

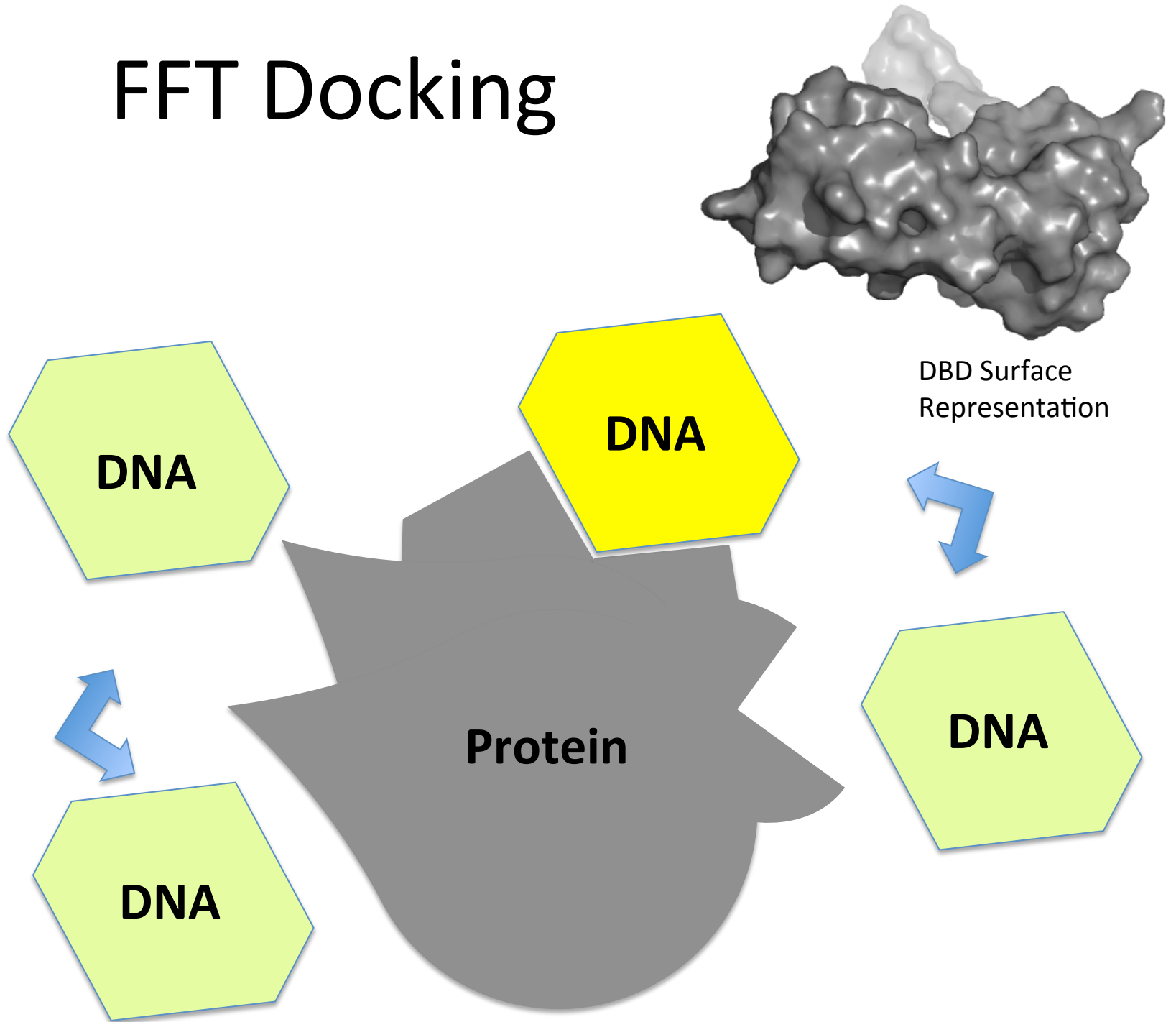
# **SASSIE Tutorial**

ACNS 2012

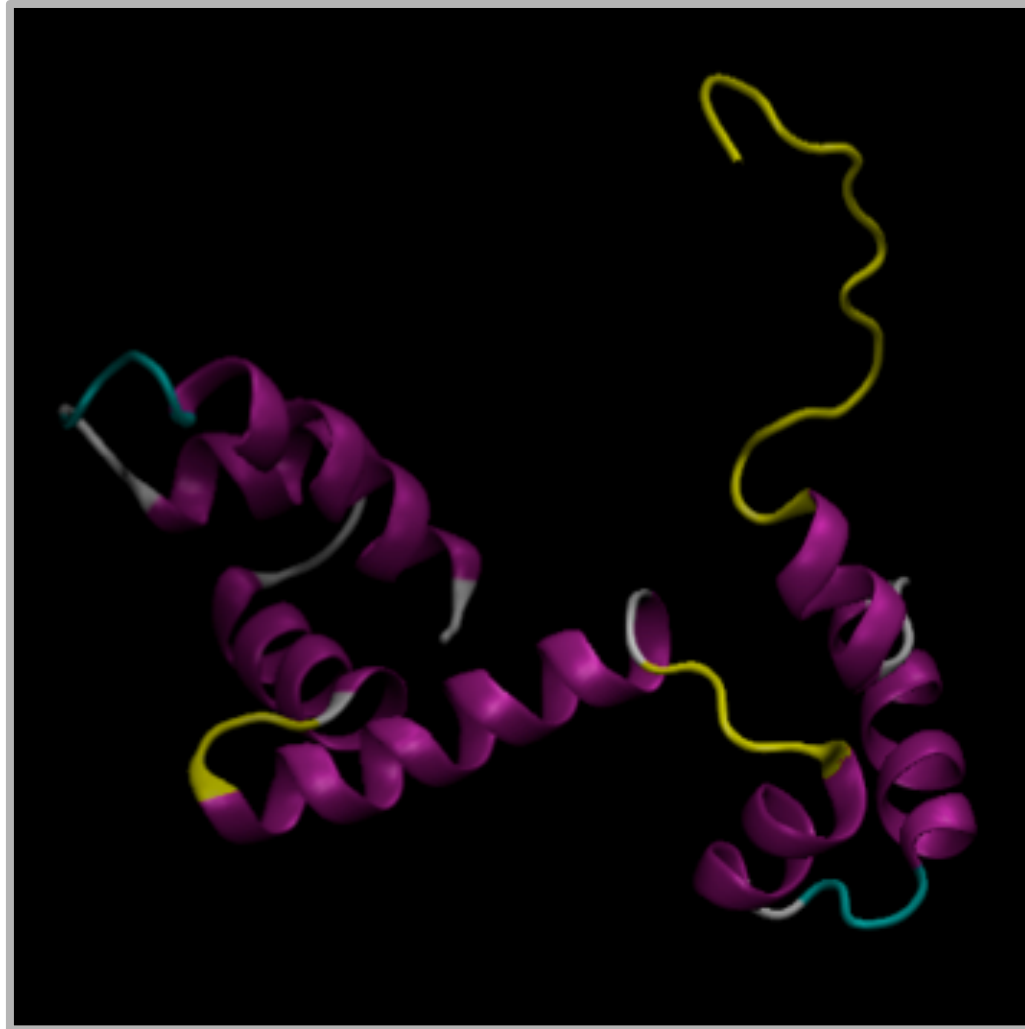
Presented By

Nicholas Clark and Hailiang Zhang

# FFT Docking

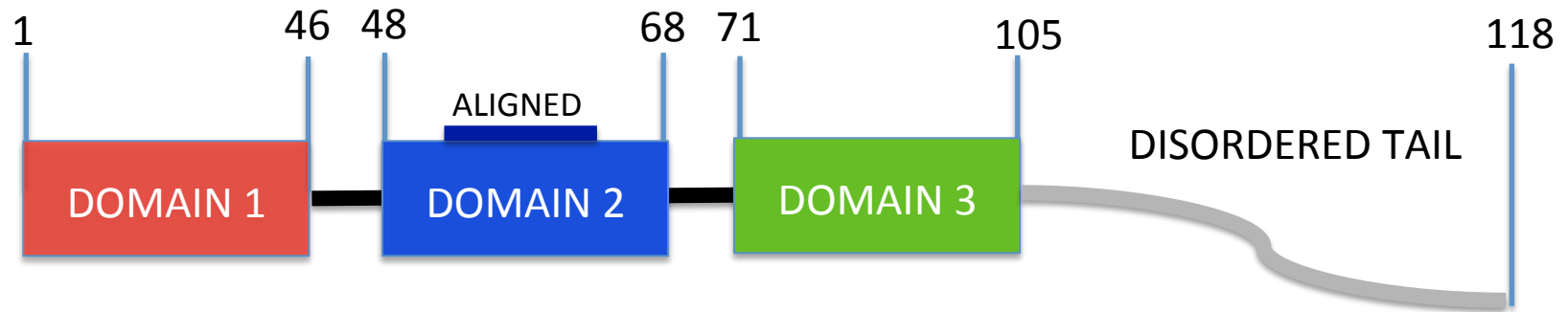


# Tutorial Example

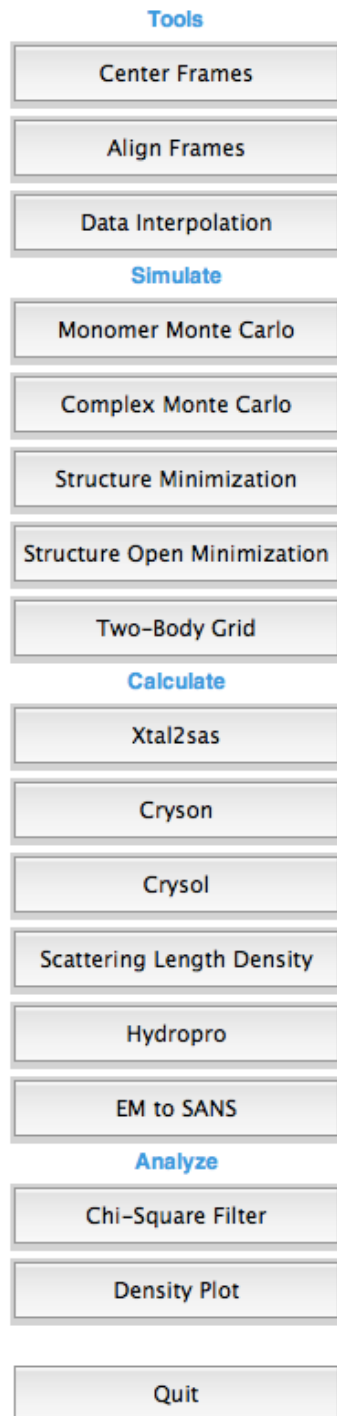


BDB Protein

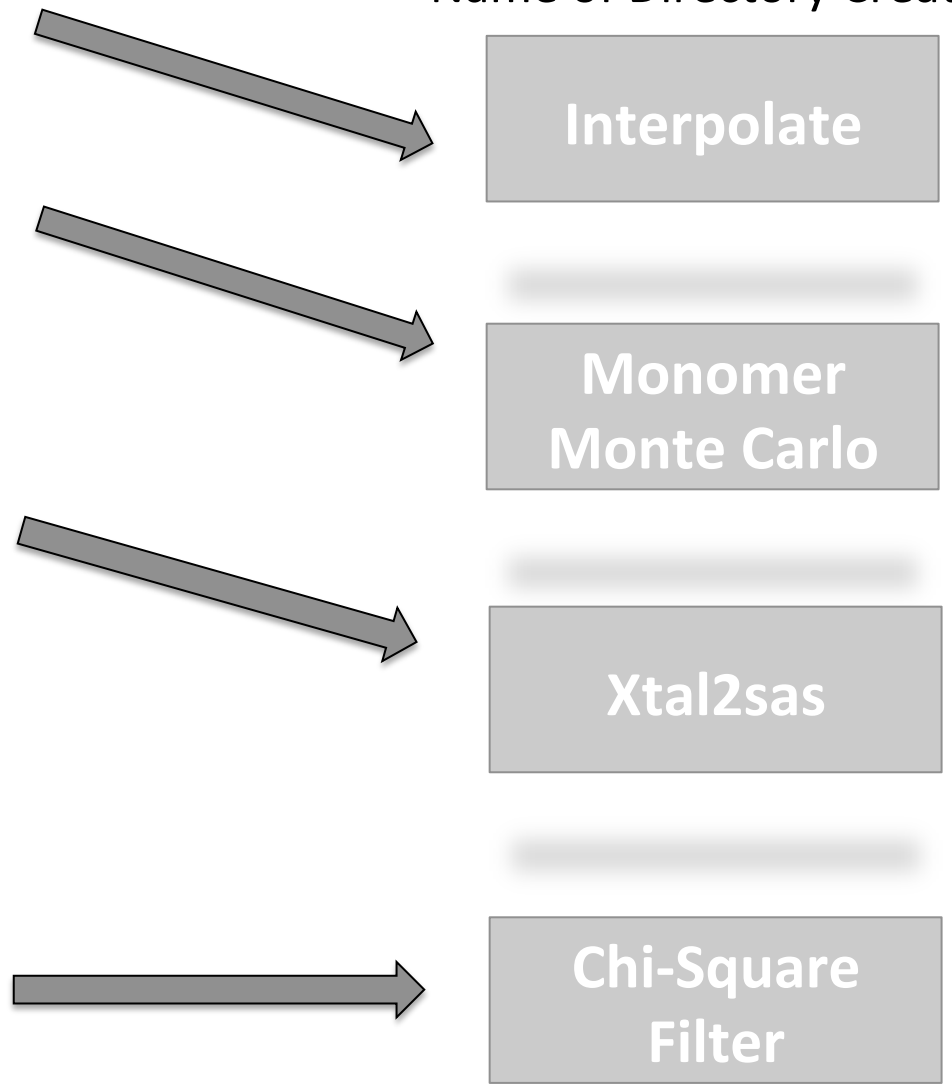
# BDB Protein Domain Organization



# File Structure of SASSIE

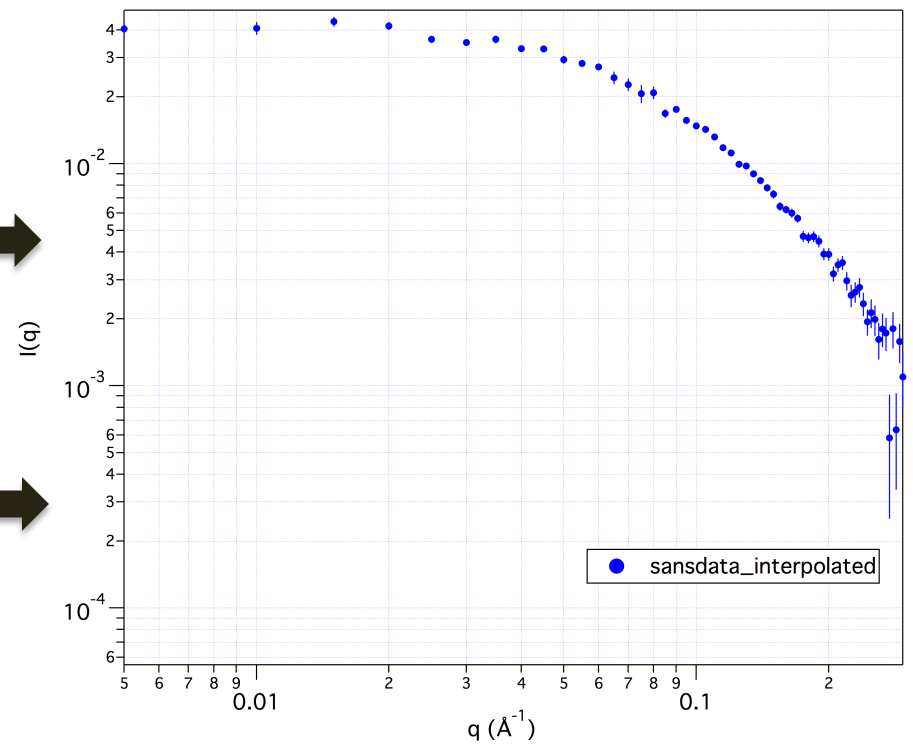
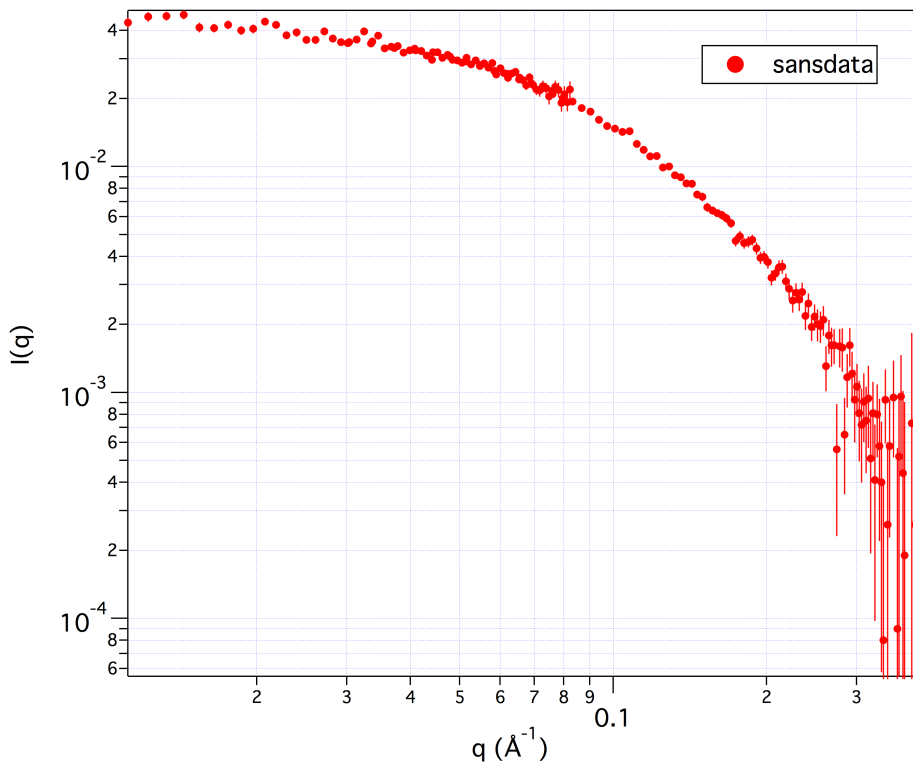


Name of Directory Created

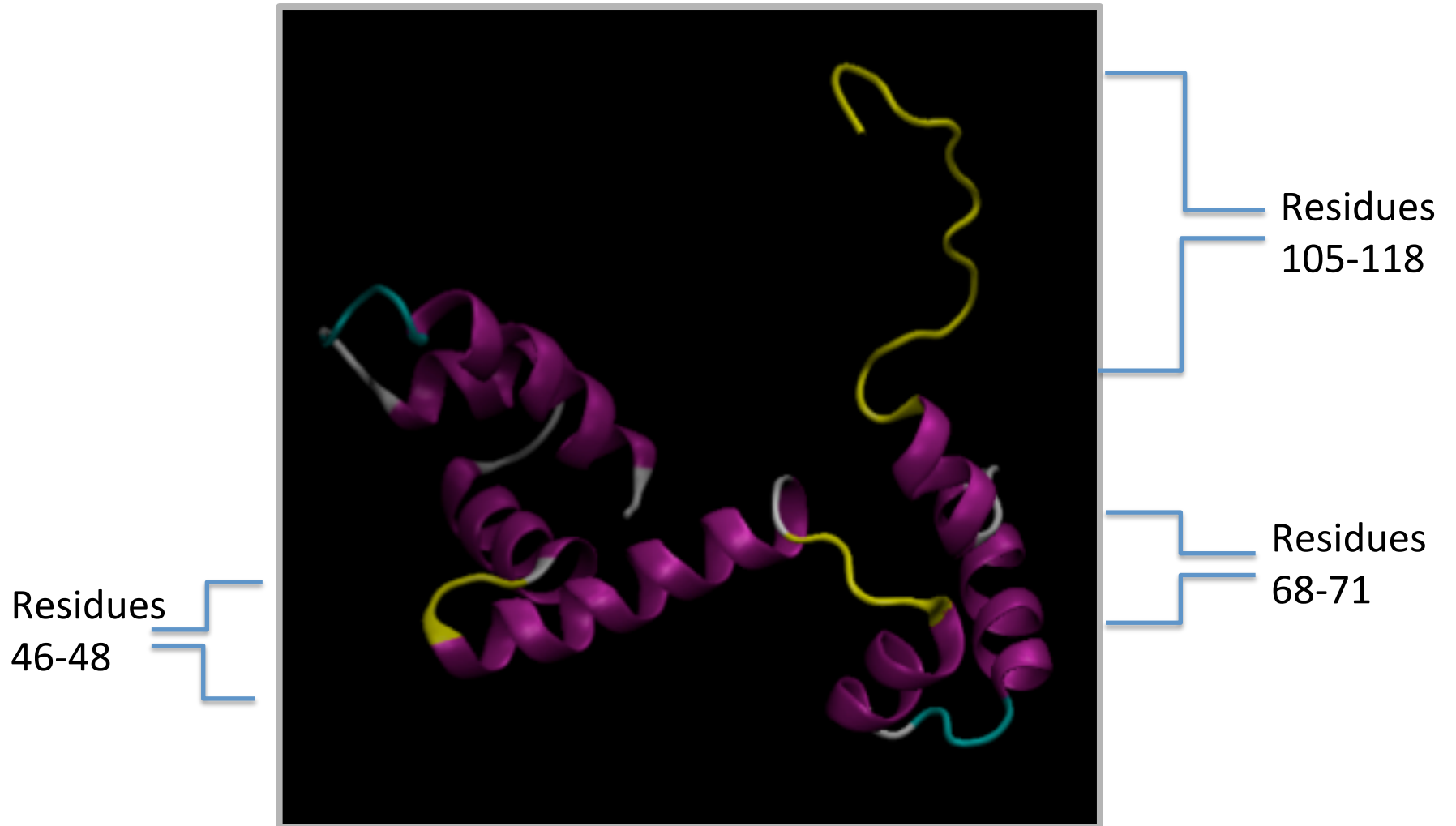


# Data Interpolation

Data Interpolation			
project name :	<input type="text" value="data"/>	input file path :	<input type="text" value="."/>
input filename :	<input type="text" value="sansdata.sub"/>	output filename :	<input type="text" value="sansdata.dat"/>
I(0) :	<input type="text" value="0.042"/>	I(0) error :	<input type="text" value="0.001"/>
new delta q :	<input type="text" value="0.005"/>	number of new points :	<input type="text" value="60"/>



# Starting Structure of Bdb Protein



# Monte Carlo Configuration Generator

Monomer Configuration Generator

**User Input Section**

project name :	<input type="text" value="test_1"/>	output filename (dcd) :	<input type="text" value="test_1.dcd"/>
input file path :	<input type="text" value="."/>	input filename (pdb) :	<input type="text" value="4309r2.pdb"/>
number of trial attempts :	<input type="text" value="10000"/>	return to previously accepted structure :	<input type="text" value="10"/>
temperature (K) :	<input type="text" value="300.0"/>	molecule type (protein or rna) :	<input type="text" value="protein"/>

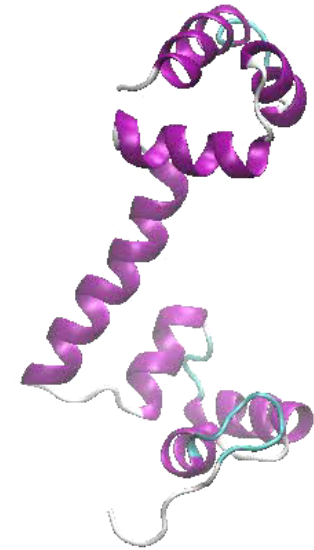
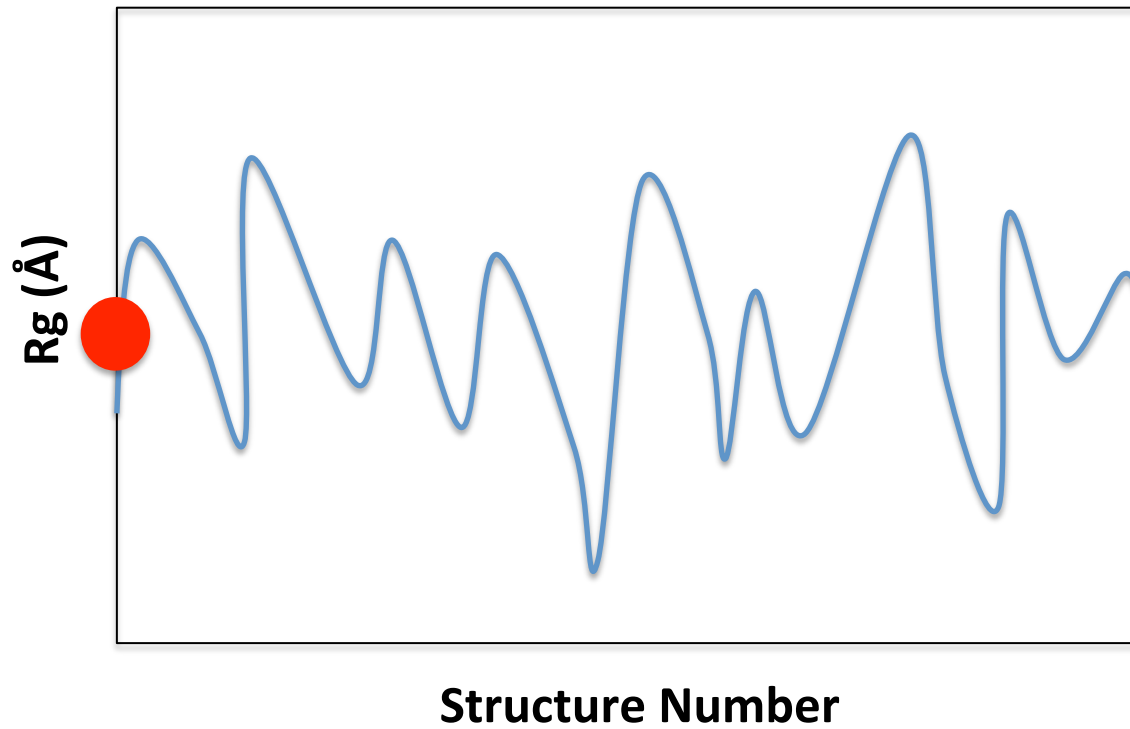
**Molecule Specific Input**

number of flexible regions to vary :	<input type="text" value="3"/>	enter MAX  dtheta  for each region :	<input type="text" value="30,30,30"/>
first residue per region :	<input type="text" value="46,68,108"/>	number contiguous residues per region :	<input type="text" value="3,4,7"/>
structure alignment: low residue :	<input type="text" value="50"/>	structure alignment: high residue :	<input type="text" value="60"/>

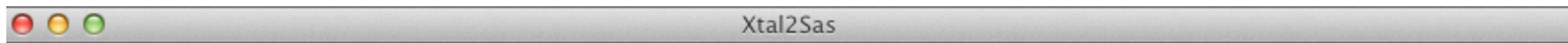
**Non-Standard / Specialized Input**

overlap basis :	<input type="text" value="CA"/>	overlap cutoff :	<input type="text" value="3.0"/>
low Rg cutoff :	<input type="text" value="0.0"/>	high Rg cutoff :	<input type="text" value="400.0"/>
Z coordinate filter (0==no, 1==yes) :	<input type="text" value="0"/>	Z cutoff (angstroms) :	<input type="text" value="0.0"/>
atomic constraints (0==no, 1==yes) :	<input type="text" value="0"/>	constraint filename :	<input type="text" value="constraints.txt"/>
non-bonding energies (0==no, 1==yes) :	<input type="text" value="0"/>	non-bonding scaling factor :	<input type="text" value="1.0"/>
psf file path :	<input type="text" value="."/>	psf file name :	<input type="text" value="dbd.psf"/>
parameter file path :	<input type="text" value="/usr/local/bin/sassie/simula"/>	parameter file name :	<input type="text" value="par_all27_prot_na.inp"/>

# Monte Carlo Configuration Generator



# Xtal2sas; SANS Curve Calculator

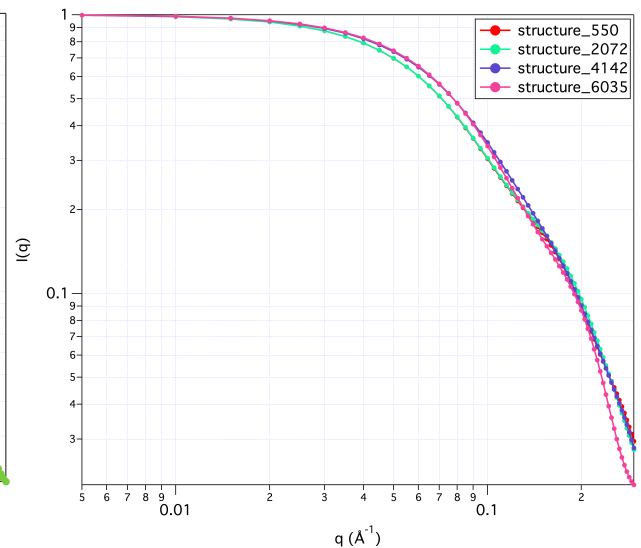
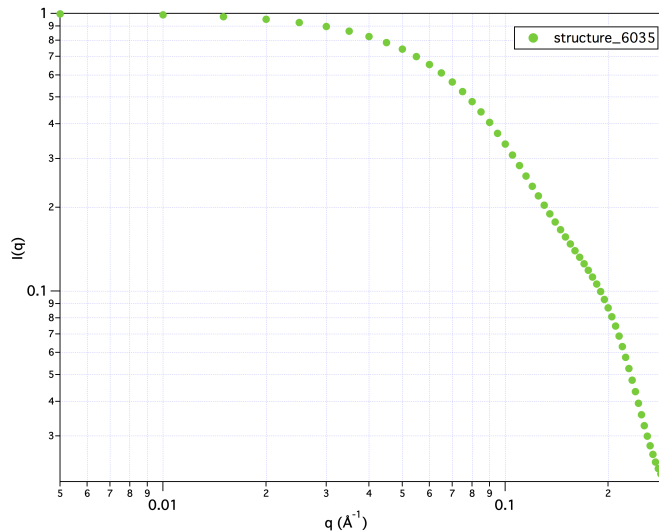
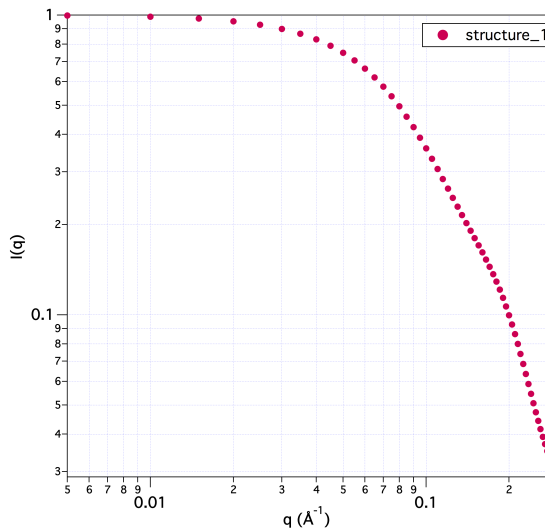


## Data Management Section

project name :	<input type="text" value="test_1"/>	input filename (dcd) :	<input type="text" value="test_1.dcd"/>
DCD input file path :	<input type="text" value="./test_1/generate/"/>	input filename (pdb) :	<input type="text" value="4309r2.pdb"/>
PDB input file path :	<input type="text" value="./test_1/generate/"/>	delete crd/ans/inf/pr files (1=Y/0=N):	<input type="text" value="1"/>
xtal2sas executable name (v4) :	<input type="text" value="/usr/local/bin/xtal2sas.exe"/>		

## Xtal2sas Input Section

X-rays or Neutrons (X/N):	<input type="text" value="N"/>	number of I(Q) values :	<input type="text" value="60"/>
maximum Q value :	<input type="text" value="0.3"/>	Intensity at I(0) :	<input type="text" value="1.0"/>
number output iterations :	<input type="text" value="1"/>	number of hits :	<input type="text" value="1000"/>

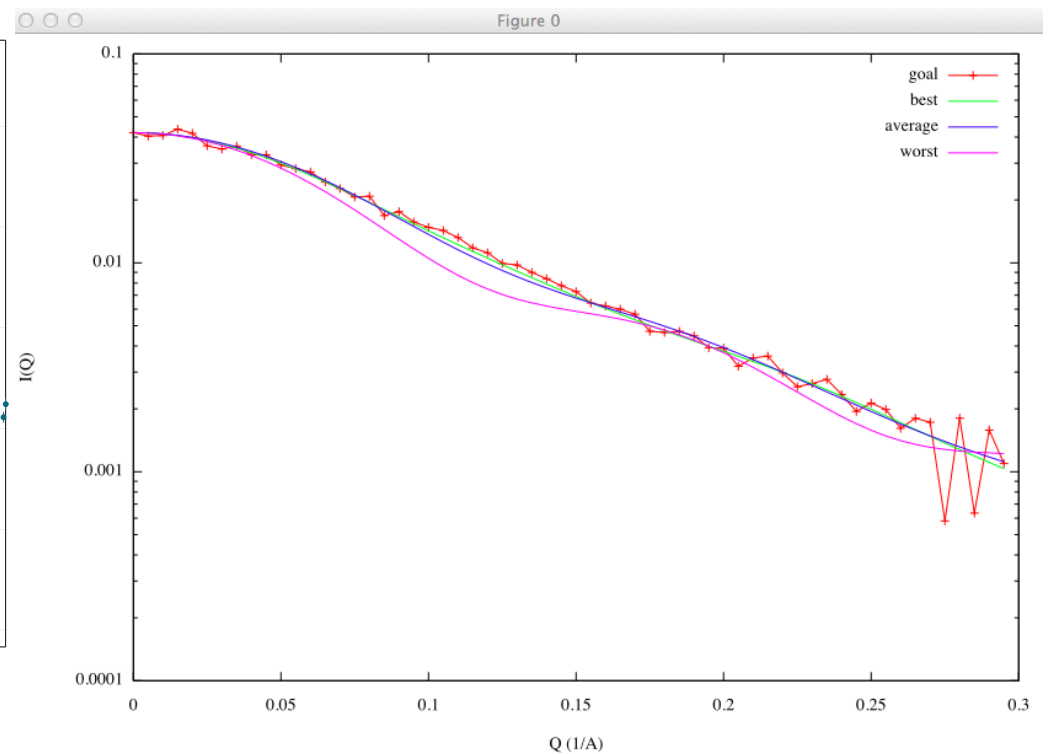
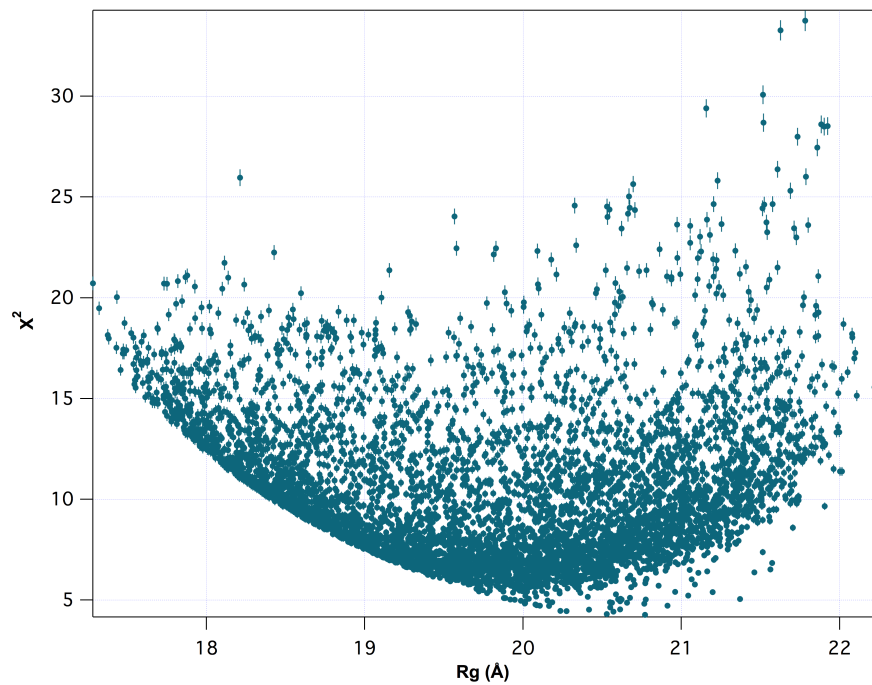


Krueger, S., Groshkova, I., Brown, J., Hoskins, J., McKenney, K. H. & Schwarz, F. P. (1998). J. Biol. Chem. 273, 20001–20008.

# X<sup>2</sup> Filtering

Chi-Square Filter

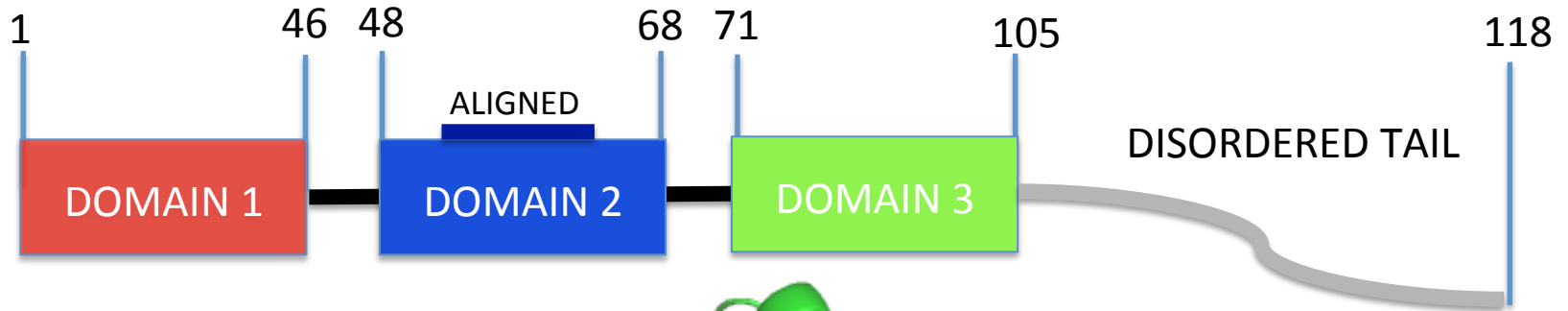
project name :	<input type="text" value="test_1"/>	path to SAS files	<input type="text" value="test_1/xtal2sas/"/>
SAS exp. data file (goal) :	<input type="text" value="./sansdata.dat"/>	I(0) :	<input type="text" value="0.042"/>
X2 high cutoff :	<input type="text" value="10.0"/>	X2 high cutoff file (output) :	<input type="text" value="x2highweights.txt"/>
X2 low cutoff :	<input type="text" value="5.0"/>	X2 low cutoff file (output) :	<input type="text" value="x2lowweights.txt"/>
Rg high cutoff :	<input type="text" value="60.0"/>	Rg high cutoff file (output) :	<input type="text" value="rghighweights.txt"/>
Rg low cutoff :	<input type="text" value="40.0"/>	Rg low cutoff file (output) :	<input type="text" value="rglowweights.txt"/>
enter SAS type (1=Xtal2sas : 2=Cryson : 3=Crysol) :	<input type="text" value="1"/>	use reduced X2 (0=no, 1=yes) :	<input type="text" value="1"/>



# Density Plots

Density Plot			
project name :	test_1	input filename :	./test_1/generate/newfile.dcc
reference pdb :	./test_1/generate/4309r2.pdb	output filename :	dbd
xlength :	150	grid spacing :	6.0
ylength :	150	occupancy basis :	calpha
zlength :	150	number of regions :	4
enter low regions :	1,50,66,105	enter high regions :	49,67,104,117
equalweights (1=yes,0=no) :	1	weights filename :	./test_1/filter/x2lowweights.txt

# BDB Protein



# Density Plots

Density Plot			
project name :	<input type="text" value="all_1"/>	input filename :	<input type="text" value="./all_1/generate/newfile.dcd"/>
reference pdb :	<input type="text" value="./all_1/generate/4309r2.pdb"/>	output filename :	<input type="text" value="dbd"/>
xlength :	<input type="text" value="150"/>	grid spacing :	<input type="text" value="6.0"/>
ylength :	<input type="text" value="150"/>	occupancy basis :	<input type="text" value="calpha"/>
zlength :	<input type="text" value="150"/>	number of regions :	<input type="text" value="4"/>
enter low regions :	<input type="text" value="1,50,66,105"/>	enter high regions :	<input type="text" value="49,67,104,117"/>
equalweights (1=yes,0=no) :	<input type="text" value="1"/>	weights filename :	<input type="text" value="./all_1/filter/x2lowweights.txt"/>

version 0.6 : 07/18/08

Thu Jun 21 12:57:06 2012

```
=====
DATA FROM RUN: Thu Jun 21 13:19:06 2012

Data stored in directory: all_1/density/

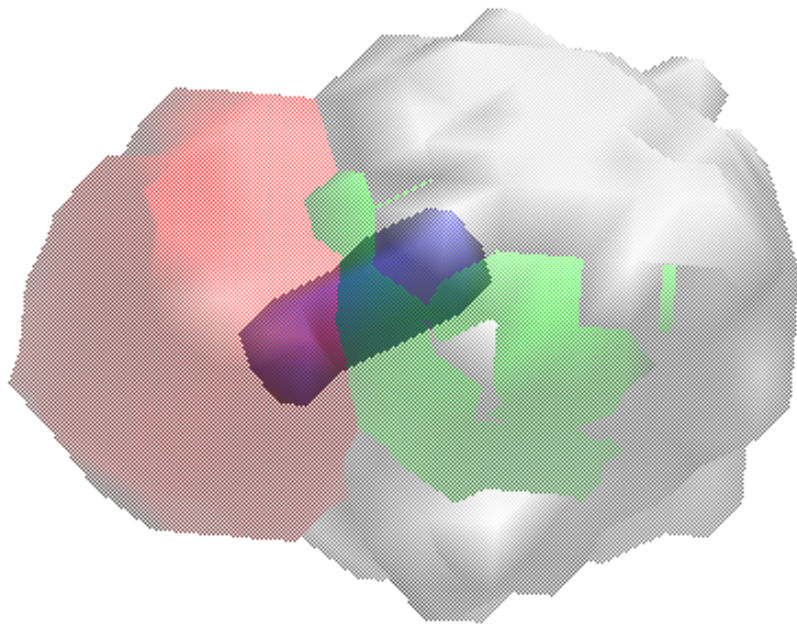
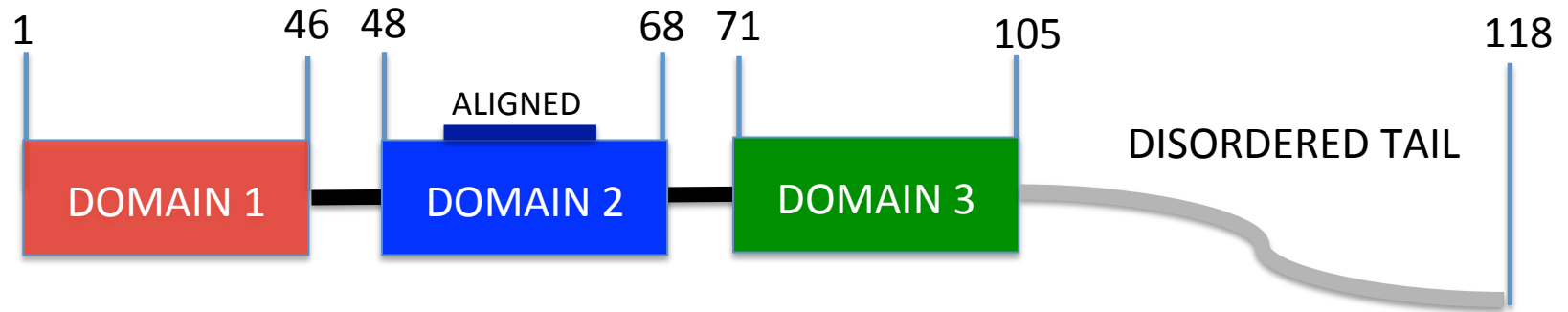
Wrote total cube data to : all_1/density/dbd_calpha_6.0_equalweights_complete.cube
Wrote cube data to : all_1/density/dbd_calpha_6.0_equalweights_region_1.cube
Wrote cube data to : all_1/density/dbd_calpha_6.0_equalweights_region_2.cube
Wrote cube data to : all_1/density/dbd_calpha_6.0_equalweights_region_3.cube
Wrote cube data to : all_1/density/dbd_calpha_6.0_equalweights_region_4.cube

=====
```

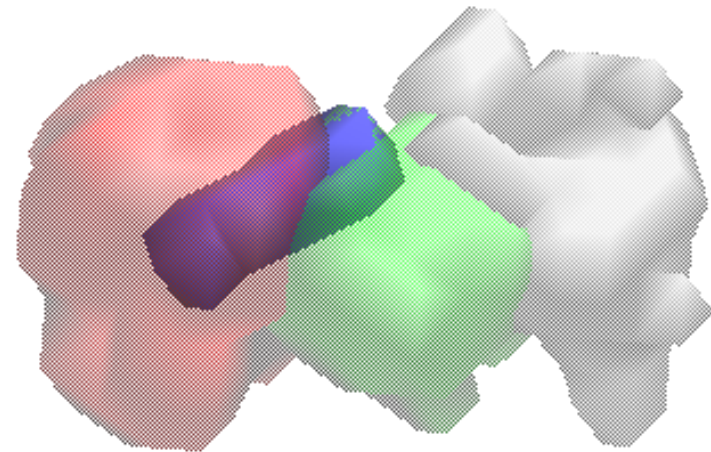
Run Density Program

100 %

# Density Plots

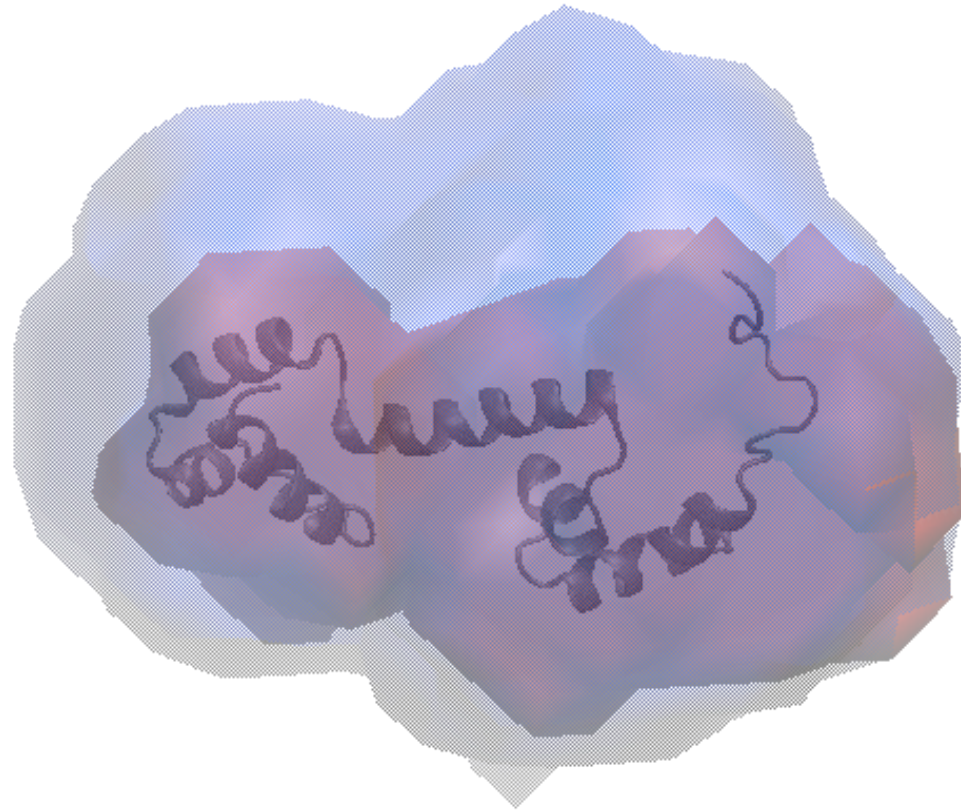


**Equal weights**



**Unequal weights**

# Density Plots



# References;

## **Xtal2sas;**

[Krueger S, Gorshkova I, Brown J, Hoskins J, McKenney KH, Schwarz FP.](#)

Determination of the conformations of cAMP receptor protein and its T127L,S128A mutant with and without cAMP from small angle neutron scattering measurements. (1998) *J Biol Chem.*, 273(32):20001-6.

## **Cryson;**

Svergun D.I., Richard S., Koch M.H.J. Sayers Z., Kuprin S., & Zaccai (1998) Protein hydration in solution: experimental observation by X-ray and neutron scattering *Proc. Natl. Acad. Sci. USA*, **95**, 768-773.S

## **Links;**

NIST Center for Neutron Research (NCNR)/ National Science Foundation (NSF)  
Summer School on Modeling Neutron Data for Biological Systems

[http://www.ncnr.nist.gov/summerschool/ss11/index\\_model.html](http://www.ncnr.nist.gov/summerschool/ss11/index_model.html)

SASSIE program webpage;

<http://www.smallangles.net/sassie/>