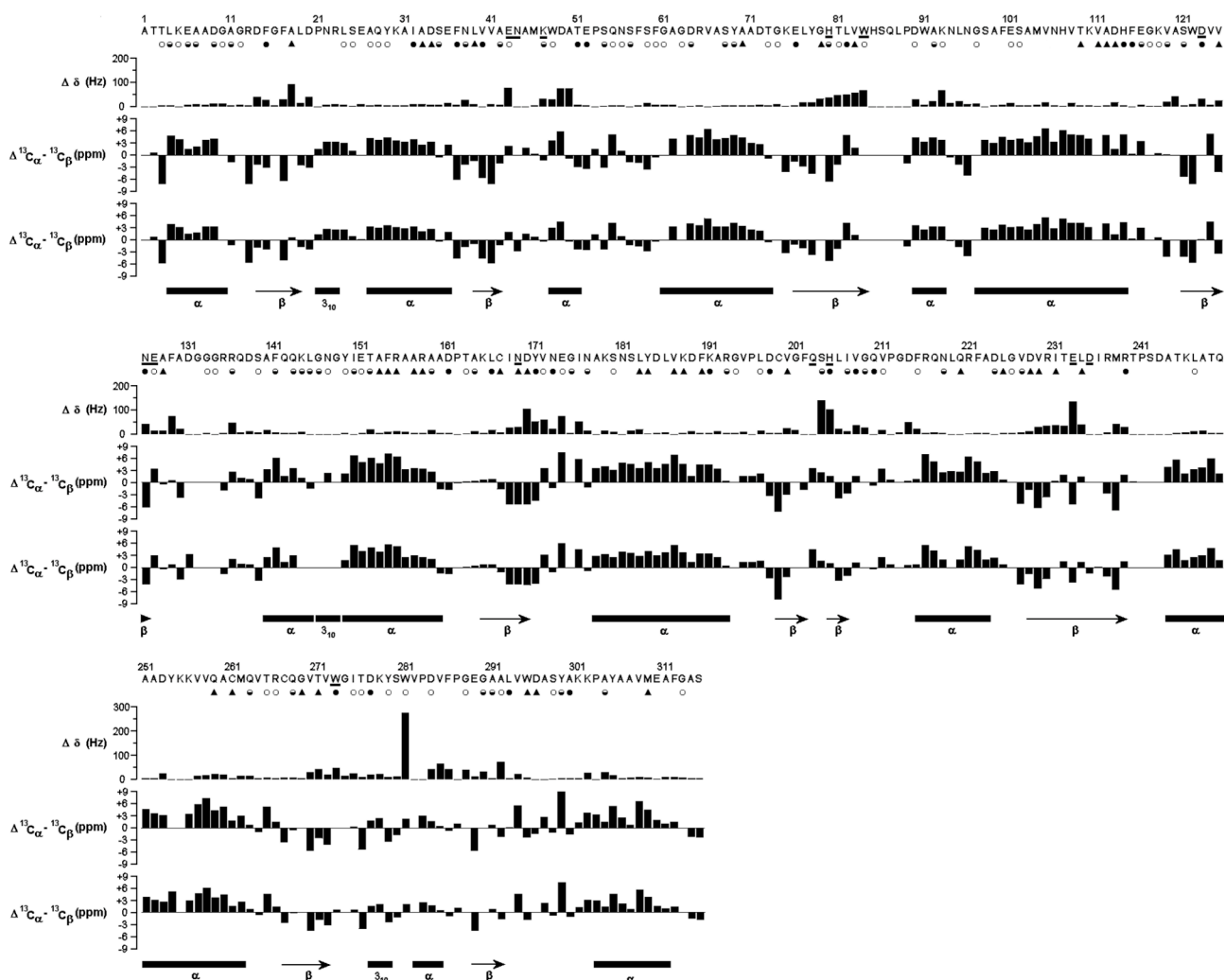


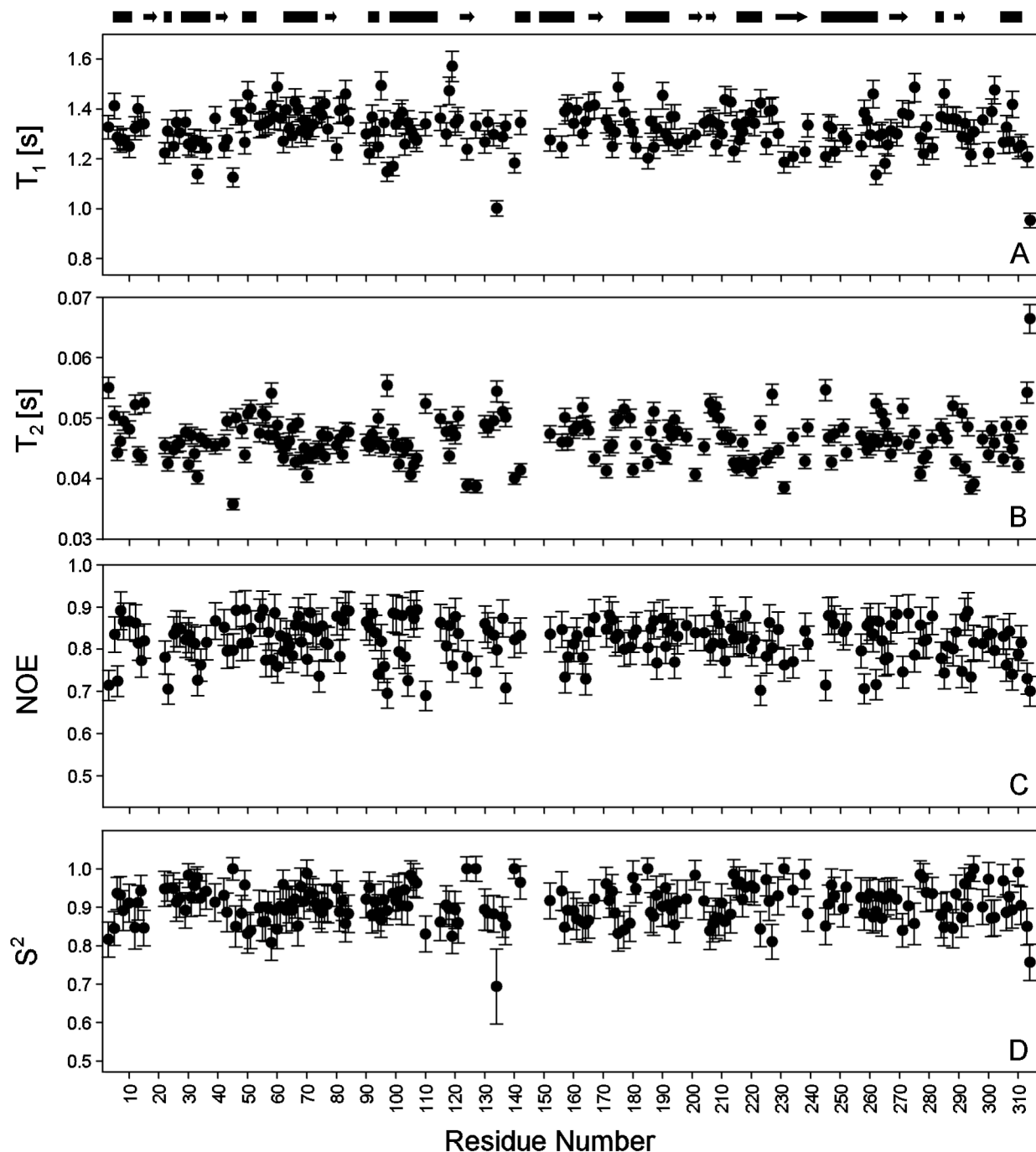
**NMR Spectroscopic Characterization of a β -(1,4)-Glycosidase along
its Reaction Pathway: Stabilization upon Formation of the
Glycosyl-Enzyme Intermediate**

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SUPPLEMENTAL FIGURE S1: Row 1: The sequence of CexCD with the active site residues underlined. Row 2: Summary of the amide proton-deuterium HX kinetics of apo-CexCD, with open circles indicating $t_{1/2} < 100$ min, half-filled circles indicating $100 \text{ min} < t_{1/2} < 65$ hrs, and filled circles indicating $t_{1/2} > 65$ hours at 30°C ; filled triangles identify amides protonated $> 70\%$ after 500 days of storage at 4°C . Row 3: Amide $^1\text{H}^{\text{N}}$ and ^{15}N chemical shift perturbations, due to the formation of the glycosyl-enzyme intermediate, are localized to the active site of the catalytic domain. Data are calculated as $[(\Delta\omega_{\text{H}})^2 + (\Delta\omega_{\text{N}})^2]^{1/2}$ at 600 MHz for apo- versus 2FCb-CexCD. Patterns of ($^{13}\text{C}^{\alpha}$ - $^{13}\text{C}^{\beta}$) chemical shift differences for apo- (Row 4) and 2FCb-CexCD (Row 5), relative to the values expected for a random coil polypeptide, are consistent with the secondary structure of CexCD determined by X-ray crystallography (Row 6 from PDB file 2EXO). Note that α -helices/ β -strands have positive and negative ($^{13}\text{C}^{\alpha}$ - $^{13}\text{C}^{\beta}$) shift differences, respectively. This measure of secondary structure also approximately compensates for ^2H isotope effects on the $^{13}\text{C}^{\alpha}$ and $^{13}\text{C}^{\beta}$ chemical shifts of an amino acid. Missing data correspond to prolines and residues with overlapped or unassigned NMR signals.



SUPPLEMENTAL FIGURE S2: Plots of the measured ^{15}N T_1 (A), T_2 (B), and heteronuclear ^1H - ^{15}N NOE (C) relaxation parameters and the fit anisotropic model free order parameters S^2 (D) as a function of residue number for 2FCb-CexCD. The secondary structural elements derived from the crystal structure of this protein (PDB: 1EXP) are shown, with bars/arrows representing α -helices/ β -strands. Missing data points correspond to prolines and residues with overlapped or unassigned NMR signals. The corresponding plots for apo-CexCD are shown in Figure 2, and the data for both proteins are provided in Supplemental Tables S1 and S2.

SUPPLEMENTAL TABLE S1: List of the measured ^{15}N T_1 , T_2 , and heteronuclear ^1H - ^{15}N NOE relaxation parameters and the fit anisotropic model free order parameters S^2 for apo-CexCD (recorded with a Varian 600 MHz NMR spectrometer at pH 6.5 and 30 °C). Missing data correspond to prolines and residues with overlapped or unassigned NMR signals. The anisotropic diffusion tensor for apo-CexCD was determined to $D_{ZZ} = 1.18 (\pm 0.02) \times 10^7 \text{ s}^{-1}$, $D_{YY} = 0.97 (\pm 0.02) \times 10^7 \text{ s}^{-1}$, and $D_{XX} = 0.94 (\pm 0.01) \times 10^7 \text{ s}^{-1}$ using the X-ray crystallographic co-ordinate file 2EXO.pdb.

<u>Residue</u>	<u>T_1 (sec)</u>	<u>T_2 (sec)</u>	<u>NOE</u>	<u>S^2</u>
A1				
T2				
T3	1.22 \pm 0.04	0.058 \pm 0.002	0.71 \pm 0.04	0.82 \pm 0.05
L4				
K5	1.31 \pm 0.05	0.051 \pm 0.001	0.76 \pm 0.04	0.87 \pm 0.05
E6	1.27 \pm 0.04	0.047 \pm 0.001	0.86 \pm 0.04	0.92 \pm 0.04
A7				
A8	1.23 \pm 0.04	0.052 \pm 0.001	0.88 \pm 0.04	0.89 \pm 0.05
D9	1.22 \pm 0.04	0.048 \pm 0.001	0.80 \pm 0.04	0.92 \pm 0.05
G10	1.21 \pm 0.04	0.050 \pm 0.001	0.87 \pm 0.04	0.90 \pm 0.04
A11	1.26 \pm 0.04	0.052 \pm 0.001	0.84 \pm 0.04	0.87 \pm 0.05
G12	1.30 \pm 0.04	0.054 \pm 0.002	0.82 \pm 0.04	0.84 \pm 0.04
R13	1.39 \pm 0.05	0.046 \pm 0.001	0.87 \pm 0.04	0.90 \pm 0.05
D14	1.29 \pm 0.04	0.049 \pm 0.001	0.83 \pm 0.04	0.90 \pm 0.05
F15	1.26 \pm 0.04	0.053 \pm 0.002	0.83 \pm 0.04	0.87 \pm 0.05
G16				
F17				
A18	1.38 \pm 0.05	0.045 \pm 0.001	0.69 \pm 0.03	0.80 \pm 0.07
L19				
D20				
P21				
N22	1.08 \pm 0.04	0.048 \pm 0.001	0.72 \pm 0.04	0.93 \pm 0.03
R23	1.34 \pm 0.05	0.044 \pm 0.001	0.89 \pm 0.04	0.94 \pm 0.04
L24				
S25	1.30 \pm 0.05	0.045 \pm 0.001	0.74 \pm 0.04	0.93 \pm 0.04
E26	1.31 \pm 0.04	0.052 \pm 0.001	0.74 \pm 0.04	0.86 \pm 0.05
A27				
Q28	1.17 \pm 0.04	0.046 \pm 0.001	0.78 \pm 0.04	0.97 \pm 0.04
Y29	1.29 \pm 0.05	0.046 \pm 0.001	0.73 \pm 0.04	0.92 \pm 0.04
K30	1.21 \pm 0.04	0.045 \pm 0.001	0.84 \pm 0.04	0.97 \pm 0.04
A31	1.21 \pm 0.04	0.047 \pm 0.001	0.86 \pm 0.04	0.95 \pm 0.04
I32	1.23 \pm 0.04	0.049 \pm 0.001	0.86 \pm 0.04	0.92 \pm 0.05
A33				
D34	1.24 \pm 0.04	0.053 \pm 0.002	0.74 \pm 0.04	0.86 \pm 0.05
S35				
E36	1.23 \pm 0.04	0.046 \pm 0.001	0.85 \pm 0.04	0.95 \pm 0.04
F37	1.29 \pm 0.04	0.054 \pm 0.002	0.87 \pm 0.04	0.85 \pm 0.05
N38	1.26 \pm 0.04	0.049 \pm 0.001	0.88 \pm 0.04	0.91 \pm 0.04
L39				
V40	1.22 \pm 0.04	0.045 \pm 0.001	0.86 \pm 0.04	0.96 \pm 0.04
V41				
A42				
E43				
N44				
A45				

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M46	1.34 ± 0.05	0.049 ± 0.001	0.83 ± 0.04	0.88 ± 0.04
K47	1.33 ± 0.05	0.048 ± 0.001	0.79 ± 0.04	0.89 ± 0.05
W48	1.33 ± 0.05	0.047 ± 0.001	0.84 ± 0.04	0.92 ± 0.05
W48-Indole	1.60 ± 0.11	0.057 ± 0.002	0.75 ± 0.04	0.86 ± 0.01
D49	1.22 ± 0.04	0.042 ± 0.001	0.86 ± 0.04	1.00 ± 0.03
A50				
T51	1.30 ± 0.04	0.053 ± 0.001	0.80 ± 0.04	0.86 ± 0.05
E52	1.25 ± 0.04	0.050 ± 0.001	0.82 ± 0.04	0.90 ± 0.05
P53				
S54	1.26 ± 0.04	0.052 ± 0.002	0.83 ± 0.04	0.88 ± 0.05
Q55	1.30 ± 0.05	0.052 ± 0.001	0.79 ± 0.04	0.87 ± 0.05
N56	1.28 ± 0.04	0.050 ± 0.001	0.81 ± 0.04	0.89 ± 0.05
S57	1.27 ± 0.04	0.050 ± 0.001	0.83 ± 0.04	0.90 ± 0.04
F58	1.39 ± 0.05	0.056 ± 0.002	0.76 ± 0.04	0.80 ± 0.05
S59	1.31 ± 0.04	0.052 ± 0.001	0.78 ± 0.04	0.86 ± 0.05
F60	1.35 ± 0.05	0.049 ± 0.001	0.82 ± 0.04	0.88 ± 0.05
G61	1.31 ± 0.05	0.046 ± 0.001	0.80 ± 0.04	0.93 ± 0.05
A62				
G63	1.35 ± 0.05	0.048 ± 0.001	0.81 ± 0.04	0.88 ± 0.05
D64	1.32 ± 0.05	0.047 ± 0.001	0.82 ± 0.04	0.91 ± 0.05
R65	1.26 ± 0.04	0.045 ± 0.001	0.84 ± 0.04	0.95 ± 0.04
V66				
A67				
S68	1.28 ± 0.04	0.046 ± 0.001	0.81 ± 0.04	0.94 ± 0.05
Y69	1.28 ± 0.04	0.044 ± 0.001	0.86 ± 0.04	0.96 ± 0.04
A70				
A71	1.33 ± 0.05	0.047 ± 0.001	0.85 ± 0.04	0.90 ± 0.04
D72	1.32 ± 0.05	0.047 ± 0.001	0.82 ± 0.04	0.91 ± 0.05
T73	1.40 ± 0.05	0.047 ± 0.001	0.86 ± 0.04	0.89 ± 0.05
G74	1.37 ± 0.05	0.050 ± 0.001	0.73 ± 0.04	0.85 ± 0.05
K75	1.33 ± 0.05	0.049 ± 0.001	0.86 ± 0.04	0.88 ± 0.04
E76	1.39 ± 0.05	0.046 ± 0.001	0.83 ± 0.04	0.90 ± 0.05
L77	1.29 ± 0.04	0.054 ± 0.002	0.76 ± 0.04	0.84 ± 0.05
Y78	1.23 ± 0.04	0.042 ± 0.001	0.72 ± 0.04	0.97 ± 0.03
G79				
H80	1.29 ± 0.04	0.048 ± 0.001	0.84 ± 0.04	0.91 ± 0.04
T81	1.35 ± 0.05	0.043 ± 0.001	0.86 ± 0.04	0.95 ± 0.04
L82				
V83	1.40 ± 0.05	0.046 ± 0.001	0.84 ± 0.04	0.90 ± 0.05
W84	1.36 ± 0.05	0.048 ± 0.001	0.83 ± 0.04	0.89 ± 0.04
W84-Indole	1.52 ± 0.19	0.053 ± 0.004	0.77 ± 0.04	0.92 ± 0.03
H85				
S86				
Q87				
L88				
P89				
D90	1.31 ± 0.04	0.050 ± 0.001	0.85 ± 0.04	0.88 ± 0.05
W91	1.22 ± 0.04	0.048 ± 0.001	0.82 ± 0.04	0.92 ± 0.04
W91-Indole	1.56 ± 0.12	0.051 ± 0.002	0.81 ± 0.04	0.92 ± 0.02
A92	1.31 ± 0.04	0.048 ± 0.001	0.75 ± 0.04	0.90 ± 0.05
K93	1.24 ± 0.04	0.049 ± 0.001	0.85 ± 0.04	0.90 ± 0.05
N94	1.21 ± 0.04	0.054 ± 0.002	0.78 ± 0.04	0.86 ± 0.04
L95				
N96	1.29 ± 0.04	0.050 ± 0.001	0.73 ± 0.04	0.87 ± 0.04
G97	1.17 ± 0.04	0.059 ± 0.002	0.69 ± 0.03	0.82 ± 0.05
S98				
A99	1.20 ± 0.04	0.051 ± 0.001	0.82 ± 0.04	0.89 ± 0.05

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F100				
E101	1.29 ± 0.04	0.044 ± 0.001	0.83 ± 0.04	0.95 ± 0.04
S102	1.31 ± 0.05	0.046 ± 0.001	0.89 ± 0.04	0.92 ± 0.05
A103				
M104	1.32 ± 0.05	0.046 ± 0.001	0.87 ± 0.04	0.92 ± 0.05
V105				
N106	1.26 ± 0.04	0.045 ± 0.001	0.87 ± 0.04	0.95 ± 0.04
H107				
V108				
T109				
K110				
V111				
A112				
D113	1.31 ± 0.05	0.043 ± 0.001	0.82 ± 0.04	0.96 ± 0.04
H114	1.28 ± 0.04	0.046 ± 0.001	0.74 ± 0.04	0.93 ± 0.04
F115	1.31 ± 0.04	0.050 ± 0.001	0.84 ± 0.04	0.88 ± 0.04
E116	1.37 ± 0.05	0.045 ± 0.001	0.82 ± 0.04	0.91 ± 0.05
G117	1.29 ± 0.04	0.051 ± 0.001	0.84 ± 0.04	0.88 ± 0.05
K118				
V119				
A120	1.32 ± 0.05	0.046 ± 0.001	0.84 ± 0.04	0.91 ± 0.05
S121	1.34 ± 0.05	0.056 ± 0.002	0.82 ± 0.04	0.82 ± 0.05
W122				
W122-Indole	1.42 ± 0.07	0.054 ± 0.005	0.82 ± 0.04	0.93 ± 0.02
D123	1.39 ± 0.05	0.051 ± 0.001	0.87 ± 0.04	0.85 ± 0.05
V124				
V125				
N126				
E127				
A128	1.26 ± 0.04	0.045 ± 0.001	0.75 ± 0.04	0.95 ± 0.04
F129	1.28 ± 0.04	0.044 ± 0.001	0.85 ± 0.04	0.96 ± 0.04
A130	1.28 ± 0.05	0.047 ± 0.001	0.77 ± 0.04	0.92 ± 0.05
D131				
G132				
G133	1.22 ± 0.04	0.050 ± 0.001	0.79 ± 0.04	0.90 ± 0.05
G134	1.00 ± 0.03	0.058 ± 0.002	0.87 ± 0.04	0.70 ± 0.10
R135	1.27 ± 0.04	0.048 ± 0.001	0.84 ± 0.04	0.91 ± 0.05
R136	1.21 ± 0.04	0.053 ± 0.002	0.82 ± 0.04	0.88 ± 0.05
Q137	1.31 ± 0.05	0.051 ± 0.001	0.76 ± 0.04	0.86 ± 0.04
D138	1.21 ± 0.04	0.047 ± 0.001	0.75 ± 0.04	0.92 ± 0.04
S139				
A140	1.18 ± 0.04	0.043 ± 0.001	0.74 ± 0.04	0.98 ± 0.03
F141	1.36 ± 0.05	0.045 ± 0.001	0.84 ± 0.04	0.91 ± 0.05
Q142	1.40 ± 0.05	0.045 ± 0.001	0.78 ± 0.04	0.91 ± 0.05
Q143	1.29 ± 0.04	0.043 ± 0.001	0.85 ± 0.04	0.97 ± 0.04
K144				
L145	1.25 ± 0.04	0.045 ± 0.001	0.79 ± 0.04	0.95 ± 0.04
G146	1.30 ± 0.05	0.051 ± 0.001	0.89 ± 0.04	0.88 ± 0.05
N147				
G148				
Y149	1.14 ± 0.04	0.046 ± 0.001	0.83 ± 0.04	0.98 ± 0.04
I150	1.18 ± 0.04	0.045 ± 0.001	0.82 ± 0.04	0.99 ± 0.03
E151	1.22 ± 0.04	0.051 ± 0.001	0.80 ± 0.04	0.90 ± 0.05
T152				
A153	1.06 ± 0.03	0.049 ± 0.001	0.88 ± 0.04	0.98 ± 0.04
F154	1.26 ± 0.04	0.043 ± 0.001	0.79 ± 0.04	0.98 ± 0.04
R155	1.26 ± 0.04	0.048 ± 0.001	0.82 ± 0.04	0.92 ± 0.05

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A156	1.19 ± 0.04	0.048 ± 0.001	0.89 ± 0.04	0.95 ± 0.04
A157	1.15 ± 0.04	0.053 ± 0.002	0.80 ± 0.04	0.91 ± 0.05
R158	1.24 ± 0.04	0.048 ± 0.001	0.75 ± 0.04	0.93 ± 0.05
A159				
A160				
D161	1.35 ± 0.05	0.050 ± 0.001	0.77 ± 0.04	0.87 ± 0.04
P162				
T163	1.27 ± 0.04	0.056 ± 0.002	0.76 ± 0.04	0.83 ± 0.05
A164	1.35 ± 0.05	0.052 ± 0.001	0.81 ± 0.04	0.84 ± 0.05
K165	1.33 ± 0.05	0.049 ± 0.001	0.89 ± 0.04	0.88 ± 0.05
L166	1.31 ± 0.05	0.052 ± 0.001	0.81 ± 0.04	0.86 ± 0.04
C167				
I168	1.13 ± 0.04	0.047 ± 0.001	0.74 ± 0.04	0.97 ± 0.04
N169				
D170				
Y171				
N172	1.28 ± 0.04	0.046 ± 0.001	0.80 ± 0.04	0.93 ± 0.05
V173	1.28 ± 0.04	0.047 ± 0.001	0.84 ± 0.04	0.92 ± 0.05
E174	1.26 ± 0.04	0.061 ± 0.002	0.71 ± 0.04	0.79 ± 0.05
G175	1.34 ± 0.05	0.054 ± 0.002	0.86 ± 0.04	0.83 ± 0.05
I176				
N177	1.34 ± 0.05	0.054 ± 0.002	0.77 ± 0.04	0.83 ± 0.04
A178				
K179	1.31 ± 0.05	0.047 ± 0.001	0.81 ± 0.04	0.90 ± 0.05
S180	1.23 ± 0.04	0.046 ± 0.001	0.80 ± 0.04	0.95 ± 0.05
N181	1.18 ± 0.04	0.050 ± 0.001	0.85 ± 0.04	0.93 ± 0.05
S182				
L183				
Y184	1.15 ± 0.04	0.046 ± 0.001	0.73 ± 0.04	0.97 ± 0.03
D185	1.21 ± 0.04	0.044 ± 0.001	0.77 ± 0.04	0.98 ± 0.03
L186	1.30 ± 0.04	0.050 ± 0.001	0.88 ± 0.04	0.89 ± 0.05
V187	1.17 ± 0.04	0.048 ± 0.001	0.80 ± 0.04	0.95 ± 0.05
K188	1.17 ± 0.04	0.046 ± 0.001	0.87 ± 0.04	0.97 ± 0.04
D189				
F190	1.28 ± 0.04	0.047 ± 0.001	0.80 ± 0.04	0.93 ± 0.04
K191	1.28 ± 0.04	0.048 ± 0.001	0.85 ± 0.04	0.91 ± 0.04
A192	1.20 ± 0.04	0.053 ± 0.002	0.87 ± 0.04	0.88 ± 0.05
R193	1.36 ± 0.05	0.052 ± 0.001	0.77 ± 0.04	0.85 ± 0.05
G194				
V195				
P196				
L197				
D198	1.25 ± 0.04	0.052 ± 0.001	0.81 ± 0.04	0.88 ± 0.05
C199				
V200				
G201	1.18 ± 0.04	0.042 ± 0.001	0.73 ± 0.04	0.98 ± 0.03
F202				
Q203				
S204	1.34 ± 0.05	0.044 ± 0.001	0.87 ± 0.04	0.93 ± 0.04
H205				
L206	1.39 ± 0.05	0.053 ± 0.002	0.76 ± 0.04	0.83 ± 0.05
I207	1.29 ± 0.04	0.054 ± 0.002	0.82 ± 0.04	0.85 ± 0.05
V208				
G209	1.32 ± 0.05	0.052 ± 0.001	0.80 ± 0.04	0.86 ± 0.05
Q210	1.24 ± 0.04	0.052 ± 0.001	0.77 ± 0.04	0.89 ± 0.05
V211	1.40 ± 0.05	0.048 ± 0.001	0.81 ± 0.04	0.87 ± 0.05
P212				

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G213	1.32 ± 0.05	0.048 ± 0.001	0.86 ± 0.04	0.90 ± 0.05
D214	1.12 ± 0.04	0.047 ± 0.001	0.82 ± 0.04	0.98 ± 0.04
F215	1.29 ± 0.04	0.046 ± 0.001	0.84 ± 0.04	0.93 ± 0.04
R216	1.23 ± 0.04	0.044 ± 0.001	0.85 ± 0.04	0.96 ± 0.04
Q217	1.31 ± 0.05	0.048 ± 0.001	0.80 ± 0.04	0.91 ± 0.05
N218	1.28 ± 0.04	0.045 ± 0.001	0.84 ± 0.04	0.95 ± 0.05
L219				
Q220	1.32 ± 0.05	0.042 ± 0.001	0.80 ± 0.04	0.97 ± 0.04
R221	1.20 ± 0.04	0.043 ± 0.001	0.85 ± 0.04	1.00 ± 0.03
F222	1.32 ± 0.04	0.042 ± 0.001	0.82 ± 0.04	0.96 ± 0.04
A223	1.25 ± 0.04	0.052 ± 0.002	0.88 ± 0.04	0.86 ± 0.05
D224	1.23 ± 0.04	0.044 ± 0.001	0.84 ± 0.04	0.98 ± 0.03
L225	1.28 ± 0.04	0.048 ± 0.001	0.85 ± 0.04	0.91 ± 0.04
G226	1.38 ± 0.05	0.048 ± 0.001	0.81 ± 0.04	0.88 ± 0.05
V227	1.32 ± 0.05	0.052 ± 0.001	0.84 ± 0.04	0.85 ± 0.05
D228				
V229				
R230	1.12 ± 0.04	0.041 ± 0.001	0.87 ± 0.04	1.00 ± 0.03
I231	1.17 ± 0.04	0.049 ± 0.001	0.84 ± 0.04	0.93 ± 0.04
T232	1.18 ± 0.04	0.039 ± 0.001	0.84 ± 0.04	1.00 ± 0.03
E233				
L234				
D235				
I236				
R237				
M238	1.17 ± 0.04	0.047 ± 0.001	0.88 ± 0.04	0.96 ± 0.04
R239	1.26 ± 0.04	0.050 ± 0.001	0.79 ± 0.04	0.89 ± 0.05
T240	1.38 ± 0.05	0.047 ± 0.001	0.86 ± 0.04	0.89 ± 0.05
P241				
S242				
D243				
A244				
T245				
K246	1.23 ± 0.04	0.052 ± 0.001	0.80 ± 0.04	0.88 ± 0.05
L247	1.25 ± 0.04	0.047 ± 0.001	0.84 ± 0.04	0.93 ± 0.05
A248	1.19 ± 0.04	0.048 ± 0.001	0.74 ± 0.04	0.94 ± 0.04
T249	1.22 ± 0.04	0.048 ± 0.001	0.85 ± 0.04	0.94 ± 0.04
Q250	1.28 ± 0.04	0.045 ± 0.001	0.85 ± 0.04	0.94 ± 0.05
A251				
A252	1.26 ± 0.04	0.048 ± 0.001	0.87 ± 0.04	0.91 ± 0.05
D253	1.24 ± 0.04	0.047 ± 0.001	0.78 ± 0.04	0.94 ± 0.05
Y254				
K255				
K256				
V257	1.25 ± 0.04	0.049 ± 0.001	0.88 ± 0.04	0.91 ± 0.04
V258				
Q259	1.22 ± 0.04	0.048 ± 0.001	0.83 ± 0.04	0.93 ± 0.05
A260	1.23 ± 0.04	0.048 ± 0.001	0.84 ± 0.04	0.93 ± 0.04
C261	1.25 ± 0.04	0.055 ± 0.002	0.84 ± 0.04	0.85 ± 0.04
M262				
Q263	1.24 ± 0.04	0.049 ± 0.001	0.86 ± 0.04	0.92 ± 0.04
V264	1.29 ± 0.04	0.053 ± 0.002	0.82 ± 0.04	0.86 ± 0.05
T265	1.19 ± 0.04	0.051 ± 0.001	0.80 ± 0.04	0.91 ± 0.05
R266				
C267	1.25 ± 0.04	0.046 ± 0.001	0.82 ± 0.04	0.94 ± 0.05
Q268	1.30 ± 0.05	0.046 ± 0.001	0.85 ± 0.04	0.92 ± 0.05
G269	1.24 ± 0.04	0.048 ± 0.001	0.88 ± 0.04	0.92 ± 0.04

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V270	1.28 ± 0.04	0.048 ± 0.001	0.82 ± 0.04	0.91 ± 0.05
T271	1.39 ± 0.05	0.052 ± 0.002	0.86 ± 0.04	0.84 ± 0.04
V272	1.26 ± 0.04	0.048 ± 0.001	0.77 ± 0.04	0.91 ± 0.05
W273	1.10 ± 0.04	0.046 ± 0.001	0.89 ± 0.04	0.99 ± 0.03
W273-Indole	1.51 ± 0.06	0.058 ± 0.003	0.81 ± 0.04	0.88 ± 0.01
G274	1.23 ± 0.04	0.051 ± 0.001	0.88 ± 0.04	0.90 ± 0.05
I275	1.33 ± 0.05	0.049 ± 0.001	0.78 ± 0.04	0.89 ± 0.04
T276				
D277	1.34 ± 0.05	0.043 ± 0.001	0.88 ± 0.04	0.94 ± 0.05
K278	1.20 ± 0.04	0.047 ± 0.001	0.73 ± 0.04	0.93 ± 0.04
Y279	1.33 ± 0.05	0.047 ± 0.001	0.75 ± 0.04	0.90 ± 0.05
S280				
W281				
W281-Indole	1.52 ± 0.30	0.059 ± 0.006	0.66 ± 0.03	0.86 ± 0.04
V282	1.24 ± 0.04	0.046 ± 0.001	0.84 ± 0.04	0.95 ± 0.04
P283				
D284	1.38 ± 0.05	0.055 ± 0.002	0.75 ± 0.04	0.82 ± 0.05
V285				
F286	1.35 ± 0.05	0.054 ± 0.002	0.72 ± 0.04	0.82 ± 0.05
P287				
G288	1.37 ± 0.05	0.055 ± 0.002	0.81 ± 0.04	0.82 ± 0.04
E289	1.35 ± 0.05	0.044 ± 0.001	0.82 ± 0.04	0.93 ± 0.05
G290	1.30 ± 0.05	0.052 ± 0.001	0.83 ± 0.04	0.86 ± 0.05
A291	1.22 ± 0.04	0.054 ± 0.002	0.80 ± 0.04	0.86 ± 0.05
A292	1.29 ± 0.05	0.044 ± 0.001	0.86 ± 0.04	0.96 ± 0.04
L293	1.24 ± 0.04	0.049 ± 0.001	0.87 ± 0.04	0.92 ± 0.04
V294				
W295				
W295-Indole	1.53 ± 0.06	0.056 ± 0.002	0.80 ± 0.04	0.88 ± 0.01
D296	1.35 ± 0.05	0.043 ± 0.001	0.87 ± 0.04	0.95 ± 0.04
A297				
S298	1.28 ± 0.04	0.050 ± 0.001	0.80 ± 0.04	0.89 ± 0.05
Y299	1.20 ± 0.04	0.044 ± 0.001	0.87 ± 0.04	0.97 ± 0.04
A300	1.23 ± 0.04	0.046 ± 0.001	0.83 ± 0.04	0.96 ± 0.04
K301	1.34 ± 0.05	0.050 ± 0.001	0.82 ± 0.04	0.86 ± 0.04
K302	1.38 ± 0.05	0.047 ± 0.001	0.72 ± 0.04	0.88 ± 0.05
P303				
A304				
Y305				
A306	1.27 ± 0.04	0.050 ± 0.001	0.83 ± 0.04	0.90 ± 0.05
A307	1.22 ± 0.04	0.051 ± 0.001	0.72 ± 0.04	0.89 ± 0.05
V308				
M309	1.27 ± 0.04	0.048 ± 0.001	0.74 ± 0.04	0.91 ± 0.04
E310	1.21 ± 0.04	0.047 ± 0.001	0.88 ± 0.04	0.95 ± 0.04
A311	1.21 ± 0.04	0.053 ± 0.002	0.85 ± 0.04	0.88 ± 0.05
F312	1.26 ± 0.04	0.049 ± 0.001	0.76 ± 0.04	0.90 ± 0.05
G313	1.17 ± 0.04	0.059 ± 0.002	0.77 ± 0.04	0.91 ± 0.07
A314				
S315				

SUPPLEMENTAL TABLE S2: List of the measured ^{15}N T_1 , T_2 , and heteronuclear ^1H - ^{15}N NOE relaxation parameters and the fit anisotropic model free order parameters S^2 for 2FCb-CexCD (recorded with a Varian 600 MHz NMR spectrometer at pH 6.5 and 30 °C). Missing data correspond to prolines and residues with overlapped or unassigned NMR signals. The anisotropic diffusion tensor for 2FCb-CexCD was determined to $D_{zz} = 1.11 (\pm 0.02) \times 10^7 \text{ s}^{-1}$, $D_{yy} = 0.94 (\pm 0.02) \times 10^7 \text{ s}^{-1}$, and $D_{xx} = 0.91 (\pm 0.01) \times 10^7 \text{ s}^{-1}$ using the X-ray crystallographic co-ordinate file 1EXP.pdb.

<u>Residue</u>	<u>T_1 (sec)</u>	<u>T_2 (sec)</u>	<u>NOE</u>	<u>S^2</u>
A1				
T2				
T3	1.33 \pm 0.05	0.055 \pm 0.002	0.71 \pm 0.04	0.82 \pm 0.05
L4				
K5	1.41 \pm 0.05	0.050 \pm 0.002	0.83 \pm 0.04	0.84 \pm 0.04
E6	1.29 \pm 0.04	0.044 \pm 0.001	0.72 \pm 0.04	0.94 \pm 0.04
A7	1.27 \pm 0.04	0.046 \pm 0.001	0.89 \pm 0.04	0.93 \pm 0.05
A8	1.28 \pm 0.04	0.050 \pm 0.001	0.87 \pm 0.04	0.89 \pm 0.05
D9				
G10	1.25 \pm 0.04	0.048 \pm 0.001	0.87 \pm 0.04	0.91 \pm 0.05
A11				
G12	1.32 \pm 0.05	0.052 \pm 0.002	0.86 \pm 0.04	0.85 \pm 0.06
R13	1.40 \pm 0.05	0.044 \pm 0.001	0.81 \pm 0.04	0.91 \pm 0.05
D14	1.34 \pm 0.05	0.043 \pm 0.001	0.77 \pm 0.04	0.94 \pm 0.04
F15	1.34 \pm 0.05	0.053 \pm 0.002	0.82 \pm 0.04	0.85 \pm 0.05
G16				
F17				
A18				
L19				
D20				
P21				
N22	1.22 \pm 0.04	0.045 \pm 0.001	0.78 \pm 0.04	0.95 \pm 0.05
R23	1.31 \pm 0.05	0.042 \pm 0.001	0.71 \pm 0.04	0.95 \pm 0.03
L24				
S25	1.25 \pm 0.04	0.045 \pm 0.001	0.84 \pm 0.04	0.95 \pm 0.04
E26	1.34 \pm 0.05	0.046 \pm 0.001	0.85 \pm 0.04	0.91 \pm 0.05
A27	1.30 \pm 0.04	0.046 \pm 0.001	0.85 \pm 0.04	0.92 \pm 0.05
Q28				
Y29	1.35 \pm 0.05	0.048 \pm 0.001	0.82 \pm 0.04	0.89 \pm 0.05
K30	1.26 \pm 0.04	0.042 \pm 0.001	0.83 \pm 0.04	0.98 \pm 0.03
A31	1.25 \pm 0.04	0.047 \pm 0.001	0.82 \pm 0.04	0.93 \pm 0.05
I32	1.27 \pm 0.04	0.044 \pm 0.001	0.81 \pm 0.04	0.96 \pm 0.04
A33	1.14 \pm 0.04	0.040 \pm 0.001	0.73 \pm 0.04	0.98 \pm 0.03
D34	1.27 \pm 0.04	0.047 \pm 0.001	0.76 \pm 0.04	0.92 \pm 0.04
S35				
E36	1.24 \pm 0.04	0.046 \pm 0.001	0.82 \pm 0.04	0.94 \pm 0.05
F37				
N38				
L39	1.36 \pm 0.05	0.045 \pm 0.001	0.87 \pm 0.04	0.91 \pm 0.05
V40				
V41				
A42	1.25 \pm 0.04	0.046 \pm 0.001	0.85 \pm 0.04	0.93 \pm 0.04
E43	1.28 \pm 0.04	0.049 \pm 0.001	0.79 \pm 0.04	0.89 \pm 0.05
N44				

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A45	1.13 ± 0.04	0.036 ± 0.001	0.80 ± 0.04	1.00 ± 0.03
M46	1.39 ± 0.05	0.050 ± 0.002	0.89 ± 0.04	0.85 ± 0.05
K47				
W48	1.36 ± 0.05	0.048 ± 0.001	0.81 ± 0.04	0.88 ± 0.05
W48-Indole	1.61 ± 0.04	0.054 ± 0.001	0.81 ± 0.04	0.88 ± 0.03
D49	1.26 ± 0.04	0.044 ± 0.001	0.89 ± 0.04	0.96 ± 0.04
A50	1.46 ± 0.05	0.051 ± 0.002	0.81 ± 0.04	0.83 ± 0.05
T51	1.40 ± 0.05	0.051 ± 0.002	0.85 ± 0.04	0.84 ± 0.05
E52				
P53				
S54	1.33 ± 0.05	0.047 ± 0.001	0.87 ± 0.04	0.90 ± 0.05
Q55	1.34 ± 0.05	0.051 ± 0.002	0.89 ± 0.04	0.86 ± 0.05
N56	1.34 ± 0.05	0.050 ± 0.002	0.77 ± 0.04	0.86 ± 0.05
S57	1.35 ± 0.05	0.047 ± 0.001	0.84 ± 0.04	0.90 ± 0.05
F58	1.41 ± 0.05	0.054 ± 0.002	0.77 ± 0.04	0.81 ± 0.05
S59	1.37 ± 0.05	0.047 ± 0.001	0.89 ± 0.04	0.89 ± 0.05
F60	1.49 ± 0.06	0.049 ± 0.001	0.76 ± 0.04	0.84 ± 0.05
G61	1.36 ± 0.05	0.046 ± 0.001	0.83 ± 0.04	0.90 ± 0.05
A62	1.27 ± 0.04	0.043 ± 0.001	0.79 ± 0.04	0.96 ± 0.04
G63	1.40 ± 0.05	0.046 ± 0.001	0.83 ± 0.04	0.89 ± 0.06
D64	1.32 ± 0.05	0.046 ± 0.001	0.81 ± 0.04	0.91 ± 0.05
R65	1.29 ± 0.05	0.048 ± 0.001	0.78 ± 0.04	0.89 ± 0.05
V66	1.43 ± 0.05	0.043 ± 0.001	0.86 ± 0.04	0.92 ± 0.05
A67	1.40 ± 0.05	0.049 ± 0.001	0.88 ± 0.04	0.85 ± 0.05
S68	1.31 ± 0.05	0.043 ± 0.001	0.82 ± 0.04	0.95 ± 0.05
Y69	1.35 ± 0.05	0.045 ± 0.001	0.85 ± 0.04	0.91 ± 0.05
A70	1.30 ± 0.05	0.041 ± 0.001	0.78 ± 0.04	0.99 ± 0.04
A71	1.33 ± 0.05	0.044 ± 0.001	0.89 ± 0.04	0.93 ± 0.05
D72	1.34 ± 0.05	0.044 ± 0.001	0.85 ± 0.04	0.93 ± 0.04
T73	1.39 ± 0.05	0.045 ± 0.001	0.84 ± 0.04	0.91 ± 0.05
G74	1.40 ± 0.05	0.045 ± 0.001	0.74 ± 0.04	0.89 ± 0.05
K75	1.37 ± 0.05	0.047 ± 0.001	0.85 ± 0.04	0.89 ± 0.05
E76	1.42 ± 0.05	0.044 ± 0.001	0.82 ± 0.04	0.91 ± 0.05
L77	1.32 ± 0.05	0.047 ± 0.001	0.81 ± 0.04	0.91 ± 0.05
Y78				
G79				
H80	1.24 ± 0.04	0.045 ± 0.001	0.88 ± 0.04	0.95 ± 0.05
T81	1.39 ± 0.05	0.047 ± 0.001	0.78 ± 0.04	0.89 ± 0.05
L82	1.40 ± 0.05	0.044 ± 0.001	0.87 ± 0.04	0.92 ± 0.05
V83	1.46 ± 0.05	0.048 ± 0.001	0.89 ± 0.04	0.86 ± 0.05
W84	1.35 ± 0.05	0.048 ± 0.001	0.89 ± 0.04	0.88 ± 0.05
W84-Indole	1.50 ± 0.05	0.053 ± 0.001	0.84 ± 0.04	0.92 ± 0.03
H85				
S86				
Q87				
L88				
P89				
D90	1.30 ± 0.04	0.046 ± 0.001	0.86 ± 0.04	0.92 ± 0.05
W91	1.22 ± 0.04	0.045 ± 0.001	0.85 ± 0.04	0.95 ± 0.04
W91-Indole	1.57 ± 0.01	0.050 ± 0.001	0.79 ± 0.04	0.92 ± 0.03
A92	1.37 ± 0.05	0.047 ± 0.001	0.88 ± 0.04	0.88 ± 0.05
K93	1.31 ± 0.05	0.046 ± 0.001	0.84 ± 0.04	0.91 ± 0.05
N94	1.25 ± 0.04	0.050 ± 0.001	0.74 ± 0.04	0.89 ± 0.05
L95	1.49 ± 0.06	0.046 ± 0.001	0.82 ± 0.04	0.87 ± 0.05
N96	1.34 ± 0.05	0.045 ± 0.001	0.76 ± 0.04	0.92 ± 0.05
G97	1.15 ± 0.04	0.055 ± 0.002	0.70 ± 0.03	0.89 ± 0.04
S98				

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A99	1.17 ± 0.04	0.048 ± 0.001	0.88 ± 0.04	0.94 ± 0.05
F100	1.34 ± 0.05	0.045 ± 0.001	0.88 ± 0.04	0.92 ± 0.05
E101	1.37 ± 0.05	0.042 ± 0.001	0.79 ± 0.04	0.94 ± 0.05
S102	1.39 ± 0.05	0.045 ± 0.001	0.88 ± 0.04	0.90 ± 0.05
A103	1.26 ± 0.04	0.045 ± 0.001	0.78 ± 0.04	0.94 ± 0.05
M104	1.34 ± 0.05	0.045 ± 0.001	0.73 ± 0.04	0.90 ± 0.05
V105	1.31 ± 0.05	0.041 ± 0.001	0.89 ± 0.04	0.98 ± 0.04
N106	1.29 ± 0.05	0.042 ± 0.001	0.87 ± 0.04	0.97 ± 0.04
H107	1.27 ± 0.04	0.043 ± 0.001	0.89 ± 0.04	0.96 ± 0.04
V108				
T109				
K110	1.34 ± 0.05	0.052 ± 0.002	0.69 ± 0.03	0.83 ± 0.05
V111				
A112				
D113				
H114				
F115	1.36 ± 0.05	0.050 ± 0.001	0.86 ± 0.04	0.86 ± 0.05
E116	±	±	±	±
G117	1.30 ± 0.05	0.048 ± 0.001	0.81 ± 0.04	0.91 ± 0.05
K118	1.47 ± 0.06	0.044 ± 0.001	0.86 ± 0.04	0.90 ± 0.05
V119	1.57 ± 0.06	0.048 ± 0.001	0.76 ± 0.04	0.82 ± 0.04
A120	1.34 ± 0.05	0.047 ± 0.001	0.88 ± 0.04	0.89 ± 0.05
S121	1.36 ± 0.05	0.050 ± 0.002	0.84 ± 0.04	0.86 ± 0.05
W122				
W122-Indole	1.47 ± 0.06	0.056 ± 0.002	0.80 ± 0.04	0.91 ± 0.03
D123				
V124	1.24 ± 0.04	0.039 ± 0.001	0.78 ± 0.04	1.00 ± 0.03
V125				
N126				
E127	1.33 ± 0.05	0.039 ± 0.001	0.75 ± 0.04	1.00 ± 0.03
A128				
F129				
A130	1.27 ± 0.04	0.049 ± 0.001	0.86 ± 0.04	0.89 ± 0.05
D131	1.35 ± 0.05	0.048 ± 0.001	0.84 ± 0.04	0.88 ± 0.05
G132				
G133	1.30 ± 0.05	0.050 ± 0.001	0.83 ± 0.04	0.88 ± 0.05
G134	1.00 ± 0.03	0.054 ± 0.002	0.80 ± 0.04	0.69 ± 0.10
R135				
R136	1.29 ± 0.04	0.051 ± 0.002	0.87 ± 0.04	0.87 ± 0.05
Q137	1.33 ± 0.05	0.050 ± 0.002	0.71 ± 0.04	0.85 ± 0.05
D138				
S139				
A140	1.18 ± 0.04	0.040 ± 0.001	0.82 ± 0.04	1.00 ± 0.03
F141				
Q142	1.34 ± 0.05	0.041 ± 0.001	0.83 ± 0.04	0.96 ± 0.04
Q143				
K144				
L145				
G146				
N147				
G148				
Y149				
I150				
E151				
T152	1.28 ± 0.04	0.047 ± 0.001	0.83 ± 0.04	0.92 ± 0.05
A153				
F154				

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R155				
A156	1.25 ± 0.04	0.046 ± 0.001	0.85 ± 0.04	0.94 ± 0.05
A157	1.39 ± 0.05	0.050 ± 0.002	0.73 ± 0.04	0.85 ± 0.04
R158	1.40 ± 0.05	0.046 ± 0.001	0.78 ± 0.04	0.89 ± 0.05
A159				
A160	1.34 ± 0.05	0.048 ± 0.001	0.81 ± 0.04	0.89 ± 0.05
D161	1.39 ± 0.05	0.049 ± 0.001	0.83 ± 0.04	0.87 ± 0.05
P162				
T163	1.30 ± 0.05	0.052 ± 0.002	0.78 ± 0.04	0.86 ± 0.05
A164	1.35 ± 0.05	0.049 ± 0.001	0.73 ± 0.04	0.86 ± 0.05
K165	1.41 ± 0.05	0.048 ± 0.001	0.84 ± 0.04	0.87 ± 0.05
L166				
C167	1.41 ± 0.05	0.043 ± 0.001	0.87 ± 0.04	0.92 ± 0.05
I168				
N169				
D170				
Y171	1.35 ± 0.05	0.041 ± 0.001	0.85 ± 0.04	0.96 ± 0.04
N172	1.33 ± 0.05	0.045 ± 0.001	0.88 ± 0.04	0.92 ± 0.04
V173	1.25 ± 0.04	0.046 ± 0.001	0.87 ± 0.04	0.94 ± 0.04
E174	1.31 ± 0.05	0.050 ± 0.001	0.83 ± 0.04	0.88 ± 0.05
G175	1.49 ± 0.06	0.050 ± 0.001	0.83 ± 0.04	0.83 ± 0.05
I176				
N177	1.39 ± 0.05	0.051 ± 0.002	0.80 ± 0.04	0.84 ± 0.05
A178				
K179	1.34 ± 0.05	0.050 ± 0.002	0.80 ± 0.04	0.86 ± 0.05
S180	1.31 ± 0.05	0.041 ± 0.001	0.83 ± 0.04	0.98 ± 0.04
N181	1.24 ± 0.04	0.046 ± 0.001	0.85 ± 0.04	0.95 ± 0.04
S182				
L183				
Y184				
D185	1.20 ± 0.04	0.042 ± 0.001	0.80 ± 0.04	1.00 ± 0.03
L186	1.35 ± 0.05	0.048 ± 0.001	0.85 ± 0.04	0.89 ± 0.05
V187	1.25 ± 0.04	0.051 ± 0.002	0.87 ± 0.04	0.88 ± 0.05
K188	1.32 ± 0.05	0.045 ± 0.001	0.77 ± 0.04	0.93 ± 0.05
D189				
F190	1.45 ± 0.05	0.044 ± 0.001	0.87 ± 0.04	0.90 ± 0.05
K191	1.30 ± 0.05	0.044 ± 0.001	0.81 ± 0.04	0.95 ± 0.04
A192	1.28 ± 0.04	0.048 ± 0.001	0.84 ± 0.04	0.91 ± 0.05
R193	1.37 ± 0.05	0.047 ± 0.001	0.86 ± 0.04	0.89 ± 0.04
G194	1.37 ± 0.05	0.050 ± 0.001	0.77 ± 0.04	0.85 ± 0.05
V195	1.26 ± 0.04	0.048 ± 0.001	0.83 ± 0.04	0.92 ± 0.05
P196				
L197				
D198	1.28 ± 0.05	0.047 ± 0.001	0.86 ± 0.04	0.92 ± 0.05
C199				
V200				
G201	1.30 ± 0.05	0.041 ± 0.001	0.84 ± 0.04	0.98 ± 0.04
F202				
Q203				
S204	1.34 ± 0.05	0.045 ± 0.001	0.84 ± 0.04	0.92 ± 0.05
H205				
L206	1.36 ± 0.05	0.052 ± 0.002	0.80 ± 0.04	0.84 ± 0.05
I207	1.35 ± 0.05	0.051 ± 0.002	0.81 ± 0.04	0.86 ± 0.05
V208	1.26 ± 0.04	0.052 ± 0.002	0.88 ± 0.04	0.87 ± 0.05
G209	1.33 ± 0.05	0.050 ± 0.002	0.86 ± 0.04	0.87 ± 0.05
Q210	1.30 ± 0.05	0.047 ± 0.001	0.81 ± 0.04	0.91 ± 0.05
V211	1.44 ± 0.05	0.047 ± 0.001	0.77 ± 0.04	0.86 ± 0.05

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P212				
G213	1.43 ± 0.05	0.047 ± 0.001	0.85 ± 0.04	0.88 ± 0.05
D214	1.23 ± 0.04	0.043 ± 0.001	0.82 ± 0.04	0.99 ± 0.04
F215	1.34 ± 0.05	0.042 ± 0.001	0.82 ± 0.04	0.96 ± 0.04
R216	1.28 ± 0.04	0.043 ± 0.001	0.83 ± 0.04	0.97 ± 0.04
Q217	1.31 ± 0.05	0.046 ± 0.001	0.83 ± 0.04	0.92 ± 0.05
N218	1.35 ± 0.05	0.042 ± 0.001	0.88 ± 0.04	0.95 ± 0.04
L219				
Q220	1.38 ± 0.05	0.041 ± 0.001	0.80 ± 0.04	0.96 ± 0.04
R221	1.34 ± 0.05	0.043 ± 0.001	0.82 ± 0.04	0.95 ± 0.04
F222				
A223	1.42 ± 0.05	0.049 ± 0.002	0.70 ± 0.04	0.84 ± 0.05
D224				
L225	1.26 ± 0.04	0.043 ± 0.001	0.78 ± 0.04	0.97 ± 0.04
G226	1.39 ± 0.05	0.044 ± 0.001	0.86 ± 0.04	0.91 ± 0.05
V227	1.39 ± 0.05	0.054 ± 0.002	0.80 ± 0.04	0.81 ± 0.05
D228				
V229	1.30 ± 0.05	0.045 ± 0.001	0.85 ± 0.04	0.93 ± 0.05
R230				
I231	1.19 ± 0.04	0.039 ± 0.001	0.76 ± 0.04	1.00 ± 0.03
T232				
E233				
L234	1.21 ± 0.04	0.047 ± 0.001	0.77 ± 0.04	0.94 ± 0.04
D235				
I236				
R237				
M238	1.23 ± 0.04	0.043 ± 0.001	0.84 ± 0.04	0.99 ± 0.04
R239	1.33 ± 0.05	0.048 ± 0.001	0.81 ± 0.04	0.88 ± 0.05
T240				
P241				
S242				
D243				
A244				
T245	1.21 ± 0.04	0.055 ± 0.002	0.71 ± 0.04	0.85 ± 0.05
K246	1.33 ± 0.05	0.047 ± 0.001	0.88 ± 0.04	0.91 ± 0.05
L247	1.32 ± 0.05	0.043 ± 0.001	0.88 ± 0.04	0.96 ± 0.04
A248	1.23 ± 0.04	0.047 ± 0.001	0.86 ± 0.04	0.93 ± 0.05
T249				
Q250				
A251	1.29 ± 0.05	0.048 ± 0.001	0.84 ± 0.04	0.90 ± 0.05
A252	1.28 ± 0.04	0.044 ± 0.001	0.85 ± 0.04	0.95 ± 0.05
D253				
Y254				
K255				
K256				
V257	1.25 ± 0.04	0.047 ± 0.001	0.80 ± 0.04	0.93 ± 0.05
V258	1.38 ± 0.05	0.046 ± 0.001	0.71 ± 0.04	0.88 ± 0.04
Q259	1.35 ± 0.05	0.045 ± 0.001	0.86 ± 0.04	0.92 ± 0.05
A260	1.30 ± 0.05	0.045 ± 0.001	0.86 ± 0.04	0.94 ± 0.04
C261	1.46 ± 0.05	0.047 ± 0.001	0.84 ± 0.04	0.87 ± 0.04
M262	1.13 ± 0.04	0.052 ± 0.002	0.72 ± 0.04	0.89 ± 0.05
Q263	1.29 ± 0.04	0.046 ± 0.001	0.86 ± 0.04	0.93 ± 0.05
V264	1.30 ± 0.05	0.051 ± 0.002	0.82 ± 0.04	0.87 ± 0.05
T265	1.18 ± 0.04	0.049 ± 0.001	0.77 ± 0.04	0.92 ± 0.05
R266	1.25 ± 0.04	0.047 ± 0.001	0.78 ± 0.04	0.93 ± 0.05
C267	1.31 ± 0.05	0.044 ± 0.001	0.86 ± 0.04	0.94 ± 0.04
Q268				

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G269	1.30 ± 0.05	0.046 ± 0.001	0.88 ± 0.04	0.92 ± 0.05
V270				
T271	1.38 ± 0.05	0.052 ± 0.002	0.75 ± 0.04	0.84 ± 0.04
V272				
W273	1.37 ± 0.05	0.046 ± 0.001	0.88 ± 0.04	0.90 ± 0.05
W273-Indole	1.64 ± 0.17	0.049 ± 0.003	0.85 ± 0.04	0.92 ± 0.04
G274				
I275	1.49 ± 0.06	0.047 ± 0.001	0.79 ± 0.04	0.86 ± 0.05
T276				
D277	1.28 ± 0.04	0.041 ± 0.001	0.86 ± 0.04	0.98 ± 0.04
K278	1.22 ± 0.04	0.043 ± 0.001	0.82 ± 0.04	0.98 ± 0.04
Y279	1.33 ± 0.05	0.044 ± 0.001	0.82 ± 0.04	0.94 ± 0.05
S280				
W281	1.24 ± 0.04	0.047 ± 0.001	0.88 ± 0.04	0.94 ± 0.04
W281-Indole	1.50 ± 0.09	0.059 ± 0.001	0.84 ± 0.04	0.87 ± 0.03
V282				
P283				
D284	1.37 ± 0.05	0.049 ± 0.001	0.78 ± 0.04	0.88 ± 0.06
V285	1.46 ± 0.05	0.048 ± 0.001	0.74 ± 0.04	0.85 ± 0.05
F286	1.36 ± 0.05	0.047 ± 0.001	0.81 ± 0.04	0.90 ± 0.04
P287				
G288	1.36 ± 0.05	0.052 ± 0.002	0.80 ± 0.04	0.84 ± 0.05
E289	1.36 ± 0.05	0.043 ± 0.001	0.84 ± 0.04	0.94 ± 0.05
G290				
A291	1.29 ± 0.04	0.051 ± 0.002	0.75 ± 0.04	0.87 ± 0.05
A292	1.34 ± 0.05	0.042 ± 0.001	0.88 ± 0.04	0.96 ± 0.04
L293	1.28 ± 0.04	0.049 ± 0.001	0.89 ± 0.04	0.90 ± 0.05
V294	1.21 ± 0.04	0.038 ± 0.001	0.73 ± 0.04	0.98 ± 0.03
W295	1.31 ± 0.05	0.039 ± 0.001	0.82 ± 0.04	1.00 ± 0.03
W295-Indole	1.54 ± 0.02	0.054 ± 0.001	0.77 ± 0.04	0.90 ± 0.03
D296				
A297				
S298	1.36 ± 0.05	0.047 ± 0.001	0.81 ± 0.04	0.90 ± 0.05
Y299	±	±	±	±
A300	1.22 ± 0.04	0.044 ± 0.001	0.83 ± 0.04	0.97 ± 0.04
K301	1.39 ± 0.05	0.048 ± 0.001	0.84 ± 0.04	0.87 ± 0.05
K302	1.48 ± 0.06	0.046 ± 0.001	0.80 ± 0.04	0.87 ± 0.05
P303				
A304				
Y305	1.27 ± 0.04	0.043 ± 0.001	0.83 ± 0.04	0.97 ± 0.04
A306	1.33 ± 0.05	0.049 ± 0.001	0.76 ± 0.04	0.89 ± 0.05
A307	1.27 ± 0.04	0.047 ± 0.001	0.84 ± 0.04	0.93 ± 0.04
V308	1.42 ± 0.05	0.045 ± 0.001	0.74 ± 0.04	0.89 ± 0.05
M309				
E310	1.24 ± 0.04	0.042 ± 0.001	0.79 ± 0.04	0.99 ± 0.03
A311	1.25 ± 0.04	0.049 ± 0.001	0.81 ± 0.04	0.90 ± 0.05
F312				
G313	1.21 ± 0.04	0.054 ± 0.002	0.73 ± 0.04	0.85 ± 0.05
A314	0.95 ± 0.03	0.066 ± 0.002	0.70 ± 0.04	0.76 ± 0.05
S315				