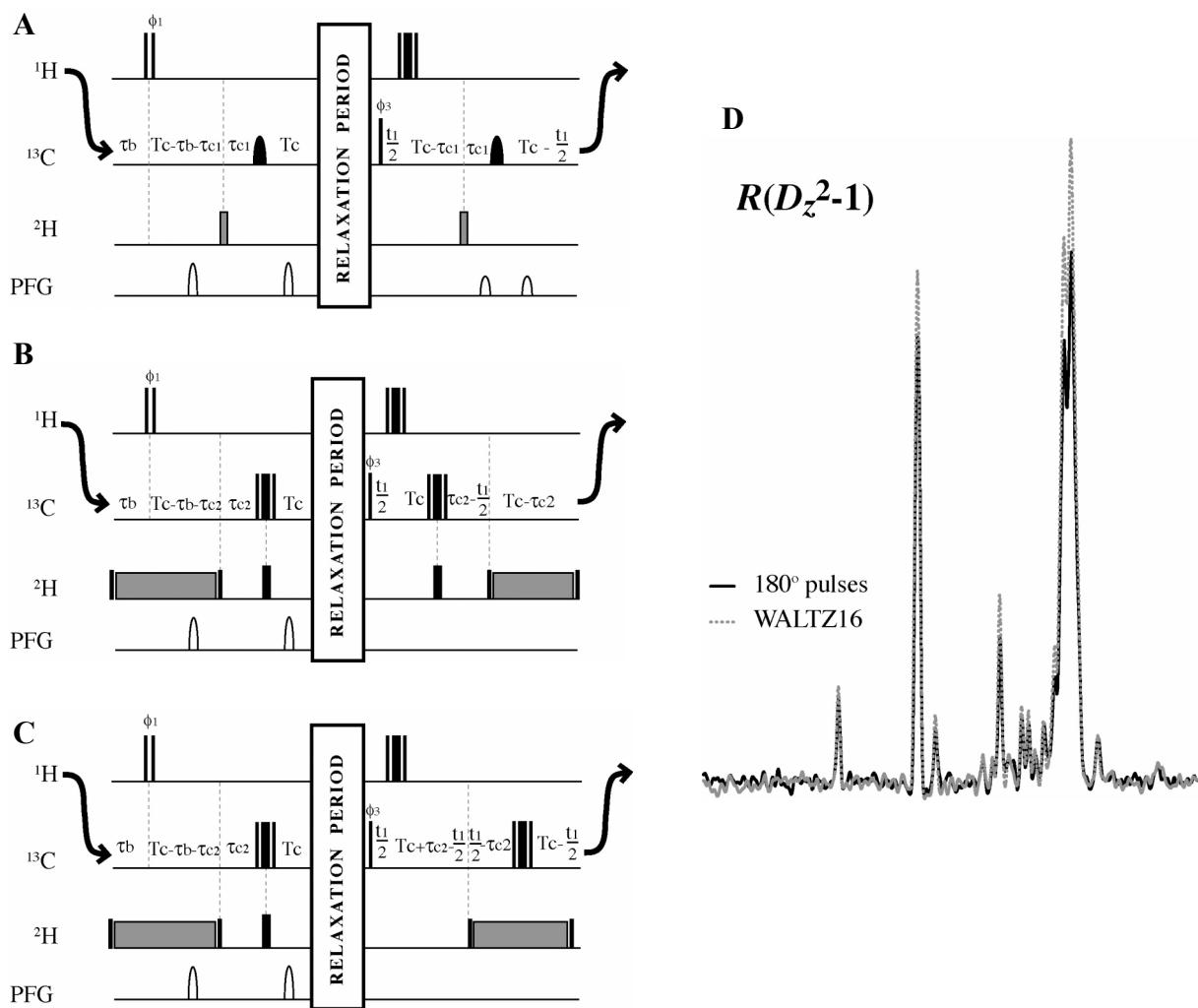
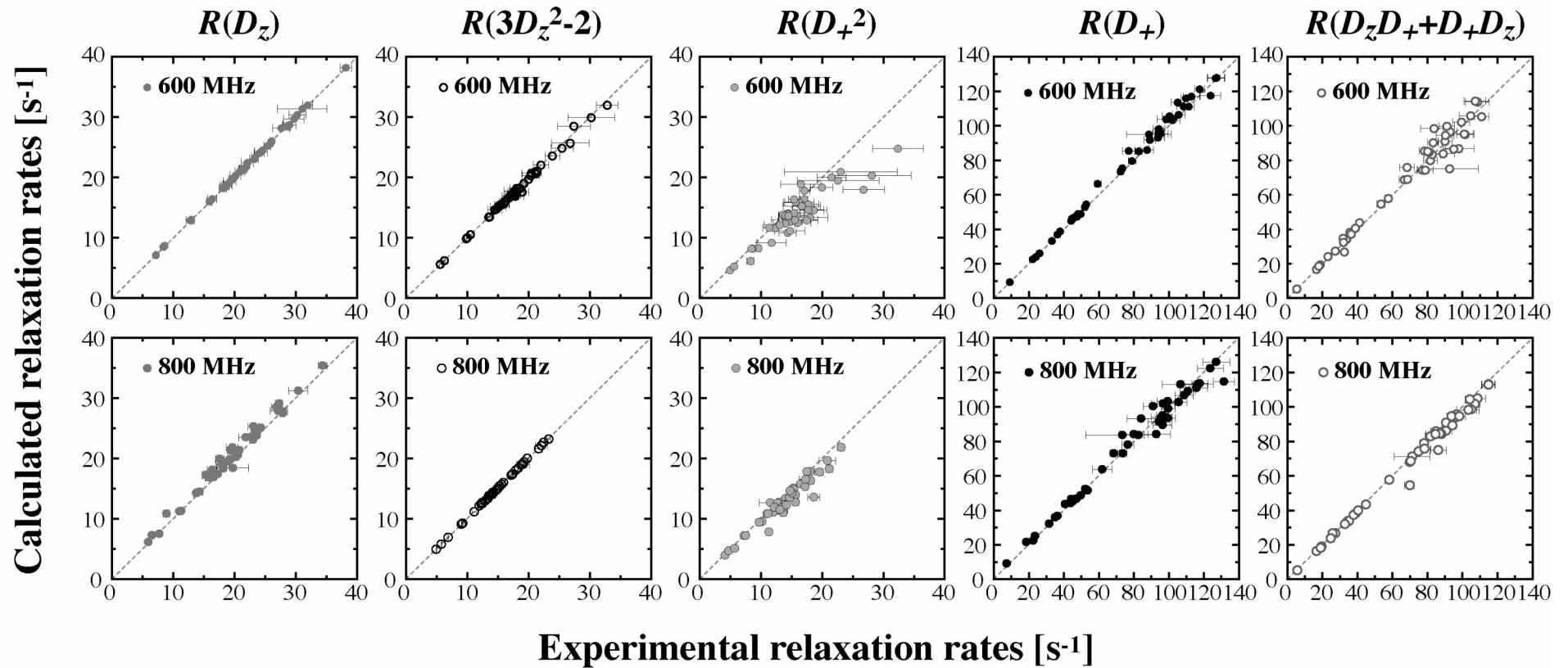


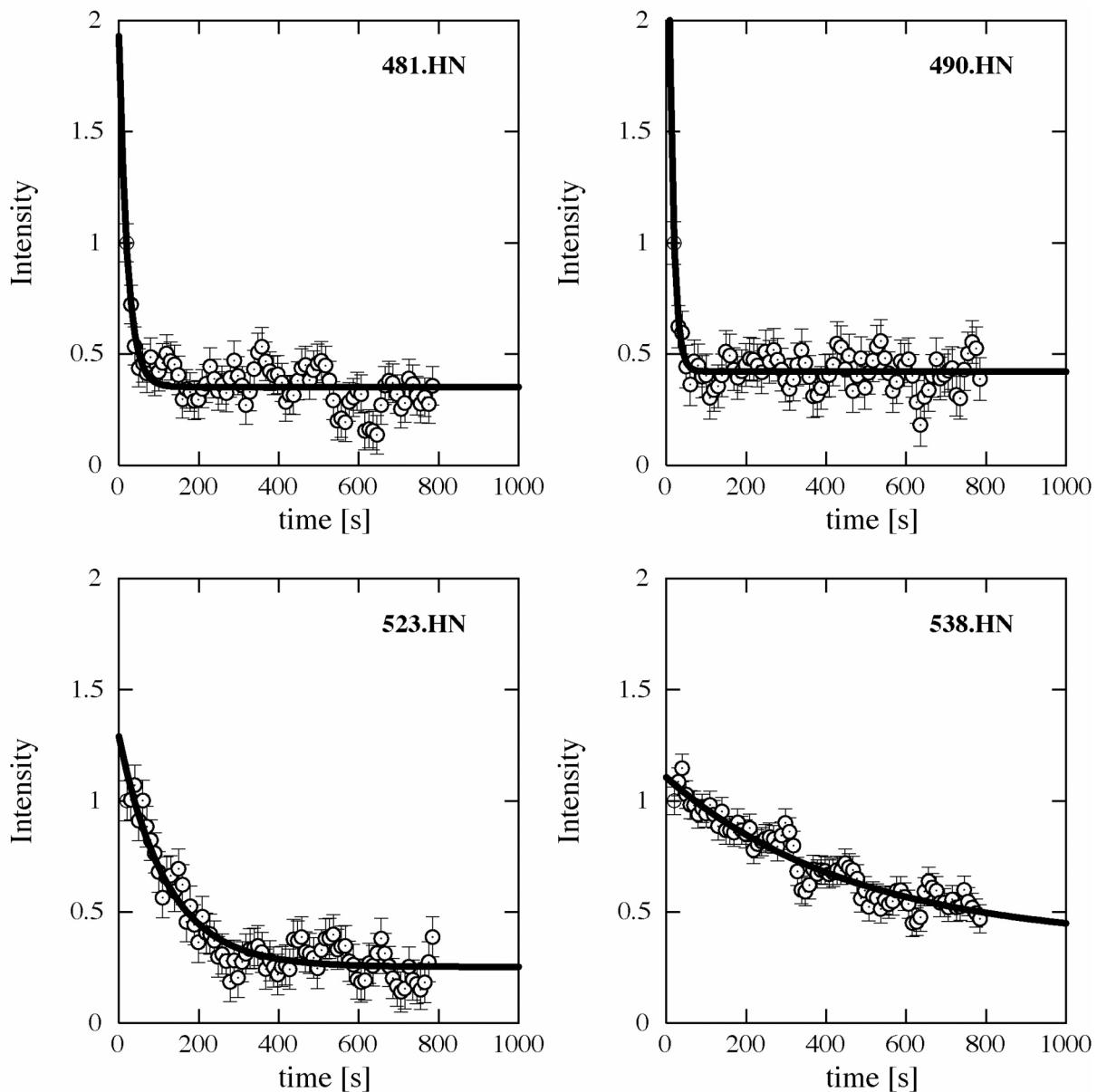
## Supplementary Material



**Figure S1:** Optimization of the pulse sequences to measure the deuterium  $R(D_xD_z)$ ,  $R(D_+^2)$  and  $R(3D_z^2-I)$  relaxation rates. **A.** Part of the pulse sequence proposed by Millet *et al.* where 2H 180° pulses are used to refocus the  ${}^1J_{CD}$  evolution **B.** Sequence where a WALTZ-16 scheme (grey boxes) is used to decouple the  ${}^1J_{CD}$  evolution, for  $\tau_{c2} > t1/2$  (**B**) and  $\tau_{c2} < t1/2$  (**C**). **D.** Comparison of a 1D proton spectrum using scheme **A** (solid black line) and scheme **B** (dashed grey line).  $\tau_b = 1/(2{}^1J_{CH}) = 3.85$  ms,  $2T_C = 1/({}^1J_{CC}) = 29$  ms,  $\tau_{CD} = 1/(2{}^1J_{CD}) = 24$  ms,  $\tau_{c1} = T_C - \tau_{CD}/2 = 2.5$  ms,  $\tau_{c2} = \tau_{CD} - T_C = 9.5$  ms.



**Figure S2:** Experimental versus back-calculated  $^2\text{H}$  relaxation rates of PX at 600 and 800 MHz. The spectral density values at 0,  $\omega_D^{600}$ ,  $\omega_D^{800}$ ,  $2\omega_D^{600}$  and  $2\omega_D^{800}$  were extracted from the ten relaxation rates according to eq. 2-6 using a linear least square fit. These values were then used to back-calculate the relaxation rates.



**Figure S3:** Intensity decay curves of PX due to H/D exchange at 25°C. A solution of 100 µl 1.3 mM  $^{15}\text{N}$  PX (2.25 M NaCl, 225 mM KPO<sub>4</sub> pH 6.0) was diluted with 350 µl D<sub>2</sub>O in the 800 MHz spectrometer by use of a syringe. Decrease of intensity was followed by immediate acquisition of subsequent SOFAST-HMQC spectra (34). Decay curves of four residues are shown. Residues 481 and 490 are located in the unstructured sub-domain of PX and exchange within one minute. Fitted exchange rates for these residues are compatible with intrinsic exchange rates at this temperature. Residues 523 and 538 are located in the structured domain of PX and are hydrogen-bonded to residues 519 and 534, respectively. These results are in agreement with H/D exchange rates measured by dissolving freeze-dried PX in D<sub>2</sub>O. The sensitivity of the D<sub>2</sub>O dilution experiment is limited by the low solubility of PX, therefore only exchange rates measured using freeze-dried PX are discussed in the main text.

**Table S-I:** Relaxation delays, scans and number of points used to measure the five  $^2\text{H}$  relaxation rates

Relaxation rate	Field	Number of scans	Number of complex data points	Relaxation delays (ms)											
$R(D_z)$	600 MHz	32 scans	512 x 83	0.05 (x2)	4.5	9.5	15	21	28 (x2)	36	45	58	71		
$R(D_+)$	600 MHz	32 scans	512 x 84	0.2 (x2)	1.5	3	4.7	6.6	8.7	10.9	13.5 (x2)	16.5	20		
$R(3D_z^2-2)$	600 MHz	64 scans	512 x 84	0.050	1.5	5	10	20	25	33	44 (x2)	54	70		
$R(D_+D_z+D_zD_+)$	600 MHz	64 scans	512 x 80	0.550	2 (x2)	4	8	10	14 (x2)	18	22	28	34		
$R(D_+^2)$	600 MHz	64 scans	512 x 80	2.350	6.5 (x2)	11	17	24	32	40	50	60 (x2)	70		
$R(D_z)$	800 MHz	16 scans	512 x 84	0.05	4.5	10	16	22	29 (x2)	39	52	70			
$R(D_+)$	800 MHz	16 scans	512 x 84	1.5 (x2)	3.0	4.7	6.6	8.7 (x2)	10.9	14.2	18.0				
$R(3D_z^2-2)$	800 MHz	16 scans	512 x 84	2.35	5	7.5	10 (x2)	16	23	31 (x2)	41	54	61		
$R(D_+D_z+D_zD_+)$	800 MHz	48 scans	512 x 104	0.7	2	4	6 (x2)	10	14	18 (x2)	22	28	34		
$R(D_+^2)$	800 MHz	16 scans	512 x 84	2.35	5	7.5	10 (x2)	16	23	31 (x2)	41	54	61	68	

**Table S-II:** Relaxation delays, scans and number of points used to measure the  $^{15}\text{N}$  relaxation rates

Relaxation rate	Field [MHz]	Conc. [mM]	Number of scans	Number of complex data points	Relaxation delays (ms)													
hetNOE	600	0.2	104	152 x 512	reference: recycle-delay 5s									saturation: recycle-delay 2s + saturation delay 3s				
hetNOE	600	1.3	32	140 x 512	reference: recycle-delay 5s									saturation: recycle-delay 2s + saturation delay 3s				
$R_1$	600	0.2	16	152 x 512	0	56	111	222	333	444 (x2)	666	888	1110	1443	1776			
$R_2(\text{CPMG})$	600	0.2	24	148 x 480	10	30	50	70	90 (x2)	110	130	150	170	210	230	250		
$R_1$	600	1.3	8	152 x 512	0	56	111	222	333	444 (x2)	666	888	1110	1443	1776			
$R_2(\text{CPMG})$	600	1.3	8	140 x 480	10	30	50	70	90 (x2)	110	130	150	170	210	230	250		
$R_1$	800	0.2	16	180 x 512	0	54	107	214 (x2)	428	642	856	1070	1338	1605				
$R_2(\text{CPMG})$	800	0.2	16	200 x 512	10	30	50	70 (x2)	90	110	130	150	170	190				
$R_2(R_{I\rho})$	800	0.2	16	200 x 512	0	10	20	30	50 (x2)	70	90	110	130	150	170			
$R_1$	800	1.3	8	180 x 512	0	54	107	214 (x2)	428	642	856	1070	1338	1605				
$R_2(\text{CPMG})$	800	1.3	8	180 x 512	10	30	50	70 (x2)	90	110	130	170	190					
$R_2(R_{I\rho})$	800	1.3	8	200 x 512	0	10	20	30	50 (x2)	70	90	110	130	150	170			

**Table S-III:**  $^{15}\text{N}$  relaxation rates [ $\text{s}^{-1}$ ] of [ $^{15}\text{N}$ ]-PX (600 MHz, 298K, ~0.2 mM)

Res	hetNOE	R <sub>1</sub>	R <sub>2</sub> (CPMG)
G462	-0.911 0.157	1.090 0.043	2.979 0.058
S463	-0.515 0.061	1.180 0.029	3.097 0.041
H464	-0.248 0.258	1.172 0.232	4.617 0.463
I470	0.093 0.053	1.560 0.036	3.993 0.045
E471	0.036 0.058	1.658 0.031	4.050 0.044
G472	-0.022 0.051	1.466 0.029	3.771 0.041
M474	0.041 0.072	1.574 0.036	3.980 0.045
K475	0.099 0.105	1.550 0.038	4.247 0.051
Y476	0.116 0.100	1.530 0.039	4.403 0.054
K477	0.188 0.155	1.594 0.040	4.281 0.058
D479	0.122 0.092	1.561 0.035	4.465 0.049
I481	0.090 0.089	1.527 0.039	4.324 0.058
R482	0.114 0.077	1.627 0.036	4.305 0.053
E483	0.183 0.045	1.576 0.029	4.425 0.045
D484	0.183 0.042	1.614 0.027	4.367 0.039
F486	0.185 0.039	1.708 0.031	4.467 0.044
R487	0.145 0.044	1.703 0.032	4.228 0.045
D488	0.184 0.042	1.635 0.029	4.177 0.040
E489	0.186 0.039	1.539 0.025	4.292 0.038
I490	0.107 0.047	1.578 0.033	4.238 0.049
N492	- -	1.616 0.028	4.833 0.049
V494	0.115 0.040	1.569 0.027	4.025 0.040
Y495	0.178 0.049	1.646 0.034	4.311 0.049
E497	0.076 0.039	1.634 0.025	3.810 0.037
R498	0.050 0.037	1.510 0.023	3.783 0.034
E501	- -	1.582 0.016	3.656 0.024
A504	-0.037 0.035	1.504 0.022	3.305 0.033
S505	-0.114 0.040	1.302 0.025	3.579 0.035
N506	-0.068 0.051	1.408 0.038	3.749 0.051
A507	-0.030 0.035	1.445 0.023	3.577 0.031
S508	-0.021 0.034	1.445 0.023	3.657 0.031
R509	0.023 0.041	1.467 0.027	3.913 0.037
L511	0.055 0.047	1.540 0.029	4.114 0.048
S513	0.107 0.057	1.442 0.032	4.421 0.052
K514	0.153 0.068	1.462 0.037	5.895 0.070
E515	0.164 0.052	1.498 0.032	4.987 0.054
K516	0.349 0.078	1.485 0.036	5.941 0.077
T518	0.498 0.108	1.509 0.072	8.266 0.175
M519	0.635 0.122	1.482 0.105	9.330 0.294
H520	0.674 0.132	1.540 0.085	10.614 0.247
S521	0.641 0.098	1.636 0.072	9.973 0.185
L522	0.792 0.155	1.491 0.083	9.778 0.244
R523	0.661 0.106	1.687 0.062	10.034 0.166
L524	0.791 0.129	1.718 0.077	13.082 0.308

V525	0.787	0.118	1.581	0.065	9.177	0.181
I526	0.671	0.154	1.410	0.098	16.044	0.547
E527	0.694	0.150	1.445	0.081	14.370	0.407
S528	0.714	0.114	1.597	0.079	11.508	0.248
S529	0.696	0.118	1.441	0.073	9.273	0.205
L531	0.771	0.195	1.468	0.116	11.370	0.414
S532	0.732	0.113	1.562	0.065	8.944	0.174
R533	0.810	0.132	1.492	0.065	9.240	0.195
A534	-	-	1.730	0.058	10.363	0.165
E535	0.742	0.102	1.638	0.071	9.408	0.188
K536	0.726	0.118	1.722	0.086	10.506	0.245
A537	0.716	0.093	1.605	0.058	11.950	0.215
A538	0.800	0.078	1.720	0.045	9.619	0.123
Y539	0.733	0.092	1.634	0.059	9.798	0.168
V540	0.750	0.146	1.738	0.084	9.664	0.242
S542	0.828	0.099	1.615	0.048	9.298	0.131
L543	0.651	0.129	1.701	0.084	9.127	0.219
S544	0.804	0.118	1.597	0.061	11.233	0.191
K545	0.669	0.142	1.642	0.086	11.507	0.296
C546	0.689	0.102	1.653	0.068	9.003	0.162
K547	0.601	0.176	1.469	0.128	8.667	0.379
T548	0.672	0.173	1.342	0.088	14.114	0.463
D549	0.598	0.097	1.630	0.091	9.766	0.256
Q550	0.659	0.103	1.592	0.055	8.597	0.138
E551	0.694	0.107	1.619	0.074	9.841	0.220
V552	0.794	0.112	1.518	0.062	9.222	0.177
K553	0.638	0.109	1.696	0.072	13.757	0.307
A554	0.799	0.106	1.727	0.060	12.343	0.212
V555	0.828	0.102	1.565	0.052	9.717	0.158
M556	0.730	0.171	1.362	0.080	16.039	0.486
E557	0.712	0.108	1.648	0.057	9.967	0.169
L558	0.682	0.136	1.540	0.080	9.874	0.255
V559	0.775	0.105	1.567	0.065	9.928	0.197
E560	0.638	0.128	1.595	0.085	17.891	0.501
E561	0.846	0.115	1.717	0.064	9.653	0.172
D562	0.798	0.102	1.713	0.058	9.387	0.152
I563	-	-	1.558	0.073	9.361	0.212
S565	0.700	0.081	1.516	0.045	9.713	0.129
L566	0.688	0.097	1.604	0.056	10.283	0.169
T567	0.383	0.055	1.531	0.035	6.043	0.065
N568	-0.037	0.031	1.335	0.018	3.349	0.028

**Table S-IV:**  $^{15}\text{N}$  relaxation rates [ $\text{s}^{-1}$ ] of [ $^{15}\text{N}$ ]-PX (600 MHz, 298K, ~1.3 mM)

Res	hetNOE	$R_1$	$R_2$ (CPMG)
G462	-0.657 0.018	- -	3.470 0.025
S463	-0.382 0.009	- -	3.350 0.020
H464	-0.177 0.051	1.277 0.177	4.198 0.218
I470	0.129 0.010	1.552 0.028	5.209 0.029
E471	0.106 0.010	1.672 0.026	4.914 0.025
G472	0.070 0.009	1.487 0.024	4.379 0.024
M474	0.096 0.011	1.587 0.026	5.294 0.028
K475	0.129 0.012	1.592 0.029	- -
Y476	0.196 0.011	1.542 0.031	5.433 0.029
K477	0.187 0.012	1.570 0.031	5.899 0.035
D479	0.202 0.011	1.538 0.028	5.523 0.028
I481	0.177 0.012	1.576 0.030	5.819 0.034
R482	0.188 0.012	1.638 0.029	5.676 0.032
E483	0.204 0.010	1.630 0.024	5.828 0.030
D484	0.220 0.008	1.634 0.022	5.816 0.027
F486	0.245 0.009	1.669 0.025	5.428 0.027
R487	0.217 0.009	1.663 0.026	5.734 0.028
D488	0.229 0.009	- -	- -
E489	0.194 0.008	1.559 0.020	5.605 0.026
I490	0.179 0.010	1.577 0.026	5.284 0.030
N492	0.165 0.010	- -	- -
V494	0.149 0.009	1.544 0.021	5.511 0.028
Y495	0.172 0.010	1.610 0.026	5.106 0.031
E497	0.109 0.008	1.577 0.020	4.866 0.022
R498	0.093 0.008	1.594 0.019	4.771 0.021
A504	-0.002 0.007	1.565 0.018	4.006 0.019
S505	-0.046 0.007	1.361 0.248	3.795 0.018
N506	-0.047 0.010	1.445 0.135	4.538 0.028
A507	-0.010 0.007	1.523 0.142	3.987 0.017
S508	0.003 0.007	1.465 0.260	4.526 0.018
R509	0.041 0.008	1.571 0.021	4.365 0.022
L511	0.050 0.010	1.490 0.023	4.986 0.030
S513	0.103 0.010	1.468 0.026	5.336 0.030
K514	0.140 0.011	1.474 0.028	7.112 0.044
E515	0.177 0.010	1.459 0.024	6.572 0.037
K516	0.292 0.013	1.414 0.029	7.030 0.048
T518	0.519 0.022	1.537 0.064	10.110 0.128
M519	0.638 0.033	1.559 0.100	12.057 0.255
H520	0.705 0.027	1.457 0.075	13.207 0.212
S521	0.699 0.022	1.519 0.062	13.194 0.168
L522	0.737 0.032	1.533 0.087	12.564 0.226
R523	0.709 0.021	1.538 0.056	13.248 0.338
L524	0.747 0.027	1.531 0.069	15.849 0.261
V525	0.702 0.021	1.528 0.062	12.288 0.161

I526	0.785	0.038	1.480	0.102	18.145	0.493
E527	0.756	0.034	1.511	0.086	17.178	0.379
S528	0.756	0.025	1.474	0.069	14.531	0.215
S529	0.677	0.025	1.428	0.071	11.961	0.190
L531	0.737	0.037	1.425	0.101	14.853	0.384
S532	0.702	0.025	1.509	0.066	11.754	0.175
R533	0.722	0.025	1.456	0.060	11.834	0.175
A534	0.755	0.020	1.571	0.051	12.863	0.145
E535	0.762	0.024	1.542	0.067	12.119	0.172
K536	0.749	0.031	1.509	0.078	13.444	0.239
A537	0.784	0.022	1.477	0.053	15.147	0.189
A538	0.760	0.016	1.519	0.039	12.864	0.118
Y539	0.794	0.023	1.591	0.056	12.443	0.148
V540	0.754	0.030	1.539	0.074	12.916	0.224
K541	-	-	-	-	-	-
S542	0.719	0.019	1.478	0.043	11.843	0.118
L543	0.735	0.029	1.571	0.075	12.019	0.212
S544	0.806	0.022	1.546	0.060	13.734	0.159
K545	0.712	0.029	1.486	0.075	14.322	0.252
C546	0.674	0.020	1.528	0.059	11.036	0.135
K547	0.687	0.045	1.392	0.121	11.747	0.357
T548	0.657	0.034	1.269	0.077	16.679	0.376
D549	0.710	0.031	1.530	0.083	12.617	0.227
Q550	0.622	0.019	1.494	0.047	11.056	0.116
E551	0.753	0.028	1.460	0.071	13.101	0.211
V552	0.709	0.024	1.536	0.065	12.464	0.173
K553	0.740	0.025	1.513	0.062	16.157	0.247
A554	0.716	0.020	1.571	0.052	14.791	0.182
V555	0.709	0.021	1.502	0.051	12.723	0.159
M556	0.681	0.030	1.505	0.084	18.432	0.387
E557	0.781	0.023	1.637	0.058	13.170	0.157
L558	0.733	0.029	1.499	0.073	12.856	0.228
V559	0.758	0.024	1.501	0.061	13.075	0.187
E560	0.711	0.029	1.586	0.082	19.689	0.400
E561	0.729	0.022	1.563	0.056	13.053	0.160
D562	0.735	0.020	1.539	0.053	12.269	0.139
I563	0.754	0.027	1.502	0.076	12.454	0.208
E564	0.732	0.022	-	-	-	-
S565	0.634	0.016	1.522	0.043	11.758	0.112
L566	0.598	0.018	1.494	0.049	12.251	0.130
T567	0.372	0.010	1.497	0.027	7.662	0.044
N568	-0.002	0.006	1.363	0.014	4.112	0.017

**Table S-V:**  $^{15}\text{N}$  relaxation rates [ $\text{s}^{-1}$ ] of  $[^{15}\text{N}]\text{-PX}$  (800 MHz, 298K, ~0.2 mM)

Res	R <sub>1</sub>	R <sub>2</sub> (CPMG)	R <sub>2</sub> (R <sub>1ρ</sub> )
G462	- -	3.253 0.044	- -
H464	1.095 0.167	4.378 0.357	4.734 0.355
I470	1.362 0.035	5.459 0.065	5.551 0.066
E471	1.335 0.053	4.988 0.048	4.999 0.069
G472	1.308 0.030	4.416 0.045	4.780 0.061
R473	1.321 0.035	4.954 0.048	4.946 0.049
M474	1.328 0.057	4.749 0.046	4.976 0.064
K475	1.316 0.078	5.014 0.054	5.158 0.076
Y476	1.335 0.092	5.114 0.053	5.708 0.086
K477	1.345 0.094	5.647 0.075	5.423 0.100
D479	1.324 0.079	5.753 0.059	5.603 0.071
L480	- -	5.381 0.051	5.650 0.092
I481	1.328 0.092	5.377 0.059	5.667 0.084
R482	1.414 0.058	5.672 0.074	5.683 0.061
E483	1.363 0.035	5.148 0.051	5.425 0.049
D484	1.376 0.027	5.781 0.054	5.251 0.048
E485	1.387 0.026	- -	- -
F486	1.401 0.030	5.470 0.056	5.575 0.055
R487	1.383 0.031	5.638 0.064	5.477 0.063
D488	1.410 0.026	5.176 0.052	5.506 0.053
E489	1.310 0.024	5.182 0.058	5.431 0.045
I490	1.351 0.031	5.330 0.051	5.700 0.065
R491	1.360 0.015	- -	- -
N492	- -	5.564 0.058	- -
V494	1.303 0.022	5.257 0.051	5.231 0.049
Y495	1.346 0.033	5.523 0.073	5.749 0.068
E497	1.356 0.022	4.326 0.048	5.066 0.042
R498	1.354 0.021	4.410 0.042	4.771 0.041
T500	- -	4.119 0.041	4.200 0.041
E501	1.348 0.013	- -	- -
A504	1.328 0.018	4.131 0.044	4.603 0.043
S505	1.201 0.019	4.182 0.039	4.440 0.037
N506	1.216 0.028	4.689 0.053	5.080 0.053
A507	1.261 0.018	4.420 0.041	4.742 0.038
S508	1.241 0.017	4.581 0.038	4.619 0.037
R509	1.283 0.023	4.691 0.047	4.996 0.047
L511	1.237 0.026	5.603 0.063	5.678 0.061
S513	1.196 0.030	5.718 0.069	5.670 0.062
K514	1.264 0.037	7.633 0.105	7.927 0.091
E515	1.229 0.029	5.998 0.064	6.374 0.072
K516	1.144 0.038	6.931 0.094	7.740 0.100
T518	1.155 0.065	10.353 0.241	10.583 0.246
M519	1.129 0.119	11.583 0.376	11.373 0.401
H520	1.134 0.074	12.864 0.269	12.994 0.296

S521	1.162	0.058	12.651	0.248	12.195	0.241
L522	1.189	0.083	13.580	0.384	12.311	0.328
R523	1.209	0.057	12.986	0.254	12.455	0.218
L524	1.109	0.087	16.430	0.469	15.097	0.385
V525	1.076	0.062	11.180	0.237	11.693	0.234
I526	1.117	0.112	20.716	0.857	16.674	0.607
E527	1.069	0.117	18.216	0.642	16.155	0.528
S528	1.099	0.064	14.804	0.313	13.841	0.330
S529	1.199	0.088	10.997	0.266	11.181	0.253
L531	1.059	0.126	15.096	0.700	14.860	0.596
S532	1.112	0.064	11.013	0.201	10.665	0.222
R533	1.083	0.069	11.163	0.233	11.895	0.255
A534	-	-	12.816	0.195	12.624	0.227
E535	1.065	0.052	11.404	0.244	11.495	0.204
K536	1.093	0.082	13.230	0.304	12.207	0.284
A537	1.125	0.051	15.462	0.276	13.761	0.239
A538	1.190	0.037	11.716	0.160	12.060	0.150
Y539	1.146	0.051	11.832	0.231	11.348	0.191
V540	1.156	0.093	12.117	0.319	12.454	0.319
K541	-	-	12.216	0.174	-	-
S542	1.147	0.042	11.305	0.170	11.345	0.166
L543	1.189	0.102	11.550	0.310	12.064	0.327
S544	-	-	12.347	0.200	12.316	0.209
K545	1.085	0.092	14.874	0.383	13.909	0.354
C546	1.121	0.068	11.399	0.219	10.664	0.205
K547	0.965	0.133	9.942	0.438	11.074	0.592
T548	0.995	0.111	18.762	0.813	14.494	0.627
D549	1.035	0.086	11.356	0.310	12.490	0.349
Q550	1.167	0.051	10.789	0.158	11.047	0.173
E551	1.087	0.061	12.108	0.289	12.312	0.286
V552	1.121	0.060	12.272	0.249	12.099	0.235
K553	1.190	0.071	18.381	0.473	15.348	0.381
A554	1.141	0.063	15.575	0.345	14.219	0.299
V555	1.091	0.046	12.066	0.209	11.863	0.180
M556	1.220	0.103	21.775	0.866	16.826	0.574
E557	1.252	0.055	12.101	0.236	12.252	0.211
L558	1.051	0.083	12.331	0.303	12.346	0.321
V559	1.147	0.056	12.450	0.239	12.590	0.228
E560	1.139	0.094	21.887	0.842	17.857	0.615
E561	1.215	0.057	12.388	0.235	12.297	0.213
D562	1.114	0.046	11.371	0.204	11.973	0.192
I563	-	-	11.098	0.271	11.370	0.268
E564	1.276	0.044	-	-	-	-
S565	1.131	0.039	11.907	0.172	11.407	0.154
L566	1.144	0.063	12.960	0.243	12.247	0.230
T567	1.211	0.029	7.421	0.070	7.273	0.077

N568	1.130 0.014	4.205 0.040
		4.220 0.036

**Table S-VI:**  $^{15}\text{N}$  relaxation rates [ $\text{s}^{-1}$ ] of [ $^{15}\text{N}$ ]-PX (800 MHz, 298K, ~1.3 mM)

<u>Res</u>	<u><math>R_1</math></u>	<u><math>R_2</math> (CPMG)</u>	<u><math>R_2(R_{1\rho})</math></u>
G462	- -	3.973 0.038	- -
S463	- -	4.060 0.030	- -
H464	1.132 0.106	5.578 0.223	4.831 0.091
I470	1.357 0.028	6.107 0.044	6.191 0.021
E471	- -	6.158 0.043	6.193 0.022
G472	1.294 0.023	5.634 0.039	5.552 0.020
R473	1.329 0.021	6.039 0.036	5.818 0.015
M474	1.345 0.033	6.448 0.044	6.225 0.019
K475	- -	6.626 0.051	6.422 0.022
Y476	1.295 0.042	7.028 0.055	6.752 0.024
K477	1.325 0.042	6.759 0.060	6.895 0.030
D479	- -	7.301 0.048	7.071 0.021
L480	- -	6.805 0.049	6.667 0.022
I481	- -	7.127 0.060	6.891 0.026
R482	1.361 0.039	6.898 0.059	7.057 0.029
E483	1.349 0.027	6.767 0.049	6.728 0.021
D484	1.353 0.021	7.164 0.043	6.872 0.018
E485	1.337 0.022	- -	- -
F486	1.363 0.022	6.903 0.043	6.571 0.017
R487	1.343 0.025	7.016 0.049	6.893 0.020
D488	1.352 0.022	6.805 0.056	6.768 0.023
E489	1.292 0.019	6.647 0.041	6.408 0.017
I490	1.335 0.025	7.080 0.059	6.811 0.024
R491	1.316 0.053	- -	- -
N492	- -	6.395 0.042	- -
V494	1.290 0.018	6.291 0.042	6.135 0.017
Y495	- -	6.419 0.051	6.749 0.023
Q496	1.311 0.011	- -	- -
E497	1.307 0.016	5.600 0.034	5.558 0.015
R498	1.333 0.016	5.393 0.032	5.426 0.013
D499	- -	- -	- -
T500	- -	4.780 0.030	4.725 0.013
E501	1.332 0.011	4.828 0.024	- -
A504	1.296 0.014	4.522 0.026	4.609 0.013
S505	1.196 0.013	4.386 0.027	4.640 0.011
N506	1.227 0.021	5.332 0.038	5.031 0.016
A507	1.266 0.013	4.615 0.027	5.095 0.013
S508	1.233 0.013	4.986 0.026	5.111 0.012
R509	1.318 0.016	5.700 0.036	- -
L511	1.224 0.018	5.968 0.046	6.491 0.021
S513	1.185 0.021	6.312 0.048	6.253 0.020

K514	1.229	0.025	8.731	0.067	8.742	0.029
E515	1.200	0.021	7.565	0.059	7.549	0.025
K516	1.141	0.029	8.605	0.078	9.152	0.036
T518	1.149	0.055	13.191	0.255	12.832	0.110
M519	1.069	0.108	15.175	0.526	14.509	0.208
H520	1.063	0.062	16.318	0.353	15.501	0.144
S521	1.054	0.048	14.964	0.294	15.059	0.118
L522	1.075	0.071	14.867	0.441	16.336	0.200
R523	1.004	0.045	16.578	0.306	15.089	0.114
L524	0.988	0.066	20.474	0.519	17.879	0.193
V525	1.038	0.055	15.182	0.304	15.325	0.128
I526	1.031	0.099	22.368	0.949	19.358	0.324
E527	1.072	0.099	21.513	0.737	18.706	0.261
S528	1.051	0.052	17.505	0.383	16.310	0.147
S529	1.010	0.065	14.789	0.332	14.093	0.135
L531	1.054	0.105	18.267	0.716	17.097	0.274
S532	1.078	0.062	13.848	0.302	14.129	0.121
R533	1.042	0.064	14.816	0.331	15.094	0.139
A534	-	-	16.447	0.276	15.676	0.111
E535	1.037	0.049	14.692	0.280	14.375	0.113
K536	1.019	0.072	16.883	0.432	15.571	0.165
A537	1.055	0.042	18.695	0.341	16.746	0.125
A538	1.060	0.031	15.403	0.194	15.270	0.083
Y539	1.081	0.044	15.299	0.260	14.972	0.103
V540	1.052	0.078	15.700	0.429	15.141	0.172
K541	1.093	0.037	-	-	-	-
S542	1.035	0.034	14.104	0.193	14.255	0.084
L543	1.047	0.085	14.526	0.383	15.352	0.170
S544	-	-	14.941	0.248	15.480	0.109
K545	0.989	0.070	17.213	0.414	16.318	0.166
C546	1.013	0.054	13.798	0.244	13.480	0.101
K547	0.986	0.116	14.016	0.702	13.288	0.281
T548	0.893	0.085	21.463	0.949	15.946	0.254
D549	1.043	0.078	15.051	0.429	15.028	0.178
Q550	1.080	0.040	12.581	0.163	12.618	0.071
E551	1.023	0.055	16.091	0.370	15.558	0.149
V552	0.988	0.051	15.524	0.322	15.354	0.134
K553	1.078	0.058	21.953	0.566	18.345	0.192
A554	1.076	0.049	19.047	0.378	17.314	0.143
V555	0.991	0.041	15.616	0.245	15.175	0.102
M556	1.070	0.078	22.689	0.841	19.898	0.287
E557	1.113	0.045	16.039	0.283	15.218	0.108
L558	1.002	0.076	16.209	0.433	15.895	0.176
V559	1.043	0.048	15.931	0.323	15.393	0.129
E560	1.081	0.076	24.465	0.919	20.743	0.294
E561	1.079	0.045	15.698	0.299	15.409	0.119

D562	1.040	0.040	15.626	0.264	15.355	0.103
I563	1.040	0.068	14.738	0.368	14.609	0.152
S565	1.053	0.032	13.916	0.181	14.321	0.078
L566	1.036	0.047	15.494	0.264	14.718	0.103
T567	1.154	0.021	9.198	0.064	8.732	0.028
N568	1.117	0.011	5.375	0.028	4.868	0.012

**Table S-VII:** Model-free analysis [<sup>15</sup>N]-PX (600 & 800 MHz, ~0.2 mM)

Res	$\tau_c$ [ns]	$S^2_f$	$S^2_s$	$\tau_e$ [ps]	$R_{ex}$
G462	5.33 0.27	0.281 0.015	-	127 15	- -
S463	4.84 0.13	0.337 0.007	-	109 7	- -
H464	5.41 0.60	0.427 0.040	-	111 36	- -
I470	4.48 0.08	0.533 0.009	-	113 10	- -
E471	4.34 0.08	0.532 0.010	-	127 12	- -
G472	4.31 0.07	0.481 0.008	-	112 8	- -
M474	4.37 0.10	0.513 0.011	-	114 12	- -
K475	4.60 0.12	0.527 0.015	-	106 17	- -
Y476	4.73 0.12	0.532 0.014	-	104 16	- -
K477	4.68 0.15	0.556 0.020	-	99 26	- -
D479	4.94 0.12	0.550 0.013	-	109 16	- -
I481	4.87 0.12	0.531 0.013	-	107 15	- -
R482	4.60 0.10	0.557 0.012	-	120 16	- -
E483	4.51 0.07	0.556 0.008	-	103 8	- -
D484	4.60 0.06	0.571 0.007	-	111 8	- -
P486	4.43 0.06	0.587 0.007	-	120 9	- -
R487	4.28 0.07	0.565 0.008	-	119 9	- -
D488	4.24 0.06	0.562 0.007	-	108 8	- -
E489	4.59 0.06	0.548 0.006	-	97 6	- -
I490	4.65 0.07	0.550 0.008	-	118 9	- -
V494	4.47 0.06	0.533 0.007	-	107 7	- -
Y495	4.47 0.07	0.566 0.008	-	108 9	- -
E497	3.92 0.06	0.516 0.006	-	112 7	- -
R498	4.11 0.05	0.500 0.006	-	109 6	- -
A504	3.83 0.05	0.467 0.005	-	111 5	- -
S505	4.50 0.06	0.437 0.005	-	105 5	- -
N506	4.64 0.09	0.470 0.008	-	111 7	- -
A507	4.25 0.05	0.469 0.005	-	107 5	- -
S508	4.40 0.05	0.475 0.005	-	107 5	- -
R509	4.45 0.06	0.495 0.006	-	109 6	- -
L511	4.81 0.07	0.525 0.007	-	112 8	- -
S513	5.13 0.09	0.527 0.008	-	99 8	- -
K514	6.09 0.12	0.613 0.011	-	129 15	- -
E515	5.27 0.08	0.567 0.008	-	105 9	- -
K516	5.84 0.11	0.624 0.012	-	80 13	- -
T518	7.00 0.01	0.776 0.000	-	- -	- -
M519	7.34 -	0.841 0.019	-	60 49	- -

H520	7.34	-	0.841	0.041	-	-	56	47	1.0	0.4
S521	7.34	-	0.827	0.032	-	-	94	39	0.8	0.3
L522	7.34	-	0.774	0.043	-	-	55	37	1.5	0.4
R523	7.34	-	0.841	0.032	-	-	133	54	0.8	0.3
L524	7.34	-	0.937	0.034	-	-	-	-	2.4	0.4
V525	7.34	-	0.830	0.012	-	-	28	34	-	-
I526	7.34	-	0.801	0.054	-	-	38	43	6.2	0.6
E527	7.34	-	0.813	0.048	-	-	26	45	4.6	0.5
S528	7.34	-	0.845	0.038	-	-	45	41	2.0	0.3
S529	7.34	-	0.823	0.014	-	-	43	36	-	-
L531	7.34	-	0.798	0.062	-	-	20	52	2.5	0.6
S532	7.34	-	0.814	0.011	-	-	50	32	-	-
R533	7.34	-	0.833	0.013	-	-	5	37	-	-
E535	7.34	-	0.848	0.013	-	-	30	34	-	-
K536	7.34	-	0.873	0.041	-	-	60	57	0.8	0.4
A537	7.34	-	0.859	0.030	-	-	49	38	2.3	0.3
A538	7.00	0.12	0.906	0.016	-	-	7	56	-	-
Y539	7.34	-	0.879	0.012	-	-	49	42	-	-
V540	7.34	-	0.885	0.017	-	-	86	82	-	-
S542	7.34	-	0.841	0.009	-	-	49	29	-	-
L543	7.34	-	0.835	0.015	-	-	120	64	-	-
S544	7.34	-	0.956	0.011	-	-	-	-	-	-
K545	7.34	-	0.849	0.046	-	-	69	57	2.0	0.4
C546	7.34	-	0.825	0.011	-	-	74	36	-	-
K547	7.34	-	0.756	0.023	-	-	49	39	-	-
T548	7.34	-	0.741	0.051	-	-	26	34	5.4	0.6
D549	7.34	-	0.854	0.016	-	-	85	48	-	-
Q550	7.34	-	0.787	0.009	-	-	97	30	-	-
E551	7.34	-	0.887	0.015	-	-	31	51	-	-
V552	7.34	-	0.779	0.031	-	-	44	26	0.8	0.3
K553	7.34	-	0.891	0.039	-	-	135	89	3.7	0.4
A554	7.34	-	0.938	0.026	-	-	-	-	1.8	0.3
V555	7.34	-	0.846	0.021	-	-	-	-	0.4	0.2
M556	7.34	-	0.788	0.050	-	-	34	43	6.8	0.6
E557	7.34	-	0.894	0.012	-	-	108	69	-	-
L558	7.34	-	0.830	0.033	-	-	-	-	0.7	0.3
V559	7.34	-	0.861	0.025	-	-	-	-	0.5	0.2
E560	7.34	-	0.885	0.048	-	-	75	73	6.7	0.5
E561	7.34	-	0.895	0.012	-	-	64	60	-	-
D562	7.34	-	0.849	0.011	-	-	55	34	-	-
S565	7.34	-	0.874	0.009	-	-	22	31	-	-
L566	7.34	-	0.932	0.012	-	-	9	77	-	-
T567	7.34	-	0.618	0.014	0.794	0.016	978	95	-	-
N568	7.34	-	0.323	0.005	0.683	0.008	873	25	-	-

**Table S-VIII:**  $^2\text{H}$  relaxation rates [ $\text{s}^{-1}$ ] of PX (600 MHz)

Res	$R(D_z)$	$R(3D_z^2 - 2)$	$R(D_+^2)$	$R(D_+)$	$R(D_x D_z)$
I470 $\gamma$ 2	21.9 0.1	18.1 0.1	14.4 0.2	45.2 0.2	33.7 0.2
I470 $\delta$ 1	12.9 0.2	10.5 0.2	9.6 0.4	23.9 0.5	16.4 0.3
I481 $\gamma$ 2	21.9 0.1	18.1 0.1	14.4 0.2	44.6 0.2	33.7 0.2
I481 $\delta$ 1	12.9 0.1	10.0 0.1	8.6 0.2	26.1 0.3	18.5 0.2
I490 $\gamma$ 2	21.9 0.1	18.1 0.1	14.4 0.2	44.6 0.2	33.7 0.2
I490 $\delta$ 1	12.9 0.1	10.0 0.1	8.5 0.2	26.1 0.3	18.5 0.2
V494 $\gamma$ 1	26.1 0.2	20.0 0.4	17.0 0.6	46.0 0.6	33.4 0.5
V494 $\gamma$ 2	22.0 0.2	17.3 0.3	13.6 0.5	37.9 0.5	27.2 0.4
T500 $\gamma$ 2	28.7 0.3	21.4 0.5	17.1 0.8	48.2 0.7	31.7 0.7
A504 $\beta$	24.5 0.2	19.3 0.3	16.5 0.6	44.2 0.5	32.0 0.4
A507 $\beta$	24.5 0.2	19.3 0.3	16.5 0.6	44.2 0.5	32.0 0.4
L511 $\delta$ 1	21.1 0.2	15.3 0.3	14.8 0.6	36.4 0.5	32.4 0.5
L511 $\delta$ 2	18.7 0.2	13.5 0.2	12.3 0.4	33.1 0.4	23.0 0.3
T518 $\gamma$ 2	22.1 0.9	18.1 1.1	18.6 2.2	101.9 4.4	90.0 4.1
M519 $\epsilon$ 1	7.2 0.1	6.3 0.1	4.9 0.2	22.3 0.3	17.8 0.2
L522 $\delta$ 1	31.1 4.0	30.3 3.8	23.0 9.2	88.6 12.8	92.6 16.3
L522 $\delta$ 2	20.8 0.7	17.9 1.2	15.9 2.4	89.0 3.3	81.6 4.0
L524 $\delta$ 1	22.0 0.3	15.4 0.4	14.0 0.7	49.8 0.8	35.5 0.7
L524 $\delta$ 2	20.1 0.2	14.8 0.3	14.2 0.6	47.5 0.7	36.2 0.6
V525 $\gamma$ 1	32.0 0.8	22.0 1.3	21.5 2.3	111.3 3.1	92.8 4.0
V525 $\gamma$ 2	15.9 0.5	15.3 0.7	14.3 1.4	94.9 2.5	78.2 2.8
I526 $\gamma$ 2	20.2 0.9	17.0 1.4	18.0 3.0	112.9 4.7	104.5 6.4
I526 $\delta$ 1	12.8 0.7	14.5 1.1	11.7 2.4	93.7 3.8	82.7 4.5
L531 $\delta$ 1	29.7 1.7	26.8 3.1	22.6 6.7	98.7 5.2	97.8 8.9
L531 $\delta$ 2	19.5 0.5	16.6 0.7	17.5 1.8	82.8 2.0	77.0 2.6
A534 $\beta$	27.6 1.4	20.5 1.6	26.8 3.4	126.8 4.9	108.5 6.8
A537 $\beta$	18.9 0.7	17.6 1.1	14.7 2.0	105.2 3.7	99.2 4.9
A538 $\beta$	24.1 0.8	20.4 1.4	16.2 2.5	127.2 4.8	107.1 6.2
V540 $\gamma$ 1	38.2 0.9	32.9 1.8	32.4 4.1	117.7 2.9	90.9 4.5
V540 $\gamma$ 2	18.3 0.7	17.6 1.1	16.0 2.2	94.5 3.4	95.0 4.7
L543 $\delta$ 1	28.5 0.6	23.9 1.2	19.9 1.8	72.5 1.7	57.6 2.1
L543 $\delta$ 2	28.5 0.6	23.9 1.2	19.9 1.8	72.5 1.7	57.6 2.1

T548γ2	29.0 1.0	25.5 1.9	16.5 3.3	108.4	3.9	90.1	5.1
V552γ1	23.4 0.6	21.1 0.9	17.7 1.7	102.2	2.5	83.1	3.0
V552γ2	30.3 1.4	27.4 2.7	28.1 6.4	123.9	5.9	83.8	7.7
A554β	18.1 0.6	17.2 1.0	14.0 1.9	105.6	3.6	101.5	4.7
V555γ1	25.4 0.6	18.5 0.8	15.6 1.7	94.1	2.1	80.9	2.7
V555γ2	18.7 0.9	15.0 1.3	13.0 2.5	87.5	3.7	68.3	4.3
M556ε1	8.4 0.2	9.9 0.3	8.3 0.5	73.5	1.2	68.4	1.3
L558δ1	24.3 1.0	17.9 1.4	16.7 3.1	77.0	3.5	78.6	4.6
L558δ2	21.3 0.6	16.0 0.8	15.1 2.1	79.0	2.2	66.6	2.7
V559γ1	21.5 0.6	18.6 0.9	15.4 1.6	94.5	2.5	80.1	2.9
V559γ2	19.2 1.0	17.7 1.8	15.5 3.8	95.1	4.4	89.0	6.3
I563γ2	21.2 0.5	16.0 0.8	14.5 1.6	109.7	2.8	111.0	4.1
I563δ1	16.3 0.8	15.6 1.2	14.7 2.5	100.5	4.2	100.9	5.7
L566δ1	23.2 0.7	19.0 1.1	17.7 2.6	59.4	2.0	53.3	2.4
L566δ2	18.8 0.4	13.7 0.5	11.3 1.0	51.9	1.2	41.2	1.1
T567γ2	25.8 0.4	21.2 0.6	15.4 0.9	52.9	0.9	38.8	0.9

**Table S-IX:**  $^2\text{H}$  relaxation rates [ $\text{s}^{-1}$ ] of PX (800 MHz)

Res	$R(D_z)$	$R(3D_z^2-2)$	$R(D_+^2)$	$R(D_+)$	$R(D_xD_z)$
I470γ2	19.3 0.1	15.6 0.0	13.3 0.0	44.0 0.4	34.4 0.1
I470δ1	11.3 0.1	9.3 0.1	7.3 0.1	22.4 0.7	16.5 0.2
I481γ2	19.1 0.1	15.6 0.0	13.3 0.0	44.0 0.4	34.4 0.1
I481δ1	11.0 0.1	9.1 0.0	7.4 0.0	23.7 0.4	19.4 0.1
I490γ2	19.3 0.1	15.6 0.0	13.3 0.0	44.0 0.4	34.4 0.1
I490δ1	11.0 0.1	9.1 0.0	7.4 0.0	23.7 0.4	19.4 0.1
V494γ1	23.6 0.2	18.4 0.1	15.3 0.1	45.4 0.8	33.9 0.3
V494γ2	19.0 0.1	14.7 0.1	12.8 0.1	36.4 0.7	27.2 0.2
T500γ2	24.3 0.2	18.9 0.1	16.5 0.1	44.1 1.0	34.9 0.3
A504β	22.7 0.2	17.4 0.1	15.3 0.1	40.9 0.6	32.6 0.2
A507β	23.1 0.2	17.2 0.1	15.3 0.1	40.9 0.6	32.6 0.2
L511δ1	20.5 0.1	14.0 0.1	12.9 0.1	35.0 0.7	25.7 0.2
L511δ2	17.3 0.1	12.5 0.1	11.0 0.1	31.7 0.7	24.4 0.2
T518γ2	19.4 0.6	17.9 0.3	15.6 0.4	105.5 4.8	90.5 2.2

M519 $\varepsilon$ 1	5.9 0.1	5.0 0.0	4.1 0.0	18.6	0.4	18.7	0.1
L522 $\delta$ 1	19.7 2.6	19.1 1.1	11.5 1.8	73.3	20.9	71.1	10.3
L522 $\delta$ 2	15.9 0.6	15.9 0.3	12.7 0.4	96.4	5.4	78.0	2.5
L524 $\delta$ 1	20.8 0.2	15.3 0.1	14.0 0.1	49.6	1.1	39.0	0.4
L524 $\delta$ 2	20.2 0.2	14.2 0.1	12.7 0.1	47.4	1.1	37.7	0.4
V525 $\gamma$ 1	27.3 0.6	19.8 0.4	21.1 0.5	110.7	4.3	96.4	2.7
V525 $\gamma$ 2	13.7 0.4	12.9 0.2	10.1 0.3	99.4	4.4	87.8	2.0
I526 $\gamma$ 2	16.4 0.8	12.3 0.5	13.7 0.7	117.0	8.6	108.5	4.8
I526 $\delta$ 1	8.9 0.5	12.4 0.4	11.3 0.5	94.3	6.3	81.6	3.0
L531 $\delta$ 1	27.7 1.0	21.7 0.6	18.0 0.7	91.0	5.4	90.4	3.5
L531 $\delta$ 2	17.9 0.4	14.2 0.2	13.8 0.3	82.6	3.0	74.7	1.6
A534 $\beta$	23.1 0.9	19.3 0.4	18.1 0.6	127.2	7.7	114.9	3.9
A537 $\beta$	16.4 0.6	14.1 0.3	12.6 0.4	115.8	6.3	107.0	3.0
A538 $\beta$	17.6 0.7	14.1 0.4	15.6 0.5	123.8	7.3	114.7	3.7
V540 $\gamma$ 1	34.4 0.7	22.5 0.4	23.0 0.5	117.7	4.5	104.8	3.2
V540 $\gamma$ 2	15.3 0.6	11.9 0.3	13.6 0.5	95.6	5.8	84.7	2.8
L543 $\delta$ 1	27.8 0.4	23.3 0.3	17.5 0.3	73.8	2.2	58.1	1.1
L543 $\delta$ 2	27.8 0.4	23.3 0.3	17.5 0.3	73.8	2.2	58.1	1.1
T548 $\gamma$ 2	26.8 0.8	18.8 0.4	19.6 0.6	108.7	5.2	96.2	2.8
V552 $\gamma$ 1	20.3 0.5	14.9 0.3	14.7 0.4	99.6	3.9	94.1	2.2
V552 $\gamma$ 2	30.4 1.6	22.1 1.0	20.8 1.3	106.7	10.5	103.2	6.5
A554 $\beta$	15.8 0.6	13.4 0.3	12.0 0.4	99.3	6.0	93.5	2.6
V555 $\gamma$ 1	23.3 0.4	15.9 0.3	17.2 0.4	96.5	3.4	87.8	2.0
V555 $\gamma$ 2	17.8 0.8	12.4 0.5	13.5 0.7	92.7	8.1	78.0	3.7
M556 $\varepsilon$ 1	6.5 0.2	6.8 0.1	5.7 0.1	68.5	2.2	70.4	0.9
L558 $\delta$ 1	27.1 1.3	13.9 0.6	17.3 1.0	80.0	8.0	86.1	4.5
L558 $\delta$ 2	18.2 0.4	15.0 0.3	12.2 0.4	76.6	3.4	69.7	1.8
V559 $\gamma$ 1	18.0 0.4	14.1 0.2	14.1 0.3	98.4	3.6	86.8	1.9
V559 $\gamma$ 2	19.6 0.9	13.5 0.6	18.6 1.0	84.2	8.1	84.5	5.5
I563 $\gamma$ 2	15.4 0.6	15.3 0.3	13.0 0.4	131.5	6.1	104.1	2.6
I563 $\delta$ 1	14.2 0.7	11.1 0.4	9.7 0.5	96.8	6.6	97.9	3.8
L566 $\delta$ 1	21.8 1.1	14.1 0.4	15.0 0.6	62.0	5.4	69.7	2.8
L566 $\delta$ 2	16.6 0.3	13.3 0.2	11.2 0.2	52.4	1.8	44.6	0.7
T567 $\gamma$ 2	23.0 0.3	17.4 0.1	14.7 0.1	53.6	1.3	40.4	0.4

**Table S-X:** Methyl side-chain model-free parameters from  $^2\text{H}$  relaxation rates (600 & 800 MHz)

Res	$S_{axis}^2$	$\tau_e$ [ps]	$\tau_c$ [ns]
I470 $\gamma$ 2	0.497 0.005	40.9 0.4	3.33 0.03
I470 $\delta$ 1	0.289 0.009	21.2 0.6	2.56 0.06
I481 $\gamma$ 2	0.502 0.005	40.6 0.3	3.30 0.03
I481 $\delta$ 1	0.282 0.005	23.0 0.3	3.25 0.05
I490 $\gamma$ 2	0.497 0.005	40.9 0.3	3.32 0.03
I490 $\delta$ 1	0.280 0.005	23.1 0.3	3.27 0.05
V494 $\gamma$ 1	0.481 0.013	51.4 0.9	3.01 0.07
V494 $\gamma$ 2	0.389 0.009	41.2 0.6	2.97 0.06
T500 $\gamma$ 2	0.468 0.015	55.6 1.0	3.03 0.08
A504 $\beta$	0.433 0.011	50.6 0.7	3.16 0.07
A507 $\beta$	0.414 0.011	51.5 0.7	3.28 0.07
L511 $\delta$ 1	0.264 0.010	47.2 0.6	4.04 0.14
L511 $\delta$ 2	0.269 0.009	39.3 0.6	3.72 0.11
T518 $\gamma$ 2	0.740 0.011	57.3 1.3	7.64 -
M519 $\varepsilon$ 1	0.230 0.004	11.9 0.3	4.71 0.08
L522 $\delta$ 1	0.552 0.046	69.3 4.7	7.64 -
L522 $\delta$ 2	0.648 0.012	49.1 1.3	7.64 -
L524 $\delta$ 1	0.240 0.002	55.3 0.4	7.64 -
L524 $\delta$ 2	0.239 0.002	51.0 0.4	7.64 -
V525 $\gamma$ 1	0.750 0.013	70.3 1.4	7.64 -
V525 $\gamma$ 2	0.732 0.011	34.6 0.9	7.64 -
I526 $\gamma$ 2	0.907 0.023	34.9 2.1	7.64 -
I526 $\delta$ 1	0.730 0.015	29.8 1.4	7.64 -
L531 $\delta$ 1	0.658 0.019	74.8 2.5	7.64 -
L531 $\delta$ 2	0.600 0.008	45.3 0.9	7.64 -
A534 $\beta$	0.936 0.020	62.2 1.9	7.64 -
A537 $\beta$	0.876 0.015	38.8 1.3	7.64 -
A538 $\beta$	0.971 0.018	41.7 1.7	7.64 -
V540 $\gamma$ 1	0.747 0.015	84.1 1.7	7.64 -
V540 $\gamma$ 2	0.731 0.013	35.4 1.3	7.64 -
L543 $\delta$ 1	0.884 0.042	55.2 2.7	3.52 0.15
L543 $\delta$ 2	0.884 0.042	55.2 2.7	3.52 0.15

T548 $\gamma$ 2	0.746 0.014	64.9 1.7	7.64	-
V552 $\gamma$ 1	0.738 0.011	48.0 1.1	7.64	-
V552 $\gamma$ 2	0.773 0.032	73.4 3.4	7.64	-
A554 $\beta$	0.812 0.013	37.2 1.3	7.64	-
V555 $\gamma$ 1	0.672 0.009	54.1 1.0	7.64	-
V555 $\gamma$ 2	0.624 0.018	38.7 1.8	7.64	-
M556 $\epsilon$ 1	0.617 0.004	13.1 0.4	7.64	-
L558 $\delta$ 1	0.578 0.020	50.2 2.1	7.64	-
L558 $\delta$ 2	0.541 0.008	48.4 1.1	7.64	-
V559 $\gamma$ 1	0.701 0.009	44.4 1.0	7.64	-
V559 $\gamma$ 2	0.695 0.024	42.1 2.3	7.64	-
I563 $\gamma$ 2	0.893 0.013	43.4 1.1	7.64	-
I563 $\delta$ 1	0.828 0.018	28.5 1.8	7.64	-
L566 $\delta$ 1	0.395 0.012	51.4 1.5	7.64	-
L566 $\delta$ 2	0.312 0.004	45.8 0.5	7.64	-
T567 $\gamma$ 2	0.530 0.019	49.9 1.3	3.69	0.11