

Advanced Building

Atomistic Modeling of Small-Angle Scattering
Data Using SASSIE-web

September 21-23, 2016

Advanced Photon Source

Argonne National Laboratory, Argonne, IL

Barriers: BUILD; EQUILIBRATE; PROPAGATE; ANALYZE

What software package(s) and force-fields do I use?

Starting structure?

How do I clean up the structure?

How do I set up a trajectory (time or space)?

How do I calculate scattering observables correctly?

Overview

Intermediate Building Tricks

Building coordinates for missing atoms/residues
Simulated annealing
Building IDPs
A trick for topological issues

“model building”

Overview

Missing bits

Typical scenarios:

- N-terminus & C-terminus missing (random or cloning artifacts)
- Single amino acid missing (or small loop)
- Large internal loop missing

Two simple solutions:

- (1) Use psfgen to add internal coordinates to fill gaps & then minimize
- (2) Use CHARMM (MD) to add internal coordinates & minimize
- (3) ROSETTA, Modeller (\$UCSF\$), . . .

Internal loops: we will then need to run some “simulated annealing” and/or Torsion Angle MD dynamics to sample configurations.

PSFGEN III

protein

Sample input file (here named: build_system_protein.psfgen):

```
>psfgen build_system_protein.psfgen >& build_protein.out &
```

sequence file only
needs on atom
per residue

```
topology /home/mdschool/toppar/top_all27_prot_na.inp
alias residue HIS HSE

segment PCLN {
  first NTER
  last CTER
  pdb output_building/icln.pdb
}

coordpdb output_building/icln.pdb PCLN

guesscoord

writepsf output_building/new_icln.psf
writepdb output_building/new_icln.pdb
```

path to pdb file (sequence)

path coordinates file (pdb)

use IC to add H etc.

PSFGEN (filling gaps)

STEP 1: Create new psf and pdb files where psfgen will add missing bits using edited PDB files as input.

LOOK AT THE STRUCTURE BEFORE MOVING TO STEP 2.

STEP 2: Set up a “fixed-atoms” PDB file so that structure is not pulled apart when you minimize the structure

STEP 3: Write NAMD input file with the addition of:
fixed atoms
IMD (so you can watch)
more minimization steps

STEP 4: Minimize the structure using NAMD (repeat w/o fixed atoms)

STEP 5: If all goes well, run a short NVE dynamics run (10 ps) . . .

If step 5 fails then go back to step 4 or maybe back to step 1 !!!

Toy system

a piece of Tral

Missing residues 1 - 11 and 342 - 400 (but we know the sequence)



PSFGEN (filling gaps)

STEP 1: Create new psf and pdb files where psfgen will add missing bits using edited PDB files as input.

Have the sequence at hand . . .

TSGIHVLDEL	SVRALSRDIM	KQNRVTVHPE	KSVPRTAGYS	DAVSVLAQDR	50
PSLAIVSGQG	GAAGQRERVA	ELVMMAREQG	REVQIIAADR	RSQMNMKQDE	100
RLSGELITGR	RQLLEGMAFT	PGSTVIVDQG	EKLSLKETLT	LLDGAARHNV	150
QVLITDSGQR	TGTGSALMAM	KDAGVNTYRW	QGGEQRPATI	ISEPDRNVRY	200
ARLAGDFAAS	VKAGEESVAQ	VSGVREQAIL	TQAIRSELKT	QGVLGLPEVT	250
MTALSPVWLD	SRSRYLRDMY	RPGMVMEQWN	PETRSHDRYV	IDRVTAQSHS	300
LTLRDAQGET	QVVRISLDS	SWSLFRPEKM	PVADGERLRV	TGKIPGLRVS	350
GGDRLQVASV	SEDAMTVVVP	GRAEPATLPV	SDSPFTALKL	ENGWVETPGH	400
SVSDSATVFA	SVTQMAMDNA	TLNGLARSGR	DVRLYSSLDE	TRTAEKLARH	450

(a) you have one pdb file with known coordinates

(b) make a copy of (a) with only the CA atoms, add in unknown residues to make a “sequence.pdb” file. **Coordinates in the sequence file do no matter.**

PSFGEN (filling gaps)

STEP 1: Create new psf and pdb files where psfgen will add missing bits using edited PDB files as input.

```
> cat coords.pdb | grep CA > ca_sequence.pdb
```

then, copy known coordinate line (say, ATOM 163 CA VAL ...) and manually change the index, rename, and resid fields. Do this for all missing atoms/AA.

```
ATOM      1  CA THR      1      35.989 -22.055 248.035  1.00  0.00      TRAI C
ATOM      2  CA SER      2      35.989 -22.055 248.035  1.00  0.00      TRAI C
ATOM      3  CA GLY      3      35.989 -22.055 248.035  1.00  0.00      TRAI C
ATOM      4  CA ILE      4      35.989 -22.055 248.035  1.00  0.00      TRAI C
ATOM      5  CA HSE      5      35.989 -22.055 248.035  1.00  0.00      TRAI C
ATOM      6  CA VAL      6      35.989 -22.055 248.035  1.00  0.00      TRAI C
ATOM      7  CA LEU      7      35.989 -22.055 248.035  1.00  0.00      TRAI C
ATOM      8  CA ASP      8      35.989 -22.055 248.035  1.00  0.00      TRAI C
ATOM      9  CA GLU      9      35.989 -22.055 248.035  1.00  0.00      TRAI C
ATOM     10  CA LEU     10      35.989 -22.055 248.035  1.00  0.00      TRAI C
ATOM     11  CA SER     11      35.989 -22.055 248.035  1.00  0.00      TRAI C
ATOM    163  CA VAL    12      35.989 -22.055 248.035  1.00  0.00      TRAI C
ATOM    179  CA ARG    13      39.541 -23.591 248.463  1.00  0.00      TRAI C
ATOM    203  CA ALA    14      41.070 -23.037 251.954  1.00  0.00      TRAI C
ATOM    213  CA LEU    15      42.765 -25.002 254.835  1.00  0.00      TRAI C
```

PSFGEN (filling gaps)

now, create a temporary pdb/psf to build the structure

Sample input file (here named: build_system_protein.psfgen):

>psfgen build_system_protein.psfgen >& build_protein.out &

```
topology /home/mdschool/research/toppar/top_all127_prot_na.inp
alias residue HIS HSE

segment TRAI {
  first NTER
  last CTER
  pdb output_building/ca_sequence.pdb
}

coordpdb output_building/coords_traI_recd_10_481_temp.pdb TRAI
guesscoord

writepsf output_building/temp_traI.psf
writepdb output_building/temp_traI.pdb
```

path to pdb file (sequence)

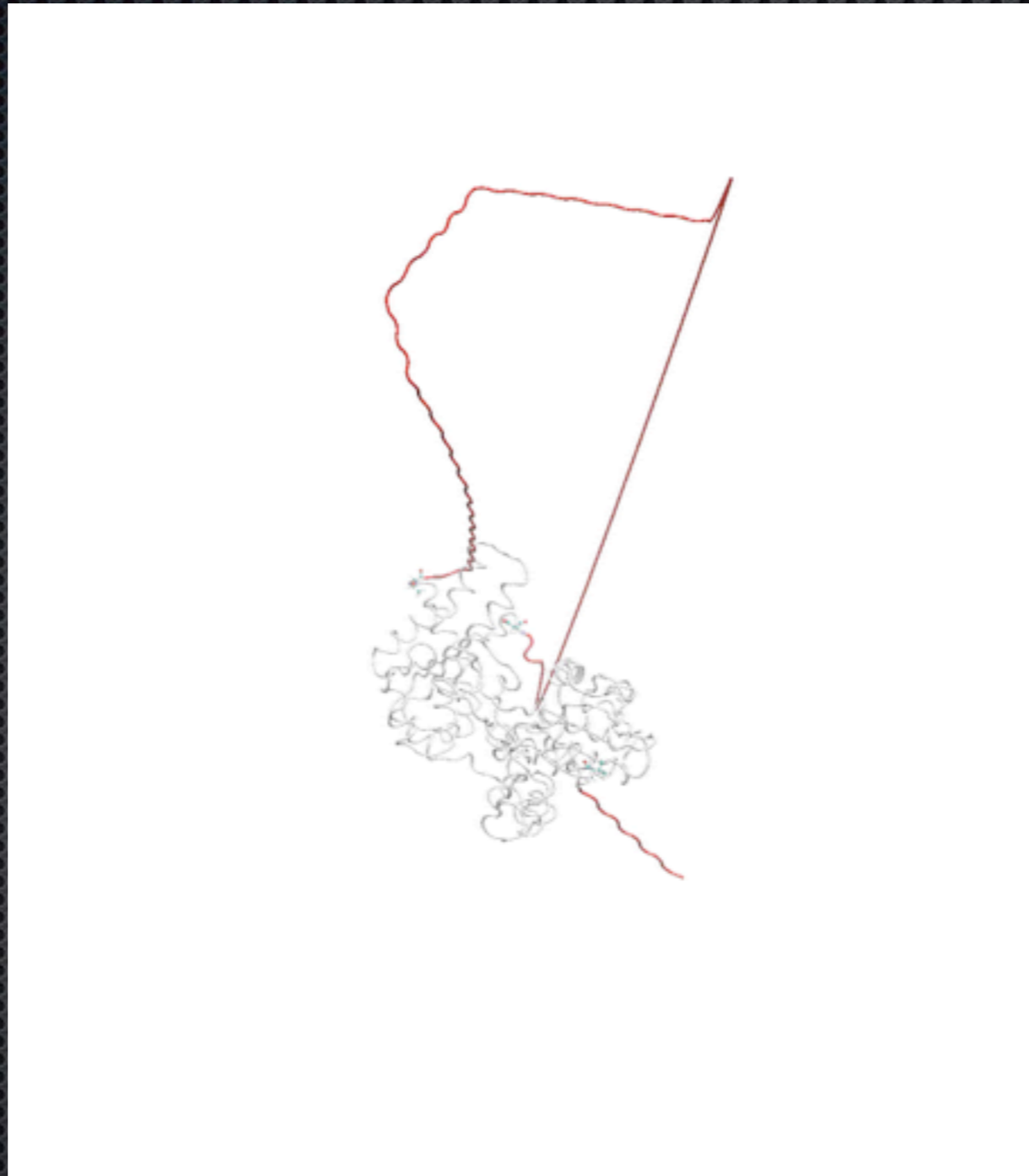
path coordinates file (pdb)

use IC to add H and
missing AA

IC will “grow” the
chain **blindly** . . .

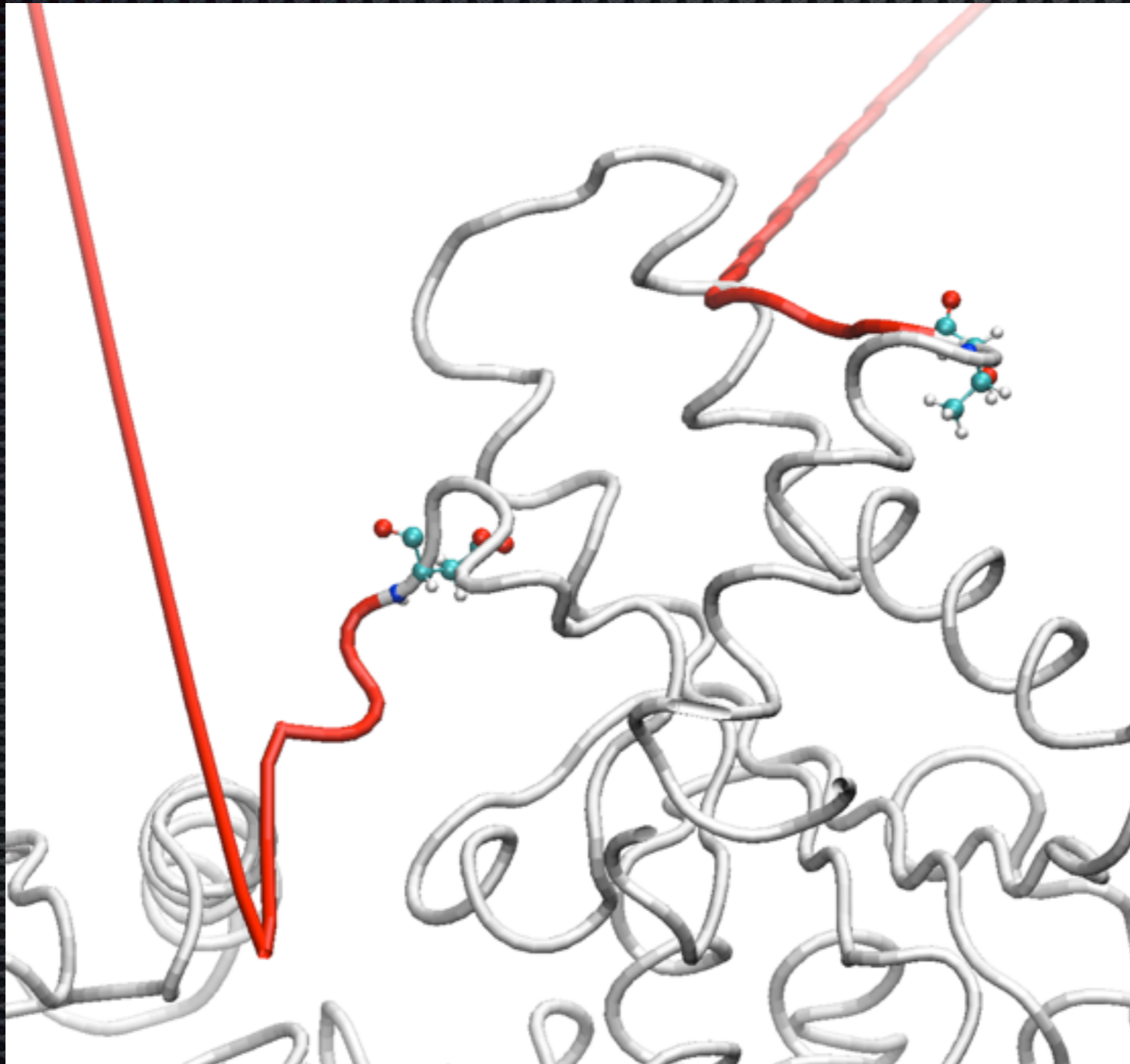
PSFGEN (filling gaps)

LOOK AT THE STRUCTURE BEFORE MOVING TO STEP 2.



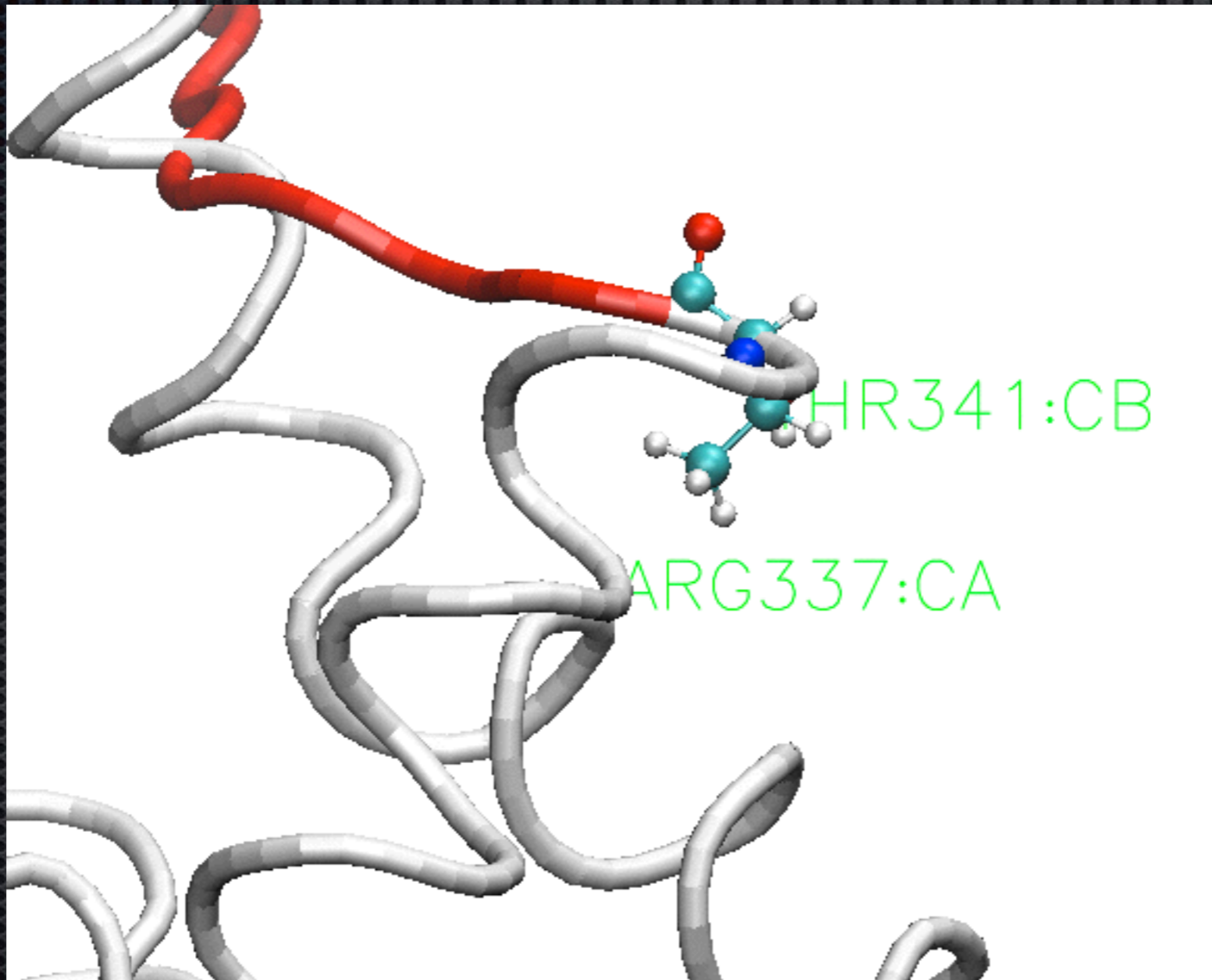
PSFGEN (filling gaps)

LOOK AT THE STRUCTURE BEFORE MOVING TO STEP 2.



PSFGEN (filling gaps)

YIKES! Welcome to the real world!!! We have overlap. Let's remove some known coordinates near the overlap and re-build the structure. You don't need to change the sequence file. Call the new coordinate file: `coords_tral_10_gap_481.pdb`



PSFGEN (filling gaps)

YIKES! Welcome to the real world!!! We have overlap. Let's remove some known coordinates near the overlap and re-build the structure. You don't need to change the sequence file. Call the new coordinate file: **coords_tral_10_gap_481.pdb**

. . .

ATOM	1621	N	LEU	D	338	-62.123	-15.211	-65.673	207.57	N
ATOM	1622	CA	LEU	D	338	-62.146	-15.489	-64.287	207.57	C
ATOM	1623	C	LEU	D	338	-62.455	-14.115	-63.597	207.57	C
ATOM	1629	N	ARG	D	339	-63.258	-13.329	-64.312	274.04	N
ATOM	1630	CA	ARG	D	339	-63.760	-11.991	-63.952	274.04	C
ATOM	1631	C	ARG	D	339	-65.237	-12.041	-64.220	274.04	C
ATOM	49	N	ALA	D	406	-47.335	-18.204	-62.224	192.55	N
ATOM	50	CA	ALA	D	406	-47.752	-17.411	-63.397	192.55	C
ATOM	51	C	ALA	D	406	-46.685	-16.573	-64.078	192.55	C
ATOM	59	N	THR	D	407	-46.016	-17.138	-65.075	244.03	N
ATOM	60	CA	THR	D	407	-45.050	-16.361	-65.852	244.03	C
ATOM	61	C	THR	D	407	-45.999	-16.025	-66.999	244.03	C

. . .

PSFGEN (filling gaps)

now, create a temporary pdb/psf to build the structure

Sample input file (here named: build_system_protein.psfgen):

>psfgen build_system_protein_ll.psfgen >& build_protein_ll.out &

```
topology /home/mdschool/toppar/top_all27_prot_na.inp
```

```
alias residue HIS HSE
```

```
segment TRAI {
```

```
  first NTER
```

```
  last CTER
```

```
  pdb output_building/ca_sequence.pdb
```

```
}
```

```
coordpdb output_building/coords_traI_10_gap_481.pdb TRAI
```

```
guesscoord
```

```
writesf output_building/temp_2_traI.psf
```

```
writpdb output_building/temp_2_traI.pdb
```

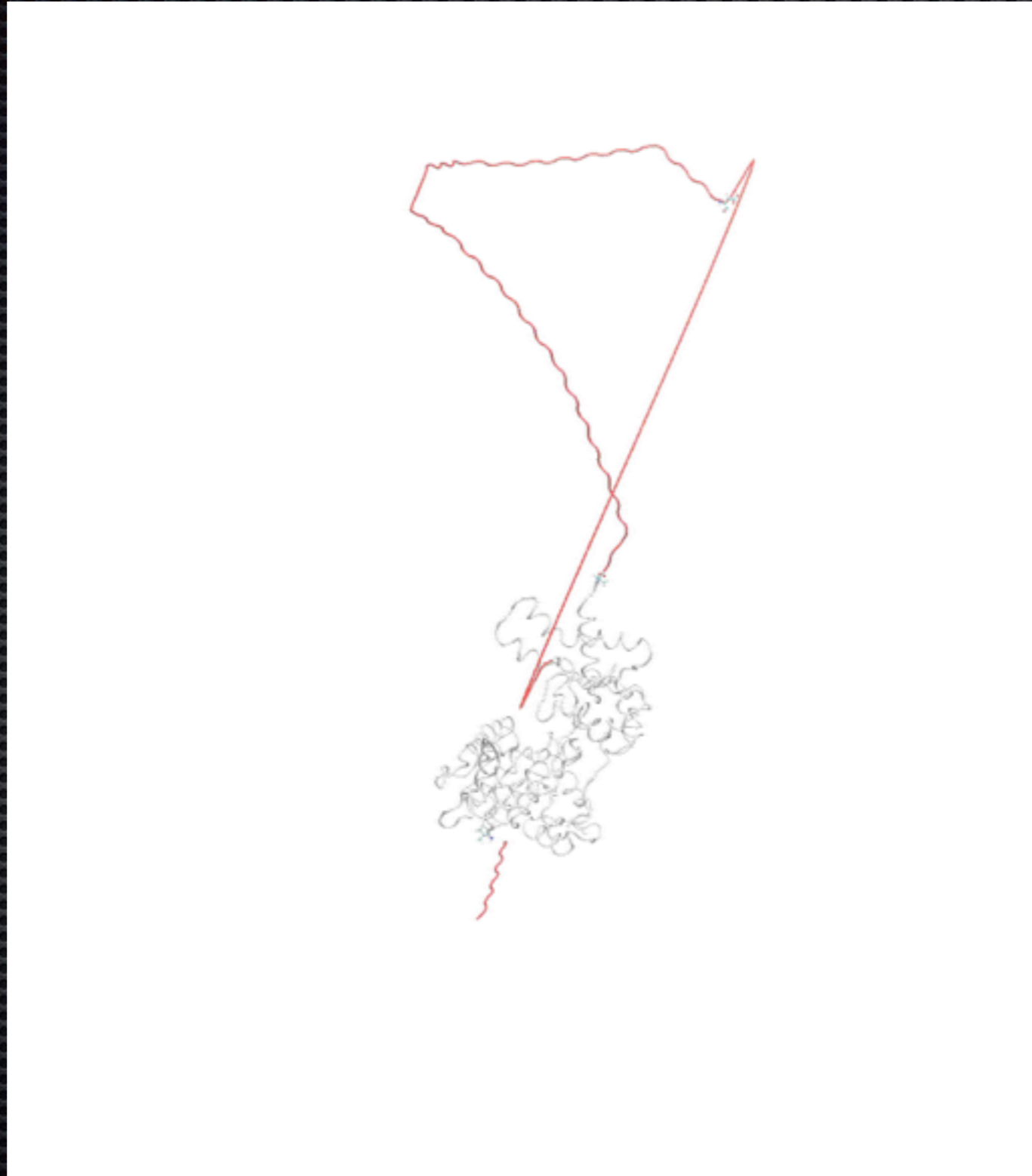
path to pdb file (sequence)

path coordinates file (pdb)

use IC to add H and
missing AA

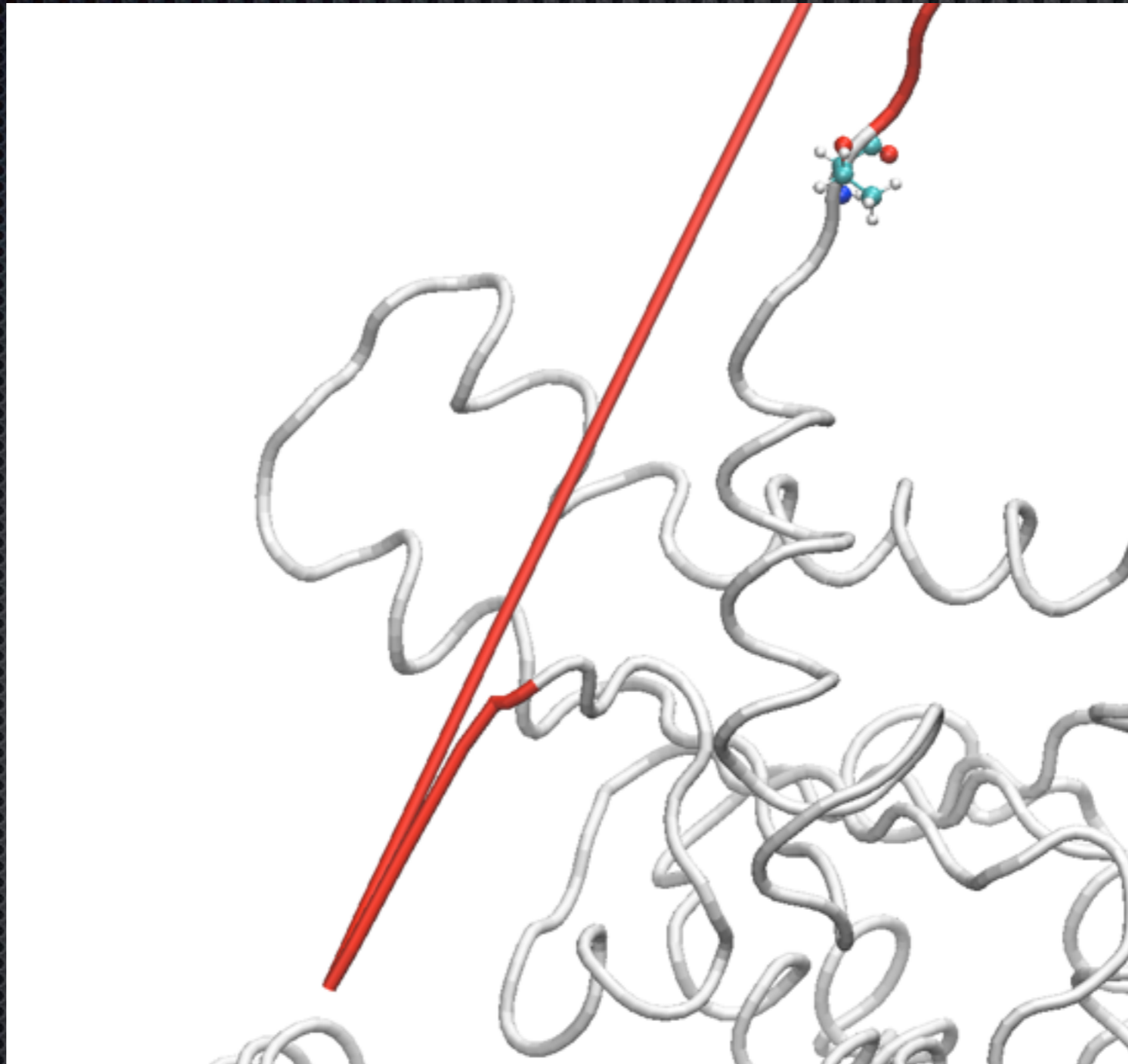
PSFGEN (filling gaps)

LOOK AT THE STRUCTURE BEFORE MOVING TO STEP 2.



PSFGEN (filling gaps)

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PSFGEN (filling gaps)

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more minimization steps

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If step 5 fails then go back to step 4 or maybe back to step 1 !!!

New PDB I

With the **temp_2_tral_piece.pdb (psf)** file open in VMD . . . at the console type:

```
vmd > set everyone [atomselect top all]
atomselect32
```

```
vmd > $everyone set beta 1.00
```

```
vmd > set sell [atomselect top "(resid > 341 and resid < 406) or (resid <
12)"]
atomselect33
```

```
vmd > $sell set beta 0.00
```

```
vmd > $everyone writepdb fixed_atoms.pdb
```

```
Info) Opened coordinate file fixed_atoms.pdb for writing.
```

```
Info) Finished with coordinate file fixed_atoms.pdb.
```

New PDB I

With the **temp_2_tral_piece.pdb (psf)** file open in VMD . . . at the console type:

```
vmd > set everyone [atomselect top all]
atomselect32
```

```
vmd > $everyone set beta 1.00
```

```
vmd > set sell [atomselect top "(resid > 341 and resid < 406) or (resid <
12)"]
atomselect33
```

```
vmd > $sell set beta 0.00
```

```
vmd > $everyone writepdb fixed_atoms.pdb
```

```
Info) Opened coordinate file fixed_atoms.pdb for writing.
```

```
Info) Finished with coordinate file fixed_atoms.pdb.
```

```
. . .
```

ATOM	6203	C	SER P 405	-46.159	-18.127	-61.621	1.00	0.00	PCLN C
ATOM	6204	O	SER P 405	-45.252	-17.351	-61.914	0.00	0.00	PCLN O
ATOM	6205	N	ALA P 406	-47.335	-18.204	-62.224	1.00	1.00	PCLN N
ATOM	6206	HN	ALA P 406	-48.017	-18.846	-61.875	0.00	1.00	PCLN H

```
. . .
```

PSFGEN (filling gaps)

STEP 1: Create new psf and pdb files where psfgen will add missing bits using edited PDB files as input.

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NAMD INPUT FILE (min0)

```
# sample NAMD configuration file for Minimization

# molecular system
coordinates      output/temp_2_tra_piece.pdb
structure        output/temp_2_tra_piece.psf
temperature      300

# restraints

fixedAtoms       on
fixedAtomsForces on
fixedAtomsFile   output/fixed_atoms.pdb
fixedAtomsCol    B

# force field
paratypecharmm   on
parameters       /home/mdschool/toppar/par_all27_prot_na.inp

# approximations
exclude          scaled1-4
1-4scaling       1.0
switching        on
switchdist       10
cutoff           12

# output

outputname       output/min0
binaryoutput     no
```

```
# interactive MD
```

```
fixedAtoms          on
fixedAtomsForces    on
fixedAtomsFile      output/fixed_atoms.pdb
fixedAtomsCol       B

# force field
paratypecharmm      on
parameters          /home/mdschool/toppar/par_all27_prot_na.inp

# approximations
exclude             scaled1-4
1-4scaling          1.0
switching           on
switchdist         10
cutoff              12

# output

outputname          output/min0
binaryoutput        no

# interactive MD

IMDon               yes
IMDport             1032
IMDfreq             10
IMDwait             no

# run control

minimize            10000
```

you will get ALOT of warnings !!!

USAGE (unix prompt):

Start a run:

```
>namd2 min0 >& min0.out &
```

Check status:

```
>tail -90f min0.out
```

Multi-processor run:

```
>charmrun ++local ++p 2 /usr/local/bin/namd/namd2 min0 >& min0.out &
```

PSFGEN (filing gaps)

ETITLE:	TS	BOND	ANGLE	DIHED	IMPRP
ELECT	VDW	BOUNDARY	MISC	KINETIC	
TOTAL	TEMP	TOTAL2	TOTAL3	TEMPAVG	

ENERGY:	0	3959878.3422	2109.1105	1825.6380	25.3996
-9900.8184	99999999.9999		0.0000	0.0000	0.0000
99999999.9999		0.0000	99999999.9999	99999999.9999	0.0000

INITIAL STEP: 1e-06

GRADIENT TOLERANCE: 1.07792e+08

Warning: Bad global exclusion count, possible error!

Warning: Increasing cutoff during minimization may avoid this.

. . .

GRADIENT TOLERANCE: 5.17843

ETITLE:	TS	BOND	ANGLE	DIHED	IMPRP
ELECT	VDW	BOUNDARY	MISC	KINETIC	
TOTAL	TEMP	TOTAL2	TOTAL3	TEMPAVG	

ENERGY:	10000	14400.1513	4244.3536	1948.5108	37.2996
-10260.9634	99999999.9999		0.0000	0.0000	0.0000
99999999.9999		0.0000	99999999.9999	99999999.9999	0.0000

WRITING EXTENDED SYSTEM TO OUTPUT FILE AT STEP 10000

WRITING COORDINATES TO OUTPUT FILE AT STEP 10000

WRITING VELOCITIES TO OUTPUT FILE AT STEP 10000

=====

PSFGEN (filling gaps)

```
ETITLE:      TS      BOND      ANGLE      DIHED      IMPRP
ELECT        VDW      BOUNDARY      MISC      KINETIC
TOTAL        TEMP      TOTAL2      TOTAL3      TEMPAVG
```

```
ENERGY:      0      3959878.3422      2109.1105      1825.6380      25.3996
-9900.8184    99999999.9999      0.0000      0.0000      0.0000
99999999.9999      0.0000      99999999.9999      99999999.9999      0.0000
```

INITIAL STEP: 1e-06

GRADIENT TOLERANCE: 1.07792e+08

Warning: Bad global exclusion count, possible error!

Warning: Increasing cutoff during minimization may avoid this.

...

GRADIENT TOLERANCE: 5.17843

```
ETITLE:      TS      BOND      ANGLE      DIHED      IMPRP
ELECT        VDW      BOUNDARY      MISC      KINETIC
TOTAL        TEMP      TOTAL2      TOTAL3      TEMPAVG
```

```
ENERGY:      10000      14400.1513      4244.3536      1948.5108      37.2996
-10260.9634    99999999.9999      0.0000      0.0000      0.0000
99999999.9999      0.0000      99999999.9999      99999999.9999      0.0000
```

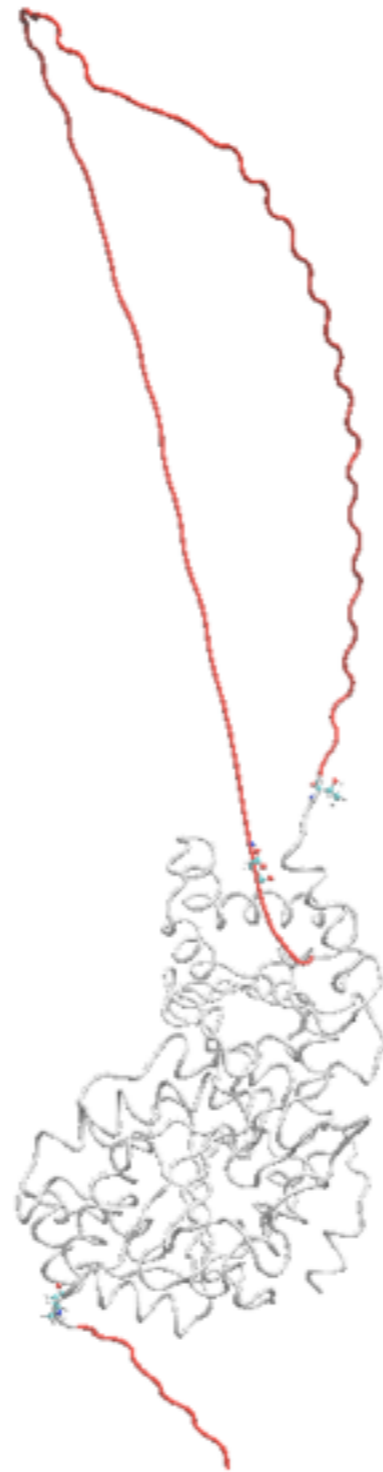
WRITING EXTENDED SYSTEM TO OUTPUT FILE AT STEP 10000

WRITING COORDINATES TO OUTPUT FILE AT STEP 10000

WRITING VELOCITIES TO OUTPUT FILE AT STEP 10000

=====

try continuing
minimization w/o fixed
atoms



MIN1 (w/o fixed atoms)

TCL: Minimizing for 10000 steps

ETITLE:	TS	BOND	ANGLE	DIHED	IMPRP
ELECT	VDW	BOUNDARY	MISC	KINETIC	
TOTAL	TEMP	TOTAL2	TOTAL3	TEMPAVG	
ENERGY:	0	14400.1137	4244.3463	1948.5042	37.3339
-10260.8912	99999999.9999		0.0000	0.0000	0.0000
99999999.9999		0.0000	99999999.9999	99999999.9999	0.0000

INITIAL STEP: 1e-06

GRADIENT TOLERANCE: 2.44629e+09

. . .

GRADIENT TOLERANCE: 0.048755

TIMING: 10000 CPU: 1535.9, 0.150397/step Wall: 1481.5, 0.144865/step, 0 hours remaining, 752124 kB of memory in use.

ETITLE:	TS	BOND	ANGLE	DIHED	IMPRP
ELECT	VDW	BOUNDARY	MISC	KINETIC	
TOTAL	TEMP	TOTAL2	TOTAL3	TEMPAVG	
ENERGY:	10000	471.9604	1640.2784	2439.1727	77.2777
-17646.7352	-1541.1823		0.0000	0.0000	0.0000
-14559.2282		0.0000	-14559.2282	-14559.2282	0.0000

WRITING EXTENDED SYSTEM TO OUTPUT FILE AT STEP 10000

WRITING COORDINATES TO OUTPUT FILE AT STEP 10000

WRITING VELOCITIES TO OUTPUT FILE AT STEP 10000

=====



DYN0: (IN LAB)

Overview

Intermediate Building Tricks

Building coordinates for missing atoms/residues

Simulated annealing

Building IDPs

A trick for topological issues

SA

Simulated Annealing (SA)

May wish to relax the structure further

May wish to explore configurations (NMR, FRET, other constraints)

For IDPs our “software” can not handle INTERNAL disordered loops

Write a TCL script (a list of commands) at the end of one of our “dyn1” NAMD input files to carry out SA.

The idea is simple. Run a series of heating and cooling cycles of your system and at the end of each cooling cycle you minimize and save the structure.

Heating allows you to cross energetic barriers.

An ensemble of such structures is representative of what might exist . . .

SA Protocol (100 cycles)

```
...
for { set x 0 } { $x < 100 } { incr x } {
if { $x == 0 } {
checkpoint
print "setting checkpoint structure"
}
for { set TEMP 300 } { $TEMP <= 1000 } { incr TEMP 50 } {
run 2000
reassignTemp $TEMP
langevinTemp $TEMP
}
run 20000
for { set TEMP 950 } { $TEMP >= 300 } { incr TEMP -50 } {
reassignTemp $TEMP
langevinTemp $TEMP
run 2000
}
run 2000
minimize 500
output output/sa0_min_$x
#revert
}
```

← at bottom of regular namd input file

← save initial structure

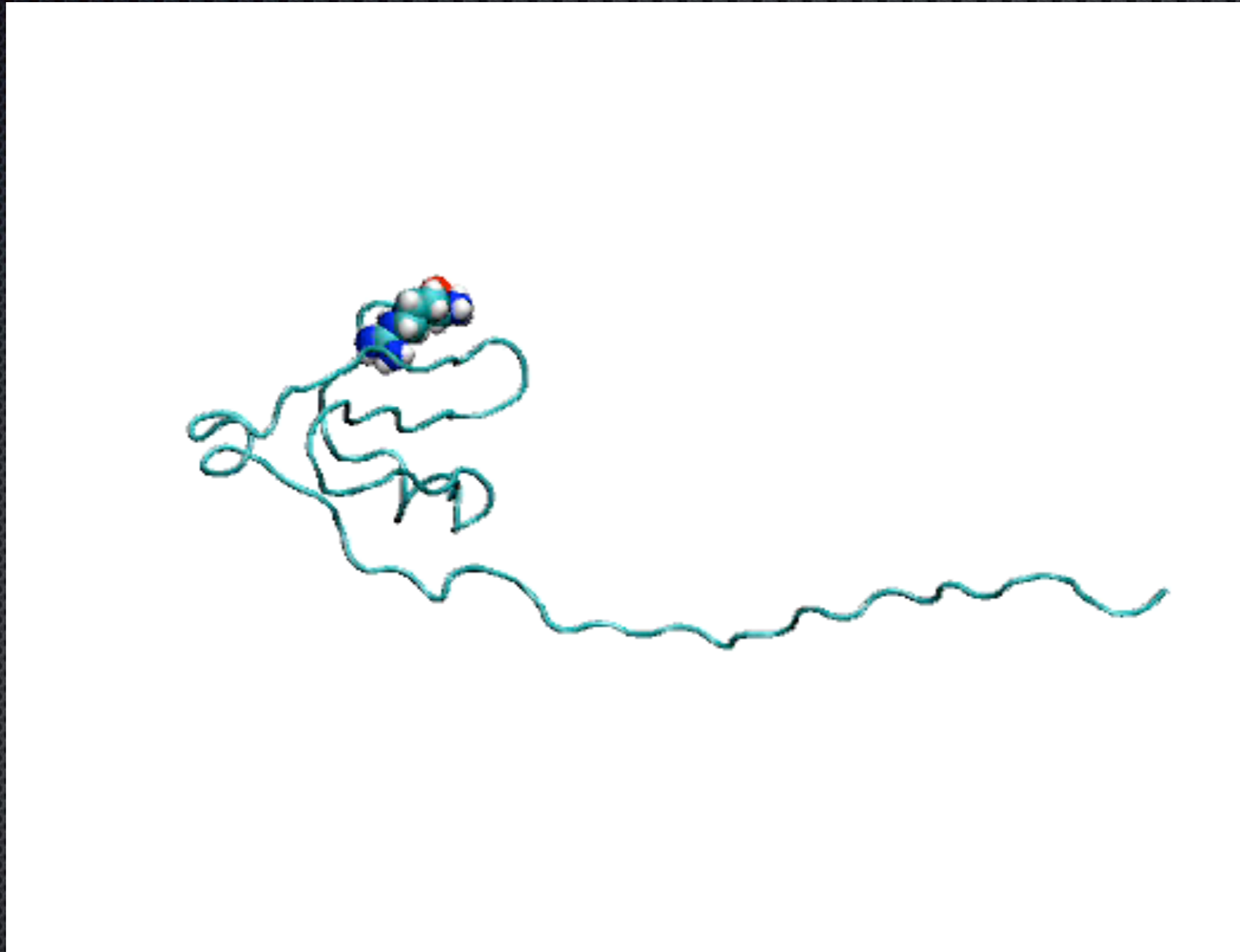
← HEAT UP

← COOL DOWN

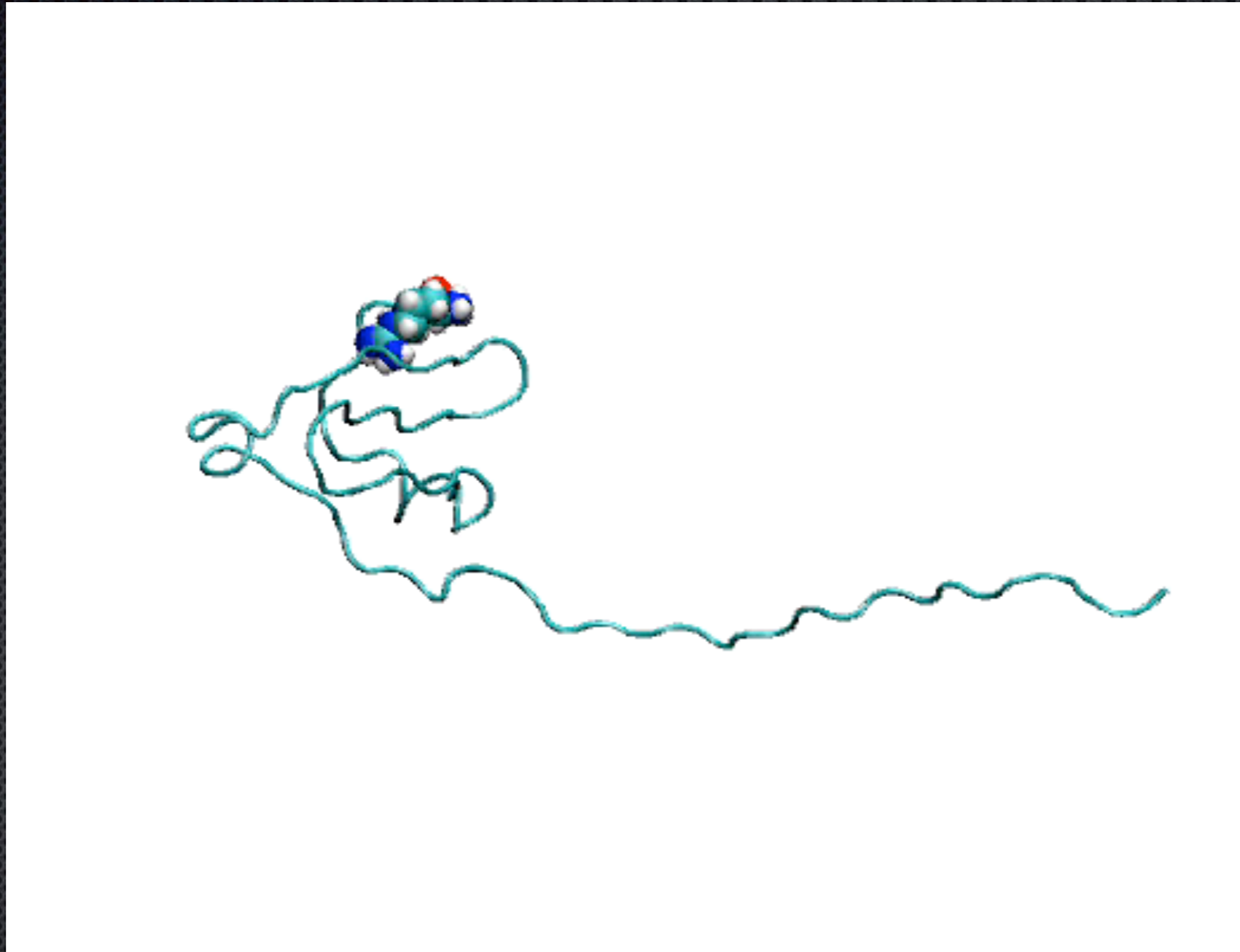
← Minimize and save structure

you probably want to
used fixed atoms!!!

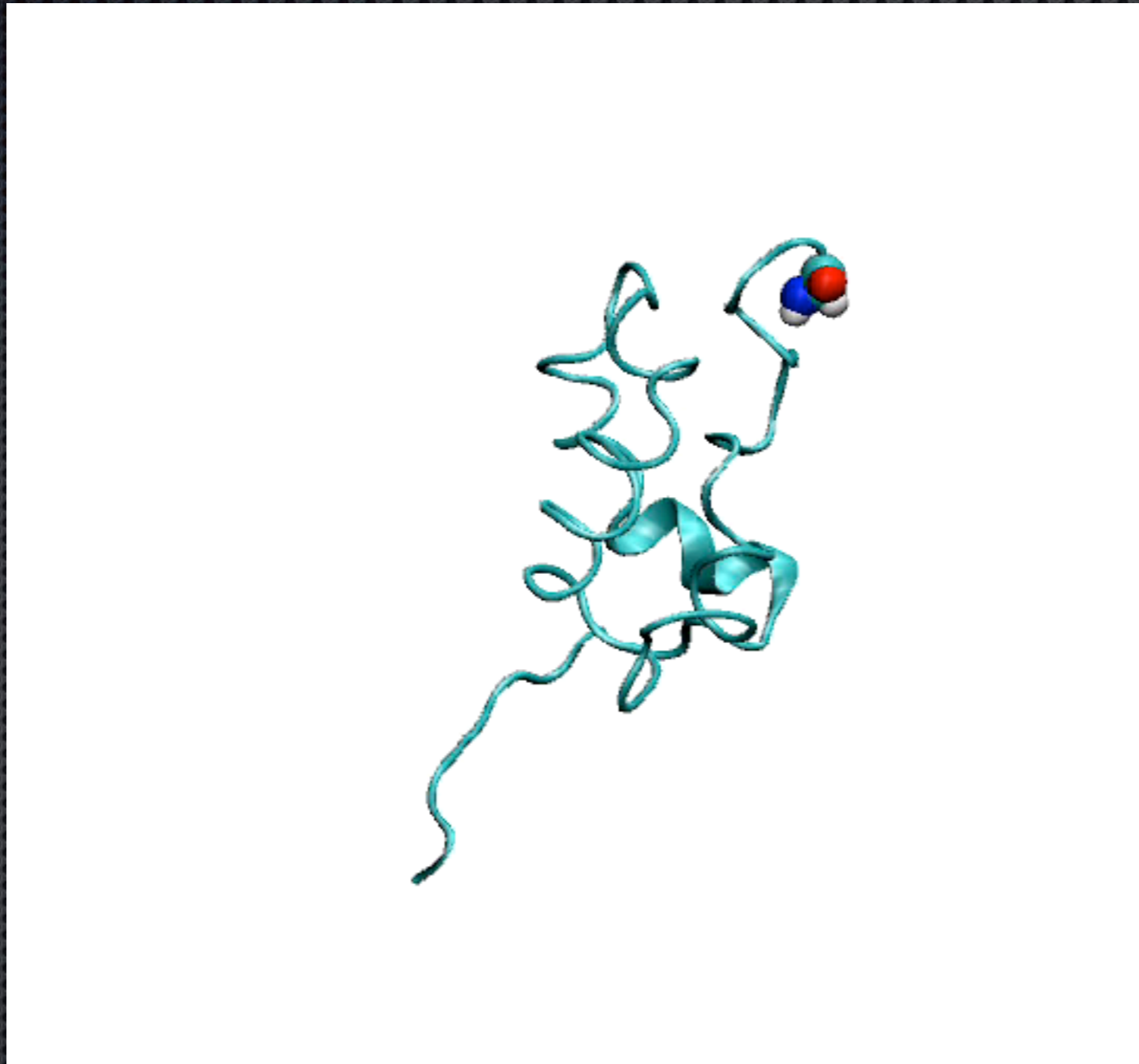
SA Examples



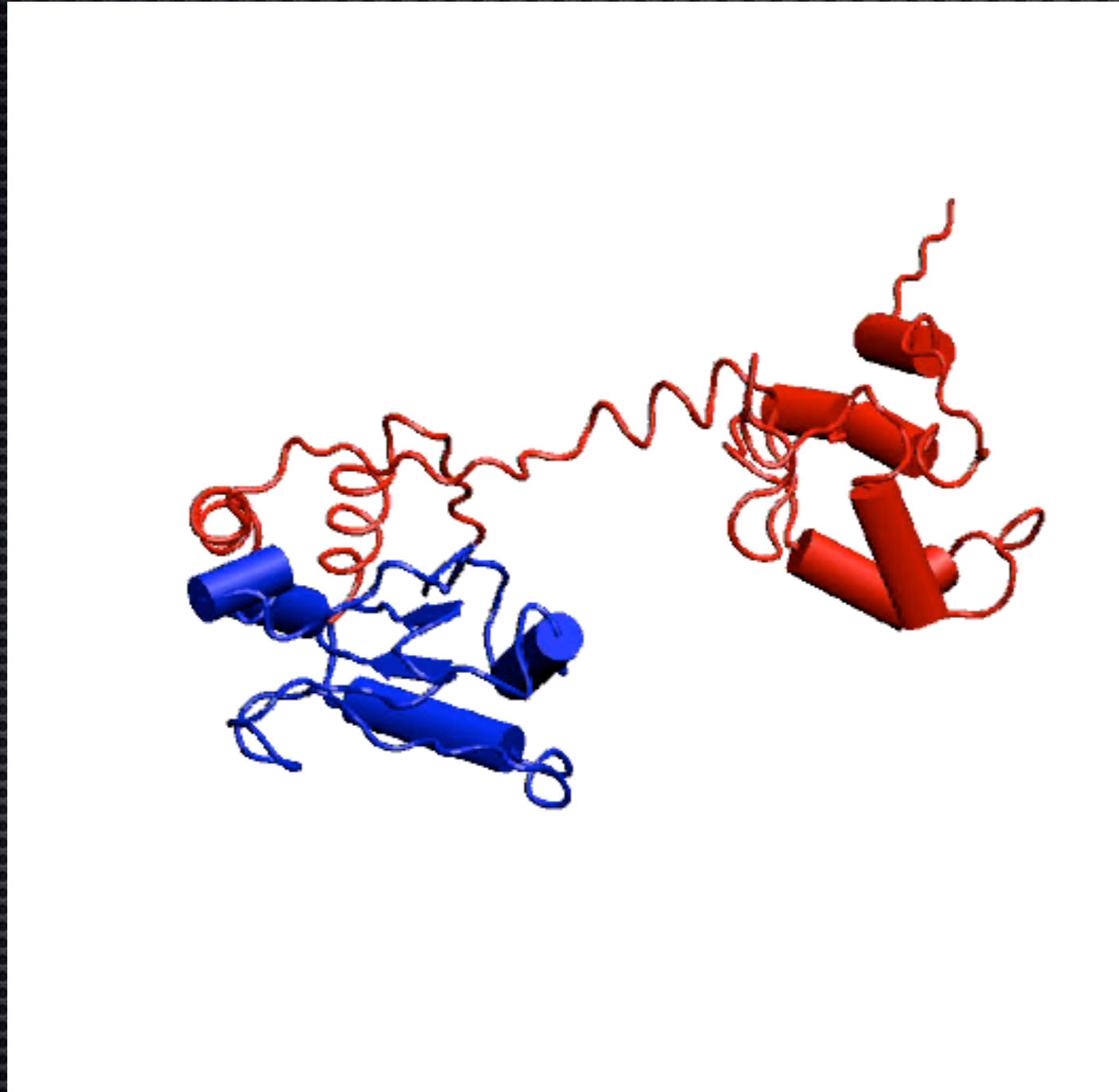
SA Examples



SA Examples



SA Examples



SA

Runs take a long time . . . adding solvent is even more CPU intensive (implicit solvent : GBSA)

Need to concatenate all the “minimized structures”. Here is a command to read in the individual sa_min0*.coor files and make a single DCD file of the ensemble.

For this example, we’ll use the PSF file and assume that the individual sa_min0*.coor files are in a directory called “output/”

```
> catdcd -o all_sa_min0.dcd -otype dcd -stype psf -s output/ .psf -filetype  
namdbin output/sa_min0*.coor
```

When you forget the options for this handy program, just type “catdcd” at the command line and the usage will print out.

SA

```
> catdcd
```

```
CatDCD 4.0
```

```
catdcd -o outputfile [-otype <filetype>] [-i indexfile]
      [-stype <filetype>] [-s structurefile]
      [-first firstframe] [-last lastframe] [-stride stride]
      [-<filetype>] inputfile1 [-<filetype>] inputfile2 ...
```

Allowed input file types:

cpmd pdb dcd Alchemy AMBERPREP BallStick MSIBGF BiosymCAR Boogie
Cacao CADPAC CHARMM Chem3d-1 Chem3d-2 CSSR FDAT GSTAT Dock
DockPDB Feature Fractional GAMESSoutput GaussianZmatrix
Gaussian92output Gaussian94output Gromos96A Gromos96N
HyperchemHIN IsisSDF M3D MacMolecule Macromodel MicroWorld
MM2Input MM2Output MM3 MMADS MDLMOL MOLIN MopacCartesian
MopacInternal MopacOutput PCModel PSGVBin PSGVBout QuantaMSF
Schakal ShelX SMILES Spartan SpartanSE SpartanMM SybylMol
SybylMol2 Conjure UniChemXYZ XYZ XED gro g96 trr trj xtc crd
crdbox namdbin binpos cube rst7 tinker POSCAR OUTCAR XDATCAR xml
dlpolyhist dlpoly3hist lammpstrj vcf vtf xyz cor molden pqr mol2
car gamess xsf bgf xbgf webpdb netcdf

Allowed output file types:

pdb dcd trr crd crdbox namdbin binpos rst7 POSCAR xyz pqr mol2
bgf xbgf

Overview

Intermediate Building Tricks

Building coordinates for missing atoms/residues

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A trick for topological issues

IDPs

Piece structures together (1) in lab VII

1. Load individual PDB files into VMD. Use “8” to grab one and sequentially move along X, rotate system, move along Y, rotate system, move along Z. Save coordinates using VMD. ((**will probably have to execute rotate TCL commands**))

“align by eye” & hope for the best. Concatentate files, renumber amino acids and atoms, make new PDB/PSF pair, minimize, 10 ps NVE MD . . .

2. Add 3 to 5 amino acids to N-terminal of the C-terminal part, then overlap these amino acids (using backbone as a basis).

Then you align the two structures (C-terminal of “A” to modified N-terminal of “B”)

Concatentate PDB files, remove the “bridging” 3 to 5 AA, renumber remaining amino acids and atoms, make new PDB/PSF pair, minimize, 10 ps NVE MD . . .

3. Insert your method here . . . etc. (pymol, mdtools, etc.)

IDPs

Many IDPs that we have built have been a combination of X-ray, NMR coordinates and homology models. Many regions are evaluated by predicting if a region has the potential to have SS or disorder etc.

SS:

<http://cib.cf.ocha.ac.jp/bitool/MIX/>

<http://bioinf.cs.ucl.ac.uk:80/psipred/>

Disorder:

<http://dis.embl.de/>

<http://mbs.cbrc.jp/poodle/poodle.html>

Homology modeling:

<http://www.sbg.bio.ic.ac.uk/~phyre/>

<http://www.smallangles.net/sassie/tra1/Tra1/Outline.html>

Do more
experiments!

CD

Enzyme digests

NMR

etc.

Overview

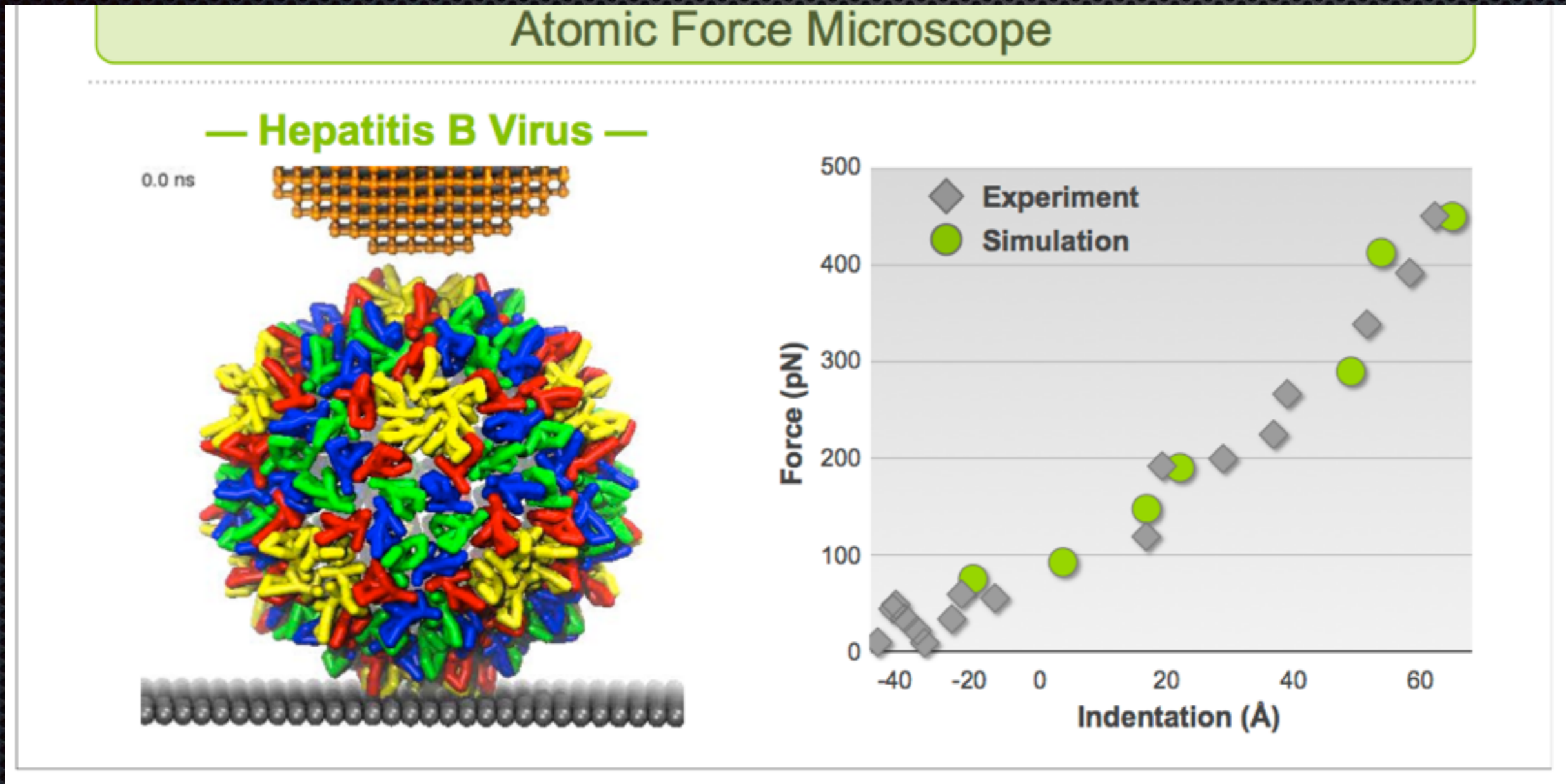
Intermediate Building Tricks

Building coordinates for missing atoms/residues
Simulated annealing
Building IDPs

A trick for topological issues

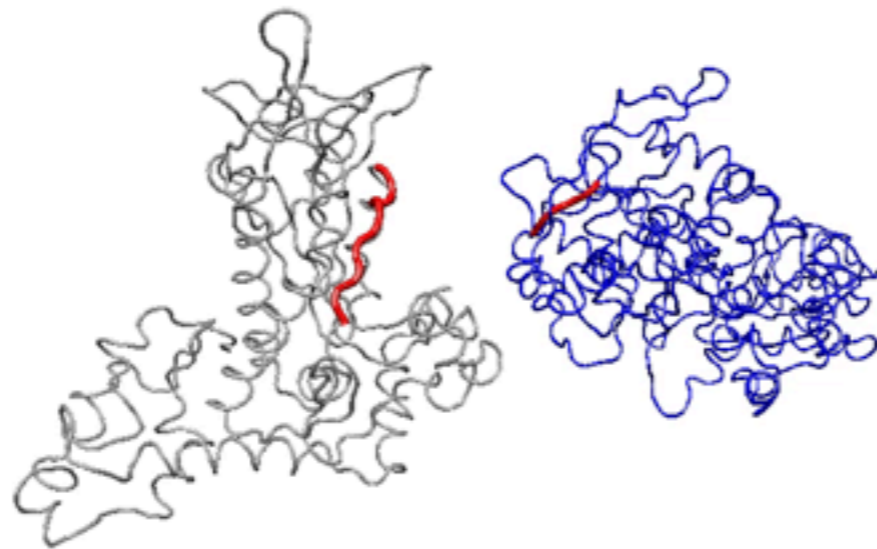
Steered MD

http://www.ks.uiuc.edu/Research/smd_imd/



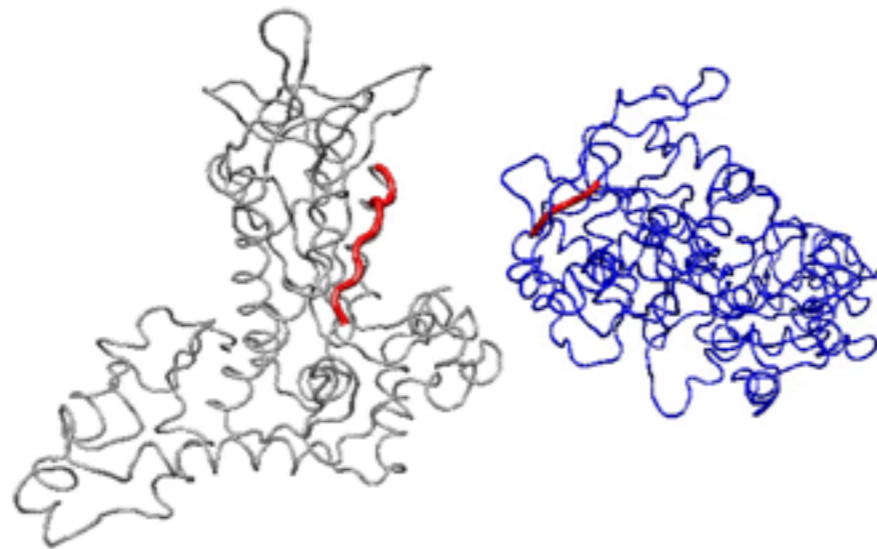
Steered MD for building

Buried disordered tails ... have to pull them out to link two structures together



Steered MD for building

Buried disordered tails ... have to pull them out to link two structures together



Steered MD for building

So, in the following movie you will see:

1. files that we are working with
2. a view of the input file (min0)
3. loading the psf and then pdb into vmd
4. initiating namd2 min0
5. starting the run via IMD in VMD
6. applying the residue specific force to pull the N-terminal out
7. a few thousand steps of MD

NOTE:

This N-terminal was known NOT to be buried and that it was unstructured. The resulting structure was minimized prior to its use in further building steps!

This example was done in the process of building a larger IDP with many known and unknown bits.

It allowed us to overlap the N-terminal AA with the “other” piece etc.

SUMMARY

What have we accomplished?

We showed some examples of how to complete structures and covered some ways to build larger structures/models from bits of known structure.

What is next?

LAB VII --> Advanced Building

LAB VIII --> Lipid & NM Labs, STUDENT PROJECTS