

Protein 2° Structure

Chou-Fasman Algorithm

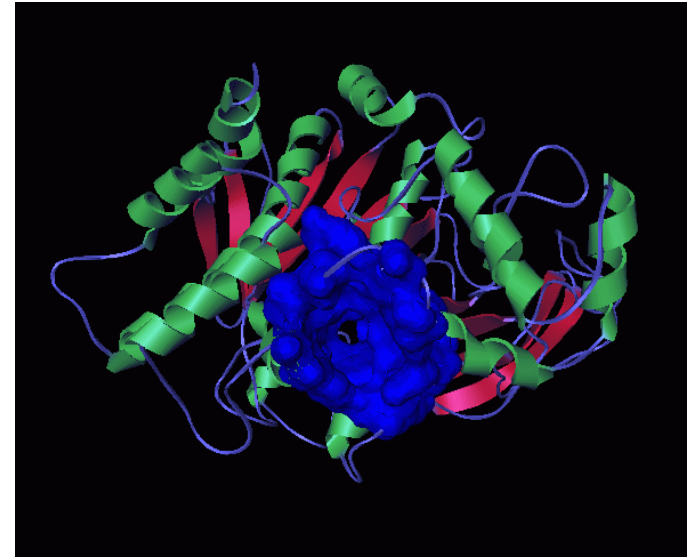
- **Conformational parameters**

for every amino acid (AA):

$P(a)$ = propensity in an **alpha helix**

$P(b)$ = propensity in a **beta sheet**

$P(\text{turn})$ = propensity in a turn



Based on observed propensities in proteins of known structure

Secondary Structure Data

P03372 (ESR1_HUMAN) ★ Reviewed, UniProtKB/Swiss-Prot

Last modified August 10, 2010. Version 164.  [History...](#)

 Clusters with [100%](#), [90%](#), [50%](#) identity |  [Documents \(6\)](#) |  [Third-party data](#)

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[Entry info](#) · [Documents](#)

Names and origin

Protein names	<i>Recommended name:</i> Estrogen receptor Short name=ER <i>Alternative name(s):</i> Estradiol receptor ER-alpha Nuclear receptor subfamily 3 group A member 1
Gene names	Name: ESR1 Synonyms:ESR, NR3A1
Organism	Homo sapiens (Human) [Complete proteome]
Taxonomic identifier	9606 [NCBI]

Secondary structure

1

Helix Strand Turn

Details...

- ☐ Turn
- ☐ Beta strand
- ☐ Beta strand
- ☐ Helix
- ☐ Beta strand
- ☐ Turn
- ☐ Helix
- ☐ Helix
- ☐ Helix
- ☐ Helix
- ☐ Helix
- ☐ Helix
- ☐ Beta strand
- ☐ Beta strand
- ☐ Helix
- ☐ Helix
- ☐ Helix
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- ☐ Helix

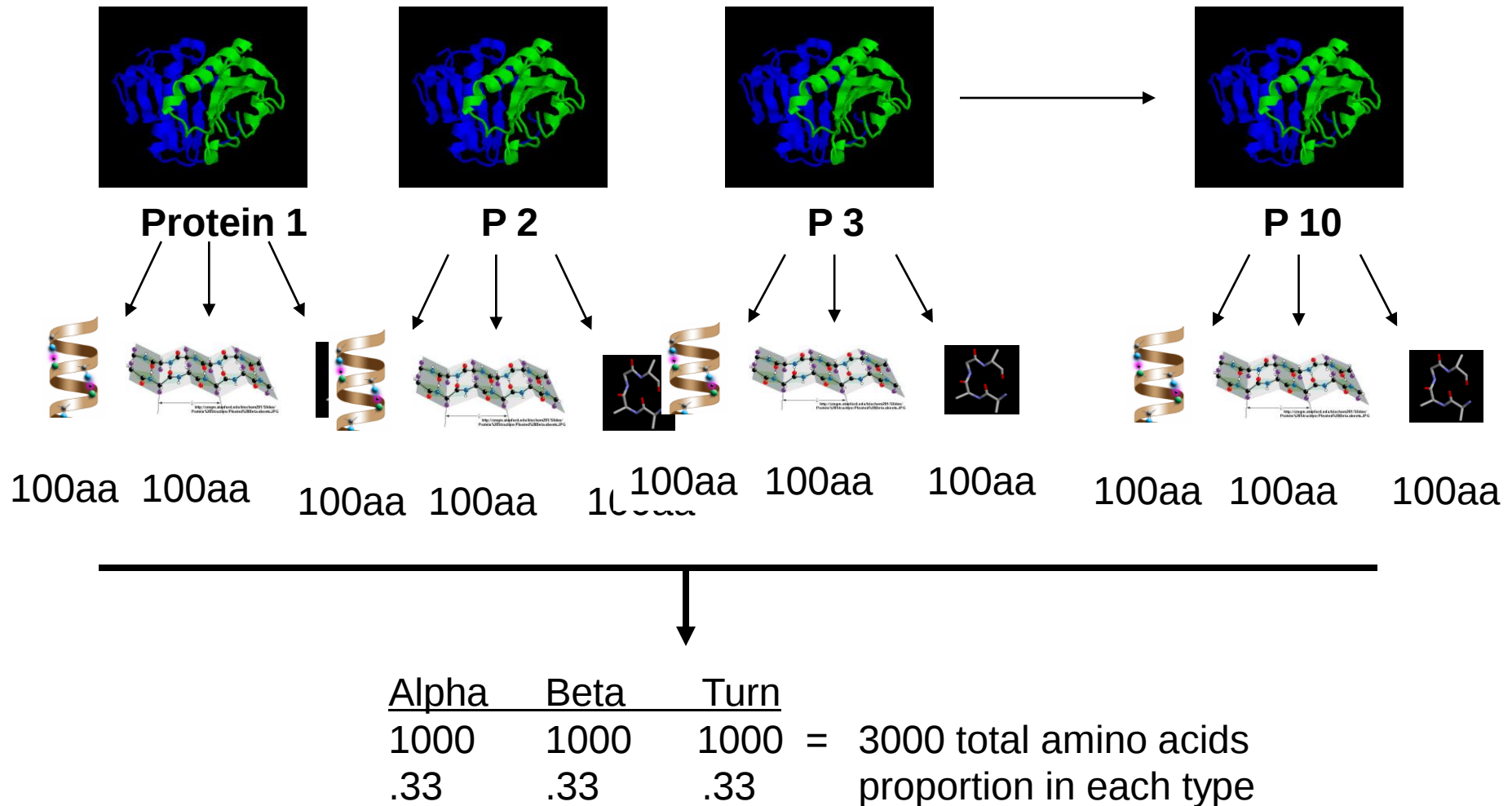
P03372[466-492], Estrogen receptor, Homo sapiens

10	20	30	40	50	60
MTMTLHTKAS	GMALLHQIQG	NELEPLNRPQ	LKIPLERPLG	EVYLDSSKPA	VYNYPEGAAY
70	80	90	100	110	120
EFNAAAAANA	QVYGQTGLPY	GPGSEAAAFG	SNGLGGFPPL	NSVSPSPLML	LHPPPQLSPF
130	140	150	160	170	180
LQPHGQQVPY	YLENEPSGYT	VREAGPPAFY	RPNSDNRRQG	GRERLASTND	KGSMAMESAK
190	200	210	220	230	240
ETRYCAVCND	YASGYHYGVW	SCEGCKAFFK	RSIQGHNDYM	CPATNQCTID	KNRRKSCQAC
250	260	270	280	290	300
RLRKCYEVGM	MKGGIRKDRR	GGRMLKHKRQ	RDDGEGRGEV	GSAGDMRAAN	LWPSPLMIKR
310	320	330	340	350	360
SKKNSLALSL	TADQMVSALL	DAEPPILYSE	YDPTRPFSEA	SMMGLLTNLA	DRELVHMINW
370	380	390	400	410	420
AKRVPGFVDL	TLHDQVHLL	CAWLEILMIG	LVWRSMHPG	KLLFAPNLLL	DRNQGKCVEG
430	440	450	460	470	480
MVEIFDMLLA	TSSRFRMMNL	QGEEFVCLKS	IILLNSGVYT	FLSSTLKSLE	EKDHIHRVLD
490	500	510	520	530	540
KITDTLIHLM	AKAGLTQQQ	HQRLAQLLLI	LSHIRHMSNK	GMEHLYSMKC	KNVVPLYDLL
550	560	570	580	590	
LEMLDAHRLH	APTSRGGASV	EETDQSHLAT	AGSTSSHSLQ	KYYITGEAEG	FPATV



DATABASE of Protein Structures

10 proteins



Proportions

Alpha	Beta	Turn	
1000	1000	1000	= 3000 total amino acids
.33	.33	.33	proportion in each type

Lysines:

Total number of Lysines in all 10 proteins = 100

Number of Lysines in alpha helices = 80

Number of Lysines in beta sheets = 15

Number of Lysines in Turns = 5

Observed (in helices) = .80

Expect (at random) = .33

Propensity = $.80 / .33$ = **2.42 (*100 = 242)**

Beta Sheets?

Turns?

Chou-Fasman Algorithm

Secondary Structure Propensities

- The “**propensity**” for an amino acid, i , to adopt the helical conformation can be calculated from the database of known structures as follows:

$$P_{\alpha}^i = \frac{\% \text{ of residues of type } i \text{ in } \alpha\text{-helix}}{\% \text{ of all residues in } \alpha\text{-helix}}$$

- e.g. for alanine

Total number of alanine in database = 2,000

Total number of all residue types in database = 20,000

Number of alanines which occur in helices = 500

Number of all residue types in helices = 5,000

$$P_{\alpha}^{ala} = \frac{500/2000}{5000/20000} = 1.0$$

- Similarly alanine propensity for beta-structure can be calculated as follows:

$$P_{\beta}^i = \frac{\% \text{ of residues of type } i \text{ in } \beta\text{-strand}}{\% \text{ of all residues in } \beta\text{-strand}}$$

- These amino acid propensities can then be used to predict the secondary structure of new protein sequence.

Chou-Fasman Algorithm

Identify **alpha helices** as follows:

STEP 1:

Find 4 out of 6 aa residues with $P(a) \geq 100$ (Window size 6)

STEP 2:

Extend to the Right (not left) until 4 contiguous residues with $P(a) < 100$ encountered. DO NOT INCLUDE THESE LAST FOUR IN THE HELIX.

STEP 3:

For each region in part 2, compute $\Sigma P(a)$ and $\Sigma P(b)$.

STEP 4:

If region > 5 AAs in length and $\Sigma P(a) > \Sigma P(b)$ then it is an alpha helix.

Chou-Fasman Algorithm

SPASEASDGQSVSV

↓
P(a) P(b)
 S: 77 75
 P: 55 55
 A: 142 83
 S: 77

SPASEASDGQFETTY

↓
P(a) P(b)
 E: 151 37
 A: 142 83
 S: 77 75
 D: 101 54
 G: 57
 Q: 111

1) 4 of 6, $P(a) \geq 100$

2) Extend RIGHT until 4 contiguous

Residues have $P(a) < 100$

3) Calculate $\Sigma P(a)$ and $\Sigma P(b)$. Is $\Sigma P(a) > \Sigma P(b)$? (Do Not Include last 4 in sum)

TABLE 7.1 The Chou-Fasman parameters for the 20 common amino acids.

Amino acid	$P(a)$	$P(b)$	$P(\text{turn})$	$f(i)$	$f(i+1)$	$f(i+2)$	$f(i+3)$
A Alanine	142	83	66	0.06	0.076	0.035	0.058
R Arginine	98	93	95	0.070	0.106	0.099	0.085
N Asparagine	67	89	156	0.161	0.083	0.191	0.091
D Aspartic acid	101	54	146	0.147	0.110	0.179	0.081
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H Histidine	100	87	95	0.140	0.047	0.093	0.054
I Isoleucine	108	160	47	0.043	0.034	0.013	0.056
L Leucine	121	130	59	0.061	0.025	0.036	0.070
K Lysine	114	74	101	0.055	0.115	0.072	0.095
M Methionine	145	105	60	0.068	0.082	0.014	0.055
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W Tryptophan	108	137	96	0.077	0.013	0.064	0.167
Y Tyrosine	69	147	114	0.082	0.065	0.114	0.125
V Valine	106	170	50	0.062	0.048	0.028	0.053

Find potential alpha helix:

MFCTYYGNNGEHIELMM

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Residues have $P(a) < 100$

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Extend Right → 4 $P(a)$'s < 100?

MFCTYYGNNGEHIELMM

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MFCTYYGNNGEH**IELMM**

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$\Sigma P(a) =$

$\Sigma P(b) =$

MFCTYYGN**NGEHIELMM**

In class Chou-Fasman calculation

Chou-Fasman Algorithm

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$$\Sigma P(a) = 1045 \quad \Sigma P(b) = 825$$

MFCTYYGNNGEHIELMM

C-F for Beta-Sheet

Now Calculate Beta-sheet on same sequence:

- 1) 4 of 6, $P(b) \geq 100$
- 2) Extend RIGHT until 4 contiguous Residues have $P(b) < 100$
(If you find 4 < 100, do not include these in calculation.)
- 3) Calculate $\Sigma P(a)$ and $\Sigma P(b)$.
- 4) If $\Sigma P(b) > \Sigma P(a)$, then region is beta-sheet

Try on same sequence:

MFCTYYGNNGEHIELMM

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N	Asparagine	67	89	156	0.161	0.083	0.191	0.091
D	Aspartic acid	101	54	146	0.147	0.110	0.179	0.081
C	Cysteine	70	119	119	0.149	0.050	0.117	0.128
E	Glutamic acid	151	37	74	0.056	0.060	0.077	0.064
Q	Glutamine	111	110	98	0.074	0.098	0.037	0.098
G	Glycine	57	75	156	0.102	0.085	0.190	0.152
H	Histidine	100	87	95	0.140	0.047	0.093	0.054
I	Isoleucine	108	160	47	0.043	0.034	0.013	0.056
L	Leucine	121	130	59	0.061	0.025	0.036	0.070
K	Lysine	114	74	101	0.055	0.115	0.072	0.095
M	Methionine	145	105	60	0.068	0.082	0.014	0.055
F	Phenylalanine	113	138	60	0.059	0.041	0.065	0.065
P	Proline	57	55	152	0.102	0.301	0.034	0.068
S	Serine	77	75	143	0.120	0.139	0.125	0.106
T	Threonine	83	119	96	0.086	0.108	0.065	0.079
W	Tryptophan	108	137	96	0.077	0.013	0.064	0.167
Y	Tyrosine	69	147	114	0.082	0.065	0.114	0.125
V	Valine	106	170	50	0.062	0.048	0.028	0.053

Regions of Overlap

- What if the alpha-helical and beta-sheet regions overlap?
- OVERLAP RULE:
 - If $\Sigma P(a) > \Sigma P(b)$, then = Alpha-helix
 - If $\Sigma P(b) > \Sigma P(a)$, then = Beta-Sheet

TEST YOURSELF

What is the overlap region on sequence below?

According to the Overlap Rule, is it Alpha or Beta?

MFCTYYMQNGEHIELMM