

Summary of integrative structure determination of Integrative model of Nucleotide excision repair complex of XPA and RPA on 5' junction substrate (PDB ID: 9A1V, PDB-Dev ID: PDBDEV 00000124)

1. Model Composition	
Entry composition	<ul style="list-style-type: none">- RPA70: chain(s) A (434 residues)- RPA32: chain(s) B (226 residues)- RPA14: chain(s) C (115 residues)- XPA: chain(s) D (239 residues)- DNA (5'-D(P*GP*GP*CP*CP*CP*GP*GP*GP*GP*CP*TP*TP*TP*TP*TP*3'): chain(s) E (18 residues)- DNA (40-MER): chain(s) F (40 residues)- ZINC ION: chain(s) G, H
Datasets used for modeling	<ul style="list-style-type: none">- SAS data, SASBDB: SASDP24- Experimental model, PDB: 1JMC- Integrative model, PDB: 9A03- Experimental model, PDB: 1L1O- Experimental model, PDB: 1DPU- Comparative model, Not available- De Novo model, Not available
2. Representation	
Number of representations	1
Scale	Atomic
Number of rigid and flexible segments	0, 12
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	<ul style="list-style-type: none">- 1 unique SASRestraint: Assembly name: Nucleotide excision repair complex of XPA and RPA 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: 166.70- Ramachandran outliers: 53- Sidechain outliers: 82
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

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