

BT3040 - Practical 6

Sunil Nagar, MM19B055

Q1 - set 1– P69905, P01946, P01942, P01966, P01958, P01959, P01965, P06635, P60529, P80043,P01980

Position	Residue	Set 1				
		Condition 1	Condition 2	Condition 3	Condition 4	Condition 5
'1'	'I'	0	1.021	5	1.019	0.943
'2'	'S'	-0.305	0.865	3.008	0.729	0.253
'3'	'L'	0	0.909	4	0.916	0.943
'4'	'S'	0	0.953	4	0.951	0.943
'5'	'D'	-1.121	0.527	1.149	0.492	-1.597
'6'	'K'	-1.16	0.561	1.157	0.439	-1.685
'7'	'D'	0	0.973	6	0.972	0.943
'8'	'K'	0	0.956	5	0.95	0.943
'9'	'A'	-1.169	0.541	1.868	0.465	-1.705
'10'	'A'	-0.305	0.917	4.661	0.77	0.253
'11'	'V'	-0.586	0.744	3.603	0.763	-0.385
'12'	'R'	-0.305	0.871	4.504	0.744	0.253
'13'	'A'	-1.034	0.567	1.909	0.566	-1.399
'14'	'L'	-1.16	0.559	1.521	0.415	-1.685
'15'	'W'	-0.305	0.943	9.306	0.888	0.253
'16'	'S'	-0.916	0.612	2.264	0.604	-1.134
'17'	'K'	0	0.956	5	0.95	0.943
'18'	'I'	-0.689	0.691	3.504	0.719	-0.618
'19'	'G'	-0.305	0.886	4.992	0.831	0.253
'20'	'K'	-1.034	0.613	2.405	0.502	-1.399
'21'	'S'	-0.886	0.713	4.372	0.627	-1.064
'22'	'A'	-0.474	0.74	2.876	0.767	-0.131
'23'	'D'	-1.034	0.624	2.24	0.517	-1.399
'24'	'A'	-0.908	0.665	2.455	0.593	-1.114
'25'	'I'	-0.886	0.757	4.314	0.679	-1.064

'26'	'G'	0	0.977	6	0.977	0.943
'27'	'N'	-0.886	0.65	1.826	0.561	-1.064
'28'	'D'	-0.305	0.922	4.512	0.784	0.253
'29'	'A'	-0.305	0.817	3.347	0.768	0.253
'30'	'L'	0	0.909	4	0.916	0.943
'31'	'S'	-0.886	0.749	3.298	0.628	-1.064
'32'	'R'	0	1.015	5	1.011	0.943
'33'	'M'	-0.305	0.933	4.008	0.944	0.253
'34'	'I'	-0.305	0.904	4.992	0.78	0.253
'35'	'V'	-1.295	0.47	0.959	0.373	-1.991
'36'	'V'	-1.367	0.472	1.132	0.386	-2.154
'37'	'Y'	-0.474	0.83	5.14	0.718	-0.131
'38'	'P'	0	0.993	7	0.993	0.943
'39'	'Q'	-0.474	0.821	3.215	0.715	-0.131
'40'	'T'	0	0.977	5	0.979	0.943
'41'	'K'	0	0.956	5	0.95	0.943
'42'	'T'	0	0.977	5	0.979	0.943
'43'	'Y'	0	1.016	7	1.012	0.943
'44'	'F'	0	0.988	6	0.989	0.943
'45'	'S'	-0.474	0.822	4.521	0.712	-0.131
'46'	'H'	0	0.969	8	0.972	0.943
'47'	'W'	-0.6	0.823	4.24	0.711	-0.417
'48'	'P'	-0.857	0.657	2.295	0.582	-1
'49'	'D'	-0.305	0.888	5.174	0.901	0.253
'50'	'V'	-0.586	0.674	2.81	0.621	-0.385
'51'	'T'	-0.6	0.776	2.752	0.605	-0.417
'52'	'P'	-0.586	0.745	3.959	0.689	-0.385
'53'	'G'	0	0.977	6	0.977	0.943
'54'	'S'	0	0.953	4	0.951	0.943
'55'	'P'	-0.6	0.73	2.322	0.628	-0.417
'56'	'H'	-0.305	0.936	4.198	0.8	0.253
'57'	'I'	-0.305	0.872	3.835	0.748	0.253

'58'	'K'	0	0.956	5	0.95	0.943
'59'	'A'	-0.86	0.596	1.835	0.687	-1.006
'60'	'H'	0	0.969	8	0.972	0.943
'61'	'G'	0	0.977	6	0.977	0.943
'62'	'K'	-0.6	0.777	3.405	0.812	-0.417
'63'	'K'	0	0.956	5	0.95	0.943
'64'	'V'	0	0.956	4	0.956	0.943
'65'	'M'	-0.76	0.66	2.124	0.612	-0.778
'66'	'G'	-0.76	0.704	2.694	0.561	-0.778
'67'	'G'	-0.305	0.817	3.355	0.692	0.253
'68'	'I'	-0.305	0.825	3.669	0.71	0.253
'69'	'A'	-0.86	0.643	2.19	0.545	-1.006
'70'	'L'	-1.673	0.36	0.124	0.382	-2.848

'71'	'A'	0	0.906	4	0.909	0.943
'72'	'V'	-0.586	0.701	2.413	0.682	-0.385
'73'	'S'	-1.594	0.406	0.934	0.359	-2.67
'74'	'K'	-0.305	0.879	6.488	0.745	0.253
'75'	'I'	-0.995	0.543	2.612	0.534	-1.312
'76'	'D'	-0.305	0.888	5.331	0.888	0.253
'77'	'D'	0	0.973	6	0.972	0.943
'78'	'L'	-0.76	0.675	3.14	0.683	-0.778
'79'	'K'	-0.6	0.807	4.446	0.618	-0.417
'80'	'T'	-0.76	0.733	3.149	0.664	-0.778
'81'	'G'	-0.305	0.817	3.355	0.692	0.253
'82'	'L'	0	0.909	4	0.916	0.943
'83'	'M'	-0.305	0.869	3.182	0.749	0.253
'84'	'E'	-1.414	0.451	0.678	0.428	-2.262
'85'	'L'	0	0.909	4	0.916	0.943
'86'	'S'	0	0.953	4	0.951	0.943
'87'	'E'	-0.305	0.888	5.331	0.763	0.253
'88'	'Q'	-0.305	0.826	3.017	0.715	0.253
'89'	'H'	0	0.969	8	0.972	0.943
'90'	'A'	0	0.906	4	0.909	0.943
'91'	'Y'	-0.76	0.731	4.967	0.618	-0.778
'92'	'K'	0	0.956	5	0.95	0.943
'93'	'L'	0	0.909	4	0.916	0.943
'94'	'R'	0	1.015	5	1.011	0.943
'95'	'V'	0	0.956	4	0.956	0.943
'96'	'D'	0	0.973	6	0.972	0.943
'97'	'P'	0	0.993	7	0.993	0.943
'98'	'A'	-0.305	0.86	3.339	0.715	0.253
'99'	'N'	0	1.012	6	1.011	0.943
'100'	'F'	0	0.988	6	0.989	0.943
'101'	'K'	0	0.956	5	0.95	0.943
'102'	'I'	-0.6	0.739	3.058	0.632	-0.417

'103'	'L'	0	0.909	4	0.916	0.943
'104'	'N'	-0.6	0.781	2.926	0.619	-0.417
'105'	'H'	-0.305	0.886	6.653	0.839	0.253
'106'	'C'	-0.305	0.937	7.306	0.962	0.253
'107'	'I'	-0.6	0.739	3.058	0.588	-0.417
'108'	'L'	-0.305	0.825	3.678	0.783	0.253
'109'	'V'	-0.474	0.784	2.215	0.844	-0.131
'110'	'V'	-0.474	0.806	3.479	0.677	-0.131
'111'	'I'	-0.6	0.735	3.24	0.58	-0.417
'112'	'S'	-0.305	0.814	3.504	0.683	0.253
'113'	'T'	-1.72	0.345	0.702	0.355	-2.955
'114'	'M'	-0.305	0.885	6.322	0.769	0.253
'115'	'F'	-0.935	0.559	1.207	0.529	-1.175
'116'	'P'	0	0.993	7	0.993	0.943
'117'	'K'	-1.846	0.302	0.562	0.299	-3.241
'118'	'E'	-0.916	0.633	3.008	0.584	-1.134
'119'	'F'	-0.305	0.893	4.992	0.837	0.253
'120'	'T'	-0.305	0.891	4.182	0.907	0.253
'121'	'P'	0	0.993	7	0.993	0.943
'122'	'E'	-0.76	0.66	2.182	0.589	-0.778
'123'	'A'	-0.886	0.695	2.736	0.519	-1.064
'124'	'H'	0	0.969	8	0.972	0.943
'125'	'V'	-0.305	0.814	3.339	0.685	0.253
'126'	'S'	0	0.953	4	0.951	0.943
'127'	'L'	0	0.909	4	0.916	0.943
'128'	'D'	0	0.973	6	0.972	0.943
'129'	'K'	0	0.956	5	0.95	0.943
'130'	'F'	0	0.988	6	0.989	0.943
'131'	'L'	-0.305	0.822	3.355	0.839	0.253
'132'	'S'	-0.86	0.595	2.289	0.528	-1.006
'133'	'G'	-1.414	0.459	1.496	0.4	-2.262
'134'	'V'	0	0.956	4	0.956	0.943
'135'	'A'	-0.6	0.769	2.909	0.577	-0.417
'136'	'L'	-0.6	0.796	3.231	0.615	-0.417
'137'	'A'	-0.305	0.86	3.339	0.715	0.253
'138'	'L'	0	0.909	4	0.916	0.943
'139'	'A'	-0.305	0.881	4.165	0.738	0.253
'140'	'E'	-0.305	0.868	3.347	0.743	0.253
'141'	'R'	-0.305	0.871	4.504	0.744	0.253
'142'	'Y'	0	1.016	7	1.012	0.943
'143'	'R'	0	1.015	5	1.011	0.943

**Set 2 - TPIS_HUMAN, TPIS_YEAST, TPIS_GRAVE, TPIS_TRYCR, TPIS_MAIZE,
TPIS_MOUSE, TPIS_DROME, TPIS_RABIT, TPIS_CAEEL**

Position	Residue	Set 2				
		Condition 1	Condition 2	Condition 3	Condition 4	Condition 5
1	-	-1.216	0.529	1.306	0.494	-1
2	-	-1.216	0.529	1.306	0.494	-1
3	-	-1.216	0.529	1.306	0.494	-1
4	-	-1.216	0.529	1.306	0.494	-1
5	-	-1.216	0.529	1.306	0.494	-1
6	-	-1.216	0.529	1.306	0.494	-1
7	-	-1.216	0.529	1.306	0.494	-1
8	-	-1.216	0.529	1.306	0.494	-1
9	-	-1.216	0.529	1.306	0.494	-1
10	-	-1.216	0.529	1.306	0.494	-1
11	-	-1.216	0.529	1.306	0.494	-1
12	-	-1.216	0.529	1.306	0.494	-1
13	-	-1.216	0.529	1.306	0.494	-1
14	-	-1.216	0.529	1.306	0.494	-1
15	-	-1.216	0.529	1.306	0.494	-1
16	-	-1.216	0.529	1.306	0.494	-1
17	-	-1.216	0.529	1.306	0.494	-1
18	-	-1.216	0.529	1.306	0.494	-1
19	-	-1.216	0.529	1.306	0.494	-1
20	-	-1.216	0.529	1.306	0.494	-1
21	-	-1.216	0.529	1.306	0.494	-1
22	-	-1.216	0.529	1.306	0.494	-1
23	-	-1.216	0.529	1.306	0.494	-1
24	-	-1.216	0.529	1.306	0.494	-1
25	-	-1.216	0.529	1.306	0.494	-1
26	-	-1.216	0.529	1.306	0.494	-1

26	-	-1.216	0.529	1.306	0.494	-1
27	-	-1.216	0.529	1.306	0.494	-1
28	-	-1.216	0.529	1.306	0.494	-1
29	-	-1.216	0.529	1.306	0.494	-1
30	-	-1.216	0.529	1.306	0.494	-1
31	-	-1.216	0.529	1.306	0.494	-1
32	-	-1.216	0.529	1.306	0.494	-1
33	-	-1.216	0.529	1.306	0.494	-1
34	-	-1.216	0.529	1.306	0.494	-1
35	-	-1.216	0.529	1.306	0.494	-1
36	-	-1.216	0.529	1.306	0.494	-1
37	-	-1.216	0.529	1.306	0.494	-1
38	-	-1.216	0.529	1.306	0.494	-1
39	-	-1.216	0.529	1.306	0.494	-1
40	-	-1.216	0.529	1.306	0.494	-1
41	-	-1.216	0.529	1.306	0.494	-1
42	-	-1.216	0.529	1.306	0.494	-1
43	-	-1.216	0.529	1.306	0.494	-1
44	-	-1.216	0.529	1.306	0.494	-1
45	-	-1.216	0.529	1.306	0.494	-1
46	-	-1.216	0.529	1.306	0.494	-1
47	-	-1.216	0.529	1.306	0.494	-1
48	-	-1.216	0.529	1.306	0.494	-1
49	-	-1.216	0.529	1.306	0.494	-1
50	-	-1.216	0.529	1.306	0.494	-1
51	-	-1.216	0.529	1.306	0.494	-1
52	-	-1.216	0.529	1.306	0.494	-1
53	M	-1.216	0.529	1.306	0.494	-1
54	A	-1.216	0.529	1.306	0.494	-1
55	S	-0.974	0.648	1.328	0.666	-0.56
56	K	-1.494	0.426	1.109	0.365	-1.507
57	P	-0.377	0.882	3.5	0.827	0.529

56	K	-1.494	0.426	1.109	0.365	-1.507
57	P	-0.377	0.882	3.5	0.827	0.529
58	Q	-0.736	0.726	2.938	0.641	-0.125
59	P	-0.377	0.884	3.828	0.83	0.529
60	I	-0.736	0.769	3.172	0.713	-0.125
61	A	-0.377	0.801	3.125	0.739	0.529
62	A	-0.377	0.812	4.656	0.754	0.529
63	A	-0.377	0.812	4.656	0.754	0.529
64	N	0	0.995	6	0.994	1.215
65	W	-0.349	0.909	8.963	0.876	0.58
66	K	0	0.962	5	0.966	1.215
67	C	-0.937	0.679	2.395	0.639	-0.492
68	N	0	0.995	6	0.994	1.215
69	G	-0.349	0.835	4	0.81	0.58
70	S	-1.311	0.51	0.79	0.53	-1.173
71	E	-1.303	0.553	1.568	0.515	-1.159
72	S	-1.523	0.401	0.901	0.372	-1.56
73	L	-1.581	0.481	0.519	0.482	-1.666
74	L	-1.061	0.526	2.667	0.514	-0.718
75	V	-1.677	0.317	0.198	0.27	-1.841
76	P	-1.003	0.64	2.025	0.597	-0.612
77	L	-0.687	0.664	3.012	0.656	-0.036
78	I	-0.965	0.55	2.716	0.557	-0.543
79	E	-1.735	0.362	0.136	0.393	-1.946
80	T	-1.003	0.663	1.815	0.595	-0.612
81	L	-0.349	0.859	3.235	0.826	0.58
82	N	-0.349	0.888	4.988	0.885	0.58
83	A	-1.003	0.591	1.951	0.549	-0.612
84	A	-0.684	0.691	2.716	0.676	-0.031
85	T	-1.889	0.305	0.383	0.302	-2.227
86	F	-1.581	0.426	0.457	0.364	-1.666
87	D	-1.149	0.604	1.543	0.553	-0.879

87	D	-1.149	0.604	1.543	0.553	-0.879
88	H	-1.677	0.372	0.383	0.348	-1.841
89	D	-1.523	0.429	1.259	0.421	-1.56
90	:	-1.216	0.529	1.306	0.494	-1
91	:	-1.216	0.529	1.306	0.494	-1
92	V	-0.687	0.645	2.222	0.684	-0.036
93	Q	-0.849	0.671	3.432	0.623	-0.331
94	C	-0.349	0.829	3.074	0.795	0.58
95	V	0	0.93	4	0.93	1.215
96	V	-1.061	0.545	2.136	0.563	-0.718
97	A	-1.003	0.594	2.062	0.557	-0.612
98	P	-0.349	0.893	5.049	0.894	0.58
99	T	-0.349	0.889	5.395	0.855	0.58
100	F	-1.215	0.498	0.889	0.51	-0.998
101	L	-1.677	0.321	0.593	0.294	-1.841
102	H	-0.684	0.808	5.247	0.771	-0.031
103	I	-0.687	0.664	3.012	0.686	-0.036
104	P	-1.149	0.595	1.272	0.564	-0.879
105	M	-1.465	0.504	1.704	0.492	-1.454
106	T	-1.149	0.509	1.704	0.45	-0.879
107	K	-0.937	0.625	2.37	0.582	-0.492
108	A	-1.215	0.541	1.556	0.505	-0.998
109	R	-1.427	0.462	0.889	0.399	-1.385
110	L	-0.349	0.85	3.407	0.809	0.58
111	T	-1.216	0.529	1.306	0.494	-1
112	N	-1.523	0.455	0.877	0.44	-1.56
113	P	-1.149	0.584	1.667	0.551	-0.879
114	K	-1.427	0.467	1.469	0.421	-1.385
115	F	-1.311	0.477	1.852	0.497	-1.173
116	Q	-1.831	0.321	-0.222	0.292	-2.121
117	I	-1.003	0.611	2.531	0.549	-0.612
118	A	-0.684	0.691	2.716	0.623	-0.031

119	A	-0.349	0.798	3.235	0.793	0.58
120	Q	0	0.994	5	0.993	1.215
121	N	0	0.995	6	0.994	1.215
122	A	-0.687	0.669	3.568	0.649	-0.036
123	I	-0.849	0.723	4	0.666	-0.331
124	:	-1.074	0.596	1.234	0.506	-0.741
125	T	-1.149	0.532	0.827	0.465	-0.879
126	R	-1.523	0.408	0.654	0.38	-1.56
127	S	-1.369	0.453	1.358	0.446	-1.279
128	G	0	0.944	6	0.951	1.215
129	A	0	0.909	4	0.905	1.215
130	F	0	1.001	6	1.006	1.215
131	T	0	0.983	5	0.984	1.215
132	G	0	0.944	6	0.951	1.215
133	E	0	0.962	5	0.96	1.215
134	V	-1.149	0.559	2	0.478	-0.879
135	S	-0.349	0.873	3.235	0.84	0.58
136	L	-1.149	0.562	1.568	0.469	-0.879
137	Q	-1.465	0.391	0.741	0.375	-1.454
138	I	-0.684	0.811	3.235	0.744	-0.031
139	L	-0.937	0.601	2.914	0.557	-0.492
140	K	-0.349	0.849	3.605	0.848	0.58
141	D	-0.349	0.883	5.012	0.878	0.58
142	Y	-1.523	0.43	1.123	0.415	-1.56
143	G	0	0.944	6	0.951	1.215
144	I	-1.003	0.58	1.778	0.529	-0.612
145	S	-1.677	0.406	0.778	0.368	-1.841
146	W	0	1.013	11	1.013	1.215
147	V	0	0.93	4	0.93	1.215
148	V	-0.687	0.644	3.506	0.676	-0.036
149	L	0	0.963	4	0.959	1.215
150	G	0	0.944	6	0.951	1.215

151	H	0	1.017	8	1.017	1.215
152	S	0	0.979	4	0.977	1.215
153	E	0	0.962	5	0.96	1.215
154	R	0	0.999	5	1	1.215
155	R	0	0.999	5	1	1.215
156	L	-1.149	0.592	1.728	0.522	-0.879
157	Y	-1.273	0.484	1.827	0.463	-1.104
158	:	-1.216	0.529	1.306	0.494	-1
159	:	-1.216	0.529	1.306	0.494	-1
160	Y	-0.849	0.703	3.346	0.65	-0.331
161	G	-0.684	0.735	3.074	0.682	-0.031
162	E	0	0.962	5	0.96	1.215
163	T	-0.684	0.768	2.704	0.7	-0.031
164	N	-0.53	0.796	4.272	0.765	0.25
165	E	-1.149	0.546	1.605	0.484	-0.879
166	I	-1.149	0.577	1.642	0.508	-0.879
167	V	-0.53	0.762	3.654	0.726	0.25
168	A	-0.687	0.601	2.42	0.643	-0.036
169	E	-1.311	0.505	1.914	0.499	-1.173
170	K	0	0.962	5	0.966	1.215
171	V	-0.995	0.535	1.679	0.492	-0.598
172	A	-1.303	0.475	1.21	0.465	-1.159
173	Q	-1.149	0.638	3.346	0.569	-0.879
174	A	0	0.909	4	0.905	1.215
175	C	-0.349	0.861	3.074	0.824	0.58
176	A	-1.427	0.419	1.136	0.381	-1.385
177	:	-1.216	0.529	1.306	0.494	-1
178	A	-1.061	0.514	1.63	0.491	-0.718
179	G	-0.349	0.837	4.79	0.813	0.58
180	F	-1.003	0.642	2.444	0.566	-0.612
181	H	-0.937	0.592	1.444	0.573	-0.492
182	V	0	0.93	4	0.93	1.215

183	I	-0.349	0.858	3.802	0.849	0.58
184	V	-1.303	0.492	0.901	0.401	-1.159
185	C	0	1.017	9	1.018	1.215
186	V	-0.53	0.762	3.654	0.726	0.25
187	G	0	0.944	6	0.951	1.215
188	E	0	0.962	5	0.96	1.215
189	T	-0.965	0.592	1.333	0.598	-0.543
190	N	-0.349	0.859	2.642	0.819	0.58
191	E	-0.637	0.706	3.778	0.782	0.056
192	E	-0.349	0.857	4.407	0.85	0.58
193	R	-0.349	0.89	4.407	0.856	0.58
194	E	-0.349	0.853	4.21	0.816	0.58
195	A	-0.349	0.802	3.407	0.766	0.58
196	G	0	0.944	6	0.951	1.215
197	R	-1.677	0.414	-0.222	0.387	-1.841
198	T	0	0.983	5	0.984	1.215
199	A	-1.831	0.35	-0.062	0.283	-2.121
200	A	-1.311	0.452	0.988	0.454	-1.173
201	V	0	0.93	4	0.93	1.215
202	V	-0.684	0.726	1.84	0.692	-0.031
203	L	-1.273	0.497	0.395	0.44	-1.104
204	T	-1.215	0.533	1.309	0.562	-0.998
205	Q	0	0.994	5	0.993	1.215
206	L	-0.965	0.604	1.543	0.623	-0.543
207	A	-1.427	0.481	0.951	0.424	-1.385
208	A	-0.637	0.629	2.222	0.712	0.056
209	V	-1.149	0.562	2.407	0.491	-0.879
210	A	-1.003	0.581	1.852	0.507	-0.612
211	Q	-0.995	0.612	3.037	0.569	-0.598
212	K	-1.215	0.519	1.593	0.511	-0.998
213	L	-1.215	0.484	1.802	0.458	-0.998
214	S	-1.216	0.529	1.306	0.494	-1

215	K	-1.216	0.529	1.306	0.494	-1
216	E	-1.003	0.635	2.136	0.568	-0.612
217	A	-0.684	0.766	3.407	0.718	-0.031
218	W	0	1.013	11	1.013	1.215
219	S	-1.003	0.658	2.086	0.617	-0.612
220	R	-1.215	0.549	2	0.558	-0.998
221	V	-0.349	0.822	3.802	0.815	0.58
222	V	0	0.93	4	0.93	1.215
223	I	-1.099	0.495	2.667	0.518	-0.787
224	A	0	0.909	4	0.905	1.215
225	Y	0	1.013	7	1.011	1.215
226	E	0	0.962	5	0.96	1.215
227	P	0	0.995	7	0.997	1.215
228	V	0	0.93	4	0.93	1.215
229	W	0	1.013	11	1.013	1.215
230	A	0	0.909	4	0.905	1.215
231	I	0	0.971	4	0.97	1.215
232	G	0	0.944	6	0.951	1.215
233	T	0	0.983	5	0.984	1.215
234	G	0	0.944	6	0.951	1.215
235	K	-0.684	0.75	2.914	0.718	-0.031
236	V	-0.937	0.591	2.037	0.535	-0.492
237	A	0	0.909	4	0.905	1.215
238	T	-0.349	0.876	4.198	0.87	0.58
239	P	-0.349	0.884	5.21	0.88	0.58
240	Q	-1.215	0.53	2.185	0.514	-0.998
241	Q	-0.349	0.888	4.025	0.853	0.58
242	A	0	0.909	4	0.905	1.215
243	Q	-0.349	0.885	4.407	0.852	0.58
244	E	-0.684	0.753	3.852	0.689	-0.031
245	V	-0.349	0.822	3.802	0.788	0.58
246	H	0	1.017	8	1.017	1.215

247	E	-0.637	0.669	2.222	0.641	0.056
248	L	-1.677	0.389	-0.074	0.351	-1.841
249	L	-0.849	0.656	2.914	0.592	-0.331
250	R	0	0.999	5	1	1.215
251	R	-1.677	0.35	0.383	0.319	-1.841
252	W	-0.53	0.822	7.296	0.792	0.25
253	V	-0.349	0.85	3.407	0.808	0.58
254	R	-1.149	0.545	1.827	0.476	-0.879
255	S	-1.303	0.564	1.778	0.525	-1.159
256	K	-0.637	0.724	3.222	0.69	0.056
257	L	-1.149	0.516	2.173	0.471	-0.879
258	G	-0.849	0.673	2.296	0.656	-0.331
259	T	-1.215	0.555	1.42	0.532	-0.998
260	D	-1.677	0.333	0.543	0.319	-1.841
261	I	-0.684	0.707	3.012	0.633	-0.031
262	A	-0.349	0.802	3.407	0.796	0.58
263	A	-1.465	0.426	1.012	0.405	-1.454
264	Q	-1.003	0.651	2.099	0.575	-0.612
265	L	-0.637	0.713	2.222	0.68	0.056
266	R	0	0.999	5	1	1.215
267	I	0	0.971	4	0.97	1.215
268	L	-0.937	0.612	1.963	0.586	-0.492
269	Y	0	1.013	7	1.011	1.215
270	G	0	0.944	6	0.951	1.215
271	G	0	0.944	6	0.951	1.215
272	S	0	0.979	4	0.977	1.215
273	V	-0.349	0.815	3.21	0.776	0.58
274	T	-0.684	0.773	3.346	0.711	-0.031
275	A	-0.965	0.53	1.765	0.521	-0.543
276	K	-1.003	0.592	1.642	0.518	-0.612
277	N	-0.637	0.733	3.222	0.814	0.056
278	A	-0.687	0.669	3.568	0.65	-0.036

279	R	-1.303	0.523	1.593	0.429	-1.159
280	T	-0.849	0.666	2.272	0.596	-0.331
281	L	-0.349	0.859	3.235	0.823	0.58
282	Y	-1.003	0.59	1.383	0.52	-0.612
283	Q	-1.465	0.444	1.111	0.427	-1.454
284	M	-0.937	0.637	2.457	0.601	-0.492
285	R	-0.684	0.777	3.802	0.707	-0.031
286	D	-0.349	0.883	5.012	0.852	0.58
287	I	-0.687	0.637	3.506	0.638	-0.036
288	N	-0.349	0.883	5.012	0.847	0.58
289	G	0	0.944	6	0.951	1.215
290	F	0	1.001	6	1.006	1.215
291	L	0	0.963	4	0.959	1.215
292	V	0	0.93	4	0.93	1.215
293	G	0	0.944	6	0.951	1.215
294	G	0	0.944	6	0.951	1.215
295	A	0	0.909	4	0.905	1.215
296	S	0	0.979	4	0.977	1.215
297	L	-0.349	0.862	3.617	0.829	0.58
298	K	0	0.962	5	0.966	1.215
299	P	0	0.995	7	0.997	1.215
300	E	-0.684	0.752	3.309	0.713	-0.031
301	F	0	1.001	6	1.006	1.215
302	V	-0.684	0.715	3.259	0.678	-0.031
303	E	-0.849	0.682	3.469	0.628	-0.331
304	I	0	0.971	4	0.97	1.215
305	I	-0.349	0.858	3.802	0.824	0.58
306	E	-0.684	0.782	3.988	0.714	-0.031
307	A	-0.53	0.714	2.963	0.663	0.25
308	T	-1.465	0.462	1.062	0.457	-1.454
309	K	-1.427	0.502	1.519	0.451	-1.385
310	:	-1.216	0.529	1.306	0.494	-1
311	:	-1.216	0.529	1.306	0.494	-1
312	:	-1.216	0.529	1.306	0.494	-1
313	:	-1.216	0.529	1.306	0.494	-1
314	:	-1.216	0.529	1.306	0.494	-1
315	:	-1.216	0.529	1.306	0.494	-1
316	:	-1.216	0.529	1.306	0.494	-1

Q2.

SET1 =>

Highest Conservation Scores:

Residue Position	Residue	Condition (i)
'1'	':'	0
'3'	'L'	0
'4'	'S'	0
'7'	'D'	0
'8'	'K'	0
'17'	'K'	0
'26'	'G'	0
'30'	'L'	0
'32'	'R'	0
'38'	'P'	0

Lowest Conservation Scores:

Residue Position	Residue	Condition (i)
'117'	'K'	-1.846
'113'	'T'	-1.72
'70'	'L'	-1.673
'73'	'S'	-1.594
'84'	'E'	-1.414
'133'	'G'	-1.414
'36'	'V'	-1.367
'35'	'V'	-1.295
'9'	'A'	-1.169
'6'	'K'	-1.16

SET2 =>

Highest Conservation Scores:

Residue Position	Residue	Condition (i)
'64'	'N'	0
'66'	'K'	0
'68'	'N'	0
'95'	'V'	0
'120'	'Q'	0
'121'	'N'	0
'128'	'G'	0
'129'	'A'	0
'130'	'F'	0
'131'	'T'	0

Lowest Conservation Scores:

Residue Position	Residue	Condition (i)
'85'	'T'	-1.889
'116'	'Q'	-1.831
'199'	'A'	-1.831
'79'	'E'	-1.735
'75'	'V'	-1.677
'88'	'H'	-1.677
'101'	'L'	-1.677
'145'	'S'	-1.677
'197'	'R'	-1.677
'248'	'L'	-1.677

Q5.

BT3040 - Practical 6

Sunil Nagar
MM19B055

Q5

For set 1

Position 9 \rightarrow A, S, T, T, A, S, T, T, G, T, T

$$f(A) = \frac{2}{11}, f(G) = \frac{1}{11}, f(S) = \frac{2}{11}, f(T) = \frac{6}{11}$$

$$C^e(9) = 0.182 \ln(0.182) + 0.182 \ln(0.182) + 0.545 \ln(0.545) + 0.09 \ln(0.09)$$

$$C^e(9) = -1.1691$$

Position 11 \rightarrow V, V, I, I, V, I, V, V, V, V, V

$$f(V) = \frac{8}{11}, f(I) = \frac{3}{11}$$

$$C^e(11) \rightarrow 0.727 \ln(0.727) + 0.273 \ln(0.273) = -0.5862$$

Position 20 \rightarrow K, S, G, G, G, G, G, G, G, A, A

$$f(K) = \frac{1}{11}, f(A) = \frac{2}{11}, f(G) = \frac{7}{11}, f(S) = \frac{1}{11}$$

$$\begin{aligned} C^e(20) &= 0.091 \ln(0.091) + 0.182 \ln(0.182) + 0.636 \ln(0.636) \\ &\quad + 0.091 \ln(0.091) \\ &= -1.0341 \end{aligned}$$

Position 22 → A, A, A, G, A, G, A, A, A, A, A

$$f(A) = \frac{9}{11} = 0.818, \quad f(G) = \frac{2}{11} = 0.182$$

$$\begin{aligned} C^e(22) &= 0.818 \ln(0.818) + 0.182 \ln(0.182) \\ &= -0.474. \end{aligned}$$

Position 30 → L, L, L, L, L, L, L, L, L, L, L

$$f(L) = \frac{11}{11} = 1$$

$$C^e(30) = 1 \ln(1) = 0$$

For set 2

Position 9 : -, -, -, -, -, -, G, -, -

$$f(G) = \frac{1}{9} = 0.111$$

$$c^e(9) = 0.111 \ln(0.111) \\ = -0.2442$$

Position 11 : -, -, -, -, -, -, G, -, -

$$f(G) = \frac{1}{9} = 0.111$$

$$c^e(11) = 0.111 \ln(0.111) = -0.2442$$

Position 20 : -, -, -, -, -, -, K, E, E

$$f(K) = \frac{1}{9} = 0.111, f(E) = \frac{2}{9} = 0.222$$

$$c^e(20) = 0.111 \ln(0.111) + 0.222 \ln(0.222) \\ = -0.5784$$

Position ~~20~~²² : -, -, -, -, -, -, E, E, E

$$f(E) = \frac{3}{9} = 0.333$$

$$c^e(22) = 0.333 \ln(0.333) = -0.3662$$

Position 30 : -, -, -, -, -, -, I, I, I

$$f(I) = \frac{3}{9} = 0.333$$

$$c^e(30) = 0.333 \ln(0.333)$$

$$= -0.3662$$

Q6.

- Go to ConSurf server
- Select analyse Amino acids, then yes for protein structure, then PDB ID = 1BTM
- Then 'No' for MSA.
- Then submit (keep the suggested parameters, can change to dig in more)

The average number of replacements between any two sequences in the alignment; A distance of 0.01 means that on average, the expected replacement for every 100 positions is 1.

Average pairwise distance: 0.99628

Lower bound: 0.10971

Upper bound: 1.89437

