Supporting Information

Temperature Dependence of Carbonyl Backbone Dynamics in Chicken Villin Headpiece Subdomain

Liliya Vugmeyster*[1], Dmitry Ostrovsky[2]

[1]*Department of Chemistry and Environment and Natural Resources Institute, University of Alaska at Anchorage, 3211 Providence Drive, Anchorage AK, 99508. Corresponding author, email: aflv@uaa.alaska.edu. Telephone: (907) 786-4709. Fax: (907) 786-4607*

[2]*Department of Mathematical Sciences, University of Alaska at Anchorage, 3211 Providence Drive, Anchorage AK, 99508*

S1. The analysis of behavior of the order parameters and internal correlation times as a function of τ_e/τ_c values using synthetic data sets.

In order to analyze the influence of the value of the τ_e/τ_c ratio on the stability of the fitted values of the order parameter and internal correlation times we have done the following analysis using synthetic R_1, $R_{C'C'-C\alpha}$ and $R_{C'C'-N}$ rates.

First, synthetic R_1, $R_{C'C'-C\alpha}$ and $R_{C'C'-N}$ rates were created with the use of the spectral density functions given by sEq. (1) of the main text for S^2 = 0.6, 0.8, 0.9 and τ_e/τ_c values between 0.1 and 0.5. C_{iso} = 175 and θ = 155°. We then fitted these synthetic rates with the χ^2 minimization procedure, taking "experimental" errors as 3%, 5%, and 7% of the average values for R_1, $R_{C'C'-C\alpha}$ and $R_{C'C'-N}$, respectively. These results are presented in Figure S1 for S^2 =0.8.

For the results presented in Figure S2, the synthetic rates were altered by adding normally distributed random noise; we have used the standard deviations of 3%, 5%, and 7% of the average values of R_1, $R_{C'C'-C\alpha}$ and $R_{C'C'-N}$, respectively. These standard deviations mimic actual experimental errors. Ten runs were done.

Results: fitted values of τ_e/τ_c reproduce input values with a reasonable accuracy only for the input values of τ_e/τ_c below a certain threshold. When no random noise in included the approximate thresholds are given by 0.45, 0.35 and 0.15 for S^2 of 0.6, 0.8, and 0.9, respectively. When the random noise is added, the thresholds change to about 0.3, 0.2 and 0.1 for S^2 of 0.6, 0.8, and 0.9, respectively. On the contrary, the fitted values of S^2 are stable for all values of τ_e/τ_c, regardless of whether the noise was added to the synthetic data. The simulated errors in S^2 values are also stable. Thus, we conclude that neither the stability of the fitted S^2 values nor their errors depend on the quality of τ_e fits and, therefore, can be well-defined even for those experimental situations which do not allow for a reliable determination of the internal correlation times.

Figure S1. Fitted internal correlation times and order parameters as a function of τ_e/τ_c ratio for S^2 =0.8. No random noise is included in the synthetic R_1, $R_{C'/C'-C\alpha}$ and $R_{C'/C'-N}$ relaxation rates.

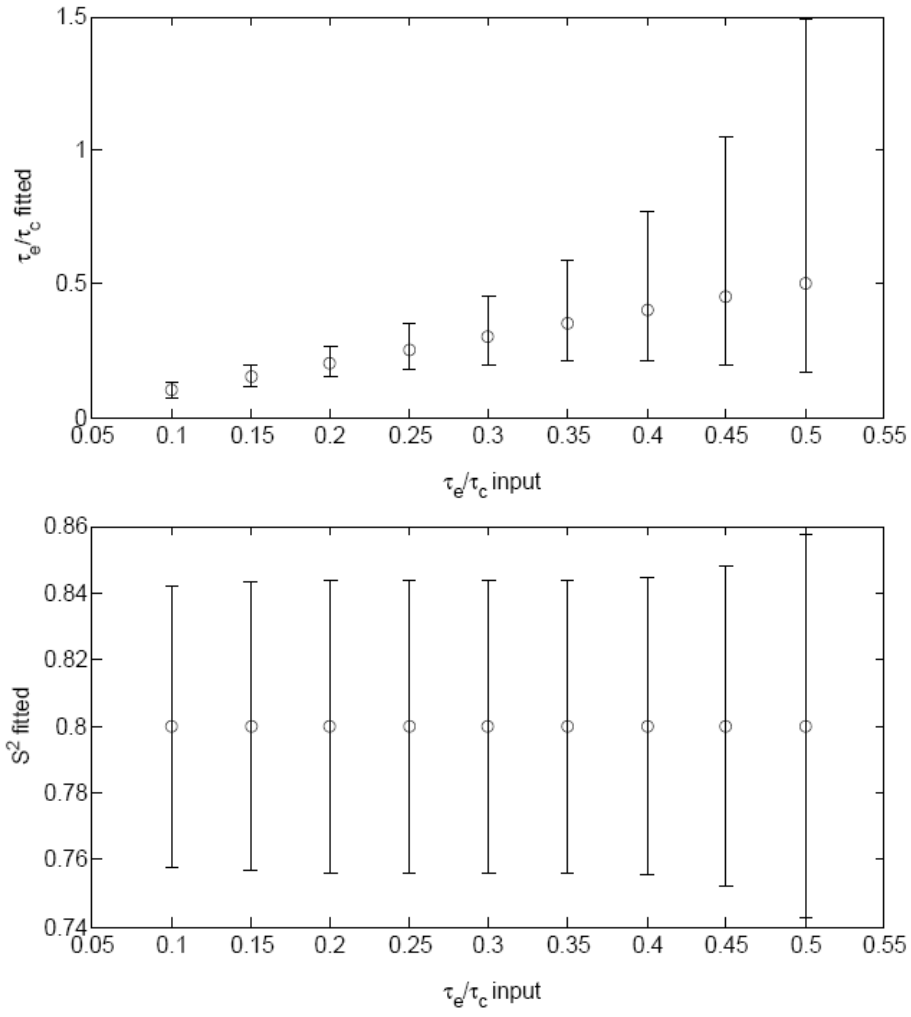
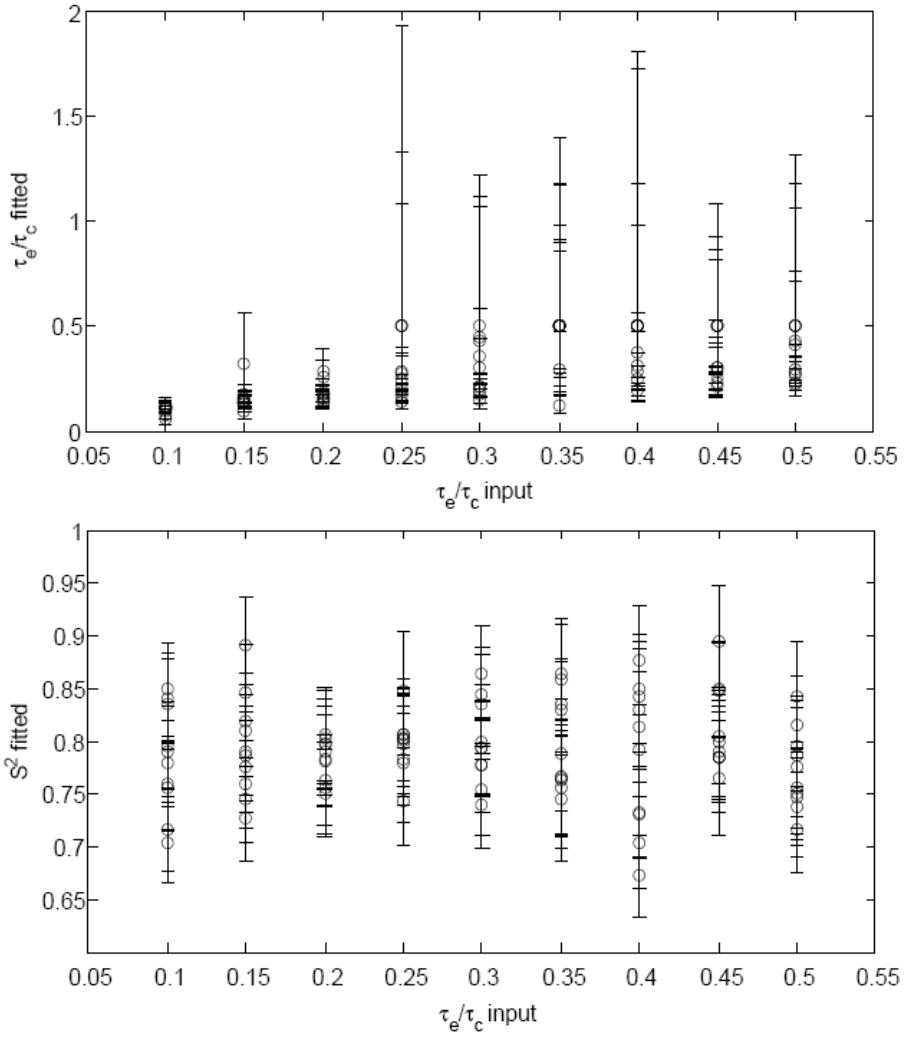


Figure S2. Fitted internal correlation times and order parameters as a function of τ_e/τ_c ratio for S^2 =0.8. Synthetic relaxation rates R_1, $R_{C'C'-C\alpha}$ and $R_{C'C'-N}$ were generated with random noise as specified in the description above.



S2. Experimental R_1, $R_{C'/C'-C\alpha}$ and $R_{C'/C'-N}$ rates.

2 °C

residue	R_1	error	$R_{C'/C'-C\alpha}$	error	$R_{C'/C'-N}$	error
41	0.887	0.039	-1.12	0.06	0.26	0.06
42	0.777	0.027	-1.10	0.09	1.00	0.13
43	0.725	0.010	-1.37	0.06	0.62	0.06
45	0.782	0.018	-1.25	0.09	0.86	0.08
47	0.756	0.007	-1.40	0.13	0.98	0.12
48	0.729	0.025	-1.11	0.06	0.76	0.06
49	0.707	0.019	-1.43	0.09	0.79	0.11
50	0.773	0.028	-1.35	0.12	0.80	0.14
51	0.788	0.026	-1.00	0.09	0.57	0.07
54	0.781	0.015	-1.14	0.07	0.68	0.06
55	0.844	0.018	-1.45	0.10	0.63	0.07
56	0.809	0.013	-1.32	0.11	1.22	0.43
57	0.833	0.032	-1.55	0.17	0.91	0.09
58	0.743	0.029	-1.34	0.09	0.59	0.06
59	0.763	0.025	-1.21	0.06	0.70	0.06
62	0.787	0.024	-1.29	0.06	0.78	0.05
63	0.769	0.019	-1.30	0.05	0.57	0.06
64	0.808	0.015	-1.64	0.19	0.56	0.16
65	0.734	0.035	-1.53	0.09	0.96	0.13
66	0.831	0.030	-1.29	0.08	0.69	0.06
67	0.790	0.024	-1.17	0.08	0.65	0.05
68	0.741	0.034	-1.35	0.13	0.84	0.14
69	0.773	0.022	-1.31	0.09	0.67	0.07
70	0.796	0.012	-1.08	0.08	0.66	0.05
71	0.755	0.019	-1.31	0.09	0.76	0.07
72	0.751	0.019	-1.11	0.07	0.64	0.05
73	0.778	0.022	-0.97	0.11	0.66	0.07
74	0.750	0.027	-1.10	0.17	0.82	0.20
75	0.802	0.014	-1.04	0.05	0.42	0.05

6 °C

residue	R_1	error	$R_{C'/C'-C\alpha}$	error	$R_{C'/C'-N}$	error
41	1.013	0.012	-1.03	0.06	0.74	0.11
42	0.888	0.014	-1.06	0.06	0.51	0.05
43	0.874	0.015	-1.00	0.04	0.51	0.03
45	0.875	0.015	-1.06	0.05	0.53	0.05
47	0.894	0.017	-0.98	0.06	0.67	0.05
48	0.856	0.012	-0.76	0.03	0.59	0.03
49	0.781	0.017	-0.97	0.05	0.63	0.05
50	0.922	0.016	-1.24	0.09	0.53	0.11
51	0.886	0.031	-0.92	0.09	0.44	0.04
54	0.873	0.033	-1.05	0.05	0.44	0.04
55	0.987	0.021	-0.91	0.05	0.55	0.04
56	0.884	0.028	-1.24	0.04	0.47	0.09
57	0.938	0.017	-0.81	0.05	0.60	0.05
58	0.877	0.021	-1.06	0.05	0.56	0.06
59	0.849	0.009	-1.00	0.04	0.48	0.04

62	0.888	0.013	-1.09	0.04	0.60	0.04
63	0.886	0.025	-1.08	0.06	0.45	0.05
64	0.878	0.028	-0.93	0.09	0.56	0.07
65	0.878	0.012	-1.11	0.06	0.46	0.05
66	0.921	0.021	-1.01	0.05	0.52	0.04
67	0.886	0.018	-0.94	0.05	0.53	0.03
68	0.870	0.021	-1.20	0.11	0.57	0.08
69	0.894	0.011	-1.03	0.05	0.56	0.04
70	0.900	0.013	-0.91	0.05	0.56	0.03
71	0.865	0.011	-0.95	0.04	0.50	0.04
72	0.906	0.018	-0.90	0.05	0.58	0.04
73	0.888	0.008	-0.75	0.03	0.58	0.07
74	0.844	0.011	-0.97	0.12	0.49	0.06
75	0.855	0.010	-0.86	0.04	0.24	0.03

12 ^{o}C

residue	R_1	error	$R_{C'C'-C\alpha}$	error	$R_{C'C'-N}$	error
41	1.128	0.058	-0.77	0.05	0.26	0.05
42	0.985	0.026	-0.80	0.05	0.50	0.04
43	0.978	0.012	-0.89	0.03	0.45	0.03
45	0.969	0.013	-0.83	0.05	0.51	0.04
47	0.995	0.026	-0.85	0.06	0.55	0.04
48	0.970	0.006	-0.87	0.03	0.48	0.03
49	0.893	0.009	-0.87	0.05	0.51	0.05
50	0.950	0.030	-1.06	0.07	0.40	0.06
51	0.990	0.018	-0.84	0.08	0.38	0.03
54	0.964	0.019	-0.88	0.04	0.44	0.04
55	1.065	0.013	-0.89	0.05	0.51	0.04
56	0.968	0.026	-0.73	0.05	0.50	0.11
57	1.020	0.017	-0.92	0.05	0.58	0.04
58	0.999	0.026	-0.91	0.04	0.51	0.04
59	0.970	0.017	-0.97	0.04	0.45	0.03
62	0.962	0.018	-0.92	0.04	0.47	0.03
63	0.946	0.025	-0.93	0.04	0.43	0.04
64	1.008	0.016	-0.88	0.09	1.16	0.17
65	0.983	0.021	-0.85	0.04	0.34	0.14
66	0.988	0.012	-1.04	0.07	0.55	0.04
67	0.999	0.018	-0.84	0.04	0.52	0.03
68	0.935	0.041	-0.96	0.07	0.35	0.03
69	0.990	0.032	-0.91	0.04	0.42	0.04
70	0.993	0.025	-0.73	0.04	0.47	0.04
71	0.964	0.017	-0.87	0.04	0.43	0.03
72	0.993	0.003	-0.80	0.04	0.48	0.04
73	0.977	0.007	-0.94	0.06	0.41	0.05
74	0.919	0.029	-0.71	0.08	0.52	0.08
75	0.873	0.009	-0.78	0.03	0.21	0.04

16 ^{o}C

residue	R_1	error	$R_{C'C'-C\alpha}$	error	$R_{C'C'-N}$	error
41	1.226	0.041	-0.69	0.06	0.32	0.05
42	1.063	0.017	-0.71	0.05	0.45	0.04

43	1.051	0.033	-0.85	0.04	0.39	0.03
45	1.022	0.029	-0.80	0.04	0.40	0.04
47	1.032	0.017	-0.77	0.05	0.48	0.06
48	1.074	0.014	-0.70	0.03	0.41	0.03
49	1.006	0.027	-0.86	0.05	0.42	0.05
50	1.043	0.015	-0.78	0.07	0.42	0.06
51	0.998	0.012	-0.72	0.07	0.38	0.03
54	1.073	0.016	-0.79	0.04	0.39	0.03
55	1.167	0.014	-0.73	0.05	0.39	0.06
56	1.078	0.014	-0.76	0.06	0.35	0.03
57	1.157	0.033	-0.62	0.04	0.39	0.03
58	1.049	0.022	-0.90	0.05	0.37	0.03
59	1.005	0.014	-0.82	0.05	0.55	0.05
62	1.078	0.019	-0.75	0.04	0.40	0.03
63	1.015	0.019	-0.84	0.05	0.34	0.03
64	1.064	0.030	-0.73	0.05	0.40	0.04
65	1.019	0.018	-0.88	0.04	0.16	0.02
66	1.060	0.016	-0.75	0.04	0.42	0.04
67	1.078	0.021	-0.76	0.04	0.41	0.04
68	0.993	0.055	-0.98	0.07	0.28	0.03
69	1.056	0.012	-0.80	0.05	0.44	0.04
70	1.069	0.029	-0.56	0.04	0.32	0.03
71	1.040	0.008	-0.72	0.04	0.52	0.05
72	1.111	0.028	-0.68	0.04	0.34	0.03
73	1.030	0.024	-1.07	0.08	0.58	0.06
74	0.950	0.009	-0.70	0.08	0.10	0.02
75	0.890	0.013	-0.72	0.03	0.21	0.02

22 ^{o}C. $R_{C'/C'-N}$ rates are reported for the relaxation delay of 80ms. The rates determined from the relaxation delay of 60ms agree within the experimental errors.

residue	R_1	error	$R_{C'/C'-C\alpha}$	error	$R_{C'/C'-N}$	error
41	1.245	0.058	-0.87	0.05	0.27	0.09
42	1.132	0.015	-0.58	0.03	0.29	0.02
43	1.118	0.015	-0.89	0.19	0.27	0.02
45	1.209	0.087	-0.59	0.07	0.38	0.02
47	1.124	0.014	-0.72	0.04	0.36	0.03
48	1.140	0.011	-0.55	0.02	0.38	0.03
49	1.051	0.015	-0.65	0.03	0.37	0.03
50	1.392	0.073	-0.58	0.02	0.32	0.03
51	1.161	0.012	-0.78	0.05	0.32	0.02
54	1.147	0.010	-0.61	0.02	0.35	0.02
55	1.295	0.024	-0.52	0.03	0.43	0.03
56	1.144	0.018	-0.66	0.02	0.24	0.03
57	1.193	0.017	-0.63	0.02	0.35	0.03
58	1.147	0.018	-0.57	0.05	0.28	0.02
59	1.101	0.016	-0.78	0.05	0.43	0.03
62	1.143	0.021	-0.58	0.03	0.35	0.02
63	1.086	0.020	-0.75	0.04	0.42	0.03
64	1.156	0.013	-0.60	0.03	0.36	0.03
65	1.141	0.018	-0.62	0.03	0.34	0.03
66	1.222	0.008	-0.73	0.03	0.45	0.03

67	1.131	0.013	-0.73	0.03	0.35	0.02
68	1.064	0.026	-0.71	0.03	0.38	0.04
69	1.236	0.210	-0.66	0.03	0.40	0.03
70	1.159	0.014	-0.60	0.03	0.32	0.02
71	1.055	0.060	-0.70	0.03	0.34	0.02
72	1.169	0.007	-0.75	0.03	0.37	0.02
73	1.096	0.011	-0.64	0.03	0.29	0.02
74	1.027	0.014	-0.41	0.04	0.29	0.03
75	0.943	0.005	-0.67	0.02	0.19	0.02

S3. Averaged fitted values of θ for those residues for which the data were obtained for at least three temperatures out of 2, 6, 12, and 16 ^{o}C..

residue	θ, degrees
41	161.6 ± 2.5
42	148.8 ± 1.8
43	154.7 ± 1.1
45	151.8 ± 1.8
47	149.2 ± 1.2
48	147.0 ± 1.4
49	152.3 ± 2.0
50	156.7 ± 3.0
51	153.7 ± 2.0
54	154.0 ± 1.3
55	156.8 ± 2.2
56	156.9 ± 4.6
57	146.6 ± 2.2
58	155.9 ± 1.5
59	154.6 ± 1.5
62	152.9 ± 1.3
63	159.2 ± 1.8
64	154.2 ± 3.2
65	165.3 ± 4.8
66	153.5 ± 1.7
67	151.3 ± 1.5
68	160.9 ± 4.1
69	154.7 ± 1.8
70	147.9 ± 1.7
71	151.9 ± 1.7
72	150.2 ± 1.5
73	148.2 ± 2.6
74	154.8 ±7.0
75	166.0± 2.3

S4. 13CO chemical shifts

res	8c	20c
41	169.7	170.0
42	175.5	175.5
43	171.4	171.8
44	176.7	176.7
45	176.5	176.7
46	175.1	175.3
46	174.6	174.8
48	176.9	177.2
49	176.7	176.9
50	174.8	174.8
51	174.1	174.4
52	170.2	170.4
53	169.7	170.0
54	173.0	173.2
55	176.9	176.9
56	173.4	173.7
57	178.6	178.6
58	174.6	174.1
59	175.1	175.3
60	173.4	173.4
62	174.8	175.3
63	175.8	175.8
64	175.1	175.3
65	175.3	175.5
66	176.0	176.2
67	176.2	176.2
68	175.3	175.5
69	176.7	176.9
70	176.2	176.5
71	177.2	177.2
72	176.2	176.5
73	174.1	174.4
74	171.4	171.6
75	172.3	172.3

SI5. Graphs of 1-*S* vs *T* for all residues for which the data were obtained for at least three temperatures out of 2, 6, 12, and 16 ^{o}C.