

Indian Institute of Technology Gandhinagar

BE623 Biocomputing

Sem1 2025-2026

Lab Assignment -3

Text processing (sed and awk)

1. Create a file with some text written every alternate line using vi. Now delete all empty lines from file using sed (Hint use wildcards for beginning and end of lines)

- Using the same file created above, add line numbers in front of each line and save in another file.

```
My name is Khushi Kamlesh Muttha
khushik@DESKTOP-DE71G03:~/Lab_session3/Lab_assignment3$ awk '{print NR, $0}' lab3.txt > lab3_output.txt
khushik@DESKTOP-DE71G03:~/Lab_session3/Lab_assignment3$ less lab3_output.txt
1 My name is Khushi Kamlesh Muttha
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50 My name is Khushi Kamlesh Muttha
```

3. Print only the header lines from `clock gene.fasta` using sed.

```
khush1@DESKTOP-DE71C03:~/Lab_session3/Lab_assignment3$ less 102_output.xls
>NC_000004.12:c5546909-55427993 Homo sapiens chromosome 4, GRCh38/GRCh38 Primary Assembly
```

4. Print all headers from protein.fasta that contain the word CLOCK.

```
NC_000004.12:c5546903-5547903 Homo sapiens chromosome 4, GRCh38.p14 Primary Assembly  
khush@DESKTOP-DE7103:~/Lab_session3/Lab_assignment3$ awk '/^> / && /CLOCK/{print}' protein.fasta  
Homo_sapiens|CLOCK_protein
```

5. Extract sequences from protein.fasta that contain at least two consecutive C's (CC).

```
[kushii@DESKTOP-DE7103 ~]$ awk '/CC/ && !/!/ {print}' protein.fasta
kushii@DESKTOP-DE7103 ~]$ Lab_assignment3$ awk '/CC/ && !/!/ {print}' protein.fasta
MADQLTQEERVQIAFEKSLFKDGGDTCTKELETLGTVRSCCQNPTTEALQOMINEVADNGNQ
kushii@DESKTOP-DE7103 ~]$ Lab_assignment3$
```

6. Count the total number of G's in clock_gene.fasta.

```
[1]: maqdltreeqafkeafslfdrgggtctklegtvirscclqmpaeelqlqmlnevdagngq  
khush@DESKTOP-DE716G03:~/Lab_session3/Lab_assignment3$ awk '{g+=gsub(/G/,"&")} END {print g}' clock_gene.fasta  
356
```

7. Print only lines 5 to 28 from clock_gene.fasta.

8. Print only the sequence ID (without >) from each header in protein.fasta.

```
khush@DESKTOP-DE71003:~/Lab_session3/Lab_assignment3$ awk '/^>/ {sub(>,""); print $1}' protein.fasta
```

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

9. From protein.fasta, extract sequence lines that start with M and end with Q.

```
khushi@DESKTOP-DE71G03:~/Lab_session3/Lab_assignment3$ sed -n '/^M.*Q$/p' protein.fasta  
MAQDLTTEQIAEKFASLFDKGDGTCTKEGLVMTRSQCMPTEAELQDMINEVDAQNGQ  
MAQSDPGLLQHNTAQKGGTLLDPTVQTLTTATCQYQWQVAGLAEKQFQ
```

10. Find the length of each sequence in protein.fasta and print it alongside the sequence ID.

```
hushui@DESKTOP-DE7A603:~/Lab_session3/Lab_assignment3$ awk '/^>/{if(seq_id) print seq_id, seqlen; seq_id=substr($1,2); seqlen=0;next} {seqlen+=length($0)} END {print seq_id, seqlen}' 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|Aradidopsis_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
```

11. Print all ATOM lines from protein.pdb that belong to chain A only.



khushif@DESKTOP-DE7IG03: ~/Lab_session3/Lab_assignment3								
ATOM	27	CG	GLU A 174	-41.381	-15.977	22.138	1.00	23.23
ATOM	28	CD	GLU A 174	-41.381	-15.977	22.138	1.00	23.23
ATOM	29	CG	GLU A 174	-45.376	-16.258	23.359	1.00	26.89
ATOM	30	CD	GLU A 174	-45.777	-15.061	24.206	1.00	27.42
ATOM	31	OEI	GLU A 174	-46.102	-14.001	23.639	1.00	29.42
ATOM	32	OEZ	GLU A 174	-45.759	-15.182	25.445	1.00	30.63
ATOM	33	PRO	A 174	-41.313	-17.867	20.372	1.00	21.55
ATOM	34	CA	PRO A 174	-39.911	-16.886	20.454	1.00	21.99
ATOM	35	C	PRO A 174	-39.565	-16.385	19.866	1.00	18.58
ATOM	36	O	PRO A 174	-38.520	-15.781	20.142	1.00	18.18
ATOM	37	CB	PRO A 174	-39.594	-18.893	19.632	1.00	20.52
ATOM	38	CG	PRO A 174	-40.908	-19.247	19.843	1.00	19.77
ATOM	39	CD	PRO A 174	-41.899	-19.017	20.148	1.00	19.73
ATOM	40	C	PRO A 174	-40.425	-18.542	20.465	1.00	19.73
ATOM	41	CA	CYS A 176	-40.212	-14.710	18.226	1.00	16.80
ATOM	42	C	CYS A 176	-40.222	-13.501	19.159	1.00	16.78
ATOM	43	O	CYS A 176	-39.363	-12.626	19.953	1.00	16.20
ATOM	44	CB	CYS A 176	-41.244	-14.528	17.116	1.00	16.50
ATOM	45	N	ARG A 177	-40.886	-13.006	19.464	1.00	15.40
ATOM	46	CA	ARG A 177	-41.200	-12.569	20.062	1.00	17.53
ATOM	47	C	ARG A 177	-41.351	-12.338	20.984	1.00	18.15
ATOM	48	O	ARG A 177	-40.135	-12.196	21.888	1.00	18.13
ATOM	49	CB	ARG A 177	-39.686	-11.088	22.853	1.00	17.51
ATOM	50	CG	ARG A 177	-42.634	-12.458	21.897	1.00	18.62
ATOM	51	CD	ARG A 177	-42.707	-12.458	21.111	1.00	17.77
ATOM	52	CD	ARG A 177	-44.227	-11.292	23.368	1.00	22.66
ATOM	53	NE	ARG A 177	-44.366	-10.263	24.391	1.00	24.94
ATOM	54	CZ	ARG A 177	-43.848	-10.348	25.616	1.00	25.91
ATOM	55	NH2	ARG A 177	-43.147	-11.413	25.983	1.00	25.04
ATOM	56	NH2	ARG A 177	-44.039	-9.366	26.477	1.00	26.28
ATOM	57	CA	ILE A 178	-39.749	-12.953	21.521	1.00	19.93
ATOM	58	CA	ILE A 178	-38.446	-13.332	23.221	1.00	18.88
ATOM	59	C	ILE A 178	-37.252	-12.846	22.394	1.00	18.95
ATOM	60	O	ILE A 178	-36.563	-11.962	22.843	1.00	19.62
ATOM	61	CB	ILE A 178	-38.154	-14.721	23.862	1.00	18.59
ATOM	62	CD1	ILE A 178	-39.133	-14.728	24.770	1.00	18.59
ATOM	63	CD2	ILE A 178	-36.818	-14.687	24.621	1.00	18.59
ATOM	64	CD1	ILE A 178	-39.754	-14.186	25.865	1.00	20.15
ATOM	65	N	GLU A 179	-37.088	-13.386	21.187	1.00	19.21
ATOM	66	CA	GLU A 179	-35.993	-12.958	20.327	1.00	19.54
ATOM	67	O	GLU A 179	-36.088	-11.449	20.843	1.00	19.29
ATOM	68	O	GLU A 179	-35.070	-12.500	20.814	1.00	19.57
ATOM	69	CB	GLU A 179	-35.908	-13.726	19.920	1.00	19.65
ATOM	70	CG	GLU A 179	-34.670	-13.469	18.245	1.00	21.79
khushif@DESKTOP-DE7IG03: ~/Lab_session3/Lab_assignment3								
ATOM	71	CG	GLU A 179	-35.848	-13.726	19.026	1.00	19.69
ATOM	72	CD	GLU A 179	-34.670	-13.469	18.345	1.00	19.11
ATOM	73	CD	GLU A 179	-34.657	-14.096	16.879	1.00	24.88
ATOM	74	OEI	GLU A 179	-33.547	-14.398	16.389	1.00	26.52
ATOM	75	OEZ	GLU A 179	-35.742	-14.303	16.292	1.00	27.10
ATOM	76	N	LEU A 180	-37.277	-18.979	19.702	1.00	19.29
ATOM	77	CA	LEU A 180	-37.907	-19.560	19.561	1.00	19.70
ATOM	78	C	LEU A 180	-36.979	-19.558	20.588	1.00	19.88
ATOM	79	O	LEU A 180	-36.226	-7.704	20.241	1.00	18.14
ATOM	80	CB	LEU A 180	-38.976	-9.273	19.106	1.00	19.11
ATOM	81	CG	LEU A 180	-39.319	-7.798	18.847	1.00	19.67
ATOM	82	CD1	LEU A 180	-39.518	-7.233	17.640	1.00	19.70
ATOM	83	CD2	LEU A 180	-40.500	-8.549	19.514	1.00	19.74
ATOM	84	N	TYR A 181	-37.358	-8.954	21.751	1.00	19.19
ATOM	85	CA	TYR A 181	-36.842	-8.229	22.914	1.00	19.73
ATOM	86	C	TYR A 181	-35.318	-8.230	22.972	1.00	19.86
ATOM	87	O	TYR A 181	-34.698	-7.175	23.148	1.00	19.98
ATOM	88	CB	TYR A 181	-37.277	-8.170	20.472	1.00	20.49
ATOM	89	CG	TYR A 181	-38.814	-8.123	24.527	1.00	20.84
ATOM	90	CD1	TYR A 181	-38.915	-7.004	25.358	1.00	21.48
ATOM	91	CD2	TYR A 181	-39.998	-8.645	23.977	1.00	20.81
ATOM	92	CE1	TYR A 181	-40.147	-6.422	25.633	1.00	22.34
ATOM	93	CE2	TYR A 181	-41.239	-8.068	24.264	1.00	21.54
ATOM	94	N	TYR A 181	-40.516	-6.373	20.342	1.00	21.54
ATOM	95	OH	TYR A 181	-42.516	-6.373	25.347	1.00	22.89
ATOM	96	N	ARG A 182	-34.717	-9.486	22.797	1.00	19.68
ATOM	97	CA	ARG A 182	-33.266	-9.544	22.849	1.00	20.85
ATOM	98	C	ARG A 182	-32.593	-8.739	21.743	1.00	19.42
ATOM	99	O	ARG A 182	-31.570	-8.071	21.998	1.00	19.22
ATOM	100	CB	ARG A 182	-32.204	-8.119	21.925	1.00	20.23
ATOM	101	CG	ARG A 182	-33.592	-11.854	23.896	1.00	23.33
ATOM	102	CD	ARG A 182	-32.691	-12.324	24.917	1.00	31.08
ATOM	103	NE	ARG A 182	-32.233	-13.693	24.676	1.00	34.53
ATOM	104	CZ	ARG A 182	-32.728	-14.777	25.285	1.00	36.34
ATOM	105	NH2	ARG A 182	-32.323	-14.686	24.918	1.00	36.34
ATOM	106	N	VAL A 183	-33.164	-8.795	20.537	1.00	37.59
ATOM	107	CA	VAL A 183	-32.586	-8.101	19.374	1.00	18.83
ATOM	108	C	VAL A 183	-32.676	-6.583	19.566	1.00	18.48
ATOM	109	O	VAL A 183	-31.693	-5.875	19.318	1.00	18.13
ATOM	110	CB	VAL A 183	-32.873	-7.606	16.895	1.00	19.78
ATOM	111	CG1	VAL A 183	-32.873	-9.975	17.689	1.00	18.64
ATOM	112	CG2	VAL A 183	-33.822	-6.106	20.034	1.00	18.63
khushif@DESKTOP-DE7IG03: ~/Lab_session3/Lab_assignment3								
ATOM	113	N	VAL A 184	-33.822	-6.106	20.034	1.00	18.63
ATOM	113	CA	VAL A 184	-34.017	-4.667	20.304	1.00	19.03
ATOM	114	C	VAL A 184	-32.987	-4.148	21.338	1.00	19.24
ATOM	115	O	VAL A 184	-32.377	-3.081	21.136	1.00	18.61
ATOM	115	CD	VAL A 184	-35.686	-4.355	20.381	1.00	20.54
ATOM	116	CG1	VAL A 184	-35.686	-4.357	21.114	1.00	20.37
ATOM	117	CG2	VAL A 184	-36.497	-4.486	19.532	1.00	18.87
ATOM	118	N	GLU A 185	-32.767	-4.919	22.395	1.00	19.25
ATOM	119	CA	GLU A 185	-31.799	-4.545	23.423	1.00	20.57
ATOM	120	O	GLU A 185	-30.359	-4.498	22.870	1.00	20.10
ATOM	121	CB	GLU A 185	-31.888	-3.948	23.448	1.00	20.76
ATOM	122	CG	GLU A 185	-30.953	-5.118	25.786	1.00	22.36
ATOM	123	CD	GLU A 185	-31.033	-6.061	26.975	1.00	22.88
ATOM	124	OEI	GLU A 185	-31.853	-7.002	26.951	1.00	27.18
ATOM	127	OEZ	GLU A 185	-32.273	-5.892	27.948	1.00	24.24
ATOM	128	N	SER A 186	-39.593	-5.917	23.139	1.00	19.34
ATOM	129	CA	SER A 186	-28.627	-5.563	21.588	1.00	20.82
ATOM	130	C	SER A 186	-28.397	-4.432	20.505	1.00	19.66
ATOM	131	O	SER A 186	-27.329	-3.816	20.487	1.00	18.81
ATOM	132	CB	SER A 186	-28.373	-6.999	20.838	1.00	20.39
ATOM	133	Og	SER A 186	-28.466	-6.171	23.162	1.00	19.21
ATOM	134	CG	LEU A 187	-29.406	-4.171	19.676	1.00	19.62
ATOM	135	CA	LEU A 187	-29.344	-3.078	18.706	1.00	19.74
ATOM	136	C	LEU A 187	-29.183	-1.718	19.393	1.00	19.37
ATOM	137	O	LEU A 187	-28.363	-0.985	18.973	1.00	19.34
ATOM	138	CB	LEU A 187	-30.593	-3.049	17.833	1.00	19.81
ATOM	139	CD	LEU A 187	-30.593	-3.969	18.210	1.00	21.81
ATOM	140	CD1	LEU A 187	-32.032	-3.091	16.973	1.00	24.65
ATOM	142	N	ALA A 187	-29.985	-1.499	20.431	1.00	19.16
ATOM	143	CA	ALA A 187	-29.908	-0.273	21.249	1.00	19.62
ATOM	144	C	ALA A 187	-28.455	-0.125	21.798	1.00	19.76
ATOM	145	O	ALA A 187	-27.877	-0.568	21.798	1.00	19.76
ATOM	146	CB	ALA A 187	-30.914	-0.334	22.398	1.00	19.86
ATOM	147	N	LYS A 188	-27.943	-1.219	22.313	1.00	19.72
ATOM	148	CA	LYS A 188	-26.592	-1.220	22.859	1.00	19.83
ATOM	149	C	LYS A 188	-25.535	-0.931	21.783	1.00	20.51
ATOM	150	O	LYS A 188	-25.537	-0.931	22.040	1.00	19.94
ATOM	151	CB	LYS A 1					

	khushiiDESKTOP-DETFCG3	\lab_resin\glu\glu_assignments3					
ATOM	155 NZ LYS A 189	-23.673	1.401	27.284	1.00	25.98	N
ATOM	156 N ALA A 190	-25.651	-1.581	20.618	1.00	19.73	N
ATOM	157 CA ALA A 190	-24.689	-1.482	19.528	1.00	20.13	C
ATOM	158 C ALA A 190	-24.697	0.933	19.811	1.00	20.31	C
ATOM	159 O ALA A 190	-23.819	0.931	19.812	1.00	20.40	O
ATOM	160 CB GLN A 189	-24.972	-2.378	18.386	1.00	20.81	C
ATOM	161 N GLN A 189	-25.879	0.633	18.973	1.00	20.86	N
ATOM	162 CA GLN A 189	-26.024	2.804	18.459	1.00	22.02	C
ATOM	163 O GLN A 189	-25.233	3.828	19.288	1.00	21.64	O
ATOM	164 D GLU A 190	-24.750	4.904	19.777	1.00	21.77	O
ATOM	165 CB GLN A 191	-27.500	2.393	18.374	1.00	22.25	C
ATOM	166 CG GLN A 191	-28.199	1.933	17.086	1.00	25.97	C
ATOM	167 CD GLN A 191	-27.735	2.695	15.851	1.00	30.74	C
ATOM	168 OE1 GLN A 191	-28.111	3.853	15.635	1.00	33.63	O
ATOM	169 NE2 GLN A 191	-28.153	2.805	15.635	1.00	32.92	N
ATOM	170 CA GLU A 192	-25.451	2.742	20.577	1.00	21.46	C
ATOM	171 C GLU A 192	-24.277	3.615	21.482	1.00	21.62	N
ATOM	172 G GLU A 192	-22.849	3.877	20.973	1.00	21.84	C
ATOM	173 T GLU A 192	-22.456	5.034	21.837	1.00	20.87	O
ATOM	174 CB GLU A 192	-24.256	3.934	20.592	1.00	21.14	C
ATOM	175 CG GLU A 192	-25.645	2.977	23.531	1.00	21.99	C
ATOM	176 CD GLU A 192	-25.689	2.475	24.965	1.00	22.37	C
ATOM	177 OE1 GLU A 192	-24.668	1.996	25.496	1.00	22.90	O
ATOM	178 OE2 GLU A 192	-26.209	2.526	25.496	1.00	22.93	O
ATOM	179 B THR A 193	-22.217	2.432	20.459	1.00	22.20	N
ATOM	180 CA THR A 193	-26.820	2.918	20.040	1.00	23.10	C
ATOM	181 C THR A 193	-28.673	2.774	18.526	1.00	24.43	C
ATOM	182 D THR A 193	-19.506	2.654	18.023	1.00	23.91	O
ATOM	183 E THR A 193	-26.820	1.479	18.023	1.00	23.11	O
ATOM	184 OG1 THR A 193	-20.622	0.538	20.378	1.00	22.12	O
ATOM	185 CG2 THR A 193	-19.949	1.957	22.207	1.00	22.37	C
ATOM	186 N SER A 194	-21.792	2.789	17.886	1.00	26.17	N
ATOM	187 CA SER A 194	-21.785	2.582	16.374	1.00	28.66	C
ATOM	188 C SER A 194	-20.347	3.552	16.377	1.00	28.53	C
ATOM	189 O SER A 194	-21.196	4.739	15.764	1.00	30.63	O
ATOM	190 CB SER A 194	-23.206	2.411	15.808	1.00	28.78	C
ATOM	191 OG SER A 194	-23.179	2.859	14.427	1.00	29.52	O
ATOM	192 H1 GLY A 195	-26.043	3.845	14.791	1.00	32.35	N
ATOM	193 CA GLY A 195	-17.879	3.908	14.795	1.00	32.45	C
ATOM	194 C GLY A 195	-19.806	4.288	12.636	1.00	36.12	C
ATOM	195 O GLY A 195	-19.172	4.964	11.819	1.00	36.57	O
ATOM	196 N GLU A 196	-21.844	3.837	12.413	1.00	37.26	N
ATOM	197 CA GLU A 196	-21.892	4.225	11.232	1.00	38.38	C
ATOM	198 C GLU A 196	-23.273	4.538	11.614	1.00	38.59	C

Atom Data												
ATOM	384	CA	CYS A 206	-43.624	-11.632	18.186	1.00	17.83	C			
ATOM	385	CB	CYS A 206	-44.518	-11.639	18.845	1.00	18.36	O			
ATOM	286	O	CYS A 206	-45.623	-10.361	14.652	1.00	18.35	O			
ATOM	287	CB	CYS A 206	-43.376	-11.456	16.612	1.00	17.73	C			
ATOM	288	SG	CYS A 206	-41.659	-11.522	17.121	1.00	17.34	S			
ATOM	289	N	CYS A 206	-45.763	-11.527	17.121	1.00	17.34	N			
ATOM	290	CA	ASN A 207	-47.282	-12.593	14.923	1.00	18.73	C			
ATOM	291	C	ASN A 207	-47.713	-12.386	16.381	1.00	19.14	C			
ATOM	292	O	ASN A 207	-46.874	-12.491	17.293	1.00	19.85	O			
ATOM	293	CB	ASN A 207	-47.931	-13.841	16.271	1.00	18.13	C			
ATOM	294	CG	ASN A 207	-47.909	-13.847	16.293	1.00	18.66	C			
ATOM	295	OD1	ASN A 207	-47.549	-15.180	16.254	1.00	18.06	O			
ATOM	296	ND2	ASN A 207	-47.442	-16.236	14.278	1.00	19.03	N			
ATOM	297	N	LYS A 208	-49.812	-12.189	16.598	1.00	19.70	N			
ATOM	298	CA	LYS A 208	-49.849	-12.189	16.598	1.00	19.71	C			
ATOM	299	C	LYS A 208	-49.491	-13.063	16.513	1.00	20.08	C			
ATOM	300	O	LYS A 208	-49.633	-12.865	20.118	1.00	20.32	O			
ATOM	301	CB	LYS A 208	-51.043	-11.459	17.773	1.00	20.47	C			
ATOM	302	CG	LYS A 208	-51.938	-11.521	17.131	1.00	20.18	C			
ATOM	303	CD	LYS A 208	-53.096	-12.312	17.559	1.00	20.10	C			
ATOM	304	CE	LYS A 208	-54.292	-13.221	16.642	1.00	20.94	C			
ATOM	305	NZ	LYS A 208	-54.187	-14.667	17.174	1.00	20.34	N			
ATOM	306	N	ASN A 209	-49.280	-14.275	18.399	1.00	19.57	N			
ATOM	307	CA	ASN A 209	-49.097	-14.275	18.399	1.00	19.58	O			
ATOM	308	C	ASN A 209	-47.633	-15.638	19.679	1.00	19.32	C			
ATOM	309	O	ASN A 209	-47.303	-16.579	20.421	1.00	19.64	O			
ATOM	310	CB	ASN A 209	-49.550	-16.730	18.508	1.00	19.75	C			
ATOM	311	CG	ASN A 209	-50.407	-16.664	18.607	1.00	19.73	C			
ATOM	312	CD1	ASN A 209	-50.811	-16.838	18.608	1.00	19.95	O			
ATOM	313	ND2	ASN A 209	-51.778	-15.856	18.251	1.00	17.82	N			
ATOM	314	N	GLY A 210	-46.771	-14.739	19.205	1.00	19.30	N			
ATOM	315	CA	GLY A 210	-45.373	-14.753	19.536	1.00	18.83	C			
ATOM	316	C	GLY A 210	-45.373	-14.753	19.536	1.00	18.84	C			
ATOM	317	O	GLY A 210	-43.363	-15.993	19.662	1.00	17.75	O			
ATOM	318	N	PHE A 211	-45.059	-16.258	17.638	1.00	18.35	N			
ATOM	319	CA	PHE A 211	-44.372	-16.984	16.632	1.00	18.84	C			
ATOM	320	C	PHE A 211	-43.852	-16.084	16.632	1.00	18.02	C			
ATOM	321	O	PHE A 211	-44.212	-16.056	15.525	1.00	19.06	O			
ATOM	322	CB	PHE A 211	-45.076	-18.238	16.160	1.00	19.96	C			
ATOM	323	CG	PHE A 211	-44.992	-19.373	17.138	1.00	19.94	C			
ATOM	324	CD1	PHE A 211	-43.851	-20.175	17.187	1.00	20.48	O			
ATOM	325	CE2	PHE A 211	-45.221	-19.757	17.187	1.00	19.75	C			
ATOM	326	CE3	PHE A 211	-43.759	-21.224	18.112	1.00	20.21	C			
ATOM	327	CD2	PHE A 211	-45.933	-20.643	18.976	1.00	21.29	C			

Atom Data												
ATOM	327	CE2	PHE A 211	-45.933	-20.643	18.976	1.00	21.29	C			
ATOM	328	CB	PHE A 211	-44.889	-21.450	19.065	1.00	20.87	C			
ATOM	329	N	PHE A 211	-45.008	-21.450	19.065	1.00	20.87	N			
ATOM	330	CA	TYR A 212	-42.776	-15.643	19.273	1.00	18.09	C			
ATOM	331	C	TYR A 212	-43.769	-15.774	12.184	1.00	18.14	C			
ATOM	332	O	TYR A 212	-44.288	-16.890	11.744	1.00	18.14	O			
ATOM	333	CG	TYR A 212	-41.449	-16.444	12.834	1.00	18.04	C			
ATOM	334	CD1	TYR A 212	-42.212	-16.757	12.834	1.00	18.04	C			
ATOM	335	CD2	TYR A 212	-40.225	-17.467	14.081	1.00	17.30	C			
ATOM	336	CD2	TYR A 212	-39.485	-15.344	13.975	1.00	17.57	C			
ATOM	337	CE1	TYR A 212	-39.221	-17.434	15.777	1.00	18.28	C			
ATOM	338	CE2	TYR A 212	-39.221	-17.434	15.777	1.00	18.28	C			
ATOM	339	OH	TYR A 212	-38.363	-16.344	15.829	1.00	16.70	O			
ATOM	340	OH	TYR A 212	-37.376	-16.282	16.786	1.00	16.15	O			
ATOM	341	N	HIS A 213	-44.028	-14.572	11.673	1.00	17.97	N			
ATOM	342	CA	HIS A 213	-44.678	-14.460	10.366	1.00	18.11	C			
ATOM	343	C	HIS A 213	-44.678	-14.464	10.366	1.00	18.06	C			
ATOM	344	O	HIS A 213	-42.635	-15.316	9.949	1.00	17.33	O			
ATOM	345	CB	HIS A 213	-44.808	-13.085	9.931	1.00	18.71	C			
ATOM	346	CG	HIS A 213	-45.862	-12.251	10.673	1.00	19.72	C			
ATOM	347	CD1	HIS A 213	-47.704	-13.567	10.569	1.00	20.50	N			
ATOM	348	CD2	HIS A 213	-45.784	-11.531	10.498	1.00	20.60	C			
ATOM	349	CE1	HIS A 213	-47.894	-11.761	11.371	1.00	21.53	C			
ATOM	350	NE2	HIS A 213	-47.060	-10.888	11.907	1.00	21.26	N			
ATOM	351	N	SER A 214	-44.533	-15.922	8.481	1.00	17.92	N			
ATOM	352	CA	SER A 214	-44.745	-15.922	8.481	1.00	17.92	C			
ATOM	353	C	SER A 214	-42.899	-15.727	6.548	1.00	18.52	C			
ATOM	354	O	SER A 214	-41.765	-16.093	6.253	1.00	18.58	O			
ATOM	355	CB	SER A 214	-44.839	-17.290	6.356	1.00	19.46	C			
ATOM	356	O	SER A 214	-42.839	-17.290	6.356	1.00	19.46	O			
ATOM	357	CG	ARG A 215	-43.344	-16.515	6.124	1.00	18.42	C			
ATOM	358	CA	ARG A 215	-42.464	-13.537	5.651	1.00	18.42	C			
ATOM	359	C	ARG A 215	-41.666	-12.820	6.745	1.00	17.97	C			
ATOM	360	O	ARG A 215	-42.248	-12.339	7.726	1.00	19.04	O			
ATOM	361	CG	ARG A 215	-42.248	-12.325	7.726	1.00	19.04	C			
ATOM	362	CD	ARG A 215	-42.421	-11.489	4.100	1.00	19.30	C			
ATOM	363	CD	ARG A 215	-43.301	-10.359	3.594	1.00	20.84	C			
ATOM	364	NE	ARG A 215	-43.854	-9.573	4.697	1.00	20.02	N			
ATOM	365	CA	NH1 ARG A 215	-45.467	-8.510	3.418	1.00	23.51	N			
ATOM	366	NH1	ARG A 215	-45.467	-8.510	3.418	1.00	23.51	N			
ATOM	367	NH2	ARG A 215	-45.282	-8.040	5.656	1.00	23.60	N			
ATOM	368	N	GLN A 216	-48.348	-12.761	6.573	1.00	17.58	N			
ATOM	369	CA	GLN A 216	-39.487	-11.936	7.424	1.00	16.83	C			
ATOM	370	C	GLN A 216	-38.810	-10.882	6.577	1.00	16.91	C			

Atom Data												
ATOM	370	C	GLN A 216	-38.810	-10.882	6.577	1.00	16.91	C			
ATOM	371	O	GLN A 216	-38.184	-11.199	5.561	1.00	16.53	O			
ATOM	372	CB	GLN A 216	-38.417	-12.769	8.150	1.00	16.94	C			
ATOM	373	CG	GLN A 216	-38.972	-13.769	9.151	1.00	16.52	C			
ATOM	374	CD1	GLN A 216	-39.502	-12.665	9.150	1.00	16.50	O			
ATOM	375	OE1	GLN A 216	-39.927	-12.452	10.222	1.00	16.64	O			
ATOM	376	NE2	GLN A 216	-40.893	-13.457	10.589	1.00	14.49	N			
ATOM	377	N	CYS A 217	-38.912	-9.625	7.014	1.00	16.94	N			
ATOM	378	CA	CYS A 217	-38.374	-8.526	6.255	1.00	16.94	C			</td

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ATOM	413	N	ASP	A	222	-35.073	4.478	5.418	1.00	20.40
ATOM	414	CA	ASP	A	222	-34.270	5.298	4.588	1.00	20.45
ATOM	415	C	ASP	A	222	-37.272	5.477	3.788	1.00	20.58
ATOM	416	O	ASP	A	222	-34.288	2.277	2.228	1.00	20.57
ATOM	417	CB	ASP	A	222	-32.856	4.725	4.386	1.00	20.76
ATOM	418	CG	ASP	A	222	-32.849	3.279	3.882	1.00	20.93
ATOM	419	OD1	ASP	A	222	-31.774	2.666	3.934	1.00	22.26
ATOM	420	OD2	ASP	A	222	-33.911	2.768	3.445	1.00	21.53
ATOM	421	N	GLY	A	223	-36.125	5.041	2.943	1.00	20.55
ATOM	422	CA	GLY	A	223	-36.815	5.176	1.658	1.00	21.58
ATOM	423	C	GLY	A	223	-36.820	5.181	0.993	1.00	21.57
ATOM	424	O	GLY	A	223	-36.861	4.134	-0.498	1.00	21.96
ATOM	425	N	GLU	A	224	-35.766	3.053	1.141	1.00	21.38
ATOM	426	CA	GLU	A	224	-35.450	1.891	0.324	1.00	21.72
ATOM	427	C	GLU	A	224	-36.126	0.661	0.914	1.00	21.14
ATOM	428	O	GLU	A	224	-36.255	0.536	2.133	1.00	20.93
ATOM	429	CB	GLU	A	224	-33.948	1.673	0.264	1.00	22.89
ATOM	430	CG	GLU	A	224	-33.943	2.076	0.586	1.00	21.77
ATOM	431	CD	GLU	A	224	-31.682	1.620	0.509	1.00	20.43
ATOM	432	OE1	GLU	A	224	-31.287	1.518	0.838	1.00	20.43
ATOM	433	OE2	GLU	A	224	-30.988	3.638	-0.483	1.00	31.11
ATOM	434	N	ALA	A	225	-36.575	-0.234	0.039	1.00	20.59
ATOM	435	CA	ALA	A	225	-37.186	-1.492	0.463	1.00	20.38
ATOM	436	C	ALA	A	225	-36.151	-2.361	1.188	1.00	19.93
ATOM	437	O	ALA	A	225	-35.813	-2.494	0.724	1.00	19.69
ATOM	438	CB	ALA	A	225	-37.123	-2.082	0.920	1.00	20.55
ATOM	439	N	GLY	A	226	-36.537	-1.937	2.327	1.00	19.20
ATOM	440	CA	GLY	A	226	-35.799	-3.955	2.988	1.00	18.85
ATOM	441	C	GLY	A	226	-35.821	-5.315	2.294	1.00	18.42
ATOM	442	O	GLY	A	226	-36.804	-5.578	1.595	1.00	18.31
ATOM	443	N	LEU	A	227	-34.808	-6.166	2.487	1.00	18.11
ATOM	444	CA	LEU	A	227	-34.812	-7.532	1.968	1.00	17.92
ATOM	445	C	LEU	A	227	-37.857	-8.162	2.738	1.00	17.33
ATOM	446	O	LEU	A	227	-36.002	-1.161	3.035	1.00	16.48
ATOM	447	CB	LEU	A	227	-33.431	-8.175	2.139	1.00	18.26
ATOM	448	CG	LEU	A	227	-32.270	-7.657	1.283	1.00	20.78
ATOM	449	CD1	LEU	A	227	-30.917	-8.132	1.816	1.00	23.35
ATOM	450	CD2	LEU	A	227	-32.451	-8.046	-0.194	1.00	21.98
ATOM	451	N	CYS	A	228	-36.584	-9.216	2.037	1.00	16.71
ATOM	452	CA	CYS	A	228	-37.472	-10.166	2.785	1.00	17.38
ATOM	453	C	CYS	A	228	-37.510	-10.000	2.059	1.00	17.41
ATOM	454	O	CYS	A	228	-36.573	-11.806	1.215	1.00	17.14
ATOM	455	CB	CYS	A	228	-38.947	-9.929	2.362	1.00	17.03
ATOM	456	SG	CYS	A	228	-39.619	-8.273	2.708	1.00	16.75

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ATOM	456	SQ	CYS	A	228	-39.619	-8.273	2.708	1.00	18.75
ATOM	457	N	TRP	A	229	-37.214	-17.533	3.178	1.00	17.59
ATOM	458	CA	TRP	A	229	-38.313	-14.754	3.622	1.00	18.01
ATOM	459	C	TRP	A	229	-39.155	-14.171	4.325	1.00	18.74
ATOM	460	O	TRP	A	229	-35.820	-14.414	3.366	1.00	19.05
ATOM	461	CB	TRP	A	229	-35.545	-14.189	4.825	1.00	19.34
ATOM	462	CD1	TRP	A	229	-35.685	-15.100	5.834	1.00	19.36
ATOM	463	CD2	TRP	A	229	-35.086	-12.975	5.446	1.00	19.75
ATOM	465	NE1	TRP	A	229	-35.345	-14.530	7.042	1.00	19.95
ATOM	466	CE2	TRP	A	229	-34.964	-13.230	6.828	1.00	19.97
ATOM	467	CE3	TRP	A	229	-34.763	-11.698	4.953	1.00	19.95
ATOM	468	CZ2	TRP	A	229	-34.324	-10.728	7.739	1.00	20.31
ATOM	469	CZ3	TRP	A	229	-34.228	-11.088	5.508	1.00	19.98
ATOM	470	CH2	TRP	A	229	-38.301	-16.079	3.454	1.00	18.85
ATOM	471	N	CYS	A	230	-39.332	-16.931	4.016	1.00	18.94
ATOM	472	C	CYS	A	230	-38.794	-17.854	5.106	1.00	18.58
ATOM	474	O	CYS	A	230	-37.736	-18.464	4.946	1.00	18.93
ATOM	475	CB	CYS	A	230	-40.004	-17.763	2.915	1.00	19.33
ATOM	476	SQ	CYS	A	230	-40.630	-16.761	1.539	1.00	21.95
ATOM	477	N	VAL	A	231	-39.537	-17.962	6.269	1.00	18.37
ATOM	478	CA	VAL	A	231	-39.114	-18.795	7.338	1.00	17.92
ATOM	479	C	VAL	A	231	-39.740	-18.700	7.737	1.00	17.70
ATOM	480	O	VAL	A	231	-41.346	-19.646	7.524	1.00	17.73
ATOM	481	CB	VAL	A	231	-39.723	-17.944	8.571	1.00	18.39
ATOM	482	CG1	VAL	A	231	-37.542	-17.099	8.238	1.00	18.20
ATOM	483	CG2	VAL	A	231	-39.946	-17.177	9.121	1.00	18.39
ATOM	484	N	TYR	A	232	-39.826	-20.793	8.525	1.00	18.07
ATOM	485	CA	TYR	A	232	-40.801	-21.624	9.208	1.00	18.02
ATOM	486	C	TYR	A	232	-41.359	-20.832	10.407	1.00	17.80
ATOM	487	O	TYR	A	232	-40.593	-20.347	11.239	1.00	17.24
ATOM	488	CG	TYR	A	232	-39.552	-23.774	8.576	1.00	18.48
ATOM	489	CD1	TYR	A	232	-40.142	-22.912	9.681	1.00	18.50
ATOM	490	CD2	TYR	A	232	-39.552	-23.774	8.570	1.00	18.40
ATOM	491	CE1	TYR	A	232	-40.379	-24.437	7.660	1.00	20.13
ATOM	492	CE2	TYR	A	232	-38.167	-23.966	8.474	1.00	18.40
ATOM	493	CE3	TYR	A	232	-39.841	-25.241	6.655	1.00	19.49
ATOM	494	CD2	TYR	A	232	-37.447	-24.767	7.459	1.00	19.57
ATOM	495	CG1	TYR	A	232	-38.465	-24.404	6.579	1.00	19.11
ATOM	496	OG	TYR	A	232	-37.038	-26.294	5.150	1.00	18.02
ATOM	497	PRO	A	233	-42.695	-26.681	10.497	1.00	18.03	
ATOM	497	CA	PRO	A	233	-43.253	-19.870	11.598	1.00	17.74
ATOM	498	C	PRO	A	233	-42.902	-20.308	13.024	1.00	17.82
ATOM	499	O	PRO	A	233	-42.882	-19.469	13.932	1.00	17.24
ATOM	500	CB	PRO	A	233	-44.765	-19.946	11.362	1.00	17.97
ATOM	501	CG	PRO	A	233	-44.897	-20.256	9.893	1.00	18.42
ATOM	502	CD	PRO	A	233	-43.750	-21.183	9.666	1.00	18.27
ATOM	503	N	TRP	A	234	-42.624	-21.598	13.224	1.00	17.63
ATOM	504	CA	TRP	A	234	-42.345	-22.098	14.563	1.00	17.85
ATOM	505	C	TRP	A	234	-46.928	-21.830	15.693	1.00	17.77
ATOM	506	O	TRP	A	234	-46.494	-20.664	16.560	1.00	18.60
ATOM	507	CB	TRP	A	234	-42.687	-23.593	14.796	1.00	17.64
ATOM	508	CD1	TRP	A	234	-41.958	-24.497	13.754	1.00	16.96
ATOM	509	CD2	TRP	A	234	-40.786	-25.179	13.983	1.00	17.91
ATOM	510	NE2	TRP	A	234	-42.363	-24.836	12.425	1.00	17.13
ATOM	511	NE1	TRP	A	234	-40.430	-25.996	12.866	1.00	16.95
ATOM	512	CE2	TRP	A	234	-41.387	-25.721	11.899	1.00	17.40
ATOM	513	CE3	TRP	A	234	-43.459	-24.488	11.625	1.00	17.41
ATOM	514	CZ2	TRP	A	234	-41.478	-26.259	10.668	1.00	17.51
ATOM	515	CZ3	TRP	A	234	-43.546	-25.004	16.342	1.00	17.72
ATOM	516	CH2	TRP	A	234	-42.555	-25.887	9.843	1.00	17.50
ATOM	517	N	ASN	A	235	-39.948	-20.584	14.565	1.00	17.27
ATOM	518	CA	ASN	A	235	-38.569	-21.115	14.560	1.00	17.39
ATOM	519	O	ASN	A	235	-37.885	-20.097	13.941	1.00	17.16
ATOM	520	CB	ASN	A	235	-36.793	-19.751	14.367	1.00	16.87
ATOM	521	CG	ASN	A	235	-37.726	-22.587	14.499	1.00	17.29
ATOM	522	CG	ASN	A	235	-37.407	-22.934			

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ATOM	524	CA	GLY A 236	-37.95
ATOM	527	CB	GLY A 236	-18.270
ATOM	528	O	GLY A 236	-35.952
ATOM	529	N	LYS A 237	-36.427
ATOM	530	CA	LYS A 237	-35.253
ATOM	531	C	LYS A 237	-35.652
ATOM	532	O	LYS A 237	-36.799
ATOM	533	CB	LYS A 237	-34.658
ATOM	534	CG	LYS A 237	-34.152
ATOM	535	CD	LYS A 237	-33.395
ATOM	537	CE	LYS A 237	-32.397
ATOM	538	NZ	LYS A 237	-32.303
ATOM	539	ARG A 238	-34.811	
ATOM	540	CA	ARG A 238	-35.854
ATOM	541	C	ARG A 238	-34.588
ATOM	542	CB	ARG A 238	-33.882
ATOM	543	CG	ARG A 238	-34.126
ATOM	544	CD	ARG A 238	-32.999
ATOM	545	NE	ARG A 238	-33.127
ATOM	546	CZ	ARG A 238	-32.372
ATOM	547	NH1	ARG A 238	-34.524
ATOM	548	NH2	ARG A 238	-32.617
ATOM	549	N	TLE A 239	-36.322
ATOM	550	CA	TLE A 239	-36.698
ATOM	551	C	TLE A 239	-35.552
ATOM	552	O	TLE A 239	-35.352
ATOM	553	CB	TLE A 239	-38.055
ATOM	554	CG1	TLE A 239	-39.067
ATOM	555	CG2	TLE A 239	-38.335
ATOM	556	CD1	TLE A 239	-40.562
ATOM	557	N	PRO A 240	-37.047
ATOM	558	CA	PRO A 240	-33.817
ATOM	559	C	PRO A 240	-34.418
ATOM	560	O	PRO A 240	-35.524
ATOM	561	CB	PRO A 240	-33.348
ATOM	562	CG	PRO A 240	-33.668
ATOM	563	CD	PRO A 240	-34.952
ATOM	564	N	GLY A 241	-33.693
ATOM	565	C	GLY A 241	-34.199
ATOM	566	C	GLY A 241	-35.899
ATOM	567	O	GLY A 241	-35.561
ATOM	568	N	SER A 242	-35.406
ATOM	569	CA	SER A 242	-36.237
			-18.270	1.00
			-19.550	19.00
			-17.543	19.00
			-19.755	18.90
			-20.079	20.87
			-20.988	20.62
			-20.687	20.15
			-21.438	20.03
			-21.504	19.85
			-21.594	20.64
			-22.819	20.64
			-22.937	20.64
			-22.601	20.64
			-19.483	21.63
			-19.483	22.74
			-20.815	23.18
			-21.765	23.36
			-21.438	23.15
			-21.504	24.78
			-17.817	29.07
			-17.584	32.71
			-16.866	33.88
			-16.865	34.50
			-16.723	34.89
			-20.928	23.39
			-22.157	24.14
			-22.310	25.20
			-21.499	25.16
			-22.159	25.16
			-21.968	24.06
			-21.450	24.06
			-21.741	23.96
			-23.658	26.67
			-23.482	26.91
			-23.932	27.37
			-25.996	26.80
			-25.369	26.50
			-24.638	26.11
			-22.777	27.81
			-22.463	28.67
			-21.234	29.09
			-20.844	29.78
			-20.645	29.22
			-19.436	28.62

	Type here to search	File	Open	Save	Cut	Paste	Copy	Find	Help	26°C Mostly cloudy	...	21-73	ENG	24-Aug-2025
ATOM	569	CA	SER	A	242	-36.237	-19.436	-0.167	1.00	28.62	C			
ATOM	570	C	SER	A	242	-35.646	-18.301	-0.992	1.00	28.58	C			
ATOM	571	O	SER	A	242	-34.427	-18.089	-0.985	1.00	28.71	C			
ATOM	572	CB	SER	A	242	-36.433	-18.977	1.290	1.00	28.97	C			
ATOM	573	OG	SER	A	242	-36.756	-17.583	1.376	1.00	27.17	O			
ATOM	574	N	PRO	A	243	-36.596	-17.572	-1.722	1.00	28.39	N			
ATOM	575	CA	PRO	A	243	-36.887	-16.359	-2.349	1.00	28.39	C			
ATOM	576	C	PRO	A	243	-36.920	-16.209	-2.309	1.00	28.40	C			
ATOM	577	O	PRO	A	243	-36.725	-15.313	0.164	1.00	27.71	O			
ATOM	578	CB	PRO	A	243	-37.167	-15.904	3.244	1.00	28.46	C			
ATOM	579	CG	PRO	A	243	-38.367	-16.690	-2.761	1.00	28.86	C			
ATOM	580	CD	PRO	A	243	-37.933	-17.828	-2.083	1.00	28.47	C			
ATOM	581	N	GLU	A	244	-34.736	-14.419	-1.613	1.00	27.88	N			
ATOM	582	CA	GLU	A	244	-34.478	-13.212	-0.837	1.00	28.29	C			
ATOM	583	C	GLU	A	244	-34.515	-12.022	-1.795	1.00	27.43	C			
ATOM	584	O	GLU	A	244	-33.628	-11.854	-2.622	1.00	27.85	O			
ATOM	585	CB	GLU	A	244	-33.138	-13.293	-0.106	1.00	28.06	C			
ATOM	586	CG	GLU	A	244	-32.866	-12.110	0.845	1.00	29.84	C			
ATOM	587	CD	GLU	A	244	-31.803	-12.400	1.897	1.00	30.20	C			
ATOM	588	OE1	GLU	A	244	-31.396	-13.572	2.032	1.00	33.67	O			
ATOM	589	OE2	GLU	A	244	-31.387	-11.453	2.609	1.00	34.03	O			
ATOM	590	N	ILE	A	245	-35.563	-11.214	-1.682	1.00	26.49	N			
ATOM	591	CA	ILE	A	245	-35.400	-10.975	-1.575	1.00	25.75	C			
ATOM	592	G	ILE	A	245	-36.217	-8.832	-1.891	1.00	25.75	O			
ATOM	593	O	ILE	A	245	-36.768	-8.951	-0.799	1.00	25.02	O			
ATOM	594	CB	ILE	A	245	-36.858	-10.402	-3.671	1.00	25.53	C			
ATOM	595	CG1	ILE	A	245	-38.173	-10.846	-3.833	1.00	25.35	C			
ATOM	596	CG2	ILE	A	245	-36.325	-11.466	-4.663	1.00	24.89	C			
ATOM	597	CD1	ILE	A	245	-39.407	-10.707	-3.934	1.00	26.20	C			
ATOM	598	N	ARG	A	246	-36.804	-7.648	-2.381	1.00	24.57	N			
ATOM	599	CA	ARG	A	246	-36.526	-6.467	-1.793	1.00	24.09	C			
ATOM	600	C	ARG	A	246	-37.988	-6.289	-2.186	1.00	23.73	C			
ATOM	601	O	ARG	A	246	-38.334	-5.370	-3.019	1.00	22.92	O			
ATOM	602	CB	ARG	A	246	-35.657	-5.290	-2.156	1.00	24.34	C			
ATOM	603	CG	ARG	A	246	-34.232	-5.365	-1.662	1.00	25.49	C			
ATOM	604	CD	ARG	A	246	-34.407	-4.461	-1.804	1.00	25.99	C			
ATOM	605	NE	ARG	A	246	-32.020	-4.466	-1.877	1.00	26.08	C			
ATOM	606	CZ	ARG	A	246	-31.617	-4.321	-0.957	1.00	28.42	C			
ATOM	607	NH1	ARG	A	246	-32.447	-3.835	0.870	1.00	27.71	N			
ATOM	608	NHZ	ARG	A	246	-30.378	-4.676	0.281	1.00	29.27	N			
ATOM	609	N	GLY	A	247	-38.835	-7.026	-1.581	1.00	23.42	N			
ATOM	610	CA	GLY	A	247	-40.259	-7.039	-1.851	1.00	24.01	C			
ATOM	611	C	GLY	A	247	-40.829	-8.273	-1.197	1.00	24.58	C			
ATOM	612	O	GLY	A	247	-40.888	-9.077	-0.649	1.00	24.29	O			

12. Extract all ATOM lines for residues LYS or ARG in protein.pdb.

```
khushik@DESKTOP-DE71GO3:~/Lab_session3/Lab_assignment3$ awk '/^ATOM/ && /LYS|ARG/ {print}' protein.pdb
ATOM 15 N LYS A 173 -42.516 -20.697 24.576 1.00 32.18 N
ATOM 16 CA LYS A 173 -43.842 -20.728 23.949 1.00 31.37 C
ATOM 17 C LYS A 173 -44.028 -19.664 22.914 1.00 29.85 C
ATOM 18 O LYS A 173 -44.831 -19.725 21.976 1.00 30.15 O
ATOM 19 CB LYS A 173 -44.935 -20.645 25.024 1.00 31.31 C
ATOM 20 CO LYS A 173 -46.343 -20.964 24.519 1.00 32.53 C
ATOM 21 CD LYS A 173 -47.425 -20.459 25.479 1.00 32.89 C
ATOM 22 CE LYS A 173 -48.818 -20.684 24.901 1.00 33.96 C
ATOM 23 NZ LYS A 173 -49.893 -20.189 25.806 1.00 34.66 N
ATOM 46 N ARG A 177 -41.200 -13.469 26.062 1.00 17.53 N
ATOM 47 CA ARG A 177 -41.351 -12.338 26.984 1.00 18.15 C
ATOM 48 C ARG A 177 -40.135 -12.196 21.880 1.00 18.13 C
ATOM 49 O ARG A 177 -39.608 -11.088 22.053 1.00 17.51 O
ATOM 50 CB ARG A 177 -42.634 -12.456 21.807 1.00 18.62 C
ATOM 51 CG ARG A 177 -42.872 -11.237 22.713 1.00 20.72 C
ATOM 52 CD ARG A 177 -44.227 -11.292 23.368 1.00 22.66 C
ATOM 53 NE ARG A 177 -44.366 -16.263 24.391 1.00 24.94 N
ATOM 54 CZ ARG A 177 -43.848 -16.348 25.616 1.00 25.91 C
ATOM 55 NH1 ARG A 177 -43.147 -11.413 25.983 1.00 25.04 N
ATOM 56 NH2 ARG A 177 -44.030 -9.366 26.477 1.00 26.28 N
ATOM 94 N ARG A 182 -34.717 -9.406 22.797 1.00 19.68 N
ATOM 95 CA ARG A 182 -33.268 -9.544 22.849 1.00 20.05 C
ATOM 96 C ARG A 182 -32.593 -8.739 21.743 1.00 19.42 C
ATOM 97 O ARG A 182 -31.576 -8.072 21.990 1.00 19.22 O
ATOM 98 CB ARG A 182 -32.874 -11.019 22.769 1.00 20.66 C
ATOM 99 CG ARG A 182 -33.592 -11.864 23.806 1.00 23.33 C
ATOM 100 CD ARG A 182 -32.691 -12.324 24.917 1.00 31.08 C
ATOM 101 NE ARG A 182 -32.238 -13.693 24.676 1.00 34.53 N
ATOM 102 CZ ARG A 182 -32.720 -14.777 25.285 1.00 36.34 C

khushik@DESKTOP-DE71GO3:~/Lab_session3/Lab_assignment3$ awk '/^ATOM/ && /LYS|ARG/ {print}' protein.pdb
ATOM 182 CZ ARG A 182 -32.720 -14.777 25.285 1.00 36.34 C
ATOM 183 NH1 ARG A 182 -32.233 -14.065 26.074 1.00 36.34 N
ATOM 184 NH2 ARG A 182 -32.223 -14.066 26.075 1.00 37.59 N
ATOM 147 N LYS A 189 -27.943 -1.219 22.313 1.00 19.72 N
ATOM 148 CA LYS A 189 -26.592 -1.228 22.859 1.00 19.83 C
ATOM 149 C LYS A 189 -25.533 -0.931 21.783 1.00 19.51 C
ATOM 150 O LYS A 189 -24.637 -0.124 22.080 1.00 19.26 O
ATOM 151 CB LYS A 189 -25.980 -0.544 21.800 1.00 19.26 C
ATOM 152 CG LYS A 189 -24.988 -2.573 24.353 1.00 21.18 C
ATOM 153 CD LYS A 189 -24.991 -1.568 25.500 1.00 23.97 C
ATOM 154 CE LYS A 189 -23.703 -1.601 26.298 1.00 25.23 C
ATOM 155 NZ LYS A 189 -23.673 -0.491 27.204 1.00 25.98 N
ATOM 156 N LYS A 200 -30.913 0.893 21.060 1.00 19.73 N
ATOM 157 CA LYS A 200 -31.745 -0.835 21.813 1.00 20.24 C
ATOM 158 C LYS A 200 -31.205 -1.828 8.880 1.00 23.56 C
ATOM 159 O LYS A 200 -30.014 -1.861 9.160 1.00 23.03 O
ATOM 232 CB LYS A 200 -31.682 -1.479 6.440 1.00 24.17 C
ATOM 233 CG LYS A 200 -32.218 -0.669 5.294 1.00 23.41 C
ATOM 234 CD LYS A 200 -32.315 -0.669 5.294 1.00 23.41 C
ATOM 235 CE LYS A 200 -32.479 -0.443 2.786 1.00 21.93 C
ATOM 236 NZ LYS A 200 -31.331 0.512 2.647 1.00 19.78 N
ATOM 297 N LYS A 204 -49.012 -12.189 16.590 1.00 19.70 N
ATOM 298 CA LYS A 204 -49.580 -11.893 17.916 1.00 20.21 C
ATOM 299 C LYS A 204 -49.635 -12.866 18.110 1.00 20.99 C
ATOM 300 O LYS A 204 -49.635 -12.866 19.110 1.00 20.32 O
ATOM 301 CB LYS A 208 -51.043 -11.459 17.773 1.00 28.47 C
ATOM 302 CG LYS A 208 -51.935 -12.512 17.115 1.00 26.38 C
ATOM 303 CD LYS A 208 -53.396 -12.222 17.359 1.00 22.18 C
ATOM 304 CE LYS A 208 -54.291 -13.224 16.642 1.00 26.94 C
ATOM 305 NZ LYS A 208 -54.507 -13.507 17.340 1.00 26.34 N
ATOM 357 N ARG A 215 -43.344 -14.515 6.254 1.00 18.42 N
ATOM 358 CA ARG A 215 -42.464 -13.537 5.651 1.00 18.42 C
ATOM 359 C ARG A 215 -41.666 -12.828 6.745 1.00 17.97 C
ATOM 360 O ARG A 215 -42.249 -12.338 7.726 1.00 19.04 O
ATOM 361 CB ARG A 215 -43.431 -11.669 4.438 1.00 19.99 C
ATOM 362 CG ARG A 215 -43.431 -11.669 4.438 1.00 19.99 C
ATOM 363 CD ARG A 215 -43.301 -10.359 3.594 1.00 20.84 C
ATOM 364 NE ARG A 215 -43.854 -9.573 4.697 1.00 20.02 N
ATOM 365 CZ ARG A 215 -44.864 -8.786 4.586 1.00 22.74 C
ATOM 366 NH1 ARG A 215 -45.467 -8.518 4.518 1.00 21.74 N
ATOM 367 NH2 ARG A 215 -45.102 -8.540 5.624 1.00 23.60 N
ATOM 529 N LYS A 237 -36.427 -19.755 11.690 1.00 18.99 N
ATOM 530 CA LYS A 237 -35.253 -20.079 10.303 1.00 20.07 C
ATOM 531 C LYS A 237 -35.652 -20.086 8.836 1.00 20.62 C

khushik@DESKTOP-DE71GO3:~/Lab_session3/Lab_assignment3$ awk '/^ATOM/ && /LYS|ARG/ {print}' protein.pdb
ATOM 531 C LYS A 237 -35.652 -20.086 8.836 1.00 20.62 C
ATOM 532 O LYS A 237 -36.709 -20.667 8.487 1.00 20.15 O
ATOM 533 CB LYS A 237 -34.656 -21.438 10.712 1.00 20.03 C
ATOM 534 CG LYS A 237 -34.152 -21.438 10.712 1.00 20.03 C
ATOM 535 CD LYS A 237 -33.165 -22.819 13.393 1.00 20.54 C
ATOM 536 CZ LYS A 237 -32.887 -22.927 13.828 1.00 20.64 C
ATOM 537 NZ LYS A 237 -32.303 -24.281 14.128 1.00 19.43 N
ATOM 538 N ARG A 238 -34.811 -19.483 7.993 1.00 21.63 N
ATOM 539 CA ARG A 238 -35.054 -19.471 6.556 1.00 22.18 C
ATOM 540 C ARG A 238 -35.050 -19.471 6.556 1.00 22.18 C
ATOM 541 O ARG A 238 -34.580 -21.765 6.321 1.00 23.36 O
ATOM 542 CB ARG A 238 -33.882 -18.738 5.842 1.00 23.15 C
ATOM 543 CG ARG A 238 -34.126 -18.455 4.367 1.00 24.78 C
ATOM 544 CD ARG A 238 -32.969 -17.817 3.729 1.00 29.07 C
ATOM 545 CZ ARG A 238 -33.738 -16.866 1.525 1.00 29.00 N
ATOM 546 CZ ARG A 238 -33.738 -16.866 1.525 1.00 29.00 N
ATOM 547 NH1 ARG A 238 -31.254 -16.265 2.028 1.00 35.38 N
ATOM 548 NH2 ARG A 238 -32.617 -16.721 0.248 1.00 34.89 N
ATOM 598 N ARG A 246 -36.004 -7.648 -2.331 1.00 24.57 N
ATOM 599 CA ARG A 246 -36.526 -6.481 -1.00 24.99 C
ATOM 600 C ARG A 246 -37.008 -6.309 -1.00 24.99 C
ATOM 601 O ARG A 246 -38.334 -5.378 -1.019 1.00 22.92 O
ATOM 602 CB ARG A 246 -35.057 -5.260 -2.156 1.00 24.34 C
ATOM 603 CG ARG A 246 -34.232 -5.365 -1.662 1.00 25.49 C
ATOM 604 CD ARG A 246 -33.350 -4.136 -1.880 1.00 25.98 C
ATOM 605 CZ ARG A 246 -33.350 -4.136 -1.880 1.00 25.98 N
ATOM 606 CZ ARG A 246 -31.517 -5.231 -0.857 1.00 24.42 C
ATOM 607 NH1 ARG A 246 -32.447 -3.835 0.870 1.00 27.71 N
ATOM 608 NH2 ARG A 246 -30.378 -4.676 0.281 1.00 29.27 N

khushik@DESKTOP-DE71GO3:~/Lab_session3/Lab_assignment3$
```

13. Replace every occurrence of LYS with ARG in protein.pdb.

```

khush1@DESKTOP-DE71G03:~/Lab_session3/Lab_assignment3$ sed -n 's/lys/arg/gp' protein.pdb
CONNECT 647 645 649
CONNECT 648 644 645
CONNECT 649 646 647
MASTER 244 0 1 1 4 0 2 6 690 1 12 7
END
khush1@DESKTOP-DE71G03:~/Lab_session3/Lab_assignment3$ sed -n 's/lys/arg/gp' protein.pdb
CONNECT 1 A 86 TRP ARG GLU PRO CYS ARG ILE GLU LEU TYR ARG VAL VAL
SEQURES 2 A 86 GLU SER LEU ALA ARG ALA GLN GLU THR SER GLY GLU GLU
SEQURES 3 A 86 GLU SER LEU ALA ARG ALA GLN GLU THR SER GLY GLU GLU
SEQURES 4 A 86 ARG ARG ILE PRO GLY SER PRO GLU ILE ARG GLY ASP PRO
SEQURES 5 A 86 ARG ARG ILE PRO GLY SER PRO GLU ILE ARG GLY ASP PRO
SHEET 1 A 2 ARG A 208 PHE A 281 O
ATOM 15 N ARG A 173 -42.516 -20.697 24.576 1.00 32.18 N
ATOM 16 CA ARG A 173 -43.845 -20.720 23.500 1.00 32.17 C
ATOM 17 CB ARG A 173 -42.918 -20.684 23.214 1.00 32.16 C
ATOM 18 O ARG A 173 -44.831 -19.725 21.976 1.00 30.15 O
ATOM 19 CB ARG A 173 -44.935 -20.645 25.924 1.00 31.31 C
ATOM 20 CG ARG A 173 -46.343 -20.964 24.519 1.00 32.53 C
ATOM 21 CD ARG A 173 -47.652 -20.964 24.500 1.00 32.50 C
ATOM 22 CE ARG A 173 -48.818 -20.684 24.091 1.00 33.06 C
ATOM 23 NZ ARG A 173 -49.893 -20.189 25.806 1.00 34.66 N
ATOM 147 N ARG A 189 -27.943 -1.219 23.313 1.00 19.72 N
ATOM 148 CA ARG A 189 -26.593 -1.203 23.313 1.00 19.81 C
ATOM 149 CB ARG A 189 -25.395 -1.251 23.173 1.00 19.51 C
ATOM 150 O ARG A 189 -24.637 -0.121 22.000 1.00 19.20 O
ATOM 151 CB ARG A 189 -26.368 -2.544 23.584 1.00 19.67 C
ATOM 152 CG ARG A 189 -24.988 -2.573 24.153 1.00 21.18 C
ATOM 153 CD ARG A 189 -26.998 -2.560 24.153 1.00 21.17 C
ATOM 154 CE ARG A 189 -23.993 -1.401 26.298 1.00 25.23 C
ATOM 155 NZ ARG A 189 -23.673 -0.401 26.204 1.00 25.98 N
ATOM 228 N ARG A 200 -30.993 0.420 7.874 1.00 26.73 N
ATOM 229 CA ARG A 200 -31.742 -0.835 7.833 1.00 26.10 C
ATOM 230 CB ARG A 200 -32.908 -0.835 7.833 1.00 26.10 C
ATOM 231 O ARG A 200 -30.014 -1.861 9.166 1.00 23.03 O
ATOM 232 CB ARG A 200 -31.682 -1.479 6.448 1.00 24.17 C
ATOM 233 CG ARG A 200 -32.216 -0.699 5.294 1.00 23.41 C
ATOM 234 CD ARG A 200 -32.852 -0.699 5.294 1.00 23.43 C
ATOM 235 CE ARG A 200 -33.479 -0.443 2.786 1.00 21.93 C
ATOM 236 NZ ARG A 200 -31.331 0.512 2.647 1.00 19.78 N
ATOM 297 N ARG A 208 -49.012 -12.189 16.598 1.00 19.70 N
ATOM 298 CA ARG A 208 -49.588 -11.897 17.316 1.00 20.21 C
ATOM 299 CB ARG A 208 -49.691 -11.863 17.316 1.00 20.20 C
ATOM 300 O ARG A 208 -49.635 -12.866 20.118 1.00 20.32 O
ATOM 301 CB ARG A 208 -51.043 -11.459 17.773 1.00 20.47 C
ATOM 302 CG ARG A 208 -51.935 -12.512 17.115 1.00 20.38 C
ATOM 303 CD ARG A 208 -53.396 -12.222 17.359 1.00 22.10 C
ATOM 304 CE ARG A 208 -54.291 -13.221 16.642 1.00 20.94 C
ATOM 305 NZ ARG A 208 -54.187 -14.607 17.174 1.00 20.34 N
ATOM 529 N ARG A 237 -36.427 -19.755 11.099 1.00 18.90 N
ATOM 530 CA ARG A 237 -35.253 -20.079 10.303 1.00 20.07 C
ATOM 531 C ARG A 237 -35.652 -20.086 8.836 1.00 20.62 C
ATOM 532 O ARG A 237 -36.709 -20.607 8.487 1.00 20.15 O
ATOM 533 CB ARG A 237 -34.658 -21.438 10.712 1.00 20.03 C
ATOM 534 CG ARG A 237 -34.152 -21.504 12.151 1.00 19.85 C
ATOM 535 CD ARG A 237 -33.395 -22.819 12.393 1.00 20.64 C
ATOM 536 CE ARG A 237 -32.887 -22.927 13.828 1.00 20.64 C
ATOM 537 NZ ARG A 237 -32.303 -24.281 14.128 1.00 19.43 N
khush1@DESKTOP-DE71G03:~/Lab_session3/Lab_assignment3$ awk '/^ATOM/{print $9}' protein.pdb
24.415
24.729
23.944
22.789
24.418
25.025
26.396
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
24.981
25.896
23.098
22.191
21.728
22.138
22.913

```

14. Print only the z-coordinate (third number in coordinates) for each atom from protein.pdb.

```

khush1@DESKTOP-DE71G03:~/Lab_session3/Lab_assignment3$ awk '/^ATOM/{print $9}' protein.pdb
24.415
24.729
23.944
22.789
24.418
25.025
26.396
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
24.981
25.896
23.098
22.191
21.728
22.138
22.913

```

khushi@DE	khushi@DES	khushi@E	khushi@DE													
22.913	16.879	21.330	19.528	10.144	12.083	14.652	14.463	8.150	3.121	2.910	9.893	3.729	1.897			
23.359	16.389	21.136	19.011	10.474	12.838	16.612	13.332	9.161	2.228	3.622	9.606	2.305	2.032			
24.206	16.292	20.725	18.652	11.457	12.483	17.121	12.184	10.339	4.386	4.325	13.224	1.525	2.609			
23.639	19.702	21.314	18.386	12.338	13.243	14.844	11.744	11.022	3.882	3.366	14.563	2.028	-1.682			
25.445	19.389	19.532	18.973	11.354	13.057	14.923	12.834	10.589	3.934	4.825	15.057	0.240	-2.583			
20.872	28.508	22.395	18.459	10.667	11.024	16.381	13.885	7.014	3.445	5.834	16.260	5.150	-1.801			
20.564	28.241	23.423	19.288	10.878	11.146	17.293	14.801	6.294	2.943	5.449	14.766	4.423	-0.700			
19.866	19.106	22.870	18.754	10.074	12.549	14.274	13.975	7.198	1.658	7.042	13.754	3.324	-3.671			
20.142	18.847	23.148	18.374	8.877	13.524	15.029	15.777	8.411	0.668	6.829	13.983	2.518	-3.033			
19.632	17.675	24.630	17.086	10.445	10.713	16.254	14.936	5.639	-0.498	4.953	12.425	3.856	-4.663			
19.043	18.614	25.786	15.851	10.822	10.948	14.278	15.829	4.537	1.141	7.739	12.866	4.997	-3.934			
20.148	21.751	26.975	15.635	11.820	11.816	16.590	16.786	6.592	0.324	5.858	11.899	3.074	-2.381			
18.986	22.914	26.951	15.035	11.792	10.324	17.916	11.673	7.216	0.914	7.234	11.625	4.571	-1.793			
18.226	22.972	27.948	20.577	12.621	12.043	18.913	10.366	7.451	2.135	3.459	10.666	3.301	-2.186			
19.159	23.148	22.196	21.482	16.722	10.551	20.118	9.348	6.663	0.268	4.016	10.342	2.275	-3.819			
19.053	24.227	21.588	20.973	10.020	11.483	17.773	9.449	6.313	-0.500	5.106	9.843	0.877	-2.156			
17.116	24.527	20.595	21.037	9.745	11.626	17.115	9.931	6.156	-0.299	4.946	14.152	0.615	-1.662			
16.044	25.358	20.487	22.992	10.616	12.635	17.359	10.673	5.225	0.038	4.953	12.425	3.856	-4.663			
20.062	23.977	20.830	23.531	10.718	13.807	16.642	10.619	5.502	-0.483	1.539	13.941	3.954	-3.934			
20.984	25.633	21.792	24.965	12.097	13.453	17.174	11.488	4.222	0.039	6.295	14.367	4.200	-0.057			
21.880	24.244	19.676	25.496	16.792	12.499	18.399	11.371	8.538	0.463	7.338	14.499	0.010	0.870			
22.053	25.082	18.796	25.568	12.539	14.148	19.242	11.987	8.838	1.188	7.737	12.950	-1.334	0.281			
21.897	25.347	19.393	20.458	8.516	15.215	19.679	8.481	8.146	0.724	7.344	12.018	-1.404	-1.580			
22.713	22.797	18.973	20.040	8.054	15.328	20.421	7.317	8.234	-0.750	8.571	12.754	-2.500	-1.851			
23.368	22.849	17.833	18.526	7.892	14.951	18.508	6.548	10.359	2.327	8.238	12.940	-0.245	-1.197			
24.391	21.743	16.619	18.023	7.759	14.232	17.661	6.253	10.934	2.988	9.121	12.295	-0.167	-0.649			
25.616	21.996	16.073	20.694	6.726	14.000	16.468	6.356	10.673	2.294	8.525	11.488	-0.992	-1.235			
25.983	22.769	15.538	20.378	5.830	13.831	18.251	6.890	7.431	1.596	9.208	11.210	-0.985	-0.633			
26.477	23.806	20.431	22.207	7.874	14.618	19.205	6.254	6.727	2.487	10.497	11.099	1.294	-1.502			
22.435	24.917	21.249	17.886	7.833	15.284	19.536	5.651	7.156	1.968	11.239	10.303	1.376	-2.651			
23.221	24.676	21.798	16.374	8.888	15.708	18.713	6.745	7.389	2.738	9.681	8.836	-1.722	-0.467			
22.394	25.285	21.788	15.607	9.160	15.352	19.862	7.726	5.226	3.945	8.579	8.487	-2.349	0.400			
22.843	26.205	22.398	15.764	6.440	12.769	17.638	4.835	4.553	2.139	7.668	10.712	-1.290	1.176			
23.862	24.975	22.313	15.808	5.294	12.495	16.632	4.100	7.222	1.283	8.470	12.151	-0.194	0.312			
24.759	20.537	22.859	14.427	3.981	13.181	15.478	3.594	7.580	1.816	6.655	12.393	-3.244	0.954			
24.621	19.374	21.783	14.791	2.786	12.655	15.535	4.697	6.636	-0.194	7.465	13.828	-2.761	-1.719			
25.865	19.560	22.008	13.965	2.647	10.987	16.160	4.586	7.002	2.037	6.570	14.128	-2.003	-1.935			
21.187	19.310	23.584	12.636	9.451	10.197	17.138	3.418	9.027	2.783	5.592	7.993	-1.613	-2.670			
20.327	18.037	24.353	11.819	10.421	8.884	17.187	5.656	10.096	2.299	10.497	6.556	-0.837	-0.842			
20.043	16.895	25.500	12.413	10.497	10.698	18.044	6.573	11.765	1.216	11.598	5.978	-1.795	0.229			
20.146	17.689	26.298	11.232	10.100	14.336	18.112	7.424	11.874	2.362	13.024	6.321	-2.622	0.415			
19.020	20.034	27.204	11.614	11.816	15.106	18.976	6.577	5.418	2.708	13.932	5.842	-0.100	-1.315			
18.245	20.304	20.618	12.751	12.254	14.845	19.005	5.561	4.508	3.178	11.362	4.367	0.845	-1.319			
16.879	21.330	19.528	10.144	12.083	14.652	14.463	8.150	9.121	2.910	9.893	9.729	1.897	-0.728			



khushi@DESKTOP-DE71G03

```
-0.728
-1.417
-2.721
-3.167
-4.308
-2.272
0.557
1.273
1.495
1.840
2.607
2.435
1.329
khushi@DESKTOP-DE71G03
```

15. Count how many lines in protein.pdb contain a GLY residue.

```
1.340
2.607
2.435
1.329
khushi@DESKTOP-DE71G03:~/Lab_session3/Lab_assignment3$ sed -n '/GLY/p' protein.pdb | wc -l
33
khushi@DESKTOP-DE71G03:~/Lab_session3/Lab_assignment3$ awk '/^ATOM.*CA|ALA|GLY/{print}' protein.pdb
```

16. Print only the C-alpha (CA) atoms for residues ALA or GLY.

```
33
khushi@DESKTOP-DE71G03:~/Lab_session3/Lab_assignment3$ awk '/^ATOM.*CA|& /ALA|GLY/{print}' protein.pdb
ATOM 143 CA ALA A 188 -29.906 -0.273 21.249 1.00 19.62 C
ATOM 157 CA ALA A 190 -24.689 -1.482 19.528 1.00 20.13 C
ATOM 193 CA GLY A 195 -19.179 3.898 13.965 1.00 34.45 C
ATOM 315 CA GLY A 210 -45.353 -14.753 19.536 1.00 18.56 C
ATOM 422 CA GLY A 223 -36.815 5.170 1.658 1.00 21.58 C
ATOM 435 CA ALA A 225 -37.186 -1.492 0.463 1.00 20.30 C
ATOM 440 CA GLY A 226 -35.705 -3.955 2.988 1.00 18.85 C
ATOM 526 CA GLY A 236 -37.957 -18.276 12.295 1.00 18.22 C
ATOM 565 CA GLY A 241 -34.199 -22.463 -1.334 1.00 28.67 C
ATOM 610 CA GLY A 247 -40.259 -7.039 -1.851 1.00 24.01 C
khushi@DESKTOP-DE71G03:~/Lab_session3/Lab_assignment3$ awk '/^ATOM/ && $3=="C" {count++} END {print count}' protein.pdb
```

17. Count how many atoms are carbon (element C) in protein.pdb. 17.

```
17
khushi@DESKTOP-DE71G03:~/Lab_session3/Lab_assignment3$ awk '/^ATOM/ && $3=="C" {count++} END {print count}' protein.pdb
80
khushi@DESKTOP-DE71G03:~/Lab_session3/Lab_assignment3$
```

Type here to search

27°C Mostly cloudy 21:39 24-08-2025

18. Print only the HETATM lines from protein.pdb.

```
lhu@lhu-DESKTOP-DET1GQ:~/Lab_session3/Lab_assignment3$ awk '/^ATOM & $3+>C/{count++} END {print count}' protein.pdb
80
lhu@lhu-DESKTOP-DET1GQ:~/Lab_session3/Lab_assignment3$ awk '/^HETATM/{print}' protein.pdb
0
lhu@lhu-DESKTOP-DET1GQ:~/Lab_session3/Lab_assignment3$ awk '/^ATOM & $3+>C/{count++} END {print count}' protein.pdb
80
HEATM 645 O HOM A 488 -29.575 -1.996 25.245 1.00 28.23 0
HEATM 645 C2 DIO A 488 -29.575 -1.996 27.132 1.00 36.34 0
HEATM 646 O HOM A 489 -28.873 -8.437 26.988 1.00 39.93 0
HEATM 646 C2 DIO A 489 -27.687 -6.281 17.262 1.00 35.99 0
HEATM 647 C2 DIO A 490 -26.684 -8.437 16.825 1.00 36.68 0
HEATM 647 O HOM A 490 -28.996 -8.072 16.254 1.00 36.78 0
HEATM 647 C2 DIO A 491 -26.684 -8.437 16.825 1.00 36.78 0
HEATM 650 O HOM A 1 -37.255 -6.228 10.647 1.00 14.97 0
HEATM 651 O HOM A 2 -22.812 -8.788 22.336 1.00 26.64 0
HEATM 652 O HOM A 3 -38.877 -3.393 4.474 1.00 26.33 0
HEATM 653 O HOM A 4 -38.877 -3.393 4.474 1.00 26.33 0
HEATM 654 O HOM A 5 -20.730 -0.315 24.894 1.00 28.65 0
HEATM 655 O HOM A 6 -44.936 -13.438 1.965 1.00 28.30 0
HEATM 656 O HOM A 7 -48.895 -18.782 15.563 1.00 27.48 0
HEATM 657 O HOM A 8 -28.996 -8.054 17.811 1.00 19.13 0
HEATM 658 O HOM A 9 -32.124 -5.065 16.006 1.00 29.82 0
HEATM 659 O HOM A 10 -46.106 -13.792 6.539 1.00 23.52 0
HEATM 660 O HOM A 11 -29.575 -1.996 25.245 1.00 28.23 0
HEATM 661 O HOM A 12 -45.642 -11.444 19.694 1.00 25.61 0
HEATM 662 O HOM A 13 -45.642 -11.444 19.694 1.00 25.61 0
HEATM 663 O HOM A 14 -38.137 -4.552 3.329 1.00 27.31 0
HEATM 664 O HOM A 15 -42.693 -7.945 15.244 1.00 19.76 0
HEATM 665 O HOM A 16 -35.986 -28.175 5.866 1.00 31.98 0
HEATM 666 O HOM A 17 -47.265 -12.454 21.564 1.00 28.48 0
HEATM 667 O HOM A 18 -47.265 -12.454 21.564 1.00 28.48 0
HEATM 668 O HOM A 19 -36.430 -3.094 -3.026 1.00 25.02 0
HEATM 669 O HOM A 20 -29.553 -5.969 12.150 1.00 34.06 0
HEATM 670 O HOM A 21 -21.462 -10.989 -5.598 1.00 24.90 0
HEATM 671 O HOM A 22 -43.889 -10.965 19.065 1.00 29.99 0
HEATM 672 O HOM A 23 -43.476 -6.477 -2.563 1.00 30.73 0
HEATM 673 O HOM A 24 -28.999 -3.283 21.951 1.00 26.71 0
HEATM 674 O HOM A 25 -50.516 -10.430 14.194 1.00 25.35 0
HEATM 675 O HOM A 26 -20.730 -5.065 16.006 1.00 29.44 0
HEATM 676 O HOM A 27 -48.424 -14.440 -0.286 1.00 61.67 0
HEATM 677 O HOM A 28 -43.808 -10.899 7.886 1.00 28.89 0
HEATM 678 O HOM A 29 -35.566 -5.280 24.699 1.00 29.22 0
HEATM 679 O HOM A 30 -39.566 -10.899 7.886 1.00 27.50 0
HEATM 680 O HOM A 31 -41.964 -17.595 25.641 1.00 37.16 0
HEATM 681 O HOM A 32 -34.312 -2.922 25.191 1.00 31.83 0
HEATM 682 O HOM A 33 -51.060 -11.051 21.823 1.00 29.98 0
HEATM 683 O HOM A 34 -32.561 -16.311 28.119 1.00 56.80 0
HEATM 684 O HOM A 35 -34.469 -16.084 9.169 1.00 24.01 0
```

19. Extract all residue names that end with “E” (e.g., ILE, PHE).

20. Delete all the lines that contain TER or END from protein.pdb.

```

khush@DESKTOP-DE71G03:/Lab/session3/Lab_assignment3$ sed '/TER/!d; /END/d' protein.pdb
HEADER PEPTIDE BINDING PROTEIN 26-MAY-05 1273
TITLE 2 ISOLATED FROM HUMAN AMNIOTIC FLUID
COMPND MOL_ID: 1;
COMPND 2 ISOLATED; INSULIN-LIKE GROWTH FACTOR BINDING PROTEIN 1;
COMPND CHAIN: A;
COMPND 5 SYNONYM: IGFBP-1, IGBP-1, IGF-BINDING PROTEIN 1, PLACENTAL PROTEIN
COMPND 6 12, PPI2
SOURCE MOL_ID: 1;
SOURCE SCIENTIFIC_NAME: HOMO SAPIENS;
SOURCE 3 ORGANISM_COMMON: HUMANS;
SOURCE 4 ORGANISM_TAXID: 9606;
SOURCE 5 OTHER_DETAILS: AMNIOTIC FLUID
KEYWDS INSULIN-LIKE GROWTH FACTOR BINDING PROTEIN-1, IGFBP-1, AMNIOTIC
X-RAY CRYSTALLOGRAPHY
AUTHOR 1 A.SALA,S.CAPALDI,M.CAMPAGNOLI,B.FAGGIONI,S.LABO,M.PERDUA,A.ROMANO,
AUTHOR 2 M.E.CARRIZO,M.VALLI,L.VISAI,L.MINCHIOTTI,H.GALLIANO,H.LI-MONACO
REVDAT 5 16-OCT-24 1273 1 REMARK
REVDAT 4 11-OCT-17 1273 1 REMARK
REVDAT 3 24-AUG-05 1273 1 VERSN
REVDAT 2 30-AUG-05 1273 1 JRNL
REVDAT 1 28-JUN-05 1273 0
JRNL AUTH 1 A.SALA,S.CAPALDI,M.CAMPAGNOLI,B.FAGGIONI,S.LABO,M.PERDUA,
JRNL AUTH 2 A.ROMANO,M.E.CARRIZO,M.VALLI,L.VISAI,L.MINCHIOTTI,
JRNL AUTH 3 H.GALLIANO,H.LI-MONACO
JRNL TITLE 2 INSULIN-LIKE GROWTH FACTOR-BINDING PROTEIN-1 ISOLATED FROM
JRNL TITL 3 HUMAN AMNIOTIC FLUID
JRNL REF 3.BIOL.CHEM., V. 28B 29812 2005
JRNL REFM 15972819
JRNL DOI 10.1017/S095042404200
REMARK 2 RESOLUTION: 1.80 ANGSTROMS.
REMARK 2
REMARK 3 Select khush@DESKTOP-DE71G03:/Lab/session3/Lab_assignment3
REMARK 2 RESOLUTION: 1.80 ANGSTROMS.
REMARK 3
REMARK 3 REFINEMENT.
REMARK 3 PROGRAM : REFMAC 5.2.0005
REMARK 3 AUTHORS : MURSHUDOV,SKUBAK,LEBEDEV,PANIN,STEINER,
REMARK 3 : NICHOLLS,WINN,LONG,VAGIN
REMARK 3
REMARK 3 REFINEMENT TARGET : MAXIMUM LIKELIHOOD
REMARK 3
REMARK 3 DATA USED IN REFINEMENT.
REMARK 3 RESOLUTION RANGE HIGH (ANGSTROMS) : 1.80
REMARK 3 RESOLUTION RANGE LOW (ANGSTROMS) : 18.92
REMARK 3 DATA CUTOFF (%) : 0.0000
REMARK 3 COMPLETENESS FOR RANGE (%) : 99.3
REMARK 3 NUMBER OF REFLECTIONS : 6091
REMARK 3
REMARK 3 FIT TO DATA USED IN REFINEMENT.
REMARK 3 CROSS-VALIDATION METHOD : THROUGHOUT
REMARK 3 FREE R VALUE TEST SET SELECTION : RANDOM
REMARK 3 R VALUE (WORKING + TEST SET) : 0.224
REMARK 3 R VALUE (WORKING SET) : 0.221
REMARK 3 FREE R VALUE : 0.275
REMARK 3 FREE R VALUE TEST SET SIZE (%) : 4.700
REMARK 3 FREE R VALUE TEST SET COUNT : 335
REMARK 3
REMARK 3 FIT IN THE HIGHEST RESOLUTION BIN.
REMARK 3 TOTAL NUMBER OF BINS USED : 28
REMARK 3 BIN RESOLUTION RANGE HIGH (A) : 1.80
REMARK 3 BIN RESOLUTION RANGE LOW (A) : 18.92
REMARK 3 REFLECTION IN BIN (WORKING SET) : 493
REMARK 3 BIN COMPLETENESS (WORKING+TEST) (%) : 96.48
REMARK 3 BIN R VALUE (WORKING SET) : 0.3210
REMARK 3 BIN FREE R VALUE SET COUNT : 28
REMARK 3 BIN FREE R VALUE : 0.2740
REMARK 3
REMARK 3 NUMBER OF NON-HYDROGEN ATOMS USED IN REFINEMENT.
REMARK 3 PROTEIN ATOMS : 642
REMARK 3 NUCLEIC ACID ATOMS : 0
REMARK 3 SOLVENT ATOMS : 42
REMARK 3
REMARK 3 B VALUES.
REMARK 3 FROM WILSON PLOT (A**2) : NULL
REMARK 3 MEAN B VALUE (OVERALL, A**2) : 23.59
REMARK 3 OVERALL ANISOTROPIC B VALUE.
REMARK 3
REMARK 3 Select khush@DESKTOP-DE71G03:/Lab/session3/Lab_assignment3
REMARK 3 OVERALL ANISOTROPIC B VALUE.
REMARK 3 ESU BASED ON R VALUE (A) : 0.168
REMARK 3 ESU BASED ON FREE R VALUE (A) : 0.161
REMARK 3 ESU BASED ON MAXIMUM LIKELIHOOD (A) : 0.165
REMARK 3 ESU FOR B VALUES BASED ON MAXIMUM LIKELIHOOD (A**2) : 3.230
REMARK 3
REMARK 3 CORRELATION COEFFICIENTS.
REMARK 3 CORRELATION COEFFICIENT FO-FC : 0.940
REMARK 3 CORRELATION COEFFICIENT FO-FC FREE : 0.885
REMARK 3
REMARK 3 RMS DEVIATIONS FROM IDEAL VALUES COUNT RMS WEIGHT
REMARK 3 BOND LENGTHS REFINED ATOMS (A): 669 : 0.008 : 0.022
REMARK 3 BOND LENGTHS OTHERS (A): NULL : NULL : NULL
REMARK 3 BOND ANGLES REFINED ATOMS (DEGREES): 969 : 1.000 : 0.050
REMARK 3 BOND ANGLES OTHERS (DEGREES): NULL : NULL : NULL
REMARK 3 TORSION ANGLES, PERIOD 1 (DEGREES): 79 : 5.849 : 5.000
REMARK 3 TORSION ANGLES, PERIOD 2 (DEGREES): 33 : 31.224 : 23.939
REMARK 3 TORSION ANGLES, PERIOD 3 (DEGREES): 113 : 13.432 : 15.000
REMARK 3 TORSION ANGLES, PERIOD 4 (DEGREES): 57 : 1.000 : 0.000
REMARK 3 GENERAL PLANES REFINED ATOMS (A): 523 : 0.004 : 0.020
REMARK 3 GENERAL PLANES OTHERS (A): NULL : NULL : NULL
REMARK 3 NON-BONDED CONTACTS REFINED ATOMS (A): 275 : 0.190 : 0.200
REMARK 3 NON-BONDED CONTACTS OTHERS (A): NULL : NULL : NULL
REMARK 3 SYMMETRY VDW REFINED ATOMS (A): 548 : 0.180 : 0.200
REMARK 3 SYMMETRY VDW OTHERS (A): NULL : NULL : NULL
REMARK 3 H-BOND (X,-Y) REFINED ATOMS (A): 45 : 0.116 : 0.200
REMARK 3 H-BOND (X,-Y) OTHERS (A): NULL : NULL : NULL
REMARK 3 POTENTIAL METAL-ION REFINED ATOMS (A): NULL : NULL : NULL
REMARK 3 POTENTIAL METAL-ION OTHERS (A): NULL : NULL : NULL
REMARK 3 SYMMETRY VDW REFINED ATOMS (A): 51 : 0.180 : 0.200
REMARK 3 SYMMETRY VDW OTHERS (A): NULL : NULL : NULL
REMARK 3 SYMMETRY H-BOND REFINED ATOMS (A): 12 : 0.121 : 0.200
REMARK 3 SYMMETRY H-BOND OTHERS (A): NULL : NULL : NULL
REMARK 3 SYMMETRY METAL-ION REFINED ATOMS (A): NULL : NULL : NULL
REMARK 3 SYMMETRY METAL-ION OTHERS (A): NULL : NULL : NULL
REMARK 3

```

```
 Select khushi@DESKTOP-DE71GO3: ~/Lab_session3/Lab_assignment3
REMARK 3 ISOTROPIC THERMAL FACTOR RESTRAINTS COUNT RMS WEIGHT
REMARK 3 MAIN-CHAIN BOND REFINED ATOMS (A**2) : 412 ; 0.731 ; 500
REMARK 3 MAIN-CHAIN BOND OTHER ATOMS (A**2) : NULL ; NULL ; NULL
REMARK 3 MAIN-CHAIN ANGLE REFINED ATOMS (A**2) : 642 ; 1.226 ; 2.000
REMARK 3 MAIN-CHAIN ANGLE OTHER ATOMS (A**2) : NULL ; NULL ; NULL
REMARK 3 SIDE-CHAIN BOND REFINED ATOMS (A**2) : 305 ; 1.609 ; 3.000
REMARK 3 SIDE-CHAIN BOND OTHER ATOMS (A**2) : NULL ; NULL ; NULL
REMARK 3 SIDE-CHAIN ANGLE REFINED ATOMS (A**2) : 263 ; 2.385 ; 4.500
REMARK 3 SIDE-CHAIN ANGLE OTHER ATOMS (A**2) : NULL ; NULL ; NULL
REMARK 3 LONG RANGE A REFINED ATOMS (A**2) : NULL ; NULL ; NULL
REMARK 3 LONG RANGE B REFINED ATOMS (A**2) : NULL ; NULL ; NULL
REMARK 3 LONG RANGE B OTHER ATOMS (A**2) : NULL ; NULL ; NULL
REMARK 3
REMARK 3 ANISOTROPIC THERMAL FACTOR RESTRAINTS COUNT RMS WEIGHT
REMARK 3 RIGID-BOND RESTRAINTS (A**2) : NULL ; NULL ; NULL
REMARK 3 SPHERICITY; FREE ATOMS (A**2) : NULL ; NULL ; NULL
REMARK 3 SPHERICITY; BONDED ATOMS (A**2) : NULL ; NULL ; NULL
REMARK 3
REMARK 3 NCS RESTRAINTS STATISTICS
REMARK 3 NUMBER OF DIFFERENT NCS GROUPS : NULL
REMARK 3
REMARK 3 TLS DETAILS
REMARK 3 NUMBER OF TLS GROUPS : NULL
REMARK 3
REMARK 3 BULK SOLVENT MODELLING.
REMARK 3 METHOD USED : MASK
REMARK 3 VDW PROBE RADIUS : 1.20
REMARK 3 ION PROBE RADIUS : 0.80
REMARK 3 SHRINKAGE RADIUS : 0.80
REMARK 3
REMARK 3 OTHER REFINEMENT REMARKS: NULL
REMARK 4 1ZT3 COMPLIES WITH FORMAT V. 3.30, 13-JUL-11
REMARK 100
REMARK 100 THIS ENTRY HAS BEEN PROCESSED BY RCSB ON 02-JUN-05.
REMARK 100 THE DEPOSITION ID IS D_1000033086.
REMARK 200
REMARK 200 EXPERIMENTAL DETAILS
REMARK 200 EXPERIMENT TYPE : X-RAY DIFFRACTION
REMARK 200 DATE OF DATA COLLECTION : 17-FEB-64
REMARK 200 TEMPERATURE (KELVIN) : 100.0
REMARK 200 PH : 7.5
REMARK 200 NUMBER OF CRYSTALS USED : 1
REMARK 200
```

Type here to search 26°C Mostly cloudy 21:58 24-08-2025

```
 Select khushi@DESKTOP-DE71GO3: ~/Lab_session3/Lab_assignment3
REMARK 200
REMARK 200 SYNCHROTRON (Y/N) : N
REMARK 200 RADIATION SOURCE : ROTATING ANODE
REMARK 200 BEAMLINE : NULL
REMARK 200 X-RAY GENERATOR MODEL : RIGAKU RU300
REMARK 200 MONOCHROMATIC OR LAUE (M/L) : M
REMARK 200 WAVELENGTH OR RANGE (Å) : 1.5418
REMARK 200 MONOCHROMATOR : XENOS MULTILAYER CONFOCAL
REMARK 200 MIRRORS : MIRRORS
REMARK 200 OPTICS : MIRRORS
REMARK 200
REMARK 200 DETECTOR TYPE : IMAGE PLATE
REMARK 200 DETECTOR MANUFACTURER : MARRESEARCH
REMARK 200 INTENSITY-INTEGRATION SOFTWARE : AUTOMAR
REMARK 200 DATA SCALING SOFTWARE : MARSCALE
REMARK 200
REMARK 200 NUMBER OF UNIQUE REFLECTIONS : 7168
REMARK 200 RESOLUTION RANGE HIGH (Å) : 1.800
REMARK 200 RESOLUTION RANGE LOW (Å) : 18.920
REMARK 200
REMARK 200 OVERALL.
REMARK 200 COMPLETENESS FOR RANGE (%) : 99.5
REMARK 200 DATA REDUNDANCY : 6.200
REMARK 200 R MERGE (I) : NULL
REMARK 200 R SYM (I) : 0.04100
REMARK 200 <SIGMA(I)> FOR THE DATA SET : 34.2000
REMARK 200
REMARK 200 IN THE HIGHEST RESOLUTION SHELL.
REMARK 200 HIGHEST RESOLUTION SHELL, RANGE HIGH (Å) : 1.80
REMARK 200 HIGHEST RESOLUTION SHELL, RANGE LOW (Å) : 1.90
REMARK 200 COMPLETENESS FOR SHELL (%) : 98.1
REMARK 200 DATA REDUNDANCY IN SHELL : NULL
REMARK 200 R MERGE FOR SHELL (I) : NULL
REMARK 200 R SYM FOR SHELL (I) : 0.27400
REMARK 200 <SIGMA(I)> FOR SHELL : 2.800
REMARK 200
REMARK 200 DIFFRACTION PROTOCOL: SINGLE WAVELENGTH
REMARK 200 SOFTWARE USED: SHARP
REMARK 200 STARTING MODEL: NULL
REMARK 200
REMARK 200 REMARK: NULL
REMARK 200
REMARK 200 CRYSTAL
REMARK 200 SOLVENT CONTENT, VS (%) : 37.40
```

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 Select khushi@DESKTOP-DE71GO3: ~/Lab_session3/Lab_assignment3
REMARK 200 SOLVENT CONTENT, VS (%) : 37.40
REMARK 200 MATTHEWS COEFFICIENT, VM (ANGSTROMS**3/DA) : 2.00
REMARK 200
REMARK 200 CRYSTALLIZATION CONDITIONS: DIOXANE, PH 7.5, VAPOR DIFFUSION,
REMARK 200 SITTING DROP, TEMPERATURE 277K
REMARK 200
REMARK 200 CRYSTALLOGRAPHIC SYMMETRY
REMARK 200 SYMMETRY OPERATORS FOR SPACE GROUP: P 21 21 2
REMARK 200
REMARK 200 SYMOP SYMMETRY
REMARK 200 NNNMNM OPERATOR
REMARK 200 1555 X,Y,Z
REMARK 200 3555 -X,-Y,Z
REMARK 200 3555 X+1/2,Y+1/2,-Z
REMARK 200 4555 X+1/2,-Y+1/2,-Z
REMARK 200 WHERE NNN -> OPERATOR NUMBER
REMARK 200 MMM -> TRANSLATION VECTOR
REMARK 200
REMARK 200 CRYSTALLOGRAPHIC SYMMETRY TRANSFORMATIONS
REMARK 200 THE FOLLOWING TRANSFORMATIONS OPERATE ON THE ATOM/HETATM
REMARK 200 RECORDS IN THIS ENTRY TO PRODUCE CRYSTALLOGRAPHICALLY
REMARK 200 RELATED MOLECULES.
REMARK 200 SMTRY1 1 0.000000 0.000000 0.000000 0.000000
REMARK 200 SMTRY2 1 0.000000 1.000000 0.000000 0.000000
REMARK 200 SMTRY3 1 0.000000 0.000000 1.000000 0.000000
REMARK 200 SMTRY1 2 -1.000000 0.000000 0.000000 0.000000
REMARK 200 SMTRY2 2 0.000000 1.000000 0.000000 0.000000
REMARK 200 SMTRY3 2 0.000000 0.000000 1.000000 0.000000
REMARK 200 SMTRY1 3 -1.000000 0.000000 0.000000 19.7600
REMARK 200 SMTRY2 3 0.000000 1.000000 0.000000 30.19500
REMARK 200 SMTRY3 3 0.000000 0.000000 -1.000000 0.000000
REMARK 200 SMTRY1 4 1.000000 0.000000 0.000000 19.27000
REMARK 200 SMTRY2 4 0.000000 -1.000000 0.000000 30.19500
REMARK 200 SMTRY3 4 0.000000 0.000000 -1.000000 0.000000
REMARK 200
REMARK 200 REMARK: NULL
REMARK 200
REMARK 300 BIOMOLECULE: 1
REMARK 300 SEE REMARK 350 FOR THE AUTHOR PROVIDED AND/OR PROGRAM
REMARK 300 GENERATED ASSEMBLY INFORMATION FOR THE STRUCTURE IN
REMARK 300 THIS ENTRY. THE REMARK MAY ALSO PROVIDE INFORMATION ON
REMARK 300 BURIED SURFACE AREA.
REMARK 350
```

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REMARK 358 SELECT KHUSHIDDESKTOP-DE71G03 -\Lab\session3\Lab_assignment
 REMARK 358 COORDINATES FOR A COMPLETE MULTIMER REPRESENTING THE KNOWN
 REMARK 358 BIOLOGICALLY SIGNIFICANT OLIGOMERIZATION STATE OF THE
 REMARK 358 PROTEIN. THIS FILE CONTAINS ALL BONDS AND BIOMOL TRANSFORMATIONS
 REMARK 358 GIVEN BELOW, BOTH NON-CRYSTALLOGRAPHIC AND
 REMARK 358 CRYSTALLOGRAPHIC OPERATIONS ARE GIVEN.
 REMARK 358
 REMARK 358 BIOMOLECULE: 1
 REMARK 358 APPLY THE FOLLOWING TO CHAINS: A
 REMARK 358 DIO 1.0 0.000000 0.000000 0.000000 0.000000
 REMARK 358 BIOMT2 1 0 0.000000 0.000000 0.000000 0.000000
 REMARK 358 BIOMT3 1 0 0.000000 0.000000 1.000000 0.000000
 REMARK 358
 REMARK 358 SITE
 REMARK 358 SITE_IDENTIFIER: ACT1
 REMARK 358 EVIDENCE_CODE: SOFTWARE
 REMARK 358 SITE_DESCRIPTION: BINDING SITE FOR RESIDUE DIO A 400
 REMARK 358 RELATED_ENTRIES:
 REMARK 358 RELATED_CHAINS: RELATED DBI; PDB
 REMARK 358 SAME PROTEIN ISOLATED FROM HUMAN AMNIOTIC FLUID COMPLEXED WITH
 REMARK 358 IRON(II)
 REMARK 358 XREF_ID: 251 UNP PBW833 IBP1_HUMAN 172 251
 SEQUES 2 A 88 TRP LYS GLU PRO CYS ARG ILE GLU LEU TYR ARG VAL VAL
 SEQUES 2 A 89 GLU SER ILE ALA LYS ALA GLN GLU THR SER GLY GLU GLU
 SEQUES 2 A 90 GLU
 SEQUES 4 A 88 PHE TYR HIS SER ARG GLN CYS GLU THR SER MET ASP GLY
 SEQUES 5 A 88 GLU ALA GLY LEU GLY TRP CYS VAL TYR PRO TRP ASP GLY
 SEQUES 6 A 88 GLU
 SEQUES 7 A 88 ASH CYS
 HET DIO DIO,4,4-DIMETHYLENE DIOXIDE
 FORMUL 2 DI 0.000000 C4 H8 O2
 FORMUL 3 HOH 42(H2O)
 KELVIN 298.15
 SHEET 1 A 2 LYS A 209 SER A 194 1 21
 SHEET 2 A 2 THR A 219 SER A 220 -1 O THR A 219 N PHE A 201
 SHEET 3 B 2 CYS A 228 CYS A 230 -1 O TRP A 229 N GLN A 216
 USBRND 3 CYS A 176 CYS A 206 1555 1555 2.05
 USBRND 3 CYS A 230 CYS A 232 1555 1555 2.05
 USBRND 3 CYS A 230 CYS A 251 1555 1555 2.04
 SITE 3 ACT1 7 HOH A 7 HOH A 40 VAL A 183 SER A 186
 SITE 3 ACT1 7 LEU A 187 PRO A 233 TRP A 234
 Type here to search 26°C Mostly cloudy ENG 23:58 24-08-2025

 Select khushiddeSKTDP-DE71G03 -\Lab\session3\Lab_assignment3
 CRYST1 2 AC1 7 LEU A 187 PRO A 233 TRP A 234
 38.546 60.398 31.240 90.000 90.000 P 21 21 2 4
 ORIGX1 1.000000 0.000000 0.000000 0.000000
 ORIGX2 0.000000 1.000000 0.000000 0.000000
 ORIGX3 0.000000 0.000000 1.000000 0.000000
 SCALE1 0.025347 0.000000 0.000000 0.000000
 SCALE2 0.000000 0.016559 0.000000 0.000000
 SCALE3 0.000000 0.000000 0.000000 0.000000
 ATOM 1 N TRP A 172 -39.136 -21.997 24.415 1.00 34.43 N
 ATOM 2 CA TRP A 172 -40.188 -20.997 24.729 1.00 34.28 C
 ATOM 3 CB TRP A 172 -41.186 -21.067 25.041 1.00 33.48 C
 ATOM 4 O TRP A 172 -39.185 -21.066 27.789 1.00 34.13 O
 ATOM 5 CB TRP A 172 -39.586 -19.534 24.418 1.00 35.12 C
 ATOM 6 CG TRP A 172 -38.161 -19.292 25.025 1.00 36.34 C
 ATOM 7 CD TRP A 172 -37.161 -19.292 25.025 1.00 36.34 C
 ATOM 8 CD2 TRP A 172 -37.032 -18.693 24.384 1.00 37.47 C
 ATOM 9 NEI TRP A 172 -36.465 -19.193 26.497 1.00 37.97 N
 ATOM 10 CE2 TRP A 172 -35.986 -18.652 25.334 1.00 37.83 C
 ATOM 11 CZ2 TRP A 172 -35.779 -18.652 25.334 1.00 37.57 C
 ATOM 12 C22 TRP A 172 -34.725 -18.128 25.037 1.00 37.51 C
 ATOM 13 C23 TRP A 172 -35.545 -17.671 22.882 1.00 37.85 C
 ATOM 14 CZ3 TRP A 172 -34.537 -17.671 22.882 1.00 37.43 C
 ATOM 15 CH2 TRP A 172 -34.516 -20.697 24.376 1.00 37.43 C
 ATOM 16 CA LYS A 173 -41.842 -20.728 23.949 1.00 31.37 C
 ATOM 17 C LYS A 173 -44.028 -19.662 22.914 1.00 29.85 C
 ATOM 18 CB LYS A 173 -43.170 -19.662 22.914 1.00 29.85 O
 ATOM 19 CD LYS A 173 -44.935 -20.645 25.024 1.00 31.31 C
 ATOM 20 CG LYS A 173 -46.343 -20.964 24.519 1.00 32.53 C
 ATOM 21 CD2 LYS A 173 -47.425 -20.474 25.479 1.00 32.89 C
 ATOM 22 CZ2 LYS A 173 -46.343 -20.474 25.479 1.00 32.89 C
 ATOM 23 NZ LYS A 173 -40.893 -20.189 25.096 1.00 34.66 N
 ATOM 24 N GLU A 174 -43.280 -18.518 23.090 1.00 27.67 N
 ATOM 25 CA GLU A 174 -43.337 -17.386 22.191 1.00 25.77 C
 ATOM 26 CB GLU A 174 -43.337 -17.386 22.191 1.00 25.77 C
 ATOM 27 O GLU A 174 -41.381 -15.977 22.138 1.00 23.23 O
 ATOM 28 CB GLU A 174 -43.933 -16.148 22.913 1.00 25.76 C
 ATOM 29 CD GLU A 174 -43.933 -16.148 22.913 1.00 25.76 C
 ATOM 30 OD GLU A 174 -45.777 -15.065 24.206 1.00 27.42 C
 ATOM 31 OE1 GLU A 174 -46.182 -14.061 23.639 1.00 29.42 O
 ATOM 32 OE2 GLU A 174 -45.756 -15.182 25.445 1.00 30.63 O
 ATOM 33 CA PRO A 175 -39.891 -17.795 26.554 1.00 20.15 N
 ATOM 34 CB PRO A 175 -39.891 -17.795 26.554 1.00 20.18 C
 ATOM 35 C PRO A 175 -39.565 -16.386 19.866 1.00 18.58 C
 ATOM 36 O PRO A 175 -39.528 -15.783 20.142 1.00 18.18 O

 Select khushiddeSKTDP-DE71G03 -\Lab\session3\Lab_assignment3
 ATOM 36 O PRO A 175 -36.520 -15.781 20.142 1.00 18.18 O
 ATOM 37 CB PRO A 175 -43.504 -18.893 19.632 1.00 20.52 C
 ATOM 38 CB PRO A 175 -40.989 -19.247 19.043 1.00 19.77 C
 ATOM 39 CD PRO A 175 -41.896 -19.915 20.148 1.00 21.28 C
 ATOM 40 CG PRO A 175 -41.896 -19.915 20.148 1.00 21.28 N
 ATOM 41 CD2 PRO A 176 -40.212 -19.710 18.726 1.00 16.80 C
 ATOM 42 C PRO A 176 -40.222 -13.501 19.159 1.00 16.78 C
 ATOM 43 O CYS A 176 -39.363 -12.626 19.953 1.00 16.20 O
 ATOM 44 CB CYS A 176 -40.222 -13.501 19.159 1.00 16.59 C
 ATOM 45 SG CYS A 176 -40.885 -13.084 16.644 1.00 15.59 S
 ATOM 46 N ARG A 177 -41.200 -13.469 20.062 1.00 17.53 N
 ATOM 47 CA ARG A 177 -41.351 -12.238 20.384 1.00 18.15 C
 ATOM 48 CB ARG A 177 -41.351 -12.238 20.384 1.00 18.15 C
 ATOM 49 O ARG A 177 -39.040 -11.088 22.053 1.00 17.51 O
 ATOM 50 CG ARG A 177 -42.634 -12.458 21.887 1.00 18.62 C
 ATOM 51 CD ARG A 177 -42.634 -11.474 22.713 1.00 20.72 C
 ATOM 52 ND ARG A 177 -44.337 -11.493 22.713 1.00 18.66 C
 ATOM 53 NE ARG A 177 -44.366 -10.263 24.391 1.00 24.94 N
 ATOM 54 CZ ARG A 177 -43.848 -10.348 25.516 1.00 25.91 C
 ATOM 55 NH1 ARG A 177 -42.384 -11.413 25.083 1.00 25.24 N
 ATOM 56 NH2 ARG A 177 -42.384 -11.413 25.083 1.00 25.28 N
 ATOM 57 N ILE A 178 -39.076 -13.324 22.435 1.00 18.26 C
 ATOM 58 CA ILE A 178 -38.446 -13.332 23.221 1.00 18.88 C
 ATOM 59 CB ILE A 178 -37.347 -12.889 23.221 1.00 18.95 C
 ATOM 60 CG ILE A 178 -36.549 -12.842 23.243 1.00 18.62 O
 ATOM 61 CB ILE A 178 -36.549 -12.842 23.243 1.00 18.62 O
 ATOM 62 CG1 ILE A 178 -39.219 -15.180 24.759 1.00 18.73 C
 ATOM 63 CG2 ILE A 178 -36.838 -12.842 24.621 1.00 18.59 C
 ATOM 64 CB ILE A 178 -36.838 -12.842 24.621 1.00 18.59 C
 ATOM 65 N ILE A 179 -37.888 -13.386 21.187 1.00 19.21 N
 ATOM 66 CA GLU A 179 -35.993 -12.958 20.327 1.00 19.54 C
 ATOM 67 CB GLU A 179 -36.975 -13.117 20.327 1.00 19.57 C
 ATOM 68 CG GLU A 179 -35.975 -13.745 20.346 1.00 19.32 C
 ATOM 69 CD GLU A 179 -35.948 -13.726 19.920 1.00 19.69 C
 ATOM 70 CG GLU A 179 -34.670 -13.469 18.245 1.00 21.79 C
 ATOM 71 CD2 GLU A 179 -34.670 -13.469 18.245 1.00 21.79 C
 ATOM 72 OE1 GLU A 179 -33.547 -14.596 18.979 1.00 18.63 O
 ATOM 73 OE2 GLU A 179 -35.742 -14.303 16.292 1.00 27.10 O
 ATOM 74 N LEU A 180 -37.277 -10.379 19.792 1.00 19.29 N
 ATOM 75 CB LEU A 180 -36.974 -10.379 19.792 1.00 19.29 C
 ATOM 76 C LEU A 180 -36.979 -8.659 20.588 1.00 19.08 C
 ATOM 77 O LEU A 180 -36.226 -7.704 20.241 1.00 18.14 O
 ATOM 78 CB LEU A 180 -38.974 -9.273 19.106 1.00 19.11 C
 ATOM 79 CG LEU A 180 -39.319 -7.798 18.847 1.00 19.07 C

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ATOM	79	LEU	A	188	-39.319	-7.798	18.847	1.00	19.97	C		
ATOM	80	CD1	LEU	A	-39.319	-7.798	18.847	1.00	21.10	C		
ATOM	81	CD2	LEU	A	188	-48.838	-7.649	18.014	1.00	19.74	C	
ATOM	82	N	TYR	A	181	-37.358	-8.954	21.751	1.00	19.10	N	
ATOM	83	CA	TYR	A	181	-36.842	-8.229	22.914	1.00	19.73	C	
ATOM	84	C	TYR	A	181	-35.332	-8.146	23.081	1.00	19.56	C	
ATOM	85	O	TYR	A	181	-35.008	-7.175	23.148	1.00	19.98	O	
ATOM	86	CB	TYR	A	181	-37.467	-8.751	24.227	1.00	20.16	C	
ATOM	87	CG	TYR	A	181	-38.813	-8.123	24.527	1.00	20.84	C	
ATOM	88	CD1	TYR	A	181	-38.915	-7.084	25.358	1.00	21.48	C	
ATOM	89	CD2	TYR	A	181	-39.319	-7.798	18.847	1.00	21.31	C	
ATOM	90	CE1	TYR	A	181	-48.147	-6.422	25.633	1.00	22.34	C	
ATOM	91	CE2	TYR	A	181	-41.238	-8.868	24.244	1.00	21.91	C	
ATOM	92	CZ	TYR	A	181	-41.308	-6.959	25.082	1.00	22.24	C	
ATOM	93	OH	TYR	A	181	-42.518	-6.773	23.785	1.00	22.59	O	
ATOM	94	CHG	TYR	A	181	-38.117	-9.443	22.797	1.00	19.68	H	
ATOM	95	CA	ARG	A	182	-33.268	-9.544	22.849	1.00	20.05	C	
ATOM	96	C	ARG	A	182	-32.593	-8.739	21.743	1.00	19.42	C	
ATOM	97	O	ARG	A	182	-31.576	-8.072	21.998	1.00	19.22	O	
ATOM	98	CB	ARG	A	182	-32.690	-8.146	21.966	1.00	19.55	C	
ATOM	99	CG	ARG	A	182	-31.592	-11.864	23.406	1.00	21.33	C	
ATOM	100	CD	ARG	A	182	-32.609	-12.324	24.417	1.00	31.98	C	
ATOM	101	NE	ARG	A	182	-32.238	-13.693	24.076	1.00	34.53	N	
ATOM	102	CE	ARG	A	182	-32.723	-14.306	23.285	1.00	35.34	C	
ATOM	103	NH1	ARG	A	182	-33.064	-14.685	23.626	1.00	35.99	N	
ATOM	104	NH2	ARG	A	182	-32.223	-15.866	24.975	1.00	37.59	N	
ATOM	105	N	VAL	A	183	-33.164	-8.795	20.537	1.00	18.69	N	
ATOM	106	CA	VAL	A	183	-32.586	-8.101	19.374	1.00	18.83	C	
ATOM	107	O	VAL	A	183	-32.679	-8.161	19.548	1.00	18.48	O	
ATOM	108	CB	VAL	A	183	-31.093	-8.875	19.318	1.00	18.13	O	
ATOM	109	CG1	VAL	A	183	-32.244	-8.558	18.037	1.00	18.63	C	
ATOM	110	CG2	VAL	A	183	-32.873	-7.606	16.895	1.00	19.70	C	
ATOM	111	OG1	VAL	A	183	-32.886	-9.939	17.689	1.00	18.83	C	
ATOM	112	OG2	VAL	A	183	-32.202	-7.606	16.895	1.00	19.53	N	
ATOM	113	CA	VAL	A	184	-34.017	-4.667	29.304	1.00	19.93	C	
ATOM	114	C	VAL	A	184	-32.987	-4.148	21.338	1.00	19.24	C	
ATOM	115	O	VAL	A	184	-32.377	-3.081	21.136	1.00	18.61	O	
ATOM	116	CB	VAL	A	184	-30.921	-4.148	21.338	1.00	19.12	C	
ATOM	117	CG1	VAL	A	184	-35.606	-2.937	11.114	1.00	20.37	C	
ATOM	118	CG2	VAL	A	184	-36.407	-4.148	19.532	1.00	18.87	C	
ATOM	119	N	GLU	A	185	-31.793	-4.545	23.423	1.00	20.57	N	
ATOM	120	CA	GLU	A	185	-30.538	-5.002	24.147	1.00	21.40	C	
ATOM	121	O	GLU	A	185	-29.614	-3.546	23.148	1.00	19.76	O	
ATOM	122	CB	GLU	A	185	-29.614	-3.546	23.148	1.00	19.76	O	

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ATOM	122	O	GLU	A	185	-29.614	-3.546	23.148	1.00	19.76	O	
ATOM	123	CB	GLU	A	185	-31.588	-5.488	24.638	1.00	20.14	C	
ATOM	124	CG	GLU	A	185	-30.953	-5.110	25.786	1.00	22.36	C	
ATOM	125	CD	GLU	A	185	-31.034	-6.061	26.975	1.00	22.86	C	
ATOM	126	OE1	GLU	A	185	-31.853	-7.082	26.951	1.00	27.18	O	
ATOM	127	OE2	GLU	A	185	-30.925	-7.082	26.951	1.00	27.18	O	
ATOM	128	N	SER	A	186	-29.073	-5.517	22.186	1.00	19.89	N	
ATOM	129	CA	SER	A	186	-28.627	-5.563	21.568	1.00	20.62	C	
ATOM	130	C	SER	A	186	-28.397	-4.432	20.505	1.00	19.65	C	
ATOM	131	O	SER	A	186	-27.329	-3.818	20.489	1.00	18.81	O	
ATOM	132	CB	SER	A	186	-29.602	-5.000	20.809	1.00	20.59	C	
ATOM	133	OG	SER	A	186	-28.358	-7.942	21.792	1.00	21.17	O	
ATOM	134	N	LEU	A	187	-29.496	-4.171	19.676	1.00	19.21	N	
ATOM	135	CA	LEU	A	187	-29.344	-3.078	18.768	1.00	19.74	C	
ATOM	136	O	LEU	A	187	-29.183	-1.718	19.393	1.00	19.37	C	
ATOM	137	D	LEU	A	187	-29.075	-1.025	19.393	1.00	19.37	O	
ATOM	138	CB	LEU	A	187	-28.559	-3.047	17.833	1.00	19.81	C	
ATOM	139	CG	LEU	A	187	-30.623	-3.969	16.619	1.00	21.86	C	
ATOM	140	CD1	LEU	A	187	-32.832	-3.991	16.073	1.00	24.65	C	
ATOM	141	CD2	LEU	A	187	-29.626	-3.528	15.532	1.00	24.78	C	
ATOM	142	N	ALA	A	188	-29.794	-2.847	21.432	1.00	21.38	N	
ATOM	143	CA	ALA	A	188	-29.866	-0.279	21.519	1.00	19.62	C	
ATOM	144	C	ALA	A	188	-28.484	-0.122	21.799	1.00	19.76	C	
ATOM	145	O	ALA	A	188	-27.877	0.958	21.768	1.00	19.78	O	
ATOM	146	CB	ALA	A	188	-30.914	-0.334	22.398	1.00	19.86	C	
ATOM	147	N	LYS	A	189	-27.459	-1.228	22.859	1.00	19.74	N	
ATOM	148	CA	LYS	A	189	-26.535	-1.229	22.859	1.00	19.63	C	
ATOM	149	O	LYS	A	189	-24.637	-0.121	22.068	1.00	19.20	O	
ATOM	150	CB	LYS	A	189	-26.308	-2.544	23.588	1.00	19.67	C	
ATOM	151	N	LYS	A	189	-24.949	-2.043	24.073	1.00	21.18	N	
ATOM	152	CA	LYS	A	189	-24.291	-1.568	24.587	1.00	21.67	C	
ATOM	153	O	LYS	A	189	-23.793	-1.681	26.298	1.00	25.23	C	
ATOM	154	CB	LYS	A	189	-23.673	-0.481	26.577	1.00	21.46	N	
ATOM	155	CG	LYU	A	192	-24.277	-3.615	21.482	1.00	21.62	C	
ATOM	156	CD2	LYU	A	192	-22.849	3.877	20.973	1.00	21.84	C	
ATOM	157	O	LYU	A	192	-22.341	5.002	21.837	1.00	20.87	O	
ATOM	158	CD1	LYU	A	192	-24.637	3.095	23.571	1.00	21.24	C	
ATOM	159	CG	LYU	A	192	-25.645	-3.577	23.531	1.00	21.00	C	
ATOM	160	CD	LYU	A	192	-25.689	2.475	24.965	1.00	22.37	C	
ATOM	161	OE1	GLU	A	192	-24.666	1.990	25.496	1.00	22.99	O	
ATOM	162	OE2	GLU	A	192	-26.783	2.565	25.568	1.00	25.93	O	
ATOM	163	N	THR	A	193	-22.217	2.832	20.458	1.00	22.20	N	
ATOM	164	CA	THR	A	193	-22.913	2.913	20.458	1.00	22.20	C	
ATOM	165	O	THR	A	193	-22.673	2.774	18.526	1.00	24.43	O	
ATOM	166	CB	THR	A	193	-28.673	-1.247	22.859	1.00	21.61	C	
ATOM	167	O	THR	A	193	-29.057	-2.654	18.023	1.00	23.11	O	
ATOM	168	CG1	THR	A	193	-28.008	0.538	20.378	1.00	22.12	C	
ATOM	169	CG2	THR	A	193	-19.949	1.958	22.267	1.00	20.80	C	
ATOM	170	SD	SER	A	194	-21.098	-0.589	21.463	1.00	26.17	N	
ATOM	171	SE	SER	A	194	-21.785	2.582	16.374	1.00	28.66	C	
ATOM	172	C	SER	A	194	-20.976	3.535	15.687	1.00	30.43	C	
ATOM	173	O	SER	A	194	-21.196	4.739	15.764	1.00	30.63	O	
ATOM	174	CB	SER	A	194	-23.206	2.411	15.888	1.00	28.78	C	
ATOM	175	OG	SER	A	194	-24.178	2.059	14.427	1.00	29.52	O	
ATOM	176	SG	SER	A	194	-20.443	3.445	14.772	1.00	29.52	N	
ATOM	177	CA	GLY	A	195	-19.179	3.890	13.965	1.00	34.45	C	
ATOM</td												

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ATOM	288	O	GLU	A	197	-26.494	-8.597	0.877	1.00	38.98
ATOM	289	CB	GLU	A	197	-25.821	3.766	10.445	1.00	39.07
ATOM	290	CD	GLU	A	197	-27.249	7.239	10.822	1.00	40.48
ATOM	291	CI	GLU	A	197	-27.277	8.398	11.829	1.00	42.86
ATOM	292	OE1	GLU	A	197	-27.259	8.199	10.749	1.00	43.49
ATOM	293	OE2	GLU	A	197	-28.241	8.474	12.621	1.00	43.51
ATOM	294	N	ILE	A	198	-26.691	3.233	10.722	1.00	37.57
ATOM	295	C	ILE	A	198	-27.441	2.181	10.820	1.00	36.57
ATOM	296	CA	ILE	A	198	-27.459	1.509	10.760	1.00	37.59
ATOM	297	O	ILE	A	198	-29.574	3.164	10.616	1.00	36.01
ATOM	298	CB	ILE	A	198	-27.389	0.782	10.718	1.00	36.84
ATOM	299	CG1	ILE	A	198	-28.087	0.874	12.705	1.00	37.53
ATOM	300	CG2	ILE	A	198	-28.441	0.875	12.703	1.00	37.54
ATOM	301	CD1	ILE	A	198	-28.621	-0.537	12.539	1.00	38.43
ATOM	302	N	SER	A	199	-29.326	2.382	8.516	1.00	33.45
ATOM	303	CA	SER	A	199	-29.296	1.303	8.899	1.00	32.72
ATOM	304	CB	SER	A	199	-31.578	1.628	9.455	1.00	29.24
ATOM	305	O	SER	A	199	-32.779	1.798	7.759	1.00	28.70
ATOM	306	CB	SER	A	199	-38.596	3.555	6.726	1.00	31.53
ATOM	307	OD1	SER	A	199	-39.501	3.595	6.740	1.00	31.46
ATOM	308	LYS	A	200	-30.993	0.420	8.874	1.00	26.73	
ATOM	309	CA	LYS	A	200	-31.745	-0.835	7.833	1.00	24.20
ATOM	310	C	LYS	A	200	-31.280	-1.829	8.889	1.00	23.56
ATOM	311	CA	LYS	A	200	-31.284	-1.824	8.884	1.00	23.53
ATOM	312	CB	LYS	A	200	-31.682	-1.479	6.448	1.00	24.17
ATOM	313	CD	LYS	A	200	-32.216	-0.669	5.294	1.00	23.41
ATOM	314	CD2	LYS	A	200	-32.280	-1.139	3.983	1.00	23.52
ATOM	315	CD	LYS	A	200	-32.779	-0.443	3.981	1.00	21.93
ATOM	316	N	PHE	A	201	-31.331	0.512	2.647	1.00	19.78
ATOM	317	C	PHE	A	201	-32.192	-2.617	9.451	1.00	22.85
ATOM	318	CA	PHE	A	201	-32.461	-2.870	11.024	1.00	22.49
ATOM	319	O	PHE	A	201	-32.776	-4.767	10.407	1.00	22.14
ATOM	320	O	PHE	A	201	-33.918	-4.484	10.190	1.00	21.35
ATOM	321	CB	PHE	A	201	-31.465	-3.031	11.816	1.00	23.03
ATOM	322	CD1	PHE	A	201	-32.345	-3.034	11.814	1.00	23.03
ATOM	323	CD2	PHE	A	201	-33.788	-2.569	12.083	1.00	25.93
ATOM	324	CZ	PHE	A	201	-33.333	0.213	12.493	1.00	24.45
ATOM	325	CD1	PHE	A	201	-33.433	-10.489	11.816	1.00	24.52
ATOM	326	CD2	PHE	A	201	-35.911	-9.476	10.324	1.00	23.91
ATOM	327	CZ	PHE	A	201	-34.317	-11.546	12.043	1.00	24.21
ATOM	328	N	TYR	A	202	-35.987	-10.524	10.551	1.00	23.78
ATOM	329	CA	TYR	A	202	-36.001	-9.925	10.579	1.00	23.70
ATOM	330	O	TYR	A	202	-36.987	-6.928	11.142	1.00	23.48
ATOM	331	CB	TYR	A	202	-33.256	-7.283	13.524	1.00	22.87

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ATOM	251	O	TYR	A	202	-33.256	-7.283	13.524	1.00	22.87
ATOM	252	CB	TYR	A	202	-32.882	-8.293	10.713	1.00	23.34
ATOM	253	CD	TYR	A	202	-32.926	-9.265	10.743	1.00	23.38
ATOM	254	CD1	TYR	A	202	-33.433	-10.489	11.816	1.00	24.52
ATOM	255	CD2	TYR	A	202	-35.911	-9.476	10.324	1.00	23.91
ATOM	256	CE1	TYR	A	202	-34.317	-11.546	12.043	1.00	24.21
ATOM	257	CE2	TYR	A	202	-35.987	-10.524	10.551	1.00	23.78
ATOM	258	CZ	TYR	A	202	-36.001	-9.925	10.579	1.00	23.48
ATOM	259	N	TYR	A	202	-36.437	-12.599	11.636	1.00	24.47
ATOM	260	CA	LEU	A	203	-35.259	-6.766	12.635	1.00	21.56
ATOM	261	CB	LEU	A	203	-36.079	-6.988	13.887	1.00	21.32
ATOM	262	C	LEU	A	203	-36.996	-8.155	13.453	1.00	20.36
ATOM	263	D	LEU	A	203	-37.494	-8.849	12.602	1.00	20.70
ATOM	264	CB	LEU	A	203	-36.957	-5.142	11.448	1.00	21.26
ATOM	265	CG	LEU	A	203	-36.545	-4.765	15.215	1.00	23.82
ATOM	266	CD1	LEU	A	203	-35.859	-4.627	15.328	1.00	23.04
ATOM	267	CD2	LEU	A	203	-37.218	-3.428	14.951	1.00	22.01
ATOM	268	CZ	LEU	A	203	-37.981	-3.259	14.800	1.00	19.27
ATOM	269	CA	PRO	A	204	-37.883	-10.360	14.800	1.00	19.39
ATOM	270	C	PRO	A	204	-39.312	-9.861	13.811	1.00	18.61
ATOM	271	O	PRO	A	204	-39.777	-9.035	14.618	1.00	18.19
ATOM	272	CB	PRO	A	204	-37.765	-11.194	15.288	1.00	19.29
ATOM	273	CG	PRO	A	204	-38.433	-10.850	15.789	1.00	19.53
ATOM	274	CD	PRO	A	204	-38.632	-9.548	15.782	1.00	19.29
ATOM	275	N	ASN	A	205	-39.969	-18.324	12.769	1.00	17.98
ATOM	276	CA	ASN	A	205	-41.355	-9.968	12.495	1.00	18.18
ATOM	277	C	ASN	A	205	-42.247	-11.006	13.181	1.00	18.05
ATOM	278	O	ASN	A	205	-42.446	-11.006	12.702	1.00	18.05
ATOM	279	CB	ASN	A	205	-41.669	-9.983	10.987	1.00	18.39
ATOM	280	CG	ASN	A	205	-40.668	-9.188	10.187	1.00	18.90
ATOM	281	OD1	ASN	A	205	-40.832	-9.161	8.888	1.00	22.20
ATOM	282	ND2	ASN	A	205	-39.657	-8.569	10.699	1.00	19.63
ATOM	283	H	CYS	A	206	-42.838	-10.204	14.338	1.00	17.88
ATOM	284	CA	CYS	A	206	-42.935	-11.532	10.596	1.00	18.63
ATOM	285	C	CYS	A	206	-45.118	-11.479	14.845	1.00	18.36
ATOM	286	O	CYS	A	206	-45.623	-10.361	14.652	1.00	18.35
ATOM	287	CB	CYS	A	206	-43.376	-11.456	16.612	1.00	17.73
ATOM	288	SG	CYS	A	206	-44.188	-11.456	17.755	1.00	17.73
ATOM	289	N	ASN	A	207	-45.824	-12.619	14.844	1.00	18.54
ATOM	290	CA	ASN	A	207	-47.282	-12.593	14.923	1.00	18.73
ATOM	291	C	ASN	A	207	-47.713	-12.386	16.381	1.00	19.14
ATOM	292	O	ASN	A	207	-46.874	-12.481	17.293	1.00	19.85
ATOM	293	CB	ASN	A	207	-47.916	-13.848	14.274	1.00	18.43
ATOM	294	CG	ASN	A	207	-47.669	-15.147	15.029	1.00	18.66

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ATOM	314	CG	ASH	A	209	-51.689	-15.147	15.629	1.00	23.95
ATOM	315	CD1	ASH	A	209	-49.747	-14.753	19.524	1.00	23.96
ATOM	316	ND2	ASH	A	209	-47.442	-16.236	14.278	1.00	19.03
ATOM	317	N	LYS	A	208	-49.812	-12.189	16.598	1.00	19.78
ATOM	318	CA	LYS	A	208	-49.588	-11.893	17.916	1.00	20.21
ATOM	319	C	LYS	A	208	-49.491	-13.063	18.913	1.00	20.88
ATOM	320	O	LYS	A	208	-49.635	-12.868	20.118	1.00	20.32
ATOM	321	CB	LYS	A	208	-51.043	-11.459	17.777	1.00	20.47
ATOM	322	CD	LYS	A	208	-53.396	-12.222	17.359	1.00	22.48
ATOM	323	CE	LYS	A	208	-54.291	-13.223	16.642	1.00	20.94
ATOM	324	NZ	LYS	A	208	-54.187	-14.667	17.174	1.00	20.34
ATOM	325	N	ASH	A	209	-49.288	-14.275	18.399	1.00	19.57
ATOM	326	CA	ASH	A	209	-49.083	-13.845	19.247	1.00	19.88
ATOM	327	O	ASH	A	209	-49.325	-15.539	19.279	1.00	22.32
ATOM	328	O	ASH	A	209	-47.304	-16.579	20.421	1.00	19.64
ATOM	329	CB	ASH	A	209	-49.558	-16.736	18.588	1.00	19.75
ATOM	330	CG	ASH							

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ATOM	337	CE1	TYR A	212	-39.221	-17.434	15.777	1.00	18.28	C
ATOM	338	CD2	TYR A	212	-38.507	-16.344	15.829	1.00	18.75	C
ATOM	339	CZ	TYR A	212	-38.563	-16.344	15.829	1.00	18.78	C
ATOM	340	OH	TYR A	212	-37.375	-16.282	16.786	1.00	18.15	O
ATOM	341	N	HIS A	213	-44.028	-14.572	11.673	1.00	17.97	N
ATOM	342	CA	HIS A	213	-44.678	-14.469	10.361	1.00	18.14	C
ATOM	343	C	HIS A	213	-43.859	-15.264	9.341	1.00	17.86	C
ATOM	344	CD1	HIS A	213	-42.632	-15.085	9.449	1.00	17.13	O
ATOM	345	CB	HIS A	213	-44.084	-13.095	9.361	1.00	18.71	C
ATOM	346	CG	HIS A	213	-45.862	-12.251	10.673	1.00	19.72	C
ATOM	347	ND1	HIS A	213	-47.197	-12.594	10.619	1.00	20.89	N
ATOM	348	CD2	HIS A	213	-45.784	-11.167	11.480	1.00	20.00	C
ATOM	349	CE1	HIS A	213	-47.894	-11.761	11.371	1.00	21.53	C
ATOM	350	NE2	HIS A	213	-47.002	-10.935	11.987	1.00	21.46	N
ATOM	351	O	ASP A	214	-44.633	-15.322	8.011	1.00	17.93	O
ATOM	352	CA	SER A	214	-43.835	-16.637	7.317	1.00	19.18	C
ATOM	353	C	SER A	214	-42.890	-15.727	6.548	1.00	18.32	C
ATOM	354	O	SER A	214	-41.765	-16.493	6.253	1.00	18.58	O
ATOM	355	CB	SER A	214	-44.838	-17.298	6.356	1.00	19.46	C
ATOM	356	OG	SER A	214	-45.258	-18.538	6.894	1.00	23.83	O
ATOM	357	SG	SER A	214	-45.393	-18.500	6.902	1.00	23.72	S
ATOM	358	CA	ARG A	215	-42.464	-13.537	5.651	1.00	18.42	C
ATOM	359	C	ARG A	215	-41.666	-12.826	6.745	1.00	17.97	C
ATOM	360	O	ARG A	215	-42.248	-12.338	7.726	1.00	19.64	O
ATOM	361	CB	ARG A	215	-43.275	-12.525	4.835	1.00	18.99	C
ATOM	362	CG	ARG A	215	-42.421	-11.489	4.108	1.00	19.38	C
ATOM	363	OD1	ARG A	215	-43.364	-10.488	3.869	1.00	20.46	O
ATOM	364	NE	ARG A	215	-43.164	-9.573	4.697	1.00	20.02	N
ATOM	365	CZ	ARG A	215	-44.864	-8.786	4.586	1.00	22.74	C
ATOM	366	NH1	ARG A	215	-45.467	-8.518	3.418	1.00	23.51	N
ATOM	367	NH2	ARG A	215	-45.282	-8.948	5.656	1.00	23.68	N
ATOM	368	N	GLN A	216	-48.348	-12.761	6.573	1.00	17.58	N
ATOM	369	CA	GLN A	216	-49.481	-11.798	7.029	1.00	18.43	C
ATOM	370	C	GLN A	216	-48.818	-10.882	6.577	1.00	18.61	C
ATOM	371	O	GLN A	216	-48.184	-11.199	5.561	1.00	16.53	O
ATOM	372	CB	GLN A	216	-48.417	-12.769	8.151	1.00	16.94	C
ATOM	373	CG	GLN A	216	-38.974	-13.769	9.161	1.00	16.52	C
ATOM	374	CD	GLN A	216	-39.649	-13.095	10.339	1.00	16.89	C
ATOM	375	OE1	GLN A	216	-39.872	-12.248	11.021	1.00	16.64	O
ATOM	376	OE2	GLN A	216	-40.103	-12.747	10.609	1.00	17.09	O
ATOM	377	N	CYS A	217	-38.912	-9.625	7.814	1.00	16.94	N
ATOM	378	CA	CYS A	217	-38.270	-8.525	6.294	1.00	16.91	C
ATOM	379	C	CYS A	217	-37.384	-7.678	7.198	1.00	16.97	C
ATOM	380	O	CYS A	217	-37.647	-7.538	8.411	1.00	16.75	O

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ATOM	380	O	CYS A	217	-37.647	-7.538	8.411	1.00	16.75	O
ATOM	381	CA	CYS A	217	-39.320	-7.622	5.639	1.00	17.22	C
ATOM	382	SG	CYS A	217	-40.478	-8.464	4.537	1.00	18.26	S
ATOM	383	N	GLU A	218	-36.340	-7.121	6.592	1.00	16.79	N
ATOM	384	CA	GLU A	218	-35.546	-6.969	7.216	1.00	18.15	C
ATOM	385	C	GLU A	218	-36.424	-4.859	7.451	1.00	17.77	C
ATOM	386	O	GLU A	218	-37.605	-4.777	6.055	1.00	17.55	O
ATOM	387	CB	GLU A	218	-34.398	-5.636	6.313	1.00	18.22	C
ATOM	388	CG	GLU A	218	-33.278	-6.626	6.156	1.00	21.61	C
ATOM	389	CD	GLU A	218	-32.280	-6.998	5.225	1.00	24.73	C
ATOM	390	OE1	GLU A	218	-31.088	-6.339	5.502	1.00	27.34	O
ATOM	391	OE2	GLU A	218	-32.550	-5.418	4.222	1.00	24.10	O
ATOM	392	N	THR A	219	-36.117	-4.151	8.538	1.00	17.82	N
ATOM	393	CA	THR A	219	-36.720	-2.866	8.838	1.00	17.58	C
ATOM	394	C	THR A	219	-35.780	-3.079	8.149	1.00	17.59	C
ATOM	395	OD1	THR A	219	-34.672	-1.753	8.324	1.00	17.92	O
ATOM	396	CB	THR A	219	-36.884	-2.634	10.359	1.00	17.50	C
ATOM	397	OG1	THR A	219	-37.707	-3.591	10.934	1.00	17.69	O
ATOM	398	CG2	THR A	219	-37.329	-1.232	10.673	1.00	16.71	C
ATOM	399	N	SER A	220	-36.592	-0.985	7.431	1.00	18.10	N
ATOM	400	CA	SER A	220	-35.936	0.177	6.727	1.00	18.76	C
ATOM	401	C	SER A	220	-36.502	1.537	7.156	1.00	18.01	C
ATOM	402	O	SER A	220	-37.691	1.676	7.389	1.00	18.11	O
ATOM	403	CB	SER A	220	-37.007	-0.810	5.039	1.00	19.06	C
ATOM	404	CG	SER A	220	-35.857	-1.208	5.553	1.00	22.71	O
ATOM	405	N	MET A	221	-35.635	2.537	7.222	1.00	18.98	N
ATOM	406	CA	MET A	221	-36.036	2.993	7.588	1.00	21.13	C
ATOM	407	C	MET A	221	-35.384	4.915	6.636	1.00	20.38	C
ATOM	408	O	MET A	221	-35.168	4.072	7.002	1.00	19.76	O
ATOM	409	CB	MET A	221	-35.626	4.216	9.027	1.00	20.63	C
ATOM	410	CG	MET A	221	-36.286	3.349	16.896	1.00	22.82	C
ATOM	411	SD	MET A	221	-35.781	3.885	11.761	1.00	20.45	S
ATOM	412	CE	MET A	221	-36.064	2.409	12.074	1.00	25.56	C
ATOM	413	N	ASP A	222	-35.873	4.479	5.418	1.00	28.49	N
ATOM	414	CA	ASP A	222	-34.270	5.298	4.508	1.00	28.45	C
ATOM	415	C	ASP A	222	-34.877	5.473	3.121	1.00	28.58	C
ATOM	416	O	ASP A	222	-34.288	5.977	2.228	1.00	28.57	O
ATOM	417	CB	ASP A	222	-32.856	4.725	4.386	1.00	20.76	C
ATOM	418	CG	ASP A	222	-32.849	3.279	3.882	1.00	20.03	C
ATOM	419	OD1	ASP A	222	-31.774	2.668	3.937	1.00	22.26	O
ATOM	420	OD2	ASP A	222	-32.935	3.030	3.945	1.00	23.53	O
ATOM	421	CA	GLY A	223	-36.125	5.041	9.943	1.00	28.55	N
ATOM	422	CA	GLY A	223	-36.815	5.170	1.658	1.00	21.58	C
ATOM	423	C	GLY A	223	-36.488	4.069	0.668	1.00	21.57	C

Select khush@DESKTOP-DE71GO3:~/Lab_session3/Lab_assignment3										
ATOM	423	C	GLY A	223	-36.480	4.069	0.668	1.00	21.57	C
ATOM	424	O	GLY A	223	-36.861	4.134	-0.498	1.00	21.96	O
ATOM	425	N	GLU A	224	-35.939	5.318	1.061	1.00	23.86	N
ATOM	426	CA	GLU A	224	-34.450	1.091	0.324	1.00	21.72	C
ATOM	427	CA	GLU A	224	-36.126	0.661	0.914	1.00	21.14	C
ATOM	428	O	GLU A	224	-36.255	0.536	2.135	1.00	20.93	O
ATOM	429	CA	GLU A	224	-33.948	1.673	0.260	1.00	22.89	C
ATOM	430	CB	GLU A	224	-33.177	2.741	-0.500	1.00	24.47	C
ATOM	431	CD	GLU A	224	-31.207	1.510	0.038	1.00	30.43	O
ATOM	432	OE1	GLU A	224	-31.207	1.510	0.038	1.00	30.43	O
ATOM	433	OE2	GLU A	224	-30.980	3.638	-0.483	1.00	31.11	O
ATOM	434	N	ALA A	225	-36.575	-0.234	0.839	1.00	29.59	N
ATOM	435	CA	ALA A	225	-37.186	-1.493	0.463	1.00	28.30	C
ATOM	436	C	ALA A	225	-37.261	-1.251	1.028	1.00	29.53	C
ATOM	437	O	ALA A	225	-35.013	-2.494	0.724	1.00	19.69	O
ATOM	438	CB	ALA A	225	-37.732	-2.236	-0.750	1.00	20.55	C
ATOM	439	N	GLY A	226	-35.537	-2.937	2.327	1.00	19.28	N
ATOM	440	CA	GLY A	226	-35.705	-3.955	2.			

Select khushi@DESKTOP-DE71G03: ~/Lab_session3/Lab_assignment3

ATOM	500	CG1 TRP A 239	-34.964 -13.238	6.679	1.00 10.97	C
ATOM	467	CE3 TRP A 239	-34.964 -13.239	6.673	1.00 10.95	C
ATOM	468	CZ2 TRP A 239	-34.541 -12.251	7.739	1.00 20.31	C
ATOM	469	CZ3 TRP A 239	-34.324 -10.728	5.858	1.00 19.70	C
ATOM	478	CH2 TRP A 239	-34.228 -11.008	7.234	1.00 19.70	C
ATOM	473	N CYS A 230	-38.301 -16.079	3.450	1.00 18.85	N
ATOM	474	O CYS A 230	-38.301 -16.079	3.450	1.00 18.85	O
ATOM	475	CA CYS A 230	-38.794 -17.854	5.106	1.00 18.59	C
ATOM	476	O CYS A 230	-37.736 -18.464	4.946	1.00 18.93	O
ATOM	478	SG CYS A 230	-40.004 -17.763	2.915	1.00 19.33	S
ATOM	479	CB CYS A 230	-40.638 -16.761	1.539	1.00 21.99	C
ATOM	480	CG CYS A 230	-40.638 -16.761	6.079	1.00 21.97	C
ATOM	478	CA VAL A 231	-39.114 -18.799	-3.338	1.00 17.92	N
ATOM	479	C VAL A 231	-40.282 -19.781	7.737	1.00 17.70	C
ATOM	480	O VAL A 231	-41.346 -19.646	7.341	1.00 17.73	O
ATOM	481	CB VAL A 231	-38.723 -17.948	8.571	1.00 18.20	C
ATOM	482	CG1 VAL A 231	-37.946 -17.948	8.121	1.00 18.39	C
ATOM	483	C2 VAL A 231	-39.946 -17.177	8.525	1.00 18.07	N
ATOM	484	N TYR A 232	-39.826 -20.793	9.268	1.00 18.07	C
ATOM	485	O TYR A 232	-40.881 -21.624	5.592	1.00 18.92	O
ATOM	486	CA TYR A 232	-41.359 -20.832	10.407	1.00 17.88	C
ATOM	487	O TYR A 232	-41.359 -20.832	10.407	1.00 17.88	O
ATOM	488	CB TYR A 232	-40.147 -22.912	9.681	1.00 18.50	C
ATOM	489	CG TYR A 232	-39.552 -23.774	8.570	1.00 18.40	C
ATOM	490	CD1 TYR A 232	-40.379 -24.437	7.660	1.00 20.13	C
ATOM	491	CD2 TYR A 232	-38.167 -23.966	8.470	1.00 18.40	C
ATOM	492	O TYR A 232	-39.946 -21.774	6.465	1.00 18.40	C
ATOM	492	CZ2 TYR A 232	-37.657 -24.774	6.570	1.00 19.11	C
ATOM	494	CZ TYR A 232	-38.465 -25.404	6.570	1.00 19.11	C
ATOM	495	OH TYR A 232	-37.938 -26.204	5.592	1.00 18.92	O
ATOM	496	N PRO A 233	-42.695 -20.681	10.497	1.00 18.03	N
ATOM	497	O PRO A 233	-42.695 -20.681	10.497	1.00 18.03	O
ATOM	498	CB PRO A 233	-42.992 -20.309	13.824	1.00 17.82	C
ATOM	499	O PRO A 233	-42.882 -19.469	13.932	1.00 17.24	O
ATOM	500	CB PRO A 233	-44.765 -19.946	11.362	1.00 17.97	C
ATOM	501	CG PRO A 233	-44.897 -20.250	9.893	1.00 18.42	C
ATOM	502	CD PRO A 233	-43.919 -20.250	10.429	1.00 18.21	C
ATOM	503	N ASN A 235	-42.634 -21.598	12.224	1.00 17.93	N
ATOM	504	O ASN A 235	-42.345 -22.099	14.563	1.00 17.85	C
ATOM	505	C TRP A 234	-40.928 -21.831	15.057	1.00 17.77	C
ATOM	506	O TRP A 234	-40.784 -21.864	16.268	1.00 18.66	O
ATOM	507	CB TRP A 234	-41.958 -24.497	13.754	1.00 16.26	C
ATOM	508	CG TRP A 234	-40.786 -25.170	13.983	1.00 17.91	C

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Select khushi@DESKTOP-DFT1GO2: ~/Lab_sessions/Lab_assignment3									
ATOM	505	CSD	IILE	A	241	-38.172	-18.846	-0.832	1.00 25..35
ATOM	506	CSD	IILE	A	245	-35.325	-11.466	-4.663	1.00 24..89
ATOM	507	CSD	IILE	A	245	-39.497	-18.707	-3.934	1.00 26..29
ATOM	508	N	ARG	A	246	-36..084	-7.648	-2.381	1.00 24..57
ATOM	509	C	ARG	A	246	-36..526	-6..407	-1.793	1.00 24..09
ATOM	600	C	ARG	A	246	-37..988	-6..209	-2.186	1.00 23..73
ATOM	601	O	ARG	A	246	-38..334	-5..376	-3..019	1.00 22..92
ATOM	602	CB	ARG	A	246	-35..657	-5..266	-2..156	1.00 24..34
ATOM	603	CD	ARG	A	246	-36..392	-5..035	-1..000	1.00 24..30
ATOM	604	CD	ARG	A	246	-33..359	-4..136	-0..804	1.00 25..90
ATOM	605	NE	ARG	A	246	-32..028	-4..466	-1..317	1.00 27..80
ATOM	606	CZ	ARG	A	246	-31..617	-4..321	-0..057	1.00 28..42
ATOM	607	NH1	ARG	A	246	-32..447	-3..835	0..878	1.00 27..71
ATOM	608	NH2	ARG	A	246	-30..378	-4..676	0..281	1.00 29..27
ATOM	609	N	GLY	A	247	-38..835	-7..026	-1..588	1.00 23..42
ATOM	610	CA	GLY	A	247	-48..259	-7..839	-1..851	1.00 24..81
ATOM	611	O	GLY	A	247	-49..157	-8..523	-1..000	1.00 24..55
ATOM	612	O	GLY	A	247	-49..888	-9..977	-0..649	1.00 24..29
ATOM	613	N	ASP	A	248	-42..149	-8..488	-1..235	1.00 25..16
ATOM	614	CA	ASP	A	248	-42..824	-9..555	-0..633	1.00 26..30
ATOM	615	C	ASP	A	248	-42..603	-10..798	-1..592	1.00 26..46
ATOM	616	O	ASP	A	248	-43..038	-10..838	-2..651	1.00 26..50
ATOM	617	CB	ASP	A	248	-44..319	-9..259	-0..467	1.00 26..46
ATOM	618	CD	ASP	A	248	-45..837	-18..213	0..488	1.00 27..46
ATOM	619	OD1	ASP	A	248	-45..273	-12..662	0..000	1.00 25..63
ATOM	620	OD2	ASP	A	248	-44..774	-11..481	0..312	1.00 29..19
ATOM	621	N	PRO	A	249	-41..919	-11..325	-0..954	1.00 27..01
ATOM	622	CA	PRO	A	249	-41..616	-13..940	-1..719	1.00 27..12
ATOM	623	C	PRO	A	249	-42..839	-13..938	-1..935	1.00 27..58
ATOM	624	O	PRO	A	249	-42..747	-14..917	-2..670	1.00 27..69
ATOM	625	CB	PRO	A	249	-48..575	-13..763	-0..842	1.00 27..25
ATOM	626	CG	PRO	A	249	-48..376	-12..767	0..238	1.00 27..27
ATOM	627	CD	PRO	A	249	-47..376	-11..765	0..115	1.00 26..62
ATOM	628	N	ASN	A	250	-43..965	-13..579	-1..315	1.00 28..06
ATOM	629	CA	ASN	A	250	-45..188	-14..384	-1..319	1.00 28..66
ATOM	630	C	ASN	A	250	-44..915	-15..768	-0..728	1.00 28..70
ATOM	631	O	ASN	A	250	-44..998	-16..798	-1..417	1.00 29..19
ATOM	632	CS	ASN	A	250	-45..827	-14..456	-2..721	1.00 29..27
ATOM	633	CG	ASN	A	250	-46..426	-13..126	-3..167	1.00 31..00
ATOM	634	OD1	ASN	A	250	-46..176	-12..000	-3..398	1.00 30..50
ATOM	635	OD2	ASN	A	250	-47..167	-11..476	-2..200	1.00 31..93
ATOM	636	N	CYS	A	251	-44..571	-15..756	0..557	1.00 28..18
ATOM	637	CA	CYS	A	251	-44..118	-16..941	1..273	1.00 27..85
ATOM	638	C	CYS	A	251	-45..248	-17..940	1..495	1.00 28..66

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[Select khushi@DESKTOP-DE71G03: ~/Lab_session3/Lab_assignment3
HETATM 682 O HOH A 33 -51.606 -11.651 21.823 1.00 29.90 0
HETATM 683 O HOH A 34 -32.561 -16.311 28.119 1.00 50.80 0
HETATM 684 O HOH A 35 -34.469 -16.004 9.163 1.00 24.81 0
HETATM 685 O HOH A 36 -31.585 -23.210 8.833 1.00 26.89 0
HETATM 686 O HOH A 37 -49.015 -19.892 20.176 1.00 31.69 0
HETATM 687 O HOH A 38 -38.973 -14.980 5.185 1.00 43.86 0
HETATM 688 O HOH A 39 -47.022 -17.146 11.346 1.00 28.11 0
HETATM 689 O HOH A 40 -38.833 -7.743 14.123 1.00 34.35 0
HETATM 690 O HOH A 41 -25.168 6.080 14.148 1.00 49.89 0
HETATM 691 O HOH A 42 -51.167 -14.258 13.359 1.00 47.34 0
CONECT 45 288
CONECT 288 45
CONECT 382 456
CONECT 456 382
CONECT 476 641
CONECT 641 476
CONECT 644 646 648
CONECT 645 647 648
CONECT 646 644 649
CONECT 647 645 649
CONECT 648 644 645
CONECT 649 646 647
khushi@DESKTOP-DE71G03:~/Lab_session3/Lab_assignment3$ sed -E '/^TER|END/!d' protein.pdb
```

21. From protein.pdb, print only the ATOM lines that do not belong to residue ARG.

```

khushi@DESKTOP-DE71GO3:~/Lab_session3/Lab_assignment3$ awk '/^ATOM/ && $4 != "ARG" {print}' protein.pdb
ATOM 1 N TRP A 172 -39.136 -21.997 24.415 1.00 34.43 N
ATOM 2 CA TRP A 172 -40.108 -20.987 24.729 1.00 34.28 C
ATOM 3 C TRP A 172 -41.493 -21.065 23.944 1.00 33.46 C
ATOM 4 O TRP A 172 -40.538 -21.065 24.418 1.00 35.12 C
ATOM 5 CB TRP A 172 -39.586 -19.534 24.418 1.00 35.12 C
ATOM 6 CG TRP A 172 -38.161 -19.292 25.025 1.00 36.34 C
ATOM 7 CD1 TRP A 172 -37.773 -19.562 26.306 1.00 37.69 C
ATOM 8 CD2 TRP A 172 -37.932 -18.693 24.384 1.00 37.47 C
ATOM 9 NE1 TRP A 172 -36.465 -19.193 26.439 1.00 37.97 N
ATOM 10 HE1 TRP A 172 -35.997 -19.209 26.334 1.00 37.93 C
ATOM 11 CE3 TRP A 172 -36.799 -18.192 23.007 1.00 37.57 C
ATOM 12 CZ2 TRP A 172 -34.725 -18.128 25.037 1.00 37.51 C
ATOM 13 CZ3 TRP A 172 -35.545 -17.671 22.802 1.00 37.85 C
ATOM 14 CH2 TRP A 172 -34.523 -17.645 23.769 1.00 37.43 C
ATOM 15 N LYS A 173 -42.355 -18.691 24.579 1.00 32.18 N
ATOM 16 CA LYS A 173 -40.342 -20.528 24.649 1.00 33.37 C
ATOM 17 C LYS A 173 -44.028 -19.684 22.914 1.00 29.85 C
ATOM 18 O LYS A 173 -44.831 -19.725 21.976 1.00 30.15 O
ATOM 19 CB LYS A 173 -44.935 -20.645 25.024 1.00 31.31 C
ATOM 20 CG LYS A 173 -46.343 -20.964 24.519 1.00 32.53 C
ATOM 21 CD LYS A 173 -47.438 -21.064 24.519 1.00 32.69 C
ATOM 22 OE1 LYS A 173 -46.318 -20.684 24.991 1.00 30.96 C
ATOM 23 NZ LYS A 173 -49.893 -20.189 25.896 1.00 34.66 N
ATOM 24 N GLU A 174 -43.288 -18.514 23.890 1.00 27.67 N
ATOM 25 CA GLU A 174 -43.337 -17.366 22.191 1.00 25.77 C
ATOM 26 C GLU A 174 -41.922 -17.014 21.728 1.00 23.54 C
ATOM 27 O GLU A 174 -41.876 -17.014 21.728 1.00 23.23 O
ATOM 28 CB GLU A 174 -43.931 -16.148 22.913 1.00 25.76 C
ATOM 29 CG GLU A 174 -43.376 -16.258 23.359 1.00 26.89 C
ATOM 30 CD GLU A 174 -45.777 -15.061 24.206 1.00 27.42 C
ATOM 31 OE1 GLU A 174 -46.102 -14.081 23.639 1.00 29.42 O
ATOM 32 OE2 GLU A 174 -45.756 -15.182 25.445 1.00 30.63 O

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khushi@DESKTOP-DE71GO3:~/Lab_session3/Lab_assignment3$ awk '/^ATOM/ && $4 != "ARG" {print}' protein.pdb
ATOM 32 OE2 GLU A 174 -45.756 -15.182 25.445 1.00 30.63 O
ATOM 33 N PRO A 175 -41.313 -17.867 20.872 1.00 21.55 N
ATOM 34 CA PRO A 175 -39.89 -17.795 20.564 1.00 20.18 C
ATOM 35 C PRO A 175 -39.565 -18.078 19.465 1.00 18.58 C
ATOM 36 O PRO A 175 -39.528 -15.781 20.142 1.00 18.18 O
ATOM 37 CB PRO A 175 -39.594 -18.893 19.632 1.00 20.52 C
ATOM 38 CG PRO A 175 -48.999 -19.247 19.043 1.00 19.77 C
ATOM 39 CD PRO A 175 -41.896 -19.015 20.148 1.00 21.28 C
ATOM 40 N CYS A 176 -48.493 -18.757 18.163 1.00 16.73 N
ATOM 41 CA CYS A 176 -47.612 -18.716 18.226 1.00 16.69 C
ATOM 42 C CYS A 176 -46.222 -13.581 19.159 1.00 16.78 C
ATOM 43 O CYS A 176 -39.363 -12.626 19.053 1.00 16.20 O
ATOM 44 CB CYS A 176 -41.244 -14.528 17.116 1.00 16.50 C
ATOM 45 SG CYS A 176 -48.895 -13.984 16.044 1.00 15.28 S
ATOM 46 N GLU A 177 -39.735 -12.953 20.325 1.00 19.25 N
ATOM 47 CA GLU A 177 -36.005 -12.549 20.043 1.00 19.49 C
ATOM 48 C GLU A 177 -37.775 -12.549 20.146 1.00 19.32 O
ATOM 49 CB GLU A 177 -35.948 -13.726 19.020 1.00 19.69 C
ATOM 50 CG GLU A 177 -34.679 -11.469 18.245 1.00 21.79 C
ATOM 51 CD GLU A 177 -37.519 -14.723 23.861 1.00 18.59 C
ATOM 52 OE1 GLU A 177 -33.564 -14.381 18.389 1.00 20.52 C
ATOM 53 OE2 GLU A 177 -35.442 -14.381 16.922 1.00 19.10 O
ATOM 54 N LEU A 180 -37.277 -10.979 19.702 1.00 19.29 N
ATOM 55 CA LEU A 180 -37.497 -9.568 19.383 1.00 19.26 C
ATOM 56 C LEU A 180 -36.979 -8.858 20.588 1.00 19.08 C
ATOM 57 O LEU A 180 -36.226 -7.704 20.241 1.00 18.14 O
ATOM 58 CB LEU A 180 -39.039 -8.565 19.643 1.00 19.13 C
ATOM 59 CG LEU A 180 -39.319 -7.798 18.847 1.00 19.07 C
ATOM 60 CD1 LEU A 180 -38.510 -7.233 17.675 1.00 21.29 C
ATOM 61 CD2 LEU A 180 -48.830 -7.649 18.614 1.00 19.74 C
ATOM 62 N TYR A 181 -37.358 -8.954 21.751 1.00 19.18 N
ATOM 63 CA TYR A 181 -50.095 -9.514 20.744 1.00 19.72 C
ATOM 64 C TYR A 181 -35.318 -8.238 22.972 1.00 19.86 C
ATOM 65 O TYR A 181 -34.698 -7.715 23.148 1.00 19.98 O
ATOM 66 CB TYR A 181 -37.467 -8.751 24.227 1.00 20.16 C

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khushi@DESKTOP-DE71GO3:~/Lab_session3/Lab_assignment3$ awk '/^ATOM/ && $4 != "ARG" {print}' protein.pdb
ATOM 86 CB TYR A 181 -37.467 -8.751 24.227 1.00 20.16 C
ATOM 87 CG TYR A 181 -38.814 -8.123 24.527 1.00 20.84 C
ATOM 88 CD1 TYR A 181 -38.915 -7.008 25.358 1.00 21.48 C
ATOM 89 CD2 TYR A 181 -39.990 -8.645 23.977 1.00 20.81 C
ATOM 90 CE3 TYR A 181 -40.147 -6.422 25.621 1.00 22.34 C
ATOM 91 CD TYR A 181 -38.990 -8.645 23.977 1.00 20.51 C
ATOM 92 CZ TYR A 181 -41.409 -8.059 25.093 1.00 20.32 C
ATOM 93 OH TYR A 181 -42.516 -6.373 25.247 1.00 22.89 O
ATOM 94 N VAL A 183 -33.164 -8.795 20.537 1.00 18.69 N
ATOM 95 CA VAL A 183 -32.586 -8.181 19.374 1.00 18.83 C
ATOM 96 C VAL A 183 -32.676 -6.583 19.560 1.00 18.48 C
ATOM 97 O VAL A 183 -31.693 -5.875 19.316 1.00 18.13 O
ATOM 98 EB VAL A 183 -33.283 -8.586 19.561 1.00 18.63 C
ATOM 99 CG VAL A 183 -35.973 -7.006 16.005 1.00 19.70 C
ATOM 100 CG2 VAL A 183 -37.894 -9.975 17.689 1.00 18.64 C
ATOM 101 N GLU A 185 -32.767 -4.919 22.305 1.00 19.25 N
ATOM 102 CA GLU A 185 -31.793 -4.545 23.423 1.00 20.57 C
ATOM 103 C GLU A 185 -30.359 -4.498 22.870 1.00 20.10 C
ATOM 104 O GLU A 185 -29.614 -3.546 23.148 1.00 19.76 O
ATOM 105 CB GLU A 185 -31.888 -5.488 24.638 1.00 20.14 C
ATOM 106 CG GLU A 185 -30.992 -5.030 25.786 1.00 21.36 C
ATOM 107 CD GLU A 185 -30.034 -6.061 24.638 1.00 22.00 C
ATOM 108 OE1 GLU A 185 -31.553 -7.082 26.951 1.00 22.78 O
ATOM 109 OE2 GLU A 185 -30.273 -7.486 19.532 1.00 20.87 C
ATOM 110 N GLU A 185 -32.767 -4.919 22.305 1.00 19.25 N
ATOM 111 CG2 GLU A 185 -31.793 -4.545 23.423 1.00 20.57 C
ATOM 112 N VAL A 184 -33.822 -6.186 20.034 1.00 18.63 N
ATOM 113 CA VAL A 184 -34.017 -4.667 26.304 1.00 19.03 C
ATOM 114 C VAL A 184 -32.987 -4.148 21.330 1.00 19.24 C
ATOM 115 O VAL A 184 -32.377 -3.081 21.136 1.00 18.61 O
ATOM 116 CB VAL A 184 -35.483 -4.352 20.725 1.00 19.12 C
ATOM 117 CG1 VAL A 184 -36.662 -2.977 20.725 1.00 19.57 C
ATOM 118 CG2 VAL A 184 -36.107 -4.486 19.532 1.00 19.87 C
ATOM 119 N GLU A 185 -32.767 -4.919 22.305 1.00 19.25 N
ATOM 120 CA GLU A 185 -31.793 -4.545 23.423 1.00 20.57 C
ATOM 121 C GLU A 185 -30.359 -4.498 22.870 1.00 20.10 C
ATOM 122 O GLU A 185 -29.614 -3.546 23.148 1.00 19.76 O
ATOM 123 CB GLU A 185 -31.888 -5.488 24.638 1.00 20.14 C
ATOM 124 CG GLU A 185 -30.992 -5.030 25.786 1.00 21.36 C
ATOM 125 CD GLU A 185 -30.034 -6.061 24.638 1.00 22.00 C
ATOM 126 OE1 GLU A 185 -31.553 -7.082 26.951 1.00 22.78 O
ATOM 127 OE2 GLU A 185 -30.273 -7.486 19.532 1.00 20.87 C
ATOM 128 N SER A 186 -29.973 -5.517 22.106 1.00 19.89 N
ATOM 129 CA SER A 186 -28.627 -5.563 21.598 1.00 20.02 C
ATOM 130 C SER A 186 -28.397 -4.432 20.505 1.00 19.66 C
ATOM 131 O SER A 186 -27.329 -3.818 20.481 1.00 18.81 O
ATOM 132 FB SER A 186 -28.397 -6.049 20.536 1.00 19.59 C
ATOM 133 OG SER A 186 -28.358 -7.042 21.702 1.00 23.17 O
ATOM 134 N LEU A 187 -29.406 -4.171 19.676 1.00 19.21 N
ATOM 135 CA LEU A 187 -29.344 -3.978 18.786 1.00 19.74 C
ATOM 136 C LEU A 187 -29.183 -1.718 19.393 1.00 19.37 C
ATOM 137 O LEU A 187 -28.362 -0.985 18.973 1.00 19.34 O
ATOM 138 CB LEU A 187 -30.593 -3.047 17.833 1.00 19.81 C
ATOM 139 CG LEU A 187 -30.623 -3.968 16.619 1.00 21.86 C
ATOM 140 CD1 LEU A 187 -32.052 -3.991 16.073 1.00 24.65 C

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ATOM	148	CD1	LEU	A	187	-32.032	-3.991	16.073	1.00	24.65	C
ATOM	149	CD2	LEU	A	187	-29.629	-3.529	16.073	1.00	24.78	C
ATOM	142	CA	ALA	A	188	-29.945	-0.090	20.431	1.00	19.15	N
ATOM	143	CA	ALA	A	188	-29.988	-0.273	21.249	1.00	19.62	C
ATOM	144	C	ALA	A	188	-28.484	-0.122	21.790	1.00	19.76	C
ATOM	145	O	ALA	A	188	-27.877	0.958	21.798	1.00	19.78	O
ATOM	146	CB	ALA	A	188	-30.914	-0.334	22.398	1.00	19.86	C
ATOM	147	N	LYS	A	189	-27.943	-1.219	22.313	1.00	19.77	N
ATOM	148	CA	LYS	A	189	-26.909	-2.073	22.313	1.00	19.63	C
ATOM	149	CA	LYS	A	189	-25.535	-0.931	21.783	1.00	19.51	C
ATOM	150	O	LYS	A	189	-24.637	-0.121	22.088	1.00	19.29	O
ATOM	151	CB	LYS	A	189	-26.384	-2.544	23.584	1.00	19.67	C
ATOM	152	CG	LYS	A	189	-24.988	-2.573	24.353	1.00	21.18	C
ATOM	153	CD	LYS	A	189	-24.991	-1.168	25.580	1.00	23.97	C
ATOM	154	CE	LYS	A	189	-27.593	-1.688	20.501	1.00	25.23	C
ATOM	155	CE	LYS	A	189	-23.673	-1.601	27.384	1.00	19.58	C
ATOM	156	N	ALA	A	190	-25.651	-1.181	20.618	1.00	19.73	N
ATOM	157	CA	ALA	A	190	-24.684	-1.402	19.528	1.00	20.13	C
ATOM	158	C	ALA	A	190	-24.697	0.033	19.811	1.00	20.31	C
ATOM	159	O	ALA	A	190	-23.654	0.575	18.652	1.00	20.46	O
ATOM	160	CB	ALA	A	190	-27.974	-2.374	18.151	1.00	20.81	C
ATOM	161	N	GLN	A	191	-25.629	0.623	19.973	1.00	20.85	N
ATOM	162	CA	GLN	A	191	-26.824	0.004	18.459	1.00	21.02	C
ATOM	163	C	GLN	A	191	-25.233	3.028	19.288	1.00	21.64	C
ATOM	164	O	GLN	A	191	-24.787	4.046	18.754	1.00	21.77	O
ATOM	165	CB	GLN	A	191	-27.586	2.393	18.374	1.00	22.25	C
ATOM	166	CG	GLN	A	191	-28.199	1.933	17.886	1.00	25.97	C
ATOM	167	CD	GLN	A	191	-27.694	2.693	18.374	1.00	21.71	C
ATOM	168	OE1	GLN	A	191	-28.111	3.553	15.635	1.00	31.63	O
ATOM	169	NE2	GLN	A	191	-26.910	2.047	15.935	1.00	32.02	N
ATOM	170	N	GLU	A	192	-25.051	2.742	20.577	1.00	21.46	N
ATOM	171	CA	GLU	A	192	-24.277	3.615	21.482	1.00	21.62	C
ATOM	172	C	GLU	A	192	-22.849	3.877	20.973	1.00	21.84	C
ATOM	173	O	GLU	A	192	-23.349	5.068	20.981	1.00	20.87	O
ATOM	174	CB	GLU	A	192	-24.166	3.924	22.092	1.00	21.74	C
ATOM	175	CG	GLU	A	192	-25.645	3.977	23.531	1.00	21.99	C
ATOM	176	CD	GLU	A	192	-25.680	2.475	24.965	1.00	22.37	C
ATOM	177	OE1	GLU	A	192	-24.666	1.990	25.496	1.00	22.90	O
ATOM	178	OE2	GLU	A	192	-26.783	2.565	25.568	1.00	25.93	O
ATOM	179	N	THR	A	193	-27.217	2.818	28.480	1.00	22.26	N
ATOM	180	CA	THR	A	193	-28.003	2.910	28.940	1.00	20.03	C
ATOM	181	C	THR	A	193	-28.673	3.774	18.526	1.00	24.43	C
ATOM	182	O	THR	A	193	-19.568	2.654	18.023	1.00	23.91	O
ATOM	183	CB	THR	A	193	-20.008	1.791	20.694	1.00	23.11	C

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ATOM	162	CD	THR	A	193	-23.056	4.704	20.604	1.00	23.41	C
ATOM	184	OE1	THR	A	193	-26.622	0.538	20.378	1.00	22.12	O
ATOM	185	CG2	THR	A	193	-19.949	1.957	22.287	1.00	22.37	C
ATOM	186	N	SER	A	194	-21.792	2.789	17.806	1.00	26.17	N
ATOM	187	CA	SER	A	194	-21.785	2.502	16.374	1.00	28.66	C
ATOM	188	C	SER	A	194	-20.976	3.535	15.607	1.00	30.43	C
ATOM	189	O	SER	A	194	-21.198	4.739	15.764	1.00	30.63	O
ATOM	190	CB	SER	A	194	-23.286	2.411	15.888	1.00	28.78	C
ATOM	191	OG	SER	A	194	-23.179	2.859	14.422	1.00	29.52	O
ATOM	192	CG	SER	A	194	-23.053	2.921	14.755	1.00	29.53	C
ATOM	193	CA	GLY	A	195	-21.179	3.898	13.965	1.00	34.45	C
ATOM	194	C	GLY	A	195	-19.886	4.288	12.636	1.00	36.12	C
ATOM	195	O	GLY	A	195	-19.172	4.956	11.819	1.00	36.57	O
ATOM	196	N	GLU	A	196	-21.944	3.837	12.413	1.00	37.26	N
ATOM	197	CA	GLU	A	196	-21.822	4.225	11.233	1.00	38.38	C
ATOM	198	C	GLU	A	196	-23.273	4.535	11.614	1.00	38.59	C
ATOM	199	O	GLU	A	196	-23.676	4.399	12.751	1.00	38.87	O
ATOM	200	GLU	A	196	-21.766	3.139	10.144	1.00	38.61	C	
ATOM	201	CG	GLU	A	196	-23.161	3.143	10.774	1.00	38.20	C
ATOM	202	CD	GLU	A	196	-21.760	0.761	10.792	1.00	42.45	C
ATOM	203	OE1	GLU	A	196	-22.418	0.352	12.338	0.50	42.52	O
ATOM	204	OE2	GLU	A	196	-20.513	0.856	11.354	1.00	43.56	O
ATOM	205	N	GLU	A	197	-24.042	5.069	10.667	1.00	38.83	N
ATOM	206	CA	GLU	A	197	-25.464	5.336	10.878	1.00	38.88	C
ATOM	207	C	GLU	A	197	-26.278	4.317	10.874	1.00	38.33	C
ATOM	208	CG	GLU	A	197	-26.494	4.560	8.877	1.00	38.98	O
ATOM	209	CB	GLU	A	197	-25.821	6.766	10.445	1.00	38.97	C
ATOM	210	CG	GLU	A	197	-23.056	3.938	10.803	1.00	38.48	C
ATOM	211	CD	GLU	A	197	-27.277	8.398	11.820	1.00	42.86	C
ATOM	212	OE1	GLU	A	197	-26.348	9.232	11.792	1.00	43.48	O
ATOM	213	OE2	GLU	A	197	-28.241	8.474	12.621	1.00	43.51	O
ATOM	214	N	ILE	A	198	-26.691	3.231	10.722	1.00	37.57	N
ATOM	215	CA	ILE	A	198	-27.447	2.184	10.020	1.00	36.57	C
ATOM	216	C	ILE	A	198	-28.889	2.619	9.745	1.00	35.29	C
ATOM	217	O	ILE	A	198	-29.574	3.169	10.610	1.00	36.61	O
ATOM	218	CB	ILE	A	198	-29.509	0.629	10.774	1.00	36.84	C
ATOM	219	CG1	ILE	A	198	-28.857	0.812	12.097	1.00	37.53	C
ATOM	220	CG2	ILE	A	198	-25.941	0.265	10.792	1.00	36.74	C
ATOM	221	CD1	ILE	A	198	-28.621	-0.537	12.539	1.00	38.43	C
ATOM	222	N	SER	A	199	-29.326	2.382	8.516	1.00	33.45	N
ATOM	223	CA	SER	A	199	-30.640	2.811	8.054	1.00	31.29	C
ATOM	224	C	SER	A	199	-31.578	1.620	7.899	1.00	29.24	C
ATOM	225	O	SER	A	199	-32.798	1.798	7.755	1.00	28.70	O
ATOM	226	CB	SER	A	199	-38.505	3.555	6.726	1.00	31.53	C

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ATOM	226	CB	SER	A	199	-38.505	3.555	6.726	1.00	31.53	C
ATOM	227	OG	SER	A	199	-29.665	2.841	5.830	1.00	33.46	O
ATOM	228	N	LYS	A	200	-30.993	0.420	7.874	1.00	26.73	N
ATOM	229	CA	LYS	A	200	-31.745	-0.835	7.833	1.00	24.20	C
ATOM	230	C	LYS	A	200	-31.288	-1.820	8.888	1.00	23.56	C
ATOM	231	O	LYS	A	200	-30.814	-1.861	9.168	1.00	23.03	O
ATOM	232	CG	LYS	A	200	-31.682	-1.479	6.448	1.00	24.17	C
ATOM	233	CD	LYS	A	200	-32.216	0.669	5.294	1.00	23.47	C
ATOM	234	CE	LYS	A	200	-32.268	1.416	5.309	1.00	23.93	C
ATOM	235	NZ	LYS	A	200	-31.779	-0.443	7.786	1.00	24.93	N
ATOM	237	N	PHE	A	201	-31.331	0.512	2.647	1.00	19.78	N
ATOM	238	CA	PHE	A	201	-32.182	-2.617	0.451	1.00	22.85	C
ATOM	239	C	PHE	A	201	-31.799	-3.649	10.421	1.00</td		

ATOM	269	CA	PRO A	284	-37.883	-10.366	14.000	1.00	19.27	C
ATOM	278	O	PRO A	284	-39.777	-10.305	14.518	1.00	19.19	O
ATOM	272	CB	PRO A	284	-37.765	-11.194	15.284	1.00	19.79	C
ATOM	273	CG	PRO A	284	-36.357	-10.992	15.708	1.00	19.73	C
ATOM	274	CD	PRO A	284	-36.032	-9.548	15.352	1.00	19.59	C
ATOM	275	N	ASN A	285	-39.969	-10.324	12.769	1.00	17.90	N
ATOM	276	CA	ASN A	285	-41.357	-9.968	12.495	1.00	18.16	C
ATOM	277	O	ASN A	285	-42.477	-10.777	13.028	1.00	18.05	O
ATOM	278	CB	ASN A	285	-42.411	-12.113	12.655	1.00	17.42	O
ATOM	279	CB	ASN A	285	-41.666	-9.983	10.987	1.00	18.39	C
ATOM	288	CG	ASN A	285	-40.666	-9.188	10.107	1.00	18.94	C
ATOM	281	OD1	ASN A	285	-40.832	-9.161	8.884	1.00	22.20	O
ATOM	282	ND2	ASN A	285	-39.057	-8.569	10.698	1.00	19.63	N
ATOM	283	N	CYS A	286	-42.910	-10.689	14.834	1.00	18.84	N
ATOM	284	CA	CYS A	286	-43.625	-11.522	15.186	1.00	17.93	C
ATOM	285	CG	CYS A	286	-45.118	-11.479	14.845	1.00	18.36	C
ATOM	286	O	CYS A	286	-45.623	-10.361	14.652	1.00	18.35	O
ATOM	287	CB	CYS A	286	-43.376	-11.456	16.612	1.00	17.73	C
ATOM	288	SG	CYS A	286	-41.654	-11.522	17.123	1.00	17.34	S
ATOM	289	N	ASN A	287	-41.822	-12.619	14.454	1.00	18.54	N
ATOM	290	CA	ASN A	287	-41.922	-12.529	14.923	1.00	17.73	C
ATOM	291	CB	ASN A	287	-47.713	-12.386	16.381	1.00	19.14	C
ATOM	292	O	ASN A	287	-46.874	-12.401	17.293	1.00	19.85	O
ATOM	293	CB	ASN A	287	-47.916	-13.848	14.274	1.00	18.43	C
ATOM	294	CG	ASN A	287	-47.680	-15.147	15.029	1.00	18.66	C
ATOM	295	OD1	ASN A	287	-47.540	-15.188	16.254	1.00	18.06	O
ATOM	296	ND2	ASN A	287	-47.747	-15.188	16.254	1.00	19.03	N
ATOM	297	N	LYS A	288	-49.812	-12.189	16.598	1.00	18.79	N
ATOM	298	CA	LYS A	288	-49.589	-11.893	17.916	1.00	20.21	C
ATOM	299	C	LYS A	288	-49.499	-13.063	18.913	1.00	20.08	C
ATOM	300	O	LYS A	288	-49.635	-12.868	20.118	1.00	20.32	O
ATOM	301	CB	LYS A	288	-51.043	-11.459	17.773	1.00	20.47	C
ATOM	302	CG	LYS A	288	-51.953	-12.530	17.188	1.00	20.38	C
ATOM	303	CD	LYS A	288	-53.056	-12.622	17.359	1.00	19.19	C
ATOM	304	CE	LYS A	288	-54.297	-13.221	16.642	1.00	20.94	C
ATOM	305	NZ	LYS A	288	-54.187	-14.607	17.174	1.00	20.34	N
ATOM	306	N	ASN A	289	-49.284	-14.275	18.399	1.00	19.57	N
ATOM	307	CA	ASN A	289	-49.083	-15.465	19.242	1.00	19.88	C
ATOM	308	C	ASN A	289	-49.633	-15.631	19.421	1.00	19.34	C
ATOM	309	O	ASN A	289	-49.757	-16.779	19.641	1.00	19.74	O
ATOM	310	CB	ASN A	289	-49.559	-16.738	18.588	1.00	19.75	C
ATOM	311	CG	ASN A	289	-50.766	-16.486	17.661	1.00	21.13	C
ATOM	312	OD1	ASN A	289	-50.811	-16.838	16.468	1.00	23.95	O

ATOM	312	CD1	ASN A	289	-50.811	-16.630	16.468	1.00	23.95	O
ATOM	313	ND2	ASN A	289	-51.778	-15.856	18.251	1.00	17.82	N
ATOM	314	N	GLY A	210	-46.771	-14.739	19.295	1.00	19.30	N
ATOM	315	CA	GLY A	210	-45.353	-14.753	19.536	1.00	18.56	C
ATOM	316	C	GLY A	210	-44.513	-15.719	18.713	1.00	18.50	C
ATOM	317	O	GLY A	210	-43.364	-15.993	19.062	1.00	17.75	O
ATOM	318	N	PHE A	211	-45.091	-16.258	17.638	1.00	18.35	N
ATOM	319	CA	PHE A	211	-46.394	-16.063	16.671	1.00	18.88	C
ATOM	320	C	PHE A	211	-45.045	-16.063	15.778	1.00	18.67	C
ATOM	321	O	PHE A	211	-44.212	-14.858	15.535	1.00	19.06	O
ATOM	322	CB	PHE A	211	-45.076	-18.238	16.158	1.00	19.06	C
ATOM	323	CG	PHE A	211	-44.992	-19.373	17.138	1.00	19.94	C
ATOM	324	CD1	PHE A	211	-43.859	-20.175	17.187	1.00	20.48	C
ATOM	325	CD2	PHE A	211	-46.021	-19.684	18.044	1.00	22.97	C
ATOM	326	CE	PHE A	211	-43.779	-21.224	18.139	1.00	20.71	C
ATOM	327	CE1	PHE A	211	-46.033	-20.453	18.776	1.00	21.29	C
ATOM	328	CE2	PHE A	211	-44.890	-21.459	19.095	1.00	20.87	C
ATOM	329	N	TYR A	212	-38.501	-15.298	14.936	1.00	14.95	C
ATOM	330	CA	TYR A	212	-42.776	-15.843	13.332	1.00	18.09	C
ATOM	331	C	TYR A	212	-43.769	-15.774	12.184	1.00	18.14	C
ATOM	332	TYR	TYR A	212	-44.288	-16.886	11.744	1.00	18.14	O
ATOM	333	OE1	TYR A	212	-41.449	-16.441	12.834	1.00	18.46	C
ATOM	334	CG	TYR A	212	-42.945	-17.572	16.077	1.00	19.57	C
ATOM	335	CD1	TYR A	212	-48.125	-17.467	14.881	1.00	17.30	C
ATOM	336	CD2	TYR A	212	-39.485	-15.344	13.975	1.00	17.57	C
ATOM	337	CE1	TYR A	212	-39.221	-17.434	15.777	1.00	18.28	C
ATOM	338	CE2	TYR A	212	-38.501	-15.298	14.936	1.00	14.95	C
ATOM	339	CZ	TYR A	212	-38.363	-16.344	15.829	1.00	16.70	C
ATOM	340	OH	TYR A	212	-37.375	-16.284	16.786	1.00	18.15	O
ATOM	341	N	HIS A	213	-46.092	-17.572	18.101	1.00	18.07	N
ATOM	342	CA	HIS A	213	-44.978	-14.469	16.568	1.00	18.14	C
ATOM	343	C	HIS A	213	-43.859	-15.264	9.348	1.00	17.86	C
ATOM	344	O	HIS A	213	-42.635	-15.316	9.449	1.00	17.33	O
ATOM	345	CB	HIS A	213	-44.894	-13.005	9.931	1.00	18.71	C
ATOM	346	CG	HIS A	213	-45.862	-12.251	16.673	1.00	19.72	C
ATOM	347	ND1	HIS A	213	-47.197	-12.594	16.619	1.00	20.89	N
ATOM	348	CD2	HIS A	213	-45.784	-11.167	11.488	1.00	18.66	C
ATOM	349	NE2	HIS A	213	-45.379	-11.601	15.153	1.00	18.66	C
ATOM	350	NE2	HIS A	213	-47.066	-18.884	11.997	1.00	21.26	N
ATOM	351	N	SER A	214	-44.533	-15.922	8.401	1.00	17.92	N
ATOM	352	CA	SER A	214	-43.835	-16.637	7.317	1.00	19.16	C
ATOM	353	C	SER A	214	-42.890	-15.727	6.548	1.00	18.52	C
ATOM	354	O	SER A	214	-41.765	-16.099	6.253	1.00	18.58	O
ATOM	355	CB	SER A	214	-44.838	-17.294	6.356	1.00	19.46	C

ATOM	355	CB	SER A	214	-44.838	-17.290	6.356	1.00	19.46	C
ATOM	356	OG	SER A	214	-36.422	-4.859	7.451	1.00	17.77	C
ATOM	368	N	GLN A	216	-48.348	-12.761	6.573	1.00	17.58	N
ATOM	369	CA	GLN A	216	-39.487	-11.938	7.424	1.00	16.83	C
ATOM	370	CA	GLN A	216	-38.819	-10.889	6.594	1.00	16.91	C
ATOM	371	O	GLN A	216	-39.889	-11.849	6.631	1.00	17.55	O
ATOM	372	CB	GLN A	216	-38.417	-12.769	8.159	1.00	16.94	C
ATOM	373	CG	GLN A	216	-39.974	-13.769	9.161	1.00	16.52	C
ATOM	374	CD	GLN A	216	-39.649	-13.099	10.339	1.00	16.09	C
ATOM	375	OE2	GLN A	216	-39.027	-12.252	11.022	1.00	15.64	O
ATOM	376	NE2	GLN A	216	-48.893	-13.457	10.589	1.00	14.49	N
ATOM	377	N	CYS A	217	-38.912	-9.625	7.014	1.00	16.94	N
ATOM	378	CA	CYS A	217	-38.229	-8.525	6.294	1.00	16.91	C
ATOM	379	O	CYS A	217	-37.769	-7.968	7.017	1.00	17.97	O
ATOM	380	O	CYS A	217	-37.647	-7.538	7.411	1.00	16.75	O
ATOM	381	CB	CYS A	217	-38.320	-7.622	5.639	1.00	17.22	C
ATOM	382	SG	CYS A	217	-46.478	-8.466	4.537	1.00	18.26	S
ATOM	383	N	GLU A	218	-36.348	-7.121	6.592	1.00	16.79	N
ATOM	384	CA	GLU A	218	-35.546	-6.869	7.216	1.00	18.15	C
ATOM	385	C	GLU A	218	-3					

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ATOM	499	CB	MET A	221	-35.626	4.216	9.027	1.00	20.63	C	
ATOM	499	CD	MET A	221	-35.626	4.216	9.027	1.00	20.63	S	
ATOM	411	SD	MET A	221	-35.787	3.838	11.765	1.00	26.61	S	
ATOM	412	CE	MET A	221	-36.444	5.498	11.874	1.00	25.56	C	
ATOM	413	N	ASP A	222	-35.073	4.478	5.418	1.00	20.40	N	
ATOM	414	CA	ASP A	222	-34.279	5.398	4.588	1.00	20.45	C	
ATOM	415	O	ASP A	222	-34.279	5.398	3.728	1.00	20.55	O	
ATOM	416	CG	ASP A	222	-34.288	5.977	2.238	1.00	20.57	C	
ATOM	417	CB	ASP A	222	-32.856	4.725	4.386	1.00	20.76	C	
ATOM	418	CG	ASP A	222	-32.849	3.279	3.882	1.00	20.03	C	
ATOM	419	OD1	ASP A	222	-31.774	2.668	3.934	1.00	22.26	O	
ATOM	420	OD2	ASP A	222	-31.774	2.668	2.134	1.00	21.51	O	
ATOM	421	CD	GLY A	223	-36.125	5.041	2.943	1.00	19.55	N	
ATOM	422	CA	GLY A	223	-36.815	5.178	1.658	1.00	21.58	C	
ATOM	423	C	GLY A	223	-36.488	4.069	0.668	1.00	21.57	C	
ATOM	424	O	GLY A	223	-36.861	4.134	-0.498	1.00	21.96	O	
ATOM	425	N	ALA A	224	-35.769	4.953	1.141	1.00	21.38	N	
ATOM	426	CA	ALA A	224	-35.569	1.048	0.724	1.00	21.72	C	
ATOM	427	C	ALA A	224	-36.126	0.661	0.914	1.00	21.14	C	
ATOM	428	O	ALA A	224	-36.255	0.536	2.135	1.00	20.93	O	
ATOM	429	CG	ALA A	224	-33.948	1.673	0.260	1.00	22.09	C	
ATOM	430	CD	GLU A	224	-33.197	2.741	-0.586	1.00	24.47	C	
ATOM	431	OD1	GLU A	224	-33.197	2.741	-0.589	1.00	24.45	O	
ATOM	432	OE1	GLU A	224	-31.297	1.518	0.638	1.00	30.43	O	
ATOM	433	OE2	GLU A	224	-30.988	3.638	-0.483	1.00	31.11	O	
ATOM	434	N	ALA A	225	-36.575	-0.734	0.030	1.00	20.59	N	
ATOM	435	CA	ALA A	225	-37.186	-1.492	0.463	1.00	20.38	C	
ATOM	436	C	ALA A	225	-36.253	-1.081	1.053	1.00	20.59	C	
ATOM	437	O	ALA A	225	-35.013	-2.494	0.724	1.00	19.69	O	
ATOM	438	CB	ALA A	225	-37.732	-2.226	-0.750	1.00	20.55	C	
ATOM	439	N	GLY A	226	-36.537	-2.937	2.327	1.00	19.20	N	
ATOM	440	CA	GLY A	226	-35.795	-3.955	2.980	1.00	18.85	C	
ATOM	441	C	GLY A	226	-35.804	-3.752	2.294	1.00	18.47	C	
ATOM	442	O	GLY A	226	-35.804	-5.578	1.065	1.00	19.31	O	
ATOM	443	N	LEU A	227	-34.888	-0.166	2.487	1.00	18.11	N	
ATOM	444	CA	LEU A	227	-34.812	-7.532	1.968	1.00	17.92	C	
ATOM	445	C	LEU A	227	-35.853	-8.348	2.738	1.00	17.33	C	
ATOM	446	O	LEU A	227	-35.069	-8.000	3.000	1.00	16.48	O	
ATOM	447	CB	LEU A	227	-33.931	8.175	2.139	1.00	19.18	C	
ATOM	448	CG	LEU A	227	-32.270	-7.857	1.283	1.00	20.78	C	
ATOM	449	CD1	LEU A	227	-30.917	-8.132	1.816	1.00	23.35	C	
ATOM	450	CD2	LEU A	227	-32.451	-8.846	-0.194	1.00	21.98	C	
ATOM	451	N	CYS A	228	-36.584	-9.216	2.037	1.00	16.71	N	
ATOM	452	CA	CYS A	228	-37.474	-16.166	2.763	1.00	17.38	C	

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ATOM	452	CA	CYS A	228	-37.472	-16.166	2.763	1.00	17.38	C	
ATOM	453	C	CYS A	228	-37.472	-11.996	2.269	1.00	17.41	C	
ATOM	454	O	CYS A	228	-36.573	-23.896	1.516	1.00	17.14	O	
ATOM	455	CB	CYS A	228	-38.047	-9.928	2.362	1.00	17.03	C	
ATOM	456	SG	CYS A	228	-39.618	-8.273	2.708	1.00	18.75	S	
ATOM	457	N	TRP A	229	-37.406	-12.535	3.178	1.00	17.59	N	
ATOM	458	CA	TRP A	229	-37.214	-13.963	2.910	1.00	18.64	C	
ATOM	459	C	TRP A	229	-37.314	-14.000	2.600	1.00	18.59	C	
ATOM	460	O	TRP A	229	-39.155	-14.171	4.325	1.00	18.74	O	
ATOM	461	CB	TRP A	229	-35.820	-14.414	3.366	1.00	19.05	C	
ATOM	462	CG	TRP A	229	-35.545	-14.189	4.825	1.00	19.34	C	
ATOM	463	CD1	TRP A	229	-35.685	-15.169	5.834	1.00	19.36	C	
ATOM	464	CD2	TRP A	229	-35.086	-12.975	5.448	1.00	19.75	C	
ATOM	465	NE1	TRP A	229	-35.345	-14.533	5.842	1.00	19.95	N	
ATOM	466	CE2	TRP A	229	-36.400	-13.030	6.152	1.00	19.97	C	
ATOM	467	CE3	TRP A	229	-34.763	-11.698	4.953	1.00	19.95	C	
ATOM	468	CZ2	TRP A	229	-34.541	-12.251	7.739	1.00	20.31	C	
ATOM	469	CZ3	TRP A	229	-34.324	-10.728	5.858	1.00	19.00	C	
ATOM	470	CH2	TRP A	229	-34.228	-11.008	7.234	1.00	19.70	C	
ATOM	471	N	CYS A	230	-38.946	-16.079	6.076	1.00	18.85	N	
ATOM	472	CA	CYS A	230	-39.332	-16.031	4.016	1.00	19.50	C	
ATOM	473	CYS	CYS A	230	-38.794	-17.854	5.106	1.00	18.50	C	
ATOM	474	O	CYS A	230	-37.736	-18.464	4.946	1.00	18.93	O	
ATOM	475	CB	CYS A	230	-40.004	-17.763	2.915	1.00	19.33	C	
ATOM	476	SG	CYS A	230	-40.630	-16.763	1.539	1.00	21.95	S	
ATOM	477	N	VAL A	231	-39.537	-17.963	6.265	1.00	18.37	N	
ATOM	478	CA	VAL A	231	-39.414	-17.905	7.931	1.00	17.97	C	
ATOM	479	O	VAL A	231	-40.382	-19.788	7.737	1.00	17.76	O	
ATOM	480	B	VAL A	231	-41.346	-19.646	7.344	1.00	17.73	O	
ATOM	481	CB	VAL A	231	-38.723	-17.944	8.571	1.00	18.29	C	
ATOM	482	CG1	VAL A	231	-37.542	-17.088	8.238	1.00	18.20	C	
ATOM	483	CG2	VAL A	231	-39.946	-17.170	8.131	1.00	18.39	C	
ATOM	484	N	VAL A	231	-39.727	-17.003	8.150	1.00	17.07	N	
ATOM	485	CA	TYR A	232	-40.891	-21.624	9.280	1.00	18.02	C	
ATOM	486	C	TYR A	232	-41.359	-20.832	10.497	1.00	17.80	C	
ATOM	487	O	TYR A	232	-40.593	-20.347	11.239	1.00	17.24	O	
ATOM	488	CB	TYR A	232	-40.142	-22.912	1.681	1.00	18.50	C	
ATOM	489	CG	TYR A	232	-39.552	-23.774	8.570	1.00	18.49	C	
ATOM	490	CD1	TYR A	232	-40.400	-23.452	8.473	1.00	18.53	C	
ATOM	491	CD2	TYR A	232	-38.167	-23.566	8.470	1.00	18.49	C	
ATOM	492	CE1	TYR A	232	-37.617	-24.241	6.655	1.00	19.48	C	
ATOM	493	CE2	TYR A	232	-37.617	-24.774	7.465	1.00	18.57	C	
ATOM	494	CZ	TYR A	232	-38.465	-25.404	6.570	1.00	19.11	C	
ATOM	495	OH	TYR A	232	-37.938	-26.264	5.592	1.00	18.92	O	

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ATOM	495	OH	TYR A	232	-37.938	-26.264	5.592	1.00	18.92	O	
ATOM	496	N	PRO A	233	-42.695	-20.681	10.497	1.00	18.03	N	
ATOM	497	CA	PRO A	233	-43.253	-19.870	11.598	1.00	17.74	C	
ATOM	498	C	PRO A	233	-42.992	-20.388	13.024	1.00	17.82	C	
ATOM	499	O	PRO A	233	-42.882	-19.469	13.932	1.00	17.24	O	
ATOM	500	CB	PRO A	233	-42.446	-19.263	11.883	1.00	17.07	C	
ATOM	501	CG	PRO A	233	-40.484	-20.256	9.893	1.00	16.42	C	
ATOM	502	CD2	PRO A	233	-40.756	-21.183	9.506	1.00	18.27	C	
ATOM	503	N	TRP A	234	-42.624	-21.598	13.224	1.00	17.63	N	
ATOM	504	CA	TRP A	234	-42.345	-22.099	14.563	1.00	17.85	C	
ATOM	505	C	TRP A	234	-40.928	-21.831	15.857	1.00	17.77	C	

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khushik@DESKTOP-DE71G03:~/Lab_session3/Lab_assignment3$ ATOM 549 N ILE A 239 -36.328 -28.928 5.150 1.00 23.39 N
ATOM 550 CA ILE A 239 -36.680 -28.600 5.423 1.00 24.14 C
ATOM 551 C ILE A 239 -35.552 -22.319 3.324 1.00 25.20 C
ATOM 552 O ILE A 239 -35.352 -21.409 2.518 1.00 25.16 O
ATOM 553 CB ILE A 239 -38.059 -22.159 3.856 1.00 23.81 C
ATOM 554 CG1 ILE A 239 -39.350 -22.059 3.856 1.00 23.96 C
ATOM 555 CG2 ILE A 239 -38.335 -23.450 4.074 1.00 23.17 C
ATOM 556 CD1 ILE A 239 -48.505 -21.711 4.571 1.00 23.96 C
ATOM 557 N PRO A 240 -34.847 -23.477 3.301 1.00 26.03 N
ATOM 558 CA PRO A 240 -33.813 -23.053 2.903 1.00 26.07 C
ATOM 559 C PRO A 240 -34.500 -23.482 3.877 1.00 25.91 C
ATOM 560 O PRO A 240 -35.524 -23.932 6.615 1.00 27.37 O
ATOM 561 CB PRO A 240 -33.346 -25.896 2.513 1.00 26.80 C
ATOM 562 CG PRO A 240 -33.668 -25.369 3.954 1.00 26.58 C
ATOM 563 CD PRO A 240 -35.000 -25.345 3.954 1.00 27.11 C
ATOM 564 N GLY A 241 -33.693 -22.777 0.610 1.00 27.81 N
ATOM 565 CA GLY A 241 -34.199 -22.463 -1.334 1.00 28.67 C
ATOM 566 C GLY A 241 -35.099 -21.233 -1.404 1.00 29.09 C
ATOM 567 O GLY A 241 -31.586 -20.821 -2.508 1.00 29.78 O
ATOM 568 N SER A 242 -35.350 -20.415 3.025 1.00 28.72 C
ATOM 569 CA SER A 242 -36.237 -19.436 -0.167 1.00 28.62 C
ATOM 570 C SER A 242 -35.646 -18.381 -0.992 1.00 28.58 C
ATOM 571 O SER A 242 -34.427 -18.089 -0.985 1.00 28.71 O
ATOM 572 N GLU A 244 -32.860 -17.453 1.299 1.00 28.57 N
ATOM 573 OGLU A 242 -36.756 -17.583 1.299 1.00 27.17 O
ATOM 574 N PRO A 243 -36.506 -17.572 -1.722 1.00 28.39 N
ATOM 575 CA PRO A 243 -36.007 -16.356 -2.349 1.00 28.39 C
ATOM 576 C PRO A 243 -35.400 -16.293 -1.909 1.00 28.20 C
ATOM 577 O PRO A 243 -33.259 -15.113 -1.194 1.00 27.71 O
ATOM 578 CB PRO A 243 -37.167 -15.904 -3.244 1.00 28.46 C
ATOM 579 CG PRO A 243 -38.367 -16.606 -2.761 1.00 28.86 C
ATOM 580 CD PRO A 243 -37.933 -17.828 -2.003 1.00 28.47 C
ATOM 581 N GLU A 244 -34.498 -17.212 -0.859 1.00 28.49 N
ATOM 582 C GLU A 244 -34.478 -13.212 -0.837 1.00 28.29 C
ATOM 583 CGLUA 244 -34.515 -12.022 -1.795 1.00 27.43 C
ATOM 584 O GLU A 244 -33.628 -11.854 -2.622 1.00 27.85 O
ATOM 585 CB GLU A 244 -31.821 -11.291 -0.813 1.00 28.00 C
ATOM 586 CG GLU A 244 -32.666 -12.140 0.845 1.00 28.54 C
ATOM 587 CD GLU A 244 -31.801 -12.400 -0.897 1.00 30.20 C
ATOM 588 OE1 GLU A 244 -31.396 -13.572 2.032 1.00 33.67 O
ATOM 589 OE2 GLU A 244 -31.387 -11.452 2.609 1.00 34.03 O
ATOM 590 N GLU A 245 -35.788 -10.875 2.583 1.00 25.65 C
ATOM 591 CA ILE A 245 -35.788 -10.875 2.583 1.00 25.65 C
ATOM 592 C ILE A 245 -36.217 -8.832 -1.801 1.00 25.29 C

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khushik@DESKTOP-DE71G03:~/Lab_session3/Lab_assignment3$ ATOM 592 C ILE A 245 -36.217 -8.832 -1.801 1.00 25.29 C
ATOM 593 O ILE A 245 -36.768 -8.951 -0.700 1.00 25.02 O
ATOM 594 CB ILE A 245 -36.856 -10.402 -3.671 1.00 25.53 C
ATOM 595 CG1 ILE A 245 -36.856 -10.402 -3.671 1.00 25.53 C
ATOM 596 CG2 ILE A 245 -36.125 -11.466 -4.663 1.00 24.89 C
ATOM 597 CD1 ILE A 245 -39.487 -10.767 -3.934 1.00 26.28 C
ATOM 598 N GLY A 247 -38.835 -7.626 -1.580 1.00 23.42 N
ATOM 599 CA GLY A 247 -40.220 -7.777 -0.851 1.00 24.03 C
ATOM 600 C GLY A 247 -40.529 -7.273 -1.167 1.00 24.58 C
ATOM 611 O GLY A 247 -40.888 -9.077 -0.649 1.00 24.29 O
ATOM 613 N ASP A 247 -42.149 -8.408 -1.235 1.00 25.16 N
ATOM 614 CA ASP A 247 -42.824 -9.555 -0.633 1.00 26.30 C
ATOM 615 C ASP A 247 -42.520 -10.203 -0.603 1.00 26.45 C
ATOM 616 O ASP A 248 -43.938 -10.630 -2.651 1.00 26.50 O
ATOM 617 CB ASP A 248 -44.319 -9.255 -0.467 1.00 26.46 C
ATOM 618 CG ASP A 248 -45.836 -10.278 0.480 1.00 27.46 C
ATOM 619 OOG ASP A 248 -46.320 -10.278 0.480 1.00 27.40 O
ATOM 620 CB ASP A 248 -44.724 -11.481 0.312 1.00 29.49 O
ATOM 621 N PRO A 249 -41.919 -11.825 -0.954 1.00 27.01 N
ATOM 622 CA PRO A 249 -41.616 -13.046 -1.710 1.00 27.12 C
ATOM 623 C PRO A 249 -42.839 -13.935 -1.020 1.00 27.58 C
ATOM 624 O PRO A 249 -41.727 -13.570 0.570 1.00 27.09 O
ATOM 625 CB PRO A 249 -40.575 -13.763 -0.842 1.00 27.25 C
ATOM 626 CG PRO A 249 -40.172 -12.767 0.222 1.00 26.22 C
ATOM 627 CD PRO A 249 -41.376 -11.986 0.415 1.00 26.82 C
ATOM 628 N ASN A 250 -42.198 -12.049 0.209 1.00 26.06 N
ATOM 629 CA ASN A 250 -45.188 -14.384 -1.319 1.00 28.66 C
ATOM 630 C ASN A 250 -44.915 -15.766 -0.728 1.00 28.76 C
ATOM 631 O ASN A 250 -44.998 -16.798 -1.417 1.00 29.19 O
ATOM 632 CB ASN A 250 -45.827 -16.456 -2.721 1.00 29.27 C
ATOM 633 CG ASN A 250 -46.386 -15.130 -3.047 1.00 29.00 C
ATOM 634 ODI ASN A 250 -46.227 -12.687 -4.308 1.00 34.38 O
ATOM 635 ND2 ASN A 250 -47.167 -12.478 -2.272 1.00 31.93 N
ATOM 636 N CYT A 251 -44.571 -15.758 0.557 1.00 28.18 N
ATOM 637 CA CYT A 251 -44.242 -16.149 0.293 1.00 28.35 C
ATOM 638 C CYT A 251 -45.248 -17.940 1.495 1.00 28.66 C
ATOM 639 O CYT A 251 -46.378 -17.574 1.840 1.00 29.48 O
ATOM 640 CB CYT A 251 -43.484 -16.541 2.607 1.00 27.05 C
ATOM 641 SG CYT A 251 -41.988 -15.536 2.439 1.00 22.88 S
ATOM 642 OXT CYT A 251 -45.044 -19.143 1.329 1.00 29.75 O

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khushik@DESKTOP-DE71G03:~/Lab_session3/Lab_assignment3$ awk '$^ATOM/ {print $3, $4, $5}' protein.pdb

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22. Extract all residues and their frequencies from chain A.

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ATOM 642 OXT CYS A 251 -45.044 -19.143 1.329 1.00 29.75 O
khushik@DESKTOP-DE71G03:~/Lab_session3/Lab_assignment3$ awk '$^ATOM/ && $5=="A" {res[$4++]} END {for(r in res) print r, res[r]}' protein.pdb
GLY 28
CYS 37
LEU 32
THR 14
GLN 18
PRO 42
ILE 32
MET 8
ASN 49
TYR 48
LYS 45
ASP 16
SER 36
PHE 22
HIS 18
GLU 81
ARG 55
TRP 42
ALA 15
VAL 21

```

23. From protein.pdb, print only atom name, residue name, and chain ID, separated by (,)

```

khushik@DESKTOP-DE71G03:~/Lab_session3/Lab_assignment3$ awk '$^ATOM/ {print $3, $4, $5}' protein.pdb

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khuhi@DESKTOP-DE71GO3: ~/Lab_session3/Lab_assignment3

Y, GLU,A
CD, GLU,A
CG, GLU,A
CD, GLU,A
OE1, GLU,A
Z, GLU,A
V, PRO,A
CA, PRO,A
C, PRO,A
U, PRO,A
CB, PRO,A
CG, PRO,A
CD, PRO,A
N, CYS,A
D, CYS,A
C, CYS,A
O, CYS,A
CB, CYS,A
SG, CYS,A
V, ARG,A
CA, ARG,A
C, ARG,A
O, ARG,A
D, ARG,A
CB, ARG,A
CG, ARG,A
CD, ARG,A
HE, ARG,A
Z, ARG,A
NH1, ARG,A
NH2, ARG,A
N, ILE,A
CA, ILE,A
C, ILE,A
O, ILE,A
CB, ILE,A
CG1, ILE,A
CD2, ILE,A
CD1, ILE,A
N, GLU,A
CA, GLU,A
C, GLU,A
O, GLU,A
CB, GLU,A
CG, GLU,A

Type here to search 26°C Mostly cloudy 22:22 24-08-2025

khuhi@DESKTOP-DE71GO3: ~/Lab_session3/Lab_assignment3

CG, GLU,A
CD, GLU,A
OE1, GLU,A
Z, GLU,A
V, LEU,A
CA, LEU,A
C, LEU,A
O, LEU,A
CB, LEU,A
CG, LEU,A
CD1, LEU,A
CD2, LEU,A
N, TYR,A
CA, TYR,A
C, TYR,A
O, TYR,A
CB, TYR,A
CG, TYR,A
CD1, TYR,A
CD2, TYR,A
CE1, TYR,A
CE2, TYR,A
CZ, TYR,A
OH1, TYR,A
NH1, TYR,A
N, VAL,A
CA, VAL,A
C, VAL,A
O, VAL,A
CB, VAL,A
CG1, VAL,A
CG2, VAL,A
N, VAL,A
CA, VAL,A

Type here to search 26°C Mostly cloudy 22:22 24-08-2025

khuhi@DESKTOP-DE71GO3: ~/Lab_session3/Lab_assignment3

CA, VAL,A
C, VAL,A
O, VAL,A
CB, VAL,A
CG1, VAL,A
CG2, VAL,A
N, GLU,A
CA, GLU,A
C, GLU,A
O, GLU,A
CB, GLU,A
CG, GLU,A
CD, GLU,A
OE1, GLU,A
OE2, GLU,A
N, SER,A
CA, SER,A
C, SER,A
O, SER,A
CB, SER,A
OG, SER,A
N, LEU,A
CA, LEU,A
C, LEU,A
O, LEU,A
CB, LEU,A
CG, LEU,A
CD1, LEU,A
CD2, LEU,A
N, ALA,A
CA, ALA,A
C, ALA,A
O, ALA,A
CB, ALA,A
N, LYS,A
CA, LYS,A
C, LYS,A
O, LYS,A
CB, LYS,A
CG, LYS,A
CD, LYS,A
CE, LYS,A
HZ, LYS,A
N, ALA,A

khushit@DESKTOP-DE71GO3: ~/Lab_session3/Lab_assignment3

N,ALA,A
D,ALA,A
C,ALA,A
D,ALA,A
CB,ALA,A
N,GLN,A
CA,GLN,A
O,GLN,A
D,GLN,A
CB,GLN,A
CG,GLN,A
CD,GLN,A
Z1,GLN,A
ME2,GLN,A
N,GLU,A
CA,GLU,A
C,GLU,A
D,GLU,A
CB,GLU,A
CG,GLU,A
CD,GLU,A
OE1,GLU,A
OE2,GLU,A
H,THR,A
CA,THR,A
C,THR,A
O,THR,A
CB,THR,A
Z1,THR,A
CG2,THR,A
N,SER,A
CA,SER,A
C,SER,A
D,SER,A
CB,SER,A
CG,SER,A
N,GLY,A
CA,GLY,A
C,GLY,A
D,GLY,A
V,GLU,A
CA,GLU,A
C,GLU,A
D,GLU,A

khushit@DESKTOP-DE71GO3: ~/Lab_session3/Lab_assignment3

O,GLU,A
CB,GLU,A
D,GLU,A
CD,GLU,A
OE1,GLU,A
OE2,GLU,A
N,GLU,A
CA,GLU,A
C,GLU,A
D,GLU,A
CB,GLU,A
CG,GLU,A
CD,GLU,A
Z1,GLU,A
Z2,GLU,A
N,ILE,A
CA,ILE,A
C,ILE,A
D,ILE,A
CB,ILE,A
CG1,ILE,A
CG2,ILE,A
CD1,ILE,A
I,SER,A
C,SER,A
D,SER,A
CB,SER,A
CG,SER,A
N,LYS,A
CA,LYS,A
C,LYS,A
D,LYS,A
CB,LYS,A
CG,LYS,A
N,PHE,A
CA,PHE,A
C,PHE,A
D,PHE,A
CB,PHE,A
CG,PHE,A

khushit@DESKTOP-DE71GO3: ~/Lab_session3/Lab_assignment3

CG,PHE,A
CD1,PHE,A
CD2,PHE,A
CE1,PHE,A
CE2,PHE,A
CZ,PHE,A
CZ,PHE,A
N,TYR,A
CA,TYR,A
C,TYR,A
D,TYR,A
CB,TYR,A
CG,TYR,A
CD1,TYR,A
CD2,TYR,A
CE1,TYR,A
CE2,TYR,A
CZ,TYR,A
CZ,TYR,A
N,LEU,A
CA,LEU,A
C,LEU,A
D,LEU,A
CB,LEU,A
CG,LEU,A
CD1,LEU,A
CD2,LEU,A
N,PRO,A
CA,PRO,A
C,PRO,A
D,PRO,A
CB,PRO,A
CG,PRO,A
CD,PRO,A
HA,PRO,A
CA,ASN,A
C,ASN,A
D,ASN,A
CB,ASN,A
CG,ASN,A
ZD1,ASN,A
ND2,ASN,A
N,CYS,A
CA,CYS,A
C,CYS,A

```
Mush@DESKTOP-DE71GO3: ~/Lab_session3/Lab_assignment3
V,CYS,A
S,CYS,A
CB,CYS,A
SG,CYS,A
H,ASN,A
CA,ASH,A
AS,ASH,A
D,ASN,A
CB,ASH,A
CG,ASH,A
CD1,ASH,A
CD2,ASH,A
NQ2,ASN,A
N,LYS,A
CA,LYS,A
D,LYS,A
D1,LYS,A
CB,LYS,A
CG,LYS,A
CD,LYS,A
E,LYS,A
NE,LYS,A
N,ASN,A
CA,ASH,A
AS,ASH,A
D,ASN,A
CB,ASH,A
CG,ASH,A
CD1,ASN,A
CD2,ASN,A
V,GLY,A
CA,GLY,A
C,GLY,A
J,GLY,A
C,PHE,A
CA,PHE,A
C,PHE,A
D,PHE,A
E,PHE,A
F,PHE,A
G,PHE,A
CD1,PHE,A
CD2,PHE,A
CE1,PHE,A
CE2,PHE,A
CZ,PHE,A
Mush@DESKTOP-DE71GO3: ~/Lab_session3/Lab_assignment3
C2,PHE,A
N,TYR,A
CA,TYR,A
C,TYR,A
D,TYR,A
CB,TYR,A
CG,TYR,A
CD1,TYR,A
CD2,TYR,A
CE1,TYR,A
CE2,TYR,A
CZ,TYR,A
OH,TYR,A
H,HIS,A
D,HIS,A
C,HIS,A
D,HIS,A
CB,HIS,A
CG,HIS,A
ND1,HIS,A
CD2,HIS,A
CE1,HIS,A
NE2,HIS,A
N,SER,A
CA,SER,A
D,SER,A
CB,SER,A
OG,SER,A
N1,ARG,A
CA,ARG,A
C,ARG,A
O,ARG,A
CB,ARG,A
G,ARG,A
D,ARG,A
NE,ARG,A
CZ,ARG,A
NH1,ARG,A
NH2,ARG,A
H,GLN,A
CA,GLN,A
C,GLN,A
O,GLN,A
Mush@DESKTOP-DE71GO3: ~/Lab_session3/Lab_assignment3
CA,ASP,A
C,ASP,A
H,ASP,A
CB,ASP,A
CG,ASP,A
CD1,ASP,A
CD2,ASP,A
H,CGLY,A
CA,GLY,A
C,GLY,A
D,GLY,A
V,GLY,A
CA,GLU,A
C,GLU,A
D,GLU,A
CB,GLU,A
CG,GLU,A
CD,GLU,A
CE1,GLU,A
CE2,GLU,A
H,ALA,A
CA,ALA,A
C,ALA,A
D,ALA,A
CB,ALA,A
CG,ALA,A
H,LEU,A
CA,LEU,A
C,LEU,A
D,LEU,A
CB,LEU,A
CG,LEU,A
CD1,LEU,A
CD2,LEU,A
H,CYS,A
CA,CYS,A
C,CYS,A
D,CYS,A
CB,CYS,A
CG,CYS,A
V,RP,A
```

```
khushit@DESKTOP-DE71GO3: ~/Lab_session3/Lab_assignment3
N, TRP, A
CA, TRP, A
C, TRP, A
O, TRP, A
CB, TRP, A
CG, TRP, A
CD1, TRP, A
CD2, TRP, A
NE1, TRP, A
CE2, TRP, A
CE3, TRP, A
CZ2, TRP, A
CZ3, TRP, A
CH2, TRP, A
H, CYS, A
CA, CYS, A
C, CYS, A
O, CYS, A
CB, CYS, A
SG, CYS, A
N, VAL, A
CA, VAL, A
C, VAL, A
O, VAL, A
CB, VAL, A
CG1, VAL, A
CG2, VAL, A
N, TYR, A
CA, TYR, A
C, TYR, A
O, TYR, A
CB, TYR, A
CG, TYR, A
CD1, TYR, A
CD2, TYR, A
CE1, TYR, A
CE2, TYR, A
CZ, TYR, A
CH, TYR, A
N, PRO, A
CA, PRO, A
C, PRO, A
O, PRO, A
CB, PRO, A
N, ASN, A
CA, ASN, A
C, ASN, A
O, ASN, A
CB, ASN, A
CG, ASN, A
O1, ASN, A
ND2, ASN, A
N, GLY, A
CA, GLY, A
C, GLY, A
O, GLY, A
N, LYS, A
CA, LYS, A
C, LYS, A
O, LYS, A
CB, LYS, A
CG, LYS, A
CD, LYS, A
CE, LYS, A
N, ARG, A
CA, ARG, A
C, ARG, A
O, ARG, A
CB, ARG, A
CG, ARG, A
CG, ARG, A
CD, ARG, A
NE, ARG, A
CZ, ARG, A
NH1, ARG, A
NH2, ARG, A
N, ILE, A
CA, ILE, A
C, ILE, A
O, ILE, A
CB, ILE, A
CG, ILE, A
CG2, ILE, A
CD1, ILE, A
N, PRO, A
CA, PRO, A
C, PRO, A
O, PRO, A
CB, PRO, A
CG, PRO, A
CD, PRO, A
N, GLU, A
CA, GLU, A
C, GLU, A
O, GLU, A
CB, GLU, A
CG, GLU, A
N, GLU, A
CA, GLU, A
C, GLU, A
O, GLU, A
CB, GLU, A
CG, GLU, A
```

```

khush@DESKTOP-DE71GO3:~/Lab_session3/Lab_assignment3
CG,GLU,A
SD,ASP,A
DE1,GLU,A
DE2,GLU,A
N,ILE,A
CA,ILE,A
H,ILE,A
D,ILE,A
CB,ILE,A
CG1,ILE,A
CG2,ILE,A
CD,ILE,A
H,ARG,A
CA,ARG,A
C,ARG,A
O,ARG,A
DP,ASP,A
CG,ARG,A
CD,ARG,A
NE,ARG,A
CZ,ARG,A
NH1,ARG,A
NH2,ARG,A
V,GLY,A
CA,GLY,A
C,GLY,A
D,GLY,A
N,ASP,A
CA,ASP,A
C,ASP,A
O,ASP,A
D,ASP,A
CG,ASP,A
CD1,ASP,A
CD2,ASP,A
N,PRO,A
CA,PRO,A
D,PRO,A
O,PRO,A
CB,PRO,A
CG,PRO,A
CD,PRO,A
N,ASN,A
CA,ASN,A
C,ASN,A
O,ASN,A
CB,ASN,A
CD,ASN,A
ND1,CYS,A
ND2,CYS,A
N,CYS,A
CA,CYS,A
C,CYS,A
D,CYS,A
CB,CYS,A
SG,CYS,A
OXT,CYS,A
khush@DESKTOP-DE71GO3:~/Lab_session3/Lab_assignment3$ 

khush@DESKTOP-DE71GO3:~/Lab_session3/Lab_assignment3
CA,ASH,A
C,ASH,A
O,ASH,A
CB,ASH,A
CD,ASH,A
ND1,CYS,A
ND2,CYS,A
N,CYS,A
CA,CYS,A
C,CYS,A
D,CYS,A
CB,CYS,A
SG,CYS,A
OXT,CYS,A
khush@DESKTOP-DE71GO3:~/Lab_session3/Lab_assignment3$ 

```

24. Replace all lowercase letters in sequences of protein.fasta with uppercase

```

khush@DESKTOP-DE71GO3:~/Lab_session3/Lab_assignment3
CG,ASN,A
CD1,ASN,A
ND2,ASN,A
N,CYS,A
CA,CYS,A
C,CYS,A
D,CYS,A
CB,CYS,A
SG,CYS,A
OXT,CYS,A
khush@DESKTOP-DE71GO3:~/Lab_session3/Lab_assignment3$ awk '{print toupper($0)}' protein.fasta
>SEQ1|HOMO_SAPIENS|CLOCK_PROTEIN
HTEYKLVVGAGCCGKSALTSQLIHFGFVDEYDPTIEDSYRKQVVIDGETCLLDILDTAG

>SEQ2|MUS_MUSCULUS|PER_PROTEIN
HSODEEVQPSLLTKGRVLQLVLSLFFGKNSDQLQSLENQLQDLLTAAQNMYSSNT

>SEQ3|DROSOPHILA_MELANOASTER|TIM_PROTEIN
HADQLTTEQIAEKFKEAFLFDKQDGCTKELGTVRSCCQNPTEAEIQLDMINEVDADGNQ

>SEQ4|DANIO_ERIO|BMAL_PROTEIN
HLSRAVCAGTGKSTLSRITAQYFKKTDVLVGPMSGAGKTTISKLLLEQLDYNQKIV

>SEQ5|ARABIDOPSIS_THALIANA|LHY_PROTEIN
HSEQNQVWDDGSIKVLVTGKCDPQRVTSQPVQLQAGLDRIFGVIRDLGGSS

>SEQ6|SACCHAROMYCES_CEREVISIAE|CYC_PROTEIN
HTEYKLVVGAGCCGKSALTSQLIHFGFVDEYDPTIEDSYRKQVVIDGETCLLDILDTAG

>SEQ7|CAENORHABDITIS_ELEGANS|CLK_PROTEIN
HADSRQRLLQNVINKAAKGKSSLLPVQDGKILVVTITGGVQVSINVLEAMKELLQ

>SEQ8|GALLUS_GALLUS|CRY_PROTEIN
HPIGSGVVRAGTVAGQLRMNNKVVGDLGAGKTTLLQSVIEMKLLGEKGTA

>SEQ9|ESCHERICHIA_COLI|RECA_PROTEIN
HMVQLKKQLKDLPGVIVLGPPIAGKGTQFVSYVLNQLPQYLKKIDVYRTKGF

>SEQ10|XENOPUS_LAEVIS|REV-ERB_PROTEIN
HADEEKLPPGWEKRMRSRSSGRVYYFNHITNASQWERPSGNSSSGSL

```

25. Find the sequence(s) in protein.fasta with the maximum length.

```
khushi@DESKTOP-DE71G03:~/Lab_session3/Lab_assignment3$ awk '/^>/ {if(seqlen){print header, seq, seqlen};header=$0; seq="" ; seqlen=0; next} {seq=seq $0; seqlen+=length($0)} END {print header, seq, seqlen}' protein.fasta | sort -n -k3 -nr | head -n 1
>seq3|Drosophila_melanogaster|TIM_protein MADQLTEEQIAEKFKEAFLSLFDKGDGTCTKELGTVMRSCCQNPEAEIQLQDMINEVDADNGQ 63
```

26. Extract unique residue names from protein.pdb and sort them alphabetically.

```
khushi@DESKTOP-DE71G03:~/Lab_session3/Lab_assignment3$ awk '/^ATOM/{print $4}' protein.pdb | sort -u
ALA
ARG
ASN
ASP
CYS
GLN
GLU
GLY
HIS
ILE
LEU
LYS
MET
PHE
PRO
SER
THR
TRP
TYR
VAL
khushi@DESKTOP-DE71G03:~/Lab_session3/Lab_assignment3$
```

27. Find how many distinct chains are present in protein.pdb.

```
VAL
khushi@DESKTOP-DE71G03:~/Lab_session3/Lab_assignment3$ awk '/^ATOM/{print $5}' protein.pdb | sort -u |wc -l
1
khushi@DESKTOP-DE71G03:~/Lab_session3/Lab_assignment3$
```

28. From clock_gene.fasta, count nucleotide frequencies (A, T, G, C) separately.

```
pscr: line 1: syntax error
khushi@DESKTOP-DE71G03:~/Lab_session3/Lab_assignment3$ awk '{a+=gsub(/A/, "&"); t+=gsub(/T/, "&"); g+=gsub(/G/, "&"); c+=gsub(/C/, "&") } END {print "A="a, "T="t, "G="g, "C="c}'
clock_gene.fasta
A=115 T=100 G=356 C=203
khushi@DESKTOP-DE71G03:~/Lab_session3/Lab_assignment3$
```

I used AI tool **Chatgpt** for some commands to understand the syntax error occurred while using them. To rectify the syntax errors and get proper outputs. To understand awk functions such as **sub(/pattern/, “replacement”)** and **substr(string,location)** use while giving command to avoid syntax error and how they give output. And also for command **awk ‘/ATOM/ && \$5== "A" {res[\$4]++} END {for(r in res) print r, res[r]}’ protein.pdb** and understood that res is an associative array in awk and \$4 residue number and thus by res[\$4]++ increment and store the count for that residue and then execute it for all residues and print its count.