# Bioinformatique: du gène à la structure

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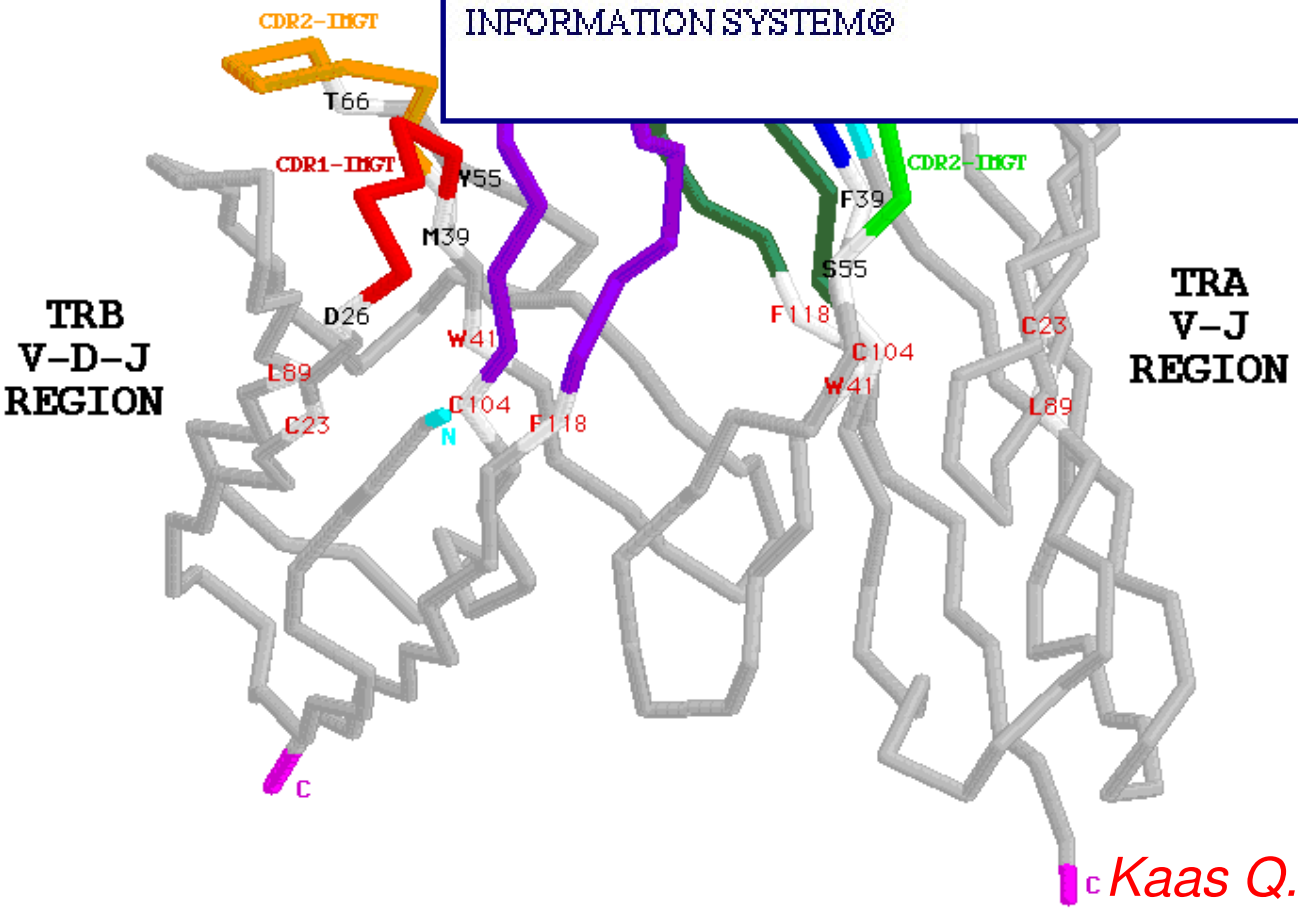


TRB
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REGION

TRA
V-J
REGION

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

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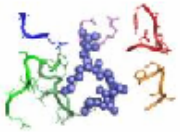
**IMGT/3Dstructure-DB card for : 1ce1**



Entry code [ ] Search

Query page

| 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

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
- ☐ (SB) Side chain/backbone

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# IMGT/3Dstructure-DB

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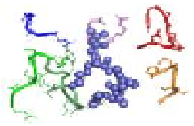
## IMGT/3Dstructure-DB card for : 1u8k



| 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 | [ IGHV_1<br>RITLKESGPPLVKPTQTLTLTCSFSGFSLSDFGVGVGWIRQPPGKALEWLAIIYSDDDKRYSPSINTRLTITKDTSKNQVVLVMTRVSPV<br>][ D ][ IGHJ_1 ] [ IG<br>DTATYFCAHRRGPTTLFGVPIARGPVNAMDVWGQGITVTISSTSTKGPSVFPLAPCSKSTAGGTAALGCLVKDYFPEPVTVSWNSGALTS<br>HC_1 ]<br>GVHTFPAVLQSSGLYSLSSVVTVPSSSLGTQTYTCNVNHKPSNTKVDKRVEPKS |
| V-DOMAIN | IMGT domain description: VH<br>IGHV gene and allele name: IGHV2-5*05 (85.00%), IGHV2-5*06 (85.00%), *Alignment details*<br>IGHJ gene and allele name: IGHJ6*01 (83.33%), IGHJ6*02 (83.33%), *Alignment details*<br>2D representation: Collier de Perles or Collier de Perles on 2 layers<br>CDR-IMGT lengths: [10.7.24]<br>Sheet composition: [A B D E] [C C" C' F G]<br>[ CDR1 ] [ CDR2 ]<br>RITLKESGP.PLVKPTQTLTLTCSFSGFSLSDFGVG..VGWIRQPPGKALEWLAIIYSDDDK...RYSPSIN.TRLTITKDTSKNQVVLV<br>[ CDR3 ]<br>MTRVSPVDTATYFCAHRRGPTTLFGVPIARGPVNAMDVWGQGITVTI |
| C-DOMAIN | IMGT domain description: CH1<br>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*<br>2D representation: Collier de Perles or Collier de Perles on 2 layers<br>Sheet composition: [A B D E] [C F G]<br>.....STKGPSVFPLAPCSKSTA...GGTAALGCLVKDYFP..EPVTVSWNSGALTS....GVHTFPAVLQSS.....GLYSLSSVVTV<br>PSSSL...GTQTYTCNVNHKP..SNTKVDKRV |

| Chain ID | 1u8k_A |
|---|---|
| IMGT chain description | L-KAPPA |
| Chain amino acid sequence | [ IGKV_1<br>ALQLTQSPSSLSASVGDRITITCRASQGVTSALAWYRQKPGSPPQLLIYDASSLESGVPSRFSGSGSGTEFTLTISTLRPEDFATYYCQQ<br>] [ IGKJ_1 ][ IGKC_1<br>LHFYPHTFGGGTRVDVRRTVAAPSVFIFPPSDRQLKSGTASVVCLLNNFYPREAKVQWKVDNALQSGNSQESVTEQDSKDSTYSLSSTLT<br>]<br>LSKADYEKHKVYECEVTHQGLSSPVTKSFNRGEC |
| V-DOMAIN | IMGT domain description: V-KAPPA<br>IGKV gene and allele name: IGKV1-13*02 (85.26%) *Alignment details*<br>IGKJ gene and allele name: IGKJ4*01 (63.64%) , IGKJ4*02 (63.64%) *Alignment details*<br>2D representation: Collier de Perles or Collier de Perles on 2 layers<br>CDR-IMGT lengths: [6.3.9]<br>Sheet composition: [A B D E] [C C" C' F G]<br>[ CDR1 ] [ CDR2 ]<br>ALQLTQSPSSLSASVGDRITITCRASQGVTSA.....LAWYRQKPGSPPQLLIYDAS.....SLESGVP.SRFSGSG..SGTEFTLT<br>[ CDR3 ]<br>ISTLRPEDFATYYCQQLHF....YPHTFGGGTRVDVR |
| C-DOMAIN | IMGT domain description: C-KAPPA<br>IGKC gene and allele name: IGKC*01 (98.13%) *Alignment details* |

| Chain ID | 1u8k_C |
|---|---|
| IMGT chain description | Peptide |
| Chain amino acid sequence | LELDKWASL |

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

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| | | |
|---|---|---|
| Chain ID | **1u8k_B** | |
| IMGT chain description | VH-CH1 | Region identification and delimitation |
| Chain amino acid sequence | [ IGHV_1<br>RITLKESGPPLVKPTQTLTLTCSFSGFSLSDFGVGVGWIRQPPGKALEWLAIIYSDDDKRYSPSLNTRLTITKDTSKNQVVLVMTRVSPV<br>][ D ][ IGHJ_1 ] [ IG<br>DTATYFCAHRRGPTTLFGVPIARGPVNAMDVWGQGITVTISSTSTKGPSVFPLAPCSKSTAGGTAALGCLVKDYFPEPVTVSWNSGALTS<br>HC_1 ]<br>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 ]<br>RITLKESGP.PLVKPTQTLTLTCSFSGFSLSDFGVG..VGWIRQPPGKALEWLAIIYSDDDK...RYSPSLN.TRLTITKDTSKNQVVLV<br>[ CDR3 ]<br>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%), |

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

# IMGT/3Dstructure-DB

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| | | |
|---|---|---|
| Chain ID | **1u8k_B** | |
| IMGT chain description | VH-CH1 | |
| Chain amino acid sequence | [<br>RITLKESGPPLVKPTQTLTLTCS<br>][ D<br>DTATYFCAHRRGPTTLFGVPIAR<br>HC_1<br>GVHTFPAVLQSSGLYSLSSVVTVPSSSLGTQTYTCNVNHKPSNTKVDKRVEPKS | ITRVSPV<br>IG<br>SGALTS<br>] |
| 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 ]<br>RITLKESGP.PLVKPTQTLTLTCSFSGFSLSDFGVG..VGWIRQPPGKALEWLAIIYSDDDK...RYSPSIN.TRLTITKDTSKNQVVLV<br>[ CDR3 ]<br>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* |

Identification of the IMGT gene and the IMGT closest allele(s)

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# IMGT/3Dstructure-DB

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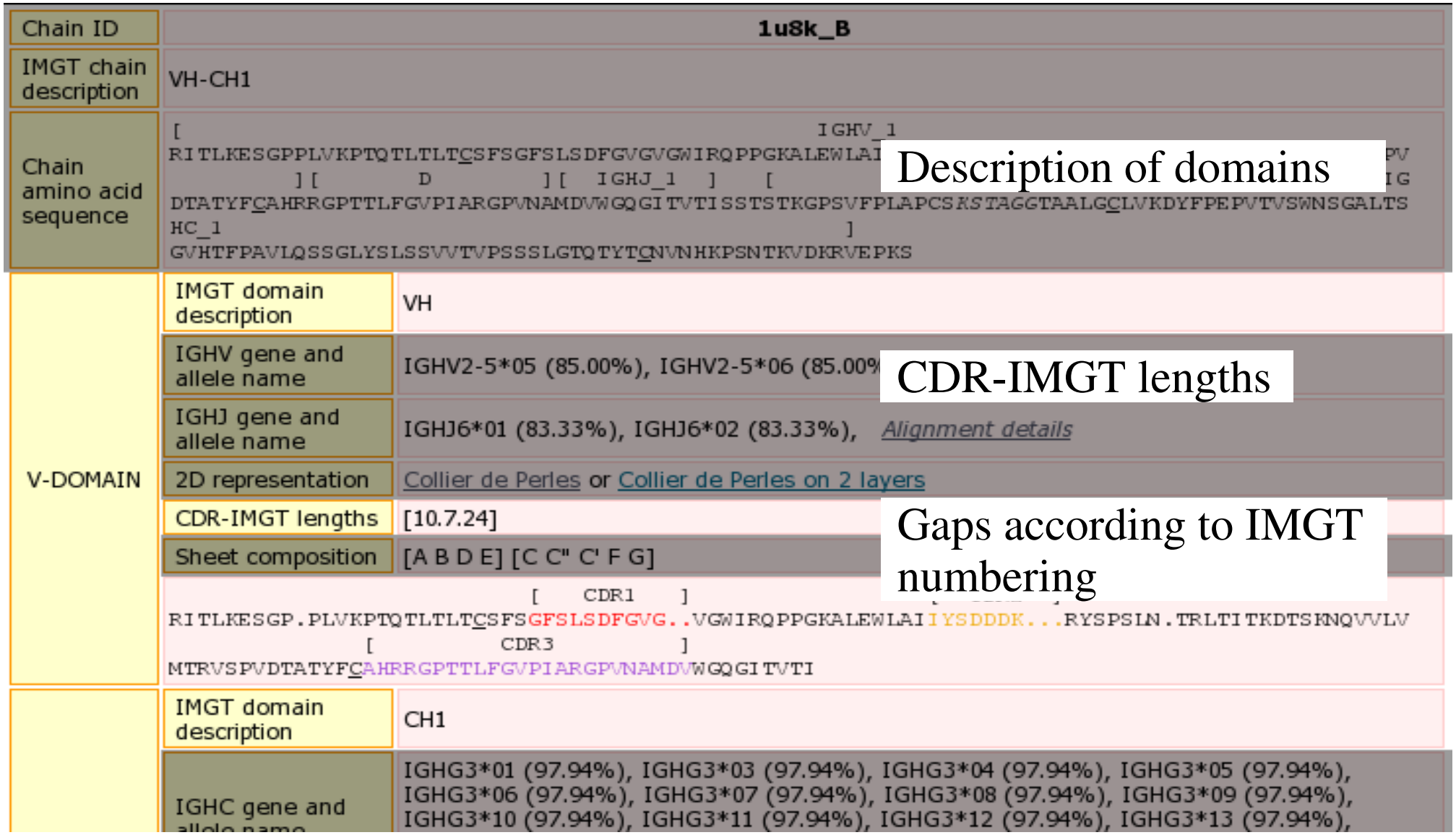

| | | |
|---|---|---|
| Chain ID | **1u8k_B** | |
| IMGT chain description | VH-CH1 | |
| Chain amino acid sequence | [ IGHV_1<br>RITLKESGPPLVKPTQTLTLTCSFSGFSLSDFGVGVGWIRQPPGKALEWLAI PV<br>][ D ][ IGHJ_1 ] [ IG<br>DTATYFCAHRRGPTTLFGVPIARGPVNAMDVWGQGITVTISSTSTKGPSVFPLAPCSKSTAGGTAALGCLVKDYFPEPVTVSWNSGALTS<br>HC_1 ]<br>GVHTFPAVLQSSGLYSLSSVVTVPSSSLGTQTYTCNVNHKPSNTKVDKRVEPKS | |
| V-DOMAIN | IMGT domain description | VH |
| | IGHV gene and allele name | IGHV2-5*05 (85.00%), IGHV2-5*06 (85.00% |
| | 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 ]<br>RITLKESGP.PLVKPTQTLTLTCSFSGFSLSDFGVG..VGWIRQPPGKALEWLAIIYSDDDK...RYSPSLN.TRLTITKDTSKNQVVLV<br>[ CDR3 ]<br>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%), |

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 |

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IMGT/3Dstructure-DB Domain pair contacts

*Contacts of* Domain **VH** Chain **1ce1_H** *with* Domain **(Ligand)** Chain **1ce1_P**

Atom contact types

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

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 | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | 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 |

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| | 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 | *with* | Domain | Chain
---|---|---|---|---|---
| **V-KAPPA** | **1cz8_X** | | **(Ligand)** | **1cz8_V**

Atom contact types

- [ ] Non covalent
- [x] Polar
- [x] 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 |

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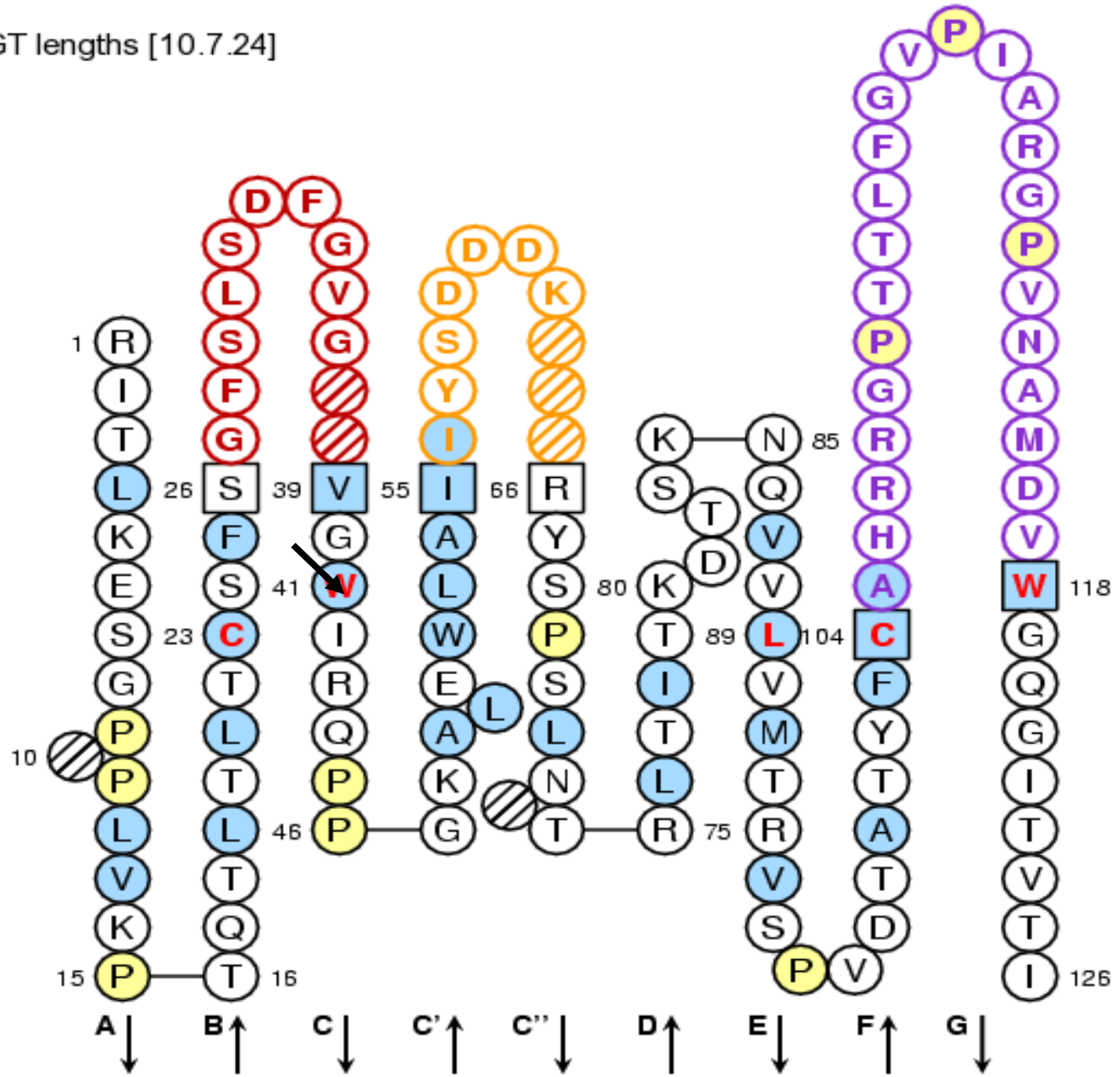
IMGT Collier de Perles : *Homo sapiens* (Human) IGHV_1 V-DOMAIN from 2F5 (PDB: 1u8k_B)

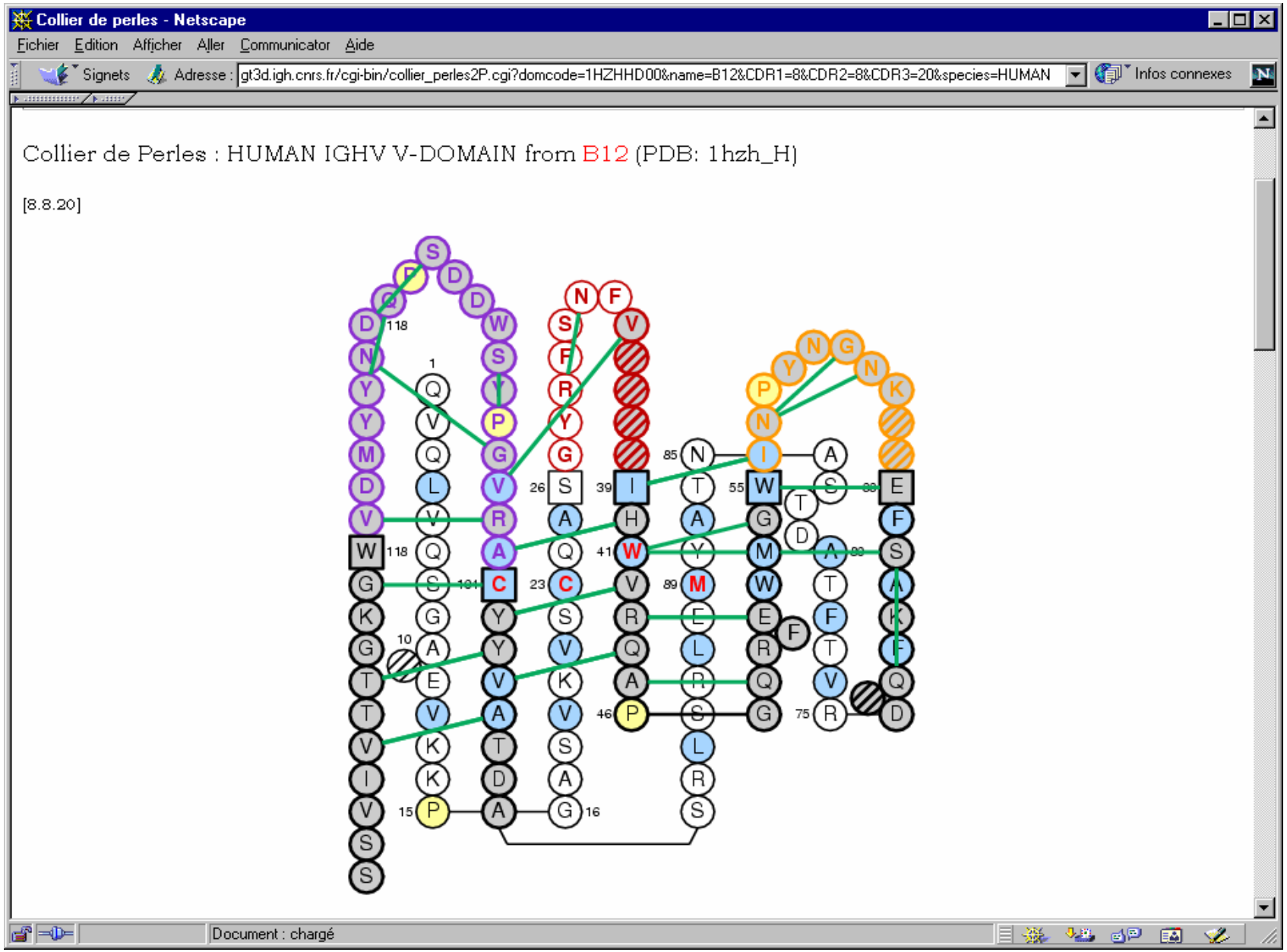
CDR-IMGT lengths [10.7.24]

http://imgt.cines.fr




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

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




http://imgt.cines.fr

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

## 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] | 108Y 114T |
| pertuzumab | [6.3.9] | |

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

# Structural domains

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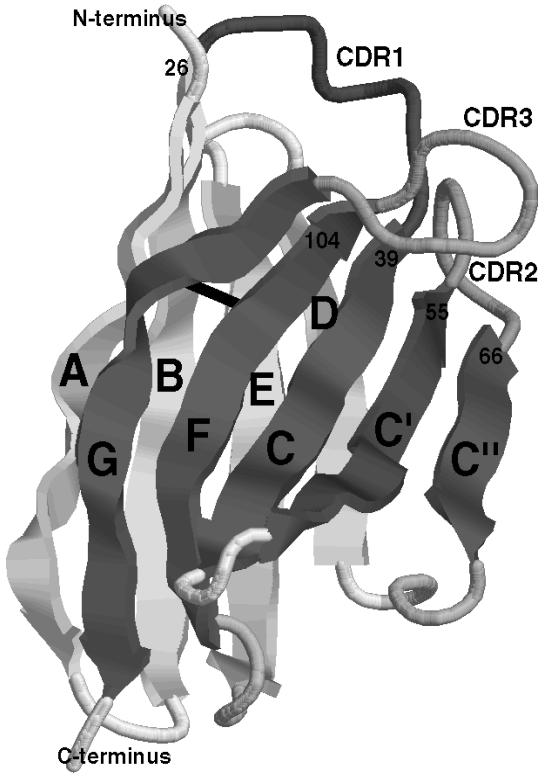
## IG and TR

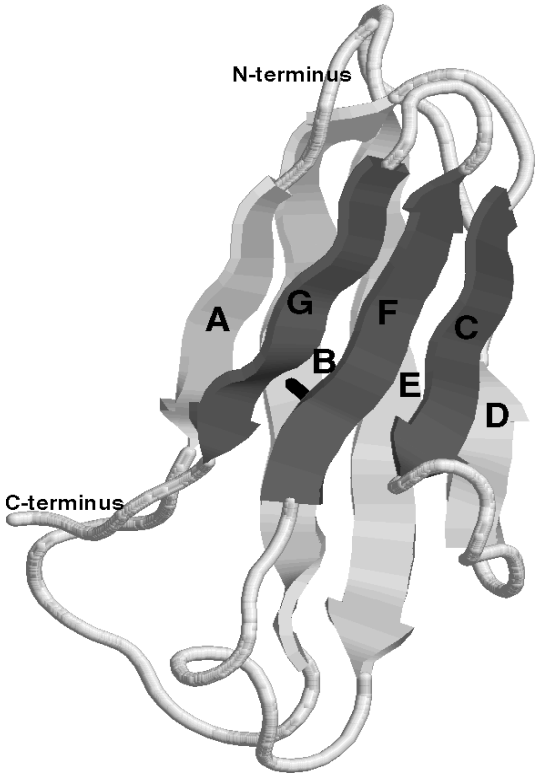
## MHC

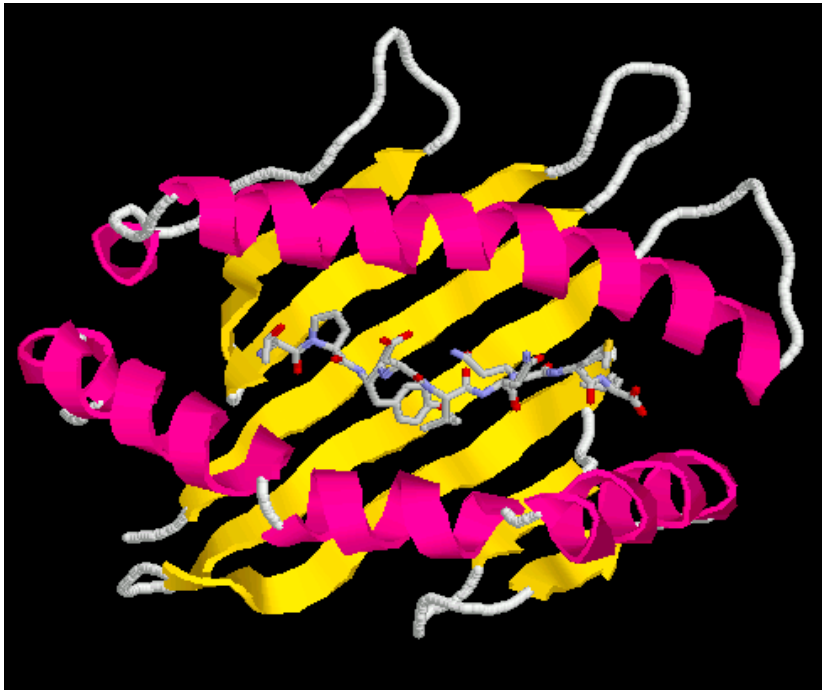
### V-DOMAIN

### C-DOMAIN

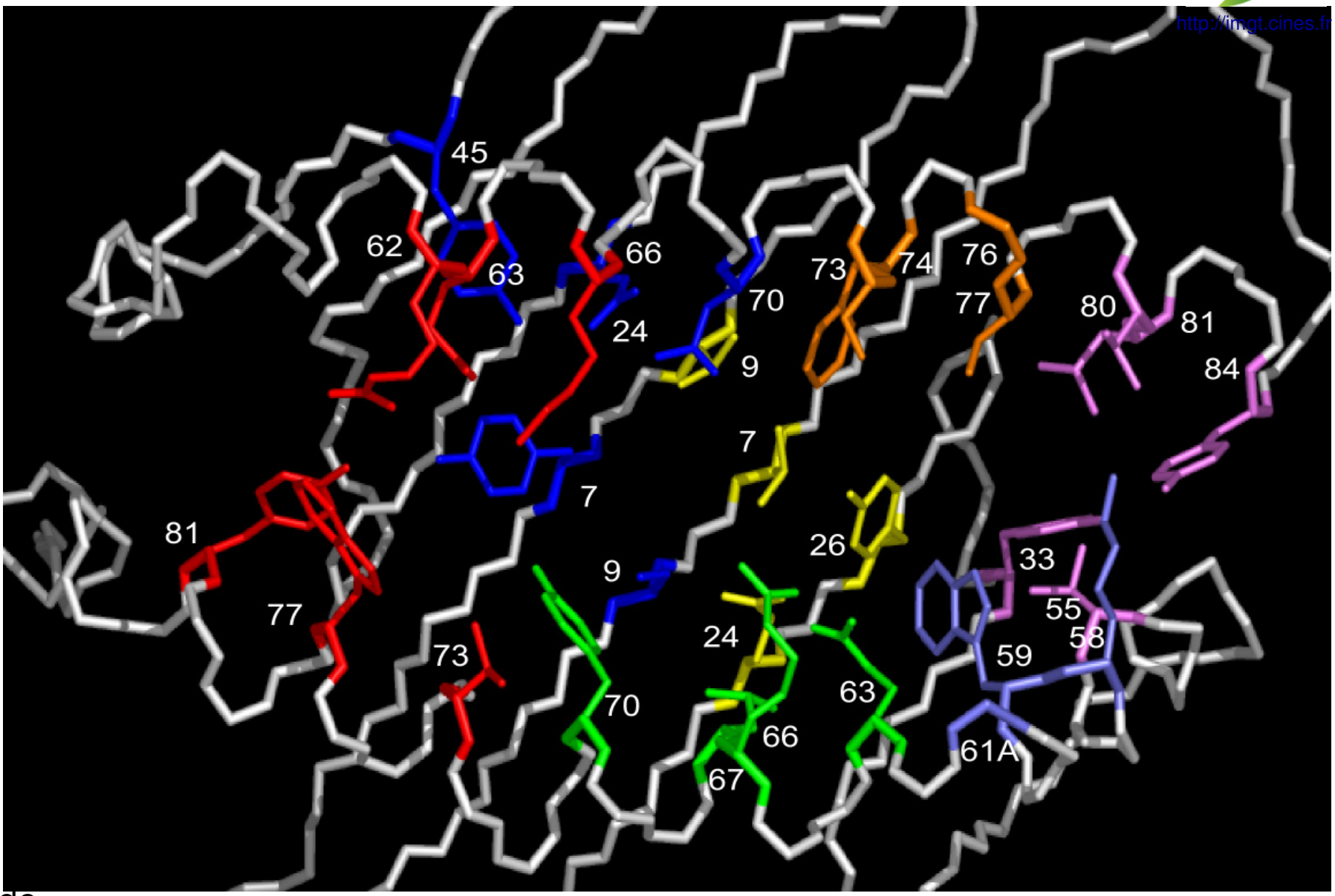
### G-DOMAINs



# 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 |

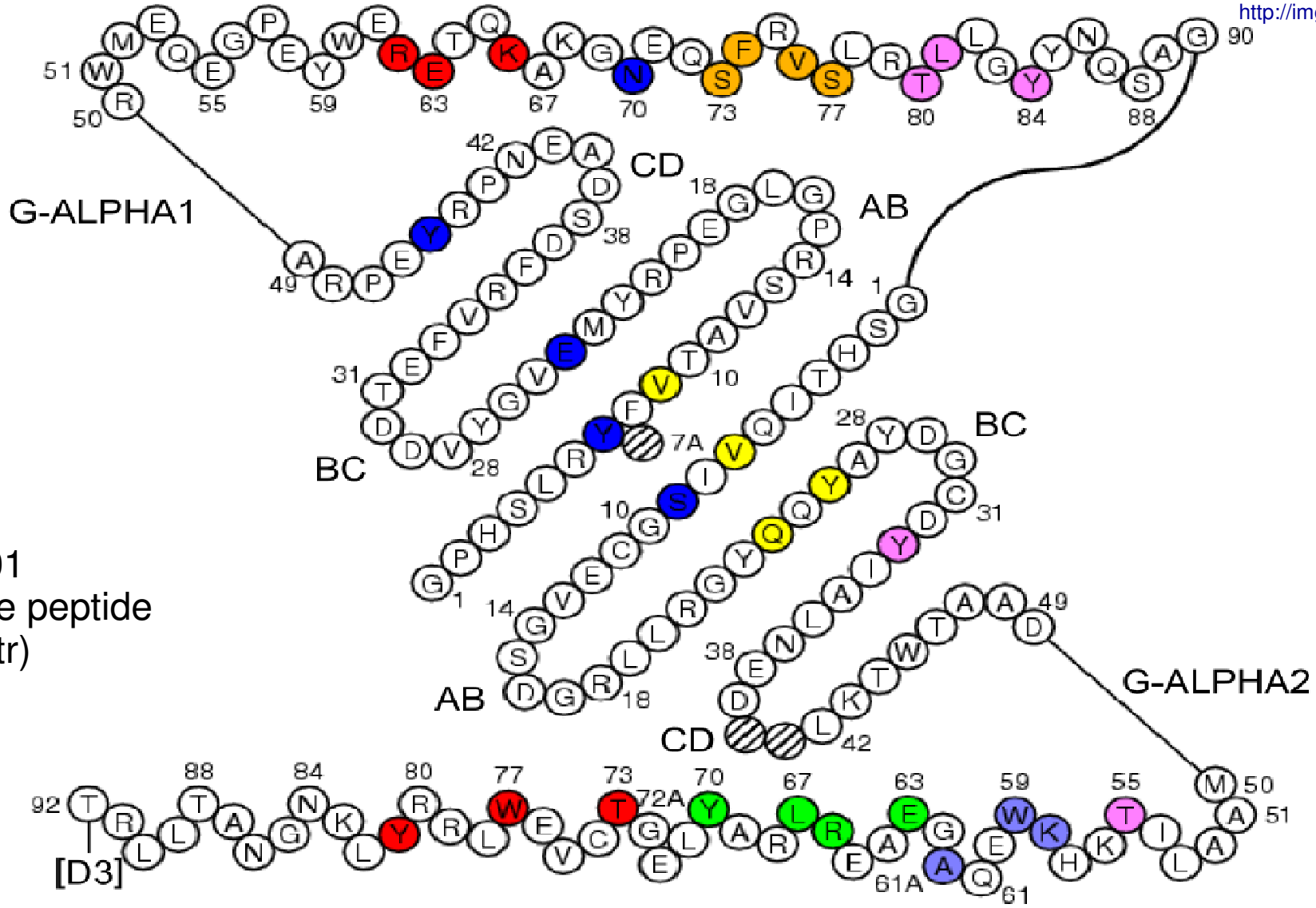
H2-K1*01
(code 1jtr)
8 residue peptide

*Kaas and Lefranc In Silico Biology 2005*

# MHC class I IMGT contact sites

http://imgt.cines.fr

| | |
|---|---|
| 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

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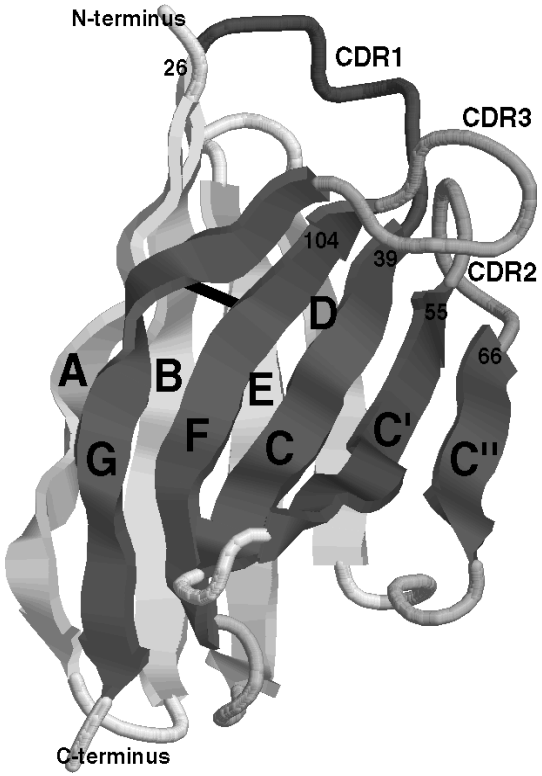
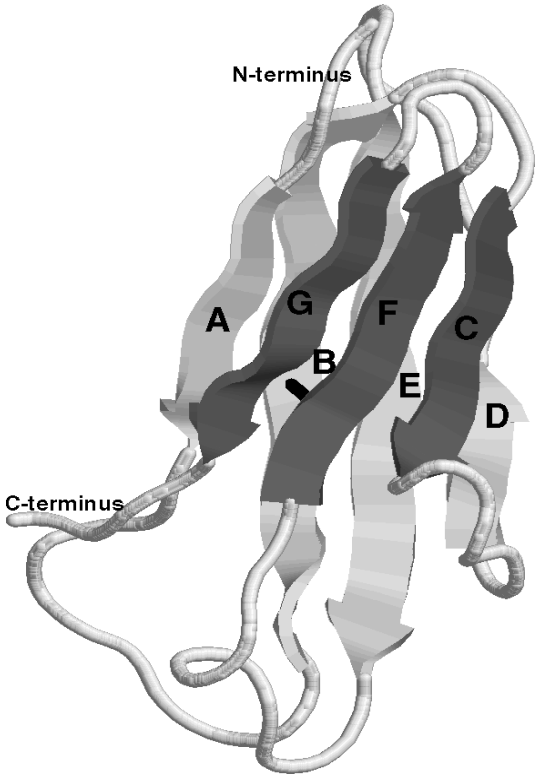
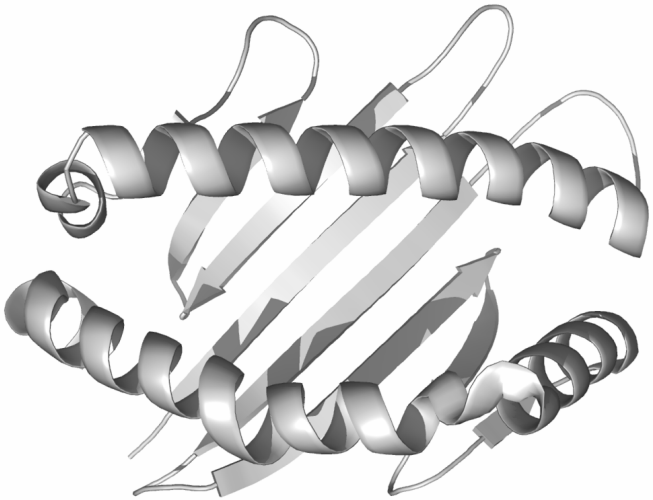
**V-DOMAIN (IG,TR)**
AND
**V-LIKE-DOMAIN**
(other than IG,TR)

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

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



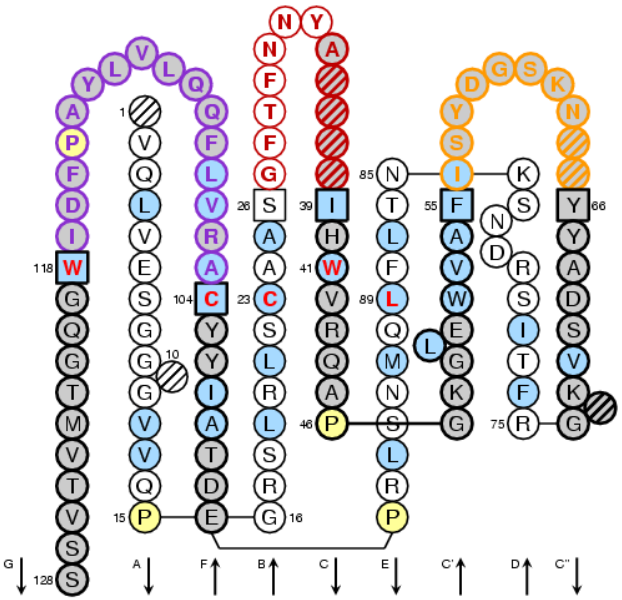



*Immunoglobulin superfamily (IgSF)*

*MHC superfamily (MhcSF)*

## V-LIKE-DOMAIN

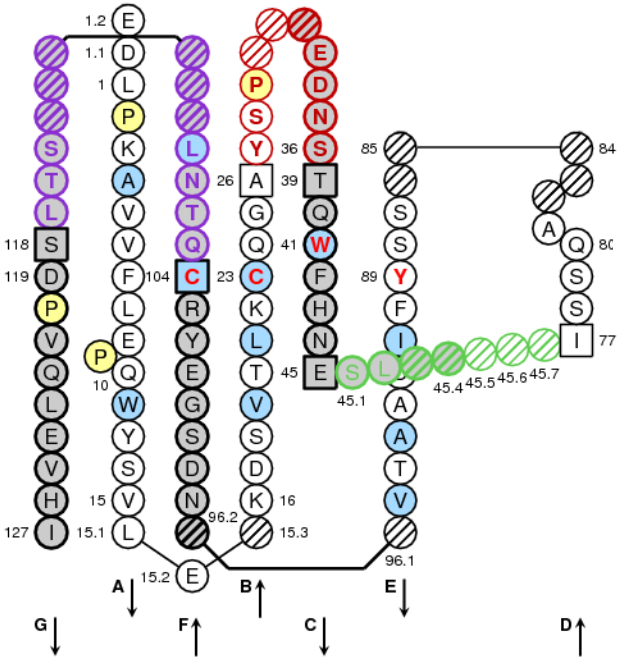
### MOG



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

## C-LIKE-DOMAIN

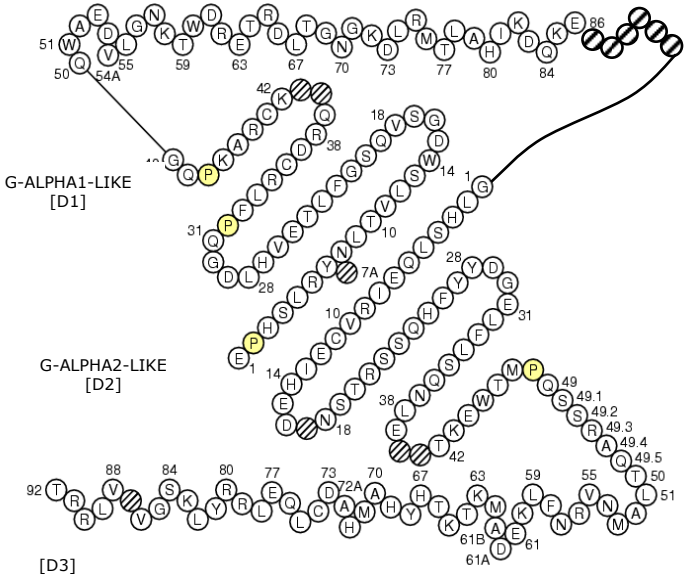
### FCGR3B



*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

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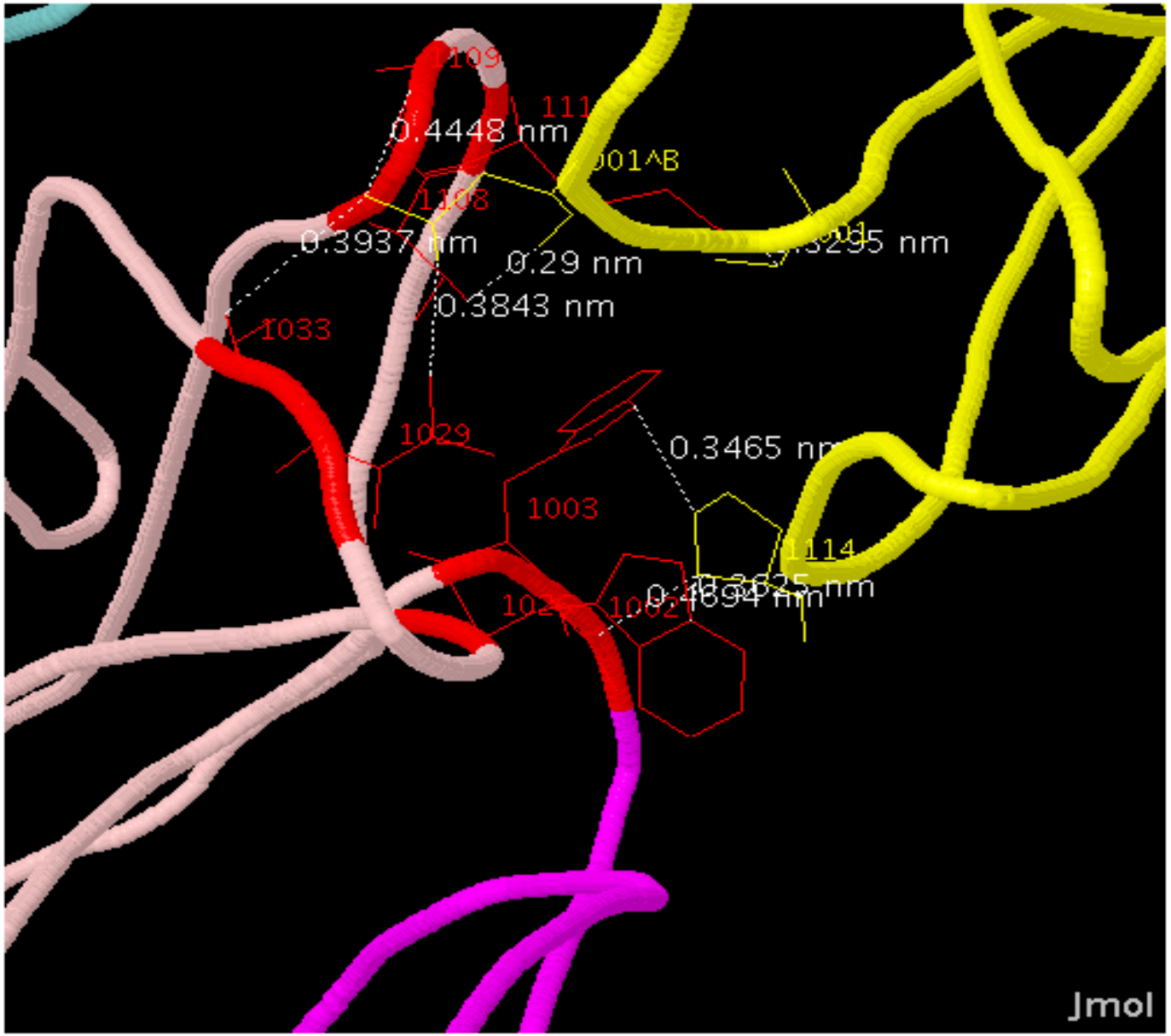
FCGR3B




IGHG1
(FC-GAMMA1)

CH2
C-DOMAIN

[D2]
C-LIKE-
DOMAIN

[D1] C-LIKE-DOMAIN

Im
Muno
Gene
Tics
Information
system®
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