

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	
<i>Entry composition</i>	<ul style="list-style-type: none"> - DNA polymerase processivity factor component A20: Chain A (124 residues) - DNA polymerase: Chain B (1010 residues)
<i>Datasets used for modeling</i>	<ul style="list-style-type: none"> - Experimental model, PDB ID: 6ZXP - Experimental model, PDB ID: 5N2E - NMR data, BMRB: 34544 - NMR data, BMRB: 34545 - Other, File: None
2. Representation	
<i>Resolution</i>	Atomic
<i>Number of rigid bodies, flexible units</i>	0, 2
<i>Flexible units</i>	<ul style="list-style-type: none"> - A: 1-124 - B: 1-1010
<i>Structural coverage (rigid bodies)</i>	100%
3. Restraints	
<i>Physical principles</i>	Information about physical principles was not provided

<p>Experimental data</p>	<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)	Model precision can not be calculated with one structure
Data quality	Data quality has not been assessed

<p><i>Model quality: assessment of atomic segments</i></p>	<ul style="list-style-type: none"> - Model-1: Clashscore = 2.79, Number of Ramachandran outliers = 4, Number of sidechain outliers = 97 - Model-2: Clashscore = 3.28, Number of Ramachandran outliers = 6, Number of sidechain outliers = 87 - Model-3: Clashscore = 3.12, Number of Ramachandran outliers = 5, Number of sidechain outliers = 96 - Model-4: Clashscore = 3.61, Number of Ramachandran outliers = 4, Number of sidechain outliers = 94 - Model-5: Clashscore = 3.17, Number of Ramachandran outliers = 3, Number of sidechain outliers = 87 - Model-6: Clashscore = 3.56, Number of Ramachandran outliers = 4, Number of sidechain outliers = 83 - Model-7: Clashscore = 3.17, Number of Ramachandran outliers = 5, Number of sidechain outliers = 96 - Model-8: Clashscore = 3.23, Number of Ramachandran outliers = 6, Number of sidechain outliers = 90 - Model-9: Clashscore = 2.35, Number of Ramachandran outliers = 8, Number of sidechain outliers = 109 - Model-10: Clashscore = 2.19, Number of Ramachandran outliers = 6, Number of sidechain outliers = 85
<p><i>Model quality: assessment of excluded volume</i></p>	<p>Not applicable</p>
<p><i>Fit to data used for modeling</i></p>	<p>Fit of model to information used to compute it has not been determined</p>
<p><i>Fit to data used for validation</i></p>	<p>Fit of model to information not used to compute it has not been determined</p>
<p>5. Methodology and Software</p>	
<p><i>1. Method</i></p>	<p>None</p>
<p><i>Name</i></p>	<p>Docking</p>
<p><i>Number of computed models</i></p>	<p>?</p>
<p><i>Software</i></p>	<p>HADDOCK (version Not available)</p>