

Supplementary Material for Neira et al.

FIGURE 1: DOSY curves for the methyl region of SAMp73 at 0M and 1 M GdmCl, at 298 K (pH 7.0).

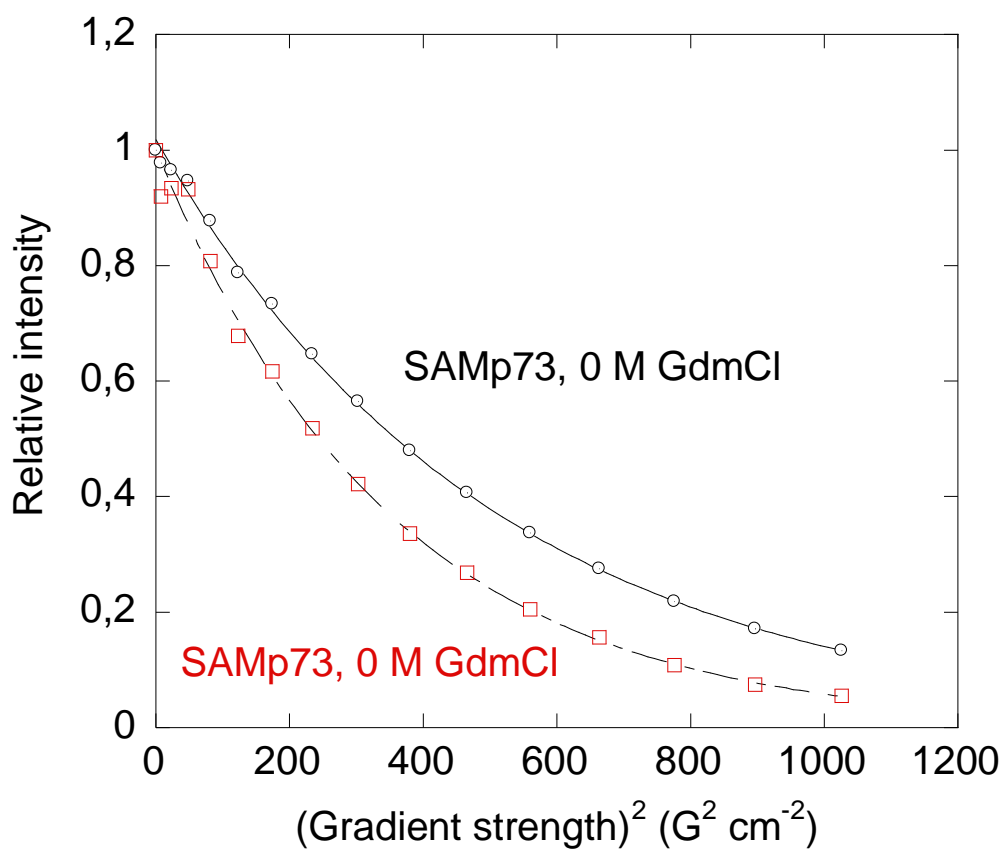
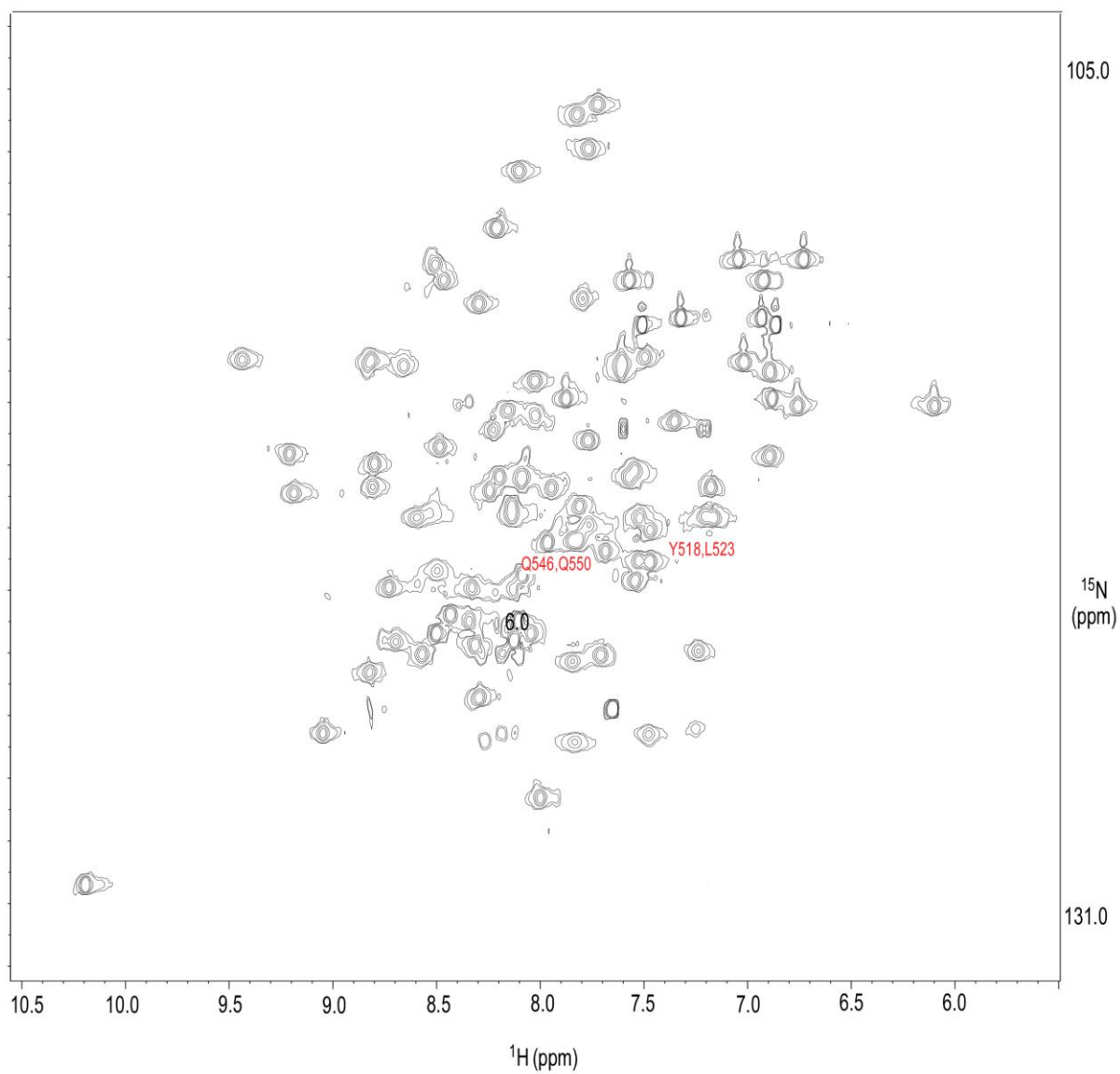


FIGURE 2: HSQC spectrum of SAMp73, at 0 M GdmCl, pH 7.0 and 298 K. The residues whose signals overlap under any of the explored conditions are indicated.



TABLES

Table 1: Experimental relaxation parameters, the reduced spectral density functions and the model-free parameters of SAMp73 at pH 7.0 and 298 K.

| Residue | R_1 (s ⁻¹) ^a | R_2 (s ⁻¹) ^a | η_{xy} (s ⁻¹) ^a | R_2^0 (s ⁻¹) ^b | NOE ^c | $J(0)$ (ns rad ⁻¹) ^b | $J(\omega_N)$ (ns rad ⁻¹) ^b | $J(0.87\omega_H)$ (ps rad ⁻¹) ^b | S^2 (S_f^2) ^d | R_{ex} (s ⁻¹) ^d | τ_c (ns) ^d |
|---------|---------------------------------------|---------------------------------------|---|---|------------------|--|---|---|--------------------------------|--|----------------------------|
| Y487 | 2.04±0.04 | 7.89±0.24 | 3.64±0.07 | 5.49±0.75 | 0.32±0.03 | 2.13±0.21 | 0.38±0.037 | 21.32±2.07 | 0.20±0.01 | 5.80±0.26 | 2.52±0.01 |
| H488 | 2.09±0.06 | 10.01±0.18 | 6.37±0.34 | 9.61±1.39 | 0.67±0.06 | 2.80±0.27 | 0.41±0.040 | 10.51±1.00 | 0.87±0.02 | 1.30±0.31 | 0.08±0.06 |
| A489 | 2.05±0.03 | 8.36±0.24 | 4.20±0.20 | 6.34±0.91 | 0.48±0.05 | 2.28±0.25 | 0.39±0.043 | 16.56±1.78 | 0.82±0.01 | | 0.18±0.003 |
| D490 | 2.31±0.06 | 10.77±0.21 | 5.57±0.02 | 8.40±1.17 | 0.73±0.06 | 3.01 ±0.26 | 0.46±0.041 | 9.66±0.86 | 0.99±0.01 | 0.78±0.33 | |
| P491 | | | | | | | | | | | |
| S492 | 2.56±0.08 | 13.18±0.40 | 6.00±0.15 | 9.05±1.24 | 0.75±0.03 | 3.72±0.25 | 0.51±0.028 | 9.85±0.54 | 0.71±0.09 | 4.41±0.54 | 6.85±1.41 |
| L493 | 2.58±0.13 | 10.02±0.19 | 7.10±0.20 | 10.71±1.47 | 0.89±0.11 | 2.73±0.31 | 0.53±0.078 | 4.27±0.57 | 0.74±0.14 | 1.21±0.80 | 6.85±2.13 |
| V494 | 2.37±0.07 | 10.16±0.30 | 4.96±0.24 | 7.48±1.07 | 0.73±0.07 | 2.81±0.26 | 0.47±0.042 | 9.77±0.77 | 0.99±0.01 | | |
| S495 | 2.44±0.09 | 10.58±0.21 | 6.60±0.30 | 9.95±1.41 | 0.72±0.06 | 2.92±0.25 | 0.49±0.044 | 10.52±0.95 | 0.83±0.09 | 1.62±0.59 | 2.97±2.16 |
| F496 | 2.52±0.13 | 10.56±0.31 | 6.80±0.20 | 10.26±1.43 | 0.83±0.07 | 2.91±0.33 | 0.51±0.052 | 6.43±0.65 | 0.98±0.01 | | |

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|------|-----------|------------|-----------|------------|-----------|-----------|------------|------------|-----------|-----------|-----------|
| L497 | 2.46±0.08 | 10.82±0.13 | 6.56±0.17 | 9.89±1.36 | 0.75±0.03 | 3.00±0.15 | 0.49±0.027 | 9.49±0.52 | 0.83±0.08 | 1.66±0.39 | 4.71±1.99 |
| T498 | 2.54±0.95 | 10.56±0.22 | 6.20±0.30 | 9.35±1.34 | 0.84±0.06 | 2.91±0.28 | 0.52±0.045 | 6.28±0.54 | 0.78±0.10 | 1.54±0.52 | 6.85±2.01 |
| G499 | 2.59±0.09 | 10.29±0.14 | 6.45±0.20 | 9.73±1.75 | 0.74±0.05 | 2.81±0.24 | 0.52±0.045 | 10.39±0.89 | 0.67±0.10 | 1.71±0.50 | 6.30±1.56 |
| L500 | 2.28±0.06 | 9.75±0.14 | 7.53±0.06 | 11.36±1.53 | 0.76±0.05 | 2.70±0.25 | 0.46±0.036 | 8.41±0.66 | 0.97±0.01 | | |
| G501 | 2.43±0.07 | 10.52±0.16 | 6.10±0.20 | 9.20±1.27 | 0.72±0.05 | 2.91±0.21 | 0.48±0.039 | 10.49±0.85 | 0.84±0.09 | 1.53±0.54 | 2.86±1.95 |
| C502 | 2.26±0.05 | 9.51±0.13 | 6.30±0.08 | 9.50±1.29 | 0.68±0.05 | 2.62±0.26 | 0.45±0.035 | 10.92±0.86 | 0.96±0.01 | | |
| P503 | | | | | | | | | | | |
| N504 | 2.37±0.08 | 9.85±0.18 | 6.20±0.20 | 9.35±1.30 | 0.79±0.05 | 2.71±0.25 | 0.48±0.038 | 7.46±0.59 | 0.99±0.01 | | |
| C505 | 2.36±0.09 | 10.21±0.11 | 6.50±0.20 | 9.80±1.35 | 0.71±0.05 | 2.82±0.25 | 0.47±0.036 | 10.39±0.82 | 0.99±0.02 | 0.31±0.22 | |
| I506 | 2.33±0.06 | 9.18±0.20 | 6.64±0.16 | 10.02±1.37 | 0.66±0.05 | 2.50±0.26 | 0.45±0.035 | 12.13±0.97 | 0.91±0.03 | | 1.01±0.8 |
| E507 | 1.62±0.23 | 6.98±0.37 | 4.46±0.06 | 6.73±0.91 | 0.42±0.04 | 1.92±0.28 | 0.31±0.032 | 14.42±1.49 | 0.68±0.03 | | 0.17±0.08 |
| Y508 | 2.28±0.05 | 10.09±0.17 | 6.80±0.10 | 10.26±1.39 | 0.77±0.05 | 2.80±0.26 | 0.46±0.038 | 7.99±0.59 | 0.99±0.01 | | |
| F509 | 2.51±0.08 | 9.80±0.67 | 3.10±0.40 | 4.67±0.87 | 0.74±0.05 | 2.67±0.28 | 0.50±0.041 | 9.93±0.81 | 0.99±0.01 | | |
| T510 | 2.68±0.09 | 11.36±0.39 | 6.20±0.20 | 9.35±1.29 | 0.65±0.07 | 3.13±0.31 | 0.53±0.059 | 14.22±1.57 | 0.53±0.10 | 3.98±0.73 | 3.59±1.37 |
| S511 | 2.35±0.09 | 11.88±0.26 | 6.19±0.27 | 9.34±1.32 | 0.69±0.05 | 3.35±0.32 | 0.47±0.042 | 11.16±0.99 | 0.99±0.02 | 1.79±0.46 | |
| Q512 | 2.40±0.07 | 11.39±0.23 | 6.11±0.06 | 9.21±1.24 | 0.50±0.03 | 3.18±0.23 | 0.46±0.038 | 18.52±1.29 | 0.60±0.08 | 4.08±0.53 | 1.78±0.30 |

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| G513 | 2.41±0.08 | 9.88±0.17 | 6.30±0.20 | 9.50±1.31 | 0.72±0.05 | 2.71±0.27 | 0.48±0.039 | 10.13±0.83 | 0.99±0.08 | | |
| L514 | 2.44±0.07 | 10.39±0.23 | 6.99±0.20 | 10.54±1.45 | 0.77±0.05 | 2.87±0.20 | 0.49±0.031 | 8.64±0.69 | 0.99±0.01 | | |
| Q515 | 2.57±0.11 | 10.12±0.26 | 7.38±0.24 | 11.13±1.54 | 0.72±0.05 | 2.76±0.23 | 0.51±0.04 | 10.85±0.94 | 0.70±0.11 | 1.65±0.67 | 4.53±1.55 |
| S516 | 2.24±0.05 | 9.85±0.20 | 5.61±0.16 | 8.46±1.16 | 0.64±0.05 | 2.73±0.27 | 0.44±0.040 | 12.44±1.11 | 0.91±0.03 | 0.80±0.31 | 0.21±0.29 |
| I517 | 1.63±0.03 | 4.32±0.09 | 1.75±0.07 | 2.64±0.37 | 0.04±0.03 | 1.03±0.81 | 0.29±0.089 | 24.48±20.34 | 0.46±0.02 | | 0.96±0.05 |
| | | | | | | | | | (0.76±0.015) | | |
| Y518 | | | | | | | | | | | 1.18±0.32 |
| H519 | 2.33±0.09 | 10.14±0.18 | 6.21±0.20 | 9.37±1.30 | 0.71±0.06 | 2.80±0.21 | 0.47±0.043 | 10.27±0.94 | 0.99±0.01 | | |
| L520 | 2.54±0.08 | 11.32±0.16 | 6.76±0.12 | 10.20±1.39 | 0.52±0.05 | 3.13±0.30 | 0.49±0.048 | 18.87±1.82 | 0.52±0.10 | 4.56±0.63 | 2.17±0.22 |
| Q521 | 2.09±0.03 | 9.37±0.20 | 6.70±0.10 | 10.11±1.37 | 0.70±0.05 | 2.60±0.20 | 0.42±0.031 | 9.53±0.71 | 0.91±0.01 | | |
| N522 | 1.66±0.47 | 5.56±0.44 | 2.38±0.08 | 3.59±0.05 | 0.10±0.06 | 1.46±0.86 | 0.30±0.18 | 23.01±13.51 | 0.53±0.06 | | 0.35±0.09 |
| L523 | | | | | | | | | | | |
| T524 | 2.23±0.05 | 9.65±0.17 | 5.60±0.30 | 8.44±1.22 | 0.71±0.06 | 2.67±0.24 | 0.44±0.039 | 10.06±0.89 | 0.96±0.01 | | |
| I525 | 2.46±0.08 | 9.63±0.23 | 5.50±0.40 | 8.30±1.27 | 0.78±0.08 | 2.63±0.29 | 0.49±0.054 | 8.09±0.87 | 0.86±0.04 | | 6.85±2.10 |
| E526 | 2.02±0.04 | 8.51±0.30 | 3.22±0.19 | 4.85±0.71 | 0.65±0.05 | 2.34±0.21 | 0.40±0.034 | 10.79±0.93 | 0.84±0.02 | | 0.07±0.03 |
| D527 | 1.94±0.06 | 7.17±0.38 | 5.44±0.13 | 8.20±1.12 | 0.39±0.02 | 1.93±0.16 | 0.37±0.023 | 18.16±1.16 | 0.44±0.01 | 2.63±0.35 | 0.034±0.00 |

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| L528 | 2.34±0.06 | 11.11±0.23 | 7.39±0.31 | 11.15±1.57 | 0.75±0.06 | 3.11±0.26 | 0.47±0.039 | 8.78±0.73 | 0.99±0.01 | 0.77±0.32 | |
| G529 | 2.35±0.08 | 10.25±0.27 | 6.40±0.20 | 9.65±1.33 | 0.87±0.05 | 2.85±0.22 | 0.48±0.035 | 4.55±0.33 | 0.99±0.01 | | |
| A530 | 2.35±0.06 | 12.51±0.31 | 7.00±0.30 | 10.56±1.49 | 0.77±0.05 | 3.55±0.28 | 0.47±0.036 | 8.19±0.62 | 0.99±0.02 | 2.48±0.35 | |
| L531 | 2.31±0.06 | 10.11±0.14 | 6.70±0.12 | 10.11±1.38 | 0.75±0.04 | 2.80±0.18 | 0.46±0.029 | 8.70±0.55 | 0.99±0.08 | | |
| K532 | 2.43±0.09 | 16.90±0.35 | 7.30±0.80 | 11.01±1.91 | 0.77±0.07 | 4.92±0.56 | 0.49 ±0.050 | 8.56±0.85 | 0.99±0.02 | 6.17±0.52 | |
| I533 | 2.33±0.12 | 7.96±0.56 | 6.96±0.19 | 10.50±1.44 | 0.72±0.09 | 2.15±0.30 | 0.51 ±0.05 | 10.85±2.15 | 0.70±0.09 | 6.85±2.75 | |
| | | | | | | | | | (0.91±0.09) | | |
| P534 | | | | | | | | | | | |
| E535 | 2.43±0.05 | 10.22±0.16 | 6.30±0.20 | 9.50±1.31 | 0.70±0.06 | 2.81±0.25 | 0.48±0.043 | 11.24±1.03 | 0.83±0.08 | 1.41±0.57 | 2.46±1.73 |
| Q536 | 2.43±0.05 | 10.45±0.19 | 6.00±0.20 | 9.05±1.26 | 0.72±0.05 | 2.89±0.25 | 0.49±0.038 | 10.41±0.82 | 0.82±0.07 | 1.42±0.53 | 3.17±1.71 |
| Y537 | 2.42±0.11 | 10.47±0.15 | 6.84±0.22 | 10.32±1.43 | 0.68±0.06 | 2.89±0.28 | 0.48±0.044 | 11.82±1.15 | 0.78±0.10 | 1.75±0.65 | 2.54±1.61 |
| R538 | 2.44±0.07 | 10.12±0.14 | 6.78±0.37 | 10.23±1.49 | 0.73±0.06 | 2.78±0.25 | 0.49±0.043 | 10.13±0.89 | 0.99±0.07 | | |
| M539 | 2.61±0.09 | 14.09±0.30 | 7.40±0.50 | 11.16±1.68 | 0.83±0.07 | 4.01±0.39 | 0.53±0.051 | 6.56±0.63 | 0.67±0.09 | 5.48±0.64 | 6.85±1.60 |
| T540 | 2.16±0.03 | 7.62±0.29 | 6.43±0.16 | 9.70±1.33 | 0.52±0.04 | 2.03±0.17 | 0.42±0.031 | 16.02±0.19 | 0.75±0.03 | 1.26±0.25 | |
| | | | | | | | | | (0.94±0.02) | | |

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| I541 | 1.82±0.11 | 5.83±0.55 | 3.15±0.11 | 4.75±0.66 | 0.51±0.25 | 1.53±0.76 | 0.35±0.17 | 13.72±6.72 | 0.66±0.12 | | 2.13±1.60 |
| W542 | 2.35±0.08 | 9.71±0.28 | 5.6±0.30 | 8.45±1.22 | 0.68±0.06 | 2.67±0.27 | 0.47±0.046 | 11.33±1.11 | 0.99±0.01 | | |
| R543 | 2.47±0.94 | 10.46±0.15 | 7.00±0.30 | 10.56±1.50 | 0.87±0.06 | 2.89±0.25 | 0.50±0.044 | 4.89±0.42 | 0.99±0.21 | 1.46±0.56 | 6.85±3.02 |
| G544 | 2.42±0.07 | 10.52±0.11 | 6.60±0.20 | 9.95±1.38 | 0.76±0.05 | 2.91±0.22 | 0.49±0.037 | 8.97±0.67 | 0.87±0.08 | 1.12±0.47 | 4.87±2.15 |
| L545 | 2.50±0.08 | 10.42±0.20 | 6.99±0.13 | 10.54±1.43 | 0.72±0.06 | 2.87±0.27 | 0.50±0.047 | 10.61±0.99 | 0.78±0.10 | 1.70±0.58 | 3.61±1.93 |
| Q546 | | | | | | | | | | | |
| D547 | 2.08±0.06 | 8.39±0.36 | 4.42±0.23 | 6.67±0.96 | 0.45±0.03 | 2.29±0.22 | 0.40±0.034 | 17.74±1.53 | 0.82±0.01 | | 0.22±0.14 |
| L548 | 2.37±0.15 | 8.95±0.63 | 7.12±0.57 | 10.74±1.68 | 0.51±0.08 | 2.42±0.31 | 0.50±0.052 | 13.72±1.52 | 0.32±0.15 | 8.95±0.03 | |
| K549 | 2.37±0.11 | 8.27±0.39 | 6.71±0.22 | 10.12±1.40 | 0.60±0.05 | 2.23±0.25 | 0.49±0.053 | 11.66±1.10 | 0.75±0.07 | | 6.85±2.35 |
| | | | | | | | | | (0.93±0.04) | | |
| Q550 | | | | | | | | | | | |
| G551 | 1.86±0.03 | 6.29±0.34 | 2.88±0.08 | 4.34±0.59 | 0.20±0.04 | 1.65±0.33 | 0.36±0.068 | 23.15±4.56 | 0.65±0.04 | | 0.73±0.16 |
| | | | | | | | | | (0.87±0.02) | | |
| H552 | 1.79±0.03 | 6.51±0.35 | 3.17±0.47 | 4.78±0.65 | 0.06±0.04 | 1.73±0.25 | 0.32±0.04 | 36.48±26.53 | 0.63±0.02 | | 0.19±0.02 |
| D553 | 1.45±0.03 | 4.51±0.12 | 2.04±0.53 | 3.08±0.90 | 0.13±0.05 | 1.16±0.41 | 0.26±0.094 | 19.50±6.93 | 0.59±0.03 | | 0.80±0.01 |
| | | | | | | | | | (0.68±0.01) | | |

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|------|-----------|-----------|-----------|-----------|-----------|-----------|------------|------------|--------------------------|-----------|
| Y554 | 1.13±0.01 | 2.96±0.05 | 1.57±0.04 | 2.37±0.32 | 0.22±0.02 | 0.73±0.07 | 0.21±0.021 | 13.71±1.74 | 0.46±0.01 (0.50±0.01) | 1.27±0.04 |
| W542 | 1.85±0.03 | 8.74±0.23 | 4.03±0.10 | 6.08±0.83 | 0.65±0.04 | 2.45±0.17 | 0.37±0.024 | 10.02±0.67 | | |
| (NH) | | | | | | | | | | |

^aErrors are fitting errors to the corresponding equations (see Materials and Methods).

^bErrors are determined by error propagation ³⁶.

^cErrors are determined by the noise level from two different experiments.

^cErrors are from Monte Carlo simulations.

Table 2: Experimental relaxation parameters, the reduced spectral density functions and the model-free parameters of SAMp73 at pH 7.0 and 288 K

| Residue | R_1 (s ⁻¹) ^a | R_2 (s ⁻¹) ^a | NOE ^b | $J(0)$ (ns rad ⁻¹) ^c | $J(\omega_N)$ (ns rad ⁻¹) ^c | $J(0.87\omega_H)$ (ps rad ⁻¹) ^c | S^2 (S_f^2) ^d | R_{ex} (s ⁻¹) ^d | τ_e (ns) ^d |
|---------|---------------------------------------|---------------------------------------|------------------|--|---|--|--------------------------------|--|----------------------------|
| Y487 | 1.99±0.09 | 6.63±0.55 | 0.43±0.15 | 1.77±1.50 | 0.57±0.43 | 17.48±8.22 | 0.20±0.01 | 5.80±0.24 | 2.51±0.12 |
| H488 | 1.92±0.01 | 7.34±0.08 | 0.63±0.10 | 1.99±0.15 | 0.38±0.06 | 10.99±1.90 | 0.87±0.03 | 1.30±0.34 | 0.08±0.05 |
| A489 | 1.94±0.04 | 5.82±0.21 | 0.65±0.32 | 1.51±0.75 | 0.38±0.19 | 10.54±5.24 | 0.82±0.01 | | 0.18±0.04 |
| D490 | 2.35±0.05 | 6.96±0.16 | 0.65±0.10 | 1.80±0.15 | 0.47±0.07 | 12.41±1.99 | 0.99±0.01 | 0.78±0.32 | |
| P491 | | | | | | | | | |
| S492 | 2.72±0.10 | 10.30±0.44 | 0.79±0.07 | 2.80±0.34 | 0.55±0.07 | 8.77±0.91 | 0.71±0.09 | 4.41±0.54 | 6.85±1.37 |
| L493 | 1.59±0.06 | 4.32±0.31 | 0.75±0.15 | 1.10±0.97 | 0.32±0.28 | 6.15±5.43 | 0.99±0.01 | | |
| V494 | 2.43±0.06 | 7.73±0.15 | 0.78±0.20 | 2.04±0.85 | 0.45±0.20 | 8.09±3.39 | 0.99±0.01 | | |
| S495 | 2.68±0.08 | 7.31±0.08 | 0.93±0.13 | 1.87±0.28 | 0.55±0.08 | 2.76±0.41 | 0.83±0.09 | 1.62±0.56 | 2.97±2.02 |
| F496 | 2.73±0.08 | 8.64±0.37 | 0.74±0.18 | 2.27±1.17 | 0.55±0.28 | 10.93±5.65 | 0.99±0.02 | | |
| L497 | 2.35±0.04 | 7.74±0.31 | 0.74±0.05 | 2.05±0.16 | 0.47±0.03 | 9.20±0.63 | 0.83±0.08 | 1.68±0.38 | 4.71±1.96 |

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|------|-----------|-----------|-----------|-----------|-----------|------------|-----------|-----------|-----------|
| T498 | 1.91±0.08 | 2.49±0.23 | 0.87±0.17 | 5.53±0.21 | 0.51±0.18 | 3.57±0.21 | 0.78±0.10 | 1.53±0.56 | 6.85±1.94 |
| G499 | 2.80±0.10 | 7.66±0.13 | 0.77±0.10 | 1.95±0.26 | 0.57±0.07 | 9.72±1.31 | 0.67±0.10 | 1.71±0.48 | 6.36±1.48 |
| L500 | 2.64±0.08 | 7.26±0.33 | 0.75±0.10 | 1.84±0.26 | 0.53±0.07 | 9.90±1.31 | 0.97±0.01 | | |
| G501 | 2.62±0.09 | 8.42±0.09 | 0.72±0.08 | 2.22±0.25 | 0.52±0.06 | 11.22±1.30 | 0.84±0.08 | 1.53±0.51 | 2.86±1.91 |
| C502 | 2.47±0.07 | 7.49±0.08 | 0.77±0.09 | 1.94±0.26 | 0.49±0.07 | 8.65±1.31 | 0.96±0.01 | | |
| P503 | | | | | | | | | |
| N504 | 2.50±0.06 | 6.77±0.12 | 0.83±0.07 | 1.73±0.26 | 0.52±0.07 | 6.43±0.65 | 0.99±0.01 | | |
| C505 | 2.60±0.09 | 6.35±0.08 | 0.96±0.12 | 1.58±0.22 | 0.54±0.07 | 1.52±0.21 | 0.99±0.02 | 0.27±0.20 | |
| I506 | 2.58±0.07 | 7.25±0.12 | 0.73±0.09 | 1.86±0.24 | 0.52±0.06 | 10.70±1.38 | 0.90±0.03 | | 1.01±0.68 |
| E507 | 1.39±0.05 | 3.85±0.22 | 0.46±0.16 | 0.97±0.57 | 0.27±0.21 | 11.54±9.01 | 0.68±0.04 | | 0.33±0.08 |
| Y508 | 2.21±0.04 | 3.81±0.12 | 0.81±0.16 | 1.16±0.88 | 0.85±0.08 | 6.37±0.03 | 0.99±0.01 | | |
| F509 | 1.93±0.04 | 44.3±7.76 | 0.76±0.23 | 1.36±0.24 | 0.41±0.18 | 9.93±1.83 | 0.99±0.02 | | |
| T510 | 2.79±0.08 | 7.20±0.26 | 0.63±0.10 | 1.82±0.65 | 0.58±0.02 | 16.03±0.15 | 0.52±0.10 | 3.98±0.79 | 3.59±1.44 |
| S511 | 2.59±0.09 | 6.13±0.29 | 0.74±0.05 | 1.54±0.68 | 0.58±0.02 | 9.93±0.15 | 0.99±0.02 | 1.79±0.45 | |
| Q512 | 2.59±0.08 | 7.36±0.08 | 0.93±0.10 | 1.90±0.22 | 0.54±0.06 | 2.60±0.30 | 0.60±0.08 | 4.08±0.51 | 1.78±0.28 |
| G513 | 2.60±0.08 | 6.98±0.15 | 0.77±0.12 | 1.77±0.29 | 0.52±0.08 | 9.03±1.49 | 0.99±0.02 | | |

| | | | | | | | | | |
|------|-----------|-----------|-----------|-----------|-----------|------------|-----------------------|-----------|-------------|
| L514 | 2.59±0.09 | 7.70±0.15 | 0.82±0.11 | 2.00±0.28 | 0.53±0.07 | 6.92±0.99 | 0.99±0.02 | | |
| Q515 | 2.41±0.23 | 4.71±0.30 | 0.76±0.06 | 1.12±1.03 | 0.54±0.39 | 8.97±0.67 | 0.70±0.12 | 1.65±0.62 | 4.53±1.73 |
| S516 | 2.59±0.06 | 7.01±0.10 | 0.72±0.11 | 1.78±0.28 | 0.52±0.08 | 10.93±1.74 | 0.91±0.03 | 0.80±0.31 | 0.34±0.21 |
| I517 | 0.74±0.04 | 0.69±0.07 | 0.77±0.14 | 0.17±0.09 | 0.27±0.15 | 9.03±1.40 | 0.46±0.02 (0.76±0.01) | | 0.96±0.06 |
| Y518 | | | | | | | | | |
| H519 | 2.72±0.12 | 2.94±0.25 | 0.76±0.25 | 0.54±0.20 | 0.65±0.24 | 8.97±3.02 | 0.99±0.01 | | |
| L520 | 2.64±0.08 | 7.97±0.18 | 0.62±0.11 | 2.07±0.37 | 0.52±0.09 | 15.59±2.82 | 0.52±0.09 | 4.56±0.60 | 2.17±0.31 |
| Q521 | 1.46±0.03 | 4.78±0.09 | 0.75±0.15 | 1.28±0.26 | 0.31±0.06 | 8.99±1.15 | 0.91±0.01 | | |
| N522 | 0.60±0.05 | 0.76±0.11 | 0.76±0.12 | 0.16±0.14 | 0.13±0.08 | 8.97±0.95 | 0.53±0.06 | | 0.38±0.09 |
| L523 | | | | | | | | | |
| T524 | 2.51±0.07 | 6.91±0.12 | 0.74±0.11 | 1.76±0.26 | 0.51±0.07 | 10.02±1.51 | 0.96±0.01 | | |
| I525 | 1.93±0.17 | 5.88±0.14 | 0.94±0.16 | 1.54±0.27 | 0.40±0.07 | 1.71±0.30 | 0.86±0.04 | | 6.85±2.16 |
| E526 | 2.11±0.02 | 5.14±0.19 | 0.70±0.11 | 1.27±0.25 | 0.42±0.06 | 9.57±1.51 | 0.84±0.16 | | 0.07±0.03 |
| D527 | 1.90±0.01 | 4.93±0.16 | 0.60±0.05 | 1.23±0.24 | 0.38±0.03 | 11.66±1.10 | 0.44±0.17 | 2.63±0.44 | 0.033±0.003 |
| L528 | 2.61±0.09 | 8.57±0.18 | 0.78±0.10 | 2.27±0.32 | 0.53±0.07 | 8.89±1.26 | 0.99±0.01 | 0.77±0.34 | |
| G529 | 2.65±0.08 | 7.40±0.15 | 0.82±0.11 | 1.90±0.27 | 0.54±0.07 | 7.15±1.00 | 0.99±0.01 | | |

| | | | | | | | | | |
|------|-----------|------------|-----------|-----------|------------|------------|-----------------------|-----------|-----------|
| A530 | 1.31±0.02 | 3.38±0.19 | 0.67±0.05 | 0.85±0.08 | 0.26±0.02 | 6.54±0.52 | 0.10±0.05 | | |
| L531 | 2.63±0.13 | 1.81±0.19 | 0.77±0.05 | 0.22±0.13 | 0.66±0.38 | 8.79±0.62 | 0.10±0.05 | | |
| K532 | 2.74±0.11 | 18.63±0.31 | 0.77±0.13 | 5.38±1.04 | 0.555±0.22 | 8.79±0.93 | 0.99±0.02 | | |
| I533 | 2.71±0.08 | 5.06 ±0.12 | 1.39±0.32 | 1.18±0.28 | 0.59±0.14 | | 0.70±0.10 (0.91±0.10) | | 6.85±2.75 |
| P534 | | | | | | | | | |
| E535 | 2.56±0.07 | 7.42±0.08 | 0.76±0.10 | 1.91±0.26 | 0.51±0.07 | 9.54±1.30 | 0.83±0.07 | 1.41±0.51 | 2.46±1.70 |
| Q536 | 2.63±0.07 | 7.80±0.14 | 0.74±0.09 | 2.02±0.25 | 0.53±0.06 | 10.41±1.51 | 0.81±0.06 | 1.42±0.46 | 3.17±1.73 |
| Y537 | 2.79±0.11 | 8.90±0.84 | 0.87±0.30 | 2.35±0.85 | 0.57±0.20 | 5.38±1.38 | 0.78±0.11 | 1.75±0.66 | 2.54±1.73 |
| R538 | 2.18±0.09 | 8.66±0.96 | 0.74±0.15 | 2.40±2.16 | 0.43±0.04 | 8.70±0.10 | 0.05±0.01 | | |
| M539 | 2.47±0.07 | 8.20±0.21 | 0.76±0.06 | 2.18±0.19 | 0.49±0.04 | 8.80±0.77 | 0.67±0.10 | 5.48±0.62 | 6.85±1.68 |
| T540 | 2.08±0.21 | 3.91±0.12 | 0.37±0.14 | 0.87±0.33 | 3.95±1.50 | 20.20±7.68 | 0.75±0.04 (0.94±0.19) | | 2.52±1.26 |
| I541 | 1.90±0.06 | 5.43±0.13 | 0.66±0.12 | 1.39±0.90 | 3.78±1.53 | 9.85±8.53 | 0.66±0.11 (0.77±0.09) | | 2.27±1.60 |
| W542 | 2.27±0.04 | 6.81±0.42 | 0.52±0.20 | 1.76±0.81 | 0.44±0.20 | 16.85±7.67 | 0.99±0.01 | | |
| R543 | 2.71±0.09 | 8.25±0.17 | 0.85±0.13 | 2.16±0.36 | 0.55±0.09 | 6.16±1.03 | 0.99±0.22 | 1.82±0.56 | 3.05±0.05 |
| G544 | 2.57±0.09 | 3.75±0.23 | 0.74±0.09 | 0.87±0.28 | 0.51±0.21 | 10.13±8.34 | 0.87±0.07 | 1.12±0.38 | 4.87±2.16 |
| L545 | 2.11±0.12 | 3.50±0.28 | 0.70±0.15 | 1.26±0.13 | 0.42±0.28 | 9.53±0.33 | 0.78±0.09 | 1.70±0.57 | 3.61±1.88 |

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|-----------|-----------|-----------|-----------|-----------|-----------|------------|-----------------------|-----------|
| Q546 | | | | | | | | |
| D547 | 2.60±0.07 | 5.59±0.13 | 0.48±0.17 | 1.35±0.21 | 0.50±0.08 | 20.61±0.89 | 0.82±0.01 | 0.22±0.18 |
| L548 | 2.66±0.09 | 9.44±0.12 | 0.58±0.06 | 2.52±0.30 | 0.52±0.06 | 17.13±2.05 | 0.010±0.005 | 8.95±0.15 |
| K549 | 2.73±0.10 | 3.66±0.18 | 1.66±0.74 | 0.75±0.25 | 0.62±0.20 | 28.43±9.35 | 0.74±0.08 (0.93±0.04) | 6.85±2.33 |
| Q550 | | | | | | | | |
| G551 | 2.07±0.13 | 5.33±0.10 | 0.30±0.07 | 1.32±0.32 | 0.38±0.09 | 22.43±5.45 | 0.65±0.05 (0.87±0.06) | 0.74±0.18 |
| H552 | 2.51±0.06 | 7.09±0.83 | 0.63±0.23 | 1.81±0.70 | 0.49±0.18 | 14.21±5.29 | 0.63±0.02 | 0.19±0.01 |
| D553 | 1.52±0.05 | 2.03±0.05 | 0.34±0.15 | 0.39±0.07 | 0.28±0.05 | 15.53±6.18 | 0.59±0.03 (0.68±0.01) | 0.80±0.01 |
| Y554 | 1.27±0.01 | 2.49±0.08 | 0.15±0.04 | 0.56±0.17 | 0.23±0.17 | 16.64±4.93 | 0.46±0.01 (0.49±0.01) | 1.27±0.04 |
| W542 (NH) | 1.97±0.02 | 5.89±0.37 | 0.72±0.08 | 1.78±0.19 | 0.46±0.04 | 8.46±0.93 | | |

^aErrors are fitting errors to the corresponding equations (see Materials and Methods).

^bErrors are determined by the noise level from two different experiments.

^cErrors are determined by error propagation ³⁶.

^dErrors are from Monte Carlo simulations.

Table 3: Experimental relaxation parameters, the reduced spectral density functions and the model-free parameters of SAMp73 at pH 7.0 and 308 K

| Residue | R_1 (s ⁻¹) | R_2 (s ⁻¹) | NOE | $J(0)$ (ns rad ⁻¹) | $J(\omega_N)$ (ns rad ⁻¹) | $J(0.87\omega_H)$ (ps rad ⁻¹) | S^2 (S_f^2) | R_{ex} (s ⁻¹) | τ_c (ns) |
|---------|--------------------------|--------------------------|-----------|--------------------------------|---------------------------------------|---|-------------------|-----------------------------|---------------|
| Y487 | 3.72±0.83 | 10.31±2.07 | 0.52±0.06 | 2.60±0.85 | 0.72±0.18 | 27.24±7.01 | 0.01±0.05 | 10.31±2.34 | 0.03±0.01 |
| H488 | 2.70±0.11 | 5.75±0.07 | 0.65±0.11 | 1.35±0.24 | 0.53±0.09 | 14.31±2.54 | 0.99±0.02 | 0.25±0.20 | |
| A489 | 2.36±0.18 | 7.21±0.48 | 0.58±0.04 | 1.86±0.28 | 0.46±0.05 | 15.23±1.55 | 0.88±0.06 | 1.63±0.62 | |
| D490 | 2.59±0.06 | 5.41±0.13 | 0.62±0.10 | 1.26±0.22 | 0.51±0.08 | 15.10±2.61 | 0.90±0.02 | 1.07±0.16 | |
| P491 | | | | | | | | | |
| S492 | 3.27±0.39 | 12.18±0.45 | 0.48±0.08 | 3.26±0.66 | 0.63±0.13 | 26.03±5.38 | 0.90±0.12 | 6.47±0.66 | 2.68±1.25 |
| L493 | 3.34±0.54 | 8.47±0.55 | 0.63±0.02 | 2.10±0.02 | 0.66±0.04 | 18.88±2.04 | 0.99±0.08 | 4.08±0.68 | 1.04±0.01 |
| V494 | 3.23±0.26 | 10.97±1.07 | 0.23±0.02 | 2.87±0.42 | 0.59±0.06 | 38.32±4.25 | 0.27±0.16 | 6.47±1.22 | 2.68±0.75 |
| S495 | 2.88±0.11 | 6.65±0.15 | 0.67±0.10 | 1.61±0.26 | 0.57±0.09 | 14.63±2.34 | 0.97±0.01 | | |
| F496 | 2.86±0.11 | 5.89±0.09 | 0.84±0.08 | 1.38±0.15 | 0.58±0.06 | 7.05±0.77 | 0.99±0.02 | 0.23±0.17 | 2.68±1.19 |
| L497 | 2.99±0.12 | 6.97±0.16 | 0.68±0.09 | 1.69±0.24 | 0.59±0.08 | 14.53±2.03 | 0.99±0.01 | | |
| T498 | 3.15±0.35 | 17.95±1.53 | 0.19±0.01 | 5.05±0.83 | 0.58±0.08 | 39.53±5.56 | 0.21±0.14 | 13.74±1.69 | 2.68±0.61 |

| | | | | | | | | | |
|------|-----------|------------|-----------|-----------|-----------|-------------|----------------------|------------|-----------|
| G499 | 3.21±0.14 | 10.93±0.58 | 0.44±0.01 | 2.88±0.12 | 0.61±0.03 | 27.32±1.08 | 0.90±0.10 | 4.78±0.72 | 2.68±1.23 |
| L500 | 2.77±0.13 | 9.98±0.44 | 0.33±0.01 | 2.65±0.20 | 0.52±0.01 | 28.63±1.54 | 0.59±0.12 | 5.16±0.53 | 2.68±0.94 |
| G501 | 2.78±0.15 | 6.81±0.19 | 0.56±0.02 | 1.67±0.81 | 0.54±0.06 | 18.93±3.45 | 0.82±0.04 | | 2.23±1.01 |
| C502 | 2.66±0.05 | 6.23±0.14 | 0.48±0.02 | 1.50±0.21 | 0.51±0.08 | 21.39±2.15 | 0.88±0.03 | | 0.41±0.36 |
| P503 | | | | | | | | | |
| N504 | 2.90±0.09 | 6.14±0.09 | 0.76±0.11 | 1.45±0.21 | 0.58±0.08 | 10.53±1.56 | 0.96±0.06(1.00±0.05) | | 2.68±1.12 |
| C505 | 2.73±0.11 | 9.08±0.25 | 0.34±0.08 | 2.37±0.62 | 0.51±0.13 | 27.73±7.29 | 0.50±0.16 | 3.87±0.66 | 2.68±0.90 |
| I506 | 2.64±0.13 | 9.16±0.32 | 0.36±0.09 | 2.48±0.62 | 0.50±0.12 | 25.59±6.95 | 0.94±0.04 | 4.23±0.40 | |
| E507 | 2.08±0.08 | 4.69±0.96 | 0.44±0.09 | 1.11±0.24 | 0.40±0.08 | 17.79±3.79 | 0.77±0.03 | | |
| Y508 | 2.80±0.12 | 8.72±0.38 | 0.62±0.01 | 2.26±0.99 | 0.55±0.06 | 16.44±5.01 | 0.99±0.03 | 2.70±0.47 | |
| F509 | 2.80±0.14 | 7.89±0.34 | 0.47±0.01 | 2.00±0.88 | 0.53±0.06 | 22.88±4.54 | 0.99±0.04 | 2.96±0.38 | |
| T510 | 3.28±0.20 | 6.67±0.12 | 0.61±0.06 | 1.54±0.42 | 0.64±0.10 | 19.77±4.18 | 0.99±0.12 | 2.11±0.24 | 2.68±1.17 |
| S511 | 2.58±0.10 | 5.06±0.08 | 0.73±0.15 | 1.16±0.24 | 0.51±0.10 | 10.41±2.17 | 0.95±0.13 | | |
| Q512 | 2.77±0.11 | 6.48±0.13 | 0.60±0.02 | 1.57±0.88 | 0.54±0.08 | 16.86±5.45 | 1.00±0.02 | 0.600±0.16 | 1.81±1.23 |
| G513 | 3.14±0.42 | 10.00±0.71 | 0.39±0.15 | 2.59±2.18 | 0.59±0.37 | 29.31±18.53 | 0.99±0.09 | 4.29±1.11 | |
| L514 | 3.39±0.37 | 24.12±2.21 | 0.28±0.06 | 6.96±6.63 | 0.63±0.60 | 37.38±29.31 | 0.54±0.16 | 20.08±2.18 | 2.68±0.84 |

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|------|-----------|------------|-----------|-----------|-----------|-------------|-----------------------|-----------|-----------|
| Q515 | 3.05±0.11 | 7.04±0.18 | 0.62±0.12 | 1.70±0.34 | 0.60±0.12 | 17.71±3.60 | 0.99±0.10 | 1.82±0.28 | 2.68±1.16 |
| S516 | 2.80±0.08 | 7.31±0.17 | 0.70±0.10 | 1.83±0.28 | 0.55±0.08 | 12.81±2.05 | 0.99±0.01 | | |
| I517 | 1.55±0.17 | 2.81±0.10 | 0.37±0.03 | 0.61±0.09 | 0.29±0.04 | 15.10±2.22 | 0.42±0.01 | | 0.27±0.03 |
| Y518 | | | | | | | | | |
| H519 | 3.20±0.23 | 16.04±1.09 | 0.29±0.15 | 4.47±0.05 | 0.60±0.05 | 35.03±2.93 | 0.99±0.04 | 4.88±0.77 | |
| L520 | | | | | | | | | |
| Q521 | 2.84±0.11 | 11.65±0.74 | 0.46±0.08 | 3.16±0.62 | 0.54±0.10 | 23.78±4.43 | 0.99±0.02 | | |
| N522 | 2.18±0.41 | 4.37±0.40 | 0.62±0.05 | 1.56±0.83 | 0.66±0.44 | 19.68±12.33 | 1.25±0.26 (0.67±0.06) | | 2.68±1.18 |
| L523 | | | | | | | | | |
| T524 | 2.53±0.11 | 7.06±0.15 | 0.52±0.09 | 1.79±0.33 | 0.49±0.09 | 18.44±3.42 | 0.93±0.04 | 0.95±0.29 | |
| I525 | 3.39±0.38 | 11.35±1.75 | 0.39±0.04 | 2.98±0.65 | 0.64±0.10 | 31.66±4.95 | 0.81±0.09 | 6.09±1.64 | 2.68±1.21 |
| E526 | 2.19±0.06 | 7.05±0.51 | 0.17±0.01 | 1.82±0.19 | 0.40±0.03 | 28.04±2.24 | 0.69±0.18 | 2.96±0.51 | 0.14±0.02 |
| D527 | 2.43±0.07 | 6.06±0.13 | 0.78±0.08 | 1.50±0.16 | 0.49±0.05 | 8.23±0.90 | 0.90±0.01 | | |
| L528 | 2.80±0.14 | 8.74±0.32 | 0.53±0.08 | 2.27±0.39 | 0.54±0.09 | 20.18±3.39 | 0.99±0.03 | 2.68±0.44 | |
| G529 | 2.91±0.10 | 7.66±0.21 | 0.47±0.05 | 1.91±0.28 | 0.56±0.06 | 23.61±2.74 | 0.99±0.03 | 2.55±0.25 | 1.06±0.21 |
| A530 | 1.07±0.13 | 3.90±0.17 | 0.86±0.08 | 1.04±0.16 | 0.21±0.03 | 2.21±0.33 | 1.45±0.47 (0.42±0.03) | | 2.68±0.99 |

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|------|-----------|------------|-----------|-----------|-----------|------------|-----------------------|------------|-----------|
| L531 | 3.06±0.17 | 15.61±0.93 | 0.19±0.01 | 4.37±0.47 | 0.56±0.05 | 38.14±3.46 | 0.26±0.21 | 11.68±1.10 | 2.68±0.91 |
| K532 | 2.82±0.15 | 12.05±0.23 | 0.55±0.02 | 3.30±0.86 | 0.55±0.06 | 19.59±4.50 | 0.99±0.03 | 6.40±0.27 | 1.21±0.99 |
| I533 | 3.34±0.44 | 3.52 ±0.09 | 0.90±0.06 | 0.57±0.15 | 0.68±0.05 | 5.00±1.49 | 1.56±0.57 (0.63±0.03) | | 2.68±1.07 |
| P534 | | | | | | | | | |
| E535 | 2.98±0.17 | 11.51±0.39 | 0.32±0.01 | 3.10±0.25 | 0.56±0.04 | 31.49±2.37 | 0.40±0.13 | 6.27±0.75 | 2.68±0.76 |
| Q536 | 3.04±0.12 | 6.93±0.22 | 0.63±0.14 | 1.67±0.40 | 0.60±0.14 | 17.14±4.09 | 0.99±0.03 | 0.57±0.42 | 2.14±1.20 |
| Y537 | 2.61±0.27 | 6.61±0.09 | 0.53±0.17 | 1.63±0.29 | 0.50±0.19 | 18.93±3.27 | 0.99±0.06 | 0.46±0.30 | |
| R538 | | | | | | | | | |
| M539 | 2.99±0.12 | 7.83±0.17 | 0.69±0.11 | 1.96±0.34 | 0.59±0.10 | 14.09±2.47 | 0.99±0.06 | 1.62±0.29 | |
| T540 | 2.99±0.19 | 6.80±0.40 | 0.54±0.12 | 1.63±0.40 | 0.58±0.14 | 21.31±5.13 | 0.99±0.02 | 1.35±0.51 | |
| I541 | 1.88±0.16 | 6.61±0.59 | 0.34±0.05 | 1.74±0.35 | 0.35±0.06 | 19.10±3.41 | 0.61±0.05 | 2.35±0.67 | 0.06±0.02 |
| W542 | 3.13±0.30 | 6.60±0.26 | 0.74±0.12 | 1.56±0.31 | 0.62±0.12 | 12.10±2.42 | 0.98±0.03 | | |
| R543 | 2.89±0.11 | 5.93±0.08 | 0.74±0.09 | 1.38±0.19 | 0.58±0.08 | 11.41±1.61 | 0.96±0.12 | | |
| G544 | 3.11±0.14 | 17.11±0.83 | 0.17±0.01 | 4.81±0.45 | 0.57±0.04 | 39.81±3.14 | 0.68±0.21 | 12.26±0.97 | 0.95±0.77 |
| L545 | 3.15±0.57 | 5.44±0.53 | 0.68±0.12 | 1.18±0.32 | 0.62±0.15 | 15.45±3.90 | 0.70±0.06 | | |
| Q546 | | | | | | | | | |

| | | | | | | | | | |
|-----------|-----------|------------|-----------|-----------|-----------|-------------|-----------------------|-----------|-------------|
| D547 | 2.36±0.04 | 3.96±0.18 | 0.42±0.09 | 0.84±0.18 | 0.45±0.09 | 21.02±4.47 | 0.80±0.12 | | |
| L548 | 2.88±0.10 | 6.84±0.19 | 0.59±0.05 | 1.66±0.18 | 0.56±0.05 | 17.95±1.85 | 0.99±0.02 | 0.44±0.27 | |
| K549 | 2.78±0.15 | 7.94±0.27 | 0.56±0.06 | 2.03±0.27 | 0.54±0.07 | 18.61±2.43 | 0.97±0.04 | 1.50±0.45 | |
| Q550 | | | | | | | | | |
| G551 | 1.83±0.04 | 5.64±0.21 | 0.16±0.01 | 1.44±0.14 | 0.33±0.03 | 23.81±21.51 | 0.56±0.01 | 2.86±0.22 | 0.064±0.004 |
| H552 | 1.47±0.10 | 4.38±0.17 | 0.78±0.28 | 1.13±0.16 | 0.30±0.04 | 8.23±5.08 | 1.60±0.72 (0.50±0.35) | | 2.68±0.60 |
| D553 | 1.76±0.04 | 4.82±0.08 | 0.75±0.13 | 1.22±0.22 | 0.35±0.06 | 6.61±1.19 | 0.65±0.01 | | |
| Y554 | 0.98±0.02 | 6.43±0.29 | 0.34±0.06 | 1.84±0.34 | 0.18±0.03 | 10.06±1.80 | 0.31±0.07 | 4.76±0.29 | 0.012±0.003 |
| W542 (NH) | 2.24±0.13 | 10.50±0.38 | 0.34±0.07 | 3.42±0.65 | 0.49±0.09 | 22.61±5.02 | | | |

^aErrors are fitting errors to the corresponding equations (see Materials and Methods).

^bErrors are determined by the noise level from two different experiments.

^cErrors are determined by error propagation ³⁶.

^dErrors are from Monte Carlo simulations.

Table 4: Experimental relaxation parameters, the reduced spectral density functions and the model-free parameters of SAMp73 at pH 7.0 and 313 K

| Residue | R_1 (s ⁻¹) ^a | R_2 (s ⁻¹) ^a | NOE ^b | $J(0)$ (ns rad ⁻¹) ^c | $J(\omega_N)$ (ns rad ⁻¹) ^c | $J(0.87\omega_H)$ (ps rad ⁻¹) ^c | S^2 (S_f^2) ^c | R_{ex} (s ⁻¹) ^d | τ_e (ns) ^d | C_p (J mol ⁻¹ K ⁻¹) ^{a,e} |
|---------|---------------------------------------|---------------------------------------|------------------|--|---|---|--------------------------------|--|----------------------------|--|
| Y487 | 2.18±0.35 | 3.03±1.05 | 0.54±0.05 | 0.59±0.58 | 0.40±0.35 | 15.54±14.83 | 0.21±0.02 | 3.11±1.32 | 0.21±0.01 | |
| H488 | 3.10±0.09 | 5.17±0.07 | 0.61±0.04 | 1.10±0.09 | 0.61±0.05 | 18.63±1.32 | 0.98±0.02 | 0.20±0.12 | 0.63±0.20 | |
| A489 | | | | | | | | | | |
| D490 | 2.69±0.05 | 4.56±0.12 | 0.56±0.05 | 0.98±0.08 | 0.52±0.04 | 18.15±1.56 | 0.82±0.05 | | 2.26±0.51 | |
| | | | | | | | (1.00±0.04) | | | |
| P491 | | | | | | | | | | |
| S492 | 3.24±0.12 | 10.20±0.31 | 0.57±0.06 | 2.65±0.33 | 0.63±0.07 | 21.53±2.63 | 1.00±0.03 | 5.32±0.32 | 2.26±0.93 | |
| L493 | 2.57±0.13 | 5.23±0.41 | 0.08±0.01 | 1.18±0.04 | 0.46±0.06 | 36.66±2.56 | 0.69±0.05 | 0.97±0.43 | 0.70±0.33 | |
| V494 | 1.35±0.07 | 3.61±0.26 | 0.12±0.01 | 1.12±0.89 | 0.36±0.24 | 18.43±12.25 | 0.41±0.02 | 1.00±0.31 | 0.05±0.004 | |
| S495 | 3.23±0.09 | 6.89±0.13 | 0.54±0.04 | 1.62±0.13 | 0.62±0.05 | 22.91±1.82 | 1.00±0.02 | 1.95±0.16 | 1.24±0.93 | |
| F496 | 3.12±0.10 | 5.76±0.13 | 0.53±0.04 | 1.28±0.10 | 0.60±0.04 | 22.31±1.67 | 1.00±0.04 | 0.87±0.18 | 2.26±1.02 | |

| | | | | | | | | | | |
|------|-----------|------------|-------------|-----------|-----------|-------------|-------------|-----------|-----------|------------|
| L497 | 3.36±0.10 | 5.55±0.14 | 0.70±0.04 | 1.18±0.09 | 0.67±0.05 | 15.39±1.12 | 1.00±0.03 | 0.89±0.18 | 0.65±0.01 | |
| T498 | 1.70±0.19 | 3.92±0.54 | 0.67±0.14 | 0.94±0.54 | 0.33±0.19 | 8.50±4.80 | 0.61±0.05 | | | |
| G499 | 3.28±0.26 | 10.36±1.07 | 0.43±0.18 | 2.68±1.98 | 0.62±0.27 | 28.92±12.41 | 1.00±0.05 | 4.78±1.14 | | |
| L500 | 3.28±0.48 | 6.89±0.22 | 0.42±0.015 | 1.60±0.12 | 0.62±0.12 | 29.16±6.35 | 1.00±0.05 | 1.88±0.36 | 1.76±0.95 | |
| G501 | 3.15±0.12 | 8.63±0.35 | 0.092±0.006 | 2.15±0.22 | 0.64±0.14 | 44.23±1.50 | 0.69±0.05 | 4.36±0.35 | 0.69±0.30 | |
| C502 | 2.88±0.09 | 8.54±0.38 | 0.28±0.09 | 2.18±1.24 | 0.54±0.34 | 32.15±4.56 | 0.77±0.09 | 3.57±0.43 | 2.26±0.98 | |
| P503 | | | | | | | | | | |
| N504 | 3.22±0.08 | 5.73±0.16 | 0.72±0.05 | 1.27±0.10 | 0.64±0.05 | 13.08±1.05 | 1.00±0.03 | 0.81±0.71 | 2.26±0.98 | |
| C505 | 2.97±0.11 | 10.35±0.17 | 0.15±0.07 | 2.72±1.28 | 0.54±0.25 | 38.93±18.25 | 0.47±0.14 | 5.18±0.67 | 2.26±0.82 | |
| I506 | 3.07±0.17 | 10.98±0.77 | 0.28±0.09 | 2.91±0.99 | 0.57±0.19 | 34.16±11.39 | 0.86±0.07 | 6.03±0.86 | 0.68±0.56 | |
| E507 | 2.47±0.05 | 4.20±0.06 | 0.49±0.05 | 0.90±0.09 | 0.47±0.05 | 19.12±1.88 | 0.87±0.07 | | 2.26±0.70 | |
| | | | | | | | (0.94±0.02) | | | |
| Y508 | 2.89±0.08 | 5.94±0.11 | 0.62±0.15 | 1.38±0.78 | 0.57±0.02 | 16.64±6.56 | 1.00±0.11 | 1.08±0.25 | 2.26±0.92 | |
| F509 | 3.22±0.17 | 9.27±1.36 | 0.59±0.14 | 2.36±0.10 | 0.63±0.03 | 20.15±2.34 | 1.00±0.03 | 3.36±1.32 | | |
| T510 | 3.35±0.20 | 6.85±0.14 | 0.51±0.09 | 1.58±0.90 | 0.65±0.16 | 25.15±4.10 | 1.00±0.07 | 2.06±0.24 | 0.89±0.64 | -397 ± 100 |

| | | | | | | | | | |
|------|-----------|------------|-----------|-----------|-----------|-------------|-------------|-----------|-----------|
| S511 | 2.71±0.01 | 5.20±0.10 | 0.58±0.05 | 1.18±0.11 | 0.53±0.05 | 17.31±1.67 | 0.91±0.04 | | 2.26±0.60 |
| | | | | | | | (1.00±0.07) | | |
| Q512 | 3.01±0.10 | 8.96±0.37 | 0.16±0.05 | 2.28±0.05 | 0.55±0.38 | 39.05±1.82 | 0.91±0.05 | 4.58±0.38 | 0.70±0.53 |
| G513 | 3.05±0.14 | 5.37±0.13 | 0.60±0.15 | 1.17±0.67 | 0.60±0.26 | 18.61±2.12 | 1.00±0.05 | 0.46±0.33 | 0.99±0.32 |
| L514 | | | | | | | | | |
| Q515 | 3.08±0.08 | 6.13±0.12 | 0.43±0.05 | 1.40±0.17 | 0.59±0.07 | 26.93±3.34 | 1.00±0.02 | 1.35±0.15 | 1.00±0.82 |
| S516 | 3.12±0.08 | 6.87±0.22 | 0.45±0.04 | 1.62±0.19 | 0.59±0.06 | 26.55±2.99 | 0.26±0.03 | | 2.26±0.12 |
| | | | | | | | (1.00±0.23) | | |
| I517 | 0.54±0.05 | 2.45±0.11 | 0.76±0.09 | 0.84±0.68 | 0.13±0.11 | 2.42±1.96 | 0.23±0.01 | | |
| Y518 | | | | | | | | | |
| H519 | | | | | | | | | |
| L520 | | | | | | | | | |
| Q521 | 2.73±0.25 | 11.38±1.92 | 0.44±0.12 | 3.15±1.51 | 0.52±0.24 | 23.42±10.85 | 1.00±0.14 | 6.30±1.92 | 1.31±0.99 |
| N522 | | | | | | | | | |
| L523 | | | | | | | | | |
| T524 | 2.87±0.09 | 7.00±0.16 | 0.36±0.04 | 1.70±0.10 | 0.68±0.54 | 28.34±3.52 | 0.88±0.04 | 1.98±0.19 | 0.70±0.47 |

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|------|-----------|------------|-----------|-----------|-----------|------------|-------------|-----------|---------------|-----------|
| I525 | 0.70±0.11 | 1.42±0.30 | 0.32±0.02 | 0.40±0.32 | 0.18±0.13 | 9.74±7.42 | 1.00±0.34 | | 2.28±0.94 | |
| | | | | | | | (0.26±0.03) | | | |
| E526 | 0.61±0.06 | 2.35±0.26 | 0.15±0.01 | 0.63±0.50 | 0.13±0.10 | 8.07±5.07 | 0.21±0.02 | 1.20±0.01 | 0.0009±0.0001 | |
| D527 | 2.76±0.05 | 5.33±0.14 | 0.71±0.03 | 1.21±0.08 | 0.55±0.03 | 12.23±0.69 | 1.00±0.09 | | 2.26±0.97 | |
| | | | | | | | (0.91±0.03) | | | |
| L528 | 3.11±0.14 | 8.75±0.38 | 0.25±0.05 | 2.20±0.48 | 0.58±0.12 | 35.57±7.72 | 1.00±0.06 | 2.89±0.44 | 2.26±0.97 | |
| G529 | 3.07±0.09 | 5.50±0.15 | 0.55±0.03 | 1.21±0.09 | 0.62±0.04 | 21.14±1.46 | 1.00±0.01 | | | |
| A530 | 1.73±0.05 | 3.93±0.123 | 0.52±0.03 | 0.94±0.08 | 0.33±0.02 | 12.61±0.76 | 0.61±0.13 | | | |
| L531 | | | | | | | | | | |
| K532 | 3.26±0.14 | 10.61±0.09 | 0.51±0.15 | 2.72±0.06 | 0.63±0.08 | 24.48±0.75 | 1.00±0.16 | 5.01±0.48 | 0.97±0.39 | |
| I533 | 3.17±0.13 | 5.41 ±0.06 | 0.68±0.04 | 1.18±0.08 | 0.63±0.04 | 15.44±1.21 | 0.99±0.01 | | | |
| P534 | | | | | | | | | | |
| E535 | 2.70±0.12 | 8.29±0.87 | 0.72±0.03 | 2.15±1.06 | 0.54±0.26 | 11.39±5.46 | 1.00±0.23 | | | |
| Q536 | 3.26±0.08 | 6.71±0.29 | 0.56±0.09 | 1.56±0.26 | 0.63±0.10 | 21.81±3.61 | 1.00±0.10 | 1.77±0.36 | 2.26±0.94 | -243 ± 24 |
| Y537 | 3.14±0.11 | 9.19±0.30 | 0.16±0.04 | 2.33±0.10 | 0.57±0.08 | 40.96±4.65 | 0.87±0.07 | 4.64±0.33 | 2.26±1.02 | |
| R538 | | | | | | | | | | |

| | | | | | | | | | | |
|------|-----------|-----------|-----------|-----------|-----------|------------|-------------|-----------|-----------|----------|
| M539 | 3.28±0.10 | 6.21±0.16 | 0.70±0.05 | 1.42±0.12 | 0.65±0.08 | 14.83±1.30 | 1.00±0.02 | 1.09±0.19 | 2.26±0.96 | |
| T540 | 2.80±0.08 | 3.63±0.15 | 0.53±0.19 | 0.67±0.13 | 0.54±0.11 | 20.23±0.34 | 0.40±0.09 | | 2.26±0.43 | |
| | | | | | | | (1.03±0.05) | | | |
| I541 | 1.98±0.21 | 5.15±0.87 | 0.32±0.09 | 1.27±1.11 | 0.37±0.35 | 20.96±5.15 | 0.68±0.06 | | 0.07±0.06 | |
| W542 | 3.17±0.32 | 5.06±0.12 | 0.67±0.09 | 1.06±0.15 | 0.63±0.08 | 16.21±2.26 | 0.91±0.02 | | | 213 ± 72 |
| R543 | 3.22±0.09 | 5.27±0.06 | 0.63±0.04 | 1.12±0.08 | 0.63±0.05 | 18.29±1.21 | 1.00±0.02 | 0.14±0.10 | 1.21±0.97 | |
| G544 | 1.53±0.20 | 2.88±0.73 | 0.10±0.06 | 0.63±0.45 | 0.27±0.20 | 21.43±0.24 | 0.48±0.05 | | 0.06±0.01 | |
| L545 | 0.79±0.11 | 3.51±0.32 | 0.65±0.14 | 1.33±0.97 | 0.22±0.15 | 4.29±1.14 | 0.28±0.04 | 1.36±0.42 | | |
| Q546 | | | | | | | | | | |
| D547 | 2.54±0.06 | 3.44±0.08 | 0.57±0.04 | 0.65±0.05 | 0.49±0.04 | 16.8±1.37 | 0.71±0.05 | | 2.26±0.36 | |
| | | | | | | | (0.84±0.02) | | | |
| L548 | 3.17±0.10 | 8.91±0.35 | 0.33±0.03 | 2.24±0.22 | 0.59±0.05 | 32.71±3.04 | 0.72±0.08 | 4.07±0.39 | 2.26±0.93 | |
| K549 | 3.19±0.12 | 9.22±0.20 | 0.35±0.05 | 2.34±0.33 | 0.60±0.08 | 31.98±4.49 | 0.77±0.07 | 4.11±0.27 | 2.26±0.99 | |
| Q550 | | | | | | | | | | |
| G551 | 1.66±0.44 | 6.49±0.31 | 0.19±0.09 | 1.74±0.08 | 0.30±0.14 | 20.81±9.77 | 0.67±0.17 | 2.95±1.00 | | |
| H552 | | | | | | | | | | |

| | | | | | | | | |
|-----------|-----------|------------|-----------|-----------|-----------|-------------|-------------|-----------|
| D553 | 2.43±0.02 | 5.07±0.11 | 0.49±0.04 | 1.18±0.10 | 0.47±0.04 | 18.98±1.55 | 0.68±0.03 | 2.26±0.27 |
| | | | | | | | (0.92±0.12) | |
| Y554 | 1.03±0.08 | 10.61±0.66 | 0.76±0.08 | 3.15±0.49 | 0.20±0.03 | 3.82±0.54 | 0.36±0.03 | 8.46±0.66 |
| W542 (NH) | 2.28±0.30 | 10.53±1.84 | 0.27±0.11 | 3.39±1.34 | 0.50±0.18 | 25.71±11.23 | | |

^aErrors are fitting errors to the corresponding equations (see Materials and Methods).

^bErrors are determined by the noise level from two different experiments.

^cErrors are determined by error propagation ³⁶.

^dErrors are from Monte Carlo simulations.

^eObtained from the slope of a straight line of the S_{conf} versus $\text{Ln}(T)$.

Table 5: Experimental relaxation parameters, the reduced spectral density functions and the model-free parameters of SAMp73 at pH 7.0, 298 K and 1 M GdmCl.

| Residue | R_1 (s ⁻¹) ^a | R_2 (s ⁻¹) ^a | NOE ^c | $J(0)$ (ns rad ⁻¹) ^b | $J(\omega_N)$ (ns rad ⁻¹) ^b | $J(0.87\omega_H)$ (ps rad ⁻¹) ^b | S^2 (S_f^2) ^d | R_{ex} (s ⁻¹) ^d | τ_c (ns) ^d |
|---------|---------------------------------------|---------------------------------------|------------------|---|--|--|--------------------------------|--|----------------------------|
| Y487 | 2.16±0.07 | 5.34±0.14 | 0.36±0.04 | 1.31±0.17 | 0.41±0.05 | 21.38±2.37 | 0.17±0.02 | 2.75±0.19 | 3.00±0.23 |
| H488 | 2.30±0.08 | 7.24±0.21 | 0.66±0.06 | 1.90±0.19 | 0.46±0.04 | 12.11±1.20 | 0.86±0.19 | | |
| A489 | 2.14±0.04 | 5.73±0.10 | 0.44±0.05 | 1.45±0.16 | 0.41±0.04 | 18.49±2.09 | 0.69±0.03 (0.86±0.02) | | 1.17±0.22 |
| D490 | 2.75±0.22 | 8.16±0.10 | 0.72±0.05 | 2.11±0.24 | 0.55±0.06 | 11.76±1.37 | 1.00±0.01 | | |
| P491 | | | | | | | | | |
| S492 | 2.74±0.10 | 10.17±0.32 | 0.71±0.04 | 2.75±0.19 | 0.55±0.03 | 12.12±0.77 | 1.00±0.02 | | |
| L493 | 2.87±0.14 | 8.43±0.20 | 0.64±0.10 | 2.18±0.38 | 0.57±0.12 | 16.02±2.81 | 1.00±0.03 | | |
| V494 | 2.75±0.12 | 9.25±0.31 | 0.49±0.05 | 2.45±0.30 | 0.53±0.06 | 21.66±2.60 | 0.39±0.20 | 3.80±0.79 | 2.60±0.69 |
| S495 | 2.21±0.07 | 7.61±0.15 | 0.61±0.04 | 2.03±0.16 | 0.43±0.03 | 13.17±1.06 | 0.79±0.03 | 1.06±0.25 | 0.06±0.02 |
| F496 | 2.86±0.12 | 8.90±0.20 | 0.69±0.08 | 2.33±0.28 | 0.57±0.06 | 13.66±1.66 | 0.55±0.20 | 1.99±0.80 | 5.26±1.14 |
| L497 | 2.65±0.10 | 8.42±0.06 | 0.75±0.03 | 2.22±0.12 | 0.53±0.03 | 10.07±0.56 | 1.00±0.01 | | |
| T498 | 2.68±0.12 | 8.09±0.18 | 0.71±0.06 | 2.10±0.19 | 0.54±0.05 | 12.08±1.06 | 0.98±0.01 | | |

| | | | | | | | | | |
|------|-----------|-----------|-----------|-----------|-----------|------------|-----------|-----------|-----------|
| G499 | 2.78±0.13 | 7.97±0.11 | 0.72±0.06 | 2.05±0.19 | 0.56±0.05 | 12.18±1.15 | 0.96±0.10 | | |
| L500 | 2.71±0.10 | 8.31±0.34 | 0.67±0.05 | 2.17±0.21 | 0.54±0.05 | 13.92±1.28 | 1.00±0.01 | | |
| G501 | 2.63±0.09 | 8.28±0.14 | 0.72±0.06 | 2.17±0.19 | 0.53±0.04 | 11.47±1.01 | 1.00±0.01 | | |
| C502 | 2.43±0.10 | 7.20±0.11 | 0.66±0.04 | 1.86±0.14 | 0.48±0.03 | 12.86±0.94 | 0.88±0.01 | | 0.24±0.09 |
| P503 | | | | | | | | | |
| N504 | 2.80±0.21 | 7.73±0.12 | 0.72±0.05 | 1.97±0.21 | 0.56±0.06 | 12.02±1.30 | 0.94±0.01 | | |
| C505 | 2.48±0.11 | 8.16±0.11 | 0.72±0.05 | 2.16±0.17 | 0.49±0.04 | 10.56±0.86 | 0.98±0.01 | | |
| I506 | 2.55±0.10 | 7.18±0.10 | 0.66±0.04 | 1.84±0.13 | 0.50±0.03 | 13.16±0.95 | 0.88±0.01 | | 0.20±0.09 |
| E507 | 1.00±0.41 | 3.09±0.10 | 0.21±0.04 | 0.80±0.36 | 0.18±0.08 | 12.30±0.56 | 0.35±0.01 | | 0.04±0.01 |
| Y508 | 2.54±0.08 | 8.64±0.15 | 0.72±0.05 | 2.30±0.17 | 0.51±0.03 | 10.80±0.79 | 1.00±0.01 | | |
| F509 | 2.72±0.11 | 8.07±0.22 | 0.68±0.05 | 2.09±0.18 | 0.54±0.04 | 13.31±1.09 | 1.00±0.01 | | |
| T510 | 2.99±0.11 | 8.75±0.21 | 0.66±0.05 | 2.26±0.12 | 0.59±0.05 | 15.61±1.41 | 0.38±0.19 | 2.60±0.63 | 5.26±0.27 |
| S511 | 2.56±0.13 | 9.52±0.20 | 0.67±0.05 | 2.57±0.23 | 0.51±0.04 | 13.18±1.17 | 0.96±0.04 | 1.51±0.44 | |
| Q512 | 2.70±0.13 | 7.77±0.28 | 0.57±0.05 | 1.99±0.21 | 0.53±0.05 | 18.01±1.86 | 0.88±0.04 | | 0.70±0.64 |
| G513 | 2.60±0.10 | 7.72±0.09 | 0.65±0.05 | 2.00±0.17 | 0.51±0.04 | 14.25±1.21 | 0.90±0.02 | | 1.09±0.87 |
| L514 | 2.66±0.09 | 8.23±0.11 | 0.64±0.05 | 2.15±0.19 | 0.53±0.04 | 14.77±1.29 | 0.88±0.11 | 0.89±0.44 | 1.24±1.16 |

| | | | | | | | | | |
|------|-----------|------------|-----------|-----------|-----------|------------|-----------------------|-------------|-----------|
| Q515 | 2.36±0.11 | 6.49±0.15 | 0.56±0.04 | 1.65±1.48 | 0.46±0.04 | 15.97±1.38 | 0.78±0.01 | 0.009±0.002 | |
| S516 | 2.36±0.13 | 7.68±0.83 | 0.72±0.05 | 2.05±0.55 | 0.55±0.12 | 10.80±0.79 | 0.88±0.04 | | |
| I517 | 1.58±0.03 | 2.97±0.06 | 0.10±0.03 | 0.68±0.17 | 0.29±0.07 | 22.12±5.93 | 0.36±0.03 (0.66±0.12) | 1.26±0.08 | |
| Y518 | | | | | | | | | |
| H519 | 2.59±0.09 | 8.01±0.08 | 0.58±0.05 | 2.09±0.19 | 0.51±0.04 | 16.74±1.55 | 0.88±0.09 | 1.04±0.34 | 0.72±0.29 |
| L520 | 2.93±0.14 | 10.10±0.40 | 0.31±0.04 | 2.67±0.41 | 0.55±0.08 | 31.09±4.63 | 0.16±0.08 | 6.38±0.57 | 2.61±0.83 |
| Q521 | 2.19±0.08 | 8.61±0.12 | 0.48±0.04 | 2.34±0.21 | 0.42±0.04 | 17.63±1.60 | 0.78±0.03 | 1.77±0.28 | 0.13±0.07 |
| N522 | 1.63±0.04 | 3.66±0.11 | 0.03±0.02 | 1.19±0.86 | 0.41±0.29 | 25.08±3.47 | 0.47±0.04 (0.72±0.02) | 0.95±0.09 | |
| L523 | | | | | | | | | |
| T524 | 2.66±0.23 | 7.54±0.13 | 0.68±0.05 | 1.93±0.22 | 0.53±0.06 | 13.14±1.50 | 0.90±0.01 | | |
| I525 | 2.55±0.10 | 7.48±0.16 | 0.73±0.08 | 1.94±0.23 | 0.51±0.06 | 10.34±1.25 | 0.91±0.02 | | |
| E526 | 2.31±0.07 | 6.48±0.22 | 0.69±0.06 | 1.66±0.17 | 0.46±0.04 | 11.01±1.11 | 0.82±0.02 | | |
| D527 | 2.60±0.13 | 9.38±0.38 | 0.79±0.05 | 2.53±0.22 | 0.52±0.04 | 8.17±0.62 | 0.96±0.04 | 1.49±0.52 | |
| L528 | 2.53±0.09 | 8.46±0.16 | 0.68±0.05 | 2.24±0.18 | 0.50±0.04 | 12.37±1.00 | 1.00±0.01 | | |
| G529 | 2.47±0.14 | 7.69±0.23 | 0.91±0.05 | 2.02±0.17 | 0.51±0.04 | 3.50±0.29 | 1.10±0.07 (0.89±0.04) | 5.26±2.21 | |
| A530 | 2.45±0.09 | 10.56±0.23 | 0.74±0.05 | 2.92±0.22 | 0.49±0.03 | 9.77±0.72 | 0.90±0.03 | 3.21±0.34 | |

| | | | | | | | | | |
|------|-----------|------------|-----------|-----------|-----------|------------|-----------------------|-----------|-----------|
| L531 | 2.46±0.09 | 7.94±0.09 | 0.69±0.05 | 2.09±0.17 | 0.49±0.04 | 11.67±0.95 | 0.95±0.01 | | |
| K532 | 2.58±0.09 | 17.53±0.40 | 0.61±0.06 | 5.09±0.56 | 0.51±0.05 | 15.64±1.70 | 0.89±0.11 | 9.96±0.64 | 0.99±0.65 |
| I533 | 2.50±0.13 | 7.04±0.24 | 0.85±0.05 | 1.81±0.16 | 0.51±0.04 | 5.77±0.47 | 0.89±0.02 | | |
| P534 | | | | | | | | | |
| E535 | 2.86±0.21 | 7.94±0.10 | 0.68±0.06 | 2.03±0.26 | 0.57±0.06 | 14.01±1.55 | 0.98±0.01 | | |
| Q536 | 2.87±0.20 | 8.02±0.10 | 0.74±0.04 | 2.05±0.19 | 0.58±0.05 | 11.18±1.09 | 0.94±0.01 | | |
| Y537 | 2.69±0.11 | 8.60±0.07 | 0.52±0.04 | 2.25±0.20 | 0.52±0.05 | 19.90±1.78 | 0.48±0.16 | 2.59±0.63 | 2.52±0.64 |
| R538 | 2.57±0.12 | 8.41±0.12 | 0.68±0.05 | 2.22±0.21 | 0.51±0.04 | 12.70±1.19 | 0.94±0.04 | 0.79±0.36 | |
| M539 | 2.98±0.23 | 11.73±0.25 | 0.79±0.08 | 3.20±0.42 | 0.60±0.08 | 9.74±1.28 | 0.88±0.20 | 4.00±0.66 | 5.26±2.21 |
| T540 | 2.63±0.14 | 8.23±0.11 | 0.73±0.05 | 2.16±0.20 | 0.53±0.04 | 10.84±1.00 | 1.00±0.02 | | |
| I541 | 2.01±0.07 | 4.42±0.10 | 0.17±0.04 | 1.04±0.25 | 0.37±0.09 | 25.95±6.36 | 0.50±0.04 (0.84±0.02) | | 1.09±0.13 |
| W542 | 2.39±0.16 | 7.35±0.28 | 0.62±0.05 | 1.91±0.22 | 0.47±0.05 | 14.05±1.54 | 0.88±0.04 | | 0.76±0.14 |
| R543 | 2.83±0.27 | 8.52±0.21 | 0.71±0.06 | 2.22±0.29 | 0.56±0.07 | 12.43±1.62 | 1.00±0.02 | | |
| G544 | 2.59±0.11 | 8.21±0.11 | 0.74±0.06 | 2.16±0.17 | 0.52±0.04 | 10.22±0.80 | 1.00±0.01 | | |
| L545 | 2.49±0.14 | 6.94±0.30 | 0.65±0.05 | 1.77±0.18 | 0.49±0.04 | 13.54±1.02 | 0.87±0.03 | | |
| Q546 | | | | | | | | | |

| | | | | | | | | | |
|-----------|-----------|------------|-----------|-----------|-----------|-------------|-----------------------|-----------|-----------|
| D547 | 2.28±0.04 | 7.42±0.18 | 0.26±0.02 | 1.94±0.19 | 0.43±0.04 | 26.06±2.55 | 0.72±0.01 | 1.32±0.20 | 0.26±0.02 |
| L548 | 2.51±0.11 | 6.33±0.39 | 0.92±0.06 | 1.59±0.17 | 0.52±0.04 | 2.98±0.27 | 0.86±0.11 (0.87±0.04) | | 5.26±2.05 |
| K549 | 2.61±0.11 | 6.75±0.05 | 0.78±0.06 | 1.70±0.15 | 0.53±0.05 | 8.69±0.79 | 0.76±0.07 (0.91±0.03) | | 5.26±1.49 |
| Q550 | | | | | | | | | |
| G551 | 1.96±0.03 | 4.58±0.08 | 0.09±0.02 | 1.09±0.33 | 0.35±0.10 | 27.76±8.41 | 0.57±0.02 (0.85±0.01) | | 0.73±0.08 |
| H552 | 1.80±0.12 | 12.42±0.96 | 0.12±0.10 | 3.75±3.06 | 0.33±0.31 | 24.45±23.56 | 0.57±0.03 | 7.35±0.98 | 0.12±0.03 |
| D553 | 1.56±0.07 | 5.61±0.18 | 0.24±0.04 | 1.49±0.29 | 0.29±0.05 | 18.43±3.57 | 0.50±0.03 | 1.42±0.25 | 0.07±0.01 |
| Y554 | 1.13±0.02 | 2.32±0.03 | 0.24±0.01 | 0.53±0.04 | 2.13±0.18 | 13.45±1.15 | 0.47±0.02 (0.46±0.07) | | 1.30±0.06 |
| W542 (NH) | 2.36±0.21 | 6.27±0.10 | 0.52±0.03 | 1.85±0.17 | 0.54±0.05 | 17.41±1.93 | | | |

^aErrors are fitting errors to the corresponding equations (see Materials and Methods).

^bErrors are determined by error propagation ³⁶.

^cErrors are determined by the noise level from two different experiments.

^dErrors are from Monte Carlo simulations.

Table 6: Experimental relaxation parameters, the reduced spectral density functions and the model-free parameters of SAMp73 at pH 7.0, 298 K and 0.5 M GdmCl.

| Residue | R_1 (s ⁻¹) ^a | R_2 (s ⁻¹) ^a | NOE ^b | $J(0)$ (ns rad ⁻¹) ^c | $J(\omega_N)$ (ns rad ⁻¹) ^c | $J(0.87\omega_H)$ (ps rad ⁻¹) ^c | S^2 (S_f^2) ^d | R_{ex} (s ⁻¹) ^d | τ_e (ns) ^d | m_{s_i} (cal mol ⁻¹ K ⁻¹ M ⁻¹) ^{a,e} |
|---------|---------------------------------------|---------------------------------------|------------------|--|---|---|--------------------------------|--|----------------------------|--|
| Y487 | 2.01±0.03 | 7.56±0.06 | 0.32±0.03 | 2.03±0.22 | 0.38±0.04 | 21.06±2.30 | 0.21±0.01 | 5.63±0.09 | 2.45±0.10 | |
| H488 | 1.97±0.05 | 9.81±0.17 | 0.74±0.08 | 2.76±0.30 | 0.39±0.04 | 7.71±0.83 | 0.91±0.01 | | | |
| A489 | 1.95±0.05 | 8.12±0.13 | 0.44±0.05 | 2.22±0.25 | 0.37±0.04 | 17.08±1.95 | 0.75±0.02 (0.92±0.02) | | 0.98±0.16 | |
| D490 | 2.15±0.05 | 11.17±0.17 | 0.71±0.05 | 3.16±0.23 | 0.43±0.03 | 9.65±0.78 | 0.96±0.02 | 1.02±0.30 | | |
| P491 | | | | | | | | | | |
| S492 | 2.40±0.07 | 15.79±0.20 | 0.56±0.03 | 4.56±0.28 | 0.47±0.03 | 16.49±1.00 | 0.64±0.07 | 7.95±0.47 | 1.98±0.30 | |
| L493 | 2.39±0.09 | 11.44±0.37 | 0.79±0.13 | 3.21±0.55 | 0.48±0.08 | 7.62±1.29 | 0.83±0.11 | 1.77±0.78 | 7.38±2.58 | -6.79±1.90 |
| V494 | 2.36±0.09 | 13.24±0.16 | 0.32±0.17 | 3.76±0.88 | 0.45±0.10 | 24.95±5.84 | 0.42±0.19 | 7.12±1.45 | 1.59±0.41 | |
| S495 | 2.23±0.06 | 10.64±0.12 | 0.69±0.05 | 2.98±0.25 | 0.44±0.04 | 10.84±0.91 | 0.93±0.05 | 0.88±0.37 | 0.99±0.90 | |
| F496 | 2.38±0.08 | 11.26±0.51 | 0.84±0.08 | 3.14±0.35 | 0.49±0.05 | 5.76±0.59 | 1.00±0.01 | | | |

| | | | | | | | | | | |
|------|------------|------------|-----------|-----------|-----------|------------|-----------|------------|-------------|------------|
| L497 | 2.29±0.07 | 12.49±0.14 | 0.56±0.03 | 3.54±0.21 | 0.45±0.03 | 15.36±0.89 | 0.73±0.07 | 4.08±0.50 | 1.57±0.39 | |
| T498 | 2.26±0.06 | 10.65±0.24 | 0.76±0.06 | 2.98±0.25 | 0.45±0.04 | 8.21±0.68 | 1.00±0.01 | | | -6.79±2.84 |
| G499 | 2.48±0.09 | 11.4±0.12 | 0.64±0.05 | 3.20±0.30 | 0.49±0.05 | 13.68±1.30 | 0.66±0.09 | 3.13±0.60 | 2.79±1.04 | |
| L500 | 2.23±0.09 | 17.21±0.58 | 0.21±0.04 | 5.03±1.19 | 0.41±0.09 | 27.25±6.39 | 0.43±0.10 | 11.05±0.92 | 1.33±0.21 | |
| G501 | 2.30±0.08 | 12.28±0.15 | 0.47±0.05 | 3.47±0.36 | 0.44±0.05 | 18.91±1.99 | 0.62±0.09 | 4.62±0.65 | 1.56±0.33 | |
| C502 | 2.11±0.05 | 10.73±0.16 | 0.56±0.04 | 3.02±0.23 | 0.41±0.03 | 14.44±1.10 | 0.88±0.02 | 1.34±0.28 | 0.26±0.25 | |
| P503 | | | | | | | | | | |
| N504 | 2.22±0.06 | 10.36±0.18 | 0.83±0.05 | 2.90±0.21 | 0.45±0.03 | 5.82±0.42 | 0.98±0.01 | | | |
| C505 | 2.21±0.06 | 10.89±0.15 | 0.58±0.04 | 3.06±0.24 | 0.43±0.03 | 14.32±1.12 | 0.78±0.06 | 1.86±0.48 | 1.44±0.40 | |
| I506 | 2.20±0.06 | 10.07±0.14 | 0.65±0.04 | 2.80±0.20 | 0.43±0.03 | 11.84±0.84 | 0.94±0.01 | | 0.51±0.39 | |
| E507 | 0.929±0.07 | 4.13±0.05 | 0.13±0.04 | 1.13±0.34 | 0.17±0.05 | 12.56±3.76 | 0.38±0.01 | | 0.044±0.001 | |
| Y508 | 2.30±0.07 | 13.77±0.30 | 0.28±0.04 | 3.93±0.58 | 0.43±0.06 | 25.68±3.80 | 0.42±0.08 | 7.57±0.56 | 1.50±0.15 | |
| F509 | 2.45±0.08 | 11.74±0.88 | 0.43±0.04 | 3.27±0.42 | 0.47±0.05 | 21.69±2.26 | 0.44±0.08 | 5.23±0.96 | 1.92±0.19 | |
| T510 | 2.48±0.07 | 12.41±0.17 | 0.61±0.05 | 3.49±0.34 | 0.49±0.05 | 14.91±1.45 | 0.62±0.08 | 4.51±0.60 | 2.49±0.58 | 0.68±0.39 |
| S511 | 2.27±0.07 | 14.07±0.24 | 0.48±0.05 | 4.04±0.41 | 0.44±0.05 | 18.34±1.86 | 0.67±0.08 | 6.16±0.61 | 1.44±0.31 | |
| Q512 | 2.29±0.08 | 15.57±0.40 | 0.23±0.07 | 4.50±1.36 | 0.42±0.12 | 27.39±8.26 | 0.38±0.10 | 9.68±0.86 | 1.47±0.16 | |

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|------|-----------|------------|-----------|-----------|-----------|-------------|-------------|------------|-----------|-----------|
| G513 | 2.27±0.06 | 11.67±0.30 | 0.41±0.04 | 3.28±0.38 | 0.43±0.05 | 20.62±2.38 | 0.60±0.07 | 4.29±0.57 | 1.41±0.21 | |
| L514 | 2.32±0.08 | 12.64±0.19 | 0.38±0.05 | 3.58±0.46 | 0.44±0.05 | 22.09±2.81 | 0.51±0.09 | 5.80±0.66 | 1.56±0.21 | |
| Q515 | 2.40±0.08 | 10.62±0.14 | 0.64±0.05 | 2.94±0.25 | 0.47±0.04 | 13.20±1.13 | 0.69±0.08 | 2.07±0.55 | 2.46±0.73 | |
| S516 | 2.09±0.05 | 10.43±0.12 | 0.74±0.05 | 2.94±0.22 | 0.42±0.03 | 8.51±0.64 | 0.97±0.01 | | | |
| I517 | 1.59±0.05 | 4.16±0.05 | 0.04±0.02 | 1.03±0.59 | 0.28±0.16 | 23.71±13.76 | 0.39±0.02 | | 1.11±0.04 | 0.36±0.23 |
| | | | | | | | (0.74±0.01) | | | |
| Y518 | | | | | | | | | | |
| H519 | 2.31±0.08 | 11.90±0.15 | 0.58±0.06 | 3.36±0.14 | 0.45±0.05 | 15.16±1.86 | 0.74±0.09 | 3.45±0.64 | 1.63±0.58 | |
| L520 | 2.57±0.13 | 16.24±1.02 | 0.34±0.11 | 4.67±1.62 | 0.48±0.16 | 26.12±8.92 | 0.23±0.06 | 11.18±1.47 | 2.01±0.29 | 3.04±0.39 |
| Q521 | 1.96±0.04 | 11.8±0.32 | 0.36±0.03 | 3.40±0.33 | 0.37±0.03 | 19.33±1.79 | 0.80±0.01 | 2.96±0.33 | 2.69±0.09 | |
| N522 | 1.66±0.06 | 4.80±0.75 | 0.07±0.03 | 1.22±0.65 | 0.30±0.16 | 24.03±12.99 | 0.43±0.10 | | 1.10±0.21 | |
| | | | | | | | (0.78±0.05) | | | |
| L523 | | | | | | | | | | |
| T524 | 2.07±0.05 | 10.52±0.11 | 0.68±0.05 | 2.97±0.23 | 0.41±0.03 | 10.19±0.80 | 0.96±0.01 | | | 2.78±2.03 |
| I525 | 2.41±0.09 | 12.27±0.15 | 0.54±0.08 | 3.45±0.53 | 0.47±0.07 | 17.21±2.65 | 0.56±0.11 | 4.58±0.82 | 2.16±0.61 | |
| E526 | 2.10±0.06 | 9.56±0.24 | 0.74±0.07 | 2.66±0.28 | 0.42±0.04 | 8.51±0.87 | 0.92±0.01 | | | |

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|------|-----------|------------|-----------|-----------|-----------|-------------|-------------|------------|-----------|------------|
| D527 | 2.20±0.08 | 12.55±0.24 | 0.78±0.04 | 3.59±0.25 | 0.44±0.03 | 7.55±0.50 | 1.00±0.02 | 1.68±0.45 | | |
| L528 | 2.17±0.06 | 11.61±0.18 | 0.74±0.05 | 3.30±0.24 | 0.43±0.03 | 8.53±0.61 | 1.05±0.01 | 0.77±0.35 | | |
| G529 | 2.22±0.08 | 10.16±0.14 | 0.83±0.03 | 2.84±0.15 | 0.45±0.02 | 5.77±0.30 | 0.96±0.01 | | | |
| A530 | 2.21±0.06 | 13.72±0.25 | 0.85±0.05 | 3.96±0.26 | 0.45±0.03 | 4.97±0.31 | 0.97±0.02 | 3.00±0.37 | | |
| L531 | 2.27±0.08 | 13.11±0.16 | 0.41±0.05 | 3.74±0.39 | 0.43±0.04 | 20.70±2.16 | 0.55±0.07 | 5.71±0.56 | 1.56±0.21 | |
| K532 | 2.27±0.06 | 19.82±0.66 | 0.43±0.06 | 5.85±0.90 | 0.43±0.06 | 20.09±3.02 | 0.58±0.07 | 12.27±0.84 | 1.55±0.19 | |
| I533 | 2.18±0.06 | 9.72±0.18 | 0.81±0.03 | 2.70±0.14 | 0.44±0.02 | 6.43±0.32 | 0.94±0.14 | | | |
| P534 | | | | | | | | | | |
| E535 | 2.27±0.06 | 10.89±0.18 | 0.67±0.06 | 3.05±0.29 | 0.45±0.04 | 11.43±1.09 | 0.84±0.07 | 1.52±0.53 | 1.77±1.20 | |
| Q536 | 2.27±0.05 | 10.95±0.17 | 0.71±0.05 | 3.07±0.21 | 0.45±0.03 | 10.04±0.64 | 0.86±0.06 | 1.24±0.46 | 2.21±1.61 | |
| Y537 | 2.34±0.08 | 13.77±0.44 | 0.21±0.04 | 3.92±0.89 | 0.43±0.09 | 28.71±6.44 | 0.30±0.08 | 8.37±0.72 | 1.56±0.12 | |
| R538 | 2.28±0.08 | 13.46±0.43 | 0.14±0.04 | 3.83±1.31 | 0.42±0.14 | 30.30±10.31 | 0.33±0.10 | 8.19±0.82 | 1.38±0.17 | |
| M539 | 2.41±0.08 | 15.49±0.37 | 0.86±0.08 | 4.48±0.46 | 0.49±0.05 | 5.18±0.52 | 0.83±0.09 | 5.87±0.65 | 7.38±2.27 | -1.89±0.78 |
| T540 | 2.36±0.08 | 12.43±0.20 | 0.56±0.05 | 3.50±0.34 | 0.46±0.04 | 15.91±1.55 | 0.66±0.09 | 4.39±0.63 | 1.87±0.38 | |
| I541 | 1.94±0.05 | 6.49±0.12 | 0.29±0.04 | 1.70±0.26 | 0.35±0.05 | 21.52±3.33 | 0.59±0.02 | | 1.11±0.10 | 0.79±0.35 |
| | | | | | | | (0.89±0.19) | | | |

| | | | | | | | | | | |
|------|-----------|------------|-----------|-----------|-----------|------------|-------------|-----------|-------------|------------|
| W542 | 2.23±0.06 | 9.83±0.22 | 0.89±0.09 | 2.73±0.31 | 0.46±0.05 | 3.61±0.40 | 0.96±0.02 | | | 5.28±0.27 |
| R543 | 2.36±0.08 | 11.34±0.12 | 0.76±0.06 | 3.18±0.29 | 0.47±0.04 | 8.68±0.79 | 0.87±0.08 | 1.64±0.50 | 4.46±2.49 | |
| G544 | 2.29±0.07 | 11.43±0.13 | 0.78±0.05 | 3.22±0.23 | 0.46±0.03 | 7.82±5.47 | 0.89±0.06 | 1.25±0.39 | 7.38±2.34 | |
| L545 | 2.08±0.05 | 8.24±0.30 | 0.11±0.03 | 2.22±0.63 | 0.38±0.10 | 28.68±8.04 | 0.55±0.08 | 1.49±0.62 | 0.89±0.18 | |
| Q546 | | | | | | | | | | |
| D547 | 2.17±0.07 | 7.25±0.43 | 0.63±0.09 | 1.92±0.31 | 0.43±0.06 | 12.28±1.89 | 0.65±0.07 | | 2.57±1.80 | |
| | | | | | | | (0.88±0.04) | | | |
| L548 | 2.20±0.07 | 9.50±0.16 | 0.86±0.04 | 2.63±0.15 | 0.45±0.02 | 4.56±0.24 | 0.87±0.0 | | 7.38±2.34 | -4.40±2.68 |
| | | | | | | | (0.94±0.02) | | | |
| K549 | 2.37±0.08 | 10.48±0.10 | 0.64±0.04 | 2.90±0.24 | 0.47±0.04 | 13.21±1.09 | 0.74±0.08 | 1.73±0.51 | 2.31±0.66 | |
| Q550 | | | | | | | | | | |
| G551 | 1.83±0.05 | 6.16±0.09 | 0.14±0.03 | 1.62±0.35 | 0.33±0.07 | 24.38±5.24 | 0.59±0.02 | | 0.82±0.07 | 0.30±0.20 |
| | | | | | | | (0.87±0.02) | | | |
| H552 | 1.85±0.03 | 8.41±0.08 | 0.22±0.06 | 2.32±0.68 | 0.34±0.10 | 22.49±6.65 | 0.72±0.02 | 0.40±0.18 | 0.21±0.03 | |
| D553 | 1.52±0.06 | 6.63±0.06 | 0.26±0.05 | 1.82±0.04 | 0.28±0.06 | 17.59±3.86 | 0.61±0.01 | | 0.09±0.01 | |
| Y554 | 1.10±0.04 | 6.21±0.26 | 0.18±0.02 | 1.76±0.12 | 0.20±0.02 | 13.99±1.58 | 0.42±0.16 | 1.66±0.29 | 0.048±0.003 | |

W542 (NH) 1.70±0.03 8.99±0.10 0.60±0.04 2.98±0.17 0.36±0.02 10.45±0.68

^aErrors are fitting errors to the corresponding equations (see Materials and Methods).

^bErrors are determined by the noise level from two different experiments.

^cErrors are determined by error propagation ³⁶.

^dErrors are from Monte Carlo simulations.

^eObtained from the slope of a straight line of the S_{conf} versus [GdmCl].

Table 7: Experimental relaxation parameters, the reduced spectral density functions and the model-free parameters of SAMp73 at pH 7.0, 298 K and 0.25 M GdmCl.

| Residue | R_1 (s ⁻¹) ^a | R_2 (s ⁻¹) ^a | NOE ^b | $J(0)$ (ns rad ⁻¹) ^c | $J(\omega_N)$ (ns rad ⁻¹) ^c | $J(0.87\omega_H)$ (ps rad ⁻¹) ^c | S^2 (S_f^2) ^d | R_{ex} (s ⁻¹) ^d | τ_c (ns) ^d |
|---------|---------------------------------------|---------------------------------------|------------------|---|--|--|--------------------------------|--|----------------------------|
| Y487 | 2.01±0.03 | 8.03±0.10 | 0.40±0.02 | 2.18±0.19 | 0.38±0.02 | 18.79±0.99 | 0.23±0.01 | 6.18±0.12 | 2.73±0.01 |
| H488 | 2.02±0.05 | 10.42±0.16 | 0.76±0.09 | 2.95±0.15 | 0.41±0.02 | 7.60±0.39 | 0.93±0.01 | | |
| A489 | 1.91±0.02 | 8.84±0.09 | 0.46±0.02 | 2.45±0.13 | 0.37±0.19 | 16.15±0.86 | 0.78±0.01(0.94±0.01) | | 0.91±0.07 |
| D490 | 2.16±0.16 | 12.54±0.17 | 0.74±0.03 | 3.59±0.18 | 0.43±0.22 | 8.58±0.43 | 0.90±0.09 | 1.99±0.53 | 2.35±2.30 |
| P491 | | | | | | | | | |
| S492 | 2.34±0.07 | 15.08±0.26 | 0.75±0.01 | 4.36±0.19 | 0.47±0.02 | 10.07±0.39 | 0.80±0.08 | 5.24±0.72 | 4.61±2.57 |
| L493 | 2.37±0.08 | 12.36±0.32 | 0.86±0.6 | 3.50±0.27 | 0.48±0.04 | 5.28±0.39 | 0.74±0.08 | 2.42±0.58 | 7.94±2.23 |
| V494 | 2.25±0.06 | 12.41±0.28 | 0.59±0.03 | 3.53±0.23 | 0.44±0.28 | 14.21±0.89 | 0.73±0.05 | 3.50±0.46 | 1.74±0.29 |
| S495 | 2.20±0.05 | 10.54±0.14 | 0.64±0.02 | 2.98±0.14 | 0.40±0.02 | 11.43±0.53 | 0.83±0.04 | 0.92±0.33 | 1.62±0.39 |
| F496 | 2.31±0.10 | 12.82±0.26 | 0.86±0.03 | 3.67±0.24 | 0.47±0.03 | 4.97±0.31 | 0.88±0.08 | 2.20±0.47 | 7.94±2.78 |
| L497 | 2.26±0.07 | 12.80±0.06 | 0.69±0.01 | 3.65±0.14 | 0.45±0.02 | 10.72±0.42 | 0.81±0.05 | 3.13±0.34 | 2.32±0.58 |
| T498 | 2.25±0.06 | 11.30±0.34 | 0.71±0.03 | 3.18±0.18 | 0.45±0.02 | 9.97±0.50 | 0.84±0.05 | 1.44±0.49 | 2.41±1.00 |

| | | | | | | | | | |
|------|-----------|------------|-----------|-----------|-----------|------------|-----------------------|-----------|-----------|
| G499 | 2.38±0.08 | 12.39±0.14 | 0.66±0.03 | 3.50±0.19 | 0.47±0.03 | 12.37±0.68 | 0.69±0.07 | 3.49±0.44 | 2.71±0.57 |
| L500 | 2.13±0.06 | 12.73±0.15 | 0.48±0.02 | 3.64±0.23 | 0.41±0.03 | 17.13±1.07 | 0.71±0.06 | 3.91±0.45 | 1.26±0.26 |
| G501 | 2.25±0.07 | 12.53±0.15 | 0.64±0.02 | 3.57±0.18 | 0.45±0.02 | 12.45±0.64 | 0.76±0.05 | 3.21±0.40 | 2.00±0.40 |
| C502 | 2.05±0.05 | 11.06±0.10 | 0.65±0.02 | 3.14±0.14 | 0.41±0.02 | 11.09±0.50 | 0.92±0.02 | 0.74±0.22 | 0.36±0.24 |
| P503 | | | | | | | | | |
| N504 | 2.16±0.06 | 11.60±0.13 | 0.74±0.02 | 3.29±0.15 | 0.44±0.02 | 8.60±0.39 | 0.90±0.04 | 1.03±0.31 | 2.42±1.23 |
| C505 | 2.15±0.06 | 12.11±0.16 | 0.65±0.02 | 3.45±0.18 | 0.43±0.02 | 11.76±0.58 | 0.83±0.05 | 2.19±0.38 | 1.61±0.48 |
| I506 | 2.10±0.06 | 11.17±0.16 | 0.76±0.03 | 3.17±0.16 | 0.42±0.02 | 7.85±0.39 | 0.99±0.08 | | |
| E507 | 1.13±0.03 | 4.36±0.08 | 0.17±0.02 | 1.18±0.13 | 0.21±0.02 | 14.51±1.62 | 0.62±0.02 (0.56±0.01) | | 0.81±0.07 |
| Y508 | 2.21±0.06 | 12.62±0.16 | 0.81±0.02 | 3.61±0.18 | 0.45±0.02 | 6.44±0.31 | 0.89±0.05 | 1.84±0.33 | 7.94±2.50 |
| F509 | 2.41±0.09 | 11.47±0.57 | 0.65±0.03 | 3.21±0.24 | 0.48±0.03 | 12.99±0.73 | 0.65±0.07 | 2.76±0.07 | 2.82±0.05 |
| T510 | 2.52±0.09 | 12.89±0.21 | 0.62±0.03 | 3.64±0.23 | 0.50±0.03 | 14.69±0.91 | 0.54±0.04 | 4.95±0.51 | 2.91±0.04 |
| S511 | 2.15±0.09 | 14.23±0.12 | 0.72±0.03 | 4.12±0.24 | 0.43±0.02 | 9.26±0.53 | 1.00±0.02 | 3.01±0.47 | |
| Q512 | 2.27±0.09 | 12.40±0.15 | 0.51±0.02 | 3.52±0.23 | 0.44±0.03 | 17.11±1.10 | 0.61±0.07 | 4.17±0.55 | 1.79±0.28 |
| G513 | 2.21±0.07 | 11.60±0.18 | 0.67±0.02 | 3.28±0.18 | 0.44±0.02 | 11.19±0.58 | 0.83±0.05 | 1.86±0.39 | 1.88±0.58 |
| L514 | 2.25±0.07 | 12.42±0.12 | 0.68±0.02 | 3.53±0.18 | 0.45±0.02 | 10.95±0.56 | 0.78±0.05 | 2.73±0.37 | 2.38±0.50 |

| | | | | | | | | | |
|------|-----------|------------|-----------|-----------|-----------|------------|-----------------------|-----------|-----------|
| Q515 | 2.29±0.10 | 11.91±0.19 | 0.70±0.02 | 3.37±0.20 | 0.46±0.03 | 10.48±0.62 | 0.78±0.08 | 2.24±0.49 | 2.82±0.83 |
| S516 | 1.98±0.08 | 11.65±0.19 | 0.67±0.02 | 3.34±0.19 | 0.39±0.02 | 10.15±0.55 | 0.91±0.03 | 1.37±0.36 | 0.33±0.13 |
| I517 | 1.61±0.03 | 4.30±0.07 | 0.05±0.01 | 1.06±0.33 | 0.29±0.09 | 23.90±7.39 | 0.37±0.01 (0.75±0.01) | | 1.17±0.02 |
| Y518 | | | | | | | | | |
| H519 | 2.18±0.07 | 12.72±0.15 | 0.60±0.03 | 3.64±0.21 | 0.43±0.02 | 13.40±0.78 | 0.78±0.06 | 3.35±0.46 | 1.52±0.40 |
| L520 | 2.49±0.10 | 14.31±0.23 | 0.33±0.03 | 4.07±0.45 | 0.47±0.05 | 25.93±2.85 | 0.27±0.09 | 8.85±0.68 | 1.88±0.16 |
| Q521 | 1.90±0.03 | 10.02±0.36 | 0.67±0.03 | 2.84±0.15 | 0.37±0.01 | 9.75±0.39 | 0.88±0.01 | | 0.09±0.02 |
| N522 | 1.70±0.03 | 5.10±0.09 | 0.08±0.02 | 1.30±0.34 | 0.31±0.08 | 24.32±6.42 | 0.42±0.01 (0.81±0.01) | | 1.15±0.03 |
| L523 | | | | | | | | | |
| T524 | 2.04±0.06 | 11.31±0.16 | 0.73±0.03 | 3.22±0.17 | 0.41±0.02 | 8.63±0.43 | 0.98±0.01 | | |
| I525 | 2.28±0.08 | 12.10±0.23 | 0.82±0.04 | 3.43±0.24 | 0.46±0.03 | 6.18±0.41 | 0.78±0.07 | 1.65±0.47 | 7.94±2.14 |
| E526 | 2.03±0.05 | 10.28±0.31 | 0.66±0.03 | 2.90±0.18 | 0.40±0.02 | 10.72±0.59 | 0.90±0.02 | | 0.92±0.44 |
| D527 | 2.36±0.17 | 13.67±0.95 | 0.71±0.02 | 3.91±0.41 | 0.47±0.03 | 10.66±0.84 | 0.72±0.13 | 4.17±1.18 | 3.61±1.51 |
| L528 | 2.16±0.07 | 13.20±0.19 | 0.80±0.03 | 3.80±0.21 | 0.43±0.03 | 6.72±0.35 | 0.89±0.06 | 2.19±0.37 | 7.94±2.58 |
| G529 | 2.10±0.08 | 11.67±0.15 | 0.86±0.03 | 3.34±0.16 | 0.44±0.01 | 4.93±0.31 | 1.00±0.05 | 0.43±0.25 | 5.83±3.35 |
| A530 | 2.11±0.07 | 13.84±0.40 | 0.74±0.02 | 4.00±0.21 | 0.42±0.02 | 8.28±0.38 | 0.94±0.04 | 3.07±0.46 | 1.44±1.19 |

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|------|-----------|------------|-----------|-----------|-----------|------------|-----------------------|------------|-----------|
| L531 | 2.11±0.07 | 12.81±0.08 | 0.55±0.02 | 3.68±0.18 | 0.41±0.02 | 14.67±0.73 | 0.76±0.05 | 3.36±0.43 | 1.35±0.35 |
| K532 | 2.22±0.07 | 19.99±0.45 | 0.66±0.03 | 5.92±0.37 | 0.44±0.03 | 11.70±0.69 | 0.76±0.07 | 10.27±0.73 | 2.24±1.14 |
| I533 | 2.08±0.09 | 11.36±0.20 | 0.80±0.08 | 3.24±0.18 | 0.43±0.02 | 6.72±0.49 | 1.00±0.10 | | |
| P534 | | | | | | | | | |
| E535 | 2.24±0.05 | 11.78±0.18 | 0.67±0.02 | 3.34±0.16 | 0.45±0.02 | 11.31±0.54 | 0.80±0.04 | 2.17±0.33 | 2.09±0.35 |
| Q536 | 2.19±0.04 | 11.91±0.17 | 0.72±0.02 | 3.38±0.13 | 0.44±0.02 | 9.46±0.36 | 0.86±0.03 | 1.65±0.24 | 2.35±0.65 |
| Y537 | 2.27±0.08 | 12.87±0.09 | 0.61±0.03 | 3.67±0.23 | 0.45±0.03 | 13.73±0.87 | 0.69±0.06 | 3.81±0.46 | 2.13±0.35 |
| R538 | 2.25±0.07 | 12.28±0.11 | 0.63±0.03 | 3.49±0.19 | 0.44±0.02 | 12.90±0.70 | 0.76±0.06 | 3.05±0.43 | 1.91±0.41 |
| M539 | 2.33±0.09 | 16.41±0.31 | 0.87±0.04 | 4.78±0.31 | 0.48±0.03 | 4.44±0.28 | 0.84±0.05 | 6.13±0.51 | 7.99±2.38 |
| T540 | 2.28±0.06 | 12.81±0.18 | 0.61±0.02 | 3.65±0.19 | 0.45±0.02 | 13.67±0.68 | 0.71±0.05 | 3.87±0.35 | 2.01±0.26 |
| I541 | 1.97±0.05 | 6.82±0.10 | 0.21±0.02 | 1.80±0.22 | 0.36±0.04 | 24.33±3.03 | 0.55±0.02 (0.94±0.17) | | 1.07±0.05 |
| W542 | 2.18±0.09 | 11.47±0.28 | 0.75±0.03 | 3.25±0.20 | 0.44±0.03 | 8.44±0.53 | 0.99±0.01 | | |
| R543 | 2.25±0.08 | 12.37±0.14 | 0.77±0.03 | 3.52±0.25 | 0.46±0.02 | 7.92±0.45 | 0.88±0.07 | 2.05±0.39 | 4.97±2.48 |
| G544 | 2.23±0.07 | 12.44±0.13 | 0.79±0.02 | 3.55±0.17 | 0.45±0.02 | 7.11±0.33 | 0.86±0.06 | 1.81±0.35 | 7.94±2.28 |
| L545 | 2.28±0.07 | 11.99±0.26 | 0.57±0.03 | 3.39±0.22 | 0.45±0.03 | 15.31±0.97 | 0.68±0.06 | 3.38±0.51 | 1.84±0.29 |
| Q546 | | | | | | | | | |

| | | | | | | | | | |
|-----------|-----------|------------|-----------|------------|-----------|-------------|-------------------------|-----------|-----------|
| D547 | 1.99±0.04 | 9.49±0.07 | 0.38±0.01 | 2.64±0.12 | 0.38±0.07 | 19.02±0.89 | 0.81±0.06 | | 0.41±0.08 |
| L548 | 2.14±0.09 | 9.48±0.20 | 0.48±0.03 | 2.67±0.14 | 0.46±0.02 | 17.13±1.07 | 0.78±0.02 | | 1.57±0.67 |
| K549 | 2.17±0.10 | 11.24±0.22 | 0.89±0.03 | 3.18±0.19 | 0.45±0.03 | 3.57±0.20 | 1.00±0.05 | 0.34±0.11 | 7.94±3.29 |
| Q550 | | | | | | | | | |
| G551 | 1.84±0.02 | 6.28±0.09 | 0.16±0.01 | 24.01±2.59 | 0.34±0.03 | 1.65±0.18 | 0.54±0.02 (0.888±0.008) | | 1.02±0.03 |
| H552 | 1.74±0.04 | 6.28±0.06 | 0.03±0.02 | 1.66±1.21 | 0.31±0.23 | 26.22±19.05 | 0.54±0.01 (0.88±0.01) | | 0.83±0.04 |
| D553 | 1.49±0.04 | 5.15±0.07 | 0.15±0.02 | 1.36±0.17 | 0.27±0.03 | 19.68±2.45 | 0.54±0.02 (0.72±0.01) | | 0.98±0.05 |
| Y554 | 1.13±0.01 | 3.43±0.03 | 0.18±0.01 | 0.88±0.05 | 0.21±0.01 | 14.47±0.85 | 0.54±0.02 (0.52±0.01) | | 0.98±0.05 |
| W542 (NH) | 1.69±0.03 | 9.94±0.16 | 0.65±0.02 | 3.33±0.12 | 0.39±0.01 | 9.22±0.39 | | | |

^aErrors are fitting errors to the corresponding equations (see Materials and Methods).

^bErrors are determined by the noise level from two different experiments.

^cErrors are determined by error propagation ³⁶.

^dErrors are from Monte Carlo simulations.

Table 8: Relaxation dispersion parameters of
SAMp73 at pH 7.0 and 298 K, 0 M GdmCl^c

| Residue | $R_2 (1/\tau_{cp} \rightarrow \infty) (s^{-1})$ | $R_{ex} (s^{-1})$ |
|-------------------|---|-------------------|
| Y487 | 5.07±0.91 | 4.44±1.13 |
| H488 | 7.31±0.58 | 4.41±0.88 |
| A489 | 5.21±0.50 | 3.95±0.62 |
| D490 | 6.69±0.73 | 4.36±1.08 |
| P491 | | |
| S492 | 7.84±0.89 | 5.70±1.34 |
| L493 | 7.57±0.92 | 4.83±1.93 |
| V494 | 5.90±0.96 | 4.50±1.41 |
| S495 | 7.49±0.71 | 4.37±1.01 |
| F496 | 6.80±0.74 | 4.57±1.13 |
| L497 | 6.39±1.79 | 4.07±1.82 |
| T498 | 7.17±0.93 | 4.34±1.46 |
| G499 | 6.41±0.65 | 3.82±0.97 |
| L500 ^c | 6.55±0.68 | 3.60±1.14 |
| G501 | [6.5] ^a | 3.54±1.05 |
| C502 | 6.08±0.56 | 4.12±1.00 |
| P503 | | |
| N504 | 6.55±0.57 | 4.39±1.08 |
| C505 | 6.01±0.60 | 4.34±0.97 |
| I506 | 5.52±0.62 | 4.08±0.94 |

| | | |
|-------------------|--------------------|------------|
| E507 | 6.86±0.88 | 8.75±1.69 |
| Y508 | 5.95±0.53 | 3.81±0.93 |
| F509 ^c | 7.81±0.27 | 2.27±0.54 |
| T510 | 8.87±2.01 | 7.76±2.82 |
| S511 | 7.29±0.81 | 3.19±1.15 |
| Q512 ^c | [6.5] ^a | 3.90±1.34 |
| G513 | 5.83±1.17 | 4.24±1.53 |
| L514 ^c | 6.51±0.77 | 3.93±1.19 |
| Q515 | 7.69±0.78 | 3.36±1.54 |
| S516 | 6.20±1.34 | 4.93±1.38 |
| I517 | 3.15±0.34 | 3.33±0.43 |
| Y518 ^b | | |
| H519 | 6.45±0.32 | 4.09±0.53 |
| L520 | 6.45±1.04 | 4.23±1.45 |
| Q521 ^c | 5.61±0.37 | 4.18±0.51 |
| N522 | [5.5] ^a | 11.19±2.43 |
| L523 ^b | | |
| T524 | 6.76±0.56 | 4.41±0.92 |
| I525 | [7.0] ^a | 4.48±1.95 |
| E526 | 3.88±0.66 | 5.56±0.80 |
| D527 | 5.41±1.26 | 2.76±2.13 |
| L528 | 7.20±0.84 | 4.18±1.40 |
| G529 | 5.84±0.31 | 4.78±0.51 |
| A530 | 6.50±0.51 | 5.29±0.96 |
| L531 | 6.47±0.93 | 4.20±1.32 |

| | | |
|-------------------|--------------------|------------|
| K532 ^c | 9.71±0.80 | 6.47±1.38 |
| I533 | 5.51±0.62 | 4.93±0.87 |
| P534 | | |
| E535 | 6.78±1.13 | 5.24±1.48 |
| Q536 | 6.91±0.93 | 6.58±1.25 |
| Y537 | 6.88±0.47 | 3.93±0.84 |
| R538 | 6.43±0.76 | 4.20±1.18 |
| M539 | 7.75±0.85 | 6.32±1.34 |
| T540 | 6.37±0.84 | 4.39±1.06 |
| I541 | 5.40±2.98 | 8.47±3.65 |
| W542 | [8.0] ^a | 3.01±1.72 |
| R543 | 6.87±0.68 | 4.34±1.11 |
| G544 | 6.21±0.71 | 10.52±1.00 |
| L545 | 6.53±0.58 | 4.34±0.84 |
| Q546 ^b | | |
| D547 | 4.78±0.64 | 3.75±0.75 |
| L548 | 5.06±0.37 | 4.98±0.44 |
| K549 | 4.77±1.97 | 4.99±1.86 |
| Q550 ^b | | |
| G551 | 4.38±0.40 | 4.08±0.52 |
| H552 | 5.54±0.90 | 7.30±1.27 |
| D553 | 4.40±0.33 | 5.93±0.99 |
| Y554 ^c | [1.9] ^a | 1.17±0.28 |
| W542 (NH) | 4.68±0.44 | 2.65±0.66 |

^aFitting was only possible when the R_2 ($1/\tau_{cp} \rightarrow \infty$)

was fixed to the value shown in brackets.

^b The variation in the intensity of the signals could

not be determined due to overlapping.

^cErrors are fitting errors to Eq. (7).