

# Ab initio modelling: Guided tutorial

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# Ressources: Atsas help - Sasdoc

SASDOC - ATASAS Documentation

File Edit View Go Bookmarks Help

Contents

ATASAS manuals

Index Bookmarks Search

Look for:

adjust  
almerge  
alpraxin  
ambimeter  
anisometry  
autorg  
average  
bodies  
bunch  
coral  
crysol  
crysol3  
cryson  
damaver  
damclust  
damesv  
damfilt  
dammif  
dammin  
damsel  
damstart

Open Pages

monsa

Written by D.I. Svergun. Contribution of M.V. Petoukhov.  
Post all your questions about MONSA to the [ATASAS Forum](#).  
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## Table of Contents

- [Manual](#)
  - [Introduction](#)
  - [Running MONSA](#)
    - [Interactive Configuration](#)
    - [Runtime Output](#)
  - [MONSA Input Files](#)
  - [MONSA Output Files](#)
  - [DAMESV](#)
    - [Running DAMESV](#)
- [Example](#)

## Manual

The following sections shortly describe the [method implemented in MONSA](#), usage in [dialog mode](#) as well as the required [input](#) and the produced [output files](#).

MONSA implements the algorithm described by:

[D.Svergun \(1999\) Restoring low resolution structure of biological macromolecules from solution scattering using simulated annealing. \*Biophys. J.\* 76, 2879-2886.](#)

[Svergun, D.I. & Nierhaus, K.H. \(2000\) A map of protein-rRNA distribution in the 70S Escherichia coli ribosome. \*J. Biol. Chem.\* 275, 14432-14439.](#)

The users are referred to these papers for details.

## Introduction

MONSA is an extended version of [DAMMIN](#) for multiphase bead modelling which allows one to fit simultaneously multiple curves (e.g. from X-ray and/or neutron contrast variation series).

## Running MONSA

MONSA reads in multiple data sets and information about the contrasts and volume fractions of the phases in a particle. The program can simultaneously fit data recorded at different instrumental settings and also with different radiations (e.g. X-rays and neutrons). The structure of the [input data](#) is therefore somewhat complicated.

The program requires:

1. a [MASTER file](#) (file \*.mst) containing the general phase information and references to CONTROL file(s);
2. [CONTROL file\(s\)](#) (\*.con) containing the smearing information for the given setting, information about contrasts and references to DATA files (\*.dat);
3. [DATA files](#) (\*.dat), containing raw experimental data at different contrasts;

# Ressources: Saxier forum

- [www.saxier.org/forum/](http://www.saxier.org/forum/)

SAXS - Index page

https://www.saxier.org/forum/

**saxier**  
SAXS  
Small Angle X-ray Scattering Initiative for Europe :: Forum

Search...

Quick links FAQ

Board index

Unanswered topics Active topics

It is currently 2019.09.17 14:53

General	Topics	Posts	Last post
<b>Announcements</b> Courses and workshops, new software releases	35	69	<b>Re: Help save SSR</b> by bmoers 2019.08.27 14:22
<b>SAS Hardware/Instrumentation</b> Detectors, sample changers, home sources, nanomanipulation tools, add-ons (Raman spectrometer, HPLC), gas phase scattering etc.	14	46	<b>X33 beam size: 2x0.6 mm<sup>2</sup></b> by AL 2017.08.14 11:41
<b>SAS Experiment Design</b> Plan your small angle X-ray or neutron scattering measurements	16	43	<b>Re: Saxs xeuss 2.0</b> by pierre38 2018.10.01 17:39
<b>Literature</b> Books and reviews on small angle scattering. Discussions and criticism on recent SAXS papers.	18	44	<b>MW determination using SAXS</b> by akshayc 2015.08.10 08:49
<b>Feedback</b> Suggestions for new topics to discuss, questions on the use of the Forum	16	56	<b>Re: ATSAS online access</b> by cborges 2019.01.04 15:10

ATSAS	Topics	Posts	Last post
<b>FAQ</b> Frequently Asked Questions about ATSAS small-angle scattering analysis program package	7	23	<b>Re: convert ab initio model b...</b> by SaxeMax 2014.07.16 11:18
<b>ATSAS Package in General</b> ATSAS for Linux and Mac, general installation issues, ATSAS online etc.	147	591	<b>Request for Python3 version o...</b> by bmoers 2019.08.27 14:37
<b>Primary Data Processing</b> Interactive and automated data processing tools (PRIMUS, GNOM, AUTORG). Scattering from simple bodies (BODIES), peak analysis (PEAK), data plotting (SASPLOTT) etc.	356	1271	<b>Re: pddffit</b> by AL 2019.08.20 13:33
<b>Ab initio Shape Determination</b> Ab initio modelling: DAMMIF, DAMMIN, GASBOR, MONSA	330	1102	<b>DAMMIN online runs only once</b> by AL 2019.07.31 10:19
<b>Rigid Body Modelling</b> Interactive modelling (MASSHA, SASpy) and global minimization programs (SASREF, BUNCH, CORAL, GLOBSYMM)	212	789	<b>SASpy</b> by AL 2019.04.25 14:46
<b>Mixtures and Flexible Systems</b> Linear (OLIGOMER) and non-linear (MIXTURE) analysis, singular value decomposition (SVDPLLOT), addition of missing fragments (BUNCH, CORAL), analysis of flexible systems (EOM/RANCH & GAJOE), flexible refinement of high-resolution models (SREFLEX)	322	1315	<b>Re: Oligomer online error - z...</b> by schmeing 2019.08.21 22:19
<b>Working with Models</b> Calculation of SAXS and SANS profiles (CRY SOL, CRYSON), superposition of models (SUPCOMB, DAMAVER, DAMCLUST), database DARA	222	726	<b>CRY SOL in fitting mode</b> by AL 2019.05.31 11:40

# Ressources: SASBDB – [www.sasbdb.org](http://www.sasbdb.org)

The screenshot shows the SASBDB website in a web browser. The browser's address bar displays <https://www.sasbdb.org>. The website header features the SASBDB logo, a search bar, and links for 'Sign in' and 'Register'. Below the header is a navigation menu with 'Home', 'Browse', 'Submit data', 'About SASBDB', and 'Help'. The main content area is titled 'Curated repository for small angle scattering data and models' and includes a brief description of the database. To the right, it states 'SASBDB currently contains: 1200 experimental data sets, 1764 models, 337 experimental data sets on hold, 592 models on hold'. Below this, a section titled 'Recent depositions:' highlights a specific entry: 'SASDGF3 – Xrn1 resistance RNA1 from Zika virus'. This entry includes a sample description, buffer details, experiment information, and a table of structural parameters. At the bottom, a row of five smaller entry cards is visible, each with a thumbnail image and a title.

Small Angle Scattering Biological Data Bank

Sign in | Register

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Advanced search E.g. SASDBF4, Lyz, Nucleic Acids Res

Home Browse Submit data About SASBDB Help

## Curated repository for small angle scattering data and models

Small angle scattering (SAS) of X-ray and neutrons provides structural information on biological macromolecules in solution at a resolution of 1-2 nm. SASBDB is a fully searchable curated repository of freely accessible and downloadable experimental data, which are deposited together with the relevant experimental conditions, sample details, derived models and their fits to the data.

**SASBDB currently contains:**  
1200 experimental data sets  
1764 models  
337 experimental data sets on hold  
592 models on hold

### Recent depositions:

#### SASDGF3 – Xrn1 resistance RNA1 from Zika virus

Sample:	Xrn1 resistance RNA2 from Zika virus monomer, 22 kDa <i>Zika virus</i> RNA	$R_g$ Guinier	2.4 nm
Buffer:	20mM Tris-HCl, 100mM NaCl, 5mM MgCl <sub>2</sub> , pH: 7.5	$D_{max}$	8.5 nm
Experiment:	SAXS data collected at 12ID-B SAXS/WAXS, Advanced Photon Source (APS), Argonne National Laboratory on 2016 Dec 9	Volume <sup>PoreD</sup>	34 nm <sup>3</sup>

Long non-coding subgenomic flavivirus RNAs have extended 3D structures and are flexible in solution *EMBO reports* (2019)  
Zhang Y, Zhang Y, Liu Z, Cheng M, Ma J, Wang Y, Qin C, Fang X

**SASDFD3 – Filamin A Ig-like d**  
Critical Structural Defects Expla

**SASDE79 – Interleukin-18 recs**  
Functional Relevance of Interleu

**SASDF86 – Human Galectin-1**  
Protein crystallization promotes

**SASDFD7 – Pseudomonas put**  
Structural and Mechanistic Insig

**SASDFD6 – Protein kinase Yor**  
Studying Conformational Chan

# Running atsas program - DAMMIN

C:\Users\blanchet\Documents\Presentations\tuto\_abinitio2020&gt;dammin

```

***      Ab initio shape determination by simulated      ***
***      annealing using a single phase dummy atoms model ***
***      Win 9x/NT, UNIX/Linux/Mac release version  5.3 ***
***      --- ***
***      Please reference: D.Svergun (1999). Biophys. J. ***
***                        76, 2879-2886. ***
***      Copyright (c) ATSAS Team ***
***      EMBL, Hamburg Outstation, 1999 - 2020 ***

```

Type dammin --help for batch mode use

===== DAMMIN started on 19-Jun-2022 16:40:20

```

Mode: <[F]>ast, [S]low, [J]ag, [K]eep,
[E]xpert ..... < Fast >: E
Log file name ..... < .log >: log_tuto
Input data, GNOM output file name ..... < .out >: SASDA96
Project identifier ..... : log_tuto
Enter project description ..... : Dammin tutorial
Initialized random seed as ..... : 258628215133905284
Data set title
Maximum diameter of the particle ..... : 4.800
Radius of gyration read ..... : 1.508
Number of GNOM data points ..... : 815
Angular units in the input file:
4*pi*sin(theta)/lambda [1/angstrom] (1)
4*pi*sin(theta)/lambda [1/nm ] (2) < 2 >:
Angular units multiplied by ..... : 0.100
Dmax and Rg divided by ..... : 0.100
Maximum s value [1/angstrom] ..... : 0.2288
Number of Shannon channels ..... : 3.496

```

Mode: how much do you want to tune the  
Fast (large beam, fast cool-down)  
Slow (smaller beads and slower cool-down)

Name of the gnom output file

Angular unit of the input file

```

Number of GNOM data points ..... : 815
Angular units in the input file:
4*pi*sin(theta)/lambda [1/angstrom] (1)
4*pi*sin(theta)/lambda [1/nm      ] (2) <          2 >:
Angular units multiplied by ..... : 0.100
Dmax and Rg divided by ..... : 0.100
Maximum s value [1/angstrom] ..... : 0.2288
Number of Shannon channels ..... : 3.496
Portion of the curve to be fitted ..... <          1.000 >:
Number of knots in the curve to fit .... <          20 >:
Constant subtraction procedure. Enter
Positive number: value to be subtracted, OR
Negative number: to skip subtraction , OR
Zero for automatic subtraction ..... <          0.000 >:
** Constant subtraction procedure skipped **
Maximum order of harmonics ..... <          20 >:
Initial DAM: type S for sphere [default],
E for ellipsoid, C for cylinder, P for parallelepiped
or start file name ..... <          .pdb >: S
Symmetry: P1...19 or Pn2 (n=1,..,12)
or P23 or P432 or PICO ..... <          P1 >:
Sphere diameter [Angstrom] ..... <          48.00 >:
Packing radius of dummy atoms ..... <          1.000 >:
Radius of the sphere generated ..... : 24.00
Number of dummy atoms ..... : 10192
Number of equivalent positions ..... : 1
Expected particle shape: <P>rolate, <O>blate,
or <U>nknown ..... <          Unknown >:
Excluded volume per atom ..... : 5.661
Radius of 1st coordination sphere ..... <          2.820 >:
Minimum number of contacts ..... : 7
Maximum number of contacts ..... : 13
Looseness penalty weight ..... < 2.0000E-003 >:

```

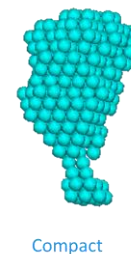
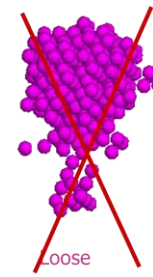
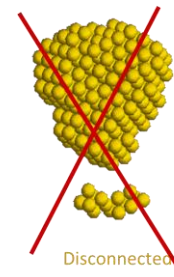
Input curve (unit, portion to be fitted, etc...)

Model (search volume, symmetry, bead size)

```

Sphere diameter [Angstrom] ..... < 48.00 >:
Packing radius of dummy atoms ..... < 1.000 >:
Radius of the sphere generated ..... : 24.00
Number of dummy atoms ..... : 10192
Number of equivalent positions ..... : 1
Expected particle shape: <P>rolate, <O>blate,
or <U>nknown ..... < Unknown >:
Excluded volume per atom ..... : 5.661
Radius of 1st coordination sphere ..... < 2.820 >:
Minimum number of contacts ..... : 7
Maximum number of contacts ..... : 13
Looseness penalty weight ..... < 2.0000E-003 >:
No of non-solvent atoms ..... : 10192
Initial DAM looseness ..... : 1.342E-03
Disconnectivity penalty weight ..... < 2.0000E-003 >:
Initial DAM # of graphs ..... : 1
Discontiguity value ..... : 0.0
Center of the initial DAM: 0.0000 0.0000 -0.0000
Peripheral penalty weight ..... < 0.3000 >:
Peripheral penalty value ..... : 0.6046
Fixing thresholds Los and Rf < 5.0000E-002, 2.0000E-002 >:
Randomize the structure [ Y / N ] ..... < Yes >:
No of non-solvent atoms ..... : 5116
Randomized DAM looseness ..... : 5.350E-02
Randomized DAM # of graphs ..... : 12
Discontiguity value ..... : 2.152E-03
Randomized peripheral penalty value ..... : 0.6026
Initial DAM shape anisotropy ..... : 7.217E-03
Initial DAM non-prolateness ..... : 5.555E-03
Initial DAM non-oblateness ..... : 0.0
Weight: 0=s^2, 1=Emphas.s->0, 2=Log .... < 1 >:
*** Porod weight with emphasis at low s ***
Initial scale factor ..... < 1.3056E-006 >:

```

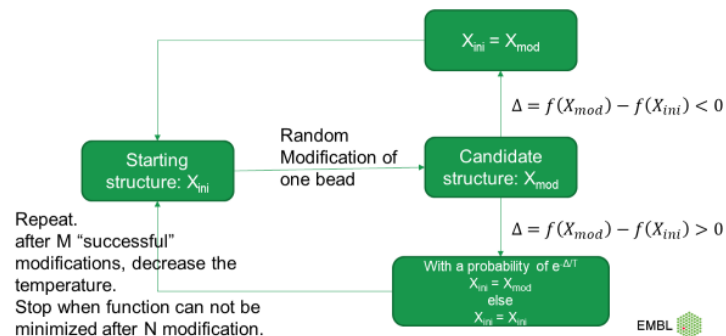


Penalty terms



```
Initial DAM non-oblateness ..... : 0.0
Weight: 0=s^2, 1=Emphas.s->0, 2=Log .... < 1 >:
*** Porod weight with emphasis at low s ***
Initial scale factor ..... < 1.3056E-006 >:
Fix the scale factor [ Y / N ] ..... < No >:
Initial R^2 factor ..... : 0.2315
Initial R factor ..... : 0.4811
Initial penalty ..... : 0.1809
Initial fVal ..... : 0.4124
Tuning the annealing parameters. Please wait...
Variation of the target function ..... : 7.469E-05
CPU per function call, seconds ..... : 1.094E-03
Initial annealing temperature ..... < 1.0000E-003 >:
Annealing schedule factor ..... < 0.9500 >:
# of independent atoms to modify ..... < 1 >:
Max # of iterations at each T ..... < 713440 >:
Max # of successes at each T ..... < 71344 >:
Min # of successes to continue ..... < 237 >:
Max # of annealing steps ..... < 200 >:
==== Simulated annealing procedure started ====
j: 1 T: 0.100E-02 Suc: 71344 Eva: 73689 CPU: 0.817E+02 SqF: 0.6273
Rf: 0.46553 Los:0.0519 Dis:0.0024 Per: 0.5891 Sca: 0.129E-05
j: 2 T: 0.950E-03 Suc: 71344 Eva: 147449 CPU: 0.163E+03 SqF: 0.6212
Rf: 0.46657 Los:0.0522 Dis:0.0035 Per: 0.5898 Sca: 0.127E-05
j: 3 T: 0.903E-03 Suc: 71344 Eva: 221346 CPU: 0.244E+03 SqF: 0.6096
Rf: 0.46121 Los:0.0545 Dis:0.0035 Per: 0.5866 Sca: 0.130E-05
j: 4 T: 0.857E-03 Suc: 71344 Eva: 295383 CPU: 0.326E+03 SqF: 0.6034
Rf: 0.46144 Los:0.0570 Dis:0.0020 Per: 0.5873 Sca: 0.135E-05
j: 5 T: 0.815E-03 Suc: 71344 Eva: 369539 CPU: 0.407E+03 SqF: 0.5980
Rf: 0.46265 Los:0.0562 Dis:0.0028 Per: 0.5868 Sca: 0.133E-05
j: 6 T: 0.774E-03 Suc: 71344 Eva: 443803 CPU: 0.488E+03 SqF: 0.5901
Rf: 0.46053 Los:0.0551 Dis:0.0020 Per: 0.5859 Sca: 0.132E-05
```

## Simulated annealing



Simulated annealing parameters

# DAMMIF command line

- For all atsas program: Use --help in command line to see available options

```
Administrator: C:\WINDOWS\system32\cmd.exe
C:\Users\blanchet\Documents\Presentations\tuto_abinitio2020>
C:\Users\blanchet\Documents\Presentations\tuto_abinitio2020>dammit --help
Usage: dammit [OPTIONS] <GNOMFILE>

rapid ab-initio shape determination in small-angle scattering

Known Arguments:
  GNOMFILE                GNOM output file with the data to fit

Known Options:
  -h, --help              Print usage information and exit
  -v, --version            Print version information and exit
  -q, --quiet             Reduce verbosity level
  --seed=<INT>            Set the seed for the random number generator
  -c, --chained            enable building of pseudo-chains in PDB output
  -u, --unit=<UNIT>        ANGSTROM, NANOMETRE or UNKNOWN (default: unknown)
  -p, --prefix=<PREFIX>   the PREFIX to prepend to any output filename (default: dammit)
  -a, --anisometry=<O|P>  Particle anisometry (Oblate/Prolate)
  --shape=<SHAPE>         Expected particle shape (default: use classifier)
  -s, --symmetry=<PXY>    Particle symmetry
  -m, --mode=<MODE>       one of: FAST, SLOW, INTERACTIVE (default: interactive)
  --omit-solvent           omit output of solvent in PREFIX-0.pdb
  --constant=<VALUE>      constant to subtract, 0 to disable constant subtraction (automatic if undefined)
  --max-bead-count=<VALUE> maximum number of beads in search space (unlimited if undefined)

Mandatory arguments to long options are mandatory for short options too.

Report bugs to <atsas@embl-hamburg.de>.

C:\Users\blanchet\Documents\Presentations\tuto_abinitio2020>
```

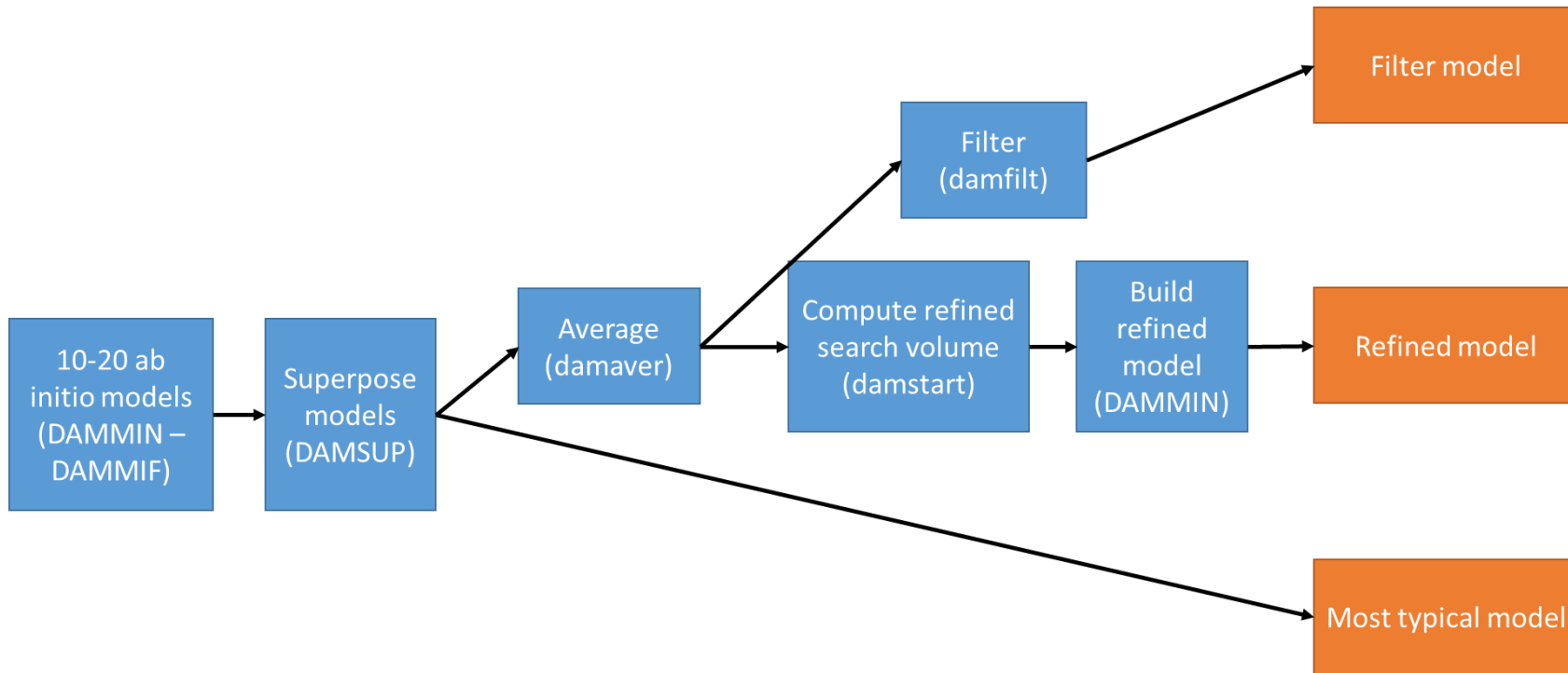
dammit lys.out --mode=slow --prefix lys1

# windows

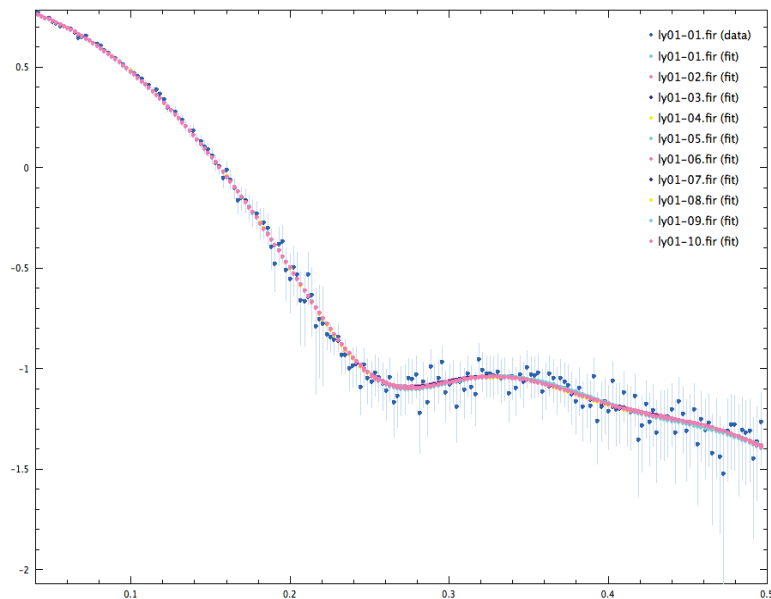
```
dammif lys.out --mode=slow --prefix lys1  
dammif lys.out --mode=slow --prefix lys2  
dammif lys.out --mode=slow --prefix lys3  
dammif lys.out --mode=slow --prefix lys4  
dammif lys.out --mode=slow --prefix lys5  
dammif lys.out --mode=slow --prefix lys6  
dammif lys.out --mode=slow --prefix lys7  
dammif lys.out --mode=slow --prefix lys8  
dammif lys.out --mode=slow --prefix lys9  
dammif lys.out --mode=slow --prefix lys10
```

# On linux/macOS

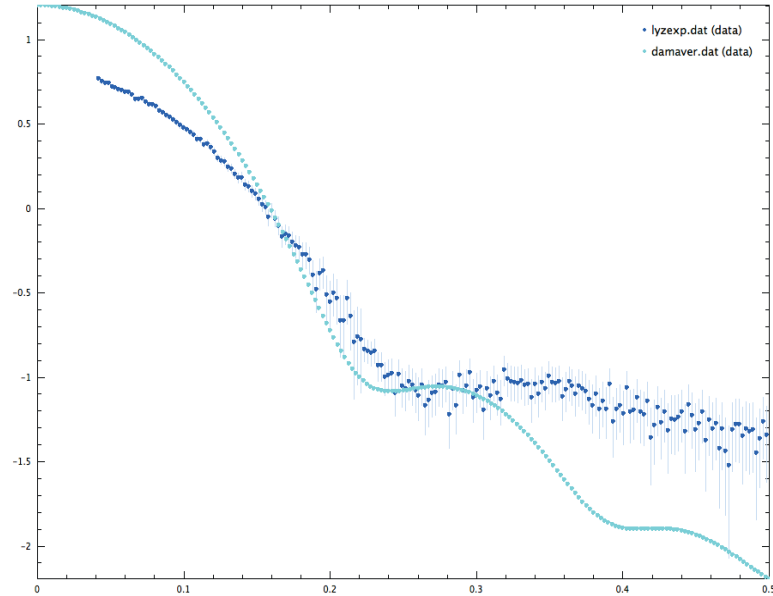
```
for i in `seq 1 10` ; do  
dammif --prefix=lys-$i --mode=slow lys.out;  
done
```



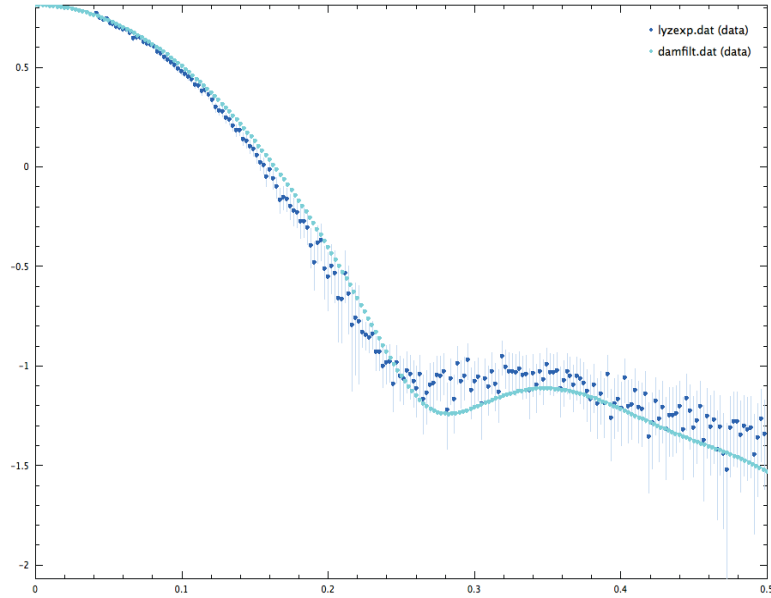
# DAMMIF fits



# DAMAVER fit

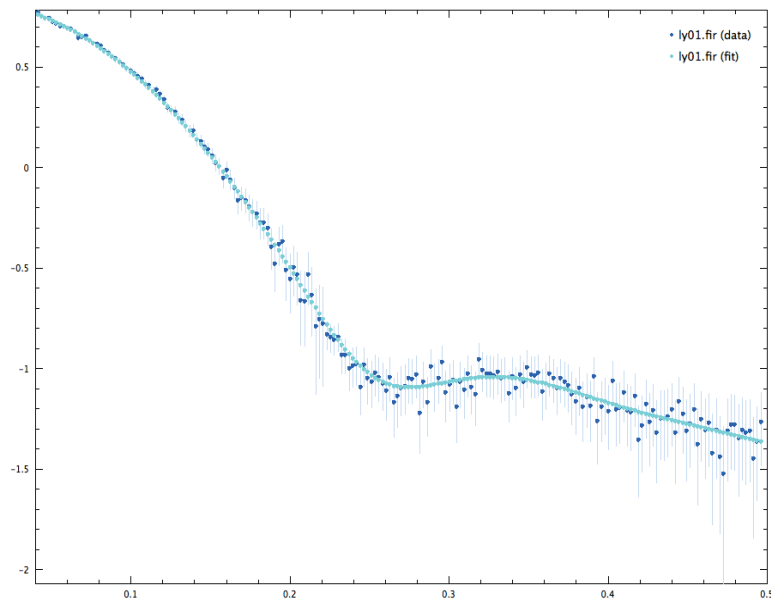


# DAMFILT fit








# DAMMIN fit



# Using Primus

# Atsas online

← | | https://www.embl-hamburg.de/biosaxs/atsas-online/ | | | Search | | | | | | |



ATSAS online

Home > Web services > ATSAS online

## ATSAS online

[Create an account](#)  
[Change password](#)  
[Forgot your password?](#)

As a courtesy to other users please do not submit more than 100 jobs at a time.  
The following services are available for registered users:

- [DAMMIN](#) - ab initio shape determination by simulated annealing using a bead model
- [DAMMIF](#) - rapid ab initio bead model shape determination
- [GASBOR](#) - ab initio reconstruction of protein structure by a chain-like ensemble of dummy residues
- [MONSA](#) - multiphase ab initio modelling
- [AMBIMETER](#) - ambiguity estimate of 3D reconstruction from a SAXS profile
- [SASRES](#) - Resolution estimate of 3D reconstructions of a protein structure
- [CRYSQL](#) - evaluation of X-ray solution scattering curves from atomic models
- [CORAL](#) - modelling of complexes made by multidomain proteins
- [SASREF](#) - modelling of multisubunit complexes from contrast variation and X-ray data
- Utility for generation of a [contact conditions file](#) to be used in SASREF 6.0 offline
- [SREFLEX](#) - flexible refinement of high-resolution models based on SAXS and normal mode analysis
- [EOM](#) - Ensemble Optimisation Method (for flexible proteins)
- [DANESSA](#) - Automated data analysis system (alpha version)
- [My Projects](#) - List of your recent projects (to check/re-run/report a problem)
- [Questions and feedback](#)

### Queue status

668916	cd25_140.cmd	atsas-online	508:31:1	Running
668947	cd25_10.cmd	atsas-online	506:19:5	Running
671222	T02.cmd	atsas-online	312:01:5	Running

# DAMMIN



Home > Web services > ATSAS online > DAMMIN

## DAMMIN online

Project description

The first 8 characters in the description will be used to generate the project identifier.

GNOM file (\*.out)  No file selected.

Angular units  s = 4 $\pi$ sin( $\theta$ )/ $\lambda$

Symmetry

Anisotropy

Mode

# DAMMIF



Home > Web services > ATSAS online > DAMMIF

## DAMMIF online

Project description

The first 8 characters in the description will be used to generate the project identifier.

GNOM file (\*.out)  No file selected.

Angular units  s = 4 $\pi$ sin( $\theta$ )/ $\lambda$

Symmetry

Anisotropy

Run DAMMIF  times

☐ Run Clustering and Resolution Assessment Algorithms (postprocessing)

# GASBOR



Home > Web services > ATSAS online > GASBOR

## GASBOR online

Use GASBOR only for proteins not bigger than 660 kDa. In other cases please use [DAMMIN](#) or [DAMMIF](#).

Project description

The first 8 characters in the description will be used to generate the project identifier.

GNOM file (\*.out)  No file selected.

Angular units  s = 4 $\pi$ sin( $\theta$ )/ $\lambda$

Symmetry

Anisotropy

Number of dummy residues in asymmetric part

Mode ☒ Reciprocal space (fit  $I(s)$ , slower)  
☐ Real space (fit  $p(r)$ , faster)  
☐ Fit to oligomer-monomer mixture

# MONSA



Home > Web services > ATSAS online > MONSA

## MONSA online

[Short tutorial](#)  
Please note that only first 1000 data points will be taken from each experimental data file.  
MONSA will guess the units of the experimental data ( $\text{\AA}^{-3}$  or  $\text{nm}^{-3}$ ). To be on the safe side you can provide the data in  $\text{\AA}^{-3}$ .  
The volumes for each phase can be either all in  $\text{\AA}^3$  or all in  $\text{nm}^3$  (only relative values are important).

Project description

The first 8 characters in the description will be used to generate the project identifier.

Overall symmetry

Search volume ☒ Sphere ☐ Ellipsoid

Sphere radius ( $D_{\text{max}}/2$ )

Number of curves

Number of phases

Phase Volume   Connectivity  Type

	1	2	Experiment	D2O fract	Presence1	Perd1	Contr1	Presence2	Perd2	O
1	-1.0	-1.0	<input type="text" value="X-ray"/>	0.0	<input type="checkbox"/>	0.0	0.0	<input type="checkbox"/>	0.0	0
2	-1.0	-1.0	<input type="text" value="X-ray"/>	0.0	<input type="checkbox"/>	0.0	0.0	<input type="checkbox"/>	0.0	0

# AMBIMETER



Home > Web services > ATSAS online > ambimeter

## ambimeter online

Project description

The first 8 characters in the description will be used to generate the project identifier.

GNOM file (\*.out)  No file selected.

# SASRES



Home > Web services > ATSAS online > SASRES

## SASRES online

Project description

The first 8 characters in the description will be used to generate the project identifier.

SAS-based Ab initio models  No file selected.  
in a single file (.zip)

Ab initio model type ☒ Bead models ☐ Dummy residue models

Test example: Ab initio bead models of lysozyme ☒ No ☐ Yes

