

# 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	9A9J
Structure Title	Complex of the closed conformation of P. furiosus Mre11-Rad50
Structure Authors	Canny, M.D.; Latham, M.P.
Deposited on	2025-02-19

*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](mailto:helpdesk@pdb-ihm.org)*

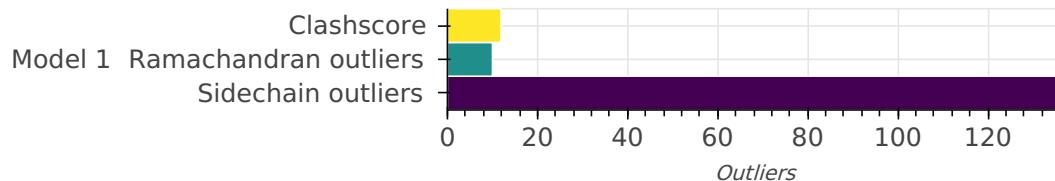
*A user guide is available at [https://pdb-ihm.org/validation\\_help.html](https://pdb-ihm.org/validation_help.html) with specific help available everywhere you see the ? symbol.*

*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 7 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					

## Datasets used for modeling ?

There are 7 unique datasets used to build the models in this entry.

ID	Dataset type	Database name	Data access code
1	Ensemble FRET data	Zenodo	<a href="https://zenodo.org/record/14990529">10.5281/zenodo.14990529</a>
2	Experimental model	PDB	<a href="https://www.rcsb.org/structure/3QKU">3QKU</a>
3	Experimental model	PDB	<a href="https://www.rcsb.org/structure/3DSC">3DSC</a>
4	Predicted contacts	Not available	Not available
5	Experimental model	PDB	<a href="https://www.rcsb.org/structure/3AV0">3AV0</a>
6	Experimental model	PDB	<a href="https://www.rcsb.org/structure/6S6V">6S6V</a>
7	Experimental model	PDB	<a href="https://www.rcsb.org/structure/3QG5">3QG5</a>

## 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
				<p>Molecular docking of the MRNBD complex was done in the GURU interface on the HADDOCK 2.4 Webserver using experimental luminescence resonance energy transfer (LRET) data as distance restraints. The PDB inputs were 3DSC (Pf Mre11 dimer) and two monomers of 3QKU (Pf Rad50NBD). Except for increasing the number of structures for rigid body docking (it0) to 3000, all settings used were default. The three linkers attaching the Pf Mre11 capping domain to the nuclease domain were allowed to be fully flexible.</p> <p>C2 symmetry was enforced between the two Rad50NBD monomers and</p>			

Step number 1	Protocol ID 1	Method name None	Method type None	Method description between the two monomers of the Mre11 dimer. HADDOCK Mre11 to Rad50 active ambiguous interaction restraints (AIRs) were based on M. jannaschii (3AV0) and E. coli (6S6V) ATP-gamma-S-bound MR structures. Passive AIRs were automatically defined by HADDOCK based on these active AIRs. Two extra passive AIRs were included on the 'back side' of the Mre11 capping domain to allow for the extended structure seen in ATP- free T. maritima MR (PDB: 3QG5). HADDOCK runs had 50% random exclusion of AIRs in each structure calculation. The experimentally measured LRET distances were input as unambiguous restraints and defined as the Cbeta-Cbeta distance between the LRET-labeled residues, +/- 5 A, or, for distance restraints greater than 75 A, +/-7 A.	Number of computed models None	Multi state modeling False	Multi scale modeling False

*There is 1 software package reported in this entry.*

ID	Software name	Software version	Software classification	Software location
1	<a href="#">HADDOCK</a>	2.40	model building	<a href="https://rascar.science.uu.nl/haddock2.4/">https://rascar.science.uu.nl/haddock2.4/</a>

## Data quality ?

### Predicted contacts

Validation for this section is under development.

### Ensemble FRET

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 1 bond angle outliers in this entry (0.01% of 16238 assessed bonds). A summary is provided below.

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
D	162	ASN	CA-CB-CG	4.07	116.67	112.60	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	11.90	284

There are 284 clashes. The table below contains the detailed list of all clashes based on a MolProbity analysis. Bad clashes are  $\geq 0.4$  Angstrom. The output is limited to 100 rows.

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:165:LYS:HD3	C:16:GLY:HA3	0.81	1	1
G:2:LYS:HE2	G:39:GLU:HG3	0.73	1	1
G:306:ILE:HB	G:330:THR:HG22	0.73	1	1
H:2:LYS:HE2	H:39:GLU:HG3	0.73	1	1
A:45:VAL:HA	A:51:LEU:HD21	0.72	1	1
A:2:LYS:NZ	A:4:GLU:HG2	0.69	1	1
G:15:GLN:HB3	G:21:ARG:HG2	0.69	1	1
H:84:ASN:HA	H:87:ARG:HG2	0.69	1	1
D:2:LYS:NZ	D:4:GLU:HG2	0.68	1	1
G:7:ALA:HB2	G:47:ALA:HB3	0.68	1	1
G:84:ASN:HA	G:87:ARG:HG2	0.68	1	1
E:70:LYS:HB2	E:72:ARG:HH21	0.67	1	1
E:102:SER:HB3	E:133:PRO:HG2	0.67	1	1
B:30:LEU:HB2	B:54:VAL:HG11	0.66	1	1
B:50:SER:HB3	H:329:ASP:HA	0.65	1	1
A:7:THR:HB	A:72:ASP:HB3	0.64	1	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
G:315:THR:HA	G:318:LYS:NZ	0.64	1	1
D:57:LYS:HB2	D:60:GLU:HB2	0.64	1	1
E:49:TYR:CE1	E:67:TRP:HB2	0.64	1	1
D:165:LYS:HD3	F:16:GLY:CA	0.64	1	1
D:172:LYS:HE3	F:23:PHE:HZ	0.63	1	1
H:7:ALA:HB2	H:47:ALA:HB3	0.63	1	1
B:109:PRO:C	B:111:PRO:HD3	0.62	1	1
E:154:ILE:HD11	E:161:SER:HB3	0.62	1	1
E:45:THR:HB	E:48:LYS:HB3	0.61	1	1
C:6:GLU:O	C:10:LYS:HE3	0.60	1	1
D:62:THR:HB	D:90:LYS:HE3	0.60	1	1
D:146:ILE:HD11	D:156:VAL:HG21	0.60	1	1
G:183:ARG:HH21	G:207:ILE:HG21	0.60	1	1
H:48:GLY:HA2	H:81:ILE:O	0.60	1	1
D:45:VAL:HA	D:51:LEU:HD21	0.60	1	1
H:63:LYS:O	H:67:LEU:HG	0.60	1	1
D:150:ASP:OD2	E:62:ARG:HA	0.59	1	1
A:28:ILE:HB	B:138:VAL:HG13	0.59	1	1
A:84:ILE:HG12	A:100:MET:HG3	0.59	1	1
A:146:ILE:HD11	A:156:VAL:HG21	0.58	1	1
B:42:ALA:HB2	B:50:SER:HA	0.58	1	1
G:48:GLY:HA2	G:81:ILE:O	0.58	1	1
B:45:THR:HG21	B:49:TYR:HD2	0.58	1	1
B:125:MET:HA	B:129:LEU:HD13	0.58	1	1
G:63:LYS:O	G:67:LEU:HG	0.58	1	1
D:153:ARG:HB3	E:61:VAL:HB	0.58	1	1
D:172:LYS:HE3	F:23:PHE:CZ	0.57	1	1
B:102:SER:HB3	B:133:PRO:HG2	0.57	1	1
H:237:ARG:HB3	H:248:ARG:HB3	0.57	1	1
A:64:VAL:HG21	E:72:ARG:NH1	0.57	1	1
H:176:VAL:HG11	H:192:LEU:HG	0.56	1	1
A:153:ARG:HB3	B:61:VAL:HB	0.56	1	1
B:19:LYS:HA	B:22:LYS:HD3	0.56	1	1
E:109:PRO:C	E:111:PRO:HD3	0.56	1	1
D:132:PHE:HA	D:136:ILE:HD12	0.56	1	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:71:ILE:HD12	A:88:PHE:HE1	0.56	1	1
A:131:ILE:HG13	A:160:VAL:HA	0.56	1	1
D:71:ILE:HD12	D:88:PHE:HE1	0.56	1	1
A:86:ARG:HD3	A:98:HIS:ND1	0.56	1	1
D:58:LYS:HA	D:61:PHE:CE2	0.55	1	1
D:84:ILE:HG12	D:100:MET:HG3	0.55	1	1
B:8:LYS:O	B:12:GLU:HG2	0.55	1	1
B:50:SER:CB	H:329:ASP:HA	0.55	1	1
D:128:PRO:HB2	D:131:ILE:HD13	0.54	1	1
D:101:LYS:HD3	D:108:TRP:HB3	0.54	1	1
G:176:VAL:HA	G:190:ILE:O	0.54	1	1
D:150:ASP:OD2	E:62:ARG:HD2	0.54	1	1
G:205:GLY:O	G:206:HIS:HB2	0.54	1	1
G:276:VAL:HG21	G:292:LEU:HD21	0.54	1	1
D:165:LYS:HD3	F:16:GLY:HA3	0.54	1	1
G:315:THR:HA	G:318:LYS:HZ3	0.54	1	1
C:17:GLU:HB2	C:19:ASP:OD1	0.54	1	1
G:281:SER:O	G:285:ILE:HG12	0.54	1	1
D:162:ASN:ND2	D:165:LYS:HB2	0.53	1	1
A:168:THR:O	A:172:LYS:HG3	0.53	1	1
A:150:ASP:OD2	B:62:ARG:HD2	0.53	1	1
H:15:GLN:HB3	H:21:ARG:HG2	0.53	1	1
B:118:ARG:HD2	B:143:GLU:OE1	0.53	1	1
H:18:LYS:O	H:21:ARG:HB3	0.53	1	1
A:151:GLU:OE2	B:60:LYS:HE3	0.53	1	1
A:140:GLN:HE21	B:108:GLU:HG3	0.53	1	1
G:3:PHE:HA	G:41:VAL:HB	0.53	1	1
G:228:ARG:HE	G:233:ASP:HB3	0.53	1	1
H:183:ARG:HH21	H:207:ILE:HG21	0.53	1	1
H:39:GLU:HG2	H:257:ILE:HD12	0.52	1	1
B:86:GLY:O	B:90:ARG:HG2	0.52	1	1
E:83:ILE:HG21	E:111:PRO:HD2	0.52	1	1
E:86:GLY:O	E:90:ARG:HG2	0.52	1	1
H:315:THR:HA	H:318:LYS:NZ	0.52	1	1
F:6:GLU:O	F:10:LYS:HE3	0.52	1	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
G:207:ILE:HG22	G:209:LYS:H	0.52	1	1
G:237:ARG:HB3	G:248:ARG:HB3	0.52	1	1
H:45:LEU:HD23	H:79:PHE:HB2	0.52	1	1
A:7:THR:HG23	A:18:VAL:HG22	0.52	1	1
H:310:LYS:HD3	H:311:PRO:HD2	0.52	1	1
A:2:LYS:HZ2	A:4:GLU:HG2	0.52	1	1
D:165:LYS:HD3	F:16:GLY:HA2	0.51	1	1
G:235:GLU:CD	G:272:PRO:HA	0.51	1	1
G:176:VAL:HG11	G:192:LEU:HG	0.51	1	1
E:30:LEU:HB2	E:54:VAL:HG11	0.51	1	1
G:45:LEU:HD23	G:79:PHE:HB2	0.51	1	1
G:306:ILE:HB	G:330:THR:CG2	0.51	1	1
H:83:GLY:O	H:145:TYR:HB3	0.51	1	1
H:176:VAL:HA	H:190:ILE:O	0.51	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	102	10

There are 10 unique backbone outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	35	GLY	1
A	148	GLU	1
D	35	GLY	1
E	69	GLY	1
G	136	LYS	1
G	206	HIS	1
H	136	LYS	1
H	177	ARG	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	964	170	136

*There are 136 unique sidechain outliers. Detailed list of outliers are tabulated below. The output is limited to 100 rows.*

Chain	Res	Type	Models (Total)
A	13	SER	1
A	15	SER	1
A	19	VAL	1
A	27	LEU	1
A	51	LEU	1
A	57	LYS	1
A	58	LYS	1
A	61	PHE	1
A	68	ASP	1
A	76	GLU	1
A	93	SER	1
A	94	SER	1
A	116	SER	1
A	120	SER	1
A	149	SER	1
A	162	ASN	1
A	163	LEU	1
A	168	THR	1
A	176	LEU	1
A	178	LYS	1
B	30	LEU	1
B	31	SER	1
B	39	GLU	1
B	50	SER	1
B	51	GLU	1
B	60	LYS	1
B	75	THR	1
B	110	THR	1
B	120	LYS	1
B	122	ILE	1
B	123	THR	1

Chain	Res	Type	Models (Total)
B	135	VAL	1
B	145	LYS	1
B	149	ASP	1
B	155	SER	1
B	163	VAL	1
C	12	ILE	1
C	14	ILE	1
C	15	LEU	1
C	18	LYS	1
C	21	ASP	1
C	24	ASP	1
C	29	LEU	1
D	15	SER	1
D	17	THR	1
D	19	VAL	1
D	27	LEU	1
D	51	LEU	1
D	57	LYS	1
D	58	LYS	1
D	60	GLU	1
D	68	ASP	1
D	76	GLU	1
D	93	SER	1
D	116	SER	1
D	120	SER	1
D	162	ASN	1
D	164	ASP	1
D	168	THR	1
D	171	LYS	1
D	178	LYS	1
D	181	ASN	1
E	8	LYS	1
E	30	LEU	1
E	39	GLU	1
E	60	LYS	1

Chain	Res	Type	Models (Total)
E	75	THR	1
E	82	ARG	1
E	115	GLU	1
E	117	ARG	1
E	120	LYS	1
E	122	ILE	1
E	123	THR	1
E	135	VAL	1
E	145	LYS	1
E	149	ASP	1
E	163	VAL	1
E	167	SER	1
F	1	SER	1
F	12	ILE	1
F	14	ILE	1
F	15	LEU	1
F	19	ASP	1
F	24	ASP	1
F	29	LEU	1
G	6	LEU	1
G	14	GLU	1
G	21	ARG	1
G	54	SER	1
G	87	ARG	1
G	147	SER	1
G	165	THR	1
G	174	GLN	1
G	210	ARG	1
G	227	GLU	1
G	228	ARG	1
G	233	ASP	1
G	240	TRP	1
G	248	ARG	1
G	253	LYS	1

### Fit of model to data used for modeling ?

#### Predicted contacts

Validation for this section is under development.

#### Ensemble FRET

Validation for this section is under development.

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### Fit of model to data used for validation ?

Validation for this section is under development.

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#### *Acknowledgments*

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