Exp 12 Structure Validation

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1 Introduction

In this final dry lab experiment, we try to confirm the validation of protein structure from others. Model validation can be checked by geometry, dihedral angels from Ramachandran plot, sterics and packing from all atom clash and B-factor.

2 Methods

1. Analyze the two Hemoglobin structure (4HHB and 2HHB) in PDB. Find which one is better and why.

2. Analyze the 2HHB structure in PyMOL considering the effects of B-factor. Find out which region is more flexible and which region is more stable and reliable?

3. Investigate the Murthy's faked structure (1BEF) using MolProbity sever. Find out why this structure is faked.

3 Results

3.1 Model quality check of 4HHB and 2HHB with PDB database

Generaly, 2HHB show more better quanlity than 4HHB(Figure 1,2).(I wonder why here are large difference from same paper!)
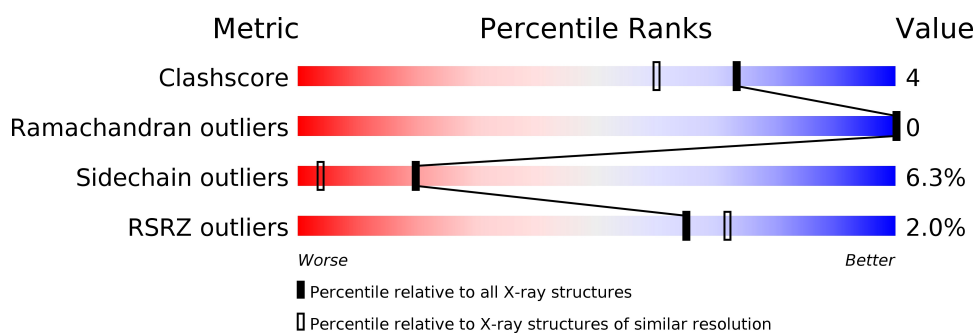

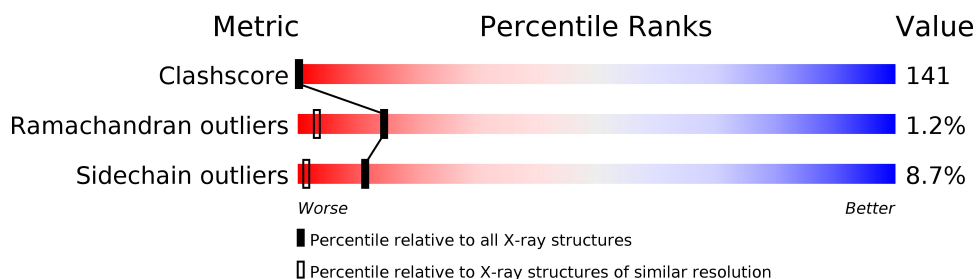**Figure 1.** The 2HHB wwPDB validation from RCSB

Figure 2. The 4HHB wwPDB validation from RCSB

3.2 Comparing by using b-factor

The red color indicates higher b-factor, suggested flexible. Othewise, blue color indicates lower b-factor, suggested stable. Most red or organal colored region present in loop, turn and terminal where almost in the surface of globin.(Figure 3) It mean loop, turn and terminal, especially located at surface, are flexible. The helix in the core are stable and reliable.
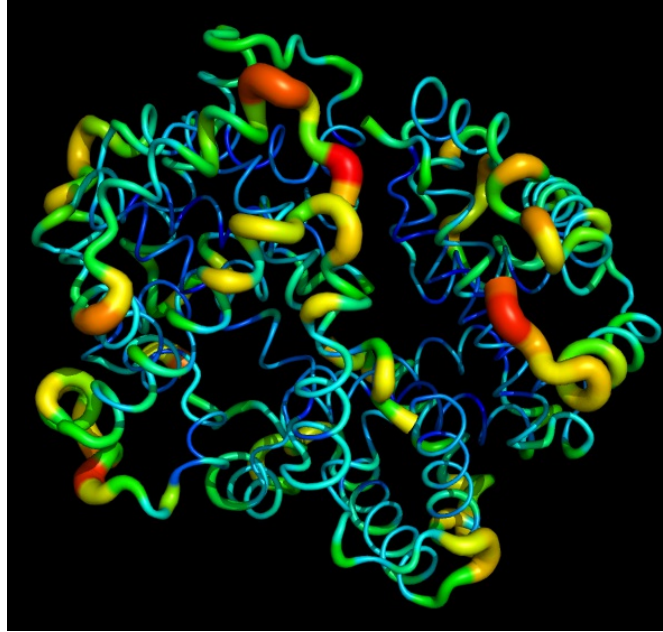
Figure 3. B-factor analysis of 2HHB. Red Color show higher b-factor, which suggest the loop, terminal and trun are more flexible than helix.

3.3 Analysis 1BEF

Figure 4. B-factor analysis of 1BEF. Most region are red, which suggests this structure may be faked.

4 Conclusion

The story of Murthy's faked protein structure, awares us to care the validation of protein form public datebase. Although here are not unique index to profile the validation of protein structure, we analysis the validation from difference factor.