

Backbone Dynamics of *Pseudomonas aeruginosa* K122-4 Pilin from ^1H - ^{15}N Heteronuclear NMR Relaxation

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Pilin is the major fibre-forming protein in type-IV pili of various pathogenic bacteria including *Pseudomonas aeruginosa*. Pilin is not only involved in the attachment of the bacterium to host cells for infection but also in the immune response as it contains a major antigenic determinant. ^{15}N -NMR relaxation measurements were exploited to probe the dynamics of an N-terminal truncated monomeric pilin from *P. aeruginosa* strain K122-4. ^{15}N - T_1 , ^{15}N - T_2 and $^{15}\text{N}\{^1\text{H}\}$ NOE experiments were measured at three different magnetic field strengths. The relaxation parameters were interpreted in terms of order parameters and motions on different time scales, and these motional parameters were corroborated by their magnetic field and temperature dependence. The structured region exhibited consistently large order parameters while the terminal and loop regions showed variable internal motions. Interestingly the functionally active C-terminal disulfide loop region was found to be relatively rigid on the ps-ns time scale but exhibited conformational exchange. It is notable that this disulfide loop has been reported to display the antigenic determinant for immune response as well as the receptor-binding domain for infection. This study suggests that the active site of pilin utilize a rigid backbone scaffold for attachment to the host cell receptor and in antigen-antibody recognition. Characterization of pilin dynamics will help our understanding of infection and immunity, and facilitate the design of more efficient antibacterial vaccines.