# Integrative Structure Validation Report

## February 18, 2025 - 08:38 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*

| | |
|---|---|
| PDB ID | 9A3X |
| PDB-Dev ID | PDBDEV_00000218 |
| Structure Title | Predicted model of tissue transglutaminase 2 (TG2) in complex with plasma fibronectin type I modules 2 and 3 (FNI2-3) |
| Structure Authors | Selcuk, K.; Leitner, A.; Le Blanc, F. |
| Deposited on | 2023-10-04 |

*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*

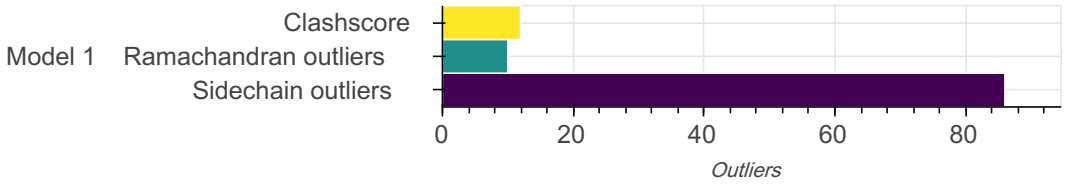
*A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the* ? symbol.

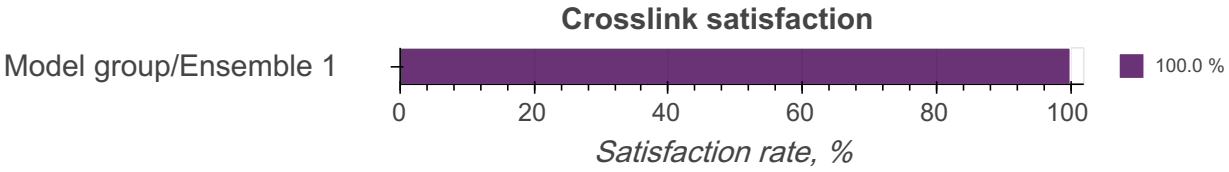
*List of references used to build this report is available here.*

## 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 3 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 | Protein-glutamine gamma-glutamyltransferase 2 | A | 687 | - | 1-687 | 100.00 / 100.00 | Atomic |
| | | 2 | Fibronectin | B | 90 | - | 1-90 | 100.00 / 100.00 | Atomic |

## Datasets used for modeling

*There are 3 unique datasets used to build the models in this entry.*

| ID | Dataset type | Database name | Data access code |
|---|---|---|---|
| 1 | Crosslinking-MS data | PRIDE | PXD043976 |
| 2 | Experimental model | PDB | 4PYG |
| 3 | Experimental model | PDB | 2CG7 |

## 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 | Refinement | Iterative Threading ASSEmbly Refinement | structural refinement of starting models guided by experimental crosslinks | None | False | False |
| 2 | 1 | satisfied/violated crosslinks identification | Validate measured chemical cross-links on a protein 3D structure | calculation of Euclidean distances between crosslinked residues | None | False | False |
| 3 | 1 | calculation of accessible area | calculates the atomic accessible area when a probe is rolled around the Van der Waal's surface of a macromolecule | calculation of accessible area | None | False | False |
| 4 | 1 | accessible interaction space | None | determine the number of complexes consistent with the restraints | None | False | False |
| 5 | 1 | docking | data-driven biomolecular docking | generates predicted model of a protein complex | None | False | False |

*There are 5 software packages reported in this entry.*

| ID | Software name | Software version | Software classification | Software location |
|---|---|---|---|---|
| 1 | I-TASSER | Not available | structure refinement | https://zhanggroup.org/I-TASSER/ |
| 3 | Xwalk | Not available | Euclidean distances calculation | https://www.xwalk.org/home.cgi |
| 2 | NACCESS | Not available | solvent accessibility | http://www.bioinf.manchester.ac.uk/naccess/ |
| 4 | DisVis | Not available | accessible interaction space | https://wenmr.science.uu.nl/disvis/ |
| 5 | HADDOCK | Not available | protein-protein docking | https://wenmr.science.uu.nl/haddock2.4/ |

## 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 no bond angle outliers.*

### 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 | 11.96 | 145 |

*There are 145 clashes. The table below contains the detailed list of all clashes based on a MolProbity analysis. Bad clashes are >= 0.4 Angstrom. The output is limited to 100 rows.*

| Atom 1 | Atom 2 | Clash(Å) | Model ID (Worst) | Models (Total) |
|---|---|---|---|---|
| A:249:VAL:HG22 | B:24:ASP:HA | 0.95 | 1 | 1 |
| A:11:ASP:HB3 | A:42:THR:HB | 0.89 | 1 | 1 |
| A:361:PRO:HA | A:369:TYR:HB3 | 0.88 | 1 | 1 |
| A:514:VAL:HG21 | A:562:LYS:HB2 | 0.83 | 1 | 1 |
| A:641:PRO:HG3 | B:39:ARG:HG3 | 0.81 | 1 | 1 |
| A:62:VAL:HG13 | A:67:PRO:HB3 | 0.74 | 1 | 1 |
| A:483:MET:HB2 | A:584:LEU:HD23 | 0.73 | 1 | 1 |
| A:12:LEU:HB3 | A:31:LEU:HD22 | 0.73 | 1 | 1 |
| A:499:THR:HG23 | A:501:GLU:H | 0.72 | 1 | 1 |
| B:27:ILE:HG12 | B:54:SER:HB3 | 0.69 | 1 | 1 |
| A:379:ILE:HD13 | A:393:VAL:HG12 | 0.68 | 1 | 1 |
| A:514:VAL:HG13 | A:518:GLY:HA2 | 0.66 | 1 | 1 |
| A:606:GLU:HB3 | A:651:ARG:HG3 | 0.65 | 1 | 1 |
| A:81:ASP:HA | A:92:VAL:HG22 | 0.65 | 1 | 1 |
| A:617:LEU:HD11 | A:668:PHE:HZ | 0.65 | 1 | 1 |
| A:200:ASN:HA | A:227:MET:SD | 0.64 | 1 | 1 |
| A:460:ASN:HB3 | A:464:LYS:HB2 | 0.63 | 1 | 1 |
| A:158:GLU:HA | A:162:THR:OG1 | 0.62 | 1 | 1 |
| A:599:GLN:HG3 | A:600:LYS:HG2 | 0.62 | 1 | 1 |
| A:262:ARG:HD2 | A:632:GLU:HG2 | 0.62 | 1 | 1 |
| A:504:VAL:HA | A:533:ASN:HA | 0.61 | 1 | 1 |
| A:374:VAL:HG21 | A:390:ALA:HA | 0.61 | 1 | 1 |
| A:259:ASP:O | A:263:ARG:HG2 | 0.60 | 1 | 1 |
| A:668:PHE:HB3 | A:676:VAL:HB | 0.58 | 1 | 1 |
| A:495:ILE:HD11 | A:507:LEU:HD22 | 0.58 | 1 | 1 |
| A:276:GLN:HG2 | A:278:TRP:CZ3 | 0.58 | 1 | 1 |
| A:196:LEU:HD12 | A:227:MET:HB3 | 0.58 | 1 | 1 |
| A:167:ILE:HB | A:178:ILE:HG23 | 0.58 | 1 | 1 |
| A:559:ASN:HB3 | A:584:LEU:HB2 | 0.57 | 1 | 1 |
| A:355:GLN:HB3 | A:373:PRO:HB2 | 0.57 | 1 | 1 |
| A:236:VAL:HG23 | A:237:LEU:HD12 | 0.56 | 1 | 1 |
| A:260:ILE:HG23 | A:272:VAL:HG21 | 0.56 | 1 | 1 |
| A:567:LEU:HB3 | A:576:LEU:HB2 | 0.56 | 1 | 1 |
| A:343:THR:HG22 | A:352:GLU:HG3 | 0.56 | 1 | 1 |
| A:565:ALA:HB3 | A:578:ALA:HB3 | 0.56 | 1 | 1 |

| Atom 1 | Atom 2 | Clash(Å) | Model ID (Worst) | Models (Total) |
|---|---|---|---|---|
| B:72:LEU:HB3 | B:86:CYS:SG | 0.55 | 1 | 1 |
| A:186:GLU:HB3 | A:189:ILE:HG12 | 0.55 | 1 | 1 |
| A:26:LEU:HD22 | A:185:PHE:HA | 0.54 | 1 | 1 |
| A:59:PHE:HB2 | A:77:PHE:CE2 | 0.54 | 1 | 1 |
| A:179:PRO:HG3 | A:679:PHE:HB3 | 0.54 | 1 | 1 |
| A:416:ILE:HD12 | A:469:GLU:HG2 | 0.53 | 1 | 1 |
| A:9:ARG:HB2 | A:44:HIS:HB3 | 0.53 | 1 | 1 |
| A:307:GLN:HE22 | A:311:LEU:HA | 0.53 | 1 | 1 |
| A:85:GLU:H | A:89:THR:HG21 | 0.52 | 1 | 1 |
| A:153:GLU:O | A:156:ARG:HG2 | 0.52 | 1 | 1 |
| A:513:THR:HG23 | A:555:LEU:HD23 | 0.52 | 1 | 1 |
| A:249:VAL:HG13 | B:24:ASP:HB3 | 0.51 | 1 | 1 |
| A:311:LEU:HD22 | A:395:ALA:HB2 | 0.51 | 1 | 1 |
| A:624:VAL:HG12 | A:666:VAL:HG12 | 0.51 | 1 | 1 |
| B:5:PHE:HD2 | B:7:LYS:HE2 | 0.51 | 1 | 1 |
| A:445:TYR:HB2 | A:452:GLU:HB3 | 0.51 | 1 | 1 |
| A:4:GLU:HG2 | A:123:THR:HB | 0.50 | 1 | 1 |
| A:50:TYR:HE1 | A:57:LEU:HB2 | 0.50 | 1 | 1 |
| A:323:ILE:HG12 | A:325:GLY:H | 0.50 | 1 | 1 |
| A:342:MET:HG2 | A:355:GLN:HG3 | 0.50 | 1 | 1 |
| A:343:THR:HA | A:352:GLU:HG3 | 0.50 | 1 | 1 |
| A:14:LEU:H | A:14:LEU:HD12 | 0.49 | 1 | 1 |
| A:112:ILE:H | A:112:ILE:HD13 | 0.49 | 1 | 1 |
| B:60:THR:HG23 | B:75:VAL:HB | 0.49 | 1 | 1 |
| A:433:ARG:HB2 | A:435:GLU:OE1 | 0.49 | 1 | 1 |
| A:56:SER:HB3 | A:122:SER:HB2 | 0.49 | 1 | 1 |
| A:548:TYR:HA | A:551:TYR:CE2 | 0.49 | 1 | 1 |
| A:67:PRO:HB2 | A:74:LYS:HB2 | 0.49 | 1 | 1 |
| A:36:GLY:H | A:106:THR:HB | 0.49 | 1 | 1 |
| A:491:VAL:HB | A:544:LEU:HB2 | 0.48 | 1 | 1 |
| A:587:PRO:HG2 | A:673:LEU:HD21 | 0.48 | 1 | 1 |
| A:509:LEU:HB2 | A:527:LYS:HB2 | 0.48 | 1 | 1 |
| A:154:GLU:HB2 | A:431:VAL:HG11 | 0.47 | 1 | 1 |
| A:445:TYR:HB3 | A:446:PRO:HD2 | 0.47 | 1 | 1 |
| A:61:VAL:O | A:74:LYS:HA | 0.47 | 1 | 1 |

| Atom 1 | Atom 2 | Clash(Å) | Model ID (Worst) | Models (Total) |
|---|---|---|---|---|
| A:532:LEU:H | A:532:LEU:HD22 | 0.47 | 1 | 1 |
| A:639:PRO:HA | B:43:THR:OG1 | 0.47 | 1 | 1 |
| A:623:THR:HB | A:635:THR:HG23 | 0.47 | 1 | 1 |
| A:21:HIS:CE1 | A:37:GLN:HB3 | 0.47 | 1 | 1 |
| A:618:GLU:CB | B:40:ILE:HG13 | 0.47 | 1 | 1 |
| A:425:LYS:HA | A:425:LYS:HD3 | 0.47 | 1 | 1 |
| A:430:SER:HB2 | A:433:ARG:HG3 | 0.47 | 1 | 1 |
| A:255:ILE:HD12 | A:625:GLU:HG2 | 0.46 | 1 | 1 |
| A:623:THR:HA | A:635:THR:HA | 0.46 | 1 | 1 |
| A:244:ASN:HD21 | B:10:GLY:HA3 | 0.46 | 1 | 1 |
| A:13:GLU:HG3 | A:16:THR:HB | 0.46 | 1 | 1 |
| A:294:PRO:HB2 | A:341:TRP:HB3 | 0.46 | 1 | 1 |
| A:201:PRO:O | A:205:LYS:HG2 | 0.46 | 1 | 1 |
| A:195:ILE:O | A:199:VAL:HG23 | 0.45 | 1 | 1 |
| A:193:CYS:HB3 | A:287:VAL:HG13 | 0.45 | 1 | 1 |
| A:328:SER:HB3 | A:519:ILE:HA | 0.45 | 1 | 1 |
| A:593:ILE:HD13 | A:680:ARG:HD2 | 0.45 | 1 | 1 |
| A:387:LYS:O | A:388:TYR:HB2 | 0.45 | 1 | 1 |
| A:497:ASN:OD1 | A:499:THR:HG22 | 0.45 | 1 | 1 |
| A:471:THR:HG22 | A:574:SER:HB3 | 0.45 | 1 | 1 |
| A:61:VAL:HB | A:115:TYR:HD2 | 0.44 | 1 | 1 |
| A:447:GLU:HA | A:452:GLU:OE1 | 0.44 | 1 | 1 |
| A:343:THR:HG22 | A:352:GLU:CG | 0.44 | 1 | 1 |
| A:362:GLN:HG3 | A:392:PHE:CZ | 0.44 | 1 | 1 |
| A:456:PHE:O | A:460:ASN:HB2 | 0.44 | 1 | 1 |
| A:492:PHE:CZ | A:543:PRO:HB3 | 0.44 | 1 | 1 |
| A:299:THR:HG23 | A:336:CYS:SG | 0.44 | 1 | 1 |
| A:505:CYS:HB2 | A:567:LEU:HD11 | 0.44 | 1 | 1 |
| A:569:GLU:OE1 | A:571:VAL:HG13 | 0.44 | 1 | 1 |
| A:81:ASP:CG | A:82:ALA:H | 0.43 | 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 | 773 | 682 | 81 | 10 |

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

| Chain | Res | Type | Models (Total) |
|---|---|---|---|
| A | 47 | GLY | 1 |
| A | 81 | ASP | 1 |
| A | 93 | VAL | 1 |
| A | 108 | ALA | 1 |
| A | 230 | CYS | 1 |
| A | 421 | ILE | 1 |
| A | 431 | VAL | 1 |
| A | 465 | LEU | 1 |
| A | 525 | GLY | 1 |
| B | 37 | ARG | 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 | 671 | 459 | 126 | 86 |

*There are 86 unique sidechain outliers. Detailed list of outliers are tabulated below.*

| Chain | Res | Type | Models (Total) |
|---|---|---|---|
| A | 26 | LEU | 1 |
| A | 29 | GLU | 1 |
| A | 46 | GLU | 1 |
| A | 56 | SER | 1 |
| A | 58 | THR | 1 |
| A | 73 | THR | 1 |
| A | 84 | GLU | 1 |
| A | 94 | ASP | 1 |
| A | 100 | LEU | 1 |
| A | 103 | GLN | 1 |
| A | 112 | ILE | 1 |
| A | 118 | SER | 1 |
| A | 129 | SER | 1 |
| A | 151 | ASP | 1 |
| A | 157 | GLN | 1 |
| A | 163 | GLN | 1 |

| Chain | Res | Type | Models (Total) |
|---|---|---|---|
| A | 164 | GLN | 1 |
| A | 166 | PHE | 1 |
| A | 184 | GLN | 1 |
| A | 186 | GLU | 1 |
| A | 209 | ARG | 1 |
| A | 211 | CYS | 1 |
| A | 215 | SER | 1 |
| A | 216 | SER | 1 |
| A | 225 | SER | 1 |
| A | 238 | LEU | 1 |
| A | 250 | SER | 1 |
| A | 255 | ILE | 1 |
| A | 257 | SER | 1 |
| A | 271 | ARG | 1 |
| A | 279 | VAL | 1 |
| A | 298 | VAL | 1 |
| A | 305 | HIS | 1 |
| A | 307 | GLN | 1 |
| A | 312 | LEU | 1 |
| A | 313 | ILE | 1 |
| A | 314 | GLU | 1 |
| A | 347 | LEU | 1 |
| A | 362 | GLN | 1 |
| A | 364 | LYS | 1 |
| A | 365 | SER | 1 |
| A | 381 | GLU | 1 |
| A | 419 | SER | 1 |
| A | 422 | VAL | 1 |
| A | 431 | VAL | 1 |
| A | 442 | THR | 1 |
| A | 447 | GLU | 1 |
| A | 478 | ARG | 1 |
| A | 483 | MET | 1 |
| A | 491 | VAL | 1 |
| A | 496 | THR | 1 |

| Chain | Res | Type | Models (Total) |
|---|---|---|---|
| A | 503 | TYR | 1 |
| A | 524 | CYS | 1 |
| A | 526 | THR | 1 |
| A | 531 | ASN | 1 |
| A | 532 | LEU | 1 |
| A | 533 | ASN | 1 |
| A | 549 | GLU | 1 |
| A | 556 | THR | 1 |
| A | 560 | LEU | 1 |
| A | 571 | VAL | 1 |
| A | 577 | LEU | 1 |
| A | 608 | SER | 1 |
| A | 617 | LEU | 1 |
| A | 618 | GLU | 1 |
| A | 621 | THR | 1 |
| A | 631 | GLU | 1 |
| A | 632 | GLU | 1 |
| A | 653 | ASP | 1 |
| A | 657 | LEU | 1 |
| A | 659 | MET | 1 |
| A | 664 | LEU | 1 |
| B | 3 | THR | 1 |
| B | 7 | LYS | 1 |
| B | 9 | THR | 1 |
| B | 12 | THR | 1 |
| B | 13 | TYR | 1 |
| B | 24 | ASP | 1 |
| B | 29 | ASP | 1 |
| B | 40 | ILE | 1 |
| B | 56 | LYS | 1 |
| B | 60 | THR | 1 |
| B | 63 | ARG | 1 |
| B | 67 | THR | 1 |
| B | 74 | CYS | 1 |
| B | 85 | THR | 1 |

# Fit of model to data used for modeling

## Fit of model(s) to crosslinking-MS data

### Restraint types

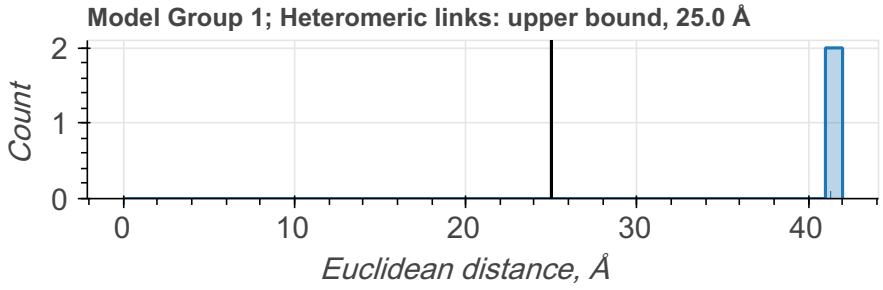
*Restraint types are summarized in the table below. Restraints assigned "by-residue" are interpreted as between CA atoms. Restraints between coarse-grained beads are indicated as "coarse-grained". Restraint group represents a set of crosslinking restraints applied collectively in the modeling.*

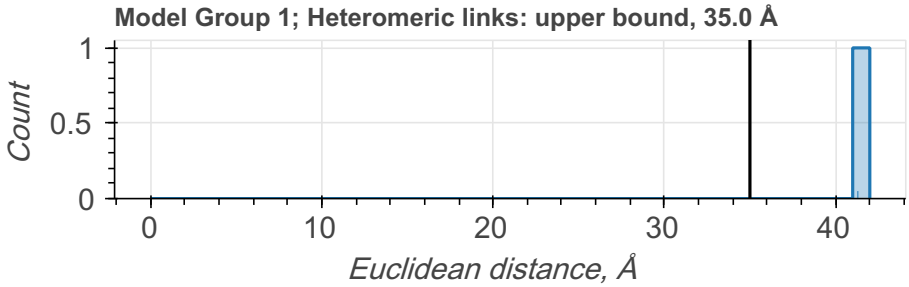
There are 53 crosslinking restraints combined in 1 restraint groups.

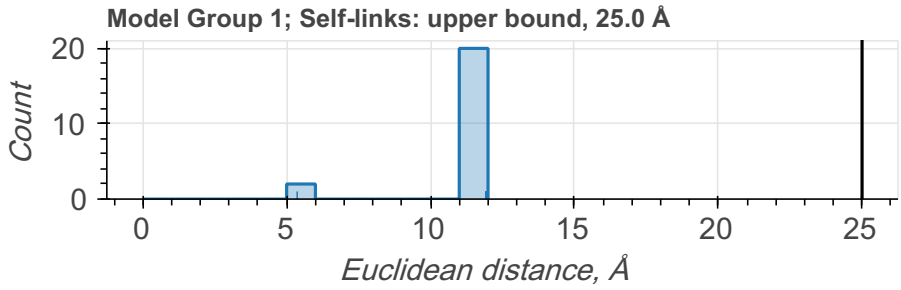
| Linker | Residue 1 | Atom 1 | Residue 2 | Atom 2 | Restraint type | Distance, Å | Count |
|---|---|---|---|---|---|---|---|
| DMTMM | GLU | CA | LYS | CA | upper bound | 25.0 | 24 |
| DMTMM | GLU | CA | LYS | CA | upper bound | 35.0 | 29 |

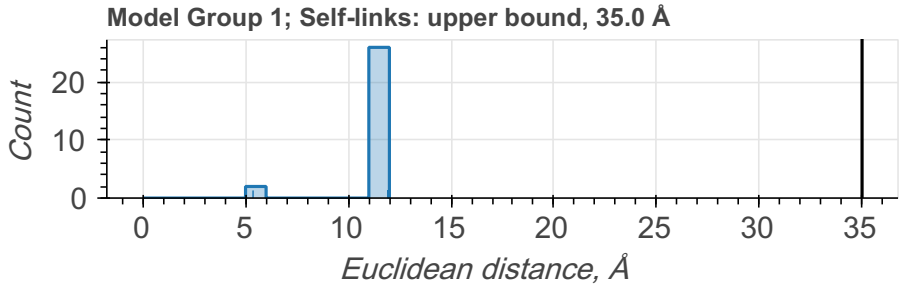
Distograms of individual restraints

*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.*





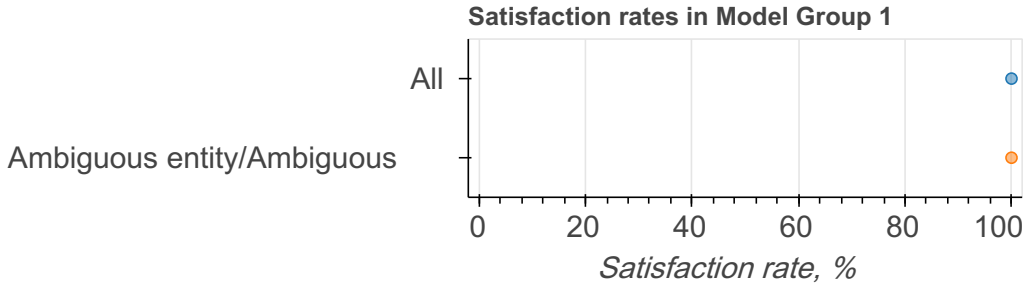

## Satisfaction of restraints

*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 | 100.00 | 0.00 | 1 |
| | | | | Ambiguous entity/ Ambiguous | 100.00 | 0.00 | 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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