BIOISIS.net Data Deposit Ready Form

SAXS Data Deposit Form Prep List

Use this form to organize the relevant information for depositing your SAXS data into BIOISIS.net.
If you need additional information or have questions, email rprambo@lbl.gov

items

1 **Title** (short)

2 **Description** (summary describing experiment, see example below)

SAXS profile of the P4-P6 domain. Refolding of the RNA produces folding artifacts that must be removed from the sample prior to SAXS data collection. In this case, the samples were thermally refolded and purified by size-exclusion chromatography immediately prior to SAXS analysis. Sample homogeneity was assessed using multi-angle light scattering methods during chromatographic separation.

3 **Where did you collect the data?**
e.g., ALS, APS, BL 12.3.1

4 **Publication**
e.g., Crystal Structure of the Lysine Riboswitch Regulatory mRNA Element, Journal of Biological Chemistry, Vol. 283, 22347-22351

OPTIONAL: if no publication, please describe purpose of the experiment in the description.
NOTE: Authors are added in a separate section.

SAXS Data Deposit Form Prep List

Experimental Conditions

5	**X-ray wavelength** *...in Angstroms,* Å	
6	**Experimental Details (**How the data was measured?)	

e.g., Data was collected as a 2/3rds dilution series starting at 3 mg/mL using dialyzed samples and extrapolated to zero concentration using the method of Zimm.

7	**Buffer** *...i.e., 20 mM MES, MOPS, HEPES, etc*	
8	**pH**	
9	**Temperature, °C**	
10	**type of monovalent salt**	
11	**salt concentration, mM**	
12	**Divalent**	
13	**Divalent Concentration, mM**	
14	**Additives? (**Please provide additional information here, such as glycerol, detergent, etc.)	

Experimental SAXS Parameters

15	**I(zero)** *...from Guinier approximation*	
16	**error I(zero)** *...in Angstroms*	
17	**Proposed Molecular Weight, ...** *in Da*	
18	**D_{max}** *...in Angstroms,* Å	
19	**Guinier R_g** *...in Angstroms,* Å	
20	**error Guinier R_g** *...in Angstroms,* Å	

SAXS Data Deposit Form Prep List		
21	**real space R_g** *...in Angstroms,* Å	
22	**error real space R_g** *...in Angstroms,* Å	
23	**Porod Volume** *...in Angstroms³,* Å³	
24	**Scattering Data File** (A 3 column text file: q, intensity, error) If you would like to upload all your data from several concentrations, use a concatenated file separating each scattering data set with a # symbol.	
25	**Pair Distribution Data File** (A 3 column text file: distance, count, error)	
26	**Transformation Method** (Please specify either GNOM, GIFT, Moore, etc.)	

Macromolecular Sequence(s)

27 The SAXS experiment will involve a biopolymer (DNA, RNA and protein), please upload the sequence for each biopolymer using single letter abbreviations. Where appropriate, please provide the GI accession number.

In addition, each sequence should have a brief annotation, *e.g., 35 kDa C-terminal helicase domain of WRN protein.*

Model(s)

Deposited SAXS data must be accompanied by one or more models listed below. Please make the appropriate choice for your data. You are allowed to upload more than one type of model during a single deposit such as a DAMMIN and GASBOR model.

a. DAMMIN/F Model
   - *ab initio* model from DAMMIN or DAMMIF

b. GASBOR Model
   - *ab initio* model from GASBOR

c. Structural Model
   - atomistic model, typically from a homology model or a crystal structure.

d. Ensemble Model
   - atomistic models derived from MD or normal mode analysis.

e. No Model
   - choose this model if you do not have a structural PDB model for your data.

SAXS Data Deposit Form Prep List

a. **DAMMIN/F Model**

Symmetry Group *...P1, P2, etc*	
Chi Square *... χ^2 fit for the best single model*	
Single Model (non averaged DAMMIN/F PDB file)	
Averaged Model (output PDB file from DAMAVER)	
Superpositioned Hi-Res PDB Model (optional)	
NSD (normalized spatial descrepancy) *...calculated from DAMAVER*	
Number of Models Used in Averaging	

b. **GASBOR Model**

Symmetry Group *...P1, P2, etc*	
Chi Square *... χ^2 fit for the best single model*	
Single Model (non averaged GASBOR PDB filel)	
Averaged Model (output PDB file from DAMAVER)	
Superpositioned PDB Model (optional)	
NSD (normalized spatial descrepancy) *...calculated from DAMAVER*	
Number of Models Used in Averaging	

c. **Structural Model**

PDB File (single hi-resolution model)	
Description ...how was the model derived? Homology? X-ray?	
Chi Square *... $\chi 2$ fit for the model to the SAXS data*	
Fit File (A 2 column text file: q, calculated I)	

SAXS Data Deposit Form Prep List

d. **Ensemble Model**

Fit File (A 2 column text file: q, calculated I)	
Selection Method *...e.g, genetic algorithm, EOM, MES, etc*	
Simulation Software *...e.g, CNS, CHARM, GAJOE*	
Simulation Algorithm *...e.g., limited torsion angle dynamics, normal modes, etc*	
Ensemble Size (starting ensemble size)	
Member Size (final size of the selected ensemble)	
Chi Square	
Diagnostic File (*.png or *.gif file describing the selection such as a histogram or chevron plot)	
PDB FIles (PDB files of the selected members)	

e. **No Model**

Description

If no reasonable structural model is available but you would like to report your SAXS data i.e., the protein is completely unfolded, please use this form and provide a concise conclusion to the data.

Example:

The protein is conformationally flexible existing in multiple conformations, or is a mixture at this pH but appears to be stabilized by ATP.

Figure File Figure supporting your hypothesis such as a native gel, DLS data, MALS, etc in *.gif or *.png format. The file should not be larger than width 600 px by height 500 px	