

Summary of integrative structure determination of Complex of the partially open conformation of P. furiosus Mre11-Rad50 bound to dsDNA (PDB ID: 9A9O)

1. Model Composition	
Entry composition	<ul style="list-style-type: none"> - DNA double-strand break repair Rad50 ATPase: chain(s) A, D (192 residues) - DNA double-strand break repair Rad50 ATPase: chain(s) B, E (167 residues) - DNA double-strand break repair protein Mre11: chain(s) C, F (32 residues) - DNA double-strand break repair protein Mre11: chain(s) G, H (333 residues) - DNA (36-MER): chain(s) I, J (36 residues)
Datasets used for modeling	<ul style="list-style-type: none"> - NMR data, Other: bmrbig115 - Integrative model, PDB: 9A9K - De Novo model, Zenodo: 10.5281/zenodo.15065939
2. Representation	
Number of representations	1
Scale	Atomic
Number of <i>rigid</i> and <i>flexible</i> segments	0, 10
3. Restraints	
Physical principles	Information about physical principles was not provided
	<ul style="list-style-type: none"> - 6 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 19.0-47.1 - 8 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 18.5-45.8 - 6 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 17.1-42.3 - 4 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 19.5-48.3 - 12 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 18.7-46.3 - 2 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 16.4-40.5 - 2 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 16.5-41.0 - 2 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 18.3-45.3 - 4 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 18.4-45.5 - 10 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 18.0-44.5 - 2 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 19.4-48.2 - 6 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 19.0-47.0

[Experimental data](#)

- 8 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 18.6-46.0
 - 4 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 19.4-48.1
 - 2 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 16.6-41.2
 - 2 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 17.7-43.9
 - 2 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 18.8-46.5
 - 4 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 19.8-49.0
 - 2 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 17.4-43.2
 - 2 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 18.0-44.7
 - 2 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 17.2-42.7
 - 4 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 17.0-42.1
 - 2 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 18.1-44.8
 - 2 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 19.3-47.8
 - 6 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 18.9-46.8
 - 2 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 17.3-42.8
 - 6 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 17.7-44.0
 - 2 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 17.9-44.3
 - 2 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 19.6-48.5
 - 2 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 17.5-43.3
 - 2 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 17.7-43.8
 - 2 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 18.5-46.0
 - 2 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 16.8-41.6
 - 2 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 19.1-47.3
 - 2 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 19.6-48.6
 - 2 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 18.4-45.6
 - 4 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 17.4-43.0
 - 4 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 18.8-46.7
 - 4 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 16.5-40.8
 - 4 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 17.8-44.0
 - 4 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 17.8-44.1
 - 4 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 19.7-48.8
 - 4 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 17.6-43.7
 - 6 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 17.8-44.2

	<ul style="list-style-type: none"> - 6 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 16.3-40.5 - 4 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 16.9-42.0 - 4 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 20.1-49.8 - 6 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 16.1-39.9 - 4 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 19.2-47.5 - 4 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 20.2-50.0 - 2 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 19.9-49.3 - 4 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 17.2-42.6 - 2 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 16.3-40.4 - 2 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 17.4-43.1 - 2 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 15.9-39.5 - 4 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 17.2-42.5 - 2 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 16.9-41.8 - 2 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 16.1-39.8 - 2 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 15.5-38.5 - 2 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 15.7-39.0 - 2 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 18.6-46.1 - 2 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 17.1-42.5 - 2 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 18.2-45.2
4. Validation	
<i>Number of ensembles</i>	0
<i>Number of models in ensembles</i>	Not applicable
<i>Number of deposited models</i>	1
<i>Model precision (uncertainty of models)</i>	Not available
<i>Data quality</i>	Data quality has not been assessed
<i>Model quality: assessment of atomic segments</i>	<ul style="list-style-type: none"> - Clashscore: 8.30 - Ramachandran outliers: 14 - Sidechain outliers: 80
<i>Fit to data used for modeling</i>	Fit of model to information used to compute it has not been determined
<i>Fit to data used for validation</i>	Fit of model to information not used to compute it has not been determined

5. Methodology and Software	
1. Name	None
Description	<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>
Software	HADDOCK (version 2.4)