

Table S2_Subtitle

Site-specific fit with site-specific $\Delta\omega_{ij}$, $\Delta\omega_{ij}$, P_{ij} , k_{ij} , and R_{ij}^2

AA Num	Res	Atom	Curveset Name	Group Name	Curveset Num	Curve Num	B_j (MHz)	Temp (°C)	Num of Curvesets	Num of Curves	Dataset Name	Exchange?	Best fit OK? *	DoF [†] (NoEx)	DoF (Ex+)	χ^2 (NoEx)	χ^2 (Ex+)	χ^2 Red [†] (NoEx)	χ^2 Red (Ex+)	F [†] (Eq)	P(E [†]) (For F-1)	$\Delta\omega_{ij}$ (ppm)	$\Delta\omega_{ij}$ (ppm)	P_{ij} (%)	k_{ij} (Hz)	R_{ij}^2 (%)	R_{ij} (Hz)	α (°)	k_{ij} (Hz)	k_{ij} (Hz)	
24	Leu	-delta_1	Leu 24-delta_1	Leu 24-delta_1 + lie 28-delta_1_25C	1	1	800.13	25.0	2	8	800-MQ-25C	TRUE	TRUE	72	66	2576.46	83.23	35.78	1.26	28.38	2.29e-31	0.00,0.0	1.360.1	96.30.7	1760.44164.7	53.50.7	26.61.4	1.40.1	64.746.1	1695.7159.1	
24	Leu	-delta_1	Leu 24-delta_1	Leu 24-delta_1 + lie 28-delta_1_25C	1	2	600.17	25.0	2	8	600-MQ-25C	TRUE	TRUE	72	66	2576.46	83.23	35.78	1.26	28.38	2.29e-31	0.00,0.0	1.360.1	96.30.7	1760.44164.7	45.41.2	14.140.6	0.90.1	64.746.1	1695.7159.1	
24	Leu	-delta_1	Leu 24-delta_1	Leu 24-delta_1 + lie 28-delta_1_25C	1	3	800.13	25.0	2	8	800-SQ-25C	TRUE	TRUE	72	66	2576.46	83.23	35.78	1.26	28.38	2.29e-31	0.00,0.0	1.360.1	96.30.7	1760.44164.7	53.50.7	26.61.4	1.40.1	64.746.1	1695.7159.1	
24	Leu	-delta_1	Leu 24-delta_1	Leu 24-delta_1 + lie 28-delta_1_25C	1	4	600.13	25.0	2	8	600-SQ-25C	TRUE	TRUE	72	66	2576.46	83.23	35.78	1.26	28.38	2.29e-31	0.00,0.0	1.360.1	96.30.7	1760.44164.7	45.41.2	14.140.6	0.90.1	64.746.1	1695.7159.1	
28	Ile	-delta_1	Ile 28-delta_1	Leu 24-delta_1 + lie 28-delta_1_25C	2	1	800.13	25.0	2	8	800-MQ-25C	TRUE	TRUE	72	66	2576.46	83.23	35.78	1.26	28.38	2.29e-31	0.00,0.0	1.260.1	96.30.7	1760.44164.7	53.50.7	26.61.4	1.40.1	64.746.1	1695.7159.1	
28	Ile	-delta_1	Ile 28-delta_1	Leu 24-delta_1 + lie 28-delta_1_25C	2	2	600.17	25.0	2	8	600-MQ-25C	TRUE	TRUE	72	66	2576.46	83.23	35.78	1.26	28.38	2.29e-31	0.00,0.0	1.260.1	96.30.7	1760.44164.7	45.41.2	14.140.6	0.90.1	64.746.1	1695.7159.1	
28	Ile	-delta_1	Ile 28-delta_1	Leu 24-delta_1 + lie 28-delta_1_25C	2	3	800.13	25.0	2	8	800-SQ-25C	TRUE	TRUE	72	66	2576.46	83.23	35.78	1.26	28.38	2.29e-31	0.00,0.0	1.260.1	96.30.7	1760.44164.7	53.50.7	26.61.4	1.40.1	64.746.1	1695.7159.1	
28	Ile	-delta_1	Ile 28-delta_1	Leu 24-delta_1 + lie 28-delta_1_25C	2	4	600.13	25.0	2	8	600-SQ-25C	TRUE	TRUE	72	66	2576.46	83.23	35.78	1.26	28.38	2.29e-31	0.00,0.0	1.260.1	96.30.7	1760.44164.7	45.41.2	14.140.6	0.90.1	64.746.1	1695.7159.1	
24	Leu	-delta_2	Leu 24-delta_2	Leu 24-delta_2 + lie 28-delta_1_25C	1	1	800.13	25.0	2	8	800-MQ-25C	TRUE	TRUE	72	66	9550.15	302.45	132.64	4.58	28.94	1.22e-31	Param Not OK	Param Not OK	Param Not OK	1399.24144.7	58.52.6	35.245.1	1.90.1	Param Not OK	Param Not OK	
24	Leu	-delta_2	Leu 24-delta_2	Leu 24-delta_2 + lie 28-delta_1_25C	1	2	600.17	25.0	2	8	600-MQ-25C	TRUE	TRUE	72	66	9550.15	302.45	132.64	4.58	28.94	1.22e-31	Param Not OK	Param Not OK	Param Not OK	1399.24144.7	45.312.1	18.941.8	1.50.5	Param Not OK	Param Not OK	
24	Leu	-delta_2	Leu 24-delta_2	Leu 24-delta_2 + lie 28-delta_1_25C	1	3	800.13	25.0	2	8	800-SQ-25C	TRUE	TRUE	72	66	9550.15	302.45	132.64	4.58	28.94	1.22e-31	Param Not OK	Param Not OK	Param Not OK	1399.24144.7	58.52.6	35.245.1	1.90.1	Param Not OK	Param Not OK	
24	Leu	-delta_2	Leu 24-delta_2	Leu 24-delta_2 + lie 28-delta_1_25C	1	4	600.13	25.0	2	8	600-SQ-25C	TRUE	TRUE	72	66	9550.15	302.45	132.64	4.58	28.94	1.22e-31	Param Not OK	Param Not OK	Param Not OK	1399.24144.7	48.811.9	20.443.3	1.90.1	Param Not OK	Param Not OK	
28	Ile	-delta_1	Ile 28-delta_1	Leu 24-delta_2 + lie 28-delta_1_25C	2	1	800.13	25.0	2	8	800-MQ-25C	TRUE	TRUE	72	66	9550.15	302.45	132.64	4.58	28.94	1.22e-31	Param Not OK	Param Not OK	Param Not OK	1399.24144.7	58.52.6	35.245.1	1.90.1	Param Not OK	Param Not OK	
28	Ile	-delta_1	Ile 28-delta_1	Leu 24-delta_2 + lie 28-delta_1_25C	2	2	600.17	25.0	2	8	600-MQ-25C	TRUE	TRUE	72	66	9550.15	302.45	132.64	4.58	28.94	1.22e-31	Param Not OK	Param Not OK	Param Not OK	1399.24144.7	45.312.1	18.941.8	1.50.5	Param Not OK	Param Not OK	
28	Ile	-delta_1	Ile 28-delta_1	Leu 24-delta_2 + lie 28-delta_1_25C	2	3	800.13	25.0	2	8	800-SQ-25C	TRUE	TRUE	72	66	9550.15	302.45	132.64	4.58	28.94	1.22e-31	Param Not OK	Param Not OK	Param Not OK	1399.24144.7	58.52.6	35.245.1	1.90.1	Param Not OK	Param Not OK	
28	Ile	-delta_1	Ile 28-delta_1	Leu 24-delta_2 + lie 28-delta_1_25C	2	4	600.13	25.0	2	8	600-SQ-25C	TRUE	TRUE	72	66	9550.15	302.45	132.64	4.58	28.94	1.22e-31	Param Not OK	Param Not OK	Param Not OK	1399.24144.7	48.811.9	20.443.3	1.90.1	Param Not OK	Param Not OK	
10	Val	-gamma_1	Val 10-gamma_1	Val 10-gamma_1_25C	1	1	800.13	25.0	1	4	800-MQ-25C	TRUE	FALSE	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK
10	Val	-gamma_1	Val 10-gamma_1	Val 10-gamma_1_25C	1	2	600.17	25.0	1	4	600-MQ-25C	TRUE	FALSE	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK
10	Val	-gamma_1	Val 10-gamma_1	Val 10-gamma_1_25C	1	3	800.13	25.0	1	4	800-SQ-25C	TRUE	FALSE	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK
10	Val	-gamma_1	Val 10-gamma_1	Val 10-gamma_1_25C	1	4	600.13	25.0	1	4	600-SQ-25C	TRUE	FALSE	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK
10	Val	-gamma_2	Val 10-gamma_2	Val 10-gamma_2_25C	1	1	800.13	25.0	1	4	800-MQ-25C	TRUE	TRUE	36	32	498.44	210.57	13.85	6.58	2.10	5.72e-02	Param Not OK	Param Not OK	Param Not OK	1590.5780.2	74.6111.8	34.112.8	2.00.5	Param Not OK	Param Not OK	
10	Val	-gamma_2	Val 10-gamma_2	Val 10-gamma_2_25C	1	2	600.17	25.0	1	4	600-MQ-25C	TRUE	TRUE	36	32	498.44	210.57	13.85	6.58	2.10	5.72e-02	Param Not OK	Param Not OK	Param Not OK	1590.5780.2	58.824.8	19.643.6	1.247	Param Not OK	Param Not OK	
10	Val	-gamma_2	Val 10-gamma_2	Val 10-gamma_2_25C	1	3	800.13	25.0	1	4	800-SQ-25C	TRUE	TRUE	36	32	498.44	210.57	13.85	6.58	2.10	5.72e-02	Param Not OK	Param Not OK	Param Not OK	1590.5780.2	74.6111.8	34.112.8	2.00.5	Param Not OK	Param Not OK	
10	Val	-gamma_2	Val 10-gamma_2	Val 10-gamma_2_25C	1	4	600.13	25.0	1	4	600-SQ-25C	TRUE	TRUE	36	32	498.44	210.57	13.85	6.58	2.10	5.72e-02	Param Not OK	Param Not OK	Param Not OK	1590.5780.2	67.810.4	18.110.2	2.00.5	Param Not OK	Param Not OK	
11	Val	-gamma_1	Val 11-gamma_1	Val 11-gamma_1_25C	1	1	800.13	25.0	1	4	800-MQ-25C	FALSE	TRUE	36	No Exch	107.32	No Exch	2.98	No Exch	No Exch	No Exch	0.00,0	0.00,0	100.00,0	0.00,0	62.00,0	0.00,0	70.0	0.00,0	0.00,0	
11	Val	-gamma_1	Val 11-gamma_1	Val 11-gamma_1_25C	1	2	600.17	25.0	1	4	600-MQ-25C	FALSE	TRUE	36	No Exch	107.32	No Exch	2.98	No Exch	No Exch	No Exch	0.00,0	0.00,0	100.00,0	0.00,0	62.00,0	0.00,0	70.0	0.00,0	0.00,0	
11	Val	-gamma_1	Val 11-gamma_1	Val 11-gamma_1_25C	1	3	800.13	25.0	1	4	800-SQ-25C	FALSE	TRUE	36	No Exch	107.32	No Exch	2.98	No Exch	No Exch	No Exch	0.00,0	0.00,0	100.00,0	0.00,0	62.00,0	0.00,0	70.0	0.00,0	0.00,0	
11	Val	-gamma_1	Val 11-gamma_1	Val 11-gamma_1_25C	1	4	600.13	25.0	1	4	600-SQ-25C	FALSE	TRUE	36	No Exch	107.32	No Exch	2.98	No Exch	No Exch	No Exch	0.00,0	0.00,0	100.00,0	0.00,0	60.80,0	0.00,0	70.0	0.00,0	0.00,0	
11	Val	-gamma_2	Val 11-gamma_2	Val 11-gamma_2_25C	1	1	800.13	25.0	1	3	800-MQ-25C	FALSE	FALSE	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	
11	Val	-gamma_2	Val 11-gamma_2	Val 11-gamma_2_25C	1	2	600.17	25.0	1	3	600-MQ-25C	FALSE	FALSE	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	
11	Val	-gamma_2	Val 11-gamma_2	Val 11-gamma_2_25C	1	3	800.13	25.0	1	3	800-SQ-25C	FALSE	FALSE	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	
12	Ile	-delta_1	Ile 12-delta_1	Ile 12-delta_1_25C	1	1	800.13	25.0	1	4	800-MQ-25C	TRUE	TRUE	36	32	2215.39	62.67	61.54	1.96	31.42	3.87e-17	Param Not OK	Param Not OK	Param Not OK	1775.8139.1	58.822.2	37.811.8	2.00.0	Param Not OK	Param Not OK	
12	Ile	-delta_1	Ile 12-delta_1	Ile 12-delta_1_25C	1	2	600.17	25.0	1	4	600-MQ-25C	TRUE	TRUE	36	32	2215.39	62.67	61.54	1.96	31.42	3.87e-17	Param Not OK	Param Not OK	Param Not OK	1775.8139.1	29.014.7	23.10.8	1.90.2	Param Not OK	Param Not OK	
12	Ile	-delta_1	Ile 12-delta_1	Ile 12-delta_1_25C	1	3	800.13	25.0	1	4	800-SQ-25C	TRUE	TRUE	36	32	2215.39	62.67	61.54	1.96	31.42	3.87e-17	Param Not OK	Param Not OK	Param Not OK	1775.8139.1	58.822.5	37.811.8	2.00.0	Param Not OK	Param Not OK	
12	Ile	-delta_1	Ile 12-delta_1	Ile 12-delta_1_25C	1	4	600.13	25.0	1	4	600-SQ-25C	TRUE	TRUE	36	32	2215.39	62.67	61.54	1.96	31.42	3.87e-17	Param Not OK	Param Not OK	Param Not OK	1775.8139.1	52.622.6	21.210.1	2.00.0	Param Not OK	Param Not OK	
15	Leu	-delta_1	Leu 15-delta_1	Leu 15-delta_1_25C	1	1	800.13	25.0	1	4	800-MQ-25C	FALSE	TRUE	36	No Exch	59.91	No Exch	1.66	No Exch	No Exch	No Exch	0.00,0	0.00,0	100.00,0	0.00,0	55.40,0	0.00,0	70.0	0.00,0	0.00,0	
15	Leu	-delta_1	Leu 15-delta_1	Leu 15-delta_1_25C	1	2	600.17	25.0	1	4	600-MQ-25C	FALSE	TRUE	36	No Exch	59.91	No Exch	1.66	No Exch	No Exch	No Exch	0.00,0	0.00,0	100.00,0	0.00,0	58.00,0	0.00,0	70.0	0.00,0	0.00,0	
15	Leu	-delta_1	Leu 15-delta_1	Leu 15-delta_1_25C	1	3	800.13	25.0	1	4	800-SQ-25C	FALSE	TRUE	36	No Exch	59.91	No Exch	1.66	No Exch	No Exch	No Exch	0.00,0	0.00,0	100.00,0	0.00,0	55.40,0	0.00,0	70.0	0.00,0	0.00,0	
15	Leu	-delta_1	Leu 15-delta_1	Leu 15-delta_1_25C	1	4	600.13	25.0	1	4	600-SQ-25C	FALSE	TRUE	36	No Exch	59.91	No Exch	1.66	No Exch	No Exch	No Exch	0.00,0	0.00,0	100.00,0	0.00,0	48.90,0	0.00,0	70.0	0.00,0	0.00,0	
15	Leu	-delta_2	Leu 15-delta_2	Leu 15-delta_2_25C	1	1	800.13	25.0																							

Table S2_Subtilis

AA Num	Res	Atom	Curvest Name	Group Name	Curvest Num	Curve Num	B ₁ (MHz)	Temp (C)	Num of Curvests	Num of Curves	Dataset Name	Exchange?	Best fit OK?	Def ¹ (NOE)	Def ¹ (Ex)	X ¹ (NOE)	X ¹ (Ex)	r ² (NOE)	r ² (Ex)	F ¹ (Ex)	F ¹ (NOE)	Δ _{NOE} (ppm)	Δ _{Ex} (ppm)	P ₁ (%)	k _{ex} (s)	R ₁ ^ρ (Hz)	R ₂ ^ρ (Hz)	α (°)	k ₁ (s)	k ₂ (s)		
22	lle	-delta_1	lle 22-delta_1	lle 22-delta_1_25C	1	1	800.13	25.0	1	4	800-MQ-25C	TRUE	TRUE	36	32	325.59	17.73	9.04	0.55	16.32	1.13e-12	0.040.0	1.5e0.2	98.680.6	1315.53272.8	45.740.5	12.040.1	0.840.3	18.444.6	1297.14323.3		
22	lle	-delta_1	lle 22-delta_1	lle 22-delta_1_25C	1	2	600.17	25.0	1	4	800-MQ-25C	TRUE	TRUE	36	32	325.59	17.73	9.04	0.55	16.32	1.13e-12	0.040.0	1.5e0.2	98.680.6	1315.53272.8	40.840.4	9.840.4	0.840.3	18.444.6	1297.14323.3		
22	lle	-delta_1	lle 22-delta_1	lle 22-delta_1_25C	1	3	800.13	25.0	1	4	800-SQ-25C	TRUE	TRUE	36	32	325.59	17.73	9.04	0.55	16.32	1.13e-12	0.040.0	1.5e0.2	98.680.6	1315.53272.8	39.540.3	8.440.5	0.840.3	18.444.6	1297.14323.3		
22	lle	-delta_1	lle 22-delta_1	lle 22-delta_1_25C	1	4	600.13	25.0	1	4	800-SQ-25C	TRUE	TRUE	36	32	325.59	17.73	9.04	0.55	16.32	1.13e-12	0.040.0	1.5e0.2	98.680.6	1315.53272.8	39.540.3	8.440.5	0.840.3	18.444.6	1297.14323.3		
24	Leu	-delta_1	Leu 24-delta_1	Leu 24-delta_1_25C	1	1	800.13	25.0	1	4	800-MQ-25C	TRUE	TRUE	36	32	1058.52	33.02	29.40	1.03	28.49	1.86e-16	0.140.0	1.0e0.2	95.543.4	1161.32171.6	55.440.5	27.741.5	1.140.3	51.949.9	1109.4211.6		
24	Leu	-delta_1	Leu 24-delta_1	Leu 24-delta_1_25C	1	2	600.17	25.0	1	4	800-MQ-25C	TRUE	TRUE	36	32	1058.52	33.02	29.40	1.03	28.49	1.86e-16	0.140.0	1.0e0.2	95.543.4	1161.32171.6	46.145.9	14.940.8	0.740.2	51.949.9	1109.4211.6		
24	Leu	-delta_1	Leu 24-delta_1	Leu 24-delta_1_25C	1	3	800.13	25.0	1	4	800-SQ-25C	TRUE	TRUE	36	32	1058.52	33.02	29.40	1.03	28.49	1.86e-16	0.140.0	1.0e0.2	95.543.4	1161.32171.6	55.440.5	27.741.5	1.140.3	51.949.9	1109.4211.6		
24	Leu	-delta_1	Leu 24-delta_1	Leu 24-delta_1_25C	1	4	600.13	25.0	1	4	800-SQ-25C	TRUE	TRUE	36	32	1058.52	33.02	29.40	1.03	28.49	1.86e-16	0.140.0	1.0e0.2	95.543.4	1161.32171.6	46.270.4	13.941.1	1.140.3	51.949.9	1109.4211.6		
24	Leu	-delta_2	Co(Leu 24-delta_2)	Leu 24-delta_2_25C	1	1	800.13	25.0	1	4	800-MQ-25C	TRUE	TRUE	36	32	8032.21	145.29	223.12	4.54	49.14	2.71e-20	0.040.0	1.0e0.1	87.342.5	1046.8103.6	61.641.9	83.347.1	1.140.2	133.0413.7	913.8494.0		
24	Leu	-delta_2	Co(Leu 24-delta_2)	Leu 24-delta_2_25C	1	2	600.17	25.0	1	4	800-MQ-25C	TRUE	TRUE	36	32	8032.21	145.29	223.12	4.54	49.14	2.71e-20	0.040.0	1.0e0.1	87.342.5	1046.8103.6	58.043.3	61.646.5	1.147	133.0413.7	913.8494.0		
24	Leu	-delta_2	Co(Leu 24-delta_2)	Leu 24-delta_2_25C	1	3	800.13	25.0	1	4	800-SQ-25C	TRUE	TRUE	36	32	8032.21	145.29	223.12	4.54	49.14	2.71e-20	0.040.0	1.0e0.1	87.342.5	1046.8103.6	61.641.9	83.347.1	1.140.2	133.0413.7	913.8494.0		
24	Leu	-delta_2	Co(Leu 24-delta_2)	Leu 24-delta_2_25C	1	4	600.13	25.0	1	4	800-SQ-25C	TRUE	TRUE	36	32	8032.21	145.29	223.12	4.54	49.14	2.71e-20	0.040.0	1.0e0.1	87.342.5	1046.8103.6	51.040.9	61.542.5	1.140.2	133.0413.7	913.8494.0		
28	lle	-delta_1	Co(Lle 28-delta_1)	lle 28-delta_1_25C	1	1	800.13	25.0	1	4	800-MQ-25C	TRUE	TRUE	36	32	1517.94	24.11	42.17	0.75	55.96	3.20e-21	0.040.0	1.4e0.2	96.342.3	2391.8237.6	52.341.0	29.741.4	1.540.2	88.349.0	2303.5423.3		
28	lle	-delta_1	Co(Lle 28-delta_1)	lle 28-delta_1_25C	1	2	600.17	25.0	1	4	800-MQ-25C	TRUE	TRUE	36	32	1517.94	24.11	42.17	0.75	55.96	3.20e-21	0.040.0	1.4e0.2	96.342.3	2391.8237.6	48.542.9	19.440.5	1.547	88.349.0	2303.5423.3		
28	lle	-delta_1	Co(Lle 28-delta_1)	lle 28-delta_1_25C	1	3	800.13	25.0	1	4	800-SQ-25C	TRUE	TRUE	36	32	1517.94	24.11	42.17	0.75	55.96	3.20e-21	0.040.0	1.4e0.2	96.342.3	2391.8237.6	52.341.0	29.741.4	1.540.2	88.349.0	2303.5423.3		
28	lle	-delta_1	Co(Lle 28-delta_1)	lle 28-delta_1_25C	1	4	600.13	25.0	1	4	800-SQ-25C	TRUE	TRUE	36	32	1517.94	24.11	42.17	0.75	55.96	3.20e-21	0.040.0	1.4e0.2	96.342.3	2391.8237.6	44.440.8	19.340.5	1.540.2	88.349.0	2303.5423.3		
38	Leu	-delta_1	Leu 38-delta_1	Leu 38-delta_1_25C	1	1	800.13	25.0	1	4	800-MQ-25C	FALSE	TRUE	36	No Exch	20.19	No Exch	0.56	No Exch	No Exch	No Exch	0.040.0	0.040.0	100.00.0	0.040.0	47.740.0	0.047	740.0	0.047	0.047	0.047	
38	Leu	-delta_1	Leu 38-delta_1	Leu 38-delta_1_25C	1	2	600.17	25.0	1	4	800-MQ-25C	FALSE	TRUE	36	No Exch	20.19	No Exch	0.56	No Exch	No Exch	No Exch	0.040.0	0.040.0	100.00.0	0.040.0	46.840.0	0.047	740.0	0.047	0.047	0.047	
38	Leu	-delta_1	Leu 38-delta_1	Leu 38-delta_1_25C	1	3	800.13	25.0	1	4	800-SQ-25C	FALSE	TRUE	36	No Exch	20.19	No Exch	0.56	No Exch	No Exch	No Exch	0.040.0	0.040.0	100.00.0	0.040.0	47.740.0	0.047	740.0	0.047	0.047	0.047	
38	Leu	-delta_1	Leu 38-delta_1	Leu 38-delta_1_25C	1	4	600.13	25.0	1	4	800-SQ-25C	FALSE	TRUE	36	No Exch	20.19	No Exch	0.56	No Exch	No Exch	No Exch	0.040.0	0.040.0	100.00.0	0.040.0	43.740.0	0.047	740.0	0.047	0.047	0.047	
38	Leu	-delta_2	Leu 38-delta_2	Leu 38-delta_2_25C	1	1	800.13	25.0	1	3	800-MQ-25C	TRUE	TRUE	36	23	74.65	5.86	2.07	0.25	8.14	9.96e-07	Param Not OK	Param Not OK	Param Not OK	1423.5216.2	51.043.5	7.040.7	7?7	Param Not OK	Param Not OK		
38	Leu	-delta_2	Leu 38-delta_2	Leu 38-delta_2_25C	1	2	600.17	25.0	1	3	800-MQ-25C	TRUE	TRUE	36	23	74.65	5.86	2.07	0.25	8.14	9.96e-07	Param Not OK	Param Not OK	Param Not OK	1423.5216.2	19.247.5	4.540.4	2.240.3	Param Not OK	Param Not OK		
38	Leu	-delta_2	Leu 38-delta_2	Leu 38-delta_2_25C	1	3	800.13	25.0	1	3	800-SQ-25C	TRUE	TRUE	36	23	74.65	5.86	2.07	0.25	8.14	9.96e-07	Param Not OK	Param Not OK	Param Not OK	1423.5216.2	51.043.5	7.040.7	7?7	Param Not OK	Param Not OK		
43	Val	-gamma_1	Val 43-gamma_1	Val 43-gamma_1_25C	1	1	800.13	25.0	1	2	800-MQ-25C	FALSE	TRUE	18	No Exch	117.93	No Exch	6.55	No Exch	No Exch	No Exch	0.040.0	0.040.0	100.00.0	0.040.0	60.340.0	0.047	740.0	0.047	0.047	0.047	
43	Val	-gamma_1	Val 43-gamma_1	Val 43-gamma_1_25C	1	2	600.17	25.0	1	2	800-SQ-25C	FALSE	TRUE	18	No Exch	117.93	No Exch	6.55	No Exch	No Exch	No Exch	0.040.0	0.040.0	100.00.0	0.040.0	60.340.0	0.047	740.0	0.047	0.047	0.047	
43	Val	-gamma_2	Val 43-gamma_2	Val 43-gamma_2_25C	1	1	800.13	25.0	1	4	800-MQ-25C	FALSE	TRUE	36	No Exch	32.49	No Exch	0.90	No Exch	No Exch	No Exch	0.040.0	0.040.0	100.00.0	0.040.0	59.240.0	0.047	740.0	0.047	0.047	0.047	
43	Val	-gamma_2	Val 43-gamma_2	Val 43-gamma_2_25C	1	2	600.17	25.0	1	4	800-MQ-25C	FALSE	TRUE	36	No Exch	32.49	No Exch	0.90	No Exch	No Exch	No Exch	0.040.0	0.040.0	100.00.0	0.040.0	61.440.0	0.047	740.0	0.047	0.047	0.047	
43	Val	-gamma_2	Val 43-gamma_2	Val 43-gamma_2_25C	1	3	800.13	25.0	1	4	800-SQ-25C	FALSE	TRUE	36	No Exch	32.49	No Exch	0.90	No Exch	No Exch	No Exch	0.040.0	0.040.0	100.00.0	0.040.0	59.240.0	0.047	740.0	0.047	0.047	0.047	
43	Val	-gamma_2	Val 43-gamma_2	Val 43-gamma_2_25C	1	4	600.13	25.0	1	4	800-SQ-25C	FALSE	TRUE	36	No Exch	32.49	No Exch	0.90	No Exch	No Exch	No Exch	0.040.0	0.040.0	100.00.0	0.040.0	55.740.0	0.047	740.0	0.047	0.047	0.047	
44	Leu	-delta_1	Leu 44-delta_1	Leu 44-delta_1_25C	1	1	800.13	25.0	1	4	800-MQ-25C	TRUE	TRUE	36	32	4490.71	172.13	124.74	5.38	23.19	4.86e-15	Param Not OK	Param Not OK	Param Not OK	1517.8147.3	72.342.4	63.945.0	2.140.0	Param Not OK	Param Not OK		
44	Leu	-delta_1	Leu 44-delta_1	Leu 44-delta_1_25C	1	2	600.17	25.0	1	4	800-MQ-25C	TRUE	TRUE	36	32	4490.71	172.13	124.74	5.38	23.19	4.86e-15	Param Not OK	Param Not OK	Param Not OK	1517.8147.3	28.644.1	41.842.1	2.140.0	Param Not OK	Param Not OK		
44	Leu	-delta_1	Leu 44-delta_1	Leu 44-delta_1_25C	1	3	800.13	25.0	1	4	800-SQ-25C	TRUE	TRUE	36	32	4490.71	172.13	124.74	5.38	23.19	4.86e-15	Param Not OK	Param Not OK	Param Not OK	1517.8147.3	72.342.4	63.945.0	2.140.0	Param Not OK	Param Not OK		
44	Leu	-delta_1	Leu 44-delta_1	Leu 44-delta_1_25C	1	4	600.13	25.0	1	4	800-SQ-25C	TRUE	TRUE	36	32	4490.71	172.13	124.74	5.38	23.19	4.86e-15	Param Not OK	Param Not OK	Param Not OK	1517.8147.3	54.942.1	35.342.7	2.140.0	Param Not OK	Param Not OK		
44	Leu	-delta_2	Leu 44-delta_2	Leu 44-delta_2_25C	1	1	800.13	25.0	1	4	800-MQ-25C	TRUE	FALSE	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK
44	Leu	-delta_2	Leu 44-delta_2	Leu 44-delta_2_25C	1	2	600.17	25.0	1	4	800-MQ-25C	TRUE	FALSE	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK
44	Leu	-delta_2	Leu 44-delta_2	Leu 44-delta_2_25C	1	3	800.13	25.0	1	4	800-SQ-25C	TRUE	FALSE	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK
44	Leu	-delta_2	Leu 44-delta_2	Leu 44-delta_2_25C	1	4	600.13	25.0	1	4	800-SQ-25C	TRUE	FALSE	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK	Fit Not OK
45	lle	-delta_1	lle 45-delta_1	lle 45-delta_1_25C	1	1	800.13	25.0	1	4	800-MQ-25C	TRUE	TRUE	36	32	587.81	20.49	16.33	0.64	25.50	1.09e-15	0.040.0	1.0e0.2	96.447.3	1679.12993.3	54.941.5	21.041.4	1.540.3	60.9411.6	1618.2408.1		
45	lle	-delta_1	lle 45-delta_1	lle 45-delta_1_25C	1	2	600.17	25.0	1	4	800-MQ-25C	TRUE	TRUE	36																		

Table S2_Subtilis

Global fit of site-specific Δ_{iso} , Δ_{iso} , and R_2 with fixed $P_{\text{ex}} = 94.8\%$ and $k_{\text{ex}} = 1629$ s

AA Num	Res	Atom	Curset Name	Group Name	Curset Num	Curve Num	B_1 (MHz)	Temp (C)	Num of Cursets	Num of Curves	Dataset Name	Exchange?	Best fit OK?	DeF ¹⁴ (NoEx)	DeF ¹³ (Ex) ⁺	χ^2 (NoEx)	χ^2 (Ex)	χ^2 Red ⁺ (NoEx)	χ^2 Red ⁺ (Ex)	F ¹⁴ (Ex)	F ¹³ (For F ¹⁴)	Δ_{iso} (ppm)	Δ_{iso} (ppm)	P_{ex} (%)	k_{ex} (s)	R_2 (Hz)	R_{ex} (Hz)	σ (°)	k_{ex} (s)	k_{ex} (s)
10	Val	-gamma_1	Val 10-gamma_1	Val 10-gamma_1_25C	1	1	800.13	25.0	1	4	800-MQ-25C	TRUE	TRUE	36	32	107.85	50.64	3.00	1.58	1.89	1:14e-01	0.160, 1	0.760, 1	94.800	1629.000	57.817	20.1438	1.740, 1	84.400	1544.600
10	Val	-gamma_1	Val 10-gamma_1	Val 10-gamma_1_25C	2	2	800.17	25.0	1	4	800-MQ-25C	TRUE	TRUE	36	32	107.85	50.64	3.00	1.58	1.89	1:14e-01	0.160, 1	0.760, 1	94.800	1629.000	57.817	20.1438	1.740, 1	84.400	1544.600
10	Val	-gamma_1	Val 10-gamma_1	Val 10-gamma_1_25C	3	3	800.13	25.0	1	4	800-MQ-25C	TRUE	TRUE	36	32	107.85	50.64	3.00	1.58	1.89	1:14e-01	0.160, 1	0.760, 1	94.800	1629.000	57.817	20.1438	1.740, 1	84.400	1544.600
10	Val	-gamma_1	Val 10-gamma_1	Val 10-gamma_1_25C	4	4	600.13	25.0	1	4	800-SQ-25C	TRUE	TRUE	36	32	107.85	50.64	3.00	1.58	1.89	1:14e-01	0.160, 1	0.760, 1	94.800	1629.000	51.3114	12.4246	1.740, 1	84.400	1544.600
10	Val	-gamma_2	Val 10-gamma_2	Val 10-gamma_2_25C	1	1	800.13	25.0	1	4	800-MQ-25C	TRUE	TRUE	36	32	498.44	215.39	13.85	6.73	2.06	6.67e-02	0.040, 1	1.040, 1	94.800	1629.000	70.0427	29.0449	1.540, 1	84.400	1544.600
10	Val	-gamma_2	Val 10-gamma_2	Val 10-gamma_2_25C	2	2	600.17	25.0	1	4	800-MQ-25C	TRUE	TRUE	36	32	498.44	215.39	13.85	6.73	2.06	6.67e-02	0.040, 1	1.040, 1	94.800	1629.000	103.2433	18.8425	1.547, 1	84.400	1544.600
10	Val	-gamma_2	Val 10-gamma_2	Val 10-gamma_2_25C	3	3	800.13	25.0	1	4	800-SQ-25C	TRUE	TRUE	36	32	498.44	215.39	13.85	6.73	2.06	6.67e-02	0.040, 1	1.040, 1	94.800	1629.000	70.0427	29.0449	1.540, 1	84.400	1544.600
10	Val	-gamma_2	Val 10-gamma_2	Val 10-gamma_2_25C	4	4	600.13	25.0	1	4	800-SQ-25C	TRUE	TRUE	36	32	498.44	215.39	13.85	6.73	2.06	6.67e-02	0.040, 1	1.040, 1	94.800	1629.000	63.2223	18.8439	1.540, 1	84.400	1544.600
11	Val	-gamma_1	Val 11-gamma_1	Val 11-gamma_1_25C	1	1	800.13	25.0	1	4	800-MQ-25C	FALSE	TRUE	36	No Exch	107.32	No Exch	2.98	No Exch	No Exch	No Exch	0.040, 0	0.040, 0	100.000	0.040	62.0400	0.047	740.0	0.047	0.047
11	Val	-gamma_1	Val 11-gamma_1	Val 11-gamma_1_25C	2	2	600.17	25.0	1	4	800-MQ-25C	FALSE	TRUE	36	No Exch	107.32	No Exch	2.98	No Exch	No Exch	No Exch	0.040, 0	0.040, 0	100.000	0.040	57.8400	0.047	740.0	0.047	0.047
11	Val	-gamma_1	Val 11-gamma_1	Val 11-gamma_1_25C	3	3	800.13	25.0	1	4	800-SQ-25C	FALSE	TRUE	36	No Exch	107.32	No Exch	2.98	No Exch	No Exch	No Exch	0.040, 0	0.040, 0	100.000	0.040	62.0400	0.047	740.0	0.047	0.047
11	Val	-gamma_1	Val 11-gamma_1	Val 11-gamma_1_25C	4	4	600.13	25.0	1	4	800-SQ-25C	FALSE	TRUE	36	No Exch	107.32	No Exch	2.98	No Exch	No Exch	No Exch	0.040, 0	0.040, 0	100.000	0.040	60.8400	0.047	740.0	0.047	0.047
11	Val	-gamma_2	Val 11-gamma_2	Val 11-gamma_2_25C	1	1	800.13	25.0	1	4	800-MQ-25C	TRUE	TRUE	36	32	75.23	37.80	2.09	1.18	1.77	1.70e-01	0.160, 1	0.460, 1	94.800	1629.000	59.4409	5.9416	1.940, 1	84.400	1544.600
11	Val	-gamma_2	Val 11-gamma_2	Val 11-gamma_2_25C	2	2	600.17	25.0	1	4	800-MQ-25C	TRUE	TRUE	36	32	75.23	37.80	2.09	1.18	1.77	1.70e-01	0.160, 1	0.460, 1	94.800	1629.000	59.8227	5.9416	1.940, 1	84.400	1544.600
11	Val	-gamma_2	Val 11-gamma_2	Val 11-gamma_2_25C	3	3	800.13	25.0	1	4	800-SQ-25C	TRUE	TRUE	36	32	75.23	37.80	2.09	1.18	1.77	1.70e-01	0.160, 1	0.460, 1	94.800	1629.000	59.4409	5.9416	1.940, 1	84.400	1544.600
11	Val	-gamma_2	Val 11-gamma_2	Val 11-gamma_2_25C	4	4	600.13	25.0	1	4	800-SQ-25C	TRUE	TRUE	36	32	75.23	37.80	2.09	1.18	1.77	1.70e-01	0.160, 1	0.460, 1	94.800	1629.000	54.2412	3.4409	1.940, 1	84.400	1544.600
12	Ile	-delta_1	Ile 12-delta_1	Ile 12-delta_1_25C	1	1	800.13	25.0	1	4	800-MQ-25C	TRUE	TRUE	36	32	2215.39	81.52	61.54	2.55	24.16	2.56e-15	0.040, 0	1.140, 0	94.800	1629.000	52.8407	34.5410	1.440, 0	84.400	1544.600
12	Ile	-delta_1	Ile 12-delta_1	Ile 12-delta_1_25C	2	2	600.17	25.0	1	4	800-MQ-25C	TRUE	TRUE	36	32	2215.39	81.52	61.54	2.55	24.16	2.56e-15	0.040, 0	1.140, 0	94.800	1629.000	64.3409	23.2408	1.447, 0	84.400	1544.600
12	Ile	-delta_1	Ile 12-delta_1	Ile 12-delta_1_25C	3	3	800.13	25.0	1	4	800-SQ-25C	TRUE	TRUE	36	32	2215.39	81.52	61.54	2.55	24.16	2.56e-15	0.040, 0	1.140, 0	94.800	1629.000	52.8407	34.5410	1.440, 0	84.400	1544.600
12	Ile	-delta_1	Ile 12-delta_1	Ile 12-delta_1_25C	4	4	600.13	25.0	1	4	800-SQ-25C	TRUE	TRUE	36	32	2215.39	81.52	61.54	2.55	24.16	2.56e-15	0.040, 0	1.140, 0	94.800	1629.000	46.9406	23.2408	1.440, 0	84.400	1544.600
15	Leu	-delta_1	Leu 15-delta_1	Leu 15-delta_1_25C	1	1	800.13	25.0	1	4	800-MQ-25C	FALSE	TRUE	36	No Exch	59.91	No Exch	1.66	No Exch	No Exch	No Exch	0.040, 0	0.040, 0	100.000	0.040	55.4400	0.047	740.0	0.047	0.047
15	Leu	-delta_1	Leu 15-delta_1	Leu 15-delta_1_25C	2	2	600.17	25.0	1	4	800-MQ-25C	FALSE	TRUE	36	No Exch	59.91	No Exch	1.66	No Exch	No Exch	No Exch	0.040, 0	0.040, 0	100.000	0.040	36.0400	0.047	740.0	0.047	0.047
15	Leu	-delta_1	Leu 15-delta_1	Leu 15-delta_1_25C	3	3	800.13	25.0	1	4	800-SQ-25C	FALSE	TRUE	36	No Exch	59.91	No Exch	1.66	No Exch	No Exch	No Exch	0.040, 0	0.040, 0	100.000	0.040	55.4400	0.047	740.0	0.047	0.047
15	Leu	-delta_1	Leu 15-delta_1	Leu 15-delta_1_25C	4	4	600.13	25.0	1	4	800-SQ-25C	FALSE	TRUE	36	No Exch	59.91	No Exch	1.66	No Exch	No Exch	No Exch	0.040, 0	0.040, 0	100.000	0.040	46.8400	0.047	740.0	0.047	0.047
15	Leu	-delta_2	Leu 15-delta_2	Leu 15-delta_2_25C	1	1	800.13	25.0	1	4	800-MQ-25C	FALSE	TRUE	36	No Exch	19.34	No Exch	0.54	No Exch	No Exch	No Exch	0.040, 0	0.040, 0	100.000	0.040	50.0400	0.047	740.0	0.047	0.047
15	Leu	-delta_2	Leu 15-delta_2	Leu 15-delta_2_25C	2	2	600.17	25.0	1	4	800-MQ-25C	FALSE	TRUE	36	No Exch	19.34	No Exch	0.54	No Exch	No Exch	No Exch	0.040, 0	0.040, 0	100.000	0.040	50.0400	0.047	740.0	0.047	0.047
15	Leu	-delta_2	Leu 15-delta_2	Leu 15-delta_2_25C	3	3	800.13	25.0	1	4	800-SQ-25C	FALSE	TRUE	36	No Exch	19.34	No Exch	0.54	No Exch	No Exch	No Exch	0.040, 0	0.040, 0	100.000	0.040	50.0400	0.047	740.0	0.047	0.047
15	Leu	-delta_2	Leu 15-delta_2	Leu 15-delta_2_25C	4	4	600.13	25.0	1	4	800-SQ-25C	FALSE	TRUE	36	No Exch	19.34	No Exch	0.54	No Exch	No Exch	No Exch	0.040, 0	0.040, 0	100.000	0.040	46.8400	0.047	740.0	0.047	0.047
19	Val	-gamma_1	Val 19-gamma_1	Val 19-gamma_1_25C	1	1	800.13	25.0	1	4	800-MQ-25C	FALSE	TRUE	36	No Exch	25.39	No Exch	0.71	No Exch	No Exch	No Exch	0.040, 0	0.040, 0	100.000	0.040	56.4400	0.047	740.0	0.047	0.047
19	Val	-gamma_1	Val 19-gamma_1	Val 19-gamma_1_25C	2	2	600.17	25.0	1	4	800-MQ-25C	FALSE	TRUE	36	No Exch	25.39	No Exch	0.71	No Exch	No Exch	No Exch	0.040, 0	0.040, 0	100.000	0.040	43.6400	0.047	740.0	0.047	0.047
19	Val	-gamma_1	Val 19-gamma_1	Val 19-gamma_1_25C	3	3	800.13	25.0	1	4	800-SQ-25C	FALSE	TRUE	36	No Exch	25.39	No Exch	0.71	No Exch	No Exch	No Exch	0.040, 0	0.040, 0	100.000	0.040	56.4400	0.047	740.0	0.047	0.047
19	Val	-gamma_1	Val 19-gamma_1	Val 19-gamma_1_25C	4	4	600.13	25.0	1	4	800-SQ-25C	FALSE	TRUE	36	No Exch	25.39	No Exch	0.71	No Exch	No Exch	No Exch	0.040, 0	0.040, 0	100.000	0.040	51.7400	0.047	740.0	0.047	0.047
19	Val	-gamma_2	Val 19-gamma_2	Val 19-gamma_2_25C	1	1	800.13	25.0	1	4	800-MQ-25C	FALSE	TRUE	36	No Exch	24.25	No Exch	0.67	No Exch	No Exch	No Exch	0.040, 0	0.040, 0	100.000	0.040	55.1400	0.047	740.0	0.047	0.047
19	Val	-gamma_2	Val 19-gamma_2	Val 19-gamma_2_25C	2	2	600.17	25.0	1	4	800-MQ-25C	FALSE	TRUE	36	No Exch	24.25	No Exch	0.67	No Exch	No Exch	No Exch	0.040, 0	0.040, 0	100.000	0.040	39.1400	0.047	740.0	0.047	0.047
19	Val	-gamma_2	Val 19-gamma_2	Val 19-gamma_2_25C	3	3	800.13	25.0	1	4	800-SQ-25C	FALSE	TRUE	36	No Exch	24.25	No Exch	0.67	No Exch	No Exch	No Exch	0.040, 0	0.040, 0	100.000	0.040	55.1400	0.047	740.0	0.047	0.047
19	Val	-gamma_2	Val 19-gamma_2	Val 19-gamma_2_25C																										

