



JOURNAL OF THE AMERICAN CHEMICAL SOCIETY

J. Am. Chem. Soc., 1998, 120(38), 9880-9887, DOI:[10.1021/ja981873k](https://doi.org/10.1021/ja981873k)

Terms & Conditions

Electronic Supporting Information files are available without a subscription to ACS Web Editions. The American Chemical Society holds a copyright ownership interest in any copyrightable Supporting Information. Files available from the ACS website may be downloaded for personal use only. Users are not otherwise permitted to reproduce, republish, redistribute, or sell any Supporting Information from the ACS website, either in whole or in part, in either machine-readable form or any other form without permission from the American Chemical Society. For permission to reproduce, republish and redistribute this material, requesters must process their own requests via the RightsLink permission system. Information about how to use the RightsLink permission system can be found at <http://pubs.acs.org/page/copyright/permissions.html>



ACS Publications

MOST TRUSTED. MOST CITED. MOST READ.

Copyright © 1998 American Chemical Society

Supplemental Table 1. NMR derived ψ values (ψ_1, ψ_2) determined from $\Gamma_{\text{H}\alpha\text{C}\alpha, \text{HN}}$ and $\Gamma_{\text{H}\alpha\text{C}\alpha, \text{C}'}$ cross-correlation rates either individually^a or in combination^b vs. ψ obtained from the x-ray structure of ubiquitin²⁰.

Residue	$\psi_1(\Gamma_{\text{H}\alpha\text{C}\alpha, \text{C}'})^a$	$\psi_2(\Gamma_{\text{H}\alpha\text{C}\alpha, \text{C}'})^a$	$\psi_1(\Gamma_{\text{H}\alpha\text{C}\alpha, \text{HN}})^a$	$\psi_2(\Gamma_{\text{H}\alpha\text{C}\alpha, \text{HN}})^a$	ψ_1^b	ψ_2^b	$\psi(\text{x-ray})$
M1	85	155	85	155	85 ^c	155	150
Q2	103	137	98	142	100	140	138
I3	81	159	77	163	78	162	163
F4	96	144	108	132	102	138	140
V5	116	124	107	133	110	130	114
K6	110	130	98	142	102	138	128
T7	78	162	75	165	76	164	171
L8	-98	-22	-92	-28	-24 ^d		-7
K11	90	150	91	149	91	149	138
T12 ^e			105	135	110	130	132
I13	93	147	92	148	92	148	142
T14			101	139	106	134	140
L15	90	150	92	148	91	149	154
E16			122	122	120	120	121
V17	83	157	73	167	76	164	171
P19	-91	-29	-89	-31	-30		-24
S20	-116	-4	-113	-7	-4		-8
D21	103	137	94	146	97	143	148
T22	91	149	86	154	88	152	160
E24	-80	-40	-77	-43	-41		-40
K27	-80	-40	-73	-47	-43		-38
A28	-85	-35	-83	-37	-36		-38
K29	-83	-37	-68	-52	-42		-37
I30	-78	-42			-69	-51	-40
Q31	-76	-44	-69	-51	-46		-49
D32	-86	-34	-82	-38	-35		-42
K33	-84	-36	-80	-40	-37		-24
E34	-110	-10	-117	-3	-8		-6
P38	-81	-39	-69	-51	-43		-32
D39	-108	-12	-111	-9	-11		-16
Q40	-113	-7	-125	5	-5		-10
Q41	117	123	115	125	117	123	130
R42	99	141	102	138	102	138	116
L43			104	136	111	129	130
I44	101	139	102	138	102	138	132
K48	102	138	94	146	97	143	143
Q49	115	125	100	140	104	136	130
L50	106	134	103	137	105	135	138
E51	97	143	100	140	99	141	140
R54	81	159	75	165	76	164	166
T55	84	156	79	161	81	159	165

L56	-82	-38	-68	-52	-42		-36
S57	-84	-36	-80	-40	-37		-30
D58	-93	-27	-99	-21	-25		-39
Y59	-122	2	-116	-4	1		5
N60	-138	18	-156	36	32		45
I61	104	136	103	137	104	136	116
Q62	76	164	72	168	73	167	170
K63	106	134	97	143	100	140	143
E64	-137	17	-154	34	19		19
S65	86	154	89	151	88	152	160
T66	113	127	111	129	112	128	127
V70	94	146	88	152	90	150	140
L71	109	131	97	143	100	140	139

^aOnly the ψ values consistent with ψ obtained by a combined fit of $\Gamma_{\text{H}\alpha\text{C}\alpha,\text{HN}}$ and $\Gamma_{\text{H}\alpha\text{C}\alpha,\text{C}'}$ cross-correlation rates are indicated.

^bValues of ψ calculated as described in Materials and Methods.

^cThere are two possible ψ values consistent with the $\Gamma_{\text{H}\alpha\text{C}\alpha,\text{HN}}$ and $\Gamma_{\text{H}\alpha\text{C}\alpha,\text{C}'}$ cross-correlation rates.

^dFor $-50^\circ \leq \psi \leq 40^\circ$ only a single ψ value is reported (see text and Figure 3b).

^e Γ value close to an extrema in the Γ vs. ψ profile. In this case an error in Γ can result in large errors in ψ , as described in the text. Values of ψ obtained from cross-correlation rates near the extrema are not included. Note that a good agreement between the x-ray derived values and ψ obtained when $\Gamma_{\text{H}\alpha\text{C}\alpha,\text{HN}}$ and $\Gamma_{\text{H}\alpha\text{C}\alpha,\text{C}'}$ are fit simultaneously is nevertheless obtained.