

Summary of integrative structure determination of Model of the vaccinia virus DNA polymerase: complex between A20-Cter and E9 (PDB ID: 9A13, PDB-Dev ID: PDBDEV_00000075)

1. Model Composition	
Entry composition	<ul style="list-style-type: none"> - DNA polymerase processivity factor component A20: chain(s) A (124 residues) - DNA polymerase: chain(s) B (1010 residues)
Datasets used for modeling	<ul style="list-style-type: none"> - Experimental model, PDB: 6ZXP - Experimental model, PDB: 5N2E - NMR data, BMRB: 34544 - NMR data, BMRB: 34545 - Other, Not available: 10.1016/j.jmb.2021.167009
2. Representation	
Number of representations	1
Scale	Atomic
Number of rigid and flexible segments	0, 2
3. Restraints	
Physical principles	Information about physical principles was not provided

Experimental data	<ul style="list-style-type: none"> - 738 unique DerivedDistanceRestraint: Upper Bound Distance: 2.0 - 1 unique DerivedDistanceRestraint: Upper Bound Distance: 3.632 - 1 unique DerivedDistanceRestraint: Upper Bound Distance: 2.838 - 1 unique DerivedDistanceRestraint: Upper Bound Distance: 2.575 - 1 unique DerivedDistanceRestraint: Upper Bound Distance: 2.765 - 1 unique DerivedDistanceRestraint: Upper Bound Distance: 3.557 - 1 unique DerivedDistanceRestraint: Upper Bound Distance: 2.16 - 1 unique DerivedDistanceRestraint: Upper Bound Distance: 2.689 - 1 unique DerivedDistanceRestraint: Upper Bound Distance: 2.442 - 1 unique DerivedDistanceRestraint: Upper Bound Distance: 3.563 - 1 unique DerivedDistanceRestraint: Upper Bound Distance: 2.548 - 1 unique DerivedDistanceRestraint: Upper Bound Distance: 2.678 - 1 unique DerivedDistanceRestraint: Upper Bound Distance: 2.451 - 1 unique DerivedDistanceRestraint: Upper Bound Distance: 3.203 - 1 unique DerivedDistanceRestraint: Upper Bound Distance: 2.33 - 1 unique DerivedDistanceRestraint: Upper Bound Distance: 2.618 - 1 unique DerivedDistanceRestraint: Upper Bound Distance: 2.655
4. Validation	
Number of ensembles	0
Number of models in ensembles	Not applicable
Number of deposited models	10
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: 2.19-3.61 - Ramachandran outliers: 3-8 - Sidechain outliers: 83-109
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
Method	Docking
Number of computed models	?
Software	HADDOCK (version Not available)