STRUCTURAL
BIOLOGY

Volume 73 (2017)

Supporting information for article:

2017 publication guidelines for structural modelling of small-angle scattering data from biomolecules in solution: an update

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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 ε (wavelength and units)			
Partial specific volume $\bar{\upsilon}$ ($cm^3\ g^{-1}$)			
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 (ºC)			
(*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 ε from sequence			
Calculation of $\Delta\bar{\rho}$ and $\bar{\upsilon}$ 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

Guinier Analysis	Sample 1	Sample 2	Sample 3, *etc.*
$I(0)$ (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	Sample 1	Sample 2	Sample 3, *etc.*
$I(0)$ (cm^{-1})			
R_g (Å)			
d_{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)

	Sample 1	Sample 2	Sample 3, *etc.*
q-range for fitting			
Symmetry/anisotropy assumptions			
Ambiguity measure(s) with definitions			
χ^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

	Sample 1	Sample 2	Sample 3, *etc.*
Method			
q-range for fitting			
Symmetry assumptions			
Any measures of model precision			

χ^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_{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.*

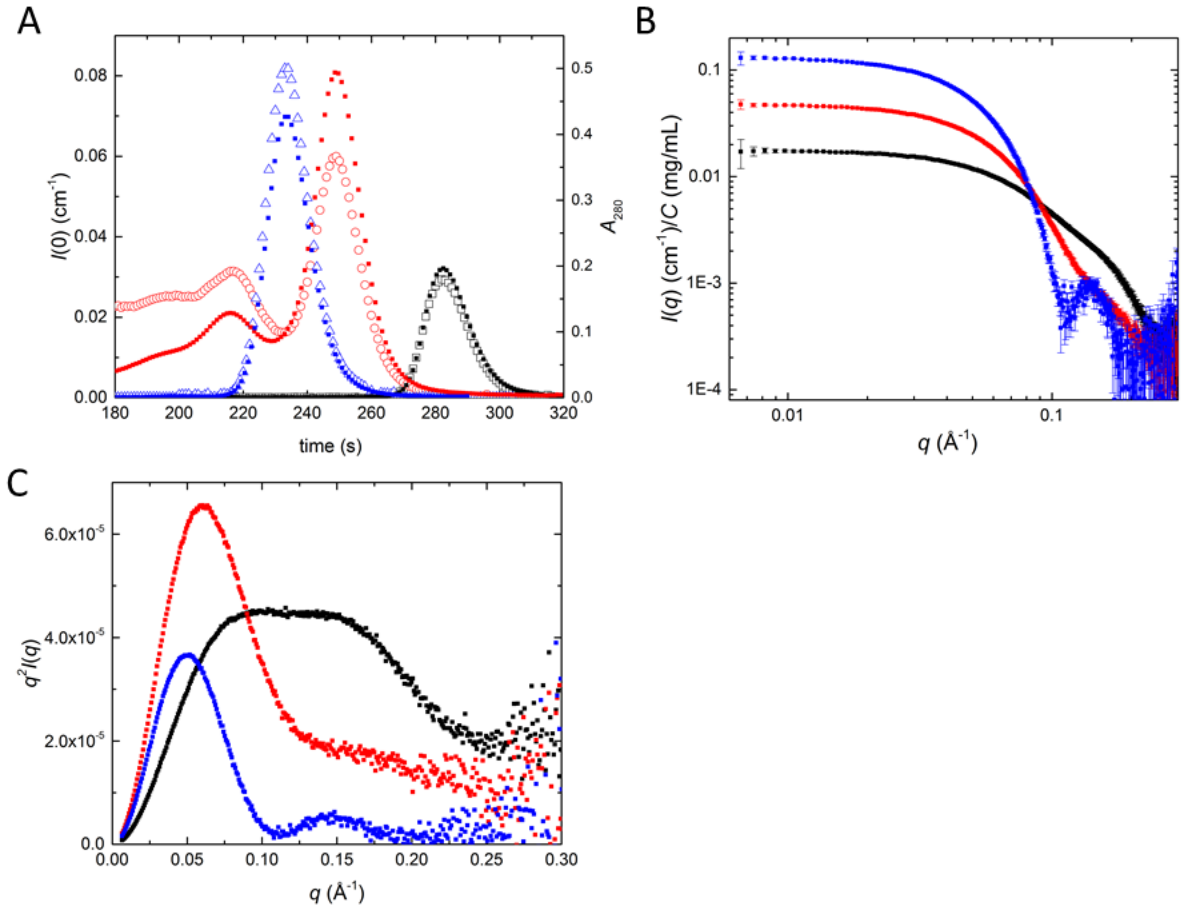

Figure S1

A. Overlaid plots of $I(0)$ (filled symbols) and A280 (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$I(q)$ v 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).