JACS
JOURNAL OF THE AMERICAN CHEMICAL SOCIETY

Supporting Information for *J. Am. Chem. Soc.*, **1989**, 111(14), 5488-5490, DOI: 10.1021/ja00196a078

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5488-5490

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Table 1. Comparison of measured J couplings, J(NMR), and values derived from the crystal structure[15], J(X-RAY), for the protein staphylococcal nuclease complexed with pdTp and Ca^{2+}.

Amino Acid	ϕ(X-RAY)	J(X-RAY)*	J(NMR)
L7	a	a	7.5
H8	-130.4	9.5	b
K9	-95.7	8.5	b
E10	-130.0	9.5	9.1
P11	-71.0		
A12	-148.3	8.1	b
T13	-121.8	9.7	10.3
L14	-58.2	4.0	c
I15	-105.3	9.2	b
K16	-169.0	5.6	5.3
A17	-82.7	7.1	5.5
I18	-97.2	8.6	8.0
D19	-158.4	6.9	5.9
G20	-58.9	4.1,6.9	b
D21	-120.2	9.7	b
T22	-129.7	9.5	10.0
V23	-145.2	8.4	8.3
K24	-93.4	8.3	8.0
L25	-127.7	9.6	b
M26	-96.5	8.6	8.6
Y27	-128.9	9.5	9.6
K28	55.4	6.9	5.6
G29	71.7	6.7,5.7	6.0,6.0
Q30	-132.4	9.4	b
P31	-67.0		
M32	-144.2	8.5	9.4
T33	-96.6	8.6	b
F34	-108.7	9.4	8.8
R35	-118.9	9.7	b
L36	-61.5	4.4	b
L37	-62.5	4.5	c
L38	59.8	6.7	b
V39	-140.4	8.8	10.1
D40	-137.8	9.0	9.3
T41	-97.8	8.7	b
P42	-56.8		
E43	-75.6	6.2	b
T44	-124.0	9.7	b
K45	-126.4	9.6	b
H46	-79.2	6.6	b
P47	-62.7		
K48	-78.8	6.6	b
K49	-123.8	9.7	b
G50	122.4	2.6,9.7	b
V51	146.1	1.8	b
E52	-55.7	3.7	b
K53	-56.7	3.8	b
Y54	78.7	6.3	b
G55	-54.6	3.6,6.8	b

P56	-60.5		
E57	-61.4	4.3	b
A58	-62.9	4.6	b
S59	-64.4	4.7	c
A60	-69.7	5.4	c
F61	-56.9	3.8	4.5
T62	-62.5	4.5	b
K63	-52.2	3.3	c
K64	-54.5	3.6	c
M65	-56.4	3.8	4.8
V66	-76.4	6.3	7.0
E67	-73.1	5.8	5.5
N68	-86.7	7.5	7.9
A69	-73.1	5.8	5.5
K70	-85.9	7.5	8.5
K71	-125.2	9.6	10.3
I72	-114.6	9.6	9.6
E73	-131.2	9.4	8.1
V74	-117.5	9.7	10.0
E75	-132.8	9.4	9.8
F76	-78.9	6.7	6.2
N77	-92.0	8.1	9.1
K78	-78.9	6.6	4.3
G79	-91.5	8.1,5.4	7.8,5.7
Q80	-50.1	3.1	4.0
R81	-104.1	9.2	b
T82	-136.1	9.2	9.5
D83	-97.5	8.7	b
K84	-63.0	4.6	b
Y85	-97.9	8.7	10.6
G86	87.7	5.7,7.7	7.0,7.0
R87	-84.3	7.3	7.1
G88	-65.1	4.8,6.9	5.7,8.3
L89	-114.9	9.6	10.5
A90	-152.2	7.7	7.9
Y91	-96.2	8.5	b
I92	-111.4	9.5	b
Y93	-119.2	9.7	9.8
A94	-117.6	9.7	10.1
D95	51.8	6.8	6.1
G96	78.1	6.4,6.5	6.2,6.2
K97	-106.6	9.3	9.5
M98	-72.2	5.7	4.8
V99	-58.4	4.0	c
N100	-54.3	3.6	c
E101	-73.3	5.9	5.5
A102	-52.1	3.3	b
L103	-60.4	4.2	c
V104	-65.3	4.8	5.0
R105	-53.2	3.4	c
Q106	-84.3	7.3	7.8
G107	72.7	6.6,5.8	5.3,5.3
L108	-101.6	9.0	8.0
A109	-164.1	6.2	b
K110	-114.4	9.6	b
V111	-75.4	6.1	6.9

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A112	-144.9	8.4	7.1
Y113	51.2	6.8	6.2
V114	-81.7	6.9	b
Y115	-114.7	9.6	9.9
K116	-56.7	3.8	b
P117	-89.1		
N118	-84.7	7.3	7.6
N119	-144.7	8.5	9.3
T120	-60.5	4.3	c
H121	-103.9	9.2	9.1
E122	-59.7	4.2	b
Q123	-63.7	4.6	b
H124	-54.5	3.6	c
L125	-62.5	4.5	5.3
R126	-67.0	5.1	c
K127	-69.1	5.3	5.0
S128	-61.1	4.3	4.7
E129	-60.6	4.3	c
A130	-60.6	4.3	c
Q131	-63.1	4.6	6.1
A132	-57.1	3.9	b
K133	-75.0	6.1	c
K134	-69.3	5.4	b
E135	-98.8	8.8	6.4
K136	52.4	6.8	6.0
L137	-84.4	7.3	6.3
N138	41.1	6.3	6.0
I139	-36.1	2.1	b
W140	-79.4	6.7	b
S141	-62.3	4.5	4.8

*calculated based on the Karplus Equation with coefficients determined from Pardi et al. (16). The ϕ values used were obtained from the crystal structure refined using isotropic B factors.

[a]residues 1-7 not observed in electron density map.

[b]J not available from NMR data.

[c]J value too small to measure (< 5 Hz).