From tilings to fibers

Archamps

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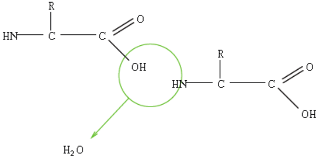
UMR 5127

Outline

Proteins

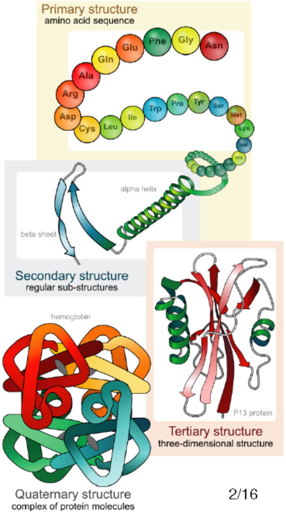
PROTEIN: sequence of amino acids that folds and realises a biological function

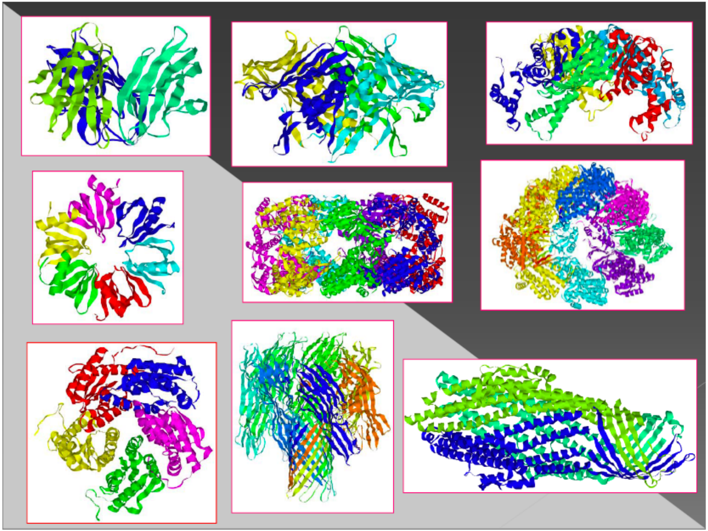


R: 20 standard amino acids = protein building blocks

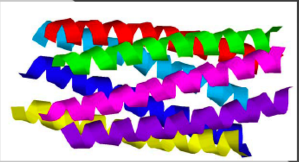
Main chain (backbone), side chain

Information flow: 1D $\longrightarrow$ 3D

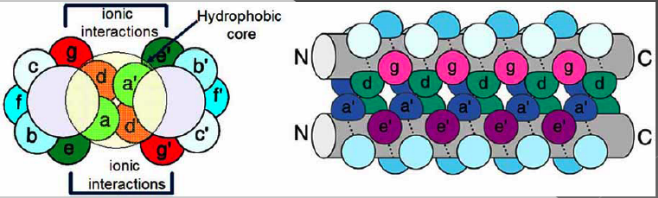




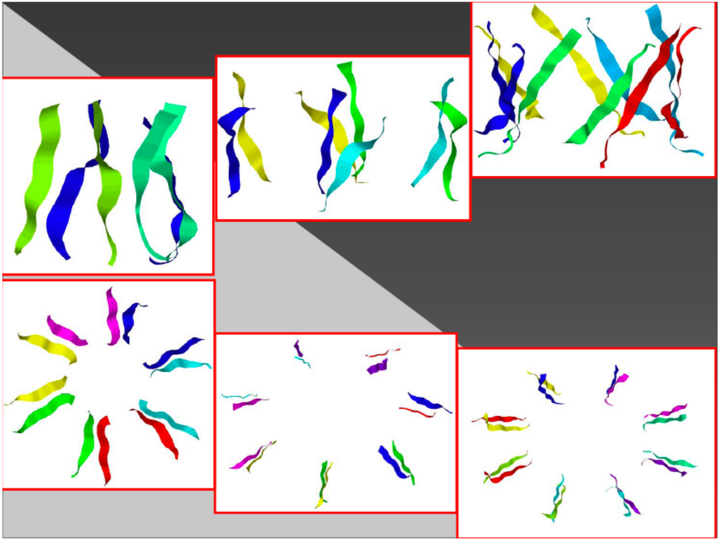
α-coiled interface



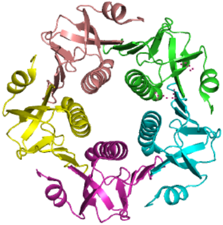
Heptad repeat: « abcdefg »

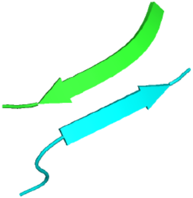


1- Crick FHC (1953). Acta Crystallogr 6: 689–697.
2- Lupas A (1996). Trends Biochem Sci 21: 375-382.



Focus on one interface geometry: two aligned β-strands



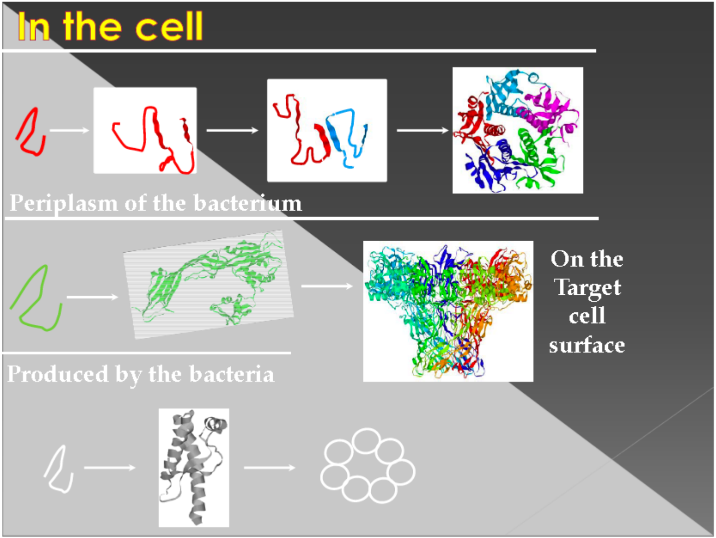


D: 96-103, E: 23-31

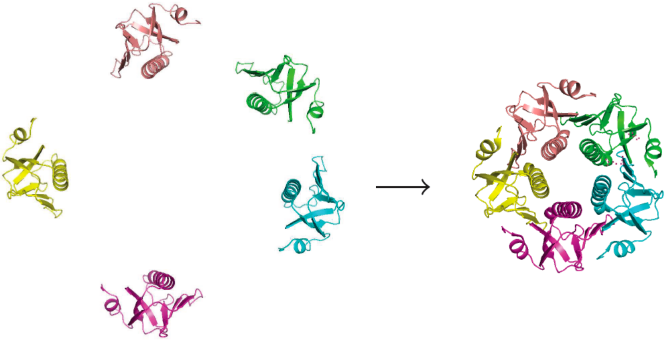
- ⋆ less understood than α-coil; "planar" geometry: much less constrained than α
- ⋆ many pathologies (Alzheimer, Parkinson, cholera, ...)

classes: continuous β-sheet, β-sandwich Guharoy, Chakrabarti 2007

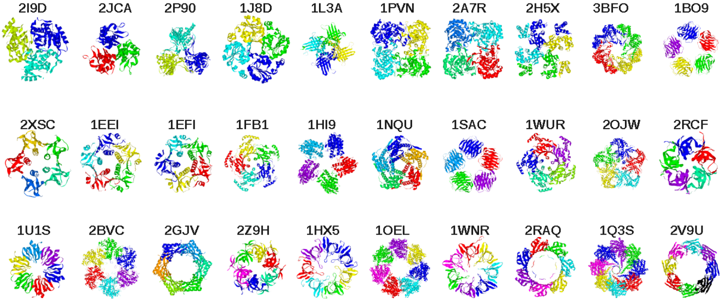
10/16

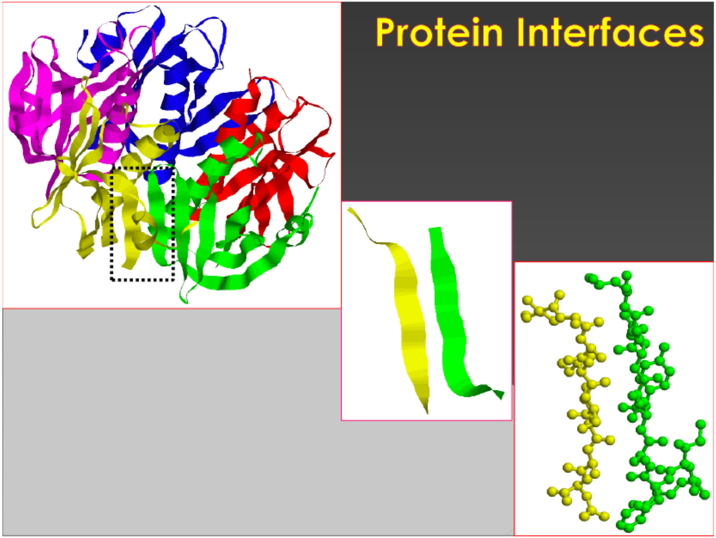

In the cell
Periplasm of the bacterium
On the Target cell surface
Produced by the bacteria

Circle



Circles


2I9D
2JCA
2P90
1J8D
1L3A
1PVN
2A7R
2H5X
3BFO
1BO9
2XSC
1EEI
1EFI
1FB1
1HI9
1NQU
1SAC
1WUR
2OJW
2RCF
1U1S
2BVC
2GJV
2Z9H
1HX5
1OEL
1WNR
2RAQ
1Q3S
2V9U


Protein Interfaces

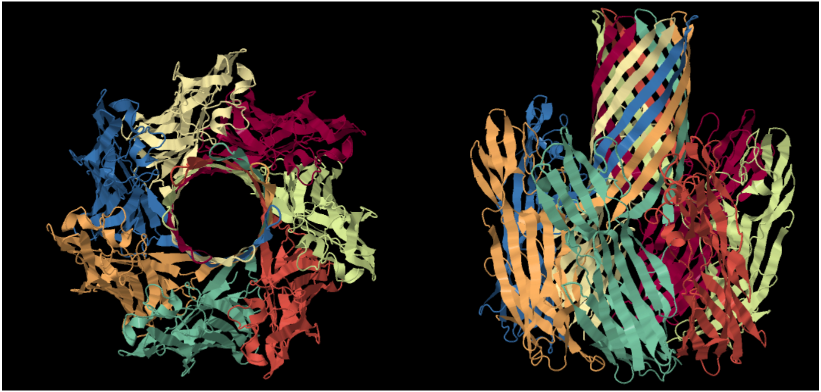
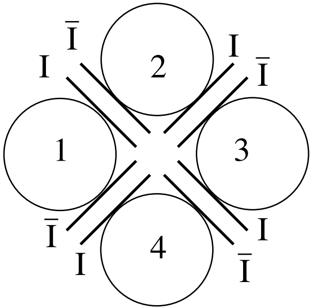


FIGURE: **Heptamer 4H56 in the PDB with each chain adjacent to 2 other chains.** Remark that in the beta barrel the adjacency between pairs of chains is the same as in the other part of the heptamer. This implies an oligomerization with exactly 1 interface.



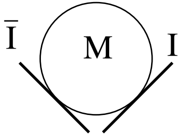
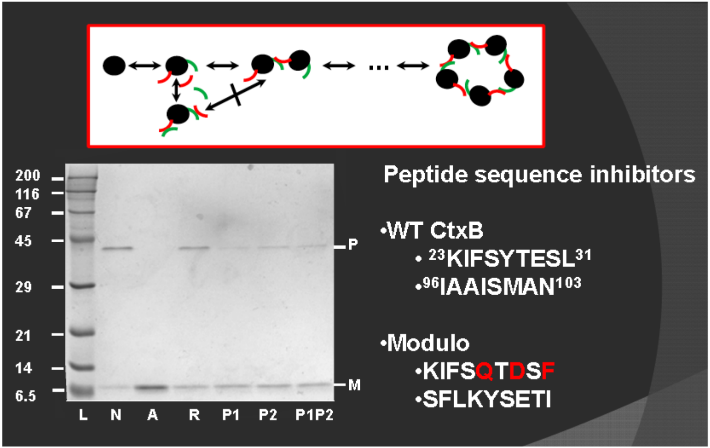


FIGURE: **Abstract view of C_4 symmetry.** A tetramer formed by a single interface between the part I and $\overline{I}$. Each chain is adjacent via the interface to exactly 2 other chains


...
200
116
67
45
29
21
14
6.5
P
M
L N A R P1 P2 P1P2
Peptide sequence inhibitors
•WT CtxB
• 23KIFSYTESL31
•96IAAISMAN103
•Modulo
•KIFSQTDSF
•SFLKYSETI

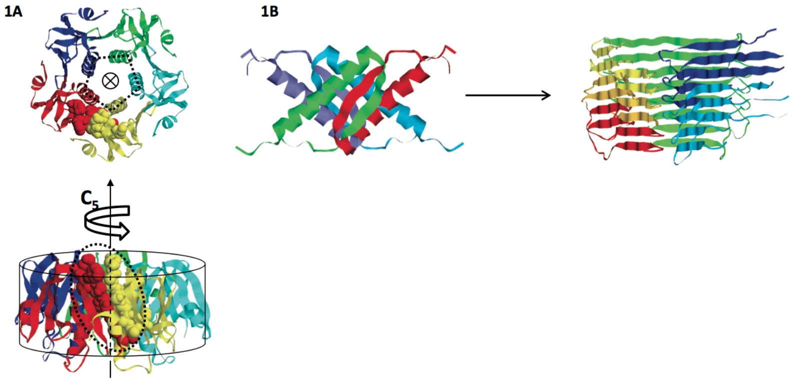
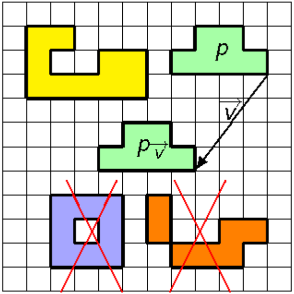


FIGURE: **Protein oligomers and fibers. A. Protein oligomer.** Cholera toxin B pentamer ($CtxB_5$) is shown (PDB code 3CHB). **B. Oligomer to fiber transition.** Each monomer is indicated by a different color.

Tilings of the plane

Définition

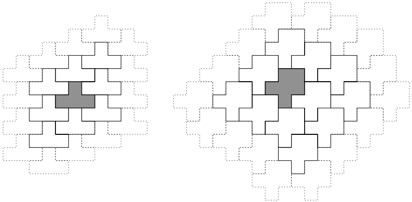
A *polyomino* is the interior of a closed non intersecting path in a square lattice.



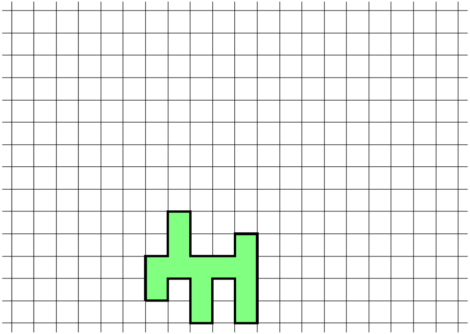
Tilings of the plane

Definitions

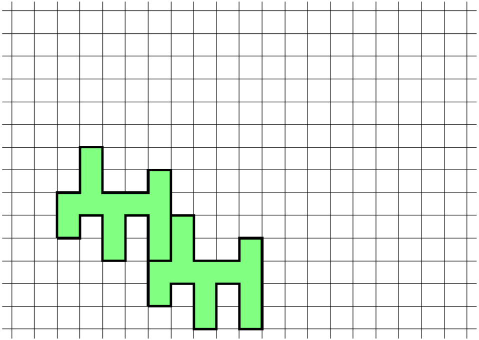
A *tiling by translation* of a polyomino P is a covering of $\mathbb{R}^2$ by translation of copies of P without overlapping or hole.



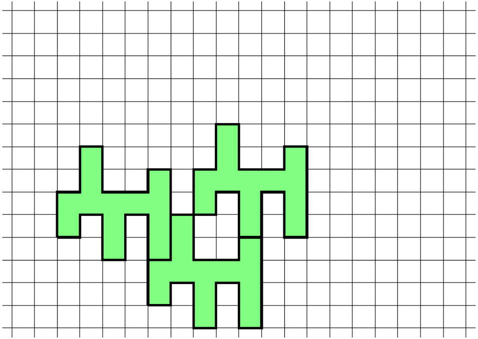
Tilings by translation



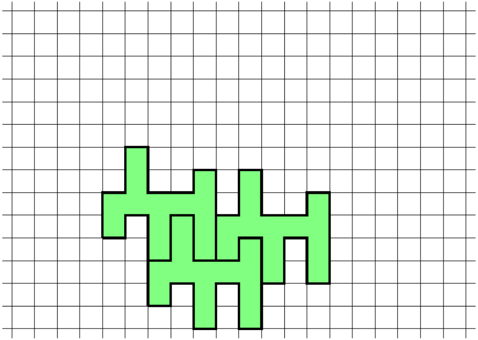
Tilings by translation



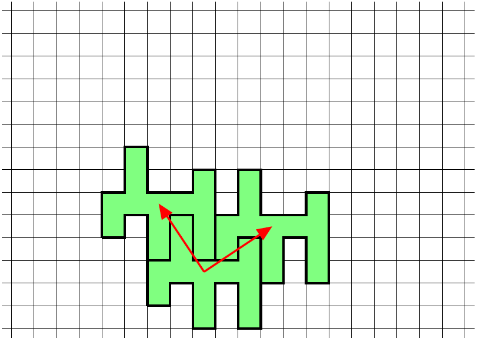
Tilings by translation



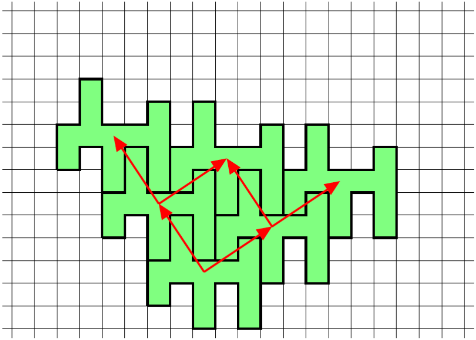
Tilings by translation



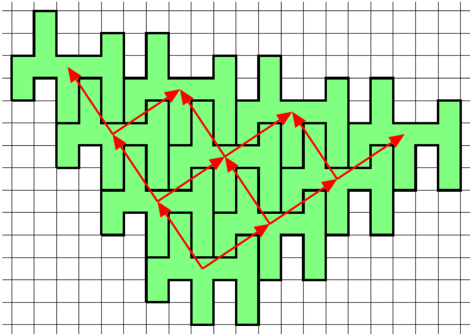
Tilings by translation



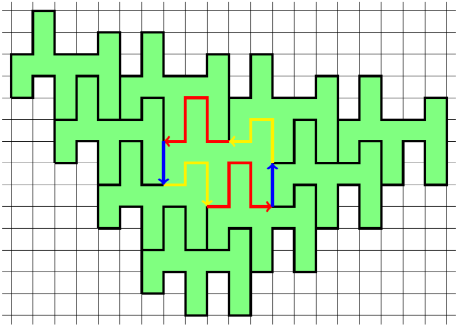
Tilings by translation



Tilings by translation

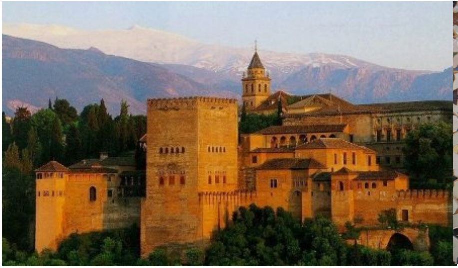


Tilings by translation



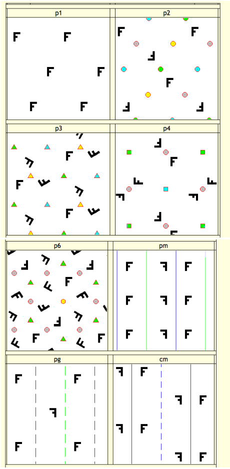
Tilings of the plane

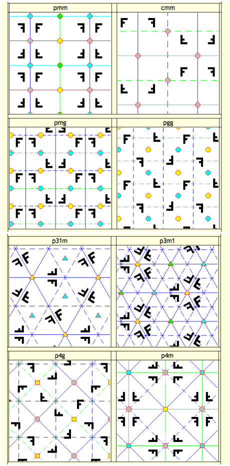
Isometries of the plane : translation, rotation, reflection and glide reflection.
17 crystalographic groups for the plane (Bravais 1847).

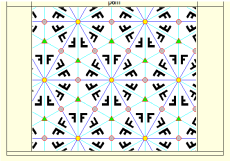



The 17 crystallographic groups are represented at the Alhambra of Grenada (by artists around 1350).

Cristallographic groups



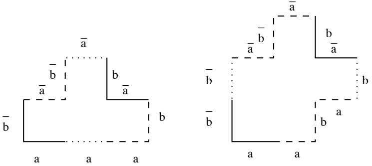




Tilings of the plane by translation

Definitions

Let *bw* be a *boundary word of P*, i.e. a word on the alphabet $\{a, b, \bar{a}, \bar{b}\}$ where a codes right step, b up step, $\bar{a}$ left step and $\bar{b}$ down step which codes the boundary of the polyomino P.



bw is defined up to circular permutations of letters.

Beauquier-Nivat's Theorem

Theorem [Beauquier-Nivat 1991]

A polyomino P tiles the plane by translation if and only if the boundary word bw of P is equal to $XYZ\,\overline{X}\,\overline{Y}\,\overline{Z}$ or $XY\,\overline{X}\,\overline{Y}$ with $X, Y, Z \in \{a, b, \bar{a}, \bar{b}\}^*$ and where $\overline{w} = \overline{w_1 w_2 \cdots w_n} = \overline{w}_n \overline{w}_{n-1} \cdots \overline{w}_1$ with $w_i \in \{a, b, \bar{a}, \bar{b}\}$.

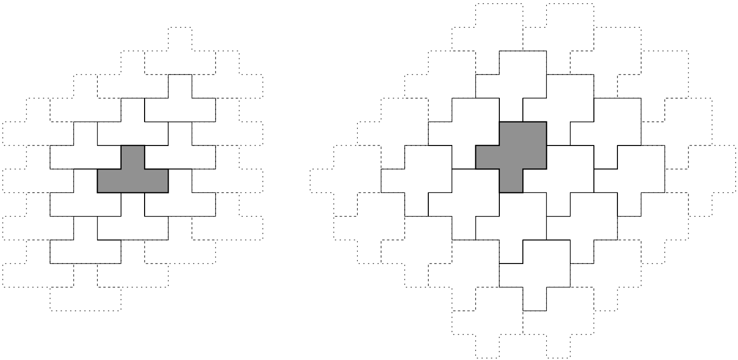
Tiling models

According to Beauquier-Nivat's Theorem, we have 2 ways of tilings the plane by translations :

If the boundary word is $XYZ\,\overline{X}\,\overline{Y}\,\overline{Z}$, we talk about pseudo-hexagon.

If the boundary word is $XY\,\overline{X}\,\overline{Y}$, we talk about pseudo-square.

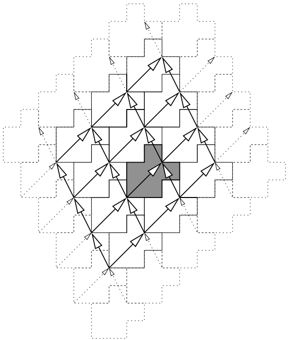
Tilings by translation



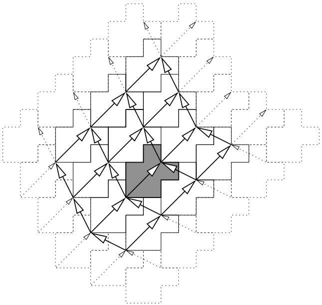
Lattice periodic tilings

Definition

A tiling is called *lattice periodic* if it is invariant under the translation by two non-collinear vectors.



a)



b)

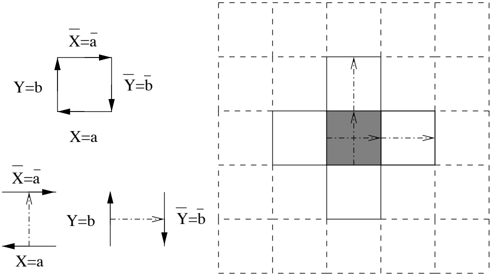


FIGURE: **Tiling by a mino and the 4 adjacent tiles of the grey mino**

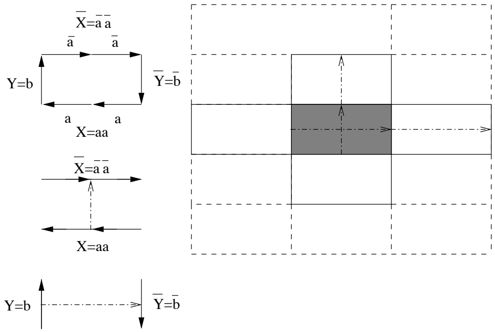


FIGURE: **Tiling of the plane by a domino like a pseudo square and the 4 adjacent tiles of the grey domino**

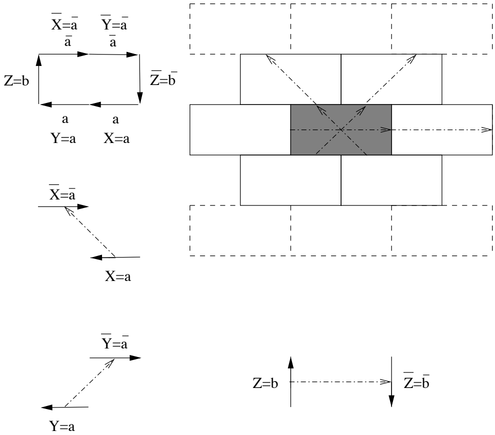


FIGURE: **Tiling of the plane by a domino like a pseudo hexagon and the 6 adjacent tiles of the grey domino**

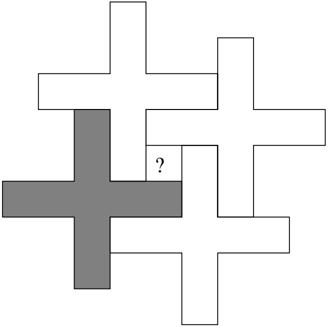


FIGURE: **A thin cross that doesn't tile the plane**

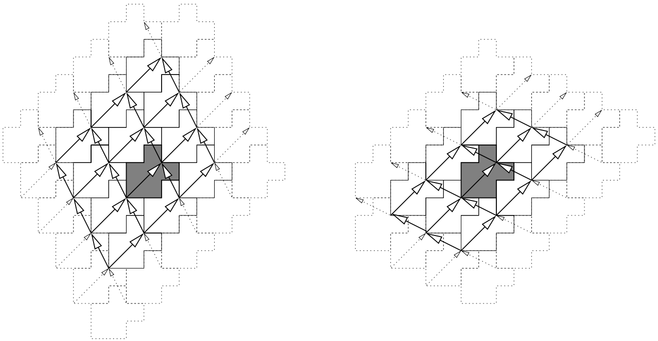


FIGURE: **Two regular tilings of the plane by the same polyomino**

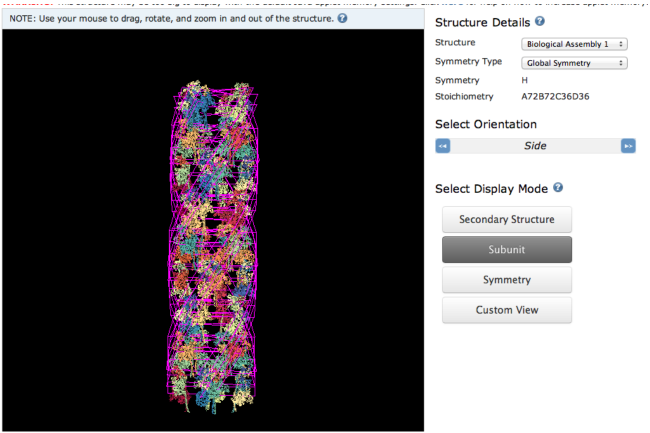


FIGURE: **Spider silk.**

From regular tilings of the plane to tilings of a fiber

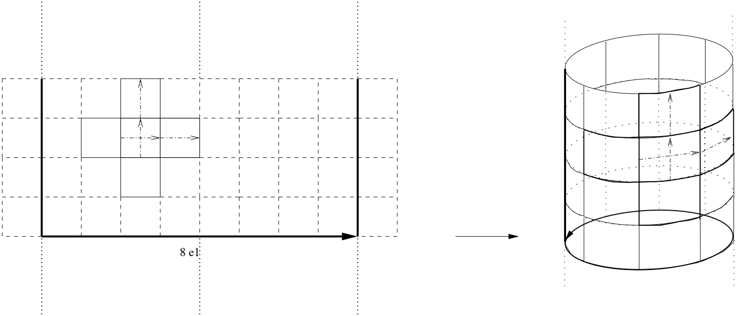


FIGURE: **From tiling to cylinder by using the translation of 8 times the vector $\vec{e}_1$.**

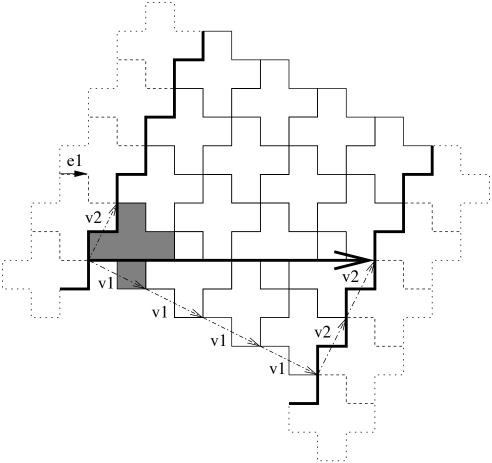


FIGURE: **Two boundaries in correspondence by the translation** $4\vec{v}_1 + 2\vec{v}_2)$

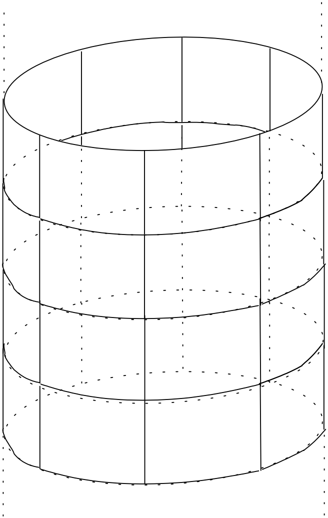


FIGURE: **Fiber with a pseudo square shape.** Each tile is surrounded by 4 tiles.

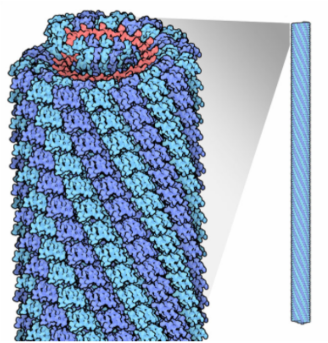


FIGURE: **Tobacco Mosaic Virus.**

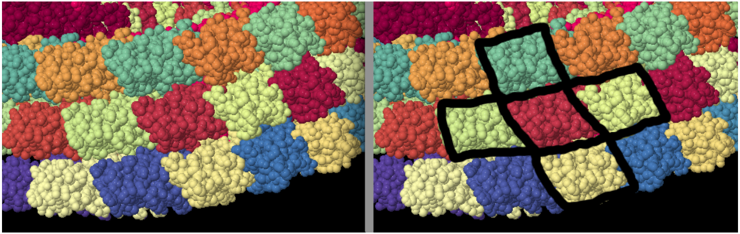


FIGURE: **Tobacco Mosaic Virus : an example of tiling of a fiber with 4 adjacent chains.**

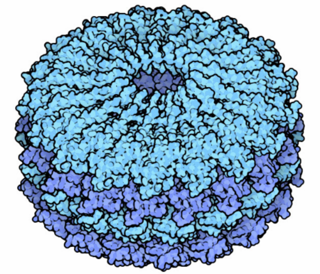


FIGURE: **Tobacco Mosaic Virus : a 17-mer.**

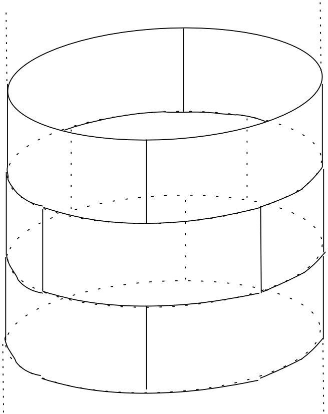


FIGURE: **Fiber with a pseudo hexagon shape.** Each tile is surrounded by 6 tiles. Remark that pseudo hexagon shapes appear in particular when there is a tilt on the fiber.

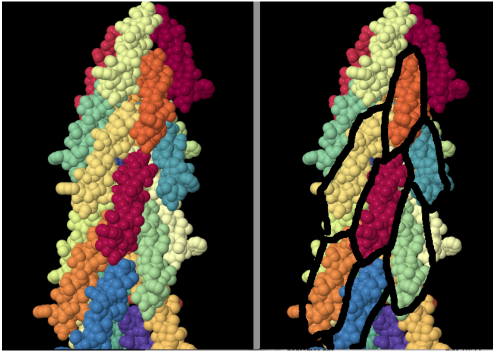


FIGURE: **3J1R : an example of tiling of a fiber with 6 adjacent chains.**

From fold plasticity to fibers : the P53 case

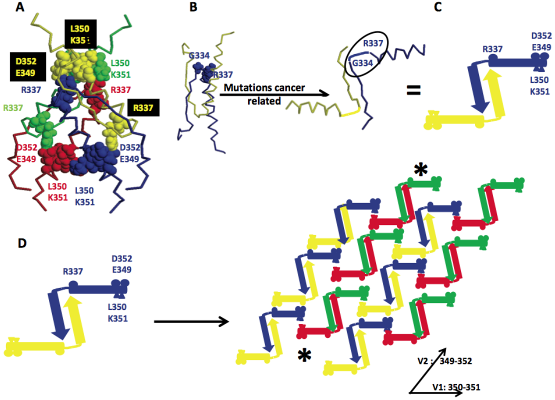


FIGURE: **A. The p53 tetrameric domain is made of 2 dimers.** Each monomer is made of a β-strand followed by a small helix ended by a long α-helix parallel to the β-strand (1SAK). The residue R337 is sensitive to mutation.

Tiling fibers by *n*-mers

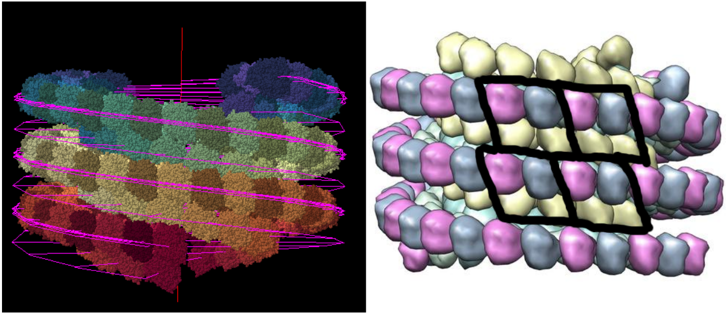


FIGURE: **Fiber 3J2U with a tetramer inside each pseudo hexagon**

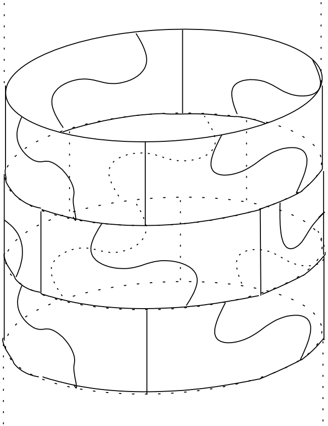


FIGURE: **Fiber with a dimer inside each pseudo hexagon**

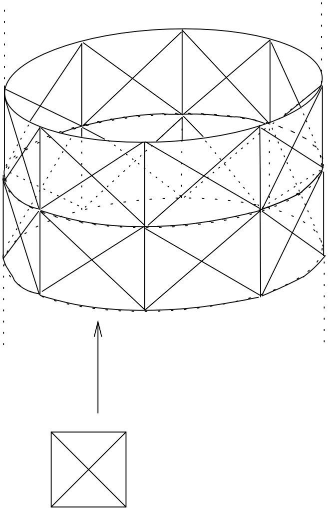


FIGURE: **Replacement of each pseudo square by a tetramer.**

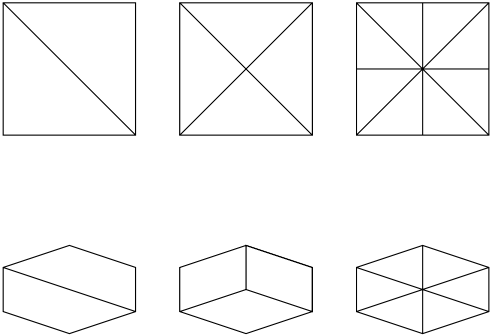


FIGURE: **Replacement of a pseudo square and of a pseudo hexagon.**

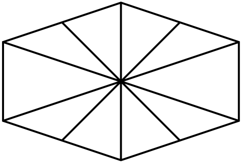


FIGURE: **Replacement of pseudo square by 2 non regular pentamers.**

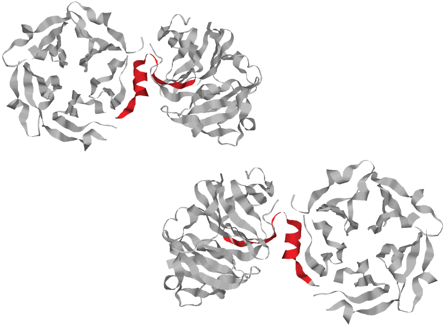


FIGURE: **Double asymmetrical pentamer (Tachylectin).**

From 1-periodical tiling to fibers

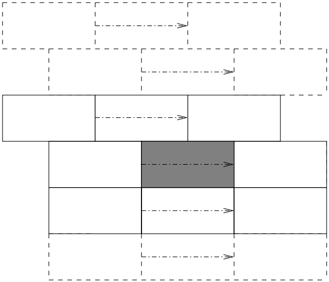


FIGURE: **Non regular tiling with dominoes.** The grey domino is surrounded by 5 dominoes thus this tiling is certainly not regular. Remark that the horizontal strips are invariant by the horizontal vector $\vec{v}_1$ and also by the vector $3\vec{v}_1$. Thus we are able to map the left border to the right border in order to form a non bounded height cylinder.

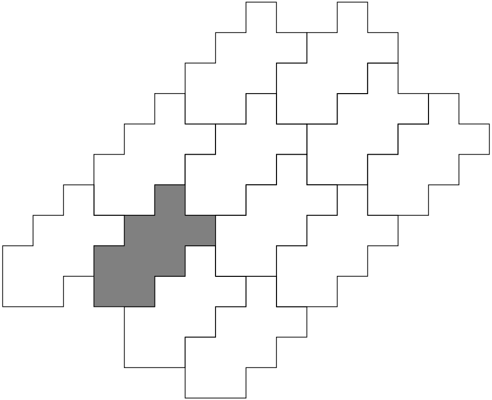


FIGURE: **Non regular tiling and stair case shape.**