| Name of parameter | Meaning |
|--------------------------------------|---|
| total_score | weighted average of all parameters |
| Transform_accept_ratio | How well the low resolution Monte Carlo stage worked. It is a number between 0 and 1 and is provided as a diagnostic |
| fa_elec | Coulombic electrostatic potential |
| fa_intra_rep | The repulsive energy within residues |
| fa_pair | Statistical residue-residue interaction potential. Very useful in protein-protein interactions |
| fa_rep | The repulsive portion of the <u>Lenard-Jones potential</u> . If high then there are clashes in the protein |
| if_X_hbond_bb_sc if_X_hbond_sc | Hydrogen bonding term between protein backbones and sidechain (ligand) |
| interface_delta_X | The energy of interactions between the ligand (chain X) and the protein |
| ligand_is_touching_X | 1 if ligand is close to the protein, 0 otherwise |
| complex_normalized | Total score of the protein complex with the ligand (holo state) normalized by the number of residues |
| dG_cross | The energy of interaction between the two sides of the complex, calculated in the holo state (protein bound to ligand) |
| dG_separated | The energy of interaction between the two sides of the complex, calculated by taking the score of the holo state, then separating the two sides of the interface, optionally repacking, and then calculating the score in the separated state. This is particularly useful if you think you have an "induced fit" type situation, and want to correct for repacking in the absence of the ligand. |
| delta_unsatHbonds | How many unsatisfied hydrogen bonds are introduced by the design. Unsatisfied hydrogen bonds are ones where the atom is able to make a hydrogen bond but does not because it's blocked by other residues |
| Packstat | How well the protein is packed. values between 0-1 with 1 being better |
| sc_value | Shape complementary score. Values between 0-1 with 1 being better. It looks at the correspondence between normal vectors of the surfaces of the protein and ligand |
| side1_normalized side2_normalized | The energies of the two sides of the interface, possibly normalized by the number of residues |