# Full wwPDB Integrative Structure Validation Report

## June 05, 2020 -- 07:28 PM

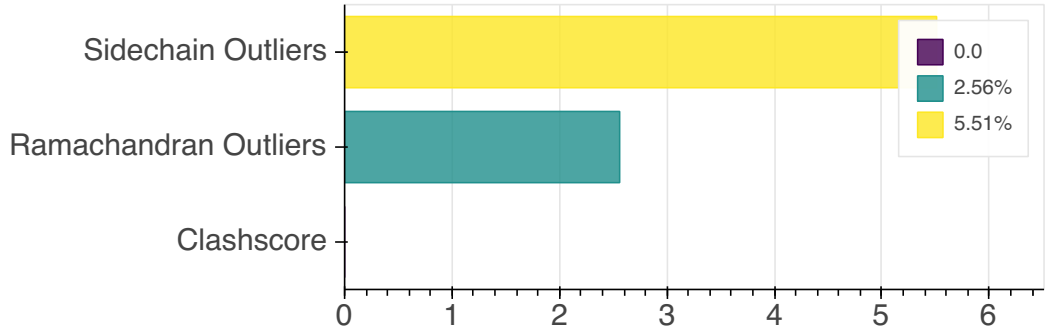
**The following software were used in the production of this report:**

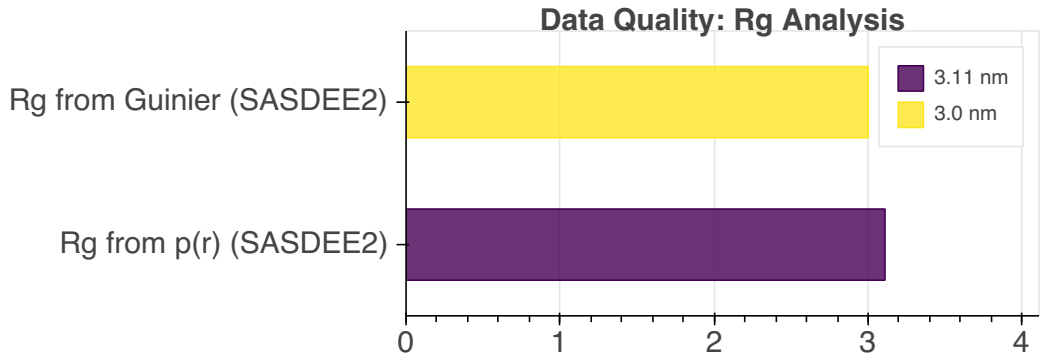
*Molprobity : Version 4.4*
*Integrative Modeling Validation Package : Version 1.0*

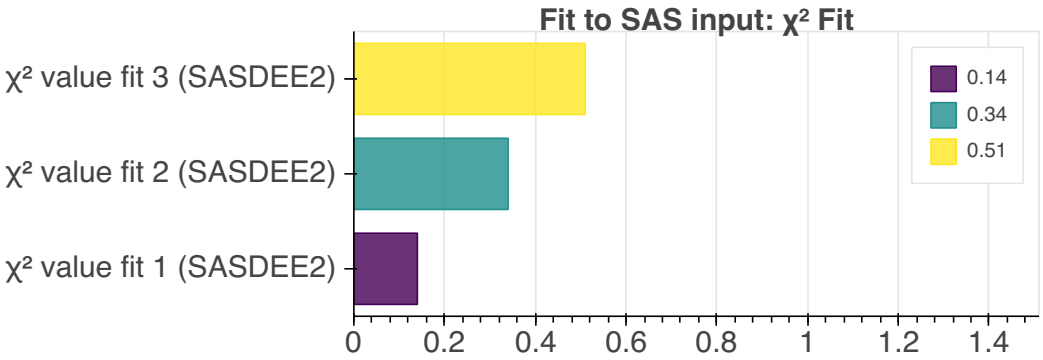
| PDB ID | PDBDEV_00000027 |
|---|---|
| Molecule Name | A metastable contact and structural disorder in the estrogen receptor transactivation domain |
| Title | A metastable contact and structural disorder in the estrogen receptor transactivation domain |
| Authors | Peng Y;Cao S;Kiselar J;Xiao X;Du Z;Hsien A;Ko S;Chen Y;Agrawal P;Zheng W;Shi W;Jiang W;Yang L;Chance MR;Surewicz WK;Buck M;Yang S |

## Overall quality

**Model Quality: Molprobity Analysis**






## Ensemble information

*This entry consists of 0 distinct ensemble.*

## Summary

*This entry consists of 10 unique models, with 1 subunits in each model. A total of 2 datasets or restraints was used to build this entry. Each model is represented by 1 rigid bodies and 0 flexible or non-rigid units.*

## Entry composition

*There are 10 unique types of models in this entry.These models are titled None/?, None/?, None/?, None/?, None/?, None/?, None/?, None/?, None/?, None/? respectively.*

| Model ID | Subunit number | Subunit ID | Subunit name | Chain ID | Total residues |
|---|---|---|---|---|---|

| Model ID | Subunit number | Subunit ID | Subunit name | Chain ID | Total residues |
|---|---|---|---|---|---|
| 1 | 1 | 1 | Estrogen receptor | A | 184 |
| 2 | 1 | 1 | Estrogen receptor | A | 184 |
| 3 | 1 | 1 | Estrogen receptor | A | 184 |
| 4 | 1 | 1 | Estrogen receptor | A | 184 |
| 5 | 1 | 1 | Estrogen receptor | A | 184 |
| 6 | 1 | 1 | Estrogen receptor | A | 184 |
| 7 | 1 | 1 | Estrogen receptor | A | 184 |
| 8 | 1 | 1 | Estrogen receptor | A | 184 |
| 9 | 1 | 1 | Estrogen receptor | A | 184 |
| 10 | 1 | 1 | Estrogen receptor | A | 184 |

## Datasets used for modeling

*There are 2 unique datasets used to build the models in this entry.*

| ID | Dataset type | Database name | Data access code |
|---|---|---|---|
| 1 | SAS data | SASBDB | SASDEE2 |
| 2 | unspecified | Not listed | None |

## Representation

*This entry has only one representation and includes 1 rigid bodies and 0 flexible units.*

| Chain ID | Rigid bodies | Non-rigid segments |
|---|---|---|
| A | 1-184:None. | - |

## Methodology and software

| Step number | Protocol ID | Method name | Method type | Number of computed models | Multi state modeling | Multi scale modeling |
|---|---|---|---|---|---|---|
| 1 | 1 | ? | Modeling estrogen receptor N-terminal domain | None | False | False |

*There is 1 software package reported in this entry.*

| ID | Software name | Software version | Software classification | Software location |
|---|---|---|---|---|
| 1 | iSPOT | None | model building | http://www.theyanglab.org/ispot/index.html |

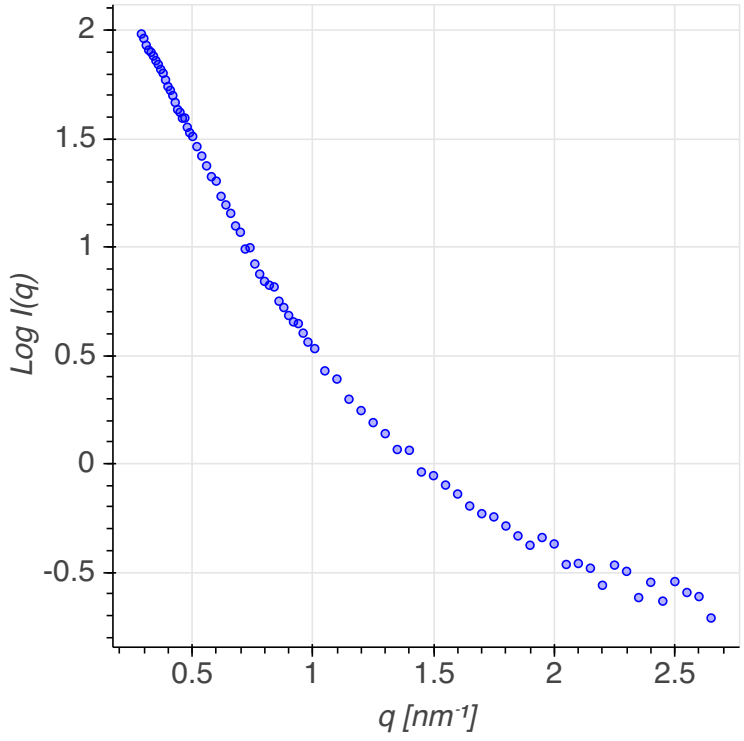
# Data quality

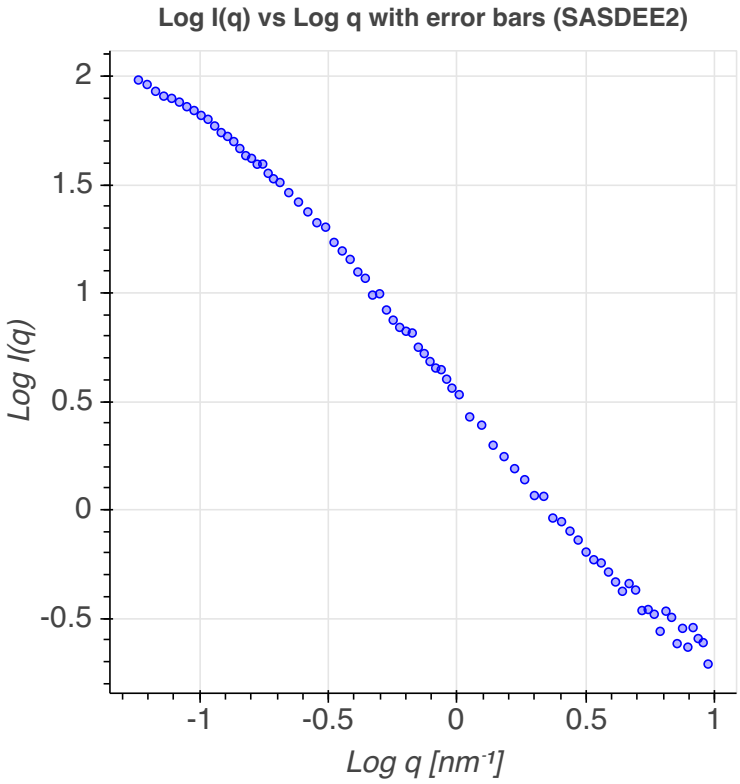
## Scattering profile

SAS data used in this integrative model was obtained from 1 deposited SASBDB entry (entries).

Scattering profile for SASDEE2: 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.

**Log I(q) vs q with error bars (SASDEE2)**






## Key experimental estimates

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

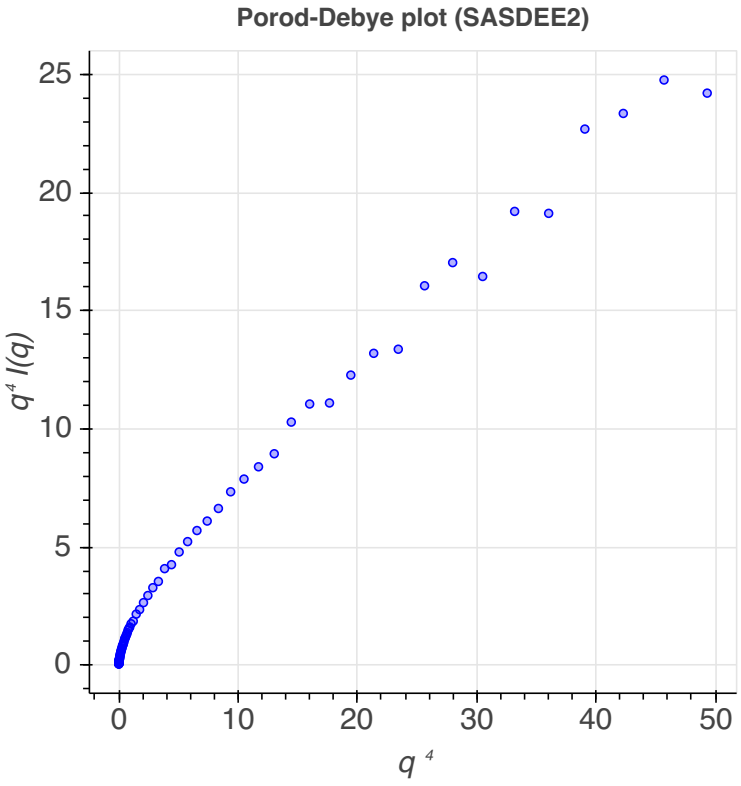
| SASDB ID | Sequence MW | Experimental MW | Porod MW |
|---|---|---|---|
| SASDEE2 | 20.175 kDa | 20.180 kDa | N/A |

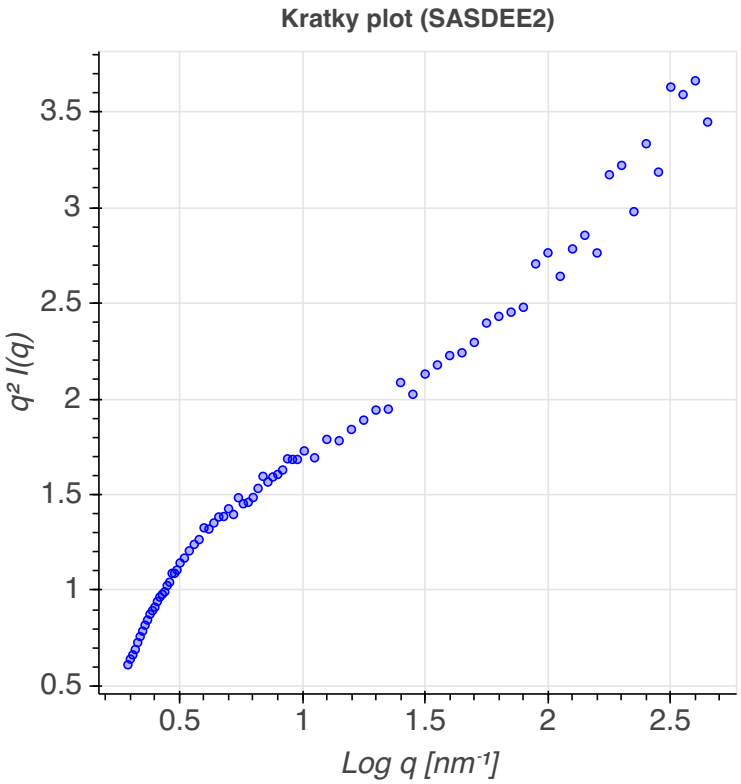
Volume estimates from experiments and analysis: estimated volume can be compared to Porod volume obtained from scattering profiles.

| SASDB ID | Estimated volume | Estimated volume method | Porod volume |
|---|---|---|---|
| SASDEE2 | None | None | N/A |

## Flexibility analysis

Flexibility analysis for SASDEE2: 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.



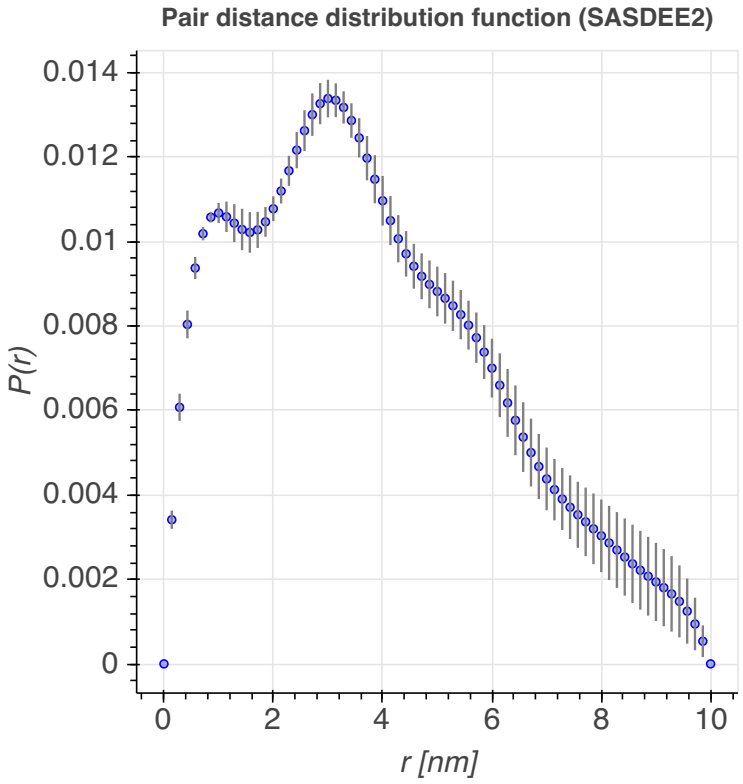

## Pair-distance distribution analysis

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). Rg can be estimated from integrating the p(r) function. Agreement between the p(r)

and Guinier-determined Rg (table below) is a good measure of the self-consistency of the SAS profile. Rg is a measure for the overall size of a macromolecule; e.g. a protein with a smaller Rg is more compact than a protein with a larger Rg, provided both have the same molecular weight (MW). The point where p(r) is decaying to zero is called Dmax and represents the maximum size of the particle.

| SASDB ID | Software used | Dmax | Dmax error | Rg | Rg error |
|---|---|---|---|---|---|
| SASDEE2 | ATSAS GNOM | 10.00 nm | N/A | 3.110 nm | None nm |

P(r) for SASDEE2: The value of P(r) should be zero beyond r=Dmax.



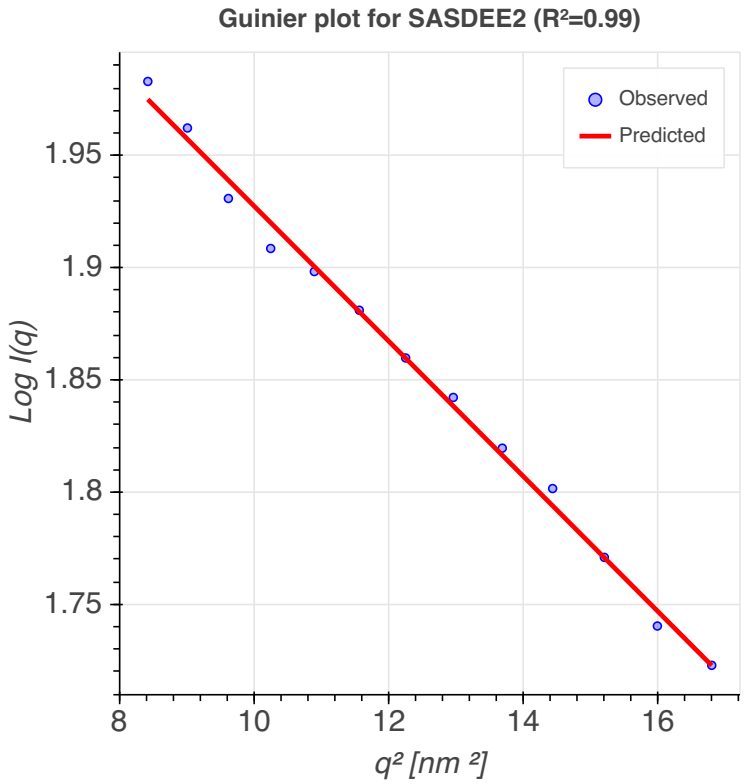

## Guinier analysis

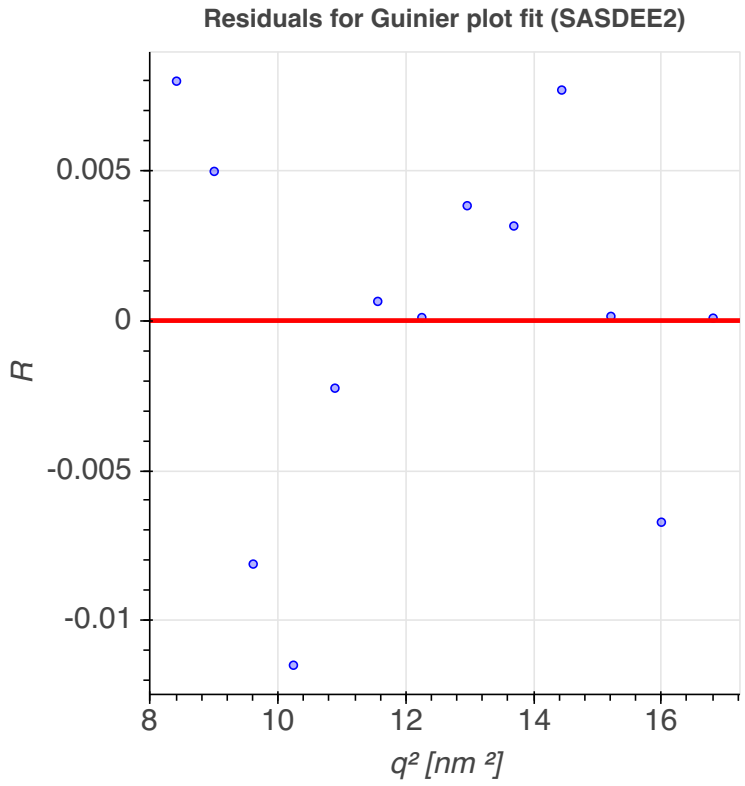
Guinier analysis: agreement between the p(r) and Guinier-determined Rg (table below) is a good measure of the self-consistency of the SAS profile. Molecular weight estimates can also be compared to Porod and sample molecular weights for consistency.

| SASDB ID | Rg | Rg error | MW | MW error |
|---|---|---|---|---|
| SASDEE2 | 3.0 nm | 0.160 nm | N/A | N/A |

Guinier analysis for SASDEE2: 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 samesize. 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.




## Model quality

### Standard geometry

*There are 13530 bond outliers in this entry.*

| Bond type | Observed distance (Å) | Ideal distance (Å) | Number of outliers |
|---|---|---|---|
| ND2--HD22 | 1.008 | 0.86 | 109 |
| N--H | 1.008 | 0.86 | 1609 |
| NE2--HE2 | 1.008 | 0.86 | 39 |
| NH1--HH12 | 1.008 | 0.86 | 89 |
| CD2--HD2 | 1.078 | 0.93 | 199 |
| CE1--HE1 | 1.078 | 0.93 | 199 |
| CE2--HE2 | 1.078 | 0.93 | 159 |
| NH1--HH11 | 1.009 | 0.86 | 89 |
| ND2--HD21 | 1.009 | 0.86 | 109 |
| NE2--HE22 | 1.009 | 0.86 | 99 |
| CZ--HZ | 1.079 | 0.93 | 49 |
| NH2--HH22 | 1.009 | 0.86 | 89 |
| NE2--HE21 | 1.008 | 0.86 | 99 |
| NE--HE | 1.009 | 0.86 | 89 |
| CD1--HD1 | 1.078 | 0.93 | 159 |
| NH2--HH21 | 1.009 | 0.86 | 89 |
| CG--HG3 | 1.089 | 0.97 | 649 |
| CA--HA | 1.088 | 0.97 | 1659 |
| CB--HB | 1.088 | 0.97 | 149 |
| CD--HD2 | 1.089 | 0.97 | 359 |
| CB--HB2 | 1.088 | 0.97 | 1509 |
| CD2--HD22 | 1.088 | 0.97 | 189 |

| Bond type | Observed distance (Å) | Ideal distance (Å) | Number of outliers |
|---|---|---|---|
| CE--HE1 | 1.088 | 0.97 | 59 |
| CB--HB3 | 1.088 | 0.97 | 1509 |
| CB--HB1 | 1.088 | 0.97 | 189 |
| CG2--HG21 | 1.089 | 0.97 | 149 |
| CA--HA2 | 1.089 | 0.97 | 179 |
| CD2--HD21 | 1.088 | 0.97 | 189 |
| CG--HG2 | 1.088 | 0.97 | 649 |
| CA--HA3 | 1.089 | 0.97 | 179 |
| CD--HD3 | 1.089 | 0.97 | 359 |
| CD1--HD11 | 1.089 | 0.97 | 209 |
| CD1--HD13 | 1.088 | 0.97 | 209 |
| NZ--HZ3 | 1.009 | 0.89 | 49 |
| CG1--HG12 | 1.089 | 0.97 | 79 |
| CG2--HG22 | 1.088 | 0.97 | 149 |
| N--H3 | 1.009 | 0.89 | 9 |
| CG2--HG23 | 1.089 | 0.97 | 149 |
| OG--HG | 0.959 | 0.84 | 139 |
| CE--HE2 | 1.089 | 0.97 | 109 |
| CD1--HD12 | 1.089 | 0.97 | 209 |
| CG1--HG11 | 1.089 | 0.97 | 59 |
| NZ--HZ2 | 1.009 | 0.89 | 49 |
| CG1--HG13 | 1.088 | 0.97 | 79 |
| CD2--HD23 | 1.089 | 0.97 | 189 |

| Bond type | Observed distance (Å) | Ideal distance (Å) | Number of outliers |
|---|---|---|---|
| OG1--HG1 | 0.959 | 0.84 | 69 |
| CE--HE3 | 1.089 | 0.97 | 109 |
| NZ--HZ1 | 1.009 | 0.89 | 49 |
| OH--HH | 0.959 | 0.84 | 109 |
| CG--HG | 1.089 | 0.97 | 189 |
| N--H2 | 1.009 | 0.89 | 9 |
| N--H1 | 1.009 | 0.89 | 9 |

*There are 316 angle outliers in this entry.*

| Angle type | Observed angle (°) | Ideal angle (°) | Number of outliers |
|---|---|---|---|
| C-N-H | 112.269 | 124.3 | 122 |
| HG2-CG-HG3 | 97.708 | 110.0 | 8 |
| CG-CB-HB2 | 120.202 | 108.0 | 7 |
| HD22-CD2-HD23 | 97.918 | 110.0 | 2 |
| HG12-CG1-HG13 | 92.282 | 110.0 | 0 |
| HB2-CB-HB3 | 97.993 | 110.0 | 31 |
| HZ1-NZ-HZ3 | 122.371 | 109.0 | 2 |
| CA-N-H | 126.273 | 114.0 | 7 |
| CB-OG1-HG1 | 93.037 | 110.0 | 0 |
| CB-CA-HA | 96.938 | 109.0 | 3 |
| N-CA-HA | 97.858 | 110.0 | 6 |
| HD21-CD2-HD22 | 97.003 | 110.0 | 1 |
| HB1-CB-HB2 | 96.99 | 110.0 | 5 |
| CG-CB-HB3 | 95.827 | 108.0 | 7 |

| Angle type | Observed angle (°) | Ideal angle (°) | Number of outliers |
|---|---|---|---|
| HD2-CD-HD3 | 122.233 | 110.0 | 7 |
| C-CA-HA | 96.951 | 109.0 | 10 |
| CE-NZ-HZ2 | 94.864 | 110.0 | 0 |
| CA-CB-HB3 | 96.927 | 109.0 | 9 |
| CA-CB-HB2 | 121.002 | 109.0 | 4 |
| HD12-CD1-HD13 | 97.874 | 110.0 | 1 |
| HD11-CD1-HD12 | 95.703 | 110.0 | 0 |
| HG22-CG2-HG23 | 96.722 | 109.0 | 3 |
| SD-CE-HE1 | 95.744 | 109.0 | 1 |
| HG21-CG2-HG23 | 95.829 | 110.0 | 0 |
| CB-CG-HG3 | 121.179 | 109.0 | 2 |
| CB-CG1-HG11 | 122.984 | 109.0 | 0 |
| CG-CD2-HD23 | 121.251 | 109.0 | 1 |
| NZ-CE-HE2 | 121.714 | 108.0 | 0 |
| HD21-CD2-HD23 | 96.708 | 110.0 | 1 |
| N-CA-HA2 | 96.384 | 110.0 | 0 |
| HE2-CE-HE3 | 96.468 | 110.0 | 0 |
| CB-CG-HG2 | 121.139 | 109.0 | 2 |
| CD-CG-HG2 | 121.262 | 108.0 | 0 |
| CB-CG2-HG22 | 97.308 | 110.0 | 1 |
| HG11-CG1-HG13 | 97.438 | 110.0 | 3 |
| SD-CE-HE2 | 121.941 | 109.0 | 0 |
| HE1-CE-HE3 | 97.073 | 110.0 | 0 |

| Angle type | Observed angle (°) | Ideal angle (°) | Number of outliers |
|---|---|---|---|
| CZ-CE2-HE2 | 107.364 | 120.2 | 0 |
| HG11-CG1-HG12 | 97.195 | 110.0 | 0 |
| CZ-OH-HH | 122.334 | 110.0 | 1 |
| HH21-NH2-HH22 | 107.333 | 120.0 | 0 |
| HB1-CB-HB3 | 97.473 | 110.0 | 1 |
| OG-CB-HB2 | 121.604 | 109.0 | 0 |
| CD-CG-HG3 | 97.925 | 110.0 | 2 |
| N-CD-HD3 | 121.548 | 109.0 | 0 |
| CG-CD1-HD12 | 121.475 | 109.0 | 0 |
| N-CD-HD2 | 121.456 | 109.0 | 0 |
| CG-CD2-HD22 | 121.003 | 109.0 | 1 |
| CD2-CG-HG | 95.7 | 108.0 | 0 |
| CZ-NH2-HH22 | 107.711 | 120.0 | 0 |
| CG2-CB-HB | 95.715 | 108.0 | 0 |
| HZ2-NZ-HZ3 | 121.179 | 109.0 | 1 |
| OG-CB-HB3 | 96.789 | 109.0 | 0 |
| CB-CG2-HG23 | 121.082 | 109.0 | 1 |
| CG-CD-HD3 | 121.18 | 109.0 | 0 |
| HD11-CD1-HD13 | 97.867 | 110.0 | 0 |
| C-CA-HA3 | 96.869 | 109.0 | 0 |
| HA2-CA-HA3 | 96.936 | 109.0 | 1 |
| CZ-NH1-HH11 | 107.88 | 120.0 | 0 |
| CG-ND2-HD21 | 107.932 | 120.0 | 0 |

| Angle type | Observed angle (°) | Ideal angle (°) | Number of outliers |
|---|---|---|---|
| CA-CB-HB1 | 121.049 | 109.0 | 0 |
| NZ-CE-HE3 | 120.023 | 108.0 | 0 |

## Too-close contacts

*The following all-atom clashscore is based on a MolProbity analysis. All-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The table below contains clashscores for all the models in this entry.*

| Model ID | Clash score | Number of clashes |
|---|---|---|
| Model 1 | 0.00 | 0 |
| Model 10 | 0.00 | 0 |
| Model 2 | 0.00 | 0 |
| Model 3 | 0.00 | 0 |
| Model 4 | 0.00 | 0 |
| Model 5 | 0.00 | 0 |
| Model 6 | 0.00 | 0 |
| Model 7 | 0.00 | 0 |
| Model 8 | 0.00 | 0 |
| Model 9 | 0.00 | 0 |

*All 0 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.*

## Torsion angles: Protein backbone

*In the following table, Ramachandran outliers are listed. The Analysed column shows the number of residues for which the backbone conformation was analysed.*

| Model ID | Analyzed | Favored | Allowed | Outliers |
|---|---|---|---|---|
| 1 | 182 | 147 | 32 | 3 |
| 2 | 182 | 150 | 28 | 4 |
| 3 | 182 | 169 | 10 | 3 |

| Model ID | Analyzed | Favored | Allowed | Outliers |
|---|---|---|---|---|
| 4 | 182 | 154 | 26 | 2 |
| 5 | 182 | 161 | 14 | 7 |
| 6 | 182 | 153 | 23 | 6 |
| 7 | 182 | 159 | 19 | 4 |
| 8 | 182 | 153 | 23 | 6 |
| 9 | 182 | 156 | 19 | 7 |
| 10 | 182 | 155 | 23 | 4 |

*Detailed list of outliers are tabulated below.*

| Model ID | Chain and res ID | Residue type |
|---|---|---|
| 1 | A:55 | PRO |
| 1 | A:74 | GLY |
| 1 | A:136 | PRO |
| 2 | A:21 | 1ASN |
| 2 | A:35 | 1LEU |
| 2 | A:55 | 1PRO |
| 2 | A:129 | 1PRO |
| 3 | A:55 | PRO |
| 3 | A:72 | VAL |
| 3 | A:124 | HIS |
| 4 | A:55 | PRO |
| 4 | A:99 | PRO |
| 5 | A:10 | SER |
| 5 | A:11 | GLY |

| Model ID | Chain and res ID | Residue type |
|---|---|---|
| 5 | A:14 | LEU |
| 5 | A:55 | PRO |
| 5 | A:76 | THR |
| 5 | A:117 | LEU |
| 5 | A:144 | ALA |
| 6 | A:55 | PRO |
| 6 | A:70 | ALA |
| 6 | A:103 | VAL |
| 6 | A:126 | GLN |
| 6 | A:146 | PRO |
| 6 | A:163 | GLU |
| 7 | A:44 | LEU |
| 7 | A:47 | SER |
| 7 | A:55 | PRO |
| 7 | A:110 | LEU |
| 8 | A:32 | LYS |
| 8 | A:55 | PRO |
| 8 | A:79 | PRO |
| 8 | A:86 | ALA |
| 8 | A:90 | GLY |
| 8 | A:144 | ALA |
| 9 | A:55 | PRO |
| 9 | A:57 | GLY |

| Model ID | Chain and res ID | Residue type |
|---|---|---|
| 9 | A:69 | ASN |
| 9 | A:70 | ALA |
| 9 | A:88 | ALA |
| 9 | A:96 | GLY |
| 9 | A:126 | GLN |
| 10 | A:42 | VAL |
| 10 | A:55 | PRO |
| 10 | A:57 | GLY |
| 10 | A:141 | VAL |

## Torsion angles: Protein sidechains

*In the following table, sidechain outliers are listed. The Analysed column shows the number of residues for which the sidechain conformation was analysed.*

| Model ID | Analyzed | Favored | Allowed | Outliers |
|---|---|---|---|---|
| 1 | 147 | 123 | 14 | 10 |
| 2 | 147 | 133 | 12 | 2 |
| 3 | 147 | 132 | 9 | 6 |
| 4 | 147 | 125 | 16 | 6 |
| 5 | 147 | 108 | 24 | 15 |
| 6 | 147 | 126 | 13 | 8 |
| 7 | 147 | 116 | 19 | 12 |
| 8 | 147 | 119 | 21 | 7 |
| 9 | 147 | 124 | 15 | 8 |
| 10 | 147 | 119 | 21 | 7 |

*Detailed list of outliers are tabulated below.*

| Model ID | Chain and res ID | Residue type |
|---|---|---|
| 1 | A:2 | THR |
| 1 | A:18 | ILE |
| 1 | A:26 | LEU |
| 1 | A:72 | VAL |
| 1 | A:109 | MET |
| 1 | A:116 | GLN |
| 1 | A:151 | ARG |
| 1 | A:165 | LEU |
| 1 | A:168 | THR |
| 1 | A:184 | TYR |
| 2 | A:106 | SER |
| 2 | A:177 | GLU |
| 3 | A:17 | GLN |
| 3 | A:26 | LEU |
| 3 | A:33 | ILE |
| 3 | A:99 | PRO |
| 3 | A:102 | SER |
| 3 | A:140 | THR |
| 4 | A:12 | MET |
| 4 | A:51 | VAL |
| 4 | A:91 | SER |
| 4 | A:97 | PHE |
| 4 | A:112 | HIS |

| Model ID | Chain and res ID | Residue type |
|---|---|---|
| 4 | A:140 | THR |
| 5 | A:14 | LEU |
| 5 | A:39 | LEU |
| 5 | A:42 | VAL |
| 5 | A:43 | TYR |
| 5 | A:60 | TYR |
| 5 | A:97 | PHE |
| 5 | A:103 | VAL |
| 5 | A:117 | LEU |
| 5 | A:120 | PHE |
| 5 | A:135 | GLU |
| 5 | A:154 | SER |
| 5 | A:164 | ARG |
| 5 | A:168 | THR |
| 5 | A:169 | ASN |
| 5 | A:181 | GLU |
| 6 | A:4 | THR |
| 6 | A:52 | TYR |
| 6 | A:85 | GLU |
| 6 | A:110 | LEU |
| 6 | A:134 | ASN |
| 6 | A:140 | THR |
| 6 | A:165 | LEU |

| Model ID | Chain and res ID | Residue type |
|---|---|---|
| 6 | A:177 | GLU |
| 7 | A:1 | MET |
| 7 | A:4 | THR |
| 7 | A:31 | LEU |
| 7 | A:35 | LEU |
| 7 | A:45 | ASP |
| 7 | A:91 | SER |
| 7 | A:126 | GLN |
| 7 | A:128 | VAL |
| 7 | A:132 | LEU |
| 7 | A:165 | LEU |
| 7 | A:180 | LYS |
| 7 | A:183 | ARG |
| 8 | A:44 | LEU |
| 8 | A:72 | VAL |
| 8 | A:108 | LEU |
| 8 | A:140 | THR |
| 8 | A:143 | GLU |
| 8 | A:159 | GLN |
| 8 | A:168 | THR |
| 9 | A:6 | HIS |
| 9 | A:15 | LEU |
| 9 | A:19 | GLN |

| Model ID | Chain and res ID | Residue type |
|---|---|---|
| 9 | A:104 | SER |
| 9 | A:126 | GLN |
| 9 | A:127 | GLN |
| 9 | A:174 | MET |
| 9 | A:178 | SER |
| 10 | A:35 | LEU |
| 10 | A:39 | LEU |
| 10 | A:42 | VAL |
| 10 | A:78 | LEU |
| 10 | A:100 | LEU |
| 10 | A:129 | PRO |
| 10 | A:176 | MET |

## Fit of model to data used for modeling

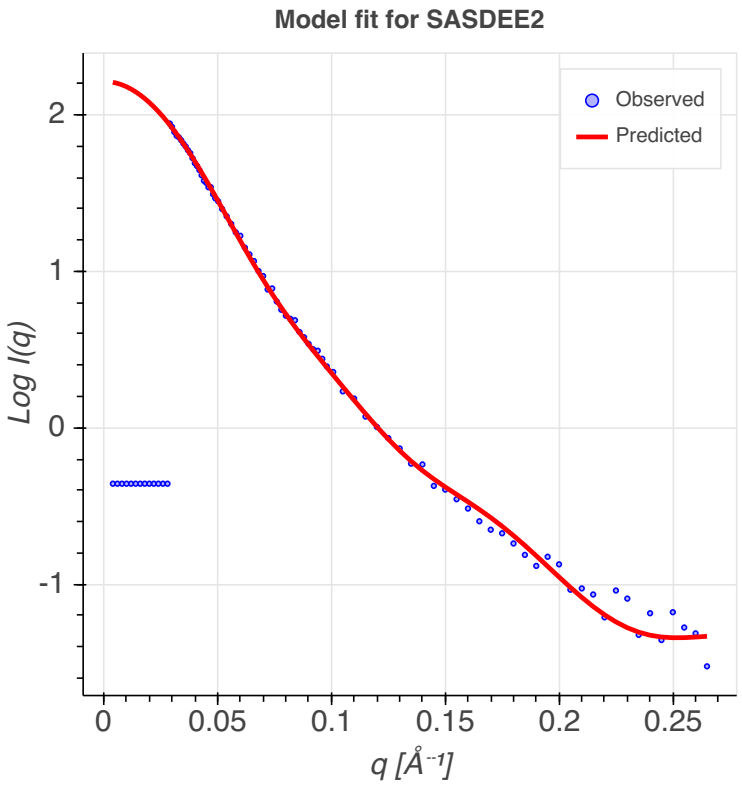
### Fit of model(s) to SAS data

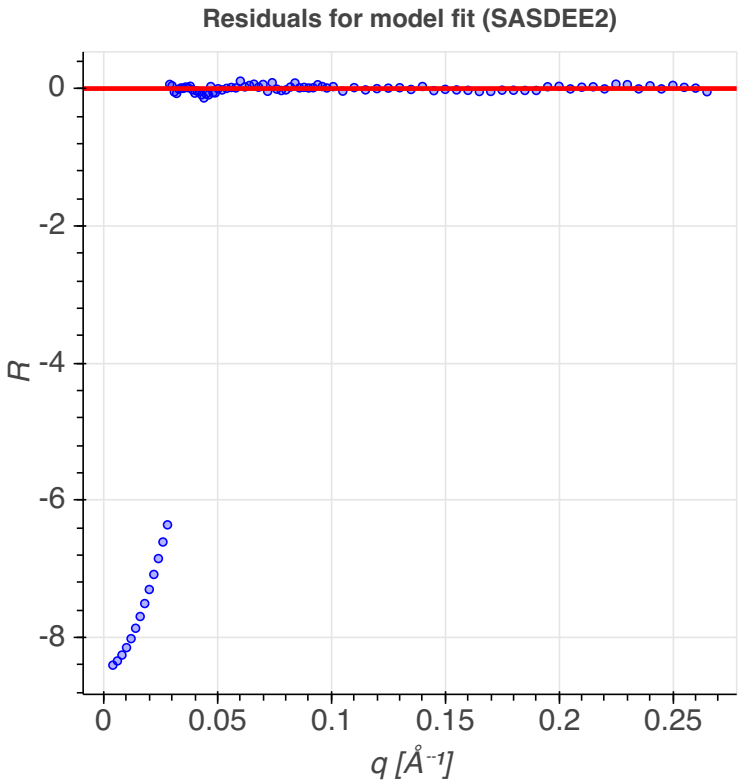
#### $\chi^2$ goodness of fit analysis

*Model and fits displayed below were obtained from SASBDB. $\chi^2$ values are a measure of fit of the model to data. A perfect fit has a $\chi^2$ value of zero.*

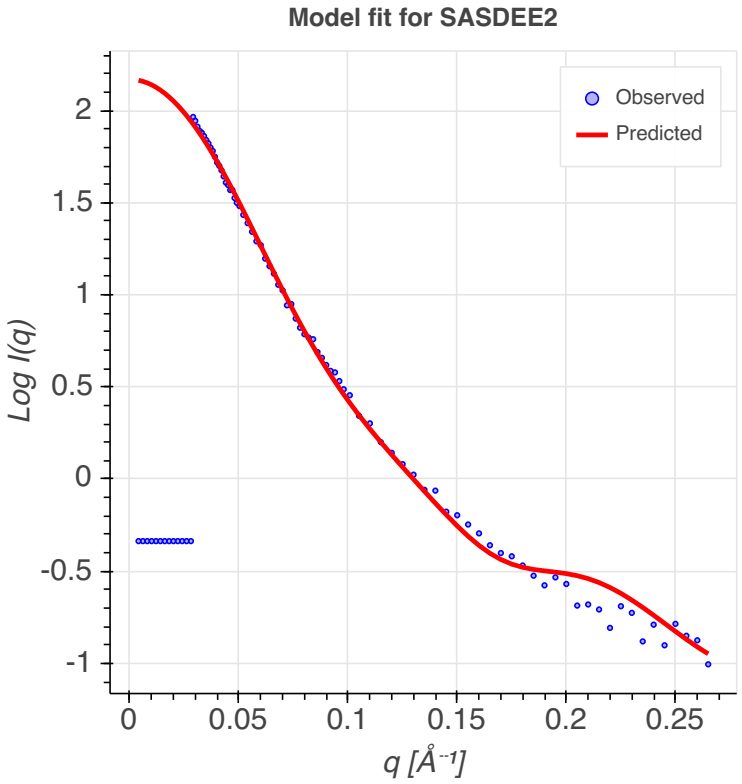
| SASDB ID | Model | $\chi^2$ |
|---|---|---|
| SASDEE2 | 1 | 2.73 |
| SASDEE2 | 2 | 2.32 |
| SASDEE2 | 3 | 1.98 |

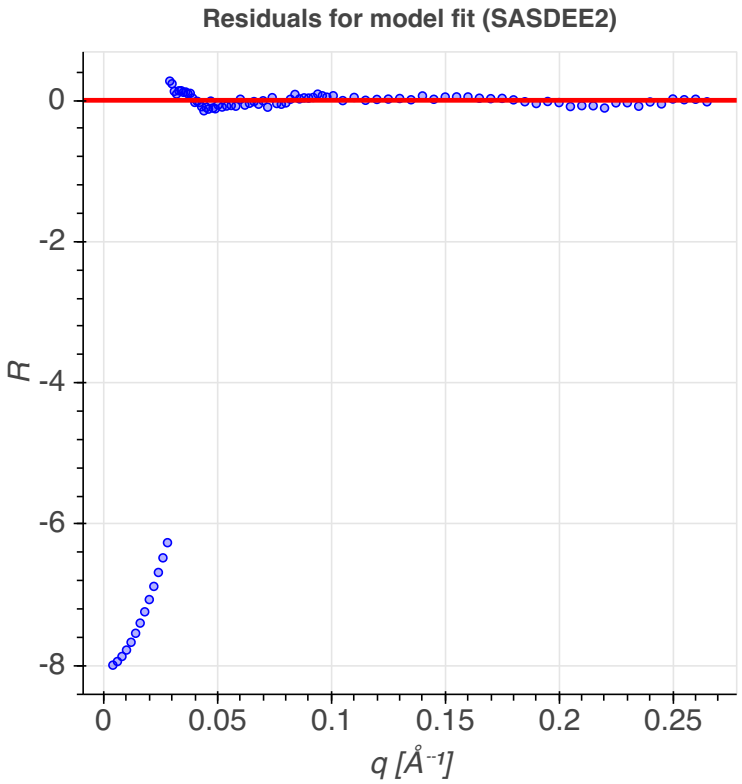
Model fit for SASDEE2 (fit/model number 1): Residual value plot is a measure to assess fit to the data. sResidual values should be equally and randomly spaced around the horizontal axis.



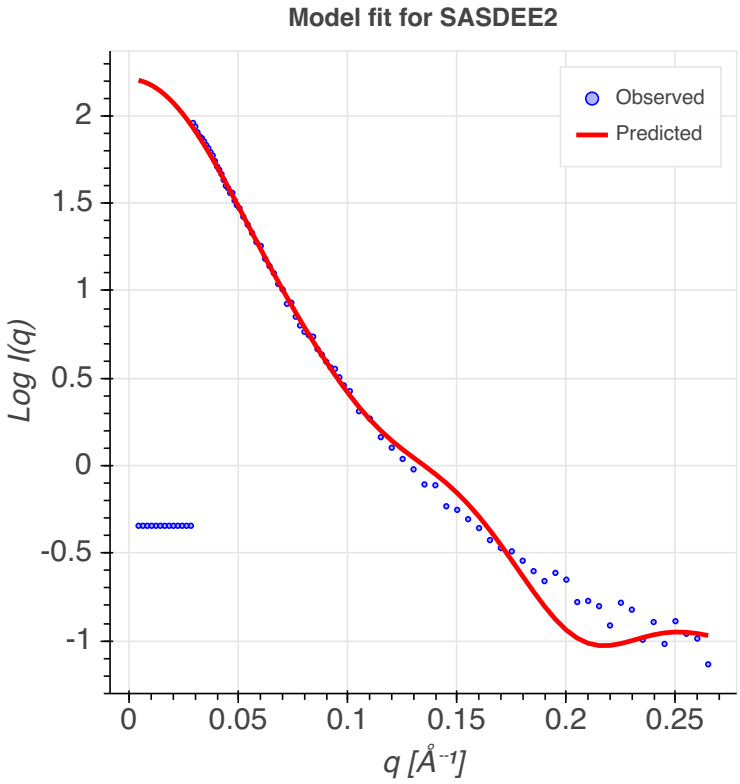



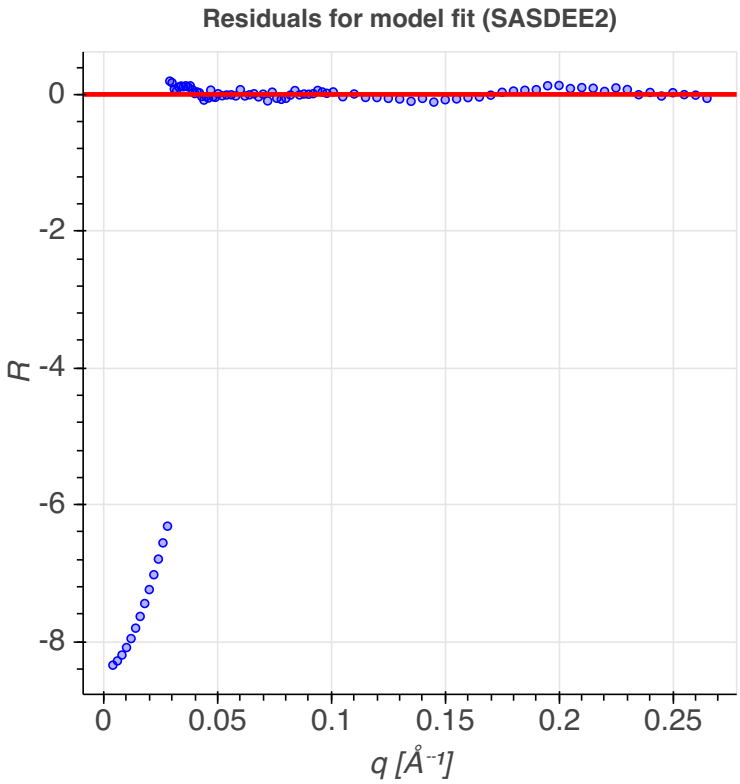
Model fit for SASDEE2 (fit/model number 2): Residual value plot is a measure to assess fit to the data. sResidual values should be equally and randomly spaced around the horizontal axis.



Model fit for SASDEE2 (fit/model number 3): Residual value plot is a measure to assess fit to the data. sResidual values should be equally and randomly spaced around the horizontal axis.



Fit of model to data not used for modeling

Uncertainty of data and model