http://www.imgt.org

Structures en immunogénétique

Introduction

Master 2 Bioinformatique, Université Montpellier 2
Montpellier, 16 Novembre 2011

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

Immunogenetics and structure

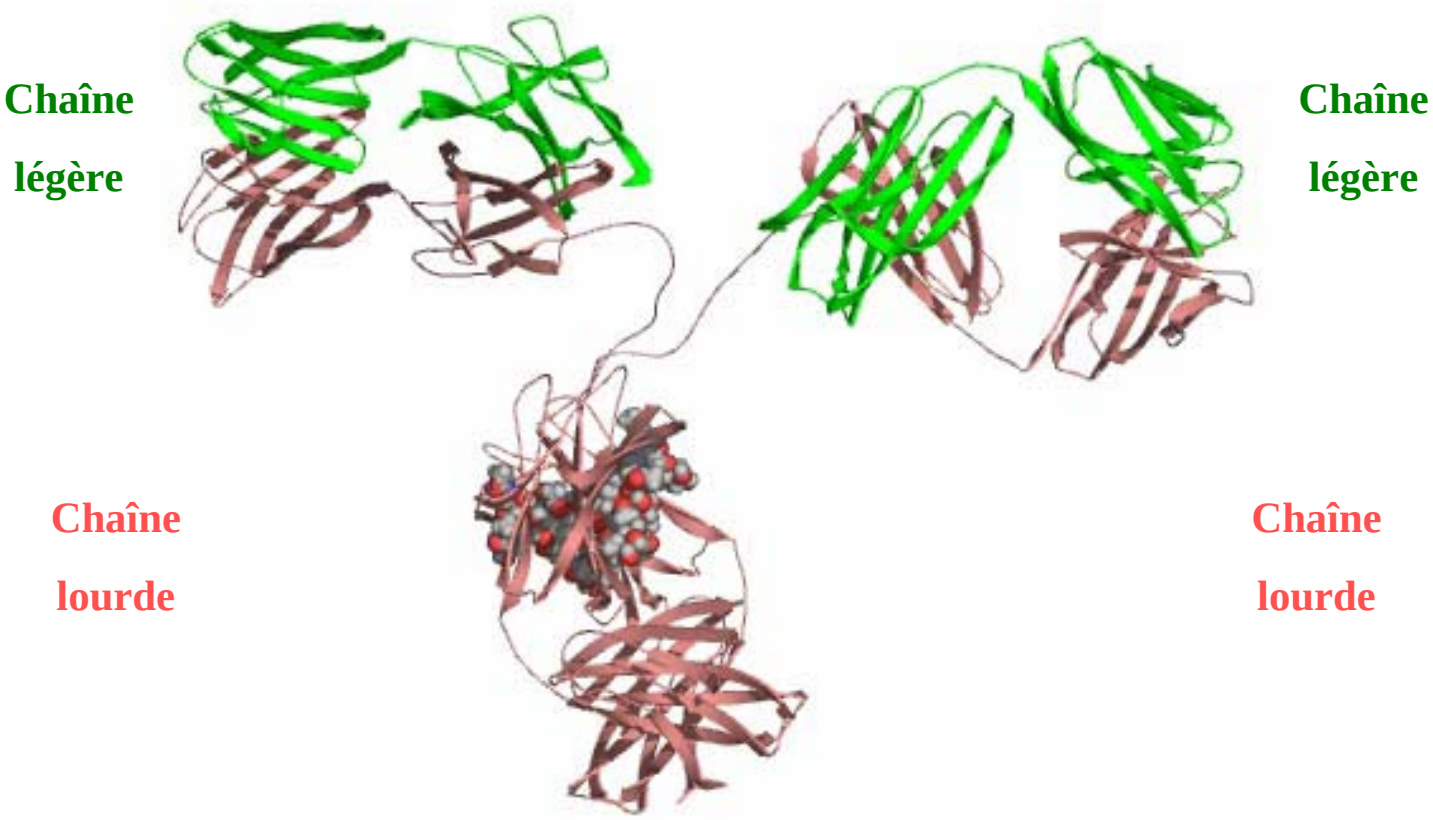
http://www.imgt.org

- Structures en immunogénétique
- Une base de données : IMGT/3Dstructure-DB
- IMGT unique numbering for V-DOMAIN, C-DOMAIN, G-DOMAIN
- IMGT Colliers de Perles (représentation 2D)
- Analyse des contacts
- Relations séquences-structures-fonctions
- Applications: ingénierie et humanisation des anticorps

  => consiste à remplacer les régions hypervariables (complementary determining region,CDR) d'un anticorps humain par des régions CDR d'origine murine.

Immunoglobulines (IG)

http://www.imgt.org



Immunoglobulin (IG) | T cell receptor (TR)

http://www.imgt.org

V-DOMAIN

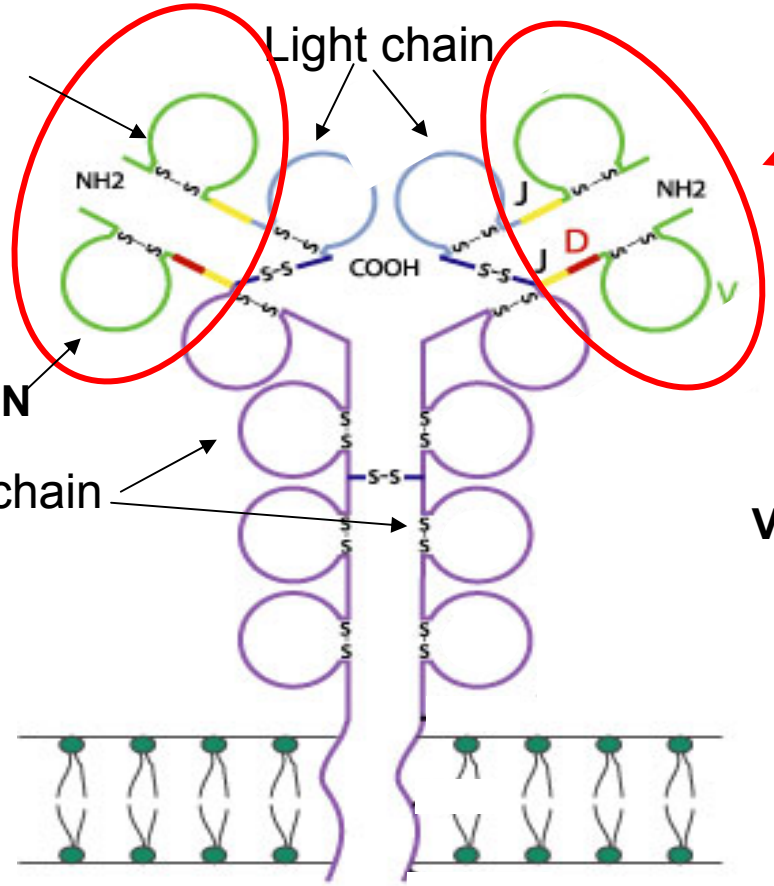
V-J-REGION

V-DOMAIN

V-D-J-REGION

Light chain

Heavy chain



Membrane IgM

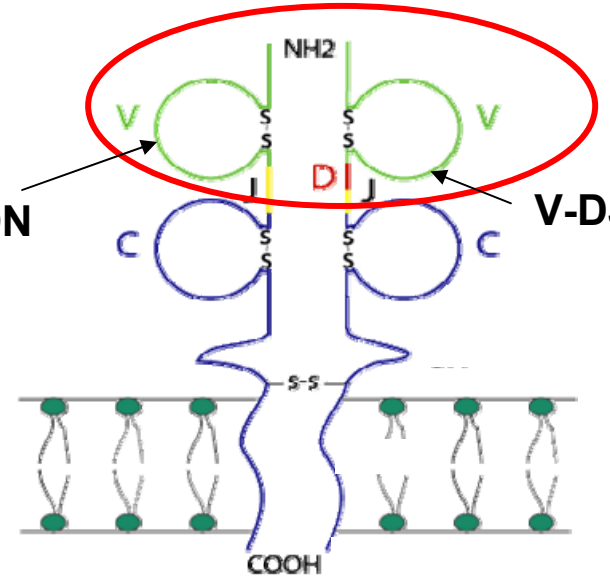
Contribution of the
2 V-DOMAINs
to the antigen binding site

Alpha - Beta

Gamma - Delta

V-J-REGION

V-DJ-REGION

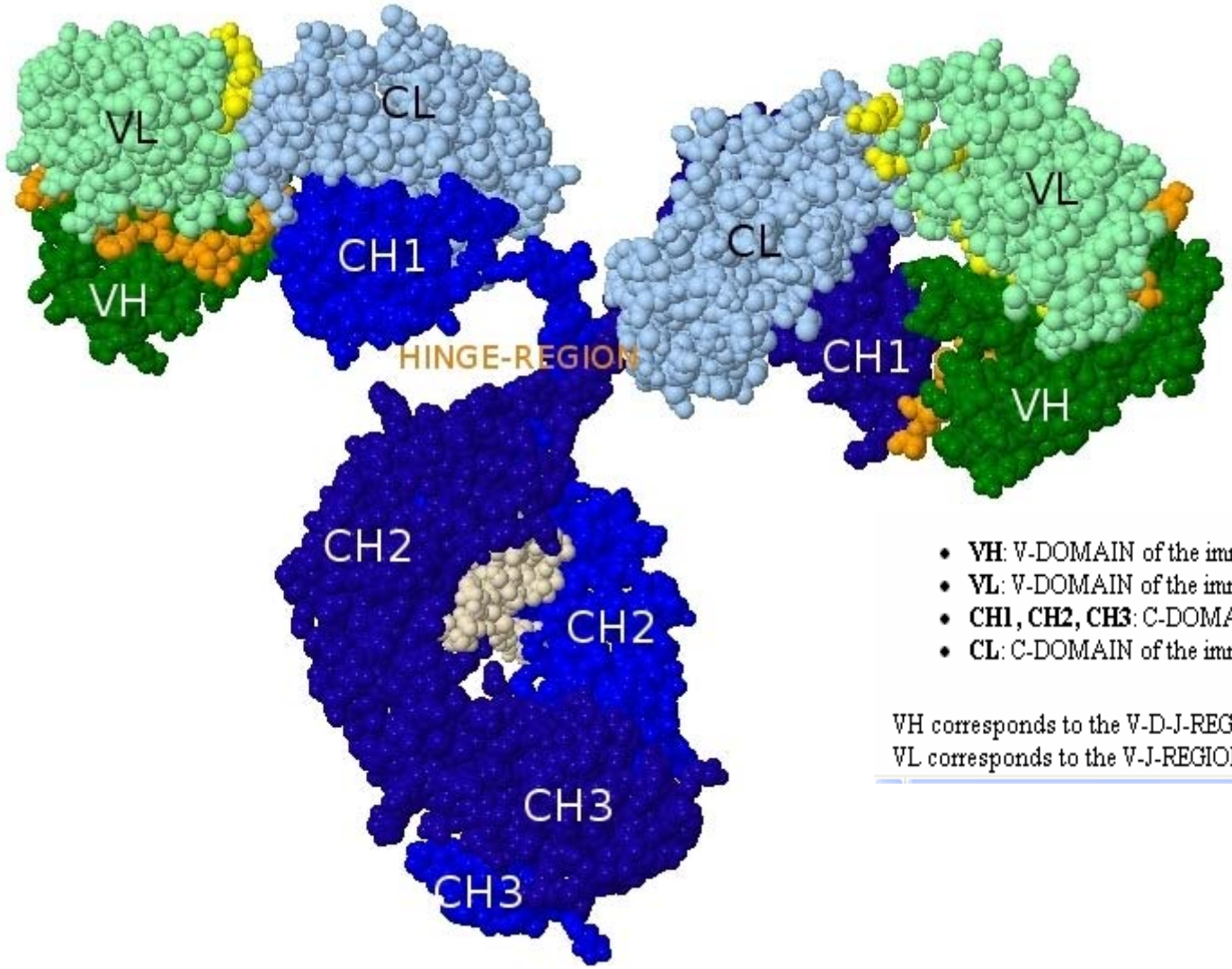


T cell receptor

The Immunoglobulin FactsBook, 2001

Immunoglobulins (IG) - Spacefill

http://www.imgt.org



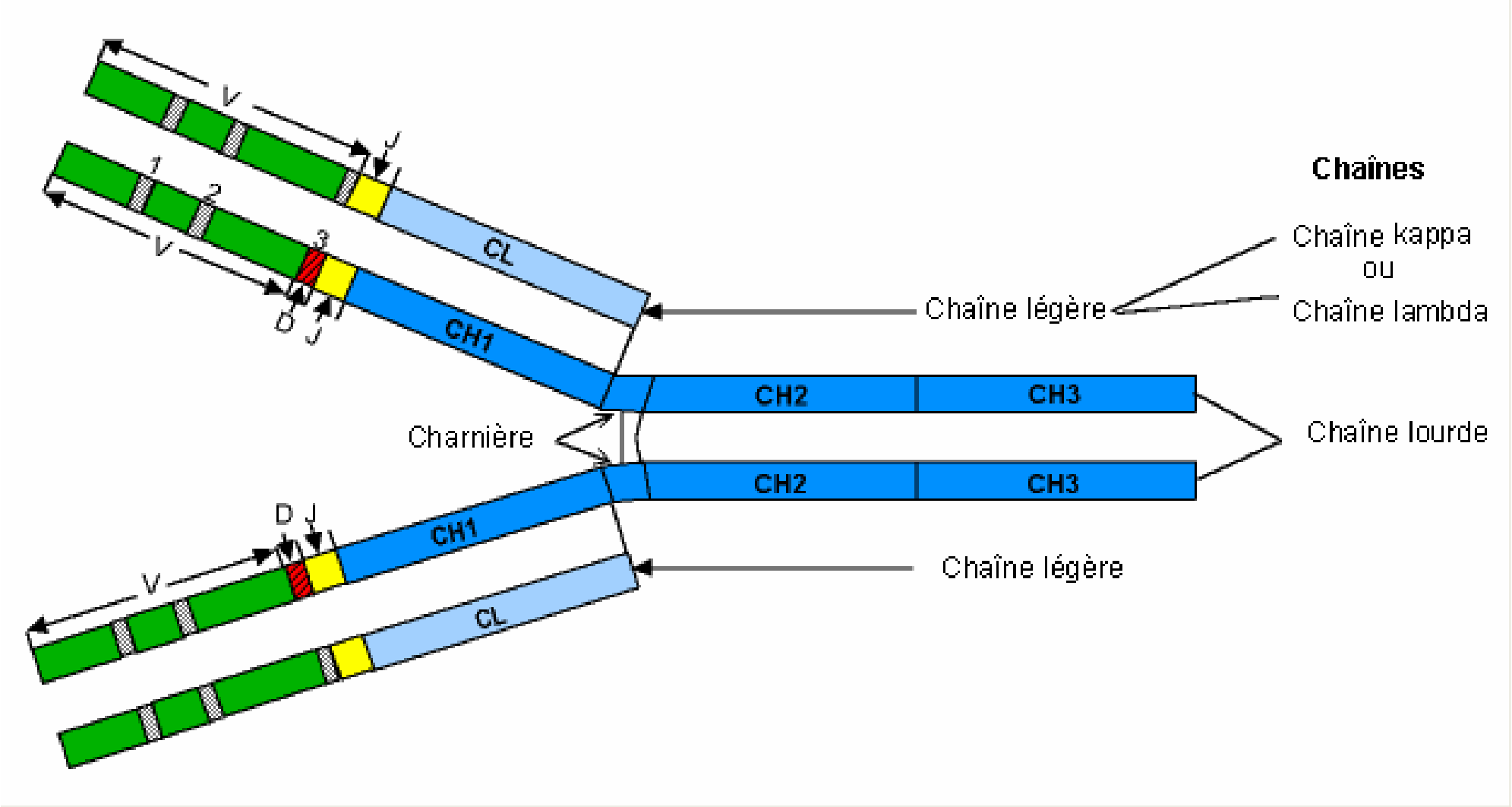
- **VH**: V-DOMAIN of the immunoglobulin heavy chain
- **VL**: V-DOMAIN of the immunoglobulin light chain
- **CH1, CH2, CH3**: C-DOMAIN of the immunoglobulin heavy chain
- **CL**: C-DOMAIN of the immunoglobulin light chain

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



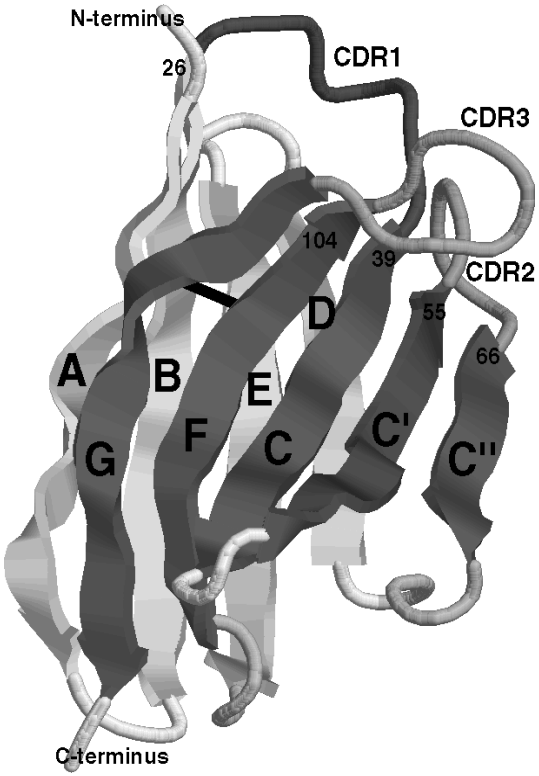
IMGT Repertoire, http://www.imgt.org

Structural domains

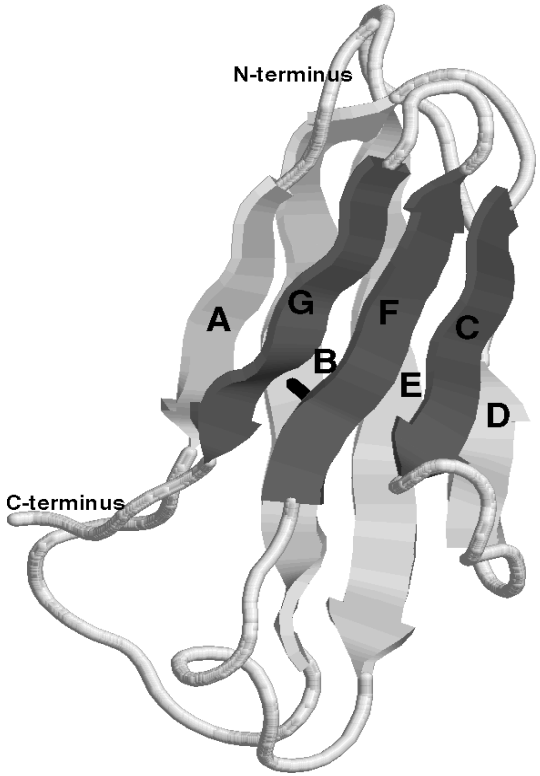
http://www.imgt.org

IG and TR

V-DOMAIN



C-DOMAIN



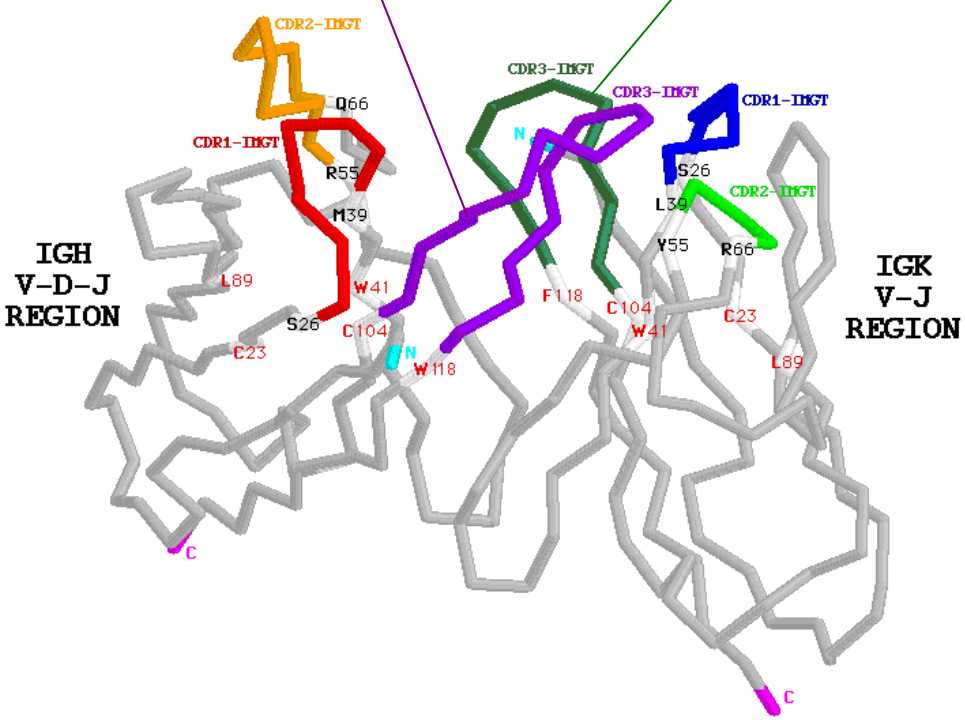
Le domaine d'IG est une structure de type sandwich bêta constituée de deux feuillets bêta antiparallèles. Les feuillets des V-DOMAINs possèdent respectivement 4 brins et 5 brins. Les V-DOMAINs possèdent trois boucles qui assurent la liaison avec un antigène. Ces boucles ou CDR (Complementarity Determining 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

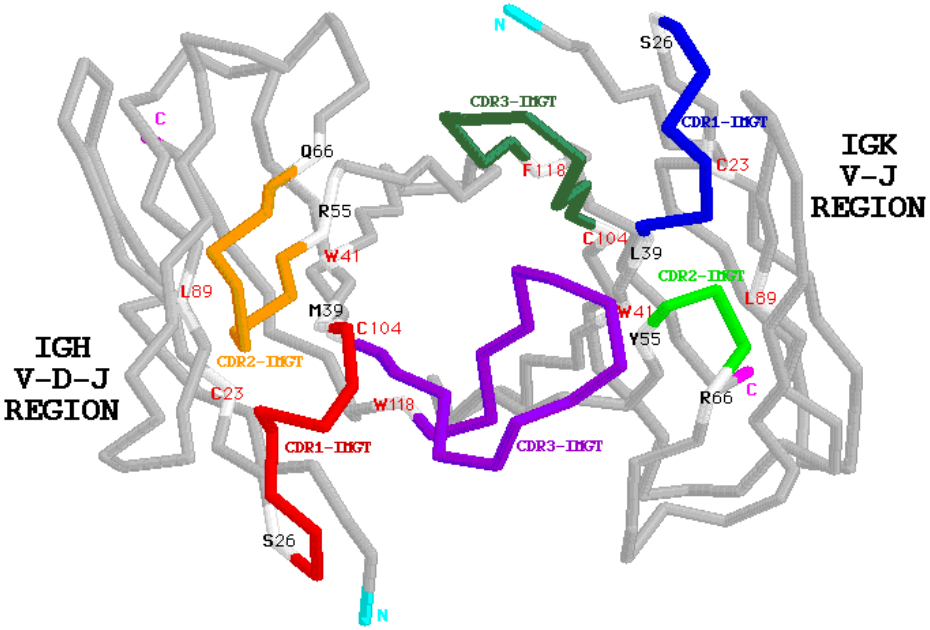
VH V-KAPPA

V-D-J junction V-J junction



Side view of the V-DOMAINs

VH V-KAPPA



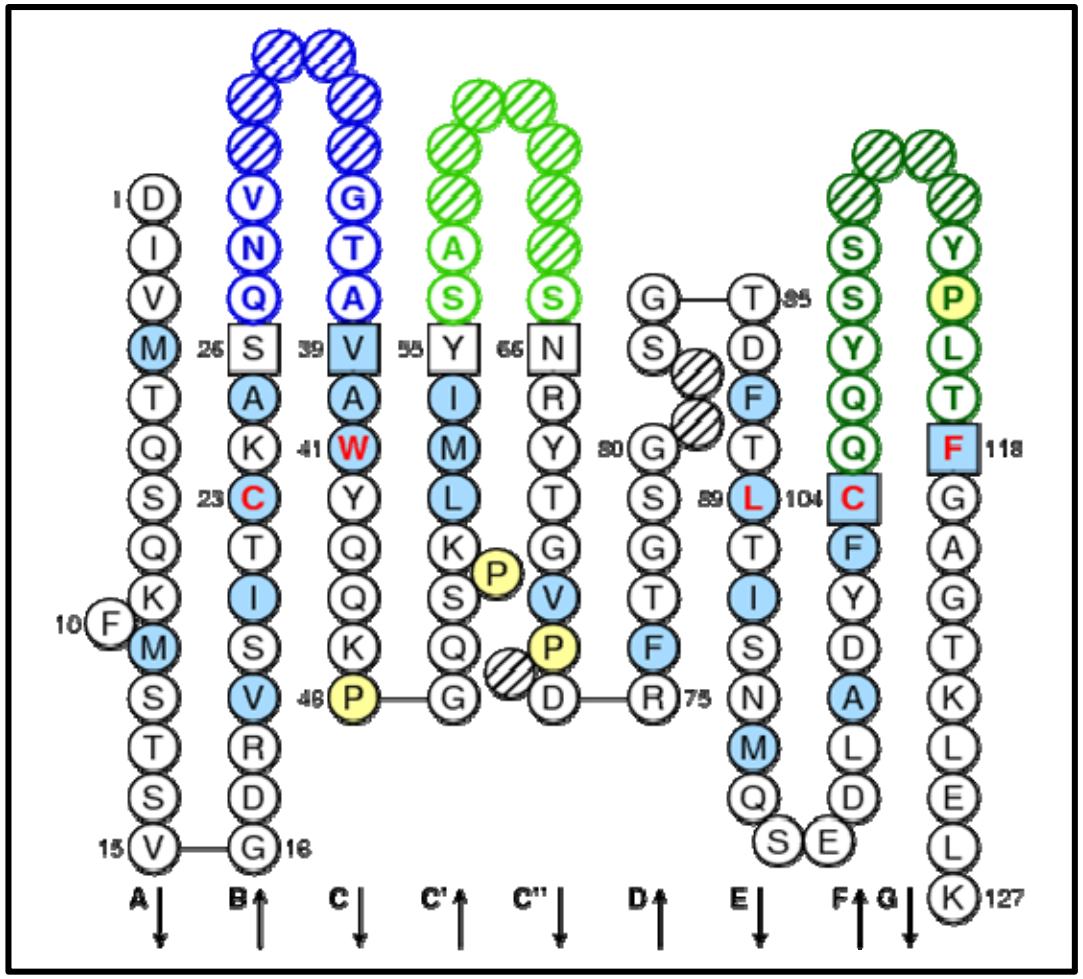
View from above the CDRs

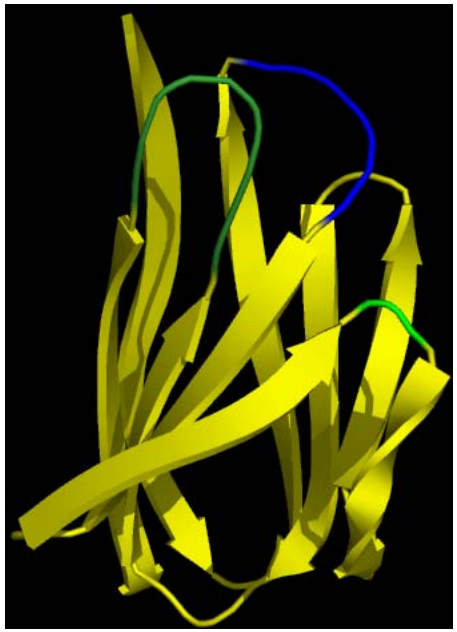
Mouse(Mus musculus) E5.2Fv

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

IMGT Collier de Perles for V-DOMAIN

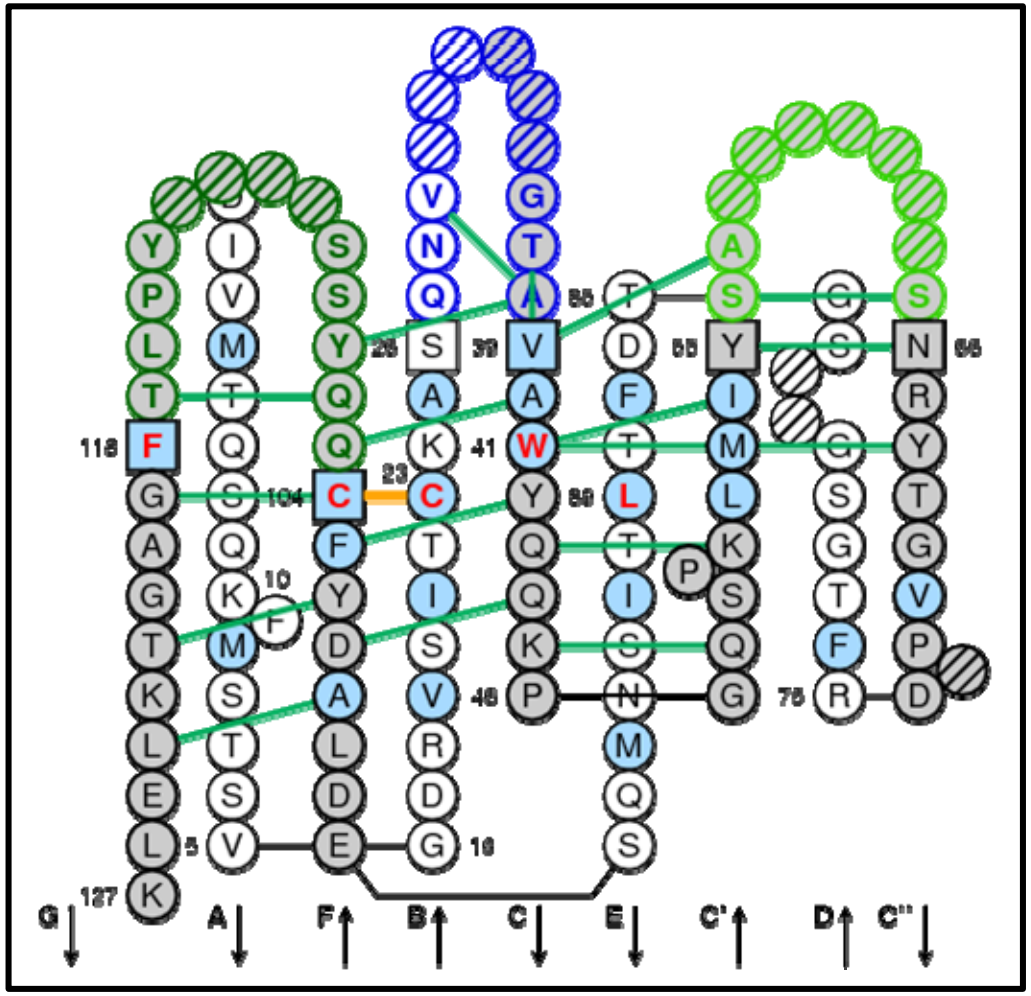
http://www.imgt.org





IMGT Collier de Perles for V-DOMAIN on two layers

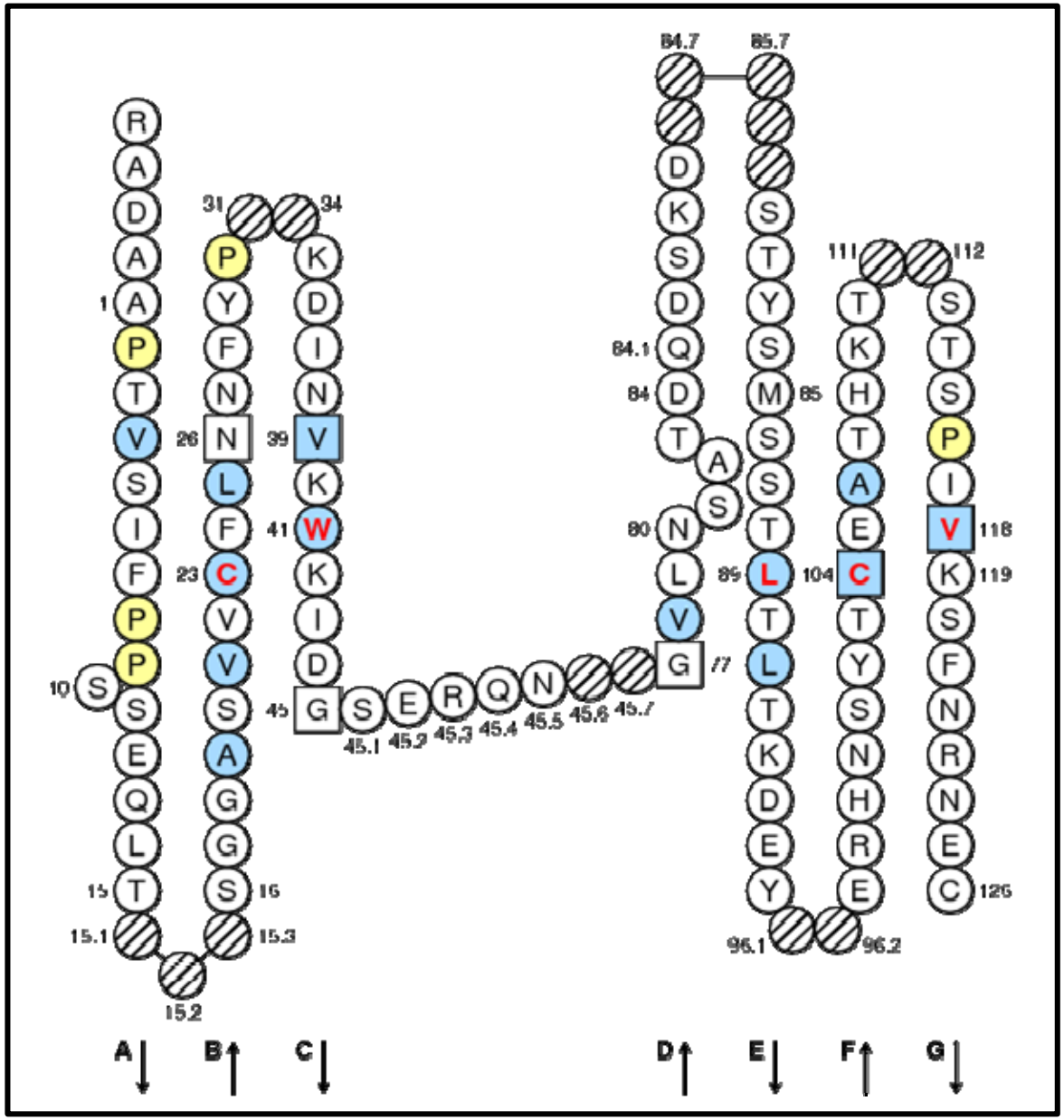
http://imgt.cines.fr

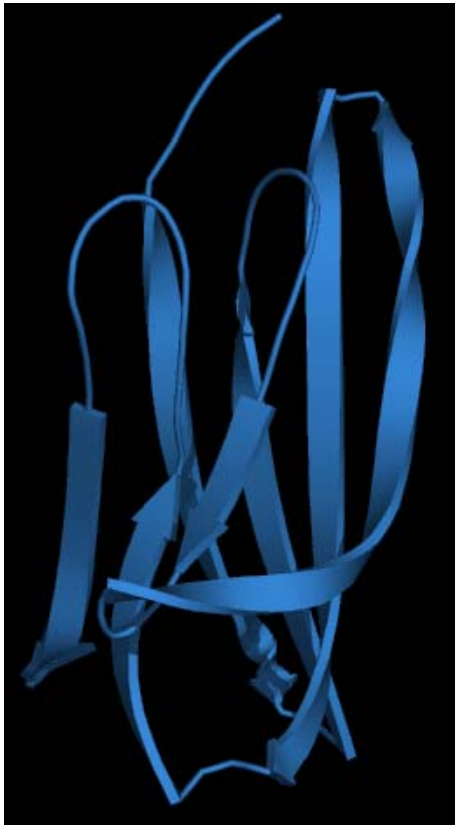


Hydrogen bonds between the amino acids of the C, C', C'', F and G strands and those of the CDR-IMGT

IMGT Collier de Perles for C-DOMAIN

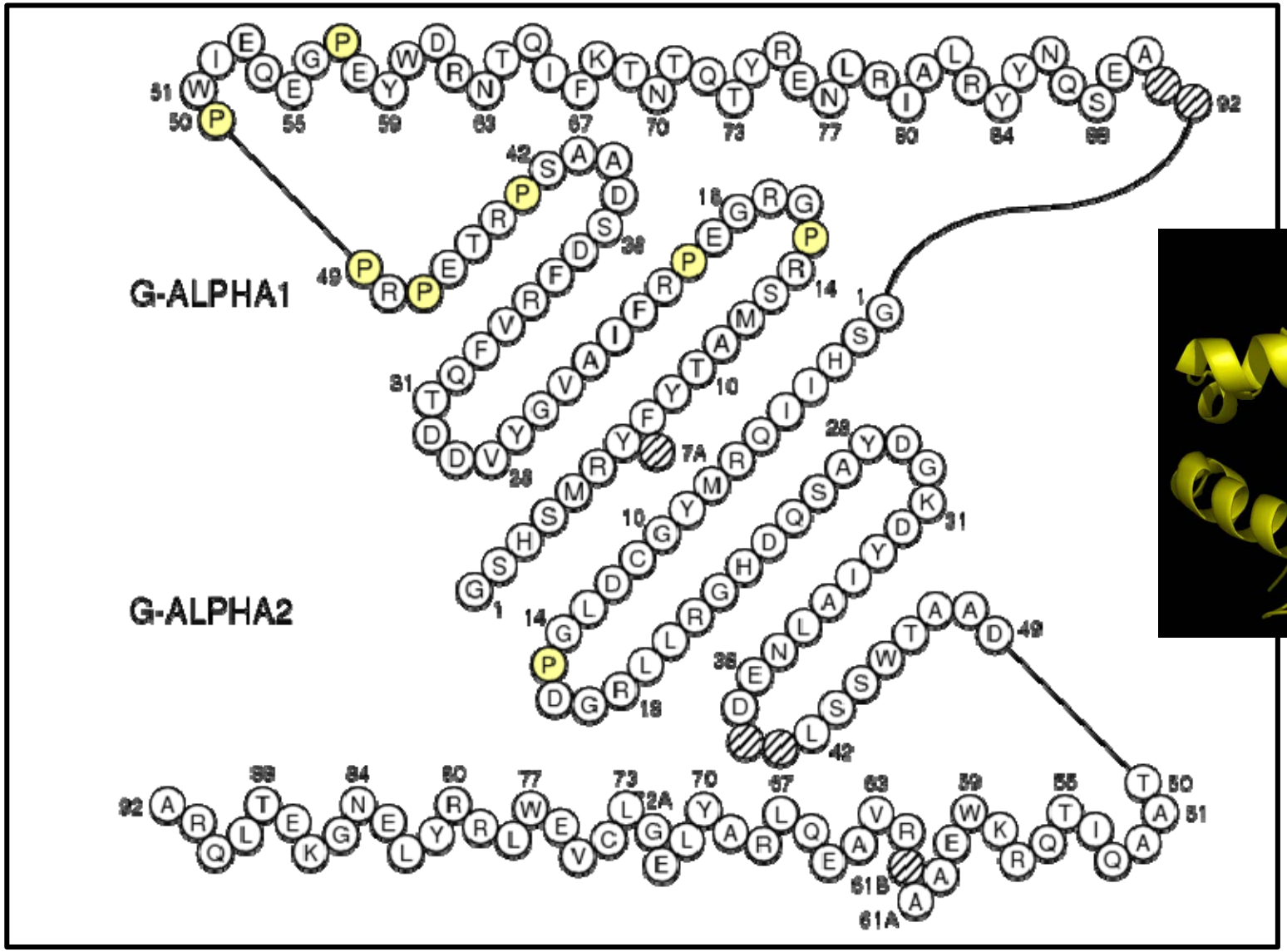
http://www.imgt.org

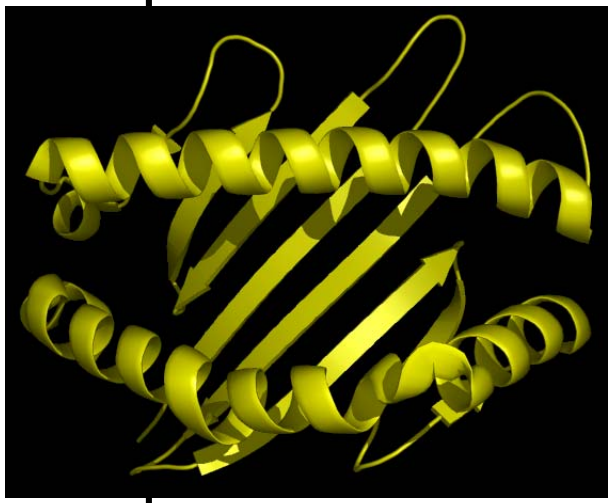




IMGT Collier de Perles for G-DOMAIN

http://www.imgt.org

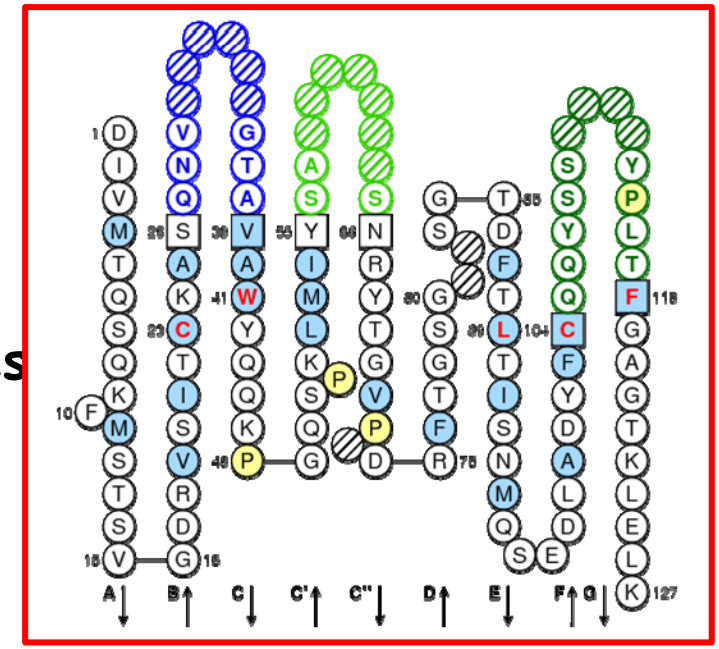




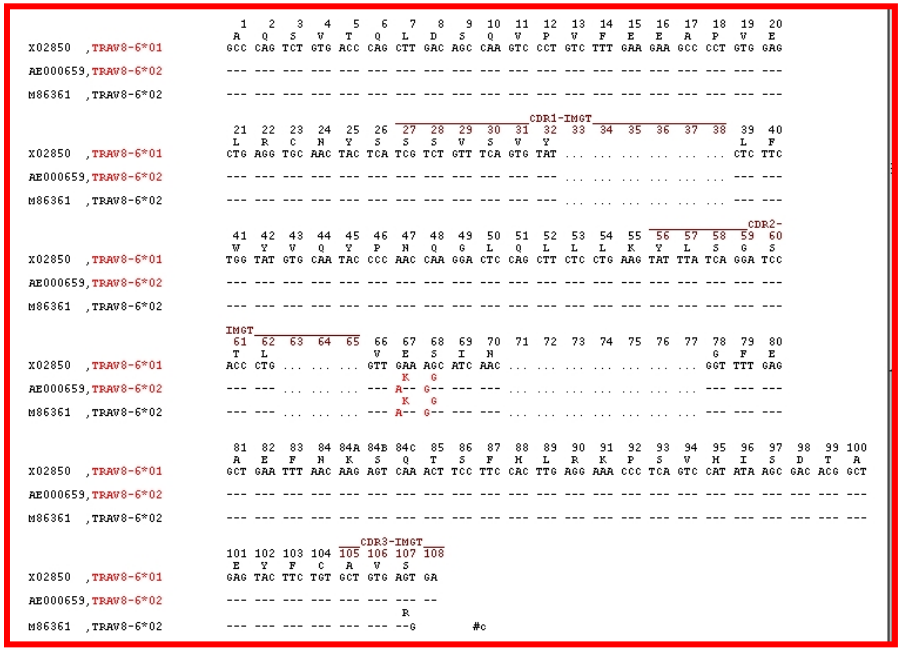
IMGT Web resources

http://www.imgt.org

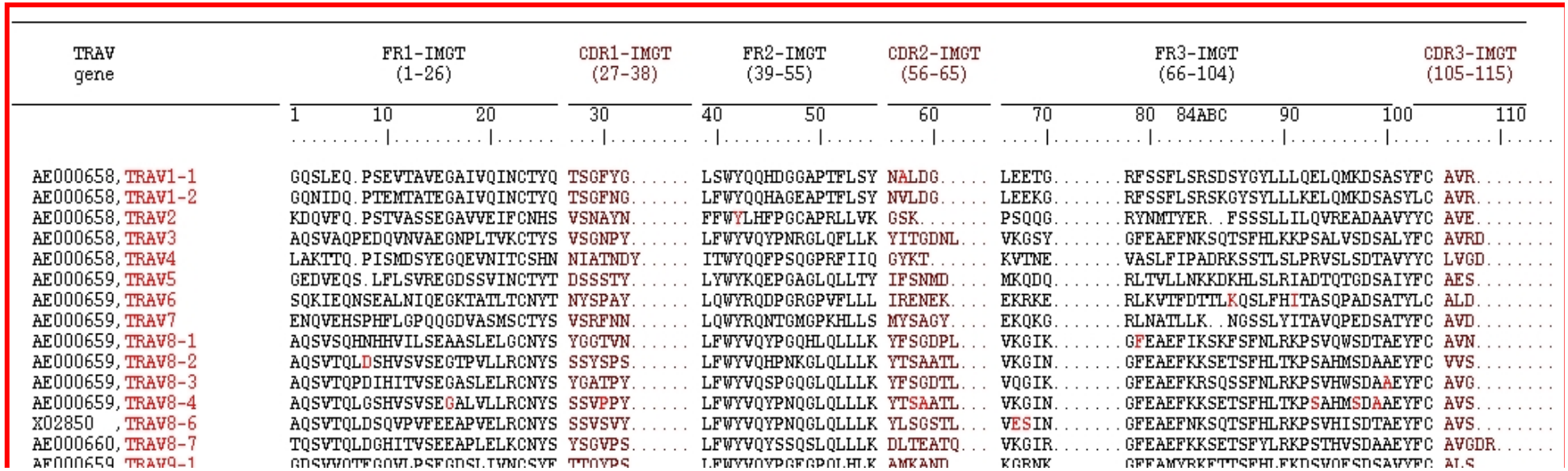
IMGT Collier de Perles



IMGT Alignment of alleles



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)
AE000658,TRAV1-1	GQSLEQ.PSEVTAVEGAIVQINCTYQ	TSGFYG.....	LSWYQQHDGGAPTFLSY	NALDG.....	LEETG.....RFSSFLSRSDSYGYLLLQELQMKDSASYFC	AVR.....
AE000658,TRAV1-2	GQNIDQ.PTEMTATEGAIVQINCTYQ	TSGFNG.....	LFWYQQHAGEAPTFLSY	NVLDG.....	LEEKG.....RFSSFLSRSKGYSYLLLKELQMKDSASYLC	AVR.....
AE000658,TRAV2	KDQVFQ.PSTVASSEGAVVEIFCNHS	VSNAYN.....	FFWYLHFPGCAPRLLVK	GSK.....	PSQQG.....RYNMTYER..FSSSLLILQVREADAAVYYC	AVE.....
AE000658,TRAV3	AQSVAQPEDQVNVAEGNPLTVKCTYS	VSGNPY.....	LFWYVQYPNRGLQFLLK	YITGDNL...	VKGSY.....GFEAEFNKSQTSFHLKKPSALVSDSALYFC	AVRD.....
AE000658,TRAV4	LAKTTQ.PISMDSYEGQEVNITCSHN	NIATNDY.....	ITWYQQFPSQGPRFIIQ	GYKT.....	KVTNE.....VASLFIPADRKSSTLSLPRVSLSDTAVYYC	LVGD.....
AE000659,TRAV5	GEDVEQS.LFLSVREGDSSVINCTYT	DSSSTY.....	LYWYKQEPGAGLQLLTY	IFSNMD....	MKQDQ.....RLTVLLNKKDKHLSLRIADTQTGDSAIYFC	AES.....
AE000659,TRAV6	SQKIEQNSEALNIQEGKTATLTCNYT	NYSPAY.....	LQWYRQDPGRGPVFLLL	IRENEK....	EKRKE.....RLKVTFDTTLKQSLFHITASQPADSATYLC	ALD.....
AE000659,TRAV7	ENQVEHSPHFLGPQQGDVASMSCTYS	VSRFNN.....	LQWYRQNTGMGPKHLLS	MYSAGY....	EKQKG.....RLNATLLK..NGSSLYITAVQPEDSATYFC	AVD.....
AE000659,TRAV8-1	AQSVSQHNHHVILSEAASLELGCNYS	YGGTVN.....	LFWYVQYPGQHLQLLLK	YFSGDPL...	VKGIK.....GFEAEFIKSKFSFNLRKPSVQWSDTAEYFC	AVN.....
AE000659,TRAV8-2	AQSVTQLDSHVSVSEGTPVLLRCNYS	SSYSPS.....	LFWYVQHPNKGLQLLLK	YTSAATL...	VKGIN.....GFEAEFKKSETSFHLTKPSAHMSDAAEYFC	VVS.....
AE000659,TRAV8-3	AQSVTQPDIHITVSEGASLELRCNYS	YGATPY.....	LFWYVQSPGQGLQLLLK	YFSGDTL...	VQGIK.....GFEAEFKRSQSSFNLRKPSVHWSDAAEYFC	AVG.....
AE000659,TRAV8-4	AQSVTQLGSHVSVSEGALVLLRCNYS	SSVPPY.....	LFWYVQYPNQGLQLLLK	YTSAATL...	VKGIN.....GFEAEFKKSETSFHLTKPSAHMSDAAEYFC	AVS.....
X02850 ,TRAV8-6	AQSVTQLDSQVPVFEEAPVELRCNYS	SSVSVY.....	LFWYVQYPNQGLQLLLK	YLSGSTL...	VESIN.....GFEAEFNKSQTSFHLRKPSVHISDTAEYFC	AVS.....
AE000660,TRAV8-7	TQSVTQLDGHITVSEEAPLELKCNYS	YSGVPS.....	LFWYVQYSSQSLQLLLK	DLTEATQ...	VKGIR.....GFEAEFKKSETSFYLRKPSTHVSDAAEYFC	AVGDR.....
AE000659,TRAV9-1	GDSVWQTFGQWLPSEGDSLIWNCSYE	TTQYPS.....	LFWYVQYPGEGPQLHLK	AMKAND....	KGRNK.....GFEAMYRKETTSFHLEKDSVQFSDSAVYFC	ALS.....

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

IMGT/3Dstructure-DB and IMGT/2D...

WELCOME!
to IMGT/3Dstructure-DB and IMGT/2Dstructure-DB

THE
INTERNATIONAL
IMMUNOGENETICS
INFORMATION SYSTEM®

http://www.imgt.org

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

Programm version: 4.8.0 (06/10/2011) **Database release:** 201142-3 (19/10/2011)

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 Tuesday, November 15 2011
IMGT/3Dstructure-DB contains 2644 entries
2181 entries PDB
128 entries INN
335 entries Kabat

IMGT 3Dstructure-DB Query Page

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

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

Search Clear

Search for complexes

Paratope/epitope	IG/Ag TR/pMH1 TR/pMH2 RPI/pMH1 RPI/pMH2
Peptide/MH	pMH1 pMH2
Ligand category	any
Peptide length	any

Terminé zotero

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

IMGT/3Dstructure-DB and IMGT/2D...

Search by IMGT entry type using IMGT-ONTOLOGY concepts

IMGT entry type ○ PDB ○ INN ○ Kabat ○ any

IDENTIFICATION

Species any

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

Options: ○ MH1 ○ MH2 ○ RPI-MH1Like

DESCRIPTION

IMGT receptor description any

Options: ○ FV ○ SCFV ○ FAB ○ FC

IMGT chain description any

IMGT domain description any

CLASSIFICATION

IMGT group any

IMGT subgroup any

IMGT gene any

IMGT allele

Search Clear

Terminé zotero

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

IMGT/3Dstructure-DB and IMGT/2D...

Search by Resolution, Release date or Experimental method

Resolution | Release date | Experimental method

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

Terminé

zotero

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

IMGT/3Dstructure-DB and IMGT/2D...

Display results

Overview

- [x] IMGT entry ID
- [x] IMGT entry type
- [x] IMGT molecule name
- [x] Species
- [x] IMGT receptor description
- [x] Ligand(s)
- [ ] Gene(s) and Allele(s)
- [x] Experimental technique
- [x] PDB release date
- [x] 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

Terminé

zotero

IMGT/3Dstructure-DB Overview

http://www.imgt.org

IMGT/3Dstructure-DB Results - Mozilla Firefox

IMGT/3Dstructure-DB Results

THANK YOU

for using IMGT/3Dstructure-DB and IMGT/2Dstructure-DB

THE
INTERNATIONAL
IMMUNOGENETICS
INFORMATION SYSTEM®

http://www.imgt.org

Overview

Entry code Search

Your query: Receptor description FAB-GAMMA-1_KAPPA

Query page

Number of results: 614

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 tec
1	12e8	2E8	PDB	FAB-GAMMA-1_KAPPA	*Mus musculus*		X-ray diffraction
2	15c8	5C8	PDB	FAB-GAMMA-1_KAPPA	*Mus musculus*		X-ray diffraction
3	1a0q	29G11	PDB	FAB-GAMMA-1_KAPPA	*Mus musculus*		X-ray diffraction
4	1a3l	13G5	PDB	FAB-GAMMA-1_KAPPA	*Mus musculus*		X-ray diffraction
5	1a4j	39-A11	PDB	FAB-GAMMA-1_KAPPA	*Chimeric*		X-ray diffraction
6	1a4k	39-A11	PDB	FAB-GAMMA-1_KAPPA	*Chimeric*		X-ray diffraction
7	1a5f	7A9	PDB	FAB-GAMMA-1_KAPPA	*Mus musculus*		X-ray diffraction
8	1acy	59.1 mAb, anti-gp120 [HIV-1]	PDB	FAB-GAMMA-1_KAPPA	*Mus musculus*		X-ray diffraction
9	1ae6	Ctm01	PDB	FAB-GAMMA-1_KAPPA	*Mus musculus*		X-ray diffraction
10	1afv	25.3 mAb, anti-p24 [HIV-1]	PDB	FAB-GAMMA-1_KAPPA	*Mus musculus*		X-ray diffraction
11	1ahw	5G9	PDB	FAB-GAMMA-1_KAPPA	*Mus musculus*		X-ray diffraction
12	1ai1	59.1	PDB	FAB-GAMMA-1_KAPPA	*Mus musculus*		X-ray diffraction
13	1aif	409.5.3	PDB	FAB-GAMMA-1_KAPPA	*Mus musculus*		X-ray diffraction
14	1aj7	48G7	PDB	FAB-GAMMA-1_KAPPA	*Chimeric*		X-ray diffraction
15	1axs	AZ-28-chimeric	PDB	FAB-GAMMA-1_KAPPA	*Chimeric*		X-ray diffraction
16	1b2w	Anti-Gamma-Interferon	PDB	FAB-GAMMA-1_KAPPA	*Humanized*		X-ray diffraction
17	1b4j	Anti-Gamma-Interferon	PDB	FAB-GAMMA-1_KAPPA	*Chimeric*		X-ray diffraction

Terminé zotero

IMGT/3Dstructure-DB Card (1)

http://www.imgt.org

IMGT/3Dstructure-DB card - Mozilla Firefox

Fichier Édition Affichage Historique Marque-pages Outils ?

http://www.imgt.org/3Dstructure-DB/cgi/details.cgi?pdbcode=1AO7

google translation

IMGT/3Dstructure-DB card

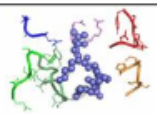
THANK YOU

for using IMGT/3Dstructure-DB and IMGT/2Dstructure-DB

THE
INTERNATIONAL
IMMUNOGENETICS
INFORMATION SYSTEM®

http://www.imgt.org

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		*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_2]
		Ion			1	[1ao7_1]

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

Rechercher : 1ao Suivant Précédent Surligner tout Respecter la casse Phrase non trouvée

Terminé zotero

IMGT/3Dstructure-DB Card (2)

http://www.imgt.org

IMGT/3Dstructure-DB card - Mozilla Firefox

http://www.imgt.org/3Dstructure-DB/cgi/details.cgi?pdbcode=1AO7

IMGT/3Dstructure-DB card

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] NAGVTQTPKFQVLKTGQSMTLQCAQDMNHEYMSWYRQDPGMGLRLIHYSVGAGITDQGEVPNGYNVSRSTTEDFPLRLLSAAPSQTSVYF](N-D)-REG[J-REGION][C-BETA-2 (11 CASRPGLAGGRPEQYFGPGTRLTVTEDLKNVFPPEVAVFEPSEAEISHTQKATLVCLATGFYPDHVELSWWVNGKEVHSGVSTDPQPLKE 4-208) [D2]] QPALNDSKYALSSRLRVSATFWQNPRNHFRCQVQFYGLSENDEWTQDRAKPVTQIVSAEAWGRAD 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]
		[CDR1] [CDR2] NAGVTQTPKFQVLKTGQSMTLQCAQDMNH.....EYMSWYRQDPGMGLRLIHYSVG....AGITDQGEVP.NGYNVSRS.TTEDFPLR [CDR3] LLSAAPSQTSVYFCASRPGLAGGRPEQYFGPGTRLTVT IMGT/DomainGapAlign results
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..TQKATLVCLATGFYP..DHVELSWWVNGKEVHS..GVSTDPQPLKEQPAL.NDSKYALSSRLRV SATFWQ.NPRNHFRCQVQFYGLSENDEWTQDRAKPVTQIVSAEAWGRA IMGT/DomainGapAlign results

Rechercher : 1ao Suivant Précédent Surligner tout Respecter la casse Phrase non trouvée

Terminé zotero

IMGT/3Dstructure-DB Contact Analysis

IMGT/3Dstructure-DB card - Mozilla Firefox

http://www.imgt.org/3Dstructure-DB/cgi/details.cgi?pdbcode=1AO7&Part=CONT_OVERVIEW

google translation

IMGT/3Dstructure-DB card

Contact analysis

Chain and domains of 1ao7

IMGT molecule name	IMGT receptor description	Chain ID	IMGT chain description	Species	Domain number	IMGT domain description
A6	TR-ALPHA_BETA-2	1ao7_D	TR-ALPHA	*Homo sapiens* (human)	[D1]	V-ALPHA
					[D2]	C-ALPHA
		1ao7_E	TR-BETA-2	*Homo sapiens* (human)	[D1]	V-BETA
					[D2]	C-BETA-2
HLA-A*0201	MH1-ALPHA_B2M	1ao7_A	I-ALPHA	*Homo sapiens* (human)	[D1]	G-ALPHA1
					[D2]	G-ALPHA2
					[D3]	C-LIKE
		1ao7_B	B2M	*Homo sapiens* (human)	[D1]	C-LIKE
Tax peptide 11-19 (Q82235)	Peptide	1ao7_C	Peptide	(Human T lymphotropic virus type 1)		
Ethyl Mercury Ion	Ion	1ao7_2	Ion			
Ethyl Mercury Ion	Ion	1ao7_1	Ion			

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

Rechercher : 1ao Suivant Précédent Surligner tout Respecter la casse Phrase non trouvée

Terminé zotero

IMGT/3Dstructure-DB Domain pair contacts

IMGT/3Dstructure-DB card - Mozilla Firefox

http://www.imgt.org/3Dstructure-DB/cgi/details.cgi#results

IMGT/3Dstructure-DB card

IMGT/3Dstructure-DB Domain pair contacts

Contacts of Domain Chain [D1] V-ALPHA 1ao7_D *with* Domain Chain (Ligand) 1ao7_C

Summary:

Residue pair contacts	Number of residues			Atom pair contact types						
	Total	From 1	From 2	Total	Noncovalent	Polar	Hydrogen	Nonpolar	Covalent	Disulfide
15	13	7	6	109	109	20	3	89	0	0

List of the Residue@Position pair contacts:

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

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

Display:

Atom pair contact types

- ☑ Noncovalent
- ☑ Polar
- ☑ Hydrogen bond
- ☑ Nonpolar
- ☑ Covalent
- ☑ Disulfide
- ○ Check all
- ○ Uncheck all

Atom pair contact categories

- ☐ (BB) Backbone/backbone
- ☐ (SS) Side chain/side chain
- ☐ (BS) Backbone/side chain
- ☐ (SB) Side chain/backbone
- ○ Check all
- ○ Uncheck all

Show

Terminé

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

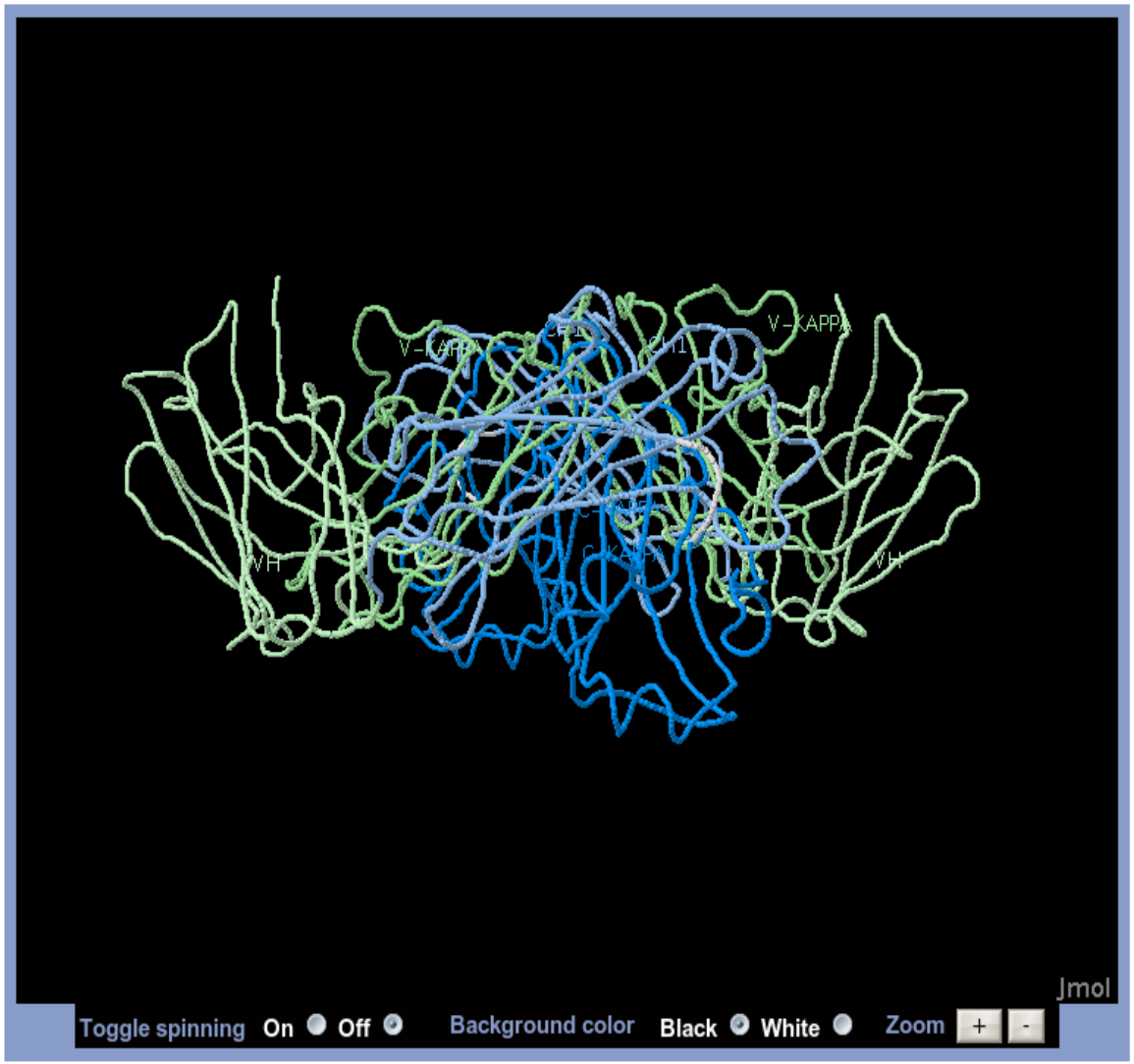
Number of covalent links

Disulfide

Number of disulfide bridges

IMGT/3Dstructure-DB Visualization

http://www.imgt.org



Selection

Predefined ensemble: All, Backbone, Sidechain, Water

IMGT receptor type: any

Chain ID: any

IMGT domain description: any

CDR type: Choose

Reset

View

wireframe, spacefill, dots, ribbons, cartoon, trace structure, meshribbon, rocket, off

Disulfide bridges: On, Off

Coloration

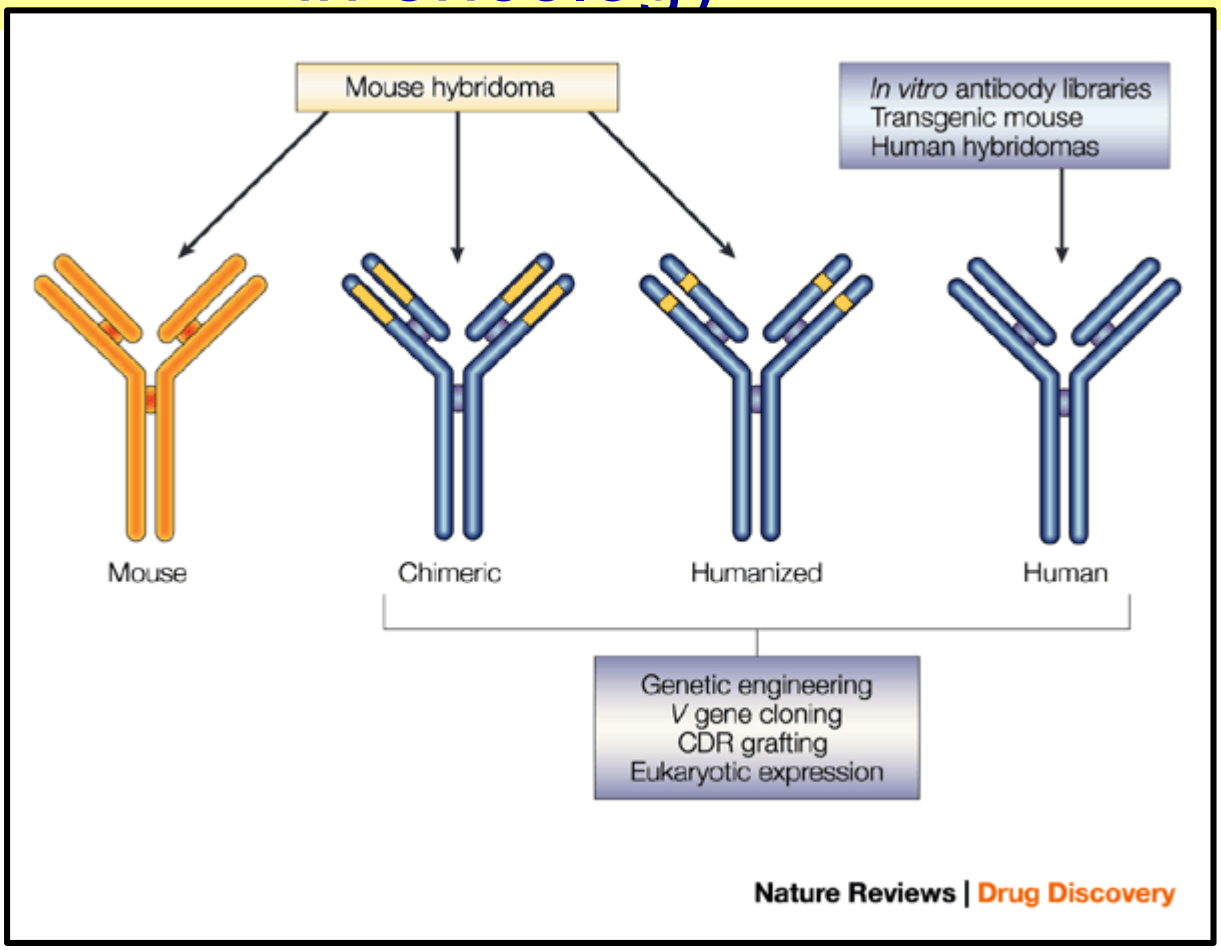
amino acid type, cpk, chain, charge, structure, green, red, yellow, blue, purple

IMGT

CDR-IMGT labels, CDR-IMGT only (side view), Domain description, Complex colored by chains and CDRs

Chimeric and humanized antibodies: application in oncology

http://www.imgt.org



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.

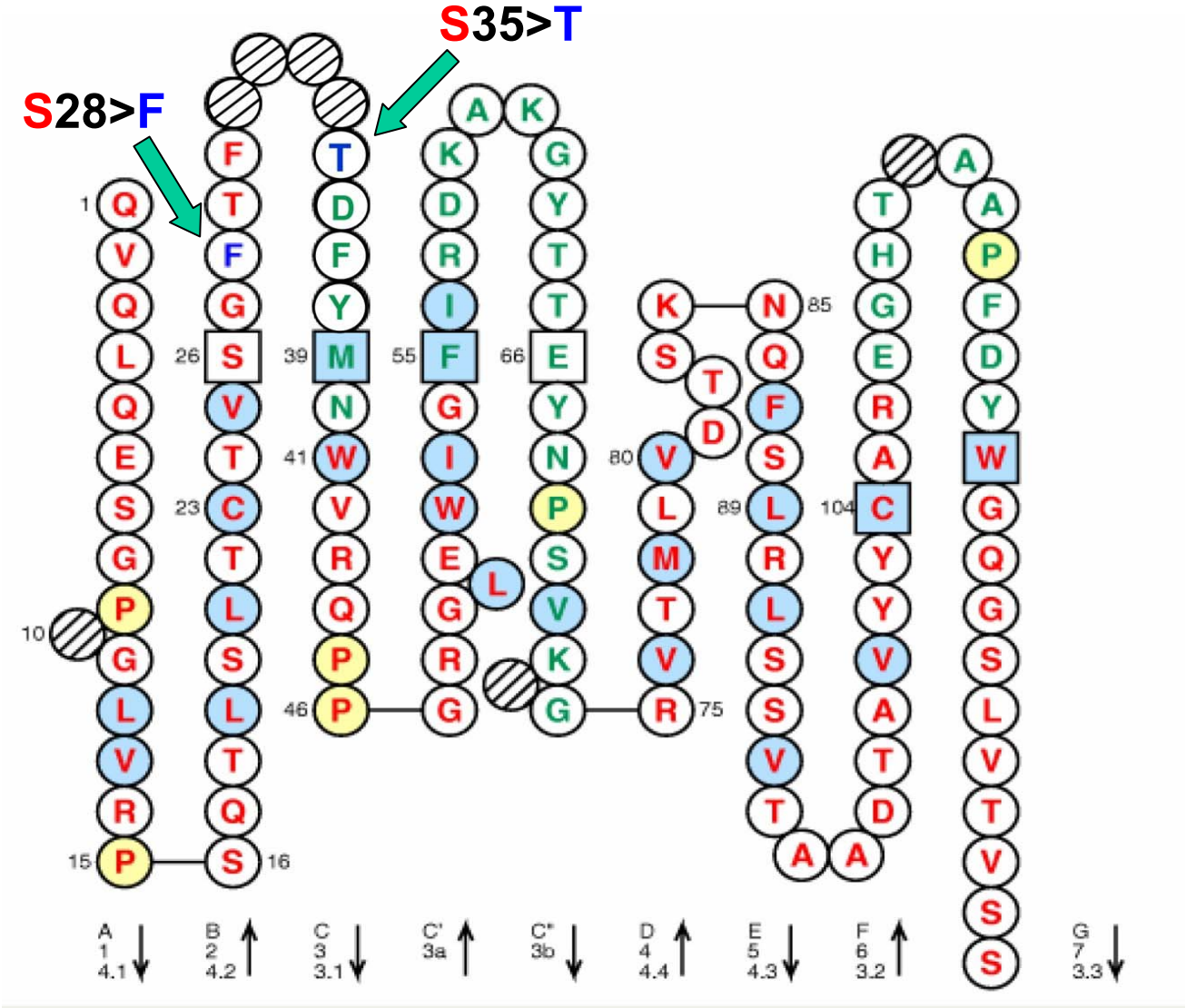
Une chaîne humanisée est une chaîne dans laquelle les CDR des domaines variables sont étrangers (provenant d'une espèce autre que l'homme, ou de synthèse), alors que le reste de la chaîne est d'origine humaine.

Antibody humanization and engineering

Alemtuzumab (CAMPATH®)

http://www.imgt.org

2 mutations:



VH domain
[8.10.12]

human

rat

IMGT® http://www.imgt.org