IMGT-ONTOLOGY for immunoglobulin or antibody, T cell receptor and major histocompatibility:
IG/Ag and TR/pMH interactions

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Montpellier, 08 November 2011

IMGT®: the adaptive immune response

Immunoglobulin

Vertebrates

B lymphocyte

T lymphocyte

peptide

MH

T cell receptor (TR)

molecular complex TR/pMH
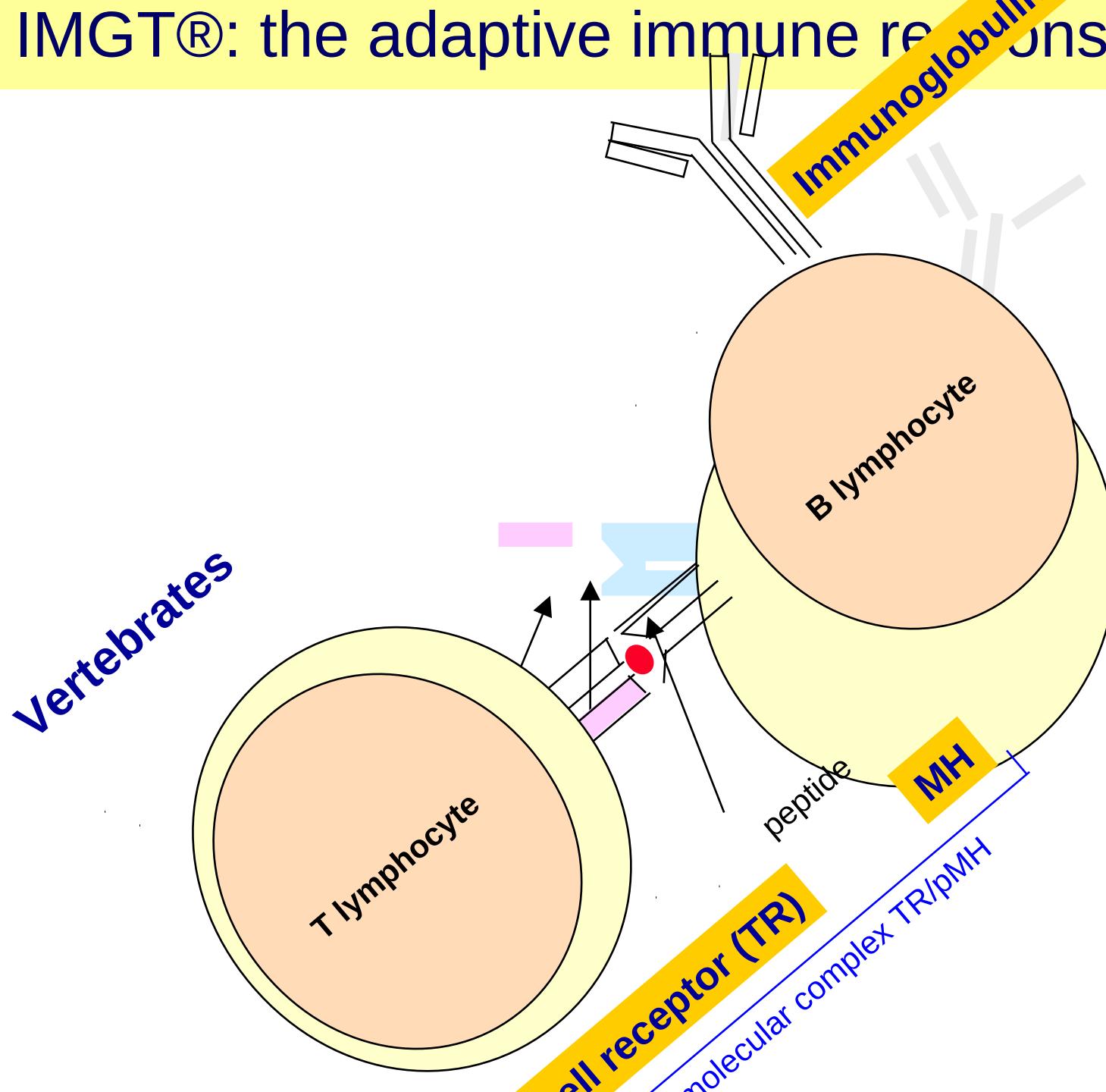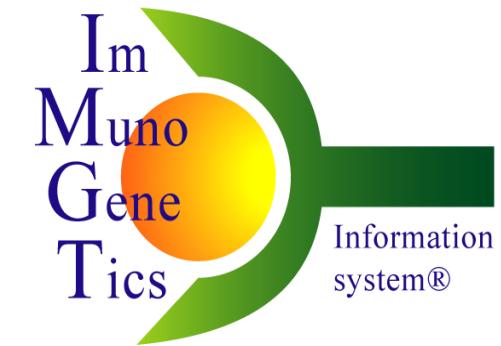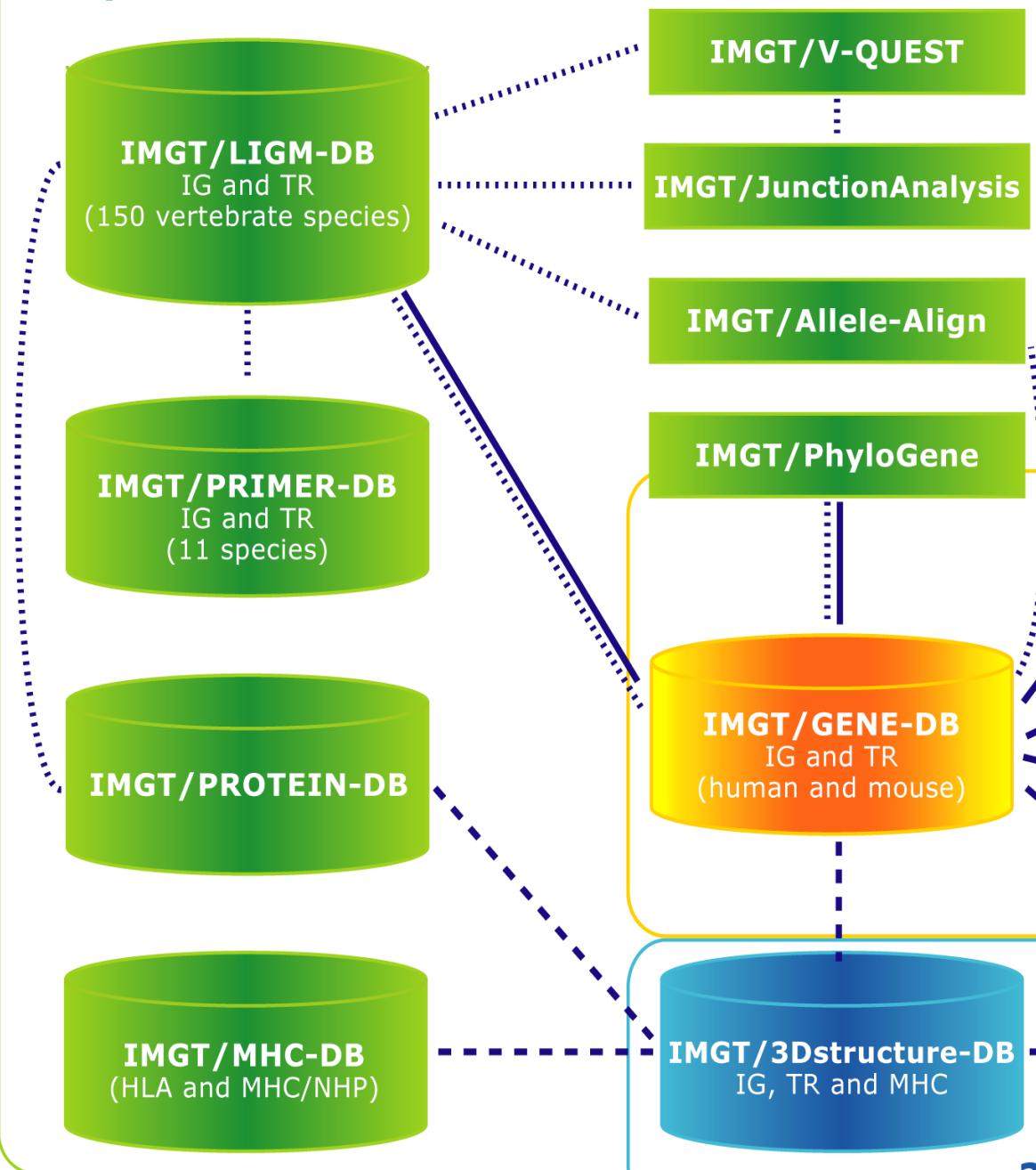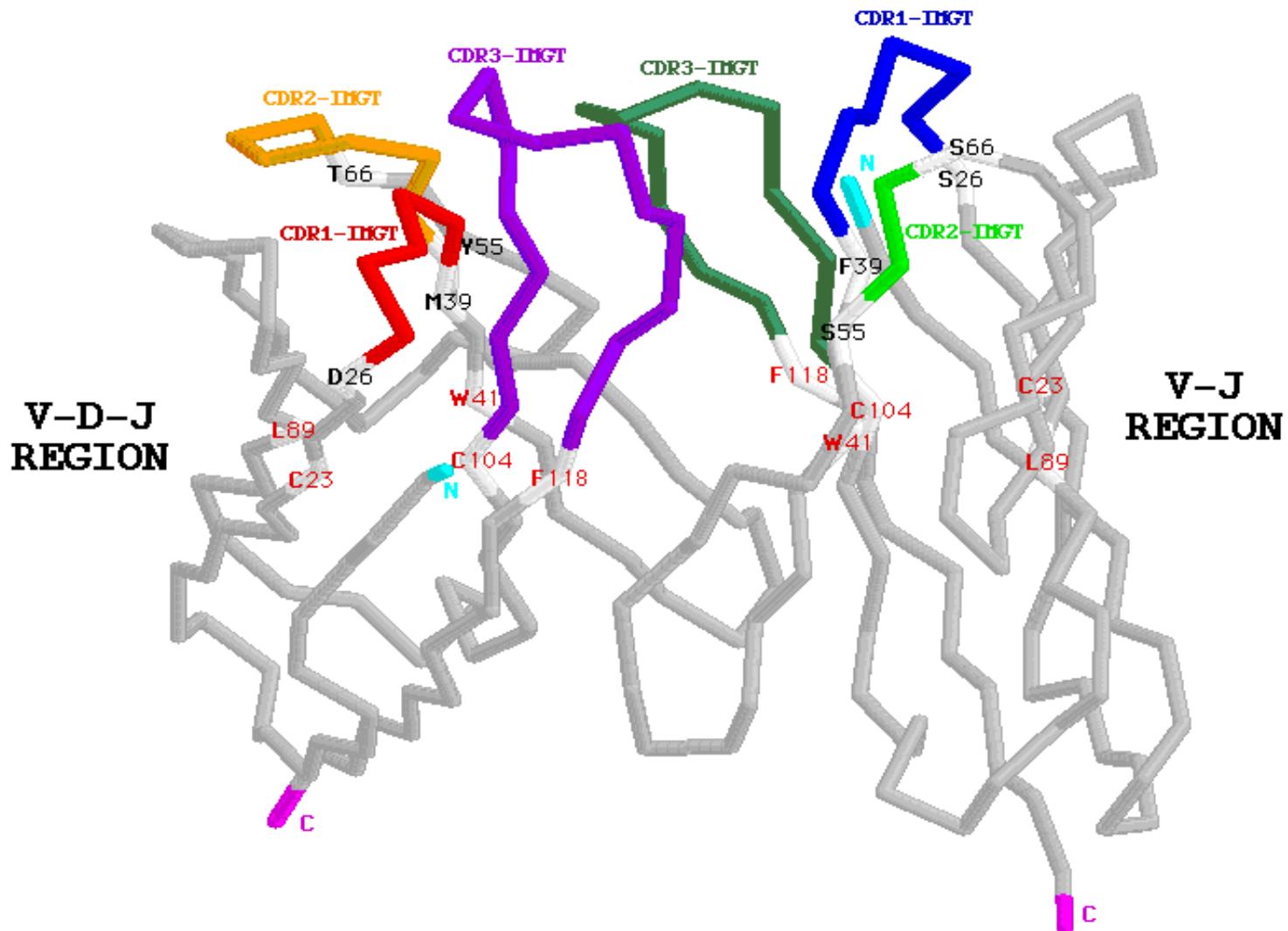
V-DOMAIN

CDR: complementarity determining region

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

IMGT Colliers de Perles for V-DOMAIN

Based on the IMGT unique numbering for V-DOMAIN

1ao7_D

1ao7_E
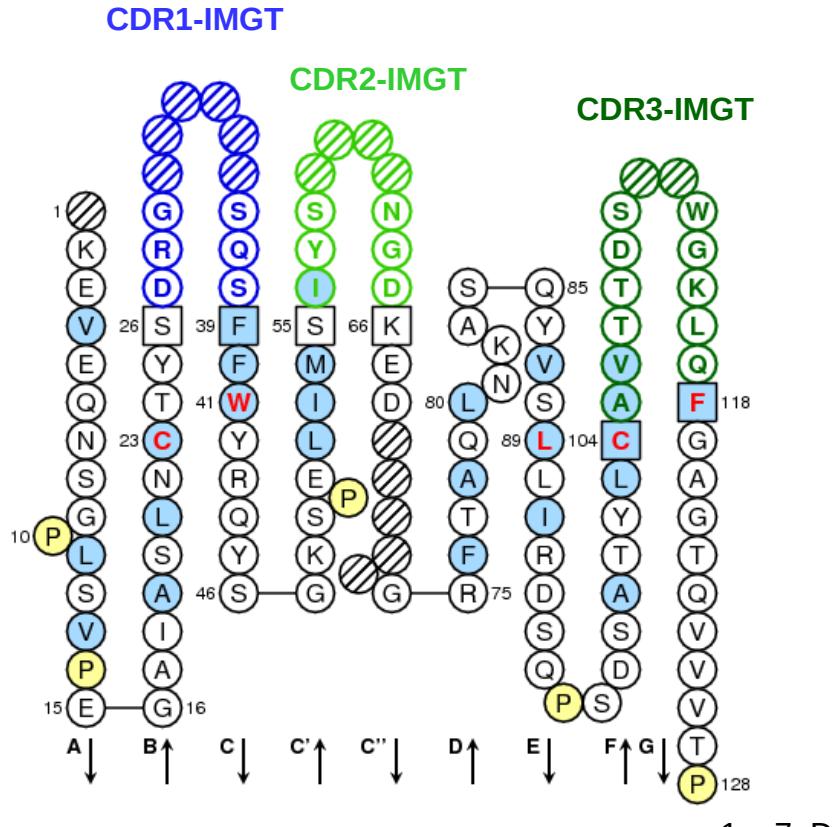
TR V-ALPHA

[6.6.11]
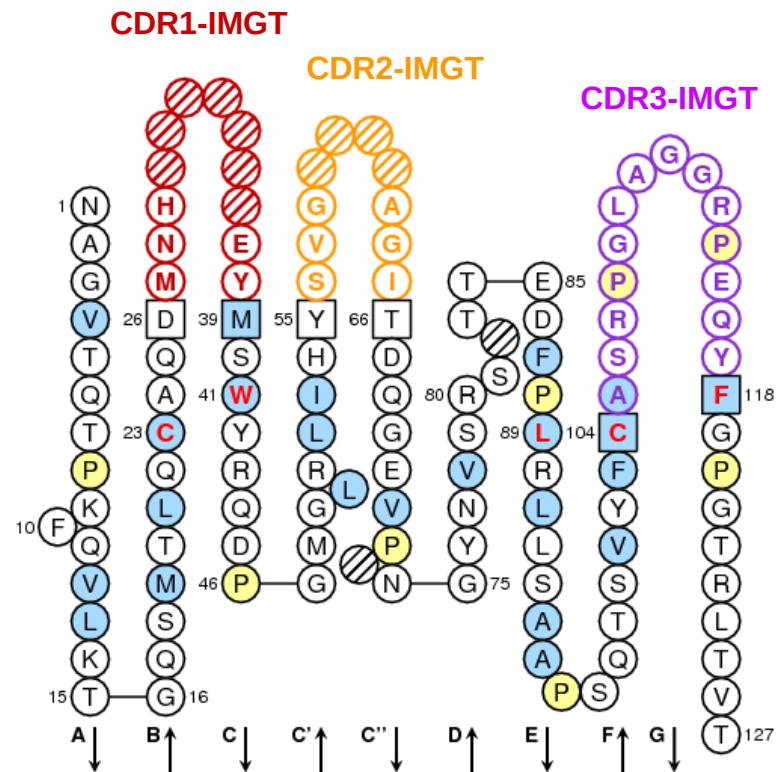
TR V-BETA

[5.6.14]

CDR: complementarity determining region

Lefranc et al., Dev. Comp. Immunol. 27, 55-77 (2003)

TR/peptide/MH (TR/pMH) complex

T cell receptor (TR)   **Peptide**   **MH1**

TR-ALPHA

V-ALPHA

C-ALPHA

C-BETA

V-BETA

TR-BETA

C

N

G-ALPHA2

I-ALPHA

C-LIKE-DOMAIN

C-LIKE-DOMAIN

G-ALPHA1

B2M
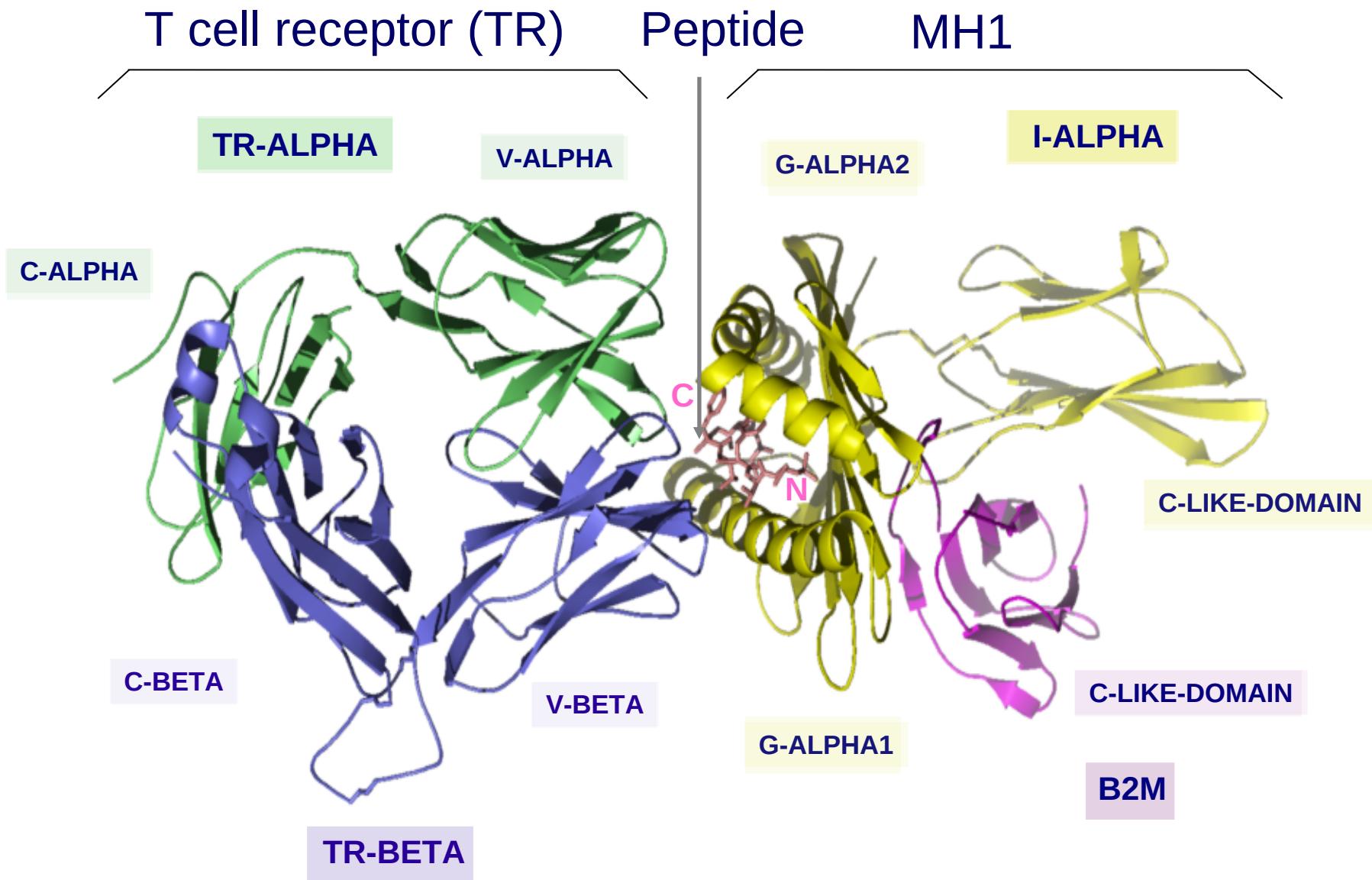
T cell receptor chains and domains

TR-ALPHA_BETA

The T cell Receptor FactsBook (2001)
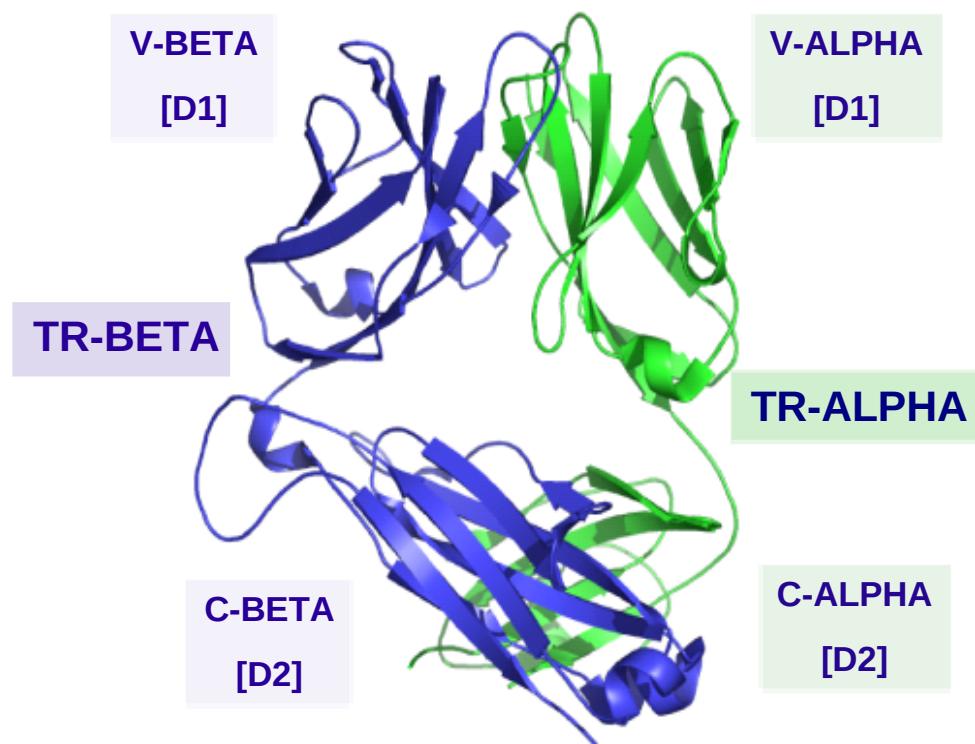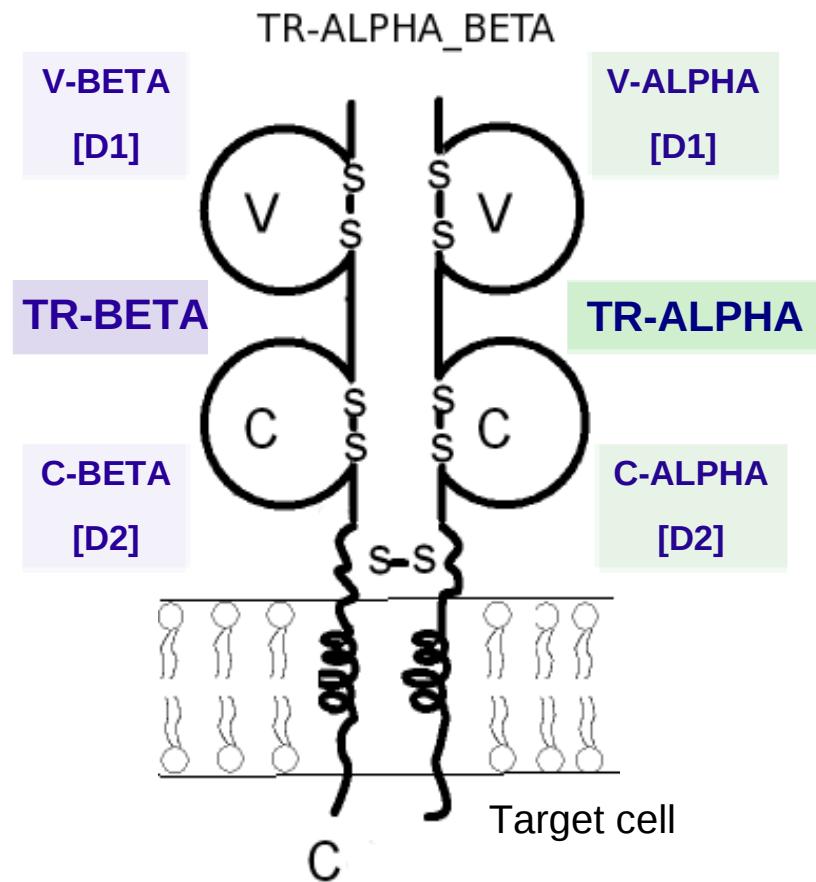
MH1 chains and domains

MH1-ALPHA_B2M

Peptide

G-ALPHA2 [D2]

G-ALPHA1 [D1]

N

C

N

I-ALPHA

B2M

C-LIKE [D3]

C-LIKE [D]

C

Target cell **(infected or tumoral cell)**

G-ALPHA2 [D2]

Peptide

G-ALPHA1 [D1]

I-ALPHA

N

B2M

C-LIKE [D3]

C-LIKE [D]

C
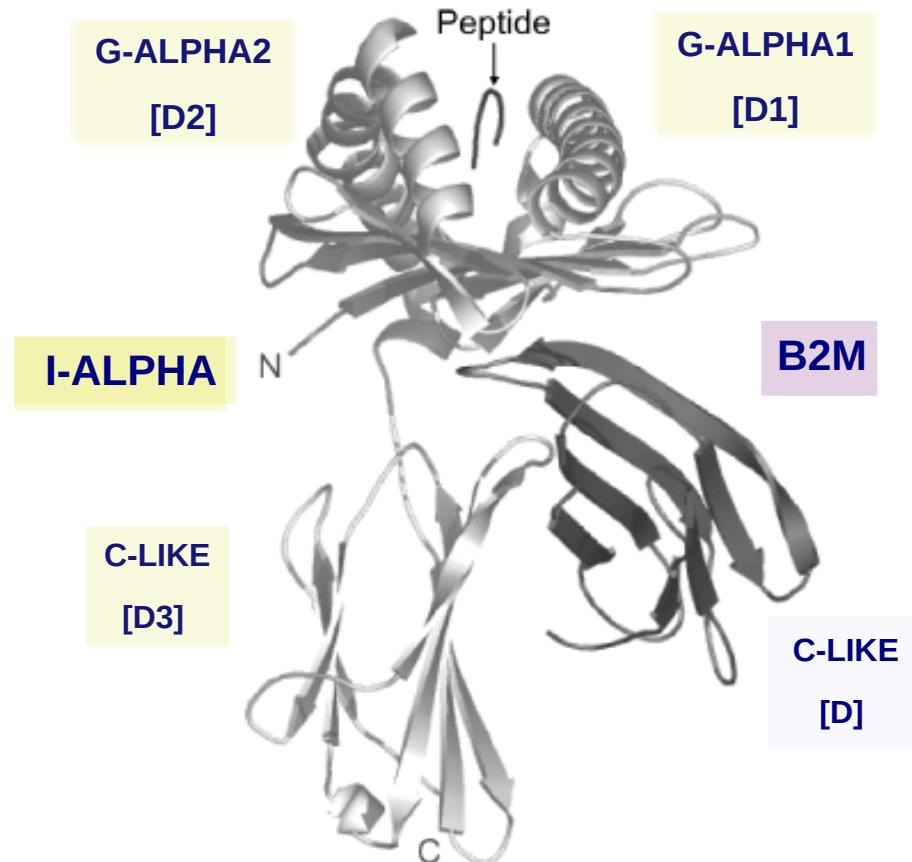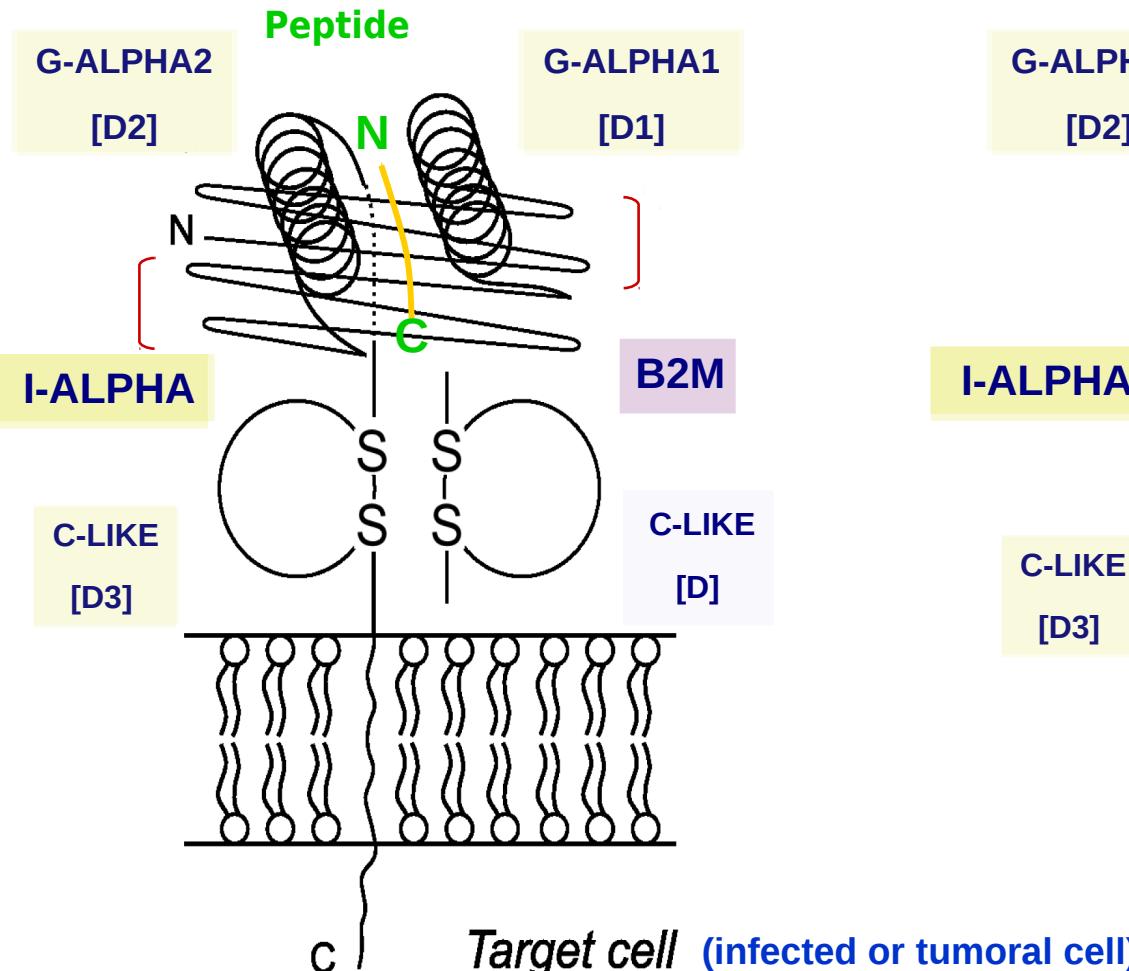
IMGT/3Dstructure-DB: Contact Analysis

Receptors **Chains** **Domains**

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

Chain and domains of 1ao7

IMGT molecule name	IMGT receptor description	Chain ID	IMGT chain description	Domain number	IMGT domain description
A6	TR-ALPHA_BETA-1	1ao7_D	TR-ALPHA	[D1]	V-ALPHA
				[D2]	C-ALPHA
		1ao7_E	TR-BETA-1	[D1]	V-BETA
				[D2]	C-BETA-1
HLA-A*0201	MHC-I-ALPHA_B2M	1ao7_A	I-ALPHA	[D1]	G-ALPHA1
				[D2]	G-ALPHA2
				[D3]	C-LIKE
		1ao7_B	B2M	[D1]	C-LIKE
Tax peptide 11-19 (Q82235)	Peptide	1ao7_C	Peptide		

Peptide

				Number of residues			Atom contact types		
	Unit 1		Unit 2	Residue contacts	Total	From 1	From 2	Total	Polar	Hydrogen
	Domain	Chain	Domain	Chain							
DomPair	V-ALPHA	1ao7_D	G-ALPHA1	1ao7_A	15	16	9	7	126	22	3
DomPair			G-ALPHA2	1ao7_A	12	15	7	8	105	17	2
DomPair			(Ligand)	1ao7_C	15	13	7	6	109	20	3

IMGT/3Dstructure-DB: Contact Analysis

Contacts between domains

	Unit 1 Domain Chain	Unit 2 Domain Chain	Residue contacts	Number of residues Total	From 1	From 2	Atom contact types Total	Polar	Hydrogen
DomPair	V-ALPHA 1ao7_D	G-ALPHA1 1ao7_A	15	16	9	7	126	22	3
DomPair		G-ALPHA2 1ao7_A	12	15	7	8	105	17	2
DomPair		(Ligand) 1ao7_C	15	13	7	6	109	20	3
DomPair		C-ALPHA 1ao7_D	4	6	4	2	27	7	1
DomPair		V-BETA 1ao7_E	57	42	20	22	401	46	7
DomPair		C-BETA-1 1ao7_E	1	2	1	1	9	2	0
DomPair	C-ALPHA 1ao7_D	V-ALPHA 1ao7_D	4	6	2	4	27	7	1
DomPair	V-BETA 1ao7_E	G-ALPHA1 1ao7_A	3	4	1	3	23	0	0
DomPair		G-ALPHA2 1ao7_A	11	10	5	5	82	17	3
DomPair		(Ligand) 1ao7_C	14	13	9	4	119	9	2
DomPair		V-ALPHA 1ao7_D	57	42	22	20	401	46	7
DomPair		C-BETA-1 1ao7_E	32	27	12	15	236	30	1

IMGT/3Dstructure-DB: Contact Analysis

Contacts of V-ALPHA with G-ALPHA1

http://www.imgt.org

Summary:

Residue contacts	Number of residues			Atom contact types		
	Total	From 1	From 2	Total	Polar	Hydrogen
15	16	9	7	126	22	3

Contacts of

Domain	Chain
V-ALPHA 1ao7_D	

with

Domain	Chain
G-ALPHA1 1ao7_A	

List of the Residue@Position pair contacts:

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

	Order IMGT Num	Residue		Domain	Chain		Order IMGT Num	Residue		Domain	Chain	Total	Polar	Hydrogen
R@P	2	LYS	K	V-ALPHA	1ao7_D	R@P	58	GLU	E	G-ALPHA1	1ao7_A	7	1	0
R@P	26	SER	S	V-ALPHA	1ao7_D	R@P	58	GLU	E	G-ALPHA1	1ao7_A	3	2	0
R@P	27	ASP	D	V-ALPHA	1ao7_D	R@P	58	GLU	E	G-ALPHA1	1ao7_A	24	6	1
R@P	28	ARG	R	V-ALPHA	1ao7_D	R@P	58	GLU	E	G-ALPHA1	1ao7_A	1	1	0
R@P	37	GLN	Q	V-ALPHA	1ao7_D	R@P	66	LYS	K	G-ALPHA1	1ao7_A	4	1	0
R@P	108	THR	T	V-ALPHA	1ao7_D	R@P	65	ARG	R	G-ALPHA1	1ao7_A	5	2	1
R@P	108	THR	T	V-ALPHA	1ao7_D	R@P	66	LYS	K	G-ALPHA1	1ao7_A	1	0	0
R@P	109	ASP	D	V-ALPHA	1ao7_D	R@P	62	GLY	G	G-ALPHA1	1ao7_A	1	1	0
R@P	109	ASP	D	V-ALPHA	1ao7_D	R@P	65	ARG	R	G-ALPHA1	1ao7_A	19	5	1
R@P	109	ASP	D	V-ALPHA	1ao7_D	R@P	66	LYS	K	G-ALPHA1	1ao7_A	14	1	0
R@P	113	TRP	W	V-ALPHA	1ao7_D	R@P	65	ARG	R	G-ALPHA1	1ao7_A	12	1	0
R@P	113	TRP	W	V-ALPHA	1ao7_D	R@P	68	LYS	K	G-ALPHA1	1ao7_A	8	0	0
R@P	113	TRP	W	V-ALPHA	1ao7_D	R@P	69	ALA	A	G-ALPHA1	1ao7_A	16	0	0
R@P	113	TRP	W	V-ALPHA	1ao7_D	R@P	72	GLN	Q	G-ALPHA1	1ao7_A	4	0	0
R@P	114	GLY	G	V-ALPHA	1ao7_D	R@P	65	ARG	R	G-ALPHA1	1ao7_A	7	1	0

Atom contacts

E 58
G 62
R 65
K 66
K 68
A 69
Q 72

K 2
S 26

D 27
R 28
Q 37

T 108
D 109
W 113
G 114

Contacts of V-ALPHA with G-ALPHA1

Involve CDR1-IMGT and CDR3-IMGT

⬭ Contact with G-ALPHA1
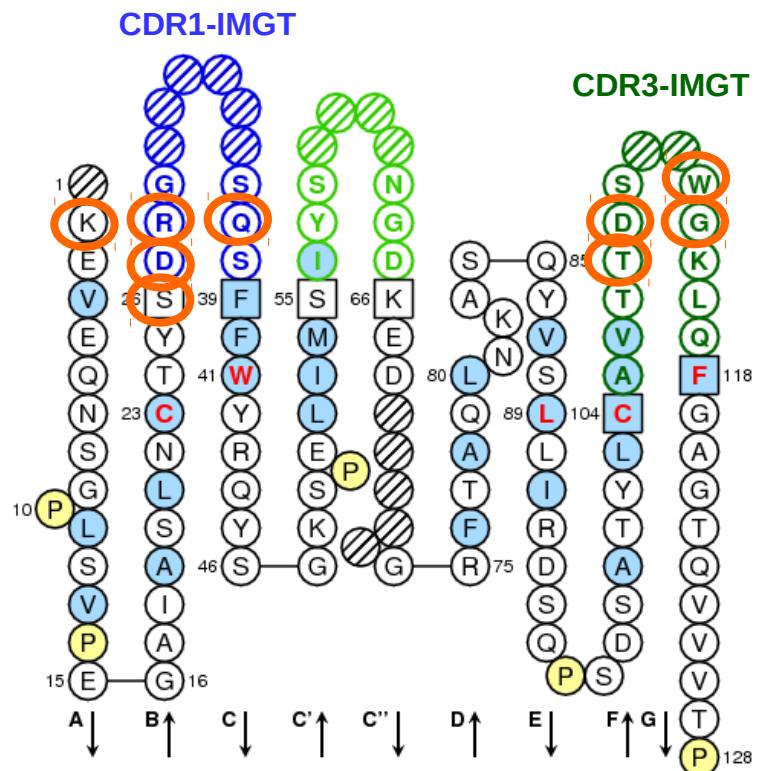
58E 62G 65R 66K 68K 69A 72Q

1ao7_D

TR V-ALPHA
[6.6.11]

G-ALPHA1
[D1]

G-ALPHA2
[D2]

I-ALPHA

1ao7_A

Kaas and Lefranc, In Silico Biology 5, 505-528 (2005)

IMGT/3Dstructure-DB: Contact Analysis

Contacts of V-BETA with G-ALPHA2

http://www.imgt.org

Summary:

Residue contacts	Number of residues			Atom contact types		
	Total	From 1	From 2	Total	Polar	Hydrogen
11	10	5	5	82	17	3

Contacts of

Domain	Chain
V-BETA 1ao7_E	

with

Domain	Chain
G-ALPHA2 1ao7_A	

List of the Residue@Position pair contacts:

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

A 61
A 61A
H 62
V 63
Q 66

A 111
G 112.1
G 112
R 113
P 114

	Order					Order					Atom contacts		
	IMGT Num	Residue		Domain	Chain		IMGT Num	Residue		Domain	Chain	Total	Polar	Hydrogen
R@P	111	ALA	A	V-BETA	1ao7_E	R@P	61A	ALA	A	G-ALPHA2	1ao7_A	1	0	0
R@P	112.1	GLY	G	V-BETA	1ao7_E	R@P	61A	ALA	A	G-ALPHA2	1ao7_A	5	0	0
R@P	112	GLY	G	V-BETA	1ao7_E	R@P	61A	ALA	A	G-ALPHA2	1ao7_A	8	2	1
R@P	112	GLY	G	V-BETA	1ao7_E	R@P	62	HIS	H	G-ALPHA2	1ao7_A	4	1	0
R@P	112	GLY	G	V-BETA	1ao7_E	R@P	63	VAL	V	G-ALPHA2	1ao7_A	4	0	0
R@P	112	GLY	G	V-BETA	1ao7_E	R@P	66	GLN	Q	G-ALPHA2	1ao7_A	10	2	1
R@P	113	ARG	R	V-BETA	1ao7_E	R@P	61	ALA	A	G-ALPHA2	1ao7_A	5	2	1
R@P	113	ARG	R	V-BETA	1ao7_E	R@P	61A	ALA	A	G-ALPHA2	1ao7_A	24	6	0
R@P	113	ARG	R	V-BETA	1ao7_E	R@P	62	HIS	H	G-ALPHA2	1ao7_A	12	2	0
R@P	113	ARG	R	V-BETA	1ao7_E	R@P	66	GLN	Q	G-ALPHA2	1ao7_A	2	1	0
R@P	114	PRO	P	V-BETA	1ao7_E	R@P	66	GLN	Q	G-ALPHA2	1ao7_A	7	1	0

Contacts of V-BETA with G-ALPHA2

Involve CDR3-IMGT

○ Contact with G-ALPHA2

CDR3-IMGT

G-ALPHA1
[D1]

G-ALPHA2
[D2]

1ao7_A

1ao7_E

TR V-BETA
[5.6.14]

66Q 63V 62H 61AA 61A

I-ALPHA

http://www.imgt.org

Kaas and Lefranc, In Silico Biology 5, 505-528 (2005)

Peptide alignment

Kaas and Lefranc, In Silico Biology 5, 505-528 (2005)

IMGT Collier de Perles pMH contact sites

Human HLA-A*0201 (MH1) and a 9-amino acid peptide

http://www.imgt.org

	9-amino acid peptides	Peptide	Pocket (approx.)
C1	1	1 L	A
C2	-	--	
C3	2	2 L	B
C4	3	3 F	D
C5	4	(4 G)	
C6	5	5 Y	
C7	-	--	
C8	6	6 P	
C9	7	7 V	E
C10	8	8 Y	
C11	9	9 V	F

Peptide chain: 1ao7_C
MHC chain: 1ao7_A

Kaas and Lefranc, In Silico Biology 5, 505-528 (2005)
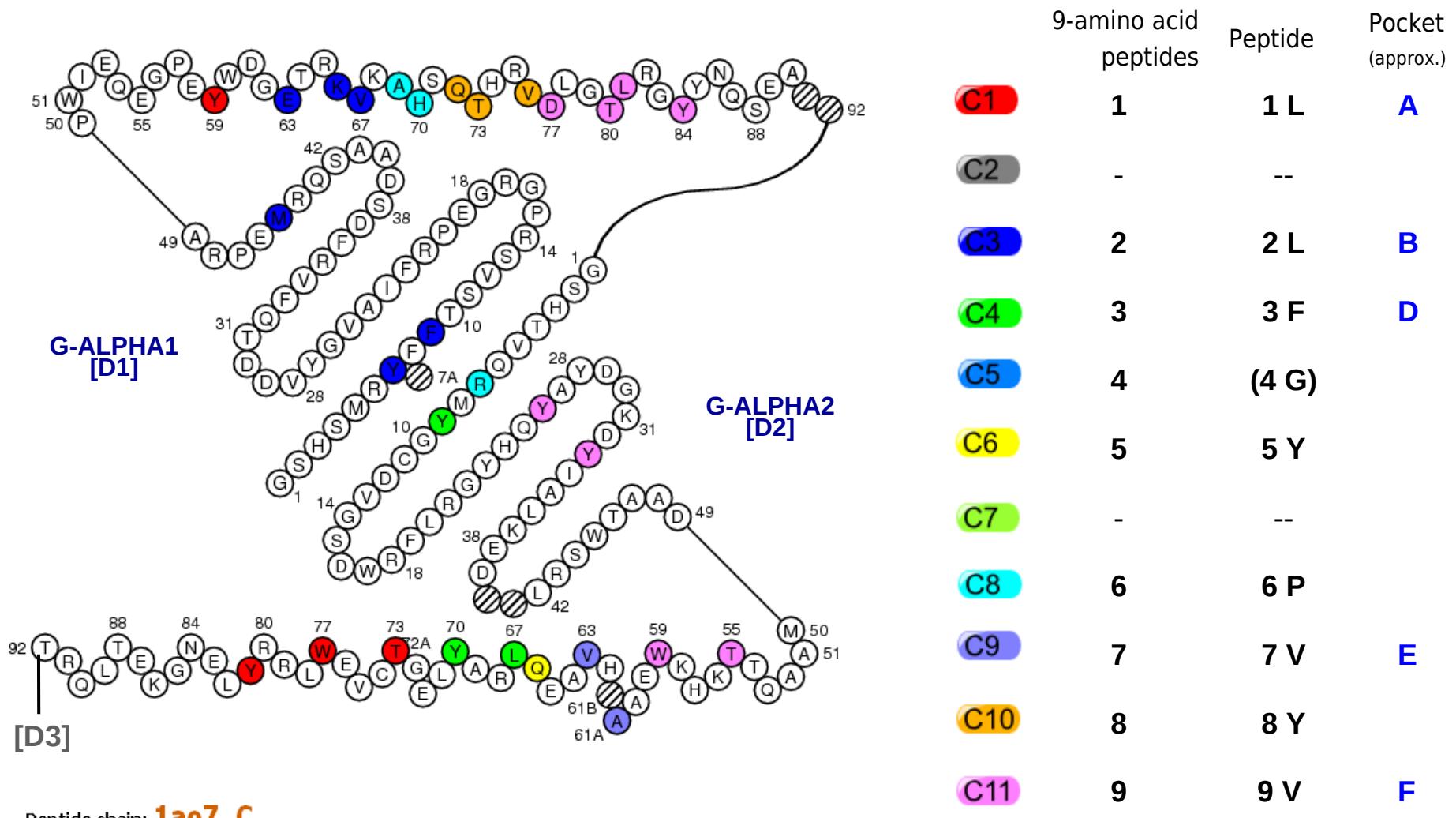
IMGT/3Dstructure-DB: Contact Analysis

IMGT Residue@Position cards

http://www.imgt.org

IMGT Residue@Position card

Residue@Position: 113 - ARG (R) - V-BETA - 1ao7_E — CDR3-IMGT

General information:

PDB file numbering	102
IMGT file numbering	113
Residue full name	Arginine
Formula	C6 H15 N4 O2 1+

IMGT LocalStructure@Position

Secondary structure	Coil
Phi (in degrees)	-89.71
Psi (in degrees)	111.56
ASA (in square angstrom)	73.2

IMGT Num	Residue		Domain	Chain	Atom contacts	Polar	Hydrogen Bond	Non Polar
61	ALA	A	G-ALPHA2	1ao7_A	5	2	1	3
61A	ALA	A	G-ALPHA2	1ao7_A	24	6	0	18
62	HIS	H	G-ALPHA2	1ao7_A	12	2	0	10
66	GLN	Q	G-ALPHA2	1ao7_A	2	1	0	1
5	TYR	Y		1ao7_C	1	0	0	1
108	PRO	P	V-BETA	1ao7_E	15	1	0	14
111	ALA	A	V-BETA	1ao7_E	6	2	0	4
112.1	GLY	G	V-BETA	1ao7_E	24	5	0	19
115	GLU	E	V-BETA	1ao7_E	17	3	0	14

G-ALPHA2

Peptide

Acknowledgements

BioSTIC-LR, ACI IMPbio, SFR BioCampus
GIS IBiSA, GIS AGENAE
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GDR ACCITH, LABEX MabImprove
«ImmunoGrid» 6th PCRDT

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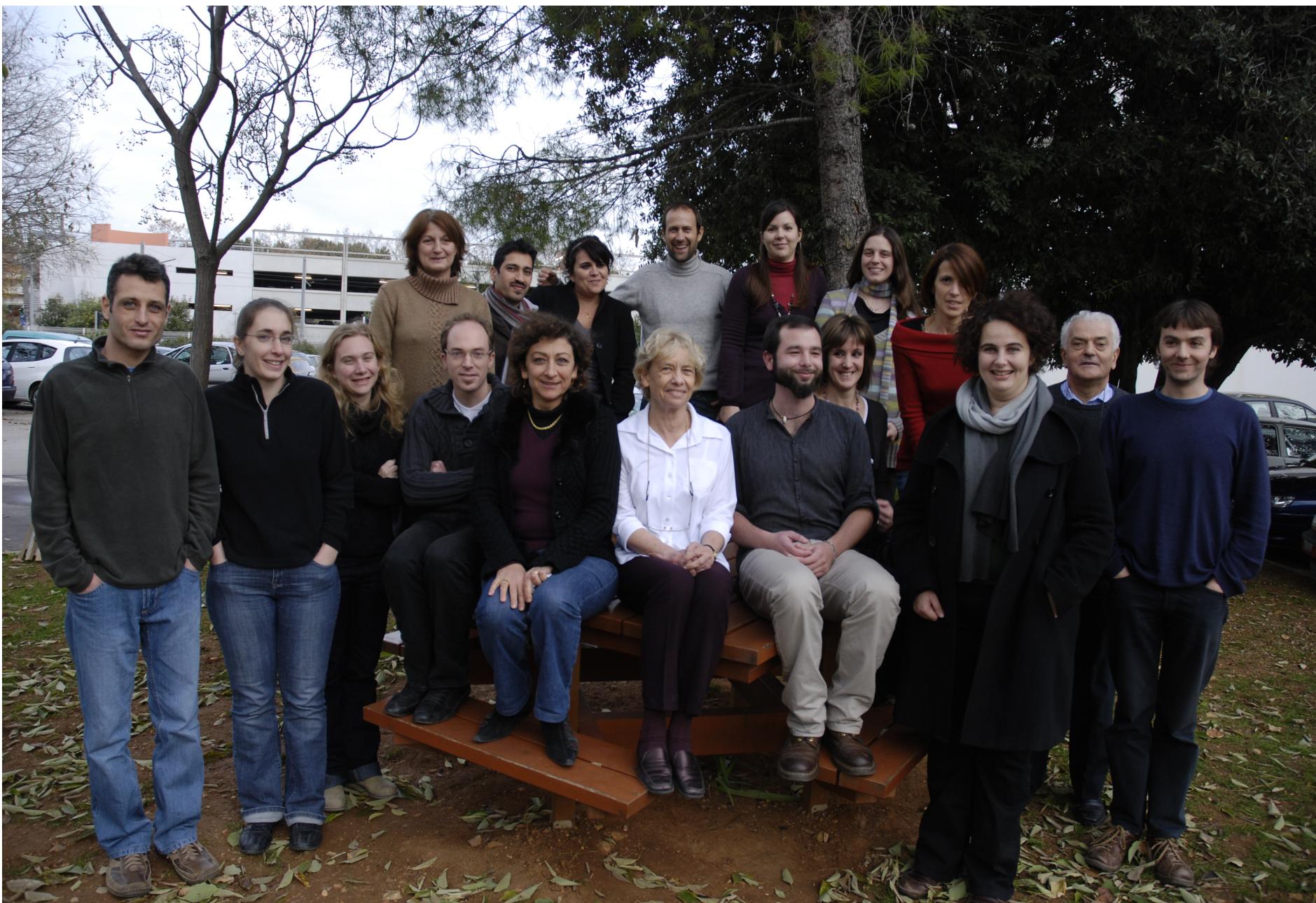
The IMGT® team, Montpellier, France

ImMunoGeneTics

Information system®

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