

Integrative Structure Validation Report ?

February 18, 2025 - 08:45 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

PyMOL Version 2.5.0

| | |
|-------------------|---|
| PDB ID | 9A83 |
| PDB-Dev ID | PDBDEV_00000368 |
| Structure Title | Encounter complex in the cross-modular condensation step of the Tomaymycin NRPS system: complex of the substrate-loaded peptidyl-carrier-protein domain from the TomA module (APCP-load) with the adaptor (BN91) of the TomB module |
| Structure Authors | Karant, M.N.; Kirkpatrick, J. P.; Carlomagno, T. |
| Deposited on | 2024-02-05 |

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

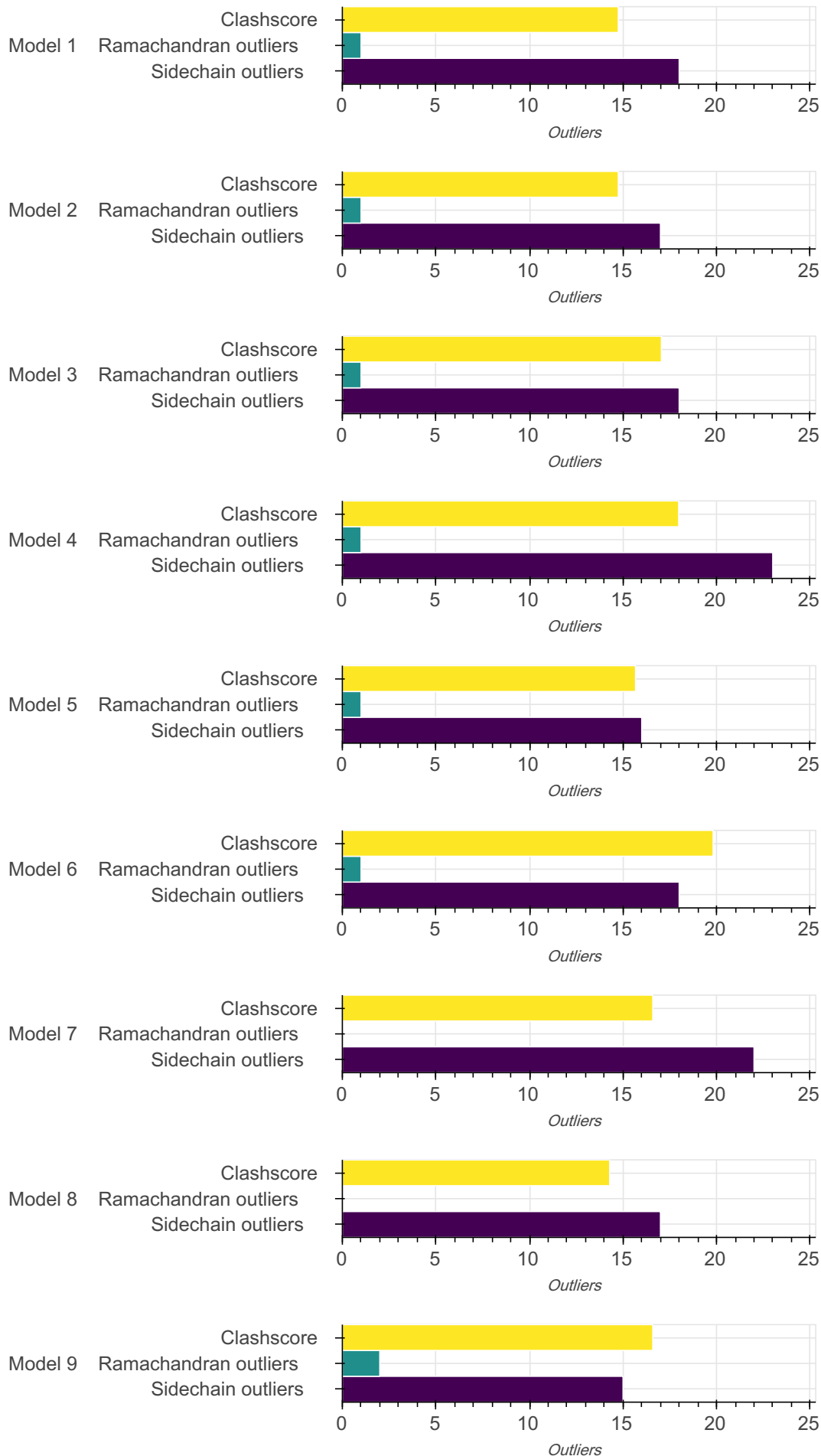
A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the ? symbol.

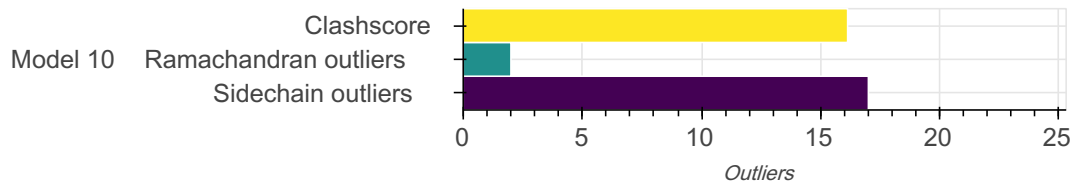
List of references used to build this report is available [here](#).

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 1 distinct ensemble(s).

Summary ?

This entry consists of 10 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 | 1-10 | 1 | Adaptor BN91 domain of Tomaymycin B module | A | 73 | - | 1-73 | 100.00 / 100.00 | Atomic |
| | | 2 | Substrate-loaded form of the peptidyl-carrier-protein (APCP) domain of the Tomaymycin A module | B | 72 | - | 1-72 | 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 | NMR data | Not available | Not available |
| 2 | Experimental model | PDB | 8Q SX |
| 3 | Experimental model | PDB | 8Q RX |

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 | None | Data-driven docking using CSP-derived distance restraints within HADDOCK. | Data-driven docking using CSP-derived distance restraints within HADDOCK. | None | False | False |

There is 1 software package reported in this entry.

| ID | Software name | Software version | Software classification | Software location |
|----|-------------------------|------------------|-------------------------|---|
| 1 | HADDOCK | 2.40 | Data-driven docking | https://wenmr.science.uu.nl/haddock2.4/ |

Data quality ?

NMR

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 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 | 14.75 | 32 |
| 2 | 14.75 | 32 |
| 3 | 17.05 | 37 |
| 4 | 17.97 | 39 |

| Model ID | Clash score | Number of clashes |
|----------|-------------|-------------------|
| 5 | 15.67 | 34 |
| 6 | 19.82 | 43 |
| 7 | 16.59 | 36 |
| 8 | 14.29 | 31 |
| 9 | 16.59 | 36 |
| 10 | 16.13 | 35 |

There are 355 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:6:THR:HG23 | B:46:ILE:HB | 0.99 | 10 | 9 |
| B:9:GLN:HA | B:12:LYS:HD2 | 0.96 | 3 | 1 |
| B:1:ASN:HB2 | B:4:GLU:HB2 | 0.92 | 4 | 6 |
| A:6:THR:HB | A:47:PHE:HZ | 0.84 | 8 | 7 |
| A:6:THR:HG21 | B:6:VAL:HG21 | 0.83 | 6 | 9 |
| A:73:ARG:HE | B:70:GLU:HB3 | 0.81 | 3 | 1 |
| B:12:LYS:HG2 | B:18:ASP:HA | 0.79 | 3 | 1 |
| B:3:LEU:HD23 | B:66:ALA:HA | 0.76 | 4 | 5 |
| A:43:LEU:HA | A:46:VAL:HG12 | 0.76 | 3 | 9 |
| A:44:THR:HG22 | A:50:GLU:HG2 | 0.75 | 10 | 5 |
| B:56:VAL:HA | B:65:LEU:HD21 | 0.70 | 3 | 1 |
| A:46:VAL:HG22 | B:6:VAL:HG23 | 0.68 | 10 | 5 |
| B:8:LEU:HD12 | B:12:LYS:HE2 | 0.67 | 7 | 1 |
| B:9:GLN:HA | B:9:GLN:HE21 | 0.67 | 7 | 1 |
| B:8:LEU:HB3 | B:62:VAL:HG21 | 0.67 | 8 | 3 |
| A:3:LEU:HD21 | B:3:LEU:HA | 0.67 | 5 | 7 |
| A:2:PRO:HG2 | B:3:LEU:HD13 | 0.67 | 1 | 3 |
| B:12:LYS:HZ2 | B:18:ASP:HA | 0.66 | 9 | 8 |
| A:4:ARG:HE | A:63:ALA:HA | 0.65 | 3 | 2 |
| B:9:GLN:HA | B:12:LYS:CD | 0.64 | 3 | 1 |
| B:44:GLN:HG2 | B:51:VAL:H | 0.63 | 5 | 6 |
| A:1:SER:HB3 | A:73:ARG:HH22 | 0.63 | 5 | 1 |
| A:48:ALA:HB2 | B:5:THR:HG21 | 0.63 | 7 | 1 |
| A:6:THR:HB | A:47:PHE:CZ | 0.61 | 8 | 5 |
| B:4:GLU:HG2 | B:22:THR:HG21 | 0.61 | 4 | 1 |
| B:3:LEU:HG | B:6:VAL:HG12 | 0.61 | 7 | 1 |

| Atom 1 | Atom 2 | Clash(Å) | Model ID (Worst) | Models (Total) |
|---------------|---------------|----------|------------------|----------------|
| | | | | |
| A:2:PRO:HG3 | B:69:VAL:HG13 | 0.61 | 7 | 1 |
| B:3:LEU:O | B:7:VAL:HG23 | 0.59 | 4 | 8 |
| A:39:LEU:HD23 | A:56:LEU:HD21 | 0.59 | 8 | 6 |
| A:51:ILE:HD12 | A:68:ARG:HD3 | 0.58 | 10 | 9 |
| B:47:PHE:HD2 | B:51:VAL:HG21 | 0.57 | 3 | 2 |
| A:1:SER:N | A:4:ARG:HH12 | 0.56 | 3 | 1 |
| A:61:THR:H | A:64:ASP:HB3 | 0.56 | 8 | 9 |
| A:10:LEU:HD11 | A:43:LEU:HD21 | 0.56 | 9 | 5 |
| A:53:GLY:HA2 | A:56:LEU:HB3 | 0.56 | 4 | 3 |
| A:32:HIS:O | A:35:LEU:HG | 0.56 | 5 | 10 |
| A:46:VAL:HG13 | B:6:VAL:HG23 | 0.56 | 8 | 1 |
| B:3:LEU:HB3 | B:66:ALA:HB1 | 0.55 | 4 | 2 |
| B:1:ASN:HB2 | B:4:GLU:CB | 0.55 | 10 | 3 |
| A:73:ARG:NE | B:70:GLU:HB3 | 0.55 | 3 | 1 |
| B:39:LEU:O | B:43:LEU:HG | 0.55 | 7 | 9 |
| A:3:LEU:HD21 | B:2:PRO:HG2 | 0.54 | 3 | 1 |
| B:12:LYS:NZ | B:18:ASP:HA | 0.54 | 1 | 8 |
| B:3:LEU:HD21 | B:47:PHE:CZ | 0.53 | 7 | 1 |
| B:41:SER:O | B:45:LYS:HG3 | 0.53 | 3 | 1 |
| B:32:ASN:HB3 | B:35:HIS:HB2 | 0.53 | 10 | 8 |
| A:69:MET:O | B:2:PRO:HG3 | 0.53 | 3 | 1 |
| B:22:THR:O | B:62:VAL:HG22 | 0.53 | 9 | 4 |
| A:3:LEU:O | A:7:VAL:HG23 | 0.52 | 2 | 5 |
| B:54:GLU:O | B:58:ARG:HG3 | 0.52 | 5 | 7 |
| A:43:LEU:HA | A:46:VAL:CG1 | 0.52 | 3 | 4 |
| A:40:ALA:HA | A:43:LEU:HD12 | 0.52 | 5 | 2 |
| B:41:SER:HA | B:44:GLN:HG3 | 0.52 | 9 | 2 |
| A:6:THR:CG2 | B:6:VAL:HG21 | 0.52 | 5 | 4 |
| A:39:LEU:O | A:43:LEU:HG | 0.51 | 5 | 4 |
| A:1:SER:HB3 | A:73:ARG:NH2 | 0.51 | 5 | 2 |
| A:47:PHE:HB3 | A:69:MET:HG2 | 0.51 | 6 | 1 |
| B:63:GLU:OE1 | B:64:GLN:HG2 | 0.50 | 4 | 5 |
| A:47:PHE:C | B:5:THR:HG21 | 0.50 | 2 | 4 |
| A:3:LEU:HD22 | A:47:PHE:HE1 | 0.50 | 9 | 1 |

| Atom 1 | Atom 2 | Clash(Å) | Model ID (Worst) | Models (Total) |
|---------------|---------------|----------|------------------|----------------|
| A:5:THR:HG21 | B:48:GLY:HA2 | 0.49 | 9 | 5 |
| B:27:LEU:H | B:27:LEU:HD12 | 0.49 | 5 | 3 |
| A:11:ALA:O | A:15:LEU:HB2 | 0.49 | 9 | 5 |
| B:7:VAL:HG21 | B:66:ALA:HB2 | 0.49 | 8 | 3 |
| B:43:LEU:HD23 | B:46:ILE:HD11 | 0.48 | 9 | 1 |
| B:40:ALA:O | B:44:GLN:HG3 | 0.48 | 4 | 7 |
| A:3:LEU:HD23 | B:3:LEU:HD12 | 0.48 | 1 | 4 |
| A:22:ALA:HA | A:62:VAL:HG22 | 0.48 | 1 | 3 |
| A:3:LEU:HD22 | A:47:PHE:CE1 | 0.48 | 2 | 5 |
| A:12:ARG:HB2 | A:17:SER:O | 0.47 | 6 | 4 |
| B:53:THR:HA | B:56:VAL:HG22 | 0.47 | 6 | 2 |
| A:3:LEU:HA | A:6:THR:OG1 | 0.47 | 2 | 3 |
| B:7:VAL:CG1 | B:62:VAL:HB | 0.47 | 4 | 2 |
| B:12:LYS:O | B:16:GLY:HA2 | 0.47 | 10 | 8 |
| B:8:LEU:HG | B:12:LYS:HE3 | 0.47 | 3 | 1 |
| B:1:ASN:O | B:4:GLU:HB2 | 0.46 | 1 | 1 |
| A:9:ASP:O | A:12:ARG:HG2 | 0.46 | 7 | 1 |
| A:72:ARG:HB3 | B:2:PRO:HA | 0.46 | 5 | 1 |
| B:22:THR:HA | B:62:VAL:HG22 | 0.45 | 3 | 1 |
| B:66:ALA:HA | B:69:VAL:HG12 | 0.45 | 7 | 1 |
| A:21:THR:HG22 | A:22:ALA:H | 0.45 | 9 | 2 |
| B:1:ASN:O | B:4:GLU:HG2 | 0.45 | 3 | 1 |
| B:20:PHE:HZ | B:62:VAL:HG13 | 0.45 | 1 | 1 |
| B:8:LEU:HD13 | B:22:THR:HG23 | 0.45 | 4 | 1 |
| A:49:VAL:HB | A:69:MET:HG3 | 0.45 | 7 | 1 |
| B:54:GLU:OE1 | B:58:ARG:HD3 | 0.45 | 7 | 1 |
| A:49:VAL:HB | A:69:MET:HE3 | 0.45 | 3 | 1 |
| A:8:LEU:HD11 | A:20:LEU:O | 0.45 | 10 | 3 |
| A:46:VAL:HA | B:9:GLN:HG3 | 0.44 | 5 | 3 |
| A:5:THR:HG21 | B:48:GLY:CA | 0.44 | 4 | 4 |
| A:26:LEU:O | A:30:CYS:HB2 | 0.44 | 7 | 4 |
| A:47:PHE:C | A:49:VAL:H | 0.44 | 6 | 1 |
| B:8:LEU:CD1 | B:12:LYS:HE2 | 0.44 | 2 | 1 |
| B:59:HIS:ND1 | B:64:GLN:HB3 | 0.44 | 3 | 2 |
| B:43:LEU:HA | B:46:ILE:HG12 | 0.44 | 6 | 1 |

| Atom 1 | Atom 2 | Clash(Å) | Model ID (Worst) | Models (Total) |
|--------------|-------------|----------|------------------|----------------|
| A:4:ARG:HB2 | A:4:ARG:NH1 | 0.43 | 3 | 1 |
| B:24:ASP:O | B:61:THR:HA | 0.43 | 1 | 2 |
| B:25:SER:HA | B:60:GLY:O | 0.43 | 10 | 1 |
| A:43:LEU:HA | A:46:VAL:HB | 0.43 | 8 | 1 |
| A:6:THR:HG23 | B:46:ILE:CB | 0.43 | 6 | 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 | 141 | 131 | 9 | 1 |
| 2 | 141 | 131 | 9 | 1 |
| 3 | 141 | 132 | 8 | 1 |
| 4 | 141 | 129 | 11 | 1 |
| 5 | 141 | 132 | 8 | 1 |
| 6 | 141 | 131 | 9 | 1 |
| 7 | 141 | 132 | 9 | 0 |
| 8 | 141 | 134 | 7 | 0 |
| 9 | 141 | 132 | 7 | 2 |
| 10 | 141 | 131 | 8 | 2 |

There are 3 unique backbone outliers. Detailed list of outliers are tabulated below.

| Chain | Res | Type | Models (Total) |
|-------|-----|------|----------------|
| A | 51 | ILE | 5 |
| B | 2 | PRO | 4 |
| A | 44 | THR | 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 | 117 | 81 | 18 | 18 |
| 2 | 117 | 84 | 16 | 17 |
| 3 | 117 | 83 | 16 | 18 |
| 4 | 117 | 84 | 10 | 23 |
| 5 | 117 | 87 | 14 | 16 |


| Model ID | Analysed | Favored | Allowed | Outliers |
|----------|----------|---------|---------|----------|
| 6 | 117 | 87 | 12 | 18 |
| 7 | 117 | 82 | 13 | 22 |
| 8 | 117 | 89 | 11 | 17 |
| 9 | 117 | 84 | 18 | 15 |
| 10 | 117 | 83 | 17 | 17 |

There are 37 unique sidechain outliers. Detailed list of outliers are tabulated below.

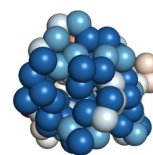
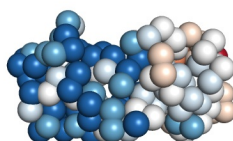
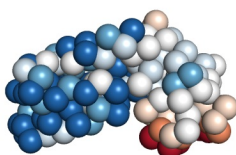
| Chain | Res | Type | Models (Total) |
|-------|-----|------|----------------|
| A | 5 | THR | 10 |
| A | 20 | LEU | 10 |
| A | 28 | ASP | 10 |
| B | 23 | THR | 10 |
| B | 33 | SER | 10 |
| B | 8 | LEU | 9 |
| B | 22 | THR | 9 |
| B | 53 | THR | 9 |
| A | 6 | THR | 8 |
| A | 52 | THR | 8 |
| A | 71 | ASP | 8 |
| B | 24 | ASP | 8 |
| B | 52 | SER | 8 |
| B | 63 | GLU | 8 |
| A | 1 | SER | 7 |
| A | 4 | ARG | 7 |
| A | 21 | THR | 6 |
| B | 9 | GLN | 6 |
| A | 62 | VAL | 5 |
| B | 6 | VAL | 3 |
| A | 37 | ASP | 2 |
| B | 5 | THR | 2 |
| B | 18 | ASP | 2 |
| B | 19 | ASP | 2 |
| B | 21 | THR | 2 |
| A | 46 | VAL | 1 |
| A | 70 | ASP | 1 |

| Chain | Res | Type | Models (Total) |
|-------|-----|------|----------------|
| B | 3 | LEU | 1 |
| B | 13 | ASP | 1 |
| B | 25 | SER | 1 |
| B | 29 | HIS | 1 |
| B | 41 | SER | 1 |
| B | 44 | GLN | 1 |
| B | 45 | LYS | 1 |
| B | 62 | VAL | 1 |
| B | 65 | LEU | 1 |
| B | 68 | PHE | 1 |

PrISM precision analysis ?

Regions of **low**  **high** precision, defined as the variability among the models that satisfy the input data and calculated as the density-weighted root mean-square fluctuation (RMSF) from the bead/atom center of density, annotated and visualized using PrISM. The per-bead precision is computed from the deposited ensemble of superposed integrative models. High- and low-precision regions are then determined by clustering beads of similar precision based on their proximity in the structure. Only coarse-grained beads (or CA atoms for atomic models) of deposited models are used for assessment and visualization, and three projections for each representative model are generated.

PrISM analysis for Ensemble 1 (models deposited/total: 10/10).



Fit of model to data used for modeling ?

NMR

Validation for this section is under development.

Fit of model to data used for validation ?

Validation for this section is under development.

Acknowledgments

The development of integrative model validation metrics, implementation of a model validation pipeline, and creation of a validation report for integrative structures are funded by NSF awards to the [PDB-IHM team](#) (DBI-1756248, DBI-2112966, DBI-2112967, DBI-2112968, and DBI-1756250) and awards from NSF, NIH, and DOE to the [RCSB PDB](#) (DBI-2321666, R01GM157729, and DE-SC0019749). The PDB-IHM team and members of the [Sali lab](#) contributed model validation metrics and software packages.

Dr. Jill Trehwella, Dr. Dina Schneidman, and members of the [SASBDB](#) repository are acknowledged for their advice and support in implementing SAS validation methods. Team members from the labs of Dr. Juri Rappsilber, Dr. Alexander Leitner, Dr. Andrea Graziadei, and members of [PRIDE](#) database are acknowledged for their advice and support in implementing crosslinking-MS validation methods. We are grateful to Dr. Shruthi Viswanath for discussions about uncertainty assessment of integrative structural models.

Members of the [wwPDB Integrative/Hybrid Methods Task Force](#) provided recommendations and community support for the project.