# Integrative Structure Validation Report ?

## July 22, 2024 - 03:53 PM PDT

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

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

| | |
|---|---|
| PDB ID | 8ZZY |
| PDB-Dev ID | PDBDEV_00000034 |
| Structure Title | Integrative threading of the DNA-PKcs sequence based on data from chemical cross-linking and hydrogen deuterium exchange |
| Structure Authors | Saltzberg DJ; Hepburn M; Pilla KB; Schriemer DC; Lees-Miller SP; Blundell TL; Sali A |

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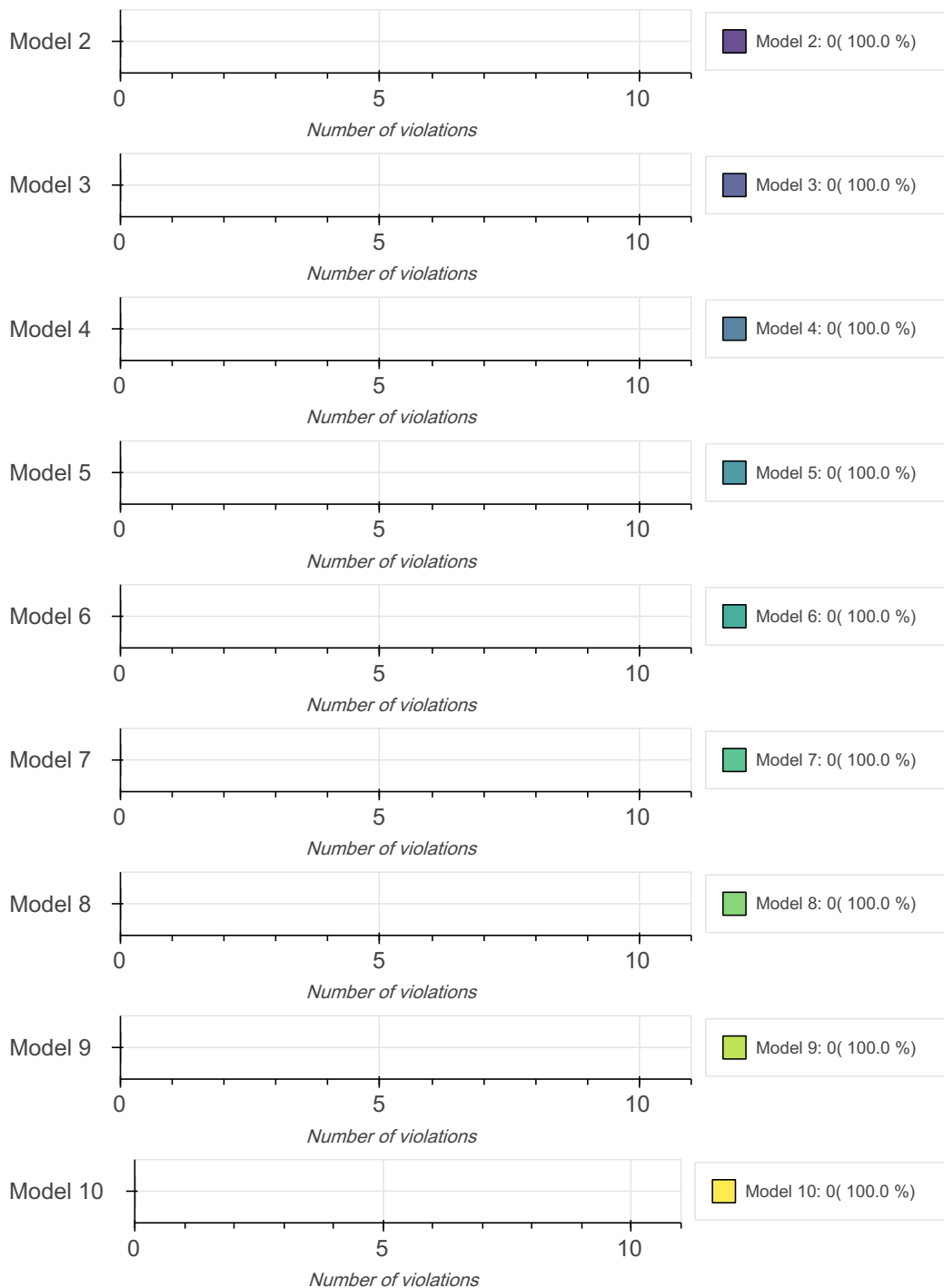
*List of references used to build this report is available here.*

## 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: Excluded Volume Analysis



Model 1: 0(100.0 %)

*Number of violations*

Model 2 — Model 2: 0( 100.0 %)

*Number of violations*

Model 3 — Model 3: 0( 100.0 %)

*Number of violations*

Model 4 — Model 4: 0( 100.0 %)

*Number of violations*

Model 5 — Model 5: 0( 100.0 %)

*Number of violations*

Model 6 — Model 6: 0( 100.0 %)

*Number of violations*

Model 7 — Model 7: 0( 100.0 %)

*Number of violations*

Model 8 — Model 8: 0( 100.0 %)

*Number of violations*

Model 9 — Model 9: 0( 100.0 %)

*Number of violations*

Model 10 — Model 10: 0( 100.0 %)

*Number of violations*

## Ensemble information ?

*This entry consists of 2 distinct ensemble(s).*

## Summary ?

*This entry consists of 10 unique models, with 1 subunits in each model. A total of 5 datasets or restraints were used to build this entry. Each model is represented by 1 rigid bodies and 0 flexible or non-rigid units.*

## Entry composition ⍰

*There are 10 unique types of models in this entry.These models are titled Example model 0 for cluster 0, Example model 1 for cluster 0, Example model 2 for cluster 0, Example model 3 for cluster 0, Example model 4 for cluster 0, Example model 0 for cluster 1, Example model 1 for cluster 1, Example model 2 for cluster 1, Example model 3 for cluster 1, Example model 4 for cluster 1 respectively.*

| Model ID | Subunit number | Subunit ID | Subunit name | Chain ID | Chain ID [auth] | Total residues |
|----------|----------------|------------|--------------|----------|-----------------|----------------|
| 1 | 1 | 1 | DNA-PKcs | A | A | 4128 |
| 2 | 1 | 1 | DNA-PKcs | A | A | 4128 |
| 3 | 1 | 1 | DNA-PKcs | A | A | 4128 |
| 4 | 1 | 1 | DNA-PKcs | A | A | 4128 |
| 5 | 1 | 1 | DNA-PKcs | A | A | 4128 |
| 6 | 1 | 1 | DNA-PKcs | A | A | 4128 |
| 7 | 1 | 1 | DNA-PKcs | A | A | 4128 |
| 8 | 1 | 1 | DNA-PKcs | A | A | 4128 |
| 9 | 1 | 1 | DNA-PKcs | A | A | 4128 |
| 10 | 1 | 1 | DNA-PKcs | A | A | 4128 |

## Datasets used for modeling ⍰

*There are 5 unique datasets used to build the models in this entry.*

| ID | Dataset type | Database name | Data access code |
|----|--------------|---------------|------------------|
| 1 | Crosslinking-MS data | File | 10.5281/zenodo.3886944 |
| 2 | Crosslinking-MS data | File | 10.5281/zenodo.3886944 |
| 3 | Crosslinking-MS data | File | 10.5281/zenodo.3886944 |
| 4 | H/D exchange data | PRIDE | PXD016595 |

| ID | Dataset type | Database name | Data access code |
|----|--------------|---------------|------------------|
| 5 | Experimental model | PDB | 5LUQ |

## Representation ?

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

| Chain ID | Rigid bodies | Non-rigid segments |
|----------|--------------|--------------------|
| A | 1-4128 | - |

## 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 | Enumeration | Production sampling | None | 2860000 | False | True |

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

| ID | Software name | Software version | Software classification | Software location |
|----|---------------|------------------|--------------------------|-------------------|
| 1 | PSIPRED | 4.0 | secondary structure prediction | http://bioinf.cs.ucl.ac.uk/psipred/ |
| 2 | Integrative Modeling Platform (IMP) | 2.2 | integrative model building | https://integrativemodeling.org |
| 3 | scikit-learn | 0.21.3 | model building | https://scikit-learn.org/stable/ |

## Data quality ?

### Crosslinking-MS

Validation for this section is under development.

### H/D exchange

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.

### Excluded volume satisfaction ?

*Excluded volume satisfaction for the models in the entry are listed below.*

| Models | Excluded Volume Satisfaction (%) | Number of violations |
|:------:|:--------------------------------:|:--------------------:|
| 1 | 100.0 | 0.0 |
| 2 | 100.0 | 0.0 |
| 3 | 100.0 | 0.0 |
| 4 | 100.0 | 0.0 |
| 5 | 100.0 | 0.0 |
| 6 | 100.0 | 0.0 |
| 7 | 100.0 | 0.0 |
| 8 | 100.0 | 0.0 |
| 9 | 100.0 | 0.0 |
| 10 | 100.0 | 0.0 |

## Fit of model to data used for modeling ?

### Crosslinking-MS

Validation for this section is under development.

### H/D exchange

Validation for this section is under development.

## Fit of model to data used for validation ❓

Validation for this section is under development.

---