# Integrative Structure Validation Report

## February 18, 2025 - 08:30 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 | 9A0K |
| PDB-Dev ID | PDBDEV_00000056 |
| Structure Title | A structural model of the endogenoushuman SWI/SNF (BAF) complex bound to the nucleosome informs disease mechanisms |
| Structure Authors | Mashtalir N; Suzuki H; Farrell DP; Sankar A; Luo J; Filipovski M; D'Avino AR; St.Pierre R; Valencia AM; Onikubo T; Roeder RG; Han Y; He Y; Ranish JA; DiMaio F; Walz T; Kadoch C |
| Deposited on | 2020-08-24 |

*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*

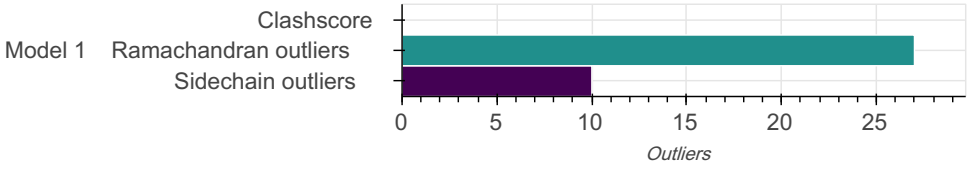
*A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the* ? symbol.

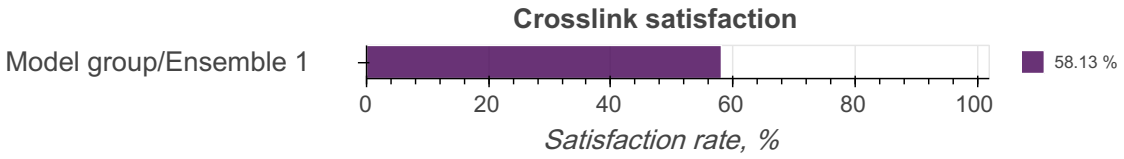
*List of references used to build this report is available here.*

## 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 49 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 | 7 | SMARCC1 | 1 | 1105 | 1-1105 | - | 100.00 / 100.00 | Atomic |
| | | 8 | SMARCC2 | 2 | 1214 | 1-1214 | - | 100.00 / 100.00 | Atomic |
| | | 5 | SMARCA4 | 4 | 1647 | 1-1647, 1-1647, 1-1647 | - | 100.00 / 100.00 | Atomic |
| | | 2 | ACTL6A | 6 | 429 | 1-429 | - | 100.00 / 100.00 | Atomic |
| | | 3 | ARID1A | A | 2285 | 1-2285 | - | 100.00 / 100.00 | Atomic |
| | | 1 | ACTB | B | 375 | 1-375 | - | 100.00 / 100.00 | Atomic |
| | | 9 | SMARCD1 | D | 515 | 1-515 | - | 100.00 / 100.00 | Atomic |
| | | 10 | SMARCE1 | E | 411 | 220-298 | - | 19.22 / 100.00 | Atomic |
| | | 4 | DPF2 | P | 391 | 1-88 | - | 22.51 / 100.00 | Atomic |
| | | 11 | H2A | V<br>v | 130 | 1-130 | - | 100.00 / 100.00 | Atomic |
| | | 12 | H2B | W<br>w | 126 | 1-126 | - | 100.00 / 100.00 | Atomic |

| ID | Model(s) | Entity ID | Molecule name | Chain(s) [auth] | Total residues | Rigid segments | Flexible segments | Model coverage/ Starting model coverage (%) | Scale |
|---|---|---|---|---|---|---|---|---|---|
| | | 13 | H3 | X | 136 | 1-136 | - | 100.00 / 100.00 | Atomic |
| | | | | x | | | | | |
| | | 14 | H4 | Y | 103 | 1-103 | - | 100.00 / 100.00 | Atomic |
| | | | | y | | | | | |
| | | 6 | SMARCB1 | b | 385 | 1-385, 1-385 | - | 100.00 / 100.00 | Atomic |
| | | 15 | 601 dna fwd | p | 196 | 1-196 | - | 100.00 / 100.00 | Atomic |
| | | 16 | 601 dna rev | q | 196 | 1-196 | - | 100.00 / 100.00 | Atomic |

## Datasets used for modeling

*There are 49 unique datasets used to build the models in this entry.*

| ID | Dataset type | Database name | Data access code |
|---|---|---|---|
| 1 | 3DEM volume | Zenodo | 10.5281/zenodo.3998811 |
| 2 | Crosslinking-MS data | PRIDE | PXD020992 |
| 3 | Comparative model | Zenodo | 10.5281/zenodo.3998811 |
| 4 | Comparative model | Zenodo | 10.5281/zenodo.3998811 |
| 5 | Comparative model | Zenodo | 10.5281/zenodo.3998811 |
| 6 | Comparative model | Zenodo | 10.5281/zenodo.3998811 |
| 7 | Comparative model | Zenodo | 10.5281/zenodo.3998811 |
| 8 | Comparative model | Zenodo | 10.5281/zenodo.3998811 |
| 9 | Comparative model | Zenodo | 10.5281/zenodo.3998811 |
| 10 | Comparative model | Zenodo | 10.5281/zenodo.3998811 |
| 11 | Comparative model | Zenodo | 10.5281/zenodo.3998811 |
| 12 | Comparative model | Zenodo | 10.5281/zenodo.3998811 |
| 13 | Comparative model | Zenodo | 10.5281/zenodo.3998811 |
| 14 | Comparative model | Zenodo | 10.5281/zenodo.3998811 |
| 15 | Comparative model | Zenodo | 10.5281/zenodo.3998811 |
| 16 | Comparative model | Zenodo | 10.5281/zenodo.3998811 |
| 17 | Comparative model | Zenodo | 10.5281/zenodo.3998811 |
| 18 | Comparative model | Zenodo | 10.5281/zenodo.3998811 |
| 19 | Comparative model | Zenodo | 10.5281/zenodo.3998811 |
| 20 | Comparative model | Zenodo | 10.5281/zenodo.3998811 |
| 21 | Comparative model | Zenodo | 10.5281/zenodo.3998811 |
| 22 | Comparative model | Zenodo | 10.5281/zenodo.3998811 |

| ID | Dataset type | Database name | Data access code |
|---|---|---|---|
| 23 | Comparative model | Zenodo | 10.5281/zenodo.3998811 |
| 24 | De Novo model | Zenodo | 10.5281/zenodo.3998811 |
| 25 | De Novo model | Zenodo | 10.5281/zenodo.3998811 |
| 26 | Experimental model | PDB | 6UXV |
| 27 | Experimental model | PDB | 6UXV |
| 28 | Experimental model | PDB | 6UCH |
| 29 | Experimental model | PDB | 6UXV |
| 30 | Experimental model | PDB | 5X0Y |
| 31 | Experimental model | PDB | 5X0Y |
| 32 | Experimental model | PDB | 5X0Y |
| 33 | Experimental model | PDB | 6UXV |
| 34 | Experimental model | PDB | 5X0Y |
| 35 | Experimental model | PDB | 5X0Y |
| 36 | Experimental model | PDB | 6UXV |
| 37 | Experimental model | PDB | 4I6M |
| 38 | Experimental model | PDB | 5X0Y |
| 39 | Experimental model | PDB | 6UXV |
| 40 | Experimental model | PDB | 4I6M |
| 41 | Experimental model | PDB | 5X0Y |
| 42 | Experimental model | PDB | 5X0Y |
| 43 | Experimental model | PDB | 6UXV |
| 44 | Experimental model | PDB | 5X0Y |
| 45 | Experimental model | PDB | 5X0Y |
| 46 | Experimental model | PDB | 4I6M |
| 47 | Experimental model | PDB | 5X0Y |
| 48 | 3DEM volume | EMDB | EMD-22476 |
| 49 | 3DEM volume | EMDB | EMD-22478 |

## 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 | Production sampling | Monte Carlo | None | None | False | False |
| 2 | 1 | trRosetta | trRosetta | None | None | False | False |
| 3 | 1 | Rosetta Hybridize | Rosetta Hybridize | None | None | False | False |

*There are 3 software packages reported in this entry.*

| ID | Software name | Software version | Software classification | Software location |
|---|---|---|---|---|
| 1 | Rosetta | Rosetta version unknown:ff8ee24ee5f65423d5064cba818ede41d012fa87 2020-08-10 10:39:53 -0700 from git@github.com:RosettaCommons/main.git | RosettaCM/hybridize and unpublished 'complex assembly' | https://www.rosettacommons.org/ |
| 2 | trRosetta | 1.0.0 | trRosetta | https://github.com/gjoni/trRosetta |
| 3 | HHpred | website | protein homology detection | https://toolkit.tuebingen.mpg.de/hhpred |

## 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.

### 3DEM volume

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 278 bond length outliers in this entry (0.69% of 40116 assessed bonds). A summary is provided below. The output is limited to 100 rows.*

| Chain | Res | Type | Atoms | \|Z\| | Observed (Å) | Ideal (Å) | Model ID (Worst) | Models (Total) |
|---|---|---|---|---|---|---|---|---|
| p | 39 | DG | N9-C4 | 26.60 | 0.85 | 1.38 | 1 | 1 |
| q | 28 | DA | N9-C4 | 21.04 | 0.96 | 1.38 | 1 | 1 |
| 4 | 1371 | SER | C-N | 19.68 | 1.05 | 1.33 | 1 | 1 |
| p | 66 | DA | N9-C8 | 17.97 | 1.73 | 1.37 | 1 | 1 |
| q | 158 | DC | C2-O2 | 17.47 | 0.89 | 1.24 | 1 | 1 |
| p | 71 | DG | N9-C8 | 16.54 | 1.70 | 1.37 | 1 | 1 |
| q | 160 | DG | C5-C6 | 16.09 | 1.09 | 1.42 | 1 | 1 |
| p | 39 | DG | C5-C6 | 15.92 | 1.10 | 1.42 | 1 | 1 |
| p | 39 | DG | C2-N3 | 15.65 | 1.64 | 1.33 | 1 | 1 |
| q | 160 | DG | N7-C5 | 14.65 | 1.68 | 1.39 | 1 | 1 |

| Chain | Res | Type | Atoms | \|Z\| | Observed (Å) | Ideal (Å) | Model ID (Worst) | Models (Total) |
|---|---|---|---|---|---|---|---|---|
| q | 126 | DC | N1-C2 | 14.46 | 1.11 | 1.40 | 1 | 1 |
| q | 157 | DA | N9-C8 | 14.31 | 1.65 | 1.37 | 1 | 1 |
| q | 158 | DC | C4'-O4' | 13.89 | 1.73 | 1.45 | 1 | 1 |
| q | 126 | DC | N3-C4 | 13.85 | 1.61 | 1.33 | 1 | 1 |
| p | 40 | DT | N3-C4 | 13.69 | 1.66 | 1.38 | 1 | 1 |
| p | 65 | DC | N1-C6 | 13.15 | 1.10 | 1.36 | 1 | 1 |
| p | 40 | DT | C4-C5 | 13.14 | 1.70 | 1.44 | 1 | 1 |
| q | 160 | DG | N9-C4 | 13.13 | 1.11 | 1.38 | 1 | 1 |
| p | 40 | DT | C2-N3 | 13.06 | 1.11 | 1.37 | 1 | 1 |
| p | 66 | DA | C5-C6 | 13.01 | 1.15 | 1.41 | 1 | 1 |
| p | 37 | DC | N3-C4 | 12.98 | 1.59 | 1.33 | 1 | 1 |
| q | 164 | DT | N1-C2 | 12.93 | 1.12 | 1.38 | 1 | 1 |
| p | 39 | DG | C2'-C1' | 12.90 | 1.27 | 1.52 | 1 | 1 |
| q | 132 | DG | N9-C8 | 12.71 | 1.63 | 1.37 | 1 | 1 |
| p | 37 | DC | C4-C5 | 12.58 | 1.68 | 1.43 | 1 | 1 |
| q | 160 | DG | C8-N7 | 12.43 | 1.06 | 1.30 | 1 | 1 |
| p | 71 | DG | N9-C4 | 12.42 | 1.13 | 1.38 | 1 | 1 |
| q | 28 | DA | C1'-N9 | 11.74 | 1.69 | 1.46 | 1 | 1 |
| p | 37 | DC | C5-C6 | 11.72 | 1.10 | 1.34 | 1 | 1 |
| q | 158 | DC | N3-C4 | 11.46 | 1.56 | 1.33 | 1 | 1 |
| q | 158 | DC | C5-C6 | 11.43 | 1.11 | 1.34 | 1 | 1 |
| q | 158 | DC | C4-C5 | 11.33 | 1.65 | 1.43 | 1 | 1 |
| q | 126 | DC | C4-C5 | 10.86 | 1.64 | 1.43 | 1 | 1 |
| p | 39 | DG | N3-C4 | 10.84 | 1.57 | 1.35 | 1 | 1 |
| p | 37 | DC | N1-C2 | 10.67 | 1.19 | 1.40 | 1 | 1 |
| q | 126 | DC | C2-N3 | 10.64 | 1.14 | 1.36 | 1 | 1 |
| q | 164 | DT | C5-C6 | 10.60 | 1.13 | 1.34 | 1 | 1 |
| 4 | 1191 | HIS | CB-CG | 10.54 | 1.35 | 1.50 | 1 | 1 |
| p | 37 | DC | N1-C6 | 10.46 | 1.15 | 1.36 | 1 | 1 |
| p | 65 | DC | C4-C5 | 10.38 | 1.63 | 1.43 | 1 | 1 |
| p | 39 | DG | C5-C4 | 10.26 | 1.17 | 1.38 | 1 | 1 |
| p | 66 | DA | C6-N6 | 10.19 | 1.13 | 1.34 | 1 | 1 |
| 4 | 445 | GLN | C-N | 10.14 | 1.47 | 1.33 | 1 | 1 |
| q | 157 | DA | C5-C6 | 10.12 | 1.21 | 1.41 | 1 | 1 |
| p | 66 | DA | C8-N7 | 10.02 | 1.11 | 1.31 | 1 | 1 |
| p | 33 | DA | N9-C8 | 10.02 | 1.57 | 1.37 | 1 | 1 |
| q | 159 | DC | C4-N4 | 9.93 | 1.14 | 1.34 | 1 | 1 |
| p | 65 | DC | N1-C2 | 9.85 | 1.20 | 1.40 | 1 | 1 |
| p | 39 | DG | O4'-C1' | 9.81 | 1.61 | 1.41 | 1 | 1 |

| Chain | Res | Type | Atoms | \|Z\| | Observed (Å) | Ideal (Å) | Model ID (Worst) | Models (Total) |
|---|---|---|---|---|---|---|---|---|
| p | 169 | DT | N1-C6 | 9.50 | 1.19 | 1.38 | 1 | 1 |
| q | 158 | DC | C2-N3 | 9.48 | 1.17 | 1.36 | 1 | 1 |
| p | 169 | DT | C4-C5 | 9.43 | 1.63 | 1.44 | 1 | 1 |
| p | 169 | DT | N1-C2 | 9.35 | 1.19 | 1.38 | 1 | 1 |
| p | 65 | DC | N3-C4 | 9.32 | 1.52 | 1.33 | 1 | 1 |
| 1 | 538 | GLN | CG-CD | 9.27 | 1.28 | 1.52 | 1 | 1 |
| q | 159 | DC | C4-C5 | 9.26 | 1.61 | 1.43 | 1 | 1 |
| q | 160 | DG | C5-C4 | 9.24 | 1.19 | 1.38 | 1 | 1 |
| p | 41 | DC | N1-C2 | 9.13 | 1.22 | 1.40 | 1 | 1 |
| P | 86 | HIS | CB-CG | 8.94 | 1.62 | 1.50 | 1 | 1 |
| q | 131 | DT | N1-C6 | 8.93 | 1.20 | 1.38 | 1 | 1 |
| b | 163 | THR | C-N | 8.62 | 1.45 | 1.33 | 1 | 1 |
| p | 33 | DA | C8-N7 | 8.52 | 1.14 | 1.31 | 1 | 1 |
| q | 28 | DA | N9-C8 | 8.48 | 1.54 | 1.37 | 1 | 1 |
| q | 157 | DA | C8-N7 | 8.34 | 1.15 | 1.31 | 1 | 1 |
| p | 65 | DC | C2-N3 | 8.23 | 1.19 | 1.36 | 1 | 1 |
| 4 | 1073 | LEU | CG-CD2 | 8.22 | 1.25 | 1.52 | 1 | 1 |
| p | 38 | DG | N1-C2 | 8.18 | 1.21 | 1.38 | 1 | 1 |
| q | 28 | DA | N7-C5 | 8.15 | 1.22 | 1.39 | 1 | 1 |
| A | 1816 | ILE | CB-CG2 | 8.12 | 1.25 | 1.52 | 1 | 1 |
| p | 40 | DT | N1-C2 | 8.09 | 1.22 | 1.38 | 1 | 1 |
| p | 39 | DG | C6-N1 | 8.01 | 1.23 | 1.39 | 1 | 1 |
| p | 71 | DG | C8-N7 | 7.94 | 1.15 | 1.30 | 1 | 1 |
| p | 39 | DG | C6-O6 | 7.94 | 1.08 | 1.24 | 1 | 1 |
| 6 | 283 | PRO | N-CD | 7.78 | 1.36 | 1.47 | 1 | 1 |
| q | 131 | DT | N1-C2 | 7.78 | 1.22 | 1.38 | 1 | 1 |
| p | 39 | DG | N1-C2 | 7.74 | 1.53 | 1.38 | 1 | 1 |
| q | 160 | DG | O4'-C1' | 7.70 | 1.26 | 1.41 | 1 | 1 |
| p | 33 | DA | N9-C4 | 7.64 | 1.22 | 1.38 | 1 | 1 |
| p | 40 | DT | C2-O2 | 7.54 | 1.07 | 1.22 | 1 | 1 |
| p | 71 | DG | N7-C5 | 7.50 | 1.24 | 1.39 | 1 | 1 |
| b | 164 | PHE | N-CA | 7.49 | 1.60 | 1.46 | 1 | 1 |
| 4 | 1212 | GLU | CG-CD | 7.40 | 1.33 | 1.52 | 1 | 1 |
| 4 | 1085 | LEU | CB-CG | 7.29 | 1.38 | 1.53 | 1 | 1 |
| q | 28 | DA | O4'-C1' | 7.28 | 1.56 | 1.41 | 1 | 1 |
| p | 169 | DT | N3-C4 | 7.20 | 1.53 | 1.38 | 1 | 1 |
| X | 67 | PRO | N-CD | 7.09 | 1.37 | 1.47 | 1 | 1 |
| p | 71 | DG | C5-C4 | 7.06 | 1.52 | 1.38 | 1 | 1 |
| B | 8 | LEU | CB-CG | 6.97 | 1.67 | 1.53 | 1 | 1 |

| Chain | Res | Type | Atoms | \|Z\| | Observed (Å) | Ideal (Å) | Model ID (Worst) | Models (Total) |
|---|---|---|---|---|---|---|---|---|
| A | 1818 | GLN | CA-C | 6.85 | 1.67 | 1.52 | 1 | 1 |
| A | 2049 | TRP | CD2-CE3 | 6.79 | 1.51 | 1.40 | 1 | 1 |
| 4 | 918 | LEU | CB-CG | 6.77 | 1.67 | 1.53 | 1 | 1 |
| 1 | 537 | TYR | CB-CG | 6.60 | 1.66 | 1.51 | 1 | 1 |
| V | 27 | PRO | N-CD | 6.54 | 1.38 | 1.47 | 1 | 1 |
| q | 28 | DA | C8-N7 | 6.54 | 1.18 | 1.31 | 1 | 1 |
| q | 132 | DG | N9-C4 | 6.53 | 1.25 | 1.38 | 1 | 1 |
| q | 159 | DC | C2-O2 | 6.49 | 1.11 | 1.24 | 1 | 1 |
| b | 385 | TRP | CZ2-CH2 | 6.46 | 1.49 | 1.37 | 1 | 1 |
| v | 27 | PRO | N-CD | 6.45 | 1.38 | 1.47 | 1 | 1 |
| p | 38 | DG | C5-C4 | 6.42 | 1.51 | 1.38 | 1 | 1 |
| b | 385 | TRP | CD2-CE3 | 6.41 | 1.50 | 1.40 | 1 | 1 |

## Standard geometry: angle outliers

*There are 547 bond angle outliers in this entry (0.99% of 55397 assessed bonds). A summary is provided below. The output is limited to 100 rows.*

| Chain | Res | Type | Atoms | \|Z\| | Observed (Å) | Ideal (Å) | Model ID (Worst) | Models (Total) |
|---|---|---|---|---|---|---|---|---|
| p | 40 | DT | O2-C2-N3 | 80.76 | 0.86 | 122.00 | 1 | 1 |
| p | 33 | DA | N9-C4-C5 | 61.76 | 13.06 | 105.70 | 1 | 1 |
| q | 160 | DG | C8-N7-C5 | 58.32 | 16.72 | 104.20 | 1 | 1 |
| q | 158 | DC | O2-C2-N3 | 56.52 | 37.13 | 121.90 | 1 | 1 |
| p | 66 | DA | N9-C4-C5 | 51.59 | 28.32 | 105.70 | 1 | 1 |
| p | 37 | DC | N1-C2-O2 | 51.12 | 42.51 | 119.20 | 1 | 1 |
| p | 71 | DG | N9-C4-C5 | 50.43 | 29.96 | 105.60 | 1 | 1 |
| q | 132 | DG | N9-C4-C5 | 50.29 | 30.16 | 105.60 | 1 | 1 |
| p | 37 | DC | O2-C2-N3 | 50.07 | 46.80 | 121.90 | 1 | 1 |
| q | 157 | DA | N9-C4-C5 | 50.00 | 30.70 | 105.70 | 1 | 1 |
| q | 158 | DC | N1-C2-O2 | 49.96 | 44.26 | 119.20 | 1 | 1 |
| p | 65 | DC | O2-C2-N3 | 49.69 | 47.36 | 121.90 | 1 | 1 |
| p | 169 | DT | O2-C2-N3 | 48.98 | 48.54 | 122.00 | 1 | 1 |
| q | 160 | DG | N9-C4-C5 | 47.98 | 33.63 | 105.60 | 1 | 1 |
| q | 126 | DC | O2-C2-N3 | 47.11 | 51.23 | 121.90 | 1 | 1 |
| p | 169 | DT | N1-C2-O2 | 46.98 | 52.73 | 123.20 | 1 | 1 |
| q | 126 | DC | N1-C2-O2 | 44.96 | 51.76 | 119.20 | 1 | 1 |
| q | 131 | DT | N1-C2-O2 | 44.06 | 57.11 | 123.20 | 1 | 1 |
| q | 28 | DA | N9-C4-C5 | 43.94 | 39.79 | 105.70 | 1 | 1 |
| q | 131 | DT | O2-C2-N3 | 43.88 | 56.18 | 122.00 | 1 | 1 |
| q | 164 | DT | N1-C2-N3 | 42.13 | 51.60 | 114.80 | 1 | 1 |
| p | 39 | DG | N9-C4-C5 | 41.68 | 43.08 | 105.60 | 1 | 1 |

| Chain | Res | Type | Atoms | \|Z\| | Observed (Å) | Ideal (Å) | Model ID (Worst) | Models (Total) |
|---|---|---|---|---|---|---|---|---|
| p | 39 | DG | C8-N7-C5 | 39.91 | 44.34 | 104.20 | 1 | 1 |
| q | 28 | DA | C8-N7-C5 | 39.08 | 45.28 | 103.90 | 1 | 1 |
| p | 65 | DC | N1-C2-O2 | 38.12 | 62.03 | 119.20 | 1 | 1 |
| p | 39 | DG | C8-N9-C4 | 37.94 | 49.09 | 106.00 | 1 | 1 |
| q | 160 | DG | C1'-N9-C4 | 37.03 | 71.46 | 127.00 | 1 | 1 |
| p | 66 | DA | C8-N9-C4 | 36.28 | 51.48 | 105.90 | 1 | 1 |
| p | 40 | DT | N1-C6-C5 | 36.25 | 68.43 | 122.80 | 1 | 1 |
| q | 157 | DA | C8-N9-C4 | 35.70 | 52.35 | 105.90 | 1 | 1 |
| q | 132 | DG | C8-N9-C4 | 34.92 | 53.62 | 106.00 | 1 | 1 |
| q | 132 | DG | C8-N7-C5 | 34.22 | 52.87 | 104.20 | 1 | 1 |
| q | 160 | DG | N9-C4-N3 | 33.57 | 176.35 | 126.00 | 1 | 1 |
| q | 164 | DT | O2-C2-N3 | 33.03 | 72.46 | 122.00 | 1 | 1 |
| q | 28 | DA | C1'-N9-C4 | 32.82 | 176.28 | 127.05 | 1 | 1 |
| q | 157 | DA | C1'-N9-C8 | 32.51 | 175.82 | 127.05 | 1 | 1 |
| q | 157 | DA | C8-N7-C5 | 32.03 | 55.86 | 103.90 | 1 | 1 |
| q | 126 | DC | N1-C6-C5 | 31.89 | 73.16 | 121.00 | 1 | 1 |
| p | 66 | DA | C8-N7-C5 | 31.60 | 56.49 | 103.90 | 1 | 1 |
| q | 160 | DG | C2-N3-C4 | 29.78 | 67.12 | 111.80 | 1 | 1 |
| p | 71 | DG | C8-N9-C4 | 29.34 | 61.99 | 106.00 | 1 | 1 |
| q | 131 | DT | C1'-N1-C6 | 29.12 | 75.68 | 119.35 | 1 | 1 |
| p | 65 | DC | N1-C6-C5 | 28.67 | 77.99 | 121.00 | 1 | 1 |
| p | 39 | DG | N9-C4-N3 | 28.15 | 83.78 | 126.00 | 1 | 1 |
| p | 169 | DT | N1-C6-C5 | 27.95 | 80.88 | 122.80 | 1 | 1 |
| p | 71 | DG | C8-N7-C5 | 27.85 | 62.42 | 104.20 | 1 | 1 |
| q | 28 | DA | C8-N9-C4 | 27.85 | 64.13 | 105.90 | 1 | 1 |
| p | 169 | DT | C2-N1-C6 | 27.80 | 162.99 | 121.30 | 1 | 1 |
| q | 131 | DT | C1'-N1-C2 | 27.24 | 78.49 | 119.35 | 1 | 1 |
| q | 158 | DC | N1-C6-C5 | 27.15 | 80.28 | 121.00 | 1 | 1 |
| q | 132 | DG | C1'-N9-C8 | 26.74 | 86.90 | 127.00 | 1 | 1 |
| p | 37 | DC | N1-C6-C5 | 26.59 | 81.11 | 121.00 | 1 | 1 |
| p | 33 | DA | C8-N7-C5 | 25.34 | 65.89 | 103.90 | 1 | 1 |
| q | 158 | DC | N1-C2-N3 | 25.01 | 81.38 | 118.90 | 1 | 1 |
| p | 65 | DC | C2-N1-C6 | 24.86 | 157.89 | 120.60 | 1 | 1 |
| p | 33 | DA | N9-C8-N7 | 24.68 | 76.78 | 113.80 | 1 | 1 |
| q | 126 | DC | C2-N3-C4 | 22.87 | 85.70 | 120.00 | 1 | 1 |
| q | 131 | DT | C2-N1-C6 | 21.91 | 154.17 | 121.30 | 1 | 1 |
| p | 40 | DT | N1-C2-O2 | 21.13 | 91.51 | 123.20 | 1 | 1 |
| p | 40 | DT | C2-N3-C4 | 21.02 | 95.47 | 127.00 | 1 | 1 |
| p | 39 | DG | C1'-N9-C4 | 20.80 | 158.20 | 127.00 | 1 | 1 |

| Chain | Res | Type | Atoms | \|Z\| | Observed (Å) | Ideal (Å) | Model ID (Worst) | Models (Total) |
|---|---|---|---|---|---|---|---|---|
| p | 37 | DC | C2-N3-C4 | 20.69 | 88.97 | 120.00 | 1 | 1 |
| p | 33 | DA | C8-N9-C4 | 20.25 | 75.53 | 105.90 | 1 | 1 |
| p | 39 | DG | N7-C5-C6 | 19.89 | 100.26 | 130.10 | 1 | 1 |
| p | 66 | DA | C1'-N9-C4 | 19.74 | 97.44 | 127.05 | 1 | 1 |
| p | 37 | DC | N1-C2-N3 | 19.72 | 89.31 | 118.90 | 1 | 1 |
| p | 66 | DA | N9-C8-N7 | 19.59 | 84.41 | 113.80 | 1 | 1 |
| q | 28 | DA | C5-C4-N3 | 19.54 | 156.21 | 126.90 | 1 | 1 |
| p | 71 | DG | C1'-N9-C8 | 19.42 | 156.13 | 127.00 | 1 | 1 |
| q | 158 | DC | C3'-O3'-P | 19.36 | 149.24 | 120.20 | 1 | 1 |
| p | 65 | DC | C2-N3-C4 | 19.32 | 91.02 | 120.00 | 1 | 1 |
| q | 164 | DT | C2-N1-C6 | 19.30 | 150.25 | 121.30 | 1 | 1 |
| D | 471 | GLY | C-N-CA | 18.02 | 154.14 | 121.70 | 1 | 1 |
| q | 160 | DG | N7-C5-C4 | 17.77 | 137.45 | 110.80 | 1 | 1 |
| q | 159 | DC | C1'-N1-C6 | 17.66 | 146.19 | 119.70 | 1 | 1 |
| q | 160 | DG | C8-N9-C4 | 17.65 | 79.52 | 106.00 | 1 | 1 |
| p | 65 | DC | C1'-N1-C2 | 17.58 | 93.32 | 119.70 | 1 | 1 |
| q | 132 | DG | N9-C4-N3 | 17.53 | 99.71 | 126.00 | 1 | 1 |
| q | 28 | DA | N7-C5-C4 | 17.52 | 136.98 | 110.70 | 1 | 1 |
| p | 71 | DG | N9-C8-N7 | 17.41 | 87.38 | 113.50 | 1 | 1 |
| q | 160 | DG | N9-C8-N7 | 16.99 | 138.98 | 113.50 | 1 | 1 |
| A | 1923 | THR | C-N-CA | 16.96 | 152.23 | 121.70 | 1 | 1 |
| q | 157 | DA | N9-C8-N7 | 16.79 | 88.62 | 113.80 | 1 | 1 |
| q | 160 | DG | C6-C5-C4 | 16.76 | 93.96 | 119.10 | 1 | 1 |
| q | 164 | DT | C4-C5-C6 | 16.52 | 94.42 | 119.20 | 1 | 1 |
| p | 38 | DG | N9-C4-N3 | 16.44 | 150.65 | 126.00 | 1 | 1 |
| D | 350 | GLN | C-N-CA | 16.26 | 150.97 | 121.70 | 1 | 1 |
| q | 158 | DC | C4'-O4'-C1' | 16.09 | 85.57 | 109.70 | 1 | 1 |
| q | 160 | DG | C1'-N9-C8 | 15.98 | 150.97 | 127.00 | 1 | 1 |
| q | 132 | DG | N9-C8-N7 | 15.75 | 89.87 | 113.50 | 1 | 1 |
| p | 169 | DT | C2-N3-C4 | 15.65 | 103.53 | 127.00 | 1 | 1 |
| 4 | 445 | GLN | O-C-N | 15.34 | 147.55 | 123.00 | 1 | 1 |
| q | 158 | DC | C2-N3-C4 | 15.24 | 97.13 | 120.00 | 1 | 1 |
| q | 131 | DT | N1-C6-C5 | 15.17 | 100.04 | 122.80 | 1 | 1 |
| p | 169 | DT | C1'-N1-C2 | 15.15 | 96.62 | 119.35 | 1 | 1 |
| p | 40 | DT | N1-C2-N3 | 14.95 | 92.37 | 114.80 | 1 | 1 |
| 4 | 445 | GLN | CA-C-N | 14.86 | 86.48 | 116.20 | 1 | 1 |
| p | 66 | DA | C1'-N9-C8 | 14.58 | 148.92 | 127.05 | 1 | 1 |
| q | 160 | DG | C5-C4-N3 | 14.41 | 150.02 | 128.40 | 1 | 1 |

| Chain | Res | Type | Atoms | \|Z\| | Observed (Å) | Ideal (Å) | Model ID (Worst) | Models (Total) |
|---|---|---|---|---|---|---|---|---|
| p | 39 | DG | C5-C6-N1 | 14.18 | 132.97 | 111.70 | 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 | 0.00 | 0 |

*There are no too-close contacts.*

## 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 | 4036 | 3849 | 160 | 27 |

*There are 27 unique backbone outliers. Detailed list of outliers are tabulated below.*

| Chain | Res | Type | Models (Total) |
|---|---|---|---|
| 4 | 718 | TYR | 1 |
| 4 | 957 | ASN | 1 |
| 4 | 984 | VAL | 1 |
| 4 | 1073 | LEU | 1 |
| 4 | 1289 | PRO | 1 |
| 4 | 1372 | ARG | 1 |
| 4 | 1382 | SER | 1 |
| 4 | 1383 | LEU | 1 |
| 6 | 71 | ASP | 1 |
| A | 1704 | PHE | 1 |
| A | 1823 | PHE | 1 |
| A | 1826 | ASP | 1 |
| A | 1935 | GLU | 1 |
| A | 2006 | GLY | 1 |
| A | 2074 | SER | 1 |
| A | 2211 | SER | 1 |
| A | 2222 | PRO | 1 |
| P | 75 | PRO | 1 |
| b | 132 | VAL | 1 |
| b | 147 | CYS | 1 |
| b | 153 | ARG | 1 |
| b | 163 | THR | 1 |
| b | 168 | PHE | 1 |
| b | 257 | GLN | 1 |

| Chain | Res | Type | Models (Total) |
|---|---|---|---|
| b | 303 | LEU | 1 |
| b | 330 | GLU | 1 |
| b | 355 | 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 | 3557 | 3516 | 31 | 10 |

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

| Chain | Res | Type | Models (Total) |
|---|---|---|---|
| 1 | 537 | TYR | 1 |
| 4 | 1014 | LYS | 1 |
| 4 | 1074 | ASP | 1 |
| 4 | 1362 | GLU | 1 |
| 4 | 1367 | PHE | 1 |
| 4 | 1375 | LYS | 1 |
| 4 | 1376 | GLU | 1 |
| 4 | 1377 | VAL | 1 |
| A | 1834 | VAL | 1 |
| A | 2124 | LYS | 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.*

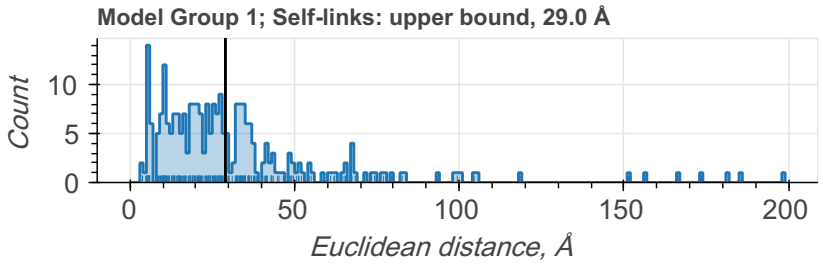
There are 1321 crosslinking restraints combined in 1188 restraint groups.

| Linker | Residue 1 | Atom 1 | Residue 2 | Atom 2 | Restraint type | Distance, Å | Count |
|---|---|---|---|---|---|---|---|
| BS3 | LYS | CA | LYS | CA | upper bound | 29.0 | 1234 |
| BS3 | LYS | CA | MET | CA | upper bound | 29.0 | 4 |
| BS3 | LYS | CA | VAL | CA | upper bound | 29.0 | 4 |
| BS3 | ILE | CA | LYS | CA | upper bound | 29.0 | 1 |
| BS3 | LYS | CA | PHE | CA | upper bound | 29.0 | 13 |
| BS3 | ALA | CA | LYS | CA | upper bound | 29.0 | 13 |
| BS3 | LYS | CA | PRO | CA | upper bound | 29.0 | 13 |

| Linker | Residue 1 | Atom 1 | Residue 2 | Atom 2 | Restraint type | Distance, Å | Count |
|---|---|---|---|---|---|---|---|
| BS3 | GLY | CA | LYS | CA | upper bound | 29.0 | 3 |
| BS3 | HIS | CA | LYS | CA | upper bound | 29.0 | 2 |
| BS3 | LYS | CA | THR | CA | upper bound | 29.0 | 1 |
| BS3 | GLU | CA | LYS | CA | upper bound | 29.0 | 4 |
| BS3 | LYS | CA | SER | CA | upper bound | 29.0 | 12 |
| BS3 | PRO | CA | SER | CA | upper bound | 29.0 | 2 |
| BS3 | ALA | CA | MET | CA | upper bound | 29.0 | 3 |
| BS3 | LEU | CA | LYS | CA | upper bound | 29.0 | 1 |
| BS3 | GLY | CA | MET | CA | upper bound | 29.0 | 1 |
| BS3 | THR | CA | VAL | CA | upper bound | 29.0 | 1 |
| BS3 | ALA | CA | VAL | CA | upper bound | 29.0 | 1 |
| BS3 | PHE | CA | VAL | CA | upper bound | 29.0 | 1 |
| BS3 | HIS | CA | PRO | CA | upper bound | 29.0 | 1 |
| BS3 | ALA | CA | THR | CA | upper bound | 29.0 | 1 |
| BS3 | ALA | CA | PHE | CA | upper bound | 29.0 | 1 |
| BS3 | PHE | CA | THR | CA | upper bound | 29.0 | 1 |
| BS3 | THR | CA | THR | CA | upper bound | 29.0 | 1 |
| BS3 | ASP | CA | SER | CA | upper bound | 29.0 | 1 |
| BS3 | GLU | CA | SER | CA | upper bound | 29.0 | 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.*



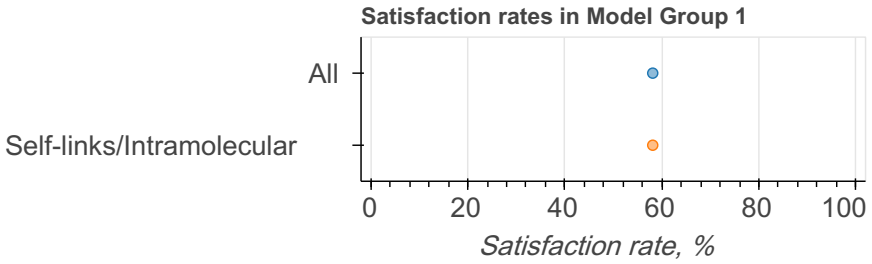

## Satisfaction of restraints

*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=1188) |
|---|---|---|---|---|---|---|---|
| 1 | 1 | 1 | 1/1 | All | 58.13 | 41.87 | 246 |
| | | | | Self-links/ Intramolecular | 58.13 | 41.87 | 246 |

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.*




## 3DEM volume

Validation for this section is under development.

## Fit of model to data used for validation

Validation for this section is under development.

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