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Re: [modeller_usage] How to set starting residue number in modeling

- To: Keehyoung Joo <newton@kias.re.kr>, modeller_usage <modeller_usage@salilab.org>
 - Subject: Re: [modeller_usage] How to set starting residue number in modeling
 - From: Modeller Caretaker <modeller-care@salilab.org>
 - Date: Thu, 27 May 2010 10:04:49 -0700
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On 5/27/10 9:17 AM, Keehyoung Joo wrote:

Today, I tried it by using `rename_segments` method.

But, I did not make model that I want.

The following is my script to model.

I add MyModel class and function `rename_segments`.

I want to build model that have chain id = 'A' and starting residue number=5.

To use `rename_segments` in combination with `automodel`, use the `special_patches()` method, as detailed at

http://salilab.org/archives/modeller_usage/2009/msg00245.html

A minimal script which should do what you want is:

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

class MyModel(automodel):
    def special_patches(self, aln):
        self.rename_segments(segment_ids='A', renumber_residues=5)

log.verbose()
env = environ()

a = MyModel(env, alnfile='alignment.ali',
            knowns='5fdl', sequence='lfdx')
a.make()
```

Ben Webb, Modeller Caretaker

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modeller-care@salilab.org <http://www.salilab.org/modeller/>
Modeller mail list: http://salilab.org/mailman/listinfo/modeller_usage

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