

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 | 9A81 |
| PDB-Dev ID | PDBDEV_00000366 |
| Structure Title | Integrative model of GRPE-DNAK by crosslinking MS and deep learning |
| Structure Authors | Kolja Stahl; Oliver Brock; Juri Rappsilber |
| Deposited on | 2024-01-24 |

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

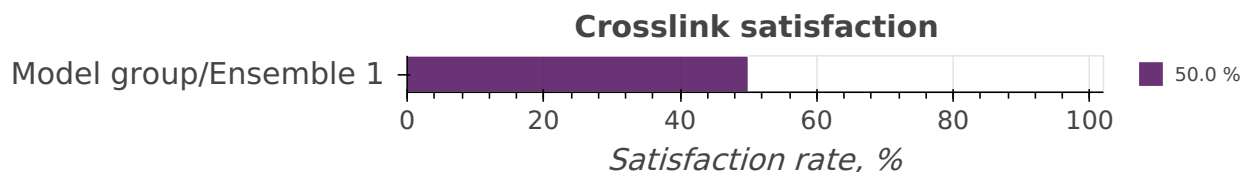
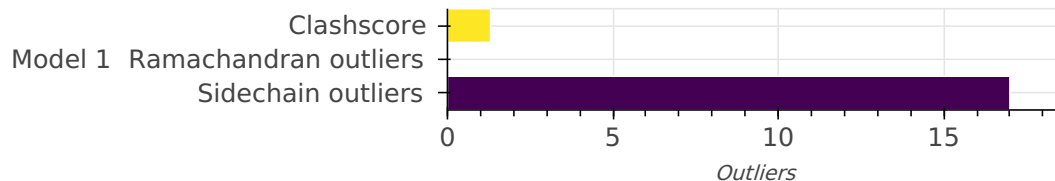
A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the ? symbol.

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 | GRPE_BACSU | A | 187 | - | 1-187 | 100.00 / 0.00 | Atomic |
| | | 2 | DNAK_BACSU | B | 611 | - | 1-611 | 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 43 bond angle outliers in this entry (0.51% of 8367 assessed bonds). A summary is provided below.

| Chain | Res | Type | Atoms | Z | Observed (Å) | Ideal (Å) | Model ID (Worst) | Models (Total) |
|-------|-----|------|------------|------|--------------|-----------|------------------|----------------|
| A | 29 | GLN | OE1-CD-NE2 | 5.46 | 117.14 | 122.60 | 1 | 1 |
| B | 348 | GLN | OE1-CD-NE2 | 5.44 | 117.16 | 122.60 | 1 | 1 |
| A | 16 | GLN | OE1-CD-NE2 | 5.16 | 117.44 | 122.60 | 1 | 1 |
| A | 168 | GLN | OE1-CD-NE2 | 5.08 | 117.52 | 122.60 | 1 | 1 |
| B | 126 | GLN | OE1-CD-NE2 | 5.07 | 117.53 | 122.60 | 1 | 1 |
| A | 187 | GLN | OE1-CD-NE2 | 5.01 | 117.59 | 122.60 | 1 | 1 |
| A | 46 | GLN | OE1-CD-NE2 | 4.94 | 117.66 | 122.60 | 1 | 1 |
| A | 122 | GLN | OE1-CD-NE2 | 4.76 | 117.84 | 122.60 | 1 | 1 |
| A | 161 | ASN | OD1-CG-ND2 | 4.73 | 117.87 | 122.60 | 1 | 1 |
| A | 28 | GLN | OE1-CD-NE2 | 4.70 | 117.90 | 122.60 | 1 | 1 |
| A | 22 | GLN | OE1-CD-NE2 | 4.66 | 117.94 | 122.60 | 1 | 1 |
| B | 562 | GLN | OE1-CD-NE2 | 4.64 | 117.96 | 122.60 | 1 | 1 |
| B | 295 | GLN | OE1-CD-NE2 | 4.60 | 118.00 | 122.60 | 1 | 1 |
| A | 60 | GLN | OE1-CD-NE2 | 4.60 | 118.00 | 122.60 | 1 | 1 |
| A | 10 | GLN | OE1-CD-NE2 | 4.58 | 118.02 | 122.60 | 1 | 1 |
| A | 78 | GLN | OE1-CD-NE2 | 4.53 | 118.07 | 122.60 | 1 | 1 |
| B | 511 | GLN | OE1-CD-NE2 | 4.52 | 118.08 | 122.60 | 1 | 1 |
| A | 108 | GLN | OE1-CD-NE2 | 4.51 | 118.09 | 122.60 | 1 | 1 |
| B | 581 | GLN | OE1-CD-NE2 | 4.50 | 118.10 | 122.60 | 1 | 1 |
| B | 95 | GLN | OE1-CD-NE2 | 4.50 | 118.10 | 122.60 | 1 | 1 |
| A | 6 | GLN | OE1-CD-NE2 | 4.49 | 118.11 | 122.60 | 1 | 1 |
| A | 39 | GLN | OE1-CD-NE2 | 4.48 | 118.12 | 122.60 | 1 | 1 |
| B | 608 | GLN | OE1-CD-NE2 | 4.47 | 118.13 | 122.60 | 1 | 1 |
| B | 515 | GLN | OE1-CD-NE2 | 4.46 | 118.14 | 122.60 | 1 | 1 |
| B | 566 | GLN | OE1-CD-NE2 | 4.46 | 118.14 | 122.60 | 1 | 1 |
| B | 204 | GLN | OE1-CD-NE2 | 4.45 | 118.15 | 122.60 | 1 | 1 |
| B | 48 | GLN | OE1-CD-NE2 | 4.43 | 118.17 | 122.60 | 1 | 1 |
| B | 87 | GLN | OE1-CD-NE2 | 4.29 | 118.31 | 122.60 | 1 | 1 |
| A | 114 | GLN | OE1-CD-NE2 | 4.29 | 118.31 | 122.60 | 1 | 1 |
| A | 140 | GLN | OE1-CD-NE2 | 4.24 | 118.36 | 122.60 | 1 | 1 |
| B | 96 | HIS | CB-CG-CD2 | 4.23 | 125.70 | 131.20 | 1 | 1 |
| B | 195 | ASN | OD1-CG-ND2 | 4.22 | 118.38 | 122.60 | 1 | 1 |
| B | 281 | HIS | CB-CG-CD2 | 4.22 | 125.71 | 131.20 | 1 | 1 |
| B | 394 | 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) |
|-------|-----|------|------------|------|--------------|-----------|------------------|----------------|
| B | 583 | GLN | OE1-CD-NE2 | 4.21 | 118.39 | 122.60 | 1 | 1 |
| B | 531 | GLN | OE1-CD-NE2 | 4.18 | 118.42 | 122.60 | 1 | 1 |
| B | 336 | ASN | OD1-CG-ND2 | 4.09 | 118.51 | 122.60 | 1 | 1 |
| A | 41 | GLN | OE1-CD-NE2 | 4.06 | 118.54 | 122.60 | 1 | 1 |
| B | 200 | ASP | CA-CB-CG | 4.04 | 116.64 | 112.60 | 1 | 1 |
| B | 608 | GLN | N-CA-C | 4.04 | 122.30 | 111.00 | 1 | 1 |
| B | 441 | GLN | OE1-CD-NE2 | 4.04 | 118.56 | 122.60 | 1 | 1 |
| B | 265 | HIS | CB-CG-CD2 | 4.02 | 125.97 | 131.20 | 1 | 1 |
| A | 101 | 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 | 1.30 | 16 |

There are 16 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:195:ASN:HD22 | B:479:ASP:CG | 0.60 | 1 | 1 |
| A:93:LEU:HD11 | A:127:LEU:CD1 | 0.56 | 1 | 1 |
| B:421:ASN:HA | B:485:MET:HE3 | 0.53 | 1 | 1 |
| B:513:VAL:HG11 | B:543:LYS:HE3 | 0.49 | 1 | 1 |
| B:196:ARG:NH1 | B:480:GLU:HG3 | 0.48 | 1 | 1 |
| A:153:ALA:HB2 | A:184:LYS:HE2 | 0.44 | 1 | 1 |
| B:367:LEU:HD11 | B:482:ILE:HG23 | 0.44 | 1 | 1 |
| A:133:GLU:HB2 | A:172:LYS:HE3 | 0.44 | 1 | 1 |
| A:65:ASN:HD21 | B:105:LEU:HA | 0.43 | 1 | 1 |
| B:151:LEU:HD11 | B:361:LEU:HD11 | 0.43 | 1 | 1 |
| B:409:HIS:CE1 | B:426:ARG:HH21 | 0.43 | 1 | 1 |
| B:196:ARG:HG3 | B:196:ARG:HH11 | 0.43 | 1 | 1 |
| B:406:VAL:HG21 | B:442:ILE:HD13 | 0.42 | 1 | 1 |
| B:421:ASN:HA | B:485:MET:CE | 0.42 | 1 | 1 |
| A:151:MET:HE2 | A:184:LYS:HE3 | 0.42 | 1 | 1 |
| B:151:LEU:HD11 | B:361:LEU:CD1 | 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 | 794 | 779 | 15 | 0 |

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 | 671 | 620 | 34 | 17 |

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

| Chain | Res | Type | Models (Total) |
|-------|-----|------|----------------|
| A | 7 | THR | 1 |
| A | 13 | THR | 1 |
| A | 37 | LEU | 1 |
| A | 56 | LEU | 1 |
| A | 57 | LEU | 1 |
| A | 123 | LEU | 1 |
| A | 125 | GLU | 1 |
| A | 150 | VAL | 1 |
| B | 119 | TYR | 1 |
| B | 229 | LEU | 1 |
| B | 250 | GLN | 1 |
| B | 302 | SER | 1 |
| B | 335 | VAL | 1 |
| B | 361 | LEU | 1 |
| B | 524 | GLU | 1 |
| B | 572 | LEU | 1 |
| B | 573 | TYR | 1 |

Fit of model to data used for modeling ?

Fit of model(s) to crosslinking-MS data

Restraint types

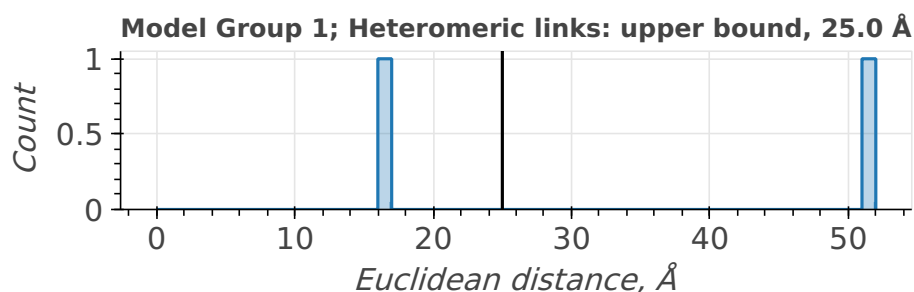
Restraint types are summarized in the table below. Restraints assigned "*by-residue*" are interpreted as between CA atoms. Restraints between coarse-grained beads are indicated as "coarse-grained". *Restraint group* represents a set of crosslinking restraints applied collectively in the modeling.

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.



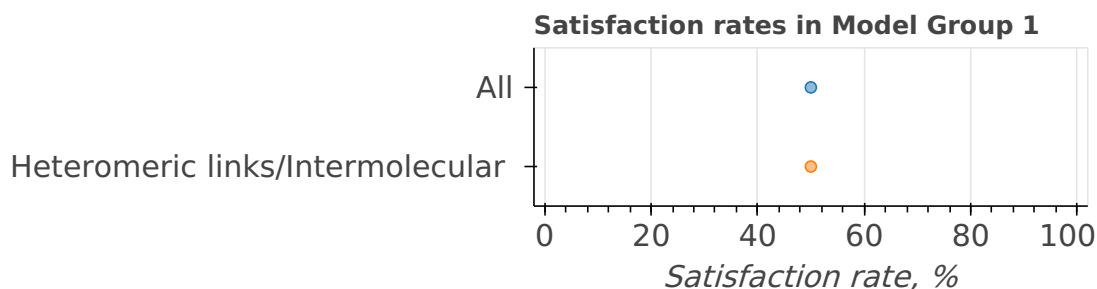
Satisfaction of restraints

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 | 50.00 | 50.00 | 2 |
| | | | | Heteromeric links/ Intermolecular | 50.00 | 50.00 | 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.

Acknowledgments

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