Questions to the paper “X-ray and NMR structure of Bet v 1, the origin of birch pollen allergy”, Gajhede et al. 1996

1. NMR-specific questions
   1. Why is the NMR structure represented as an ensemble of 20 structures?

   2. Does the ensemble of structures reflect the structures of all possible conformations in the real protein? Why/why not?

   3. What is the atomic RMS deviation of the NMR structure? How is it calculated? What does the RMSD from the paper tell about the structure?

   4. An NMR structure is often presented using a table of different parameters used in the structure calculation and statistics of the structural ensemble like Table 2.
      a. What kind of experimental restraints are used for the structure calculations? How are they obtained?
      b. Why is it important to describe the number of distance restraints in each category (intra-residual, sequential, medium, long range)?

2. X-ray-specific questions
   1. How was the structure solved?
      a. Are the requirements for the method met?

   2. Given the resolution of the final structure, consider the following:
      a. What data and refinement parameters contain information on the quality of the final model (see the Methods section)?
      b. How large uncertainties are associated with this structure? How do they compare to the scale of the model?
      c. How was the solvent in the crystal included in the final model?
      d. Does the structure seem to be well ordered?

   3. Is the RMSD between the X-ray structure and the NMR structure (ensemble) reasonable?
3. General (biological) questions

1. What kind of structural elements are described? (See the section “The structure”)

2. Why is it unusual to find large cavities in protein structures?

3. How does the structure contribute to the understanding of the analysis of the sequences of Fagales family of allergens?

4. How is the structure used for prediction of the function of Bet v 1?

5. In Fig. 1e is shown the structure of rabbit muscle phosphoglucomutase, which is similar to the structure of Bet v 1.
   a. What does the text explain about the sequence similarity between the two proteins?
   b. What can be concluded about the conservation of protein structure relative to the conservation of protein sequence?

6. What does the conservation of surface patches on Bet v 1 suggest about birch pollen allergy in general? Why is the size of the patches important?