

1. Given the structural coordinates (X, Y, Z in Angstroms, see highlighted bold font for atom 1) from a PDB file of SPERM WHALE MYOGLOBIN (*pdb code: 102M*) below:

ATOM	1	N	MET A 0	<b>24.512</b>	<b>8.259</b>	<b>-9.688</b>	1.00	33.83	N
ATOM	2	CA	MET A 0	24.523	9.740	-9.865	1.00	32.90	C
ATOM	3	C	MET A 0	25.889	10.228	-10.330	1.00	31.90	C
ATOM	4	O	MET A 0	26.886	9.516	-10.198	1.00	32.07	O
ATOM	5	CB	MET A 0	24.143	10.414	-8.560	1.00	34.34	C
ATOM	6	CG	MET A 0	24.891	9.880	-7.378	1.00	35.66	C
ATOM	7	SD	MET A 0	24.111	10.428	-5.871	1.00	38.66	S
ATOM	8	CE	MET A 0	24.454	12.221	-5.988	1.00	36.36	C
ATOM	9	N	VAL A 1	25.922	11.435	-10.891	1.00	30.10	N
ATOM	10	CA	VAL A 1	27.161	12.020	-11.393	1.00	27.92	C
ATOM	11	C	VAL A 1	27.260	13.522	-11.114	1.00	26.21	C
ATOM	12	O	VAL A 1	26.304	14.278	-11.304	1.00	26.54	O
ATOM	13	CB	VAL A 1	27.312	11.769	-12.919	1.00	27.99	C
ATOM	14	CG1	VAL A 1	28.557	12.455	-13.466	1.00	27.68	C
ATOM	15	CG2	VAL A 1	27.395	10.282	-13.189	1.00	28.05	C
ATOM	16	N	LEU A 2	28.407	13.938	-10.599	1.00	23.68	N
ATOM	17	CA	LEU A 2	28.641	15.349	-10.324	1.00	20.97	C
ATOM	18	C	LEU A 2	29.285	15.976	-11.549	1.00	19.50	C
ATOM	19	O	LEU A 2	29.976	15.300	-12.306	1.00	18.60	O
ATOM	20	CB	LEU A 2	29.602	15.516	-9.142	1.00	20.07	C
ATOM	21	CG	LEU A 2	29.003	15.462	-7.742	1.00	19.76	C
ATOM	22	CD1	LEU A 2	28.734	14.017	-7.356	1.00	18.96	C
ATOM	23	CD2	LEU A 2	29.966	16.142	-6.762	1.00	18.40	C
ATOM	24	N	SER A 3	29.056	17.260	-11.759	1.00	18.20	N
ATOM	25	CA	SER A 3	29.690	17.929	-12.882	1.00	17.70	C
ATOM	26	C	SER A 3	31.086	18.341	-12.420	1.00	17.23	C
ATOM	27	O	SER A 3	31.404	18.261	-11.230	1.00	16.47	O
ATOM	28	CB	SER A 3	28.882	19.155	-13.301	1.00	17.59	C
ATOM	29	OG	SER A 3	28.766	20.060	-12.225	1.00	17.97	O
ATOM	30	N	GLU A 4	31.935	18.742	-13.356	1.00	11.50	N
ATOM	31	CA	GLU A 4	33.283	19.175	-13.008	1.00	13.15	C
ATOM	32	C	GLU A 4	33.188	20.387	-12.086	1.00	16.93	C
ATOM	33	O	GLU A 4	33.964	20.514	-11.147	1.00	15.15	O
ATOM	34	CB	GLU A 4	34.074	19.549	-14.275	1.00	17.13	C
ATOM	35	CG	GLU A 4	35.473	20.111	-14.013	1.00	17.78	C
ATOM	36	CD	GLU A 4	36.414	19.122	-13.332	1.00	19.05	C
ATOM	37	OE1	GLU A 4	36.132	17.911	-13.343	1.00	29.34	O
ATOM	38	OE2	GLU A 4	37.452	19.559	-12.792	1.00	24.04	O
ATOM	39	N	GLY A 5	32.218	21.261	-12.358	1.00	13.76	N
ATOM	40	CA	GLY A 5	32.027	22.458	-11.553	1.00	13.72	C
ATOM	41	C	GLY A 5	31.722	22.137	-10.101	1.00	13.60	C
ATOM	42	O	GLY A 5	32.186	22.833	-9.197	1.00	13.74	O
ATOM	1207	N	GLN A 152	24.446	-4.753	3.940	1.00	34.79	N

ATOM	1208	CA	GLN A 152	23.530	-3.665	3.569	1.00	37.20	C
ATOM	1209	C	GLN A 152	22.709	-3.098	4.737	1.00	38.24	C
ATOM	1210	O	GLN A 152	21.671	-2.466	4.532	1.00	38.67	O
ATOM	1211	CB	GLN A 152	22.597	-4.059	2.422	1.00	38.53	C
ATOM	1212	CG	GLN A 152	22.461	-2.974	1.348	1.00	47.32	C
ATOM	1213	CD	GLN A 152	22.386	-1.558	1.909	1.00	53.70	C
ATOM	1214	OE1	GLN A 152	23.408	-0.957	2.246	1.00	62.61	O
ATOM	1215	NE2	GLN A 152	21.174	-1.020	2.010	1.00	72.20	N
ATOM	1216	N	GLY A 153	23.174	-3.342	5.957	1.00	39.00	N
ATOM	1217	CA	GLY A 153	22.479	-2.839	7.122	1.00	40.00	C
ATOM	1218	C	GLY A 153	22.703	-1.350	7.301	1.00	40.37	C
ATOM	1219	O	GLY A 153	22.020	-0.745	8.154	1.00	40.86	O
ATOM	1220	OXT	GLY A 153	23.555	-0.774	6.580	1.00	40.85	O
TER	1221		GLY A 153						

calculate the following:

- a) End to End distance in the chain, *i.e.* residue 1 to 153
  - b) Distance between C-Alpha atoms of adjacent amino acids, calculate at least three to see variations
  - c) Dihedral angles: phi, psi and omega. Plot these in Ramachandran map to see their secondary structure.
  - d) Distance between hydrogen bond donor and acceptor
2. Write a mathematical equation to trace the path of helix
  3. Trace the C-alpha backbone in a folded protein and an unstructured protein using the following PDB codes: 1BTA and 1B7D
  4. Compare the structure of two proteins with PDB codes 1BTA and 1ADN and compute their RMSD
  5. Why are non-polar amino acid residues like Ile, Leu, Val, Trp, Phe buried inside the protein interior while charged groups like Lys, Glu are exposed to solvent on the surface?
  6. Explain KEY non-covalent interactions that play a role in folding a protein in an aqueous medium
  7. What is the volume occupied by 1 gram of the protein? Calculate this for multiple proteins and compare the values? What name is given to this volume parameter?
  8. What are INTRINSICALLY DISORDERED proteins? How are they different from normal folded globular proteins in terms of structure and function?