Supporting information
Xu et al. Solution Structure of the *Pfu* Rpp21-Rpp29 Protein Complex

Figures

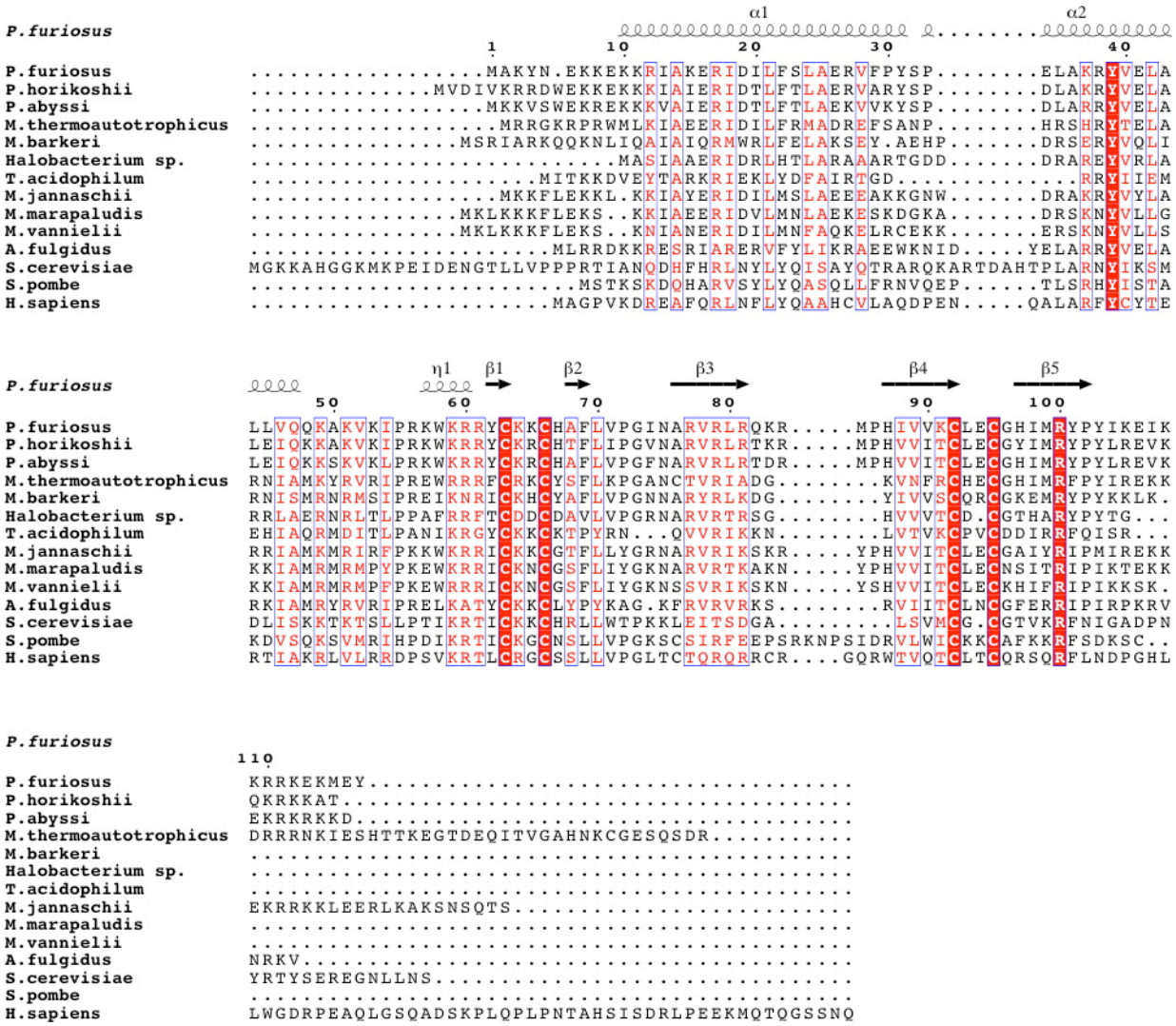

Figure S1: Sequence alignment of select RPP21 homologs from Archaea and Eukarya. The alignment was generated with CLUSTALW, and illustrated using ESPRIPT2.2, in which red letters indicate a global similarity score of 0.7, and red boxed letters indicate invariant residues. Secondary structural elements represented in cartoon are observed in the NMR ensemble of *Pfu* RPP21 in complex with *Pfu* RPP29. Aligned sequences are form *Pyrococcus furiosis* (NCBI entry NP_579342), *Pyrococcus horikoshii* (NP_143456), *Pyrococcus abyssi* (NP_126253), *Methanobacterium thermoautotrophicum* (NP_276730), *Methanosarcina barkeri* (NCBI_entry YP_304815), *Halobacterium sp.* (NP_279631), *Thermoplasma acidophilum* (NP_393654), *Methanococcus jannaschii* (NP_247957), *Methanococcus marapaludis* (YP_001549778), *Methanococcus vannielii* (YP_001322736), *Archaeoglobus fulgidus* (NP_068950), *Saccharomyces cerevisiae* (NP_012280), *Schizosaccharomyces pombe* (NP_596472) and *Homo sapiens* (NP_079115).

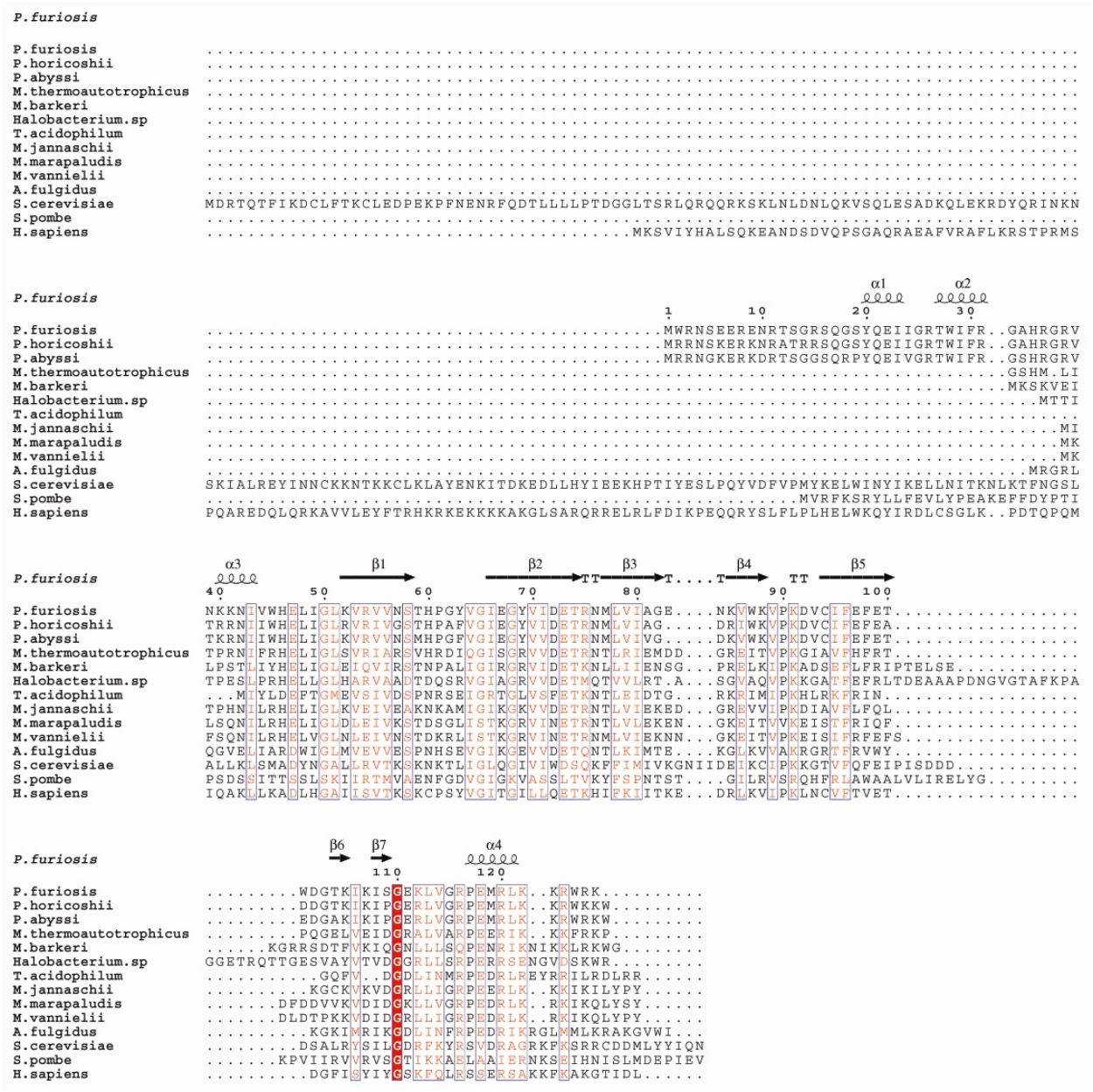

Figure S2: Sequence alignment of select RPP29 homologues from Archaea and Eukarya. The alignment was generated with CLUSTALW, and illustrated using ESPRIPT2.2, in which red letters indicate a global similarity score of 0.7, and red boxed letters indicate invariant residues. Secondary structural elements represented in cartoon are observed in the NMR ensemble of *Pfu* RPP29 in complex with *Pfu* RPP21. Aligned sequences are form *Pyrococcus furiosis* (NCBI entry NP_579545), *Pyrococcus horikoshii* (NP_143607), *Pyrococcus abyssi* (NP_126024), *Methanobacterium thermoautotrophicum* (10QK_A), *Methanosarcina barkeri* (YP_303669), *Halobacterium sp.* (NP_280464), *Thermoplasma acidophilum* (NP_394719), *Methanococcus jannaschii* (NP_247439), *Methanococcus marapaludis* (YP_001549311), *Methanococcus vannielii* (YP_001323236), *Archaeoglobus fulgidus* (1TSF_A), *Saccharomyces cerevisiae* (NP_009816), *Schizosaccharomyces pombe* (NP_588479) and *Homo sapiens* (NP_006618).

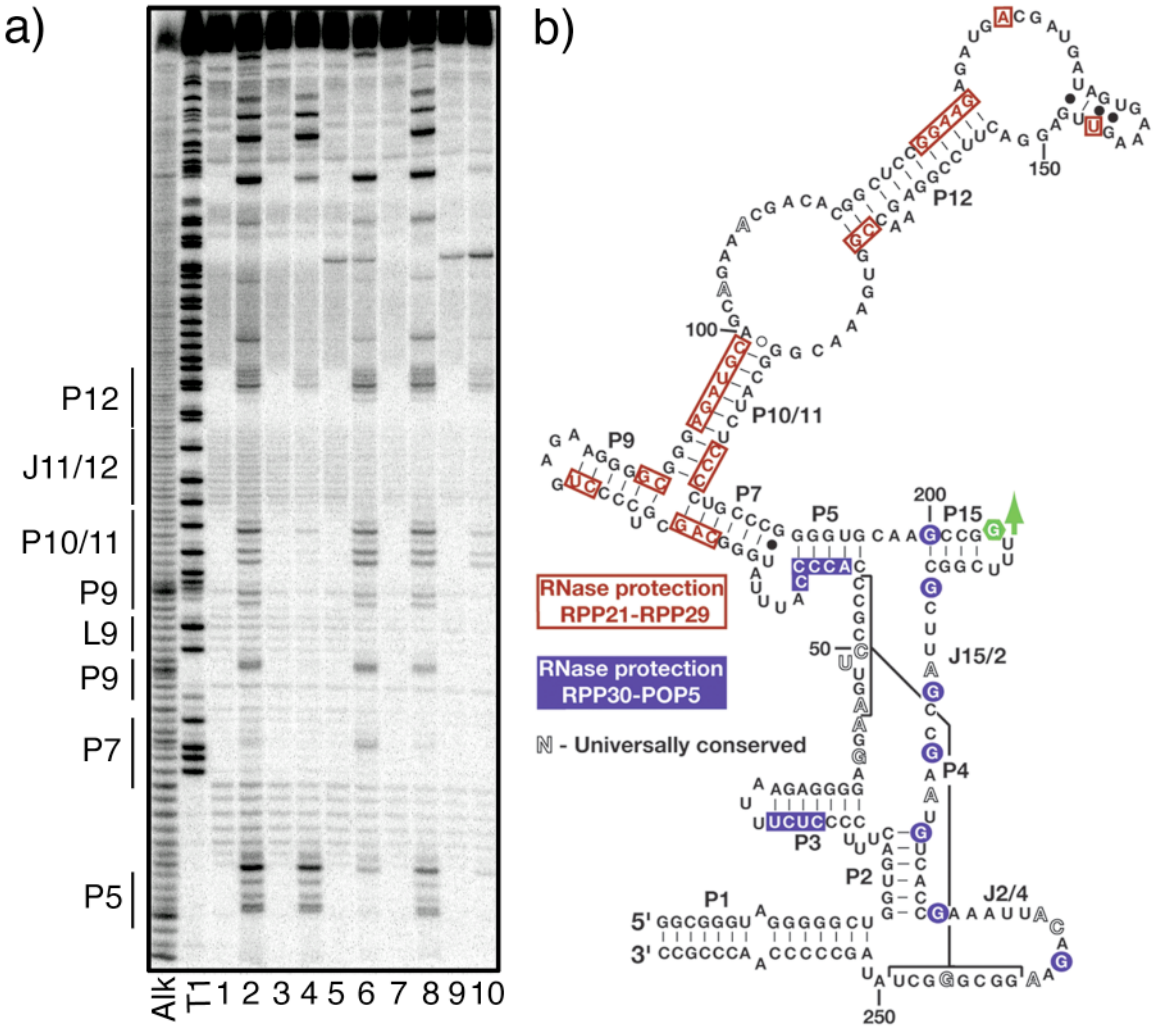

Figure S3. Footprinting using RNase V1 and RNase T1 to identify RPP-binding sites in *Mja* RPR. (a) Same as panel a in Figure 6 except this is a longer electrophoretic run, which was required to map protection patterns distal to the labeled termini. *Mja* RPR labeled at the 5'-end was incubated either without (lanes 1, 3, 5, 7 and 9) or with (lanes 2, 4, 6, 8 and 10) RNase V1 (panel a) or RNase T1 (panel b). *Mja* RPR was present either alone (lanes 1, 2, 7 and 8), with RPP21-RPP29 (lanes 3 and 4), with RPP30-POP5 (lanes 5 and 6) or with both binary complexes (lanes 9 and 10). Since reconstitution of the RPR with each binary RPP complex is performed in a buffer different from that used for reconstitution with both binary complexes together, two different control RNase T1/V1 digestions of the RPR are shown (lanes 1, 2 for binary RPPs and lanes 7, 8 for both binary pairs). "Alk." and "T1" represent molecular size ladders generated by subjecting end-labeled, denatured *Mja* RPRs to alkaline hydrolysis and partial RNase T1 digestion, respectively. The RNase T1 cleavage sites were also mapped by using primer extension assays. (b) Summary of the RPP footprinting data depicted on a secondary-structure model of *Mja* RPR. Circled and boxed nucleotides indicate protection to RNase T1 and RNase V1, respectively; blue and red colors indicate regions of protection by RPP30-POP5 and RPP21-RPP29, respectively. The green arrow indicates an RPR position that showed increased susceptibility to RNase T1 in the presence of either RPP30-POP5 or all four RPPs. RNase V1 cleavages around nucleotides 130-150 suggest that the secondary structure as drawn may need to be revised.

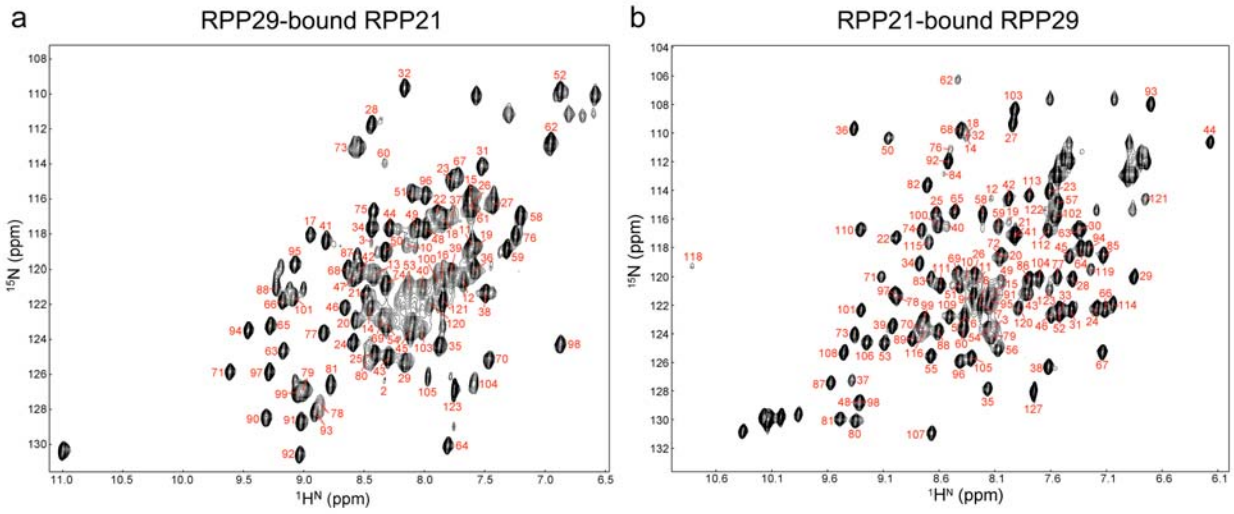

Figure S4: Two-dimensional ^{1}H-^{15}N NMR spectra of *Pfu* RPP21 (a) and RPP29 (b) in complex with its (unlabeled) partner. Backbone amide assignments are indicated in red as the residue number.

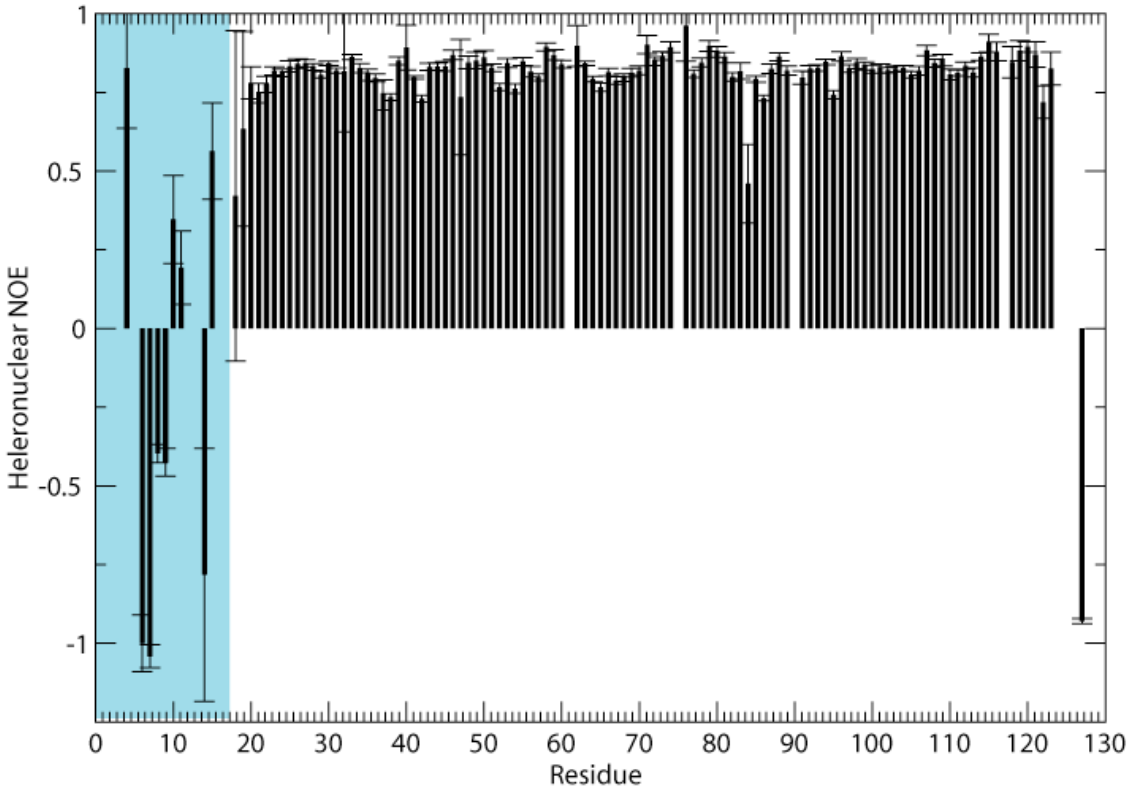

Figure S5: Heteronuclear {^{1}H)-^{15}N NOE data of *Pfu* RPP29 in the presence of *Pfu* RPP21 shows that the N-terminus (residues 1-16, highlighted in cyan) remains flexible, indicating this segment is not involved in binding to RPP21.

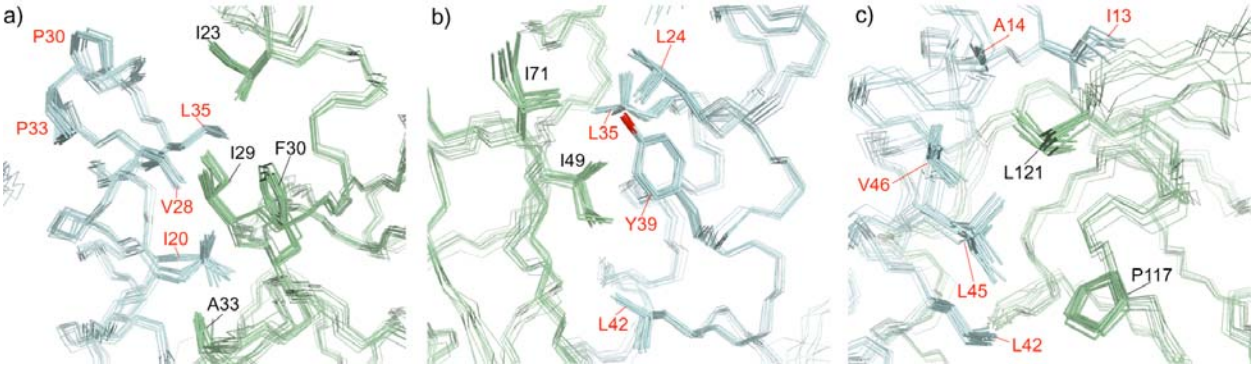

Figure S6: Interface of the *Pfu* RPP29-RPP21 complex in the ensemble. The backbones are shown in lines (RPP21 in cyan and RPP29 in cyan). The residues involving in protein-protein interactions are shown in sticks. Panels a-c are similar zoom-in regions as panel c-e in Figure 3.

Table S1. Inter-molecular NOEs identified from chemical shifts in the ^{13}C-filtered/edited NOESY spectrum recorded on [U-^{13}C,^{15}N]-RPP21 (*) and unlabeled RPP29.[†]

RPP21*	RPP29
K10Hβ	L121Mδ-
K10Hα	L121Mδ+
K10Hα	L121Mδ-
I13Mγ2	W45Hδ
I13Mγ2	W45Hβ-
I13Mγ2	H46Hδ2
I13Mδ	W45Hζ3
I13Mγ2	N42Hα
I13Mγ2	N42Hβ-
I13Mγ2	L121Mδ-
I13Mγ2	N42Hβ+
I13Mδ	W45Hε3
I13Mδ	H46Hε1
A14Hα	L121Mδ-
A14Mβ	L121Mδ-
A14Mβ	L121Mδ+
A14Mβ	L121Hβ-
A14Hα	L121Mδ+
A14Mβ	L121Hβ+
E16Hγ-	H46Hε1
E16Hβ-	H46Hε1
E16Hγ+	H46Hδ2
E16Hγ+	H46Hε1
E16Hβ+	H46Hε1
E16Hα	H46Hε1
R17Hα	E47Hβ
I20Mγ2	H34Hβ+
I20Mγ2	E47Hγ+
I20Mγ2	E47Hβ
I20Mγ2	E47Hγ-
I20Mγ2	H34Hδ2
I20Mγ2	H34Hβ-
L21Mδ-	I49Hβ
L21Mδ-	I49Mγ2
L21Mδ-	I49Mδ
L21Mδ+	I49Mδ
L21Mδ-	E47Hγ-
S23Hα	A33Mβ
S23Hβ	A33Mβ
L24Mδ+	I49Mδ
L24Mδ-	G50Hα+
L24Mδ-	F30Hβ+

RPP21*	RPP29
K10Hβ	L121Mδ-
K10Hα	L121Mδ+
K10Hα	L121Mδ-
I13Mγ2	W45Hδ
S32Hβ-	E22Hβ+
S32Hβ-	E22Hγ
L35Mδ-	I71Mδ
L35Mδ-	Y20Hδ
L35Mδ+	I71Mδ
L35Mδ-	I23Hβ
L35Mδ+	I23Hβ
L35Mδ+	I71Mγ2
L35Mδ-	Y20Hε
L35Mδ-	D72Hβ-
L35Mδ-	D72Hβ+
L35Mδ+	Y20Hδ
L35Mδ-	I23Mγ1
L35Mδ+	Y20Hε
L35Mδ+	F30Hζ
L35Mδ+	I23Mδ
L35Mδ+	I23Mγ1
L35Mδ+	D72Hβ-
L35Mδ-	I71Hα
L35Mδ-	I71Mγ2
L42Mδ+	P117Hγ
L42Mδ-	P117Hβ-
L42Mδ+	I49Mδ
L24Mδ-	A33Hα
L24Mδ+	A33Hα
L24Mδ-	F30Hδ
L24Mδ+	F30Hδ
L24Mδ-	F30Hα
L24Mδ+	F30Hε
L24Mδ-	I49Mγ2
L24Mδ-	A33Mβ
L24Mδ-	F30Hε
L24Mδ+	G50Hα+
L24Mδ+	A33Mβ
L24Mδ+	I49Hβ
L24Mδ+	I49Mγ2
L24Mδ+	G50Hα-
L24Mδ-	G50Hα-

RPP21*	RPP29
K10Hβ	L121Mδ-
K10Hα	L121Mδ+
K10Hα	L121Mδ-
I13Mγ2	W45Hδ
L24Mδ+	F30Hβ-
R27Hα	I29Hβ
V28Hβ	I23Mδ
V28Mγ-	I29Mγ1
V28Mγ-	I23Mδ
V28Mγ-	I29Hβ
V28Hβ	I29Mδ
V28Mγ+	I29Hβ
V28Mγ+	I23Mδ
V28Mγ+	F30Hζ
V28Mγ-	I29Mγ2
V28Mγ-	F30Hε
V28Mγ-	I29Mδ
V28Mγ+	I23Mγ1
V28Mγ+	I29Mγ1
V28Mγ+	F30Hβ-
V28Mγ+	I29Mδ
V28Mγ-	F30Hζ
V28Hα	I29Mδ
V28Hα	I23Mδ
V28Mγ+	F30Hε
V28Mγ+	I29Mγ2
V28Hα	I29Mγ2
V28Mγ-	I23Mγ1
P30Hγ+	I29Hβ
S32Hα	E22Hγ
S32Hβ-	I23Mδ
RPP21	RPP29
L42Mδ+	I49Mγ2
L42Mδ+	P117Hβ-
L42Mδ-	P117Hγ
L42Mδ-	P117Hβ+
L42Mδ-	I49Mδ
L42Mδ-	P117Hδ-
L42Mδ+	P117Hβ+
L42Mδ-	E118Hα
L45Mδ+	P117Hδ-
L45Mδ+	L121Hα

RPP21*	RPP29
K10Hβ	L121Mδ-
K10Hα	L121Mδ+
K10Hα	L121Mδ-
I13Mγ2	W45Hδ
L45Mδ-	P117Hδ-
L45Mδ-	P117Hγ
L45Mδ+	P117Hγ
V46Hγ	L121Hα
V46Hγ	L121Mδ-

RPP21*	RPP29
K10Hβ	L121Mδ-
K10Hα	L121Mδ+
K10Hα	L121Mδ-
I13Mγ2	W45Hδ
V46Hγ	P117Hβ-
V46Hγ	L121Mδ+
V46Hα	L121Hα
V46Hα	L121Mδ+
A50Mβ	L121Mδ+

RPP21*	RPP29
K10Hβ	L121Mδ-
K10Hα	L121Mδ+
K10Hα	L121Mδ-
I13Mγ2	W45Hδ
A50Mβ	L121Mδ-
A50Hα	L121Mδ+
A50Mβ	L121Hβ+

† The downfield and upfield-shifted non-stereoassigned, but spectroscopically distinct diastereotopic methyl groups and methylene protons are indicated by “+” and “-“, respectively.

Table S2. Inter-molecular NOEs identified from chemical shifts in the ^{13}C-filtered/edited NOESY spectrum recorded on unlabeled RPP21 and [U-^{13}C,^{15}N]-RPP29 (*).[†]

RPP29*	RPP21
S19Hβ	P33Hβ
S19Hβ	L35Mδ-
S19Hβ	L35Mδ+
S19Hβ	L35Hα
S19Hα	E34Hβ1/2
S19Hβ	E34Hβ1/2
Y20Hα	L35Mδ-
Y20Hα	L35Mδ+
I23Mγ2	Y31Hβ-
I23Mγ2	V28Mγ-
I23Mδ	V28Mγ+
I23Mγ2	L35Hβ-
I23Mγ2	Y31Hδ
I23Mγ1	L35Mδ+
I23Mδ	S32Hβ+
I23Mδ	Y31Hδ
I23Mδ	S32Hβ-
I23Mγ2	Y31Hβ+
I23Mδ	Y31Hβ-
I23Mγ2	S32Hβ-
I23Mδ	V28Hβ
I23Mγ2	L35Hγ
I23Mγ2	V28Hβ
I23Mγ2	S32Hβ+
I23Mγ2	V28Hα
I23Mδ	V28Hα
R26Hγ+	Y31Hε
R26Hδ-	Y31Hε
R26Hδ+	Y31Hε
R26Hδ+	Y31Hδ
R26Hγ+	Y31Hδ
R26Hδ-	Y31Hβ+
R26Hδ-	Y31Hδ
I29Hβ	R27Hγ
I29Mδ	R27Hα
I29Mγ2	L24Mδ-
I29Mγ1	R27Hβ
I29Mγ1	Y31Hδ
I29Mδ	R27Hβ
I29Mγ2	V28Mγ+
I29Mγ2	R27Hδ+
I29Mγ2	Y31Hε

RPP29*	RPP21
S19Hβ	P33Hβ
S19Hβ	L35Mδ-
S19Hβ	L35Mδ+
RPP29	RPP21
W45Hβ-	I13Mγ2
W45Hβ+	I13Mγ2
H46Hα	I13Mδ
E47Hα	R17Hβ
E47Hα	R17Hα
E47Hβ	R17Hα
I49Mγ2	L42Mδ+
I49Mδ	Y39Hε
I49Mδ	L21Mδ-
I49Mγ2	L24Hβ
I49Mγ2	L21Mδ-
I49Mδ	L42Hβ-
I49Mγ2	L42Hβ-
I49Mγ2	L24Hα
I49Mγ2	L24Hγ
I49Mγ2	L24Mδ+
I49Hα	L24Mδ+
I49Mδ	L42Mδ+
I49Mδ	L24Mδ+
I49Mγ2	R38Hδ+
I49Hβ	L21Mδ-
I49Mγ2	Y39Hε
I49Mγ2	Y39Hδ
I49Mδ	R38Hδ+
I49Mδ	Y39Hδ
I49Hβ	L24Mδ+
G50Hα+	L24Mδ+
G50Hα+	L24Mδ-
G50Hα-	L24Mδ+
G50Hα-	L24Mδ-
I71Mγ2	Y39Hδ
I71Mδ	L35Mδ+
I71Mγ2	L35Mδ-
I71Mγ2	L35Mδ+
I29Mδ	R27Hδ-
I29Hα	R27Hδ-
I29Hβ	R27Hβ
I29Mδ	Y31Hε

RPP29*	RPP21
S19Hβ	P33Hβ
S19Hβ	L35Mδ-
S19Hβ	L35Mδ+
I29Mγ2	L24Hα
I29Mδ	Y31Hδ
I29Mδ	V28Mγ+
I29Mγ2	Y31Hδ
I29Mγ2	R27Hδ-
I29Mδ	V28Hβ
I29Mγ2	R27Hβ
I29Mγ2	R27Hα
I29Mδ	L24Hα
I29Mγ2	V28Hα
I29Mγ2	V28Hβ
I29Hα	R27Hδ+
I29Mδ	R27Hγ
I29Mγ2	R27Hγ
I29Mγ1	V28Mγ+
I29Mδ	V28Hα
I29Mδ	L24Mδ-
F30Hα	L24Mδ-
A33Hα	L24Mδ-
A33Mβ	L24Mδ+
A33Mβ	L24Mδ-
A33Hα	R27Hβ
A33Mβ	R27Hδ+
A33Mβ	R27Hδ-
A33Mβ	L24Hα
A33Mβ	R27Hβ
H34Hβ+	I20Mγ2
H34Hα	I20Hβ
H34Hα	I20Hα
H34Hβ-	I20Mγ2
H34Hα	I20Mδ
H34Hα	I20Mγ2
N42Hα	I13Mγ2
N42Hβ+	I13Mγ2
N42Hβ-	I13Mγ2
W45Hβ+	I13Mδ
W45Hα	I13Mγ2
W45Hβ-	I13Mδ
RPP29	RPP21

RPP29*	RPP21
S19Hβ	P33Hβ
S19Hβ	L35Mδ-
S19Hβ	L35Mδ+
I71Mδ	L35Mδ+
I71Mδ	L35Mδ-
I71Hβ	L35Mδ-
I71Hα	L35Mδ+
D72Hα	Y39Hδ
P117Hβ+	L42Mδ-
P117Hδ+	L42Mδ-
P117Hγ	L42Mδ-
P117Hα	L42Mδ-
P117Hβ-	L42Mδ-
E118Hα	K49Hδ
E118Hα	L42Mδ+
E118Hα	V46Hα

RPP29*	RPP21
S19Hβ	P33Hβ
S19Hβ	L35Mδ-
S19Hβ	L35Mδ+
E118Hα	L45Hβ+
E118Hα	L45Mδ-
L121Mδ-	I13Mγ2
L121Mδ+	I13Mδ
L121Mδ+	A50Mβ
L121Mδ+	L45Mδ-
L121Mδ-	L45Mδ-
L121Mδ+	K49Hβ+
L121Mδ+	K10Hα
L121Mδ+	R17Hβ
L121Mδ-	V46Hα
L121Mδ-	K10Hα
L121Mδ-	A50Mβ

RPP29*	RPP21
S19Hβ	P33Hβ
S19Hβ	L35Mδ-
S19Hβ	L35Mδ+
L121Mδ-	R17Hα
L121Mδ-	A50Hα
L121Mδ-	I13Mδ
L121Mδ-	K10Hβ
L121Mδ+	A50Hα
L121Mδ+	V46Hα
L121Mδ+	R17Hα

† The downfield and upfield-shifted non-stereoassigned, but spectroscopically distinct diastereotopic methyl groups and methylene protons are indicated by “+” and “-“, respectively.

Table S3. Inter-molecular NOEs identified by iterative structure-based assignment in ^{13}C-separated NOESY spectra recorded on [U-^{13}C,^{15}N]-RPP21 (*) and unlabeled RPP29.†

RPP21*	RPP29
I13Hα	H46Hα
I13Mγ2	W45Hδ1
I13Mγ2	N42Hα
I13Mγ2	H46Hα
I13Mδ	W45Hε3
I13Mδ	W45Hδ1
I13Mδ	W45Hζ3
I13Mδ	W45Hβ-
I13Mδ	L121Mδ-
A14Hα	L121Hβ+
A14Mβ	L121Mδ+
E16HN	H46Hε1
E16Hγ+	N42Hβ+
E16Hγ+	H46Hε1
E16Hβ+	H46Hε1
R17Hα	E47Hγ-
I18HN	E47Hγ+
I20HN	E47Hγ+
I20HN	E47Hβ
I20Hα	H34Hα
I20Mγ2	H34Hδ2
I20Mγ2	G50Hα+
I20Mγ2	H34Hα
I20Mγ2	H34Hβ-
I20Mγ2	E47Hβ
I20Mγ2	E47Hγ-
I20Mγ2	I49Hβ
I20Mγ2	A33Mβ
L21HN	E47Hγ+
L21HN	I49Hβ
L21Hα	I49Mγ2
L21Mδ+	E47Hγ+
L21Mδ+	E47Hβ
L21Mδ+	E47Hγ-
S23Hα	A33Mβ
S23Hβ	A33Mβ
L24Hα	A33Mβ
L24Mδ-	A33Mβ
L24Mδ-	F30Hβ+
L24Mδ-	H34Hβ-
L24Mδ-	I49Hα
L24Mδ-	G50Hα-
A50HN	L121Mδ+
A50Hα	L121Mδ+
L24Mδ-	A33Hα
L24Mδ-	H34Hα
L24Mδ-	G50Hα+
L24Mδ-	F30Hδ
L24Mδ-	F30Hε
L24Mδ-	F30Hζ
L24Mδ+	F30Hβ-
L24Mδ+	G50Hα-
L24Mδ+	I29Hα
L24Mδ+	G50Hα+
L24Mδ+	F30Hε
R27HN	I23Mδ
V28HN	I29Hβ
V28HN	I29Mδ
V28HN	I29Mγ2
V28Hα	I29Mδ
V28Hα	I29Mγ2
V28Mγ-	I29Mδ
V28Mγ-	F30Hζ
F29HN	I29Mδ
P30Hγ+	I29HB
Y31HN	I29Mδ
S32HN	I23Mδ
S32HN	I29Mδ
S32Hα	E22Hγ
S32Hβ-	E22Hβ+
L35HN	S19Hβ
L35Mδ+	F30Hζ
L35Mδ+	I71Hα
L35Mδ+	Y20Hα
L35Mδ+	I23Mδ
Y39HN	I49Mδ
L42Mδ-	E73Hβ
L42Mδ-	P117Hγ
L42Mδ-	P117Hβ+
L42Mδ-	P117Hδ-
L45Mδ-	P117Hβ+
L45Mδ-	R116Hα
V46HN	L121Hβ+
V46Hα	L121Hβ+
V46Hα	L121Mδ+
A50HN	L121Hβ+
A50Mβ	L121Mδ+

† The downfield and upfield-shifted non-stereoassigned, but spectroscopically distinct diastereotopic methyl groups and methylene protons are indicated by “+” and “-“, respectively.

Table S4. Inter-molecular NOEs identified by iterative structure-based assignment in ^{13}C-separated NOESY spectra recorded on [U-^{13}C,^{15}N]-RPP29 (*) and unlabeled RPP21.†

RPP29	RPP21
S19Hβ	S32Hα
E22Hγ	S32Hβ+
E22Hγ	Y31Hα
E22Hγ	S32Hα
I23Hα	Y31Hβ+
I23Mγ2	V28Hβ
I23Mγ2	Y31Hβ+
I23Mγ2	S32Hβ-
I23Mγ2	S32Hβ+
I23Mγ2	S32Hα
I23Mγ2	Y31Hδ
I23Mδ	V28Hβ
I23Mδ	S32Hβ-
I23Mδ	S32Hβ+
I23Mδ	Y31Hα
I23Mδ	S32Hα
R26Hβ-	Y31Hβ-
R26Hβ-	Y31Hε
R26Hβ-	Y31Hδ
I29Hα	R27Hδ+
I29Hβ	R27Hγ
I29Mδ	Y31Hδ
I29Mδ	Y31Hα
I29Mδ	R27Hα
I29Mδ	V28Hα
I29Mδ	R27Hδ+
I29Mδ	Y31Hβ+
I29Mδ	V28Hβ
I29Mδ	P30Hγ+
I29Mγ2	Y31Hβ-
I29Mγ2	Y31Hβ+
I29Mγ2	R27Hα
I29Mγ2	V28Hα
I29Mγ2	Y31Hε
F30HN	L24Mδ-
F30Hα	V28Mγ+
F30Hβ+	L24Mδ-
F30Hβ+	L24Mδ+
G32Hα+	R27Hδ+
A33HN	L24Mδ-

RPP29	RPP21
S19Hβ	S32Hα
E22Hγ	S32Hβ+
A33Hα	L24Mδ-
A33Mβ	L24Mδ-
RPP29	RPP21
I71Mγ2	L35Hγ
D72Hα	Y39Hδ
D72Hα	L35Mδ-
E73HN	Y39Hδ
E73HN	L42Hγ
P117Hβ+	L42Mδ-
P117Hγ	L42Hβ+
P117Hγ	L42Mδ-
E118Hα	V46Hα
L121Hβ-	A50Hα
A33Mβ	L24Mδ+
A33Mβ	R27Hβ
A33Mβ	R27Hδ-
A33Mβ	R27Hδ+
A33Mβ	I20Hα
A33Mβ	S23Hα
H34HN	I20Mγ2
H34Hα	I20Mδ
H34Hβ+	I20Mγ2
H34Hβ-	I20Mγ2
R35HN	I20Hβ
R35HN	I20Mδ
G36HN	R17Hα
G36HN	E16Hβ-
G36HN	I20Mδ
G36HN	I20Mγ2
G36Hα+	E16Hβ-
G36Hα-	R17Hα
W45HN	I13Mγ2
W45Hβ-	I13Mγ2
W45Hβ-	I13Mδ
W45Hβ+	I13Mγ2
W45Hβ+	I13Mδ
H46HN	I13Hβ
H46HN	I13Mγ2

RPP29	RPP21
S19Hβ	S32Hα
E22Hγ	S32Hβ+
E47Hα	L42Hβ-
I49Mδ	L42Hγ
I49Mδ	Y39Hβ-
I49Mδ	Y39Hα
I49Mδ	Y39Hε
I49Mδ	Y39Hδ
I49Mγ2	Y39Hβ-
I49Mγ2	L21Hα
I49Mγ2	L24Hα
I49Mγ2	Y39Hα
I49Mγ2	Y39Hε
I49Mγ2	Y39Hδ
G50Hα+	L24Mδ-
G50Hα+	L24Mδ+
G50Hα-	L24Mδ+
G50Hα-	L24Mδ-
I71Mγ2	L35Hβ-
RPP29	RPP21
L121Mδ+	L13Mδ+
L121Mδ+	I18Hβ
L121Mδ+	V46Hβ
L121Mδ+	V46Hα
L121Mδ+	A50Hα
L121Mδ+	A14Hα
L121Mδ-	L13Mδ+
L121Mδ-	A14Mβ
L121Mδ-	A14Hα
K122Hγ-	L45Hβ+

† The downfield and upfield-shifted non-stereoassigned, but spectroscopically distinct diastereotopic methyl groups and methylene protons are indicated by “+” and “-“, respectively.