

Summary of integrative structure determination of Complex of the partially open conformation of P. furiosus Mre11-Rad50 (PDB ID: 9A9K)

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)
Datasets used for modeling	<ul style="list-style-type: none"> - Ensemble FRET data, Zenodo: 10.5281/zenodo.14990529 - Experimental model, PDB: 3QKU - Experimental model, PDB: 3DSC - Predicted contacts, Not available - Experimental model, PDB: 3AV0 - Experimental model, PDB: 6S6V - Experimental model, PDB: 3QG5
2. Representation	
Number of representations	1
Scale	Atomic
Number of rigid and flexible segments	0, 8
3. Restraints	
Physical principles	Information about physical principles was not provided

Experimental data	<ul style="list-style-type: none"> - 1 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 32.7-42.7 - 2 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 46.1-56.1 - 2 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 42.6-52.6 - 1 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 46.5-56.5 - 1 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 45.7-55.7 - 1 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 30.7-40.7 - 2 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 28.7-38.7 - 2 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 30.6-40.6 - 1 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 30.4-40.4 - 2 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 42.8-52.8 - 2 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 43.3-53.3 - 1 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 31.2-41.2 - 4 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 45.4-55.4 - 2 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 30.5-40.5 - 2 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 28.4-38.4 - 2 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 29.7-39.7 - 2 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 32.0-42.0 - 2 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 45.0-55.0 - 2 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 47.7-57.7 - 265 unique PredictedContactRestraint: Distance: 4.0
4. Validation	
Number of ensembles	0
Number of models in ensembles	Not applicable
Number of deposited models	1
Model precision (uncertainty of models)	Not available
Data quality	Data quality has not been assessed
Model quality: assessment of atomic segments	<ul style="list-style-type: none"> - Clashscore: 10.94 - Ramachandran outliers: 6 - Sidechain outliers: 128
Fit to data used for modeling	Fit of model to information used to compute it has not been determined

Fit to data used for validation	Fit of model to information not used to compute it has not been determined
5. Methodology and Software	
1. Name	None
Description	<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. C2 symmetry was enforced between the two Rad50NBD monomers and 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.</p>
Software	HADDOCK (version 2.4)