

Integrative Structure Validation Report

February 18, 2025 - 08:44 AM PST

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

pyHMMER Version 0.11.0

| | |
|-------------------|---|
| PDB ID | 9A7G |
| PDB-Dev ID | PDBDEV_00000345 |
| Structure Title | Integrative model of ODPa-ODP2 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

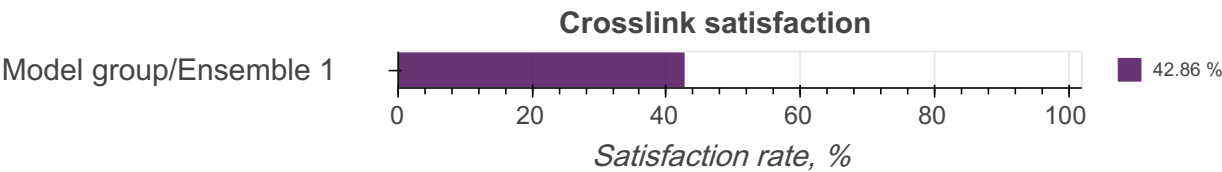
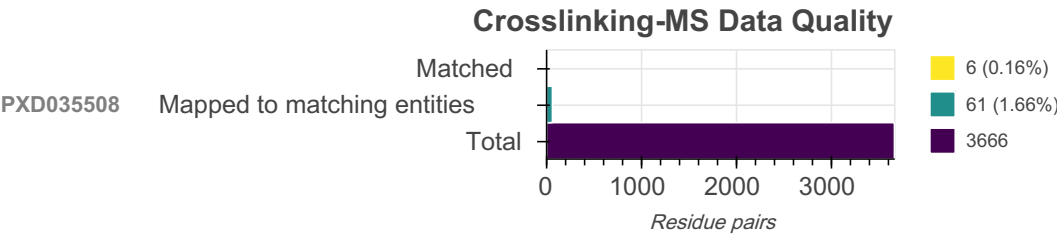
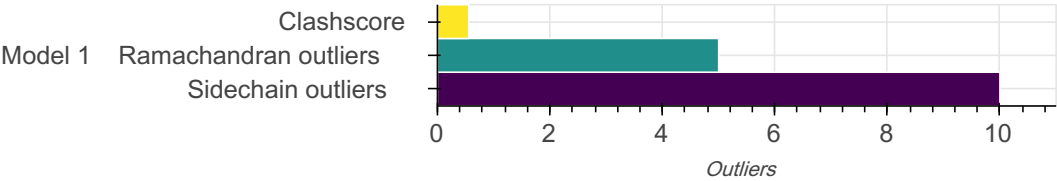
A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the  symbol.

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 | ODPA_BACSU | A | 371 | - | 1-371 | 100.00 / 0.00 | Atomic |
| | | 2 | ODP2_BACSU | B | 442 | - | 1-442 | 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 ([PRIDE ID](#))

[PXD035508](#)

Number of entities in the crosslinking-MS dataset:

810

Number of entities in the entry:

2

Matching entities:

| Entity ID | Molecule name | Crosslinking-MS Entity ID | E-value | Exact match |
|-----------|---------------|---------------------------|---------|-------------|
| 1 | ODPA_BACSU | dbseq_P21881_target | 0.00 | True |
| 2 | ODP2_BACSU | dbseq_P21883_target | 0.00 | True |

Residue pairs stats:

| Source | Total | In matched entities | Total matched |
|-----------|-------|---------------------|---------------|
| 9A7G | 7 | 7 (100.00%) | 6 (85.71%) |
| PXD035508 | 3666 | 61 (1.66%) | 6 (0.16%) |

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 49 bond angle outliers in this entry (0.57% of 8623 assessed bonds). A summary is provided below.

| Chain | Res | Type | Atoms | Z | Observed (Å) | Ideal (Å) | Model ID (Worst) | Models (Total) |
|-------|-----|------|------------|-------|--------------|-----------|------------------|----------------|
| B | 184 | GLU | C-N-CA | 10.64 | 140.86 | 121.70 | 1 | 1 |
| B | 189 | GLU | C-N-CA | 7.80 | 135.73 | 121.70 | 1 | 1 |
| B | 187 | PRO | C-N-CA | 7.00 | 134.29 | 121.70 | 1 | 1 |
| B | 186 | ALA | CA-C-N | 6.17 | 126.15 | 116.90 | 1 | 1 |
| B | 186 | ALA | N-CA-C | 6.16 | 128.25 | 111.00 | 1 | 1 |
| B | 189 | GLU | CA-C-N | 5.71 | 127.62 | 116.20 | 1 | 1 |
| B | 189 | GLU | O-C-N | 5.62 | 114.01 | 123.00 | 1 | 1 |
| B | 184 | GLU | CA-C-N | 5.45 | 127.11 | 116.20 | 1 | 1 |
| B | 184 | GLU | O-C-N | 5.40 | 114.36 | 123.00 | 1 | 1 |
| B | 109 | GLN | C-N-CA | 5.14 | 130.95 | 121.70 | 1 | 1 |
| B | 131 | GLN | OE1-CD-NE2 | 5.14 | 117.46 | 122.60 | 1 | 1 |
| A | 84 | GLN | OE1-CD-NE2 | 5.11 | 117.49 | 122.60 | 1 | 1 |
| B | 187 | PRO | CA-C-N | 5.07 | 126.34 | 116.20 | 1 | 1 |
| B | 187 | PRO | O-C-N | 4.92 | 115.13 | 123.00 | 1 | 1 |

| Chain | Res | Type | Atoms | Z | Observed (Å) | Ideal (Å) | Model ID (Worst) | Models (Total) |
|-------|-----|------|------------|------|--------------|-----------|------------------|----------------|
| B | 133 | GLU | C-N-CA | 4.89 | 130.51 | 121.70 | 1 | 1 |
| B | 427 | HIS | CB-CG-CD2 | 4.85 | 124.90 | 131.20 | 1 | 1 |
| A | 224 | GLN | OE1-CD-NE2 | 4.80 | 117.80 | 122.60 | 1 | 1 |
| B | 183 | GLN | OE1-CD-NE2 | 4.75 | 117.85 | 122.60 | 1 | 1 |
| A | 291 | ASN | OD1-CG-ND2 | 4.70 | 117.90 | 122.60 | 1 | 1 |
| B | 109 | GLN | OE1-CD-NE2 | 4.69 | 117.91 | 122.60 | 1 | 1 |
| B | 118 | GLN | OE1-CD-NE2 | 4.59 | 118.01 | 122.60 | 1 | 1 |
| B | 237 | HIS | CB-CG-CD2 | 4.58 | 125.24 | 131.20 | 1 | 1 |
| B | 40 | GLN | OE1-CD-NE2 | 4.58 | 118.02 | 122.60 | 1 | 1 |
| A | 295 | GLN | OE1-CD-NE2 | 4.52 | 118.08 | 122.60 | 1 | 1 |
| B | 129 | GLN | OE1-CD-NE2 | 4.51 | 118.09 | 122.60 | 1 | 1 |
| A | 150 | GLN | OE1-CD-NE2 | 4.48 | 118.12 | 122.60 | 1 | 1 |
| B | 110 | ASP | CA-CB-CG | 4.44 | 117.04 | 112.60 | 1 | 1 |
| B | 128 | GLN | OE1-CD-NE2 | 4.41 | 118.19 | 122.60 | 1 | 1 |
| B | 190 | THR | CA-CB-OG1 | 4.40 | 116.19 | 109.60 | 1 | 1 |
| B | 263 | GLN | OE1-CD-NE2 | 4.39 | 118.21 | 122.60 | 1 | 1 |
| B | 116 | GLN | OE1-CD-NE2 | 4.36 | 118.24 | 122.60 | 1 | 1 |
| B | 436 | GLN | OE1-CD-NE2 | 4.35 | 118.25 | 122.60 | 1 | 1 |
| B | 102 | GLN | OE1-CD-NE2 | 4.31 | 118.29 | 122.60 | 1 | 1 |
| B | 252 | HIS | CB-CG-CD2 | 4.31 | 125.60 | 131.20 | 1 | 1 |
| A | 27 | GLN | OE1-CD-NE2 | 4.26 | 118.34 | 122.60 | 1 | 1 |
| A | 22 | GLN | OE1-CD-NE2 | 4.24 | 118.36 | 122.60 | 1 | 1 |
| A | 48 | GLN | OE1-CD-NE2 | 4.21 | 118.39 | 122.60 | 1 | 1 |
| B | 85 | GLN | OE1-CD-NE2 | 4.19 | 118.41 | 122.60 | 1 | 1 |
| B | 194 | GLN | OE1-CD-NE2 | 4.19 | 118.41 | 122.60 | 1 | 1 |
| B | 100 | GLN | OE1-CD-NE2 | 4.12 | 118.48 | 122.60 | 1 | 1 |
| A | 15 | GLN | OE1-CD-NE2 | 4.12 | 118.48 | 122.60 | 1 | 1 |
| B | 288 | ASN | OD1-CG-ND2 | 4.12 | 118.48 | 122.60 | 1 | 1 |
| B | 130 | ASP | C-N-CA | 4.10 | 129.08 | 121.70 | 1 | 1 |
| B | 300 | GLN | OE1-CD-NE2 | 4.09 | 118.51 | 122.60 | 1 | 1 |
| A | 65 | ARG | NE-CZ-NH2 | 4.06 | 122.86 | 119.20 | 1 | 1 |
| B | 188 | GLN | OE1-CD-NE2 | 4.04 | 118.56 | 122.60 | 1 | 1 |
| A | 361 | GLN | OE1-CD-NE2 | 4.02 | 118.58 | 122.60 | 1 | 1 |
| A | 153 | GLN | OE1-CD-NE2 | 4.01 | 118.59 | 122.60 | 1 | 1 |
| A | 64 | GLN | OE1-CD-NE2 | 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 | 0.56 | 7 |

There are 7 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:298:VAL:HG22 | B:415:MET:HE1 | 0.54 | 1 | 1 |
| B:273:VAL:HG11 | B:385:ILE:HD11 | 0.47 | 1 | 1 |
| A:44:LEU:HD21 | A:245:TYR:CZ | 0.47 | 1 | 1 |
| B:119:GLU:HB3 | B:120:PRO:HD3 | 0.45 | 1 | 1 |
| B:119:GLU:CB | B:120:PRO:HD3 | 0.45 | 1 | 1 |
| B:243:GLU:O | B:429:LYS:HE3 | 0.43 | 1 | 1 |
| B:94:ASP:C | B:96:LYS:H | 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 | 809 | 760 | 44 | 5 |

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

| Chain | Res | Type | Models (Total) |
|-------|-----|------|----------------|
| A | 209 | ILE | 1 |
| B | 93 | ASP | 1 |
| B | 95 | ALA | 1 |
| B | 110 | ASP | 1 |
| B | 120 | 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 | 656 | 627 | 19 | 10 |

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

| Chain | Res | Type | Models (Total) |
|-------|-----|------|----------------|
| A | 5 | THR | 1 |
| B | 97 | THR | 1 |
| B | 104 | THR | 1 |
| B | 111 | VAL | 1 |
| B | 114 | GLU | 1 |
| B | 119 | GLU | 1 |
| B | 124 | THR | 1 |
| B | 190 | THR | 1 |
| B | 413 | HIS | 1 |
| B | 440 | MET | 1 |

Fit of model to data used for modeling ?

Fit of model(s) to crosslinking-MS data

Restraint types

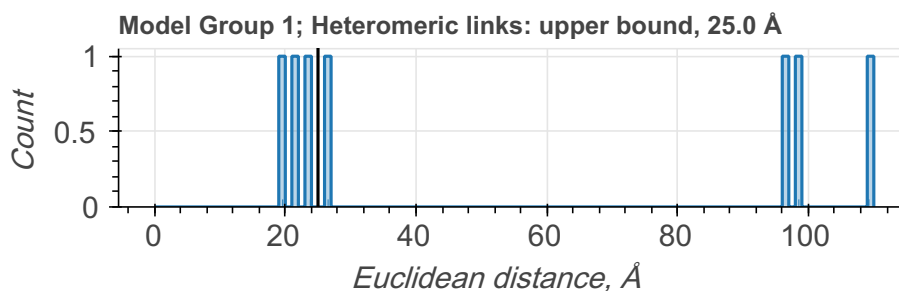
Restraint types are summarized in the table below. Restraints assigned "by-residue" are interpreted as between CA atoms. Restraints between coarse-grained beads are indicated as "coarse-grained". *Restraint group* represents a set of crosslinking restraints applied collectively in the modeling.

There are 7 crosslinking restraints combined in 7 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 | 5 |
| SDA | ALA | 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.



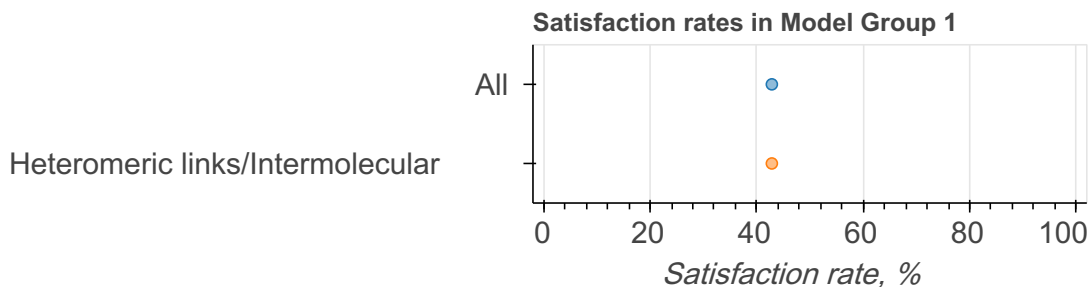
Satisfaction of restraints

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=7) |
|-------------|-------|-------------|-----------------------------|----------------------------------|---------------|--------------|-----------------|
| 1 | 1 | 1 | 1/1 | All | 42.86 | 57.14 | 7 |
| | | | | Heteromeric links/Intermolecular | 42.86 | 57.14 | 7 |

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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