Bioinformatique: du gène à la structure

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26 septembre 2012

IMGT/3Dstructure-DB

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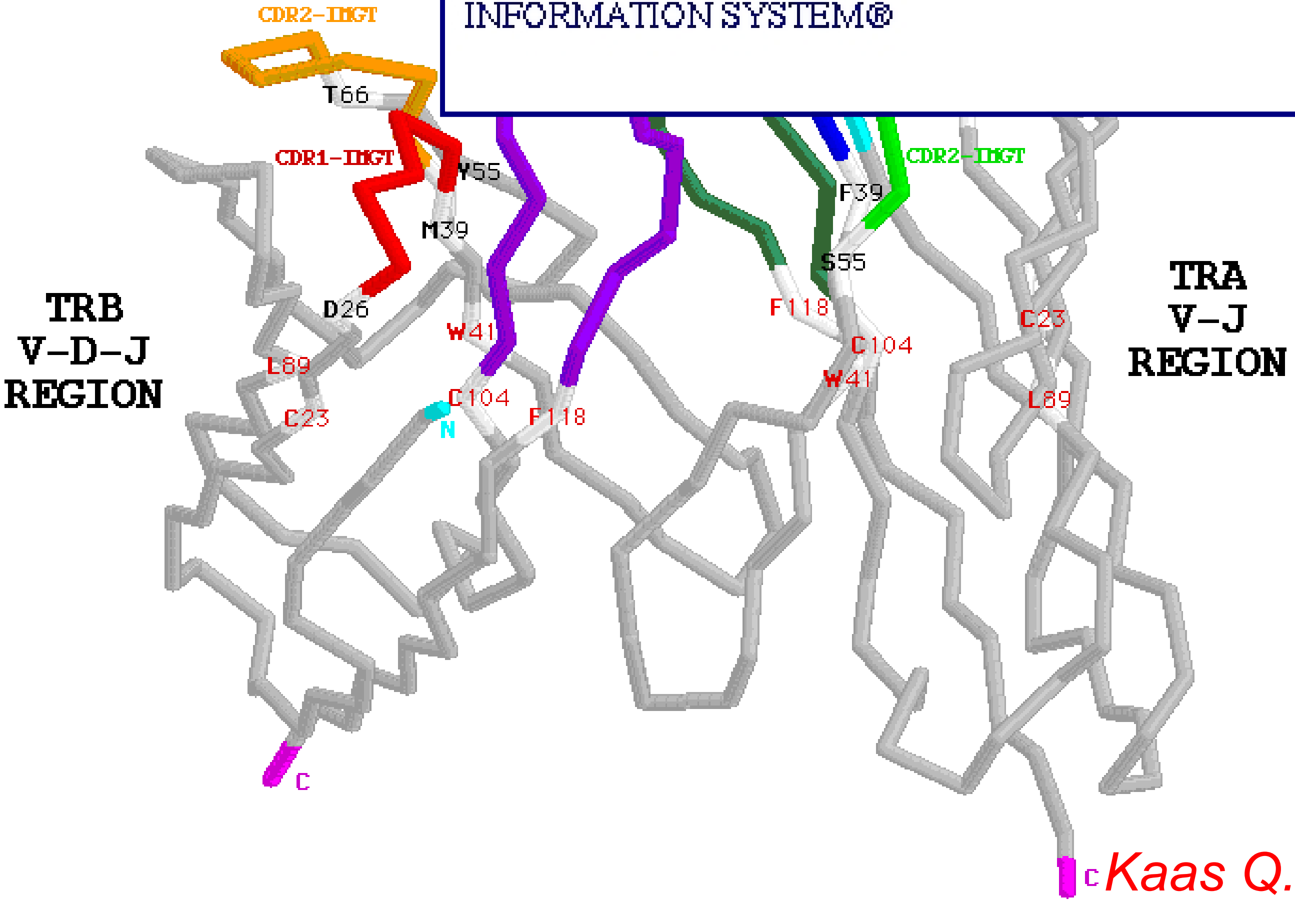

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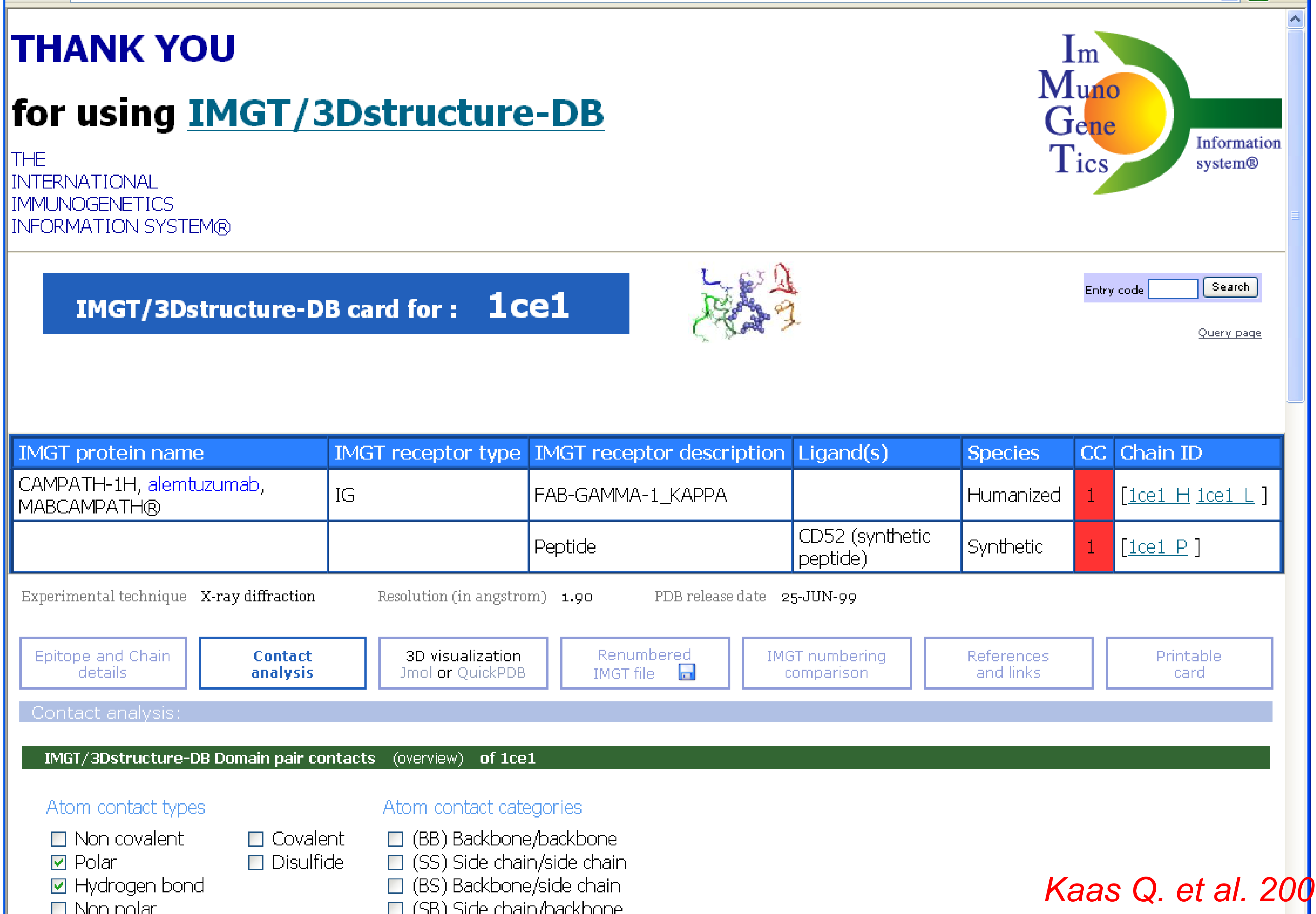

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IMGT/3Dstructure-DB card for : 1ce1

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

Contact analysis:

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

Atom contact types

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

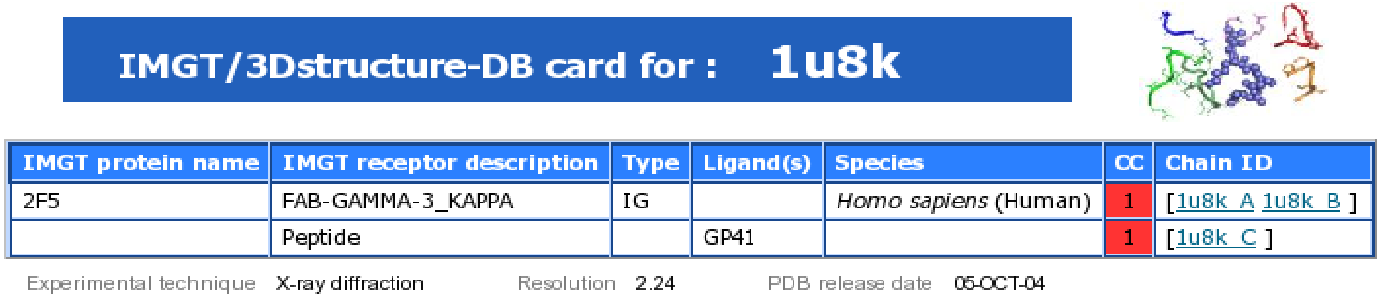
Atom contact categories

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

Kaas Q. et al. 2004)

IMGT/3Dstructure-DB

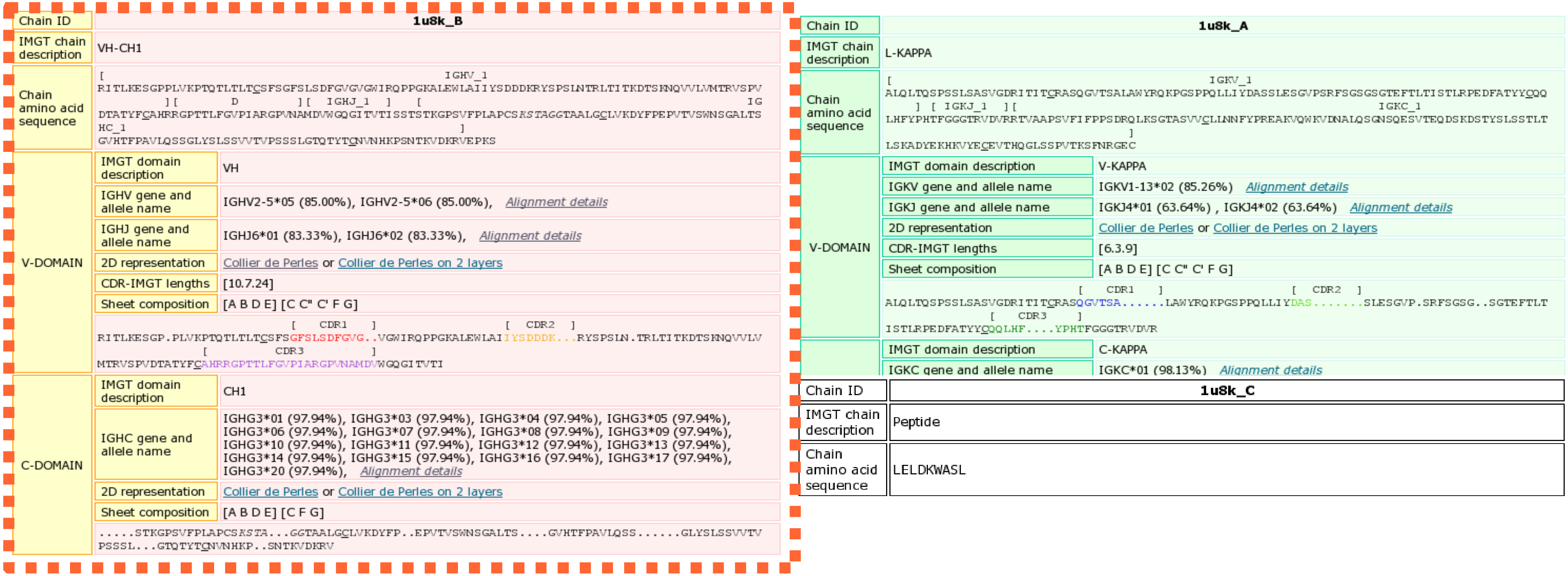
http://www.imgt.org



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	see below	

```
[                                                                  IGHV_1
RITLKESGPPLVKPTQTLTLTCSFSGFSLSDFGVGVGWIRQPPGKALEWLAIIYSDDDKRYSPSLNTRLTITKDTSKNQVVLVMTRVSPV
             ][          D           ][   IGHJ_1   ]     [                                  IG
DTATYFCAHRRGPTTLFGVPIARGPVNAMDVWGQGITVTISSTSTKGPSVFPLAPCSKSTAGGTAALGCLVKDYFPEPVTVSWNSGALTS
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]

```
.....STKGPSVFPLAPCSKSTA...GGTAALGCLVKDYFP..EPVTVSWNSGALTS....GVHTFPAVLQSS......GLYSLSSVVTV
PSSSL...GTQTYTCNVNHKP..SNTKVDKRV
```

Chain ID	1u8k_A	
IMGT chain description	L-KAPPA	
Chain amino acid sequence	see below	

```
[                                                           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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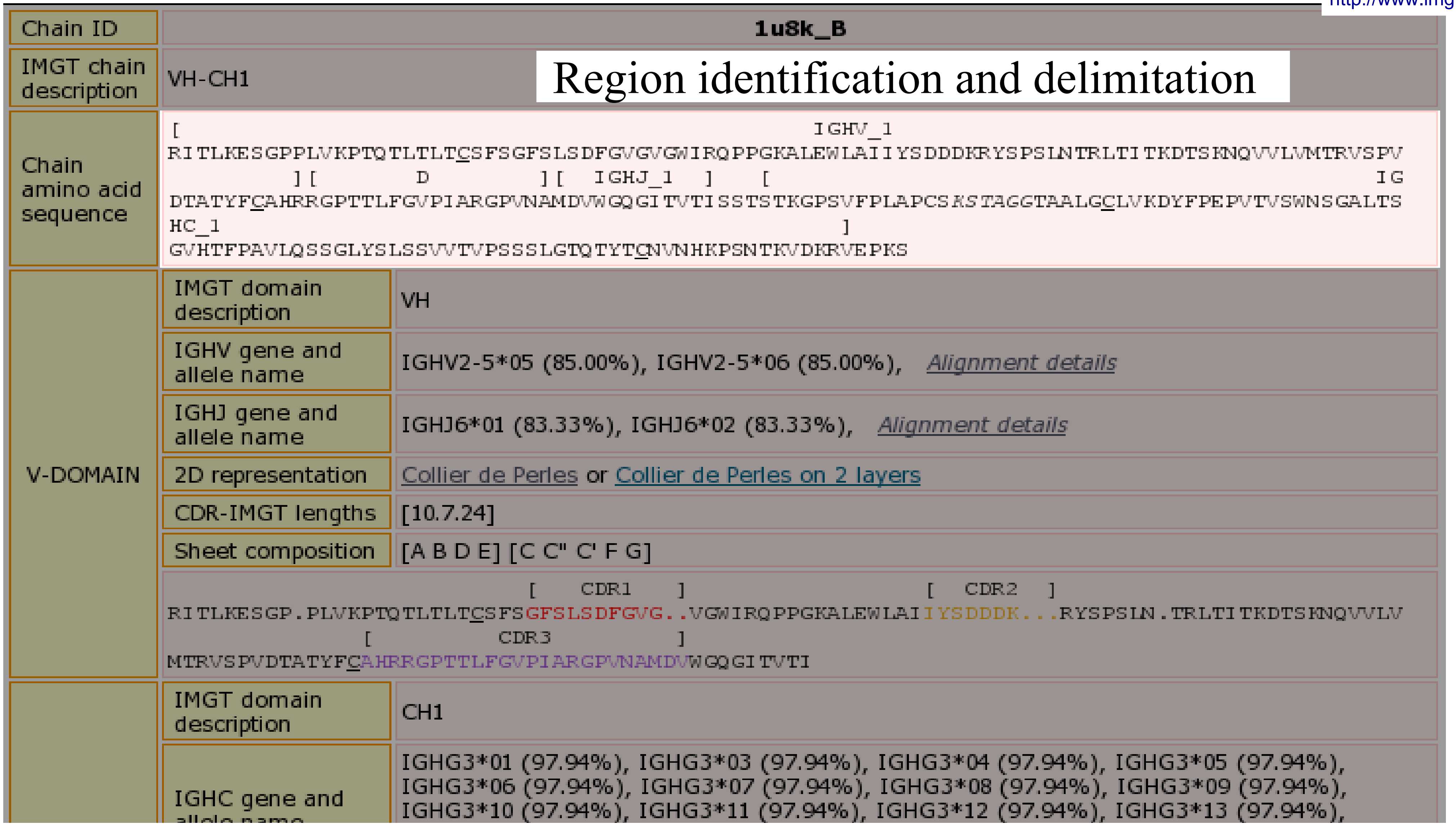
IMGT/3Dstructure-DB

http://www.imgt.org



Region identification and delimitation

Chain ID	1u8k_B	
IMGT chain description	VH-CH1	
Chain amino acid sequence	see below	

```
[                                                IGHV_1
RITLKESGPPLVKPTQTLTLTCSFSGFSLSDFGVGVGWIRQPPGKALEWLAIIYSDDDKRYSPSLNTRLTITKDTSKNQVVLVMTRVSPV
         ][       D          ][  IGHJ_1   ]    [                                          IG
DTATYFCAHRRGPTTLFGVPIARGPVNAMDVWGQGITVTISSTSTKGPSVFPLAPCSKSTAGGTAALGCLVKDYFPEPVTVSWNSGALTS
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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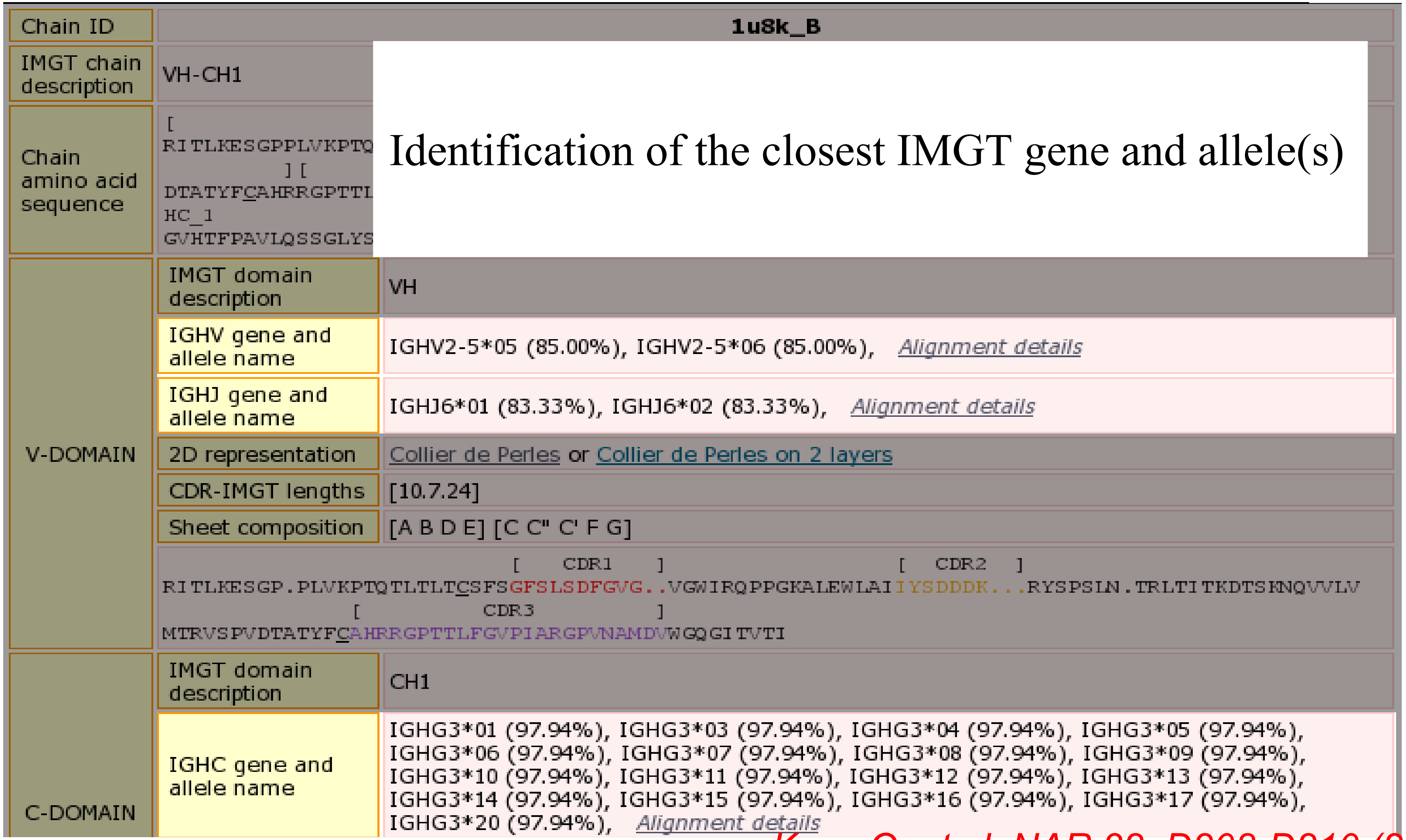
IMGT/3Dstructure-DB

http://www.imgt.org



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...RYSPSIN.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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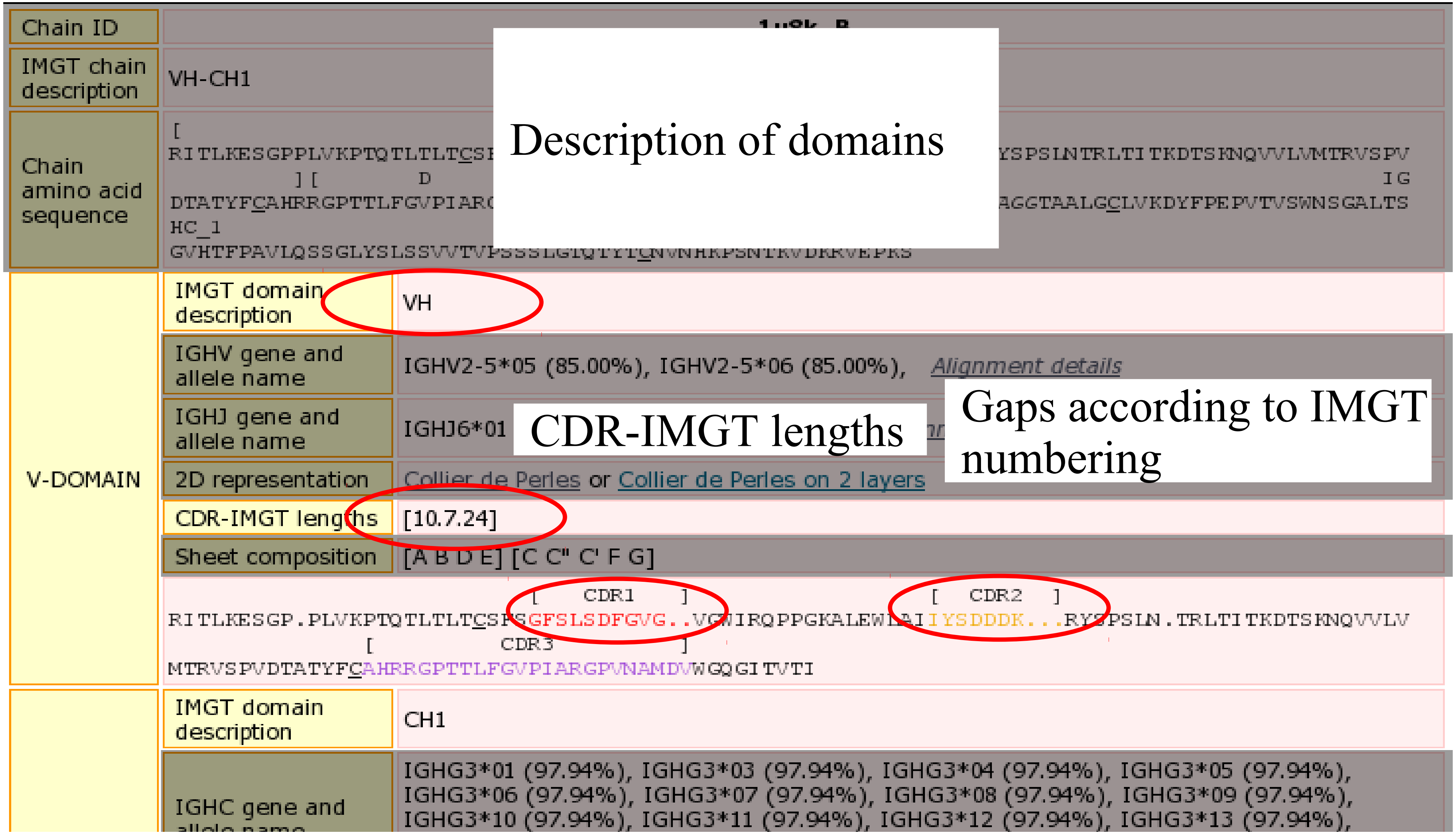
IMGT/3Dstructure-DB

http://www.imgt.org



Chain ID		1u8k_B
IMGT chain description		VH-CH1
Chain amino acid sequence		see below
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
	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]
	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%),

Chain amino acid sequence:

```
[
RITLKESGPPLVKPTQTLTLTCSF                                    YSPSINTRLTITKDTSKNQVVLVMTRVSPV
           ] [         D                                                                IG
DTATYFCAHRRGPTTLFGVPIARC                                    AGGTAALGCLVKDYFPEPVTVSWNSGALTS
HC_1
GVHTFPAVLQSSGLYSLSSVVTVPSSSLGTQTYTCNVNHKPSNTKVDKRVEPKS
```

V-DOMAIN sequence:

```
                               [    CDR1    ]                        [   CDR2   ]
RITLKESGP.PLVKPTQTLTLTCSFSGFSLSDFGVG..VGWIRQPPGKALEWLAIIYSDDDK...RYSPSIN.TRLTITKDTSKNQVVLV
                    [            CDR3            ]
MTRVSPVDTATYFCAHRRGPTTLFGVPIARGPVNAMDVWGQGITVTI
```

Description of domains

CDR-IMGT lengths

Gaps according to IMGT numbering

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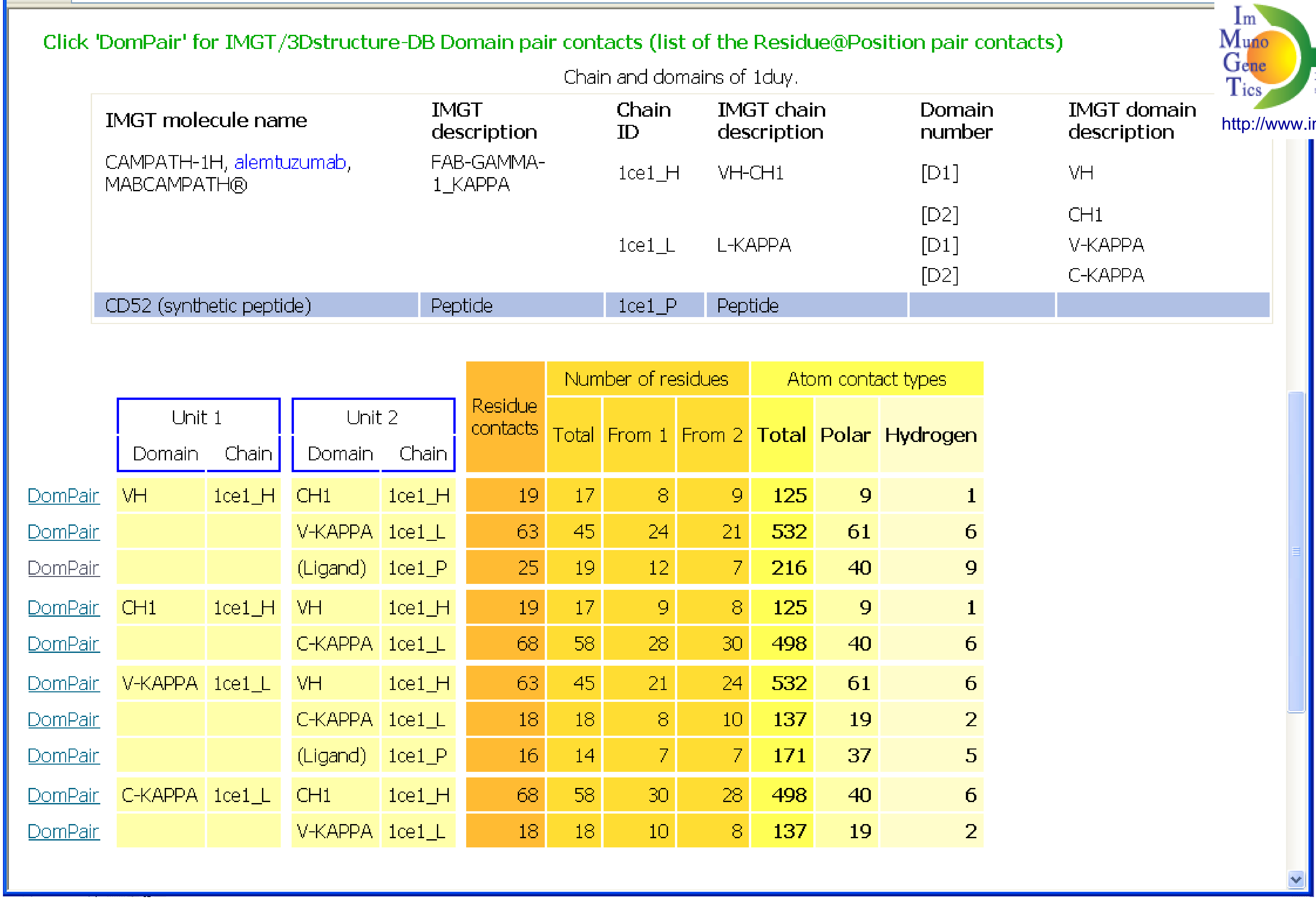


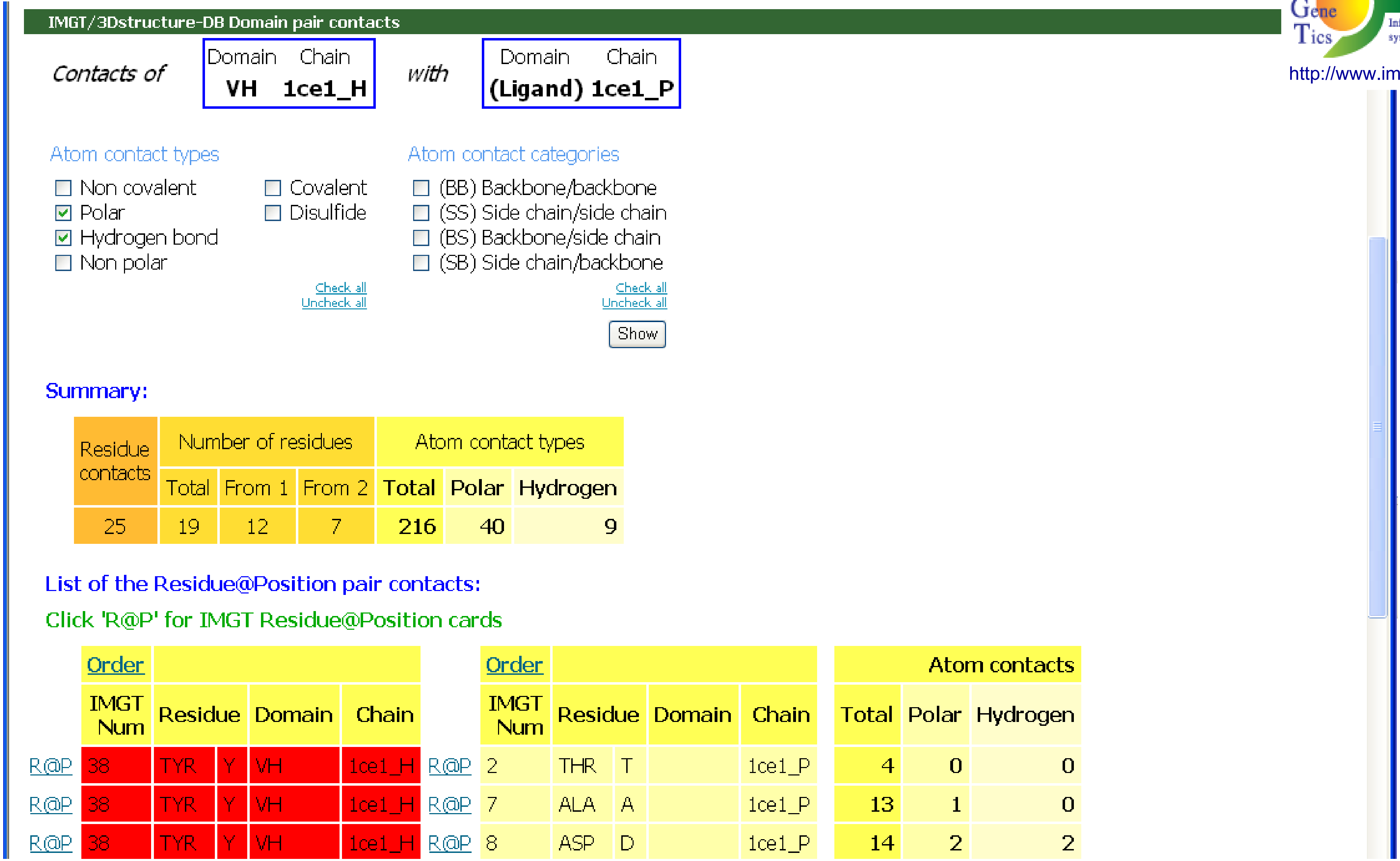
Click 'DomPair' for IMGT/3Dstructure-DB Domain pair contacts (list of the Residue@Position pair contacts)

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**

Kaas Q. et al. 2004)



IMGT/3Dstructure-DB Domain pair contacts

Contacts of

Domain	Chain
VH	**1ce1_H**

with

Domain	Chain
(Ligand)	**1ce1_P**

Atom contact types

☐ Non covalent
☑ Polar
☑ 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

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:

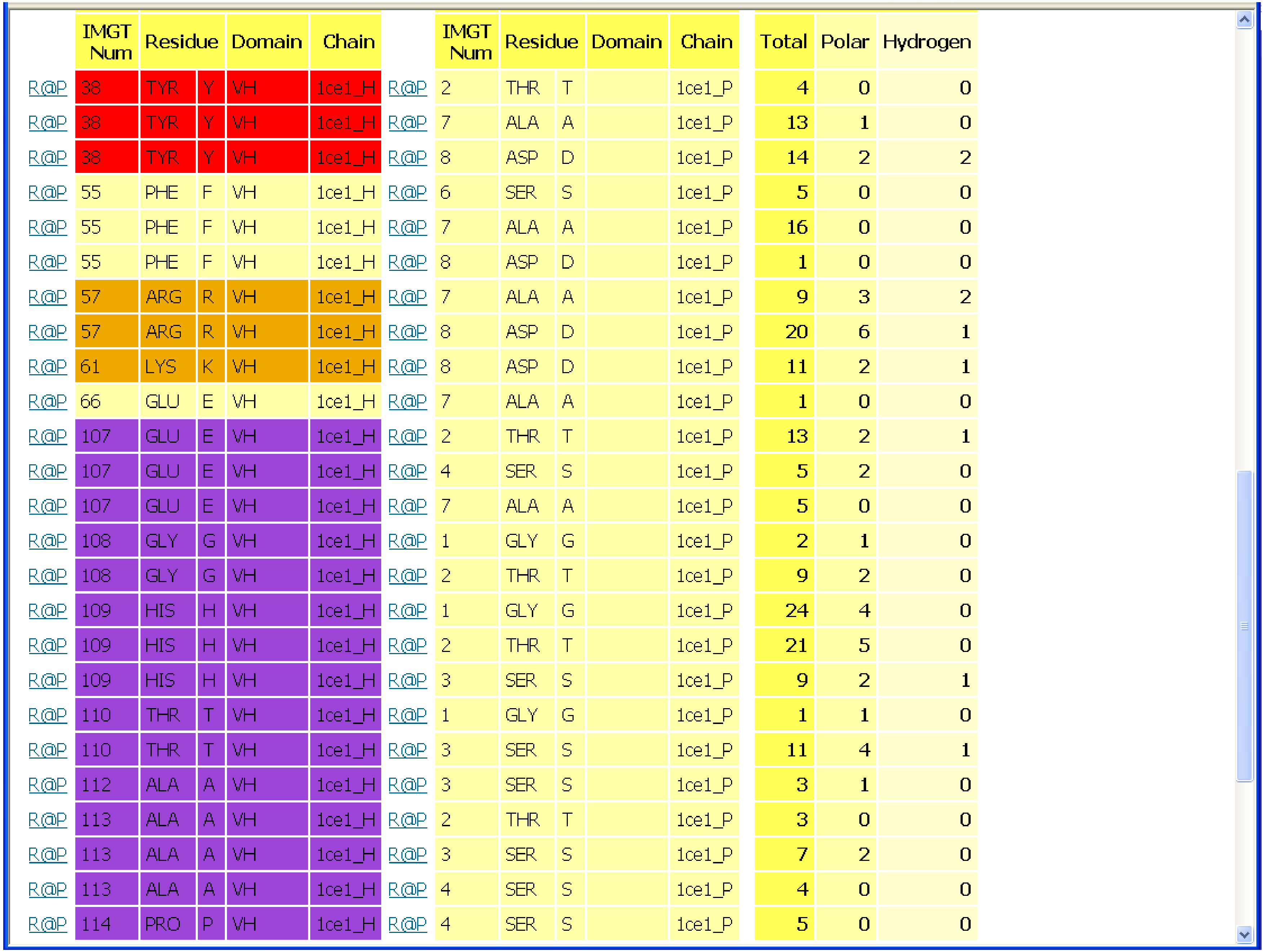
Click 'R@P' for IMGT Residue@Position cards

	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

http://www.imgt.org

Kaas Q. et al. 2004)

http://www.imgt.org



	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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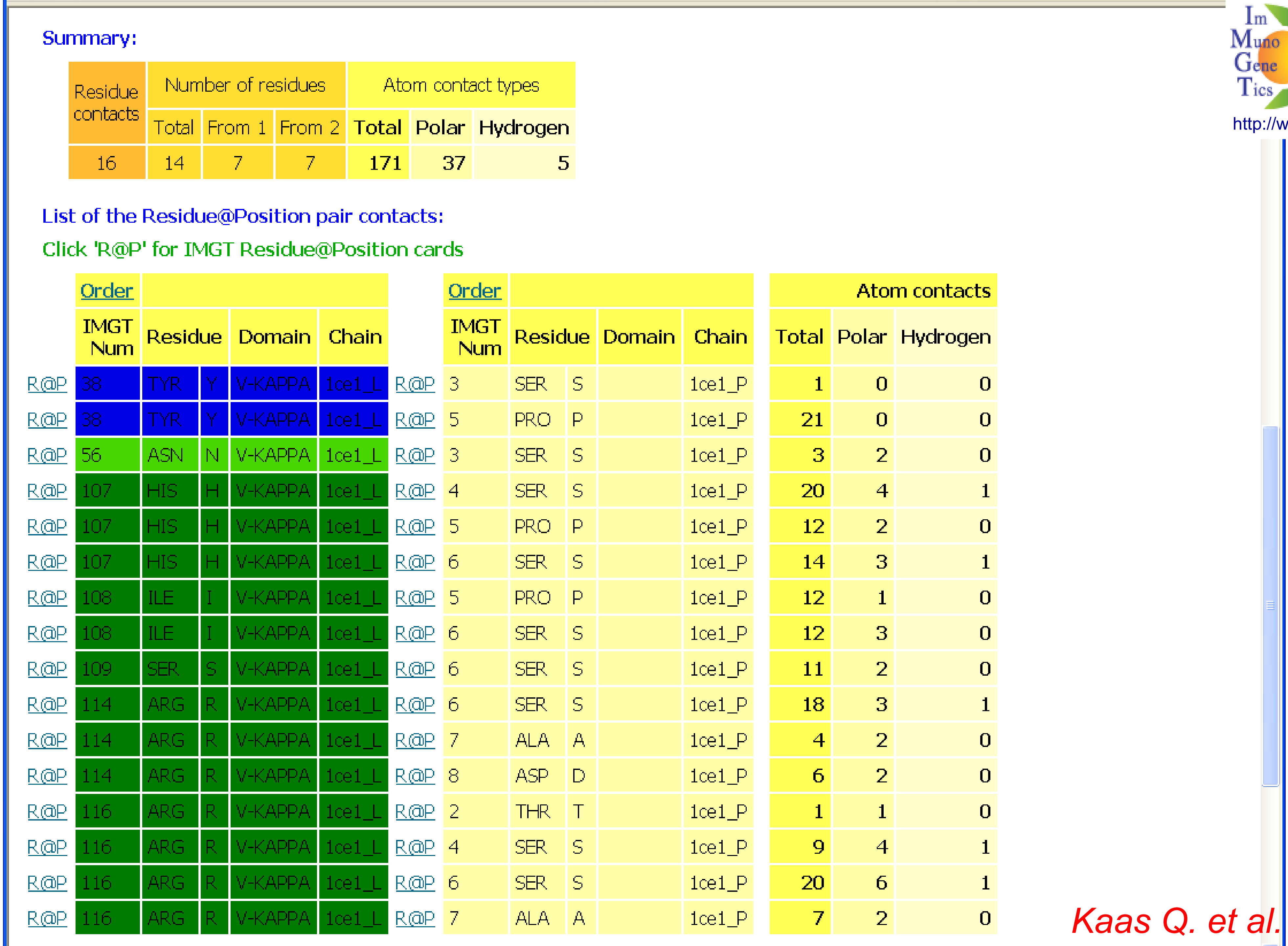


Summary:

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

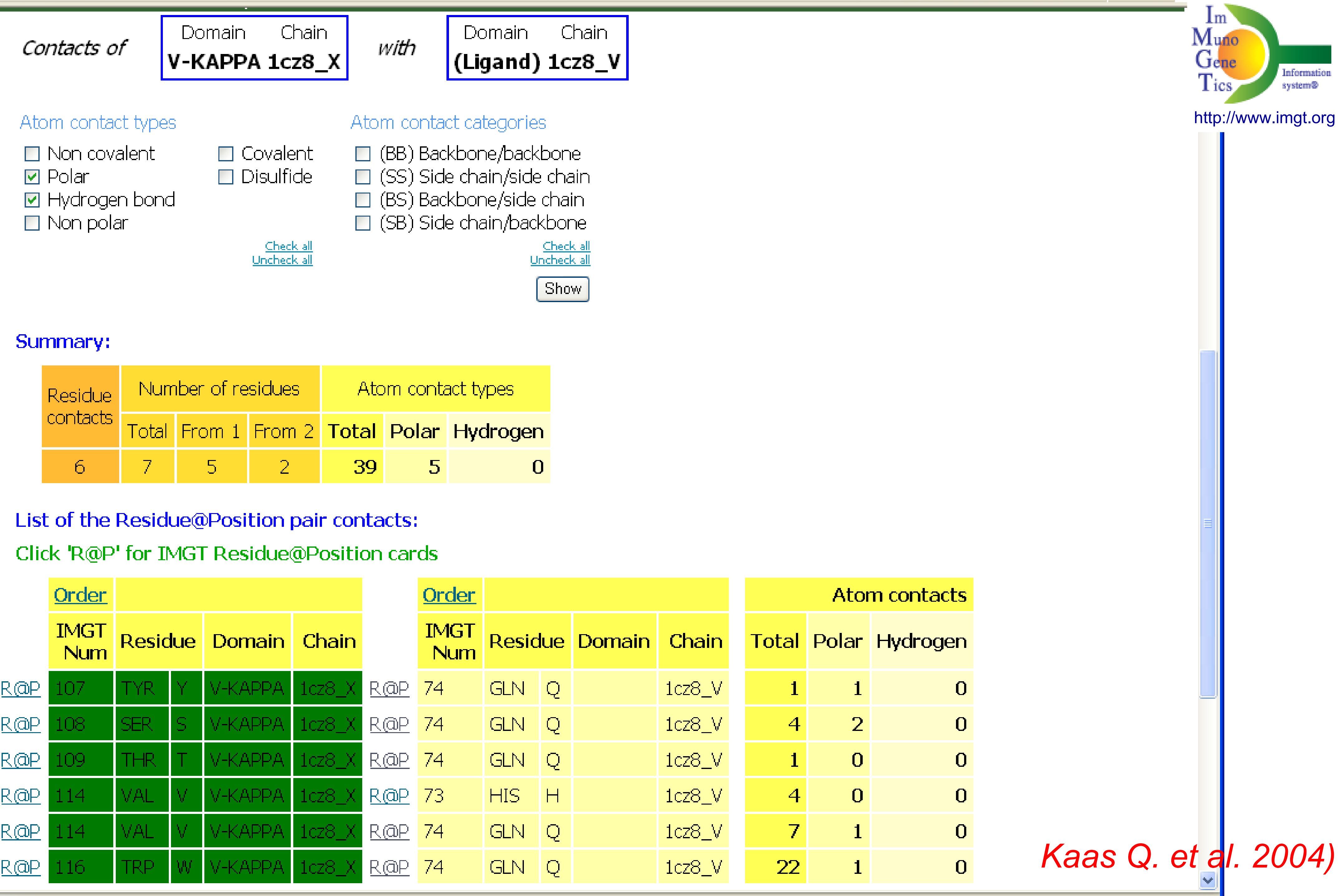
List of the Residue@Position pair contacts:

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

http://www.imgt.org

Kaas Q. et al. 2004)



Contacts of

Domain	Chain
V-KAPPA	**1cz8_X**

with

Domain	Chain
(Ligand)	**1cz8_V**

Atom contact types

☐ Non covalent
☑ Polar
☑ 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

Kaas Q. et al. 2004)

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

CDR-IMGT lengths [10.7.24]

Im Muno Gene Tics Information system®

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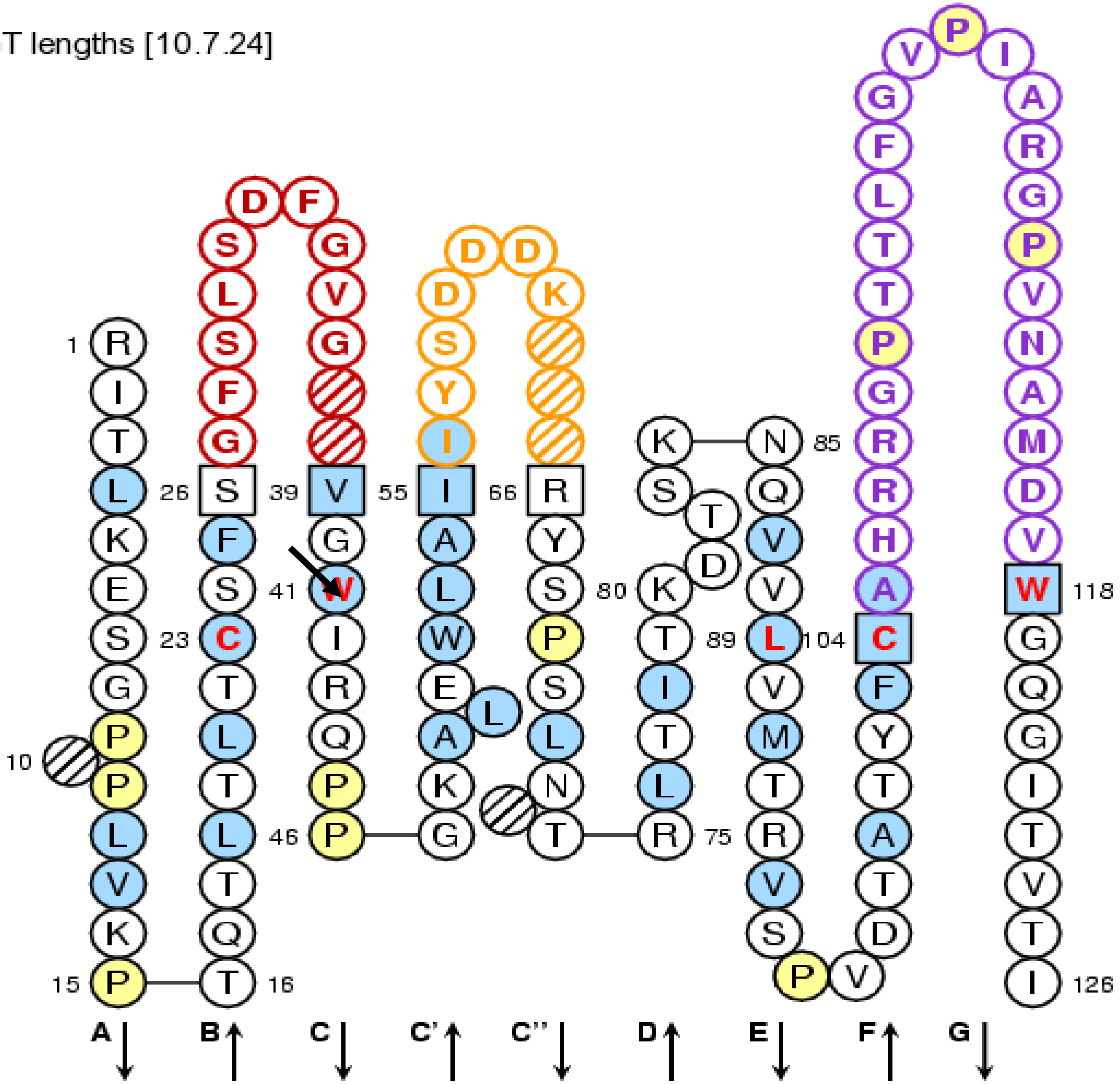
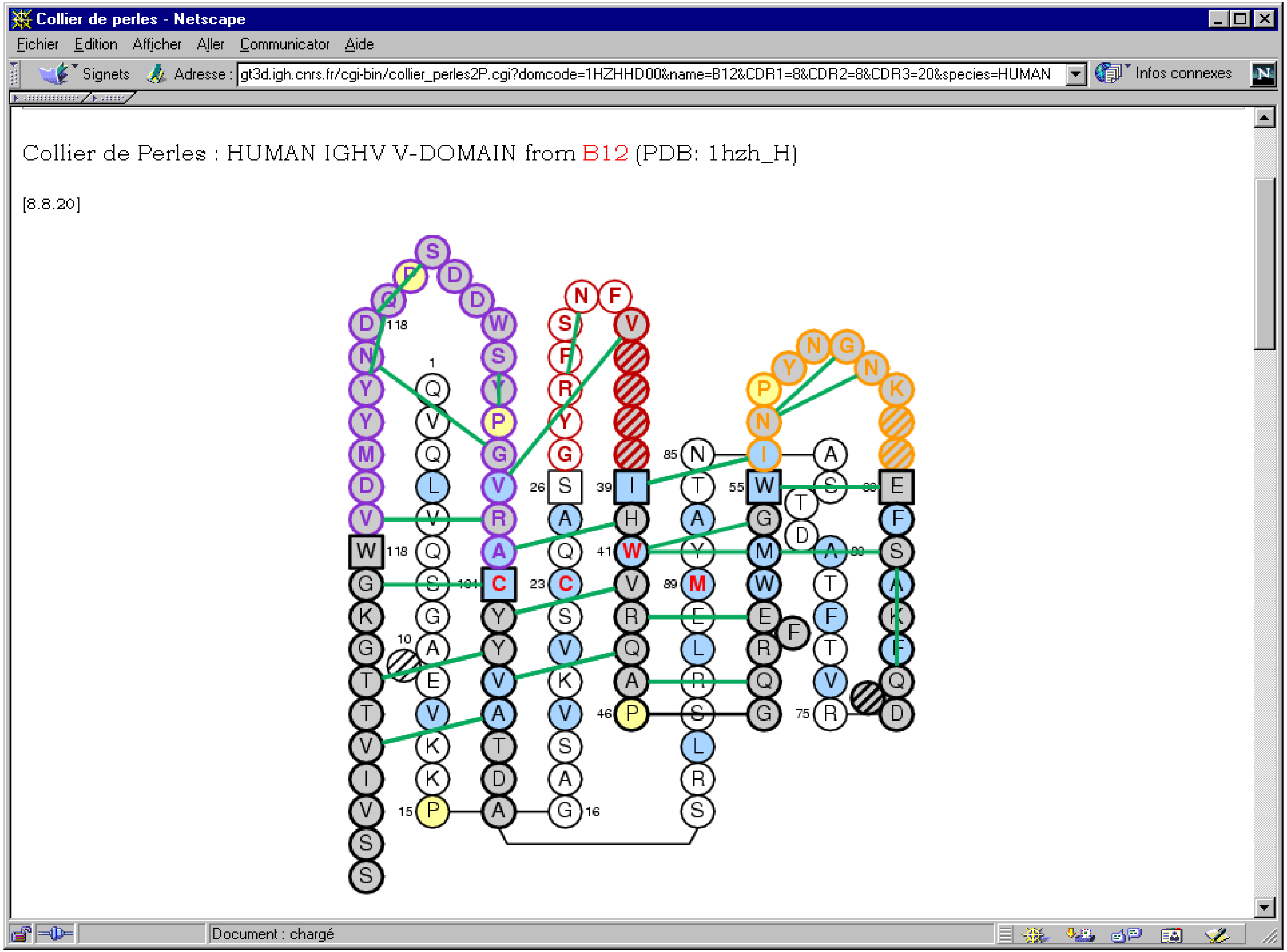


Kaas Q. et al. NAR 32, D208-D210 (2004)

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

http://www.imgt.org



Adresse : gt3d.igh.cnrs.fr/cgi-bin/collier_perles2P.cgi?domcode=1HZHHD00&name=B12&CDR1=8&CDR2=8&CDR3=20&species=HUMAN

Collier de Perles : HUMAN IGHV V-DOMAIN from B12 (PDB: 1hzh_H)

[8.8.20]

Document : chargé

Kaas Q. et al. NAR 32, D208-D210 (2004)

http://www.imgt.org

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 111.1G 112.1S
trastuzumab	[8.8.13]		55R	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]			

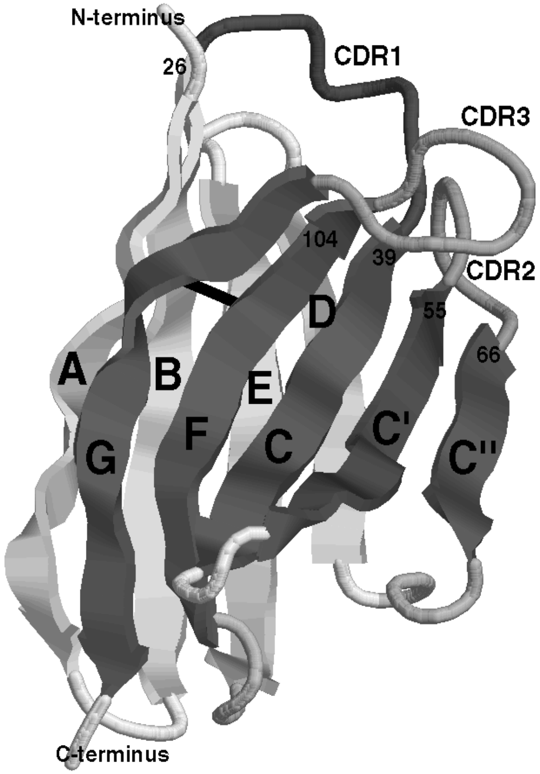
Magdelaine-Beuzelin C. et al. Crit. Rev. Oncol. Hemat. 2007

Structural domains

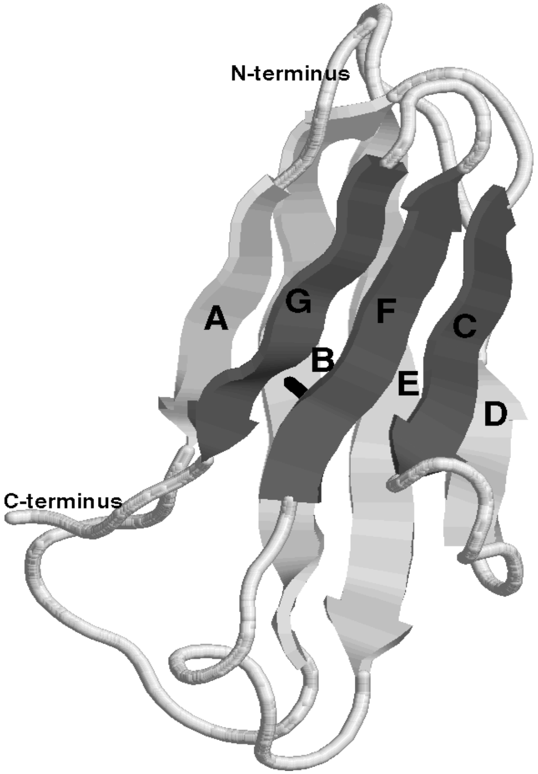
http://www.imgt.org

IG and TR

V-DOMAIN

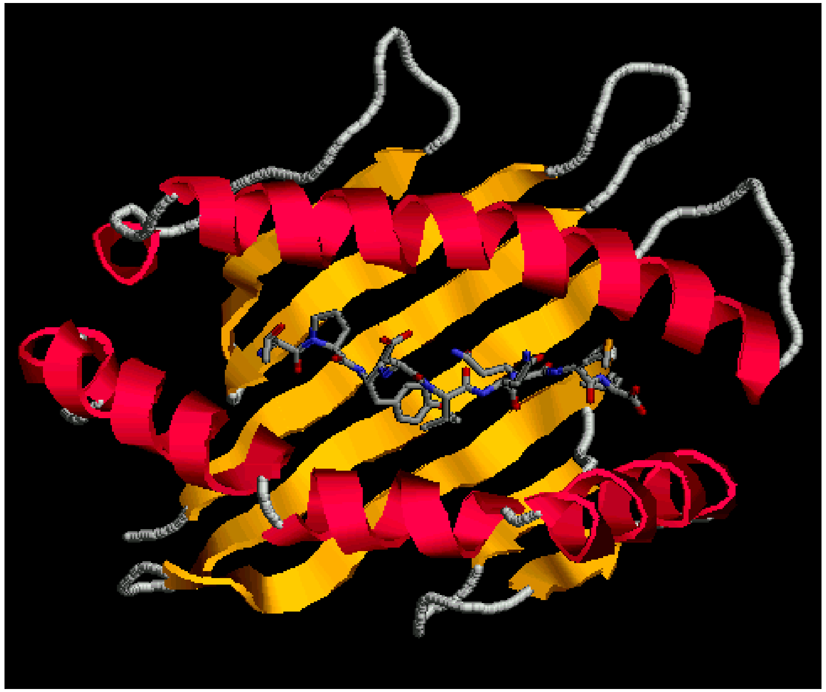


C-DOMAIN



MHC

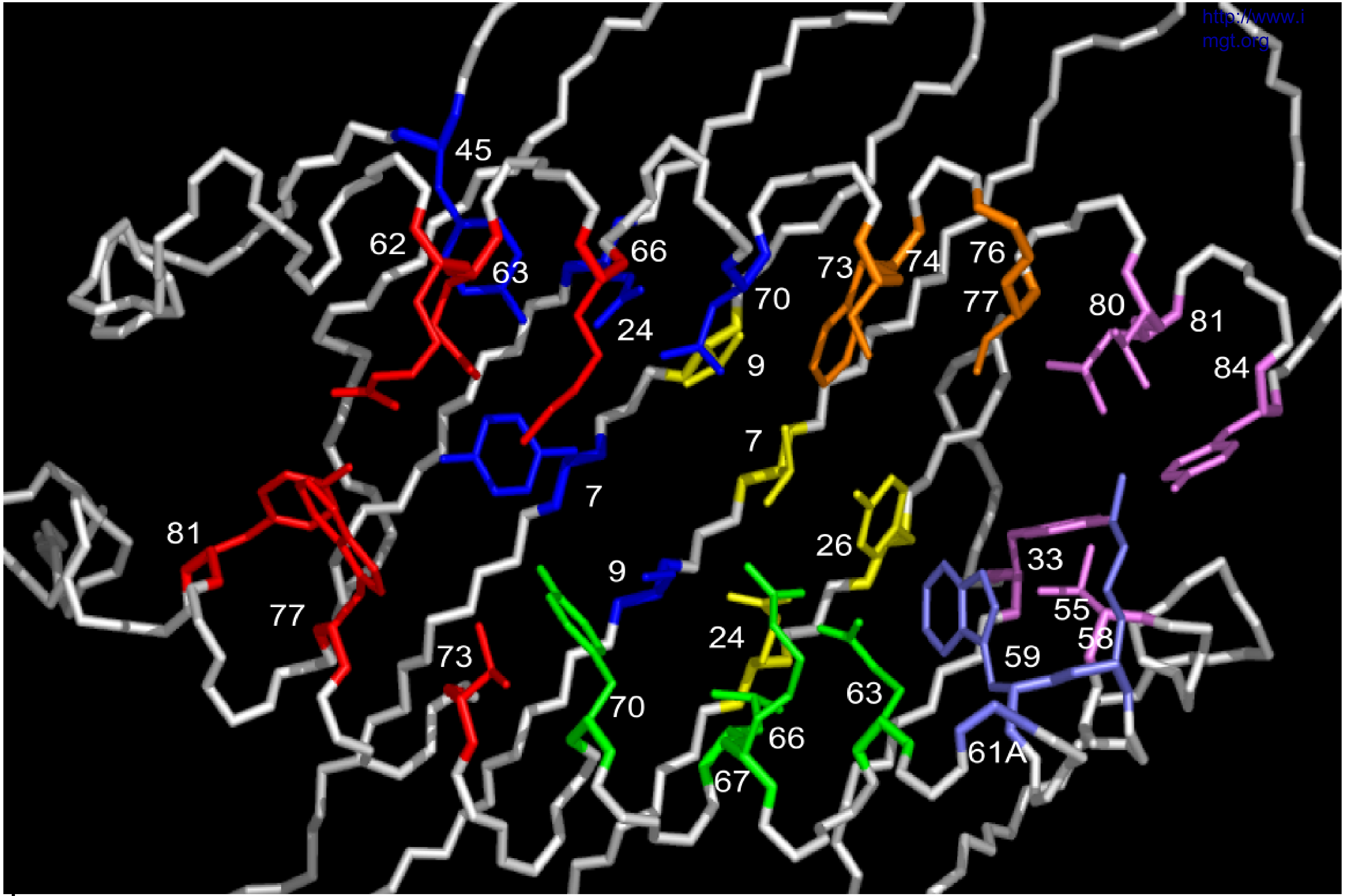
G-DOMAINs



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



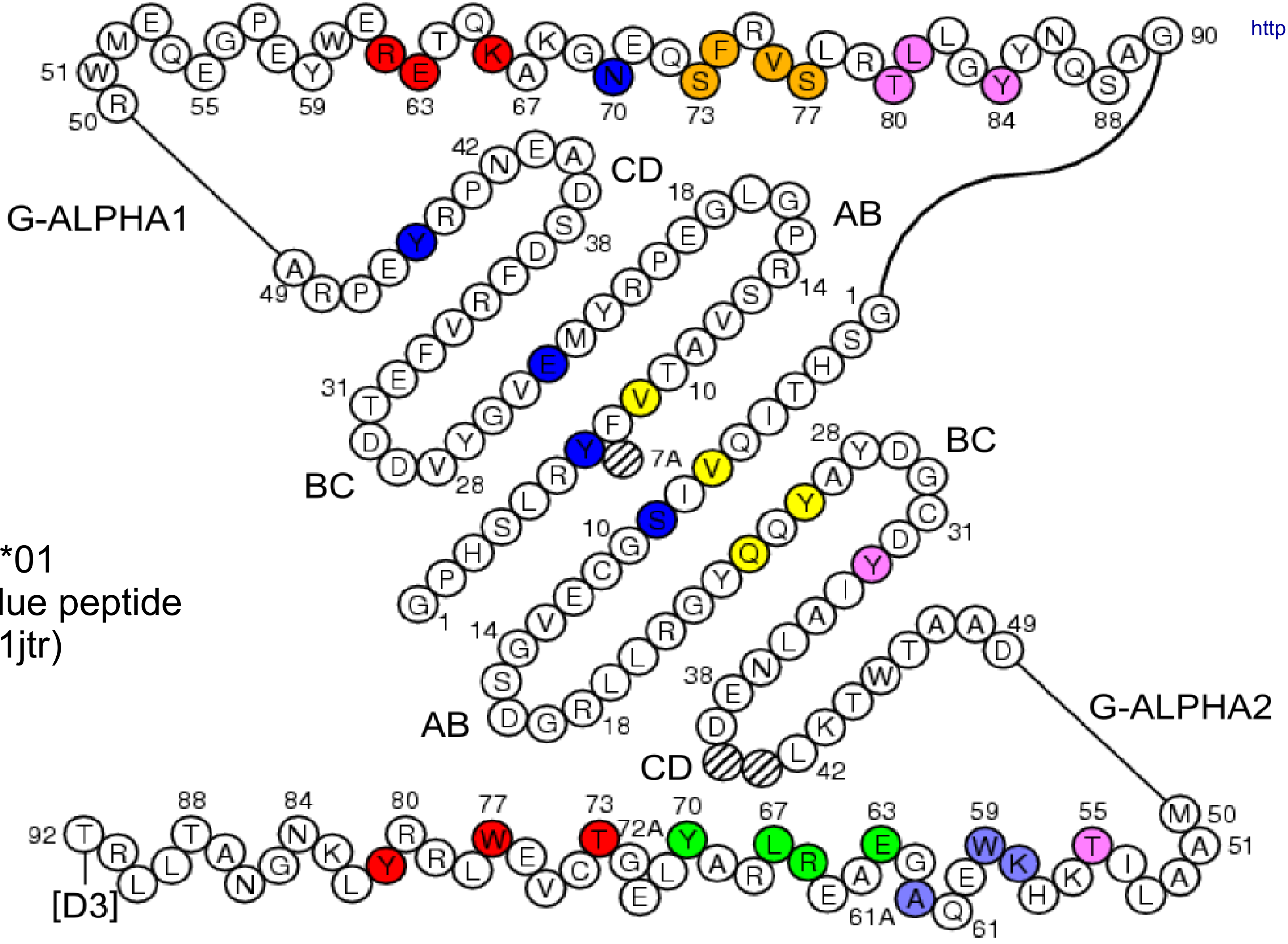
H2-K1*01
(code 1jtr)
8 residue peptide

Kaas and Lefranc In Silico Biology 2005

MHC class I IMGT contact sites

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

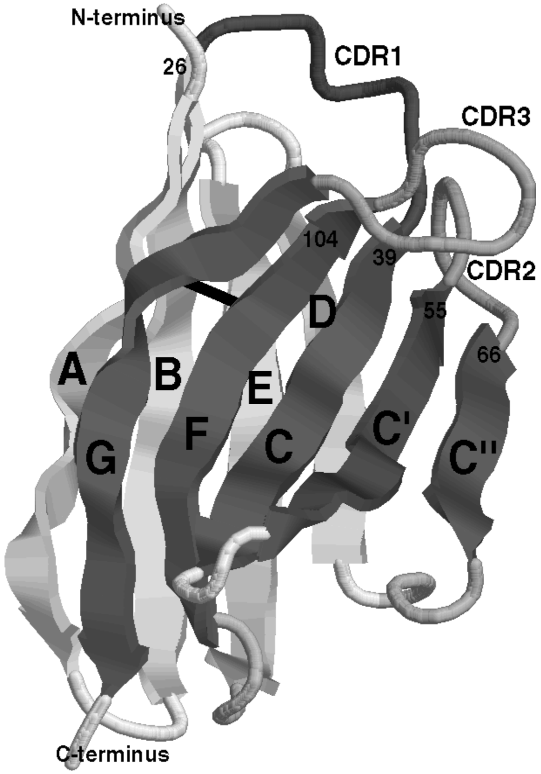
http://www.imgt.org

V-DOMAIN (IG,TR)

AND

V-LIKE-DOMAIN

(other than IG,TR)

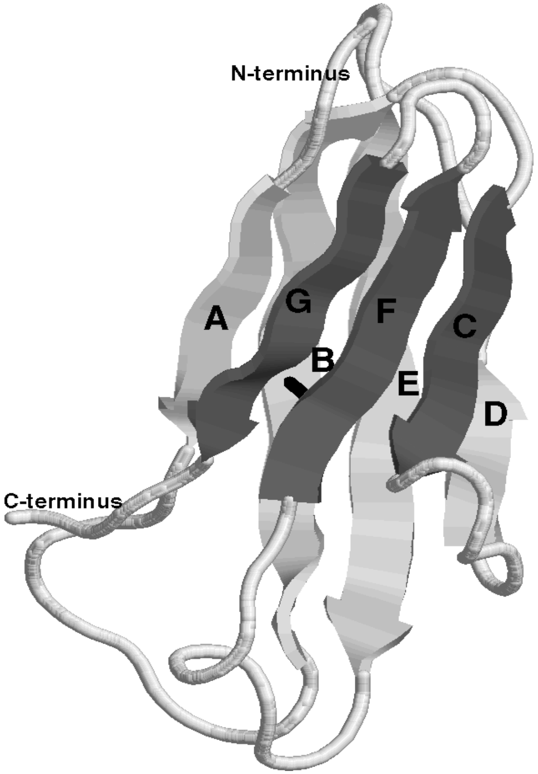


C-DOMAIN (IG,TR)

AND

C-LIKE-DOMAIN

(other than IG,TR)

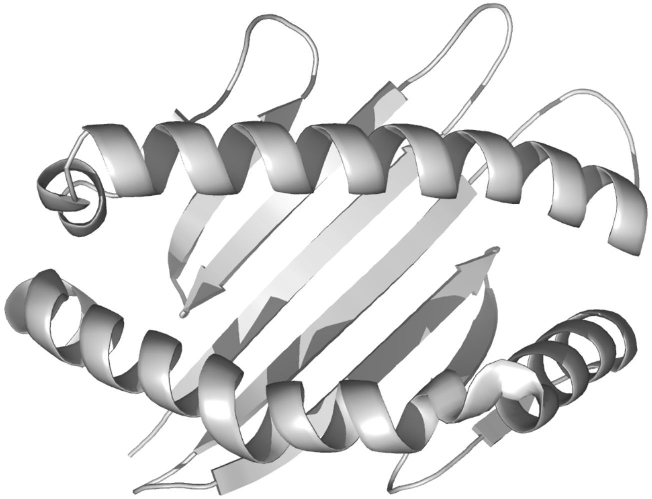


G-DOMAIN (MHC)

AND

G-LIKE-DOMAIN

(other than MHC)

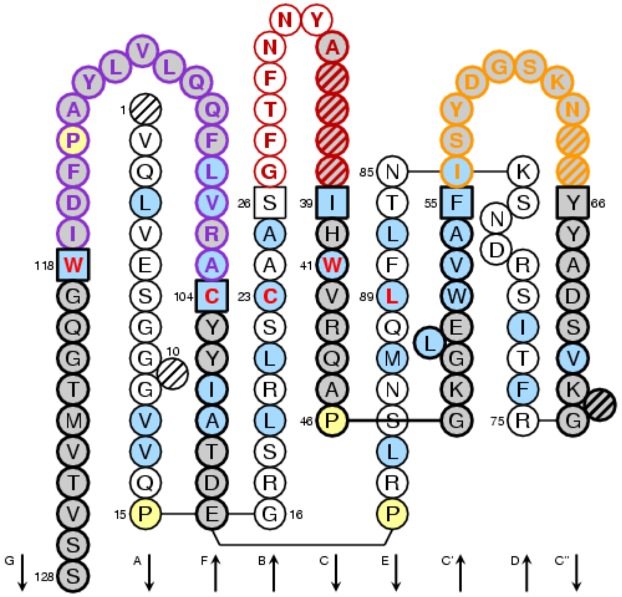


Immunoglobulin superfamily (IgSF)

MHC superfamily (MhcSF)

V-LIKE-DOMAIN

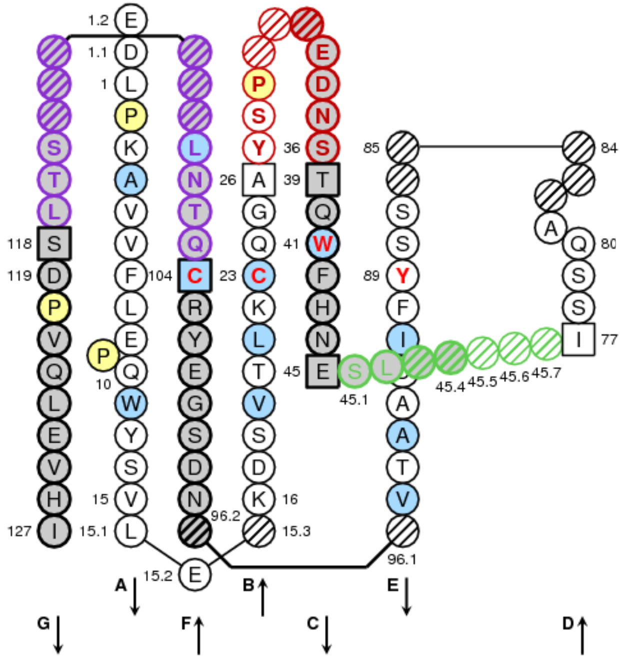
MOG



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

C-LIKE-DOMAIN

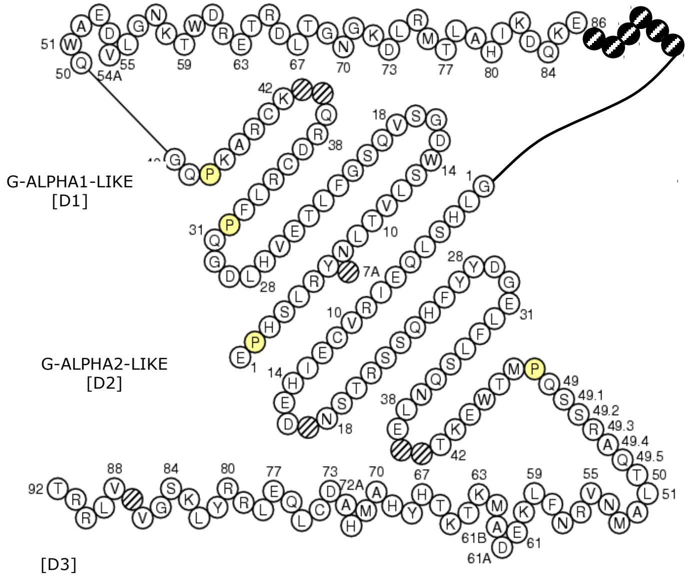
FCGR3B



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

G-LIKE-DOMAIN

MICA



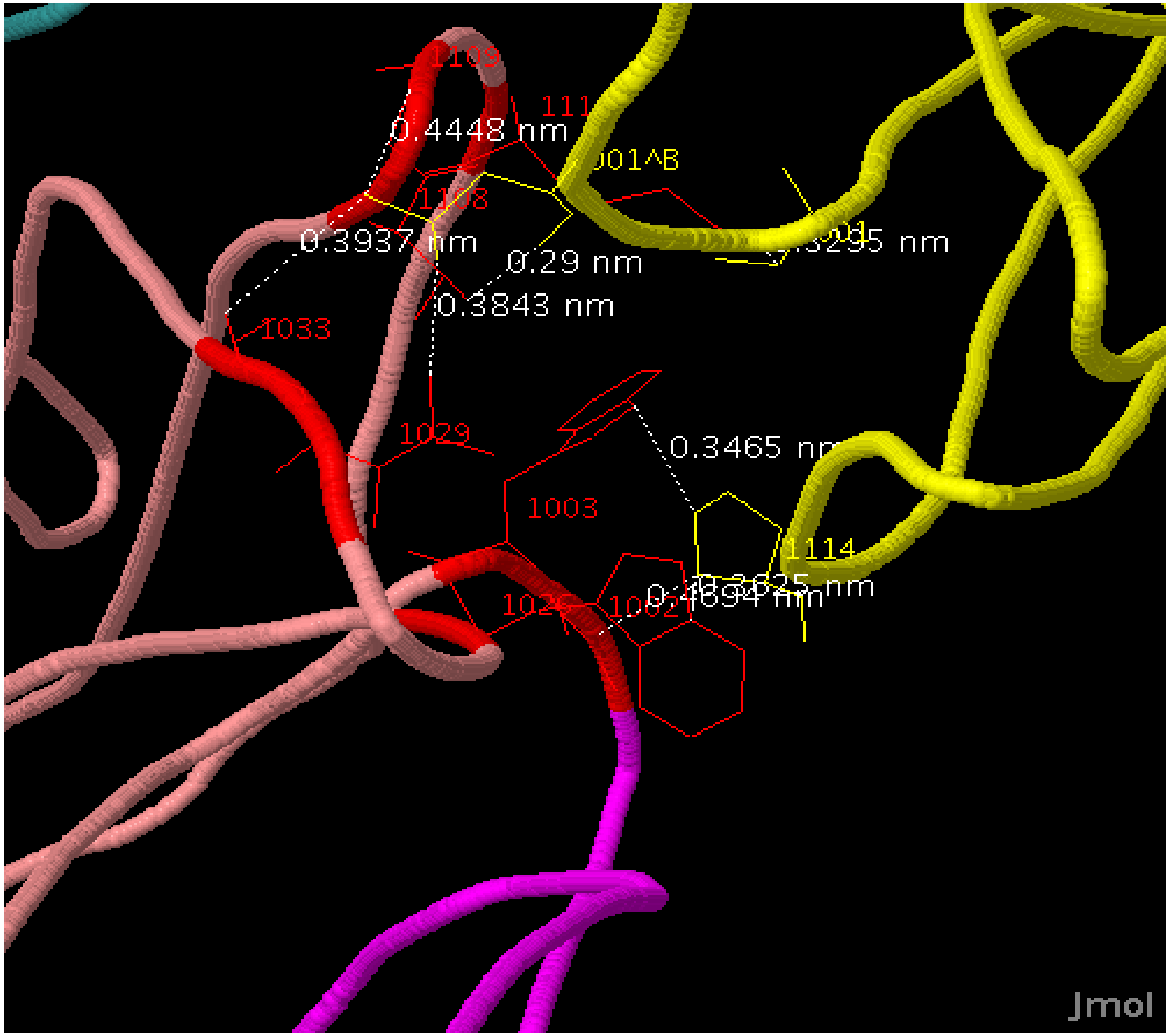
Frigoul, A. et al., Recent Res. Develop. Human Genet., 3, 95-145 (2005)

Interactions between domains

IMGT logo
http://www.imgt.org

FCGR3B

[D2]
C-LIKE-
DOMAIN



IGHG1
(FC-GAMMA1)

CH2
C-DOMAIN

[D1] C-LIKE-DOMAIN