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	- DNA (5'-D(P*GP*GP*CP*CP*CP*GP*CP*GP*GP*CP*TP*TP*TP*TP*TP*T 3'): Chain E (18 residues) - XPA: Chain D (239 residues) - RPA70: Chain A (434 residues) - DNA (40-MER): Chain F (40 residues) - RPA32: Chain B (226 residues) - ZINC ION: Chain G (Not available residues) - RPA14: Chain C (115 residues) - ZINC ION ON 3-FOLD CRYSTAL AXIS: Chain H (Not available residues)
Datasets used for modeling	- SAS data, SASBDB: SASDP24 - Experimental model, PDB ID: 1JMC - Integrative model, PDB-Dev: PDBDEV_00000039 - Experimental model, PDB ID: 1L1O - Experimental model, PDB ID: 1DPU - Comparative model, template PDB ID: Not available - De Novo model, Not available
2. Representation	
Resolution	Atomic
Number of rigid bodies, flexible units	0, 14
Flexible units	- A: 1-238, 239-253, 254-434 - B: 1-128, 129-226 - C: 1-115 - D: 1-28, 29-48, 49-97, 98-239 - E: 1-18 - F: 1-40 - G: None-None - H: None-None
Structural coverage (rigid bodies)	100%
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	- 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)	Model precision can not be calculated with one structure
Data quality	

Model quality: assessment of atomic segments	Model-1: Clashscore = 166.7, Number of Ramachandran outliers = 53, Number of sidechain outliers = 82
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	None
Name	None
Number of computed models	1
Software	- Modeller (version 9v4) - FoXSDock (version main.c2a7893)