

Integrative Structure Validation Report ?

April 03, 2025 - 08:30 AM PDT

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	9A9N
Structure Title	Complex of the closed conformation of P. furiosus Mre11-Rad50 bound to dsDNA
Structure Authors	Canny, M.D.; Beikzadeh, M.; Kaur, N.; Pendse, R.; Latham, M.P.
Deposited on	2025-03-17

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

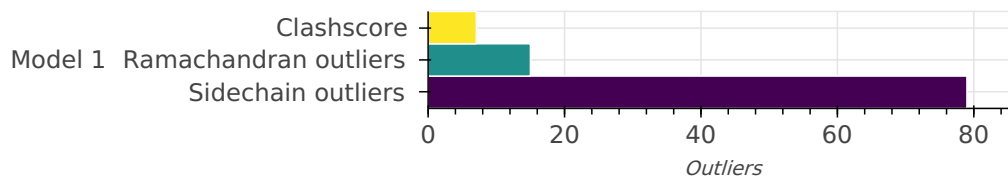
A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the ? symbol.

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 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	1	DNA double-strand break repair Rad50 ATPase	A	192	-	1-192	100.00 / 100.00	Atomic
				D					
		2	DNA double-strand break repair Rad50 ATPase	B	167	-	1-167	100.00 / 100.00	Atomic
				E					
		3	DNA double-strand break repair protein Mre11	C	32	-	1-32	100.00 / 100.00	Atomic
				F					
		4	DNA double-strand break repair protein Mre11	G	333	-	1-333	100.00 / 100.00	Atomic
				H					
		5	DNA (36-MER)	I	36	-	1-36	100.00 / 100.00	Atomic
				J					

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	Other	bmrbig115
2	Integrative model	PDB	9A9j
3	De Novo model	Zenodo	10.5281/zenodo.15065939

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	None	<p>This model was calculated using NMR paramagnetic relaxation enhancement (PRE) data as distance restraints in the 'Guru' and 'multi-body' interface of the HADDOCK v2.4 webserver. The starting structural model of the P. furiosus Closed MR(NBD) complex (PDBIHM id 9A9J) was obtained from previous HADDOCK calculations using LRET measurements as distance restraints to dock a Mre11 dimer and two Rad50 monomers (https://doi.org/10.7554/elife.69579). Two hairpin dsDNA ensembles were used as the starting structural models for the DNA. When HADDOCK performed the docking simulations, one of the dsDNA structures from the ensemble of 20 was randomly selected for each run. During the rigid body energy minimization, 3000 structures were calculated, and the 200 best solutions based on the inter-molecular energy were selected for the semiflexible simulated annealing followed by explicit water refinement.</p>	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	model building	https://rascar.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 2 bond angle outliers in this entry (0.01% of 18762 assessed bonds). A summary is provided below.

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
J	27	DC	C4'-O4'-C1'	5.06	102.11	109.70	1	1
J	30	DG	C4'-O4'-C1'	4.20	103.40	109.70	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	7.08	185

There are 185 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)
G:306:ILE:HB	G:330:THR:HG22	0.86	1	1
H:176:VAL:HG11	H:192:LEU:HG	0.74	1	1
G:176:VAL:HG11	G:192:LEU:HG	0.73	1	1
H:207:ILE:HG22	H:209:LYS:H	0.73	1	1
E:30:LEU:HB2	E:54:VAL:HG11	0.70	1	1
B:70:LYS:HB2	B:72:ARG:HH21	0.70	1	1
A:57:LYS:HB2	A:60:GLU:HB2	0.69	1	1
J:23:DT:H2''	J:24:DC:C5	0.68	1	1
H:63:LYS:O	H:67:LEU:HG	0.67	1	1
D:146:ILE:HD11	D:156:VAL:HG21	0.66	1	1
G:63:LYS:O	G:67:LEU:HG	0.65	1	1
H:15:GLN:HB3	H:21:ARG:HG2	0.64	1	1
J:15:DC:H2''	J:16:DT:H5'	0.63	1	1
G:15:GLN:HB3	G:21:ARG:HG2	0.63	1	1
D:131:ILE:HG13	D:160:VAL:HA	0.61	1	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
B:30:LEU:HB2	B:54:VAL:HG11	0.60	1	1
B:45:THR:HB	B:48:LYS:HB3	0.59	1	1
A:146:ILE:HD11	A:156:VAL:HG21	0.59	1	1
G:207:ILE:HG22	G:209:LYS:H	0.59	1	1
G:7:ALA:HB2	G:47:ALA:HB3	0.59	1	1
D:165:LYS:HD3	F:16:GLY:HA3	0.58	1	1
B:125:MET:HA	B:129:LEU:HD13	0.58	1	1
E:109:PRO:C	E:111:PRO:HD3	0.58	1	1
B:73:PRO:HG2	B:76:PHE:HB2	0.57	1	1
A:131:ILE:HG13	A:160:VAL:HA	0.57	1	1
D:128:PRO:HB2	D:131:ILE:HD13	0.57	1	1
B:49:TYR:CE1	B:67:TRP:HB2	0.57	1	1
G:252:ASN:HD22	G:267:GLU:HB2	0.56	1	1
G:183:ARG:HH21	G:207:ILE:HG21	0.56	1	1
A:67:ARG:HH22	J:26:DA:H3'	0.56	1	1
G:57:SER:HA	H:55:ARG:HG2	0.56	1	1
J:28:DG:H1'	J:29:DT:H5'	0.56	1	1
H:183:ARG:HH21	H:207:ILE:HG21	0.55	1	1
G:281:SER:O	G:285:ILE:HG12	0.55	1	1
D:7:THR:HB	D:72:ASP:HB3	0.55	1	1
A:132:PHE:HA	A:136:ILE:HD12	0.55	1	1
A:183:ARG:O	A:187:TYR:HB2	0.55	1	1
B:109:PRO:C	B:111:PRO:HD3	0.55	1	1
D:58:LYS:HE2	D:93:SER:HB3	0.54	1	1
H:7:ALA:HB2	H:47:ALA:HB3	0.54	1	1
H:306:ILE:HB	H:330:THR:HG22	0.54	1	1
G:143:MET:H	G:172:LEU:HD23	0.54	1	1
H:143:MET:H	H:172:LEU:HD23	0.54	1	1
D:183:ARG:O	D:187:TYR:HB2	0.54	1	1
E:73:PRO:HG2	E:76:PHE:HB2	0.54	1	1
D:71:ILE:HD12	D:88:PHE:HE2	0.53	1	1
J:27:DC:H2''	J:28:DG:H5'	0.53	1	1
E:45:THR:HG21	E:49:TYR:HD2	0.53	1	1
A:74:ILE:HG12	A:83:ARG:HG3	0.53	1	1
B:122:ILE:HG23	B:147:ALA:HB2	0.53	1	1
H:281:SER:O	H:285:ILE:HG12	0.53	1	1
I:28:DG:H2''	I:29:DT:H72	0.53	1	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
B:49:TYR:CD1	B:65:VAL:HB	0.52	1	1
J:23:DT:H2''	J:24:DC:C6	0.52	1	1
D:184:ILE:HG12	E:4:LEU:HB3	0.52	1	1
B:83:ILE:HG21	B:111:PRO:HD2	0.52	1	1
D:168:THR:O	D:172:LYS:HG3	0.51	1	1
H:298:LYS:H	H:298:LYS:HD3	0.51	1	1
E:50:SER:HB2	H:330:THR:H	0.51	1	1
E:86:GLY:O	E:90:ARG:HG2	0.51	1	1
D:74:ILE:HG12	D:83:ARG:HG3	0.51	1	1
D:58:LYS:HA	D:61:PHE:CZ	0.51	1	1
E:125:MET:HA	E:129:LEU:HD13	0.51	1	1
G:55:ARG:HG2	H:57:SER:HA	0.51	1	1
A:128:PRO:HB2	A:131:ILE:HD13	0.50	1	1
A:71:ILE:HD12	A:88:PHE:HE2	0.50	1	1
D:136:ILE:HG12	E:101:ILE:HG21	0.50	1	1
E:110:THR:HA	E:113:LEU:HD12	0.50	1	1
D:84:ILE:HG12	D:100:MET:HG3	0.49	1	1
A:27:LEU:HA	B:137:LEU:O	0.49	1	1
B:45:THR:HG21	B:49:TYR:HD2	0.49	1	1
G:70:ILE:HB	G:71:PRO:HD3	0.49	1	1
I:28:DG:C2'	I:29:DT:H72	0.49	1	1
G:276:VAL:HG21	G:292:LEU:HD21	0.49	1	1
A:7:THR:HB	A:72:ASP:HB3	0.48	1	1
D:132:PHE:HA	D:136:ILE:HD12	0.48	1	1
G:180:SER:HB3	G:185:GLU:HB2	0.48	1	1
H:116:ASN:HD21	H:119:LEU:HD12	0.48	1	1
H:70:ILE:HB	H:71:PRO:HD3	0.48	1	1
E:83:ILE:HG21	E:111:PRO:HD2	0.48	1	1
D:27:LEU:HA	E:137:LEU:O	0.48	1	1
E:30:LEU:H	E:30:LEU:HD13	0.48	1	1
G:228:ARG:NE	G:233:ASP:HB3	0.48	1	1
E:70:LYS:HB2	E:72:ARG:NH2	0.48	1	1
I:11:DG:H2''	I:12:DA:C8	0.48	1	1
B:154:ILE:HD11	B:161:SER:HB3	0.47	1	1
D:34:SER:HA	E:156:LEU:HB2	0.47	1	1
G:138:LEU:HD21	G:169:ILE:HD12	0.47	1	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
G:116:ASN:HD21	G:119:LEU:HD12	0.47	1	1
G:315:THR:HA	G:318:LYS:NZ	0.47	1	1
H:124:LEU:HD22	H:161:LEU:HD22	0.47	1	1
H:305:ASN:HB3	H:331:TRP:HE1	0.47	1	1
H:291:ARG:HA	H:291:ARG:HE	0.47	1	1
B:86:GLY:O	B:90:ARG:HG2	0.47	1	1
E:50:SER:CB	H:329:ASP:HA	0.47	1	1
B:140:HIS:HB2	E:114:ASP:HB3	0.47	1	1
D:27:LEU:HD12	E:137:LEU:HB2	0.47	1	1
D:28:ILE:HB	E:138:VAL:HG13	0.46	1	1
G:291:ARG:HA	G:291:ARG:HE	0.46	1	1
G:11:LEU:H	G:51:PHE:HA	0.46	1	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	1432	1320	97	15

There are 15 unique backbone outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	12	ARG	1
A	35	GLY	1
A	162	ASN	1
A	190	SER	1
B	58	GLU	1
B	69	GLY	1
D	12	ARG	1
D	162	ASN	1
D	190	SER	1
E	58	GLU	1
G	136	LYS	1
G	206	HIS	1
H	136	LYS	1
H	206	HIS	1
H	268	ILE	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	1270	1079	112	79

There are 79 unique sidechain outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	51	LEU	1
A	58	LYS	1
A	60	GLU	1
A	61	PHE	1
A	76	GLU	1
A	162	ASN	1
A	176	LEU	1
B	8	LYS	1
B	30	LEU	1
B	35	GLU	1
B	39	GLU	1
B	60	LYS	1
B	120	LYS	1
B	122	ILE	1
B	135	VAL	1
B	163	VAL	1
C	6	GLU	1
C	12	ILE	1
C	15	LEU	1
C	24	ASP	1
C	29	LEU	1
D	20	GLU	1
D	27	LEU	1
D	51	LEU	1
D	58	LYS	1
D	61	PHE	1
D	68	ASP	1
D	76	GLU	1
D	176	LEU	1
E	30	LEU	1
E	50	SER	1
E	120	LYS	1

Chain	Res	Type	Models (Total)
E	135	VAL	1
E	163	VAL	1
F	6	GLU	1
F	12	ILE	1
F	15	LEU	1
F	18	LYS	1
F	21	ASP	1
F	24	ASP	1
G	21	ARG	1
G	87	ARG	1
G	147	SER	1
G	174	GLN	1
G	178	GLU	1
G	228	ARG	1
G	240	TRP	1
G	248	ARG	1
G	260	ASP	1
G	267	GLU	1
G	268	ILE	1
G	269	LYS	1
G	283	GLU	1
G	284	GLU	1
G	287	LYS	1
G	298	LYS	1
G	326	LEU	1
G	332	ARG	1
H	21	ARG	1
H	54	SER	1
H	63	LYS	1
H	87	ARG	1
H	115	GLU	1
H	123	ARG	1
H	174	GLN	1
H	178	GLU	1
H	228	ARG	1
H	233	ASP	1
H	248	ARG	1

Chain	Res	Type	Models (Total)
H	268	ILE	1
H	269	LYS	1
H	283	GLU	1
H	284	GLU	1
H	287	LYS	1
H	298	LYS	1
H	303	ARG	1
H	324	GLU	1
H	326	LEU	1
H	331	TRP	1

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.