

Supporting Information for

Protein Side-chain-DNA Contacts Probed by Fast Magic-Angle Spinning NMR

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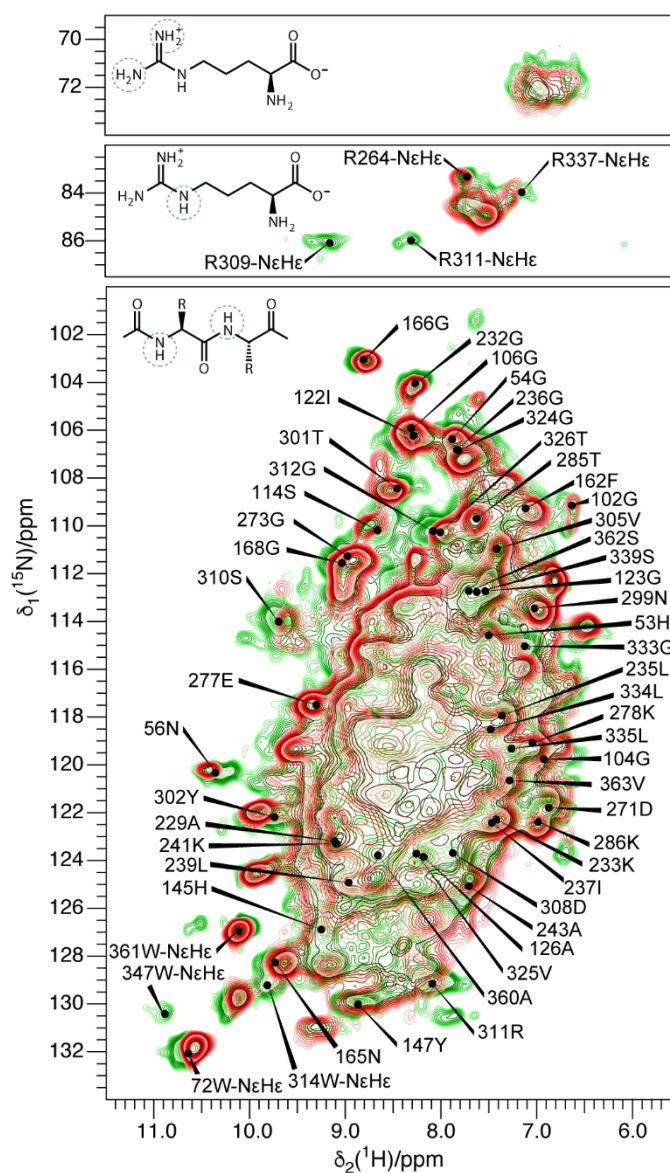


Figure S1: 2D hNH spectra of pRN1:ATP:DNA (green) and pRN1:DNA (red) with a set of representative resonances assigned by solid-state NMR at 288 K.

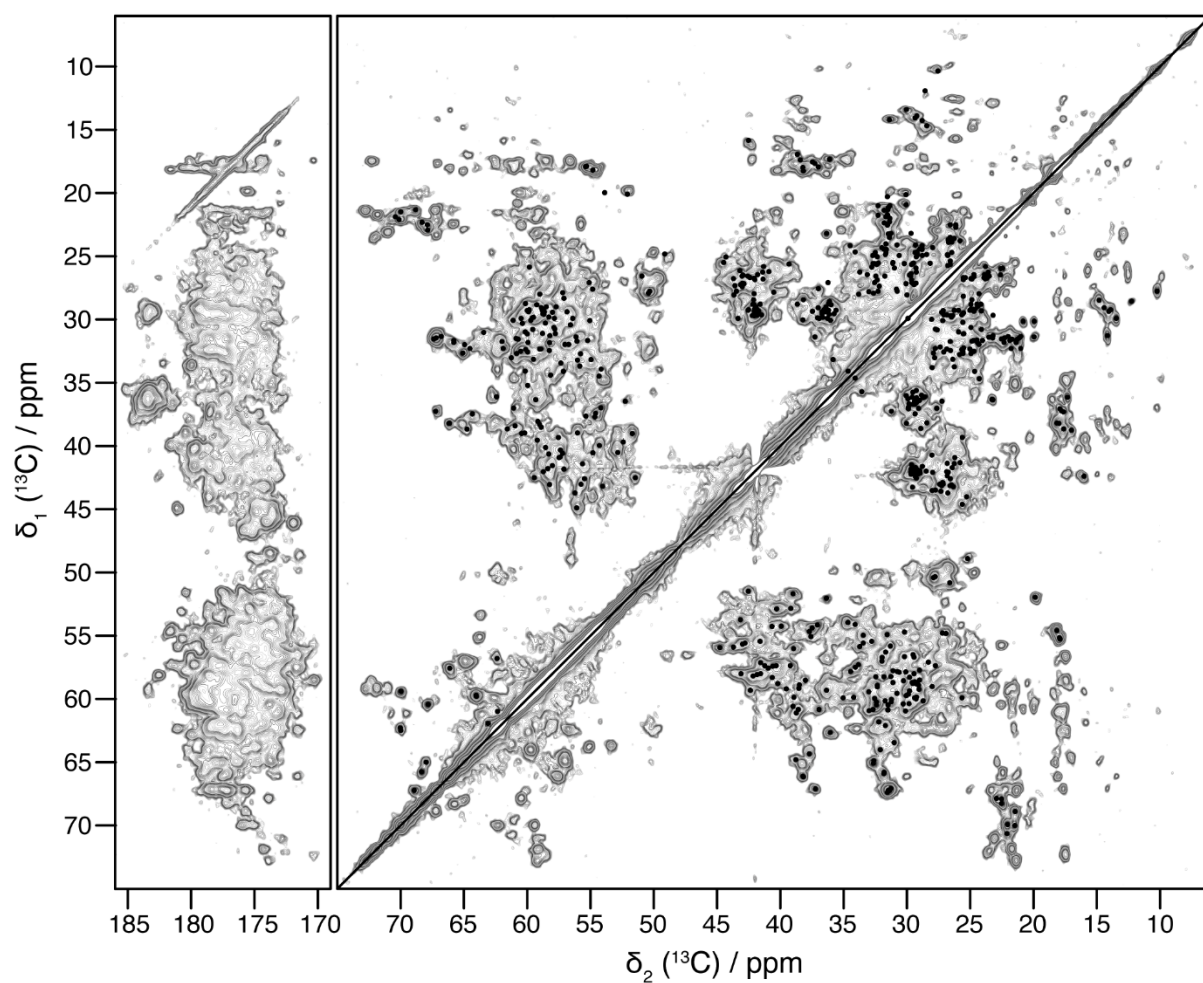


Figure S2: ^{13}C - ^{13}C 20 ms DARR correlation spectrum of pRN1:ATP:DNA. The black dots indicate back-predicted peaks of the HBD:ATP:DNA solution-state assignment.

Table S1: Experimental solid-state NMR parameters.

Experiment	(pRN1:ATP: DNA)	(pRN1:DNA)
	hNH 2D	hNH 2D
MAS frequency/ kHz	109	105
Field/ T	20	20
Transfer I	HN-CP	HN-CP
¹ H field/ kHz	89	85
X field/ kHz	14	14
Shape	Tangent ¹ H	Tangent ¹ H
Carrier ¹⁵ N / ppm	117.5	117.5
Time/ ms	0.9	0.7
Transfer II	NH-CP	NH-CP
¹ H field/ kHz	89	85
¹⁵ N field/ kHz	14	14
Shape	Tangent ¹ H	Tangent ¹ H
Time/ ms	1.0	1.0
Carrier ¹ H/ ppm	4.8	4.8
Time/ ms	1.0	1.0
t1 increments	300	300
Sweep width (t1)/ ppm	120	120
Acquisition time (t1)/ ms	14.5	14.5
t2 increments	2048	2048
Sweep width (t2)/ ppm	47	47
Acquisition time (t2)/ ms	25.8	25.8
¹ H swfTPPM decoupling/ kHz	10	10
¹⁵ N WALTZ64 decoupling/ kHz	5	5
MISSISSIPPI wat.suppl./ kHz	20	20
Inter-scan delay/ s	1.2	1.2
Number of scans	96	80
Measurement time/ h	11	9

Experiment	(pRN1:ATP: DNA)	(pRN1:DNA)
	hCH 2D	hCH 2D
MAS frequency/ kHz	109	110
Field/ T	20	20
Transfer I	HC-CP	HC-CP
¹ H field/ kHz	78	135
X field/ kHz	16	39
Shape	Tangent ¹ H	Tangent ¹ H
Carrier ¹⁵ N / ppm	56	56
Time/ ms	0.5	0.4
Transfer II	CH-CP	CH-CP
¹ H field/ kHz	78	135
¹⁵ N field/ kHz	16	39
Shape	Tangent ¹ H	Tangent ¹ H
Time/ ms	0.5	0.3
Carrier ¹ H/ ppm	4.8	4.8
Time/ ms	1.0	1.0
t1 increments	822	822
Sweep width (t1)/ ppm	200	200
Acquisition time (t1)/ ms	9.6	9.6
t2 increments	2048	3072
Sweep width (t2)/ ppm	47	47
Acquisition time (t2)/ ms	25.8	38.7
¹ H swfTPPM decoupling/ kHz	10	10
¹³ C WALTZ64 decoupling/ kHz	5	5
MISSISSIPPI wat.sup./ kHz	20	20
InterScan delay/ s	0.9	0.9
Number of scans	32	72
Measurement time/ h	8	17.5

Experiment	(pRN1:ATP:DNA)			
	hCANH 3D	hCAcoNH 3D	hNCAH 3D	hNcoCAH 3D
MAS frequency/ kHz	109	109	109	109
Field/ T	20	20	20	20
Transfer I	HC-CP	HC-CP	HN-CP	HN-CP
¹ H field/ kHz	85	85	86	85
X field/ kHz	17	17	15	15
Shape	Tangent ¹ H	Tangent ¹ H	Tangent ¹ H	Tangent ¹ H
Carrier / ppm	52	52	117.5	117.5
Time/ ms	0.75	0.75	1.5	1.0
Transfer II	CN-CP	CC DREAM	NC-CP	NC-CP
¹³ C field/ kHz	75	49	75	71
¹⁵ N field/ kHz	33	-	31	36
Shape	Tangent ¹³ C	Tangent ¹³ C	Tangent ¹³ C	Tangent ¹³ C
Carrier/ ppm	117.5	185	52	176
Time/ ms	15.0	8.0	17.0	18.0
Transfer III	NH-CP	CN-CP	CH-CP	CC DREAM
¹ H field/ kHz	86	-	90	-
¹³ C field/ kHz	-	75	16	51
¹⁵ N field/ kHz	16	33	-	-
Shape	Tangent ¹ H	Tangent ¹³ C	Tangent ¹ H	Tangent ¹³ C
Carrier/ ppm	4.8	117.5	4.8	175
Time/ ms	1.0	18.0	0.6	9.5
Transfer IV	-	NH-CP	-	CH-CP
¹ H field/ kHz	-	86	-	89
X field/ kHz	-	16	-	15
Shape	-	Tangent ¹ H	-	Tangent ¹ H
Carrier/ ppm	-	4.8	-	4.8
Time/ ms	-	1.0	-	0.7
t1 increments	96	96	50	50
Sweep width (t1)/ ppm	30	30	40	40
Acquisition time (t1)/ ms	7.4	7.4	7.3	7.3
t2 increments	50	50	96	96
Sweep width (t2)/ ppm	40	40	30	30
Acquisition time (t2)/ ms	7.3	7.3	7.4	7.4
t3 increments	3072	3072	3072	3072
Sweep width (t3)/ ppm	46.7	46.7	46.7	46.7
Acquisition time (t3)/ ms	38.7	38.7	38.7	38.7
¹ H swfTPPM decoupling/ kHz	10	10	10	10
¹⁵ N WALTZ64 decoupling/ kHz	5	5	5	5
¹³ C WALTZ64 decoupling/ kHz	5	5	5	5
MISSISSIPPI wat.suppl./ kHz	20	20	20	20
InterScan delay/ s	1.0	1.0	1.0	1.0
Number of scans	56	88	56	112
Measurement time/ h	89	140.5	89	118

Experiment	(pRN1:ATP: DNA)	(pRN1:DNA)
	hnCH(Trp)	hnCH(Trp)
MAS frequency/ kHz	100	100
Field/ T	20	20
Transfer I	HN-CP	HN-CP
¹ H field/ kHz	80	84
X field/ kHz	15	15
Shape	Tangent ¹ H	Tangent ¹ H
Carrier / ppm	120	120
Time/ ms	0.9	0.9
Transfer II	NC-CP	NC-CP
¹³ C field/ kHz	64	65
¹⁵ N field/ kHz	32	32
Shape	Tangent ¹³ C	Tangent ¹³ C
Carrier/ ppm	130	130
Time/ ms	18.0	18.0
Transfer III	CH-CP	CH-CP
¹ H field/ kHz	75	75
¹³ C field/ kHz	17	17
Shape	Tangent ¹ H	Tangent ¹ H
Carrier/ ppm	4.8	4.8
Time/ ms	0.4	0.6
t1 increments	320	320
Sweep width (t1)/ ppm	100	100
Acquisition time (t1)/ ms	7.5	7.5
t2 increments	3072	3072
Sweep width (t2)/ ppm	47	47
Acquisition time (t2)/ ms	38.7	38.7
¹ H swfTPPM decoupling/ kHz	10	10
¹⁵ N WALTZ64 decoupling/ kHz	5	5
¹³ C WALTZ64 decoupling/ kHz	5	5
MISSISSIPPI wat.supp./ kHz	20	20
InterScan delay/ s	1.0	1.0
Number of scans	688	814
Measurement time/ h	72	86