

## Evaluation of structure quality tutorial, using RCSB PDB tools

The PDB ID of the molecule studied is \_\_\_\_\_.

The protein name is \_\_\_\_\_.

The high resolution is \_\_\_\_\_ and the R-factor is \_\_\_\_\_.

### A. Reviewing the Atlas Summary Page

1. Look at the Atlas Summary page. How many chains are in your structure?

2. List 5 pieces of information you can obtain from this page.

3. What is a biological unit?

Does your structure have a biological unit different from the asymmetric unit? YES NO  
If so, how is it different?

4. Can you locate the chains in the asymmetric unit? YES NO

If your biological unit is different from the asymmetric unit, how many chains per biological unit can you see?

5. View the crystal packing picture to see how the molecule or complex is packed in the crystal.

### B. Reviewing the Validation Summary Letter

6. Open the validation summary letter. Are there any close contacts? YES NO

How many? \_\_\_\_\_

Are the close contacts within the asymmetric unit or between symmetry related molecules?

What does it mean (i.e. are the close contacts protein-protein, protein-water, water-water, protein-ligand, etc)?

How does it reflect on the quality of the structure?

7. What is the overall RMS deviation for covalent bonds? \_\_\_\_\_  
Are there deviations more than 6 \*RMSD? YES NO  
Which covalent bond deviation is the highest (absolute value)? \_\_\_\_\_  
How does it reflect on the quality of the structure?

8. What is the overall RMS deviation for covalent bond angles? \_\_\_\_\_  
Are there deviations more than 6 \*RMSD? YES NO  
Which covalent bond angle deviation is the highest (absolute value)? \_\_\_\_\_  
How does it reflect on the quality of the structure?

9. Are there any chirality errors in the structure? YES NO  
If yes, what are the chirality errors?

How does it reflect on the quality of the structure?

10. Are there waters further than 3.5Angstroms away from the macromolecule? YES NO  
How many? \_\_\_\_\_

11. Are any other errors or warnings listed in the letter (i.e. Missing residues? Missing atoms?)  
YES NO

List as many as you see in your report.

**C. Reviewing the SFCheck report**

12. Open the SFCheck report. Look at the number of reflections in the refinement and structure factors section of the SFCheck report. Do the number of reflections and resolution limits match? YES NO  
What does it mean when the values don't match?

13. What is the correlation factor in the Model vs. Structure factors section of the report?

14. Do the R-factors reported in the refinement section agree with those calculated for the model? YES NO

15. Do you think this structure factor file corresponds to this structure? YES NO

**D. Review the PROCHECK reports**

16. Review the Ramachandran plot. How many residues are in the disallowed and generously allowed regions? \_\_\_\_\_  
How does this reflect on the quality of the structure?

**E. Overview**

17. Considering the questions you just answered, what is the overall quality of this structure?

Would you use this structure in your computational research? YES NO