

Supplemental Material for: Assignment of $^1\text{H}^{\text{N}}$, ^{15}N , $^{13}\text{C}^{\alpha}$, ^{13}CO and $^{13}\text{C}^{\beta}$ resonances in a 67 kDa p53 dimer using 4D-TROSY spectroscopy. Mulder et al.

Table 1S

Assignments of the main chain and C β resonances for dimeric p53
M340Q/L344R 82-360^a

res	HN	N	CO	C α	C β	res	HN	N	CO	C α	C β
pro82	-	-	176.2	62.4	30.8	thr140	8.06	118.1	173.6	65.2	68.2
ala83	8.24	125.0	176.8	51.5	18.1	cys141	9.19	127.7	172.4	54.9	27.3
ala84	8.15	125.4	175.1	49.7	17.1	pro142	-	-	175.3	61.3	30.4
pro85	-	-	176.0	62.0	30.8	val143	8.95	125.6	174.0	61.4	34.1
ala86	8.22	126.1	175.2	49.7	17.0	gln144	8.18	122.2	175.0	52.8	28.8
pro87	-	-	176.0	62.0	30.7	leu145	9.23	120.2	175.3	52.8	40.9
ala88	8.26	126.2	175.3	49.7	17.0	trp146	8.85	127.7	174.1	55.8	28.5
pro89	-	-	176.2	62.2	30.7	val147	8.01	111.5	176.2	58.5	33.9
ser90	8.09	116.8	173.4	57.1	62.9	asp148	9.03	122.6	176.4	55.0	41.1
trp91	7.96	124.7	174.2	54.0	28.6	ser149	7.78	114.2	172.2	56.2	64.0
pro92	-	-	177.1	62.2	31.0	thr150	8.12	118.3	172.3	61.2	69.0
leu93	8.27	123.3	177.2	54.1	41.1	pro151	-	-	-	-	-
ser94	8.79	115.0	175.4	57.9	63.4	pro152	-	-	-	-	-
ser95	8.07	118.6	173.8	57.8	63.4	pro153	-	-	177.4	63.1	30.4
ser96	8.10	116.5	172.6	56.3	64.4	gly154	8.71	113.7	173.9	44.4	-
val97	8.27	121.9	173.4	58.6	33.1	thr155	7.54	118.5	173.9	63.7	67.8
pro98	-	-	175.0	61.6	30.9	arg156	9.60	128.9	172.9	54.7	33.4
ser99	8.28	115.4	174.5	57.7	62.9	val157	9.00	120.9	175.1	60.1	32.1
gln100	8.45	121.5	175.6	53.6	29.1	arg158	9.53	108.7	172.9	53.9	32.0
lys101	7.74	124.1	176.4	56.5	31.7	ala159	8.66	127.7	175.3	49.9	20.9
thr102	8.74	125.8	174.0	64.1	68.2	met160	8.09	119.1	172.2	53.9	37.5
tyr103	9.24	128.7	173.8	55.8	39.6	ala161	9.37	128.0	175.6	49.0	20.5
gln104	9.12	128.9	179.0	57.8	27.9	ile162	8.35	112.2	174.8	58.8	41.8
gly105	7.23	105.6	174.2	44.6	-	tyr163	9.07	123.0	174.1	60.4	36.5
ser106	9.19	117.4	174.8	60.1	62.0	lys164	7.58	119.3	177.1	57.2	34.8
tyr107	8.58	118.0	175.4	57.6	34.6	gln165	8.93	117.2	177.9	55.1	28.7
gly108	7.36	110.7	172.7	47.4	-	ser166	-	-	176.3	61.4	65.8
phe109	8.23	120.6	174.2	57.0	39.6	gln167	9.18	119.9	175.5	57.3	26.2
arg110	8.43	125.5	172.6	54.8	31.1	his168	7.54	116.9	176.2	54.5	30.9
leu111	8.39	118.3	178.1	52.2	41.9	met169	7.37	119.3	179.0	60.1	32.6
gly112	8.36	107.8	169.1	43.2	-	thr170	8.37	110.4	172.4	62.5	68.0
phe113	7.64	115.8	175.6	55.8	41.8	glu171	7.98	124.7	175.7	55.6	28.9
leu114	9.05	123.6	177.3	54.2	41.3	val172	8.94	128.7	177.2	63.5	31.2
his115	8.67	122.5	175.1	55.4	29.0	val173	8.52	130.6	174.7	62.9	29.7
ser116	8.60	120.4	174.2	57.6	64.2	arg174	7.70	126.5	173.9	53.8	31.7
gly117	8.59	111.3	174.0	44.2	-	arg175	7.79	116.8	175.8	56.5	31.4
thr118	8.29	110.2	173.7	59.9	68.5	cys176	8.55	124.9	172.0	55.9	28.7
ala119	8.01	124.9	178.0	52.4	18.1	pro177	-	-	178.5	65.0	30.8
lys120	8.30	119.1	176.7	57.8	31.5	his178	7.84	116.2	177.4	58.9	29.1
ser121	7.64	112.4	174.4	57.2	62.7	his179	8.96	120.9	177.4	62.0	29.1
val122	7.72	122.9	175.9	62.0	31.7	glu180	8.74	121.0	177.4	58.5	28.8
thr123	8.43	115.4	174.4	62.2	68.9	arg181	7.12	115.3	176.7	55.7	29.6
cys124	7.32	120.2	172.5	57.7	27.4	cys182	7.39	119.0	174.5	59.1	26.6
thr125	9.52	123.6	180.0	59.4	68.1	ser183	8.21	118.9	174.3	57.3	61.6
tyr126	8.69	130.4	172.9	55.8	40.3	asp184	7.96	122.4	177.3	52.4	40.8
ser127	8.31	120.7	-	52.7	63.7	ser185	8.33	116.8	174.8	58.5	62.8
pro128	-	-	179.1	63.6	30.9	asp186	8.08	125.1	176.5	53.2	40.0
ala129	8.04	119.4	179.1	54.1	17.7	gly187	8.40	109.9	173.3	44.6	-
leu130	6.97	113.7	176.3	53.2	42.9	leu188	8.18	122.4	176.4	55.2	43.0
asn131	7.88	120.0	172.8	53.0	36.2	ala189	8.81	125.0	174.6	49.2	17.2
lys132	6.77	118.2	172.2	53.5	38.4	pro190	-	-	-	-	-
met133	9.43	129.2	172.5	53.4	34.7	pro191	-	-	176.0	64.4	31.6
phe134	9.14	126.7	174.4	54.8	39.8	gln192	8.43	113.7	176.6	56.8	27.6
cys135	9.20	120.3	171.6	54.5	32.0	his193	7.15	118.8	176.4	57.2	30.6
gln136	7.77	118.7	176.2	53.9	30.8	leu194	-	-	174.2	57.5	41.3
leu137	8.51	126.2	176.7	56.5	40.8	ile195	7.63	116.0	175.6	60.4	37.5
ala138	8.90	124.0	175.3	54.0	16.6	arg196	8.72	122.4	175.8	53.2	33.8
lys139	7.38	118.4	177.1	53.4	32.0	val197	7.22	118.2	175.1	60.5	32.9

res	HN	N	CO	C α	C β
glu198	8.50	129.3	176.4	54.1	30.6
gly199	8.65	111.6	173.7	45.8	-
asn200	8.10	118.0	175.2	52.0	39.6
leu201	8.74	126.6	177.4	55.4	40.5
arg202	8.46	119.6	174.1	54.8	28.1
val203	6.79	119.0	172.9	60.1	32.1
glu204	8.60	126.3	173.6	54.4	32.3
tyr205	8.78	123.7	175.3	57.8	38.4
leu206	9.27	126.6	174.7	53.7	43.4
asp207	8.27	123.1	175.1	52.1	40.9
asp208	8.15	124.6	178.4	54.8	42.8
arg209	9.03	128.7	175.3	57.4	28.9
asn210	8.68	115.4	175.9	54.0	39.3
thr211	8.61	110.2	175.3	61.0	69.7
phe212	7.53	114.1	174.4	57.3	35.7
arg213	7.53	116.3	176.5	55.8	29.8
his214	7.71	123.5	176.6	52.0	31.5
ser215	9.27	115.6	171.1	58.3	65.5
val216	8.31	116.7	174.2	58.0	32.6
val217	9.13	131.0	174.5	59.0	34.4
val218	8.29	117.8	172.6	56.7	32.4
pro219	-	-	177.2	62.1	30.6
tyr220	8.51	124.2	173.7	58.9	37.0
glu221	7.06	131.5	170.7	51.5	30.0
pro222	-	-	-	-	-
pro223	-	-	176.7	61.8	31.0
glu224	8.29	123.1	175.9	55.1	29.1
val225	8.20	122.0	177.5	64.2	30.3
gly226	8.74	116.4	173.8	44.3	-
ser227	8.23	117.0	172.9	56.4	63.9
asp228	8.39	120.6	174.0	53.8	42.0
cys229	7.39	112.7	171.6	54.2	27.4
thr230	7.66	120.1	172.8	61.5	69.7
thr231	8.68	124.5	173.0	61.8	68.9
ile232	9.01	129.9	173.1	59.2	39.0
his233	8.35	125.0	172.9	53.3	29.3
tyr234	8.33	123.5	176.0	57.3	40.3
asn235	8.96	118.0	171.9	51.8	43.6
tyr236	9.97	122.2	178.1	57.7	40.4
met237	8.50	117.3	174.8	53.6	28.3
cys238	7.21	120.7	173.3	60.4	33.7
asn239	8.32	118.8	177.4	53.3	39.5
ser240	9.49	120.5	174.1	63.4	62.4
ser241	8.01	110.0	175.1	57.8	63.0
cys242	7.69	122.7	177.7	63.8	28.6
met243	8.92	129.9	177.4	56.4	-
gly244	8.79	111.0	173.3	44.8	-
gly245	7.24	108.9	-	43.4	-
met246	-	-	-	-	-
asn247	-	-	-	-	-
arg248	-	-	-	-	-
arg249	-	-	-	-	-
pro250	-	-	177.3	62.1	32.5
ile251	7.03	112.7	174.2	58.4	42.3
leu252	9.18	119.3	177.9	52.5	44.0
thr253	8.81	115.3	171.3	61.8	68.9
ile254	9.23	127.3	175.6	59.6	38.4
ile255	9.19	131.1	175.4	57.7	36.4
thr256	9.36	116.4	172.4	57.5	69.1
leu257	8.02	125.1	175.8	51.9	41.9
glu258	9.12	126.3	175.1	53.4	33.8
asp259	8.33	120.0	177.6	52.0	40.4
ser260	8.48	113.6	175.2	60.6	62.3

res	HN	N	CO	C α	C β
ser261	8.01	117.4	173.9	57.8	63.0
gly262	7.96	109.6	174.3	44.1	-
asn263	8.62	121.2	174.9	52.9	37.3
leu264	8.47	124.0	176.5	55.8	41.2
leu265	9.55	124.8	177.7	54.2	42.6
gly266	7.83	107.1	170.3	44.9	-
arg267	10.17	125.3	173.9	56.1	33.9
asn268	9.53	129.3	173.2	53.0	43.4
ser269	9.67	114.4	172.5	57.5	66.3
phe270	8.05	113.5	172.7	55.6	39.3
glu271	8.54	123.6	174.6	55.0	29.3
val272	7.92	123.5	174.1	59.8	34.5
arg273	8.45	128.2	172.9	54.4	32.7
val274	8.51	130.5	177.3	59.5	30.7
cys275	9.82	124.8	172.6	54.8	30.9
ala276	8.37	122.8	178.9	54.4	18.4
cys277	8.61	116.6	171.2	54.6	26.8
pro278	-	-	176.8	65.7	31.6
gly279	8.88	105.3	175.1	46.5	-
arg280	7.14	122.5	178.4	58.2	29.2
asp281	8.12	121.8	177.1	57.1	38.4
arg282	7.70	121.2	176.7	58.7	27.5
arg283	7.25	118.3	178.8	58.8	28.6
thr284	8.29	116.7	176.4	65.7	68.0
glu285	8.08	121.8	180.2	60.4	28.5
glu286	8.53	120.6	179.2	59.2	27.9
glu287	8.28	121.9	178.6	58.4	27.9
asn288	7.88	118.0	176.9	54.8	37.3
leu289	7.46	121.2	178.3	56.6	40.7
arg290	7.66	119.7	177.6	57.2	29.1
lys291	7.88	120.0	177.1	56.8	31.4
lys292	7.85	121.0	177.1	56.6	31.4
gly293	7.99	109.1	173.5	44.4	-
glu294	7.96	122.4	174.4	53.7	28.7
pro295	-	-	-	-	-
his296	-	-	-	-	-
his297	-	-	174.1	54.8	29.2
glu298	8.46	123.2	175.7	55.6	29.4
leu299	8.31	125.5	174.5	52.3	40.4
pro300	-	-	-	-	-
pro301	-	-	177.6	62.8	30.7
gly302	8.47	110.3	174.4	44.6	-
ser303	8.01	116.2	174.8	58.2	63.2
thr304	8.13	116.6	174.3	61.5	69.1
lys305	8.19	124.6	176.2	55.7	31.7
arg306	8.18	123.4	175.5	55.3	29.6
ala307	8.21	126.5	177.0	51.5	18.2
leu308	8.16	123.8	175.2	52.3	40.3
pro309	-	-	176.4	62.5	30.8
asn310	8.40	119.2	174.7	52.7	37.9
asn311	8.35	120.0	175.2	52.8	38.0
thr312	8.10	114.8	174.5	61.5	69.1
ser313	8.27	118.5	174.2	57.8	62.9
ser314	8.23	118.3	174.2	57.8	62.9
ser315	8.20	118.3	-	57.7	63.0
pro316	-	-	176.5	62.5	30.9
gln317	8.35	122.5	173.8	52.9	28.0
pro318	-	-	176.5	62.4	31.0
lys319	8.32	122.6	176.3	55.5	31.9
lys320	8.23	123.7	176.0	55.3	32.0
lys321	8.31	125.3	174.2	53.6	31.3
pro322	-	-	176.7	62.4	30.9
leu323	8.27	122.7	177.0	54.7	40.9

res	HN	N	CO	C α	C β
asp324	8.21	121.8	176.1	53.8	40.6
gly325	8.12	109.5	172.9	44.3	–
glu326	7.94	121.3	174.2	55.4	29.8
tyr327	7.83	120.3	174.9	56.7	39.9
phe328	9.20	121.9	174.7	56.1	42.1
thr329	8.34	115.5	172.9	60.8	69.9
leu330	8.94	127.4	174.4	52.8	45.9
gln331	8.60	125.8	174.8	54.5	28.8
ile332	9.31	127.2	173.6	59.2	40.4
arg333	9.70	130.9	175.6	55.3	30.0
gly334	8.60	115.4	173.5	43.7	–
arg335	8.83	127.1	177.4	58.8	28.5
glu336	8.64	119.4	178.7	59.3	27.5
arg337	7.87	122.5	178.1	58.7	28.7
phe338	8.38	120.4	176.0	61.1	37.7
glu339	8.56	119.3	179.0	58.5	27.6
gln340	7.69	119.2	179.5	58.3	27.3
phe341	8.12	120.7	177.3	60.7	38.1
arg342	9.25	122.5	178.3	59.2	28.1
glu343	8.11	119.9	179.2	59.0	28.2
arg344	7.43	120.2	178.5	58.2	28.9
asn345	8.72	119.1	176.7	56.9	38.9
glu346	8.72	119.1	178.9	58.9	28.5
ala347	7.74	122.0	180.9	54.5	16.8
leu348	7.78	120.5	179.2	57.2	39.5
glu349	8.33	119.9	179.9	58.8	27.9
leu350	8.16	122.9	179.2	57.2	40.3
lys351	7.47	120.2	179.3	58.2	30.6
asp352	7.98	120.9	177.8	56.2	39.5
ala353	7.71	122.2	178.9	53.2	17.4
gln354	7.90	118.2	176.4	55.9	27.8
ala355	7.81	123.5	178.1	52.5	17.8
gly356	8.14	108.2	173.8	44.6	–
lys357	7.87	121.1	176.1	55.3	31.9
glu358	8.37	124.3	174.4	53.8	28.5
pro359	–	–	176.2	62.8	31.1
gly360	7.94	116.0	178.8	45.2	–

local minor form of folded oligomerization domain (dimer)

gly325	8.06	109.4	172.9	44.4	–
glu326	7.67	119.9	174.6	53.4	29.2

unfolded oligomerization domain (monomer)

res	HN	N	CO	C α	C β
asp324	8.16	121.2	176.4	54.0	40.4
gly325	8.18	109.4	174.0	44.8	–
glu326	8.10	121.2	176.1	56.0	29.2
tyr327	8.04	121.1	175.5	57.8	37.8
phe328	7.97	121.3	175.6	57.7	38.3
thr329	7.87	116.0	174.1	61.5	68.9
leu330	7.99	124.3	177.1	54.9	41.0
gln331	8.13	121.5	175.7	55.5	28.1
ile332	7.97	122.5	176.0	60.7	37.3
arg333	8.29	125.3	176.6	55.8	29.5
gly334	8.35	110.8	174.1	44.9	–
arg335	8.10	121.3	176.3	55.8	29.3
glu336	8.50	122.1	176.4	56.5	28.8
arg337	8.14	121.5	176.0	55.8	29.5
phe338	8.09	121.2	175.7	57.4	38.2
glu339	8.24	122.5	176.1	56.2	29.3
gln340	8.13	121.1	175.6	55.8	28.3
phe341	8.11	121.3	175.4	57.3	38.2
arg342	7.94	123.1	175.8	55.7	29.8
glu343	8.29	122.3	176.3	56.2	29.0
arg344	8.24	122.3	175.8	55.8	29.4
asn345	8.41	120.7	175.2	52.9	37.9
glu346	8.42	122.6	176.2	56.7	29.0
ala347	8.10	124.2	177.8	52.2	17.8
leu348	7.88	121.2	177.3	55.0	41.0
glu349	8.16	121.6	176.3	56.0	28.9
leu350	8.06	123.6	177.3	54.8	40.7
lys351	8.12	122.4	176.4	56.1	31.7
asp352	8.18	121.5	176.1	54.0	40.2
ala353	8.11	125.0	177.8	52.5	17.9
gln354	8.21	119.0	175.8	55.2	28.3
ala355	8.01	125.1	178.0	52.2	17.9
gly356	8.28	108.8	173.7	44.5	–
lys357	7.93	121.2	176.2	55.3	32.0
glu358	8.41	124.4	174.4	53.8	28.4

^a All ¹⁵N and HN shifts are for the TROSY multiplet component. Nuclei for which assignments are impossible to obtain from existing experiments are indicated by dashed lines (note that pro HN and gly c β are not present). Blank spaces denote cases where assignments are not available due to missing correlations (from conformational exchange, for example).

