Atomic Contact Energies

Max Emil Schön, Adrian Geißler

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1 Introduction

The free energy functions needed to model Protein structures are made up of multiple components including van-der-Waals energies, electrostatics, dipole interactions, torsions and others. Here, we focus on atomic contact energies (ACE) of Proteins.
Zhang et al. (1997) describe a method to compute contact energies based on atoms rather than residue interactions, as proposed by Miyazawa and Jernigan (1996).

2 Material and Methods

2.1 Energy computation

We implemented the Computation of atomic contact energies as proposed by Zhang et al. (1997). Only heavy atoms were considered as potential pair members. We scanned every pair of atoms in a peptide chain for possible contact pairs. A contact pair is defined by Zhang et al. (1997) as two atoms that have a distance $\leq 6\,\text{Å}$ and are located at least ten bonds of the backbone away from each other. The bond distance criterion is implemented in terms of residues and the atoms' connectivity classes (Appendix in Zhang et al. (1997)).
For every valid contact pair an energy is given by Table 1 in Zhang et al. (1997), which is based on the idea of grouping atoms into atom types with similar contact energy behaviour. As Zhang et al. (1997), we used 18 atom types. To compute the overall energy of a given structure, we summed over all such contact pairs.

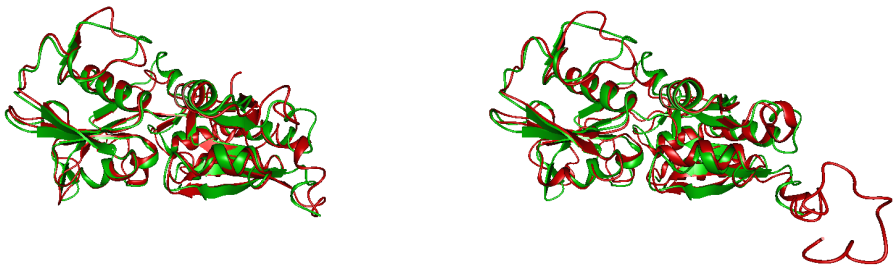
2.2 Data

The Critical Assessment of protein Structure Prediction (CASP) experiments[1] provides a variety of protein structure predictions from different researchers worldwide. We used 4 Protein targets (T0762, T0769, T0776, T0784) and the respective predictions from the current CASP11 experiment to test our energy computation from 2.1.

2.3 RMSD

For the evaluation of the predicted structures we aligned the backbone Cα atoms of the prediction with those of the target experimental structure (Hamelryck and Manderick, 2003).

3 Results



(a) (b)

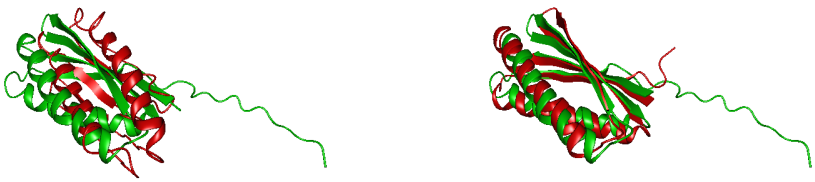
Figure 1: Best scoring predictions of T0762 evaluated using (a) atomic contact energies (008) and (b) the RMSD between prediction and experimental structure (251). Both predictions were visualized in BALLView (Moll et al., 2006). green: target experimental stucture. red: predicted structure.

4 Discussion

References

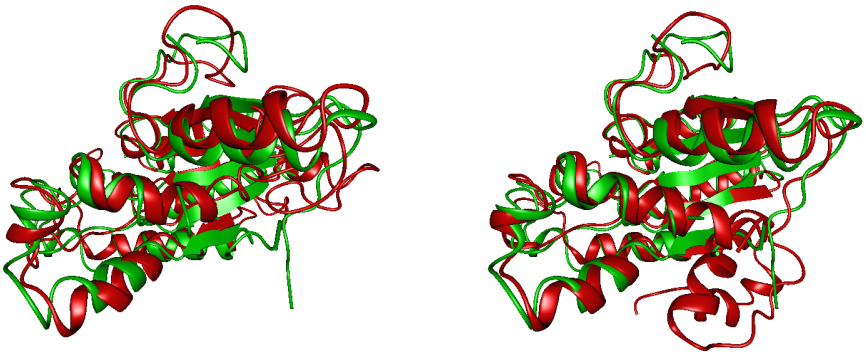
T. Hamelryck and B. Manderick. PDB file parser and structure class implemented in Python. *Bioinformatics*, 19(17):2308–2310, 2003.

[1] `http://www.predictioncenter.org/casp11` (last accessed: June 15, 2015)



(a) (b)

Figure 2: Best scoring predictions of T0769 evaluated using (a) atomic contact energies (442) and (b) the RMSD between prediction and experimental structure (241). Both predictions were visualized in BallView (Moll et al., 2006). green: target experimental stucture. red: predicted structure.

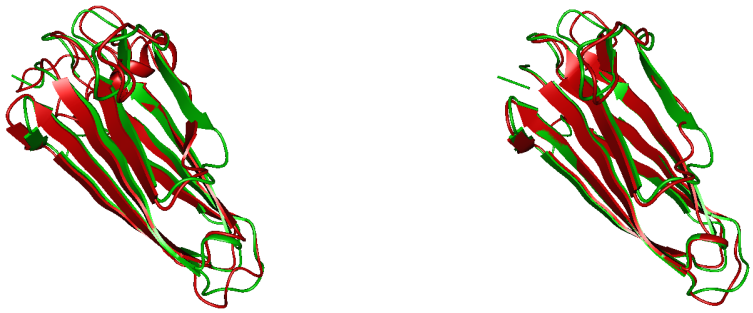


(a) (b)

Figure 3: Best scoring predictions of T0776 evaluated using (a) atomic contact energies (300) and (b) the RMSD between prediction and experimental structure (420). Both predictions were visualized in BallView (Moll et al., 2006). green: target experimental stucture. red: predicted structure.

S. Miyazawa and R. L. Jernigan. Residue-residue potentials with a favorable contact pair term and an unfavorable high packing density term, for simulation and threading. *Journal of molecular biology*, 256(3):623–644, 1996.

A. Moll, A. Hildebrandt, H.-P. Lenhof, and O. Kohlbacher. BALLView: a



(a) (b)

Figure 4: Best scoring predictions of T0776 evaluated using (a) atomic contact energies (117) and (b) the RMSD between prediction and experimental structure (156). Both predictions were visualized in BallView (Moll et al., 2006). green: target experimental stucture. red: predicted structure.

tool for research and education in molecular modeling. *Bioinformatics*, 22(3):365–366, 2006.

C. Zhang, G. Vasmatzis, J. L. Cornette, and C. DeLisi. Determination of atomic desolvation energies from the structures of crystallized proteins. *Journal of molecular biology*, 267(3):707–726, 1997.

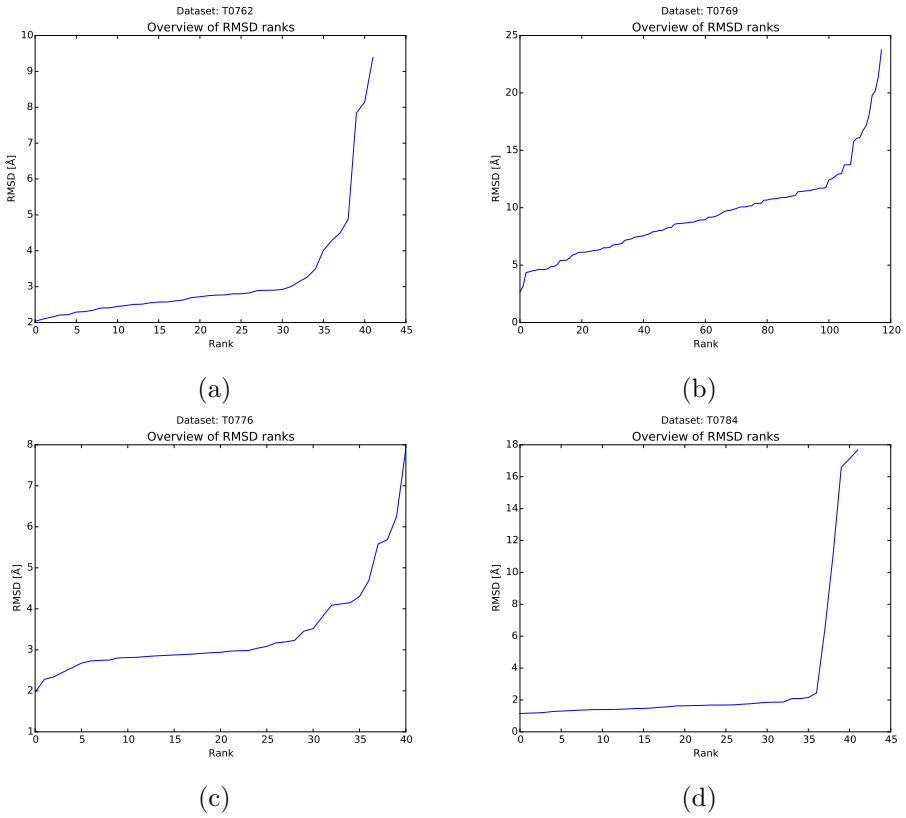


Figure 5: RMSD VS. Rank in original CASP11 exeperiment. (a) T0762 (b) T0769 (c) T0776 (d) T0784