Integrative Structure Validation Report ?

July 22, 2024 - 03:43 PM PDT

The following software was used in the production of this report:

Python-IHM Version 1.3
ATSAS Version 3.2.1 (r14885)
Integrative Modeling Validation Version 1.2

PDB ID	8ZZH
PDB-Dev ID	PDBDEV_00000017
Structure Title	Molecular architecture of the major membrane ring component, Pom152, of the yeast nuclear pore complex
Structure Authors	Upla P; Kim SJ; Sampathkumar P; Dutta K; Cahill SM; Chemmama IE; Williams R; Bonanno JB; Rice WJ; Stokes DL; Cowburn D; Almo SC; Sali A; Rout MP; Fernandez-Martinez J

This is a PDB-Dev IM Structure Validation Report for a publicly released PDB-Dev entry.

We welcome your comments at pdb-dev@mail.wwpdb.org

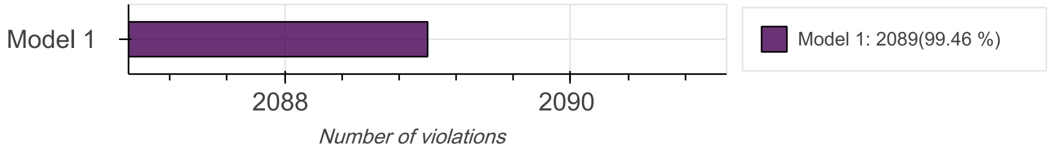
A user guide is available at https://pdb-dev.wwpdb.org/validation_help.html with specific help available everywhere you see the ? symbol.

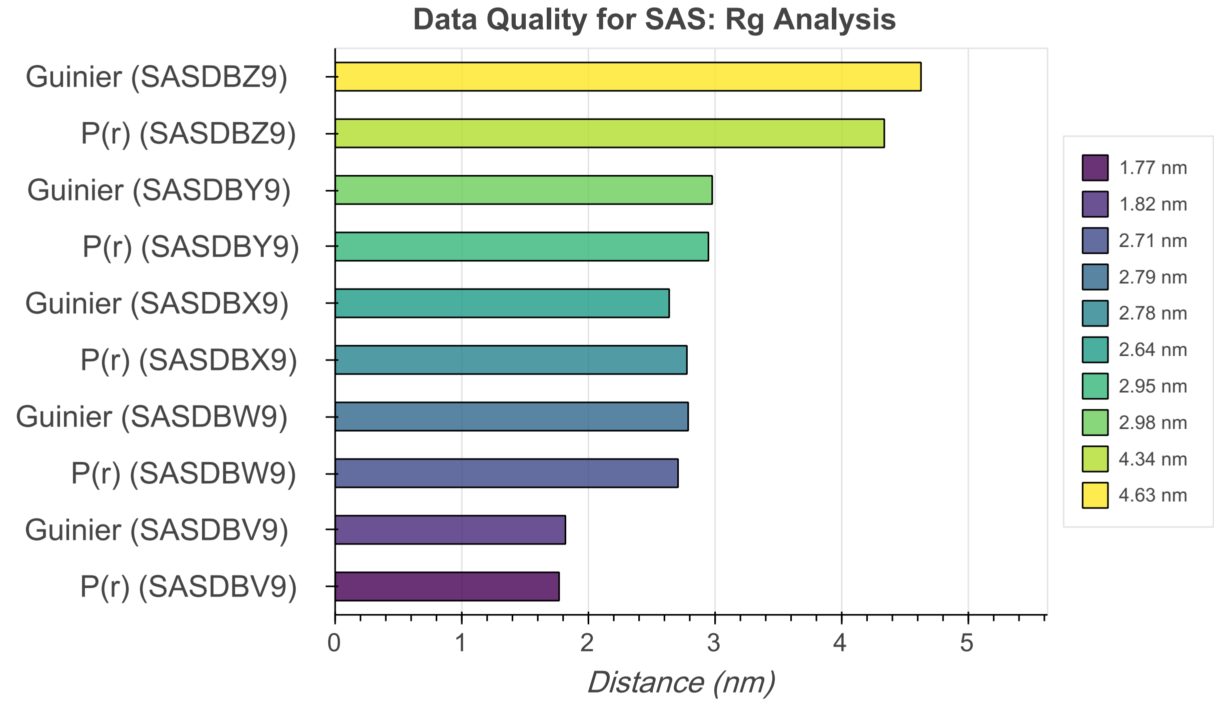
List of references used to build this report is available here.

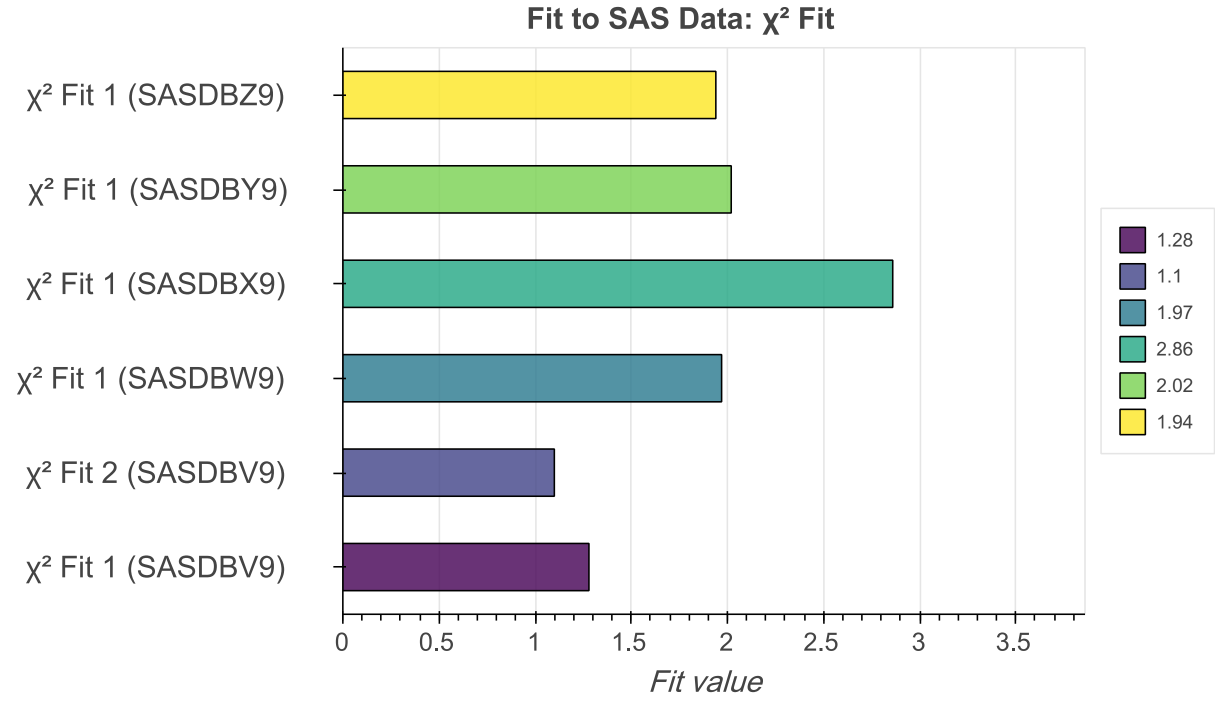
Overall quality ?

This validation report contains model quality assessments for all structures, data quality assessment for SAS datasets and fit to model assessments for SAS datasets. Data quality and fit to model assessments for other datasets and model uncertainty are under development. Number of plots is limited to 256.

Model Quality: Excluded Volume Analysis







Ensemble information

This entry consists of 1 distinct ensemble(s).

Summary ?

This entry consists of 1 unique models, with 1 subunits in each model. A total of 22 datasets or restraints were used to build this entry. Each model is represented by 9 rigid bodies and 9 flexible or non-rigid units.

Entry composition?

There is 1 unique type of models in this entry.This model is titled Cluster 0/None.

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	1	1	pom152	A	A	1337

Datasets used for modeling ?

There are 22 unique datasets used to build the models in this entry.

ID	Dataset type	Database name	Data access code
1	Experimental model	PDB	5TVZ
2	Comparative model	File	10.5281/zenodo.1231518
3	Comparative model	File	10.5281/zenodo.1231518
4	Comparative model	File	10.5281/zenodo.1231518
5	Comparative model	File	10.5281/zenodo.1231518
6	Comparative model	File	10.5281/zenodo.1231518
7	Comparative model	File	10.5281/zenodo.1231518
8	3DEM volume	EMDB	EMD-8543
9	3DEM volume	File	10.5281/zenodo.1231518
10	2DEM class average	File	10.5281/zenodo.1231518
11	2DEM class average	File	10.5281/zenodo.1231518
12	2DEM class average	File	10.5281/zenodo.1231518

ID	Dataset type	Database name	Data access code
13	2DEM class average	File	10.5281/zenodo.1231518
14	2DEM class average	File	10.5281/zenodo.1231518
15	2DEM class average	File	10.5281/zenodo.1231518
16	2DEM class average	File	10.5281/zenodo.1231518
17	2DEM class average	File	10.5281/zenodo.1231518
18	SAS data	SASBDB	SASDBV9
19	SAS data	SASBDB	SASDBW9
20	SAS data	SASBDB	SASDBX9
21	SAS data	SASBDB	SASDBY9
22	SAS data	SASBDB	SASDBZ9

Representation ?

This entry has only one representation and includes 9 rigid bodies and 9 flexible units

Chain ID	Rigid bodies	Non-rigid segments
A	379-472, 520-611, 616-714, 722-818, 824-918, 931-1026, 1036-1141, 1150-1229, 1244-1337	1-378, 473-519, 612-615, 715-721, 819-823, 919-930, 1027-1035, 1142-1149, 1230-1243

Methodology and software ?

This entry is a result of 1 distinct protocol(s).

Step number	Protocol ID	Method name	Method type	Method description	Number of computed models	Multi state modeling	Multi scale modeling
1	1	Replica exchange monte carlo	Sampling	None	100000	False	True

There are 3 software packages reported in this entry.

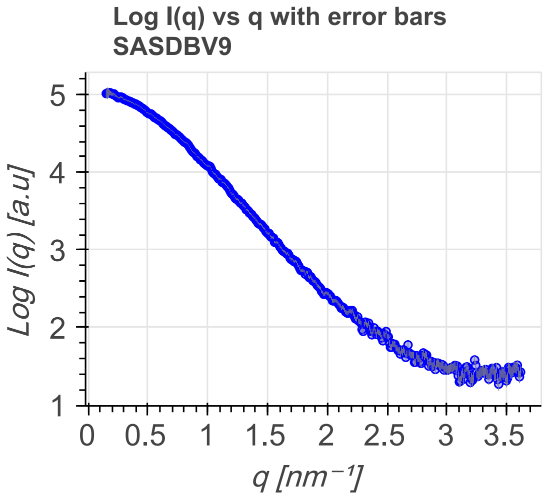
ID	Software name	Software version	Software classification	Software location
1	Integrative Modeling Platform (IMP)	develop-0a5706e202	integrative model building	https://integrativemodeling.org
2	IMP PMI module	67456c0	integrative model building	https://integrativemodeling.org
3	MODELLER	9.13	comparative modeling	https://salilab.org/modeller/

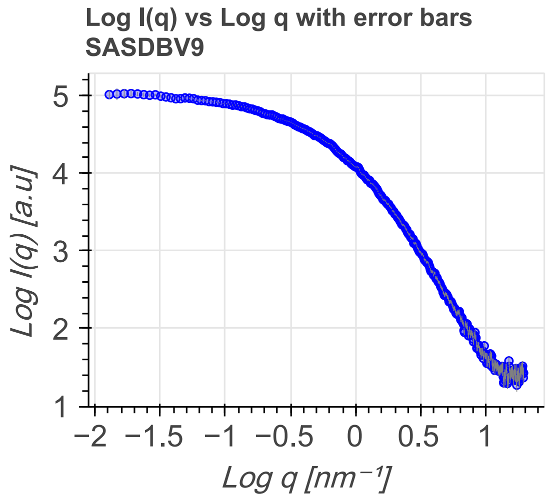
Data quality ?

Scattering profile ?

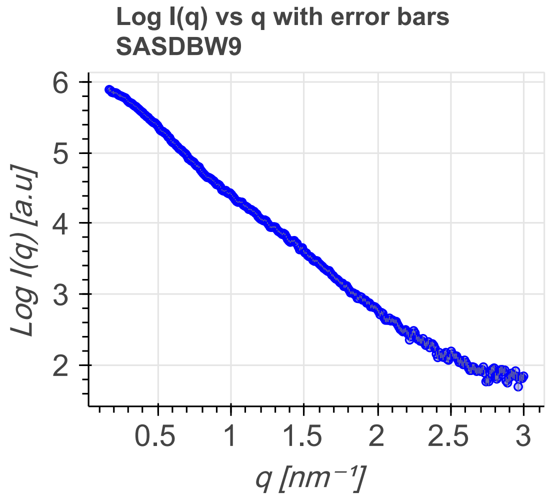
SAS data used in this integrative model was obtained from 5 deposited SASBDB entry (entries).

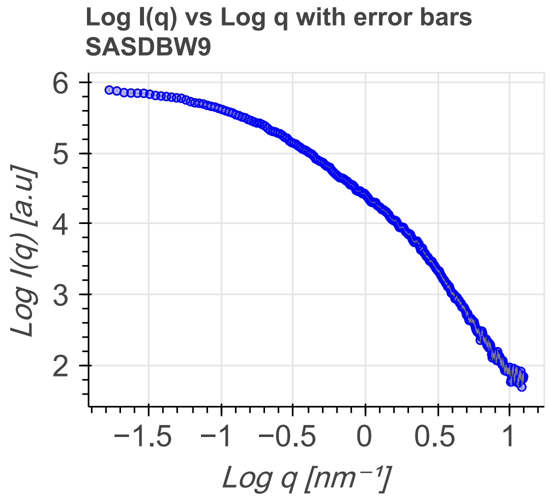
Scattering profile for SASDBV9: data from solutions of biological macromolecules are presented as both log I(q) vs q and log I(q) vs log (q) based on SAS validation task force (SASvtf) recommendations. I(q) is the intensity (in arbitrary units) and q is the modulus of the scattering vector.



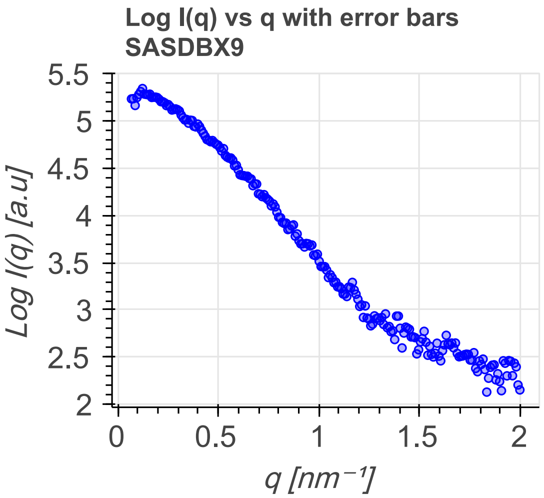


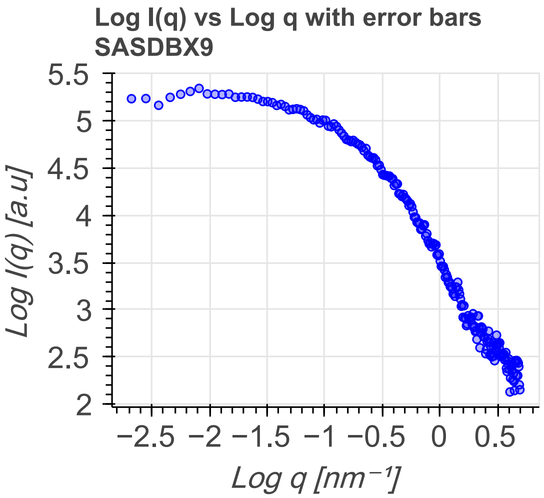
Scattering profile for SASDBW9: data from solutions of biological macromolecules are presented as both log I(q) vs q and log I(q) vs log (q) based on SAS validation task force (SASvtf) recommendations. I(q) is the intensity (in arbitrary units) and q is the modulus of the scattering vector.



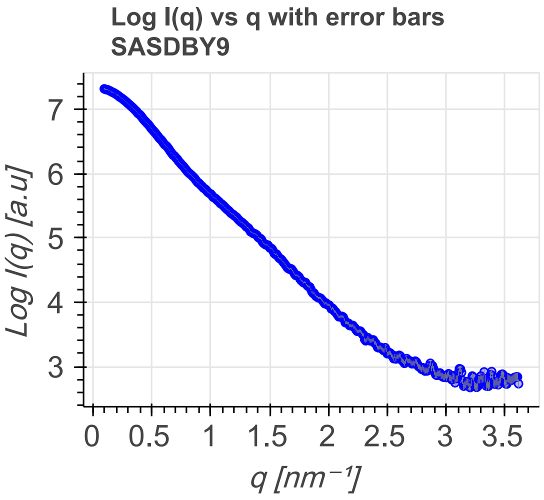


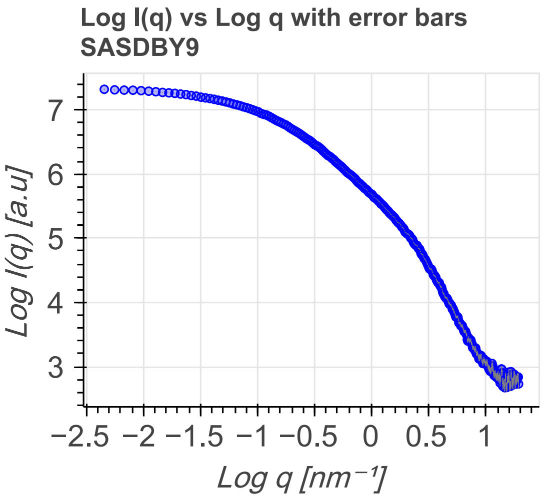
Scattering profile for SASDBX9: data from solutions of biological macromolecules are presented as both log I(q) vs q and log I(q) vs log (q) based on SAS validation task force (SASvtf) recommendations. I(q) is the intensity (in arbitrary units) and q is the modulus of the scattering vector.



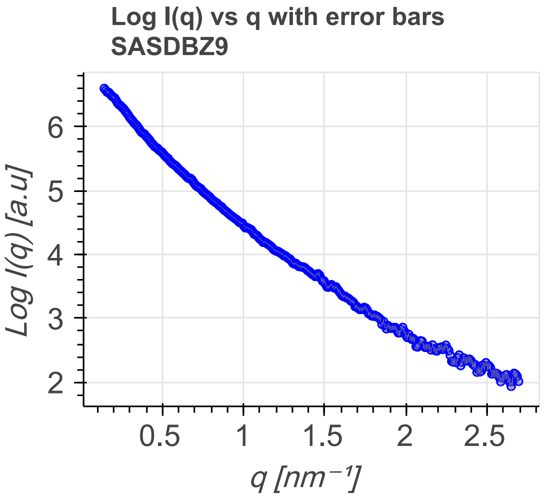


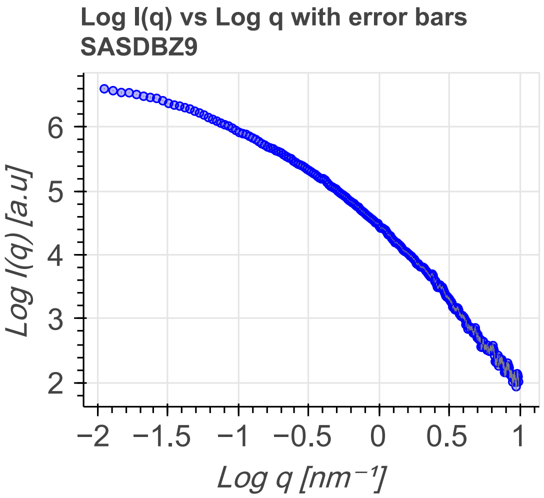
Scattering profile for SASDBY9: data from solutions of biological macromolecules are presented as both log I(q) vs q and log I(q) vs log (q) based on SAS validation task force (SASvtf) recommendations. I(q) is the intensity (in arbitrary units) and q is the modulus of the scattering vector.





Scattering profile for SASDBZ9: data from solutions of biological macromolecules are presented as both log I(q) vs q and log I(q) vs log (q) based on SAS validation task force (SASvtf) recommendations. I(q) is the intensity (in arbitrary units) and q is the modulus of the scattering vector.





Key experimental estimates ?

Molecular weight (MW) estimates from experiments and analysis true molecular weight can be compared to the Porod estimate from scattering profiles.

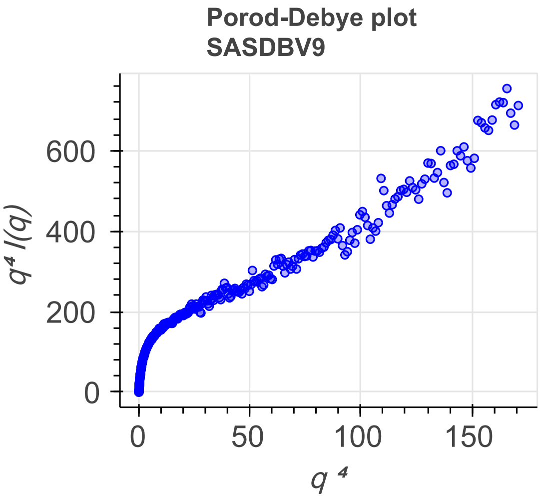
SASDB ID	Chemical composition MW	Standard MW	Porod Volume/MW
SASDBV9	12.6 kDa	12.2 kDa	N/A
SASDBW9	24.1 kDa	25.2 kDa	N/A
SASDBX9	12.5 kDa	14.7 kDa	N/A
SASDBY9	25.9 kDa	25.2 kDa	N/A
SASDBZ9	49.4 kDa	48.3 kDa	N/A

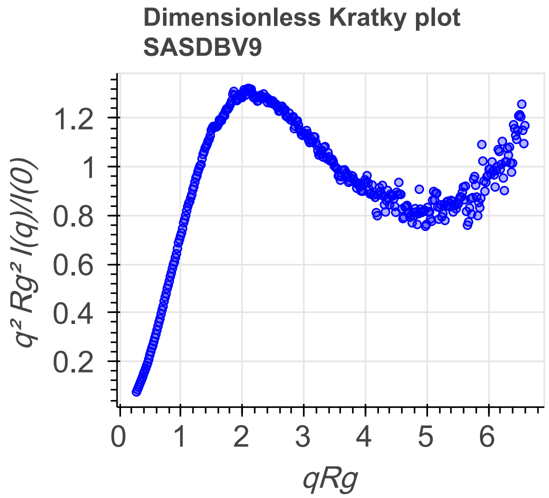
Volume estimates from experiments and analysis: estimated volume can be compared to Porod volume obtained from scattering profiles.

SASDB ID	Estimated Volume	Porod Volume	Specific Volume	Sample Contrast	Sample Concentration
SASDBV9	N/A	17.94 nm³	N/A	N/A	N/A
SASDBW9	N/A	22.50 nm³	N/A	N/A	N/A
SASDBX9	N/A	56.68 nm³	N/A	N/A	N/A
SASDBY9	N/A	27.97 nm³	N/A	N/A	N/A
SASDBZ9	N/A	66.59 nm³	N/A	N/A	N/A

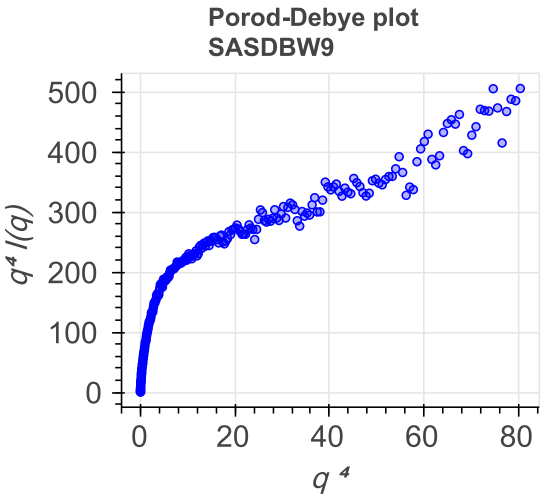
Flexibility analysis

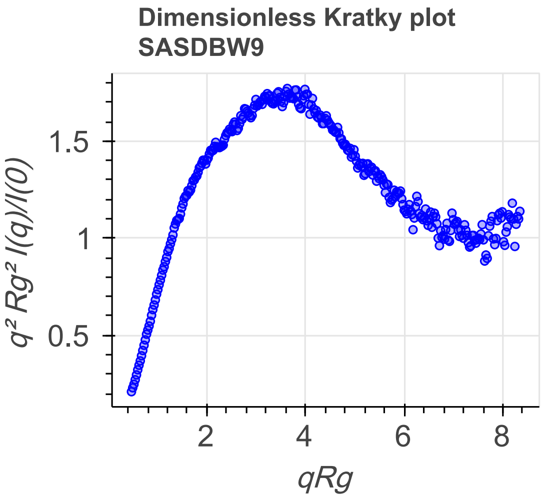
Flexibility analysis for SASDBV9: In a Porod-Debye plot, a clear plateau is observed for globular (partial or fully folded) domains, whereas, fully unfolded domains are devoid of any discernable plateau. For details, refer to Figure 5 in Rambo and Tainer, 2011 . In a Kratky plot, a parabolic shape is observed for globular (partial or fully folded) domains and a hyperbolic shape is observed for fully unfolded domains.



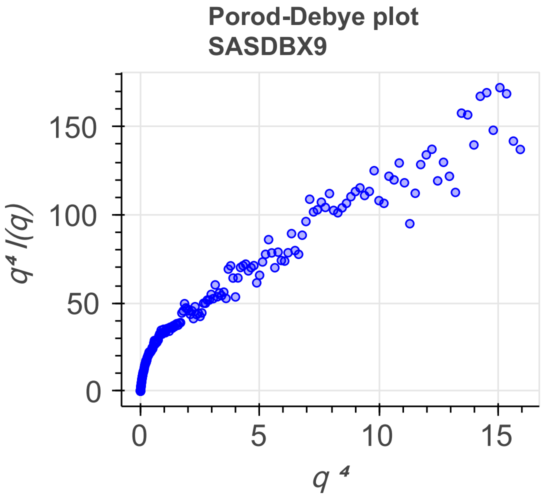


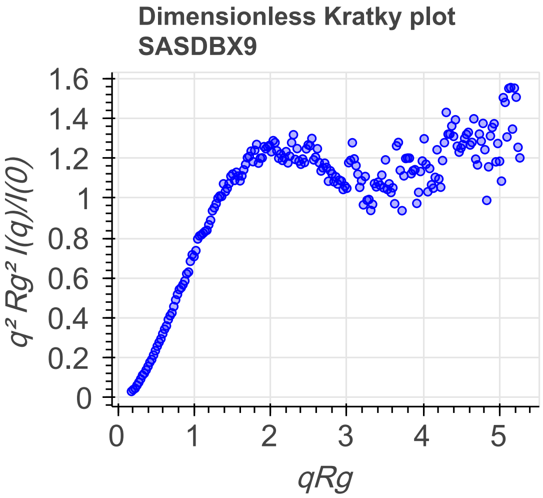
Flexibility analysis for SASDBW9: In a Porod-Debye plot, a clear plateau is observed for globular (partial or fully folded) domains, whereas, fully unfolded domains are devoid of any discernable plateau. For details, refer to Figure 5 in Rambo and Tainer, 2011 . In a Kratky plot, a parabolic shape is observed for globular (partial or fully folded) domains and a hyperbolic shape is observed for fully unfolded domains.



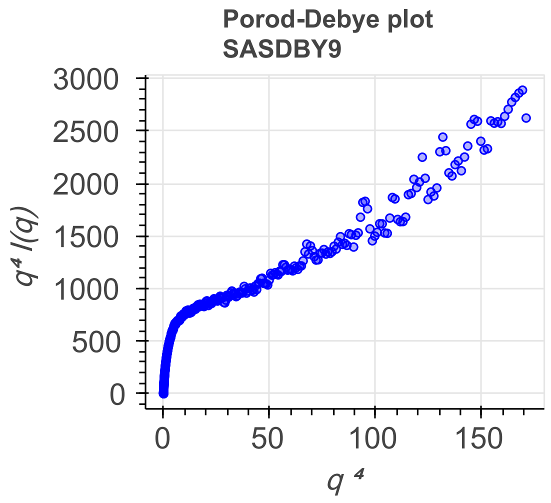


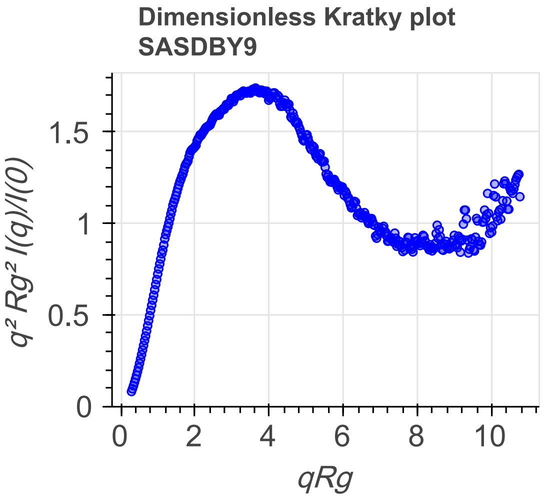
Flexibility analysis for SASDBX9: In a Porod-Debye plot, a clear plateau is observed for globular (partial or fully folded) domains, whereas, fully unfolded domains are devoid of any discernable plateau. For details, refer to Figure 5 in Rambo and Tainer, 2011 . In a Kratky plot, a parabolic shape is observed for globular (partial or fully folded) domains and a hyperbolic shape is observed for fully unfolded domains.



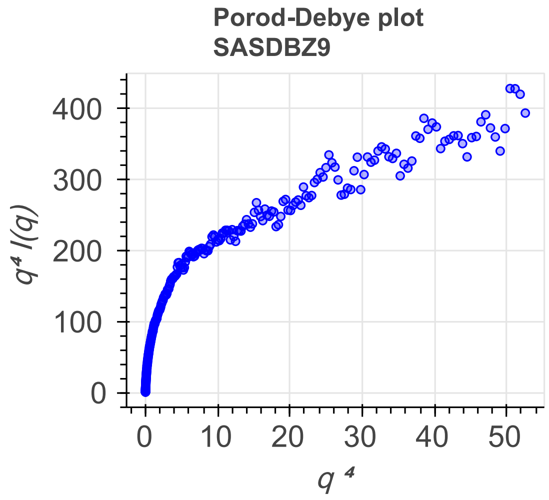


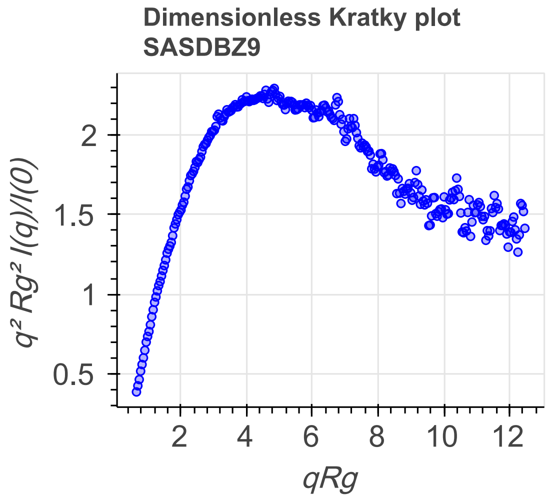
Flexibility analysis for SASDBY9: In a Porod-Debye plot, a clear plateau is observed for globular (partial or fully folded) domains, whereas, fully unfolded domains are devoid of any discernable plateau. For details, refer to Figure 5 in Rambo and Tainer, 2011 . In a Kratky plot, a parabolic shape is observed for globular (partial or fully folded) domains and a hyperbolic shape is observed for fully unfolded domains.





Flexibility analysis for SASDBZ9: In a Porod-Debye plot, a clear plateau is observed for globular (partial or fully folded) domains, whereas, fully unfolded domains are devoid of any discernable plateau. For details, refer to Figure 5 in Rambo and Tainer, 2011 . In a Kratky plot, a parabolic shape is observed for globular (partial or fully folded) domains and a hyperbolic shape is observed for fully unfolded domains.


Porod-Debye plot
SASDBZ9

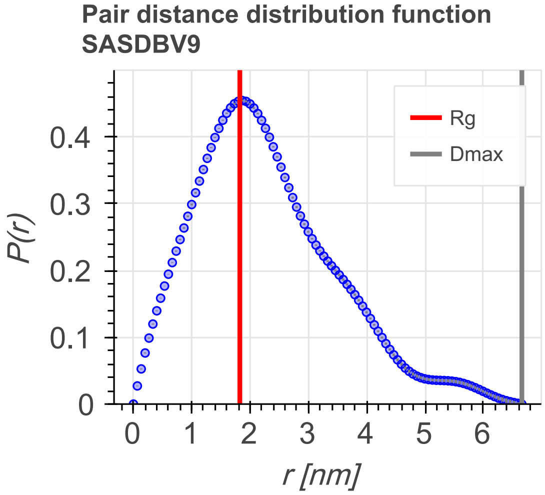

Dimensionless Kratky plot
SASDBZ9

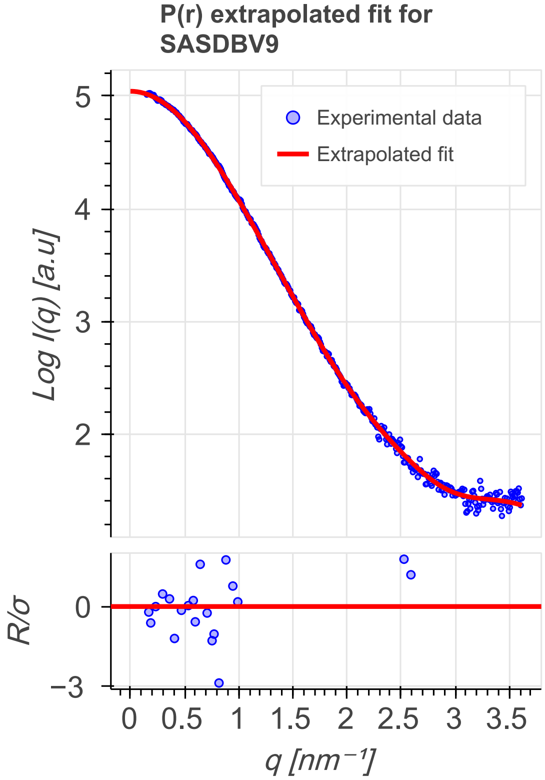
Pair-distance distribution analysis

P(r) analysis: P(r) represents the distribution of distances between all pairs of atoms within the particle weighted by the respective electron densities. P(r) is the Fourier transform of I(s) (and vice versa). R_g can be estimated from integrating the P(r) function. Agreement between the P(r) and Guinier-determined R_g (table below) is a good measure of the self-consistency of the SAS profile. R_g is a measure for the overall size of a macromolecule; e.g. a protein with a smaller R_g is more compact than a protein with a larger R_g, provided both have the same molecular weight (MW). The point where P(r) is decaying to zero is called D_{max} and represents the maximum size of the particle.

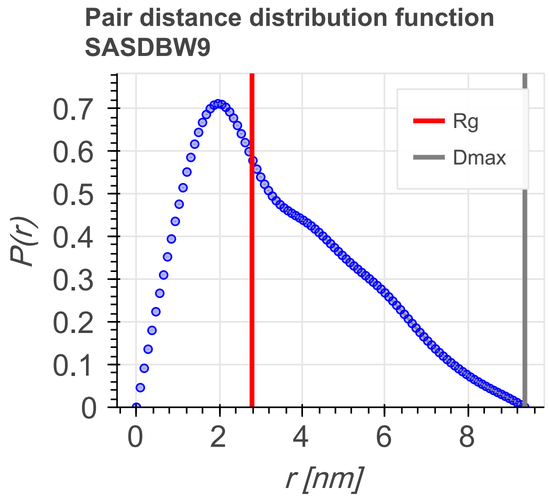
SASDB ID	Software used	Dmax	Dmax error	Rg	Rg error
SASDBV9	GNOM 4.5a	6.660 nm	N/A	1.824 nm	0.006 nm
SASDBW9	GNOM 4.5a	9.370 nm	N/A	2.787 nm	0.007 nm
SASDBX9	GNOM 4.5a	7.930 nm	N/A	2.636 nm	0.008 nm
SASDBY9	GNOM 4.5a	10.450 nm	N/A	2.976 nm	0.005 nm
SASDBZ9	GNOM 4.5a	15.430 nm	N/A	4.629 nm	0.011 nm

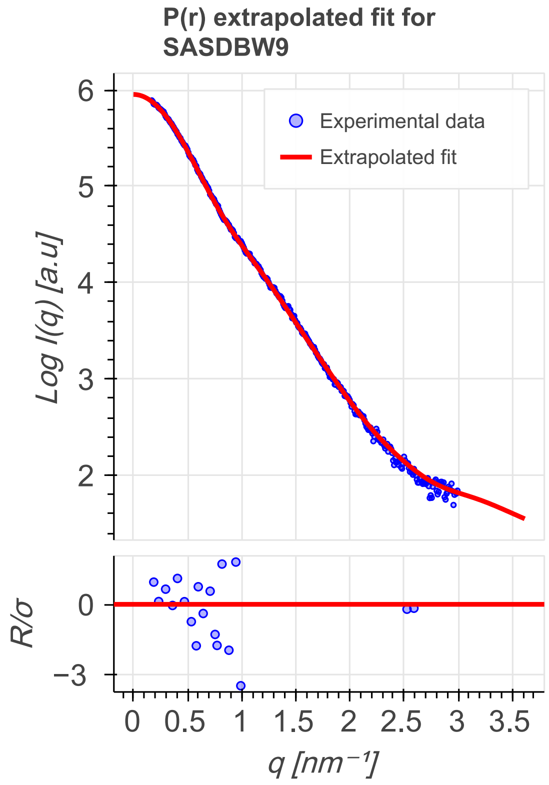
P(r) for SASDBV9: The value of P(r) should be zero beyond r=D_{max}.



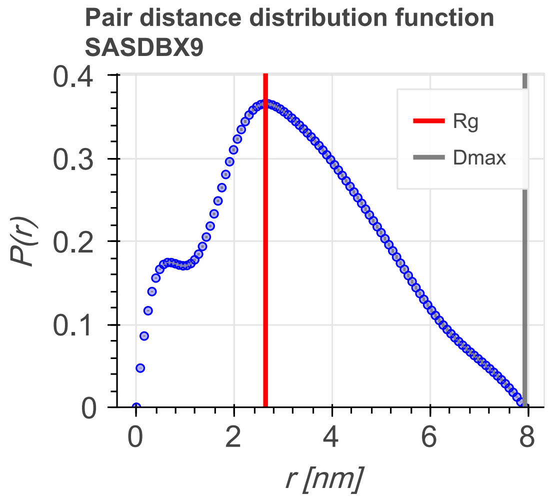


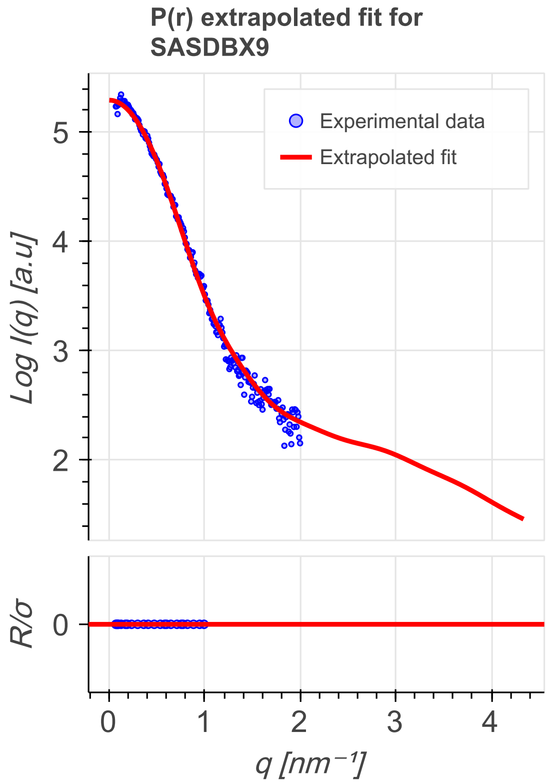
P(r) for SASDBW9: The value of P(r) should be zero beyond r=D_{max}.



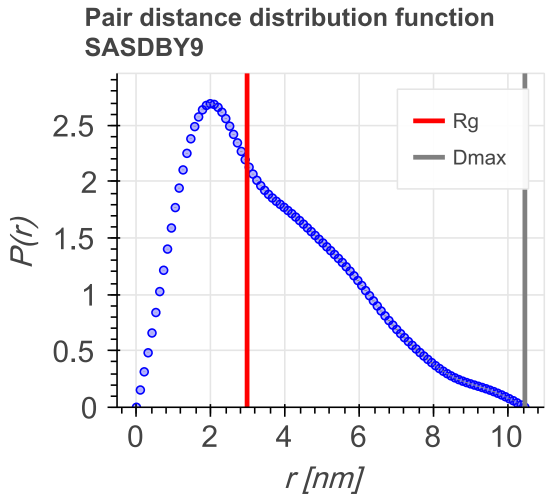


P(r) for SASDBX9: The value of P(r) should be zero beyond r=D_{max}.

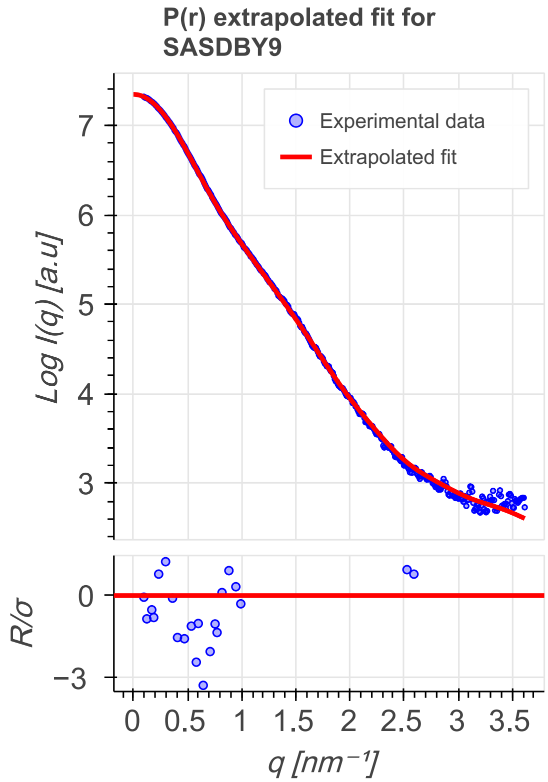

Pair distance distribution function SASDBX9


P(r) extrapolated fit for SASDBX9

P(r) for SASDBY9: The value of P(r) should be zero beyond r=D_{max}.

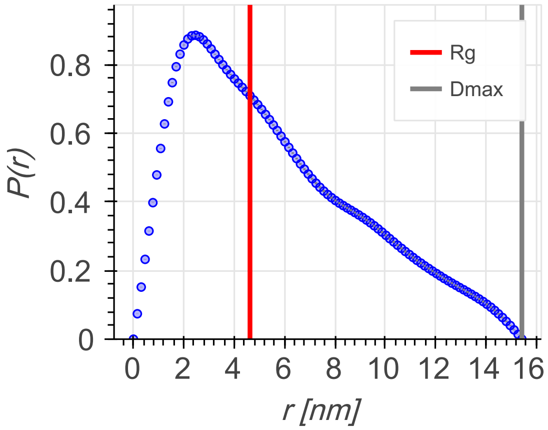


Pair distance distribution function SASDBY9

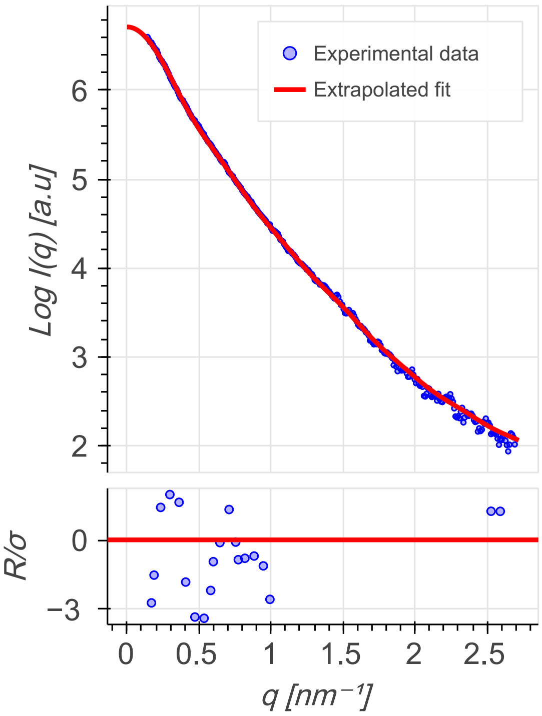


P(r) extrapolated fit for SASDBY9

P(r) for SASDBZ9: The value of P(r) should be zero beyond r=D_{max}.



Pair distance distribution function
SASDBZ9



P(r) extrapolated fit for
SASDBZ9

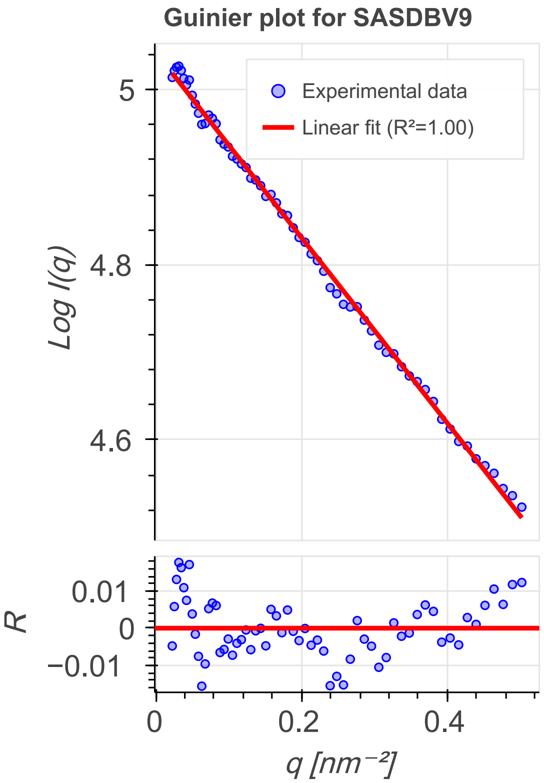
Guinier analysis ?

Guinier analysis: agreement between the P(r) and Guinier-determined R_g (table below) is a good measure of the self-consistency of the SAS profile. Molecular weight estimates can also be compared to Porod and sample molecular weights for consistency.

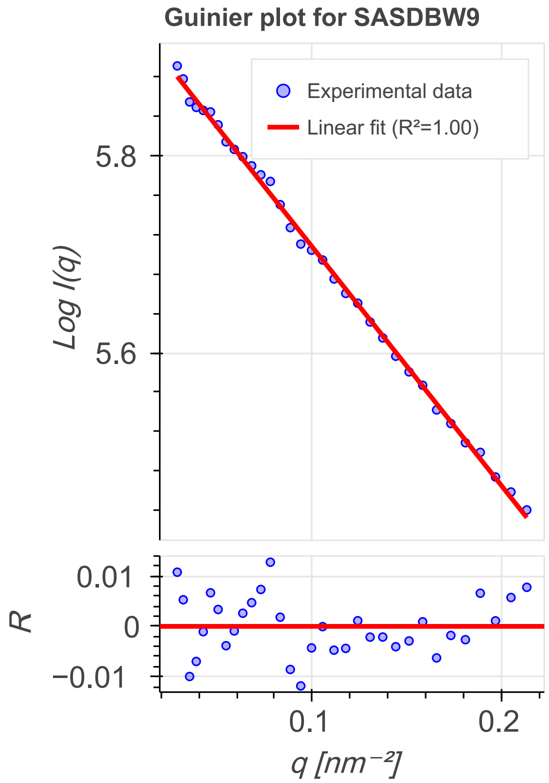
SASDB ID	Rg	Rg error	MW	MW error
SASDBV9	1.77 nm	0.05 nm	12.2 kDa	N/A
SASDBW9	2.71 nm	0.06 nm	25.2 kDa	N/A

SASDB ID	Rg	Rg error	MW	MW error
SASDBX9	2.78 nm	0.18 nm	14.7 kDa	N/A
SASDBY9	2.95 nm	0.11 nm	25.2 kDa	N/A
SASDBZ9	4.34 nm	0.17 nm	48.3 kDa	N/A

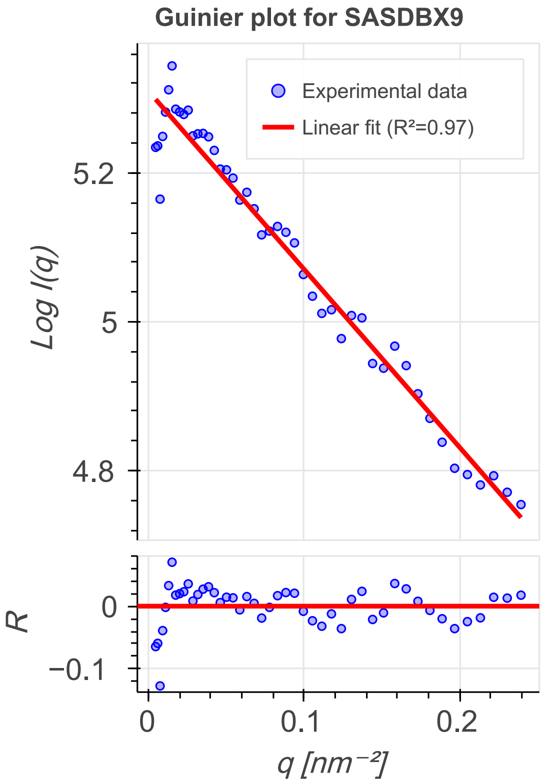
Guinier analysis for SASDBV9: the linearity of the Guinier plot is a sensitive indicator of the quality of the experimental SAS data; a linear Guinier plot is a necessary but not sufficient demonstration that a solution contains monodisperse particles of the same size. Deviations from linearity usually point to strong interference effects, polydispersity of the samples or improper background subtraction. Residual value plot and coefficient of determination (R^2) are measures to assess linear fit to the data. A perfect fit has an R^2 value of 1. Residual values should be equally and randomly spaced around the horizontal axis.



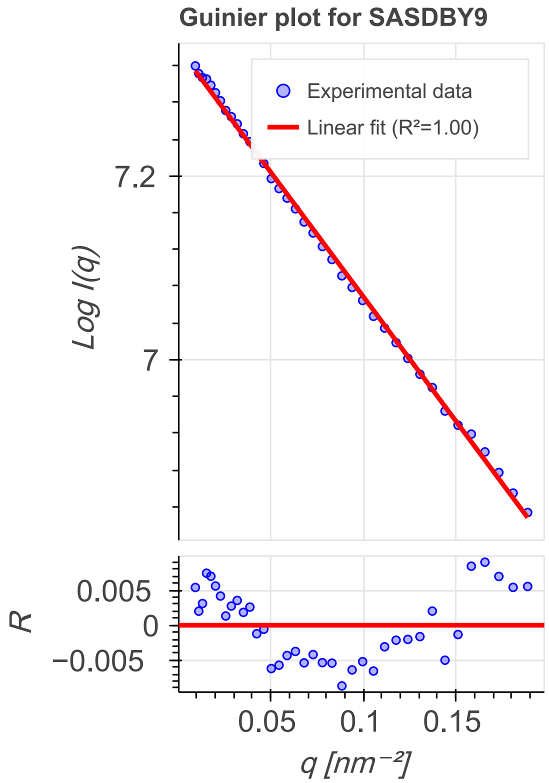
Guinier analysis for SASDBW9: the linearity of the Guinier plot is a sensitive indicator of the quality of the experimental SAS data; a linear Guinier plot is a necessary but not sufficient demonstration that a solution contains monodisperse particles of the same size. Deviations from linearity usually point to strong interference effects, polydispersity of the samples or improper background subtraction. Residual value plot and coefficient of determination (R^2) are measures to assess linear fit to the data. A perfect fit has an R^2 value of 1. Residual values should be equally and randomly spaced around the horizontal axis.



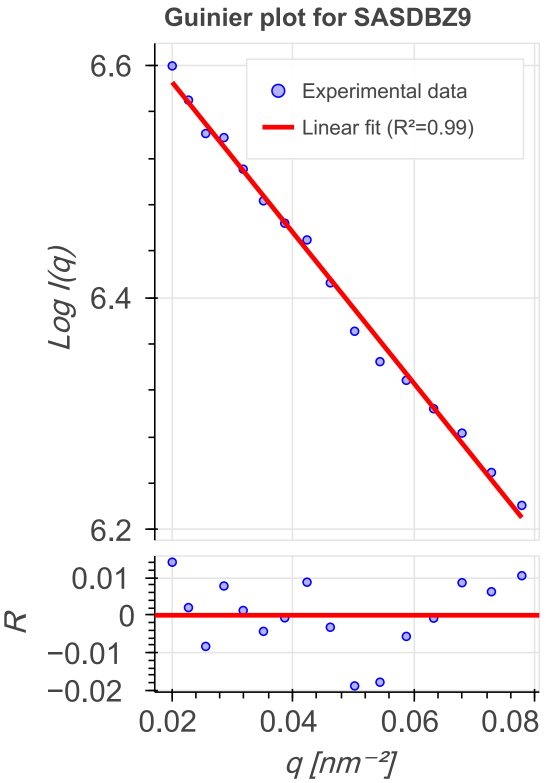
Guinier analysis for SASDBX9: the linearity of the Guinier plot is a sensitive indicator of the quality of the experimental SAS data; a linear Guinier plot is a necessary but not sufficient demonstration that a solution contains monodisperse particles of the same size. Deviations from linearity usually point to strong interference effects, polydispersity of the samples or improper background subtraction. Residual value plot and coefficient of determination (R^2) are measures to assess linear fit to the data. A perfect fit has an R^2 value of 1. Residual values should be equally and randomly spaced around the horizontal axis.



Guinier analysis for SASDBY9: the linearity of the Guinier plot is a sensitive indicator of the quality of the experimental SAS data; a linear Guinier plot is a necessary but not sufficient demonstration that a solution contains monodisperse particles of the same size. Deviations from linearity usually point to strong interference effects, polydispersity of the samples or improper background subtraction. Residual value plot and coefficient of determination (R^2) are measures to assess linear fit to the data. A perfect fit has an R^2 value of 1. Residual values should be equally and randomly spaced around the horizontal axis.



<u>Guinier analysis for SASDBZ9:</u> the linearity of the Guinier plot is a sensitive indicator of the quality of the experimental SAS data; a linear Guinier plot is a necessary but not sufficient demonstration that a solution contains monodisperse particles of the same size. Deviations from linearity usually point to strong interference effects, polydispersity of the samples or improper background subtraction. Residual value plot and coefficient of determination (R^2) are measures to assess linear fit to the data. A perfect fit has an R^2 value of 1. Residual values should be equally and randomly spaced around the horizontal axis.



3DEM volume

Validation for this section is under development.

2DEM class average

Validation for this section is under development.

Model quality ?

For models with atomic structures, molprobity analysis is performed. For models with coarse-grained or multi-scale structures, excluded volume analysis is performed.

Excluded volume satisfaction ?

Excluded volume satisfaction for the models in the entry are listed below.

Models	Excluded Volume Satisfaction (%)	Number of violations
1	99.46	2089.0

Fit of model to data used for modeling ?

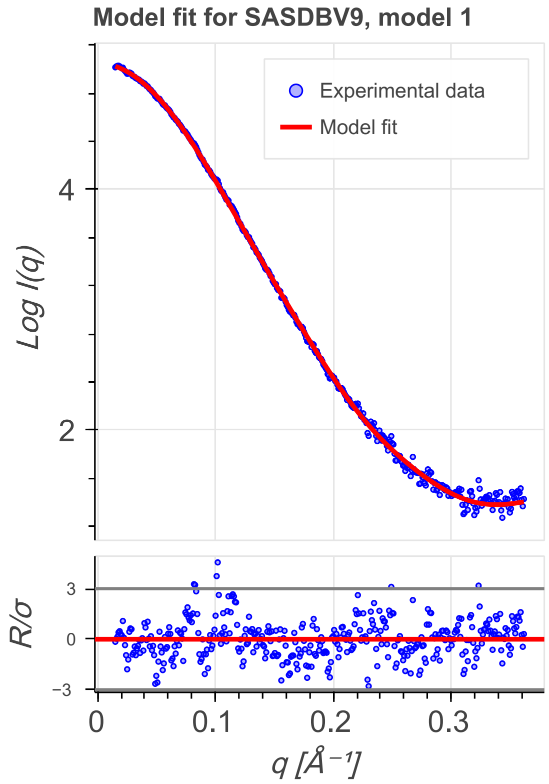
Fit of model(s) to SAS data

χ² goodness of fit and cormap analysis ?

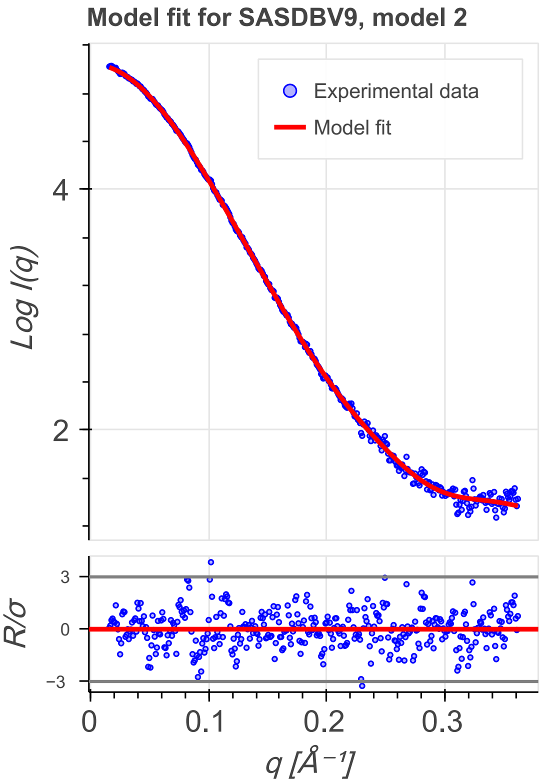
Model and fits displayed below were obtained from SASBDB. χ² values are a measure of fit of the model to data. A perfect fit has a χ² value of 1.0. ATSAS datcmp was used for hypothesis testing. All data sets are similar (i.e. the fit and the data collected) is the null hypothesis. p-value is a measure of evidence against the null hypothesis, smaller the value, the stronger the evidence that you should reject the null hypothesis.

SASDB ID	Model	χ²	p-value
SASDBV9	1	1.28	2.22E-02
SASDBV9	2	1.10	5.56E-03
SASDBW9	1	1.97	1.10E-05
SASDBX9	1	2.86	0.00E+00
SASDBY9	1	2.02	3.00E-06
SASDBZ9	1	1.94	0.00E+00

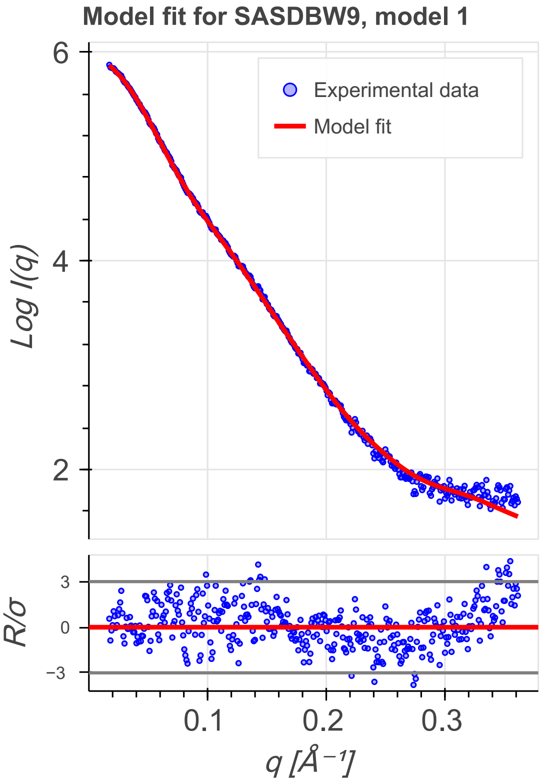
Model fit for SASDBV9 (fit/model number 1): Residual value plot is a measure to assess fit to the data. Residual values should be equally and randomly spaced around the horizontal axis.



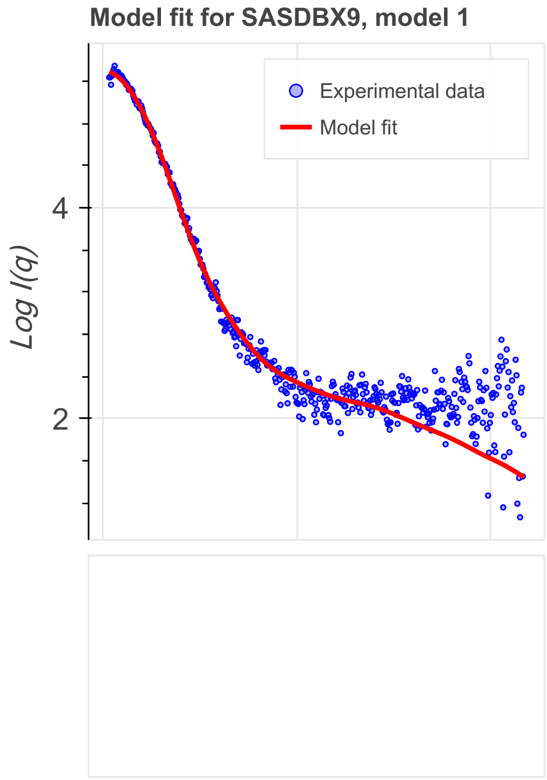
Model fit for SASDBV9 (fit/model number 2): Residual value plot is a measure to assess fit to the data. Residual values should be equally and randomly spaced around the horizontal axis.



Model fit for SASDBW9 (fit/model number 1): Residual value plot is a measure to assess fit to the data. Residual values should be equally and randomly spaced around the horizontal axis.

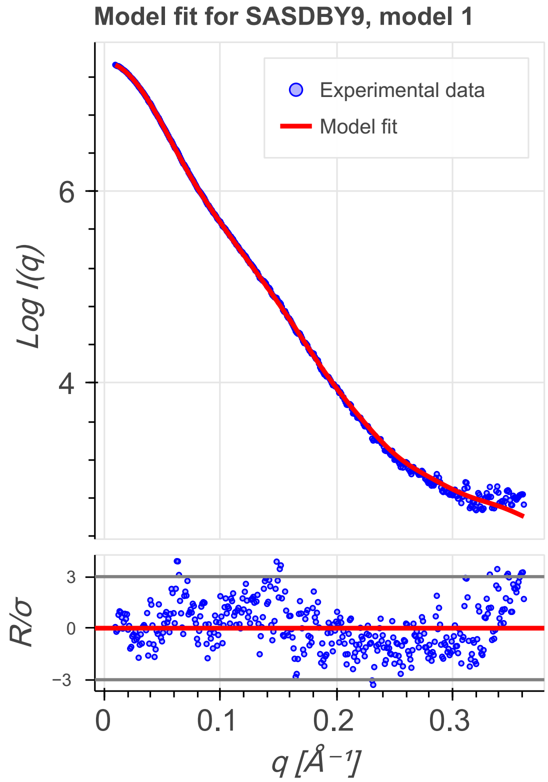


Model fit for SASDBX9 (fit/model number 1): Residual value plot is a measure to assess fit to the data. Residual values should be equally and randomly spaced around the horizontal axis.



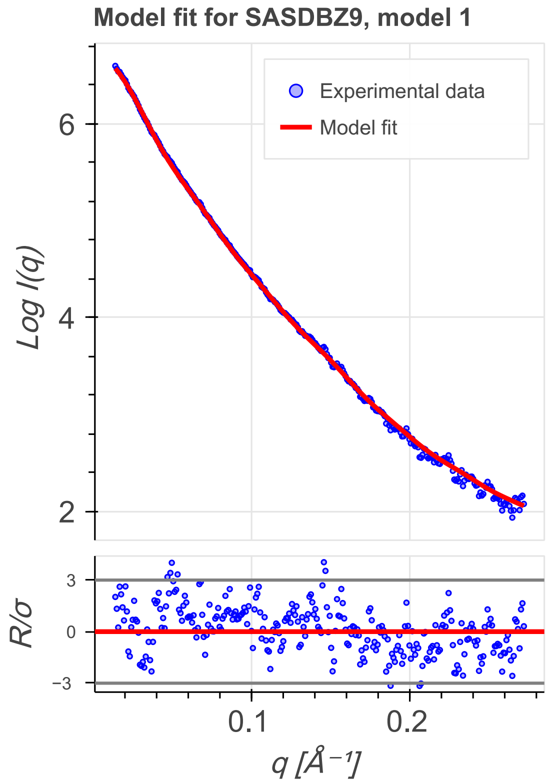
Model fit for SASDBX9, model 1

Model fit for SASDBY9 (fit/model number 1): Residual value plot is a measure to assess fit to the data. Residual values should be equally and randomly spaced around the horizontal axis.



Model fit for SASDBY9, model 1

Model fit for SASDBZ9 (fit/model number 1): Residual value plot is a measure to assess fit to the data. Residual values should be equally and randomly spaced around the horizontal axis.



3DEM volume

Validation for this section is under development.

2DEM class average

Validation for this section is under development.

Fit of model to data used for validation ?

Validation for this section is under development.

Acknowledgements

Development of integrative model validation metrics, implementation of a model validation pipeline, and creation of a validation report for integrative structures, are funded by NSF ABI awards (DBI-1756248, DBI-2112966, DBI-2112967, DBI-2112968, and DBI-1756250). The PDB-Dev team and members of Sali labcontributed model validation metrics and software packages.

Implementation of validation methods for SAS data and SAS-based models are funded byRCSB PDB (grant number DBI-1832184). Dr. Stephen Burley, Dr. John Westbrook, and Dr. Jasmine Young from RCSB PDB, Dr. Jill Trewhella, Dr. Dina Schneidman, and members of the SASBDB repository are acknowledged for their advice and support in implementing SAS validation methods.

Members of the wwPDB Integrative/Hybrid Methods Task Force provided recommendations and community support for the project.