

**Summary of integrative structure determination of Integrative model of Nucleotide excision repair complex of XPA and RPA on 3' junction substrate (PDB ID: 9A1Y, PDB-Dev ID: PDBDEV\_00000128)**

<b>1. Model Composition</b>	
<a href="#">Entry composition</a>	<ul style="list-style-type: none"> <li>- RPA70: chain(s) A (434 residues)</li> <li>- RPA32: chain(s) B (226 residues)</li> <li>- RPA14: chain(s) C (115 residues)</li> <li>- XPA: chain(s) D (239 residues)</li> <li>- DNA (40-MER): chain(s) E (40 residues)</li> <li>- DNA (5'-D(P*TP*TP*TP*TP*TP*TP*TP*TP*GP*CP*CP*CP*GP*CP*GP 3'): chain(s) F (17 residues)</li> <li>- ZINC ION: chain(s) G [E], H</li> </ul>
<a href="#">Datasets used for modeling</a>	<ul style="list-style-type: none"> <li>- SAS data, SASBDB: <a href="#">SASDH44</a></li> <li>- Experimental model, PDB: <a href="#">1JMC</a></li> <li>- Integrative model, PDB: <a href="#">9A03</a></li> <li>- Experimental model, PDB: <a href="#">1L1O</a></li> <li>- Experimental model, PDB: <a href="#">1DPU</a></li> <li>- Comparative model, Not available</li> <li>- De Novo model, Not available</li> </ul>
<b>2. Representation</b>	
<a href="#">Number of representations</a>	1
<a href="#">Scale</a>	Atomic
Number of <a href="#">rigid</a> and <a href="#">flexible</a> segments	0, 12
<b>3. Restraints</b>	
<a href="#">Physical principles</a>	Information about physical principles was not provided
<a href="#">Experimental data</a>	- 1 unique SASRestraint: Assembly name: Nucleotide Excision repair complex of XPA and RPA Fitting method: FoXS Multi-state: False
<b>4. Validation</b>	
<a href="#">Number of ensembles</a>	0
<a href="#">Number of models in ensembles</a>	Not applicable
<a href="#">Number of deposited models</a>	1
<a href="#">Model precision (uncertainty of models)</a>	Not available
<a href="#">Data quality</a>	
<a href="#">Model quality: assessment of atomic segments</a>	<ul style="list-style-type: none"> <li>- Clashscore: 30.10</li> <li>- Ramachandran outliers: 37</li> <li>- Sidechain outliers: 61</li> </ul>
<a href="#">Fit to data used for modeling</a>	Fit of model to information used to compute it has not been determined
<a href="#">Fit to data used for validation</a>	Fit of model to information not used to compute it has not been determined
<b>5. Methodology and Software</b>	

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1. <a href="#"><i>Name</i></a>	None
<a href="#"><i>Method</i></a>	None
<a href="#"><i>Number of computed models</i></a>	1
<a href="#"><i>Software</i></a>	<ul style="list-style-type: none"><li>- <a href="#">Modeller</a> (version 9v4)</li><li>- <a href="#">FoXSDock</a> (version main.c2a7893)</li></ul>