

IMGT/3Dstructure-DB and tools for immunoglobulins (IG) or antibodies, T cell receptors (TR), MHC, IgSF and MhcSF structural data

François Ehrenmann Tuesday, September 7, 2010





http://www.imgt.org



Data origin and Scientific Chart



3D structures database (IG, TR, MHC, IgSF and MhcSF)

Card

IMG	T/3Dstructur	e-DB ca	ard for: 1	n0	x	R	3				Entry code Search	
IMGT molec	ule name		IMGT receptor t	ype	IMGT receptor des	scription	Ligand(s)	Species		СС	Chain ID	
h10 noutralizi	ing mAb anti gn10	0 [LIIV 4]	IG		FAB-GAMMA-1_K	APPA		Homo sapier	ns (Human)	1	[<u>1n0x H</u> <u>1n0x L</u>]	
DIZ NEUtralizi	ing mab, anti-gp12	0 [[[]]	IG		FAB-GAMMA-1_K	APPA		Homo sapier	os (Human)	2	[1n0x K 1n0x M]	
					Protein		P2.1 peptide	Synthetic (Sy	/nthetic)	2	[<u>1n0x R</u>]	
					Protein		BZ. I peptide	Synthetic (Sy	/nthetic)	1	[<u>1n0x P</u>]	
Experimental t	technique X-ray diffi	raction	Resolution (in ang	strom) 1.80 PDB re	elease date	13-APR-04					
Chain details	Contac analysi	t s	Paratope and epitope	3D Jmo) visualization bl or QuickPDB	Renumbere MGT file	ed IMG	iT numbering parison 🗖	Reference and link	es s	Printable card	
For the IMGT Re Differences wit Chain details	esidue@Position card th the closest IMGT al s of b12 neutralizin	d of a given re l <mark>lele sequenc</mark> g mAb, anti	esidue, click on its lett ce are in orange. I-gp120 [HIV-1], IG	erina , FAB	a sequence. 9-GAMMA-1_KAPPA h	lomo sapiel	ns (Human) [1n0x_H,1n0x_L]				
Chain ID	1n0x_H											
Chain length	230											
IMGT chain	VH-CH1											
description	= VH (1-127) [D1] + C	H1 (128-219	9) [D2]									
Chain sequence	<pre></pre>											
	Sequence in FASTA	format Seq	uence in IMGT forma									
	IMGT domain description	VH (1-127) [D1]									
	IMGT gene and allele name	IGHV1-3*01	(79.60%)(Human) <u>Al</u>	ignme	ent details							
	IMGT gene and allele name	IGHJ6*03 (9	3.80%)(Human) <u>Aligr</u>	iment	<u>details</u>							
	2D representation	IMGT Collier	de Perles or IMGT C	ollier	de Perles on 2 layers							

IMGT/3Dstructure-DB

provides the closest genes and alleles that are expressed in the amino acid sequences of the 3D structures, by aligning these sequences with the IMGT domain reference directory.

- Chain and domain details
- Contact analysis
- Paratope and epitope
- 3D visualization
- Renumbered files
- Numbering comparison
- References and links

IMGT Colliers de Perles

2D representations of V, C and G domains based on the **IMGT unique numbering**

- delimitation of the framework (**FR-IMGT**) and complementarity determining region (**CDR-IMGT**) is standardized

- **CDR-IMGT lengths** are crucial information which characterize variable regions

- conserved AA (and codons) are always at the **same positions**:

- 23 1st-CYS
- 41 CONSERVED-TRP
- 89 hydrophobic
- 104 2nd-CYS
- 118 J-PHE, J-TRP



IGHV, VH domain, one layer CDR-IMGT lengths [8.8.13]

Contact analysis and IMGT Colliers de Perles

List	List of the Residue@Position pair contacts: Domain pair contacts Click 'R@P' for IMGT Residue@Position cards											ts		
Cilc	Order			Residue	e@F0Siti	on care	Order						Ato	m contacts
	IMGT Num	Resid	ue	Domain	Chain		IMGT Num	Resid	lue	Domain	Chain	Total	Polar	Hydrogen
<u>R@P</u>	38	TYR	Y	VH	1ce1_H	<u>R@P</u>	2	THR	Т		1ce1_P	4	0	0
<u>R@P</u>	38	TYR	Y	VH	1ce1_H	<u>R@P</u>	7	ALA	А		1ce1_P	13	1	0
<u>R@P</u>	38	TYR	Y	VH	1ce1_H	<u>R@P</u>	8	ASP	D		1ce1_P	14	2	2
<u>R@P</u>	55	PHE	F	VH	1ce1_H	<u>R@P</u>	6	SER	S		1ce1_P	5	0	0
<u>R@P</u>	55	PHE	F	VH	1ce1_H	<u>R@P</u>	7	ALA	А		1ce1_P	16	0	0
<u>R@P</u>	55	PHE	F	VH	1ce1_H	<u>R@P</u>	8	ASP	D		1ce1_P	1	0	0
<u>R@P</u>	57	ARG	R	VH	1ce1_H	<u>R@P</u>	7	ALA	А		1ce1_P	9	3	2
<u>R@P</u>	57	ARG	R	VH	1ce1_H	<u>R@P</u>	8	ASP	D		1ce1_P	20	6	1
<u>R@P</u>	61	LYS	ĸ	VH	1ce1_H	<u>R@P</u>	8	ASP	D		1ce1_P	11	2	1
<u>R@P</u>	66	GLU	Е	VH	1ce1_H	<u>R@P</u>	7	ALA	А		1ce1_P	1	0	0
<u>R@P</u>	107	GLU	Е	VH	1ce1_H	<u>R@P</u>	2	THR	т		1ce1_P	13	2	1
<u>R@P</u>	107	GLU	Е	VH	1ce1_H	<u>R@P</u>	4	SER	s		1ce1_P	5	2	0
<u>R@P</u>	107	GLU	Е	VH	1ce1_H	<u>R@P</u>	7	ALA	А		1ce1_P	5	0	0
<u>R@P</u>	108	GLY	G	VH	1ce1_H	<u>R@P</u>	1	GLY	G		1ce1_P	2	1	0
R@P	108	GLY	G	VH	1ce1_H	<u>R@P</u>	2	THR	т		1ce1_P	9	2	0
<u>R@P</u>	109	HIS	н	VH	1ce1_H	<u>R@P</u>	1	GLY	G		1ce1_P	24	4	0
<u>R@P</u>	109	HIS	н	VH	1ce1_H	<u>R@P</u>	2	THR	т		1ce1_P	21	5	0
<u>R@P</u>	109	HIS	н	VH	1ce1_H	<u>R@P</u>	3	SER	s		1ce1_P	9	2	1
<u>R@P</u>	110	THR	т	VH	1ce1_H	<u>R@P</u>	1	GLY	G		1ce1_P	1	1	0
<u>R@P</u>	110	THR	т	VH	1ce1_H	<u>R@P</u>	3	SER	S		1ce1_P	11	4	1
<u>R@P</u>	112	ALA	А	VH	1ce1_H	<u>R@P</u>	3	SER	S		1ce1_P	3	1	0
<u>R@P</u>	113	ALA	А	VH	1ce1_H	<u>R@P</u>	2	THR	Т		1ce1_P	3	0	0
<u>R@P</u>	113	ALA	А	VH	1ce1_H	<u>R@P</u>	3	SER	s		1ce1_P	7	2	0
<u>R@P</u>	113	ALA	А	VH	1ce1_H	<u>R@P</u>	4	SER	s		1ce1_P	4	0	0
<u>R@P</u>	114	PRO	Ρ	VH	1ce1_H	<u>R@P</u>	4	SER	S		1ce1_P	5	0	0

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IGHV, VH domain, two layers with Hydrogen bonds CDR-IMGT lengths [8.8.13]

IMGT/Collier-de-Perles

2D graphical representations of protein domains

 Domain type Number of layers CDR-IMGT color type Background color Domain sequence 	Variable (V) 1 1 1 1 (RPI,IGH,TRB,TRD) 50% Hydrophobic positions QVTLKESGP.GILQPSQTLSLTCSFSGFSLSTYGMGVGWIRQPSGKGLEWLAH IWWDDVKRYNPALK.SRLTISKDTSGSQVFLKIASVDTSDTATYYCARMGSD YDVWFDYWGOGTLVTVSA	IMGT/Collier-de-Perles tool: • provides 2D representations of V, C and G type domains • can be customized - to display CDR-IMGT according to the IMGT Color menu - to visualize the amino acids according to their hydropathy, volume or IMGT physicochemical classes
 Amino acid insertions CDR3-IMGT length Your domain title 	Position Length Numbering labels Image: Draw! ADD	
	$10 \bigcirc E \bigcirc V \bigcirc C \land C \land A = B \land C \downarrow C \land A = B \land$	$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$

IMGT/DomainGapAlign

Amino acid sequences analysis per domain

Paste your protein sequence(s) in <u>FASTA format</u> below >alemtuzumab_VH QVQLQESGPGLVRPSQTLSLTCTVSGFTFTDFYMNWVRQPPGRGLEWIGFIRDKAKGYTTEY HTAAPFDYWGQGSLVTVSSASTKGPSVFPLAPSSKSTSGGTAALGCLVKDYFPEPVTVSWNS NVNHKPSNTKVDKKVE	NPSVKGRVTMLVDTSKNQFSLRLSSVTAADTAVYYCAREG GALTSGVHTFPAVLQSSGLYSLSSVVTVPSSSLGTQTYIC Sequence name: <u>alemtuzumab</u>	 For an antibody V domain sequence, IMGT/DomainGapAlign: identifies the closest V domain creates gaps according to the IMGT unique numbering delimits FR- and CDR-IMGT highlights differences with the closest reference
Ø Sequence names must be different !		
Upload a file	Move your mouse over the amino acids below the alignment for the	e characterization of AA changes
Select a domain type	Closest reference gene and allele(s) from the IMG	T V domain directory: <i>Homo sapiens</i> (Human)
Select a species All species	V gene and allele Species Domain IGHV4-59*01 Homo sapiens 1	Smith-Waterman Score V-REGION percentage of identity Overlap Align your sequence with 494 73.0 100 Image: Content of the second
Displayed alignments Display IMGT Colliers de Perles Align and IMGT-gap my sequence(s)	J gene and allele Species Domain IGHJ4*01 Homo sapiens 1 IGHJ4*02 Homo sapiens 1 IGHJ4*03 Homo sapiens 1	Smith-Waterman Score J-REGION percentage of identity Overlap 94 92.9 14 94 92.9 14 94 92.9 14
	 Alignment with the closest gene and allele from the FR1-IMGT (1-26) A B (1-15) A (1-26) A (1-15) A (1-15)	ne IMGT V domain directory: Homo sapiens (Human) DR1-IMGT FR2-IMGT CDR2-IMGT FR3-IMGT CDR3-IMGT FR4-IMGT (27-38) (39-55) (56-65) (66-104) (105-117) (118-128) BC C C' C'C' C'' D E F FG G (27-38) (39-46) (47-55) (56-65) (66-74) (75-84) (85-96) (97-104) (105-117) (118-128) 38 3941 46 47 55 56 65 66 74 75 80 84 89 96 97 104 105 1112 118 128

IMGT/DomainGapAlign

Towards «Potential immunogenicity evaluation»

Comparison with the statistical profiles of the human expressed repertoires is useful to identify potential immunogenic residues at given positions in chimeric or humanized antibodies or to evaluate immunogenicity of primate antibodies.



Collier de Perles on one layer

Conclusion

- IMGT/3Dstructure-DB, IMGT Colliers de Perles and the IMGT/DomainGapAlign tool
- 1. are widely used by researchers, particularly for antibody engineering and humanization design
- 2. allow to precisely define and to easily compare amino acid sequences of the FR and CDR-IMGT
- 3. facilitate the identification of potential immunogenic residues at given positions in chimeric or humanized antibodies.
- 4. Therapeutic applications emphasize the importance of the IMGT/3Dstructure-DB standardized approach that bridges the gap between sequences and 3D structures whatever the species.

THANKS FOR YOUR ATTENTION

And thanks to IMGT Team !

Poster n° 9: IMGT/3Dstructure-DB and tools for immunoglobulins (IG) or antibodies, T cell receptors (TR), MHC, IgSF and MhcSF structural data







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					<u> </u>	ard			
IMC	GT/3Dstructu	re-DB c	ard for: 1n	0x 🕺	61		Entry code Search	IMGT/3Dstructure-DB	
MGT mole	cule name		IMGT receptor type	e IMGT receptor description	n Ligand(s)	Species	CC Chain ID	provides the closest ge	ile
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- nouu diiz	and an and a second pro-	.5 (mv-1)	IG	FAB-GAMMA-1_KAPPA		Homo sapiens (Human)	2 [1n0x K 1n0x M]		
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IMGT/DomainGapAlign Towards «Potential immunogenicity evaluation»

Comparison with the statistical profiles of the human expressed repertoires is useful to identify potential immunogenic residues at given positions in chimeric or humanized antibodies or to evaluate immunogenicity of primate antibodies.



Conclusion

IMGT/3Dstructure-DB, IMGT Colliers de Perles and the IMGT/DomainGapAlign tool

- 1. are widely used by researchers, particularly for antibody engineering and humanization design
- 2. allow to precisely define and to easily compare amino acid sequences of the FR and CDR-IMGT
- 3. facilitate the identification of potential immunogenic residues at given positions in chimeric or humanized antibodies.
- 4. Therapeutic applications emphasize the importance of the IMGT/3Dstructure-DB standardized approach that bridges the gap between sequences and 3D structures whatever the species.

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