

# Protein Prediction and Structure Analysis of N- terminal of E3L Protein in SPPV

绵羊痘病毒E3L蛋白N端结构与功能预测和分析

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报告: 卢昌

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# 1. Background

The E3 protein of vaccinia virus, the prototypic member of orthopoxviruses, functions as an inhibitor of innate immune signaling and is essential for vaccinia replication in vivo and in many human cell culture systems.

E3L is vary conserved in variola and related viruses and plays a key role in cirumventing the IFN-mediated defense of host cells.(Moss.B, J.L.Shisler. Immunology 101 at poxvirus U: immune evasion genes. Semin Immunol, 2001,13:59-66.)

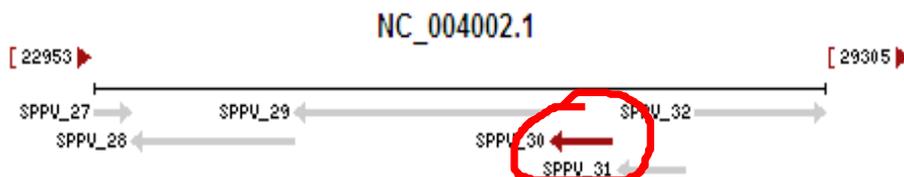
TABLE 1. SPPV AND GTPV ORFS

ORF no. <sup>a</sup>	Accession no. <sup>b</sup>	SPPV						GTPV			LSDV		MYXV ORF <sup>g</sup>	VACV ORF <sup>h</sup>				
		TU		SA		NK	PL		GV	% Id vs. SA	PL	Predicted structure and/or function <sup>f</sup>						
		Position	Length <sup>c</sup>	Changes <sup>d</sup> vs. SA	vs. NK	Length	Changes vs. NK	% Id <sup>e</sup> vs. PL	Length						Position	Length	Changes vs. GV	Length
001	M28823	589-113		Q/H		H/Q	97		648-172			159	96	99		M003.1	B15R	
002	M28823											131				M003.2		
003	M28823	2167-1235	311	+72 aa	+72 aa		97		2056-1337			240	97	99	ER-localized apoptosis regulator	M004	B9R	
004												57				M004.1		
005		2243-2746	168				92	168	2333-2842			170	93	93	IL-10			
006		3455-2763					95		3551-2859			231	96	96	IL-1R		B16R	
007		4545-3481					96		4640-3576			355	98	98			C10L	
008		5454-4630		I/N	I/N		94		5530-4706			275	94	95	Interferon-γ receptor	M007	B8R	
009												230			α-Amanitin sensitive protein	M139R	N2L	
010		6646-6161		V/A			93		6631-6146			162	95	94	LAP/PHD-finger protein	M153R		
011	S78201	7818-6697	374	A/T	A/T	374	92	374	7826-6684			381	92	95	G protein-coupled chemokine receptor			
012	S78201	8557-7925					95		8562-7930			211	95	95	Ankyrin repeat protein	M149R	B4R	
013	S78201											341			IL-1R		B16R	
014		9918-9652					93		9903-9637			89	96	96	eIF2α-like PKR inhibitor	M156R	K3L	
015		10390-9908					94		10375-9893			161	95	96	IL-18 binding protein			
016		10698-10399	100			100	92	100	10683-10396	96		89	96	97	EGF-like growth factor	M010L	C11R	
017		11219-10692		D/N	D/N		95		11204-10677			176	94	96	Antiapoptotic virulence factor	M011L		
018		11701-11264					99		11683-11246			146	98	97	dUTPase	M012L	F2L	
019 (a)		13452-11746					93		13414-11729	562		569	95	95	Kelch-like protein	M014L	F3L	
(b)												282						
020		14488-13526					97		14444-13482			321	98	98	Ribonucleotide reductase, small subunit	M015L	F4L	
021		14767-14531	79	A/S		79	S/A	86	14719-14483	79		86	81	82		M016L		
022		15148-14840	103			103	85	103	15114-14791	108		112	83	87				
023		15557-15342					95		15534-15319			72	97	97		M018L	F8L	
024		16286-15639					97		16265-15618			216	98	98		M019L	F9L	
025		17607-16267					99		17586-16246			447	98	99	Ser/Thr protein kinase; virus assembly	M020L	F10L	
026												302					F11L	
027		20390-18474	639	R/K,-N	R/K,-N	640	96	640	20429-18513	639		638	97	97	EEV maturation	M021L	F12L	
028	AF119594	21509-20400		T/A	G/C,T/A	G/C	98		21548-20439			370	98	99	Palmitoylated EEV envelope protein	M022L	F13L	
029		22148-21714					99		22187-21753			145	99	100		M024L	F15L	
030		22881-22225					96		22919-22263			219	97	97		M025L	F16L	
031		22953-23264					95		22994-23305			104	96	95	DNA-binding virion core protein	M026L	F17L	
032		24695-23274		K/N	K/N		97		24736-23315			474	97	98	Fcyl(A) polymerase large subunit PAP <sub>L</sub>	M027L	E1L	
033		24696-24695					97		24696-24695			752	97	97		M028L	E2L	
034		27444-26914		I/M			97		27530-26955	192		192	177	97	97	dsRNA-binding PKR inhibitor	M029L	E3L
035		28120-28002	222			222	97	222	28095-28002	222		222	98	98		M031R	E5R	
036		28087-27506	194	D/E,K/N	D/E,K/N	194	96	194	28150-27548			201	95	97	RNA polymerase subunit RPO30	M030L	E4L	
037		29315-31012		S/R			98		29376-31073			566	99	98		M032R	E6R	
038		31025-31819	265			265	99	265	31086-31880	265	N/D	265	96	99		M033R	E8R	
039		34851-31822		S/L,A/S	S/L,A/S		97		34912-31883			1010	98	98	DNA polymerase	M034L	E9L	
040		34885-35169		S/T		S/T	95		34946-35230			95	98	96	IMV redox protein, virus assembly	M035R	E10R	
041		35561-35172					92		35622-35233			130	93	97	Virion core protein		E11L	
042		37602-35551		H/N	H/N		96		37663-35612			684	97	97		M036L	O1L	
043		38652-37711					99		38713-37772			314	99	99	DNA-binding virion core protein	M038L	I1L	
044		38874-38662	71			71	97	71	38935-38723	71		71	92	95	95		M039L	I2L
045		39705-38878		V/I	V/I		95		39766-38939			276	96	97	DNA-binding phosphoprotein	M040L	I3L	
046		40001-39768					97		40049-39816			78	100	97	IMV membrane protein	M041L	I5L	
047		41203-40022					98		41251-40070			394	98	99		M042L	I6L	
048		42497-41199					99		42545-41247			433	99	99	Virion core protein	M043L	I7L	
049		43117-41778					98		43168-41781			400	97	97	TH-II, DNA polymerase	M044R	I8R	
050		46317-44533	595			595	98	595	46363-44581	595		596	98	98	Metalloprotease, virion morphogenesis	M045L	G1L	
051		46640-47305					98		46688-47353			222	98	100	Putative transcriptional elongation factor	M047L	G2F	
052		47000-47325					98		47000-47325			126	99	99		M048L	G4L	
053		47652-47275					98		47700-47325						Glutaredoxin 2, virion morphogenesis			

Comparison of CaPV genomes and vaccinia virus genomes. (E.R. Tulman, C.L. Afonso, et al. The Genomes of Sheepox and Goatpox Viruses. Journal of Virology, 2002, 76:6054-6061.)

Genomic context

Sequence: NC\_004002.1 (26911..27444, complement)

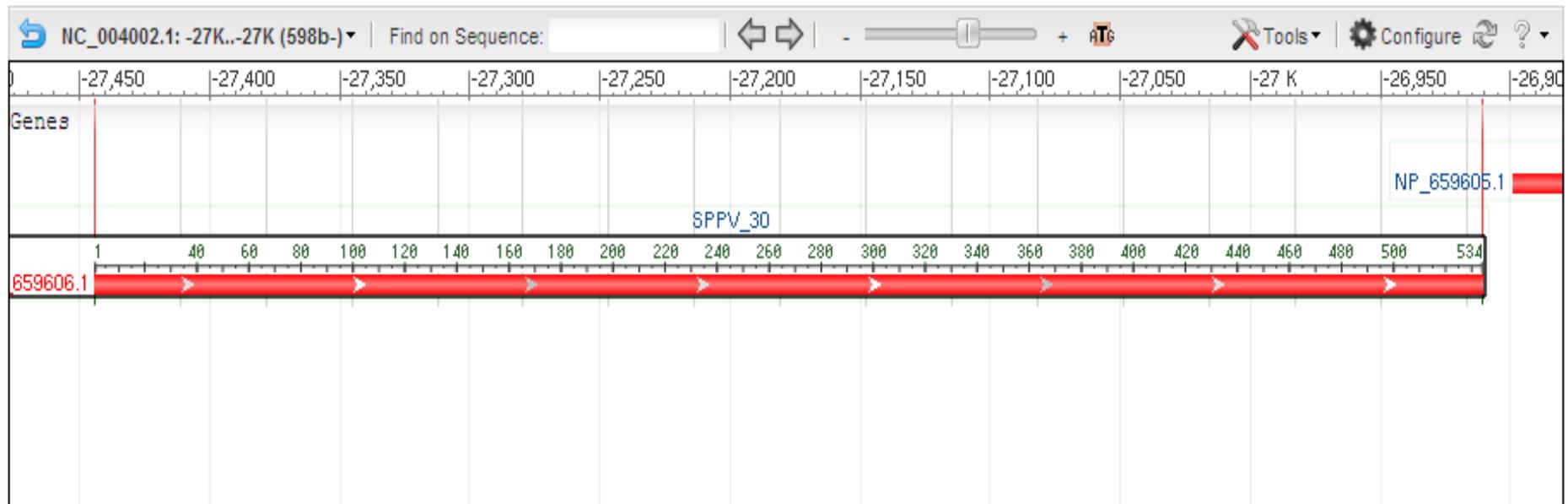


Genomic regions, transcripts, and products

Genomic Sequence

[Go to reference sequence details](#)

[Go to nucleotide](#) [Graphics](#) [FASTA](#) [GenBank](#)



- The E3 protein is composed of a carboxy-terminal dsRNA binding domain and an amino-terminal Z-DNA binding domain. While wild-type vaccinia virus displays a broad cellular tropism and is highly resistant to effects of interferon(IFN), deletion of E3 results in restricted tropism and sensitivity to IFNs.

- The ability to bind Z-DNA is essential for E3L activity. A replacement of the N-terminal domain of E3L with a domain defective in Z-DNA binding results in a less pathogenic or nonpathogenic virus.

- Z-DNA-forming sequences found near the transcription start site can flip into the Z-conformation in some actively transcribing genes , and E3L may bind to the Z-DNA segment of such genes.

## 2. Basic protein information

LOCUS NP\_659606 177 aa linear VRL 26-MAR-2010  
DEFINITION dsRNA-binding PKR inhibitor [Sheeppox virus].  
ACCESSION NP\_659606  
VERSION NP\_659606.1 GI:21492487  
DBLINK Project: [14196](#)  
DBSOURCE REFSEQ: accession [NC 004002.1](#)  
KEYWORDS .  
SOURCE Sheeppox virus  
ORGANISM [Sheeppox virus](#)  
Viruses; dsDNA viruses, no RNA stage; Poxviridae; Chordopoxvirinae;  
Capripoxvirus.  
REFERENCE 1 (residues 1 to 177)  
AUTHORS Tulman,E.R., Afonso,C.L., Lu,Z., Zsak,L., Sur,J.H., Sandybaev,N.T.,  
Kerembekova,U.Z., Zaitsev,V.L., Kutish,G.F. and Rock,D.L.  
TITLE The genomes of sheeppox and goatpox viruses  
JOURNAL J. Virol. 76 (12), 6054-6061 (2002)  
PUBMED [12021338](#)  
REFERENCE 2 (residues 1 to 177)  
CONSTRM NCBI Genome Project  
TITLE Direct Submission  
JOURNAL Submitted (14-JUN-2002) National Center for Biotechnology  
Information, NIH, Bethesda, MD 20894, USA  
REFERENCE 3 (residues 1 to 177)  
AUTHORS Tulman,E.R., Afonso,C.L., Lu,Z., Zsak,L., Sur,J.-H.,  
Sandybaev,N.T., Kerembekova,U.Z., Zaitsev,V.L., Kutish,G.F. and  
Rock,D.L.  
TITLE Direct Submission  
JOURNAL Submitted (31-JAN-2002) African Swine Fever Research, Plum Island  
Animal Disease Center, U.S. Dept. Agriculture, Agricultural  
Research Service, P.O. Box 848, Greenport, NY 11944-0848, USA  
COMMENT PROVISIONAL [REFSEQ](#): This record has not yet been subject to final  
NCBI review. The reference sequence was derived from SPPV\_30.  
Method: conceptual translation.  
FEATURES Location/Qualifiers  
source 1..177  
/organism="Sheeppox virus"

[Run BLAST](#)

[Identify Conserved Domains](#)

[Highlight Sequence Features](#)

[Find in this Sequence](#)

### Articles about the SPPV\_30 gene

The genomes of sheeppox and goatpox viruses.  
[J Virol. 2002]

[See all...](#)

### Protein clusters for NP\_659606.1

Double-strand RNA-binding protein - double-strand RNA-binding protein; has adenosine deaminase activity (converts adenosines to Total proteins: 18  
Total genera: 6  
Conserved in: Chordopoxvirinae

### More about the gene SPPV\_30

SPPV\_30 gene  
Also Known As: SPPV\_30

### Related information

[BLink](#)

[Related Sequences](#)

[BioProject](#)

[CDD Search Results](#)

[Conserved Domains \(Conserved\)](#)

[Protein](#) 1..177  
/product="double-strand RNA-binding protein"  
/calculated\_mol\_wt=20401

[Region](#) 1..177  
/region\_name="PHA03103"  
/note="double-strand RNA-binding protein; Provisional"  
/db\_xref="CDD:177529"

[Region](#) <33..66  
/region\_name="z-alpha"  
/note="Adenosine deaminase z-alpha domain; cl02659"  
/db\_xref="CDD:287691"

[Region](#) 104..169  
/region\_name="DSRM"  
/note="Double-stranded RNA binding motif. Binding is not sequence specific but is highly specific for double stranded RNA. Found in a variety of proteins including dsRNA dependent protein kinase PKR, RNA helicases, Drosophila staufer protein, E. coli RNase III; cd00048"  
/db\_xref="CDD:28930"

[Site](#) order(104,110..111,152..155,158)  
/site\_type="other"  
/note="dsRNA binding site [nucleotide binding]"  
/db\_xref="CDD:28930"

[CDS](#) 1..177  
/locus\_tag="SPPV\_30"  
/coded\_by="complement(NC\_004002.1:26911..27444)"  
/note="double-strand RNA-binding protein; has adenosine deaminase activity (converts adenosines to inosines); involved in viral immune evasion, The poxviridae are enveloped unsegmented dsDNA viruses; unlike many dsDNA viruses that replicate in the host nucleus poxviruses encode their own replication machinery and therefore replicate in the cytoplasm; viral genes are expressed in a bi-phasic manner with early genes encoding non-structural proteins involved in genome replication and late genes encoding the viral structural proteins"  
/db\_xref="GeneID:944663"

Protein Clusters

PubMed

PubMed (RefSeq)

PubMed (Weighted)

Related Structures (List)

Related Structures (Summary)

Taxonomy

### Recent activity

[Turn Off](#) [Clear](#)

 dsRNA-binding PKR inhibitor [Sheeppox virus] Protein

 dsRNA-binding PKR inhibitor[All Fields] (119) Protein

 dsRNA-binding PKR inhibitor (119) Protein

[See more...](#)

# Alignment of E3I in SPPV and VACV

Pairwise Alignment Result

LENGTH	SCORE	IDENTITY	SIMILARITY	GAPS
191	297.0	66/191 (34.6%)	96/191 (50.3%)	16/191 ( 8.4%)

```

VACV  - 1 MSKIY-IDERSNAEIVCEAIKTIG-IEGATAAQLTRQLNMEKREVNKALY      48
      :| .||...:|:|:..... .|..||:.....:|:|..|||.||
SPPV  - 1 ---MYSCDEVDSYELVKKIVNNLSESESTITAEISKKLNIEKSNVKNQLY      47
      .|.....:.....||:|..... |.:|.....:.....:|
      49 DLQRSAMVYSSDDIPFRWFMTTEADKPDADAMADVIDDVSRKSMREDHK      98
      .|.....:.....||:|..... |.:|.....:.....:|
      48 KLHNDGFIFMIRSNPPKWFKNKG-----IDNDDNENNNTKKLNK      86
      99 SFDDVIPAKKIIDWKGANPVTVINEYCQITRRDWSFRIESVGPNSPTFY      148
      ||.|.||..||:|.||..||:|||||.|||.||..|.||..|.||.
      87 SFSDTIPYYKIVLWKEKNPCSAINEYCQFTSRDWYINISSCGNGRKPMFL      136
      149 ACVDIDGRVFDKADGKSKRDAKNNAAKLAVDKLLGYVIIRF      189
      |.|.||..|.||:|:|:|..:|.||:|..:|..:|..:|..:|
      137 ASVIISGKIFPPEIGNTKKEAKQKSTKRTIDFLINTSIIKF      177
  
```

## PEPSTATS of dsRNA-binding from 1 to 177

Molecular weight = 20532.49 Residues = 177Average Residue Weight = 116.003 Charge = 8.5Isoelectric Point = 9.6391

A280 Molar Extinction Coefficient = 26030

A280 Extinction Coefficient 1mg/ml = 1.27

Improbability of expression in inclusion bodies = 0.911

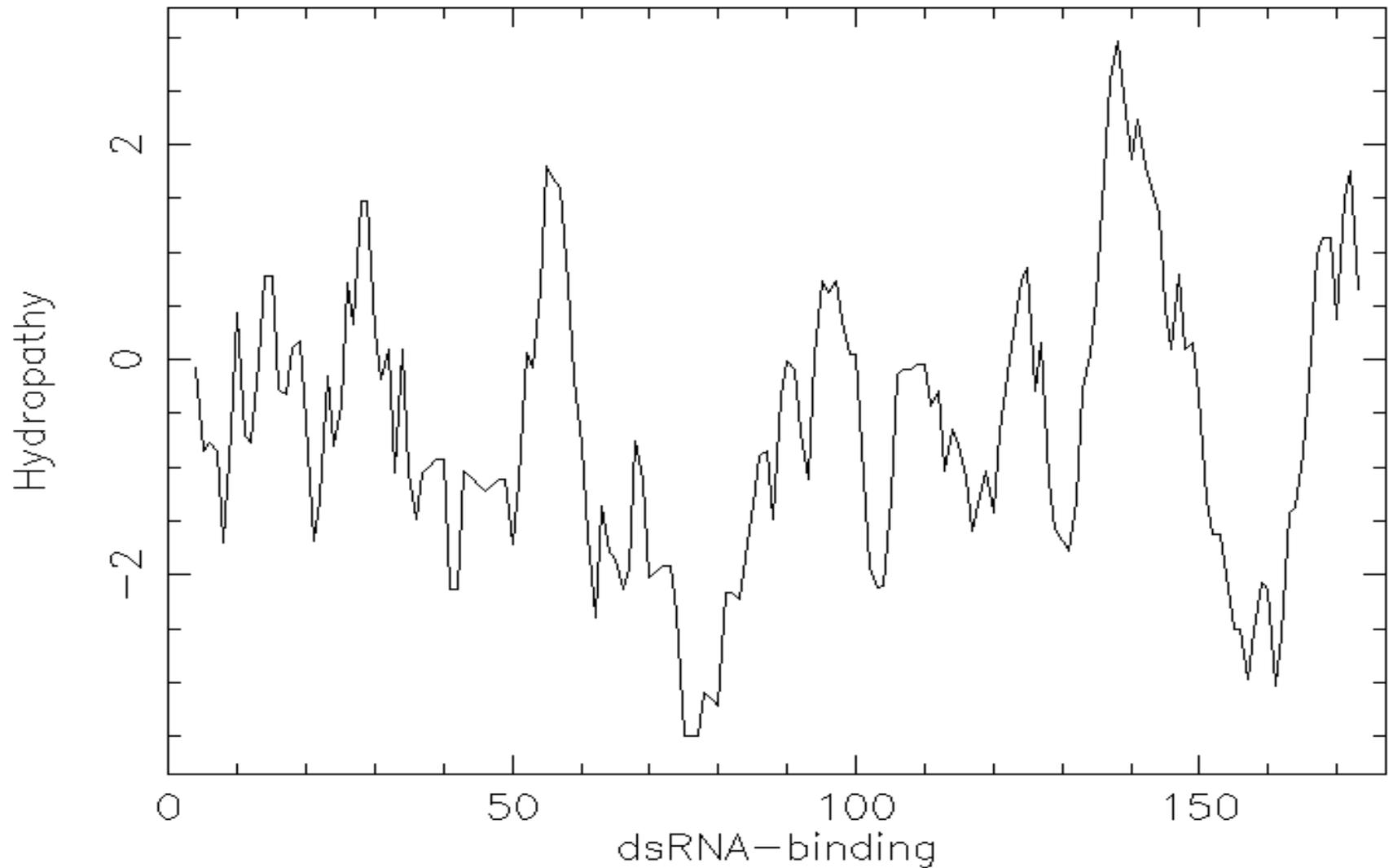
Residue	Number	Mole%	DayhoffStat
A = Ala	4	2.260	0.263
B = Asx	0	0.000	0.000
C = Cys	4	2.260	0.779
D = Asp	9	5.085	0.924
E = Glu	11	6.215	1.036
F = Phe	10	5.650	1.569
G = Gly	6	3.390	0.404
H = His	1	0.565	0.282
I = Ile	21	11.864	2.637
J = ---	0	0.000	0.000
K = Lys	24	13.559	2.054
L = Leu	9	5.085	0.687
M = Met	3	1.695	0.997
N = Asn	20	11.299	2.628
O = ---	0	0.000	0.000
P = Pro	6	3.390	0.652
Q = Gln	3	1.695	0.435
R = Arg	4	2.260	0.461
S = Ser	18	10.169	1.453
T = Thr	8	4.520	0.741
U = ---	0	0.000	0.000
V = Val	6	3.390	0.514
W = Trp	3	1.695	1.304
X = Xaa	0	0.000	0.000
Y = Tyr	7	3.955	1.163
Z = Glx	0	0.000	0.000

Property	Residues	Number	Mole%	DayhoffStat
Tiny	(A+C+G+S+T)	40	22.599	22.599
Small	(A+B+C+D+G+N+P+S+T+V)	81	45.763	45.763
Aliphatic	(A+I+L+V)	40	22.599	22.599
Aromatic	(F+H+W+Y)	21	11.864	11.864
Non-polar	(A+C+F+G+I+L+M+P+V+W+Y)	79	44.633	44.633
Polar	(D+E+H+K+N+Q+R+S+T+Z)	98	55.367	55.367
Charged	(B+D+E+H+K+R+Z)	49	27.684	27.684
Basic	(H+K+R)	29	16.384	16.384
Acidic	(B+D+E+Z)	20	11.299	11.299

# hydropathy

Kyte-Doolittle Plot



# Average flexibility

## ProtScale

User-provided sequence:

```
10      20      30      40      50      60
M Y S C D E V D S Y  E L V K K I V N N L  S E S E S I T A I E  I S K K L N I E K S  N V N K Q L Y K L H  N D G F I F M I R S

70      80      90      100     110     120
N P P K W F K K N G  I D N D D N E N N N  T K K L N K S F S D  T I P Y Y K I V L W  K E K N P C S A I N  E Y C Q F T S R D W

130     140     150     160     170
Y I N I S S C G N G  R K P M F L A S V I  I S G I K F F F E I  G N T K K E A R Q K  S T K R T I D F L I  N T S I I K F
```

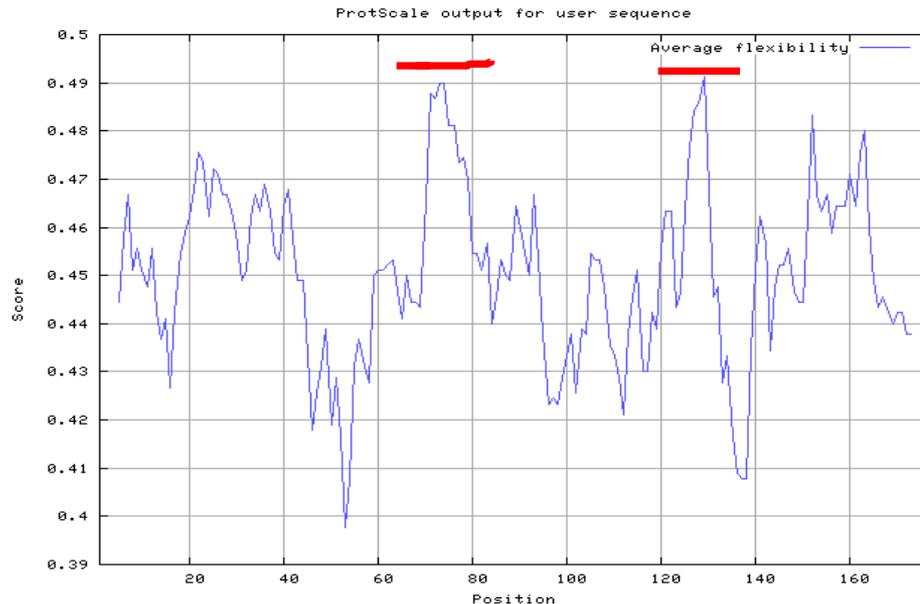
SEQUENCE LENGTH: 177

Using the scale **Average flexibility**, the individual values for the 20 amino acids are:

Ala:	0.360	Arg:	0.530	Asn:	0.460	Asp:	0.510	Cys:	0.350	Gln:	0.490
Glu:	0.500	Gly:	0.540	His:	0.320	Ile:	0.460	Leu:	0.370	Lys:	0.470
Met:	0.300	Phe:	0.310	Pro:	0.510	Ser:	0.510	Thr:	0.440	Trp:	0.310
Tyr:	0.420	Val:	0.390	: 0.485		: 0.495		: 0.428			

Weights for window positions 1,...,9, using **linear weight variation model**:

1	2	3	4	5	6	7	8	9
1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00
edge				center				edge



Protocol

Macro

Utility

Resource



User Space

My Data

My Literature

My MetaPackage

My Toolbox

History



Account

My Account

My Group

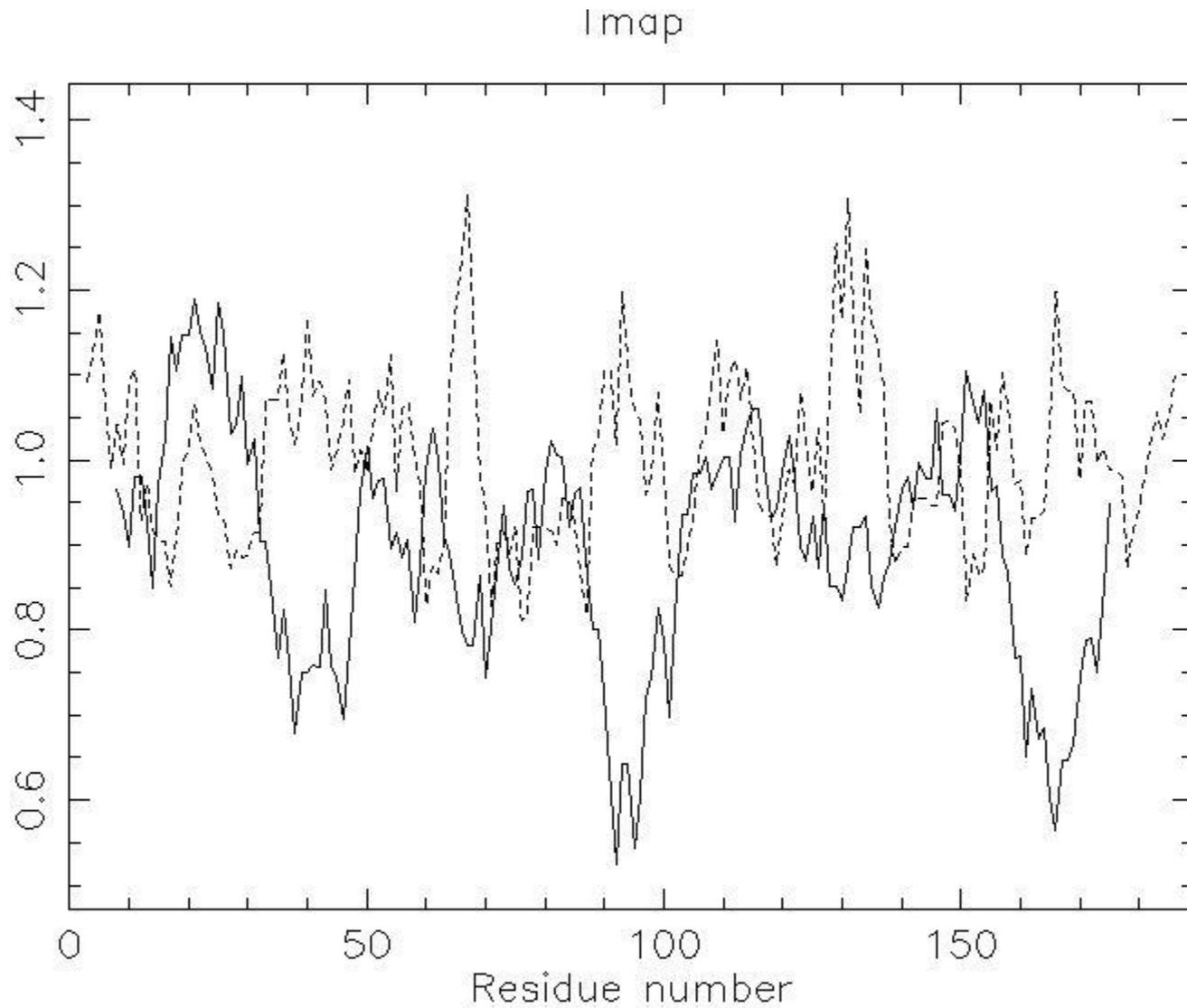
Logout

```

# Please cite:
# Garnier, Osguthorpe and Robson (1978) J. Mol. Biol. 120:97-120
#
#
#-----
      10      20      30      40      50
MYSCEVDSYELVKKIVNLSSESEITALEISKLNIEKSNVVKQLYKLVH
helix  WXXXXXXXXXX  XXXXXXXXXXXXXXXXXXXX  XXXXX
sheet E EE      EE      XXXXX
turns T T      T      T
coil      CCCC      C
      60      70      80      90      100
NDGFIFMIRSNPPKWFKKNGIDNDNENNTKLNKSFSDTIPYYKIVLW
helix  XXXXX      EE      EE  EE  EEEEE  H
sheet  EEEEE      EE      EE  EE  EEEEE
turns TTT  T  TTT  TTT  TT  T  TTT  TT
coil      CCC      CCCCC  C
      110     120     130     140     150
KEKNPCSAINEYCQFTSRDWWYINISSCGNGRKFPLASVIISGIKFFPEI
helix H      MH      H
sheet      EE      EE      EEEEE  EEE  EEE
turns TT TTTT  TTTTTTTTTT  TTTTTT      T  T
coil      C      CC      CC
      160     170
GNTKKEAKQKSTKRTIDFLINTSLIKF
helix  XXXXXXXXXXXX
sheet      EEEEEEE  EEE
turns T      TT
coil      CCCC
#-----
#
# Residue totals: H: 52  E: 50  T: 50  C: 25
#      percent: H: 32.3 E: 31.1 T: 31.1 C: 15.5
#
#-----
# Total_sequences: 1
# Total_hitcount: 52
#-----

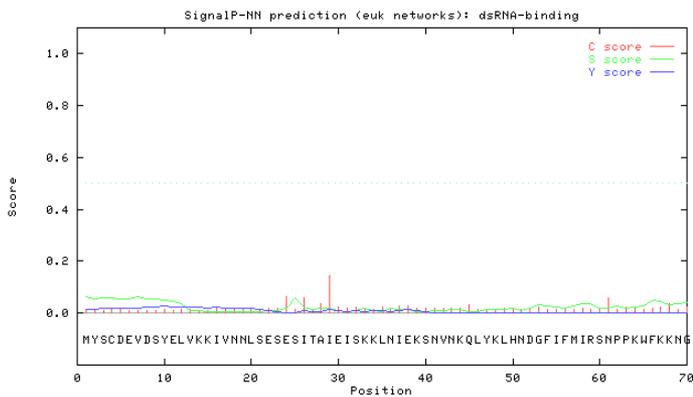
```

# Trans membrane



# SignalP predictions

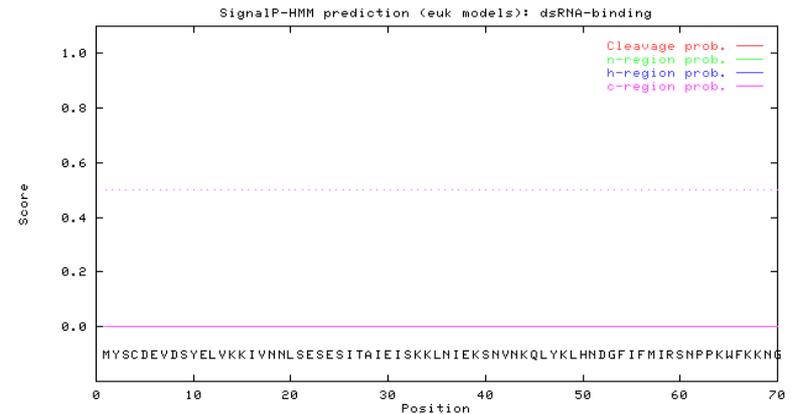
## SignalP-NN result:



# data

```
>dsRNA-binding          length = 70
# Measure  Position  Value  Cutoff  signal peptide?
max. C    29      0.146  0.33   NO
max. Y    10      0.026  0.32   NO
max. S     1      0.063  0.82   NO
mean S    1-9     0.057  0.47   NO
```

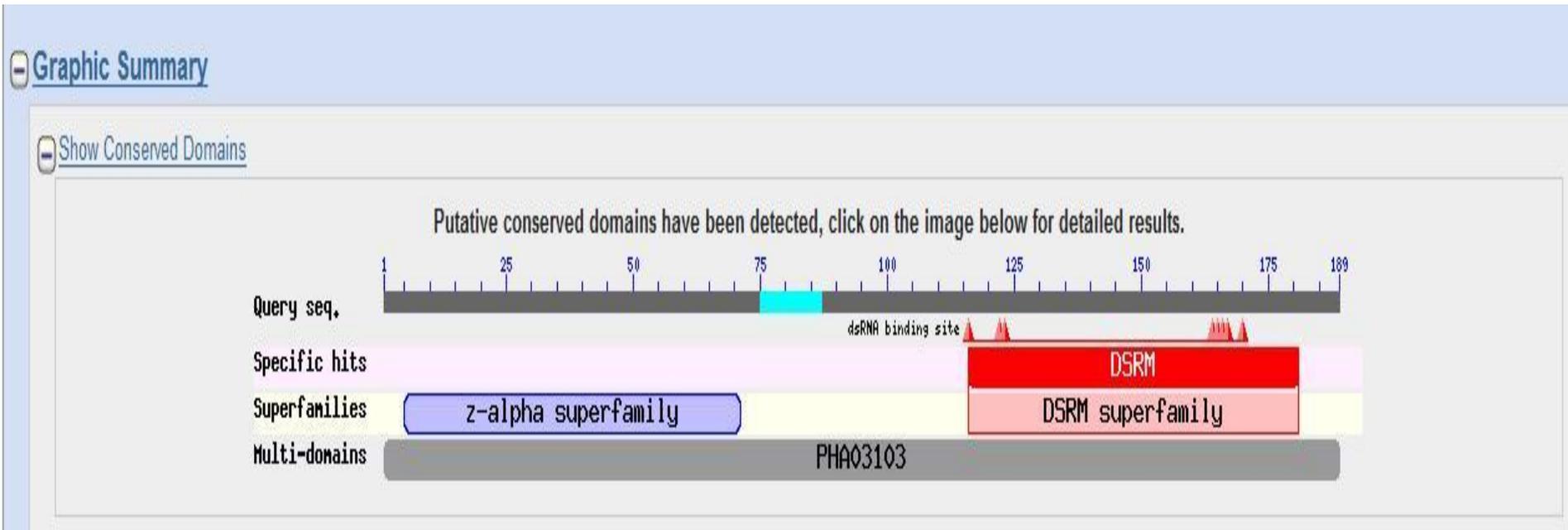
## SignalP-HMM result:



# data

```
>dsRNA-binding
Prediction: Non-secretory protein
Signal peptide probability: 0.000
Signal anchor probability: 0.000
Max cleavage site probability: 0.000 between pos. -1 and 0
```

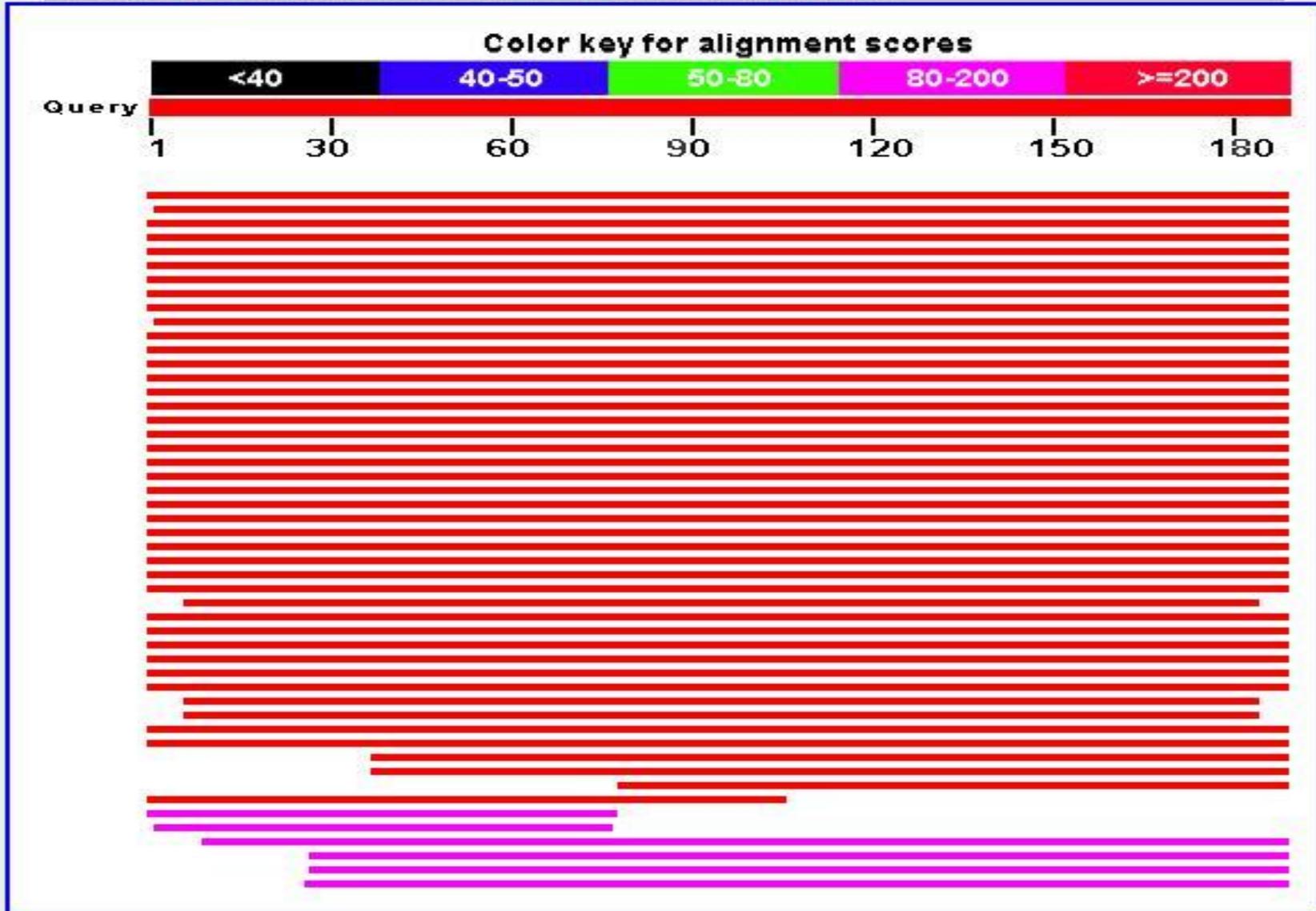
# Using BLAST to search the similar sequence of E3L in the protein database.



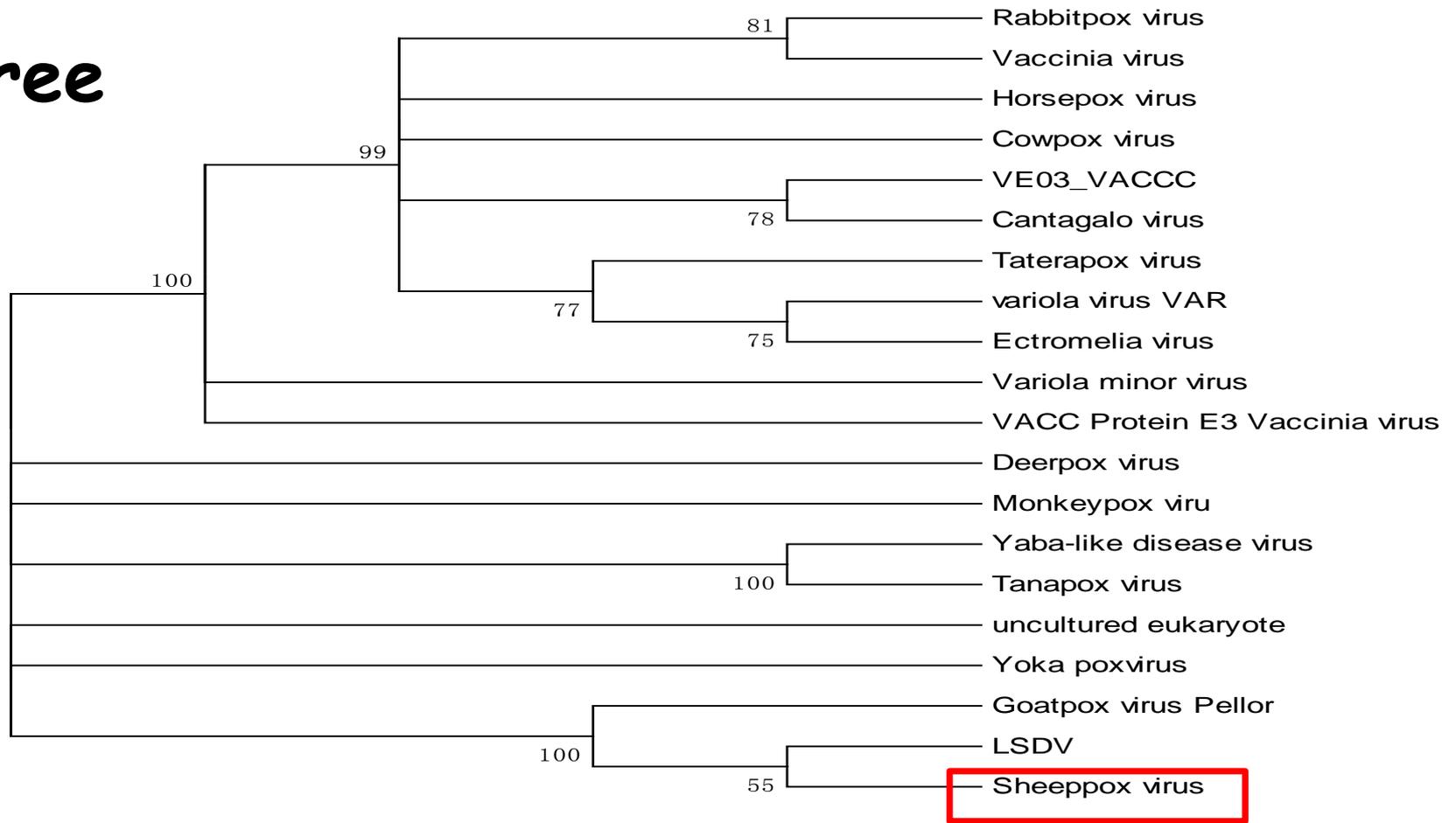
The result shows that there exist sequences when align conserved domain using blastp. From the above image we can see E3L protein consists of two superfamilies, z-alpha superfamily and DSRM superfamily

# Distribution of 50 Blast Hits on the Query Sequence

Mouse-over to show define and scores, click to show alignments



# Tree



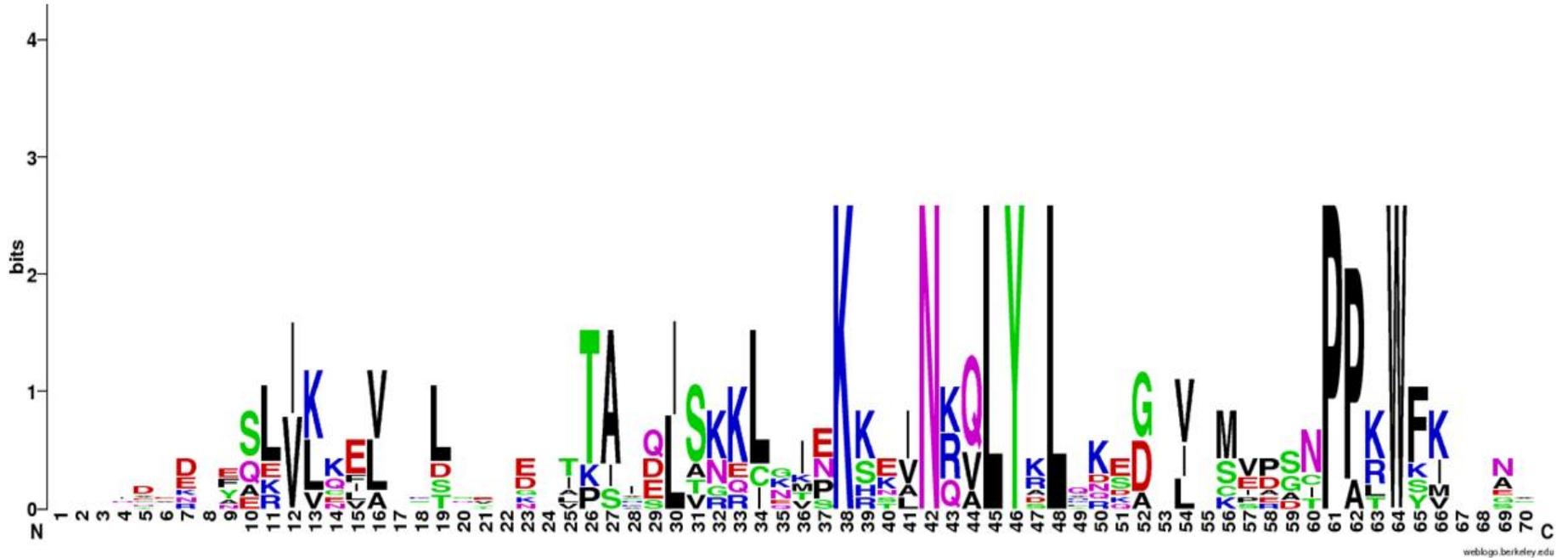
## Figure. Evolutionary relationships of taxa

The evolutionary history was inferred using the Neighbor-Joining method. The percentage of replicate trees in which the associated taxa clustered together in the bootstrap test are shown next to the branches. The evolutionary distances were computed using the Poisson correction method and are in the units of the number of amino acid substitutions per site. The analysis involved 20 amino acid sequences. All positions containing gaps and missing data were eliminated. Evolutionary analyses were conducted in MEGA5.

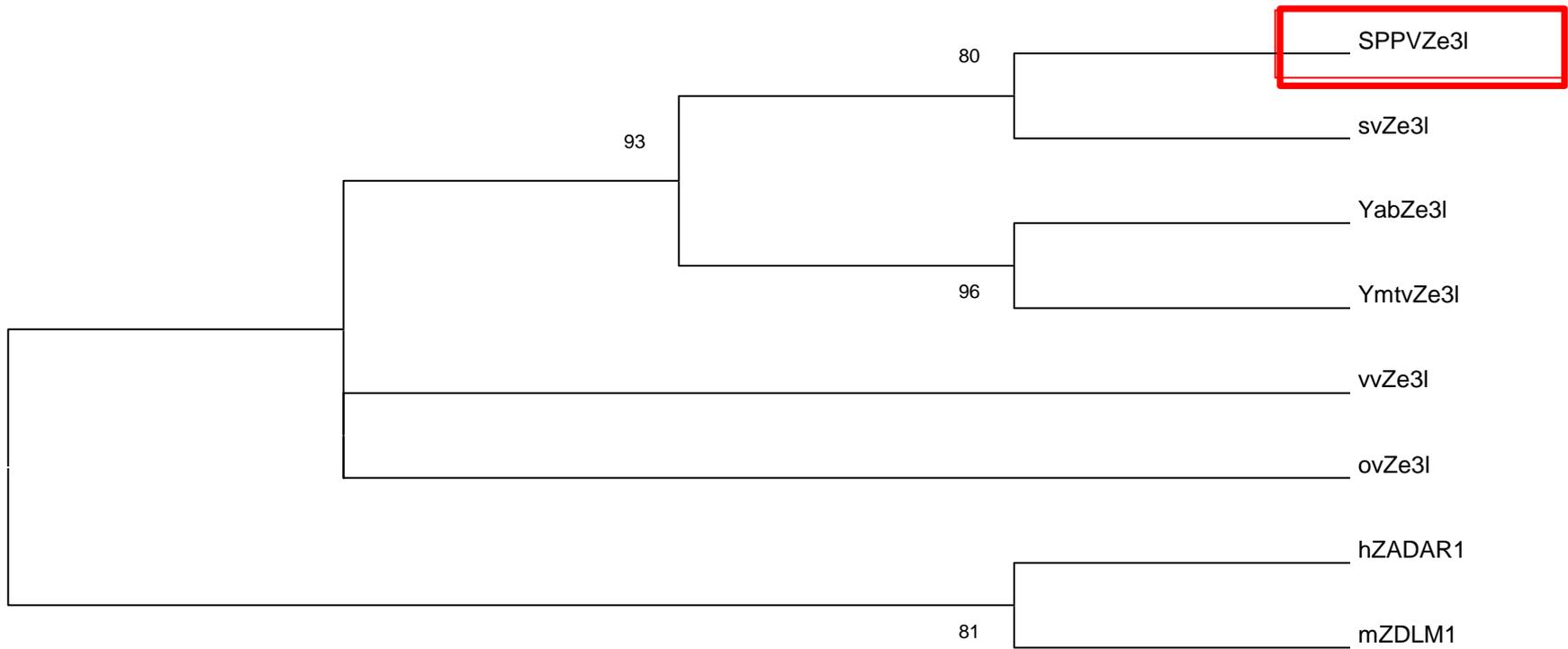
3. Sequence analysis  
of Za family and  
SPPVZae31

- >SPPVZae3l
- SCDEVDSYELVKKIVNNLSESE SITAIEISKKLNIEKSNV NKQLYKLHNDG  
FIFMIRSNPPKWFKNNGI
- >YabZae3l
- CTVNDAEIFSLVKKEVLSLNTNDYTTAISLSNRLKINKKKINQQLYKLQKE  
DTVKMVPSNPPKWFKNYNC
- >YmtvZae3l
- GCENDVKTFSLVKNEVMMLNVDEYTTSIDISNKLKINKKKINKQLYKLQK  
EGVLKMVPSNPPKWFKN CNC
- >vvZae3l
- KIYIDERSNAEIVCEAIKTIGIEGATAAQLTRQLNMEKREVNKALYDLQR  
SAMVYSSDDIPPRWFMTTEA
- >ovZae3l
- MACECASLILELLRKSDDKLP AKQIAKELGISKHEANRQLYRL LDSDEV CCE  
DGNPPRWFVECAP
- >svZae3l
- SDISNEDVYSLVKQEVD SLPVGNFITAVEISKKIEKEKSSINRQLYALYQQ  
GYIDMVPACPPKWK-RNQ
- >hZaADAR1
- ELSIYQDQEQRILKFLEELGEGKATTAHDL SGKLGTPKKEINRVLYSLAKKG  
KLQKEAGTPPLWKIAVST
- >mZaDLM1
- DLSTGDNLEQKILQVLSDDGGPVKIGQLVKKCQVPKKT LNQVLYRLKKEDR  
VSSPEPATWSIGGAA





The Z-DNA binding domain of the Za family.(Used WebLogo.  
<http://weblogo.berkeley.edu/>)



The Za family evolutionary history was inferred using the Neighbor-Joining method. The bootstrap consensus tree inferred 500 replicates is taken to represent the evolutionary history of the Za family analysed. The percentage of replicate trees in which the associated taxa clustered together in the bootstrap test (500 replicates) are shown next to the branches. The tree is drawn to scale, with branch lengths in the same units as those of the evolutionary distances used to infer the phylogenetic tree. The evolutionary distances were computed using the Poisson correction method and are in the units of the number of amino acid substitutions per site. The analysis involved 8 amino acid sequences. All positions containing gaps and missing data were eliminated. There were a total of 61 positions in the final dataset. Evolutionary analyses were conducted in MEGA5.

## Pairwise Alignment Result

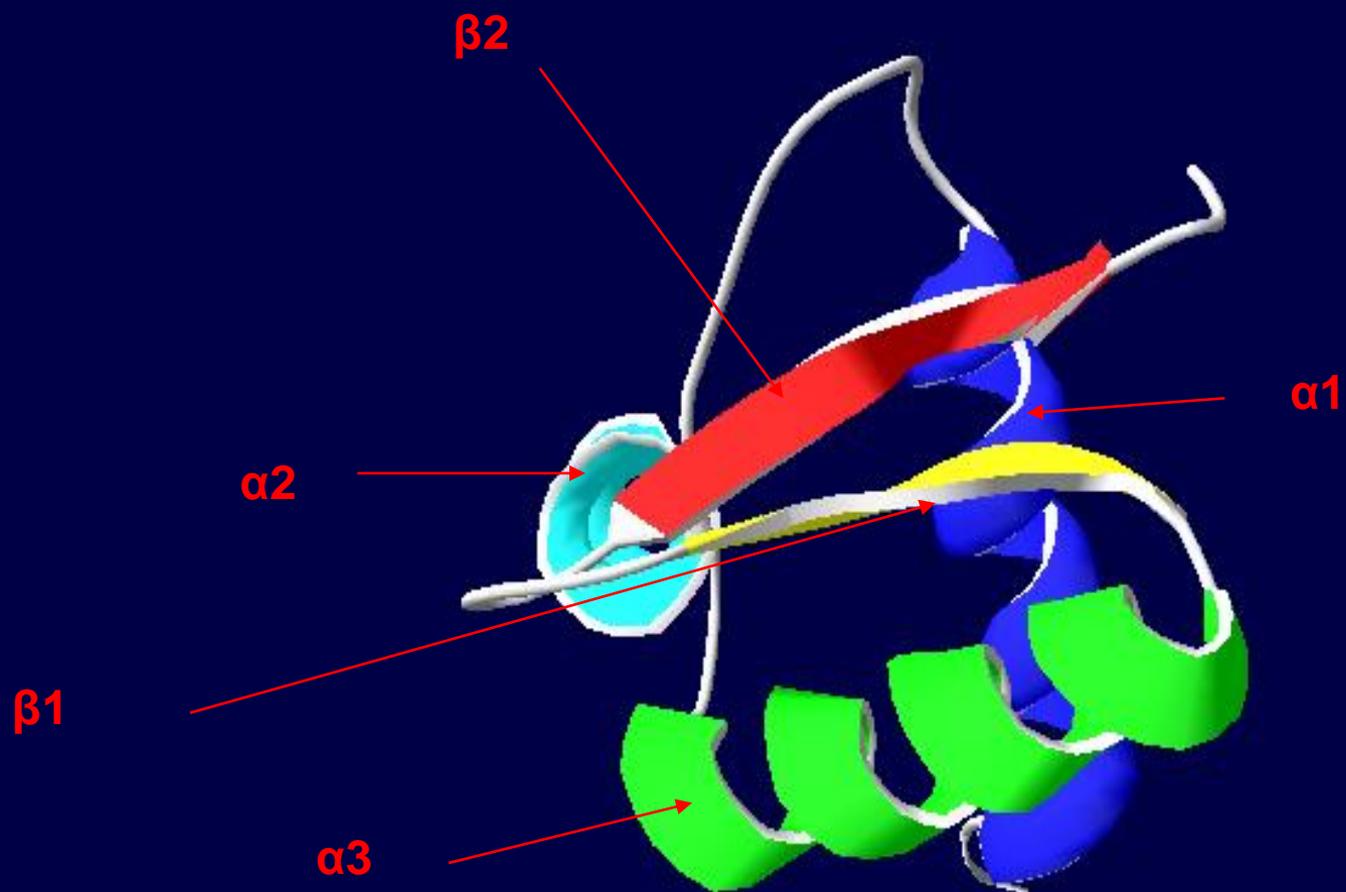
LENGTH	SCORE	IDENTITY	SIMILARITY	GAPS
70	149.0	28/70 (40.0%)	44/70 (62.9%)	1/70 ( 1.4%)

SPPVZ??e31	1	-SCDEVDSYELVKKIVNNLSESE <sup>o</sup> SITAEISKKLNIEKSNV <sup>o</sup> NKQIYKLHN	49
		: : : : : :         .   : : : : : :       : : :   .   .   . :   :       . .	
YabZ??e31	1	CTVNDAEIFSLVKKEVLSLNTNDYTTAISLSNRLKINKKK <sup>o</sup> NQ <sup>o</sup> QIYKLQK	50
SPPVZ??e31	50	DGFIFMIRSNPP <sup>o</sup> WFKKNGI	69
		: : : :   :                 . . . . .	
YabZ??e31	51	EDTVKMVPSNPP <sup>o</sup> WFKNYNC	70

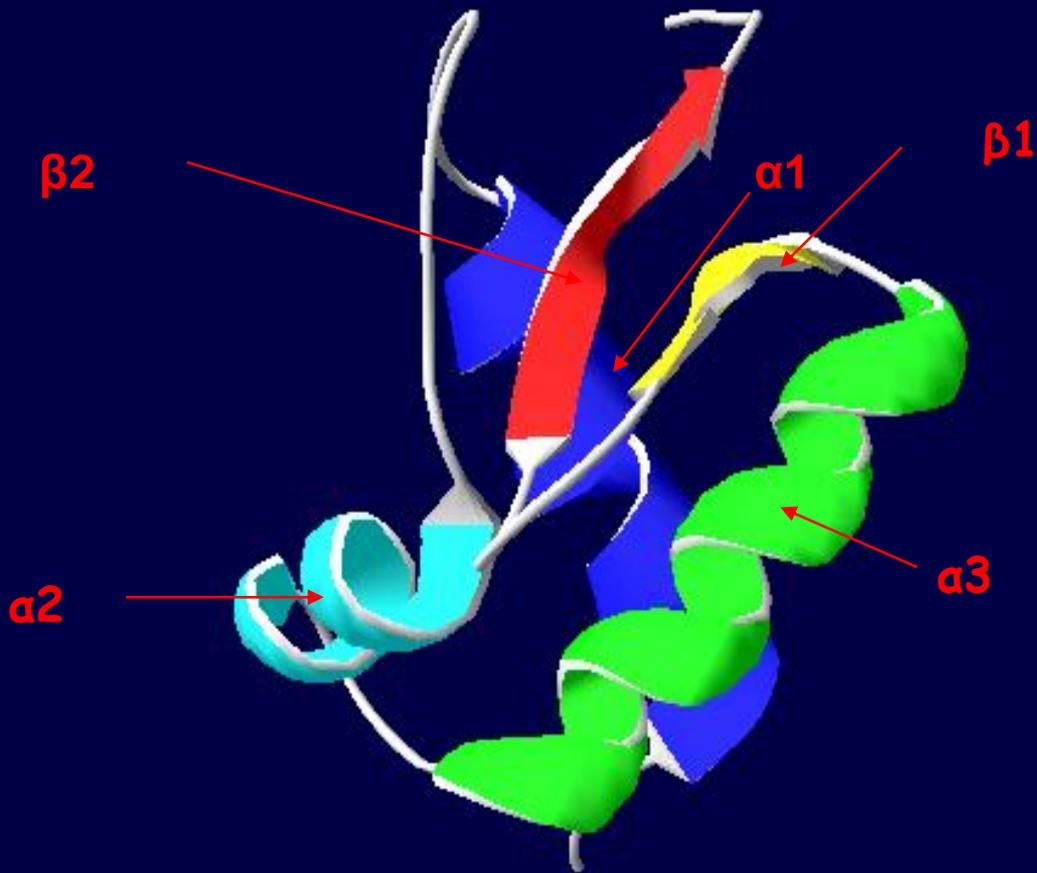
Sequence Alignment result of SPPVZae31 and YabZae31.

# 4. 3D structure analysis of SPPVZae31

- The predicted structure of sppvZaE3L suggests that it may belong to the Za family of helix-turn-helix (HTH), winged-helix Z-DNA-binding protein. It has an  $\alpha/\beta$  architecture, consisting of two  $\beta$ -strands and three  $\alpha$ -helices, although there are three  $\beta$ -strands in YabZaE3L- and vvZaE3L. The three  $\alpha$ -helices ( $\alpha_1, \alpha_2, \alpha_3$ ) form a core domain, which is flanked by a  $\beta$ -sheet of two antiparallel strands ( $\beta_1$  and  $\beta_2$ ).  $\alpha_2$  and  $\alpha_3$  form an HTH motif and two antiparallel  $\beta$ -strands form the wing. (Sung Chul Ha, Neratur K. Lokanath, et al. A poxvirus protein forms a complex with left-handed Z-DNA: Crystal structure of a Yatapoxvirus Za bound to DNA [J]. PANS, 2004, 40: 14367-14372.)



The 3D structure of YabZae31.



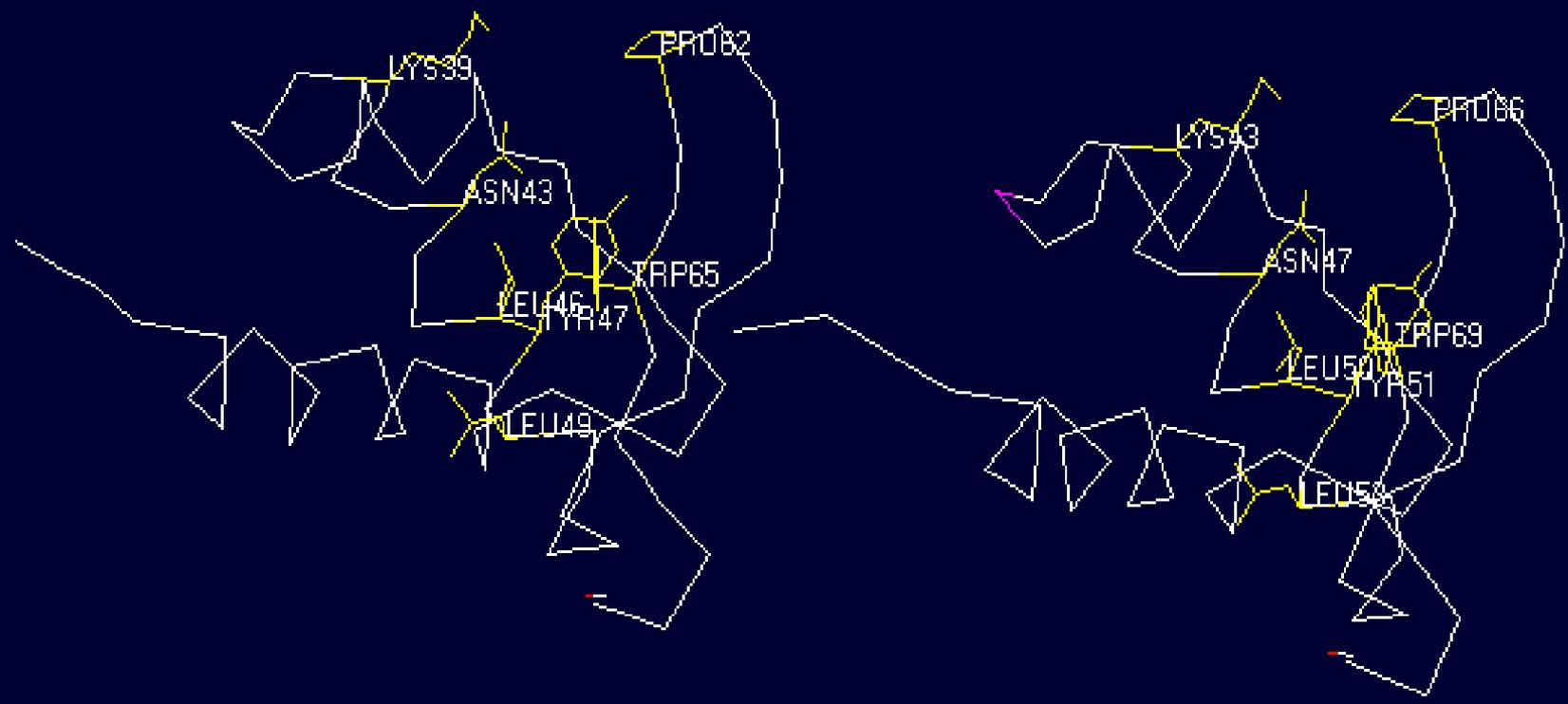
The 3D structure of SPPVZae3I.

- The interaction between members of the Za family and Z-DNA is made up of residues in the  $\alpha 3$  helix and the "wing". Three residues, Asn-47, Tyr-51, and Trp-69 as numbered in YabZaE3L-, central to interaction with Z-DNA, are completely conserved with Za family. We can find those three residues (Asn-43, Tyr-47, Trp-65) in sppvZaE3L at the relative positions by these two sequences alignment.



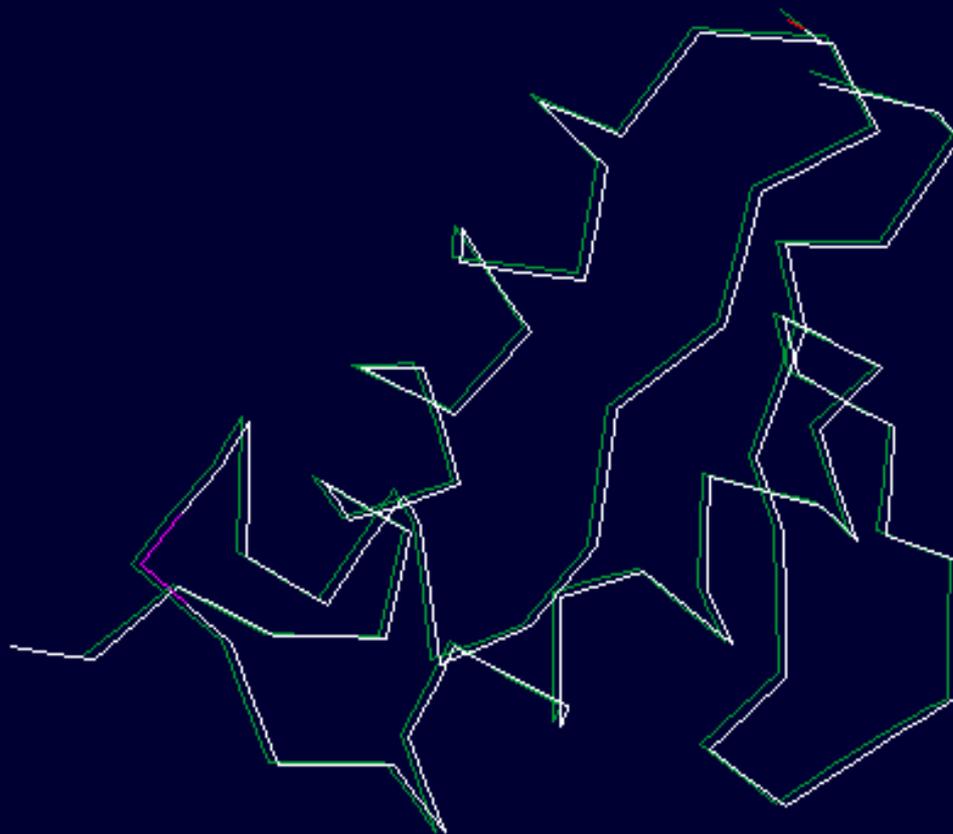
1SFU\_B 8.6 0.0 CTVNDAEI FSLVKKEVL SLNTNDYTTAI SLSNRLKIN KKI QQ K QKEDTVKMVPSN PK FKNYNC >  
QMEAN\_plotscolo 100.0 100.0 SCDEVDSYELVKKI VNNLSESESI TAI EISKKLNI E SNV KQ K HNDGFI FMI RSN PK FKNNGI >

(B): VAL8

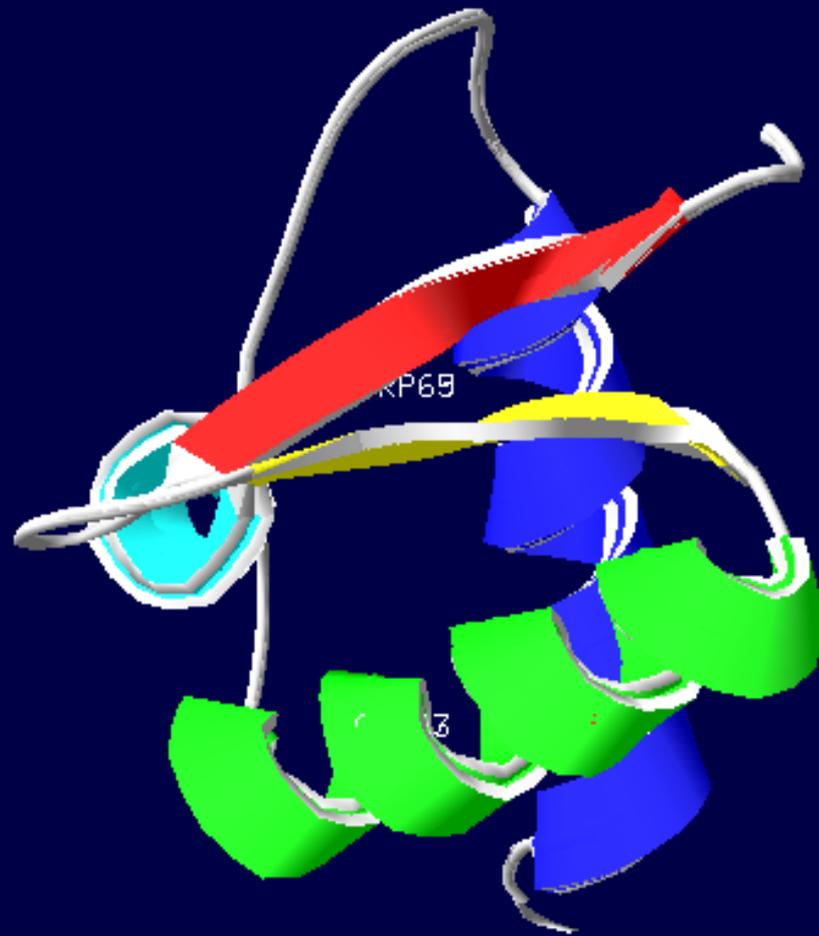


YabZaE3L

sppvZaE3L

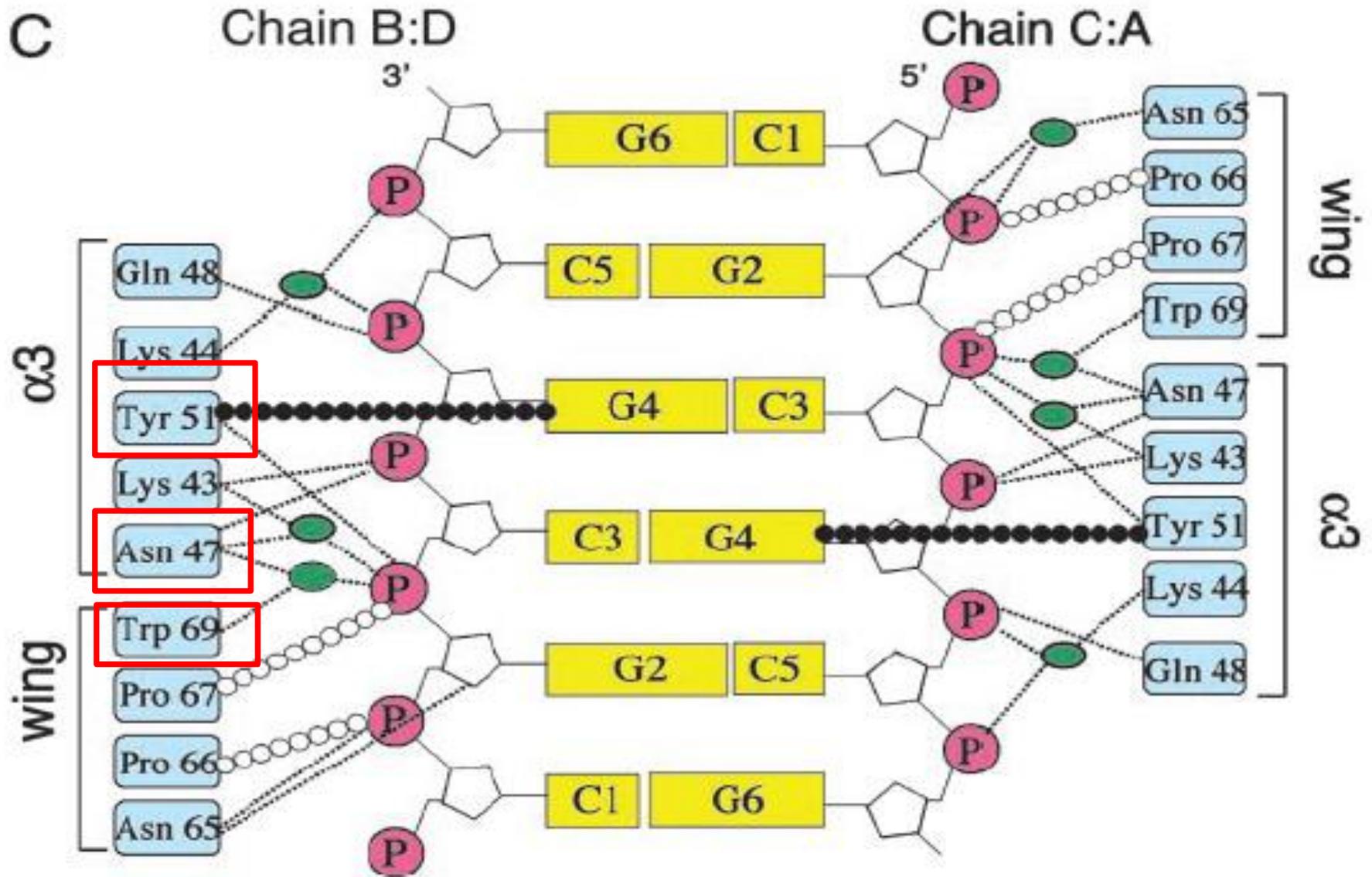


The carbon alpha (CA) fit of SPPVZae3l and YabZae3l. SPPVZae3l is shown by green line. YabZae3l is shown by white line. RMS (CA)=0.06 Å.



The picture of fit molecule. RMS=0.

- Asn-47 and Trp-69 make water-mediated hydrogen bonds to the phosphate backbone and Tyr-51 makes a direct hydrogen bond to a phosphate in the DNA backbone in YabZαE3L. Asn-43 and Trp-65 may make water-mediated hydrogen bonds to the phosphate backbone and Tyr-47 may makes a direct hydrogen bond to a phosphate in the DNA backbone in sppvZαE3L.



Sung Chul Ha, Neratur K.Lokanath, et al. A poxvirus protein forms a complex with left-handed Z-DNA: Crystal structure of a Yatapoxvirus Za bound to DNA [J]. PANS, 2004, 40: 14367-14372.

# 5. Conclusion

- The E3 protein in SPPV might be composed of a Za domain and a DSRM domain. There are three  $\alpha$ -helices ( $\alpha_1, \alpha_2, \alpha_3$ ) and two antiparallel strands ( $\beta_1$  and  $\beta_2$ ).  $\alpha_2$  and  $\alpha_3$  form an HTH motif and two antiparallel  $\beta$ -strands form the wing. There are also three conserved residues, Asn, Tyr and Trp in sppvZaE3L.

- The sppvZαE3L might play an important role in the pathogenicity of SPPV. This result may allow the design of a class of antiviral agents against SPPV.

# Acknowledge

- Thank you for Pro. Luo!
- Thank you for the efforts of all group members!