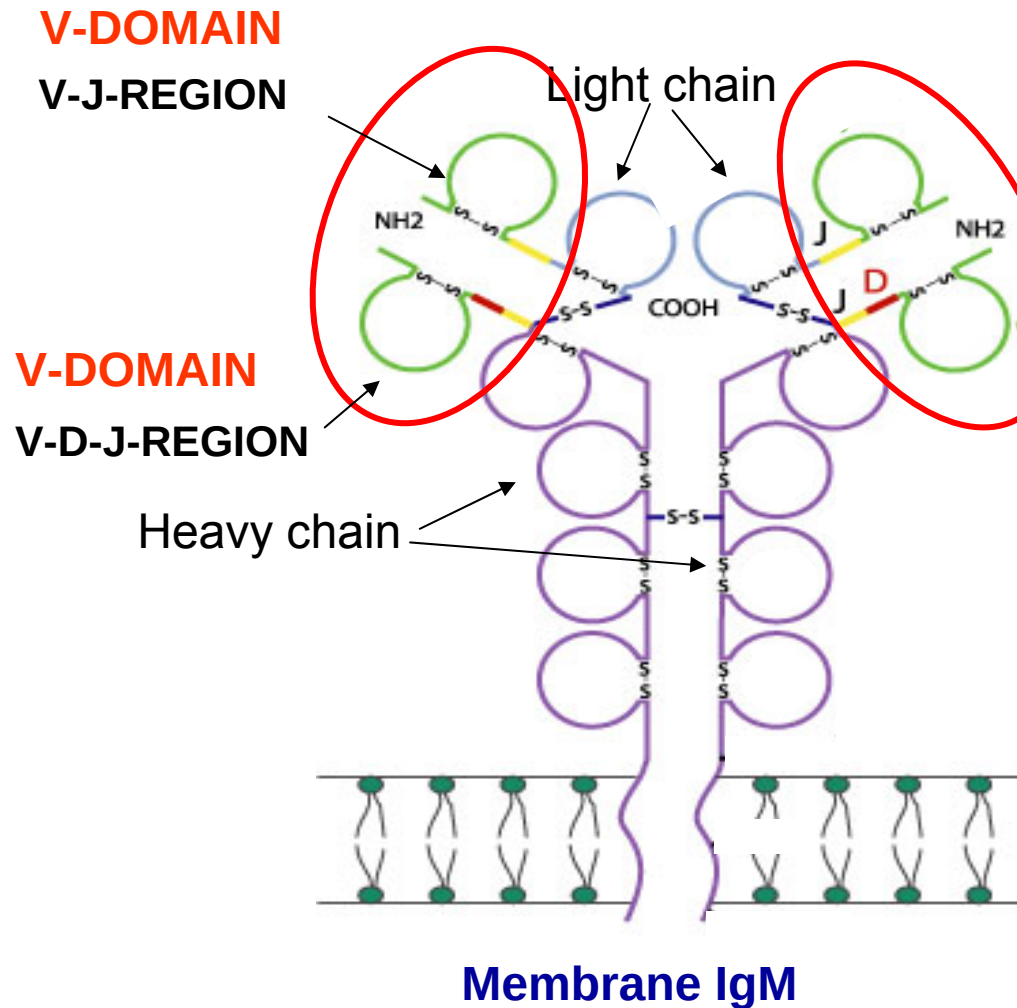
4. Immunoglobulin IgG



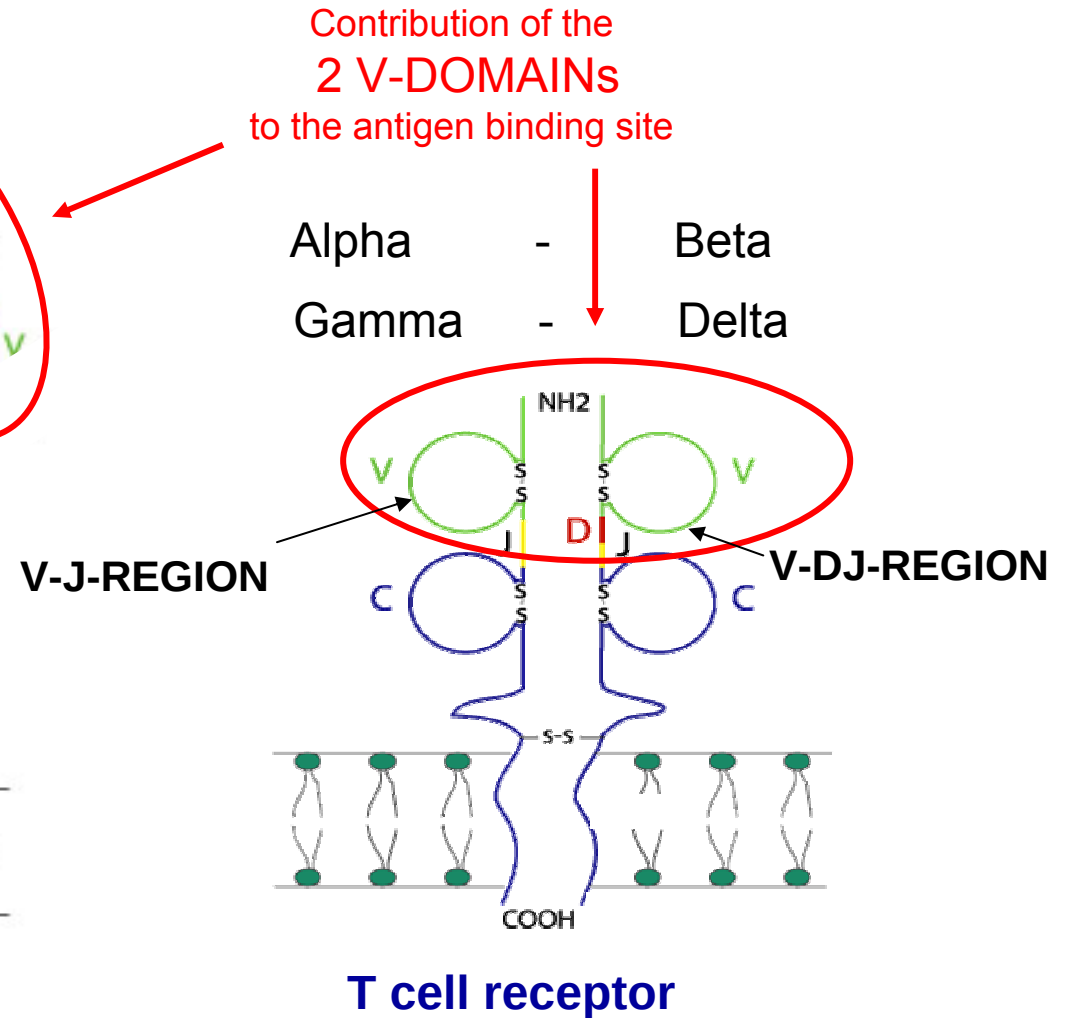
4.

Antigen receptors

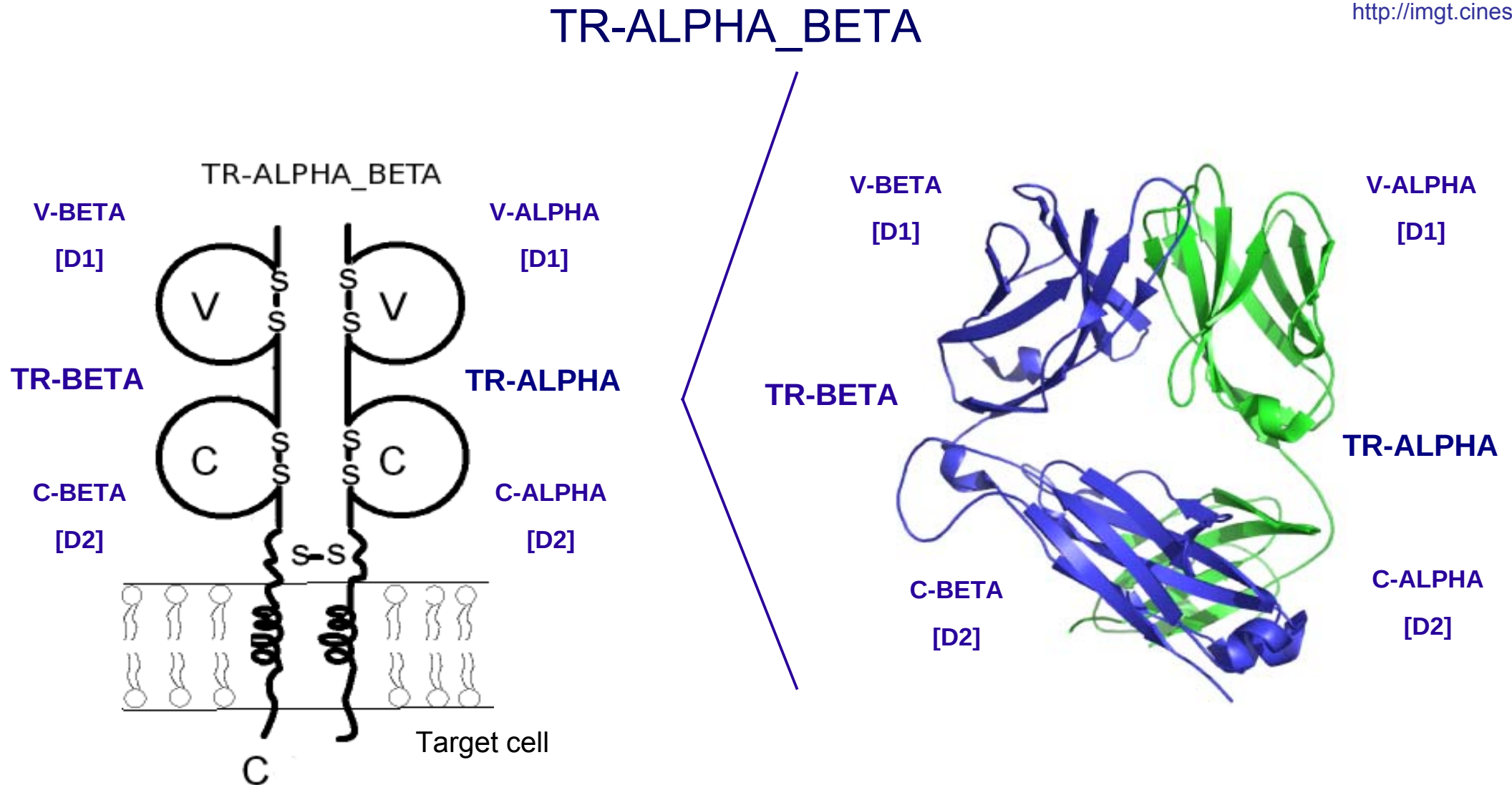
Immunoglobulin (IG)



T cell receptor (TR)



T cell receptor chains and domains

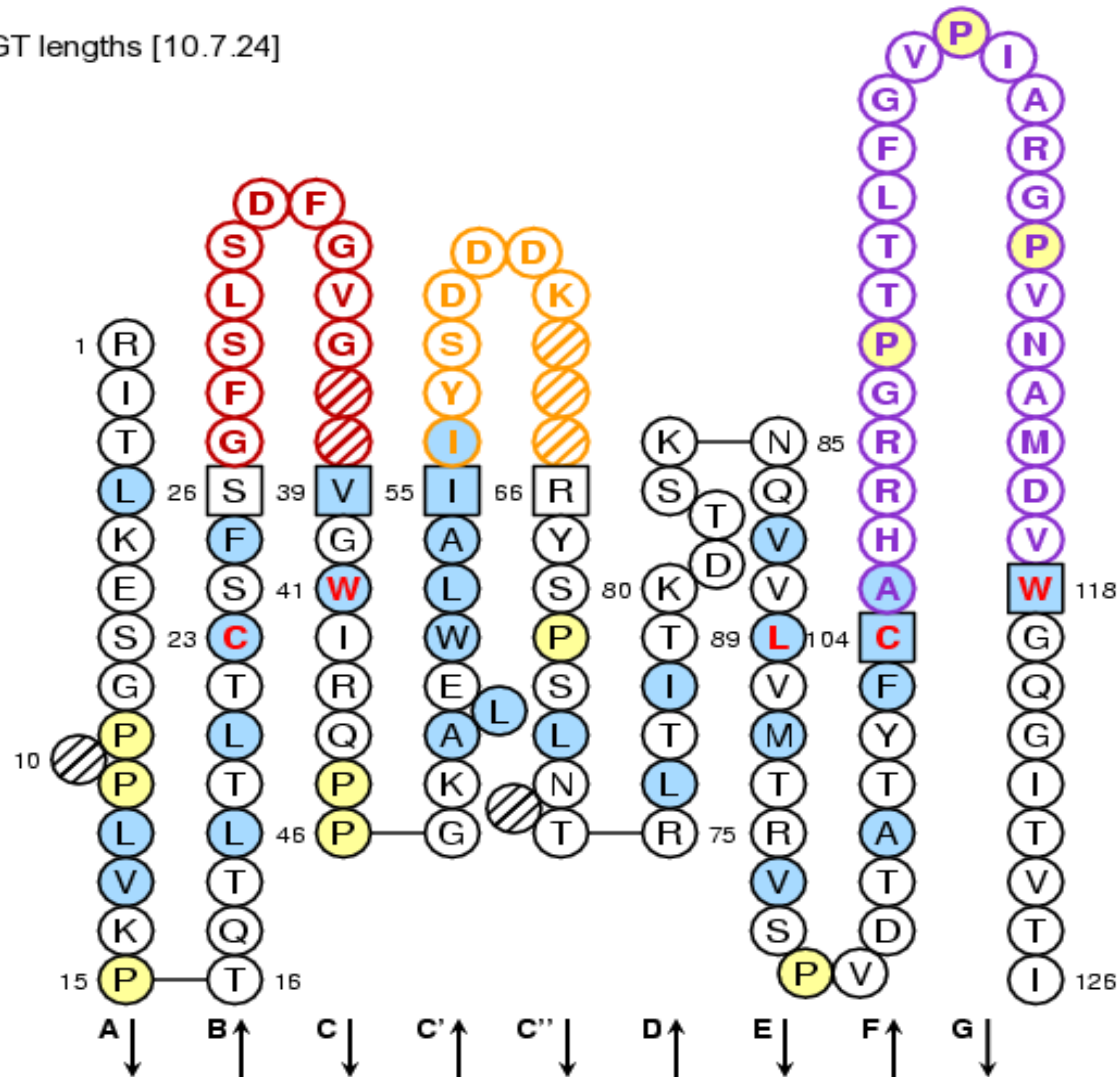


4. NUMEROTATION axiom

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

CDR-IMGT lengths [10.7.24]

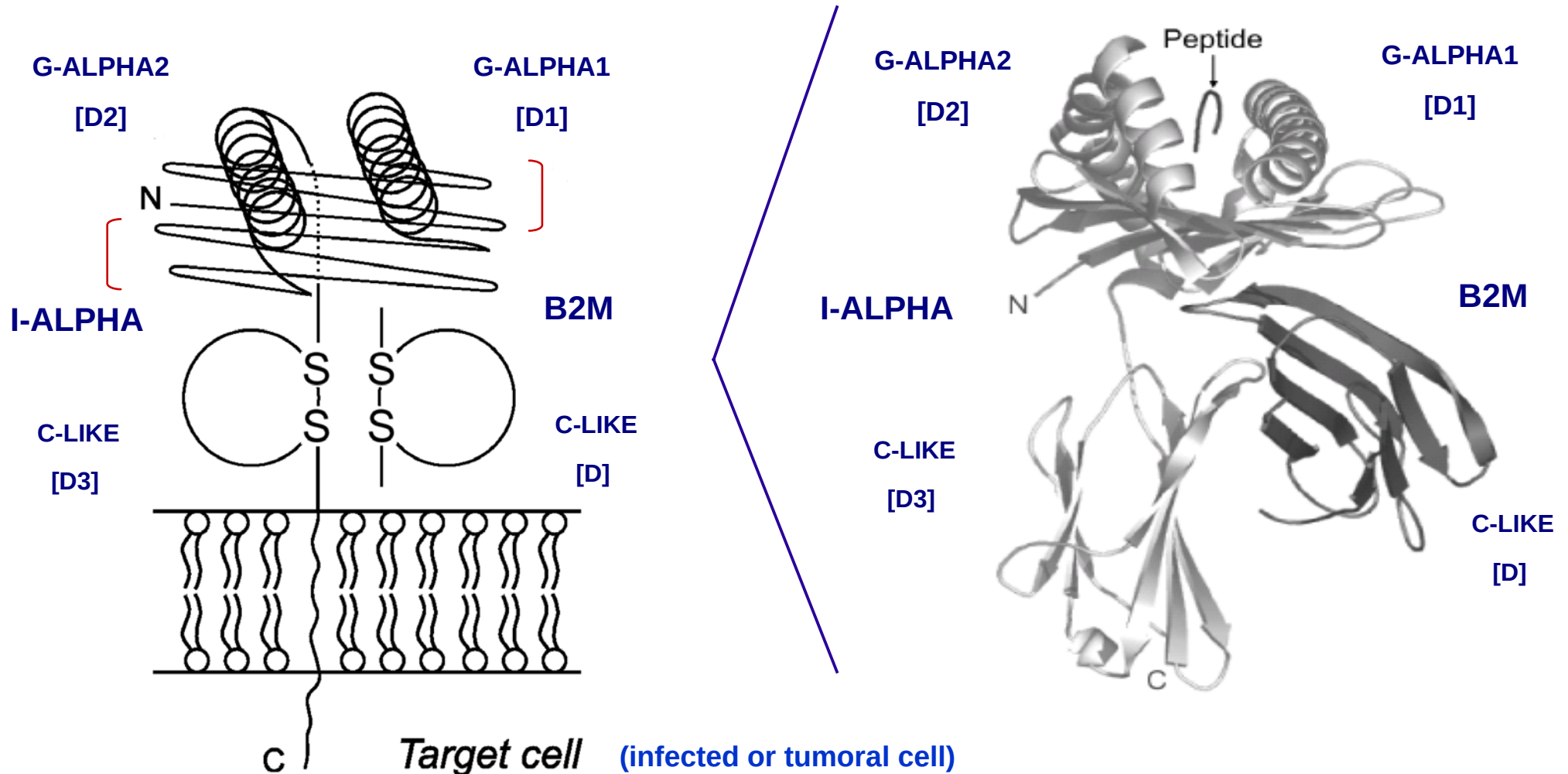
IMGT
Collier
de
Perles



IMGT Colliers de Perles and IMGT unique numbering

MHC-I chains and domains

MHC-I-ALPHA_B2M

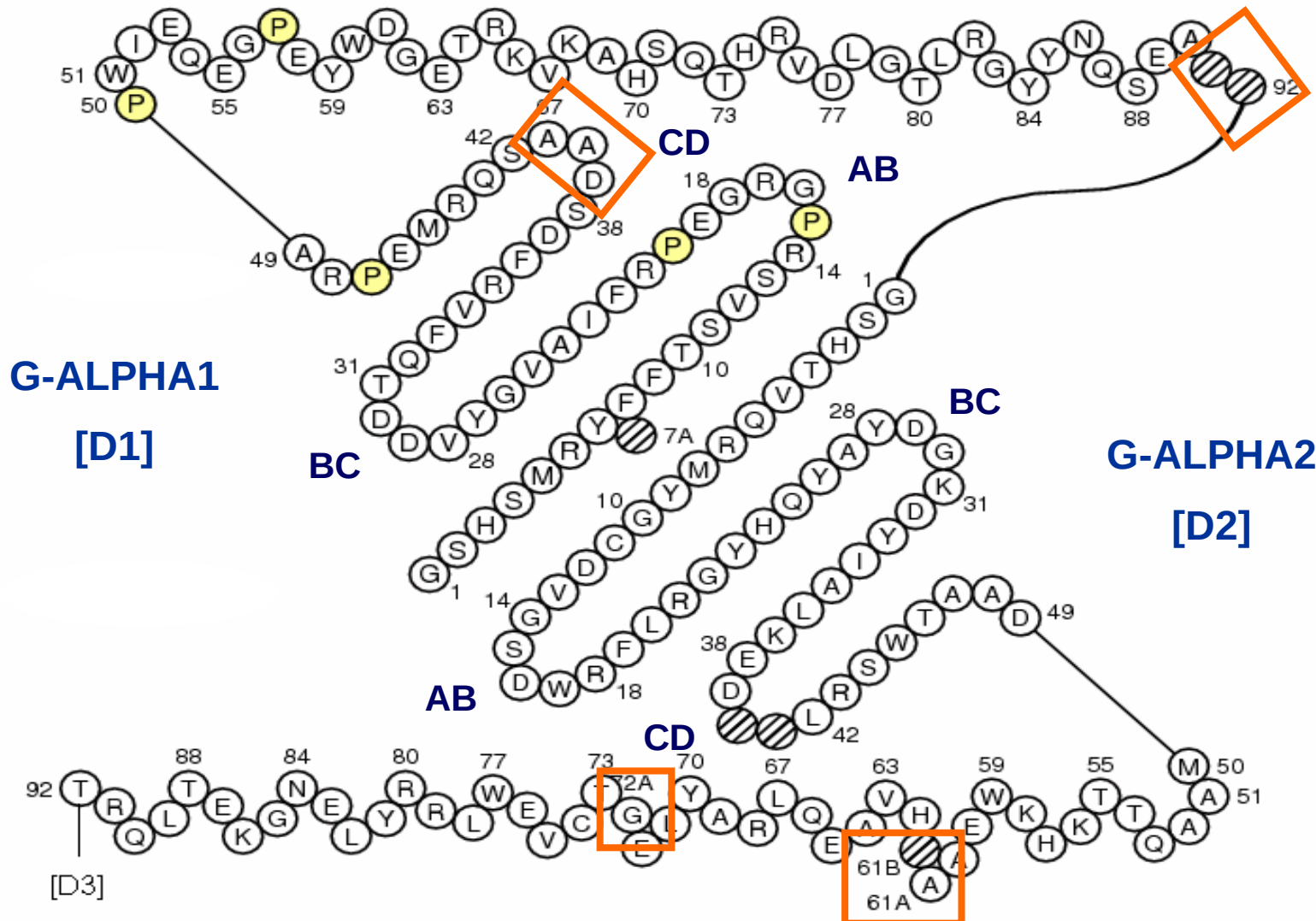


Lefranc et al., Dev. Comp. Immunol. 29, 917-938 (2005)

IMGT Colliers de Perles for G-DOMAIN

Based on the IMGT unique numbering for G-DOMAIN

MHC-I



Lefranc et al., Dev. Comp. Immunol. 29, 917-938 (2005)

4. Notion of structural domains

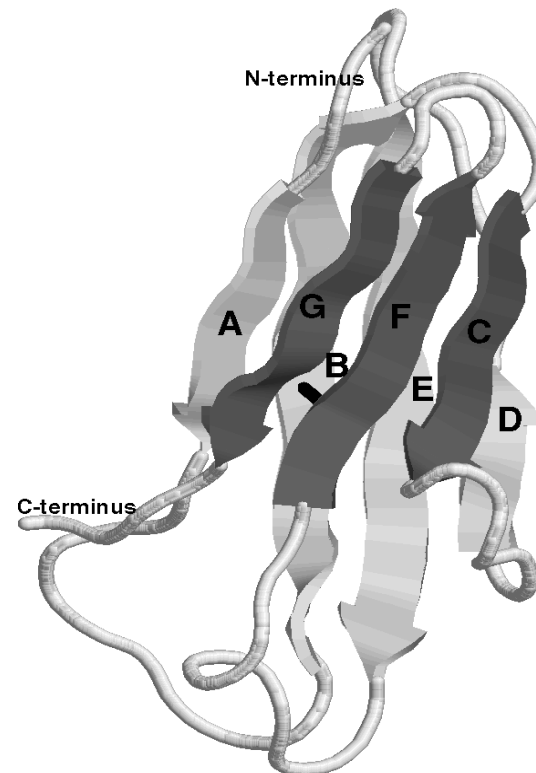
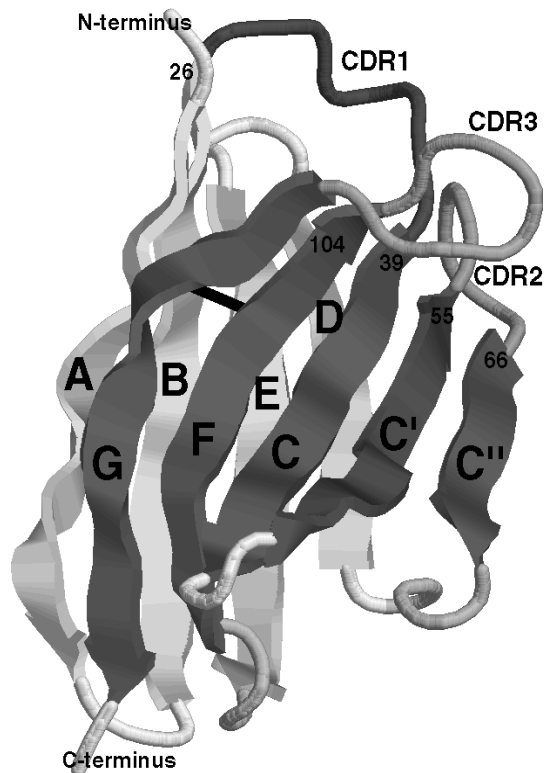
IG and TR

MHC

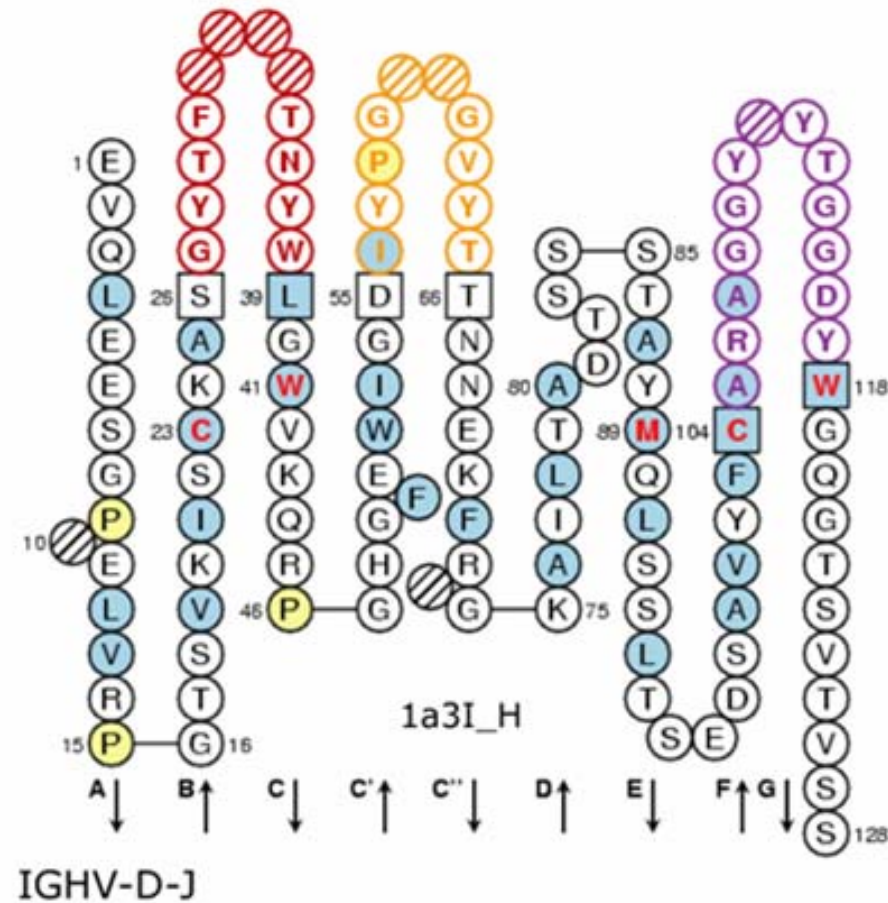
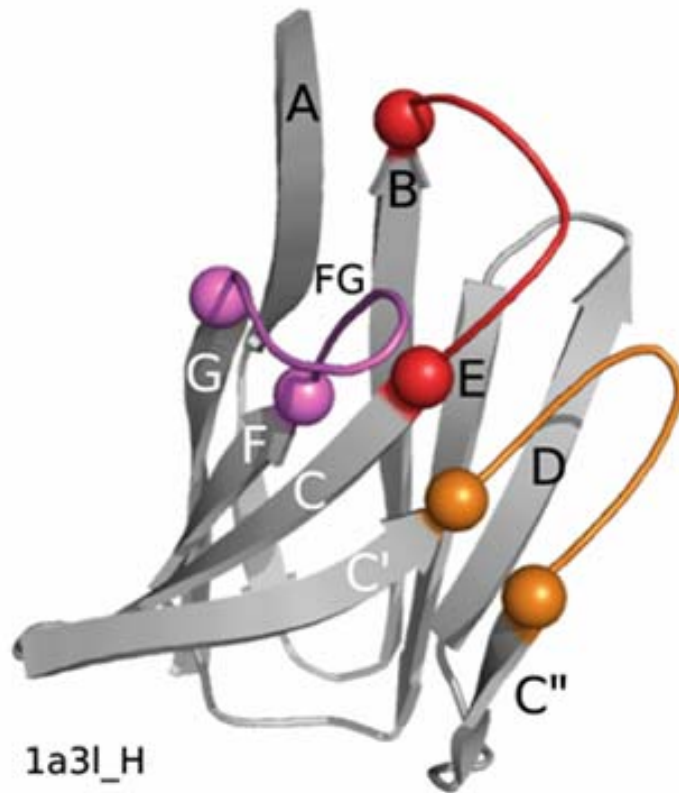
V-DOMAIN

C-DOMAIN

G-DOMAINS



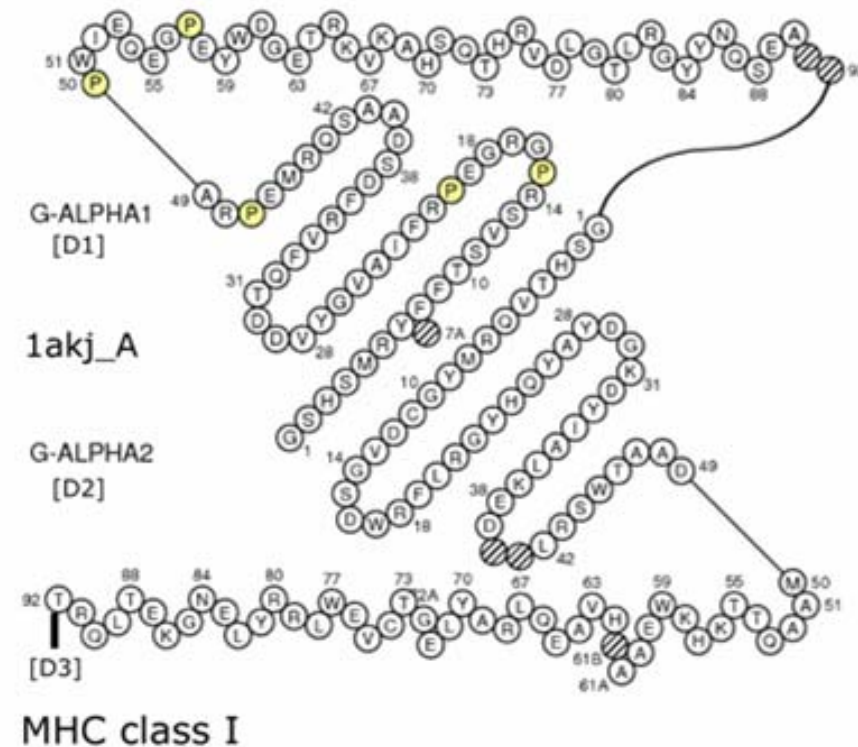
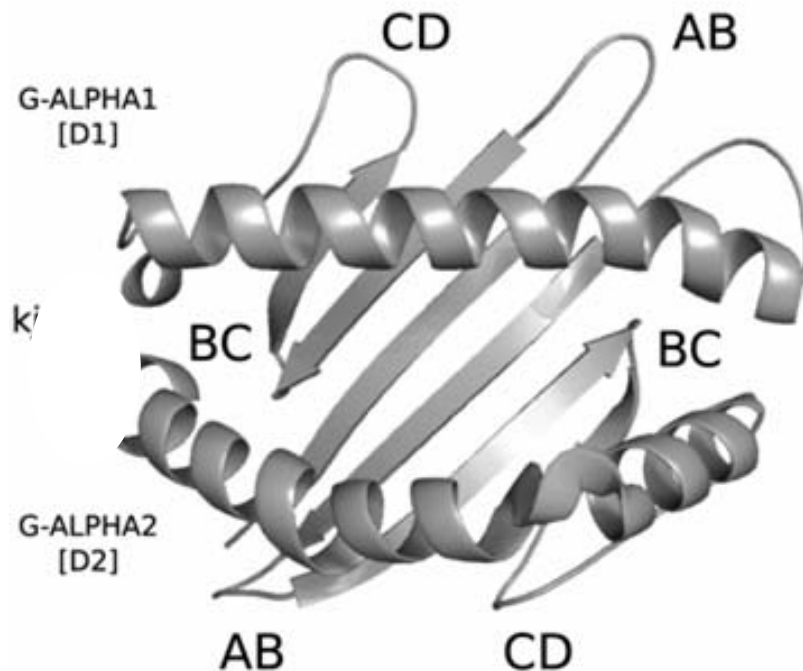
4. V type domain and IMGT Collier de Perles



ImMunoGeneTics
Information system®

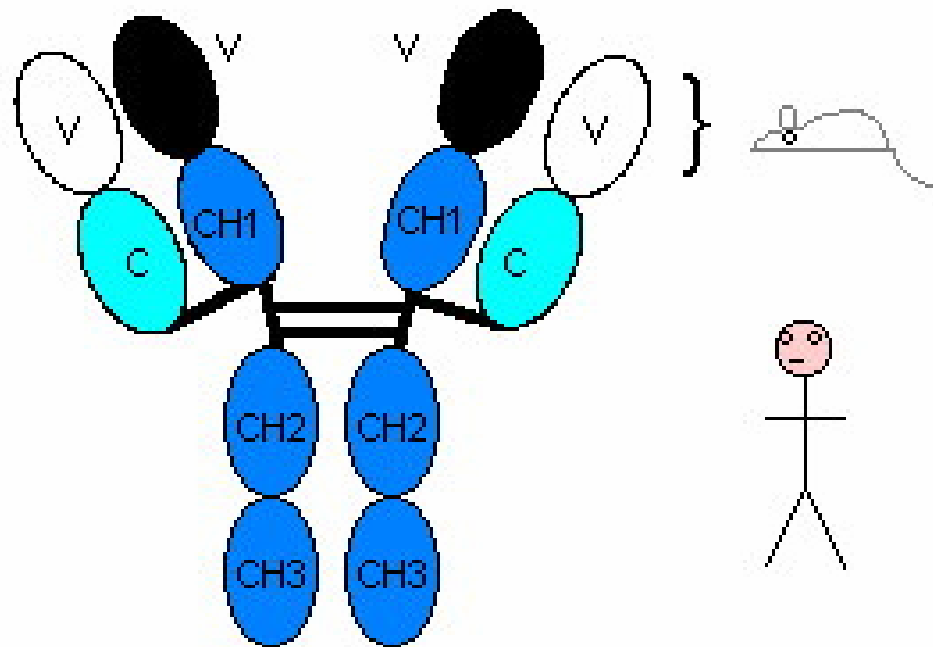
[illegible]

4. G type domain and IMGT Collier de Perles

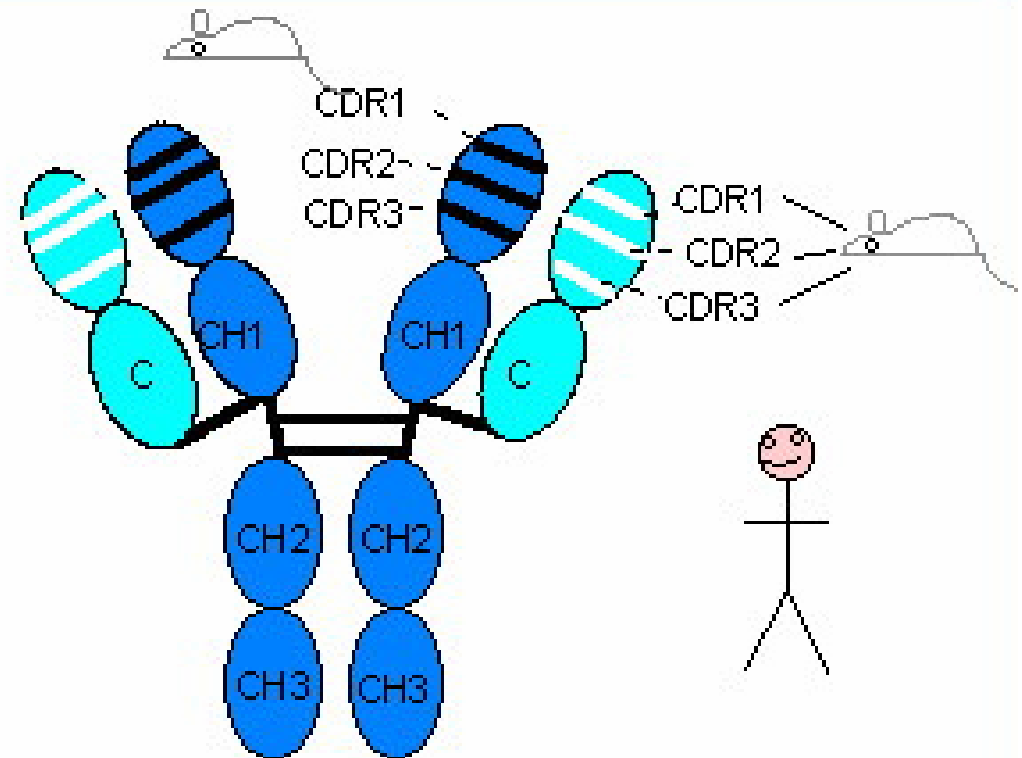


**What do we learn from IMGT-
ONTOLOGY and IMGT Colliers
de Perles ?**

Chimeric and humanized antibodies



chimeric antibody



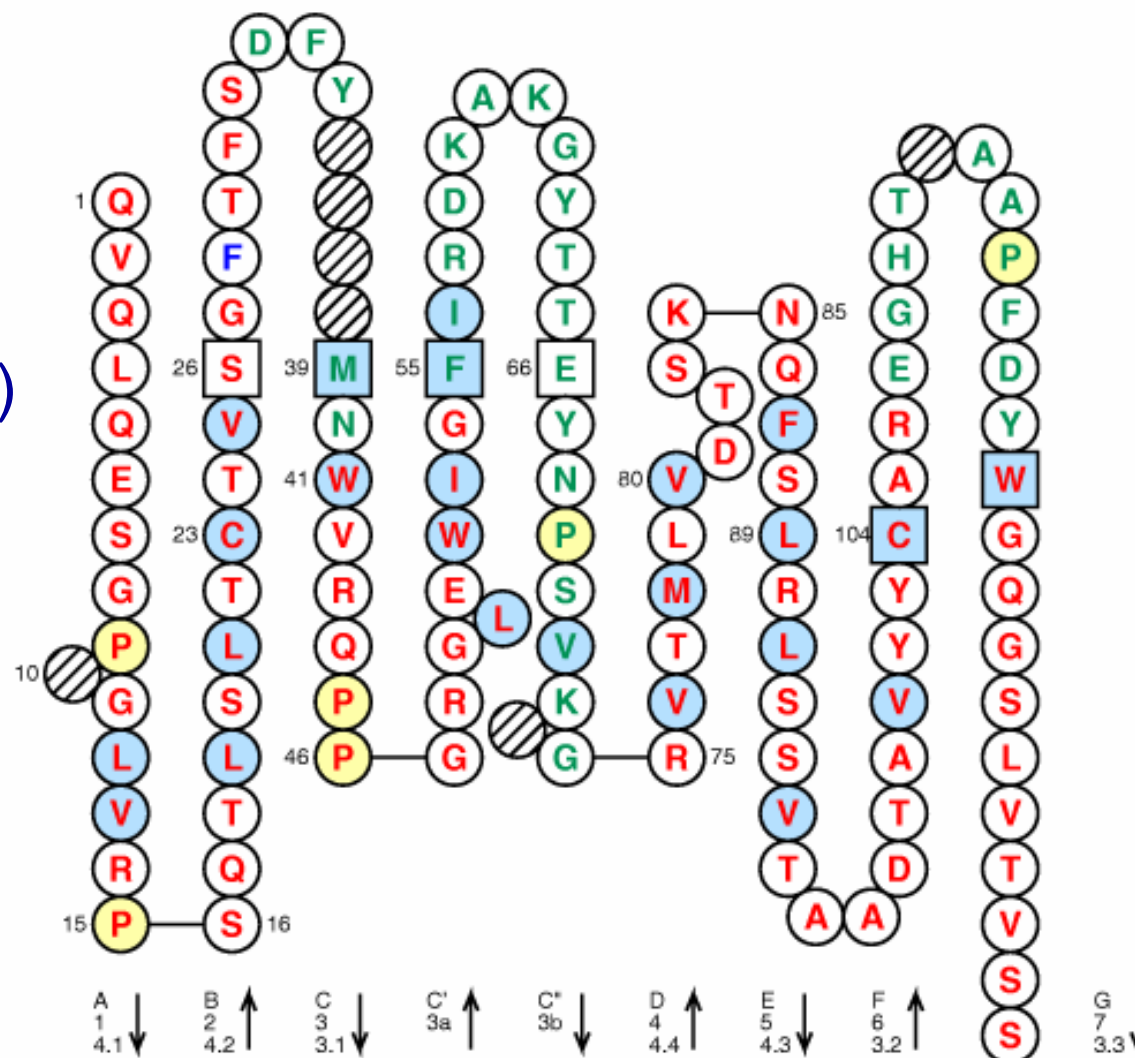
humanized antibody

Humanized CAMPATH-1H mutant 1

VH domain
(V-D-J-REGION)

[8.10.12]

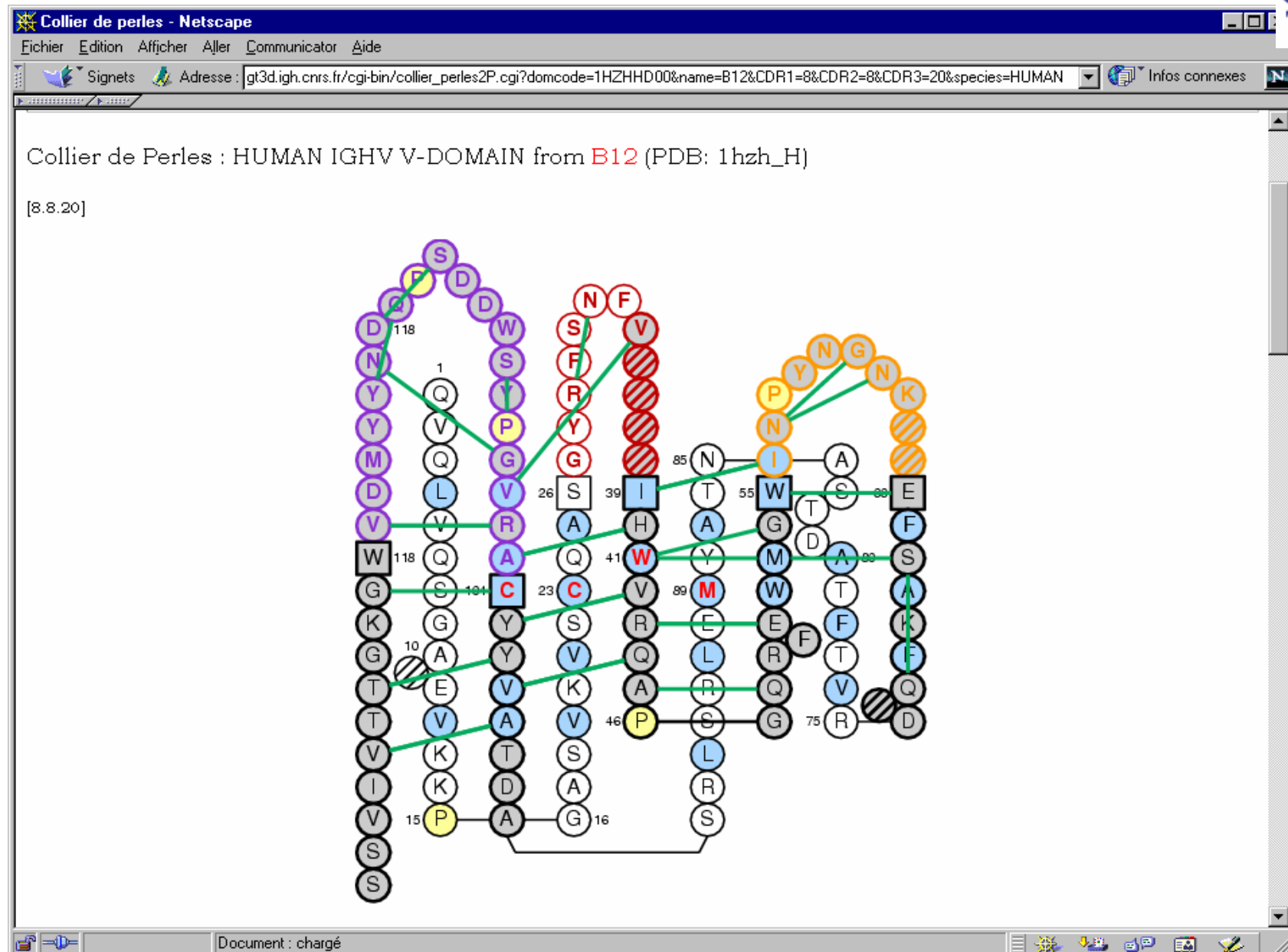
■ human
■ rat



Mutant 1: S28>F

Mutant 2:
alemtuzumab
S31>T

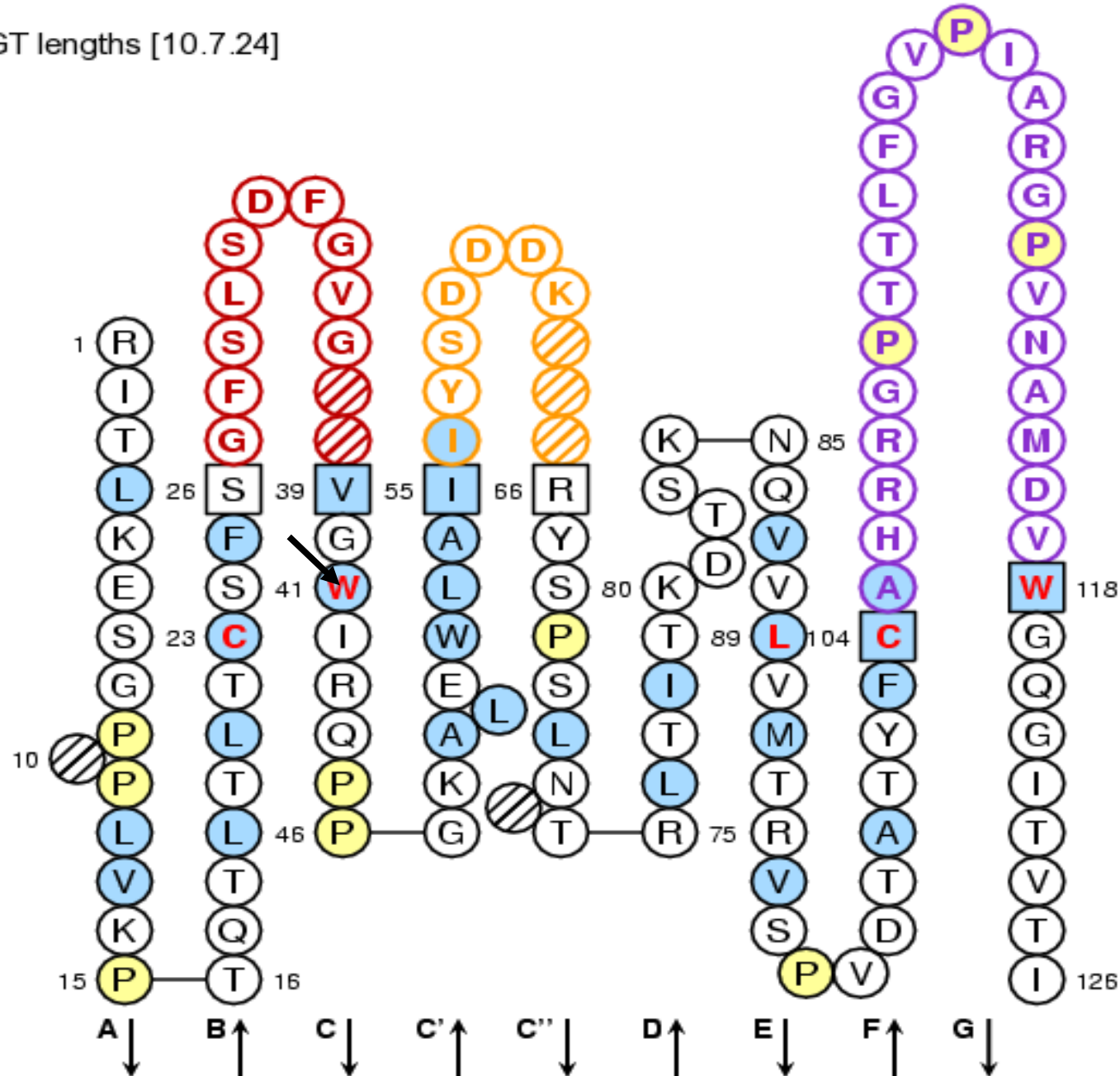
IMGT Collier de Perles on two layers



Kaas Q. et al. NAR 32, D208-D210 (2004)

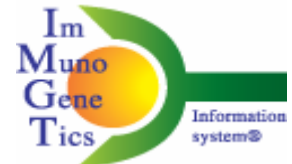
IMGT Collier de Perles : *Homo sapiens* (Human) IGHV_1 V-DOMAIN from 2F5 (PDB: 1u8k_E

CDR-IMGT lengths [10.7.24]



IMGT/3Dstructure-DB: Contact Analysis

IMGT Residue@Position cards



<http://imgt.cines.fr>

IMGT Residue@Position card

Residue@Position: **113 - ARG (R) - V-BETA - 1ao7_E** CDR3-IMGT

General information:

PDB file numbering 102
 IMGT file numbering 113
 Residue full name Arginine
 Formula C6 H15 N4 O2 1+

IMGT LocalStructure@Position

Secondary structure Coil
 Phi (in degrees) -89.71
 Psi (in degrees) 111.56
 ASA (in square angstrom) 73.2

IMGT Num	Residue	Domain	Chain	Atom contacts	Polar	Hydrogen Bond	Non Polar	
61	ALA	A	G-ALPHA2	1ao7_A	5	2	1	3
61A	ALA	A	G-ALPHA2	1ao7_A	24	6	0	18
62	HIS	H	G-ALPHA2	1ao7_A	12	2	0	10
66	GLN	Q	G-ALPHA2	1ao7_A	2	1	0	1
5	TYR	Y		1ao7_C	1	0	0	1
108	PRO	P	V-BETA	1ao7_E	15	1	0	14
111	ALA	A	V-BETA	1ao7_E	6	2	0	4
112.1	GLY	G	V-BETA	1ao7_E	24	5	0	19
115	GLU	E	V-BETA	1ao7_E	17	3	0	14

G-ALPHA2

Peptide

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

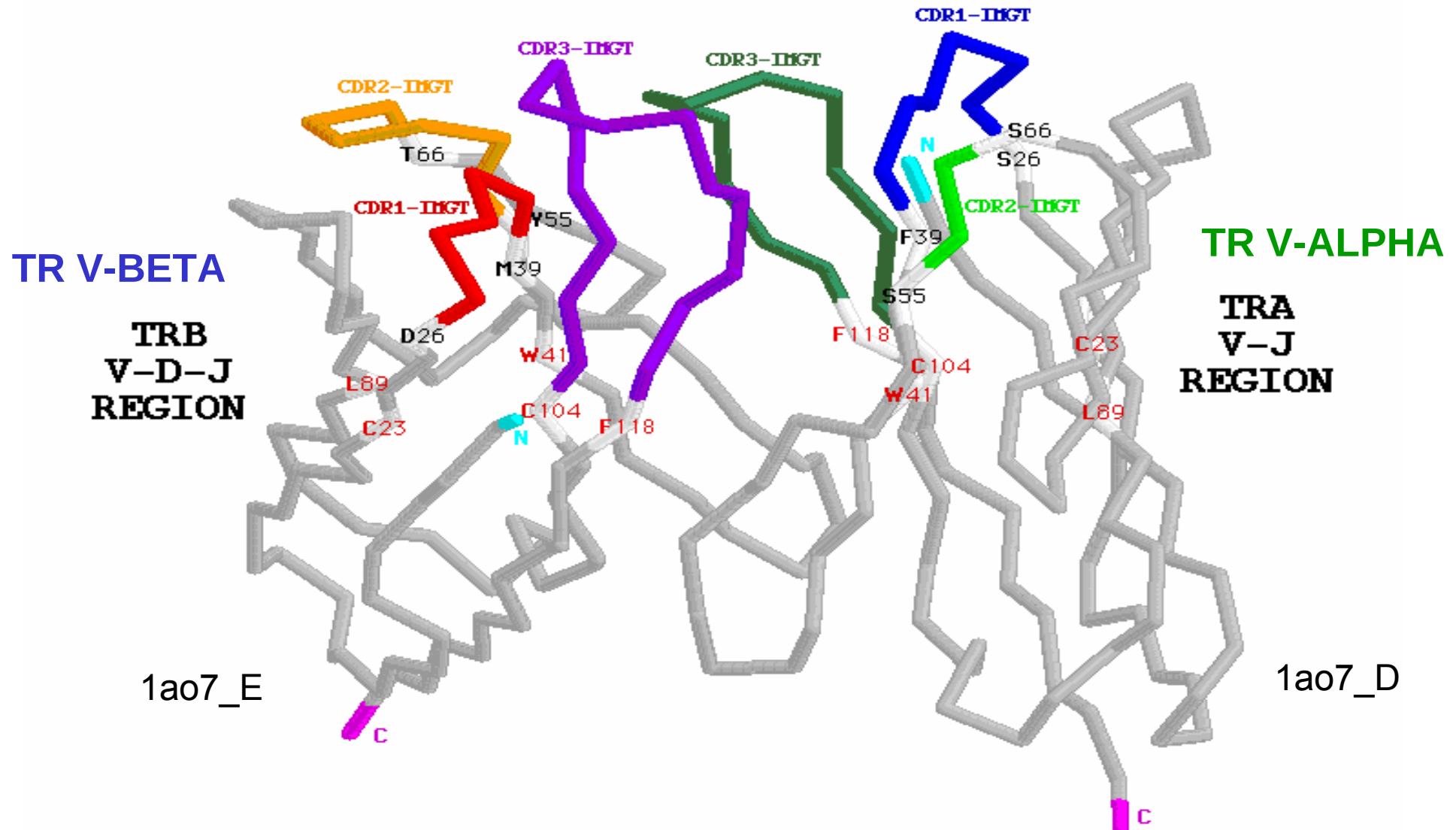
Residue local structure

	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
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

T cell receptor V-DOMAINS

Human TR $\alpha\beta$ A6



CDR: complementarity determining region

IMGT Repertoire, <http://imgt.cines.fr>

Immunoglobulin V-D-J generation of sequence diversity



JUNCTION

C A P Y R G D T Y D Y S W

tgt gcg cca tac cgg ggt gac act tat gat tac tcc tgg

IMGT/JunctionAnalysis Results

Locus IGH
Species Homo sapiens
IMGTrepertoire link [Locus representation](#)

Maximum number of mutations :
V-REGION : 2; D-REGION : 4; J-REGION : 2
Deletion criterium : Using patterns
Best D gene choice for a same score : Less mutations

Description of the JUNCTIONS

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

Input	V name	V-REGION	P	N1	D-REGION	N2	P	J-REGION	J name	D name	Vmut	Dmut	Jmut	Ngc
#1	Z70256	IGHV2-26*01		tgtgtgt	gcagcgcctgttac	ccaaatatc		...actttgaccactgg	IGHJ4*02	IGHD6-13*01	1	2	1	5/15
#2	Z70257	IGHV3-7*02		ggatgg	cagctcttatgcc	cgccc		ctactggtacttcgatctctgg	IGHJ2*01	IGHD2-2*01	0	2	0	9/11
#3	Z70606	IGHV4-31*03		c	.gactacg.....	cact		..atgcttttgatgtctgg	IGHJ3*01	IGHD4-17*01	0	0	0	3/5
#4	Z70608	IGHV4-39*05		cagagta	acgatttttgagtggttatt....	ccccggggga		..atgcttttgatatctgg	IGHJ3*02	IGHD3-3*01	0	0	0	12/17
#5	Z70610	IGHV4-34*09		tcgggag	cgatttttgagtggttatt....	cccga	ca	tgatgcttttgatatctgg	IGHJ3*02	IGHD3-3*01	0	0	0	9/12
#6	Z70611	IGHV4-59*01		ca	tggttaactataa.	tgccggcggttg		...actggttcgaccctgg	IGHJ5*02	IGHD3-9*01	0	2	0	9/13
#7	Z70613	IGHV4-59*01			cagcagctgttac	ctccct		ctttgactactgg	IGHJ4*02	IGHD6-13*01	0	0	0	4/6
#8	Z70614	IGHV4-59*01		cactataa	ttcggggacttat.....	cccctc		gactactgg	IGHJ4*02	IGHD3-16*01	0	2	0	7/14
#9	Z70615	IGHV4-59*01		ggctg	gtaaagaggg.....	tttcggaa		.tactggtacttcgatctctgg	IGHJ2*01	IGHD5-24*01	0	2	0	7/13
#10	Z70616	IGHV4-34*01		cgg	gtttggg.....	ttccc		...actggttcgaccctgg	IGHJ5*02	IGHD3-16*01	0	0	0	6/8
#11	Z70620	IGHV4-30-4*01		cc	ggggcgggatggtt....	cgg		.gatgcttttgatatctgg	IGHJ3*02	IGHD3-16*01	1	4	0	5/5
#12	Z70621	IGHV4-39*01		ccacgatttatgg	ttcggggagtt.....	tgacccc		ttgactactgg	IGHJ4*02	IGHD3-16*01	0	1	0	12/21
#13	Z70622	IGHV4-39*06	t	tgccccgcctcctgccccaaat	gtattactatggttcgggga.....	tatgtacg		ttgactactgg	IGHJ4*03	IGHD3-10*01	0	0	0	15/28

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

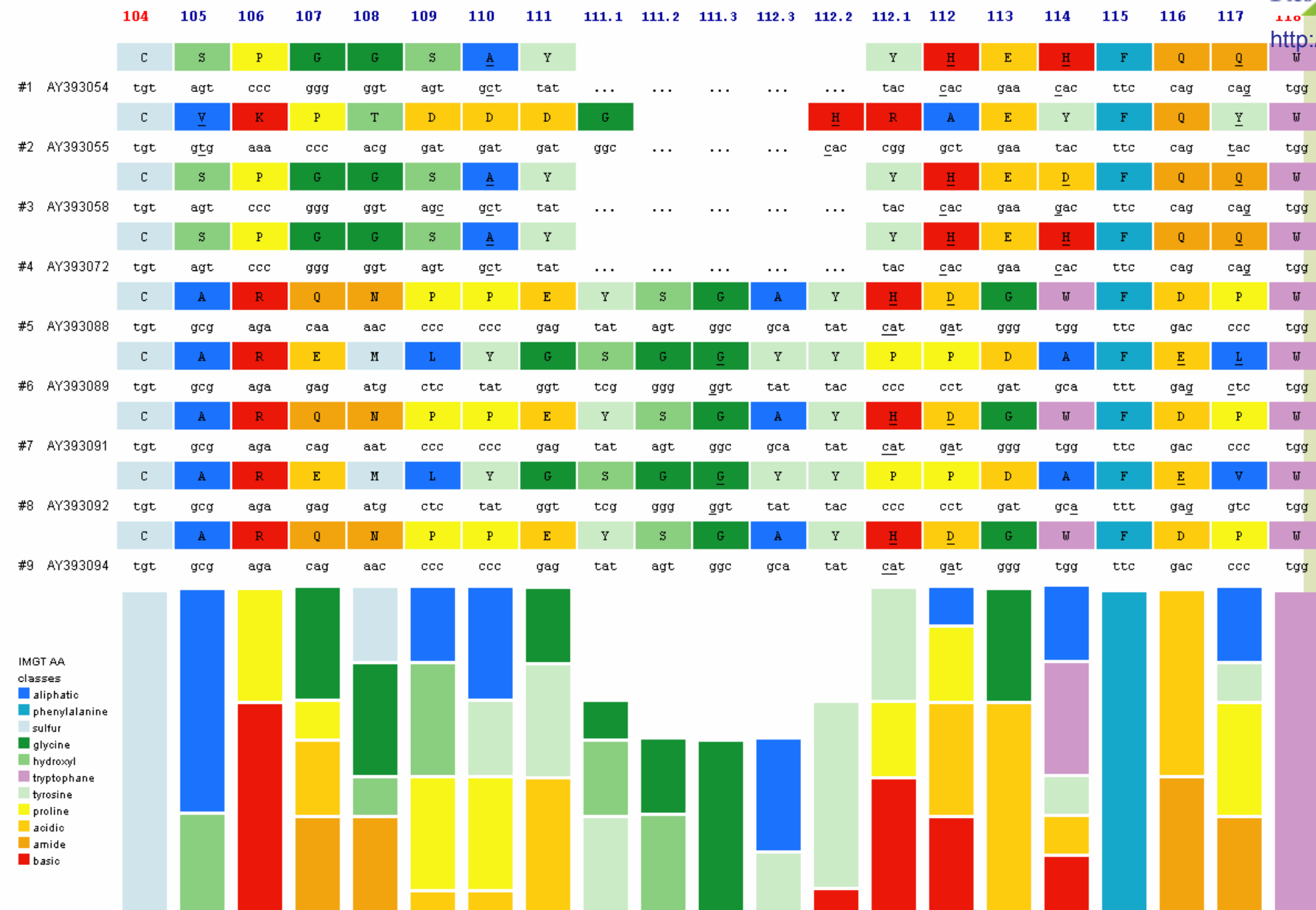
'Volume' classes		'Hydropathy' classes			
	in Å ³	Hydrophobic		Neutral	Hydrophilic
Very large	189-228	F	W	Y	
Large	162-174	I L	M		K R
Medium	138-154	V			H
Small	108-117		C	P	T
Very small	60-90	A		G	S
		Aliphatic		Sulfur	
				Hydroxyl	
					Basic
					Acidic
					Amide
		Nonpolar		Uncharged	Charged
					Uncharged
				Polar	

JUNCTION alignments with translation and IMGT AA classes

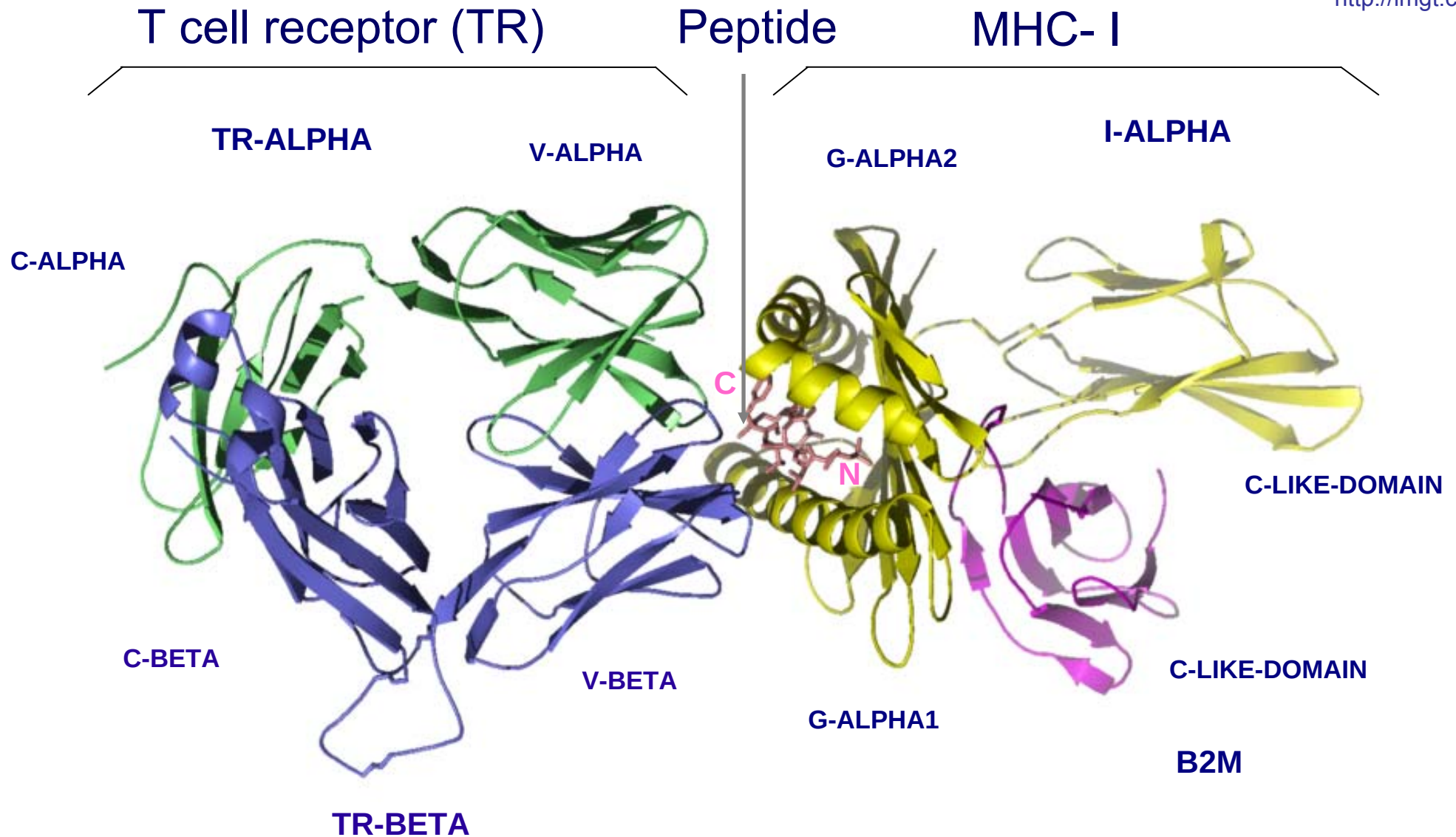
Click on mutated (underlined) amino acid to see the original one:



<http://imgt.cines.fr>



TR/peptide/MHC complex



IMGT/3Dstructure-DB



<http://imgt.cines.fr>

THANK YOU

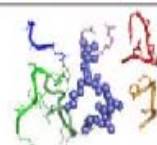
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IMGT/3Dstructure-DB card for : **1ao7**



Entry code Search

[Query page](#)

IMGT protein name	IMGT receptor type	IMGT receptor description	Ligand(s)	Species	CC	Chain ID
A6	TR	TR-ALPHA_BETA-1		<i>Homo sapiens</i> (Human)	1	[1ao7 D 1ao7 E]
HLA-A*0201	MHC	MHC-I-ALPHA_B2M		<i>Homo sapiens</i> (Human)	1	[1ao7 A 1ao7 B]
		Peptide	Tax peptide 11-19 (Q82235)	Human T lymphotropic virus type 1	1	[1ao7 C]

Experimental technique **X-ray diffraction**

Resolution (in angstrom) **2.6**

PDB release date **17-SEP-97**

Epitope and Chain
details

Contact
analysis

3D visualization
Jmol or QuickPDB

Renumbered
IMGT file 

IMGT numbering
comparison

References
and links

Printable
card

Reference 1ao7: *Garboczi et al., Nature 384, 134-141 (1996)*

IMGT/3Dstructure-DB: Contact Analysis

Receptors

Chains

Domains

Click 'DomPair' for IMGT/3Dstructure-DB Domain pair contacts (list of Residue@Position pair contacts)

Chain and domains of 1ao7					
IMGT molecule name	IMGT receptor description	Chain ID	IMGT chain description	Domain number	IMGT domain description
A6	TR-ALPHA_BETA-1	1ao7_D	TR-ALPHA	[D1]	V-ALPHA
		1ao7_E	TR-BETA-1	[D2]	C-ALPHA
HLA-A*0201	MHC-I-ALPHA_B2M	1ao7_A	I-ALPHA	[D1]	V-BETA
				[D2]	C-BETA-1
		1ao7_B	B2M	[D1]	G-ALPHA1
				[D2]	G-ALPHA2
Tax peptide 11-19 (Q82235)	Peptide	1ao7_C	Peptide	[D3]	C-LIKE
				[D1]	C-LIKE

Peptide

				Residue contacts	Number of residues			Atom contact types			
Unit 1		Unit 2			Total	From 1	From 2	Total	Polar	Hydrogen	
	Domain	Chain	Domain	Chain							
DomPair	V-ALPHA	1ao7_D	G-ALPHA1	1ao7_A	15	16	9	7	126	22	3
DomPair			G-ALPHA2	1ao7_A	12	15	7	8	105	17	2
DomPair			(Ligand)	1ao7_C	15	13	7	6	109	20	3

IMGT/3Dstructure-DB: Contact Analysis

Contacts between domains

	Unit 1		Unit 2		Residue contacts	Number of residues			Atom contact types		
	Domain	Chain	Domain	Chain		Total	From 1	From 2	Total	Polar	Hydrogen
DomPair	V-ALPHA	1ao7_D	G-ALPHA1	1ao7_A	15	16	9	7	126	22	3
DomPair			G-ALPHA2	1ao7_A	12	15	7	8	105	17	2
DomPair			(Ligand)	1ao7_C	15	13	7	6	109	20	3
DomPair			C-ALPHA	1ao7_D	4	6	4	2	27	7	1
DomPair			V-BETA	1ao7_E	57	42	20	22	401	46	7
DomPair			C-BETA-1	1ao7_E	1	2	1	1	9	2	0
DomPair	C-ALPHA	1ao7_D	V-ALPHA	1ao7_D	4	6	2	4	27	7	1
DomPair	V-BETA	1ao7_E	G-ALPHA1	1ao7_A	3	4	1	3	23	0	0
DomPair			G-ALPHA2	1ao7_A	11	10	5	5	82	17	3
DomPair			(Ligand)	1ao7_C	14	13	9	4	119	9	2
DomPair			V-ALPHA	1ao7_D	57	42	22	20	401	46	7
DomPair			C-BETA-1	1ao7_E	32	27	12	15	236	30	1

IMGT/3Dstructure-DB: Contact Analysis

Contacts of V-ALPHA with G-ALPHA1

Summary:

Residue contacts	Number of residues			Atom contact types		
	Total	From 1	From 2	Total	Polar	Hydrogen
15	16	9	7	126	22	3

Contacts of

Domain	Chain
V-ALPHA	1ao7_D

with

Domain	Chain
G-ALPHA1	1ao7_A

List of the Residue@Position pair contacts:

Click 'R@P' for IMGT Residue@Position cards

	Order						Order					Atom contacts		
	IMGT Num	Residue	Domain	Chain	IMGT Num		Residue	Domain	Chain	Total	Polar	Hydrogen		
R@P	2	LYS	K	V-ALPHA	1ao7_D	R@P	58	GLU	E	G-ALPHA1	1ao7_A	7	1	0
R@P	26	SER	S	V-ALPHA	1ao7_D	R@P	58	GLU	E	G-ALPHA1	1ao7_A	3	2	0
R@P	27	ASP	D	V-ALPHA	1ao7_D	R@P	58	GLU	E	G-ALPHA1	1ao7_A	24	6	1
R@P	28	ARG	R	V-ALPHA	1ao7_D	R@P	58	GLU	E	G-ALPHA1	1ao7_A	1	1	0
R@P	37	GLN	Q	V-ALPHA	1ao7_D	R@P	66	LYS	K	G-ALPHA1	1ao7_A	4	1	0
R@P	108	THR	T	V-ALPHA	1ao7_D	R@P	65	ARG	R	G-ALPHA1	1ao7_A	5	2	1
R@P	108	THR	T	V-ALPHA	1ao7_D	R@P	66	LYS	K	G-ALPHA1	1ao7_A	1	0	0
R@P	109	ASP	D	V-ALPHA	1ao7_D	R@P	62	GLY	G	G-ALPHA1	1ao7_A	1	1	0
R@P	109	ASP	D	V-ALPHA	1ao7_D	R@P	65	ARG	R	G-ALPHA1	1ao7_A	19	5	1
R@P	109	ASP	D	V-ALPHA	1ao7_D	R@P	66	LYS	K	G-ALPHA1	1ao7_A	14	1	0
R@P	113	TRP	W	V-ALPHA	1ao7_D	R@P	65	ARG	R	G-ALPHA1	1ao7_A	12	1	0
R@P	113	TRP	W	V-ALPHA	1ao7_D	R@P	68	LYS	K	G-ALPHA1	1ao7_A	8	0	0
R@P	113	TRP	W	V-ALPHA	1ao7_D	R@P	69	ALA	A	G-ALPHA1	1ao7_A	16	0	0
R@P	113	TRP	W	V-ALPHA	1ao7_D	R@P	72	GLN	Q	G-ALPHA1	1ao7_A	4	0	0
R@P	114	GLY	G	V-ALPHA	1ao7_D	R@P	65	ARG	R	G-ALPHA1	1ao7_A	7	1	0

K 2
S 26

D 27
R 28
Q 37

T 108
D 109
W 113
G 114

K 2
S 26

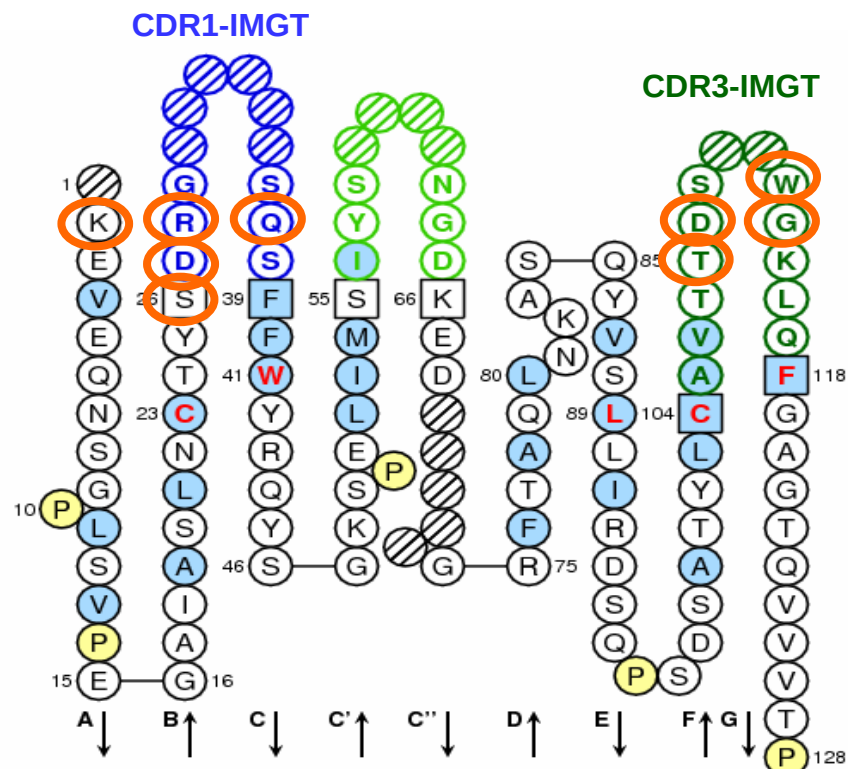
D 27
R 28
Q 37

T 108
D 109
W 113
G 114

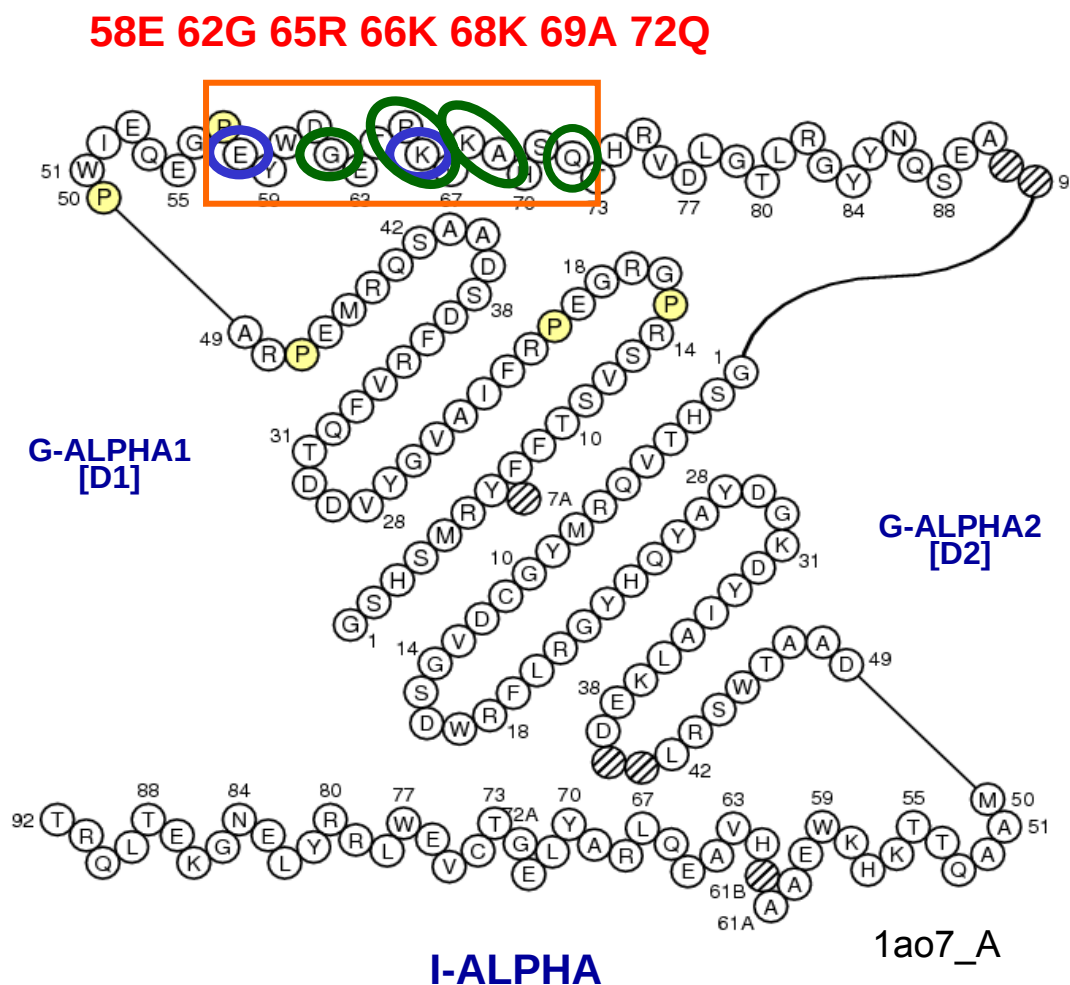
Contacts of V-ALPHA with G-ALPHA1

Involve CDR1-IMGT and CDR3-IMGT

○ Contact with G-ALPHA1



TR V-ALPHA
[6.6.11]



Kaas and Lefranc, In Silico Biology 5, 505-528 (2005)

IMGT/3Dstructure-DB: Contact Analysis

Contacts of V-ALPHA with G-ALPHA2

Summary:

Residue contacts	Number of residues			Atom contact types		
	Total	From 1	From 2	Total	Polar	Hydrogen
12	15	7	8	105	17	2

Contacts of

Domain	Chain
V-ALPHA	1ao7_D

with

Domain	Chain
G-ALPHA2	1ao7_A

List of the Residue@Position pair contacts:

Click 'R@P' for IMGT Residue@Position cards

Order					Order					Atom contacts		
IMG	Residue	Domain	Chain		IMG	Residue	Domain	Chain		Total	Polar	Hydrogen
R@P	28	ARG	R	V-ALPHA 1ao7_D	R@P	77	TRP	W	G-ALPHA2 1ao7_A	14	1	0
R@P	28	ARG	R	V-ALPHA 1ao7_D	R@P	80	ARG	R	G-ALPHA2 1ao7_A	13	5	0
R@P	29	GLY	G	V-ALPHA 1ao7_D	R@P	77	TRP	W	G-ALPHA2 1ao7_A	6	0	0
R@P	37	GLN	Q	V-ALPHA 1ao7_D	R@P	70	TYR	Y	G-ALPHA2 1ao7_A	8	0	0
R@P	37	GLN	Q	V-ALPHA 1ao7_D	R@P	73	THR	T	G-ALPHA2 1ao7_A	10	2	0
R@P	57	TYR	Y	V-ALPHA 1ao7_D	R@P	65	GLU	E	G-ALPHA2 1ao7_A	4	0	0
R@P	57	TYR	Y	V-ALPHA 1ao7_D	R@P	66	GLN	Q	G-ALPHA2 1ao7_A	16	1	0
R@P	57	TYR	Y	V-ALPHA 1ao7_D	R@P	69	ALA	A	G-ALPHA2 1ao7_A	7	1	0
R@P	58	SER	S	V-ALPHA 1ao7_D	R@P	69	ALA	A	G-ALPHA2 1ao7_A	3	1	0
R@P	63	ASN	N	V-ALPHA 1ao7_D	R@P	76	GLU	E	G-ALPHA2 1ao7_A	4	2	0
R@P	82	LYS	K	V-ALPHA 1ao7_D	R@P	73	THR	T	G-ALPHA2 1ao7_A	5	2	1
R@P	82	LYS	K	V-ALPHA 1ao7_D	R@P	76	GLU	E	G-ALPHA2 1ao7_A	15	2	1

E 65
Q 66
A 69
Y 70
T 73
E 76
W 77
R 80

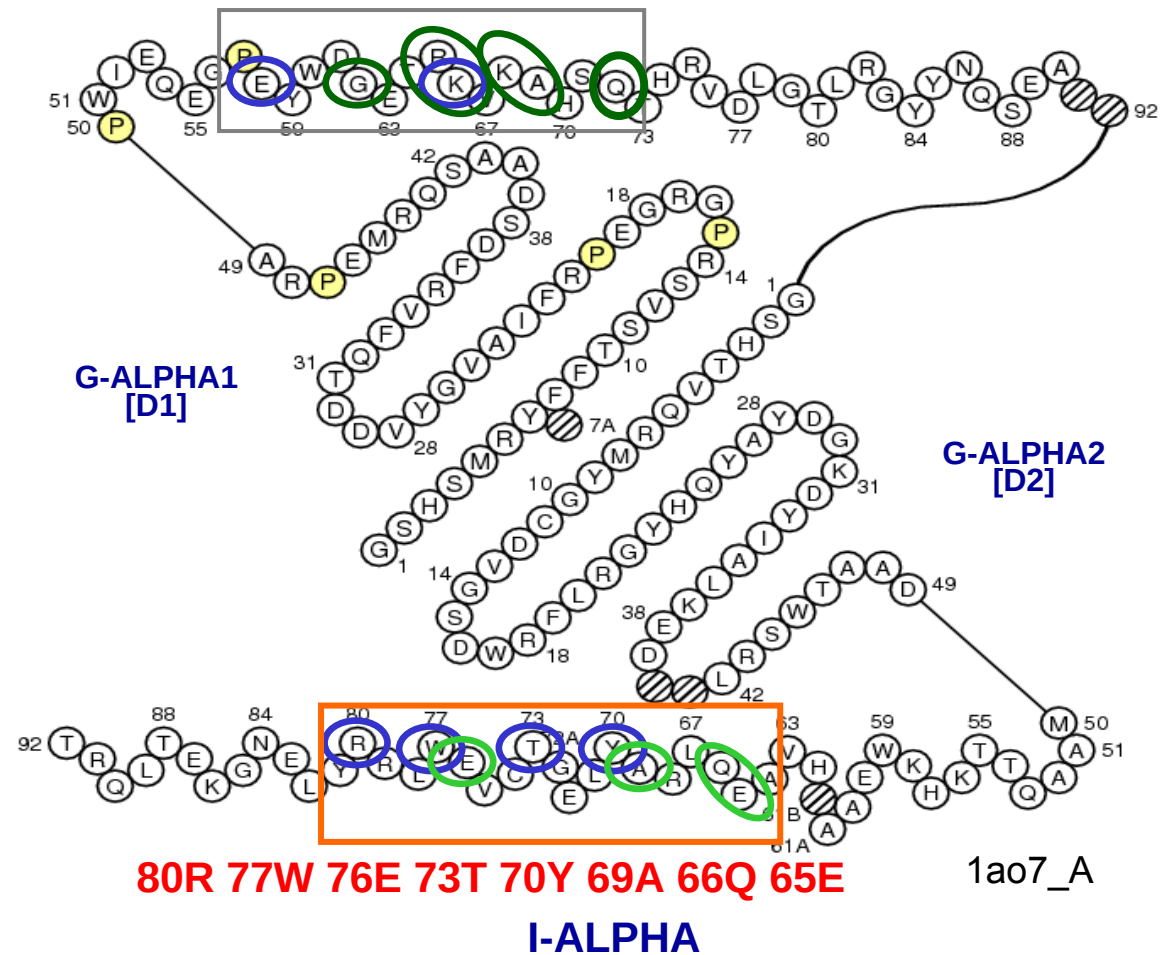
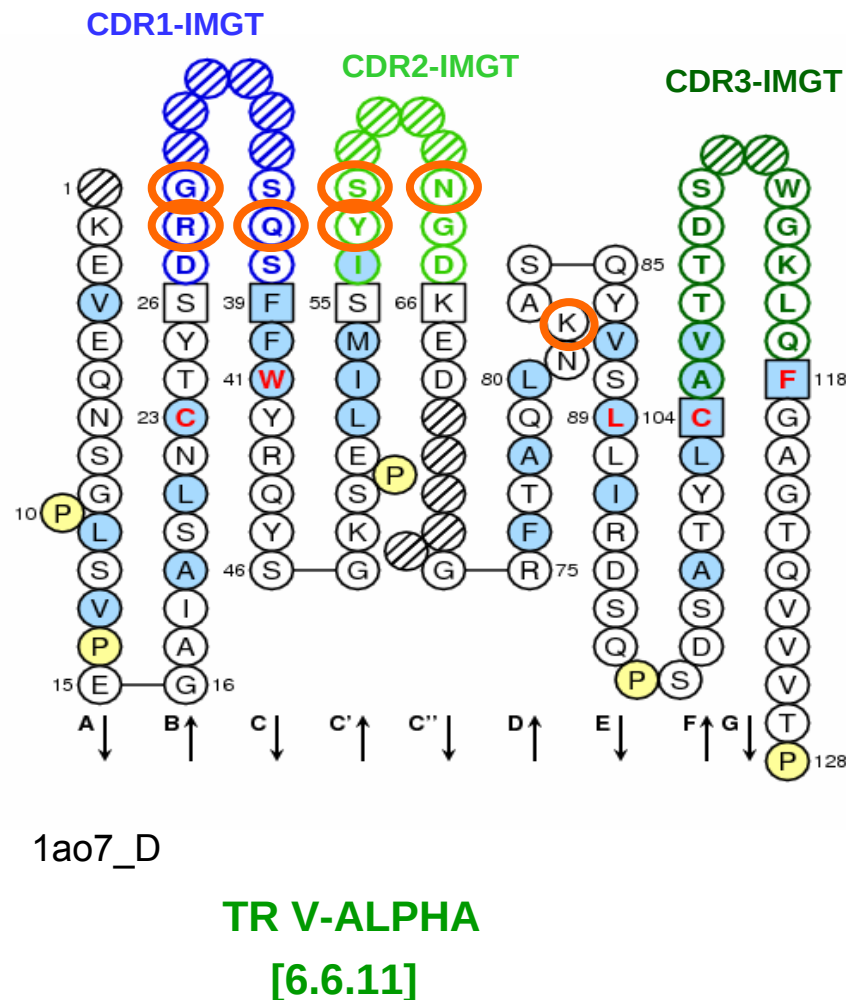
R 28
G 29
Q 37

Y 57
S 58
N 63

K 82

Contacts of V-ALPHA with G-ALPHA2

○ Contact with G-ALPHA2



Kaas and Lefranc, In Silico Biology 5, 505-528 (2005)

IMGT/3Dstructure-DB: Contact Analysis

Contacts of V-BETA with G-ALPHA2

Summary:

Residue contacts	Number of residues			Atom contact types		
	Total	From 1	From 2	Total	Polar	Hydrogen
11	10	5	5	82	17	3

Contacts of

Domain	Chain
V-BETA	1ao7_E

with

Domain	Chain
G-ALPHA2	1ao7_A

List of the Residue@Position pair contacts:

Click 'R@P' for IMGT Residue@Position cards

Order						Order						Atom contacts		
IMGT Num	Residue	Domain	Chain			IMGT Num	Residue	Domain	Chain			Total	Polar	Hydrogen
R@P	111	ALA	A	V-BETA	1ao7_E	R@P	61A	ALA	A	G-ALPHA2	1ao7_A	1	0	0
R@P	112.1	GLY	G	V-BETA	1ao7_E	R@P	61A	ALA	A	G-ALPHA2	1ao7_A	5	0	0
R@P	112	GLY	G	V-BETA	1ao7_E	R@P	61A	ALA	A	G-ALPHA2	1ao7_A	8	2	1
R@P	112	GLY	G	V-BETA	1ao7_E	R@P	62	HIS	H	G-ALPHA2	1ao7_A	4	1	0
R@P	112	GLY	G	V-BETA	1ao7_E	R@P	63	VAL	V	G-ALPHA2	1ao7_A	4	0	0
R@P	112	GLY	G	V-BETA	1ao7_E	R@P	66	GLN	Q	G-ALPHA2	1ao7_A	10	2	1
R@P	113	ARG	R	V-BETA	1ao7_E	R@P	61	ALA	A	G-ALPHA2	1ao7_A	5	2	1
R@P	113	ARG	R	V-BETA	1ao7_E	R@P	61A	ALA	A	G-ALPHA2	1ao7_A	24	6	0
R@P	113	ARG	R	V-BETA	1ao7_E	R@P	62	HIS	H	G-ALPHA2	1ao7_A	12	2	0
R@P	113	ARG	R	V-BETA	1ao7_E	R@P	66	GLN	Q	G-ALPHA2	1ao7_A	2	1	0
R@P	114	PRO	P	V-BETA	1ao7_E	R@P	66	GLN	Q	G-ALPHA2	1ao7_A	7	1	0

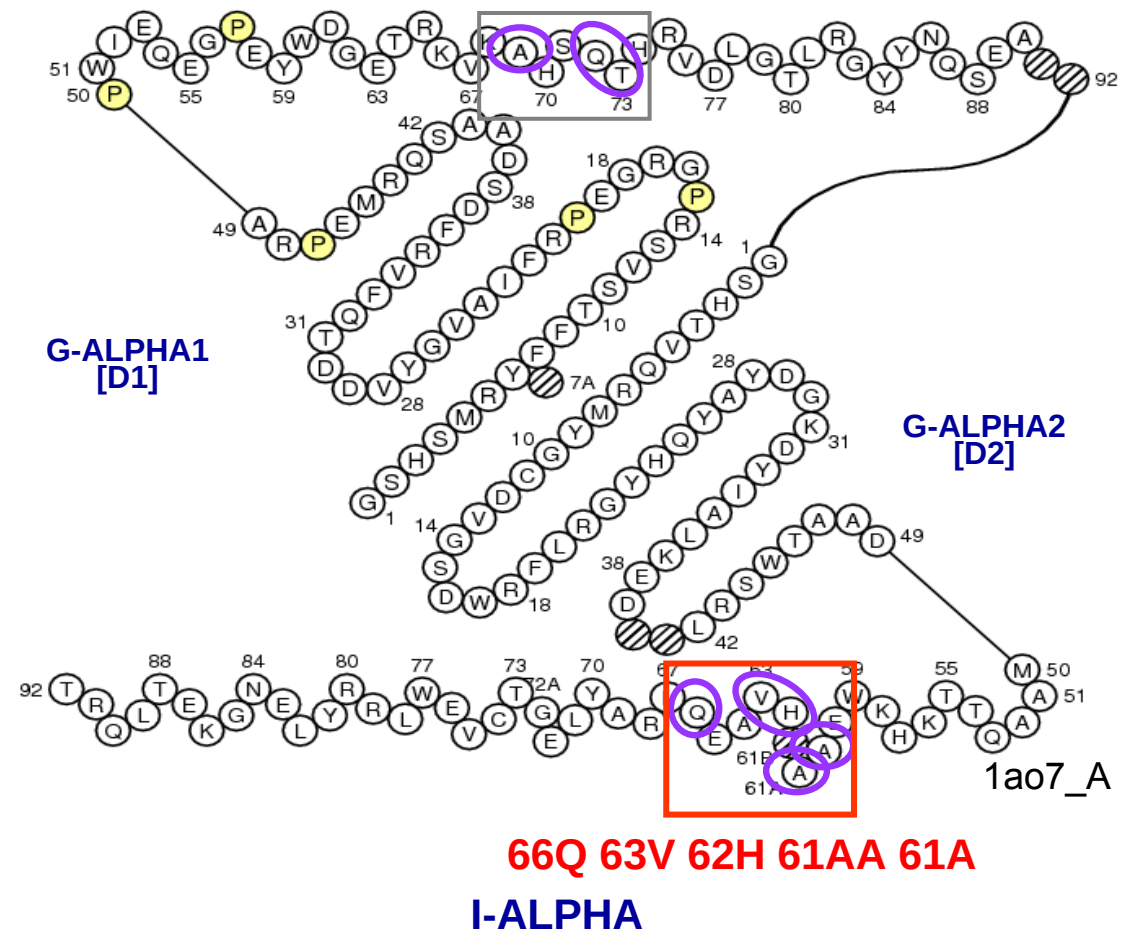
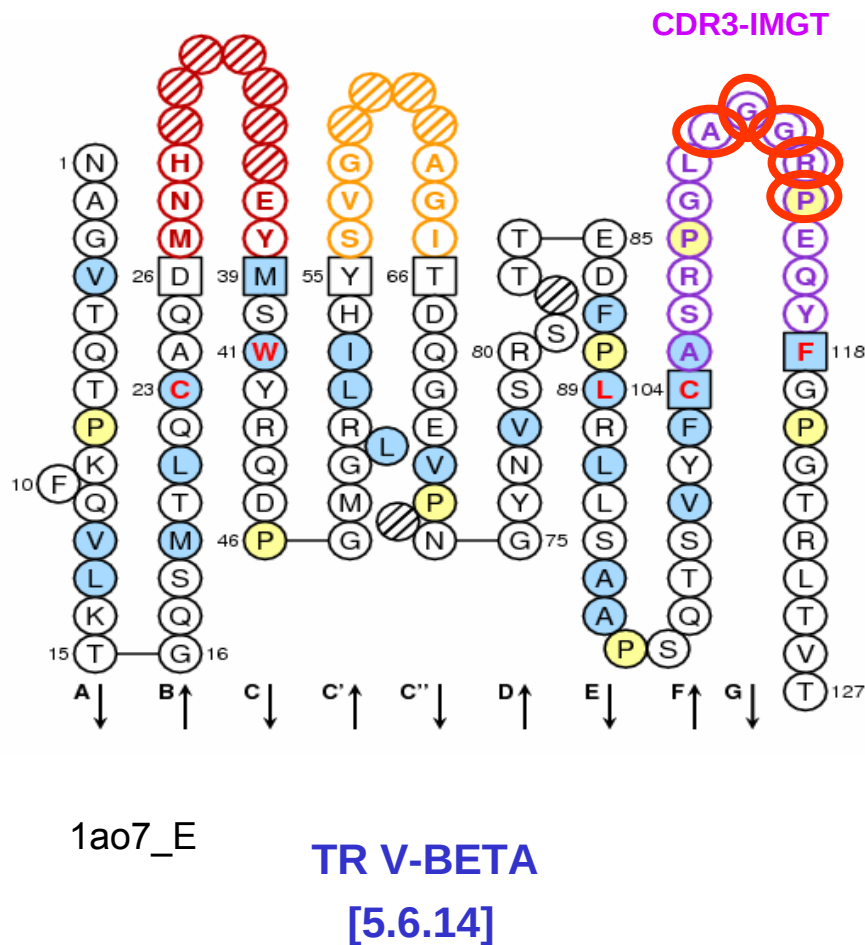
A 61
A 61A
H 62
V 63
Q 66

A 111
G 112.1
G 112
R 113
P 114

Contacts of V-BETA with G-ALPHA2

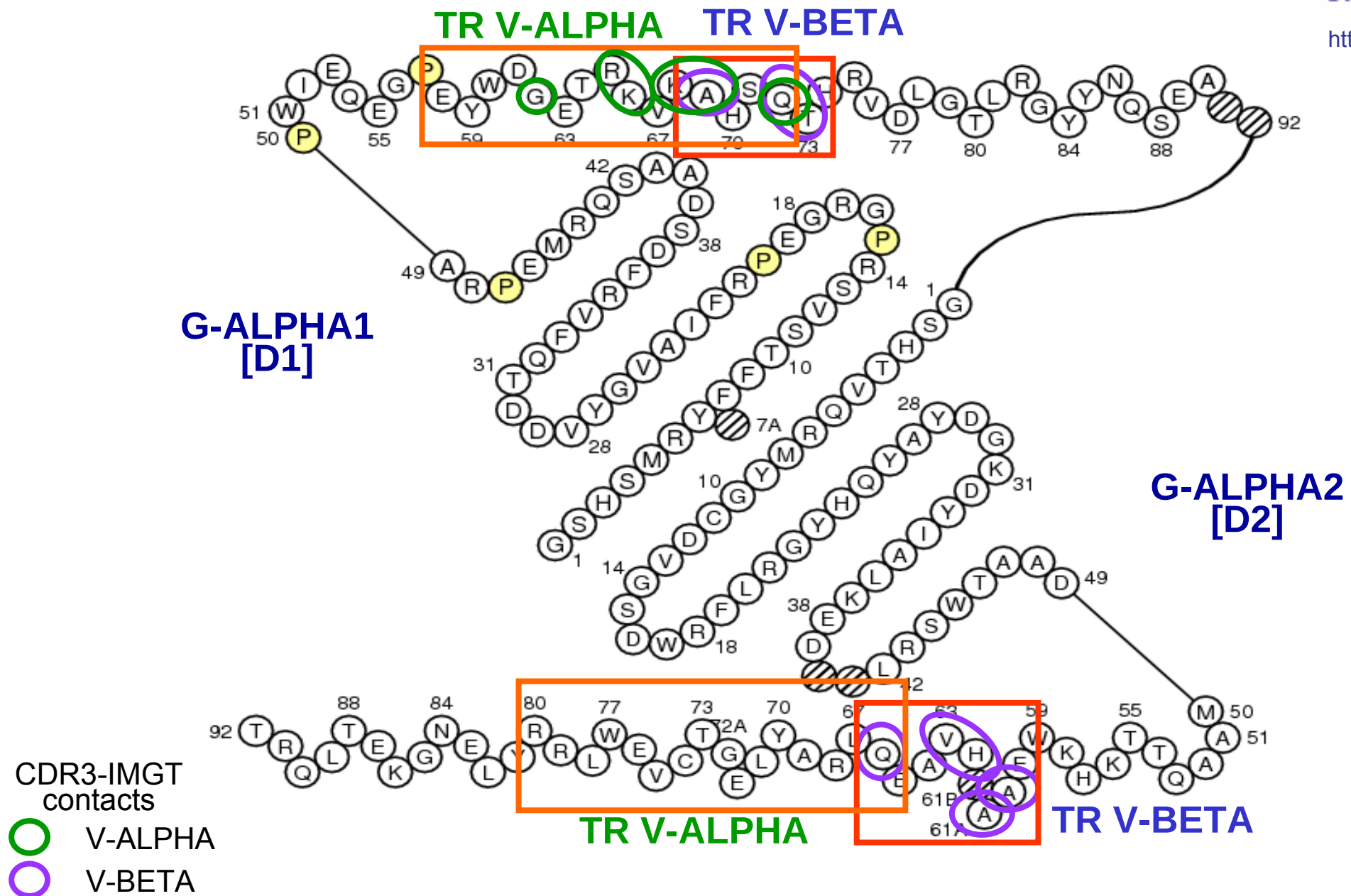
Involve CDR3-IMGT

○ Contact with G-ALPHA2



Kaas and Lefranc, In Silico Biology 5, 505-528 (2005)

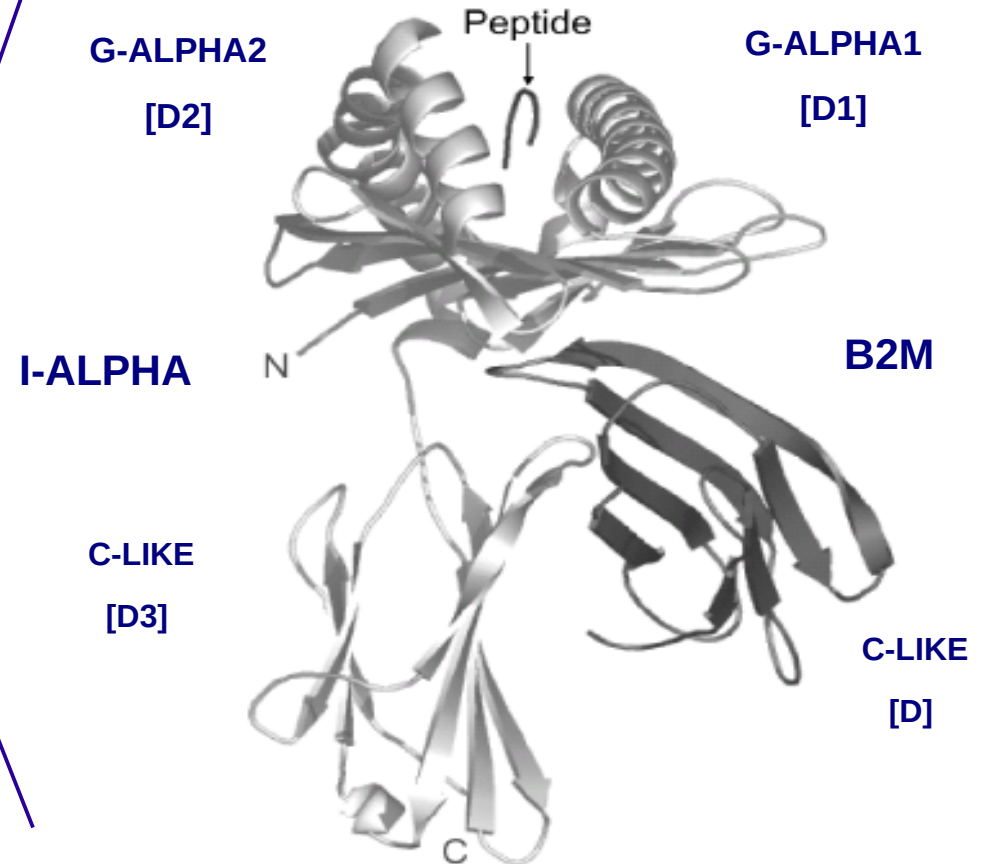
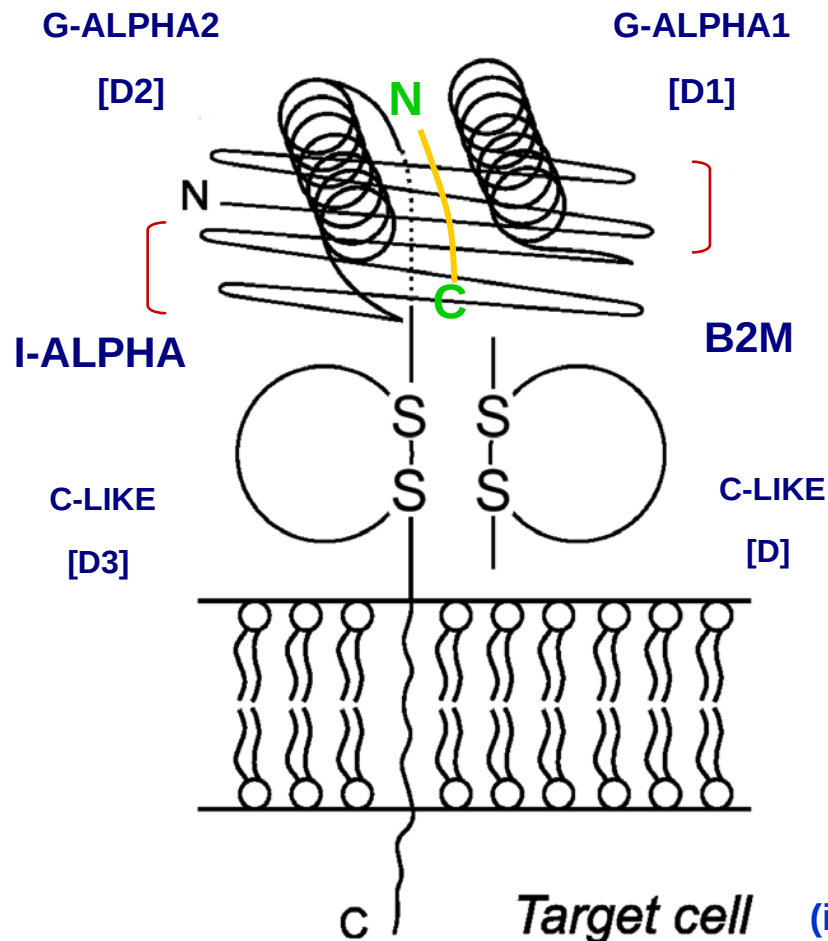
HLA-A*0201 regions in contact with TR $\alpha\beta$ A6



MHC-I chains and domains

MHC-I-ALPHA_B2M

Peptide 8, 9 or 10 amino acids
Groove with "closed" ends



Lefranc et al., Dev. Comp. Immunol. 29, 917-938 (2005)

Peptide alignment

	Number of residues	Peptide sequence
MHC-I	8 amino acids 1jtr_Q	E - Q Y (K) F - - Y S V
	9 amino acids 1ao7_C	L - L F (G) Y - P V Y V
	10 amino acids 1bii_P	R - G P (G) R A F V T I
IMGT pMHC contact sites		C1 C2 C3 C4 C5 C6 C7 C8 C9 C10 C11
MHC-II	13 amino acids 1j8h_C	P K Y V K Q (N) T - - L K L A T

Kaas and Lefranc, In Silico Biology 5, 505-528 (2005)

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Kaas and Lefranc, In Silico Biology 5, 505-528 (2005)

Why are IMGT Colliers de Perles so useful?

The IMGT Colliers de Perles

1. bridge the gaps between sequences and structures
2. are used whatever the IG,TR, MHC and whatever the species.

	MHC-Ia	MHC-Ib	MHC-IIa	MHC-IIb
	HLA-A,-B,-C	HLA-E,-F,-G	HLA-DPA,-DQA, - DRA HLA-DPB,-DQB, - DRB	HLA-DMA, DOA HLA-DMB, DOB
	H2-D,-K,-L	H2-M,-Q,-T	H2-AA,-EA H2-AB,-EB	H2-DMA,-DOA H2-DMB,-DOB

3. have been extended to the IgSF proteins and MhcSF proteins (CD1, FCRN, RAET, HFE, MICA, AZGP1,...).

Interestingly, only one additional position **54A** in **G-ALPHA1-LIKE** was needed to extend the IMGT unique numbering for G-DOMAIN to the G-LIKE-DOMAIN.



Many thanks to the IMGT® team at Montpellier, France