PNAS

Supporting Information for

TapA acts as specific chaperone in TasA filament formation by strand complementation

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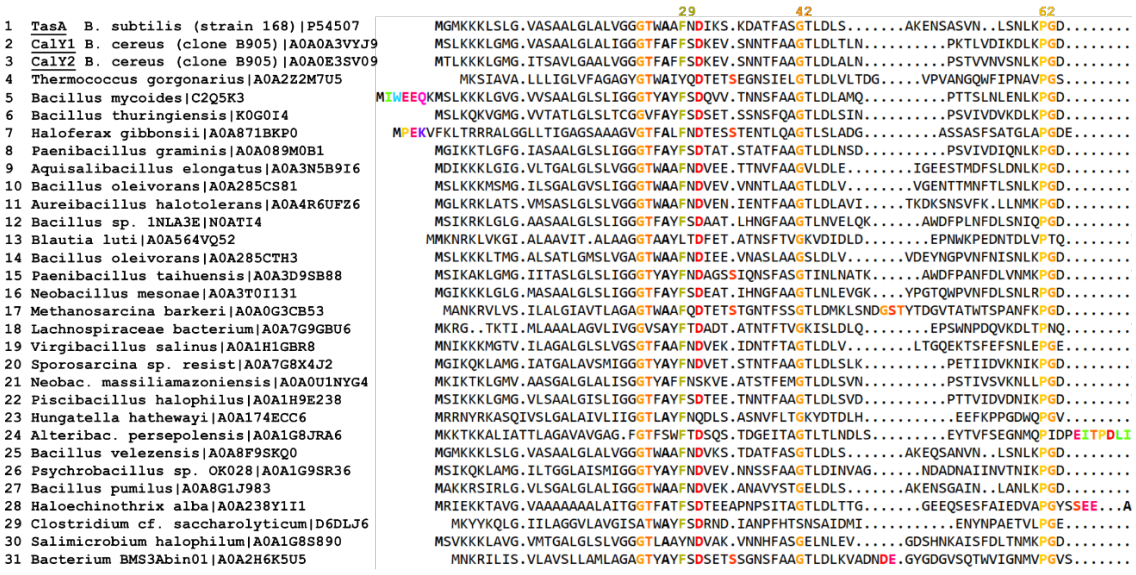


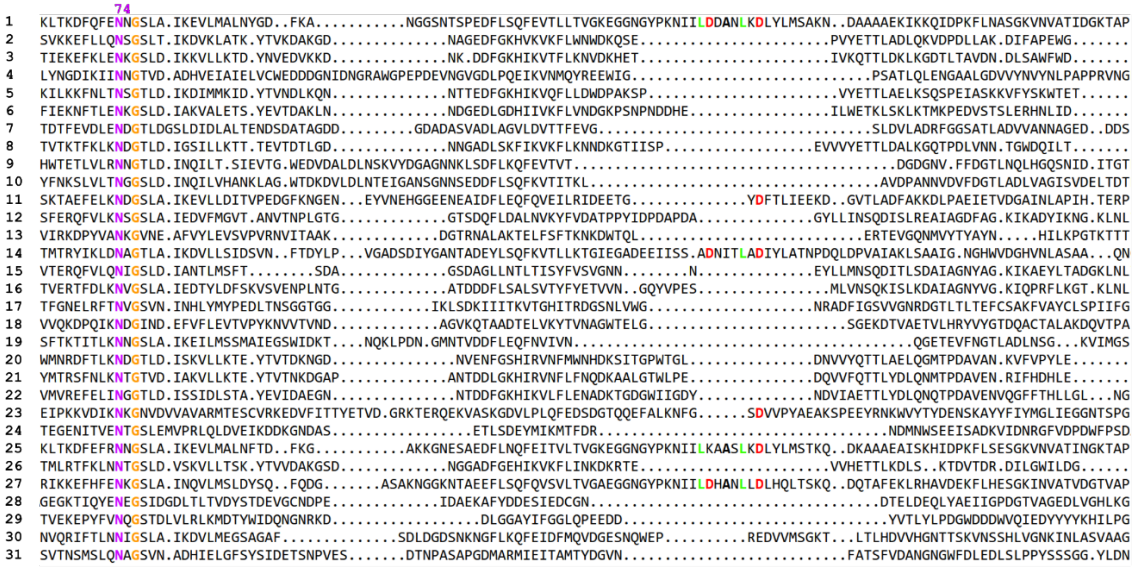


Fig. S1. Sequence alignment of *Bacillus subtilis* TasA, *Bacillus cereus* CalY1/CalY2, and close primary sequences from organisms with varying evolutionary distance generated by ClustalW, covering *Bacillicae*, *Chlostridia*, *Haloferacaceae*, and *Archea*. Residues conserved in more than 90% of the sequences are colored according to the Taylor coloring scheme provided by strap (https://www.bioinformatics.org/strap/aa/) (1). A precise description of the alignment workflow can be found in the Material and Methods section. The conserved last alanine of the signal peptide (residue 27 in TasA) is shown in bold.

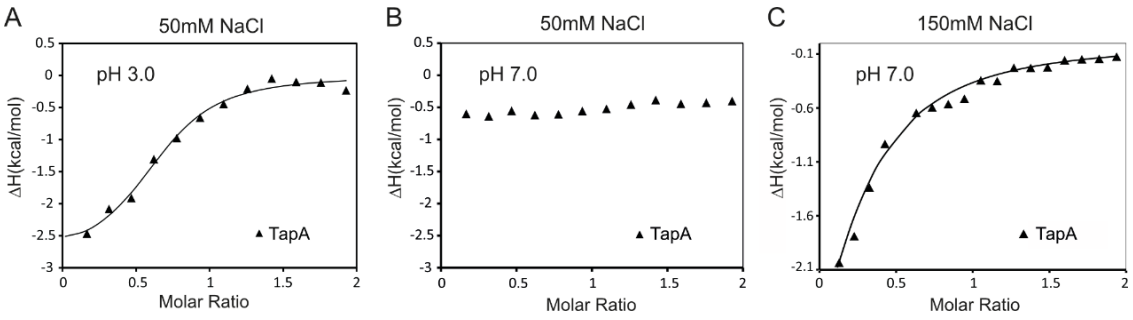


Fig. S2. ITC titration of TapA to TasA in 20 mM Tris HCl buffer with (**A**) 50 mM NaCl at pH 3.0, (**B**) 50 mM NaCl at pH 7.0 and (**C**) 150 mM NaCl at pH 7.0. At physiological pH the interaction necessitates a higher salt concentration. At acidic pH the proteins interact with lower salt but form a different, Thioflavin T stainable, fibril (as shown in SI Appendix, Fig. S3).

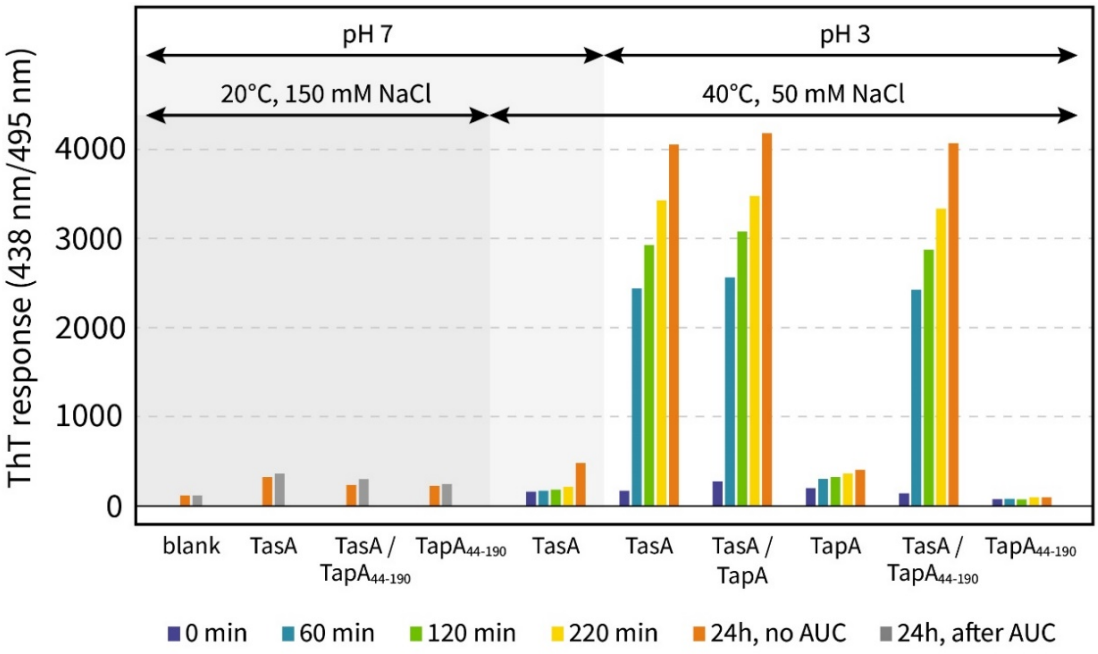


Fig. S3. Thioflavin T (ThT) assay probing stainable fiber formation upon varying multiple factors (pH, temperature, and salt concentration). For ThT response measurements, samples of 10 µl were drawn, diluted with 90 µl of the appropriate buffer and mixed with 100 µl 40 µM pH 7 buffered ThT.
At a sample condition of pH 7 at 20 °C in 20 mM phosphate buffer with 150 mM NaCl, incubation was performed with 100 µM mature $TasA_{28-261}$, $TapA_{44-190}$ and a mixture of both (each 100 µM) for 24 h. Under these conditions, TasA/TapA interaction was shown by ITC (SI Appendix, Fig. S2). Little to no signal is observed in the ThT assay under these conditions, indicative of no amyloid fiber species in the sample. Subsequent ultracentrifugation (as performed for filament collection) does not yield a significantly higher ThT response ensuring fiber-free samples for further experiments.
Increasing the temperature to 40 °C and decreasing the salt concentration to 50 mM in 20 mM HEPES causes a minor rise in signal for TasA (see the orange bar after 24 h) while still showing little absolute ThT response.
However, at pH 3 mature $TasA_{28-261}$ and TapA at 50 µM (each 50 µM when mixed) a different result is observed. Incubation at 40 °C in 20 mM HEPES and 50 mM NaCl shows a strong ThT response for TasA and TasA/TapA mixtures starting with the first datapoint measured after incubation (light blue bar, 60 min). For TapA alone, no significant response is observed. The same tendency remains when truncating the TapA C-terminus ($TapA_{44-190}$) with TapA itself showing a reduced signal.
Notably, the ThT response for mixtures of TasA and TapA is always smaller than the sum of the individual bars despite the total protein amount being doubled. This speaks toward a fold-protecting effect of TapA that prevents formation of ThT stainable, and thus likely amyloid, fibers when starting from folded protein. This effect is especially pronounced at pH 7, 20 °C and 150 mM NaCl, here shown for $TapA_{44-190}$.

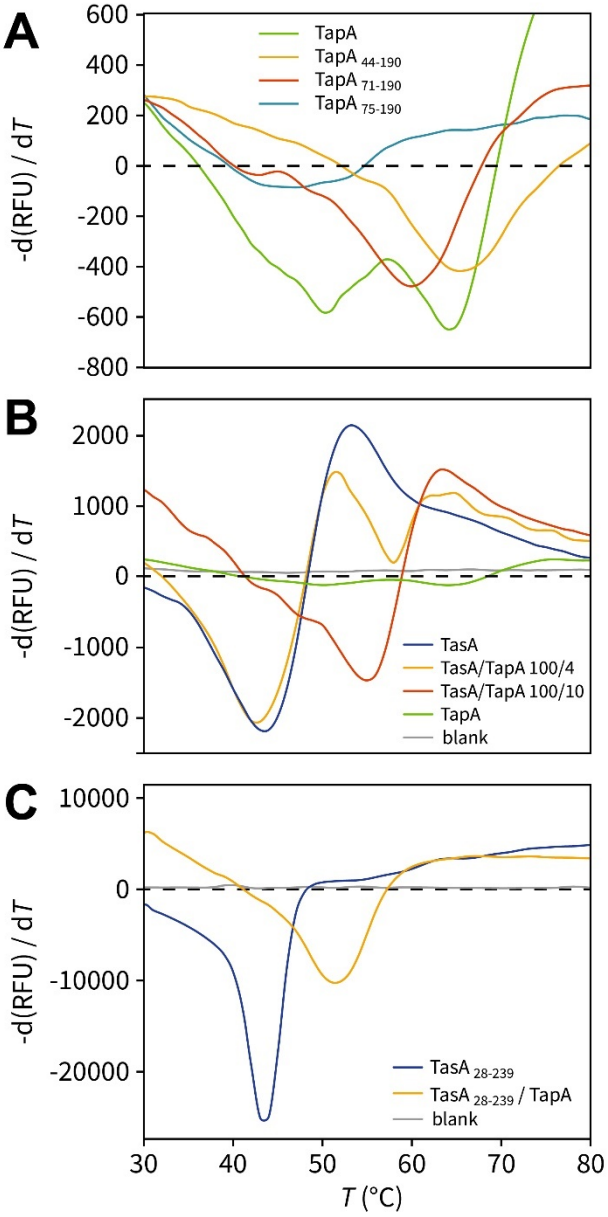
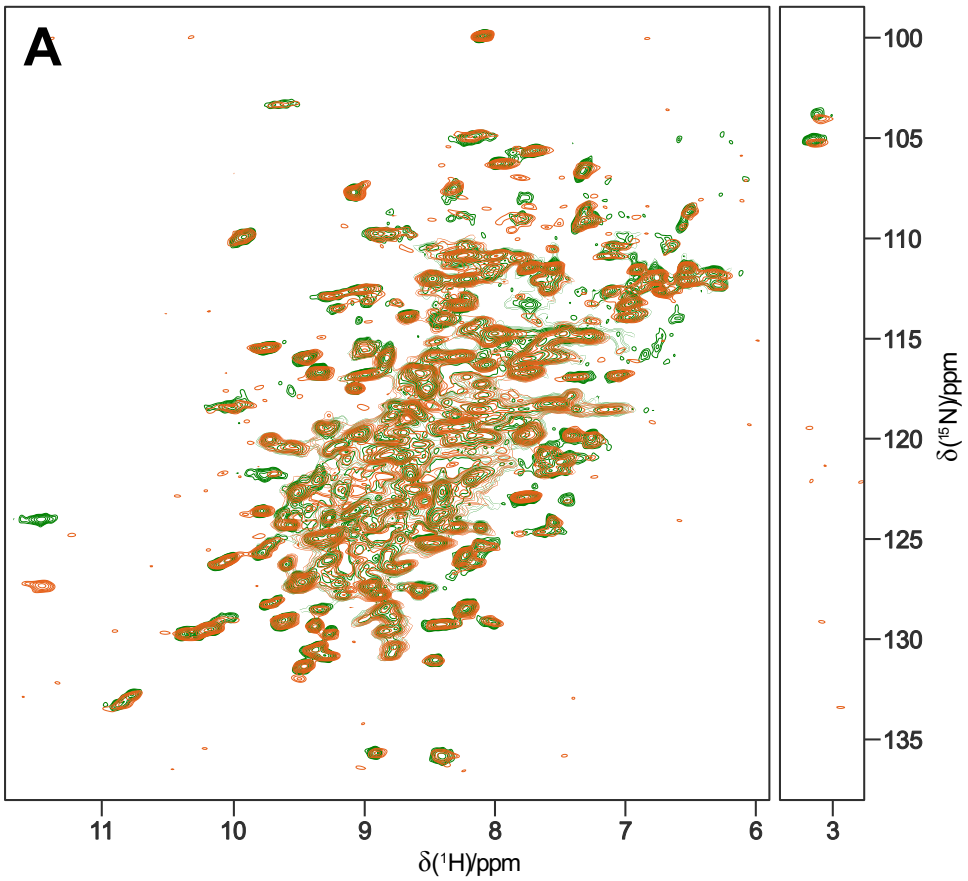


Fig. S4. Thermal shift assays (TSA) probing stability of different TapA variants and the interaction with TasA. All experiments were performed with mature TapA$_{44-253}$ and TasA$_{28-261}$ unless stated otherwise. First derivative calculations of the observed intensity show the melting curve of the individually measured samples.
(**A**) The highest stability is observed for TapA$_{44-190}$ with a T_m of 66 °C. In comparison, TapA$_{71-190}$ is slightly less stable with a T_m of 60 °C, pinpointing a minor contribution of N-terminal residues 44-71. A further truncation of 3 residues at the N-terminus, resulting in TapA$_{75-190}$, shows a significantly lower stability with a T_m of 46°C. Using the mature TapA, a biphasic melting profile with two peaks is observed with one at 64 °C (which likely reflects the melting of the folded domain) and one at 50 °C indicative for the C-terminus losing its association to the folded domain. Interestingly, in our X-Ray studies the most stable construct TapA$_{44-190}$ failed to crystallize in contrast to TapA$_{71-190}$ and TapA$_{75-190}$ despite the latter missing the aromatic ring packing of W74 against Y170 and P171 (Fig. 3G).
(**B**) TapA influences stability of TasA filaments for different mixture ratios, measured after 17 h at 20 °C. Pure TasA is shown in blue with a T_m of 43 °C. With addition of 1/10 of TapA to TasA

an T_m increase by almost 12 °C is detected (red curve). A ratio of 1/25 TapA to TasA is not sufficient to affect the TasA profile (yellow curve).
(**C**) C-terminally truncated $TasA_{28-239}$ (250 µM) shows a melting temperature of 44 °C. Addition of 50 µM TapA increased T_m to 53 °C showing a less pronounced effect than for the mature protein shown in **B**. A blank buffer measurement is shown in gray.


A
100
105
110
115
120
125
130
135
δ(15N)/ppm
11
10
9
8
7
6
3
δ(1H)/ppm

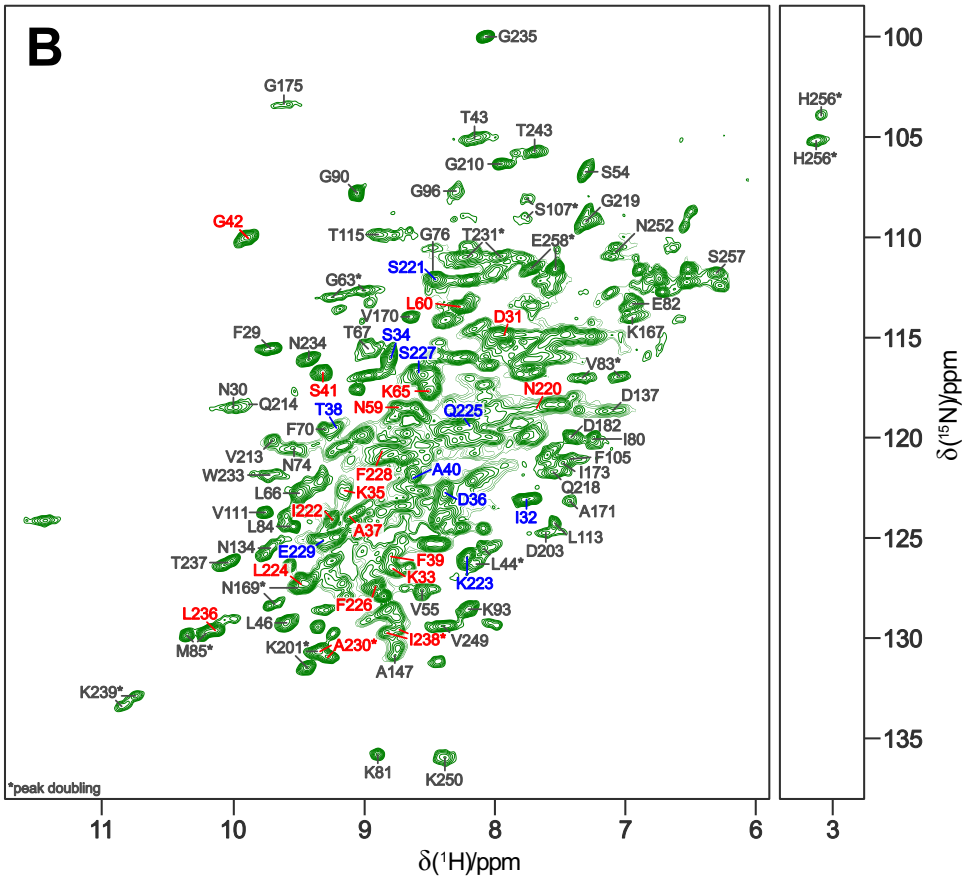

B
G235
G175
T43
T243
G210
S54
G90
G96
S107*
G219
G42
T115
G76
T231*
E258*
N252
S257
S221
G63*
E82
L60
V170
D31
K167
F29
N234
T67
S34
S227
V83*
N30
S41
K65
N220
D137
Q214
T38
N59
Q225
D182
F70
I80
V213
N74
F105
W233
F228
A40
I173
L66
K35
D36
Q218
V111
I222
I32
A171
L84
A37
L113
N134
E229
D203
T237
L224
F39
L44*
N169*
K33
K223
L236
F226
V55
K93
L46
M85*
K201*
A230*
I238*
V249
A147
K239*
K81
K250
H256*
H256*
*peak doubling
100
105
110
115
120
125
130
135
δ(15N)/ppm
11
10
9
8
7
6
3
δ(1H)/ppm

Fig. S5. (**A**) Comparison of ^{1}H-^{15}N spectra from TapA-induced filaments of ^{2}H,^{13}C,^{15}N-labeled (100% back-exchanged) TasA (green) collected by ultracentrifugation with isotopically mixed (^{2}H,^{15}N/[2-^{13}C]; 50/50) TasA filaments generated at pH 7 through concentration (orange). The histidine sidechain signal at ~11.5 ppm ^{1}H chemical shift is aliased, its position varies due to differing spectral widths in the ^{15}N dimension. (**B**) Solid-state NMR ^{1}H-^{15}N correlation of TapA-fibrillated TasA filaments as shown in **A** with assignments indicated for resolved signals. Asterisks indicate residues with peak doubling. Residues that give rise to intense signals presented in SI Appendix, Fig. S8B (antiparallel inter-strand contacts from β0 and β9) and SI Appendix, Fig. S8C (parallel inter-strand contacts) are indicated in red. Further signals arising from β0 (D31-S41) and β9 (A230-N220) are highlighted in blue. For β0 and β9 see also SI Appendix, Fig. S6 which includes strip plots used for assignment. A complete list of assigned chemical shifts can be found in SI Appendix, Tab. S2.

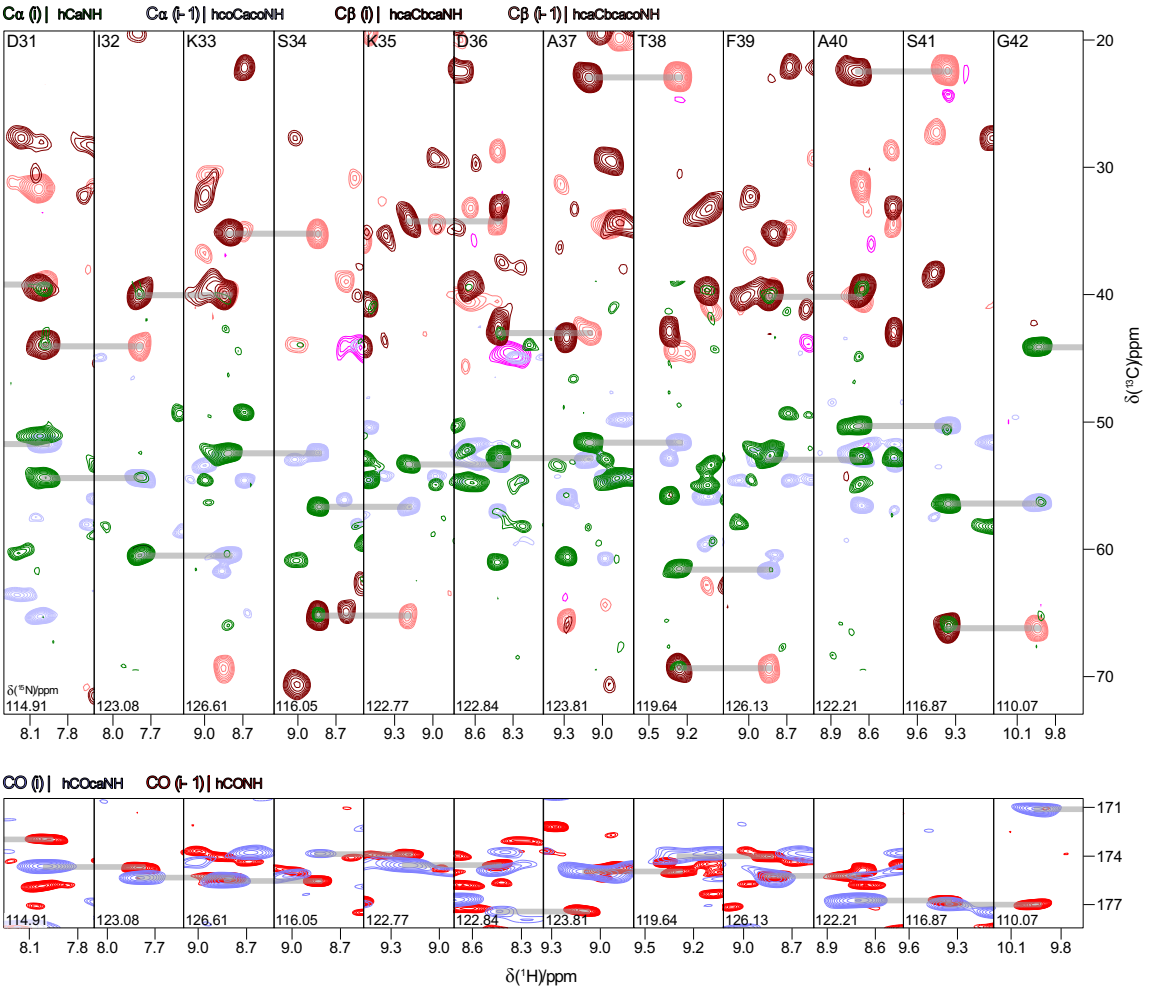


Fig. S6. Strip plots displaying NMR assignment spectra for stretches 31-42 and 220-231 (next page). Spectra are shown in green (hCaNH), light blue (hcoCAcoNH), brown (hcaCbcaNH) and light orange/pink (positive/negative contours of hcaCbcacoNH) for aliphatic carbons on the top and in light blue (hCOcaNH) and red (hCONH) for carbonyls on the bottom. The spectra description above the strip plots denote whether atoms from the amino acid itself (i) or the preceding one (i-1) are measured. Connecting sequential links are highlighted with grey bars. Doubling of peaks is observed for asterisk marked residues 229, 230 and 231 (next page) wheras 231 shows clearly separated peaks in the ^{1}H and ^{13}C dimensions. For the other residues the effect is less pronounced and manifests as line broadening in ^{1}H and ^{13}C for 230 and in ^{1}H for 229.

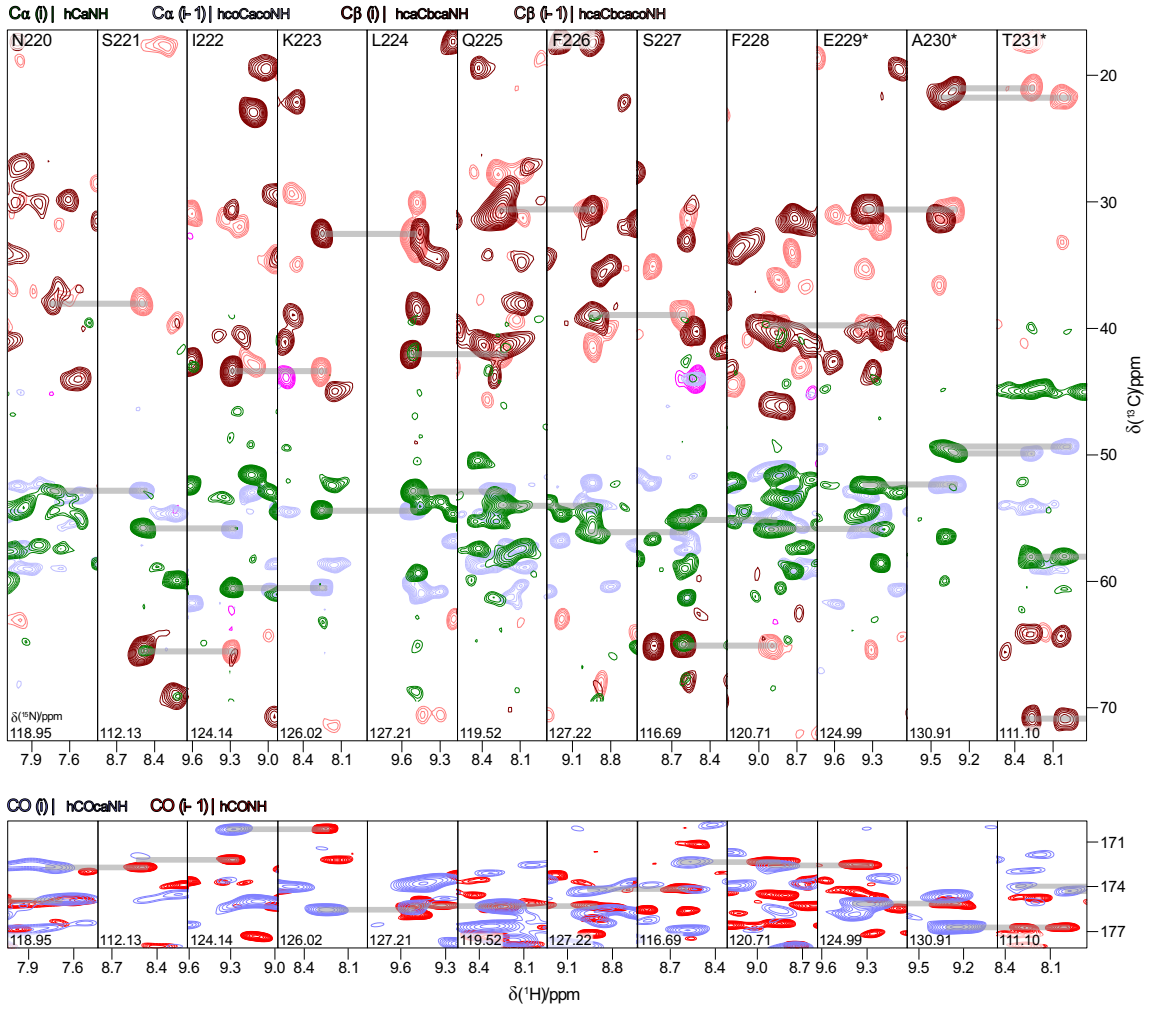


Fig. S6. continued

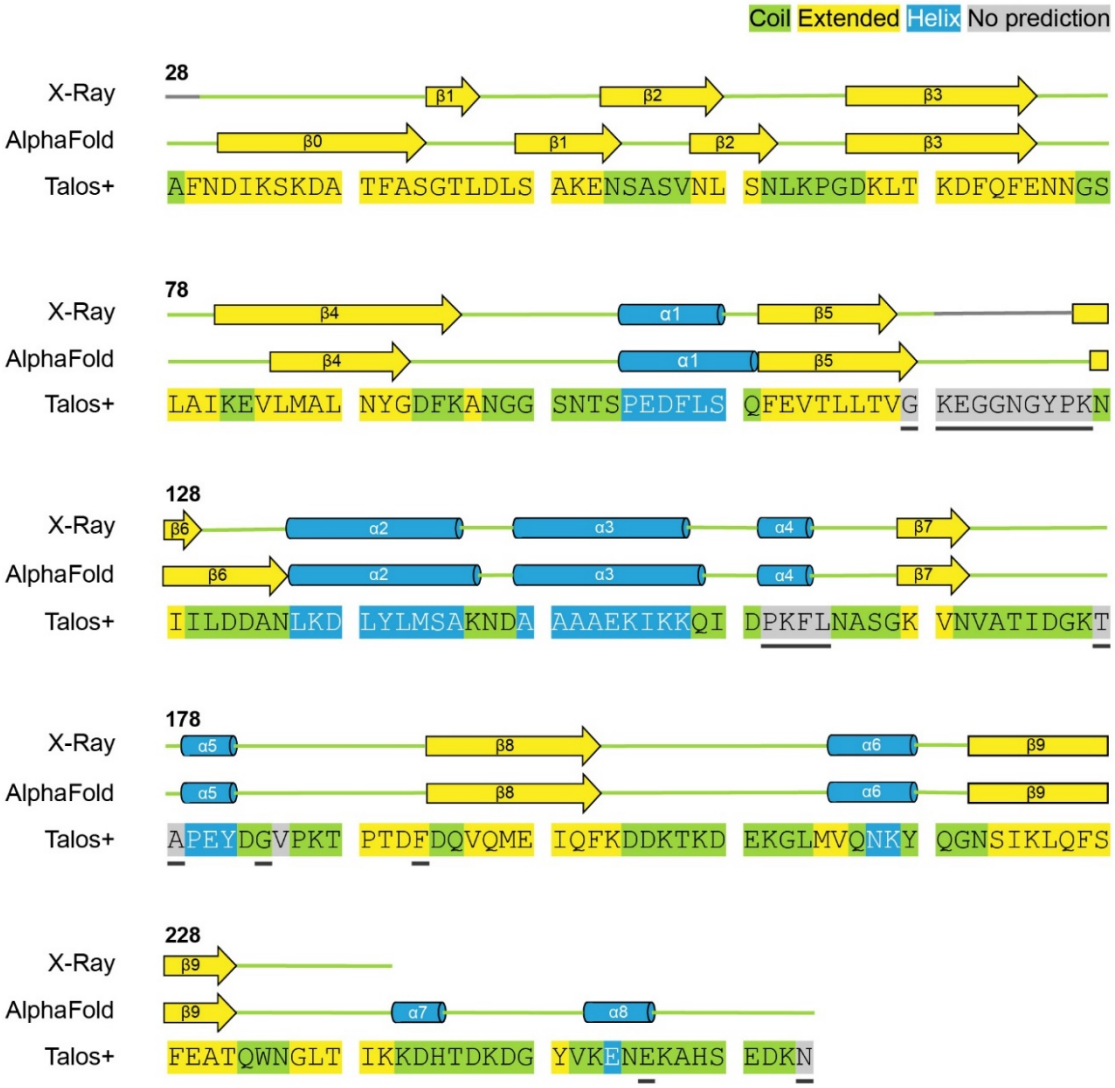


Fig. S7. Comparison of secondary structure information obtained from the X-Ray structure of monomeric TasA (PDB 5OF1), filamentous TasA predicted from AlphaFold multimer and the TALOS+ prediction based on assigned chemical shifts (SI Appendix, Tab. S2). Sheets are colored in yellow, helices in blue, coiled regions in green and not predicted (NMR) or missing regions (X-Ray) in gray. Residues lacking NMR assignments are underlined. For P185 only the Cα shift is known. Fig. 3B in the main text visualized the TALOS+ prediction plotted on the X-Ray structure, SI Appendix, Fig. S11 does the same for the AlphaFold multimer model. Noteworthy is that the stretch between β0 and β1 is present in an extended conformation in the AlphaFold prediction and β6 manifests as an irregular β-sheet in X-Ray and AlphaFold.

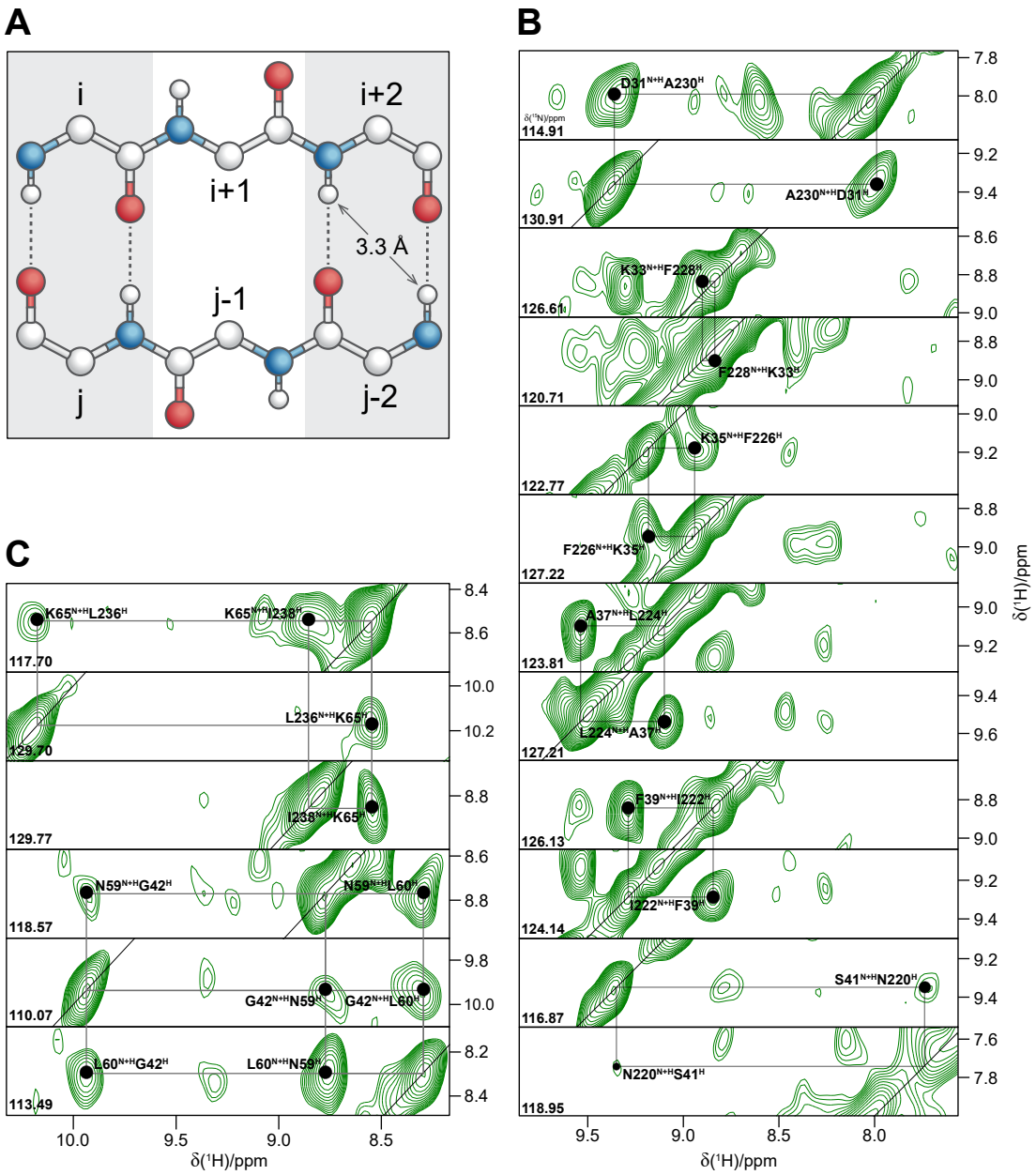


Fig. S8. NMR contacts that can be unambiguously assigned due to typical secondary structure patterns. (**A**) Schematic pattern of an antiparallel β-sheet with the cross-strand H^N-H^N distance of 3.3 Å indicated. (**B**) Slices from the solid-state NMR 3D hNHH spectrum recorded on TapA-fibrillated ^2H,^{13}C,^{15}N-labeled and 100% back-exchanged TasA filaments showing H^N-H^N contacts. Symmetric cross-peaks are characteristic for the antiparallel strands and can be attributed to β0 and β9 (Fig. 3D and 4C, left). (**C**) Additional slices from the spectrum shown in **B**. Contacts between K65 and L236/I238 (Fig. 4C, right), part of a short parallel β-sheet, are displayed on the top. On the bottom, residues G42, N59 and L60 are shown that form a less regular interaction (4C, left).
The peak doubling previously observed for A230 (SI Appendix, Figs. S5B and S6) and I238 (SI Appendix, Fig. S5B) is not resolved and appears as an increase in peak linewidth.

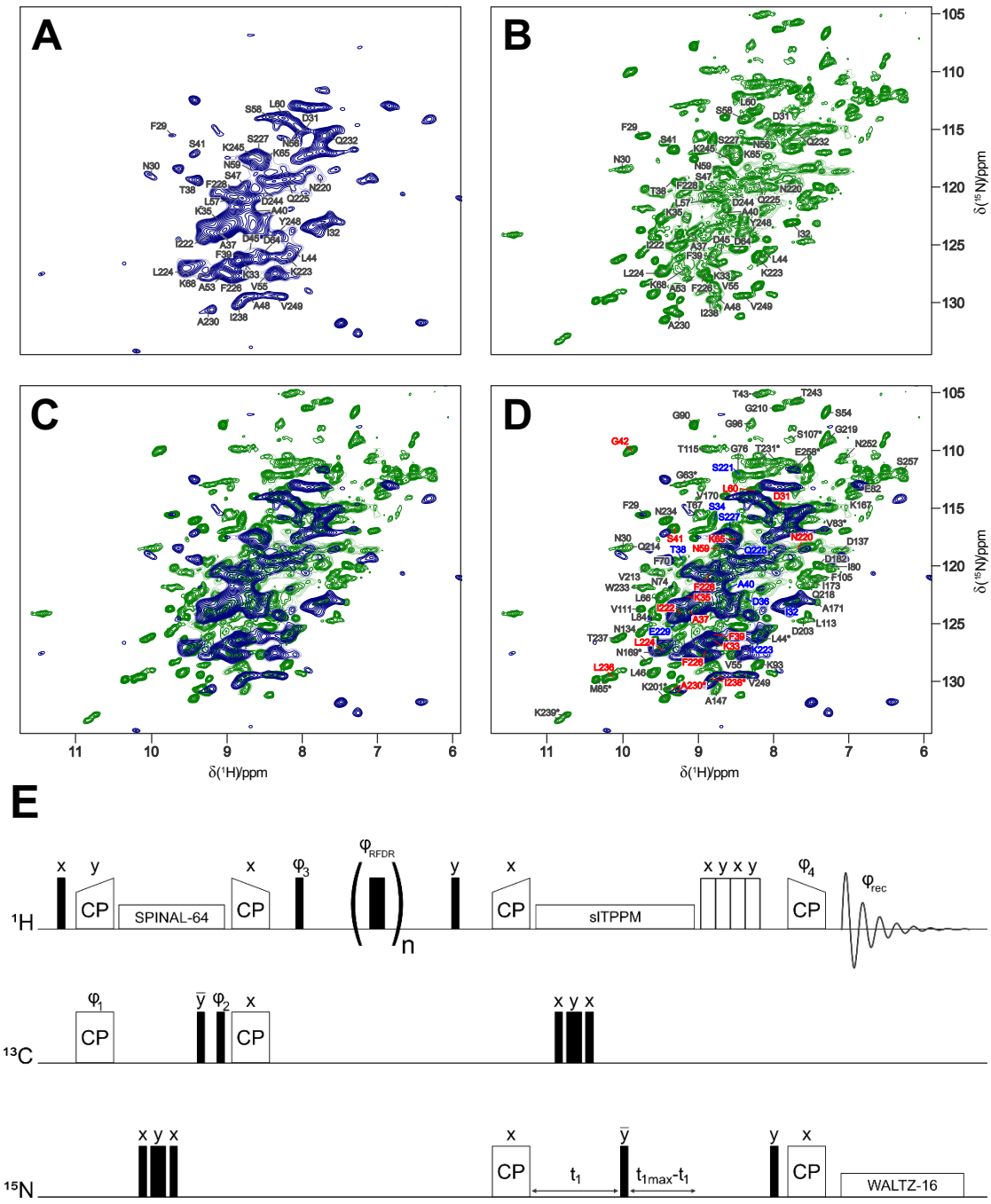


Fig. S9. Intermolecular contacts of TasA filaments monitored by NMR. (**A**) NH plane of a hchhNH experiment acquired on a sample in aqueous buffer prepared with a mixed labeling scheme (^{2}H,^{15}N/[2-^{13}C]; 50/50). Detectable peaks present at the interface are labeled. (**B**) hNH spectrum shown in SI Appendix, Fig. S5 with peak labeling as presented in **A**. (**C**) Superposition of **A** and **B** without labels. (**D**) Superposition of **A** and **B** with peak labeling as presented in SI Appendix, Fig. S5B. (**E**) Pulse sequence used to acquire the spectrum shown in **A**. Initial ^{1}H polarization is produced by a $\pi/2$ pulse. Afterwards, it is transferred to ^{13}C nuclei and back using a $^{1}H/^{13}C$ CP block which functions as a filter for non ^{13}C labeled material. The magnetization, now at ^{1}H again, is transferred through space to adjacent ^{1}H nuclei using an rotor-synchronized 3 ms RFDR (2) pulse train (n=180 at 60 kHz MAS). Subsequently a second CP block is applied, this time on $^{1}H/^{15}N$ filtering everything lacking ^{15}N isotopes. At the end of the pulse sequence, only magnetization that was transferred through space and experienced both ^{13}C and ^{15}N remains. For our labelling pattern this is solely true for inter-molecular cross peaks. Black rectangles depict hard pulses (narrow: $\pi/2$; broad: π), empty rectangles are used for decoupling sequences (either SPINAL-64, slTPPM or WALTZ-16), cross-polarization (CP) pulses and the

MISSISSIPPI solvent suppression scheme (xyxy pulse train prior to the last CP). Phase cycling is applied for pulses labeled with φ. φ_1=00002222, φ_2=13, φ_3=3311, φ_4=00001111, φ_{RFDR}=01011010 (cycled within the RFDR sequence), φ_{rec}=20021331.

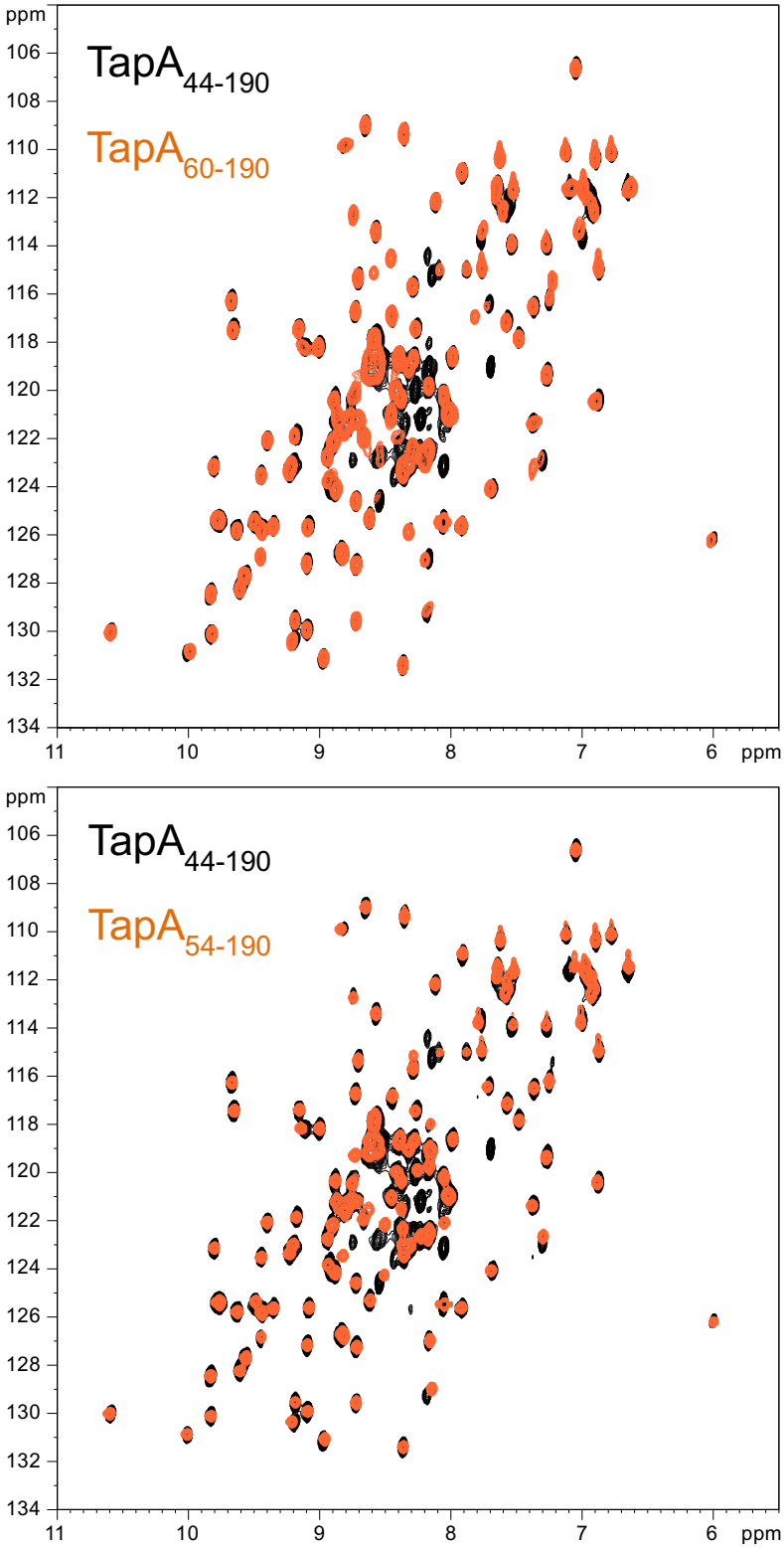


Fig. S10. Overlay of 2D solution NMR ^{1}H-^{15}N correlation spectra of $TapA_{44\text{-}190}$ (black) with $TapA_{60\text{-}190}$ (orange, top) and $TapA_{54\text{-}190}$ (orange, bottom). Black signals without orange overlap are only present in spectral regions characteristic of disordered stretches and indicate an unfolded N-terminus.

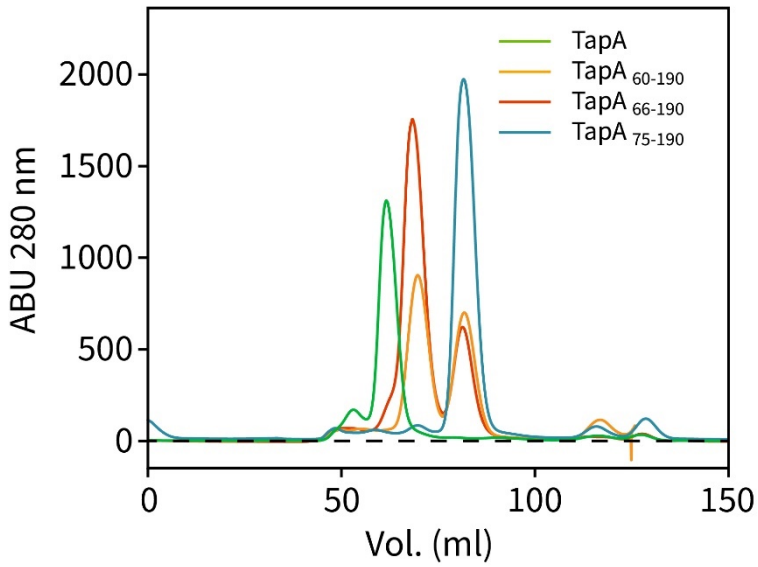


Fig. S11. TapA variants monitored by gel filtration on a Superdex 75 column (total volume 120 ml, buffer: 20 mM phosphate pH 7.0, 150 mM NaCl). Mature TapA (green curve) shows one elution maxima, characteristic of a defined monomer. For TapA variants with three cysteines like $TapA_{60\text{-}190}$ (orange curve) and $TapA_{66\text{-}190}$ (red curve) two maxima occur indicating an additional species, likely a dimer. As this effect is not present in the presence of reducing agents it can be attributed to the unbound C68 forming a disulfide bridge between two monomers. Truncating more N-terminal residues and removing C68 ($TapA_{75\text{-}190}$, blue curve) yields a monomeric profile again.
Taken together it can be concluded that C68 is likely being bound to C58 in the mature protein forming a second disulfide bridge in addition to the one observed in the crystal structure (Fig. 3E, C92-C188).

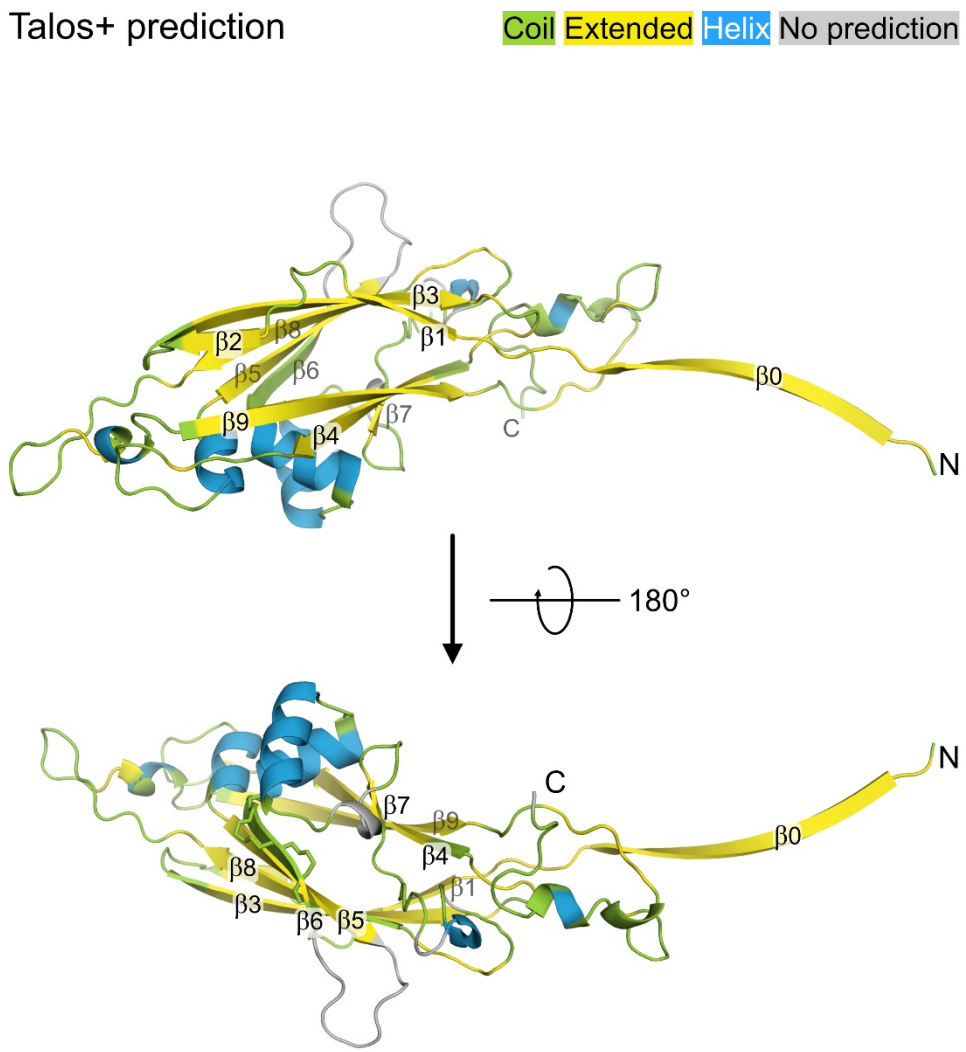


Fig. S12. TALOS+ secondary structure prediction based on solid-state NMR chemical shifts displayed on a cartoon representation of a protomer extracted from an AlphaFold multimer filament (SI Appendix, Fig. S7 and Tab. S2). Predicted helices are shown in blue, sheets in yellow, and loops in green. Regions lacking a prediction are indicated in gray. β6 exists in an irregular conformation, similar to what is observed in the X-Ray structure (PDB 5OF1) and which is represented by the backbone trace shown on the bottom panel.

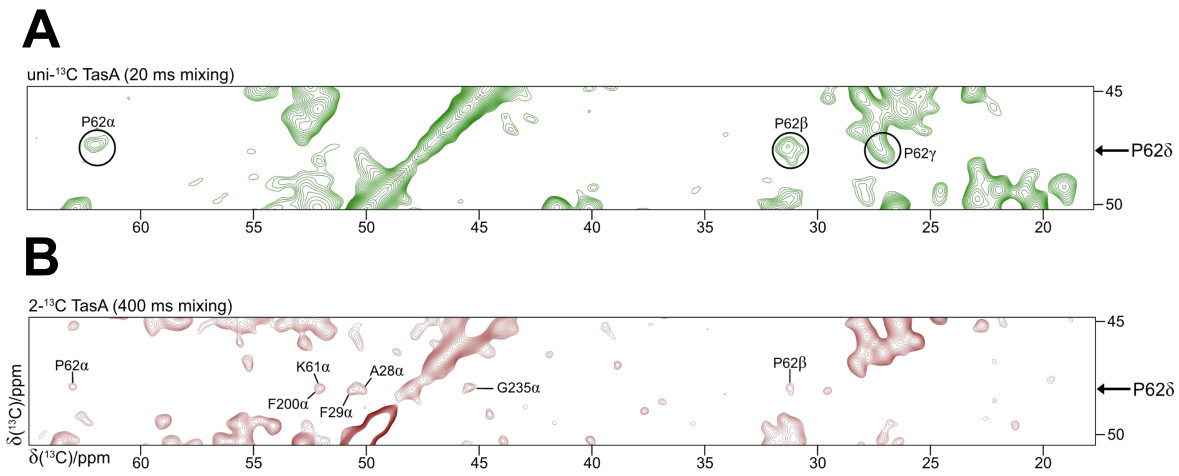


Fig. S13. ^{13}C-^{13}C DARR spectra showing separated peaks of P62. (**A**) Spectrum of uniformly ^{13}C, ^{15}N-labeled TasA fibers at a short mixing time of 20 ms showing intra-residue crosspeaks of P62. (**B**) Spectrum of sparsely labeled TasA fibers composed of [2-^{13}C]-glycerol and uniformly ^{15}N-labeled protein recorded with 400 ms mixing time. P62 shows crosspeaks to A28, F29, K61, F200 and G235 consistent with the predicted interface area shown in Fig. 4E. Assignment of crosspeaks was conducted by applying a correction (3) to the chemical shifts observed for the perdeuterated protein (SI Appendix, Tab. S2).

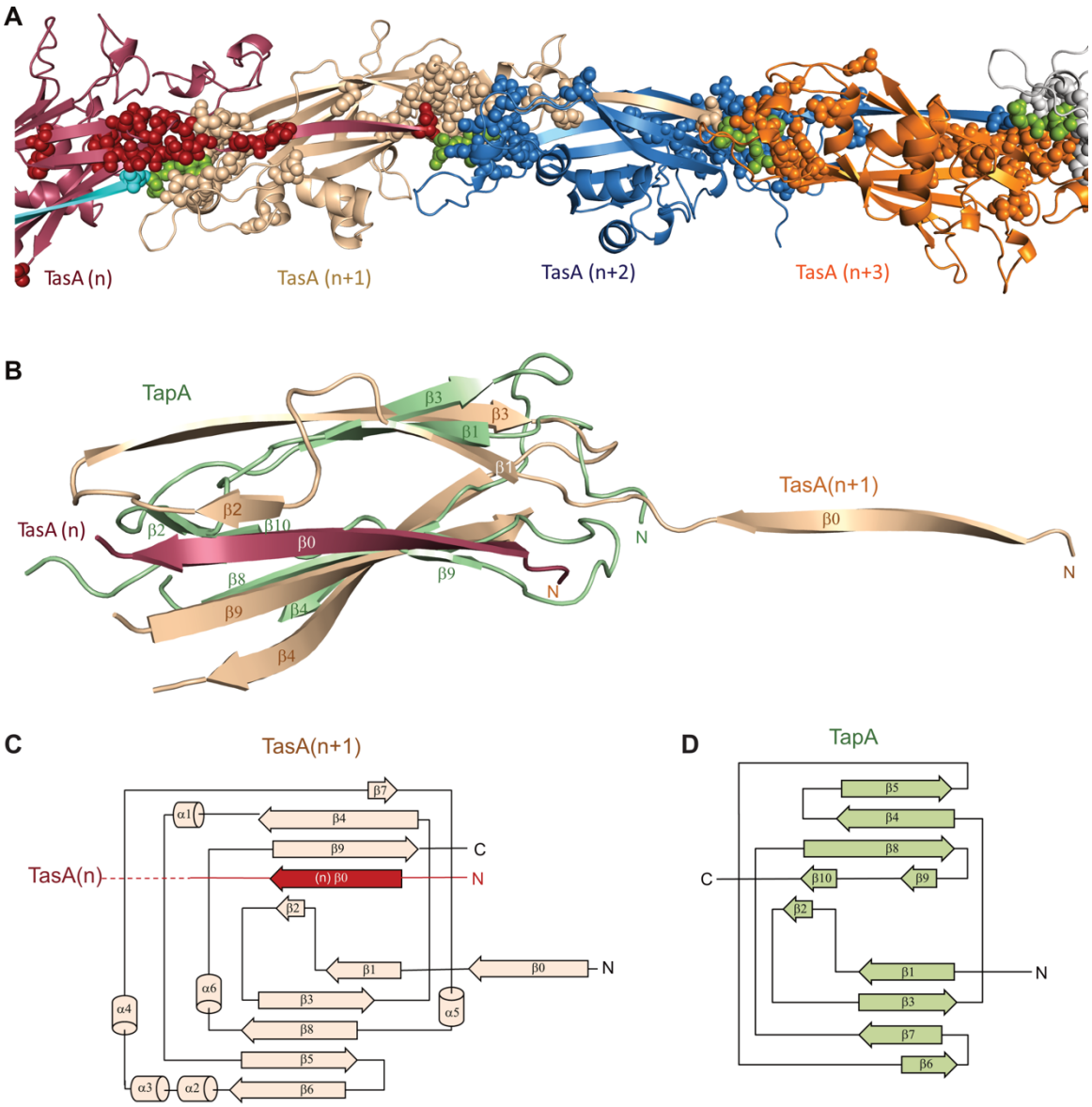


Fig. S14. (**A**) AlphaFold predicted TasA filament chain with the side chains of the most conserved residues indicated as spheres (see SI Appendix, Figs. S1 and Fig. 4A). All phenylalanine and alanine residues at the N-termini (A28, F29) are shown in green, other residues in the color of their protomer. (**B**) Overlay of TapA (green) with filamentous TasA (beige and dark red). Secondary structure topology plots of filamentous TasA (**C**) and TapA (**D**) with the same colours as in **B**.

Table S1. Results of AUC measurements: *s*-values, frictional ratios and apparent molecular weights.

Protein sample	Conc. [µM]	f/f_0	Monomer		Oligomer[a,b,e]	
			$S_{20,w}$	MW [kDa]	$S_{20,w}$	MW [kDa]
$TapA_{44\text{-}62\ mutant}$[d]	85	1.28	0.60	2.8	-	-
$TapA_{75\text{-}190}$	100	1.24	1.69	14.9	-	-
$TapA_{44\text{-}190}$	100	1.33	1.81	17.5	-	-
$TapA_{44\text{-}253}$	100	1.74	1.90	27.0	-	-
$TasA_{28\text{-}261}$	100	1.45	2.15	25.4	-	-
$TasA_{28\text{-}261}$[c]	100	1.35	2.97	37.2	-	-
$TasA_{28\text{-}261}$+$TapA_{44\text{-}62\ mutant}$[d]	100 + 250	1.69	2.15	32.1	9.7	~ 300
$TasA_{28\text{-}261}$ + $TapA_{75\text{-}190}$	100 + 100	1.37	1.93	20.5	-	-
$TasA_{28\text{-}261}$ + $TapA_{44\text{-}190}$	100 + 100	1.67	1.83	24.9	6.7	~ 170
$TasA_{28\text{-}261}$ + $TapA_{44\text{-}253}$	100 + 1	1.54	2.17	28.3	-	-
$TasA_{28\text{-}261}$ + $TapA_{44\text{-}253}$	100 + 2	1.58	2.18	29.4	9.8	~ 280
$TasA_{28\text{-}261}$ + $TapA_{44\text{-}253}$	100 + 4	1.81	2.05	33.0	9.6	~ 330
$TasA_{28\text{-}261}$ + $TapA_{44\text{-}253}$	100 + 10	1.95	1.94	34.3	8.8	~ 330
$TasA_{28\text{-}261}$ + $TapA_{44\text{-}253}$	100 + 70	1.98	1.87	32.3	6.0	~ 190
$TasA_{28\text{-}261}$[c] + $TapA_{44\text{-}253}$	100 + 100	2.17	1.83	36.8	10.5	~ 500

[a] Largest oligomeric species formed over the course of the sedimentation velocity experiment.

[b] Potential protein fibrils could not be detected due to the high rotor speed of 40,000 rpm

[c] Experiment performed with isotopic labeled $^{2}H,^{13}C,^{15}N$-$TasA_{28\text{-}261}$

[d] $TapA_{44\text{-}62\ wt}$: AFHDIETFDVSLQTCKDFQ; $TapA_{44\text{-}62\ mutant}$: AFHDIETFDVSLQT**S**KD**A**Q.

[e] Heterogeneous samples such as TapA-induced TasA filaments only allow to determine an approximate MW.

Table S2. Backbone assignments obtained from solid-state NMR of TasA filaments. Signal sets arising form doubled peaks are shown in italics.
Determined chemical shifts, peak lists and raw datasets have been deposited in the BMRB with the accession code 51785. Processed spectra and the CCPN 2.4.2 assignment project are uploaded to zenodo (10.5281/zenodo.7534572).

Res.	Nuc.	Shift	Res.	Nuc.	Shift	Res.	Nuc.	Shift	Res.	Nuc.	Shift
A28	C	172.04	**I80**	CB	38.76	***A143***	*CA*	*52.93*	**E208**	HN	9.01
A28	CA	50.20	**I80**	HN	7.22	***A143***	*CB*	*19.49*	**E208**	N	116.90
A28	CB	19.53	**I80**	N	120.18	***A143***	*HN*	*9.00*	**K209**	C	176.61
F29	C	176.38	**K81**	C	173.48	***A143***	*N*	*124.21*	**K209**	CA	55.27
F29	CA	50.80	**K81**	CA	59.09	**K144**	C	176.35	**K209**	CB	31.38
F29	CB	39.77	**K81**	CB	30.32	**K144**	CA	53.64	**K209**	HN	8.28
F29	HN	9.76	**K81**	HN	8.93	**K144**	CB	31.55	**K209**	N	119.44
F29	N	115.61	**K81**	N	135.94	**K144**	HN	6.55	**G210**	C	174.22
N30	C	172.98	**E82**	C	173.94	**K144**	N	112.25	**G210**	CA	44.35
N30	CA	51.81	**E82**	CA	53.36	**N145**	C	174.84	**G210**	HN	7.98
N30	CB	39.28	**E82**	CB	31.74	**N145**	CA	53.14	**G210**	N	106.36
N30	HN	10.04	**E82**	HN	6.99	**N145**	CB	36.99	**L211**	C	177.26
N30	N	118.55	**E82**	N	112.92	**N145**	HN	7.73	**L211**	CA	53.22
D31	C	174.68	**V83**	C	173.69	**N145**	N	119.52	**L211**	CB	40.80
D31	CA	54.39	**V83**	CA	61.63	**D146**	C	176.45	**L211**	HN	8.39
D31	CB	43.97	**V83**	CB	31.00	**D146**	CA	54.65	**L211**	N	123.77
D31	HN	7.98	**V83**	HN	7.37	**D146**	CB	44.06	**M212**	C	175.36
D31	N	114.89	**V83**	N	117.06	**D146**	HN	7.53	**M212**	CA	53.30
I32	C	175.36	***V83***	*C*	*173.60*	**D146**	N	118.43	**M212**	CB	33.02
I32	CA	60.48	***V83***	*CA*	*61.75*	**A147**	C	180.05	**V213**	C	172.79
I32	CB	39.98	***V83***	*CB*	*31.01*	**A147**	CA	54.58	**V213**	CA	58.58
I32	HN	7.79	***V83***	*HN*	*7.07*	**A147**	CB	17.82	**V213**	CB	35.12
I32	N	123.08	***V83***	*N*	*116.97*	**A147**	HN	8.79	**V213**	HN	9.73
K33	C	175.52	**L84**	C	176.59	**A147**	N	130.76	**V213**	N	120.21
K33	CA	52.43	**L84**	CA	52.39	**A148**	C	181.25	**Q214**	C	176.71
K33	CB	35.21	**L84**	CB	42.72	**A148**	CA	54.47	**Q214**	CA	57.53
K33	HN	8.81	**L84**	HN	9.60	**A148**	CB	16.77	**Q214**	CB	27.66
K33	N	126.61	**L84**	N	124.23	**A148**	HN	8.20	**Q214**	HN	9.82
S34	C	173.90	**M85**	C	174.37	**A148**	N	122.19	**Q214**	N	118.23
S34	CA	56.68	**M85**	CA	54.62	**A149**	C	179.60	**N215**	C	178.40
S34	CB	65.18	**M85**	CB	34.95	**A149**	CA	54.46	**N215**	CA	55.43
S34	HN	8.83	**M85**	HN	10.39	**A149**	CB	18.80	**N215**	CB	37.94
S34	N	116.05	**M85**	N	129.89	**A149**	HN	8.75	**N215**	HN	8.11
K35	C	174.57	***M85***	*C*	*174.38*	**A149**	N	123.42	**N215**	N	117.36
K35	CA	53.32	***M85***	*CA*	*54.28*	**A150**	C	179.51	**K216**	C	174.77
K35	CB	34.15	***M85***	*CB*	*34.79*	**A150**	CA	54.46	**K216**	CA	57.53
K35	HN	9.19	***M85***	*HN*	*10.25*	**A150**	CB	17.28	**K216**	CB	29.83
K35	N	122.78	***M85***	*N*	*129.76*	**A150**	HN	8.03	**K216**	HN	7.62
D36	C	177.43	**A86**	C	173.85	**A150**	N	118.26	**K216**	N	118.35
D36	CA	52.94	**A86**	CA	49.32	***A150***	*C*	*179.49*	**Y217**	C	176.83
D36	CB	42.77	**A86**	CB	22.14	***A150***	*CA*	*54.30*	**Y217**	CA	57.08
D36	HN	8.42	**A86**	HN	8.69	***A150***	*CB*	*17.42*	**Y217**	CB	37.55
D36	N	122.84	**A86**	N	126.47	***A150***	*HN*	*8.12*	**Y217**	HN	7.74
A37	C	174.98	***A86***	*C*	*174.02*	***A150***	*N*	*118.07*	**Y217**	N	116.12
A37	CA	51.59	***A86***	*CA*	*49.45*	**E151**	C	178.86	***Y217***	*C*	*176.77*
A37	CB	22.92	***A86***	*CB*	*22.09*	**E151**	CA	58.62	***Y217***	*CA*	*57.37*

A37	HN	9.11	***A86***	*HN*	*8.45*	**E151**	CB	28.42	***Y217***	*CB*	*37.51*
A37	N	123.81	***A86***	*N*	*125.36*	**E151**	HN	7.81	***Y217***	*HN*	*7.55*
T38	C	174.04	**L87**	C	173.49	**E151**	N	116.26	***Y217***	*N*	*116.08*
T38	CA	61.62	**L87**	CA	52.63	**K152**	C	179.96	**Q218**	C	176.66
T38	CB	69.30	**L87**	CB	45.57	**K152**	CA	58.84	**Q218**	CA	58.33
T38	HN	9.27	**L87**	HN	7.74	**K152**	CB	31.35	**Q218**	CB	27.60
T38	N	119.64	**L87**	N	120.02	**K152**	HN	7.41	**Q218**	HN	7.56
F39	C	175.12	**N88**	C	173.13	**K152**	N	118.18	**Q218**	N	121.62
F39	CA	52.89	**N88**	CA	50.40	**I153**	C	178.72	**G219**	C	174.94
F39	CB	40.16	**N88**	CB	41.58	**I153**	CA	62.18	**G219**	CA	45.19
F39	HN	8.85	**N88**	HN	8.35	**I153**	CB	35.06	**G219**	HN	7.32
F39	N	126.13	**N88**	N	120.10	**I153**	HN	8.09	**G219**	N	109.25
A40	C	176.77	**Y89**	C	173.63	**I153**	N	120.00	**N220**	C	172.67
A40	CA	50.32	**Y89**	CA	55.75	**K154**	C	177.99	**N220**	CA	52.83
A40	CB	22.45	**Y89**	CB	41.57	**K154**	CA	59.05	**N220**	CB	38.00
A40	HN	8.69	**Y89**	HN	8.27	**K154**	CB	31.48	**N220**	HN	7.74
A40	N	122.22	**Y89**	N	116.00	**K154**	HN	8.76	**N220**	N	118.82
S41	C	177.00	**G90**	C	171.28	**K154**	N	119.79	**S221**	C	172.21
S41	CA	56.42	**G90**	CA	44.10	**K155**	C	177.11	**S221**	CA	55.82
S41	CB	66.18	**G90**	HN	9.09	**K155**	CA	57.47	**S221**	CB	65.55
S41	HN	9.36	**G90**	N	107.82	**K155**	CB	31.54	**S221**	HN	8.49
S41	N	116.79	**D91**	C	174.31	**K155**	HN	7.29	**S221**	N	112.13
G42	C	171.05	**D91**	CA	54.69	**K155**	N	114.85	**I222**	C	170.14
G42	CA	44.11	**D91**	CB	40.34	**Q156**	C	174.62	**I222**	CA	60.55
G42	HN	9.93	**D91**	HN	8.50	**Q156**	CA	54.85	**I222**	CB	43.37
G42	N	110.07	**D91**	N	117.01	**Q156**	CB	30.20	**I222**	HN	9.28
T43	C	172.22	**F92**	C	175.54	**Q156**	HN	8.06	**I222**	N	124.14
T43	CA	58.66	**F92**	CA	57.69	**Q156**	N	115.26	**K223**	C	175.55
T43	CB	71.63	**F92**	CB	39.50	**I157**	CA	59.31	**K223**	CA	54.43
T43	HN	8.20	**F92**	HN	8.61	**I157**	CB	40.49	**K223**	CB	32.50
T43	N	105.17	**F92**	N	118.65	**I157**	HN	7.63	**K223**	HN	8.25
L44	C	173.95	**K93**	C	173.48	**I157**	N	120.81	**K223**	N	126.02
L44	CA	52.44	**K93**	CA	54.13	**D158**	CA	53.58	**L224**	C	175.38
L44	CB	45.01	**K93**	CB	34.72	**D158**	HN	9.08	**L224**	CA	52.90
L44	HN	8.18	**K93**	HN	8.23	**D158**	N	119.92	**L224**	CB	42.04
L44	N	126.30	**K93**	N	128.59	**N163**	C	176.13	**L224**	HN	9.52
L44	*CA*	*52.11*	**A94**	CA	52.50	**N163**	CA	51.90	**L224**	N	127.28
L44	*CB*	*44.79*	**A94**	CB	18.26	**N163**	CB	41.74	**Q225**	C	175.34
L44	*HN*	*8.05*	**A94**	HN	8.30	**A164**	C	177.97	**Q225**	CA	54.01
L44	*N*	*125.49*	**A94**	N	124.50	**A164**	CA	54.25	**Q225**	CB	30.66
D45	C	173.07	**N95**	C	174.99	**A164**	CB	17.50	**Q225**	HN	8.24
D45	CA	53.08	**N95**	HN	8.78	**A164**	HN	8.94	**Q225**	N	119.52
D45	CB	43.29	**N95**	N	121.42	**A164**	N	127.46	**F226**	C	174.15
D45	HN	8.80	**G96**	C	175.03	**S165**	C	174.76	**F226**	CA	56.14
D45	N	125.55	**G96**	CA	44.90	**S165**	CA	58.88	**F226**	CB	38.95
L46	C	175.36	**G96**	HN	8.33	**S165**	CB	64.11	**F226**	HN	8.95
L46	CA	53.06	**G96**	N	107.64	**S165**	HN	8.29	**F226**	N	127.22
L46	CB	44.09	**G97**	C	173.92	**S165**	N	111.43	**S227**	C	172.35
L46	HN	9.62	**G97**	CA	45.03	**G166**	C	171.90	**S227**	CA	55.16
L46	N	129.31	**G97**	HN	7.84	**G166**	CA	44.65	**S227**	CB	65.05
S47	C	173.55	**G97**	N	111.04	**G166**	HN	8.18	**S227**	HN	8.62

S47	CA	55.97	**S98**	C	176.37	**G166**	N	110.81	**S227**	N	116.69
S47	CB	62.39	**S98**	CA	59.51	**K167**	C	174.67	**F228**	C	172.57
S47	HN	8.69	**S98**	CB	62.75	**K167**	CA	55.46	**F228**	CA	55.91
S47	N	119.77	**S98**	HN	8.48	**K167**	CB	36.03	**F228**	CB	39.81
S47	*CA*	*56.04*	**S98**	N	115.89	**K167**	HN	6.99	**F228**	HN	8.90
S47	*CB*	*62.96*	**N99**	C	173.88	**K167**	N	113.61	**F228**	N	120.71
S47	*HN*	*8.84*	**N99**	CA	54.83	**V168**	C	175.87	**E229**	C	175.11
S47	*N*	*119.12*	**N99**	CB	39.66	**V168**	CA	60.13	**E229**	CA	52.42
A48	C	174.75	**N99**	HN	9.05	**V168**	CB	33.75	**E229**	CB	30.64
A48	CA	49.77	**N99**	N	119.89	**V168**	HN	7.72	**E229**	HN	9.33
A48	CB	20.08	**T100**	C	174.41	**V168**	N	116.74	**E229**	N	124.99
A48	HN	8.80	**T100**	CA	60.02	**N169**	C	173.92	**A230**	C	176.76
A48	N	130.00	**T100**	CB	69.03	**N169**	CA	52.70	**A230**	CA	49.87
A48	*C*	*174.75*	**T100**	HN	8.23	**N169**	CB	38.01	**A230**	CB	21.11
A48	*CA*	*49.89*	**T100**	N	112.14	**N169**	HN	9.49	**A230**	HN	9.33
A48	*CB*	*19.87*	**S101**	CA	52.99	**N169**	N	127.30	**A230**	N	130.91
A48	*HN*	*8.77*	**S101**	CB	62.80	***N169***	*C*	*174.16*	***A230***	*C*	*176.74*
A48	*N*	*128.93*	**S101**	HN	7.45	***N169***	*CA*	*53.24*	***A230***	*CA*	*49.42*
K49	C	174.76	**S101**	N	115.01	***N169***	*CB*	*38.45*	***A230***	*CB*	*21.67*
K49	CA	54.40	**P102**	C	178.59	***N169***	*HN*	*9.73*	***A230***	*HN*	*9.40*
K49	CB	34.44	**P102**	CA	63.64	***N169***	*N*	*128.33*	***A230***	*N*	*130.81*
K49	HN	8.86	**P102**	CB	31.37	**V170**	C	173.82	**T231**	C	174.31
K49	N	123.69	**E103**	C	178.41	**V170**	CA	58.57	**T231**	CA	58.00
K49	*C*	*174.62*	**E103**	CA	60.22	**V170**	CB	30.22	**T231**	CB	70.90
K49	*CA*	*54.41*	**E103**	CB	27.67	**V170**	HN	8.68	**T231**	HN	8.00
K49	*CB*	*34.80*	**E103**	HN	8.17	**V170**	N	114.01	**T231**	N	111.10
K49	*HN*	*8.71*	**E103**	N	114.51	**A171**	C	176.73	***T231***	*C*	*173.98*
K49	*N*	*123.49*	**D104**	C	179.95	**A171**	CA	49.40	***T231***	*CA*	*58.00*
E50	C	175.20	**D104**	CA	57.02	**A171**	CB	17.63	***T231***	*CB*	*70.83*
E50	CA	54.74	**D104**	CB	38.00	**A171**	HN	7.45	***T231***	*HN*	*8.27*
E50	CB	29.51	**D104**	HN	8.08	**A171**	N	123.09	***T231***	*N*	*110.99*
E50	HN	8.94	**D104**	N	119.89	**T172**	C	174.83	**Q232**	C	177.11
E50	N	123.63	**F105**	C	177.34	**T172**	CA	61.36	**Q232**	CA	53.52
N51	C	174.31	**F105**	CA	58.90	**T172**	HN	9.03	**Q232**	CB	32.17
N51	CA	51.80	**F105**	CB	37.76	**T172**	N	121.05	**Q232**	HN	7.69
N51	CB	38.78	**F105**	HN	7.48	**I173**	C	175.81	**Q232**	N	115.50
N51	HN	8.48	**F105**	N	121.13	**I173**	CA	58.28	***Q232***	*C*	*177.15*
N51	N	125.46	**L106**	C	177.63	**I173**	CB	34.36	***Q232***	*CA*	*53.53*
S52	C	173.18	**L106**	CA	57.45	**I173**	HN	7.50	***Q232***	*CB*	*31.93*
S52	CA	56.95	**L106**	CB	40.83	**I173**	N	121.34	***Q232***	*HN*	*7.50*
S52	CB	62.79	**L106**	HN	8.37	**D174**	C	177.20	***Q232***	*N*	*114.88*
S52	HN	7.32	**L106**	N	118.31	**D174**	CA	55.05	**W233**	C	173.89
S52	N	114.88	***L106***	*CA*	*57.41*	**D174**	CB	40.67	**W233**	CA	57.54
A53	C	177.90	***L106***	*CB*	*40.85*	**D174**	HN	9.28	**W233**	CB	27.19
A53	CA	54.67	***L106***	*HN*	*8.42*	**D174**	N	129.82	**W233**	HN	9.75
A53	CB	17.29	***L106***	*N*	*119.43*	**G175**	C	173.36	**W233**	N	121.95
A53	HN	9.19	**S107**	C	175.12	**G175**	CA	45.19	**N234**	C	173.29
A53	N	127.60	**S107**	CA	58.98	**G175**	HN	9.61	**N234**	CA	52.38
S54	C	173.76	**S107**	CB	63.11	**G175**	N	103.43	**N234**	CB	38.22
S54	CA	57.07	**S107**	HN	7.82	**K176**	C	177.11	**N234**	HN	9.45
S54	CB	64.28	**S107**	N	109.02	**K176**	CA	59.68	**N234**	N	116.10

S54	HN	7.34	***S107***	*CA*	*58.84*	**K176**	CB	33.18	**G235**	C	172.42
S54	N	106.73	***S107***	*CB*	*63.07*	**K176**	HN	7.80	**G235**	CA	45.24
V55	C	175.85	***S107***	*HN*	*7.77*	**K176**	N	120.02	**G235**	HN	8.10
V55	CA	65.26	***S107***	*N*	*108.15*	**P179**	C	178.57	**G235**	N	100.02
V55	CB	31.70	**Q108**	C	172.55	**P179**	CA	64.35	**L236**	C	175.59
V55	HN	8.59	**Q108**	CA	54.03	**P179**	CB	31.12	**L236**	CA	52.47
V55	N	127.68	**Q108**	CB	27.06	**E180**	C	177.52	**L236**	CB	45.29
N56	C	174.58	**Q108**	HN	8.00	**E180**	CA	57.82	**L236**	HN	10.18
N56	CA	51.12	**Q108**	N	118.86	**E180**	CB	30.12	**L236**	N	129.72
N56	CB	39.41	***Q108***	*CA*	*54.19*	**E180**	HN	8.66	**T237**	C	174.52
N56	HN	8.02	***Q108***	*CB*	*27.14*	**E180**	N	118.52	**T237**	CA	63.05
N56	N	114.86	***Q108***	*HN*	*8.08*	***E180***	*CA*	*57.93*	**T237**	CB	66.09
L57	C	175.64	***Q108***	*N*	*119.29*	***E180***	*CB*	*30.54*	**T237**	HN	10.08
L57	CA	53.36	**F109**	C	174.99	***E180***	*HN*	*8.79*	**T237**	N	126.29
L57	CB	46.20	**F109**	CA	55.90	***E180***	*N*	*118.98*	**I238**	C	176.94
L57	HN	8.93	**F109**	CB	41.24	**Y181**	C	174.52	**I238**	CA	61.51
L57	N	121.14	**F109**	HN	7.68	**Y181**	CA	58.75	**I238**	CB	36.43
L57	*CA*	*53.54*	**F109**	N	116.06	**Y181**	CB	38.85	**I238**	HN	8.86
L57	*CB*	*46.21*	**E110**	C	174.75	**Y181**	HN	8.08	**I238**	N	129.69
L57	*HN*	*8.81*	**E110**	CA	53.30	**Y181**	N	116.49	***I238***	*C*	*176.94*
L57	*N*	*120.76*	**E110**	CB	32.31	**D182**	CA	53.76	***I238***	*CA*	*61.56*
S58	C	174.53	**E110**	HN	9.08	**D182**	CB	42.31	***I238***	*CB*	*36.27*
S58	CA	55.39	**E110**	N	117.64	**D182**	HN	7.45	***I238***	*HN*	*8.78*
S58	CB	64.06	**V111**	C	175.62	**D182**	N	119.94	***I238***	*N*	*129.68*
S58	HN	8.41	**V111**	CA	61.23	**V184**	CA	64.95	**K239**	C	177.95
S58	N	114.23	**V111**	CB	31.53	**V184**	CB	30.04	**K239**	CA	52.99
N59	C	174.31	**V111**	HN	9.79	**V184**	HN	8.52	**K239**	CB	33.99
N59	CA	53.07	**V111**	N	123.74	**V184**	N	117.06	**K239**	HN	10.85
N59	CB	39.49	**T112**	C	175.84	**P185**	CA	63.18	**K239**	N	133.26
N59	HN	8.77	**T112**	CA	61.39	**K186**	CA	56.18	**K240**	C	178.29
N59	N	118.47	**T112**	CB	67.96	**K186**	CB	31.30	**K240**	CA	59.16
L60	C	176.60	**T112**	HN	8.58	**K186**	HN	7.85	**K240**	CB	31.32
L60	CA	55.00	**T112**	N	116.83	**K186**	N	118.17	**K240**	HN	8.73
L60	CB	44.52	**L113**	C	174.01	**T187**	CA	58.91	**K240**	N	121.05
L60	HN	8.29	**L113**	CA	55.80	**T187**	CB	71.51	**D241**	C	176.80
L60	N	113.49	**L113**	CB	44.27	**T187**	HN	7.59	**D241**	CA	55.10
K61	C	171.72	**L113**	HN	7.58	**T187**	N	115.01	**D241**	CB	39.48
K61	CA	52.16	**L113**	N	124.23	**P188**	C	172.83	**D241**	HN	8.24
K61	CB	33.96	**L114**	C	174.94	**P188**	CA	58.68	**D241**	N	113.03
K61	HN	9.19	**L114**	CA	53.49	**P188**	CB	34.79	**H242**	C	175.70
K61	N	120.42	**L114**	CB	44.04	**T189**	C	173.04	**H242**	CA	55.77
P62	C	175.83	**L114**	HN	7.61	**T189**	CA	61.15	**H242**	CB	33.46
P62	CA	63.17	**L114**	N	118.40	**T189**	CB	70.73	**H242**	HN	7.84
P62	CB	30.58	**T115**	CA	58.50	**T189**	HN	8.96	**H242**	N	116.81
G63	C	175.02	**T115**	CB	70.96	**T189**	N	124.47	**T243**	C	175.28
G63	CA	44.03	**T115**	HN	8.91	**D190**	CA	53.00	**T243**	CA	58.61
G63	HN	9.27	**T115**	N	109.96	**D190**	CB	45.72	**T243**	CB	71.88
G63	N	113.03	**V116**	CA	61.22	**D190**	HN	9.39	**T243**	HN	7.73
G63	*C*	*175.07*	**V116**	CB	34.21	**D190**	N	129.44	**T243**	N	105.78
G63	*CA*	*44.06*	**V116**	HN	8.34	**D192**	C	177.97	**D244**	C	179.25
G63	*HN*	*9.03*	**V116**	N	119.55	**D192**	CA	54.48	**D244**	CA	51.88

G63	*N*	*112.70*	**N127**	C	173.64	**D192**	CB	40.26	**D244**	CB	41.33
D64	C	175.23	**N127**	CA	52.16	**Q193**	C	174.61	**D244**	HN	8.58
D64	CA	55.70	**N127**	CB	38.73	**Q193**	CA	56.91	**D244**	N	120.38
D64	CB	41.16	**I128**	C	175.64	**Q193**	CB	28.76	**K245**	CA	58.36
D64	HN	8.53	**I128**	CA	61.64	**Q193**	HN	8.62	**K245**	CB	30.59
D64	N	125.28	**I128**	CB	36.33	**Q193**	N	123.77	**K245**	HN	8.55
K65	C	174.15	**I128**	HN	8.74	**V194**	C	174.94	**K245**	N	117.27
K65	CA	54.52	**I128**	N	125.02	**V194**	CA	61.08	**G247**	C	173.01
K65	CB	35.75	**I129**	C	175.50	**V194**	CB	33.19	**G247**	CA	45.11
K65	HN	8.53	**I129**	CA	63.14	**V194**	HN	8.43	**G247**	HN	8.26
K65	N	117.69	**I129**	CB	37.82	**V194**	N	122.79	**G247**	N	111.13
L66	C	174.95	**I129**	HN	8.82	**Q195**	C	174.01	**Y248**	C	178.00
L66	CA	52.91	**I129**	N	129.01	**Q195**	CA	54.27	**Y248**	CA	58.09
L66	CB	44.02	**L130**	C	179.25	**Q195**	CB	32.42	**Y248**	CB	37.88
L66	HN	9.54	**L130**	CA	52.80	**Q195**	HN	9.46	**Y248**	HN	8.25
L66	N	122.79	**L130**	CB	41.15	**Q195**	N	127.37	**Y248**	N	123.23
T67	C	175.18	**L130**	HN	7.64	**M196**	C	174.46	**V249**	C	176.07
T67	CA	60.83	**L130**	N	115.41	**M196**	CA	53.29	**V249**	CA	61.55
T67	CB	70.60	**D131**	C	173.03	**M196**	CB	35.29	**V249**	CB	27.79
T67	HN	9.00	**D131**	CA	53.18	**M196**	HN	9.37	**V249**	HN	8.42
T67	N	115.62	**D131**	CB	43.80	**M196**	N	122.21	**V249**	N	129.44
K68	C	173.49	**D131**	HN	8.31	**E197**	C	175.89	**K250**	C	179.75
K68	CA	53.76	**D131**	N	119.49	**E197**	CA	54.44	**K250**	CA	56.91
K68	CB	34.22	**D132**	C	175.50	**E197**	CB	30.07	**K250**	CB	30.98
K68	HN	9.44	**D132**	CA	55.59	**E197**	HN	9.35	**K250**	HN	8.42
K68	N	127.23	**D132**	CB	39.98	**E197**	N	125.30	**K250**	N	135.93
K68	*CA*	*53.60*	**D132**	HN	7.50	**I198**	C	173.60	**E251**	C	177.60
K68	*CB*	*34.48*	**D132**	N	118.38	**I198**	CA	59.39	**E251**	CA	57.97
K68	*HN*	*9.30*	**A133**	C	176.23	**I198**	CB	38.98	**E251**	CB	28.92
K68	*N*	*126.95*	**A133**	CA	49.73	**I198**	HN	9.47	**E251**	HN	8.20
D69	C	174.44	**A133**	CB	18.69	**I198**	N	127.35	**E251**	N	120.00
D69	CA	52.77	**A133**	HN	8.12	**Q199**	C	174.56	**N252**	C	178.86
D69	CB	44.40	**A133**	N	124.59	**Q199**	CA	52.71	**N252**	CA	52.50
D69	HN	8.12	**N134**	C	177.15	**Q199**	CB	31.79	**N252**	CB	37.29
D69	N	121.83	**N134**	CA	55.07	**Q199**	HN	9.28	**N252**	HN	7.12
F70	C	173.62	**N134**	CB	41.20	**Q199**	N	126.16	**N252**	N	110.75
F70	CA	55.80	**N134**	HN	9.74	**F200**	C	175.22	**K254**	C	175.19
F70	CB	43.00	**N134**	N	125.45	**F200**	CA	52.45	**K254**	CA	54.75
F70	HN	9.34	**L135**	C	178.53	**F200**	CB	36.44	**K254**	CB	34.15
F70	N	119.58	**L135**	CA	58.05	**F200**	HN	8.86	**A255**	C	176.03
Q71	C	174.08	**L135**	CB	40.23	**F200**	N	128.57	**A255**	CA	51.23
Q71	CA	53.14	**L135**	HN	9.05	**K201**	C	174.76	**A255**	CB	18.06
Q71	CB	31.53	**L135**	N	125.77	**K201**	CA	56.65	**A255**	HN	8.04
Q71	HN	8.64	**K136**	C	178.07	**K201**	CB	31.38	**A255**	N	120.23
Q71	N	120.19	**K136**	CA	59.63	**K201**	HN	9.46	***A255***	*C*	*177.22*
F72	C	175.01	**K136**	CB	28.84	**K201**	N	131.47	***A255***	*CA*	*51.21*
F72	CA	55.87	**K136**	HN	8.15	***K201***	*C*	*174.64*	***A255***	*CB*	*19.79*
F72	CB	41.16	**K136**	N	118.68	***K201***	*CA*	*56.48*	**H256**	C	172.52
E73	C	173.66	**D137**	C	177.97	***K201***	*CB*	*31.56*	**H256**	CA	58.62
E73	CA	53.54	**D137**	CA	57.40	***K201***	*HN*	*9.38*	**H256**	CB	23.98
E73	CB	33.40	**D137**	CB	39.43	***K201***	*N*	*130.64*	**H256**	HN	3.18

E73	HN	9.03	**D137**	HN	7.15	**D202**	C	175.20	**H256**	N	105.23
E73	N	119.85	**D137**	N	118.68	**D202**	CA	52.61	***H256***	*C*	*173.22*
N74	C	175.00	**L138**	C	180.06	**D202**	CB	39.75	***H256***	*CA*	*57.76*
N74	CA	52.72	**L138**	CA	57.68	**D202**	HN	8.66	***H256***	*CB*	*25.04*
N74	CB	38.77	**L138**	CB	41.02	**D202**	N	121.88	***H256***	*HN*	*3.14*
N74	HN	9.54	**L138**	HN	8.12	**D203**	C	177.18	***H256***	*N*	*104.07*
N74	N	120.61	**L138**	N	119.37	**D203**	CA	52.24	**S257**	C	171.17
N75	C	175.42	**Y139**	C	175.41	**D203**	CB	41.15	**S257**	CA	54.13
N75	CA	51.83	**Y139**	CA	59.37	**D203**	HN	7.65	**S257**	CB	59.77
N75	CB	39.69	**Y139**	CB	36.81	**D203**	N	124.75	**S257**	HN	6.33
N75	HN	8.80	**Y139**	HN	8.43	**K204**	C	175.86	**S257**	N	111.94
N75	N	125.69	**Y139**	N	123.97	**K204**	CA	55.51	**E258**	C	175.79
G76	C	172.14	**L140**	C	180.27	**K204**	CB	30.63	**E258**	CA	51.89
G76	CA	44.03	**L140**	CA	57.40	**K204**	HN	8.95	**E258**	CB	33.25
G76	HN	8.52	**L140**	CB	40.08	**K204**	N	127.46	**E258**	HN	7.58
G76	N	110.59	**L140**	HN	8.65	**T205**	C	174.68	**E258**	N	111.57
S77	C	173.11	**L140**	N	120.90	**T205**	CA	65.02	***E258***	*C*	*175.72*
S77	CA	58.88	**M141**	C	176.89	**T205**	CB	67.90	***E258***	*CA*	*52.09*
S77	CB	64.16	**M141**	CA	59.08	**T205**	HN	8.21	***E258***	*CB*	*33.40*
S77	HN	8.47	**M141**	CB	33.03	**T205**	N	117.12	***E258***	*HN*	*7.75*
S77	N	115.32	**M141**	HN	8.59	**K206**	C	176.47	***E258***	*N*	*111.56*
L78	C	175.67	**M141**	N	117.05	**K206**	CA	54.51	**D259**	C	174.69
L78	CA	51.72	**S142**	C	175.42	**K206**	CB	36.23	**D259**	CA	54.85
L78	CB	43.34	**S142**	CA	60.71	**K206**	HN	8.88	**D259**	CB	39.41
L78	HN	7.91	**S142**	CB	64.45	**K206**	N	127.91	**D259**	HN	8.64
L78	N	121.42	**S142**	HN	8.04	**D207**	C	178.41	**D259**	N	122.72
A79	C	173.79	**S142**	N	111.75	**D207**	CA	51.64	**K260**	CA	59.95
A79	CA	52.99	**A143**	C	179.69	**D207**	CB	40.64	**K260**	CB	33.87
A79	CB	18.37	**A143**	CA	52.96	**D207**	HN	8.85	**K260**	HN	8.12
A79	HN	8.41	**A143**	CB	19.54	**D207**	N	121.00	**K260**	N	118.66
A79	N	122.49	**A143**	HN	9.08	**E208**	C	177.49			
I80	C	176.84	**A143**	N	124.93	**E208**	CA	58.24			
I80	CA	59.44	***A143***	*C*	*179.70*	**E208**	CB	27.78			

Table S3. X-Ray diffraction data collection and refinement statistics.

	$TapA_{71-190}$	$TapA_{75-190}$
Data collection		
Space group	$P2_12_12_1$	$P2_1$
Cell dimensions		
a, *b*, *c* (Å)	39.2, 52.9, 167.7	30.1, 61.1, 34.3
α, β, γ (°)	90.0, 90.0, 90.0	90.0, 106.9, 90.0
Resolution (Å)*	44.77-1.07 (1.13-1.07)	32.8-1.28 (1.36-1.28)
R_{meas}*	6.6 (154.2)	4.5 (177.0)
$< I / \sigma(I) >$*	9.77 (0.8)	14.2 (0.8)
Completeness (%)*	98.8 (97.9)	98.4 (97.2)
Multiplicity*	3.5	4.4
Refinement		
No. reflections	151,026	30,250
R_{work}/ R_{free}	0.148/0.176	0.147/0.197
No. atoms		
Protein	2949	943
Ligand/ion	28	15
Water	742	212
Mean B factor (Å^2)	17.8	28.0
R.m.s deviations		
Bond lengths (Å)	0.012	0.012
Bond angles (º)	1.632	1.685
Ramachandran		
Outlier (%)	0	0
Favored (%)	96.6	95.6

* Data in highest resolution shell are indicated in parenthesis.

Table S4. H^N-H^N contacts observed by NMR within TasA filaments including those shown in SI Appendix, Fig. S8. Contacts shown in column 1 are located in antiparallel β-sheets and are involved in cross-strand hydrogen bonds, the remaining show validated contacts in loop and helical regions.

D31	-	A230	K65	-	L236	N145	-	D146	G219	-	N220
K33	-	F228	K65	-	I138	A147	-	A148	H242	-	T243
K35	-	F226	G42	-	N59	A148	-	A149	K250	-	E251
A37	-	L224	G42	-	L60	A149	-	A150	E251	-	N252
F39	-	I222	N59	-	L60	A150	-	E151			
S41	-	N220	E103	-	D104	E151	-	K152			
S58	-	V249	D104	-	F105	K152	-	I153			
K49	-	Q71	F105	-	L106	I153	-	K154			
G63	-	F200	S107	-	Q108	K154	-	K155			
K68	-	M196	Q108	-	F109	K155	-	Q156			
F70	-	V194	Y139	-	L140	Q156	-	I157			
M85	-	V168	L140	-	M141	E180	-	Y181			
L84	-	E229	M141	-	S142	Y181	-	D182			
G90	-	K223	S142	-	A143	N215	-	K216			
K93	-	S221	A143	-	K144	K216	-	Y217			
V111	-	A133	K144	-	N145	Y217	-	Q218			

Table S5. Primer used for cloning different TapA fragments into pCA528.

$TapA_{44-253}$	**BsmI XhoI $TapA_{44-253}$**
Forward 1	5‘CCAGTG**CGTCTC**AGGTGGTGCTTTTCATGATATTGAAAC
Reverse 1	5‘TCGA**CTCGAG**ttaCTGATCAGCTTCATTGC
$TapA_{44-190/33-190}$	mutation for stop codon generation at AA 191
Forward 2	5‘CAAAATGCGATGAATAACCGACAGTCCCTAAAAAAG
Reverse 2	5‘AGGGACTGTCGGTTATTCATCGCATTTTGCAAGCCTC
$TapA_{54-190}$	$TapA_{54ff}$ C-terminus Sumo
Forward 3	5‘TCACTTCAAACGTGTAAAGACTTTCAGCATACAG
Reverse 3	5‘TACACGTTTGAAGTGAACCACCAATCTGTTCTCTGTGAGCCTC
$TapA_{60-190}$	$TapA_{60ff}$ C-terminus Sumo
Forward 4	5‘GACTTTCAGCATACAGATAAAAACTGCCATTATG
Reverse 4	5‘TCTGTATGCTGAAAGTCACCACCAATCTGTTCTCTGTGAGCCTC
$TapA_{66-190}$	$TapA_{66ff}$ C-terminus Sumo
Forward 5	5‘AAAAACTGCCATTATGATAAACGCTGGGATCAAAG
Reverse 5	5‘TCATAATGGCAGTTTTTACCACCAATCTGTTCTCTGTGAGCCTC
$TapA_{71-190}$	$TapA_{71ff}$ C-terminus Sumo
Forward 6	5‘GATAAACGCTGGGATCAAAGTGATTTGCACATATCAGATC
Reverse 6	5‘CCAGCGTTTATCACCACCAATCTGTTCTCTGTGAGCCTC
$TapA_{75-190}$	C-terminus Sumo $TapA_{75ff}$
Forward 7	5’AGAGAACAGATTGGTGGTGCTGATCAAAGTGATTTGCACATATCAGATCAAACGG
Reverse 7	5‘TGTGCAAATCACTTTGATCAGCACCACCAATCTGTTCTCTGTGAGCCTCAATAATATCG

Table S6. Primers for Biofilm experiments.

Primer	Sequence	Used for
RK221	ACAT gcatgc TTATTCATCGCATTTTGCAAGCCTC	pKXD2, pKXD3, pKXD4, pKXD5
RK222	ACAT gcatgc TTACTGATCAGCTTCATTGC	pKXD6, pKXD7
RK224	CCGATGATACAAGCGCTGCT GATCAAAGTGATTTG	pKXD3
RK225	GATATGTGCAAATCACTTTGATC AGCAGCGCTTGTATC	pKXD3
RK226	CCGATGATACAAGCGCTGCT GATAAACGCTGGGATC	pKXD4
RK227	CACTTTGATCCCAGCGTTTATC AGCAGCGCTTGTATC	pKXD4
RK228	CATTTTCAGTCTGACTGCCGCAATA GCTTTTCATGATATTG	pKXD5, pKXD6
RK229	CAAATGTTTCAATATCATGAAAAGC TATTGCGGCAGTCAG	pKXD5, pKXD6
RK234	CACAATCAGCAAAAGGCGAAGCAATCAGACCAGAAGG	pKXD13
RK235	CCCGCTTTCCTTCTGGTCTGATTGCTTCGCCTTTTGCTGATTG	pKXD13
RK239	TGGCGAATTCTCAGAGTTAAATGGTATTGCTTCACT	pKXD13
RK240	GACTAGTCC TTAATTTTTATCCTCGCTATGCGC	pKXD13
RK242	TCCCCCCGGGGGGATCAGAGTTAAATGGTATTGCTTCACT	pKXD2-7
RK243	GCTCTAGAGCCTCAGAGTTAAATGGTATTGCTTCACT	pKXD13
KD117	aCGTTTGAAGTGAGACATC	pKXD23
KD118	AAGCATGCAAGCTAATTC	pKXD23

Table S7. Plasmids for Biofilm experiments.

Plasmid	Genotype	Construction of strain
pKXD2	pBS2E-P_{tapA}-*tapA190*	BKD34
pKXD3	pBS2E-P_{tapA}-*tapAΔ45-74*	BKD35
pKXD4	pBS2E-P_{tapA}-*tapAΔ45-70*	BKD36
pKXD5	pBS2E-P_{tapA}-*tapAΔ34-43*	BKD37
pKXD6	pBS2E-P_{tapA}-*tapA253Δ34-43*	BKD38
pKXD7	pBS2E-P_{tapA}-*tapA*	BKD39
pKXD13	pBS1K-P_{tapA}-*tapAΔ13-234-sipW-tasA*	BKD30
pKXD23	pBS2E-P_{tapA}-*tapA1-57*	BKD121

Table S8. Strains for Biofilm experiments.

Strain	Genotype	Reference
DK1042	NCIB 3610 *comIQ12L*	(4)
BRK49	*comIQ12L ΔtapA-sipW-tasA::spc*	(5)
BRK263	*ΔsipW::erm*	(5)
BKD30	*comIQ12L ΔtapA-sipW-tasA::spc amyE:: P_{tapA}-tapAΔ13-234-sipW-tasA-kan*	This study
BKD34	*comIQ12L ΔtapA-sipW-tasA::spc amyE:: P_{tapA}-tapAΔ13-234-sipW-tasA-kan lacA:: P_{tapA}-tapA190-erm*	This study
BKD35	*comIQ12L ΔtapA-sipW-tasA::spc amyE:: P_{tapA}-tapAΔ13-234-sipW-tasA-kan lacA::P_{tapA}-tapA190Δ45-74-erm*	This study
BKD36	*comIQ12L ΔtapA-sipW-tasA::spc amyE:: P_{tapA}-tapAΔ13-234-sipW-tasA-kan lacA:: P_{tapA}-tapA190Δ45-70-erm*	This study
BKD37	*comIQ12L ΔtapA-sipW-tasA::spc amyE:: P_{tapA}-tapAΔ13-234-sipW-tasA-kan lacA:: P_{tapA}-tapA190Δ34-43-erm*	This study
BKD38	*comIQ12L ΔtapA-sipW-tasA::spc amyE:: P_{tapA}-tapAΔ13-234-sipW-tasA-kan lacA:: P_{tapA}-tapAΔ34-43-erm*	This study
BKD39	*comIQ12L ΔtapA-sipW-tasA::spc amyE:: P_{tapA}-tapAΔ13-234-sipW-tasA-kan lacA:: P_{tapA}-tapA-erm*	This study
BKD121	*comIQ12L ΔtapA-sipW-tasA::spc amyE:: P_{tapA}-tapAΔ13-234-sipW-tasA-kan lacA:: P_{tapA}-tapA57-erm*	This study

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