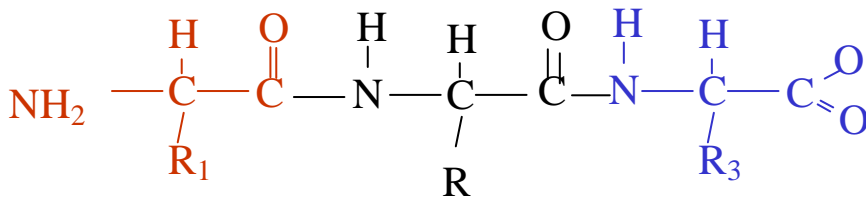


## Revision Übung GST

For 16 Dec 2009

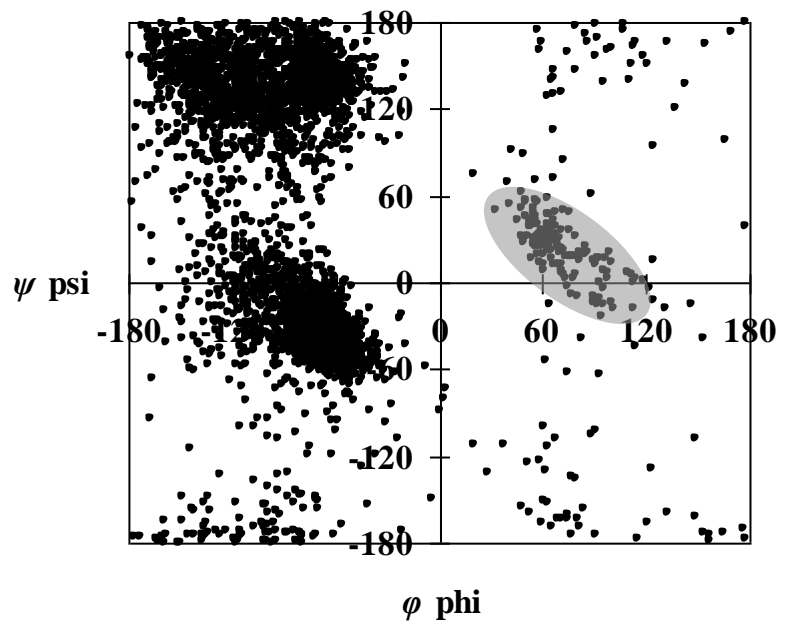
All written exams will be in German. One can answer in English or German.

1. What order of magnitude is a chemical bond (in Å) ?
2. On the diagram, mark the two backbone angles which can rotate in a normal protein. You only need do this for one residue.



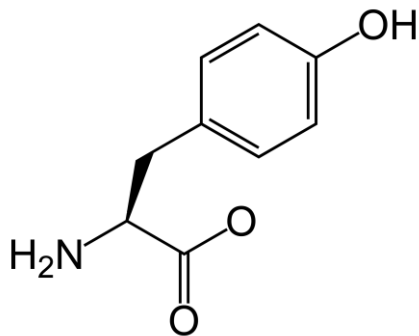
3. Mark the angle which is nearly planar (flat).
4. Why can I not have a short  $\alpha$ -helix which is only 2 residues long ?
5. Name a small amino acid.
6. Name a large hydrophobic amino acid.
7. Name the amino acid which often forms covalent bonds from its side-chain.

8. If you consider a Ramachandran plot for a protein, there is a region where only one amino acid is found, marked on the diagram by the grey oval.



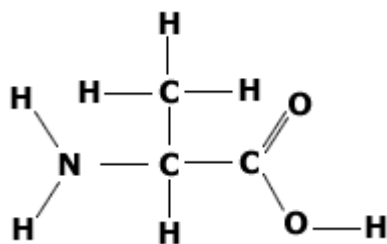
Which amino acid is this? Why can it occupy this area?

9. Why can proline not be part of a perfect  $\alpha$ -helix?
10. Name three elements, with the correct nuclei, which are relevant to biochemistry and NMR.
11. In an NMR spectrum, the hydrogen in the hydroxyl group is not normally seen.



Why?

12. In the structure of alanine, which protons would be  $J$  (spin/spin) coupled to another?



13. When calculating a protein structure based on NMR data, what information does one get from the size of a  $J$  (spin-spin) coupling constant?
14. Why are only some values of the coupling constant useful?

15. You use the metric matrix method to calculate the structure of a protein, but you do not have any experimental data.
- a. What would you expect if you generate 20 structures ?
16. In a distance geometry calculation, I have a set of atoms  $i-j-k-l-m-n$ . What stops atoms  $i$  and  $n$  ending on top of each other ? If I know nothing about the angles in the structure, what is the minimum distance  $d_{ik}$  ?
17. Draw a graph that corresponds to this distance matrix

	A	B	C	D	E
A	0		4		
B		0	2	5	3
C			0	2	1
D				0	
E					0

What is the maximum distance between points D and E ?

18. What is an advantage of the variable target function method compared to the metric matrix method of distance geometry ?
19. The metric matrix method has  $O(n^3)$  running time. Explain in one sentence.
20. What is the running time of the variable target function method ?
21. Write a wave equation in any format you like. Explain each term
22. Given  $F_{hkl} = \sum_{j=1}^n e^{2\pi i(x_j + ky_j + lz_j)}$ , explain what  $F_{hkl}$  is. What are  $x$ ,  $y$  and  $z$  ?
23. Given  $\rho_{x,y,z} = V^{-1} \sum_h \sum_k \sum_l F_{h,k,l} e^{-2\pi i(x+ky+lz)}$ , explain what each of the terms are.
24. Explain why you cannot simply Fourier transform to recover  $\rho_{x,y,z}$ .
25. In MIR (heavy atom phasing), you have recorded data of protein alone and protein with heavy atoms. What is the first step to using this for phasing ? Describe the difference between an  $R$  factor and  $R_{free}$ .