

# Integrative Structure Validation Report ?

April 09, 2025 - 04:30 PM PDT

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

*Integrative Modeling Validation Version 2.0*

*Python-IHM Version 1.8*

*MolProbity Version 4.5.2*

*ATSAS Version 3.2.1 (r14885)*

*PyMOL Version 2.5.0*

|                   |   |
|-------------------|---|
| PDB ID            | 8ZZZ  |
| PDB-Dev ID        | PDBDEV_00000035   |
| Structure Title   | Rosetta model of human LRH-1 nuclear receptor generated with XL-MS, HDX-MS, and SAXS data |
| Structure Authors | Seacrist CD; Kuenze G; Hoffmann R; Burke J; Meiler J; Blind RD                            |
| Deposited on      | 2019-09-13  |

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

*We welcome your comments at [helpdesk@pdb-ihm.org](mailto:helpdesk@pdb-ihm.org)*

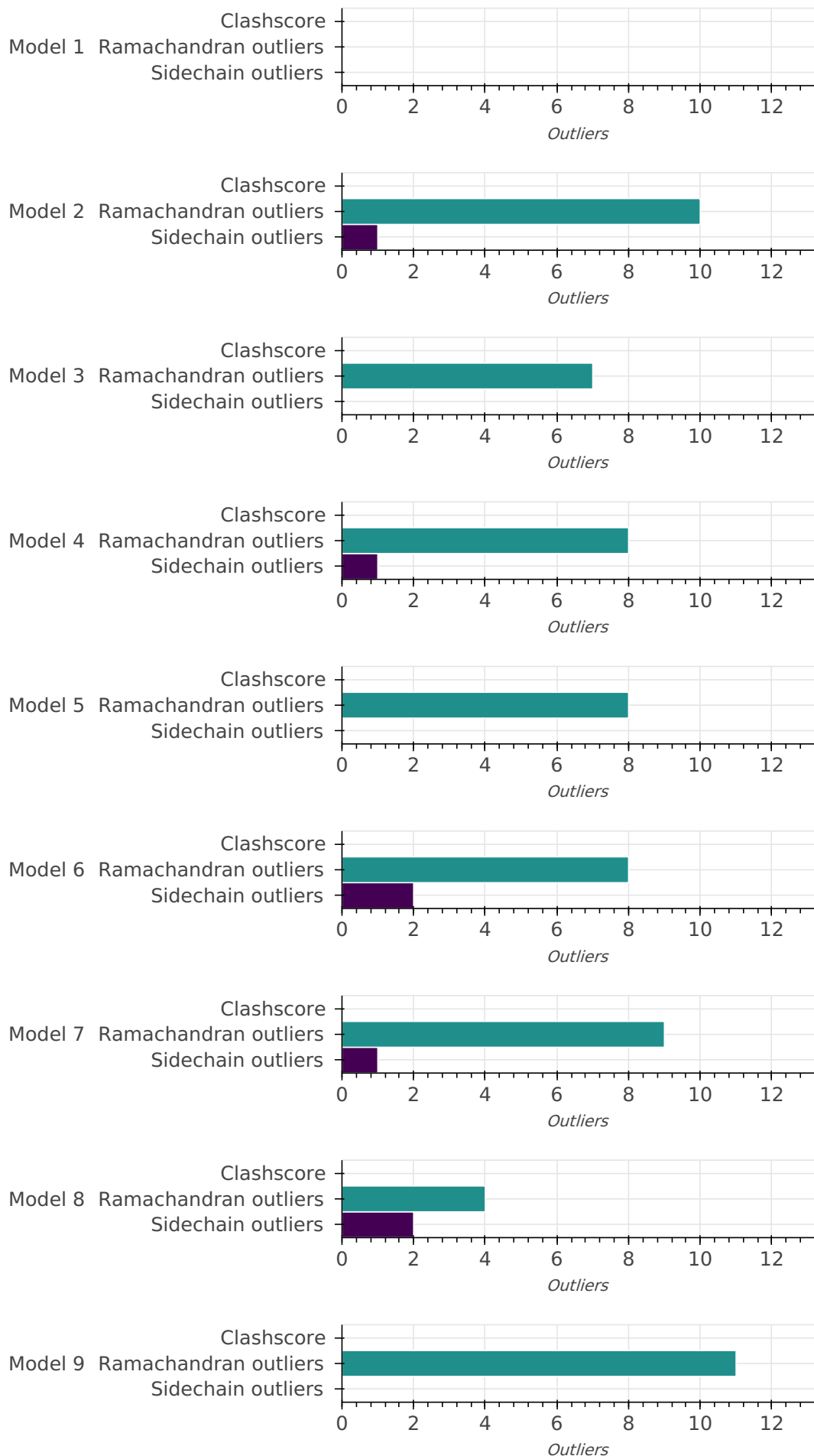
*A user guide is available at [https://pdb-ihm.org/validation\\_help.html](https://pdb-ihm.org/validation_help.html) with specific help available everywhere you see the ? symbol.*

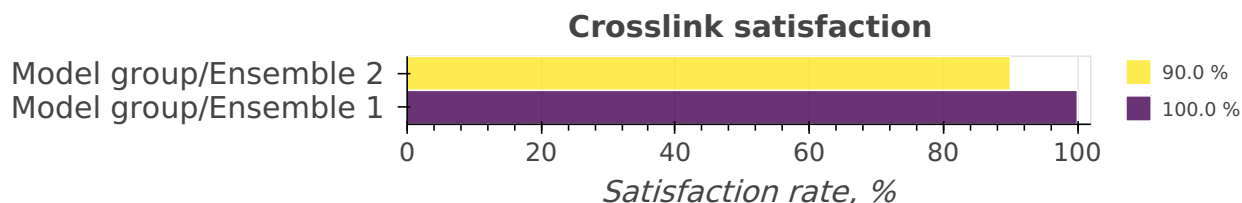
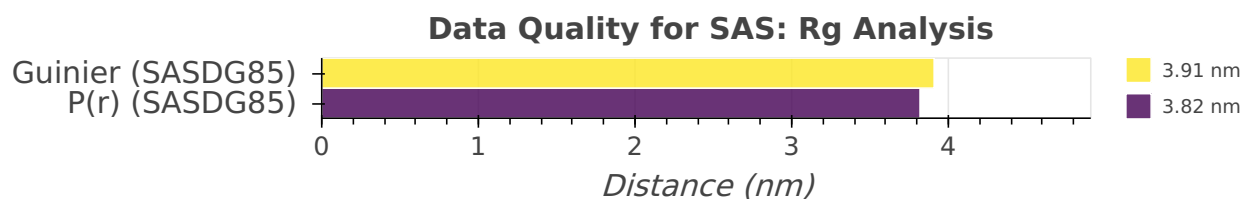
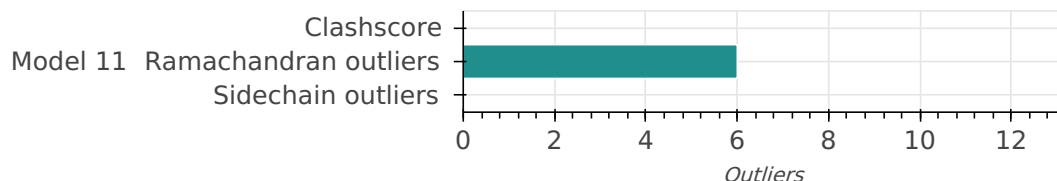
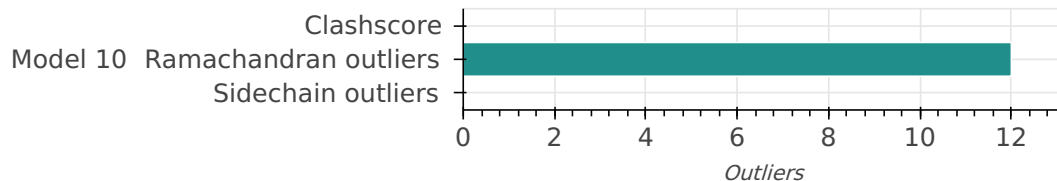
*List of references used to build this report is available [here](#).*

## Overall quality ?

*This validation report contains model quality assessments for all structures, data quality and fit to model assessments for SAS and crosslinking-MS 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: MolProbity Analysis





### Ensemble information ?

*This entry consists of 1 distinct ensemble(s).*

### Summary ?

*This entry consists of 11 model(s). A total of 9 datasets were used to build this entry.*

### Representation ?

*This entry has 2 representation(s).*

| ID | Model(s) | Entity ID | Molecule name | Chain(s) [auth] | Total residues | Rigid segments | Flexible segments | Model coverage/ Starting model coverage (%) | Scale |
|----|----------|-----------|---------------|-----------------|----------------|----------------|-------------------|---|-------|
|    |          |           |               |                 |                |                |                   |   |       |

| ID | Model(s) | Entity ID | Molecule name                  | Chain(s) [auth] | Total residues | Rigid segments | Flexible segments | Model coverage/<br>Starting model coverage (%) | Scale  |
|----|----------|-----------|--------------------------------|-----------------|----------------|----------------|-------------------|--|--------|
| 1  | 1        | 1         | LRH-1 DNA-binding domain       | A               | 102            | -              | 1-102             | 100.00 / 100.00                                | Atomic |
|    |          | 2         | LRH-1 Ligand-binding domain    | B               | 240            | -              | 1-240             | 100.00 / 100.00                                | Atomic |
|    |          | 4         | PGC1-alpha coactivator peptide | D               | 10             | -              | 1-10              | 100.00 / 100.00                                | Atomic |
|    |          | 5         | DNA strand 1                   | E               | 12             | 1-12           | -                 | 100.00 / 100.00                                | Atomic |
|    |          | 6         | DNA strand 2                   | F               | 12             | 1-12           | -                 | 100.00 / 100.00                                | Atomic |
|    |          | 7         | Phospholipid ligand            | X               | Non-polymeric  | -              | -                 | Not available / Not available                  | Atomic |
|    |          | 8         | Zinc ion                       | Y               | Non-polymeric  | -              | -                 | Not available / Not available                  | Atomic |
|    |          |           |                                | Z               |                |                |                   |  |        |
| 2  | 2-11     | 3         | LRH-1 full length polypeptide  | C               | 538            | -              | 1-538             | 100.00 / 100.00                                | Atomic |
|    |          | 4         | PGC1-alpha coactivator peptide | D               | 10             | 1-10           | -                 | 100.00 / 100.00                                | Atomic |
|    |          | 5         | DNA strand 1                   | E               | 12             | 1-12           | -                 | 100.00 / 100.00                                | Atomic |
|    |          | 6         | DNA strand 2                   | F               | 12             | 1-12           | -                 | 100.00 / 100.00                                | Atomic |
|    |          | 7         | Phospholipid ligand            | X               | Non-polymeric  | -              | -                 | Not available / Not available                  | Atomic |
|    |          |           |                                |                 |                |                |                   |  |        |

| ID | Model(s) | Entity ID | Molecule name | Chain(s) [auth] | Total residues | Rigid segments | Flexible segments | Model coverage/<br>Starting model coverage (%) | Scale  |
|----|----------|-----------|---------------|-----------------|----------------|----------------|-------------------|--|--------|
|    |          | 8         | Zinc ion      | Y               | Non-polymeric  | -              | -                 | Not available /<br>Not available               | Atomic |
|    |          |           |               | Z               |                |                |                   |  |        |

### Datasets used for modeling ?

There are 9 unique datasets used to build the models in this entry.

| ID | Dataset type         | Database name | Data access code                       |
|----|----------------------|---------------|--|
| 1  | Experimental model   | PDB           | <a href="#">2A66</a>                   |
| 2  | Experimental model   | PDB           | <a href="#">1YOK</a>                   |
| 3  | Comparative model    | Zenodo        | <a href="#">10.5281/zenodo.3405545</a> |
| 4  | Comparative model    | Zenodo        | <a href="#">10.5281/zenodo.3405545</a> |
| 5  | Crosslinking-MS data | Zenodo        | <a href="#">10.5281/zenodo.3405545</a> |
| 6  | H/D exchange data    | Zenodo        | <a href="#">10.5281/zenodo.3405545</a> |
| 7  | Integrative model    | Zenodo        | <a href="#">10.5281/zenodo.3405545</a> |
| 8  | Crosslinking-MS data | Zenodo        | <a href="#">10.5281/zenodo.3405545</a> |
| 9  | SAS data             | SASBDB        | <a href="#">SASDG85</a>                |

### Methodology and software ?

This entry is a result of 2 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           | Loop modeling   | RosettaRemodel            | None               | 100                       | False                | False                |
| 2           | 1           | Docking         | RosettaDock               | None               | 40000                     | False                | False                |
| 1           | 2           | Linker modeling | Ranch and RosettaMinimize | None               | 45000                     | False                | False                |

There are 3 software packages reported in this entry.

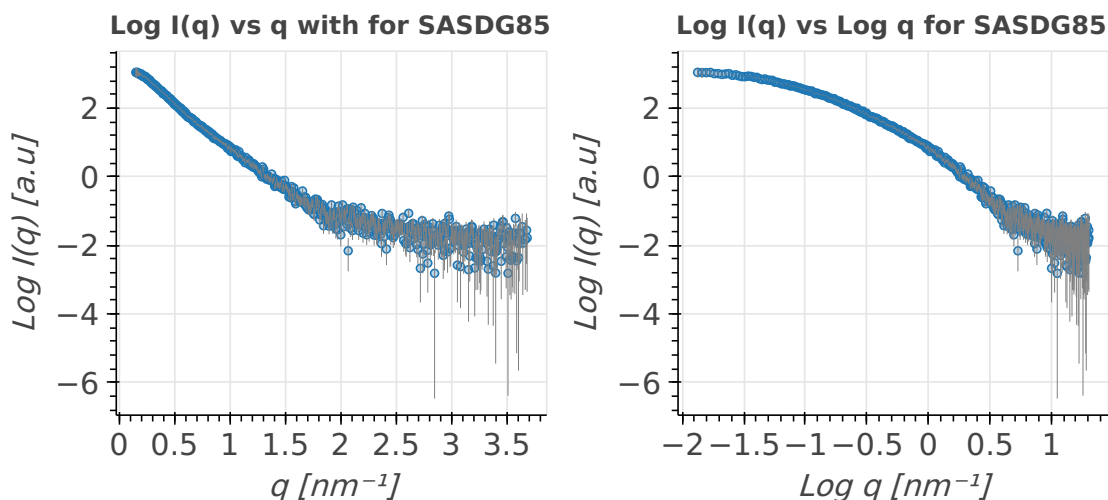
| ID | Software name           | Software version | Software classification          | Software location   |
|----|-------------------------|------------------|----------------------------------|---|
| 1  | <a href="#">Rosetta</a> | 3.10             | model building, model validation | <a href="https://www.rosettacommons.org/">https://www.rosettacommons.org/</a>                                     |
| 2  | <a href="#">ATSAS</a>   | 2.8.4            | model building, model validation | <a href="https://www.embl-hamburg.de/biosaxs/software.html">https://www.embl-hamburg.de/biosaxs/software.html</a> |
| 3  | <a href="#">REMO</a>    | 1                | model building                   | <a href="https://zhanglab.ccmb.med.umich.edu/REMO/">https://zhanglab.ccmb.med.umich.edu/REMO/</a>                 |

## Data quality ?

### Scattering profile ?

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

Scattering profile for [SASDG85](#): 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.

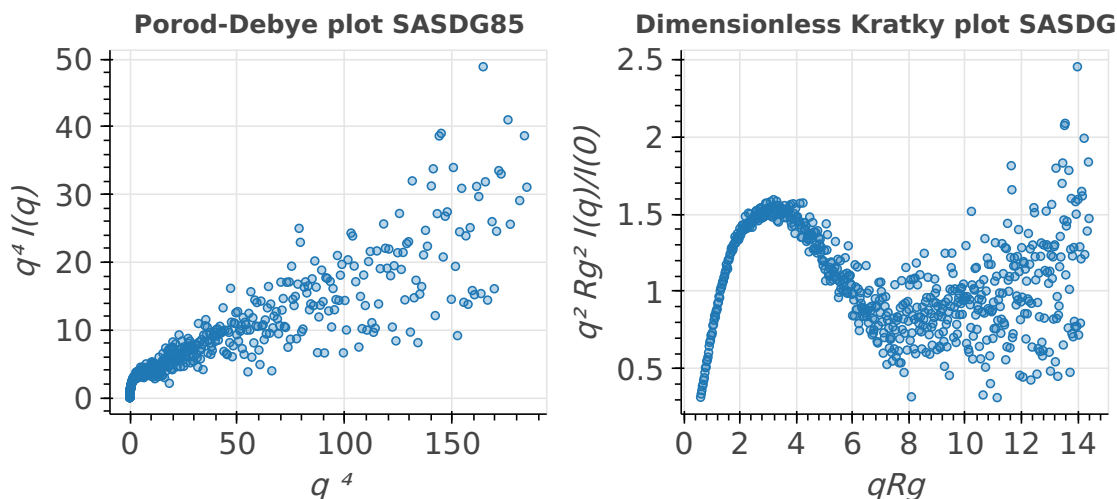
| SASDB ID | Chemical composition MW | Standard MW   | Porod Volume/MW |
|----------|-------------------------|---------------|-----------------|
| SASDG85  | 67.0 kDa                | Not available | Not available   |

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 |
|----------|------------------|-----------------------|-----------------|-----------------|----------------------|
| SASDG85  | Not available    | 76.00 nm <sup>3</sup> | Not available   | Not available   | 7.50 mg/mL           |

## Flexibility analysis ?

**Flexibility analysis for SASDG85:** 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.

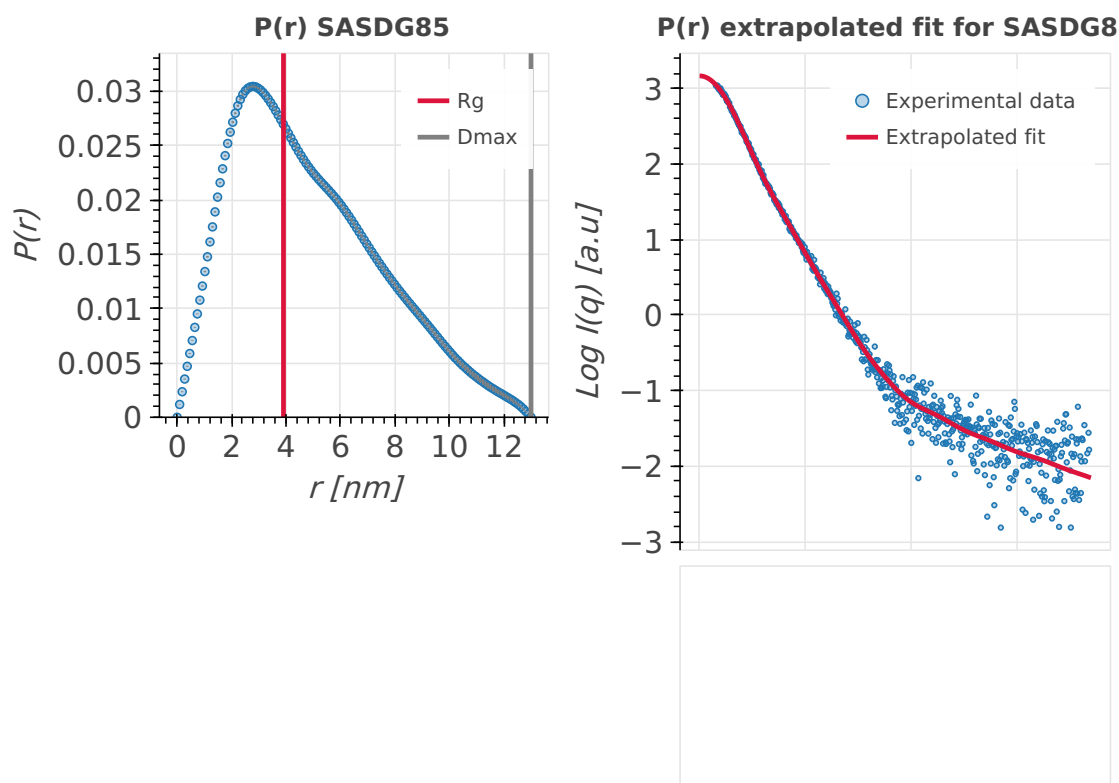


## Pair-distance distribution analysis ?

**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).  $R_g$  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 | $D_{max}$ | $D_{max}$ error | $R_g$    | $R_g$ error |
|----------|---------------|-----------|-----------------|----------|-------------|
| SASDG85  | GNOM 4.6      | 13.000 nm | Not available   | 3.907 nm | 0.020 nm    |

**P(r) for SASDG85:** The value of P(r) should be zero beyond  $r=D_{max}$ .



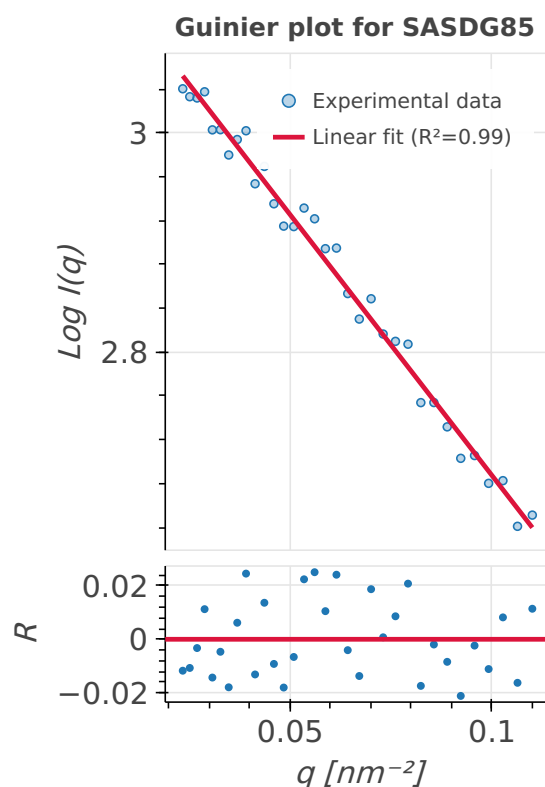
### Guinier analysis ?

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 | $R_g$   | $R_g$ error | MW            | MW error      |
|----------|---------|-------------|---------------|---------------|
| SASDG85  | 3.82 nm | 0.05 nm     | Not available | Not available |

Guinier analysis: 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.





### Crosslinking-MS

*At the moment, data validation is only available for crosslinking-MS data deposited as a fully [compliant](#) dataset in the [PRIDE Crosslinking](#) database. Correspondence between crosslinking-MS and entry entities is established using [pyHMMER](#). Only residue pairs that passed the reported threshold are used for the analysis. The values in the report have to be interpreted in the context of the experiment (i.e. only a minor fraction of in-situ or in-vivo dataset can be used for modeling).*

Crosslinking-MS dataset is not available in the [PRIDE Crosslinking](#) database.

### H/D exchange

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.

### Standard geometry: bond outliers ?

*There are 119 bond length outliers in this entry (0.22% of 53875 assessed bonds). A summary is provided below.*

| Chain | Res | Type | Atoms   | Z     | Observed (Å) | Ideal (Å) | Model ID (Worst) | Models (Total) |
|-------|-----|------|---------|-------|--------------|-----------|------------------|----------------|
| C     | 44  | LYS  | CB-CG   | 94.02 | 4.34         | 1.52      | 6                | 3              |
| C     | 43  | PRO  | N-CD    | 17.06 | 1.71         | 1.47      | 8                | 3              |
| C     | 79  | ASP  | C-N     | 16.53 | 1.56         | 1.33      | 4                | 2              |
| C     | 34  | PRO  | N-CD    | 13.22 | 1.66         | 1.47      | 9                | 1              |
| C     | 298 | PRO  | C-N     | 12.84 | 1.51         | 1.33      | 2                | 1              |
| C     | 80  | GLU  | N-CA    | 12.47 | 1.69         | 1.46      | 4                | 2              |
| C     | 298 | PRO  | CG-CD   | 11.97 | 1.91         | 1.50      | 2                | 1              |
| C     | 82  | LEU  | CG-CD2  | 11.08 | 1.16         | 1.52      | 4                | 2              |
| C     | 78  | TYR  | CB-CG   | 10.08 | 1.73         | 1.51      | 4                | 1              |
| C     | 44  | LYS  | CG-CD   | 9.48  | 1.80         | 1.52      | 6                | 2              |
| X     | 1   | P6L  | C33-C34 | 9.43  | 1.52         | 1.33      | 7                | 11             |
| C     | 44  | LYS  | CA-CB   | 9.39  | 1.72         | 1.53      | 6                | 4              |
| X     | 1   | P6L  | C22-C23 | 9.36  | 1.52         | 1.33      | 9                | 11             |
| C     | 298 | PRO  | N-CD    | 9.27  | 1.60         | 1.47      | 2                | 1              |
| C     | 76  | TYR  | CE2-CZ  | 8.47  | 1.17         | 1.38      | 11               | 1              |
| C     | 250 | PRO  | N-CD    | 8.34  | 1.59         | 1.47      | 8                | 1              |
| C     | 76  | TYR  | CG-CD2  | 8.21  | 1.22         | 1.39      | 11               | 1              |
| C     | 46  | GLU  | CB-CG   | 7.96  | 1.28         | 1.52      | 3                | 2              |
| C     | 43  | PRO  | C-N     | 7.41  | 1.43         | 1.33      | 2                | 5              |
| C     | 82  | LEU  | CB-CG   | 7.03  | 1.67         | 1.53      | 4                | 1              |
| C     | 231 | PRO  | N-CD    | 6.76  | 1.57         | 1.47      | 10               | 1              |
| C     | 298 | PRO  | CB-CG   | 6.72  | 1.83         | 1.49      | 2                | 1              |
| C     | 265 | PRO  | N-CD    | 6.68  | 1.38         | 1.47      | 11               | 1              |
| C     | 83  | GLU  | CB-CG   | 6.27  | 1.33         | 1.52      | 3                | 2              |
| C     | 76  | TYR  | CE1-CZ  | 6.11  | 1.23         | 1.38      | 11               | 1              |
| C     | 78  | TYR  | CE2-CZ  | 6.09  | 1.23         | 1.38      | 4                | 1              |
| C     | 84  | GLU  | C-N     | 5.96  | 1.41         | 1.33      | 8                | 1              |
| C     | 76  | TYR  | CD1-CE1 | 5.88  | 1.56         | 1.38      | 11               | 1              |
| C     | 83  | GLU  | CG-CD   | 5.87  | 1.37         | 1.52      | 4                | 2              |
| C     | 81  | ASP  | CB-CG   | 5.56  | 1.65         | 1.52      | 3                | 1              |
| C     | 106 | CYS  | CB-SG   | 5.54  | 1.99         | 1.81      | 11               | 10             |
| C     | 204 | PRO  | N-CD    | 5.51  | 1.55         | 1.47      | 5                | 2              |
| A     | 24  | CYS  | CB-SG   | 5.51  | 1.99         | 1.81      | 1                | 1              |
| C     | 44  | LYS  | N-CA    | 5.49  | 1.56         | 1.46      | 2                | 5              |
| C     | 83  | GLU  | CD-OE2  | 5.42  | 1.15         | 1.25      | 3                | 1              |

| Chain | Res | Type | Atoms  | Z    | Observed (Å) | Ideal (Å) | Model ID (Worst) | Models (Total) |
|-------|-----|------|--------|------|--------------|-----------|------------------|----------------|
| C     | 276 | PRO  | N-CD   | 5.15 | 1.55         | 1.47      | 2                | 1              |
| C     | 78  | TYR  | CE1-CZ | 5.09 | 1.26         | 1.38      | 4                | 1              |
| C     | 239 | PRO  | N-CD   | 5.05 | 1.40         | 1.47      | 8                | 1              |
| C     | 76  | TYR  | CG-CD1 | 4.97 | 1.28         | 1.39      | 11               | 1              |
| C     | 78  | TYR  | CG-CD1 | 4.96 | 1.28         | 1.39      | 4                | 1              |
| C     | 43  | PRO  | N-CA   | 4.96 | 1.54         | 1.47      | 2                | 1              |
| C     | 83  | GLU  | C-N    | 4.95 | 1.40         | 1.33      | 3                | 1              |
| C     | 244 | PRO  | N-CD   | 4.87 | 1.54         | 1.47      | 7                | 2              |
| C     | 78  | TYR  | CG-CD2 | 4.77 | 1.49         | 1.39      | 4                | 1              |
| C     | 44  | LYS  | CA-C   | 4.60 | 1.62         | 1.52      | 6                | 3              |
| X     | 1   | P6L  | C1-O12 | 4.58 | 1.50         | 1.41      | 6                | 11             |
| C     | 41  | MET  | C-N    | 4.57 | 1.39         | 1.33      | 2                | 1              |
| C     | 42  | LEU  | CA-C   | 4.49 | 1.62         | 1.52      | 2                | 1              |
| C     | 44  | LYS  | C-N    | 4.43 | 1.39         | 1.33      | 3                | 1              |
| C     | 34  | PRO  | N-CA   | 4.36 | 1.53         | 1.47      | 9                | 1              |
| C     | 84  | GLU  | N-CA   | 4.21 | 1.54         | 1.46      | 3                | 1              |
| C     | 32  | PRO  | N-CD   | 4.17 | 1.41         | 1.47      | 8                | 1              |
| C     | 76  | TYR  | CB-CG  | 4.05 | 1.60         | 1.51      | 11               | 1              |
| C     | 83  | GLU  | CA-C   | 4.00 | 1.61         | 1.52      | 3                | 1              |

### Standard geometry: angle outliers ?

There are 387 bond angle outliers in this entry (0.53% of 73684 assessed bonds). A summary is provided below. The output is limited to 100 rows.

| Chain | Res | Type | Atoms     | Z     | Observed (Å) | Ideal (Å) | Model ID (Worst) | Models (Total) |
|-------|-----|------|-----------|-------|--------------|-----------|------------------|----------------|
| C     | 79  | ASP  | C-N-CA    | 24.23 | 165.32       | 121.70    | 4                | 3              |
| C     | 298 | PRO  | C-CA-CB   | 23.44 | 65.56        | 110.10    | 2                | 1              |
| C     | 18  | LEU  | C-N-CA    | 22.58 | 162.34       | 121.70    | 10               | 1              |
| C     | 82  | LEU  | C-N-CA    | 22.23 | 161.71       | 121.70    | 5                | 3              |
| C     | 209 | ILE  | CA-CB-CG1 | 22.11 | 72.82        | 110.40    | 2                | 1              |
| C     | 81  | ASP  | C-N-CA    | 21.09 | 159.66       | 121.70    | 11               | 1              |
| C     | 20  | PRO  | C-N-CA    | 20.82 | 159.17       | 121.70    | 10               | 1              |
| C     | 54  | ARG  | C-N-CA    | 19.98 | 157.67       | 121.70    | 9                | 1              |
| C     | 298 | PRO  | N-CA-C    | 19.94 | 62.25        | 112.10    | 2                | 1              |
| C     | 37  | GLY  | C-N-CA    | 19.72 | 157.19       | 121.70    | 5                | 1              |
| C     | 7   | THR  | C-N-CA    | 19.31 | 156.46       | 121.70    | 8                | 1              |

| Chain | Res | Type | Atoms      | Z     | Observed (Å) | Ideal (Å) | Model ID (Worst) | Models (Total) |
|-------|-----|------|------------|-------|--------------|-----------|------------------|----------------|
| C     | 64  | GLU  | C-N-CA     | 19.10 | 156.08       | 121.70    | 5                | 1              |
| C     | 21  | ILE  | C-N-CA     | 19.03 | 155.95       | 121.70    | 10               | 1              |
| C     | 221 | LYS  | C-N-CA     | 19.02 | 155.93       | 121.70    | 9                | 1              |
| C     | 57  | GLY  | C-N-CA     | 18.52 | 155.04       | 121.70    | 11               | 1              |
| C     | 298 | PRO  | N-CA-CB    | 18.39 | 123.23       | 103.00    | 2                | 1              |
| C     | 237 | ARG  | C-N-CA     | 17.97 | 154.04       | 121.70    | 4                | 1              |
| C     | 277 | TYR  | C-N-CA     | 17.83 | 153.79       | 121.70    | 4                | 1              |
| C     | 213 | ILE  | C-N-CA     | 17.34 | 152.91       | 121.70    | 5                | 1              |
| C     | 258 | TYR  | C-N-CA     | 17.30 | 152.84       | 121.70    | 3                | 2              |
| C     | 209 | ILE  | CA-CB-CG2  | 16.77 | 81.99        | 110.50    | 2                | 1              |
| C     | 24  | GLY  | C-N-CA     | 16.68 | 151.72       | 121.70    | 11               | 1              |
| C     | 32  | PRO  | C-N-CA     | 16.58 | 151.54       | 121.70    | 7                | 2              |
| C     | 185 | LEU  | C-N-CA     | 16.56 | 151.52       | 121.70    | 7                | 1              |
| C     | 80  | GLU  | C-CA-CB    | 16.08 | 79.55        | 110.10    | 3                | 2              |
| C     | 209 | ILE  | CG1-CB-CG2 | 14.65 | 154.64       | 110.70    | 2                | 1              |
| C     | 81  | ASP  | CA-CB-CG   | 14.41 | 127.01       | 112.60    | 3                | 2              |
| C     | 34  | PRO  | CA-N-CD    | 13.86 | 92.60        | 112.00    | 9                | 1              |
| C     | 80  | GLU  | N-CA-C     | 13.84 | 149.76       | 111.00    | 4                | 3              |
| C     | 83  | GLU  | C-N-CA     | 12.40 | 144.03       | 121.70    | 8                | 1              |
| C     | 298 | PRO  | C-N-CA     | 11.84 | 100.39       | 121.70    | 9                | 2              |
| C     | 53  | ALA  | C-CA-CB    | 11.58 | 93.14        | 110.50    | 9                | 1              |
| C     | 79  | ASP  | CA-C-N     | 11.29 | 138.78       | 116.20    | 4                | 1              |
| C     | 33  | ILE  | C-N-CD     | 10.51 | 81.90        | 125.00    | 9                | 1              |
| C     | 43  | PRO  | CA-N-CD    | 10.50 | 97.30        | 112.00    | 8                | 1              |
| C     | 44  | LYS  | CA-CB-CG   | 10.48 | 135.05       | 114.10    | 8                | 5              |
| C     | 33  | ILE  | C-N-CA     | 10.36 | 174.42       | 122.60    | 9                | 1              |
| C     | 44  | LYS  | N-CA-CB    | 10.14 | 93.27        | 110.50    | 10               | 2              |
| C     | 82  | LEU  | CD1-CG-CD2 | 10.08 | 132.97       | 110.80    | 7                | 2              |
| C     | 298 | PRO  | CA-CB-CG   | 9.77  | 85.94        | 104.50    | 2                | 1              |
| C     | 76  | TYR  | CB-CG-CD1  | 9.33  | 134.79       | 120.80    | 11               | 1              |
| C     | 242 | THR  | OG1-CB-CG2 | 9.00  | 127.30       | 109.30    | 8                | 1              |
| C     | 44  | LYS  | CB-CG-CD   | 8.87  | 131.70       | 111.30    | 6                | 2              |

| Chain | Res | Type | Atoms      | Z    | Observed (Å) | Ideal (Å) | Model ID (Worst) | Models (Total) |
|-------|-----|------|------------|------|--------------|-----------|------------------|----------------|
| C     | 260 | THR  | OG1-CB-CG2 | 8.78 | 126.85       | 109.30    | 11               | 1              |
| C     | 44  | LYS  | C-CA-CB    | 8.71 | 93.54        | 110.10    | 8                | 4              |
| C     | 78  | TYR  | C-N-CA     | 8.71 | 137.37       | 121.70    | 4                | 1              |
| C     | 44  | LYS  | C-N-CA     | 8.66 | 137.28       | 121.70    | 4                | 5              |
| C     | 199 | VAL  | CA-CB-CG1  | 8.63 | 125.07       | 110.40    | 10               | 1              |
| C     | 82  | LEU  | N-CA-CB    | 8.41 | 96.21        | 110.50    | 4                | 2              |
| C     | 84  | GLU  | C-N-CA     | 8.36 | 106.65       | 121.70    | 8                | 2              |
| C     | 83  | GLU  | N-CA-C     | 8.32 | 134.31       | 111.00    | 4                | 2              |
| C     | 79  | ASP  | CA-C-O     | 8.25 | 106.77       | 120.80    | 4                | 1              |
| C     | 41  | MET  | C-N-CA     | 8.07 | 136.23       | 121.70    | 3                | 2              |
| C     | 68  | VAL  | CA-CB-CG2  | 7.89 | 123.82       | 110.40    | 6                | 1              |
| C     | 82  | LEU  | CB-CG-CD2  | 7.88 | 87.05        | 110.70    | 3                | 1              |
| C     | 233 | THR  | OG1-CB-CG2 | 7.87 | 125.03       | 109.30    | 8                | 1              |
| C     | 84  | GLU  | CA-C-N     | 7.76 | 131.71       | 116.20    | 8                | 1              |
| C     | 42  | LEU  | N-CA-C     | 7.58 | 132.23       | 111.00    | 2                | 2              |
| C     | 287 | TYR  | C-N-CA     | 7.45 | 135.11       | 121.70    | 5                | 1              |
| C     | 82  | LEU  | CA-C-O     | 7.36 | 108.29       | 120.80    | 4                | 1              |
| C     | 83  | GLU  | CB-CG-CD   | 7.28 | 100.22       | 112.60    | 3                | 2              |
| C     | 80  | GLU  | N-CA-CB    | 7.21 | 122.76       | 110.50    | 4                | 1              |
| C     | 84  | GLU  | CA-C-O     | 7.18 | 108.60       | 120.80    | 8                | 1              |
| C     | 84  | GLU  | N-CA-C     | 7.07 | 130.81       | 111.00    | 8                | 2              |
| C     | 191 | LEU  | C-N-CA     | 7.07 | 134.42       | 121.70    | 2                | 1              |
| C     | 6   | ASP  | CA-CB-CG   | 7.04 | 119.64       | 112.60    | 3                | 1              |
| X     | 1   | P6L  | O12-P11-O9 | 6.93 | 115.34       | 94.56     | 9                | 11             |
| C     | 76  | TYR  | CB-CG-CD2  | 6.91 | 110.44       | 120.80    | 11               | 1              |
| C     | 67  | GLN  | C-N-CA     | 6.89 | 134.09       | 121.70    | 6                | 1              |
| C     | 298 | PRO  | CA-N-CD    | 6.87 | 102.39       | 112.00    | 2                | 1              |
| C     | 45  | VAL  | C-CA-CB    | 6.83 | 98.42        | 111.40    | 3                | 1              |
| C     | 202 | ALA  | C-N-CA     | 6.73 | 133.82       | 121.70    | 9                | 1              |
| C     | 240 | PHE  | CA-CB-CG   | 6.62 | 120.42       | 113.80    | 6                | 1              |
| C     | 79  | ASP  | CA-CB-CG   | 6.59 | 119.19       | 112.60    | 4                | 1              |
| C     | 294 | GLN  | C-N-CA     | 6.57 | 133.53       | 121.70    | 4                | 1              |
| C     | 242 | THR  | C-N-CA     | 6.56 | 133.51       | 121.70    | 10               | 1              |

| Chain | Res | Type | Atoms      | Z    | Observed (Å) | Ideal (Å) | Model ID (Worst) | Models (Total) |
|-------|-----|------|------------|------|--------------|-----------|------------------|----------------|
| C     | 83  | GLU  | N-CA-CB    | 6.51 | 99.43        | 110.50    | 3                | 1              |
| C     | 208 | THR  | C-N-CA     | 6.51 | 133.42       | 121.70    | 6                | 1              |
| C     | 34  | PRO  | N-CD-CG    | 6.49 | 112.94       | 103.20    | 9                | 1              |
| C     | 210 | SER  | C-N-CA     | 6.42 | 133.26       | 121.70    | 11               | 4              |
| C     | 46  | GLU  | C-N-CA     | 6.15 | 132.77       | 121.70    | 3                | 2              |
| C     | 82  | LEU  | N-CA-C     | 6.13 | 128.16       | 111.00    | 4                | 2              |
| C     | 62  | MET  | CA-C-N     | 6.10 | 126.05       | 116.90    | 5                | 1              |
| C     | 43  | PRO  | N-CA-C     | 6.02 | 127.14       | 112.10    | 6                | 3              |
| C     | 76  | TYR  | CA-CB-CG   | 5.95 | 124.61       | 113.90    | 11               | 1              |
| C     | 72  | LYS  | C-N-CA     | 5.88 | 132.29       | 121.70    | 7                | 1              |
| C     | 34  | PRO  | N-CA-CB    | 5.88 | 109.47       | 103.00    | 9                | 1              |
| C     | 55  | SER  | C-N-CA     | 5.85 | 132.23       | 121.70    | 7                | 1              |
| C     | 71  | PHE  | CA-CB-CG   | 5.83 | 107.97       | 113.80    | 6                | 1              |
| C     | 80  | GLU  | C-N-CA     | 5.75 | 132.04       | 121.70    | 4                | 2              |
| C     | 47  | THR  | C-N-CA     | 5.73 | 132.01       | 121.70    | 5                | 1              |
| C     | 281 | PRO  | C-N-CA     | 5.72 | 131.99       | 121.70    | 10               | 1              |
| C     | 66  | MET  | C-N-CA     | 5.64 | 131.84       | 121.70    | 6                | 1              |
| C     | 269 | ILE  | CG1-CB-CG2 | 5.63 | 127.60       | 110.70    | 2                | 1              |
| C     | 80  | GLU  | CA-CB-CG   | 5.63 | 125.36       | 114.10    | 3                | 1              |
| C     | 231 | PRO  | C-CA-CB    | 5.62 | 120.78       | 110.10    | 9                | 1              |
| C     | 22  | GLY  | N-CA-C     | 5.55 | 97.22        | 113.30    | 8                | 1              |
| C     | 29  | HIS  | CA-CB-CG   | 5.48 | 108.32       | 113.80    | 2                | 1              |
| C     | 83  | GLU  | C-CA-CB    | 5.47 | 99.70        | 110.10    | 4                | 1              |
| C     | 83  | GLU  | CA-C-N     | 5.47 | 127.15       | 116.20    | 8                | 1              |

### 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 atomic models in this entry.

| Model ID | Clash score | Number of clashes |
|----------|-------------|-------------------|
| 1        | 0.00        | 0                 |
| 2        | 0.00        | 0                 |
| 3        | 0.00        | 0                 |
| 4        | 0.00        | 0                 |

| Model ID | Clash score | Number of clashes |
|----------|-------------|-------------------|
| 5        | 0.00        | 0                 |
| 6        | 0.00        | 0                 |
| 7        | 0.00        | 0                 |
| 8        | 0.00        | 0                 |
| 9        | 0.00        | 0                 |
| 10       | 0.00        | 0                 |
| 11       | 0.00        | 0                 |

There are no too-close contacts.

### 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 | Analysed | Favored | Allowed | Outliers |
|----------|----------|---------|---------|----------|
| 1        | 346      | 340     | 6       | 0        |
| 2        | 544      | 500     | 34      | 10       |
| 3        | 544      | 511     | 26      | 7        |
| 4        | 544      | 507     | 29      | 8        |
| 5        | 544      | 505     | 31      | 8        |
| 6        | 544      | 509     | 27      | 8        |
| 7        | 544      | 500     | 35      | 9        |
| 8        | 544      | 511     | 29      | 4        |
| 9        | 544      | 497     | 36      | 11       |
| 10       | 544      | 494     | 38      | 12       |
| 11       | 544      | 508     | 30      | 6        |

There are 54 unique backbone outliers. Detailed list of outliers are tabulated below.

| Chain | Res | Type | Models (Total) |
|-------|-----|------|----------------|
| C     | 44  | LYS  | 4              |
| C     | 249 | MET  | 4              |
| C     | 19  | THR  | 3              |
| C     | 45  | VAL  | 3              |
| C     | 200 | ILE  | 3              |
| C     | 203 | MET  | 3              |
| C     | 31  | SER  | 2              |
| C     | 41  | MET  | 2              |
| C     | 43  | PRO  | 2              |

| Chain | Res | Type | Models (Total) |
|-------|-----|------|----------------|
| C     | 47  | THR  | 2              |
| C     | 48  | GLU  | 2              |
| C     | 62  | MET  | 2              |
| C     | 68  | VAL  | 2              |
| C     | 81  | ASP  | 2              |
| C     | 82  | LEU  | 2              |
| C     | 186 | ILE  | 2              |
| C     | 216 | ILE  | 2              |
| C     | 241 | VAL  | 2              |
| C     | 254 | SER  | 2              |
| C     | 265 | PRO  | 2              |
| C     | 287 | TYR  | 2              |
| C     | 7   | THR  | 1              |
| C     | 14  | LEU  | 1              |
| C     | 15  | LYS  | 1              |
| C     | 21  | ILE  | 1              |
| C     | 34  | PRO  | 1              |
| C     | 40  | VAL  | 1              |
| C     | 42  | LEU  | 1              |
| C     | 55  | SER  | 1              |
| C     | 60  | GLY  | 1              |
| C     | 74  | VAL  | 1              |
| C     | 83  | GLU  | 1              |
| C     | 84  | GLU  | 1              |
| C     | 199 | VAL  | 1              |
| C     | 201 | GLN  | 1              |
| C     | 205 | SER  | 1              |
| C     | 208 | THR  | 1              |
| C     | 209 | ILE  | 1              |
| C     | 210 | SER  | 1              |
| C     | 213 | ILE  | 1              |
| C     | 217 | HIS  | 1              |
| C     | 230 | LEU  | 1              |
| C     | 231 | PRO  | 1              |
| C     | 242 | THR  | 1              |



| Chain | Res | Type | Models (Total) |
|-------|-----|------|----------------|
| C     | 262 | GLY  | 1              |
| C     | 264 | PHE  | 1              |
| C     | 267 | ARG  | 1              |
| C     | 269 | ILE  | 1              |
| C     | 271 | SER  | 1              |
| C     | 275 | ASP  | 1              |
| C     | 283 | SER  | 1              |
| C     | 284 | ILE  | 1              |
| C     | 290 | MET  | 1              |
| C     | 298 | PRO  | 1              |

### Torsion angles : Protein sidechains ?


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

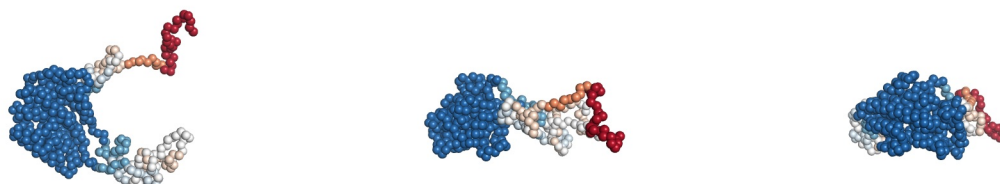
| Model ID | Analysed | Favored | Allowed | Outliers |
|----------|----------|---------|---------|----------|
| 1        | 315      | 312     | 3       | 0        |
| 2        | 484      | 479     | 4       | 1        |
| 3        | 484      | 480     | 4       | 0        |
| 4        | 484      | 478     | 5       | 1        |
| 5        | 484      | 481     | 3       | 0        |
| 6        | 484      | 477     | 5       | 2        |
| 7        | 484      | 478     | 5       | 1        |
| 8        | 484      | 478     | 4       | 2        |
| 9        | 484      | 480     | 4       | 0        |
| 10       | 484      | 478     | 6       | 0        |
| 11       | 484      | 479     | 5       | 0        |

There are 7 unique sidechain outliers. Detailed list of outliers are tabulated below.

| Chain | Res | Type | Models (Total) |
|-------|-----|------|----------------|
| C     | 43  | PRO  | 1              |
| C     | 68  | VAL  | 1              |
| C     | 82  | LEU  | 1              |
| C     | 239 | PRO  | 1              |
| C     | 250 | PRO  | 1              |
| C     | 278 | THR  | 1              |
| C     | 298 | PRO  | 1              |

### PrISM precision analysis ?

Regions of **low**  **high** precision, defined as the variability among the models that satisfy the input data and calculated as the density-weighted root mean-square fluctuation (RMSF) from the bead/atom center of density, annotated and visualized using PrISM. The per-bead precision is computed from the deposited ensemble of superposed integrative models. High- and low-precision regions are then determined by clustering beads of similar precision based on their proximity in the structure. Only coarse-grained beads (or CA atoms for atomic models) of deposited models are used for assessment and visualization, and three projections for each representative model are generated. PrISM analysis for Ensemble 1 (models deposited/total: 10/10).



### Fit of model to data used for modeling ?

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

#### $\chi^2$ goodness of fit and cormap analysis ?

Model(s) and/or fit for this entry have not been deposited.

#### Fit of model(s) to crosslinking-MS data

#### Restraint types

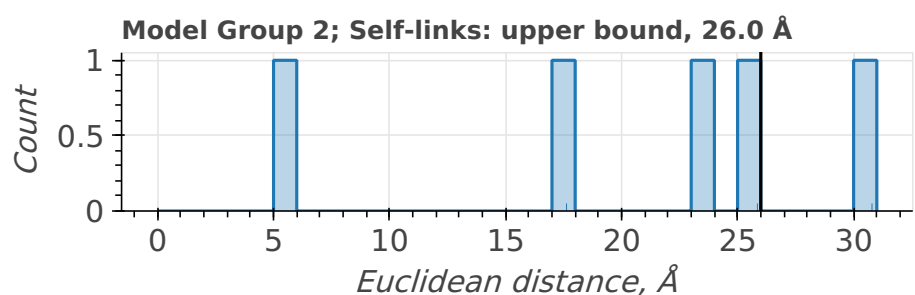
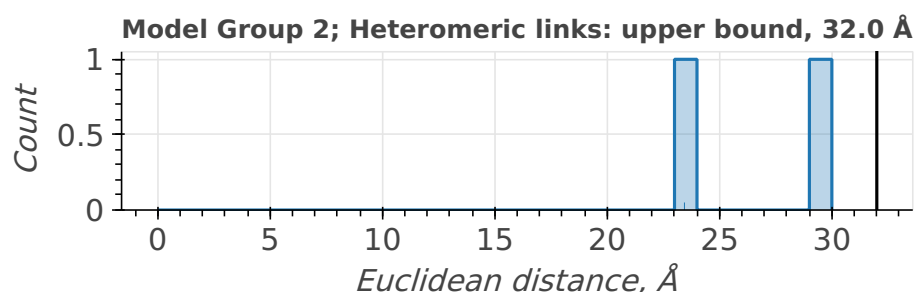
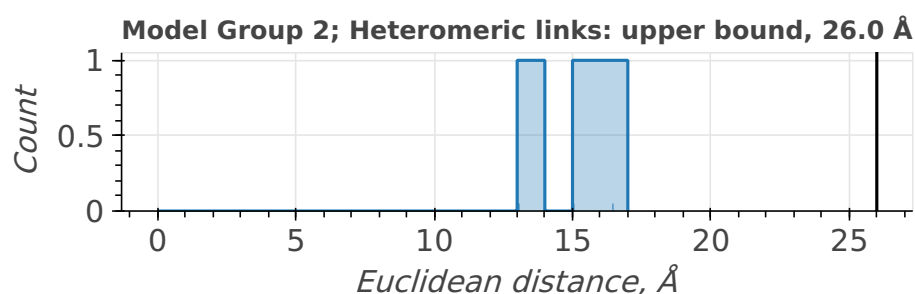
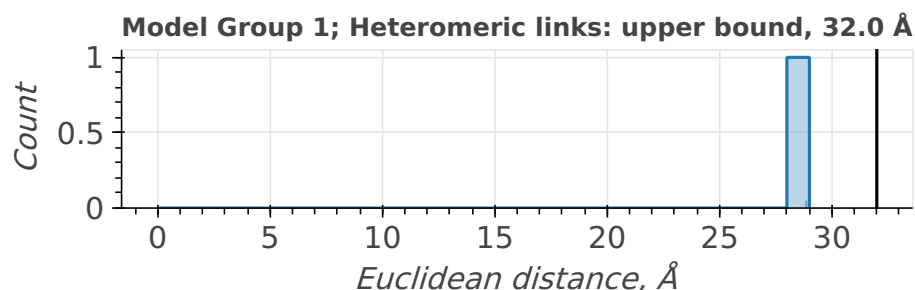
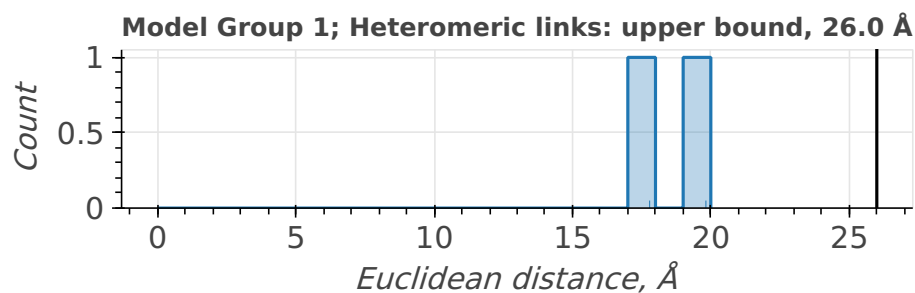
Restraint types are summarized in the table below. Restraints assigned "*by-residue*" are interpreted as between CA atoms. Restraints between coarse-grained beads are indicated as "*coarse-grained*". *Restraint group* represents a set of crosslinking restraints applied collectively in the modeling.

There are 13 crosslinking restraints combined in 13 restraint groups.

| Linker | Residue 1 | Atom 1 | Residue 2 | Atom 2 | Restraint type | Distance, Å | Count |
|--------|-----------|--------|-----------|--------|----------------|-------------|-------|
| BS3    | LYS       | CA     | LYS       | CA     | upper bound    | 26.0        | 7     |
| BS3    | LYS       | CA     | PRO       | CA     | upper bound    | 32.0        | 1     |
| BS3    | LEU       | CA     | LYS       | CA     | upper bound    | 32.0        | 2     |
| BS3    | LEU       | CA     | LYS       | CA     | upper bound    | 26.0        | 3     |

#### Distograms of individual restraints

Restraints with identical thresholds are grouped into one plot. Only the best distance per restraint per model group/ensemble is plotted. Inter- and intramolecular (including self-links) restraints are also grouped into one plot. Distance for a restraint between coarse-grained beads is calculated as a minimal distance between shells; if beads intersect, the distance will be reported as 0.0. A bead with the highest available resolution for a given residue is used for the assessment.



### Satisfaction of restraints

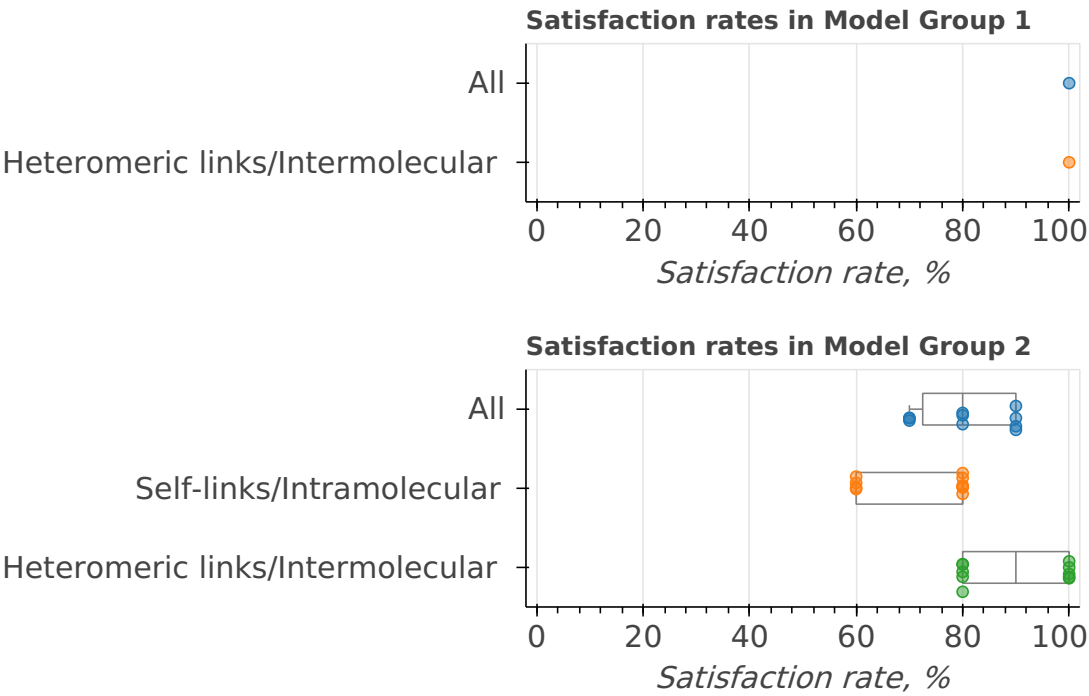
*Satisfaction of restraints is calculated on a [restraint group](#) (a set of crosslinking restraints applied collectively in the modeling) level. Satisfaction of a restraint group depends on satisfaction of individual restraints in the group and the conditionality (all/any). A restraint group is considered satisfied, if the condition was met in at least one model of the model group/ensemble. The number of measured restraints can be smaller than the total number of restraint groups if crosslinks involve non-*

modeled residues. Only deposited models are used for validation right now.

| State group | State | Model group | # of Deposited models/Total | Restraint group type              | Satisfied (%) | Violated (%) | Count (Total=13) |
|-------------|-------|-------------|-----------------------------|-----------------------------------|---------------|--------------|------------------|
| 1           | 1     | 1           | 1/1                         | All                               | 100.00        | 0.00         | 3                |
|             |       |             |                             | Heteromeric links/ Intermolecular | 100.00        | 0.00         | 3                |
| 1           | 1     | 2           | 10/10                       | All                               | 90.00         | 10.00        | 10               |
|             |       |             |                             | Self-links/ Intramolecular        | 80.00         | 20.00        | 5                |
|             |       |             |                             | Heteromeric links/ Intermolecular | 100.00        | 0.00         | 5                |

Per-model satisfaction rates in ensembles

Every point represents one model in a model group/ensemble. Where possible, boxplots with quartile marks are also plotted.



H/D exchange

Validation for this section is under development.

Fit of model to data used for validation ?

Validation for this section is under development.

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