Thursday, April 23rd

Today's Theoretical Seminar:

Prediction of Secondary Structures Elements

What's behind DSSP (and STRIDE)?

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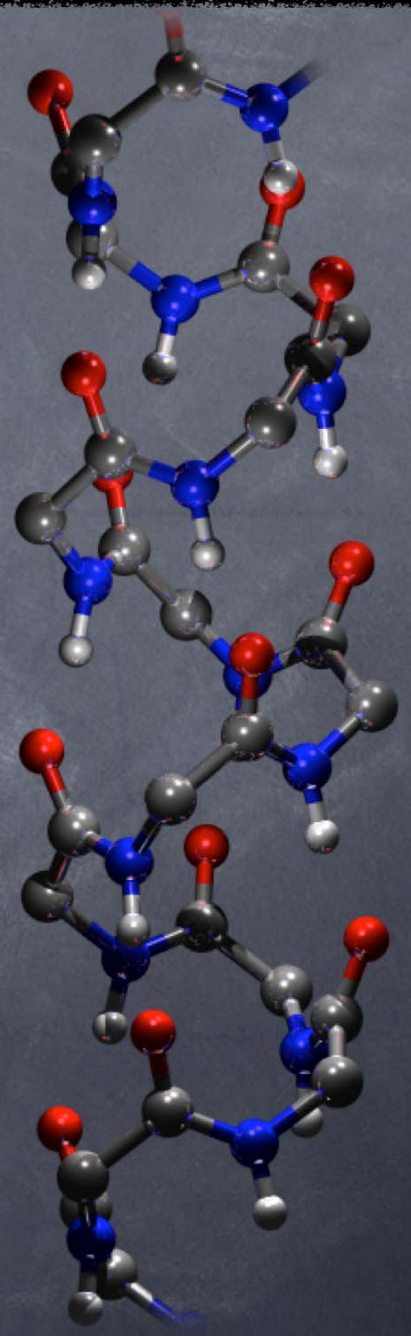
Determination ~~Prediction~~ of Secondary Structures Elements

What's behind DSSP (and STRIDE)?

What's a Secondary Structure Element (SSE)?

It looks like a helix. But how can it be clearly (and simply) defined?



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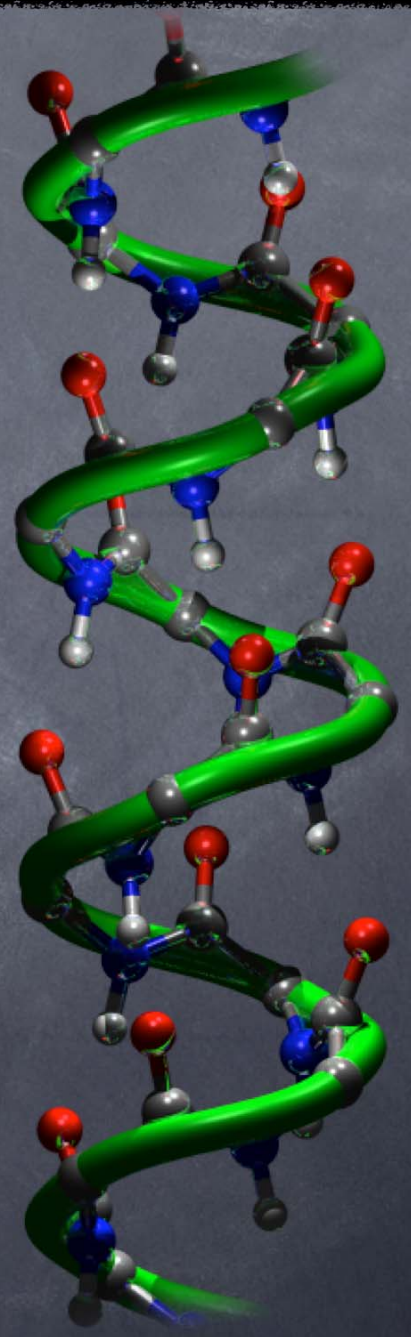

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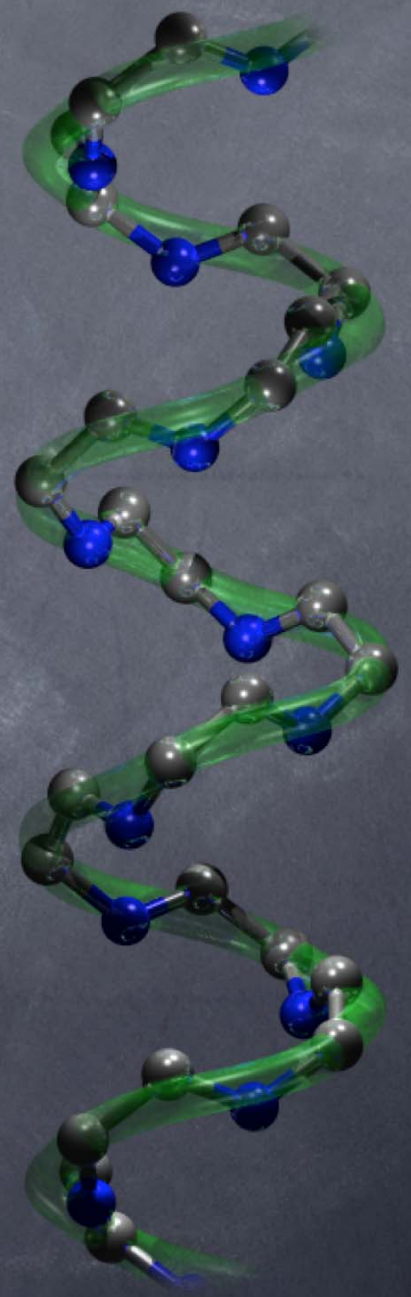
Two main definitions:
1. Using the backbone Φ and Ψ dihedrals (Ramanchandran's plot)



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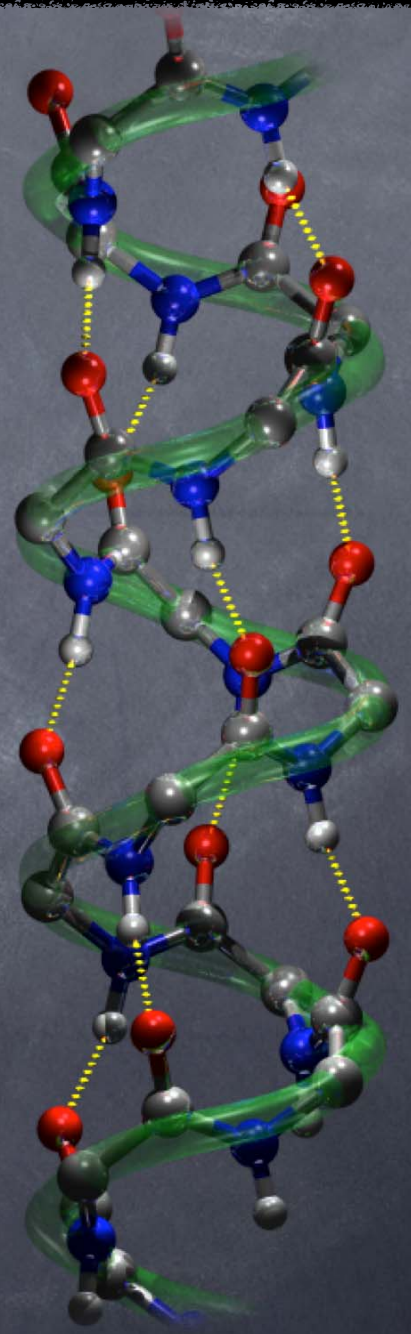

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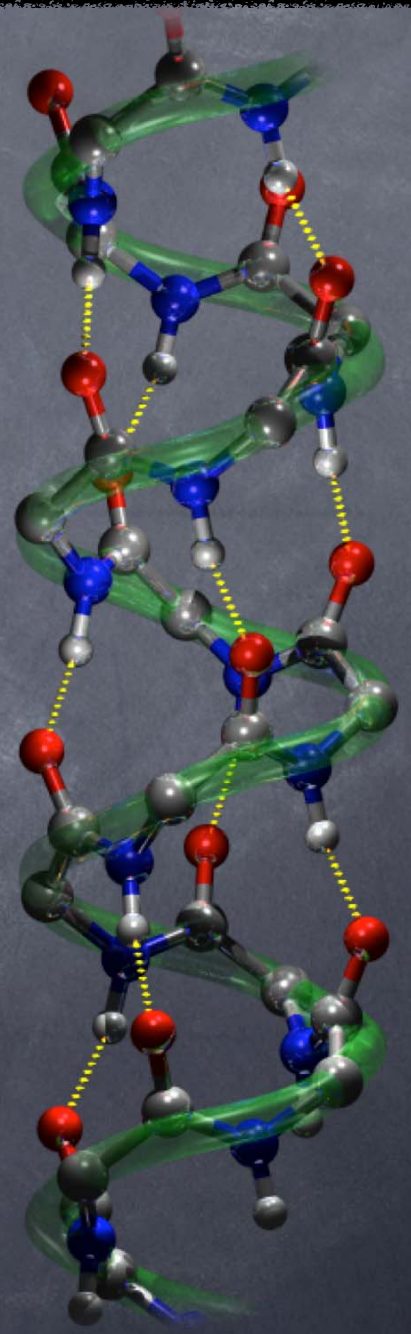
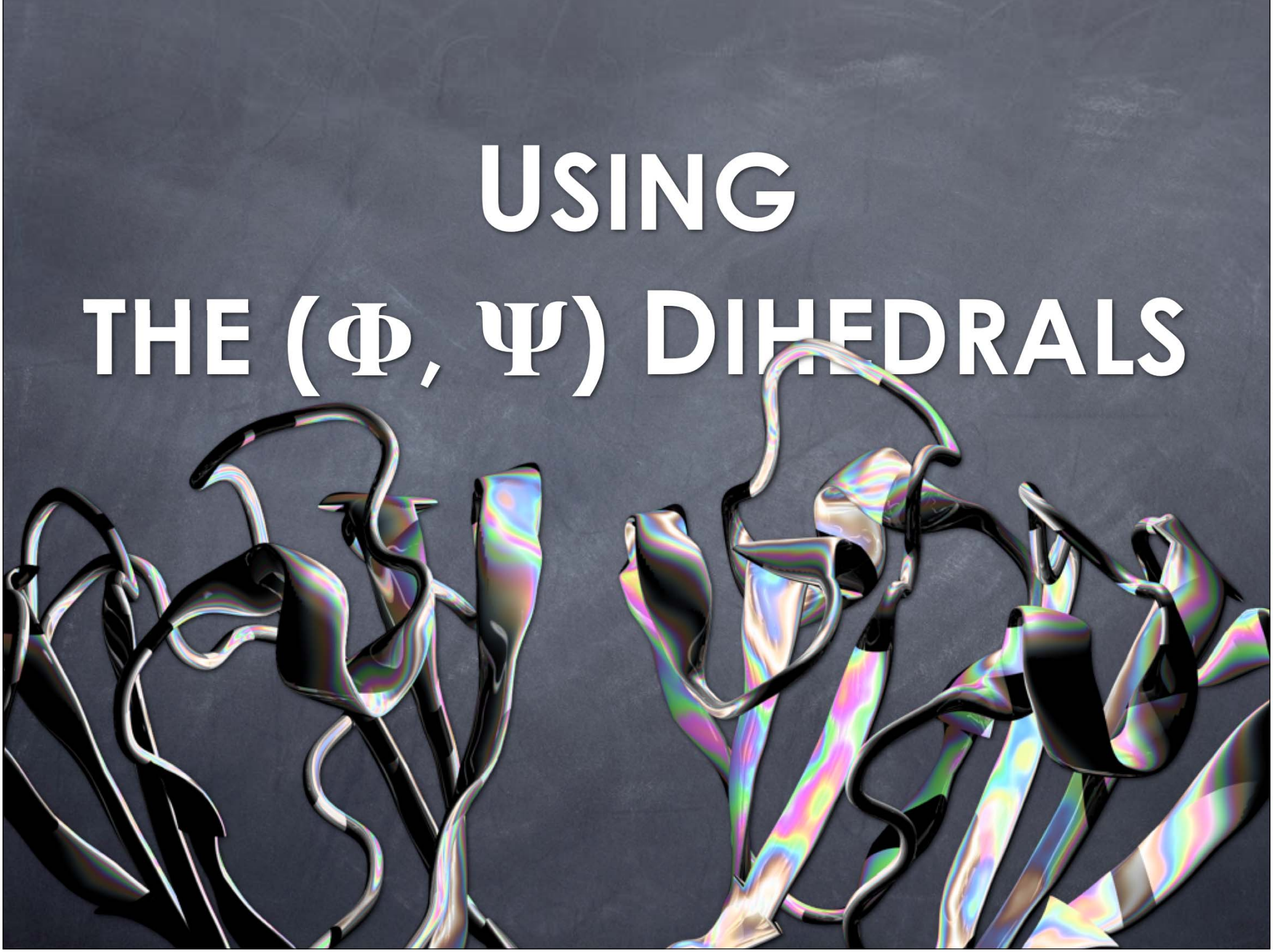
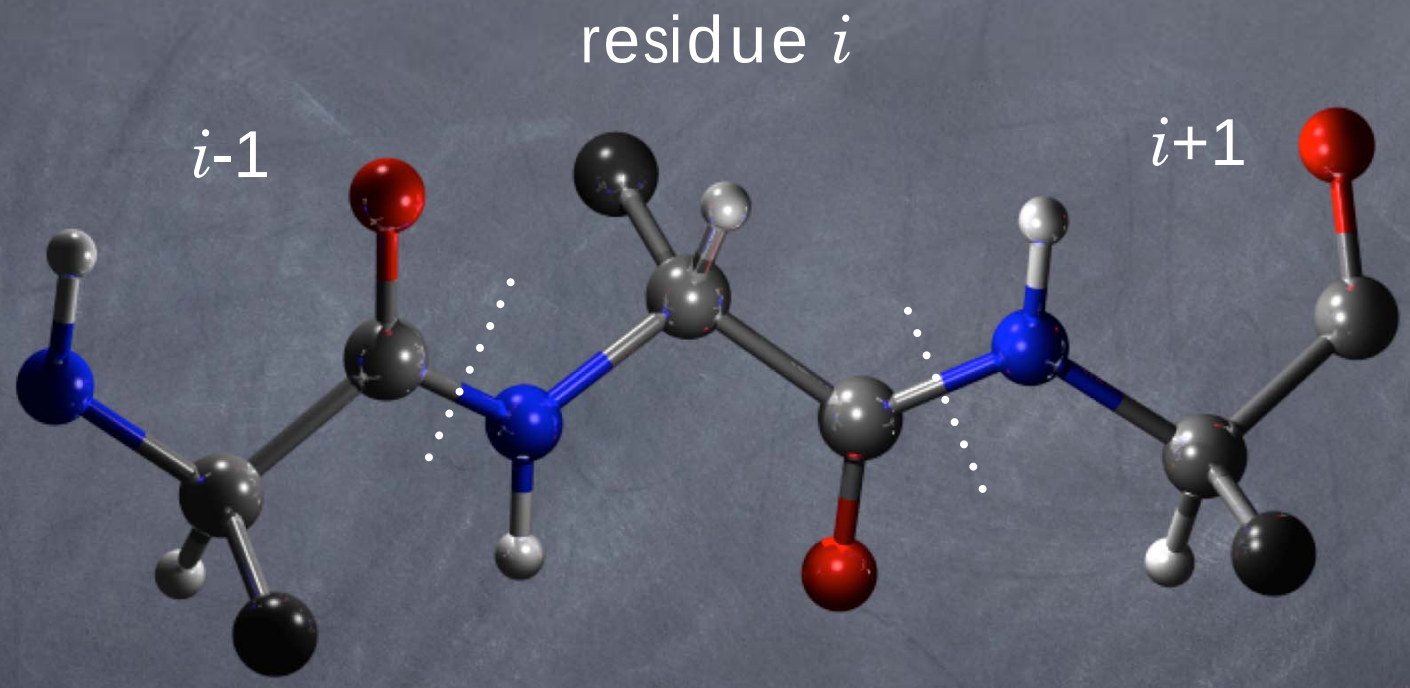
- SSE are defined with the backbone atoms only



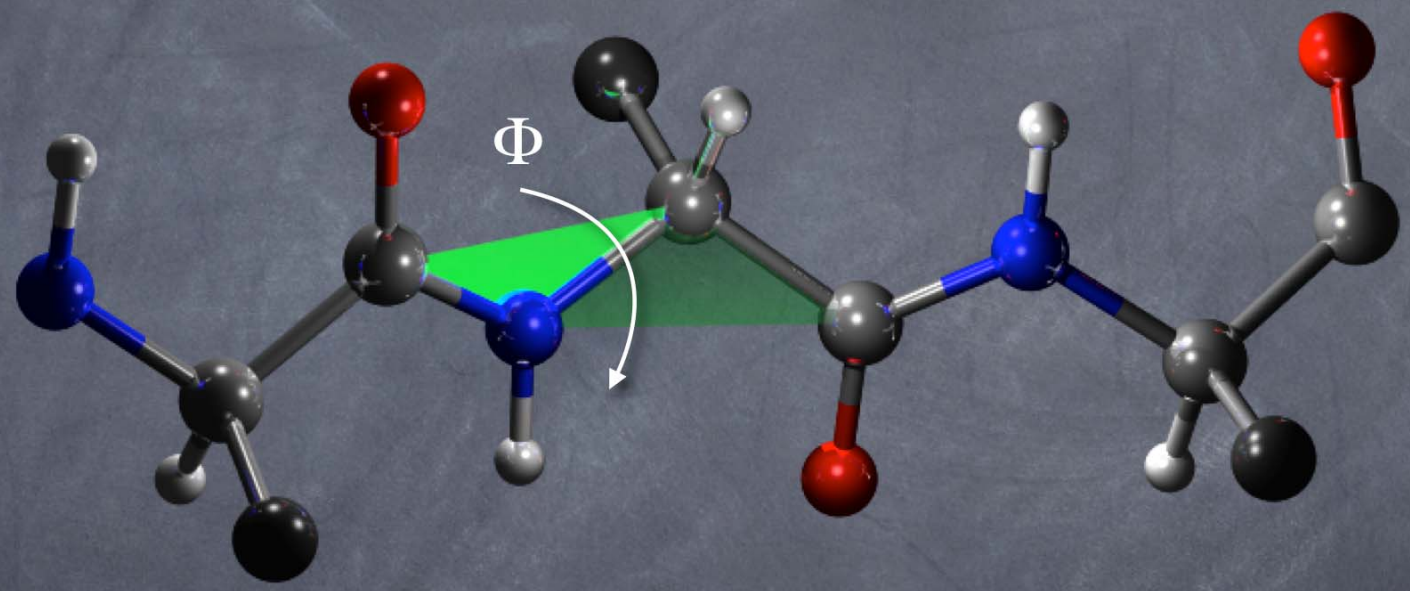
Using the (Φ, Ψ) Dihedrals



Φ, Ψ *and* ω

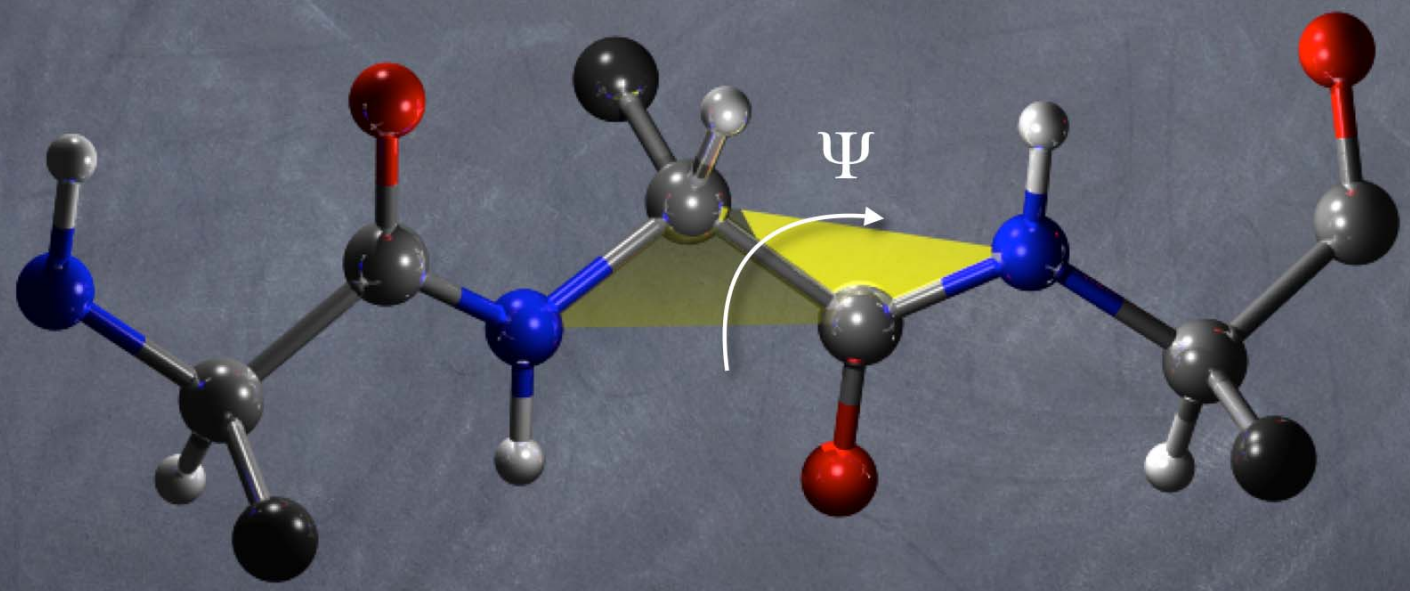


Φ, Ψ *and* ω



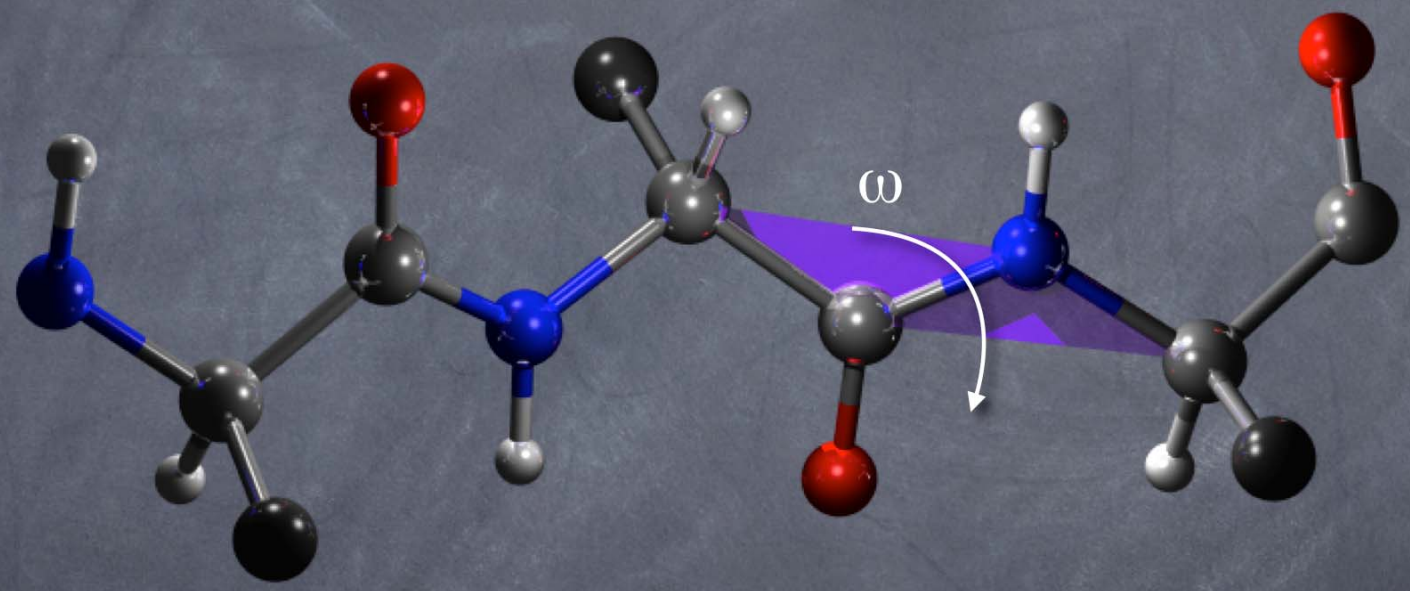
$\Phi=(C^{i-1}, N^{i}, C_{\alpha}^{i}, C^{i})$

Φ, Ψ *and* ω



$\Psi=(N^{i}, C_{\alpha}^{i}, C^{i}, N^{i+1})$

Φ, Ψ *and* ω



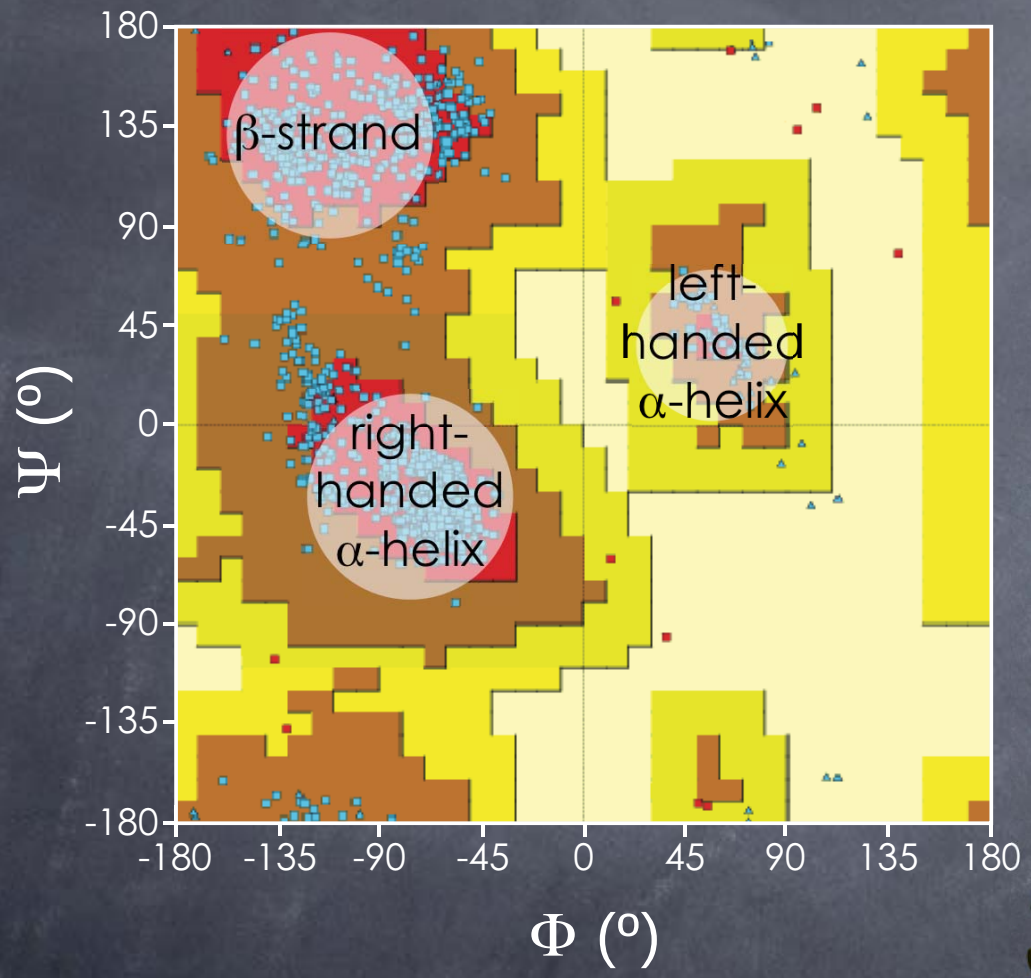
$\omega=(C_\alpha^{i}, C^{i}, N^{i+1}, C_\alpha^{i+1})$

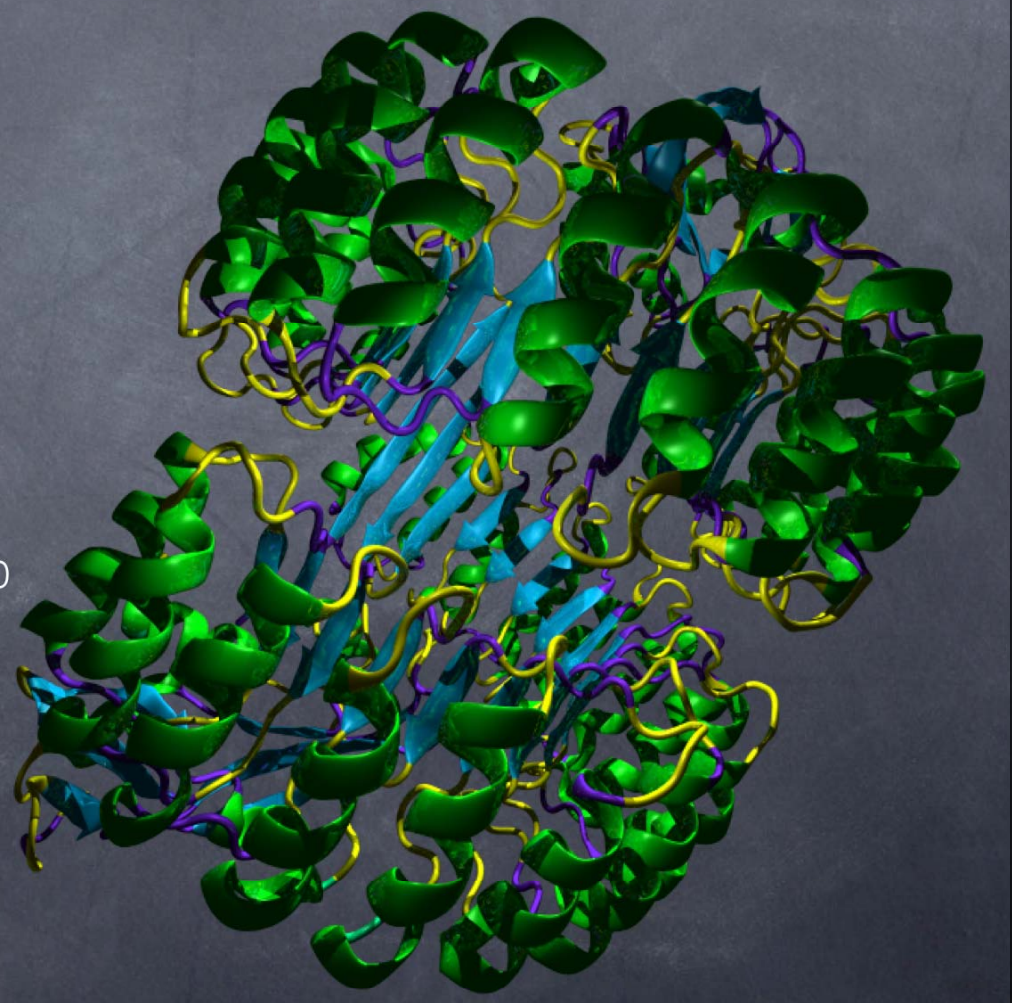
2 isomers: *Z* or *E*

Using Φ and Ψ to determine SSE

Repeating values of Φ and Ψ along the chain result in regular structures that can be identified on a map of the (Φ,Ψ) values: Ramanchandran's plot.

Using Φ and Ψ to determine SSE





Human placental RNase inhibitor in complex with the human angiogenin.

Using Φ and Ψ to determine SSE

Repeating values of Φ and Ψ along the chain result in regular structures that can be identified on a map of the (Φ,Ψ) values: Ramanchandran's plot.

SSE are defined from the repetition of characteristic average values of (Φ,Ψ) found:

α-helix	-50°,-50°
β-sheet	-110°,-140°
	+110,+135°
3_{10}-helix	-50°,-30°
π-helix	-60°,-80°
α_L-helix	+50°,+50°
polyGly, polyPro	-80°,+150°

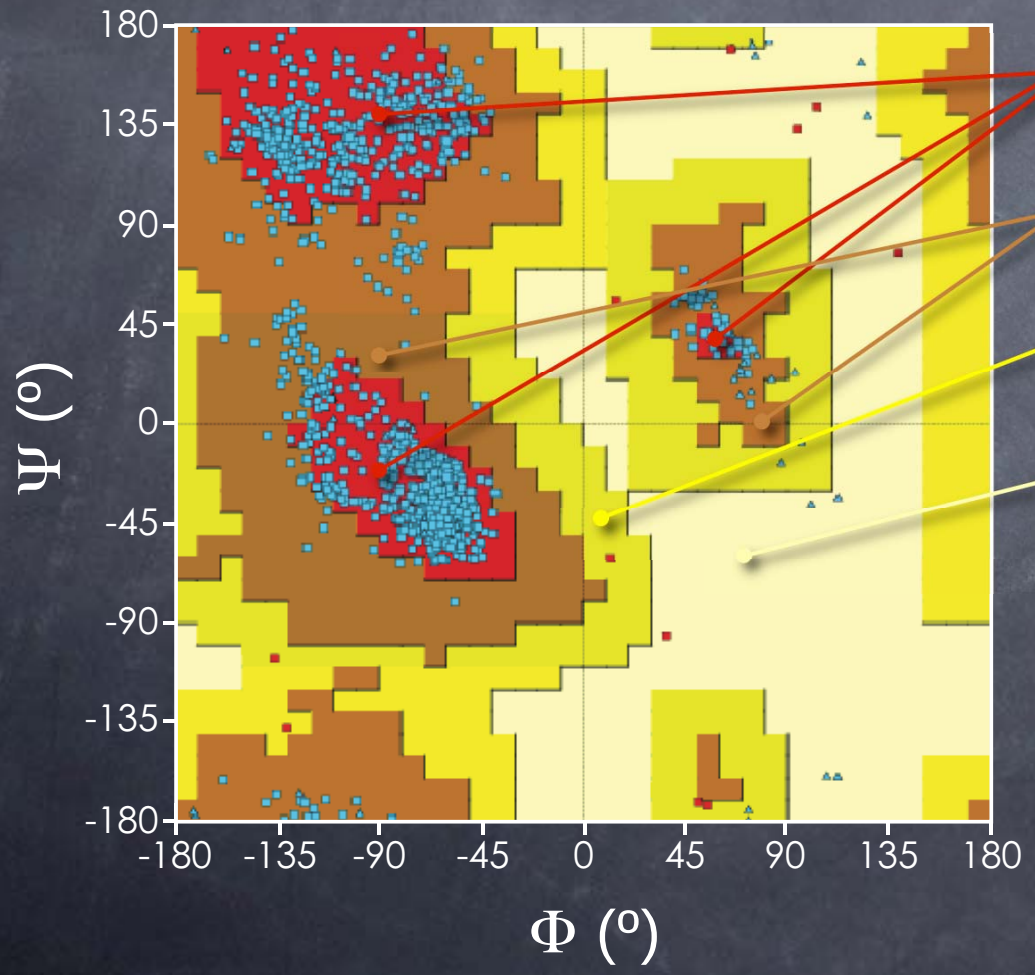
Using Φ and Ψ to determine SSE

Turn types are also defined using the (Φ,Ψ) values of the second and third residues.

	Φ_2,Ψ_2	Φ_3,Ψ_3
turn I	-60°,-30°	-90°,0
turn II	-60°,+120°	+80°,0
turn III	-60°,-30°	-60,-30°
turn IV	*not otherwise classified*	
turn V	-80°,+80°	+80°,-80°
turn VIa	-60°,+120°	-90°,0
turn VIb	-120°,+120°	-60°,0
turn VII	Ψ_2=+180°	Φ_3<+60°
	Ψ_2<+160°	Φ_3=+180°
turn VIII	-60°,-30°	-120°,+120°

Using Φ and Ψ to determine SSE

Today (Φ,Ψ) values are mostly used to validate/test the quality of a structure.



Most favoured regions

Additional allowed regions

Generously allowed regions

Disallowed regions

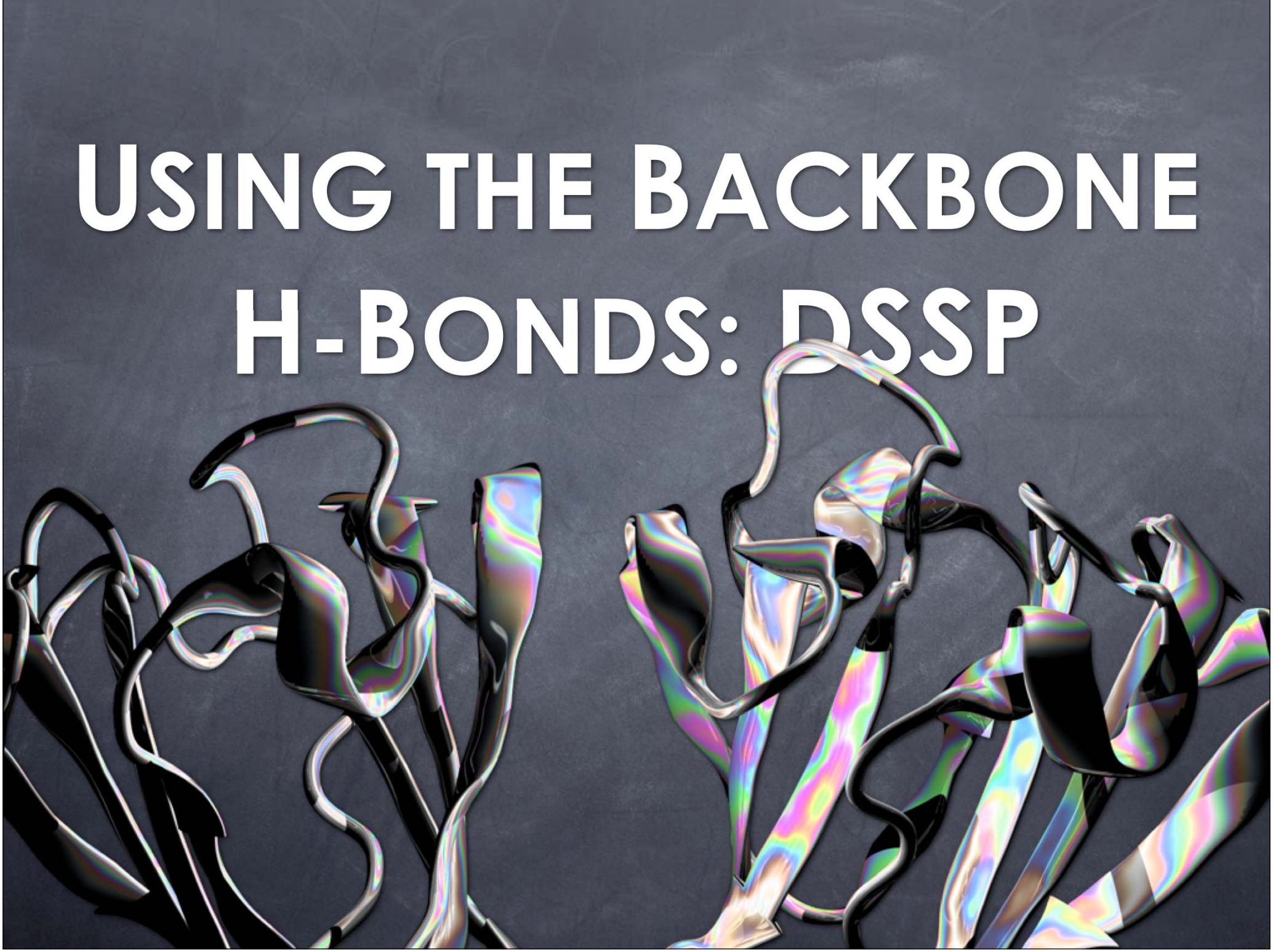
Programs:

PROCHECK

PDBsum (online)

plugins in various viewers

Using the Backbone H-Bonds: DSSP



Define Secondary Structure of Protein (DSSP)

Kabsch W & Sander C (1983) *Biopolymers* **22**, 2577-2637

Based on the X-ray structure of 62 different globular proteins (resolution 1.4–3.0 Å)

Only one parameter is used to define SSEs: H-bonds between backbone C=O and N-H.

H-bonds are defined with a Coulombian electrostatic interaction energy:

$$E = q_1 q_2 f \left(\frac{1}{r_{\mathrm{ON}}} + \frac{1}{r_{\mathrm{CH}}} + \frac{1}{r_{\mathrm{OH}}} + \frac{1}{r_{\mathrm{CN}}} \right)$$

q_1 = 0.42e

q_2 = 0.20e

f = 332 (E in kcal·mol^{-1} and r in Å)

Define Secondary Structure of Protein (DSSP)

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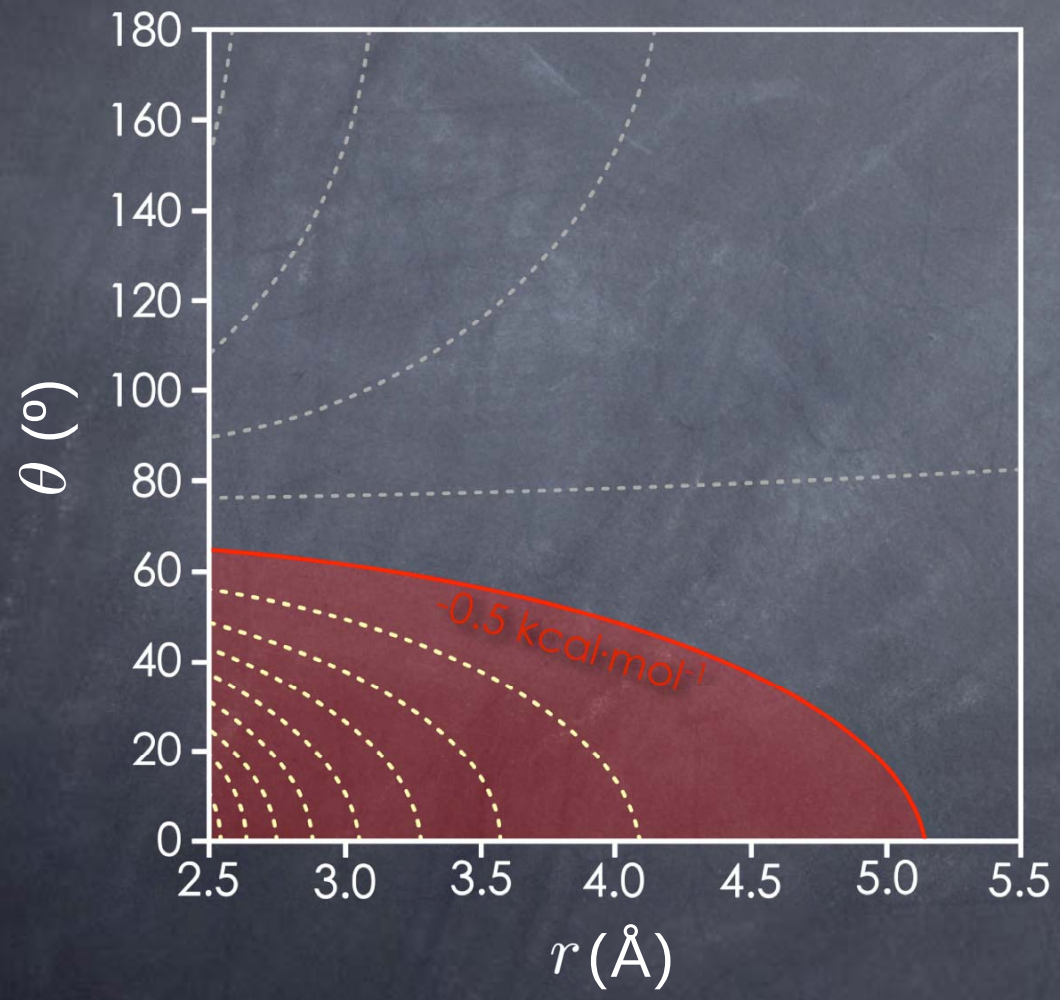
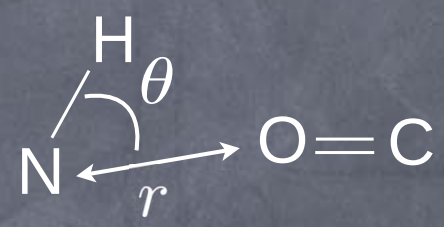




Energy cutoff for H-bonds:
$E \leq$ -0.5 kcal·mol^{-1}

r_{max} = 5.2 Å
θ_{max} = 63º

Define Secondary Structure of Protein (DSSP)

Kabsch W & Sander C (1983) *Biopolymers* **22**, 2577-2637

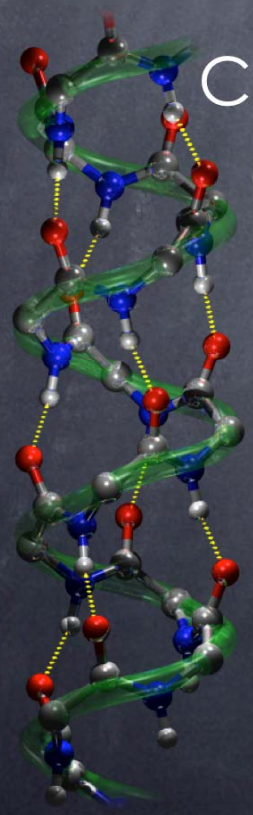
H-bonds between nearby residues

yes

n-turn

C=O^{i}···H-N^{i+n}

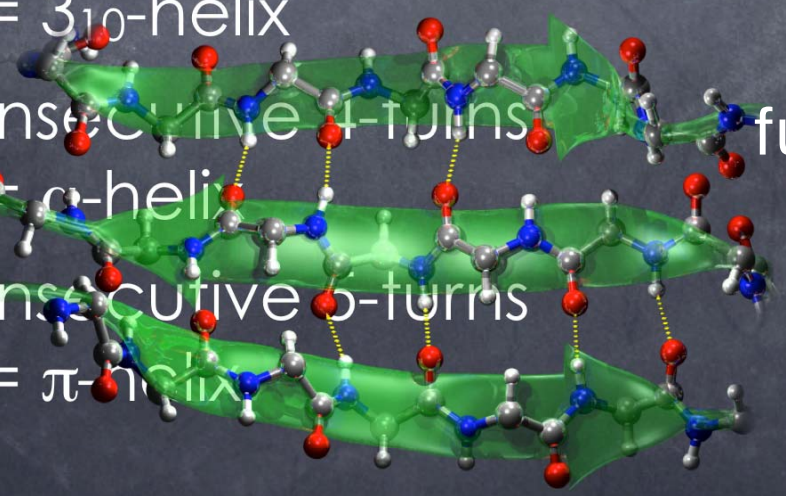
(n = 3,4,5)



→ consecutive 3-turns = 3_{10}-helix

→ consecutive 4-turns = α-helix

→ consecutive 5-turns = π-helix

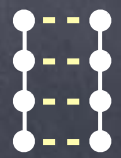


no

β-bridge

↓

consecutive β-bridges = β-ladder



↓

fused β-ladders = β-sheet

Define Secondary Structure of Protein (DSSP)

Kabsch W & Sander C (1983) *Biopolymers* **22**, 2577-2637

Easy and simple definition of SSEs:

n-helix: ≥ 2 consecutive n-turns

β-elements: a β-bridge between 2 residues i and j is defined when there are 2 H-bonds between 2 non-overlapping stretches of 3 consecutive residues each (i-1, i, i+1 and j-1, j, j+1).

- parallel β-bridge:
  (i-1, j) and (j, i+1) <u>or</u> (j-1, i) and (i, j+1)
- antiparallel β-bridge:
  (i, j) and (j, i) <u>or</u> (i-1, j+1) and (j-1, i+1)

Using DSSP

Download: http://swift.cmbi.kun.nl/gv/dssp/

GROMACS do_dssp uses DSSP (but as a black box).

DSSP provides a lot of geometrical and HB-related data, besides the basic assignment of secondary structures.

A DSSP Output File

```
==== Secondary Structure Definition by the program DSSP, updated CMBI version by ElmK / April 1,2000 ====
REFERENCE W. KABSCH AND C.SANDER, BIOPOLYMERS 22 (1983) 2577-2637
HEADER    TRANSFERASE/GROWTH FACTOR                10-SEP-02   1MOX
COMPND   2 MOLECULE: EPIDERMAL GROWTH FACTOR RECEPTOR;
SOURCE   2 ORGANISM_SCIENTIFIC: HOMO SAPIENS;
AUTHOR    T.P.J.GARRETT,N.M.MCKERN,M.LOU,T.C.ELLEMAN,T.E.ADAMS,
 1097  5 40 39  1 TOTAL NUMBER OF RESIDUES, NUMBER OF CHAINS, NUMBER OF SS-BRIDGES(TOTAL,INTRACHAIN,INTERCHAIN)
 49778.0   ACCESSIBLE SURFACE OF PROTEIN (ANGSTROM**2)
  692 63.1   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(J)  , SAME NUMBER PER 100 RESIDUES
  156 14.2   TOTAL NUMBER OF HYDROGEN BONDS IN     PARALLEL BRIDGES, SAME NUMBER PER 100 RESIDUES
  109  9.9   TOTAL NUMBER OF HYDROGEN BONDS IN ANTIPARALLEL BRIDGES, SAME NUMBER PER 100 RESIDUES
    8  0.7   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I-5), SAME NUMBER PER 100 RESIDUES
   10  0.9   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I-4), SAME NUMBER PER 100 RESIDUES
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    6  0.5   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I+5), SAME NUMBER PER 100 RESIDUES
  1  2  3  4  5  6  7  8  9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30     *** HISTOGRAMS OF ***
  0  0  0  4  0  2  0  0  0  0  0  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0    RESIDUES PER ALPHA HELIX
 14 17  6  5  4  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0    PARALLEL BRIDGES PER LADDER
 19  5  6  2  1  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0    ANTIPARALLEL BRIDGES PER LADDER
  6  1  3  4  6  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0    LADDERS PER SHEET

#  RESIDUE AA STRUCTURE BP1 BP2  ACC     N-H-->O    O-->H-N    N-H-->O    O-->H-N    TCO  KAPPA ALPHA  PHI   PSI   X-CA Y-CA Z-CA
  1    1 A L              0   0  118      0, 0.0     2,-0.1     0, 0.0   233,-0.0   0.000 360.0 360.0 360.0 -24.2 -10.7 44.3 21.8
  2    2 A E        -     0   0   79      1,-0.1     0, 0.0   231,-0.1     0, 0.0  -0.618 360.0-176.9-150.0  80.4  -7.4 42.5 20.8
  3    3 A E        -     0   0  182     -2,-0.1    -1,-0.1     3,-0.0     2,-0.0   0.908  15.3-142.7 -42.2-106.2  -5.4 41.6 23.9
  4    4 A K        -     0   0   83      2,-0.1    32,-0.1    32,-0.0    31,-0.0   0.331  31.0 -93.4 125.4 105.4  -1.9 40.0 23.4
  5    5 A K        -     0   0  137     30,-0.1    30,-2.9    29,-0.1    31,-1.8  -0.122  51.5-168.1 -41.1 113.1  -0.4 37.3 25.6
  6    6 A V  E     -a   36  0A   82     29,-0.2     2,-0.3    28,-0.2    31,-0.2  -0.786   7.3-174.2-110.8 154.1   1.6 39.1 28.2
  7    7 A a  E     -a   37  0A   19     29,-2.2    31,-2.1    -2,-0.3    32,-0.4  -0.955  29.0-110.7-145.1 165.0   4.1 37.8 30.7
  8    8 A Q        -     0   0  102     -2,-0.3    31,-1.9    29,-0.2     2,-0.2   0.984  39.6-151.7 -57.5 -79.2   6.3 38.8 33.7
  9    9 A G        -     0   0   16     21,-0.2     2,-0.3    29,-0.2    32,-0.2  -0.651  12.5-100.4 121.9 179.1  10.0 38.7 32.8
 10   10 A T  B     -F   40  0B   25     30,-1.5    30,-0.6    -2,-0.2     3,-0.0  -0.891  13.6-162.5-139.9 168.9  13.1 38.1 34.8
 11   11 A S        +     0   0   75     -2,-0.3  1032,-0.7    28,-0.1     3,-0.1  -0.206  51.5 119.4-144.8  46.4  16.1 39.7 36.6
 12   12 A N    >   -     0   0   20      1,-0.3     3,-3.1  1030,-0.2  1033,-0.1   0.403  46.6-171.8 -92.4  -0.2  18.7 37.0 37.2
 13   13 A K  T 3  S-     0   0   83      1,-0.3    -1,-0.3  1020,-0.1  1020,-0.1  -0.150  70.5 -13.2  43.2-121.3  21.3 38.8 35.1
 14   14 A L  T 3  S+     0   0    8   1018,-0.1    -1,-0.3    -3,-0.1     2,-0.1   0.309 106.2 120.0 -93.5  11.2  24.2 36.4 34.7
 15   15 A T    <   -     0   0    3     -3,-3.1     2,-0.4  1018,-0.1  1020,-0.2  -0.424  55.1-138.9 -76.6 148.7  23.1 33.9 37.3
 16   16 A Q  B     -g 1035  0C   13   1018,-2.9  1020,-2.1    -2,-0.1     2,-1.0  -0.872   7.2-140.2-107.0 141.2  22.3 30.3 36.5
 17   17 A L        -     0   0   19     -2,-0.4     2,-0.2  1018,-0.2     9,-0.2  -0.674  61.0 -66.3-103.0  79.9  19.4 28.5 38.1
 18   18 A G  S    S+     0   0   13     -2,-1.0  1018,-0.1  1018,-0.5  1019,-0.1  -0.514 104.7   3.8  79.0-148.1  20.7 25.1 38.9
 19   19 A T  S  > S-     0   0   77     -2,-0.2     4,-3.2     1,-0.1     5,-0.2  -0.075  78.9-104.9 -63.9 168.5  21.7 22.7 36.0
 20   20 A F  H  > S+     0   0   88      2,-0.2     4,-2.5     1,-0.2     5,-0.2   0.964 124.6  46.2 -60.0 -50.2  21.6 23.8 32.4
 21   21 A E  H  > S+     0   0  113      2,-0.2     4,-2.3     1,-0.2     5,-0.2   0.931 114.0  47.1 -58.3 -49.7  18.4 21.7 31.9
```

A DSSP Output File

```
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SOURCE    2 ORGANISM_SCIENTIFIC: HOMO SAPIENS;
AUTHOR    T.P.J.GARRETT,N.M.MCKERN,M.LOU,T.C.ELLEMAN,T.E.ADAMS,
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  0  0  0  4  0  2  0  0  0  0  0  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0    RESIDUES PER ALPHA HELIX
 14 17  6  5  4  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0    PARALLEL BRIDGES PER LADDER
 19  5  6  2  1  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0    ANTIPARALLEL BRIDGES PER LADDER
  6  1  3  4  6  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0    LADDERS PER SHEET

#  RESIDUE AA STRUCTURE BP1 BP2  ACC     N-H-->O    O-->H-N    N-H-->O    O-->H-N    TCO  KAPPA ALPHA  PHI   PSI   X-CA Y-CA Z-CA
  1    1 A L              0   0  118      0, 0.0     2,-0.1     0, 0.0   233,-0.0   0.000 360.0 360.0 360.0 -24.2 -10.7 44.3 21.8
  2    2 A E        -     0   0   79      1,-0.1     0, 0.0   231,-0.1     0, 0.0  -0.618 360.0-176.9-150.0  80.4  -7.4 42.5 20.8
  3    3 A E        -     0   0  182     -2,-0.1    -1,-0.1     3,-0.0     2,-0.0   0.908  15.3-142.7 -42.2-106.2  -5.4 41.6 23.9
  4    4 A K        -     0   0   83      2,-0.1    32,-0.1    32,-0.0    31,-0.0   0.331  31.0 -93.4 125.4 105.4  -1.9 40.0 23.4
  5    5 A K        -     0   0  137     30,-0.1    30,-2.9    29,-0.1    31,-1.8  -0.122  51.5-168.1 -41.1 113.1  -0.4 37.3 25.6
  6    6 A V  E     -a   36  0A   82     29,-0.2     2,-0.3    28,-0.2    31,-0.2  -0.786   7.3-174.2-110.8 154.1   1.6 39.1 28.2
  7    7 A a  E     -a   37  0A   19     29,-2.2    31,-2.1    -2,-0.3    32,-0.4  -0.955  29.0-110.7-145.1 165.0   4.1 37.8 30.7
  8    8 A Q        -     0   0  102     -2,-0.3    31,-1.9    29,-0.2     2,-0.2   0.984  39.6-151.7 -57.5 -79.2   6.3 38.8 33.7
  9    9 A G        -     0   0   16     21,-0.2     2,-0.3    29,-0.2    32,-0.2  -0.651  12.5-100.4 121.9 179.1  10.0 38.7 32.8
 10   10 A T  B     -F   40  0B   25     30,-1.5    30,-0.6    -2,-0.2     3,-0.0  -0.891  13.6-162.5-139.9 168.9  13.1 38.1 34.8
 11   11 A S        +     0   0   75     -2,-0.3  1032,-0.7    28,-0.1     3,-0.1  -0.206  51.5 119.4-144.8  46.4  16.1 39.7 36.6
 12   12 A N    >   -     0   0   20      1,-0.3     3,-3.1  1030,-0.2  1033,-0.1   0.403  46.6-171.8 -92.4  -0.2  18.7 37.0 37.2
 13   13 A K  T 3  S-     0   0   83      1,-0.3    -1,-0.3  1020,-0.1  1020,-0.1  -0.150  70.5 -13.2  43.2-121.3  21.3 38.8 35.1
 14   14 A L  T 3  S+     0   0    8   1018,-0.1    -1,-0.3    -3,-0.1     2,-0.1   0.309 106.2 120.0 -93.5  11.2  24.2 36.4 34.7
 15   15 A T    <   -     0   0    3     -3,-3.1     2,-0.4  1018,-0.1  1020,-0.2  -0.424  55.1-138.9 -76.6 148.7  23.1 33.9 37.3
 16   16 A Q  B     -g 1035  0C   13   1018,-2.9  1020,-2.1    -2,-0.1     2,-1.0  -0.872   7.2-140.2-107.0 141.2  22.3 30.3 36.5
 17   17 A L        -     0   0   19     -2,-0.4     2,-0.2  1018,-0.2     9,-0.2  -0.674  61.0 -66.3-103.0  79.9  19.4 28.5 38.1
 18   18 A G  S    S+     0   0   13     -2,-1.0  1018,-0.1  1018,-0.5  1019,-0.1  -0.514 104.7   3.8  79.0-148.1  20.7 25.1 38.9
 19   19 A T  S  > S-     0   0   77     -2,-0.2     4,-3.2     1,-0.1     5,-0.2  -0.075  78.9-104.9 -63.9 168.5  21.7 22.7 36.0
 20   20 A F  H  > S+     0   0   88      2,-0.2     4,-2.5     1,-0.2     5,-0.2   0.964 124.6  46.2 -60.0 -50.2  21.6 23.8 32.4
 21   21 A E  H  > S+     0   0  113      2,-0.2     4,-2.3     1,-0.2     5,-0.2   0.931 114.0  47.1 -58.3 -49.7  18.4 21.7 31.9
```

Remarks from the header of the PDB file

A DSSP Output File

```
==== Secondary Structure Definition by the program DSSP, updated CMBI version by ElmK / April 1,2000 ====
REFERENCE W. KABSCH AND C.SANDER, BIOPOLYMERS 22 (1983) 2577-2637
HEADER    TRANSFERASE/GROWTH FACTOR                10-SEP-02   1MOX
COMPND   2 MOLECULE: EPIDERMAL GROWTH FACTOR RECEPTOR;
SOURCE   2 ORGANISM_SCIENTIFIC: HOMO SAPIENS;
AUTHOR    T.P.J.GARRETT,N.M.MCKERN,M.LOU,T.C.ELLEMAN,T.E.ADAMS,
 1097  5 40 39  1 TOTAL NUMBER OF RESIDUES, NUMBER OF CHAINS, NUMBER OF SS-BRIDGES(TOTAL,INTRACHAIN,INTERCHAIN)
 49778.0   ACCESSIBLE SURFACE OF PROTEIN (ANGSTROM**2)
  692 63.1   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(J)  , SAME NUMBER PER 100 RESIDUES
  156 14.2   TOTAL NUMBER OF HYDROGEN BONDS IN     PARALLEL BRIDGES, SAME NUMBER PER 100 RESIDUES
  109  9.9   TOTAL NUMBER OF HYDROGEN BONDS IN ANTIPARALLEL BRIDGES, SAME NUMBER PER 100 RESIDUES
    8  0.7   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I-5), SAME NUMBER PER 100 RESIDUES
   10  0.9   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I-4), SAME NUMBER PER 100 RESIDUES
    5  0.5   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I-3), SAME NUMBER PER 100 RESIDUES
    0  0.0   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I-2), SAME NUMBER PER 100 RESIDUES
    0  0.0   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I-1), SAME NUMBER PER 100 RESIDUES
    0  0.0   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I+0), SAME NUMBER PER 100 RESIDUES
    0  0.0   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I+1), SAME NUMBER PER 100 RESIDUES
  132 12.0   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I+2), SAME NUMBER PER 100 RESIDUES
  145 13.2   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I+3), SAME NUMBER PER 100 RESIDUES
   56  5.1   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I+4), SAME NUMBER PER 100 RESIDUES
    6  0.5   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I+5), SAME NUMBER PER 100 RESIDUES
```


```
 1097  5 40 39  1 TOTAL NUMBER OF RESIDUES,NUMBER OF CHAINS,NUMBER OF SS-BRIDGES(TOTAL,INTRACHAIN,INTERCHAIN)
 49778.0   ACCESSIBLE SURFACE OF PROTEIN (ANGSTROM**2)
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    0  0.0   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I-2), SAME NUMBER PER 100 RESIDUES
    0  0.0   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I-1), SAME NUMBER PER 100 RESIDUES
    0  0.0   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I+0), SAME NUMBER PER 100 RESIDUES
    0  0.0   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I+1), SAME NUMBER PER 100 RESIDUES
  132 12.0   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I+2), SAME NUMBER PER 100 RESIDUES
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   56  5.1   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I+4), SAME NUMBER PER 100 RESIDUES
    6  0.5   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I+5), SAME NUMBER PER 100 RESIDUES
```


```
#    1    2 A E         -     0   0   79     1,-0.1     0, 0.0   231,-0.1     0, 0.0  -0.618 360.0-176.9-150.0  80.4  -7.4 42.5 20.8
     2    3 A E         -     0   0  182    -2,-0.1    -1,-0.1     3,-0.0     2,-0.0   0.908  15.3-142.7 -42.2-106.2  -5.4 41.6 23.9
     3    4 A K         -     0   0   83     2,-0.1    32,-0.1    32,-0.0    31,-0.0   0.931  31.0  93.4 [illegible]  [illegible] [illegible] [illegible] 23.4
     4    5 A K         -     0   0  137    30,-0.1    30,-2.9    29,-0.1    31,-0.1   [illegible]  [illegible] [illegible] [illegible] [illegible] [illegible] [illegible] 25.6
     5    6 A V   E    -a    36  0A   82    29,-0.2     2,-0.3    28,-0.2    31,-0.2  -0.786   7.3-174.2-110.8 154.1   1.6 39.1 28.2
     6    7 A a   E    -a    37  0A   19    29,-2.2    31,-2.1    -2,-0.3    32,-0.4  -0.955  29.0-110.7-145.1 165.0   4.1 37.8 30.7
     7    8 A Q         -     0   0  102    -2,-0.3    31,-1.9    29,-0.2     2,-0.2   0.984  39.6-151.7 -57.5 -79.2   6.3 38.8 33.7
     8    9 A G         -     0   0   16    21,-0.2     2,-0.3    29,-0.2    32,-0.2  -0.651  12.5-100.4 121.9 179.1  10.0 38.7 32.8
    9   10 A T   B    -F    40  0B   25    30,-1.5    30,-0.6    -2,-0.2     3,-0.0  -0.891  13.6-162.5-139.9 168.9  13.1 38.1 34.8
    10   11 A S         +     0   0   75    -2,-0.3  1032,-0.7    28,-0.1     3,-0.1  -0.206  51.5 119.4-144.8  46.4  16.1 39.7 36.6
    11   12 A N    >    -     0   0   20     1,-0.3     3,-3.1  1030,-0.2  1033,-0.1   0.403  46.6-171.8 -92.4  -0.2  18.7 37.0 37.2
    12   13 A K   T 3  S-     0   0   83     1,-0.3    -1,-0.3  1020,-0.1  1020,-0.1  -0.150  70.5 -13.2  43.2-121.3  21.3 38.8 35.1
    13   14 A L   T 3  S+     0   0    8  1018,-0.1    -1,-0.3    -3,-0.1     2,-0.1   0.309 106.2 120.0 -93.5  11.2  24.2 36.4 34.7
    14   15 A T    <   -     0   0    3    -3,-3.1     2,-0.4  1018,-0.1  1020,-0.2  -0.424  55.1-138.9 -76.6 148.7  23.1 33.9 37.3
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    16   17 A L         -     0   0   19    -2,-0.4     2,-0.2  1018,-0.2     9,-0.2  -0.674  61.0 -66.3-103.0  79.9  19.4 28.5 38.1
    17   18 A G   S    S+     0   0   13    -2,-1.0  1018,-0.1  1018,-0.5  1019,-0.1  -0.514 104.7   3.8  79.0-148.1  20.7 25.1 38.9
    18   19 A T   S  > S-     0   0   77    -2,-0.2     4,-3.2     1,-0.1     5,-0.2  -0.075  78.9-104.9 -63.9 168.5  21.7 22.7 36.0
    19   20 A F   H  > S+     0   0   88     2,-0.2     4,-2.5     1,-0.2     5,-0.2   0.964 124.6  46.2 -60.0 -50.2  21.6 23.8 32.4
    20   21 A E   H  > S+     0   0  113     2,-0.2     4,-2.3     1,-0.2     5,-0.2   0.931 114.0  47.1 -58.3 -49.7  18.4 21.7 31.9
```

H-Bonds and SSE stats

A DSSP Output File

```
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REFERENCE W. KABSCH AND C.SANDER, BIOPOLYMERS 22 (1983) 2577-2637
HEADER    TRANSFERASE/GROWTH FACTOR                10-SEP-02   1MOX
COMPND   2 MOLECULE: EPIDERMAL GROWTH FACTOR RECEPTOR;
SOURCE   2 ORGANISM_SCIENTIFIC: HOMO SAPIENS;
AUTHOR    T.P.J.GARRETT,N.M.MCKERN,M.LOU,T.C.ELLEMAN,T.E.ADAMS,
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   10  0.9   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I-4), SAME NUMBER PER 100 RESIDUES
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    0  0.0   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I-2), SAME NUMBER PER 100 RESIDUES
    0  0.0   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I-1), SAME NUMBER PER 100 RESIDUES
    0  0.0   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I+0), SAME NUMBER PER 100 RESIDUES
    0  0.0   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I+1), SAME NUMBER PER 100 RESIDUES
  132 12.0   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I+2), SAME NUMBER PER 100 RESIDUES
  145 13.2   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I+3), SAME NUMBER PER 100 RESIDUES
   56  5.1   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I+4), SAME NUMBER PER 100 RESIDUES
    6  0.5   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I+5), SAME NUMBER PER 100 RESIDUES
```

β-bridges

H-Bonds and SSE stats

A DSSP Output File

```
==== Secondary Structure Definition by the program DSSP, updated CMBI version by ElmK / April 1,2000 ====
REFERENCE W. KABSCH AND C.SANDER, BIOPOLYMERS 22 (1983) 2577-2637
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COMPND   2 MOLECULE: EPIDERMAL GROWTH FACTOR RECEPTOR;
SOURCE   2 ORGANISM_SCIENTIFIC: HOMO SAPIENS;
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  109  9.9   TOTAL NUMBER OF HYDROGEN BONDS IN ANTIPARALLEL BRIDGES, SAME NUMBER PER 100 RESIDUES
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    5  0.5   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I-3), SAME NUMBER PER 100 RESIDUES
    0  0.0   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I-2), SAME NUMBER PER 100 RESIDUES
    0  0.0   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I-1), SAME NUMBER PER 100 RESIDUES
    0  0.0   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I+0), SAME NUMBER PER 100 RESIDUES
    0  0.0   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I+1), SAME NUMBER PER 100 RESIDUES
  132 12.0   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I+2), SAME NUMBER PER 100 RESIDUES
  145 13.2   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I+3), SAME NUMBER PER 100 RESIDUES
   56  5.1   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I+4), SAME NUMBER PER 100 RESIDUES
    6  0.5   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I+5), SAME NUMBER PER 100 RESIDUES
```

γ-turns

H-Bonds and SSE stats

```
#  RESIDUE AA STRUCTURE BP1 BP2  ACC     N-H-->O    O-->H-N    N-H-->O    O-->H-N    TOTAL     PHI     PSI  X-CA   Y-CA   Z-CA
  1    2 A E        -    0   0   79    0, 0.0     0, 0.0   231,-0.1     0, 0.0  -0.618 360.0-176.9-150.0  80.4   -7.4  44.3  21.8
  2    3 A E        -    0   0  182   -2,-0.1    -1,-0.1     3,-0.0     2, 0.0   0.908  15.3-142.7 -42.2-106.2   -5.4  41.6  23.9
  3    4 A K        -    0   0   83    2,-0.1    32,-0.1    32,-0.0    31,-0.0   0.931  31.1 -93.4 -120.9 -90.0   -0.0  40.0  23.4
  4    5 A K        -    0   0  137   30,-0.1    30,-2.9    29,-0.1    31,-0.1   0.931  [illegible]  [illegible]  [illegible]  [illegible]  [illegible]  [illegible]  25.6
  5    6 A V  E    -a   36  0A   82   29,-0.2     2,-0.3    28,-0.2    31,-0.2  -0.786   7.3-174.2-110.8 154.1   1.6  39.1  28.2
  6    7 A a  E    -a   37  0A   19   29,-2.2    31,-2.1    -2,-0.3    32,-0.4  -0.955  29.0-110.7-145.1 165.0   4.1  37.8  30.7
  7    8 A Q        -    0   0  102   -2,-0.3    31,-1.9    29,-0.2     2,-0.2   0.984  39.6-151.7 -57.5 -79.2   6.3  38.8  33.7
  8    9 A G        -    0   0   16   21,-0.2     2,-0.3    29,-0.2    32,-0.2  -0.651  12.5-100.4 121.9 179.1  10.0  38.7  32.8
  9   10 A T  B    -F   40  0B   25   30,-1.5    30,-0.6    -2,-0.2     3,-0.0  -0.891  13.6-162.5-139.9 168.9  13.1  38.1  34.8
 10   11 A S       +    0   0   75   -2,-0.3  1032,-0.7    28,-0.1     3,-0.1  -0.206  51.5 119.4-144.8  46.4  16.1  39.7  36.6
 11   12 A N    >  -    0   0   20    1,-0.3     3,-3.1  1030,-0.2  1033,-0.1   0.403  46.6-171.8 -92.4  -0.2  18.7  37.0  37.2
 12   13 A K  T 3  S-    0   0   83    1,-0.3    -1,-0.3  1020,-0.1  1020,-0.1  -0.150  70.5 -13.2  43.2-121.3  21.3  38.8  35.1
 13   14 A L  T 3  S+    0   0    8 1018,-0.1    -1,-0.3    -3,-0.1     2,-0.1   0.309 106.2 120.0 -93.5  11.2  24.2  36.4  34.7
 14   15 A T    <  -    0   0    3   -3,-3.1     2,-0.4  1018,-0.1  1020,-0.2  -0.424  55.1-138.9 -76.6 148.7  23.1  33.9  37.3
 15   16 A Q  B    -g 1035  0C   13 1018,-2.9  1020,-2.1    -2,-0.1     2,-1.0  -0.872   7.2-140.2-107.0 141.2  22.3  30.3  36.5
 16   17 A L       -    0   0   19   -2,-0.4     2,-0.2  1018,-0.2     9,-0.2  -0.674  61.0 -66.3-103.0  79.9  19.4  28.5  38.1
 17   18 A G  S    S+   0   0   13   -2,-1.0  1018,-0.1  1018,-0.5  1019,-0.1  -0.514 104.7   3.8  79.0-148.1  20.7  25.1  38.9
 18   19 A T  S  > S-   0   0   77   -2,-0.2     4,-3.2     1,-0.1     5,-0.2  -0.075  78.9-104.9 -63.9 168.5  21.7  22.7  36.0
 19   20 A F  H  > S+   0   0   88    2,-0.2     4,-2.5     1,-0.2     5,-0.2   0.964 124.6  46.2 -60.0 -50.2  21.6  23.8  32.4
 20   21 A E  H  > S+   0   0  113    2,-0.2     4,-2.3     1,-0.2     5,-0.2   0.931 114.0  47.1 -58.3 -49.7  18.4  21.7  31.9
```

A DSSP Output File

```
==== Secondary Structure Definition by the program DSSP, updated CMBI version by ElmK / April 1,2000 ====
REFERENCE W. KABSCH AND C.SANDER, BIOPOLYMERS 22 (1983) 2577-2637
HEADER    TRANSFERASE/GROWTH FACTOR                10-SEP-02   1MOX
COMPND   2 MOLECULE: EPIDERMAL GROWTH FACTOR RECEPTOR;
SOURCE   2 ORGANISM_SCIENTIFIC: HOMO SAPIENS;
AUTHOR    T.P.J.GARRETT,N.M.MCKERN,M.LOU,T.C.ELLEMAN,T.E.ADAMS,
 1097  5 40 39  1 TOTAL NUMBER OF RESIDUES, NUMBER OF CHAINS, NUMBER OF SS-BRIDGES(TOTAL,INTRACHAIN,INTERCHAIN)
 49778.0   ACCESSIBLE SURFACE OF PROTEIN (ANGSTROM**2)
  692 63.1   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(J)  , SAME NUMBER PER 100 RESIDUES
  156 14.2   TOTAL NUMBER OF HYDROGEN BONDS IN     PARALLEL BRIDGES, SAME NUMBER PER 100 RESIDUES
  109  9.9   TOTAL NUMBER OF HYDROGEN BONDS IN ANTIPARALLEL BRIDGES, SAME NUMBER PER 100 RESIDUES
    8  0.7   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I-5), SAME NUMBER PER 100 RESIDUES
   10  0.9   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I-4), SAME NUMBER PER 100 RESIDUES
    5  0.5   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I-3), SAME NUMBER PER 100 RESIDUES
    0  0.0   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I-2), SAME NUMBER PER 100 RESIDUES
    0  0.0   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I-1), SAME NUMBER PER 100 RESIDUES
    0  0.0   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I+0), SAME NUMBER PER 100 RESIDUES
    0  0.0   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I+1), SAME NUMBER PER 100 RESIDUES
  132 12.0   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I+2), SAME NUMBER PER 100 RESIDUES
  145 13.2   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I+3), SAME NUMBER PER 100 RESIDUES
   56  5.1   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I+4), SAME NUMBER PER 100 RESIDUES
    6  0.5   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I+5), SAME NUMBER PER 100 RESIDUES
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3_{10}-helices

H-Bonds and SSE stats

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#  RESIDUE AA STRUCTURE BP1 BP2  ACC     N-H-->O    O-->H-N    N-H-->O    O-->H-N    TOTAL     TCO  KAPPA   ALPHA    PHI    PSI    X-CA   Y-CA   Z-CA
  1    2 A E        -     0   0   79    0, 0.0     0, 0.0   231,-0.1     0, 0.0  -0.618 360.0-176.9-150.0  80.4  -7.4  42.5  20.8
  2    3 A E        -     0   0  182   -2,-0.1    -1,-0.1     3,-0.0     2, 0.0   0.908  15.3-142.7 -42.2 106.2  -5.4  41.6  23.9
  3    4 A K        -     0   0   83    2,-0.1    32,-0.1    32,-0.0    31,-0.0   0.931  31.6 -93.4 -120.9 -90.0  -0.0  40.0  23.4
  4    5 A K        -     0   0  137   30,-0.1    30,-2.9    29,-0.1    31,-0.2  -0.786   7.3-174.2-110.8 154.1   1.6  39.1  25.6
  5    6 A V  E     -a   36  0A   82   29,-0.2     2,-0.3    28,-0.2    31,-0.4  -0.955  29.0-110.7-145.1 165.0   4.1  37.8  28.2
  6    7 A a  E     -a   37  0A   19   29,-2.2    31,-2.1    -2,-0.3    32,-0.4   0.984  39.6-151.7 -57.5 -79.2   6.3  38.8  33.7
  7    8 A Q        -     0   0  102   -2,-0.3    31,-1.9    29,-0.2     2,-0.2  -0.651  12.5-100.4 121.9 179.1  10.0  38.7  32.8
  8    9 A G        -     0   0   16   21,-0.2     2,-0.3    29,-0.2    32,-0.2  -0.891  13.6-162.5-139.9 168.9  13.1  38.1  34.8
  9   10 A T  B     -F   40  0B   25   30,-1.5    30,-0.6    -2,-0.2     3,-0.0  -0.206  51.5 119.4-144.8  46.4  16.1  39.7  36.6
 10   11 A S        +     0   0   75   -2,-0.3  1032,-0.7    28,-0.1     3,-0.1   0.403  46.6-171.8 -92.4  -0.2  18.7  37.0  37.2
 11   12 A N    >   -     0   0   20    1,-0.3     3,-3.1  1030,-0.2  1033,-0.1  -0.150  70.5 -13.2  43.2-121.3  21.3  38.8  35.1
 12   13 A K  T 3  S-     0   0   83    1,-0.3    -1,-0.3  1020,-0.1  1020,-0.1   0.309 106.2 120.0 -93.5  11.2  24.2  36.4  34.7
 13   14 A L  T 3  S+     0   0    8 1018,-0.1    -1,-0.3    -3,-0.1     2,-0.1  -0.424  55.1-138.9 -76.6 148.7  23.1  33.9  37.3
 14   15 A T    <   -     0   0    3   -3,-3.1     2,-0.4  1018,-0.1  1020,-0.2  -0.872   7.2-140.2-107.0 141.2  22.3  30.3  36.5
 15   16 A Q  B     -g 1035  0C   13 1018,-2.9  1020,-2.1    -2,-0.1     2,-1.0  -0.674  61.0 -66.3-103.0  79.9  19.4  28.5  38.1
 16   17 A L        -     0   0   19   -2,-0.4     2,-0.2  1018,-0.2     9,-0.2  -0.514 104.7   3.8  79.0-148.1  20.7  25.1  38.9
 17   18 A G  S    S+     0   0   13   -2,-1.0  1018,-0.1  1018,-0.5  1019,-0.1   0.075  78.9-104.9 -63.9 168.5  21.7  22.7  36.0
 18   19 A T  S  > S-     0   0   77   -2,-0.2     4,-3.2     1,-0.1     5,-0.2   0.964 124.6  46.2 -60.0 -50.2  21.6  23.8  32.4
 19   20 A F  H  > S+     0   0   88    2,-0.2     4,-2.5     1,-0.2     5,-0.2   0.931 114.0  47.1 -58.3 -49.7  18.4  21.7  31.9
 20   21 A E  H  > S+     0   0  113    2,-0.2     4,-2.3     1,-0.2     5,-0.2
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A DSSP Output File

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==== Secondary Structure Definition by the program DSSP, updated CMBI version by ElmK / April 1,2000 ====
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SOURCE   2 ORGANISM_SCIENTIFIC: HOMO SAPIENS;
AUTHOR    T.P.J.GARRETT,N.M.MCKERN,M.LOU,T.C.ELLEMAN,T.E.ADAMS,
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    0  0.0   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I-2), SAME NUMBER PER 100 RESIDUES
    0  0.0   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I-1), SAME NUMBER PER 100 RESIDUES
    0  0.0   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I+0), SAME NUMBER PER 100 RESIDUES
    0  0.0   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I+1), SAME NUMBER PER 100 RESIDUES
  132 12.0   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I+2), SAME NUMBER PER 100 RESIDUES
  145 13.2   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I+3), SAME NUMBER PER 100 RESIDUES
   56  5.1   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I+4), SAME NUMBER PER 100 RESIDUES
    6  0.5   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I+5), SAME NUMBER PER 100 RESIDUES
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α-helices

H-Bonds and SSE stats

A DSSP Output File

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    0  0.0   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I-1), SAME NUMBER PER 100 RESIDUES
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  132 12.0   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I+2), SAME NUMBER PER 100 RESIDUES
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```

π-helices

```
#  RESIDUE AAA STRUCTURE BP1 BP2  ACC     N-H-->O  O-->H-N    N-H-->O  O-->H-N    TCO  KAPPA  PHI   PSI    X-CA   Y-CA   Z-CA
  1    2 A E        -     0   0   79      1,-0.1     0, 0.0   231,-0.1     0, 0.0  -0.618 360.0-176.9-150.0  80.4  -7.4  42.5  20.8
  2    3 A E        -     0   0  182     -2,-0.1    -1,-0.1     3,-0.0     2, 0.0   0.908  15.3-142.7 -42.2 106.2  -5.4  41.6  23.9
  3    4 A K        -     0   0   83      2,-0.1    32,-0.1    32,-0.0    31,-0.0   0.931  31.6 -93.4 -121.7 -62.3  -0.0  40.0  23.4
  4    5 A K        -     0   0  137     30,-0.1    30,-2.9    29,-0.1    31,-0.2   0.786  25.6 -113.3 -93.4 -121.7 -62.3  -3.3  25.6
  5    6 A V  E     -a   36  0A   82     29,-0.2     2,-0.3    28,-0.2    31,-0.2  -0.786   7.3-174.2-110.8 154.1   1.6  39.1  28.2
  6    7 A a  E     -a   37  0A   19     29,-2.2    31,-2.1    -2,-0.3    32,-0.4  -0.955  29.0-110.7-145.1 165.0   4.1  37.8  30.7
  7    8 A Q        -     0   0  102     -2,-0.3    31,-1.9    29,-0.2     2,-0.2   0.984  39.6-151.7 -57.5 -79.2   6.3  38.8  33.7
  8    9 A G        -     0   0   16     21,-0.2     2,-0.3    29,-0.2    32,-0.2  -0.651  12.5-100.4 121.9 179.1  10.0  38.7  32.8
  9   10 A T  B     -F   40  0B   25     30,-1.5    30,-0.6    -2,-0.2     3,-0.0  -0.891  13.6-162.5-139.9 168.9  13.1  38.1  34.8
 10   11 A S        +     0   0   75     -2,-0.3  1032,-0.7    28,-0.1     3,-0.1  -0.206  51.5 119.4-144.8  46.4  16.1  39.7  36.6
 11   12 A N    >   -     0   0   20      1,-0.3     3,-3.1  1030,-0.2  1033,-0.1   0.403  46.6-171.8 -92.4  -0.2  18.7  37.0  37.2
 12   13 A K  T 3  S-     0   0   83      1,-0.3    -1,-0.3  1020,-0.1  1020,-0.1  -0.150  70.5 -13.2  43.2-121.3  21.3  38.8  35.1
 13   14 A L  T 3  S+     0   0    8   1018,-0.1    -1,-0.3    -3,-0.1     2,-0.1   0.309 106.2 120.0 -93.5  11.2  24.2  36.4  34.7
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   56  5.1   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I+4), SAME NUMBER PER 100 RESIDUES
    6  0.5   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I+5), SAME NUMBER PER 100 RESIDUES
  1  2  3  4  5  6  7  8  9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30     *** HISTOGRAMS OF ***
  0  0  0  4  0  2  0  0  0  0  0  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0    RESIDUES PER ALPHA HELIX
  1  2  3  4  5  6  7  8  9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30     *** HISTOGRAMS OF ***
  0  0  0  4  0  2  0  0  0  0  0  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0    RESIDUES PER ALPHA HELIX
 14 17  6  5  4  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0    PARALLEL BRIDGES PER LADDER
 19  5  6  2  1  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0    ANTIPARALLEL BRIDGES PER LADDER
  6  1  3  4  6  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0    LADDERS PER SHEET
#  RESIDUE AA STRUCTURE BP1 BP2 ACC     N-H-->O    O-->H-N    N-H-->O    O-->H-N    TCO  KAPPA  PHI   PSI    X-CA   Y-CA   Z-CA
  1    1 A L              0   0  118      0, 0.0     2,-0.1     0, 0.0   233,-0.0   0.000 360.0 360.0 360.0 -24.2 -10.7  44.3 21.8
  2    2 A E        -     0   0   79      1,-0.1     0, 0.0   231,-0.1     0, 0.0  -0.618 360.0-176.9-150.0  80.4  -7.4  42.5 20.8
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  4    4 A K        -     0   0   83      2,-0.1    32,-0.1    32,-0.0    31,-0.0   0.331  31.0 -93.4 125.4 -43.4  -0.0  40.0 23.4
  5    5 A K        -     0   0  137     30,-0.1    30,-2.9    29,-0.1    31,-1.8  -0.122  51.5-168.1 -41.1 113.1  -0.4  37.3 25.6
  6    6 A V  E     -a   36  0A   82     29,-0.2     2,-0.3    28,-0.2    31,-0.2  -0.786   7.3-174.2-110.8 154.1   1.6  39.1 28.2
  7    7 A a  E     -a   37  0A   19     29,-2.2    31,-2.1    -2,-0.3    32,-0.4  -0.955  29.0-110.7-145.1 165.0   4.1  37.8 30.7
  8    8 A Q        -     0   0  102     -2,-0.3    31,-1.9    29,-0.2     2,-0.2   0.984  39.6-151.7 -57.5 -79.2   6.3  38.8 33.7
  9    9 A G        -     0   0   16     21,-0.2     2,-0.3    29,-0.2    32,-0.2  -0.651  12.5-100.4 121.9 179.1  10.0  38.7 32.8
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 13   13 A K  T 3  S-     0   0   83      1,-0.3    -1,-0.3  1020,-0.1  1020,-0.1  -0.150  70.5 -13.2  43.2-121.3  21.3  38.8 35.1
 14   14 A L  T 3  S+     0   0    8   1018,-0.1    -1,-0.3    -3,-0.1     2,-0.1   0.309 106.2 120.0 -93.5  11.2  24.2  36.4 34.7
 15   15 A T    <   -     0   0    3     -3,-3.1     2,-0.4  1018,-0.1  1020,-0.2  -0.424  55.1-138.9 -76.6 148.7  23.1  33.9 37.3
 16   16 A Q  B     -g 1035  0C   13   1018,-2.9  1020,-2.1    -2,-0.1     2,-1.0  -0.872   7.2-140.2-107.0 141.2  22.3  30.3 36.5
 17   17 A L        -     0   0   19     -2,-0.4     2,-0.2  1018,-0.2     9,-0.2  -0.674  61.0 -66.3-103.0  79.9  19.4  28.5 38.1
 18   18 A G  S    S+     0   0   13     -2,-1.0  1018,-0.1  1018,-0.5  1019,-0.1  -0.514 104.7   3.8  79.0-148.1  20.7  25.1 38.9
 19   19 A T  S  > S-     0   0   77     -2,-0.2     4,-3.2     1,-0.1     5,-0.2  -0.075  78.9-104.9 -63.9 168.5  21.7  22.7 36.0
 20   20 A F  H  > S+     0   0   88      2,-0.2     4,-2.5     1,-0.2     5,-0.2   0.964 124.6  46.2 -60.0 -50.2  21.6  23.8 32.4
 21   21 A E  H  > S+     0   0  113      2,-0.2     4,-2.3     1,-0.2     5,-0.2   0.931 114.0  47.1 -58.3 -49.7  18.4  21.7 31.9
```

SSE stats

A DSSP Output File

```
==== Secondary Structure Definition by the program DSSP, updated CMBI version by ElmK / April 1,2000 ====
REFERENCE W. KABSCH AND C.SANDER, BIOPOLYMERS 22 (1983) 2577-2637
HEADER    TRANSFERASE/GROWTH FACTOR                10-SEP-00   1MOK
COMPND    2 MOLECULE: EPIDERMAL GROWTH FACTOR RECEPTOR;
SOURCE    2 ORGANISM_SCIENTIFIC: HOMO SAPIENS;
AUTHOR    T.P.J.GARRETT,N.M.MCKERN,M.LOU,T.C.ELLEMAN,T.E.ADAMS,
 1097  5 40 39  1 TOTAL NUMBER OF RESIDUES, NUMBER OF CHAINS, NUMBER OF SS-BRIDGES(TOTAL,INTRACHAIN,INTERCHAIN)
 49778.0   ACCESSIBLE SURFACE OF PROTEIN (ANGSTROM**2)
  692 63.1   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(J)  , SAME NUMBER PER 100 RESIDUES
  156 14.2   TOTAL NUMBER OF HYDROGEN BONDS IN PARALLEL BRIDGES, SAME NUMBER PER 100 RESIDUES
  109  9.9   TOTAL NUMBER OF HYDROGEN BONDS IN ANTIPARALLEL BRIDGES, SAME NUMBER PER 100 RESIDUES
    8  0.7   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I-5), SAME NUMBER PER 100 RESIDUES
   10  0.9   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I-4), SAME NUMBER PER 100 RESIDUES
    5  0.5   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I-3), SAME NUMBER PER 100 RESIDUES
    0  0.0   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I-2), SAME NUMBER PER 100 RESIDUES
    0  0.0   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I-1), SAME NUMBER PER 100 RESIDUES
    0  0.0   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I+0), SAME NUMBER PER 100 RESIDUES
    0  0.0   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I+1), SAME NUMBER PER 100 RESIDUES
  132 12.0   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I+3), SAME NUMBER PER 100 RESIDUES
  145 13.2   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I+4), SAME NUMBER PER 100 RESIDUES
   56  5.1   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I+5), SAME NUMBER PER 100 RESIDUES
    6  0.5   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I+6), SAME NUMBER PER 100 RESIDUES
  1  2  3  4  5  6  7  8  9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30  *** HISTOGRAMS OF ***
  0  0  0  4  0  2  0  0  0  0  0  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  RESIDUES PER ALPHA HELIX
 14  1  2  3  4  5  6  7  8  9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30  PARALLEL BRIDGES PER LADDER
 19  0  0  0  4  0  2  0  0  0  0  0  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  ANTIPARALLEL BRIDGES PER LADDER
  6 14 17  6  5  4  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  LADDERS PER SHEET
  6  1  3  4  6  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
```

Length of SSEs

6 2 4 6 8 10 12 14 16 18 20

Number of SSEs

1 3 4 5 6 7 8 9 10 11 12 13

"There are 4, 2 and 2 α-helices of length 4, 6 and 12 residues, respectively."

SSE stats

α-helices

Parallel β-bridges per ladder

Antiparallel β-bridges per ladder

β-ladders per sheet

A DSSP Output File

```
==== Secondary Structure Definition by the program DSSP, updated CMBI version by ElmK / April 1,2000 ====
REFERENCE W. KABSCH AND C.SANDER, BIOPOLYMERS 22 (1983) 2577-2637
HEADER    TRANSFERASE/GROWTH FACTOR                10-SEP-02   1MOX
COMPND   2 MOLECULE: EPIDERMAL GROWTH FACTOR RECEPTOR;
SOURCE   2 ORGANISM_SCIENTIFIC: HOMO SAPIENS;
AUTHOR    T.P.J.GARRETT,N.M.MCKERN,M.LOU,T.C.ELLEMAN,T.E.ADAMS,
 1097  5 40 39  1 TOTAL NUMBER OF RESIDUES, NUMBER OF CHAINS, NUMBER OF SS-BRIDGES(TOTAL,INTRACHAIN,INTERCHAIN)
 49778.0   ACCESSIBLE SURFACE OF PROTEIN (ANGSTROM**2)
  692 63.1   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(J)    SAME NUMBER PER 100 RESIDUES
  156 14.2   TOTAL NUMBER OF HYDROGEN BONDS IN     PARALLEL BRIDGES, SAME NUMBER PER 100 RESIDUES
  109  9.9   TOTAL NUMBER OF HYDROGEN BONDS IN ANTIPARALLEL BRIDGES, SAME NUMBER PER 100 RESIDUES
    8  0.7   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I-5), SAME NUMBER PER 100 RESIDUES
   10  0.9   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I-4), SAME NUMBER PER 100 RESIDUES
    5  0.5   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I-3), SAME NUMBER PER 100 RESIDUES
    0  0.0   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I-2), SAME NUMBER PER 100 RESIDUES
    0  0.0   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I-1), SAME NUMBER PER 100 RESIDUES
    0  0.0   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I+0), SAME NUMBER PER 100 RESIDUES
    0  0.0   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I+1), SAME NUMBER PER 100 RESIDUES
  132 12.0   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I+2), SAME NUMBER PER 100 RESIDUES
  145 13.2   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I+3), SAME NUMBER PER 100 RESIDUES
   56  5.1   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I+4), SAME NUMBER PER 100 RESIDUES
    6  0.5   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I+5), SAME NUMBER PER 100 RESIDUES
  1  2  3  4  5  6  7  8  9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30    *** HISTOGRAMS OF ***
  0  0  0  4  0  2  0  0  0  0  0  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0    RESIDUES PER ALPHA HELIX
 14 17  6  5  4  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0    PARALLEL BRIDGES PER LADDER
 19  5  6  2  1  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0    ANTIPARALLEL BRIDGES PER LADDER
  6  1  3  4  6  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0    LADDERS PER SHEET

#  RESIDUE AA STRUCTURE BP1 BP2  ACC     N-H-->O    O-->H-N    N-H-->O    O-->H-N    TCO  KAPPA ALPHA  PHI   PSI   X-CA Y-CA Z-CA
  1    1 A L              0   0  118     0, 0.0     2,-0.1     0, 0.0   233,-0.0   0.000 360.0 360.0 360.0 -24.2 -10.7 44.3 21.8
  2    2 A E          -   0   0   0     0, 0.0     0, 0.0     0, 0.0     0, 0.0  -0.618 360.0-176.9-150.0  80.4  -7.4 42.5 20.8
  3    3 A E          -   0   0  182   -2,-0.1    -1,-0.1     3,-0.0     2,-0.0   0.908  15.3-142.7 -42.2-106.2  -5.4 41.6 23.9
  4    4 A K          -   0   0  83     2,-0.1    32,-0.1    32,-0.0    31,-0.0   0.331  31.0 -93.4 125.4 105.4  -1.9 40.0 23.4
  5    5 A K          -   0   0  123   30,-0.1    -2,-0.2    29,-0.1    31,-1.8  -0.122  51.5-168.1 -41.1 113.1  -0.4 37.3 25.6
  6    6 A V  E       -a  6   0  83    29,-0.2    -2,-0.3    28,-0.2    31,-0.2  -0.786   7.3-174.2-110.8 154.1   1.6 39.1 28.2
  7    7 A a  E       -a  7   0  14    29,-0.2    31,-2.1    -2,-0.3    32,-0.4  -0.955  29.0-110.7-145.1 165.0   4.1 37.8 30.7
  8    8 A Q          -   0   0  107   -2,-0.2    -1,-0.1    29,-0.2     2,-0.2   0.984  39.6-151.7 -57.5 -79.2   6.3 38.8 33.7
  9    9 A G          -   0   0  0     21,-0.2     2,-0.3    29,-0.2    32,-0.2  -0.651  12.5-100.4 121.9 179.1  10.0 38.7 32.8
 10   10 A T  B       -F  10  0  22    30,-1.5    30,-0.6    -2,-0.2     3,-0.0  -0.891  13.6-162.5-139.9 168.9  13.1 38.1 34.8
 11   11 A S          +   0   0  75    -2,-0.3  1032,-0.7    28,-0.1     3,-0.1  -0.206  51.5 119.4-144.8  46.4  16.1 39.7 36.6
 12   12 A N     >    -   0   0  20     1,-0.3    3,-3.1  1030,-0.2  1033,-0.1   0.403  46.6-171.8 -92.4  -0.2  18.7 37.0 37.2
 13   13 A K  T 3  S-   0   0  83     1,-0.2    [illegible]  [illegible]  1020,-0.1  -0.150  70.5 -13.2  43.2-121.3  21.3 38.8 35.1
 14   14 A L  T 3  S+   0   0   8  1018,-0.1    [illegible]  [illegible]    2,-0.1   0.309 106.2 120.0 -93.5  11.2  24.2 36.4 34.7
 15   15 A T     <    -   0   0   3    -3,-3.1     2,-0.4  1018,-0.1  1020,-0.2  -0.424  55.1-138.9 -76.6 148.7  23.1 33.9 37.3
 16   16 A Q  B       -g 1035  0C  13  1018,-2.9  1020,-2.1    -2,-0.1     2,-1.0  -0.872   7.2-140.2-107.0 141.2  22.3 30.3 36.5
 17   17 A L          -   0   0  19    -2,-0.4     2,-0.2  1018,-0.2     9,-0.2  -0.674  61.0 -66.3-103.0  79.9  19.4 28.5 38.1
 18   18 A G  S    S+   0   0  13    -2,-1.0  1018,-0.1  1018,-0.5  1019,-0.1  -0.514 104.7   3.8  79.0-148.1  20.7 25.1 38.9
 19   19 A T  S  > S-   0   0  77    -2,-0.2     4,-3.2     1,-0.1     5,-0.2  -0.075  78.9-104.9 -63.9 168.5  21.7 22.7 36.0
 20   20 A F  H  > S+   0   0  88     2,-0.2     4,-2.5     1,-0.2     5,-0.2   0.964 124.6  46.2 -60.0 -50.2  21.6 23.8 32.4
 21   21 A E  H  > S+   0   0 113     2,-0.2     4,-2.3     1,-0.2     5,-0.2   0.931 114.0  47.1 -58.3 -49.7  18.4 21.7 31.9
```

H	α-helix
G	3_{10}-helix
I	π-helix
B	residue in isolated β-bridge
E	extended β-strand
T	H-bonded turn

```
#  RESIDUE AA STRUCTURE BP1 BP2
  12   12 A N    >   -    0   0
  13   13 A K  T 3  S-   0   0
  14   14 A L  T 3  S+   0   0
  15   15 A T    <   -    0   0
```

SSE notation

A DSSP Output File

```
==== Secondary Structure Definition by the program DSSP, updated CMBI version by ElmK / April 1,2000 ====
REFERENCE W. KABSCH AND C.SANDER, BIOPOLYMERS 22 (1983) 2577-2637
HEADER    TRANSFERASE/GROWTH FACTOR                10-SEP-02   1MOX
COMPND   2 MOLECULE: EPIDERMAL GROWTH FACTOR RECEPTOR;
SOURCE   2 ORGANISM_SCIENTIFIC: HOMO SAPIENS;
AUTHOR    T.P.J.GARRETT,N.M.MCKERN,M.LOU,T.C.ELLEMAN,T.E.ADAMS,
 1097  5 40 39  1 TOTAL NUMBER OF RESIDUES, NUMBER OF CHAINS, NUMBER OF SS-BRIDGES(TOTAL,INTRACHAIN,INTERCHAIN)
 49778.0   ACCESSIBLE SURFACE OF PROTEIN (ANGSTROM**2)
  692 63.1   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(J)  , SAME NUMBER PER 100 RESIDUES
  156 14.2   TOTAL NUMBER OF HYDROGEN BONDS IN     PARALLEL BRIDGES, SAME NUMBER PER 100 RESIDUES
  109  9.9   TOTAL NUMBER OF HYDROGEN BONDS IN ANTIPARALLEL BRIDGES, SAME NUMBER PER 100 RESIDUES
    8  0.7   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I-5), SAME NUMBER PER 100 RESIDUES
   10  0.9   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I-4), SAME NUMBER PER 100 RESIDUES
    5  0.5   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I-3), SAME NUMBER PER 100 RESIDUES
    0  0.0   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I-2), SAME NUMBER PER 100 RESIDUES
    0  0.0   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I-1), SAME NUMBER PER 100 RESIDUES
    0  0.0   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I+0), SAME NUMBER PER 100 RESIDUES
    0  0.0   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I+1), SAME NUMBER PER 100 RESIDUES
  132 12.0   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I+2), SAME NUMBER PER 100 RESIDUES
  145 13.2   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I+3), SAME NUMBER PER 100 RESIDUES
   56  5.1   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I+4), SAME NUMBER PER 100 RESIDUES
    6  0.5   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I+5), SAME NUMBER PER 100 RESIDUES
  1  2  3  4  5  6  7  8  9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30      *** HISTOGRAMS OF ***
  0  0  0  4  0  2  0  0  0  0  0  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  RESIDUES PER ALPHA HELIX
 14 17  6  5  4  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  PARALLEL BRIDGES PER LADDER
 19  5  6  2  1  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  ANTIPARALLEL BRIDGES PER LADDER
  6  1  3  4  6  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  LADDERS PER SHEET

#  RESIDUE AA STRUCTURE BP1 BP2  ACC     N-H-->O    O-->H-N    N-H-->O    O-->H-N    TCO  KAPPA ALPHA  PHI   PSI   X-CA Y-CA Z-CA
  1    1 A L           0   0  118     0, 0.0     2,-0.1     0, 0.0   233,-0.0   0.000 360.0 360.0 360.0 -24.2 -10.7 44.3 21.8
  2    2 A E         -     0   0   0     0, 0.0     0, 0.0     0, 0.0     0, 0.0   -0.618 360.0-176.9-150.0  80.4  -7.4 42.5 20.8
  3    3 A E         -     0   0  182    -2,-0.1    -1,-0.1     3,-0.0     2,-0.0   0.908  15.3-142.7 -42.2-106.2  -5.4 41.6 23.9
  4    4 A K         -     0   0   83     2,-0.1    32,-0.1    32,-0.0    31,-0.0   0.331  31.0 -93.4 125.4 105.4  -1.9 40.0 23.4
  5    5 A K         -     0   0  113    30,-0.1    30,-2.9    29,-0.2    31,-1.8  -0.122  51.5-168.1 -41.1 113.1  -0.4 37.3 25.6
  6    6 A V   E     -a    6   0   85    29,-0.2     2,-0.3    28,-0.2    31,-0.2  -0.786   7.3-174.2-110.8 154.1   1.6 39.1 28.2
  7    7 A a   E     -a    7   0   14    29,-0.2    31,-2.1     2,-0.3    32,-0.4  -0.955  29.0-110.7-145.1 165.0   4.1 37.8 30.7
  8    8 A Q         -     0   0   0    -2,-0.1    29,-1.9    29,-0.2     2,-0.2   0.984  39.6-151.7 -57.5 -79.2   6.3 38.8 33.7
  9    9 A G         -     0   0   2    21,-0.2     2,-0.3    29,-0.2    32,-0.2  -0.651  12.5-100.4 121.9 179.1  10.0 38.7 32.8
 10   10 A T   B     -F    10  0   2    30,-1.5    30,-0.6     -2,-0.2     3,-0.0  -0.891  13.6-162.5-139.9 168.9  13.1 38.1 34.8
 11   11 A S         +     0   0   75    -2,-0.3  1032,-0.7    28,-0.1     3,-0.1  -0.206  51.5 119.4-144.8  46.4  16.1 39.7 36.6
 12   12 A N     >   -     0   0   20     1,-0.3     3,-3.1  1030,-0.2  1033,-0.1   0.403  46.6-171.8 -92.4  -0.2  18.7 37.0 37.2
 13   13 A K   T 3  S-     0   0   83     1,-0.2    -1,-0.1    -1,-0.1  1020,-0.1  -0.150  70.5 -13.2  43.2-121.3  21.3 38.8 35.1
 14   14 A L   T 3  S+     0   0    8  1018,-0.1     1,-0.3     3,-0.1     2,-0.1   0.309 106.2 120.0 -93.5  11.2  24.2 36.4 34.7
 15   15 A T     <   -     0   0    3    -3,-3.1     2,-0.4  1018,-0.1  1020,-0.2  -0.424  55.1-138.9 -76.6 148.7  23.1 33.9 37.3
 16   16 A Q   B     -g 1035   0C  13  1018,-2.9  1020,-2.1    -2,-0.1     2,-1.0  -0.872   7.2-140.2-107.0 141.2  22.3 30.3 36.5
 17   17 A L         -     0   0   19    -2,-0.4     2,-0.2  1018,-0.2     9,-0.2  -0.674  61.0 -66.3-103.0  79.9  19.4 28.5 38.1
 18   18 A G   S    S+     0   0   13    -2,-1.0  1018,-0.1  1018,-0.5  1019,-0.1  -0.514 104.7   3.8  79.0-148.1  20.7 25.1 38.9
 19   19 A T   S  > S-     0   0   77    -2,-0.2     4,-3.2     1,-0.1     5,-0.2  -0.075  78.9-104.9 -63.9 168.5  21.7 22.7 36.0
 20   20 A F   H  > S+     0   0   88     2,-0.2     4,-2.5     1,-0.2     5,-0.2   0.964 124.6  46.2 -60.0 -50.2  21.6 23.8 32.4
 21   21 A E   H  > S+     0   0  113     2,-0.2     4,-2.3     1,-0.2     5,-0.2   0.931 114.0  47.1 -58.3 -49.7  18.4 21.7 31.9
```

First and last H-bonds
Type of turn (n=3,4,5)

```
#  RESIDUE AA STRUCTURE BP1 BP2
 12   12 A N     >   -     0   0
 13   13 A K   T 3  S-     0   0
 14   14 A L   T 3  S+     0   0
 15   15 A T     <   -     0   0
```

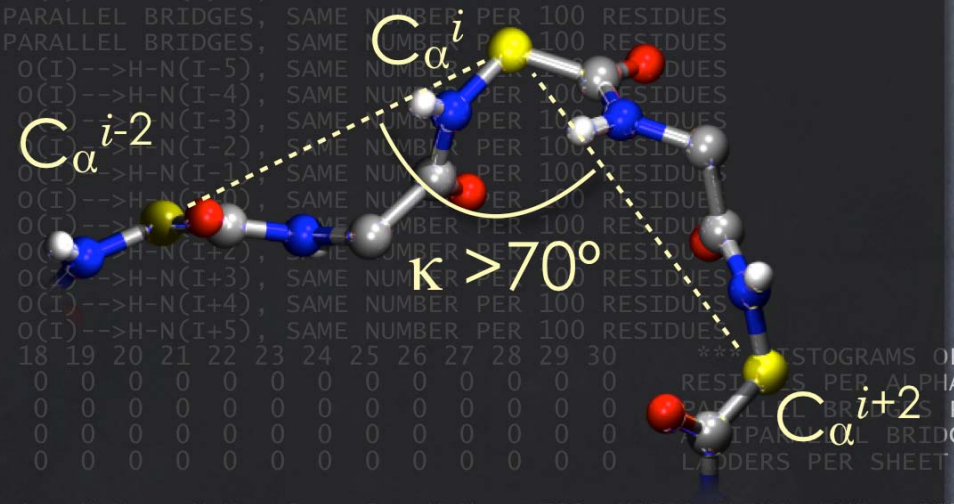
SSE notation

A DSSP Output File

```
==== Secondary Structure Definition by the program DSSP, updated CMBI version by ElmK / April 1,2000 ====
REFERENCE W. KABSCH AND C.SANDER, BIOPOLYMERS 22 (1983) 2577-2637
HEADER    TRANSFERASE/GROWTH FACTOR                              10-SEP-02   1MOX
COMPND    2 MOLECULE: EPIDERMAL GROWTH FACTOR RECEPTOR;
SOURCE    2 ORGANISM_SCIENTIFIC: HOMO SAPIENS;
AUTHOR    T.P.J.GARRETT,N.M.MCKERN,M.LOU,T.C.ELLEMAN,T.E.ADAMS,
 1097  5 40 39  1 TOTAL NUMBER OF RESIDUES, NUMBER OF CHAINS, NUMBER OF SS-BRIDGES(TOTAL,INTRACHAIN,INTERCHAIN)
 49778.0   ACCESSIBLE SURFACE OF PROTEIN (ANGSTROM**2)
  692 63.1   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I), SAME NUMBER PER 100 RESIDUES
  156 14.2   TOTAL NUMBER OF HYDROGEN BONDS IN     PARALLEL BRIDGES, SAME NUMBER PER 100 RESIDUES
  109  9.9   TOTAL NUMBER OF HYDROGEN BONDS IN ANTIPARALLEL BRIDGES, SAME NUMBER PER 100 RESIDUES
    8  0.7   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I-5), SAME NUMBER PER 100 RESIDUES
   10  0.9   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I-4), SAME NUMBER PER 100 RESIDUES
    5  0.5   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I-3), SAME NUMBER PER 100 RESIDUES
    0  0.0   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I-2), SAME NUMBER PER 100 RESIDUES
    0  0.0   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I-1), SAME NUMBER PER 100 RESIDUES
    0  0.0   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I), SAME NUMBER PER 100 RESIDUES
    0  0.0   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I+1), SAME NUMBER PER 100 RESIDUES
  132 12.0   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I+2), SAME NUMBER PER 100 RESIDUES
  145 13.2   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I+3), SAME NUMBER PER 100 RESIDUES
   56  5.1   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I+4), SAME NUMBER PER 100 RESIDUES
    6  0.5   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I+5), SAME NUMBER PER 100 RESIDUES
  1  2  3  4  5  6  7  8  9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30   *** HISTOGRAMS OF ***
  0  0  0  4  0  2  0  0  0  0  0  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0   RESIDUES PER ALPHA HELIX
 14 17  6  5  4  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0   PARALLEL BRIDGES PER LADDER
 19  5  6  2  1  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0   ANTIPARALLEL BRIDGES PER LADDER
  6  1  3  4  6  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0   LADDERS PER SHEET

#  RESIDUE AA STRUCTURE BP1 BP2  ACC     N-H-->O    O-->H-N    N-H-->O    O-->H-N    TCO  KAPPA ALPHA  PHI   PSI   X-CA Y-CA Z-CA
  1    1 A L              0   0  118   0, 0.0     2,-0.1     0, 0.0   233,-0.0   0.000 360.0 360.0 360.0 -24.2 -10.7 44.3 21.8
  2    2 A E            -     0   0   0   0, 0.0     0, 0.0     0, 0.0     0, 0.0     0, 0.0   0.0   0.0   0.0   0.0   80.4  -7.4 42.5 20.8
  3    3 A E            -     0   0  182  -2,-0.1    -1,-0.1     3,-0.0     2,-0.0     0.908  15.3-142.7 -42.2-106.2  -5.4 41.6 23.9
  4    4 A K            -     0   0   83   2,-0.1    32,-0.1    32,-0.0    31,-0.0     0.331  21.0 -93.4 125.4 105.4  -1.9 40.0 23.4
  5    5 A K            -     0   0   83  30,-0.1    -2,-0.2    29,-0.1    31,-0.1     0.403  46.6-171.8 113.1  -0.4 37.3 25.6
  6    6 A V    E       -a    6   0   83  29,-0.2     2,-0.3    28,-0.2    31,-0.2    -0.150  70.5 -13.2  43.2-121.3 154.1   1.6 39.1 28.2
  7    7 A a    E       -a    7   0   118 29,-0.2    31,-2.1     2,-0.3    32,-0.2     0.309 106.2 120.0 -93.5  11.2 165.0   4.1 37.8 30.7
  8    8 A Q            -     0   0   0  -2,-0.2    -1,-1.9    29,-0.2     2,-0.2    -0.424  55.1-138.9 -76.6 148.7 -79.2   6.3 38.8 33.7
  9    9 A G            -     0   0   0  21,-0.2     2,-0.3    29,-0.2    32,-0.2    -0.206  51.5 119.4-144.8  46.4 179.1  10.0 38.7 32.8
 10   10 A T    B       -F    10  0   2  30,-1.5    30,-0.6     -2,-0.2     3,-0.1     0.891  16.1 -61.9 -16.9 168.9  13.1 38.1 34.8
 11   11 A S            +     0   0   75  -2,-0.3  1032,-0.7    28,-0.1     3,-0.1    -0.206  51.5 119.4-144.8  46.4  16.1 39.7 36.6
 12   12 A N      >     -     0   0   20   1,-0.3    3,-3.1  1030,-0.2  1033,-0.1     0.403  46.6-171.8 -92.4  -0.2  18.7 37.0 37.2
 13   13 A K    T 3   S-      0   0   83   1,-0.2   -1,-0.1  1031,-0.2  1020,-0.1    -0.150  70.5 -13.2  43.2-121.3  21.3 38.8 35.1
 14   14 A L    T 3   S+      0   0    8 1018,-0.1   1,-0.3     3,-0.1     2,-0.1     0.309 106.2 120.0 -93.5  11.2  24.2 36.4 34.7
 15   15 A T      <   -       0   0    3  -3,-3.1    2,-0.4  1018,-0.1  1020,-0.2    -0.424  55.1-138.9 -76.6 148.7  23.1 33.9 37.3
 16   16 A Q    B       -g 1035   0C  13 1018,-2.9  1020,-2.1    -2,-0.1     2,-1.0    -0.872   7.2-140.2-107.0 141.2  22.3 30.3 36.5
 17   17 A L            -     0   0   19  -2,-0.4    2,-0.2  1018,-0.2     9,-0.2    -0.674  61.0 -66.3-103.0  79.9  19.4 28.5 38.1
 18   18 A G    S     S+      0   0   13  -2,-1.0  1018,-0.1  1018,-0.5  1019,-0.1    -0.514 104.7   3.8  79.0-148.1  20.7 25.1 38.9
 19   19 A T    S   > S-      0   0   77  -2,-0.2    4,-3.2     1,-0.1     5,-0.2    -0.075  78.9-104.9 -63.9 168.5  21.7 22.7 36.0
 20   20 A F    H   > S+      0   0   88   2,-0.2    4,-2.5     1,-0.2     5,-0.2     0.964 124.6  46.2 -60.0 -50.2  21.6 23.8 32.4
 21   21 A E    H   > S+      0   0  113   2,-0.2    4,-2.3     1,-0.2     5,-0.2     0.931 114.0  47.1 -58.3 -49.7  18.4 21.7 31.9
```

Bend: high chain curvature centered at "S"




```
#  RESIDUE AA STRUCTURE BP1 BP2
 12   12 A N      >     -     0   0
 13   13 A K    T 3   S-      0   0
 14   14 A L    T 3   S+      0   0
 15   15 A T      <   -       0   0
```

```
TCO   KAPPA ALPHA
0.403  46.6-171.8
-0.150  70.5 -13.2
0.309 106.2 120.0
-0.424  55.1-138.9
```

SSE notation

A DSSP Output File

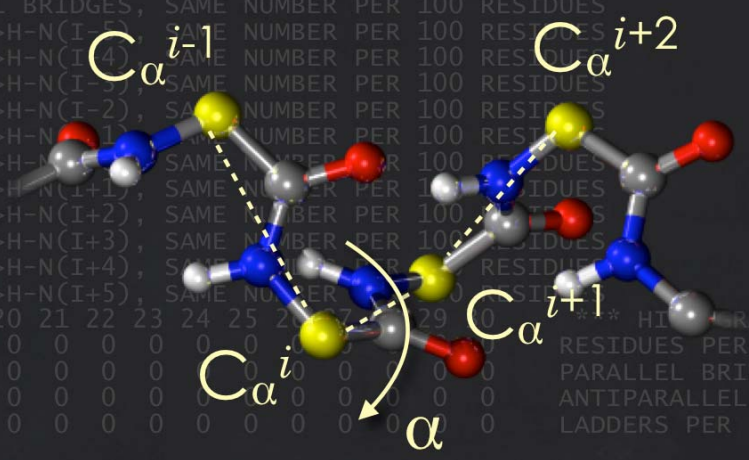
```
==== Secondary Structure Definition by the program DSSP, updated CMBI version by ElmK / April 1,2000 ====
REFERENCE W. KABSCH AND C.SANDER, BIOPOLYMERS 22 (1983) 2577-2637
HEADER    TRANSFERASE/GROWTH FACTOR                              10-SEP-93  1EGF
COMPND    2 MOLECULE: EPIDERMAL GROWTH FACTOR RECEPTOR;
SOURCE    2 ORGANISM_SCIENTIFIC: HOMO SAPIENS;
AUTHOR    T.P.J.GARRETT,N.M.MCKERN,M.LOU,T.C.ELLEMAN,T.L.ADAMS,
 1097  5 40 39  1 TOTAL NUMBER OF RESIDUES, NUMBER OF CHAINS, NUMBER OF SS-BRIDGES(TOTAL,INTRACHAIN,INTERCHAIN)
 49778.0   ACCESSIBLE SURFACE OF PROTEIN (ANGSTROM**2)
  692 63.1   TOTAL NUMBER OF HYDROGEN BONS OF TYPE O(I)-->H-N(I+5), SAME NUMBER PER 100 RESIDUES
  156 14.2   TOTAL NUMBER OF HYDROGEN BONS IN     PARALLEL BRIDGES, SAME NUMBER PER 100 RESIDUES
  109  9.9   TOTAL NUMBER OF HYDROGEN BONS IN ANTIPARALLEL BRIDGES, SAME NUMBER PER 100 RESIDUES
    8  0.7   TOTAL NUMBER OF HYDROGEN BONS OF TYPE O(I)-->H-N(I+4), SAME NUMBER PER 100 RESIDUES
   10  0.9   TOTAL NUMBER OF HYDROGEN BONS OF TYPE O(I)-->H-N(I+3), SAME NUMBER PER 100 RESIDUES
    5  0.5   TOTAL NUMBER OF HYDROGEN BONS OF TYPE O(I)-->H-N(I+2), SAME NUMBER PER 100 RESIDUES
    0  0.0   TOTAL NUMBER OF HYDROGEN BONS OF TYPE O(I)-->H-N(I-2), SAME NUMBER PER 100 RESIDUES
    0  0.0   TOTAL NUMBER OF HYDROGEN BONS OF TYPE O(I)-->H-N(I-3), SAME NUMBER PER 100 RESIDUES
    0  0.0   TOTAL NUMBER OF HYDROGEN BONS OF TYPE O(I)-->H-N(I-4), SAME NUMBER PER 100 RESIDUES
    0  0.0   TOTAL NUMBER OF HYDROGEN BONS OF TYPE O(I)-->H-N(I-5), SAME NUMBER PER 100 RESIDUES
  132 12.0   TOTAL NUMBER OF HYDROGEN BONS OF TYPE O(I)-->H-N(I+1), SAME NUMBER PER 100 RESIDUES
  145 13.2   TOTAL NUMBER OF HYDROGEN BONS OF TYPE O(I)-->H-N(I+2), SAME NUMBER PER 100 RESIDUES
   56  5.1   TOTAL NUMBER OF HYDROGEN BONS OF TYPE O(I)-->H-N(I+3), SAME NUMBER PER 100 RESIDUES
    6  0.5   TOTAL NUMBER OF HYDROGEN BONS OF TYPE O(I)-->H-N(I+4), SAME NUMBER PER 100 RESIDUES
    6  0.5   TOTAL NUMBER OF HYDROGEN BONS OF TYPE O(I)-->H-N(I+5), SAME NUMBER PER 100 RESIDUES
  1  2  3  4  5  6  7  8  9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48 49 50
  0  0  0  4  0  2  0  0  0  0  0  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  *** HISTOGRAMS OF ***
 14 17  6  5  4  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  RESIDUES PER ALPHA HELIX
 19  5  6  2  1  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  PARALLEL BRIDGES PER LADDER
  6  1  3  4  6  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  ANTIPARALLEL BRIDGES PER LADDER
                                                                                                                                                                                                                                  LADDERS PER SHEET

#  RESIDUE AA STRUCTURE BP1 BP2  ACC     N-H-->O    O-->H-N    N-H-->O    O-->H-N    TCO  KAPPA ALPHA  PHI   PSI    X-CA Y-CA Z-CA
  1    1 A L              0   0   118   0, 0.0     2,-0.1     0, 0.0   233,-0.0  0.000 360.0 360.0 360.0 -24.2 -10.7 44.3 21.8
  2    2 A E            -  0   0   182  -2,-0.1    -1,-0.1     3,-0.0     0, 0.0  -0.908  15.3-142.7 -42.2-106.2  -7.4 42.5 20.8
  3    3 A E            -  0   0    83   2,-0.1    32,-0.1    32,-0.0     2,-0.0   0.331  31.0 -93.4 125.4 105.4  -5.4 41.6 23.9
  4    4 A K            -  0   0    83   0, 0.0    -2,-0.2    -2,-0.1    31,-0.0   0.331  31.0 -93.4 125.4 105.4  -1.9 40.0 23.4
  5    5 A K            -  0   0   136  30,-0.2    -2,-0.2    -2,-0.2    31,-1.8  -0.[illegible]  -0.4 37.3 25.6
  6    6 A V  E         -a 6   0    83  29,-0.2     2,-0.3    28,-0.2    31,-0.2  -0.[illegible]   1.6 39.1 28.2
  7    7 A a  E         -a 7   0    [illegible]  29,-0.2    31,-2.1    -2,-0.3    32,-0.4  -0.[illegible]   4.1 37.8 30.7
  8    8 A Q            -  0   0    [illegible]  -2,-0.2    -2,-1.9    29,-0.2     2,-0.2   0.[illegible]   6.3 38.8 33.7
  9    9 A G            -  0   0    [illegible]  21,-0.2     2,-0.3    29,-0.2    32,-0.2  -0.[illegible]  10.0 38.7 32.8
 10   10 A T  B         -F 10  0    [illegible]  30,-1.5    30,-0.6    -2,-0.2     3,-0.0  -0.[illegible]  13.1 38.1 34.8
 11   11 A S            +  0   0   75   -2,-0.3  1032,-0.7    28,-0.1     3,-0.1  -0.206  51.5 119.4-144.8  46.4  16.1 39.7 36.6
 12   12 A N    >       -  0   0   20    1,-0.3    3,-3.1  1030,-0.2  1033,-0.1   0.403  46.6-171.8 -92.4  -0.2  18.7 37.0 37.2
 13   13 A K  T 3  S-   0   0   83    1,-0.[illegible]  1020,-0.1  -0.150  70.5 -13.2  43.2-121.3  21.3 38.8 35.1
 14   14 A L  T 3  S+   0   0    8 1018,-0.[illegible]  2,-0.1   0.309 106.2 120.0 -93.5  11.2  24.2 36.4 34.7
 15   15 A T    <       -  0   0    3   -3,-3.1    2,-0.4  1018,-0.1  1020,-0.2  -0.424  55.1-138.9 -76.6 148.7  23.1 33.9 37.3
 16   16 A Q  B         -g 1035 0C  13 1018,-2.9  1020,-2.1    -2,-0.1     2,-1.0  -0.872   7.2-140.2-107.0 141.2  22.3 30.3 36.5
 17   17 A L            -  0   0   19   -2,-0.4    2,-0.2  1018,-0.2     9,-0.2  -0.674  61.0 -66.3-103.0  79.9  19.4 28.5 38.1
 18   18 A G  S         S+ 0   0   13   -2,-1.0  1018,-0.1  1018,-0.5  1019,-0.1  -0.514 104.7   3.8  79.0-148.1  20.7 25.1 38.9
 19   19 A T  S    > S- 0   0   77   -2,-0.2    4,-3.2    1,-0.1     5,-0.2  -0.075  78.9-104.9 -63.9 168.5  21.7 22.7 36.0
 20   20 A F  H    > S+ 0   0   88    2,-0.2    4,-2.5    1,-0.2     5,-0.2   0.964 124.6  46.2 -60.0 -50.2  21.6 23.8 32.4
 21   21 A E  H    > S+ 0   0  113    2,-0.2    4,-2.3    1,-0.2     5,-0.2   0.931 114.0  47.1 -58.3 -49.7  18.4 21.7 31.9
```

Chirality for every residue i

"+": $0 < \alpha < 180°$: right-handed

"–": $-180° < \alpha < 0$: left-handed



#	RESIDUE	AA	STRUCTURE	BP1	BP2	KAPPA	ALPHA	PHI
12	12	A	N > -	0	0	46.6	-171.8	-92.4
13	13	A	K T 3 S-	0	0	70.5	-13.2	43.2
14	14	A	L T 3 S+	0	0	106.2	120.0	-93.5
15	15	A	T < -	0	0	55.1	-138.9	-76.6

SSE notation

A DSSP Output File

```
==== Secondary Structure Definition by the program DSSP, updated CMBI version by ElmK / April 1,2000 ====
REFERENCE W. KABSCH AND C.SANDER, BIOPOLYMERS 22 (1983) 2577-2637
HEADER    TRANSFERASE/GROWTH FACTOR                10-SEP-02   1MOX
COMPND   2 MOLECULE: EPIDERMAL GROWTH FACTOR RECEPTOR;
SOURCE   2 ORGANISM_SCIENTIFIC: HOMO SAPIENS;
AUTHOR    T.P.J.GARRETT,N.M.MCKERN,M.LOU,T.C.ELLEMAN,T.E.ADAMS,
 1097  5 40 39  1 TOTAL NUMBER OF RESIDUES, NUMBER OF CHAINS, NUMBER OF SS-BRIDGES(TOTAL,INTRACHAIN,INTERCHAIN)
 49778.0   ACCESSIBLE SURFACE OF PROTEIN (ANGSTROM**2)
  692 63.1   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(J)  , SAME NUMBER PER 100 RESIDUES
  156 14.2   TOTAL NUMBER OF HYDROGEN BONDS IN     PARALLEL BRIDGES, SAME NUMBER PER 100 RESIDUES
  109  9.9   TOTAL NUMBER OF HYDROGEN BONDS IN ANTIPARALLEL BRIDGES, SAME NUMBER PER 100 RESIDUES
    8  0.7   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I-5), SAME NUMBER PER 100 RESIDUES
   10  0.9   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I-4), SAME NUMBER PER 100 RESIDUES
    5  0.5   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I-3), SAME NUMBER PER 100 RESIDUES
    0  0.0   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I-2), SAME NUMBER PER 100 RESIDUES
    0  0.0   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I-1), SAME NUMBER PER 100 RESIDUES
    0  0.0   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I+0), SAME NUMBER PER 100 RESIDUES
    0  0.0   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I+1), SAME NUMBER PER 100 RESIDUES
  132 12.0   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I+2), SAME NUMBER PER 100 RESIDUES
  145 13.2   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I+3), SAME NUMBER PER 100 RESIDUES
   56  5.1   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I+4), SAME NUMBER PER 100 RESIDUES
    6  0.5   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I+5), SAME NUMBER PER 100 RESIDUES
  1  2  3  4  5  6  7  8  9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30     *** HISTOGRAMS OF ***
  0  0  0  4  0  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0    RESIDUES PER ALPHA HELIX
 14 17  6  5  4  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0    PARALLEL BRIDGES PER LADDER
 19  5  6  2  1  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0    ANTIPARALLEL BRIDGES PER LADDER
  6  1  3  4  6  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0    LADDERS PER SHEET

#  RESIDUE AA STRUCTURE BP1 BP2  ACC     N-H-->O    O-->H-N    N-H-->O    O-->H-N    TCO  KAPPA ALPHA  PHI   PSI   X-CA Y-CA Z-CA
  1    1 A L           0   0  118     0, 0.0     2,-0.1     0, 0.0   233,-0.0   0.000 360.0 360.0 360.0 -24.2 -10.7 44.3 21.8
  2    2 A E         -     0   0   0     0, 0.0     0, 0.0     0, 0.0     0, 0.0   0, 0.0   0, 0.0   0, 0.0   0, 0.0   0, 0.0
  3    3 A E         -     0   0  182    -2,-0.1    -1,-0.1     3,-0.0     2,-0.0   0.908  15.3-142.7 -42.2-106.2  -5.4 41.6 23.9
  4    4 A K         -     0   0   83     2,-0.1    32,-0.1    32,-0.0    31,-0.0   0.331  31.0 -93.4 125.4 105.4  -1.9 40.0 23.4
  5    5 A K         -     0   0  113    30,-0.1    -2,-0.2    29,-0.1    31,-1.8  -0.122  51.5-168.1 -41.1 113.1  -0.4 37.3 25.6
  6    6 A V   E     -a    6   0  82     29,-0.2     2,-0.3    28,-0.2    31,-0.2  -0.786   7.3-174.2-110.8 154.1   1.6 39.1 28.2
  7    7 A a   E     -a    7   0  14     29,-0.2    31,-2.1     2,-0.3    32,-0.4  -0.955  29.0-110.7-145.1 165.0   4.1 37.8 30.7
  8    8 A Q         -     0   0  101    -2,-0.2    -1,-1.9    29,-0.2     2,-0.2   0.984  39.6-151.7 -57.5 -79.2   6.3 38.8 33.7
  9    9 A G         -     0   0   0    21,-0.2     2,-0.3    29,-0.2    32,-0.2  -0.651  12.5-100.4 121.9 179.1  10.0 38.7 32.8
 10   10 A T   B     -F    10  0  22    30,-1.5    30,-0.6     -2,-0.2     3,-0.0  -0.891  13.6-162.5-139.9 168.9  13.1 38.1 34.8
 11   11 A S         +     0   0   75    -2,-0.3  1032,-0.7    28,-0.1     3,-0.1  -0.206  51.5 119.4-144.8  46.4  16.1 39.7 36.6
 12   12 A N    >    -     0   0   20     1,-0.3     3,-3.1  1030,-0.2  1033,-0.1   0.403  46.6-171.8 -92.4  -0.2  18.7 37.0 37.2
 13   13 A K   T 3  S-     0   0   83     1,-0.2    -1,-0.1    -2,-0.1  1020,-0.1  -0.150  70.5 -13.2  43.2-121.3  21.3 38.8 35.1
 14   14 A L   T 3  S+     0   0    8  1018,-0.1     1,-0.3     3,-0.1     2,-0.1   0.309 106.2 120.0 -93.5  11.2  24.2 36.4 34.7
 15   15 A T    <   -      0   0    3    -3,-3.1     2,-0.4  1018,-0.1  1020,-0.2  -0.424  55.1-138.9 -76.6 148.7  23.1 33.9 37.3
 16   16 A Q   B     -g 1035  0C  13  1018,-2.9  1020,-2.1    -2,-0.1     2,-1.0  -0.872   7.2-140.2-107.0 141.2  22.3 30.3 36.5
 17   17 A L         -     0   0   19    -2,-0.4     2,-0.2  1018,-0.2     9,-0.2  -0.674  61.0 -66.3-103.0  79.9  19.4 28.5 38.1
 18   18 A G   S    S+     0   0   13    -2,-1.0  1018,-0.1  1018,-0.5  1019,-0.1  -0.514 104.7   3.8  79.0-148.1  20.7 25.1 38.9
 19   19 A T   S  > S-     0   0   77    -2,-0.2     4,-3.2     1,-0.1     5,-0.2  -0.075  78.9-104.9 -63.9 168.5  21.7 22.7 36.0
 20   20 A F   H  > S+     0   0   88     2,-0.2     4,-2.5     1,-0.2     5,-0.2   0.964 124.6  46.2 -60.0 -50.2  21.6 23.8 32.4
 21   21 A E   H  > S+     0   0  113     2,-0.2     4,-2.3     1,-0.2     5,-0.2   0.931 114.0  47.1 -58.3 -49.7  18.4 21.7 31.9
```

Residue number of first and second bridge partner

```
#  RESIDUE AA STRUCTURE BP1 BP2
 12   12 A N    >    -     0   0
 13   13 A K   T 3  S-     0   0
 14   14 A L   T 3  S+     0   0
 15   15 A T    <   -      0   0
```

SSE notation

A DSSP Output File

```
==== Secondary Structure Definition by the program DSSP, updated CMBI version by ElmK / April 1,2000 ====
REFERENCE W. KABSCH AND C.SANDER, BIOPOLYMERS 22 (1983) 2577-2637
HEADER    TRANSFERASE/GROWTH FACTOR                10-SEP-02   1MOX
COMPND   2 MOLECULE: EPIDERMAL GROWTH FACTOR RECEPTOR;
SOURCE   2 ORGANISM_SCIENTIFIC: HOMO SAPIENS;
AUTHOR    T.P.J.GARRETT,N.M.MCKERN,M.LOU,T.C.ELLEMAN,T.E.ADAMS,
 1097  5 40 39  1 TOTAL NUMBER OF RESIDUES, NUMBER OF CHAINS, NUMBER OF SS-BRIDGES(TOTAL,INTRACHAIN,INTERCHAIN)
 49778.0   ACCESSIBLE SURFACE OF PROTEIN (ANGSTROM**2)
  692 63.1   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(J)  , SAME NUMBER PER 100 RESIDUES
  156 14.2   TOTAL NUMBER OF HYDROGEN BONDS IN     PARALLEL BRIDGES, SAME NUMBER PER 100 RESIDUES
  109  9.9   TOTAL NUMBER OF HYDROGEN BONDS IN ANTIPARALLEL BRIDGES, SAME NUMBER PER 100 RESIDUES
    8  0.7   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I-5), SAME NUMBER PER 100 RESIDUES
   10  0.9   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I-4), SAME NUMBER PER 100 RESIDUES
    5  0.5   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I-3), SAME NUMBER PER 100 RESIDUES
    0  0.0   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I-2), SAME NUMBER PER 100 RESIDUES
    0  0.0   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I-1), SAME NUMBER PER 100 RESIDUES
    0  0.0   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I+0), SAME NUMBER PER 100 RESIDUES
    0  0.0   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I+1), SAME NUMBER PER 100 RESIDUES
  132 12.0   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I+2), SAME NUMBER PER 100 RESIDUES
  145 13.2   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I+3), SAME NUMBER PER 100 RESIDUES
   56  5.1   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I+4), SAME NUMBER PER 100 RESIDUES
    6  0.5   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I+5), SAME NUMBER PER 100 RESIDUES
  1  2  3  4  5  6                                                                  RESIDUES PER ALPHA HELIX
  0  0  0  4  0  2                                                                  PARALLEL BRIDGES PER LADDER
 14 17  6  5  4  0                                                                  ANTIPARALLEL BRIDGES PER LADDER
 19  5  6  2  1  2
  6  1  3  4  6  0                                                                  LADDERS PER SHEET

#  RESIDUE AA STRUCTURE BP1 BP2  ACC     N-H-->O    O-->H-N    N-H-->O    O-->H-N    TCO  KAPPA   PHI   PSI  X-CA  Y-CA  Z-CA
  1    1 A L              0   0  118   0, 0.0     0, 0.0     0, 0.0     0, 0.0  0.000 360.0 360.0 360.0 -24.2 -10.7  44.3  21.8
  2    2 A E              0   0   79   1, 0.1     0, 0.0   291,-0.1     0, 0.0 -0.618 360.0 170.9 150.0  88.4   7.4  42.5  20.8
  3    3 A E              0   0  182   2, 0.1    -1,-0.1     3,-0.0     3,-0.0  0.908  15.3 142.7  42.2-106.2  -5.4  41.6  23.9
  4    4 A K              0   0   83   32,-0.2    30,-0.2     3,-0.0     3,-0.0  0.331  5.0  -125.4 105.4  -1.9  40.0  23.4
  5    5 A K              0   0  137   30,-0.2    31,-0.2    31,-0.2    31,-0.2  0.122  5.0  -141.1 113.1  -0.4  37.3  25.6
  6    6 A V  E     -a    36  0A   82   29,-0.2     2,-0.3    28,-0.2    31,-0.2  -0.786  7.5 174.2 -110.8 154.1   1.6  39.1  28.2
  7    7 A a  E     -a    37  0A   19   29,-2.2    31,-2.1    -2,-0.3    32,-0.4  -0.955 29.0-110.7-145.1 165.0   4.1  37.8  30.7
  8    8 A Q        -     0   0  102   -2,-0.3    31,-1.9    29,-0.2     2,-0.2  -0.981 39.6-151.7 -57.5 -79.2   6.3  38.8  33.7
  9    9 A G        -     0   0   16   21,-0.2     2,-0.3    29,-0.2    32,-0.2  -0.[illegible] [illegible] [illegible] 121.9 179.1  10.0  38.7  32.8
 10   10 A T  B     -F   40  0B   25   30,-1.5    30,-0.6    -2,-0.2     3,-0.0  -0.891 13.6-162.5-139.9 168.9  13.1  38.1  34.8
 11   11 A S        +     0   0   75   -2,-0.3  1032,-0.7    28,-0.1     3,-0.1  -0.206  51.5 119.4-144.8  46.4  16.1  39.7  36.6
 12   12 A N    >   -     0   0   20    1,-0.3     3,-3.1  1030,-0.2  1033,-0.1   0.403  46.6-171.8 -92.4  -0.2  18.7  37.0  37.2
 13   13 A K  T 3  S-     0   0   83    1,-0.3    -1,-0.3  1020,-0.1  1020,-0.1  -0.150  70.5 -13.2  43.2-121.3  21.3  38.8  35.1
 14   14 A L  T 3  S+     0   0    8 1018,-0.1    -1,-0.3    -3,-0.1     2,-0.1   0.309 106.2 120.0 -93.5  11.2  24.2  36.4  34.7
 15   15 A T    <   -     0   0    3   -3,-3.1     2,-0.4  1018,-0.1  1020,-0.2  -0.424  55.1-138.9 -76.6 148.7  23.1  33.9  37.3
 16   16 A Q  B     -g 1035  0C   13 1018,-2.9  1020,-2.1    -2,-0.1     2,-1.0  -0.872   7.2-140.2-107.0 141.2  22.3  30.3  36.5
 17   17 A L        -     0   0   19   -2,-0.4     2,-0.2  1018,-0.2     9,-0.2  -0.674  61.0 -66.3-103.0  79.9  19.4  28.5  38.1
 18   18 A G  S    S+     0   0   13   -2,-1.0  1018,-0.1  1018,-0.5  1019,-0.1  -0.514 104.7   3.8  79.0-148.1  20.7  25.1  38.9
 19   19 A T  S  > S-     0   0   77   -2,-0.2     4,-3.2     1,-0.1     5,-0.2  -0.075  78.9-104.9 -63.9 168.5  21.7  22.7  36.0
 20   20 A F  H  > S+     0   0   88    2,-0.2     4,-2.5     1,-0.2     5,-0.2   0.964 124.6  46.2 -60.0 -50.2  21.6  23.8  32.4
 21   21 A E  H  > S+     0   0  113    2,-0.2     4,-2.3     1,-0.2     5,-0.2   0.931 114.0  47.1 -58.3 -49.7  18.4  21.7  31.9
```

H-bond interactions

A-->B H-bond between group A of residue i

m,e and group B of residue $j=i+m$ with a H-bond energy of e (kcal·mol^{-1})

H-bonds

A DSSP Output File

```
==== Secondary Structure Definition by the program DSSP, updated CMBI version by ElmK / April 1,2000 ====
REFERENCE W. KABSCH AND C.SANDER, BIOPOLYMERS 22 (1983) 2577-2637
HEADER    TRANSFERASE/GROWTH FACTOR                     10-SEP-02   1MOX
COMPND   2 MOLECULE: EPIDERMAL GROWTH FACTOR RECEPTOR;
SOURCE   2 ORGANISM_SCIENTIFIC: HOMO SAPIENS;
AUTHOR    T.P.J.GARRETT,N.M.MCKERN,M.LOU,T.C.ELLEMAN,T.E.ADAMS,
 1097  5 40 39  1 TOTAL NUMBER OF RESIDUES, NUMBER OF CHAINS, NUMBER OF SS-BRIDGES(TOTAL,INTRACHAIN,INTERCHAIN)
 49778.0   ACCESSIBLE SURFACE OF PROTEIN (ANGSTROM**2)
  692 63.1   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(J)  , SAME NUMBER PER 100 RESIDUES
  156 14.2   TOTAL NUMBER OF HYDROGEN BONDS IN     PARALLEL BRIDGES, SAME NUMBER PER 100 RESIDUES
  109  9.9   TOTAL NUMBER OF HYDROGEN BONDS IN ANTIPARALLEL BRIDGES, SAME NUMBER PER 100 RESIDUES
    8  0.7   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I-5), SAME NUMBER PER 100 RESIDUES
   10  0.9   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I-4), SAME NUMBER PER 100 RESIDUES
    5  0.5   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I-3), SAME NUMBER PER 100 RESIDUES
    0  0.0   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I-2), SAME NUMBER PER 100 RESIDUES
    0  0.0   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I-1), SAME NUMBER PER 100 RESIDUES
    0  0.0   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I+0), SAME NUMBER PER 100 RESIDUES
    0  0.0   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I+1), SAME NUMBER PER 100 RESIDUES
  132 12.0   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I+2), SAME NUMBER PER 100 RESIDUES
  145 13.2   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I+3), SAME NUMBER PER 100 RESIDUES
   56  5.1   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I+4), SAME NUMBER PER 100 RESIDUES
    6  0.5   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I+5), SAME NUMBER PER 100 RESIDUES
  1  2  3  4  5  6  7  8  9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30     *** HISTOGRAMS OF ***
  0  0  0  4  0  2  0  0  0  0  0  2  0                                                         RESIDUES PER ALPHA HELIX
 14 17  6  5  4  0  0  0  0  0  0  0  0                                                         PARALLEL BRIDGES PER LADDER
 19  5  6  2  1  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0     ANTIPARALLEL BRIDGES PER LADDER
  6  1  3  4  6  0  0  0  0  0  0  0  0                                                         LADDERS PER SHEET

#  RESIDUE AA STRUCTURE BP1 BP2  ACC     N-H-->O    O-->H-N    N-H-->O    O-->H-N    TCO  KAPPA ALPHA  PHI   PSI    X-CA   Y-CA   Z-CA
  1    1 A L              0   0  118      0, 0.0     2,-0.1     0, 0.0   233,-0.0   0.000 360.0 360.0 360.0 -24.2  -10.7  44.3  21.8
  2    2 A E        -     0   0   79      1,-0.1                                                                               20.8
  3    3 A E        -     0   0  182     -2,-0.1                                                                               23.9
  4    4 A K        -     0   0   83      2,-0.1                                                                               23.4
  5    5 A K        -     0   0  137     30,-0.1                                                                               25.6
  6    6 A V  E     -a   36   0A  82     29,-0.2                                                                               28.2
  7    7 A a  E     -a   37   0A  19     29,-2.2                                                                               30.7
  8    8 A Q        -     0   0  102     -2,-0.3                                                                               33.7
  9    9 A G        -     0   0   16     21,-0.2                                                                               32.8
 10   10 A T  B     -F   40   0B  25     30,-1.5                                                                               34.8
 11   11 A S        +     0   0   75     -2,-0.3  1032,-0.7    28,-0.1     3,-0.1  -0.206  51.5 119.4-144.8  46.4   16.1  39.7  36.6
 12   12 A N    >   -     0   0   20      1,-0.3     3,-3.1  1030,-0.2  1033,-0.1   0.403  46.6-171.8 -92.4  -0.2   18.7  37.0  37.2
 13   13 A K  T 3  S-     0   0   83      1,-0.3    -1,-0.3  1020,-0.1  1020,-0.1  -0.150                                      35.1
 14   14 A L  T 3  S+     0   0    8   1018,-0.1    -1,-0.3    -3,-0.1     2,-0.1   0.309                                      34.7
 15   15 A T    <   -     0   0    3     -3,-3.1     2,-0.4  1018,-0.1  1020,-0.2  -0.424  55.1-138.9 -76.6 148.7   23.1  33.9  37.3
 16   16 A Q  B     -g 1035   0C  13   1018,-2.9  1020,-2.1    -2,-0.1     2,-1.0  -0.872   7.2-140.2-107.0 141.2   22.3  30.3  36.5
 17   17 A L        -     0   0   19     -2,-0.4     2,-0.2  1018,-0.2     9,-0.2  -0.674  61.0 -66.3-103.0  79.9   19.4  28.5  38.1
 18   18 A G  S    S+     0   0   13     -2,-1.0  1018,-0.1  1018,-0.5  1019,-0.1  -0.514 104.7   3.8  79.0-148.1   20.7  25.1  38.9
 19   19 A T  S  > S-     0   0   77     -2,-0.2     4,-3.2     1,-0.1     5,-0.2  -0.075  78.9-104.9 -63.9 168.5   21.7  22.7  36.0
 20   20 A F  H  > S+     0   0   88      2,-0.2     4,-2.5     1,-0.2     5,-0.2   0.964 124.6  46.2 -60.0 -50.2   21.6  23.8  32.4
 21   21 A E  H  > S+     0   0  113      2,-0.2     4,-2.3     1,-0.2     5,-0.2   0.931 114.0  47.1 -58.3 -49.7   18.4  21.7  31.9
```

Cosine of the angle between C=O of residue i and C=O of residue i-1 (α-helices, ≈ +1, for β-sheets ≈-1)

```
   TCO  KAPPA ALPHA  PHI   PSI    X-CA Y-CA Z-CA

 0.403  46.6-171.8 -92.4  -0.2  18.7 37.0 37.2
-0.150  70.5 -13.2  43.2-121.3  21.3 38.8 35.1
 0.309 106.2 120.0 -93.5  11.2  24.2 36.4 34.7
-0.424  55.1-138.9 -76.6 148.7  23.1 33.9 37.3
```

Local geometry

A DSSP Output File

```
==== Secondary Structure Definition by the program DSSP, updated CMBI version by ElmK / April 1,2000 ====
REFERENCE W. KABSCH AND C.SANDER, BIOPOLYMERS 22 (1983) 2577-2637
HEADER    TRANSFERASE/GROWTH FACTOR                10-SEP-02   1MOX
COMPND   2 MOLECULE: EPIDERMAL GROWTH FACTOR RECEPTOR;
SOURCE   2 ORGANISM_SCIENTIFIC: HOMO SAPIENS;
AUTHOR    T.P.J.GARRETT,N.M.MCKERN,M.LOU,T.C.ELLEMAN,T.E.ADAMS,
 1097  5 40 39  1 TOTAL NUMBER OF RESIDUES, NUMBER OF CHAINS, NUMBER OF SS-BRIDGES(TOTAL,INTRACHAIN,INTERCHAIN)
 49778.0   ACCESSIBLE SURFACE OF PROTEIN (ANGSTROM**2)
  692 63.1   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(J)  , SAME NUMBER PER 100 RESIDUES
  156 14.2   TOTAL NUMBER OF HYDROGEN BONDS IN     PARALLEL BRIDGES, SAME NUMBER PER 100 RESIDUES
  109  9.9   TOTAL NUMBER OF HYDROGEN BONDS IN ANTIPARALLEL BRIDGES, SAME NUMBER PER 100 RESIDUES
    8  0.7   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I-5), SAME NUMBER PER 100 RESIDUES
   10  0.9   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I-4), SAME NUMBER PER 100 RESIDUES
    5  0.5   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I-3), SAME NUMBER PER 100 RESIDUES
    0  0.0   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I-2), SAME NUMBER PER 100 RESIDUES
    0  0.0   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I-1), SAME NUMBER PER 100 RESIDUES
    0  0.0   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I+0), SAME NUMBER PER 100 RESIDUES
    0  0.0   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I+1), SAME NUMBER PER 100 RESIDUES
  132 12.0   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I+2), SAME NUMBER PER 100 RESIDUES
  145 13.2   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I+3), SAME NUMBER PER 100 RESIDUES
   56  5.1   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I+4), SAME NUMBER PER 100 RESIDUES
    6  0.5   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I+5), SAME NUMBER PER 100 RESIDUES
  1  2  3  4  5  6  7  8  9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30     *** HISTOGRAMS OF ***
  0  0  0  4  0  2  0  0  0  0  0  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0    RESIDUES PER ALPHA HELIX
 14 17  6  5  4  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0    PARALLEL BRIDGES PER LADDER
 19  5  6  2  1  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0    ANTIPARALLEL BRIDGES PER LADDER
  6  1  3  4  6  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0    ANTIPARALLEL BRIDGE PER LADDER

#  RESIDUE AA STRUCTURE BP1 BP2  ACC     N-H-->O    O-->H-N    N-H-->O    O-->H-N    TCO  KAPPA ALPHA  PHI   PSI  X-CA Y-CA Z-CA
  1    1 A L              0   0  118     0, 0.0     2,-0.1     0, 0.0   233,-0.0  0.000 360.0 360.0 360.0 -24.2 -10.7 44.3 21.8
  2    2 A E        -     0   0   79     1,-0.1     0, 0.0     0, 0.0     0, 0.0  0.000 360.0 360.0 360.0 360.0 -10.7 44.3 20.8
  3    3 A E        -     0   0  182    -2,-0.1    -1,-0.1     3,-0.0     2,-0.0  0.908  15.3-142.7 -42.2-106.2  -5.4 41.6 23.9
  4    4 A K        -     0   0   83     2,-0.1    32,-0.1    32,-0.0    31,-0.0  0.331  31.0  93.4 125.4 105.4  -1.9 40.0 23.4
  5    5 A K        -     0   0  137    30,-0.1     3,-0.1     2,-0.1     3,-0.1  0.403  46.6-171.8 -92.4  -0.2  18.7 37.0 37.2 25.6
  6    6 A V  E     -a   36  0A   82    29,-0.2    -2,-0.1    -2,-0.2    -2,-0.1 -0.150  70.5 -13.2  43.2-121.3  21.3 38.8 35.1 28.2
  7    7 A a  E     -a   37  0A   19    29,-2.2    31,-0.1    -3,-0.1    -3,-0.1  0.309 106.2 120.0 -93.5  11.2  24.2 36.4 34.7 30.7
  8    8 A Q        -     0   0  102    -2,-0.3    -3,-0.1    -4,-0.1    -4,-0.1 -0.424  55.1-138.9 -76.6 148.7  23.1 33.9 37.3 33.7
  9    9 A G        -     0   0   16    21,-0.2    -2,-0.2    -2,-0.2    -2,-0.2  0.403  46.6-171.8 -92.4  -0.2  18.7 37.0 37.2 32.8
 10   10 A T  B     -F   40  0B   25    30,-1.5    -3,-0.1    -4,-0.1    -4,-0.1 -0.150  70.5 -13.2  43.2-121.3  21.3 38.8 35.1 34.8
 11   11 A S        +     0   0   75    -2,-0.3  1032,-0.7    28,-0.1     3,-0.1  0.309 106.2 120.0 -93.5  11.2  24.2 36.4 34.7 36.6
 12   12 A N    >   -     0   0   20     1,-0.3     3,-3.1  1030,-0.2  1033,-0.1 -0.424  55.1-138.9 -76.6 148.7  23.1 33.9 37.3 37.2
 13   13 A K  T 3  S-     0   0   83     1,-0.3    -1,-0.3  1020,-0.1  1020,-0.1  0.872   7.2-140.2-107.0 141.2  22.3 30.3 36.5 35.1
 14   14 A L  T 3  S+     0   0    8  1018,-0.1    -1,-0.3    -3,-0.1     2,-0.1  0.674  61.0 -66.3-103.0  79.9  19.4 28.5 38.1 34.7
 15   15 A T    <   -     0   0    3    -3,-3.1     2,-0.4  1018,-0.1  1020,-0.2 -0.514 104.7   3.8  79.0-148.1  20.7 25.1 38.9 37.3
 16   16 A Q  B     -g 1035  0C   13  1018,-2.9  1020,-2.1    -2,-0.1     2,-1.0 -0.075  78.9-104.9 -63.9 168.5  21.7 22.7 36.0 36.5
 17   17 A L        -     0   0   19    -2,-0.4     2,-0.2  1018,-0.2     9,-0.2  0.964 124.6  46.2 -60.0 -50.2  21.6 23.8 32.4 38.1
 18   18 A G  S    S+     0   0   13    -2,-1.0  1018,-0.1  1018,-0.5  1019,-0.1  0.931 114.0  47.1 -58.3 -49.7  18.4 21.7 31.9 38.9
 19   19 A T  S  > S-     0   0   77    -2,-0.2     4,-3.2     1,-0.1     5,-0.2
 20   20 A F  H  > S+     0   0   88     2,-0.2     4,-2.5     1,-0.2     5,-0.2
 21   21 A E  H  > S+     0   0  113     2,-0.2     4,-2.3     1,-0.2     5,-0.2
```

Angle κ and dihedrals α, Φ and Ψ

Local geometry

A DSSP Output File

```
==== Secondary Structure Definition by the program DSSP, updated CMBI version by ElmK / April 1,2000 ====
REFERENCE W. KABSCH AND C.SANDER, BIOPOLYMERS 22 (1983) 2577-2637
HEADER    TRANSFERASE/GROWTH FACTOR                10-SEP-02   1MOX
COMPND   2 MOLECULE: EPIDERMAL GROWTH FACTOR RECEPTOR;
SOURCE   2 ORGANISM_SCIENTIFIC: HOMO SAPIENS;
AUTHOR    T.P.J.GARRETT,N.M.MCKERN,M.LOU,T.C.ELLEMAN,T.E.ADAMS,
 1097  5 40 39  1 TOTAL NUMBER OF RESIDUES, NUMBER OF CHAINS, NUMBER OF SS-BRIDGES(TOTAL,INTRACHAIN,INTERCHAIN)
 49778.0   ACCESSIBLE SURFACE OF PROTEIN (ANGSTROM**2)
  692 63.1   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(J)  , SAME NUMBER PER 100 RESIDUES
  156 14.2   TOTAL NUMBER OF HYDROGEN BONDS IN     PARALLEL BRIDGES, SAME NUMBER PER 100 RESIDUES
  109  9.9   TOTAL NUMBER OF HYDROGEN BONDS IN ANTIPARALLEL BRIDGES, SAME NUMBER PER 100 RESIDUES
    8  0.7   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I-5), SAME NUMBER PER 100 RESIDUES
   10  0.9   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I-4), SAME NUMBER PER 100 RESIDUES
    5  0.5   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I-3), SAME NUMBER PER 100 RESIDUES
    0  0.0   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I-2), SAME NUMBER PER 100 RESIDUES
    0  0.0   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I-1), SAME NUMBER PER 100 RESIDUES
    0  0.0   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I+0), SAME NUMBER PER 100 RESIDUES
    0  0.0   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I+1), SAME NUMBER PER 100 RESIDUES
  132 12.0   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I+2), SAME NUMBER PER 100 RESIDUES
  145 13.2   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I+3), SAME NUMBER PER 100 RESIDUES
   56  5.1   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I+4), SAME NUMBER PER 100 RESIDUES
    6  0.5   TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(I+5), SAME NUMBER PER 100 RESIDUES
  1  2  3  4  5  6  7  8  9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30     *** HISTOGRAMS OF ***
  0  0  0  4  0  2  0  0  0  0  0  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0    RESIDUES PER ALPHA HELIX
 14 17  6  5  4  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0    PARALLEL BRIDGES PER LADDER
 19  5  6  2  1  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0    ANTIPARALLEL BRIDGES PER LADDER
  6  1  3  4  6  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0    LADDERS PER SHEET

#  RESIDUE AA STRUCTURE BP1 BP2  ACC     N-H-->O    O-->H-N    N-H-->O    O-->H-N    TCO  KAPPA ALPHA  PHI   PSI  X-CA Y-CA Z-CA
  1    1 A L              0   0  118     0, 0.0     2,-0.1     0, 0.0   233,-0.0   0.000 360.0 360.0 360.0 -24.2 -10.7 44.3 21.8
  2    2 A E        -     0   0   79     1,-0.1     0, 0.0     3,-0.0     0, 0.0   0.000 360.0 -60.0 -60.0 -36.8 -13.8 41.5 20.8
  3    3 A E        -     0   0  182    -2,-0.1    -1,-0.1     3,-0.0     2,-0.0   0.908  15.3-142.7 -42.2-106.2  -5.4 41.6 23.9
  4    4 A K        -     0   0   83     2,-0.1    32,-0.1    32,-0.0    31,-0.0   0.331  31.0  93.4 125.4 105.4  -1.9 40.0 23.4
  5    5 A K        -     0   0  137    30,-0.1    -2,-0.2    -2,-0.2    -3,-0.2   0.403  46.6-171.8 -92.4  -0.2  18.7 37.0 37.2 25.6
  6    6 A V  E     -a   36  0A   82    29,-0.2    -2,-0.2    31,-0.2    -4,-0.2  -0.150  70.5 -13.2  43.2-121.3  21.3 38.8 35.1 28.2
  7    7 A a  E     -a   37  0A   19    29,-2.2    31,-0.2    -2,-0.2    -5,-0.2   0.309 106.2 120.0 -93.5  11.2  24.2 36.4 34.7 30.7
  8    8 A Q        -     0   0  102    -2,-0.3    -2,-0.2    -2,-0.2    -6,-0.2  -0.424  55.1-138.9 -76.6 148.7  23.1 33.9 37.3 33.7
  9    9 A G        -     0   0   16    21,-0.2    -2,-0.2    -2,-0.2    -7,-0.2   0.403  46.6-171.8 -92.4  -0.2  18.7 37.0 37.2 32.8
 10   10 A T  B     -F   40  0B   25    30,-1.5    -2,-0.2    -2,-0.2    -8,-0.2  -0.150  70.5 -13.2  43.2-121.3  21.3 38.8 35.1 34.8
 11   11 A S        +     0   0   75    -2,-0.3  1032,-0.7    28,-0.1     3,-0.1  -0.206  51.5 119.4-144.8  46.4  16.1 39.7 36.6
 12   12 A N    >   -     0   0   20     1,-0.3     3,-3.1  1030,-0.2  1033,-0.1   0.403  46.6-171.8 -92.4  -0.2  18.7 37.0 37.2
 13   13 A K  T 3  S-     0   0   83     1,-0.3    -1,-0.3  1020,-0.1  1020,-0.1  -0.150  70.5 -13.2  43.2-121.3  21.3 38.8 35.1
 14   14 A L  T 3  S+     0   0    8  1018,-0.1    -1,-0.3    -3,-0.1     2,-0.1   0.309 106.2 120.0 -93.5  11.2  24.2 36.4 34.7
 15   15 A T    <   -     0   0    3    -3,-3.1     2,-0.4  1018,-0.1  1020,-0.2  -0.424  55.1-138.9 -76.6 148.7  23.1 33.9 37.3
 16   16 A Q  B     -g 1035  0C   13  1018,-2.9  1020,-2.1    -2,-0.1     2,-1.0  -0.872   7.2-140.2-107.0 141.2  22.3 30.3 36.5
 17   17 A L        -     0   0   19    -2,-0.4     2,-0.2  1018,-0.2     9,-0.2  -0.674  61.0 -66.3-103.0  79.9  19.4 28.5 38.1
 18   18 A G  S     S+    0   0   13    -2,-1.0  1018,-0.1  1018,-0.5  1019,-0.1  -0.514 104.7   3.8  79.0-148.1  20.7 25.1 38.9
 19   19 A T  S  > S-     0   0   77    -2,-0.2     4,-3.2     1,-0.1     5,-0.2  -0.075  78.9-104.9 -63.9 168.5  21.7 22.7 36.0
 20   20 A F  H  > S+     0   0   88     2,-0.2     4,-2.5     1,-0.2     5,-0.2   0.964 124.6  46.2 -60.0 -50.2  21.6 23.8 32.4
 21   21 A E  H  > S+     0   0  113     2,-0.2     4,-2.3     1,-0.2     5,-0.2   0.931 114.0  47.1 -58.3 -49.7  18.4 21.7 31.9
```

Position of C_α^i

Local geometry

BEYOND DSSP: STRIDE

STRuctural IDEntification (STRIDE)

Frishman D & Argos P (1995) *Proteins* **23**, 566-579

Basically: SSEs are assigned using the weighted contribution of both H-bonds and (Φ, Ψ) values.

statistically derived propensities of aminoacids to occur in α-helices and β-sheets.

⊕ STRIDE was parameterized using 226 X-ray/NMR structures.

⊕ Relatively weak H-bonds can be compensated for by correct backbone geometry

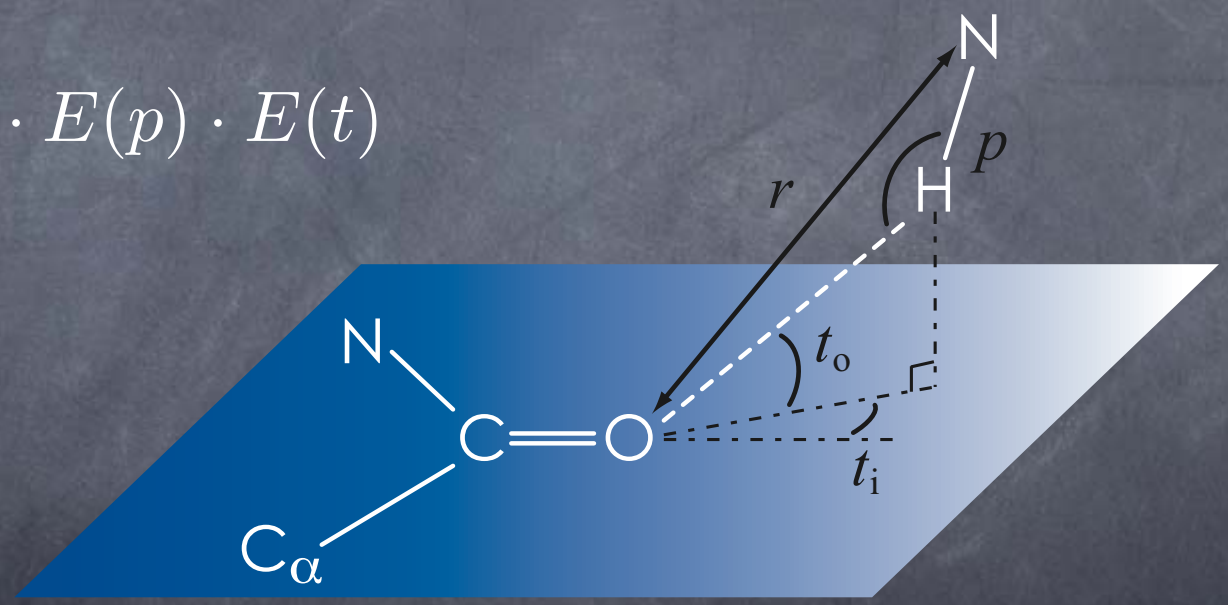
⊕ (Φ, Ψ) values can disfavour the assignment of SSEs in spite of a strong H-bond pattern (e.g. 3_{10}- and α-helices)

STRIDE: The H-Bond Contribution

Frishman D & Argos P (1995) *Proteins* **23**, 566-579

The H-bond energy term is more sophisticated than in DSSP.
Emphasis on the geometry of the C=O···H–N complex.

$$E_{\mathrm{HB}} = E(r) \cdot E(p) \cdot E(t)$$



$$E(r) = \frac{C}{r^8} + \frac{D}{r^6}$$

$$C = -3E_{\mathrm{m}} r_{\mathrm{m}}^8$$

$$D = -4E_{\mathrm{m}} r_{\mathrm{m}}^6$$

E_{m} ,r_{m}: optimal terms
E_{m} = -2.8 kcal·mol^{-1}
r_{m} = 3 Å

STRIDE: The H-Bond Contribution

Frishman D & Argos P (1995) *Proteins* **23**, 566-579

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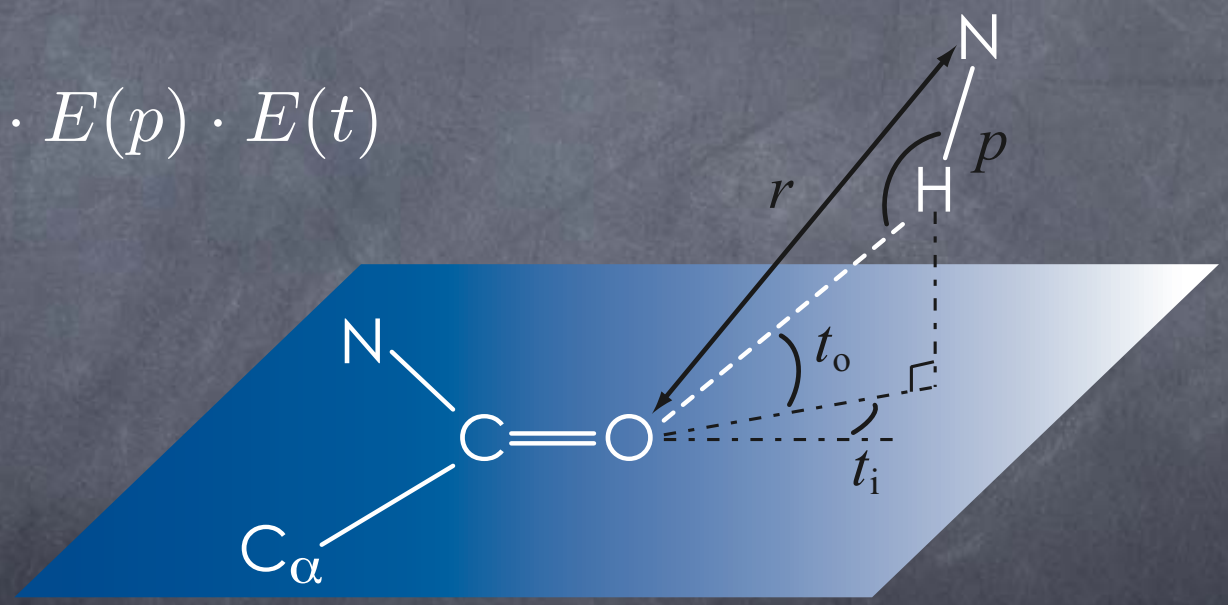


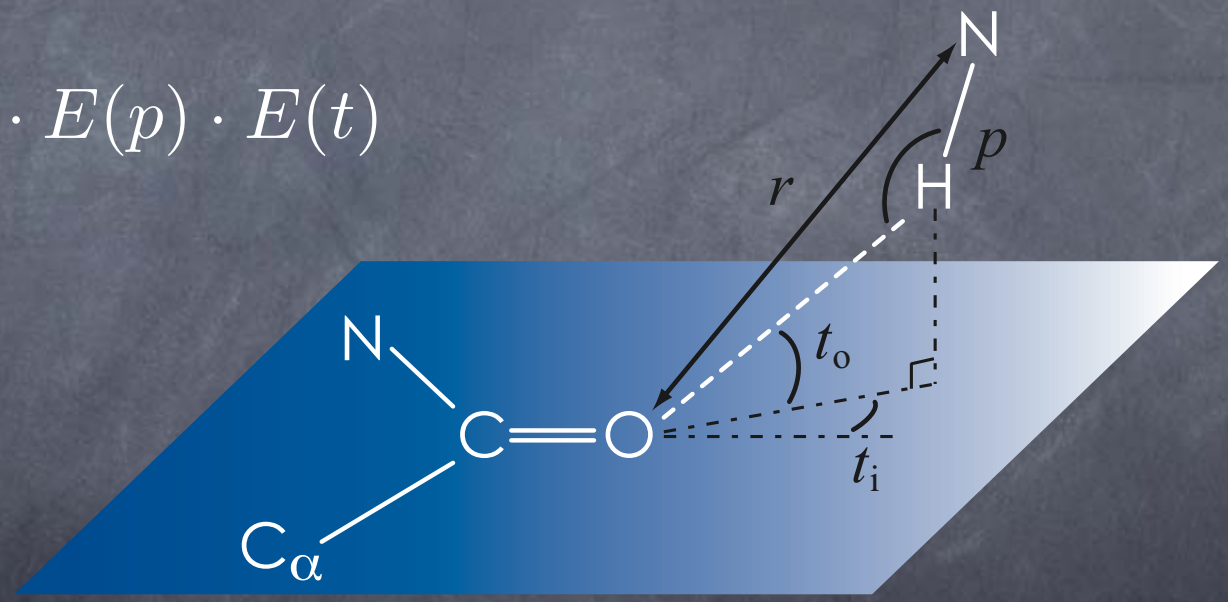
$$E(p) = \cos^2 p$$

STRIDE: The H-Bond Contribution

Frishman D & Argos P (1995) *Proteins* **23**, 566-579

The H-bond energy term is more sophisticated than in DSSP.
Emphasis on the geometry of the C=O···H–N complex.

$$E_{\mathrm{HB}} = E(r) \cdot E(p) \cdot E(t)$$

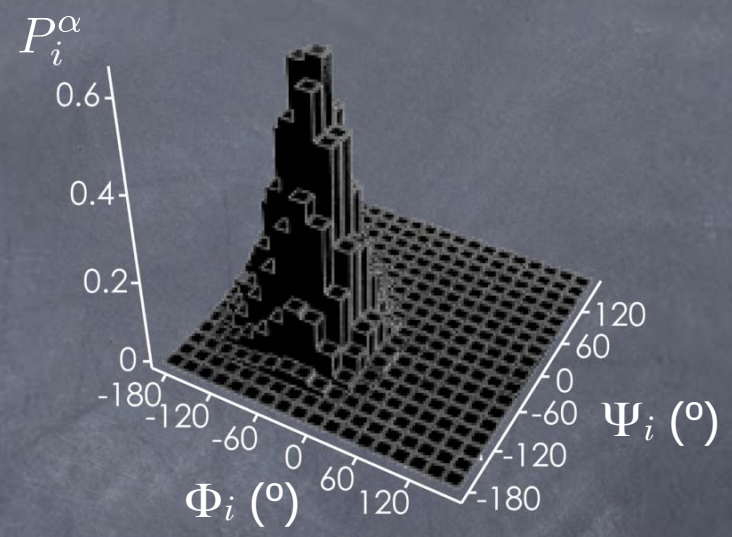


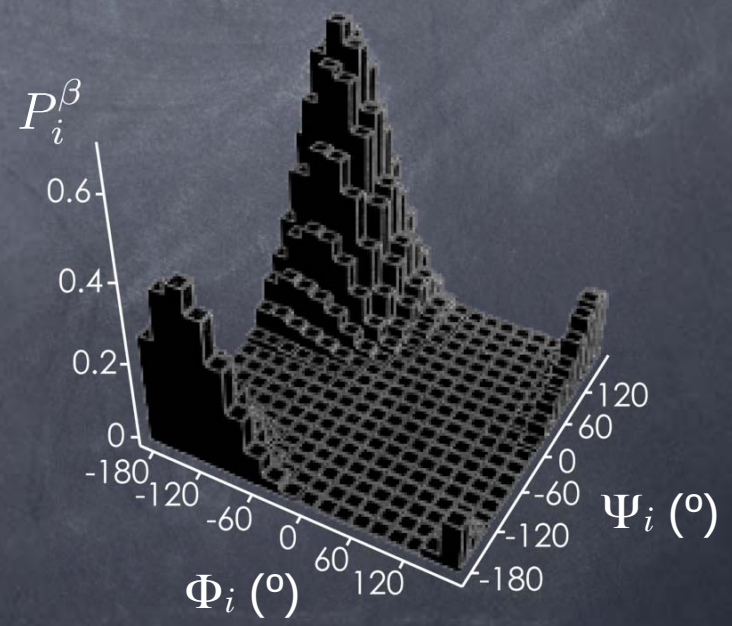
$$E(t) = \begin{cases} (0.9 + 0.1 \sin 2t_i) \cos t_0 & , 0 < t_i < 90^\circ \\ k_1 (k_2 - \cos^2 t_i)^3 \cos t_0 & , 90^\circ < t_i < 110^\circ \\ 0 & , \quad t_i > 110^\circ \end{cases}$$

STRIDE: The (Φ,Ψ) Contribution

Frishman D & Argos P (1995) *Proteins* **23**, 566-579

Probabilities P_i^α and P_i^β that a residue is in an α-helix or a β-sheet at position i calculated from the HELIX and SHEET records in PDB files.





Definition of α-helices and β-sheets

α-helices: similarly to DSSP, an α-helix is defined when there are 2 consecutive HBs (i, i+4) and (i+1, i+5). STRIDE will assign the α-helix from residue i+1 to residue i+4 (and possibly to i and i+5 with specific thresholds).

$$E_{\mathrm{HB}}^{i,i+4} \cdot W^{\alpha}(P_i^{\alpha}, P_{i+4}^{\alpha}) < T^{\alpha}$$

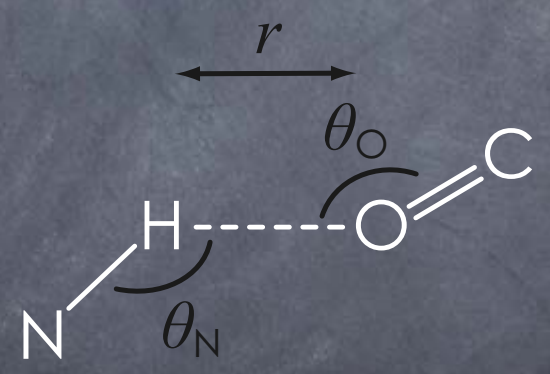
β-sheets: they are defined by two consecutive β-bridges. A β-bridge between 2 residues i and j requires that 2 conditions are fulfilled:

$$\begin{cases} E_{\mathrm{HB}}^{i} \cdot W^{\beta}(P_i^{\beta}, P_j^{\beta}) < T^{\beta} \\ E_{\mathrm{HB}}^{j} \cdot W^{\beta}(P_i^{\beta}, P_j^{\beta}) < T^{\beta} \end{cases}$$

W^s, T^s: weighting function and threshold for the element s, respectively (specific W and T for antiparallel and parallel β-bridges).

Definition of 3_{10}- and π-helices and turns

3_{10}-helices, π-helices: assigned as in DSSP, but HBs are defined differently by taking into account various parameters, *e.g.* r, θ_N, θ_O, chemical elements, atomic hybridization, environment, planarity, *etc* (Stickle *et al.*, 1992).



Turns: definition from Richardson (1981) and Wilmot and Thornton (1990).

DSSP or STRIDE?

DSSP and STRIDE give roughly the same results (identical in 11% of the protein chains tested).

α-Helices and β-strands tend to be 1-2 residues longer with STRIDE than with DSSP.

DSSP tends to split long α-helices into 2 separate helices.

DSSP tends to assign short α-helices where the local geometry is not typical of α-helices.

STRIDE assigns longer α-helices at the expense of residues that DSSP would find in 3_{10}-helices or in turns.

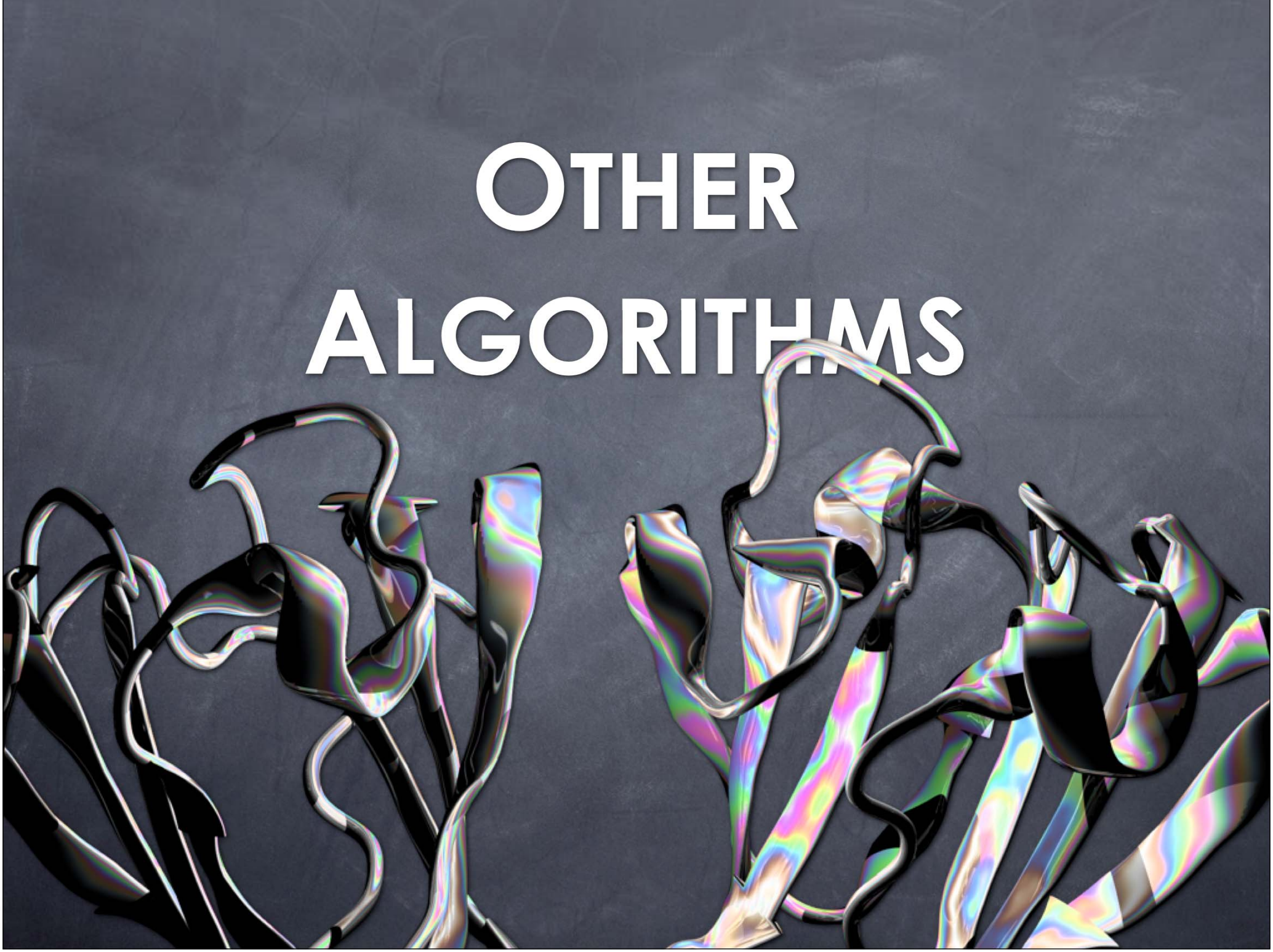
DSSP or STRIDE?

DSSP can be used with GROMACS (do_dssp).
For STRIDE, you need to write your own do_stride *(I have one, but slower than do_dssp)*.

In viewers:

- Rasmol: uses DSSP
- VMD: uses STRIDE
- PyMOL: if there is no HELIX/SHEET record in the PDB file, it has its own assignment method (dss) but it is close to DSSP
- Chimera: same as PyMOL with its own algorithm (ksdssp)
- DeepView/Swiss-PdbViewer: has its own method; doesn't use the HELIX/SHEET records

Other Algorithms



Using C_α Traces

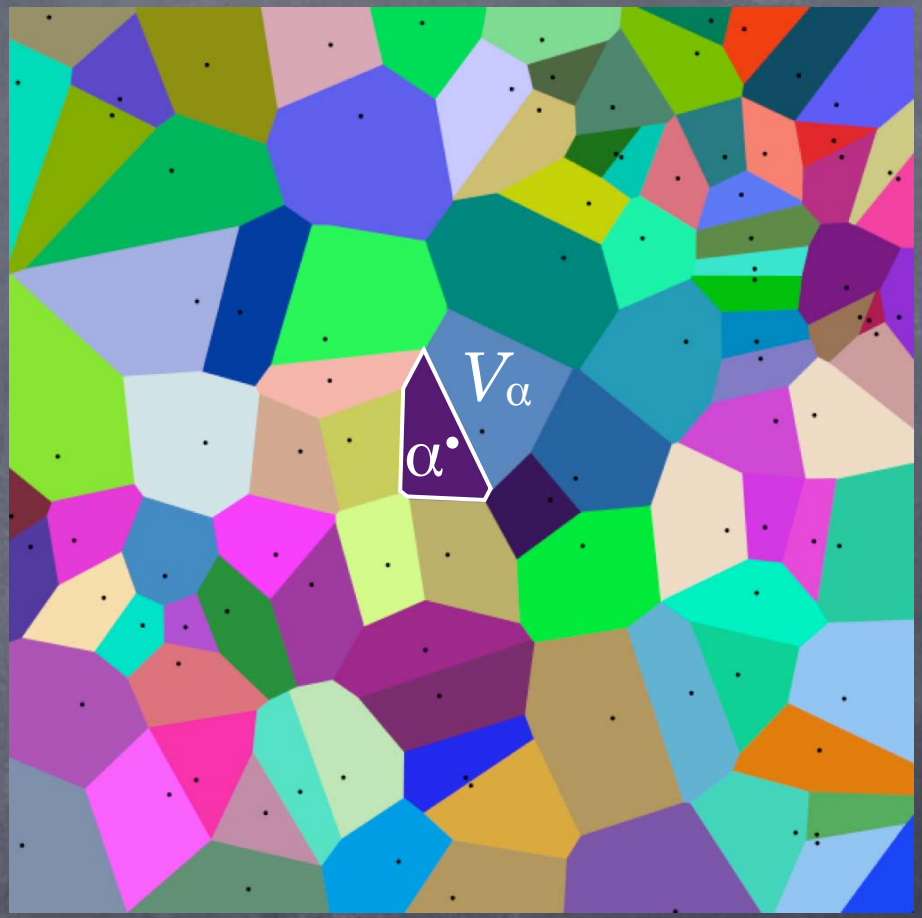
DEFINE (Richards & Kundrot (1988) *Proteins* **3**, 71-84): uses a matrix of the distances between the C_α atoms of a protein chain. DEFINE can assign α- and 3_{10}-helices, β-strands, β-sheets, turns and Ω-loops.

P-SEA (Labesse *et al.* (1997) *Comput Appl Biosci* **13**, 291-295): uses the distances (i-1, i+1), (i-1, i+2) and (i-1, i+3), the angles (i-1, i, i+1) and the dihedrals (i-1, i, i+1, i+2) between the C_α atoms.

VoTAP (Dupuis *et al.* (2004) *Proteins* **55**, 519-528): uses 3D Voronoï tessellation. Each residue is associated with a Voronoï polyhedron (using C_α's only) and the contacts between them allow to define SSE.

Using C_α Traces

Each cell V_α consists of all the points closer to α than to any other site. The segments of the Voronoï diagram are all the points in the plane that are equidistant to two sites.

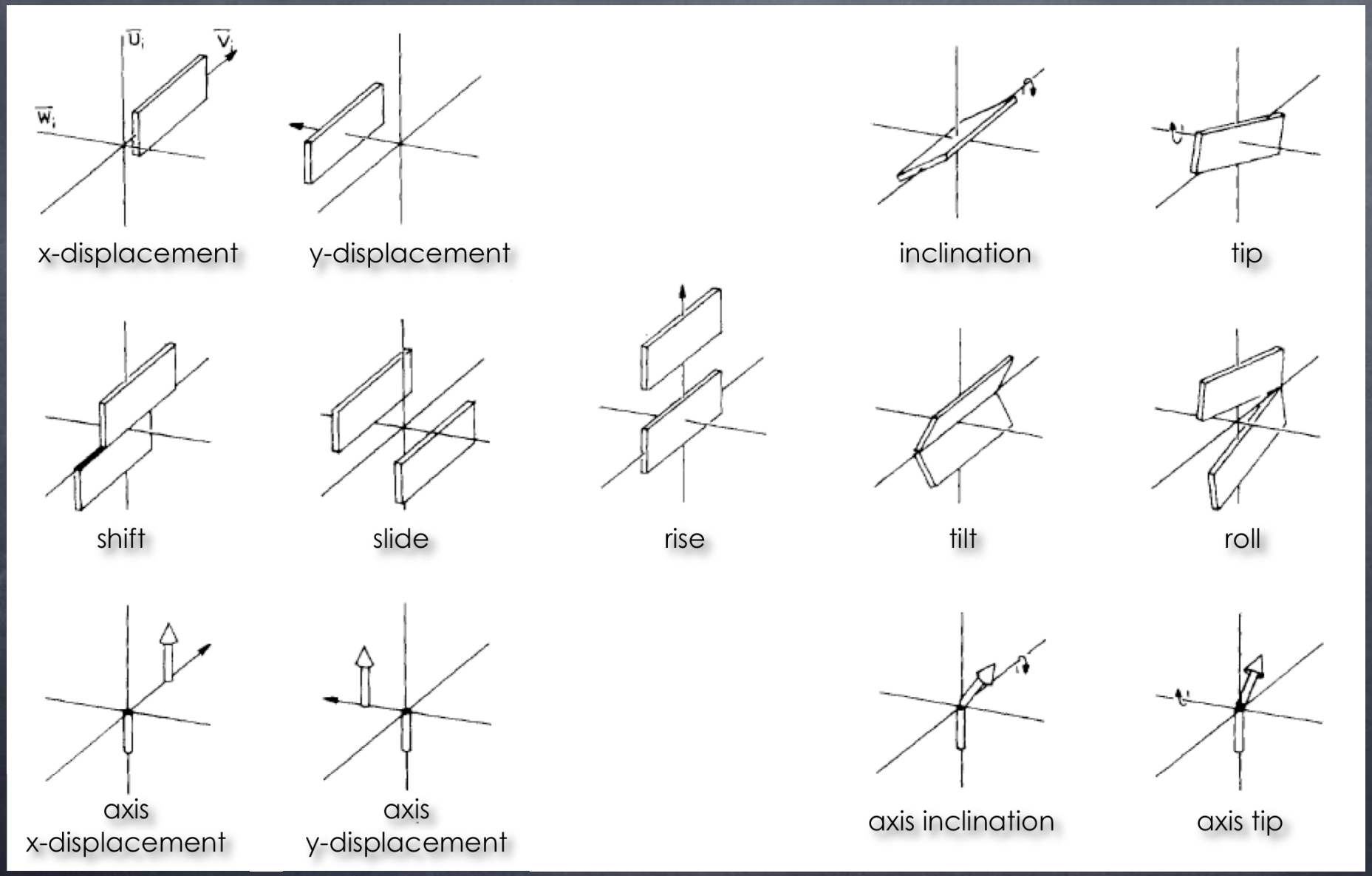


VoTAP (Dupuis *et al.* (2004) *Proteins* **55**, 519-528): uses 3D Voronoï tessellation. Each residue is associated with a Voronoï polyhedron (using C_α's only) and the contacts between them allow to define SSE.

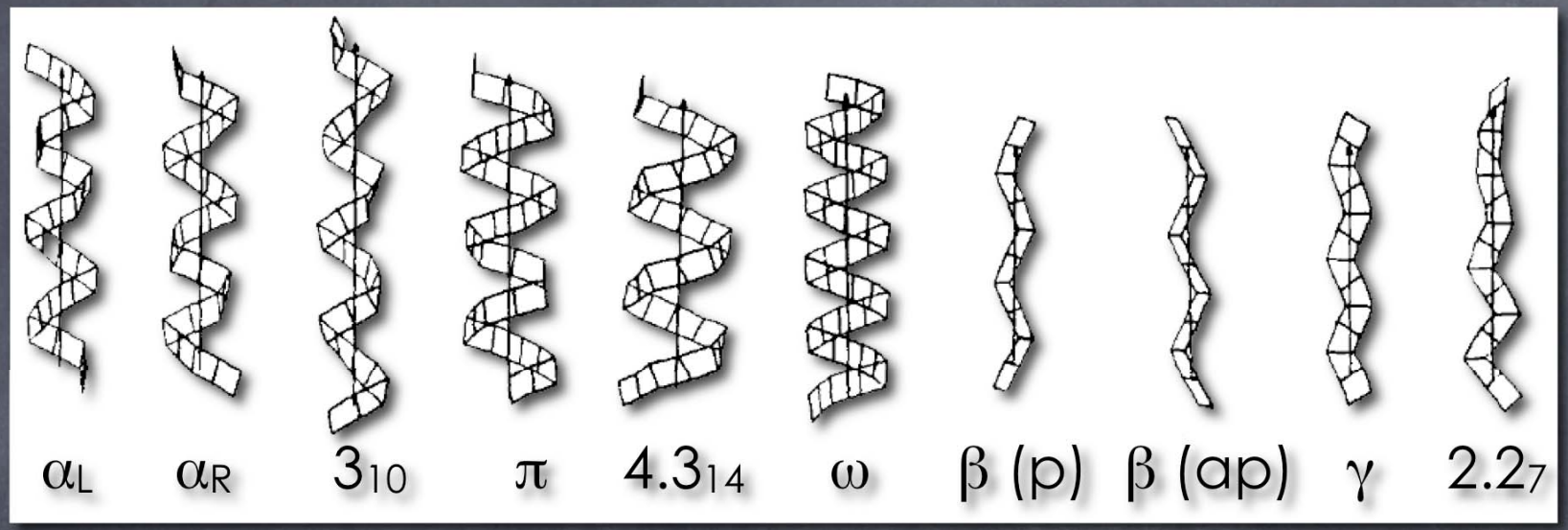
Using the Backbone Geometry

P-CURVE (Sklenar *et al.* (1989) *Proteins* **6**, 46-60): it is an extension to proteins of the widely used program CURVE for nucleic acids. Each aminoacid i defines a unit which comprises the atoms C_α^i, C^i, O^i, N^{i+1} and H^{i+1}. From the relative arrangements between units, helicoidal parameters are derived exactly like with nucleic acids (x-displacement, y-displacement, inclination,tip, shift, slide, rise, tilt, roll, twist, axis x-displacement, axis y-displacement, axis inclination and axis tip).

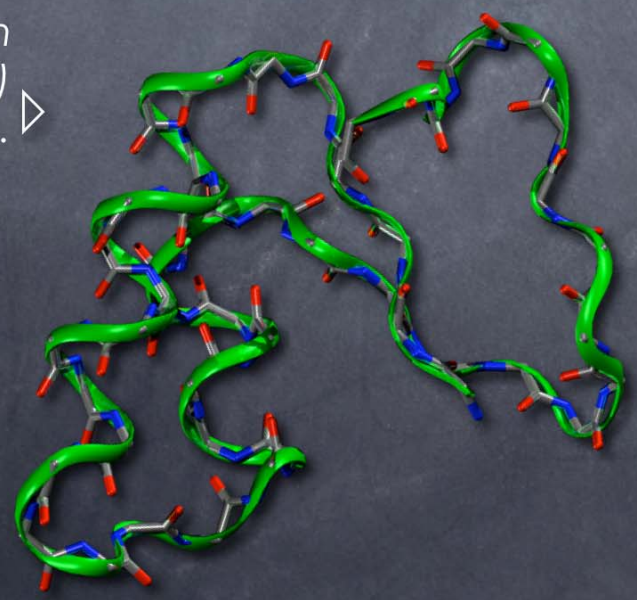
Using the Backbone Geometry: P-CURVE

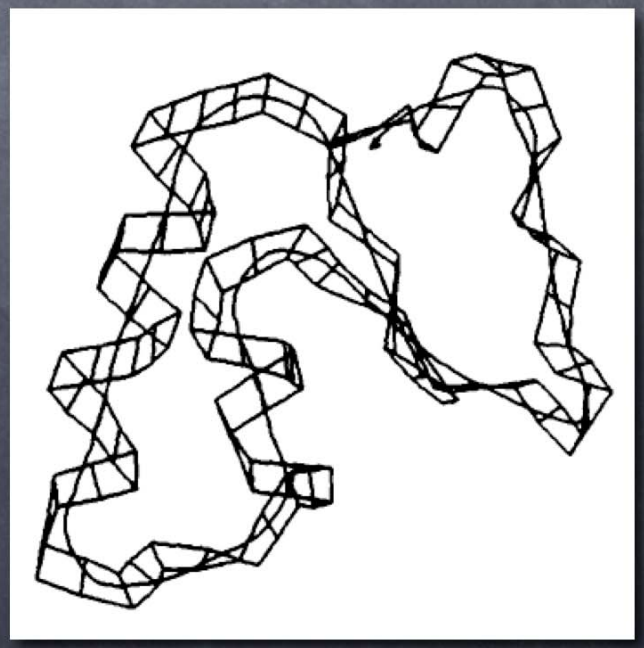


Using the Backbone Geometry: P-CURVE



Example of Crambin at 1.5 Å (1CRN) Teeter (1984).





To put it in a nutshell...

Most methods give similar results, generally difference at edges (1-2 residues more or less).

Sensitivity to 3_{10}-helices and π-helices can still be improved.

A combination of several methods can be used to get consensus SSEs.

Be aware that some methods underestimate/ overestimate the presence or the extent of some SSEs.