Sidechains

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Introduction

The file seeks to define the plausible conformations of the peptides for the purpose of creating a protein folding test.

SIDECHAINS

Plausible peptides

The *myosin* molecule has an alpha helical portion which consists of 645 turns.[1] Each of the residues lies in one of the three axially parallel columns of the helix. An examination of each of the three columns shows that there is at least one instance where a lysine residue is columnarly adjacent to each of the other nineteen types of residues in each of the two axial directions. This suggests that the residues fit in the space defined by the pitch of the alpha helical turn. Within this constraint, each of the plausible representations of each of the peptide units has been constructed and these are presented in the figure encaptioned *Plausible peptides viewed along alpha helical axis*. The viewing direction is parallel to the alpha helical axis.

Plausibility was determined by the suitability of a terminal atom to make a join.

Each of the plausible peptides is shown in a projection which is perpendicular to the alpha helical axis. In this projection, the suitability of the peptide for making sheet joins is apparent.

Single conformaton peptides

Seven peptides are shown in only one conformation–glycine, alanine, cysteine, methionine, isoleucine, phenylalanine, and tryptophan. Glycine is essentially the main chain portion and is fixed so that it may produce the identified protein substructures. There is only one likely way of joining the C_β to the C_α and that allows for only one alanine. There are multiple ways for the S-atom to join to the C_β to form cysteine but only one permits a cleft-to-cleft join between the S-atoms of the fifteen residue chain of insulin. It is inferred from this that the S-atom of methionine is joined to the C_δ atom in an identical manner. Isoleucine is grouped with two possible leucines. It might be true that one of the leucines could be isoleucine. The C_6-ring of phenylalanine fits within the allowed sidechain space only when it is joined to the C_β in the way that is shown. Tryptophan is shown in just one way, but other ways might be possible.

Multiple conformation peptides

Each of the peptides for which the sidechain conformation is ambiguous are shown in the following figures. They include serine, valine, threonine, leucine/isoleucine, aspartate/asparagine, glutamine/glutamate, lysine, tyrosine, proline, arginine, and histidine.

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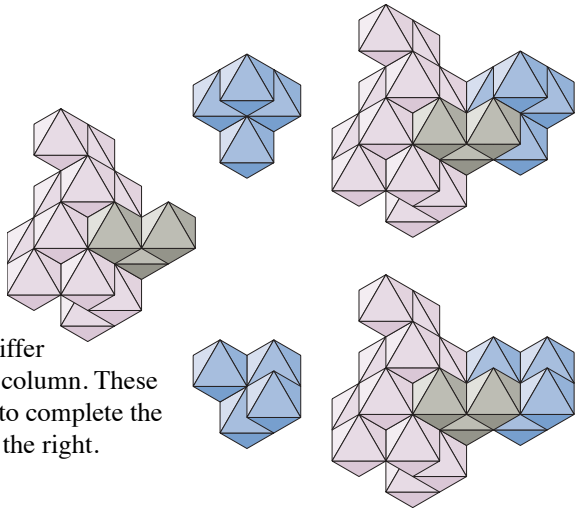
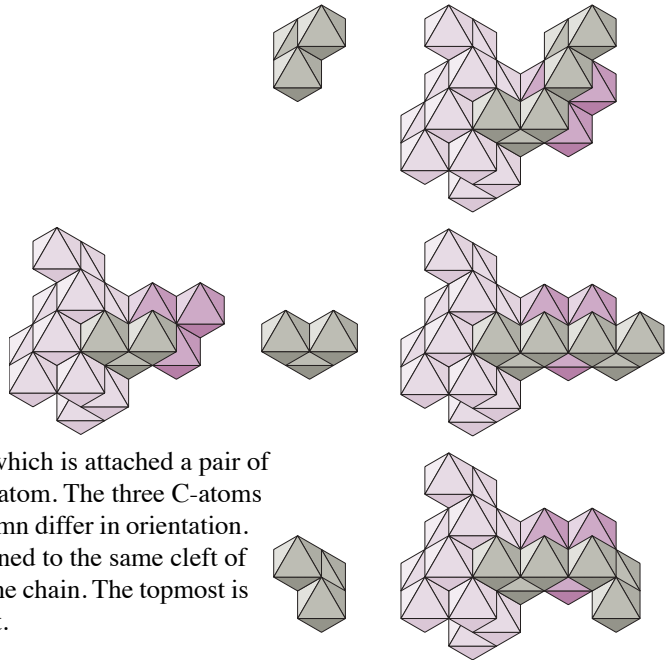
1. T. Jaenicke *et al* "The complete sequence of the human beta-myosin heavy chain gene and a comparative analysis of its product", *Genomics* **8** (2), 194-206 (1990)

Serine



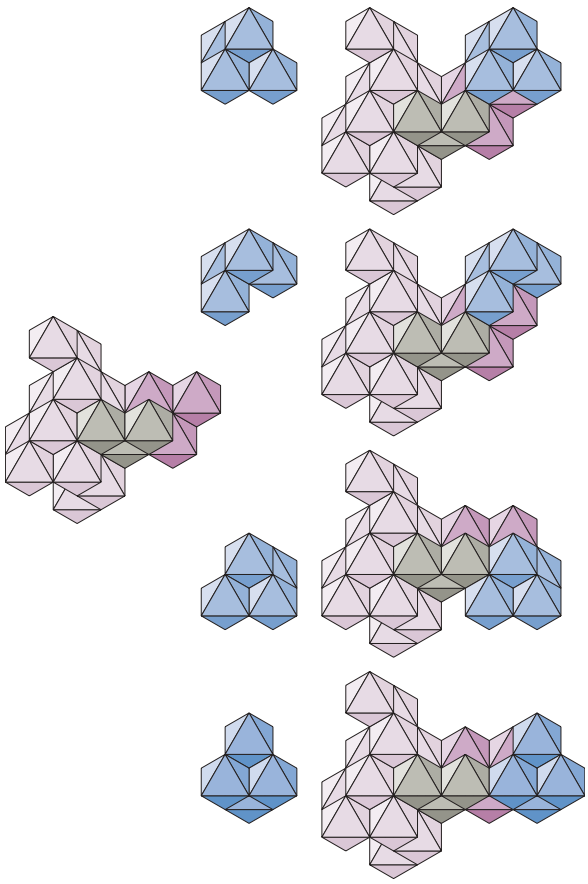
Serine
Serine consists of a main chain portion to which is attached a C-atom and an O-atom. Two O-atoms which differ in orientation are shown in the central column. These attach to the same cleft of the C-atom to complete the serine groups shown in the column on the right.

Valine



Valine
Valine consists of a main chain portion to which is attached a pair of C-atoms and a third C-atom. The three C-atoms shown in the third column differ in orientation. The bottom two are joined to the same cleft of the second C-atom of the chain. The topmost is joined to the other cleft.

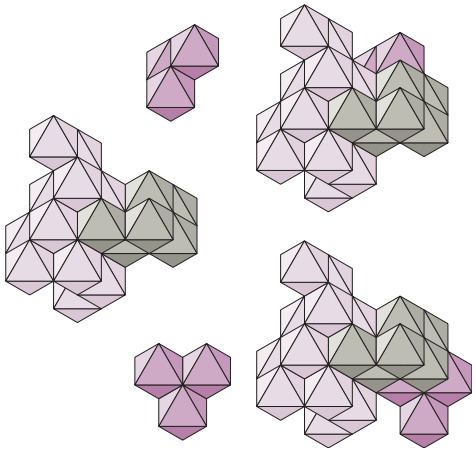
Threonine



Threonine

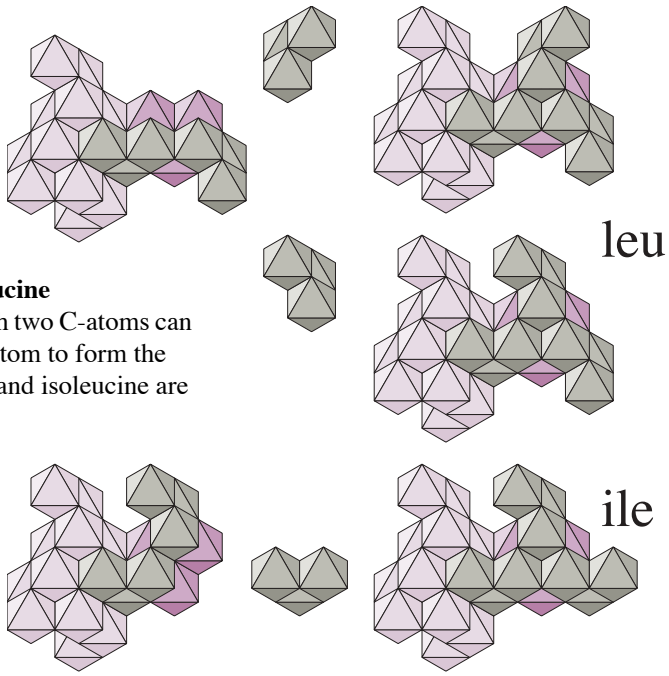
An O-atom can be attached in four ways to produce four plausible threonine side chains. The O-atoms are shown in the middle column, they differ by orientation. The top two join to one C-atom cleft, the bottom two to the other C-atom cleft.

Proline



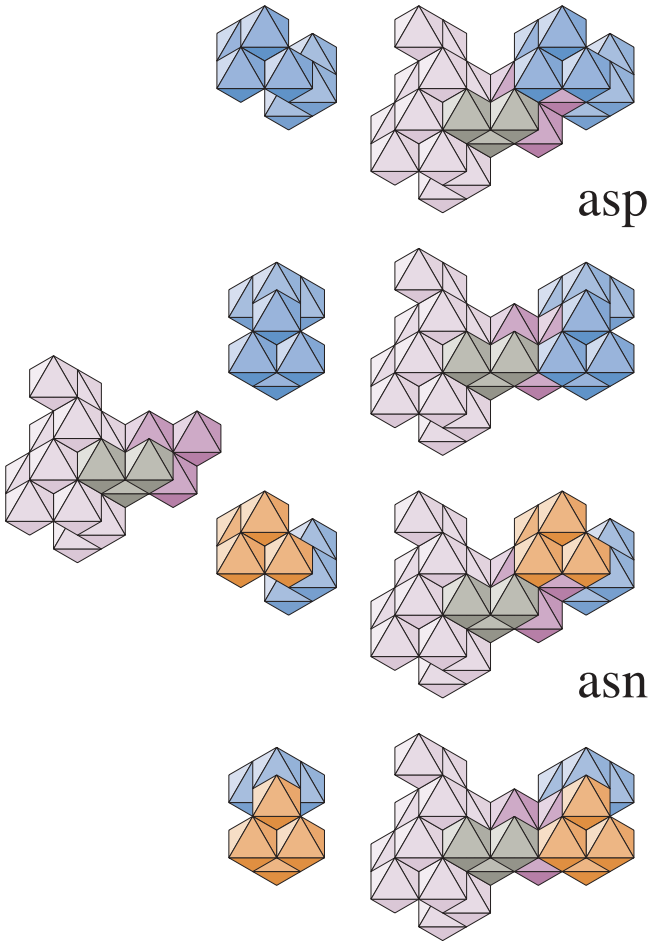
Proline
There are two ways of attaching the third C-atom to the second C-atom of the proline side chain.

Leucine/Isoleucine



Leucine and Isoleucine
Three ways in which two C-atoms can join to the second C-atom to form the sidechains of leucine and isoleucine are shown here.

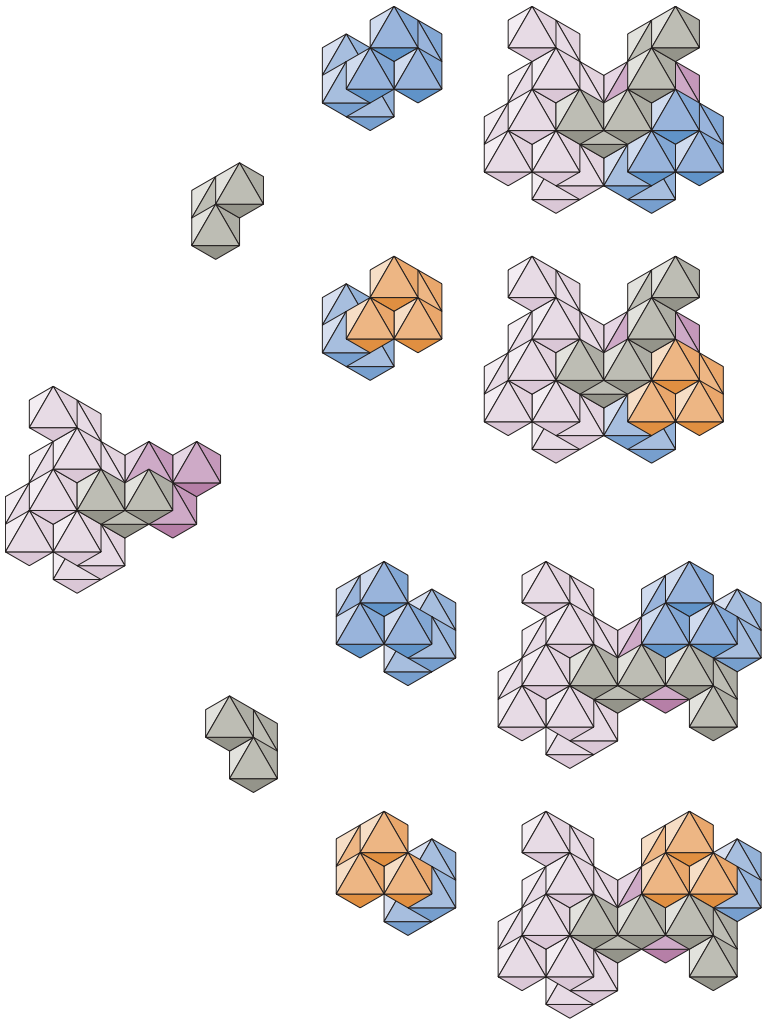
Aspartate/Asparagine



Aspartate and asparagine

Two ways of attaching an O_2-group to the second C-atom of the sidechain produes the two possible aspartates shown at the top of the figure. The two asparagines at the bottom have the same conformation as the aspartates but an NH_2-group replaces one of the O-atoms.

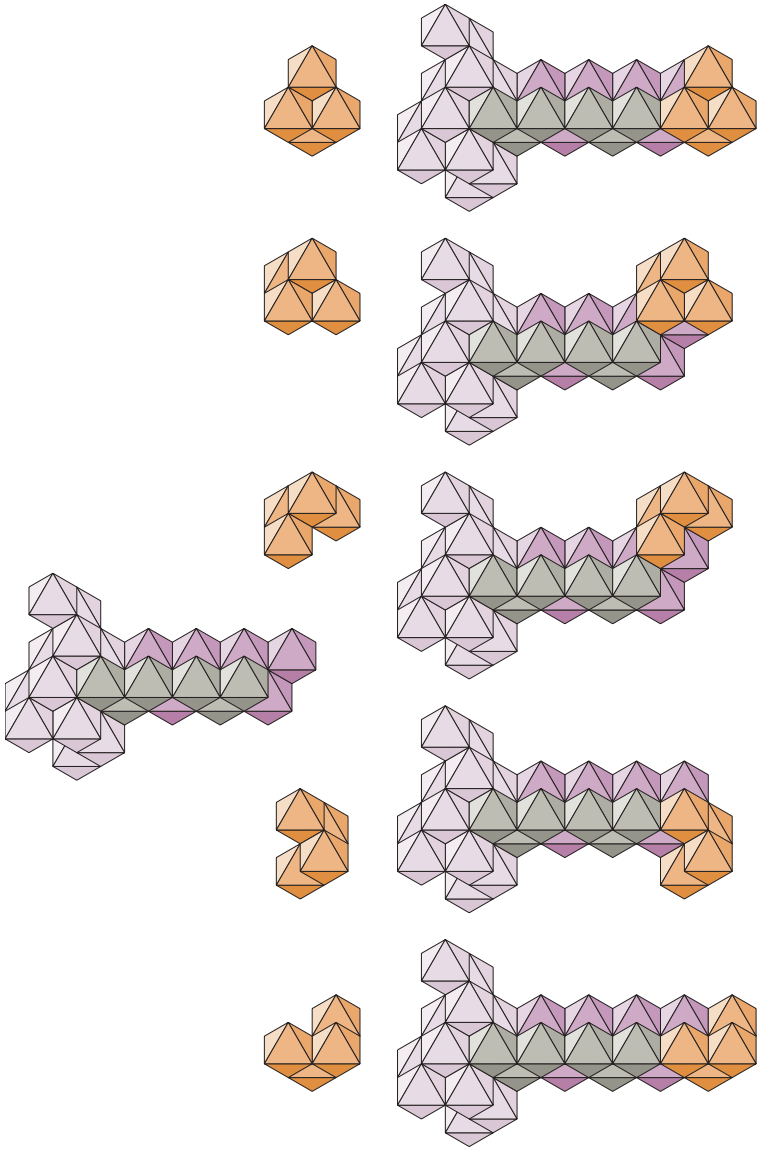
Glutamine/Glutamate



Glutamine & Glutamate

The sidechains of glutamine and glutamate begin with a pair of C-atoms. The side chain is extended with a third C-atom which can be attached is two ways. An O_2-group is attached to the remaining cleft of the second C-atom to produce glutamate; an NH_2-group is attached to the same position produces glutamine.

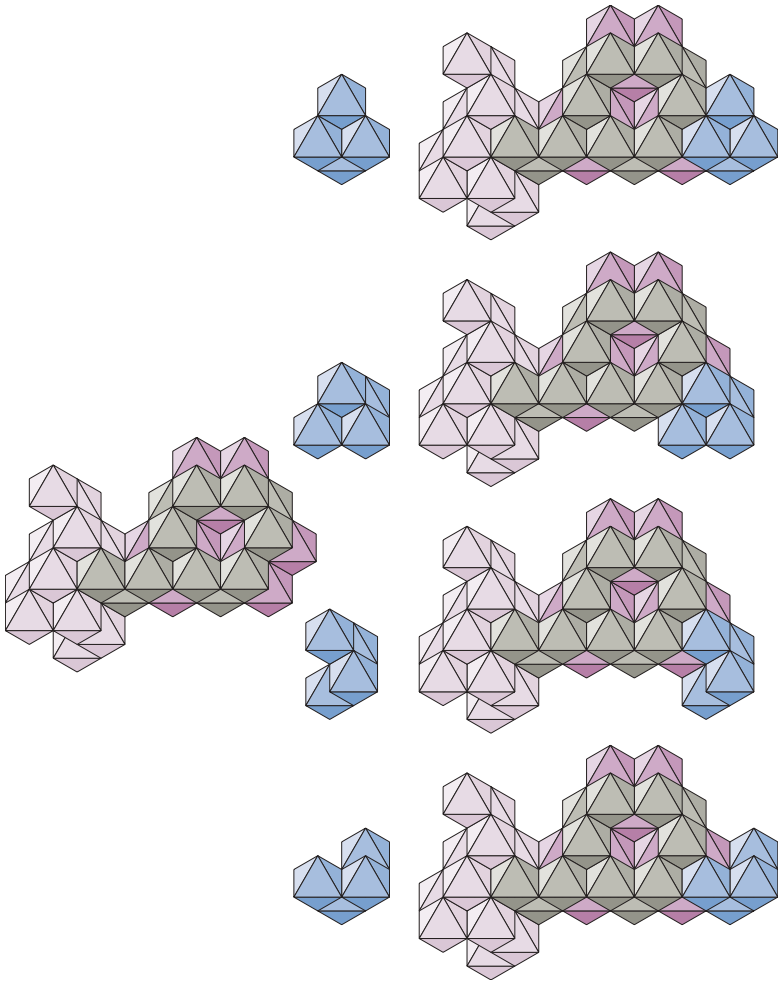
Lysine



Lysine

Lysine consists of a main chain portion to which is appended a chain of three C-atoms and an NH_2-group. The five NH_2-groups in the middle column which differ in orientation are joined to the C-atom at the end of the chain. Three of the NH_2-groups–the topmost, next to bottommost, and bottommost–are attached to the same cleft of the C-atom. The remaining two are attached to the other cleft.

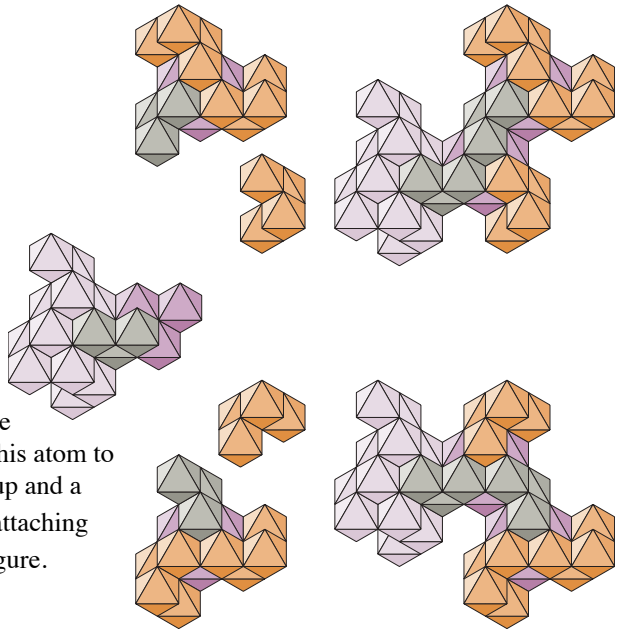
Tyrosine



Tyrosine

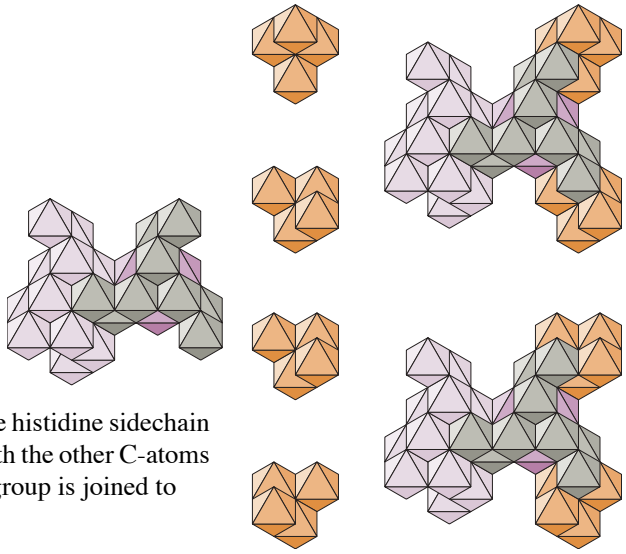
Tyrosine consists of a phenylalanine portion to which an O-atom is appended. The figure shows the phenylalanine portion on the left. To its right are four O-atoms which differ in orientation that are joined to phenylalanine to produce four different tyrosine groups which are depicted on the right. Each of the O-atoms is joined to the same C-atom cleft.

Arginine



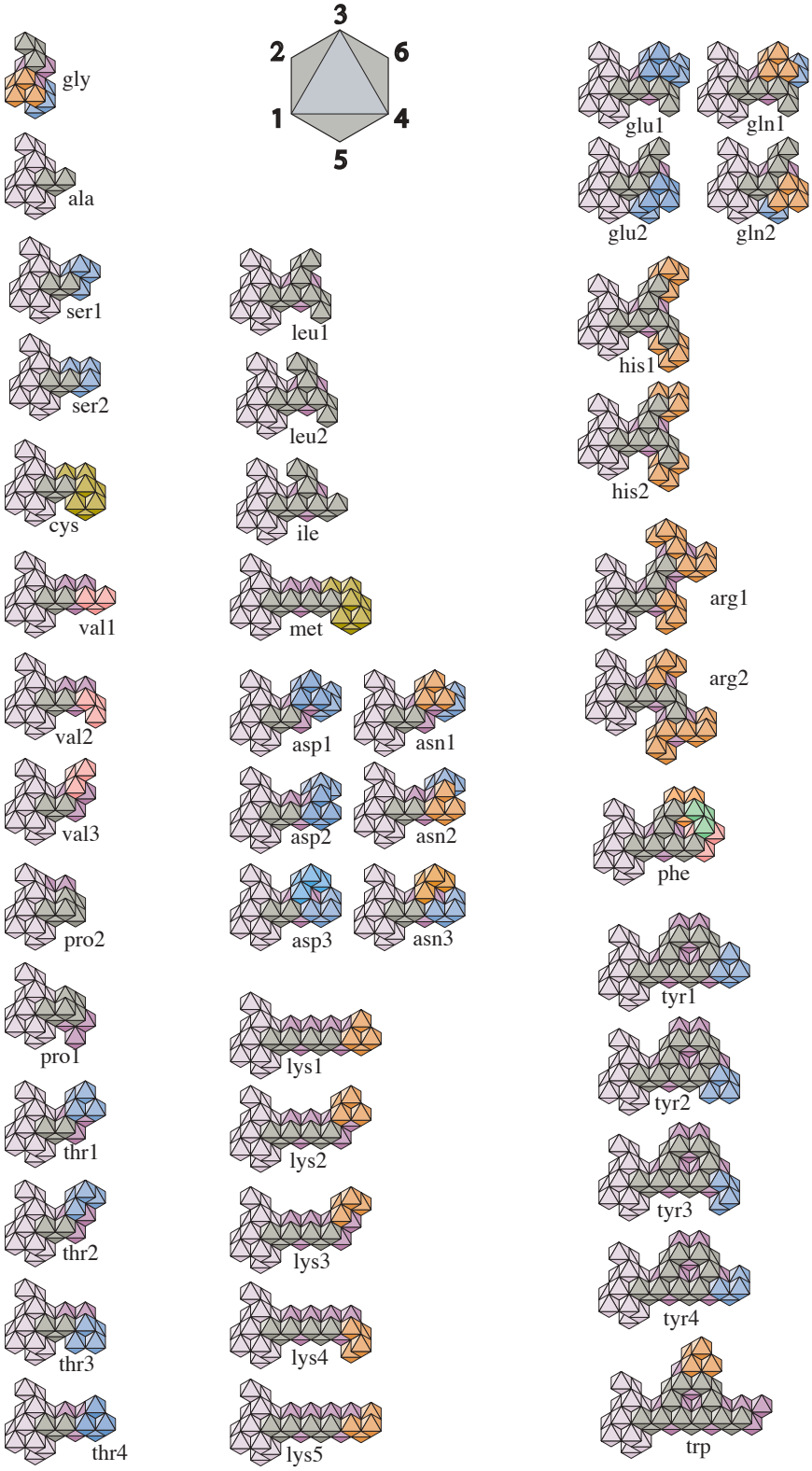
Arginine
The sidechain of arginine begins with two C-atoms. The end C-atom has two clefts available for joining. Two groups attach to this atom to complete the residue–an NH_2-group and a $CCNH_2NH_2$ group. Two ways of attaching the two groups are shown in the figure.

Histidine

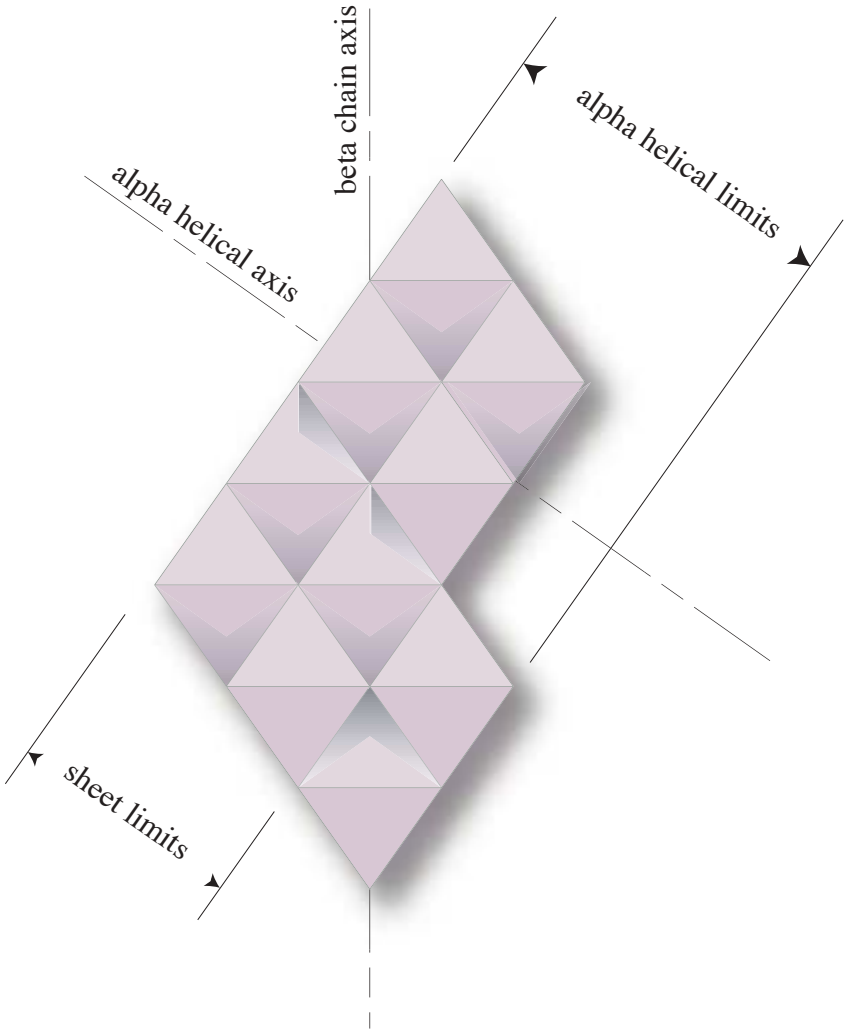


Histidine
The second C-atom of the histidine sidechain is right-handedly joined with the other C-atoms of the sidechain. An NH_2-group is joined to each of the outer C-atoms.

Plausible peptides viewed along alpha helical axis



Peptide limits

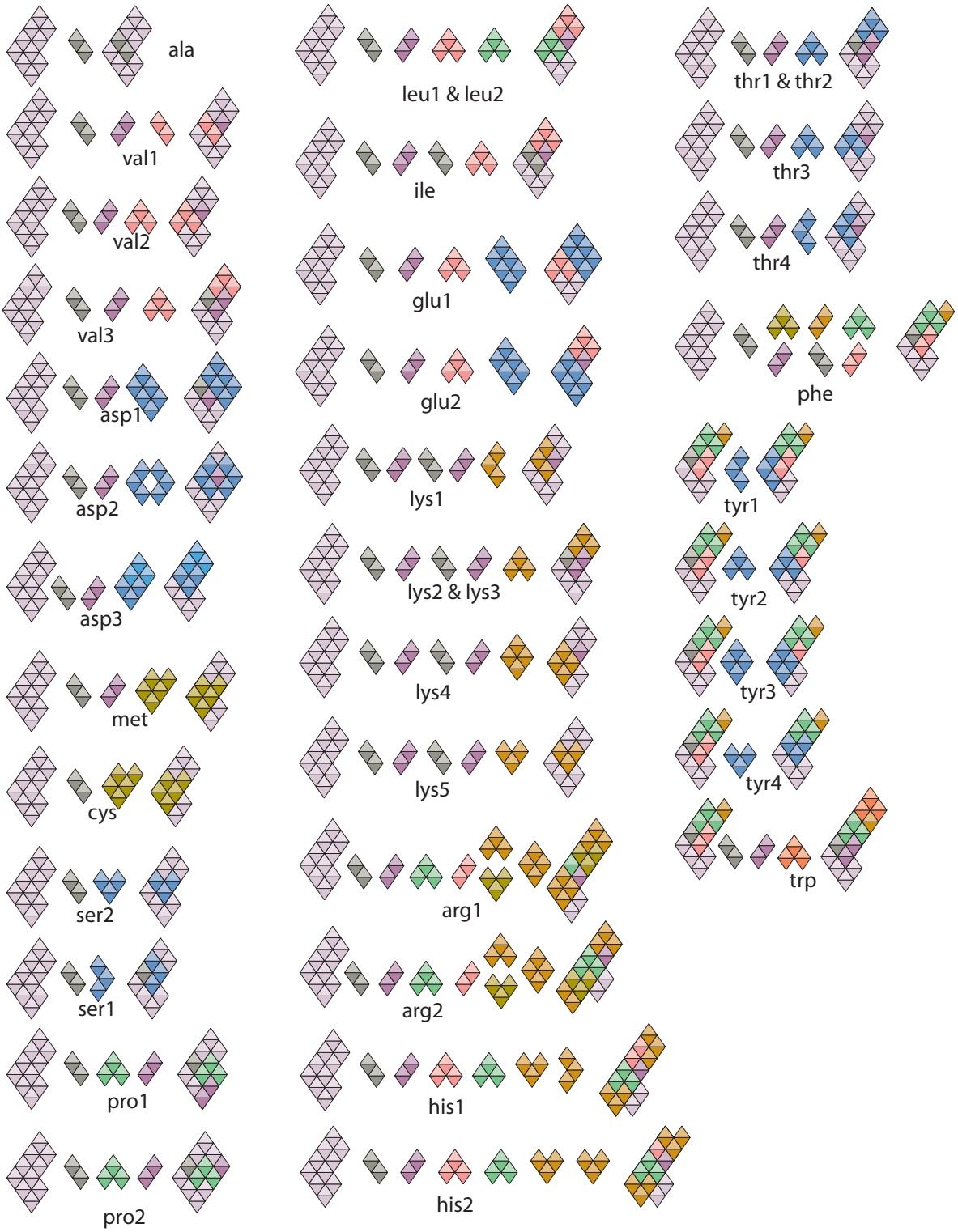


Peptide: Side chain limits

The figure shows the main chain portion of a peptide as it appears in a projection normal to the plane of a pleated sheet. In this view, the axis of the side chain is towards the viewer. This same view shows the peptide as it would appear as part of an alpha helix when viewed perpendicular to the axis of the helix. The relationship of the axis of the beta chain to the main chain unit is shown as is the relationship of the alpha helix to the unit. The permissible limits for the side chain units for both the sheet and the alpha helix are indicated. Peptides whose side chains lie within the respective limits can fit within alpha helixes and pleated sheets.

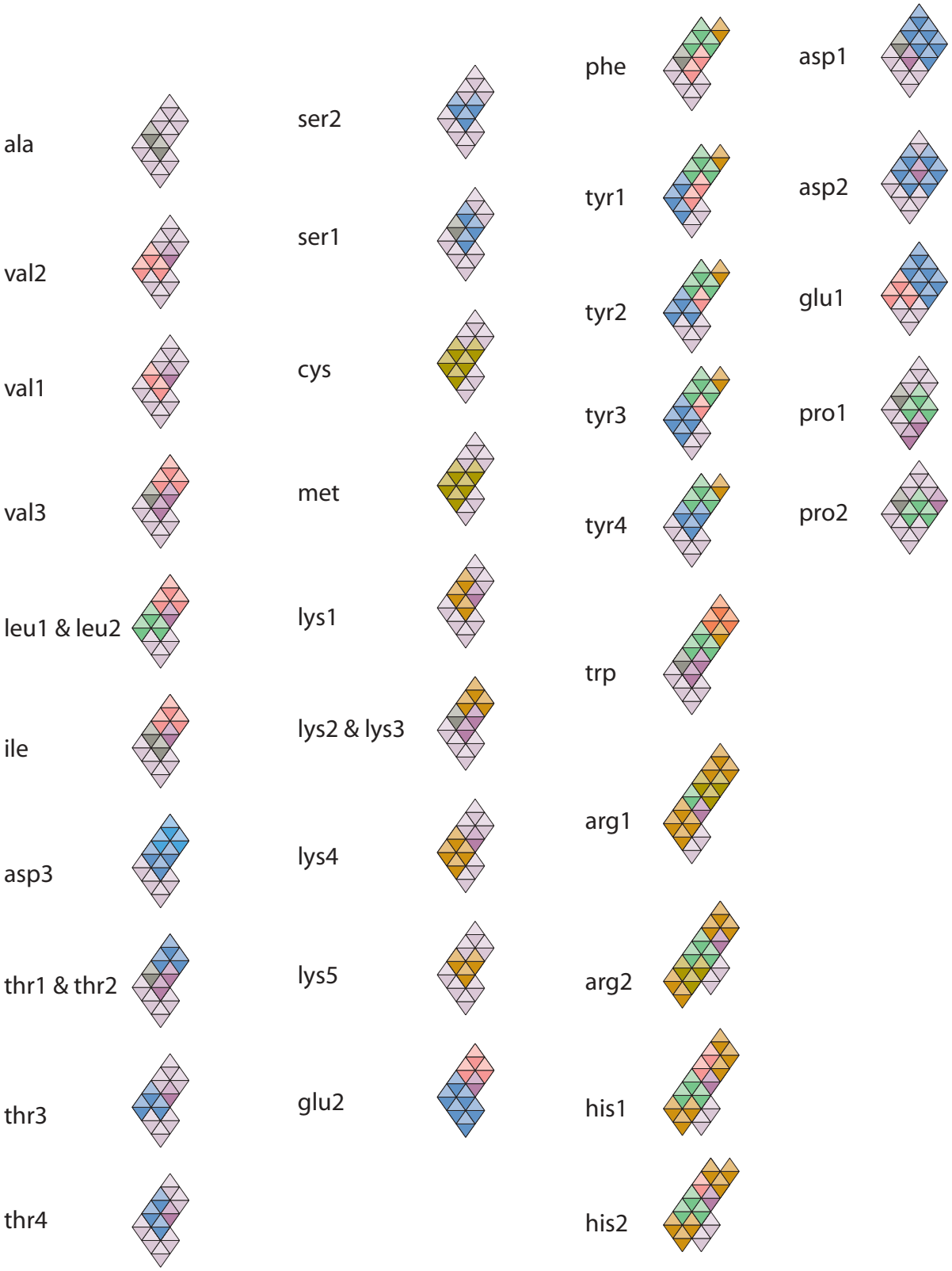
Peptides: radial projections

Peptides viewed parallel to the sidechain axes showing the components of thier sidechains.



Peptide projections

Peptides viewed parallel to sidechain axes



Peptide atoms

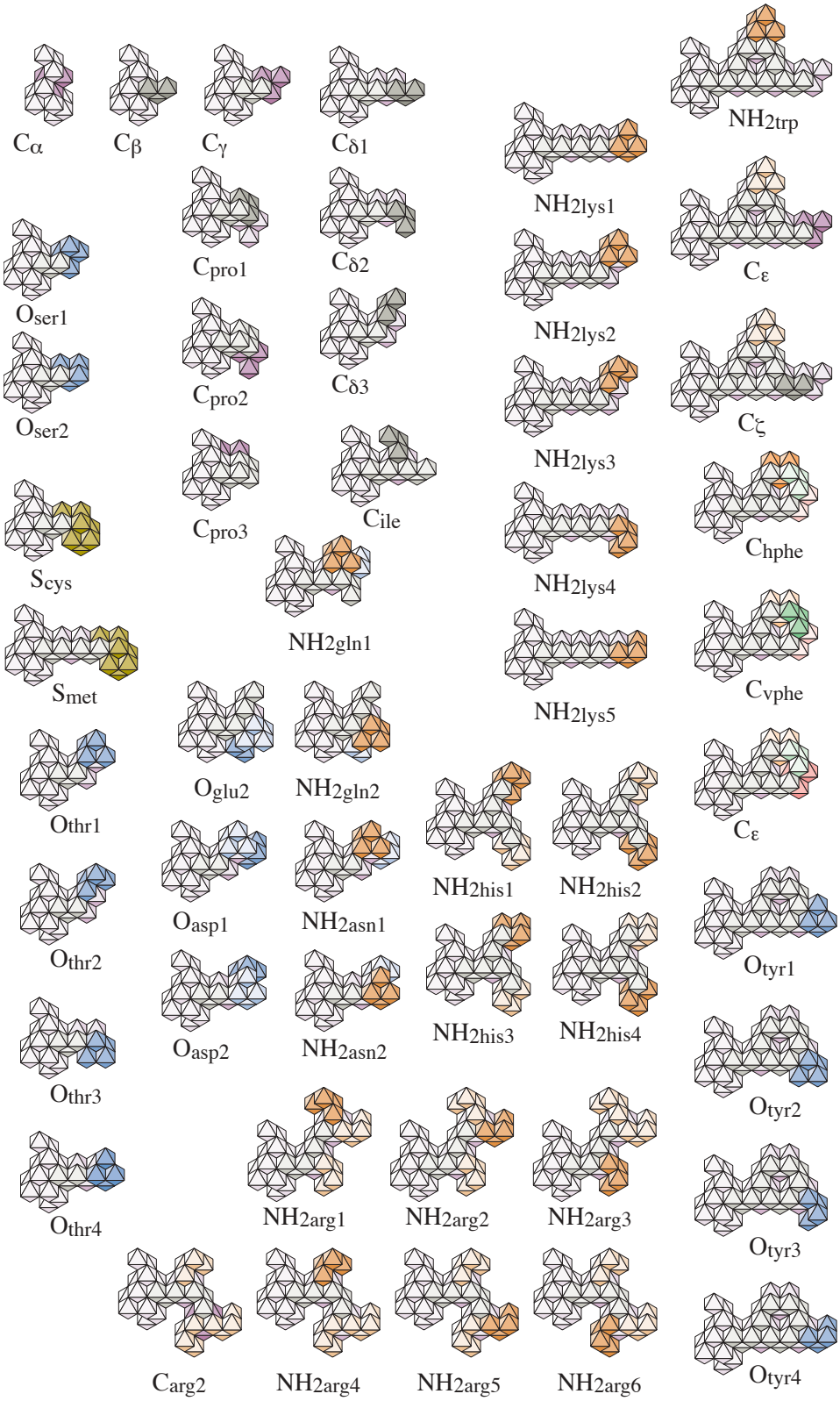


Table 1: Peptide sidechain atoms

	Atoms									
gly										
ala	C_{β}									
ser1	C_{β}	O_{ser1}								
ser2	C_{β}	O_{ser2}								
cys	C_{β}	S_{cys}								
pro1	C_{β}	C_{pro1}	C_{pro2}							
pro2	C_{β}	C_{pro1}	C_{pro3}							
thr1	C_{β}	$C\gamma$	O_{thr1}							
thr2	C_{β}	$C\gamma$	O_{thr2}							
thr3	C_{β}	$C\gamma$	O_{thr3}							
thr4	C_{β}	$C\gamma$	O_{thr4}							
asp1	C_{β}	$C\gamma$	O_{thr1}	O_{asp1}						
asp2	C_{β}	$C\gamma$	O_{thr4}	O_{asp2}						
asn1	C_{β}	$C\gamma$	NH_{2asn1}	O_{asp1}						
asn2	C_{β}	$C\gamma$	NH_{2asn2}	O_{asp2}						
val1	C_{β}	$C\gamma$	$C_{\delta 1}$							
val2	C_{β}	$C\gamma$	$C_{\delta 2}$							
val3	C_{β}	$C\gamma$	$C_{\delta 3}$							
ile	C_{β}	$C\gamma$	$C_{\delta 1}$	C_{ile}						
leu1	C_{β}	$C\gamma$	$C_{\delta 2}$	$C_{\delta 3}$						
leu2	C_{β}	$C\gamma$	$C_{\delta 2}$	C_{ile}						
glu1	C_{β}	$C\gamma$	$C_{\delta 2}$	O_{thr1}	O_{asp1}					
glu2	C_{β}	$C\gamma$	$C_{\delta 3}$	O_{thr3}	O_{glu2}					
gln1	C_{β}	$C\gamma$	$C_{\delta 2}$	NH_{2gln1}	O_{asp1}					
gln2	C_{β}	$C\gamma$	$C_{\delta 3}$	NH_{2gln2}	O_{glu2}					
met	C_{β}	$C\gamma$	$C_{\delta 1}$	S_{met}						

Table 1: Peptide sidechain atoms

	Atoms									
phe	C_β	$C\gamma$	$C_{\delta 1}$	$C_{\delta 3}$	C_ε	C_{hphe}	C_{vphe}			
tyr1	C_β	$C\gamma$	$C_{\delta 1}$	$C_{\delta 3}$	C_ε	C_{hphe}	C_{vphe}	O_{tyr1}		
tyr2	C_β	$C\gamma$	$C_{\delta 1}$	$C_{\delta 3}$	C_ε	C_{hphe}	C_{vphe}	O_{tyr2}		
tyr3	C_β	$C\gamma$	$C_{\delta 1}$	$C_{\delta 3}$	C_ε	C_{hphe}	C_{vphe}	O_{tyr3}		
tyr4	C_β	$C\gamma$	$C_{\delta 1}$	$C_{\delta 3}$	C_ε	C_{hphe}	C_{vphe}	O_{tyr4}		
his1	C_β	$C\gamma$	$C_{\delta 2}$	$C_{\delta 3}$	NH_{2his1}	NH_{2his2}				
his2	C_β	$C\gamma$	$C_{\delta 2}$	$C_{\delta 3}$	NH_{2his3}	NH_{2his4}				
arg1	C_β	$C\gamma$	$C_{\delta 3}$	C_{hphe}	NH_{2arg1}	NH_{2arg2}	NH_{2arg3}			
arg2	C_β	$C\gamma$	$C_{\delta 2}$	C_{arg2}	NH_{2arg4}	NH_{2arg5}	NH_{2arg6}			
lys1	C_β	$C\gamma$	$C_{\delta 1}$	C_ε	NH_{2lys1}					
lys2	C_β	$C\gamma$	$C_{\delta 1}$	C_ε	NH_{2lys2}					
lys3	C_β	$C\gamma$	$C_{\delta 1}$	C_ε	NH_{2lys3}					
lys4	C_β	$C\gamma$	$C_{\delta 1}$	C_ε	NH_{2lys4}					
lys5	C_β	$C\gamma$	$C_{\delta 1}$	C_ε	NH_{2lys5}					
trp	C_β	$C\gamma$	$C_{\delta 1}$	$C_{\delta 3}$	C_ε	C_{hphe}	C_{vphe}	C_ζ	C_η	NH_{2trp}

He-octa numbers

When each of the plausible peptides is placed in a common orientation with its joining He-octa at the origin of the coordinate axes, it is found that there are just seventy-nine unique xyz-addresses for their combined He-octas. These addresses have been assigned a numeric code from 1 to 79 inclusive. The numeric codes 1 through 14 are assigned to the He-octas of the main chain unit. The He-octas of the side chains have the codes from 15 through 79.

The table shows both the literal symbol and the standard three letter abreviation for each of the peptides. The numeral added to the literal symbol is used to differentiate those peptides where there is more than one plausible configuration.

Table 2: Peptide symbols

Symbols with abbreviations			
G gly	T thr	L leu	Y tyr
A ala	D asp	E glu	H his
S ser	N asn	Q gln	R arg
C cys	V val	M met	K lys
P pro	I ile	F phe	W trp

Numeric codes

List of the numeric codes of the He-octas with the peptides in which the He-octa is included.

Main chain He-octas

Each of the peptides contains the fourteen He-octas of the main chain unit.

1 through 14
G A S1 S2 C P1 P2 T1 T2 T3 T4 D1 D2 N1 N2 V1 V2 V3 I L2 L1 E1 E2 Q1 Q2 M F Y1 Y2 Y3 Y4 H1 H2 R1 R2 K1 K2 K3 K4 K5 W

Side chain He-octas

15
A S1 S2 C P1 P2 T1 T2 T3 T4 D1 D2 N1 N2 V1 V2 V3 I L2 L1 E1 E2 Q1 Q2 M F Y1 Y2 Y3 Y4 H1 H2 R1 R2 K1 K2 K3 K4 K5 W

16
A S1 S2 C P1 P2 T1 T2 T3 T4 D1 D2 N1 N2 V1 V2 V3 I L2 L1 E1 E2 Q1 Q2 M F Y1 Y2 Y3 Y4 H1 H2 R1 R2 K1 K2 K3 K4 K5 W

17
A S1 S2 C P1 P2 T1 T2 T3 T4 D1 D2 N1 N2 V1 V2 V3 I L2 L1 E1 E2 Q1 Q2 M F Y1 Y2 Y3 Y4 H1 H2 R1 R2 K1 K2 K3 K4 K5 W

18
S1 S2 C P1 P2 T1 T2 T3 T4 D1 D2 N1 N2 V1 V2 V3 I L2 L1 E1 E2 Q1 Q2 M F Y1 Y2 Y3 Y4 H1 H2 R1 R2 K1 K2 K3 K4 K5 W

19
S1 S2 C T1 T2 T3 T4 D1 D2 N1 N2 V1 V2 V3 I L2 L1 E1 E2 Q1 Q2 M F Y1 Y2 Y3 Y4 H1 H2 R1 R2 K1 K2 K3 K4 K5 W

20
S1 S2 C P1 P2 T1 T2 T3 T4 D1 D2 N1 N2 V1 V2 V3 I L2 L1 E1 E2 Q1 Q2 M F Y1 Y2 Y3 Y4 H1 H2 R1 R2 K1 K2 K3 K4 K5 W

21
C T3 T4 D2 N2 V1 V2 I L2 L1 E1 E2 Q1 Q2 M F Y1 Y2 Y3 Y4 H1 H2 R1 R2 K1 K2 K3 K4 K5 W

22
C S2 T3 T4 D2 N2 V1 V2 I L2 L1 E1 E2 Q1 Q2 M F Y1 Y2 Y3 Y4 H1 H2 R1 R2 K1 K2 K3 K4 K5 W

23
T4 D2 N2 V1 I M F Y1 Y2 Y3 Y4 K1 K2 K3 K4 K5 W

24
S1 T1 T2 D1 N1 V3 I L2 L1 E1 E2 Q1 Q2 F

Y1 Y2 Y3 Y4 H1 H2 R1 R2 W

25
T1 T2 D1 N1 V3 I L2 L1 E1 E2 Q1 Q2 F Y1 Y2 Y3 Y4 H1 H2 R1 R2 W

26
T1 T2 D1 N1 V3 L1 E1 E2 Q1 Q2 F Y1 Y2 Y3 Y4 H1 H2 R1 R2 W

27
C T3 V2 L2 L1 E1 E2 Q1 Q2 H1 H2 R1 R2

28
MFY1Y2Y3Y4K1K2K3K4K5W

29
M Y1 Y2 Y3 Y4 K4 K5 W

30
D1 N1 E1 Q1 MF Y1 Y2 Y3 Y4 K1 K2 K3 K4 K5 W

31
C T3 E2 Q2

32
M F Y1 Y2 Y3 Y4 K1 K2 K3 K4 K5 W

33
T1 T4 D1 D2 N1 N2 E1 Q1

34
M Y1 Y2 Y3 Y4 K1 K4 K5 W

35
P1 E2 Q2 H1

36
T2 D2 N2 F Y1 Y2 Y3 Y4 H1 H2 R1 W

37
F Y1 Y2 Y3 Y4 K2 K3 W

38
D1 D2 N1 N2 E1 Q1

39
C H1 H2 R1 R2

40
D1 D2 N1 N2 E1 Q1

41
D1 D2 N1 N2 E1 Q1

42
I L2

43
E2 Q2

44
M Y3 R1 K4

45
M Y2 Y3 K4

46
M Y2

47
P1 E2 Q2

48
P1 E2 Q2

49
P1 P 2

50
P2

51
P2

52
F Y1 Y2 Y3 Y4 R1 K2 K3 W

53
F Y1 Y2 Y3 Y4 H2 R1 W

54
F Y1 Y2 Y3 Y4 H1 H2 R1 R2 W

55
F Y1 Y2 Y3 Y4 H1 H2 R1 W

56
Y1 Y4 K1 K5 W

57
Y 1K1 K2

58
Y4 K1 K5 W

59
H1 R2

60
H1 H2 R2

61
H1 R1 W

62
H2 R2

63
H2 R2

64
R1 L2 L3

65
R1

66
R1 W

67
R1

68
R1

69
R2

70
R2

71
R2

73
R2

74
L3

75
W

76
W.

77
W

78
W

79
P2

Peptide symbols

List of peptides showing the numeric codes of their side chain He-octas

A
15 16 17

S1
15-20 24

S2
15-20 22

C
15-22 27 31 39

P1
15-18 20 35 47-49

P2
15-18 20 49-51 79

T1

15-20 24-26 33

T2
15-20 24-26 36

T3
15-22 27 31

T4
15-23 33

D1 & N1
15-20 24-26 30 33 38 40-41

D2 & N2
15-23 33 36 38 40-41

V1
15-23

V2
15-22 27

V3
15-20 24-26

I
15-25 42

L2
15-22 24-25 27 42

L1
15-22 24-27

E1 & Q1
15-22 24-27 30 33 38 40-41

E2 & Q2
15-22 24-27 31 35 43 47-48

M
15-23 28-30 32 34 44-46

F
15-26 28 30 32 36-37 52-55

Y1
15-26 28-30 32 34 36-37 52-57

Y2
15-26 28-30 32 34 36-37 45-46 52-55

Y3
15-26 28-30 32 34 36-37 44-45 52-55

Y4
15-26 28-30 32 34 36-37 52-56 58

H1
15-22 24-27 35-36 39 54-55 59-61

H2
15-22 24-27 36 39 53-55 60 62-63

R1
15-22 24-27 36 39 52-55 61 64-68

R2
15-22 24-27 39 44 54 59-60 62-63 69-73

K1
15-23 28 30 32 34 56-58

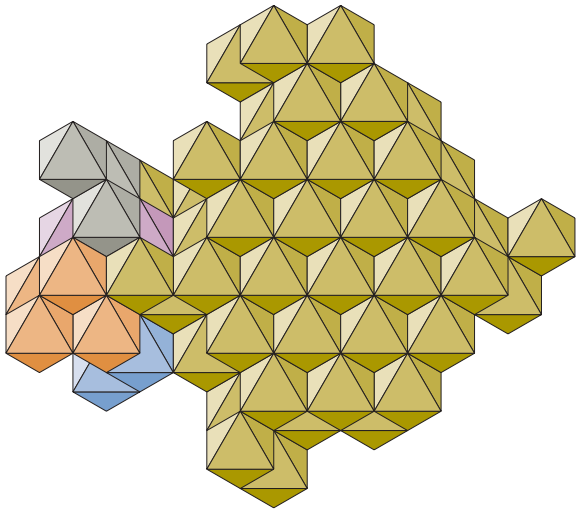
K2
15-23 28 30 32 37 52 57 64

K3
15-23 28 30 32 37 52 64 74

K4
15-23 28-30 32 34 44-45

K5
15-23 28-30 32 34 56 58

W
15-26 28-30 32 34 36-37 52-56 58 61 66 75-



Sidechain tester

The figure shows the sidechain testing assembly which contains a He-octa for each of the unique xyz-addresses which occur in the plausible peptides. The main chain unit contains fourteen He-octas and these are colored according the atoms or atomic groups. The fifty-five sidechain He-octas are colored yellow. The unit is used to test for interference between any two plausible peptides which are related by their positions within a chain with a given conformation.

Protein folding

The assembly depicted above includes a He-octa for each of the unique xyz-addresses which occur in the plausible peptides. Identical assemblies are used as the terminal residues of a protein chain of a length *n*. The chain is folded into each of the 6^(n-1) possible conformations and the xyz-addresses of the terminal residuues are tested for duplication. Where duplicates occur, the numerical codes of the two octas are noted along with the join codes for that conformation.

In this manner, each of the plausible peptides is tested at any two positions within each of the possible protein conformations for a given chain length at one time.

The following table lists each of the He-octas of each atom of the plausible peptides. They are arranged in order by the numerical codes which have been assigned to their xyz-addresses.

Table 3: Peptide He-octas

Number	Atom	Octa	X	Y	Z
1	O_{main}	2	-5	-1	0
2	O_{main}	1	-4	-2	0
3	O_{main}	4	-4	-1	1
4	O_{main}	3	-4	0	0
5	NH_{2main}	4	-3	-2	-1
6	NH_{2main}	2	-3	-1	-1
7	C_{α}	3	-3	-1	0
8	NH_{2main}	3	-3	0	-1
9	NH_{2main}	1	-2	-1	-1
10	C_{α}	2	-2	-1	1
11	C_{α}	1	-2	0	0
12	C_{male}	2	-1	-1	0
13	C_{male}	3	-1	0	1
14	C_{male}	1	0	0	0
15	C_{β}	2	-2	-3	1
16	C_{β}	1	-2	-2	0
17	C_{β}	3	-3	-2	1
18	$C\gamma$	3	-3	-3	2
	O_{ser1}	2			
	O_{ser2}	4			
	S_{cys}	6			
	C_{pro1}	2			

Table 3: Peptide He-octas

Number	Atom	Octa	X	Y	Z
19	$C\gamma$	2	-2	-3	3
	O_{ser1}	4			
	O_{ser2}	3			
	S_{cys}	3			
20	$C\gamma$	1	-2	-2	2
	O_{ser1}	3			
	O_{ser2}	2			
	S_{cys}	2			
	C_{pro1}	1			
21	$C_{\delta 1}$	3	-3	-4	3
	$C_{\delta 2}$	3			
	O_{thr3}	4			
	O_{thr4}	4			
	S_{cys}	4			
	NH_{2arg3}	4			
	NH_{2asn2}	4			
	NH_{2gln2}	4			
22	$C_{\delta 1}$	1	-2	-4	2
	$C_{\delta 2}$	1			
	O_{thr3}	1			
	O_{thr4}	1			
	O_{ser2}	1			
	S_{cys}	1			
	NH_{2arg3}	1			
	NH_{2asn2}	2			
	NH_{2gln2}	1			

Table 3: Peptide He-octas

Number	Atom	Octa	X	Y	Z
23	$C_{\delta 1}$	2	-2	-5	3
	O_{thr4}	2			
	NH_{2asn2}	3			
24	$C_{\delta 3}$	2	-1	-3	2
	O_{thr1}	2			
	O_{thr2}	2			
	O_{ser1}	1			
	C_{ile}	2			
	NH_{2arg4}	2			
	NH_{2asn1}	3			
	NH_{2gln1}	2			
25	$C_{\delta 3}$	3	-1	-2	3
	O_{thr1}	4			
	O_{thr2}	4			
	C_{ile}	3			
	NH_{2arg4}	3			
	NH_{2asn1}	2			
	NH_{2gln1}	4			
26	$C_{\delta 3}$	1	0	-3	3
	O_{thr1}	1			
	O_{thr2}	1			
	NH_{2arg4}	1			
	NH_{2asn1}	1			
	NH_{2gln1}	1			

Table 3: Peptide He-octas

Number	Atom	Octa	X	Y	Z
27	$C_{\delta 2}$	2	-3	-5	2
	O_{thr3}	2			
	S_{cys}	8			
	NH_{2arg3}	2			
	NH_{2gln2}	3			
28	C_{ε}	2	-2	-5	5
	S_{met}	3			
29	C_{ζ}	1	-2	-6	4
	O_{tyr1}	1			
	O_{tyr2}	1			
	O_{tyr3}	1			
	O_{tyr4}	1			
	S_{met}	1			
	NH_{2lys4}	1			
	NH_{2lys5}	1			
30	C_{ε}	1	-2	-4	4
	S_{met}	2			
	O_{asp1}	1			
31	O_{thr3}	3	-3	-4	1
	S_{cys}	7			
	NH_{2gln2}	2			
32	C_{ε}	3	-3	-5	4
	S_{met}	6			

Table 3: Peptide He-octas

Number	Atom	Octa	X	Y	Z
33	O_{thr1}	3	-1	-4	3
	O_{thr4}	3			
	NH_{2asn1}	4			
	NH_{2asn2}	1			
	NH_{2gln1}	3			
34	C_{ζ}	3	-3	-6	5
	O_{tyr1}	4			
	O_{tyr2}	4			
	O_{tyr3}	4			
	O_{tyr4}	4			
	S_{met}	4			
	NH_{2lys1}	4			
	NH_{2lys4}	3			
	NH_{2lys5}	3			
35	O_{glu2}	3	-5	-3	2
	NH_{2his2}	2			
	C_{pro2}	1			
36	C_{hphe}	3	-1	-3	4
	O_{thr2}	3			
	O_{asp2}	1			
	NH_{2his1}	2			
	NH_{2his3}	4			
37	C_{vphe}	2	-1	-5	4
	NH_{2lys3}	1			
	NH_{2lys2}	3			
38	O_{asp1}	4	-3	-3	4
	O_{asp2}	2			

Table 3: Peptide He-octas

Number	Atom	Octa	X	Y	Z
39	S_{cys}	5	-4	-4	2
	NH_{2his2}	3			
	NH_{2his4}	3			
	C_{arg2}	2			
	NH_{2arg3}	3			
40	O_{asp1}	3	-2	-3	5
	O_{asp2}	4			
41	O_{asp1}	2	-2	-2	4
	O_{asp2}	3			
42	C_{ile}	3	0	-2	2
43	O_{glu2}	1	-4	-3	1
44	O_{tyr3}	3	-4	-6	4
	S_{met}	5			
	NH_{2arg5}	4			
	NH_{2lys4}	4			
45	O_{tyr2}	3	-3	-7	4
	O_{tyr3}	2			
	S_{met}	8			
	NH_{2lys4}	2			
46	O_{tyr2}	2	-3	-6	3
	S_{met}	7			
47	O_{glu2}	2	-4	-3	3
	C_{pro2}	2			
48	O_{glu2}	4	-4	-2	2
	C_{pro2}	3			
49	C_{pro1}	3	-3	-2	3

Table 3: Peptide He-octas

Number	Atom	Octa	X	Y	Z
50	C_{pro3}	3	-3	-1	2
51	C_{pro3}	2	-2	-1	3
52	C_{vphe}	3	-1	-4	5
	NH_{2lys3}	3			
	NH_{2lys2}	2			
	NH_{2arg2}	4			
53	C_{vphe}	1	0	-4	4
	NH_{2his3}	1			
	NH_{2arg2}	1			
54	C_{hphe}	2	0	-3	5
	NH_{2his1}	4			
	NH_{2his3}	3			
	NH_{2arg4}	4			
55	C_{hphe}	1	0	-2	4
	NH_{2his1}	3			
	NH_{2his3}	2			
56	C_{ζ}	2	-2	-7	5
	O_{tyr1}	2			
	O_{tyr4}	2			
	NH_{2lys1}	2			
	NH_{2lys5}	2			
57	O_{tyr1}	3	-1	-6	5
	NH_{2lys2}	4			
	$NH2_{lys1}$	3			

Table 3: Peptide He-octas

Number	Atom	Octa	X	Y	Z
58	C_{η}	1	-2	-6	6
	O_{tyr4}	3			
	NH_{2lys5}	4			
	NH_{2lys1}	4			
59	NH_{2his2}	1	-4	-6	2
	NH_{2arg5}	1			
60	NH_{2his2}	4	-4	-5	3
	NH_{2his4}	4			
	C_{arg2}	3			
61	NH_{2trp}	1	1	-3	4
	NH_{2his1}	1			
	NH_{2arg1}	1			
62	NH_{2his4}	1	-5	-5	2
	C_{arg2}	1			
63	NH_{2his4}	2	-4	-5	1
	NH_{2arg6}	1			
64	NH_{2lys3}	2	0	-5	5
	NH_{2lys2}	1			
	NH_{2arg2}	2			
65	NH_{2arg2}	3	0	-4	6
66	NH_{2trp}	3	1	-2	5
	NH_{2arg1}	3			
67	NH_{2arg1}	4	1	-1	4
68	NH_{2arg1}	2	2	-2	4
69	NH_{2arg6}	2	-6	-5	1
70	NH_{2arg5}	3	-5	-6	3

Table 3: Peptide He-octas

Number	Atom	Octa	X	Y	Z
71	NH_{2arg6}	3	-5	-5	0
72	NH_{2arg6}	4	-5	-4	1
73	NH_{2arg5}	2	-4	-7	3
74	NH_{2lys3}	4	-1	-5	6
75	C_{η}	3	-3	-7	6
76	C_{η}	2	-2	-7	7
77	NH_{2trp}	4	1	-4	5
78	NH_{2trp}	2	2	-3	5
79	C_{pro3}	1	-2	0	2

Interference compacting

A program written in Visual Basic for Microsoft Access calculates the xyz-addresses of the He-octas of the two terminal peptides for duplication.

The following He-octas are grouped because each He-octa in the group is present if any of the other He-octas are present. Interference with one of the He-octas has the same effect as interference with any other.

1-14 block all
15-17 blocks all but G
18 & 20 blocks all but G & A
28 & 32 blocks M, Y1 to Y4, K1 to K5, W
38 & 40 & 41 blocks D1, D2, N1, N2, E1, Q1
47 & 48 blocks P1, E2, Q2
50 & 51 & 79 block P2
62 & 63 blocks H2, R2
65 & 67 & 68 blocks R1
69-73 blocks R2
75-78 blocks W

TO BE CONTINUED