Supporting information for

Solvation and the secondary structure of a proline-containing dipeptide: Insights from VCD spectroscopy

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1. Additional spectra

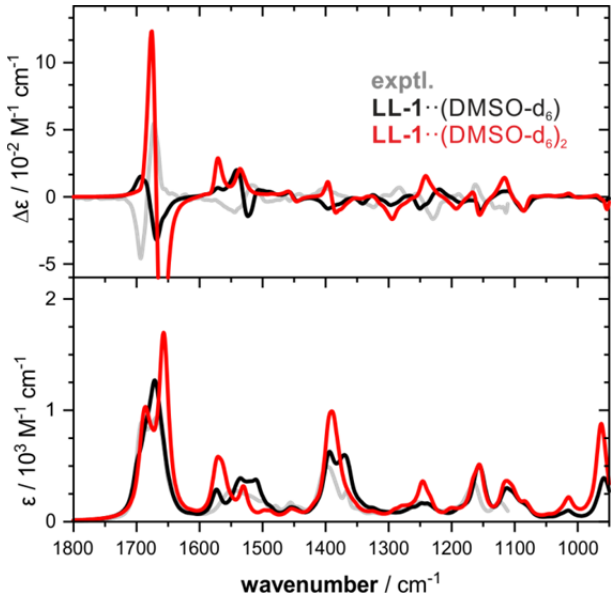


Figure S1. Mono- vs. twofold solvation of LL-**1** with DMSO-d_6**:** Comparison of the experimental IR and VCD spectra of DD- and DL-**1** recorded in DMSO-d_6 (grey) with the computed spectra of LL- and LD-**1**··(DMSO-d_6) and LL- and LD-**1**··(DMSO-d_6)$_2$

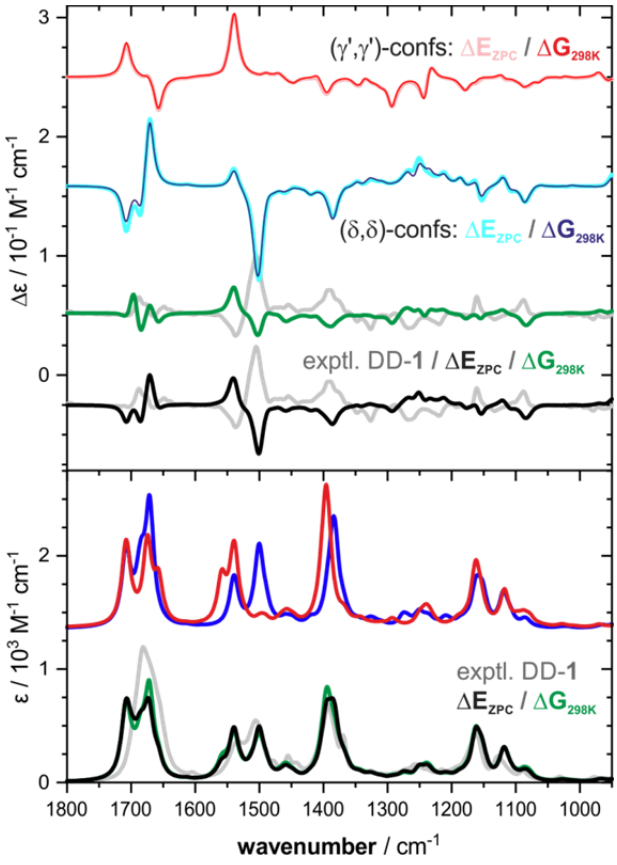


Figure S2. Conformer families of LL-**1** computed based on ΔG_{298K}: Comparison of the experimental IR and VCD spectra of DD-**1** with several sets of computed spectra of LL-**1**.

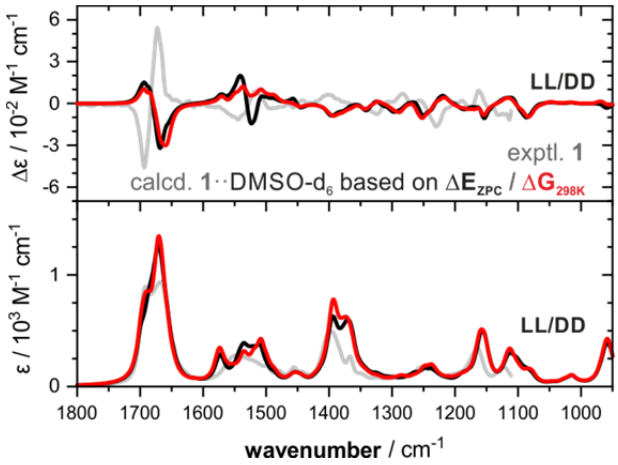


Figure S3. ΔG_{298K}-based spectra of LL-**1**··DMSO-d_6**:** Comparison of the experimental IR and VCD spectra of DD- and DL-**1** recorded in DMSO-d_6 (grey) with the computed spectra of LL-**1**··DMSO-d_6 using Boltzmann weights based on ΔE_{ZPC} (black) and ΔG_{298K} (red).

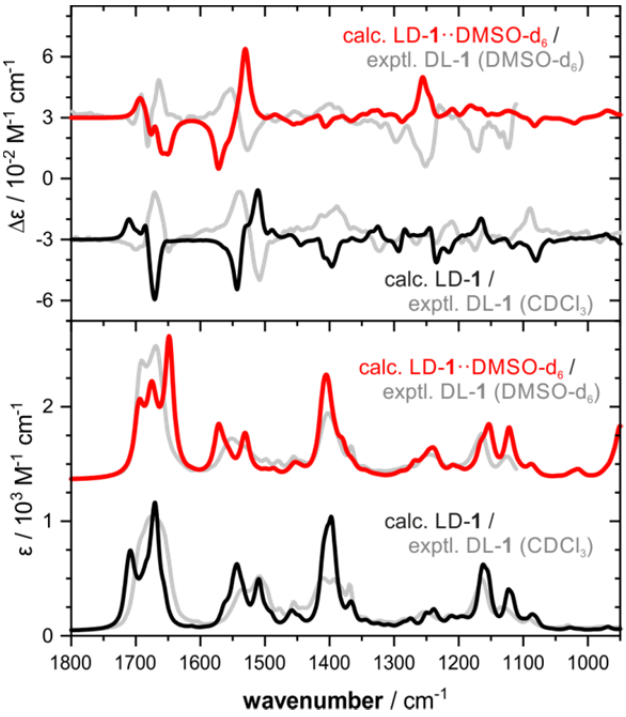
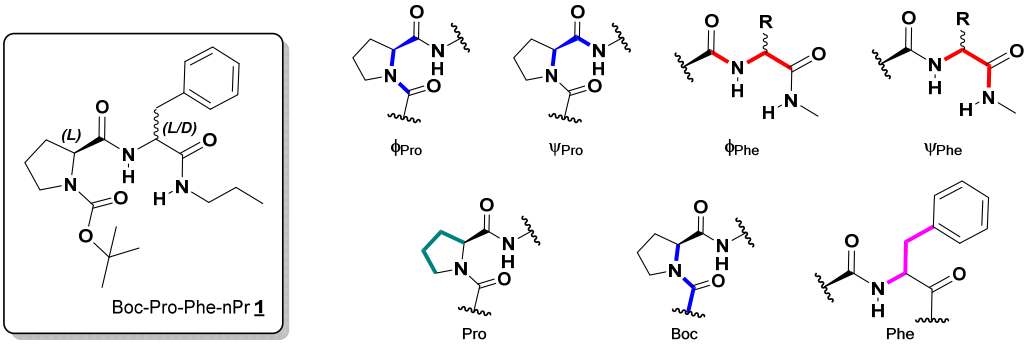


Figure S4. Computed IR and VCD spectra of LD-**1** and LD-**1**··DMSO-d_6

2. Conformational analysis



Scheme S1. Definition of torsional angles used in the conformational analysis of LL- and LD-**1**. Note that the calculations were carried out on a truncated model, in which the n-propyl group was replaced by methyl.

Table S1. Summary of the conformational analysis of LL-1 by conformer family. Populations *p* of the conformer families are given in percentage. [1] Not computed; [2] Not possible; [3] bifurcated hydrogen bond to DMSO-d_6; [4] Combined with (pp_{II},α)

	monomeric LL-**1** ($CHCl_3$)				LL-**1**··DMSO-d_6			
	#conf	***p*(ΔE_{ZPC})**	***p*(ΔG_{298K})**	***p*(ΔG_{corr})**	**#conf**	***p*(ΔE_{ZPC})**	***p*(ΔG_{298K})**	***p*(ΔG_{corr})**
(δ,α)	[1]				11	6.4	1.7	5.1
(δ,β)	12	3.7	13	2.6	23	27.8	35.3	33.0
(δ,δ)	11	51.7	25.7	43.6	6	19.7	1.7	17.6
(δ,γ')	9	4.6	4.5	5.2	7	7.2	0.4	7.5
(γ',α)	5	1.3	1.5	1.2	9	2.0	0.6	1.8
(γ',α')	12	0.2	0.3	0.2	7	0	0	
(γ',β)	12	5.5	8.8	5.7	15	22.4	31.2	21.0
(γ',δ)	13	5.6	3.7	6.7	12	3.1	1	3.3
(γ',γ)	10	1.7	1.3	2.1	[1]			
(γ',γ')	7	22.6	28.3	30.1	[2]			
(pp_{II},α')	2	0	0	0	10	2.2	3.5	2.0
(pp_{II},α)	2	0	0	0	10[3]	3.2	4.7	2.7
(pp_{II},β)	6	1	7.8	0.7	12	4.2	13.0	4.3
(pp_{II},δ)	5	0.5	0.7	0.5	[4]			
(pp_{II},γ')	11	0.9	3.5	0.8	6	1.3	6.0	0.5
In list:	117	99.3	99.1	99.4	128	99.4	99.1	98.8
Total:	144				169			

Table S2. Conformational analysis of LL-1. Optimized geometries and relative energies were obtained at the B3LYP/6-31G(2d,p)/IEFPCM($CHCl_3$) level of theory. ΔG_{corr} are the entropy-corrected relative free energies obtained following Cramer and Trular (*J. Phys. Chem. B* 115 **2011** 14556-14562). [1)] Conformer family names are assigned for the main conformer classes according to the Ramachandran regions' nomenclature presented in Figure 2.

				torsional angles (definition see Scheme S1)							rel. energies			populations		
Conf.[1)]	**Pro**	**Phe**	**Boc**	**ϕ_{Pro}**	**ψ_{Pro}**	**ϕ_{Phe}**	**ψ_{Phe}**	**Pro**	**Phe**	**Boc**	**ΔE_{ZPC}**	**ΔG_{298K}**	**ΔG_{corr}**	***p*(ΔE)**	***p*(ΔG)**	***p*(ΔG_{corr})**
(δ,δ)	A	(g-)	(trans)	-78.4	-6.0	-96.8	2.8	-37.3	-62.1	14.9	1.02	1.25	0.97	4.6	2.6	4.3
(δ,δ)	A	(g-)	(cis)	-94.7	-1.4	-105.0	4.6	-37.4	-64.0	-163.6	3.13	2.47	3.21	0.1	0.3	0.1
(δ,δ)	A	(g+)	(trans)	-78.0	-7.2	-95.7	6.0	-37.2	54.9	13.5	0.00	0.50	0.00	26.0	9.2	22.3
(δ,δ)	A	(g+)	(cis)	-94.8	-2.0	-109.2	8.4	-37.6	55.8	-162.7	2.80	3.45	2.71	0.2	0.1	0.2
(δ,δ)	A	(t)	(trans)	-80.9	-2.7	-93.5	-2.0	-37.4	-162.5	15.7	3.59	3.15	3.54	0.1	0.1	0.1
(δ,δ)	B	(g-)	(trans)	-65.1	-24.4	-94.5	6.7	37.8	-64.2	12.0	1.15	0.68	1.21	3.8	6.8	2.9
(δ,δ)	B	(g-)	(cis)	-81.1	-21.1	-110.7	7.3	37.2	-62.9	-163.4	3.74	3.81	3.75	0.0	0.0	0.0
(δ,δ)	B	(g+)	(trans)	-66.2	-21.0	-88.2	3.0	37.4	57.0	10.8	0.26	0.71	0.30	16.7	6.4	13.4
(δ,δ)	B	(g+)	(cis)	-81.0	-21.6	-113.7	11.5	36.8	55.2	-162.9	3.07	3.27	3.08	0.1	0.1	0.1
(δ,δ)	B	(t)	(trans)	-66.2	-23.1	-73.4	-17.2	37.6	-166.5	11.7	3.72	3.31	3.72	0.0	0.1	0.0
(δ,δ)	B	(t)	(cis)	-83.5	-18.1	-85.8	-18.1	36.7	-169.3	-164.7	6.57	6.31	6.58	0.0	0.0	0.0
(δ,γ')	A	(g-)	(trans)	-92.6	-2.8	-85.0	69.0	-37.6	-56.5	12.2	1.87	2.62	1.37	1.1	0.3	2.2
(δ,γ')	A	(g+)	(trans)	-88.3	-9.8	-83.6	58.8	-37.3	40.8	11.0	2.13	2.17	2.14	0.7	0.6	0.6
(δ,γ')	A	(t)	(trans)	-90.5	-6.8	-84.0	76.4	-37.8	-161.4	12.7	2.47	1.78	2.38	0.4	1.1	0.4
(δ,γ')	B	(g-)	(trans)	-74.4	-21.4	-85.3	68.2	37.1	-54.0	9.8	2.69	2.07	2.74	0.3	0.6	0.2
(δ,γ')	B	(g-)	(cis)	-74.5	-18.6	-83.6	76.4	37.1	-54.6	-172.3	2.06	1.75	2.17	0.8	1.1	0.6
(δ,γ')	B	(g+)	(trans)	-70.6	-25.4	-82.8	57.0	37.0	41.5	7.8	2.71	2.69	2.75	0.3	0.2	0.2
(δ,γ')	B	(g+)	(cis)	-77.6	-18.7	-81.5	53.0	37.0	44.0	-167.3	2.48	2.74	2.54	0.4	0.2	0.3
(δ,γ')	B	(t)	(trans)	-63.7	-32.4	-80.9	81.3	37.6	-164.5	8.5	2.99	3.36	2.86	0.2	0.1	0.2
(δ,γ')	B	(t)	(cis)	-75.9	-17.9	-81.1	84.2	37.1	-164.9	-171.2	2.34	2.49	2.28	0.5	0.3	0.5
NA[1)]	A	(t)	(cis)	-93.3	-4.3	-142.4	37.0	-37.7	-150.5	-162.6	5.38	5.07	5.38	0.0	0.0	0.0
(δ,β)	A	(g-)	(trans)	-82.6	-12.5	-126.6	146.8	-37.0	-58.9	7.6	3.60	3.08	3.69	0.1	0.1	0.0
(δ,β)	A	(g-)	(cis)	-88.2	-6.9	-120.2	144.3	-37.5	-59.7	-165.7	2.71	2.53	2.81	0.3	0.3	0.2
(δ,β)	A	(g+)	(trans)	-78.8	-13.6	-153.4	166.1	-36.7	58.7	5.8	2.95	1.89	3.11	0.2	0.9	0.1
(δ,β)	A	(g+)	(cis)	-85.0	-7.5	-147.7	166.9	-37.5	58.6	-166.3	2.61	1.54	2.78	0.3	1.6	0.2
(δ,β)	A	(t)	(trans)	-82.6	-9.3	-154.0	157.4	-37.4	-169.8	7.1	2.27	1.15	2.36	0.6	3.1	0.4
(δ,β)	A	(t)	(cis)	-88.1	-0.5	-149.2	158.6	-38.0	-169.1	-166.2	1.81	0.94	1.91	1.2	4.4	0.9
(δ,β)	B	(g-)	(trans)	-66.1	-30.3	-122.7	148.4	36.9	-60.5	5.2	3.71	3.02	3.89	0.0	0.1	0.0
(δ,β)	B	(g-)	(cis)	-76.8	-21.4	-120.0	143.0	37.1	-59.5	-165.4	3.07	2.76	3.19	0.1	0.2	0.1
(δ,β)	B	(g+)	(trans)	-64.0	-29.2	-148.9	166.9	37.3	58.8	3.4	3.43	2.70	3.58	0.1	0.2	0.1
(δ,β)	B	(g+)	(cis)	-75.1	-21.2	-144.1	166.9	37.5	59.2	-166.7	3.18	2.30	3.34	0.1	0.4	0.1
(δ,β)	B	(t)	(trans)	-65.0	-27.4	-148.7	160.3	37.0	-169.2	4.0	2.85	2.22	2.92	0.2	0.5	0.2
(δ,β)	B	(t)	(cis)	-74.6	-19.9	-146.3	161.4	37.5	-167.4	-166.9	2.37	1.75	2.45	0.5	1.1	0.4
NA[1)]	A	(g+)	(trans)	-91.0	-8.1	-174.3	-30.7	-38.3	58.0	13.5	7.64	7.57	7.61	0.0	0.0	0.0
NA[1)]	A	(t)	(trans)	-88.2	-10.7	-161.7	-47.4	-37.8	-170.9	12.7	8.32	7.20	8.39	0.0	0.0	0.0
NA[1)]	B	(g+)	(trans)	-72.5	-25.8	-173.8	-29.8	37.3	56.9	10.5	7.95	7.43	8.03	0.0	0.0	0.0
NA[1)]	B	(t)	(trans)	-70.7	-28.6	-161.0	-49.0	37.4	-172.6	10.2	8.74	7.76	8.87	0.0	0.0	0.0
(γ',α')	A	(g-)	(trans)	-87.1	61.1	67.1	25.5	-38.0	-60.7	12.7	3.00	2.62	2.93	0.2	0.3	0.2
(γ',α')	A	(g-)	(cis)	-94.4	53.5	67.7	27.2	-37.9	-58.9	-166.2	4.99	4.72	5.06	0.0	0.0	0.0
(γ',α')	A	(g+)	(trans)	-86.5	63.4	48.2	41.3	-37.8	52.9	12.1	5.92	6.21	5.81	0.0	0.0	0.0
(γ',α')	A	(g+)	(cis)	-94.7	58.4	48.0	42.9	-37.8	51.5	-167.1	8.50	8.73	8.49	0.0	0.0	0.0
(γ',α')	A	(t)	(trans)	-86.1	58.5	62.9	35.4	-38.0	-133.5	12.8	4.67	4.58	4.48	0.0	0.0	0.0

(γ',α')	A	(t)	(cis)	-94.4	55.2	64.2	34.2	-37.8	-133.2	-166.5	7.17	6.80	7.09	0.0	0.0	0.0
(γ',α')	B	(g-)	(trans)	-85.2	63.8	67.9	24.3	32.5	-59.0	11.4	4.15	3.60	4.08	0.0	0.0	0.0
(γ',α')	B	(g-)	(cis)	-94.8	54.9	66.2	28.5	29.5	-60.1	-165.6	6.32	6.03	6.35	0.0	0.0	0.0
(γ',α')	B	(g+)	(trans)	-84.7	65.1	47.2	41.9	32.5	52.1	10.6	7.14	7.36	7.02	0.0	0.0	0.0
(γ',α')	B	(g+)	(cis)	-94.7	65.4	47.7	42.5	29.3	51.1	-167.1	9.76	9.33	9.78	0.0	0.0	0.0
(γ',α')	B	(t)	(trans)	-84.4	62.0	61.7	37.4	32.5	-136.5	11.3	5.79	5.21	5.65	0.0	0.0	0.0
(γ',α')	B	(t)	(cis)	-94.5	58.0	62.7	36.4	29.4	-135.4	-166.4	8.44	7.92	8.36	0.0	0.0	0.0
(γ',α)	A	(g+)	(trans)	-85.2	78.4	-86.8	-10.0	-37.1	66.1	9.8	1.91	1.79	1.87	1.0	1.0	1.0
(γ',α)	A	(t)	(trans)	-84.9	69.1	-80.5	-26.3	-37.5	-171.1	10.7	3.49	3.03	3.40	0.1	0.1	0.1
(γ',α)	A	(t)	(cis)	-94.9	64.2	-76.2	-28.8	-37.4	-171.6	-167.0	6.54	6.35	6.53	0.0	0.0	0.0
(γ',α)	B	(g+)	(trans)	-82.0	84.4	-90.0	-8.4	32.9	65.5	7.8	2.89	2.52	2.84	0.2	0.3	0.2
(γ',α)	B	(t)	(trans)	-82.7	73.1	-79.8	-27.8	32.4	-171.6	9.1	4.52	3.49	4.48	0.0	0.1	0.0
(γ',β)	A	(g-)	(trans)	-86.6	62.4	-129.9	136.4	-37.8	-59.9	9.6	2.19	3.42	1.69	0.6	0.1	1.3
(γ',β)	A	(g-)	(cis)	-92.6	48.8	-132.9	141.0	-37.6	-59.0	-170.7	2.66	2.95	2.68	0.3	0.1	0.2
(γ',β)	A	(g+)	(trans)	-88.2	59.1	-160.2	163.2	-37.6	61.3	10.9	2.50	2.54	2.54	0.4	0.3	0.3
(γ',β)	A	(g+)	(cis)	-93.4	62.7	-157.9	159.7	-37.1	61.7	-171.9	2.59	3.61	2.58	0.3	0.0	0.3
(γ',β)	A	(t)	(trans)	-86.4	67.2	-158.5	146.4	-37.3	-172.4	9.1	1.60	1.17	1.52	1.7	3.0	1.7
(γ',β)	A	(t)	(cis)	-93.9	60.3	-158.9	149.4	-37.4	-171.3	-169.8	1.70	1.04	1.71	1.5	3.7	1.3
(γ',β)	B	(g-)	(trans)	-85.3	65.9	-132.0	136.8	30.2	-60.3	8.7	3.46	2.60	3.57	0.1	0.3	0.1
(γ',β)	B	(g-)	(cis)	-92.4	51.9	-133.9	139.6	27.1	-58.9	-171.1	4.02	3.47	4.11	0.0	0.1	0.0
(γ',β)	B	(g+)	(trans)	-87.1	62.6	-160.6	163.0	31.9	60.9	10.1	3.59	3.79	3.18	0.1	0.0	0.1
(γ',β)	B	(g+)	(cis)	-93.7	65.9	-159.9	158.3	27.8	60.8	-172.1	3.82	4.73	3.84	0.0	0.0	0.0
(γ',β)	B	(t)	(trans)	-84.4	72.7	-159.0	144.1	31.6	-172.6	7.9	2.67	1.82	2.64	0.3	1.0	0.3
(γ',β)	B	(t)	(cis)	-94.4	63.9	-160.5	148.7	27.7	-170.7	-169.9	3.12	2.71	3.09	0.1	0.2	0.1
NA[1)]	A	(g-)	(trans)	-81.6	73.1	69.9	170.9	-36.6	-57.9	3.8	5.72	6.12	5.60	0.0	0.0	0.0
NA[1)]	A	(g+)	(trans)	-85.3	64.6	36.9	-116.7	-38.1	60.0	10.7	8.80	9.47	8.56	0.0	0.0	0.0
NA[1)]	A	(t)	(trans)	-80.6	73.8	62.5	-167.5	-36.6	-155.6	2.7	5.44	5.81	5.34	0.0	0.0	0.0
NA[1)]	B	(g-)	(trans)	-78.9	78.0	69.0	172.6	29.9	-57.3	0.7	6.83	6.79	6.74	0.0	0.0	0.0
NA[1)]	B	(g+)	(trans)	-83.2	68.9	36.5	-118.1	31.6	60.5	8.7	9.91	10.10	9.75	0.0	0.0	0.0
NA[1)]	B	(t)	(trans)	-78.9	77.6	62.1	-167.4	30.2	-156.4	1.5	6.66	7.20	6.50	0.0	0.0	0.0
(γ',γ')	A	(g-)	(trans)	-87.1	55.4	-86.9	68.9	-38.0	-70.3	15.2	0.96	0.99	0.89	5.2	4.0	5.0
(γ',γ')	A	(g+)	(trans)	-85.4	88.8	-80.6	45.4	-36.5	52.0	8.7	2.51	2.91	2.34	0.4	0.2	0.4
(γ',γ')	A	(t)	(trans)	-84.9	63.5	-85.8	77.3	-37.7	-162.6	11.3	0.38	0.00	0.16	13.7	21.4	17.0
(γ',γ')	A	(t)	(cis)	-90.5	33.2	-82.4	83.6	-38.0	-165.5	-163.9	2.35	1.71	2.29	0.5	1.2	0.5
(γ',γ')	B	(g-)	(trans)	-84.6	54.8	-86.9	69.5	32.9	-69.6	14.3	2.18	2.07	2.11	0.7	0.7	0.6
(γ',γ')	B	(g+)	(trans)	-78.2	99.9	-83.3	50.1	34.5	48.5	5.6	3.25	3.00	3.15	0.1	0.1	0.1
(γ',γ')	B	(t)	(trans)	-83.0	68.7	-86.5	76.2	32.5	-161.5	9.7	1.49	2.02	0.74	2.1	0.7	6.4
(γ',δ)	A	(g-)	(trans)	-86.8	65.2	-123.5	12.3	-37.7	-64.1	11.9	1.32	1.46	1.25	2.8	1.8	2.7
(γ',δ)	A	(g-)	(cis)	-92.6	60.7	-123.0	11.4	-37.3	-64.8	-169.7	3.75	4.09	3.73	0.0	0.0	0.0
(γ',δ)	A	(g-)	(trans)	-86.7	64.4	-119.0	9.2	-37.9	-57.8	12.6	1.83	3.26	1.26	1.2	0.1	2.7
(γ',δ)	A	(g+)	(trans)	-87.6	53.7	-140.5	19.9	-38.1	55.1	15.6	2.01	1.76	2.05	0.9	1.1	0.7
(γ',δ)	A	(g+)	(cis)	-98.2	48.4	-127.5	17.8	-38.0	55.3	-162.4	3.47	3.80	3.52	0.1	0.0	0.1
(γ',δ)	A	(t)	(trans)	-85.2	71.5	-145.7	37.2	-37.2	-150.1	10.6	3.06	2.64	2.94	0.1	0.2	0.2
(γ',δ)	A	(t)	(cis)	-94.0	66.7	-148.4	38.0	-37.3	-150.0	-168.1	5.57	5.23	5.57	0.0	0.0	0.0
(γ',δ)	B	(g-)	(trans)	-84.5	66.9	-125.5	13.6	31.3	-65.3	10.6	2.68	2.93	2.58	0.3	0.2	0.3
(γ',δ)	B	(g-)	(cis)	-93.4	62.0	-125.2	13.5	27.4	-65.1	-168.8	5.16	5.32	5.16	0.0	0.0	0.0
(γ',δ)	B	(g+)	(trans)	-86.1	57.1	-143.9	21.5	32.5	55.1	14.5	3.31	3.00	3.35	0.1	0.1	0.1

(γ',δ)	B	(g+)	(cis)	-98.7	49.1	-125.9	17.1	29.0	55.9	-160.9	4.84	4.62	4.92	0.0	0.0	0.0
(γ',δ)	B	(t)	(trans)	-83.2	76.4	-147.9	36.3	32.5	-149.2	9.0	4.07	3.18	4.01	0.0	0.1	0.0
(γ',δ)	B	(t)	(cis)	-93.5	73.0	-149.7	36.6	28.9	-150.1	-168.6	6.89	6.49	6.87	0.0	0.0	0.0
(γ',γ)	A	(g-)	(trans)	-85.1	66.2	73.4	-53.6	-37.6	-57.9	11.2	1.84	1.86	1.63	1.2	0.9	1.4
(γ',γ)	A	(g-)	(cis)	-94.4	53.4	74.3	-52.8	-37.9	-58.0	-165.4	4.23	4.44	4.14	0.0	0.0	0.0
(γ',γ)	A	(g+)	(trans)	-85.9	64.7	52.1	-27.4	-37.7	67.6	11.5	5.48	5.83	5.22	0.0	0.0	0.0
(γ',γ)	A	(g+)	(cis)	-94.1	63.4	53.9	-27.5	-37.5	68.5	-167.1	8.30	8.34	8.17	0.0	0.0	0.0
(γ',γ)	A	(t)	(trans)	-85.3	65.2	71.7	-62.6	-37.6	-171.9	11.3	2.70	3.11	2.43	0.3	0.1	0.4
(γ',γ)	A	(t)	(cis)	-93.3	67.2	72.5	-62.5	-37.4	-171.8	-167.1	5.43	5.27	5.32	0.0	0.0	0.0
(γ',γ)	B	(g-)	(trans)	-83.4	68.4	72.4	-53.8	32.7	-57.6	10.0	2.93	2.85	2.75	0.2	0.2	0.2
(γ',γ)	B	(g+)	(trans)	-83.3	72.2	53.7	-27.0	32.8	70.4	9.0	6.76	7.11	6.52	0.0	0.0	0.0
(γ',γ)	B	(t)	(trans)	-83.4	70.6	71.7	-61.8	32.6	-172.2	9.6	3.87	3.76	3.66	0.0	0.0	0.0
(γ',γ)	B	(t)	(cis)	-76.3	110.0	69.6	-72.7	34.9	-170.4	-173.9	5.93	6.27	5.81	0.0	0.0	0.0
NA[1)]	A	(g+)	(trans)	-82.9	67.8	-178.3	-21.9	-37.3	59.2	9.3	4.06	4.83	4.07	0.0	0.0	0.0
NA[1)]	A	(g+)	(cis)	-96.6	53.3	-157.2	-42.9	-37.8	65.8	-164.8	7.56	7.39	7.67	0.0	0.0	0.0
NA[1)]	A	(t)	(trans)	-82.7	70.6	-166.9	-45.0	-37.3	-172.8	9.7	5.17	4.15	5.25	0.0	0.0	0.0
NA[1)]	A	(t)	(cis)	-95.4	55.8	-154.4	-63.5	-37.7	-175.1	-166.4	7.94	7.30	8.04	0.0	0.0	0.0
NA[1)]	B	(g+)	(trans)	-81.0	72.3	177.3	-23.4	31.9	59.3	7.2	5.19	5.84	5.20	0.0	0.0	0.0
NA[1)]	B	(g+)	(cis)	-96.8	54.2	-157.5	-44.2	29.0	65.7	-164.1	8.88	10.38	8.42	0.0	0.0	0.0
NA[1)]	B	(t)	(trans)	-80.0	75.1	-169.2	-47.4	32.5	-173.1	7.0	6.41	6.28	6.37	0.0	0.0	0.0
NA[1)]	B	(t)	(cis)	-96.3	58.9	-154.6	-63.2	28.1	-174.3	-165.5	9.30	8.56	9.40	0.0	0.0	0.0
(pp_{II},α')	A	(g+)	(trans)	-61.4	130.6	45.1	37.7	-36.3	53.0	1.5	6.21	7.17	6.10	0.0	0.0	0.0
(pp_{II},α')	B	(g+)	(trans)	-55.1	128.4	45.2	37.4	37.1	53.3	1.1	5.81	6.55	5.79	0.0	0.0	0.0
(pp_{II},α)	A	(g-)	(cis)	-67.8	159.1	-71.9	-27.2	-37.3	-60.4	175.7	5.49	4.83	5.67	0.0	0.0	0.0
(pp_{II},α)	A	(t)	(cis)	-66.0	146.5	-78.5	-29.6	-37.0	-173.2	176.1	7.29	5.89	7.46	0.0	0.0	0.0
(pp_{II},β)	A	(g-)	(trans)	-80.8	137.0	-130.6	148.9	-36.9	-72.5	4.9	4.39	3.96	4.50	0.0	0.0	0.0
(pp_{II},β)	A	(g+)	(trans)	-69.0	149.0	-156.1	164.2	-37.1	63.3	-2.1	2.60	2.14	2.68	0.3	0.6	0.2
(pp_{II},β)	A	(t)	(trans)	-67.5	145.4	-159.5	155.9	-36.9	-168.2	-2.0	2.80	0.91	2.93	0.2	4.6	0.2
(pp_{II},β)	B	(g-)	(trans)	-71.2	135.6	-128.0	149.0	35.7	-75.5	3.7	5.00	3.99	5.14	0.0	0.0	0.0
(pp_{II},β)	B	(g+)	(trans)	-60.6	144.8	-154.5	164.0	36.1	64.4	-1.6	2.94	2.67	3.00	0.2	0.2	0.1
(pp_{II},β)	B	(t)	(trans)	-56.4	136.6	-161.9	157.1	36.7	-164.0	-1.5	2.88	1.32	3.00	0.2	2.3	0.1
(pp_{II},δ')	A	(g-)	(trans)	-62.4	134.4	71.8	9.8	-36.6	-58.3	0.5	2.69	2.43	2.67	0.3	0.4	0.2
(pp_{II},δ')	A	(g+)	(trans)	-59.4	138.5	80.3	-11.4	-36.5	129.1	-0.9	9.06	9.63	9.04	0.0	0.0	0.0
(pp_{II},δ')	A	(t)	(trans)	-64.8	131.0	65.5	21.1	-36.6	-124.6	2.9	4.70	4.49	4.64	0.0	0.0	0.0
(pp_{II},δ')	B	(g-)	(trans)	-55.8	130.4	70.7	10.9	37.3	-60.2	0.8	2.55	2.38	2.54	0.3	0.4	0.3
(pp_{II},δ')	B	(g+)	(trans)	-52.4	136.0	82.5	-15.3	37.0	127.1	-1.8	8.72	9.36	8.71	0.0	0.0	0.0
(pp_{II},δ')	B	(t)	(trans)	-57.5	128.9	66.3	19.5	37.0	-123.1	1.7	4.52	4.44	4.44	0.0	0.0	0.0
(pp_{II},γ')	A	(g-)	(trans)	-69.9	152.7	-82.7	71.9	-36.8	-56.2	-1.4	3.55	2.05	3.67	0.1	0.7	0.0
(pp_{II},γ')	A	(g-)	(cis)	-67.2	164.9	-80.9	71.6	-37.1	-60.8	174.0	3.44	2.98	3.56	0.1	0.1	0.1
(pp_{II},γ')	A	(g+)	(trans)	-68.4	141.8	-84.5	56.4	-36.5	42.9	-0.2	3.09	2.06	3.04	0.1	0.7	0.1
(pp_{II},γ')	A	(g+)	(cis)	-66.6	150.4	-82.5	55.8	-36.8	42.9	176.7	3.34	2.93	3.34	0.1	0.2	0.1
(pp_{II},γ')	A	(t)	(cis)	-66.5	149.3	-83.9	78.4	-36.9	-162.6	176.4	3.21	2.21	3.28	0.1	0.5	0.1
(pp_{II},γ')	B	(g-)	(trans)	-57.8	134.9	-85.9	69.9	36.8	-57.4	0.0	3.77	4.34	3.77	0.0	0.0	0.0
(pp_{II},γ')	B	(g-)	(cis)	-62.3	161.3	-79.7	72.0	35.4	-62.3	176.7	3.91	4.16	3.96	0.0	0.0	0.0
(pp_{II},γ')	B	(g+)	(trans)	-58.3	133.0	-86.3	57.1	36.7	42.5	0.0	3.19	2.13	3.16	0.1	0.6	0.1
(pp_{II},γ')	B	(g+)	(cis)	-60.1	148.9	-82.6	57.1	36.2	42.5	178.3	3.67	3.72	3.62	0.1	0.0	0.0
(pp_{II},γ')	B	(t)	(trans)	-58.3	136.4	-86.0	77.7	36.5	-162.7	-0.5	3.16	2.27	3.13	0.1	0.5	0.1

(pp_{II},γ')	B	(t)	(cis)	-59.4	147.7	-83.9	78.6	36.1	-163.1	177.2	3.45	2.77	3.51	0.1	0.2	0.1
(pp_{II},δ)	A	(g-)	(trans)	-81.2	137.8	-113.6	8.3	-36.6	-73.3	4.7	5.41	4.86	5.49	0.0	0.0	0.0
(pp_{II},δ)	A	(g+)	(trans)	-66.6	134.8	-126.2	12.7	-36.5	57.0	0.1	2.77	2.42	2.73	0.2	0.4	0.2
(pp_{II},δ)	A	(g+)	(cis)	-68.8	156.4	-111.8	6.5	-37.3	57.4	176.7	4.41	4.24	4.40	0.0	0.0	0.0
(pp_{II},δ)	B	(g-)	(trans)	-63.6	138.4	-104.2	2.2	35.9	-68.1	-0.6	5.77	5.51	5.84	0.0	0.0	0.0
(pp_{II},δ)	B	(g+)	(trans)	-55.7	132.0	-126.4	12.2	36.8	57.8	-1.1	2.69	2.45	2.66	0.3	0.3	0.3
(pp_{II},pp_{II})	A	(g-)	(trans)	-71.7	153.6	-61.5	143.4	-36.6	-58.5	-1.2	5.38	3.85	5.58	0.0	0.0	0.0
(pp_{II},pp_{II})	B	(g-)	(trans)	-57.6	138.6	-61.7	129.8	36.5	-56.5	-1.3	5.71	4.33	5.91	0.0	0.0	0.0

Table S3. Conformational analysis of LL-1··DMSO-d_6. Optimized geometries and relative energies were obtained at the B3LYP/6-31G(2d,p)/IEFPCM(DMSO) level of theory. ΔG_{corr} are the entropy-corrected relative free energies obtained following Cramer and Trular (*J. Phys. Chem. B* 115 **2011** 14556-14562). [1)] Conformer family names are assigned for the main conformer classes according to the Ramachandran regions' nomenclature presented in Figure 2.

				torsional angles (definition see Scheme S1)				rel. energies						populations	
Conf.[1)]	**Pro**	**Phe**	**Boc**	**ϕ_{Pro}**	**ψ_{Pro}**	**ϕ_{Phe}**	**ψ_{Phe}**	**Pro**	**Phe**	**Boc**	**ΔE_{ZPC}**	**ΔG_{298K}**	**ΔG_{corr}**	***p*(ΔE)**	***p*(ΔG)**	***p*(ΔG_{corr})**
NA[1)]	B	(g-)	(cis)	-103.0	20.4	71.8	23.5	27.7	-60.6	-163.8	6.90	9.19	6.42	0.0	0.0	0.0
(δ,δ)	A	(g-)	(trans)	-74.1	-14.6	-100.2	8.2	-36.4	-63.8	11.3	0.35	1.39	0.46	6.2	1.0	4.8
(δ,δ)	A	(g-)	(cis)	-89.4	-7.9	-103.3	0.9	-36.5	-64.4	-167.5	1.21	2.64	1.21	1.5	0.1	1.4
(δ,δ)	A	(t)	(trans)	-72.9	-14.7	-79.5	-14.4	-36.2	-170.7	12.2	3.62	4.66	3.66	0.0	0.0	0.0
(δ,δ)	B	(g-)	(trans)	-60.1	-30.1	-98.2	9.8	37.5	-64.8	7.4	0.00	1.80	0.00	**11.2**	0.5	10.6
(δ,δ)	B	(g-)	(cis)	-75.0	-26.5	-108.2	3.9	36.2	-63.5	-169.1	1.60	3.07	1.59	0.8	0.1	0.7
(δ,δ)	B	(t)	(trans)	-60.8	-27.6	-74.6	-18.1	37.8	-172.0	8.6	3.32	3.63	3.46	0.0	0.0	0.0
$(\delta,\alpha)_{bifuHB}$	A	(g-)	(trans)	-88.6	-11.0	-99.9	-45.6	-36.9	-61.6	11.5	2.62	2.74	2.84	0.1	0.1	0.1
$(\delta,\alpha)_{bifuHB}$	A	(g-)	(cis)	-90.6	-6.1	-97.8	-47.5	-37.2	-60.7	-166.1	0.98	1.77	1.12	2.1	0.5	1.6
$(\delta,\alpha)_{bifuHB}$	A	(g+)	(trans)	-76.3	-25.7	-143.5	-4.7	-35.6	66.2	11.5	5.07	6.77	5.05	0.0	0.0	0.0
$(\delta,\alpha)_{bifuHB}$	A	(g+)	(cis)	-78.3	-21.8	-131.1	-13.6	-35.8	64.9	-168.5	2.91	4.65	2.93	0.1	0.0	0.1
$(\delta,\alpha)_{bifuHB}$	A	(t)	(trans)	-82.6	-14.7	-110.0	-56.6	-37.1	-177.1	10.1	3.18	3.26	3.32	0.1	0.0	0.0
$(\delta,\alpha)_{bifuHB}$	A	(t)	(cis)	-81.9	-15.6	-111.0	-54.9	-36.9	-177.9	-170.0	1.57	2.01	1.67	0.8	0.4	0.6
$(\delta,\alpha)_{bifuHB}$	B	(g-)	(trans)	-69.4	-28.2	-97.5	-44.4	37.8	-59.7	9.1	2.50	2.71	1.06	0.2	0.1	1.8
$(\delta,\alpha)_{bifuHB}$	B	(g-)	(cis)	-72.1	-28.1	-109.6	-50.6	37.0	-61.2	-171.2	0.99	2.16	2.60	2.1	0.3	0.1
$(\delta,\alpha)_{bifuHB}$	B	(g+)	(cis)	-68.6	-33.1	-129.1	-14.4	37.3	64.6	-170.8	2.59	4.61	3.32	0.1	0.0	0.0
$(\delta,\alpha)_{bifuHB}$	B	(t)	(trans)	-67.6	-34.7	-111.4	-55.9	37.9	-177.8	9.2	3.46	4.25	3.52	0.0	0.0	0.0
$(\delta,\alpha)_{bifuHB}$	B	(t)	(cis)	-70.5	-28.4	-111.0	-55.6	37.3	-177.9	-171.2	1.58	2.32	1.62	0.8	0.2	0.7
(δ,β)	A	(g-)	(cis)	-86.1	-11.1	-119.6	146.3	-37.5	-65.9	-166.7	0.21	0.82	1.71	**7.8**	2.7	0.6
(δ,β)	A	(g+)	(cis)	-83.5	-10.7	-139.6	160.2	-37.2	62.8	-167.0	1.52	1.92	1.09	0.9	0.4	1.7
(δ,β)	A	(t)	(trans)	-81.1	-12.0	-134.5	130.6	-37.1	-178.5	7.5	1.63	1.01	0.23	0.7	1.9	7.2
(δ,β)	A	(t)	(cis)	-85.9	-5.3	-126.0	128.4	-37.7	-177.8	-165.8	0.98	0.43	1.09	2.1	5.2	1.7
(δ,β)	B	(g-)	(trans)	-66.8	-31.2	-122.5	148.7	37.0	-66.4	6.1	1.01	1.27	0.54	2.0	1.3	4.3
(δ,β)	B	(g-)	(cis)	-74.7	-25.0	-119.2	146.5	37.1	-65.9	-166.6	0.55	1.50	2.19	4.4	0.8	0.3
(δ,β)	B	(g+)	(trans)	-64.7	-30.4	-136.8	159.5	37.3	63.5	4.3	2.15	1.70	1.83	0.3	0.6	0.5
(δ,β)	B	(g+)	(cis)	-75.3	-21.9	-133.4	158.6	37.2	64.6	-167.1	1.76	1.16	1.97	0.6	1.5	0.4
(δ,β)	B	(t)	(trans)	-66.4	-28.2	-127.8	130.6	37.1	-178.4	5.5	1.75	0.13	1.50	0.6	8.5	0.8
(δ,β)	B	(t)	(cis)	-74.6	-23.5	-113.6	125.0	37.4	-177.7	-166.4	1.46	1.78	0.87	1.0	0.5	2.4
(δ,β)	A	(g-)	(trans)	-82.5	-13.6	-118.8	144.9	-37.2	-65.2	10.2	0.79	0.39	0.21	3.0	5.5	7.5
(δ,β)	A	(g+)	(trans)	-75.8	-21.0	-132.2	155.0	-36.2	61.3	6.2	2.13	1.36	5.07	0.3	1.1	0.0
(δ,β)	A	(g+)	(cis)	-72.0	-23.4	-139.2	167.2	-35.5	64.3	-173.1	4.93	6.45	5.83	0.0	0.0	0.0
(δ,β)	A	(g+)	(trans)	-73.9	-25.4	-146.7	161.3	-35.2	64.4	9.3	5.67	6.99	1.65	0.0	0.0	0.7
(δ,β)	A	(t)	(trans)	-80.3	-14.3	-126.1	127.8	-37.0	-178.7	8.1	1.53	0.79	0.95	0.8	2.8	2.1
(δ,β)	A	(t)	(cis)	-86.5	-6.3	-118.7	125.7	-37.7	-178.3	-166.2	1.00	1.40	1.01	2.1	1.0	1.9
(δ,β)	B	(g-)	(trans)	-67.1	-28.4	-125.9	143.2	36.9	-60.4	5.6	2.63	2.09	2.83	0.1	0.3	0.1
(δ,β)	B	(g-)	(cis)	-75.4	-21.0	-123.8	139.8	37.1	-60.2	-166.0	2.11	2.56	2.20	0.3	0.1	0.3
(δ,β)	B	(g+)	(trans)	-64.6	-29.3	-144.5	159.9	37.4	60.7	4.1	2.98	2.55	3.09	0.1	0.1	0.1
(δ,β)	B	(g+)	(cis)	-68.0	-28.8	-140.7	153.5	37.8	60.7	-168.6	2.75	2.36	2.85	0.1	0.2	0.1
(δ,β)	B	(g+)	(trans)	-57.6	-43.2	-147.1	160.6	38.9	65.0	5.7	5.06	6.70	5.17	0.0	0.0	0.0
(δ,β)	B	(t)	(trans)	-66.9	-26.5	-133.9	131.4	37.2	-177.9	5.3	2.90	1.84	3.10	0.1	0.5	0.1
(δ,β)	B	(t)	(cis)	-70.1	-27.8	-146.5	121.1	37.4	-175.9	-170.9	1.83	2.32	1.98	0.5	0.2	0.4

(δ,γ')	A	(g-)	(cis)	-83.4	-27.3	-87.6	75.1	-35.4	-66.7	-171.3	0.55	2.59	0.51	4.5	0.1	4.5
(δ,γ')	A	(g-)	(trans)	-100.5	-4.7	-86.6	76.4	-37.9	-62.4	14.3	1.19	2.82	1.04	1.5	0.1	1.8
(δ,γ')	A	(t)	(cis)	-80.0	-36.1	-91.8	83.8	-35.4	-167.1	-171.9	1.96	3.57	1.88	0.4	0.0	0.4
(δ,γ')	A	(t)	(trans)	-66.5	-28.9	-83.3	79.7	-35.5	-163.4	5.7	3.75	3.78	3.83	0.0	0.0	0.0
(δ,γ')	B	(g-)	(trans)	-69.1	-38.5	-89.4	70.5	36.7	-66.5	8.2	2.01	3.11	2.03	0.4	0.1	0.3
(δ,γ')	B	(t)	(cis)	-72.1	-42.5	-95.0	87.9	36.5	-168.3	-173.1	1.98	3.12	1.94	0.4	0.1	0.4
(δ,γ')	B	(t)	(trans)	-55.6	-37.7	-82.2	82.0	37.1	-164.3	2.6	3.79	4.29	3.81	0.0	0.0	0.0
(δ,γ)	A	(g-)	(trans)	-88.8	-3.7	74.8	-58.6	-37.7	-58.3	10.5	4.07	5.71	3.95	0.0	0.0	0.0
(δ,γ)	A	(g+)	(trans)	-79.3	-7.7	61.7	-44.5	-37.1	65.7	7.0	6.65	7.65	3.35	0.0	0.0	0.0
(δ,γ)	A	(t)	(trans)	-77.5	-10.6	76.2	-62.6	-36.9	-171.2	6.5	3.02	3.67	6.62	0.1	0.0	0.0
(δ,γ)	B	(g-)	(trans)	-74.1	-12.8	74.3	-60.5	35.9	-59.8	6.0	3.86	6.23	2.95	0.0	0.0	0.1
(δ,γ)	B	(g+)	(trans)	-64.2	-23.4	63.3	-44.3	36.1	70.5	3.4	7.41	8.34	3.75	0.0	0.0	0.0
(δ,γ)	B	(t)	(trans)	-62.4	-25.8	76.9	-63.2	36.4	-171.6	3.0	3.45	3.49	3.33	0.0	0.0	0.0
(δ,α')	A	(g-)	(cis)	-96.6	7.7	69.8	56.2	-37.6	-58.0	-171.6	3.22	3.55	4.69	0.0	0.0	0.0
(δ,α')	A	(t)	(cis)	-87.2	-0.4	71.8	64.2	-37.7	-154.2	-172.4	3.68	3.68	7.39	0.0	0.0	0.0
(δ,α')	B	(g-)	(cis)	-80.4	-14.3	67.9	57.0	35.6	-61.5	-175.4	4.70	5.97	3.45	0.0	0.0	0.0
(δ,α')	B	(t)	(cis)	-71.2	-19.6	73.7	66.8	36.5	-156.0	-176.9	4.19	4.99	4.18	0.0	0.0	0.0
NA[1)]	A	(g+)	(trans)	-71.9	-39.3	165.9	-34.3	-34.0	64.7	10.3	9.69	11.32	9.64	0.0	0.0	0.0
NA[1)]	A	(g+)	(cis)	-86.2	-22.8	167.5	-32.7	-36.0	63.7	-164.7	9.02	11.09	8.93	0.0	0.0	0.0
NA[1)]	A	(t)	(trans)	-73.0	-39.6	176.3	-53.4	-34.8	179.6	10.6	9.55	10.18	9.61	0.0	0.0	0.0
NA[1)]	A	(t)	(cis)	-87.1	-23.4	176.0	-50.2	-36.5	-179.5	-164.6	8.77	9.85	8.84	0.0	0.0	0.0
NA[1)]	B	(g+)	(trans)	-60.7	-44.7	166.3	-34.2	36.6	65.7	7.5	9.49	10.81	9.50	0.0	0.0	0.0
NA[1)]	B	(g+)	(cis)	-76.4	-31.6	167.4	-32.0	36.5	63.8	-165.9	8.84	10.34	8.84	0.0	0.0	0.0
NA[1)]	B	(t)	(trans)	-58.4	-45.5	168.2	-50.2	37.0	179.3	6.9	9.52	10.65	9.56	0.0	0.0	0.0
NA[1)]	B	(t)	(cis)	-74.0	-33.5	172.7	-47.3	36.9	-179.5	-165.9	8.97	10.17	9.01	0.0	0.0	0.0
NA[1)]	A	(g+)	(trans)	-85.9	63.0	54.9	-24.4	-38.0	70.7	11.6	10.48	9.67	10.37	0.0	0.0	0.0
NA[1)]	A	(g-)	(cis)	-94.0	51.3	73.4	-93.1	-37.9	-56.4	-165.7	8.16	8.49	8.22	0.0	0.0	0.0
NA[1)]	A	(g+)	(cis)	-94.6	58.7	55.3	-23.7	-37.7	70.3	-167.2	12.91	12.69	12.76	0.0	0.0	0.0
(γ',α)	B	(g-)	(trans)	-84.1	69.6	-115.1	7.1	32.2	-66.2	10.4	2.81	3.04	2.85	0.1	0.1	0.1
(γ',α)	A	(g-)	(trans)	-87.4	65.8	-113.3	7.1	-37.7	-65.7	11.0	1.38	1.93	1.43	1.1	0.4	1.0
(γ',α)	A	(g+)	(trans)	-89.9	66.0	-89.3	-6.3	-38.0	64.1	12.7	1.90	3.84	1.84	0.5	0.0	0.5
(γ',α)	A	(t)	(trans)	-84.9	63.1	-71.6	-30.6	-37.8	-173.0	9.5	2.51	3.39	2.46	0.2	0.0	0.2
(γ',α)	B	(g-)	(trans)	-85.0	69.6	-114.8	6.3	31.4	-66.1	9.2	2.82	3.66	2.83	0.1	0.0	0.1
(γ',α)	B	(g-)	(cis)	-95.2	46.3	-118.4	22.0	29.0	-63.5	-163.2	4.16	5.61	4.08	0.0	0.0	0.0
(γ',α)	B	(g+)	(trans)	-87.6	68.5	-89.6	-6.7	31.7	64.2	11.2	3.21	4.68	3.22	0.0	0.0	0.0
(γ',α)	B	(t)	(trans)	-82.8	65.3	-71.9	-31.0	31.7	-172.7	8.0	3.73	4.13	3.74	0.0	0.0	0.0
(γ',β)	A	(t)	(trans)	-86.1	67.6	-153.3	126.2	-37.5	-175.6	10.0	1.76	0.00	1.87	0.6	10.6	0.5
(γ',β)	A	(t)	(cis)	-93.0	63.3	-153.6	128.5	-37.3	-176.4	-170.5	2.34	1.50	2.40	0.2	0.8	0.2
(γ',β)	B	(t)	(trans)	-83.9	69.3	-135.6	122.8	32.4	-177.8	9.2	1.91	1.79	1.82	0.4	0.5	0.5
(γ',β)	A	(g-)	(trans)	-86.7	60.8	-128.7	141.7	-37.8	-64.6	10.4	0.02	0.05	0.07	**10.8**	9.8	9.5
(γ',β)	A	(g-)	(cis)	-92.6	46.9	-130.9	140.3	-37.6	-63.9	-170.2	0.69	0.99	0.70	3.5	2.0	3.2
(γ',β)	A	(g+)	(trans)	-88.4	55.9	-150.8	155.5	-37.9	64.1	12.0	1.63	1.60	1.62	0.7	0.7	0.7
(γ',β)	A	(g+)	(cis)	-93.3	55.7	-148.5	153.2	-37.5	63.2	-171.0	2.05	2.88	1.95	0.4	0.1	0.4
(γ',β)	A	(t)	(trans)	-86.1	65.0	-133.5	123.4	-37.7	-177.9	10.8	0.73	0.63	0.64	3.2	3.6	3.6
(γ',β)	A	(t)	(cis)	-92.9	53.6	-136.8	124.7	-37.6	-178.2	-169.6	1.45	2.03	1.34	1.0	0.3	1.1
(γ',β)	B	(g-)	(trans)	-85.1	63.6	-129.8	142.2	31.3	-65.2	9.6	1.38	0.98	1.43	1.1	2.0	0.9
(γ',β)	B	(g-)	(cis)	-92.9	47.9	-131.3	141.0	27.9	-64.1	-169.7	2.23	2.30	2.24	0.3	0.2	0.2

(γ',β)	B	(g+)	(trans)	-86.6	60.4	-158.2	155.9	32.1	61.5	10.6	3.27	3.69	3.22	0.0	0.0	0.0
(γ',β)	B	(g+)	(cis)	-93.4	60.8	-156.9	153.9	28.7	63.1	-170.9	3.70	4.35	3.68	0.0	0.0	0.0
(γ',β)	B	(t)	(trans)	-83.7	71.9	-152.6	123.8	32.4	-176.3	8.9	2.69	1.95	2.71	0.1	0.4	0.1
(γ',β)	B	(t)	(cis)	-92.9	66.4	-153.8	126.0	28.5	-176.9	-170.5	3.50	3.22	3.52	0.0	0.0	0.0
NA[1)]	B	(g-)	(trans)	-84.7	50.1	-84.8	76.5	33.2	-62.2	13.9	4.83	5.76	4.82	0.0	0.0	0.0
(γ',δ)	A	(g-)	(trans)	-86.1	60.1	-121.1	24.0	-37.9	-63.8	11.8	1.04	1.86	0.96	1.9	0.5	2.1
(γ',δ)	A	(g-)	(cis)	-94.9	52.5	-120.2	20.3	-37.9	-63.2	-165.1	2.60	3.96	2.57	0.1	0.0	0.1
(γ',δ)	A	(g+)	(trans)	-88.0	52.2	-131.1	31.7	-38.2	52.1	16.0	2.01	2.89	1.97	0.4	0.1	0.4
(γ',δ)	A	(g+)	(cis)	-97.6	48.0	-122.4	25.3	-38.1	53.0	-161.9	2.51	4.18	2.50	0.2	0.0	0.2
(γ',δ)	A	(t)	(trans)	-85.4	61.2	-134.6	45.0	-37.9	-154.1	11.6	2.60	2.36	2.51	0.1	0.2	0.2
(γ',δ)	A	(t)	(cis)	-95.6	52.7	-134.4	43.0	-38.0	-152.7	-164.9	4.36	4.92	4.35	0.0	0.0	0.0
(γ',δ)	B	(g-)	(trans)	-84.1	63.0	-122.0	24.5	31.8	-65.0	10.3	2.21	2.34	2.19	0.3	0.2	0.3
(γ',δ)	B	(g-)	(cis)	-94.8	53.6	-118.7	19.3	28.4	-63.6	-164.8	3.87	4.67	3.89	0.0	0.0	0.0
(γ',δ)	B	(g+)	(trans)	-85.9	53.2	-130.7	31.8	32.8	52.2	15.0	3.26	3.95	3.22	0.0	0.0	0.0
(γ',δ)	B	(g+)	(cis)	-97.5	48.4	-121.8	25.5	29.3	53.4	-161.0	3.93	5.54	3.88	0.0	0.0	0.0
(γ',δ)	B	(t)	(trans)	-83.2	64.7	-134.7	44.8	32.7	-154.1	10.1	3.77	3.27	3.69	0.0	0.0	0.0
(γ',δ)	B	(t)	(cis)	-95.8	53.3	-133.1	41.8	29.2	-152.5	-163.9	5.73	6.14	5.71	0.0	0.0	0.0
(γ‘,α‘)	A	(g-)	(trans)	-86.0	49.4	57.2	39.9	-37.8	-61.5	13.0	4.27	4.80	4.24	0.0	0.0	0.0
(γ‘,α‘)	A	(g+)	(trans)	-86.1	54.4	43.3	48.3	-37.7	49.9	11.1	6.56	7.71	6.47	0.0	0.0	0.0
(γ‘,α‘)	A	(g+)	(cis)	-94.8	58.4	42.2	53.1	-37.6	49.6	-168.5	7.55	9.87	7.44	0.0	0.0	0.0
(γ‘,α‘)	B	(g-)	(trans)	-79.4	72.4	69.6	28.8	35.7	-59.9	8.0	6.07	7.72	5.88	0.0	0.0	0.0
(γ‘,α‘)	B	(g+)	(trans)	-79.2	75.8	48.7	44.4	35.5	52.5	6.3	8.16	10.25	7.97	0.0	0.0	0.0
(γ‘,α‘)	B	(g+)	(cis)	-93.7	59.3	41.6	53.8	28.7	49.2	-168.5	8.88	10.88	8.78	0.0	0.0	0.0
(γ‘,α‘)	B	(t)	(trans)	-81.7	55.7	58.8	48.5	34.2	-150.9	9.6	7.68	8.36	7.61	0.0	0.0	0.0
NA[1)]	A	(g+)	(trans)	-82.1	95.4	154.6	-23.6	-36.0	67.5	6.5	8.04	8.39	8.06	0.0	0.0	0.0
NA[1)]	A	(t)	(trans)	-88.7	52.8	-162.5	-57.0	-37.9	-177.3	14.5	5.60	6.28	5.65	0.0	0.0	0.0
NA[1)]	B	(g+)	(trans)	-75.8	102.5	149.7	-25.2	34.3	70.6	3.7	8.55	8.34	8.64	0.0	0.0	0.0
NA[1)]	B	(t)	(trans)	-85.4	51.8	-163.2	-56.8	33.0	-177.4	13.2	6.58	6.88	6.66	0.0	0.0	0.0
NA[1)]	B	(g+)	(trans)	-83.6	37.6	-177.6	-26.7	33.9	59.0	16.6	8.35	9.47	8.39	0.0	0.0	0.0
(pp_{II},α')	A	(g-)	(trans)	-63.6	133.3	66.7	17.8	-36.6	-58.3	2.2	2.33	1.85	2.40	0.2	0.5	0.2
(pp_{II},α')	A	(g-)	(cis)	-82.9	125.9	62.4	26.4	-36.7	-59.4	-168.4	3.88	4.15	4.01	0.0	0.0	0.0
(pp_{II},α')	A	(g-)	(cis)	-82.8	124.6	60.1	28.9	-36.8	-61.5	-168.1	3.92	4.15	4.02	0.0	0.0	0.0
(pp_{II},α')	A	(g+)	(trans)	-61.9	134.8	46.7	35.8	-36.5	55.1	1.3	5.51	5.21	5.55	0.0	0.0	0.0
(pp_{II},α')	A	(g+)	(cis)	-78.5	130.7	45.6	39.9	-36.7	53.0	-170.4	6.71	7.51	6.70	0.0	0.0	0.0
(pp_{II},α')	B	(g-)	(trans)	-56.3	130.1	64.6	19.8	37.5	-62.2	1.7	1.99	1.58	2.07	0.4	0.7	0.3
(pp_{II},α')	B	(g-)	(cis)	-79.7	123.6	59.2	29.1	35.6	-64.7	-167.1	4.28	4.68	4.36	0.0	0.0	0.0
(pp_{II},α')	B	(g+)	(trans)	-55.2	131.9	47.8	33.9	37.2	56.6	0.4	4.31	5.84	4.21	0.0	0.0	0.0
(pp_{II},α')	B	(g+)	(cis)	-76.0	129.5	45.8	38.6	35.5	53.9	-169.1	7.16	7.54	7.14	0.0	0.0	0.0
(pp_{II},α')	B	(g-)	(trans)	-56.2	132.3	69.0	13.5	37.5	-61.1	0.0	1.16	0.92	1.18	1.6	2.3	1.4
(pp_{II},α)$_{bifuHB}$	A	(g-)	(trans)	-86.3	125.9	-121.7	-26.8	-36.7	-73.0	8.2	2.15	2.72	2.18	0.3	0.1	0.3
(pp_{II},α)$_{bifuHB}$	A	(g+)	(trans)	-69.4	141.6	-135.7	-4.5	-36.7	61.1	0.1	1.44	1.15	1.59	1.0	1.5	0.7
(pp_{II},α)$_{bifuHB}$	A	(t)	(trans)	-80.4	122.9	-122.5	-52.6	-36.1	-176.4	3.9	2.08	1.96	2.12	0.3	0.4	0.3
(pp_{II},α)$_{bifuHB}$	A	(t)	(cis)	-65.3	158.3	-81.9	-46.0	-37.2	-177.8	173.2	3.01	1.07	3.24	0.1	1.7	0.0
(pp_{II},α)$_{bifuHB}$	B	(g-)	(trans)	-77.5	127.4	-121.4	-29.4	35.2	-75.4	5.3	2.88	3.32	2.91	0.1	0.0	0.1
(pp_{II},α)$_{bifuHB}$	B	(g-)	(cis)	-87.5	132.1	-118.4	-6.3	33.0	-81.4	-169.4	6.14	6.69	6.16	0.0	0.0	0.0
(pp_{II},α)$_{bifuHB}$	B	(g+)	(trans)	-64.1	133.9	-143.9	-11.2	36.5	65.9	0.4	1.46	2.59	1.47	1.0	0.1	0.9
(pp_{II},α)$_{bifuHB}$	B	(g+)	(cis)	-61.1	154.3	-114.2	-6.4	36.4	63.5	177.4	2.50	3.41	2.56	0.2	0.0	0.1

$(pp_{II},\alpha)_{bifuHB}$	B	(t)	(trans)	-66.0	127.5	-132.6	-51.9	36.1	-175.2	0.3	2.32	1.88	2.41	0.2	0.4	0.2
$(pp_{II},\alpha)_{bifuHB}$	B	(t)	(cis)	-60.6	153.4	-85.2	-43.4	36.2	-176.7	176.8	3.21	2.22	3.37	0.0	0.3	0.0
(pp_{II},β)	A	(g-)	(trans)	-70.6	150.9	-120.6	145.2	-36.8	-66.5	-1.4	1.65	2.03	1.74	0.7	0.3	0.6
(pp_{II},β)	A	(g-)	(trans)	-73.0	149.8	-105.9	131.8	-37.0	-62.1	-0.8	1.59	2.97	1.09	0.8	0.1	1.7
(pp_{II},β)	A	(g+)	(trans)	-69.6	146.8	-150.5	156.5	-37.0	63.6	-0.5	1.98	1.36	2.04	0.4	1.1	0.3
(pp_{II},β)	A	(g+)	(cis)	-67.5	160.7	-121.9	153.5	-37.2	63.7	175.1	2.96	1.64	3.08	0.1	0.7	0.1
(pp_{II},β)	A	(t)	(trans)	-68.8	147.7	-133.0	127.2	-36.6	-178.3	-0.1	2.37	1.41	2.48	0.2	1.0	0.2
(pp_{II},β)	A	(t)	(cis)	-76.3	141.8	-124.4	121.3	-36.8	-176.9	-175.0	1.38	0.42	1.60	1.1	5.2	0.7
(pp_{II},β)	A	(t)	(cis)	-68.5	152.7	-130.7	128.3	-36.6	-179.7	176.8	2.32	1.10	2.51	0.2	1.7	0.2
(pp_{II},β)	A	(t)	(trans)	-68.7	148.1	-116.4	116.8	-36.9	-175.7	-1.0	1.91	1.17	1.98	0.4	1.5	0.4
(pp_{II},β)	B	(g+)	(trans)	-59.9	145.2	-152.8	157.5	36.5	64.6	-0.8	2.44	2.34	2.49	0.2	0.2	0.2
(pp_{II},β)	B	(g+)	(cis)	-64.6	164.5	-139.4	157.4	35.3	66.9	177.8	4.24	3.62	4.37	0.0	0.0	0.0
(pp_{II},β)	B	(t)	(trans)	-57.8	140.4	-150.4	128.6	36.7	-176.3	-0.8	2.99	1.67	3.19	0.1	0.6	0.0
(pp_{II},β)	B	(t)	(cis)	-64.7	150.8	-145.6	129.7	35.7	-177.9	178.9	3.27	1.68	3.57	0.0	0.6	0.0
(pp_{II},δ')	A	(t)	(trans)	-60.2	139.1	80.0	-10.5	-36.8	129.6	-1.9	11.62	12.66	3.02	0.0	0.0	0.1
(pp_{II},δ')	B	(t)	(trans)	-52.9	136.7	81.2	-13.3	36.9	129.2	-3.6	11.37	12.75	1.76	0.0	0.0	0.5
(pp_{II},γ')	A	(t)	(cis)	-67.7	146.4	-83.9	77.6	-36.9	-164.7	178.3	2.82	1.03	11.54	0.1	1.9	0.0
(pp_{II},γ')	A	(t)	(trans)	-71.9	140.2	-84.3	77.7	-36.5	-164.6	0.6	1.75	1.02	11.30	0.6	1.9	0.0
(pp_{II},γ')	B	(g-)	(trans)	-59.7	141.5	-85.7	69.4	36.6	-69.3	-0.6	2.49	2.14	2.57	0.2	0.3	0.1
(pp_{II},γ')	B	(g+)	(cis)	-59.8	148.7	-88.0	70.6	36.5	45.7	177.8	5.10	5.26	5.25	0.0	0.0	0.0
(pp_{II},γ')	B	(g+)	(trans)	-59.3	141.8	-89.2	71.4	36.7	44.7	0.0	5.00	5.20	5.07	0.0	0.0	0.0
(pp_{II},γ')	B	(t)	(trans)	-60.2	138.8	-84.4	77.8	36.5	-164.5	-1.4	1.96	1.00	2.00	0.4	2.0	0.4
(pp_{II},γ)	A	(g-)	(trans)	-70.2	142.3	72.9	-54.1	-36.5	-59.0	0.2	2.65	1.97	2.70	0.1	0.4	0.1
(pp_{II},γ)	A	(g-)	(cis)	-68.4	147.3	72.9	-50.2	-36.9	-60.1	179.8	3.65	3.07	3.82	0.0	0.1	0.0
(pp_{II},γ)	A	(g+)	(trans)	-69.9	143.2	55.5	-26.3	-36.5	70.0	-0.3	6.20	6.29	6.08	0.0	0.0	0.0
(pp_{II},γ)	A	(g+)	(cis)	-65.8	147.6	56.5	-24.7	-36.8	70.2	178.3	6.94	7.30	6.97	0.0	0.0	0.0
(pp_{II},γ)	A	(t)	(trans)	-70.3	143.7	73.4	-59.9	-36.5	-172.8	-0.1	3.10	2.44	3.08	0.1	0.2	0.1
(pp_{II},γ)	A	(t)	(cis)	-67.0	146.4	73.6	-57.8	-36.8	-173.2	178.6	4.13	3.32	4.22	0.0	0.0	0.0
(pp_{II},γ)	B	(g-)	(trans)	-57.2	139.2	72.4	-52.3	37.2	-59.2	-1.9	2.93	3.05	2.93	0.1	0.1	0.1
(pp_{II},γ)	B	(g-)	(cis)	-64.3	143.2	72.1	-50.4	37.0	-60.5	-177.7	3.95	3.43	4.11	0.0	0.0	0.0
(pp_{II},γ)	B	(g+)	(trans)	-58.2	139.3	54.2	-24.9	36.4	69.5	-2.6	6.22	6.24	6.12	0.0	0.0	0.0
(pp_{II},γ)	B	(g+)	(cis)	-61.7	143.6	54.8	-24.3	36.6	70.4	-179.3	6.95	7.70	6.89	0.0	0.0	0.0
(pp_{II},γ)	B	(t)	(trans)	-57.7	139.8	72.7	-59.3	36.7	-172.9	-2.2	3.22	2.98	3.16	0.0	0.1	0.1
(pp_{II},γ)	B	(t)	(cis)	-63.5	145.1	73.7	-57.4	36.4	-173.2	-178.8	4.20	3.94	4.26	0.0	0.0	0.0

Table S4. Summary of the conformational analysis of LD-1 by conformer family. Populations *p* of the conformer families are given in percentage. [1)] Not possible

	monomeric LD-**1** ($CHCl_3$)				LD-**1**··DMSO-d_6			
	#conf	***p*(ΔE_{ZPC})**	***p*(ΔG_{298K})**	***p*(ΔG_{corr})**	**#conf**	***p*(ΔE_{ZPC})**	***p*(ΔG_{298K})**	***p*(ΔG_{corr})**
(δ,$^{D}\beta$)	9	1.7	7.6	1.2	11	1.6	5.6	1.4
(δ,$^{D}\alpha$)$_{bifuHB}$	[2)]				6	0.7	0.9	0.6
(δ,$^{D}\gamma$)	6	0.6	0.2	0.6				
(δ,$^{D}\gamma'$)	8	1.6	1.3	1.6				
(γ',$^{D}\beta$)	11	6	11.4	5.4	13	7.1	8.9	8.8
(γ',$^{D}\delta$)	6	4.7	7	4.4	7	0.2	0.1	0.3
(γ',$^{D}\gamma$)	7	2.9	0.8	3.1				
(γ',$^{D}\gamma'$)	8	34.4	31.2	38.5	[2)]			
(pp_{II},$^{D}\beta$)	6	0.4	3.6	0.3	11	1.6	6.3	1.3
(pp_{II},$^{D}\delta$)	7	45.6	34.2	43	7	78.0	46.6	77.8
(pp_{II},$^{D}\alpha$)$_{bifuHB}$	[2)]				9	1.3	3.7	1
(pp_{II},$^{D}\gamma'$)	6	0.9	2.1	0.8	8	8.7	27.2	8
In list:	74	98.8	99.4	98.9	72	99.2	99.3	99.2
Total:	109				103			

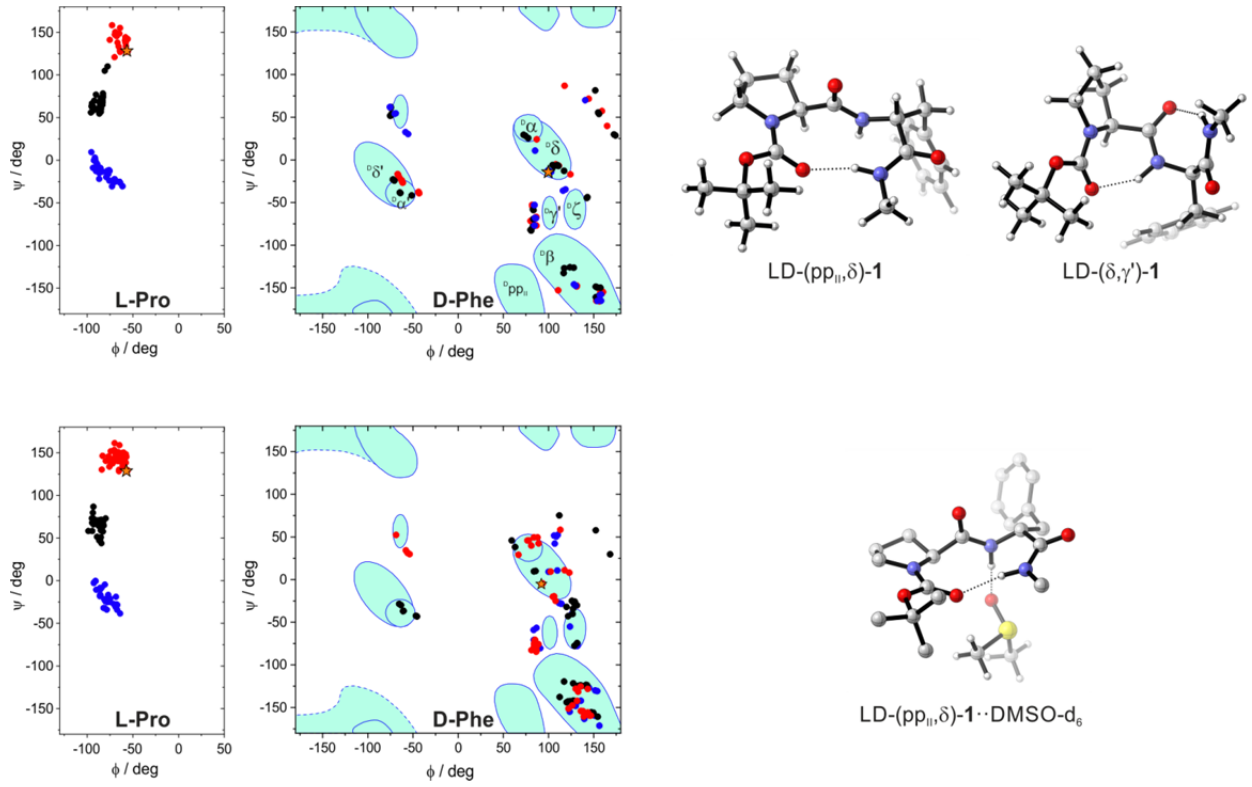


Figure S5. Ramachandran plots for LD-**1** and LD-**1**··DMSO

Table S5. Conformational analysis of LD-1. Optimized geometries and relative energies were obtained at the B3LYP/6-31G(2d,p)/IEFPCM($CHCl_3$) level of theory. ΔG_{corr} are the entropy-corrected relative free energies obtained following Cramer and Trular (*J. Phys. Chem. B* 115 **2011** 14556-14562). [1)] Conformer family names are assigned for the main conformer classes according to the Ramachandran regions' nomenclature presented in Figure 2, but rotated by 180°.

				torsional angles (definition see Scheme S1)							rel. energies			populations		
Conf.[1)]	**Pro**	**Phe**	**Boc**	**ϕ_{Pro}**	**ψ_{Pro}**	**ϕ_{Phe}**	**ψ_{Phe}**	**Pro**	**Phe**	**Boc**	**ΔE_{ZPC}**	**ΔG_{298K}**	**ΔG_{corr}**	***p*(ΔE)**	***p*(ΔG)**	***p*(ΔG_{corr})**
(δ,$^{D}\alpha'$)	A	(g-)	(trans)	-70.0	-22.0	-43.1	-39.1	-34.9	-52.2	12.5	6.45	7.44	6.41	0.0	0.0	0.0
(δ,$^{D}\alpha'$)	A	(g+)	(trans)	-75.6	-12.6	-66.1	-19.4	-37.0	59.8	13.2	2.58	2.75	2.58	0.3	0.1	0.3
(δ,$^{D}\alpha'$)	A	(t)	(trans)	-76.1	-11.7	-61.3	-26.7	-36.6	128.5	14.1	4.53	4.44	4.47	0.0	0.0	0.0
(δ,$^{D}\alpha'$)	B	(g-)	(trans)	-61.3	-30.4	-43.9	-37.5	37.8	-53.8	9.8	6.20	7.62	6.10	0.0	0.0	0.0
(δ,$^{D}\alpha'$)	B	(g+)	(trans)	-64.1	-26.0	-67.0	-16.7	37.6	59.1	10.7	2.47	2.89	2.44	0.3	0.1	0.3
(δ,$^{D}\alpha'$)	B	(t)	(trans)	-64.0	-25.9	-62.5	-23.9	37.8	126.3	11.1	4.40	4.50	4.37	0.0	0.0	0.0
(δ,$^{D}\beta$)	A	(g+)	(trans)	-91.5	3.0	131.4	-147.4	-38.2	65.3	12.1	2.91	2.25	3.07	0.2	0.3	0.1
(δ,$^{D}\beta$)	A	(g+)	(cis)	-93.6	-8.9	110.7	-152.8	-38.3	62.0	-167.2	4.23	3.74	4.37	0.0	0.0	0.0
(δ,$^{D}\beta$)	A	(t)	(trans)	-89.0	-4.7	159.0	-156.6	-37.9	169.7	11.0	2.33	0.94	2.46	0.4	2.6	0.3
(δ,$^{D}\beta$)	A	(t)	(cis)	-87.1	-8.5	158.5	-156.1	-37.6	168.8	-167.4	2.35	0.91	2.53	0.4	2.7	0.3
(δ,$^{D}\beta$)	A	(g-)	(trans)	-92.6	-0.2	156.5	-165.6	-38.2	-68.0	13.1	2.67	2.13	2.84	0.2	0.3	0.2
(δ,$^{D}\beta$)	B	(g+)	(trans)	-78.0	-12.3	131.3	-148.4	36.5	69.4	9.2	4.07	3.15	4.27	0.0	0.1	0.0
(δ,$^{D}\beta$)	B	(t)	(trans)	-69.8	-25.5	160.3	-154.8	37.3	170.2	8.4	2.86	1.64	3.04	0.2	0.8	0.1
(δ,$^{D}\beta$)	B	(t)	(cis)	-75.8	-23.9	157.5	-154.6	37.1	170.2	-168.3	2.78	1.64	2.98	0.2	0.8	0.1
(δ,$^{D}\beta$)	B	(g-)	(trans)	-79.0	-19.7	152.8	-165.1	36.7	-70.7	11.4	3.90	3.63	4.02	0.0	0.0	0.0
(δ,$^{D}\gamma$)	A	(g-)	(trans)	-69.4	-22.9	-43.3	-38.8	-34.8	-52.5	12.5	6.42	7.25	6.40	0.0	0.0	0.0
(δ,$^{D}\gamma$)	A	(g+)	(trans)	-76.0	-11.8	-65.3	-20.4	-36.9	60.2	13.5	2.61	2.99	2.56	0.3	0.1	0.3
(δ,$^{D}\gamma$)	A	(t)	(trans)	-75.6	-12.3	-61.7	-26.2	-36.6	128.6	14.1	4.50	4.47	4.43	0.0	0.0	0.0
(δ,$^{D}\gamma$)	B	(g-)	(trans)	-61.4	-30.3	-43.9	-37.6	37.7	-53.8	9.9	6.20	7.46	6.12	0.0	0.0	0.0
(δ,$^{D}\gamma$)	B	(g+)	(trans)	-64.2	-26.0	-66.4	-17.3	37.6	59.9	10.8	2.45	2.91	2.42	0.3	0.1	0.3
(δ,$^{D}\gamma$)	B	(t)	(trans)	-64.5	-25.3	-62.4	-24.0	37.8	126.5	11.0	4.39	4.59	4.33	0.0	0.0	0.0
(δ,$^{D}\gamma'$)	A	(g+)	(trans)	-95.4	9.5	86.5	-66.9	-38.4	81.4	14.6	2.82	2.59	2.81	0.2	0.2	0.2
(δ,$^{D}\gamma'$)	A	(t)	(trans)	-90.1	-2.6	85.9	-76.6	-37.9	162.5	13.0	2.28	1.72	2.21	0.5	0.7	0.5
(δ,$^{D}\gamma'$)	A	(g-)	(trans)	-90.7	-11.7	81.8	-52.8	-37.8	-45.1	13.5	2.54	2.94	2.51	0.3	0.1	0.3
(δ,$^{D}\gamma'$)	A	(g-)	(cis)	-86.7	-15.1	82.1	-54.3	-37.2	-43.8	-168.6	2.42	2.80	2.40	0.4	0.1	0.4
(δ,$^{D}\gamma'$)	B	(g+)	(trans)	-77.8	-13.9	85.1	-67.7	36.9	88.3	11.8	3.95	3.50	4.01	0.0	0.0	0.0
(δ,$^{D}\gamma'$)	B	(g+)	(cis)	-86.9	-21.9	80.1	-71.5	36.6	65.5	-160.8	3.69	3.70	3.77	0.0	0.0	0.0
(δ,$^{D}\gamma'$)	B	(g+)	(trans)	-83.1	-13.5	83.1	-70.3	36.6	70.4	13.6	4.18	3.78	4.25	0.0	0.0	0.0
(δ,$^{D}\gamma'$)	B	(t)	(trans)	-71.1	-23.0	86.6	-76.9	37.4	162.6	10.1	2.85	2.45	2.82	0.2	0.2	0.2
(γ',$^{D}\beta$)	A	(g-)	(cis)	-94.8	62.6	155.8	-159.9	-37.7	-60.7	-166.5	2.69	3.02	2.74	0.2	0.1	0.2
(γ',$^{D}\beta$)	A	(t)	(cis)	-94.3	63.8	157.4	-149.9	-37.5	170.4	-168.2	1.87	2.16	1.83	0.9	0.3	0.9
(γ',$^{D}\beta$)	B	(g-)	(cis)	-95.2	63.3	155.8	-159.2	29.1	-58.5	-165.9	4.09	5.08	4.07	0.0	0.0	0.0
(γ',$^{D}\beta$)	A	(g-)	(trans)	-86.5	67.6	154.2	-162.3	-37.4	-61.3	8.9	2.59	2.03	2.65	0.3	0.4	0.2
(γ',$^{D}\beta$)	A	(g+)	(trans)	-85.5	65.2	116.9	-132.7	-37.5	61.7	9.1	2.18	1.24	2.26	0.5	1.5	0.5
(γ',$^{D}\beta$)	A	(t)	(trans)	-85.7	64.1	123.6	-125.8	-37.6	176.6	9.5	1.61	0.67	1.67	1.4	4.0	1.2
(γ',$^{D}\beta$)	B	(g-)	(trans)	-85.1	70.8	152.4	-160.8	31.8	-61.5	8.3	3.71	3.33	3.76	0.0	0.0	0.0
(γ',$^{D}\beta$)	B	(g+)	(trans)	-84.0	70.6	117.3	-126.9	31.8	61.6	8.4	3.38	2.57	3.46	0.1	0.2	0.1
(γ',$^{D}\beta$)	B	(t)	(trans)	-83.9	68.5	127.9	-126.3	31.7	176.4	8.1	2.82	1.53	2.87	0.2	1.0	0.2
(γ',$^{D}\beta$)	A	(t)	(trans)	-86.1	62.9	153.7	-149.3	-37.6	170.2	9.4	1.41	0.88	1.43	2.0	2.8	1.8
(γ',$^{D}\beta$)	B	(t)	(trans)	-84.7	66.7	152.4	-148.6	31.7	170.8	8.2	2.61	1.48	2.64	0.3	1.0	0.2
(γ',$^{D}\alpha$)	A	(t)	(trans)	-86.8	60.6	74.6	28.2	-37.9	170.9	13.1	3.74	3.19	3.76	0.0	0.1	0.0
(γ',$^{D}\alpha$)	A	(t)	(cis)	-95.9	55.9	77.5	25.6	-37.7	172.4	-166.2	6.34	5.92	6.39	0.0	0.0	0.0

(γ',^{D}α)	B	(t)	(trans)	-84.9	62.6	72.5	29.4	32.6	171.8	11.8	4.89	4.12	4.93	0.0	0.0	0.0
(γ',^{D}α')	A	(g+)	(trans)	-85.8	64.6	-70.5	-24.4	-37.3	61.0	11.4	2.56	2.66	2.56	0.3	0.1	0.3
(γ',^{D}α')	A	(t)	(trans)	-85.1	70.1	-64.0	-38.7	-37.4	137.7	10.6	4.40	3.83	4.29	0.0	0.0	0.0
(γ',^{D}α')	B	(g-)	(trans)	-83.5	69.4	-51.4	-41.6	31.1	-52.1	8.4	6.57	7.41	6.50	0.0	0.0	0.0
(γ',^{D}α')	B	(g+)	(trans)	-84.0	66.6	-72.3	-23.0	32.0	59.7	9.9	3.78	4.27	3.74	0.0	0.0	0.0
(γ',^{D}α')	B	(t)	(trans)	-82.9	74.5	-64.6	-38.2	32.3	137.0	9.0	5.45	4.40	5.38	0.0	0.0	0.0
(γ',^{D}δ)	A	(g-)	(trans)	-88.9	59.1	104.5	-6.1	-37.8	-59.5	13.4	1.40	1.86	1.38	2.0	0.5	2.0
(γ',^{D}δ)	A	(g+)	(trans)	-86.7	54.6	110.9	-7.0	-38.0	63.6	14.1	1.38	0.47	1.41	2.1	5.7	1.9
(γ',^{D}δ)	B	(g-)	(trans)	-86.8	62.1	106.1	-7.4	32.5	-58.8	12.3	2.54	2.31	2.58	0.3	0.3	0.3
(γ',^{D}δ)	B	(g+)	(trans)	-85.0	56.9	109.6	-6.0	32.6	63.9	12.7	2.68	1.87	2.68	0.2	0.5	0.2
(γ',^{D}δ)	B	(g+)	(cis)	-94.7	66.5	117.2	-12.9	29.2	64.0	-168.0	5.48	4.99	5.52	0.0	0.0	0.0
(γ',^{D}γ)	A	(g+)	(trans)	-85.1	63.1	-74.7	51.9	-37.1	58.9	10.6	1.32	1.86	1.27	2.3	0.5	2.4
(γ',^{D}γ)	A	(g+)	(cis)	-92.1	69.8	-74.0	53.6	-36.9	60.3	-168.5	4.11	4.85	4.12	0.0	0.0	0.0
(γ',^{D}γ)	A	(t)	(trans)	-85.3	66.2	-74.7	60.9	-37.7	172.2	11.2	2.69	2.76	2.49	0.2	0.1	0.3
(γ',^{D}γ)	A	(t)	(cis)	-94.2	57.7	-74.7	62.0	-37.8	172.1	-166.9	5.21	5.34	5.12	0.0	0.0	0.0
(γ',^{D}γ)	B	(g+)	(trans)	-83.3	64.9	-75.3	51.8	32.2	58.8	9.5	2.54	3.22	2.46	0.3	0.1	0.3
(γ',^{D}γ)	B	(t)	(trans)	-83.6	67.9	-74.9	61.7	32.6	172.3	10.3	3.88	3.61	3.70	0.0	0.0	0.0
(γ',^{D}γ)	B	(t)	(cis)	-93.5	63.1	-74.9	62.0	29.2	172.1	-167.3	6.60	8.15	5.92	0.0	0.0	0.0
(γ',^{D}γ')	A	(g-)	(trans)	-85.1	72.9	83.4	-58.8	-37.3	-42.2	10.3	1.50	2.48	1.35	1.7	0.2	2.1
(γ',^{D}γ')	A	(g+)	(trans)	-84.9	63.4	83.5	-69.3	-37.8	62.7	11.5	0.19	0.03	0.12	15.7	12.0	16.7
(γ',^{D}γ')	A	(g+)	(cis)	-80.8	104.9	80.9	-82.9	-35.9	60.6	-173.0	3.00	3.57	2.99	0.1	0.0	0.1
(γ',^{D}γ')	A	(t)	(trans)	-84.9	67.1	82.9	-77.9	-37.5	162.2	10.8	0.32	0.05	0.18	12.7	11.5	15.0
(γ',^{D}γ')	B	(g-)	(trans)	-82.7	78.3	82.8	-58.1	32.9	-42.1	8.3	2.58	3.75	2.41	0.3	0.0	0.3
(γ',^{D}γ')	B	(g+)	(trans)	-83.1	67.7	83.2	-69.2	32.6	62.5	10.0	1.35	0.43	1.32	2.2	6.1	2.2
(γ',^{D}γ')	B	(g+)	(cis)	-77.7	110.1	80.2	-82.0	34.6	61.0	-173.6	3.34	3.76	3.30	0.1	0.0	0.1
(γ',^{D}γ')	B	(t)	(trans)	-82.7	73.6	82.7	-78.4	32.5	162.8	8.8	1.53	1.34	1.38	1.6	1.3	2.0
(γ',^{D}ζ)	A	(t)	(trans)	-86.5	58.8	143.1	-43.6	-37.9	152.4	12.7	3.33	2.95	3.32	0.1	0.1	0.1
(γ',^{D}ζ)	B	(t)	(trans)	-84.7	60.4	142.5	-44.6	32.5	152.8	11.5	4.58	4.19	4.55	0.0	0.0	0.0
(pp$_{II}$,^{D}γ')	A	(g-)	(trans)	-64.7	148.5	84.2	-53.0	-36.7	-43.9	-2.3	3.03	2.62	3.04	0.1	0.2	0.1
(pp$_{II}$,^{D}γ')	A	(g+)	(trans)	-67.3	148.4	86.1	-68.3	-36.8	59.9	-1.3	2.78	1.64	2.89	0.2	0.8	0.2
(pp$_{II}$,^{D}γ')	A	(t)	(trans)	-67.6	145.4	84.6	-76.8	-36.7	162.2	-0.4	2.94	2.10	3.00	0.2	0.4	0.1
(pp$_{II}$,^{D}γ')	B	(g-)	(trans)	-55.7	142.1	84.5	-52.8	36.6	-44.2	-1.6	3.07	2.80	3.06	0.1	0.1	0.1
(pp$_{II}$,^{D}γ')	B	(g+)	(trans)	-57.7	140.3	85.0	-68.0	36.7	59.8	-0.4	2.88	1.91	3.00	0.2	0.5	0.1
(pp$_{II}$,^{D}γ')	B	(t)	(trans)	-57.8	138.8	84.2	-76.7	36.8	161.8	0.4	2.99	2.68	3.00	0.1	0.1	0.1
(pp$_{II}$,^{D}β)	A	(g-)	(trans)	-69.2	150.2	158.1	-165.1	-37.2	-58.1	-1.7	3.79	2.51	3.92	0.0	0.2	0.0
(pp$_{II}$,^{D}β)	A	(g+)	(trans)	-67.6	147.2	128.2	-145.9	-36.7	59.6	-1.8	4.01	2.86	4.19	0.0	0.1	0.0
(pp$_{II}$,^{D}β)	A	(t)	(trans)	-69.7	147.2	158.1	-157.7	-37.0	167.9	-1.2	2.89	1.07	3.04	0.2	2.1	0.1
(pp$_{II}$,^{D}β)	B	(g-)	(trans)	-57.9	137.8	154.0	-165.2	36.7	-60.5	-0.7	4.06	3.28	4.13	0.0	0.0	0.0
(pp$_{II}$,^{D}β)	B	(g+)	(trans)	-58.0	142.4	130.2	-147.6	35.8	60.0	-2.5	4.38	3.02	4.54	0.0	0.1	0.0
(pp$_{II}$,^{D}β)	B	(t)	(trans)	-58.5	140.3	156.9	-158.7	36.5	168.6	-1.2	3.11	1.44	3.26	0.1	1.1	0.1
(pp$_{II}$,^{D}δ)	A	(g-)	(trans)	-64.1	128.4	99.6	-12.2	-36.5	-55.8	1.0	0.30	0.62	0.24	13.0	4.4	13.6
(pp$_{II}$,^{D}δ)	A	(g+)	(trans)	-63.9	128.3	103.0	-14.2	-36.5	64.6	0.2	0.91	0.47	0.99	4.6	5.7	3.9
(pp$_{II}$,^{D}δ)	A	(t)	(trans)	-63.9	126.8	118.7	-34.5	-36.4	150.9	0.3	2.96	2.53	3.00	0.1	0.2	0.1
(pp$_{II}$,^{D}δ)	A	(t)	(trans)	-70.0	120.8	85.1	10.9	-36.4	166.0	5.2	3.75	3.27	3.82	0.0	0.0	0.0
(pp$_{II}$,^{D}δ)	B	(g-)	(trans)	-56.5	128.2	99.8	-14.3	36.9	-55.4	-0.4	0.00	0.09	0.00	21.6	10.9	20.5
(pp$_{II}$,^{D}δ)	B	(g+)	(trans)	-57.0	127.0	101.3	-13.9	36.8	64.4	-0.5	0.75	0.00	0.86	6.0	12.6	4.8
(pp$_{II}$,^{D}δ)	B	(t)	(trans)	-55.6	127.6	116.0	-36.0	36.9	152.1	-1.2	2.70	2.06	2.78	0.2	0.4	0.2

(pp_{II},$^{D}\gamma$)	A	(g-)	(trans)	-75.2	141.1	-55.5	30.4	-36.5	-76.3	4.2	7.83	8.31	7.81	0.0	0.0	0.0
(pp_{II},$^{D}\gamma$)	A	(g+)	(trans)	-72.8	158.3	-70.2	54.1	-36.9	67.4	-0.8	4.13	4.31	4.12	0.0	0.0	0.0
(pp_{II},$^{D}\gamma$)	A	(t)	(trans)	-66.8	137.9	-75.1	61.7	-36.2	170.5	-0.2	5.40	4.72	5.42	0.0	0.0	0.0
(pp_{II},$^{D}\gamma$)	B	(g-)	(trans)	-65.5	133.4	-58.3	32.5	36.4	-79.7	3.7	8.05	8.52	8.04	0.0	0.0	0.0
(pp_{II},$^{D}\gamma$)	B	(g+)	(trans)	-63.9	155.1	-69.1	54.6	35.4	69.4	-1.3	4.53	4.29	4.57	0.0	0.0	0.0
(pp_{II},$^{D}\gamma$)	B	(t)	(trans)	-57.6	133.7	-75.5	62.1	36.6	171.5	-0.4	5.34	4.71	5.36	0.0	0.0	0.0
NA[1)]	B	(g-)	(trans)	-72.9	-30.7	111.4	-6.8	37.7	-58.0	13.3	4.17	4.04	4.24	0.0	0.0	0.0
NA[1)]	B	(g+)	(trans)	-85.4	-9.0	124.2	-16.9	35.5	76.5	12.4	5.18	4.45	5.28	0.0	0.0	0.0
NA[1)]	B	(t)	(trans)	-69.7	-25.2	87.0	24.1	37.7	171.5	11.1	6.92	5.64	7.07	0.0	0.0	0.0
NA[1)]	A	(t)	(trans)	-91.3	1.1	159.2	57.4	-38.0	175.4	13.7	7.48	5.78	7.74	0.0	0.0	0.0
NA[1)]	B	(g+)	(trans)	-79.0	-13.7	117.8	86.9	36.7	74.6	10.9	8.75	8.00	8.95	0.0	0.0	0.0
NA[1)]	B	(g-)	(trans)	-76.8	-16.1	164.9	39.8	37.2	-66.9	11.0	7.59	7.57	7.74	0.0	0.0	0.0
NA[1)]	B	(t)	(trans)	-71.2	-25.3	144.4	71.7	37.5	174.8	10.5	8.42	7.31	8.64	0.0	0.0	0.0
NA[1)]	A	(g-)	(trans)	-90.2	-12.8	107.9	-5.2	-37.1	-59.1	16.2	3.82	3.86	3.88	0.0	0.0	0.0
NA[1)]	A	(g-)	(trans)	-85.1	70.2	172.4	29.9	-37.5	-58.1	10.9	4.89	4.59	4.87	0.0	0.0	0.0
NA[1)]	A	(t)	(trans)	-84.8	65.4	154.9	55.5	-37.6	174.4	10.7	5.17	4.25	5.26	0.0	0.0	0.0
NA[1)]	A	(t)	(cis)	-90.4	77.0	151.7	81.5	-36.6	172.8	-171.8	8.72	8.82	8.75	0.0	0.0	0.0
NA[1)]	B	(g-)	(trans)	-82.7	76.0	174.1	28.7	32.5	-57.8	9.1	5.98	5.49	5.95	0.0	0.0	0.0
NA[1)]	B	(t)	(trans)	-83.0	70.3	155.9	53.8	32.1	174.6	9.1	6.28	5.12	6.43	0.0	0.0	0.0
NA[1)]	B	(t)	(cis)	-58.0	144.3	140.6	70.0	36.0	174.7	175.7	8.34	7.31	8.60	0.0	0.0	0.0

Table S6. Conformational analysis of LD-1··DMSO-d_6. Optimized geometries and relative energies were obtained at the B3LYP/6-31G(2d,p)/IEFPCM(DMSO) level of theory. ΔG_{corr} are the entropy-corrected relative free energies obtained following Cramer and Trular (*J. Phys. Chem. B* 115 **2011** 14556-14562). [1)] Conformer family names are assigned for the main conformer classes according to the Ramachandran regions' nomenclature presented in Figure 2 Figure 2, but rotated by 180°.

				torsional angles (definition see Scheme S1)				rel. energies					populations		
Conf.[1)]	**Pro**	**Phe**	**Boc**	ϕ_{Pro}	ψ_{Pro}	ϕ_{Phe}	ψ_{Phe}	**Pro**	**Phe**	**Boc**	ΔE_{ZPC}	ΔG_{298K}	ΔG_{corr}	$p(\Delta E)$	$p(\Delta G)$	$p(\Delta G_{corr})$
(δ,$^{D}\beta$)	B	(t)	(cis)	-75.6	-25.0	151.6	-129.9	37.1	176.9	-168.7	4.54	3.01	4.70	0.0	0.1	0.0
(δ,$^{D}\beta$)	B	(g+)	(cis)	-85.5	-16.8	123.5	-154.8	35.5	67.1	-168.5	4.99	4.13	5.00	0.0	0.0	0.0
(δ,$^{D}\beta$)	B	(t)	(trans)	-68.3	-27.8	145.0	-126.8	37.4	177.4	8.5	3.39	1.59	3.52	0.1	1.6	0.1
(δ,$^{D}\beta$)	B	(g+)	(trans)	-76.9	-16.6	130.1	-148.0	36.7	70.7	9.0	3.17	2.60	3.23	0.2	0.3	0.2
(δ,$^{D}\beta$)	B	(g-)	(trans)	-76.1	-22.0	156.3	-171.3	36.9	-75.2	10.6	4.38	3.06	4.39	0.0	0.1	0.0
(δ,$^{D}\beta$)	A	(t)	(trans)	-85.7	-10.2	153.9	-130.7	-37.6	176.8	11.2	4.13	2.27	4.24	0.0	0.5	0.0
(δ,$^{D}\beta$)	A	(g+)	(trans)	-91.1	-0.3	130.3	-145.4	-38.1	67.1	12.0	2.41	1.77	2.40	0.7	1.2	0.7
(δ,$^{D}\beta$)	A	(g+)	(trans)	-90.7	-0.5	135.8	-142.0	-38.1	64.7	12.1	3.46	2.46	3.57	0.1	0.4	0.1
(δ,$^{D}\beta$)	A	(g-)	(trans)	-81.5	-21.6	139.6	-163.2	-37.5	-67.5	12.9	6.66	7.71	6.78	0.0	0.0	0.0
(δ,$^{D}\beta$)	A	(g-)	(trans)	-92.5	-2.3	150.9	-159.3	-38.2	-70.1	13.2	3.00	2.32	2.99	0.2	0.5	0.2
(δ,$^{D}\beta$)	A	(g-)	(trans)	-92.8	-2.7	147.1	-156.6	-38.2	-69.9	13.4	3.33	2.01	3.36	0.1	0.8	0.1
(δ,$^{D}\alpha$)$_{bifuHB}$	B	(t)	(cis)	-71.1	-27.3	108.5	50.4	36.7	176.8	-173.3	3.10	2.85	3.19	0.2	0.2	0.2
(δ,$^{D}\alpha$)$_{bifuHB}$	A	(t)	(cis)	-86.0	-8.4	106.3	51.7	-37.5	176.4	-171.4	2.71	2.38	2.82	0.4	0.4	0.3
(δ,$^{D}\alpha$)$_{bifuHB}$	B	(t)	(trans)	-67.1	-28.3	110.2	52.4	36.8	176.5	5.0	4.12	3.11	4.30	0.0	0.1	0.0
(δ,$^{D}\alpha$)$_{bifuHB}$	B	(t)	(trans)	-67.8	-27.8	109.1	51.2	36.8	177.2	5.6	4.23	3.79	4.35	0.0	0.0	0.0
(δ,$^{D}\alpha$)$_{bifuHB}$	B	(g+)	(trans)	-74.8	-21.1	107.0	42.3	36.0	77.5	7.5	4.32	3.44	4.52	0.0	0.1	0.0
(δ,$^{D}\alpha$)$_{bifuHB}$	B	(g-)	(trans)	-64.0	-38.5	109.9	10.7	38.3	-65.1	8.5	4.76	5.32	4.80	0.0	0.0	0.0
(δ,$^{D}\gamma'$)	B	(t)	(cis)	-67.3	-34.0	87.3	-81.8	37.1	166.2	-173.0	3.45	3.49	3.42	0.1	0.1	0.1
(δ,$^{D}\gamma'$)	A	(t)	(cis)	-84.2	-8.2	89.4	-80.2	-37.0	165.3	-169.0	3.66	4.29	3.58	0.1	0.0	0.1
(δ,$^{D}\gamma'$)	B	(g+)	(cis)	-79.5	-22.1	83.8	-70.8	36.0	72.0	-168.3	5.02	5.92	4.99	0.0	0.0	0.0
(δ,$^{D}\gamma'$)	A	(g-)	(cis)	-86.1	-18.2	86.6	-56.7	-37.0	-43.5	-167.8	7.63	6.91	7.63	0.0	0.0	0.0
(δ,$^{D}\gamma'$)	A	(g-)	(cis)	-90.1	-10.5	83.6	-59.0	-36.4	-44.7	-166.2	8.68	8.44	8.75	0.0	0.0	0.0
(δ,$^{D}\gamma'$)	B	(g+)	(trans)	-68.6	-18.9	89.0	-76.1	36.2	89.0	6.7	3.98	4.73	3.94	0.0	0.0	0.0
(δ,$^{D}\gamma'$)	A	(t)	(trans)	-80.6	-4.5	90.8	-80.4	-37.2	165.4	9.0	3.10	3.54	3.03	0.2	0.1	0.2
(δ,$^{D}\zeta$)	A	(t)	(cis)	-80.0	-23.9	131.7	-77.7	-35.2	164.4	-168.7	4.68	3.98	4.69	0.0	0.0	0.0
(δ,$^{D}\zeta$)	A	(t)	(cis)	-80.0	-23.9	131.7	-77.7	-35.2	164.4	-168.7	4.68	3.98	4.69	0.0	0.0	0.0
(δ,$^{D}\zeta$)	A	(g-)	(cis)	-82.0	-32.0	114.2	-28.2	-35.5	-53.6	-167.1	5.01	5.73	4.82	0.0	0.0	0.0
(δ,$^{D}\zeta$)	A	(t)	(trans)	-77.8	-25.0	132.2	-75.3	-34.9	163.0	11.2	4.57	2.95	4.59	0.0	0.2	0.0
(δ,$^{D}\zeta$)	A	(g+)	(trans)	-85.8	-16.8	123.7	-55.0	-36.5	73.6	12.3	4.39	4.17	4.35	0.0	0.0	0.0
(δ,$^{D}\zeta$)	A	(g-)	(trans)	-78.5	-34.0	111.6	-27.4	-34.7	-53.8	13.3	5.44	5.56	5.34	0.0	0.0	0.0
(δ,$^{D}\zeta$)	A	(g-)	(trans)	-80.7	-32.2	114.0	-28.3	-35.5	-54.1	14.2	5.05	5.86	4.86	0.0	0.0	0.0
(γ',$^{D}\alpha'$)	B	(g+)	(trans)	-82.7	64.0	-65.3	-28.4	32.1	59.1	8.6	4.70	5.05	4.61	0.0	0.0	0.0
(γ',$^{D}\alpha'$)	B	(t)	(trans)	-82.6	65.6	-61.0	-37.0	32.3	135.5	9.3	6.64	5.88	6.55	0.0	0.0	0.0
(γ',$^{D}\alpha'$)	B	(g-)	(trans)	-83.8	62.2	-46.8	-42.3	31.4	-51.6	9.5	7.72	8.13	7.60	0.0	0.0	0.0
(γ',$^{D}\alpha'$)	A	(t)	(trans)	-84.5	64.1	-60.4	-36.7	-37.9	134.8	10.0	5.34	5.37	5.16	0.0	0.0	0.0
(γ',$^{D}\alpha'$)	A	(g+)	(trans)	-85.1	62.0	-63.3	-29.9	-37.6	60.8	10.1	3.48	4.50	3.33	0.1	0.0	0.1
(γ',$^{D}\alpha'$)	A	(g-)	(trans)	-85.1	59.0	-45.6	-43.2	-38.1	-51.5	10.7	6.25	6.78	6.09	0.0	0.0	0.0
(γ',$^{D}\beta$)	B	(g+)	(cis)	-93.2	86.7	124.1	-142.4	30.1	66.6	-169.7	3.61	3.34	3.53	0.1	0.1	0.1
(γ',$^{D}\beta$)	A	(g+)	(cis)	-93.8	79.6	127.7	-141.9	-36.8	66.8	-168.4	2.51	2.62	2.41	0.6	0.3	0.6
(γ',$^{D}\beta$)	A	(t)	(cis)	-93.2	66.0	141.9	-125.2	-37.5	177.5	-168.2	2.81	2.09	2.76	0.3	0.7	0.4
(γ',$^{D}\beta$)	B	(g-)	(cis)	-94.9	73.0	147.3	-155.6	29.2	-65.5	-168.2	4.51	3.74	4.45	0.0	0.0	0.0
(γ',$^{D}\beta$)	A	(g-)	(cis)	-94.5	67.9	149.6	-156.0	-37.5	-63.9	-167.5	3.25	3.50	3.14	0.2	0.1	0.2

(γ',^{D}β)	B	(t)	(trans)	-83.9	67.4	136.9	-124.4	32.1	177.3	8.4	2.92	2.56	2.82	0.3	0.3	0.3
(γ',^{D}β)	B	(t)	(trans)	-83.9	70.7	117.2	-119.5	32.1	176.7	8.5	2.80	2.74	2.67	0.3	0.2	0.4
(γ',^{D}β)	B	(g-)	(trans)	-85.3	71.1	148.7	-157.1	32.2	-65.6	9.0	3.91	2.85	3.84	0.1	0.2	0.1
(γ',^{D}β)	A	(t)	(trans)	-85.5	63.7	135.3	-123.8	-37.5	177.3	9.4	1.94	1.02	1.89	1.5	4.3	1.6
(γ',^{D}β)	B	(g+)	(trans)	-84.8	70.0	112.3	-137.6	32.1	65.5	9.5	2.47	3.42	1.85	0.6	0.1	1.7
(γ',^{D}β)	A	(t)	(trans)	-85.3	62.4	142.6	-123.8	-37.8	176.4	9.8	2.81	2.38	2.77	0.3	0.4	0.3
(γ',^{D}β)	A	(g-)	(trans)	-87.6	64.6	146.5	-156.8	-37.7	-64.9	10.6	2.78	2.22	2.67	0.4	0.6	0.4
(γ',^{D}β)	A	(g+)	(trans)	-87.2	65.8	121.5	-142.9	-37.7	66.7	10.8	1.63	1.60	1.54	2.5	1.6	2.8
(γ‘,^{D}δ)	B	(g-)	(trans)	-82.8	57.6	119.9	-31.9	30.7	-50.6	9.3	4.78	4.42	4.72	0.0	0.0	0.0
(γ‘,^{D}δ)	B	(t)	(trans)	-85.5	62.9	131.6	-74.3	27.3	163.3	9.3	5.10	4.30	5.06	0.0	0.0	0.0
(γ‘,^{D}δ)	B	(g+)	(cis)	-94.4	58.3	126.6	-40.2	25.7	64.0	-167.9	6.71	6.88	6.66	0.0	0.0	0.0
(γ‘,^{D}δ)	A	(g-)	(trans)	-82.7	67.5	129.1	-25.8	-35.4	-53.8	7.2	4.02	4.44	3.97	0.0	0.0	0.0
(γ‘,^{D}δ)	A	(g-)	(trans)	-82.0	64.7	128.3	-27.8	-36.7	-52.9	7.6	3.74	4.36	3.65	0.1	0.0	0.1
(γ‘,^{D}δ)	B	(g+)	(trans)	-79.8	73.1	125.9	-24.9	34.2	63.5	7.8	4.72	4.86	4.64	0.0	0.0	0.0
(γ‘,^{D}δ)	A	(g+)	(trans)	-83.8	62.2	127.1	-34.3	-36.2	63.0	8.4	3.57	3.59	3.49	0.1	0.1	0.1
(pp$_{II}$,^{D}β)	B	(g-)	(cis)	-60.9	141.6	142.7	-158.0	36.7	-63.9	-179.3	3.75	2.32	3.88	0.1	0.5	0.1
(pp$_{II}$,^{D}β)	B	(g+)	(trans)	-59.4	142.5	131.6	-142.2	36.3	60.8	-0.7	4.55	3.34	4.72	0.0	0.1	0.0
(pp$_{II}$,^{D}β)	A	(t)	(trans)	-68.6	150.3	143.4	-128.1	-37.0	177.6	-0.7	3.54	2.05	3.67	0.1	0.8	0.1
(pp$_{II}$,^{D}β)	A	(g-)	(trans)	-68.8	147.4	145.5	-159.3	-37.0	-65.3	-0.4	3.98	2.53	3.98	0.0	0.3	0.0
(pp$_{II}$,^{D}β)	B	(g-)	(trans)	-58.8	141.4	146.9	-159.4	36.6	-65.3	-0.4	3.88	2.40	3.92	0.1	0.4	0.0
(pp$_{II}$,^{D}β)	A	(g+)	(trans)	-68.8	147.8	126.3	-147.4	-36.7	65.8	-0.1	2.94	1.83	3.02	0.3	1.1	0.2
(pp$_{II}$,^{D}β)	B	(t)	(trans)	-61.4	142.6	130.1	-128.0	36.7	178.5	1.4	3.60	2.13	3.74	0.1	0.7	0.1
(pp$_{II}$,^{D}β)	B	(g+)	(cis)	-57.1	145.3	132.7	-131.4	35.4	62.4	173.3	3.93	3.18	4.12	0.1	0.1	0.0
(pp$_{II}$,^{D}β)	A	(g+)	(cis)	-69.3	143.7	122.1	-151.1	-36.2	65.3	174.7	2.41	1.90	2.52	0.7	1.0	0.5
(pp$_{II}$,^{D}β)	A	(g-)	(cis)	-72.1	137.5	139.1	-160.6	-36.1	-65.0	177.0	3.73	2.63	3.79	0.1	0.3	0.1
(pp$_{II}$,^{D}β)	A	(t)	(cis)	-68.2	145.3	135.7	-125.3	-36.9	177.7	178.9	3.10	1.78	3.34	0.2	1.2	0.1
(pp$_{II}$,^{D}δ)	A	(t)	(cis)	-84.0	130.2	66.6	29.2	-36.6	173.6	-169.9	0.22	0.08	0.21	26.8	20.9	26.3
(pp$_{II}$,^{D}δ)	B	(t)	(trans)	-55.6	129.3	107.8	-24.9	37.1	156.7	-1.9	2.76	2.45	2.73	0.4	0.4	0.4
(pp$_{II}$,^{D}δ)	B	(g-)	(trans)	-56.8	130.0	104.7	-20.0	37.0	-55.6	-1.8	1.03	2.19	0.93	6.9	0.6	7.8
(pp$_{II}$,^{D}δ)	B	(g+)	(trans)	-57.1	128.5	92.0	-5.2	37.1	63.4	-0.8	0.00	0.00	0.00	39.1	23.9	37.5
(pp$_{II}$,^{D}δ)	A	(g-)	(trans)	-65.1	130.1	106.2	-19.7	-36.4	-54.9	0.4	3.53	2.08	3.69	0.1	0.7	0.1
(pp$_{II}$,^{D}δ)	A	(t)	(trans)	-65.7	129.2	94.9	-4.1	-36.5	164.4	1.4	5.90	5.08	6.01	0.0	0.0	0.0
(pp$_{II}$,^{D}δ)	A	(g+)	(trans)	-65.3	128.4	93.5	-4.5	-36.6	63.6	1.7	1.25	2.67	1.11	4.8	0.3	5.8
(pp$_{II}$,^{D}α)$_{bifuHB}$	B	(g-)	(cis)	-66.9	150.3	123.1	8.2	35.6	-62.3	-178.7	3.18	3.48	3.24	0.2	0.1	0.2
(pp$_{II}$,^{D}α)$_{bifuHB}$	B	(g-)	(trans)	-60.4	144.8	117.8	11.0	36.2	-61.4	-2.1	3.56	3.54	3.57	0.1	0.1	0.1
(pp$_{II}$,^{D}α)$_{bifuHB}$	B	(t)	(trans)	-59.8	138.3	87.9	49.4	36.5	178.4	-1.3	3.40	2.10	3.49	0.1	0.7	0.1
(pp$_{II}$,^{D}α)$_{bifuHB}$	B	(g+)	(trans)	-60.6	138.5	89.1	42.4	36.6	59.9	-0.7	2.83	1.99	2.91	0.3	0.8	0.3
(pp$_{II}$,^{D}α)$_{bifuHB}$	A	(g-)	(trans)	-73.2	149.6	108.3	10.1	-37.0	-60.1	0.2	3.21	2.84	3.28	0.2	0.2	0.1
(pp$_{II}$,^{D}α)$_{bifuHB}$	A	(t)	(trans)	-71.9	140.5	78.1	46.0	-36.6	177.2	0.5	3.74	2.65	3.86	0.1	0.3	0.1
(pp$_{II}$,^{D}α)$_{bifuHB}$	B	(t)	(trans)	-61.1	135.1	83.8	49.5	36.7	178.1	0.9	4.64	3.40	4.79	0.0	0.1	0.0
(pp$_{II}$,^{D}δ)$_{bifuHB}$	A	(g+)	(trans)	-73.1	138.6	80.9	39.9	-36.5	60.0	1.0	2.95	1.67	3.14	0.3	1.4	0.2
(pp$_{II}$,^{D}α)$_{bifuHB}$	B	(t)	(cis)	-57.8	148.3	113.0	58.4	36.7	178.8	178.0	4.68	3.70	4.77	0.0	0.0	0.0
(pp$_{II}$,^{D}γ)	A	(g-)	(cis)	-83.2	146.3	-56.1	31.6	-36.6	-78.4	-172.5	9.65	9.09	9.69	0.0	0.0	0.0
(pp$_{II}$,^{D}γ)	B	(g-)	(cis)	-76.5	145.8	-57.9	34.3	34.9	-83.0	-172.3	10.27	9.81	10.29	0.0	0.0	0.0
(pp$_{II}$,^{D}γ)	B	(g+)	(trans)	-64.7	158.8	-68.8	52.4	35.4	66.8	-1.2	5.10	3.56	5.20	0.0	0.1	0.0
(pp$_{II}$,^{D}γ)	B	(g-)	(trans)	-66.2	140.2	-56.0	31.4	36.2	-77.8	1.6	7.62	7.55	7.54	0.0	0.0	0.0
(pp$_{II}$,^{D}γ)	A	(g-)	(trans)	-77.3	141.0	-53.8	29.9	-36.5	-74.3	4.2	7.32	7.61	7.19	0.0	0.0	0.0

(pp_{II},$^{D}\gamma'$)	B	(t)	(cis)	-65.3	150.2	86.4	-84.6	35.9	166.2	-179.9	3.29	2.93	3.31	0.1	0.2	0.1
(pp_{II},$^{D}\gamma'$)	B	(g+)	(cis)	-66.0	150.6	87.7	-77.0	36.1	63.5	-179.1	2.38	2.96	2.36	0.7	0.2	0.7
(pp_{II},$^{D}\gamma'$)	A	(g+)	(trans)	-69.1	142.6	84.7	-71.5	-36.6	63.6	-0.2	1.63	0.57	1.69	2.5	9.1	2.2
(pp_{II},$^{D}\gamma'$)	A	(t)	(trans)	-67.6	143.7	84.8	-79.5	-36.7	165.9	0.3	2.45	1.55	2.43	0.6	1.7	0.6
(pp_{II},$^{D}\gamma'$)	B	(t)	(trans)	-57.8	138.3	84.0	-79.6	37.0	165.5	0.4	2.35	0.60	2.36	0.7	8.7	0.7
(pp_{II},$^{D}\gamma'$)	B	(g+)	(trans)	-58.6	138.3	84.0	-75.2	37.0	61.7	0.4	1.50	0.80	1.52	3.1	6.3	2.9
(pp_{II},$^{D}\gamma'$)	A	(g+)	(cis)	-70.0	161.2	88.8	-75.7	-37.2	65.9	175.8	2.42	2.06	2.51	0.7	0.7	0.5
(pp_{II},$^{D}\gamma'$)	A	(t)	(cis)	-70.3	153.3	86.6	-82.8	-37.3	166.2	178.9	2.99	2.59	3.00	0.2	0.3	0.2
NA[1)]	B	(t)	(trans)	-82.3	69.8	152.3	57.8	32.5	176.2	8.5	6.46	4.86	6.57	0.0	0.0	0.0
NA[1)]	A	(g-)	(trans)	-84.4	71.6	168.1	29.7	-37.3	-56.7	8.8	6.83	8.16	6.72	0.0	0.0	0.0
NA[1)]	B	(g-)	(trans)	-85.0	51.0	83.8	9.7	30.8	-64.1	13.6	7.03	8.00	7.02	0.0	0.0	0.0
NA[1)]	A	(t)	(trans)	-86.9	47.2	59.2	45.9	-38.0	177.1	14.1	5.90	6.18	5.92	0.0	0.0	0.0
NA[1)]	A	(g-)	(trans)	-89.3	51.5	85.7	10.0	-37.7	-64.2	15.0	5.62	6.68	5.61	0.0	0.0	0.0
NA[1)]	A	(t)	(cis)	-98.7	58.3	112.0	75.3	-37.5	172.4	-165.5	7.54	6.46	7.57	0.0	0.0	0.0

3. Effect of GD3BJ corrections

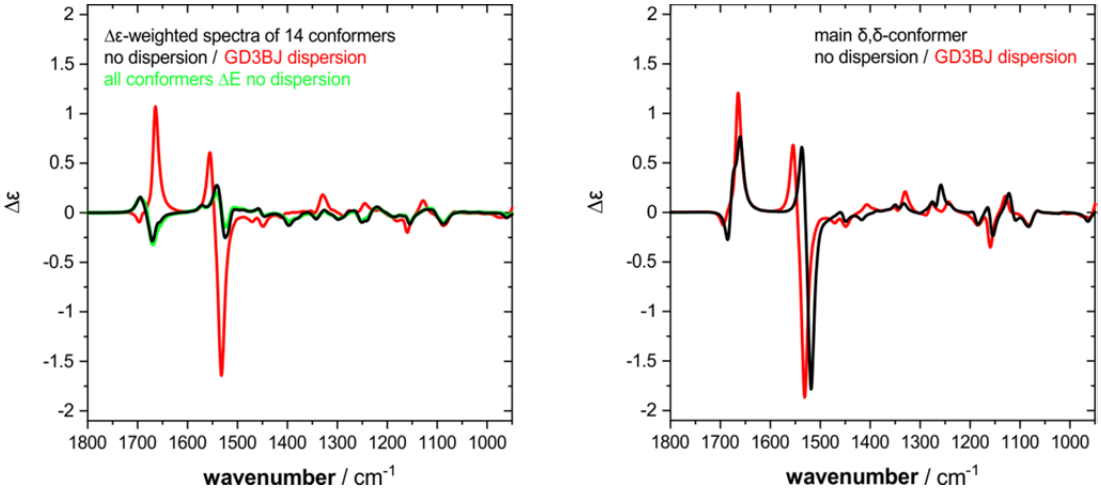


Figure S4. Computed VCD spectra of LL-1··DMSO-d6 with and without inclusion of GD3BJ dispersion correction. Left: Comparison of ΔE-weighted VCD spectra show that the predicted conformational equilibrium is off when GD3BJ is included. Right: Single-conformer spectra of (δ,δ)-conformers.

Table S7. Conformer energies ΔE_{ZPC} of the 14 lowest energy conformers of LL-1··DMSO-d_6

	B3LYP, no dispersion			B3LYP+GD3BJ	
	ΔE	pop(ΔE)$_{full}$	pop(ΔE)$_{subset}$	ΔE	pop(ΔE)
(δ,δ)	0.35	6.18	9.5	0.00	58.5
(δ,δ)	0.00	11.20	17.2	0.34	33.2
(δ,α)$_{bifurcHB}$	0.98	2.13	3.3	1.87	2.5
(δ,α)$_{bifurcHB}$	0.99	2.11	3.2	2.25	1.3
(δ,β)	0.21	7.80	12.0	5.11	0.0
(δ,β)	0.98	2.13	3.3	6.77	0.0
(δ,β)	1.01	2.05	3.1	5.24	0.0
(δ,β)	0.55	4.41	6.8	7.75	0.0
(δ,β)	0.79	2.96	4.6	6.49	0.0
(δ,β)	1.00	2.07	3.2	6.21	0.0
(δ,γ')	0.55	4.45	6.8	1.53	4.4
(γ',β)	0.02	10.84	16.7	4.24	0.0
(γ',β)	0.69	3.48	5.4	4.46	0.0
(γ',β)	0.73	3.25	5.0	8.24	0.0

4. Selected Cartesian coordinates

LL-(δ,δ)-1

C	1.24765600	3.66671100	-1.10199100
C	1.43508100	2.77001100	-2.33627700
C	2.14795300	1.53635400	-1.77107300
N	1.58780000	1.43150700	-0.41322500
C	0.93735400	2.66791800	0.03434600
C	-0.56945200	2.54409100	0.31224600
O	-1.17096300	3.47728700	0.82696600
C	1.90242900	0.45614500	0.48521700
O	1.46037600	0.43807500	1.63024100
O	2.72379800	-0.45154000	-0.06028000
C	3.11285300	-1.67876400	0.66572100
C	1.86945600	-2.51352800	0.97606800
C	4.00478400	-2.39101600	-0.35135400
C	3.90675300	-1.31439200	1.92176100
C	-2.60971000	0.16133600	1.61418200
N	-1.14847300	1.36680100	-0.02870500
C	-2.50662000	1.01313100	0.32874500
C	-3.24304600	0.32240200	-0.84305800
O	-3.70304500	-0.27633100	1.96819100
N	-1.47740300	-0.04657800	2.31076600
C	-1.49804400	-0.78996200	3.55765500
H	0.45603600	4.40926900	-1.20919300
H	2.17780600	4.19538500	-0.87359400
H	1.95330900	0.62362200	-2.33732900
H	3.23374900	1.68304400	-1.72710100
H	1.36426100	2.99617900	0.98558100
H	2.17545900	-3.47449400	1.40058400
H	1.22169300	-2.00727400	1.69144600
H	1.30183100	-2.71062600	0.06158100
H	4.37072500	-3.33132900	0.06987500
H	4.86632400	-1.77002400	-0.61205000
H	3.44772400	-2.61457800	-1.26539600
H	4.75780600	-0.67718300	1.66289500
H	3.28161700	-0.79312000	2.64595100
H	4.29509100	-2.22814400	2.38195900
H	-0.56970000	0.66510900	-0.46691600
H	-3.02019400	1.95109500	0.55856600
H	-3.37814500	1.05964300	-1.63968000
H	-0.58866200	0.31311200	1.98207400
H	-0.48671700	-0.81066400	3.96534300
H	-2.16814000	-0.31821100	4.28279800
H	-1.84320700	-1.81693400	3.40011400
H	-4.23050700	0.04229000	-0.46931200
H	2.01003900	3.25027100	-3.13022800
H	0.46209100	2.48388200	-2.74981000
C	-2.51585900	-0.89099300	-1.38230300
C	-1.70683500	-0.79301600	-2.52137100
C	-2.61464600	-2.13305500	-0.73990700
C	-1.00886300	-1.90071400	-3.00417600
H	-1.63557200	0.15722500	-3.04354900
C	-1.91950100	-3.24081400	-1.22007500
H	-3.24368500	-2.22468600	0.13951800
C	-1.11204700	-3.12858000	-2.35286000
H	-0.39359400	-1.80488000	-3.89328600
H	-2.01407600	-4.19580800	-0.71293100
H	-0.57633400	-3.99379400	-2.72968300

LL-(γ‘, γ‘)-1

C	2.38177900	3.28640300	-0.80406500
C	2.88149300	2.61936300	-2.09566900

C	3.42672700	1.26899500	-1.61551500
N	2.59032100	0.96602800	-0.44222700
C	1.78308900	2.12041200	-0.00814400
C	0.27725300	1.91895300	-0.29986600
O	-0.34728000	2.65251800	-1.06947000
C	2.75269400	-0.11789200	0.35689400
O	2.09630400	-0.30715700	1.38073000
O	3.70409600	-0.93284800	-0.12340000
C	4.02737900	-2.21495600	0.53392500
C	2.79845500	-3.12637400	0.54192300
C	5.11673500	-2.78260200	-0.37649000
C	4.57439700	-1.95555300	1.93898900
C	-2.60322800	1.34251100	1.04543600
N	-0.28757800	0.89325200	0.36718000
C	-1.67545000	0.48560500	0.14835400
C	-1.84241600	-1.01829300	0.41981300
O	-3.08307100	0.92077400	2.09222600
N	-2.80719800	2.59099700	0.56771500
C	-3.54321300	3.59666900	1.31095000
H	1.64044500	4.06350300	-0.98548500
H	3.21744700	3.71510400	-0.24278700
H	3.64072100	3.20530800	-2.61722200
H	2.03965400	2.46570700	-2.77718800
H	3.34237900	0.47877100	-2.36486000
H	4.47935100	1.33975900	-1.31799700
H	1.89356200	2.24592700	1.07341400
H	3.08304400	-4.11448700	0.91617800
H	2.01233700	-2.72371800	1.18005100
H	2.40802900	-3.24827200	-0.47309700
H	5.45338900	-3.75061200	0.00447100
H	5.97666900	-2.10831300	-0.41720100
H	4.73723900	-2.92323800	-1.39241100
H	5.42246100	-1.26548200	1.89516800
H	3.80735100	-1.53422700	2.58823900
H	4.92496300	-2.89760900	2.37156500
H	0.31526900	0.34346800	0.97808200
H	-1.90848200	0.70517000	-0.89788900
H	-1.82493100	-1.17542700	1.50198700
H	-2.22988000	2.87613200	-0.21708800
H	-4.08076300	4.24819300	0.61781000
H	-4.25850000	3.09227900	1.96130200
H	-2.88385300	4.21408100	1.93342600
H	-0.97530000	-1.52987900	-0.01025100
C	-3.11146700	-1.59342800	-0.17470900
C	-4.31031500	-1.61342500	0.54744300
C	-3.10526400	-2.11405700	-1.47422200
C	-5.47151000	-2.13923900	-0.01702500
H	-4.32581200	-1.19921200	1.54908300
C	-4.26496100	-2.63878500	-2.04178700
H	-2.18012500	-2.11356000	-2.04444600
C	-5.45353400	-2.65327800	-1.31296100
H	-6.39188400	-2.14860800	0.55865400
H	-4.23828100	-3.04083800	-3.04976700
H	-6.35757700	-3.06432700	-1.75077100

LL-(γ‘,β)-1··DMSO-d_6

C	-1.25686000	-1.26710400	3.29380100
C	-1.90923600	-2.43464400	2.53613000
C	-2.96827400	-1.75234700	1.66029100
N	-2.40166700	-0.41365700	1.42338600
C	-1.20848600	-0.14924300	2.24666000
C	0.09450400	-0.18438200	1.40766800
O	0.99892100	-0.98393700	1.64605800
C	-3.03939000	0.58458900	0.76551000
O	-2.58016300	1.72103300	0.65123700
O	-4.21081500	0.16040200	0.26392200

C	-5.08613300	1.05441400	-0.51936000
C	-4.36632500	1.51726400	-1.78768600
C	-6.26114800	0.14007100	-0.86772800
C	-5.55074100	2.22399600	0.35109200
C	1.70022900	2.32018400	-0.55040600
N	0.13363300	0.73429400	0.42149100
C	1.23174200	0.85965100	-0.51573700
C	0.82541200	0.42153900	-1.94870100
O	0.89347500	3.25009500	-0.52099200
N	3.03073200	2.48725500	-0.65450300
C	3.62266700	3.80716600	-0.77676000
H	-0.26122400	-1.50406000	3.66655000
H	-1.88604700	-0.95098000	4.13121300
H	-2.34763700	-3.18573300	3.19593000
H	-1.16163500	-2.92629300	1.90681000
H	-3.14000400	-2.27216700	0.71479600
H	-3.92957300	-1.66546100	2.17866800
H	-1.29441000	0.84897200	2.68606100
H	-5.06200200	2.08687200	-2.41139400
H	-3.51168200	2.14934800	-1.54801900
H	-4.02255200	0.65458600	-2.36689800
H	-6.99722700	0.69018400	-1.46020900
H	-6.74984800	-0.22429500	0.04019500
H	-5.92151400	-0.72109000	-1.44994900
H	-6.01436000	1.85255900	1.27005200
H	-4.71774100	2.87602400	0.61245900
H	-6.29837500	2.80741200	-0.19472000
H	-0.64875100	1.38002800	0.33930100
H	2.03798300	0.21478700	-0.16984900
H	1.66789100	0.64583700	-2.61259800
H	3.63305400	1.66274500	-0.64968100
H	3.22614200	4.33811700	-1.64811200
H	3.42111800	4.41744700	0.10991800
H	4.70197800	3.69721000	-0.89055100
H	-0.01769500	1.03846000	-2.27668700
C	0.47573100	-1.04542600	-2.03926300
C	1.48741800	-2.01452100	-2.00689200
C	-0.85279300	-1.46845200	-2.14179600
C	1.17648800	-3.37055400	-2.07491900
H	2.52255500	-1.69640000	-1.91473300
C	-1.16815300	-2.82656200	-2.20997600
H	-1.64707800	-0.72853600	-2.17465900
C	-0.15377000	-3.78177000	-2.17682200
H	1.97262300	-4.10817500	-2.05064800
H	-2.20546700	-3.13522800	-2.29455000
H	-0.39599200	-4.83815700	-2.23247500
S	5.16118000	-0.74648200	0.46969300
O	4.41582900	-0.07530800	-0.68173600
C	4.36194400	-0.18920100	2.00477500
H(Iso=2)	3.33772600	-0.56910800	1.98103400
H(Iso=2)	4.90848900	-0.60830800	2.85275100
H(Iso=2)	4.36590300	0.90253300	2.03599100
C	6.72781400	0.15805100	0.65875300
H(Iso=2)	6.51644700	1.22470100	0.75849200
H(Iso=2)	7.25135500	-0.22461300	1.53759500
H(Iso=2)	7.31595500	-0.03535400	-0.23950600

LL-(δ,δ)-1··DMSO-d_6

C	0.74012800	-2.11403500	2.48483400
C	-0.30739700	-3.20095700	2.20522400
C	-1.20808300	-2.56031000	1.14268900
N	-1.15375100	-1.12744000	1.47964700
C	-0.07086300	-0.80009700	2.41160800
C	0.80947600	0.38989700	2.02555600
O	1.36440700	1.04023200	2.90766100
C	-2.11717500	-0.21537500	1.20490200

O	-2.06738700	0.94832800	1.60090300
O	-3.10018500	-0.74378300	0.45224100
C	-4.35019000	-0.00018400	0.18609600
C	-4.06198900	1.23616400	-0.66685500
C	-5.18028000	-1.01663300	-0.59850200
C	-5.03853700	0.34809400	1.50777200
C	1.01408800	2.98548300	-0.15138000
N	0.96823600	0.63017500	0.70369200
C	1.80392400	1.71199200	0.22073700
C	2.68962300	1.26655800	-0.96394500
O	1.58065000	3.92439400	-0.71100600
N	-0.28521300	3.02023400	0.19944000
C	-1.09457000	4.20173100	-0.03750900
H	1.50750400	-2.11669700	1.70355800
H	1.23785700	-2.22190700	3.44954900
H	-0.81522800	-2.71357300	0.13213800
H	-2.23696300	-2.91944200	1.17586300
H	-0.48319100	-0.54530900	3.39358900
H	-5.00847300	1.68727400	-0.98049000
H	-3.48969700	1.97516900	-0.10756400
H	-3.50245500	0.95881600	-1.56506600
H	-6.15908100	-0.59075300	-0.83530200
H	-5.33157500	-1.92738200	-0.01255700
H	-4.68680100	-1.28275700	-1.53722500
H	-5.19758200	-0.55518900	2.10457600
H	-4.44707600	1.05724600	2.08655700
H	-6.01572400	0.79389600	1.29944500
H	0.50063000	0.04463500	0.01007600
H	2.44691000	2.00483800	1.05709900
H	3.18646800	2.16460300	-1.33785500
H	-0.71286600	2.22621400	0.66348700
H	-2.02367700	4.10947400	0.52653100
H	-0.56361300	5.09958900	0.29012300
H	-1.33684000	4.32115900	-1.09960300
H	2.04034200	0.88830800	-1.75929000
H	-0.88656200	-3.40971900	3.11063900
H	0.13509900	-4.13827100	1.86173100
C	3.70382500	0.21228600	-0.58422300
C	4.92656200	0.57638300	-0.00769700
C	3.43995300	-1.14755700	-0.78996900
C	5.86139000	-0.39016400	0.35959500
H	5.14970100	1.62816800	0.15067400
C	4.37421000	-2.11729100	-0.42383500
H	2.49621100	-1.43960000	-1.24092300
C	5.58743300	-1.74229600	0.15262800
H	6.80555800	-0.08719600	0.80140400
H	4.15507600	-3.16697800	-0.59407500
H	6.31522600	-2.49635200	0.43466200
S	-0.93797600	-0.64738900	-2.68690400
O	0.09696100	-0.95631600	-1.60929300
C	-1.84623100	-2.19664800	-2.96630100
H(Iso=2)	-2.42374300	-2.38318100	-2.06015600
H(Iso=2)	-2.51549600	-2.06498000	-3.81932000
H(Iso=2)	-1.13141100	-3.00277500	-3.14328700
C	-0.03042700	-0.61311600	-4.26190900
H(Iso=2)	0.56921100	-1.52165400	-4.34684400
H(Iso=2)	-0.74901200	-0.53490400	-5.08062400
H(Iso=2)	0.60922200	0.27027700	-4.24164600

LD-(pp_{II},$^{D}\delta$)-1

C	0.94057700	3.43704300	-0.50192600
C	2.30840700	3.84273500	0.06669600
C	3.15220200	2.57660400	-0.11511200
N	2.16475300	1.50268400	0.05121100
C	0.78070600	1.96185800	-0.07754900
C	0.02324700	1.15108300	-1.14068400

O	0.45958500	1.02577000	-2.27606600
C	2.44333300	0.20939100	0.33781300
O	1.57571700	-0.64351700	0.51244500
O	3.76867000	0.00415800	0.41334300
C	4.32970600	-1.32870400	0.70228800
C	3.94427200	-2.30808800	-0.40817100
C	5.83523200	-1.06049500	0.68703500
C	3.87931000	-1.80096200	2.08646300
C	-1.85339100	-1.71674500	-1.28516100
N	-1.15783700	0.62695900	-0.72510100
C	-2.00012600	-0.20354100	-1.56441700
C	-3.48262200	0.23099500	-1.50015200
O	-2.67104500	-2.51090800	-1.74769900
N	-0.79259800	-2.09758200	-0.55107200
C	-0.53032600	-3.50167800	-0.29384500
H	0.95799900	3.48381900	-1.59462000
H	0.11611400	4.05455400	-0.14104800
H	2.22360600	4.08549300	1.13105600
H	2.73977600	4.70597600	-0.44434900
H	3.60216000	2.53256500	-1.11438500
H	3.95013600	2.47811600	0.62193800
H	0.27174900	1.88076900	0.89103300
H	4.45722200	-3.26107100	-0.24643100
H	2.86932500	-2.48544000	-0.42247100
H	4.25103100	-1.91732700	-1.38292900
H	6.38073700	-1.98723800	0.88507200
H	6.10573100	-0.32903700	1.45374500
H	6.14870500	-0.67512500	-0.28706000
H	4.12989600	-1.05174500	2.84373300
H	2.80544700	-1.98359400	2.11130400
H	4.40183700	-2.72812700	2.34114700
H	-1.42241700	0.73417300	0.24331800
H	-1.64050400	-0.05594300	-2.58739100
H	-4.04110300	-0.47424600	-2.11911600
H	-0.10592900	-1.41877700	-0.23995100
H	0.27511300	-3.57652200	0.43796200
H	-1.42480100	-3.98948100	0.10271800
H	-0.23408000	-4.03232000	-1.20585900
H	-3.56124700	1.22142600	-1.95795300
C	-4.05416400	0.26829100	-0.09854000
C	-4.53263800	-0.89687100	0.51708100
C	-4.10552800	1.46970500	0.61926700
C	-5.04405100	-0.85885800	1.81233700
H	-4.49704300	-1.83312500	-0.02956000
C	-4.61613000	1.50979500	1.91701900
H	-3.75311300	2.38463700	0.15102900
C	-5.08707200	0.34413200	2.51766000
H	-5.41463200	-1.77056500	2.27041900
H	-4.65178900	2.45281800	2.45342900
H	-5.48924100	0.37273700	3.52518000

LD-(δ,^{D}γ‘)-1

C	1.06438300	1.19287000	3.27061800
C	2.20629800	2.09161200	2.77002900
C	2.94012700	1.20911600	1.75323900
N	1.87189000	0.34338500	1.22556500
C	0.62724900	0.43596400	2.01114700
C	-0.48972700	1.17734600	1.23695700
O	-0.97647100	2.23748800	1.63858500
C	2.06670600	-0.65295400	0.32633400
O	1.17074000	-1.41124500	-0.04664400
O	3.34103500	-0.68641100	-0.08896000
C	3.78943300	-1.63142500	-1.13195000
C	3.02920700	-1.37367000	-2.43424900
C	5.26701100	-1.26986800	-1.28627400
C	3.63200300	-3.06950500	-0.63396000
C	-1.53198500	2.13909000	-1.69305200
N	-0.88791800	0.55816000	0.11024100

C	-1.99633400	1.02890600	-0.71654200
C	-2.63061600	-0.14438900	-1.47972100
O	-1.47649000	1.96356100	-2.90473500
N	-1.21616700	3.30015800	-1.07385500
C	-0.69219600	4.45157000	-1.78274700
H	0.23713300	1.75519000	3.70179300
H	1.43335700	0.47712900	4.01136000
H	2.86789000	2.43259400	3.56867200
H	1.78841800	2.97200200	2.27294800
H	3.40967300	1.77778700	0.94752600
H	3.71557600	0.59924300	2.23080300
H	0.26545600	-0.57383200	2.22604500
H	3.45637600	-1.99077100	-3.23048500
H	1.97240100	-1.61798000	-2.33059100
H	3.12460200	-0.32455700	-2.72993500
H	5.72980800	-1.91127700	-2.04121400
H	5.79957000	-1.40760500	-0.34113900
H	5.37972900	-0.22850300	-1.60031400
H	4.15025200	-3.20015900	0.32091000
H	2.58152400	-3.32891200	-0.50588900
H	4.07959300	-3.75550400	-1.35958600
H	-0.38218900	-0.28572500	-0.15619800
H	-2.73188300	1.47041900	-0.03524800
H	-1.87125300	-0.59139800	-2.12875700
H	-1.22924500	3.29718900	-0.05799500
H	0.37472300	4.60090400	-1.57935900
H	-0.82518300	4.28111900	-2.85126200
H	-1.23123700	5.35835200	-1.49257800
H	-3.39206000	0.27265500	-2.14407200
C	-3.23917500	-1.18796800	-0.57015300
C	-2.53082600	-2.34101500	-0.21456800
C	-4.52860800	-1.01279700	-0.05379800
C	-3.09266200	-3.29093400	0.63810000
H	-1.53145000	-2.49970200	-0.60947600
C	-5.09403200	-1.95916200	0.79803900
H	-5.09674500	-0.12785000	-0.32764400
C	-4.37618100	-3.10288400	1.14758300
H	-2.52728700	-4.17978400	0.89990000
H	-6.09700900	-1.80636500	1.18397800
H	-4.81613100	-3.84314600	1.80798600

LD-(pp$_{II}$,^{D}δ)-1··DMSO-d$_6$

C	0.07574200	-2.98776900	1.21697500
C	-1.16698700	-3.58095600	1.89629500
C	-2.31921100	-3.06991900	1.02534900
N	-1.83056500	-1.75910900	0.57606400
C	-0.38254000	-1.59053600	0.74882400
C	0.29332700	-1.19393100	-0.57279600
O	0.12713800	-1.84893700	-1.59824700
C	-2.60064700	-0.75786200	0.09764700
O	-2.15975500	0.35178800	-0.20975400
O	-3.88750100	-1.13373700	0.01047200
C	-4.93171800	-0.23413400	-0.51561600
C	-4.63643300	0.10397900	-1.97811300
C	-6.19041100	-1.09581400	-0.40461500
C	-5.05277100	1.01198400	0.36371700
C	1.04096900	1.51238500	-2.40749300
N	1.08487800	-0.10301300	-0.48996200
C	1.81059600	0.42482400	-1.62596900
C	3.18998500	0.97581600	-1.19741500
O	1.58836900	2.10814000	-3.33507400
N	-0.22494900	1.76061300	-2.02287400
C	-1.04213100	2.73112000	-2.72833000
H	0.34328700	-3.58179600	0.33800100
H	0.94623100	-2.92756200	1.87241100
H	-1.26853700	-3.19148000	2.91445700
H	-1.14124500	-4.67126600	1.95082200
H	-2.49699600	-3.72835000	0.16612000

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H       -3.25804100   -2.96070300    1.56953800
H       -0.18098500   -0.83042700    1.51054100
H       -5.46999700    0.67821700   -2.39362000
H       -3.72443100    0.69335500   -2.07054200
H       -4.52803300   -0.81245100   -2.56598600
H       -7.05440700   -0.54260400   -0.78262300
H       -6.38220700   -1.36815300    0.63706400
H       -6.08283200   -2.01302200   -0.99022500
H       -5.19213500    0.72601100    1.41070200
H       -4.16742700    1.64167400    0.28264800
H       -5.92703800    1.59104300    0.05105800
H        1.12790400    0.41475900    0.39323800
H        1.95461600   -0.40028300   -2.33099800
H        3.03403500    1.76477200   -0.45294300
H       -0.66748400    1.18948600   -1.31089700
H       -1.97060300    2.87322600   -2.17407600
H       -0.51892800    3.68820100   -2.80289300
H       -1.28218500    2.39789100   -3.74457600
H        3.62855700    1.44457800   -2.08101300
C        4.11113500   -0.08320100   -0.63806000
C        4.18189700   -0.31922500    0.74005600
C        4.90462500   -0.85879900   -1.49149600
C        5.02308700   -1.30751400    1.25111600
H        3.56898600    0.27485600    1.41179400
C        5.74567100   -1.84783400   -0.98405500
H        4.86618500   -0.68211700   -2.56305900
C        5.80760700   -2.07516700    0.39093700
H        5.06760500   -1.47537500    2.32278200
H        6.35672500   -2.43613900   -1.66145000
H        6.46457800   -2.84212100    0.78838300
S        0.57906900    2.67079900    2.07298800
O        1.22759600    1.28643000    2.01352500
C        1.13467500    3.40447400    3.63914400
H(Iso=2) 2.20418900    3.59465800    3.53915500
H(Iso=2) 0.60031700    4.34410700    3.79483900
H(Iso=2) 0.94234700    2.69984400    4.45059500
C       -1.15892200    2.39042200    2.52141900
H(Iso=2)-1.20123500    1.79815000    3.43804400
H(Iso=2)-1.64868700    3.35800600    2.65313100
H(Iso=2)-1.60483600    1.84524300    1.68667400
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