

Cyclic

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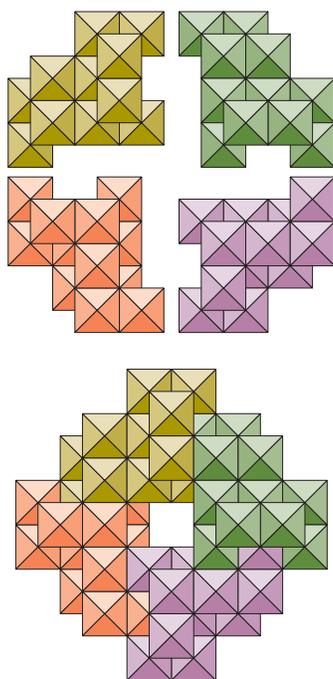
<http://web.me.com/whitby/Octahedron/Welcome.html>

Reference

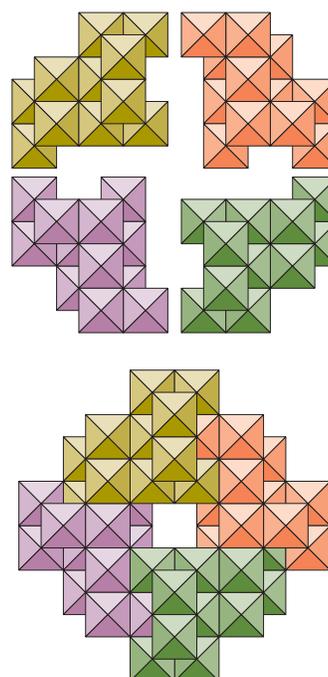
Octahedron1stEd.pdf–bookmark CYCLIC–pages 363-383

Introduction

This material is excerpted from *Octahedron*. It shows how the main chain portions of the peptides join as assemblies in which the protein chain has no termini..

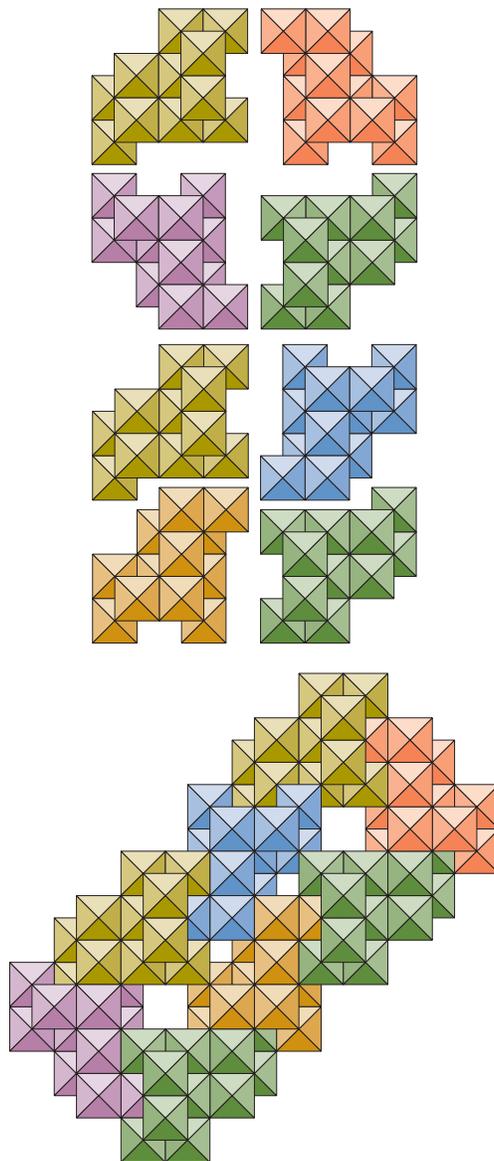
CYCLIC**Cyclic peptide LDLD****Cyclic peptide LLDD.****Cyclic peptide LLDD.**

A ring can be formed using two L-units and two D-units. The L-units differ by a rotation of a quarter turn about an axis parallel to the viewing direction. The same is true for the D-units. The L-units are colored yellow or green. The L-units are joined alpha helically. The D-units are colored red or violet. They, too, are joined alpha helically.

**Cyclic peptide LDLD.**

The same units can be used to form another ring. The L-units differ here by a half revolution. This is true for the D-units too.

Cyclic peptide LLLDLLLL

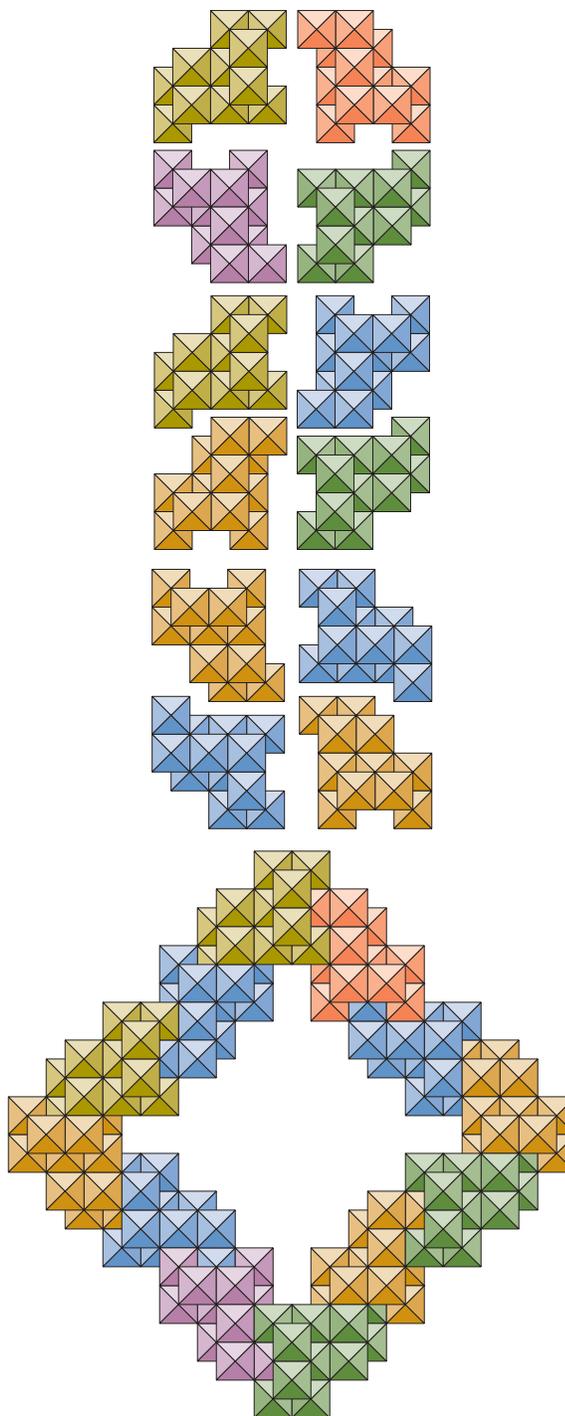


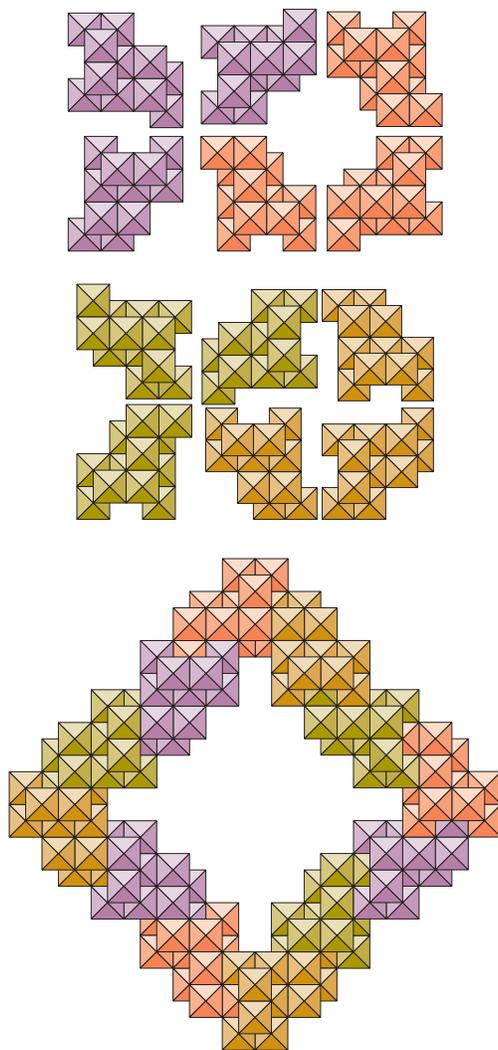
Cyclic peptide LLLDLLLL.

The ring shown in the last figure is extended by the addition of one pair of L-units between the yellow and purple units and a second pair of L-units between the red and green units. The cyclic peptide which results has the form LLLDLLLL.

Cyclic peptide LLLLLDLLLLLD.

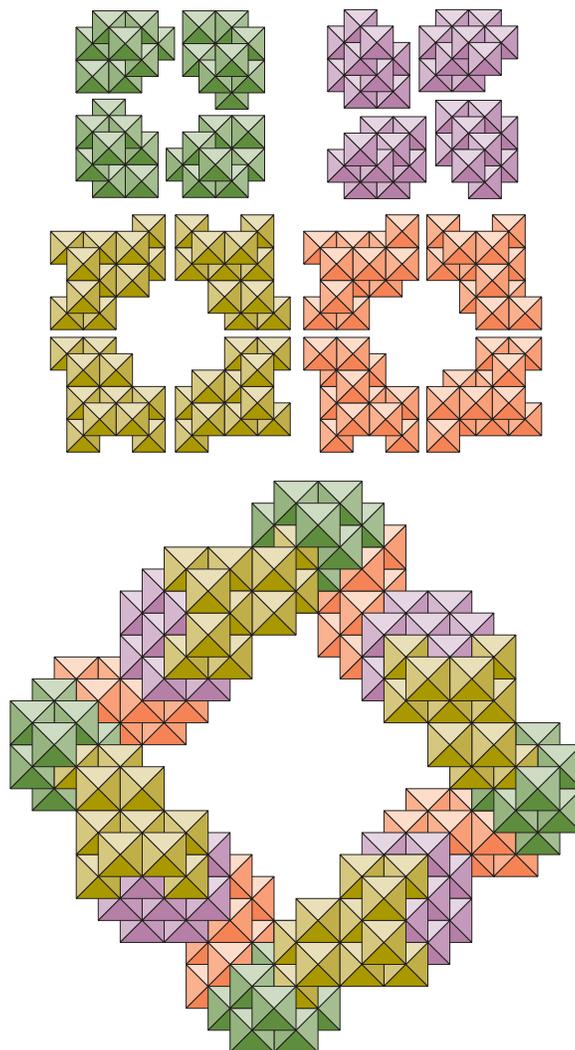
Cyclic peptide LLLLLDLLLLLD.
 The ring is extended in a direction at right angles to the previous extension in the next figure. Two L-units are inserted between the violet and yellow units and another two L-units are inserted between the red and green units. The twelve unit ring is of the form LLLLLDLLLLLD. The two units colored red and violet are the D-units.



Cyclic peptide LLDDLLDDLLDD**Cyclic peptide LLDDLLDDLLDD**

The units which form the peptide are shown in two groups of six each at the top of the figure. Those colored red or violet are D-gly and those colored yellow or orange are L-gly.

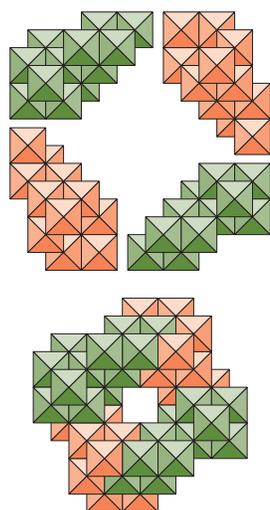
Cyclic peptide 4LDLD



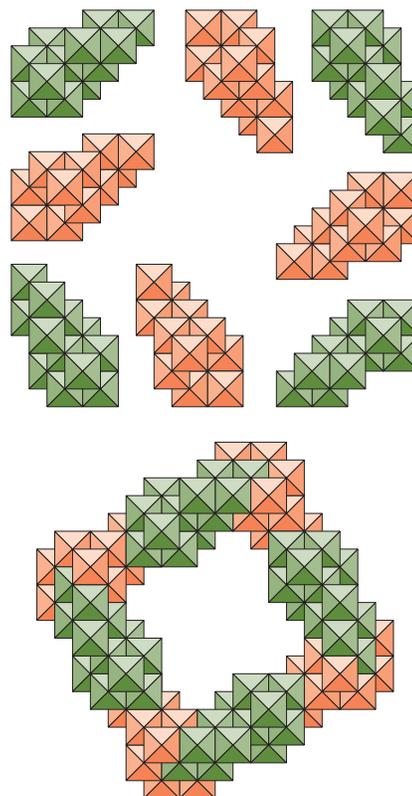
Cyclic peptide 4LDLD

The figure shows the sixteen units which constitute the cyclic peptide¹ in groups of four each at the top. Each group of four contains identical units which differ by a rotation of a quarter of a revolution about an axis parallel to the viewing direction. The units which are colored red or violet are D-units; the units colored green or yellow are L-units. The join between L-units is epsilon helical. There is a 3₂chain join between D-units. The peptide is viewed parallel to its axis of fourfold symmetry.

1. H. N. Rydon, editor, *MTP International Review of Science*, Organic Chemistry Series Two, Volume 6, Butterworths, London, 1976, p. 243, Fig. 7.11.

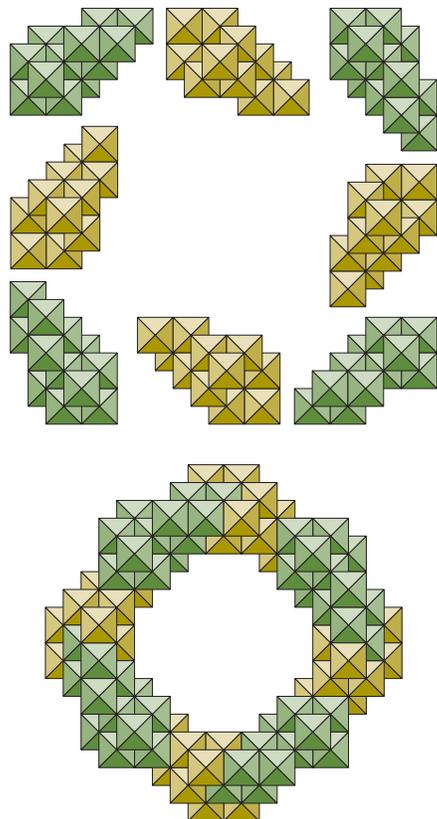
Cyclic peptide LDLD**Cyclic Peptide LDLD.**

A four unit cyclic peptide with twofold symmetry about a vertical axis is shown in the next figure. There are two L-units colored green and two D-units colored red. The pattern is LDLD.

Cyclic peptide LDLDLDL**Cyclic peptide LDLDLDL.**

This ring is extended by the addition of two L-units and two D-units to form a four-fold ring in the next figure. The added units are in the same orientation as those in the previous figure but differ from them by a rotation of a quarter of a revolution. The pattern is LDLDLDL. D-units are colored red and L-units are colored green.

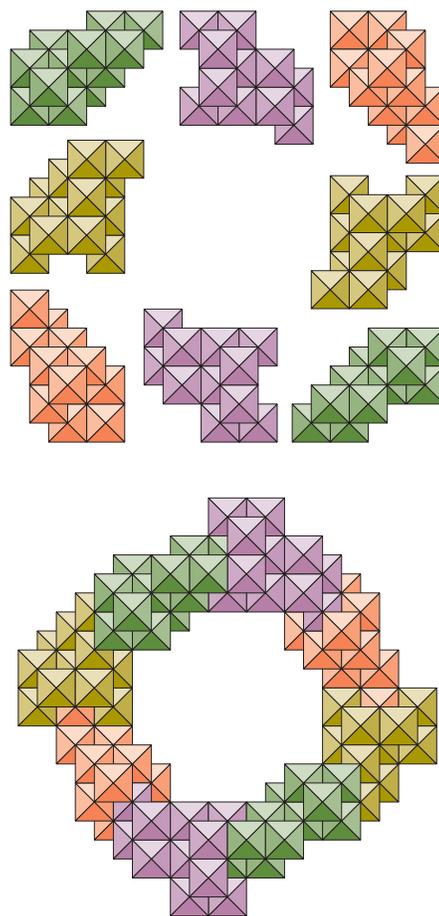
Cyclic peptide LLLLLLLL



Cyclic peptide of eight L-units.

The four L-units of the LDLD-LDL D assembly are combined with four additional L-units to provide a cyclic peptide consisting of eight L-units. The additional L-units are inverted relative to the previous L-units. They are colored yellow. The join between the male end of the green unit and the female end of the yellow unit is $\beta 32$ chain. The male end of the yellow unit is joined to the female end of the green unit in a $\beta 180$ join.

Cyclic peptide LLDDLDD

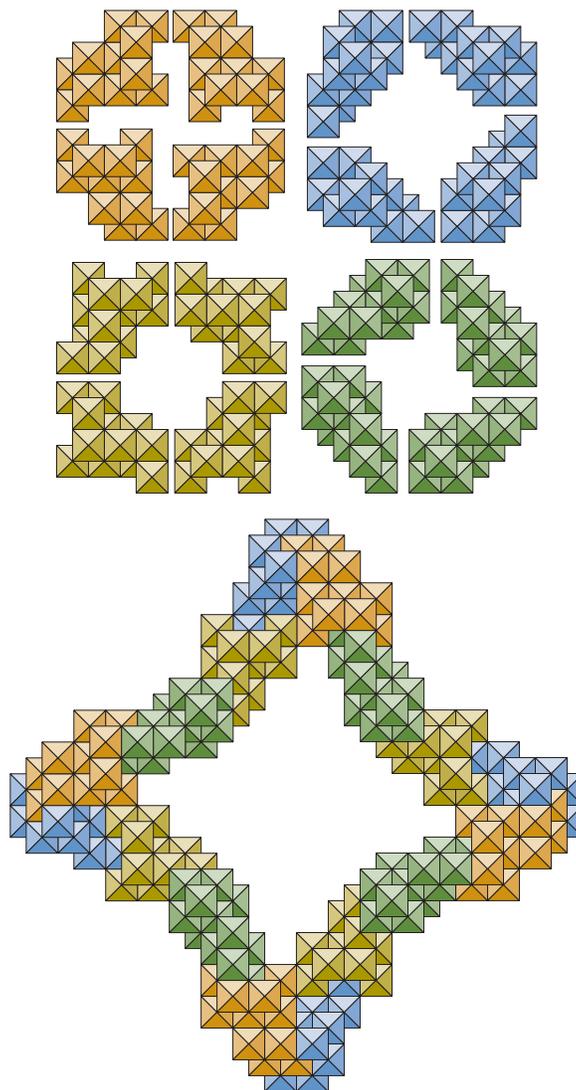


Cyclic peptide LLDDLDD.

This ring is based on the LDLD ring shown previously. The ring has been extended by the insertion of two L-units and two D-units. The units of each pair differ by a rotation of a half revolution about an axis parallel to the viewing direction. The pattern becomes LLDDLDD.¹ The L-units are colored yellow or green and the D-units are red or violet. The join between the L-units is $\beta 90$. The join between D-units is $\beta 90$ as well.

1. Lubert Stryer, *Biochemistry* 2d ed., W. H. Freeman, San Francisco, 1981, Fig. 36-19, p. 873.

Cyclic peptide of sixteen L units.

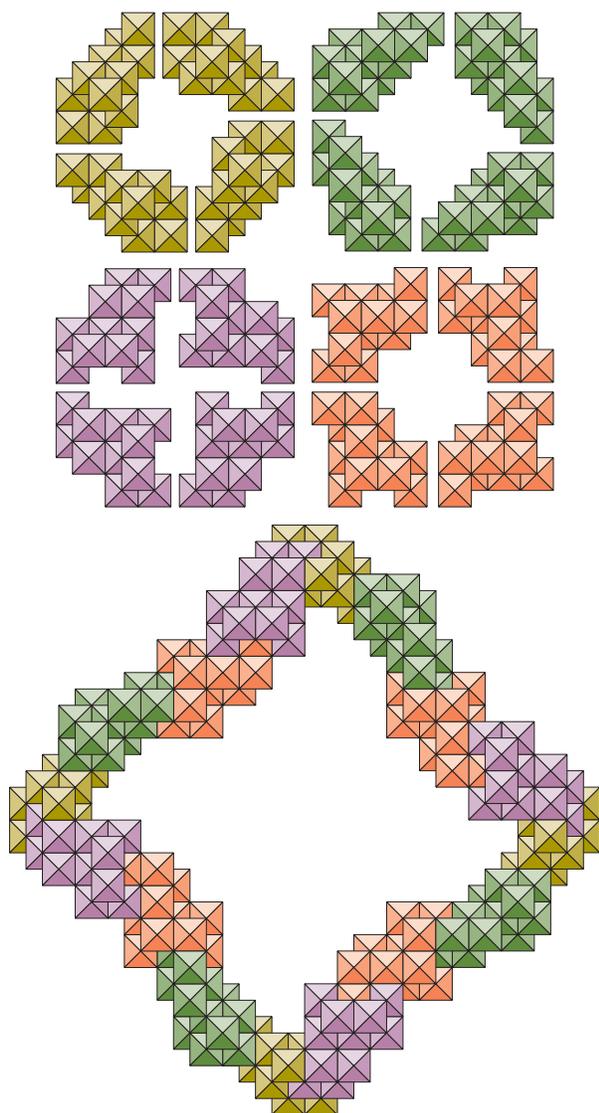


Cyclic peptide of sixteen L-units.

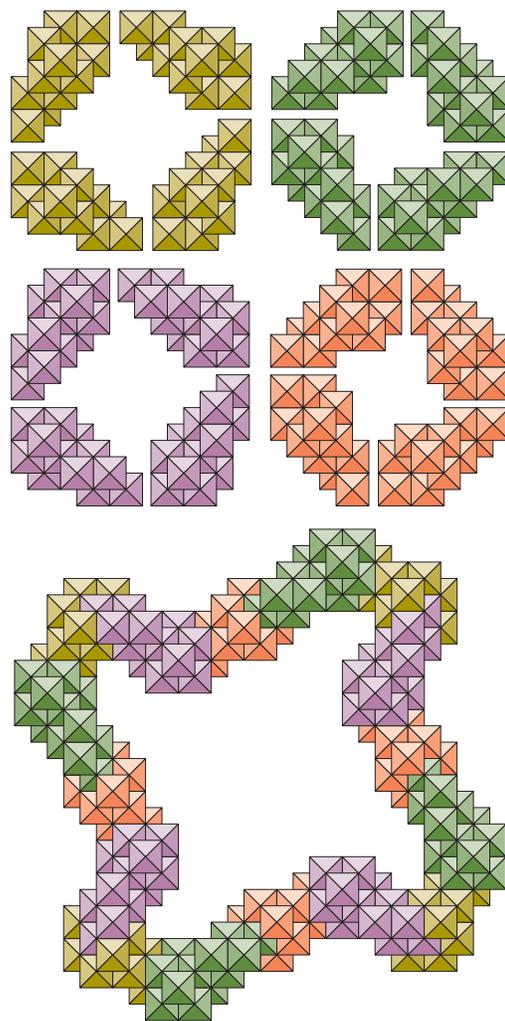
The L-units of the eight L-unit ring appear here¹ with eight additional L-units. The new units are in two sets of four. These sets differ by an inversion. Within each set, the L-units differ by a quarter turn rotation about an axis parallel to the viewing direction.

Blue and orange units are joined alpha helically. Yellow is joined with blue in a beta90 join. Green is joined with yellow in a beta90 join as well. Orange is joined with green in a beta90 join. From alpha helical join to alpha helical join the four L-units constitute a single turn of beta90 helix. The ring is composed of single turns of beta90 helix joined one to the other by an alpha helical join.

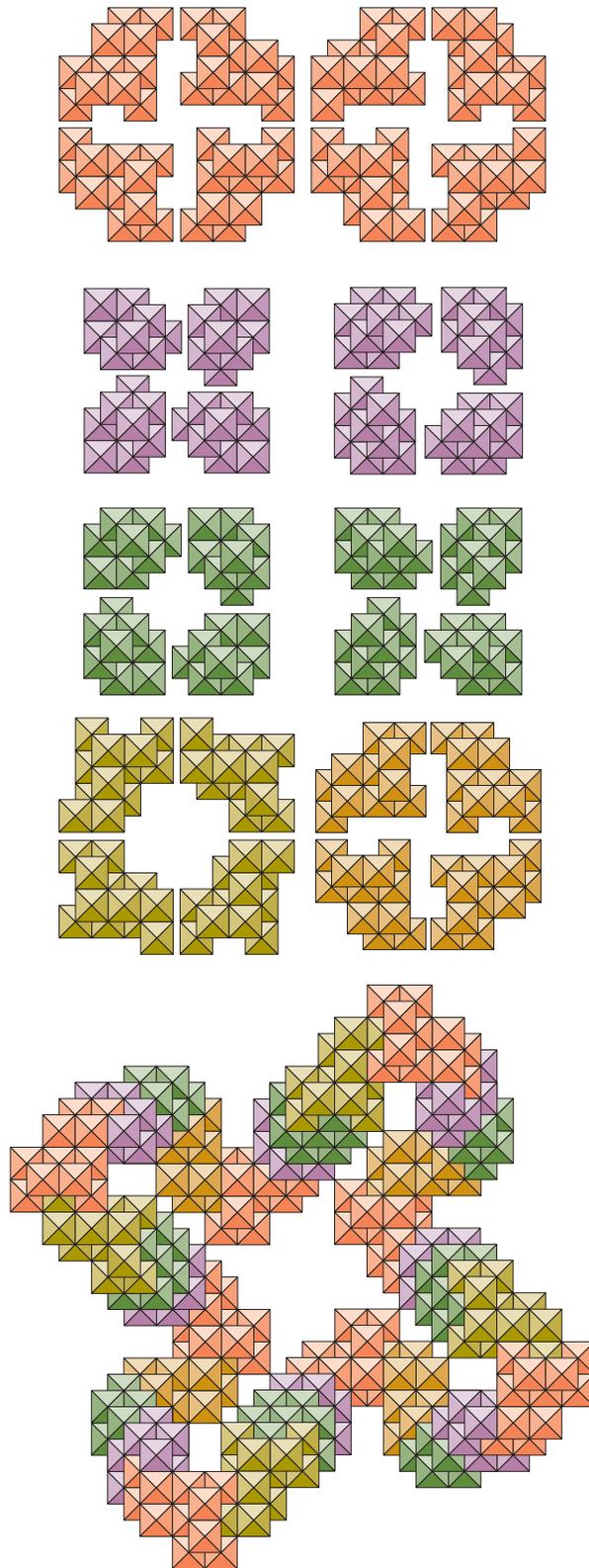
1. Rydon *ibid.* Fig 7.11(b) p. 243.

Cyclic peptide 4LLDD

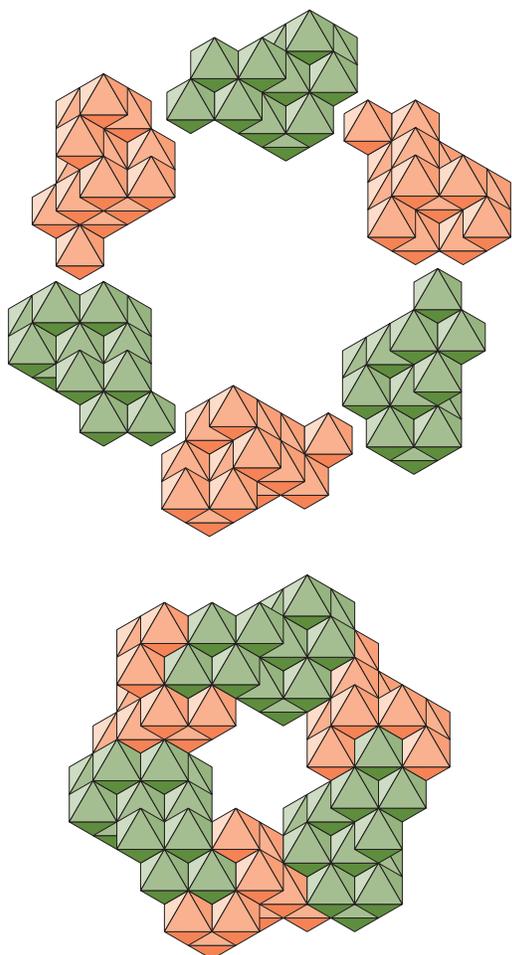
**Sixteen residue ring with vertical axis,
Type A**

Cyclic peptide 4LLDD

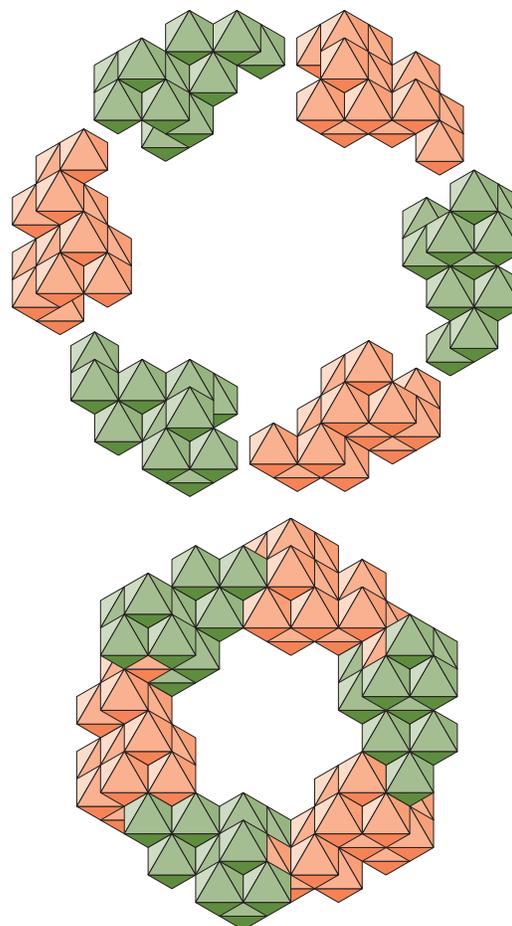
**Sixteen residue ring with vertical axis,
Type B**

Cyclic peptide 4LLD DLLDD**Cyclic peptide 4LLD DLLDD**

The thirty-two residues which form this ring are shown at the top of the figure in eight groups of four each. Red and violet colored residues are D-gly and yellow and green colored residues are L-gly.

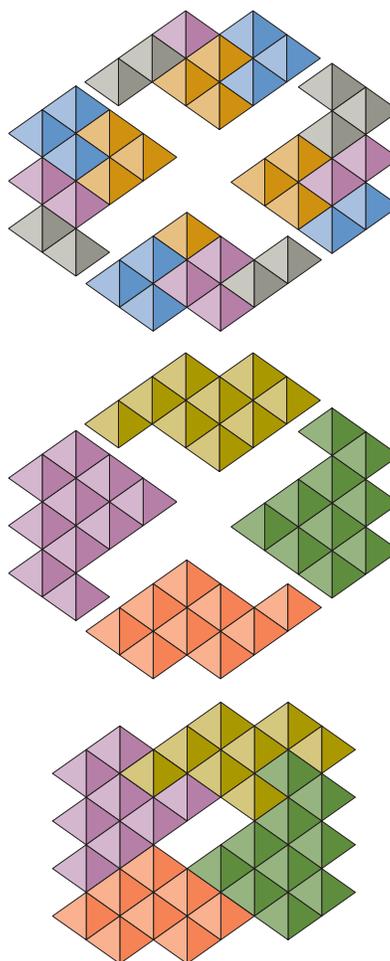
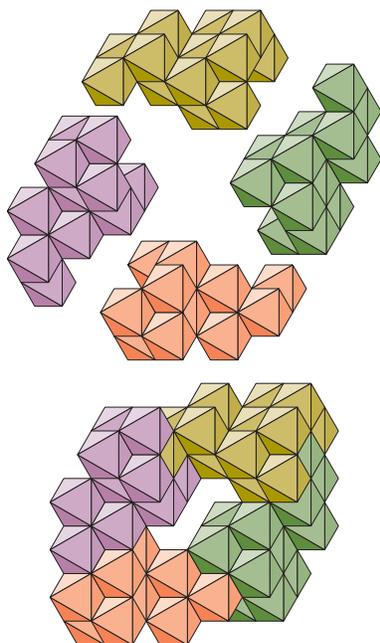
Cyclic peptide LDLDLD type A**Cyclic peptide LDLDLD type A**

The ring is made of two sets of three units each. Those colored green are L-units and those colored red are D-units. Units within a set differ by a rotation of one third of a revolution about the viewing direction. This ring is three He-octa facial diameters in thickness.

Cyclic peptide LDLDLD type B**Cyclic peptide LDLDLD type B**

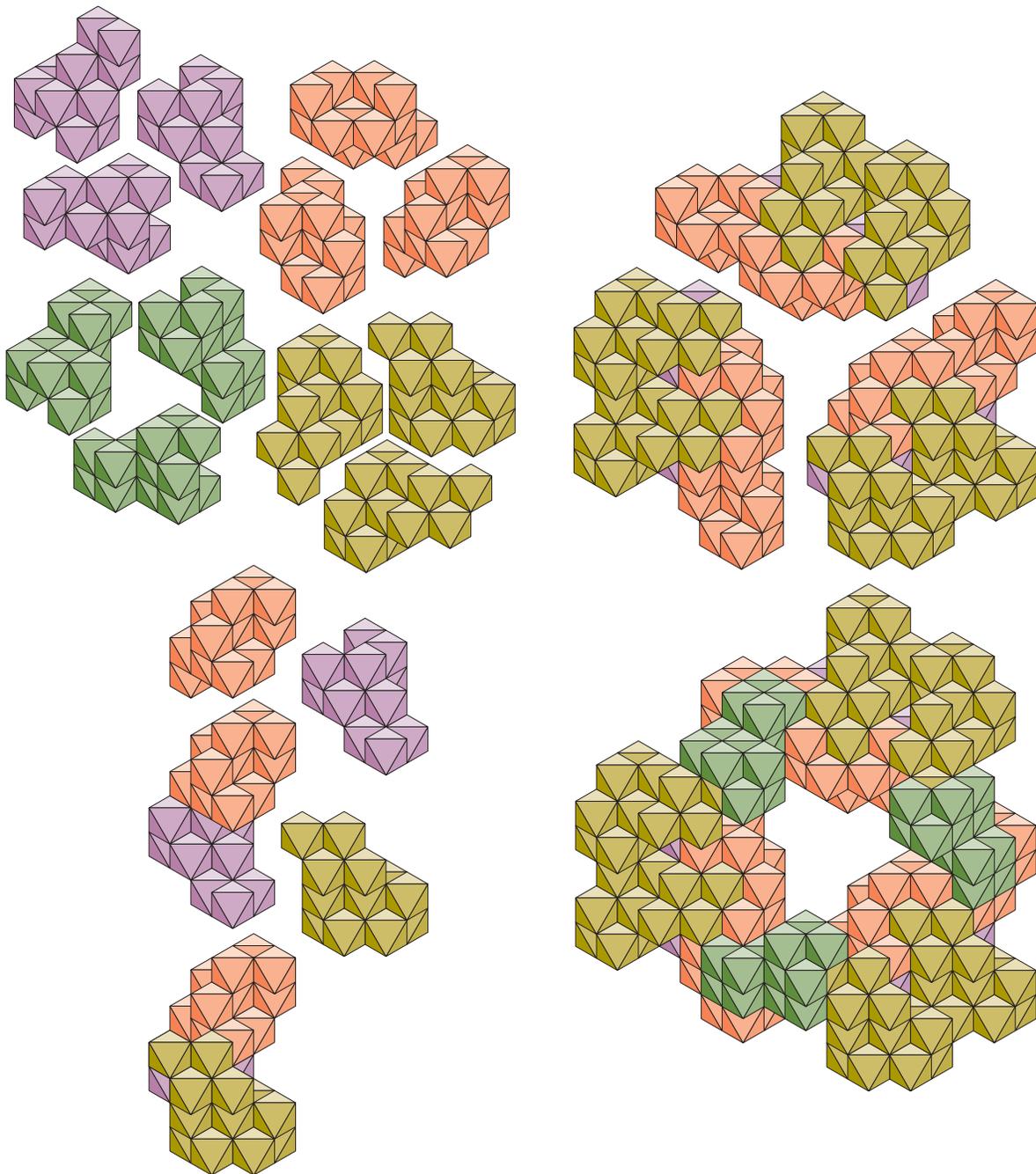
The ring is composed of six main chain units. The green colored units are L-units and the red colored units are D-units. Each set is in the orientation to produce a single turn of alpha helix. The pitch that results from the join of L-unit to D-unit is negated by the pitch which results from the join of D-unit to L-unit. This ring is four He-octa facial diameters in thickness.

Cyclic peptide LLDD



Cyclic peptide LLDD

A pair of L-units joined alpha helically can form a ring with a pair of D-units joined alpha helically. The helical axis of the D-pair is inverted relative to the helical axis of the L-pair. The L-units are colored yellow or green; the D-units are colored violet or red. In the figure on the left the view is parallel to the helical axes. On the right, the view is parallel to the axis of the ring itself. The top group shows the units with their atoms defined by color. The blue colored octas belong to O-atoms, those colored orange belong to NH₂ groups, the gray colored octas belong to the carbonyl C-atom while the violet colored octas belong to the alpha C-atom.



Three alpha helices linked by beta180 chains.

Cyclic peptide, facial axis: Three alpha helixes linked by beta180 chains

A ring can be formed using three alpha helixes of two turns each which are then joined in a single chain by a main chain unit. Only L-units are used here. The main chain units are shown at the top of the left column of the last figure. Below the four groups of three, the assembly of one turn of one helix is shown. An identical turn extends the helix by joining the yellow unit of one turn with red unit of the other turn. The red, violet, and yellow units form the alpha helixes; the green units are the links between the helixes. At the top of the right hand column of the figure, the three helixes are shown. Below them is the completed cyclic peptide.

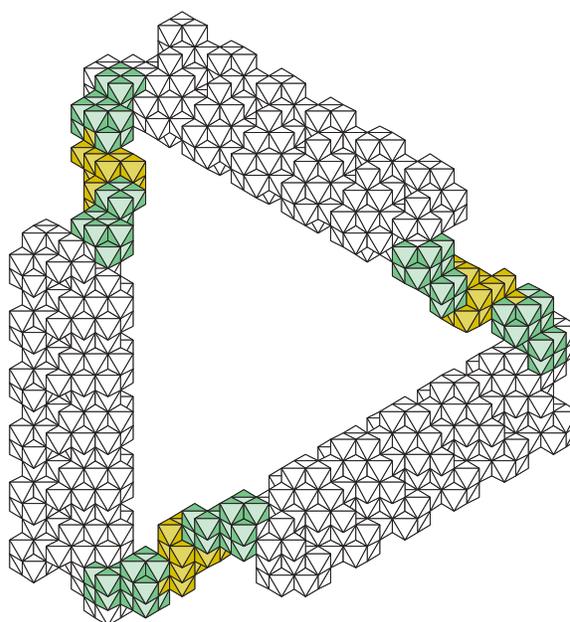
A larger ring formed by extending each of the alpha helixes from two turns to six turns is viewed along the threefold axis in the next figure. The link between each pair of helixes becomes a beta180 chain of three units which are colored green or yellow in the figure. The axis of each of the helixes is inclined to the viewing plane. Each of the helixes rises toward the viewer when moving in a clockwise direction around the ring. The beta180 chain descends away from the viewer when moving around the ring in the same clockwise direction.

Each beta180 unit moves two He-octa facial diameters away from the viewer. Each alpha helical turn moves one He-octa facial diameters towards the viewer. To make the connection, the number of beta180 units must be odd. The formula for calculating the number of units is where N is the number of units in the ring, n is any integer. The number of beta180 units per link is $2 \times n - 1$, the number of units per alpha helix is $2 \text{ turns} \times (2 \times n - 1) \times 3 (\text{units/turn})$ and the number of link-helix groups in the ring is three.

$$N = 21(2n - 1)$$

Table 22: Cyclic peptides using three alpha helixes

beta180 units	alpha helical turns	total units
1	2	21
3	6	63
5	10	105
7	14	147



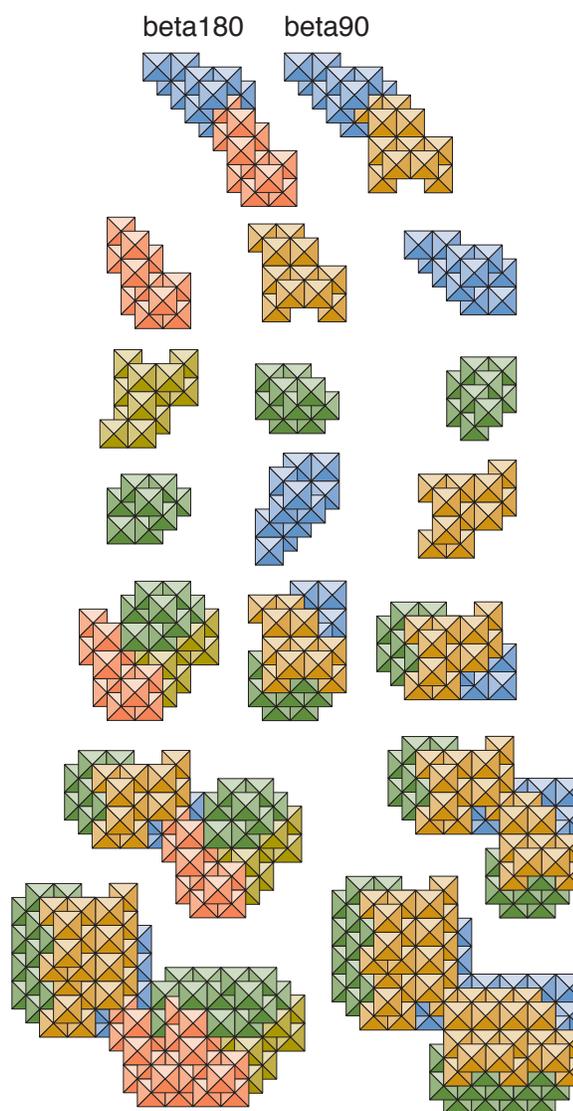
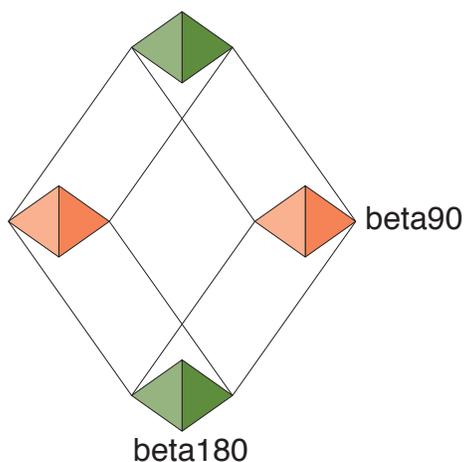
Cyclic peptide: three alpha helixes

Direct joining of alpha helices

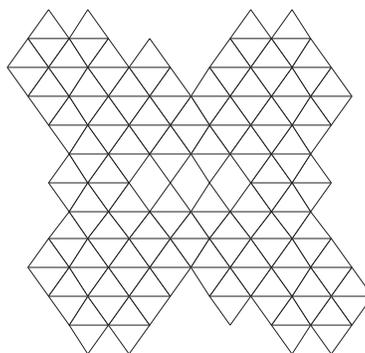
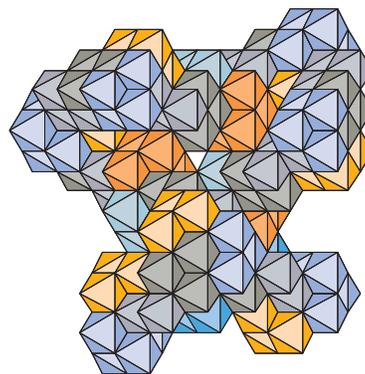
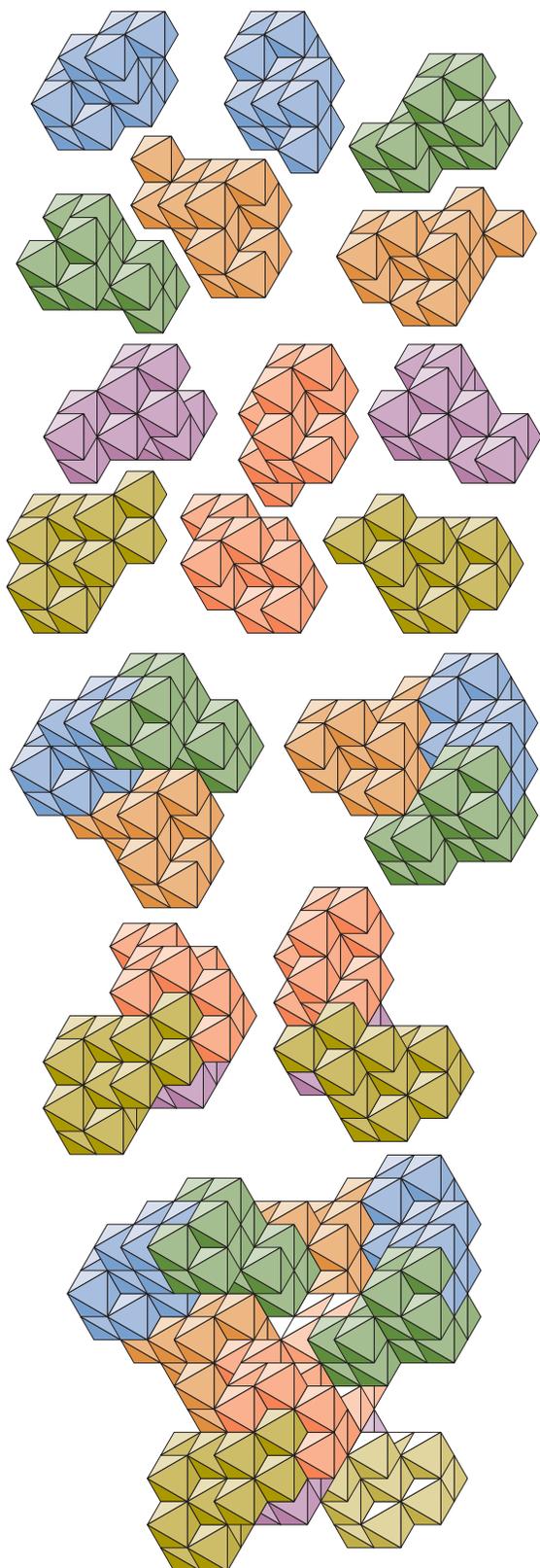
Joins between alpha helices

Alpha helices can join directly in two ways noncoaxial ways. The join between the terminal residues in these cases is either beta90 or beta180. The axes of the joined helices can lie parallel to an edgial plane of the octahedron. This is shown in the diagram below. The lines connecting the vertexes of the red and green octahedra are parallel to the axes of the alpha helices which are in oriented identically to the octahedra which compose the atoms of which the helices are made. The angle between the axes of the helices which are beta90 joined is the same angle as that between the faces of the octahedron at an edge; the angle between the axes of the helices which are beta180 joined is the same angle as that between the faces of the octahedron across a vertex.

At the top of the figure on the right are residues which are beta180 and beta90 joined. Below the two pairs, the three residues in each of the three columns combine to form a turn of alpha helix which appears below them. The turn on the right is combined with either of the two remaining turns in either a beta180 join or a beta90 join. At the bottom, each of the joined helices is extended an additional turn.



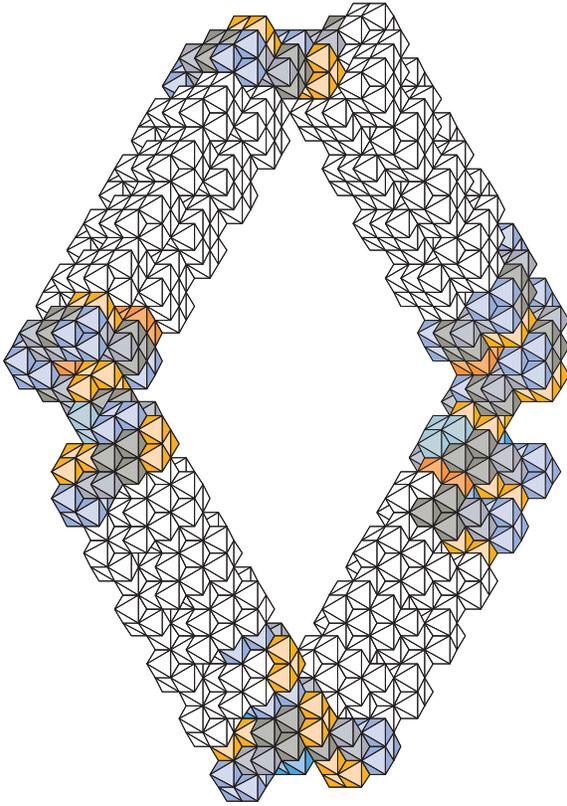
Cyclic Peptide, edgial axis: Four alpha helixes directly joined



Cyclic Peptide, edgial axis: four alpha helixes

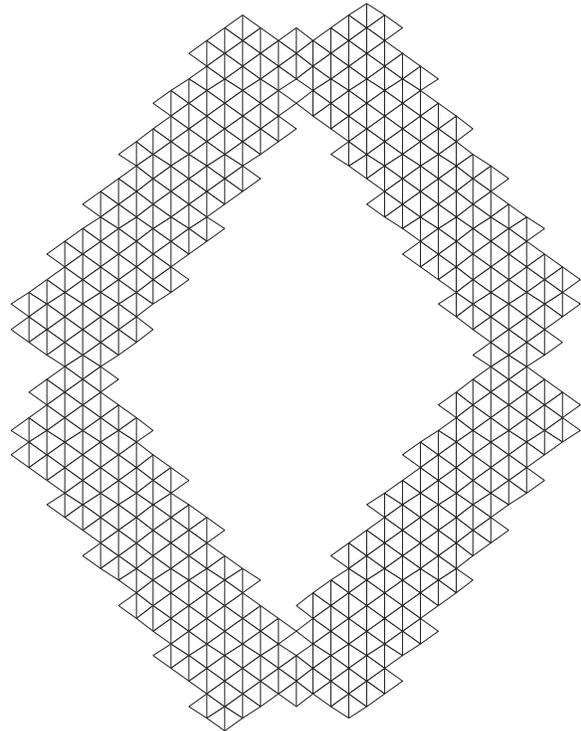
In the figure on the left, the four groups of three main chain units at the top combine to form the four single turns of alpha helix shown in the middle. These are combined to form the cyclic peptide at the bottom.

The assembly is shown at the top on the right colored so as to differentiate the atoms. Just below this figure, the assembly is viewed in a direction normal to the plane of the cyclic peptide.

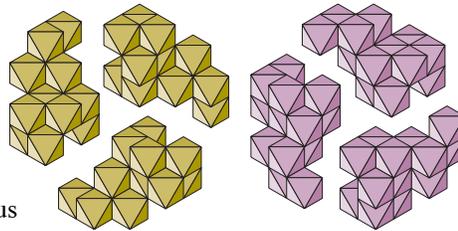


Cyclic Peptide, edgial axised: four alpha helices

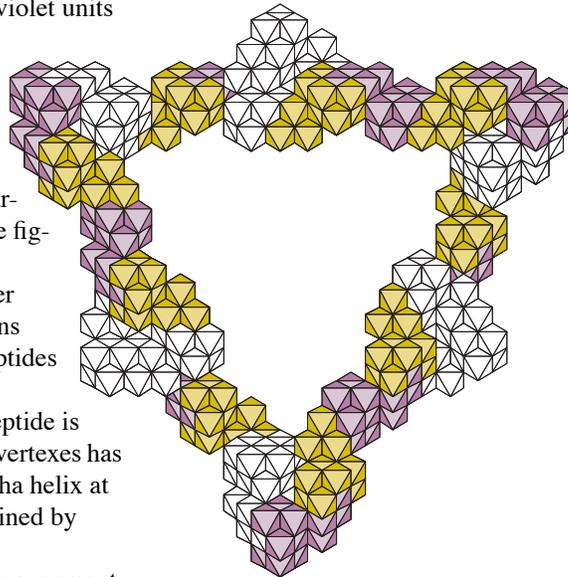
The cyclic peptide depicted here is composed of four alpha helices which are joined the same as the previous cyclic peptide but the helices have been extended several turns. In the view on the left, the atoms of the two turns of each helix which are adjacent to each of the interhelical joins have been colored. The view below is of the same cyclic peptide viewed normally to its plane.



Six alpha helix, facial axis



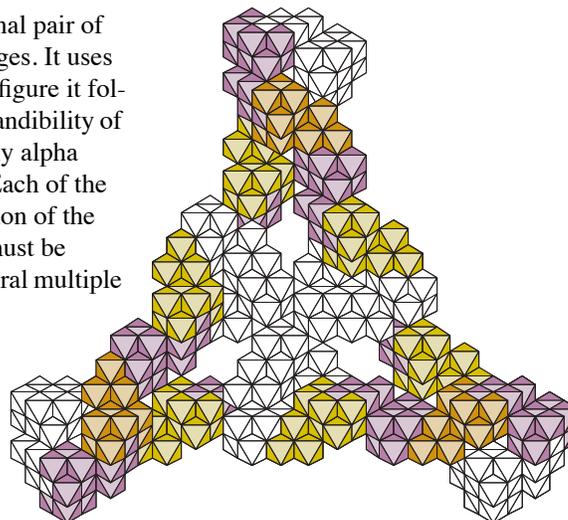
The three yellow units in the previous figure are in the orientations which can produce an alpha helix with its axis parallel to the viewing direction. The three violet units are in orientations which can produce an alpha helix which is inverted relative to that produced by the yellow units. The yellow and purple units can form 32chains whose axes are parallel to the projection plane of the figure. Units having only these orientations and which have either 32chain joins or alpha helical joins combine to produce the cyclic peptides depicted in the next four figures.

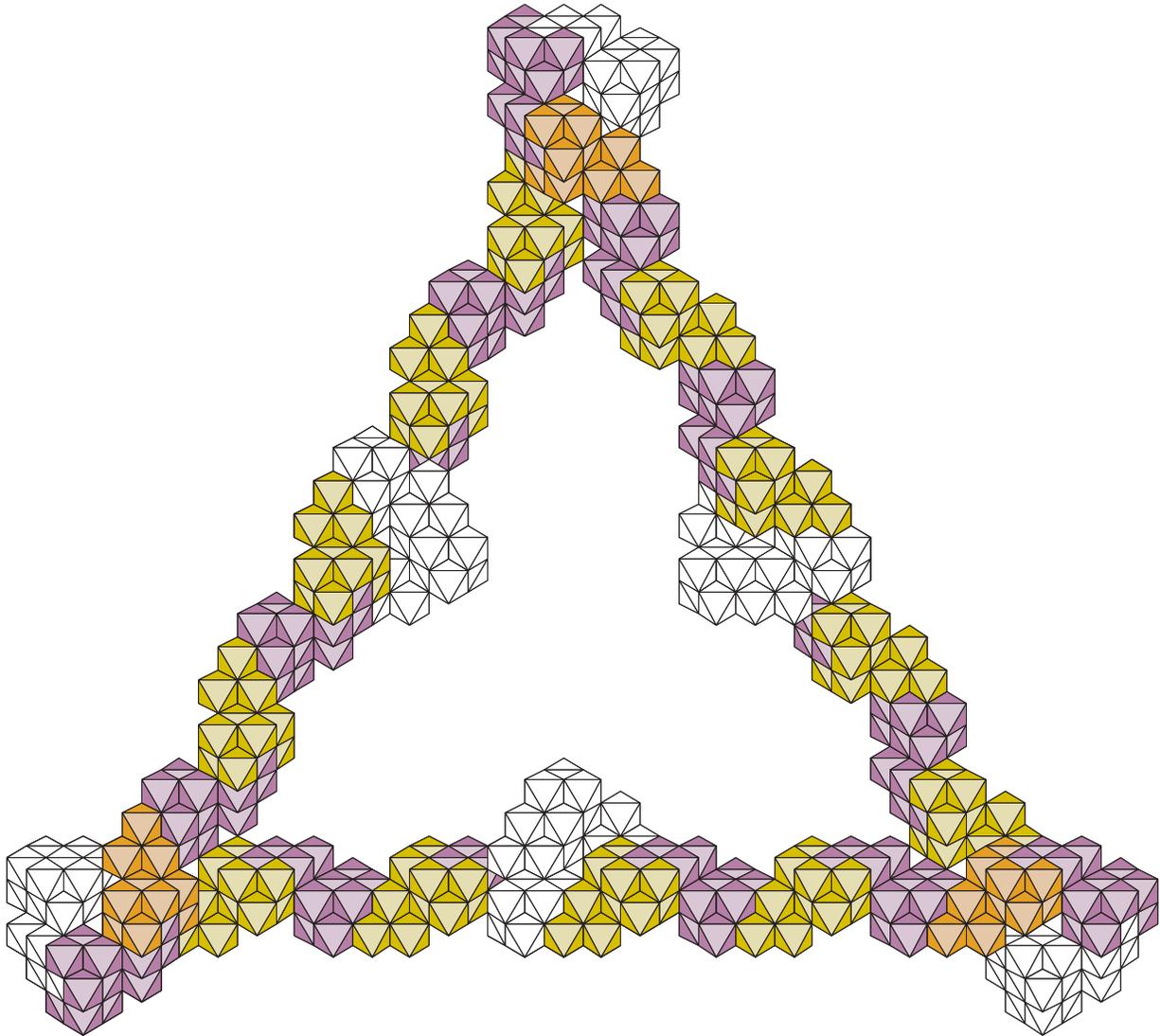


In the next figure, the cyclic peptide is triangular. Each of the triangular vertexes has an alpha helix and there is an alpha helix at each midedge. The helices are joined by 32chains.

The next figure has the same arrangement of alpha helices as the previous. The 32chains have been extended.

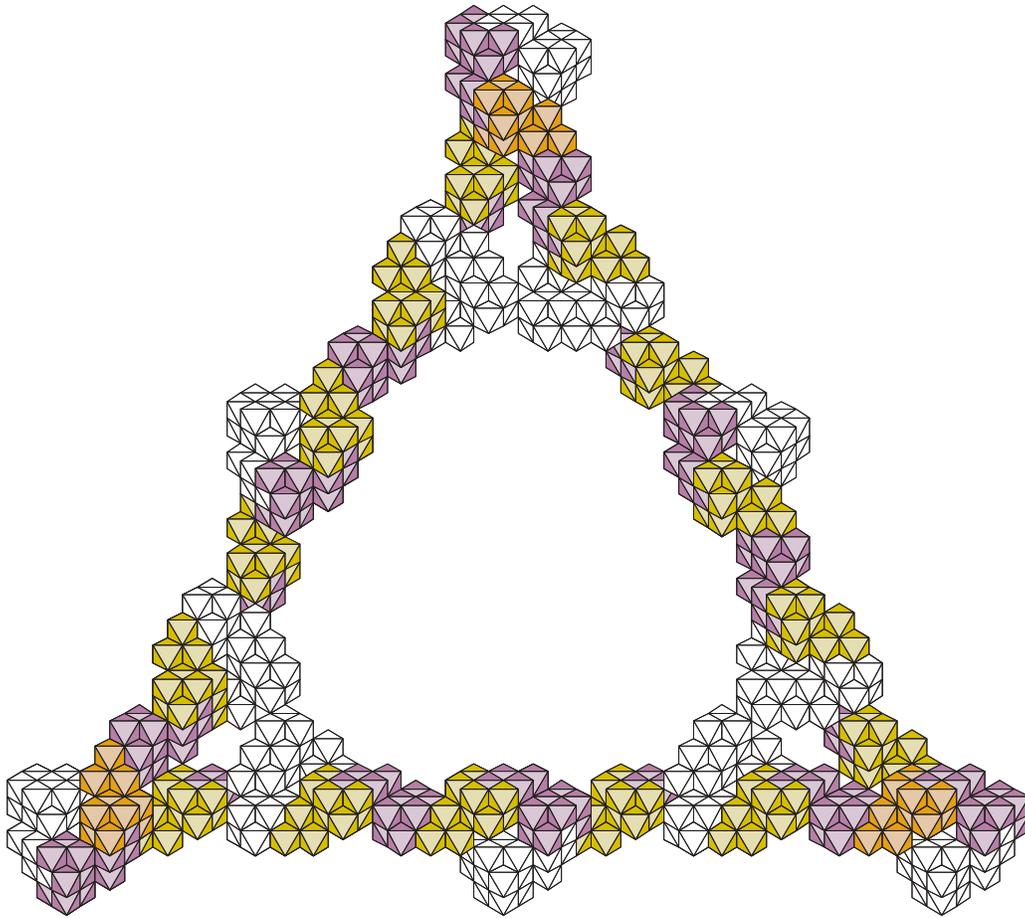
The last figure adds an additional pair of alpha helices each of its three edges. It uses the same vertexial helices as the figure it follows. These figures show the expandibility of the cyclic peptides which use only alpha helices connected by 32chains. Each of the figures is extensible in the direction of the axes of the alpha helices. Each must be extended by a full turn or an integral multiple thereof.





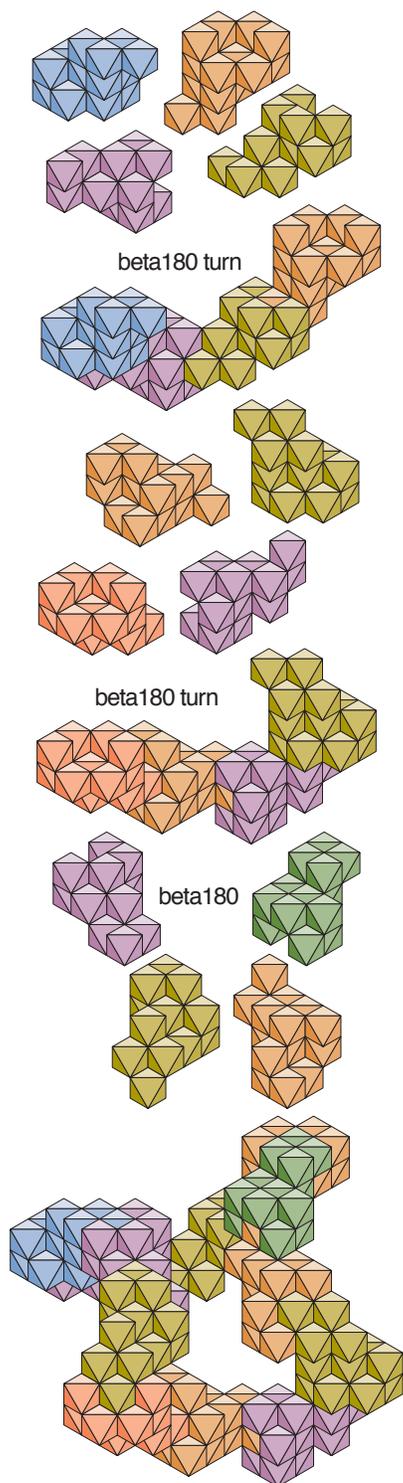
Cyclic peptide: six alpha helices

Twelve helix, facial axis



Cyclic peptide: twelve alpha helices

Cyclic peptide, sheet forming.



Cyclic peptide, sheet forming

This ring incorporates a pair of antiparallel beta180 chains whose separation is sufficient to accommodate a third beta180 chain to form a pleated sheet. At the top of the figure is a group of four units which combine to form the beta180 turn just below them. This is followed by a second group of units which form a second beta180 turn. Beneath the second turn are two groups of two units each which form the links between the two turns. The combined assembly is at the bottom of the figure.

See "Cyclic peptide sheet joined with beta chain" on page 327

