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Publications

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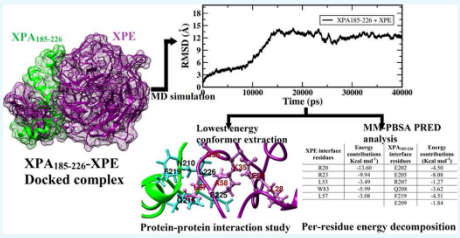
Characterizing the Binding Interactions between DNA-Binding Proteins, XPA and XPE: A Molecular Dynamics Approach

Sushmita Pradhan, Pundarikaksha Das, and Venkata Satish Kumar Mattaparthi*

Molecular Modelling and Simulation Laboratory, Department of Molecular Biology and Biotechnology, Tezpur University, Tezpur 784 028, Assam, India

Supporting Information

ABSTRACT: The scaffold nature of *Xeroderma pigmentosum* complementation group A (XPA) protein makes it an important member of nucleotide excision repair (NER) that removes bulky DNA lesions with the help of various protein−protein interactions (PPI) and DNA−protein interactions. However, many structural insights of XPA's interaction and the binding patterns with other NER proteins are yet to be understood. Here, we have studied one such crucial PPI of XPA with another NER protein, *Xeroderma pigmentosum* complementation group A (XPE), by using the previously identified binding site of XPA (residues 185−226) in the Assisted Model Building With Energy Refinement force-field-mediated dynamic system. We studied the relationship between $XPA_{185-226}$−XPE complex using three different docked models. The major residues observed in all of the models that were responsible for the PPI of this complex were Arg20, Arg47, Asp51, and Leu57 from XPE and the residues Leu191, Gln192, Val193, Trp194, Glu198, Glu202, Glu205, Arg207, Glu209, Gln216, and Phe219 from $XPE_{185-226}$. During the simulation study, the orientation of XPA was also noted to be changed by almost 180° in models 1 and 3, which remain unchanged in model 2, indicating that XPA interacts with XPE with its N-terminal end facing downward and C-terminal end facing upward. The same was concurrent with the binding of DNA-binding domain region of XPA (aa98−239) with XPE. The N-terminal of XPE was stretched for accommodating XPA. Using the per-residue energy decomposition analysis for the interface residues of all models, the binding affinity between these proteins were found to be dependent on R20, R47, and L57 of XPE and the residues L191, V193, W194, E198, E202, E205, R207, and F219 of XPA. The net binding free energy of the $XPA_{185-226}$−XPE protein complex was found to be −48.3718 kcal mol^{-1} for model 1, −49.09 kcal mol^{-1} for model 2, and −56.51 kcal mol^{-1} for model 3.



1. INTRODUCTION

DNA is always under constant threats and attacks from entities of endogenous or exogenous nature, which makes DNA repair response a crucial mechanism in all living beings. Nucleotide excision repair (NER) is one such DNA repair pathway that addresses bulky DNA damages, such as cyclobutane pyrimidine dimers (CPD), 6-4 photoproducts (6-4PP), and helix-distorting platinum (Pt) cross-links, which are inflicted upon DNA by various mutagens.[1−3] This process is mediated in a multistep fashion by the coordinated interaction of more than 20 different proteins, which is mainly overseen and systematized by *Xeroderma pigmentosum* complementation group A (XPA) protein, earning itself a title of "scaffolding protein". XPA functions as a primary damage recognition protein in both global genome NER (GG-NER) and transcription-coupled NER (TC-NER).[3−7] As a result, any alteration in the XPA gene or in the protein function leads to classical *Xeroderma pigmentosum* (XP) disease that is characterized by extreme sun sensitivity, neurological damages, and is often linked with skin cancers.[4,6,8−18]

The highly conserved XPA,[19−21] consisting of 273 residues,[22] with its disordered N- and C-terminals, has been reported to bind and interact with many proteins of NER as well as with the damaged DNA.[23−25] The DNA-interacting region of XPA was mapped initially to the globular DNA-binding domain (DBD), which spans between 98 and 219 amino acid residues,[26,27] but since the earlier DBD lacked a significant amount of positive residues for the strong bonding with the negatively charged DNA, the DBD of XPA has been now redefined between 98 and 239 amino acid residues.[28−30] To date, only a small number of the XPA's protein−protein interactions (PPI) with other NER proteins have been explored. Some of the well-documented PPIs of XPA are with (i) helicase, transcription factor II H (TFIIH) complex,[3,11,31] (ii) GG-NER damage verifier, *Xeroderma pigmentosum* complementation group C (XPC) protein,[32−34] (iii) excision-repair cross-complementing group 1 endonu-

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Investigation of the probable homo-dimer model of the *Xeroderma pigmentosum* complementation group A (XPA) protein to represent the DNA-binding core

Sushmita Pradhan, Himakshi Sarma and Venkata Satish Kumar Mattaparthi

Molecular Modelling and Simulation Laboratory, Department of Molecular Biology and Biotechnology, Tezpur University, Tezpur, India

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ABSTRACT

The *Xeroderma pigmentosum* complementation group A (XPA) protein functions as a primary damage verifier and as a scaffold protein in nucleotide excision repair (NER) in all higher organisms. New evidence of XPA's existence as a dimer and the redefinition of its DNA-binding domain (DBD) raises new questions regarding the stability and functional position of XPA in NER. Here, we have investigated XPA's dimeric status with respect to its previously defined DBD (XPA_{98-219}) as well as with its redefined DBD (XPA_{98-239}). We studied the stability of XPA_{98-210} and XPA_{98-239} homo-dimer systems using all-atom molecular dynamics simulation, and we have also characterized the protein–protein interactions (PPI) of these two homo-dimeric forms of XPA. After conducting the root mean square deviation (RMSD) analyses, it was observed that the XPA_{98-239} homo-dimer has better stability than XPA_{98-210}. It was also found that XPA_{98-239} has a larger number of hydrogen bonds, salt bridges, and hydrophobic interactions than the XPA_{98-210} homo-dimer. We further found that Lys, Glu, Gln, Asn, and Arg residues shared the major contribution toward the intermolecular interactions in XPA homo-dimers. The binding free energy (BFE) analysis, which used the molecular mechanics Poisson–Boltzmann method (MM-PBSA) and the generalized Born and surface area continuum solvation model (GBSA) for both XPA homo-dimers, also substantiated the positive result in favor of the stability of the XPA_{98-239} homo-dimer.

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1. Introduction

The *Xeroderma pigmentosum* complementation group A (XPA) protein is an obligate member of the nucleotide excision repair (NER) pathway that identifies and repairs very large DNA-distorting lesions. The most common types of lesions repaired by NER are cyclo-butane pyrimidine dimers (CPD), photoproducts and cisplatin-DNA intra-strand cross-links rendered by environmental mutagens, ultra-violet radiations, or antitumor agents (Paquet, Perez, Leng, Lancelot, & Malinge, 1996; Rabik & Dolan, 2007; Scharer, 2013; Volker et al., 2001). Based on the multiple steps of this repair process, NER involves more than 30 different proteins which perform specific functions at each step, forming multi-protein complexes that are coordinated largely by XPA during the initial steps. The primary role of XPA lies entirely in verifying early damage, and in assembling other NER proteins to the DNA damage site (DiGiovanna & Kraemer, 2012; Lehmann, 2012; Saijo, Takedachi, & Tanaka, 2011).

The smooth functioning of NER, and the proper excision of the DNA lesions are often dependent wholly on the sequential assembly and coordination of different proteins to the damage site. Therefore, any defect on these repair proteins, which hinders their ability to perform their tasks, can have repercussions in the form of various skin cancers and genetic disorders, such as *Xeroderma pigmentosum* (XP), Cockayne syndrome, and Trichothiodystrophy (Cheng et al., 2007; DiGiovanna & Kraemer, 2012; Feltes & Bonatto, 2015; Lehmann, 2012; Li et al., 2015; Negureanu & Salsbury, 2012; Ninaber & Goodfellow, 1998). Because XPA is common in both global genome NER (GG-NER), and transcription-coupled NER (TC-NER) (Fuss & Tainer, 2011; Krasikova, Rechkunova, Maltseva, Petruseva, & Lavrik, 2010; Scharer, 2013; Sugasawa et al., 1998), any deficits/mutations in XPA can result in a total NER failure, thereby causing classical XP disease phenotype that is characterized by extreme photoreactivity, neurological disorders and often, skin cancers (Amr, Messaoud, El Darouti, Abdelhak, & El-Kamah, 2014; DiGiovanna & Kraemer, 2012; Fassihi et al., 2016, Feltes & Bonatto, 2015; Kang, Reardon, & Sancar, 2011; Lehmann, 2012; Liu et al., 2015; Naegeli & Sugasawa, 2011; Qian et al., 2011; Satokata, Tanaka, Yuba, & Okada, 1992).

During the NER process, XPA interacts with various types of damaged DNA, as well with fellow repair proteins as part of its scaffolding nature. XPA has been known to exclusively interact with damaged strands by using its globular DBD, which earlier spanned between residues 98-219 (Buchko et al., 2001; Missura

CONTACT mvenkatasatishkumar@gmail.com; venkata@tezu.ernet.in
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Structural dynamics and interactions of Xeroderma pigmentosum complementation group A (XPA_{98-210}) with damaged DNA

Sushmita Pradhan & Venkata Satish Kumar Mattaparthi

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