

The porin AaxA protein model from *Chlamydia pneumoniae*

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Abstract:

Chlamydophila pneumoniae is an intracellular pathogen accountable for various acute respiratory infections. *C. pneumoniae* has a gene cluster which encodes a putative outer membrane porin (aaxA), arginine decarboxylase (CPn1032 or aaxB) and a putative cytoplasmic membrane transporter (CPn1031 or aaxC). Therefore, it is of interest to document a molecular protein model of porin AaxA from *Chlamydia pneumoniae* to gain structure to functional insight on the protein.

Keywords: *Chlamydophila pneumoniae*, AaxA, homology modelling

Background:

Chlamydomophila pneumonia is a species of Chlamydomophila. It is a microscopic, gram negative, intracellular bacterium that infects humans. It is the main cause of pneumonia. *C. pneumoniae* is transmitted directly from person to person through the respiratory system [1-2]. The incubation time is several weeks longer than that for several other respiratory pathogens [3]. *C. pneumoniae* is capable of developing an intracellular niche where it facilitates the survival or death of the host cell, modulates the hormonal signalling pathway of the host cell, and bypasses the defensive mechanisms of the host cell. *C. pneumoniae* causes a persistent infection due to the inability of the host to remove the pathogen [4-6]. Porin AaxA protein enhances the absorption of L-arginine as part of the AaxABC system. Therefore, it is of interest to document a molecular Porin AaxA protein model from *Chlamydia pneumonia* to gain functional insight.

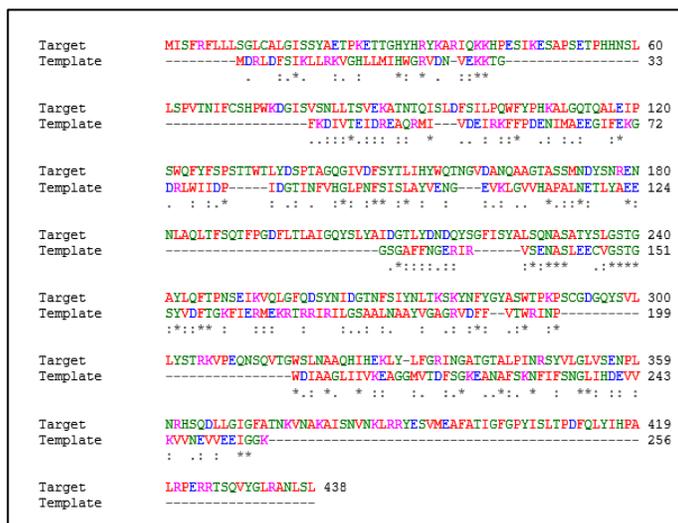


Figure 1: Alignment of porin AaxA with template (PDB: ID2P3N) protein sequence using clustal omega. Asterisks indicates identical amino acids, dots indicate similar amino acids.

Materials and Methods:

Template sequence Alignment:

The porin AaxA protein sequence was obtained from the UniProtKB/Swissprot database (Q9Z6M6) [7]. The Brook Heaven Protein Data Bank (PDB) was used to find the correct template (PDB ID: 2P3N) for modelling the porin AaxA protein with default parameters. The alignment between the target and the template (identity score of 37%) was done using the omega cluster [8].



Figure 2: The best modeled structure of porin AaxA protein obtained using Modeller 9v9.19. Red colour indicate alpha helices, yellow colour indicate the beta sheets and green colour indicate the loops

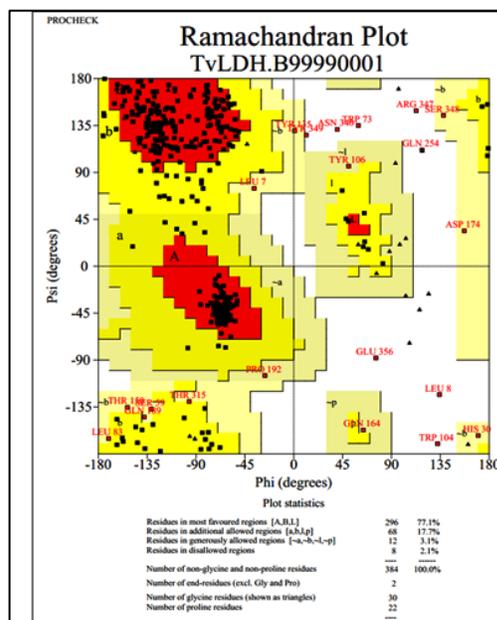


Figure 3: Ramachandran plot for the porin AaxA protein obtained using PROCHECK

Molecular Modelling of porin AaxA protein:

The homology of the porin AaxA protein modelling was conducted using the template structure with PDB ID: 2P3N using the modeller9v9.19 software [9]. PYMOL was used to visualize the modelled structure [10]. All modelled structures were graded on the basis of the internal score function (DOPE score). Models with the lowest internal score were chosen as the final model for accuracy assessment [11, 12].

Validation of the model:

The model was evaluated using energy and stereo chemical geometry [13]. The stereo chemical consistency of the modeled protein was checked using the Phi / Psi distributions in the Ramachandran plot generated with PROCHECK in SAVS (Structure Analysis Verification Server) [14].

Results and Discussion:

The target protein sequences (porin AaxA) and the template (PDB ID: 2P3N) were matched and the alignment result was shown in **Figure 1**. The asterisk indicated the identity of the amino acids found in the two protein sequences. MODELLER9.19 was used to generate a model for the target protein porin AaxA (**Figure 2**). We selected TvLTH.B99990001.pdb porin AaxA protein model using the minimum dope score rating. SAVS (Structure Alignment Verification Server) was used to verify the modelled structures. The

measurements of the Ramachandran plot are computed using the PROCHECK software (**Figure 3**). The preliminary predicted model data is available with the authors for further analysis to gain functional insights on the protein.

Conclusion:

We report a molecular protein model data of porin AaxA from *Chlamydia pneumonia* to gain structure to functional insight.

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