http://www.imgt.org

Structures en immunogénétique

Introduction

Master 2 STIC Santé UE GMIN304 « Structure des molécules »

4 Décembre 2013

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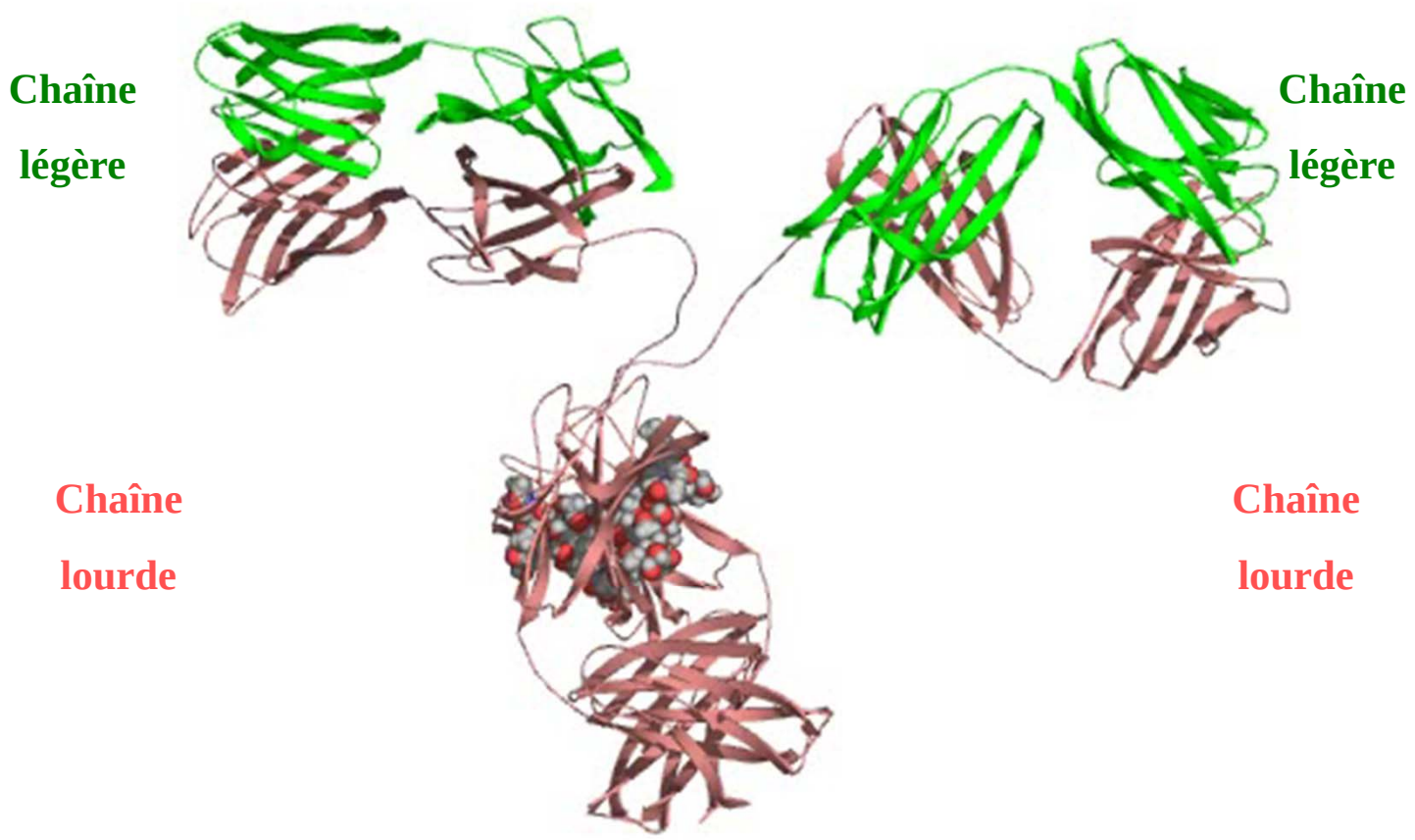
Immunoglobulines (IG)

tp://www.imgt.org



Immunoglobulin (IG)

T cell receptor (TR)

http://www.imgt.org

V-DOMAIN

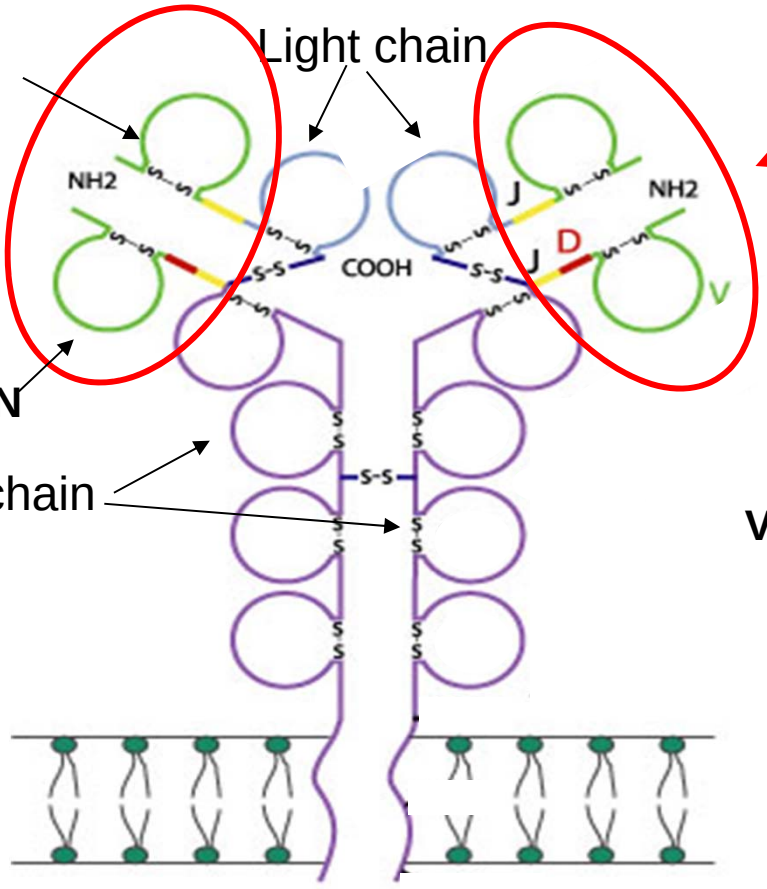
V-J-REGION

V-DOMAIN

V-D-J-REGION

Light chain

Heavy chain

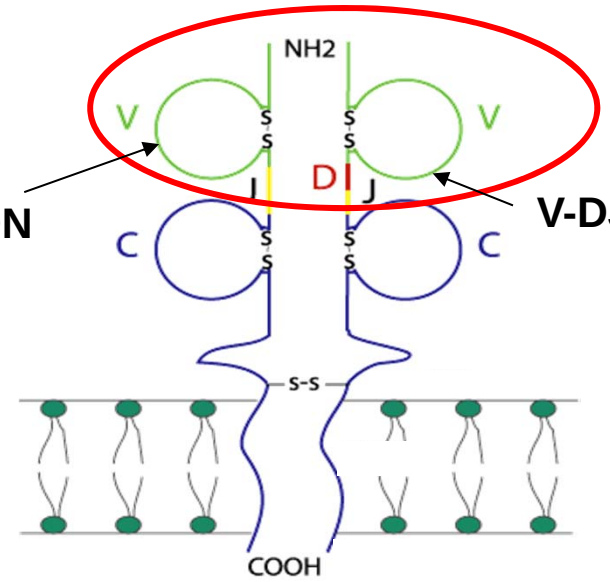


Membrane IgM

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

Alpha - Beta

Gamma - Delta



V-J-REGION

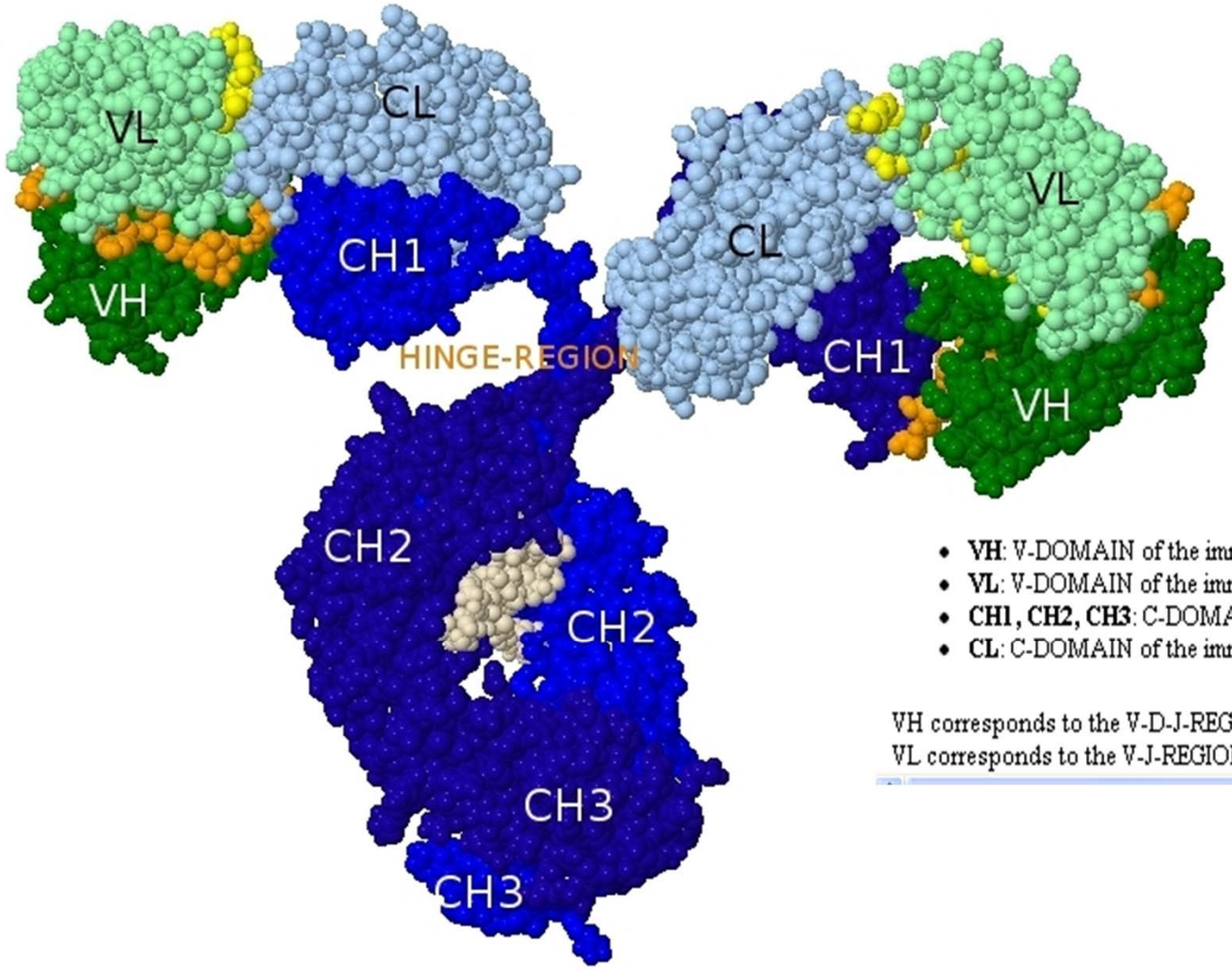
V-DJ-REGION

T cell receptor

The Immunoglobulin FactsBook, 2001

Immunoglobulins (IG) - Spacefill

http://www.imgt.org



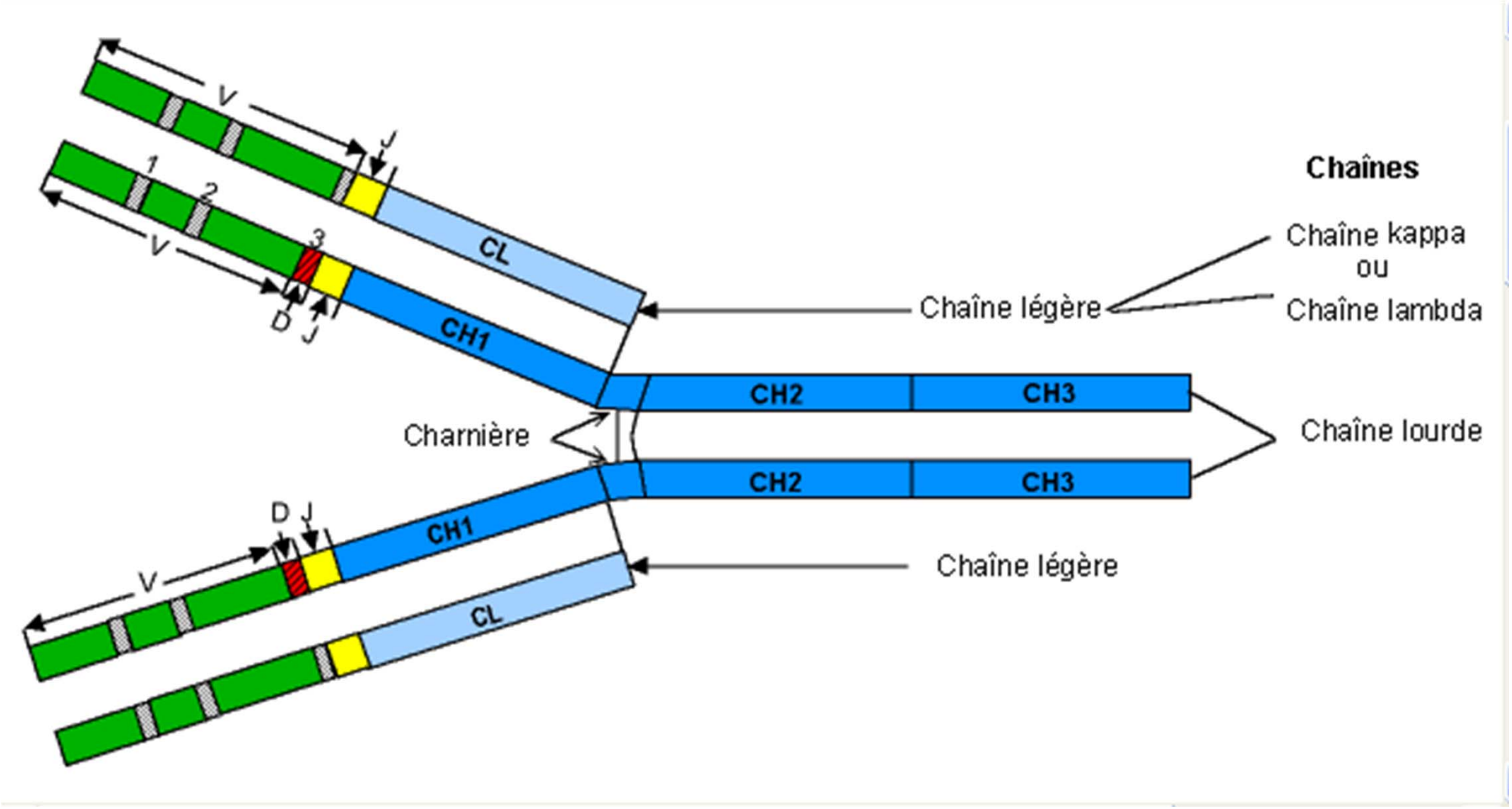
- **VH**: V-DOMAIN of the immunoglobulin heavy chain
- **VL**: V-DOMAIN of the immunoglobulin light chain
- **CH1, CH2, CH3**: C-DOMAIN of the immunoglobulin heavy chain
- **CL**: C-DOMAIN of the immunoglobulin light chain

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.

The Immunoglobulin FactsBook, 2001

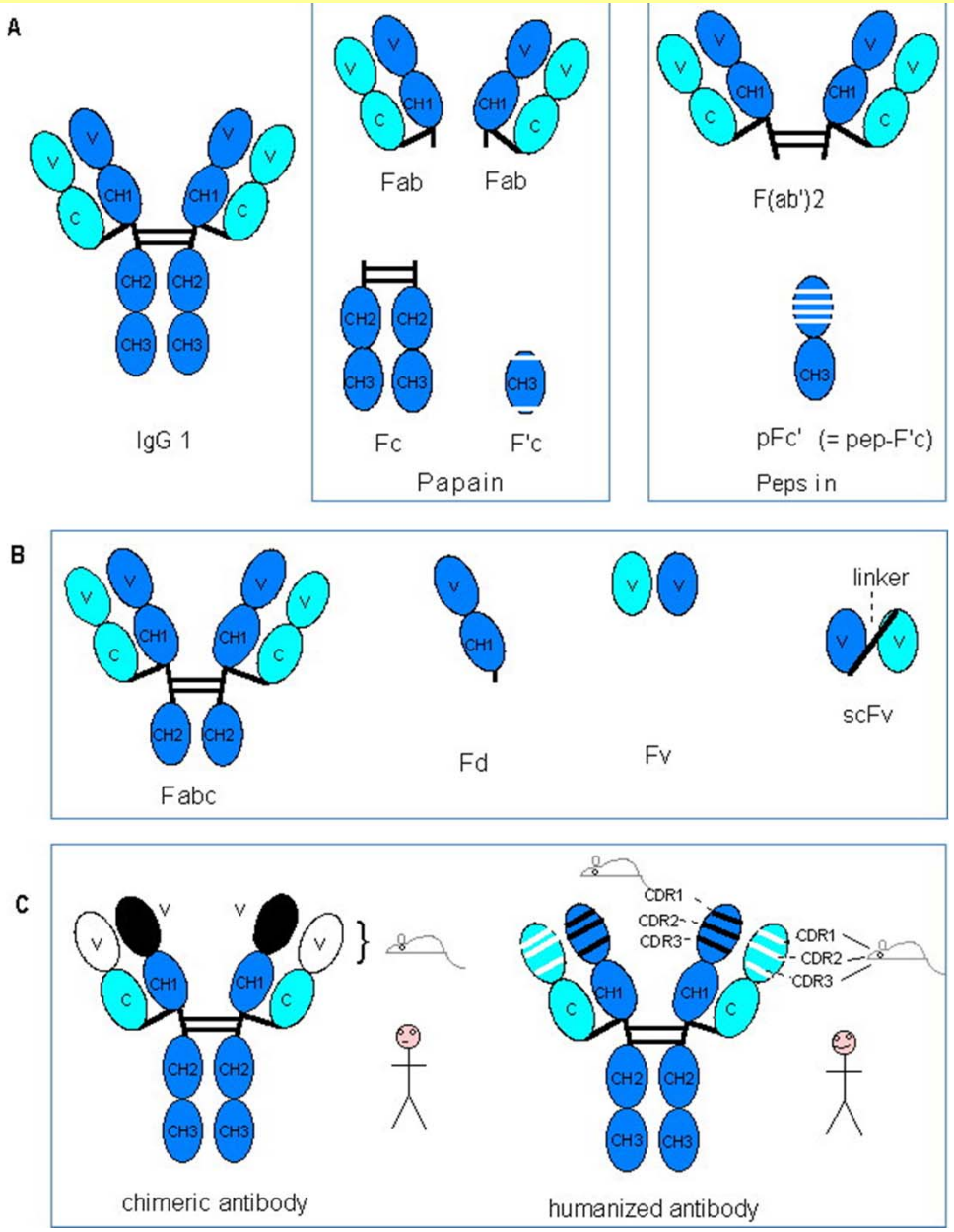
Immunoglobulin IgG

http://www.imgt.org



IMGT Repertoire, http://www.imgt.org

Organization in domains of an IgG1 immunoglobulin and of its fragments

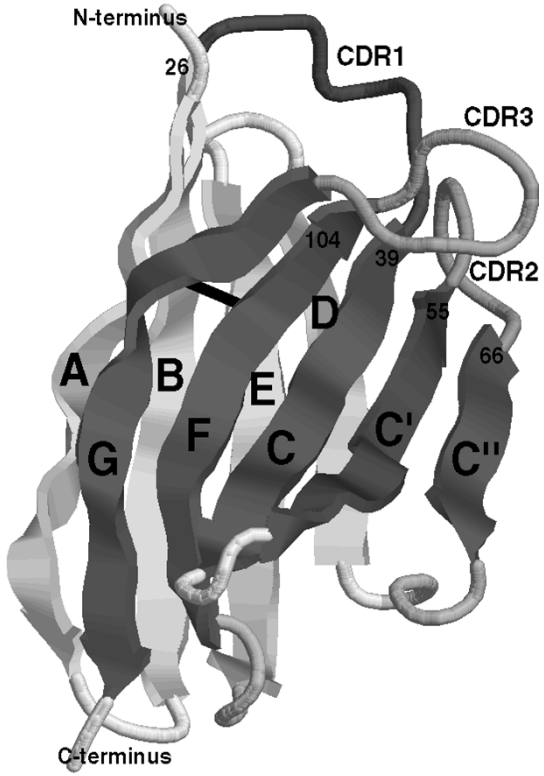


Structural domains

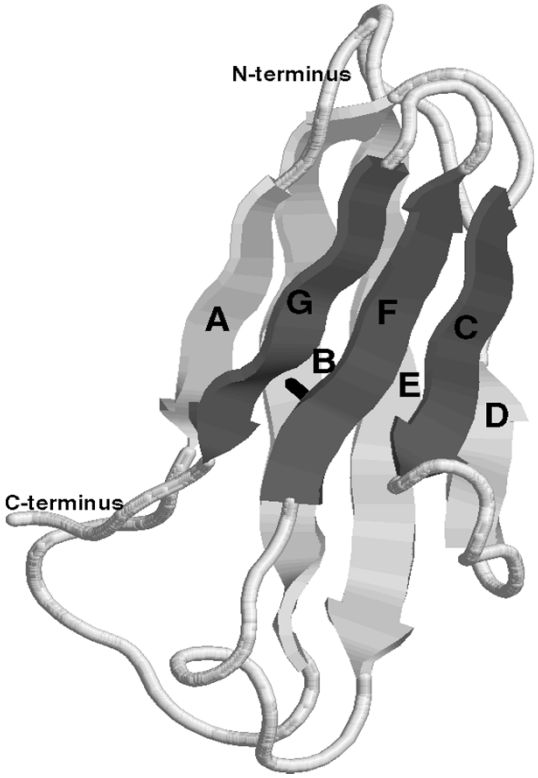
http://www.imgt.org

IG and TR

V-DOMAIN



C-DOMAIN



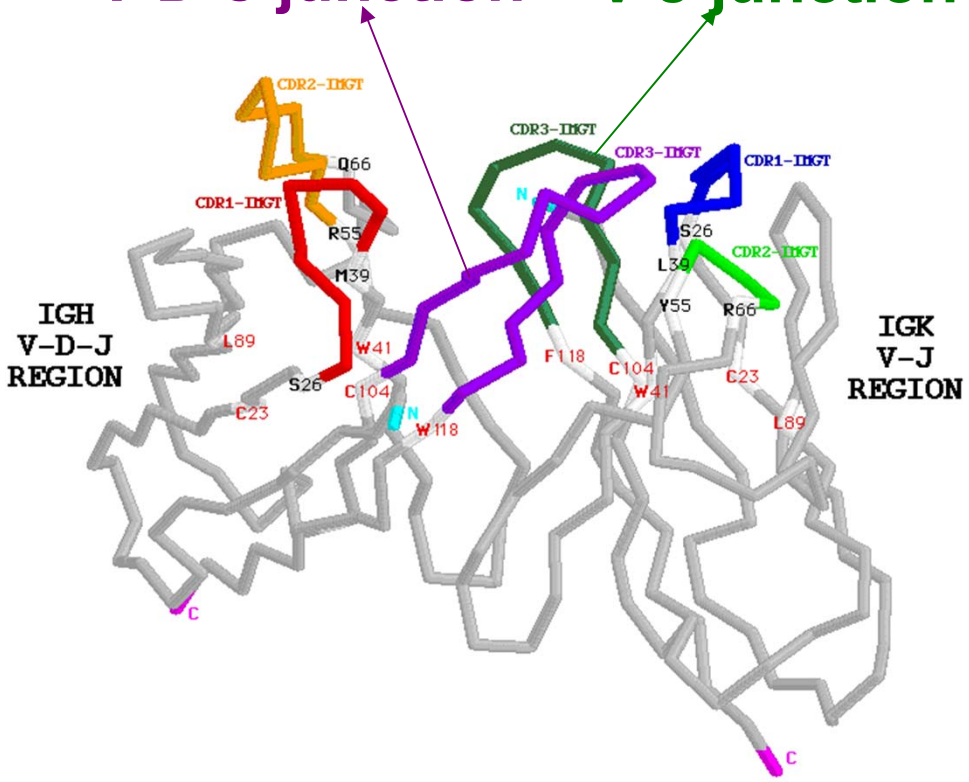
Le domaine d'IG est une structure de type sandwich bêta constituée de deux feuillets bêta antiparallèles. Les feuillets des V-DOMAINs possèdent respectivement 4 brins et 5 brins. Les V-DOMAINs possèdent trois boucles qui assurent la liaison avec un antigène. Ces boucles ou CDR (Complementarity Determining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

V-DOMAINs : VH and V-KAPPA

http://www.imgt.org

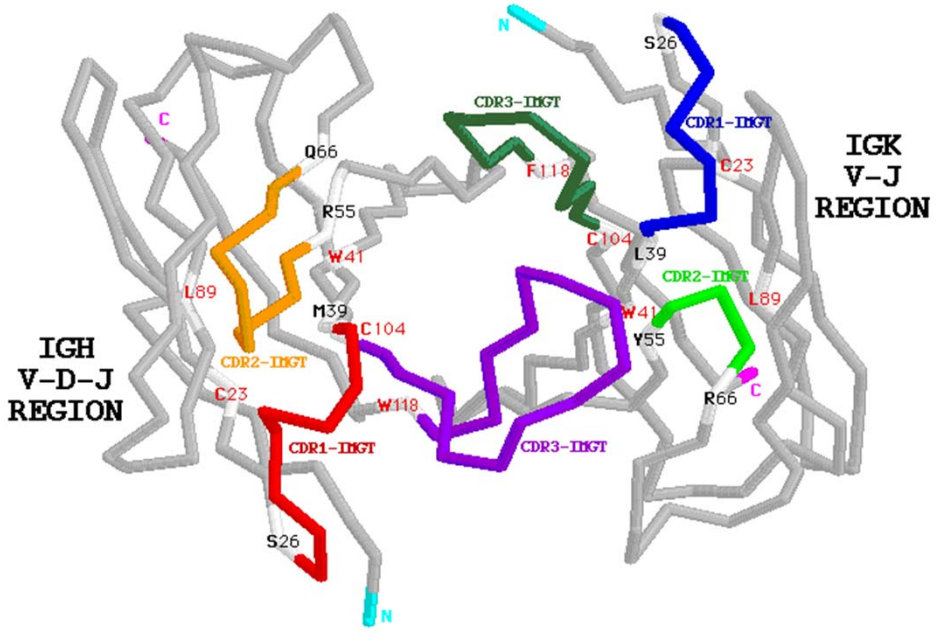
VH **V-KAPPA**

V-D-J junction **V-J junction**



Side view of the V-DOMAINs

VH **V-KAPPA**



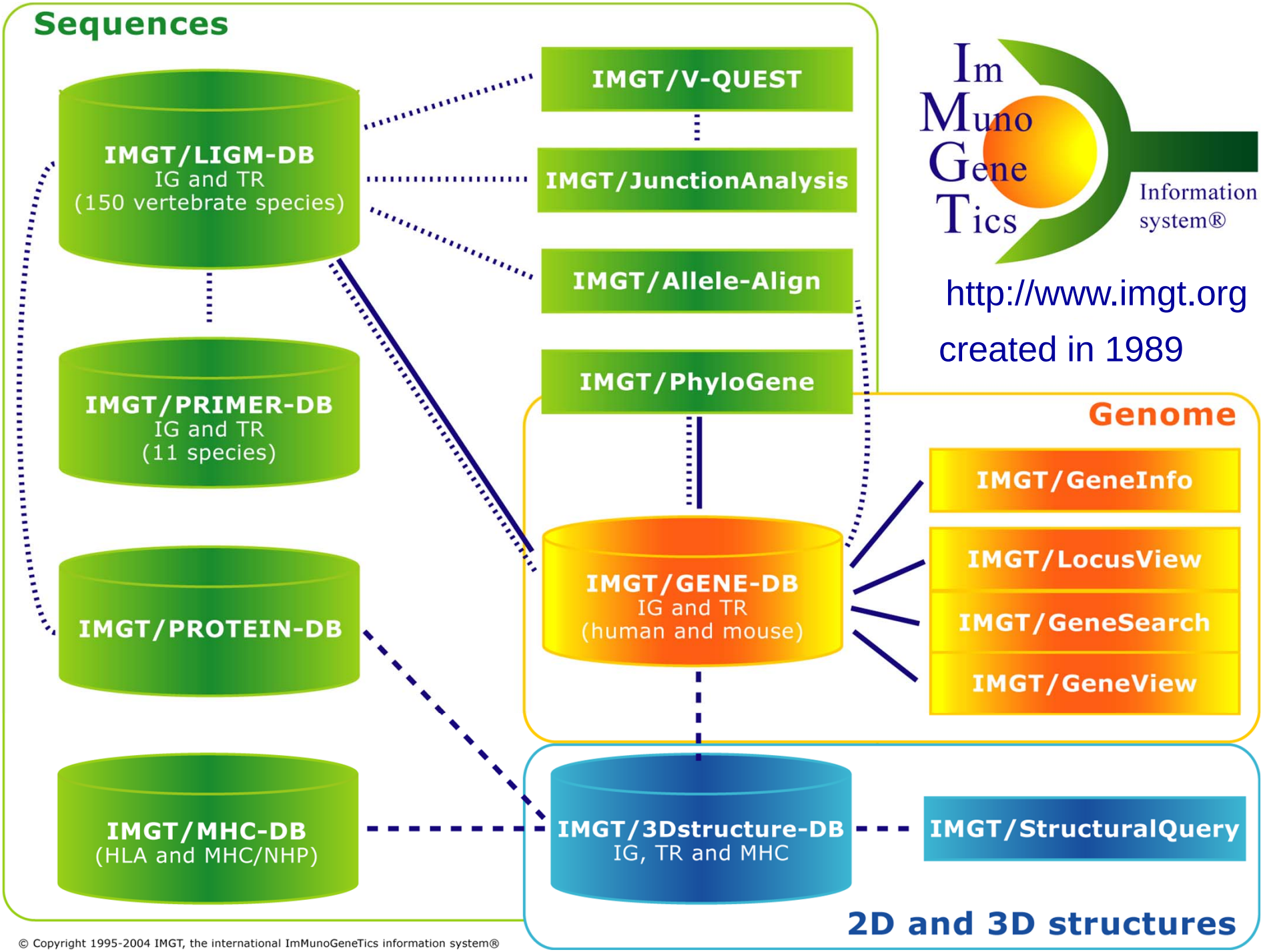
View from above the CDRs

***Mouse(Mus musculus)* E5.2Fv**

CDR3-IMGT= Complementarity determining region (105-117)

V-J junction (104-118)

V-D-J junction (104-118)


Sequences
IMGT/LIGM-DB
IG and TR
(150 vertebrate species)
IMGT/V-QUEST
IMGT/JunctionAnalysis
IMGT/Allele-Align
IMGT/PRIMER-DB
IG and TR
(11 species)
IMGT/PhyloGene
IMGT/PROTEIN-DB
IMGT/GENE-DB
IG and TR
(human and mouse)
Genome
IMGT/GeneInfo
IMGT/LocusView
IMGT/GeneSearch
IMGT/GeneView
IMGT/MHC-DB
(HLA and MHC/NHP)
IMGT/3Dstructure-DB
IG, TR and MHC
IMGT/StructuralQuery
2D and 3D structures
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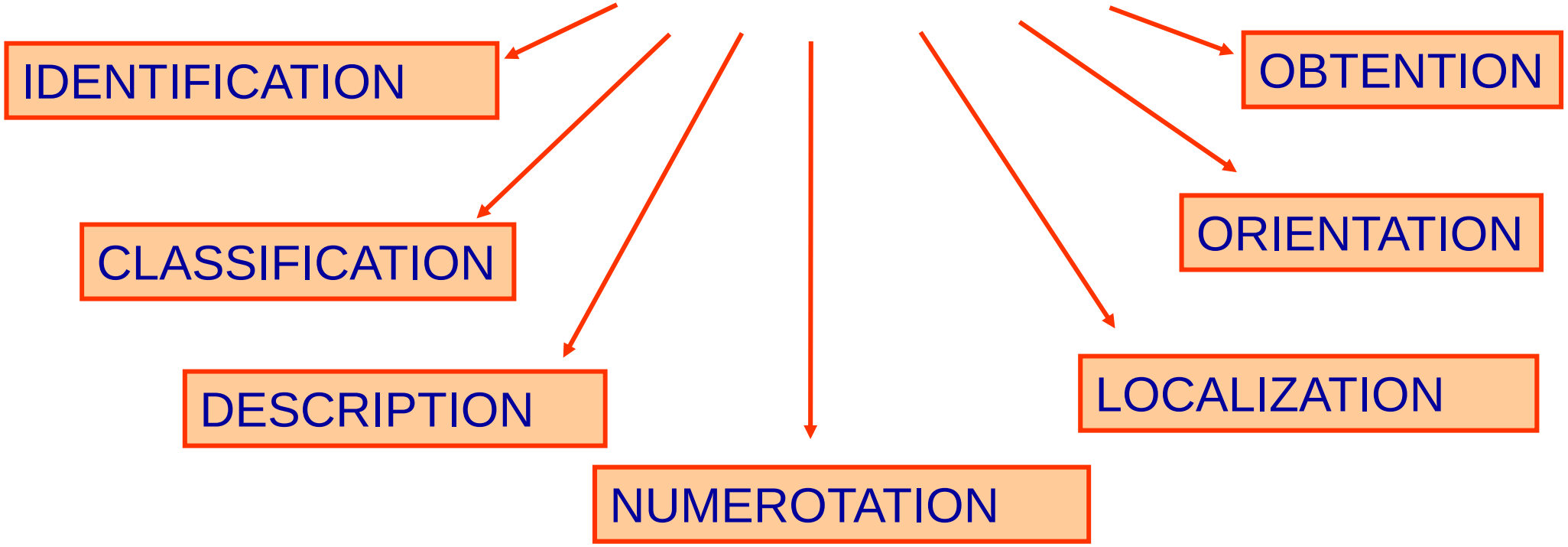
IMGT-ONTOLOGY seven axioms:

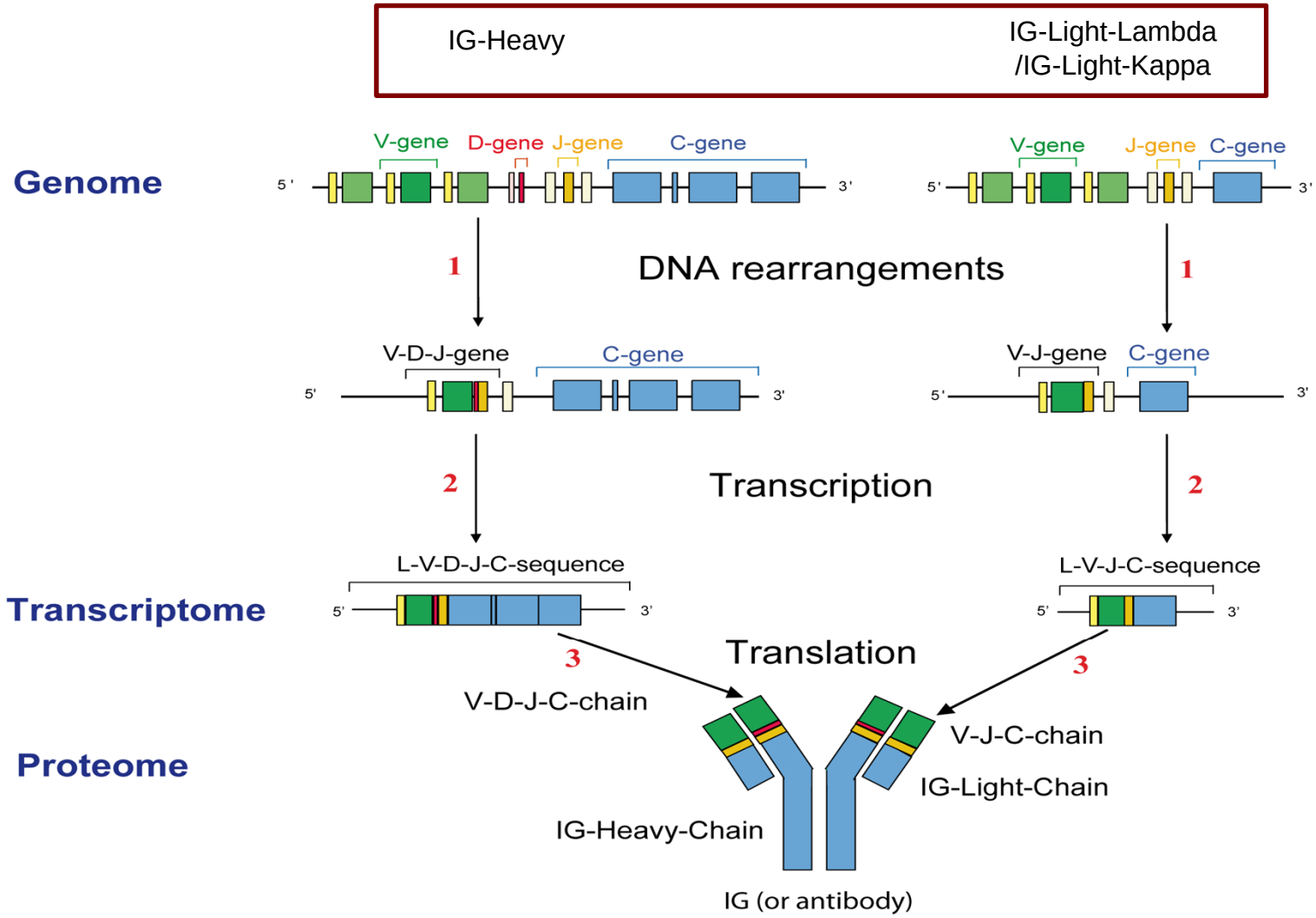
To share, reuse and represent knowledge
in Immunogenetics and Life Sciences



Giudicelli and Lefranc, Bioinformatics (1999)

Concepts of IDENTIFICATION : IMGT standardized keywords

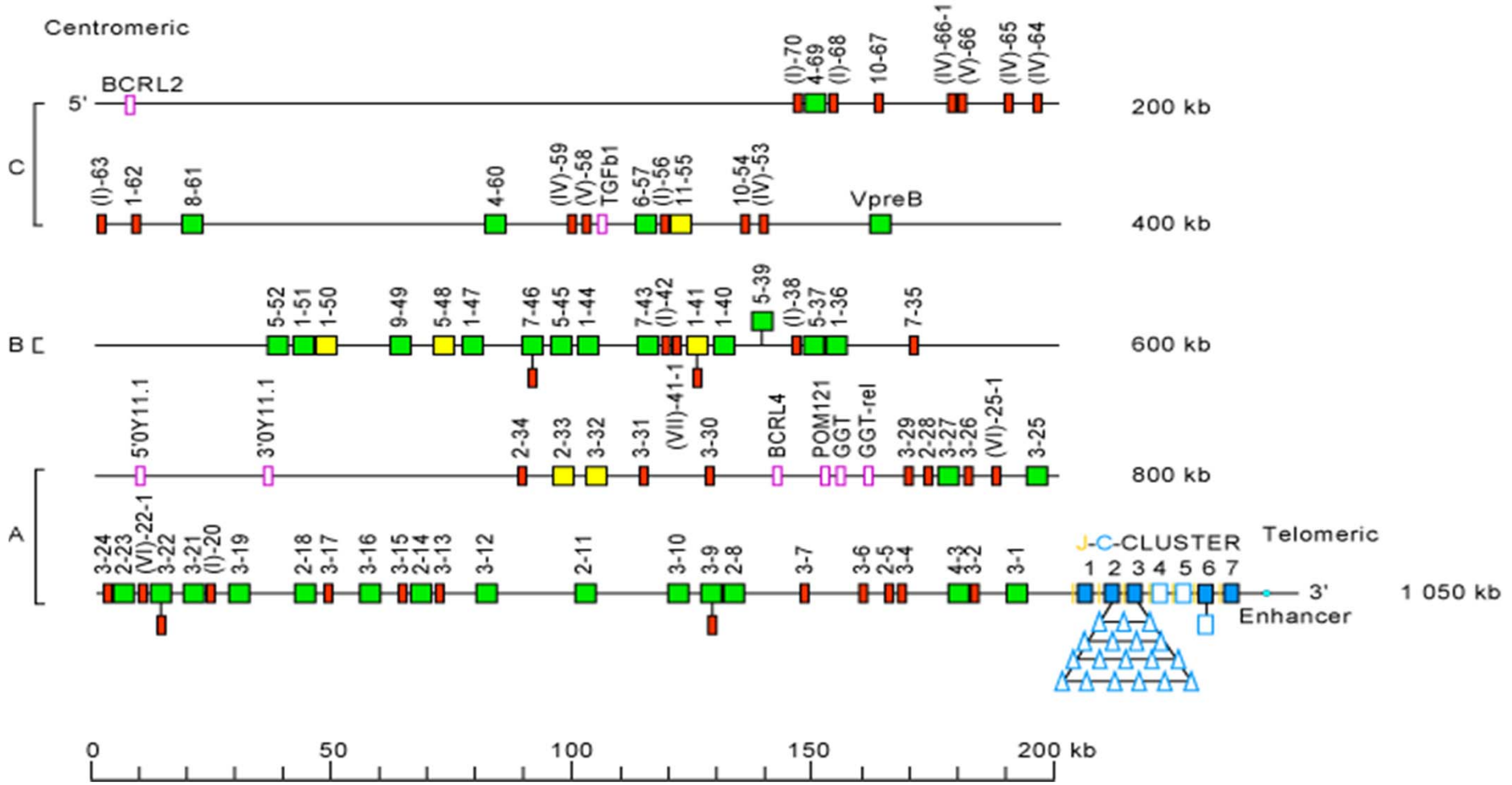
http://www.imgt.org



"MoleculeType" concept	"ConfigurationType" concept
gDNA	germline
gDNA	rearranged
mRNA (or *in vitro* cDNA)	rearranged
protein	rearranged

Concepts of CLASSIFICATION : the IG and TR gene nomenclature

- Approved by HUGO Nomenclature Committee (HGNC) in 1999



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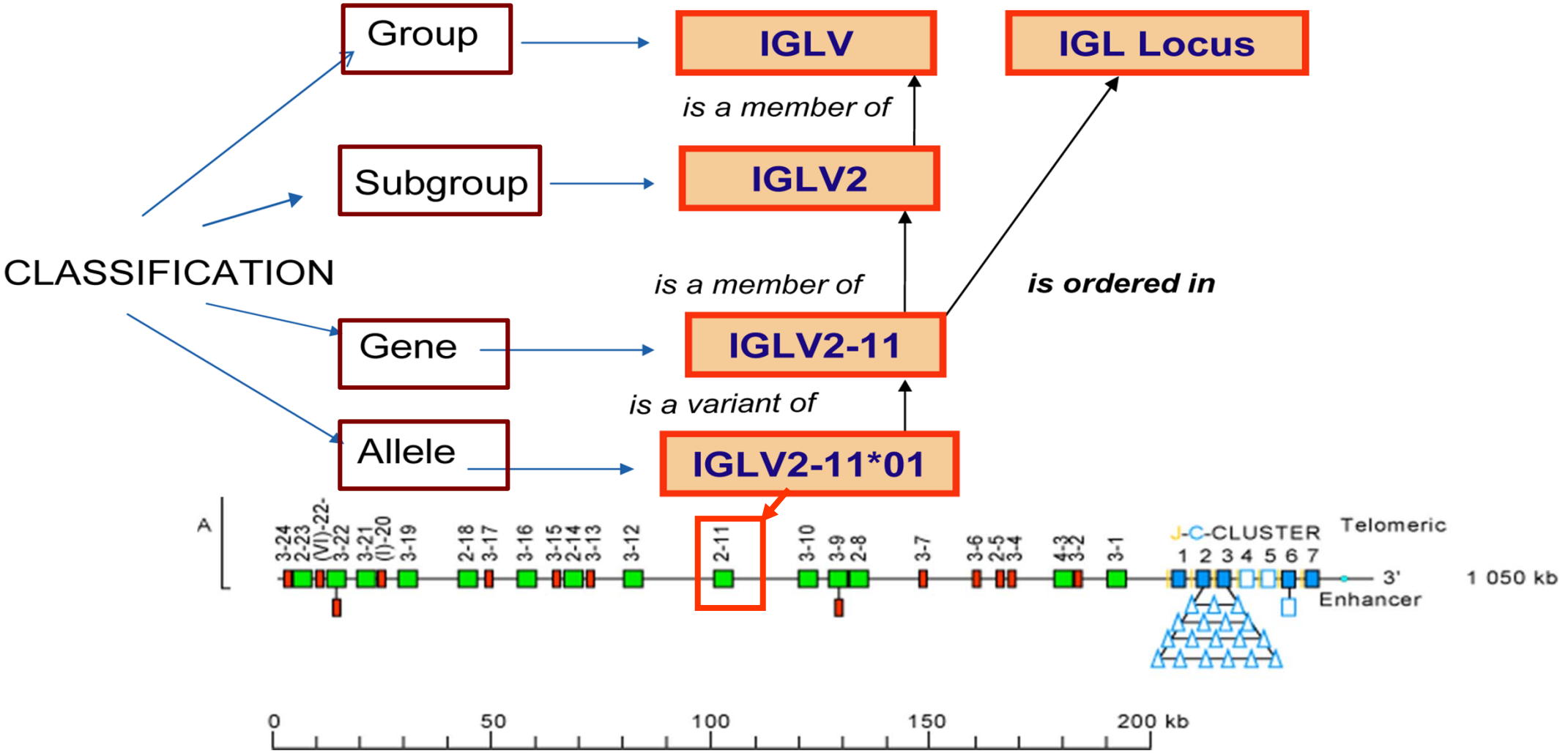
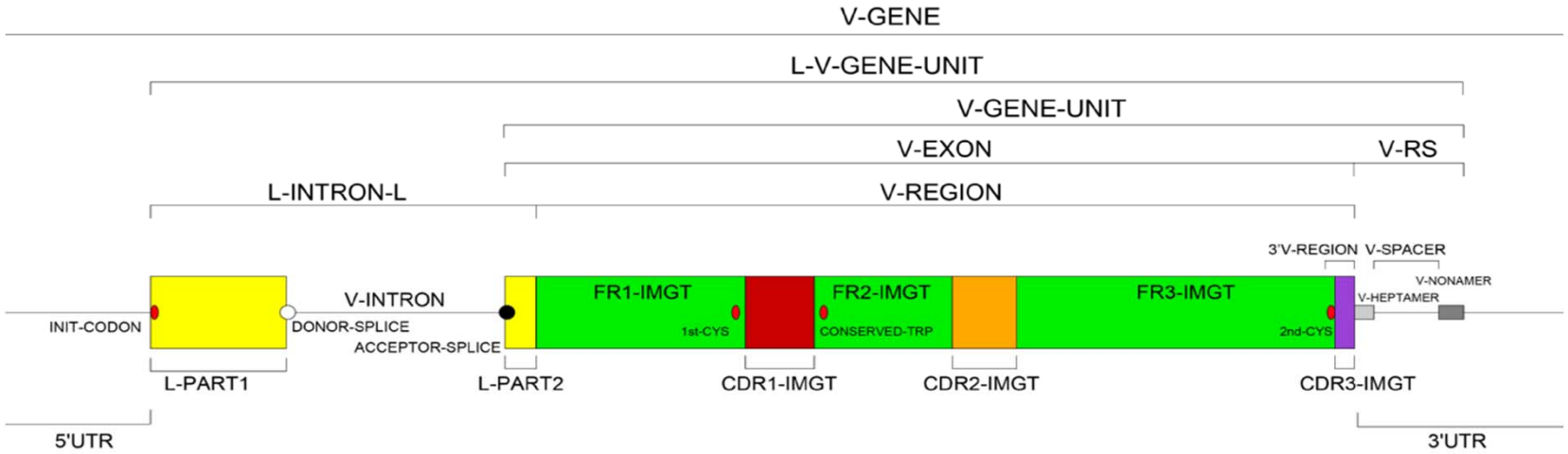


Concepts of DESCRIPTION: IMGT labels

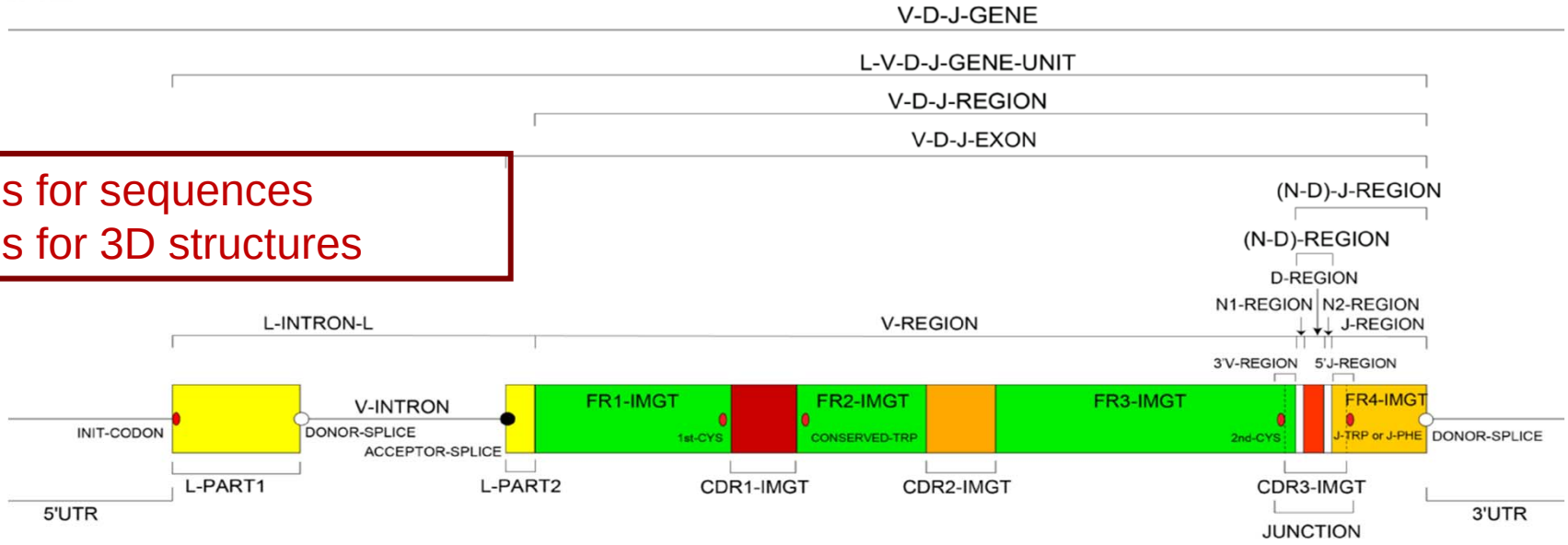
http://www.imgt.org

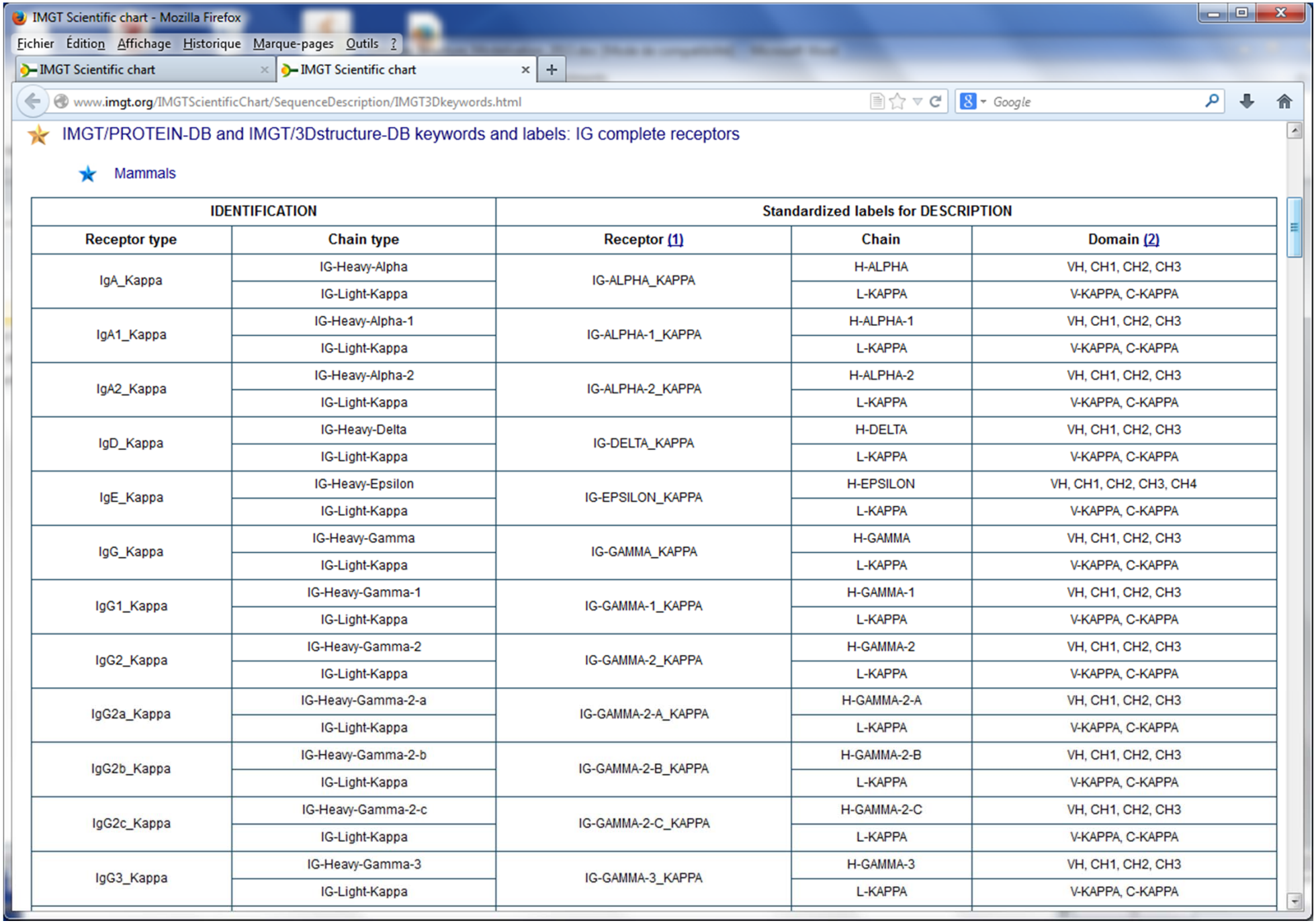
Labels for a germline V-GENE in gDNA



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

287 labels for sequences
370 labels for 3D structures





IMGT/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

http://www.imgt.org

IMGT Collier de Perles

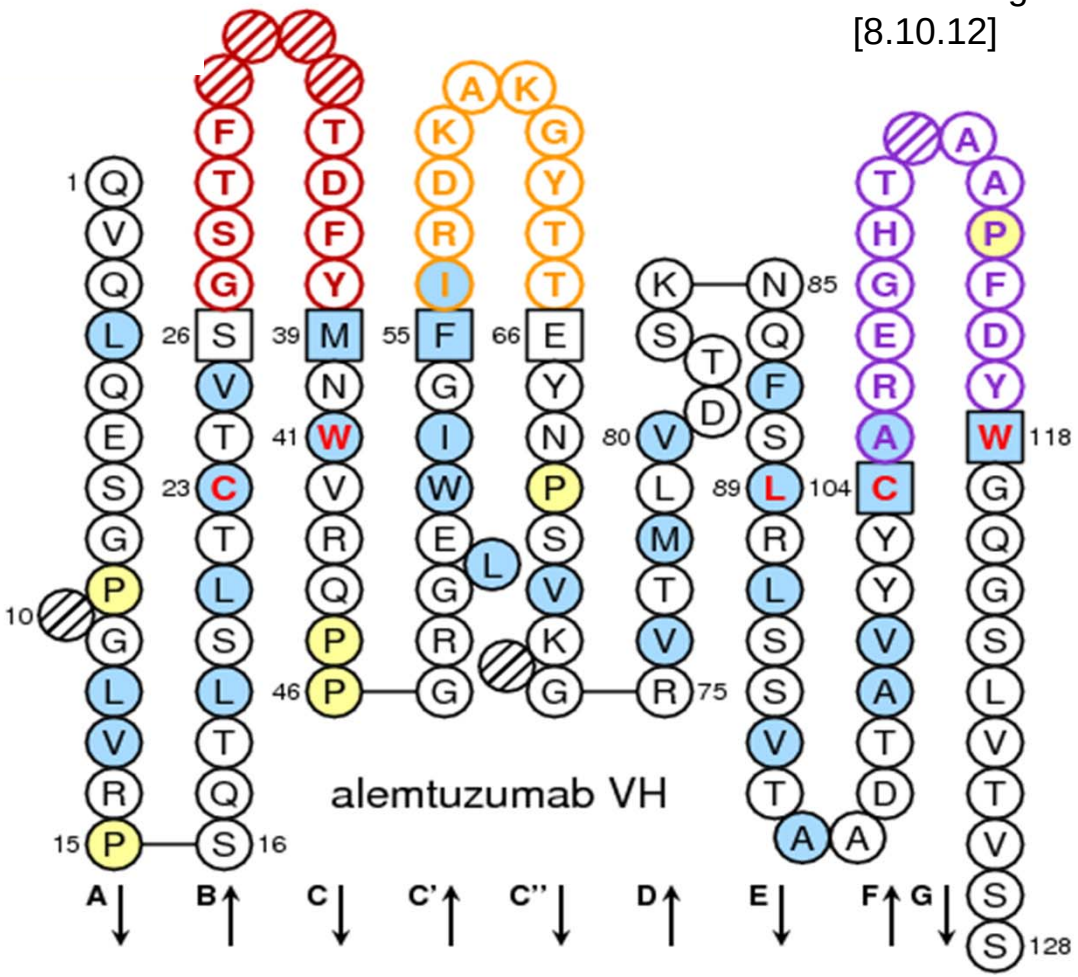
Based on the IMGT unique numbering (first one in 1997)

- 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

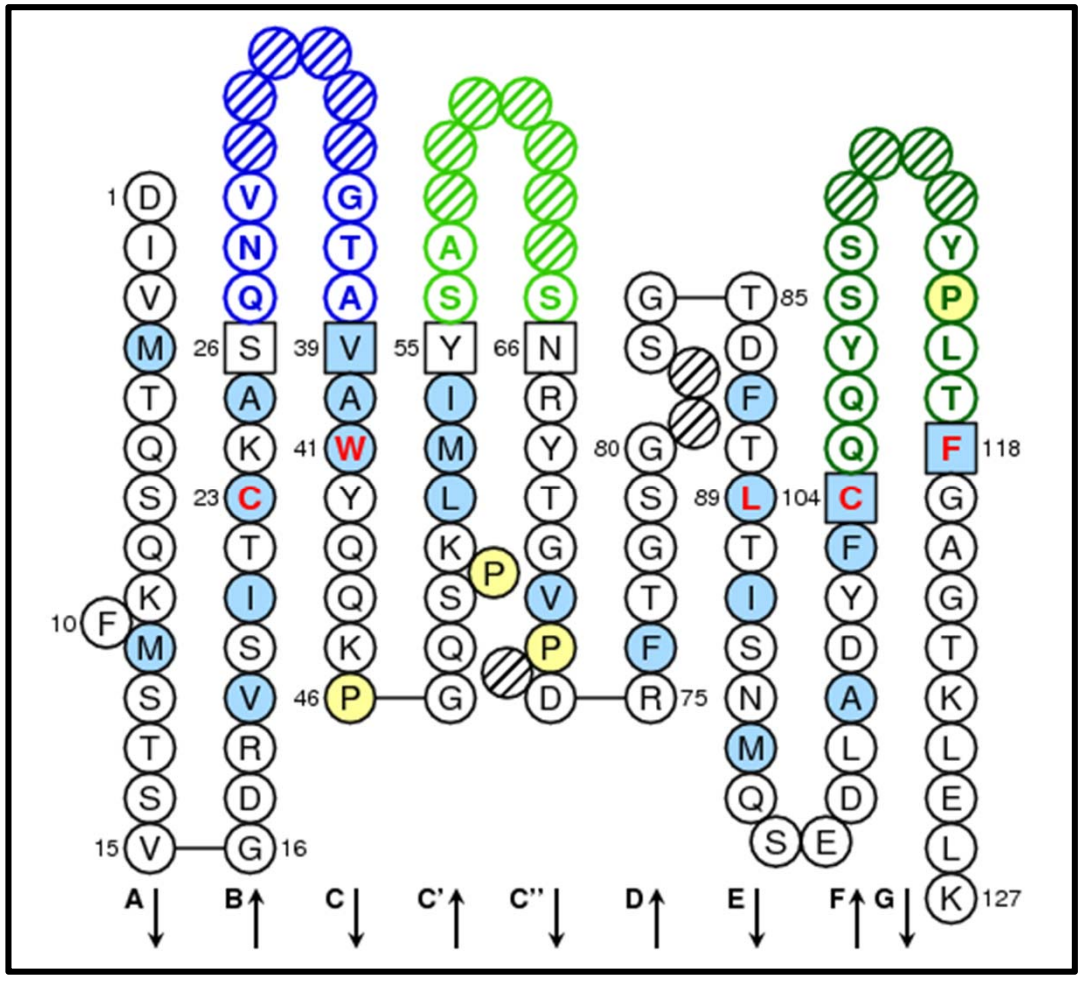
CDR-IMGT lengths
[8.10.12]

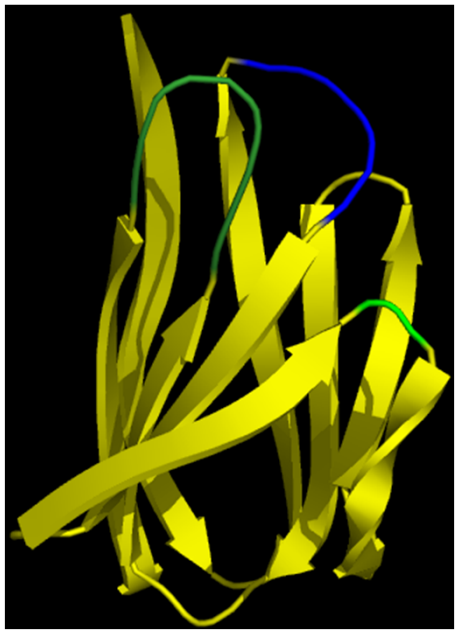


Lefranc et al. Dev. Comp. Immunol. 27, 55-77 (2003)

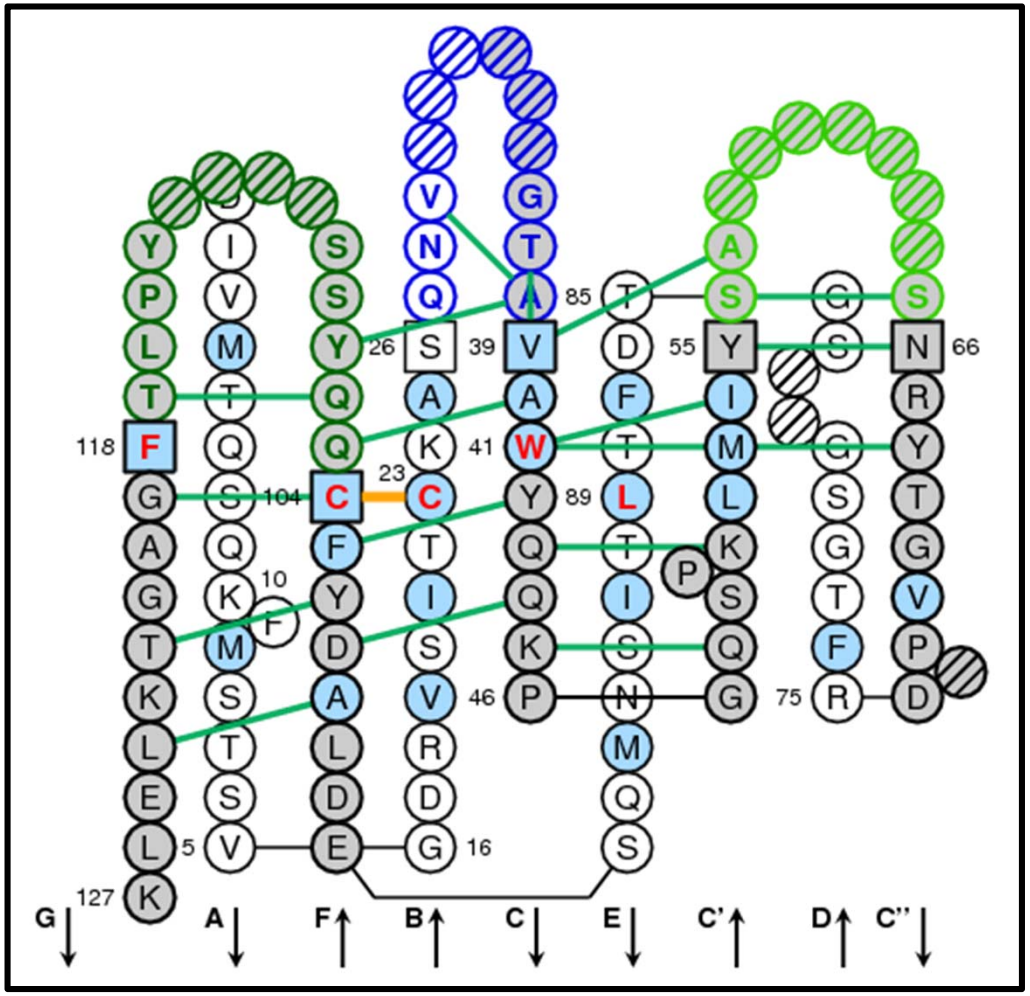
IMGT Collier de Perles for V-DOMAIN

http://www.imgt.org





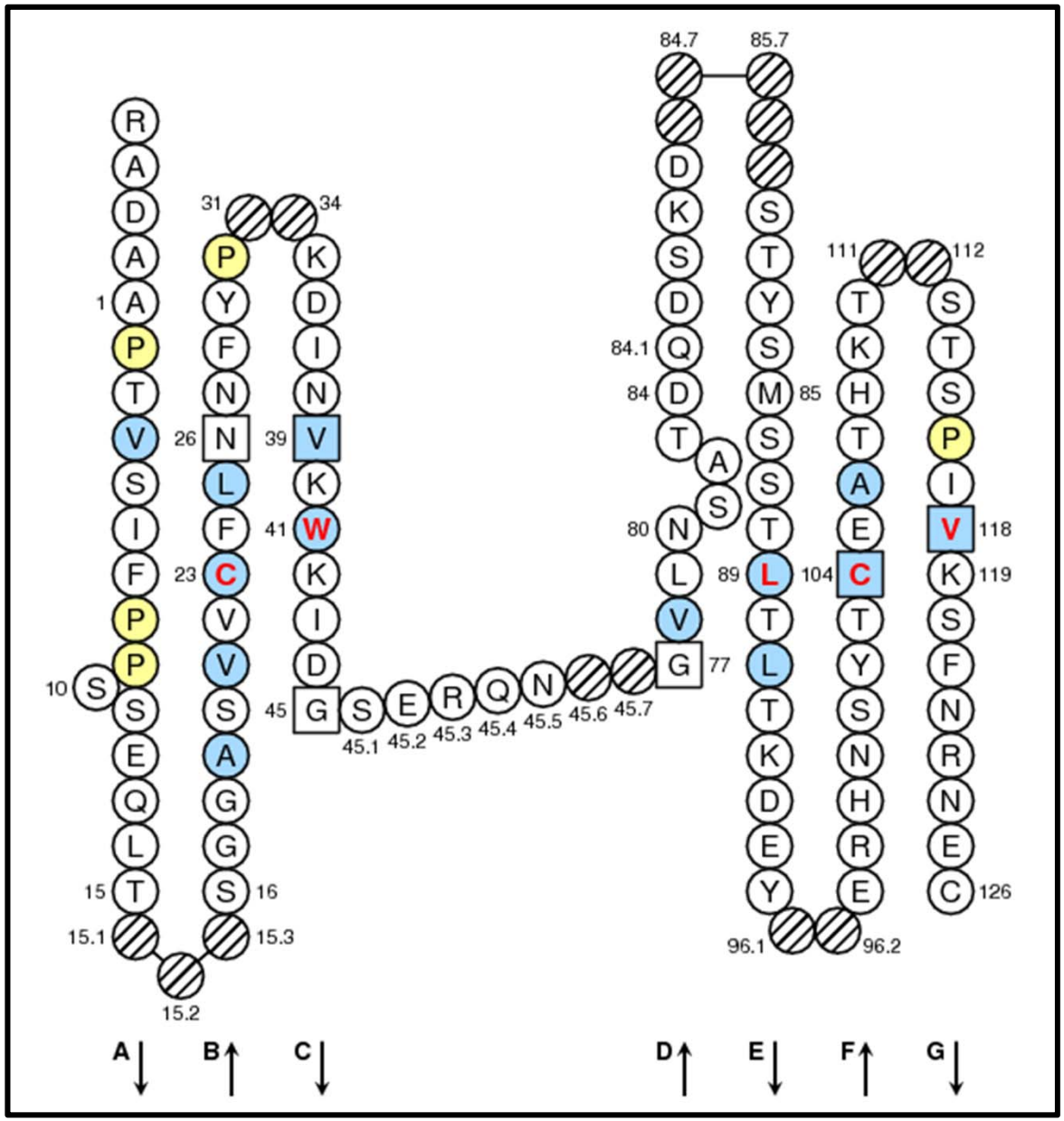
IMGT Collier de Perles for V-DOMAIN on two layers



Hydrogen bonds between the amino acids of the C, C', C'', F and G strands and those of the CDR-IMGT

IMGT Collier de Perles for C-DOMAIN

http://www.imgt.org



IMGT Collier de Perles for G-DOMAIN

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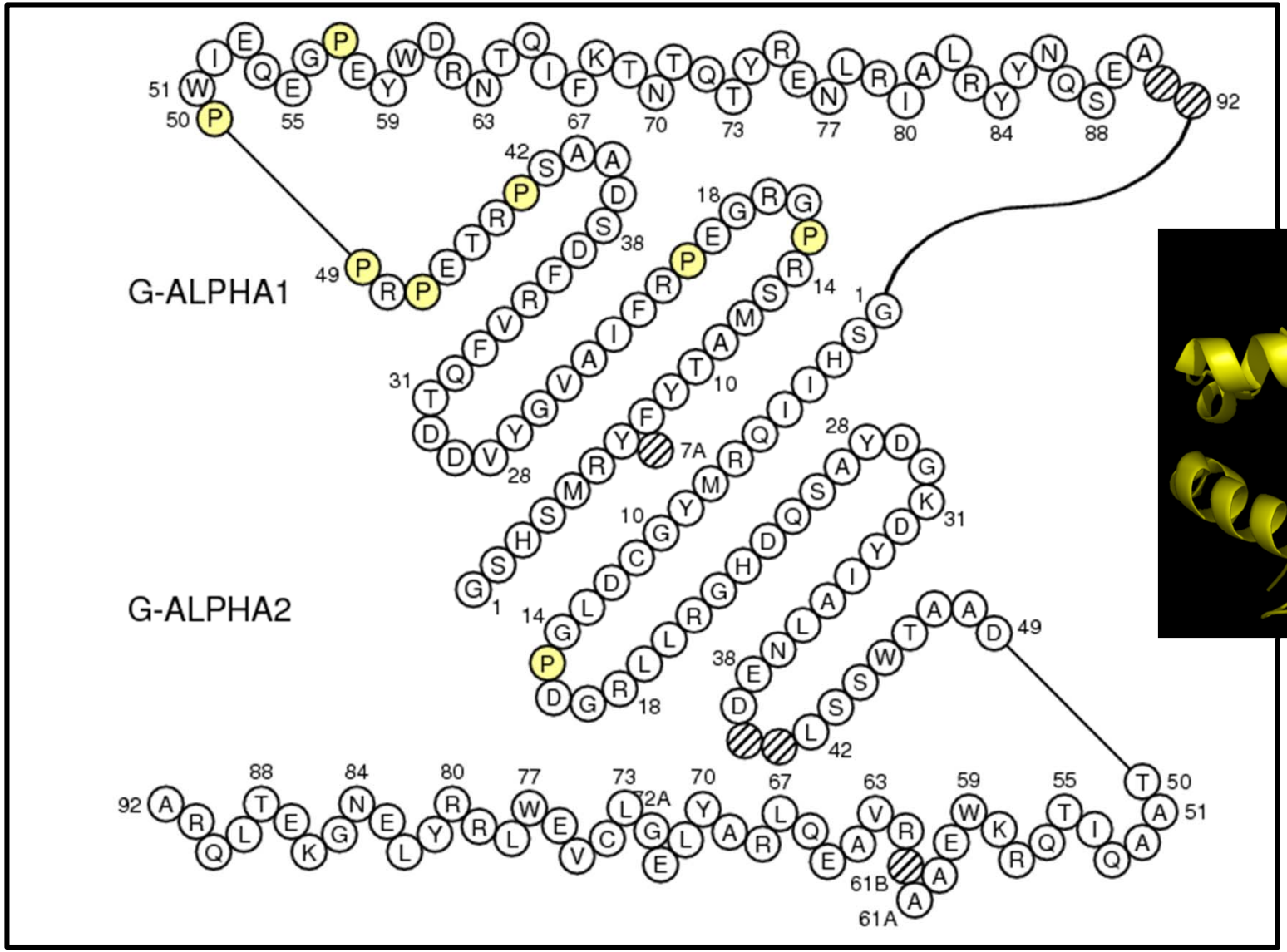

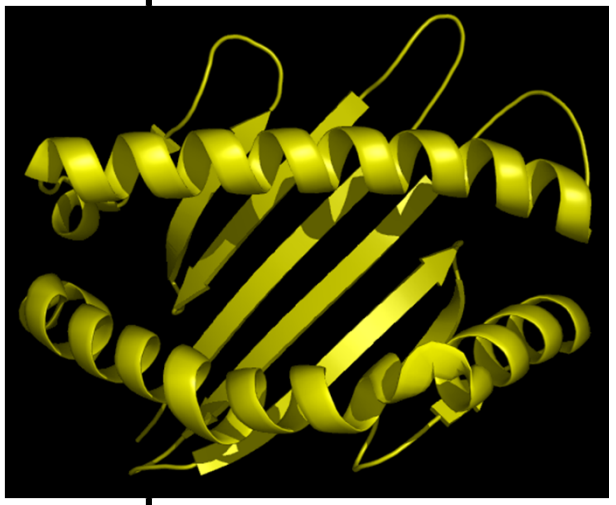

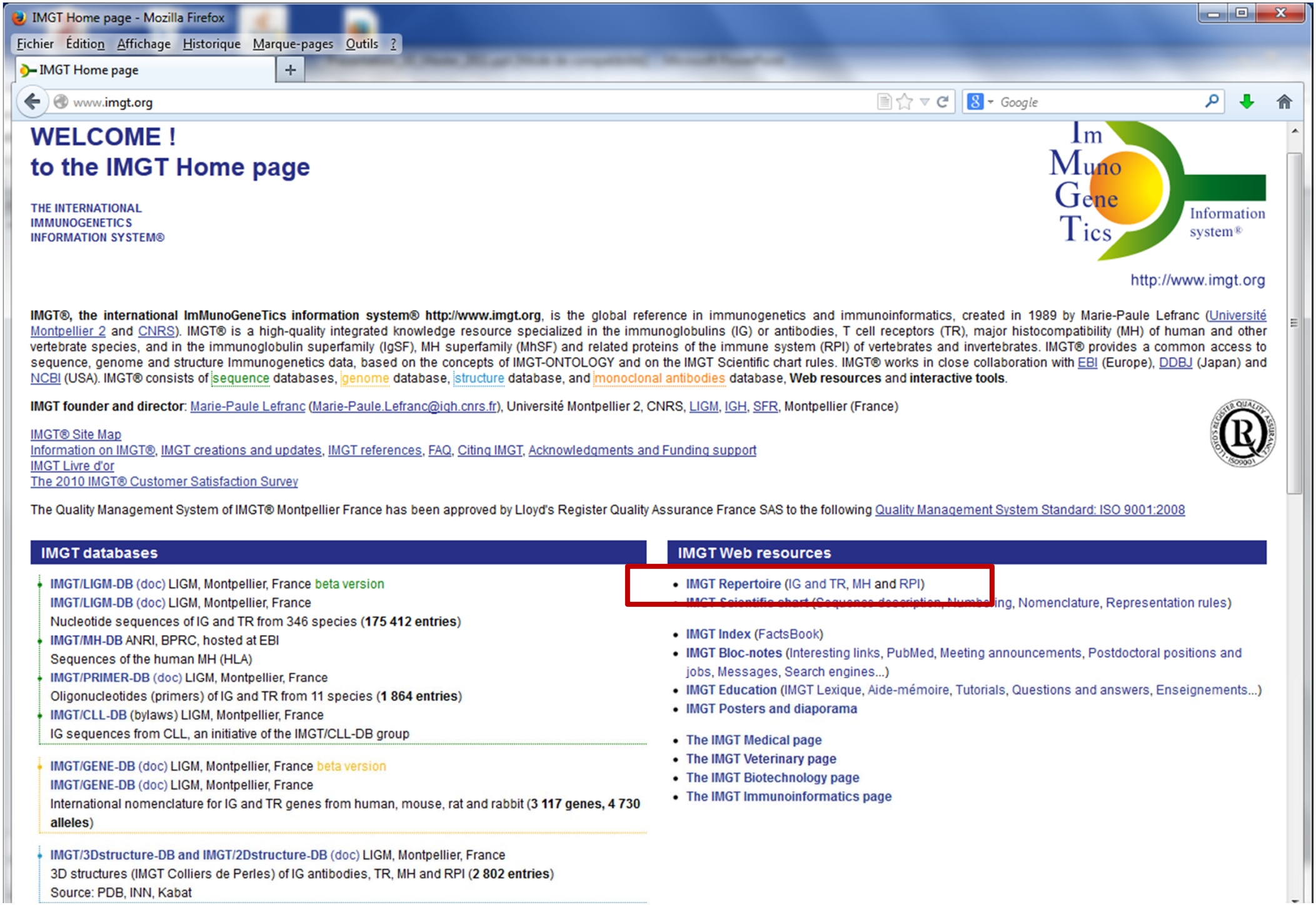

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IMGT founder and director: Marie-Paule Lefranc (Marie-Paule.Lefranc@igh.cnrs.fr), Université Montpellier 2, CNRS, LIGM, IGH, SFR, Montpellier (France)

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- IMGT/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**)
- IMGT/MH-DB ANRI, BPRC, hosted at EBI
  Sequences of the human MH (HLA)
- IMGT/PRIMER-DB (doc) LIGM, Montpellier, France
  Oligonucleotides (primers) of IG and TR from 11 species (**1 864 entries**)
- IMGT/CLL-DB (bylaws) LIGM, Montpellier, France
  IG sequences from CLL, an initiative of the IMGT/CLL-DB group

- IMGT/GENE-DB (doc) LIGM, Montpellier, France beta version
  IMGT/GENE-DB (doc) LIGM, Montpellier, France
  International nomenclature for IG and TR genes from human, mouse, rat and rabbit (**3 117 genes, 4 730 alleles**)

- 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** (Sequence description, Numbering, Nomenclature, Representation rules)

- **IMGT Index** (FactsBook)
- **IMGT Bloc-notes** (Interesting links, PubMed, Meeting announcements, Postdoctoral positions and jobs, Messages, Search engines...)
- **IMGT Education** (IMGT Lexique, Aide-mémoire, Tutorials, Questions and answers, Enseignements...)
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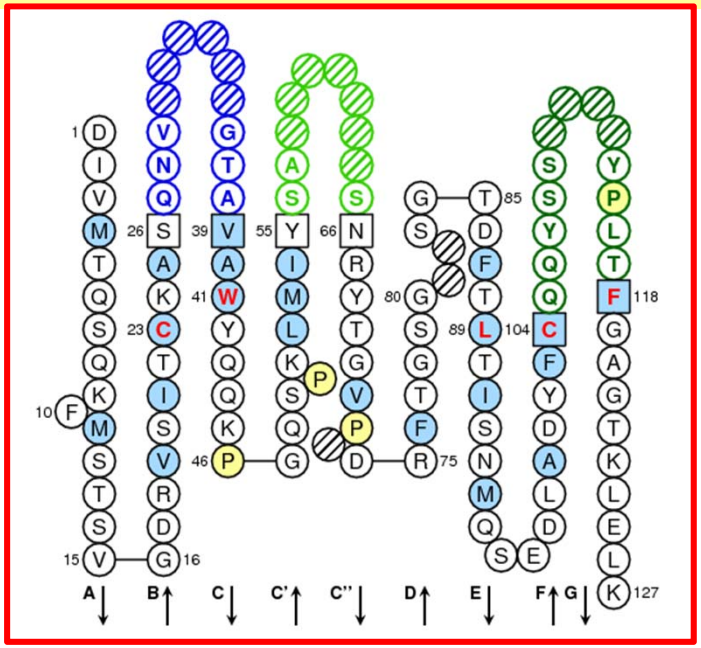
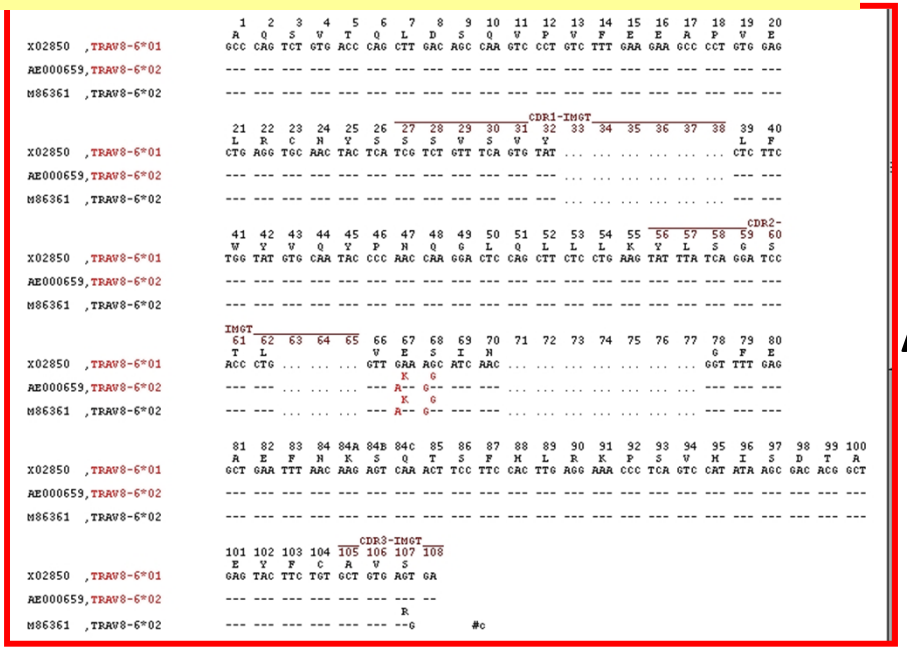
IMGT Collier de Perles



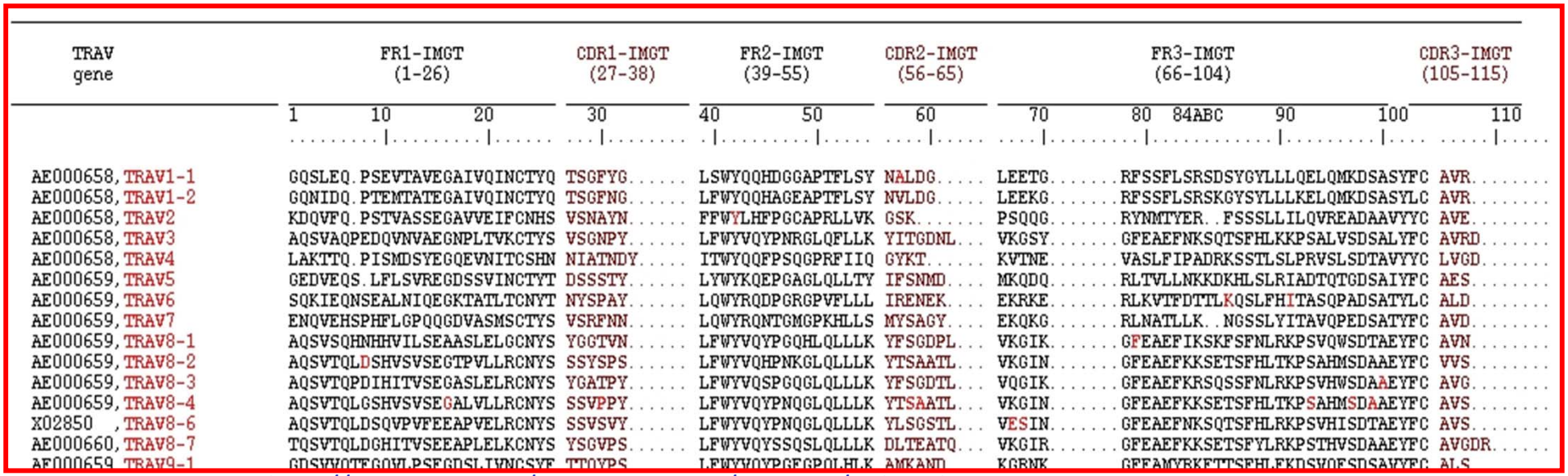
http://www.imgt.org/IMGTrepertoire/2D-3Dstruct/#h1_0

IMGT Alignment of alleles



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

IMGT Protein Display



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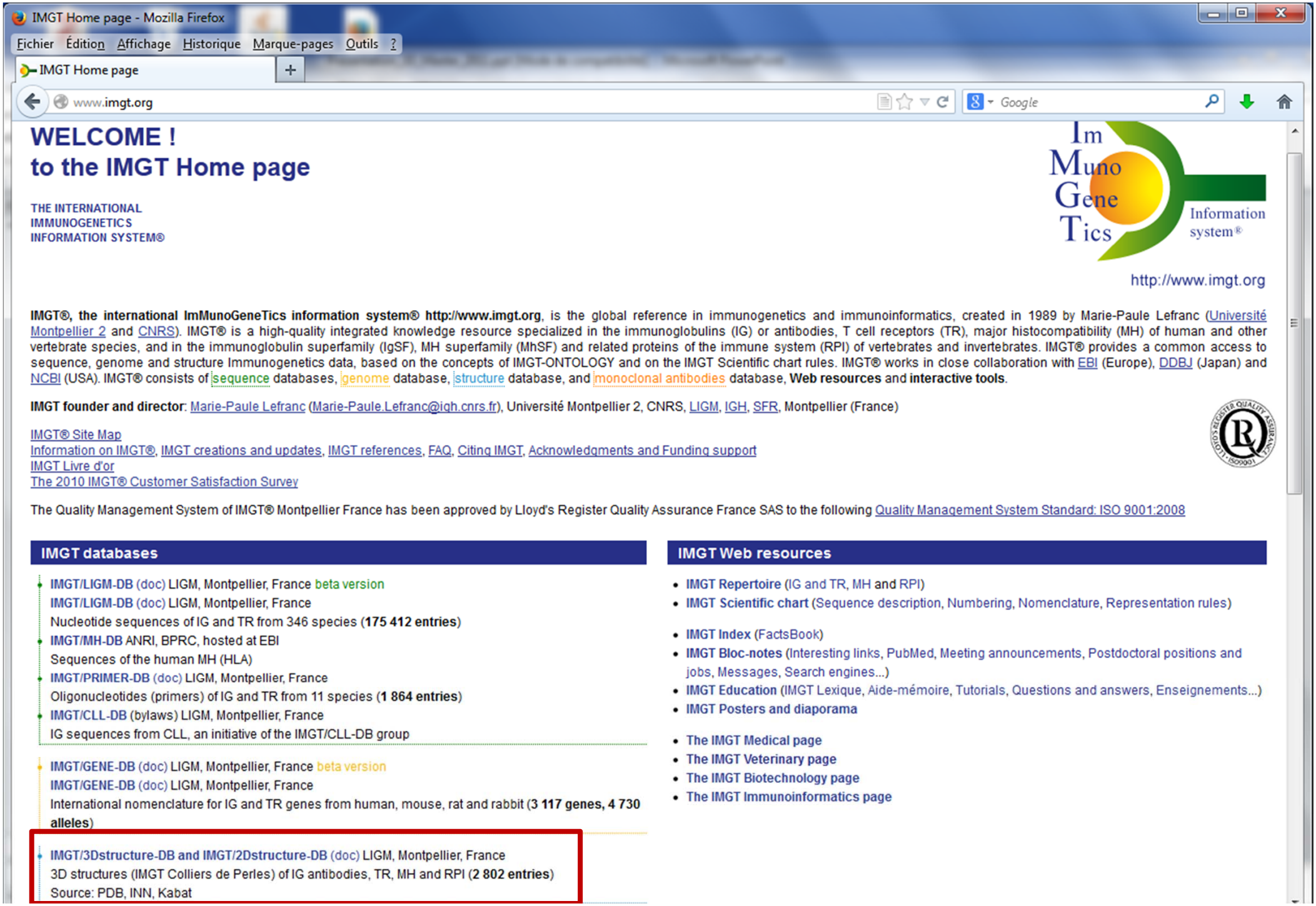

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  IMGT/GENE-DB (doc) LIGM, Montpellier, France
  International nomenclature for IG and TR genes from human, mouse, rat and rabbit (**3 117 genes, 4 730 alleles**)

- 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

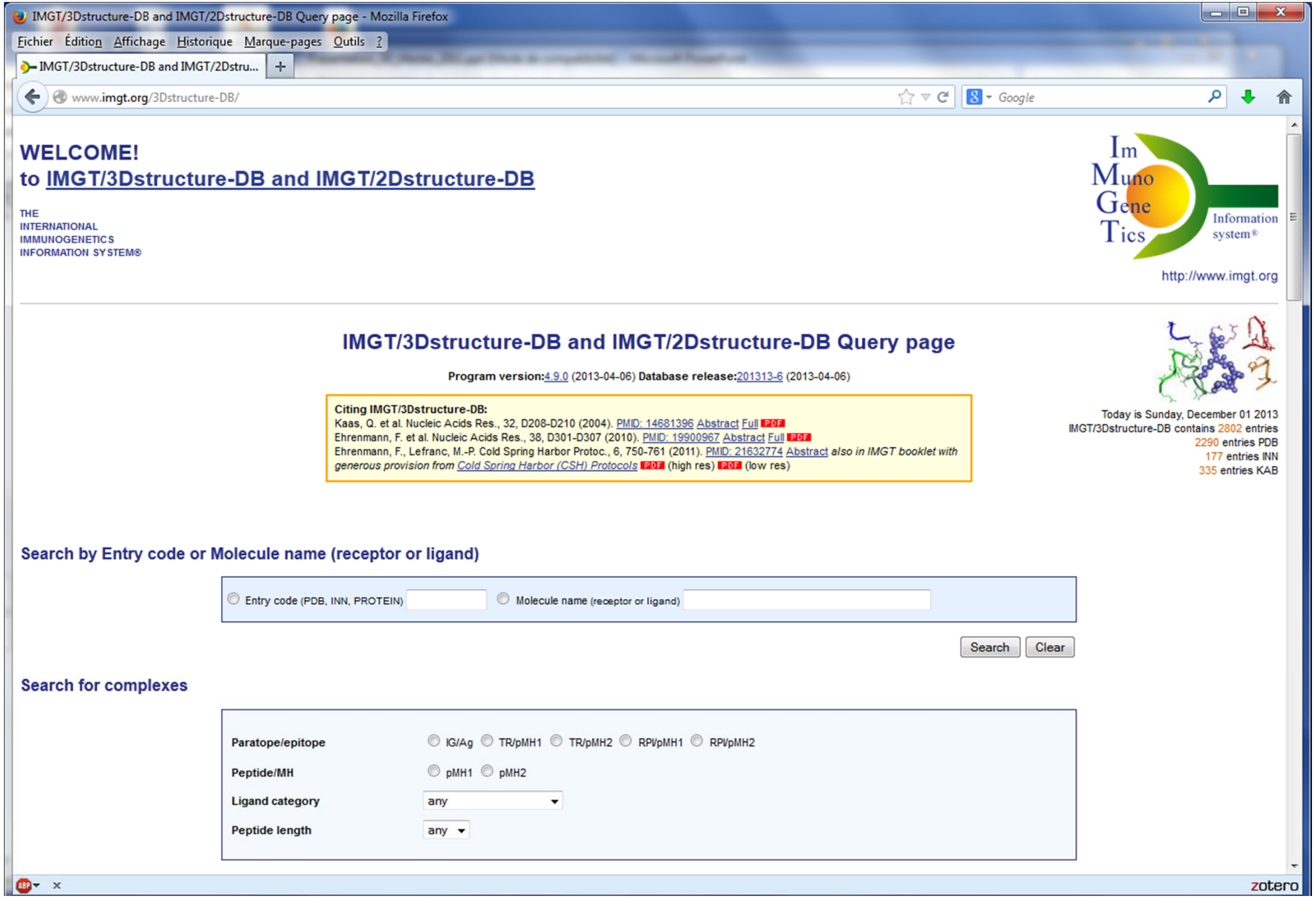
IMGT Web resources

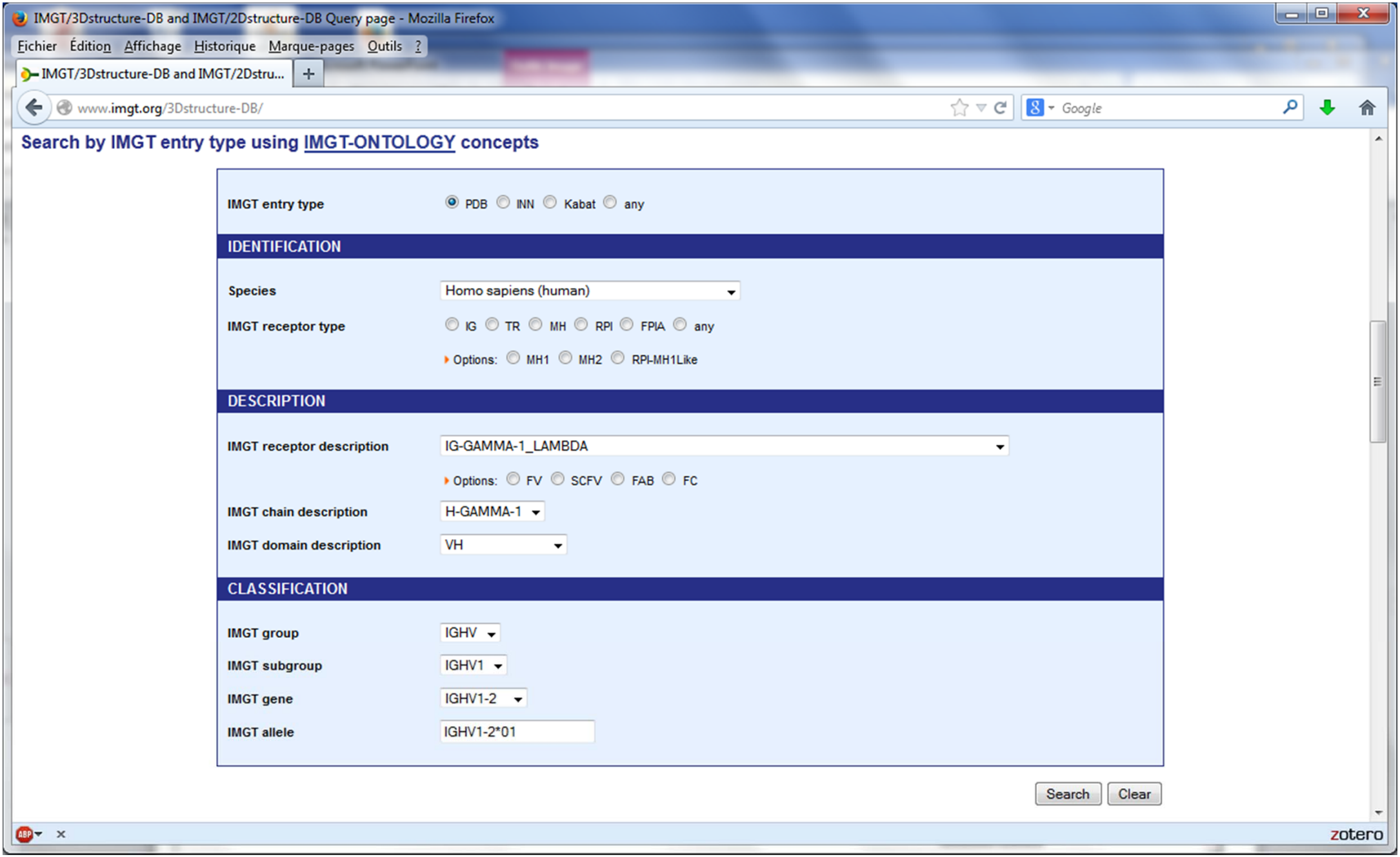
- **IMGT Repertoire** (IG and TR, MH and RPI)
- **IMGT Scientific chart** (Sequence description, Numbering, Nomenclature, Representation rules)

- **IMGT Index** (FactsBook)
- **IMGT Bloc-notes** (Interesting links, PubMed, Meeting announcements, Postdoctoral positions and jobs, Messages, Search engines...)
- **IMGT Education** (IMGT Lexique, Aide-mémoire, Tutorials, Questions and answers, Enseignements...)
- **IMGT Posters and diaporama**

- **The IMGT Medical page**
- **The IMGT Veterinary page**
- **The IMGT Biotechnology page**
- **The IMGT Immunoinformatics page**

IMGT 3Dstructure-DB Query Page

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www.imgt.org/3Dstructure-DB/
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Search by IMGT entry type using IMGT-ONTOLOGY concepts
IMGT entry type
PDB INN Kabat any
IDENTIFICATION
Species
Homo sapiens (human)
IMGT receptor type
IG TR MH RPI FPIA any
Options: MH1 MH2 RPI-MH1Like
DESCRIPTION
IMGT receptor description
IG-GAMMA-1_LAMBDA
Options: FV SCFV FAB FC
IMGT chain description
H-GAMMA-1
IMGT domain description
VH
CLASSIFICATION
IMGT group
IGHV
IMGT subgroup
IGHV1
IMGT gene
IGHV1-2
IMGT allele
IGHV1-2*01
Search
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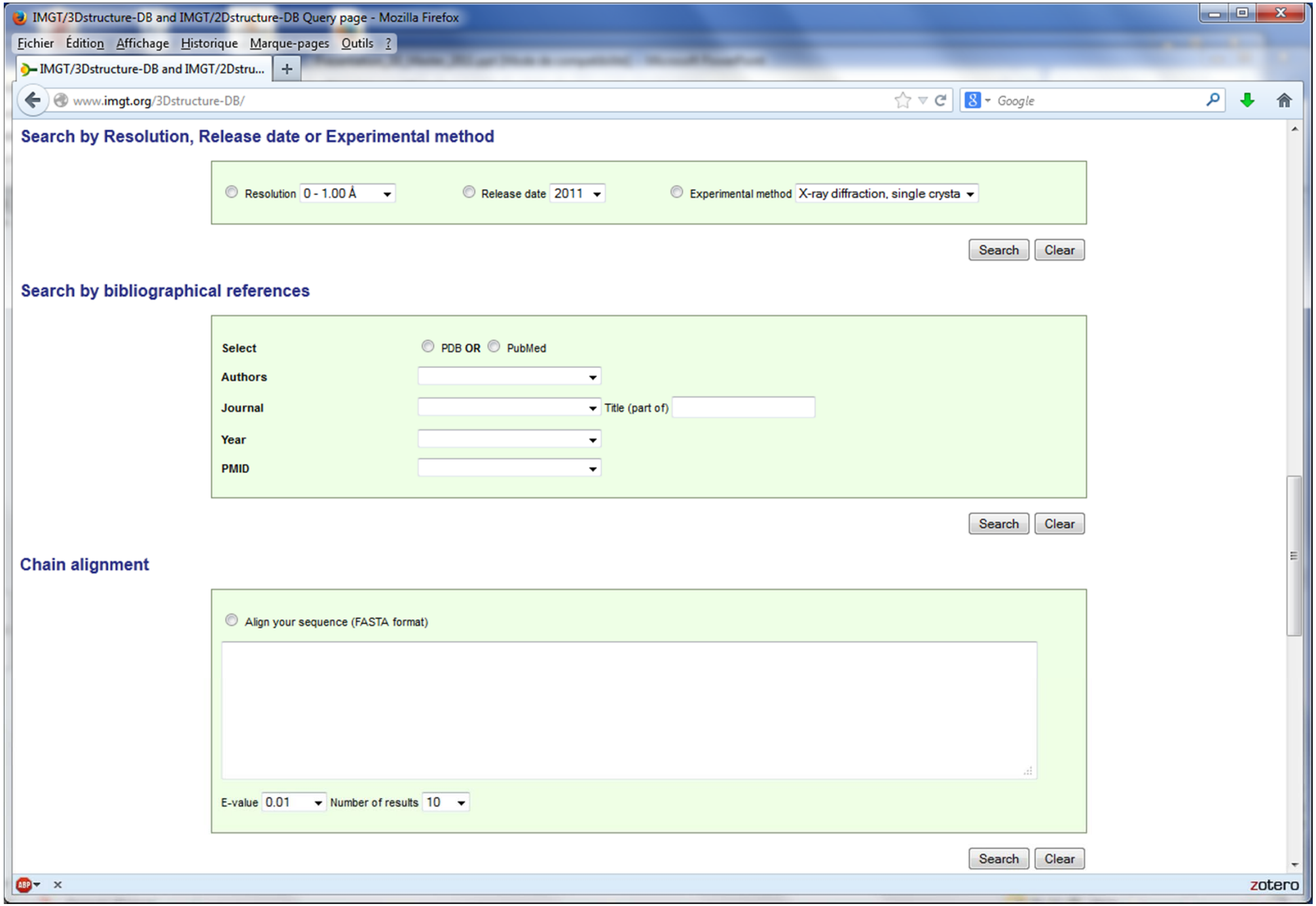
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Release date 2011
Experimental method X-ray diffraction, single crysta
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Search by bibliographical references
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PDB OR
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Journal
Title (part of)
Year
PMID
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Chain alignment
Align your sequence (FASTA format)
E-value 0.01
Number of results 10
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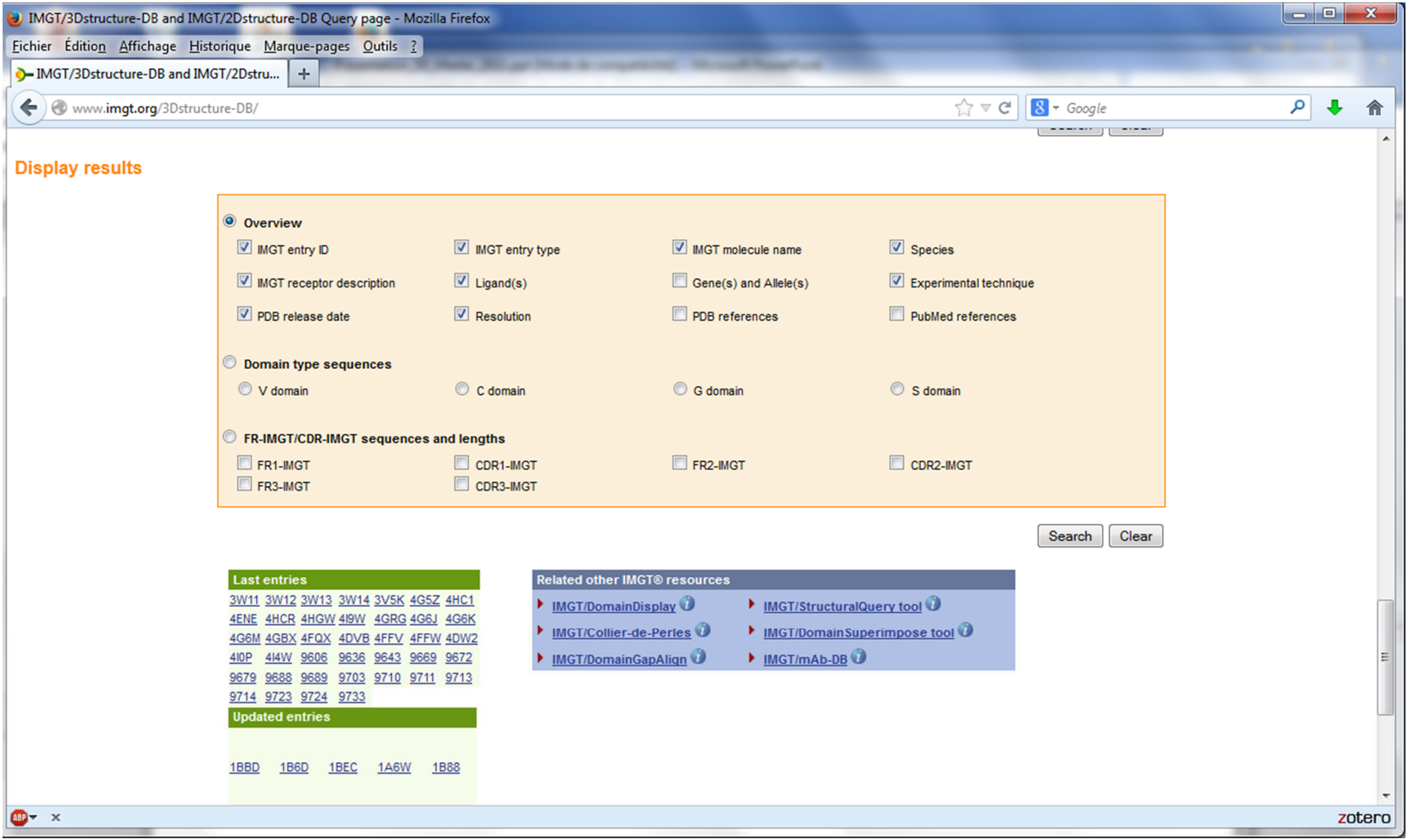
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Display results
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Species
IMGT receptor description
Ligand(s)
Gene(s) and Allele(s)
Experimental technique
PDB release date
Resolution
PDB references
PubMed references
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C domain
G domain
S domain
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CDR1-IMGT
FR2-IMGT
CDR2-IMGT
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CDR3-IMGT
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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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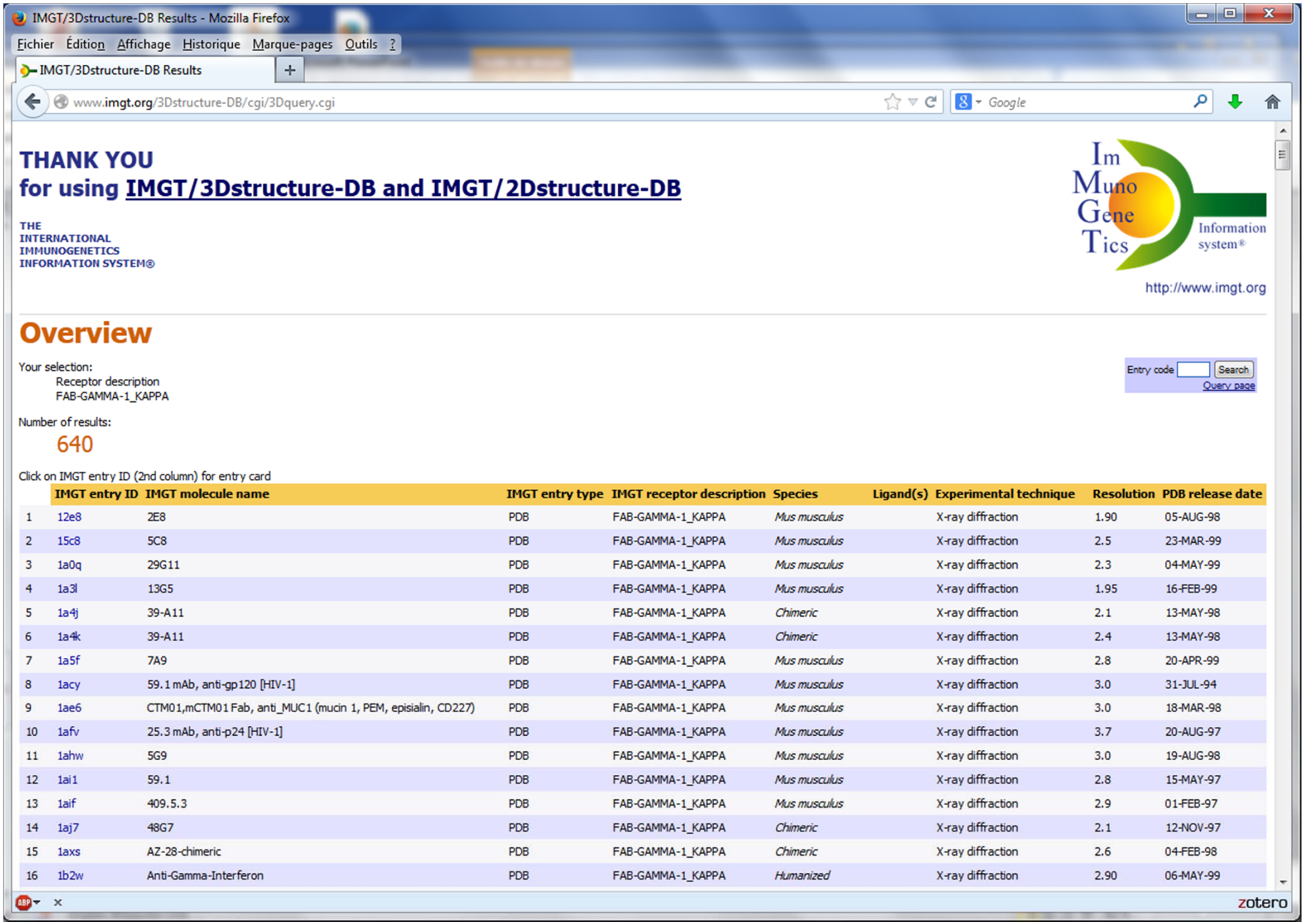
IMGT/3Dstructure-DB Overview



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1	12e8	2E8	PDB	FAB-GAMMA-1_KAPPA	*Mus musculus*		X-ray diffraction	1.90	05-AUG-98
2	15c8	5C8	PDB	FAB-GAMMA-1_KAPPA	*Mus musculus*		X-ray diffraction	2.5	23-MAR-99
3	1a0q	29G11	PDB	FAB-GAMMA-1_KAPPA	*Mus musculus*		X-ray diffraction	2.3	04-MAY-99
4	1a3l	13G5	PDB	FAB-GAMMA-1_KAPPA	*Mus musculus*		X-ray diffraction	1.95	16-FEB-99
5	1a4j	39-A11	PDB	FAB-GAMMA-1_KAPPA	*Chimeric*		X-ray diffraction	2.1	13-MAY-98
6	1a4k	39-A11	PDB	FAB-GAMMA-1_KAPPA	*Chimeric*		X-ray diffraction	2.4	13-MAY-98
7	1a5f	7A9	PDB	FAB-GAMMA-1_KAPPA	*Mus musculus*		X-ray diffraction	2.8	20-APR-99
8	1acy	59.1 mAb, anti-gp120 [HIV-1]	PDB	FAB-GAMMA-1_KAPPA	*Mus musculus*		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	*Mus musculus*		X-ray diffraction	3.0	18-MAR-98
10	1afv	25.3 mAb, anti-p24 [HIV-1]	PDB	FAB-GAMMA-1_KAPPA	*Mus musculus*		X-ray diffraction	3.7	20-AUG-97
11	1ahw	5G9	PDB	FAB-GAMMA-1_KAPPA	*Mus musculus*		X-ray diffraction	3.0	19-AUG-98
12	1ai1	59.1	PDB	FAB-GAMMA-1_KAPPA	*Mus musculus*		X-ray diffraction	2.8	15-MAY-97
13	1aif	409.5.3	PDB	FAB-GAMMA-1_KAPPA	*Mus musculus*		X-ray diffraction	2.9	01-FEB-97
14	1aj7	48G7	PDB	FAB-GAMMA-1_KAPPA	*Chimeric*		X-ray diffraction	2.1	12-NOV-97
15	1axs	AZ-28-chimeric	PDB	FAB-GAMMA-1_KAPPA	*Chimeric*		X-ray diffraction	2.6	04-FEB-98
16	1b2w	Anti-Gamma-Interferon	PDB	FAB-GAMMA-1_KAPPA	*Humanized*		X-ray diffraction	2.90	06-MAY-99

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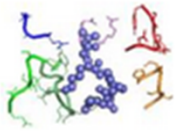

Entry code [ ] Search
Query page

IMGT molecule name	IMGT receptor type	IMGT receptor description	Ligand(s)	Species	CC	Chain ID
A6	TR	TR-ALPHA_BETA-2		*Homo sapiens* (human)	1	[1ao7_D 1ao7_E]
HLA-A*0201	MH	MH1-ALPHA_B2M		*Homo sapiens* (human)	1	[1ao7_A 1ao7_B]
		Peptide	Tax peptide 11-19 (Q82235)	*Human T-lymphotropic virus 1*	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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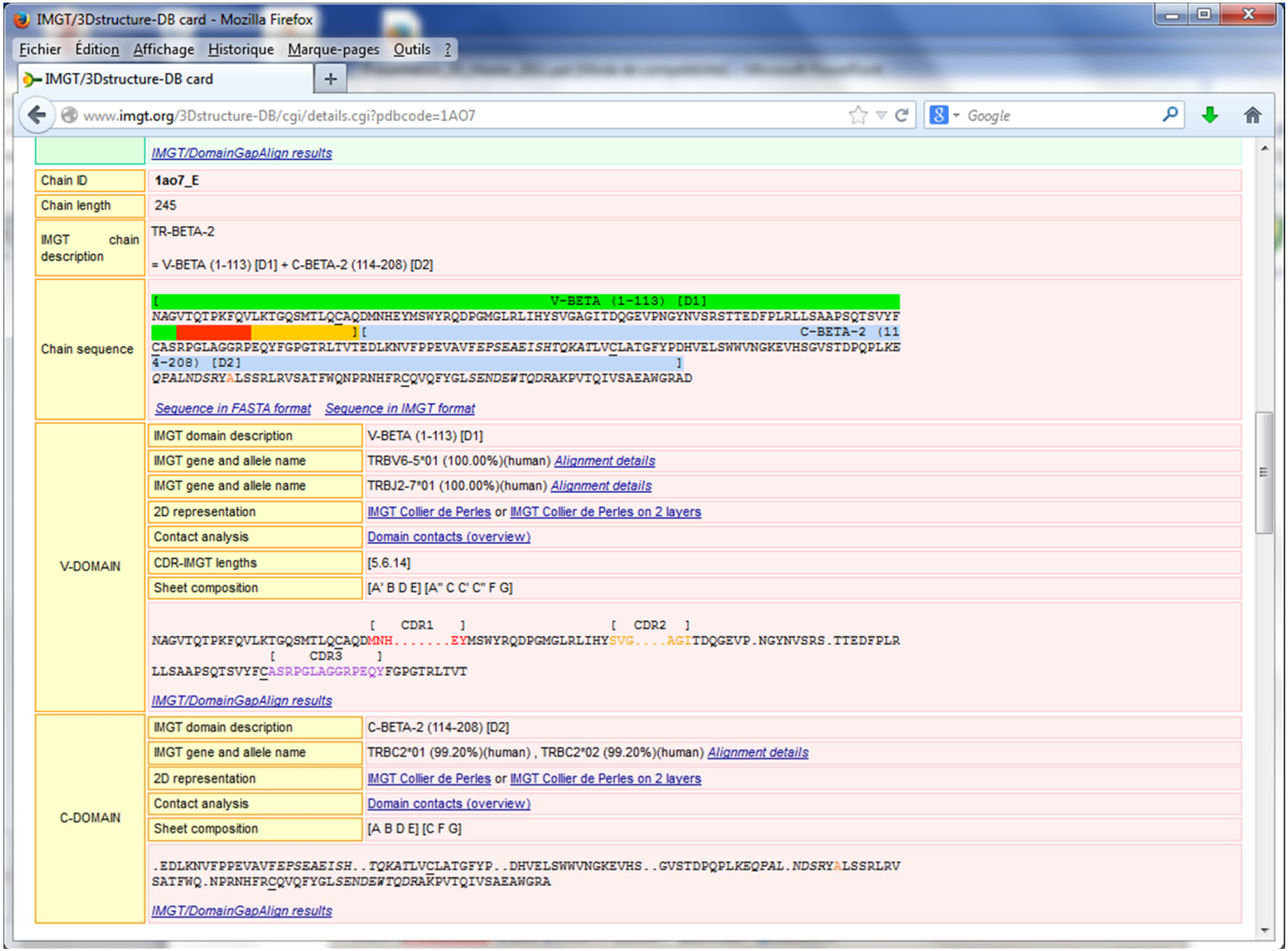
IMGT/3Dstructure-DB Card (2)



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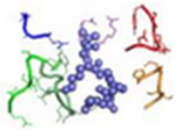

Entry code [ ] Search
Query page

IMGT molecule name	IMGT receptor type	IMGT receptor description	Ligand(s)	Species	CC	Chain ID
A6	TR	TR-ALPHA_BETA-2		*Homo sapiens* (human)	1	[1ao7_D 1ao7_E]
HLA-A*0201	MH	MH1-ALPHA_B2M		*Homo sapiens* (human)	1	[1ao7_A 1ao7_B]
		Peptide	Tax peptide 11-19 (Q82235)	*Human T-lymphotropic virus 1*	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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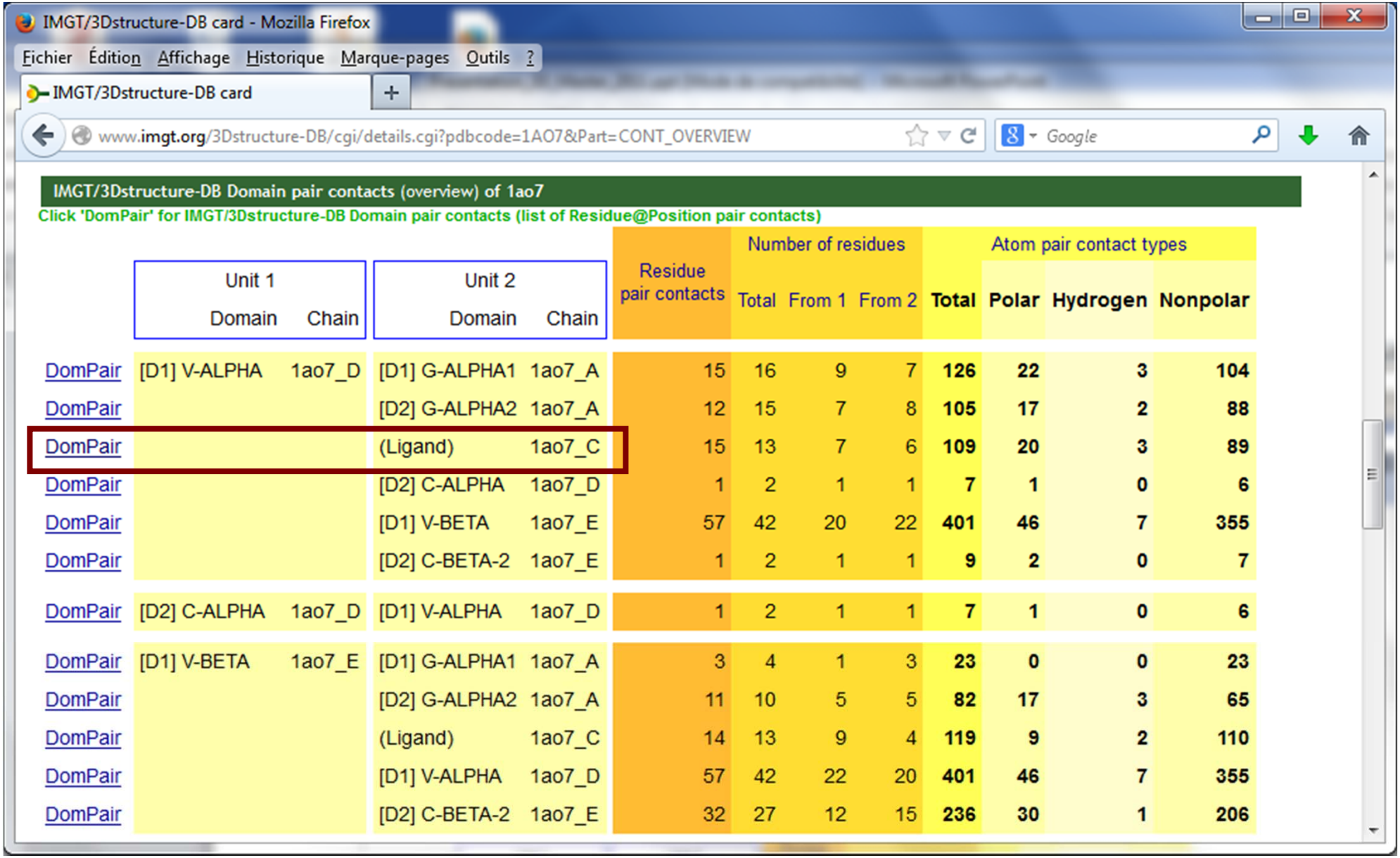
IMGT/3Dstructure-DB Contact Analysis



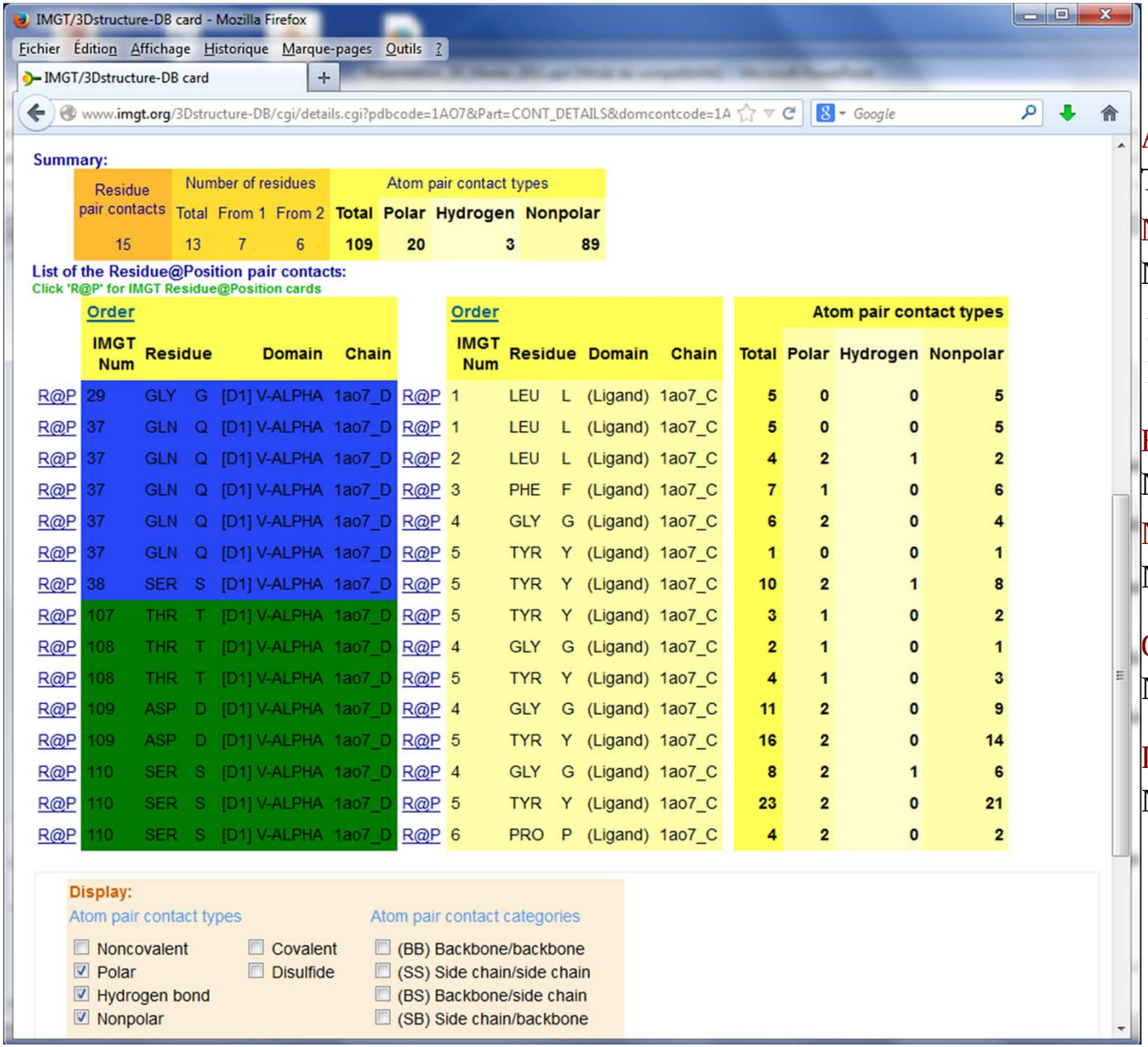
IMGT/3Dstructure-DB Domain pair contacts (overview) of 1ao7

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

	Unit 1 Domain	Unit 1 Chain	Unit 2 Domain	Unit 2 Chain	Residue pair contacts	Number of residues Total	From 1	From 2	Atom pair contact types 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



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

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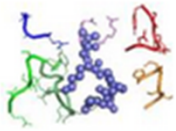

Entry code [ ] Search
Query page

IMGT molecule name	IMGT receptor type	IMGT receptor description	Ligand(s)	Species	CC	Chain ID
A6	TR	TR-ALPHA_BETA-2		*Homo sapiens* (human)	1	[1ao7_D 1ao7_E]
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		Peptide	Tax peptide 11-19 (Q82235)	*Human T-lymphotropic virus 1*	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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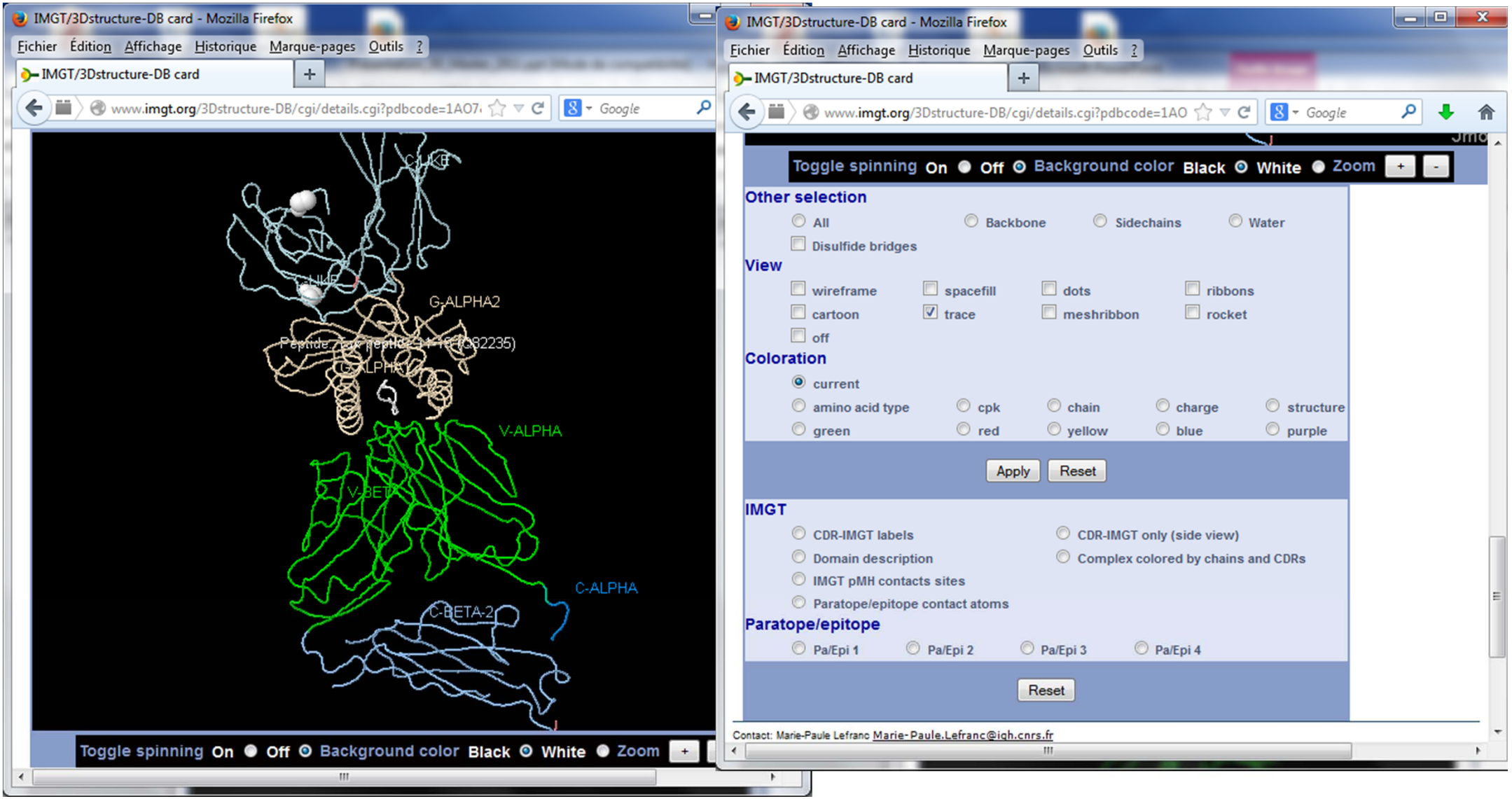
IMGT/3Dstructure-DB Visualization

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

http://www.imgt.org



Chimeric and humanized antibodies: application in oncology

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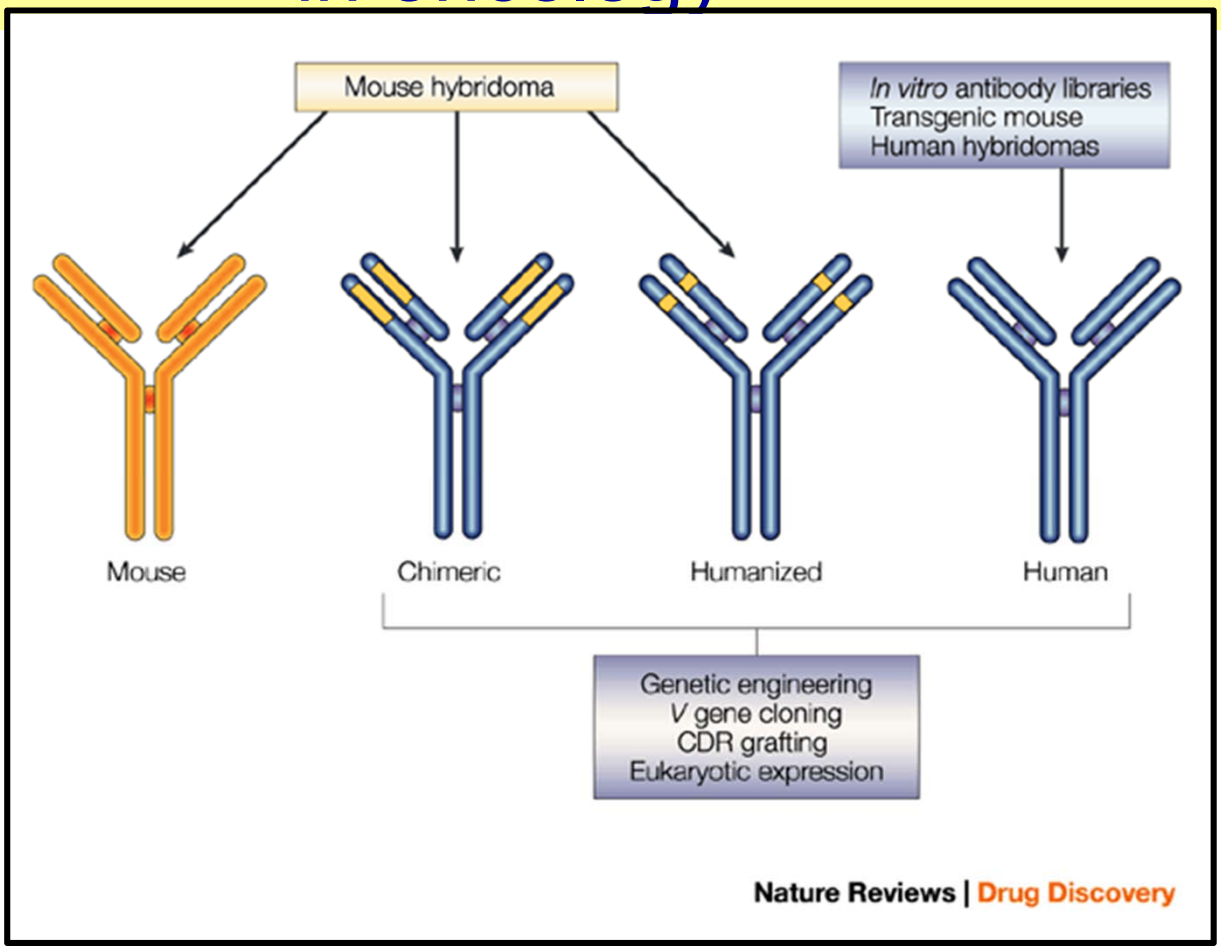
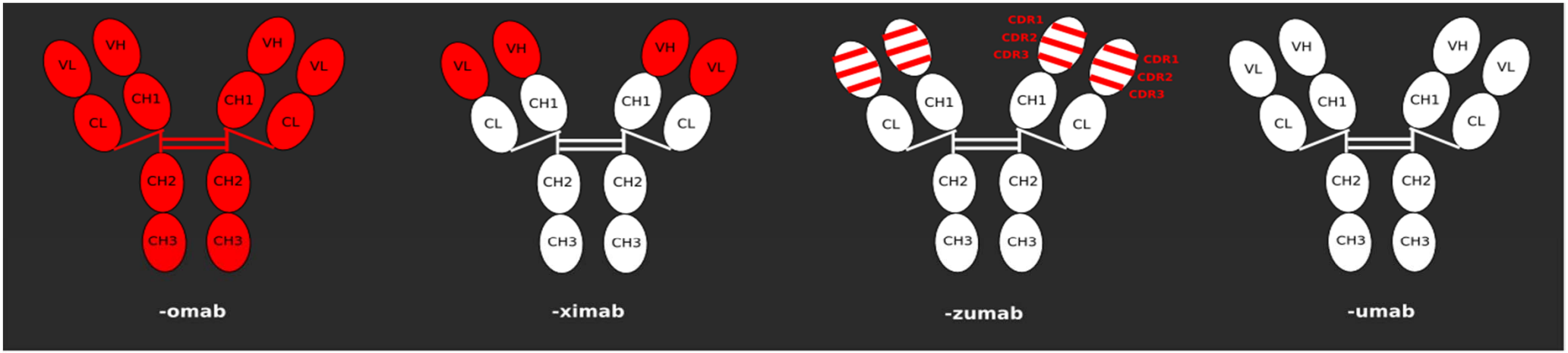


Une chaîne dite chimérique est une chaîne qui contient un domaine variable étranger (V-D-J-REGION) (provenant d'une espèce autre que l'homme, ou synthétiques) liées à une région constante (C-REGION) d'origine humaine.

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)	

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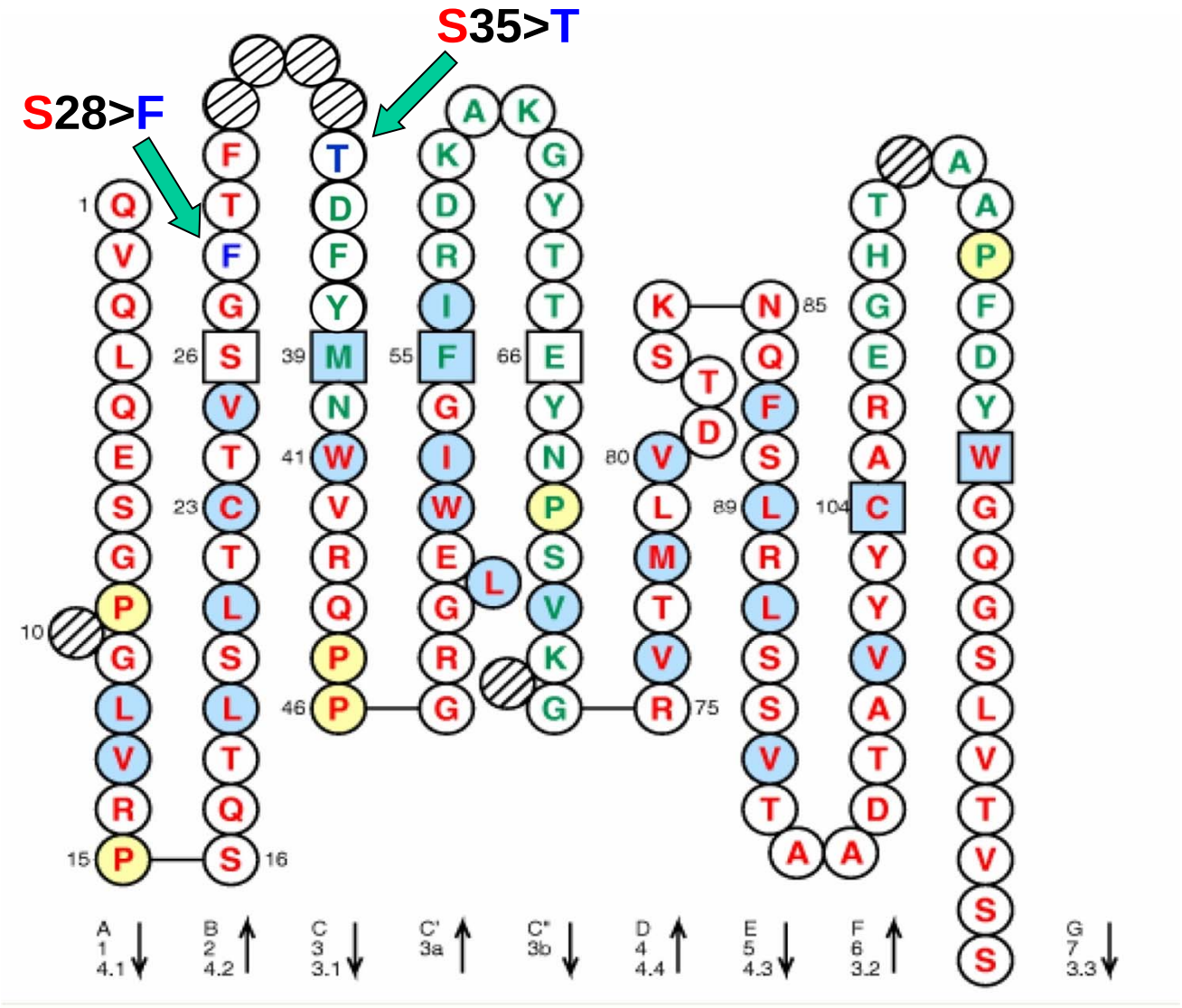

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