Evaluation of a Structure Paper. X-ray

1. How good are the data?
    a. Completeness. What percentage of the possible F's (reflections) were measured in each resolution shell?
        60-90%=good, <20%=poor.
    b. Precision. Ho many times was each reflection measured and how well to equivalent measurements agree?
        Rsym=Σ[I-<I>]/Σ<I>
        <0.05 = good
        <0.10 = typical
        > 0.10 = poor but typical at high resolution
2. Are the heavy atom derivatives isomorphous? Did metal binding change the unit cell dimensions?
    Σ[Fph-Fp]/Σp = constant with f(Θ)
3. How many derivatives were used?
    a. The more the better
    b. Were the sites different (same site no new phase info)
    c. What was the mean fraction isomorphous difference?
        Σ[(Fph-Fp)2]/Σp <0.10 = poor derivative
4. What other sources of phase information were used?
    a. Noncrystallographic symmetry averages subunits.
    b. Solvent flattening can wipe out surface loops.
    c. Molecular replacement: What was done to eliminate bias?
5. Is it a good electron density map?
    a. Is the chain continuous and was there little ambiguity in the chain tracing?
    b. Does the sequence fit the density?
    c. What is the mean figure of merit?
        <0.7 = trouble, >0/75 = interpretable map if resolution 3A.
6. Was the model refined against the data?
    a. If no, then positional errors can approach resolution/3.
    b. If yes, then what is the R value? At <2A resolution
        > 0.25 = mistakes still possible
        > 0.20 = side chains could be misplaced
        <0.20 = some side chain errors but no major problems likely.
    c. Is the geometry good? Bond angles within 3^{o} and lengths within 0.03A
    d. Are the peptides within allowed regions of the Ramachandran plot?
7. Are the conclusions compatible with the resolution of data nd accuracy of the structure?
    a. Resolution.
        6A. Secondary structures distinquishable but not strands or side chains. -Bsheet looks continuous in both direction. Big positional errors.
        3.5-3. Chain can be traced and shapes of rigid side chains distinguished.
        <2 and R<20%. Average positional errors < 0.2A. Regions with B values > 50 are poorly defined.
    b. Hydrogen bond lengths sypically 2.6 to 3.2 A, Van der Walls contacts typically 3.2 to 3.5 A. Would the conclusions be different if the positions of critical groups were off by the average error in the coordinates?

Evaluation of a Structure Paper. NMR

1. How good are the data
    a. What choice of resonance and NOESY assignment strategy was used?
    b. How was assignment ambiguity assessed and treated?
    c. Number of restraints per residue
        >10 minimum
        > 15 good
        > 20 excellent

2. Agreement of structure with experimental data
    a. Distance violations, number and size
    b. R-factor, agreement with model (accuracy)

3. Agreement within the NMR ensemble (precision).
    a. Root mean square deviations
    b. Average pair wise RMSD
    c. Average RMSD to mean coordinates

4. Agreement of structures with molecular geometry
    a. Bond angles
    b. Bond lengths
    c. Ramachandran plot
    d. Homology
    e. Etc