

Integrative Structure Validation Report ?

February 18, 2025 - 08:37 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 | 9A3D |
| PDB-Dev ID | PDBDEV_00000198 |
| Structure Title | Model of E. coli BamB by in-cell photo-crosslinking MS and deep learning |
| Structure Authors | Stahl, K.; Graziadei, A.; Dau, T.; Brock, O.; Rappsilber, J. |
| Deposited on | 2023-02-03 |

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

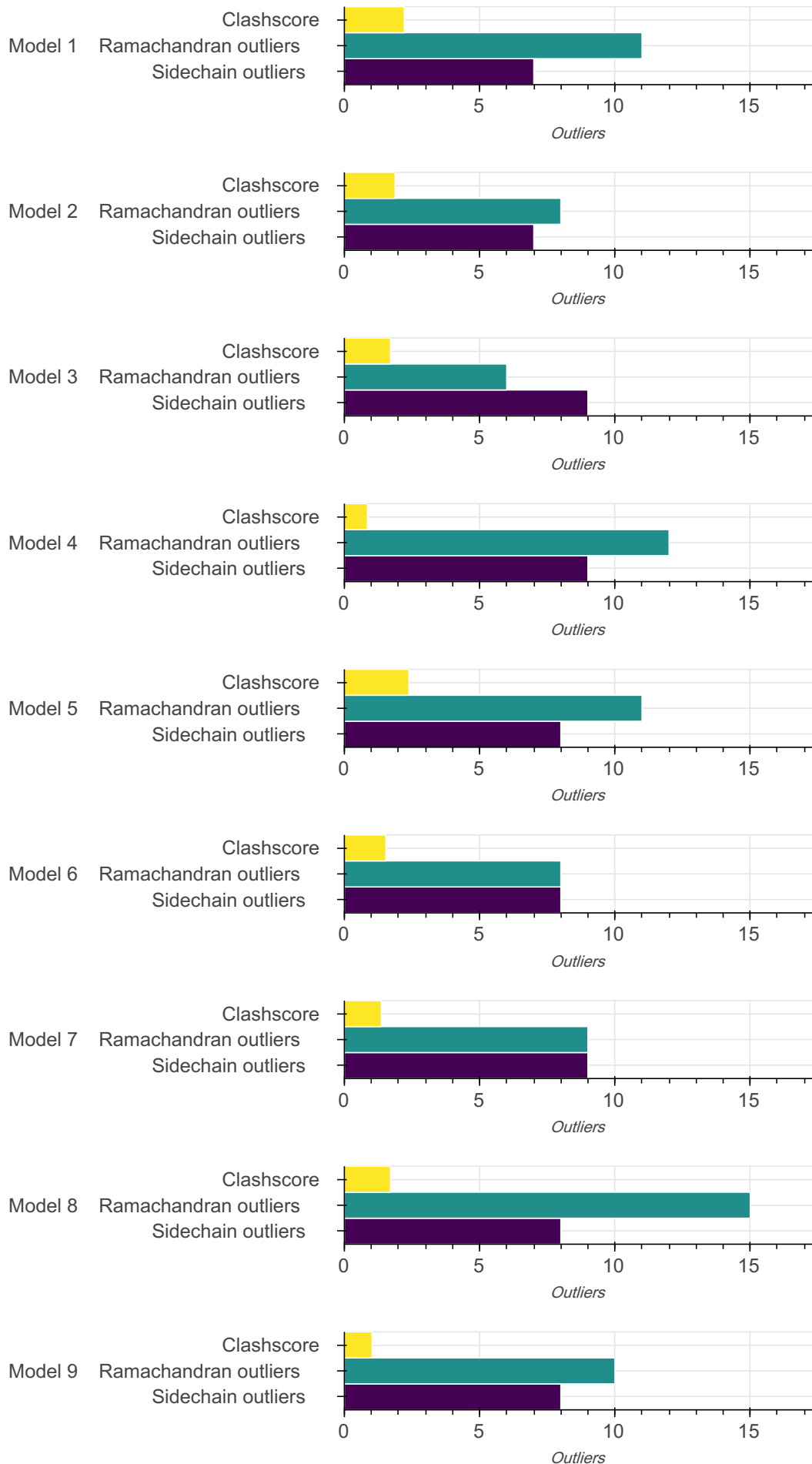
A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the ? symbol.

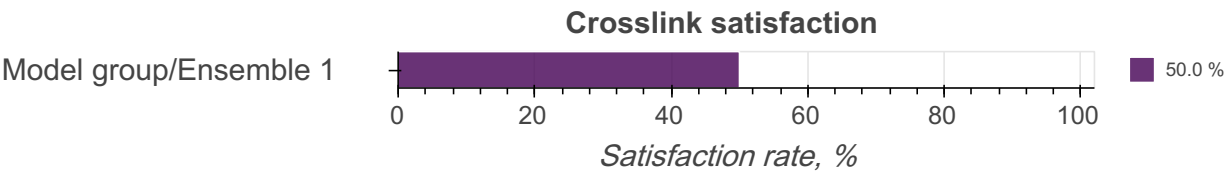
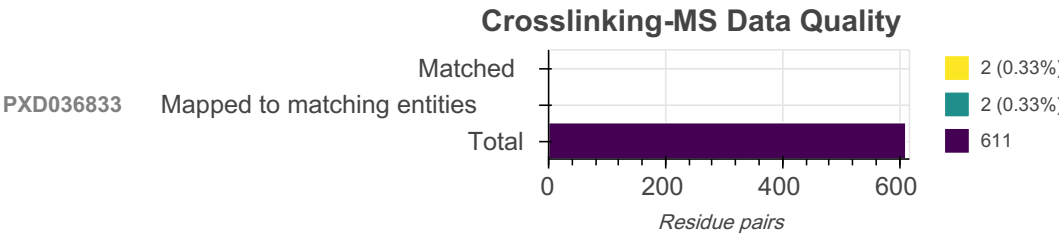
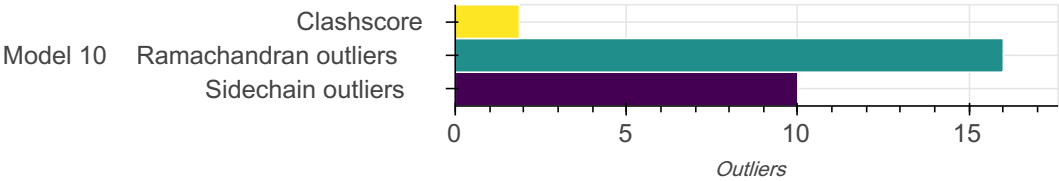
List of references used to build this report is available [here](#).

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 10 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 | 1-10 | 1 | P77774 | A | 392 | - | 1-392 | 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 | jPOSTrepo | JPST001851 |

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 | AlphaLink | AlphaLink with 10 msa subsamples | None | 10 | False | False |

There is 1 software package reported in this entry.

| ID | Software name | Software version | Software classification | Software location |
|----|---------------------------|------------------|-------------------------|---|
| 1 | AlphaLink | 1.00 | model building | https://github.com/lhatsk/AlphaLink |

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](#)) [PXD036833](#)

Number of entities in the crosslinking-MS dataset: 1102

Number of entities in the entry: 1

Matching entities:

| Entity ID | Molecule name | Crosslinking-MS Entity ID | E-value | Exact match |
|-----------|---------------|---------------------------|---------|-------------|
| 1 | P77774 | dbseq_P77774_target | 0.00 | True |

Residue pairs stats:

| Source | Total | In matched entities | Total matched |
|-----------|-------|---------------------|---------------|
| 9A3D | 2 | 2 (100.00%) | 2 (100.00%) |
| PXD036833 | 611 | 2 (0.33%) | 2 (0.33%) |

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 214 bond angle outliers in this entry (0.52% of 40920 assessed bonds). A summary is provided below.

| Chain | Res | Type | Atoms | Z | Observed (Å) | Ideal (Å) | Model ID (Worst) | Models (Total) |
|-------|-----|------|------------|------|--------------|-----------|------------------|----------------|
| A | 2 | GLN | C-N-CA | 8.85 | 137.63 | 121.70 | 7 | 3 |
| A | 223 | GLN | OE1-CD-NE2 | 6.33 | 116.27 | 122.60 | 9 | 10 |
| A | 194 | LEU | C-N-CA | 6.17 | 132.81 | 121.70 | 7 | 1 |
| A | 6 | LEU | C-N-CA | 6.09 | 132.66 | 121.70 | 6 | 1 |
| A | 8 | LEU | CA-C-N | 5.87 | 125.70 | 116.90 | 3 | 2 |
| A | 368 | GLN | OE1-CD-NE2 | 5.86 | 116.74 | 122.60 | 1 | 9 |
| A | 76 | ASP | CA-CB-CG | 5.65 | 118.25 | 112.60 | 9 | 10 |
| A | 324 | HIS | CB-CG-CD2 | 5.62 | 123.90 | 131.20 | 6 | 1 |
| A | 242 | ASP | CA-CB-CG | 5.59 | 118.19 | 112.60 | 1 | 6 |
| A | 62 | ASN | OD1-CG-ND2 | 5.56 | 117.04 | 122.60 | 2 | 1 |
| A | 341 | ASP | CA-CB-CG | 5.55 | 118.15 | 112.60 | 9 | 8 |
| A | 229 | GLN | OE1-CD-NE2 | 5.52 | 117.08 | 122.60 | 1 | 3 |
| A | 360 | GLN | OE1-CD-NE2 | 5.51 | 117.09 | 122.60 | 2 | 8 |
| A | 301 | GLN | OE1-CD-NE2 | 5.37 | 117.23 | 122.60 | 4 | 6 |
| A | 19 | GLY | C-N-CA | 5.31 | 131.26 | 121.70 | 1 | 1 |
| A | 170 | GLN | OE1-CD-NE2 | 5.29 | 117.31 | 122.60 | 9 | 7 |
| A | 9 | PRO | CA-N-CD | 5.27 | 104.63 | 112.00 | 9 | 2 |
| A | 319 | GLN | OE1-CD-NE2 | 5.18 | 117.42 | 122.60 | 2 | 2 |
| A | 172 | GLN | OE1-CD-NE2 | 5.15 | 117.45 | 122.60 | 3 | 10 |
| A | 4 | ARG | C-N-CA | 4.96 | 130.62 | 121.70 | 3 | 3 |

| Chain | Res | Type | Atoms | Z | Observed (Å) | Ideal (Å) | Model ID (Worst) | Models (Total) |
|-------|-----|------|------------|------|--------------|-----------|------------------|----------------|
| A | 234 | GLN | OE1-CD-NE2 | 4.94 | 117.66 | 122.60 | 1 | 10 |
| A | 168 | ASN | OD1-CG-ND2 | 4.93 | 117.67 | 122.60 | 3 | 7 |
| A | 26 | GLU | O-C-N | 4.89 | 115.18 | 123.00 | 10 | 1 |
| A | 64 | HIS | CB-CG-CD2 | 4.89 | 124.85 | 131.20 | 2 | 3 |
| A | 62 | ASN | CA-CB-CG | 4.85 | 117.45 | 112.60 | 2 | 1 |
| A | 187 | LEU | C-N-CA | 4.83 | 130.39 | 121.70 | 4 | 3 |
| A | 230 | GLN | OE1-CD-NE2 | 4.75 | 117.85 | 122.60 | 3 | 10 |
| A | 130 | GLN | OE1-CD-NE2 | 4.68 | 117.92 | 122.60 | 2 | 6 |
| A | 211 | GLY | C-N-CA | 4.66 | 130.09 | 121.70 | 1 | 1 |
| A | 266 | ASN | OD1-CG-ND2 | 4.66 | 117.94 | 122.60 | 4 | 9 |
| A | 359 | GLN | OE1-CD-NE2 | 4.64 | 117.96 | 122.60 | 1 | 2 |
| A | 39 | GLU | C-N-CA | 4.64 | 130.05 | 121.70 | 2 | 1 |
| A | 41 | GLN | OE1-CD-NE2 | 4.57 | 118.03 | 122.60 | 1 | 7 |
| A | 40 | ASN | OD1-CG-ND2 | 4.54 | 118.06 | 122.60 | 1 | 4 |
| A | 1 | MET | C-N-CA | 4.50 | 129.80 | 121.70 | 2 | 2 |
| A | 195 | ARG | NH1-CZ-NH2 | 4.47 | 113.49 | 119.30 | 9 | 1 |
| A | 215 | ARG | NE-CZ-NH1 | 4.44 | 125.94 | 121.50 | 4 | 1 |
| A | 276 | GLN | OE1-CD-NE2 | 4.43 | 118.17 | 122.60 | 6 | 10 |
| A | 190 | PRO | CA-N-CD | 4.40 | 105.85 | 112.00 | 7 | 1 |
| A | 26 | GLU | CA-C-N | 4.39 | 124.98 | 116.20 | 10 | 1 |
| A | 347 | HIS | CB-CG-CD2 | 4.38 | 125.51 | 131.20 | 7 | 8 |
| A | 363 | ASP | CA-CB-CG | 4.37 | 108.23 | 112.60 | 9 | 1 |
| A | 175 | ASN | OD1-CG-ND2 | 4.36 | 118.24 | 122.60 | 9 | 3 |
| A | 188 | ASP | CA-CB-CG | 4.35 | 116.95 | 112.60 | 1 | 1 |
| A | 7 | LEU | N-CA-CB | 4.35 | 103.10 | 110.50 | 6 | 1 |
| A | 264 | ASN | OD1-CG-ND2 | 4.33 | 118.27 | 122.60 | 1 | 2 |
| A | 246 | ASP | C-CA-CB | 4.32 | 118.31 | 110.10 | 1 | 1 |
| A | 325 | ARG | NE-CZ-NH2 | 4.32 | 123.09 | 119.20 | 6 | 1 |
| A | 3 | LEU | C-N-CA | 4.25 | 129.34 | 121.70 | 10 | 1 |
| A | 295 | ARG | NH1-CZ-NH2 | 4.23 | 113.80 | 119.30 | 6 | 1 |
| A | 24 | ASN | OD1-CG-ND2 | 4.23 | 118.37 | 122.60 | 4 | 2 |
| A | 5 | LYS | C-N-CA | 4.20 | 129.27 | 121.70 | 8 | 2 |
| A | 355 | ARG | NE-CZ-NH2 | 4.20 | 122.98 | 119.20 | 6 | 1 |
| A | 58 | ASN | OD1-CG-ND2 | 4.16 | 118.44 | 122.60 | 4 | 2 |
| A | 10 | GLY | C-N-CA | 4.15 | 129.17 | 121.70 | 8 | 1 |

| Chain | Res | Type | Atoms | Z | Observed (Å) | Ideal (Å) | Model ID (Worst) | Models (Total) |
|-------|-----|------|------------|------|--------------|-----------|------------------|----------------|
| A | 300 | ASP | C-CA-CB | 4.14 | 117.96 | 110.10 | 1 | 1 |
| A | 195 | ARG | N-CA-CB | 4.12 | 103.49 | 110.50 | 6 | 1 |
| A | 57 | GLY | C-N-CA | 4.12 | 129.11 | 121.70 | 2 | 1 |
| A | 195 | ARG | N-CA-C | 4.11 | 122.52 | 111.00 | 7 | 1 |
| A | 193 | SER | C-N-CA | 4.11 | 129.10 | 121.70 | 7 | 1 |
| A | 2 | GLN | O-C-N | 4.11 | 116.43 | 123.00 | 7 | 1 |
| A | 154 | ARG | NE-CZ-NH2 | 4.10 | 122.89 | 119.20 | 2 | 1 |
| A | 26 | GLU | C-N-CA | 4.09 | 129.06 | 121.70 | 10 | 1 |
| A | 2 | GLN | OE1-CD-NE2 | 4.09 | 118.51 | 122.60 | 10 | 1 |
| A | 28 | ASP | N-CA-C | 4.08 | 99.58 | 111.00 | 10 | 1 |
| A | 215 | ARG | NH1-CZ-NH2 | 4.07 | 114.01 | 119.30 | 4 | 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 | 2.21 | 13 |
| 2 | 1.87 | 11 |
| 3 | 1.70 | 10 |
| 4 | 0.85 | 5 |
| 5 | 2.38 | 14 |
| 6 | 1.53 | 9 |
| 7 | 1.36 | 8 |
| 8 | 1.70 | 10 |
| 9 | 1.02 | 6 |
| 10 | 1.87 | 11 |

There are 97 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:5:LYS:HB3 | A:6:LEU:HD12 | 0.68 | 6 | 1 |
| A:35:LEU:HD21 | A:324:HIS:CE1 | 0.67 | 6 | 1 |
| A:360:GLN:HE22 | A:390:ILE:HG23 | 0.63 | 2 | 1 |
| A:42:PHE:CZ | A:44:PRO:HG3 | 0.62 | 2 | 1 |
| A:235:ALA:HB1 | A:243:ARG:HA | 0.61 | 1 | 1 |
| A:35:LEU:HD21 | A:324:HIS:NE2 | 0.59 | 6 | 1 |

| Atom 1 | Atom 2 | Clash(Å) | Model ID (Worst) | Models (Total) |
|----------------|----------------|----------|------------------|----------------|
| A:261:LEU:HD21 | A:286:VAL:HB | 0.55 | 1 | 4 |
| A:62:ASN:HB3 | A:369:THR:HG22 | 0.55 | 5 | 1 |
| A:286:VAL:HA | A:300:ASP:HA | 0.54 | 1 | 7 |
| A:41:GLN:NE2 | A:355:ARG:HH12 | 0.54 | 5 | 6 |
| A:150:GLU:CD | A:195:ARG:HH21 | 0.53 | 9 | 1 |
| A:189:MET:HE1 | A:212:ASP:OD2 | 0.53 | 3 | 1 |
| A:261:LEU:HD21 | A:286:VAL:CG1 | 0.52 | 3 | 6 |
| A:64:HIS:CE1 | A:154:ARG:HH11 | 0.51 | 1 | 1 |
| A:190:PRO:CD | A:213:ASN:HD21 | 0.51 | 8 | 1 |
| A:194:LEU:HD12 | A:244:LEU:HD11 | 0.50 | 5 | 1 |
| A:169:GLY:HA2 | A:189:MET:HE3 | 0.50 | 1 | 1 |
| A:308:LEU:HD23 | A:315:THR:HA | 0.50 | 7 | 2 |
| A:48:TRP:CE2 | A:389:SER:HB2 | 0.49 | 2 | 5 |
| A:213:ASN:ND2 | A:215:ARG:HH21 | 0.49 | 1 | 1 |
| A:63:LEU:O | A:369:THR:HG21 | 0.49 | 5 | 1 |
| A:212:ASP:HA | A:246:ASP:HA | 0.49 | 1 | 1 |
| A:44:PRO:HB2 | A:360:GLN:HE21 | 0.49 | 2 | 1 |
| A:189:MET:SD | A:211:GLY:HA3 | 0.48 | 2 | 1 |
| A:64:HIS:NE2 | A:154:ARG:HD3 | 0.48 | 9 | 2 |
| A:152:LEU:CD1 | A:195:ARG:HB3 | 0.48 | 4 | 1 |
| A:265:GLY:HA3 | A:284:GLY:O | 0.47 | 10 | 4 |
| A:331:VAL:HG11 | A:371:PRO:O | 0.47 | 5 | 2 |
| A:295:ARG:HH12 | A:352:GLU:HA | 0.47 | 10 | 6 |
| A:24:ASN:C | A:26:GLU:H | 0.46 | 10 | 1 |
| A:285:SER:HB2 | A:301:GLN:CD | 0.46 | 3 | 1 |
| A:64:HIS:CE1 | A:154:ARG:HD3 | 0.46 | 1 | 1 |
| A:167:SER:HA | A:197:GLU:OE2 | 0.46 | 3 | 1 |
| A:73:TYR:CD1 | A:117:VAL:HG21 | 0.43 | 5 | 5 |
| A:193:SER:HB2 | A:212:ASP:CB | 0.43 | 6 | 1 |
| A:249:THR:HG21 | A:261:LEU:HD23 | 0.43 | 1 | 1 |
| A:152:LEU:HB3 | A:196:GLY:HA2 | 0.42 | 2 | 1 |
| A:297:TYR:CD1 | A:337:LEU:HD11 | 0.42 | 5 | 1 |
| A:165:HIS:NE2 | A:189:MET:CE | 0.42 | 1 | 1 |
| A:238:SER:HA | A:242:ASP:OD2 | 0.42 | 2 | 1 |
| A:303:ASP:OD1 | A:325:ARG:HA | 0.42 | 2 | 1 |

| Atom 1 | Atom 2 | Clash(Å) | Model ID (Worst) | Models (Total) |
|----------------|----------------|----------|------------------|----------------|
| A:307:ALA:C | A:308:LEU:HD12 | 0.42 | 5 | 1 |
| A:83:ALA:HB2 | A:93:TRP:CE2 | 0.41 | 7 | 6 |
| A:156:VAL:HG21 | A:200:PRO:O | 0.41 | 7 | 1 |
| A:52:VAL:O | A:80:LEU:HD23 | 0.41 | 3 | 1 |
| A:26:GLU:HB3 | A:28:ASP:H | 0.41 | 10 | 1 |
| A:285:SER:HB3 | A:301:GLN:CD | 0.41 | 10 | 2 |
| A:121:HIS:HB2 | A:123:TYR:CZ | 0.41 | 2 | 2 |
| A:26:GLU:HA | A:27:GLU:C | 0.41 | 10 | 1 |
| A:38:VAL:HG12 | A:40:ASN:H | 0.40 | 7 | 1 |
| A:173:ALA:HB2 | A:183:TRP:CZ2 | 0.40 | 6 | 1 |
| A:59:PHE:HB3 | A:60:TYR:CD2 | 0.40 | 8 | 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 | 390 | 347 | 32 | 11 |
| 2 | 390 | 349 | 33 | 8 |
| 3 | 390 | 366 | 18 | 6 |
| 4 | 390 | 351 | 27 | 12 |
| 5 | 390 | 361 | 18 | 11 |
| 6 | 390 | 357 | 25 | 8 |
| 7 | 390 | 354 | 27 | 9 |
| 8 | 390 | 351 | 24 | 15 |
| 9 | 390 | 354 | 26 | 10 |
| 10 | 390 | 355 | 19 | 16 |

There are 39 unique backbone outliers. Detailed list of outliers are tabulated below.

| Chain | Res | Type | Models (Total) |
|-------|-----|------|----------------|
| A | 28 | ASP | 9 |
| A | 105 | SER | 8 |
| A | 26 | GLU | 7 |
| A | 11 | LEU | 5 |
| A | 16 | LEU | 5 |
| A | 312 | GLY | 5 |
| A | 9 | PRO | 4 |

| Chain | Res | Type | Models (Total) |
|-------|-----|------|----------------|
| A | 21 | SER | 4 |
| A | 188 | ASP | 4 |
| A | 2 | GLN | 3 |
| A | 5 | LYS | 3 |
| A | 15 | THR | 3 |
| A | 17 | LEU | 3 |
| A | 20 | CYS | 3 |
| A | 29 | VAL | 3 |
| A | 3 | LEU | 2 |
| A | 4 | ARG | 2 |
| A | 12 | LEU | 2 |
| A | 13 | SER | 2 |
| A | 14 | VAL | 2 |
| A | 18 | SER | 2 |
| A | 19 | GLY | 2 |
| A | 27 | GLU | 2 |
| A | 59 | PHE | 2 |
| A | 106 | LYS | 2 |
| A | 167 | SER | 2 |
| A | 195 | ARG | 2 |
| A | 196 | GLY | 2 |
| A | 6 | LEU | 1 |
| A | 7 | LEU | 1 |
| A | 8 | LEU | 1 |
| A | 25 | SER | 1 |
| A | 30 | VAL | 1 |
| A | 31 | LYS | 1 |
| A | 40 | ASN | 1 |
| A | 103 | TRP | 1 |
| A | 114 | GLY | 1 |
| A | 190 | PRO | 1 |
| A | 323 | LEU | 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 | 321 | 308 | 6 | 7 |
| 2 | 321 | 303 | 11 | 7 |
| 3 | 321 | 304 | 8 | 9 |
| 4 | 321 | 309 | 3 | 9 |
| 5 | 321 | 302 | 11 | 8 |
| 6 | 321 | 306 | 7 | 8 |
| 7 | 321 | 306 | 6 | 9 |
| 8 | 321 | 305 | 8 | 8 |
| 9 | 321 | 302 | 11 | 8 |
| 10 | 321 | 302 | 9 | 10 |

There are 22 unique sidechain outliers. Detailed list of outliers are tabulated below.

| Chain | Res | Type | Models (Total) |
|-------|-----|------|----------------|
| A | 300 | ASP | 10 |
| A | 8 | LEU | 9 |
| A | 6 | LEU | 8 |
| A | 12 | LEU | 8 |
| A | 11 | LEU | 7 |
| A | 76 | ASP | 7 |
| A | 3 | LEU | 6 |
| A | 15 | THR | 4 |
| A | 16 | LEU | 4 |
| A | 189 | MET | 3 |
| A | 285 | SER | 3 |
| A | 18 | SER | 2 |
| A | 194 | LEU | 2 |
| A | 212 | ASP | 2 |
| A | 21 | SER | 1 |
| A | 37 | THR | 1 |
| A | 99 | GLU | 1 |
| A | 192 | LEU | 1 |
| A | 270 | LEU | 1 |
| A | 281 | ARG | 1 |
| A | 329 | SER | 1 |
| A | 369 | THR | 1 |

Fit of model to data used for modeling ?

Fit of model(s) to crosslinking-MS data

Restraint types

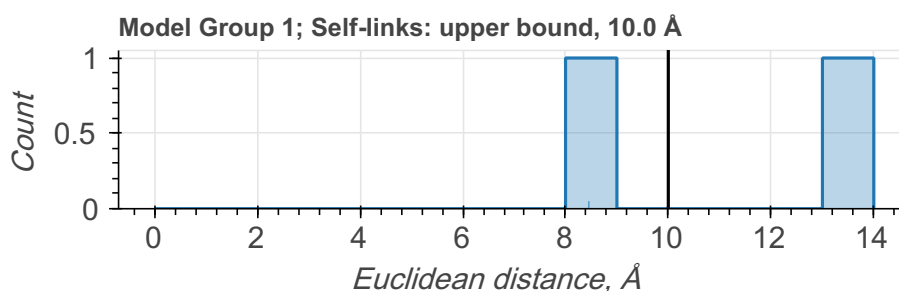
Restraint types are summarized in the table below. Restraints assigned "by-residue" are interpreted as between CA atoms. Restraints between coarse-grained beads are indicated as "coarse-grained". *Restraint group* represents a set of crosslinking restraints applied collectively in the modeling.

There are 2 crosslinking restraints combined in 2 restraint groups.

| Linker | Residue 1 | Atom 1 | Residue 2 | Atom 2 | Restraint type | Distance, Å | Count |
|-----------------|-----------|--------|-----------|--------|----------------|-------------|-------|
| L-Photo-Leucine | ALA | CA | LEU | CA | upper bound | 10.0 | 1 |
| L-Photo-Leucine | ASN | CA | LEU | CA | upper bound | 10.0 | 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

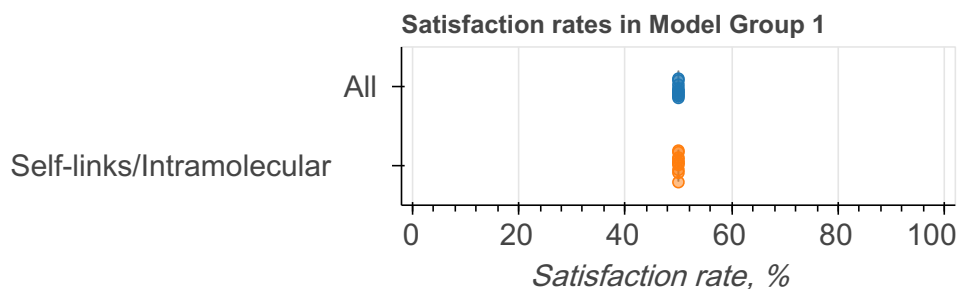
Satisfaction of restraints is calculated on a *restraint group* (a set of crosslinking restraints applied collectively in the modeling) level. Satisfaction of a restraint group depends on satisfaction of individual restraints in the group and the conditionality (all/any). A restraint group is considered 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=2) |
|-------------|-------|-------------|-----------------------------|----------------------------|---------------|--------------|-----------------|
| 1 | 1 | 1 | 10/10 | All | 50.00 | 50.00 | 2 |
| | | | | Self-links/ Intramolecular | 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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