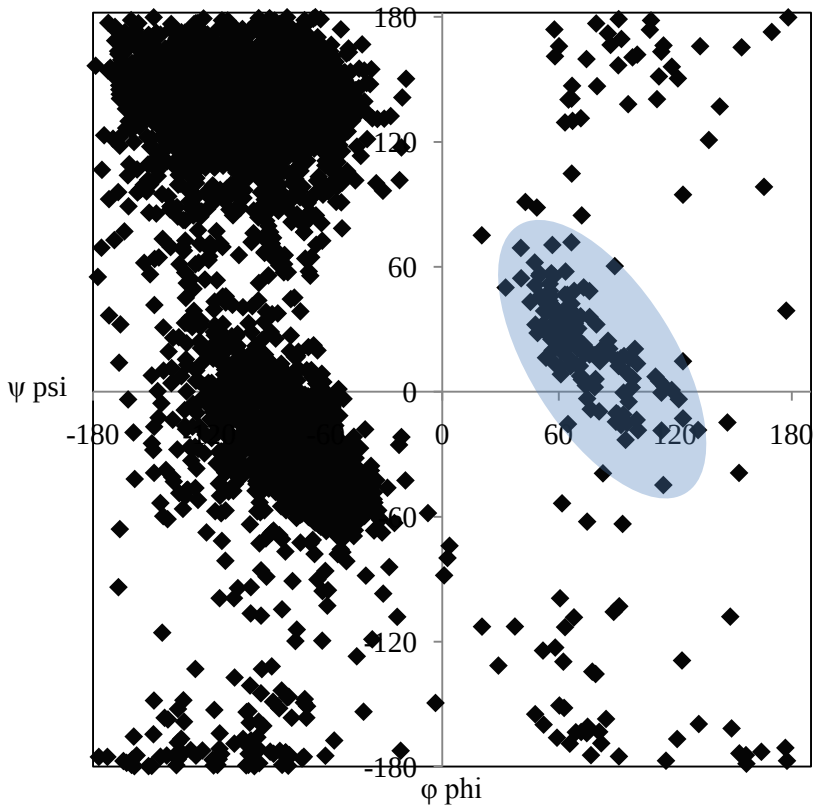
Revision Übung Jan 2011

These are typical of exam questions.

The final exam will be in German.

Really easy questions will not be discussed in the Übung time. They are just given as examples. There will be more questions on X-ray crystallography later.

1. Name a large amino acid, a small amino acid and a polar (uncharged) amino acid.
2. Why is proline never part of an α-helix ?
3. Which amino acid can occupy the area of the Ramachandran plot marked by the oval below ?



Why ?

4. A crystallographer has a model for uncertainty in atomic coordinates. How is this uncertainty represented ?
5. How is uncertainty in protein coordinates from NMR represented ?
6. Which experimental phenomenon provides most of the structural information for determining a structure by NMR ?

7. What structural information may be provided by ^3J coupling measurements ? Which atoms are involved ?
8. If one could record the ^3J coupling between all coupled protons perfectly, why would it not always provide useful structural information ?
9. Draw three atoms with distances between them, which are not possible in 3-dimensional space.
10. Aside from experimental distance information, what information does one add to a metric matrix distance geometry calculation, before applying the triangle inequality (bound smoothing).
11. Why is the triangle inequality applied twice during a metric matrix distance geometry calculation ?
12. In the metric matrix distance geometry method, one generates a trial matrix. Imagine you have no experimental errors. All your distance measurements are correct to 10^{-20} m. Would you expect the trial matrix to correspond to a set of 3-dimensional coordinates ?
13. What is the running time of the bound smoothing step in this kind of distance geometry ?
14. Name an advantage of the variable target function method, compared to the metric matrix method for distance geometry.
15. The R-factor used by protein crystallographers is given by $R = 100 \frac{\sum_{hkl} \left\| F_{obs} \right| - \left| F_{calc} \right\|}{\sum_{hkl} \left| F_{obs} \right|}$

    What is the purpose of the equation / when does a crystallographer use it ?
16. What is the difference between R and R_{free} ?