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Adding additional restraints to the defaults

You can add your own restraints to the restraints file, with the homology-derived restraints, by redefining the **automodel.special_restraints()** routine (by default it does nothing). This can be used, for example, to add information from NMR experiments or to add regions of known secondary structure. Symmetry restraints, excluded pairs, or rigid body definitions can also be added in this routine (see Section 2.2.11 for a symmetry example). The example below enforces an additional restraint on a single CA-CA distance, adds some known secondary structure, and shows how to add restraints from a file. (See Section 5.3 for further information on how to specify restraints, and Section 6.8 for details on secondary structure restraints.)

Note that the residue numbers for any restraints refer to the model, *not* the templates. See Section 2.2.6 for more discussion.

Example: examples/automodel/model-addrsr.py

```
# Addition of restraints to the default ones
from modeller import *
from modeller.automodel import *    # Load the automodel class

log.verbose()
env = environ()

# directories for input atom files
env.io.atom_files_directory = ['.', '../atom_files']

class MyModel(automodel):
    def special_restraints(self, aln):
        rsr = self.restraints
        at = self.atoms
#       Add some restraints from a file:
#       rsr.append(file='my_rsrs1.rsr')

#       Residues 20 through 30 should be an alpha helix:
        rsr.add(secondary_structure.alpha(self.residue_range('20:', '30:')))
#       Two beta-strands:
        rsr.add(secondary_structure.strand(self.residue_range('1:', '6:')))
        rsr.add(secondary_structure.strand(self.residue_range('9:', '14:')))
#       An anti-parallel sheet composed of the two strands:
        rsr.add(secondary_structure.sheet(at['N:1'], at['O:14'],
                                          sheet_h_bonds=-5))
#       Use the following instead for a *parallel* sheet:
#       rsr.add(secondary_structure.sheet(at['N:1'], at['O:9'],
#                                         sheet_h_bonds=5))

#       Restrain the specified CA-CA distance to 10 angstroms (st. dev.=0.1)
```

```
#       Use a harmonic potential and X-Y distance group.
        rsr.add(forms.gaussian(group=physical.xy_distance,
                               feature=features.distance(at['CA:35'],
                                                         at['CA:40']),
                               mean=10.0, stdev=0.1))

a = MyModel(env,
            alnfile  = 'alignment.ali',     # alignment filename
            knowns   = '5fd1',              # codes of the templates
            sequence = '1fdx')              # code of the target
a.starting_model= 1                 # index of the first model
a.ending_model  = 1                 # index of the last model
                                    # (determines how many models to calculate)
a.make()                            # do homology modeling
```

Automatic builds 2013-06-11