

Chapter 2

Command Scripts and Data Structure

All commands related to sets of atoms have a syntax of the form

will modify the atoms in set 1 such that residues 3 to 20 and 34 to 40 will become helical and residues 24 to 30 and 44 to 50 will become sheet.

Chapter 3

Identification of the rigid part of a protein

Please

Aspartate Aminotransferase (Section 3.2) Compare ve di erent models of Aspartate

```
! finito  
stop();
```



```
! 1TAS
aset_egen(sset=4, esd_model =dpi u, npar=25408, nobs=17636, cpl =87. 9, rfree=30. 0, dmi n=2. 8);

! 1TAT
aset_egen(sset=5, esd_model =dpi u, npar=25408, nobs=18194, cpl =97. 0, dmi n=3. 0, rfree=30. 0);

ddm(
  setl ={1-5},
  esd_scaled=on,
  l o l i m=2. 0, h i l i m=5. 0,
  sspl ot=on,
  rbpl ot=on
);

stop();
```

The first run on all the models is used to decide which conformers are identical. For this purpose, a table is printed in the log- file:

reactions take place at two active centers which are separated by a distap 1 45=-a k 1 1 Torce25

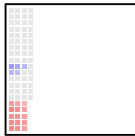
pstype=eps,

! make an eps-file


```
    esd_scaled=on,           ! esd-scaling is used
    lolim=3.0,hi lim=5.0,    ! low and high limit for DD-matrix
    psfname=ddm_mers_all.ps  ! postscript output file
);

stop();
```

```
seta=1, setb=2,  
l o l i m=3. 0, h i l i m=5. 0,  
v x 1=170, v y 1=630, v x 2=240, v y 2=700,  
t y p e=both, e s d _ s c a l e d=on,  
l i m i t=150,  
t i c k s=off, c o m m e n t s=off,  
x t i c k s=off, y t i c k s=off,  
l e g e n d=on,  
l e g e n d x=340, l e g e n d y=200,  
l e g e n d w=180  
);
```



—

4.2 Stu

4.2.1 Change residue names

Chapter 5

Tips and Tricks

Chapter 6

Release Notes

Known Bugs

For multiple chain analyses, the rigid body display on the bottom of the DD-matrices is sometimes messed up. However, the calculations and the RASMOL, and mol script files are correct.

Version 0.2d, 11-Apr-2002

Some problems with automatic consistency checking of atom lists were fixed.

The Pairwise comparison table now contains a line with the mean estimated error for the atoms that are actually compared. This allows to easily pick out the best determined atom set from a set of redundant conformers.

STDOUT is now flushed regularly to make monitoring easier.

Version 0.2c, 1-Mar-2002

A warning is now given, if a pdb-file contains B-values that are smaller or equal 0.0 - such B-values would mess up the error-estimation.

The manual is again available in pdf-format !

The plotting of DD-matrices for multi-chain problems is still not perfect (loads of book-keeping to do ...) but it is getting better.

If more than two atom sets were selected using the setI -keyword in the ddm-command, the auto-

Bibliography

[1] K. S. Anderson, E. W. Miles, and K. A. Johnson. Serine Modulates Substrate Channeling in Tryptophan Synthase. *J.Biol.Chem*, 266:8020{8033, 1991.

[2]