

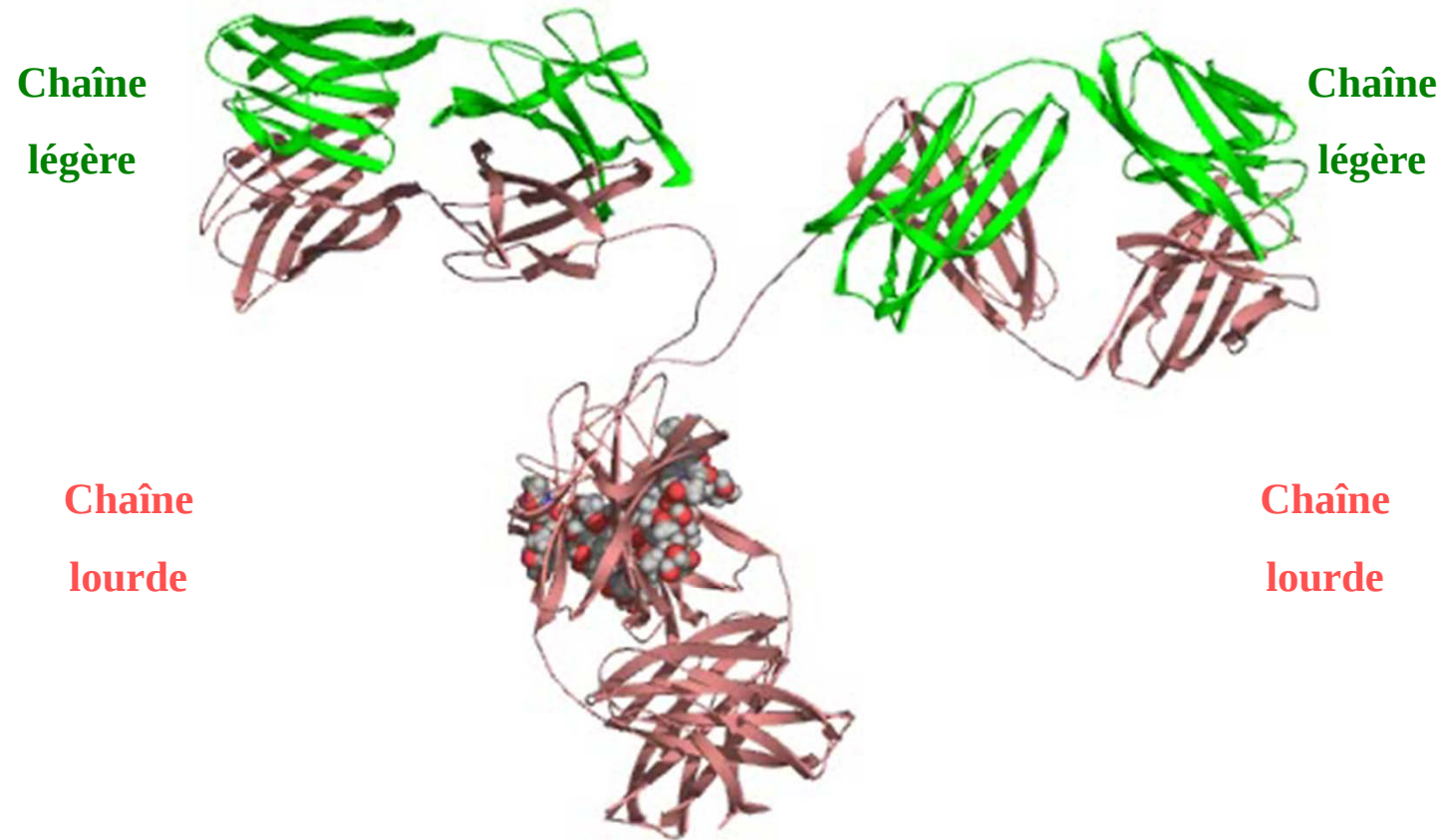
Structures en immunogénétique

Introduction

Master 2 STIC Santé UE GMIN304 « Structure des molécules »
4 Décembre 2013

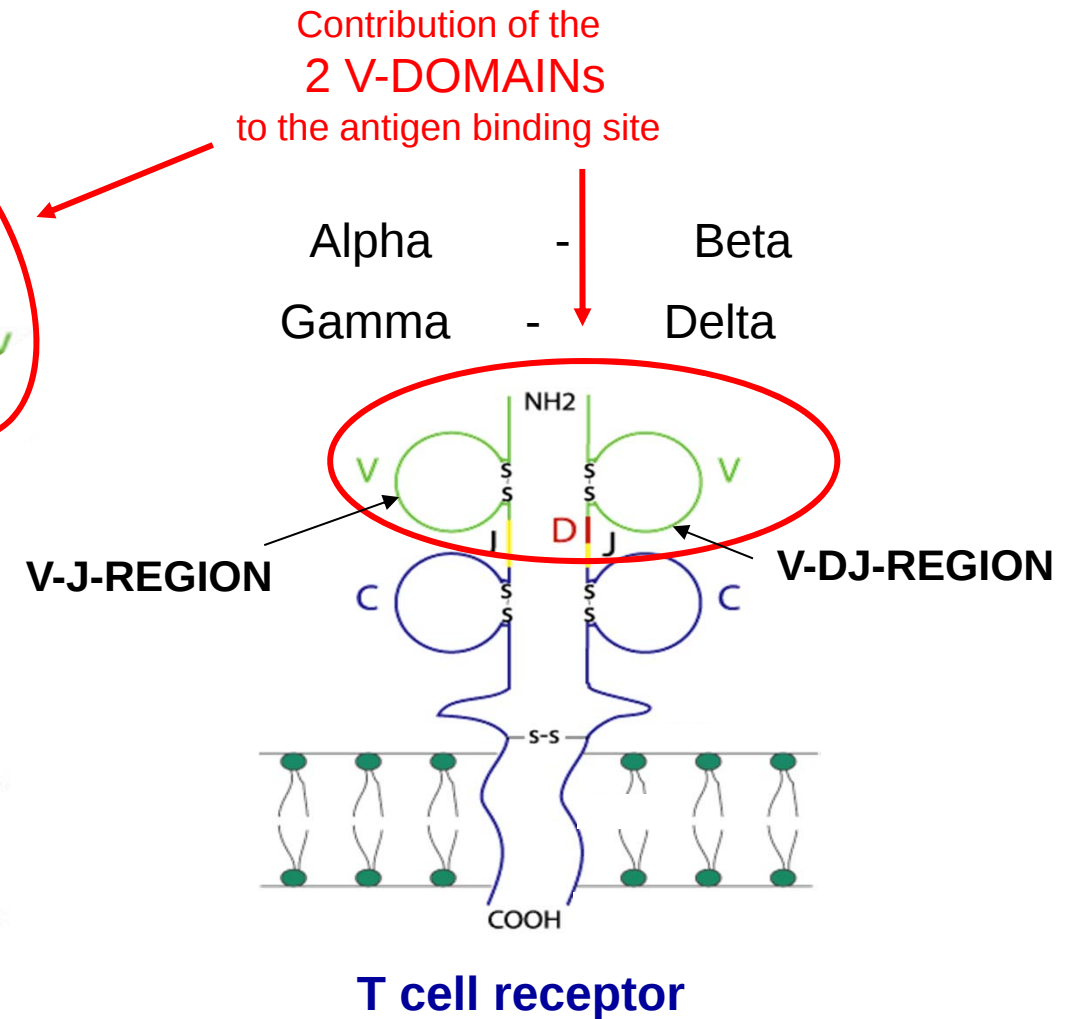
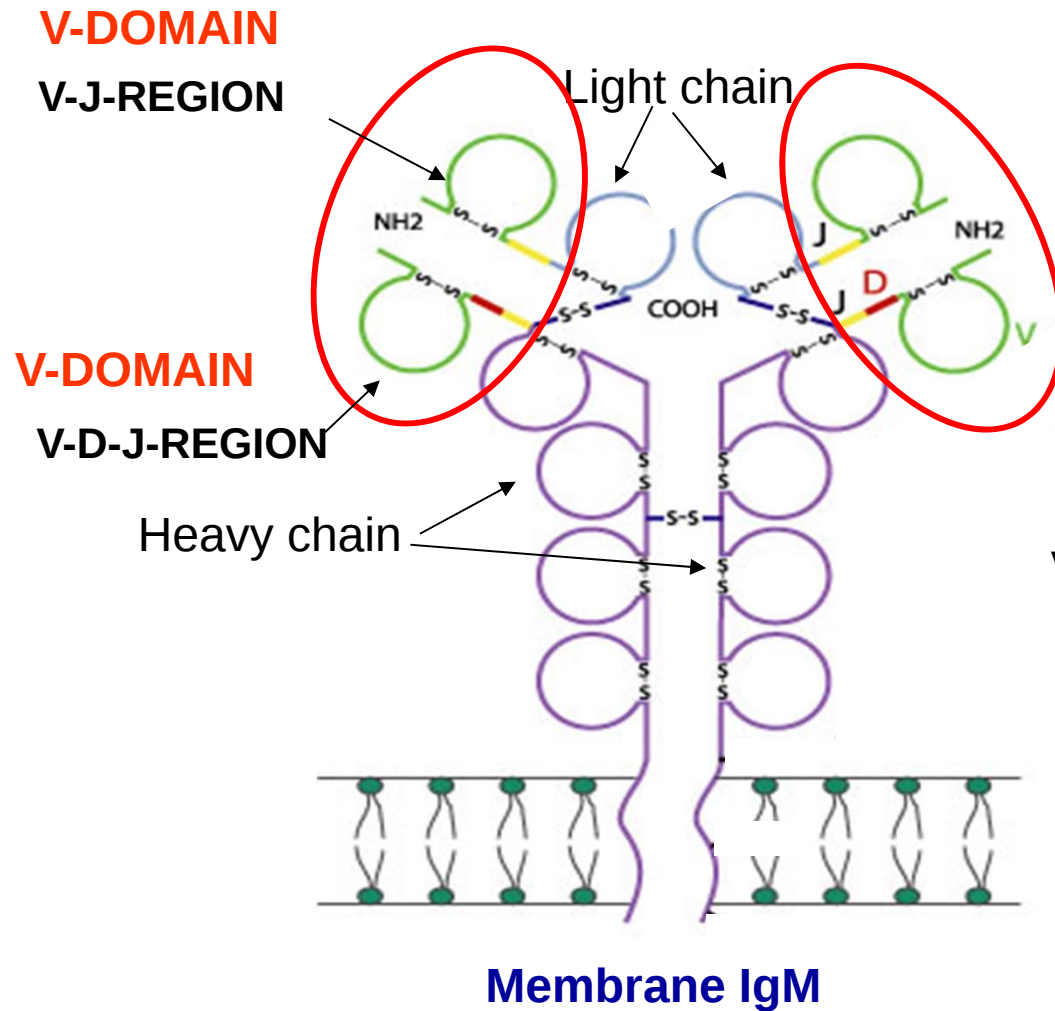
Véronique Giudicelli
LIGM, IGH, UPR CNRS 1142
141 rue de la Cardonille
34296 Montpellier Cedex 5
tel: 04.34.35.99.28 fax: 04.34.35.99.01
e-mail: Veronique.Giudicelli@igh.cnrs.fr

Immunoglobulines (IG)

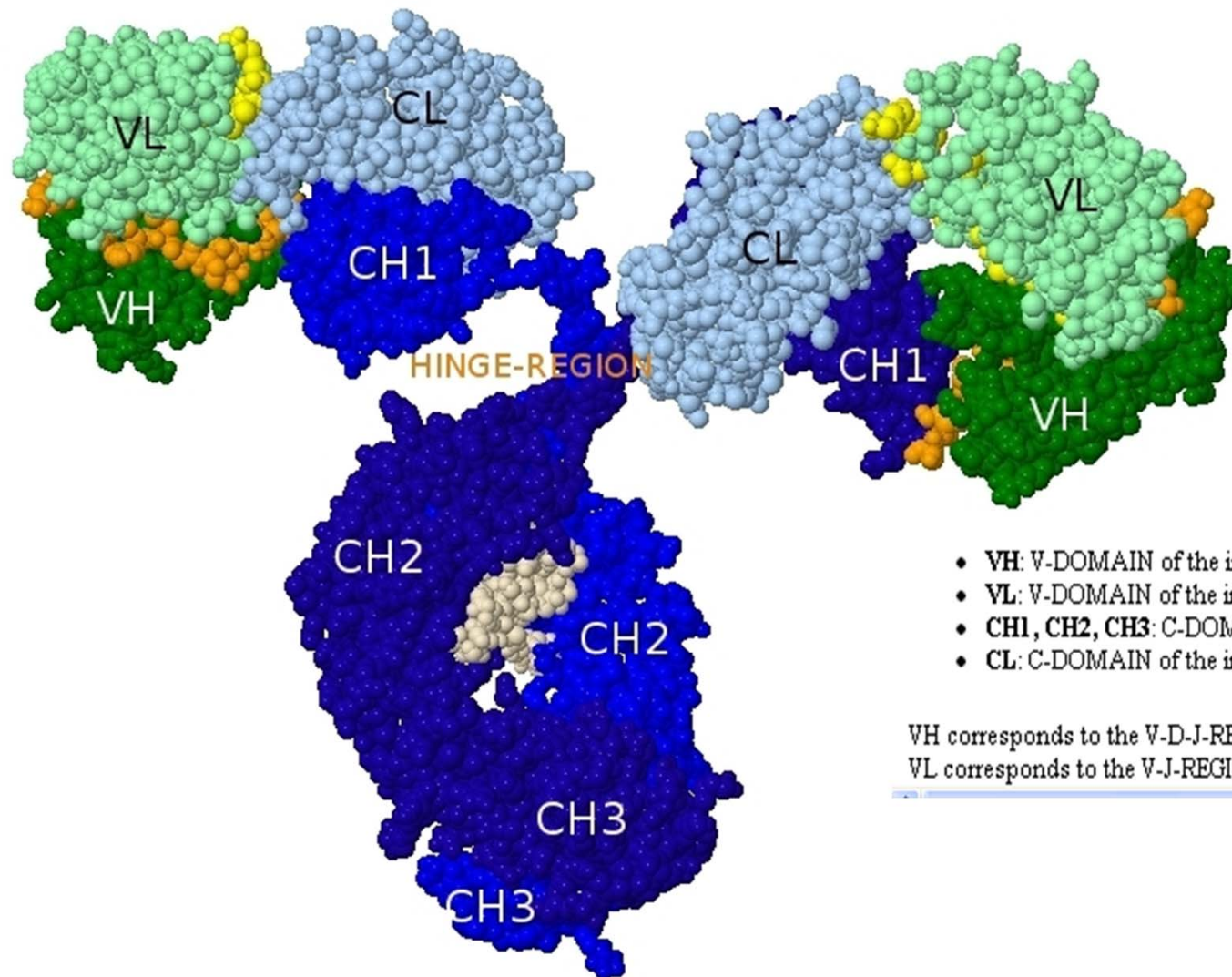


Immunoglobulin (IG)

T cell receptor (TR)



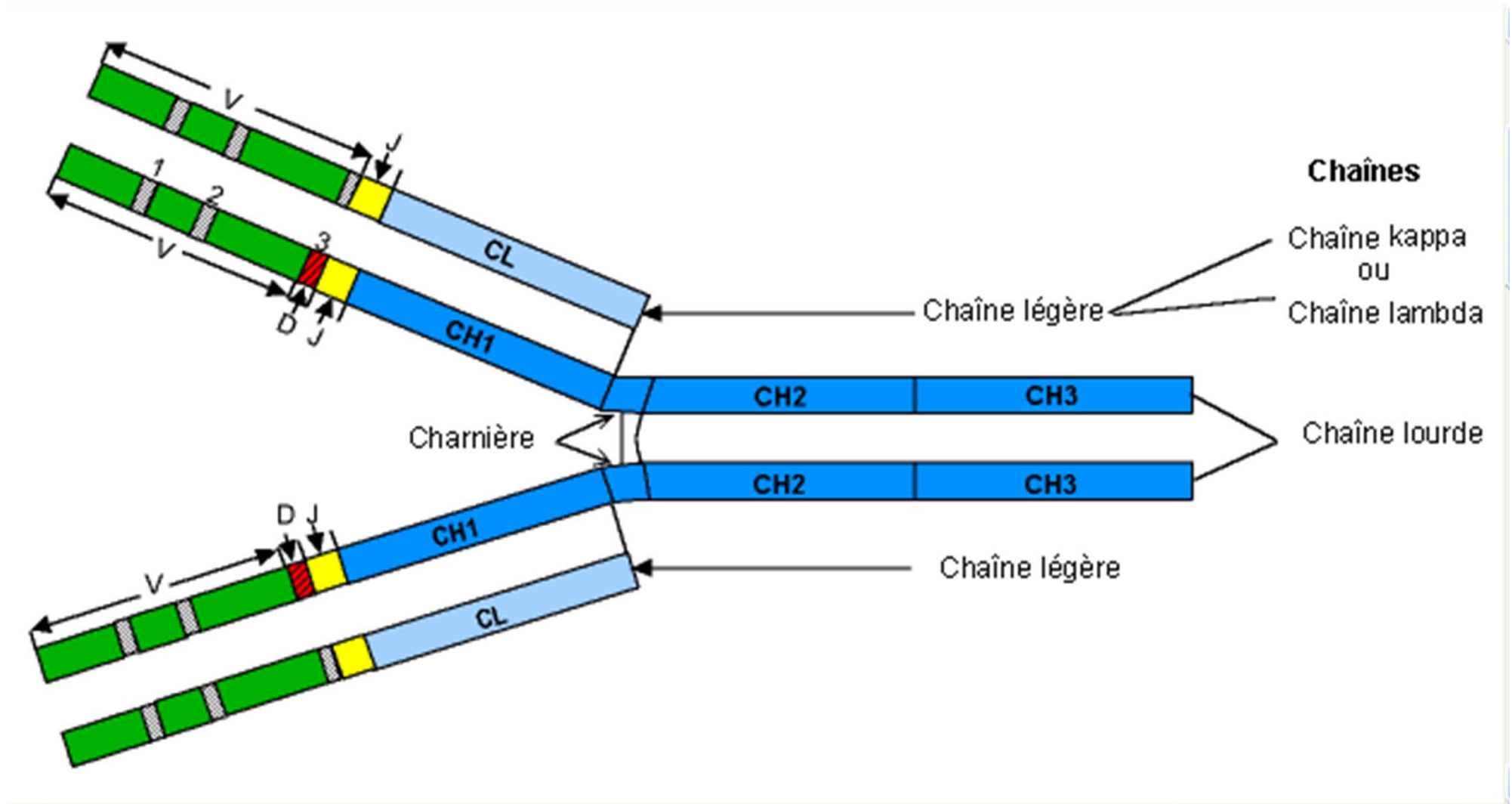
Immunoglobulins (IG) - Spacefill



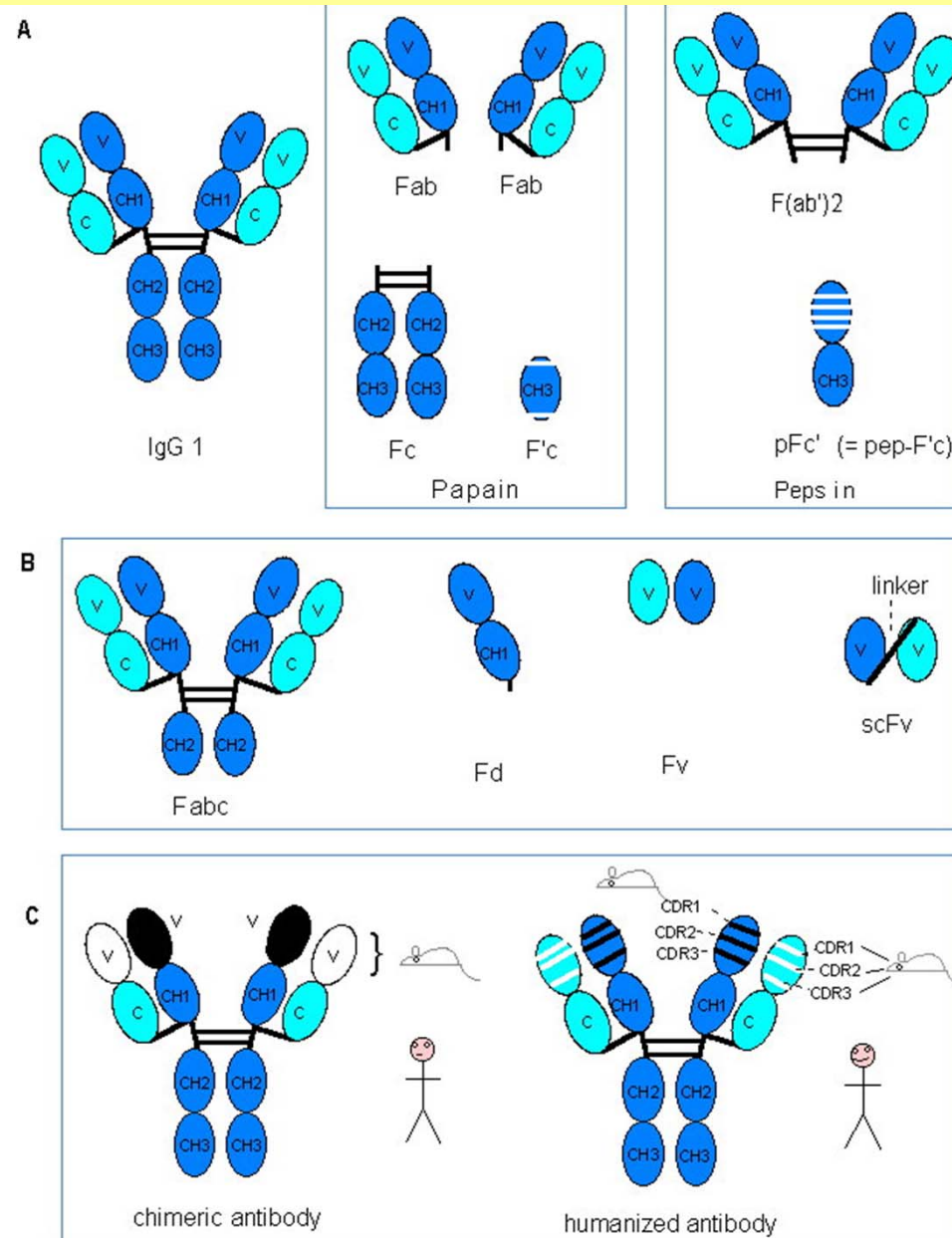
- VH: V-DOMAIN of the immunoglobulin heavy chain
- VL: V-DOMAIN of the immunoglobulin light chain
- CH1, CH2, CH3: C-DOMAIN of the immunoglobulin heavy chain
- CL: C-DOMAIN of the immunoglobulin light chain

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 IgG



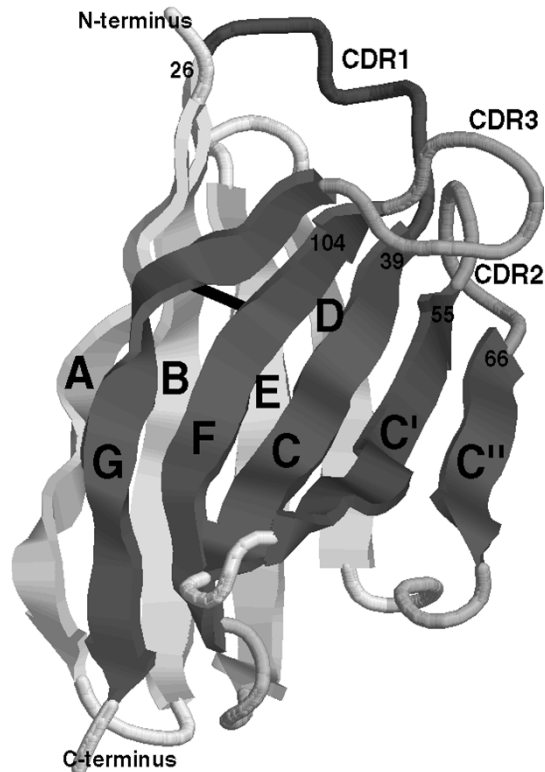
Organization in domains of an IgG1 immunoglobulin and of its fragments



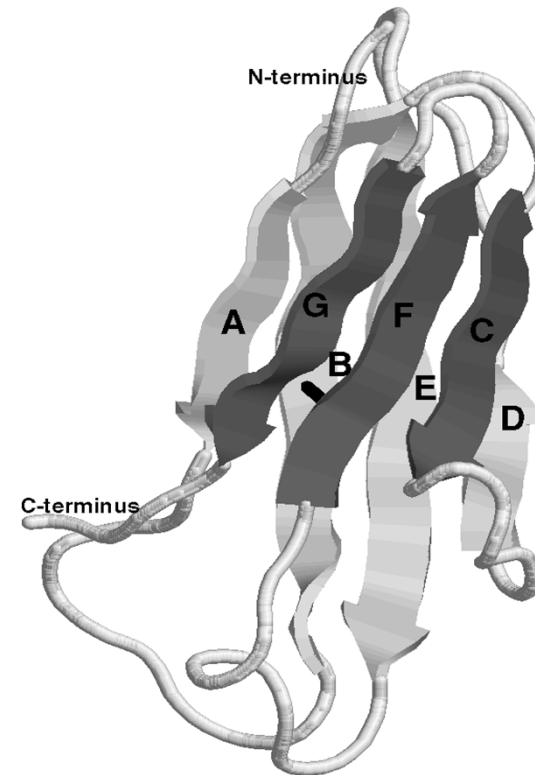
Structural domains

IG and TR

V-DOMAIN



C-DOMAIN

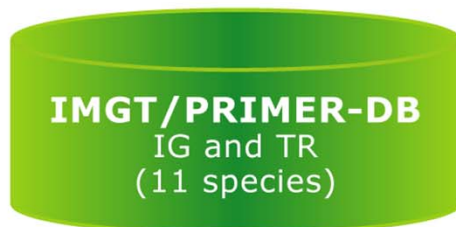


Le domaine d'IG est une structure de type sandwich bêta constituée de deux feuillets bêta antiparallèles. Les feuillets des V-DOMAINS possèdent respectivement 4 brins et 5 brins. Les V-DOMAINS possèdent trois boucles qui assurent la liaison avec un antigène. Ces boucles ou CDR (Complementarity Determining Region) sont les régions les plus variables en séquence des V-DOMAINS et sont également appelées boucles hypervariables.

ImMunoGeneTics
Information system®

View from above the CDRs

Sequences



<http://www.imgt.org>

created in 1989

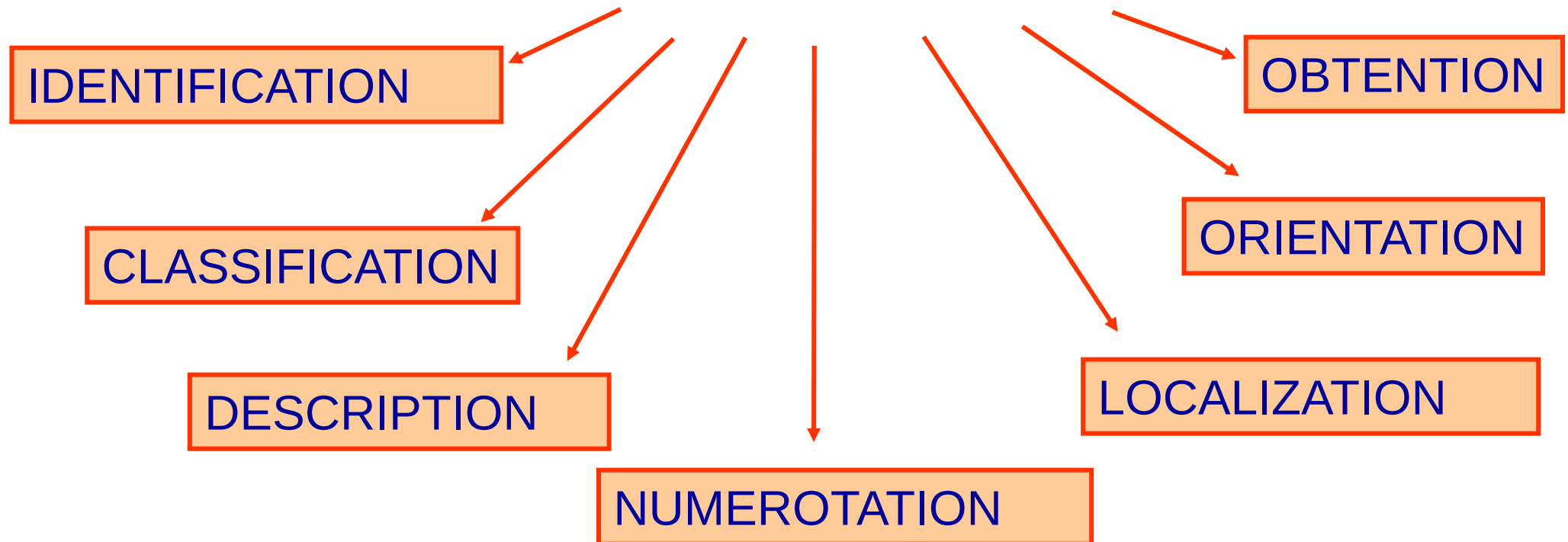
Genome



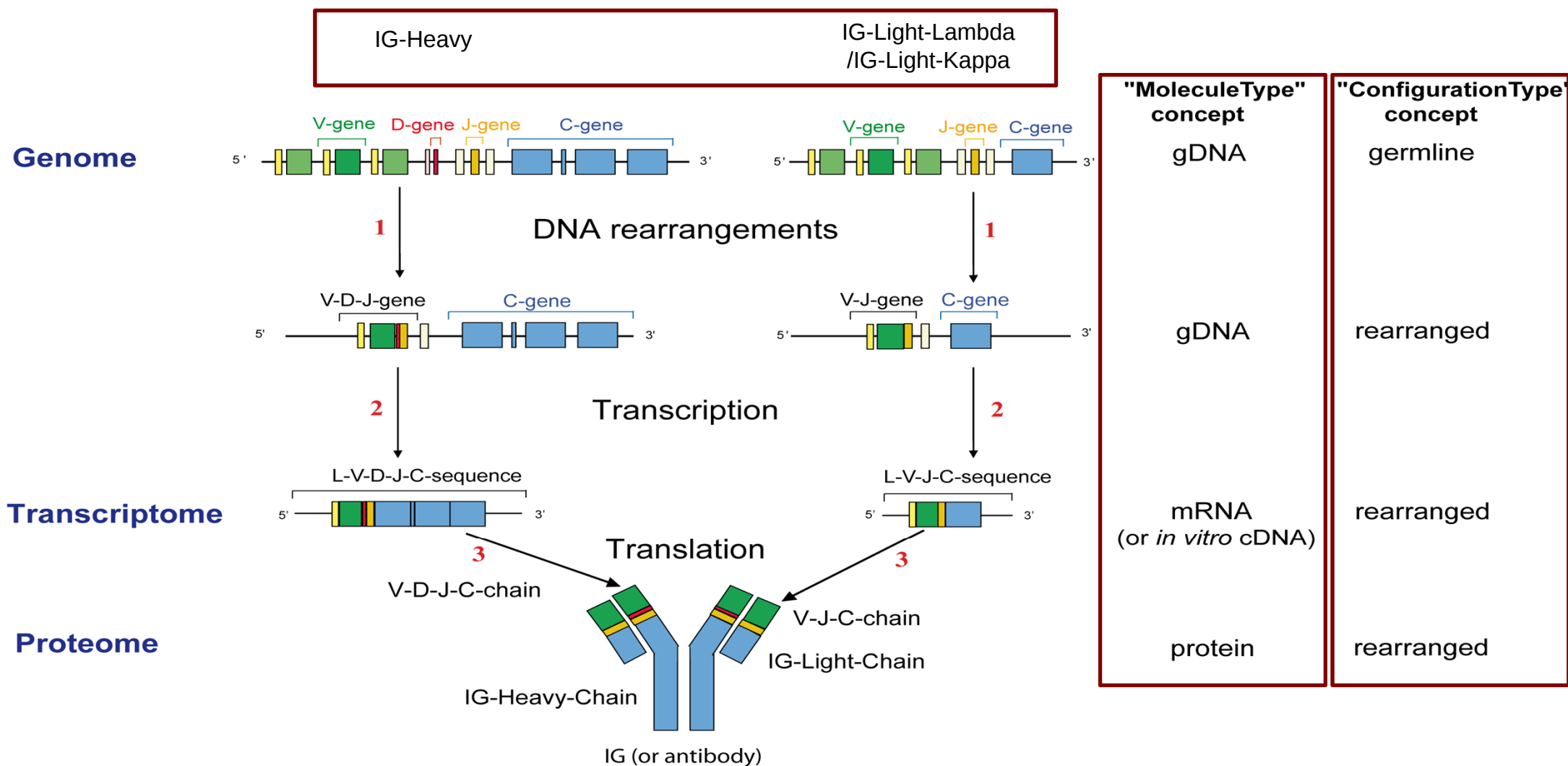
2D and 3D structures

IMGT-ONTOLOGY seven axioms:

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

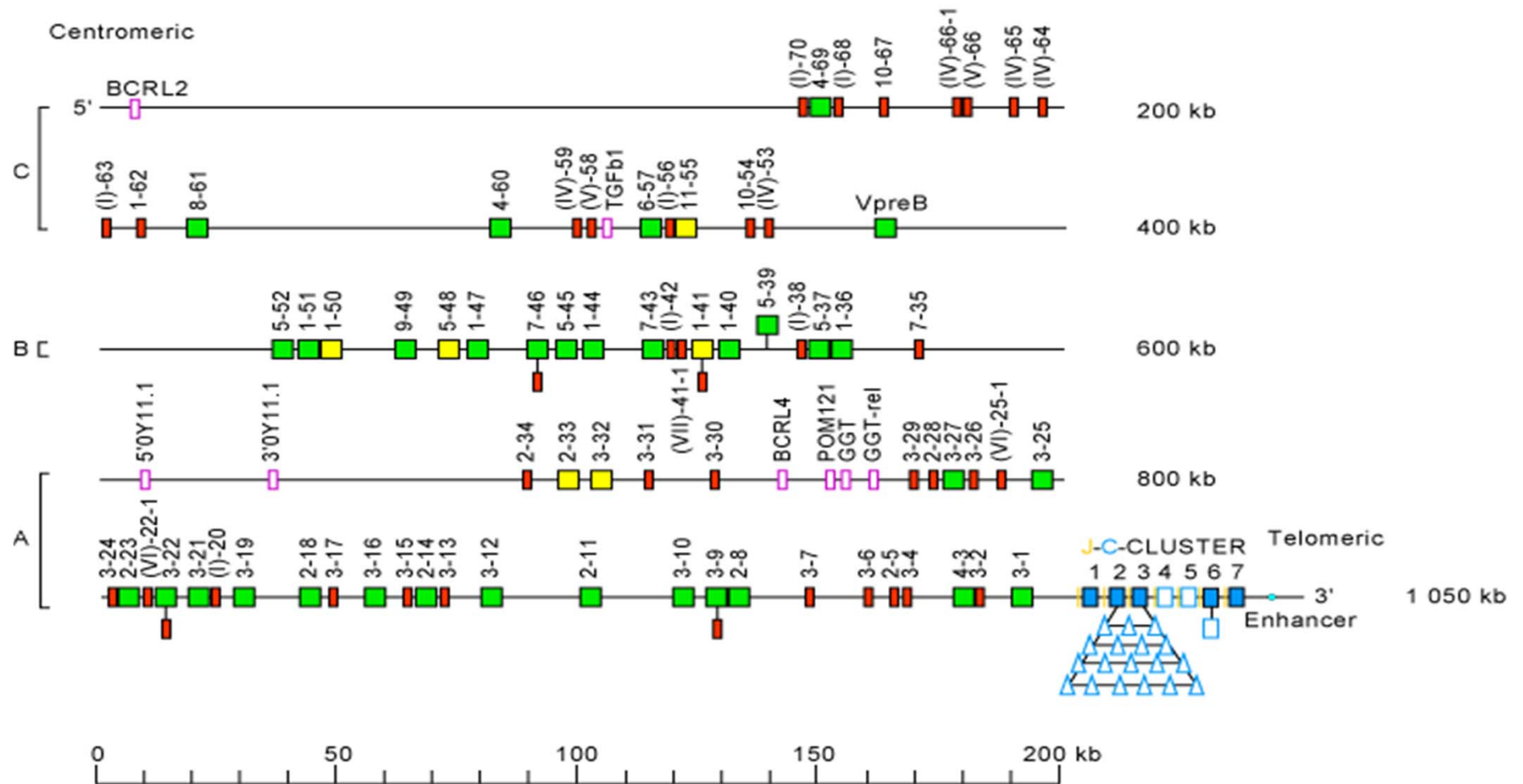


Concepts of IDENTIFICATION : IMGT standardized keywords



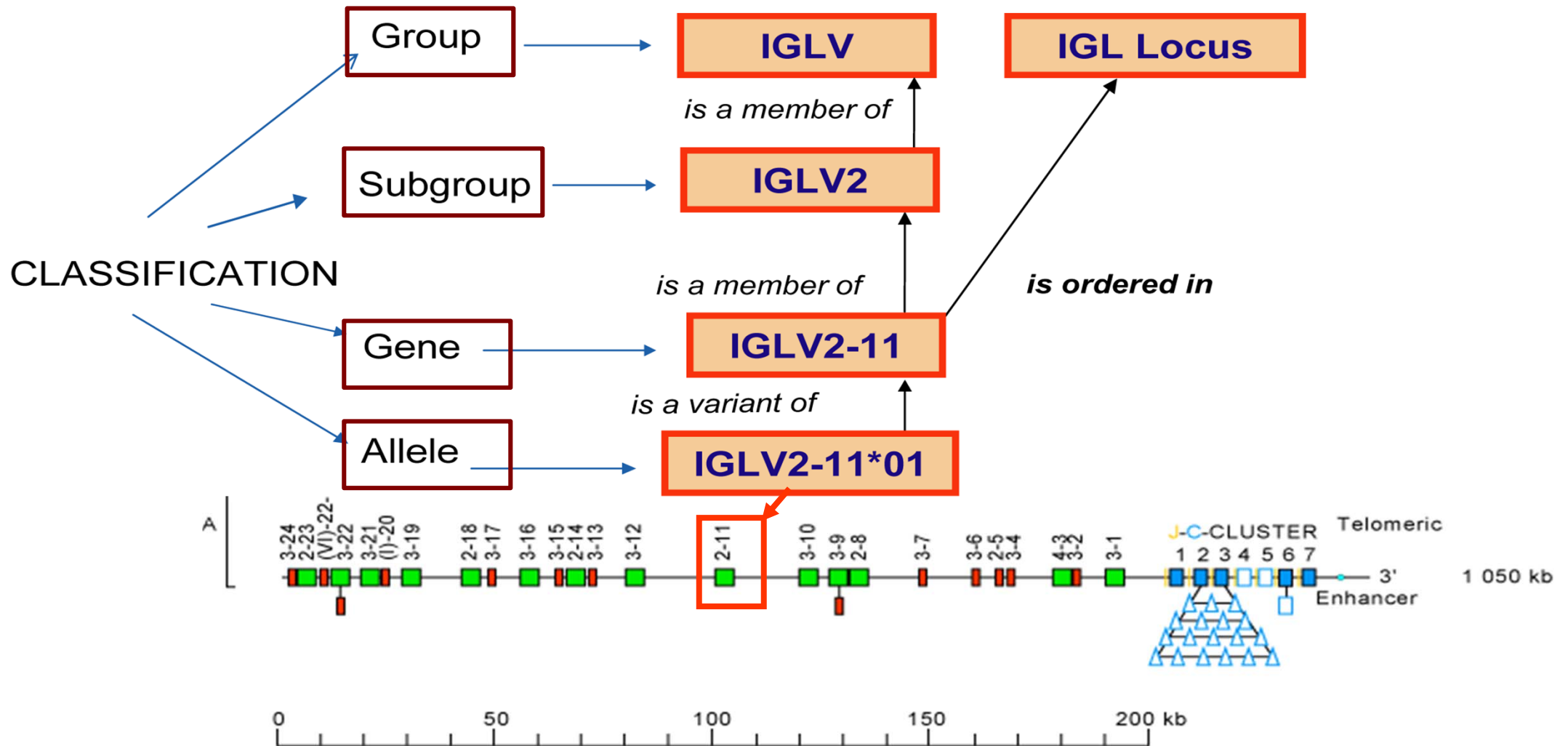
Concepts of CLASSIFICATION : the IG and TR gene nomenclature

- Approved by HUGO Nomenclature Committee (HGNC) in 1999



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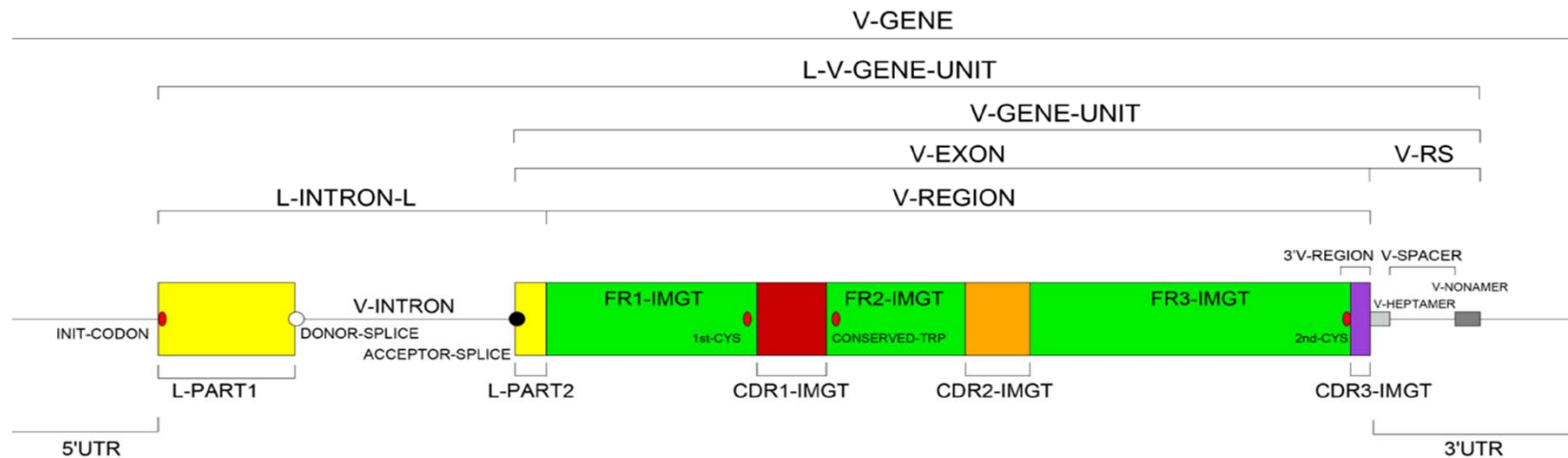


Concepts of DESCRIPTION: IMGT labels

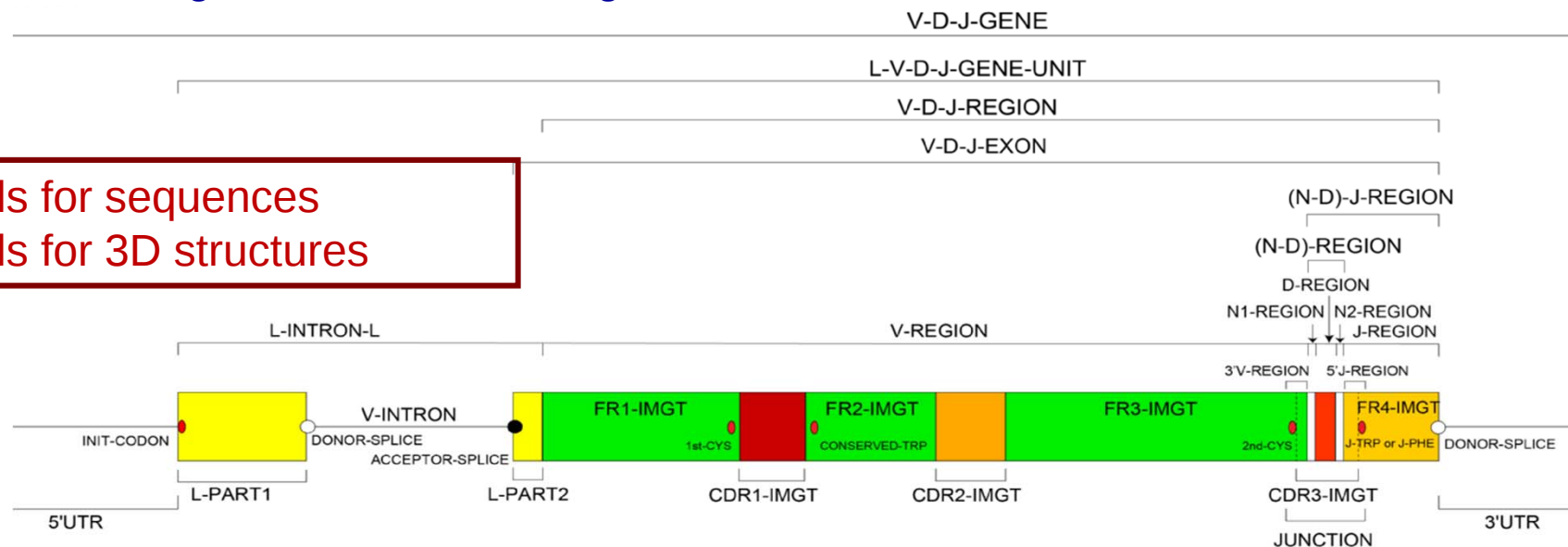


<http://www.imgt.org>

Labels for a germline V-GENE in gDNA



Labels for a rearranged V-D-J-GENE in gDNA



287 labels for sequences
370 labels for 3D structures

IMGT Scientific chart - Mozilla Firefox

Fichier Édition Affichage Historique Marque-pages Outils ?

IMGT Scientific chart

www.imgt.org/IMGTScientificChart/SequenceDescription/IMGT3Dkeywords.html

IMGT/PROTEIN-DB and IMGT/3Dstructure-DB keywords and labels: IG complete receptors

Mammals

IDENTIFICATION		Standardized labels for DESCRIPTION		
Receptor type	Chain type	Receptor (1)	Chain	Domain (2)
IgA_Kappa	IG-Heavy-Alpha	IG-ALPHA_KAPPA	H-ALPHA	VH, CH1, CH2, CH3
	IG-Light-Kappa		L-KAPPA	V-KAPPA, C-KAPPA
IgA1_Kappa	IG-Heavy-Alpha-1	IG-ALPHA-1_KAPPA	H-ALPHA-1	VH, CH1, CH2, CH3
	IG-Light-Kappa		L-KAPPA	V-KAPPA, C-KAPPA
IgA2_Kappa	IG-Heavy-Alpha-2	IG-ALPHA-2_KAPPA	H-ALPHA-2	VH, CH1, CH2, CH3
	IG-Light-Kappa		L-KAPPA	V-KAPPA, C-KAPPA
IgD_Kappa	IG-Heavy-Delta	IG-DELTA_KAPPA	H-DELTA	VH, CH1, CH2, CH3
	IG-Light-Kappa		L-KAPPA	V-KAPPA, C-KAPPA
IgE_Kappa	IG-Heavy-Epsilon	IG-EPSILON_KAPPA	H-EPSILON	VH, CH1, CH2, CH3, CH4
	IG-Light-Kappa		L-KAPPA	V-KAPPA, C-KAPPA
IgG_Kappa	IG-Heavy-Gamma	IG-GAMMA_KAPPA	H-GAMMA	VH, CH1, CH2, CH3
	IG-Light-Kappa		L-KAPPA	V-KAPPA, C-KAPPA
IgG1_Kappa	IG-Heavy-Gamma-1	IG-GAMMA-1_KAPPA	H-GAMMA-1	VH, CH1, CH2, CH3
	IG-Light-Kappa		L-KAPPA	V-KAPPA, C-KAPPA
IgG2_Kappa	IG-Heavy-Gamma-2	IG-GAMMA-2_KAPPA	H-GAMMA-2	VH, CH1, CH2, CH3
	IG-Light-Kappa		L-KAPPA	V-KAPPA, C-KAPPA
IgG2a_Kappa	IG-Heavy-Gamma-2-a	IG-GAMMA-2-A_KAPPA	H-GAMMA-2-A	VH, CH1, CH2, CH3
	IG-Light-Kappa		L-KAPPA	V-KAPPA, C-KAPPA
IgG2b_Kappa	IG-Heavy-Gamma-2-b	IG-GAMMA-2-B_KAPPA	H-GAMMA-2-B	VH, CH1, CH2, CH3
	IG-Light-Kappa		L-KAPPA	V-KAPPA, C-KAPPA
IgG2c_Kappa	IG-Heavy-Gamma-2-c	IG-GAMMA-2-C_KAPPA	H-GAMMA-2-C	VH, CH1, CH2, CH3
	IG-Light-Kappa		L-KAPPA	V-KAPPA, C-KAPPA
IgG3_Kappa	IG-Heavy-Gamma-3	IG-GAMMA-3_KAPPA	H-GAMMA-3	VH, CH1, CH2, CH3
	IG-Light-Kappa		L-KAPPA	V-KAPPA, C-KAPPA

Concepts of NUMEROTATION

IMGT Collier de Perles

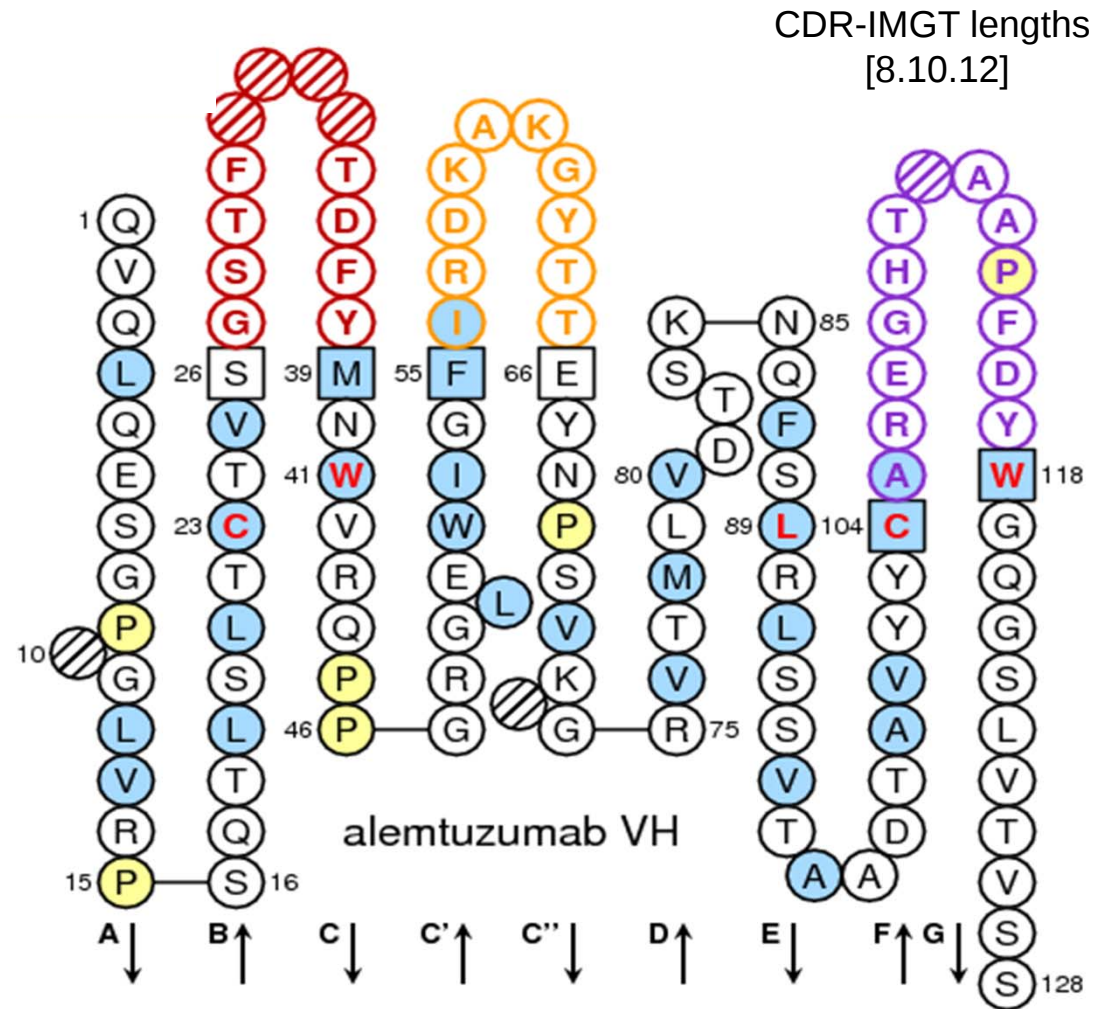
Based on the **IMGT** unique numbering
(first one in 1997)

- conserved AA (and codons)
are always at the **same positions**:

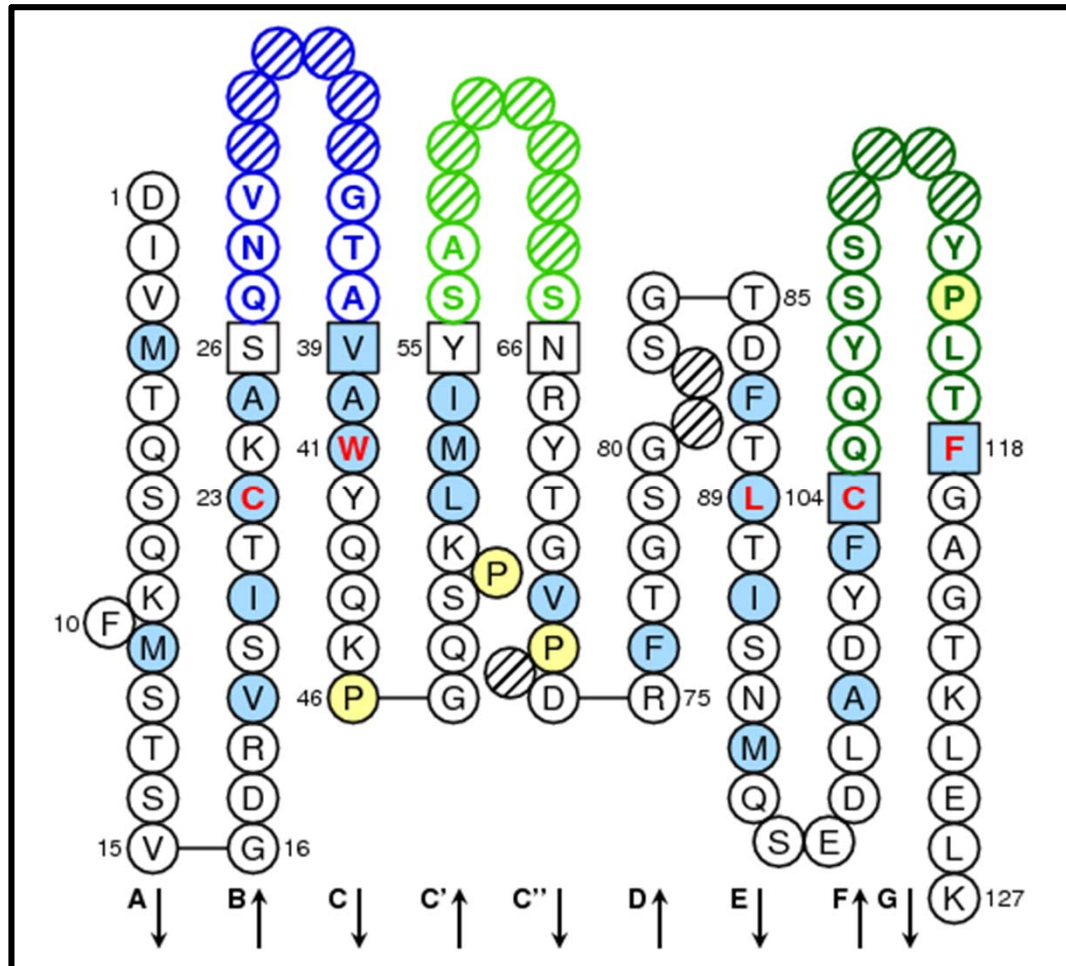
23 1st-CYS
41 CONSERVED-TRP
89 hydrophobic
104 2nd-CYS
118 J-PHE, J-TRP

- delimitation of the **FR-IMGT**
and **CDR-IMGT** is standardized

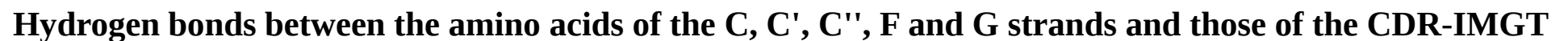
- **CDR-IMGT lengths** are crucial
information



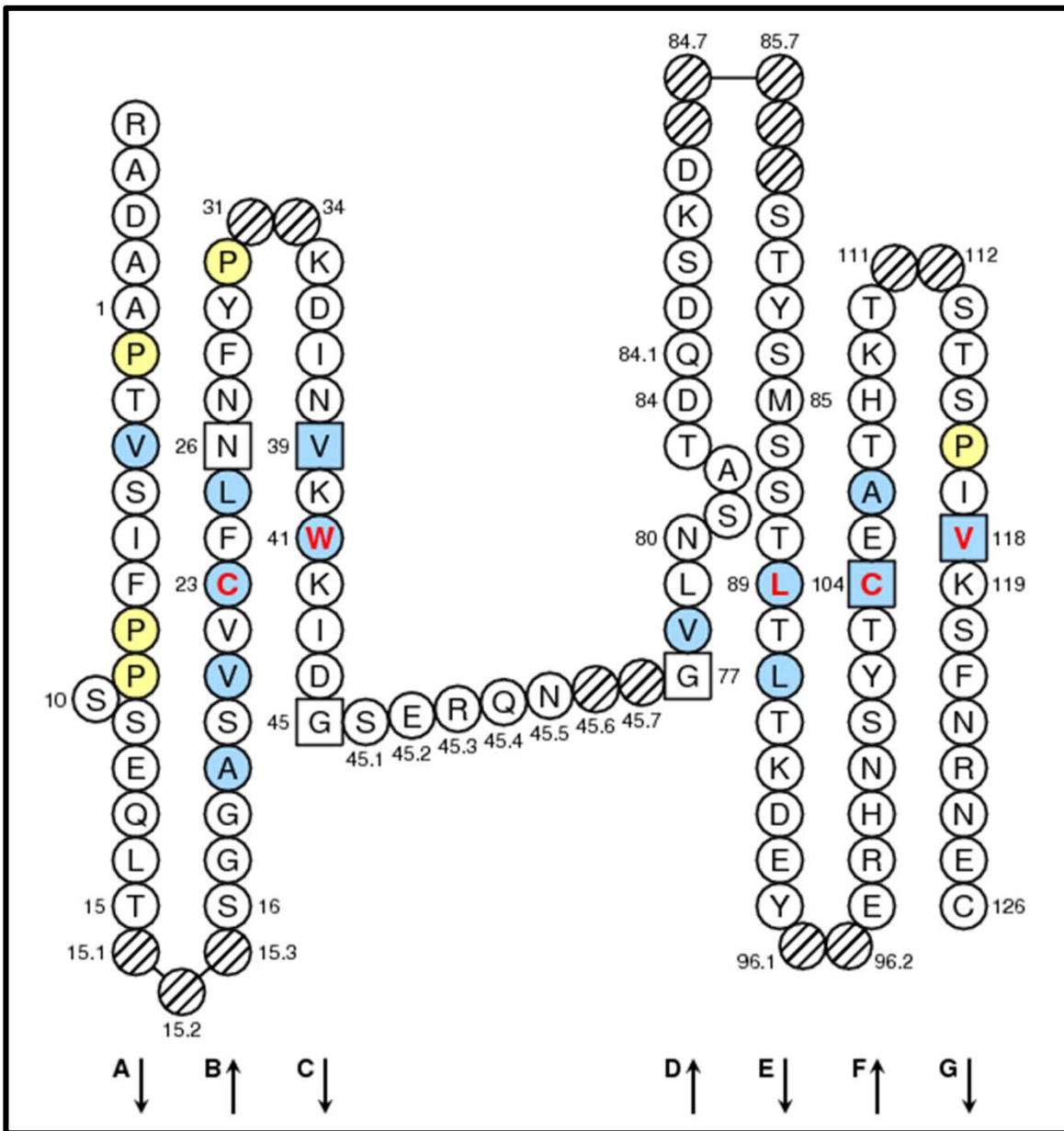
IMGT Collier de Perles for V-DOMAIN



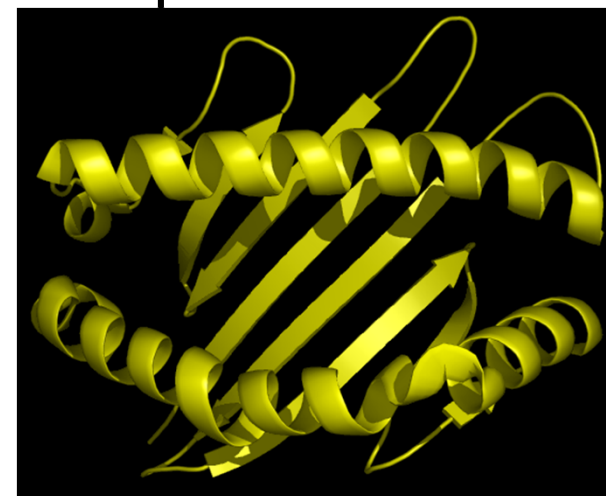
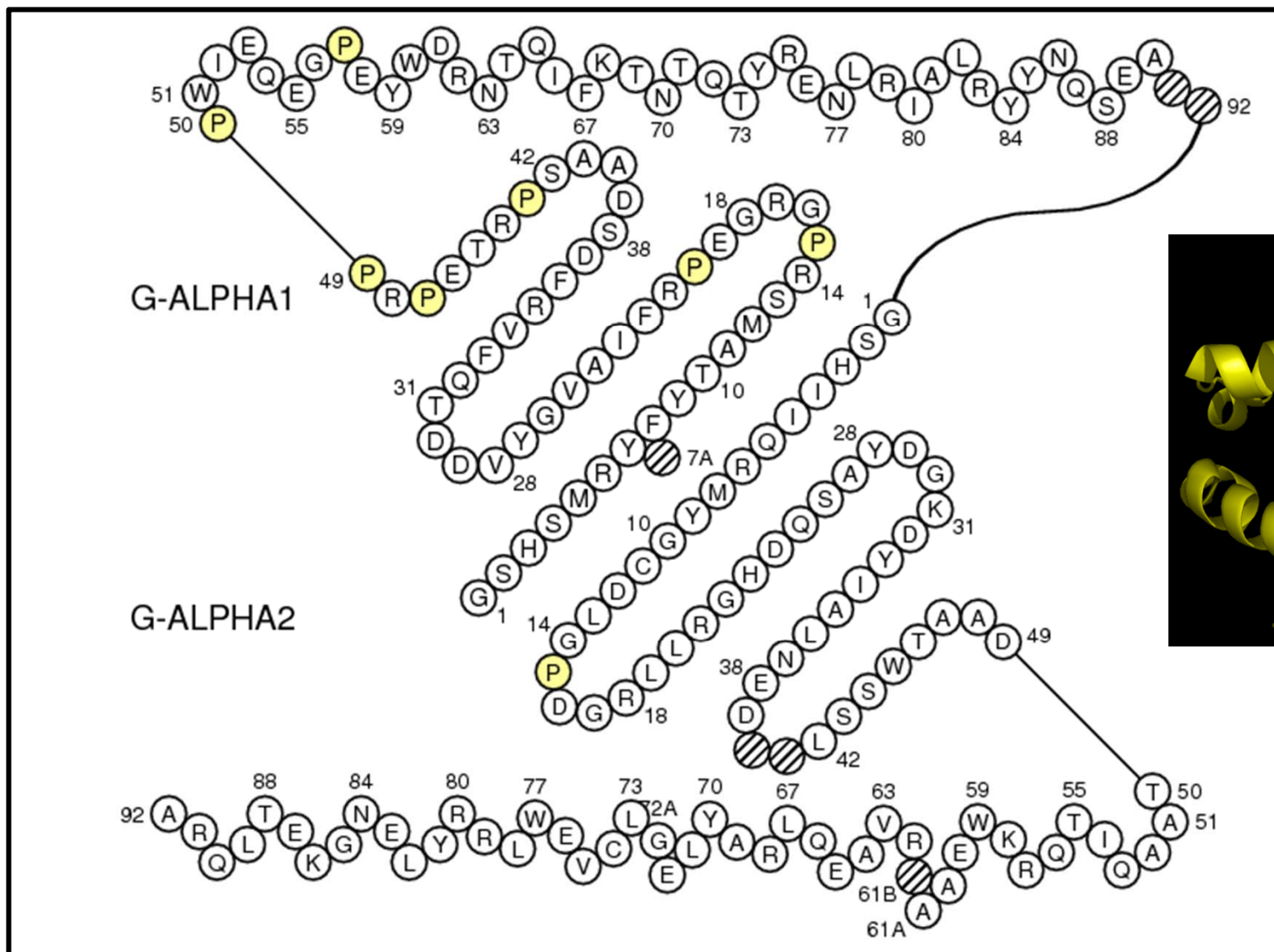
<http://imgt.cines.fr>



IMGT Collier de Perles for C-DOMAIN

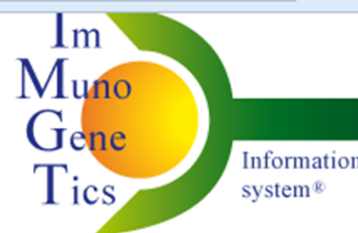


IMGT Collier de Perles for G-DOMAIN



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to the IMGT Home page

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IMMUNOGENETICS
INFORMATION SYSTEM®



<http://www.imgt.org>

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IMGT founder and director: Marie-Paule Lefranc (Marie-Paule.Lefranc@igh.cnrs.fr), Université Montpellier 2, CNRS, LIGM, IGH, SFR, Montpellier (France)

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The 2010 IMGT® Customer Satisfaction Survey



The Quality Management System of IMGT® Montpellier France has been approved by Lloyd's Register Quality Assurance France SAS to the following Quality Management System Standard: ISO 9001:2008

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- [IMGT/LIGM-DB \(doc\)](#) LIGM, Montpellier, France **beta version**
[IMGT/LIGM-DB \(doc\)](#) LIGM, Montpellier, France
Nucleotide sequences of IG and TR from 346 species (**175 412 entries**)
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-
- [IMGT/GENE-DB \(doc\)](#) LIGM, Montpellier, France **beta version**
[IMGT/GENE-DB \(doc\)](#) LIGM, Montpellier, France
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 - [IMGT/3Dstructure-DB and IMGT/2Dstructure-DB \(doc\)](#) LIGM, Montpellier, France
3D structures (IMGT Colliers de Perles) of IG antibodies, TR, MH and RPI (**2 802 entries**)
Source: PDB, INN, Kabat

IMGT Web resources

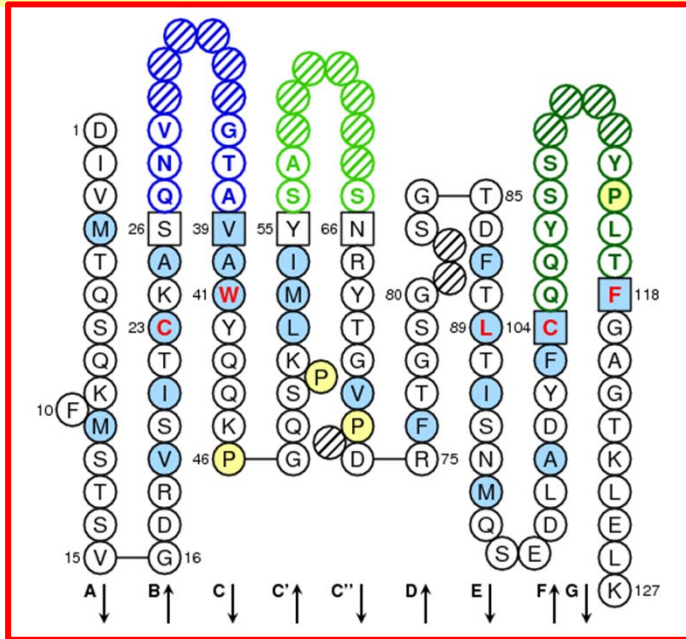
- [IMGT Repertoire \(IG and TR, MH and RPI\)](#)
- [IMGT Scientific chart \(Sequences description, Numbering, Nomenclature, Representation rules\)](#)
- [IMGT Index \(FactsBook\)](#)
- [IMGT Bloc-notes](#) (Interesting links, PubMed, Meeting announcements, Postdoctoral positions and jobs, Messages, Search engines...)
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IMGT Web resources



<http://www.imgt.org>

IMGT
Collier
de Perles



	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	P	V	F	E	E	A	P	V	E
AE000659, TRAV8-6*02	GCC	CAG	TCT	GTG	ACC	CAG	CTT	GAC	AGC	CAR	GTC	CCT	CTC	TTT	GAA	GAA	GCC	CCT	GTG	GAG
H86361 , TRAV8-6*02	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---
	CDR1-IMGT																			
X02850 , TRAV8-6*01	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40
AE000659, TRAV8-6*02	L	R	C	N	Y	S	S	S	V	S	V	V	V	V	V	V	V	V	L	F
H86361 , TRAV8-6*02	CTG	AGG	TGC	AAC	TAC	TCA	TGG	TCT	GTT	TCA	GTG	TAT	---	---	---	---	---	---	CTC	TTC

	CDR2-																			
X02850 , TRAV8-6*01	41	42	43	44	45	46	47	48	49	50	51	52	53	54	55	56	57	58	59	60
AE000659, TRAV8-6*02	W	Y	V	Q	Y	P	N	Q	G	L	Q	L	L	L	K	Y	L	S	G	S
H86361 , TRAV8-6*02	TGG	TAT	GTG	CAR	TAC	CCC	ACC	CAR	GGA	CTC	CAG	CTT	CTC	CTG	AGG	TAT	TCA	GGA	TCC	---

	IMGT																			
X02850 , TRAV8-6*01	61	62	63	64	65	66	67	68	69	70	71	72	73	74	75	76	77	78	79	80
AE000659, TRAV8-6*02	T	L	---	---	---	V	E	S	I	N	---	---	---	---	---	---	---	---	---	---
H86361 , TRAV8-6*02	ACC	CTG	---	---	---	GTT	GAA	AGC	ATC	ACC	---	---	---	---	---	---	---	GGT	TTT	GAG

	A-- G--																			
	K G																			
	A-- G--																			

IMGT
Alignment
of alleles

http://www.imgt.org/IMGTrepertoire/2D-3Dstruct/#h1_0

<http://www.imgt.org/IMGTrepertoire/Proteins/index.php#B>

IMGT
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)
	1 10 20	30	40 50	60	70 80 84ABC 90 100 110	
AE000658, TRAV1-1	GQSLEQ.PSEVTAVEGAIVQINCTYQ	TSGFYG.....	LSWYQQHGGCAPTFLSY	NALDG.....	LEETG.....	RFSSFLSRSDSYGYLLQLQMKDSASYFC
AE000658, TRAV1-2	GQNIDQ.PTEMTATEGAIVQINCTYQ	TSGFNG.....	LFWYQQHAGEAPTFLSY	NVLDG.....	LEETG.....	RFSSFLSRSGYSYLLQLQMKDSASYLC
AE000658, TRAV2	KDQVFQ.PSTVASSEGAIVVEIFCNHS	VSNAYN.....	FFWYLFHFGCAPRLLVK	GSK.....	PSQQG.....	RYNMTYER.FSSSLILQVREADAAVYFC
AE000658, TRAV3	AQSVAQPEDQVNAEGNPLTVKCTYS	VSGNPY.....	LFWYVQYPNRGLQLLLK	YITGDNL.....	VKGSY.....	GFEAEFNKSTSFHLKPSALVSDSALYFC
AE000658, TRAV4	LAKTTQ.PISMDSYEGQEVNITCSHN	NIATNDY.....	ITWYQQFSPSQPRFIIQ	GYKT.....	KVTNE.....	VASLFIPADRKSSSTLSLPRVSLSDTAVYFC
AE000659, TRAV5	GEDVEQS.LFLSVREGDSSVINCTYT	DSSSTY.....	LYWYKQEPGAGLQLLTY	IFSND.....	MKQDQ.....	RLTVLLNKKDKHLSLRIADTQTGDSAIYFC
AE000659, TRAV6	SQKIEQNSEALNIQEGKTATLTCTNYT	NYSPAY.....	LQWYRQDPGRGPVFLLL	IRENEK.....	EKRKE.....	RLKVTFTDTLTKQSLFHITASQPADSATYLC
AE000659, TRAV7	ENQVEHSPHFLGPQQGDVASMCTYS	VSRFNN.....	LQWYRQNTGMGPKHLIS	MYSAGY.....	EKQKG.....	RLNATLLK.NGSSLYITAVQPEDSATYFC
AE000659, TRAV8-1	AQSVSQNHVHILSEAASLELGCNYS	YGGTVN.....	LFWYVQYPPGQHLQLLLK	YFSGDPL.....	VKGIK.....	GFEAEFIKSKFSFNLKPSVQWSDTAIEYFC
AE000659, TRAV8-2	AQSVTQLDGHVSVSEGTPLVLRNYS	SSYSPS.....	LFWYVQHPNKGQLQLLLK	YTSAAITL.....	VKGIN.....	GFEAEFKKSETSFHLTKPSAHMSDAIEYFC
AE000659, TRAV8-3	AQSVTQPDIIHITVSEGASLELRNYS	YGATPY.....	LFWYVQSPGQGLQLLLK	YFSGDTL.....	VQGIK.....	GFEAEFKRSQSSFNLRKPSVHWSDAIEYFC
AE000659, TRAV8-4	AQSVTQLGSHVSVSEGTPLVLRNYS	SSVPPY.....	LFWYVQYPPGQHLQLLLK	YTSAAITL.....	VKGIN.....	GFEAEFKKSETSFHLTKPSAHMSDAIEYFC
X02850 , TRAV8-6	AQSVTQLDSQVPVFEEAPVELRCNYS	SSVSVY.....	LFWYVQYPPGQGLQLLLK	YLSGSL.....	VESIN.....	GFEAEFNKSTSFHLKPSVHISDAIEYFC
AE000660, TRAV8-7	TQSVTQLDGHITVSEEAPLELKNYS	YSGVPS.....	LFWYVQYSSQSLQLLLK	DLTEATQ.....	VKGIR.....	GFEAEFKKSETSFYLRKPSVHWSDAIEYFC
AE000659, TRAV9-1	GDVYVQTFGQVLPSEFGSLIVNCSYF	TTQVPS.....	LFWYVQYPPGQGLQLLLK	AMKAND.....	KGRNK.....	GFFAMYRKFTTSFHLKFNDSVHWSDAIEYFC

<http://www.imgt.org/IMGTrepertoire/Proteins/index.php>

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IMGT founder and director: [Marie-Paule Lefranc](#) (Marie-Paule.Lefranc@igh.cnrs.fr), Université Montpellier 2, CNRS, [LIGM](#), [IGH](#), [SFR](#), Montpellier (France)

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IMGT 3Dstructure-DB Query Page

IMGT/3Dstructure-DB and IMGT/2Dstructure-DB Query page - Mozilla Firefox

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IMGT/3Dstructure-DB and IMGT/2Dstructure-DB Query page

Program version: [4.9.0](#) (2013-04-06) Database release: [201313-6](#) (2013-04-06)

Citing IMGT/3Dstructure-DB:
Kaas, Q. et al. Nucleic Acids Res., 32, D208-D210 (2004). PMID: 14681396 [Abstract Full](#) [PDF](#)
Ehrenmann, F. et al. Nucleic Acids Res., 38, D301-D307 (2010). PMID: 19900967 [Abstract Full](#) [PDF](#)
Ehrenmann, F., Lefranc, M.-P. Cold Spring Harbor Protoc., 6, 750-761 (2011). PMID: 21632774 [Abstract](#) also in IMGT booklet with generous provision from [Cold Spring Harbor \(CSH\) Protocols](#) [PDF](#) (high res) [PDF](#) (low res)

Today is Sunday, December 01 2013
IMGT/3Dstructure-DB contains **2802** entries
2290 entries PDB
177 entries INN
335 entries KAB

Search by Entry code or Molecule name (receptor or ligand)

☐ Entry code (PDB, INN, PROTEIN) ☐ Molecule name (receptor or ligand)

Search for complexes

Paratope/epitope ☐ IG/Ag ☐ TR/pMH1 ☐ TR/pMH2 ☐ RPI/pMH1 ☐ RPI/pMH2

Peptide/MH ☐ pMH1 ☐ pMH2

Ligand category

Peptide length

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Search by IMGT entry type using IMGT-ONTOLOGY concepts

IMGT entry type ☒ PDB ☐ INN ☐ Kabat ☐ any

IDENTIFICATION

Species

IMGT receptor type ☐ IG ☐ TR ☐ MH ☐ RPI ☐ FPIA ☐ any

Options: ☐ MH1 ☐ MH2 ☐ RPI-MH1Like

DESCRIPTION

IMGT receptor description

Options: ☐ FV ☐ SCFV ☐ FAB ☐ FC

IMGT chain description

IMGT domain description

CLASSIFICATION

IMGT group

IMGT subgroup

IMGT gene

IMGT allele

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☆ Google

Search by Resolution, Release date or Experimental method

☐ Resolution 0 - 1.00 Å ☐ Release date 2011 ☐ Experimental method X-ray diffraction, single crysta

Search Clear

Search by bibliographical references

Select ☐ PDB OR ☐ PubMed

Authors

Journal Title (part of)

Year

PMID

Search Clear

Chain alignment

☐ Align your sequence (FASTA format)

E-value 0.01 Number of results 10

Search Clear

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Display results

Overview

☒ IMGT entry ID
 ☒ IMGT entry type
 ☒ IMGT molecule name
 ☒ Species

☒ IMGT receptor description
 ☒ Ligand(s)
 ☐ Gene(s) and Allele(s)
 ☒ Experimental technique

☒ PDB release date
 ☒ Resolution
 ☐ PDB references
 ☐ PubMed references

Domain type sequences

☐ V domain
 ☐ C domain
 ☐ G domain
 ☐ S domain

FR-IMGT/CDR-IMGT sequences and lengths

☐ FR1-IMGT
 ☐ CDR1-IMGT
 ☐ FR2-IMGT
 ☐ CDR2-IMGT

☐ FR3-IMGT
 ☐ CDR3-IMGT

Search Clear

Last entries

[3W11](#)
[3W12](#)
[3W13](#)
[3W14](#)
[3V5K](#)
[4G5Z](#)
[4HC1](#)

[4ENE](#)
[4HCR](#)
[4HGW](#)
[4I9W](#)
[4GRG](#)
[4G6J](#)
[4G6K](#)

[4G6M](#)
[4GBX](#)
[4FQX](#)
[4DVB](#)
[4FFV](#)
[4FFW](#)
[4DW2](#)

[4I0P](#)
[4I4W](#)
[9606](#)
[9636](#)
[9643](#)
[9669](#)
[9672](#)

[9679](#)
[9688](#)
[9689](#)
[9703](#)
[9710](#)
[9711](#)
[9713](#)

[9714](#)
[9723](#)
[9724](#)
[9733](#)

Updated entries

[1BBD](#)
[1B6D](#)
[1BEC](#)
[1A6W](#)
[1B88](#)

Related other IMGT® resources

[IMGT/DomainDisplay](#)
[IMGT/StructuralQuery tool](#)

[IMGT/Collier-de-Perles](#)
[IMGT/DomainSuperimpose tool](#)

[IMGT/DomainGapAlign](#)
[IMGT/mAb-DB](#)

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IMGT/3Dstructure-DB Overview

IMGT/3Dstructure-DB Results - Mozilla Firefox

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IMGT/3Dstructure-DB Results

www.imgt.org/3Dstructure-DB/cgi/3Dquery.cgi

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Overview

Your selection:
Receptor description
FAB-GAMMA-1_KAPPA

Number of results:
640

Entry code: Search
[Query page](#)

Click on IMGT entry ID (2nd column) for entry card

	IMGT entry ID	IMGT molecule name	IMGT entry type	IMGT receptor description	Species	Ligand(s)	Experimental technique	Resolution	PDB release date
1	12e8	2E8	PDB	FAB-GAMMA-1_KAPPA	<i>Mus musculus</i>		X-ray diffraction	1.90	05-AUG-98
2	15c8	5C8	PDB	FAB-GAMMA-1_KAPPA	<i>Mus musculus</i>		X-ray diffraction	2.5	23-MAR-99
3	1a0q	29G11	PDB	FAB-GAMMA-1_KAPPA	<i>Mus musculus</i>		X-ray diffraction	2.3	04-MAY-99
4	1a3l	13G5	PDB	FAB-GAMMA-1_KAPPA	<i>Mus musculus</i>		X-ray diffraction	1.95	16-FEB-99
5	1a4j	39-A11	PDB	FAB-GAMMA-1_KAPPA	<i>Chimeric</i>		X-ray diffraction	2.1	13-MAY-98
6	1a4k	39-A11	PDB	FAB-GAMMA-1_KAPPA	<i>Chimeric</i>		X-ray diffraction	2.4	13-MAY-98
7	1a5f	7A9	PDB	FAB-GAMMA-1_KAPPA	<i>Mus musculus</i>		X-ray diffraction	2.8	20-APR-99
8	1acy	59.1 mAb, anti-gp120 [HIV-1]	PDB	FAB-GAMMA-1_KAPPA	<i>Mus musculus</i>		X-ray diffraction	3.0	31-JUL-94
9	1ae6	CTM01,mCTM01 Fab, anti_MUC1 (mucin 1, PEM, episialin, CD227)	PDB	FAB-GAMMA-1_KAPPA	<i>Mus musculus</i>		X-ray diffraction	3.0	18-MAR-98
10	1afv	25.3 mAb, anti-p24 [HIV-1]	PDB	FAB-GAMMA-1_KAPPA	<i>Mus musculus</i>		X-ray diffraction	3.7	20-AUG-97
11	1ahw	5G9	PDB	FAB-GAMMA-1_KAPPA	<i>Mus musculus</i>		X-ray diffraction	3.0	19-AUG-98
12	1ai1	59.1	PDB	FAB-GAMMA-1_KAPPA	<i>Mus musculus</i>		X-ray diffraction	2.8	15-MAY-97
13	1aif	409.5.3	PDB	FAB-GAMMA-1_KAPPA	<i>Mus musculus</i>		X-ray diffraction	2.9	01-FEB-97
14	1aj7	48G7	PDB	FAB-GAMMA-1_KAPPA	<i>Chimeric</i>		X-ray diffraction	2.1	12-NOV-97
15	1axs	AZ-28-chimeric	PDB	FAB-GAMMA-1_KAPPA	<i>Chimeric</i>		X-ray diffraction	2.6	04-FEB-98
16	1b2w	Anti-Gamma-Interferon	PDB	FAB-GAMMA-1_KAPPA	<i>Humanized</i>		X-ray diffraction	2.90	06-MAY-99

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

Entry code Search [Query page](#)

IMGT molecule name	IMGT receptor type	IMGT receptor description	Ligand(s)	Species	CC	Chain ID
A6	TR	TR-ALPHA_BETA-2		<i>Homo sapiens</i> (human)	1	[1ao7_D 1ao7_E]
HLA-A*0201	MH	MH1-ALPHA_B2M		<i>Homo sapiens</i> (human)	1	[1ao7_A 1ao7_B]
		Peptide	Tax peptide 11-19 (Q82235)	<i>Human T-lymphotropic virus 1</i>	1	[1ao7_C]
		Ion	Ethyl Mercury Ion		1	[1ao7_1]
		Ion			1	[1ao7_2]

Experimental technique X-ray diffraction Resolution (in angstrom) 2.6 PDB release date 17-SEP-97

Chain details Contact analysis Paratope and epitope 3D visualization Jmol or QuickPDB Renumbered IMGT file IMGT numbering comparison References and links Printable card

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IMGT/3Dstructure-DB Card (2)

IMGT/3Dstructure-DB card - Mozilla Firefox

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IMGT/3Dstructure-DB card

www.imgt.org/3Dstructure-DB/cgi/details.cgi?pdbcode=1A07

IMGT/DomainGapAlign results

Chain ID	1ao7_E	
Chain length	245	
IMGT chain description	TR-BETA-2 = V-BETA (1-113) [D1] + C-BETA-2 (114-208) [D2]	
Chain sequence	V-BETA (1-113) [D1] NAGVTQTPKFQVLKGTQSMILQCAQDMNHEYSWYRQDPGMGLRLIHYSVGAGITDQGEVPGNGYNVSRSTTEDFPLRLLSAAPSQTSVYF C-BETA-2 (114-208) [D2] CASRPGLAGGRPEQYFGPGTRLTIVTDLKNVFPPEVAVFEPSEAEISHTQKATLVCLATGFYDPHVELSWWVNGKEVHSGVSTDPQPLKE QFALNDSRYALSSRLRVSATFWQNPFRNHFRQVQFYGLSENDEWTQDRAKPVTVQIVSAEAWGRAD Sequence in FASTA format Sequence in IMGT format	
V-DOMAIN	IMGT domain description	V-BETA (1-113) [D1]
	IMGT gene and allele name	TRBV6-5*01 (100.00%)(human) Alignment details
	IMGT gene and allele name	TRBJ2-7*01 (100.00%)(human) Alignment details
	2D representation	IMGT Collier de Perles or IMGT Collier de Perles on 2 layers
	Contact analysis	Domain contacts (overview)
	CDR-IMGT lengths	[5.6.14]
	Sheet composition	[A' B D E] [A" C C' C" F G]
C-DOMAIN	IMGT domain description	C-BETA-2 (114-208) [D2]
	IMGT gene and allele name	TRBC2*01 (99.20%)(human) , TRBC2*02 (99.20%)(human) Alignment details
	2D representation	IMGT Collier de Perles or IMGT Collier de Perles on 2 layers
	Contact analysis	Domain contacts (overview)
	Sheet composition	[A B D E] [C F G]
		EDLKNVFPPEVAVFEPSEAEISH . TQKATLVCLATGFY . DHVELSWWVNGKEVHS . GVSTDPQPLKEQPAL . NDSRYALSSRLRV SATFWQ . NFRNHFRQVQFYGLSENDEWTQDRAKPVTVQIVSAEAWGRAD IMGT/DomainGapAlign results

IMGT/3Dstructure-DB Card (1)



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

Entry code Search [Query page](#)

IMGT molecule name	IMGT receptor type	IMGT receptor description	Ligand(s)	Species	CC	Chain ID
A6	TR	TR-ALPHA_BETA-2		<i>Homo sapiens</i> (human)	1	[1ao7_D 1ao7_E]
HLA-A*0201	MH	MH1-ALPHA_B2M		<i>Homo sapiens</i> (human)	1	[1ao7_A 1ao7_B]
		Peptide	Tax peptide 11-19 (Q82235)	<i>Human T-lymphotropic virus 1</i>	1	[1ao7_C]
		Ion			1	[1ao7_1]
		Ion	Ethyl Mercury Ion		1	[1ao7_2]

Experimental technique X-ray diffraction Resolution (in angstrom) 2.6 PDB release date 17-SEP-97

Chain details Contact analysis Paratope and epitope 3D visualization Jmol or QuickPDB Renumbered IMGT file IMGT numbering comparison References and links Printable card

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IMGT/3Dstructure-DB Contact Analysis

IMGT/3Dstructure-DB card - Mozilla Firefox

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IMGT/3Dstructure-DB card

www.imgt.org/3Dstructure-DB/cgi/details.cgi?pdbcode=1ao7&Part=CONT_OVERVIEW

IMGT/3Dstructure-DB Domain pair contacts (overview) of 1ao7

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

	Unit 1		Unit 2		Residue pair contacts	Number of residues			Atom pair contact types			
	Domain	Chain	Domain	Chain		Total	From 1	From 2	Total	Polar	Hydrogen	Nonpolar
DomPair	[D1] V-ALPHA	1ao7_D	[D1] G-ALPHA1	1ao7_A	15	16	9	7	126	22	3	104
DomPair			[D2] G-ALPHA2	1ao7_A	12	15	7	8	105	17	2	88
DomPair			(Ligand)	1ao7_C	15	13	7	6	109	20	3	89
DomPair			[D2] C-ALPHA	1ao7_D	1	2	1	1	7	1	0	6
DomPair			[D1] V-BETA	1ao7_E	57	42	20	22	401	46	7	355
DomPair			[D2] C-BETA-2	1ao7_E	1	2	1	1	9	2	0	7
DomPair	[D2] C-ALPHA	1ao7_D	[D1] V-ALPHA	1ao7_D	1	2	1	1	7	1	0	6
DomPair	[D1] V-BETA	1ao7_E	[D1] G-ALPHA1	1ao7_A	3	4	1	3	23	0	0	23
DomPair			[D2] G-ALPHA2	1ao7_A	11	10	5	5	82	17	3	65
DomPair			(Ligand)	1ao7_C	14	13	9	4	119	9	2	110
DomPair			[D1] V-ALPHA	1ao7_D	57	42	22	20	401	46	7	355
DomPair			[D2] C-BETA-2	1ao7_E	32	27	12	15	236	30	1	206

IMGT/3Dstructure-DB Domain pair contacts

http://www.imgt.org/IMGTeducation/Aide-memoire/_UK/ContactAnalysis.html

IMGT/3Dstructure-DB card - Mozilla Firefox

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IMGT/3Dstructure-DB card

www.imgt.org/3Dstructure-DB/cgi/details.cgi?pdbcode=1A07&Part=CONT_DETAILS&domcontcode=1A

Summary:

Residue pair contacts	Number of residues			Atom pair contact types		
	Total	From 1	From 2	Total	Polar	Nonpolar
15	13	7	6	109	20	89

List of the Residue@Position pair contacts:
Click 'R@P' for IMGT Residue@Position cards

Order					Order					Atom pair contact types			
IMGT Num	Residue	Domain	Chain		IMGT Num	Residue	Domain	Chain		Total	Polar	Hydrogen	Nonpolar
R@P 29	GLY	G [D1] V-ALPHA	1ao7_D		R@P 1	LEU	L (Ligand)	1ao7_C		5	0	0	5
R@P 37	GLN	Q [D1] V-ALPHA	1ao7_D		R@P 1	LEU	L (Ligand)	1ao7_C		5	0	0	5
R@P 37	GLN	Q [D1] V-ALPHA	1ao7_D		R@P 2	LEU	L (Ligand)	1ao7_C		4	2	1	2
R@P 37	GLN	Q [D1] V-ALPHA	1ao7_D		R@P 3	PHE	F (Ligand)	1ao7_C		7	1	0	6
R@P 37	GLN	Q [D1] V-ALPHA	1ao7_D		R@P 4	GLY	G (Ligand)	1ao7_C		6	2	0	4
R@P 37	GLN	Q [D1] V-ALPHA	1ao7_D		R@P 5	TYR	Y (Ligand)	1ao7_C		1	0	0	1
R@P 38	SER	S [D1] V-ALPHA	1ao7_D		R@P 5	TYR	Y (Ligand)	1ao7_C		10	2	1	8
R@P 107	THR	T [D1] V-ALPHA	1ao7_D		R@P 5	TYR	Y (Ligand)	1ao7_C		3	1	0	2
R@P 108	THR	T [D1] V-ALPHA	1ao7_D		R@P 4	GLY	G (Ligand)	1ao7_C		2	1	0	1
R@P 108	THR	T [D1] V-ALPHA	1ao7_D		R@P 5	TYR	Y (Ligand)	1ao7_C		4	1	0	3
R@P 109	ASP	D [D1] V-ALPHA	1ao7_D		R@P 4	GLY	G (Ligand)	1ao7_C		11	2	0	9
R@P 109	ASP	D [D1] V-ALPHA	1ao7_D		R@P 5	TYR	Y (Ligand)	1ao7_C		16	2	0	14
R@P 110	SER	S [D1] V-ALPHA	1ao7_D		R@P 4	GLY	G (Ligand)	1ao7_C		8	2	1	6
R@P 110	SER	S [D1] V-ALPHA	1ao7_D		R@P 5	TYR	Y (Ligand)	1ao7_C		23	2	0	21
R@P 110	SER	S [D1] V-ALPHA	1ao7_D		R@P 6	PRO	P (Ligand)	1ao7_C		4	2	0	2

Display:

Atom pair contact types

☐ Noncovalent ☐ Covalent ☐ Disulfide

☒ Polar ☐ Hydrogen bond ☒ Nonpolar

Atom pair contact categories

☐ (BB) Backbone/backbone ☐ (SS) Side chain/side chain ☐ (BS) Backbone/side chain ☐ (SB) Side chain/backbone

Atom contacts

Total number of atomic pair contacts

Non Covalent

Number of non covalent atomic

Polar

Number of polar atomic pair contacts

Hydrogen Bond

Number of hydrogen bonds

Non Polar

Number of non polar atomic pair contacts

Covalent

Number of covalent links

Disulfide

Number of disulfide bridges

IMGT/3Dstructure-DB Card (1)



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

Entry code Search [Query page](#)

IMGT molecule name	IMGT receptor type	IMGT receptor description	Ligand(s)	Species	CC	Chain ID
A6	TR	TR-ALPHA_BETA-2		<i>Homo sapiens</i> (human)	1	[1ao7_D 1ao7_E]
HLA-A*0201	MH	MH1-ALPHA_B2M		<i>Homo sapiens</i> (human)	1	[1ao7_A 1ao7_B]
		Peptide	Tax peptide 11-19 (Q82235)	<i>Human T-lymphotropic virus 1</i>	1	[1ao7_C]
		Ion	Ethyl Mercury Ion		1	[1ao7_1]
		Ion			1	[1ao7_2]

Experimental technique X-ray diffraction Resolution (in angstrom) 2.6 PDB release date 17-SEP-97

[Chain details](#)
[Contact analysis](#)
[Paratope and epitope](#)
[3D visualization Jmol or QuickPDB](#)
[Renumbered IMGT file](#)
[IMGT numbering comparison](#)
[References and links](#)
[Printable card](#)

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IMGT/3Dstructure-DB Visualization

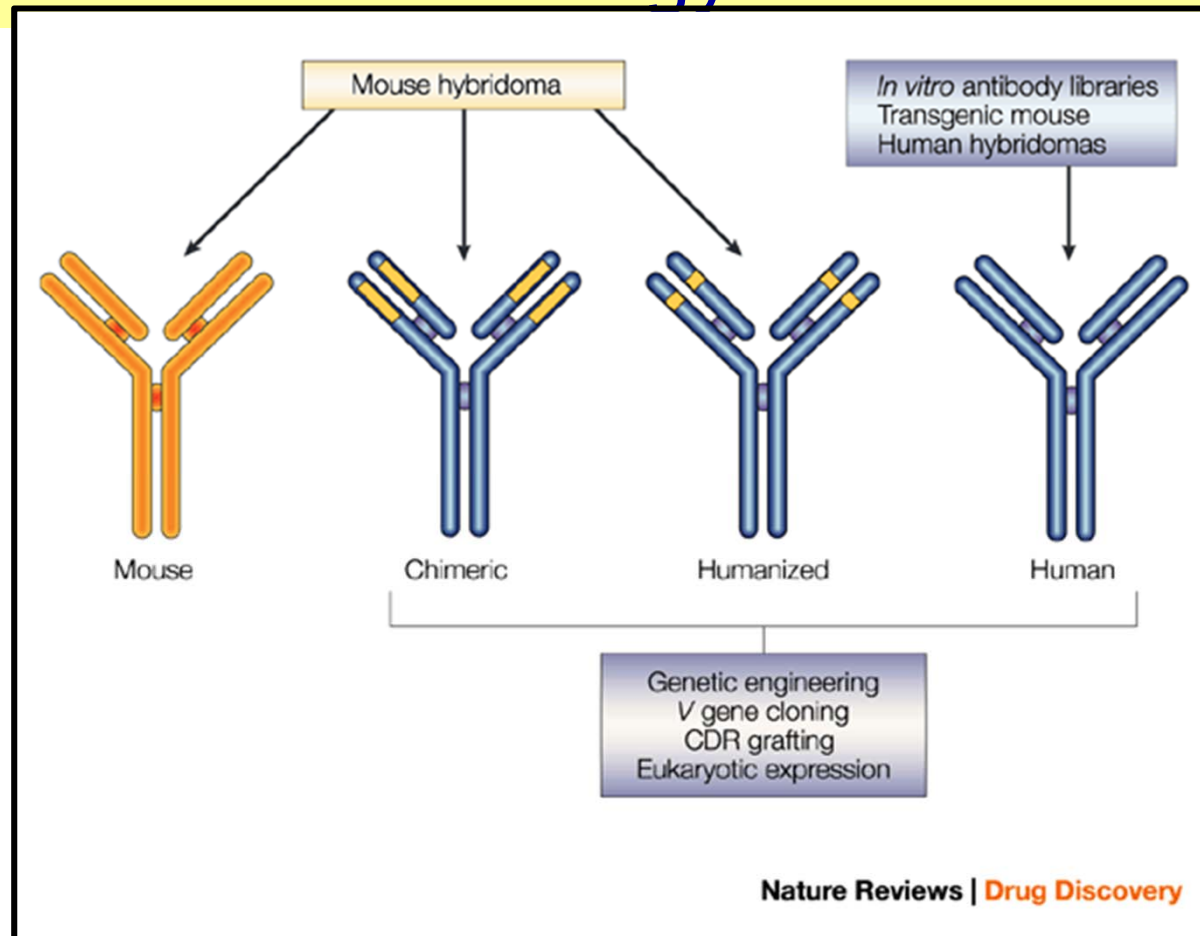
Documentation: http://www.imgt.org/3Dstructure-DB/doc/IMGT3DstructureDBHelp.shtml#h2_129

The image displays two overlapping browser windows from Mozilla Firefox showing the IMGT/3Dstructure-DB interface. The left window shows a 3D visualization of a protein structure (PDB code 1A07) with various regions labeled: G-ALPHA2, Peptide, G-ALPHA1, V-ALPHA, V-BETA, C-ALPHA, and C-BETA-2. The right window shows the configuration panel for the same structure.

Configuration Panel (Right Window):

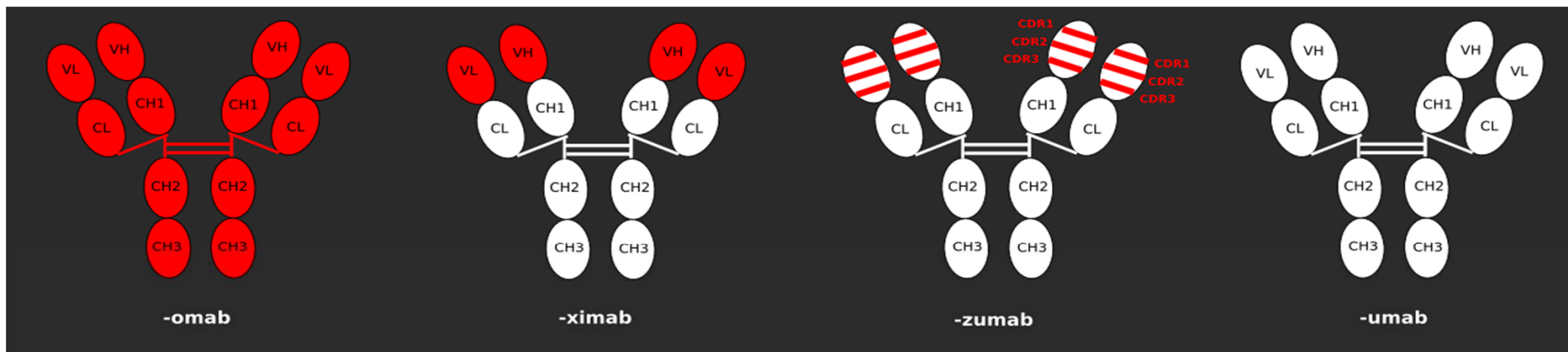
- Toggle spinning:** On (selected), Off, Background color: Black (selected), White, Zoom: +, -
- Other selection:**
 - ☐ All, ☐ Backbone, ☐ Sidechains, ☐ Water
 - ☐ Disulfide bridges
- View:**
 - ☐ wireframe, ☐ spacefill, ☐ dots, ☐ ribbons
 - ☐ cartoon, ☒ trace, ☐ meshribbon, ☐ rocket
 - ☐ off
- Coloration:**
 - ☒ current
 - ☐ amino acid type, ☐ cpk, ☐ chain, ☐ charge, ☐ structure
 - ☐ green, ☐ red, ☐ yellow, ☐ blue, ☐ purple
- Buttons:** Apply, Reset
- IMGT:**
 - ☐ CDR-IMGT labels, ☐ CDR-IMGT only (side view)
 - ☐ Domain description, ☐ Complex colored by chains and CDRs
 - ☐ IMGT pMH contacts sites
 - ☐ Paratope/epitope contact atoms
- Paratope/epitope:**
 - ☐ Pa/Epi 1, ☐ Pa/Epi 2, ☐ Pa/Epi 3, ☐ Pa/Epi 4
- Buttons:** Reset
- Contact:** Marie-Paule Lefranc Marie-Paule.Lefranc@igh.cnrs.fr

Chimeric and humanized antibodies: application in oncology



Une chaîne dite chimérique est une chaîne qui contient un domaine variable étranger (V-D-J-REGION) (provenant d'une espèce autre que l'homme, ou synthétiques) liées à une région constante (C-REGION) d'origine humaine.

Une chaîne humanisée est une chaîne dans laquelle les CDR des domaines variables sont étrangers (provenant d'une espèce autre que l'homme, ou de synthèse), alors que le reste de la chaîne est d'origine humaine.



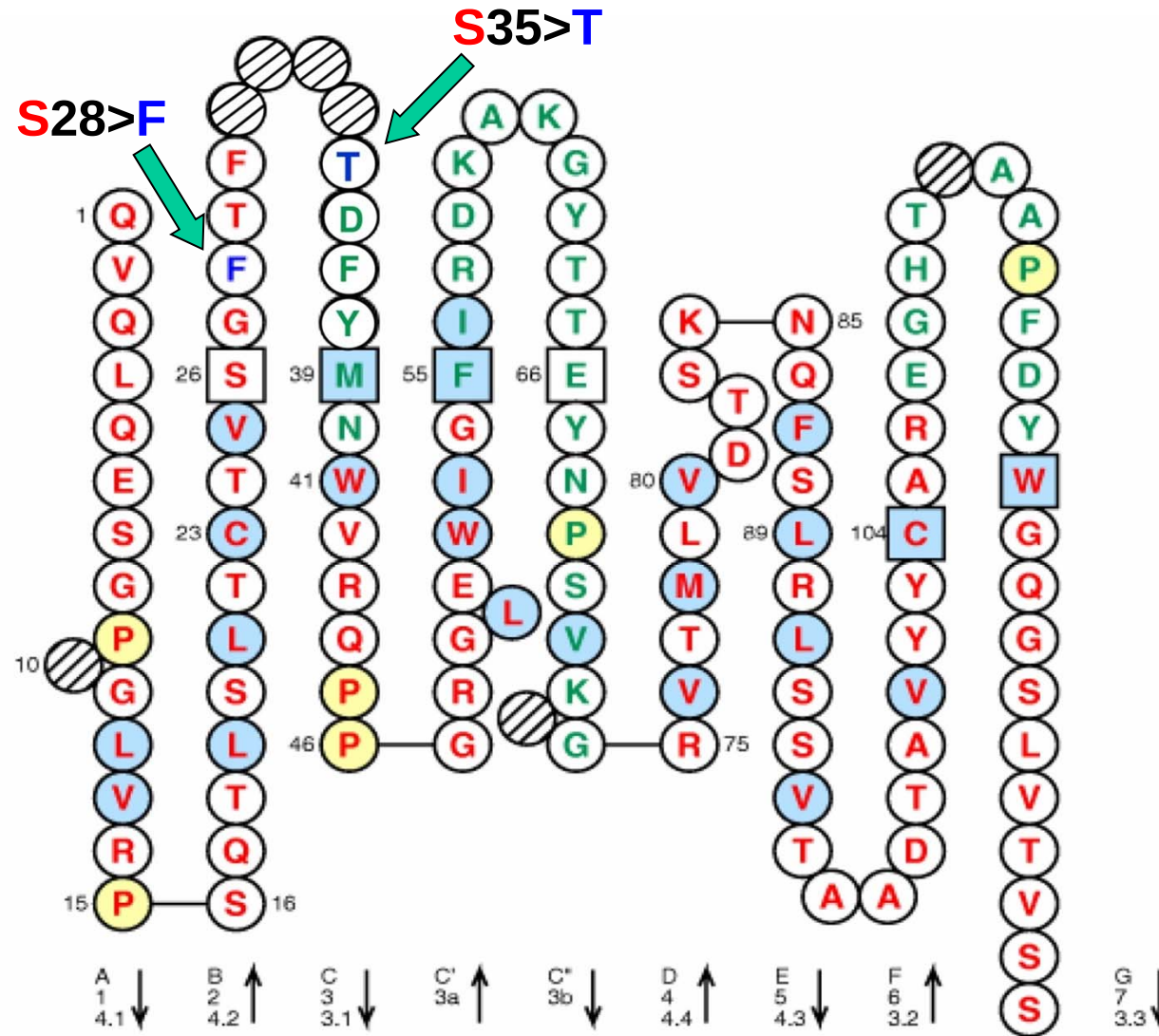
Immunogenicity

-omab	-ximab	-zumab	-umab
muromonab (1986)	abciximab (1994)	daclizumab (1997)	adalimumab (2002)
edrecolomab (1995)	rituximab (1997)	palivizumab (1998)	panitumumab (2006)
ibritumomab tiuxetan (2002)	basiliximab (1998)	trastuzumab (1998)	
tositumomab (2003)	infliximab (1998)	gemtuzumab ozogamicin (2000)	
	cetuximab (2004)	alemtuzumab (2001)	
		efalizumab (2003)	
		omalizumab (2003)	
		bevacizumab (2004)	
		natalizumab (2004)	
		nimotuzumab (2004)	
		ranibizumab (2006)	
		eculizumab (2007)	
		certolizumab pegol (2008)	

Antibody humanization and engineering

Alemtuzumab (CAMPATH®)

2 mutations:



VH domain
[8.10.12]