

Supplementary material for ‘Multiple binding modes for palmitate to barley lipid transfer protein facilitated by the presence of proline 12’.

Comparison of r^{-3} averaged distances calculated from the simulation trajectories with the 25 inter-proton distances between palmitate and barley LTP derived from the experimental NOE cross-peak intensities. In each case the difference between the distance averaged over the simulation and the corresponding NMR-derived upper distance bound is listed (in nm). A negative value indicates that the distance in the simulation is shorter than the NMR-derived upper distance bound and so there is no violation. The data for the 1be2 NMR structure are given for comparison.

NOE number	Atom 1	Atom 2	NMR structure	WT_LA_310	WT_LA_NOE_310	WT_LAH_310	WT_LB_NOE_400	M12_LAH_310	M12,70_LAH_310
10	PLM H3*	9 Lys HD*	-0.143	-0.209	-0.041	0.316	0.02	0.795	0.498
11	PLM H2*	9 Lys HE*	-0.100	-0.251	-0.081	0.472	0.0190	1.003	0.542
12	PLM H2*	69 Ile HG11	-0.111	0.880	0.084	-0.185	-0.112	-0.164	0.749
13	PLM H2*	10 Met HG*	-0.380	0.290	-0.349	0.036	-0.05	0.730	0.470
14	PLM H2*	14 Leu HD*	-0.467	0.592	-0.357	-0.340	-0.120	0.305	-0.114
15	PLM H2*	81 Ile HD*	-0.398	0.624	-0.105	-0.091	-0.262	0.955	0.0800
16	PLM H2*	81 Ile HG2	-0.409	0.741	-0.013	-0.077	-0.0380	0.938	0.387
17	PLM H3*	14 Leu HD*	-0.290	0.531	-0.349	-0.415	-0.278	0.255	-0.133
18	PLM H3*	81 Ile HD*	-0.203	0.556	-0.118	-0.116	-0.315	0.900	0.0350
19	PLM H3*	81 Ile HG2	-0.276	0.668	-0.058	-0.079	-0.116	0.897	0.332
20	PLM H3*	27 Cys HB2	-0.229	0.420	-0.125	-0.231	-0.256	0.0910	0.598
21	PLM H3*	69 Ile HG2	-0.252	0.553	-0.092	-0.255	-0.184	-0.230	0.529
22	PLM H4*	27 Cys HN	-0.040	0.339	-0.032	-0.111	-0.0110	0.180	0.558
23	PLM H4*	13 Cys HB*	-0.265	0.219	-0.324	-0.092	-0.247	-0.010	0.108
24	PLM HG*	79 Tyr HA	-0.074	-0.040	-0.063	0.073	-0.105	0.030	0.112
25	PLM HG*	79 Tyr HE*	-0.349	0.043	-0.204	-0.104	-0.105	0.263	0.479
26	PLM HG*	35 His HD2	-0.025	0.047	-0.199	-0.272	-0.101	0.320	-0.157
27	PLM HG*	48 Cys HA	-0.292	0.076	-0.188	-0.131	-0.261	-0.219	-0.010

28	PLM HG*	45 Gln HN	-0.112	0.483	-0.061	-0.005	-0.0640	0.287	0.376
29	PLM HG*	44 Arg HA	-0.280	0.101	-0.319	-0.340	-0.297	0.044	0.060
30	PLM HE*	85 Ile HG2	-0.215	0.190	0.008	0.204	-0.0620	0.087	0.133
31	PLM HE*	51 Leu HD*	-0.590	-0.502	-0.443	-0.405	-0.475	-0.280	-0.526
32	PLM HE*	47 Val HG1	-0.347	-0.028	-0.363	-0.341	-0.289	-0.076	-0.242
33	PLM HD*	34 Leu HD2	-0.222	-0.324	-0.225	-0.067	-0.0980	-0.310	-0.094
34	PLM HD*	47 Val HG2	-0.176	0.082	-0.276	-0.149	-0.304	0.192	0.133