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A Survey on π-π Stackings and π-Cations in Prion Protein Structures

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Abstract

π-π stackings and π-cations clearly do some contributions to maintain the structural stability of a normal cellular prion protein (PrP). This short article is to do a survey on the π-π stackings and π-cations in all the PrP structures listed in the PDB (www.rcsb.org) Bank. We find the following important π-π stackings: Y218–F175– Y169 (around the β2-α2 loop), Y162–Y128 (linking the two β-strands), F141–Y150– Y157 (in α-helix 1), H187–F198 (linking α-helix 2 and the α2-α3 loop); and we also find the following important π-cations: F141–R208.(N)NH2 (linking the β1-α1 loop and α- helix 3), Y128–R164.(N)NH2–Y169 (linking β-strand 1 and the β2-α2 loop). Thus, for PrPs, there exists a long "π-chain" Y218–F175–Y169–R164–Y128–Y162 covering the β2-α2 loop, and there exists another long "π-chain" R208–Y141–Y150–Y157–F198– H187 covering the α-helix 1. This short article can be acted as a "quick reference card" for PrP protein structure π-interaction studies in laboratories or in theories.

Keywords: π-π Stackings; π-chains; Prion protein PrP structures; Two long π-chains

π-π and π-cation interactions play an important role in maintaining the structural stability of PrP. In this short article, we consider all the PrP structures listed in the PDB Bank: first we use the Swiss-PdbViewer 4.1.0 (spdbv.vital-it.ch) to relax (i.e. do Energy Minimisation in the use of Steepest Descent - Conjugate Gradients -Steepest Descent optimization methods) all the PrP structures, and then we use Maestro 10.1 2015–1 (Academic use only) (www.schrodinger.com) to find the π interactions see Table 1, where the code in the ( ) bracket is the PBD ID for each PrP species).

Let us denote some notations for a PrP structure: L0 is the N-terminal structured region before the β-strand 1, B1 is β-strand 1, L1 is the loop between B1 and α- helix 1, H1 is the α-helix 1, L2 is the loop between H1 and β-strand 2, B2 is β- strand 2, L3 is the loop between B2 and α-helix 2, H2 is the α-helix 2, L4 is the loop between H2 and α-helix 3, and H3 is the α-helix 3. From Table 1, we may see that there are π-π stackings (Figure 1): Y218–F175–Y169 (linking H3–H2–L3), H187–F198 (linking H2–L4), F141–Y150–Y157 (in H1), Y225–Y226 (in H3), Y162–Y128 (linking B2–B1), etc. From Table 1, we also see the following π-cations (Figure 1): F141– R208.(N) NH2 (linking L1–H3), Y162–L125.(N)N–Y128–R164.(N)NH2–Y169 (linking B2–L0–B1–L3), F198–R156.(N)NH2 (linking L4–L2), H155–R136.(N)NH2 (linking L2– L1), Y127–L125.(N)N (in L0), etc. The above bioinformatics might be acted as a "quick reference card" for PrP protein structure π-interaction studies [1,2].

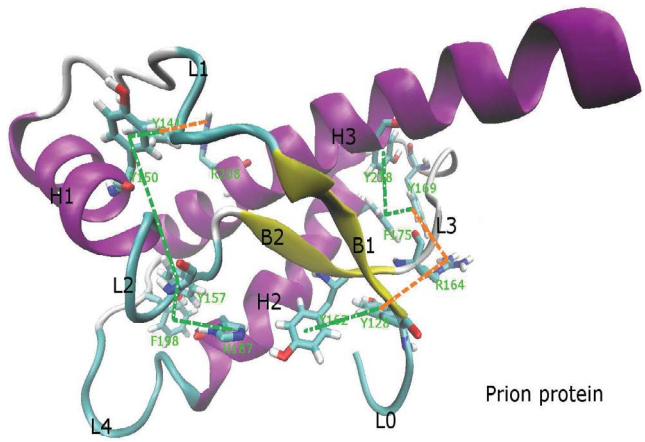

Figure 1: Some selected π-interactions of PrPs, where the green dashed-lines denote the π-π stackings and the orange colored dashed-lines denote the π-cations

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Species	π-π-stacking	π-cation
mousePrP (1AG2)	F175–Y218,Y162–Y128,H187–F198	F141–R208.(N)NH2
(1XYX)	Y169–Y218	
humanPrP (1QLX)		Y169–R164.(N)NH2
(1QLZ)		
(1QM0/1/2/3)		
(2LSB)	F175–Y218	Y128–R164.(N)NH2, F198–R156.(N)NH2,
		H155–R136.(N)NH2
bovinePrP (1DWY)		Y128–R164.(N)NH2
(1DWZ)		
(1DX0/1)		
SyrianHamsterPrP (1B10)	Y169–F175–Y218	
(2LH8)	Y169–F175–Y218	
caninePrP (1XYK)		
catPrP (1XYJ)		Y150–R156.(N)NH2
sheepPrP (1UW3)	F141–Y150, Y169–F175–Y218	
mousePrP[N174T] (1Y15)	F141–Y150, Y169–F175–Y218	Y128–R164.(N)NH2
humanPrP[Q212P]-M129 (2KUN)		H237–R228.(N)NH2
rabbitPrP[S173N]-NMR (2JOH)		Y127–L124.(N)N, Y144–R147.(N)NH2
rabbitPrP[I214V]-NMR (2JOM)	H139–Y149	Y148–R155.(N)NH2
rabbitPrP[S170N]-X-ray (4HLS)	Y169–F175	F141–R208.(N)NH2
rabbitPrP[S174N]-X-ray (4HMM)	Y169–F175	F141–R208.(N)NH2
rabbitPrP[S170N,S174N] (4HMR)	Y169–F175	F141–R208.(N)NH2
mousePrP - at 37°C (2L39)		Y169-R164.(N)NH2
mousePrP[V166A] (2KFO)	Y169–F175	
mousePrP[D167S] (2KU5)	F175–Y218	
mousePrP[D167S, N173K] (2KU6)	F175–Y218, H187–F198	
mousePrP[Y169G] (2L1D)	F141–Y150, F175–Y218, Y225–Y226	Y128–R164.(N)NH2
mousePrP[Y169A] (2L40)	W145–Y149, H187–F198	
mousePrP[S170N] (2K1O)	Y225–Y226	
mousePrP[S170N, N174T] (1Y16)		Y169–R164.(N)NH2
mousePrP[F175A] (2L1E)	Y163–Y218	F141–R208.(N)NH2
mousePrP[Y225A,Y226A] (2KFM)	Y169–F175–Y218	
mousePrP[Y169A, Y225A, Y226A] (2L1K)		
elkPrP (1XYW)	Y169–F175–Y218	
pigPrP (1XYQ)		
bankVolePrP (2K56)	Y169–F175–Y218	Y169–R164.(N)NH2
tammarWallabyPrP (2KFL)		F198–R156.(N)NH2
rabbitPrP-NMR (2FJ3)	F140–Y149	Y127–L124.(N)N
rabbitPrP-X-ray (3O79)	Y169–F175	
horsePrP (2KU4)		F198–R156.(N)NH2
humanPrP-pH7 (1HJM)		F141–R208.(N)NH2
(1HJN)	H187–F198, Y218–F175–Y169	
humanPrP(118–224) (4N9O)	F175–Y218	Y128–R164.(N)NH2
humanPrP-V129 (3HAK)	Y225–Y226, F175–Y218	F141–R208.(N)NH2
humanPrP-M166C/E221C (1H0L)	F175–Y218–Y169	

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humanPrP-M166V (1E1G)		Y225–R228.(N)NH2, Y128–L125.(N)N
(1E1J)		Y128–L125.(N)N
humanPrP-S170N (1E1P)	H187–F198	
(1E1S)	F141–Y150	T128–R164.(N)NH2
humanPrP-D178N (2K1D)	Y128–Y162, Y150–F141–	F141–R208.(N)NH2
humanPrP-D178N-M129 (3HEQ)	Y225–Y226, F175–Y218	
humanPrP-D178N-V129 (3HJX)		
humanPrP-F198S-M129 (3HES)	F175–Y218	F141–R208.(N)NH2
humanPrP-F198S-V129 (3HER)	F175–Y218, Y225–Y226	
humanPrP-R200K (1FKC)	F175–Y218, Y150–Y157	Y162–L125.(N)N
(1FO7)	F175–Y218, Y150–Y157	Y162–L125.(N)N
humanPrP-V209M-M129 (2M8T)		
humanPrP-V210I-M129 (2LEJ)	Y150–Y157	H187–R136.(N)NH2
(2LV1)	Y225–Y226	F141–R208.(N)NH2, W99=K101.(N)NZ
humanPrP-E219K-M129 (2LFT)	Y157–Y198, F175–Y218	
humanPrP-R220K (1E1U)	Y225–Y226	H155–R136.(N)NH2
(1E1W)	Y225–Y226, Y218–F175–Y169	H155–R136.(N)NH2
chickenPrP (1U3M)	Y235–Y238, F148–W156	
turtlePrP (1U5L)	F141–W150, Y162–Y188, Y166–F176	
xenopusLeavisPrP (1XU0)	Y149–Y153	
sheepPrP-H168 (1XYU)	F175–Y218, F141–Y150, H187–F198	Y128–R164.(N)NH2–Y169
ovinePrP-R168 (1Y2S)	Y150–Y157, H187–F198	

Table 1: π-π-stackings and π-cations for each (optimized) PrP.