

# Integrative Structure Validation Report ?

April 09, 2025 - 11:19 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            | 9A7I  |
| PDB-Dev ID        | PDBDEV_00000347   |
| Structure Title   | Integrative model of NUSA-RPOC 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)*

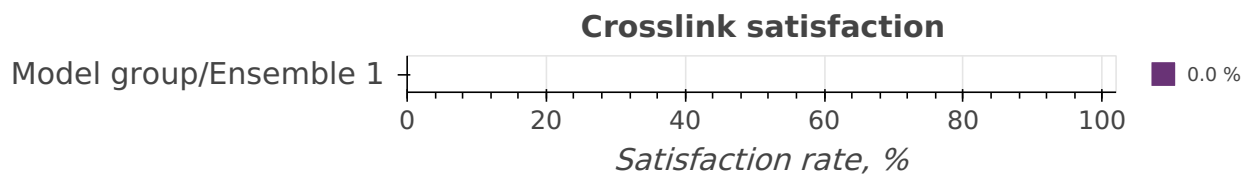
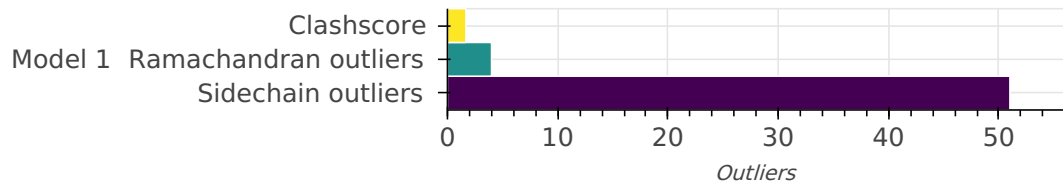
*A user guide is available at [https://pdb-ihm.org/validation\\_help.html](https://pdb-ihm.org/validation_help.html) with specific help available everywhere you see the ? symbol.*

*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         | NUSA_BACSU    | A               | 371            | -              | 1-371             | 100.00 / 0.00                                  | Atomic |
|    |          | 2         | RPOC_BACSU    | B               | 1199           | -              | 1-1199            | 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         | <a href="#">PXD035508</a> |

## 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 70 bond angle outliers in this entry (0.41% of 16960 assessed bonds). A summary is provided below.*

| Chain | Res  | Type | Atoms      | Z    | Observed (Å) | Ideal (Å) | Model ID (Worst) | Models (Total) |
|-------|------|------|------------|------|--------------|-----------|------------------|----------------|
| A     | 367  | ALA  | C-N-CA     | 7.01 | 134.31       | 121.70    | 1                | 1              |
| A     | 370  | ASP  | C-N-CA     | 6.63 | 133.63       | 121.70    | 1                | 1              |
| B     | 803  | ARG  | NE-CZ-NH2  | 6.38 | 124.94       | 119.20    | 1                | 1              |
| A     | 366  | THR  | N-CA-C     | 6.14 | 128.18       | 111.00    | 1                | 1              |
| B     | 1124 | THR  | CA-CB-OG1  | 5.94 | 118.51       | 109.60    | 1                | 1              |
| A     | 366  | THR  | CA-C-N     | 5.82 | 127.84       | 116.20    | 1                | 1              |
| B     | 449  | ASP  | CA-CB-CG   | 5.74 | 118.34       | 112.60    | 1                | 1              |
| A     | 312  | GLN  | OE1-CD-NE2 | 5.45 | 117.15       | 122.60    | 1                | 1              |
| A     | 369  | SER  | N-CA-C     | 5.44 | 126.23       | 111.00    | 1                | 1              |
| B     | 668  | ASP  | CA-CB-CG   | 5.40 | 118.00       | 112.60    | 1                | 1              |
| A     | 193  | GLN  | OE1-CD-NE2 | 5.35 | 117.25       | 122.60    | 1                | 1              |
| B     | 713  | GLN  | OE1-CD-NE2 | 5.24 | 117.36       | 122.60    | 1                | 1              |
| A     | 43   | GLN  | OE1-CD-NE2 | 5.17 | 117.43       | 122.60    | 1                | 1              |
| A     | 41   | GLN  | OE1-CD-NE2 | 5.14 | 117.46       | 122.60    | 1                | 1              |
| B     | 253  | ASP  | CA-CB-CG   | 5.07 | 117.67       | 112.60    | 1                | 1              |
| B     | 585  | ASN  | OD1-CG-ND2 | 5.03 | 117.57       | 122.60    | 1                | 1              |
| A     | 367  | ALA  | N-CA-C     | 4.98 | 124.94       | 111.00    | 1                | 1              |
| B     | 439  | HIS  | CB-CG-CD2  | 4.97 | 124.74       | 131.20    | 1                | 1              |
| A     | 143  | GLN  | OE1-CD-NE2 | 4.96 | 117.64       | 122.60    | 1                | 1              |
| A     | 368  | GLU  | N-CA-C     | 4.87 | 124.63       | 111.00    | 1                | 1              |
| B     | 994  | GLN  | OE1-CD-NE2 | 4.84 | 117.76       | 122.60    | 1                | 1              |
| B     | 670  | GLN  | OE1-CD-NE2 | 4.78 | 117.82       | 122.60    | 1                | 1              |
| B     | 329  | GLN  | OE1-CD-NE2 | 4.78 | 117.82       | 122.60    | 1                | 1              |
| A     | 116  | GLN  | OE1-CD-NE2 | 4.78 | 117.82       | 122.60    | 1                | 1              |
| B     | 988  | GLN  | OE1-CD-NE2 | 4.69 | 117.91       | 122.60    | 1                | 1              |
| B     | 527  | GLN  | OE1-CD-NE2 | 4.64 | 117.96       | 122.60    | 1                | 1              |
| B     | 394  | GLN  | OE1-CD-NE2 | 4.64 | 117.96       | 122.60    | 1                | 1              |
| B     | 180  | GLN  | OE1-CD-NE2 | 4.64 | 117.96       | 122.60    | 1                | 1              |
| B     | 957  | GLN  | OE1-CD-NE2 | 4.63 | 117.97       | 122.60    | 1                | 1              |
| B     | 925  | GLN  | OE1-CD-NE2 | 4.61 | 117.99       | 122.60    | 1                | 1              |
| B     | 887  | ARG  | NE-CZ-NH2  | 4.59 | 123.33       | 119.20    | 1                | 1              |
| B     | 768  | ARG  | NE-CZ-NH2  | 4.55 | 123.30       | 119.20    | 1                | 1              |
| B     | 737  | ASN  | CA-CB-CG   | 4.55 | 117.15       | 112.60    | 1                | 1              |
| A     | 363  | GLU  | CA-C-N     | 4.54 | 123.71       | 116.90    | 1                | 1              |

| Chain | Res  | Type | Atoms      | Z    | Observed (Å) | Ideal (Å) | Model ID (Worst) | Models (Total) |
|-------|------|------|------------|------|--------------|-----------|------------------|----------------|
| B     | 1044 | GLN  | OE1-CD-NE2 | 4.50 | 118.10       | 122.60    | 1                | 1              |
| A     | 108  | GLN  | OE1-CD-NE2 | 4.48 | 118.12       | 122.60    | 1                | 1              |
| A     | 256  | GLN  | OE1-CD-NE2 | 4.46 | 118.14       | 122.60    | 1                | 1              |
| B     | 737  | ASN  | OD1-CG-ND2 | 4.44 | 118.16       | 122.60    | 1                | 1              |
| B     | 968  | GLN  | OE1-CD-NE2 | 4.42 | 118.18       | 122.60    | 1                | 1              |
| B     | 1140 | GLN  | OE1-CD-NE2 | 4.40 | 118.20       | 122.60    | 1                | 1              |
| B     | 753  | ASN  | OD1-CG-ND2 | 4.40 | 118.20       | 122.60    | 1                | 1              |
| B     | 1022 | GLN  | OE1-CD-NE2 | 4.39 | 118.21       | 122.60    | 1                | 1              |
| B     | 1058 | GLN  | OE1-CD-NE2 | 4.39 | 118.21       | 122.60    | 1                | 1              |
| B     | 726  | ILE  | CA-CB-CG2  | 4.36 | 103.09       | 110.50    | 1                | 1              |
| B     | 1190 | GLN  | OE1-CD-NE2 | 4.31 | 118.29       | 122.60    | 1                | 1              |
| B     | 243  | GLN  | OE1-CD-NE2 | 4.30 | 118.30       | 122.60    | 1                | 1              |
| A     | 38   | ASN  | OD1-CG-ND2 | 4.25 | 118.35       | 122.60    | 1                | 1              |
| B     | 955  | ARG  | NE-CZ-NH2  | 4.25 | 115.38       | 119.20    | 1                | 1              |
| B     | 324  | GLN  | OE1-CD-NE2 | 4.24 | 118.36       | 122.60    | 1                | 1              |
| A     | 166  | GLN  | OE1-CD-NE2 | 4.24 | 118.36       | 122.60    | 1                | 1              |
| A     | 112  | GLN  | OE1-CD-NE2 | 4.22 | 118.38       | 122.60    | 1                | 1              |
| A     | 357  | ASP  | CA-CB-CG   | 4.19 | 116.79       | 112.60    | 1                | 1              |
| B     | 803  | ARG  | NH1-CZ-NH2 | 4.18 | 113.86       | 119.30    | 1                | 1              |
| B     | 1066 | HIS  | CB-CG-CD2  | 4.17 | 125.78       | 131.20    | 1                | 1              |
| B     | 318  | HIS  | CB-CG-CD2  | 4.15 | 125.80       | 131.20    | 1                | 1              |
| A     | 84   | HIS  | CB-CG-CD2  | 4.14 | 125.82       | 131.20    | 1                | 1              |
| B     | 201  | GLN  | OE1-CD-NE2 | 4.13 | 118.47       | 122.60    | 1                | 1              |
| B     | 608  | GLN  | OE1-CD-NE2 | 4.12 | 118.48       | 122.60    | 1                | 1              |
| B     | 553  | GLN  | OE1-CD-NE2 | 4.12 | 118.48       | 122.60    | 1                | 1              |
| B     | 424  | GLN  | OE1-CD-NE2 | 4.10 | 118.50       | 122.60    | 1                | 1              |
| B     | 753  | ASN  | CA-CB-CG   | 4.10 | 116.70       | 112.60    | 1                | 1              |
| B     | 1086 | THR  | CA-CB-CG2  | 4.10 | 117.47       | 110.50    | 1                | 1              |
| B     | 532  | HIS  | CB-CG-CD2  | 4.10 | 125.87       | 131.20    | 1                | 1              |
| B     | 686  | GLN  | OE1-CD-NE2 | 4.08 | 118.52       | 122.60    | 1                | 1              |
| B     | 349  | HIS  | CB-CG-CD2  | 4.06 | 125.93       | 131.20    | 1                | 1              |
| B     | 951  | GLN  | OE1-CD-NE2 | 4.05 | 118.55       | 122.60    | 1                | 1              |

| Chain | Res | Type | Atoms      | Z    | Observed (Å) | Ideal (Å) | Model ID (Worst) | Models (Total) |
|-------|-----|------|------------|------|--------------|-----------|------------------|----------------|
| B     | 478 | ASN  | OD1-CG-ND2 | 4.03 | 118.57       | 122.60    | 1                | 1              |
| B     | 542 | ASN  | OD1-CG-ND2 | 4.03 | 118.57       | 122.60    | 1                | 1              |
| B     | 854 | HIS  | CB-CG-CD2  | 4.01 | 125.99       | 131.20    | 1                | 1              |
| B     | 493 | 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        | 1.68        | 42                |

There are 42 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) |
|----------------|-----------------|----------|------------------|----------------|
| B:113:ARG:HH11 | B:212:VAL:HG22  | 0.88     | 1                | 1              |
| B:808:ALA:HB2  | B:1070:MET:HE1  | 0.84     | 1                | 1              |
| B:808:ALA:CB   | B:1070:MET:HE1  | 0.78     | 1                | 1              |
| B:441:LEU:HD21 | B:495:MET:HE1   | 0.68     | 1                | 1              |
| B:726:ILE:HG21 | B:741:PHE:CE1   | 0.66     | 1                | 1              |
| B:234:ILE:HD11 | B:316:LEU:HD21  | 0.62     | 1                | 1              |
| B:371:MET:CE   | B:383:ILE:HG23  | 0.62     | 1                | 1              |
| B:113:ARG:NH1  | B:212:VAL:HG22  | 0.61     | 1                | 1              |
| B:2:LEU:HD22   | B:7:PHE:HZ      | 0.57     | 1                | 1              |
| B:930:PRO:HB3  | B:1060:VAL:HG11 | 0.56     | 1                | 1              |
| B:820:THR:HG22 | B:887:ARG:HH21  | 0.56     | 1                | 1              |
| B:720:LEU:HD11 | B:741:PHE:CE2   | 0.56     | 1                | 1              |
| B:214:GLU:OE1  | B:1089:LEU:HD21 | 0.56     | 1                | 1              |
| B:317:SER:HB3  | B:321:LYS:HE2   | 0.54     | 1                | 1              |
| B:539:VAL:HG21 | B:565:LEU:HD11  | 0.53     | 1                | 1              |
| B:234:ILE:HG22 | B:235:PRO:HD2   | 0.52     | 1                | 1              |
| B:208:LYS:O    | B:212:VAL:HG23  | 0.52     | 1                | 1              |
| A:99:PRO:HD2   | A:102:PHE:CG    | 0.51     | 1                | 1              |
| B:808:ALA:HB1  | B:1070:MET:HE1  | 0.50     | 1                | 1              |

| Atom 1          | Atom 2          | Clash(Å) | Model ID (Worst) | Models (Total) |
|-----------------|-----------------|----------|------------------|----------------|
| B:1086:THR:HG22 | B:1106:VAL:HG21 | 0.49     | 1                | 1              |
| B:978:VAL:HG22  | B:1018:ILE:HD11 | 0.48     | 1                | 1              |
| B:506:ARG:HH21  | B:723:LEU:HD22  | 0.47     | 1                | 1              |
| B:495:MET:HE3   | B:644:LYS:HA    | 0.47     | 1                | 1              |
| A:1:MET:HA      | A:4:GLU:OE1     | 0.47     | 1                | 1              |
| B:978:VAL:CG2   | B:1018:ILE:HD11 | 0.47     | 1                | 1              |
| B:441:LEU:CD2   | B:495:MET:HE1   | 0.46     | 1                | 1              |
| B:895:PRO:HA    | B:1097:HIS:CD2  | 0.46     | 1                | 1              |
| A:99:PRO:HG2    | A:102:PHE:CD1   | 0.46     | 1                | 1              |
| B:930:PRO:CB    | B:1060:VAL:HG11 | 0.46     | 1                | 1              |
| B:118:LEU:HD23  | B:182:ILE:HD11  | 0.45     | 1                | 1              |
| B:991:ILE:HD11  | B:1010:LEU:CD2  | 0.44     | 1                | 1              |
| A:97:VAL:O      | A:99:PRO:HD3    | 0.43     | 1                | 1              |
| B:726:ILE:HG21  | B:741:PHE:HE1   | 0.43     | 1                | 1              |
| B:328:ARG:NH2   | B:1139:PHE:CE2  | 0.42     | 1                | 1              |
| B:317:SER:CB    | B:321:LYS:HE2   | 0.42     | 1                | 1              |
| B:346:VAL:HG22  | B:450:PHE:CE2   | 0.42     | 1                | 1              |
| B:119:ASP:HB2   | B:209:ARG:CZ    | 0.41     | 1                | 1              |
| B:1158:LEU:HD22 | B:1167:ILE:CD1  | 0.41     | 1                | 1              |
| B:234:ILE:HD11  | B:316:LEU:CD2   | 0.41     | 1                | 1              |
| B:1070:MET:HA   | B:1070:MET:HE2  | 0.41     | 1                | 1              |
| B:705:TRP:CD2   | B:762:PRO:HG3   | 0.41     | 1                | 1              |
| B:890:PHE:CE1   | B:1068:GLU:HA   | 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        | 1566     | 1521    | 41      | 4        |

There are 4 unique backbone outliers. Detailed list of outliers are tabulated below.

| Chain | Res | Type | Models (Total) |
|-------|-----|------|----------------|
| A     | 357 | ASP  | 1              |
| A     | 363 | GLU  | 1              |
| A     | 367 | ALA  | 1              |
| A     | 368 | GLU  | 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        | 1353     | 1225    | 77      | 51       |

There are 51 unique sidechain outliers. Detailed list of outliers are tabulated below.

| Chain | Res | Type | Models (Total) |
|-------|-----|------|----------------|
| A     | 5   | LEU  | 1              |
| A     | 221 | GLU  | 1              |
| A     | 258 | VAL  | 1              |
| A     | 348 | ILE  | 1              |
| A     | 362 | THR  | 1              |
| A     | 366 | THR  | 1              |
| B     | 1   | MET  | 1              |
| B     | 24  | SER  | 1              |
| B     | 55  | THR  | 1              |
| B     | 76  | ASP  | 1              |
| B     | 107 | PHE  | 1              |
| B     | 125 | LEU  | 1              |
| B     | 159 | LEU  | 1              |
| B     | 195 | LEU  | 1              |
| B     | 234 | ILE  | 1              |
| B     | 287 | MET  | 1              |
| B     | 327 | PHE  | 1              |
| B     | 345 | VAL  | 1              |
| B     | 357 | LEU  | 1              |
| B     | 373 | GLU  | 1              |
| B     | 431 | VAL  | 1              |
| B     | 444 | THR  | 1              |
| B     | 449 | ASP  | 1              |
| B     | 453 | ASP  | 1              |
| B     | 474 | LEU  | 1              |
| B     | 488 | VAL  | 1              |
| B     | 497 | LEU  | 1              |
| B     | 504 | LEU  | 1              |
| B     | 646 | LEU  | 1              |



| Chain | Res  | Type | Models (Total) |
|-------|------|------|----------------|
| B     | 657  | THR  | 1              |
| B     | 666  | LEU  | 1              |
| B     | 692  | ILE  | 1              |
| B     | 716  | LEU  | 1              |
| B     | 761  | LEU  | 1              |
| B     | 780  | THR  | 1              |
| B     | 809  | GLN  | 1              |
| B     | 813  | ILE  | 1              |
| B     | 816  | THR  | 1              |
| B     | 949  | ILE  | 1              |
| B     | 957  | GLN  | 1              |
| B     | 974  | ILE  | 1              |
| B     | 977  | THR  | 1              |
| B     | 999  | THR  | 1              |
| B     | 1003 | THR  | 1              |
| B     | 1018 | ILE  | 1              |
| B     | 1040 | LEU  | 1              |
| B     | 1041 | THR  | 1              |
| B     | 1042 | THR  | 1              |
| B     | 1124 | THR  | 1              |
| B     | 1161 | LEU  | 1              |
| B     | 1171 | VAL  | 1              |

## Fit of model to data used for modeling ?

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

#### Restraint types

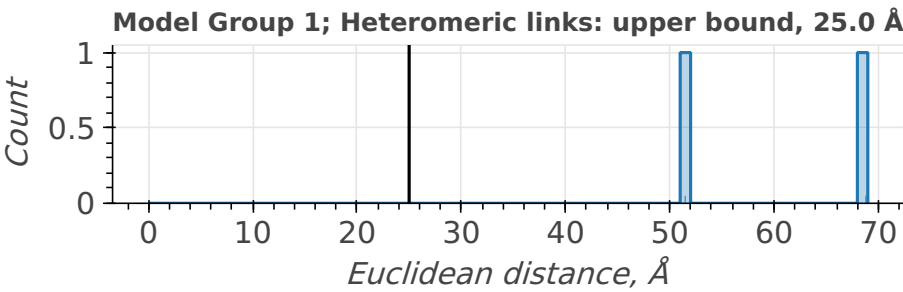
*Restraint types are summarized in the table below. Restraints assigned "by-residue" are interpreted as between CA atoms. Restraints between coarse-grained beads are indicated as "coarse-grained". **Restraint group** represents a set of crosslinking restraints applied collectively in the modeling.*

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.



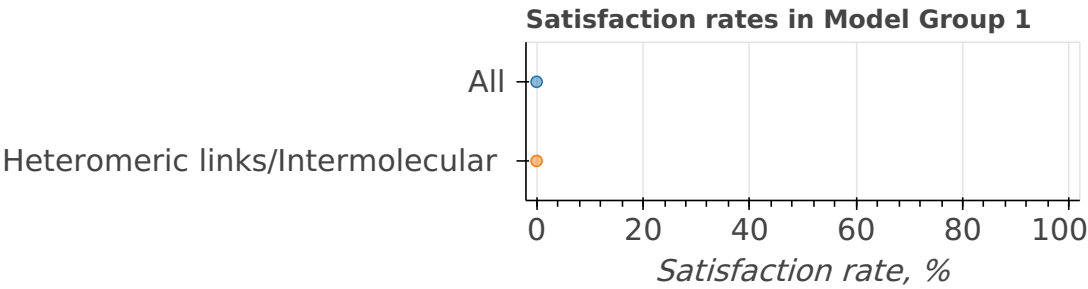
Satisfaction of restraints

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                               | 0.00          | 100.00       | 2               |
|             |       |             |                             | Heteromeric links/ Intermolecular | 0.00          | 100.00       | 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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