

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 | 9A4P |
| PDB-Dev ID | PDBDEV_00000246 |
| Structure Title | Integrative model of YJCM-YJCN by crosslinking MS and deep learning |
| Structure Authors | Kolja Stahl; Oliver Brock; Juri Rappsilber |
| Deposited on | 2024-01-23 |

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

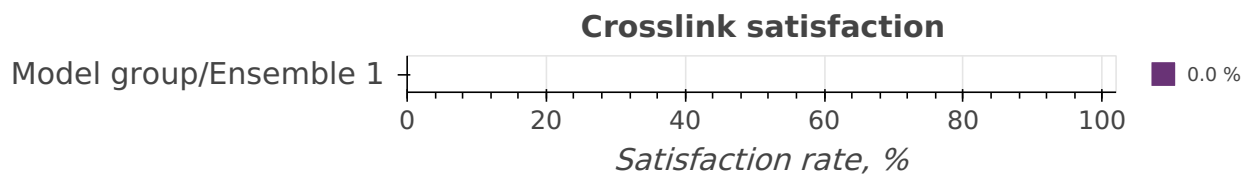
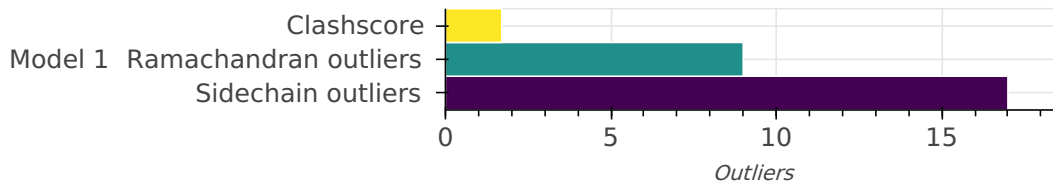
A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the ? symbol.

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 | YJCM_BACSU | A | 409 | - | 1-409 | 100.00 / 0.00 | Atomic |
| | | 2 | YJCN_BACSU | B | 106 | - | 1-106 | 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 22 bond angle outliers in this entry (0.39% of 5681 assessed bonds). A summary is provided below.

| Chain | Res | Type | Atoms | Z | Observed (Å) | Ideal (Å) | Model ID (Worst) | Models (Total) |
|-------|-----|------|------------|------|--------------|-----------|------------------|----------------|
| A | 167 | ASN | C-N-CA | 6.00 | 132.50 | 121.70 | 1 | 1 |
| A | 200 | ASN | CA-CB-CG | 5.79 | 118.39 | 112.60 | 1 | 1 |
| A | 219 | GLN | OE1-CD-NE2 | 5.47 | 117.13 | 122.60 | 1 | 1 |
| A | 50 | ASP | CA-CB-CG | 5.38 | 117.98 | 112.60 | 1 | 1 |
| B | 83 | GLN | OE1-CD-NE2 | 5.15 | 117.45 | 122.60 | 1 | 1 |
| A | 10 | VAL | CA-CB-CG1 | 4.95 | 118.81 | 110.40 | 1 | 1 |
| A | 203 | GLU | C-N-CA | 4.92 | 130.55 | 121.70 | 1 | 1 |
| B | 68 | ASN | OD1-CG-ND2 | 4.89 | 117.71 | 122.60 | 1 | 1 |
| A | 402 | ARG | NE-CZ-NH2 | 4.60 | 123.34 | 119.20 | 1 | 1 |
| A | 183 | GLN | OE1-CD-NE2 | 4.49 | 118.11 | 122.60 | 1 | 1 |
| B | 73 | ASN | CA-CB-CG | 4.49 | 108.11 | 112.60 | 1 | 1 |
| A | 171 | GLN | OE1-CD-NE2 | 4.42 | 118.18 | 122.60 | 1 | 1 |
| A | 150 | GLN | OE1-CD-NE2 | 4.42 | 118.18 | 122.60 | 1 | 1 |
| A | 314 | ASN | OD1-CG-ND2 | 4.42 | 118.18 | 122.60 | 1 | 1 |
| A | 200 | ASN | OD1-CG-ND2 | 4.40 | 118.20 | 122.60 | 1 | 1 |
| A | 383 | SER | C-N-CA | 4.37 | 129.57 | 121.70 | 1 | 1 |
| A | 360 | ASP | CA-CB-CG | 4.31 | 116.91 | 112.60 | 1 | 1 |
| A | 245 | SER | C-N-CA | 4.26 | 129.37 | 121.70 | 1 | 1 |
| A | 188 | GLN | OE1-CD-NE2 | 4.10 | 118.50 | 122.60 | 1 | 1 |
| A | 5 | LEU | C-N-CA | 4.06 | 129.00 | 121.70 | 1 | 1 |
| A | 2 | LYS | N-CA-C | 4.05 | 122.33 | 111.00 | 1 | 1 |
| A | 203 | GLU | N-CA-CB | 4.02 | 103.67 | 110.50 | 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 | 1.70 | 14 |

There are 14 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) |
|---------------|----------------|----------|------------------|----------------|
| A:206:SER:HB3 | A:357:ARG:HH22 | 0.68 | 1 | 1 |

| Atom 1 | Atom 2 | Clash(Å) | Model ID (Worst) | Models (Total) |
|----------------|----------------|----------|------------------|----------------|
| A:204:TYR:CE1 | B:89:TYR:CE2 | 0.63 | 1 | 1 |
| A:252:ALA:HB1 | A:329:LYS:HD3 | 0.59 | 1 | 1 |
| B:74:TRP:CH2 | B:86:HIS:CD2 | 0.54 | 1 | 1 |
| A:9:LEU:HG | A:10:VAL:HG23 | 0.51 | 1 | 1 |
| A:284:LYS:CE | B:104:THR:HG21 | 0.47 | 1 | 1 |
| A:204:TYR:CD1 | B:87:LEU:HB3 | 0.45 | 1 | 1 |
| A:330:MET:HE3 | A:407:ILE:HG13 | 0.45 | 1 | 1 |
| A:284:LYS:NZ | B:104:THR:HG21 | 0.44 | 1 | 1 |
| A:202:GLU:OE1 | B:103:GLY:HA3 | 0.43 | 1 | 1 |
| A:204:TYR:CE1 | B:87:LEU:HB3 | 0.42 | 1 | 1 |
| A:206:SER:C | A:208:VAL:H | 0.41 | 1 | 1 |
| A:305:TRP:HB2 | A:321:TYR:CE2 | 0.41 | 1 | 1 |
| A:138:ILE:HG22 | A:198:TYR:CD2 | 0.41 | 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 | 511 | 456 | 46 | 9 |

There are 9 unique backbone outliers. Detailed list of outliers are tabulated below.

| Chain | Res | Type | Models (Total) |
|-------|-----|------|----------------|
| A | 163 | SER | 1 |
| A | 183 | GLN | 1 |
| A | 185 | ASN | 1 |
| A | 186 | VAL | 1 |
| A | 203 | GLU | 1 |
| A | 246 | ASN | 1 |
| A | 248 | LEU | 1 |
| A | 250 | VAL | 1 |
| A | 253 | THR | 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 | 465 | 431 | 17 | 17 |

There are 17 unique sidechain outliers. Detailed list of outliers are tabulated below.

| Chain | Res | Type | Models (Total) |
|-------|-----|------|----------------|
| A | 5 | LEU | 1 |
| A | 9 | LEU | 1 |
| A | 11 | LEU | 1 |
| A | 18 | LEU | 1 |
| A | 20 | SER | 1 |
| A | 29 | THR | 1 |
| A | 147 | SER | 1 |
| A | 152 | SER | 1 |
| A | 155 | THR | 1 |
| A | 162 | PHE | 1 |
| A | 208 | VAL | 1 |
| A | 249 | THR | 1 |
| A | 251 | THR | 1 |
| A | 405 | SER | 1 |
| B | 5 | THR | 1 |
| B | 9 | LEU | 1 |
| B | 12 | LEU | 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*".

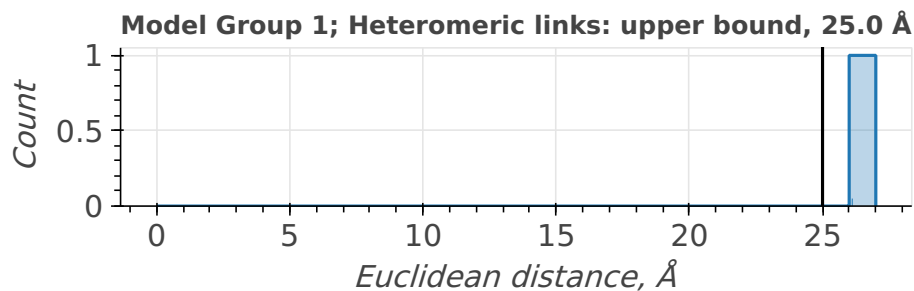
Restraint group represents a set of crosslinking restraints applied collectively in the modeling.

There are 1 crosslinking restraints combined in 1 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 | 1 |

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.



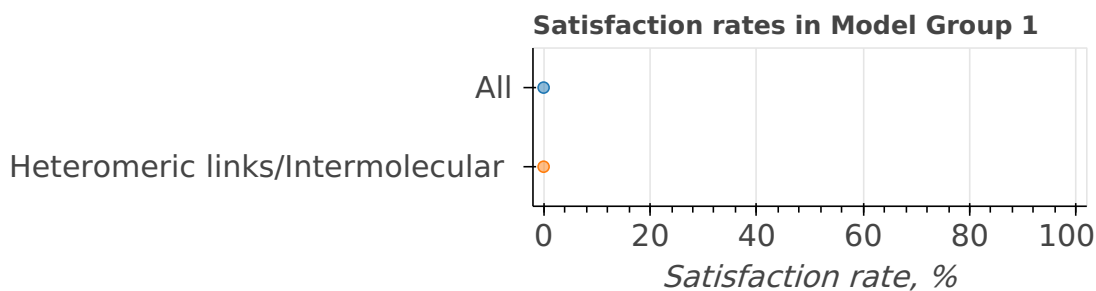
Satisfaction of restraints

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

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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