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Appendices

PIR file

```
>P1;target
sequence:target:::::0.00: 0.00
MVGKALGLEFNKKIINTLKGEQMNPDFIKINPQHSIPTLV DNGFTIWESR
AILVYLVEKYGKDDALYPKDIQKQAVINQRLYFDMALMYPTLANYYYYKAF
TTGQFGSEEDYKQVQETFDLNTFLEGQDYVAGDQYTVADIAILANVSNF
DVVGFDISKYPNVARWYDHVKKITPGWEENWAGALDVKKRIEEKQNAAK*
```

comparetemplates.py

```
from modeller import *

env = environ()
aln = alignment(env)
for (pdb, chain) in (('1jlv', 'A'), ('1pn9', 'A'), ('3f6f', 'A'),
                    ('3ein', 'A'), ('3mak', 'A'), ('3gh6', 'A')):
    m = model(env, file=pdb, model_segment=('FIRST:'+chain,
                                           'LAST:'+chain))
    aln.append_model(m, atom_files=pdb, align_codes=pdb+chain)
aln.malign()
aln.malign3d()
aln.compare_structures()
aln.id_table(matrix_file='family.mat')
env.dendrogram(matrix_file='family.mat', cluster_cut=-1.0)
```

targettemplatealign.py

```
from modeller import *

env = environ()
aln = alignment(env)
mdl = model(env, file='3ein', model_segment=('FIRST:A', 'LAST:A'))
aln.append_model(mdl, align_codes='3einA', atom_files='3ein.pdb')
aln.append(file='sequence.ali', align_codes='target')
aln.align2d()
aln.write(file='sequence-3einA.ali', alignment_format='PIR')
aln.write(file='sequence-3einA.pap', alignment_format='PAP')
```

builmodel.py

```
from modeller import *
from modeller.automodel import *

env = environ()
a = automodel(env, alnfile='sequence-3einA.ali',
              knowns='3einA', sequence='target',
              assess_methods=(assess.DOPE, assess.GA341))
a.starting_model = 1
a.ending_model = 100
a.make()
```