

Integrative Structure Validation Report ?

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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

| | |
|-------------------|--|
| PDB ID | 9A4A |
| PDB-Dev ID | PDBDEV_00000231 |
| Structure Title | Model of YLAN-FUR by crosslinking MS and deep learning |
| Structure Authors | Kolja Stahl; Oliver Brock; Juri Rappsilber |
| Deposited on | 2023-12-19 |

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

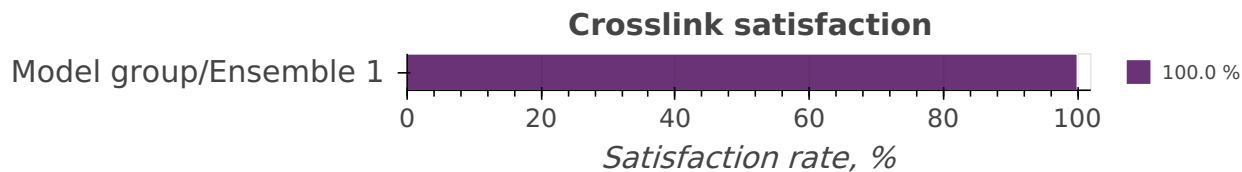
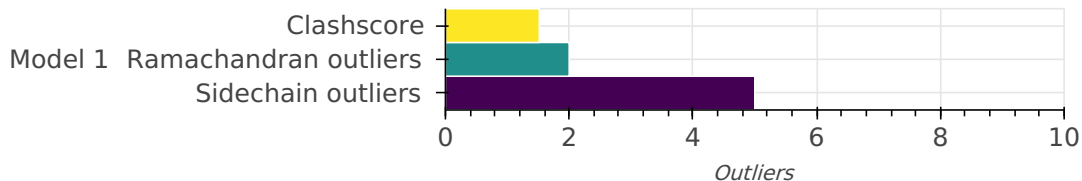
A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the ? symbol.

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 0 distinct ensemble(s).

Summary ?

This entry consists of 1 model(s). A total of 1 datasets were used to build this entry.

Representation ?

This entry has 1 representation(s).

| ID | Model(s) | Entity ID | Molecule name | Chain(s) [auth] | Total residues | Rigid segments | Flexible segments | Model coverage/ Starting model coverage (%) | Scale |
|----|----------|-----------|---------------|-----------------|----------------|----------------|-------------------|---|--------|
| 1 | 1 | 1 | YLAN_BACSU | A | 93 | - | 1-93 | 100.00 / 0.00 | Atomic |
| | | 2 | FUR_BACSU | B | 149 | - | 1-149 | 100.00 / 0.00 | Atomic |

Datasets used for modeling ?

There is 1 unique dataset used to build the models in this entry.

| ID | Dataset type | Database name | Data access code |
|----|----------------------|---------------|------------------|
| 1 | Crosslinking-MS data | PRIDE | PXD035508 |

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 | AlphaLink2 | AlphaLink2 | None | 1 | False | False |

There is 1 software package reported in this entry.

| ID | Software name | Software version | Software classification | Software location |
|----|----------------------------|------------------|-------------------------|---|
| 1 | AlphaLink2 | 1.00 | model building | https://github.com/Rappsilber-Laboratory/AlphaLink2 |

Data quality ?

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.

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 no bond length outliers.

Standard geometry: angle outliers ?

There are 10 bond angle outliers in this entry (0.37% of 2694 assessed bonds). A summary is provided below.

| Chain | Res | Type | Atoms | Z | Observed (Å) | Ideal (Å) | Model ID (Worst) | Models (Total) |
|-------|-----|------|------------|------|--------------|-----------|------------------|----------------|
| B | 96 | HIS | CB-CG-CD2 | 5.06 | 124.63 | 131.20 | 1 | 1 |
| B | 33 | ASN | OD1-CG-ND2 | 4.72 | 117.88 | 122.60 | 1 | 1 |
| A | 11 | GLN | OE1-CD-NE2 | 4.69 | 117.91 | 122.60 | 1 | 1 |
| A | 31 | GLN | OE1-CD-NE2 | 4.65 | 117.95 | 122.60 | 1 | 1 |
| A | 87 | HIS | CB-CG-CD2 | 4.52 | 125.33 | 131.20 | 1 | 1 |
| B | 132 | HIS | CB-CG-CD2 | 4.40 | 125.48 | 131.20 | 1 | 1 |
| B | 4 | ARG | NE-CZ-NH2 | 4.30 | 123.07 | 119.20 | 1 | 1 |
| A | 50 | GLN | OE1-CD-NE2 | 4.26 | 118.34 | 122.60 | 1 | 1 |
| B | 97 | HIS | CB-CG-CD2 | 4.25 | 125.68 | 131.20 | 1 | 1 |
| B | 95 | HIS | CB-CG-CD2 | 4.07 | 125.91 | 131.20 | 1 | 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 | 1.52 | 6 |

There are 6 clashes. The table below contains the detailed list of all clashes based on a MolProbity analysis. Bad clashes are ≥ 0.4 Angstrom.

| Atom 1 | Atom 2 | Clash(Å) | Model ID (Worst) | Models (Total) |
|----------------|----------------|----------|------------------|----------------|
| B:114:LEU:HD11 | B:134:LEU:HD22 | 0.47 | 1 | 1 |
| B:98:LEU:HD23 | B:136:PHE:HB2 | 0.43 | 1 | 1 |
| A:43:TYR:CZ | B:45:LEU:HD11 | 0.41 | 1 | 1 |
| B:74:LYS:HE3 | B:82:SER:HB3 | 0.40 | 1 | 1 |
| B:4:ARG:HH12 | B:34:GLU:CD | 0.40 | 1 | 1 |
| B:134:LEU:HD21 | B:136:PHE:CZ | 0.40 | 1 | 1 |

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 | 238 | 235 | 1 | 2 |

There are 2 unique backbone outliers. Detailed list of outliers are tabulated below.

| Chain | Res | Type | Models (Total) |
|-------|-----|------|----------------|
| A | 35 | LEU | 1 |

| Chain | Res | Type | Models (Total) |
|-------|-----|------|----------------|
| A | 39 | GLN | 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 | 219 | 210 | 4 | 5 |

There are 5 unique sidechain outliers. Detailed list of outliers are tabulated below.

| Chain | Res | Type | Models (Total) |
|-------|-----|------|----------------|
| A | 1 | MET | 1 |
| B | 12 | LEU | 1 |
| B | 13 | HIS | 1 |
| B | 51 | SER | 1 |
| B | 148 | THR | 1 |

Fit of model to data used for modeling ?

Fit of model(s) to crosslinking-MS data

Restraint types

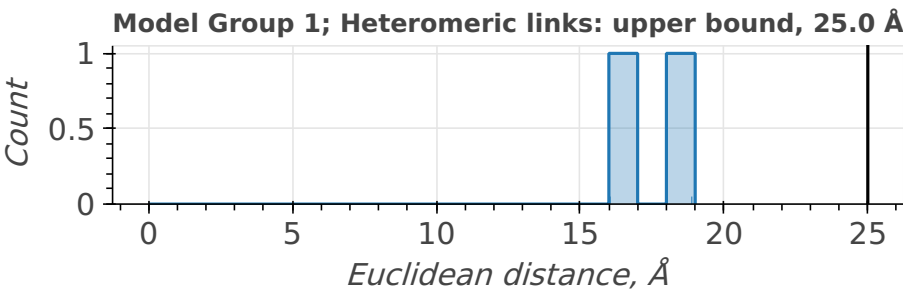
Restraint types are summarized in the table below. Restraints assigned "*by-residue*" are interpreted as between CA atoms. Restraints between coarse-grained beads are indicated as "*coarse-grained*". *Restraint group* represents a set of crosslinking restraints applied collectively in the modeling.

There are 2 crosslinking restraints combined in 2 restraint groups.

| Linker | Residue 1 | Atom 1 | Residue 2 | Atom 2 | Restraint type | Distance, Å | Count |
|--------|-----------|--------|-----------|--------|----------------|-------------|-------|
| SDA | LYS | CA | LYS | CA | upper bound | 25.0 | 2 |

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.



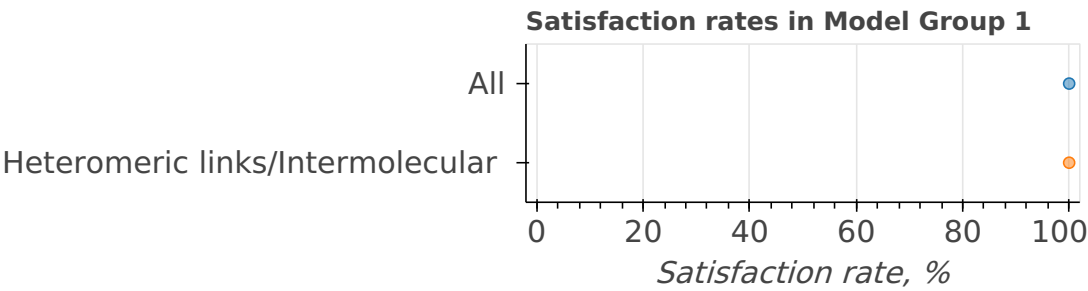
Satisfaction of restraints

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=2) |
|-------------|-------|-------------|-----------------------------|----------------------------------|---------------|--------------|-----------------|
| 1 | 1 | 1 | 1/1 | All | 100.00 | 0.00 | 2 |
| | | | | Heteromeric links/Intermolecular | 100.00 | 0.00 | 2 |

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.



Fit of model to data used for validation ?

Validation for this section is under development.

The 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 awards to the [PDB-IHM team](#) (DBI-1756248, DBI-2112966, DBI-2112967, DBI-2112968, and DBI-1756250) and awards from NSF, NIH, and DOE to the [RCSB PDB](#) (DBI-2321666, R01GM157729, and DE-SC0019749). The PDB-IHM team and members of the [Sali lab](#) contributed model validation metrics and software packages.

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