

Summary of integrative structure determination of Integrative model of 5' Nucleotide excision repair complex of XPA-DBD and RPA70AB (PDB ID: 9A04, PDB-Dev ID: PDBDEV_00000040)

1. Model Composition	
Entry composition	<ul style="list-style-type: none"> - Subunit A: chain(s) A (238 residues) - Subunit B: chain(s) B (142 residues) - DNA short arm: chain(s) C (14 residues) - DNA long arm: chain(s) D (22 residues)
Datasets used for modeling	<ul style="list-style-type: none"> - NMR data, BMRB: 27131 - SAS data, SASBDB: SASDH44 - Experimental model, PDB: 1JMC - Experimental model, PDB: 5A39 - Comparative model, Not available - Other, Not available - Other, Not available - Other, Not available
2. Representation	
Number of representations	1
Scale	Atomic
Number of rigid and flexible segments	4, 0
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	<ul style="list-style-type: none"> - 1 unique SASRestraint: Assembly name: Complete assembly Fitting method: FoXS Multi-state: False
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	
Model quality: assessment of atomic segments	<ul style="list-style-type: none"> - Clashscore: 0.00 - Ramachandran outliers: 4 - Sidechain outliers: 21
Fit to data used for modeling	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. <i>Name</i>	Homolgy Modeling of XPA
<i>Method</i>	MODELLER
<i>Number of computed models</i>	10
2. <i>Name</i>	Extension of C-terminal Helix of XPA
<i>Method</i>	ROSETTA Remodel
<i>Number of computed models</i>	1000
3. <i>Name</i>	Docking of DNA to XPA
<i>Method</i>	HADDOCK
<i>Number of computed models</i>	1000
4. <i>Name</i>	Randomization and Rigid Body Energy Minimization
<i>Method</i>	HADDOCK
<i>Number of computed models</i>	1000
5. <i>Name</i>	Semi-flexible simulated annealing
<i>Method</i>	HADDOCK
<i>Number of computed models</i>	1000
6. <i>Name</i>	Flexible explicit solvent refinement
<i>Method</i>	HADDOCK
<i>Number of computed models</i>	200
7. <i>Name</i>	Stepwise addition of nucleotide linker
<i>Method</i>	ROSETTA stepwise
<i>Number of computed models</i>	100
<i>Software</i>	<ul style="list-style-type: none"> - HADDOCK (version Not available) - ROSETTA (version Not available) - MODELLER (version Not available) - FOXS (version Not available)