

Supporting Information

Quantitative Analysis of Solid-State Homonuclear Correlation Spectra of Antiparallel β -Sheet Alanine Tetramers

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Table S1. Effective inter-nuclear distances $r_{j,k}^{eff}(\text{obs})$ obtained from 2D DARR experimentsand $r_{j,k}^{eff}(\text{calc})$ of AP- β -sheet A₄ arrangement obtained from X-ray diffraction data.²⁹Minimum inter-nuclear distances of inter- and intra-strand pairs for P- β -sheet Ala₄ crystals.¹²

Cross peak	$r_{j,k}^{eff}(\text{obs})$ (Å)	$r_{j,k}^{eff}(\text{calc})$ (Å)	Inter nuclear pair	Minimum distance of Intra-strand pair (Å)	Minimum distance of Inter- strand pair (Å)
P1-P4	1.775	1.532	C4-C α 4	1.54	4.13
P2-P5	1.689	1.490	C2-C α 2 C2-C α 3	1.55 2.47	4.48 4.87
P3-P5	1.644	1.502	C1-C α 2 C1-C α 3 C3-C α 2 C3-C α 3	2.47 5.57 4.80 1.55	5.20 6.89 4.73 4.51
P3-P6	1.665	1.494	C1-C α 1 C3-C α 1	1.55 7.89	4.37 6.36
P4-P9	1.681	1.534	C α 4-C β 4	1.53	4.89
P5-P7	1.668	1.529	C α 2-C β 3 C α 3-C β 3	4.71 1.53	4.06 4.24
P5-P8	1.668	1.516	C α 2-C β 1 C α 2-C β 2 C α 3-C β 1 C α 3-C β 2	4.84 1.53 7.17 4.70	4.14 4.71 7.26 4.40
P6-P8	1.696	1.525	C α 1-C β 1 C α 1-C β 2	1.52 4.83	4.08 4.27
P1-P9	2.243	2.445	C4-C β 4	2.50	4.37
P2-P8	2.268	2.408	C2-C β 1 C2-C β 2	5.62 2.47	5.44 5.01
P3-P4	2.910	2.443	C1-C α 4 C3-C α 4	9.00 2.47	4.48 5.19
P3-P7	2.243	2.413	C1-C β 3 C3-C β 3	5.86 2.47	6.27 3.62
P3-P8	2.181	2.313	C1-C β 1 C1-C β 2 C3-C β 1 C3-C β 2	2.49 3.49 8.48 5.37	3.71 5.35 6.26 3.62
P1-P3	3.419	3.396	C4-C1 C4-C3	>10.0 3.63	4.13 5.02
P2-P3	3.040	3.104	C2-C1 C2-C3	3.55 3.57	5.15 5.17
P2-P7	3.083	2.980	C2-C β 3	3.47	3.90
P3-P9	2.962	3.018	C1-C β 4	9.12	3.54

			C3-Cb4	3.32	5.28
P4-P5	3.239	3.586	C α 4-C α 2	6.79	5.12
			C α 4-C α 3	3.86	5.19
P5-P6	3.206	3.500	C α 2-C α 1	3.84	4.94
			C α 3-C α 1	6.54	7.65
P2-P6	3.879	4.357	C2-C α 1	4.66	6.37
P4-P7	3.731	3.929	C α 4-C β 3	4.71	4.37
P5-P9	3.406	3.872	C α 2-C β 4	6.74	3.81
			C α 3-C β 4	4.61	4.38
P1-P7	4.411	4.524	C4-C β 3	5.46	5.49
P7-P8	3.323	3.189	C β 3-C β 1	7.03	7.10
			C β 3-C β 2	5.84	3.78
P7-P9	3.781	3.881	C β 3-C β 4	5.75	3.80
P1-P2	5.656	5.415	C4-C2	6.75	5.53
P2-P9	4.861	5.077	C2-C β 4	5.76	3.73
P6-P7	4.367	4.504	C α 1-C β 3	6.66	7.52
P1-P8	4.032	3.767	C4-C β 1	>10.0	3.73
			C4-C β 2	8.19	3.91
P4-P6	3.942	3.831	C α 4-C α 1	>10.0	4.70
P1-P6	4.383	3.769	C4-C α 1	>10.0	3.93
P6-P9	3.821	3.691	C α 1-C β 4	>10.0	4.16

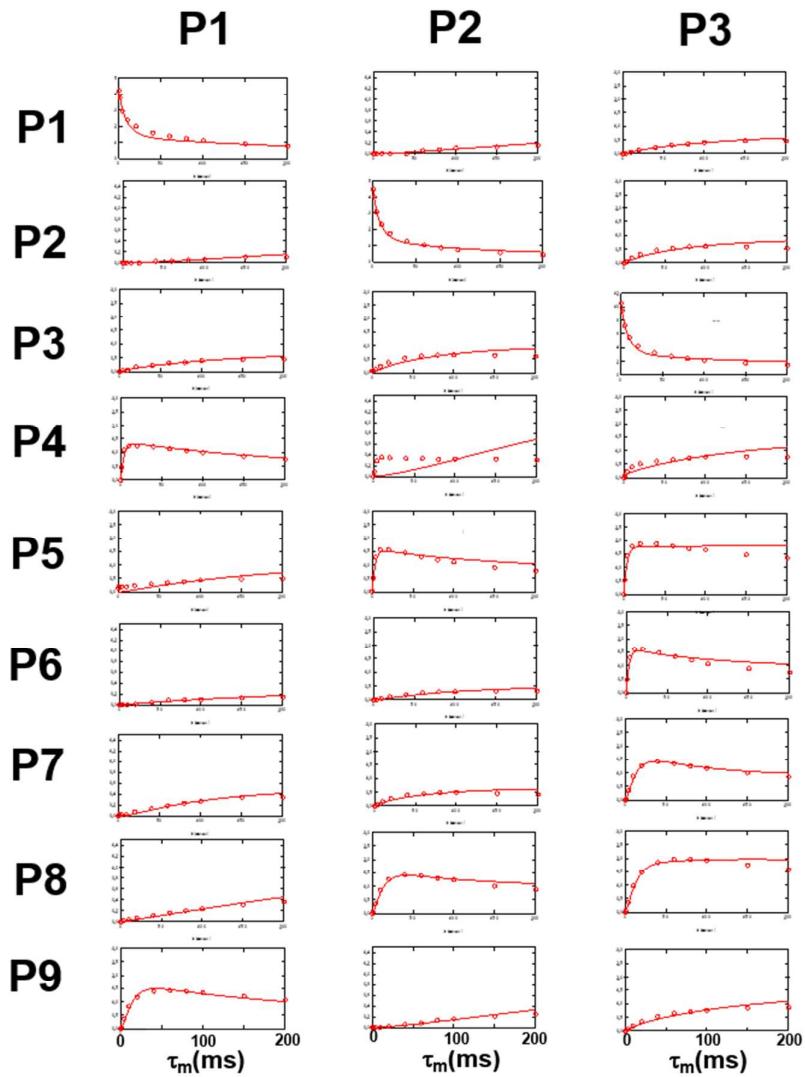


Figure S1(a). Build-up curves of (P1-3, P1-9) cross peaks in AP- β -Ala₄ crystals obtained from 2D DARR experiments.

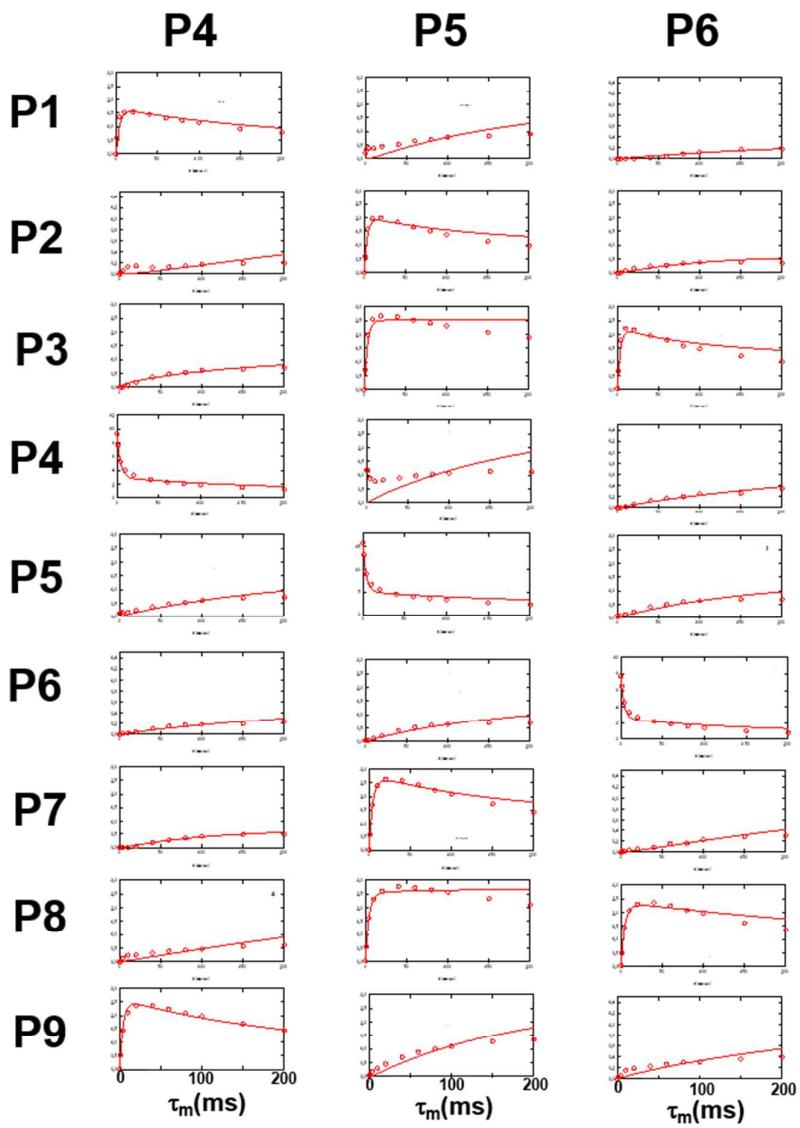


Figure S1(b). Build-up curves of (P4-6, P1-9) cross peaks in AP- β -Ala₄ crystals obtained from 2D DARR experiments.

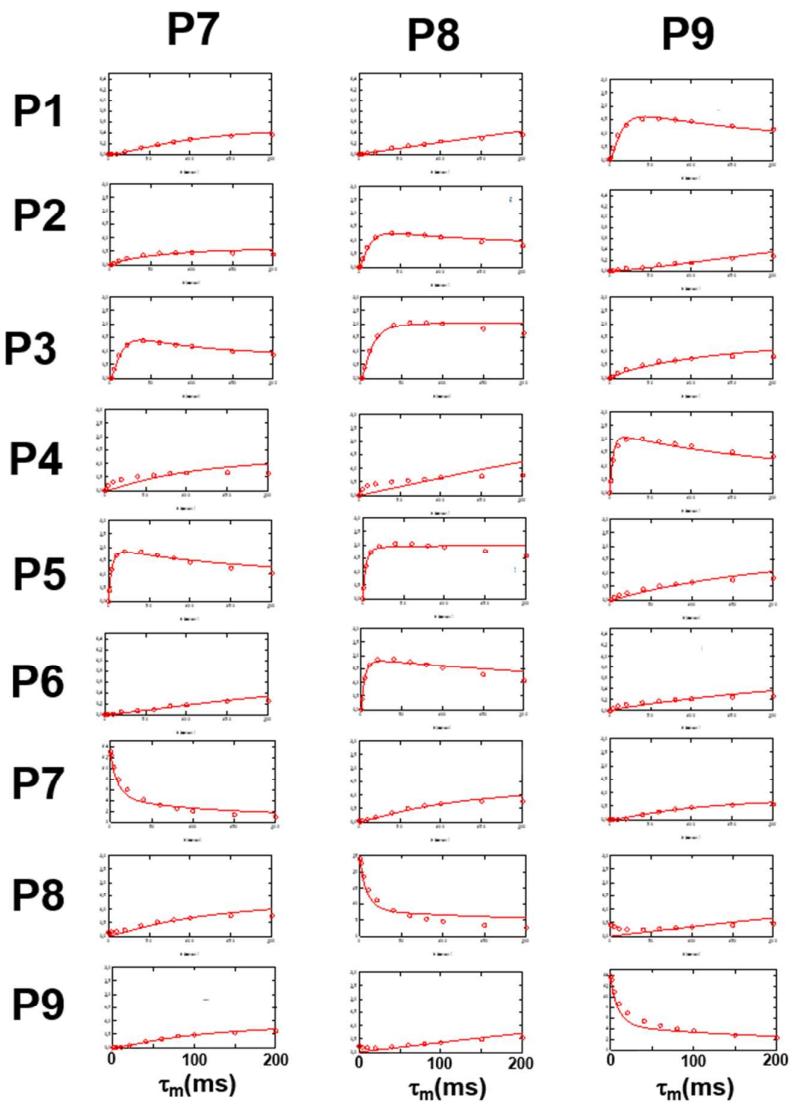


Figure S1(c). Build-up curves of (P7-9, P1-9) cross peaks in AP- β -Ala₄ crystals obtained from 2D DARR experiments

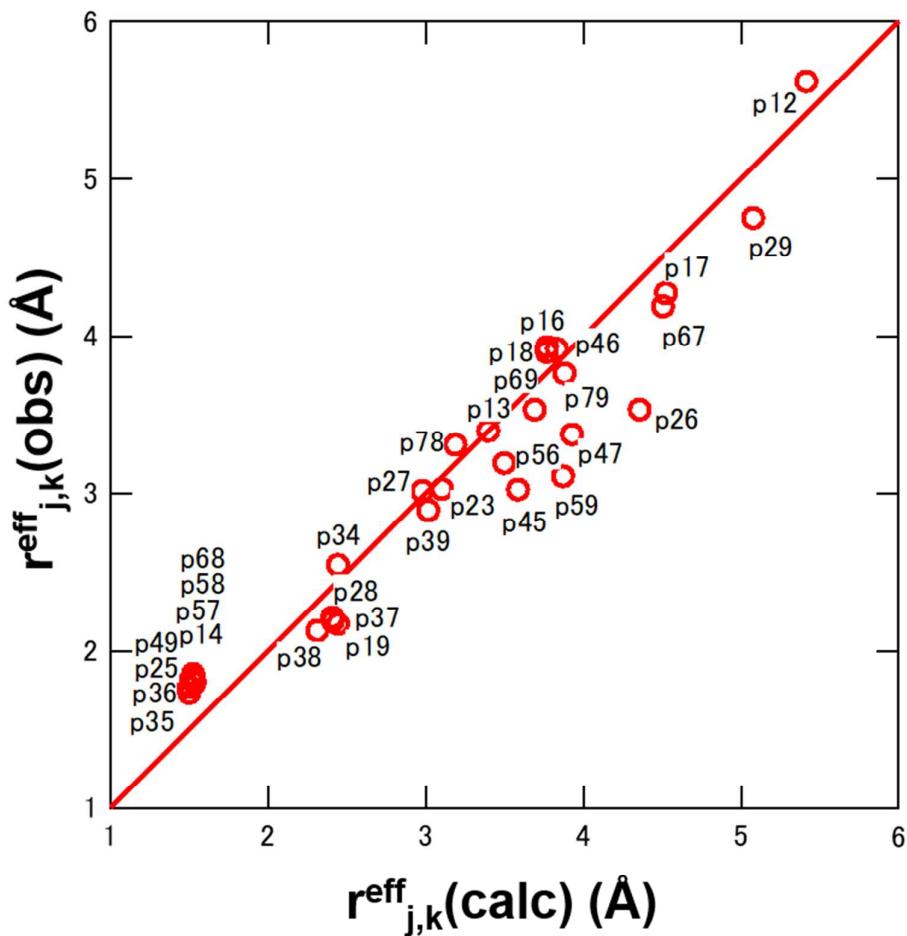


Figure S2. Correlation between $r^{eff}_{j,k}(\text{obs})$ and $r^{eff}_{j,k}(\text{calc})$. Zero-quntum line shape functions of Eqs. [5] and [6] in the text are included. Standard deviation is 0.296 Å.

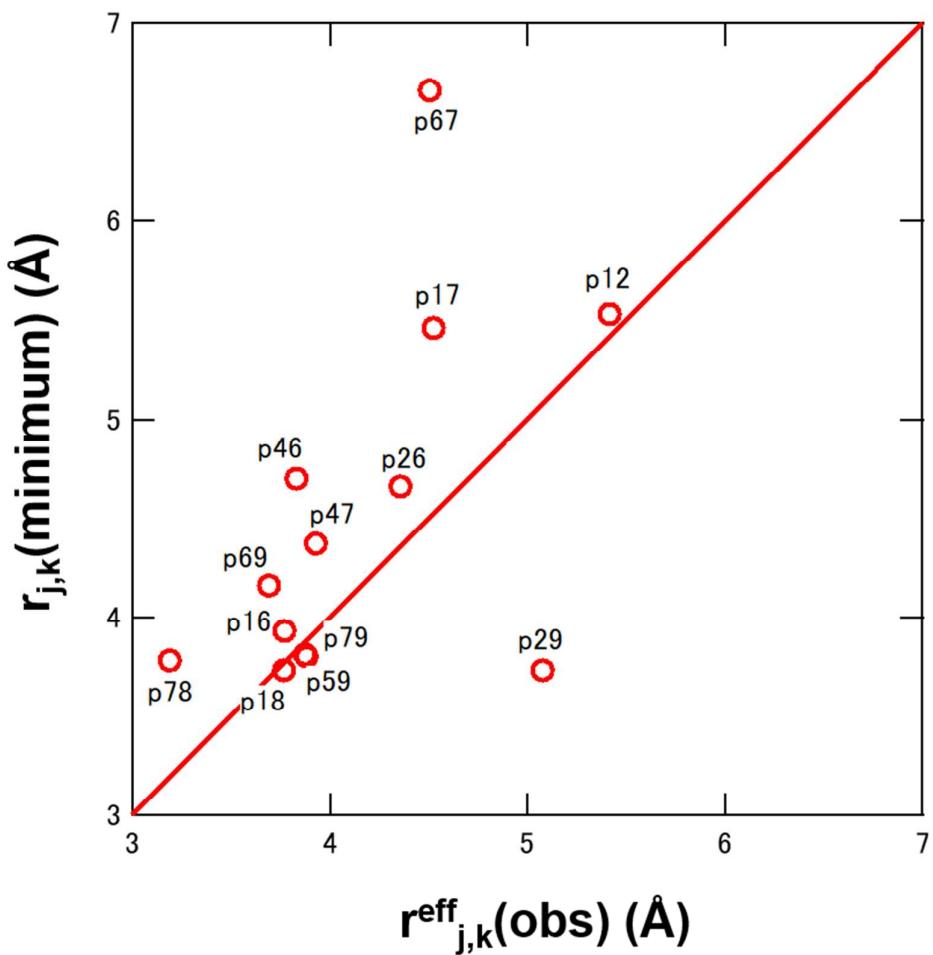


Figure S3. Correlation between $r_{j,k}^{eff}(\text{obs})$ and $r_{j,k}(\text{minimum})$ for P- β -sheet Ala_4 packing arrangement.