

Integrative Structure Validation Report ?

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

Python-IHM Version 1.3
Integrative Modeling Validation Version 1.2

| | |
|-------------------|---|
| PDB ID | 9A2B |
| PDB-Dev ID | PDBDEV_00000154 |
| Structure Title | Integrative structure of the human MHR complex |
| Structure Authors | Arvindekar S; Jackman MJ; Low JKK; Landsberg MJ; Mackay JP; Viswanath S |

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

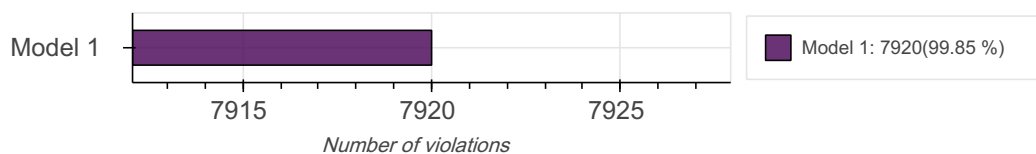
A user guide is available at https://pdb-dev.wwpdb.org/validation_help.html with specific help available everywhere you see the ? symbol.

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



Ensemble information

This entry consists of 1 distinct ensemble(s).

Summary

This entry consists of 1 unique models, with 8 subunits in each model. A total of 16 datasets or restraints were used to build this entry. Each model is represented by 18 rigid bodies and 34 flexible or non-rigid units.

Entry composition

There is 1 unique type of models in this entry. This model is titled Cluster 0/None.

| Model ID | Subunit number | Subunit ID | Subunit name | Chain ID | Chain ID [auth] | Total residues |
|----------|----------------|------------|--------------|----------|-----------------|----------------|
| 1 | 1 | 1 | MTA1 | A | A | 715 |
| 1 | 2 | 1 | MTA1 | B | B | 715 |
| 1 | 3 | 2 | HDAC1 | C | C | 482 |
| 1 | 4 | 2 | HDAC1 | D | D | 482 |
| 1 | 5 | 3 | RBBP4 | E | E | 425 |
| 1 | 6 | 3 | RBBP4 | F | F | 425 |
| 1 | 7 | 3 | RBBP4 | G | G | 425 |
| 1 | 8 | 3 | RBBP4 | H | H | 425 |

Datasets used for modeling

There are 16 unique datasets used to build the models in this entry.

| ID | Dataset type | Database name | Data access code |
|----|----------------------|---------------|------------------|
| 12 | Crosslinking-MS data | PRIDE | PXD010111 |

| ID | Dataset type | Database name | Data access code |
|----|----------------------|---------------|------------------------|
| 13 | Crosslinking-MS data | PRIDE | PXD010111 |
| 14 | Crosslinking-MS data | PRIDE | PXD010111 |
| 2 | Comparative model | File | 10.5281/zenodo.6674232 |
| 4 | De Novo model | File | 10.5281/zenodo.6674232 |
| 6 | Comparative model | File | 10.5281/zenodo.6674232 |
| 9 | Comparative model | File | 10.5281/zenodo.6674232 |
| 10 | De Novo model | File | 10.5281/zenodo.6674232 |
| 11 | Comparative model | File | 10.5281/zenodo.6674232 |
| 15 | 3DEM volume | EMDB | EMD-27557 |
| 16 | 3DEM volume | File | 10.5281/zenodo.6674232 |
| 1 | Experimental model | PDB | 2FVU |
| 3 | Experimental model | PDB | 4BKX |
| 7 | Experimental model | PDB | 5FXV |
| 8 | Experimental model | PDB | 4PBZ |
| 5 | Experimental model | PDB | 2GAT |

Representation

This entry has only one representation and includes 18 rigid bodies and 34 flexible units

| Chain ID | Rigid bodies | Non-rigid segments |
|----------|--|--|
| D | 8-376 | 1-7, 377-482 |
| C | 8-376 | 1-7, 377-482 |
| B | 1-164, 165-333, 334-353, 389-431, 468-546, 670-691 | 229-236, 354-388, 432-467, 519-528, 547-669, 692-715 |

| Chain ID | Rigid bodies | Non-rigid segments |
|----------|--|--|
| A | 1-164, 165-333, 334-353, 389-431, 468-546, 670-691 | 229-236, 354-388, 432-467, 519-528, 547-669, 692-715 |
| H | 10-411 | 1-9, 90-102, 164-165, 176-179, 212-213, 412-425 |
| E | 2-411 | 1-1, 90-113, 412-425 |
| F | 2-411 | 1-1, 90-113, 412-425 |
| G | 10-411 | 1-9, 90-102, 164-165, 176-179, 212-213, 412-425 |

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 | Replica exchange monte carlo | Sampling | None | 500000 | False | True |

There are 2 software packages reported in this entry.

| ID | Software name | Software version | Software classification | Software location |
|----|---|------------------|----------------------------|---|
| 1 | IMP PMI module | 2.16.0 | integrative model building | https://integrativemodeling.org |
| 2 | Integrative Modeling Platform (IMP) | 2.16.0 | integrative model building | https://integrativemodeling.org |

Data quality ?

Crosslinking-MS

Validation for this section is under development.

3DEM volume

Validation for this section is under development.

Model quality ?

For models with atomic structures, molprobrity 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 | 99.85 | 7920.0 |

Fit of model to data used for modeling ?

Crosslinking-MS

Validation for this section is under development.

3DEM volume

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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