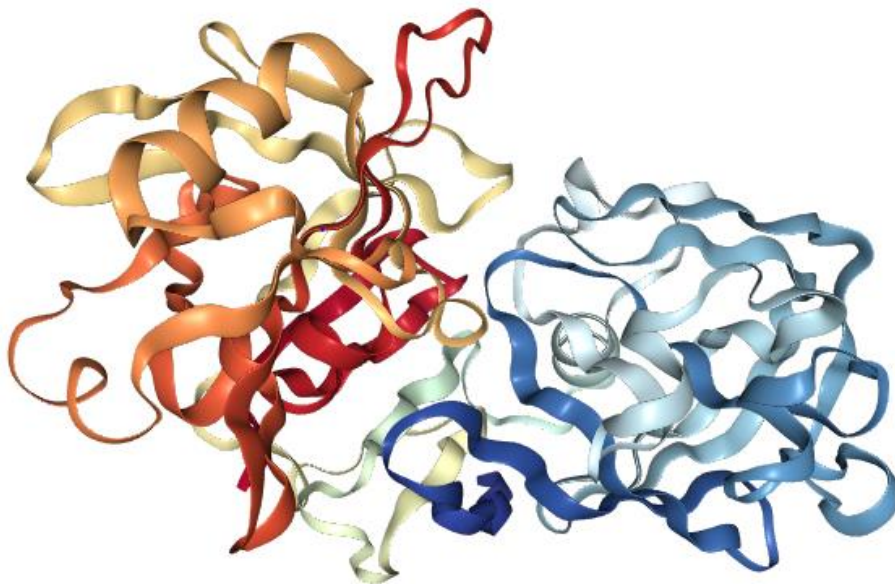


BIOPHYSICS PROJECT
ANALYSIS OF PROTEIN WITH PDB ID 5PEP



INDRANEEL GHOSH

(2016B1A70938P)

Sequence Assigned For Analysis: PDB ID: 5PEP

5PEP Sequence

IGDEPLENYL DTEYFGTIGI GTPAQDFTVI FDTGSSNLWV PSVYCSSLAC SDHNQFNPDD
SSTFEATSQE LSITYGTGSM TGILGYDTVQ VGGISDTNQI FGLSETEPGS FLYYAPFDGI
LGLAYPSISA SGATPVFDNL WDQGLVSQDL FSVYLSSNDD SGSVVLLGGI DSSYYTGSLN
WVPVSVEGYW QITLDSITMD GETIACSGGC QAIVDTGTSL LTGPTSAIAN IQSDIGASEN
SDGEMVISCS SIASLPDIVF TINGVQYPLS PSAYILQDDD SCTSGFEGMD VPTSSGELWI
LGDVFIRQYY TVFDRANNKV GLAPVA

Protein Structure and Model

The protein is a hydrolase (Aspartic Proteinase) which is found in the organism *Sus scrofa*. Based on the Biophysical Parameter Analysis carried out by Protcalc, the following conclusions were drawn about the given protein:

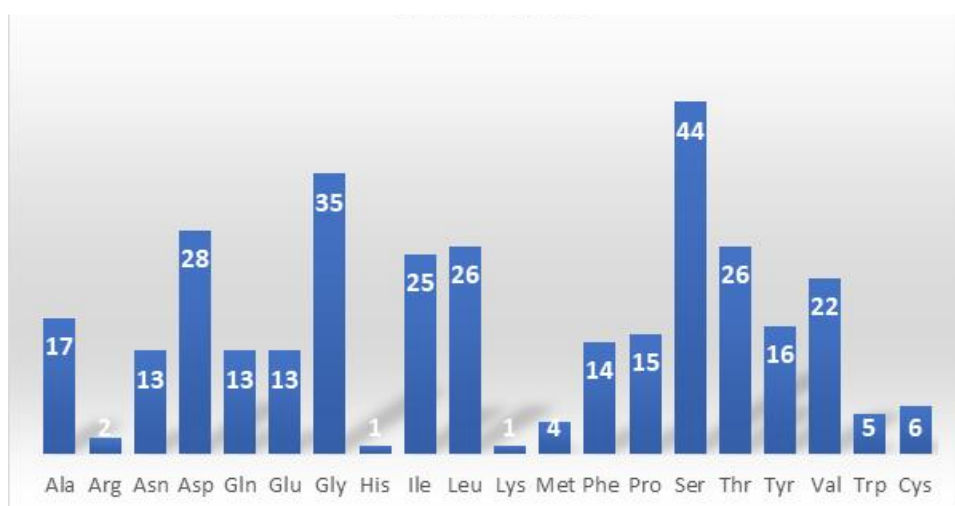
The compound was identified by the Protcalc software as X-RAY ANALYSES OF ASPARTIC PROTEASES. II. THREE-DIMENSIONAL OF THE HEXAGONAL CRYSTAL FORM OF PORCINE PEPSIN AT 2.3 ANGS RESOLUTION

- It was solved by X-RAY DIFFRACTION at a resolution of 2.34 Å.
- 1 chain(s) is/are present [1 unique chain(s)] containing a total of 326 residues are present.
- Protein consists of main chains and side chains
- 371 hetero group(s) is/are present.
- Refinement was carried out in RESTRAIN.
- R = 0.196

The individual Amino Acid constitution for the 326 residue sequence is as follows:

Residue		Number Found
A	Ala Alanine	17
R	Arg Arginine	2
N	Asn Asparagine	13
D	Asp Aspartate	28
Q	Gln Glutamine	13
E	Glu Glutamate	13
G	Gly Glycine	35
H	His Histidine	1
I	Ile Isoleucine	25
L	Leu Leucine	26
K	Lys Lysine	1
M	Met Methionine	4
F	Phe Phenylalanine	14
P	Pro Proline	15
S	Ser Serine	44
T	Thr Threonine	26
Y	Tyr Tyrosine	16
V	Val Valine	22
W	Trp Tryptophan	5
C	Cys Cysteine	6

The graph for the distribution is as follows:



An atom-wise distribution for the sequence is as follows:

Atom Count

Type	Number Found
Carbon	1529
Nitrogen	366
Oxygen	521
Sulfur	10
Hydrogen	2300

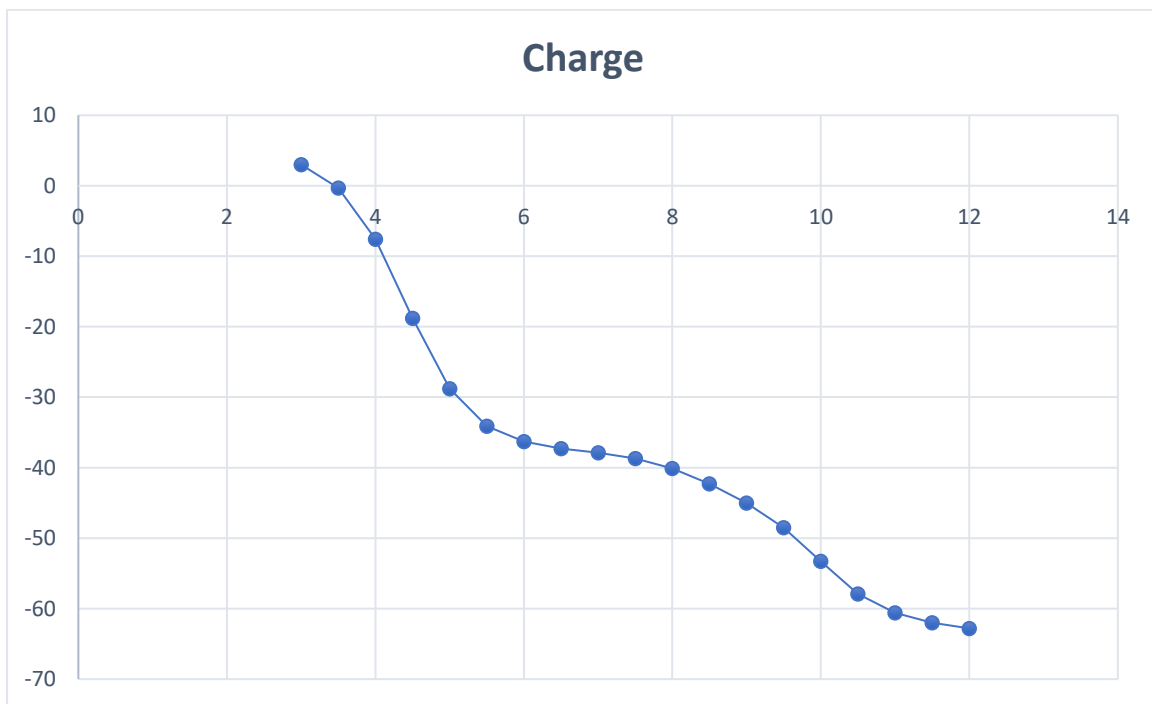
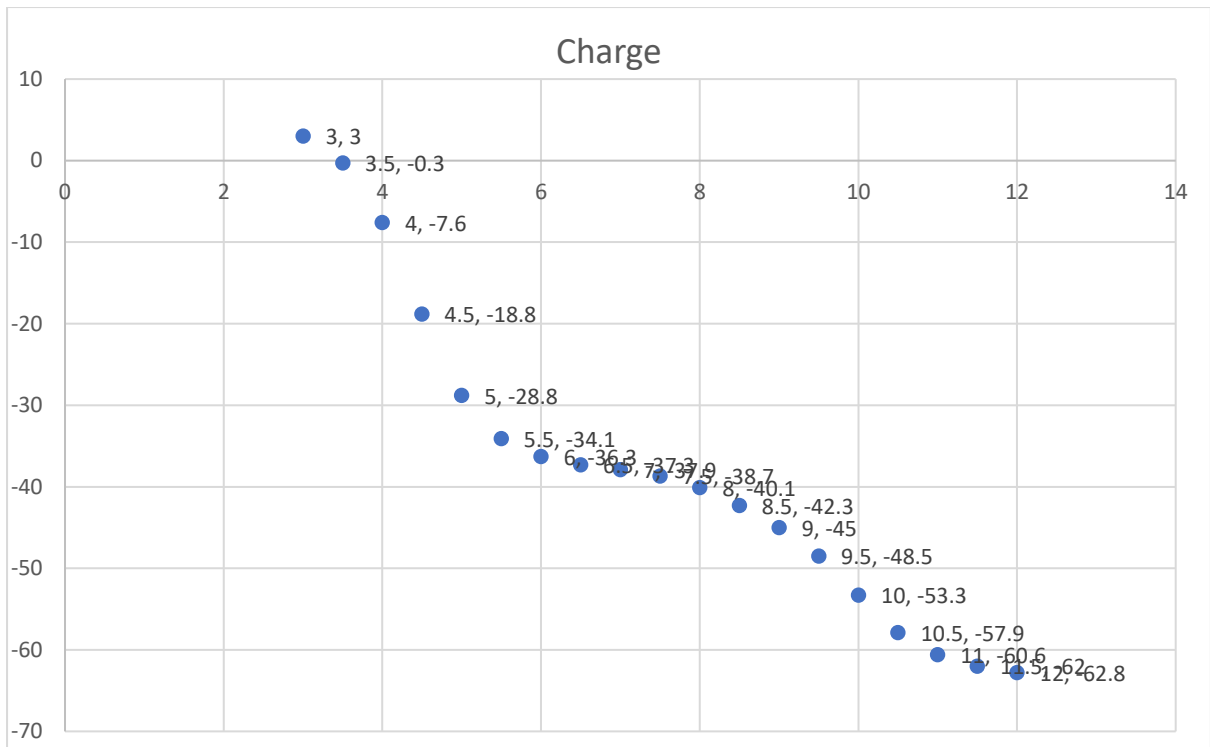
Isotopically Averaged Molecular Weight = 34465.7305

pH Based Analysis

Estimated charge at pH 7.00 = -37.9

We also find out the pH vs the charge of the molecule.

pH	Charge
3	3
3.5	-0.3
4	-7.6
4.5	-18.8
5	-28.8
5.5	-34.1
6	-36.3
6.5	-37.3
7	-37.9
7.5	-38.7
8	-40.1
8.5	-42.3
9	-45
9.5	-48.5
10	-53.3
10.5	-57.9
11	-60.6
11.5	-62
12	-62.8



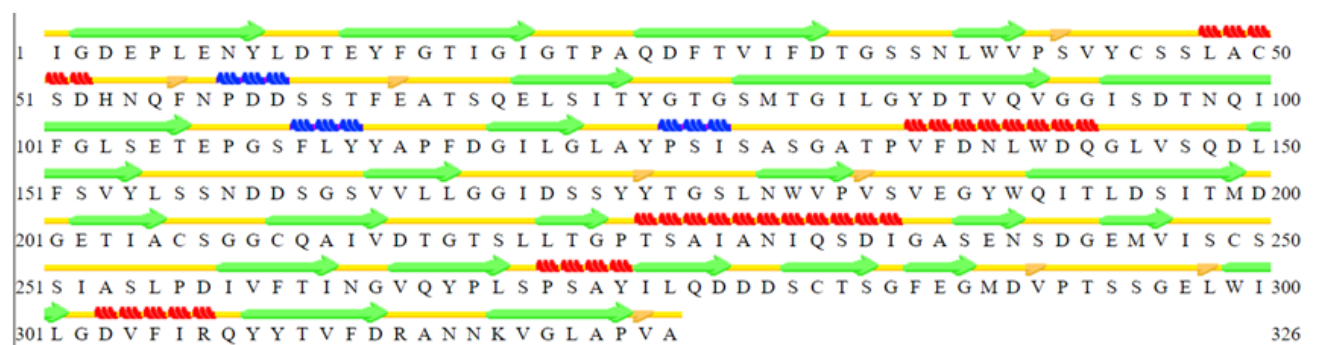
We then identify the hydrophobic residues as can be observed in the map designed below. The primary software used for this activity was Chimera.

```
5PEP:A|PDBID|CHAIN|SEQUENCE I G D E P L E N Y L D T E Y F G T I G I G T P A Q D F T V I F D T G S S N L W V P S V Y C S S L A C 50
5PEP:A|PDBID|CHAIN|SEQUENCE S D H N Q F N P D D S S T F E A T S Q E L S I T Y G T G S M T G I L G Y D T V Q V G G I S D T N Q I 100
5PEP:A|PDBID|CHAIN|SEQUENCE F G L S E T E P G S F L Y Y A P F D G I L G L A Y P S I S A S G A T P V F D N L W D Q G L V S Q D L 150
5PEP:A|PDBID|CHAIN|SEQUENCE F S V Y L S S N D D S G S V V L L G G I D S S Y Y T G S L N W V P V S V E G Y W Q I T L D S I T M D 200
5PEP:A|PDBID|CHAIN|SEQUENCE G E T I A C S G G C Q A I V D T G T S L L T G P T S A I A N I Q S D I G A S E N S D G E M V I S C S 250
5PEP:A|PDBID|CHAIN|SEQUENCE S I A S L P D I V F T I N G V Q Y P L S P S A Y I L Q D D D S C T S G F E G M D V P T S S G E L W I 300
5PEP:A|PDBID|CHAIN|SEQUENCE L G D V F I R Q Y Y T V F D R A N N K V G L A P V A 326
```

Key: The residues labelled in green are hydrophobic in nature.

(For individual residue analysis you may refer to Appendix A.)

Analysing for the Secondary Structure of the Protein Sequence (PDB ID: 5PEP)



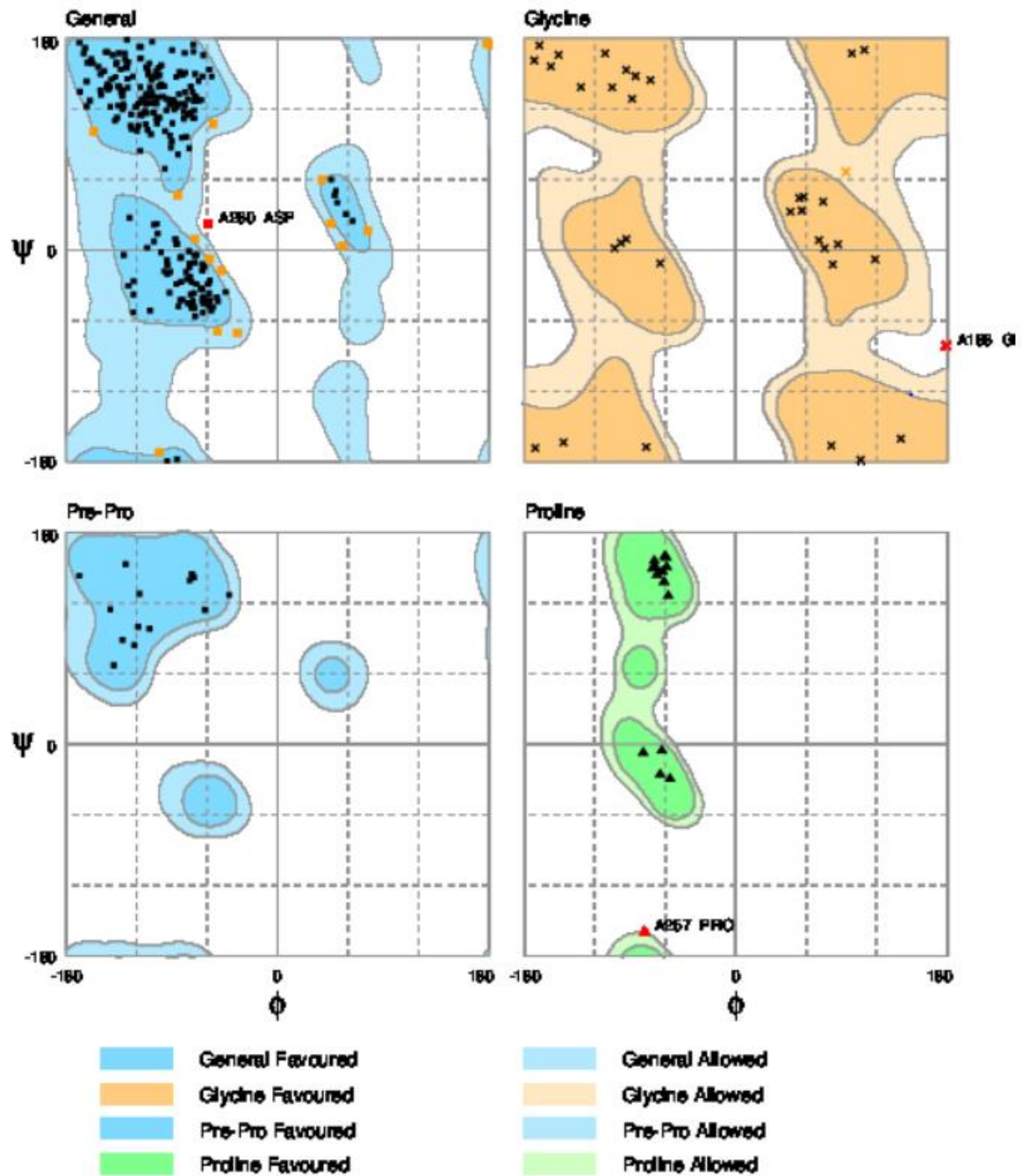
Legend of secondary structure icons:

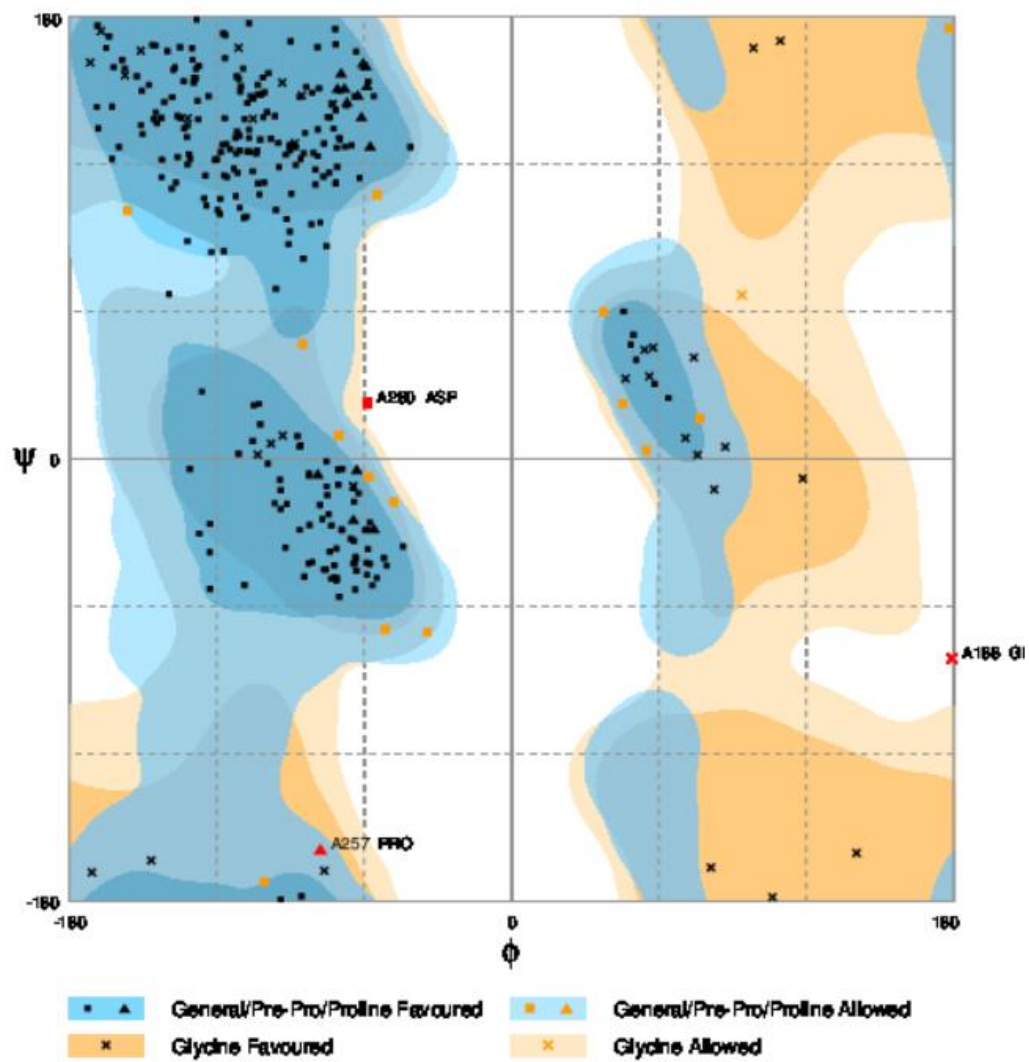
	H Alpha-Helix		T Turn
	E Extended Configuration (Beta-sheet)		C or " " Coil
	B Isolated Beta Bridge		G 3-10 Helix
	b Isolated Beta Bridge (Type 3 Fig 4,cd)		I Pi-Helix

The secondary structure of 5PEP consists of 13% helix (9 helices; 43 residues) and 45% beta sheet (32 strands; 148 residues). The helix found include the 3-10 helix and alpha helix. It also consists of turns and coils. The structure consists of two predominantly beta sheet lobes. A large portion of the residues which are absolutely conserved are polar and buried.

(For an in-depth analysis of the individual sequences, please refer to Appendix A.)

Ramachandran's Plots



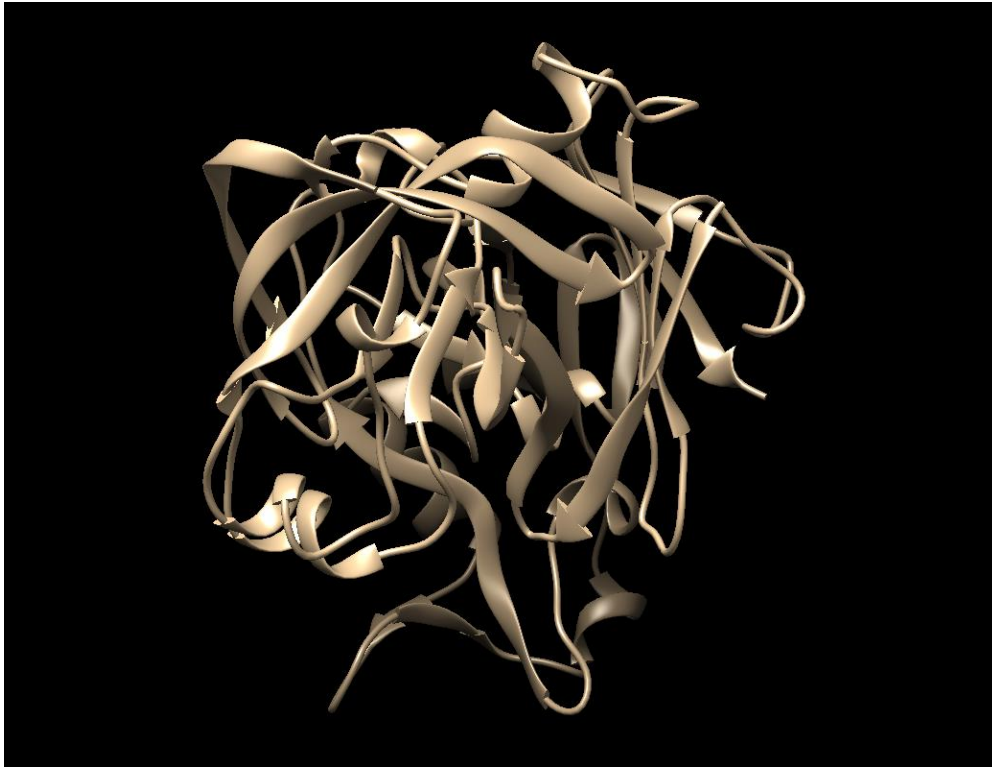


Evaluation of the residues in the sequence for the Ramachandran's plot

Evaluation of residues

```
Residue [A 11 :ASP] ( 45.44, 22.50) in Allowed region
Residue [A 124 :ALA] (-100.62,-172.00) in Allowed region
Residue [A 131 :SER] ( 76.76, 16.54) in Allowed region
Residue [A 149 :ASP] ( -85.01, 46.67) in Allowed region
Residue [A 158 :ASN] ( 37.58, 59.77) in Allowed region
Residue [A 159 :ASP] ( 54.97, 3.52) in Allowed region
Residue [A 172 :SER] ( -58.11, -7.29) in Allowed region
Residue [A 185 :SER] ( -51.26, -69.28) in Allowed region
Residue [A 205 :ALA] ( 178.20, 175.28) in Allowed region
Residue [A 242 :SER] ( -34.23, -70.44) in Allowed region
Residue [A 244 :GLY] ( 93.85, 66.66) in Allowed region
Residue [A 249 :SER] ( -54.73, 107.49) in Allowed region
Residue [A 250 :CYS] ( -47.83, -17.52) in Allowed region
Residue [A 252 :SER] ( -70.32, 9.54) in Allowed region
Residue [A 290 :MET] (-156.35, 100.99) in Allowed region
Residue [A 188 :GLY] ( 179.25, -81.14) in Outlier region
Residue [A 257 :PRO] ( -77.74,-158.75) in Outlier region
Residue [A 280 :ASP] ( -58.84, 22.73) in Outlier region
Number of residues in favoured region (~98.0% expected) : 306 ( 94.4%)
Number of residues in allowed region (~2.0% expected) : 15 ( 4.6%)
Number of residues in outlier region : 3 ( 0.9%)
```

Cartoon model of 5PEP



Z value Calculation, Hydrophobicity Analysis and Predicting the Location of Protein in the cell

Symbol	Symbol2	Amino Acid	Column3	Ratio	ΔG	E*X	J/K	Hydrophobicity
A	Ala	Alanine	17	0.0521	0.87	0.045327	NONE	H-
R	Arg	Arginine	2	0.006	2.99	0.01794	K	H+
N	Asn	Asparagine	13	0.0398	0.3	0.01194	K	H+
D	Asp	Aspartate	28	0.0858	-2.46	-0.21107	K	H+
Q	Gln	Glutamine	13	0.0398	0.3	0.01194	NONE	H+
E	Glu	Glutamate	13	0.0398	-2.53	-0.10069	K	H+
G	Gly	Glycine	35	0.1073	1.01	0.108373	K	H-
H	His	Histidine	1	0.003	0.92	0.00276	K	H+
I	Ile	Isoleucine	25	0.0766	2.16	0.165456	J	H-
L	Leu	Leucine	26	0.0797	2.29	0.182513	J	H-
K	Lys	Lysine	1	0.003	2.49	0.00747	K	H+
M	Met	Methionine	4	0.012	1.71	0.02052	J	H-
F	Phe	Phenylalanine	14	0.043	2.68	0.11524	J	H-
P	Pro	Proline	15	0.046	0.9	0.0414	NONE	H-
S	Ser	Serine	44	0.135	0.85	0.11475	NONE	H+
T	Thr	Threonine	26	0.0797	0.95	0.075715	NONE	H+
Y	Tyr	Tyrosine	16	0.049	1.67	0.08183	J	H+
V	Val	Valine	22	0.067	1.61	0.10787	J	H-
W	Trp	Tryptophan	5	0.015	2.96	0.0444	NONE	H+
C	Cys	Cysteine	6	0.018	1.23	0.02214	NONE	H+

Calculations:

$$H(\psi) = \sum (E_i X_i)$$

$$R3 = \sum(\chi(k)) / \sum(\chi(J))$$

$$Z = -0.345 * R3 + 0.5 * H(\psi)$$

$$R3 = 0.8691$$

$$H(\psi) = 0.865822$$

$$Z = 0.2196537$$

Therefore, referring to the given values, the given 5PEP sequence is most likely an external membrane protein. (Refer to lecture slides for the values of R3 and Z for classification)

Appendix A

LOC Alpha Helix	LEU	48 A	ASP	52 A	5PEP
LOC Alpha Helix	VAL	136 A	GLN	143 A	5PEP
LOC Alpha Helix	THR	225 A	ILE	236 A	5PEP
LOC Alpha Helix	PRO	272 A	TYR	275 A	5PEP
LOC Alpha Helix	ASP	304 A	ARG	308 A	5PEP
LOC 310Helix	PRO	58 A	ASP	60 A	5PEP
LOC 310Helix	PHE	111 A	TYR	113 A	5PEP
LOC 310Helix	PRO	126 A	ILE	128 A	5PEP
LOC Strand	GLY	2 A	TYR	9 A	5PEP
LOC Strand	GLU	13 A	ILE	20 A	5PEP
LOC Strand	GLN	25 A	ASP	32 A	5PEP
LOC Strand	LEU	38 A	VAL	40 A	5PEP
LOC Strand	GLU	70 A	THR	74 A	5PEP
LOC Strand	SER	79 A	VAL	91 A	5PEP
LOC Strand	ILE	94 A	THR	106 A	5PEP
LOC Strand	GLY	119 A	GLY	122 A	5PEP
LOC Strand	LEU	150 A	TYR	154 A	5PEP
LOC Strand	VAL	164 A	LEU	167 A	5PEP
LOC Strand	ASN	180 A	PRO	183 A	5PEP
LOC Strand	GLN	191 A	MET	199 A	5PEP
LOC Strand	GLU	202 A	ALA	205 A	5PEP
LOC Strand	CYS	210 A	VAL	214 A	5PEP
LOC Strand	LEU	221 A	GLY	223 A	5PEP
LOC Strand	SER	239 A	ASN	241 A	5PEP
LOC Strand	GLU	245 A	VAL	247 A	5PEP
LOC Strand	ILE	259 A	ILE	263 A	5PEP
LOC Strand	VAL	266 A	LEU	270 A	5PEP
LOC Strand	ILE	276 A	ASP	279 A	5PEP
LOC Strand	SER	282 A	SER	285 A	5PEP
LOC Strand	PHE	287 A	GLY	289 A	5PEP
LOC Strand	TRP	300 A	LEU	302 A	5PEP
LOC Strand	TYR	310 A	ASP	315 A	5PEP
LOC Strand	LYS	320 A	PRO	325 A	5PEP
LOC TurnIV	ASN	8 A	ASP	11 A	5PEP
LOC TurnI'	TYR	9 A	THR	12 A	5PEP
LOC TurnIV	LEU	10 A	GLU	13 A	5PEP
LOC TurnIV	GLY	21 A	ALA	24 A	5PEP
LOC TurnI	ASP	32 A	SER	35 A	5PEP
LOC TurnI	SER	42 A	CYS	45 A	5PEP
LOC TurnI	SER	61 A	PHE	64 A	5PEP
LOC TurnIV	TYR	75 A	GLY	78 A	5PEP
LOC TurnIV	GLN	90 A	GLY	93 A	5PEP

LOC TurnI'	VAL	91 A	ILE	94 A	5PEP
LOC TurnIV	ASP	96 A	GLN	99 A	5PEP
LOC TurnIV	SER	104 A	GLU	107 A	5PEP
LOC TurnII	SER	129 A	GLY	132 A	5PEP
LOC TurnIV	ALA	130 A	ALA	133 A	5PEP
LOC TurnIV	SER	156 A	ASP	159 A	5PEP
LOC TurnI'	SER	157 A	ASP	160 A	5PEP
LOC TurnIV	LEU	166 A	GLY	169 A	5PEP
LOC TurnI	ASP	171 A	TYR	174 A	5PEP
LOC TurnI	SER	172 A	TYR	175 A	5PEP
LOC TurnVIII	VAL	184 A	GLU	187 A	5PEP
LOC TurnIV	GLU	187 A	TRP	190 A	5PEP
LOC TurnIV	THR	198 A	GLY	201 A	5PEP
LOC TurnI'	MET	199 A	GLU	202 A	5PEP
LOC TurnII	CYS	206 A	GLY	209 A	5PEP
LOC TurnI	ASP	215 A	THR	218 A	5PEP
LOC TurnI	ASN	241 A	GLY	244 A	5PEP
LOC TurnI	SER	249 A	SER	252 A	5PEP
LOC TurnI	CYS	250 A	ILE	253 A	5PEP
LOC TurnIV	SER	251 A	ALA	254 A	5PEP
LOC TurnIV	SER	252 A	SER	255 A	5PEP
LOC TurnIV	ILE	253 A	LEU	256 A	5PEP
LOC TurnIV	THR	262 A	GLY	265 A	5PEP
LOC TurnI'	ILE	263 A	VAL	266 A	5PEP
LOC TurnIV	ASP	279 A	SER	282 A	5PEP
LOC TurnI	THR	294 A	GLY	297 A	5PEP
LOC TurnIV	ASP	315 A	ASN	318 A	5PEP
LOC TurnI	ARG	316 A	ASN	319 A	5PEP
LOC Gammalnv	GLU	202 A	ILE	204 A	5PEP
LOC Disulfide	CYS	45 A	CYS	50 A	PDB 5PEP
LOC Disulfide	CYS	206 A	CYS	210 A	PDB 5PEP
LOC Disulfide	CYS	250 A	CYS	283 A	PDB 5PEP
REM	5PEP				

REM ----- Detailed secondary structure assignment----- 5PEP

REM 5PEP

REM |---Residue---| |--Structure--| |--Phi-| |--Psi-| |--Area-| 5PEP

ASG	ILE A	1	1	C	Coil	360.00	101.05	156.4	5PEP
ASG	GLY A	2	2	E	Strand	-85.29	147.89	0.8	5PEP
ASG	ASP A	3	3	E	Strand	-136.61	112.54	86.1	5PEP
ASG	GLU A	4	4	E	Strand	-118.64	99.69	11.0	5PEP
ASG	PRO A	5	5	E	Strand	-62.49	148.14	89.5	5PEP
ASG	LEU A	6	6	E	Strand	-127.76	145.67	12.3	5PEP
ASG	GLU A	7	7	E	Strand	-94.63	118.77	113.5	5PEP
ASG	ASN A	8	8	E	Strand	-76.52	114.88	18.7	5PEP

ASG TYR A	9	9	E	Strand	-110.63	102.18	97.0	5PEP
ASG LEU A	10	10	T	Turn	50.82	40.34	93.6	5PEP
ASG ASP A	11	11	T	Turn	45.44	22.50	26.2	5PEP
ASG THR A	12	12	T	Turn	-122.70	-26.41	45.3	5PEP
ASG GLU A	13	13	E	Strand	-142.33	121.78	33.5	5PEP
ASG TYR A	14	14	E	Strand	-112.20	106.93	11.0	5PEP
ASG PHE A	15	15	E	Strand	-116.41	172.51	14.2	5PEP
ASG GLY A	16	16	E	Strand	-150.89	166.06	1.7	5PEP
ASG THR A	17	17	E	Strand	-100.48	149.08	60.8	5PEP
ASG ILE A	18	18	E	Strand	-140.10	165.87	3.9	5PEP
ASG GLY A	19	19	E	Strand	-131.77	138.58	3.9	5PEP
ASG ILE A	20	20	E	Strand	-131.24	124.03	0.0	5PEP
ASG GLY A	21	21	T	Turn	106.28	-178.31	4.9	5PEP
ASG THR A	22	22	T	Turn	-142.41	114.58	56.9	5PEP
ASG PRO A	23	23	T	Turn	-59.29	160.07	106.8	5PEP
ASG ALA A	24	24	T	Turn	-70.14	130.62	42.2	5PEP
ASG GLN A	25	25	E	Strand	-103.47	125.45	41.7	5PEP
ASG ASP A	26	26	E	Strand	-86.18	147.24	101.3	5PEP
ASG PHE A	27	27	E	Strand	-150.80	135.83	3.0	5PEP
ASG THR A	28	28	E	Strand	-90.29	127.53	29.0	5PEP
ASG VAL A	29	29	E	Strand	-128.43	158.72	0.0	5PEP
ASG ILE A	30	30	E	Strand	-89.77	127.76	16.4	5PEP
ASG PHE A	31	31	E	Strand	-90.21	92.50	8.2	5PEP
ASG ASP A	32	32	E	Strand	-89.57	107.86	14.2	5PEP
ASG THR A	33	33	T	Turn	-86.25	4.99	0.5	5PEP
ASG GLY A	34	34	T	Turn	-103.28	1.68	12.1	5PEP
ASG SER A	35	35	T	Turn	-134.92	167.47	7.8	5PEP
ASG SER A	36	36	C	Coil	-130.90	-4.16	1.8	5PEP
ASG ASN A	37	37	C	Coil	-98.90	156.98	9.1	5PEP
ASG LEU A	38	38	E	Strand	-124.60	115.36	10.1	5PEP
ASG TRP A	39	39	E	Strand	-141.34	145.18	0.8	5PEP
ASG VAL A	40	40	E	Strand	-129.33	153.10	0.0	5PEP
ASG PRO A	41	41	C	Coil	-58.80	151.89	0.0	5PEP
ASG SER A	42	42	B	Bridge	-130.04	167.12	0.0	5PEP
ASG VAL A	43	43	T	Turn	-75.35	-0.97	66.0	5PEP
ASG TYR A	44	44	T	Turn	-104.93	21.83	117.2	5PEP
ASG CYS A	45	45	T	Turn	-115.80	114.64	3.1	5PEP
ASG SER A	46	46	C	Coil	-99.23	-1.91	114.9	5PEP
ASG SER A	47	47	C	Coil	-58.29	153.58	25.6	5PEP
ASG LEU A	48	48	H	AlphaHelix	-64.11	-17.40	128.3	5PEP
ASG ALA A	49	49	H	AlphaHelix	-82.17	-26.92	0.4	5PEP
ASG CYS A	50	50	H	AlphaHelix	-86.22	-28.80	0.0	5PEP
ASG SER A	51	51	H	AlphaHelix	-69.20	-28.75	85.7	5PEP
ASG ASP A	52	52	H	AlphaHelix	-77.04	-24.54	69.2	5PEP
ASG HIS A	53	53	C	Coil	-128.20	178.77	24.7	5PEP
ASG ASN A	54	54	C	Coil	-67.19	143.80	93.4	5PEP

ASG	GLN	A	55	55	C	Coil	-120.57	121.68	69.4	5PEP
ASG	PHE	A	56	56	B	Bridge	-67.74	127.04	0.0	5PEP
ASG	ASN	A	57	57	C	Coil	-108.91	98.12	35.7	5PEP
ASG	PRO	A	58	58	G	310Helix	-64.34	-24.49	7.4	5PEP
ASG	ASP	A	59	59	G	310Helix	-62.18	-14.01	122.6	5PEP
ASG	ASP	A	60	60	G	310Helix	-111.04	2.05	107.4	5PEP
ASG	SER	A	61	61	T	Turn	-106.57	124.86	10.6	5PEP
ASG	SER	A	62	62	T	Turn	-77.94	-18.71	101.4	5PEP
ASG	THR	A	63	63	T	Turn	-102.26	14.07	61.0	5PEP
ASG	PHE	A	64	64	T	Turn	-81.10	148.98	38.6	5PEP
ASG	GLU	A	65	65	B	Bridge	-159.80	126.88	142.5	5PEP
ASG	ALA	A	66	66	C	Coil	-78.92	167.54	75.8	5PEP
ASG	THR	A	67	67	C	Coil	-144.85	168.18	34.9	5PEP
ASG	SER	A	68	68	C	Coil	-93.90	-12.73	120.7	5PEP
ASG	GLN	A	69	69	C	Coil	-65.06	127.61	82.9	5PEP
ASG	GLU	A	70	70	E	Strand	-101.15	155.17	136.4	5PEP
ASG	LEU	A	71	71	E	Strand	-138.04	147.22	7.2	5PEP
ASG	SER	A	72	72	E	Strand	-144.28	136.60	73.1	5PEP
ASG	ILE	A	73	73	E	Strand	-142.54	138.65	16.1	5PEP
ASG	THR	A	74	74	E	Strand	-116.00	128.21	124.0	5PEP
ASG	TYR	A	75	75	T	Turn	-110.98	154.64	36.6	5PEP
ASG	GLY	A	76	76	T	Turn	-64.40	-11.10	77.5	5PEP
ASG	THR	A	77	77	T	Turn	-122.72	-52.87	95.9	5PEP
ASG	GLY	A	78	78	T	Turn	-111.11	167.29	6.4	5PEP
ASG	SER	A	79	79	E	Strand	-129.11	155.15	44.1	5PEP
ASG	MET	A	80	80	E	Strand	-157.40	158.80	3.8	5PEP
ASG	THR	A	81	81	E	Strand	-150.23	132.23	48.7	5PEP
ASG	GLY	A	82	82	E	Strand	-170.74	-168.24	0.2	5PEP
ASG	ILE	A	83	83	E	Strand	-111.87	155.67	29.7	5PEP
ASG	LEU	A	84	84	E	Strand	-101.84	148.22	2.5	5PEP
ASG	GLY	A	85	85	E	Strand	-157.35	156.10	0.0	5PEP
ASG	TYR	A	86	86	E	Strand	-105.11	146.73	86.2	5PEP
ASG	ASP	A	87	87	E	Strand	-168.50	176.35	2.1	5PEP
ASG	THR	A	88	88	E	Strand	-91.84	123.81	29.1	5PEP
ASG	VAL	A	89	89	E	Strand	-106.84	130.61	0.0	5PEP
ASG	GLN	A	90	90	E	Strand	-103.13	112.05	99.1	5PEP
ASG	VAL	A	91	91	E	Strand	-133.21	134.50	2.0	5PEP
ASG	GLY	A	92	92	T	Turn	46.48	32.64	6.9	5PEP
ASG	GLY	A	93	93	T	Turn	87.07	4.93	79.4	5PEP
ASG	ILE	A	94	94	E	Strand	-111.68	133.20	20.7	5PEP
ASG	SER	A	95	95	E	Strand	-81.38	95.52	62.5	5PEP
ASG	ASP	A	96	96	E	Strand	-84.73	81.47	0.0	5PEP
ASG	THR	A	97	97	E	Strand	-63.71	147.52	52.3	5PEP
ASG	ASN	A	98	98	E	Strand	48.64	46.52	108.0	5PEP
ASG	GLN	A	99	99	E	Strand	-87.95	126.79	0.8	5PEP
ASG	ILE	A	100	100	E	Strand	-78.79	123.20	10.0	5PEP

ASG	PHE	A	101	101	E	Strand	-136.99	159.35	1.7	5PEP
ASG	GLY	A	102	102	E	Strand	-93.29	153.15	0.5	5PEP
ASG	LEU	A	103	103	E	Strand	-118.51	105.81	0.4	5PEP
ASG	SER	A	104	104	E	Strand	-55.99	147.56	0.0	5PEP
ASG	GLU	A	105	105	E	Strand	-127.10	-30.42	67.3	5PEP
ASG	THR	A	106	106	E	Strand	-145.55	138.34	52.5	5PEP
ASG	GLU	A	107	107	T	Turn	-139.38	67.07	3.3	5PEP
ASG	PRO	A	108	108	C	Coil	-66.93	145.33	59.1	5PEP
ASG	GLY	A	109	109	C	Coil	109.52	170.17	58.7	5PEP
ASG	SER	A	110	110	C	Coil	-82.63	-42.54	82.4	5PEP
ASG	PHE	A	111	111	G	310Helix	-64.44	-42.61	81.0	5PEP
ASG	LEU	A	112	112	G	310Helix	-70.53	-10.53	8.5	5PEP
ASG	TYR	A	113	113	G	310Helix	-81.01	-41.99	95.3	5PEP
ASG	TYR	A	114	114	C	Coil	-82.43	-5.90	178.3	5PEP
ASG	ALA	A	115	115	C	Coil	-74.75	139.15	10.6	5PEP
ASG	PRO	A	116	116	C	Coil	-78.81	-5.99	40.9	5PEP
ASG	PHE	A	117	117	C	Coil	-106.07	147.46	9.0	5PEP
ASG	ASP	A	118	118	C	Coil	-84.33	-47.92	10.2	5PEP
ASG	GLY	A	119	119	E	Strand	-146.66	-163.36	0.2	5PEP
ASG	ILE	A	120	120	E	Strand	-134.70	138.71	12.2	5PEP
ASG	LEU	A	121	121	E	Strand	-119.57	101.28	1.0	5PEP
ASG	GLY	A	122	122	E	Strand	-72.60	144.47	1.4	5PEP
ASG	LEU	A	123	123	C	Coil	-125.99	27.39	5.2	5PEP
ASG	ALA	A	124	124	C	Coil	-100.62	-172.00	0.8	5PEP
ASG	TYR	A	125	125	C	Coil	-71.50	141.88	2.8	5PEP
ASG	PRO	A	126	126	G	310Helix	-62.92	-4.16	50.9	5PEP
ASG	SER	A	127	127	G	310Helix	-63.55	-39.89	80.3	5PEP
ASG	ILE	A	128	128	G	310Helix	-102.78	22.39	63.1	5PEP
ASG	SER	A	129	129	T	Turn	-80.59	124.44	12.5	5PEP
ASG	ALA	A	130	130	T	Turn	-71.11	126.59	23.9	5PEP
ASG	SER	A	131	131	T	Turn	76.76	16.54	62.1	5PEP
ASG	GLY	A	132	132	T	Turn	56.19	33.59	63.8	5PEP
ASG	ALA	A	133	133	T	Turn	-76.30	128.34	9.2	5PEP
ASG	THR	A	134	134	C	Coil	-61.78	114.26	55.8	5PEP
ASG	PRO	A	135	135	C	Coil	-60.37	161.26	5.3	5PEP
ASG	VAL	A	136	136	H	AlphaHelix	-63.60	-53.08	3.7	5PEP
ASG	PHE	A	137	137	H	AlphaHelix	-59.53	-28.87	3.9	5PEP
ASG	ASP	A	138	138	H	AlphaHelix	-73.88	-37.73	19.3	5PEP
ASG	ASN	A	139	139	H	AlphaHelix	-73.27	-27.07	22.6	5PEP
ASG	LEU	A	140	140	H	AlphaHelix	-73.38	-48.79	0.2	5PEP
ASG	TRP	A	141	141	H	AlphaHelix	-58.79	-47.12	100.5	5PEP
ASG	ASP	A	142	142	H	AlphaHelix	-57.72	-42.73	111.6	5PEP
ASG	GLN	A	143	143	H	AlphaHelix	-87.07	9.32	67.8	5PEP
ASG	GLY	A	144	144	C	Coil	54.18	44.37	57.7	5PEP
ASG	LEU	A	145	145	C	Coil	-94.21	-8.52	65.4	5PEP
ASG	VAL	A	146	146	C	Coil	-127.53	138.18	9.2	5PEP

ASG SER A 147 147 C	Coil	-63.93	-42.49	101.9	5PEP
ASG GLN A 148 148 C	Coil	-123.27	147.59	96.5	5PEP
ASG ASP A 149 149 C	Coil	-85.01	46.67	19.2	5PEP
ASG LEU A 150 150 E	Strand	-146.24	168.39	5.6	5PEP
ASG PHE A 151 151 E	Strand	-147.60	152.22	1.4	5PEP
ASG SER A 152 152 E	Strand	-133.42	153.64	0.2	5PEP
ASG VAL A 153 153 E	Strand	-135.87	139.51	4.7	5PEP
ASG TYR A 154 154 E	Strand	-120.25	121.62	38.1	5PEP
ASG LEU A 155 155 C	Coil	-112.34	130.71	3.3	5PEP
ASG SER A 156 156 T	Turn	-70.23	149.82	1.0	5PEP
ASG SER A 157 157 T	Turn	-109.16	158.76	27.1	5PEP
ASG ASN A 158 158 T	Turn	37.58	59.77	115.5	5PEP
ASG ASP A 159 159 T	Turn	54.97	3.52	85.1	5PEP
ASG ASP A 160 160 T	Turn	-63.20	165.73	93.9	5PEP
ASG SER A 161 161 C	Coil	-89.90	169.95	112.4	5PEP
ASG GLY A 162 162 C	Coil	118.64	-7.94	37.9	5PEP
ASG SER A 163 163 C	Coil	-69.76	130.06	3.2	5PEP
ASG VAL A 164 164 E	Strand	-152.52	155.69	8.8	5PEP
ASG VAL A 165 165 E	Strand	-116.97	115.37	0.4	5PEP
ASG LEU A 166 166 E	Strand	-100.60	112.54	12.2	5PEP
ASG LEU A 167 167 E	Strand	-84.58	124.34	2.4	5PEP
ASG GLY A 168 168 T	Turn	57.75	45.30	1.0	5PEP
ASG GLY A 169 169 T	Turn	-171.49	161.28	7.3	5PEP
ASG ILE A 170 170 C	Coil	-132.15	131.03	57.3	5PEP
ASG ASP A 171 171 T	Turn	-125.12	105.96	66.0	5PEP
ASG SER A 172 172 T	Turn	-58.11	-7.29	84.4	5PEP
ASG SER A 173 173 T	Turn	-74.37	-22.55	90.4	5PEP
ASG TYR A 174 174 T	Turn	-93.86	-20.40	54.7	5PEP
ASG TYR A 175 175 B	Bridge	-129.81	162.36	36.1	5PEP
ASG THR A 176 176 C	Coil	-110.05	151.49	72.4	5PEP
ASG GLY A 177 177 C	Coil	81.29	-166.21	67.7	5PEP
ASG SER A 178 178 C	Coil	-103.26	152.17	97.1	5PEP
ASG LEU A 179 179 C	Coil	-71.44	112.03	26.7	5PEP
ASG ASN A 180 180 E	Strand	-90.16	125.45	57.1	5PEP
ASG TRP A 181 181 E	Strand	-108.58	138.30	87.6	5PEP
ASG VAL A 182 182 E	Strand	-117.53	127.92	3.8	5PEP
ASG PRO A 183 183 E	Strand	-69.33	157.14	65.6	5PEP
ASG VAL A 184 184 B	Bridge	-87.82	119.56	22.4	5PEP
ASG SER A 185 185 T	Turn	-51.26	-69.28	44.6	5PEP
ASG VAL A 186 186 T	Turn	-130.82	122.14	62.7	5PEP
ASG GLU A 187 187 T	Turn	-74.20	116.49	102.9	5PEP
ASG GLY A 188 188 T	Turn	179.25	-81.14	7.3	5PEP
ASG TYR A 189 189 T	Turn	-85.52	-177.92	78.6	5PEP
ASG TRP A 190 190 T	Turn	-95.93	69.17	0.4	5PEP
ASG GLN A 191 191 E	Strand	-79.81	117.72	8.0	5PEP
ASG ILE A 192 192 E	Strand	-127.29	159.90	3.4	5PEP

ASG	THR	A	193	193	E	Strand	-94.85	128.63	56.9	5PEP
ASG	LEU	A	194	194	E	Strand	-100.99	139.01	0.0	5PEP
ASG	ASP	A	195	195	E	Strand	-91.99	-36.14	64.2	5PEP
ASG	SER	A	196	196	E	Strand	-163.86	171.91	21.8	5PEP
ASG	ILE	A	197	197	E	Strand	-138.32	109.99	0.0	5PEP
ASG	THR	A	198	198	E	Strand	-116.56	163.10	22.8	5PEP
ASG	MET	A	199	199	E	Strand	-162.60	122.15	7.2	5PEP
ASG	ASP	A	200	200	T	Turn	63.88	24.82	131.6	5PEP
ASG	GLY	A	201	201	T	Turn	75.76	1.60	80.5	5PEP
ASG	GLU	A	202	202	E	Strand	-102.32	129.96	91.5	5PEP
ASG	THR	A	203	203	E	Strand	-75.26	86.61	67.9	5PEP
ASG	ILE	A	204	204	E	Strand	-68.90	-4.08	8.8	5PEP
ASG	ALA	A	205	205	E	Strand	178.20	175.28	13.7	5PEP
ASG	CYS	A	206	206	T	Turn	49.67	50.46	14.4	5PEP
ASG	SER	A	207	207	T	Turn	-72.41	134.43	96.2	5PEP
ASG	GLY	A	208	208	T	Turn	70.92	8.46	93.1	5PEP
ASG	GLY	A	209	209	T	Turn	98.67	167.21	29.7	5PEP
ASG	CYS	A	210	210	E	Strand	-165.01	167.16	19.5	5PEP
ASG	GLN	A	211	211	E	Strand	-103.13	148.29	41.1	5PEP
ASG	ALA	A	212	212	E	Strand	-144.77	141.02	0.2	5PEP
ASG	ILE	A	213	213	E	Strand	-110.44	149.38	6.6	5PEP
ASG	VAL	A	214	214	E	Strand	-91.52	97.57	3.3	5PEP
ASG	ASP	A	215	215	T	Turn	-112.99	118.05	16.8	5PEP
ASG	THR	A	216	216	T	Turn	-82.52	-6.84	13.5	5PEP
ASG	GLY	A	217	217	T	Turn	-97.88	6.21	31.1	5PEP
ASG	THR	A	218	218	T	Turn	-118.25	124.85	28.8	5PEP
ASG	SER	A	219	219	C	Coil	-72.05	-43.36	25.6	5PEP
ASG	LEU	A	220	220	C	Coil	-106.76	177.25	35.7	5PEP
ASG	LEU	A	221	221	E	Strand	-102.61	107.59	2.0	5PEP
ASG	THR	A	222	222	E	Strand	-99.50	141.09	1.3	5PEP
ASG	GLY	A	223	223	E	Strand	-167.15	174.13	0.0	5PEP
ASG	PRO	A	224	224	C	Coil	-57.49	127.41	10.0	5PEP
ASG	THR	A	225	225	H	AlphaHelix	-44.10	-35.57	70.5	5PEP
ASG	SER	A	226	226	H	AlphaHelix	-71.20	-49.58	99.0	5PEP
ASG	ALA	A	227	227	H	AlphaHelix	-54.80	-48.37	25.8	5PEP
ASG	ILE	A	228	228	H	AlphaHelix	-68.89	-28.88	9.2	5PEP
ASG	ALA	A	229	229	H	AlphaHelix	-50.82	-43.41	44.6	5PEP
ASG	ASN	A	231	230	H	AlphaHelix	-59.04	-42.34	94.5	5PEP
ASG	ILE	A	232	231	H	AlphaHelix	-72.34	-48.36	1.4	5PEP
ASG	GLN	A	233	232	H	AlphaHelix	-63.18	-40.54	14.2	5PEP
ASG	SER	A	234	233	H	AlphaHelix	-58.40	-36.65	97.7	5PEP
ASG	ASP	A	235	234	H	AlphaHelix	-75.49	-44.98	70.1	5PEP
ASG	ILE	A	236	235	H	AlphaHelix	-85.79	5.44	9.0	5PEP
ASG	GLY	A	237	236	C	Coil	74.36	41.30	43.6	5PEP
ASG	ALA	A	238	237	C	Coil	-78.34	150.82	14.1	5PEP
ASG	SER	A	239	238	E	Strand	-135.93	122.84	71.3	5PEP

ASG	GLU	A	240	239	E	Strand	-77.78	96.19	135.9	5PEP
ASG	ASN	A	241	240	E	Strand	-71.70	174.86	63.6	5PEP
ASG	SER	A	242	241	T	Turn	-34.23	-70.44	130.1	5PEP
ASG	ASP	A	243	242	T	Turn	-70.54	-4.34	150.1	5PEP
ASG	GLY	A	244	243	T	Turn	93.85	66.66	46.4	5PEP
ASG	GLU	A	245	244	E	Strand	-161.90	159.44	104.6	5PEP
ASG	MET	A	246	245	E	Strand	-117.09	84.46	44.5	5PEP
ASG	VAL	A	247	246	E	Strand	-93.95	-179.18	35.6	5PEP
ASG	ILE	A	248	247	C	Coil	-150.56	149.82	14.5	5PEP
ASG	SER	A	249	248	T	Turn	-54.73	107.49	82.8	5PEP
ASG	CYS	A	250	249	T	Turn	-47.83	-17.52	30.5	5PEP
ASG	SER	A	251	250	T	Turn	-91.37	-18.35	101.4	5PEP
ASG	SER	A	252	251	T	Turn	-70.32	9.54	57.0	5PEP
ASG	ILE	A	253	252	T	Turn	-71.20	-36.56	32.1	5PEP
ASG	ALA	A	254	253	T	Turn	-56.56	-51.42	93.0	5PEP
ASG	SER	A	255	254	T	Turn	-71.10	-48.49	114.7	5PEP
ASG	LEU	A	256	255	T	Turn	-41.12	126.85	30.2	5PEP
ASG	PRO	A	257	256	C	Coil	-77.74	-158.75	45.3	5PEP
ASG	ASP	A	258	257	C	Coil	-110.57	131.49	63.2	5PEP
ASG	ILE	A	259	258	E	Strand	-85.83	122.09	1.2	5PEP
ASG	VAL	A	260	259	E	Strand	-116.73	138.59	18.8	5PEP
ASG	PHE	A	261	260	E	Strand	-110.75	125.50	0.2	5PEP
ASG	THR	A	262	261	E	Strand	-105.29	117.01	20.2	5PEP
ASG	ILE	A	263	262	E	Strand	-119.95	122.01	1.0	5PEP
ASG	ASN	A	264	263	T	Turn	58.30	30.52	87.2	5PEP
ASG	GLY	A	265	264	T	Turn	82.58	-12.35	55.1	5PEP
ASG	VAL	A	266	265	E	Strand	-84.01	132.61	54.0	5PEP
ASG	GLN	A	267	266	E	Strand	-78.79	134.14	134.4	5PEP
ASG	TYR	A	268	267	E	Strand	-131.95	88.61	4.4	5PEP
ASG	PRO	A	269	268	E	Strand	-70.79	150.90	56.1	5PEP
ASG	LEU	A	270	269	E	Strand	-124.18	103.08	0.6	5PEP
ASG	SER	A	271	270	C	Coil	-73.04	144.63	43.2	5PEP
ASG	PRO	A	272	271	H	AlphaHelix	-56.00	-28.16	12.4	5PEP
ASG	SER	A	273	272	H	AlphaHelix	-64.16	-12.04	93.9	5PEP
ASG	ALA	A	274	273	H	AlphaHelix	-108.67	-51.35	2.9	5PEP
ASG	TYR	A	275	274	H	AlphaHelix	-75.19	-11.24	1.0	5PEP
ASG	ILE	A	276	275	E	Strand	-111.50	116.41	3.8	5PEP
ASG	LEU	A	277	276	E	Strand	-83.45	151.36	35.8	5PEP
ASG	GLN	A	278	277	E	Strand	-162.63	143.30	97.9	5PEP
ASG	ASP	A	279	278	E	Strand	-107.44	144.82	113.5	5PEP
ASG	ASP	A	280	279	T	Turn	-58.84	22.73	158.6	5PEP
ASG	ASP	A	281	280	T	Turn	-122.81	-37.90	147.7	5PEP
ASG	SER	A	282	281	E	Strand	-168.18	134.54	72.2	5PEP
ASG	CYS	A	283	282	E	Strand	-89.94	127.01	0.2	5PEP
ASG	THR	A	284	283	E	Strand	-117.33	173.11	39.7	5PEP
ASG	SER	A	285	284	E	Strand	-96.33	139.50	4.7	5PEP

ASG	GLY	A	286	285	C	Coil	-93.07	9.46	0.6	5PEP
ASG	PHE	A	287	286	E	Strand	-97.84	130.34	8.3	5PEP
ASG	GLU	A	288	287	E	Strand	-131.84	135.69	85.0	5PEP
ASG	GLY	A	289	288	E	Strand	-88.16	128.53	30.1	5PEP
ASG	MET	A	290	289	C	Coil	-156.35	100.99	73.0	5PEP
ASG	ASP	A	291	290	C	Coil	-71.43	112.47	76.6	5PEP
ASG	VAL	A	292	291	B	Bridge	-122.06	84.18	35.3	5PEP
ASG	PRO	A	293	292	C	Coil	-67.95	151.02	98.9	5PEP
ASG	THR	A	294	293	T	Turn	-158.53	162.35	56.7	5PEP
ASG	SER	A	295	294	T	Turn	-51.90	-40.28	139.7	5PEP
ASG	SER	A	296	295	T	Turn	-65.43	-32.51	67.2	5PEP
ASG	GLY	A	297	296	T	Turn	140.55	-160.35	31.1	5PEP
ASG	GLU	A	298	297	C	Coil	-79.80	111.75	79.6	5PEP
ASG	LEU	A	299	298	B	Bridge	-73.81	138.96	1.8	5PEP
ASG	TRP	A	300	299	E	Strand	-103.84	124.36	12.0	5PEP
ASG	ILE	A	301	300	E	Strand	-107.49	125.10	11.4	5PEP
ASG	LEU	A	302	301	E	Strand	-90.74	87.37	1.2	5PEP
ASG	GLY	A	303	302	C	Coil	-76.19	-167.51	0.0	5PEP
ASG	ASP	A	304	303	H	AlphaHelix	-57.56	-25.78	2.0	5PEP
ASG	VAL	A	305	304	H	AlphaHelix	-63.05	-45.54	0.6	5PEP
ASG	PHE	A	306	305	H	AlphaHelix	-76.27	-44.97	0.2	5PEP
ASG	ILE	A	307	306	H	AlphaHelix	-64.13	-33.24	1.0	5PEP
ASG	ARG	A	308	307	H	AlphaHelix	-58.81	-28.62	9.2	5PEP
ASG	GLN	A	309	308	C	Coil	-96.40	-18.03	56.6	5PEP
ASG	TYR	A	310	309	E	Strand	-131.92	119.84	17.2	5PEP
ASG	TYR	A	311	310	E	Strand	-70.94	118.86	1.4	5PEP
ASG	THR	A	312	311	E	Strand	-106.79	134.00	0.2	5PEP
ASG	VAL	A	313	312	E	Strand	-114.53	126.01	0.0	5PEP
ASG	PHE	A	314	313	E	Strand	-107.87	98.58	0.0	5PEP
ASG	ASP	A	315	314	E	Strand	-95.89	101.25	14.2	5PEP
ASG	ARG	A	316	315	T	Turn	-74.92	-14.64	42.6	5PEP
ASG	ALA	A	317	316	T	Turn	-70.09	-56.11	55.0	5PEP
ASG	ASN	A	318	317	T	Turn	-105.26	7.31	98.7	5PEP
ASG	ASN	A	319	318	T	Turn	45.66	60.01	43.4	5PEP
ASG	LYS	A	320	319	E	Strand	-137.57	158.25	78.8	5PEP
ASG	VAL	A	321	320	E	Strand	-112.03	124.24	0.0	5PEP
ASG	GLY	A	322	321	E	Strand	-105.17	138.41	0.0	5PEP
ASG	LEU	A	323	322	E	Strand	-128.43	154.87	3.4	5PEP
ASG	ALA	A	324	323	E	Strand	-168.77	143.23	0.0	5PEP
ASG	PRO	A	325	324	E	Strand	-61.05	139.34	51.3	5PEP
ASG	VAL	A	326	325	B	Bridge	-71.53	168.72	33.0	5PEP
ASG	ALA	A	327	326	C	Coil	-105.84	360.00	108.7	5PEP

Please cite: F.Eisenhaber & P.Argos, J.Comp.Chem. 14, 1272-1280, 1993

Pictorial Representation of different segments Detailed analysis

References

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