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Supporting information for article:

2022 update of template tables for reporting biomolecular structural modelling of small-angle scattering data

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Table S1: Currently available SAS Data Reduction, Analysis and Modelling Software.

Software	SAXS/SANS or both (SAS)	Image/Data reduction	Data analysis and modelling	Reference
ATSAS	SAS	✓	✓	(Manalastas-Cantos *et al.*, 2021, Franke *et al.*, 2017)
AXES	SAXS		✓	(Grishaev *et al.*, 2010)
AquaSAXS	SAXS		✓	(Poitevin *et al.*, 2011)
BioXTAS RAW	SAXS	✓	✓	(Hopkins *et al.*, 2017)
CCP-SAS & SASSIE-Web	SAS		✓	(Perkins *et al.*, 2016)
D+	SAXS		✓	(Ginsburg *et al.*, 2019)
DAWN	SAXS	✓		(Filik *et al.*, 2017)
DENSS	SAS		✓	(Grant, 2018)
DPDAK	SAXS	✓		(Benecke *et al.*, 2014)
ESRF SAXS Programs	SAXS	✓		(Narayanan *et al.*, 2018)
FIT2D	SAS	✓		(Hammersley, 2016)
FoXS	SAXS		✓	(Schneidman-Duhovny *et al.*, 2016)
GRASP	SANS	✓		Dewhurst C. https://www.ill.eu/users/support-labs-infrastructure/software-scientific-tools/grasp
GIFT	SAS		✓	(Bergmann *et al.*, 2000)
IMAGEJ	SAS	✓		
IRENA	SAS		✓	(Ilavsky & Jemian, 2009)
Mantid	SANS	✓		(Arnold *et al.*, 2014)
NIKA	SAS	✓		(Ilavsky, 2012)
NIST software package	SANS	✓	✓	(Kline, 2006)
Pepsi-SAXS/Pepsi-SANS	SAS		✓	(Grudinin *et al.*, 2017)
ScÅtter	SAXS		✓	Rambo, R. B. Request download at https://bl1231.als.lbl.gov/scatter/
SCATTER	SAXS	✓	✓	(Förster *et al.*, 2010)
SASfit	SAS		✓	(Breßler *et al.*, 2015)
sasPDF	SAS		✓	(Liu *et al.*, 2020)
sasView	SAS		✓	Download at http://www.sasview.org/
SAXSquant	SAXS	✓		Anton Paar
SASTBX	SAS	✓	✓	(Liu *et al.*, 2012)
SAXSutilities		✓	✓	(Sztucki, 2021)
US-SOMO	SAXS		✓	(Brookes & Rocco, 2018, Brookes *et al.*, 2016)
WAXSiS	SAXS		✓	(Knight & Hub, 2015, Chen & Hub, 2014)
WillItFit	SAS		✓	(Pedersen *et al.*, 2013)

Table S2: Useful web-based resources related to software in **Table S1**.

SAS Community forums data repositories & deposition resources	
Community forums	http://smallangle.org/ https://www.saxier.org/forum/
canSAS initiative	http://www.cansas.org
Protein Ensemble Database	https://proteinensemble.org
PDB-Dev prototype archiving system for structural models	https://pdb-dev.wwpdb.org/
Small Angle Scattering Biological Data Bank (SASBDB)	https://www.sasbdb.org/
UniProt	www.uniprot.org
wwPDB OneDep System	https://deposit-2.wwpdb.org/
ılculators and tables	
MULCh: ModULes for the analysis of Contrast variation data	https://smb-research.smb.usyd.edu.au/NCVWeb/
Biomolecular scattering length density calculator	http://psldc.isis.rl.ac.uk/Psldc/
NIST Scattering length density, mass attenuation calculators and other tools	https://www.ncnr.nist.gov/resources/activation/ https://www.nist.gov/pml/x-ray-mass-attenuation-coefficients https://www.nist.gov/pml/xcom-photon-cross-sections-database https://www.ncnr.nist.gov/resources/
SAXSMoW (SAXS Molecular Weight)	http://saxs.ifsc.usp.br/
SAS Software packages	
General software list	http://smallangle.org/content/software
Argonne National Laboratory SAXS and USAXS packages (Irena, Nika Indra),	https://usaxs.xray.aps.anl.gov/software-description
ATSAS online and web services, European Molecular Biology Laboratory	https://www.embl-hamburg.de/biosaxs/online.html https://www.embl-hamburg.de/biosaxs/software.html
AXES:	https://spin.niddk.nih.gov/bax/nmrserver/saxs1/axes.html
CCP-SAS project:	http://ccpsas.org/about.html
DENSS:	https://denss.ccr.buffalo.edu
ESRF SAXS software tools	https://www.esrf.eu/home/UsersAndScience/Experiments/CBS/ID02/available_software.html https://www.esrf.eu/home/UsersAndScience/Experiments/CBS/ID02/available_software/saxs-program-package.html https://www.esrf.eu/UsersAndScience/Experiments/CRG/BM26/SaxsWaxs/DataAnalysis/Scatter https://www.esrf.eu/computing/scientific/FIT2D/
foXS:	https://modbase.compbio.ucsf.edu/foxs/
ImageJ	https://imagej.nih.gov/ij/
Institut Laue-Langevin (ILL) - GRASP SANS analysis and data reduction	https://www.ill.eu/users/support-labs-infrastructure/software-scientific-tools/grasp
Mantid	https://www.mantidproject.org/Main_Page
NIST SANS and USANS data reduction and analysis software	https://www.nist.gov/ncnr/data-reduction-analysis/sans-software
Paul Scherrer Institute, PSI, SASfit package	https://www.psi.ch/en/sinq/sansi/sasfit
Pepsi-SAXS	https://team.inria.fr/nano-d/software/pepsi-saxs/
Pepsi-SANS	https://team.inria.fr/nano-d/software/pepsi-sans/
SasView	https://www.sasview.org/
SASSIE-web	https://sassie-web.chem.utk.edu/sassie2/
SASTBX	https://sastbx-document.readthedocs.io/en/latest/

SAXSutilities	https://www.saxsutilities.eu
ScÅtter, Lawrence Berkeley National Laboratory, Advanced Light Source	https://bl1231.als.lbl.gov/saxs_protocols/
US-SOMO	https://somo.aucsolutions.com/
WAXSIS	http://waxsis.uni-goettingen.de/

Table S3 SAS sample details, data collection, analysis, and 3D modelling details for biomolecules in solution.

If some descriptions are too long for the table format, *e.g.,* in the case of multiple samples, give abbreviated title(s) with details footnoted. Delete rows that are not relevant and remove or add columns as needed for the number of samples.

(*a*) Sample details				
Organism				
Source (Catalogue No. or reference)				
	Sample 1	Sample 2	Sample 3	Sample 4, *etc*
Scattering particle composition				
Protein(s)[a]				
DNA/RNA(s)[b]				
Carbohydrates/glycans[c]				
Stoichiometry of components				
Sample environment/configuration				
Solvent composition[d]				
Sample temperature (°C)				
In beam sample cell[e]				
Batch measurements				
Sample concentration(s), mg/ml or g/cm^3				
Size Exclusion Chromatography SEC-SAS				
Sample injection concentration, mg/ml or g/cm^3				
Sample injection volume, mL				
SEC column type				
SEC flowrate, mL/min				
(*b*) SAS data collection				
Data acquisition/reduction software				
Source/instrument description or reference				
Measured q-range ($q_{min} - q_{max}$; Å^{-1}, nm^{-1})				
Method for scaling intensities[f]				
Exposure time(s), number of exposures. For SEC-SAS, final number of sample frames used for averaging.				
Additional relevant details[g]				
(*c*) SAS-derived structural parameters				
Methods/Software				
Guinier Analysis	Sample 1	Sample 2	Sample 3	Sample 4, *etc*
$I(0) \pm \sigma$ (cm$^{-1;}$ a.u)				
$R_g \pm \sigma$ (Å, nm)				
$min < qR_g < max$ limit (or data point range)				
Linear fit assessment (definition)[h]				
PDDF/P(r) analysis	Sample 1	Sample 2	Sample 3	Sample 4, *etc*
$I(0) \pm \sigma$ (cm$^{-1;}$ a.u.)				

R_g ± σ (Å, nm)				
d_{max} (Å, nm)				
q-range (Å^{-1}, nm^{-1})				
$P(r)$ fit assessment (definition)[i]				
(*d*) Scattering particle size				
Methods/Software				
	Sample 1	Sample 2	Sample 3	Sample 4, *etc*
Volume estimates				
Porod volume, V_p (Å^3, nm^3)				
Molecular weight (M) estimates (kDa)				
From chemical composition				
From SAS, concentration independent method[j]				
From $I(0)$/concentration[k]				
Partial specific volume, ν (cm^3/g)				
Contrast, $\Delta\rho$ (cm^{-2})				
From SAS-independent measure[l] (method)				
(*e*) Modelling (a complete sub-panel for each method)				
Shape modelling method(s) (if used)				
	Sample 1	Sample 2	Sample 3	Sample 4, *etc*
Software				
q-range for fit (q_{min} – q_{max}; Å^{-1}, nm^{-1})				
Symmetry/anisotropy assumptions				
Number of individual model reconstructions				
χ^2, CorMap P-values for fit				
For multiple phase models: R_g values (Å, nm) and relative phase volumes (Å^3, nm^3)				
Atomistic modelling methods (if used)				
	Sample 1	Sample 2	Sample 3.	Sample 4, *etc*
Software				
q-range for fit (q_{min} – q_{max}; Å^{-1}, nm^{-1})				
Symmetry/anisotropy assumptions				
Number of individual model reconstructions				
χ^2, CorMap P-values for fit				
(*f*) Data and model deposition				
	Sample 1	Sample 2	Sample 3	Sample 4, *etc*
SASBDB IDs				

[a] Recommended description is UniProt ID (https://www.uniprot.org/), including the recommended UniProt name with the amino acid sequence range of the construct measured by SAS, plus any tags, post-translational modifications, ligands, cofactors, metals, etc. If UniProt ID's are not available the recommendation is to quote the NCBI accession and protein name (https://www.ncbi.nlm.nih.gov/guide/proteins/). If a sequence has neither UniProt nor NCBI identifiers, or if the description is too long for the table format, provide an abbreviated title with a reference to the location where exact sequences with modifications, etc., can be found.

[b] If possible, quote the relevant GenBank (https://www.ncbi.nlm.nih.gov/genbank/), RNACentral (https://rnacentral.org/) or ENA accession number (https://www.ebi.ac.uk/ena/browser/home), specifying any

modifications, derivatives, *etc*. If the description is too long for the table format, provide an abbreviated title with a reference to where the exact sequence with modifications, *etc.*, can be found.

[c] If possible, quote the GlyTouCan (https://glytoucan.org/) accession code, or information from GlyGen (https://www.glygen.org/). For chemical groups, use standard nomenclature, *e.g.*, for glycans, it is recommended to adhere to the Symbol Nomenclature for Glycans (SNFG) protocols (https://pubmed.ncbi.nlm.nih.gov/31184695/) and /or IUPAC nomenclature (https://iupac.org/what-we-do/nomenclature/).

[d] Provide complete solvent description (including buffer with pH, salts and any additives, *e.g.*, free radical scavengers).

[e] *e.g.*, cell type, pathlength, flow cell, coflow, etc.

[f] Strongly recommend absolute scaling of the scattering intensities, cm^{-1}, with reference to a standard, otherwise specify relative or arbitrary units (a.u.).

[g] *e.g.*, data smearing/desmearing, data merging, data re-binning, data normalization, standard experimental errors or otherwise, *etc*. For SANS recommend wavelength λ, $\Delta\lambda/\lambda$, sample-to-detector distances, source/sample to aperture distances, and collimation distances.

[h] *e.g.*, linear correlation coefficient.

[i] Recommend reciprocal space fit to experimental data (χ^2; CorMap *P*).

[j] *e.g.*, estimated from V_p and knowledge of partial specific volume and hydration (Trewhella *et al.*, 2017), or using volume of correlation V_c (Rambo & Tainer, 2013), SAXSMow (Piiadov *et al.*, 2019), or DatBayes (Hajizadeh *et al.*, 2018) from the ATSAS suite (Manalastas-Cantos *et al.*, 2021).

[k] Either from equation 1 (Trewhella *et al.*, 2017) or relative to a standard.

[l] *e.g.*, Multiple Angle Laser Light Scattering (MALLS), Analytical Ultra-Centrifugation (AUC), *etc*.

Table S4 SAS-cv sample details, data collection, analysis, and 3D modelling details for biomolecules in solution.

If some descriptions are too long for the table format, *e.g.,* in the case of multiple samples, give abbreviated title(s) with details footnoted. Delete rows that are not relevant and remove or add columns as needed for the number of samples.

(*a*) Sample details				
Organism				
Source				
Description of complex				
Scattering particle composition				
	Component 1	Component 2	Component 3	Component 4, *etc*
Protein(s)[a]				
DNA/RNA[b]				
Carbohydrates[c]				
Average non-exchangeable macromolecule deuteration (*if relevant*)				
Sample environment/configuration				
Solvent composition[d]				
(for SAXS-cv; contrast agent composition and concentration, mM)				
Sample temperature (°C)				
In beam sample cell[e]				
Batch measurements				
Sample concentrations(s), mg/mL or g/cm^3				
Size exclusions chromatography, SEC-SAS				
Sample injection concentration, mg/ml or g/cm^3				
Sample injection volume, mL				
SEC column type				
SEC flowrate, mL/min				

(*b*) SAS data collection		
	SAXS	SANS
Data acquisition/reduction software		
Source/instrument description or reference		
Measured q-range(s) ($q_{min} - q_{max}$; Å^{-1}, nm^{-1})		
Method for scaling intensities[f]		
Exposure time(s), number of exposures. For SEC-SAS		

include final number of sample frames used for averaging

Additional relevant details[g]

(*c*) SAS-derived structural parameters								
Methods/Software								
SAXS (*c*, contrast agent, mM) or SANS (% D_2O) contrast points	contrast-1	contrast-2	contrast-3	contrast-4	contrast-5	contrast-6	contrast-7	contrast-8
Guinier analysis								
$I(0) \pm \sigma$ (cm^{-1})								
$R_g \pm \sigma$ (Å, nm)								
$min < qR_g < max$ limit (or data point range)								
Linear fit assessment[h]								
P(*r*) analysis								
$I(0) \pm \sigma$ (cm^{-1})								
$R_g \pm \sigma$ (Å, nm)								
d_{max} (Å, nm)								
q-range ($Å^{-1}$, nm^{-1})								
P(*r*) fit assessment (definition)[i]								

(*d*) Scattering particle size and solvent match points					
Methods/Software					
	Complex	Component 1	Component 2	Component 3	Component 4, etc
Solvent match points					
Calculated					
Experimental					
Partial specific volume, ν (cm^3/g)					
Molecular weight (M) estimates (Da)					
M from chemical composition					
M from SAS-independent measure[j]					

M from SAS contrast data								
SAXS (*c*, contrast agent, mM) or SANS contrast points	contrast-1	contrast-2	contrast-3	contrast-4	contrast-5	contrast-6	contrast-7	contrast-8
M (kDa) from *I*(0)[k]								

Contrast $\Delta\rho$ (10^{10} cm^{-2})								
V_p where relevant								
(*e*) Modelling (a complete sub-panel for each method used)								
Shape modelling (if used)								
Method/Software								
Symmetry assumptions								
For multiple phase models: R_g values (Å, nm) and relative phase volumes (Å^3, nm^3)								
Number of individual model reconstructions								
Fit parameters for SAXS (*c*, contrast agent, mM) or SANS contrast points	contrast-1	contrast-2	contrast-3	contrast-4	contrast-5	contrast-6	contrast-7	contrast-8
q-range for fit (Å^{-1}, nm^{-1})								
χ^2 value								
CorMap *P*-value								
Atomistic modelling (if used)								
Method/Software								
Symmetry/anisotropy assumptions								
Number of individual model reconstructions								
Fit parameters for SAXS (*c*, contrast agent, mM) or SANS contrast points	contrast-1	contrast-2	contrast-3	contrast-4	contrast-5	contrast-6	contrast-7	contrast-8
q-range for fit (Å^{-1}, nm^{-1})								
χ^2 value								
CorMap *P*-value								
(*f*) Component structural parameters for a 2-component scattering density system								
Methods/Software								
V_p for the complex from $I_{\text{homogeneous}}(q)$[1]								
Parameters from 2-	Component 1 in complex R_g (Å,	Component 1 in complex R_g (Å, nm)	Component centre of mass (Å,		Component 1 d_{max}	Component 2 d_{max} (Å,		

component analyses	nm)	nm) separation	(Å, nm)	nm)
Stuhrmann plot			not relevant	not relevant
Parallel axis theorem			not relevant	not relevant
Component scattering functions		not relevant		
(*g*) Data and model deposition				
SASBDB IDs				

[a] Recommended description is UniProt ID (https://www.uniprot.org/), including the recommended UniProt name with the amino acid sequence range of the construct measured by SAS, plus any tags, post-translational modifications, ligands, cofactors, metals, etc. If UniProt ID's are not available the recommendation is to quote the NCBI accession and protein name (https://www.ncbi.nlm.nih.gov/guide/proteins/). If a sequence has neither UniProt nor NCBI identifiers, or if the description is too long for the table format, provide an abbreviated title with a reference to the location where exact sequences with modifications, etc., can be found.

[b] If possible, quote the relevant GenBank (https://www.ncbi.nlm.nih.gov/genbank/), RNACentral (https://rnacentral.org/) or ENA accession number (https://www.ebi.ac.uk/ena/browser/home), specifying any modifications, derivatives, etc. If the description is too long for the table format, provide an abbreviated title with a reference to where exact sequence with modifications, *etc.*, can be found.

[c] For chemical groups, use standard nomenclature, *e.g.*, for glycans, it is recommended to adhere to the Symbol Nomenclature for Glycans (SNFG) protocols (https://pubmed.ncbi.nlm.nih.gov/31184695/) and /or IUPAC nomenclature (https://iupac.org/what-we-do/nomenclature/). If possible, quote the GlyTouCan (https://glytoucan.org/) accession code, or information from GlyGen (https://www.glygen.org/).

[d] Provide complete solvent description (including buffer with pH, salts and any additives, *etc.*).

[e] *e.g.*, cell type, pathlength, flow cell, coflow, etc.

[f] Strongly recommend absolute scaling of the scattering intensities, cm^{-1}, with reference to a standard, otherwise specify relative or arbitrary units (a.u.).

[g] *e.g.*, data smearing/desmearing, data merging, data re-binning, data normalization, standard experimental errors or otherwise, *etc*. For SANS recommend wavelength λ, Δλ/λ, sample-to-detector distances, source/sample to aperture distances, and collimation distances.

[h] *e.g.*, linear correlation coefficient.

[i] Recommend reciprocal space fit to experimental data (χ^2; CorMap *P*).

[j] *e.g.*, Multiple Angle Laser Light Scattering (MALLS), Analytical Ultra-Centrifugation (AUC), etc.

[k] From equation 1 (Trewhella *et al.*, 2017)

[l] As the V_p calculation is not valid for inhomogeneous scattering contrast systems, in the case of a 2-scatteting density complex the composite scattering functions can be summed to give the scattering profile of the protein complex with homogeneous contrast ($I_{\text{homogeneous}}(q) = I_1(q) + I_2(q) + I_{12}(q)$ and V_p can be determined from this curve.

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