Figure S1 The structure analysis for SGC1, (a) the first 15 clusters for the all-atom based and (b) backbone based cluster analysis; (c) The RMSD calculation profile; (d) the structure of the first cluster of all-atom based cluster analysis.
Figure S2 The structure analysis for SGB1, (a) the first 15 clusters for the all-atom based and (b) backbone based cluster analysis; (c) The RMSD calculation profile; (d) the structure of the first cluster of all-atom based cluster analysis.
Figure S3 The structure analysis for SGD1, (a) the first 15 clusters for the all-atom based and (b) backbone based cluster analysis; (c) The RMSD calculation profile; (d) the structure of the first cluster and (e) the fifth cluster of all-atom based cluster analysis.
Figure S4 Three binding modes for R defined together with PMF curves. (a) T-edge to B-edge (b) B-edge to B-edge (c) T-edge to T-edge. The right-hand side axis of the graphs refer to PMF curve (kJ/mol) shown in purple line, with the error bars included (±1σ). The left-hand axis is the average intermolecular H-bond counts (blue line), and minimum salt-bridge distances at the polar charged residues at two different sides of β-sheet in nm; Lys16-Glu22, Asp23 (green line), and Glu22, Asp23-Lys16 (red line). The horizontal axis is the separation of the centres of mass in nm. (modified from Mehrazma et al.)
Figure S5 The backbone structure analysis for $R^1$-SGD1, (a) cluster analysis, (b) RMSD, and cluster analysis and also for $R^6$-SGD1 (c) cluster analysis (d) RMSD.
Figure S6 The structure analysis for SGB1 homodimer, (a) the clusters from all-atom based and (b) backbone based cluster analysis, (c) The RMSD calculation profile based on all-atom.

References:

(1) Mehrazma, B.; Petoyan, A.; Opare, S. K. A.; Rauk, A. Interaction of the N-AcAβ(13–23)NH2 Segment of the Beta Amyloid Peptide with Beta-Sheet-Blocking Peptides: Site and Edge Specificity. *Can. J. Chem.* **2016**, *6* (94), 583–592.
Table S2. $\alpha\beta$-SG1 energy analysis: $\alpha\beta$-SG1 (SG1 = PP) energy analysis (kJ/mol). The clusters are listed by the hierarchy of their appearance in the trajectory.

| Cluster number | $P_i$ | $V_{gas}(\alpha\beta^*)$ | $V_{gas}(PP^*)$ | $V_{int}(PP^*-\alpha\beta^*)$ | $V_{gas}(PP-\alpha\beta)$ | $\Delta G_{PBSA}(PP-\alpha\beta)$ | $\Delta G_{gas-PBSA}(PP-\alpha\beta)$ | $\Delta G_{GLIE-D}$ | $\Delta G_{GLIE-DR}$ |
|----------------|-------|--------------------------|-----------------|-------------------------------|--------------------------|--------------------------------|--------------------------------|-----------------|-----------------|
| Ba1            | 0.80  | 4501 ±7                  | 708 ±3          | -349 ±3                       | 4861 ±4                  | -2525 ±11                      | 2335 ±13                        | -33 ±4          | -26 ±11         |
| Bb2            | 0.13  | 4793 ±17                 | 611 ±3          | -617 ±14                      | 4787 ±16                 | -2439 ±13                      | 2243 ±15                        | -14 ±3           | -58 ±7          |
| Bb3            | 0.11  | 4754 ±5                  | 615 ±2          | -624 ±5                       | 4745 ±5                  | -2544 ±20                      | 2241 ±21                        | -16 ±14          | -67 ±4          |
| Bb1            | 0.58  | 4706 ±8                  | 629 ±1          | -668 ±7                       | 4666 ±7                  | -2445 ±16                      | 2221 ±8                         | -37 ±32          | -64 ±4          |
| Bc1            | 0.12  | 4238 ±10                 | 624 ±1          | -402 ±1                       | 4460 ±8                  | -2103 ±10                      | 2357 ±12                        | 100 ±29          | -33 ±3          |
| Bc4            | 0.08  | 4490 ±5                  | 576 ±1          | -567 ±8                       | 4499 ±7                  | -2192 ±35                      | 2307 ±35                        | 50 ±44           | -60 ±5          |
| Monomer        |       |                          |                 |                               |                          |                                |                                 |                 |                 |

Table S3. $\alpha\beta$-SGD1 energy analysis: $\alpha\beta$-SGD1 (SGD1 = PP) energy analysis (kJ/mol). The clusters are listed by the hierarchy of their appearance in the trajectory.

| Cluster number | $P_i$ | $V_{gas}(\alpha\beta^*)$ | $V_{gas}(PP^*)$ | $V_{int}(PP^*-\alpha\beta^*)$ | $V_{gas}(PP-\alpha\beta)$ | $\Delta G_{PBSA}(PP-\alpha\beta)$ | $\Delta G_{gas-PBSA}(PP-\alpha\beta)$ | $\Delta G_{GLIE-D}$ | $\Delta G_{GLIE-DR}$ |
|----------------|-------|--------------------------|-----------------|-------------------------------|--------------------------|--------------------------------|--------------------------------|-----------------|-----------------|
| Da1            | 0.24  | 4459 ±5                  | 706 ±1          | -351 ±3                       | 4814 ±4                  | -2476 ±13                      | 2337 ±14                        | -37 ±3           | -35 ±40         |
| Da2            | 0.23  | 4499 ±13                 | 707 ±1          | -339 ±3                       | 4866 ±11                 | -2539 ±22                      | 2327 ±24                        | 45 ±33           | -40 ±42         |
| Db1            | 0.25  | 4584 ±23                 | 617 ±4          | -616 ±29                      | 4586 ±32                 | -2288 ±12                      | 2298 ±35                        | 16 ±43           | -48 ±4          |
| Db2            | 0.23  | 4584 ±7                  | 616 ±1          | -594 ±5                       | 4606 ±6                  | -2313 ±36                      | 2293 ±37                        | 11 ±62           | -47 ±5          |
| Dc1            | 0.62  | 4606 ±5                  | 691 ±1          | -663 ±5                       | 4633 ±5                  | -1971 ±11                      | 2656 ±12                        | 374 ±29          | -67 ±3          |
| Dd2            | 0.09  | 4651 ±42                 | 597 ±2          | -598 ±32                      | 4650 ±36                 | -2334 ±15                      | 2224 ±16                        | -58 ±31          | -56 ±3          |
| Dd3            | 0.08  | 4589 ±19                 | 593 ±2          | -460 ±7                       | 4722 ±14                 | -2481 ±13                      | 2241 ±19                        | -41 ±32          | -48 ±4          |
| Dd1            | 0.33  | 4476 ±11                 | 611 ±1          | -568 ±3                       | 4519 ±8                  | -2180 ±17                      | 2339 ±19                        | 58 ±32           | -54 ±3          |
| Dd5            | 0.03  | 4365 ±7                  | 605 ±3          | -419 ±3                       | 4551 ±6                  | -2291 ±15                      | 2261 ±16                        | -21 ±31          | -41 ±3          |
| Monomer        |       |                          |                 |                               |                          |                                |                                 |                 |                 |

Table S2: $\alpha\beta$-SG1 energy analysis: $\alpha\beta$-SG1 (SG1 = PP) energy analysis (kJ/mol). The clusters are listed by the hierarchy of their appearance in the trajectory.

Table S3: $\alpha\beta$-SGD1 energy analysis: $\alpha\beta$-SGD1 (SGD1 = PP) energy analysis (kJ/mol). The clusters are listed by the hierarchy of their appearance in the trajectory.
