3D-ModelFit

3DModelFit - program for the estimation of quality of 3D model structure of protein
Program accepts model and real (target) 3D structures of protein in PDB format (indexing of residues in files should be identical). Program calculates their optimal superposition and estimates following scores for model quality estimation:
Model N - number of model residues
Target N - number of target residues
Model NP - number of model residues that presented in target structure
Target NP - number of target residues that presented in model structure
RMS_Buried - RMS for buried area of residues in model and target structure
RMS_Polar_fract - RMS for polar fraction buried of residues in model and target structure
SS_Match - fraction of secondary structure match for residues in model and target structure
LCS_score - LCS_TS score (Zemla A. (2003), Nucleic Acids Res. 31:3370-3374)
GDT_score - GDT_TS score (Zemla A. (2003), Nucleic Acids Res. 31:3370-3374)
CHI1_match - fraction of residues matching their chi1 angle
CHI2_match - fraction of residues matching their chi2 angle
CHI12_match - fraction of residues matching their chi1 and chi2 angles
RMS_CA - RMS on CA atoms.
If 'Output format' is set to "Extended" value, program outputs PDB file with structural superposition of model (chain M) and target (chain T) structures.
Remark fields in output file represent also residue to residue correspondence of model and target structutes, for example:

```
REMARK  50 Structure quality:
REMARK  50 M:  G    D    S    V    E    N    Q    S
REMARK  50 N:  15   16   17   18   19   20   21   22
REMARK  50 T:  -    -    -    -    -    -    q    S
```

where M: model amino acid, N: residue index, T: target amino acid. Missed residues are indicated as gaps ('-'); residues with missed side chains are indicated as small letters.
Detailed description of LCS and GDT scores is also presented in remark fields.