

# Integrative Structure Validation Report ?

April 09, 2025 - 08:54 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*

|                   |   |
|-------------------|---|
| PDB ID            | 9A4Z  |
| PDB-Dev ID        | PDBDEV_00000256   |
| Structure Title   | Integrative model of YXKC-DACA 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](mailto:helpdesk@pdb-ihm.org)*

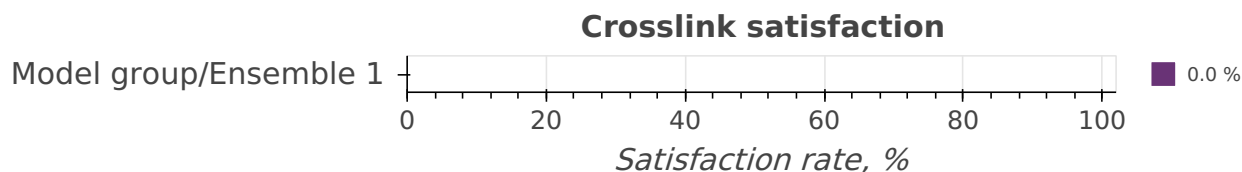
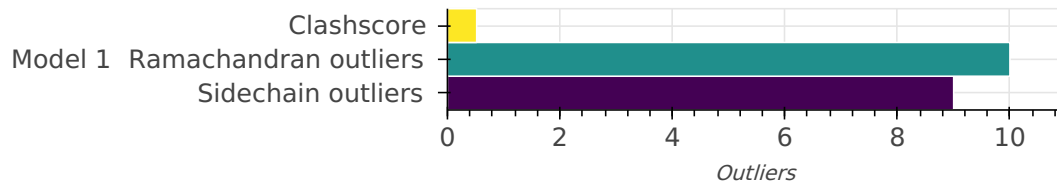
*A user guide is available at [https://pdb-ihm.org/validation\\_help.html](https://pdb-ihm.org/validation_help.html) with specific help available everywhere you see the ? symbol.*

*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 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/<br>Starting model coverage (%) | Scale  |
|----|----------|-----------|---------------|-----------------|----------------|----------------|-------------------|--|--------|
| 1  | 1        | 1         | YXKC_BACSU    | A               | 180            | -              | 1-180             | 100.00 / 0.00                                  | Atomic |
|    |          | 2         | DACA_BACSU    | B               | 443            | -              | 1-443             | 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  | <a href="#">AlphaLink2</a> | 1.00             | model building          | <a href="https://github.com/Rappsilber-Laboratory/AlphaLink2">https://github.com/Rappsilber-Laboratory/AlphaLink2</a> |

## 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 40 bond angle outliers in this entry (0.61% of 6539 assessed bonds). A summary is provided below.*

| Chain | Res | Type | Atoms      | Z    | Observed (Å) | Ideal (Å) | Model ID (Worst) | Models (Total) |
|-------|-----|------|------------|------|--------------|-----------|------------------|----------------|
| A     | 9   | ILE  | C-N-CA     | 8.23 | 136.51       | 121.70    | 1                | 1              |
| A     | 10  | LEU  | C-N-CA     | 6.82 | 133.97       | 121.70    | 1                | 1              |
| A     | 12  | VAL  | C-N-CA     | 6.80 | 133.93       | 121.70    | 1                | 1              |
| A     | 18  | ILE  | C-N-CA     | 6.44 | 133.29       | 121.70    | 1                | 1              |
| A     | 7   | THR  | C-N-CA     | 5.92 | 132.36       | 121.70    | 1                | 1              |
| A     | 3   | HIS  | C-N-CA     | 5.85 | 132.23       | 121.70    | 1                | 1              |
| A     | 1   | MET  | C-N-CA     | 5.76 | 132.06       | 121.70    | 1                | 1              |
| A     | 3   | HIS  | CA-C-N     | 5.75 | 127.70       | 116.20    | 1                | 1              |
| A     | 178 | LYS  | CG-CD-CE   | 5.51 | 98.64        | 111.30    | 1                | 1              |
| A     | 12  | VAL  | CA-CB-CG1  | 5.47 | 119.70       | 110.40    | 1                | 1              |
| A     | 3   | HIS  | C-CA-CB    | 5.42 | 120.39       | 110.10    | 1                | 1              |
| A     | 119 | ASP  | CA-CB-CG   | 5.38 | 107.22       | 112.60    | 1                | 1              |
| B     | 261 | SER  | C-N-CA     | 5.03 | 130.75       | 121.70    | 1                | 1              |
| A     | 173 | ASN  | OD1-CG-ND2 | 4.97 | 117.63       | 122.60    | 1                | 1              |
| A     | 12  | VAL  | CA-C-N     | 4.87 | 125.95       | 116.20    | 1                | 1              |
| A     | 66  | ASP  | CA-CB-CG   | 4.87 | 117.47       | 112.60    | 1                | 1              |
| A     | 14  | VAL  | CA-CB-CG2  | 4.78 | 118.52       | 110.40    | 1                | 1              |
| A     | 73  | GLN  | OE1-CD-NE2 | 4.71 | 117.89       | 122.60    | 1                | 1              |
| B     | 125 | GLN  | OE1-CD-NE2 | 4.69 | 117.91       | 122.60    | 1                | 1              |
| A     | 13  | VAL  | CG1-CB-CG2 | 4.66 | 100.56       | 110.80    | 1                | 1              |
| A     | 3   | HIS  | O-C-N      | 4.65 | 115.56       | 123.00    | 1                | 1              |
| B     | 269 | PHE  | CA-CB-CG   | 4.59 | 118.39       | 113.80    | 1                | 1              |
| A     | 10  | LEU  | O-C-N      | 4.54 | 115.73       | 123.00    | 1                | 1              |
| A     | 8   | PHE  | CA-CB-CG   | 4.54 | 118.34       | 113.80    | 1                | 1              |
| B     | 292 | HIS  | CA-CB-CG   | 4.45 | 109.35       | 113.80    | 1                | 1              |
| B     | 303 | PHE  | CA-CB-CG   | 4.44 | 118.24       | 113.80    | 1                | 1              |
| A     | 3   | HIS  | CB-CG-CD2  | 4.40 | 125.48       | 131.20    | 1                | 1              |
| B     | 240 | PHE  | CA-CB-CG   | 4.37 | 118.17       | 113.80    | 1                | 1              |
| A     | 14  | VAL  | N-CA-C     | 4.34 | 123.16       | 111.00    | 1                | 1              |
| B     | 292 | HIS  | CB-CG-CD2  | 4.34 | 125.56       | 131.20    | 1                | 1              |
| A     | 12  | VAL  | O-C-N      | 4.34 | 116.06       | 123.00    | 1                | 1              |
| A     | 18  | ILE  | CA-C-N     | 4.23 | 124.66       | 116.20    | 1                | 1              |
| A     | 7   | THR  | CA-C-N     | 4.21 | 124.61       | 116.20    | 1                | 1              |
| B     | 103 | GLN  | OE1-CD-NE2 | 4.21 | 118.39       | 122.60    | 1                | 1              |

| Chain | Res | Type | Atoms      | Z    | Observed (Å) | Ideal (Å) | Model ID (Worst) | Models (Total) |
|-------|-----|------|------------|------|--------------|-----------|------------------|----------------|
| A     | 18  | ILE  | O-C-N      | 4.19 | 116.29       | 123.00    | 1                | 1              |
| A     | 5   | ILE  | C-N-CA     | 4.18 | 129.23       | 121.70    | 1                | 1              |
| B     | 183 | GLN  | OE1-CD-NE2 | 4.12 | 118.48       | 122.60    | 1                | 1              |
| A     | 10  | LEU  | CA-C-N     | 4.08 | 124.37       | 116.20    | 1                | 1              |
| B     | 190 | ASN  | OD1-CG-ND2 | 4.03 | 118.57       | 122.60    | 1                | 1              |
| B     | 352 | ASN  | OD1-CG-ND2 | 4.01 | 118.59       | 122.60    | 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        | 0.52        | 5                 |

There are 5 clashes. The table below contains the detailed list of all clashes based on a MolProbity analysis. Bad clashes are  $\geq 0.4$  Angstrom.

| Atom 1         | Atom 2         | Clash(Å) | Model ID (Worst) | Models (Total) |
|----------------|----------------|----------|------------------|----------------|
| A:12:VAL:HA    | A:13:VAL:HG23  | 0.56     | 1                | 1              |
| B:292:HIS:HA   | B:295:ARG:HH21 | 0.51     | 1                | 1              |
| A:5:ILE:HA     | A:6:ILE:HG13   | 0.42     | 1                | 1              |
| B:335:GLU:CD   | B:335:GLU:H    | 0.40     | 1                | 1              |
| A:126:VAL:HG22 | B:292:HIS:CD2  | 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        | 619      | 570     | 39      | 10       |

There are 10 unique backbone outliers. Detailed list of outliers are tabulated below.

| Chain | Res | Type | Models (Total) |
|-------|-----|------|----------------|
| A     | 4   | LYS  | 1              |
| A     | 8   | PHE  | 1              |
| A     | 10  | LEU  | 1              |
| A     | 11  | ALA  | 1              |
| A     | 13  | VAL  | 1              |

| Chain | Res | Type | Models (Total) |
|-------|-----|------|----------------|
| A     | 14  | VAL  | 1              |
| A     | 27  | GLY  | 1              |
| A     | 38  | SER  | 1              |
| B     | 26  | MET  | 1              |
| B     | 27  | SER  | 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        | 526      | 503     | 14      | 9        |

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

| Chain | Res | Type | Models (Total) |
|-------|-----|------|----------------|
| A     | 14  | VAL  | 1              |
| A     | 18  | ILE  | 1              |
| A     | 123 | ASP  | 1              |
| B     | 9   | LEU  | 1              |
| B     | 10  | LEU  | 1              |
| B     | 11  | MET  | 1              |
| B     | 13  | LEU  | 1              |
| B     | 18  | LEU  | 1              |
| B     | 264 | SER  | 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*".

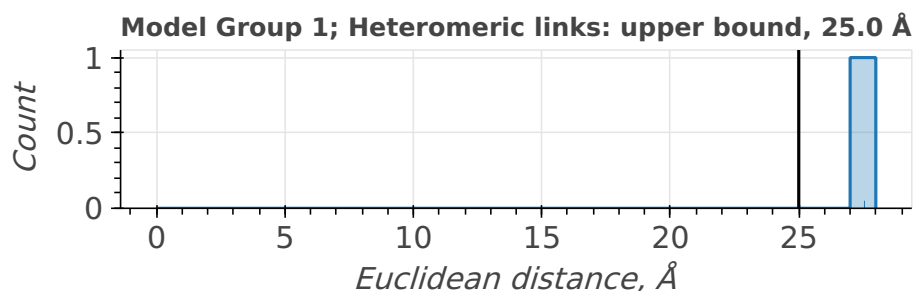
*Restraint group* represents a set of crosslinking restraints applied collectively in the modeling.

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.



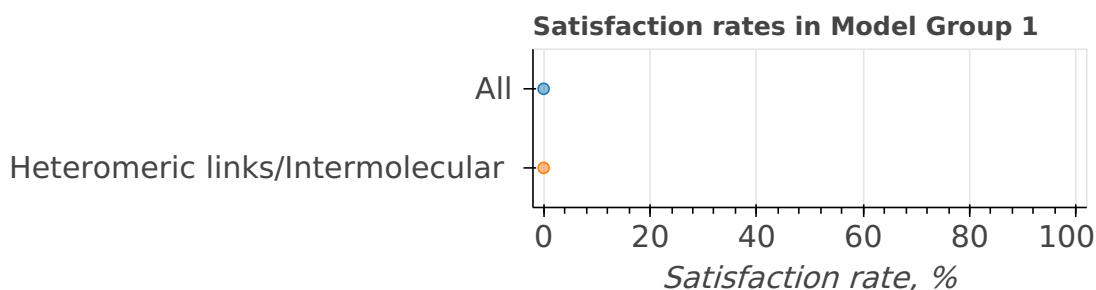
### Satisfaction of restraints

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.

### Acknowledgments

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