2017 publication guidelines for structural modelling of small-angle scattering data from biomolecules in solution: an update
Jill Trewhella, Anthony P. Duff, Dominique Durand, Frank Gabel, J. Mitchell Guss, Wayne A. Hendrickson, Greg L. Hura, David A. Jacques, Nigel M. Kirby, Ann H. Kwan, Javier Pérez, Lois Pollack, Timothy M. Ryan, Andrej Sali, Dina Schneidman-Duhovny, Torsten Schwede, Dmitri I. Svergun, Masaaki Sugiyama, John A. Tainer, Patrice Vachette, John Westbrook and Andrew E. Whitten
Supporting Information

Table S1  Reporting template for tabulating essential SAS data acquisition, sample details, data analysis, modelling fitting and software used.

(a) Sample details

|                | Sample 1 | Sample 2 | Sample 3, etc. |
|----------------|----------|----------|-----------------|
| Organism       |          |          |                 |
| Source (Catalogue No. or reference) |          |          |                 |
| Description: sequence (including Uniprot ID + uncleaved tags), bound ligands/modifications, etc. |          |          |                 |
| Extinction coefficient $\varepsilon$ (wavelength and units) |          |          |                 |
| Partial specific volume $\bar{v}$ (cm$^3$ g$^{-1}$) |          |          |                 |
| Mean solute and solvent scattering length densities and mean scattering contrast $\Delta \bar{\rho}$ (cm$^2$) |          |          |                 |
| Molecular mass $M$ from chemical composition (Da) |          |          |                 |
| For SEC-SAS, loading volume/concentration, (mg ml$^{-1}$) |          |          |                 |
| injection volume (µl), flow rate (ml min$^{-1}$) |          |          |                 |
| Concentration (range/values) measured and method |          |          |                 |
| Solvent composition and source |          |          |                 |

(b) SAS data collection parameters

|                |          |          |                 |
|----------------|----------|----------|-----------------|
| Source, instrument and description or reference |          |          |                 |
| Wavelength (Å) |          |          |                 |
| Beam geometry (size, sample-to-detector distance) |          |          |                 |
| $q$-measurement range (Å$^{-1}$ or nm$^{-1}$) |          |          |                 |
| Absolute scaling method |          |          |                 |
| Basis for normalization to constant counts |          |          |                 |
| Method for monitoring radiation damage, X-ray dose where relevant |          |          |                 |
| Exposure time, number of exposures |          |          |                 |
| Sample configuration including path length and flow rate where relevant |          |          |                 |
| Sample temperature (°C) |          |          |                 |

(c) Software employed for SAS data reduction, analysis and interpretation

|                |          |          |                 |
|----------------|----------|----------|-----------------|
| SAS data reduction to sample–solvent scattering, and extrapolation, merging, desmearing etc. as relevant |          |          |                 |
| Calculation of $\varepsilon$ from sequence |          |          |                 |
| Calculation of $\Delta \bar{\rho}$ and $\bar{v}$ values from chemical composition |          |          |                 |
Basic analyses: Guinier, $P(r)$, scattering particle volume (e.g. Porod volume $V_P$ or volume of correlation $V_c$)
Shape/bead modelling
Atomic structure modelling (homology, rigid body, ensemble)
Modelling of missing sequence from PDB files
Molecular graphics

(d) Structural parameters

| Parameter | Sample 1 | Sample 2 | Sample 3, etc. |
|-----------|----------|----------|----------------|
| Guinier Analysis | | | |
| $I(0)$ (cm$^{-1}$) | | | |
| $R_g$ (Å) | | | |
| $q$-range (Å$^{-1}$) | | | |
| Quality-of-fit parameter (with definition) | | | |
| $M$ from $I(0)$ (ratio to expected value) | | | |
| $P(r)$ analysis | | | |
| $I(0)$ (cm$^{-1}$) | | | |
| $R_g$ (Å) | | | |
| $d_{\text{max}}$ (Å) | | | |
| $q$-range (Å$^{-1}$) | | | |
| Quality-of-fit parameter (with definition) | | | |
| $M$ from $I(0)$ (ratio to expected value) | | | |
| Volume (e.g. $V_P$ and/or $V_c$) | | | |

(e) Shape modelling results (a complete panel for each method)

| Parameter | Sample 1 | Sample 2 | Sample 3, etc. |
|-----------|----------|----------|----------------|
| $q$-range for fitting | | | |
| Symmetry/anisotropy assumptions | | | |
| Ambiguity measure(s) with definitions | | | |
| $\chi^2$ value/range | | | |
| $P$ value, any other quality-of-fit parameters | | | |
| Adjustable parameters in the model fit | | | |
| Model volume and/or $M$ estimate | | | |
| Model precision/resolution | | | |
| For multiple phase shape models, $R_g$ values and relative phase volumes | | | |

(f) Atomistic modelling

| Parameter | Sample 1 | Sample 2 | Sample 3, etc. |
|-----------|----------|----------|----------------|
| Method | | | |
| $q$-range for fitting | | | |
| Symmetry assumptions | | | |
| Any measures of model precision | | | |
$\chi^2$ value/range

$P$ value, any other quality-of-fit parameters

Adjustable parameters in the model fit

Relevant output parameters (e.g. predicted $R_g/d_{\text{max}}$ values, weights for multi-state models, etc.)

Domain/subunit coordinates and contacts, regions of presumed flexibility as appropriate

| (g) Data and model deposition IDs | Sample 1 | Sample 2 | Sample 3 etc. |
|----------------------------------|----------|----------|---------------|
|                                  |          |          |               |
Supporting information, sup-4

Figure S1
A. Overlaid plots of $I(0)$ (filled symbols) and $A_{280}$ (hollow symbols) as a function of time/measurement frame showing the good correspondence in peak shape that facilitates concentration estimates for a set of 1 second measurement frames. These plots are raw values and have not been corrected for the shortened pathlengths for the shear-flow cell of UV cell. B. $\log I(q) \times \log q$ plots showing the expected near zero slope at low-$q$ expected for monodisperse scattering particles of similar size. C. Kratky plots for GI, BSA, and CaM. The rising Kratky plot for $q$ values $> 0.25$ Å$^{-1}$ for BSA and CaM are indicative of flexibility in these proteins. Color key is as in main figures: GI (blue), CaM (black) and BSA (red).