Bioinformatique: du gène à la structure

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FMBS312, Master recherche 2 Bio-Med, TC3,
Universités Montpellier 1 et 2, ENSCM, 1 octobre 2009

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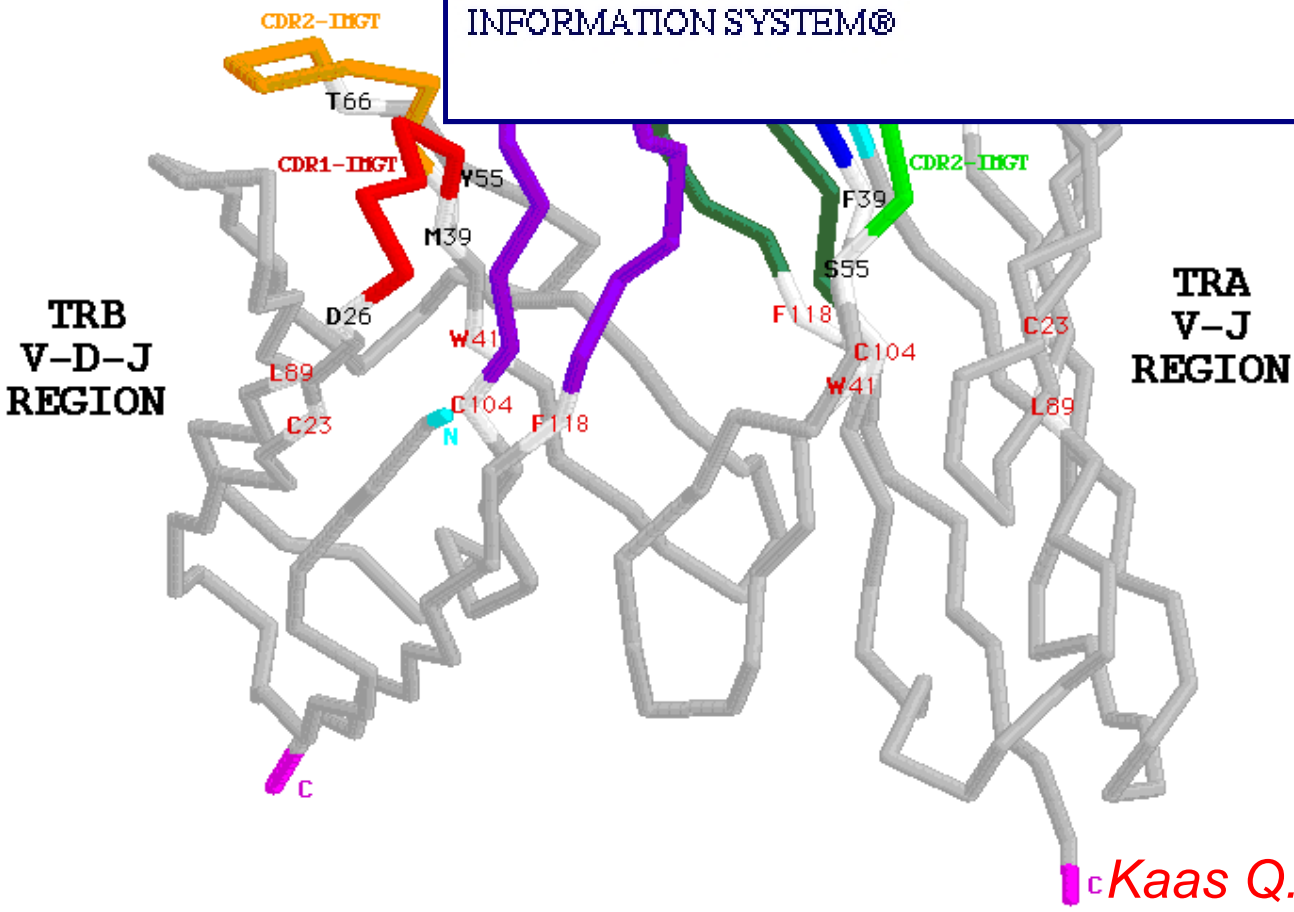

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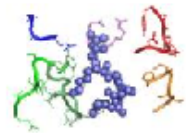
IMGT/3Dstructure-DB card for : 1ce1



Entry code [ ] Search

Query page

IMGT protein name	IMGT receptor type	IMGT receptor description	Ligand(s)	Species	CC	Chain ID
CAMPATH-1H, alemtuzumab, MABCAMPATH®	IG	FAB-GAMMA-1_KAPPA		Humanized	1	[1ce1_H 1ce1_L]
		Peptide	CD52 (synthetic peptide)	Synthetic	1	[1ce1_P]

Experimental technique X-ray diffraction Resolution (in angstrom) 1.90 PDB release date 25-JUN-99

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

Contact analysis:

IMGT/3Dstructure-DB Domain pair contacts (overview) **of 1ce1**

Atom contact types

- ☐ Non covalent
- ☐ Covalent
- ☑ Polar
- ☐ Disulfide
- ☑ Hydrogen bond
- ☐ Non polar

Atom contact categories

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

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IMGT/3Dstructure-DB

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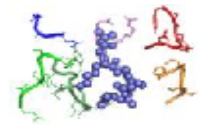
IMGT/3Dstructure-DB card for : 1u8k



IMGT protein name	IMGT receptor description	Type	Ligand(s)	Species	CC	Chain ID
2F5	FAB-GAMMA-3_KAPPA	IG		*Homo sapiens* (Human)	1	[1u8k_A 1u8k_B]
	Peptide		GP41		1	[1u8k_C]

Experimental technique X-ray diffraction Resolution 2.24 PDB release date 05-OCT-04

Chain ID	1u8k_B
IMGT chain description	VH-CH1
Chain amino acid sequence	[IGHV_1 RITLKESGPPLVKPTQTLTLTCSFSGFSLSDFGVGVGWIRQPPGKALEWLAIIYSDDDKRYSPSLNTRLTITKDTSKNQVVLVMTRVSPV][D][IGHJ_1] [IG DTATYFCAHRRGPTTLFGVPIARGPVNAMDVWGQGITVTISSTSTKGPSVFPLAPCSRSTAGGTAALGCLVKDYFPEPVTVSWNSGALTS HC_1] GVHTFPAVLQSSGLYSLSSVVTVPSSSLGTQTYTCNVNHKPSNTKVDKRVEPKS
V-DOMAIN	IMGT domain description: VH IGHV gene and allele name: IGHV2-5*05 (85.00%), IGHV2-5*06 (85.00%), *Alignment details* IGHJ gene and allele name: IGHJ6*01 (83.33%), IGHJ6*02 (83.33%), *Alignment details* 2D representation: Collier de Perles or Collier de Perles on 2 layers CDR-IMGT lengths: [10.7.24] Sheet composition: [A B D E] [C C" C' F G] [CDR1] [CDR2] RITLKESGP.PLVKPTQTLTLTCSFSGFSLSDFGVG..VGWIRQPPGKALEWLAIIYSDDDK...RYSPSLN.TRLTITKDTSKNQVVLV [CDR3] MTRVSPVDTATYFCAHRRGPTTLFGVPIARGPVNAMDVWGQGITVTI
C-DOMAIN	IMGT domain description: CH1 IGHC gene and allele name: IGHG3*01 (97.94%), IGHG3*03 (97.94%), IGHG3*04 (97.94%), IGHG3*05 (97.94%), IGHG3*06 (97.94%), IGHG3*07 (97.94%), IGHG3*08 (97.94%), IGHG3*09 (97.94%), IGHG3*10 (97.94%), IGHG3*11 (97.94%), IGHG3*12 (97.94%), IGHG3*13 (97.94%), IGHG3*14 (97.94%), IGHG3*15 (97.94%), IGHG3*16 (97.94%), IGHG3*17 (97.94%), IGHG3*20 (97.94%), *Alignment details* 2D representation: Collier de Perles or Collier de Perles on 2 layers Sheet composition: [A B D E] [C F G] .....STKGPSVFPLAPCSRSTA...GGTAALGCLVKDYFP..EPVTVSWNSGALTS....GVHTFPAVLQSS.....GLYSLSSVVTV PSSSL...GTQTYTCNVNHKP..SNTKVDKRV

Chain ID	1u8k_A
IMGT chain description	L-KAPPA
Chain amino acid sequence	[IGKV_1 ALQLTQSPSSLSASVGDRITITCRASQGVTSALAWYRQKPGSPPQLLIYDASSLESGVPSRFSGSGSGTEFTLTISTLRPEDFATYYCQQ] [IGKJ_1][IGKC_1 LHFYPHTFGGGTRVDVRRTVAAPSVFIFPPSDRQLKSGTASVVCLLNNFYPREAKVQWKVDNALQSGNSQESVTEQDSKDSTYSLSSTLT] LSKADYEKHKVYECEVTHQGLSSPVTKSFNRGEC
V-DOMAIN	IMGT domain description: V-KAPPA IGKV gene and allele name: IGKV1-13*02 (85.26%) *Alignment details* IGKJ gene and allele name: IGKJ4*01 (63.64%) , IGKJ4*02 (63.64%) *Alignment details* 2D representation: Collier de Perles or Collier de Perles on 2 layers CDR-IMGT lengths: [6.3.9] Sheet composition: [A B D E] [C C" C' F G] [CDR1] [CDR2] ALQLTQSPSSLSASVGDRITITCRASQGVTSA.....LAWYRQKPGSPPQLLIYDAS.....SLESGVP.SRFSGSG..SGTEFTLT [CDR3] ISTLRPEDFATYYCQQLHF....YPHTFGGGTRVDVR
	IMGT domain description: C-KAPPA IGKC gene and allele name: IGKC*01 (98.13%) *Alignment details*

Chain ID	1u8k_C
IMGT chain description	Peptide
Chain amino acid sequence	LELDKWASL

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Region identification and delimitation

Chain ID	**1u8k_B**	
IMGT chain description	VH-CH1	
Chain amino acid sequence	[IGHV_1 RITLKESGPPLVKPTQTLTLTCSFSGFSLSDFGVGVGWIRQPPGKALEWLAIIYSDDDKRYSPSLNTRLTITKDTSKNQVVLVMTRVSPV][D][IGHJ_1] [IG DTATYFCAHRRGPTTLFGVPIARGPVNAMDVWGQGITVTISSTSTKGPSVFPLAPCS*KSTAGG*TAALGCLVKDYFPEPVTVSWNSGALTS HC_1] GVHTFPAVLQSSGLYSLSSVVTVPSSSLGTQTYTCNVNHKPSNTKVDKRVEPKS	
V-DOMAIN	IMGT domain description	VH
	IGHV gene and allele name	IGHV2-5*05 (85.00%), IGHV2-5*06 (85.00%), *Alignment details*
	IGHJ gene and allele name	IGHJ6*01 (83.33%), IGHJ6*02 (83.33%), *Alignment details*
	2D representation	Collier de Perles or Collier de Perles on 2 layers
	CDR-IMGT lengths	[10.7.24]
	Sheet composition	[A B D E] [C C" C' F G]
	[CDR1] [CDR2] RITLKESGP.PLVKPTQTLTLTCSFSGFSLSDFGVG..VGWIRQPPGKALEWLAIIYSDDDK...RYSPSLN.TRLTITKDTSKNQVVLV [CDR3] MTRVSPVDTATYFCAHRRGPTTLFGVPIARGPVNAMDVWGQGITVTI	
	IMGT domain description	CH1
	IGHC gene and allele name	IGHG3*01 (97.94%), IGHG3*03 (97.94%), IGHG3*04 (97.94%), IGHG3*05 (97.94%), IGHG3*06 (97.94%), IGHG3*07 (97.94%), IGHG3*08 (97.94%), IGHG3*09 (97.94%), IGHG3*10 (97.94%), IGHG3*11 (97.94%), IGHG3*12 (97.94%), IGHG3*13 (97.94%),

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IMGT/3Dstructure-DB

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Identification of the closest IMGT gene and allele(s)

Chain ID		1u8k_B
IMGT chain description		VH-CH1
Chain amino acid sequence		[RITLKESGPPLVKPTQ] [DTATYFCAHRRGPTTL HC_1 GVHTFPAVLQSSGLYS
V-DOMAIN	IMGT domain description	VH
	IGHV gene and allele name	IGHV2-5*05 (85.00%), IGHV2-5*06 (85.00%), *Alignment details*
	IGHJ gene and allele name	IGHJ6*01 (83.33%), IGHJ6*02 (83.33%), *Alignment details*
	2D representation	Collier de Perles or Collier de Perles on 2 layers
	CDR-IMGT lengths	[10.7.24]
	Sheet composition	[A B D E] [C C" C' F G]
		[CDR1] [CDR2] RITLKESGP.PLVKPTQTLTLTCSFSGFSLSDFGVG..VGWIRQPPGKALEWLAIIYSDDDK...RYSPSLN.TRLTITKDTSKNQVVLV [CDR3] MTRVSPVDTATYFCAHRRGPTTLFGVPIARGPVNAMDVWGQGITVTI
C-DOMAIN	IMGT domain description	CH1
	IGHC gene and allele name	IGHG3*01 (97.94%), IGHG3*03 (97.94%), IGHG3*04 (97.94%), IGHG3*05 (97.94%), IGHG3*06 (97.94%), IGHG3*07 (97.94%), IGHG3*08 (97.94%), IGHG3*09 (97.94%), IGHG3*10 (97.94%), IGHG3*11 (97.94%), IGHG3*12 (97.94%), IGHG3*13 (97.94%), IGHG3*14 (97.94%), IGHG3*15 (97.94%), IGHG3*16 (97.94%), IGHG3*17 (97.94%), IGHG3*20 (97.94%), *Alignment details*

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IMGT/3Dstructure-DB

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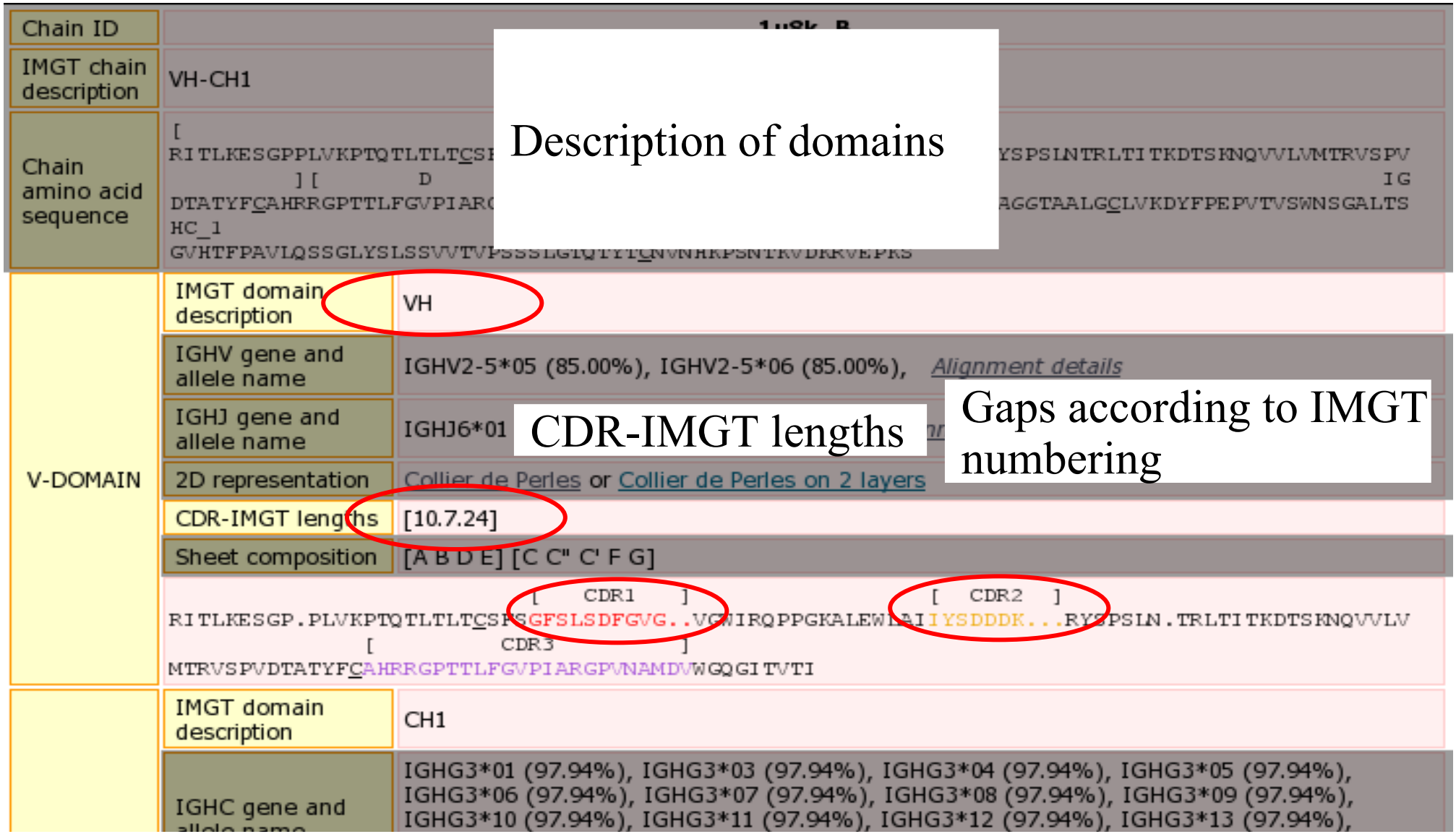

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Click 'DomPair' for IMGT/3Dstructure-DB Domain pair contacts (list of the Residue@Position pair contacts)

Chain and domains of 1duy.

IMGT molecule name	IMGT description	Chain ID	IMGT chain description	Domain number	IMGT domain description
CAMPATH-1H, alemtuzumab, MABCAMPATH®	FAB-GAMMA-1_KAPPA	1ce1_H	VH-CH1	[D1]	VH
				[D2]	CH1
		1ce1_L	L-KAPPA	[D1]	V-KAPPA
				[D2]	C-KAPPA
CD52 (synthetic peptide)	Peptide	1ce1_P	Peptide		

	Unit 1		Unit 2		Residue contacts	Number of residues			Atom contact types		
	Domain	Chain	Domain	Chain		Total	From 1	From 2	Total	Polar	Hydrogen
DomPair	VH	1ce1_H	CH1	1ce1_H	19	17	8	9	125	9	1
DomPair			V-KAPPA	1ce1_L	63	45	24	21	532	61	6
DomPair			(Ligand)	1ce1_P	25	19	12	7	216	40	9
DomPair	CH1	1ce1_H	VH	1ce1_H	19	17	9	8	125	9	1
DomPair			C-KAPPA	1ce1_L	68	58	28	30	498	40	6
DomPair	V-KAPPA	1ce1_L	VH	1ce1_H	63	45	21	24	532	61	6
DomPair			C-KAPPA	1ce1_L	18	18	8	10	137	19	2
DomPair			(Ligand)	1ce1_P	16	14	7	7	171	37	5
DomPair	C-KAPPA	1ce1_L	CH1	1ce1_H	68	58	30	28	498	40	6
DomPair			V-KAPPA	1ce1_L	18	18	10	8	137	19	2

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IMGT/3Dstructure-DB Domain pair contacts

Contacts of Domain VH Chain 1ce1_H *with* Domain (Ligand) Chain 1ce1_P

Atom contact types

- [ ] Non covalent
- [x] Polar
- [x] Hydrogen bond
- [ ] Non polar
- [ ] Covalent
- [ ] Disulfide

Check all Uncheck all

Atom contact categories

- [ ] (BB) Backbone/backbone
- [ ] (SS) Side chain/side chain
- [ ] (BS) Backbone/side chain
- [ ] (SB) Side chain/backbone

Check all Uncheck all

Show

Summary:

Residue contacts	Number of residues			Atom contact types		
	Total	From 1	From 2	Total	Polar	Hydrogen
25	19	12	7	216	40	9

List of the Residue@Position pair contacts:

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

	Order						Order					Atom contacts		
	IMGT Num	Residue		Domain	Chain		IMGT Num	Residue		Domain	Chain	Total	Polar	Hydrogen
R@P	38	TYR	Y	VH	1ce1_H	R@P	2	THR	T		1ce1_P	4	0	0
R@P	38	TYR	Y	VH	1ce1_H	R@P	7	ALA	A		1ce1_P	13	1	0
R@P	38	TYR	Y	VH	1ce1_H	R@P	8	ASP	D		1ce1_P	14	2	2

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	IMGT Num	Residue		Domain	Chain		IMGT Num	Residue		Domain	Chain	Total	Polar	Hydrogen
R@P	38	TYR	Y	VH	1ce1_H	R@P	2	THR	T		1ce1_P	4	0	0
R@P	38	TYR	Y	VH	1ce1_H	R@P	7	ALA	A		1ce1_P	13	1	0
R@P	38	TYR	Y	VH	1ce1_H	R@P	8	ASP	D		1ce1_P	14	2	2
R@P	55	PHE	F	VH	1ce1_H	R@P	6	SER	S		1ce1_P	5	0	0
R@P	55	PHE	F	VH	1ce1_H	R@P	7	ALA	A		1ce1_P	16	0	0
R@P	55	PHE	F	VH	1ce1_H	R@P	8	ASP	D		1ce1_P	1	0	0
R@P	57	ARG	R	VH	1ce1_H	R@P	7	ALA	A		1ce1_P	9	3	2
R@P	57	ARG	R	VH	1ce1_H	R@P	8	ASP	D		1ce1_P	20	6	1
R@P	61	LYS	K	VH	1ce1_H	R@P	8	ASP	D		1ce1_P	11	2	1
R@P	66	GLU	E	VH	1ce1_H	R@P	7	ALA	A		1ce1_P	1	0	0
R@P	107	GLU	E	VH	1ce1_H	R@P	2	THR	T		1ce1_P	13	2	1
R@P	107	GLU	E	VH	1ce1_H	R@P	4	SER	S		1ce1_P	5	2	0
R@P	107	GLU	E	VH	1ce1_H	R@P	7	ALA	A		1ce1_P	5	0	0
R@P	108	GLY	G	VH	1ce1_H	R@P	1	GLY	G		1ce1_P	2	1	0
R@P	108	GLY	G	VH	1ce1_H	R@P	2	THR	T		1ce1_P	9	2	0
R@P	109	HIS	H	VH	1ce1_H	R@P	1	GLY	G		1ce1_P	24	4	0
R@P	109	HIS	H	VH	1ce1_H	R@P	2	THR	T		1ce1_P	21	5	0
R@P	109	HIS	H	VH	1ce1_H	R@P	3	SER	S		1ce1_P	9	2	1
R@P	110	THR	T	VH	1ce1_H	R@P	1	GLY	G		1ce1_P	1	1	0
R@P	110	THR	T	VH	1ce1_H	R@P	3	SER	S		1ce1_P	11	4	1
R@P	112	ALA	A	VH	1ce1_H	R@P	3	SER	S		1ce1_P	3	1	0
R@P	113	ALA	A	VH	1ce1_H	R@P	2	THR	T		1ce1_P	3	0	0
R@P	113	ALA	A	VH	1ce1_H	R@P	3	SER	S		1ce1_P	7	2	0
R@P	113	ALA	A	VH	1ce1_H	R@P	4	SER	S		1ce1_P	4	0	0
R@P	114	PRO	P	VH	1ce1_H	R@P	4	SER	S		1ce1_P	5	0	0

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Summary:

Residue contacts	Number of residues			Atom contact types		
	Total	From 1	From 2	Total	Polar	Hydrogen
16	14	7	7	171	37	5

List of the Residue@Position pair contacts:

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

	Order						Order					Atom contacts		
	IMGT Num	Residue		Domain	Chain		IMGT Num	Residue		Domain	Chain	Total	Polar	Hydrogen
R@P	38	TYR	Y	V-KAPPA	1ce1_L	R@P	3	SER	S		1ce1_P	1	0	0
R@P	38	TYR	Y	V-KAPPA	1ce1_L	R@P	5	PRO	P		1ce1_P	21	0	0
R@P	56	ASN	N	V-KAPPA	1ce1_L	R@P	3	SER	S		1ce1_P	3	2	0
R@P	107	HIS	H	V-KAPPA	1ce1_L	R@P	4	SER	S		1ce1_P	20	4	1
R@P	107	HIS	H	V-KAPPA	1ce1_L	R@P	5	PRO	P		1ce1_P	12	2	0
R@P	107	HIS	H	V-KAPPA	1ce1_L	R@P	6	SER	S		1ce1_P	14	3	1
R@P	108	ILE	I	V-KAPPA	1ce1_L	R@P	5	PRO	P		1ce1_P	12	1	0
R@P	108	ILE	I	V-KAPPA	1ce1_L	R@P	6	SER	S		1ce1_P	12	3	0
R@P	109	SER	S	V-KAPPA	1ce1_L	R@P	6	SER	S		1ce1_P	11	2	0
R@P	114	ARG	R	V-KAPPA	1ce1_L	R@P	6	SER	S		1ce1_P	18	3	1
R@P	114	ARG	R	V-KAPPA	1ce1_L	R@P	7	ALA	A		1ce1_P	4	2	0
R@P	114	ARG	R	V-KAPPA	1ce1_L	R@P	8	ASP	D		1ce1_P	6	2	0
R@P	116	ARG	R	V-KAPPA	1ce1_L	R@P	2	THR	T		1ce1_P	1	1	0
R@P	116	ARG	R	V-KAPPA	1ce1_L	R@P	4	SER	S		1ce1_P	9	4	1
R@P	116	ARG	R	V-KAPPA	1ce1_L	R@P	6	SER	S		1ce1_P	20	6	1
R@P	116	ARG	R	V-KAPPA	1ce1_L	R@P	7	ALA	A		1ce1_P	7	2	0

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Contacts of Domain Chain **V-KAPPA 1cz8_X** *with* Domain Chain **(Ligand) 1cz8_V**

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Atom contact types

- [ ] Non covalent
- [x] Polar
- [x] Hydrogen bond
- [ ] Non polar
- [ ] Covalent
- [ ] Disulfide

Check all Uncheck all

Atom contact categories

- [ ] (BB) Backbone/backbone
- [ ] (SS) Side chain/side chain
- [ ] (BS) Backbone/side chain
- [ ] (SB) Side chain/backbone

Check all Uncheck all

Show

Summary:

Residue contacts	Number of residues			Atom contact types		
	Total	From 1	From 2	Total	Polar	Hydrogen
6	7	5	2	39	5	0

List of the Residue@Position pair contacts:

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

	Order						Order					Atom contacts		
	IMGT Num	Residue		Domain	Chain		IMGT Num	Residue		Domain	Chain	Total	Polar	Hydrogen
R@P	107	TYR	Y	V-KAPPA	1cz8_X	R@P	74	GLN	Q		1cz8_V	1	1	0
R@P	108	SER	S	V-KAPPA	1cz8_X	R@P	74	GLN	Q		1cz8_V	4	2	0
R@P	109	THR	T	V-KAPPA	1cz8_X	R@P	74	GLN	Q		1cz8_V	1	0	0
R@P	114	VAL	V	V-KAPPA	1cz8_X	R@P	73	HIS	H		1cz8_V	4	0	0
R@P	114	VAL	V	V-KAPPA	1cz8_X	R@P	74	GLN	Q		1cz8_V	7	1	0
R@P	116	TRP	W	V-KAPPA	1cz8_X	R@P	74	GLN	Q		1cz8_V	22	1	0

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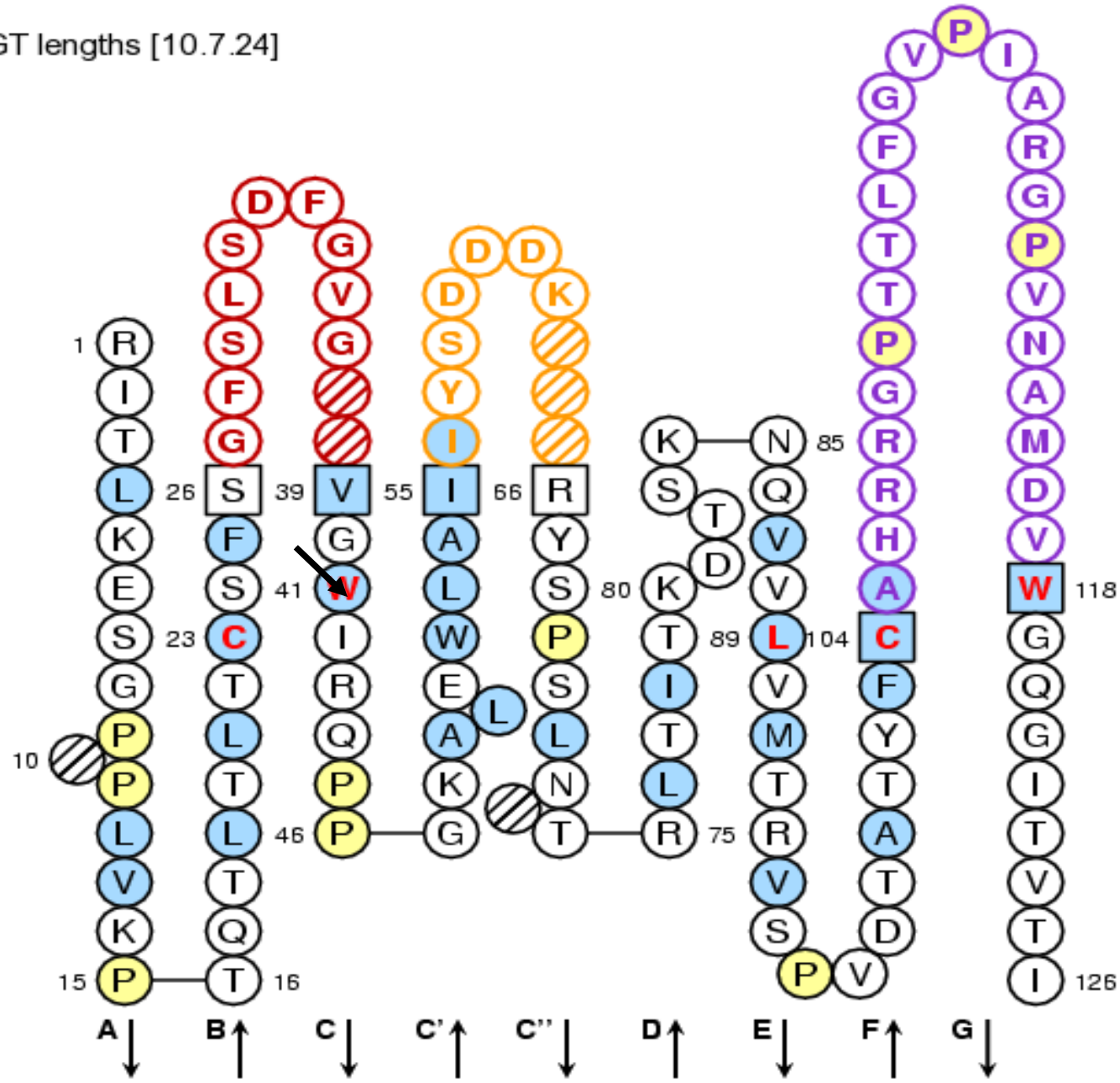
IMGT Collier de Perles : *Homo sapiens* (Human) IGHV_1 V-DOMAIN from 2F5 (PDB: 1u8k_B)

CDR-IMGT lengths [10.7.24]



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IMGT/3Dstructure-DB: analysis of 3D structures

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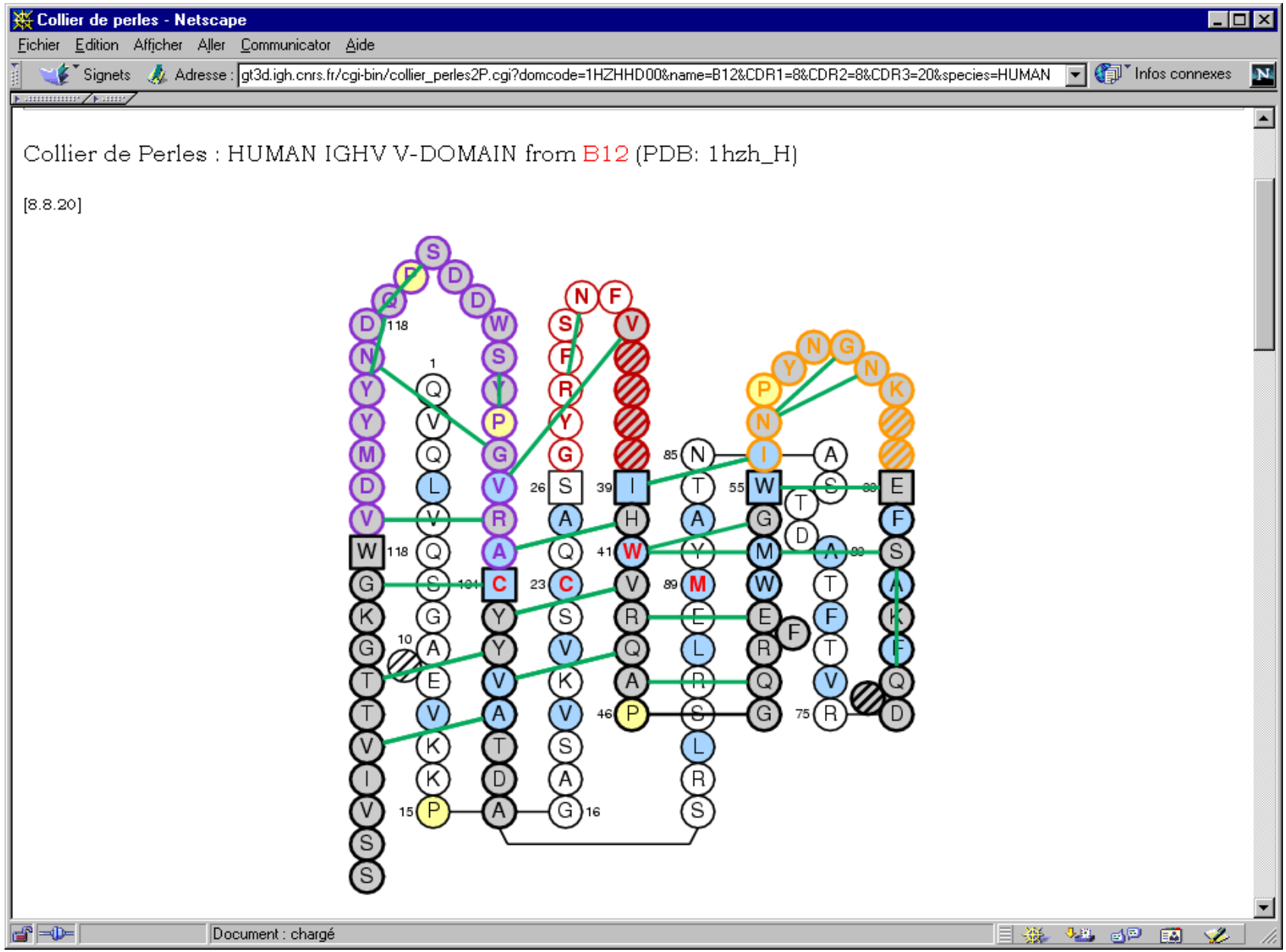

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Number of H bonds with the ligand

	Total	VH	V-KAPPA
cetuximab (1yy9)	**6**	5	1
alemtuzumab (1ce1)	**14**	9	5
bevacizumab (1bj1)	**14**	14	0
trastuzumab (1n8z)	**6**	2	4
pertuzumab (1s78)	**9**	9	0

VH		CDR1-IMGT	CDR2-IMGT	CDR3-IMGT
cetuximab	[8.7.13]		59G	111Y 112D 113Y
alemtuzumab	[8.10.12]	38Y	**57**R 61K	107E 109H 110T
bevacizumab	[8. 8.16]	38G	55W 58T	107Y 108P **110**Y
trastuzumab	[8.8.13]		55R	111.1G 112.1S 111G
pertuzumab	[8.8.12]	36D 37Y	57N 58P **59**N	110P 114Y

V-KAPPA				
cetuximab	[6.3.9]			114W
alemtuzumab	[6.3.9]			107H 114R 116R
bevacizumab	[6.3.9]			
trastuzumab	[6.3.9]	36N		108Y 114T
pertuzumab	[6.3.9]			

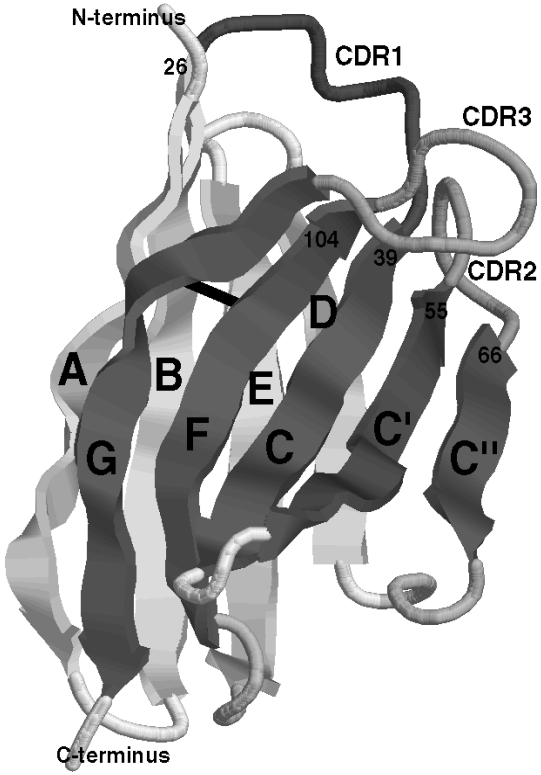
Magdelaine-Beuzelin C. et al. Crit. Rev. Oncol. Hemat. 2007

Structural domains

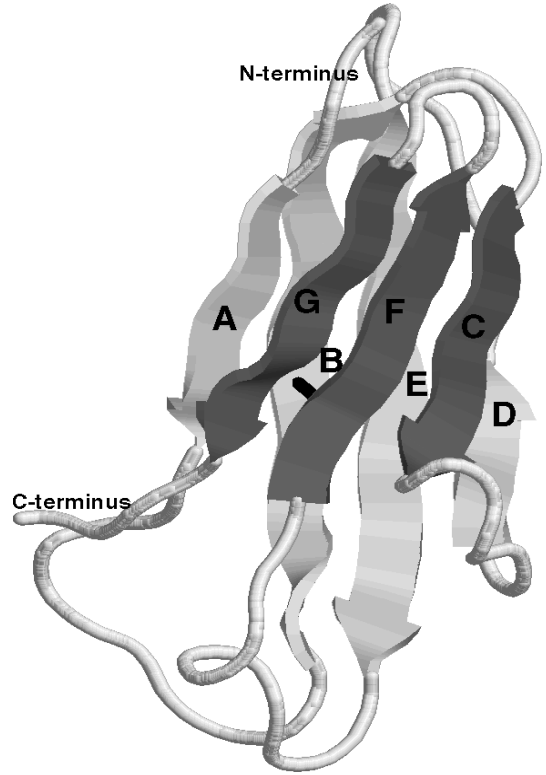
http://www.imgt.org

IG and TR

V-DOMAIN

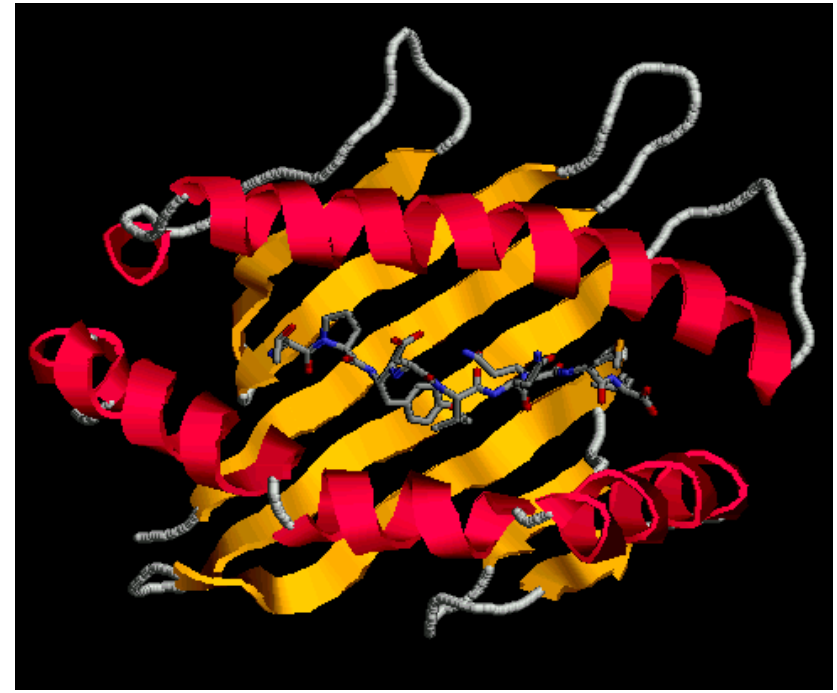


C-DOMAIN



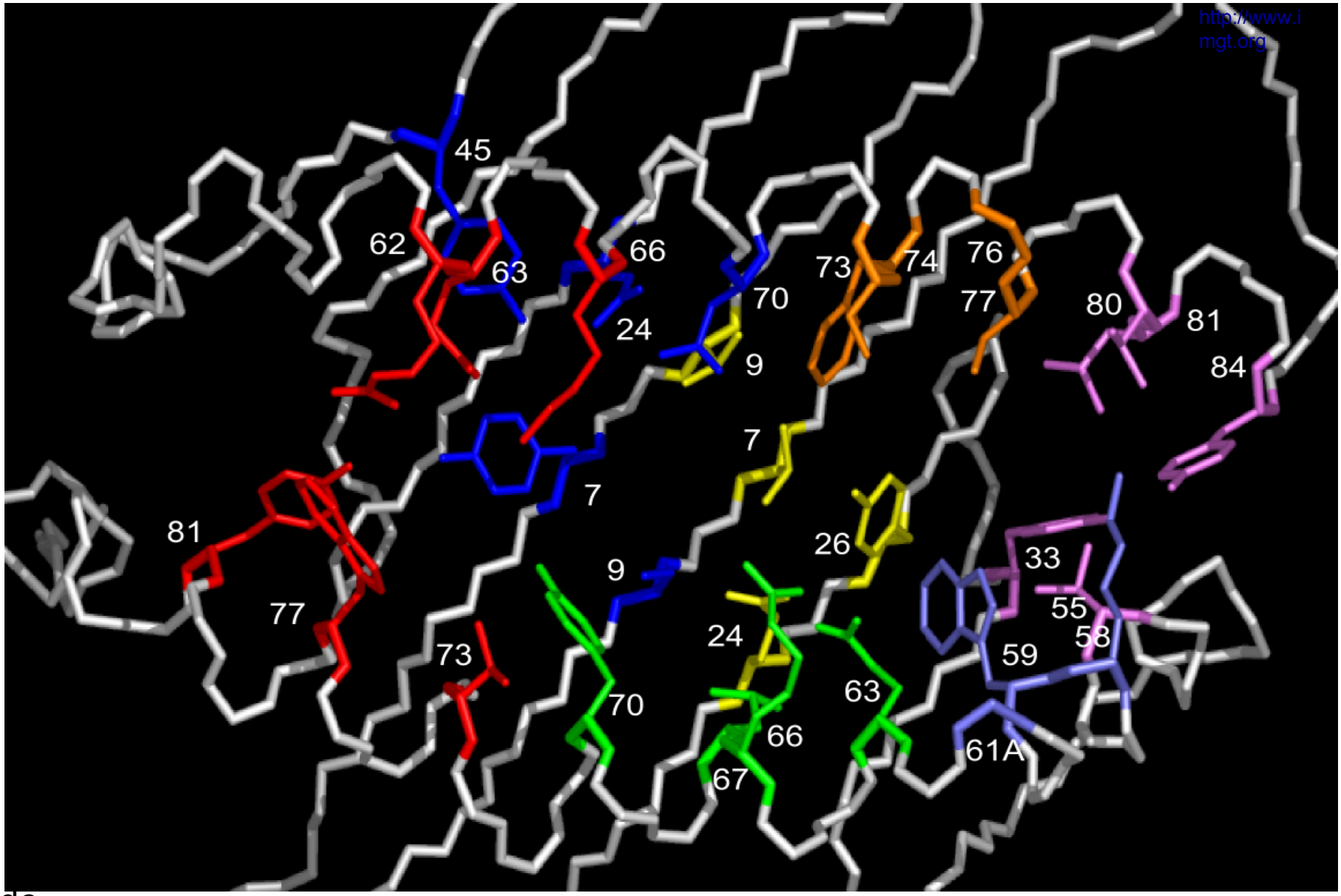
MHC

G-DOMAINs



Kaas Q. and Lefranc M.-P. Current Bioinformatics, 2, 21-30 (2007)

MHC class I IMGT contact sites



C1		1 E
C2		--
C3		2 Q
C4		3 Y
C5		(4 K)
C6		5 F
C7		--
C8		--
C9		6 Y
C10		7 S
C11		8 V

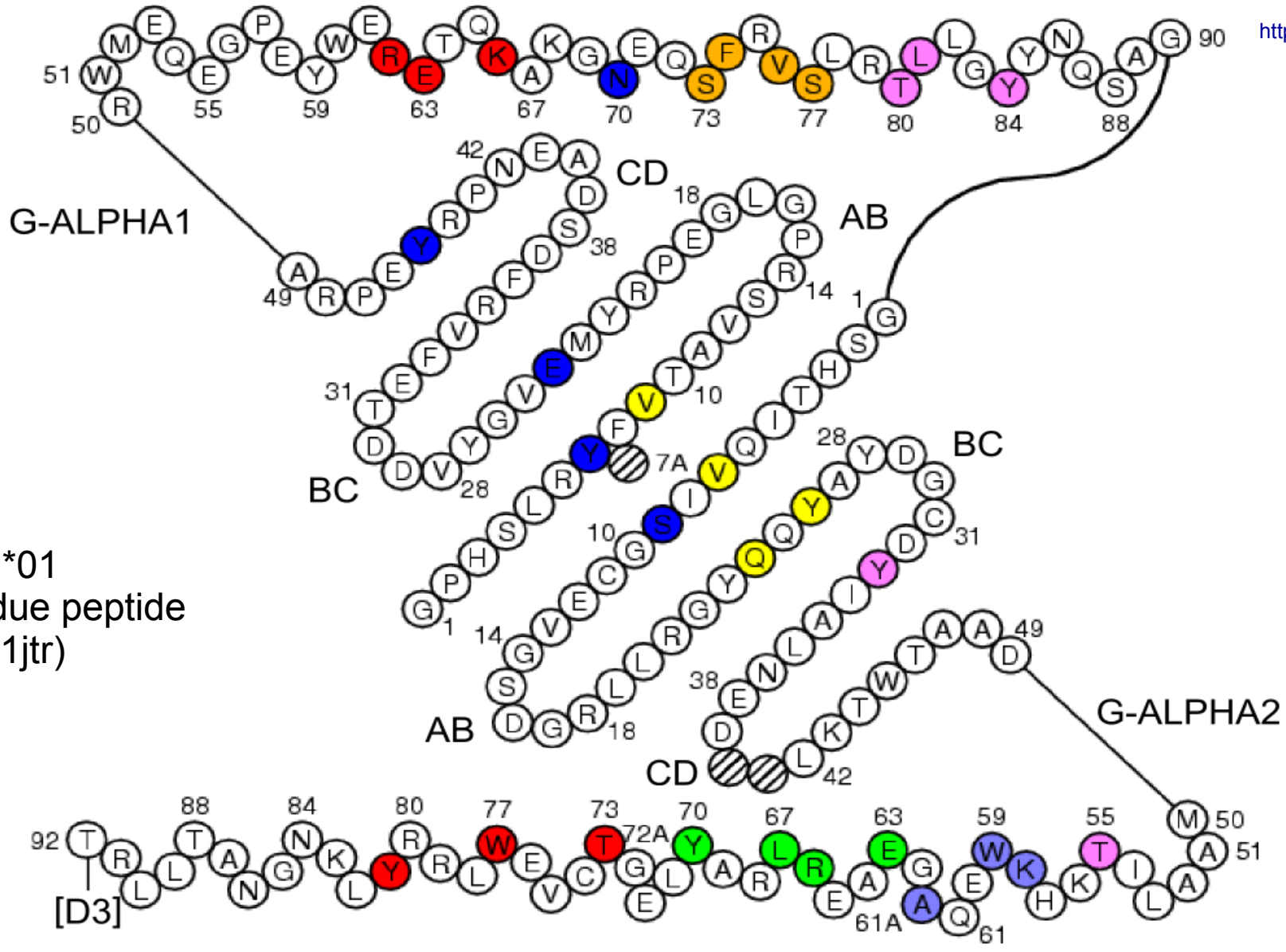
H2-K1*01
(code 1jtr)
8 residue peptide

Kaas and Lefranc In Silico Biology 2005

MHC class I IMGT contact sites

Im Muno Gene Tics Information system®
http://www.imgt.org

C1	1 E
C2	--
C3	2 Q
C4	3 Y
C5	(4 K)
C6	5 F
C7	--
C8	--
C9	6 Y
C10	7 S
C11	8 V



H2-K1*01
8 residue peptide
(code 1jtr)

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

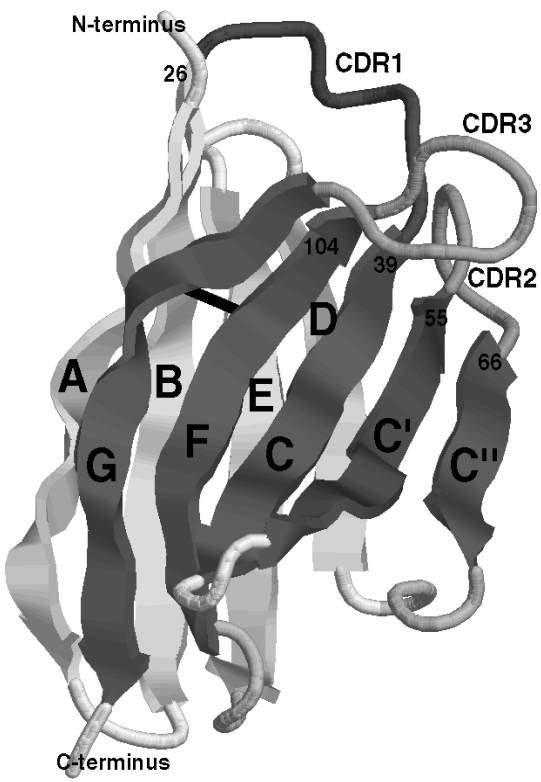
IMGT unique numbering

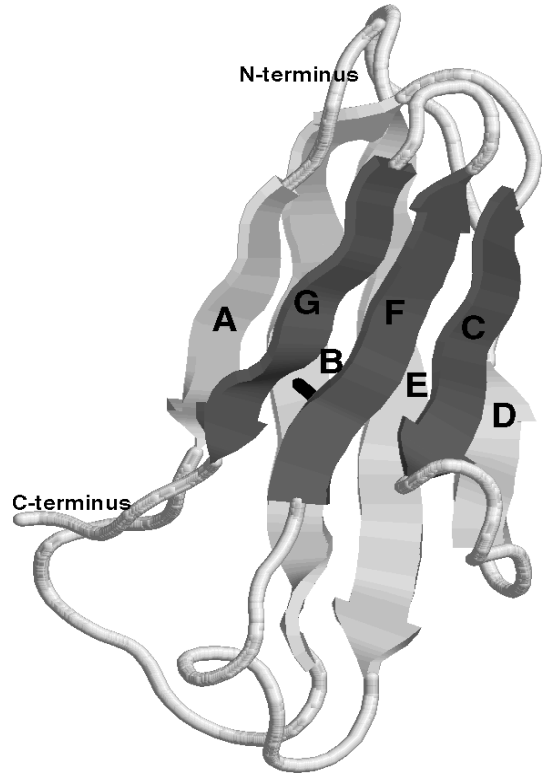
http://www.imgt.org

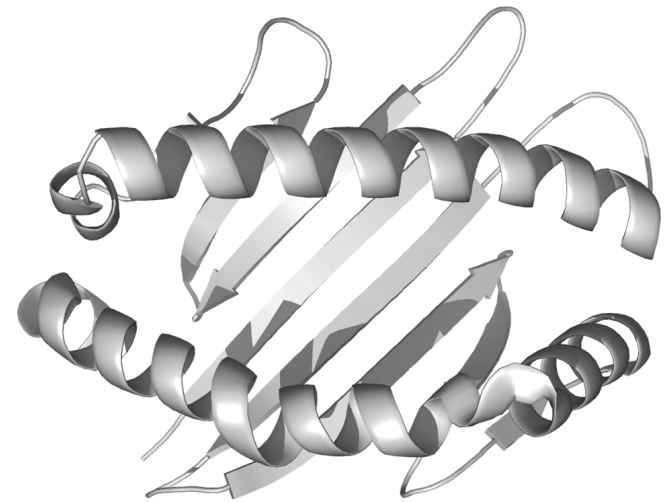
V-DOMAIN (IG,TR)
AND
V-LIKE-DOMAIN
(other than IG,TR)

C-DOMAIN (IG,TR)
AND
C-LIKE-DOMAIN
(other than IG,TR)

G-DOMAIN (MHC)
AND
G-LIKE-DOMAIN
(other than MHC)





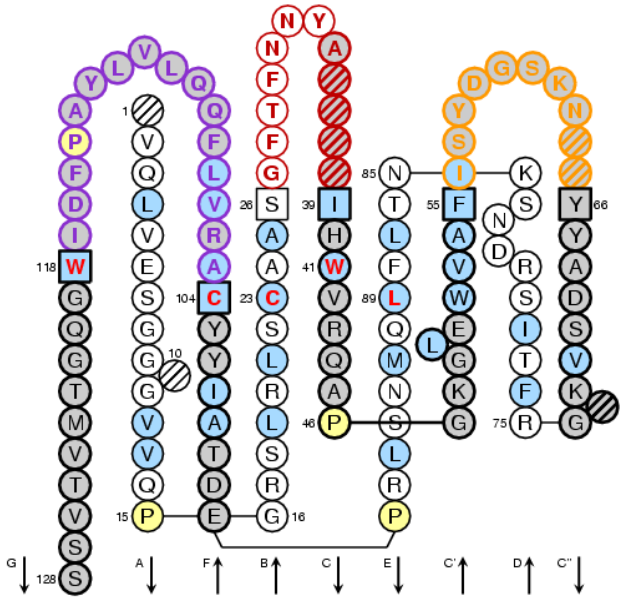


Immunoglobulin superfamily (IgSF)

MHC superfamily (MhcSF)

V-LIKE-DOMAIN

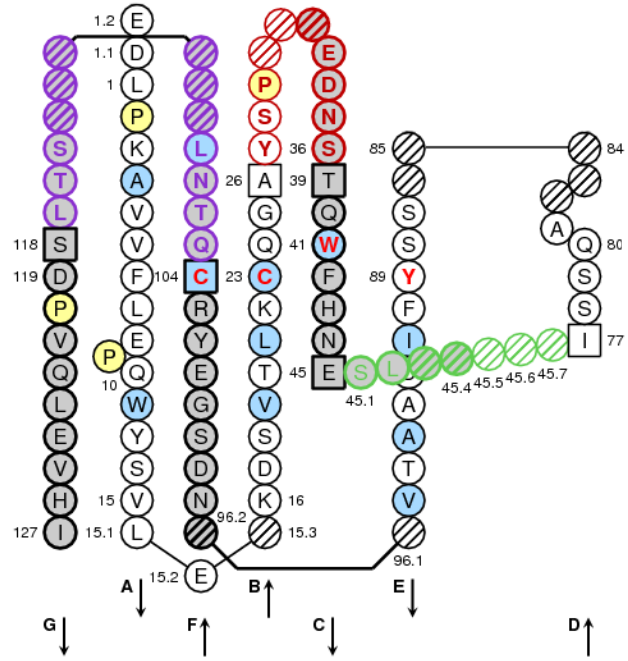
MOG



Duprat, E. et al., Recent Res. Develop. Human Genet., 2, 111-136 (2004)

C-LIKE-DOMAIN

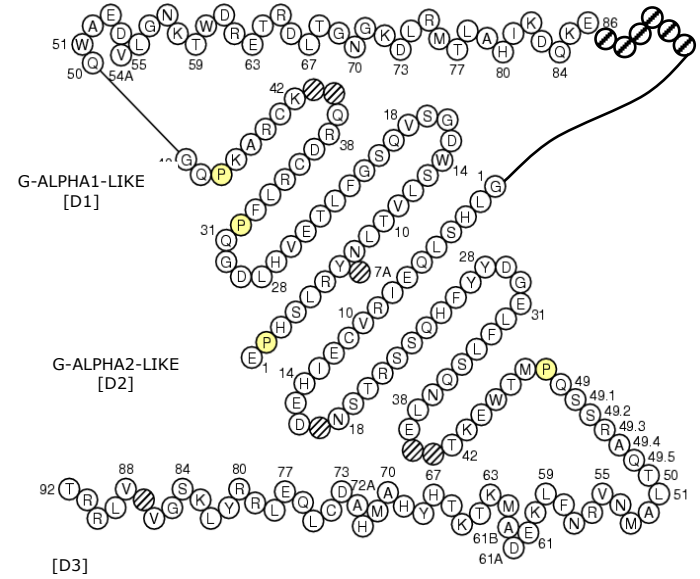
FCGR3B



Bertrand, G. et al., Tissue Antigens, 64, 119-131 (2004)

G-LIKE-DOMAIN

MICA



Frigoul, A. et al., Recent Res. Develop. Human Genet., 3, 95-145 (2005)

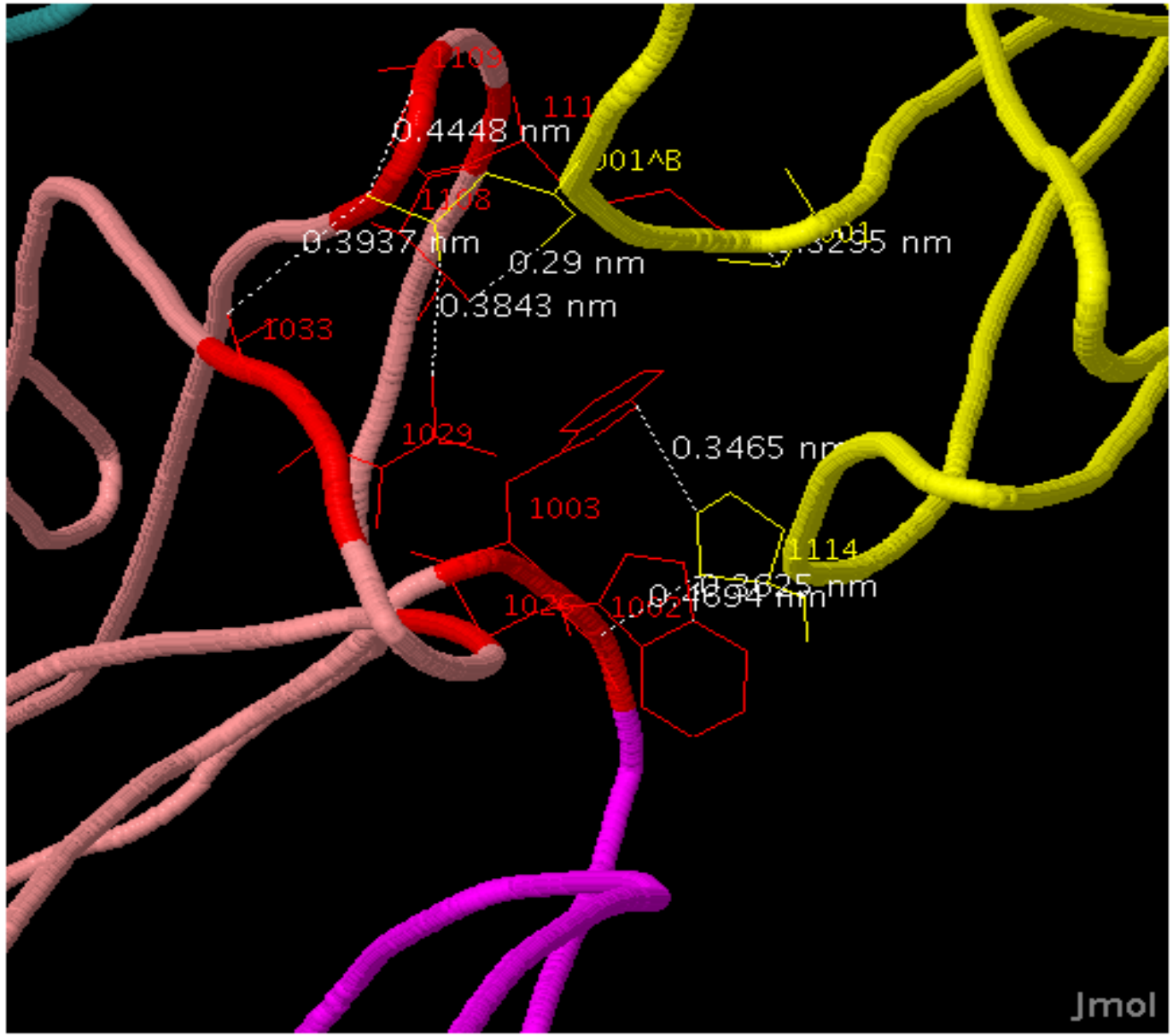
Interactions between domains

http://www.imgt.org

IGHG1
(FC-GAMMA1)

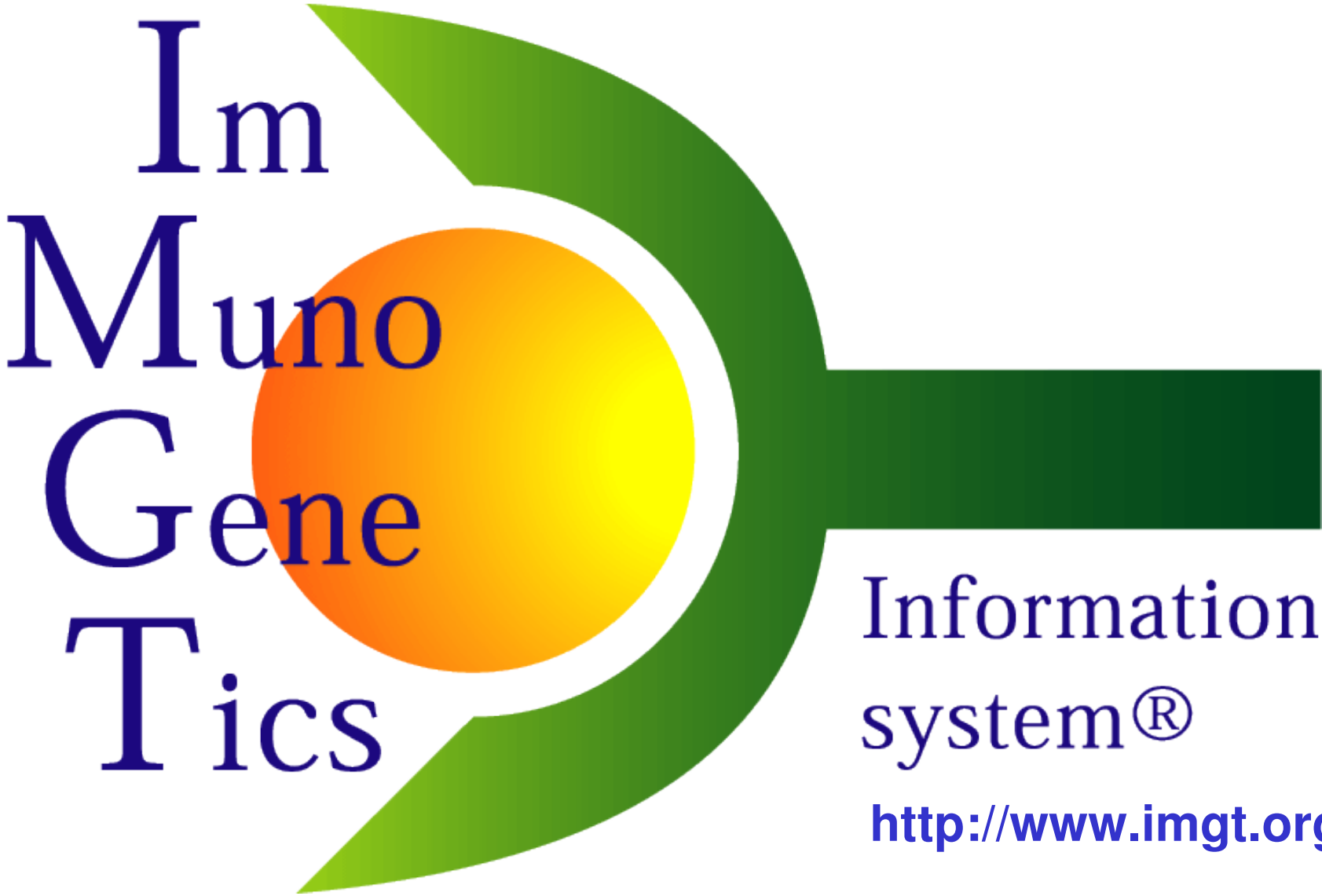
CH2
C-DOMAIN

FCGR3B



[D2]
C-LIKE-
DOMAIN

[D1] C-LIKE-DOMAIN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