

Protein files excerpted from Octahedron1stEd.pdf

Robert William Whitby

4 July 2004

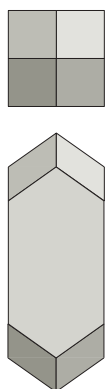
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PROTEIN

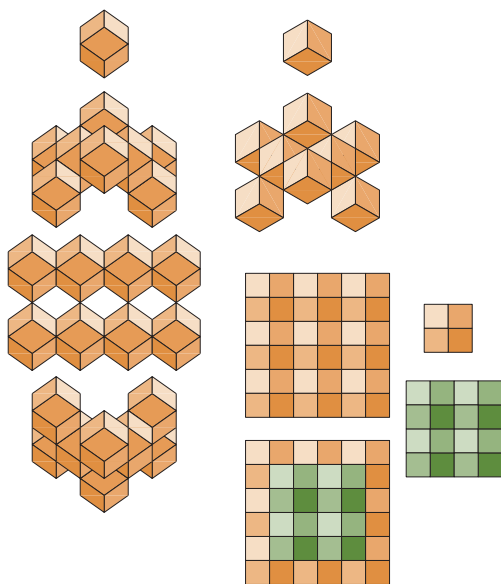
Crystalline form¹ of cytochrome

1. A. L. Lehninger, *Biochemistry* 2d ed., Worth, 1975, <Figure 3-1 Crystals of horse cytochrome C>, p. 57



Cytochrome crystalline form.

The top view is along the fourfold axis. The bottom view is of a prism face and is normal to the fourfold axis. The crystalline form is that of a rhombic dodecahedron which is elongated along a fourfold axis. Each face of the crystal is defined by octahedral edges.

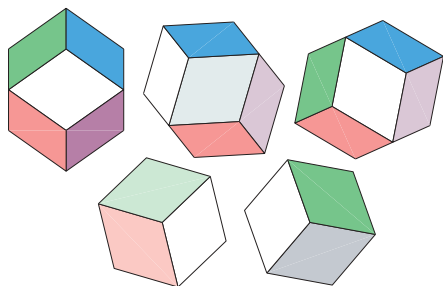


The cytochrome crystal can be formed of identical rhombic dodecahedral units. The left column show three assemblies of rhombic dodecahedra. The first assembly defines the two pyramidal faces of the crystal shown at the top of the facial view of the crystal form in the previous figure. To its right the same assembly is shown in an orientation which is rotated slightly. The second assembly shows the arrangement of the rhombic dodecahedra which define the prism plane of the crystal. The bottom assembly defines the two faces of the pyramid which are visible at the bottom of the facial view.

The relationship of the rhombic dodecahedra normal to the fourfold axis is shown in the lower right. The first layer is a three by three square. The second layer is a two by two square. The positions of the dodecahedra in alternate layers differ by an a translation in the fourfold axial direction..

Crystalline form of neuraminidase

A photograph of neuraminidase crystals obtained from an influenza virus shows that their common form is that of the rhombic dodecahedron.¹ The prominence of the rhombic dodecahedra suggests a CFU of the same shape.



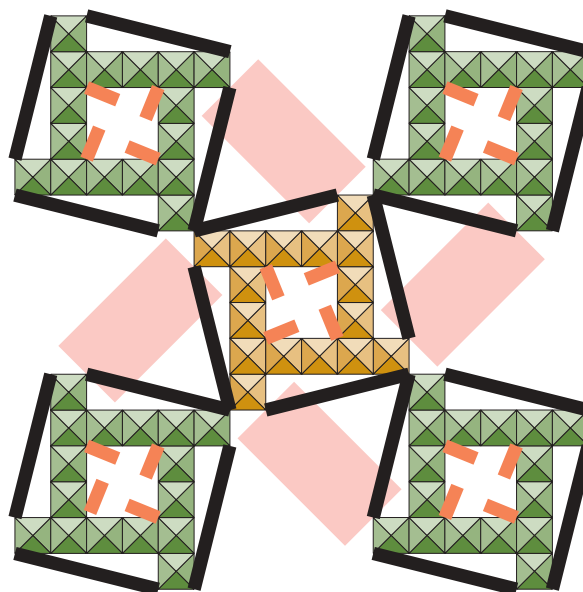
Neuraminidase crystals.

Rhombic dodecahedral forms in orientations suggested by a photograph of neuraminidase crystals. The top row shows three units in facial view which differ by a rotation about the viewing axis. The bottom row shows two units in threefold-axial view which differ by a rotation about the viewing direction.

Myelin protein P₀

A computer-generated image of crystals of myelin protein P₀ suggests the structure shown

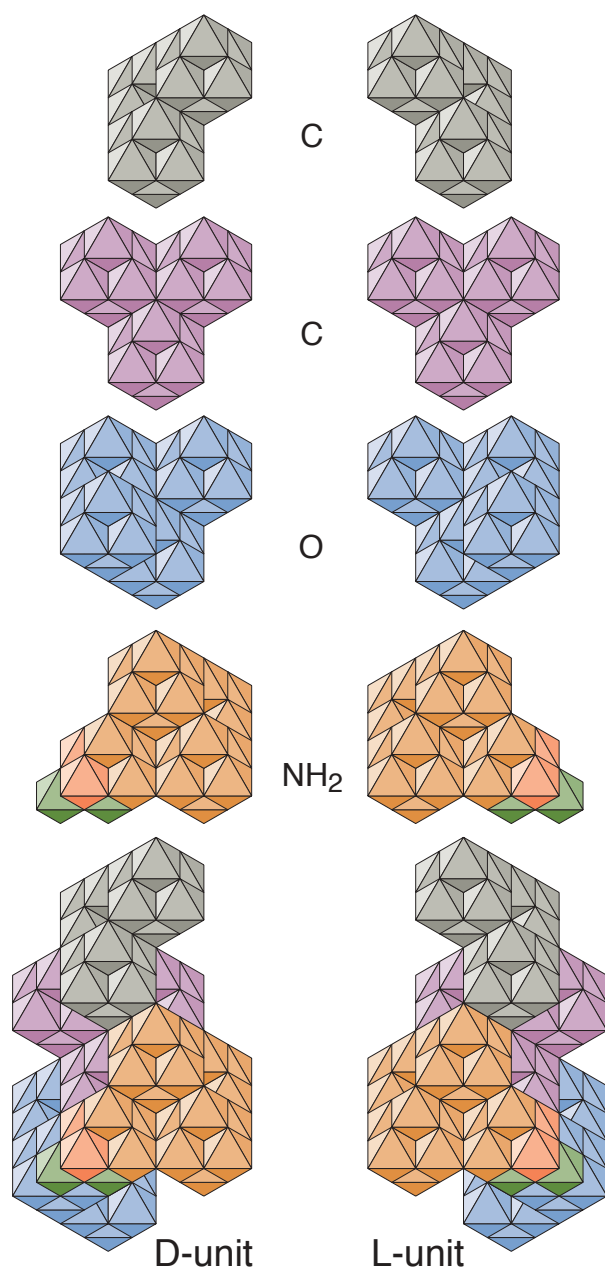
schematically in the figure. The heavy black



borders represent the boundaries of the squares delineated by what appear to be protein strands. The broad pink bands represent the parallel strands which link the central square to the outer squares. The short red lengths within the square represent the four chains which extend from the square periphery into the square area in each of the square formations. These chains and the angular relationships between the square units show that the central unit is equivalent to the four outer units except that it is inverted. The whole pattern is consistent with a vertexial projection of the regular octahedron. The octahedral assemblies in each of the squares are a minimum representation of how the sides of the squares are defined. Each broad black line is defined by a vertex of two octahedra. The borders of the four pink bands are parallel to the two vertexial diameters of the regular octahedron in the viewing plane.

1. W. Graeme Laver *et al*, Disarming Flu Viruses, *SciAm* Jan 1999, pp. 78-87. See the photograph of the rhombic dodecahedral crystals on page 82.

AMINO

**Amino main chain unit.**

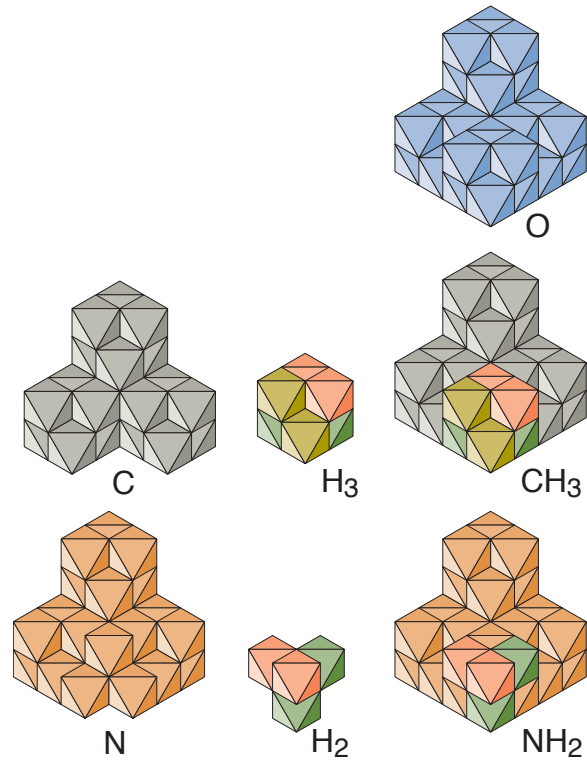
The figure depicts the assemblies of the main chain portions of both D- and L- units. The D-unit is on the left and the L- unit is on the right.

Amino acids

The forms of the amino acids are determined by the forms of the atoms and the joins between them. The principal substructures of the proteins are defined by the backbone or mainchain conformation. An examination of the alpha helix, the epsilon helix, the pleated sheets, and the beta annulus, reveals that there is an association of two C-atoms and an NH₂O group which is invariant in each of the structures. It is this invariant unit in regular association with identical units which defines the structures. This invariant unit is the base for the side chains which define each of the amino acids in the form in which it is a link in the main chain of a protein. This invariant unit is inflexible, it is rigid, it has no hinges, it has no swivels. The NH₂ group has the form of an O-atom and the NH₂O portion is essentially a "socket" for the He-octa "ball" of the carbonyl C-atom. Each of the residues in each of the structures has an NH₂O group in identical orientation with a pair of lefthandedly cleftly joined C-atoms.

In the aminos depicted below, each of the N-atoms has been depicted as an O-atom, as if each was an NH₂ group. This is because the sidechains of asparagine and glutamine terminate with an NH₂O group which suggests that each of these side chains can make the same kind of join as exists between the main chain units. Each of these two residues could link directly with a C-atom terminus of alanine, valine, isoleucine, leucine, proline, tryptophan, or phenylalanine. Aspartic acid and glutamic acid terminate with an OO-group that could make a similar join with an NH₂-group of lysine, arginine, tryptophan, or histidine.

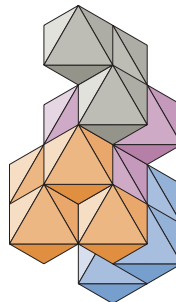
Since it is expected that the OO-group will combine so that an O-atom is replaced by an NH₂ of another sidechain, only one O-atom is



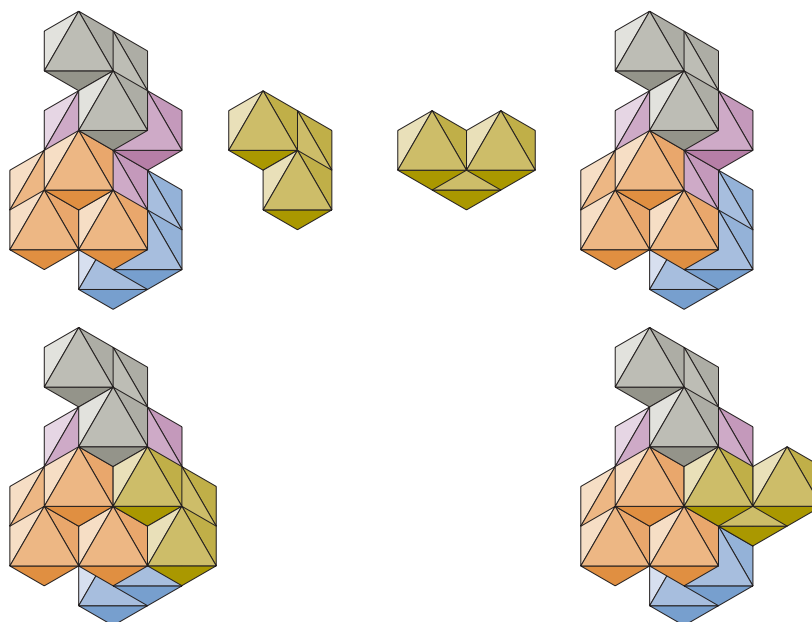
O-atom homomorphs.

The assemblies are shown on the right
and their constituents are to their left,

Glycine.



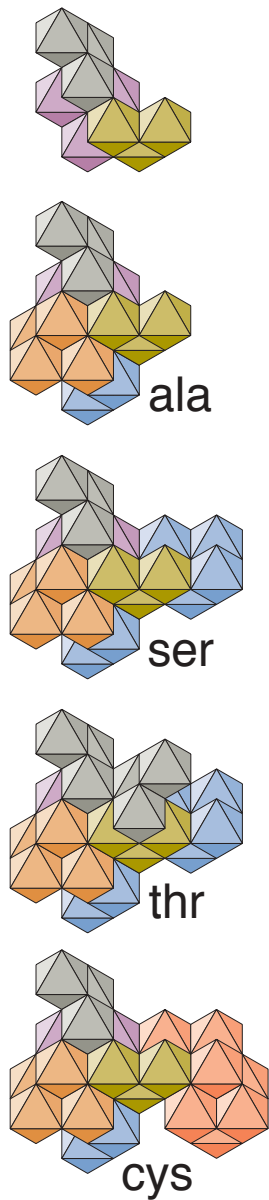
C₃ family of aminos.



The first C-atom of the side chain.

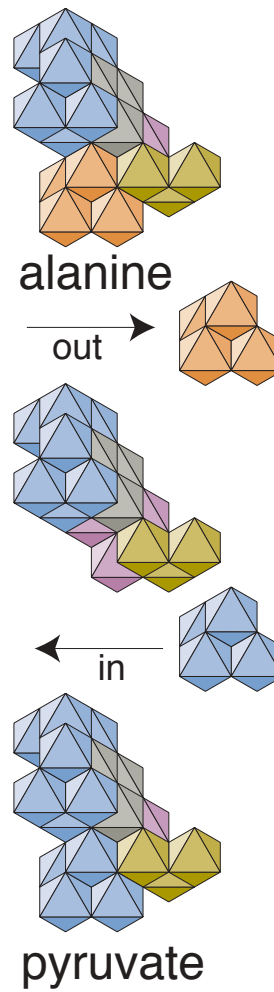
The figure depicts the only two possible assemblies of a C-atom and a main chain unit. In the top row are two main chain units with two C-atoms between. The C-atom on the left is oriented so as to make a right-hand join with the alpha C-atom of the main chain unit. The C-atom on the right is oriented for making a left-hand join. The completed assemblies are shown in the bottom row. The C-atom joined right-handedly to the alpha C-atom abuts the NH₂-group so that it cannot make a join with another atom. The C-atom that is left-handedly joined has two clefts available for joining with other atoms. The latter, then, is the manner in which a third C-atom is added to the amino acid.

The C₃ aminos ready for chaining.



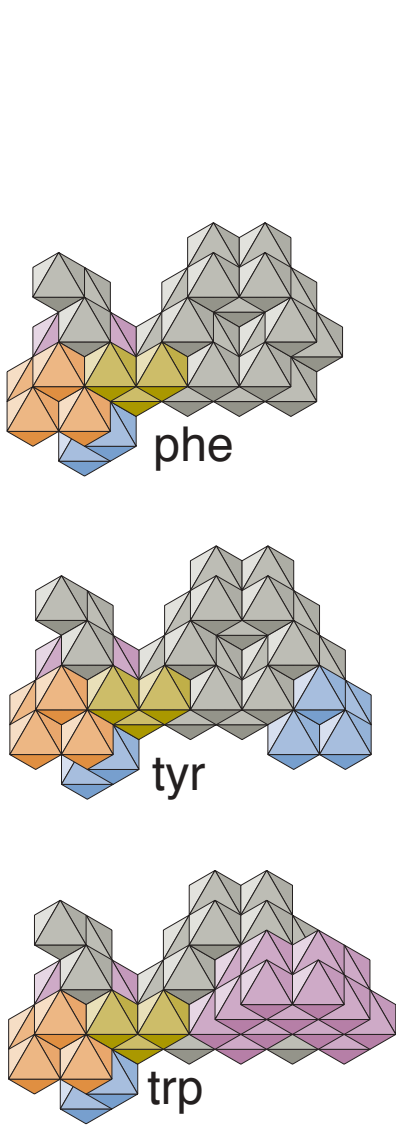
C₃ family of aminos.

Conversion of alanine to pyruvate

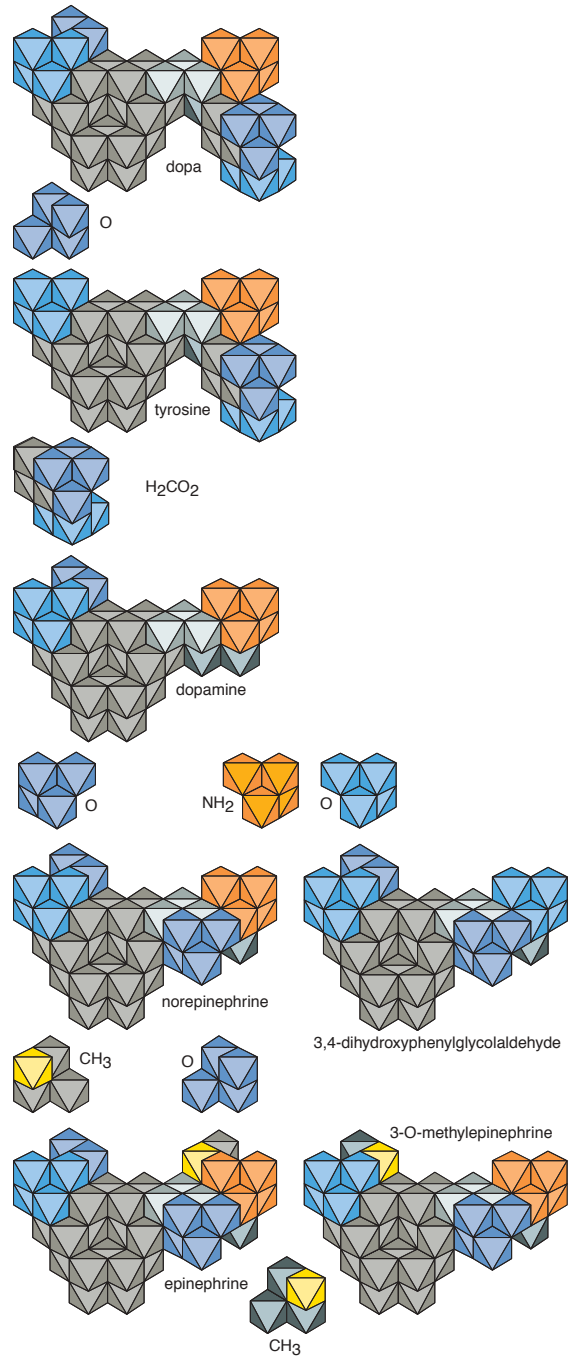


Alanine to pyruvate.
 Alanine conversion involves removal of the NH₂ group and replacement with an O-atom.

Aromatic aminos

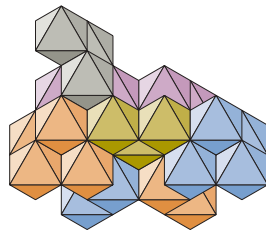
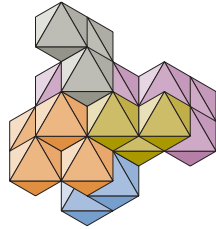
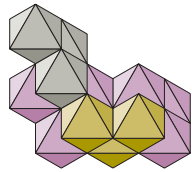


Aromatic aminos.



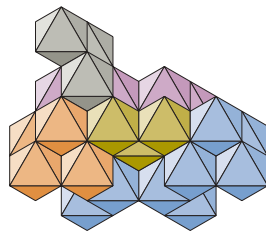
Pathway: Tyrosine and the catecholamine neurotransmitters.

C₄ family of aminos

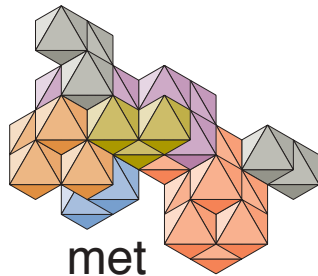


asn

C₄ family of aminos.



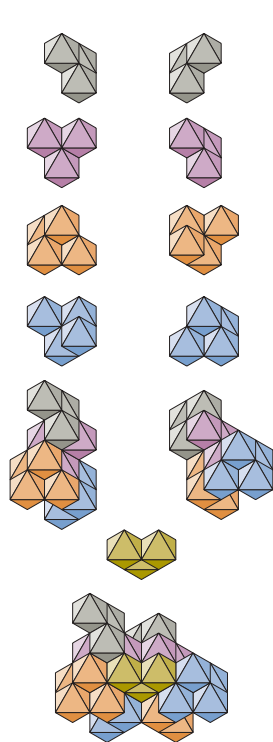
asp



met

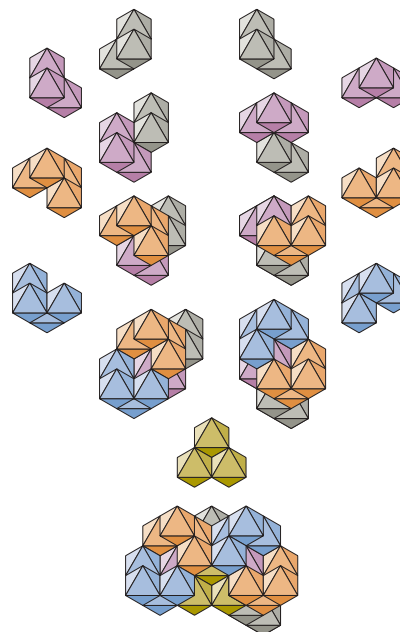
C₅ family of aminos.

The relationship between the five C-atoms of the amino acids of the C₅ family is established by the conversion of histidine to glutamine. The conversion results in the main chain group shifting from one end of the five C-atom chain to the other. That fixes the conformation of the chain as that between two main chain groups sharing a common C-atom side chain.



Histidine to glutamate.

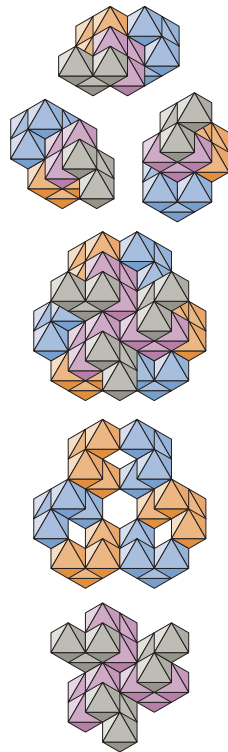
The conversion of histidine to glutamate shows the five C-atoms which the two have in common must be in the configuration of two main chain units sharing a single C-atom side chain. The figure shows the assembly of each of the main chain units in the left and right columns and their linkage by the C-atom at the bottom.



Two main chain units linked by a C-atom.

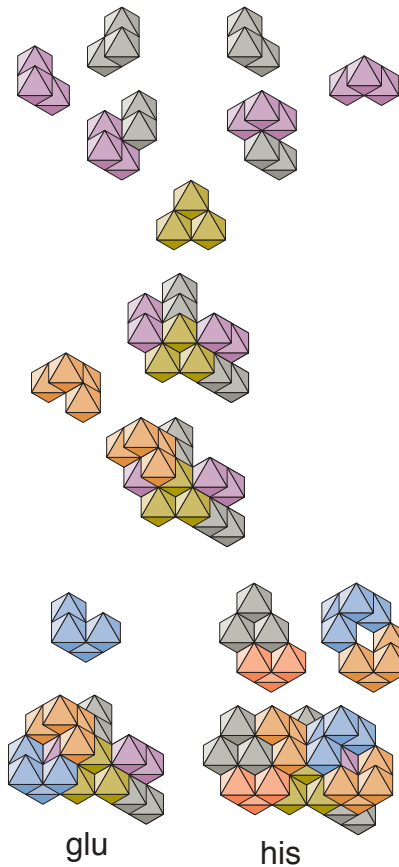
Two main chain units are assembled at the top and then joined together by a C-atom at the bottom. This is the relationship suggested by the conversion of histidine into glutamate.

Relationship of histidine and glutamate



Three main chain units in epsilon helical orientations.

At the top of the figure, the three main chain units are depicted separately. Each differs from its two circumferential neighbors by a 120° rotation about the viewing direction. The three are shown as joined in the next view. The next to last depiction is of the NH_2O groups of the three units and the bottom depiction is of the C-atoms of the three units.

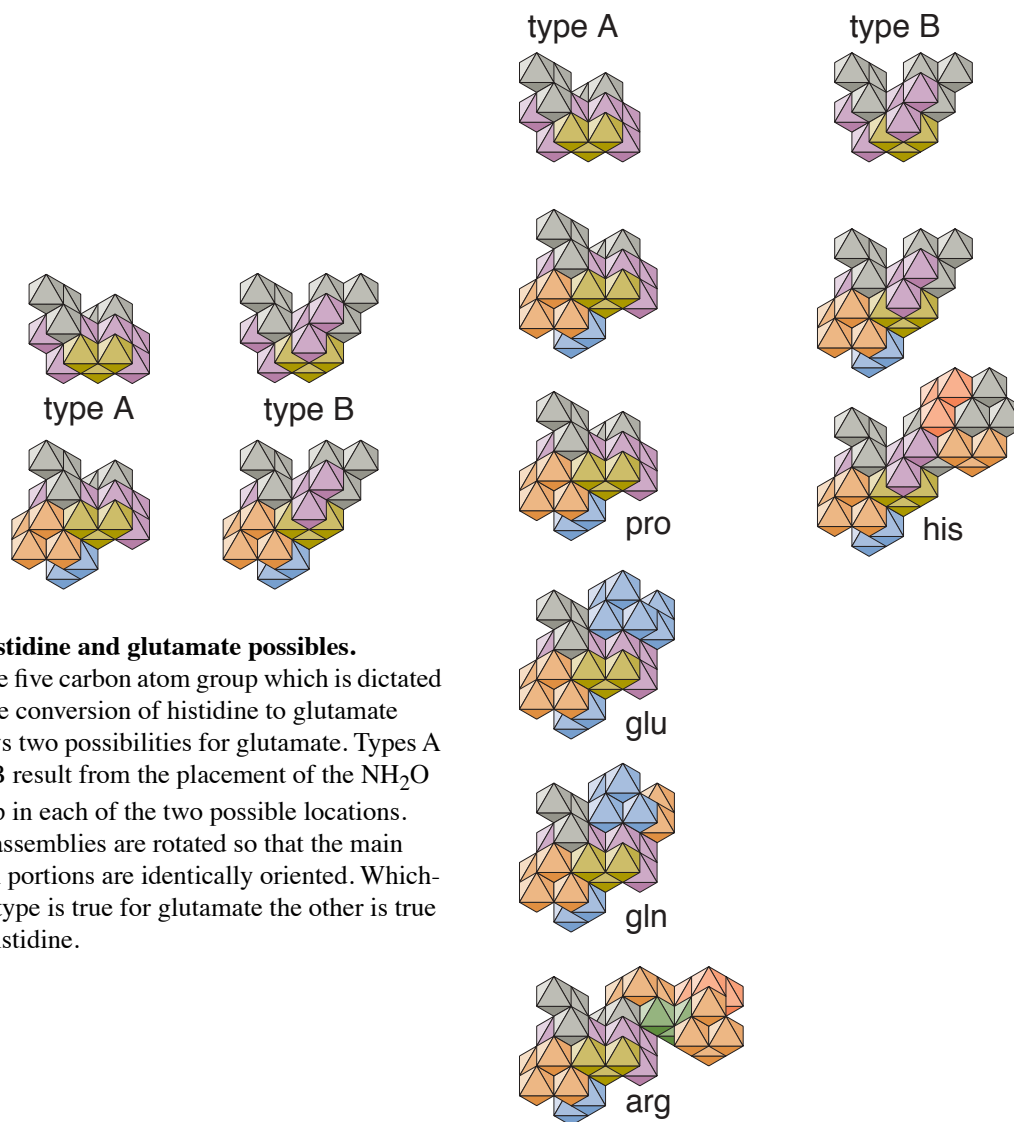


Assembling glutamate and histidine.

At the top, two identical pairs of C-atoms are formed which differ by a rotation of 120° about the viewing direction. The pairs are then joined by another C-atom to make the five C-atom group common to glutamate and histidine. An NH_2 group is then added and this assembly provides the base for the two aminos.

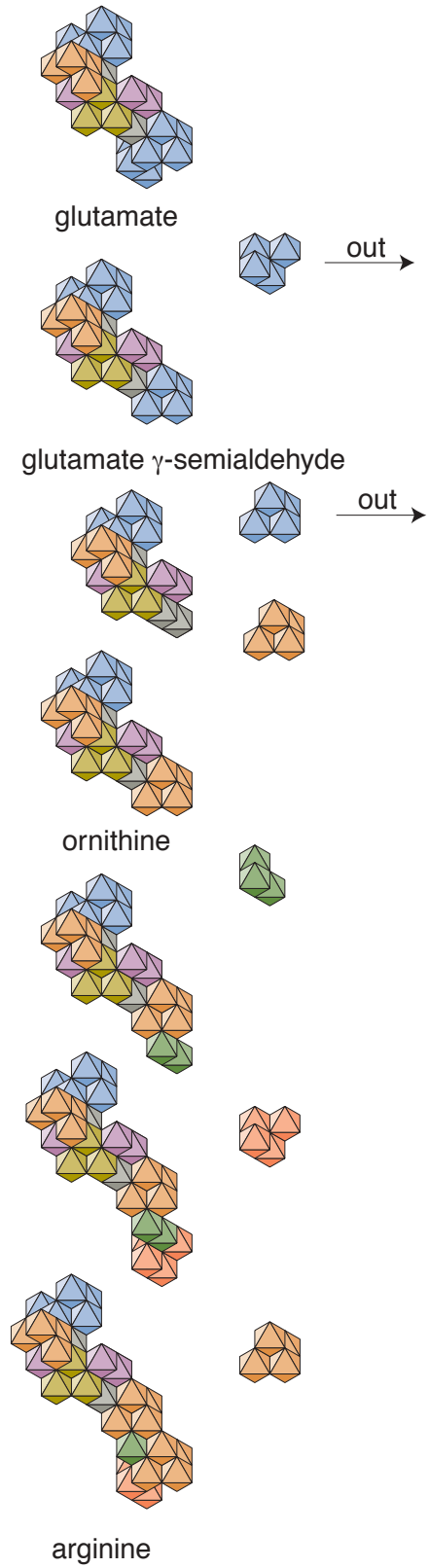
An O-atom addition provides a glutamate assembly shown at the bottom on the left.

An addition of a CNH_2 group and an NH_2O group to the base produces a histidine assembly at the bottom on the right.

C₅ family of aminos**Histidine and glutamate possibles.**

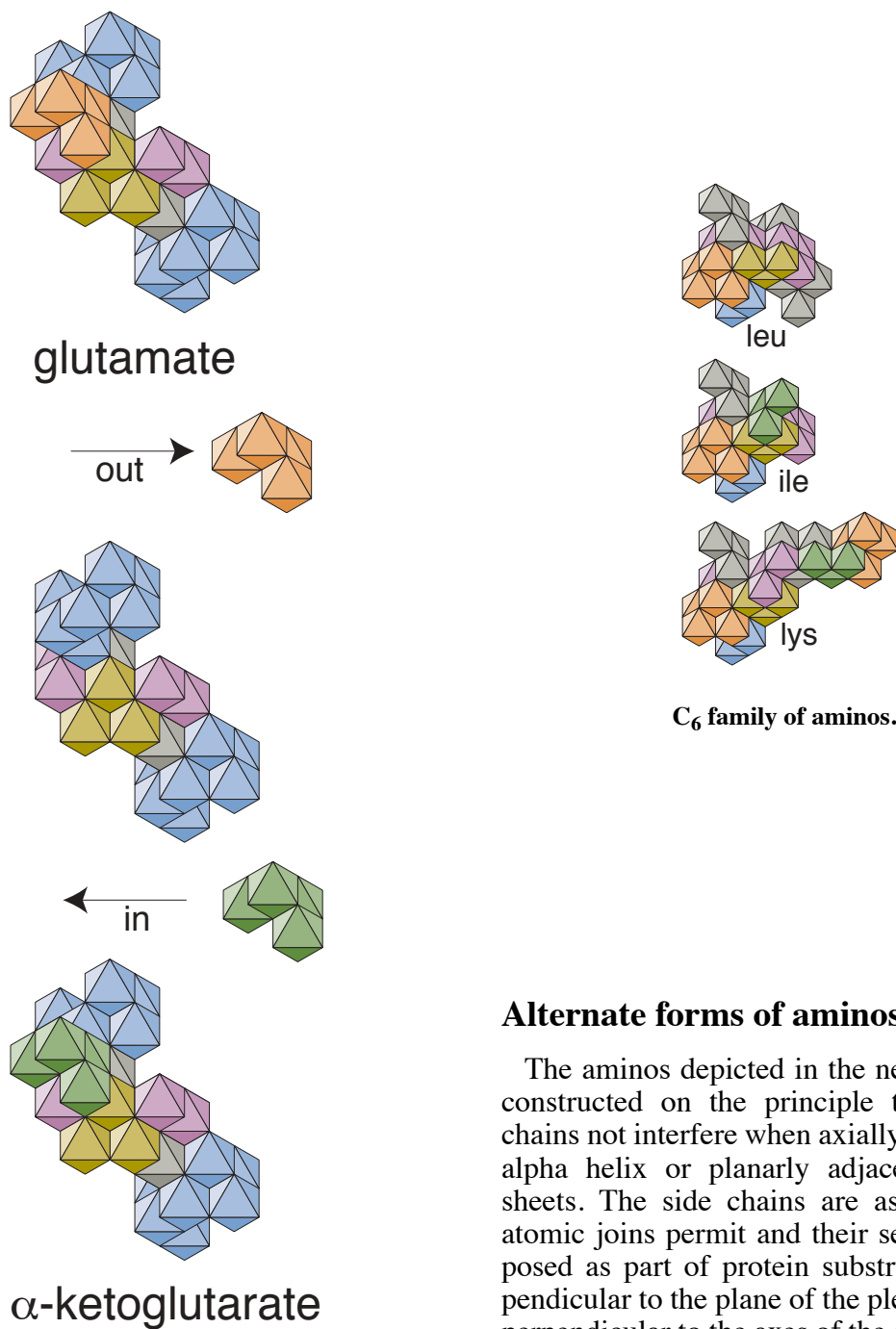
The five carbon atom group which is dictated by the conversion of histidine to glutamate allows two possibilities for glutamate. Types A and B result from the placement of the NH₂O group in each of the two possible locations. The assemblies are rotated so that the main chain portions are identically oriented. Whichever type is true for glutamate the other is true for histidine.

C₅ family of aminos.



Pathway: Glutamate to arginine

C₆ family of aminos



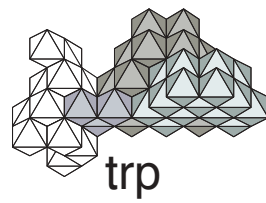
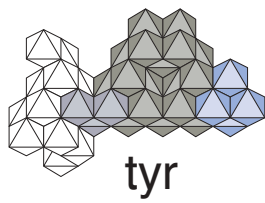
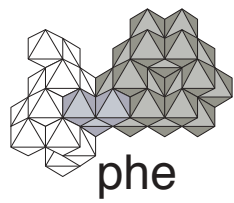
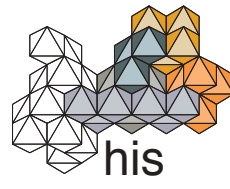
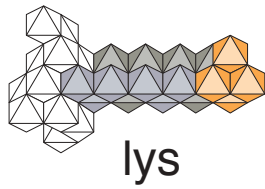
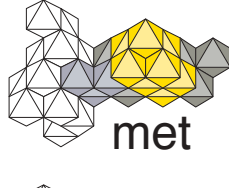
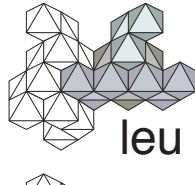
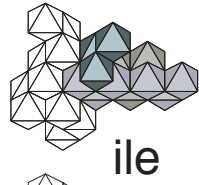
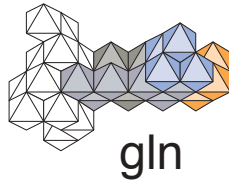
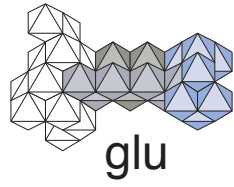
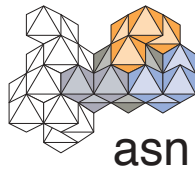
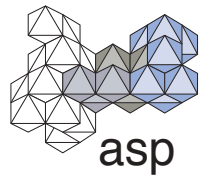
Glutamate to α -ketoglutarate.

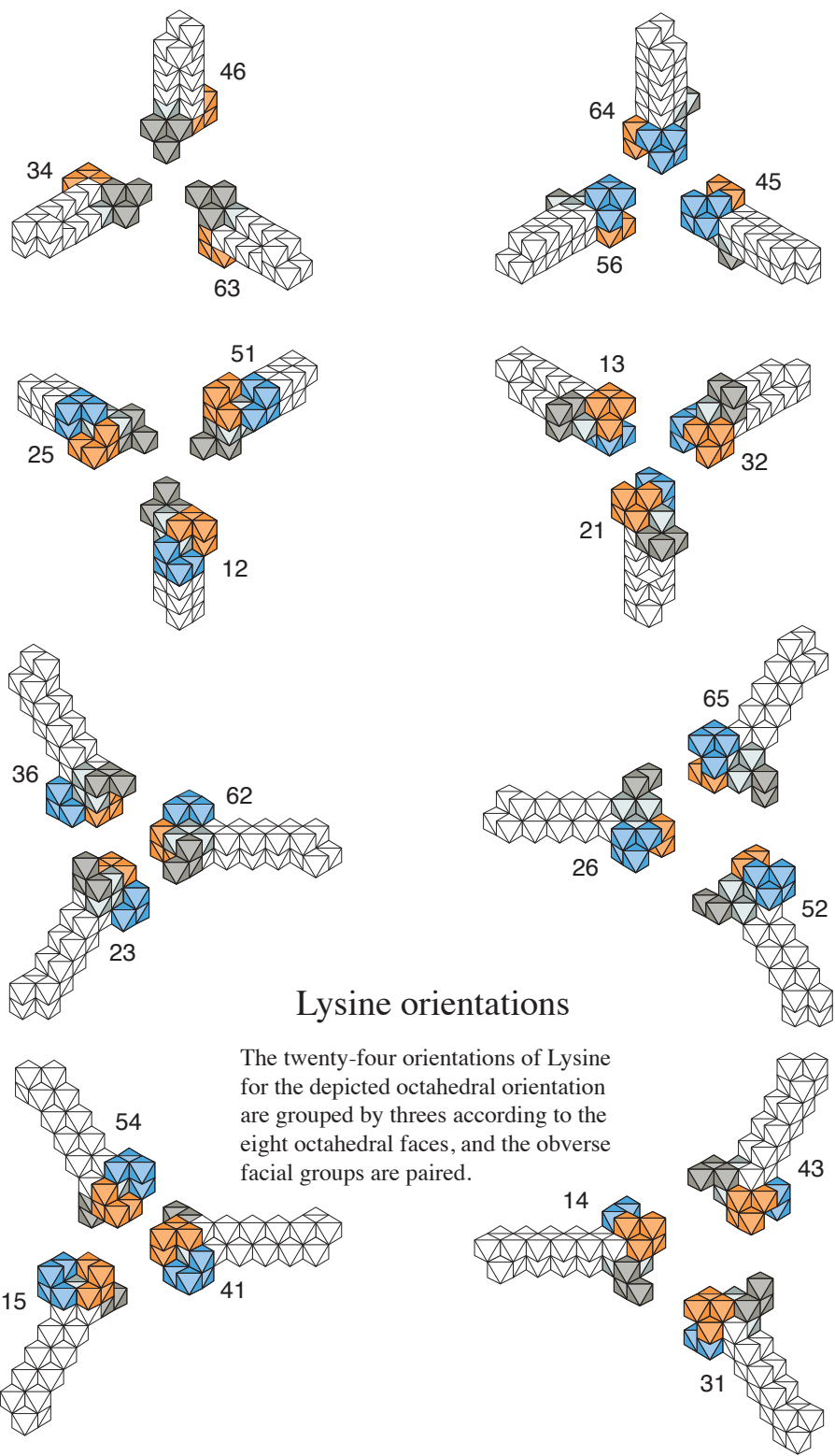
The figure shows the removal of an NH₂ group from glutamate and its replacement with an O atom.

Alternate forms of aminos

The aminos depicted in the next figure were constructed on the principle that their side chains not interfere when axially adjacent in an alpha helix or planarly adjacent in pleated sheets. The side chains are as linear as the atomic joins permit and their sense when disposed as part of protein substructures is perpendicular to the plane of the pleated sheet and perpendicular to the axes of the alpha and epsilon helices.

The lysine of this group is shown in each of the twenty-four possible orientations which are possible in a simple protein which is viewed perpendicularly to a face of the octahedron. Lysine was chosen from this group of aminos because of its long straight C-atom chain.





PROTEIN CHAIN

The main chain unit

A He-octa of a C-atom of one main chain unit fits into a space in the NH₂O group of an adjoining unit like a ball into a socket to form a protein chain. There are six such joins for a pair of main chain units. In each of the six joinings, the He-octas of each of the atoms of the pair are in identical orientation. If units are repetitively added to form a chain by using just one of the six joins the resulting form will be an alpha-helix or an epsilon-helix or a 1/2-turn-beta chain or a 1/4-turn-beta chain or a 3/2-chain, or a 4-helix. The six joins are depicted in the next figure. The adding unit is shown on the right and the joined pair is shown on the left. In each pairing, the first unit of each of the pairs is in the same orientation as shown in the previous figure. It is uncolored in each of the joined pairs. The adding unit is joined to the female end of the first unit.

No change in the atomic arrangement of the main chain unit is required to produce these joins. If the relationship of any part of a crys-

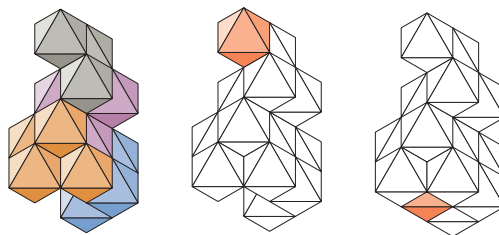
talline group relative to the remaining portion group is altered, the group is no longer the same entity. Any change in the main chain unit precludes its use in the structures.

Peptide joins

Each of the joins between peptides in a chain, excepting perhaps proline, when the chain is stably and crystallinely folded, requires a rotation between adjoining units which produces a helix.

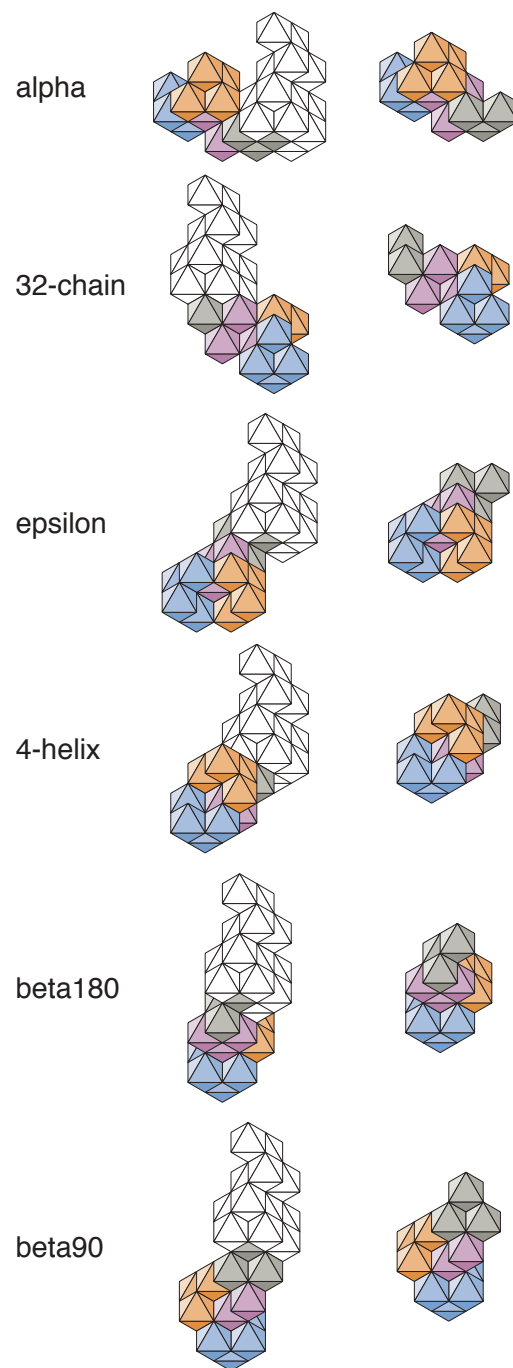
Table 15: Peptide chain joins

Join	Axis	Rotation	Occurrence
beta180	vertexial	half	pleated sheets
beta90		quarter	
4helix		quarter	beta annulus
3/2chain	edgial	half	
alpha	facial	third	alpha helix
epsilon		third	epsilon helix



Amino joining octa.

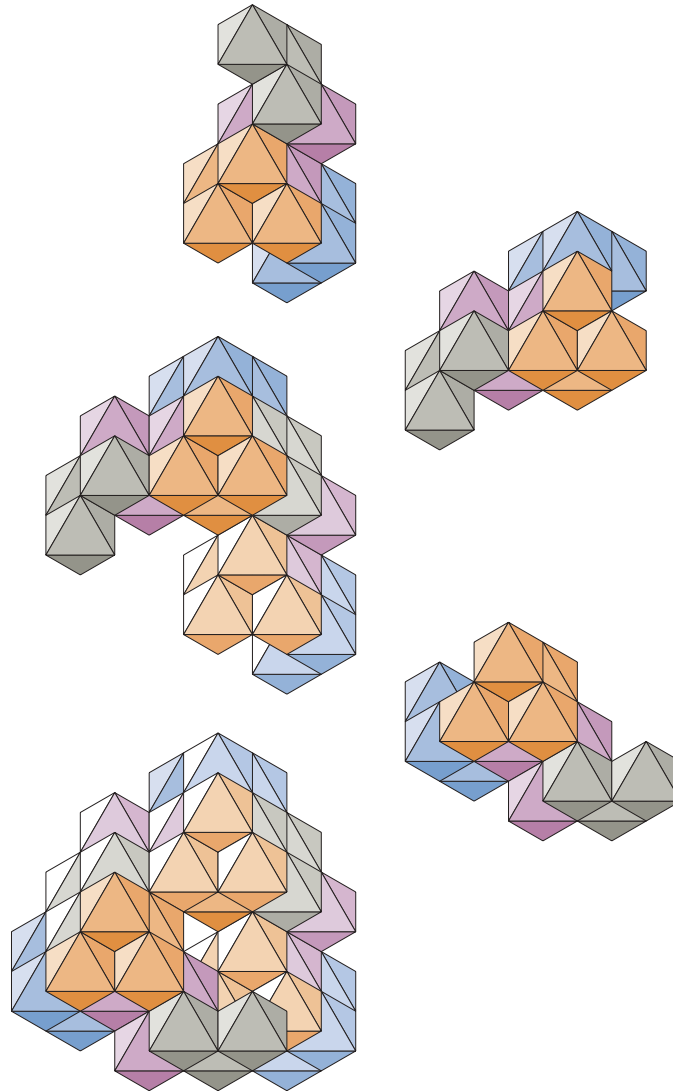
The drawing on the left is the main chain portion of an amino acid. The middle drawing shows the joining octa colored red. The right hand drawing shows a joining octa occupying the socket formed by the NH₂O group.



Amino main chain joins.

The figure depicts the six ways that two main chain units can join. The pairs are shown on the left and the joining units are shown on the right. The base unit is uncolored and is in the same orientation in each of the pairings.

Alpha helix

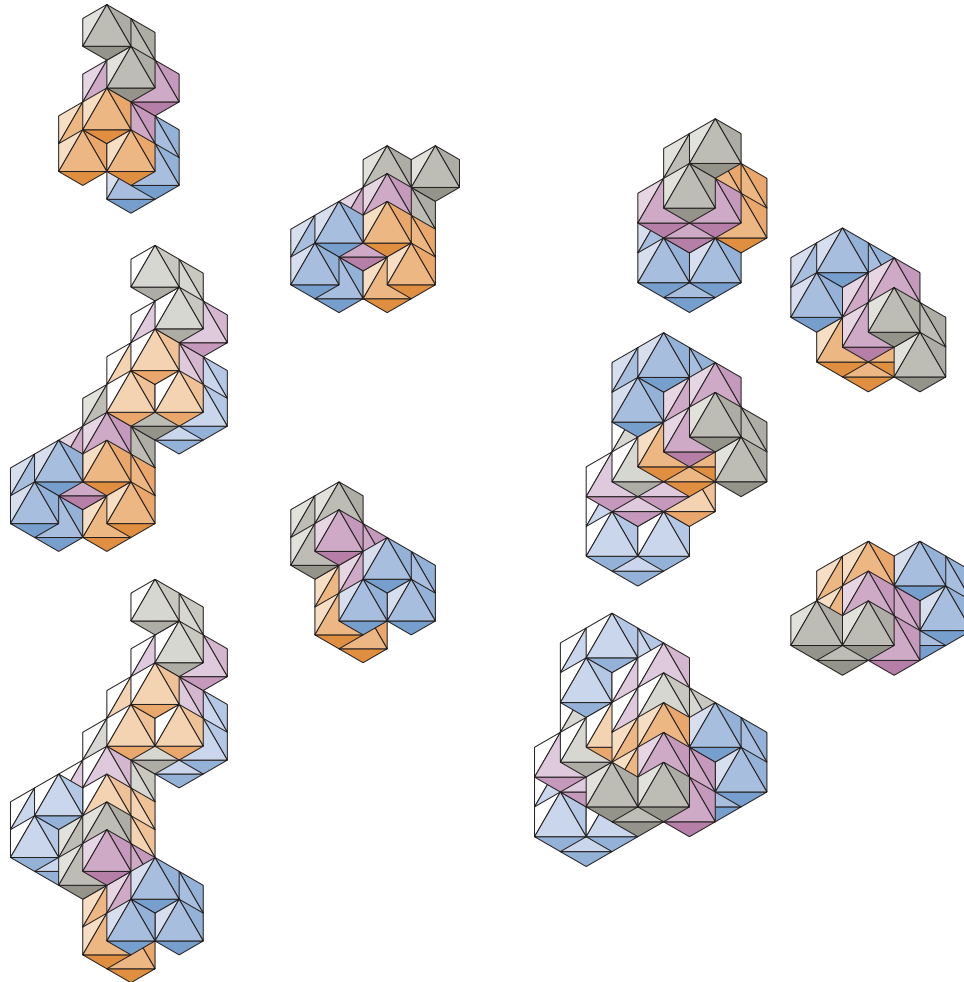


Protein substructure: Alpha helix.

The assembly of one turn of an alpha helix is depicted in the figure. The growth direction is towards the viewer and in a counter-clockwise sense. The units are added to the male end of the growing helix.

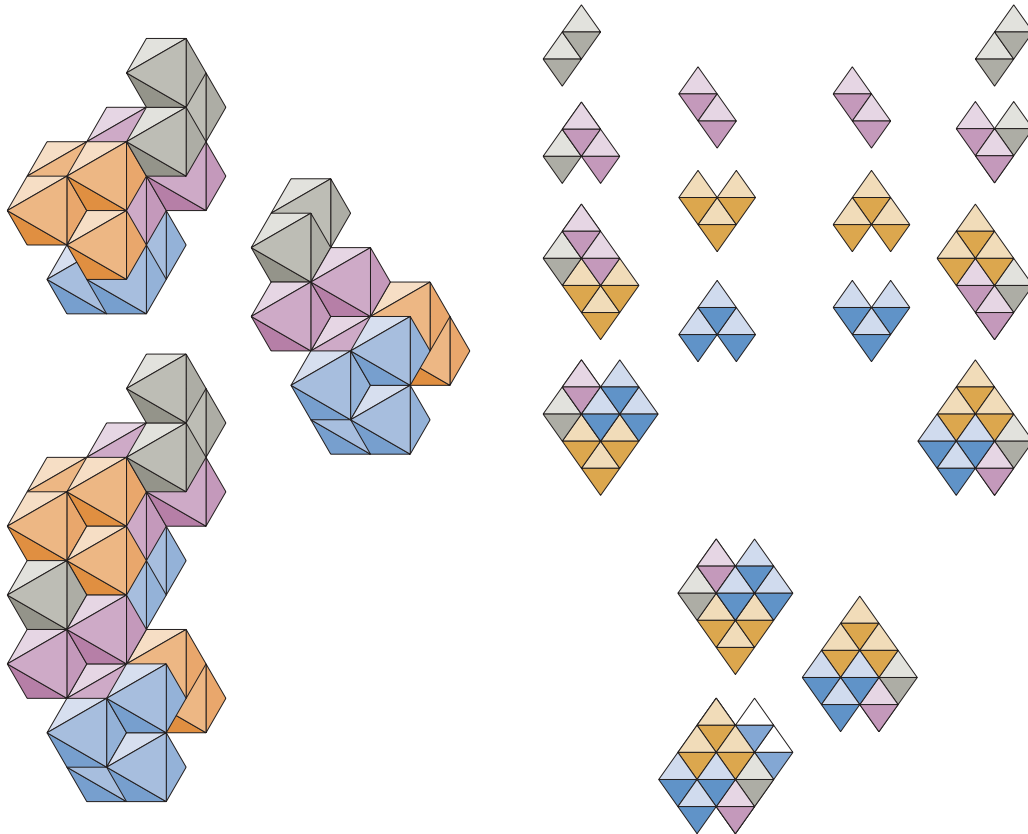
Adjoining units differ by a rotation of 120° about the helical axis.

Epsilon helix



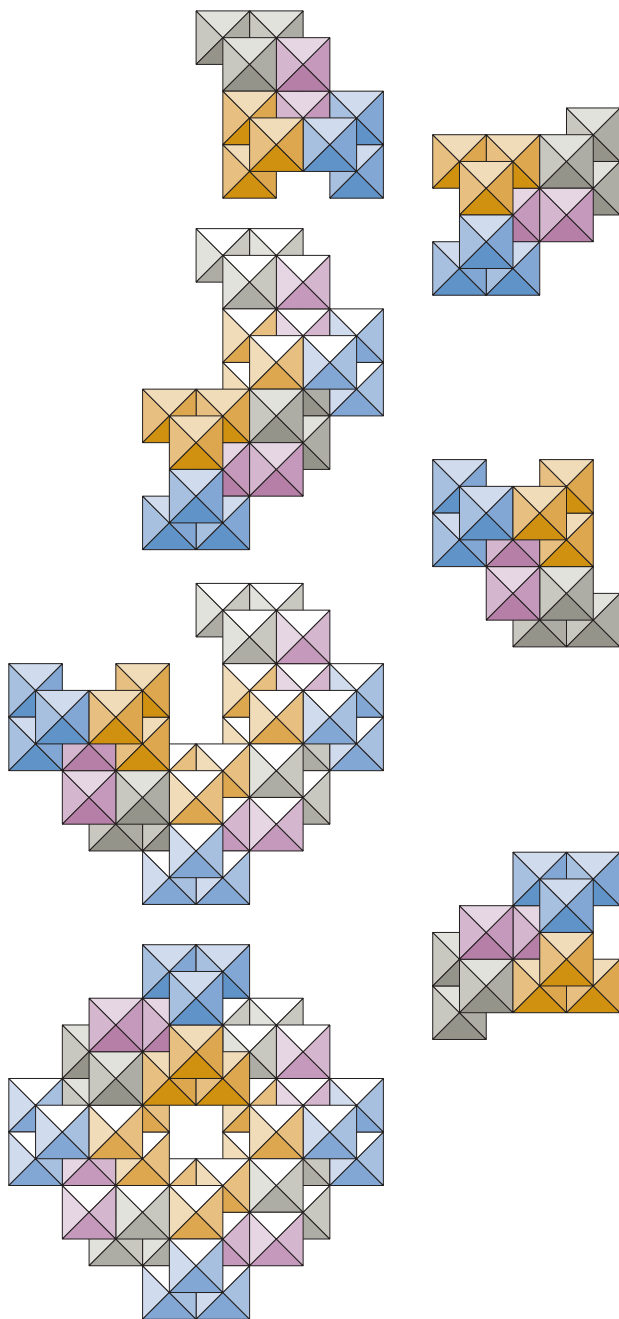
Protein substructure: Epsilon helix

The assembly of one turn of an epsilon helix is shown in the figure on the left. The growth direction is towards the bottom of the page and obliquely towards the viewer. Adjoining units differ by a rotation of 120° about the helical axis. The figure on the right shows the assembly of an epsilon helical turn as viewed along the helical axis from the male terminus.

32chain**Protein substructure: 32chain**

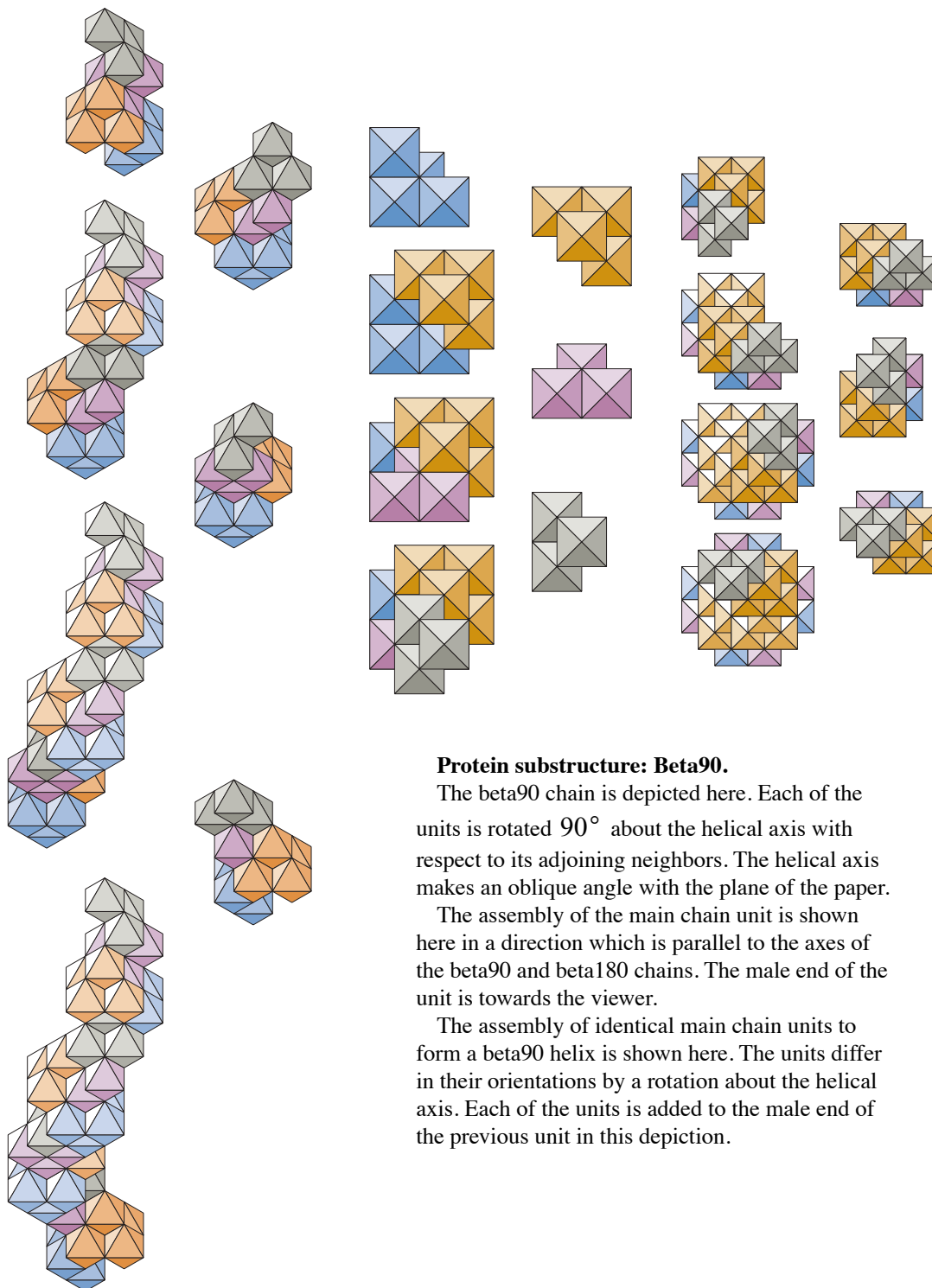
The figure on the left shows the assembly of the 32-chain. The repeat unit consists of two main chain units which are rotated 180° relative to each other about the chain axis. The axis is parallel to the plane of the paper.

The edge views on the right show the assembly of the residues and their assembly in turn to form the 32-chain in a view which is parallel to the chain axis.

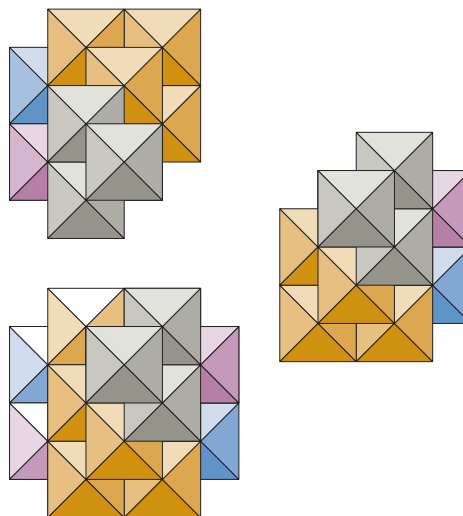
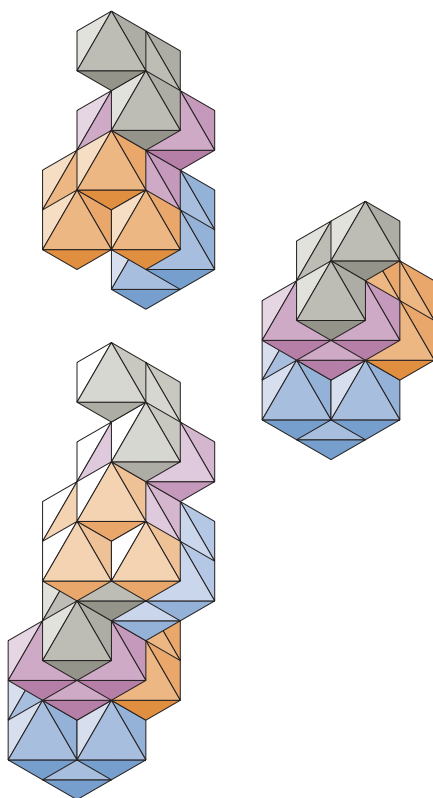
4helix**Protein substructure:
4helix.**

The figure depicts the assembly of a turn of a 4helix. Adjoining units are rotated 90° to the helical axis. The axis makes an oblique angle with the plane of the paper.

Beta90



Beta180



Protein substructure: Beta180

The assembly of one turn of beta180 helix is depicted here. Adjoining units are rotated 180° about the helical axis. The axis makes an oblique angle with the plane of the paper.

The next figure shows a beta180 turn as viewed along the helical axis.

Orientations of chain units.

Orientations of the regular octahedron

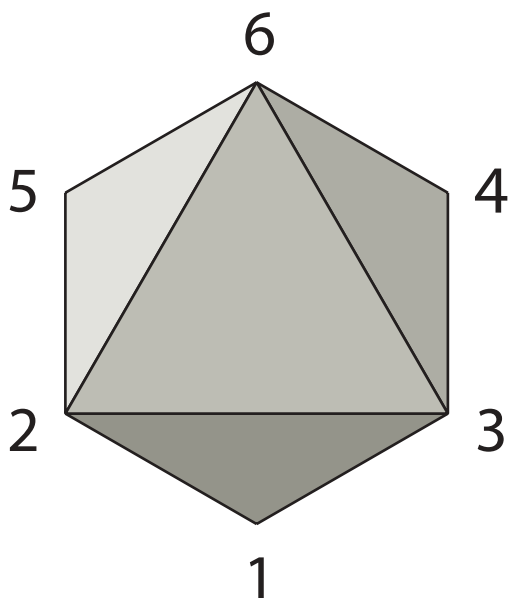
Each of the twenty-four orientations of the regular octahedron results in a different arrangement of its vertexes. Looking at the octahedron facially, each of the vertexes lies on the perimeter of a regular hexagon. The numbers of the vertexes can then be read in counter-clockwise order about the perimeter for each of the twenty-four orientations. The first and the last digit are adjacent, since the vertexes lie on the perimeter of a polygon. Each of the digits refers to a specific vertex. Any pair of adjacent digits defines an edge. Any pair of digits separated by a single intervening digit also defines an edge. The orientation of any unit relative to another unit is

defined by specifying the vertexial numbers of an identical edge. These will be in the same digit location for each of the orientation numbers.

A pair of digits which are separated by two intervening digits are diametrically opposite.

Table 16: Orientation numbers

125643	236451	463215	512364
132654	213465	456231	541326
143625	346521	415263	645123
154632	314562	431256	634152
251436	321546	564312	623145
265413	362514	526341	652134



Facial view of a regular octahedron with its vertices numerically labelled

The relative orientations between a pair of joined units can be specified by the numbers of the two vertices of any common edge in either of two orders. Since there are twelve edges and two orders for each edge, then there are twenty-four ways of specifying the same relative orientation between a pair of units. In the example of a pair of beta180,m joined units the combinations are listed below.

Table 17: Twenty-four ways of specifying the same relative orientation

15,65	54,52	46,21	63,13	32,34	21,46
51,56	45,25	64,12	36,31	23,43	12,64
14,62	56,51	43,23	62,14	31,36	25,45
41,26	65,15	34,32	26,41	13,63	52,54

The direction numbers relative to the reference orientation define the x, y, and z directions.

The moves for a residue added to the female terminus of the reference residue are not affected by the type of join because the reference He-octa for the residue occupies the

Table 18: Relative location of added residue

Join	Orientat ion	Move	x	y	z
reference	154632		0	0	0
beta180,m	652134	3,2	41,1	4	-1
beta90,m	251436	3,2	21,1	4	1
alpha,m	321546	1,2	52,1	-1	1
32chn,m	645123	2,2	31,1	1	4
epsilon,m	415263	2,2	36,1	1	4
4helix,m	314562	1,2	32,1	1	1
beta180,f	652134	5,2	41,1	-4	-1
beta90,f	456231	5,2	41,1	-4	-1
alpha,f	463215	5,2	41,1	-4	-1
32chn,f	645123	5,2	41,1	-4	-1
epsilon,f	541326	5,2	41,1	-4	-1
4helix,f	564312	5,2	41,1	-4	-1
para41	154632		41,2	0	-2
para62	154632		62,2	0	2
anti41	236451	5,2	41,3	-4	-3
anti62	236451	5,2	62,1	-4	1
32stack	541326	45,2	41,1	-2	-3

socket which is defined by the He-octas of the reference residue and whose location is fixed relative to the location of reference residue. But the female terminus of the added residue is defined by the type of the join, with each join providing a new female location that is unique for that join.

For the residue which is added to the male end of the reference residue, the location of its male He-octa is defined by the orientation of the added residue and this is determined by the type of the join.

