SUPPORTING INFORMATION

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SUPPORTING FIGURES AND TABLES

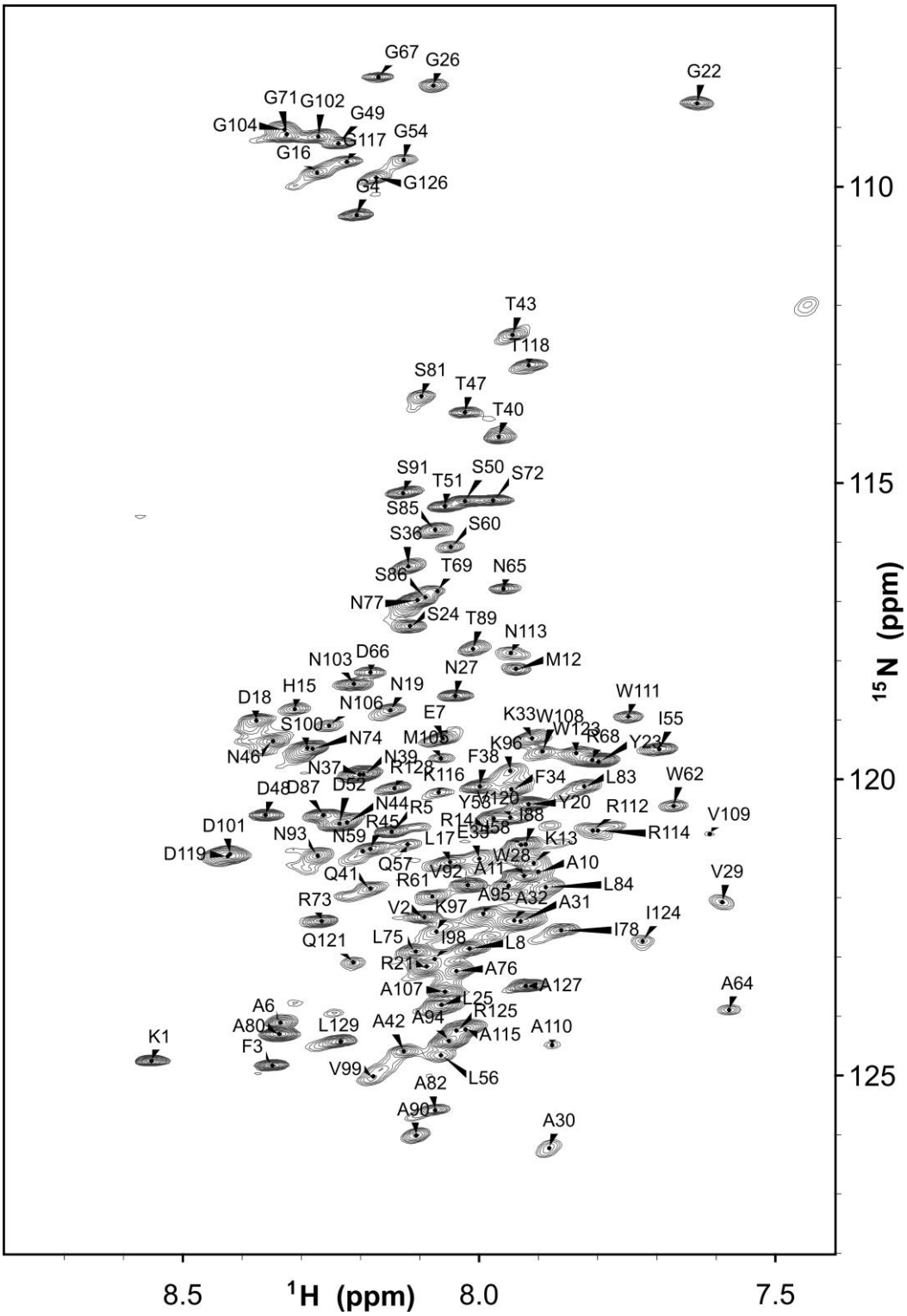


Figure S1: ^{1}H-^{15}N-HSQC of WT^{Ala} measured at 600MHz, 293K and a protein concentration of 300µM in water pH 2.0.

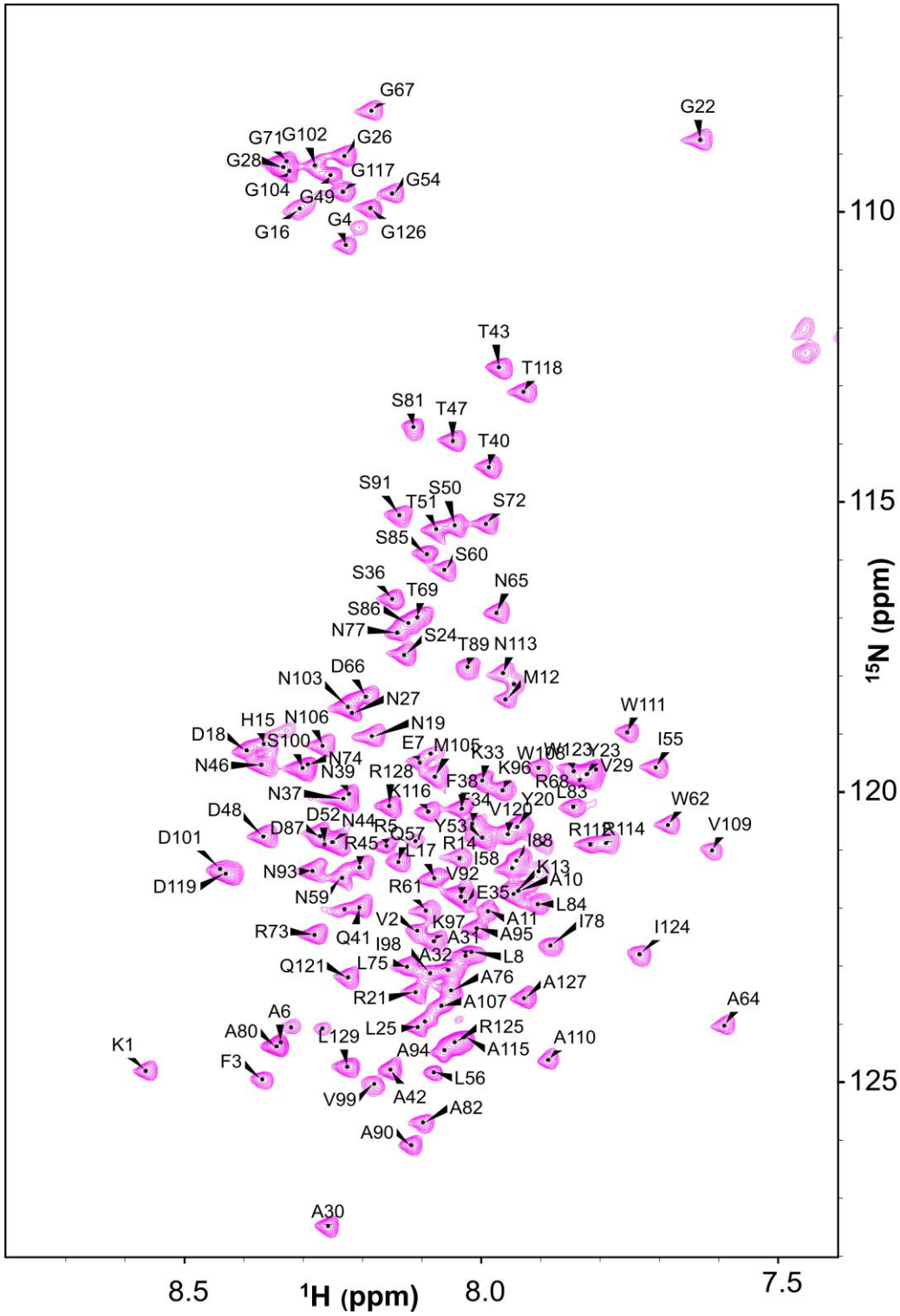


Figure S2: ^{1}H-^{15}N-HSQC of W28G measured at 600MHz, 293K and a protein concentration of 300µM in water pH 2.0.

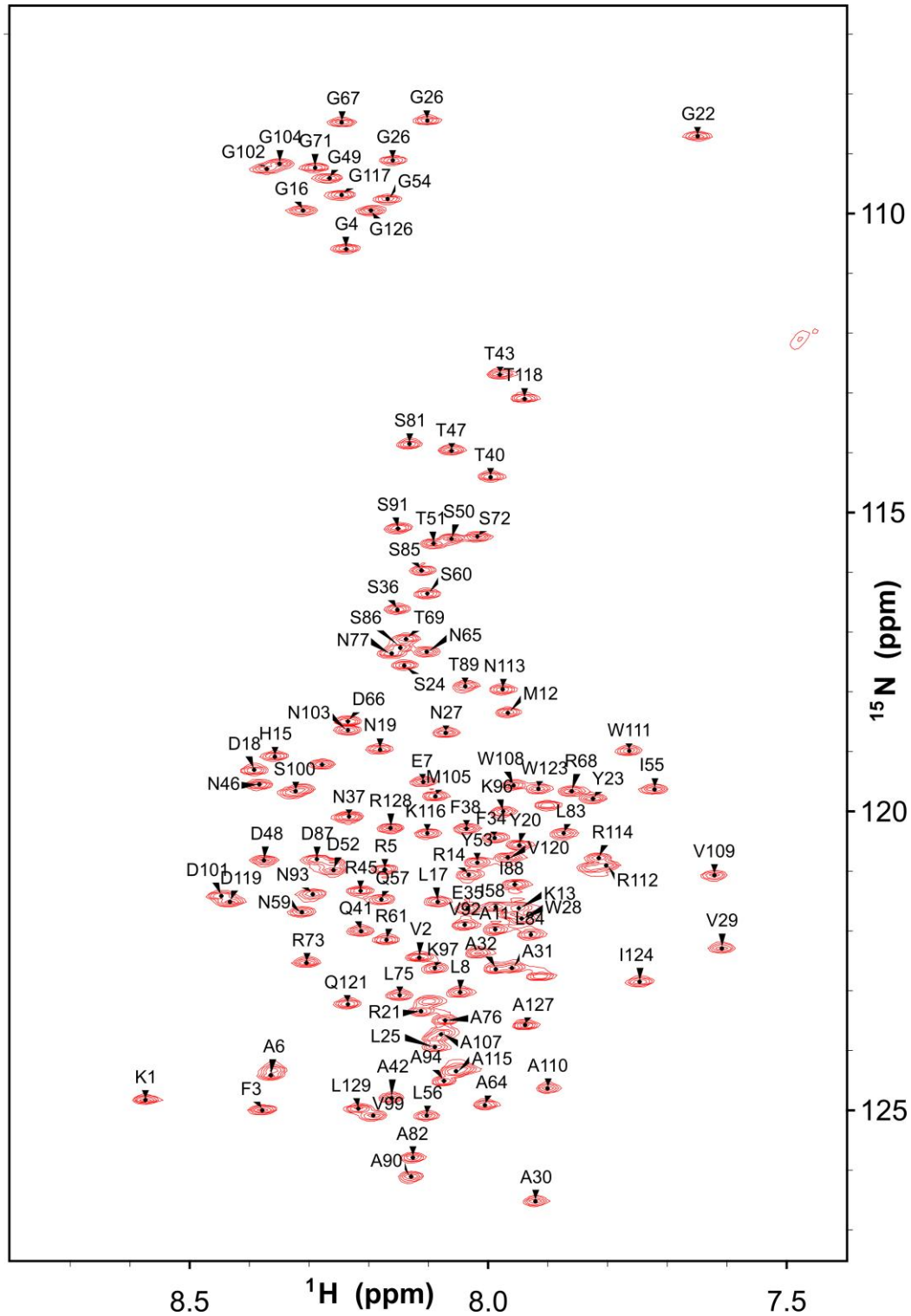


Figure S3: ^{1}H-^{15}N-HSQC of W62G measured at 600MHz, 293K and a protein concentration of 300µM in water pH 2.0.

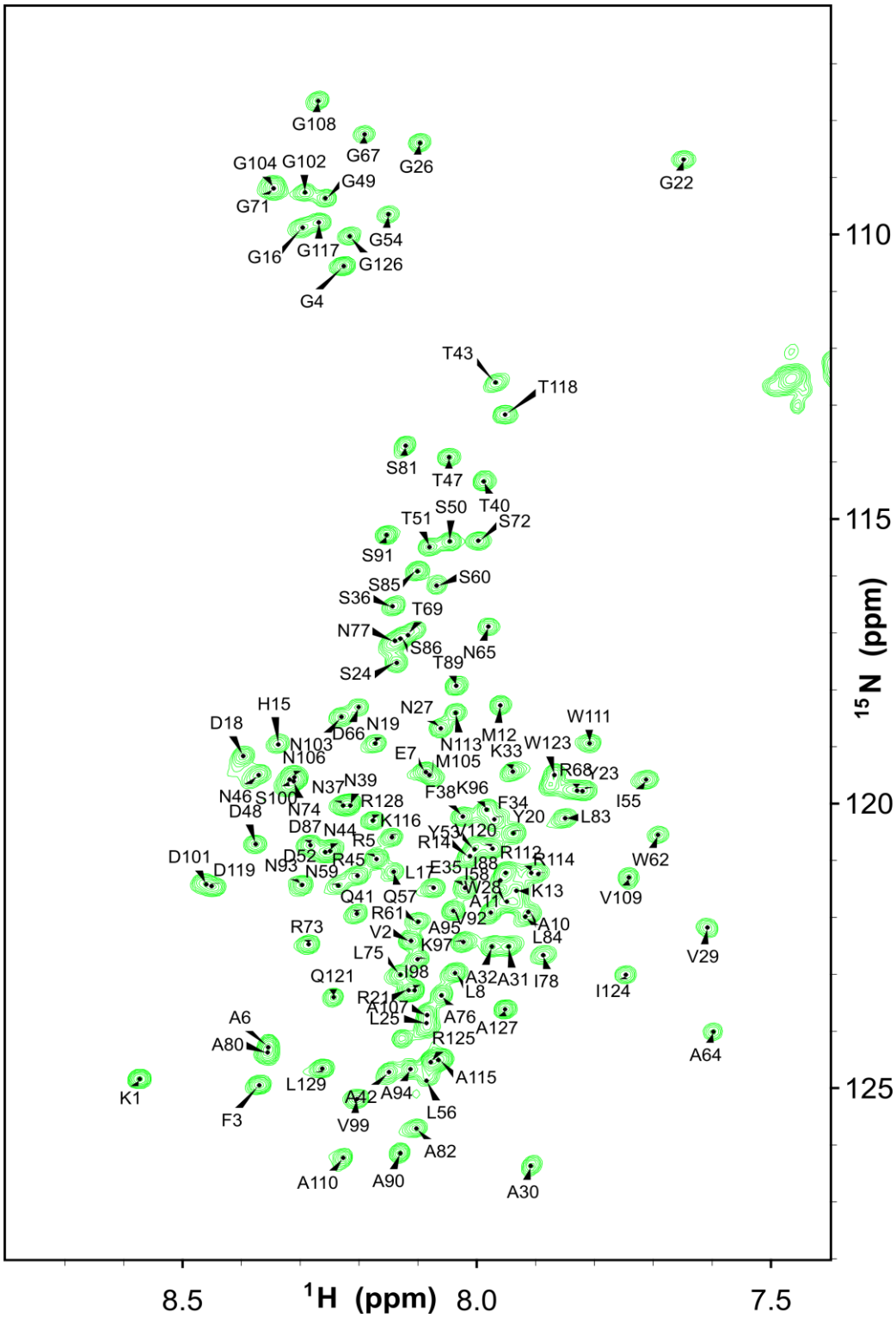


Figure S4: ^{1}H-^{15}N-HSQC of W108G measured at 600MHz, 293K and a protein concentration of 300µM in water pH 2.0.

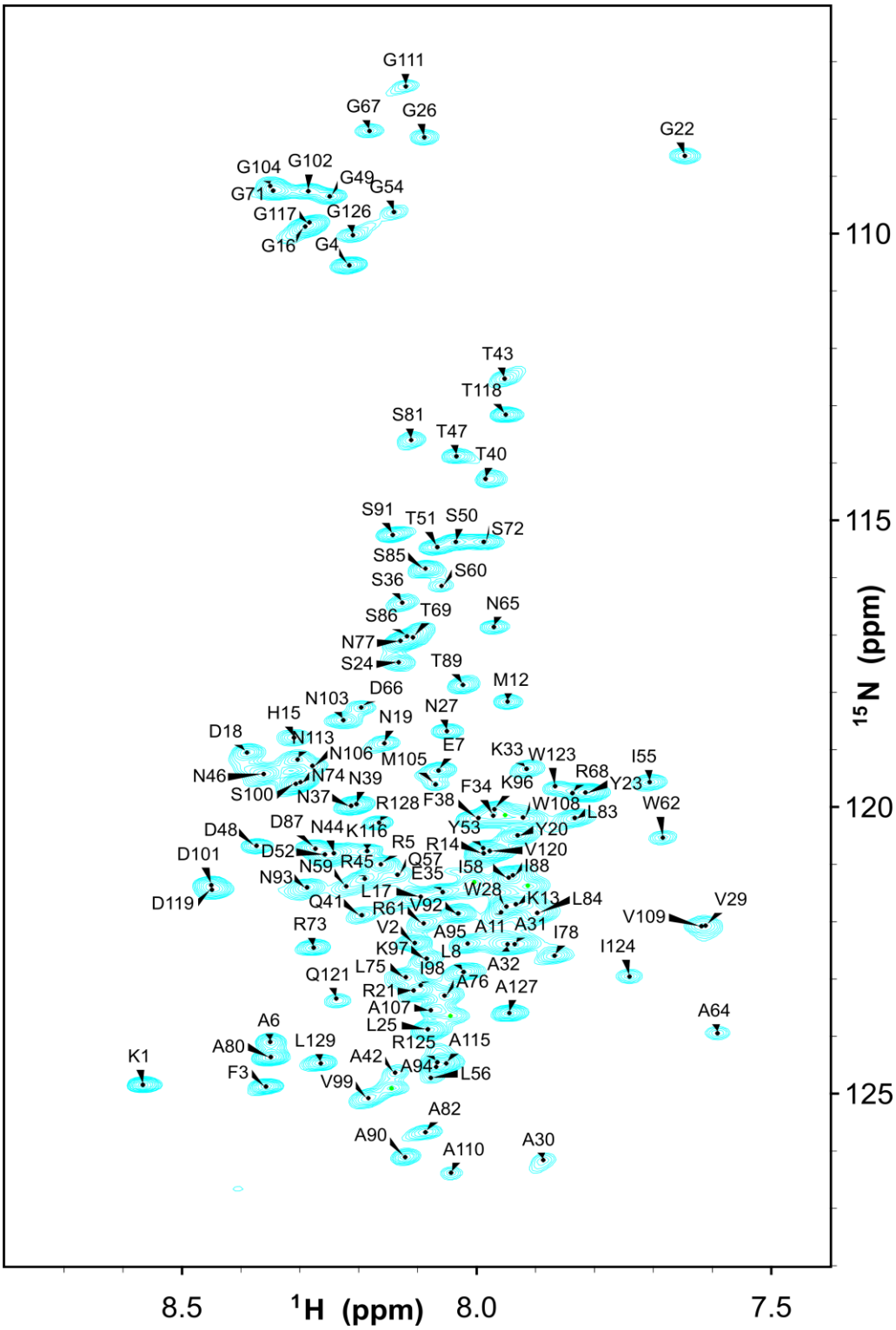


Figure S5: ^{1}H-^{15}N-HSQC of W111G measured at 600MHz, 293K and a protein concentration of 300µM in water pH 2.0.

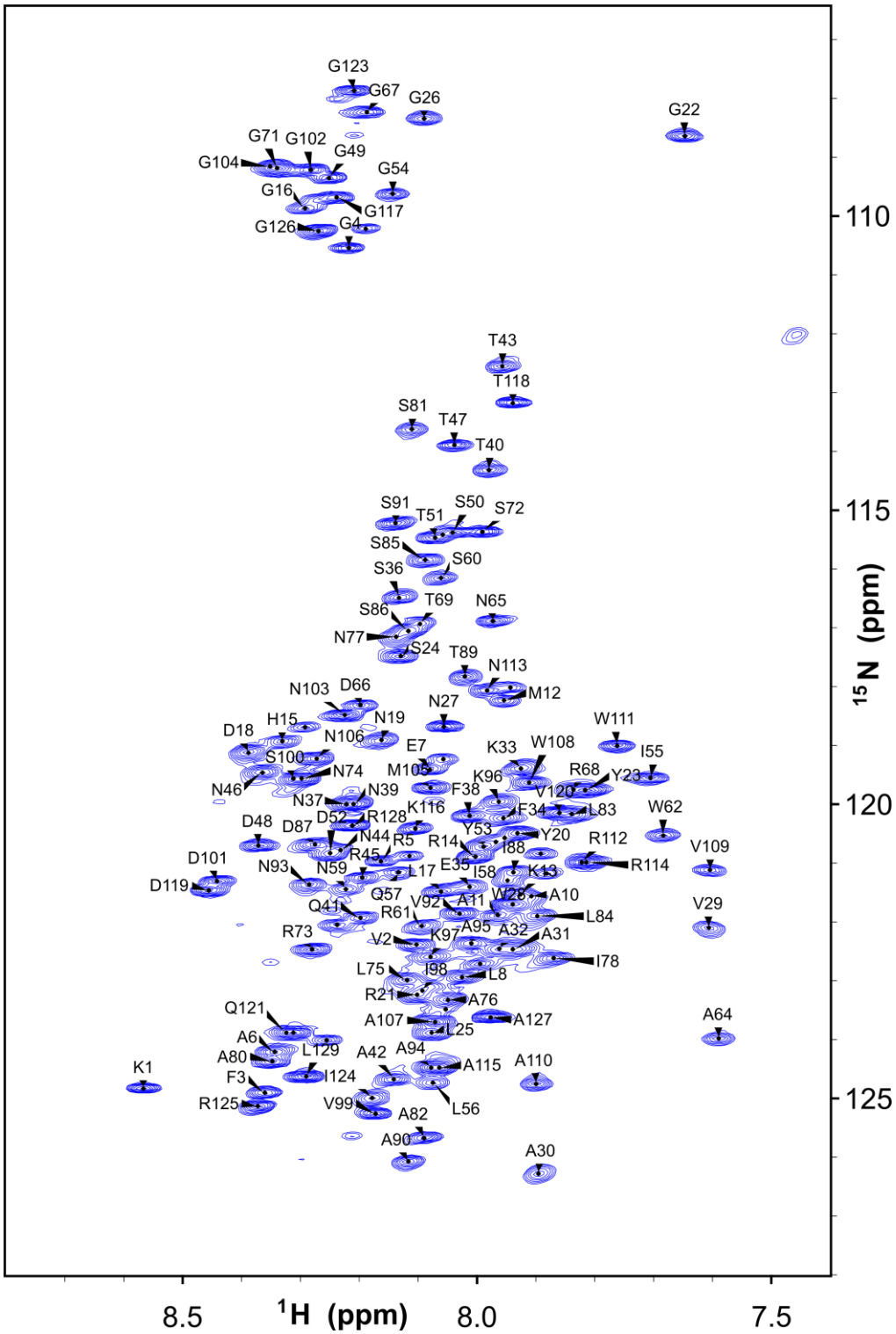


Figure S6: ^{1}H-^{15}N-HSQC of W123G measured at 600MHz, 293K and a protein concentration of 300µM in water pH 2.0.

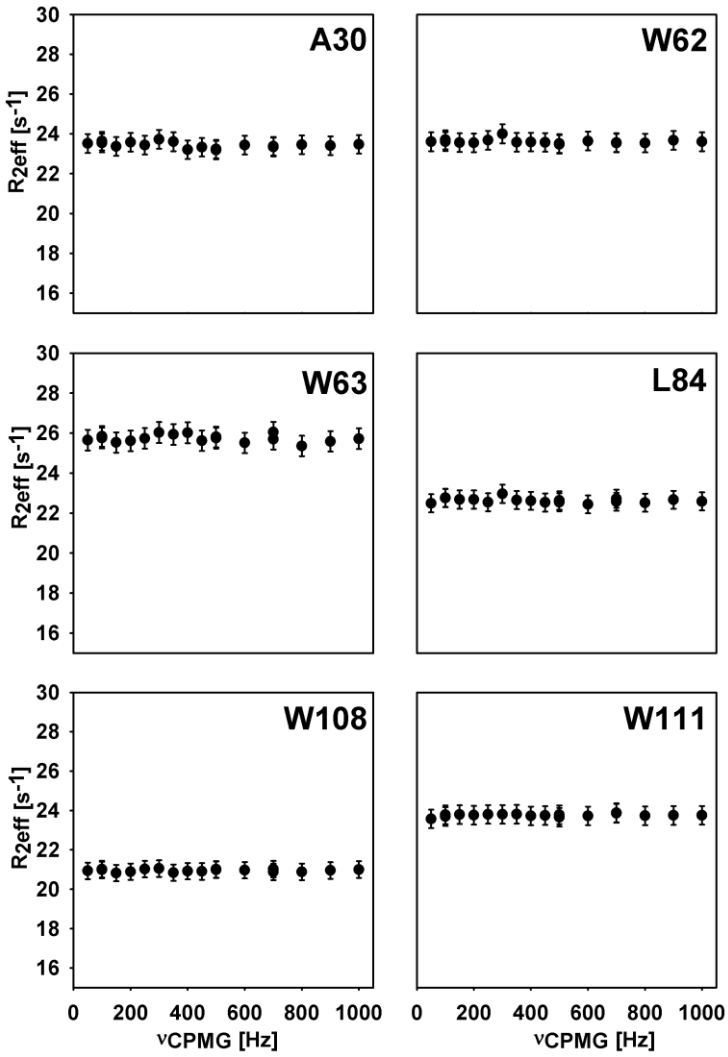
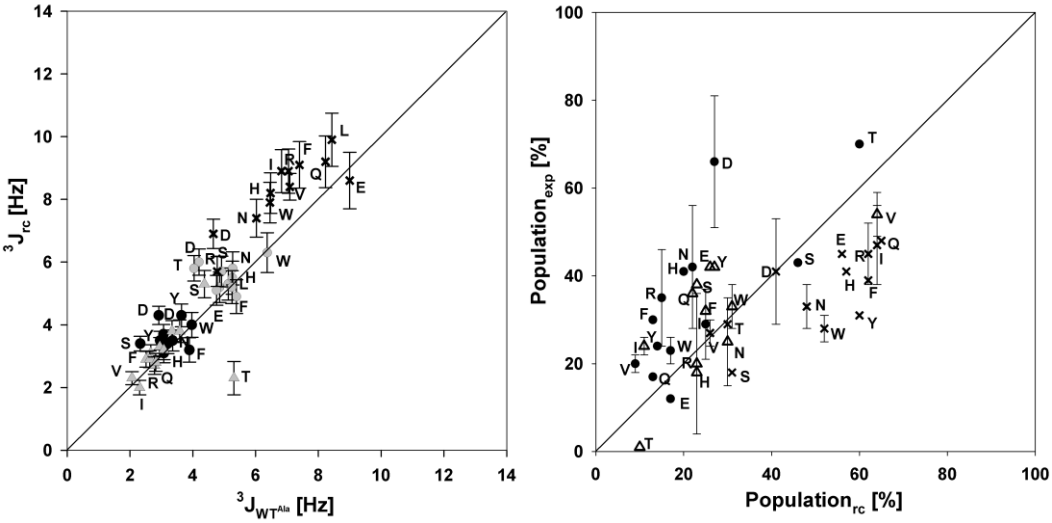


Figure S7: Relaxation dispersion data of WT^{Ala} for exemplary amino acids A30, W62, W63, L84, W108, W111.



S8: $^3J(CO,H^\beta)$ and $^3J(H^\alpha,H^\beta)$ coupling constants of WT^{Ala} (left) compared with random-coil predictions; black circle: $^3J(H^\alpha,H^{\beta2})$, grey triangle: $^3J(H^\alpha,H^{\beta3})$, black cross: $^3J(CO,H^{\beta2})$, grey circle: $^3J(CO,H^{\beta3})$. Right: Mean percentage populations of WT^{Ala} vs. random-coil (cross: -60°, circle: 60°, triangle: 180°). All experiments have been carried out at field strength corresponding to a ^1H frequency of 600MHz, using 300µM protein at pH2, T=293K.

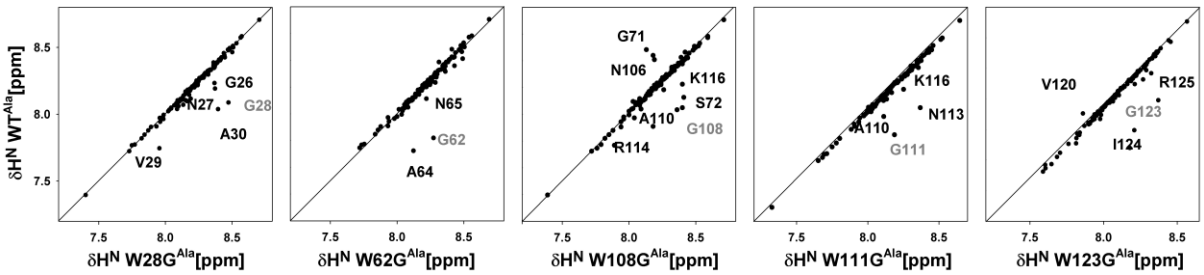


Figure S9: H^N chemical shift correlation of the mutants versus wildtype. The mutation site is highlighted (grey) deviating residues are indicated. All experiments were performed at field strength corresponding to a ^1H frequency of 600MHz, using 300µM ^{15}N-labelled protein at pH2, T=293K

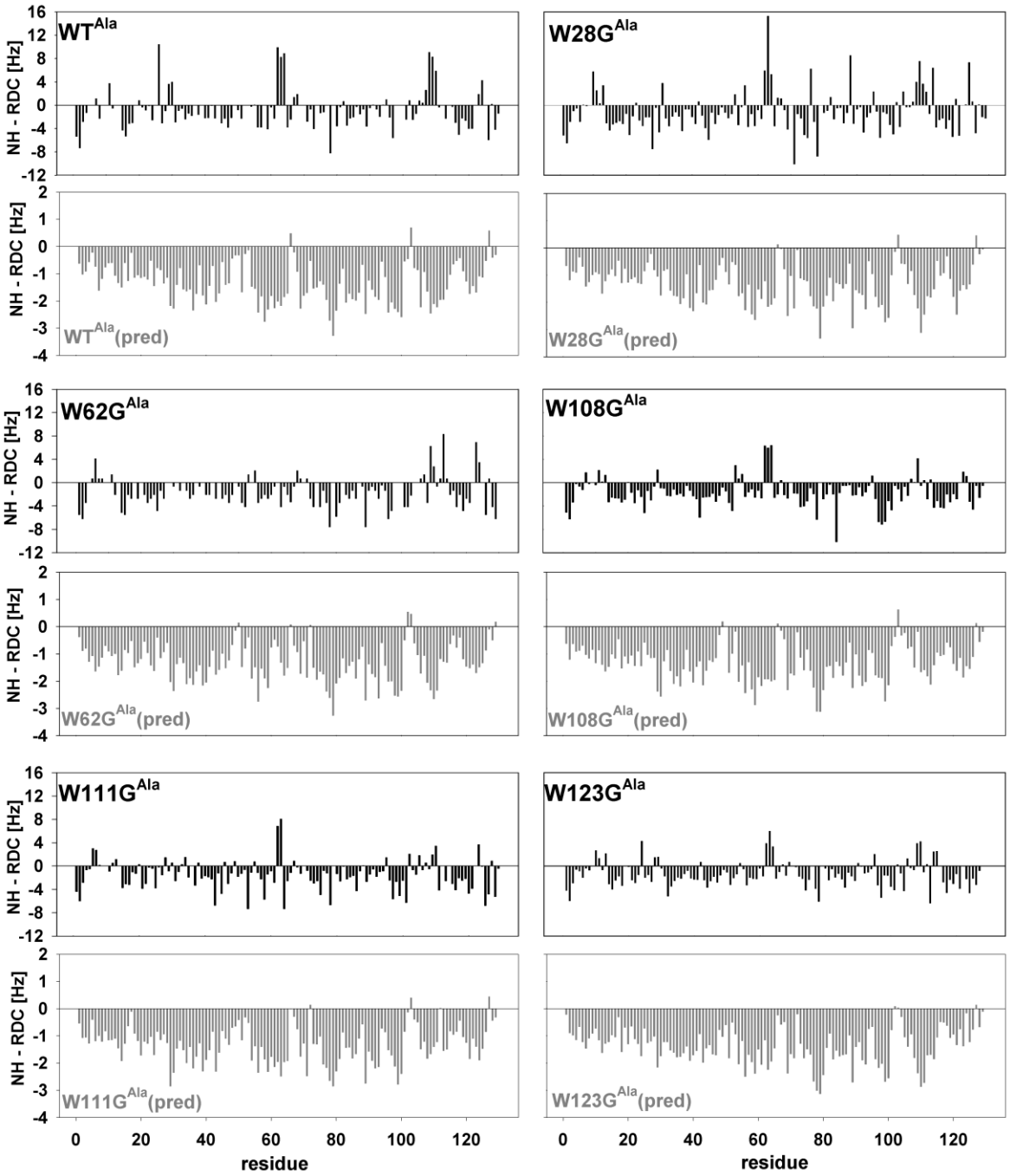


Figure S10: Experimental and predicted RDCs of WT^{Ala} and the mutants $W28G^{Ala}$, $W62G^{Ala}$, $W108G^{Ala}$, $W111G^{Ala}$, $W123G^{Ala}$, black: experimental; grey: predicted from flexible meccano.

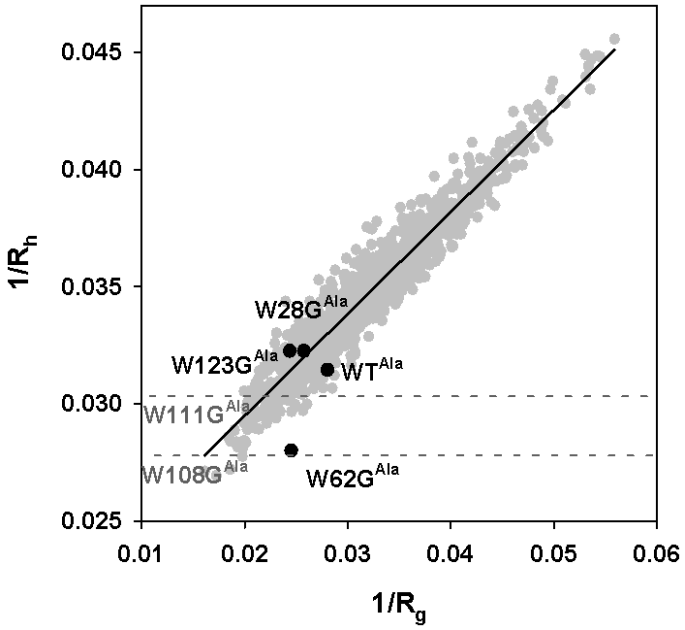


Figure S11: 1/Rh from NMR diffusion measurements of WT^{Ala} and five mutants plotted against $1/R_g$ obtained from SAXS measurements (data fit by EOM).

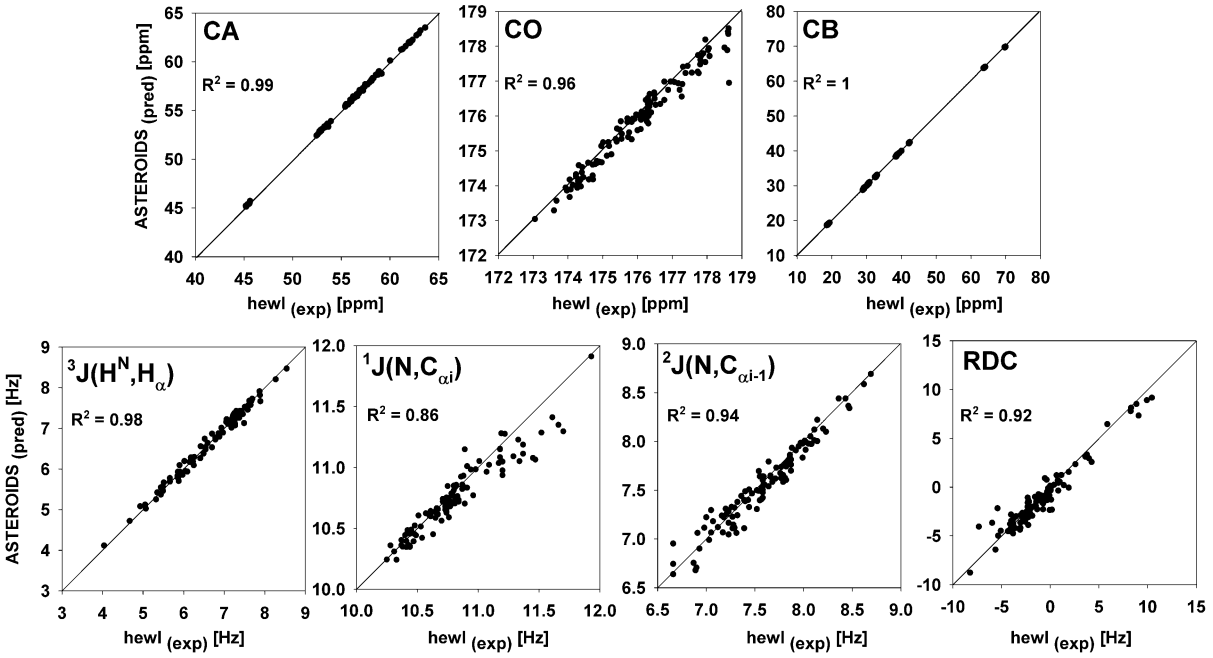


Figure S12: ASTEROIDS correlation **of** experimental chemical shifts, J-couplings and RDCs with predictions from ASTEROIDS calculations.

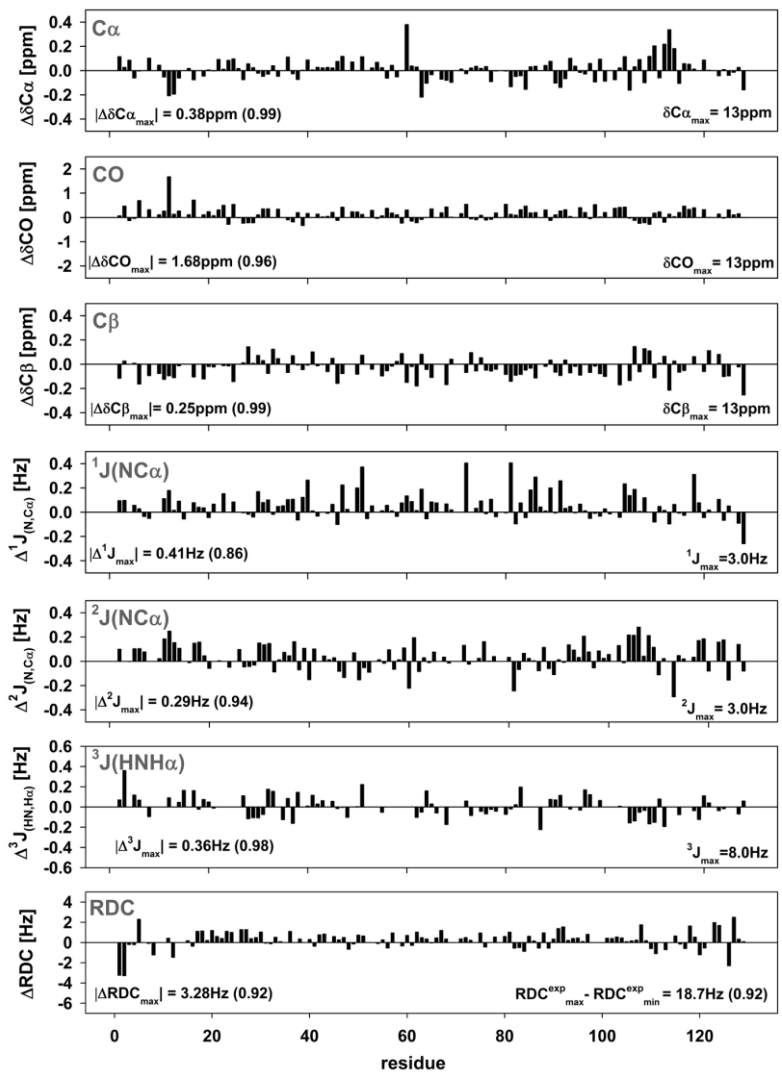


Figure S13: Differences of experimental data and data from ASTEROIDS calculations of chemical shifts (C_α, CO, C_β) and coupling constants ($^3J(H^N,H_\alpha)$, $^1J(N,C_{\alpha i})$, $^2J(N,C_{\alpha i-1})$, and RDC; data derive from backcalculation of selected structures (200 pdbs) of a flexible meccano ensemble of 15.000 structures. Absolute maximum Δ values (left) are provided, with R^2 correlation between experimental and predicted data in brackets. Maximal data spread of chemical shift δ_{max} data is given by the BMRB database (http://www.bmrb.wisc.edu/). Maximal data spread of coupling constants $^1J_{max}$, $^2J_{max}$ and $^3J_{max}$ is given by[1-3]. Maximal data spread of RDC data (RDC^{exp}_{max}-RDC^{exp}_{min}) is given by experimental data.

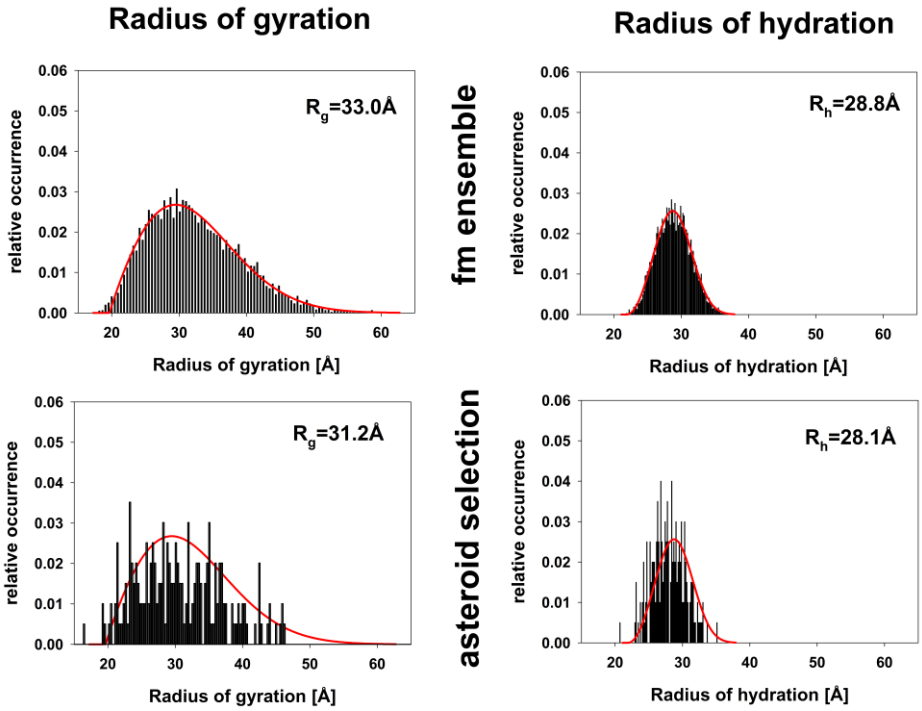


Figure S14: Comparison of R_g and R_h of the ensemble from flexible meccano and selected ensembles from ASTEROIDS.

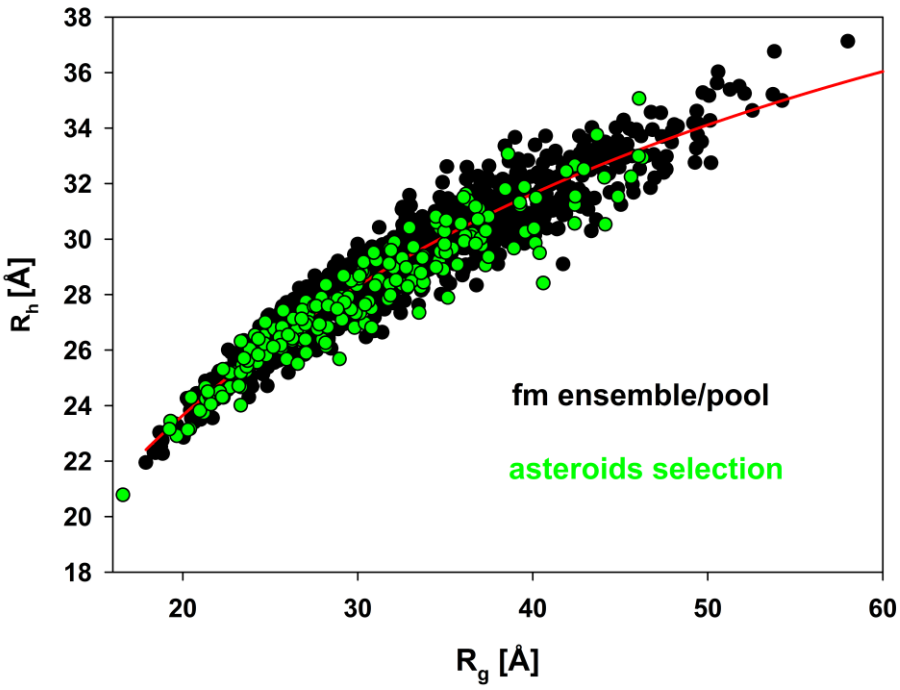
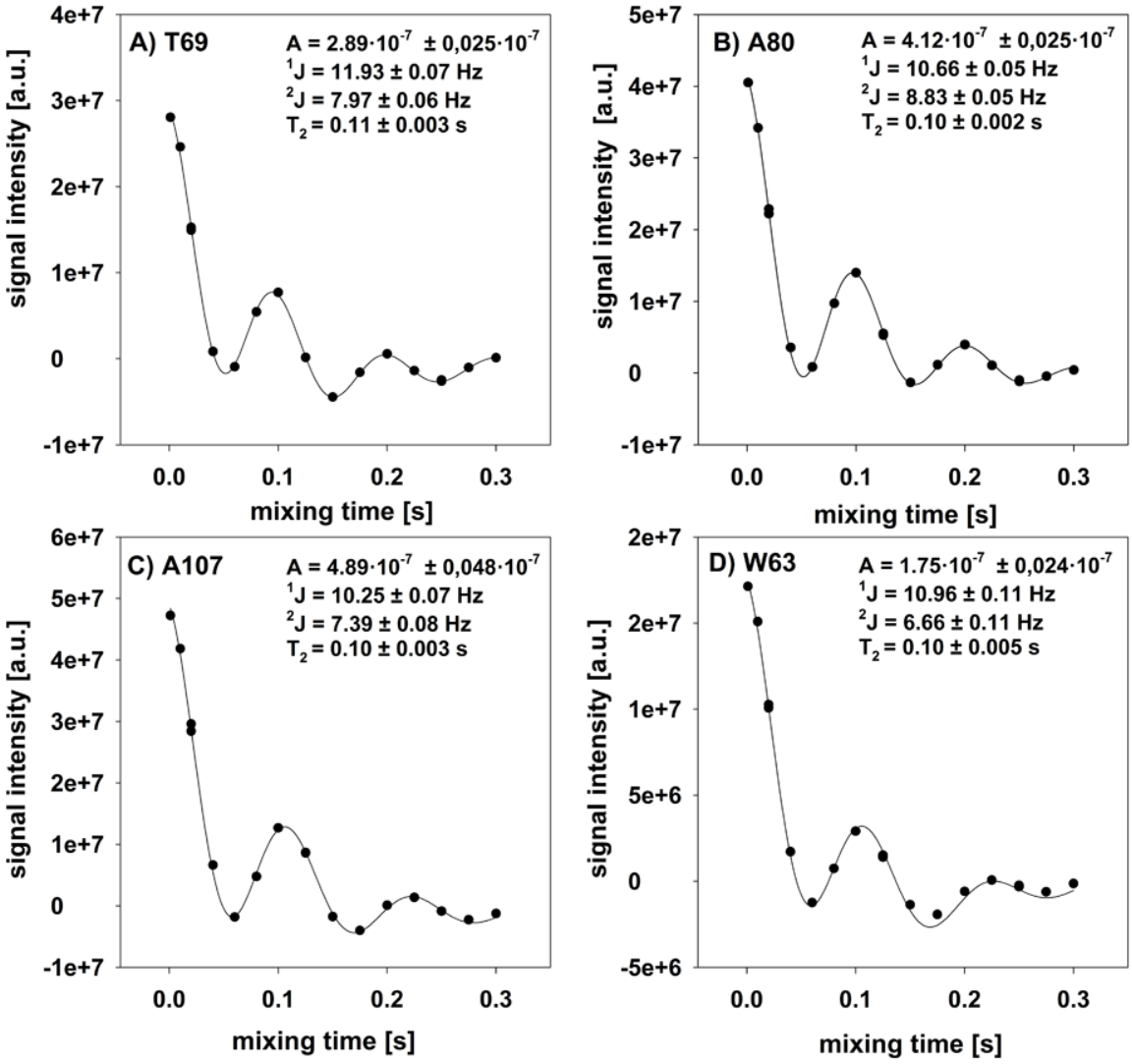


Figure S15: Correlation of R_g and R_h of ensembles from flexible meccano and selected ensembles from ASTEROIDS.



Fitting function: $I_{NC\alpha}^{\exp} = A\cos(\pi\,{}^{1}J\tau)\cos(\pi\,{}^{2}J\tau)\cdot e^{\frac{-\tau}{T_2}}$

Figure S16: Evolution profiles of residues (A) T69, (B) A80, (C) A107 and (D) W63 for the determination of $^{1}J(N_i, C^{\alpha}_i)$ and $^{2}J(NC^{\alpha}_{i-1})$. Fitting function and parameters are given.

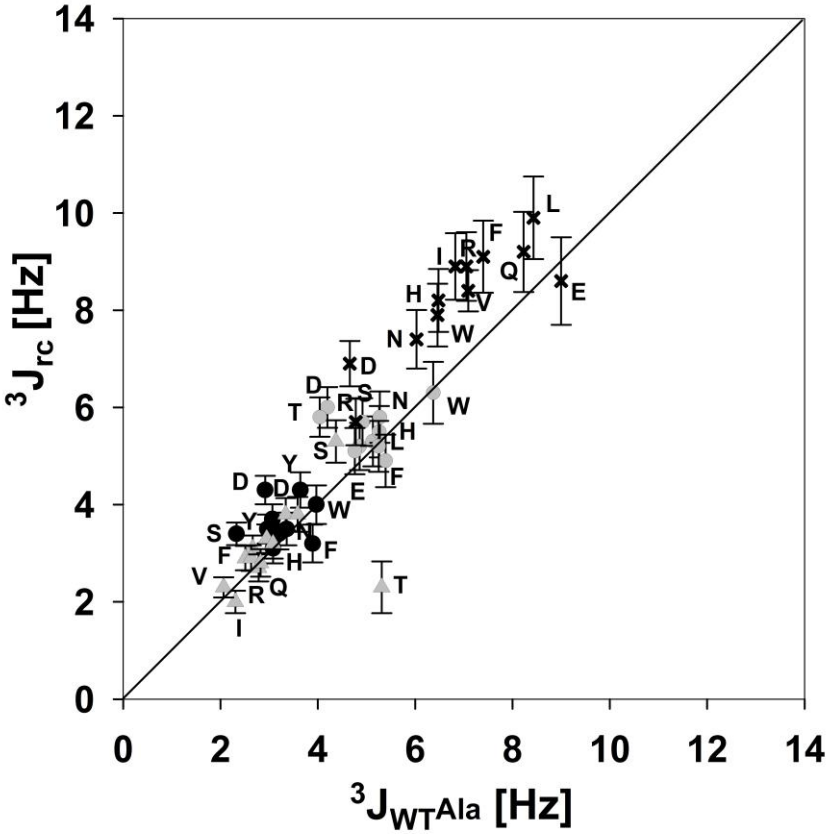


Figure S17: Blow-up of the upper left graph of Figure 5

Table S1: table of chemical shifts $^{1}H_{N}$, ^{15}N, $^{1}H^{\alpha}$, $^{1}H^{\beta2\beta3}$, $^{13}C^{\alpha}$, $^{13}C^{\beta}$, $^{13}C'$ [ppm], $^{3}J(H^{\alpha},H^{\beta})$, $^{3}J(CO,H^{\beta})$ [Hz], $^{1}J(NC^{\alpha})$ and $^{2}J(NC^{\alpha})$, of WT^{Ala}.

	$^{1}H_{N}$	^{15}N	$^{1}H^{\alpha}$	$^{1}H^{\beta2}$	$^{1}H^{\beta3}$	$^{13}C^{\alpha}$	$^{13}C^{\beta}$	$^{13}C'$	$^{3}J_{\alpha\beta2}$	$^{3}J_{\alpha\beta3}$	$\sum_{J\alpha\beta}$	$^{3}J_{C'\beta2}$	$^{3}J_{C'\beta3}$	$\sum_{JC'\beta}$	$^{1}J_{NC}{}^{\alpha}$	$\Delta^{1}J_{NC}{}^{\alpha}$	$^{2}J_{NC}{}^{\alpha}$	$\Delta^{2}J_{NC}{}^{\alpha}$
K1	8.71	126.11	4.41	1.25		56.23	32.82	173.33	7.86						10.88	0.06	9.10	0.06
V2	8.25	123.71	4.14		1.53	61.83	32.79	173.41		7.31			2.01		10.80	0.06	8.59	0.06
F3	8.51	126.24	4.70	2.55	2.69	57.50	39.80	173.95	7.40	5.13		3.59	2.79		11.18	0.04	8.11	0.04
G4	8.36	111.82	3.99				45.02	171.91										
R5	8.31	122.25	4.25	1.42	1.86	57.02	30.31	174.81	7.66	5.36				3.72	10.75	0.08	8.69	0.09
A6	8.49	125.48	4.29	0.97		53.22	18.52	176.44			8.68			7.03	10.48	0.07	7.17	0.08
E7	8.22	120.72	4.30	1.57		56.62	28.01	174.69	7.78					3.68	10.45	0.07	7.58	0.08
L8	8.17	124.22				55.85	41.92	175.66							10.42	0.07	7.32	0.08
A9				0.98							8.68							
A10	8.04	122.87	4.24	0.98		53.47	18.47	176.48			8.86							
A11	8.11	123.13	4.25	0.99		53.39	18.41	176.47			8.67			6.93	10.74	0.07	7.52	0.08
M12	8.09	119.51	4.22	1.63		56.02	32.46	176.49			7.74				10.63	0.08	7.23	0.09
K13	8.06	122.81	4.29			56.69	32.51	174.74							10.53	0.07	7.31	0.08
R14	8.15	122.21	4.30	1.32		56.38	30.38	174.15	7.05					3.67	10.77	0.08	7.55	0.09
H15	8.46	120.17	4.74	2.86	2.74	55.38	28.70	172.65	6.48	5.26		3.36	2.95		11.22	0.07	8.02	0.08
G16	8.43	111.09	4.01				45.13	171.83										
L17	8.20	122.70	4.39	1.18		55.23	42.20	175.13	7.93					3.24	10.81	0.08	8.43	0.09
D18	8.53	120.36	4.68	2.32	2.40	52.82	37.64	172.56	5.96	4.78				3.55	10.88	0.07	7.79	0.08
N19	8.30	120.16	4.71	2.23	2.28	52.91	38.30	172.57	6.40	5.67				3.82	10.80	0.06	7.99	0.06
Y20	8.07	121.73	4.55	2.53	2.63	58.10	38.30	173.62	8.48	6.94				4.59	10.94	0.07	7.60	0.08
R21	8.25	124.54	4.23	1.18	1.32	56.09	30.11	174.14	7.39	5.11		3.04	2.68		10.43	0.07	7.58	0.08
G22	7.77	109.88	3.89				45.03	171.46										
Y23	7.94	121.02	4.61	2.47	2.54	57.77	38.78	173.69	7.16	5.59		3.87	3.03		11.20	0.08	8.01	0.09
S24	8.27	118.77	4.47	3.67	3.36	57.92	63.90	172.17			5.84		4.44		11.31	0.06	7.95	0.06
L25	8.23	125.17	4.35	1.18		55.51	42.01	175.62	7.88					3.49	10.44	0.08	7.59	0.08
G26	8.23	109.59	3.87				45.21	171.79										
N27	8.19	119.93	4.73			53.08	38.41	172.87							10.98	0.07	8.46	0.08
W28	8.09	122.98	4.61	2.81		57.91	29.07	174.10			7.38			5.06	10.44	0.07	7.21	0.07
V29	7.75	123.47	3.87		1.46	62.52	32.58	173.57		7.33			2.12		10.45	0.11	7.18	0.11
A30	8.04	127.55	4.22	0.91		52.62	18.66	175.69						6.90	10.76	0.07	7.29	0.07
A31	8.10	123.75	4.23	0.92		52.64	18.70	175.93			8.91			6.81	10.74	0.06	7.79	0.06
A32	8.12	123.79	4.23	0.89		52.64	18.69	175.93			8.95			6.97	10.74	0.06	7.79	0.06
K33	8.07	120.70	4.20	1.24		56.62	32.54	174.35	7.43						10.61	0.07	7.77	0.08
F34	8.11	121.59	4.62	2.88	2.98	57.89	39.25	173.59				4.17	2.69		10.88	0.07	7.40	0.08
E35	8.16	122.68	4.36	1.49	1.63	55.55	28.53	173.60	9.00	4.86		3.20	2.66		10.77	0.08	7.66	0.09
S36	8.27	117.77	4.38	3.66	3.37	58.59	63.67	172.09		4.99					11.33	0.05	8.05	0.06
N37	8.35	121.28	4.70	2.24		53.32	38.54	172.82	6.52					4.07	10.84	0.06	7.57	0.06
F38	8.15	121.48	4.60	2.85	2.99	58.01	39.09	173.40			7.75	3.92	2.05		10.86	0.06	7.57	0.07
N39	8.35	121.25	4.76	2.26	2.39	53.24	38.49	173.38	5.10	4.90		3.31	3.92		10.84	0.06	7.57	0.06
T40	8.12	115.60	4.32	4.14		62.13	69.50	172.64					5.53		11.20	0.05	8.08	0.05
Q41	8.33	123.18	4.35	1.56	1.68	55.90	28.96	173.78	8.23	5.25		3.08	2.63		10.76	0.09	6.91	0.09
A42	8.28	125.97	4.37	0.96		52.64	18.82	175.89			8.76			6.92	10.71	0.04	7.64	0.05
T43	8.10	113.86	4.33	4.20		61.89	69.70	172.26							11.49	0.03	8.10	0.04
N44	8.38	122.09	4.75	2.35	2.38	53.13	38.46	173.04	5.12	5.00				4.11	10.71	0.07	7.27	0.08
R45	8.33	122.54	4.36	1.30	1.42	56.14	30.34	173.96	7.38	4.65		2.97	2.83		10.65	0.06	8.00	0.07
N46	8.50	120.70	4.80	2.33	2.42	53.34	38.49	173.57	4.82	4.30					10.91	0.06	7.59	0.06
T47	8.18	115.17	4.36			61.90	69.47	172.57					5.60		11.20	0.06	8.14	0.07
D48	8.51	121.95	4.76	2.46	2.79	53.08	37.67	173.49	5.71					3.96	10.87	0.05	6.98	0.05
G49	8.39	110.62	4.03				45.31	172.15										

S50	8.18	116.63	4.54	3.46	3.43	58.50	63.79	172.77	5.36	5.32			4.24		11.61	0.07	8.20	0.08
T51	8.21	116.76	4.33			61.89	69.59	172.00							11.45	0.06	7.64	0.07
D52	8.39	122.12	4.75	2.29	2.42	53.01	38.33	172.60	5.33	4.98		2.46	2.68		10.88	0.07	7.23	0.08
Y53	8.14	121.98	4.50	2.78	2.93	58.52	38.11	174.25	7.80			3.41	2.62		10.77	0.08	7.55	0.09
G54	8.28	110.88	3.93				45.37	172.09										
I55	7.85	120.85	4.18	1.43		61.41	38.30	174.20	6.48			2.38			10.61	0.11	7.92	0.12
L56	8.22	126.06	4.37	1.20	1.10	55.33	42.01	175.15	8.42	5.30				3.32	10.67	0.14	7.05	0.14
Q57	8.27	122.46	4.34			55.66	28.83	174.04							10.65	0.12	7.68	0.13
I58	8.10	122.63	4.06	1.37		61.74	38.21	173.95	6.94			2.45			10.37	0.08	7.44	0.09
N59	8.36	122.71	4.75	2.33	2.65	53.29	38.41	173.27	5.72					4.07	10.91	0.09	7.40	0.10
S60	8.20	117.45	4.29	3.42	3.34	58.95	63.54	172.83	4.79	4.41		2.41	4.24		11.17	0.06	7.87	0.07
R61	8.23	123.34	4.07	1.09		56.44	29.50	174.34	7.03					3.17	10.33	0.13	7.00	0.14
W62	7.82	121.80	4.57	2.75		57.71	29.02	174.16			7.21			4.85	10.67	0.12	6.90	0.12
W63	7.40	121.87	4.47	2.50	1.95	57.26	28.96	173.82	5.62	5.10		3.97	3.11		10.96	0.11	6.66	0.11
A64	7.72	125.22	4.18	0.77		52.57	18.66	175.30			8.31			6.88	10.57	0.07	6.93	0.07
N65	8.11	118.12	4.66	2.23	2.39	53.16	38.41	173.11	6.43	5.66		3.24	3.69		10.79	0.07	7.72	0.08
D66	8.33	119.53	4.66	2.67	2.76	53.09	37.56	173.35	5.60			2.95	3.53		10.73	0.06	7.58	0.07
G67	8.32	109.46	3.89				45.44	171.94										
R68	7.96	120.99	4.45	1.31	1.39	55.75	30.63	174.13	6.55	3.99		2.84	2.59		11.09	0.09	7.84	0.10
T69	8.25	118.25				59.82	69.51	170.91							11.93	0.06	7.97	0.06
P70																		
G71	8.48	110.54	4.01				45.13	172.15										
S72	8.13	116.63	4.47	3.43		58.53	63.83	172.58			5.24		4.34		11.70	0.07	8.23	0.08
R73	8.42	123.75	4.36	1.59	1.69	56.08	30.42	173.72				2.49	2.02		10.72	0.08	7.58	0.08
N74	8.44	120.85	4.72	2.26	2.41	53.09	38.39	173.02	6.28	5.87		2.98	3.64		11.18	0.05	7.86	0.05
L75	8.27	124.28	4.35	1.20		55.21	41.98	174.92	8.67					3.01	10.44	0.06	8.02	0.07
A76	8.19	124.58	4.31	0.93		52.40	18.87	175.17			8.66				10.80	0.05	7.27	0.06
N77	8.28	118.42	4.71	2.25	2.35	52.73	38.54	172.44				3.19	3.36		11.07	0.05	7.95	0.05
I78	8.02	123.96				58.66	38.43	172.23							10.82	0.10	7.81	0.11
P79																		
A80	8.49	125.66	4.26	0.98		53.16	18.53	176.36			8.71			7.02	10.66	0.05	8.83	0.05
S81	8.26	114.97	4.37	3.46	3.40	58.68	63.41	172.69	4.60	4.24			4.63		11.47	0.06	7.77	0.07
A82	8.23	126.97	4.37	0.96		52.62	18.78	175.75			8.62			6.79	10.51	0.04	7.05	0.05
L83	7.98	121.50	4.34	1.21		55.38	41.97	175.42	8.71					3.55	10.47	0.08	7.26	0.09
L84	8.04	123.18	4.42	1.24		55.30	42.04	175.59	8.77					3.26	10.48	0.10	7.23	0.11
S85	8.23	117.14	4.45	3.48	3.42	58.69	63.57	172.70	5.21	4.97					11.37	0.05	7.66	0.05
S86	8.27	118.36	4.49	3.48	3.43	58.68	63.59	172.30	4.75	4.69			4.31		11.34	0.05	7.47	0.06
D87	8.40	121.99	4.80	2.42	2.50	53.01	37.58	173.12	3.72	3.68					10.74	0.06	7.16	0.06
I88	8.08	122.49	4.23	1.48		61.77	38.16	174.51	7.07			2.27			10.37	0.08	7.44	0.09
T89	8.17	119.20	4.30	4.13		62.07	69.54	172.27					5.20		11.29	0.06	7.32	0.06
A90	8.26	127.34	4.37	0.98		52.70	18.84	175.91			8.70			7.00	10.78	0.04	7.20	0.05
S91	8.28	116.55	4.48	3.93	3.75	58.65	63.57	172.98			6.21	2.25	4.50		11.37	0.06	7.99	0.07
V92	8.18	123.21	4.12		1.67	62.93	32.24	174.18		6.54			2.18		10.38	0.08	7.39	0.09
N93	8.43	122.59	4.71	2.60	2.69	53.44	38.48	173.23	7.21			2.72	3.26		10.87	0.04	7.28	0.05
A94	8.21	125.74	4.29	0.97		52.74	18.74	175.60			8.51			6.94	10.60	0.04	7.71	0.04
A95	8.15	123.60	4.30	0.97		52.60	18.70	175.81			8.40			6.97	10.83	0.06	7.43	0.06
K96	8.11	121.23	4.29	1.32		56.25	32.73	174.38	7.77						10.87	0.08	7.79	0.09
K97	8.21	123.85	4.34	1.31		56.18	32.69	174.16	7.33					3.48	10.80	0.07	7.82	0.08
I98	8.23	124.42	4.20	1.40		60.94	38.30	174.17	7.86			2.11			10.61	0.11	7.88	0.12
V99	8.32	126.35	4.20			62.09	32.53	173.90							10.61	0.09	7.76	0.10
S100	8.46	120.92	4.53	3.71	3.40	58.03	63.75	172.19			6.07		4.40		11.18	0.05	7.86	0.05
D101	8.58	122.59	4.83	2.77		52.68	37.70	173.47						4.49	10.74	0.06	7.87	0.07
G102	8.41	110.46	4.01				45.44	171.91										
N103	8.36	119.71	4.77		2.38	53.19	38.62	173.86		5.56					11.01	0.06	8.47	0.07
G104	8.48	110.41	4.00				45.36	172.46							11.52	0.04	8.11	0.05
M105	8.22	120.99	4.47	1.57		55.73	32.19	174.23			7.41			3.70	10.70	0.08	7.82	0.09

N106	8.41	120.43	4.64	2.28		53.73	38.29	173.35	7.67			3.33			10.89	0.06	7.52	0.07
A107	8.21	124.94	4.25	0.88		53.46	18.51	175.81			8.92			6.87	10.25	0.07	7.39	0.08
W108	8.05	120.93	4.58	2.87	2.82	58.35	28.90	174.63	6.46	6.37		3.97	3.08		10.54	0.09	7.03	0.09
V109	7.77	122.35	3.78		1.45	63.42	32.34	174.21		7.61			1.95		10.31	0.13	6.89	0.13
A110	8.03	125.82	4.13	0.92		53.44	18.33	176.46			8.54			6.92	10.28	0.10	6.87	0.10
W111	7.91	120.32	4.48	2.86		58.37	28.75	175.03			7.79				10.49	0.11	7.07	0.11
R112	7.97	122.18	3.96	1.09	1.21	57.05	29.92	174.34	7.10	5.52		3.46	3.02		10.41	0.11	6.66	0.11
N113	8.10	119.17	4.63	2.23	2.40	53.47	38.36	173.26	8.05	5.52					10.75	0.07	7.12	0.07
R114	7.91	122.14	4.24	1.45		56.44	30.17	173.99	6.91						10.41	0.11	6.66	0.11
A115	8.18	125.59	4.28	0.88		52.56	18.72	175.67			8.38			6.81	10.73	0.04	7.54	0.05
K116	8.22	121.58	4.29	1.31	1.39	56.56	32.65	175.07	7.26	4.69				3.50	10.81	0.08	8.07	0.09
G117	8.38	110.91	4.05				45.15	172.13										
T118	8.07	114.32	4.39	3.78		61.82	69.75	172.23	4.04				4.92		11.66	0.05	8.62	0.05
D119	8.57	122.63	4.80	2.39	2.50	52.68	37.71	172.94	4.29	4.13		3.35	3.81		10.74	0.06	7.87	0.07
V120	8.10	122.04	4.02		1.59	62.77	32.19	174.12		6.64			2.07		10.40	0.09	7.81	0.10
Q121	8.37	124.49				55.97	28.67	173.69							10.65	0.07	7.36	0.07
A122				0.89							8.65			6.76				
W123	8.00	120.96	4.68	3.09	2.78	57.20	29.08	174.09			6.44			4.74	10.81	0.09	7.58	0.10
I124	7.88	124.16	4.04	1.29		61.11	38.43	173.73	8.21						10.42	0.09	7.29	0.09
R125	8.19	125.59	4.14	1.28	1.36	56.50	30.07	174.63	6.85	5.31					10.73	0.04	7.54	0.05
G126	8.33	111.20	3.97				45.00	171.53										
A127	8.07	124.83	4.33	0.90		52.26	19.13	175.24			8.83			6.90	11.19	0.05	8.14	0.06
R128	8.30	121.51	4.33			55.72	30.36	173.98							10.89	0.07	8.36	0.08
L129	8.39	125.83				53.98	41.69	176.97										

Table S2: table of ^{15}N-^{1}H RDCs [Hz] and R_2 [s^{-1}] relaxation rates of $W28G^{Ala}$, $W62G^{Ala}$, $W108G^{Ala}$, $W111G^{Ala}$, $W123G^{Ala}$.

	^{15}N-^{1}H RDC [Hz]					R_2 [s^{-1}]				
	$W28G^{Ala}$	**$W62G^{Ala}$**	**$W108G^{Ala}$**	**$W111G^{Ala}$**	**$W123G^{Ala}$**	**$W28G^{Ala}$**	**$W62G^{Ala}$**	**$W108G^{Ala}$**	**$W111G^{Ala}$**	**$W123G^{Ala}$**
K1	-4.92	-5.54	-5.10	-4.38	-5.88	1.07	1.23	1.04	1.13	0.97
V2	-6.18	-6.24	-6.24	-6.00	-8.40	1.52	1.52	1.30	1.61	1.26
F3	-2.70	-3.47	-3.36	-2.82	-4.14	1.47	1.67	1.54	1.72	1.45
G4	-0.96	0.00	-0.18	-0.66	-0.84	1.54	2.45	1.67	1.73	1.68
R5	-0.54	0.69	-0.60	-0.48	-1.20	2.14	2.44	2.52	2.33	2.27
A6	-2.70	4.13	-1.20	3.00	-2.76	2.58	2.37	2.59	2.76	2.58
E7	0.06	0.70	1.68	2.70	-0.54	2.33	2.59	2.40	2.64	2.47
L8	-0.12	0.70	-0.18	0.12	-1.02	2.41		2.57	2.75	2.58
A9										
A10	5.46		-0.36		3.72	2.75	3.10	2.66		3.10
A11	2.40	1.39	2.10	-0.90	1.86	2.72	2.91	2.93	4.01	3.04
M12	0.30	-2.08	0.12	0.48	-0.96	2.60	2.83	2.88	3.10	2.86
K13	3.24		1.26	1.14	3.00	2.68	2.88	3.41	3.51	3.33
R14	-2.94	-5.15	-3.30	-17.22	-4.32	2.88	2.60	3.06	2.99	2.41
H15	-4.08	-5.53	-2.52	-3.72	-5.64	2.40	2.28	2.81	3.01	2.71
G16	-3.12	-2.08	-2.64	-3.06	-3.48	2.11	2.61	2.21	2.07	2.47
L17	-2.88	-2.78	-2.70	-3.18	-2.46	2.51	2.49	2.66	2.61	2.70
D18	-2.58		-3.36	-1.02	-4.74	2.27	2.44	2.51	2.68	2.53
N19	-3.06	-2.77	-2.88	-1.26	36.48	2.31	2.81	2.56	2.78	2.62
Y20	-1.38	0.00	0.06	0.24	-0.18	2.63	2.73	2.80	2.65	2.81
R21	-4.86	-2.09	-1.68	-3.84	-3.36	2.57	2.51	2.65	2.78	2.72
G22	-1.80	-3.47	-3.48	-3.00	-4.08	2.43	2.79	2.77	3.09	2.91
Y23	0.36	-2.77	-1.26	-0.24	-2.16	2.42	2.76	2.87	3.12	2.92
S24	-2.46	-2.08	-2.40	-0.42	6.00	2.35	2.52	2.78	3.13	2.89
L25	-3.36	-4.85	-5.16	-3.78	-2.82	2.03		2.67	2.72	2.68
G26	-1.98	-1.38	-1.38	-0.18	-2.16	2.05	2.66	2.85	3.30	2.86
N27	-1.98	-2.77	-3.00	-1.50	-3.78	2.12	2.84	2.85	3.16	2.90
G28	-7.14		-0.60	1.44	2.10	2.12	3.05	3.11	3.56	3.10
V29	-0.42	0.00	2.16	-0.84	2.16	2.13		3.47	3.72	3.53
A30	-4.38	-0.69	-0.90	0.54	-0.60		2.77			
A31	3.60		-0.96	-2.52	-2.46	2.40	2.87	2.91	3.50	2.99
A32	-2.16	-1.38	-2.22	-0.96	-7.26	2.32		2.91	3.44	2.98
K33	-3.42		-2.28	0.24	-4.86	2.59	3.14	3.04	3.42	3.11
F34	-1.86	-1.39	-1.14	1.50	-3.54	2.67	3.04	3.02	2.57	3.30
E35	-1.14	-2.77	-2.04	-1.92	-2.70	2.46	2.70	3.35	2.76	3.36
S36	-1.86	-2.08	-1.86	0.00	-3.00	2.45	2.40	2.83	3.24	3.01
N37	-4.20		-2.34	-3.30	-1.92	2.49	2.48	2.63	2.82	2.66
F38	-0.66	-0.69	-0.48	0.54	-1.14	2.55		2.60	2.54	2.65
N39	-0.66		-1.32	-2.10	-2.94	2.42	2.29	2.63	2.87	2.70
T40	-1.92	-2.08	-2.28	-1.68	-3.24	2.31	2.67	2.46	2.54	2.43
Q41	-3.06	-2.09	-2.82	-1.86	-3.30	2.50	2.33	2.68	3.32	2.44
A42	0.60	-0.01	-5.94	-2.22	0.96	2.33	2.17	2.39	2.73	2.41
T43	-1.68	-2.77	-2.52	-6.72	-3.36	2.19	2.90	2.50	2.65	2.80
N44	-3.72		-2.46	-1.20	-5.16	2.54		2.60	2.72	2.62
R45	-5.64	-2.77	-2.40	-4.74	-3.60	2.38	2.41	2.63	3.11	2.76
N46	-1.20	-2.08	-1.86	0.66	-2.58	2.44	2.16	2.47	2.63	2.48
T47	-3.06	-3.47	-3.24	-3.00	-3.96	2.26	2.44	2.38	2.52	2.35
D48	-1.56	-2.08	-2.22	-1.20	-2.22	2.44	2.10	2.69	2.56	2.39
G49	-0.36	-0.01	-0.78	0.78	-0.90	2.08	2.26	2.14	2.41	2.21

S50	-1.20	-0.69	-1.44	-1.80	-1.50	2.26	2.42	2.34	2.55	2.39
T51	-2.10	-3.48	-3.42	-1.26	-4.50	2.42	3.02	2.57	2.81	2.62
D52	-1.44	-4.17	-4.80	-0.60	-2.88	2.61	3.14	2.90	2.66	2.90
Y53	1.74	1.39	2.94	-7.32	-1.98	3.00	2.83	3.02	2.82	3.03
G54	-3.24	0.00	0.66	-1.08	0.66	3.02	2.97	3.16	3.54	3.17
I55	-0.30	2.08	1.44	0.72	-0.72	3.32	3.06	3.33	3.71	3.39
L56	3.24	-3.46	-2.40	-1.14	-4.62	3.39	3.12	2.33	3.64	3.20
Q57	-3.54	-2.77	-1.62	-2.22	-2.82	3.52	3.06	3.94	3.97	3.91
I58	-1.44	-2.09	-1.08	-5.70	-3.06	3.35	3.18	4.00	3.02	3.96
N59	-3.36	-2.77	-2.52	-1.38	-3.12	3.64	2.74	4.03	4.02	4.15
S60	-0.78	-2.08	-1.32	-0.84	-0.54	3.57	3.30	3.80	4.27	4.11
R61	-2.22	-0.69	-2.64	-2.82	-2.46	3.91	2.59	3.63	4.56	4.15
W62	5.64	0.00	6.30	6.84	5.46	3.98		4.19	4.41	4.39
W63	14.52	-4.17	5.94	8.04	8.40	4.18	2.58	4.52	5.01	4.73
A64	5.04	-0.70	6.36	-7.32	4.68		2.53	3.85	4.23	3.88
N65	-3.42	-2.08	-2.58	-2.52	-3.00	3.19	2.26	3.34	3.74	3.43
D66	1.20	-3.32	-1.98	-1.14	-1.38	3.08	2.90	3.18	3.46	3.60
G67	1.08	-0.69	0.36	0.84	0.36	3.26	2.41	3.29	4.00	3.25
R68	-0.78	2.08	-2.10	-0.18	-2.28	2.97	2.48	2.87	2.99	2.92
T69	-3.96	0.69	-2.70	-1.26	0.96	2.58		2.62	2.85	2.65
P70										
G71	-9.60	0.68	-1.80	-0.78	-0.24	2.50	1.94	2.00	2.34	2.34
S72	-1.44	-2.77	-1.86	-2.46	-2.52	2.54	2.27	2.55	2.82	2.56
R73	-2.16	-4.16	-4.14	-2.94	-3.06	2.39	2.17	2.54	2.78	2.59
N74	-4.86		-4.02	-2.52	-5.82	2.31	2.27	2.32	2.53	2.47
L75	-5.34	-4.16	-3.18	-4.92	-3.30	2.52	2.38	2.34	2.53	2.53
A76	5.94	-1.38	-0.90	-0.78	-0.06	2.61	2.30	2.55	2.78	2.73
N77	-2.70	-3.47	-1.92	-1.20	-5.46	2.54	2.66	2.50	2.75	2.65
I78	-8.34	-7.62	-6.30	-6.66	-8.52	2.67		2.56	2.91	2.76
P79										
A80	-1.26	-5.83	-2.82	-1.32	-0.54	2.58	2.73	2.59	2.79	2.55
S81	-0.90	-3.47	-1.98	-2.58	-3.42	2.76	2.83	2.88	2.89	2.93
A82	1.32	-0.01	-0.30	-0.06	-0.72	2.91	2.43		3.65	3.27
L83	-2.28	-2.08	-1.98	-2.22	-2.70	2.71	2.63	2.62	2.79	1.95
L84	-0.48	-2.77	-10.14	-1.86	-1.86	2.67	2.44	2.66	3.33	2.69
S85	-0.42	-1.38	-1.74	-1.62	-3.18	2.56	2.52	2.52	2.85	2.62
S86	-2.94	-2.77	-0.48	-4.26	-5.16	2.56	2.89	2.52	2.82	2.57
D87	-1.26		-0.48	-0.84	-1.56	2.80	2.72	2.42	2.40	2.56
I88	8.10	-0.69	-0.36	0.06	-2.46	2.91	2.83		2.60	2.88
T89	-3.00	-7.63	-2.16	-2.64	-3.54	2.89		2.74	2.97	2.97
A90	-0.66	-1.38	-2.10	-1.38	0.72	3.20	2.40			
S91	-0.30	-0.70	-0.72	-0.54	-0.12	2.41	2.85	2.33	2.45	2.37
V92	-4.44	-1.39	-2.28	-1.80	-1.74	2.74	3.03	2.42	2.87	2.48
N93	-1.98	-2.78	-1.62	-0.96	-1.50	2.82	2.40		2.68	2.93
A94	-1.26	-0.48	-0.48	-0.84	-0.72	2.57	2.52	2.27	2.49	2.43
A95	2.22	-1.39	1.14	1.44	2.88	2.64	2.55	2.40	2.73	2.69
K96	-1.02	-6.23	-2.76	-2.40	-4.62	2.70	2.60	2.32	2.60	2.57
K97	-5.28	-4.84	-6.72	-5.64	-7.62	2.67		2.29	2.63	2.60
I98	-1.14		-7.14	-2.64	-2.22	2.64	2.57		2.77	2.70
V99	-1.38		-6.66	-5.10	-2.28	2.67	2.32	2.29	2.36	1.80
S100	-3.18		-3.12	-2.46	-4.92	2.47	2.56	2.27	2.51	2.50
D101	-4.74	-4.16	-4.68	-6.24	-5.76	2.55	2.11	2.09	1.83	2.17
G102	0.48	-4.16	-0.48	2.04	0.36	2.07	2.63	1.75	1.98	2.03
N103	-3.54	-2.20	-1.08	-0.66	-1.74	2.02	1.99	1.84	2.05	2.20
G104	2.22	0.00	-3.18	-1.44	-6.00	1.83	2.44	2.00	2.15	2.22
M105	-0.30	0.00	-0.66	1.80	1.80	2.56		2.25	2.21	2.48

N106	-0.30	0.69	-2.22	-0.66	-0.48	2.77	2.66	2.20	2.36	2.54
A107	0.54	1.39	0.60	0.54	-0.96	2.98	2.77	2.80	2.84	2.95
W108	3.78	-3.47	0.06	-0.48	5.46	3.55	3.53		2.54	3.22
V109	7.14	6.24	4.14	1.92	5.88	3.86	3.83	2.88	3.61	3.71
A110	3.48	2.77	-0.48	3.42	-1.44	3.98	3.70			3.50
W111	2.16	-0.68	0.36	-4.14	0.42	3.69	3.01	2.36		3.46
R112	-1.38	0.69	-2.82		-8.94	3.74	3.51	2.67		3.28
N113	6.06	8.31	0.48	-2.52	3.48	3.56	2.74	2.68	2.37	3.35
R114	-3.60	0.70	-4.26		3.60	3.15	2.55	2.77		3.23
A115	-2.40	-2.08	-3.12	-3.00	-0.06	2.58	2.57	2.33	2.54	2.43
K116	-2.16	-1.38	-4.20	-4.08	-3.90	2.76	2.09	2.20	1.81	2.33
G117	-3.84	-4.17	-4.32	-2.04	-6.42	2.13	2.01	2.00	2.21	2.05
T118	-2.40	-2.09	-1.98	-2.46	-3.30	2.29	2.38	1.91	1.81	2.21
D119	-5.16	-4.84	-3.30	-2.16	-4.26	2.29	2.33	2.09	2.34	1.91
V120	1.02	-2.78	-1.92	-4.68	-1.92	2.45	2.40	2.38	2.77	1.53
Q121	-4.98	-3.47		-3.84		2.58		2.29	2.49	2.32
A122			-2.82		-5.46		3.35			
W123	0.12	6.93	1.80	3.66	-3.12	2.52	2.36	2.63	2.36	2.06
I124	6.96	3.47	1.08	-0.06	-6.48	2.48		2.18	2.26	2.42
R125	0.60		-3.24	-6.78	-3.00	2.73	1.88	2.33	2.51	1.78
G126	-4.56	-5.53	-4.56	-4.80	-4.50	1.96	1.68	1.77	1.84	1.35
A127	0.12	0.69	-0.48	0.84	-1.14	1.70	1.48	1.53	1.69	1.47
R128	-1.92	-4.17	-2.58	-5.22	0.00	1.55	1.17	1.30	1.23	1.34
L129	-2.16	-6.24	-0.48	-0.42		1.22	2.65	1.12	1.24	1.04

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