# **Indian Institute of Technology Gandhinagar**

# BE623 Biocomputing Sem1 2025-2026 Lab Assignment -3

# Text processing (sed and awk)

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M.Tech Biological Engineering

# Q1) Output-

### **Q2**)

## Output-

# Q3)

### Output-

```
bhavya@BhavyaSharma:~/lab_session_3$ sed -n '/^>/p' clock_gene.fasta
>NC_000004.12:c55546909-55427903 Homo sapiens chromosome 4, GRCh38.p14
Primary Assembly
```

# **Q4**)

## **Output-**

```
bhavya@BhavyaSharma:~/lab_session_3$ sed -n '/^>.*CLOCK/p' protein.fas
ta
>seq1|Homo_sapiens|CLOCK_protein
```

### **Q5**)

# **Output-**

bhavya@BhavyaSharma:~/lab\_session\_3\$ sed -n '/CC/p' protein.fasta
MTEYKLVVVGAGCCGKSALTIQLInhfgFVDEYDPTIEDSYRKQVVIDGETCLLDILDTAG
MADQLTEEQIAEFKEAFSLFDKDGDGTCCTKELGTVMRSCCQNPTEAELQDMINEVDADGNGQ

# **Q6**)

## **Output-**

```
bhavya@BhavyaSharma:~/lab_session_3$ grep -v "^>" clock_gene.fasta | grep -o "G" | wc -l
355
```

### **Q7**)

#### Output-

### **Q8**)

### **Output-**

```
bhavya@BhavyaSharma:~/lab_session_3$ grep '^>' protein.fasta | awk '{s
ub(/^>/, ""); print}'
seq1|Homo_sapiens|CLOCK_protein
seq2|Mus_musculus|PER_protein
seq3|Drosophila_melanogaster|TIM_protein
seq4|Danio_rerio|BMAL_protein
seq5|Arabidopsis_thaliana|LHY_protein
seq6|Saccharomyces_cerevisiae|CYC_protein
seq7|Caenorhabditis_elegans|CLK_protein
seq8|Gallus_gallus|CRY_protein
seq9|Escherichia_coli|RecA_protein
seq10|Xenopus_laevis|REV-ERB_protein
```

# **Q9**)

## **Output-**

bhavya@BhavyaSharma:~/lab\_session\_3\$ sed -n '/^[^>].\*M.\*Q\$/p' protein.fasta MADQLTEEQIAEFKEAFSLFDKDGDGTCCTKELGTVMRSCCQNPTEAELQDMINEVDADGNGQ MADSQRRLLQNVINKAAGKSSTLLPVDGDKILVVTTGGQVVQSNVLEAMKELLQ

```
bhavya@BhavyaSharma:~/lab_session_3$ awk '/^>/ {if (sequenceid) print sequenceid, lengthseq; sequenceid=substr($1,2); lengthseq=0; next} {le ngthseq+=length($0)} END{if (sequenceid) print sequenceid, lengthseq}' protein.fasta seq1|Homo_sapiens|CLOCK_protein 61 seq2|Mus_musculus|PER_protein 56 seq3|Drosophila_melanogaster|TIM_protein 63 seq4|Danio_rerio|BMAL_protein 58 seq5|Arabidopsis_thaliana|LHY_protein 54 seq6|Saccharomyces_cerevisiae|CYC_protein 57 seq7|Caenorhabditis_elegans|CLK_protein 54 seq8|Gallus_gallus|CRY_protein 54 seq9|Escherichia_coli|RecA_protein 52 seq10|Xenopus_laevis|REV-ERB_protein 47
```

# Q10) Output-

bhayya	ARhavv	2 Sh 21	oma ' c	. /1	lah d	session_3\$ awk '/^ATG	M/ CC ¢F	=="A"! protein ndb	
ATOM	1	N N			172			1.00 34.43	N
ATOM	2	CA			172			1.00 34.43	C
ATOM	3	C			172	-41.403 -21.065		1.00 33.46	c
ATOM	4	0			172	-41.385 -21.496		1.00 33.48	0
ATOM	5	СВ			172	-39.506 -19.534		1.00 35.12	c
ATOM	6	CG			172			1.00 36.34	c
ATOM	7				172			1.00 37.69	c
ATOM	8				172			1.00 37.47	c
ATOM	9				172				N
ATOM	10				172		25.334	1.00 37.83	C
ATOM	11				172			1.00 37.57	Ċ
ATOM	12				172	-34.725 -18.128	25.037	1.00 37.51	Č
ATOM	13				172	-35.545 -17.671		1.00 37.85	Ċ
ATOM	14		TRP			-34.523 -17.646	23.769	1.00 37.43	Ċ
ATOM	15	N			173			1.00 32.18	N
ATOM	16	CA			173			1.00 31.37	C
ATOM	17	С	LYS	Α	173	-44.028 -19.604		1.00 29.85	С
ATOM	18	0	LYS	Α	173	-44.831 -19.725	21.976	1.00 30.15	0
ATOM	19	СВ	LYS	Α	173	-44.935 -20.645	25.024	1.00 31.31	С
ATOM	20	CG	LYS	Α	173	-46.343 -20.964	24.519	1.00 32.53	С
ATOM	21	CD	LYS	Α	173	-47.425 -20.459	25.479	1.00 32.89	Ċ
ATOM	22	CE	LYS	Α	173	-48.818 -20.684	24.901	1.00 33.96	С
ATOM	23	NZ	LYS	Α	173	-49.893 -20.189	25.806	1.00 34.66	N
ATOM	24	N	GLU	Α	174	-43.280 -18.518	23.090	1.00 27.67	N
ATOM	25	CA	GLU	Α	174	-43.337 -17.366	22.191	1.00 25.77	С
ATOM	26	С	GLU	Α	174	-41.922 -17.014	21.728	1.00 23.54	С
ATOM	27	0	GLU	Α	174	-41.381 -15.977	22.138	1.00 23.23	0
ATOM	28	СВ	GLU	Α	174	-43.933 -16.148	22.913	1.00 25.76	С
ATOM	29	CG			174	-45.376 -16.258	23.359	1.00 26.89	C C
ATOM	30	CD			174	-45.777 -15.061		1.00 27.42	
ATOM	31				174	-46.102 -14.001		1.00 29.42	0
ATOM	32	0E2	GLU	Α	174	-45.756 -15.182	25.445	1.00 30.63	0

(Printed all the ATOM lines with Chain A- The output was quite large so pasting this snippet here to avoid taking up too much space.)

# Q11) Output-

```
bhavya@BhavyaSharma:~/lab_session_3$ awk '/^ATOM/ && ($4=="LYS" || $4=="ARG" ) {print $0}' protein.pdb
```

ATOM ATOM	15 16	N CA	LYS A			-20.697 -20.728	24.576 23.949	1.00 32.18 1.00 31.37	N C
ATOM	17	c	LYS A			-19.604	22.914	1.00 29.85	Č
ATOM	18	0	LYS A			-19.725	21.976	1.00 30.15	0
ATOM ATOM	19 20	CB CG	LYS A			-20.645 -20.964	25.024 24.519	1.00 31.31 1.00 32.53	c c
MOTA	21	CD	LYS A			-20.459	25.479	1.00 32.89	c
ATOM	22	CE	LYS A			-20.684	24.901	1.00 33.96	C
ATOM ATOM	23 46	NZ N	LYS A	177		-20.189 -13.469	25.806 20.062	1.00 34.66 1.00 17.53	N N
ATOM	47	CA	ARG A	177	-41.351	-12.338	20.984	1.00 18.15	С
ATOM ATOM	48 49	C 0	ARG A			-12.196 -11.088	21.880 22.053	1.00 18.13 1.00 17.51	C 0
ATOM	50	СВ	ARG A			-12.450	21.807	1.00 17.51	Č
ATOM	51	CG	ARG A	177	-42.872	-11.237	22.713	1.00 20.72	С
ATOM ATOM	52 53	CD NE	ARG A			-11.292 -10.263	23.368 24.391	1.00 22.66 1.00 24.94	C N
ATOM	54	CZ	ARG A	177	-43.848	-10.348	25.616	1.00 25.91	č
ATOM ATOM	55 56		ARG A			-11.413	25.983	1.00 25.04	N
ATOM	94	N	ARG A		-44.030 -34.717		26.477 22.797	1.00 26.28 1.00 19.68	N N
ATOM	95	CA	ARG A		-33.268		22.849	1.00 20.05	C
ATOM ATOM	96 97	C 0	ARG A		-32.593 -31.576		21.743 21.990	1.00 19.42 1.00 19.22	C 0
MOTA	98	СВ	ARG A		-32.874	-11.019	22.769	1.00 20.66	c
ATOM	99	CG	ARG A			-11.864	23.806	1.00 23.33	C
ATOM ATOM	100 101	CD NE	ARG A			-12.324 -13.693	24.917 24.676	1.00 31.08 1.00 34.53	C N
ATOM	102	CZ	ARG A			-14.777	25.285	1.00 36.34	С
ATOM ATOM	103 104		ARG A			-14.685 -15.966	26.205 24.975	1.00 37.09 1.00 37.59	N N
ATOM	147	N	LYS A	189	-27.943	-1.219	22.313	1.00 19.72	N
ATOM ATOM	148 149	CA C	LYS A		-26.592 -25.535		22.859 21.783	1.00 19.83 1.00 19.51	c c
ATOM	150	0	LYS A		-25.535 -24.637		22.008	1.00 19.31	0
ATOM	151	СВ	LYS A		-26.300		23.584	1.00 19.67	c
ATOM ATOM	152 153	CG CD	LYS A		-24.980 -24.991		24.353 25.500	1.00 21.18 1.00 23.97	c c
ATOM	154	CE	LYS A		-23.703	-1.601	26.298	1.00 25.23	С
ATOM	155	NZ	LYS A		-23.673		27.204	1.00 25.98	N
ATOM ATOM	228 229	N CA	LYS A		-30.993 -31.745		7.874 7.833	1.00 26.73 1.00 24.20	N C
ATOM	230	C	LYS A		-31.208	-1.820	8.880	1.00 23.56	С
ATOM ATOM	231 232	O CB	LYS A		-30.014 -31.682		9.160 6.440	1.00 23.03 1.00 24.17	0 C
ATOM	233	CG	LYS A	200	-32.216	-0.609	5.294	1.00 23.41	С
ATOM ATOM	234 235	CD CE	LYS A		-32.263 -32.479		3.981 2.786	1.00 22.93 1.00 21.93	c c
ATOM	236	NZ	LYS A		-31.331		2.647	1.00 19.78	N
ATOM	297	N	LYS A			-12.189	16.590	1.00 19.70	N
ATOM ATOM	298 299	CA C	LYS A			-11.893 -13.063	17.916 18.913	1.00 20.21 1.00 20.08	c c
ATOM	300	0	LYS A	208	-49.635	-12.860	20.118	1.00 20.32	0
ATOM ATOM	301 302	CB CG	LYS A			-11.459 -12.512	17.773 17.115	1.00 20.47 1.00 20.38	c c
MOTA	303	CD	LYS A	208	-53.396	-12.222	17.359	1.00 22.10	С
ATOM ATOM	304 305	CE NZ	LYS A			-13.221 -14.607	16.642 17.174	1.00 20.94 1.00 20.34	C N
ATOM	357	N	ARG A		-43.344	-14.515	6.254	1.00 18.42	N
ATOM ATOM	358	CA	ARG A			-13.537	5.651	1.00 18.42	C
ATOM	359 360	C 0	ARG A			-12.820 -12.338	6.745 7.726	1.00 17.97 1.00 19.04	C 0
ATOM	361	СВ	ARG A			-12.525	4.835	1.00 18.99	c
ATOM ATOM	362 363	CG CD	ARG A			-11.489 -10.359	4.100 3.594	1.00 19.30 1.00 20.84	C C
ATOM	364	NE	ARG A	215	-43.854	-9.573	4.697	1.00 20.02	N
ATOM	365	CZ	ARG A		-44.864 -45.467		4.586	1.00 22.74	C
ATOM ATOM	366 367		ARG A		-45.467 -45.282		3.418 5.656	1.00 23.51 1.00 23.60	N N
ATOM	529	N	LYS A	237	-36.427	-19.755	11.099	1.00 18.90	N
ATOM ATOM	530 531	CA C	LYS A			-20.079 -20.086	10.303 8.836	1.00 20.07 1.00 20.62	C C
MOTA	532	0	LYS A		-36.709	-20.607	8.487	1.00 20.15	0
ATOM	533	CB	LYS A			-21.438	10.712	1.00 20.03	C
ATOM ATOM	534 535	CG CD	LYS A			-21.504 -22.819	12.151 12.393	1.00 19.85 1.00 20.64	C C
ATOM	536	CE	LYS A	237	-32.887	-22.927	13.828	1.00 20.64	С
ATOM ATOM	537 538	NZ N	LYS A ARG A			-24.281 -19.483	14.128 7.993	1.00 19.43 1.00 21.63	N N
MOTA	539	CA	ARG A	238	-35.054	-19.421	6.556	1.00 22.74	С
ATOM ATOM	540 541	C 0	ARG A			-20.815 -21.765	5.978 6.321	1.00 23.18 1.00 23.36	C 0
ATOM	542	СВ	ARG A			-18.738	5.842	1.00 23.36	С
ATOM	543 544	CG	ARG A			-18.455	4.367	1.00 24.78	c
ATOM ATOM	544 545	CD NE	ARG A			-17.817 -17.584	3.729 2.305	1.00 29.07 1.00 32.71	C N
ATOM	546	CZ	ARG A	238	-32.328	-16.860	1.525	1.00 33.80	С
ATOM ATOM	547 548		ARG A			-16.265 -16.721	2.028 0.240	1.00 35.30 1.00 34.89	N N
ATOM	598	N	ARG A	246	-36.004	-7.648	-2.381	1.00 24.57	N
ATOM ATOM	599 600	CA C	ARG A		-36.526 -37.988		-1.793 -2.186	1.00 24.09 1.00 23.73	C C
MOTA	601	0	ARG A	246	-38.334		-3.019	1.00 22.92	0
ATOM	602	CB	ARG A		-35.657	-5.200	-2.156	1.00 24.34	С
ATOM ATOM	603 604	CG CD	ARG A		-34.232 -33.359		-1.662 -1.804	1.00 25.49 1.00 25.90	C C
MOTA	605	NE	ARG A	246	-32.020	-4.466	-1.317	1.00 27.00	N
ATOM ATOM	606 607	CZ NH1	ARG A		-31.617 -32.447		-0.057 0.870	1.00 28.42 1.00 27.71	C N
ATOM	608		ARG A		-30.378		0.281	1.00 29.27	N.
_	_		_	_					

### Q12)

#### **Output-**

```
A@BhavyaSharma: ~/lab_session_3$ sed 's/LYS/AR

PEPTIDE BINDING PROTEIN 26-MAY-05 1ZT3
C-TERMINAL DOMAIN OF INSULIN-LIKE GROWTH FACTOR BINDING PROTEIN-1
2 ISOLATED FROM HUMAN AMNIOTIC FLUID

MOL_ID: 1;
2 MOLECULE: INSULIN-LIKE GROWTH FACTOR BINDING PROTEIN 1;
3 CHAIN: A;
4 FRAGMENT: C-TERMINAL DOMAIN;
5 SYNONYM: IGFBP-1, IBP- 1, IGF-BINDING PROTEIN 1, PLACENTAL PROTEIN
6 12, PP12

MOL_ID: 1;
2 ORGANISM_SCIENTIFIC: HOMO SAPIENS;
3 ORGANISM_COMMON: HUMAN;
4 ORGANISM_COMMON: HUMAN;
4 ORGANISM_TAXID: 9606;
5 OTHER_DETAILS: AMNIOTIC FLUID
INSULIN-LIKE GROWTH FACTOR BINDING PROTEIN-1, IGFBP-1, AMNIOTIC
2 FLUID, C-TERMINAL DOMAIN, METAL-BINDING, PEPTIDE BINDING PROTEIN
X-RAY DIFFRACTION
A.SALA,S.CAPALDI,M.CAMPAGNOLI,B.FAGGION,S.LABO,M.PERDUCA,A.ROMANO,
2 M.E.CARRIZO,M.VALLI,L.VISAI,L.MINCHIOTTI,M.GALLIANO,H.L.MONACO
5 16-OCT-24 1ZT3 1 REMARK
4 11-OCT-17 1ZT3 1 REMARK
3 24-FEB-09 1ZT3 1 VERSN
2 30-AUG-05 1ZT3 0 JRNL
1 28-JUN-05 1ZT3 0
AUTH A.SALA,S.CAPALDI,M.CAMPAGNOLI,B.FAGGION,S.LABO,M.PERDUCA,
AUTH 2 A.ROMANO,M.E.CARRIZO,M.VALLI,L.VISAI,L.MINCHIOTTI.
                                                                                                                                                                                                                                                                                                                                                                                                                                                               3$ sed 's/LYS/ARG/g' protein.pdb
   bhavya@BhavyaSharma:~/lab_session
HEADER
TITLE
TITLE
COMPND
   COMPND
COMPND
     COMPND
   COMPND
 SOURCE
SOURCE
   SOURCE
SOURCE
SOURCE
KEYWDS
   KEYWDS
EXPDTA
   AUTHOR
AUTHOR
AUTHOR
REVDAT
REVDAT
REVDAT
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REVDAT
                                                                                                  AUTH A.SALA,S.CAPALDI,M.CAMPAGNOLI,B.FAGGION,S.LABO,M.PERDUCA,
AUTH 2 A.ROMANO,M.E.CARRIZO,M.VALLI,L.VISAI,L.MINCHIOTTI,
AUTH 3 M.GALLIANO,H.L.MONACO
TITL STRUCTURE AND PROPERTIES OF THE C-TERMINAL DOMAIN OF
TITL 2 INSULIN-LIKE GROWTH FACTOR-BINDING PROTEIN-1 ISOLATED FROM
TITL 3 HUMAN AMNIOTIC FLUID
   JRNL
   JRNL
JRNL
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      JRNL
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DOI
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2 RESOLUTION.
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REMARK
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                                                                          3 REFINEMENT.
3 PROGRAM
3 AUTHORS
REMARK
REMARK
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: MURSHUDOV, SKUBAK, LEBEDEV, PANNU, STEINER
 REMARK
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                                                                                                                                       TRP A 172
ARG A 173
ARG A 175
FRO A 175
                                                                                                                                                                                                                                                           -39.136 -2.997
-40.108 -26.997
-41.403 -21.965
-41.385 -21.496
-39.506 -19.534
-38.161 -19.292
-37.773 -19.568
-37.032 -18.693
-36.465 -19.196
-35.985 -18.650
-36.799 -18.192
-34.725 -18.128
-35.545 -17.671
-34.523 -17.646
-42.516 -20.697
-43.842 -20.728
-44.928 -19.604
-44.831 -19.725
-44.935 -20.648
-49.883 -20.189
-43.280 -18.518
-43.337 -17.366
-41.922 -17.014
-41.381 -15.977
-43.933 -16.148
-45.777 -15.061
-46.102 -14.001
-45.756 -15.182
-41.313 -17.867
-39.891 -17.705
-39.565 -16.385
-38.520 -15.781
-39.594 -18.893
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ATOM
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29.656
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29.6566
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29.656
29.6
MOTA
MOTA
 MOTA
MOTA
 MOTA
MOTA
MOTA
                                                                                                         MOTA
MOTA
 ATOM
ATOM
 MOTA
MOTA
MOTA
 ATOM
ATOM
 ATOM
ATOM
                                                                                                                                                                                                                                                                                                                                                                                                                                                                           1.00 32.89
1.00 33.96
1.00 24.66
1.00 25.76
1.00 25.76
1.00 23.23
1.00 25.76
1.00 26.89
1.00 27.42
1.00 29.42
1.00 30.63
 MOTA
MOTA
 ATOM
ATOM
   ATOM
 MOTA
MOTA
 ATOM
ATOM
   MOTA
MOTA
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              .00
.00
.00
.00
 MOTA
MOTA
MOTA
MOTA
MOTA
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      21.
20.
18.
                                                                                                        N
CA
C
CB
CG
CD
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                58
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  18
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      20
19
21
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                52
                                                                                                                                                                                                                                                                -40.909
-41.896
                                                                                                                                                                                                                                                                                                                                    -19.247
-19.015
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                00
00
```

(Replaced every occurrence of LYS with ARG in protein.pdb. The output was quite large, so I'm pasting this snippet here to avoid taking up too much space.)

# Q13)

# Output-

bhavya@BhavyaSharma:~/lab\_session\_3\$ awk '/^ATOM/ {print \$9}' protein.pdb

24.415 24.729 23.944 22.789 24.418 25.025 26.306 24.384 26.497 25.334 23.097 25.037 22.802 23.769 24.576 23.949 22.914 21.976 25.024 24.519 25.479 24.901 25.806 23.090 22.191 21.728 22.138 22.913 23.359 24.206 23.639 25.445 20.872 20.564 19.866

(Printed only the z-coordinate (third number in coordinates) for each atom from protein.pdb. The output was quite large, so I'm pasting this snippet here to avoid taking up too much space.)

# Q14)

20.142 19.632

# **Output-**

bhavya@BhavyaSharma:~/lab\_session\_3\$ awk '/GLY/ {count++} END {print count}' protein.pdb 33

## Q15)

# **Output-**

```
$4=="GLY")' protein.pdb
                                                                                                                                 && ($4=="ALA"
                                                                 -29.906
-24.689
-19.179
-45.353
                                                                                                                               19.62
20.13
ATOM
ATOM
ATOM
                                    ALA
                           CA
CA
CA
CA
CA
CA
CA
                                                188
                                            A A A A A A A A
                                                                                                                                                                  0000000000
                 157
                                    ALA
                                                190
                                                195
210
223
225
                                   GLY
                 193
315
                                                                                      3.890
                                                                                                     13.965
                                                                                                                     1.00
1.00
1.00
1.00
1.00
1.00
                                                                                                                                34.45
18.56
ATOM
ATOM
                                                                                                     19.536
                                                                                  -14.753
                                                                 -45.353
-36.815
-37.186
-35.705
-37.957
-34.199
-40.259
                 422
435
                                   GLY
ALA
                                                                                   5.170
-1.492
-3.955
                                                                                                                                21.58
20.30
                                                                                                       1.658
ATOM
ATOM
                                                                                                       0.463
                                                226
236
241
247
                                                                                                                               18.85
18.22
28.67
24.01
                                   GLY
GLY
                                                                                                     2.980
12.295
-1.334
                 440
                                                                                  -18.276
-22.463
-7.039
                 526
565
ATOM
                                   GLY
GLY
ATOM
                 610
                                                                                                     -1.851
ATOM
```

# Q16)

#### **Output-**

```
bhavya@BhavyaSharma:~/lab_session_3$ awk '$1=="ATOM" && $12=="C"' protein.pd b | wc -l 401
```

### Q17)

### **Output-**

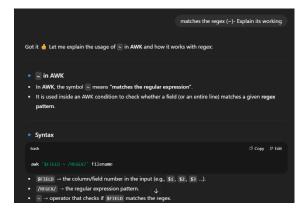
```
| Shanyageshayasharms: -/ Led. 3655301. $ awr /*HelaIm/* protein.pdo | Cherath | G44 C1 DIO A 400 | -29.644 -6.946 | 17.132 | 1.00 36.92 | Cherath | G45 C2 DIO A 400 | -28.8973 | -9.661 | 16.720 | 1.00 36.92 | Cherath | G45 C2 DIO A 400 | -27.687 | -6.281 | 17.202 | 1.00 35.99 | Cherath | G47 C2' DIO A 400 | -26.684 | -8.437 | 16.825 | 1.00 36.68 | Cherath | G49 C1 DIO A 400 | -28.996 | -8.972 | 16.254 | 1.00 36.68 | Cherath | G49 C1 DIO A 400 | -28.996 | -8.972 | 16.254 | 1.00 36.68 | Cherath | G49 C1 DIO A 400 | -28.996 | -8.972 | 16.254 | 1.00 36.28 | Oherath | G50 C1 DIO A 400 | -28.996 | -8.972 | 16.254 | 1.00 36.28 | Oherath | G50 C1 DIO A 400 | -28.996 | -8.972 | 16.254 | 1.00 26.28 | Oherath | G50 C1 DIO A 400 | -28.996 | -8.972 | 16.254 | 1.00 20.36 | Oherath | G50 C1 DIO A 400 | -28.996 | -8.972 | 16.254 | 1.00 20.36 | Oherath | G50 C1 DIO A 400 | -28.996 | -8.972 | 16.254 | 1.00 20.33 | Oherath | G51 C1 DIO A 400 | -38.877 | -3.991 | 4.471 | 1.00 20.33 | Oherath | G52 C1 DIO A 400 | -38.877 | -3.991 | 4.471 | 1.00 20.33 | Oherath | G52 C1 DIO A 400 | -38.877 | -3.991 | 4.471 | 1.00 20.33 | Oherath | G54 C1 DIO A 400 | -44.936 | -13.438 | 1.965 | 1.00 28.30 | Oherath | G55 C1 DIO A 400 | -48.895 | -18.702 | 15.563 | 1.00 28.30 | Oherath | G55 C1 DIO A 400 | -48.895 | -18.702 | 15.563 | 1.00 28.30 | Oherath | G56 C1 DIO A 400 | -48.895 | -18.702 | 15.563 | 1.00 28.30 | Oherath | G56 C1 DIO A 400 | -48.895 | -18.702 | 15.563 | 1.00 29.352 | Oherath | G56 C1 DIO A 400 | -48.895 | -18.702 | 15.563 | 1.00 29.352 | Oherath | G56 C1 DIO A 400 | -48.895 | -18.702 | 15.563 | 1.00 29.352 | Oherath | G56 C1 DIO A 400 | -49.5642 | -11.444 | 19.694 | 1.00 29.80 | Oherath | G56 C1 DIO A 400 | -49.5642 | -11.444 | 19.694 | 1.00 29.80 | Oherath | G56 C1 DIO A 400 | -49.5642 | -11.444 | 19.694 | 1.00 29.80 | Oherath | G56 C1 DIO A 400 | -49.5642 | -11.444 | 19.694 | 1.00 29.80 | Oherath | G56 C1 DIO A 400 | -49.5664 | -49.304 | -49.604 | -49.604 | -49.604 | -49.604 | -49.604 | -49.604 | -49.604 | -49.604 | -49.604 | -
```

# Q18)

# Output-

```
bhavya@BhavyaSharma:~/lab_session_3$ awk '/^ATOM/ {if($4 ~ /E$/) print $4}' protein.pdb
ILE
PHE
ILE
```

# Used ChatGPT-



## Q19)

## **Output-**

```
$ sed '/^TER/d; /^END/d' protein.pdb
bhavya@BhavyaSharma:
HEADER PEPTIDE BI
                    PEPTIDE BINDING PROTEIN
                                                                                                      26-MAY-05
                                                                                                                             1ZT3
                  C-TERMINAL DOMAIN OF INSULIN-LIKE GROWTH FACTOR BINDING PROTEIN-1
2 ISOLATED FROM HUMAN AMNIOTIC FLUID
TITLE
TITLE
                  MOL_ID: 1;
2 MOLECULE: INSULIN-LIKE GROWTH FACTOR BINDING PROTEIN 1;
3 CHAIN: A;
4 FRAGMENT: C-TERMINAL DOMAIN;
COMPND
COMPND
COMPND
COMPND
                                        IGFBP-1, IBP- 1, IGF-BINDING PROTEIN 1, PLACENTAL PROTEIN
COMPND
                 5 SYNONYM: IGFBP-1, IBP- 1, IGF-BINDING PROTEIN 1, PLACENING
6 12, PP12
MOL_ID: 1;
2 ORGANISM_SCIENTIFIC: HOMO SAPIENS;
3 ORGANISM_COMMON: HUMAN;
4 ORGANISM_TAXID: 9606;
5 OTHER_DETAILS: AMNIOTIC FLUID
INSULIN-LIKE GROWTH FACTOR BINDING PROTEIN-1, IGFBP-1, AMNIOTIC
2 FLUID, C-TERMINAL DOMAIN, METAL-BINDING, PEPTIDE BINDING PROTEIN
X-RAY DIFFRACTION
A.SALA,S.CAPALDI,M.CAMPAGNOLI,B.FAGGION,S.LABO,M.PERDUCA,A.ROMANO,
2 M.E.CARRIZO,M.VALLI,L.VISAI,L.MINCHIOTTI,M.GALLIANO,H.L.MONACO
5 16-OCT-24 1ZT3 1 REMARK
                   5 SYNONYM:
COMPND
SOURCE
SOURCE
SOURCE
SOURCE
SOURCE
KEYWDS
KEYWDS
EXPDTA
AUTHOR
AUTHOR
                          16-0CT-24 1ZT3
11-0CT-17 1ZT3
REVDAT
REVDAT
                                                                               REMARK
                          24-FEB-09 1ZT3
                                                                               VERSN
REVDAT
                                                               1
                          30-AUG-05 1ZT3
REVDAT
                                                               1
                                                                               JRNI
                       30-AUG-05 1ZT3 1 JRNL
28-JUN-05 1ZT3 0
AUTH A.SALA,S.CAPALDI,M.CAMPAGNOLI,B.FAGGION,S.LABO,M.PERDUCA,
AUTH 2 A.ROMANO,M.E.CARRIZO,M.VALLI,L.VISAI,L.MINCHIOTTI,
AUTH 3 M.GALLIANO,H.L.MONACO
TITL STRUCTURE AND PROPERTIES OF THE C-TERMINAL DOMAIN OF
TITL 2 INSULIN-LIKE GROWTH FACTOR-BINDING PROTEIN-1 ISOLATED FROM
TITL 3 HUMAN AMNIOTIC FLUID

DEE 1 BIOL CHEM V 280 20812 2005
REVDAT
JRNL
JRNL
JRNL
JRNL
JRNL
JRNL
JRNL
                        REF
                                      J.BIOL.CHEM.
                                                                                                   V. 280 29812 2005
                        REFN
                                                                       ISSN 0021-9258
JRNL
JRNL
                        PMID
                                       15972819
                                      10.1074/JBC.M504304200
 JRNL
                        DOI
REMARK
REMARK
                      RESOLUTION.
                                                     1.80 ANGSTROMS.
REMARK
REMARK
                   3 REFINEMENT.
                                                   : REFMAC 5.2.0005
: MURSHUDOV, SKUBAK, LEBEDEV, PANNU, STEINER,
REMARK
                          PROGRAM
                          AUTHORS
REMARK
```

(Deleted all the lines that contain TER or END from protein.pdb. The output was quite large so pasting this snippet here to avoid taking up too much space.)

# Q20) Output-

```
- ARG"' protein.pdb
                                                          vk '/^ATOM/ && $4!="ARG"'
−21.997 24.415 1.00 <u>3</u>4
                                                on_3$ awk
-39.136 -:
ATOM
                          TRP A
                                                                                                                   \mathbf{N}
                                                                                      .00 34.28
ATOM
                   CA
                          TRP
                                  172
                                               -40.108
                                                          -20.907
                                                                        24.729
MOTA
                          TRP
                                  172
                                               -41.403
                                                          -21.065
                                                                        23.944
                                                                                      .00
ATOM
                   0
                          TRP A
                                  172
                                               -41.385
                                                          -21.496
                                                                        22.789
                                                                                    1.00
ATOM
               5
                   СВ
                         TRP
                                  172
                                               -39.506
                                                          -19.534
                                                                        24.418
                                                                                      .00
                                               -38.161 -19.292
-37.773 -19.568
MOTA
                   CG
                          TRP
                               A 172
                                                                        25.025
                                                                                    1.00
                                                                                           36.34
                                              -37.773
-37.032
ATOM
                   CD1
                         TRP
                                  172
                                                                        26.306
                                                                                      . 00
                                                                                           37.69
ATOM
                   CD2
                         TRP A 172
                                                          -18.693
                                                                        24.384
                                                                                      .00
                                                                                           37.47
ATOM
                   NE1
                          TRP
                                  172
                                               -36.465
                                                          -19.190
                                                                        26.497
                                                                                       . 00
                                                                                           37.97
             10
11
12
13
14
15
16
17
18
19
20
21
22
23
24
25
ATOM
                   CE2
                          TRP
                                               -35.985 -18.650
                                                                        25.334
                                                                                      . 00
                                                                                           37.83
                                              -36.799 -18.192
-34.725 -18.128
-35.545 -17.674
-34.523 -17.646
                                  172
ATOM
                   CE3
                         TRP
                                                                        23.097
                                                                                      . 00
                                                                                           37.57
                         TRP A 172
                                                                        25.037
                                                                                           37.51
ATOM
                   CZ2
                                                                                      . 00
                   CZ3
                                  172
                                                                                           37.85
ATOM
                          TRP
                                                                        22.802
                                                                                    1.00
                   CH2
                         TRP A 172
ATOM
                                                                        23.769
                                                                                      .00
                                                                                           37.43
                                              -42.516 -20.697
-43.842 -20.728
-44.028 -19.604
                               A 173
A 173
                                                                        24.576
23.949
                   N
CA
ATOM
                         LYS
                                                                                    1.00
                                                                                           32.18
                                                                                       .00 31.37
.00 29.85
.00 30.15
ATOM
                                                                                      . 00
                         LYS
                         LYS A 173
                                                                        22.914
                                                                                    1.00
ATOM
                   C CB CCD CE NZ N CA
                                              -44.831 -19.725
-44.935 -20.645
-46.343 -20.964
-47.425 -20.459
                                                                        21.976
                         LYS A 173
ATOM
                         LYS A 173
ATOM
                                                                        25.024
                                                                                    1.00
                                                                                           31.31
ATOM
                         LYS A 173
                                                                        24.519
                                                                                      . 00
                                                                                           32.53
                                                                        25.479
                         LYS
                                  173
                                                                                    1.00
ATOM
                                                                                           32.89
                                              -48.818 -20.684
-49.893 -20.189
-43.280 -18.518
-43.337 -17.364
                                                                        24.901
                                                                                       . 00
                               A 173
ATOM
                         LYS
                                                                                           33.96
                         LYS A 173
GLU A 174
GLU A 174
ATOM
                                                                        25.806
                                                                                    1.00 34.66
ATOM
                                                                        23.090
                                                                                    1.00 27.67
                                                                                    1.00 25.77
1.00 23.54
ATOM
                                                                        22.191
                         GLU A 174
GLU A 174
GLU A 174
GLU A 174
                                                          -17.014
ATOM
             26
27
28
29
30
31
32
33
34
35
                                               -41.922
                                                                        21.728
                   O
CB
CG
                                               -41.381 -15.977
ATOM
                                                                        22.138
                                                                                    1.00 23.23
                                              -43.933 -16.148
-45.376 -16.258
ATOM
                                                                        22.913
                                                                                    1.00 25.76
ATOM
                                                                                    1.00
                                                                                           26.89
                                                                        23.359
                   CD
OE1
                                              -45.777 -15.061
-46.102 -14.001
ATOM
ATOM
ATOM
                         GLU A 174
GLU A 174
                                                                        24.206
                                                                                    1.00 27.42
                                                                                    1.00
                                                                        23.639
                                                                                           29.42
                   0E2
                         GLU A 174
PRO A 175
                                              -45.756
-41.313
                                                          -15.182
-17.867
                                                                        25.445
                                                                                    1.00
                                                                                           30.63
ATOM
ATOM
ATOM
ATOM
ATOM
                   N
CA
                         PRO
                                                                        20.872
                                                                                    1.00
                                                                                           21.55
                                              -39.891
-39.565
                         PRO A
                                                          -17.705
-16.385
                                                                                    1.00
                                                                                           20.10
18.58
                                  175
                                                                        20.564
                                                                        19.866
                                                                                    1.00
                                  175
             36
37
                   ō
                                               -38.520
                                                          -15.781
-18.893
                         PRO A
                                  175
                                                                                    1.00
                                                                                           18.18
20.52
                                                                        20.142
                         PRO A
                   СВ
                                               -39.594
                                                                        19.632
                                  175
                                                                                    1.00
                                                                                           19.77
ATOM
             38
                   CG
                                  175
                                               -40.909
                                                          -19.247
                                                                        19.043
                                                                                    1.00
```

(From protein.pdb, printed only the ATOM lines that do not belong to residue ARG. The output was quite large, so I'm pasting this snippet here to avoid taking up too much space.)

# Q21) Output-

```
3$ awk '/^ATOM/ && $5 == "A"
bhavya@BhavyaSharma:~/
                                                                  {residue[$4]+
+} END {for (r in residue) {print r, residue[r]}}' protein.pdb
GLY 28
CYS 37
LEU 32
THR 14
GLN 18
PRO 42
ILE 32
MET
    8
ASN 40
TYR 48
LYS 45
ASP 16
SER 36
PHE 22
HIS 10
GLU 81
ARG 55
TRP 42
ALA 15
VAL
    21
```

### Q22)

# **Output-**

```
bhavya@BhavyaSharma:~/lab_session_3$ awk '/^ATOM/ {print $3 "," $4 "," $5}' protein.pdb
N,TRP,A
C,TRP,A
C,TRP,A
C,TRP,A
CG,TRP,A
CG,TRP,A
CD1,TRP,A
CD2,TRP,A
NE1,TRP,A
CE2,TRP,A
CE3,TRP,A
CZ3,TRP,A
CZ3,TRP,A
CZ4,TRP,A
CZ5,TRP,A
CZ5,TRP,A
CZ5,TRP,A
CZ5,TRP,A
CZ5,TRP,A
CZ5,TRP,A
CZ6,TRP,A
CZ7,TRP,A
CZ7,TRP,
```

From protein.pdb, printed only the atom name, residue name, and chain ID, separated by commas. The output was quite large, so I pasted this snippet here to avoid taking up too much space.)

```
3$ sed 's/[a-z]/\U&/g' protein.fasta
>SEQ1|HOMO_SAPIENS|CLOCK_PROTEIN
MTEYKLVVVGAGCCGKSALTIQLINHFGFVDEYDPTIEDSYRKQVVIDGETCLLDILDTAG
>SEQ2|MUS_MUSCULUS|PER_PROTEIN
MSDDEEVQPSLLTKDGRVLQVLQSLFFGKNSDQLQSLENQLQDLLTAAQNNYSSST
>SEQ3|DROSOPHILA_MELANOGASTER|TIM_PROTEIN
MADOLTEEQIAEFKEAFSLFDKDGDGTCCTKELGTVMRSCCONPTEAELODMINEVDADGNGO
>SEQ4|DANIO_RERIO|BMAL_PROTEIN
MLSRAVCGTSGTGKSTLSRIIAQYFKKTDVVLVGPSGAGKTTISKLLEQLDYLNQKNV
>SEQ5|ARABIDOPSIS_THALIANA|LHY_PROTEIN
MSEQNGVVVDDGSIKVLVTGNKCDPQQRVTSQPVLQAGLDRIFGVIRDLGGSSS
>SEQ6|SACCHAROMYCES_CEREVISIAE|CYC_PROTEIN
MTEYKLVVVGDVGKSTIVKQMQNHFVDEYDPTIEDSYRKQVVIDGETCLLDILDTAG
>SEQ7|CAENORHABDITIS_ELEGANS|CLK_PROTEIN
MADŠORRLLONVINKAAGKSSTLLPVDGDKILVVTTGGQVVQSNVLEAMKELLO
>SEQ8|GALLUS_GALLUS|CRY_PROTEIN
MPGSGYVVRAGTVAGQLRIMNNKVVVVGDLGAGKTTLLQSVIEMLKLLGEKGTA
>SEQ9|ESCHERICHIA_COLI|RECA_PROTEIN
MNVOLKKOLKDLPGVIVLGPPGAGKGTOFVSYVLNOLPOYLKKIDVYRTKGF
>SEQ10|XENOPUS_LAEVIS|REV-ERB_PROTEIN
MADEEKLPPGWEKRMSRSSGRVYYFNHITNASQWERPSGNSSSGSLS
```

#### Q23)

#### **Output-**

For this question, I took the help of Gemini AI to understand the logic behind this problem-Prompt given-

Explain me the logic as to how to solve this problem in concise manner and don't write code- Find the sequence(s) in protein.fasta with the maximum length.

### Output-

To find the longest sequence in a FASTA file, you can follow a straightforward logic that processes the file step by step.

#### Step 1: Initialize Variables

First, you'll need two variables: one to keep track of the maximum length found so far (let's call it max\_len) and another to store the current sequence being built (current\_sequence).
Initialize max\_len to zero.

#### Step 2: Read the File Line by Line

Iterate through the <u>protein.fasta</u> file, processing one line at a time. The key is to distinguish between **header lines** (which start with ) and **sequence lines** (which contain the actual protein sequence).

#### Step 3: Handle Header and Sequence Lines

- · When you encounter a new header line:
  - · This signals the end of the previous sequence.
  - Calculate the length of the current\_sequence.
  - Compare this length to max\_len
     miss\_len

     with the new length
     and save the header and sequence. If the length is equal, you should save this new
     sequence as well, as there might be multiple sequences with the same maximum length.
  - After the comparison, reset the current\_sequence variable to an empty string to start building the next sequence.
- When you encounter a sequence line:
  - Simply append this line of text to the current sequence variable.

#### Step 4: Final Check

After the entire file has been read, perform one last check. The logic in Step 3 only checks the length of a sequence when it encounters the *next* header. Therefore, the very last sequence in the file would not have been checked. Compare the length of this final sequence with max\_len and update if necessary.

#### Step 5: Print the Result

Finally, print the header(s) and sequence(s) that correspond to the final max\_len value.

### The code that I wrote and got the output is as follows-

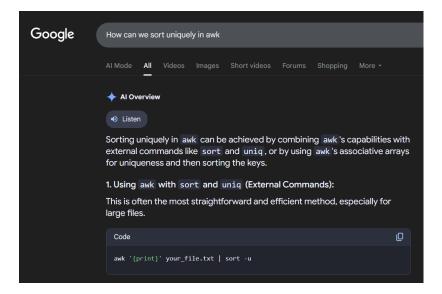
```
bhavya@BhavyaSharma:~/lab_session_3$ awk 'BEGIN {maximum_len=0} /^>/ {
if (length(sequence) > maximum_len) {maximum_len = length(sequence); m
aximum_header = header; maximum_sequence = sequence;} header = $0; seq
uence = ""; next;} {sequence=sequence $0;} END {print maximum_header;
print maximum_sequence;}' protein.fasta
>seq3|Drosophila_melanogaster|TIM_protein
MADQLTEEQIAEFKEAFSLFDKDGDGTCCTKELGTVMRSCCQNPTEAELQDMINEVDADGNGQ
```

# Q24) Output-

```
bhavya@BhavyaSharma:~/lab_session_3$ awk '/^ATOM/ {print$4}' protein.p
db | sort -u
ALA
ARG
ASN
ASP
CYS
GLN
GLU
GLY
HIS
ILE
LEU
LYS
MET
PHE
PRO
SER
THR
TRP
TYR
VAL
```

In this question, I used a Google search to understand how to sort uniquely in awk.

This is the output I got-



### Q25)

#### Output-

```
bhavya@BhavyaSharma:~/lab_session_3$ awk '/^ATOM/ {print$5}' protein.p
db | sort -u | wc -l
1
```

# **Q26)**

# Output-

```
bhavya@BhavyaSharma:~/lab_session_3$ awk '/^>/{ next } {sequence=seque
nce $0} END {countofA=0;countofT=0;countofG=0;countofC=0;for(i=1;i<=le
ngth(sequence); i++){nuc=substr(sequence,i,1);if(nuc=="A"){countofA++}
else if(nuc=="T"){countofT++}else if(nuc=="G"){countofG++}else if(nuc
=="C"){countofC++}}; print "Frequencies of nucleotides";print "A:" cou
ntofA;print"T:" countofT;print "G:" countofG;print "C:" countofC}' clo
ck_gene.fastae.fasta
Frequencies of nucleotides
A:114
T:100
G:355
C:201</pre>
```