

BIOCHEMISTRY

including biophysical chemistry & molecular biology

Biochemistry, 1998, 37(39), 13453-13462, DOI:[10.1021/bi9811664](https://doi.org/10.1021/bi9811664)

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

Additional material to the manuscript:

**Structure determination of the Ras-binding domain of the
Ral-specific guanine nucleotide exchange factor Rlf[†]**

Dirk Esser,[†] Bettina Bauer,[†] Rob M.F. Wolthuis,[#] Alfred Wittinghofer,[†] Robbert
H. Cool^{†,*} and Peter Bayer[†]

Max-Planck-Institut für molekulare Physiologie, Abteilung Strukturelle Biologie,[†]
Abteilung Physikalische Biochemie, [†]Rheinlanddamm 201, 44139 Dortmund,
Germany, Laboratory for Physiological Chemistry, [#] Utrecht University,
Universiteitsweg 100, 3584 CG Utrecht, The Netherlands

SUPPORTING INFORMATION AVAILABLE

- a list of hydrogen bonds
- a table with the coupling constants
- a figure with the HSQC spectrum plus assignments
- a figure with the chain tracing of amino acids H82 to R90 in the fingerprint region
(overlay of TOCSY and NOESY-spectra)

List of hydrogen bonds. Donors and acceptors of hydrogen bridges are shown. N means the number of structures in which distances and geometry were favourable for hydrogen bonds. *, visible in $^2\text{H}_2\text{O}$ as pointed out in Materials and Methods.

Donor (HN)	Acceptor (CO)	N	Donor (HN)	Acceptor (CO)	N
R6	V26	10 *	S47	N43	7
I8	I24	10 *	E52	A50	10
R9	H82	10 *	E54	R87	10 *
V10	K22	10 *	V56	L85	10 *
Q11	F84	10 *	Q57	R63	10 *
M12	S19	7	L58	D83	10 *
L14	M12	8	D62	Q57	10
S19	M12	8	L65	L55	10 *
I24	I8	10 *	T66	E64	6
V26	R6	10 *	H69	I67	9
Q29	T27	6	V73	A71	10
D30	T27	6	A76	F74	9
A32	D30	8	M77	V73	10
I36	P33	7	M77	F74	9
S37	S34	7	D78	F74	10 *
R38	V35	8	A80	D78	8
R38	I36	6	H82	I7	9 *
V39	V35	10 *	F84	R9	10 *
L40	I36	8	L85	V56	10 *
K41	R38	9	L86	Q11	10 *
K42	R38	10 *	R87	E54	10 *
K42	V39	7	R89	E52	10
N43	V39	9	R89	R87	10
N44	L40	10	R90	E52	7

List of $^3J_{\text{HN}-\text{H}\alpha}$ coupling constants. All coupling constants that were used for structure calculation are given in Hz. Coupling constants were fitted from HSQC or DQF-COSY spectra with a crude or simplex algorithm using the NDEE program package.

amino acid	$^3J_{\text{HN}-\text{H}\alpha}$ (Hz)	amino acid	$^3J_{\text{HN}-\text{H}\alpha}$ (Hz)	amino acid	$^3J_{\text{HN}-\text{H}\alpha}$ (Hz)
D4	7.9	S34	3.1	E64	8.1
C 5	7.9	V35	4.4	L65	8.9
R 6	8.1	I36	5.0	T66	5.7
I7	8.1	S37	5.0	H69	6.3
I 8	5.6	R38	5.0	S70	7.3
R 9	9.2	V39	3.7	A71	6.2
V 10	9.2	L40	5.0	N72	2.7
Q 11	8.2	K41	5.0	V73	2.1
M 12	7.1	K42	5.0	F74	5.0
E13	6.1	N43	8.8	Y75	4.8
L14	8.4	N44	2.8	A76	6.1
E16	3.0	R45	9.3	M77	5.0
D17	7.5	D46	6.0	D78	4.4
S19	7.1	S47	5.2	A80	4.5
V20	8.8	A48	4.0	S81	6.8
S23	7.4	V49	8.3	H82	7.0
I24	9.9	S51	5.0	D83	8.7
L25	6.6	E52	6.8	F84	8.5
V26	9.9	F53	9.7	L85	8.6
T27	8.6	E54	9.8	L86	8.6
S28	9.0	L55	8.2	R87	8.2
Q29	9.1	V56	8.7	Q88	3.0
D30	2.4	Q57	4.3	R89	3.5
K31	7.0	D62	7.7	R90	8.2
A32	7.3	R63	9.6		



