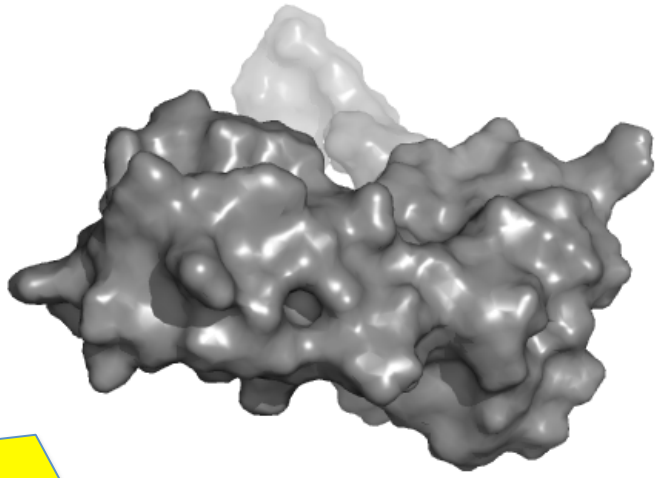
# SASSIE Tutorial

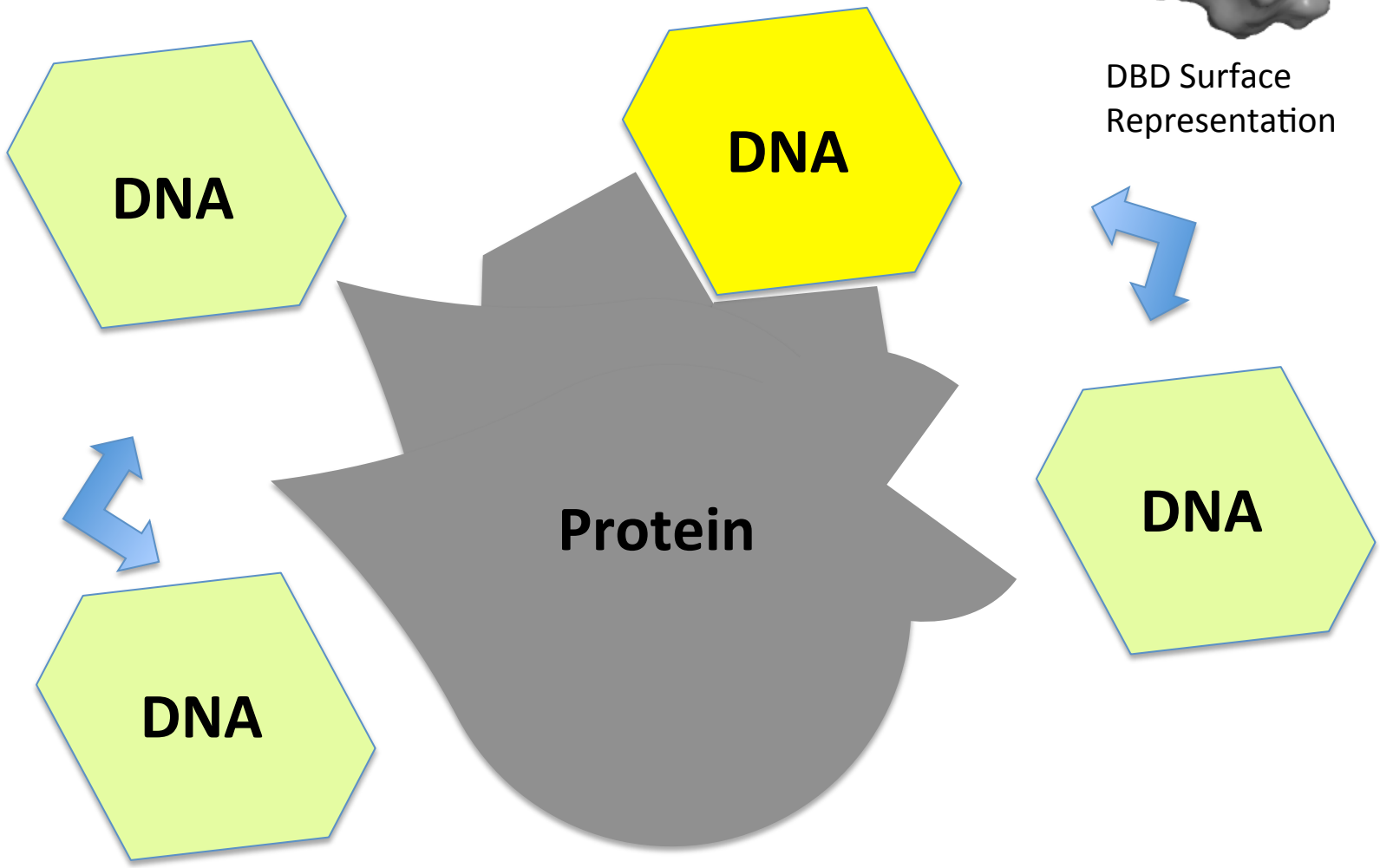
ACNS 2012

Presented By
Nicholas Clark and Hailiang Zhang

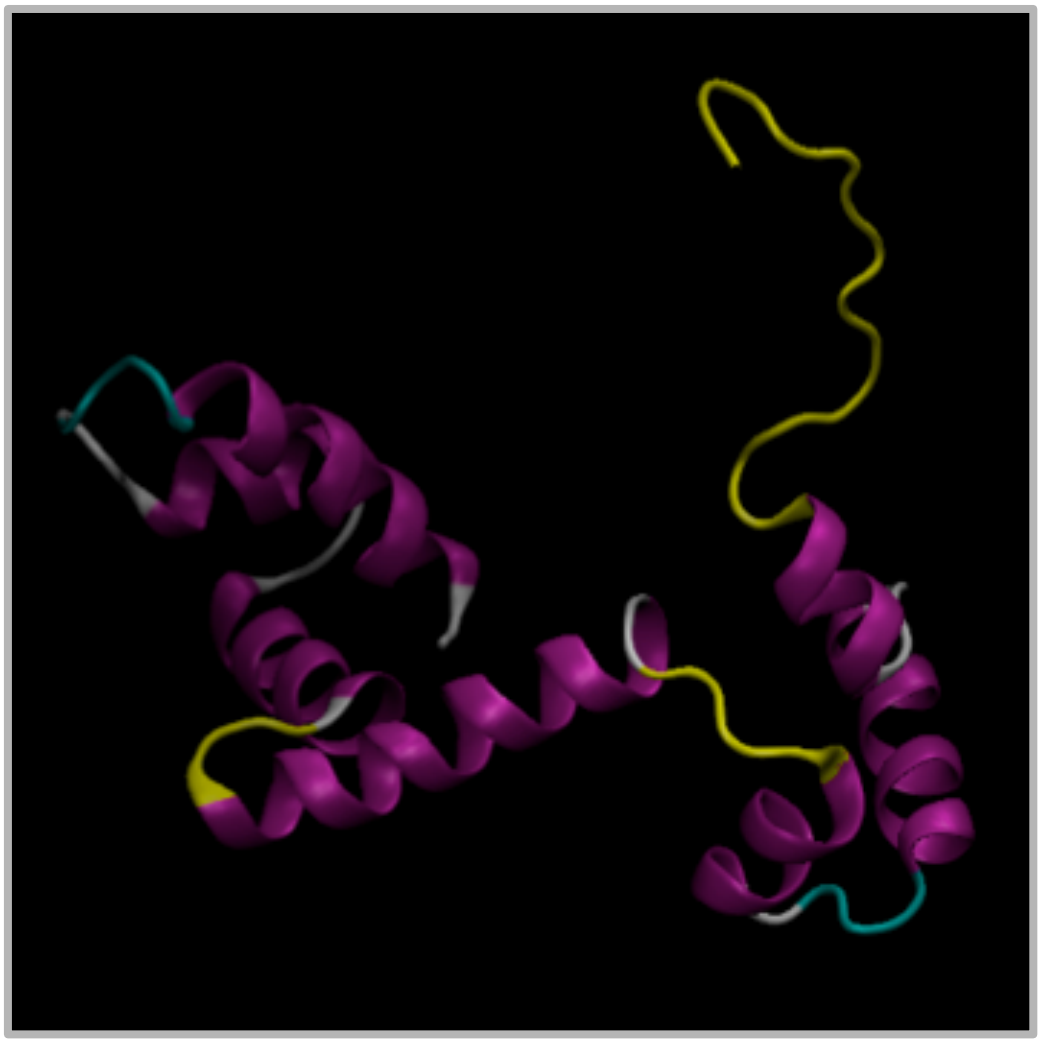
# FFT Docking



DBD Surface Representation

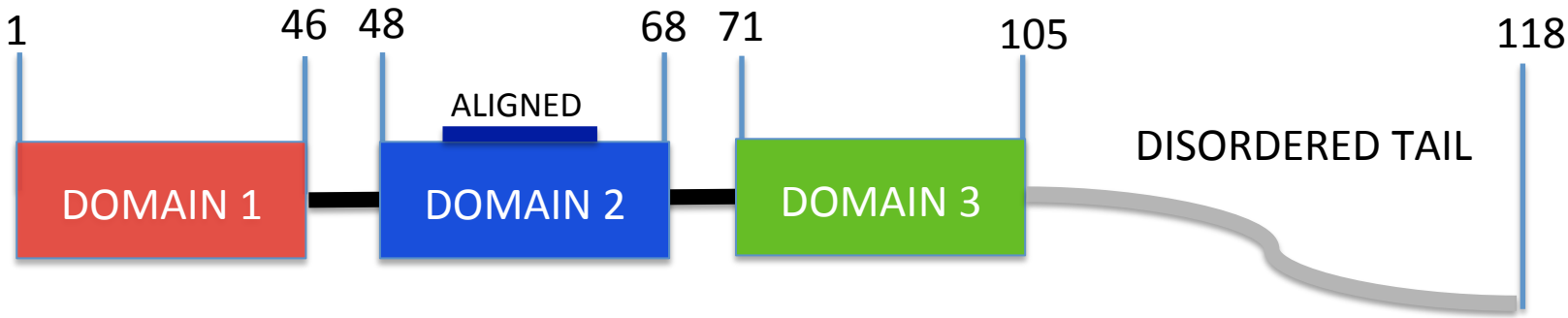


# Tutorial Example

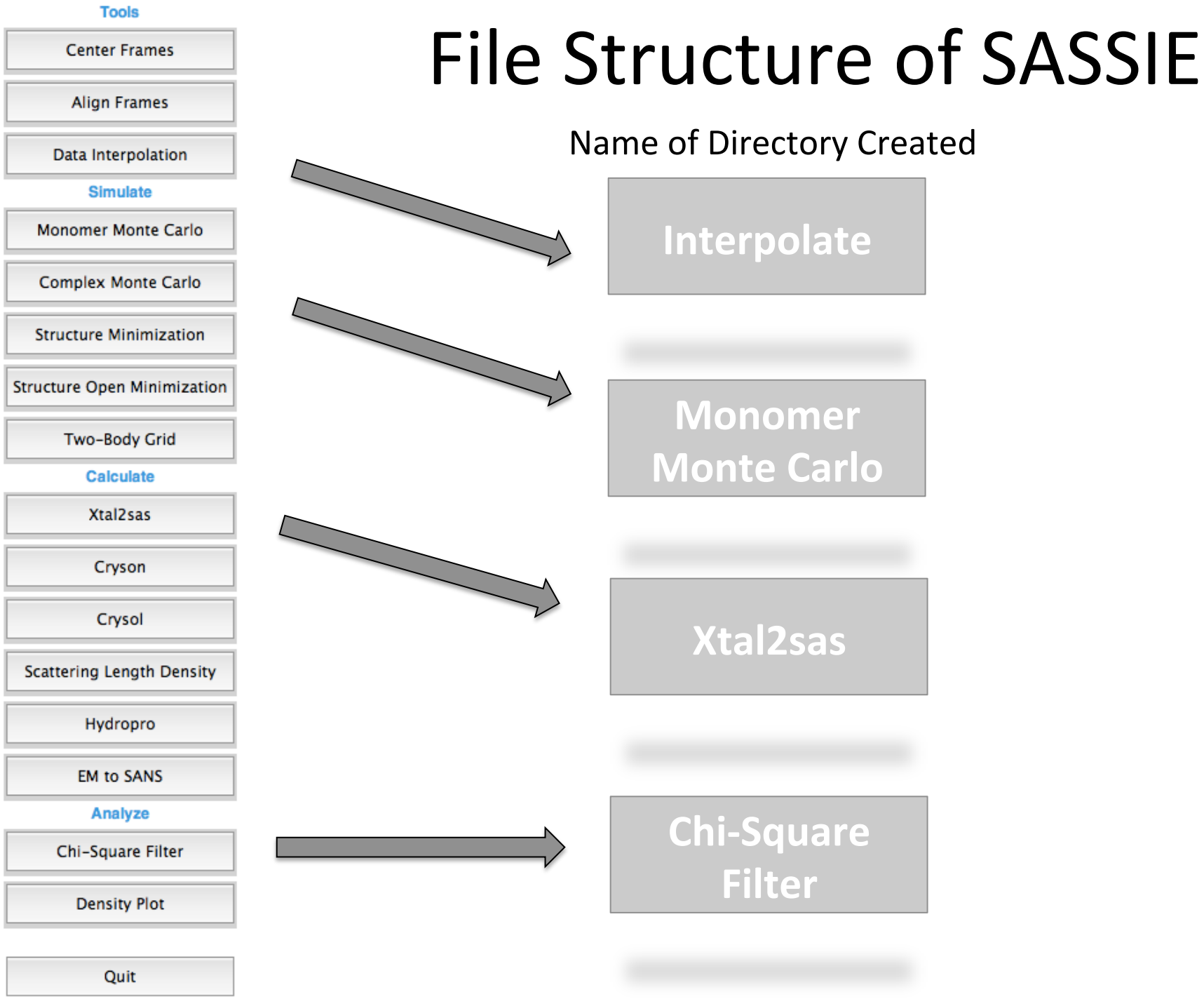


BDB Protein

# BDB Protein Domain Organization



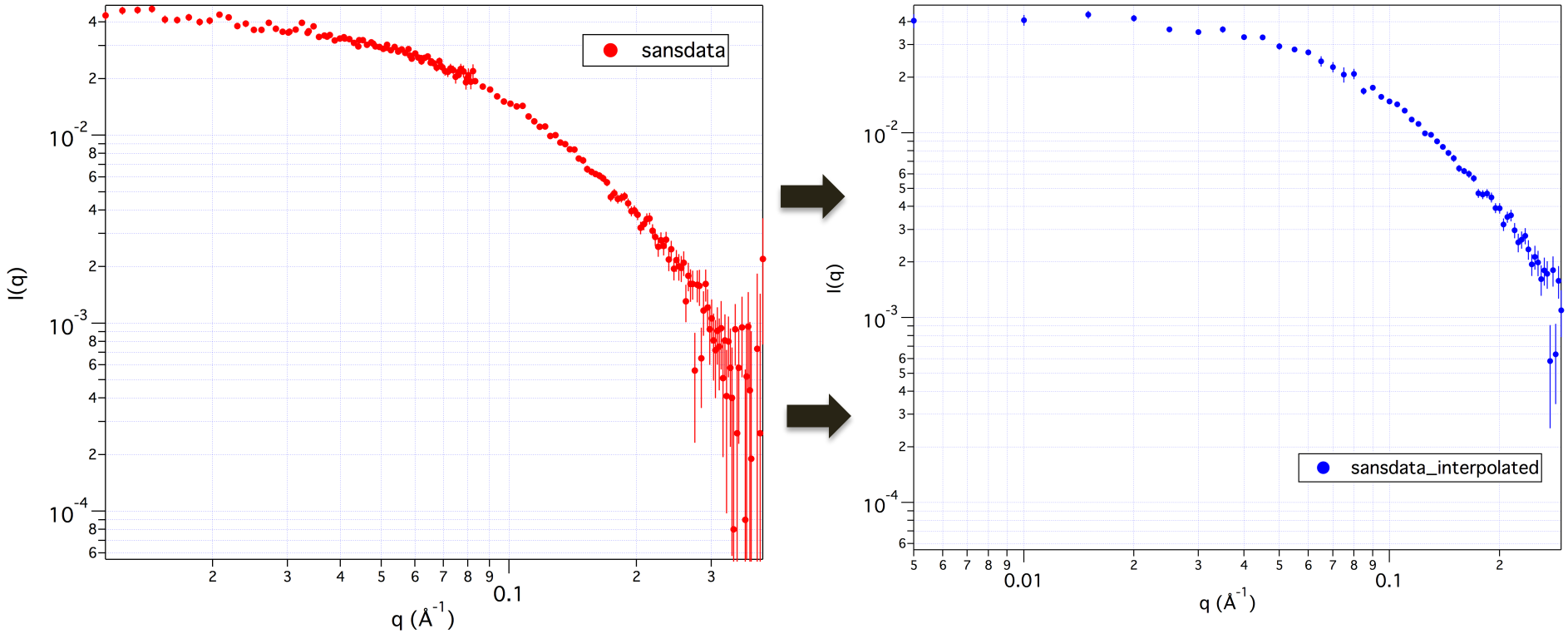

# File Structure of SASSIE



# Data Interpolation

Data Interpolation

| | | | |
|---|---|---|---|
| project name : | data | input file path : | ./ |
| input filename : | sansdata.sub | output filename : | sansdata.dat |
| I(0) : | 0.042 | I(0) error : | 0.001 |
| new delta q : | 0.005 | number of new points : | 60 |



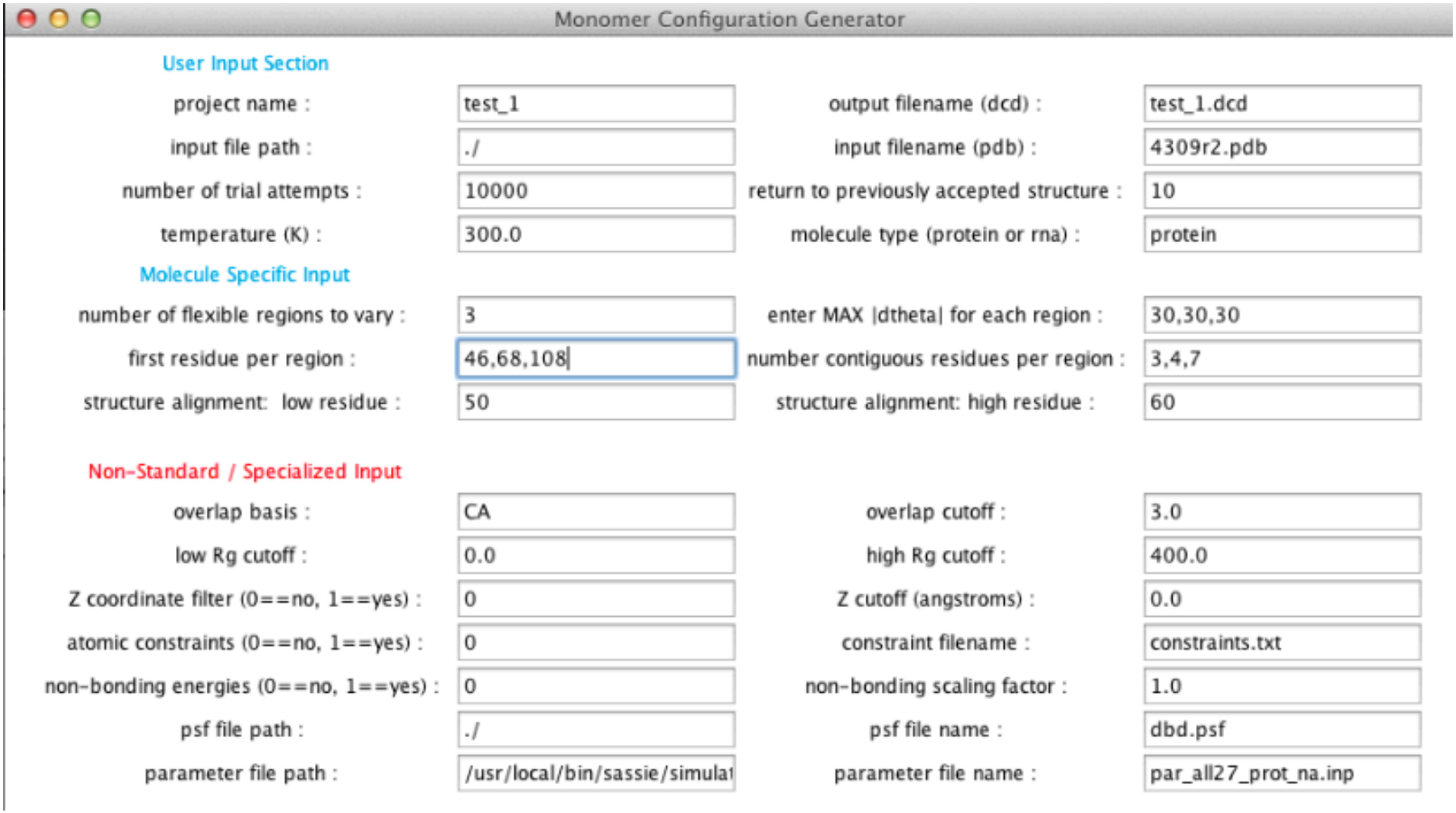
# Starting Structure of Bdb Protein

Residues
105-118

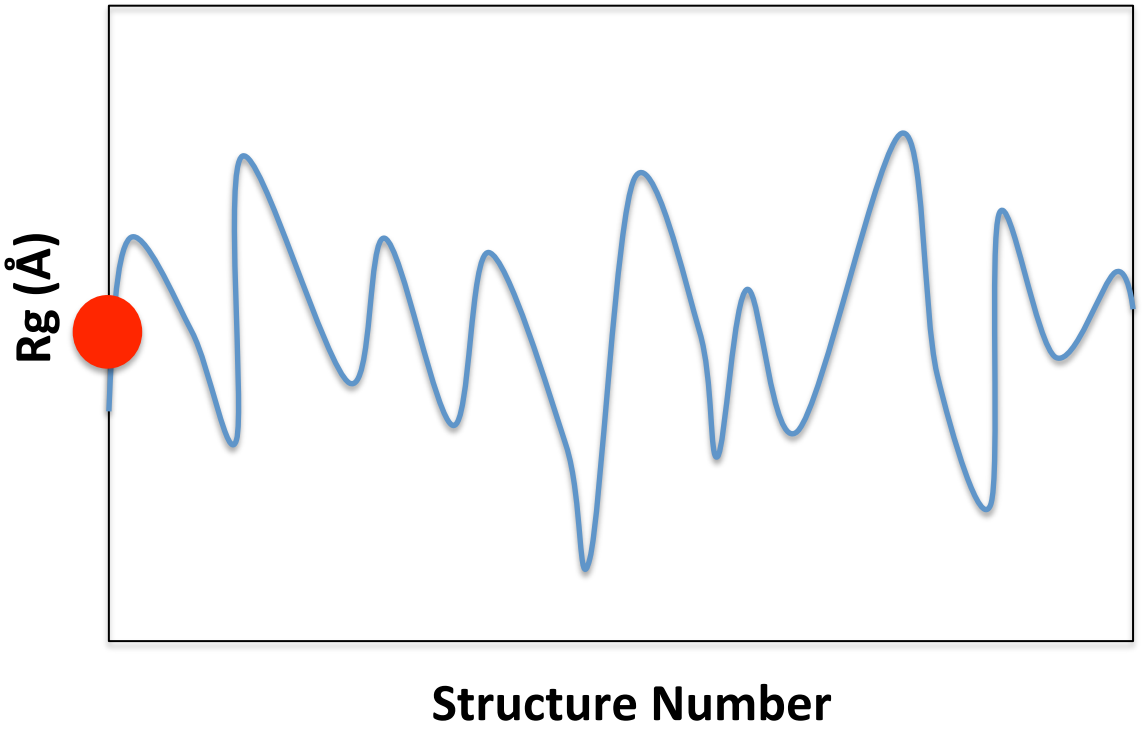
Residues
68-71

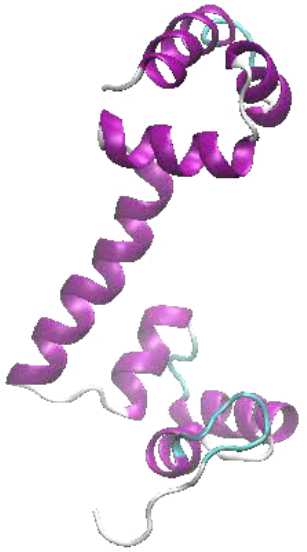
Residues
46-48

# Monte Carlo Configuration Generator



# Monte Carlo Configuration Generator



# Xtal2sas; SANS Curve Calculator

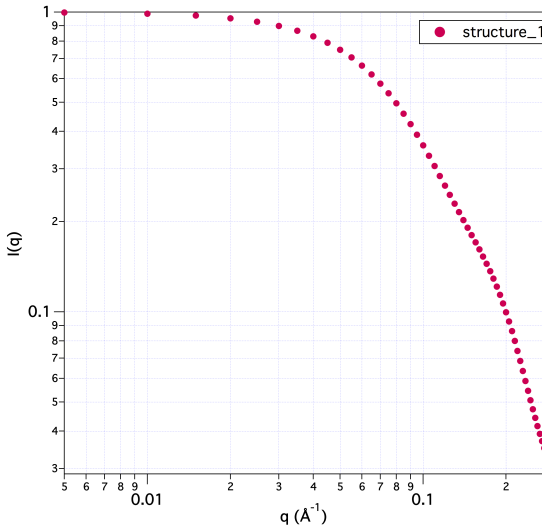
Xtal2Sas

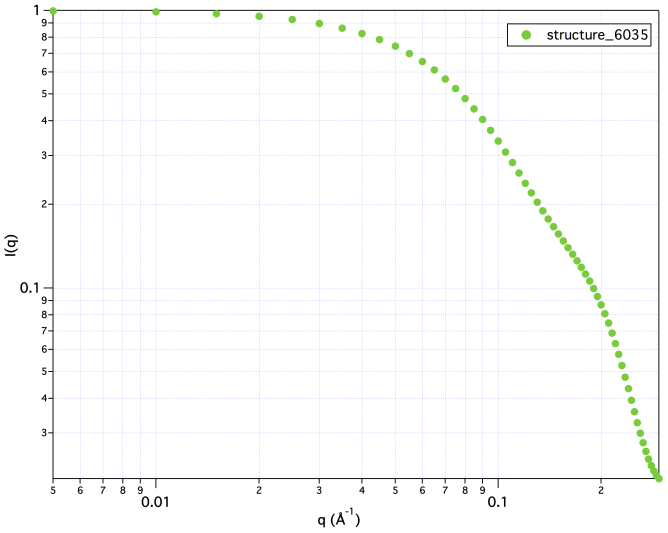
**Data Management Section**

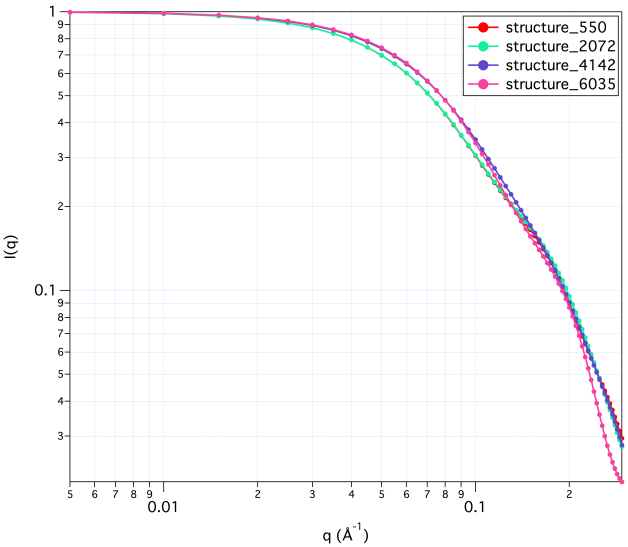
| | | | |
|---|---|---|---|
| project name : | test_1 | | |
| DCD input file path : | ./test_1/generate/ | input filename (dcd) : | test_1.dcd |
| PDB input file path : | ./test_1/generate/ | input filename (pdb) : | 4309r2.pdb |
| xtal2sas executable name (v4) : | /usr/local/bin/xtal2sas.exe | delete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

**Xtal2sas Input Section**

| | | | |
|---|---|---|---|
| X-rays or Neutrons (X/N): | N | number of I(Q) values : | 60 |
| maximum Q value : | 0.3 | Intensity at I(0) : | 1.0 |
| number output iterations : | 1 | number of hits : | 1000 |



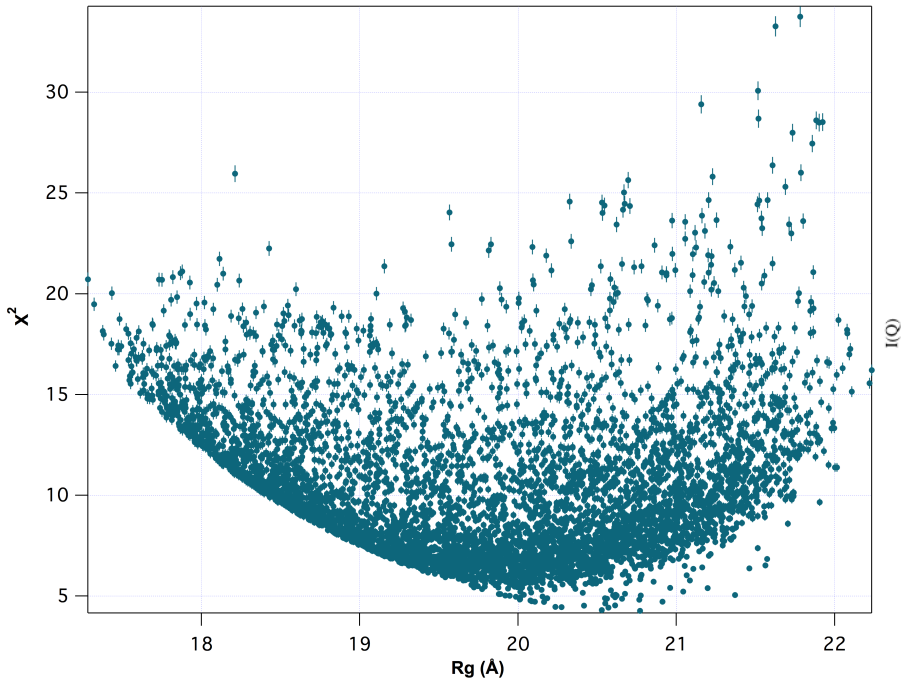



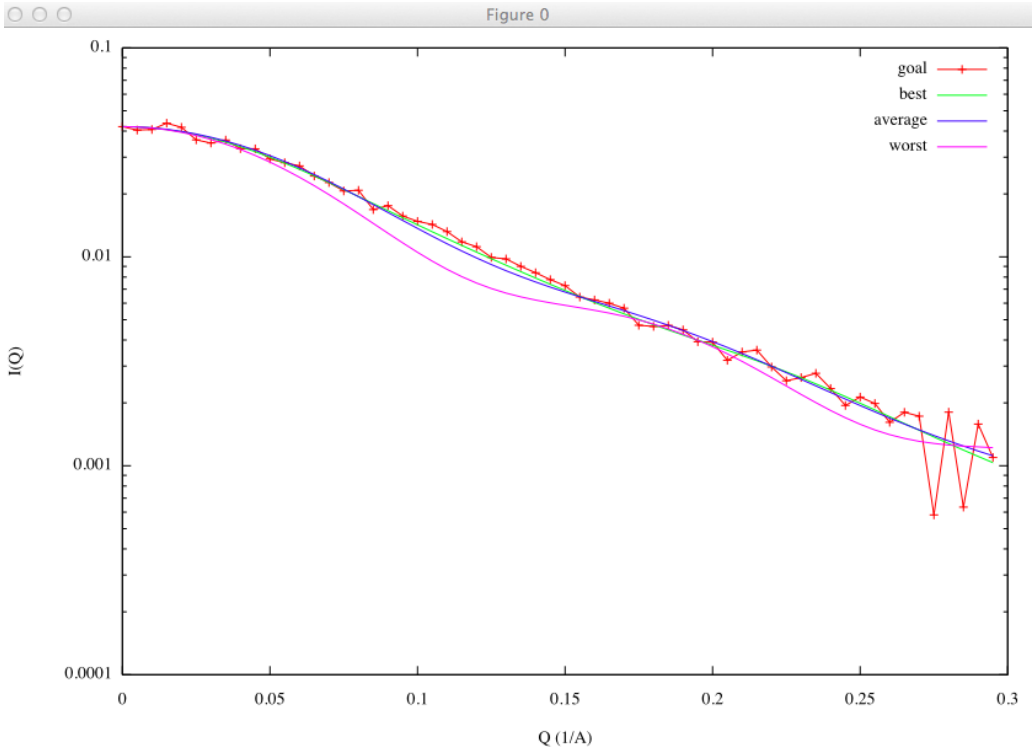

Krueger, S., Groshkova, I., Brown, J., Hoskins, J., McKenney, K. H. & Schwarz, F. P. (1998). J. Biol. Chem. 273, 20001–20008.

# $X^2$ Filtering

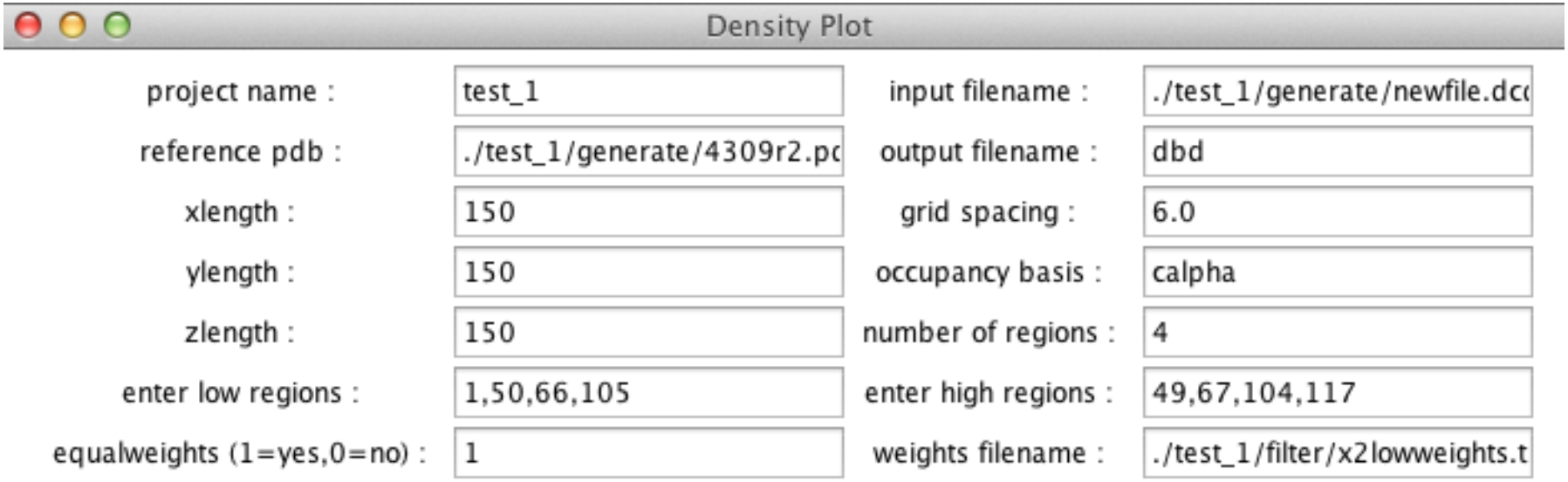
Chi-Square Filter

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

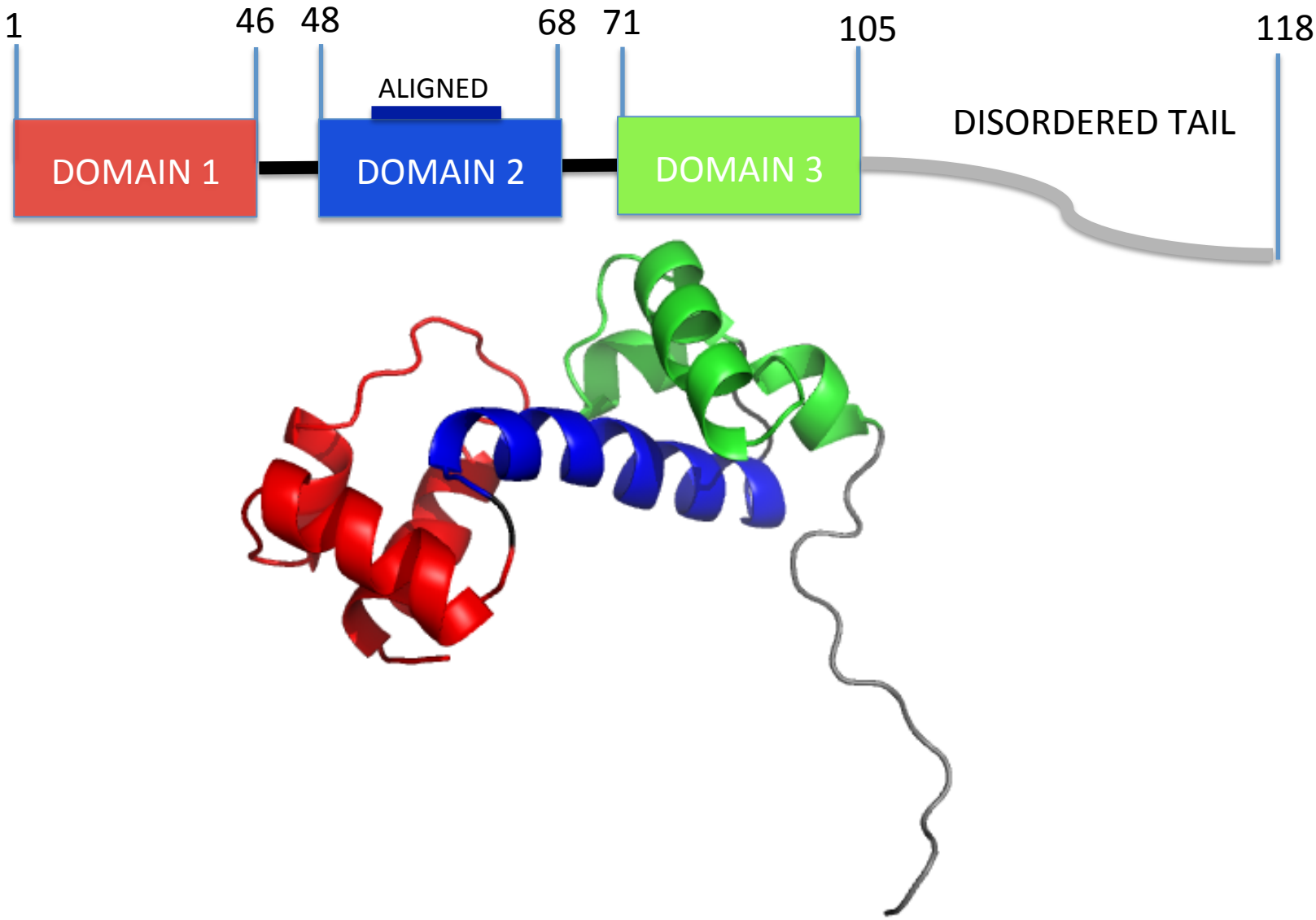


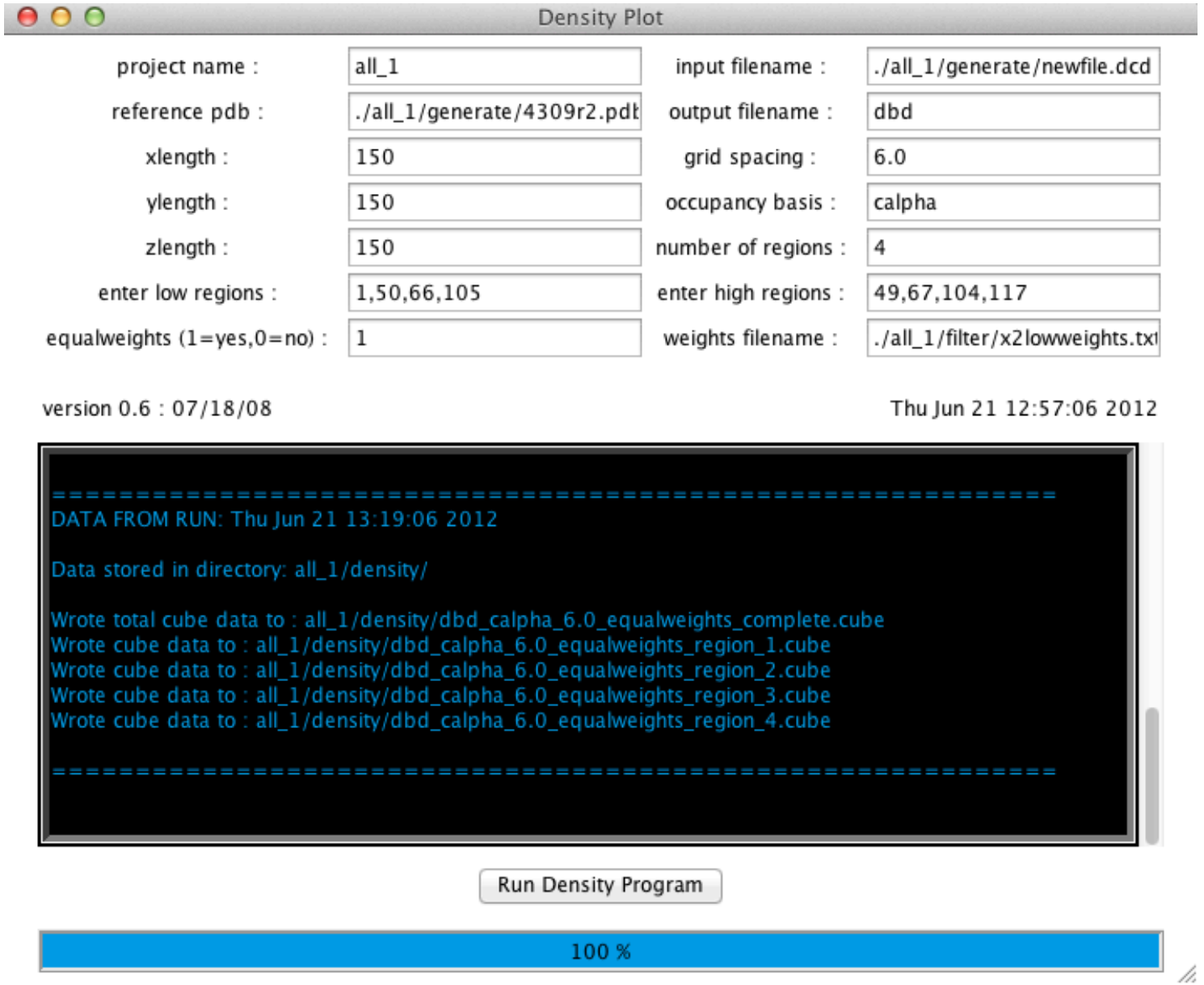
# Density Plots



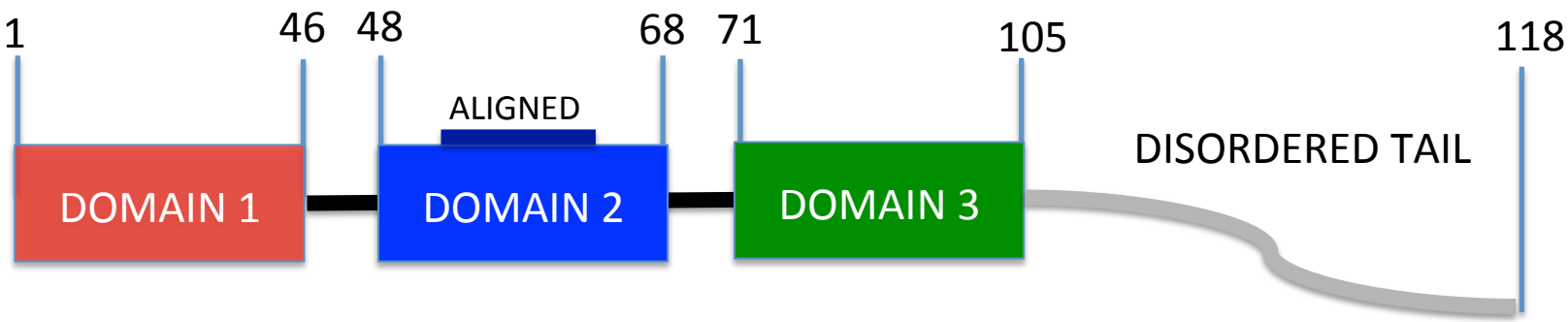
# BDB Protein

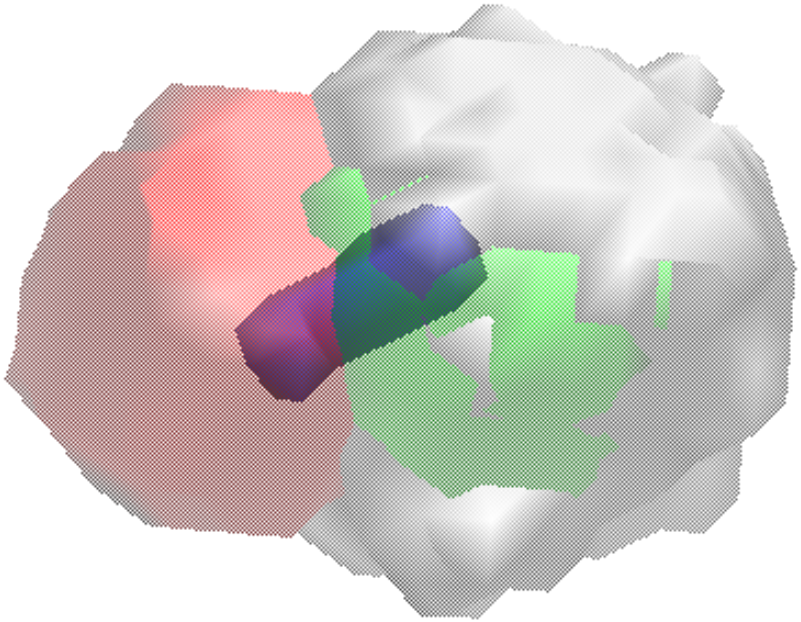

1
46
48
68
71
105
118
ALIGNED
DOMAIN 1
DOMAIN 2
DOMAIN 3
DISORDERED TAIL

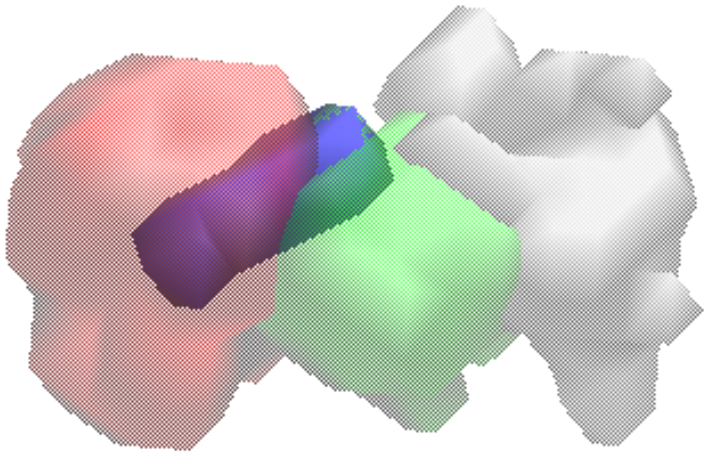
# Density Plots



# Density Plots



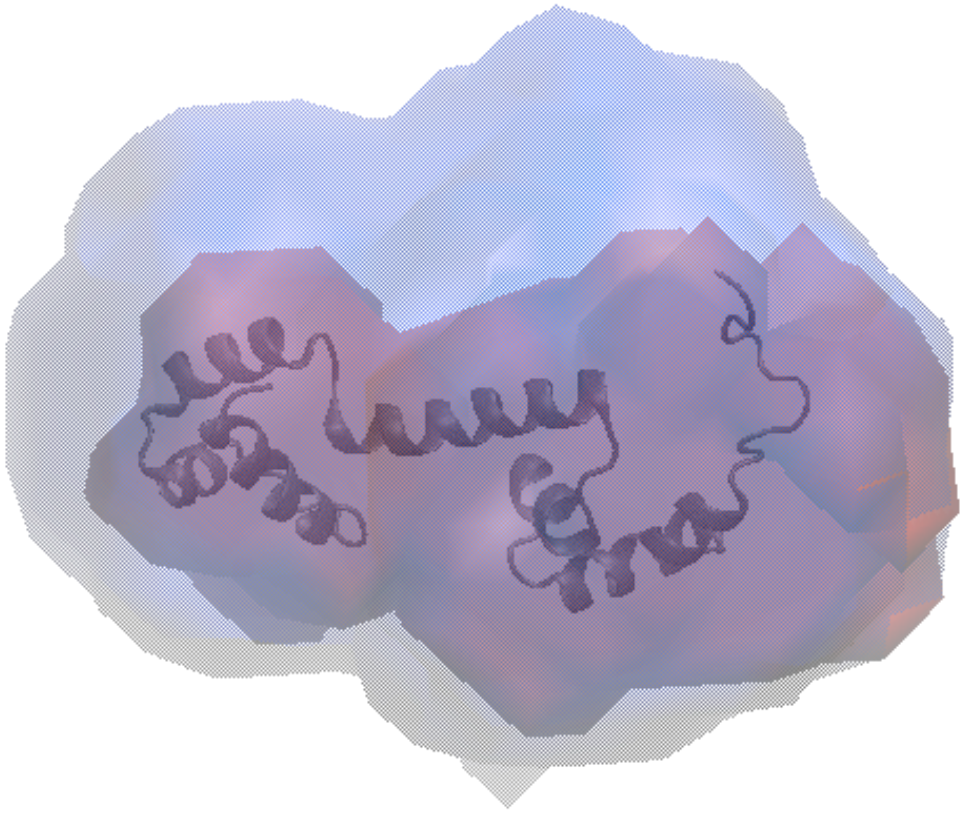





**Equal weights**

**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

SASSIE program webpage;

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