# Integrative Structure Validation Report

## July 22, 2024 - 05:02 PM PDT

**The following software was used in the production of this report:**

*Python-IHM Version 1.3*
*MolProbity Version 4.5.2*
*Integrative Modeling Validation Version 1.2*

| | |
|---|---|
| PDB ID | 9A2N |
| PDB-Dev ID | PDBDEV_00000172 |
| Structure Title | Model of E. coli Pal by in-cell photo-crosslinking MS and deep learning |
| Structure Authors | Stahl, K.; Graziadei, A.; Dau, T.; Brock, O.; Rappsilber, J. |

*This is a PDB-Dev IM Structure Validation Report for a publicly released PDB-Dev entry.*

*We welcome your comments at pdb-dev@mail.wwpdb.org*

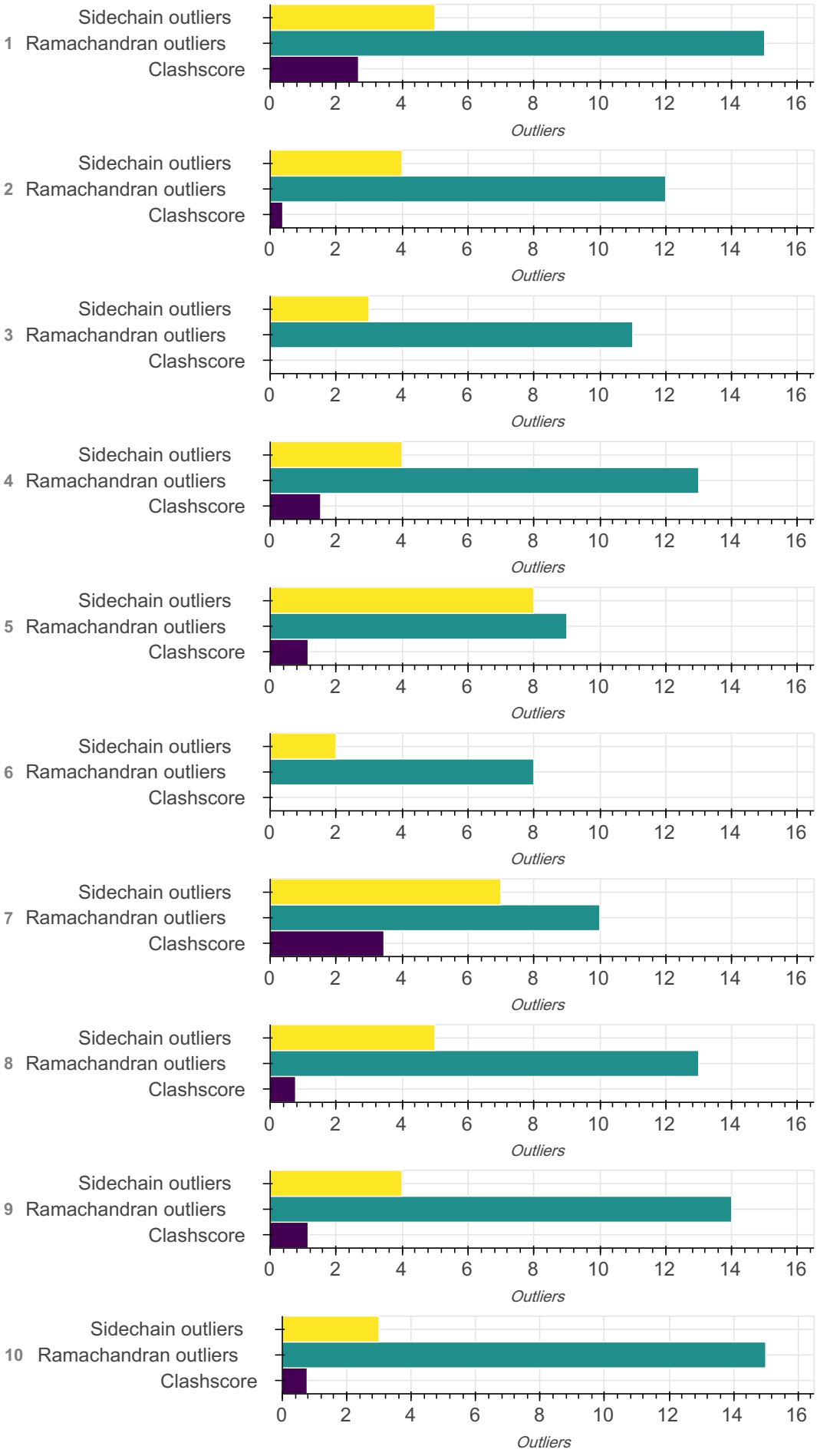
*A user guide is available at https://pdb-dev.wwpdb.org/validation_help.html with specific help available everywhere you see the* ? symbol.

*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 assessment for SAS datasets and fit to model assessments for SAS 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


Sidechain outliers
1 Ramachandran outliers
Clashscore
0 2 4 6 8 10 12 14 16
Outliers
Sidechain outliers
2 Ramachandran outliers
Clashscore
0 2 4 6 8 10 12 14 16
Outliers
Sidechain outliers
3 Ramachandran outliers
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0 2 4 6 8 10 12 14 16
Outliers
Sidechain outliers
4 Ramachandran outliers
Clashscore
0 2 4 6 8 10 12 14 16
Outliers
Sidechain outliers
5 Ramachandran outliers
Clashscore
0 2 4 6 8 10 12 14 16
Outliers
Sidechain outliers
6 Ramachandran outliers
Clashscore
0 2 4 6 8 10 12 14 16
Outliers
Sidechain outliers
7 Ramachandran outliers
Clashscore
0 2 4 6 8 10 12 14 16
Outliers
Sidechain outliers
8 Ramachandran outliers
Clashscore
0 2 4 6 8 10 12 14 16
Outliers
Sidechain outliers
9 Ramachandran outliers
Clashscore
0 2 4 6 8 10 12 14 16
Outliers
Sidechain outliers
10 Ramachandran outliers
Clashscore
0 2 4 6 8 10 12 14 16
Outliers

## Ensemble information

*This entry consists of 0 distinct ensemble(s).*

## Summary

*This entry consists of 10 unique models, with 1 subunits in each model. A total of 1 datasets or restraints were used to build this entry. Each model is represented by 0 rigid bodies and 1 flexible or non-rigid units.*

## Entry composition

*There are 10 unique types of models in this entry.These models are titled None, None, None, None, None, None, None, None, None, None respectively.*

| Model ID | Subunit number | Subunit ID | Subunit name | Chain ID | Chain ID [auth] | Total residues |
|---|---|---|---|---|---|---|
| 1 | 1 | 1 | P0A912 | A | A | 173 |
| 2 | 1 | 1 | P0A912 | A | A | 173 |
| 3 | 1 | 1 | P0A912 | A | A | 173 |
| 4 | 1 | 1 | P0A912 | A | A | 173 |
| 5 | 1 | 1 | P0A912 | A | A | 173 |
| 6 | 1 | 1 | P0A912 | A | A | 173 |
| 7 | 1 | 1 | P0A912 | A | A | 173 |
| 8 | 1 | 1 | P0A912 | A | A | 173 |
| 9 | 1 | 1 | P0A912 | A | A | 173 |
| 10 | 1 | 1 | P0A912 | A | A | 173 |

## 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 |

## Representation

*This entry has only one representation and includes 0 rigid bodies and 1 flexible units*

| Chain ID | Rigid bodies | Non-rigid segments |
|---|---|---|
| A | - | 1-173 |

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

*There is 1 software package reported in this entry.*

| ID | Software name | Software version | Software classification | Software location |
|---|---|---|---|---|
| 1 | AlphaLink | 1.0 | model building | https://github.com/lhatsk/AlphaLink |

## Data quality

### Crosslinking-MS

Validation for this section is under development.

## 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 12920 bond outliers in this entry. A summary is provided below, and a detailed list of outliers can be found here.*

| Bond type | Observed distance (Å) | Ideal distance (Å) | Number of outliers |
|---|---|---|---|
| CD--HD2 | 1.09 | 0.97 | 220 |
| NZ--HZ2 | 1.01 | 0.89 | 100 |
| CG2--HG22 | 1.09 | 0.97 | 210 |
| CG1--HG13 | 1.09 | 0.97 | 180 |
| CB--HB3 | 1.09 | 0.97 | 1360 |
| CB--HB | 1.09 | 0.97 | 210 |
| CG1--HG11 | 1.09 | 0.97 | 110 |
| CB--HB1 | 1.09 | 0.97 | 190 |
| CG--HG | 1.09 | 0.97 | 140 |
| CD1--HD13 | 1.09 | 0.97 | 210 |
| CD--HD3 | 1.09 | 0.97 | 220 |
| CG--HG2 | 1.09 | 0.97 | 500 |
| CE--HE2 | 1.09 | 0.97 | 190 |
| CA--HA3 | 1.09 | 0.97 | 160 |
| CA--HA | 1.09 | 0.97 | 1570 |
| OH--HH | 0.96 | 0.84 | 80 |
| CA--HA2 | 1.09 | 0.97 | 160 |
| CD2--HD22 | 1.09 | 0.97 | 140 |
| CG1--HG12 | 1.09 | 0.97 | 180 |
| CB--HB2 | 1.09 | 0.97 | 1360 |
| OG--HG | 0.96 | 0.84 | 140 |
| CD2--HD21 | 1.09 | 0.97 | 140 |

| Bond type | Observed distance (Å) | Ideal distance (Å) | Number of outliers |
|---|---|---|---|
| CG2--HG21 | 1.09 | 0.97 | 210 |
| CG--HG3 | 1.09 | 0.97 | 500 |
| CD1--HD12 | 1.09 | 0.97 | 210 |
| CG2--HG23 | 1.09 | 0.97 | 210 |
| NZ--HZ1 | 1.01 | 0.89 | 100 |
| CD2--HD23 | 1.09 | 0.97 | 140 |
| CD1--HD11 | 1.09 | 0.97 | 210 |
| CE--HE1 | 1.09 | 0.97 | 90 |
| CE--HE3 | 1.09 | 0.97 | 190 |
| NZ--HZ3 | 1.01 | 0.89 | 100 |
| N--H2 | 1.01 | 0.89 | 10 |
| N--H1 | 1.01 | 0.89 | 10 |
| OG1--HG1 | 0.96 | 0.84 | 30 |
| N--H3 | 1.01 | 0.89 | 10 |
| SG--HG | 1.33 | 1.20 | 1 |
| SG--HG | 1.34 | 1.20 | 9 |
| NH2--HH22 | 1.01 | 0.86 | 80 |
| N--H | 1.01 | 0.86 | 1680 |
| NH2--HH21 | 1.01 | 0.86 | 80 |
| ND2--HD21 | 1.01 | 0.86 | 140 |
| NE2--HE22 | 1.01 | 0.86 | 100 |
| CE1--HE1 | 1.08 | 0.93 | 140 |
| CE2--HE2 | 1.08 | 0.93 | 110 |

| Bond type | Observed distance (Å) | Ideal distance (Å) | Number of outliers |
|---|---|---|---|
| CD2--HD2 | 1.08 | 0.93 | 140 |
| NH1--HH12 | 1.01 | 0.86 | 80 |
| ND2--HD22 | 1.01 | 0.86 | 140 |
| CZ--HZ | 1.08 | 0.93 | 30 |
| CD1--HD1 | 1.08 | 0.93 | 110 |
| NH1--HH11 | 1.01 | 0.86 | 80 |
| NE--HE | 1.01 | 0.86 | 80 |
| NE2--HE21 | 1.01 | 0.86 | 100 |
| ND1--HD1 | 1.01 | 0.86 | 30 |

## Standard geometry: angle outliers

*There are 124 angle outliers in this entry. A summary is provided below, and a detailed list of outliers can be found here.*

| Angle type | Observed angle (°) | Ideal angle (°) | Number of outliers |
|---|---|---|---|
| C-N-CA | 121.70 | 134.53 | 1 |
| C-N-CA | 121.70 | 134.00 | 1 |
| C-N-CA | 121.70 | 133.18 | 1 |
| C-N-CA | 121.70 | 132.28 | 1 |
| C-N-CA | 121.70 | 131.99 | 1 |
| C-N-CA | 121.70 | 131.55 | 1 |
| C-N-CA | 121.70 | 131.23 | 1 |
| CA-CB-CG | 112.60 | 117.88 | 1 |
| C-N-CA | 121.70 | 131.17 | 1 |
| C-N-CA | 121.70 | 131.09 | 1 |
| C-N-CA | 121.70 | 130.71 | 1 |

| Angle type | Observed angle (°) | Ideal angle (°) | Number of outliers |
|---|---|---|---|
| CA-CB-CG | 112.60 | 117.56 | 1 |
| C-N-CA | 121.70 | 130.59 | 1 |
| C-N-CA | 121.70 | 130.55 | 1 |
| C-N-CA | 121.70 | 130.52 | 1 |
| C-N-CA | 121.70 | 130.33 | 1 |
| C-N-CA | 121.70 | 130.29 | 1 |
| C-N-CA | 121.70 | 130.28 | 1 |
| C-N-CA | 121.70 | 130.24 | 1 |
| C-N-CA | 121.70 | 130.20 | 1 |
| C-N-CA | 121.70 | 130.19 | 1 |
| CA-CB-CG | 112.60 | 117.31 | 1 |
| C-N-CA | 121.70 | 130.09 | 1 |
| OE1-CD-NE2 | 122.60 | 117.96 | 1 |
| CA-C-N | 116.20 | 125.48 | 1 |
| C-N-CA | 121.70 | 129.97 | 1 |
| C-N-CA | 121.70 | 129.92 | 1 |
| OE1-CD-NE2 | 122.60 | 118.04 | 1 |
| C-N-CA | 121.70 | 129.90 | 1 |
| CA-CB-CG | 112.60 | 117.15 | 1 |
| OE1-CD-NE2 | 122.60 | 118.11 | 2 |
| C-N-CA | 121.70 | 129.78 | 1 |
| C-N-CA | 121.70 | 129.73 | 1 |
| OE1-CD-NE2 | 122.60 | 118.14 | 2 |

| Angle type | Observed angle (°) | Ideal angle (°) | Number of outliers |
|---|---|---|---|
| OE1-CD-NE2 | 122.60 | 118.17 | 1 |
| C-CA-CB | 110.10 | 118.50 | 1 |
| OE1-CD-NE2 | 122.60 | 118.18 | 1 |
| C-N-CA | 121.70 | 129.65 | 1 |
| OE1-CD-NE2 | 122.60 | 118.19 | 1 |
| OE1-CD-NE2 | 122.60 | 118.20 | 1 |
| OE1-CD-NE2 | 122.60 | 118.21 | 3 |
| CA-CB-CG | 112.60 | 116.99 | 1 |
| OE1-CD-NE2 | 122.60 | 118.22 | 2 |
| C-N-CA | 121.70 | 129.59 | 1 |
| OE1-CD-NE2 | 122.60 | 118.23 | 2 |
| CA-CB-CG | 112.60 | 116.97 | 1 |
| C-N-CA | 121.70 | 129.55 | 1 |
| C-N-CA | 121.70 | 129.53 | 1 |
| OE1-CD-NE2 | 122.60 | 118.25 | 1 |
| OE1-CD-NE2 | 122.60 | 118.26 | 2 |
| C-N-CA | 121.70 | 129.48 | 1 |
| CA-CB-CG | 112.60 | 116.92 | 1 |
| C-N-CA | 121.70 | 129.46 | 1 |
| OE1-CD-NE2 | 122.60 | 118.30 | 1 |
| OE1-CD-NE2 | 122.60 | 118.31 | 2 |
| OE1-CD-NE2 | 122.60 | 118.32 | 3 |
| C-N-CA | 121.70 | 129.41 | 1 |

| Angle type | Observed angle (°) | Ideal angle (°) | Number of outliers |
|---|---|---|---|
| OE1-CD-NE2 | 122.60 | 118.33 | 3 |
| OE1-CD-NE2 | 122.60 | 118.34 | 1 |
| OE1-CD-NE2 | 122.60 | 118.35 | 1 |
| C-N-CA | 121.70 | 129.32 | 1 |
| OE1-CD-NE2 | 122.60 | 118.37 | 3 |
| C-N-CA | 121.70 | 129.29 | 1 |
| OE1-CD-NE2 | 122.60 | 118.38 | 2 |
| C-N-CA | 121.70 | 129.28 | 1 |
| OE1-CD-NE2 | 122.60 | 118.42 | 1 |
| C-N-CA | 121.70 | 129.21 | 1 |
| OE1-CD-NE2 | 122.60 | 118.44 | 1 |
| N-CA-C | 111.00 | 122.64 | 1 |
| OE1-CD-NE2 | 122.60 | 118.46 | 1 |
| CB-CG-CD2 | 131.20 | 125.83 | 1 |
| OD1-CG-ND2 | 122.60 | 118.47 | 1 |
| OE1-CD-NE2 | 122.60 | 118.47 | 1 |
| C-N-CA | 121.70 | 129.12 | 1 |
| OE1-CD-NE2 | 122.60 | 118.48 | 2 |
| OE1-CD-NE2 | 122.60 | 118.49 | 2 |
| CB-CG-CD2 | 131.20 | 125.87 | 2 |
| O-C-N | 123.00 | 116.44 | 1 |
| OE1-CD-NE2 | 122.60 | 118.51 | 2 |
| OE1-CD-NE2 | 122.60 | 118.53 | 2 |

| Angle type | Observed angle (°) | Ideal angle (°) | Number of outliers |
|---|---|---|---|
| CB-CG-CD2 | 131.20 | 125.92 | 1 |
| C-N-CA | 121.70 | 129.00 | 1 |
| OE1-CD-NE2 | 122.60 | 118.55 | 1 |
| OE1-CD-NE2 | 122.60 | 118.56 | 1 |
| N-CA-C | 111.00 | 122.30 | 1 |
| OE1-CD-NE2 | 122.60 | 118.57 | 1 |
| N-CA-C | 111.00 | 122.27 | 1 |
| OE1-CD-NE2 | 122.60 | 118.59 | 1 |
| C-N-CA | 121.70 | 128.91 | 1 |
| OE1-CD-NE2 | 122.60 | 118.60 | 2 |
| C-N-H | 111.97 | 124.30 | 1 |
| C-N-H | 110.59 | 124.30 | 1 |
| C-N-H | 109.94 | 124.30 | 1 |
| C-N-H | 109.69 | 124.30 | 1 |
| C-N-H | 109.51 | 124.30 | 1 |
| C-N-H | 109.42 | 124.30 | 1 |
| C-N-H | 109.14 | 124.30 | 1 |
| C-N-H | 108.86 | 124.30 | 1 |
| C-N-H | 108.82 | 124.30 | 1 |
| C-N-H | 108.33 | 124.30 | 2 |
| HH21-NH2-HH22 | 99.74 | 120.00 | 1 |
| HH21-NH2-HH22 | 97.92 | 120.00 | 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 the models in this entry.*

| Model ID | Clash score | Number of clashes |
|---|---|---|
| 1 | 2.68 | 7 |
| 2 | 0.38 | 1 |
| 3 | 0.00 | 0 |
| 4 | 1.53 | 4 |
| 5 | 1.15 | 3 |
| 6 | 0.00 | 0 |
| 7 | 3.45 | 9 |
| 8 | 0.77 | 2 |
| 9 | 1.15 | 3 |
| 10 | 0.77 | 2 |

*All 31 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.*

| Model ID | Atom-1 | Atom-2 | Clash overlap (Å) |
|---|---|---|---|
| 1 | A:62:MET:HE1 | A:173:TYR:CD1 | 0.687 |
| 1 | A:119:ILE:HG13 | A:149:GLY:HA3 | 0.562 |
| 1 | A:62:MET:HE2 | A:94:PHE:CZ | 0.498 |
| 1 | A:119:ILE:CG1 | A:149:GLY:HA3 | 0.488 |
| 1 | A:48:GLY:C | A:50:GLY:H | 0.471 |
| 1 | A:62:MET:HE2 | A:94:PHE:CE1 | 0.469 |
| 1 | A:71:VAL:HG22 | A:87:MET:HE1 | 0.467 |
| 2 | A:45:ALA:C | A:47:GLY:H | 0.464 |
| 4 | A:45:ALA:C | A:47:GLY:H | 0.494 |
| 4 | A:75:LEU:HD13 | A:112:ARG:NH2 | 0.475 |

| Model ID | Atom-1 | Atom-2 | Clash overlap (Å) |
|---|---|---|---|
| 4 | A:75:LEU:HD13 | A:112:ARG:CZ | 0.427 |
| 4 | A:66:GLN:NE2 | A:173:TYR:H | 0.415 |
| 5 | A:75:LEU:HD13 | A:112:ARG:NH2 | 0.613 |
| 5 | A:75:LEU:HD13 | A:112:ARG:CZ | 0.482 |
| 5 | A:45:ALA:C | A:47:GLY:H | 0.437 |
| 7 | A:62:MET:HE1 | A:173:TYR:CD1 | 0.660 |
| 7 | A:119:ILE:CG1 | A:149:GLY:HA3 | 0.571 |
| 7 | A:119:ILE:HG13 | A:149:GLY:HA3 | 0.557 |
| 7 | A:62:MET:HE2 | A:94:PHE:CZ | 0.517 |
| 7 | A:75:LEU:HD13 | A:112:ARG:NH2 | 0.488 |
| 7 | A:62:MET:HE2 | A:94:PHE:CE1 | 0.462 |
| 7 | A:119:ILE:HG12 | A:149:GLY:HA3 | 0.440 |
| 7 | A:45:ALA:C | A:47:GLY:H | 0.414 |
| 7 | A:119:ILE:HG13 | A:149:GLY:CA | 0.408 |
| 8 | A:45:ALA:C | A:47:GLY:H | 0.451 |
| 8 | A:75:LEU:HD13 | A:112:ARG:NH2 | 0.415 |
| 9 | A:62:MET:HE1 | A:173:TYR:CD1 | 0.628 |
| 9 | A:62:MET:HE2 | A:94:PHE:CZ | 0.448 |
| 9 | A:62:MET:HE2 | A:94:PHE:CE1 | 0.411 |
| 10 | A:111:GLU:CD | A:158:HIS:HD1 | 0.465 |
| 10 | A:45:ALA:C | A:47:GLY:H | 0.422 |

## 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 | Analyzed | Favored | Allowed | Outliers |
|---|---|---|---|---|
| 1 | 171 | 146 | 10 | 15 |
| 2 | 171 | 146 | 13 | 12 |
| 3 | 171 | 144 | 16 | 11 |
| 4 | 171 | 146 | 12 | 13 |
| 5 | 171 | 147 | 15 | 9 |
| 6 | 171 | 149 | 14 | 8 |
| 7 | 171 | 143 | 18 | 10 |
| 8 | 171 | 143 | 15 | 13 |
| 9 | 171 | 146 | 11 | 14 |
| 10 | 171 | 138 | 18 | 15 |

*Detailed list of outliers are tabulated below.*

## Torsion angles: Protein sidechains

*In the following table, sidechain outliers are listed. The Analysed column shows the number of residues for which the sidechain conformation was analysed.*

| Model ID | Analyzed | Favored | Allowed | Outliers |
|---|---|---|---|---|
| 1 | 138 | 129 | 4 | 5 |
| 2 | 138 | 130 | 4 | 4 |
| 3 | 138 | 133 | 2 | 3 |
| 4 | 138 | 132 | 2 | 4 |
| 5 | 138 | 125 | 5 | 8 |
| 6 | 138 | 126 | 10 | 2 |
| 7 | 138 | 124 | 7 | 7 |
| 8 | 138 | 129 | 4 | 5 |
| 9 | 138 | 132 | 2 | 4 |
| 10 | 138 | 125 | 10 | 3 |

*Detailed list of outliers are tabulated below.*

| Model ID | Chain | Residue ID | Residue type |
|---|---|---|---|
| 1 | A | 3 | LEU |
| 1 | A | 7 | LEU |
| 1 | A | 14 | LEU |
| 1 | A | 17 | MET |
| 1 | A | 24 | SER |
| 2 | A | 3 | LEU |
| 2 | A | 7 | LEU |
| 2 | A | 36 | MET |
| 2 | A | 51 | ASN |
| 3 | A | 7 | LEU |
| 3 | A | 14 | LEU |
| 3 | A | 36 | MET |
| 4 | A | 3 | LEU |
| 4 | A | 7 | LEU |
| 4 | A | 14 | LEU |
| 4 | A | 36 | MET |
| 5 | A | 1 | MET |
| 5 | A | 3 | LEU |
| 5 | A | 7 | LEU |
| 5 | A | 14 | LEU |
| 5 | A | 25 | ASN |
| 5 | A | 29 | SER |

| Model ID | Chain | Residue ID | Residue type |
|---|---|---|---|
| 5 | A | 36 | MET |
| 5 | A | 41 | THR |
| 6 | A | 3 | LEU |
| 6 | A | 14 | LEU |
| 7 | A | 7 | LEU |
| 7 | A | 10 | LEU |
| 7 | A | 14 | LEU |
| 7 | A | 17 | MET |
| 7 | A | 23 | SER |
| 7 | A | 36 | MET |
| 7 | A | 43 | MET |
| 8 | A | 7 | LEU |
| 8 | A | 17 | MET |
| 8 | A | 31 | ASP |
| 8 | A | 36 | MET |
| 8 | A | 41 | THR |
| 9 | A | 3 | LEU |
| 9 | A | 7 | LEU |
| 9 | A | 10 | LEU |
| 9 | A | 41 | THR |
| 10 | A | 11 | MET |
| 10 | A | 14 | LEU |
| 10 | A | 36 | MET |

## Fit of model to data used for modeling

### Crosslinking-MS

Validation for this section is under development.

## Fit of model to data used for validation

Validation for this section is under development.

*Acknowledgements*

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