

Integrative Structure Validation Report ?

February 18, 2025 - 08:34 AM PST

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

Integrative Modeling Validation Version 2.0

Python-IHM Version 1.8

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
Deposited on	2022-08-02

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

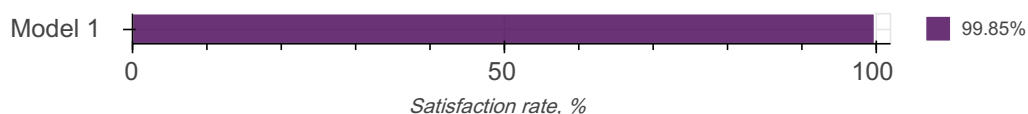
A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the ? symbol.

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

Overall quality ?

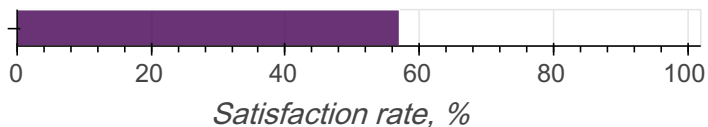
This validation report contains model quality assessments for all structures, data quality and fit to model assessments for SAS and crosslinking-MS datasets. Data quality and fit to model assessments for other datasets and model uncertainty are under development. Number of plots is limited to 256.

Model Quality: Excluded Volume Analysis



Crosslink satisfaction

Model group/Ensemble 1



57.06 %

Ensemble information ?

This entry consists of 1 distinct ensemble(s).

Summary ?

This entry consists of 1 model(s). A total of 16 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	1	MTA1	A	715	1-164, 165-333, 334-353, 389-431, 468-546, 670-691	229-236, 354-388, 432-467, 519-528, 547-669, 692-715	100.00 / 69.51	Multiscale: Coarse-grained: 1 - 30 residue(s) per bead
				B					
		2	HDAC1	C	482	8-376	1-7, 377-482	100.00 / 76.56	Multiscale: Coarse-grained: 1 - 30 residue(s) per bead
				D					
		3	RBBP4	E	425	2-411	1, 90-113, 412-425	100.00 / 96.47	Multiscale: Coarse-grained: 1 - 14 residue(s) per bead
				F					

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
		3	RBBP4	G	425	10-411	1-9, 90-102, 164-165, 176-179, 212-213, 412-425	100.00 / 94.59	Multiscale: Coarse-grained: 1 - 14 residue(s) per bead
				H					

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	Zenodo	10.5281/zenodo.6674232
13	Crosslinking-MS data	Zenodo	10.5281/zenodo.6674232
14	Crosslinking-MS data	Zenodo	10.5281/zenodo.6674232
2	Comparative model	Zenodo	10.5281/zenodo.6674232
4	De Novo model	Zenodo	10.5281/zenodo.6674232
6	Comparative model	Zenodo	10.5281/zenodo.6674232
9	Comparative model	Zenodo	10.5281/zenodo.6674232
10	De Novo model	Zenodo	10.5281/zenodo.6674232
11	Comparative model	Zenodo	10.5281/zenodo.6674232
15	3DEM volume	Zenodo	10.5281/zenodo.6674232
16	3DEM volume	Zenodo	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

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	Sampling	Replica exchange monte carlo	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

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.

Excluded volume satisfaction ?

Excluded volume satisfaction for the models in the entry are listed below. The Analysed column shows the number of particle-particle or particle-atom pairs for which excluded volume was analysed.

Model ID	Analysed	Number of violations	Excluded Volume Satisfaction (%)
1	5403828	7920	99.85

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 1964 crosslinking restraints combined in 361 restraint groups.

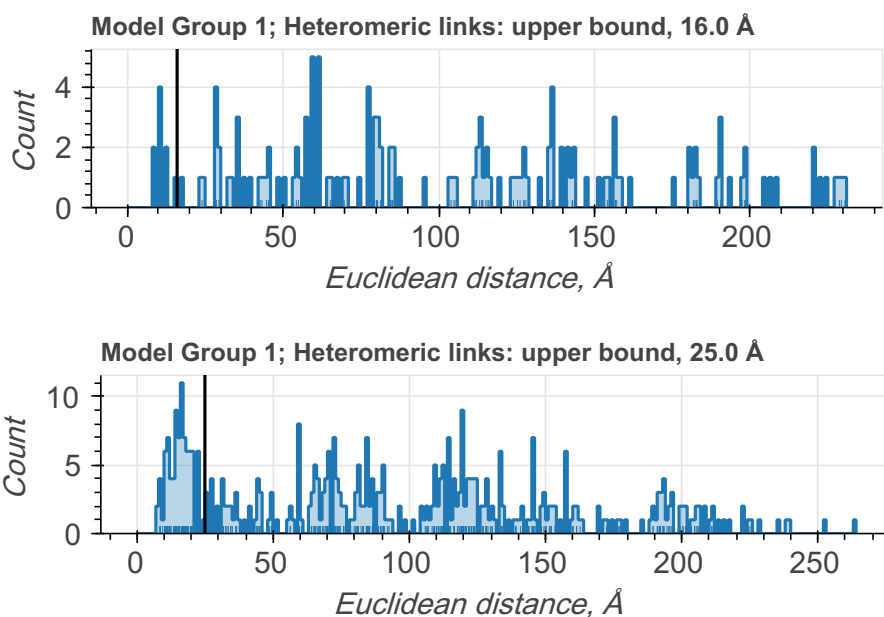
Linker	Residue 1	Atom 1	Residue 2	Atom 2	Restraint type	Distance, Å	Count
ADH	GLU	coarse-grained	GLU	coarse-grained	upper bound	25.0	36
ADH	GLU	CA	GLU	CA	upper bound	25.0	80
ADH	ASP	CA	GLU	CA	upper bound	25.0	64
ADH	ASP	coarse-grained	GLU	coarse-grained	upper bound	25.0	32
BS3	LYS	CA	LYS	CA	upper bound	25.0	168
BS3	LYS	coarse-grained	LYS	coarse-grained	upper bound	25.0	176
BS3	LYS	CA	SER	CA	upper bound	25.0	112
BS3	LYS	coarse-grained	SER	coarse-grained	upper bound	25.0	252
BS3	LYS	CA	MET	CA	upper bound	25.0	16
BS3	ARG	CA	SER	CA	upper bound	25.0	32
BS3	SER	coarse-grained	SER	coarse-grained	upper bound	25.0	36
BS3	GLY	coarse-grained	SER	coarse-grained	upper bound	25.0	8
BS3	ARG	CA	LYS	CA	upper bound	25.0	64
BS3	MET	CA	THR	CA	upper bound	25.0	4
BS3	THR	coarse-grained	VAL	coarse-grained	upper bound	25.0	8
BS3	LEU	coarse-grained	LYS	coarse-grained	upper bound	25.0	52
BS3	MET	CA	SER	CA	upper bound	25.0	16
BS3	SER	coarse-grained	TYR	coarse-grained	upper bound	25.0	12
BS3	GLU	CA	SER	CA	upper bound	25.0	8
BS3	ARG	coarse-grained	LYS	coarse-grained	upper bound	25.0	20
BS3	LEU	coarse-grained	VAL	coarse-grained	upper bound	25.0	8
BS3	ARG	coarse-grained	LEU	coarse-grained	upper bound	25.0	12
BS3	SER	coarse-grained	THR	coarse-grained	upper bound	25.0	12
BS3	LYS	coarse-grained	TYR	coarse-grained	upper bound	25.0	20
BS3	GLN	coarse-grained	THR	coarse-grained	upper bound	25.0	8
BS3	LYS	coarse-grained	THR	coarse-grained	upper bound	25.0	20
BS3	LYS	CA	THR	CA	upper bound	25.0	64
BS3	LYS	CA	TYR	CA	upper bound	25.0	116

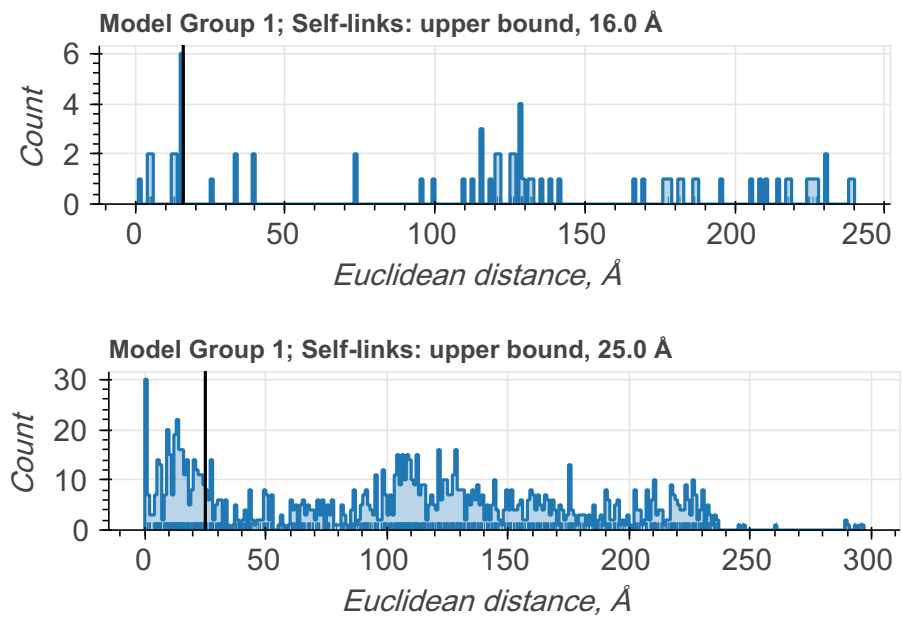
Linker	Residue 1	Atom 1	Residue 2	Atom 2	Restraint type	Distance, Å	Count
BS3	ARG	coarse-grained	GLY	coarse-grained	upper bound	25.0	4
BS3	ARG	CA	GLN	CA	upper bound	25.0	4
BS3	SER	CA	TYR	CA	upper bound	25.0	28
BS3	ALA	CA	ARG	CA	upper bound	25.0	4
BS3	ARG	CA	MET	CA	upper bound	25.0	4
BS3	SER	CA	THR	CA	upper bound	25.0	16
BS3	TYR	CA	TYR	CA	upper bound	25.0	4
BS3	ARG	CA	TYR	CA	upper bound	25.0	4
BS3	LEU	coarse-grained	TYR	coarse-grained	upper bound	25.0	4
BS3	SER	coarse-grained	VAL	coarse-grained	upper bound	25.0	8
BS3	SER	CA	SER	CA	upper bound	25.0	4
BS3	MET	CA	TYR	CA	upper bound	25.0	12
BS3	GLN	CA	LYS	CA	upper bound	25.0	4
BS3	GLU	CA	TYR	CA	upper bound	25.0	4
BS3	GLU	CA	THR	CA	upper bound	25.0	8
BS3	GLU	CA	LYS	CA	upper bound	25.0	20
BS3	ARG	CA	THR	CA	upper bound	25.0	20
BS3	ALA	CA	LYS	CA	upper bound	25.0	4
BS3	ARG	CA	GLU	CA	upper bound	25.0	8
BS3	ARG	coarse-grained	VAL	coarse-grained	upper bound	25.0	12
BS3	LYS	coarse-grained	VAL	coarse-grained	upper bound	25.0	28
BS3	LEU	coarse-grained	SER	coarse-grained	upper bound	25.0	4
BS3	ARG	CA	ARG	CA	upper bound	25.0	8
BS3	MET	coarse-grained	SER	coarse-grained	upper bound	25.0	4
BS3	GLY	coarse-grained	LYS	coarse-grained	upper bound	25.0	8
BS3	ARG	coarse-grained	SER	coarse-grained	upper bound	25.0	8
BS3	TYR	coarse-grained	VAL	coarse-grained	upper bound	25.0	4
BS3	LYS	coarse-grained	MET	coarse-grained	upper bound	25.0	4
BS3	GLY	coarse-grained	THR	coarse-grained	upper bound	25.0	4
BS3	GLU	coarse-grained	VAL	coarse-grained	upper bound	25.0	4
BS3	ARG	coarse-grained	ASN	coarse-grained	upper bound	25.0	4
BS3	ARG	coarse-grained	PRO	coarse-grained	upper bound	25.0	4
BS3	PRO	coarse-grained	VAL	coarse-grained	upper bound	25.0	4
BS3	GLN	coarse-grained	LYS	coarse-grained	upper bound	25.0	4
BS3	ARG	coarse-grained	THR	coarse-grained	upper bound	25.0	4

Linker	Residue 1	Atom 1	Residue 2	Atom 2	Restraint type	Distance, Å	Count
BS3	ARG	coarse-grained	MET	coarse-grained	upper bound	25.0	4
BS3	GLU	coarse-grained	GLY	coarse-grained	upper bound	25.0	4
BS3	MET	coarse-grained	VAL	coarse-grained	upper bound	25.0	4
BS3	LEU	coarse-grained	MET	coarse-grained	upper bound	25.0	4
BS3	GLU	coarse-grained	SER	coarse-grained	upper bound	25.0	4
Other	GLU	coarse-grained	LYS	coarse-grained	upper bound	16.0	96
Other	GLU	CA	LYS	CA	upper bound	16.0	68
Other	GLU	coarse-grained	LEU	coarse-grained	upper bound	16.0	8
Other	ASP	coarse-grained	LYS	coarse-grained	upper bound	16.0	16
Other	LEU	coarse-grained	TYR	coarse-grained	upper bound	16.0	4
Other	ASP	CA	LYS	CA	upper bound	16.0	16
Other	ARG	coarse-grained	ASN	coarse-grained	upper bound	16.0	4
Other	ARG	coarse-grained	ASP	coarse-grained	upper bound	16.0	4

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=361)
1	1	1	1/12913	All	57.06	42.94	361
				Self-links/ Ambiguous	56.02	43.98	266
				Heteromeric links/ Intermolecular	60.00	40.00	95

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.

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.

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