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Mathematical Formulas for Prion All Cross-Structures Listed in the Protein Data Bank

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Abstract

Prion protein (PrP) has two regions: unstructured region PrP(1-120) and structured region PrP(119-231). In the structured region, there are many segments which have the property of amyloid fibril formation. By theoretical calculations, PrP(126-133), PrP(137-143), PrP(170-175), PrP(177-182), PrP(211-216) have the amyloid fibril forming property. PrP(142-166) has a X-ray crystallography experimental *β*-hairpin structure, instead of a pure cross-*β* amyloid fibril structure; thus we cannot clearly find it by our theoretical calculations. However, we can predict that there must be a laboratory X-ray crystal structure in PrP(184-192) segment that will be produced in the near future. The experiments of X-ray crystallography laboratories are agreeing with our theoretical calculations. This article summarized mathematical formulas of prion amyloid fibril cross-*β* structures of all the above PrP segments currently listed in the Protein Data Bank.

Keywords: PrP structured region; Amyloid fibril formation peptides; Theoretical calculations; Experimental laboratories; Mathematical formulas

Table 1 lists the cross-*β* structures of all PrP segments that were listed in the Protein Data Bank (PDB, www.rcsb.org), produced by X-ray crystallography experiments. In the below, 1- 24 give some mathematical formulas to describe all these cross-*β* structures.

1. Figure 1, the mathematical formula for B Chain got from A Chain is

$$B=\begin{pmatrix}-1 & 0 & 0\\ 0 & 1 & 0\\ 0 & 0 & -1\end{pmatrix}A+\begin{pmatrix}0\\ 4.8655\\ 0\end{pmatrix}. \qquad (1)$$

PrP segment	Species	PDB ID	Class of the cross-β
1 PrP(126–131)	human	4TUT	Class 7 [1,4]
2	human	4UBY	Class 8 [1,4]
3	human	4UBZ	Class 8 [1,4]
4 PrP(126–132)	human	4W5L	Class 8 [1,4]
5	human	4W5M	Class 8 [1,4]
6	human	4W5P	Class 8 [1,4]
7 PrP(127–133)	human	4W5Y	Class 6 [1,4]
8	human	4W67	Class 6 [1,4]
9	human	4W71	Class 6 [1,4]
10 PrP(127–132)	human	4WBU	Class 8 [1,4]
11	human	4WBV	Class 8 [1,4]
12	human	3MD4	antiparallel (P $2_1 2_1 2_1$)
13	human	3MD5	parallel (P 1 2_1 1)
14	human-M129	3NHC	Class 8 [1]
15	human-V129	3NHD	Class 8 [1]
16 PrP(137–142)	mouse	3NVG	Class 1 [1]
17 PrP(137–143)	mouse	3NVH	Class 1 [1]
18 PrP(138–143)	Syrian hamster	3NVE	Class 6 [1]
19	human	3NVF	Class 1 [1]
20 PrP(142–166)	sheep	1G04	*β*-hairpin [3]
21 PrP(170–175)	human	2OL9	Class 2 [1]
22	elk	3FVA	Class 1 [1]
23 PrP(177–182, 211–216)	human	4E1I	*β*-prism I fold [2] (P $2_1 2_1 2_1$)
24	human	4E1H	*β*-prism I fold [2] (P $2_1 2_1 2_1$)

Table 1: The cross-*β* structures known in the PDB Bank of PrP segments.

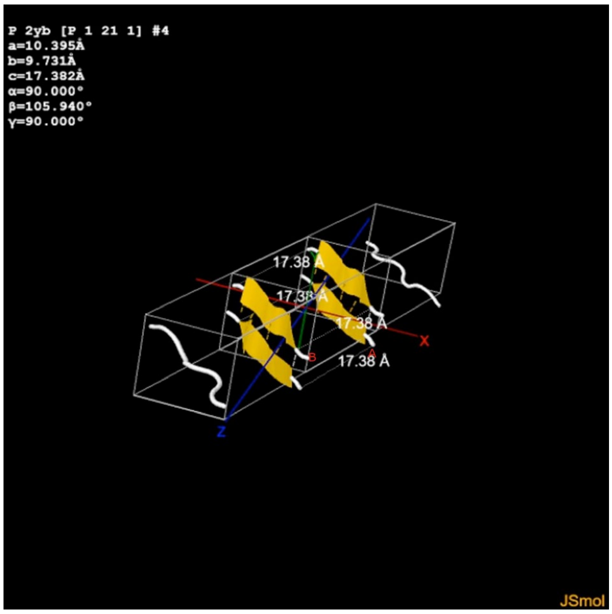

Figure 1: Protein fibril structure of human M129 prion GGYMLG (126–131) (PDB ID: 4TUT). The dashed lines denote the hydrogen bonds. A, B, C, D denote the chains of the fibril.

2. Figure 2, mathematical formulas for EFGH, IJKL, MNOP Chains obtained from ABCD Chains respectively are

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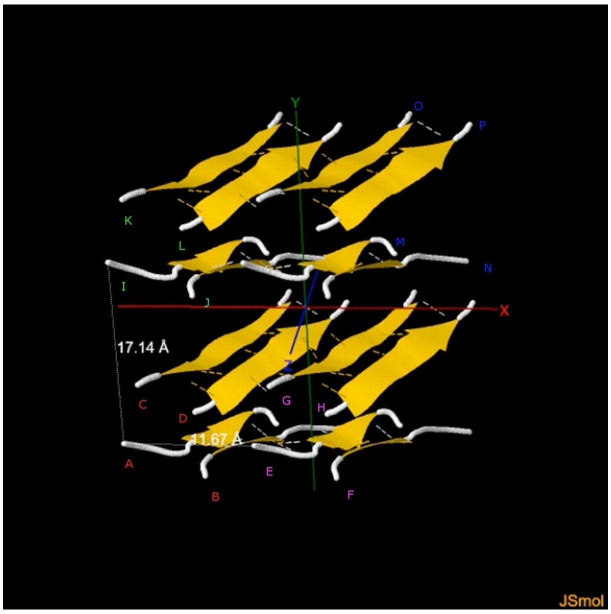

Figure 2: Protein fibril structure of human V129 prion GGYVLG (126–131) (PDB ID: 4UBY). The dashed lines denote the hydrogen bonds. A, B, C, D denote the chains of the fibril.

$$E(F/G/H)=\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}A(B/C/D)+\begin{pmatrix}11.666\\0\\0\end{pmatrix}, \tag{2}$$

$$I(J/K/L)=\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}A(B/C/D)+\begin{pmatrix}-0.05985\\17.1449\\0\end{pmatrix}, \tag{3}$$

$$M(N/O/P)=\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}A(B/C/D)+\begin{pmatrix}11.60615\\17.1449\\0\end{pmatrix}. \tag{4}$$

3. Figure 3, mathematical formulas for CD, EF, GH, IJ, KL Chains obtained from AB Chains respectively are

$$C(D)=\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}A(B)+\begin{pmatrix}11.609\\0\\0\end{pmatrix}, \tag{5}$$

$$E(F)/I(J)=\begin{pmatrix}-1&0&0\\0&1&0\\0&0&-1\end{pmatrix}A(B)+\begin{pmatrix}0\\\pm 9.0535\\0\end{pmatrix}, \tag{6}$$

$$G(H)/K(L)=\begin{pmatrix}-1&0&0\\0&1&0\\0&0&-1\end{pmatrix}A(B)+\begin{pmatrix}11.609\\\pm 9.0535\\0\end{pmatrix}. \tag{7}$$

4. Figure 4, mathematical formulas for CD, EF, GH, IJ, KL Chains obtained from the basic AB Chains respectively are

$$C(D)=\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}A(B)+\begin{pmatrix}0\\0\\9.429\end{pmatrix}, \tag{8}$$

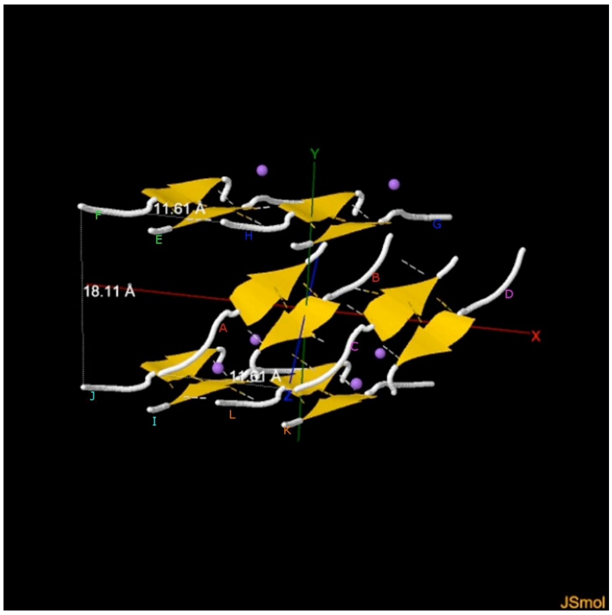

Figure 3: Protein fibril structure of human L129 prion GGYLLG (126–131) (PDB ID: 4UBZ). The dashed lines denote the hydrogen bonds. A, B denote the basic chains of the fibril.

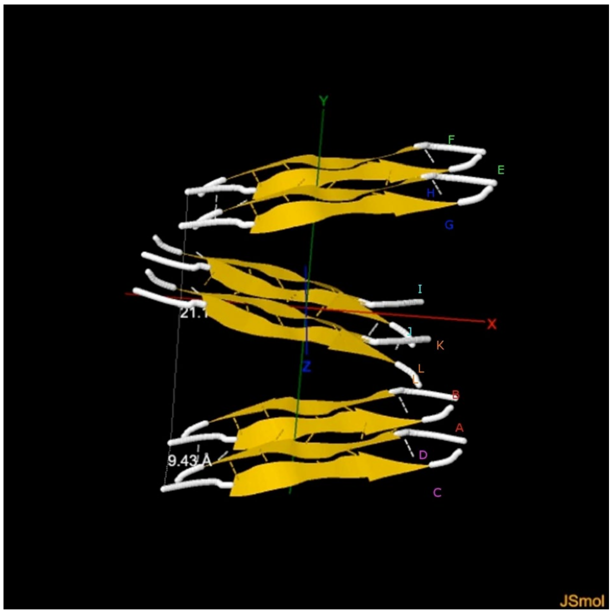

Figure 4: Protein fibril structure of human L129 prion GGYLLGS (126–132) (PDB ID: 4W5L). The dashed lines denote the hydrogen bonds. A, B denote the basic chains of the fibril.

$$E(F)=\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}A(B)+\begin{pmatrix}0\\21.113\\0\end{pmatrix}, \tag{9}$$

$$G(H)=\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}A(B)+\begin{pmatrix}0\\21.113\\9.429\end{pmatrix}, \tag{10}$$

$$I(J)=\begin{pmatrix}-1 & 0 & 0\\ 0 & 1 & 0\\ 0 & 0 & -1\end{pmatrix}A(B)+\begin{pmatrix}25.2415\\ 10.5565\\ 0\end{pmatrix}, \tag{11}$$

$$K(L)=\begin{pmatrix}-1 & 0 & 0\\ 0 & 1 & 0\\ 0 & 0 & -1\end{pmatrix}A(B)+\begin{pmatrix}25.2415\\ 10.5565\\ 9.429\end{pmatrix}. \tag{12}$$

$$K(L)=\begin{pmatrix}1 & 0 & 0\\ 0 & -1 & 0\\ 0 & 0 & -1\end{pmatrix}A(B)+\begin{pmatrix}25.2415\\ 10.5565\\ 0\end{pmatrix}. \tag{13}$$

5. Figure 5, mathematical formulas for CD, EF, GH, IJ Chains obtained from the basic AB Chains respectively are

$$C(D)/I(J)=\begin{pmatrix}-1 & 0 & 0\\ 0 & 1 & 0\\ 0 & 0 & -1\end{pmatrix}A(B)+\begin{pmatrix}25.2415\\ \pm 4.7185\\ 0\end{pmatrix}, \tag{14}$$

$$E(F)/G(H)=\begin{pmatrix}-1 & 0 & 0\\ 0 & 1 & 0\\ 0 & 0 & -1\end{pmatrix}A(B)+\begin{pmatrix}21.69816\\ \pm 4.7185\\ 22.52862\end{pmatrix}. \tag{15}$$

$$\begin{pmatrix}1 & 0 & 0\\ 0 & 1 & 0\\ 0 & 0 & 1\end{pmatrix}A(B)+\begin{pmatrix}23.7405\\ 4.7185\\ 0\end{pmatrix}. \tag{16}$$

6. Figure 6, mathematical formulas for CD, EF, GH Chains obtained from the basic AB Chains respectively are

$$C(D)=\begin{pmatrix}1 & 0 & 0\\ 0 & 1 & 0\\ 0 & 0 & 1\end{pmatrix}A(B)+\begin{pmatrix}11.593\\ 0\\ 0\end{pmatrix}, \tag{17}$$

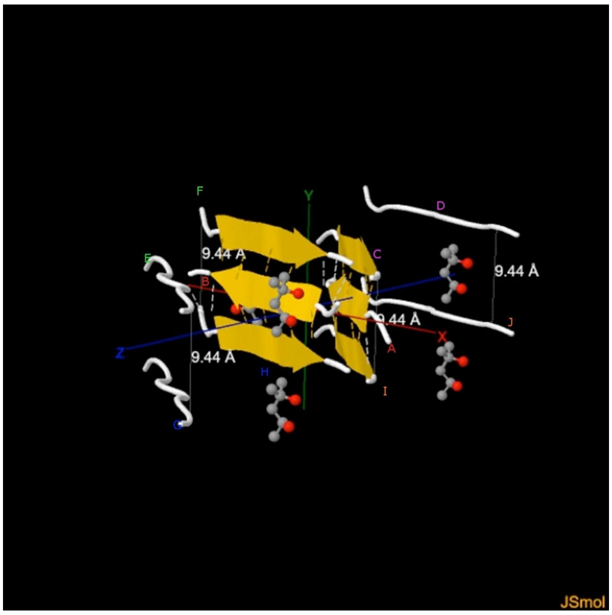

Figure 5: Protein fibril structure of human M129 prion GGYMLGS (126–132) (PDB ID: 4W5M). The dashed lines denote the hydrogen bonds. A, B denote the basic chains of the fibril.

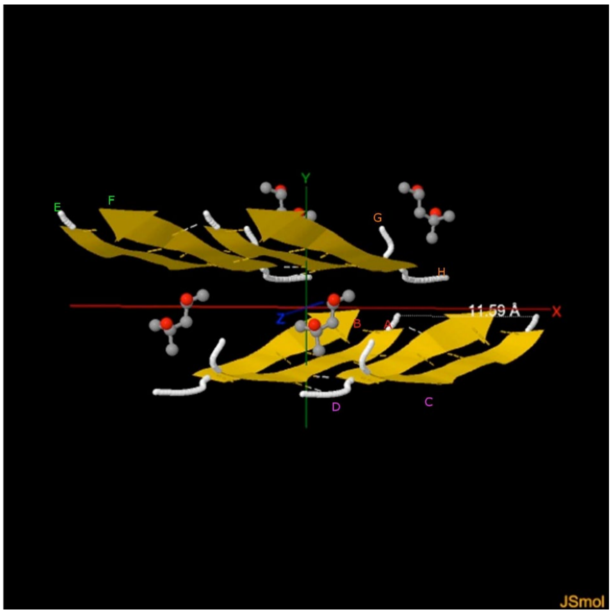

Figure 6: Protein fibril structure of human V129 prion GGYVLGS (126–132) (PDB ID: 4W5P). The dashed lines denote the hydrogen bonds. A, B, C, D, E, F, G, H denote the chains of the fibril.

$$E(F)=\begin{pmatrix}-1 & 0 & 0\\ 0 & 1 & 0\\ 0 & 0 & -1\end{pmatrix}A(B)+\begin{pmatrix}0\\ 8.576\\ 0\end{pmatrix}, \tag{18}$$

$$G(H)=\begin{pmatrix}-1 & 0 & 0\\ 0 & 1 & 0\\ 0 & 0 & -1\end{pmatrix}A(B)+\begin{pmatrix}11.593\\ 8.576\\ 0\end{pmatrix}. \tag{19}$$

7. Figure 7, mathematical formulas for CD, EF, G H Chains obtained from the basic AB Chains respectively are

$$C(D)=\begin{pmatrix}1 & 0 & 0\\ 0 & 1 & 0\\ 0 & 0 & 1\end{pmatrix}A(B)+\begin{pmatrix}9.467\\ 0\\ 0\end{pmatrix}, \tag{20}$$

$$E(F)=\begin{pmatrix}1 & 0 & 0\\ 0 & 1 & 0\\ 0 & 0 & 1\end{pmatrix}A(B)+\begin{pmatrix}\pm 4.12073\\ \pm 9.59126\\ 0\end{pmatrix}, \tag{21}$$

$$G=\begin{pmatrix}1 & 0 & 0\\ 0 & 1 & 0\\ 0 & 0 & 1\end{pmatrix}A+\begin{pmatrix}13.58773\\ \pm 9.59126\\ 0\end{pmatrix}, \tag{22}$$

$$H=\begin{pmatrix}1 & 0 & 0\\ 0 & 1 & 0\\ 0 & 0 & 1\end{pmatrix}B+\begin{pmatrix}5.34627\\ -9.59126\\ 0\end{pmatrix}. \tag{23}$$

8. Figure 8, mathematical formulas for CD, EF, GH Chains obtained from the basic AB Chains respectively are

$$C(D)=\begin{pmatrix}1 & 0 & 0\\ 0 & 1 & 0\\ 0 & 0 & 1\end{pmatrix}A(B)+\begin{pmatrix}8.519\\ 0\\ 0\end{pmatrix}, \tag{24}$$

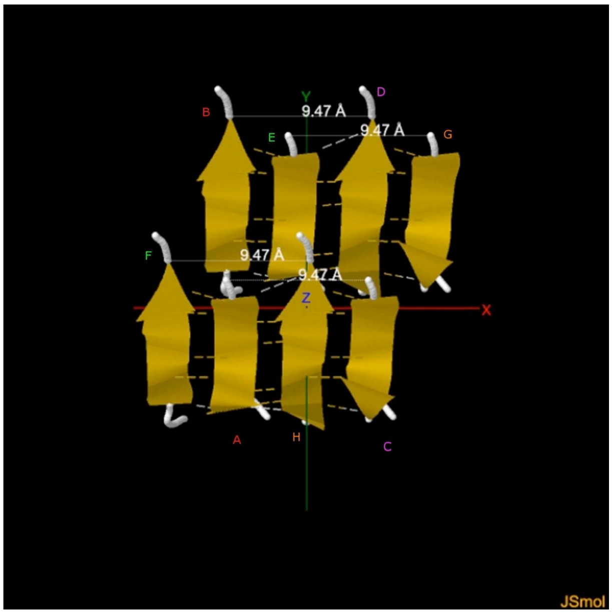

Figure 7: Protein fibril structure of human M129 prion GYMLGSA (127–133) (PDB ID: 4W5Y). The dashed lines denote the hydrogen bonds. A, B denote the basic chains of the fibril.

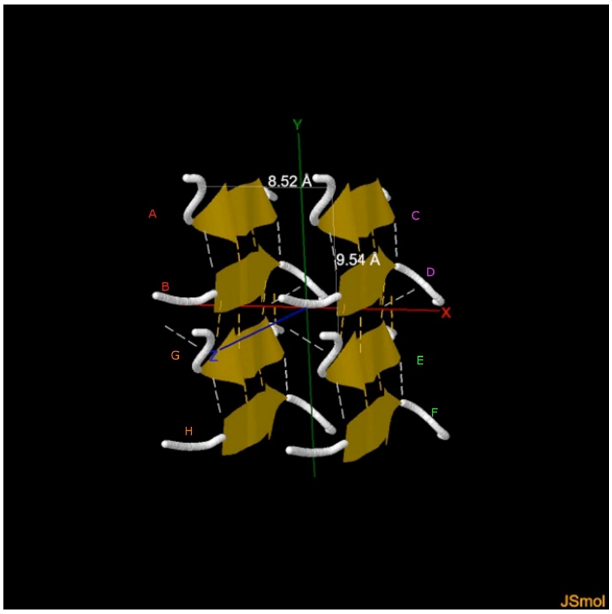

Figure 8: Protein fibril structure of human V129 prion GYVLGSA (127–133) (PDB ID: 4W67). The dashed lines denote the hydrogen bonds. A, B denote the basic chains of the fibril.

$$E(F)(/G(H))=\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}A(B)+\begin{pmatrix}8.53565(/0.01665)\\-9.53999\\0\end{pmatrix}, \qquad (25)$$

9. Figure 9, mathematical formulas for CD, EF, GH Chains obtained from the basic AB Chains respectively are

$$C(D)=\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}A(B)+\begin{pmatrix}9.467\\0\\0\end{pmatrix}, \qquad (26)$$

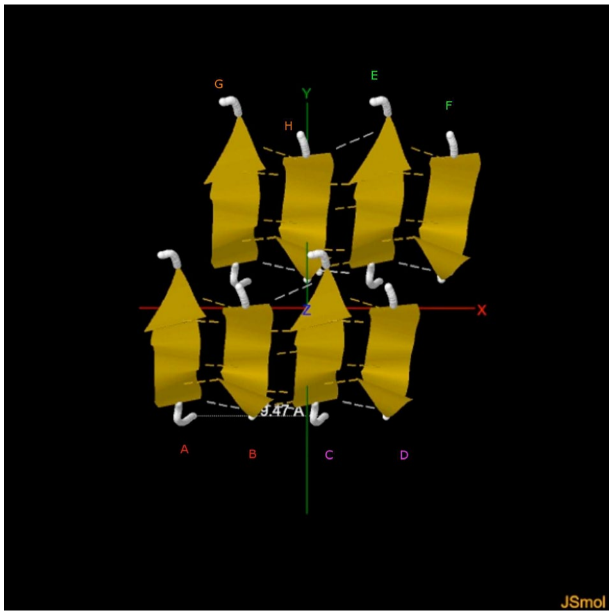

Figure 9: Protein fibril structure of human L129 prion GYLLGSA (127–133) (PDB ID: 4W71). The dashed lines denote the hydrogen bonds. A, B denote the basic chains of the fibril.

$$E(F)(/G(H))=\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}A(B)+\begin{pmatrix}13.36456(/3.89756)\\9.62263\\0\end{pmatrix}. \qquad (27)$$

10. Figure 10, mathematical formulas for CD, EF, GH Chains obtained from the basic AB Chains respectively are

$$C(D)=\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}A(B)+\begin{pmatrix}9.439\\0\\0\end{pmatrix}, \qquad (28)$$

$$E(F)=\begin{pmatrix}-1&0&0\\0&1&0\\0&0&-1\end{pmatrix}A(B)+\begin{pmatrix}9.439\\8.896\\22.2805\end{pmatrix}, \qquad (29)$$

$$G(H)=\begin{pmatrix}-1&0&0\\0&1&0\\0&0&-1\end{pmatrix}A(B)+\begin{pmatrix}18.878\\8.896\\22.2805\end{pmatrix}. \qquad (30)$$

11. Figure 11, mathematical formulas for CD, EF, GH Chains obtained from the basic AB Chains respectively are

$$C(D)(/E(F))=\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}A(B)+\begin{pmatrix}-1.00212\\0(/-9.459\\19.64646\end{pmatrix}, \qquad (31)$$

$$G(H)=\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}A(B)+\begin{pmatrix}0\\-9.459\\0\end{pmatrix}. \qquad (32)$$

$$\begin{pmatrix}-1&0&0\\0&1&0\\0&0&-1\end{pmatrix}A(B)+\begin{pmatrix}0\\4.7295\\0\end{pmatrix}. \qquad (33)$$

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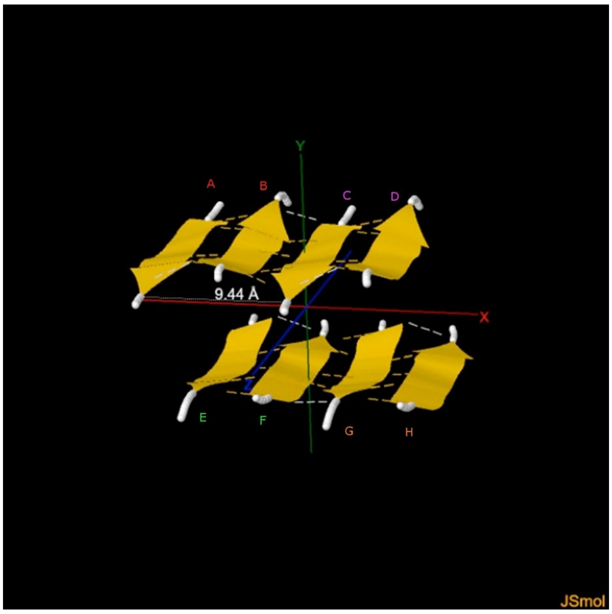

Figure 10: Protein fibril structure of human M129 prion GYMLGS (127–132) (PDB ID: 4WBU). The dashed lines denote the hydrogen bonds. A, B denote the basic chains of the fibril.

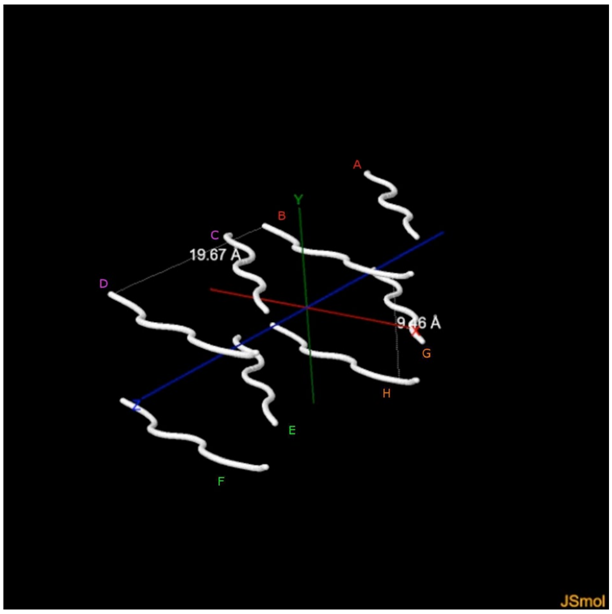

Figure 11: Protein fibril structure of human V129 prion GYVLGS (127–132) (PDB ID: 4WBV). A, B denote the basic chains of the fibril.

12. Figure 12, basing on AB Chains, other chains CD, EF, GH in the asym-metric one unit cell can be obtained by the mathematical formulas

$$C(D)=\begin{pmatrix}-1 & 0 & 0\\ 0 & -1 & 0\\ 0 & 0 & 1\end{pmatrix}A(B)+\begin{pmatrix}4.7195\\ 0\\ 22.2805\end{pmatrix}, \tag{34}$$

$$E(F)=\begin{pmatrix}-1 & 0 & 0\\ 0 & 1 & 0\\ 0 & 0 & -1\end{pmatrix}A(B)+\begin{pmatrix}0\\ 8.896\\ 22.2805\end{pmatrix}, \tag{35}$$

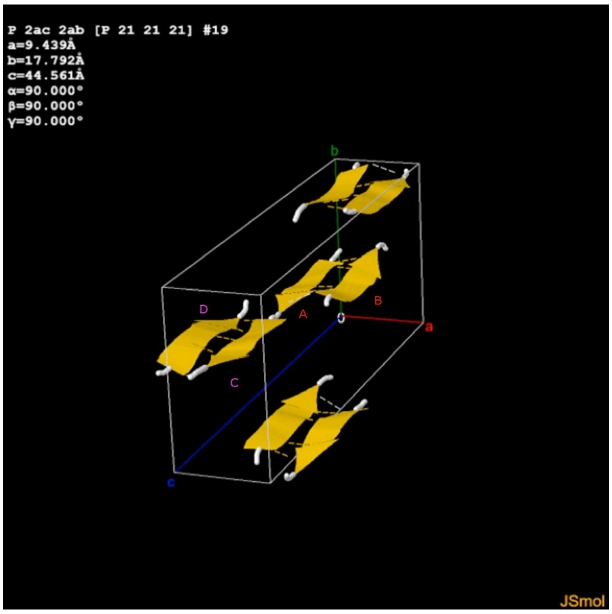

Figure 12: Protein fibril structure of human M129 prion GYMLGS (127–132) (PDB ID: 3MD4). The dashed lines denote the hydrogen bonds. A, B, C, D, E, F, G, H denote the chains of the fibril.

$$G(H)=\begin{pmatrix}1 & 0 & 0\\ 0 & -1 & 0\\ 0 & 0 & -1\end{pmatrix}A(B)+\begin{pmatrix}4.7195\\ 8.896\\ 0\end{pmatrix}. \tag{36}$$

13. Figure 13, basing on AB Chains, other Chains CD in the asymmetric unit cell can be obtained by mathematical formula

$$C(D)=\begin{pmatrix}-1 & 0 & 0\\ 0 & 1 & 0\\ 0 & 0 & -1\end{pmatrix}A(B)+\begin{pmatrix}0\\ 4.7295\\ 0\end{pmatrix}. \tag{37}$$

14. Figure 14 we see that G(H) chains (i.e., β-sheet 2) of 3NHC.pdb can be obtained from A(B) chains (i.e., β-sheet 1) by

$$G(H)=\begin{pmatrix}1 & 0 & 0\\ 0 & -1 & 0\\ 0 & 0 & -1\end{pmatrix}A(B)+\begin{pmatrix}9.07500\\ 4.77650\\ 0.00000\end{pmatrix}, \tag{38}$$

and other chains can be got by

$$I(J)=G(H)+\begin{pmatrix}0\\ 9.5530\\ 0\end{pmatrix}, K(L)=G(H)+\begin{pmatrix}0\\ -9.5530\\ 0\end{pmatrix}, \tag{39}$$

$$C(D)=A(B)+\begin{pmatrix}0\\ 9.5530\\ 0\end{pmatrix}, E(F)=A(B)+\begin{pmatrix}0\\ -9.5530\\ 0\end{pmatrix}. \tag{40}$$

15. By observations of the 3rd column of coordinates of 3NHD.pdb and Figure 15, G(H) chains (i.e., β-sheet 2) of 3NHD.pdb can be calculated from A(B) chains (i.e., β-sheet 1) by Equation (41) and other chains can be calculated by Equations (42)~(43):

$$G(H)=\begin{pmatrix}-1 & 0 & 0\\ 0 & 1 & 0\\ 0 & 0 & -1\end{pmatrix}A(B)+\begin{pmatrix}-20.5865\\ 9.48\\ 0\end{pmatrix}, \tag{41}$$

$$K(L)=G(H)+\begin{pmatrix}0\\ 0\\ 9.59\end{pmatrix}, I(J)=G(H)+\begin{pmatrix}0\\ 0\\ -9.59\end{pmatrix}, \tag{42}$$

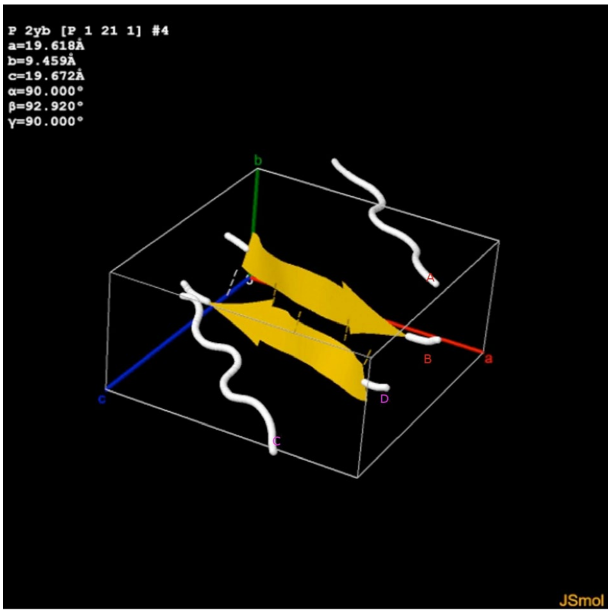

Figure 13: Protein fibril structure of human V129 prion GYMLGS (127–132) (PDB ID: 3MD5). The dashed lines denote the hydrogen bonds. A, B, C, D denote the chains of the fibril.

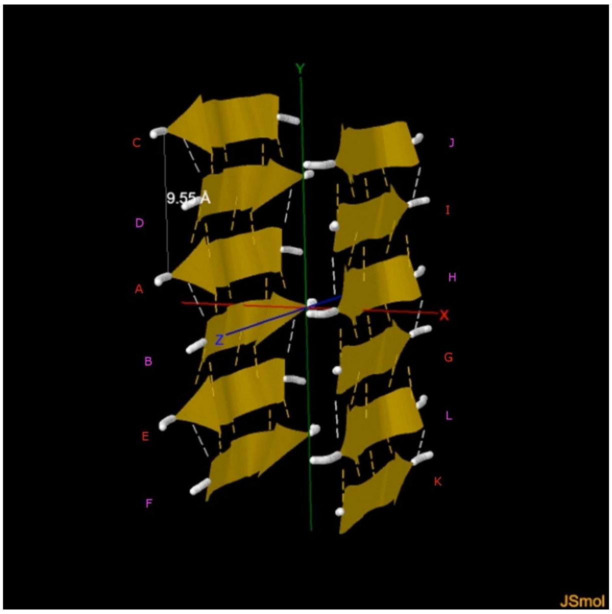

Figure 14: Protein fibril structure of human M129 prion GYMLGS (127–132) (PDB ID: 3NHC). The dashed lines denote the hydrogen bonds. A, B ... K, L denote the chains of the fibril.

$$C(D) = A(B) + \begin{pmatrix} 0 \\ 0 \\ 9.59 \end{pmatrix}, E(F) = A(B) + \begin{pmatrix} 0 \\ 0 \\ -9.59 \end{pmatrix}. \tag{43}$$

16. In Figure 16 we see that H Chain (i.e., β-sheet 2) of 3NVG.pdb can be obtained from A Chain (i.e., *β*-sheet 1) by

$$H = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix} A + \begin{pmatrix} -27.28 \\ 2.385 \\ 15.738 \end{pmatrix}, \tag{44}$$

and other chains can be got by

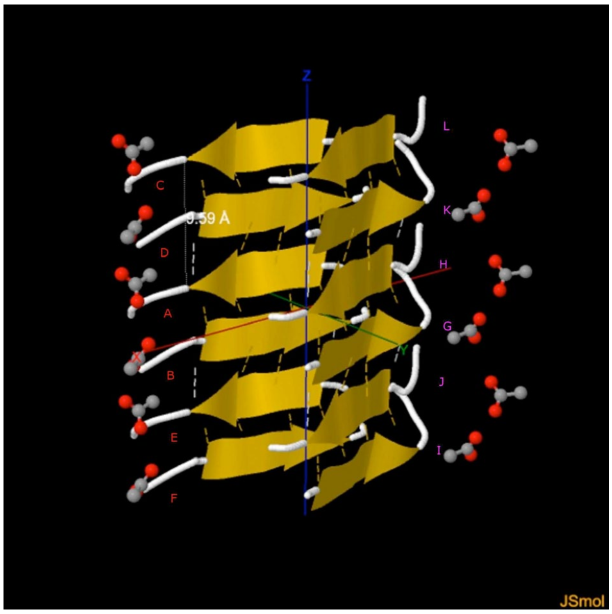

Figure 15: Protein fibril structure of human V129 prion GYVLGS (127-132) (PDB ID: 3NHD). The dashed lines denote the hydrogen bonds. A, B ... K, L denote the chains of the fibril.

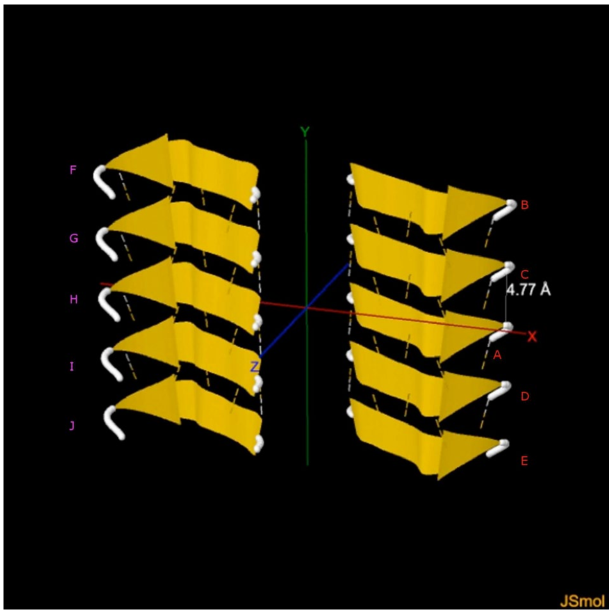

Figure 16: Protein fibril structure of MIHFGN segment 137–142 from mouse prion (PDB ID: 3NVG). The purple dashed lines denote the hydrogen bonds. A, B, ..., I, J denote the 10 chains of the fibril.

$$C(G) = A(H) + \begin{pmatrix} 0 \\ 4.77 \\ 0 \end{pmatrix}, B(F) = A(H) + 2\begin{pmatrix} 0 \\ 4.77 \\ 0 \end{pmatrix}, \tag{45}$$

$$D(I) = A(H) - \begin{pmatrix} 0 \\ 4.77 \\ 0 \end{pmatrix}, E(J) = A(H) - 2\begin{pmatrix} 0 \\ 4.77 \\ 0 \end{pmatrix}. \tag{46}$$

17. In Figure 17 we see that H chain (i.e., β-sheet 2) of 3NVH.pdb can be obtained from A chain (i.e., *β*-sheet 1) by

$$H=\begin{pmatrix}-1 & 0 & 0\\ 0 & 1 & 0\\ 0 & 0 & -1\end{pmatrix}A+\begin{pmatrix}0\\ 2.437\\ -15.553\end{pmatrix}, \tag{47}$$

and other chains can be got by

$$C(G)=A(H)+\begin{pmatrix}0\\ 4.87\\ 0\end{pmatrix}, B(F)=A(H)+2\begin{pmatrix}0\\ 4.87\\ 0\end{pmatrix}, \tag{48}$$

$$D(I)=A(H)-\begin{pmatrix}0\\ 4.87\\ 0\end{pmatrix}, E(J)=A(H)-2\begin{pmatrix}0\\ 4.87\\ 0\end{pmatrix}. \tag{49}$$

18. In Figure 18 we see that G(H) chains (i.e., β-sheet 2) of 3NVE.pdb can be obtained from A(B) chains (i.e., β-sheet 1) by

$$G(H)=A(B)+\begin{pmatrix}0\\ 11.784\\ 0\end{pmatrix}, \tag{50}$$

and other chains can be got by

$$C(D)=A(B)+\begin{pmatrix}9.513\\ 0\\ 0\end{pmatrix}, E(F)=A(B)+\begin{pmatrix}-9513\\ 0\\ 0\end{pmatrix}, \tag{51}$$

$$J(I)=H(G)+\begin{pmatrix}9.513\\ 0\\ 0\end{pmatrix}, L(K)=H(G)+\begin{pmatrix}-9513\\ 0\\ 0\end{pmatrix}. \tag{52}$$

19. In Figure 19 we see that H chain (i.e., β-sheet 2) of 3NVF.pdb can be obtained from A chain (i.e., β-sheet 1) by

$$H=\begin{pmatrix}-1 & 0 & 0\\ 0 & -1 & 0\\ 0 & 0 & 1\end{pmatrix}A+\begin{pmatrix}27.546\\ 0\\ 0\end{pmatrix}, \tag{53}$$

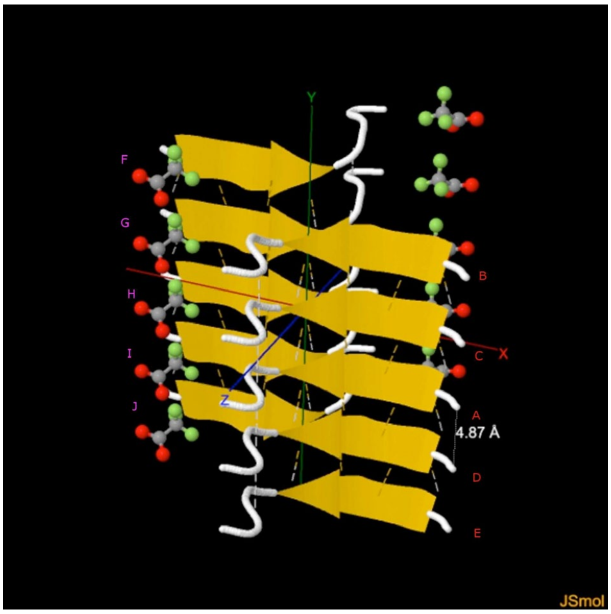

Figure 17: Protein fibril structure of MIHFGND segment 137–143 from mouse prion (PDB ID: 3NVH). The purple dashed lines denote the hydrogen bonds. A, B, ..., I, J denote the 10 chains of the fibril.

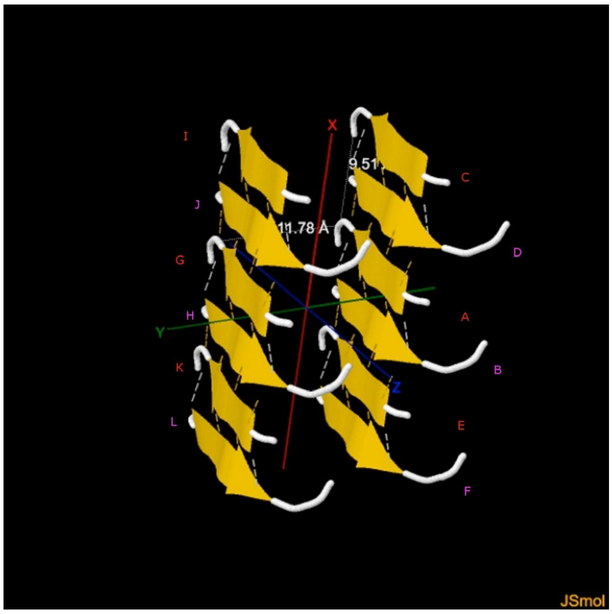

Figure 18: Protein fibril structure of MMHFGN segment 138–143 from Syrian Hamster prion (PDB ID: 3NVE). The purple dashed lines denote the hydrogen bonds. A, B, ..., K, L denote the 12 chains of the fibril.

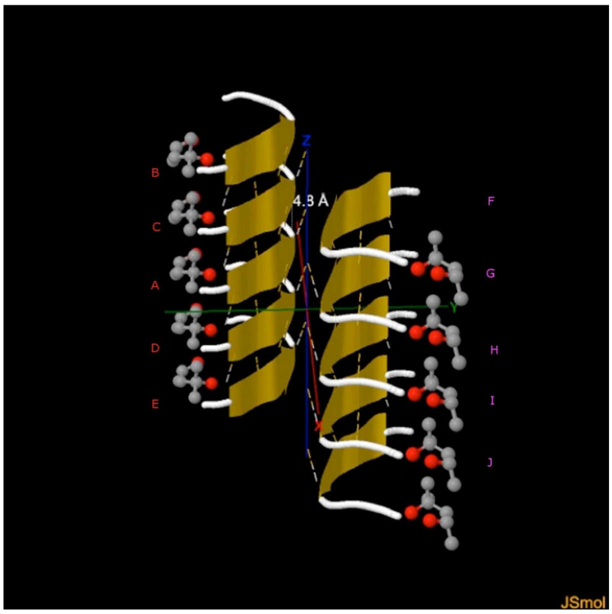

Figure 19: Protein fibril structure of IIHFGS segment 138–143 from human prion (PDB ID: 3NVF). The purple dashed lines denote the hydrogen bonds. A, B, ..., I, J denote the 10 chains of the fibrils.

and other chains can be got by

$$C(G)=A(H)+\begin{pmatrix}0\\ 0\\ 4.8\end{pmatrix}, B(F)=A(H)+2\begin{pmatrix}0\\ 0\\ 4.8\end{pmatrix}, \tag{54}$$

$$D(I)=A(H)-\begin{pmatrix}0\\ 0\\ 4.8\end{pmatrix}, E(J)=A(H)-2\begin{pmatrix}0\\ 0\\ 4.8\end{pmatrix}. \tag{55}$$

20. Figure 20.

21. In Figure 21, we see that the D chain (i.e., β-sheet 2) of 2OL9.pdb can

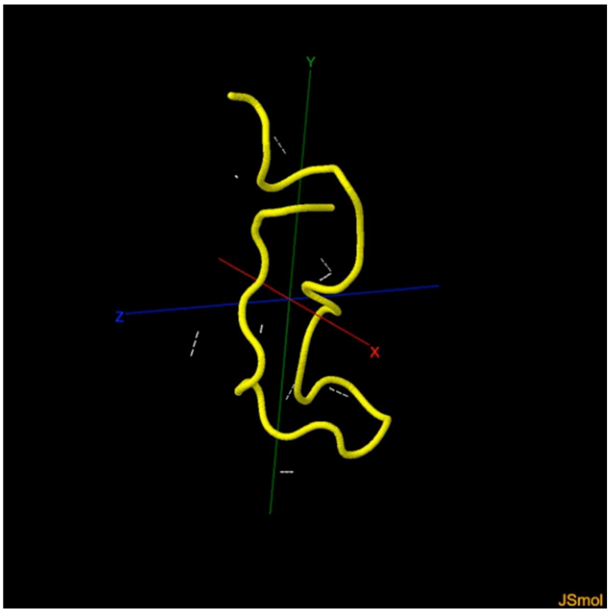

Figure 20: Protein β-hairpin structure of segment 142–166 from sheep prion (PDB ID: 1G04). The dashed lines denote the hydrogen bonds.

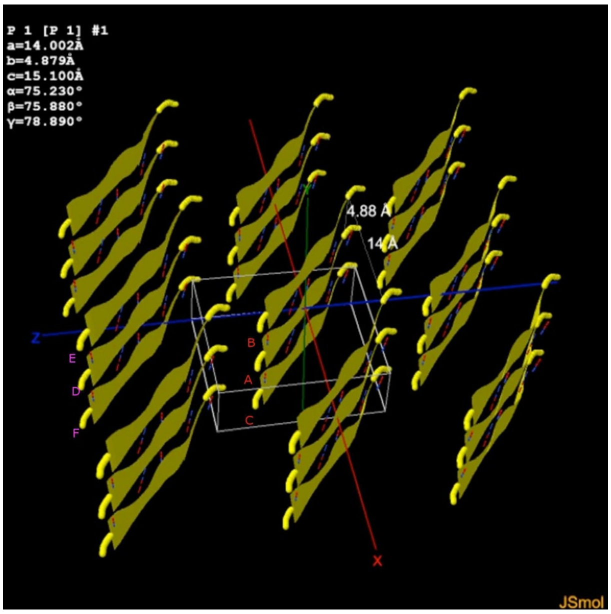

Figure 21: Protein fibril structure of NNQNTF segment 170–175 from human prion (PDB ID: 2OL9). The dashed lines denote the hydrogen bonds. A, B, C, D, E, F denote the 6 chains of the fibrils.

be obtained from A Chain (i.e., β-sheet 1) using the mathematical formula

$$D=\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}A+\begin{pmatrix}0.94015\\4.78756\\0\end{pmatrix}, \qquad (56)$$

and other chains can be got by

$$B(E)=A(D)+\begin{pmatrix}0\\4.88\\0\end{pmatrix}, \qquad (57)$$

$$C(F)=A(D)-\begin{pmatrix}0\\4.88\\0\end{pmatrix}. \qquad (58)$$

22. In Figure 22, we see that the D chain (i.e., β-sheet 2) of 3FVA.pdb can be obtained from A Chain (i.e., β-sheet 1) using the mathematical formula

$$D=\begin{pmatrix}-1&0&0\\0&1&0\\0&0&-1\end{pmatrix}A+\begin{pmatrix}-14.31482\\2.42\\-21.03096\end{pmatrix}, \qquad (59)$$

and other chains can be got by

$$B(E)=A(D)+\begin{pmatrix}0\\4.88\\0\end{pmatrix}, \qquad (60)$$

$$C(F)=A(D)-\begin{pmatrix}0\\4.88\\0\end{pmatrix}. \qquad (61)$$

23. Figure 23.
24. Figure 24.

All the above X-ray crystallography structures show to us, in the PrP(119-231) structured region, there are many segments of peptides which can formulate into amyloid fibrils. The author's theoretical calculations [5,6] (Figures 25 and 26, where -26 kcal/mol is the threshold energy of amyloid fibril formation: if energy is less than -26 kcal/mol it will have amyloid fibril forming property [7]) also show this point.

Last, seeing Figure 26, we may think there must be a laboratory X-ray crystal β-type structure in PrP(184-192) segment that will be produced by a X-ray lab in the near future.

In conclusion, this short article described about the comparison study of theoretical calculations and X-ray crystallography study

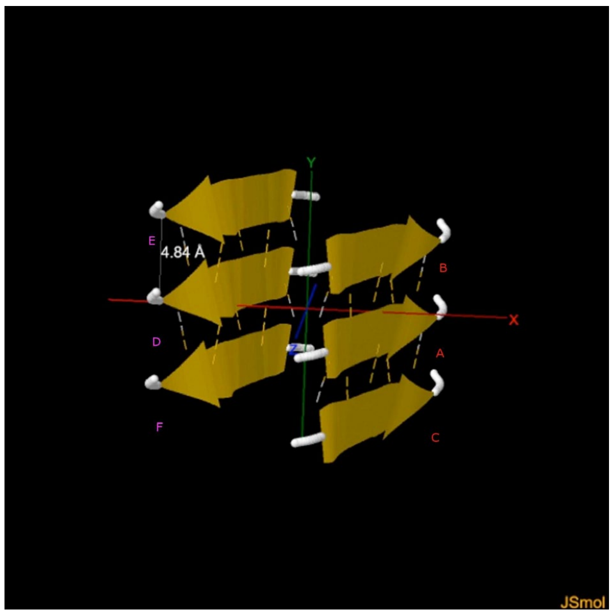

Figure 22: Protein fibril structure of NNQNTF segment 170–175 from elk prion (PDB ID: 3FVA). The dashed lines denote the hydrogen bonds. A, B, C, D, E, F denote the 6 chains of the fibrils.

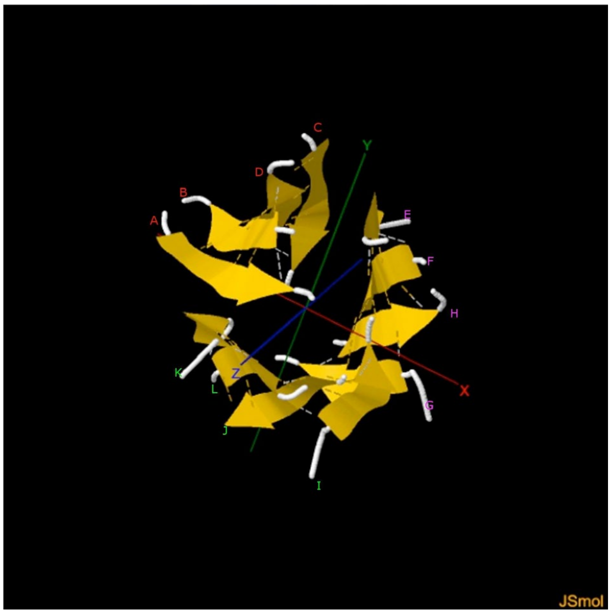

Figure 23: Protein *β*-prism fibril structure of segments 177–182, 211–216 from human prion (PDB ID: 4E1I). The dashed lines denote the hydrogen bonds. A, B, C, D, E, F, G, H, I, J, K, L denote the 12 chains of the fibrils.

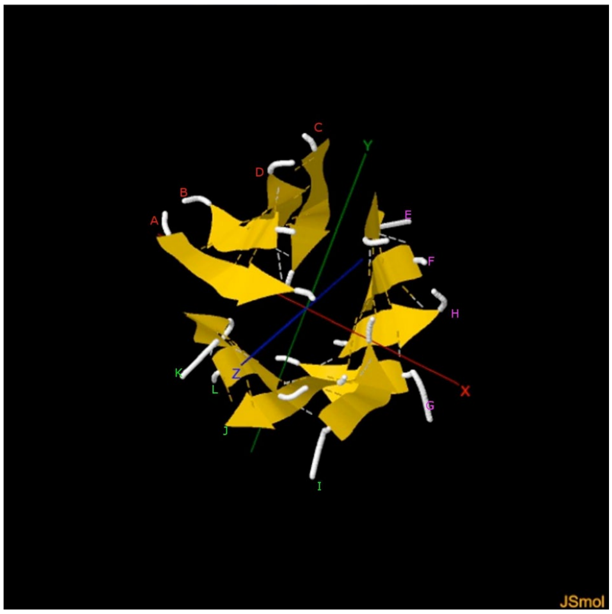

Figure 24: Protein *β*-prism fibril structure of segments 177–182, 211–216 from human prion (PDB ID: 4E1H). The dashed lines denote the hydrogen bonds. A, B, C, D, E, F, G, H, I, J, K, L denote the 12 chains of the fibrils.

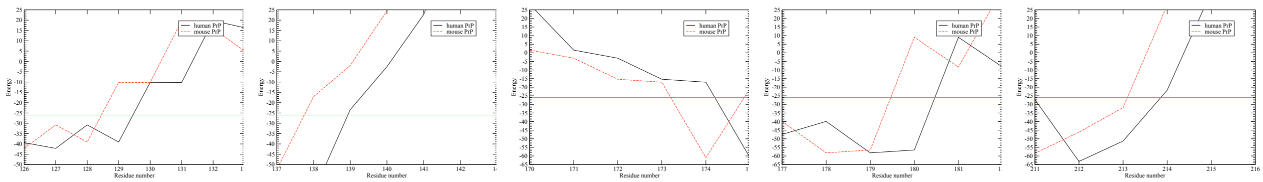

Figure 25: By theoretical calculations of the author, PrP(126-133), PrP(137-143), PrP(170-175), PrP(177-182), PrP(211-216) were identified owning the amyloid fibril forming property respectively (the graphs from left to right).

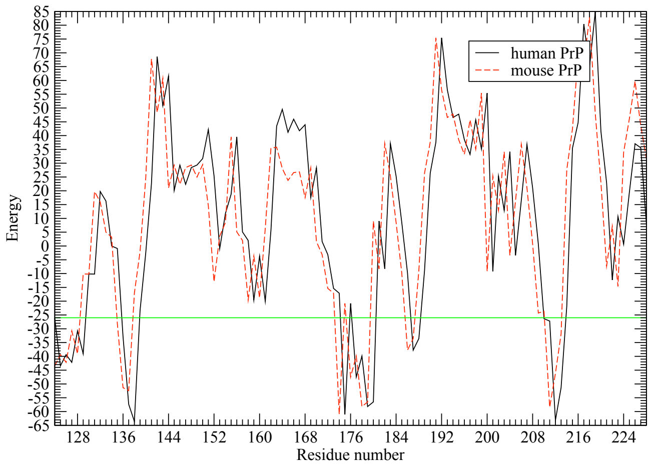

Figure 26: To identify the segments owning the amyloid fibril forming property in the whole PrP structured region: if the energy is less than -26 kcal/mol it will have amyloid fibril forming property [7].

of prion protein cross-beta structures. The author has very good prediction of theoretical calculations using mathematical formulas of unstructured region and structured region of prion proteins in detail well demonstrated. Moreover, the X-ray crystallography structures showed, in the PrP(119–231) structured region, there are many segments of peptides which can formulate into amyloid fibrils. The author's theoretical calculations for Figures 25 and 26 were shown threshold energy as -26 kcal/mol, which supports to the amyloid fibril formation. Even if the threshold energy is less than -26 kcal/mol also they will have amyloid fibril forming property. This is a good piece of work useful for the medicinal chemists. The author presented the results very well in the article, and provided an introduction of the structures to understand the significance in the biological use of amyloid fibrils [8-14].

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