

Integrative Structure Validation Report

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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	9A9O
Structure Title	Complex of the partially open 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	2025-03-20

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

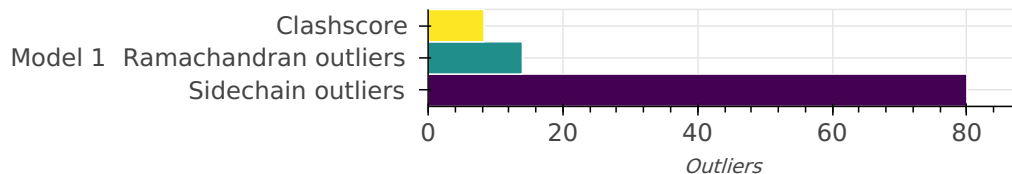
A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the  symbol.

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	9A9K
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 no bond angle outliers.

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	8.30	217

There are 217 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)
I:35:DA:H5''	I:36:DC:H5'	0.88	1	1
G:306:ILE:HB	G:330:THR:HG22	0.87	1	1
J:35:DA:H5''	J:36:DC:H5'	0.82	1	1
G:235:GLU:HG3	G:272:PRO:HA	0.80	1	1
A:53:ILE:HD12	A:56:ILE:HD12	0.77	1	1
E:151:VAL:H	E:167:SER:HB2	0.76	1	1
G:176:VAL:HG11	G:192:LEU:HG	0.69	1	1
B:125:MET:HA	B:129:LEU:HD13	0.68	1	1
H:302:VAL:HG23	H:326:LEU:HG	0.68	1	1
H:176:VAL:HG11	H:192:LEU:HG	0.68	1	1
H:63:LYS:O	H:67:LEU:HG	0.66	1	1
J:7:DC:H2'	J:8:DG:C8	0.66	1	1
I:7:DC:H2'	I:8:DG:C8	0.66	1	1
G:63:LYS:O	G:67:LEU:HG	0.66	1	1
H:19:PRO:HD3	J:35:DA:C2	0.65	1	1
B:114:ASP:HA	E:114:ASP:HB2	0.65	1	1
E:30:LEU:H	E:30:LEU:HD13	0.63	1	1
D:131:ILE:HG13	D:160:VAL:HA	0.63	1	1
G:7:ALA:HB2	G:47:ALA:HB3	0.62	1	1
A:131:ILE:HG13	A:160:VAL:HA	0.61	1	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
H:269:LYS:HA	H:269:LYS:HE2	0.61	1	1
B:154:ILE:HD11	B:161:SER:HB3	0.61	1	1
E:125:MET:HA	E:129:LEU:HD13	0.60	1	1
E:83:ILE:HG21	E:111:PRO:HD2	0.60	1	1
A:25:ILE:HG23	B:137:LEU:HD23	0.58	1	1
H:7:ALA:HB2	H:47:ALA:HB3	0.58	1	1
G:57:SER:HA	H:55:ARG:HG2	0.57	1	1
G:18:LYS:HB2	G:21:ARG:HB3	0.57	1	1
I:1:DC:H1'	I:2:DA:N7	0.57	1	1
B:45:THR:HB	B:48:LYS:HB3	0.56	1	1
E:110:THR:N	E:111:PRO:HD3	0.56	1	1
G:90:ARG:HG2	J:2:DA:H4'	0.56	1	1
A:128:PRO:HB2	A:131:ILE:HD13	0.56	1	1
D:7:THR:HB	D:72:ASP:HB3	0.56	1	1
A:47:LEU:HD23	A:84:ILE:HD12	0.55	1	1
B:83:ILE:HG21	B:111:PRO:HD2	0.55	1	1
B:110:THR:N	B:111:PRO:HD3	0.55	1	1
G:19:PRO:HD3	I:35:DA:C2	0.55	1	1
D:71:ILE:HD12	D:88:PHE:HE2	0.54	1	1
J:1:DC:H1'	J:2:DA:N7	0.54	1	1
A:74:ILE:HG12	A:83:ARG:HG3	0.54	1	1
G:124:LEU:HD21	G:130:LEU:HB2	0.54	1	1
A:183:ARG:O	A:187:TYR:HB2	0.54	1	1
G:281:SER:O	G:285:ILE:HG12	0.54	1	1
D:183:ARG:O	D:187:TYR:HB2	0.54	1	1
D:84:ILE:HG12	D:100:MET:HG3	0.54	1	1
B:151:VAL:H	B:167:SER:HB2	0.53	1	1
D:47:LEU:HD23	D:84:ILE:HD12	0.53	1	1
H:302:VAL:CG2	H:326:LEU:HG	0.53	1	1
J:1:DC:H4'	J:2:DA:O5'	0.53	1	1
A:25:ILE:HD12	B:130:LYS:HE3	0.52	1	1
E:86:GLY:O	E:90:ARG:HG2	0.52	1	1
B:86:GLY:O	B:90:ARG:HG2	0.52	1	1
D:128:PRO:HB2	D:131:ILE:HD13	0.52	1	1
A:84:ILE:HG12	A:100:MET:HG3	0.52	1	1
A:168:THR:O	A:172:LYS:HG3	0.52	1	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
I:1:DC:H4'	I:2:DA:O5'	0.52	1	1
H:292:LEU:HG	H:296:ILE:HD11	0.51	1	1
G:143:MET:H	G:172:LEU:HD23	0.51	1	1
G:292:LEU:HG	G:296:ILE:HD11	0.51	1	1
D:74:ILE:HG12	D:83:ARG:HG3	0.51	1	1
G:308:TRP:CE2	G:311:PRO:HA	0.51	1	1
H:146:MET:HA	H:146:MET:HE2	0.51	1	1
A:7:THR:HB	A:72:ASP:HB3	0.51	1	1
D:25:ILE:HD12	E:130:LYS:HE3	0.51	1	1
H:281:SER:O	H:285:ILE:HG12	0.51	1	1
D:165:LYS:HD3	F:16:GLY:HA3	0.50	1	1
B:30:LEU:H	B:30:LEU:HD13	0.50	1	1
E:8:LYS:O	E:12:GLU:HG2	0.50	1	1
G:5:HIS:CE1	G:223:PRO:HD3	0.50	1	1
E:125:MET:HE1	E:144:LEU:HD22	0.50	1	1
H:306:ILE:HB	H:330:THR:HG22	0.50	1	1
G:70:ILE:HB	G:71:PRO:HD3	0.50	1	1
A:132:PHE:HA	A:136:ILE:HD12	0.50	1	1
H:82:GLU:HG2	H:144:LYS:HB2	0.50	1	1
G:146:MET:HA	G:146:MET:HE2	0.49	1	1
B:8:LYS:O	B:12:GLU:HG2	0.49	1	1
A:165:LYS:HD3	C:16:GLY:HA3	0.49	1	1
H:231:PHE:HE2	H:325:TYR:HE2	0.49	1	1
H:124:LEU:HD21	H:130:LEU:HB2	0.49	1	1
B:110:THR:HA	B:113:LEU:HD12	0.49	1	1
H:70:ILE:HB	H:71:PRO:HD3	0.49	1	1
B:23:ALA:O	B:27:GLU:HB2	0.49	1	1
H:202:TYR:HB2	H:220:VAL:HA	0.49	1	1
G:291:ARG:HA	G:291:ARG:HE	0.48	1	1
I:1:DC:H1'	I:2:DA:C8	0.48	1	1
D:45:VAL:O	D:49:TRP:HB2	0.48	1	1
A:71:ILE:HD12	A:88:PHE:HE2	0.48	1	1
G:302:VAL:HG23	G:326:LEU:HG	0.48	1	1
B:49:TYR:CD1	B:65:VAL:HB	0.48	1	1
E:42:ALA:HB2	E:50:SER:HA	0.48	1	1
B:49:TYR:CE1	B:67:TRP:HB2	0.48	1	1
G:55:ARG:HG2	H:57:SER:HA	0.48	1	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
E:110:THR:HA	E:113:LEU:HD12	0.48	1	1
H:15:GLN:HB3	H:21:ARG:HG2	0.48	1	1
G:124:LEU:HD22	G:161:LEU:HD22	0.47	1	1
H:83:GLY:O	H:87:ARG:HB3	0.47	1	1
E:70:LYS:HA	E:70:LYS:HD3	0.46	1	1
A:45:VAL:O	A:49:TRP:HB2	0.46	1	1
H:90:ARG:HG2	I:2:DA:H4'	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	1324	94	14

There are 14 unique backbone outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	12	ARG	1
A	162	ASN	1
A	190	SER	1
B	58	GLU	1
D	12	ARG	1
D	136	ILE	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	1077	113	80

There are 80 unique sidechain outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	20	GLU	1
A	51	LEU	1
A	53	ILE	1
A	58	LYS	1
A	61	PHE	1
A	76	GLU	1
A	120	SER	1
A	176	LEU	1
B	26	ARG	1
B	30	LEU	1
B	36	LEU	1
B	44	PHE	1
B	54	VAL	1
B	60	LYS	1
B	120	LYS	1
B	135	VAL	1
B	141	ASP	1
B	163	VAL	1
C	6	GLU	1
C	12	ILE	1
C	15	LEU	1
C	21	ASP	1
C	24	ASP	1
C	29	LEU	1
D	15	SER	1
D	51	LEU	1
D	58	LYS	1
D	61	PHE	1
D	68	ASP	1
D	76	GLU	1
D	120	SER	1
D	176	LEU	1
E	26	ARG	1
E	30	LEU	1
E	44	PHE	1
E	54	VAL	1

Chain	Res	Type	Models (Total)
E	60	LYS	1
E	114	ASP	1
E	116	GLU	1
E	135	VAL	1
F	6	GLU	1
F	12	ILE	1
F	18	LYS	1
F	21	ASP	1
F	24	ASP	1
G	21	ARG	1
G	87	ARG	1
G	146	MET	1
G	147	SER	1
G	174	GLN	1
G	178	GLU	1
G	228	ARG	1
G	248	ARG	1
G	260	ASP	1
G	267	GLU	1
G	268	ILE	1
G	269	LYS	1
G	271	ARG	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	87	ARG	1
H	146	MET	1
H	174	GLN	1
H	178	GLU	1
H	228	ARG	1
H	248	ARG	1
H	260	ASP	1
H	269	LYS	1

Chain	Res	Type	Models (Total)
H	284	GLU	1
H	287	LYS	1
H	298	LYS	1
H	302	VAL	1
H	303	ARG	1
H	326	LEU	1
H	330	THR	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.

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