

MHC: what do we learn from IMGT Colliers de Perles ?

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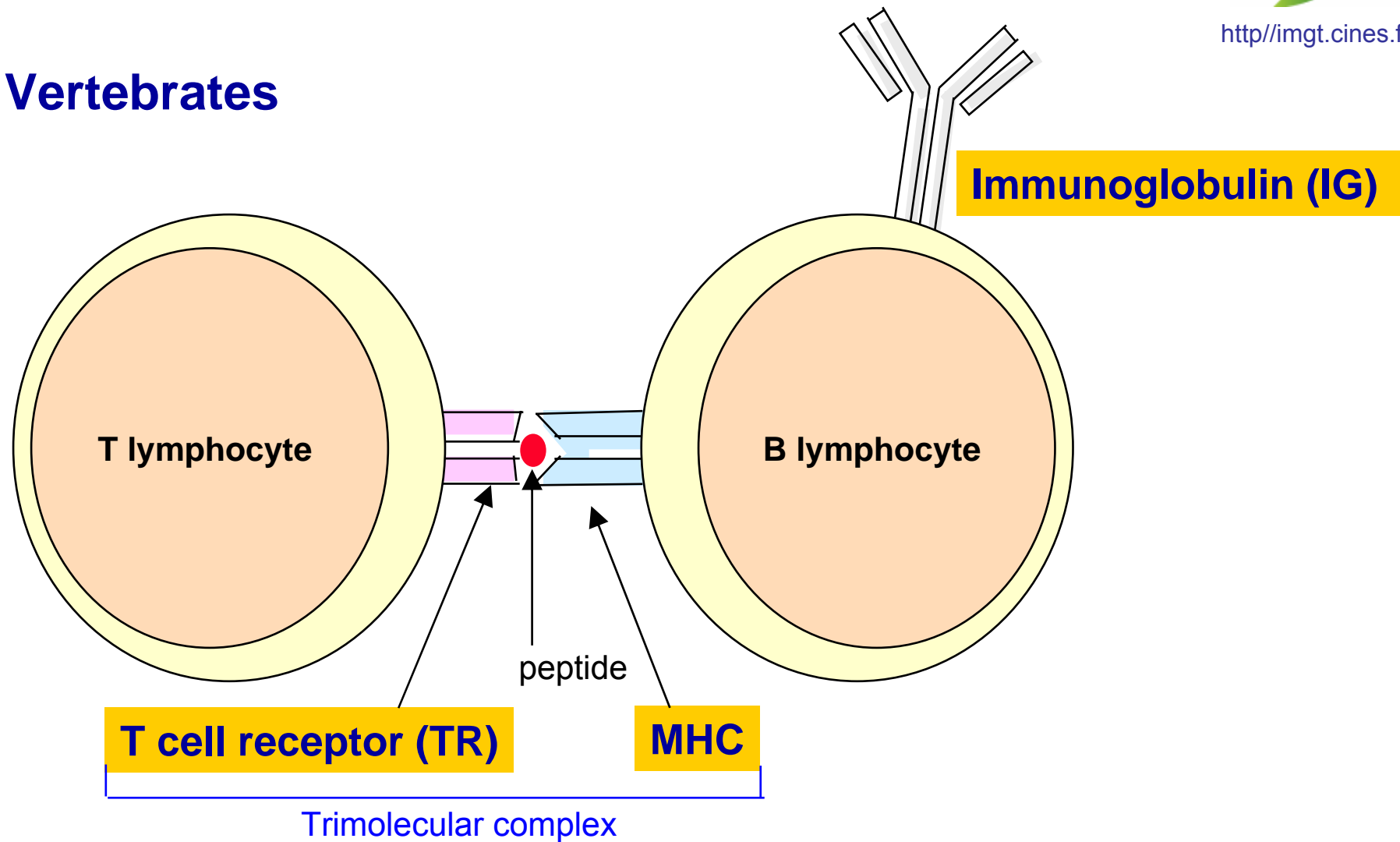


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IMGT founder and director: M.-P. Lefranc

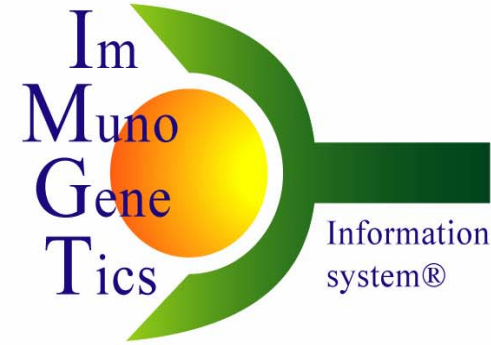
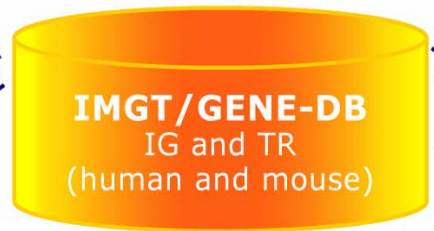
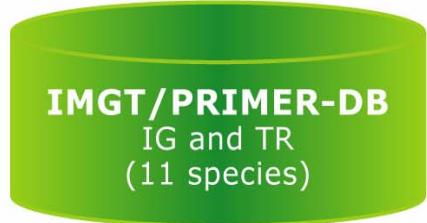


IMGT®: the adaptive immune response

Vertebrates



Sequences



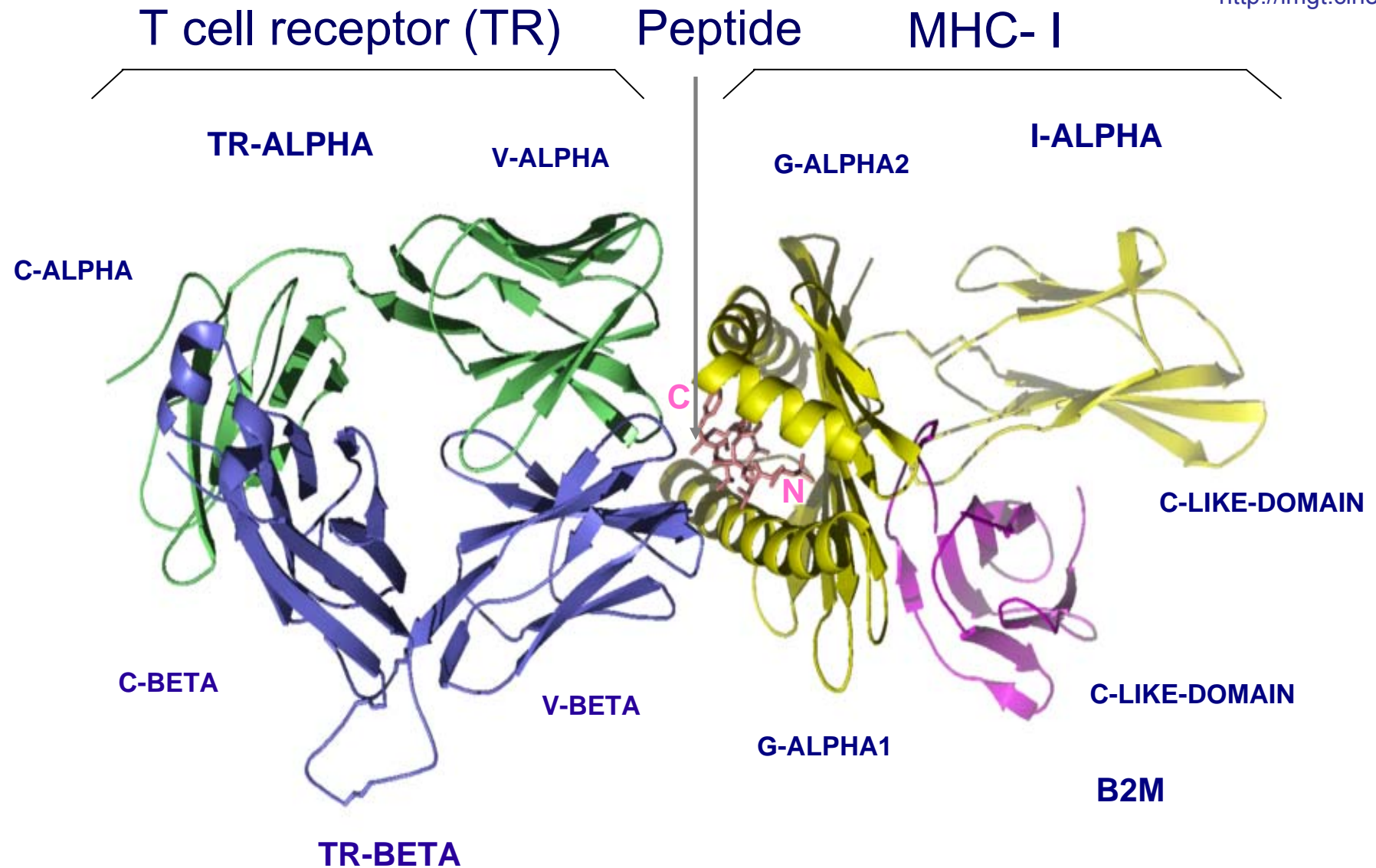
<http://imgt.cines.fr>

Genome

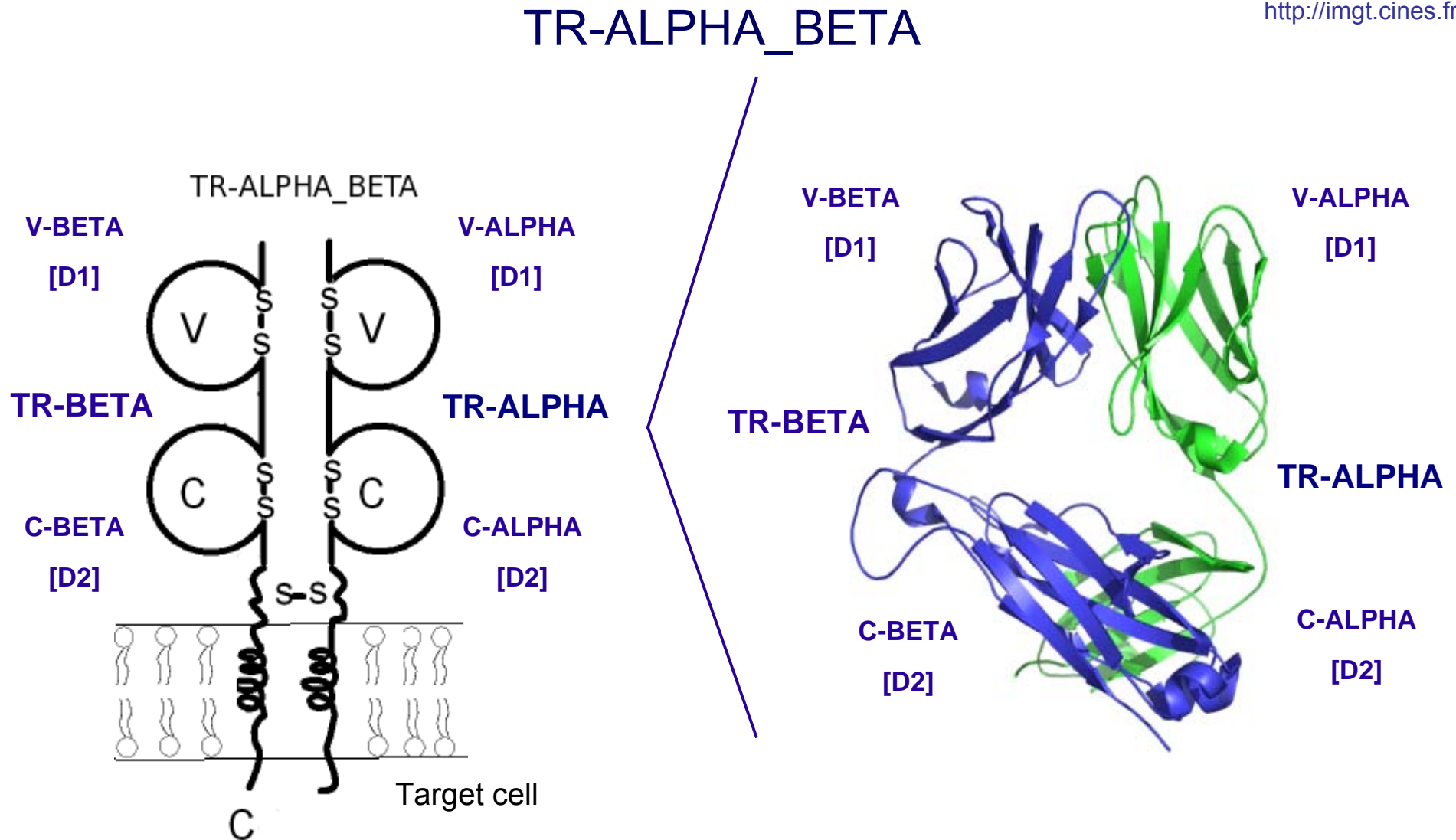


2D and 3D structures

TR/peptide/MHC complex



T cell receptor chains and domains

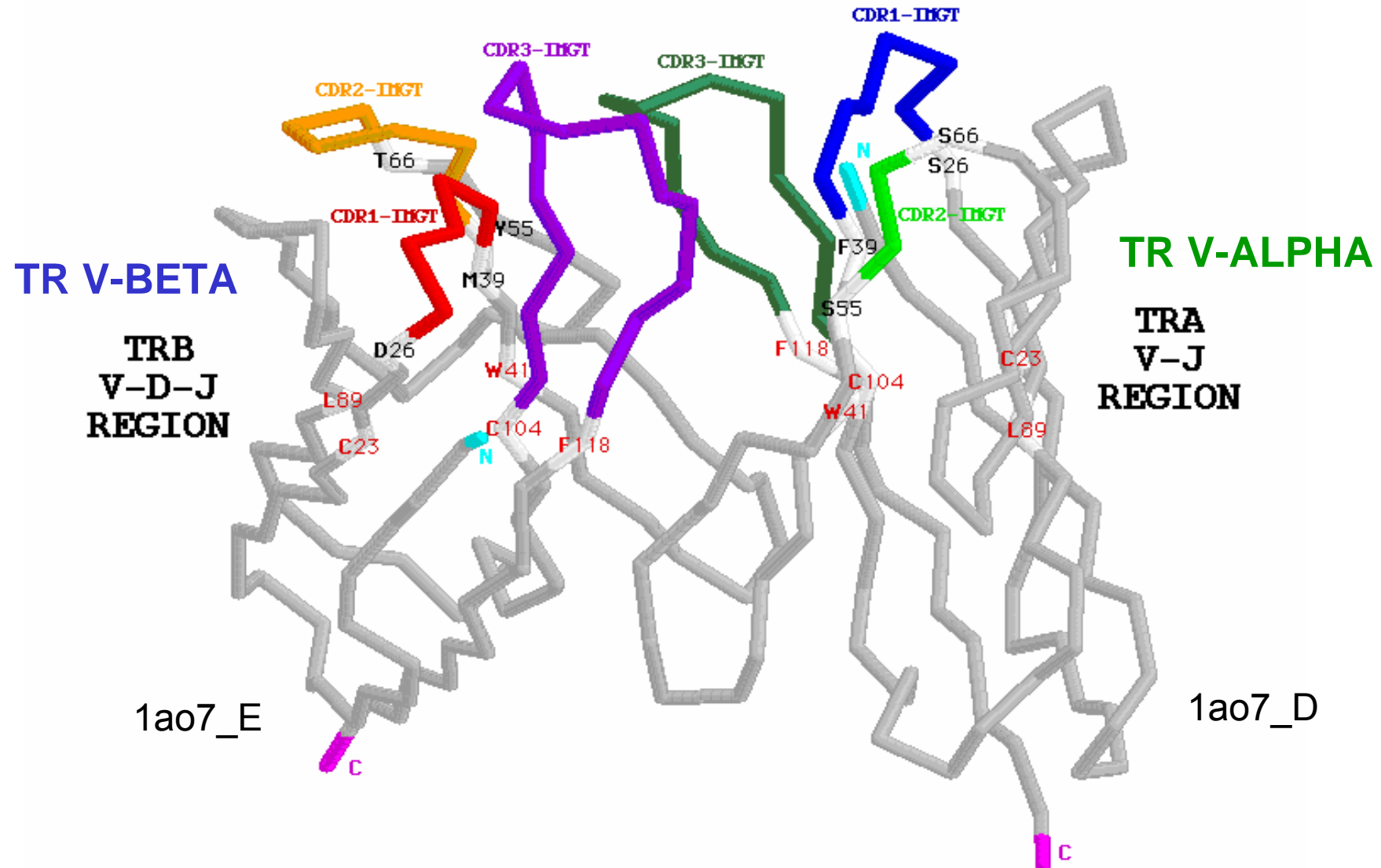


T cell receptor V-DOMAINS

Human TR $\alpha\beta$ A6



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CDR: complementarity determining region

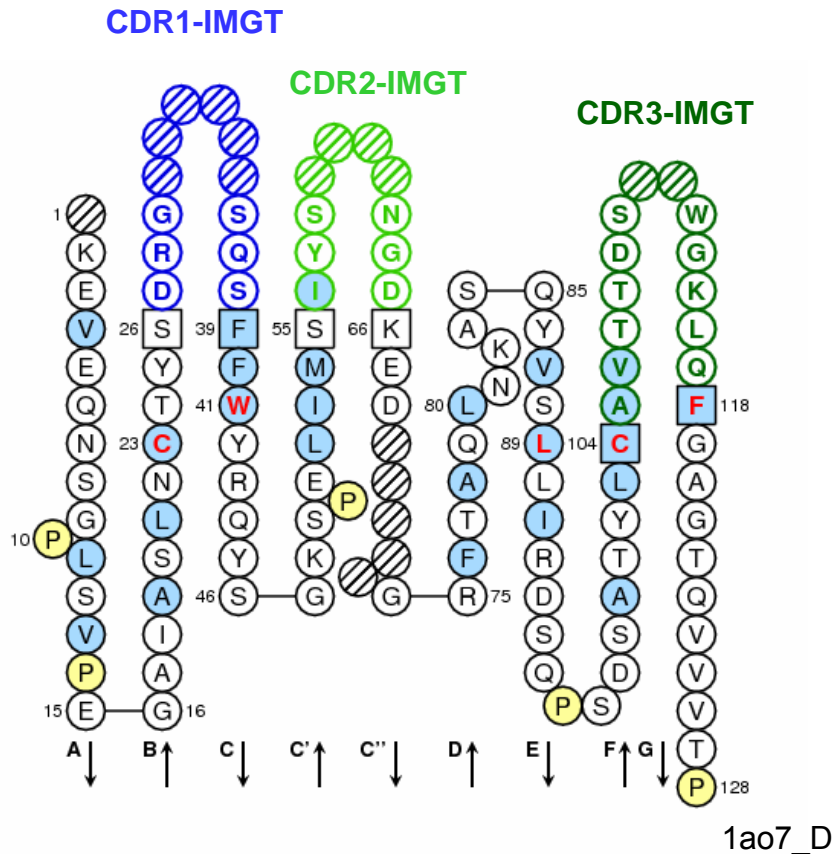
IMGT Repertoire, <http://imgt.cines.fr>

IMGT Colliers de Perles for V-DOMAIN

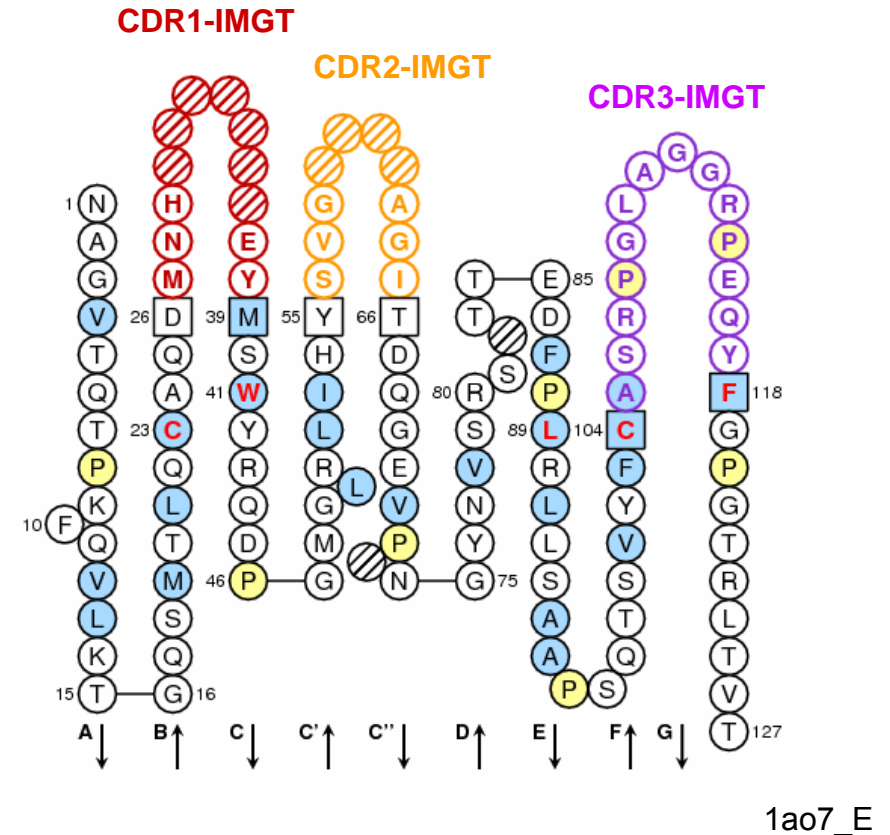


<http://imgt.cines.fr>

Based on the IMGT unique numbering for V-DOMAIN



TR V-ALPHA
[6.6.11]



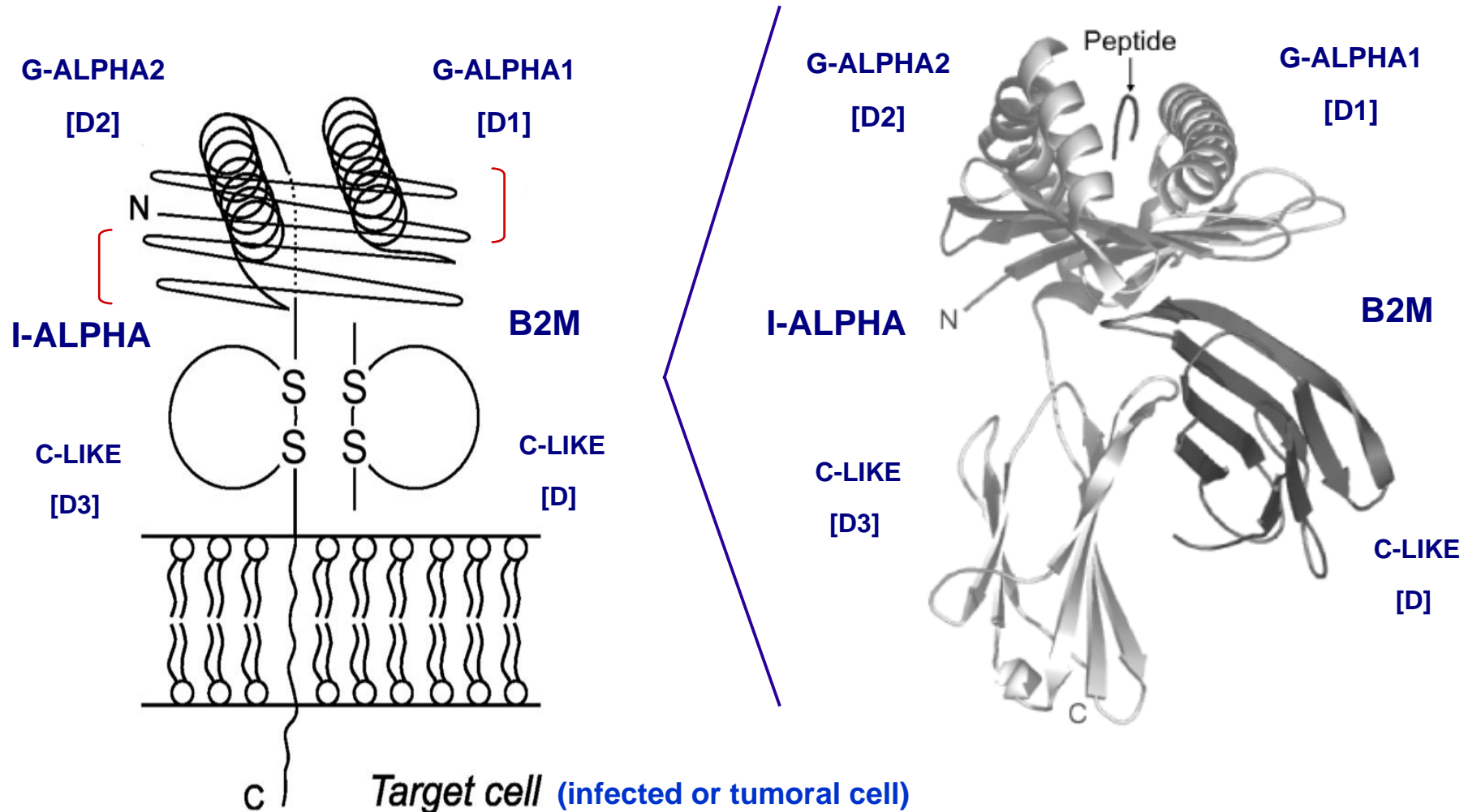
TR V-BETA
[5.6.14]

CDR: complementarity determining region

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

MHC-I chains and domains

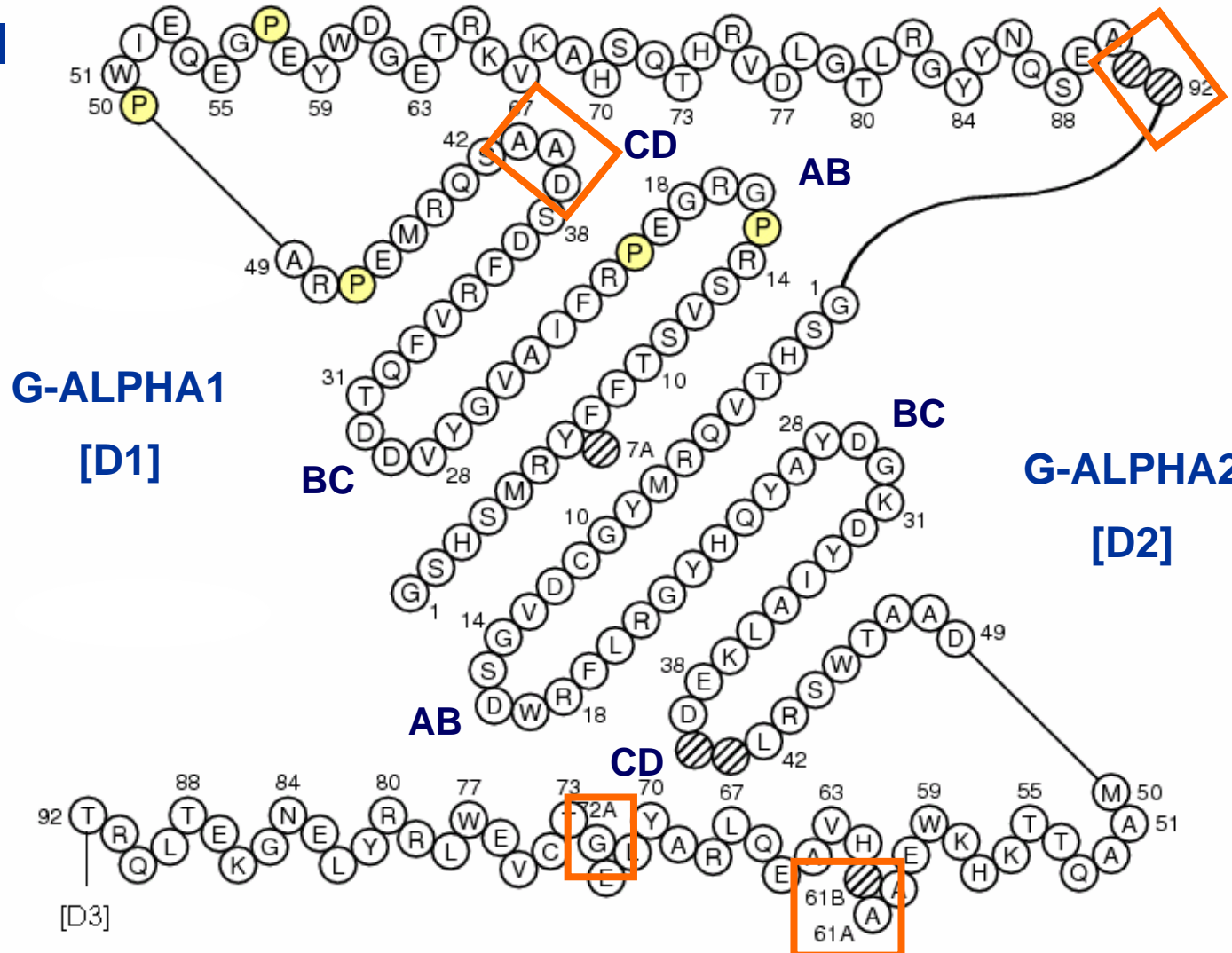
MHC-I-ALPHA_B2M



IMGT Colliers de Perles for G-DOMAIN

Based on the IMGT unique numbering for G-DOMAIN

MHC-I



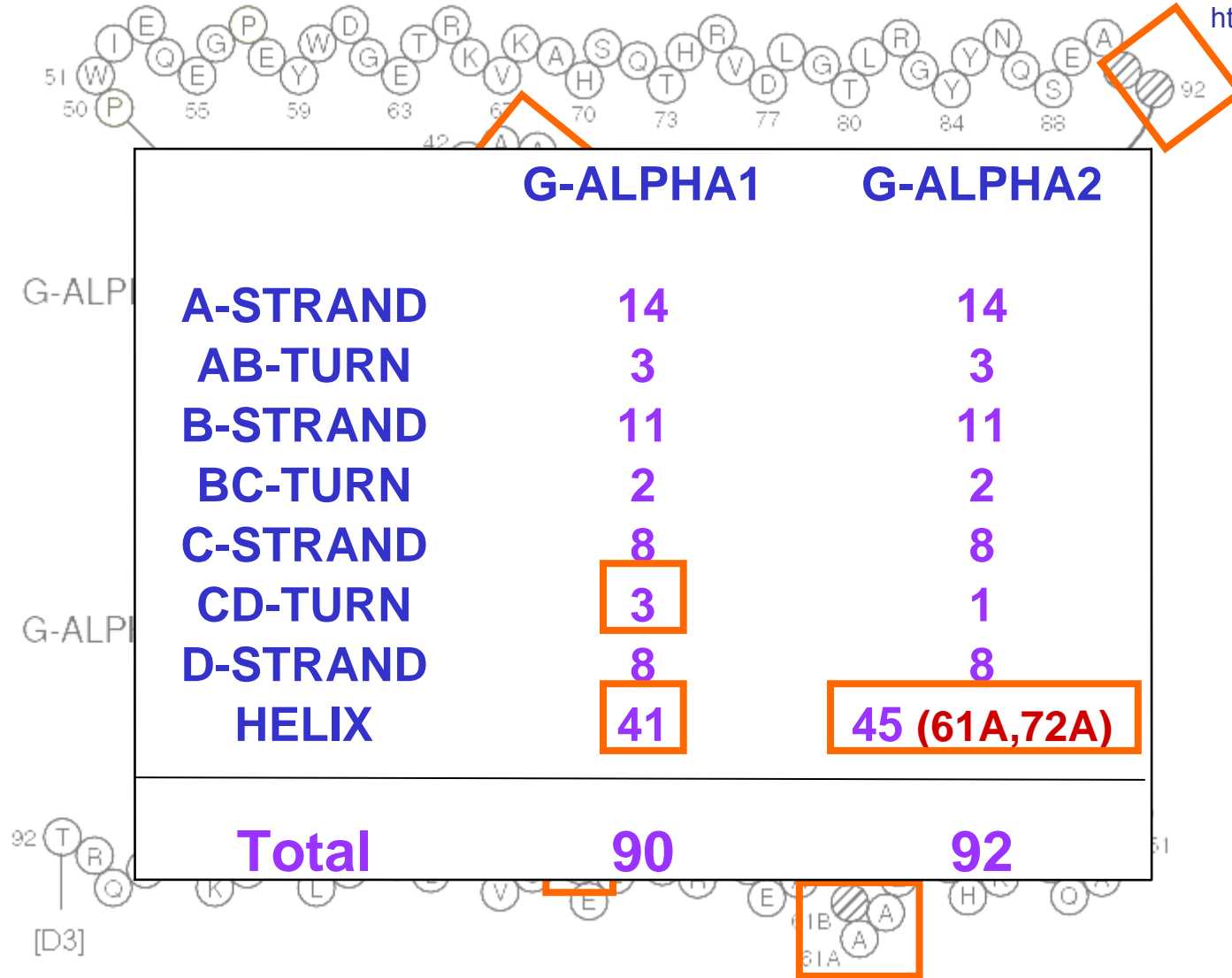
Lefranc et al., Dev. Comp. Immunol. 29, 917-938 (2005)

MHC-I G-DOMAINS

Strand, turn and helix lengths



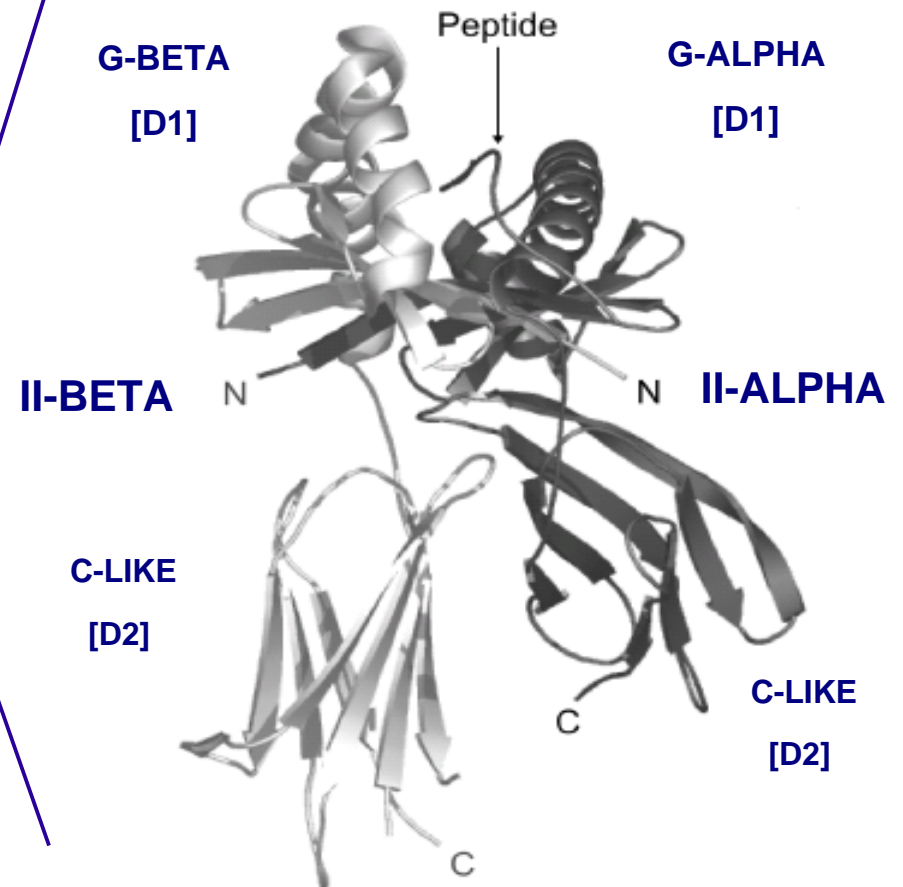
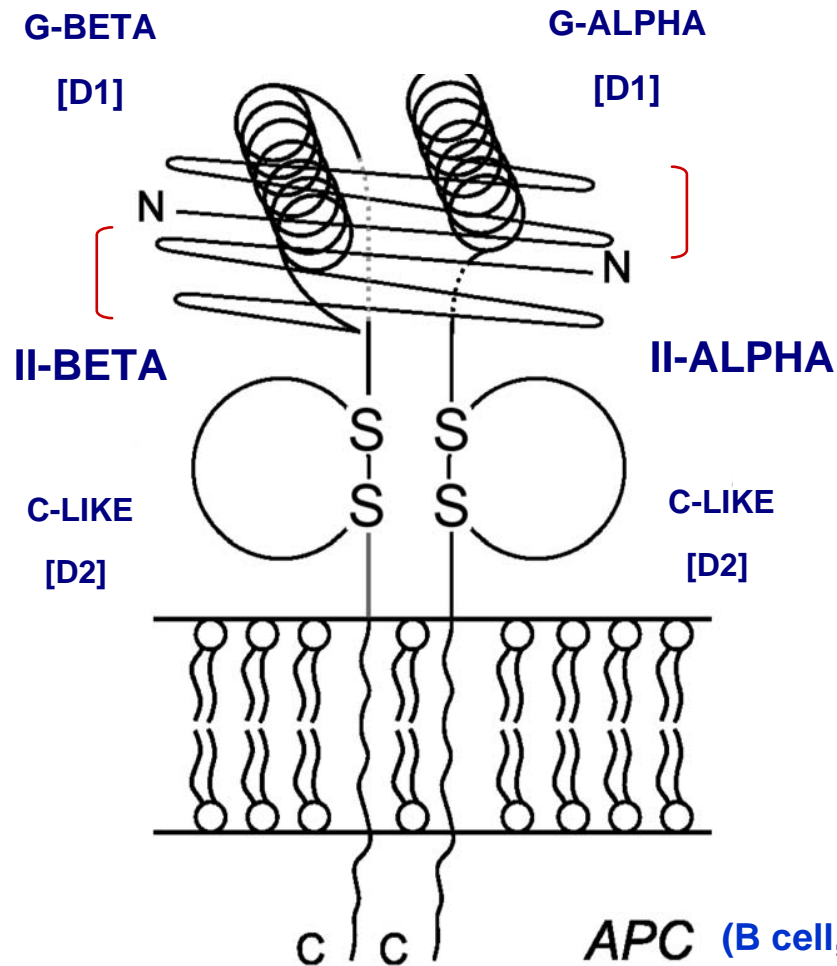
<http://imgt.cines.fr>



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

MHC-II chains and domains

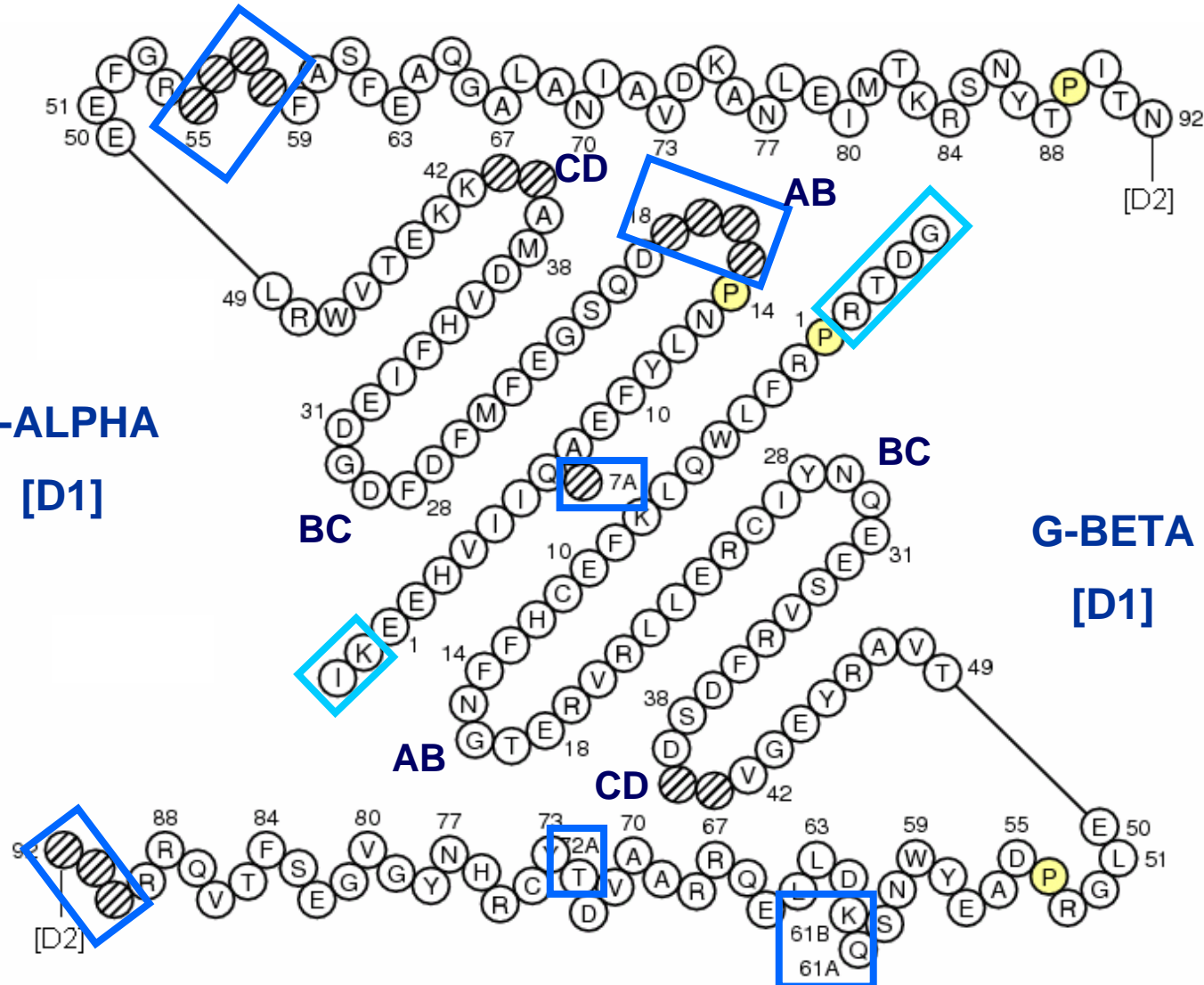
MHC-II-ALPHA_BETA



IMGT Colliers de Perles for G-DOMAIN

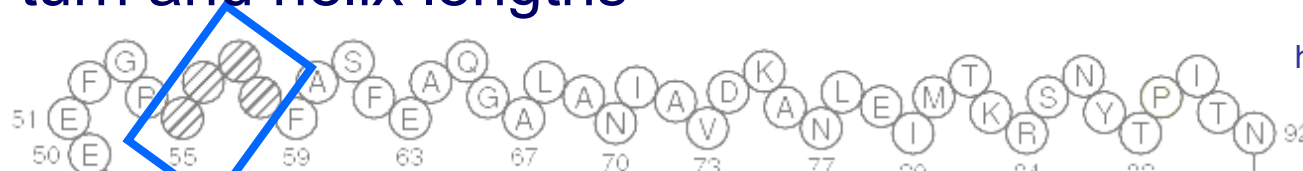
Based on the IMGT unique numbering for G-DOMAIN

MHC-II

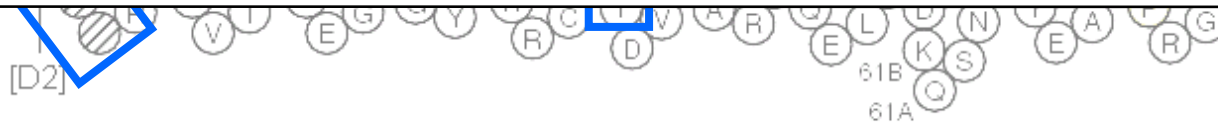


MHC-II G-DOMAINS

Strand, turn and helix lengths



	G-ALPHA	G-BETA
A-STRAND	14-15 (7A) +2	14 +4
AB-TURN	0	3
B-STRAND	10	11
BC-TURN	2	2
C-STRAND	8	8
CD-TURN	1	1
D-STRAND	8	8
HELIX	39	43 (61A,61B,72A)
Total	84-85	94



MHC-I and MHC-II G-DOMAINS



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Strand, turn and helix lengths

	MHC-I	MHC-II	MHC-I	MHC-II
	G-ALPHA1	G-ALPHA	G-ALPHA2	G-BETA
A-STRAND	14	14-15(7A)+2	14	14+4
AB-TURN	3	0	3	3
B-STRAND	11	10	11	11
BC-TURN	2	2	2	2
C-STRAND	8	8	8	8
CD-TURN	3	1	1	1
D-STRAND	8	8	8	8
HELIX	41	39	45 (61A,72A)	43 (61A,61B,72A)
Total	90	84-85	92	94

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

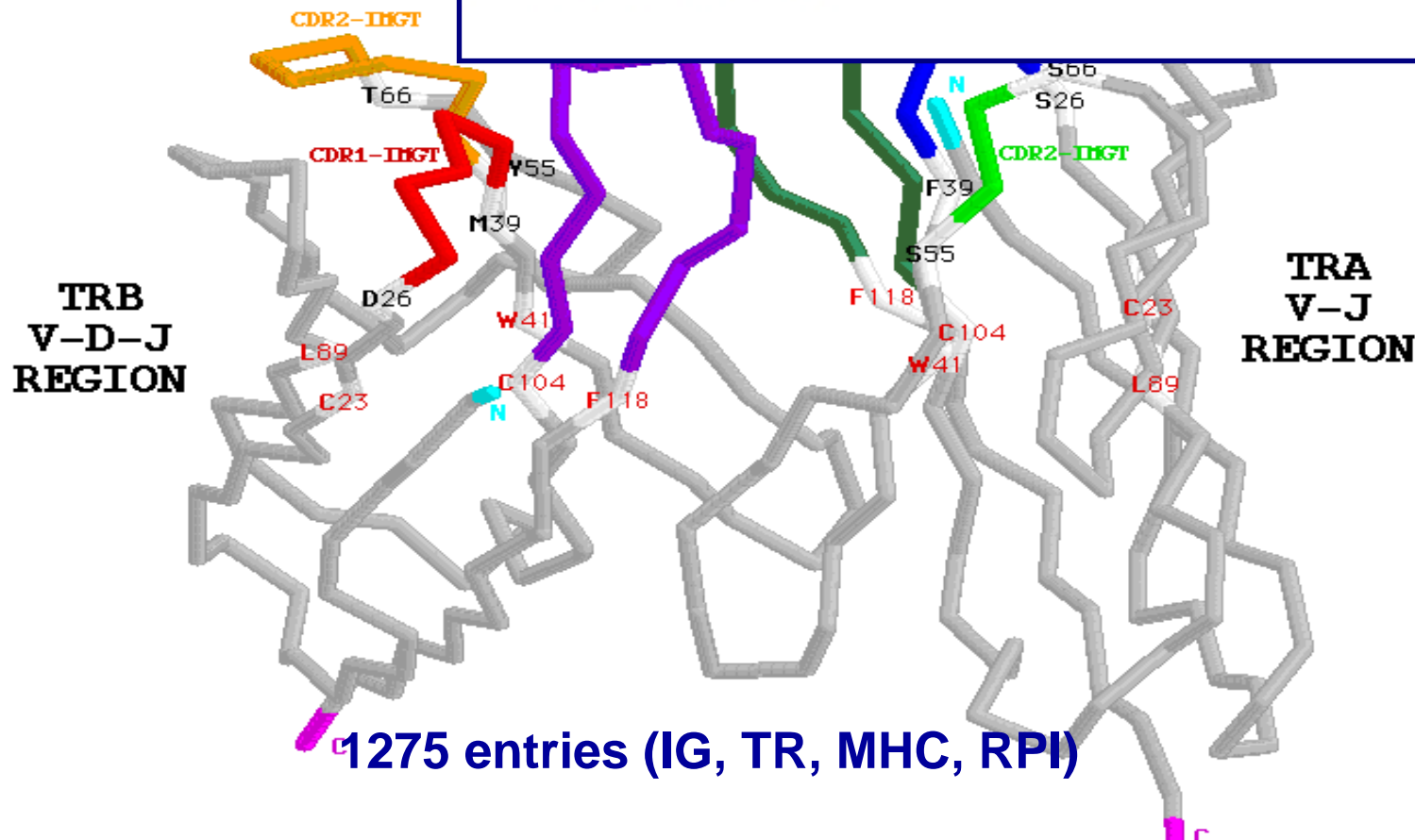
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Quentin KAAS

Kaas et al., Nucl. Acids Res. 32, D208-210 (2004)

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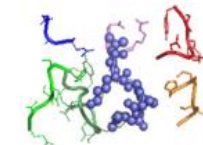
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SEARCH BY PDB CODE OR PROTEIN NAME OR REFERENCES:

PDB code OR IMGT protein name OR [References](#)

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Choose a species: and then an English name

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Kaas et al., Nucl. Acids Res. 32, D208-210 (2004)

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IMGT/3Dstructure-DB card for : **1ao7**



Entry code Search

[Query page](#)

IMGT protein name	IMGT receptor type	IMGT receptor description	Ligand(s)	Species	CC	Chain ID
A6	TR	TR-ALPHA_BETA-1		<i>Homo sapiens</i> (Human)	1	[1ao7 D 1ao7 E]
HLA-A*0201	MHC	MHC-I-ALPHA_B2M		<i>Homo sapiens</i> (Human)	1	[1ao7 A 1ao7 B]
		Peptide	Tax peptide 11-19 (Q82235)	Human T lymphotropic virus type 1	1	[1ao7 C]

Experimental technique **X-ray diffraction**

Resolution (in angstrom) **2.6**

PDB release date **17-SEP-97**

Epitope and Chain
details

Contact
analysis

3D visualization
Jmol or Quid:PDB

Renumbered
IMGT file

IMGT numbering
comparison

References
and links

Printable
card

Reference 1ao7: *Garboczi et al., Nature 384, 134-141 (1996)*

IMGT/3Dstructure-DB: Contact Analysis



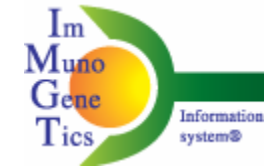
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Click 'DomPair' for IMGT/3Dstructure-DB Domain pair contacts (list of Residue@Position pair contacts)

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		

	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	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



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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
		1ao7_E	TR-BETA-1	[D2]	C-ALPHA
				[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

	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	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



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Contacts between domains

	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	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



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Contacts of V-ALPHA with G-ALPHA1

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					Order					Atom contacts		
IMGT Num	Residue	Domain	Chain		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

K 2	
S 26	
<hr/>	
D 27	
R 28	
Q 37	
<hr/>	
T 108	
D 109	
W 113	
G 114	

IMGT/3Dstructure-DB: Contact Analysis



http://imgt.cines.fr

Contacts of V-ALPHA with G-ALPHA1

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					Order					Atom contacts		
IMGT Num	Residue	Domain	Chain		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

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

K 2
S 26

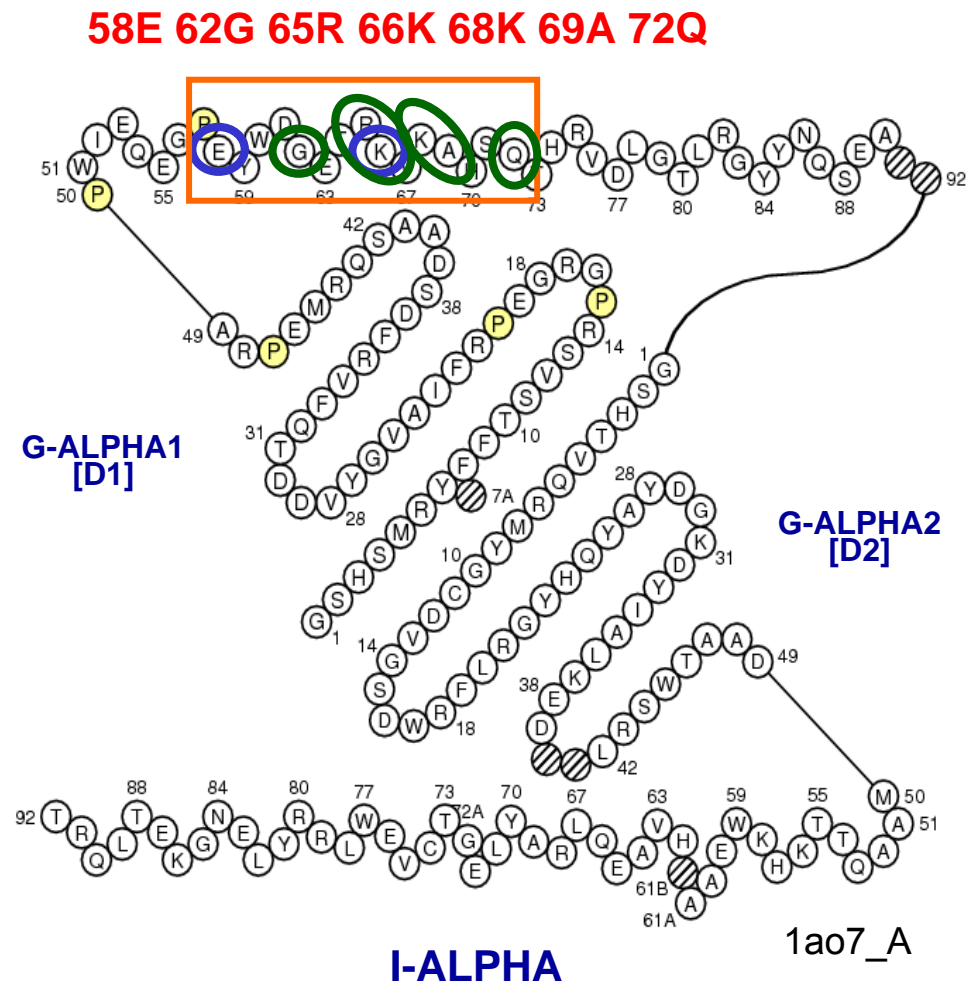
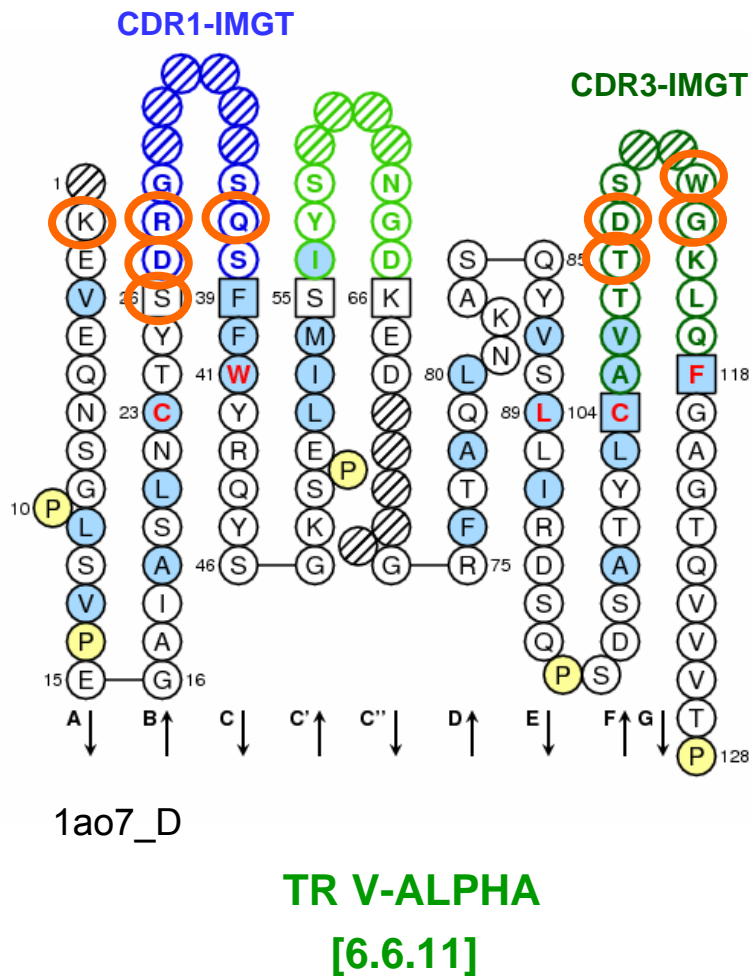
D 27
R 28
Q 37

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



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

IMGT/3Dstructure-DB: Contact Analysis

Contacts of V-ALPHA with G-ALPHA2

Summary:

Residue contacts	Number of residues			Atom contact types		
	Total	From 1	From 2	Total	Polar	Hydrogen
12	15	7	8	105	17	2

Contacts of

Domain Chain
V-ALPHA 1ao7_D

with

Domain Chain
G-ALPHA2 1ao7_A

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	28	ARG	R	V-ALPHA 1ao7_D	R@P	77	TRP	W	G-ALPHA2 1ao7_A	14	1	0
R@P	28	ARG	R	V-ALPHA 1ao7_D	R@P	80	ARG	R	G-ALPHA2 1ao7_A	13	5	0
R@P	29	GLY	G	V-ALPHA 1ao7_D	R@P	77	TRP	W	G-ALPHA2 1ao7_A	6	0	0
R@P	37	GLN	Q	V-ALPHA 1ao7_D	R@P	70	TYR	Y	G-ALPHA2 1ao7_A	8	0	0
R@P	37	GLN	Q	V-ALPHA 1ao7_D	R@P	73	THR	T	G-ALPHA2 1ao7_A	10	2	0
R@P	57	TYR	Y	V-ALPHA 1ao7_D	R@P	65	GLU	E	G-ALPHA2 1ao7_A	4	0	0
R@P	57	TYR	Y	V-ALPHA 1ao7_D	R@P	66	GLN	Q	G-ALPHA2 1ao7_A	16	1	0
R@P	57	TYR	Y	V-ALPHA 1ao7_D	R@P	69	ALA	A	G-ALPHA2 1ao7_A	7	1	0
R@P	58	SER	S	V-ALPHA 1ao7_D	R@P	69	ALA	A	G-ALPHA2 1ao7_A	3	1	0
R@P	63	ASN	N	V-ALPHA 1ao7_D	R@P	76	GLU	E	G-ALPHA2 1ao7_A	4	2	0
R@P	82	LYS	K	V-ALPHA 1ao7_D	R@P	73	THR	T	G-ALPHA2 1ao7_A	5	2	1
R@P	82	LYS	K	V-ALPHA 1ao7_D	R@P	76	GLU	E	G-ALPHA2 1ao7_A	15	2	1

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Y 70
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E 76
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R 80

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G 29
Q 37

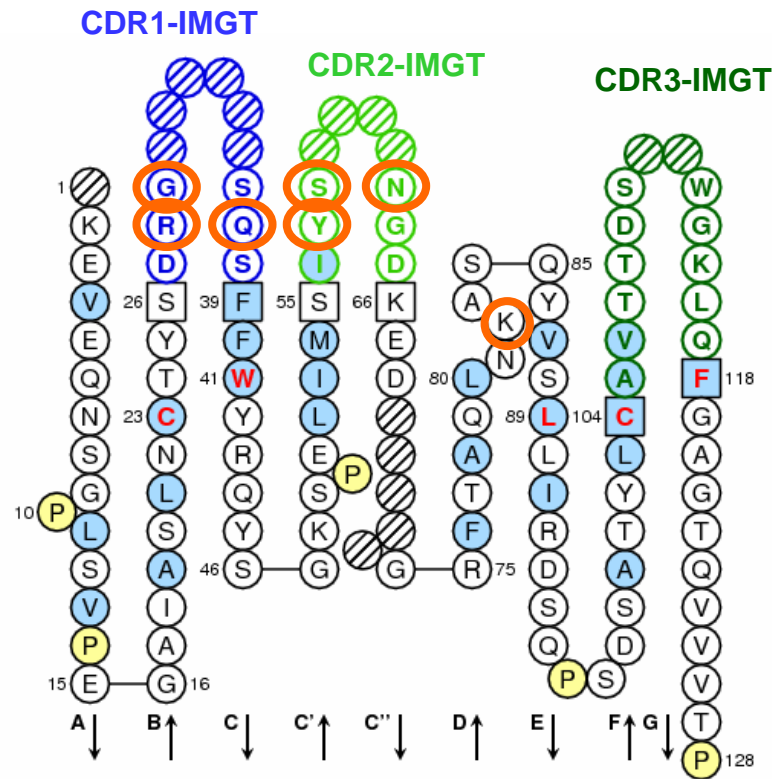
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K 82

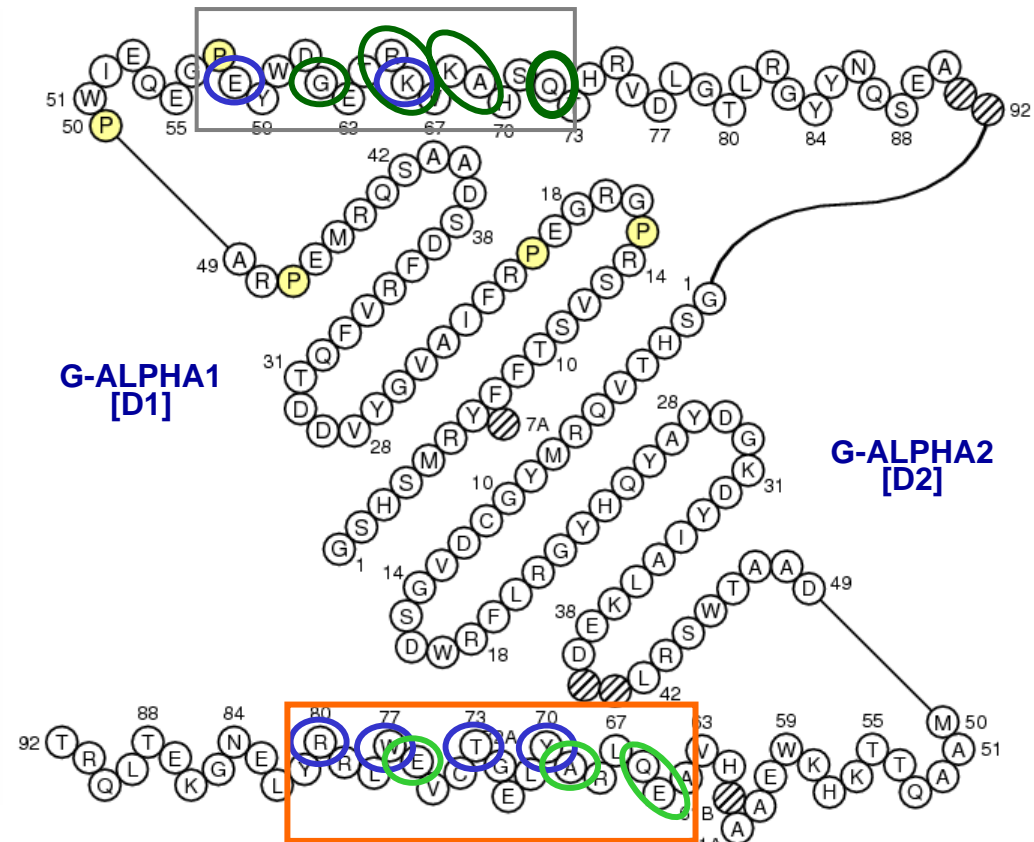
Contacts of V-ALPHA with G-ALPHA2

Involve CDR1-IMGT and CDR2-IMGT

○ Contact with G-ALPHA2



TR V-ALPHA
[6.6.11]



80R 77W 76E 73T 70Y 69A 66Q 65E 1ao7_A

I-ALPHA

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

Contact sites of TR V-ALPHA with MHC-I (1ao7)



<http://imgt.cines.fr>

TR V-ALPHA [6.6.11]	G-ALPHA1	G-ALPHA2
CDR1-IMGT		
27	58	-
28	58	77,80
29	-	77
37	66	70,73
CDR2-IMGT		
57	-	65,66,69
58	-	69
63	-	76
CDR3-IMGT		
108	65,66	-
109	62,65,66	-
113	65,68,69,72	-
114	65	-

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

IMGT/3Dstructure-DB: Contact Analysis



http://imgt.cines.fr

Contacts of V-BETA with G-ALPHA1

Summary:

Residue contacts	Number of residues			Atom contact types		
	Total	From 1	From 2	Total	Polar	Hydrogen
3	4	1	3	23	0	0

Contacts of

Domain	Chain	with	Domain	Chain
V-BETA	1ao7_E		G-ALPHA1	1ao7_A

List of the Residue@Position pair contacts:

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

<u>Order</u>	<u>IMGT Num</u>	<u>Residue</u>	<u>Domain</u>	<u>Chain</u>	<u>Order</u>	<u>IMGT Num</u>	<u>Residue</u>	<u>Domain</u>	<u>Chain</u>	<u>Atom contacts</u>				
										Total	Polar	Hydrogen		
R@P	110	LEU	L	V-BETA	1ao7_E	R@P	69	ALA	A	G-ALPHA1	1ao7_A	9	0	0
R@P	110	LEU	L	V-BETA	1ao7_E	R@P	72	GLN	Q	G-ALPHA1	1ao7_A	4	0	0
R@P	110	LEU	L	V-BETA	1ao7_E	R@P	73	THR	T	G-ALPHA1	1ao7_A	10	0	0

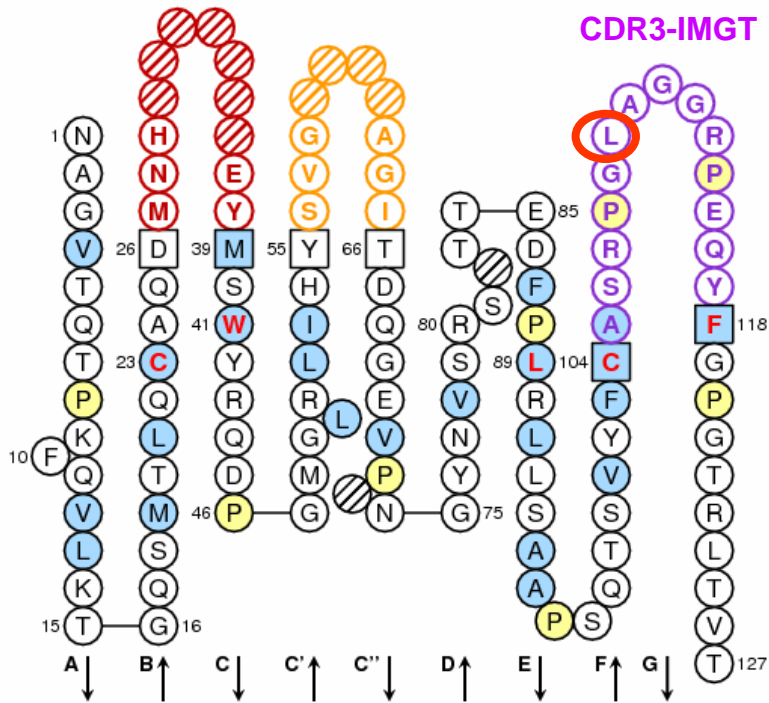
A 69
Q 72
T 73

L 110

Contacts of V-BETA with G-ALPHA1

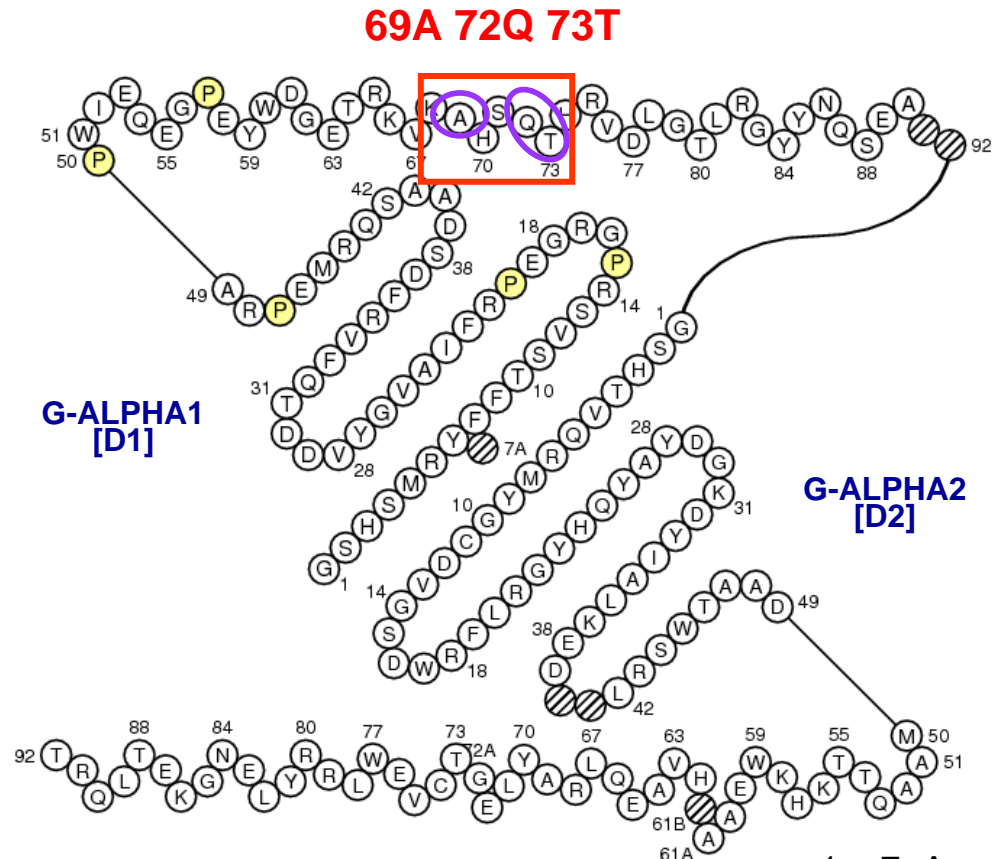
Involve CDR3-IMGT

 Contact with G-ALPHA1



1ao7_E

TR V-BETA
[5.6.14]



I-ALPHA

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

IMGT/3Dstructure-DB: Contact Analysis



http://imgt.cines.fr

Contacts of V-BETA with G-ALPHA2

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

Order	Residue@Position				Order	Residue@Position				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

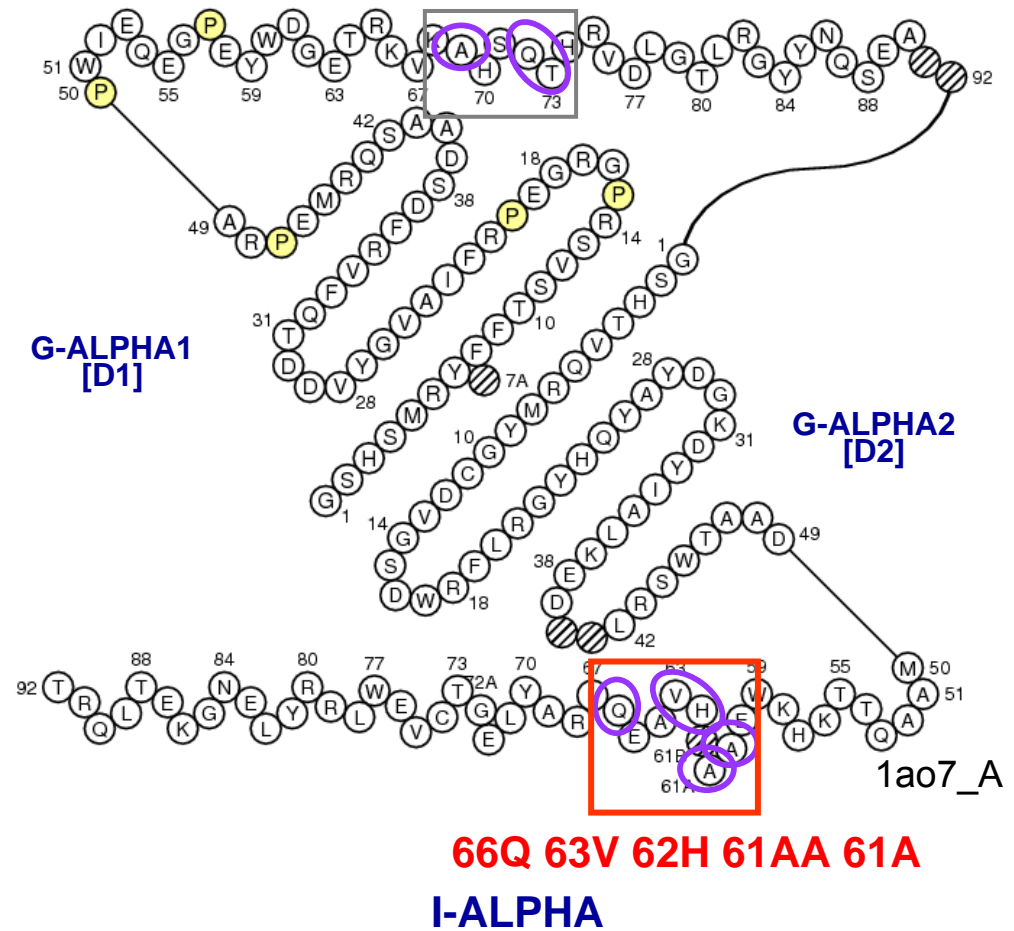
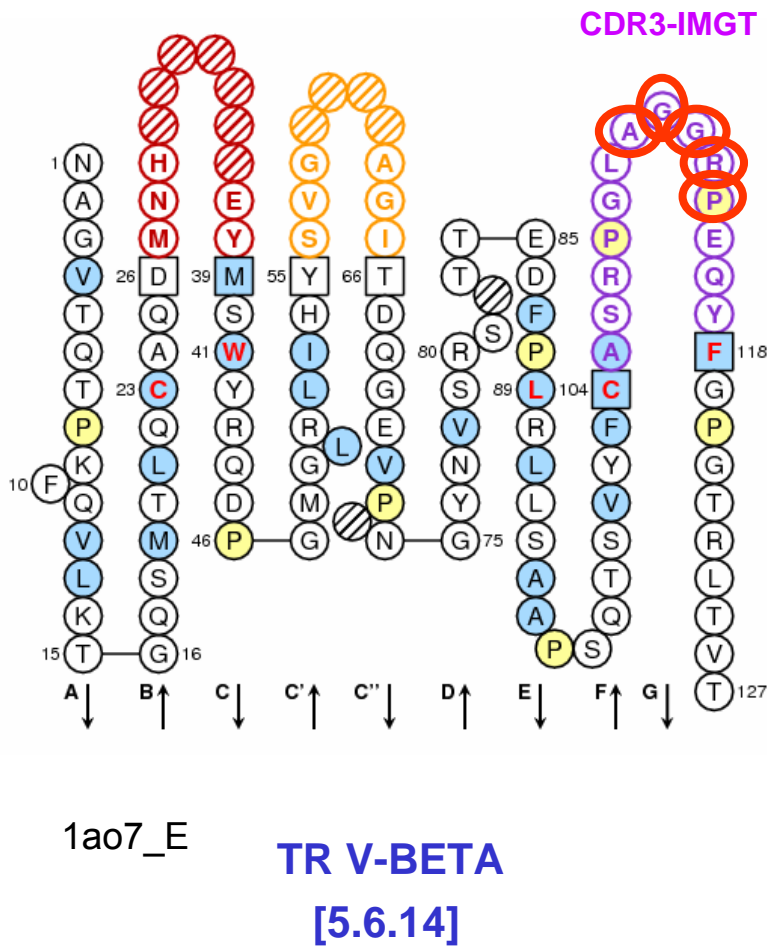
A 61
A 61A
H 62
V 63
Q 66

A 111
G 112.1
G 112
R 113
P 114

Contacts of V-BETA with G-ALPHA2

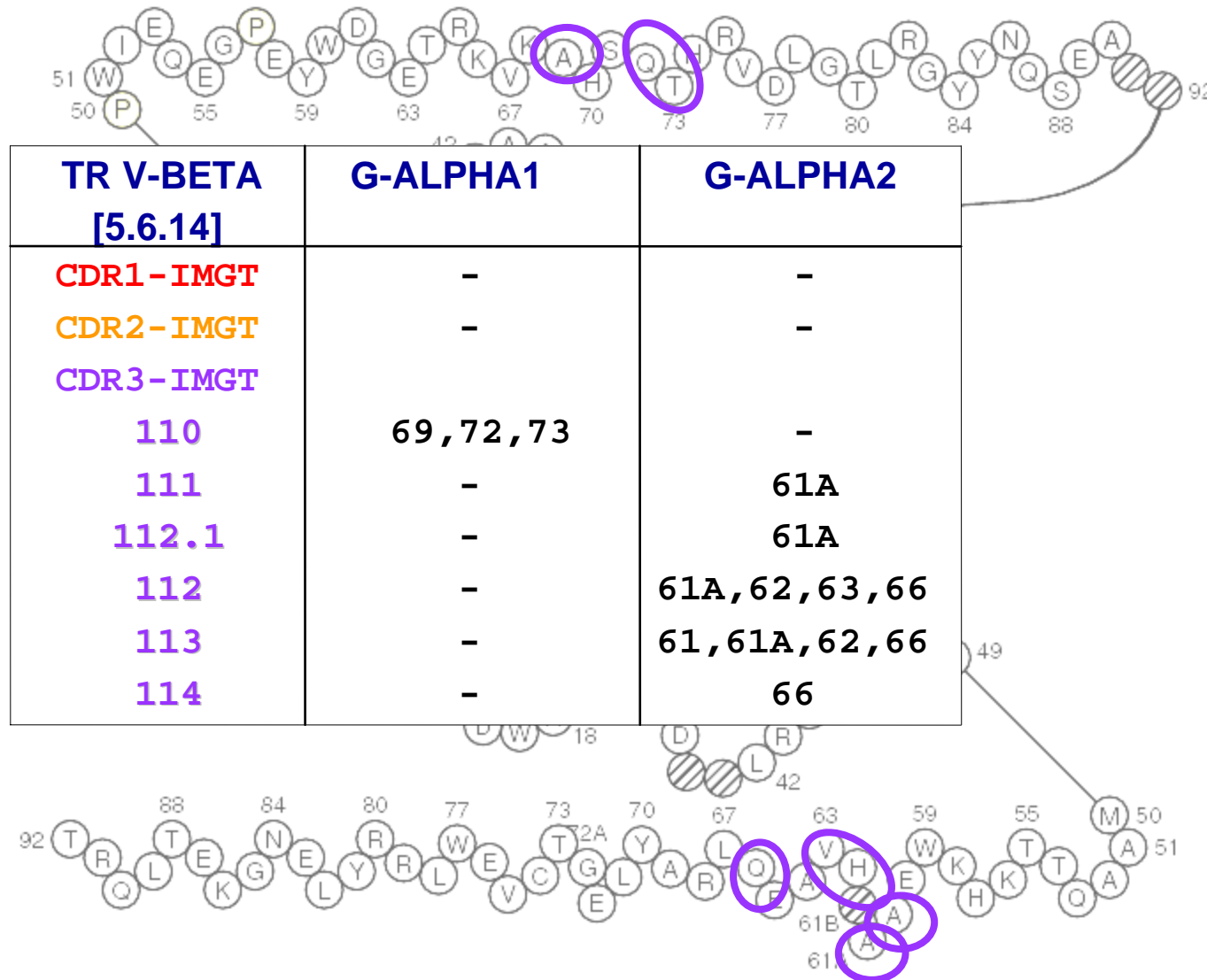
Involve CDR3-IMGT

 Contact with G-ALPHA2



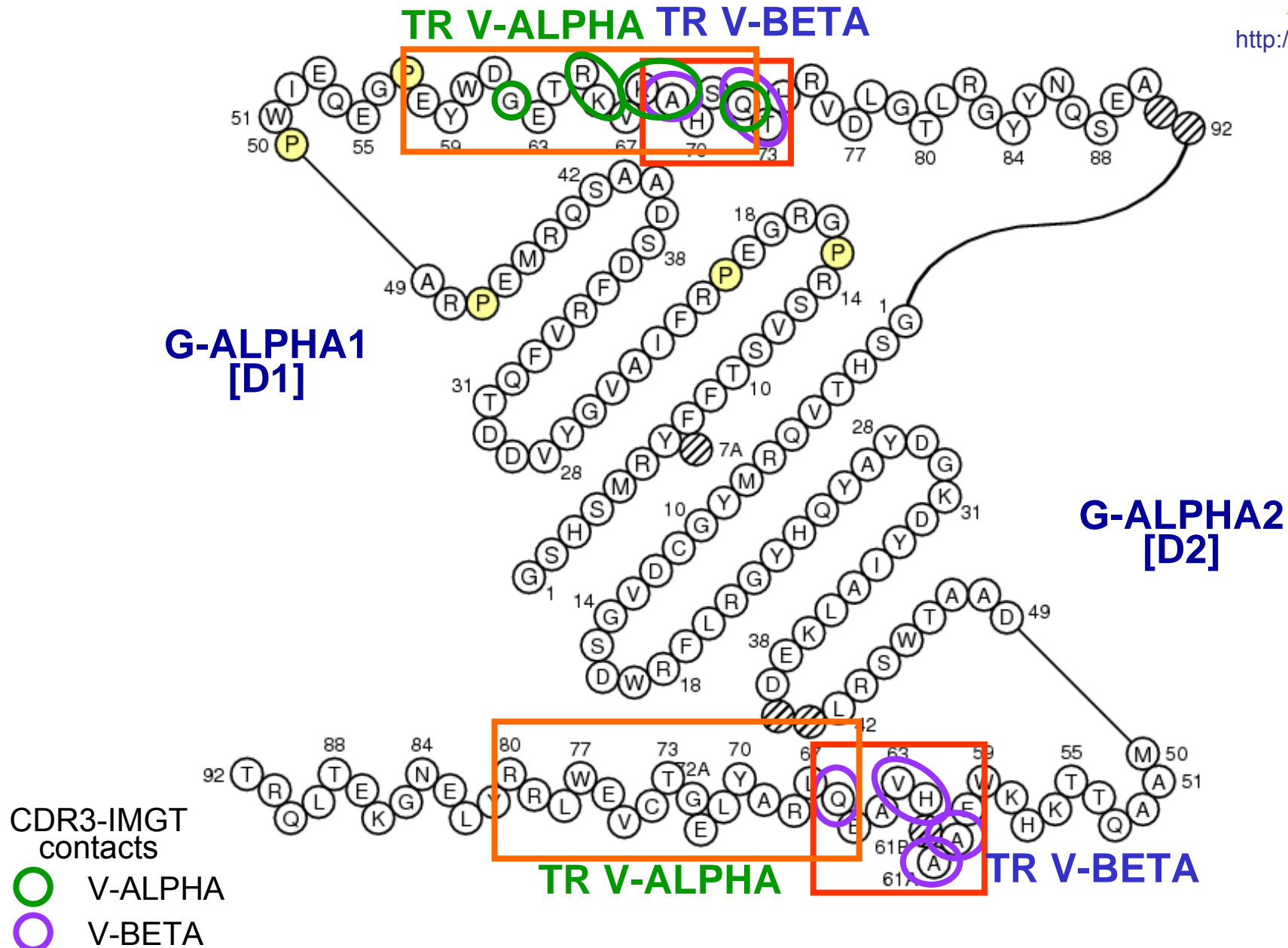
Kaas and Lefranc, In Silico Biology 5, 505-528 (2005)

Contact sites of TR V-BETA with MHC-I (1ao7)

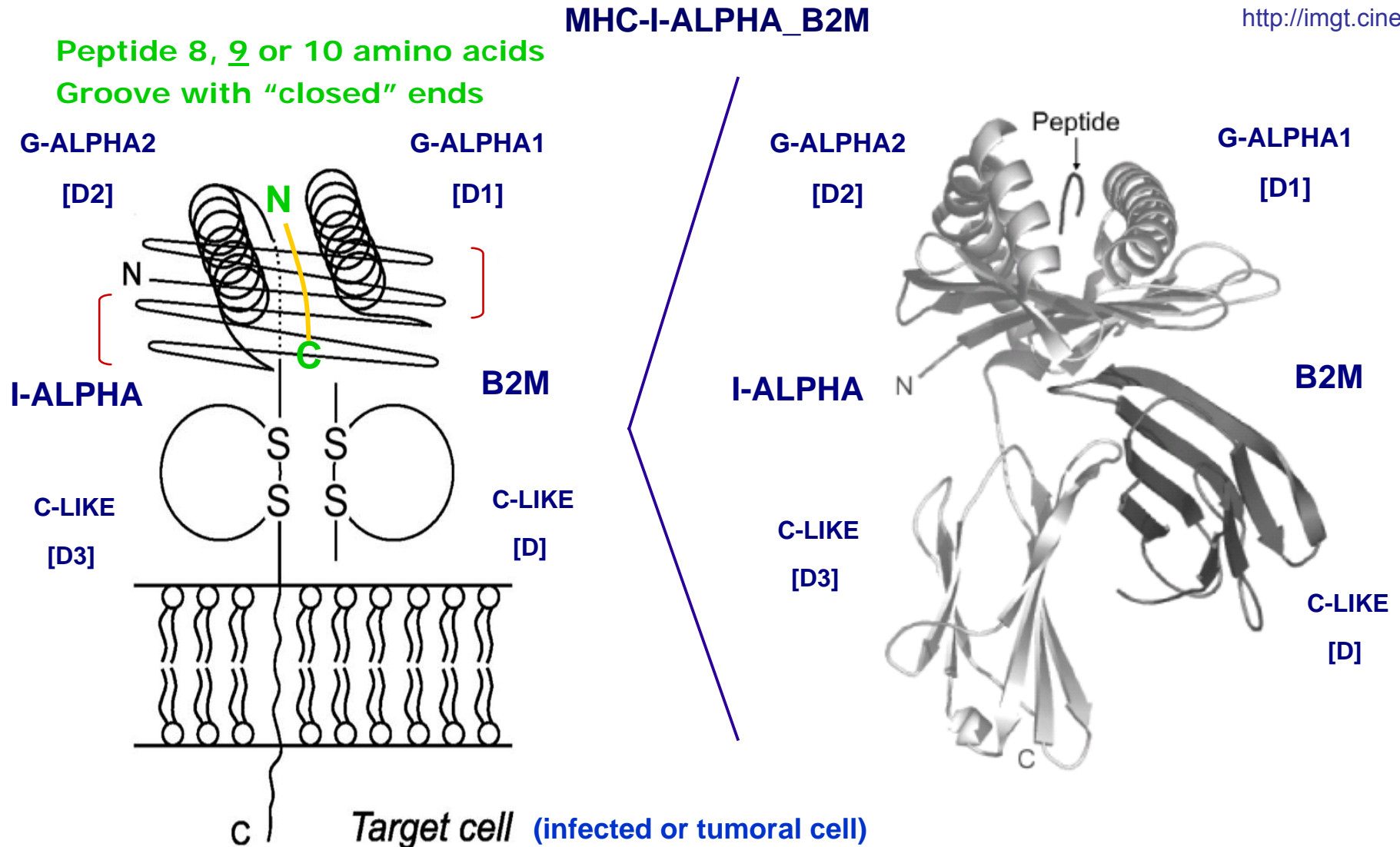


Kaas and Lefranc, In Silico Biology 5, 505-528 (2005)

HLA-A*0201 regions in contact with TR $\alpha\beta$ A6



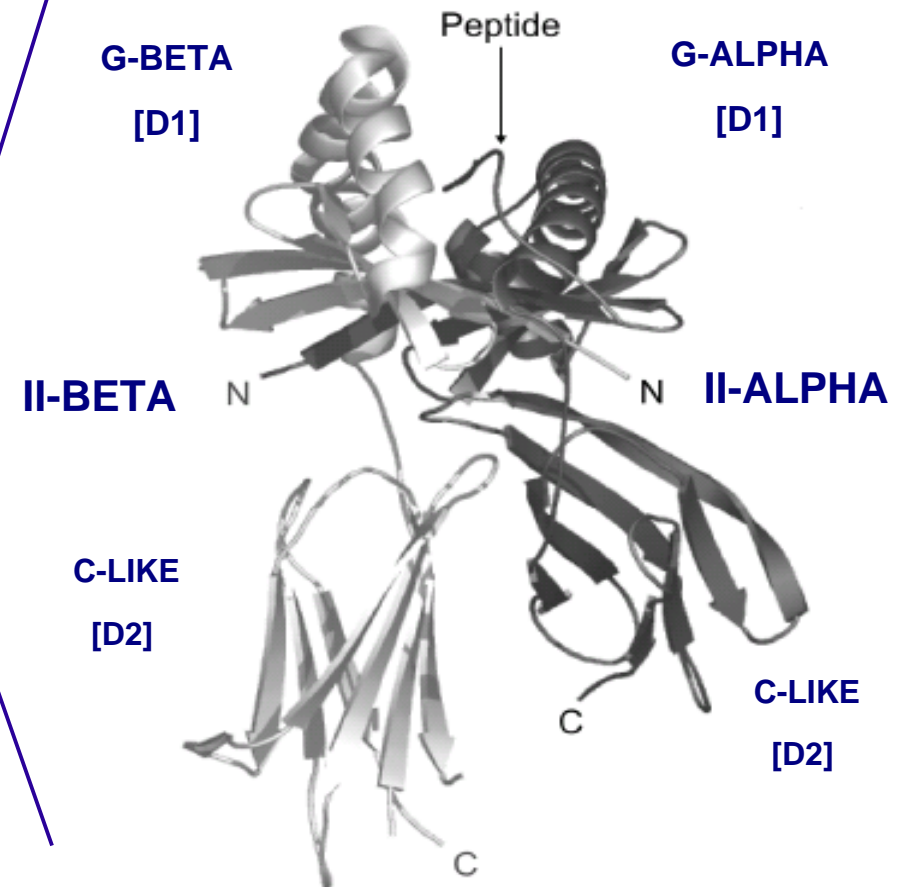
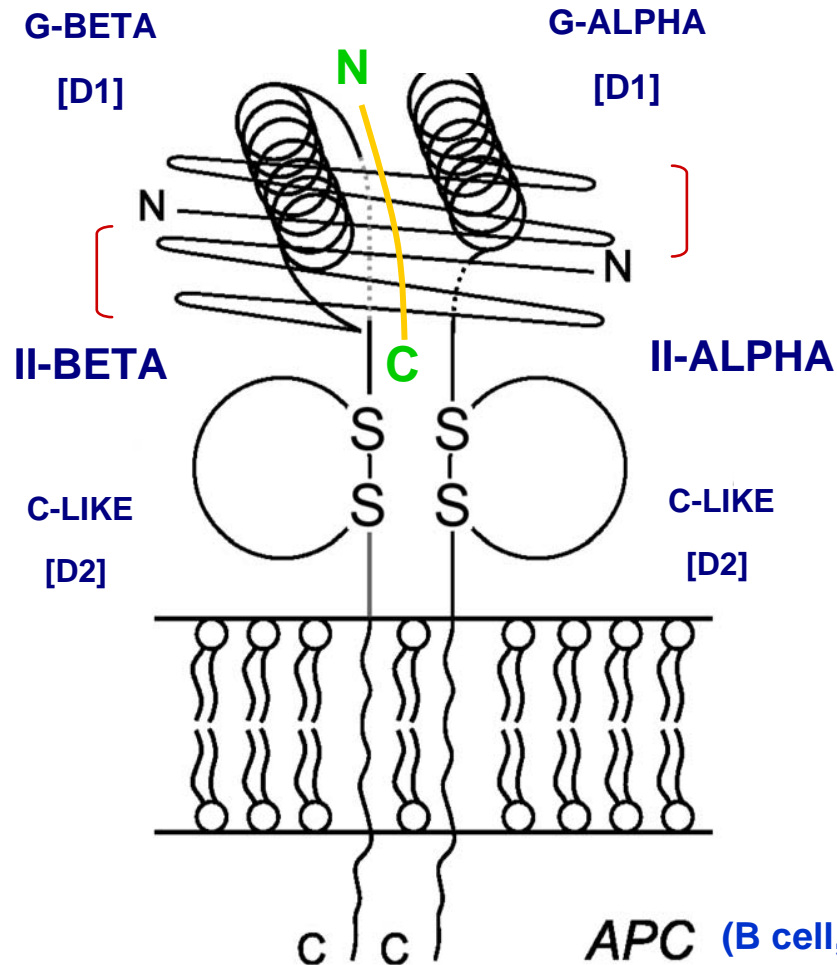
MHC-I chains and domains



MHC-II chains and domains

Peptide 13-17 amino acids
Groove with "open" ends

MHC-II-ALPHA_BETA



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

Peptide alignment



<http://imgt.cines.fr>

	Number of residues	Peptide sequence
MHC-I	8 amino acids 1jtr_Q	E Q Y K F Y S V
	9 amino acids 1ao7_C	L L F G Y P V Y V
	10 amino acids 1bij_P	R G P G R A F V T I
MHC-II	13 amino acids 1j8h_C	P K Y V K Q N T L K L A T

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

Peptide alignment



<http://imgt.cines.fr>

	Number of residues	Peptide sequence												
MHC-I	8 amino acids 1jtr_Q	E	Q	Y	K	F	Y	S	V					
	9 amino acids 1ao7_C	L	L	F	G	Y	P	V	Y	V				
	10 amino acids 1bii_P	R	G	P	G	R	A	F	V	T	I			
MHC-II	13 amino acids 1j8h_C	P	K	Y	V	K	Q	N	T	L	K	L	A	T

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

Peptide alignment



<http://imgt.cines.fr>

	Number of residues	Peptide sequence
MHC-I	8 amino acids 1jtr_Q	E - Q Y (K) F - - Y S V
	9 amino acids 1ao7_C	L - L F (G) Y - P V Y V
	10 amino acids 1bii_P	R - G P (G) R A F V T I
IMGT pMHC contact sites		
MHC-II	13 amino acids 1j8h_C	P K Y V K Q (N) T - - L K L A T

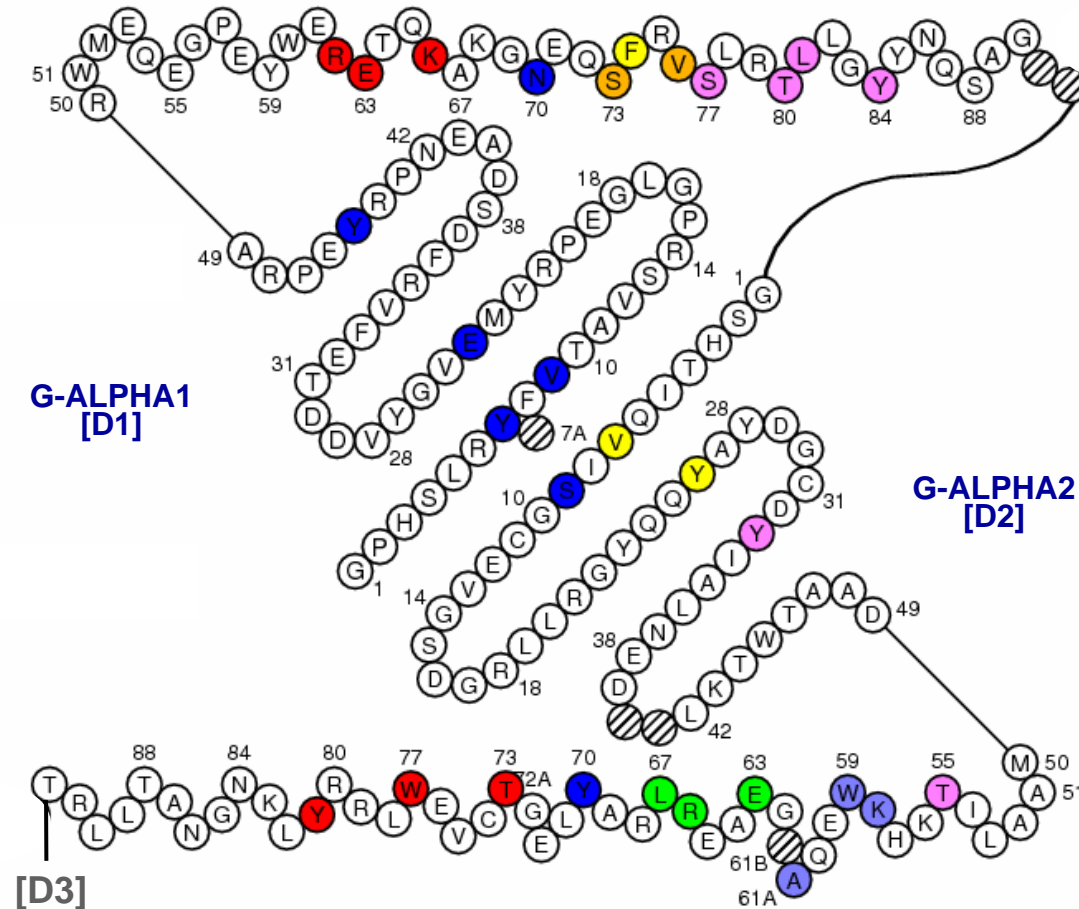
Kaas and Lefranc, In Silico Biology 5, 505-528 (2005)

IMGT Collier de Perles pMHC contact sites



Mouse H2-K1 (MHC-I) and a 8-amino acid peptide

<http://imgt.cines.fr>



8-amino acid peptides

Peptide

Pocket (approx.)

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

Peptide chain: **1jtr_Q**

MHC chain: **1jtr_I**

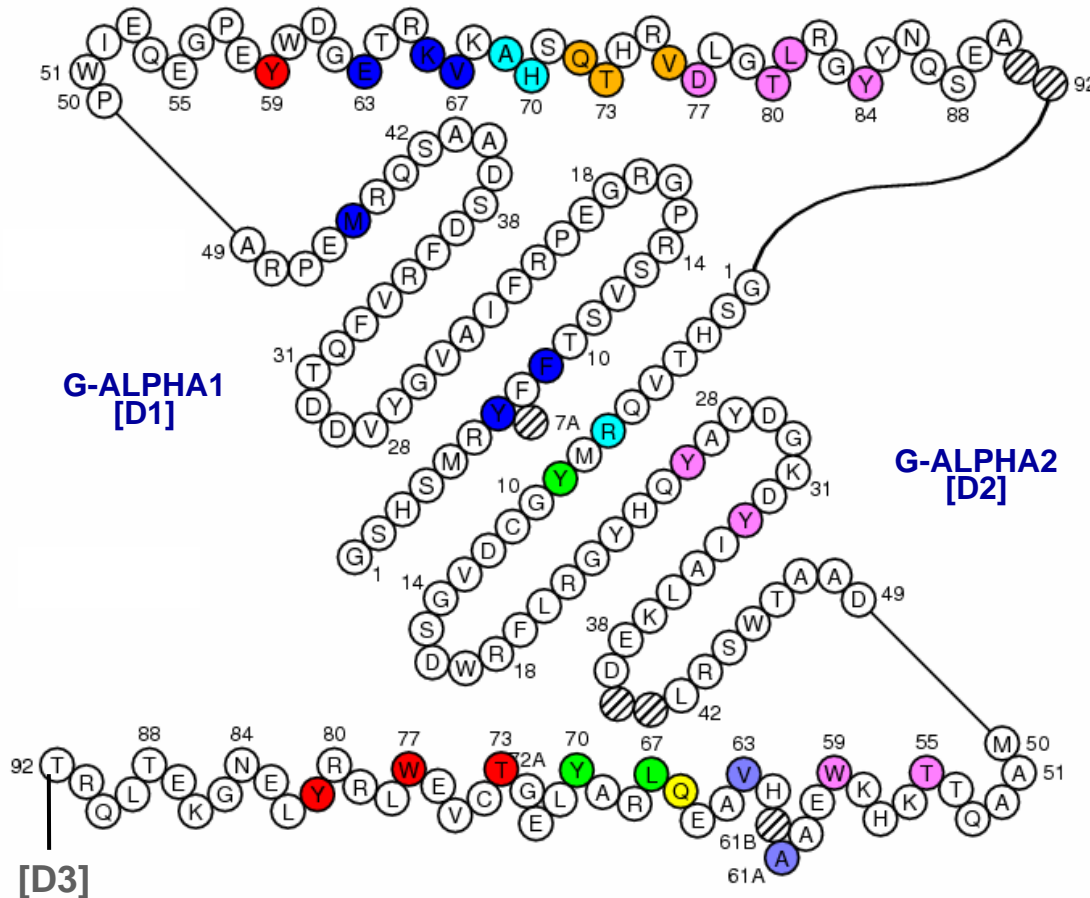
Kaas and Lefranc, In Silico Biology 5, 505-528 (2005)

IMGT Collier de Perles pMHC contact sites



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

<http://imgt.cines.fr>



Peptide chain: **1ao7_C**

MHC chain: **1ao7_A**

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

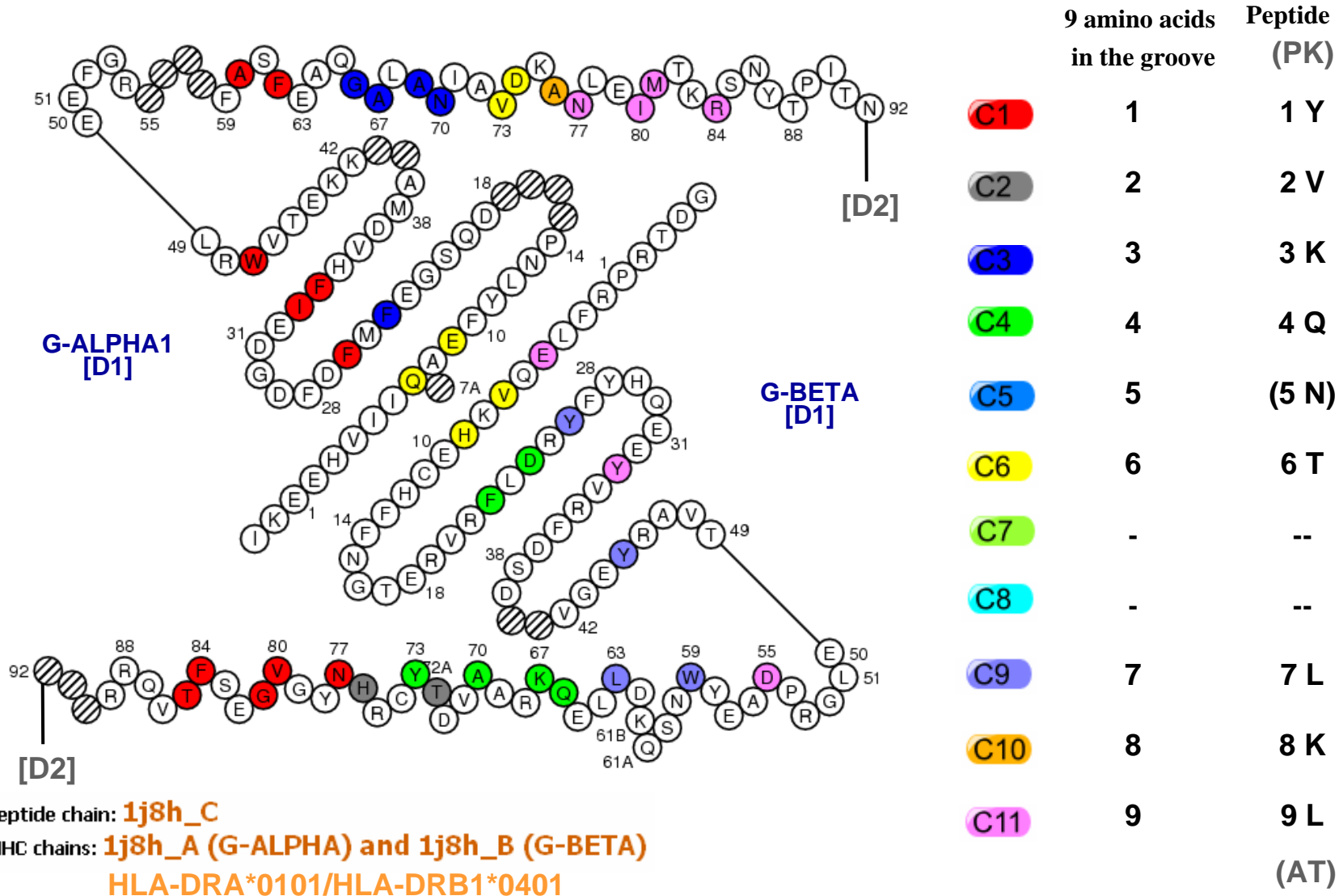
Kaas and Lefranc, In Silico Biology 5, 505-528 (2005)

IMGT Collier de Perles pMHC contact sites



<http://imgt.cines.fr>

Human HLA-DRA/DRB1 (MHC-II) and
9 amino acids of the peptide located in the groove



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

IMGT/3Dstructure-DB: Contact Analysis



<http://imgt.cines.fr>

IMGT Residue@Position cards



IMGT Residue@Position card

Residue@Position: **27 - ASP (D) - V-ALPHA - 1ao7_D** CDR1-IMGT

General information:

PDB file numbering 26
 IMGT file numbering 27
 Residue full name Aspartic Acid
 Formula C4 H7 N1 O4

IMGT LocalStructure@Position

Secondary structure Turn
 Phi (in degrees) -71.12
 Psi (in degrees) 108.09
 ASA (in square angstrom) 22.0

IMGT Num	Residue	Domain	Chain	Atom contacts	Polar	Hydrogen Bond	Non Polar
58	GLU E	G-ALPHA1	1ao7_A	24	6	1	18
2	LYS K	V-ALPHA	1ao7_D	18	0	0	18
25	TYR Y	V-ALPHA	1ao7_D	14	1	0	13
29	GLY G	V-ALPHA	1ao7_D	15	3	0	12
36	SER S	V-ALPHA	1ao7_D	19	5	2	14
85	GLN Q	V-ALPHA	1ao7_D	6	2	0	4
108	THR T	V-ALPHA	1ao7_D	4	0	0	4

G-ALPHA1

IMGT/3Dstructure-DB: Contact Analysis

IMGT Residue@Position cards



<http://imgt.cines.fr>

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



Why are IMGT Colliers de Perles so useful?



<http://imgt.cines.fr>

The IMGT Colliers de Perles

1. bridge the gaps between sequences and structures
2. are used whatever the MHC and whatever the species.

	MHC-Ia	MHC-Ib	MHC-IIa	MHC-IIb
	HLA-A,-B,-C	HLA-E,-F,-G	HLA-DPA,-DQA, -DRA HLA-DPB,-DQB, -DRB	HLA-DMA, -DOA HLA-DMB, -DOB
	H2-D,-K,-L	H2-M,-Q,-T	H2-AA,-EA H2-AB,-EB	H2-DMA,-DOA H2-DMB,-DOB

3. have been extended to the MHC-I-like proteins (CD1, FCRN, RAET, HFE, MICA, AZGP1,...).

Interestingly, only one additional position **54A** in **G-ALPHA1-LIKE** was needed to extend the IMGT unique numbering for G-DOMAIN to the G-LIKE-DOMAIN.



Many thanks to the IMGT® team at Montpellier, France