Interchain joins

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http://homepage.mac.com/whitby/

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Reference

Octahedron1stEd.pdf–bookmark INTERCHAIIN JOINS–pages 327-350

Introduction

This material is excerpted from *Octahedron*. It shows one protein chain joins with another.

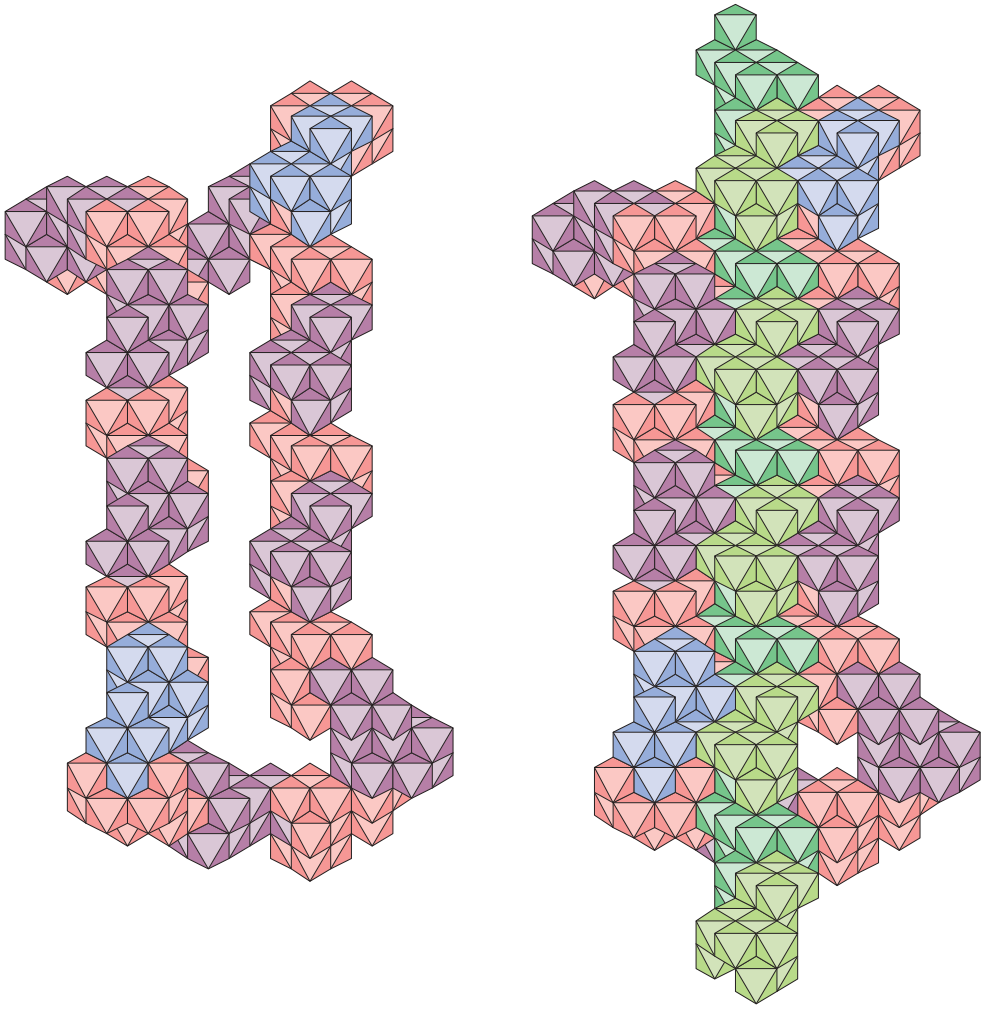
INTERCHAIN JOINS

Pleated sheet

Cyclic peptide sheet joined with beta chain

A cyclic peptide can be formed which has a pair of extensible beta180-chain segments which are separated by the width of a beta180 chain.

A second chain can form a sheet with the two beta-chains of the cyclic peptide and extend beyond the end turns without interference. The cyclic peptide is shown in this figure with a beta180 chain joined to its two beta180-chain segments to form a three chain pleated sheet. The sheet join is antiparallel on the left side of the added chain and parallel on its right

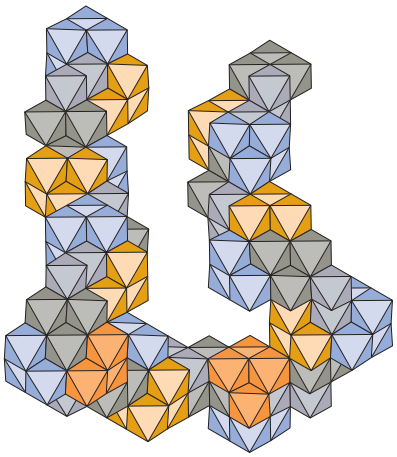


Cyclic peptide sheet joined with beta-chain

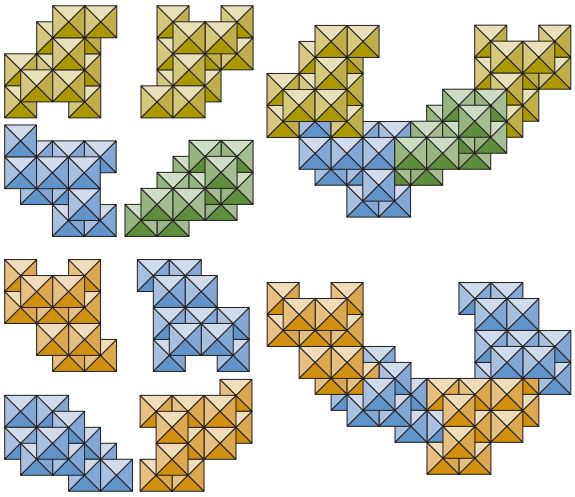
The cyclic peptide on the left consists of two beta180 chains linked by identical at either terminus. The separation between the chains accommodates a length of beta180 chain to form a three chain pleated sheet. This is shown in the figure on the right.

side.

The beta180 chain segments are joined at either end by the turn shown below. The turn is



examined in detail in the next two figures. The first of these shows the assembly of each of the

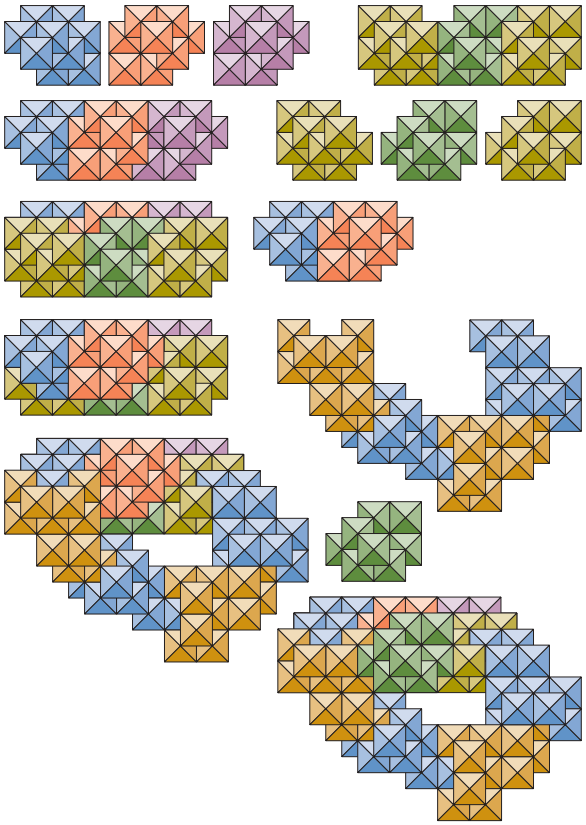


turns of the previous loop from a direction parallel to the axes of the beta180 chains which form the sheet. The two turns are in the right hand column and the units which form them are grouped on the left side of the figure. The top turn is the far turn which appears at the top of the loop figure. The bottom is the near turn and appears at the bottom of the loop figure. The turns are identical except for their orientations. They differ by a half revolution about an axis parallel to the rightmost edge of the octahedron of which they are composed.

The joins between the units in the top turn are 4helix between the yellow and blue, epsilon between the blue and green, and beta90 between the green and the second yellow.

The joins between the units in the bottom turn are 4helix between the blue and the orange at the male end of the turn, epsilon between the orange and the second blue, and beta90 between the blue and the orange at the female end of the turn.

The next figure shows the relationship of the



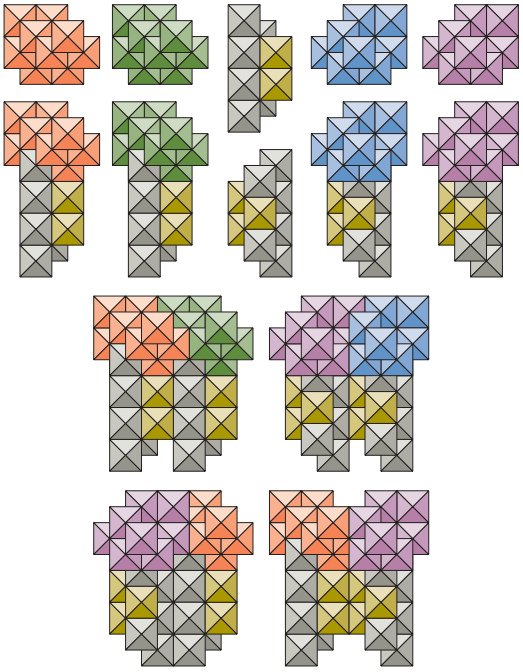
beta180 chains which form the sheet. The center chain is the added chain and the outer chains are part of the loop. The chain on the left is antiparallel to the other two chains. Its male terminus is towards the viewer. In the top left of the figure, three units are shown separated from one another which are colored blue, red, or violet. Just below them they are shown

sheet joined. To the right a second set of units is shown separated and in a sheet join which are colored yellow or green. These units are rotated one half turn about the beta180 chain axes relative to the first set of units. The two sets are combined to form a sheet consisting of one turn each of three beta180 chains on the left side of the third row of the figure. The red and blue units on the right of the third row are in the same orientation as those of the same color in the first set of units. These extend the left two chains when they are added as shown in the fourth row on the left side. The near turn is shown on the right side of the fourth row. This is joined to the sheet assembly in the bottom of the left column. The middle chain is extended by the addition of the green unit in the bottom of the right column.

The join between the blue unit of the beta180 chain on the left and the orange unit of the female end of the turn is alpha helical. The join between the yellow unit of the beta180 chain on the right and the blue unit at the male end of the turn is 32chain.

The alpha C-atom of the unit and the beta C-atom of the sidechain establish a chain direction which is normal to the plane of the sheet. Extending the chain with an identical pair of C-atoms shows the arrangement of the side chains as seen in the axial view of the beta180 units which make up the sheet. The top row of the figure shows identical main chain units in two different orientations. The red and green units are in the same orientation. The blue and violet units are in the same orientation, too. The different orientation between the two pairs of units allows antiparallel sheet joining. Between the pairs of units in the top row is a three C-atom chain which is to act as the side chain for the red and green units. Directly under it is the side chain for the blue and violet units. The chains are identical except for their orientations.

The second row shows the units with side chains attached. In the third row the red and green units are joined in parallel sheet. The blue and violet units are also paired as parallel sheet units. In the bottom row the red and violet units are paired as antiparallel sheet units. These pairs are not identical. The gray colored



C-atoms are in contact where the violet unit is to the left of the red unit; the yellow C-atoms are in contact where the violet unit is to the right of the red unit.

In the next figure, the side chains are viewed along the C-chain axes towards the main chain units to which they are joined.

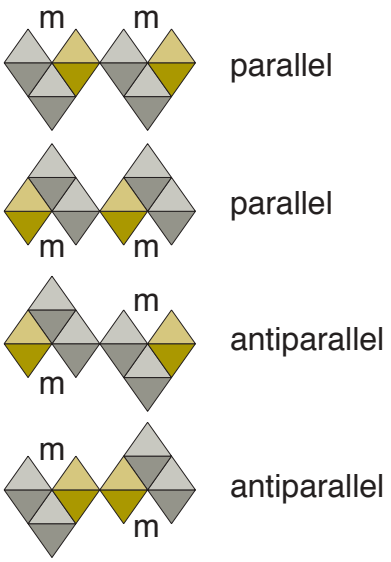


Table 19: Possible join adjacencies upon termini of sheet chains

	Sheet	beta180	beta90	alpha	32chain	epsilon	4helix
beta180	mp41m	*					*
	fp41f	*	*	*	*	*	*
	mp62m	*	*	*	*	*	*
	fp62f	*		*			
	ma41f	*		*			
	fa41m	*	*	*	*	*	*
	ma62f	*	*	*	*	*	*
	fa62m	*					*
beta90	mp41m	*	*	*	*		*
	fp41f		*	*	*	*	*
	mp62m		*			*	
	fp62f	*	*	*			
	ma41f	*	*	*			
	fa41m		*	*	*	*	*
	ma62f						
	fa62m	*					*
alpha	mp41m	*					*
	fp41f	*	*	*	*	*	*
	mp62m		*			*	
	fp62f	*	*	*			
	ma41f	*	*	*			
	fa41m	*	*	*	*	*	*
	ma62f						
	fa62m	*					*

Table 19: Possible join adjacencies upon termini of sheet chains

	Sheet	beta180	beta90	alpha	32chain	epsilon	4helix
32chain	mp41m	*					*
	fp41f						
	mp62m		*			*	
	fp62f	*	*	*		*	
	ma41f	*	*	*			
	fa41m						
	ma62f						
	fa62m	*					*
epsilon	mp41m	*	*	*	*		*
	fp41f				*		
	mp62m						
	fp62f	*	*	*			
	ma41f	*	*	*			
	fa41m						
	ma62f						
	fa62m	*					*
4helix	mp41m	*					*
	fp41f						
	mp62m	*	*	*	*	*	*
	fp62f	*	*	*			
	ma41f	*	*	*			
	fa41m						
	ma62f	*	*	*	*	*	*
	fa62m	*					*

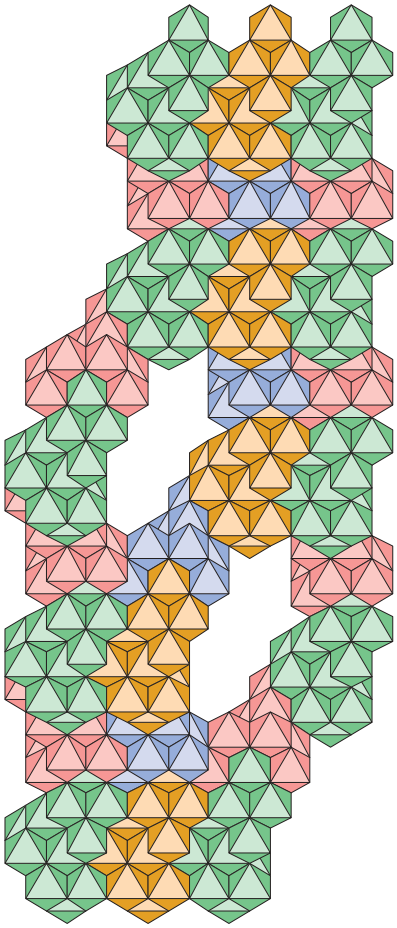
Key to table
m male end of chain
f female end of chain
p parallel sheet
a anti-parallel sheet
41 direction relative to the columnar residue join
62 direction relative to the columnar residue join
***** denotes adjacency for the pair of joins is possible

Linking chains of pleated sheet

A residue may be joined to either terminus of a solitary beta-chain with any of the six possible joins. When the beta-chain is part of a sheet, the type of join is limited, because a residue of one type of join on one chain may occupy a portion of the space required by a residue in one or more joins on an adjacent chain of the same sheet. Each of the combinations for each type of join and each type of sheet association is tabulated above.

A sheet offset

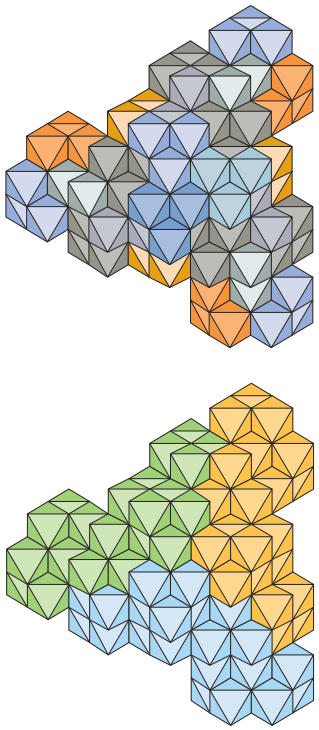
Three parallel strands can participate in the formation of multiple sheets which are offset from one another and define separate planes. The 32chn-join permits this. The offset requires pairs of 32chn-joins within each chain. The chain at the extreme 62-side of the sheet must be offset first. The chain next adjacent continues with a pair of beta180-joins and then it is offset by a pair of 32chn-joins. A sheet of any number of parallel chains may be offset in this manner. The 62-direction of the sheet is determined by the orientation of the terminal residues at the commencement of the offset from the male ends. If the offset commences from the female termini, then the chain at the extreme 41-side is offset first. The offset from the male direction is in the 32 direction and from the female it is in the 54-direction.



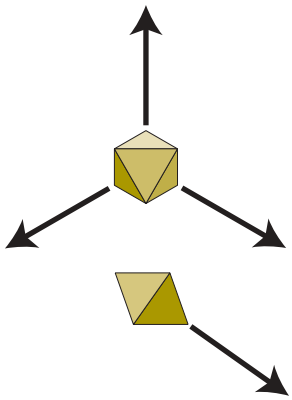
Pleated sheet offset
Three beta-chains forming two parallel sheets

Beta annulus

Three anti-parallel chains can form three sheets with a common junction. Each of the chains is sheet joined to each of the other two chains. Two depictions of the beta annulus viewed parallel to its axis of threefold symmetry are shown in the next figure. The He-octas of the top view are colored to differentiate the atoms; those of the bottom view are colored to differentiate the three chains. Each of the depicted chains consists of just two main chain units. The join between them is 4helical. The sheets are anti-parallel.

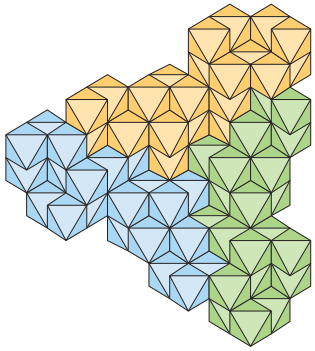


The three axial directions of the sheet chains relative to the octahedral orientation are shown in the facial view of the figure. Each of the



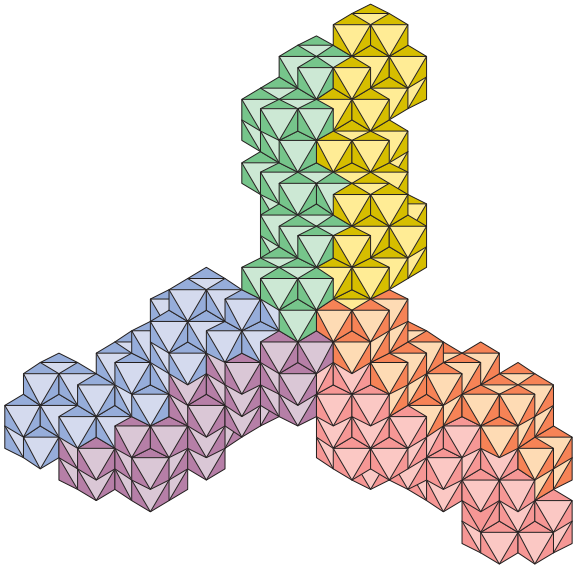
directions is parallel to a vertexial diameter of the octahedron. The arrows proceed away from the octahedron and away from the viewer. The edgial view shows one of the sheet directions in a view normal to the facial view.

The annulus is shown here from a direction that is opposite to that of the previous figure. The annulus is rotated 180° about an axis parallel to the top of the page.



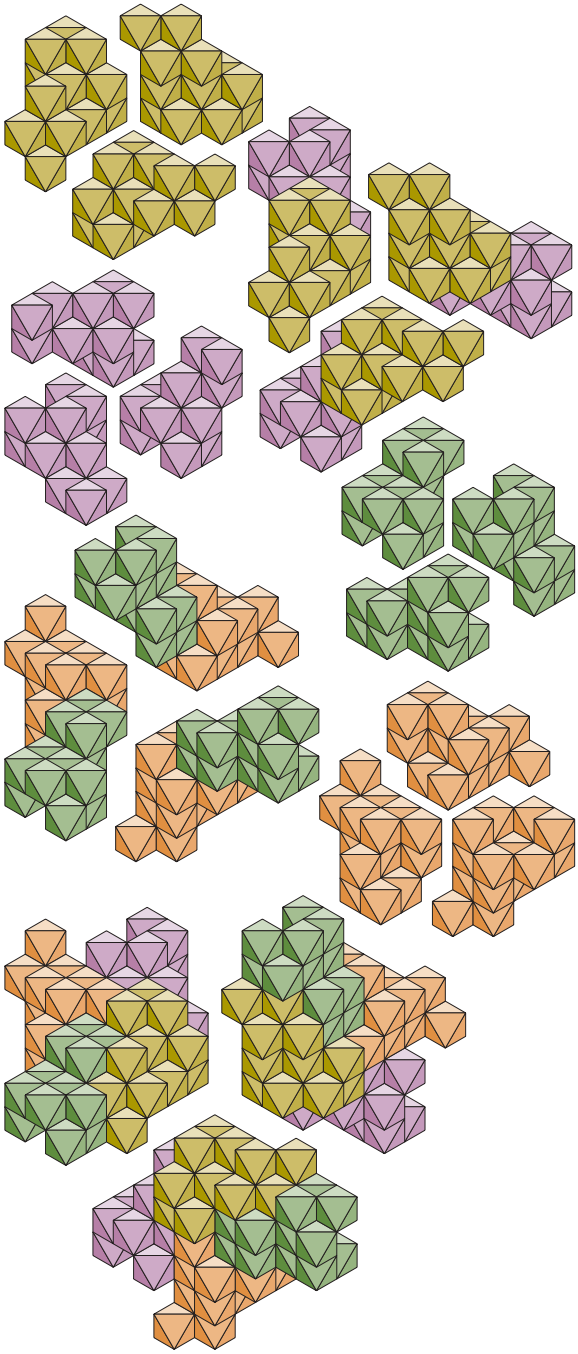
Three sheet junction

The coloration in the next figure differentiates the portions of each chain which belong to the three sheets. The chains have been extended. The green chain and the yellow chain are one sheet, the blue and violet another, and the red and orange a third. The red and yellow are one chain, the green and blue another, and the violet and red are a third.



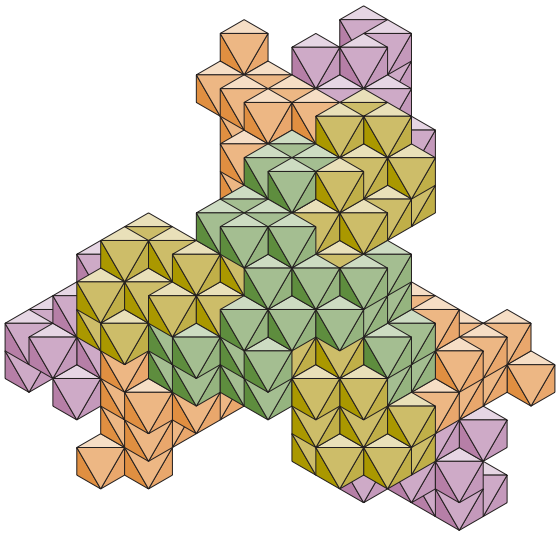
Three sheet junction, extended

The beta annulus requires main units in twelve orientations. These are shown in the next figure which details the assembly of the

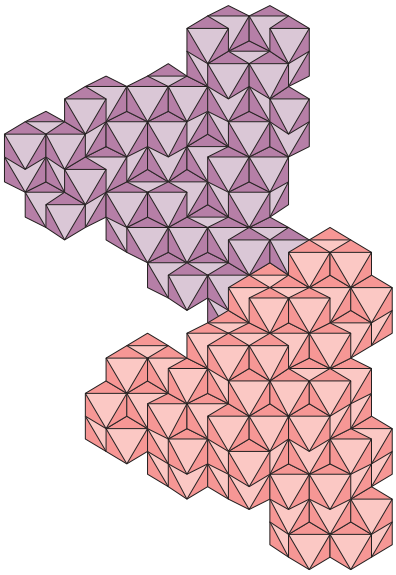


annulus. Within the colored groupings, the units differ by an orientation of one third of a revolution.The orange group is the obverse of the yellow group and the green group is the obverse of the violet group. The yellow and violet units form three beta180 pairings as do the green and orange groups. The yellow-violet pairs and the green-orange pairs form three pleated sheets which are shown at the bottom of the figure

The three sheets are joined as an annulus in the next figure.



Annulus assemblies



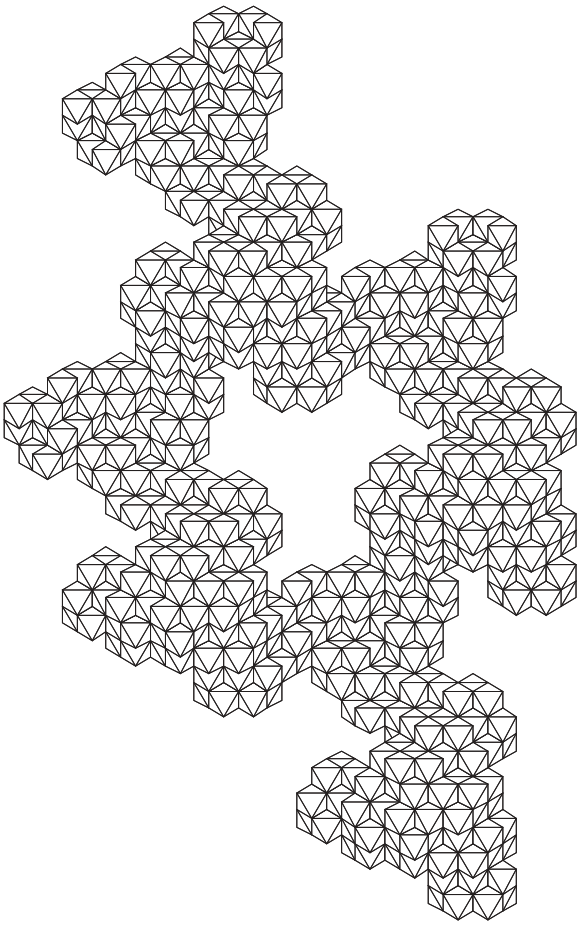
Pair of three sheet junctions

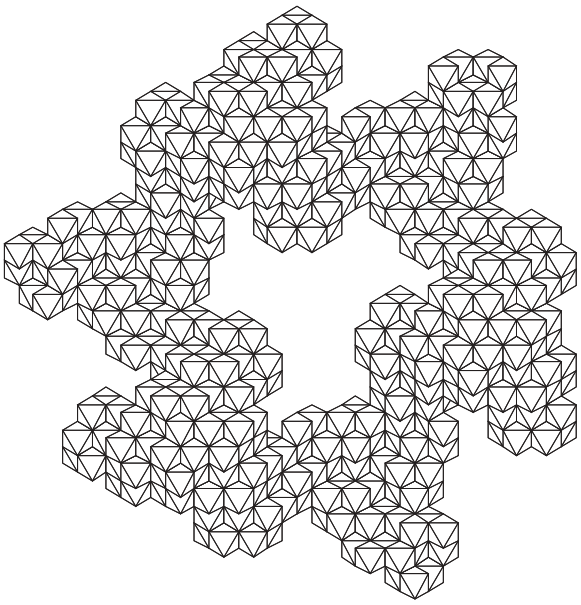
One beta annulus can join to another so that the male terminus of one of its chains joins to the female terminus of another. This is depicted in the figure which shown an inverted annulus colored purple joined to another annu-

lus colored red.

The pair can join with like pairs in the same manner to produce a planar crystal. The figure shows four pairs joined and this is extensible throughout the plane.

The ring which appears when the four pairs are joined is shown separately. This ring consists of six annuluses. Alternate annuluses are in the same orientation. Adjacent annuluses are inverted one to the other.



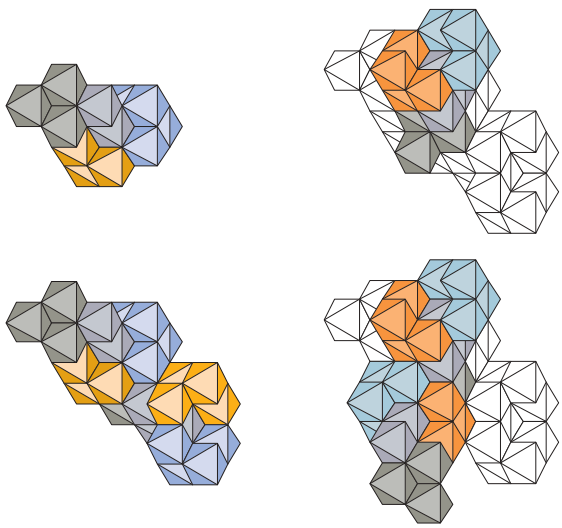


Assembly of beta annulus pairs.

The group on the left is composed of four identical beta annulus pairs indicating the formation of a planar crystal. The ring which is formed can exist as the separate structure shown on the right. It is composed of two groups of three beta annuluses each. Adjoining annuluses are inverted to one another.

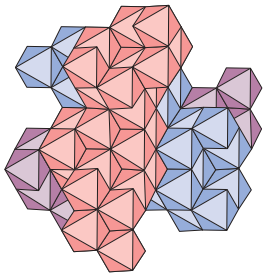
32chain stack assemblies

The edgially axised 32chain lies between a pair of parallel planes which are defined by the He-octa faces of the peptides. The planes are separated by three facial diameters of a He-octa. The thickness of the chain perpendicular to these planes is at regular intervals only two facial diameters of a He-octa. The chain alternates between contacting first one plane and then the other. The space between planes is a pocket into which an identical chain crossing at 120° fits. The axes of the two chains are separated by two facial diameters of a He-octa. The next figure shows the assembly of a two



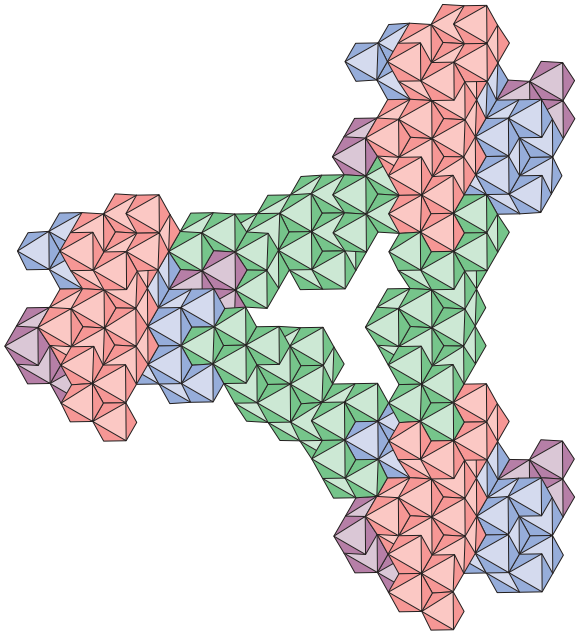
pair stack. The leftmost figure is a projection of an amino-main. The figure to its right is the same except for the addition of a second peptide to the female end of the first in a 32chain join. The pocket is towards the viewer, and lies between the two groups of He-octas on the nearest plane of He-octas. One group of four belongs to the first residue, and the second group of four belongs to the added residue. In the third figure from the left, a third residue has been placed in the 32-stack join which fills the pocket while its male-He-octa protrudes and is available for joining the fourth residue in a 32chain join. The rightmost figure is the completed two-pair stack. The second pair is rotated 1/3 turn counter-clockwise about an axis perpendicular to the plane of the paper.

A third pair of 32chain joined residues added atop the first two pairs is rotated 1/3 turn counter-clockwise to the second pair and a fourth pair atop the three is rotated in the same manner and results in an orientation for the pair which is identical with the first pair. The stack is a helical. The pitch is two facial diameters of a He-octa in 1/3 revolution. The stack is shown in the next figure in a view parallel to the helical axis.



Helical stack of 32chain pairs

Identical stacks can be joined by pairs of 32chain joined residues. The stacks differ only by a translation perpendicular to their axes. The joining pair extends the 32chain of one stack through the pair in identical orientation and identical axial elevation in another stack. In the following figure, the three stacks are



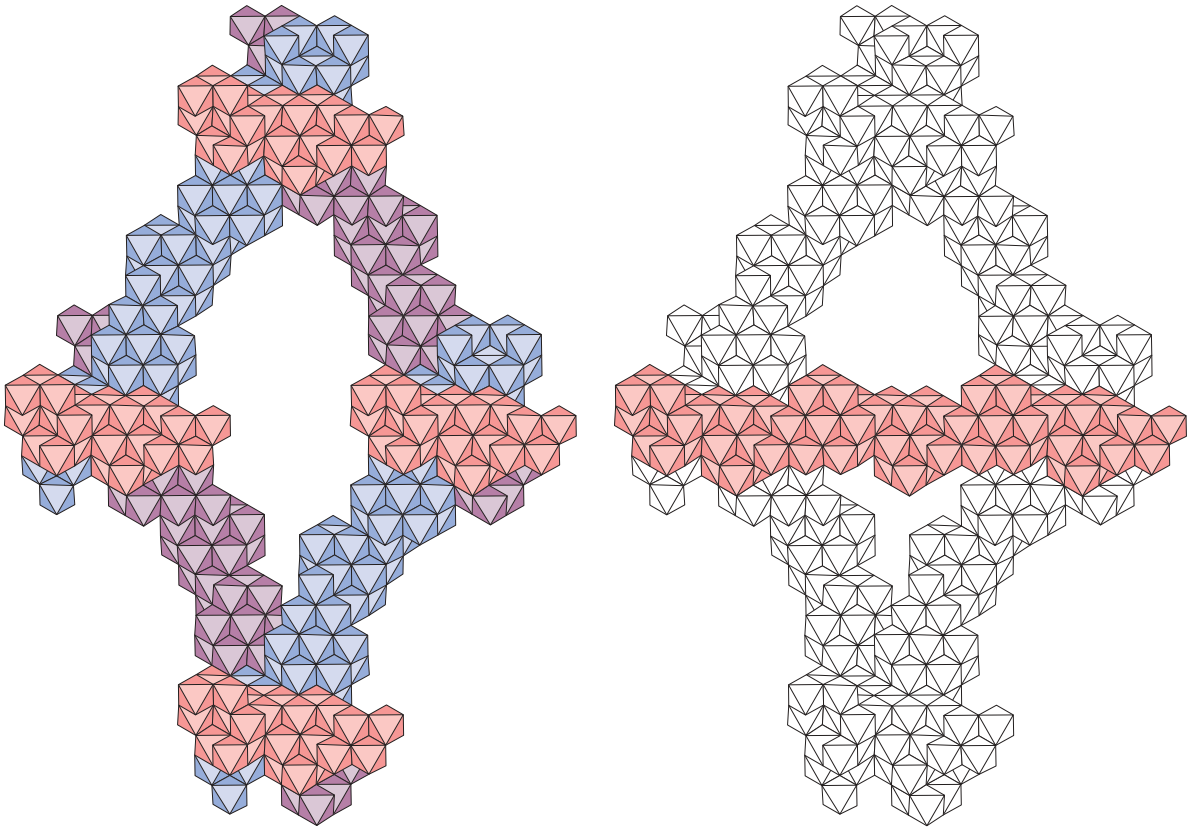
joined so that the axes of the three extended

chains project as an equilateral triangle.

The chains which are identically oriented lie on the same plane or are axially translated in multiples of six facial diameters of a He-octa. Parallel chains in the same plane do not abut like the beta-chains do in the sheet formations. When the stacks are separated by pairs of residues, the separation increases. The effect is shown in the next figure in which four stacks are joined by four pairs of residues. The axes of the chains project as a 60^0 rhombus.

Four stacks can be joined by five pairs of residues so that the rhombus is divided into two equilateral triangles. This is shown in the next figure.

The triangles are of two types, open or closed, depending upon whether the NH_2O groups protrude into the triangle. Open triangles share their sides only with closed triangles and vice versa. This triangular pattern can be extended perpendicularly to the helical axes and axially by stacking. Each chain is formed by 32-joins and the linkage between chains is the stack. The chain may be extended by additions to either its male terminus or its female terminus. The stacks differ in a translation in each of the six chain directions by five edgial-diameters of a He-octa for each pair of residues between their axes. These directions define a regular hexagon. The stack dimension is six facial-diameters of a He-Octa per revolution. These are the dimensions of a regular hexagonal prism which could be the cfu for a hexagonal crystal. In the next figure, the pairs of the four stacks are directly joined without the intervening pairs.

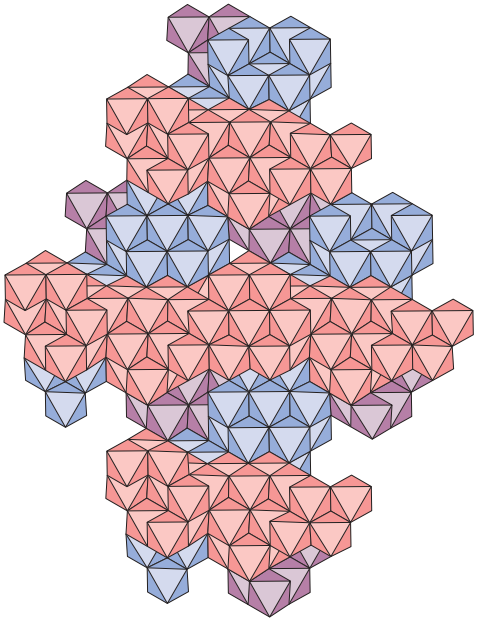


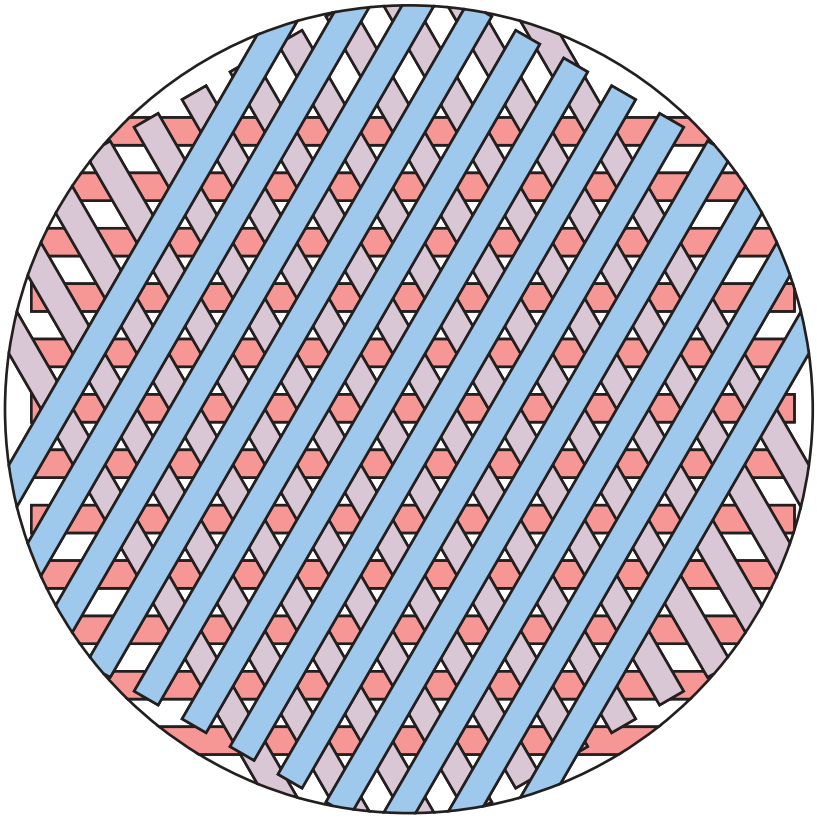
Four stacks joined by 32chain pairs rhombally

The figure on the left shows four 32chain stacks lined by 32chain pairs. The figure on the right shows the red chains of the middle stacks joined by a 32chain pair.

Lattice of 32chains

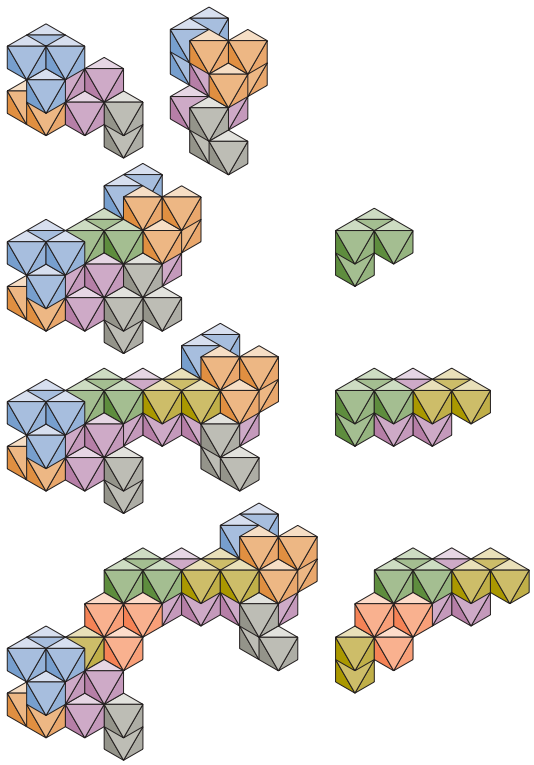
The four 32chain stacks when joined by additional 32chain peptide links form a lattice. The chains of a given color are parallel and lie in the same plane. The chains of adjacent planes are rotated one third of a revolution. This pattern is extensible in the axial directions of the chains and by additional chains within the plane and by additional planes of chains in the 32stack direction normal to the planes. The spacing of the stacks could vary to provide larger openings and a lighter structure. Also, the stack joins could be staggered from plane to plane.



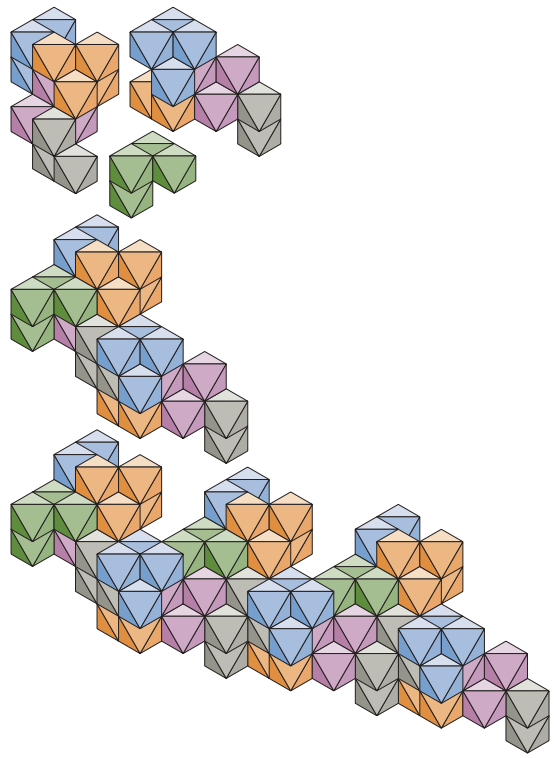


Side chain joins between 32chains.

32chains can be linked by side chains so that they form a planar crystal parallel to a pair of octahedral faces. The simplest link is an O-atom which is cleftly joined to the alpha C-atoms of two main chain units. This type linkage can be extended by the insertion of pairs of C-atoms between the O-atom and either of the main chain units. At the top of the figure are two main chain units which differ by a half revolution about the edgial axis of the 32chain. In the second row, they are linked by an O-atom. In the third row, they are linked by an O-atom to which has been added a pair of C-atoms. The bottom row shows the pair joined by the same O-atom to which has been added two pairs of C-atoms.

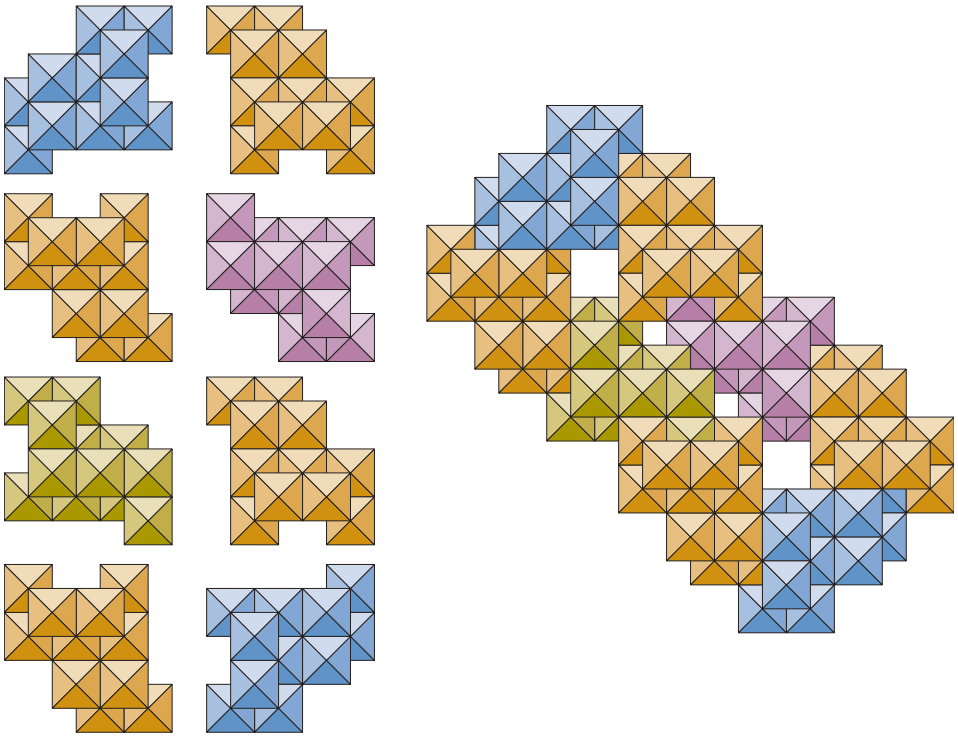


The following figure shows the unpaired main chain units at the top and an O-atom. The second row contains two main chain units joined to form a single turn of 32chain. The O-atom is attached to the unit on the left. The bottom units is composed of three identical turns of 32chain which are linked by O-atoms.



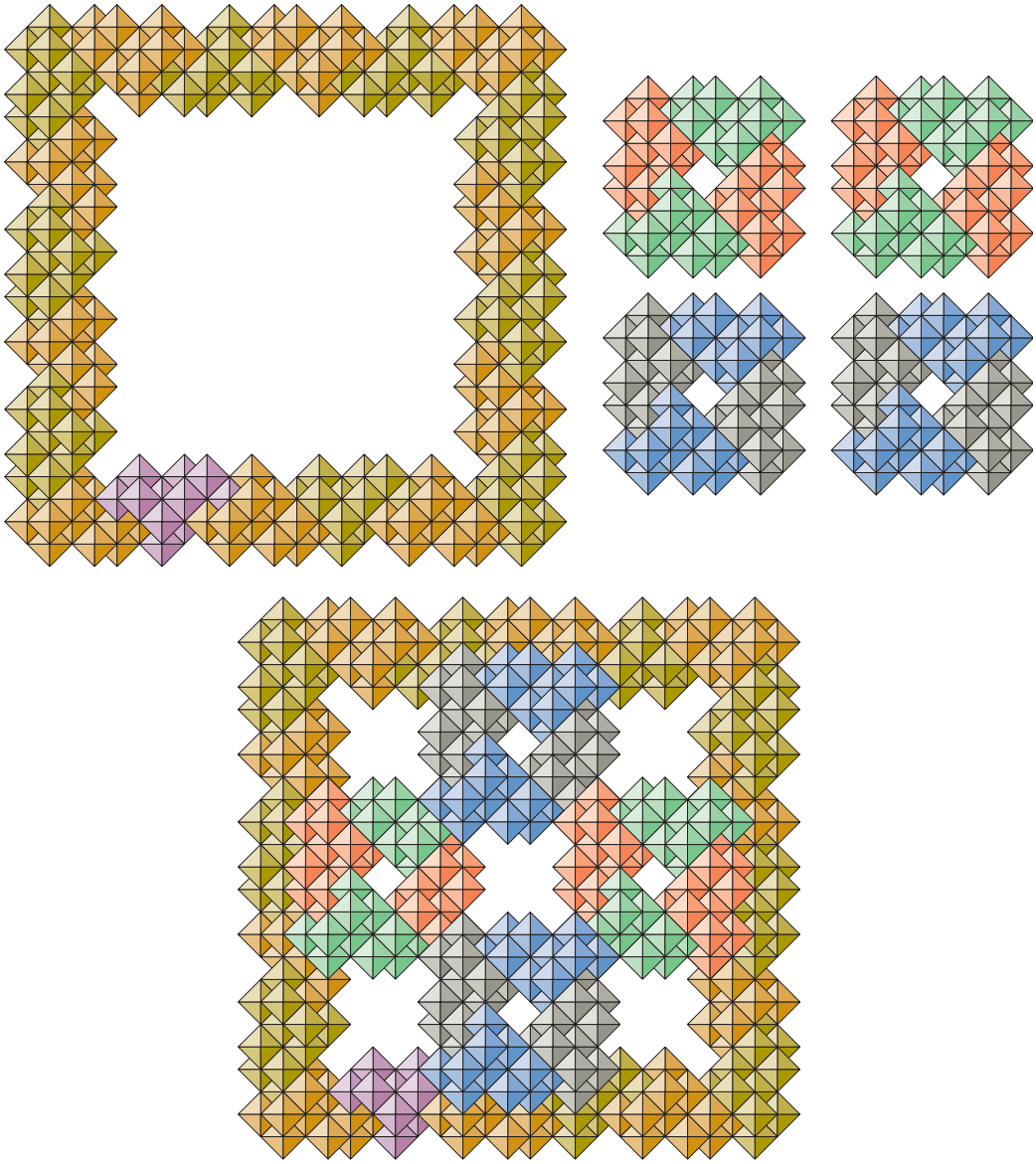
4helix assemblies

The turn of a 4helix can be extended by the addition of pairs of beta180 residues. Within a pair extended 4helix, a one residue per turn 4helix can join in sheet formation with each of the turns along one side with the central residue of the turn of the larger 4helix with parallel axes. This can be repeated for each side of the larger helix resulting in the larger helix connecting the four smaller helixes through pleated sheet joins. Each of the smaller helixes contacts two of the other smaller helixes. Direct sheet-joins between 4helixes is not possible unless the one is within the other. The size of the helixes may be extended permitting extensive variations in size and pattern. The shape of the helix can be altered from the square to the rectangular, and this adds to the pattern variations permitted by the 4helix and the sheet-join.



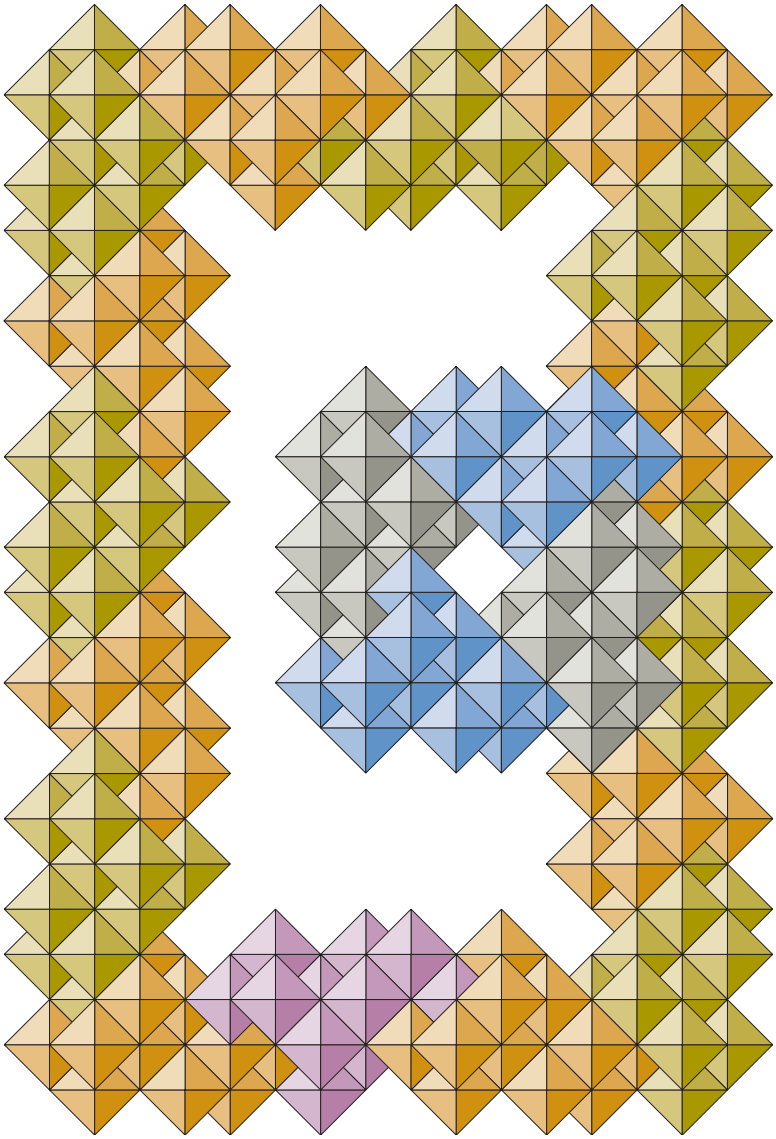
Rectangular 4helix

On the left are the eight units which form the rectangular 4helix on the right. The helix is viewed parallel to its axis. It begins with the violet colored unit and proceeds in a clockwise toward the viewer sense to the orange unit above and to the left of the violet unit.



Four 4helixes sheet-joined to larger 4helix

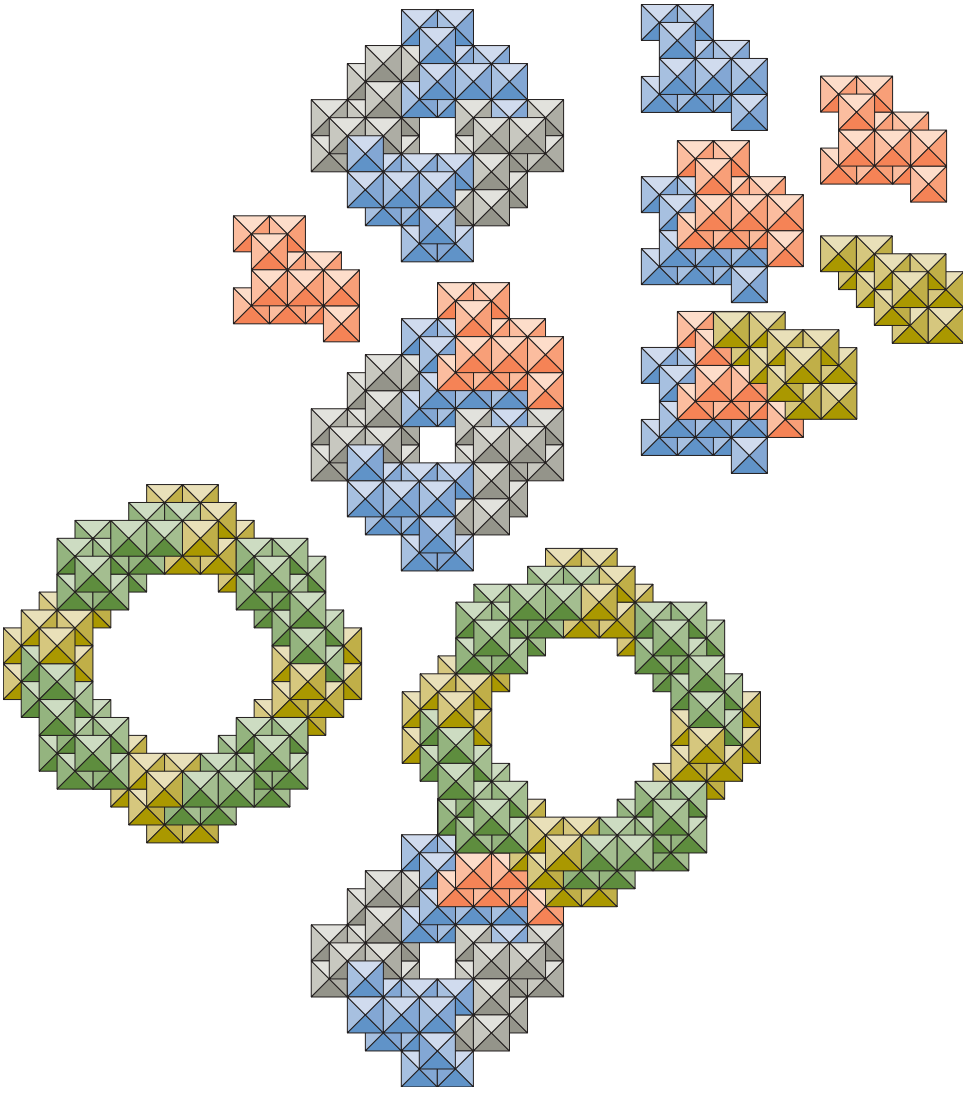
An extended leg 4helix is at the upper left of the figure. The residue at the near terminus of the helix is colored violet. In the upper right of the figure is a group of identical 4helixes. The near terminus of these helixes is the blue or red colored residue which is at the lower left of each helix. The inner 4helixes are sheet joined to the extended helix at the bottom of the figure.



Rectangular 4helix with sheet-joined 4helix

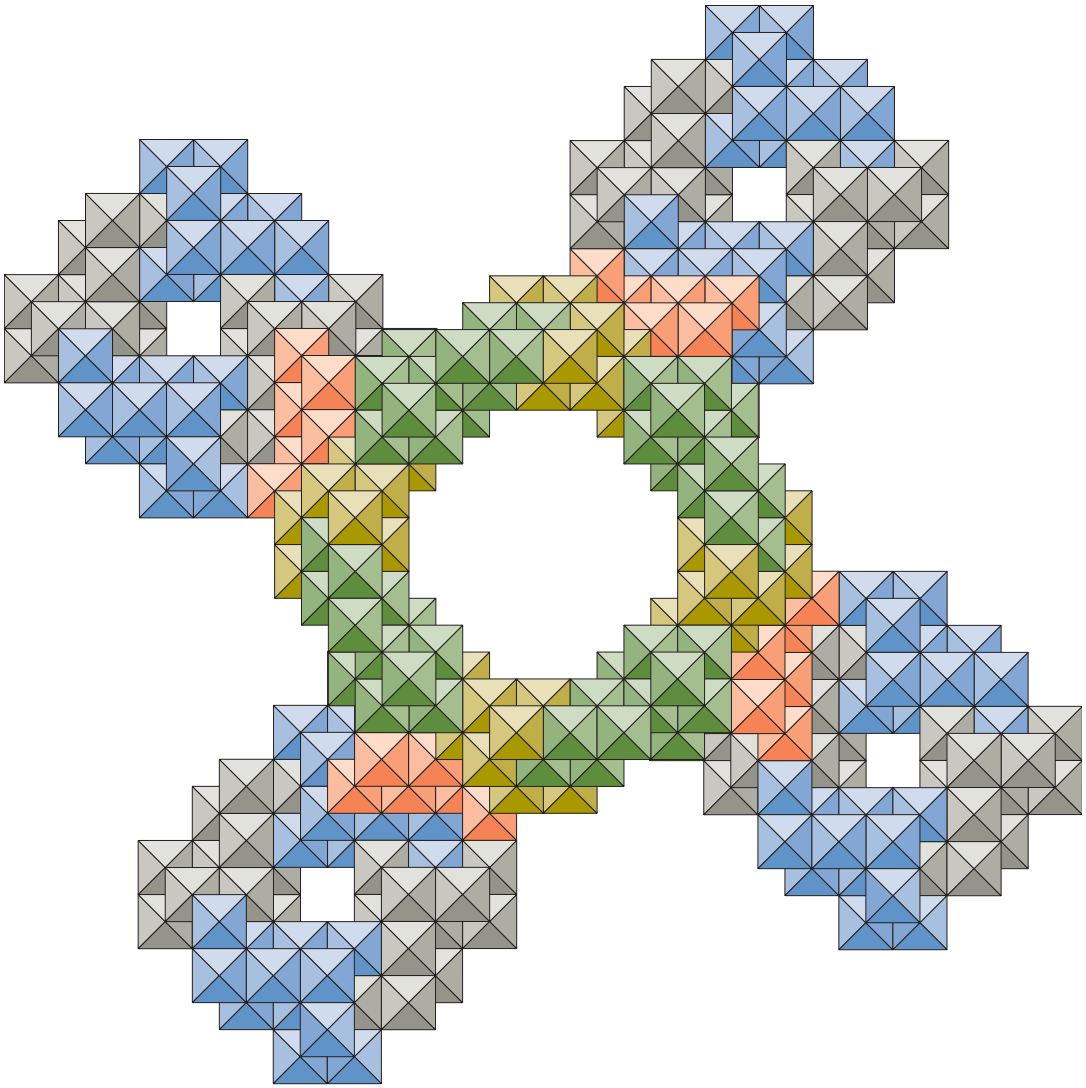
The figure shows an extended 4helix which has a rectangular form. A single 4helix is sheet joined to it. The residue which is the near terminus of the extended 4helix is colored violet.

A 4helix can be joined by to a vertexial-ring by a pair of residues to form a 4-strand sheet which includes a residue of the ring, the two linking residues, and a residue of the 4helix. The ring can join four helixes in this manner. This results in the axis of the 4helix being parallel to the normal to the ring-plane. A pattern of rings and helixes can be formed in this manner.



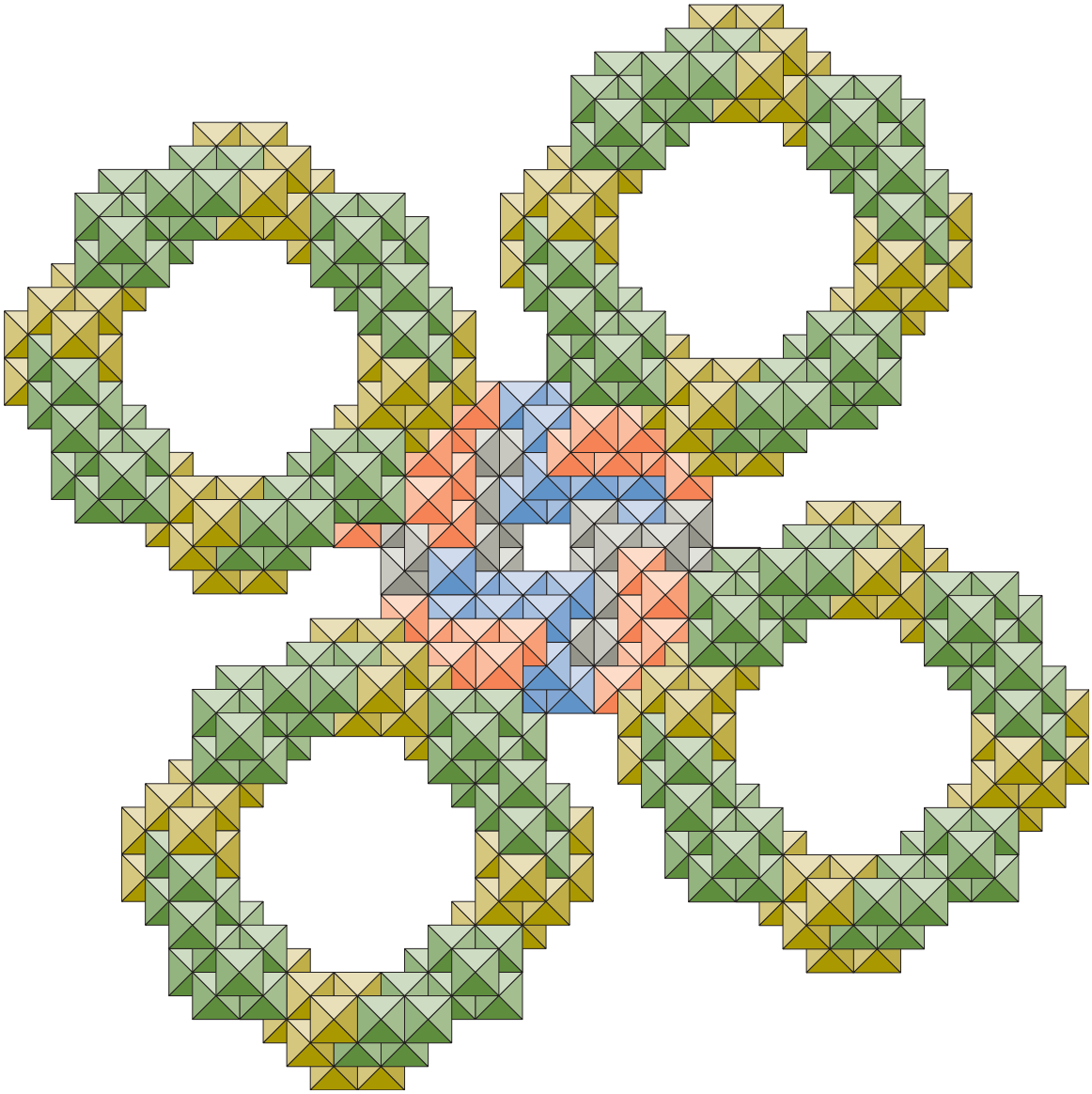
A 4helixes sheet-joined to cyclic peptide

The figure shows the joining of a 4helix to a cyclic peptide by sheet a sheet join. The assembly begins at the top with the 4helix which is composed blue and gray colored residues. A lone residue is anti-parallel sheet joined to the four helix in the next step. The ring joins to the red colored residue in a parallel sheet join to complete the assembly. In the upper right of the figure the sheet joins between the residues is shown. The blue residue is from the 4helix, the red is solitary residue, and the yellow is a residue from the ring.



Ring with four 4helixes adjoining

The 4helixes are identical and their near termini are colored blue and are located at the lower edge of the projected helix. The red residue enables a sheet join between the 4helix, itself, and the ring.



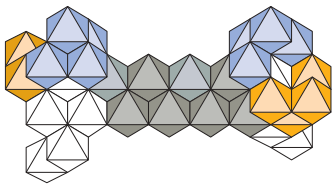
Four cyclic peptides sheet joined to a 4helix.

This figure shows a 4helix to which four rings have been sheet joined with the aid of the red colored glycine. This assembly is analogous to that shown in the previous figure.

Side chain connections of peptides

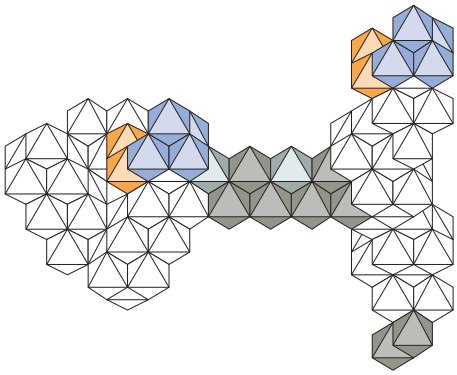
Gly-4C-gly

Two main chain units can be connected by a straight length of carbon chain which is cleftly joined to the alpha C-atom of each unit.



Pair of glycines linked by chain of four C-atoms

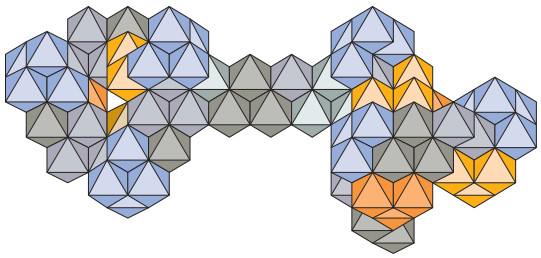
In the next figure the same relationship between residues and carbon chain links an alpha helix and a beta180 chain. The alpha helix is on the left and its axis is parallel to the viewing direction. The terminal NH_2O groups of the alpha helix and the beta180 chain have been colored. The C-atom at the male end of the beta180 chain has also been colored.



Alpha helix linked to a beta chain by a chain of four C-atoms

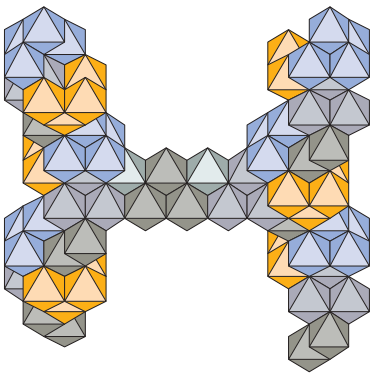
This same linkage is shown in the figure the next page. The beta180 chain has been joined by two identical chains to form a parallel pleated sheet, the linking chain of C-atoms has been extended, and an additional turn has been added to the alpha helix. The view is a perspective projection. In the second figure, the carbon chain has been extended to eight C-atoms and the alpha helix has been extended by a turn. The orientations of sheet, helix, and chain are the same as in the first figure. The axis of the alpha helix is parallel to the plane of the pleated sheet.

The join in the next figure is between two alpha helixes. The helix on the left is viewed parallel to its axis, that on the right is angled to the viewing direction. The helix on the right consists of a single turn.

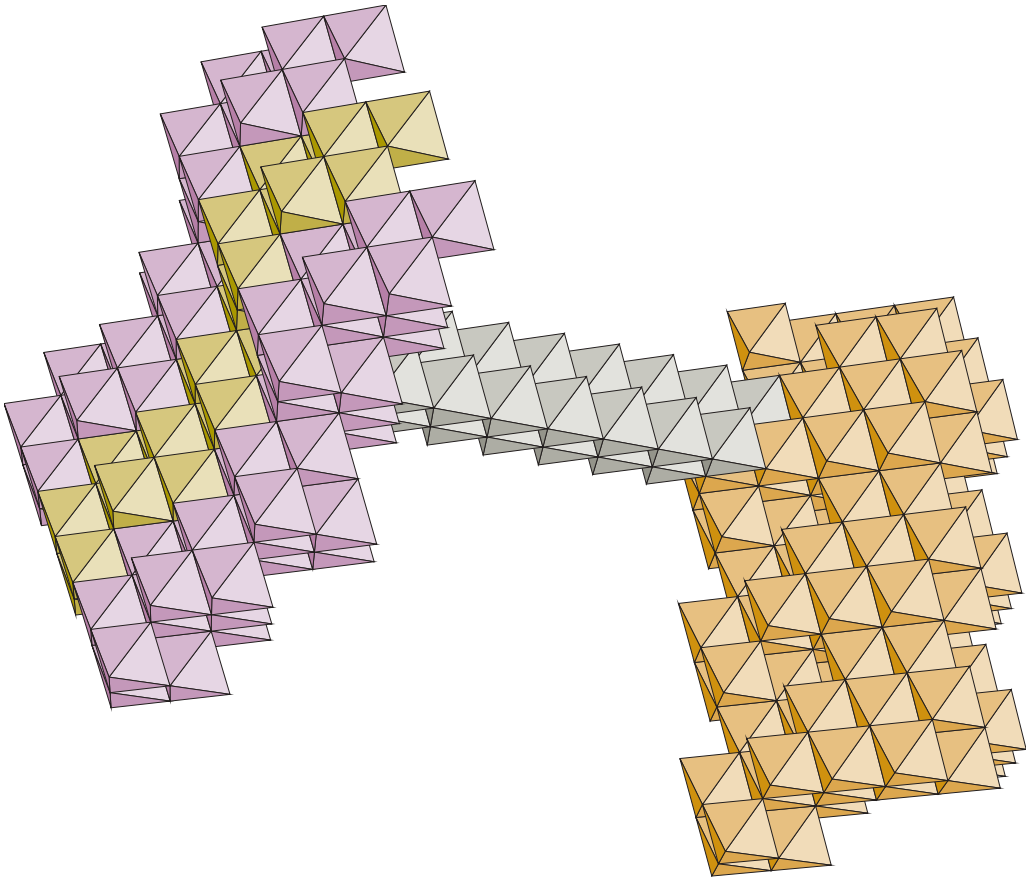


Two alpha helixes linked by a chain of four C-atoms

Two beta180 chains having the same carbon chain linkage is depicted here. Each chain has three units. Their axes are parallel. The two end units of each chain have the same orientation as the middle unit of the other chain.

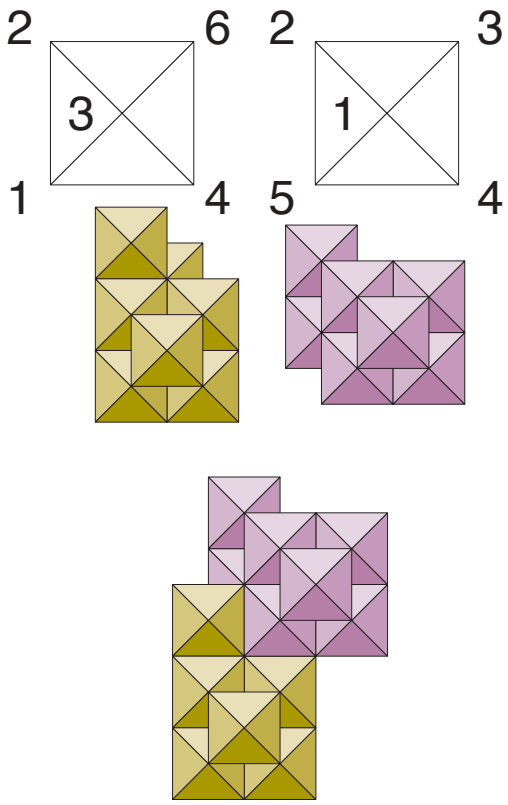


Two beta chains linked by a chain of four C-atoms



Alpha helix linked to parallel pleated sheet by a chain of eight C-atoms.

Cys-cys loop in insulin.



S to S join in cys-cys loop.

The "A" chain of insulin has a cys-cys join between unit #6 and unit #11. The S-atom has four clefts. One cleft is required for joining with the beta C-atom of the cys-unit to which it belongs. One of the three remaining clefts is required for joining with the S-atom of the other cys-unit. There are five residue to residue joins between the first cys-unit and the cys-unit to which it is joined. Each combination of C-atom to S-atom to S-atom to C-atom was tried for each combination of the six possible types of main unit joining which could link the six main chain units without interference and have the first and sixth unit cleftly joined to each of the given CSSC assemblies. Only one combination fit. The orientations of the residues and the joins between them are listed in the table.

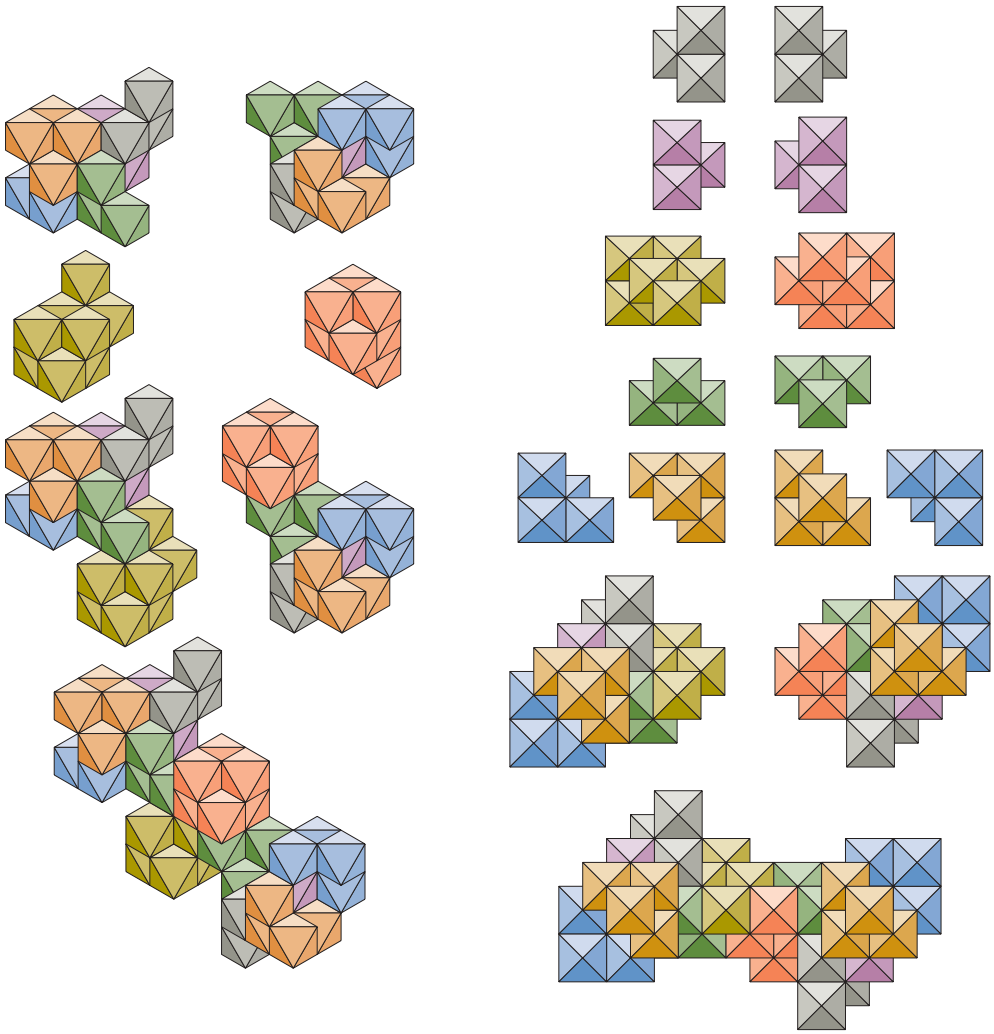
Table 20: Cys-cys loop chain joins

Unit	Orientation	Join
1	125643	
2	634152	32chain
3	265413	epsilon
4	652134	alpha
5	512364	4helix
6	526341	beta90

The next table shows the disposition of the clefts of the two S-atoms whose cleft join effects the "A" chain cys-cys join of insulin.

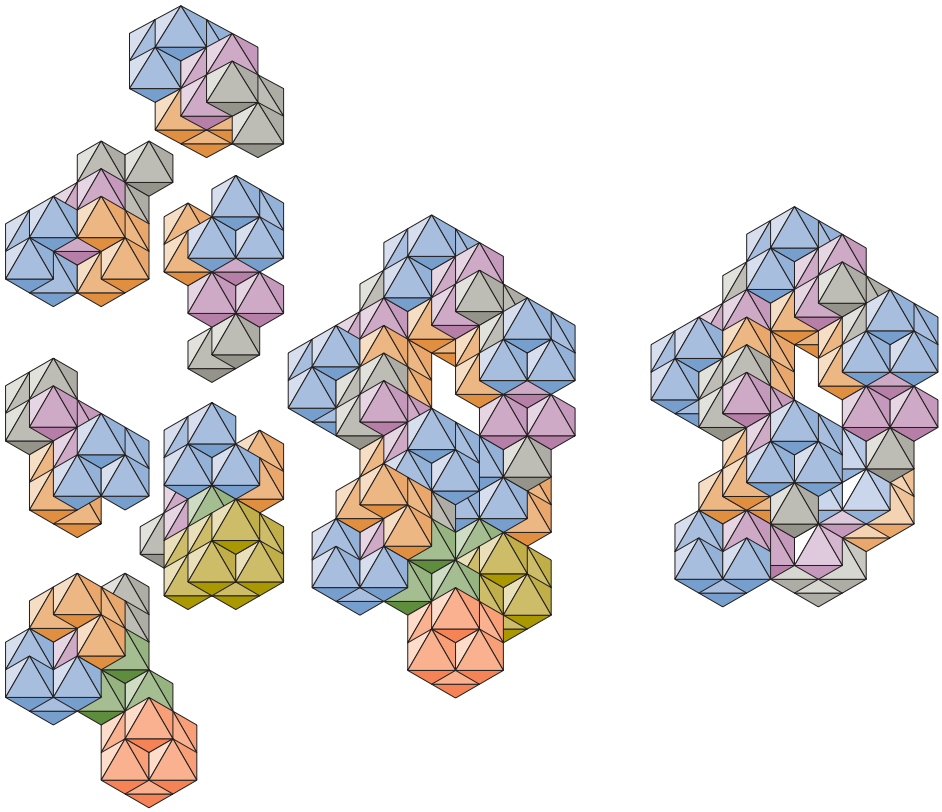
Table 21: S-atom clefts

Cleft	S-atom female end	S-atom male end
Be-S	beta C-atom	beta C-atom
Ne-Si	open	S-atom female end
Mg-Si	blocked	open
Si-S	S-atom male end	open



Cys-cys pair 3651a

The figure shows the atoms which constitute each of the cys-units and then shows the atoms assembled as the two cys-units. The two units are identical in conformation but are rotated 180° with respect to one another. The S-atom to S-atom joined units are at the bottom of the figure.



Cys-cys loop of insulin

At the left of the figure the residues #6 through #11 of the "A"-chain of insulin are shown unassembled. The completed assembly is shown just to the right of them. Residues #6 and #11 are cys-residues which form a cys-cys join. The S-atom of one is colored red and the S-atom of the other is colored yellow. On the right, the side chains of the cys residues have been removed to show the conformation of the main chain.