SUPPORTING INFORMATION

Structural effects of single mutations in a filamentous viral capsid across multiple length scales

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FIGURE S1: COMPARISON OF NMR DARR100 SPECTRA FOR SAMPLES PRECIPITATED AT TWO PEG8K CONCENTRATIONS

5% - cyan, 40% - red. Differences are negligible and are under 0.1 ppm.

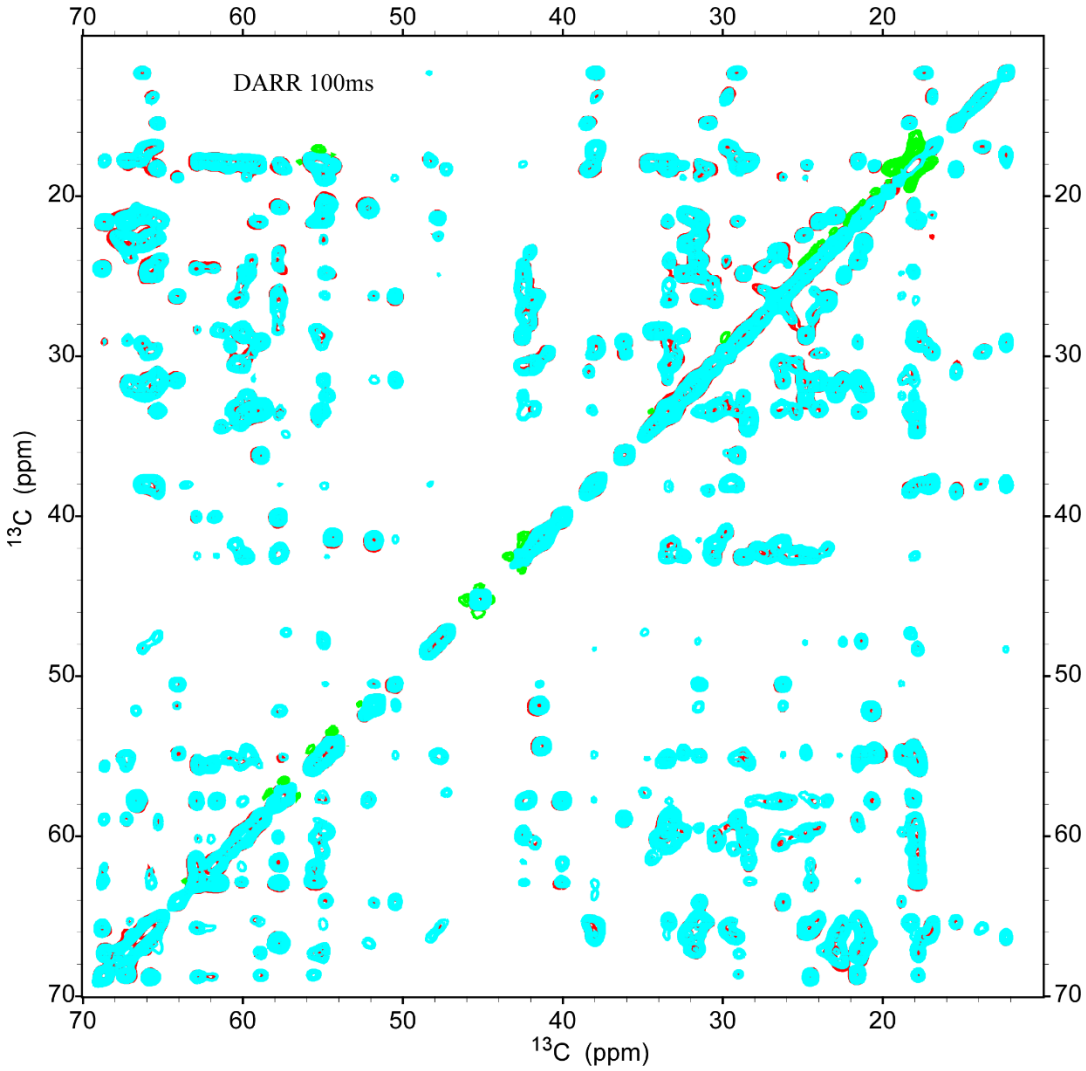

FIGURE S2: COMPARISON OF SAXS PLOTS AT TWO DIFFERENT PEG MOLECULAR WEIGHTS: PEG8K, PEG20K.

SAXS profiles for fd (left) and Y21M (right) under two osmolytes: PEG8K (solid line) and PEG 20K (dashed line) in 150 mM NaCl buffer. The PEG wt% were chosen to reach as close as possible osmotic pressures for both PEG wt%. Values of the osmotic pressure are denoted in the legend in $\log_{10}\Pi$, where Π is given in atm units.

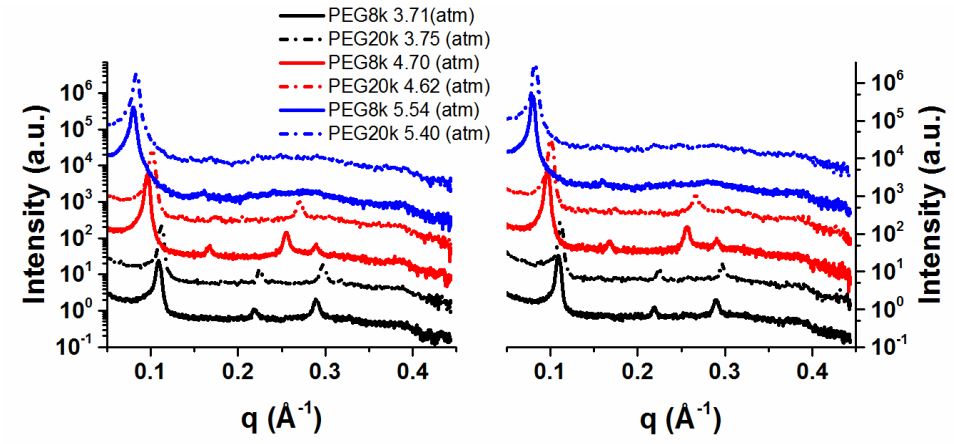

FIGURE S3: N/C'/Cα/Cβ CHEMICAL SHIFT PERTURBATIONS BETWEEN FD AND FD-Y21M

Chemical shift perturbations (CSPs) are given in absolute values as $|\delta(\text{fd})-\delta(\text{Y21M})|$. Significant shifts are above the horizontal line drawn at 0.3 ppm. The average and standard deviation (in parenthesis) of all measured CSPs for Y21M are 0.44 (0.42), 0.35 (0.53), 0.19 (0.21), and 0.19 (0.19), For N, C', Cα, and Cβ, respectively. For the D12N mutation, as reported in a prior publication (Morag et al., J. Phys. Chem B, 2011, 115, 15370-15379), they are 0.37 (0.52), 0.20 (0.39), 0.09 (0.08), 0.10 (0.09), hence they are significantly lower. The total number of significant CSPs for the D12N mutations are also much smaller. There are 11 significant CSPs for the D12N mutant and for Y21M there are 57 such CSPs.

Red circles denote residues in the DNA interface according to those observed experimentally in Morag et al., J. Am. Chem. Soc. 2014, 136, 2292-2301. Green circles denote residues, for which more than three non-ambiguous contacts were detected in the structure calculation of the M13 phage (Table S2 and Figure S4 of Morag et al., PNAS 2015, 112, 971-976). There is a clear difference between the significant CSPs of residues involved in the inter-subunit interface, and negligible CSPs for residues involved in DNA contacts.

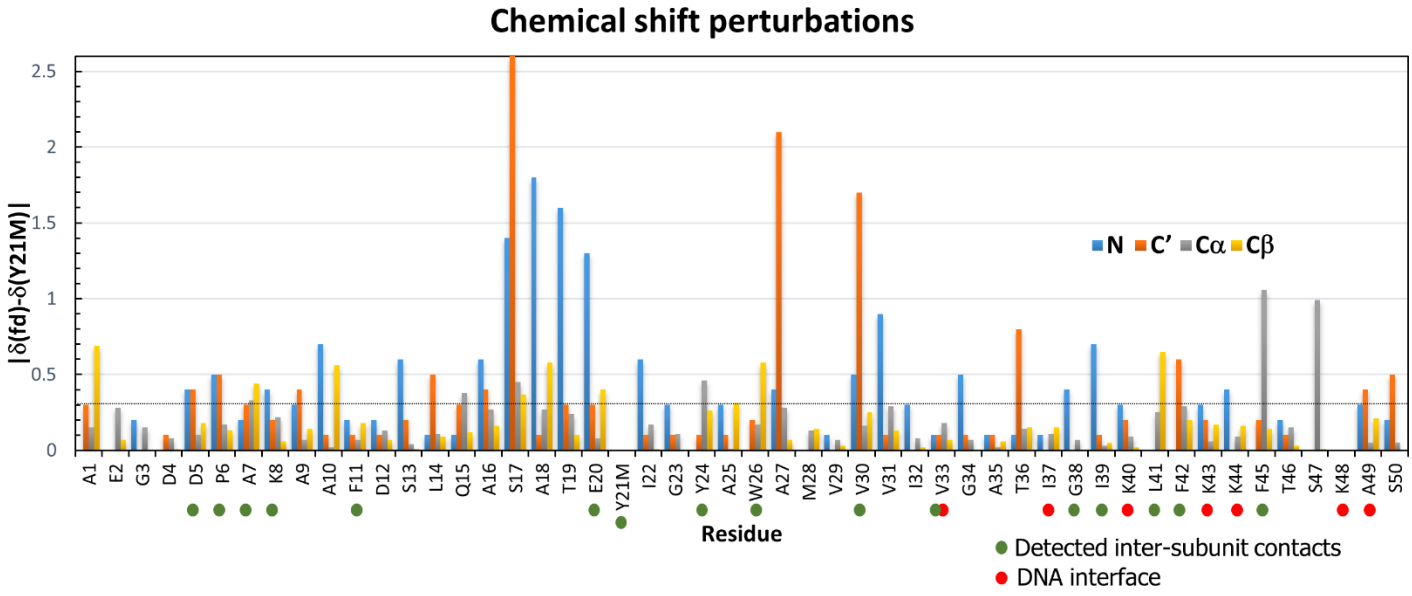

FIGURE S4: SAXS PLOTS FOR ALL BUFFER CONDITIONS

The profiles are vertically shifted for clarity. The characteristic correlation peaks are indexed to hexagonal phase (arrows).

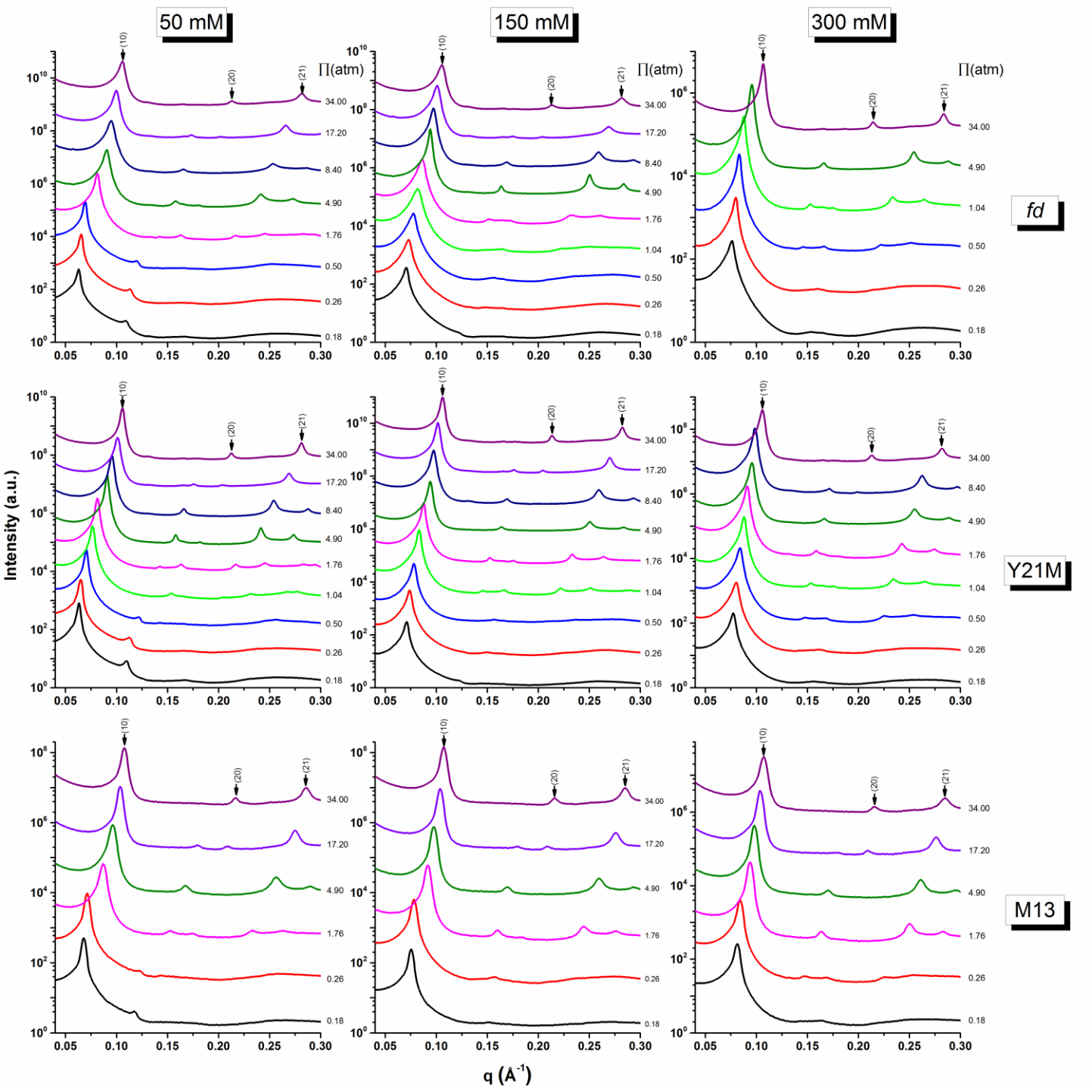

TABLE S1: 2D & 3D MAS SSNMR EXPERIMENTAL PARAMETERS OF ^{13}C, ^{15}N-LABELED Y21M PHAGE

	y21mDARR10*	y21mDARR100	y21mNCA	y21mNCACX	y21mNCOCX
PROBE	^{1}H-^{13}C-^{15}N 4 mm Efree (Bruker)				
SPIN RATE/TEMPERATURE	12 kHz/-5°C	12 kHz/-5°C	12 kHz/-5°C	12 kHz/-5°C	12 kHz/-5°C
RECYCLE DELAY/SCANS	4 s/16	4 s/16	3.5 s/32	3 s/16	3 s/32
ACQUISITION POINTS $T_1/T_2/T_3$	2000/4990	2000/4990	600/4990	64/128/4990	82/72/4990
ACQUISITION TIME $T_1/T_2/T_3$	25/25 ms	25/25 ms	25/25 ms	10.67/10.67/25 ms	13.67/12/25 ms
SPECTRAL WIDTH $T_1/T_2/T_3$	40/100 kHz	40/100 kHz	12/100 kHz	3/6/100 kHz	3/3/100 kHz
CARRIER FREQUENCY	^{13}C 99.9 ppm	^{13}C 99.9 ppm	^{13}CX 99.9 ppm $^{13}C\alpha$ 47.5 ppm ^{15}N 70 ppm	^{13}CX 99.9 ppm $^{13}C\alpha$ 54 ppm ^{15}N 120 ppm	^{13}CX 99.9 ppm ^{13}CO 177.9 ppm ^{15}N 120 ppm
CP CONTACT TIME	2 ms	2 ms	3 ms	3 ms	3 ms
RADIOFREQUENCY FIELD	^{1}H 92 kHz ^{13}C 50 kHz	^{1}H 92 kHz ^{13}C 50 kHz	^{1}H 92 kHz ^{13}C 50 kHz ^{15}N 45.45 kHz	^{1}H 100 kHz ^{13}C 50 kHz ^{15}N 45.45 kHz	^{1}H 100 kHz ^{13}C 50 kHz ^{15}N 45.45 kHz
^{1}H DECOUPLING (SW_F-TPPM[1])	90 kHz/6 µs	90 kHz/6 µs	85 kHz/ 6 µs	83 kHz/ 6 µs	83 kHz/ 6 µs
DARR MIXING TIME	10 ms	100 ms	50 ms	50 ms	50 ms
DCP[2] SHAPE	-	-	tan (^{13}C) 80-120%	tan (^{13}C) 80-120%	tan (^{13}C) 80-120%
DCP POWER	-	-	$1.5\omega_r$ ^{13}C $2.5\omega_r$ ^{15}N	$1.5\omega_r$ ^{13}C $2.5\omega_r$ ^{15}N	$2.5\omega_r$ ^{13}C $1.5\omega_r$ ^{15}N
DCP CONTACT TIME	-	-	3 ms	5.5 ms	3 ms
TOTAL EXPERIMENTAL TIME	1d:12h	1d:13h	19h	4d:17h:20 min	6d:19h:40min
PROCESSING SOFTWARE	NMRPipe				
WINDOW FUNCTION T_1/T_2	Lorentz to Gauss transformation (both dimensions) Inverse exponential 40 Hz Gaussian broadening 80 Hz		Lorentz to Gauss transformation (all dimensions) Inverse exponential 40 Hz Gaussian broadening 80 Hz		
ZERO-FILLING POINTS $T_1/T_2/T_3$	8192/8192		8192/8192	256/512/8192	256/512/8192

*y21mDARR10: sample: Y21M; experiment: DARR; mixing time: 10ms

TABLE S2: CHEMICAL SHIFT ASSIGNMENTS OF THE Y21M MUTANT OF FD PHAGE / BMRB 26910

	A1	E2	G3	D4	D5	P6	A7	K8	A9	A10	F11	D12	S13	L14	Q15	A16	S17	A18	T19	E20	M21	I22	G23	Y24	A25
N	na	na	111.2	120.3	121.5	138.2	119.5	119.3	119.3	121.1	118.9	119.2	116.2	124.6	120.9	123.6	115.8	124.1	113.0	122.9	118.3	119.8	106.4	122.4	123.2
C	174.7	na	174.2	175.9	174.6	178.5	179.0	178.3	180.7	180.6	178.9	179.9	177.6	179.7	179.2	180.8	177.5	178.9	177.5	178.7	177.9	177.9	177.7	179.0	179.8
Cα	51.9	57.7	45.3	54.4	51.9	64.2	54.9	59.8	54.7	54.9	63.8	57.9	61.7	57.9	60.2	55.5	62.0	55.6	67.3	59.0	59.3	65.4	47.3	57.4	55.1
Cβ	18.9	29.9	-	41.4	41.5	31.5	18.8	32.5	18.1	20.5	38.1	40.1	62.9	42.5	28.5	17.9	62.8	17.8	68.7	29.1	33.4	38.5	-	34.9	18.2
Cγ	-	36.1	-	180.1	180.1	26.3	-	24.9	-	-	141.3	178.9	-	27.6	34.2	-	-	-	-	36.2	na	-	-	129.1	-
Cγ1	-	-	-	-	-	-	-	-	-	-	-		-	-	-	-	-	-	-	-	-	31.0	-	-	-
Cγ2	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	21.6	-	-	18.3	-	-	-
Cδ	-	184.1	-	-	-	50.5	-	28.8	-	-	-	-	-	-	178.1	-	-	-	-	183.6	-	-	-	-	-
Cδ1	-	-	-	-	-	-	-	-	-	-	130.6	-	-	na	-	-	-	-	-	-	-	15.5	-	132.4	-
Cδ2	-	-	-	-	-	-	-	-	-	-	130.6	-	-	24.3	-	-	-	-	-	-	-	-	-	132.4	-
Cε	-	-	-	-	-	-	-	42.6	-	-	-	-	-	-	-	-	-	-	-	-	17.9	-	-	-	-
cε1	-	-	-	-	-	-	-	-	-	-	na	-	-	-	-	-	-	-	-	-	-	-	-	117.7	-
cε2	-	-	-	-	-	-	-	-	-	-	na	-	-	-	-	-	-	-	-	-	-	-	-	117.7	-
cε3	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
cζ	-	-	-	-	-	-	-	-	-	-	na	-	-	-	-	-	-	-	-	-	-	-	-	157.5	-
cζ2	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
cζ3	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
cη2	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Nε1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Nε2	-	-	-	-	-	-	-	-	-	-	-	-	-	-	108.0	-	-	-	-	-	-	-	-	-	-
Nζ	-	-	-	-	-	-	-	35.5	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-

	W26	A27	M28	V29	V30	V31	I32	V33	G34	A35	T36	I37	G38	I39	K40	L41	F42	K43	K44	F45	T46	S47	K48	A49	S50
N	118.1	120.1	117.8	120.6	119.9	121.7	121.2	122.1	107.2	123.2	112.8	123.3	110.1	122.2	121.0	124.6	123.2	121.1	120.2	115.4	109.3	116.1	na	119.5	110.9
C	178.8	180.2	178.2	177.9	179.8	178.6	178.9	178.3	177.2	179.0	179.1	178.1	175.8	177.8	179.2	179.1	179.2	177.9	179.3	178.7	177.4	176.2	180.3	173.6	179.4
Cα	60.9	55.2	59.5	65.3	67.2	66.2	65.7	66.0	47.9	55.1	67.4	61.5	48.4	66.3	60.1	57.9	62.2	60.5	59.5	62.8	65.8	61.9	59.9	52.3	57.8
Cβ	29.4	17.9	33.5	31.5	31.8	32.3	38.0	31.6	-	21.4	67.4	34.5	-	38.1	33.5	42.1	40.1	33.4	33.1	38.0	68.9	62.9	33.4	20.8	66.7
Cγ	113.6	-	-	-	-	-	-	-	-	-	-	-	-	-	25.5	26.6	138.8	26.5	24.0	144.2	-	-	na	-	-
Cγ1	-	-	-	24.1	24.0	23.0	29.8	24.9	-	-	-	28.4	-	29.2	-	-	-	-	-	-	-	-	-	-	-
Cγ2	-	-	-	21.6	21.5	21.2	17.0	22.5	-	-	22.8	17.9	-	17.4	-	-	-	-	-	-	24.6	-	-	-	-
Cδ	-	-	-	-	-	-	-	-	-	-	-	-	-	-	30.6	-	-	30.5	29.8	-	-	-	30.8	-	-
Cδ1	127.7	-	-	-	-	-	13.9	-	-	-	-	8.5	-	12.3	-	na	130.7	-	-	130.7	-	-	-	-	-
Cδ2	129.2	-	-	-	-	-	-	-	-	-	-	-	-	-	-	23.5	130.7	-	-	130.7	-	-	-	-	-
Cε	-	-	17.9*	-	-	-	-	-	-	-	-	-	-	-	42.6	-	-	41.8	41.0	-	-	-	42.5	-	-
cε1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	na	-	-	na	-	-	-	-	-
cε2	139.9	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	na	-	-	na	-	-	-	-	-
cε3	120.8	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
cζ	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	na	-	-	na	-	-	-	-	-
cζ2	114.0	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
cζ3	119.8	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
cη2	na	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Nε1	125.9	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Nε2	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Nζ	-	-	-	-	-	-	-	-	-	-	-	-	-	-	na	-	-	34.1	34.3	-	-	-	na	-	-

[na: no assignment was obtained. '-': atom does not exist in that amino acid]

TABLE S3: CHEMICAL SHIFT PERTURBATIONS BETWEEN WILD-TYPE FD AND ITS MUTANT Y21M

All values are given in absolute values as $|\delta_{fd}-\delta_{Y21M}|$. Significant chemical shift perturbations are colored.

	N	C'	Cα	Cβ	Cγ/Cγ1/Cγ2	Cδ/Cδ1/Cδ2
A1		0.3	0.1	0.7		
E2			0.3	0.1	0.0	
G3	0.2	0	0.1			
D4		0.1	0.1	0.0	0.1	
D5	0.4	0.4	0.1	0.2	0.0	
P6	0.5	0.5	0.2	0.1	0.3	0.2
A7	0.2	0.3	0.3	0.4		
K8	0.4	0.2	0.2	0.1	0.2	0.2
A9	0.3	0.4	0.1	0.1		
A10	0.7	0.1	0.0	0.6		
F11	0.2	0.1	0.1	0.2	1.0	0.1
D12	0.2	0.1	0.1	0.1	0.2	
S13	0.6	0.2	0.0	0.0		
L14	0.1	0.5	0.1	0.1	1.2	0.8
Q15	0.1	0.3	0.4	0.1	0.0	
A16	0.6	0.4	0.3	0.2		
S17	1.4	2.6	0.5	0.4		
A18	1.8	0.1	0.3	0.6		
T19	1.6	0.3	0.2	0.1	0.0	
E20	1.3	0.3	0.1	0.4	0.5	0.3
Y21M*						
I22	0.6	0.1	0.2	0.0	0.0	0.0
G23	0.3	0.1	0.1			
Y24	0	0.1	0.5	0.3	0.3	0.2
A25	0.3	0.1	0.0	0.3		
W26		0.2	0.2	0.6	0.3	0.2
A27	0.4	2.1	0.3	0.1		
M28			0.1	0.1		
V29	0.1	0	0.1	0.0	0.3	
V30	0.5	1.7	0.2	0.3		
V31	0.9	0.1	0.3	0.1	0.2	
I32	0.3	0	0.1	0.0	0.1	0.2
V33	0.1	0.1	0.2	0.1	0.2	
G34	0.5	0.1	0.1			
A35	0.1	0.1	0.0	0.1		
T36	0.1	0.8	0.1	0.2		
I37	0.1	0	0.1	0.1	0.2	0.1
G38	0.4	0	0.1			
I39	0.7	0.1	0.0	0.0	0.2	0.1
K40	0.3	0.2	0.1	0.0	0.8	
L41			0.3	0.6		
F42		0.6	0.3	0.2	0.4	0.0
K43	0.3	0.2	0.1	0.2	0.1	0.1
K44	0.4		0.1	0.2	0.0	0.1
F45		0.2	1.1	0.1	2.9	0.1
T46	0.2	0.1	0.2	0.0	0.5	
S47	0		1.0	0.0		
K48						
A49	0.3	0.4	0.0	0.2		
S50	0.2	0.5	0.1	0.0		

(1) Thakur, R. S.; Kurur, N. D.; Madhu, P. K. *Chem. Phys. Lett.* **2006**, *426*, 459–463.

(2) Baldus, M.; Petkova, A. T.; Herzfeld, J.; Griffin, R. G. *Mol. Phys.* **1998**, *95*, 1197–1207.