# Supporting Information

## Replacing the Axial Ligand Tyrosine 75 or its Hydrogen Bond Partner Histidine 83 minimally affects hemin acquisition by the Hemophore HasAp from *Pseudomonas aeruginosa*[§ξ]

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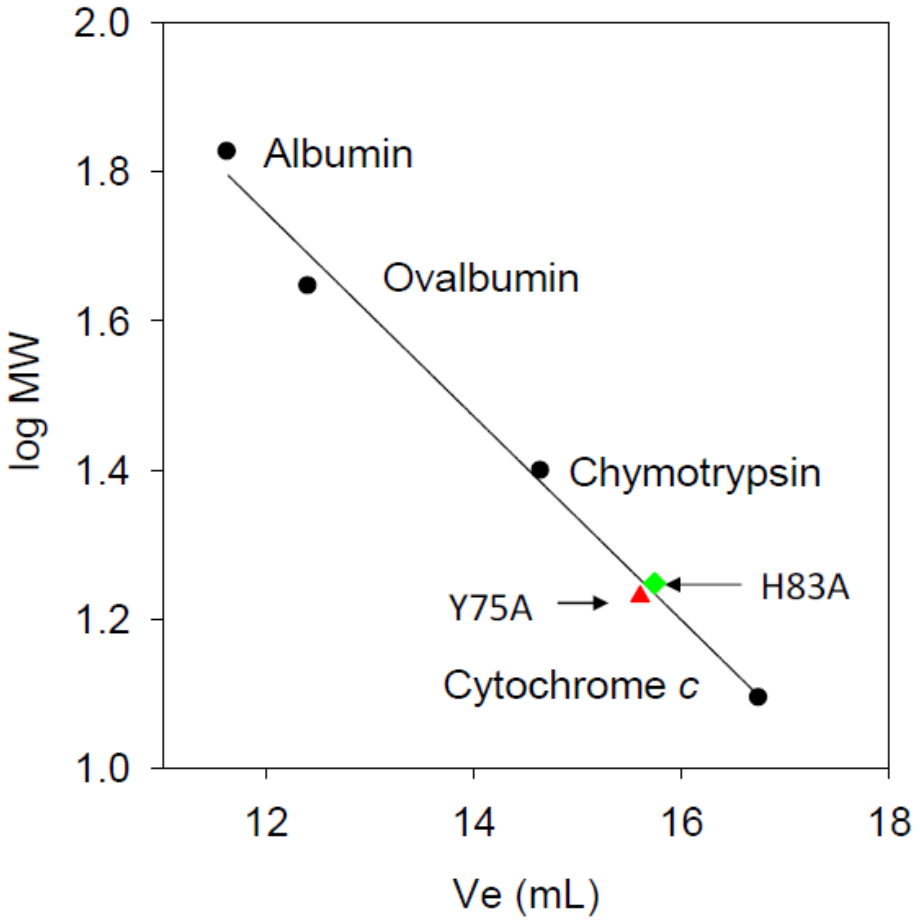


**Figure S1.** Elution volumes (*Ve*) from a calibrated Superdex 75 column and estimated molecular weight of Y75A HasAp (red triangle) and H83A HasAp (green diamond). The Superdex 75 column was calibrated with albumin (67 kDa), ovalbumin (44 kDa), chymotrypsin (25 kDa), and cytochrome *c* (12.4 kDa) shown in black filled circles.

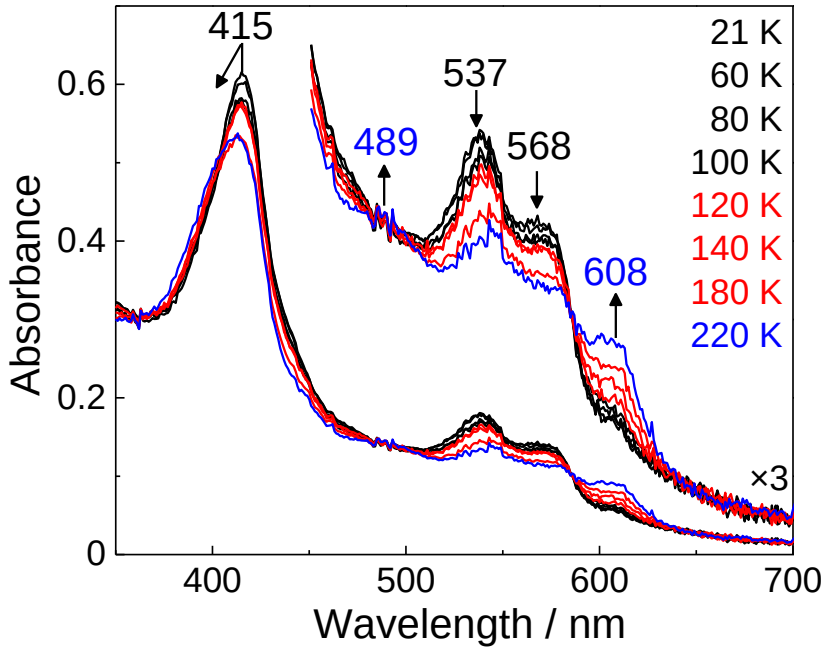


**Figure S2.** Temperature dependence of UV-vis spectra of H83A holo-HasAp

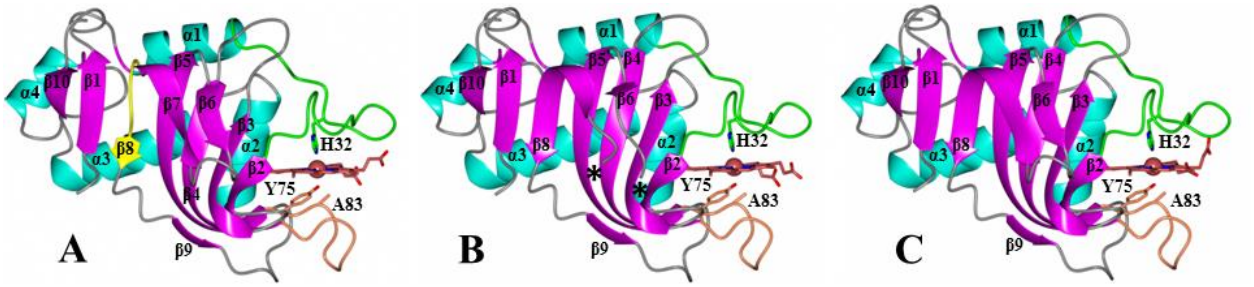


**Figure S3.** The overall structure of the H83A mutants is very similar to that of wild type HasAp (PDB: 3ELL). $C_\alpha$-RMSD values from comparing the wild type structure to the structure of H83A$^{ortho}$-HasAp (A) is 0.564 Å, H83A$^{mono}$- HasAp, (B) is 0.448 Å, and H83A$^{pH5.4}$-HasAp (C) is 0.532 Å. Secondary structures are colored cyan (α-helices), magenta (β-strands) and grey (loops). Loss in secondary structure is colored yellow (A). Missing electron density in (B) is delimited by black asterisks. Residues Ser2 to Ala183 were used to calculate the RMSD values using the secondary structure matching algorithm in the program Superpose (*1*) via the CCP4 interface (*2*).

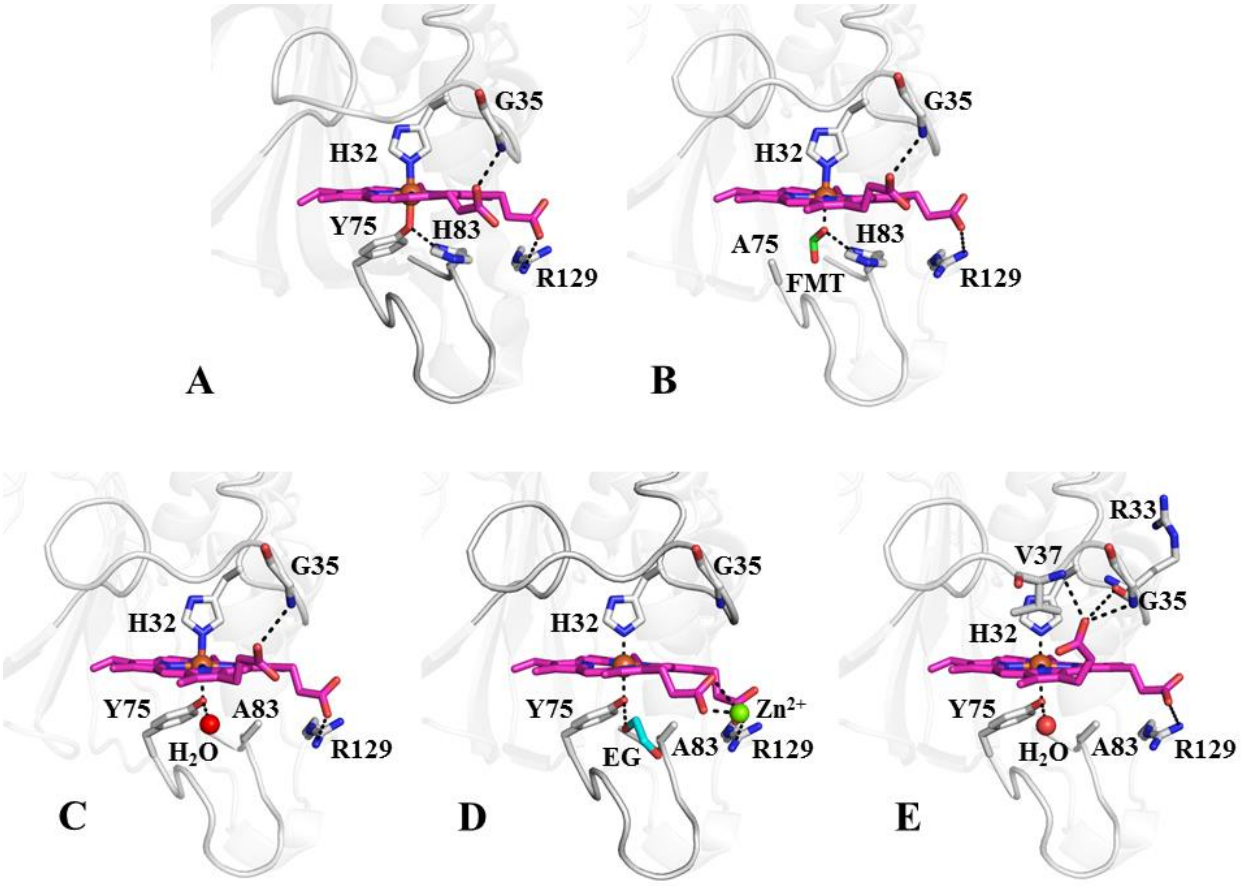


**Figure S4.** Heme propionate interactions in (A) wt holo-HasAp monomer B (PDB: 3ELL), (B) Y75A-HasAp, (C) H83A$^{ortho}$-HasAp, (D) H83A$^{mono}$-HasAp; the zinc ion coordinating the heme propionate is shown as a green sphere and (E) H83A$^{pH5.4}$-HasAp.

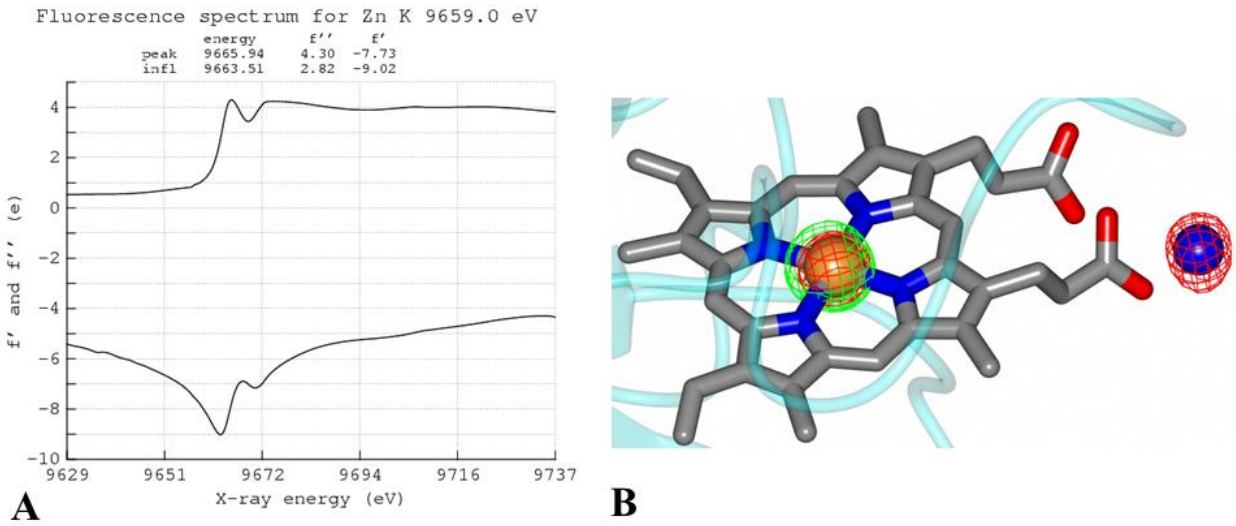


**Figure S5.** (A) X-ray fluorescence scan of the H83A$^{mono}$-HasAp crystal (B) A zinc ion coordinates the heme propionates in H83A$^{mono}$-HasAp. Phased anomalous difference map using data collected at λ=1.000 Å (red mesh) and low energy 1.28414 Å (green mesh) contoured at 4σ. Note that the anomalous difference density increases at the heme Fe atom and disappears at the Zn ion site in the data acquired at low energy.

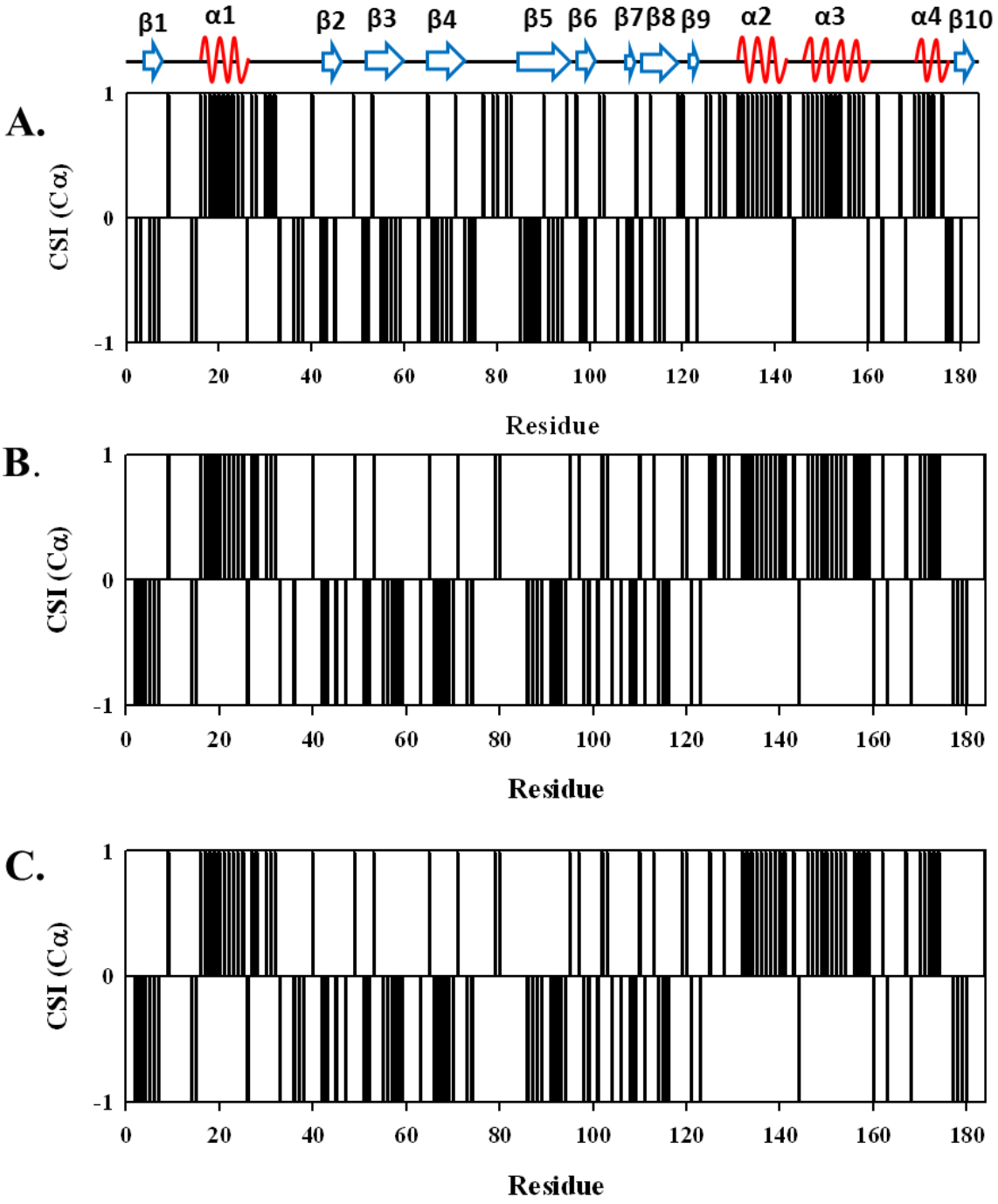


**Figure S6.** (A) Elements of secondary structure in wt apo-HasAp, derived from the plot of $C_\alpha$ chemical shift indexes are consistent with elements of secondary structure obtained from the crystal structure of wild type apo-HasAp. Chemical-shift index plots ($C_\alpha$) for apo-Y75A-HasAp (B) and apo-H83A-HasAp (C) indicate that the mutations did not introduce significant structural perturbations in the mutant apo-proteins relative to the wt apo-hemophore.

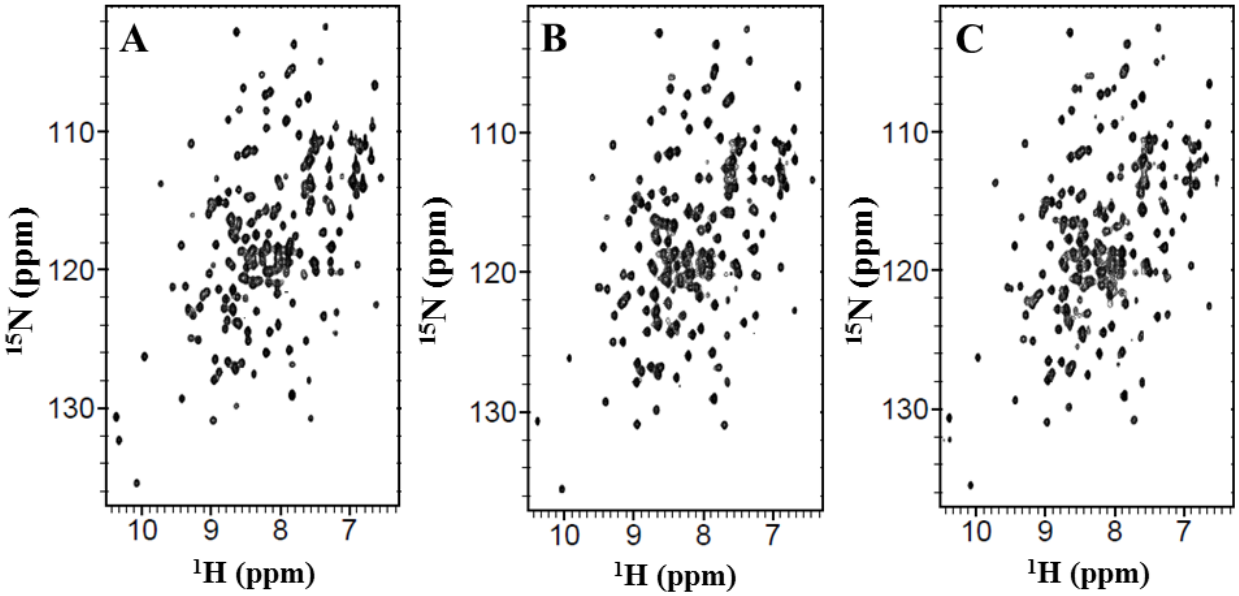


**Figure S7.** $^{1}$H,$^{15}$N-HSQC spectra of wt apo-HasAp (A), Y75A apo-HasAp (B), and H83A apo-HasAp (C). Spectra were taken at 32 °C using a 600MHz Bruker spectrometer. Acquisition parameters are as follows: 2048 ($^{1}$H) × 256 ($^{15}$N) complex points; 10.7 kHz ($^{1}$H) and 2.4 kHz ($^{15}$N) spectral widths; 32 scans per increment; d1=1sec.

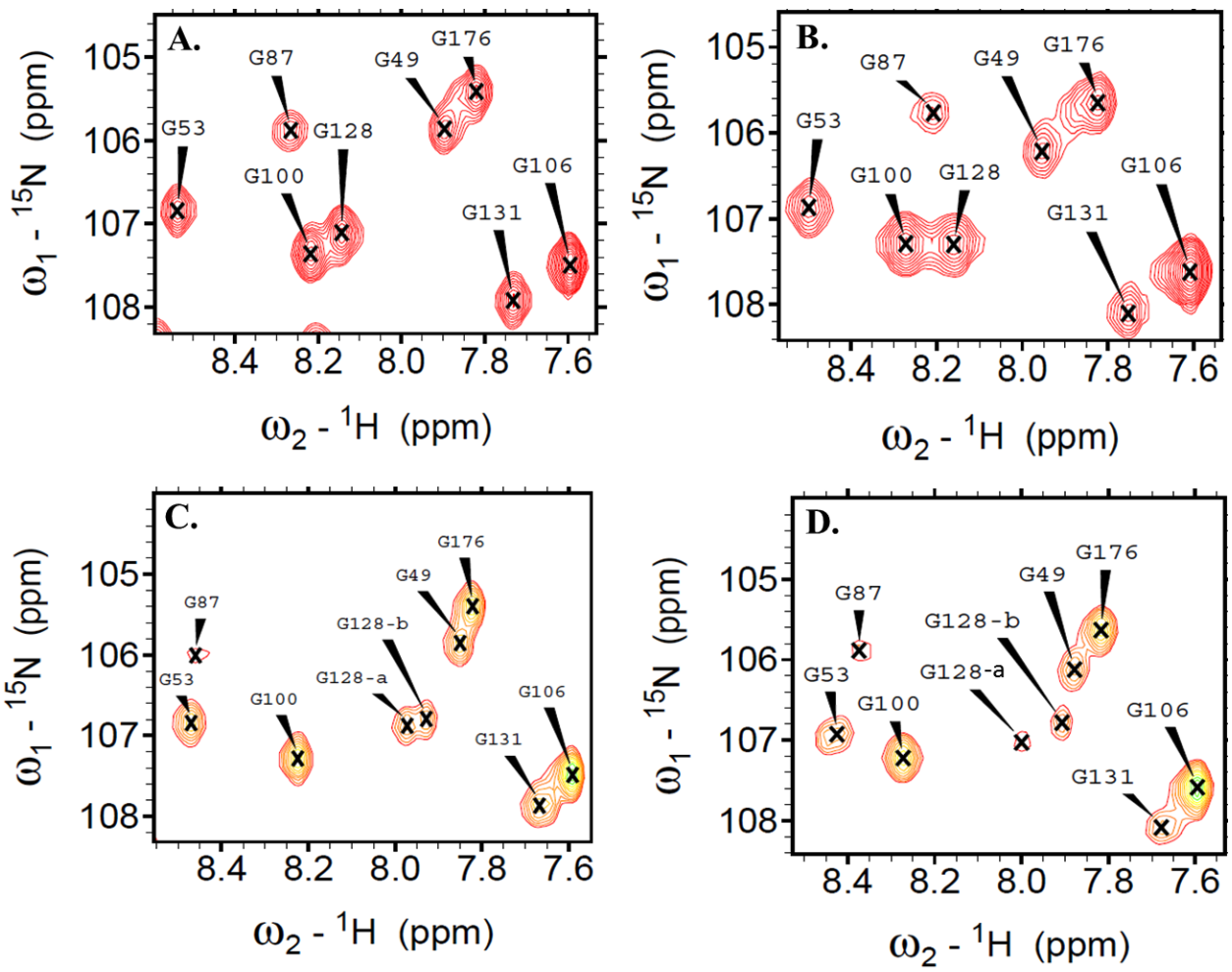


**Figure S8.** Portion of the $^{1}$H-$^{15}$N-HSQC spectra of wt apo-HasAp at 32 °C (A) and 15 °C (B), and Y75A apo-HasAp at 32 °C (C) and 15 °C (D), illustrating the temperature dependence of the two cross peaks originating from G128 in Y75A apo-HasAp.

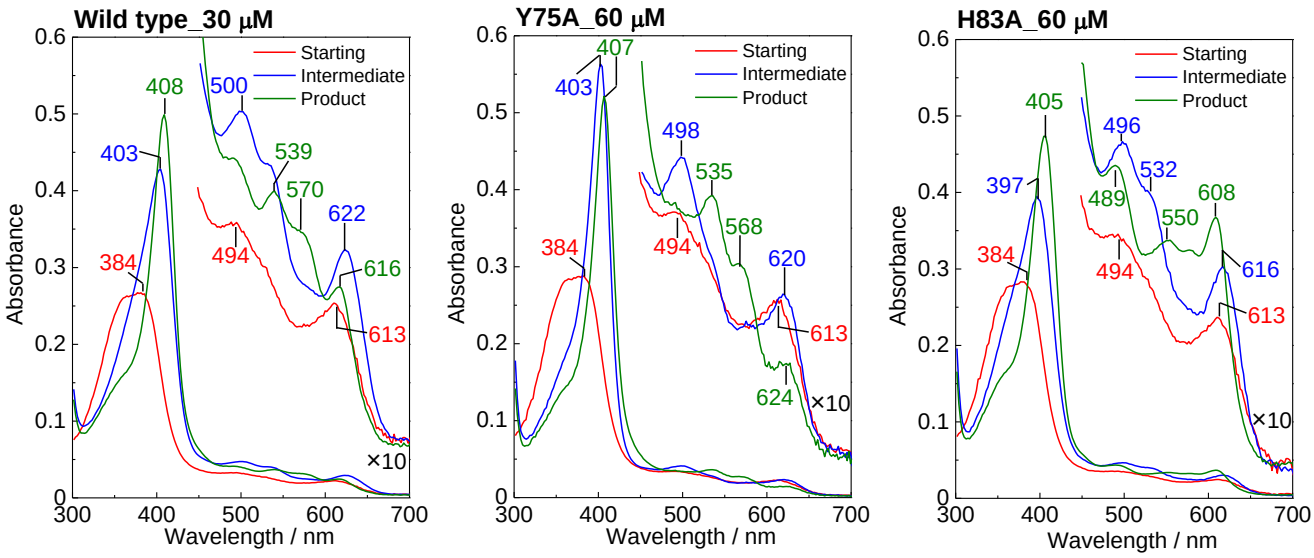


**Figure S9.** Individual spectral components from global analysis of Stopped-flow data

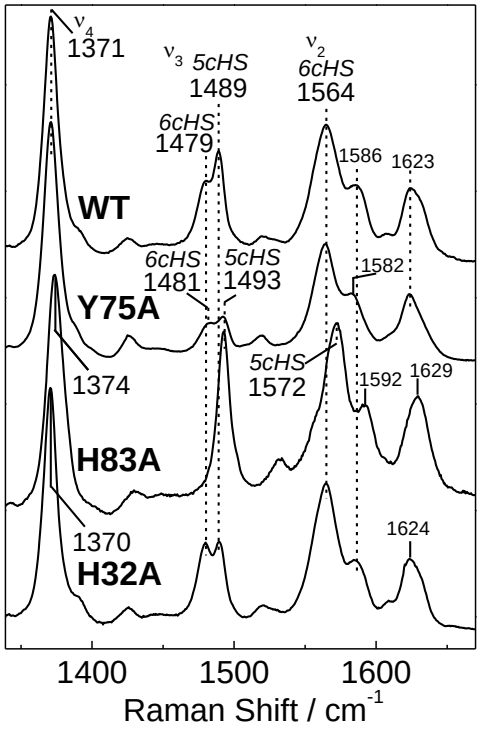


**Figure S10.** RR spectra of 6-ms RFQ samples

**Table S1:** Backbone resonance assignments for wt apo-HasAp

| Residue | $^{1}H_{N}$ | $^{15}N_{H}$ | $^{13}C_{\alpha}$ |
|---|---|---|---|
| M1 | | | |
| S2 | | | 57.52 |
| I3 | 8.52 | 121.98 | 61.44 |
| S4 | 8.03 | 118.36 | |
| I5 | 8.65 | 127.18 | 59.92 |
| S6 | 8.81 | 124.28 | 56.29 |
| Y7 | 7.89 | 120.15 | 54.66 |
| S8 | | | |
| T9 | 8.431 | 118.75 | 65.44 |
| T10 | | | |
| Y11 | | | |
| S12 | | | |
| G13 | | | |
| W14 | 8.68 | 122.88 | 57.03 |
| T15 | 8.76 | 109.08 | 60.03 |
| V16 | 7.26 | 120.10 | 66.35 |
| A17 | 8.49 | 119.73 | 55.39 |
| D18 | 8.38 | 119.56 | 57.38 |
| Y19 | 8.82 | 122.74 | 63.35 |
| L20 | 8.75 | 119.35 | 58.31 |
| A21 | 8.16 | 120.11 | 55.02 |
| D22 | 7.83 | 122.32 | 58.52 |
| W23 | 8.70 | 119.81 | 63.57 |
| S24 | 8.76 | 114.36 | 63.54 |
| A25 | 7.88 | 125.69 | 54.82 |
| Y26 | 8.16 | 120.89 | 57.00 |
| F27 | 8.69 | 122.72 | 60.93 |
| G28 | 7.35 | 102.41 | 46.28 |
| D29 | 7.52 | 119.32 | 54.57 |
| V30 | 7.60 | 128.01 | 63.83 |
| N31 | 8.04 | 115.40 | 54.67 |
| A32 | 8.28 | 118.57 | 59.67 |
| R33 | 7.30 | 115.31 | 52.91 |
| P34 | | | 63.66 |
| G35 | 8.61 | 111.72 | 45.43 |
| Q36 | 7.88 | 118.66 | 55.05 |
| V37 | 8.38 | 117.54 | 60.16 |
| V38 | 8.45 | 124.92 | 61.72 |
| D39 | 10.74 | 131.50 | 53.99 |
| G40 | 9.69 | 113.58 | 46.40 |
| S41 | 8.46 | 117.49 | 58.65 |
| N42 | 7.93 | 121.52 | 52.47 |
| T43 | 8.40 | 114.58 | 61.97 |
| G44 | 7.91 | 109.17 | 44.95 |
| G45 | 8.21 | 108.42 | 44.21 |
| F46 | 8.72 | 116.14 | 58.46 |
| N47 | | | |
| P48 | | | 65.52 |
| G49 | 7.90 | 105.82 | 46.36 |
| P50 | | | 64.27 |

| | | | |
|---|---|---|---|
| F51 | 8.70 | 116.49 | 56.32 |
| D52 | 6.56 | 113.33 | 52.00 |
| G53 | 8.54 | 106.79 | 47.64 |
| S54 | 8.60 | 114.17 | 58.15 |
| Q55 | 7.97 | 116.78 | 54.16 |
| Y56 | 9.12 | 121.85 | 57.72 |
| A57 | 7.56 | 130.70 | 48.83 |
| L58 | 7.11 | 120.04 | 54.76 |
| K59 | 7.20 | 124.48 | 53.21 |
| S60 | 8.26 | 119.34 | 58.00 |
| T61 | 8.04 | 113.50 | 62.60 |
| A62 | 8.55 | 126.68 | 52.32 |
| S63 | 7.59 | 112.18 | 56.33 |
| D64 | 9.28 | 116.05 | 54.18 |
| A65 | 7.36 | 123.30 | 53.48 |
| A66 | 9.06 | 121.55 | 51.30 |
| F67 | 8.46 | 114.69 | 55.31 |
| I68 | 8.97 | 115.40 | 61.11 |
| A69 | 10.09 | 135.37 | 50.24 |
| G70 | 9.29 | 110.80 | 43.66 |
| G71 | 8.52 | 111.54 | 46.56 |
| D72 | 9.43 | 129.27 | 54.45 |
| L73 | 8.35 | 122.94 | 54.29 |
| H74 | 8.17 | 117.28 | 54.56 |
| Y75 | 8.63 | 121.88 | 55.56 |
| T76 | 8.72 | 117.24 | 63.09 |
| L77 | | | |
| F78 | | | |
| S79 | 7.68 | 120.10 | 65.61 |
| N80 | 7.77 | 117.50 | 58.27 |
| P81 | | | 62.13 |
| S82 | 8.58 | 123.90 | 59.30 |
| H83 | 8.97 | 119.60 | 57.94 |
| T84 | 8.01 | 113.89 | 62.99 |
| L85 | 11.32 | 136.10 | 54.00 |
| W86 | 9.33 | 122.74 | 55.45 |
| G87 | 8.28 | 105.84 | 43.59 |
| K88 | 8.40 | 121.06 | 54.91 |
| L89 | 8.76 | 126.56 | 53.65 |
| D90 | 9.30 | 124.90 | 55.11 |
| S91 | 8.47 | 111.28 | 56.77 |
| I92 | 9.03 | 120.22 | 58.95 |
| A93 | 8.98 | 130.88 | 50.61 |
| L94 | 8.88 | 121.33 | 53.83 |
| G95 | 8.58 | 108.36 | 47.65 |
| D96 | 8.89 | 127.33 | 54.38 |
| T97 | 8.99 | 114.94 | 68.53 |
| L98 | 7.82 | 126.84 | 54.22 |
| T99 | 9.04 | 116.04 | 59.88 |
| G100 | 8.21 | 107.22 | 45.22 |
| G101 | 6.64 | 106.55 | 43.62 |
| A102 | 8.51 | 123.30 | 55.13 |
| S103 | | | 59.59 |

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|---|---|---|---|
| S104 | 7.34 | 114.79 | 57.66 |
| G105 | 7.89 | 109.04 | 45.37 |
| G106 | 7.59 | 107.43 | 43.93 |
| Y107 | 9.37 | 121.16 | 59.20 |
| A108 | 8.63 | 123.75 | 51.29 |
| L109 | 8.20 | 120.01 | 52.87 |
| D110 | 9.18 | 125.02 | 57.03 |
| S111 | 7.73 | 110.24 | 55.82 |
| Q112 | 8.95 | 127.87 | 56.44 |
| E113 | 8.63 | 129.79 | 58.69 |
| V114 | 7.24 | 115.61 | 60.32 |
| S115 | 8.65 | 117.68 | 56.26 |
| F116 | 9.27 | 123.25 | 56.05 |
| S117 | 9.44 | 118.16 | 57.62 |
| N118 | 8.22 | 118.08 | 53.78 |
| L119 | 8.80 | 115.18 | 57.19 |
| G120 | 8.64 | 102.73 | 47.41 |
| L121 | 7.27 | 118.36 | 54.46 |
| D122 | 8.47 | 124.40 | 54.05 |
| S123 | 9.17 | 122.68 | 55.82 |
| P124 | | | 61.80 |
| I125 | 7.63 | 125.10 | 64.41 |
| A126 | 7.28 | 119.46 | 54.11 |
| Q127 | 6.97 | 113.46 | 56.72 |
| G128 | 8.15 | 107.05 | 46.65 |
| R129 | 8.77 | 123.58 | 57.15 |
| D130 | 7.56 | 115.13 | 54.60 |
| G131 | 7.74 | 107.86 | 45.68 |
| T132 | 8.56 | 120.48 | 66.88 |
| V133 | 8.80 | 122.07 | 69.02 |
| H134 | 8.40 | 120.82 | 62.21 |
| K135 | 8.32 | 115.92 | 60.85 |
| V136 | 8.61 | 116.83 | 66.49 |
| V137 | 8.49 | 119.08 | 67.14 |
| Y138 | 9.57 | 121.19 | 61.42 |
| G139 | 7.42 | 104.90 | 48.21 |
| L140 | 7.18 | 123.04 | 58.25 |
| M141 | 7.81 | 115.92 | 59.24 |
| S142 | 7.41 | 110.61 | 57.43 |
| G143 | 7.67 | 112.50 | 46.28 |
| D144 | 8.05 | 120.93 | 52.76 |
| S145 | 8.59 | 118.63 | 57.72 |
| S146 | 8.69 | 121.41 | 63.08 |
| A147 | 8.64 | 127.01 | 55.32 |
| L148 | 8.06 | 119.86 | 58.28 |
| Q149 | 8.93 | 118.14 | 60.64 |
| G150 | 7.81 | 103.63 | 47.42 |
| Q151 | 7.50 | 119.51 | 57.43 |
| I152 | 8.41 | 118.45 | 63.88 |
| D153 | 8.19 | 118.43 | 58.98 |
| A154 | 7.15 | 117.17 | 55.23 |
| L155 | 8.01 | 119.43 | 57.88 |
| L156 | 8.51 | 120.60 | 58.02 |

| | | | |
|---|---|---|---|
| K157 | 7.88 | 118.34 | 58.37 |
| A158 | 7.25 | 118.26 | 53.63 |
| V159 | 7.48 | 120.03 | 65.45 |
| D160 | 7.72 | 118.73 | 52.34 |
| P161 | | | 64.42 |
| S162 | 8.89 | 114.95 | 59.84 |
| L163 | 8.15 | 124.41 | 53.89 |
| S164 | 8.21 | 109.67 | 58.21 |
| I165 | 8.92 | 113.33 | 62.31 |
| N166 | 8.42 | 116.53 | 53.57 |
| S167 | 7.89 | 119.38 | 60.17 |
| T168 | 8.37 | 111.26 | 59.92 |
| F169 | | | |
| D170 | | | 57.45 |
| Q171 | 8.06 | 121.72 | 59.12 |
| L172 | 8.33 | 120.69 | 57.43 |
| A173 | 8.95 | 126.47 | 54.86 |
| A174 | 8.04 | 123.98 | 54.84 |
| A175 | 7.37 | 117.20 | 52.27 |
| G176 | 7.83 | 105.34 | 45.98 |
| V177 | 7.61 | 113.90 | 62.08 |
| A178 | 6.89 | 119.57 | 48.94 |
| H179 | 8.60 | 116.22 | 55.16 |
| A180 | 8.40 | 127.56 | 50.79 |
| T181 | 8.50 | 117.80 | 59.11 |
| P182 | | | 63.08 |
| A183 | 8.22 | 125.92 | 52.46 |
| A184 | 7.84 | 128.98 | 53.79 |

**Table S2:** Backbone resonance assignments for Y75A apo-HasAp

| Residue | $^{1}H_{N}$ | $^{15}N_{H}$ | $^{13}C_{\alpha}$ |
|---|---|---|---|
| M1 | | | |
| S2 | | | 57.37 |
| I3 | 8.51 | 122.21 | 61.40 |
| S4 | 7.98 | 118.61 | 56.26 |
| I5 | 8.61 | 127.26 | 59.90 |
| S6 | 8.77 | 124.25 | 56.14 |
| Y7 | 7.87 | 119.97 | 54.59 |
| S8 | | | |
| T9 | 8.40 | 118.69 | 65.46 |
| T10 | | | |
| Y11 | | | |
| S12 | | | |
| G13 | | | 44.78 |
| W14 | 8.65 | 122.89 | 56.96 |
| T15 | 8.72 | 109.02 | 59.94 |
| V16 | 7.21 | 120.00 | 66.44 |
| A17 | 8.47 | 119.68 | 55.21 |
| D18 | 8.35 | 119.27 | 57.27 |
| Y19 | 8.78 | 122.69 | 63.37 |
| L20 | 8.72 | 119.34 | 58.24 |
| A21 | 8.12 | 119.92 | 54.84 |
| D22 | 7.80 | 122.22 | 58.44 |
| W23 | 8.68 | 119.79 | 63.59 |
| S24 | 8.72 | 114.38 | 63.60 |
| A25 | 7.84 | 125.62 | 54.64 |
| Y26 | 8.18 | 120.95 | 56.89 |
| F27 | 8.63 | 122.67 | 60.90 |
| G28 | 7.32 | 102.42 | 45.81 |
| D29 | 7.49 | 119.20 | 54.29 |
| V30 | 7.63 | 127.96 | 63.88 |
| N31 | 8.00 | 115.21 | 54.46 |
| A32 | 8.25 | 118.67 | 59.66 |
| R33 | 7.27 | 115.23 | 52.58 |
| P34 | | | 63.58 |
| G35 | 8.64 | 111.68 | 45.30 |
| Q36 | 7.90 | 118.93 | 55.21 |
| V37 | | | |
| V38 | | | |
| D39 | | | |
| G40 | 9.56 | 113.06 | 46.11 |
| S41 | | | |
| N42 | 7.91 | 121.56 | 52.37 |
| T43 | 8.39 | 114.62 | 61.93 |
| G44 | 7.90 | 109.21 | 44.45 |
| G45 | 8.23 | 108.52 | 44.02 |
| F46 | 8.62 | 116.18 | 58.47 |
| N47 | 8.68 | 116.03 | 48.83 |
| P48 | | | 65.48 |
| G49 | 7.83 | 105.74 | 45.82 |
| P50 | | | |

| | | | |
|---|---|---|---|
| F51 | | | 56.54 |
| D52 | 6.41 | 113.29 | 51.75 |
| G53 | 8.43 | 106.72 | 47.22 |
| S54 | 8.55 | 114.05 | 58.09 |
| Q55 | 7.90 | 116.65 | 53.94 |
| Y56 | 9.10 | 121.93 | 57.89 |
| A57 | 7.64 | 130.82 | 48.55 |
| L58 | 7.17 | 120.10 | 54.65 |
| K59 | | | 52.93 |
| S60 | 8.21 | 119.19 | 57.93 |
| T61 | 8.03 | 113.06 | 62.49 |
| A62 | 8.56 | 126.66 | 52.13 |
| S63 | 7.56 | 112.26 | 56.12 |
| D64 | 9.39 | 116.07 | 53.69 |
| A65 | 7.39 | 123.61 | 53.36 |
| A66 | 9.06 | 121.67 | 51.05 |
| F67 | 8.50 | 114.86 | 55.12 |
| I68 | 8.96 | 115.37 | 61.31 |
| A69 | 10.01 | 135.45 | 50.03 |
| G70 | 9.26 | 110.77 | 43.32 |
| G71 | 8.46 | 111.41 | 46.26 |
| D72 | 9.37 | 129.17 | 54.16 |
| L73 | 8.25 | 122.90 | 54.07 |
| H74 | 8.01 | 116.91 | 54.24 |
| A75 | | | |
| T76 | 8.69 | 117.23 | |
| L77 | | | |
| F78 | | | |
| S79 | 7.63 | 119.99 | 65.71 |
| N80 | 7.77 | 117.49 | 58.23 |
| P81 | | | |
| S82 | | | |
| H83 | | | |
| T84 | | | |
| L85 | | | |
| W86 | | | 55.69 |
| G87 | 8.39 | 105.87 | 43.15 |
| K88 | 8.39 | 121.08 | 54.80 |
| L89 | 8.71 | 126.58 | 53.44 |
| D90 | 9.26 | 124.86 | 54.88 |
| S91 | 8.44 | 111.32 | 56.63 |
| I92 | 9.00 | 120.11 | 58.81 |
| A93 | 8.91 | 130.75 | 50.33 |
| L94 | 8.85 | 121.18 | 53.68 |
| G95 | 8.55 | 108.27 | 47.23 |
| D96 | 8.84 | 126.86 | 54.19 |
| T97 | 8.95 | 114.43 | 68.85 |
| L98 | 7.73 | 126.65 | 53.99 |
| T99 | 9.03 | 116.09 | 59.89 |
| G100 | 8.22 | 107.19 | 44.99 |
| G101 | 6.59 | 106.53 | 43.26 |
| A102 | 8.50 | 123.35 | 55.03 |
| S103 | | | 59.50 |

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|---|---|---|---|
| S104 | 7.30 | 114.77 | 57.56 |
| G105 | 7.86 | 108.96 | 45.17 |
| G106 | 7.57 | 107.40 | 43.77 |
| Y107 | 9.35 | 121.06 | 59.08 |
| A108 | 8.62 | 123.68 | 51.05 |
| L109 | 8.19 | 119.97 | 52.66 |
| D110 | 9.11 | 124.81 | 56.92 |
| S111 | 7.72 | 110.19 | 55.66 |
| Q112 | 8.95 | 127.77 | 56.26 |
| E113 | 8.65 | 129.80 | 58.51 |
| V114 | 7.21 | 115.52 | 60.23 |
| S115 | 8.62 | 117.56 | 56.10 |
| F116 | 9.24 | 123.03 | 55.84 |
| S117 | 9.40 | 118.09 | 57.50 |
| N118 | 8.16 | 118.01 | 53.52 |
| L119 | 8.76 | 115.14 | 57.07 |
| G120 | 8.60 | 102.74 | 46.97 |
| L121 | 7.24 | 118.22 | 54.23 |
| D122 | 8.45 | 124.21 | 53.90 |
| S123 | 9.14 | 122.15 | 55.56 |
| P124 | | | 61.88 |
| I125 | 7.63 | 124.51 | 63.85 |
| A126 | | | 54.01 |
| Q127 | 6.99 | 113.38 | 56.59 |
| G128 | 7.97 | 106.82 | 46.42 |
| R129 | | | 57.12 |
| D130 | 7.62 | 115.02 | 54.54 |
| G131 | 7.65 | 107.82 | 45.45 |
| T132 | 8.53 | 120.30 | 66.85 |
| V133 | | | 69.17 |
| H134 | 8.31 | 120.56 | 62.11 |
| K135 | | | 60.82 |
| V136 | 8.50 | 116.39 | 66.60 |
| V137 | 8.47 | 119.08 | 67.38 |
| Y138 | 9.46 | 120.99 | 61.28 |
| G139 | 7.30 | 104.68 | 47.89 |
| L140 | 7.20 | 122.92 | 58.22 |
| M141 | 7.82 | 116.06 | 59.31 |
| S142 | 7.42 | 110.66 | 57.35 |
| G143 | 7.63 | 112.56 | 45.76 |
| D144 | 8.06 | 121.08 | 52.58 |
| S145 | 8.52 | 118.47 | 57.60 |
| S146 | 8.65 | 121.38 | 63.07 |
| A147 | 8.64 | 126.97 | 55.12 |
| L148 | 7.99 | 119.75 | 58.17 |
| Q149 | 8.89 | 118.07 | 60.61 |
| G150 | 7.77 | 103.57 | 46.95 |
| Q151 | 7.46 | 119.42 | 57.32 |
| I152 | 8.36 | 118.48 | 63.88 |
| D153 | 8.15 | 118.33 | 58.87 |
| A154 | 7.11 | 117.12 | 55.04 |
| L155 | 7.97 | 119.42 | 57.73 |
| L156 | 8.48 | 120.55 | 57.95 |

| | | | |
|---|---|---|---|
| K157 | 7.85 | 118.48 | 58.42 |
| A158 | 7.22 | 118.18 | 53.44 |
| V159 | 7.45 | 119.97 | 65.54 |
| D160 | 7.69 | 118.69 | 52.14 |
| P161 | | | 64.41 |
| S162 | 8.85 | 114.87 | 59.81 |
| L163 | 8.13 | 124.40 | 53.69 |
| S164 | 8.17 | 109.60 | 58.15 |
| I165 | 8.88 | 113.19 | 62.38 |
| N166 | 8.39 | 116.34 | 53.40 |
| S167 | 7.86 | 119.40 | 60.19 |
| T168 | 8.35 | 111.24 | 59.94 |
| F169 | | | |
| D170 | | | 57.37 |
| Q171 | 8.03 | 121.64 | 59.08 |
| L172 | 8.30 | 120.57 | 57.35 |
| A173 | 8.94 | 126.50 | 54.66 |
| A174 | 8.01 | 123.96 | 54.76 |
| A175 | 7.37 | 117.26 | 52.11 |
| G176 | 7.79 | 105.35 | 45.42 |
| V177 | 7.60 | 113.92 | 62.06 |
| A178 | 6.86 | 119.49 | 48.61 |
| H179 | 8.55 | 116.09 | 54.99 |
| A180 | 8.37 | 127.47 | 50.60 |
| T181 | 8.49 | 117.56 | 58.98 |
| P182 | | | 63.10 |
| A183 | 8.20 | 125.92 | 52.29 |
| A184 | 7.82 | 129.01 | 53.58 |

**Table S3.** Backbone resonance assignments for H83A apo-HasAp

| Residue | $^{1}H_{N}$ | $^{15}N_{H}$ | $^{13}C_{\alpha}$ |
|---|---|---|---|
| M1 | | | |
| S2 | | | 57.37 |
| I3 | 8.50 | 122.11 | 61.43 |
| S4 | 8.00 | 118.62 | 56.28 |
| I5 | 8.64 | 127.00 | 59.92 |
| S6 | 8.79 | 124.24 | 56.19 |
| Y7 | 7.87 | 119.99 | 54.66 |
| S8 | | | |
| T9 | 8.45 | 118.76 | |
| T10 | | | |
| Y11 | | | |
| S12 | | | |
| G13 | | | 44.78 |
| W14 | 8.66 | 122.79 | 56.88 |
| T15 | 8.73 | 109.02 | 59.89 |
| V16 | 7.22 | 120.03 | 66.39 |
| A17 | 8.48 | 119.69 | 55.18 |
| D18 | 8.36 | 119.46 | 57.22 |
| Y19 | 8.79 | 122.70 | 63.30 |
| L20 | 8.73 | 119.37 | 58.21 |
| A21 | 8.13 | 119.92 | 54.85 |
| D22 | 7.81 | 122.21 | 58.47 |
| W23 | 8.70 | 119.79 | 63.57 |
| S24 | 8.76 | 114.43 | 63.58 |
| A25 | 7.85 | 125.60 | 54.60 |
| Y26 | 8.19 | 121.00 | 56.83 |
| F27 | 8.64 | 122.77 | 60.92 |
| G28 | 7.31 | 102.41 | 45.82 |
| D29 | 7.48 | 119.28 | 54.29 |
| V30 | 7.62 | 127.99 | 63.84 |
| N31 | 7.99 | 115.13 | 54.53 |
| A32 | 8.26 | 118.51 | 59.63 |
| R33 | 7.26 | 115.40 | 52.66 |
| P34 | | | 63.58 |
| G35 | 8.64 | 111.77 | 45.29 |
| Q36 | 7.90 | 118.85 | 55.12 |
| V37 | 8.41 | 117.53 | 59.92 |
| V38 | 8.37 | 124.22 | 61.57 |
| D39 | 10.75 | 131.59 | 53.68 |
| G40 | 9.61 | 113.19 | 46.12 |
| S41 | | | |
| N42 | 7.87 | 121.58 | 52.34 |
| T43 | 8.45 | 114.50 | 61.88 |
| G44 | 7.97 | 109.41 | 44.48 |
| G45 | 8.19 | 108.64 | 44.15 |
| F46 | 8.94 | 116.17 | 58.21 |
| N47 | 8.69 | 116.21 | 48.79 |
| P48 | | | 65.56 |
| G49 | 7.88 | 105.83 | 45.84 |
| P50 | | | 64.30 |

| | | | |
|---|---|---|---|
| F51 | 8.72 | 116.67 | 56.73 |
| D52 | 6.50 | 113.12 | 52.02 |
| G53 | 8.56 | 106.71 | 47.25 |
| S54 | 8.61 | 114.21 | 58.14 |
| Q55 | 7.95 | 116.68 | 54.01 |
| Y56 | 9.08 | 121.71 | 57.41 |
| A57 | 7.70 | 130.70 | 48.44 |
| L58 | 7.19 | 120.26 | 54.59 |
| K59 | | | 52.94 |
| S60 | 8.20 | 119.12 | 57.86 |
| T61 | 8.03 | 113.03 | 62.49 |
| A62 | 8.54 | 126.67 | 52.13 |
| S63 | 7.56 | 112.20 | 56.19 |
| D64 | 9.34 | 116.16 | 53.72 |
| A65 | 7.38 | 123.53 | 53.40 |
| A66 | 9.05 | 121.71 | 51.04 |
| F67 | 8.51 | 115.02 | 55.13 |
| I68 | 8.96 | 115.41 | 61.16 |
| A69 | 10.06 | 135.45 | 50.04 |
| G70 | 9.26 | 110.75 | 43.32 |
| G71 | 8.51 | 111.56 | 46.36 |
| D72 | 9.41 | 129.29 | 54.29 |
| L73 | 8.39 | 123.49 | 54.01 |
| H74 | 8.10 | 117.01 | 54.37 |
| Y75 | | | |
| T76 | | | |
| L77 | | | |
| F78 | | | |
| S79 | 7.66 | 119.98 | 65.80 |
| N80 | 7.77 | 117.46 | 58.22 |
| P81 | | | |
| S82 | | | |
| A83 | | | |
| T84 | | | |
| L85 | | | |
| W86 | | | 55.43 |
| G87 | 8.30 | 105.87 | 43.05 |
| K88 | 8.41 | 120.99 | 54.82 |
| L89 | 8.73 | 126.36 | 53.44 |
| D90 | 9.30 | 124.84 | 54.85 |
| S91 | 8.44 | 111.25 | 56.62 |
| I92 | 9.00 | 120.10 | 58.81 |
| A93 | 8.92 | 130.80 | 50.34 |
| L94 | 8.87 | 121.23 | 53.71 |
| G95 | 8.59 | 108.31 | 47.24 |
| D96 | 8.85 | 127.04 | 54.28 |
| T97 | 8.95 | 114.54 | 68.90 |
| L98 | 7.85 | 126.83 | |
| T99 | 9.02 | 115.79 | 59.88 |
| G100 | 8.20 | 107.18 | 45.00 |
| G101 | 6.58 | 106.42 | 43.30 |
| A102 | 8.56 | 122.88 | 55.00 |
| S103 | | | 59.49 |

| | | | |
|---|---|---|---|
| S104 | 7.30 | 114.74 | 57.44 |
| G105 | 7.87 | 108.94 | 45.26 |
| G106 | 7.57 | 107.39 | 43.83 |
| Y107 | 9.33 | 121.00 | 59.06 |
| A108 | 8.61 | 123.69 | 51.05 |
| L109 | 8.19 | 119.96 | 52.61 |
| D110 | 9.11 | 124.82 | 56.84 |
| S111 | 7.72 | 110.21 | 55.68 |
| Q112 | 8.95 | 127.77 | 56.26 |
| E113 | 8.65 | 129.79 | 58.49 |
| V114 | 7.22 | 115.55 | 60.20 |
| S115 | 8.63 | 117.58 | 56.00 |
| F116 | 9.25 | 123.12 | 55.72 |
| S117 | 9.41 | 118.14 | 57.53 |
| N118 | 8.20 | 118.04 | 53.46 |
| L119 | 8.78 | 115.11 | 57.08 |
| G120 | 8.62 | 102.71 | 46.96 |
| L121 | 7.25 | 118.18 | 54.27 |
| D122 | 8.46 | 124.36 | 53.96 |
| S123 | 9.15 | 122.36 | 55.68 |
| P124 | | | |
| I125 | 7.61 | 124.73 | 64.07 |
| A126 | 7.40 | 120.09 | |
| Q127 | 6.94 | 113.38 | 56.55 |
| G128 | 8.08 | 107.06 | 46.40 |
| R129 | | | |
| D130 | | | 54.56 |
| G131 | 7.69 | 107.94 | 45.46 |
| T132 | 8.54 | 120.50 | 66.93 |
| V133 | 8.75 | 121.88 | 69.16 |
| H134 | 8.36 | 120.69 | 62.16 |
| K135 | 8.26 | 115.76 | 60.89 |
| V136 | 8.55 | 116.52 | 66.62 |
| V137 | 8.45 | 119.14 | 67.24 |
| Y138 | 9.54 | 121.13 | 61.33 |
| G139 | 7.38 | 104.83 | 47.88 |
| L140 | 7.18 | 122.89 | 58.17 |
| M141 | 7.84 | 116.24 | 59.30 |
| S142 | 7.37 | 110.31 | 57.34 |
| G143 | 7.65 | 112.53 | 45.69 |
| D144 | 8.05 | 121.07 | 52.59 |
| S145 | 8.53 | 118.60 | 57.61 |
| S146 | 8.66 | 121.43 | 63.08 |
| A147 | 8.64 | 126.98 | 55.15 |
| L148 | 8.05 | 119.82 | 58.18 |
| Q149 | 8.89 | 118.12 | 60.60 |
| G150 | 7.78 | 103.62 | 46.95 |
| Q151 | 7.48 | 119.56 | 57.35 |
| I152 | 8.38 | 118.52 | 63.88 |
| D153 | 8.15 | 118.32 | 58.93 |
| A154 | 7.13 | 117.17 | 55.09 |
| L155 | 7.99 | 119.40 | 57.72 |
| L156 | 8.48 | 120.60 | 57.93 |

| | | | |
|---|---|---|---|
| K157 | 7.86 | 118.53 | 58.37 |
| A158 | 7.23 | 118.19 | 53.46 |
| V159 | 7.46 | 120.01 | 65.53 |
| D160 | 7.70 | 118.72 | 52.15 |
| P161 | | | 64.41 |
| S162 | 8.86 | 114.94 | 59.82 |
| L163 | 8.13 | 124.45 | 53.71 |
| S164 | 8.19 | 109.61 | 58.14 |
| I165 | 8.89 | 113.17 | 62.34 |
| N166 | 8.40 | 116.47 | 53.39 |
| S167 | 7.87 | 119.38 | 60.17 |
| T168 | 8.36 | 111.29 | 59.92 |
| F169 | | | |
| D170 | | | 57.36 |
| Q171 | 8.04 | 121.70 | 59.07 |
| L172 | 8.31 | 120.50 | 57.33 |
| A173 | 8.92 | 126.44 | 54.61 |
| A174 | 8.02 | 123.99 | 54.68 |
| A175 | 7.34 | 117.17 | 52.06 |
| G176 | 7.80 | 105.39 | 45.41 |
| V177 | 7.58 | 113.91 | 62.11 |
| A178 | 6.87 | 119.52 | 48.62 |
| H179 | 8.57 | 116.03 | 54.96 |
| A180 | 8.39 | 127.58 | 50.57 |
| T181 | 8.49 | 117.62 | 59.02 |
| P182 | | | 63.11 |
| A183 | 8.21 | 125.93 | 52.31 |
| A184 | 7.83 | 128.98 | 53.65 |

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