# Summary of integrative structure determination of Integrative model of 3' Nucleotide excision repair complex of XPA-DBD and RPA70AB (PDB ID: 9A03, PDB-Dev ID: PDBDEV_00000039)

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| ***1. Model Composition*** | |
| *Entry composition* | - DNA short arm: Chain C (13 residues)<br>- Subunit B: Chain B (142 residues)<br>- DNA long arm: Chain D (22 residues)<br>- Subunit A: Chain A (238 residues) |
| *Datasets used for modeling* | - NMR data, BMRB: 27131<br>- SAS data, SASBDB: SASDH54<br>- Experimental model, PDB ID: 1JMC<br>- Experimental model, PDB ID: 5A39<br>- Comparative model, template PDB ID: Not available<br>- Other, Not available<br>- Other, Not available<br>- Other, Not available |
| ***2. Representation*** | |
| *Resolution* | Atomic |
| *Number of rigid bodies, flexible units* | 4, 0 |
| *Rigid bodies* | - A: 1-238<br>- B: 1-142<br>- C: 1-13:None<br>- D: 1-22:None |
| *Structural coverage (rigid bodies)* | 100% |
| ***3. Restraints*** | |
| *Physical principles* | Information about physical principles was not provided |
| *Experimental data* | - 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)* | Model precision can not be calculated with one structure |
| *Data quality* | |

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| *Model quality: assessment of atomic segments* | Model-1: Clashscore = 0.0, Number of Ramachandran outliers = 1, Number of sidechain outliers = 34 |
| *Model quality: assessment of excluded volume* | Not applicable |
| *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. Method* | Homolgy Modeling of XPA |
| *Name* | MODELLER |
| *Number of computed models* | 10 |
| *2. Method* | Extension of C-terminal Helix of XPA |
| *Name* | ROSETTA Remodel |
| *Number of computed models* | 1000 |
| *3. Method* | Docking of DNA to XPA |
| *Name* | HADDOCK |
| *Number of computed models* | 1000 |
| *4. Method* | Randomization and Rigid Body Energy Minimization |
| *Name* | HADDOCK |
| *Number of computed models* | 1000 |
| *5. Method* | Semi-flexible simulated annealing |
| *Name* | HADDOCK |
| *Number of computed models* | 1000 |
| *6. Method* | Flexible explicit solvent refinement |
| *Name* | HADDOCK |
| *Number of computed models* | 200 |
| *7. Method* | Stepwise addition of nucleotide linker |
| *Name* | ROSETTA stepwise |

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|---|---|
| *Number of computed models* | 100 |
| *Software* | - HADDOCK (version Not available)<br>- ROSETTA (version Not available)<br>- MODELLER (version Not available)<br>- FOXS (version Not available) |