

Bioinformatique: du gène à la structure

Marie-Paule Lefranc

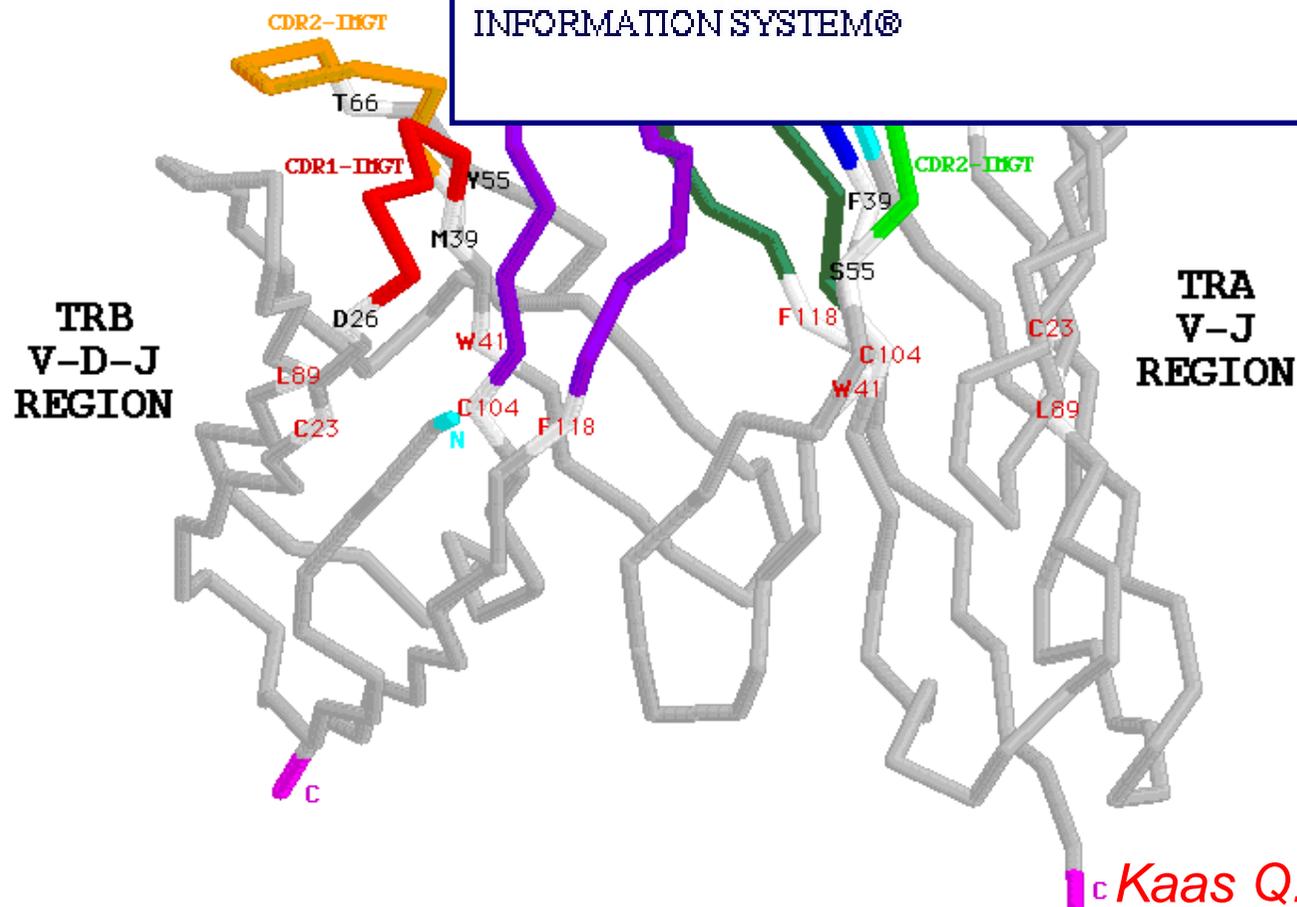
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FMBS312, Master recherche 2 Bio-Med, TC3,
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30 septembre 2013

IMGT/3Dstructure-DB

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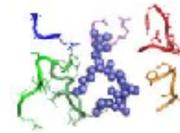
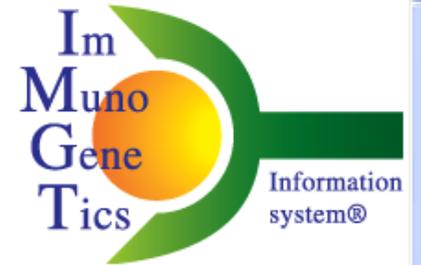


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Entry code

[Query page](#)

IMGT/3Dstructure-DB card for : 1ce1

IMGT protein name	IMGT receptor type	IMGT receptor description	Ligand(s)	Species	CC	Chain ID
CAMPATH-1H, alemtezumab , 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
- Polar
- Hydrogen bond
- Non polar
- Covalent
- Disulfide

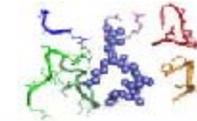
Atom contact categories

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

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IMGT/3Dstructure-DB

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		<i>Homo sapiens</i> (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	<pre>[RITLKESGPPLVKPTQTLTLTQSFSGFSLDFGVGVGWIROPPGKALEWLAIYSDDDKRYSPSINTRLTI TKDTSRNQVLLMMTRVSPV][D][IGJ1][IG DTATYFCAHRRGPTTLFGVPIARGPVNAMDVWQGI TVTI SSTSTKGPSVFPPLAPCSASTAGGTAALGCLVKDYFPEPVTVSWNSGALTS HC1 GVHTFPAVLQSSGLYSLSSVVTVPSSSLGTQTYTQNVNHNKPSNTKVDKRVKPS</pre>	
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]
		<pre>[CDR1] [CDR2] RITLKESGP . PLVKPTQTLTLTQSFSGFSLDFGVG . . VGIROPPGKALEWLAIYSDDDK . . . RYSPSIN . TRLTI TKDTSRNQVLLV [CDR3] MTRVSPVDTATYFCAHRRGPTTLFGVPIARGPVNAMDVWQGI TVTI</pre>
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]

Chain ID		1u8k_A
IMGT chain description	L-KAPPA	
Chain amino acid sequence	<pre>[ALQLTQSPSSLSASVGDRI TI TGRASQGVTSALAWYRQKPGSPPOQLLIYDASSLESQVPSRFRSGSGTEFTLTI STLRPEDFATYYCQQ][IGK1][LHFYPHTFGGTRVDVRRITVAAPSVFIPFPPSDRLKSGTASVVLINNFYPREARQVQVMDNALQSGNSQESVTEQDSKDSYSLSSSTLT] LSKADYEKHKVYEQGVTHQGLSSPVTKSFNRGEC</pre>	
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]
		<pre>[CDR1] [CDR2] ALQLTQSPSSLSASVGDRI TI TGRASQGVTS LAWYRQKPGSPPOQLLIYDAS SLESQVPSRFRSGSG . . SGTFTLTI [CDR3] ISTLRPEDFATYYCQQ LHF YPHTFGGTRVDVR</pre>
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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Chain ID	1u8k_B	
IMGT chain description	VH-CH1	
Chain amino acid sequence	<pre> [RI TLKESGPPLVKPTQTLTLTCSFSGFSLSDFGVGVGWIRQPPGKALEWLAI I YSDDDKRYSPSINTRLTI TKDTSKNQVVLVMTRVSPV] [D] [IGHJ_1] [DTATYFCAHRRGPTTLFGVPIARGPVNAMDVWGQGI TVTI SSTSTKGPSVFPLAPCS KSTAGGTAALGCLVKDYFPEPVTVSWNSGALTS HC_1] GVHTFPAVLQSSGLYSLSVVTVPSSSLGTQTYTQNVNHKPSNTKVDKRVEPKS </pre>	
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]
	<pre> [CDR1] [CDR2] RI TLKESGP . PLVKPTQTLTLTCSFSGFSLSDFGVG . . VGWIRQPPGKALEWLAI I YSDDDK . . RYSPSIN . TRLTI TKDTSKNQVVLV [CDR3] MTRVSPVDTATYFCAHRRGPTTLFGVPIARGPVNAMDVWGQGI TVTI </pre>	
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>

Chain ID	1u8k_B	
IMGT chain description	VH-CH1	
Chain amino acid sequence	<pre>[RI TLKESGPPLVKPTQ] [DTATYFCAHRRGPTTL HC_1 GVHTFPAVLQSSGLYS</pre>	
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]
	<pre> [CDR1] [CDR2] RI TLKESGP . PLVKPTQTLTLTCSFS GFSLSDFGVG . . VGWIRQPPGKALEWLAI IYSDDDK . . RYSPSIN . TRLTI TKDTSKNQVVLV [CDR3] MTRVSPVDTATYFCAHRRGPTTLFGVPIARGPVNAMDVWGQGI TVTI</pre>	
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	<div style="border: 1px solid black; padding: 5px; display: inline-block;">Description of domains</div> [RI TLKESGPPLVKPTQTLTLTCS... YSPSINTRLTI TKDTSKNQVVLVMTRVSPV] [D IG DTATYFCAHRRGPTTLFGVPIAR... AGGTAALGCLVKDYFPEPVTVSWNSGALTS HC_1 GVHTFPAVLQSSGLYSLSSVVTVPSSSLGIQTYTQNVNHRPSNTRVDRRVEPKS	
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]
	[CDR1] [CDR2] RI TLKESGP . PLVKPTQTLTLTCS... SGFSLSDFGVG . . VQWIRQPPGKALEWLA I IYSDDDK . . . RYSPSIN . TRLTI TKDTSKNQVVLV [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%),	

Gaps according to IMGT numbering

CDR-IMGT lengths

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, alemtezumab , 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

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](#)

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		
IMG T Num	Residue	Domain	Chain		IMG T 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

	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

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

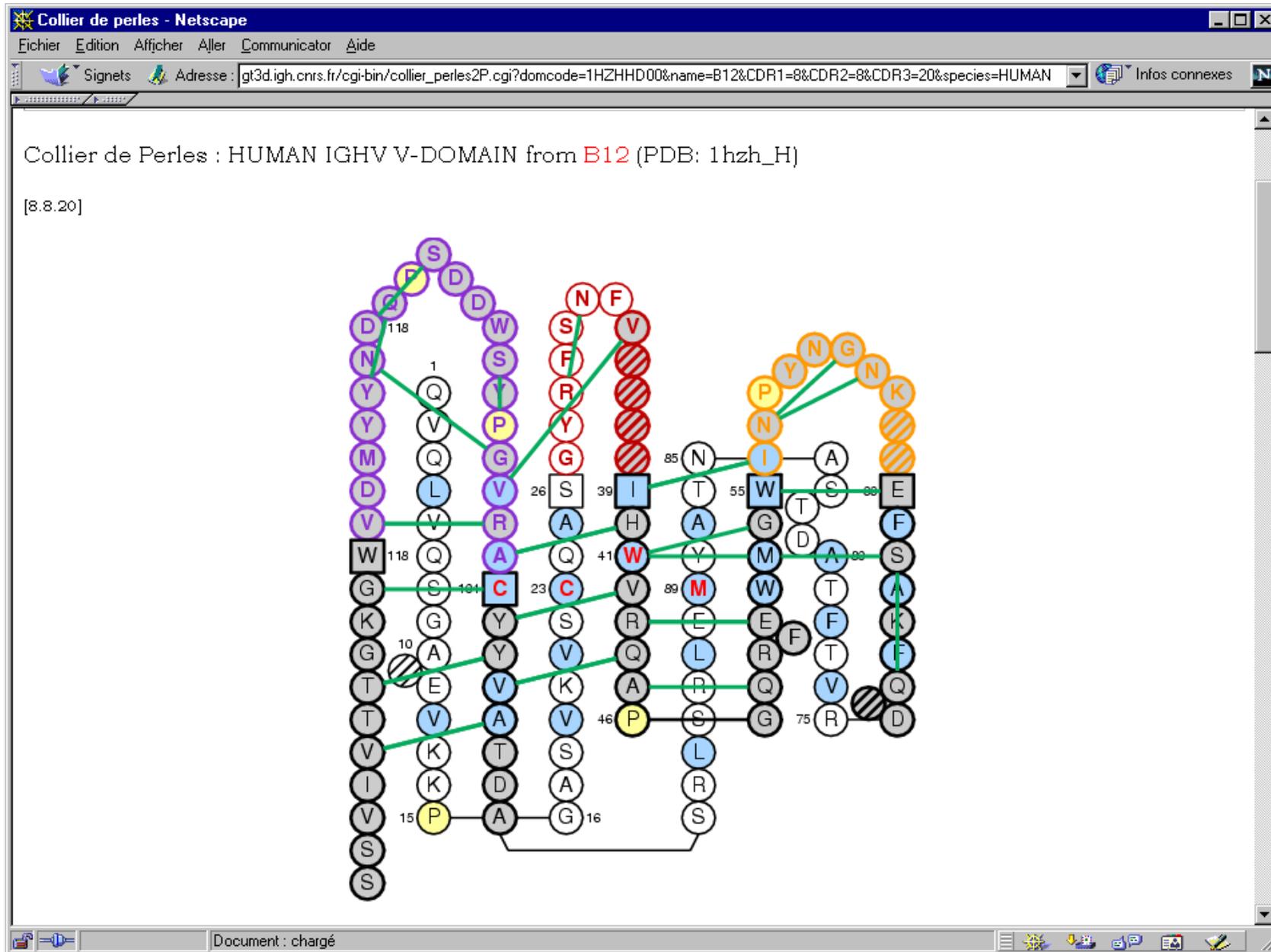
List of the Residue@Position pair contacts:

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

R@P	Order					R@P	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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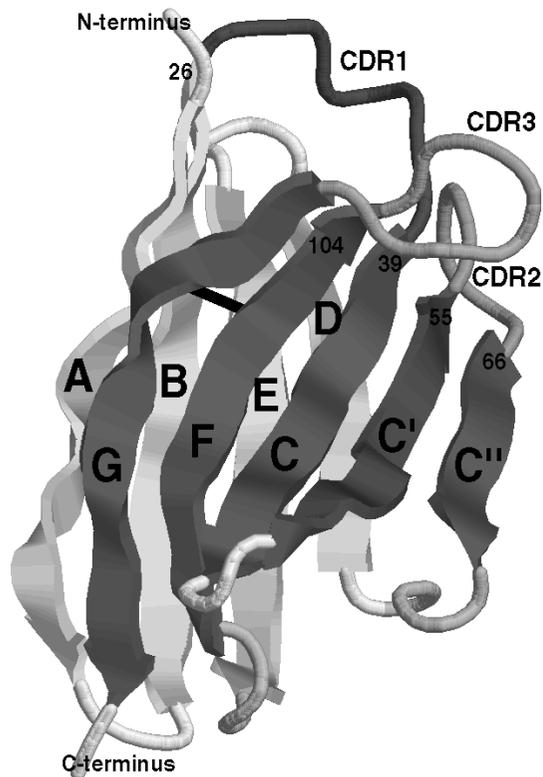
IMGT/3Dstructure-DB: analysis of 3D structures



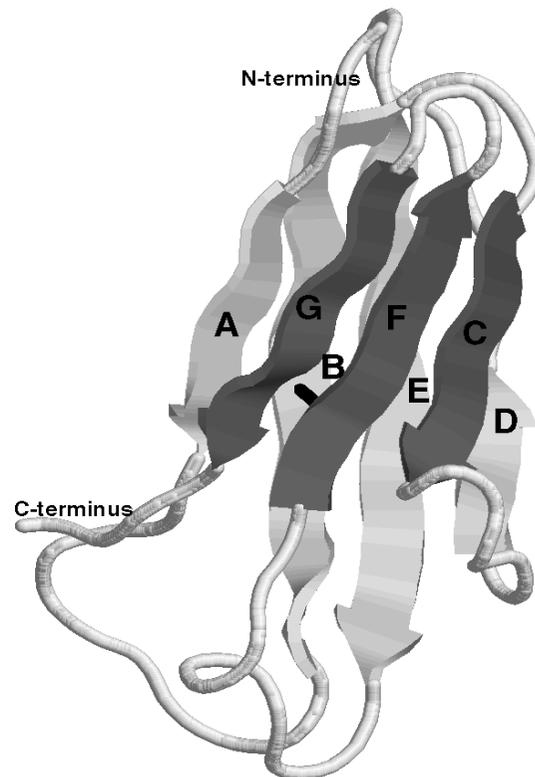
Structural domains

IG and TR

V-DOMAIN



C-DOMAIN



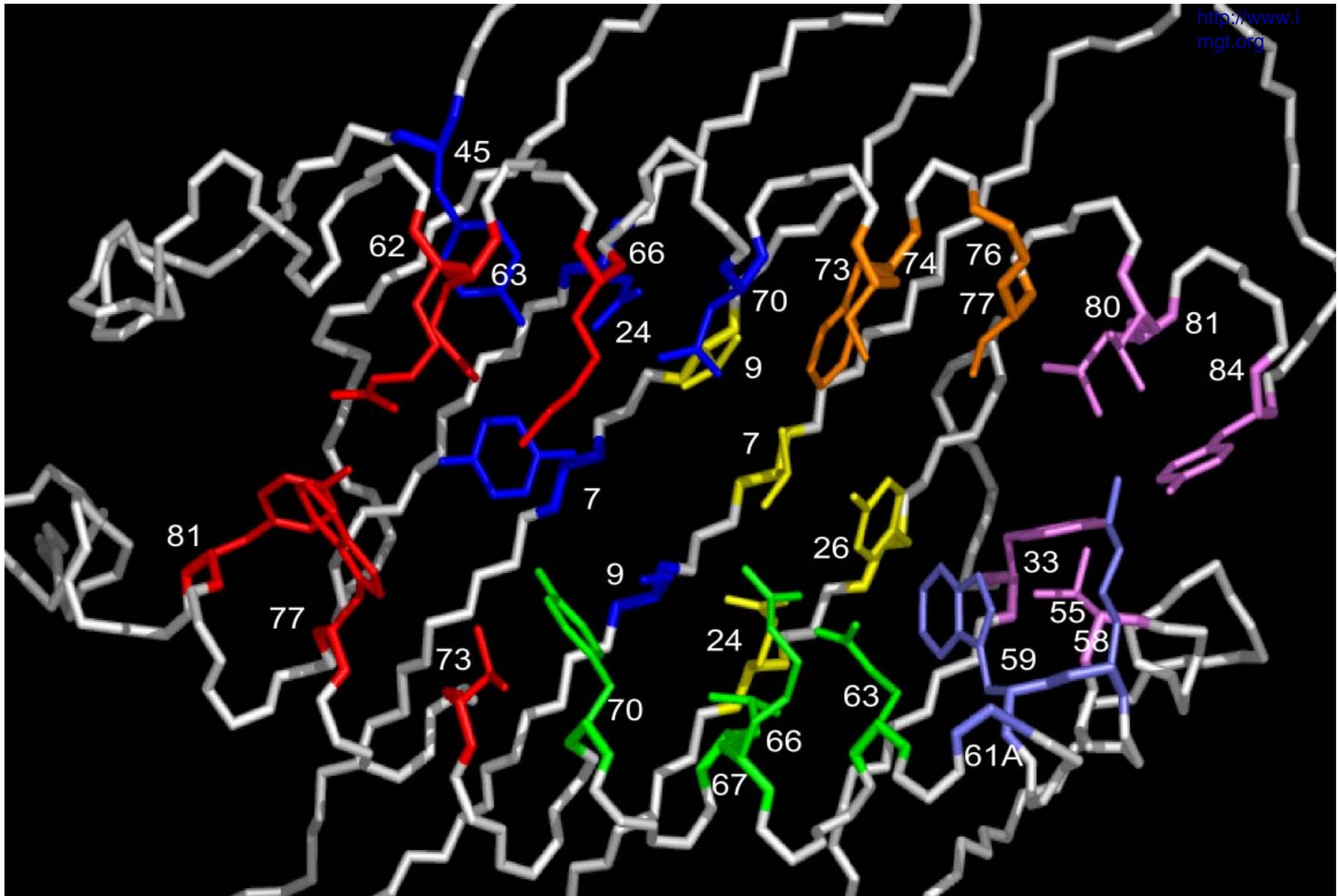
MHC

G-DOMAINS



MHC class I IMGT contact sites

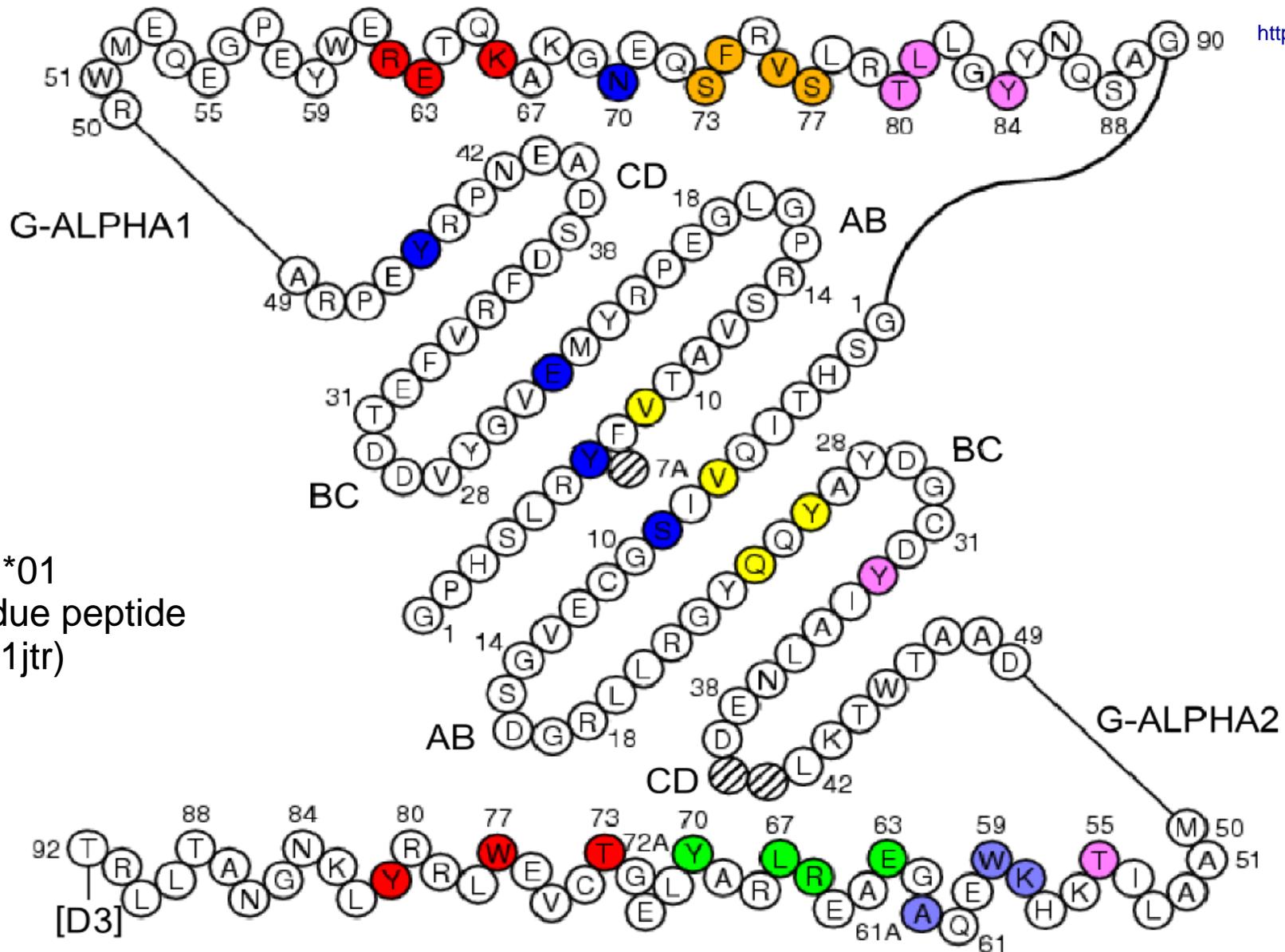
C1	■	1 E
C2	■	--
C3	■	2 Q
C4	■	3 Y
C5	■	(4 K)
C6	■	5 F
C7	■	--
C8	■	--
C9	■	6 Y
C10	■	7 S
C11	■	8 V



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

MHC class I IMGT contact sites

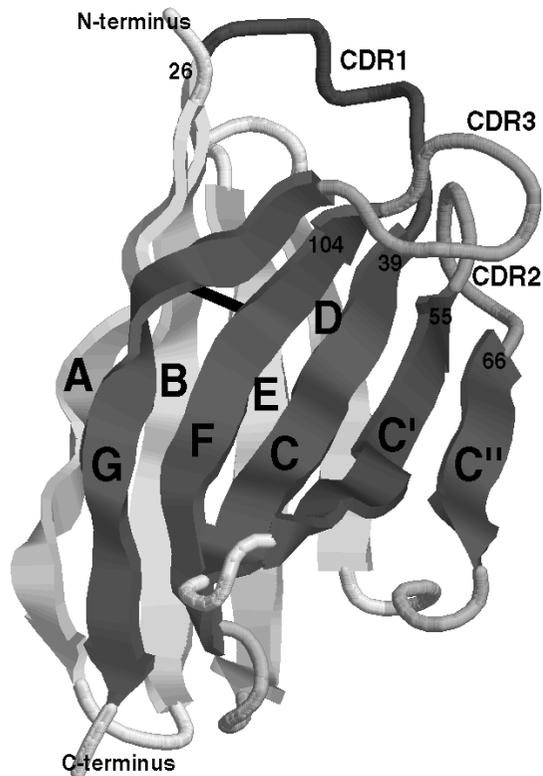
C1	1 E
C2	--
C3	2 Q
C4	3 Y
C5	(4 K)
C6	5 F
C7	--
C8	--
C9	6 Y
C10	7 S
C11	8 V



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

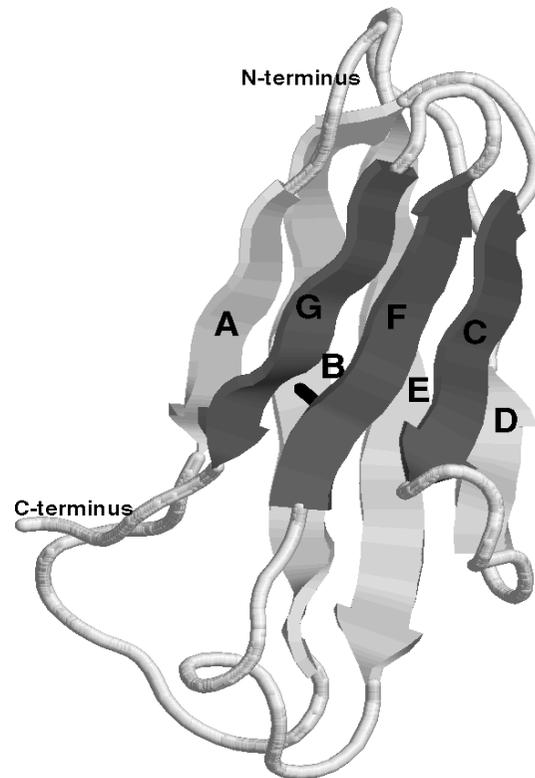
IMGT unique numbering

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

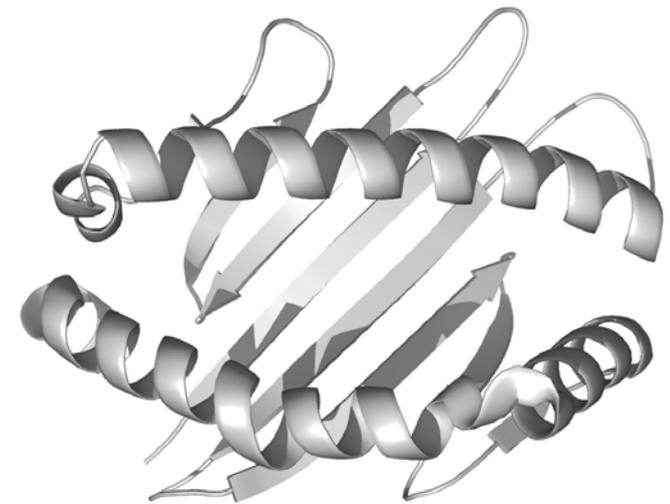


Immunoglobulin superfamily (IgSF)

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



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



MHC superfamily (MhcSF)

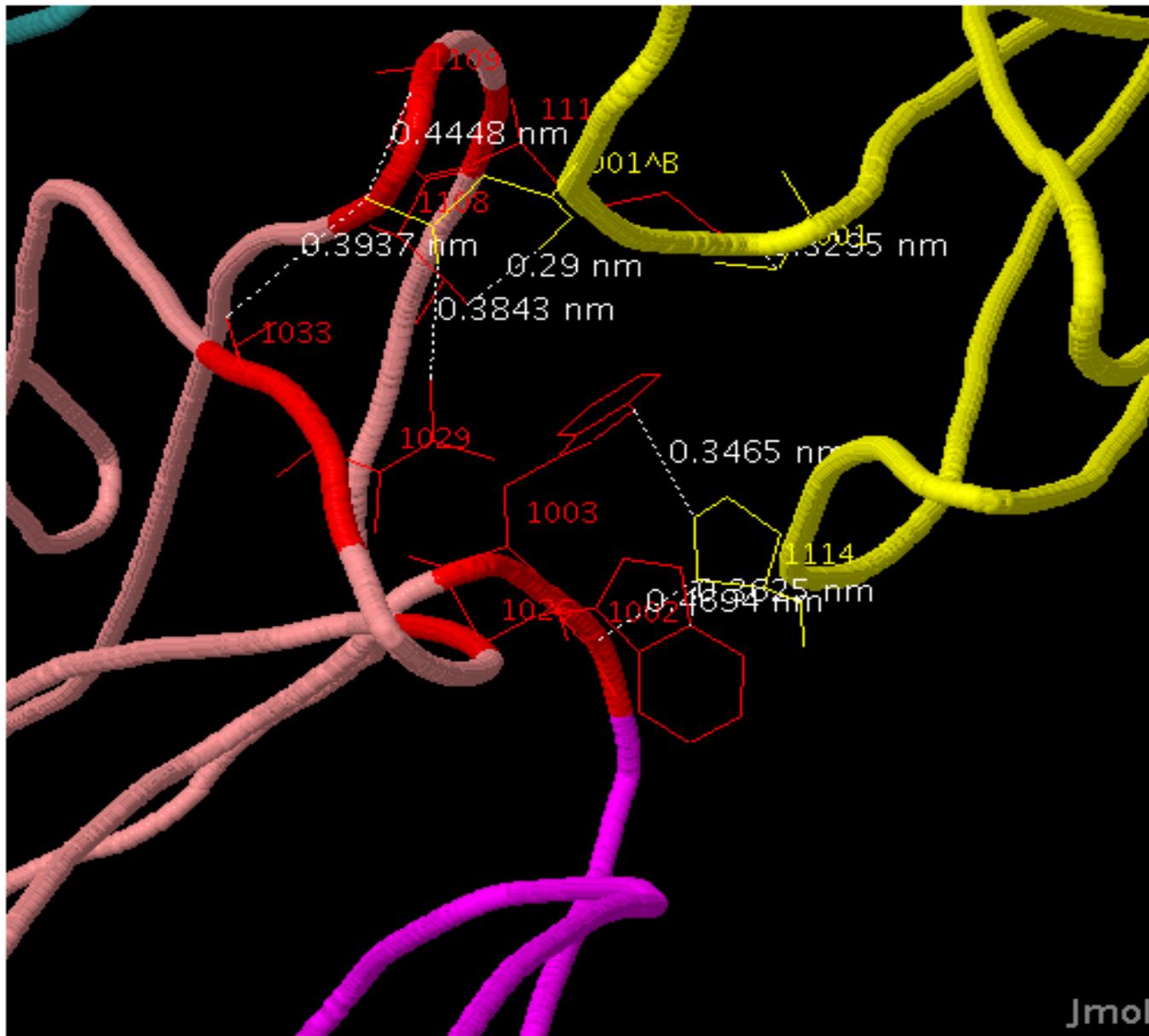
Interactions between domains

IGHG1
(FC-GAMMA1)

CH2
C-DOMAIN

FCGR3B

[D2]
C-LIKE-
DOMAIN



[D1] C-LIKE-DOMAIN

Jmol

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Muno
Gene
Tics



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