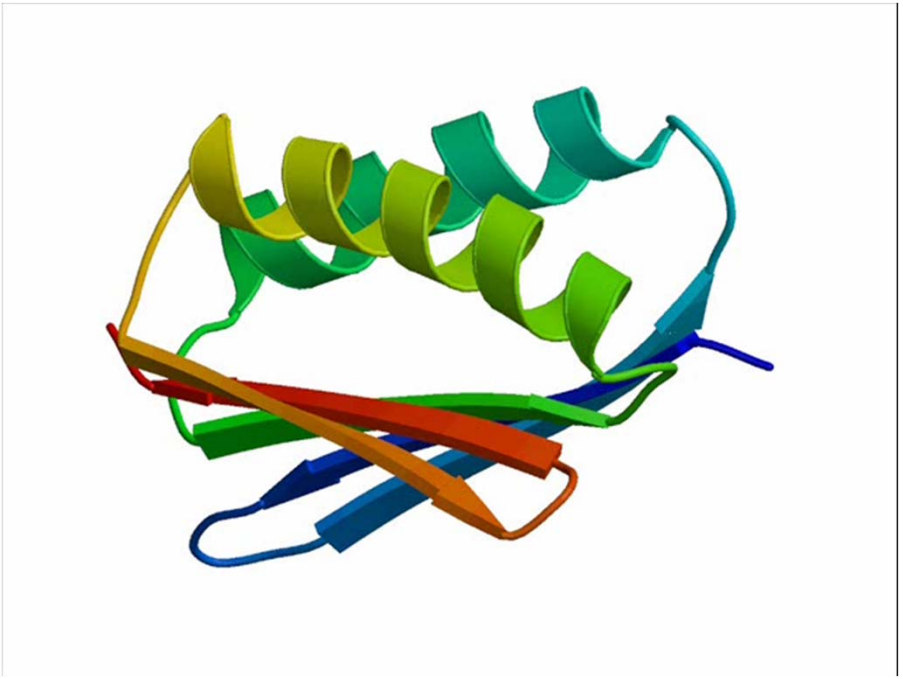
Rosetta First Application

Repack the Structure

Fixbb

- Used for design, but also repacks structure
- Example:

python clean_pdb.py 1qys A



fixbb.linuxgccrelease -database <database> -s 1qysA.pdb -ex1 -ex2 -packing:repack_only

Output

core.init: Mini-Rosetta version 40406M from https://svn.rosettacommons.org/source/branches/releases/rosetta-3.2/rosetta_source
core.init: command: /home/delucasl/release/rosetta-3.2/rosetta_source/bin/fixbb.linuxgccrelease -database /home/delucasl/release/rosetta-3.2/rosetta_database/ -s 1qysA.pdb -ex1 -ex2 -packing:repack_only
core.init: 'RNG device' seed mode, using '/dev/urandom', seed=-1081785084 seed_offset=0 real_seed=-1081785084
core.init.random: RandomGenerator:init: Normal mode, seed=-1081785084 RG_type=mt19937
core.scoring.ScoreFunctionFactory: SCOREFUNCTION: standard
core.scoring.ScoreFunctionFactory: SCOREFUNCTION PATCH: score12
core.scoring.etable: Starting energy table calculation
core.scoring.etable: smooth_etable: changing atr/rep split to bottom of energy well
core.scoring.etable: smooth_etable: spline smoothing lj etables (maxdis = 6)
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core.io.database: Database file opened: /home/delucasl/release/rosetta-3.2/rosetta_database/scoring/score_functions/hbonds/standard_params/HBEval.csv
core.io.database: Database file opened: /home/delucasl/release/rosetta-3.2/rosetta_database/P_AA
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core.io.database: Database file opened: /home/delucasl/release/rosetta-3.2/rosetta_database/P_AA_pp
core.io.database: Database file opened: /home/delucasl/release/rosetta-3.2/rosetta_database/Rama_smooth_dyn.dat_ss_6.4

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Output

```
protocols.jd2.PDBJobInputter: Instantiate PDBJobInputter
protocols.jd2.PDBJobInputter: PDBJobInputter::fill_jobs
protocols.jd2.PDBJobInputter: pushing 1qysA.pdb nstruct index 1
protocols.jd2.PDBJobInputter: PDBJobInputter::pose_from_job
core.conformation.Conformation: [ WARNING ] missing heavyatom:  CG  on residue LYS 13
core.conformation.Conformation: [ WARNING ] missing heavyatom:  CD  on residue LYS 13
core.conformation.Conformation: [ WARNING ] missing heavyatom:  CE  on residue LYS 13
core.conformation.Conformation: [ WARNING ] missing heavyatom:  NZ  on residue LYS 13
core.conformation.Conformation: [ WARNING ] missing heavyatom:  OXT on residue LEU_p:CtermProteinFull 92
core.pack.task: Packer task: initialize from command line()
core.pack.pack_missing_sidechains: packing residue number 13 because of missing atom number 6 atom name  CG
core.scoring.dunbrack: Dunbrack library took 0.07 seconds to load from binary
core.pack.interaction_graph.interaction_graph_factory: Instantiating DensePDInteractionGraph
core.pack.pack_rotamers: built 174 rotamers at 12 positions.
core.pack.pack_rotamers: IG: 19084 bytes
protocols.jd2.PDBJobInputter: filling pose from PDB 1qysA.pdb
core.pack.task: Packer task: initialize from command line()
core.pack.interaction_graph.interaction_graph_factory: Instantiating DensePDInteractionGraph
core.pack.pack_rotamers: built 1786 rotamers at 92 positions.
core.pack.pack_rotamers: IG: 2230152 bytes
protocols.jd2.JobDistributor: 1qysA_0001 reported success in 4 seconds
protocols.jd2.JobDistributor: no more batches to process...
protocols.jd2.JobDistributor: 1 jobs considered, 1 jobs attempted in 4 seconds
```

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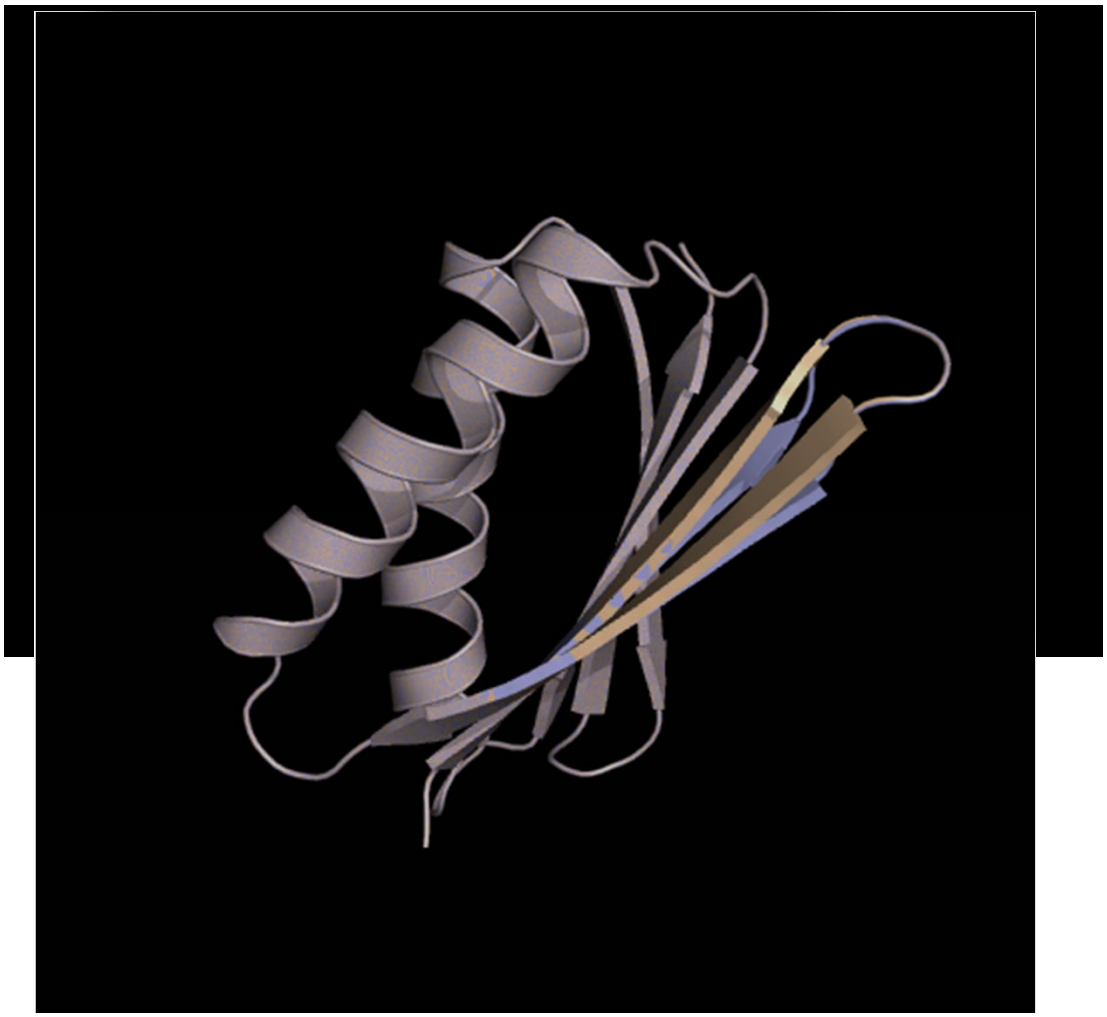
Rotamers



Inside the PDB

label fa_atr fa_rep fa_sol fa_intra_rep pro_close fa_pair hbond_sr_bb hbond_lr_bb hbond_bb_sc hbond_sc dslf_ss_dst dslf_cs_ang dslf_ss_dih dslf_ca_dih rama omega fa_dun p_aa_pp ref total

weights 0.8 0.44 0.65 0.004 1 0.49 0.585 1.17 1.17 1.1 0.5 2 5 5 0.2 0.5 0.56 0.32 1 NA

pose -313.243 199.97 149.915 0.868231 0 -6.48358 -20.779 -38.1733 -1.56429 -4.22078 0 0 0 0 14.0365 0.987027 54.6831 -4.97079 -24.92 6.10469

ASP_p:NtermProteinFull_1 -1.75204 0.0795558 1.72169 0.0144971 0 -0.0431825 0 0 0 0 0 0 0 0 0 0.000230759 0.221268 0 -0.67 -0.427986

ILE_2 -3.58032 0.184875 1.47699 0.0199879 0 0 0 0 0 0 0 0 0 0 -0.190036 0.00129203 0.194077 -0.268257 0.24 -1.92139

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