

Structures en immunogénétique

Introduction

Master 2 STIC Santé, Université Montpellier 2
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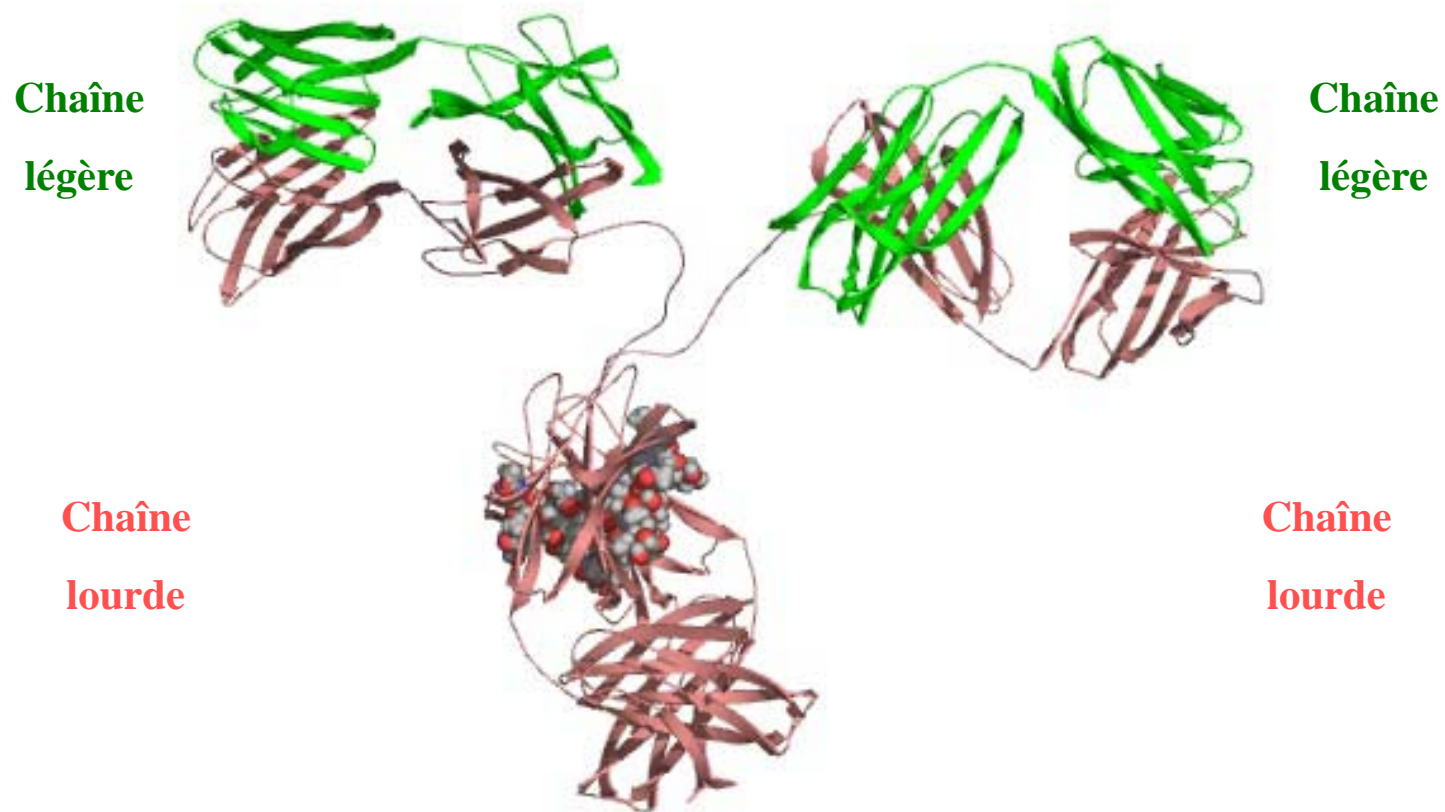
Immunogenetics and structure



<http://www.imgt.org>

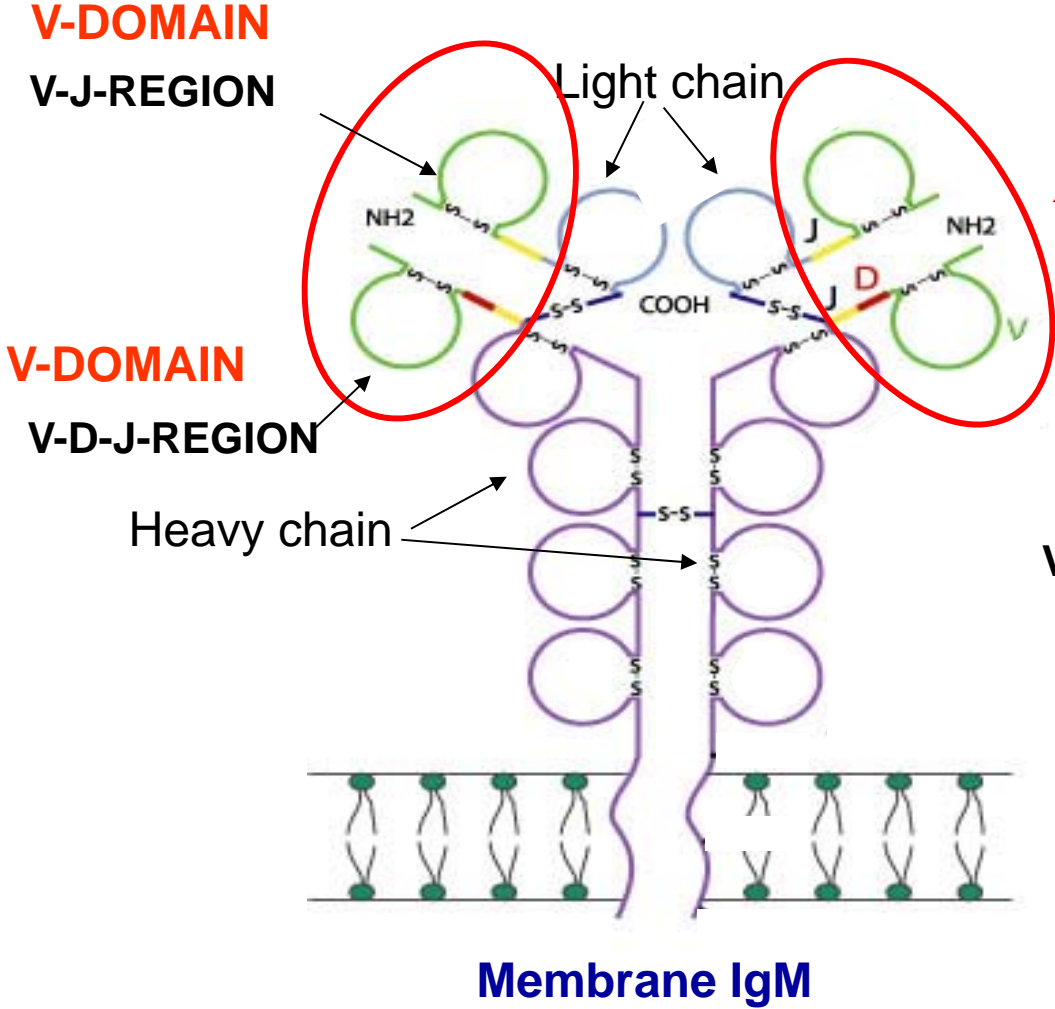
- Structures en immunogénétique
- Une base de données : **IMGT/3Dstructure-DB**
- IMGT unique numbering for V-DOMAIN, C-DOMAIN, G-DOMAIN
- IMGT Colliers de Perles (représentation 2D)
- Analyse des contacts
- Relations séquences-structures-fonctions
- Applications: ingénierie et humanisation des anticorps
=> consiste à remplacer les régions hypervariables (complementary determining region, CDR) d'un anticorps humain par des régions CDR d'origine murine.

Immunoglobulines (IG)

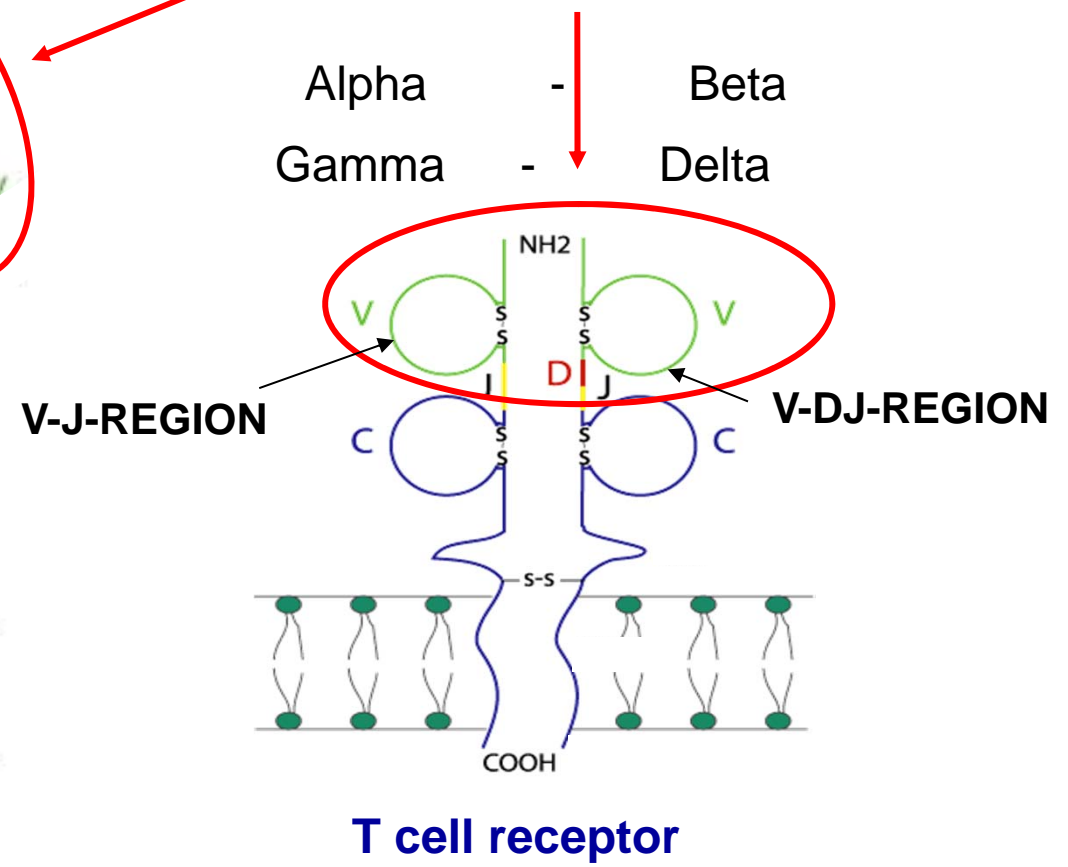


Immunoglobulin (IG)

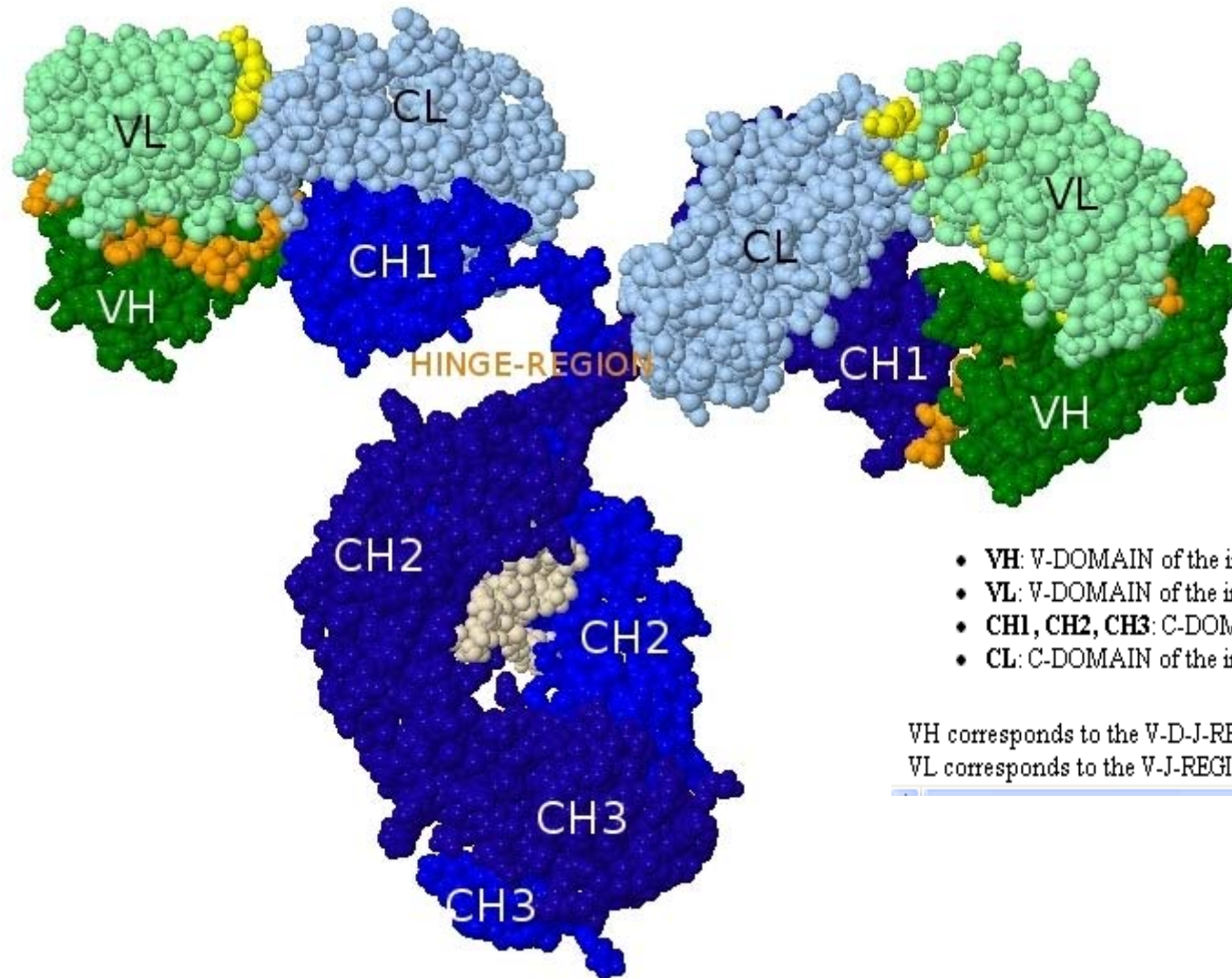
T cell receptor (TR)



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



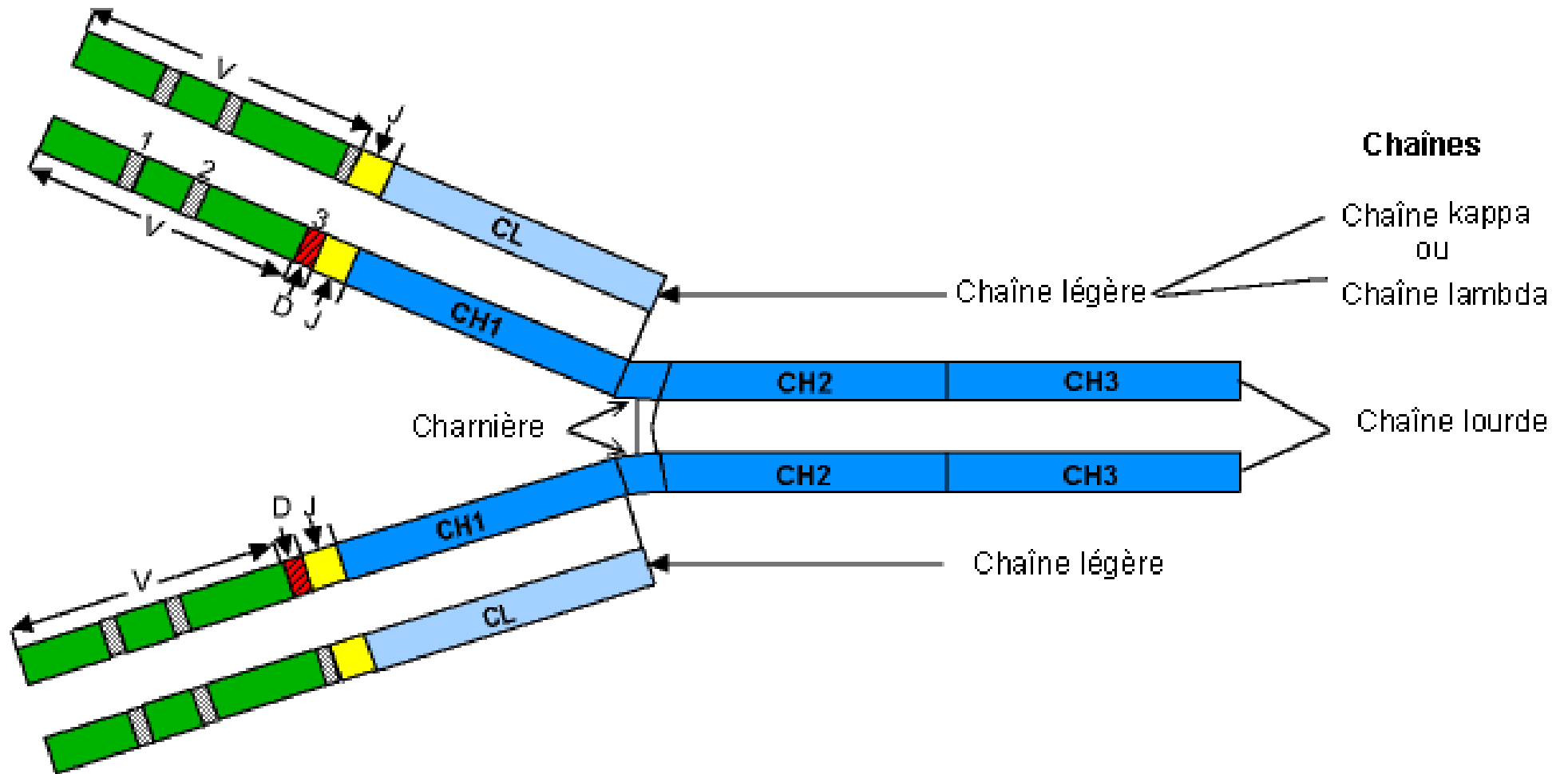
Immunoglobulins (IG) - Spacefill



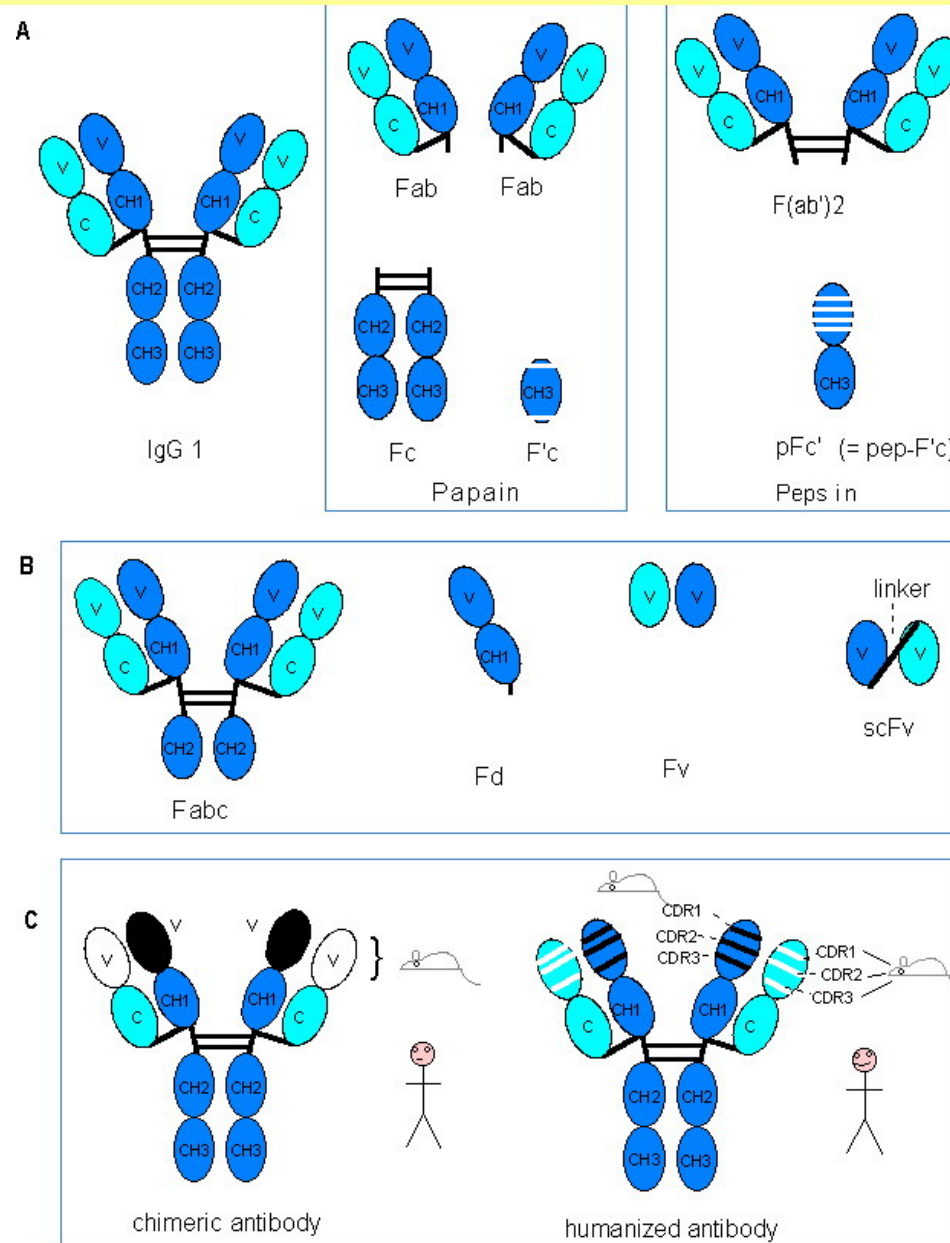
- **VH:** V-DOMAIN of the immunoglobulin heavy chain
- **VL:** V-DOMAIN of the immunoglobulin light chain
- **CH1, CH2, CH3:** C-DOMAIN of the immunoglobulin heavy chain
- **CL:** C-DOMAIN of the immunoglobulin light chain

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



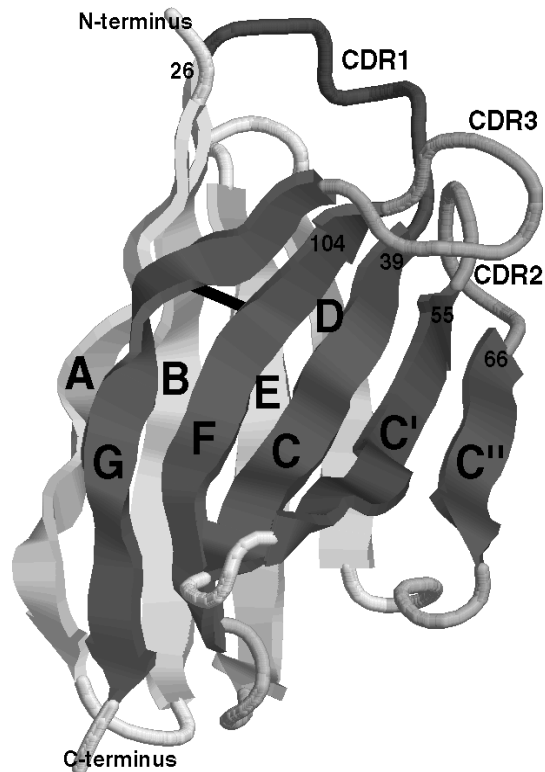
Organization in domains of an IgG1 immunoglobulin and of its fragments



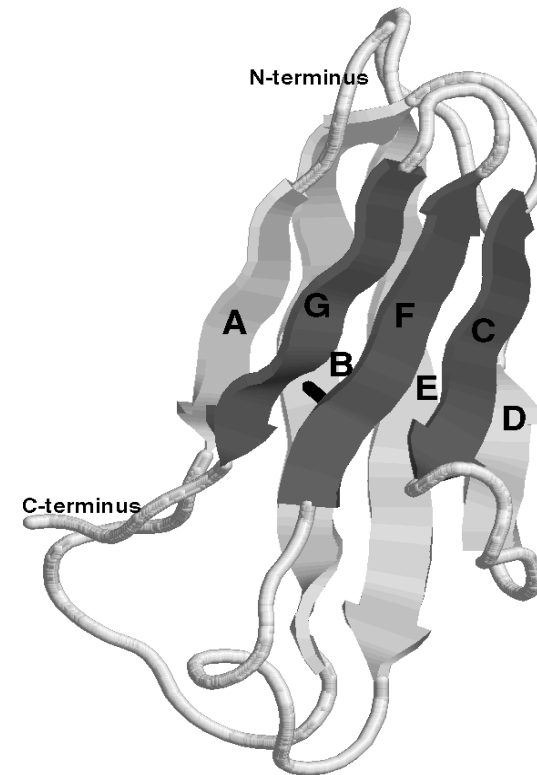
Structural domains

IG and TR

V-DOMAIN

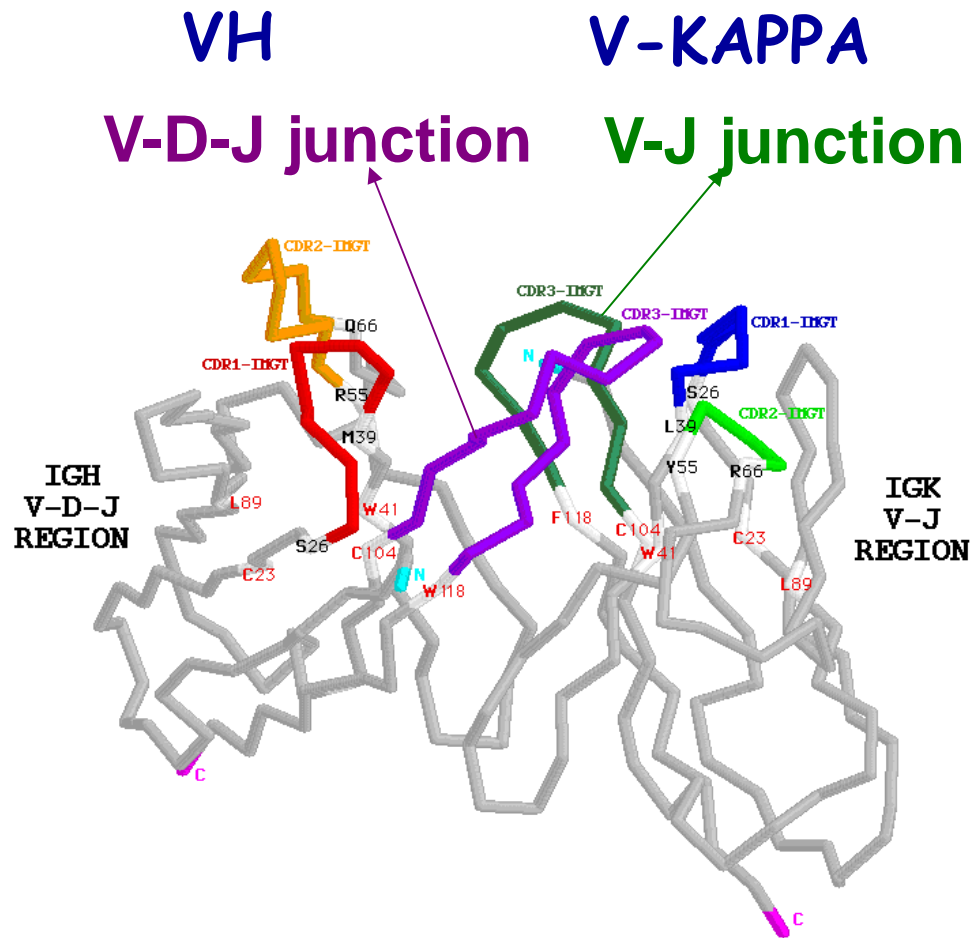


C-DOMAIN

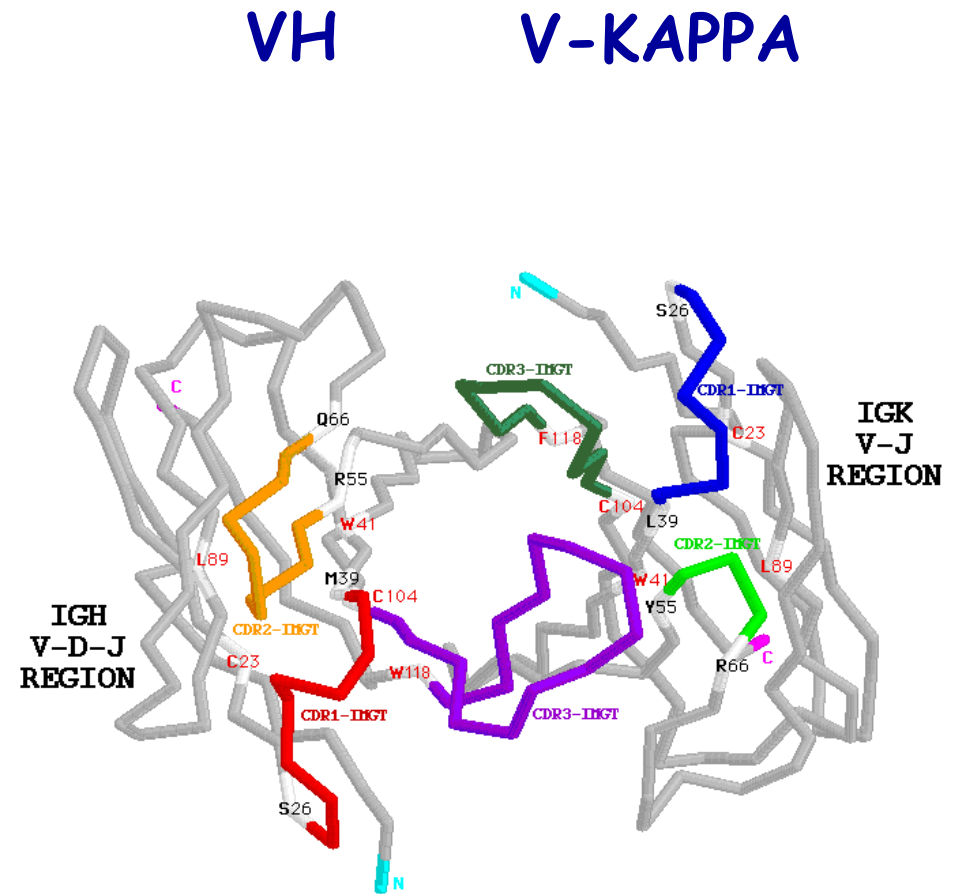


Le domaine d'IG est une structure de type sandwich bêta constituée de deux feuillets bêta antiparallèles. Les feuillets des V-DOMAINS possèdent respectivement 4 brins et 5 brins. Les V-DOMAINS possèdent trois boucles qui assurent la liaison avec un antigène. Ces boucles ou CDR (Complementarity Determining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

V-DOMAINS : VH and V-KAPPA



Side view of the V-DOMAINS



View from above the CDRs

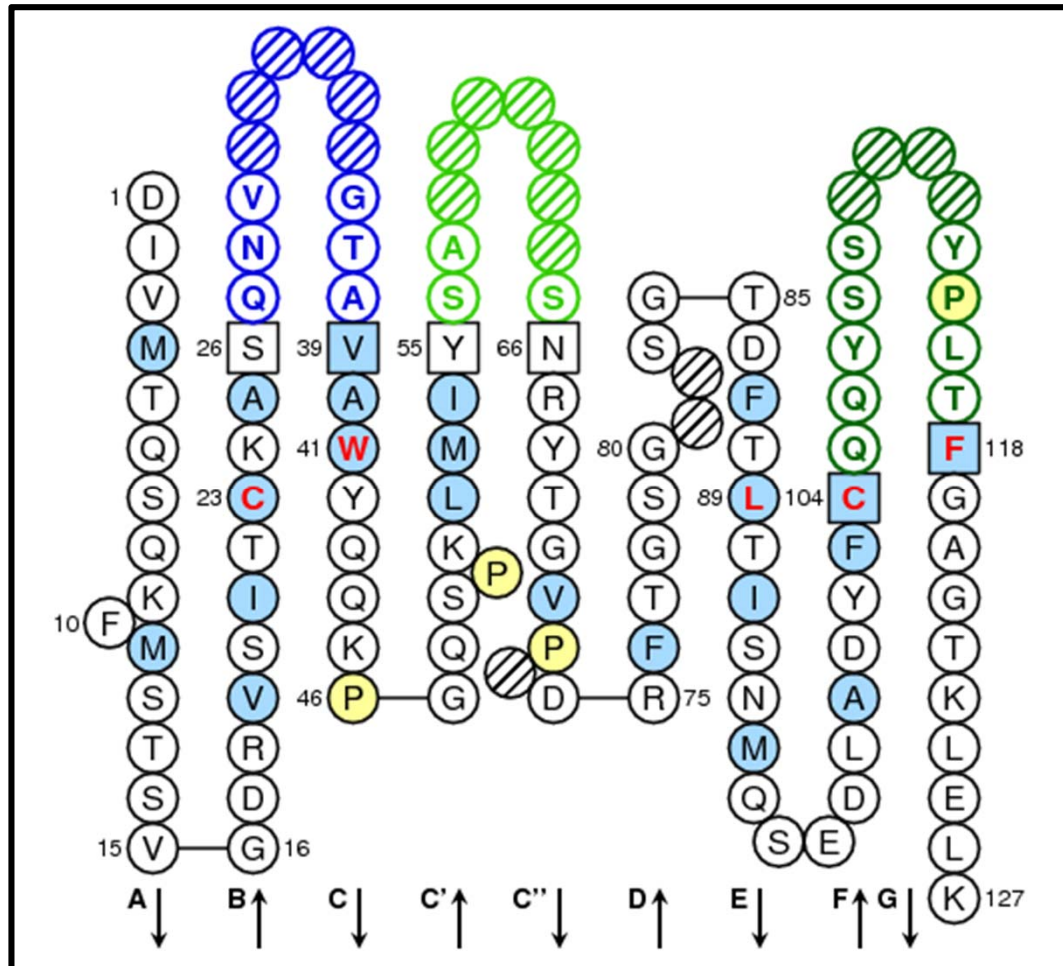
Mouse (Mus musculus) E5.2Fv

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

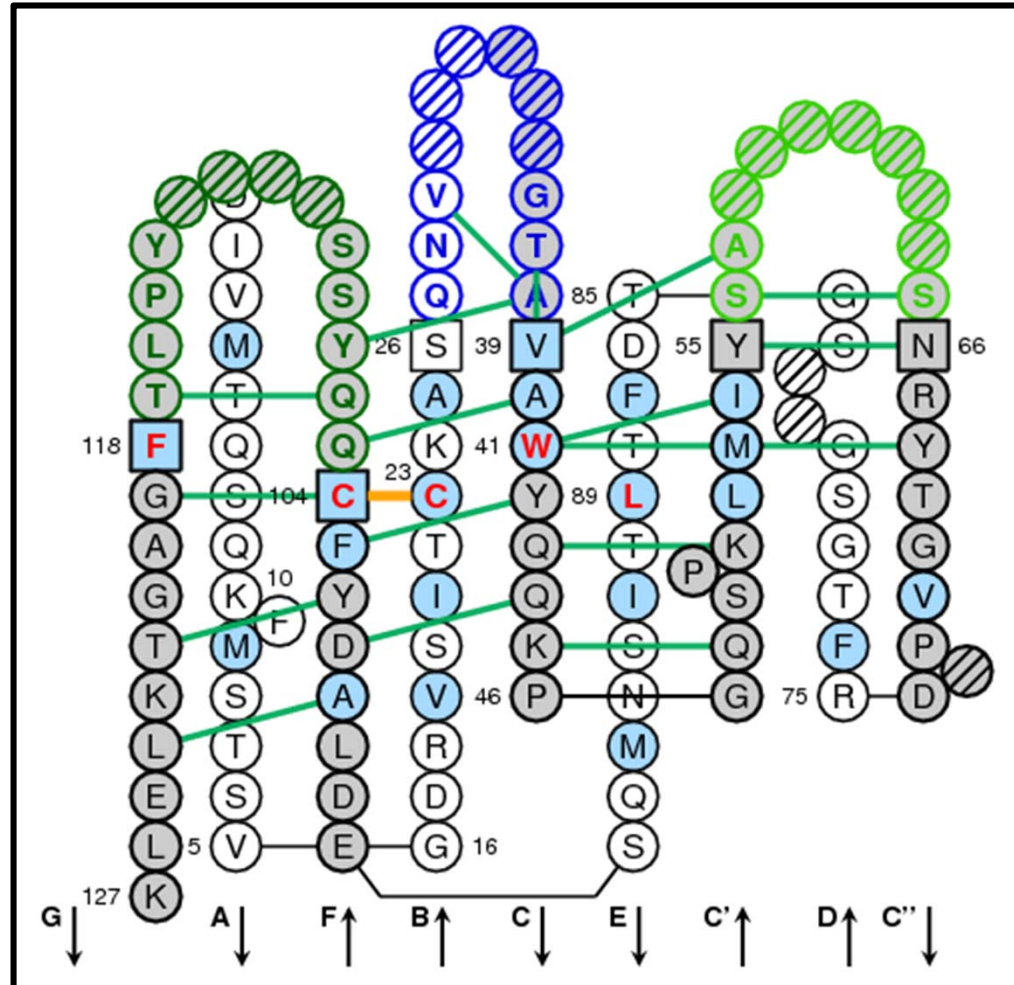
V-J junction (104-118)

V-D-J junction (104-118)

IMGT Collier de Perles for V-DOMAIN

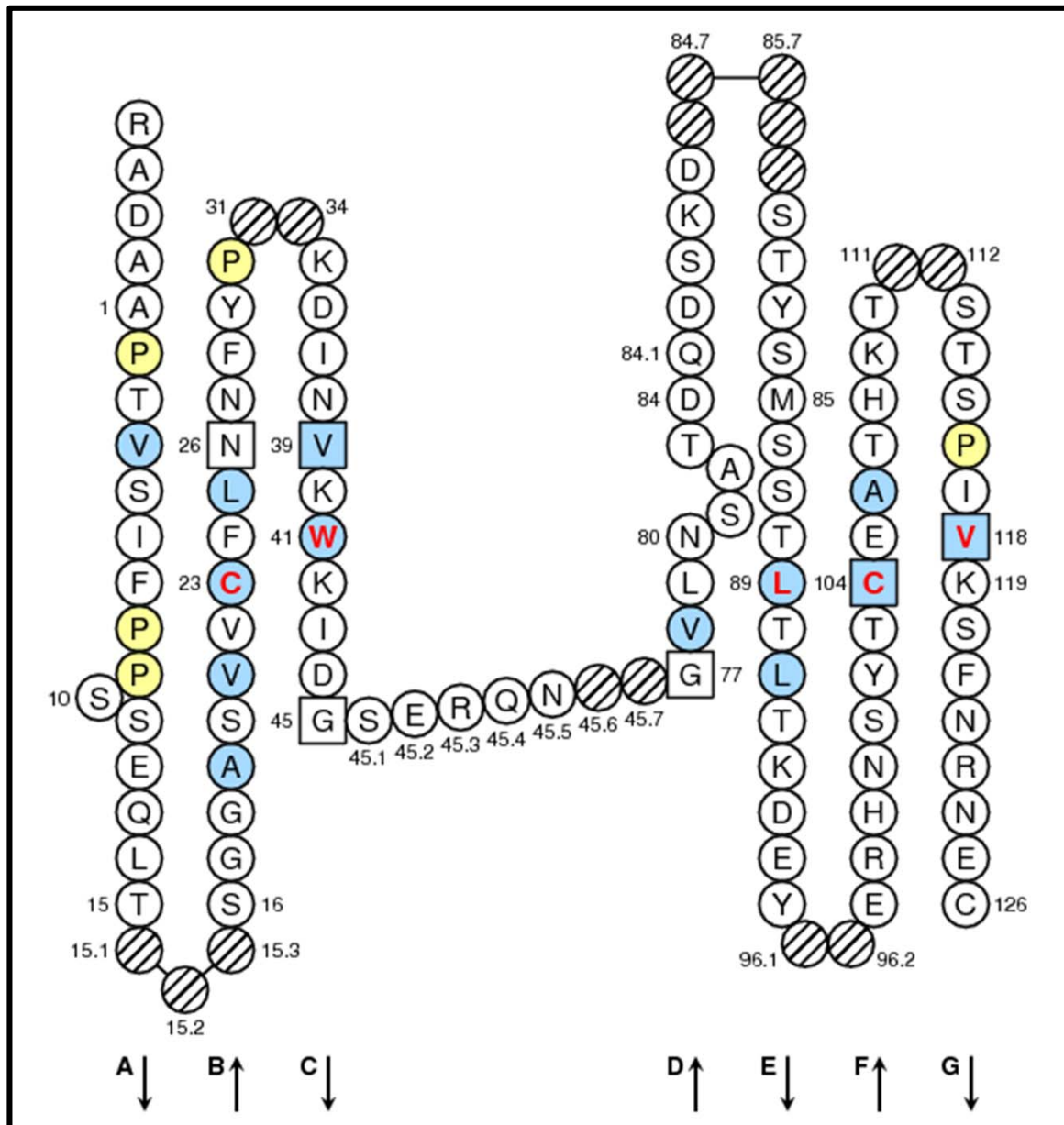


IMGT Collier de Perles for V-DOMAIN on two layers

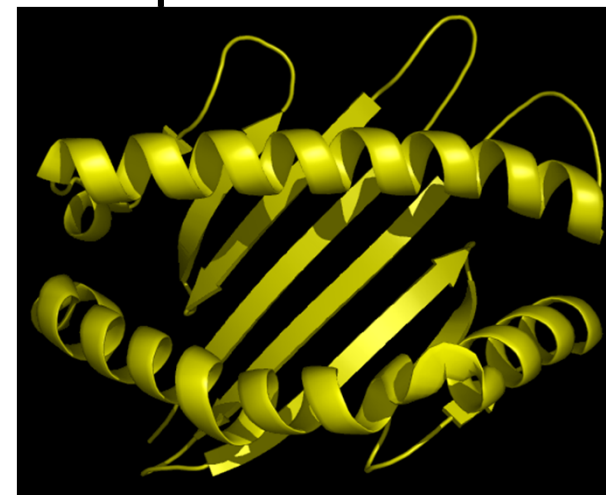
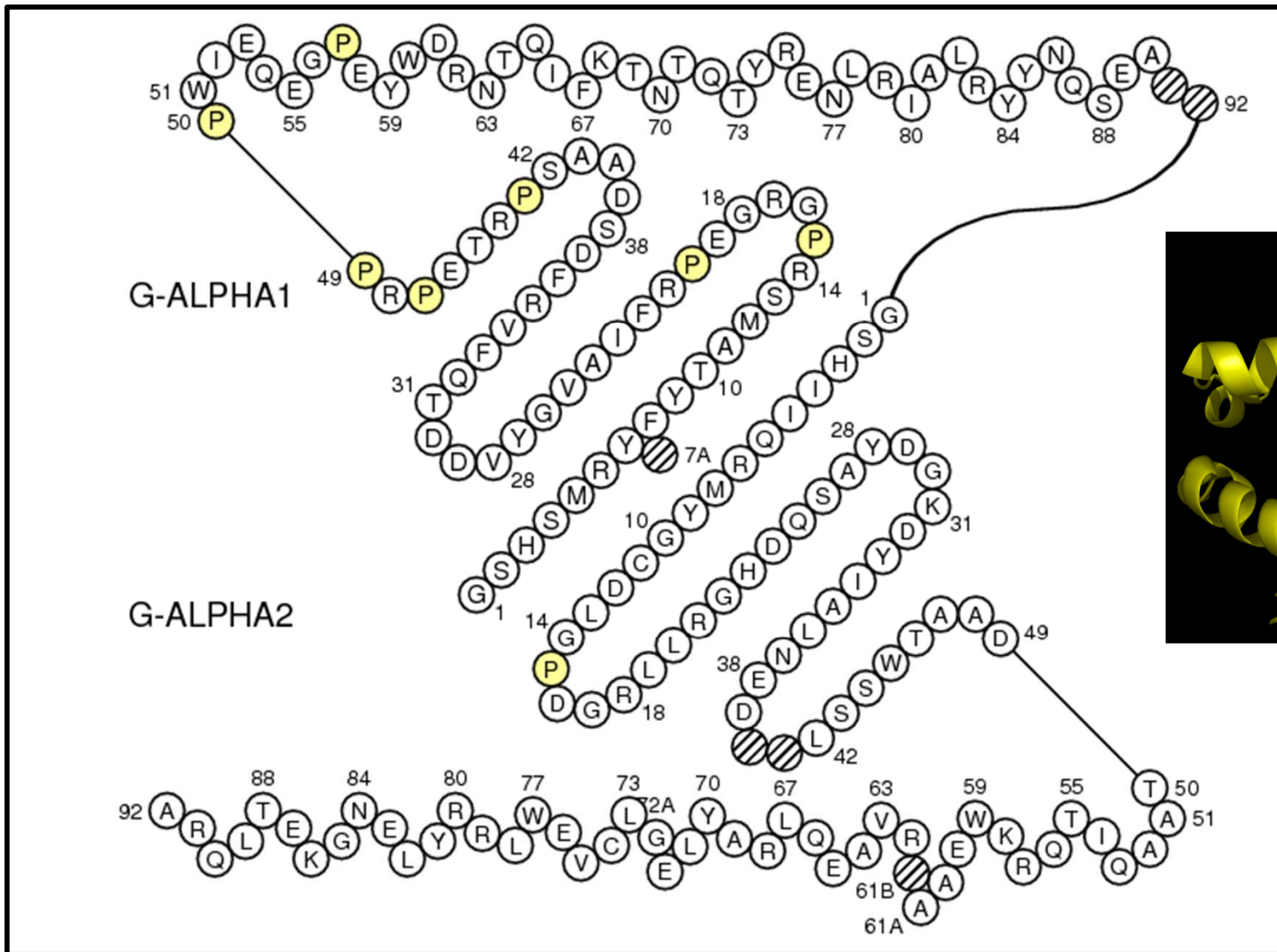


Hydrogen bonds between the amino acids of the C, C', C'', F and G strands and those of the CDR-IMGT

IMGT Collier de Perles for C-DOMAIN



IMGT Collier de Perles for G-DOMAIN

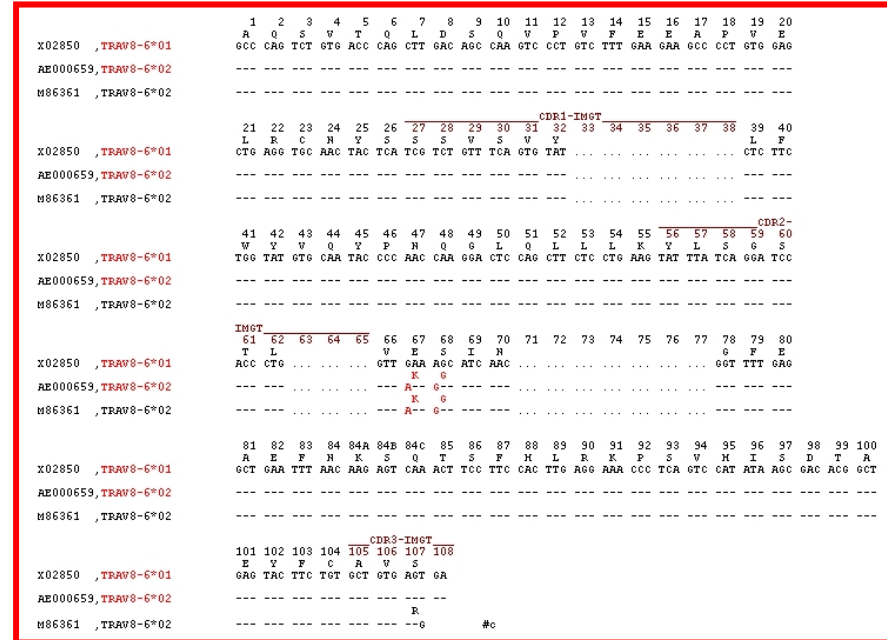
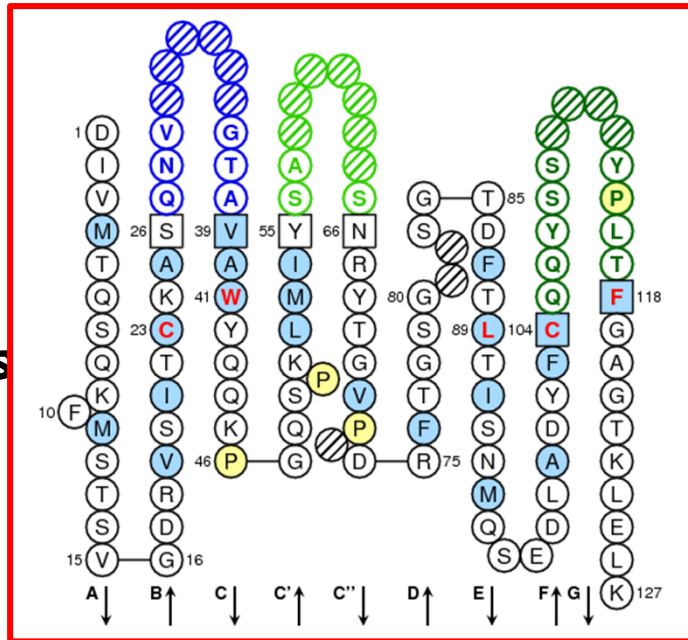


IMGT Web resources



<http://www.igmt.org>

IMGT
Collier
de Perles



IMGT
Alignment
of alleles

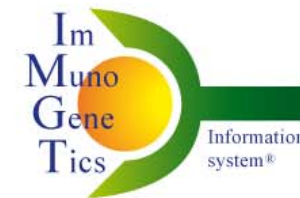
IMGT
Protein
Display

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.....	LSWYQQHGGAPITFLSY	NALDGL.....	LEETG.....	RFSSFLSRSDSYGYLLQLQMKDSASYFC
AE000658, TRAV1-2	GQNIIDQ.PTEMTATEGAIVQINCTYQ	TSGFNG.....	LFWYQQHAGEAPTFLSY	NVLDTG.....	LEEKG.....	RFSSFLSRKGYSLLLKELQMKDSASYLC
AE000658, TRAV2	KDQWFQ.PSTVASSEGAVVEIFCNHS	VSNAVY.....	FFWYHHPGCCAPRLLVK	GSK.....	PSQQG.....	RYNMTYER.FSSLLILQVREADAAVYFC
AE000658, TRAV3	AQSVAQPEDQVNVVAEGNPLTVKCTYS	VSGNPY.....	LFWYVQYPPRGLQLLLK	YITGDNL.....	VKGSY.....	GFEAEFNKSTSFHLKPKSALVSDASYFC
AE000658, TRAV4	LAKITQ.PISMSDYEGQEVNITCSHN	NIATNDY.....	ITWYQQPPSQGPRFIIQ	GYKT.....	KVINE.....	VASLFIPADRKSSSTLSLPRVSLSDTAVYFC
AE000659, TRAV5	GEDWEQS.LFLSVREGDSSVINCTYQ	DSSSTY.....	LYWKQEPGAGLQLLTY	IFSNMD.....	MKQDQ.....	RLTVLLNKKDKHLRLRIADTQTGDSAIYFC
AE000659, TRAV6	SQKIEQNSEALNIQEGKTATLTCNYT	NYSPAY.....	LQWYRQDPGRGPVFLLL	IRENEK.....	EKRKE.....	RLKVTFDITLTKQSLFHITASQPADSATYLC
AE000659, TRAV7	ENQVEHSPHFLGPQQGDVASMSTYS	VSRFNN.....	LQWYRQNTGMGPKHLLS	MYSAGY.....	EKQKG.....	RLNATLLK.NGSSLYITAVQPEDSATYFC
AE000659, TRAV8-1	AQSVSQNHVILSEAASLELGCNYS	YGGTVN.....	LFWYVQYPPRGLQLLLK	YFSGDPL.....	VKGIK.....	GFEAEFIKSKPSFLRKP SVQWSDTAEYFC
AE000659, TRAV8-2	AQSVTQLD SHVSVSECTPVLLRCNYS	SSYSPS.....	LFWYVQHPNKGLQLLLK	YTSAAITL.....	VKGIN.....	GFEAEFKKSETSFHLTKPSAHMSDAAEYFC
AE000659, TRAV8-3	AQSVTQPDIIHITVSEGASLELRCNYS	YGATPY.....	LFWYVQSPGQGLQLLLK	YFSGDITL.....	VQGIK.....	GFEAEFKRSQSSFLRKP SVHWSDAEYFC
AE000659, TRAV8-4	AQSVTQLGSHVSVSEGALVLLRCNYS	SSVPPY.....	LFWYVQYPPRGLQLLLK	YTSAAITL.....	VKGIN.....	GFEAEFKKSETSFHLTKPSAHMSDAAEYFC
X02850, TRAV8-6	AQSVTQLDSQVPVFEEAPVELRCNYS	SSVSZY.....	LFWYVQYPPRGLQLLLK	YLSGSTL.....	VESIN.....	GFEAEFNKSTSFHLRKP SVHISDTAEYFC
AE000660, TRAV8-7	TQSVTQLDGHITVSEEAPELEKCNYS	YSGVPS.....	LFWYVQYSSQLQLLLK	DLTEATQ.....	VKGIK.....	GFEAEFKKSETSFHLRKP STHVSDAAEYFC
AE000659, TRAV9-1	QNSVWQTFQGWV.PSFRQSLTVNDSYF	TDVQVS.....	LFWYVQYPPRGRDILHLK	AMKANN.....	KGRNK.....	GFFAMVYKFTTSPHLEKNSQVDFSDAVYFC

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

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IMGT 3Dstructure-DB Query Page



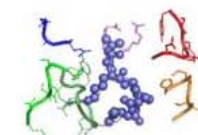
http://www.imgt.org

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

Version: version number [4.8.1](#) (05/03/2012) Database release: [201242-4](#) (2012-10-18)

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 20 2012
IMGT/3Dstructure-DB contains **2763** entries
2267 entries PDB
161 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 Clear

Search for complexes

Paratope/epitope I/Ag TR/pMH1 TR/pMH2 RPI/pMH1 RPI/pMH2

Peptide/MH pMH1 pMH2

Ligand category

Peptide length

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

• 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

Display results

Overview

- | | | | |
|---|---|--|--|
| <input checked="" type="checkbox"/> IMG/3Dstructure-DB entry ID | <input checked="" type="checkbox"/> IMG/2Dstructure-DB entry type | <input checked="" type="checkbox"/> IMG/3Dstructure-DB molecule name | <input checked="" type="checkbox"/> Species |
| <input checked="" type="checkbox"/> IMG/3Dstructure-DB receptor description | <input checked="" type="checkbox"/> Ligand(s) | <input type="checkbox"/> Gene(s) and Allele(s) | <input checked="" type="checkbox"/> Experimental technique |
| <input checked="" type="checkbox"/> PDB release date | <input checked="" type="checkbox"/> Resolution | <input type="checkbox"/> PDB references | <input type="checkbox"/> PubMed references |

Domain type sequences

- | | | | |
|--------------------------------|--------------------------------|--------------------------------|--------------------------------|
| <input type="radio"/> V domain | <input type="radio"/> C domain | <input type="radio"/> G domain | <input type="radio"/> S domain |
|--------------------------------|--------------------------------|--------------------------------|--------------------------------|

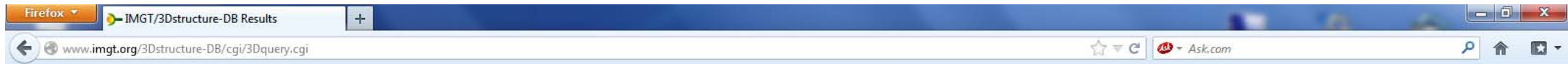
FR-IMG/3Dstructure-DB/CDR-IMG/2Dstructure-DB sequences and lengths

- | | | | |
|---|--|---|--|
| <input type="checkbox"/> FR1-IMG/3Dstructure-DB | <input type="checkbox"/> CDR1-IMG/2Dstructure-DB | <input type="checkbox"/> FR2-IMG/3Dstructure-DB | <input type="checkbox"/> CDR2-IMG/2Dstructure-DB |
| <input type="checkbox"/> FR3-IMG/3Dstructure-DB | <input type="checkbox"/> CDR3-IMG/2Dstructure-DB | | |

Search

Clear

IMGT/3Dstructure-DB Overview



THANK YOU

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

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Overview

Entry code Search

Your query: Receptor description **FAB-GAMMA-1_KAPPA**

[Query page](#)

Number of results: **632**

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
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	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	<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	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
17	1b4j	Anti-Gamma-Interferon	PDB	FAB-GAMMA-1_KAPPA	Chimeric		X-ray diffraction	2.9	15-JUN-99
18	1baf	An02	PDB	FAB-GAMMA-1_KAPPA	<i>Mus musculus</i>		X-ray diffraction	2.9	31-JAN-94
19	1bey	alemtuzumab, CAMPATH-1H, MABCAMPATH®	PDB	FAB-GAMMA-1_KAPPA	Humanized		X-ray diffraction	3.25	27-JAN-99
20	1bj1	bevacizumab Fab, 12-IgG1 Fab, F(ab)-12 IgG1, Fab-12 IgG1, rhuMAb-VEGF Fab, A/ASTIN®	PDB	FAB-GAMMA-1_KAPPA	Humanized		X-ray diffraction	2.4	13-JAN-99
21	1hm3	OPG2	PDB	FAB-GAMMA-1_KAPPA	<i>Mus musculus</i>		X-ray diffraction	2.00	14-FEB-00

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=1A07

IMGT/3Dstructure-DB card

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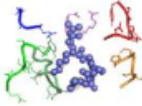
for using **IMGT/3Dstructure-DB and IMGT/2Dstructure-DB**

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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 11-18 (Q82235)	<i>Human T-lymphotropic virus 1</i>	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

Terminé

IMGT/3Dstructure-DB Card (2)

IMGT/3Dstructure-DB card - Mozilla Firefox
 http://www.imgt.org/3Dstructure-DB/cgi/details.cgi?pdbcode=1A07

Chain ID	1a07_E	
Chain length	245	
IMGT chain description	TR-BETA-2 = V-BETA (1-113) [D1] + C-BETA-2 (114-208) [D2]	
Chain sequence	<pre> [V-BETA (1-113) [D1] NAGVVTQTPKFOVLKLTGQSMTLQCAQDMNHEYMSWYRQDPGMGLRLLIHYSVGAGITDQGEVFNQYVNSRSTTEDFPLRLLSAAPSQTSVYF] (N-D) - REG [J-REGION] [C-BETA-2 (114-208) [D2] CASRPGLAGGRPEQYFGPGTRLTIVTEDLKNVFPPEVAVFE PSEAEI SHTQKATLVCLATGFPYDHVELSMMVNGKEVHSGVSTDPQLKE QPALNDSRYALSSRLRVSATFWQNFNHRFCQVQFYGLSENDEWTQDRAKPVTVQIVSAEAWGRAD </pre> <p>Sequence in FASTA format Sequence in IMGT format</p>	
V-DOMAIN	IMGT domain description	V-BETA (1-113) [D1]
	IMGT gene and allele name	TRBV8-5*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	[5.8.14]
	Sheet composition	[A' B D E] [A" C C' C" F G]
	<pre> [CDR1] [CDR2] NAGVVTQTPKFOVLKLTGQSMTLQCAQDMNH.....EYMSWYRQDPGMGLRLLIHYSVG....AGITDQGEVFNQYVNSRSTTEDFPLR [CDR3] LLSAAPSQTSVYFPCASRPGLAGGRPEQYFGPGTRLTIVT </pre> <p>IMGT/DomainGapAlign results</p>	
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]
		<pre> . EDLKNVFPPEVAVFE PSEAEI SH. . TQKATLVCLATGFPY. . DHVELSMMVNGKEVHS. . GVSTDPQLKEQPAL. NDSRYALSSRLRV SATFWQ. NPRNHRFCQVQFYGLSENDEWTQDRAKPVTVQIVSAEAWGRA </pre> <p>IMGT/DomainGapAlign results</p>

Rechercher : 1a07 SUIVANT PRECEDENT SYLIGNER TOUT RESPECTER LA CASSE PHRASE NON TROUVEE

Terminé zotero

IMGT/3Dstructure-DB Contact Analysis

IMGT/3Dstructure-DB card - Mozilla Firefox

http://www.imgt.org/3Dstructure-DB/cgi/details.cgi?pdbcode=1A07&Part=CONT_OVERVIEW

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	<i>Homo sapiens</i> (human)	[D1]	V-ALPHA
		1ao7_E	TR-BETA-2	<i>Homo sapiens</i> (human)	[D2]	C-ALPHA
HLA-A*0201	MH1-ALPHA_B2M	1ao7_A	I-ALPHA	<i>Homo sapiens</i> (human)	[D1]	V-BETA
		1ao7_B	B2M	<i>Homo sapiens</i> (human)	[D2]	C-BETA-2
		1ao7_C	Peptide	(Human T lymphotropic virus type 1)	[D3]	G-ALPHA1
Tax peptide 11-19 (Q82235)	Peptide	1ao7_C	Peptide	(Human T lymphotropic virus type 1)	[D1]	G-ALPHA2
Ethyl Mercury Ion	Ion	1ao7_2	Ion			C-LIKE
Ethyl Mercury Ion	Ion	1ao7_1	Ion			C-LIKE

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

Terminé

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				Atom pair contact types						
IMGT Num	Residue	Domain	Chain	IMGT Num	Residue	Domain	Chain	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 Covalent (BB) Backbone/backbone

Polar Disulfide (SS) Side chain/side chain

Hydrogen bond (BS) Backbone/side chain

Nonpolar (SB) Side chain/backbone

Check all Uncheck all

Check all Uncheck all

Show

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

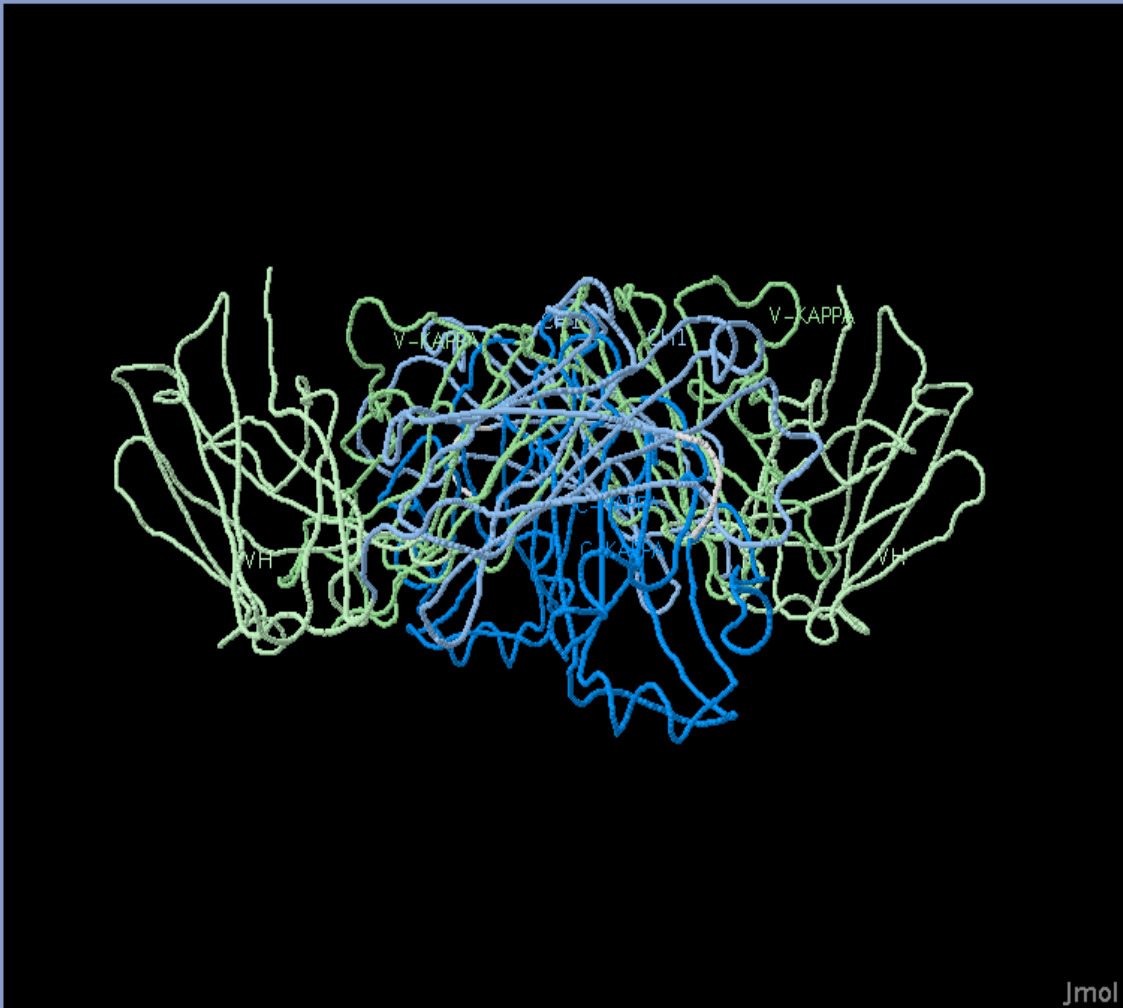
Covalent

Number of covalent links

Disulfide

Number of disulfide bridges

IMGT/3Dstructure-DB Visualization



Selection

Predefined ensemble All Backbone Sidechain Water

IMGT receptor type

Chain ID

IMGT domain description

CDR type

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

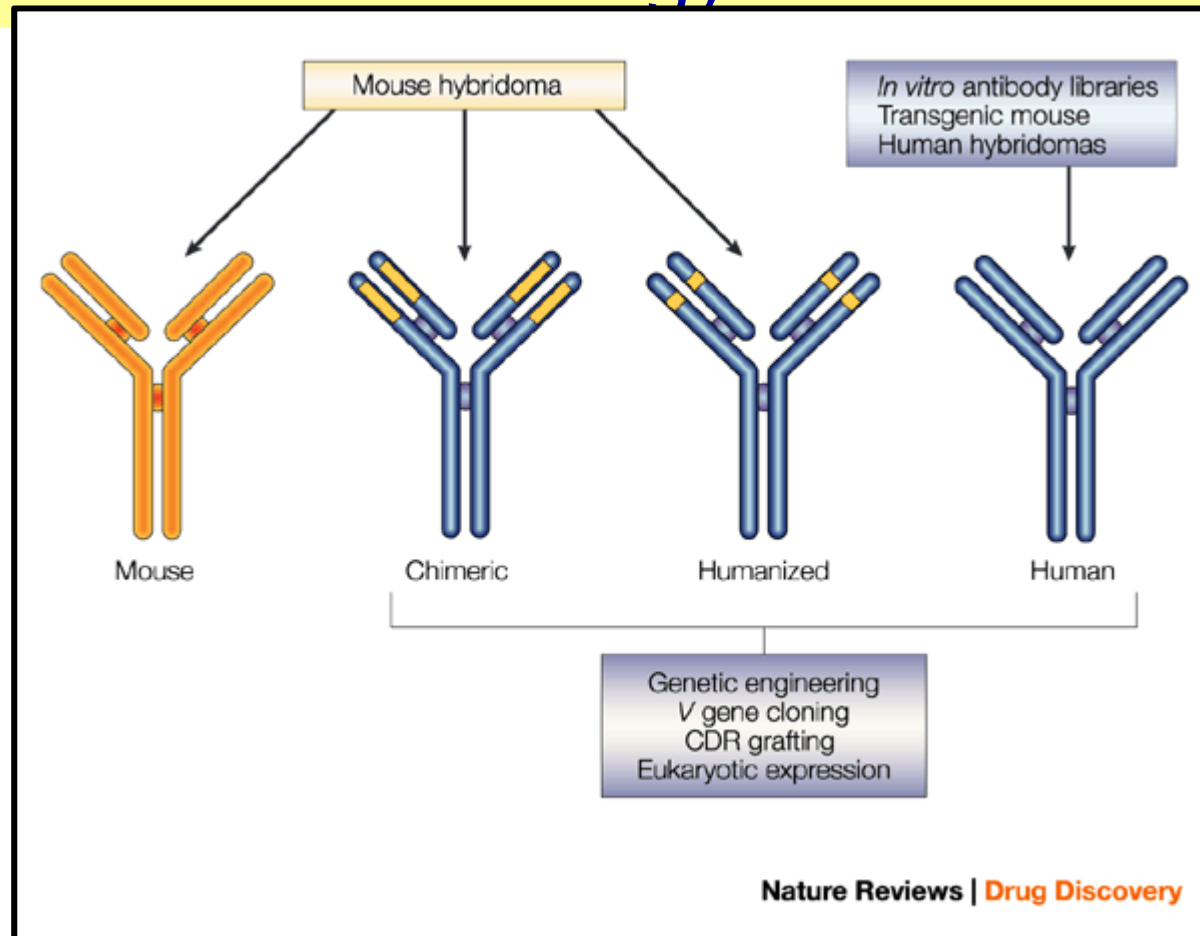
CDR-IMGT labels CDR-IMGT only (side view)

Domain description Complex colored by chains and CDRs

Toggle spinning On Off Background color Black White Zoom

Jmol

Chimeric and humanized antibodies: application in oncology



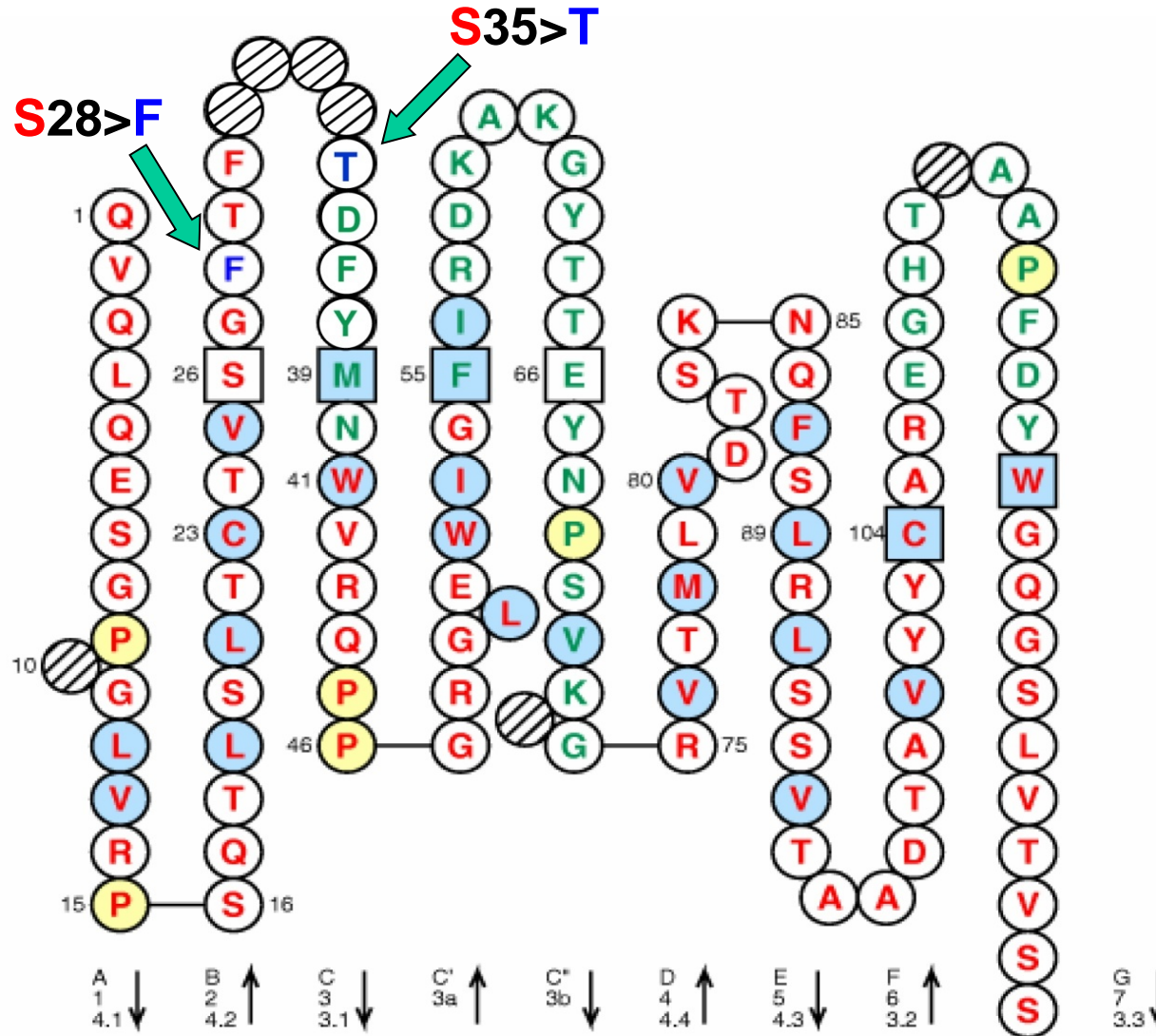
Une chaîne dite chimérique est une chaîne qui contient un domaine variable étranger (V-D-J-REGION) (provenant d'une espèce autre que l'homme, ou synthétiques) liées à une région constante (C-REGION) d'origine humaine.

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.

Antibody humanization and engineering

Alemtuzumab (CAMPATH®)

2 mutations:



VH domain
[8.10.12]

■ human
■ rat

THANK YOU

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

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INFORMATION SYSTEM®



http://www.imgt.org

Overview

Entry code Search

Your query: Entry type **INN**

Number of results: **161**

[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	Proposed
1	7164	daclizumab	INN	IG-GAMMA-1_KAPPA	Humanized	L78 (1997)
2	7602	infliximab, cA2, REMICADE®	INN	FV-HEAVY_KAPPA	Chimeric	L77 (1997)
3	7609	rituximab, IDEC-C2B8, RITUXAN®, MABTHERA®	INN	IG-GAMMA-1_KAPPA	Chimeric	L77 (1997)
4	7637	trastuzumab, 4D5-humanized variant 8, Herceptin, HERCEPTIN®	INN	IG-GAMMA-1_KAPPA	Humanized	L78 (1997)
5	7783	etanercept, TNFR-immunoadhesin, ENBREL®	INN	FUSION-TNFRSF1B-FC-GAMMA-1	Homo sapiens	L81 (1999)
6	7860	adalimumab, D2E7, LU200134, HUMIRA®	INN	FV-HEAVY_KAPPA	Homo sapiens	L82 (1999)
7	7906	cetuximab, IMC-225, Fab C225 [IgG1k], ERBITUX®	INN	IG-GAMMA-1_KAPPA	Chimeric	L82 (1999)
8	8005	alemtuzumab, CAMPATH-1H, LDP-03, MABCAMPATH®	INN	IG-GAMMA-1_KAPPA	Humanized	L83 (2000)
9	8017	bevacizumab, 12-IgG1, F(ab)-12 IgG1, Fab-12 IgG1, rhuMab-VEGF, AVASTIN®	INN	IG-GAMMA-1_KAPPA	Humanized	L83 (2000)
10	8039	omalizumab, IGE25, olizumab, rhuMab-E25	INN	IG-GAMMA-1_KAPPA	Humanized	L84 (2000)
11	8122	efalizumab, hu1124	INN	IG-GAMMA-1_KAPPA	Humanized	L85 (2001)
12	8313	ranibizumab, Fab-12 variant Y0317, RhuFab, LUCENTIS®	INN	FAB-GAMMA-1_KAPPA	Humanized	L90 (2004)
13	8380	pertuzumab, rhuMAB 2C4 OMNITARG™, PERJETA™	INN	FAB-GAMMA-1_KAPPA	Humanized	L89 (2003)
14	8394	tocilizumab, RO4877533	INN	IG-GAMMA-1_KAPPA	Humanized	L90 (2004)
15	8598	naptumomab estafenatox, ABR-217620, ANYARA, TTS CD3	INN	FAB-GAMMA-1-SAG_KAPPA	Mus musculus	L96 (2006)
16	8651	tadocizumab, C4G1, YM-337	INN	FAB-GAMMA-1_KAPPA	Humanized	L94 (2005)
17	8658	efungumab, HSP90mab, anti- Candida albicans heat shock protein 90 homolog , MYCOGRAB	INN	SCFV-HEAVY-KAPPA	Homo sapiens	L95 (2006)
18	8659	abagovomab, ACA125 MEN-2234	INN	IG-GAMMA-1_KAPPA	Mus musculus	L95 (2006)
19	8669	atacicept, TACI-Fc, TACI-Ig	INN	FUSION-TNFRSF13B-FC-GAMMA-1	Homo sapiens	L95 (2006)
20	8693	motavizumab, MEDI-524	INN	IG-GAMMA-1_KAPPA	Humanized	L95 (2006)
21	8734	haviximab, Tanvacin, ch3G4	INN	IG-GAMMA-1_KAPPA	Chimeric	L95 (2006)