A prevalent intraresidue hydrogen bond stabilizes proteins

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Supplementary Table 1 | Donor–acceptor distances (Å) for various conformations of AcGlyNHMe.

	ϕ (°)								
ψ (°)	–180	–170	–160	–150	–140	–130	–120	–110	–100
180	2.182	2.197	2.241	2.311	2.403	2.513	2.633	2.761	2.891
170	2.197	2.199	2.230	2.290	2.373	2.475	2.591	2.716	2.845
160	2.241	2.230	2.249	2.297	2.369	2.463	2.572	2.693	2.820
150	2.311	2.289	2.296	2.332	2.393	2.477	2.579	2.694	2.817
140	2.402	2.371	2.368	2.392	2.443	2.518	2.611	2.719	2.837
130	2.510	2.472	2.460	2.475	2.517	2.582	2.666	2.767	2.879
120	2.630	2.587	2.568	2.576	2.609	2.665	2.742	2.835	2.940
110	2.756	2.710	2.687	2.689	2.715	2.764	2.833	2.919	3.018
100	2.884	2.838	2.813	2.811	2.832	2.874	2.937	3.016	3.108

Supplementary Table 2 | Sequences and T_m values of TrpZip peptides.

Peptide	Sequence	T_m (K)
TrpZip2-A	Ac-S-W-T-W-E-N-G-K-W-T-W-K-NH_2	346.3 ± 0.4
TrpZip2-B	Ac-S-W-T*W-E-N-G-K-W-T-W-K-NH_2	330.4 ± 0.5
TrpZip2-C	Ac-S-W-T-W-E-N-G-K-W*T-W-K-NH_2	ND
TrpZip2-D	Ac-S-W-T*W-E-N-G-K-W*T-W-K-NH_2	ND
TrpZip2-E	Ac-W-T-W-E-N-G-K-W-T-W-K-NH_2	351.7 ± 0.5
TrpZip2-F	Ac-W-T-W-E-N-G-K-W-T-W-K-OMe	349.5 ± 0.4
TrpZip2-G	Ac-S-W-T-W-E-N-G-K-W-T-W-NH_2	325.8 ± 1.2
TrpZip2-H	F_3C-S-W-T-W-E-N-G-K-W-T-W-NH_2	330.0 ± 1.0

*Denotes ester linkage.

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Supplementary Table 3 |
^{1}H Chemical shifts of TrpZip2-A.

Residue	Atom	δ
Ser1	H^{α}	3.803
Ser1	H^{β}	3.429
Ser1	NH	7.343
Trp2	H^{α}	4.986
Trp2	$H^{\beta1}$	3.012
Trp2	$H^{\beta2}$	2.818
Trp2	NH	8.190
Thr3	H^{α}	4.703
Thr3	H^{β}	3.890
Thr3	H^{γ}	0.996
Thr3	NH	9.524
Trp4	H^{α}	4.410
Trp4	$H^{\beta1}$	2.671
Trp4	$H^{\beta2}$	1.627
Trp4	NH	8.679
Glu5	H^{α}	4.083
Glu5	$H^{\beta1}$	1.683
Glu5	$H^{\beta2}$	1.563
Glu5	H^{γ}	1.859
Glu5	NH	8.256
Asn6	H^{α}	3.970
Asn6	$H^{\beta1}$	2.726
Asn6	$H^{\beta2}$	2.418
Asn6	NH	8.918
Gly7	$H^{\alpha1}$	3.615
Gly7	$H^{\alpha2}$	3.006
Gly7	NH	7.216
Lys8	H^{α}	4.075
Lys8	H^{δ}	1.479
Lys8	H^{ε}	2.821
Lys8	H^{γ}	1.036
Lys8	NH	6.595
Trp9	H^{α}	5.035
Trp9	$H^{\beta1}$	3.030
Trp9	$H^{\beta2}$	2.765
Trp9	NH	8.309
Thr10	H^{α}	4.715
Thr10	H^{β}	3.850
Thr10	H^{γ}	1.011
Thr10	NH	9.614
Trp11	H^{α}	4.415
Trp11	$H^{\beta1}$	2.570
Trp11	$H^{\beta2}$	1.542
Trp11	NH	8.570
Lys12	H^{α}	3.871
Lys12	H^{δ}	1.402
Lys12	H^{γ}	1.062
Lys12	NH	7.775

Supplementary Table 4 |
^{1}H Chemical shifts of TrpZip2-B.

Residue	Atom	δ
Ser1	H^{α}	4.102
Ser1	H^{β}	3.450
Ser1	NH	6.935
Trp2	H^{α}	4.783
Trp2	$H^{\beta1}$	2.696
Trp2	$H^{\beta2}$	2.413
Trp2	NH	8.216
Thr3	H^{α}	4.739
Thr3	H^{β}	4.143
Thr3	H^{γ}	0.899
Thr3	NH	8.790
Glu5	H^{α}	4.210
Glu5	$H^{\beta1}$	1.749
Glu5	$H^{\beta2}$	1.587
Glu5	H^{γ}	1.873
Glu5	NH	8.596
Asn6	H^{α}	4.138
Asn6	$H^{\beta1}$	2.797
Asn6	$H^{\beta2}$	2.525
Asn6	NH	9.090
Gly7	$H^{\alpha1}$	3.016
Gly7	$H^{\alpha2}$	2.577
Gly7	NH	5.511
Lys8	H^{α}	4.340
Lys8	H^{δ}	1.548
Lys8	H^{ε}	2.842
Lys8	H^{γ}	1.144
Lys8	NH	7.216
Trp9	H^{α}	4.651
Trp9	$H^{\beta1}$	3.003
Trp9	$H^{\beta2}$	2.573
Trp9	NH	8.630
Thr10	H^{α}	4.519
Thr10	H^{β}	3.742
Thr10	H^{γ}	0.908
Thr10	NH	8.436
Trp11	H^{α}	3.978
Trp11	$H^{\beta1}$	2.514
Trp11	$H^{\beta2}$	1.624
Trp11	NH	8.395
Lys12	H^{α}	3.907
Lys12	H^{δ}	1.253
Lys12	H^{γ}	0.972
Lys12	NH	7.793

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Supplementary Table 5 | Ranked changes in ^{1}H chemical shift from TrpZip2-A to TrpZip2-B.

Residue	Atom	$\Delta\delta$ (ppm)
Gly7	NH	–1.705
Thr10	NH	–1.178
Thr3	NH	–0.734
Gly7	$H^{\alpha 1}$	–0.599
Trp11	H^{α}	–0.437
Gly7	$H^{\alpha 2}$	–0.429
Ser1	NH	–0.408
Trp2	$H^{\beta 2}$	–0.405
Trp9	H^{α}	–0.384
Trp2	$H^{\beta 1}$	–0.316
Trp2	H^{α}	–0.203
Thr10	H^{α}	–0.196
Trp9	$H^{\beta 2}$	–0.192
Trp11	NH	–0.175
Lys12	H^{δ}	–0.149
Thr10	H^{β}	–0.108
Thr10	H^{γ}	–0.103
Thr3	H^{γ}	–0.097
Lys12	H^{γ}	–0.090
Trp11	$H^{\beta 1}$	–0.056
Trp9	$H^{\beta 1}$	–0.027
Glu5	H^{γ}	0.014
Lys12	NH	0.018
Lys8	H^{ε}	0.021
Ser1	H^{β}	0.021
Glu5	$H^{\beta 2}$	0.024
Trp2	NH	0.026
Thr3	H^{α}	0.036
Lys12	H^{α}	0.036
Glu5	$H^{\beta 1}$	0.066
Lys8	H^{δ}	0.069
Asn6	$H^{\beta 1}$	0.071
Trp11	$H^{\beta 2}$	0.082
Asn6	$H^{\beta 2}$	0.107
Lys8	H^{γ}	0.108
Glu5	H^{α}	0.127
Asn6	H^{α}	0.168
Asn6	NH	0.172
Thr3	H^{β}	0.253
Lys8	H^{α}	0.265
Ser1	H^{α}	0.299
Trp9	NH	0.321
Glu5	NH	0.340
Lys8	NH	0.621

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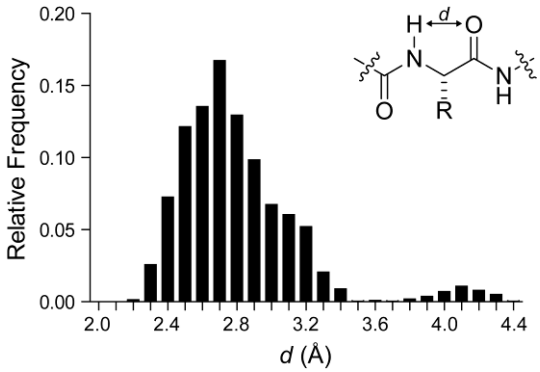
Supplementary Table 6 | Data used to generate Fig. 4a.

	ϕ (°)								
ψ (°)	–180	–170	–160	–150	–140	–130	–120	–110	–100
180	1.44	1.28	0.89	0.47	0.17	0.03			
170	1.28	1.32	1.08	0.69	0.32	0.10	0.01		
160	0.90	1.08	1.03	0.76	0.44	0.18	0.04		
150	0.50	0.7	0.78	0.67	0.45	0.23	0.08	0.01	
140	0.21	0.36	0.47	0.47	0.37	0.22	0.10	0.03	
130	0.07	0.15	0.23	0.26	0.24	0.17	0.09	0.04	
120	0.01	0.04	0.09	0.12	0.13	0.11	0.07	0.03	0.01
110		0.01	0.03	0.04	0.06	0.05	0.04	0.03	0.01
100				0.01	0.02	0.02	0.02	0.02	0.01



Supplementary Figure 1 | Frequencies of C5 hydrogen-bond donor–acceptor distances in β-sheets. Values of the NH⋯O distance (*d*) are from sub-Å protein crystal structures with assigned hydrogen coordinates.

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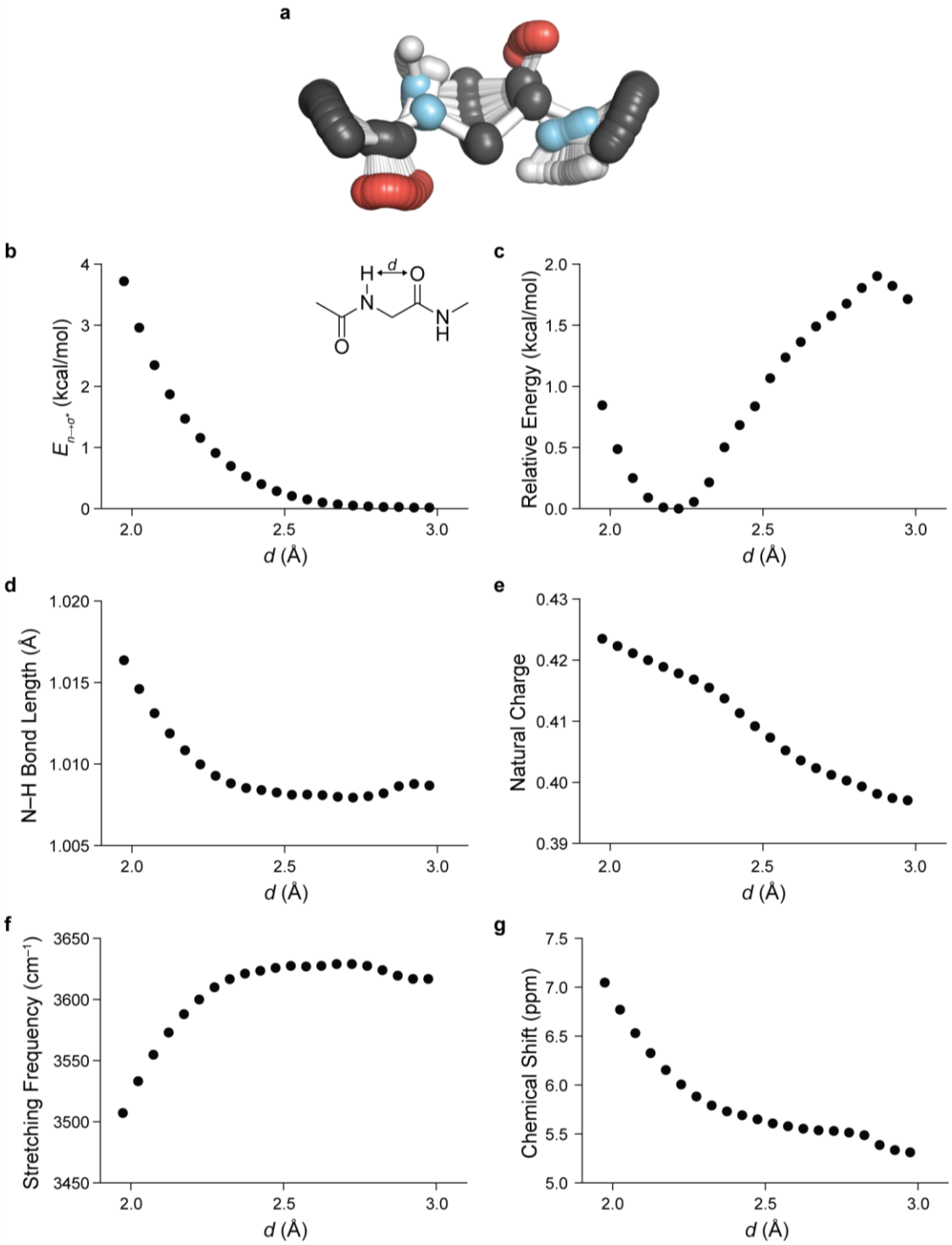

Supplementary Figure 2 | Computational characterization of AcGlyNHMe conformations. **a,** Overlay of AcGlyNHMe conformations generated by scanning the potential energy surface along the donor–acceptor distance. **b,** C5 hydrogen-bonding energy, **c,** zero-point corrected B3LYP energy relative to the local minimum, **d,** N–H bond length, **e,** NPA hydrogen charge, **f,** N–H stretching frequency, and **g,** donor ^{1}H chemical shift calculated for AcGlyNHMe conformations as a function of the C5 donor–acceptor distance.

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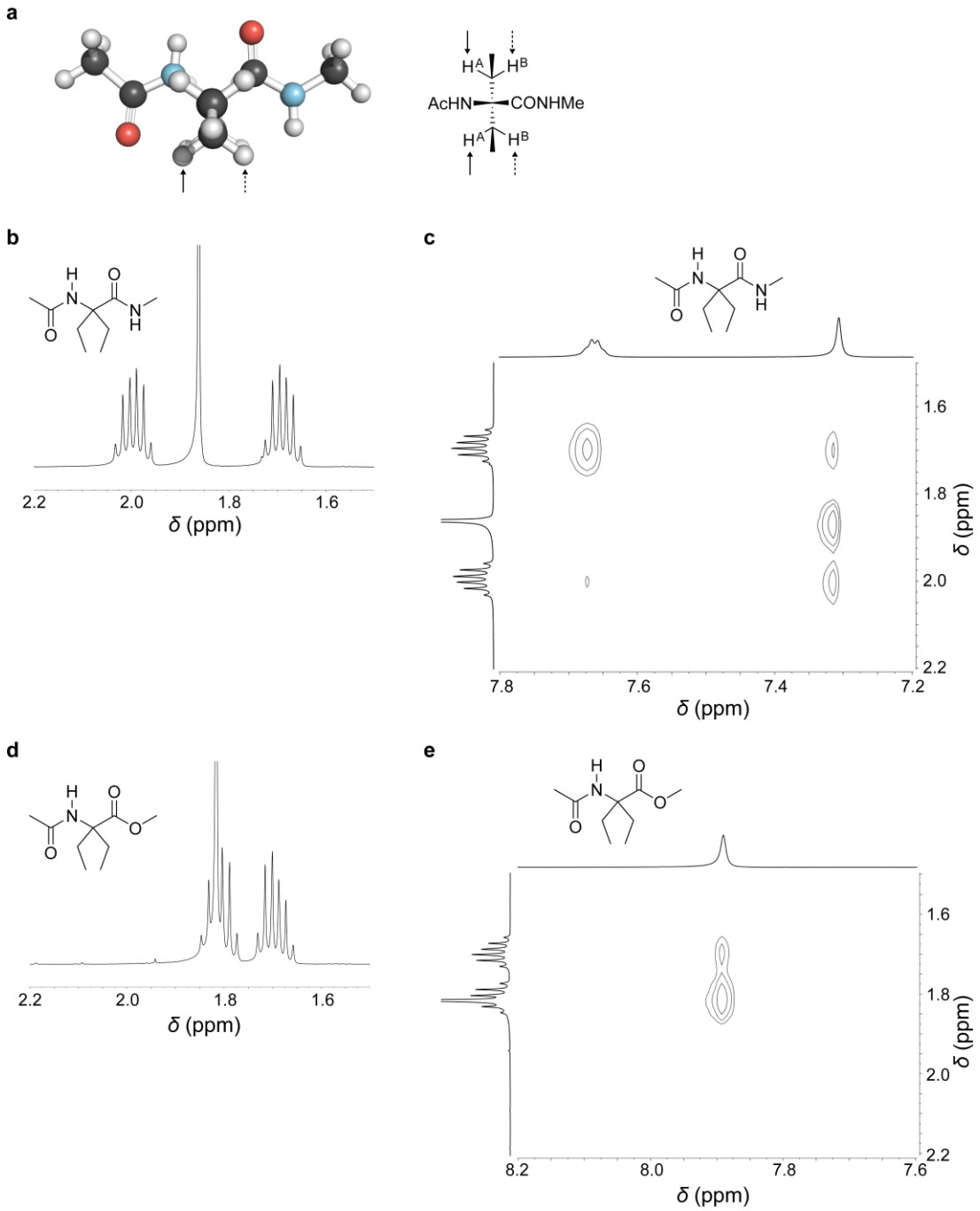

Supplementary Figure 3 | Conformational analysis of AcDegNHMe and AcDegOMe by NMR spectroscopy. **a,** Structural model of AcDegNHMe in the C5 geometry. **b,** ^{1}H and **c,** ^{1}H–^{1}H NOESY spectra of AcDegNHMe in DMSO-d_6. **d,** ^{1}H and **e,** ^{1}H–^{1}H NOESY spectra of AcDegOMe in DMSO-d_6. The one-dimensional ^{1}H NMR spectra shows two signals for the methylene groups with coupling constants consistent with gem splitting. These signals can be assigned as one proton on each methylene unit (marked with arrows in panel **a**) and indicate that the ethyl groups do not rotate freely on the NMR timescale. Moreover, the internal amide proton shows relatively equal NOEs to both methylene signals, indicating that it is oriented away from

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the ethyl groups; in contrast, the terminal amide proton has much stronger NOEs for one methylene signal over the other, indicating that it is oriented proximal to the ethyl groups. These correlations strongly suggest that the two carbonyl groups are oriented in opposite directions in solution. Similarity in the splitting patterns and coupling constants between AcDegNHMe and AcDegOMe indicates that they adopt similar conformations.

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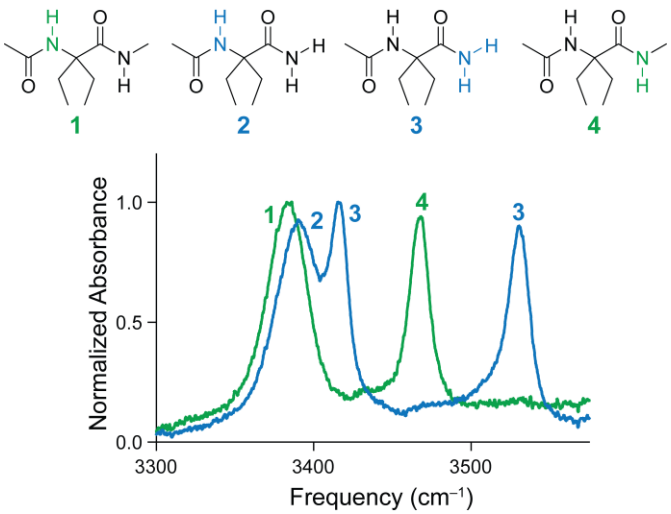
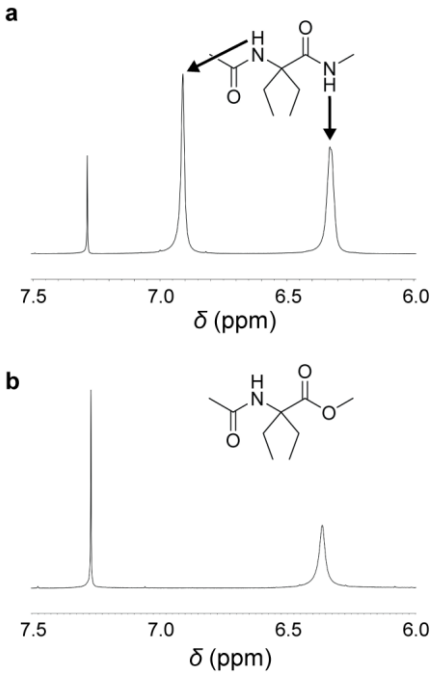


Supplementary Figure 4 | Fourier transform infrared spectra of AcDegNHMe and $AcDegNH_2$. Only the N–H stretching reagion is shown. Spectra were acquired in $CDCl_3$.



Supplementary Figure 5 | ^{1}H NMR spectra of AcDegNHMe and AcDegOMe. Only the amide region is shown Spectra were acquired in $CDCl_3$. **a,** AcDegNHMe and **b,** AcDegOMe.

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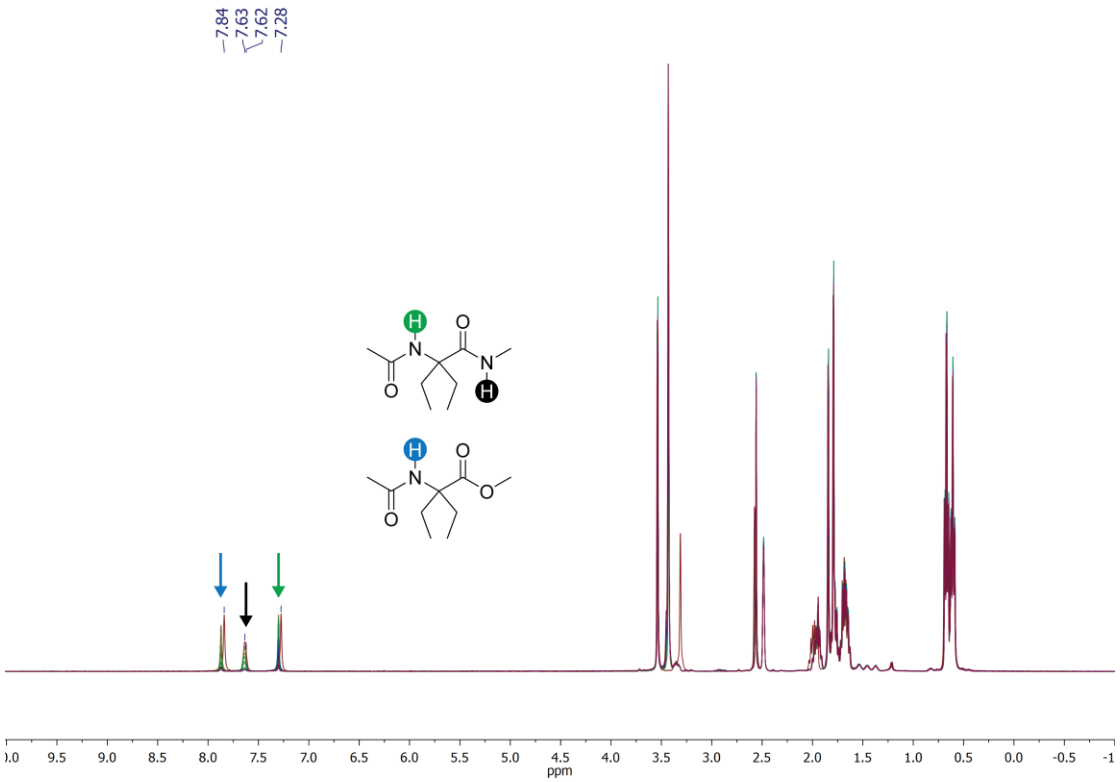

Supplementary Figure 6 | Representative ^{1}H NMR spectra during H/D exchange of AcDegNHMe and AcDegOMe. The overlayed spectra were acquired during an H/D exchange experiment with an equimolar mixture of AcDegNHMe and AcDegOMe (50 mM) in DMSO-d_6 containing 2% v/v D_2O. This experiment was performed in triplicate, and the data were averaged to generate Fig. 2c.

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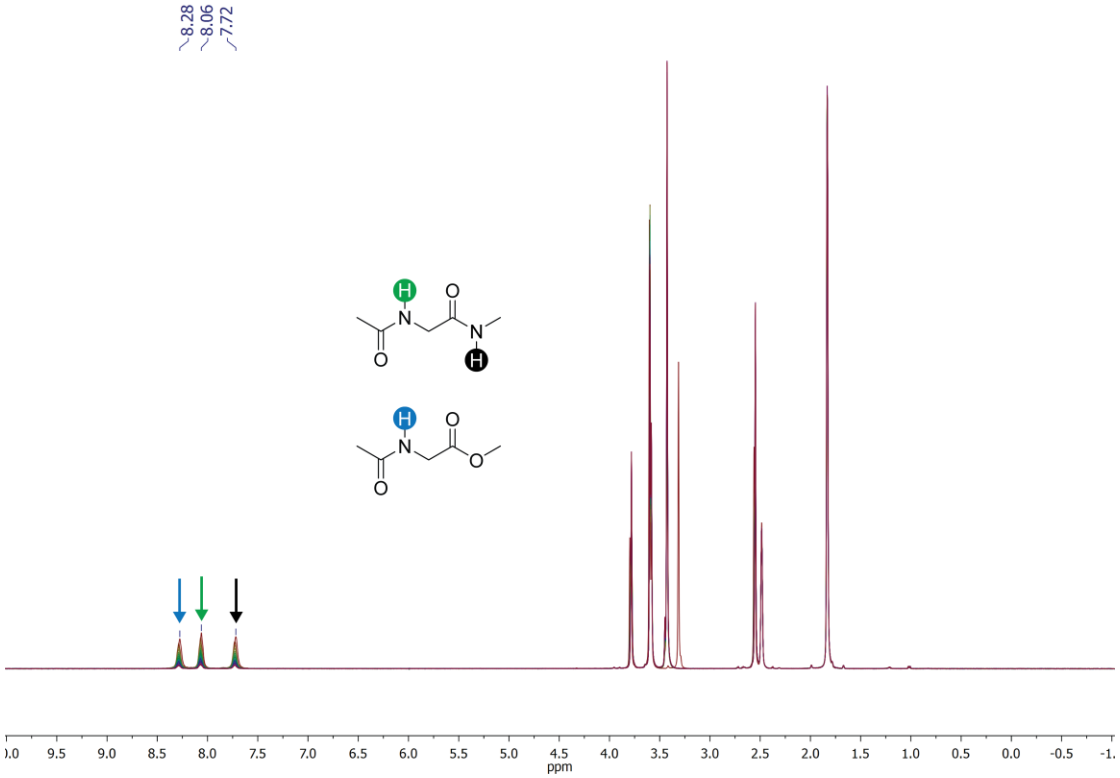

Supplementary Figure 7 | Representative ^{1}H NMR spectra during H/D exchange of AcGlyNHMe and AcGlyOMe. The overlayed spectra were acquired during an H/D exchange experiment with an equimolar mixture of AcGlyNHMe and AcGlyOMe (50 mM) in DMSO-d_6 containing 2% v/v D_2O. This experiment was performed in triplicate, and the data were averaged to generate Fig. 2d.

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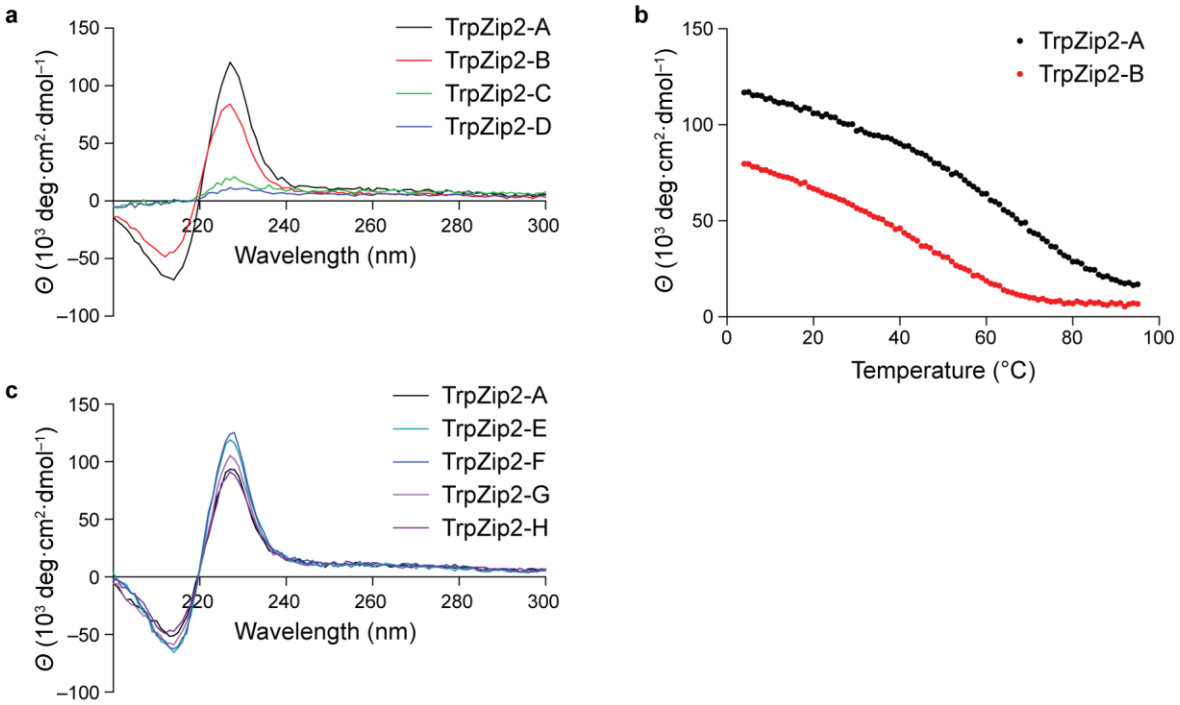

Supplementary Figure 8 | Far-UV circular dichroism spectra of TrpZip peptides. **a,** Spectra of TrpZip2 peptides A–D at 4 °C. **b,** Thermal denaturation of TrpZip2-A and TrpZip2-B observed at 228 nm. **c,** Far-UV circular dichroism spectra of TrpZip2 peptides E–F at 4 °C.

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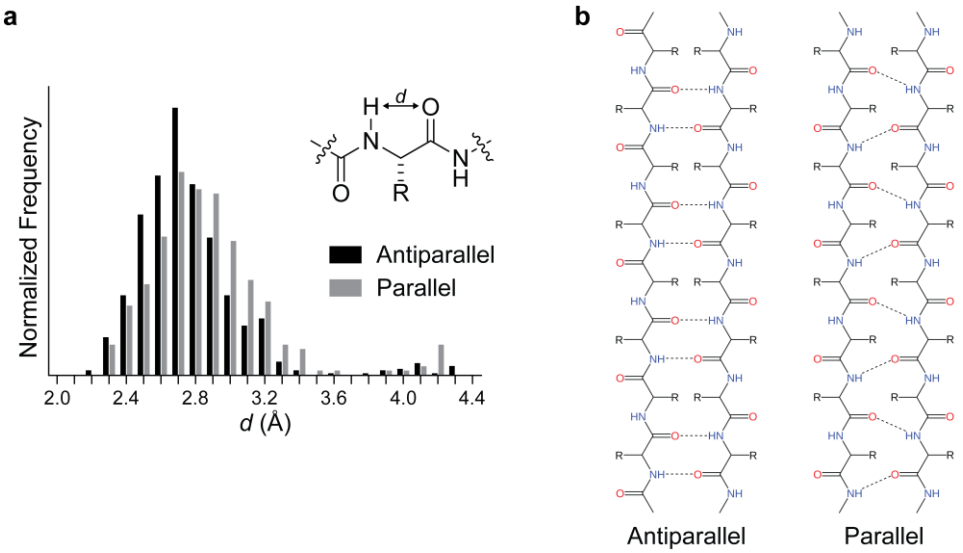

Supplementary Figure 9 | C5 hydrogen bonds in antiparallel or parallel β-sheets. **a,** Frequencies of C5 hydrogen-bond distances in parallel or antiparallel β-sheets. Values of the NH⋯O distance (*d*) are from sub-Å protein crystal structures with assigned hydrogen coordinates. **b,** Canonical hydrogen bonds in antiparallel and parallel β-sheets.

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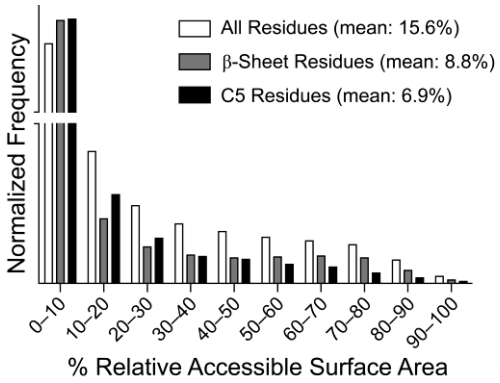
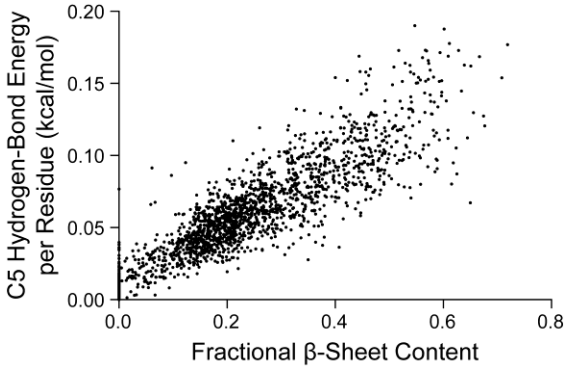


Supplementary Figure 10 | Solvent accessibility of residues engaged in C5 hydrogen bonds. Frequencies are for relative backbone solvent-accessible surface areas of residues in high-resolution protein crystal structures.



Supplementary Figure 11 | Relationship of C5 hydrogen-bonding energy with β-sheet content in proteins. Data are from high-resolution protein crystal structures.

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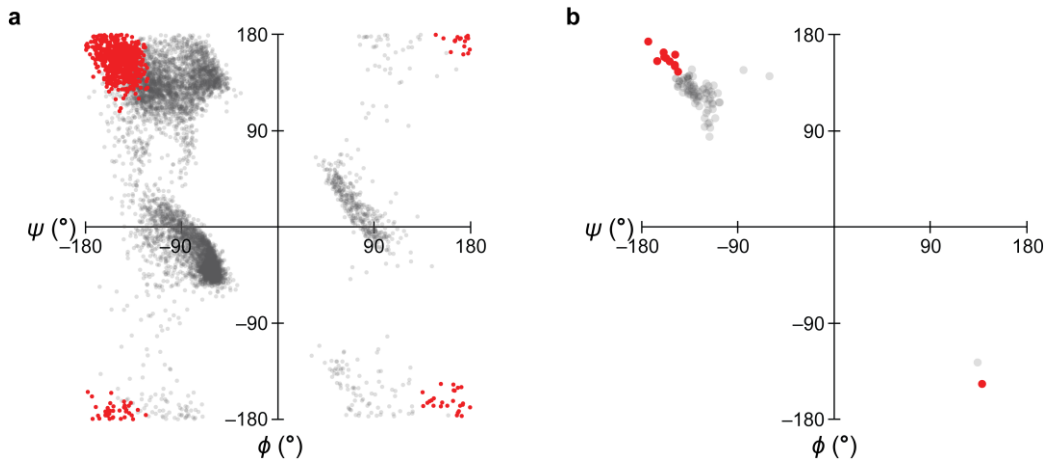

Supplementary Figure 12 | Ramachandran plots of residues engaged in C5 hydrogen bonds. **a,** Ramachandran plot of residues in sub-Å protein crystal structures with assigned hydrogen coordinates. Residues with hydrogen-bond donor–acceptor distances (*d*) <2.5 Å are shown in red. **b,** Ramachandran plot of residues in amyloid structures[1,2]. Residues with $|\phi| > 140°$ and $|\psi| > 140°$ are shown in red.

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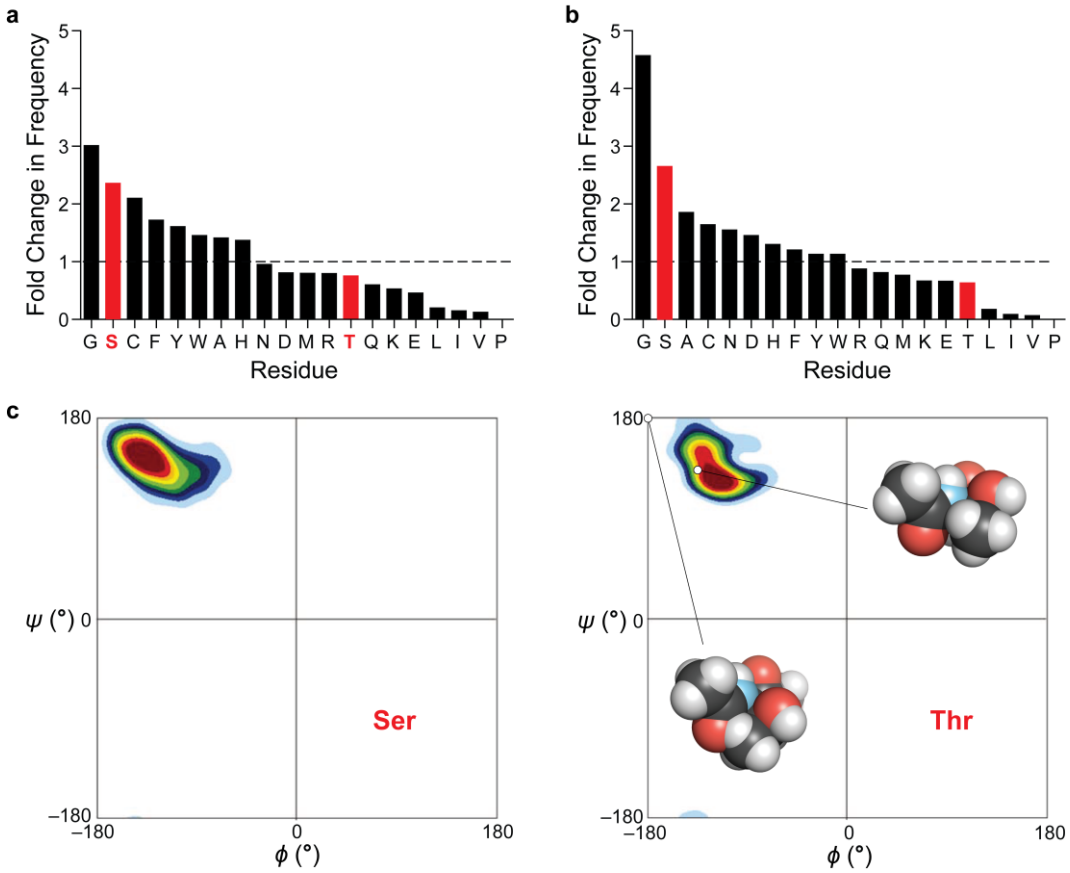

Supplementary Figure 13 | C5 hydrogen bonds in different amino acid residue-types. **a** and **b,** Relative frequency of amino acid residue-types engaged in C5 hydrogen bonds. C5 Hydrogen bonds are defined as residues having $|\phi| > 150°$ and $|\psi| > 150°$, and are shown relative to their frequency in the entire dataset (panel a) or β-sheets (panel b). Stringent criteria were employed for identifying C5 interactions so as allow comparisons between the C5 propensity of an amino acid and its propensity for β-sheet formation. **c,** Ramachandran plots of serine and threonine residues in β-sheets, along with space-filling models of a threonine residue with $\phi,\psi = -180,180$ or $\phi,\psi = -135,135$. The Ramachandran plots are adapted from ref. [3].

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Supplementary Note 1 | Calculated Cartesian coordinates

Optimized geometry of AcDegNHMe (Corrected SCF Energy = –613.721928 Hartree)

C	-2.37544800	-0.00505700	0.25980000
O	-2.81007900	-0.01134900	-0.88575700
N	-1.05319900	-0.00027100	0.56445800
H	-0.75466900	0.00713000	1.53171700
C	0.05311900	0.00110400	-0.39137100
C	1.32649400	0.00652100	0.49660800
O	1.26463900	0.01587300	1.72048600
N	2.51152000	0.00799500	-0.15323100
H	2.52213800	-0.03697900	-1.15766600
C	3.77630700	-0.00622100	0.56602500
H	4.58634400	0.13950200	-0.14702500
H	3.79960200	0.79545000	1.30429200
H	3.92605800	-0.95321200	1.08942500
C	-3.31467300	-0.00272000	1.45394200
H	-2.80121900	0.00365800	2.41613600
H	-3.96048700	0.87409500	1.38610600
H	-3.95424200	-0.88472000	1.39450200
C	0.02054400	-1.26891000	-1.28361300
H	0.83455200	-1.20263200	-2.01285900
H	-0.90813300	-1.22696700	-1.85395700
C	0.10984800	-2.59565100	-0.53057300
H	-0.70894900	-2.70125500	0.18288500
H	0.04753000	-3.43119200	-1.23089200
H	1.04807800	-2.69502200	0.02142600
C	0.01433700	1.26764000	-1.28849900
H	-0.91299200	1.21786800	-1.86051100
H	0.83140500	1.20375400	-2.01415300
C	0.09409200	2.59748900	-0.54002600
H	0.02743200	3.42989900	-1.24368400
H	-0.72624900	2.70091300	0.17202600
H	1.03134200	2.70429200	0.01205900

Optimized geometry of AcDegOMe (Corrected SCF Energy = –633.8604528 Hartree)

C	2.37371900	-0.00000500	0.23849700
O	2.78349200	-0.00002700	-0.91439500
N	1.05514700	-0.00000400	0.56915100
H	0.78976400	0.00001200	1.54362300
C	-0.06518500	-0.00001000	-0.37445000
C	-1.32210900	0.00000700	0.50696900
O	-1.31579400	0.00002100	1.71625000
C	-3.67891900	0.00002300	0.51797800
H	-4.46555200	0.00002100	-0.23154800
H	-3.74309700	-0.88846700	1.14491900
H	-3.74308400	0.88852700	1.14490000
C	3.33584500	0.00004000	1.41427900
H	2.84258300	-0.00007700	2.38711500
H	3.97711200	-0.87932100	1.33782500
H	3.97689300	0.87957300	1.33793500
C	-0.05969000	1.26748600	-1.27075900
H	-0.90636300	1.18951600	-1.95540700
H	0.85053300	1.22090000	-1.86921900
C	-0.12008900	2.59568800	-0.51737300
H	0.71952300	2.70487700	0.17139100
H	-0.07833900	3.42828900	-1.22255000
H	-1.04283500	2.70253200	0.05979700
C	-0.05970300	-1.26752700	-1.27072900
H	0.85051700	-1.22096000	-1.86919600
H	-0.90638000	-1.18956900	-1.95537400
C	-0.12010300	-2.59571200	-0.51731200
H	-0.07836400	-3.42832800	-1.22247100
H	0.71951500	-2.70488900	0.17144700
H	-1.04284500	-2.70253700	0.05986800
O	-2.44372200	0.00000600	-0.22431900

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AcGlyNHMe optimized at *d* = 2.974 Å

C	-1.82497500	-0.26278800	-0.06248700
O	-1.52832200	-1.21275700	-0.77410300
N	-1.16143000	0.93011400	-0.13304900
H	-1.24362800	1.57558200	0.63769100
C	0.04560600	1.05745800	-0.93668400
H	0.18323100	2.10360400	-1.20697800
H	-0.08441400	0.46259400	-1.83850200
C	1.25374100	0.62234900	-0.10779800
O	1.72189300	1.37129800	0.73717400
N	1.70493100	-0.63200500	-0.35573900
H	1.10359000	-1.22788800	-0.90705800
C	-2.97468900	-0.32611800	0.91989500
H	-3.09377400	0.58482600	1.50755400
H	-3.89570400	-0.51282500	0.36525700
H	-2.81736600	-1.17197800	1.59022200
C	2.74235900	-1.25104200	0.45270800
H	3.29800500	-1.96742300	-0.15261100
H	3.41771200	-0.47388700	0.80381200
H	2.32701200	-1.76684500	1.32376000

AcGlyNHMe optimized at *d* = 2.924 Å

C	-1.84461900	-0.27386000	-0.05635100
O	-1.55731200	-1.25346800	-0.72974900
N	-1.17071400	0.91021900	-0.17325000
H	-1.24893400	1.58595800	0.57166100
C	0.04050400	0.99332700	-0.97518000
H	0.17770600	2.02236800	-1.30622900
H	-0.08446200	0.34747400	-1.84185200
C	1.24614100	0.61142200	-0.11692400
O	1.66384800	1.38427800	0.73306600
N	1.76068400	-0.62117500	-0.34922800
H	1.20452900	-1.24725400	-0.91328800
C	-2.99418600	-0.28799200	0.92845900
H	-3.11632700	0.65250800	1.46686700
H	-3.91439600	-0.50793300	0.38497800
H	-2.83355700	-1.09598300	1.64344300
C	2.81340100	-1.18586700	0.47921200
H	3.41494700	-1.87487500	-0.11388900
H	3.44243300	-0.37479300	0.83948300
H	2.40854200	-1.71943500	1.34433200

AcGlyNHMe optimized at *d* = 2.874 Å

C	-1.88760800	-0.28680400	-0.04110300
O	-1.62296500	-1.32397000	-0.63134100
N	-1.18219500	0.86714500	-0.24411000
H	-1.26387700	1.60824300	0.43520300
C	0.03632700	0.86020000	-1.03669200
H	0.17543500	1.84401600	-1.48596900
H	-0.08293300	0.11933900	-1.82474800
C	1.24230900	0.58367700	-0.13797000
O	1.59179400	1.40905400	0.69321600
N	1.85217500	-0.61235700	-0.32485900
H	1.36458200	-1.29425500	-0.88604300
C	-3.04190100	-0.19311900	0.93452000
H	-3.16950700	0.80159500	1.36309100
H	-3.95854900	-0.47864800	0.41668400
H	-2.88023800	-0.91343100	1.73792400
C	2.93682500	-1.06756500	0.52978200
H	3.58460900	-1.74112500	-0.03130600
H	3.50990600	-0.20153600	0.85396200
H	2.56437300	-1.58672000	1.41775400

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AcGlyNHMe optimized at *d* = 2.824 Å

C	-1.96325400	-0.29978100	0.00062600
O	-1.73327900	-1.44051600	-0.37143600
N	-1.19716800	0.76442100	-0.38686900
H	-1.29601100	1.63677900	0.10881400
C	0.03703000	0.56759300	-1.12334500
H	0.19028600	1.41075300	-1.80003100
H	-0.07278600	-0.34113700	-1.71207400
C	1.24112400	0.51456100	-0.17877900
O	1.48386300	1.44888300	0.57052600
N	2.00191500	-0.60501900	-0.25948300
H	1.62477300	-1.38993200	-0.76714500
C	-3.13972900	0.02765400	0.89673200
H	-3.22905100	1.08987700	1.12744600
H	-4.05452400	-0.31007100	0.40785500
H	-3.03678300	-0.53423700	1.82624600
C	3.14413800	-0.82875100	0.61193800
H	3.87952400	-1.44796900	0.09803200
H	3.58805100	0.13438400	0.85422300
H	2.85277000	-1.31886200	1.54533500

AcGlyNHMe optimized at *d* = 2.774 Å

C	-2.02555800	-0.29156100	0.03876600
O	-1.84879600	-1.48774000	-0.13415200
N	-1.19385800	0.65719500	-0.48785400
H	-1.27828400	1.60745600	-0.16226500
C	0.04309200	0.28995700	-1.14616800
H	0.20928000	0.94781500	-2.00320800
H	-0.07393100	-0.73006400	-1.50801200
C	1.25052700	0.44427600	-0.21550400
O	1.43317300	1.47768100	0.40993700
N	2.10006300	-0.61253600	-0.18387600
H	1.78853300	-1.47916800	-0.59273200
C	-3.20354000	0.23580700	0.83219700
H	-3.26685800	1.32461300	0.84687000
H	-4.12099500	-0.17136900	0.40582700
H	-3.12530800	-0.13127000	1.85687700
C	3.28276100	-0.63127300	0.66202700
H	4.04983800	-1.25470300	0.20243500
H	3.65467200	0.38634800	0.76030100
H	3.06091300	-1.01503700	1.66184000

AcGlyNHMe optimized at *d* = 2.724 Å

C	-2.07649100	-0.27686300	0.07022000
O	-1.95070300	-1.49164500	0.08021000
N	-1.18623500	0.55019300	-0.55610300
H	-1.24991500	1.54242600	-0.39066200
C	0.04998500	0.04536700	-1.11267100
H	0.22804000	0.50032500	-2.09171600
H	-0.07498100	-1.02773100	-1.24957300
C	1.25982800	0.37909500	-0.23290200
O	1.39179300	1.48326600	0.27207100
N	2.17995200	-0.61156400	-0.11858200
H	1.92518200	-1.53339100	-0.43522000
C	-3.25353200	0.40960300	0.73265500
H	-3.25006500	1.49377100	0.61294300
H	-4.17497900	0.00544300	0.31161300
H	-3.24341600	0.16722500	1.79639200
C	3.39325300	-0.45965600	0.66839600
H	4.19455100	-1.05037400	0.22383200
H	3.67537300	0.59096300	0.66813100
H	3.24722000	-0.77729500	1.70462000

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AcGlyNHMe optimized at *d* = 2.674 Å

C	-2.11427500	-0.26128500	0.08343700
O	-2.04152000	-1.47672700	0.17883000
N	-1.17317600	0.48497100	-0.56893200
H	-1.20596200	1.48865600	-0.48180200
C	0.05412300	-0.10247500	-1.05788900
H	0.23185700	0.20666200	-2.09307700
H	-0.08209400	-1.18310600	-1.04298700
C	1.27293100	0.33724500	-0.23987700
O	1.38777900	1.48219600	0.16925900
N	2.22429400	-0.61567400	-0.07138000
H	1.99228100	-1.56625900	-0.31087700
C	-3.27800000	0.51619200	0.66404900
H	-3.22102400	1.58981800	0.47997200
H	-4.20399600	0.12822700	0.23768000
H	-3.31136600	0.33895500	1.74004700
C	3.45693600	-0.36515700	0.65834800
H	4.25973600	-0.97287900	0.24025300
H	3.71036500	0.68791900	0.55729300
H	3.35201600	-0.59395200	1.72255900

AcGlyNHMe optimized at *d* = 2.624 Å

C	-2.14634000	-0.24773700	0.08861200
O	-2.12281200	-1.46108500	0.22692900
N	-1.15973200	0.44058700	-0.55925300
H	-1.16058800	1.44774100	-0.51575100
C	0.05660800	-0.20610300	-0.99679300
H	0.22870300	-0.01210500	-2.06116900
H	-0.08872300	-1.27816700	-0.86737700
C	1.28597800	0.30627700	-0.24026200
O	1.39266500	1.47736200	0.08965500
N	2.25688200	-0.61914700	-0.03412400
H	2.03750400	-1.58631600	-0.21073700
C	-3.29498600	0.59209800	0.60958400
H	-3.19227800	1.65580300	0.39099600
H	-4.22326500	0.22403500	0.17074200
H	-3.36402200	0.45381200	1.68960200
C	3.50592000	-0.30213300	0.63969400
H	4.30760900	-0.92022400	0.23483300
H	3.73547700	0.74695500	0.46612300
H	3.43762500	-0.46624300	1.71869600

AcGlyNHMe optimized at *d* = 2.574 Å

C	-2.18641200	-0.23337500	0.08870400
O	-2.21772700	-1.44296200	0.25691600
N	-1.14389400	0.39936000	-0.52559100
H	-1.11327200	1.40702900	-0.52543400
C	0.05908500	-0.30517100	-0.90465100
H	0.21999700	-0.23906000	-1.98704200
H	-0.09338700	-1.35470400	-0.65311300
C	1.30301100	0.27674200	-0.22782500
O	1.40142200	1.46833800	0.02149300
N	2.29596600	-0.61957000	0.00176500
H	2.09091100	-1.59844300	-0.11879600
C	-3.32273700	0.66365300	0.53645400
H	-3.16734300	1.71675800	0.29843300
H	-4.24420600	0.32148400	0.06363500
H	-3.44639800	0.55516300	1.61499300
C	3.56936100	-0.24391800	0.59466900
H	4.37393700	-0.82398300	0.14136200
H	3.73588100	0.81420600	0.40558100
H	3.57596700	-0.40757600	1.67578500

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AcGlyNHMe optimized at *d* = 2.524 Å

C	-2.23128200	-0.21878200	0.08294000
O	-2.32124300	-1.42548600	0.25289300
N	-1.12590500	0.36779700	-0.46024600
H	-1.06319200	1.37344600	-0.49238500
C	0.06032000	-0.38987700	-0.78305400
H	0.19942500	-0.45535000	-1.86937900
H	-0.09376100	-1.40300900	-0.41059500
C	1.32358300	0.25089100	-0.20444700
O	1.41745700	1.45655600	-0.03290500
N	2.33835600	-0.61914800	0.03179000
H	2.14590500	-1.60560400	-0.03666900
C	-3.35759000	0.72518500	0.45313900
H	-3.13634900	1.77256500	0.24346400
H	-4.25325000	0.43159700	-0.09606000
H	-3.57161100	0.61030500	1.51663700
C	3.63893800	-0.19663600	0.52549600
H	4.42952900	-0.74780000	0.01444600
H	3.75056000	0.86597300	0.32224900
H	3.73205700	-0.35590600	1.60314000

AcGlyNHMe optimized at *d* = 2.474 Å

C	-2.26106500	-0.20789500	0.07560500
O	-2.39414600	-1.41253500	0.23302200
N	-1.11219600	0.34710300	-0.40418600
H	-1.01899300	1.35019300	-0.44543500
C	0.06002200	-0.44793900	-0.68418400
H	0.17817800	-0.61069600	-1.76317900
H	-0.09009100	-1.42581700	-0.22488500
C	1.33651200	0.23075500	-0.18559300
O	1.42470200	1.44354700	-0.06944400
N	2.36914800	-0.61828400	0.04842500
H	2.18718100	-1.60882400	0.02546400
C	-3.37626900	0.76749200	0.39508000
H	-3.11219300	1.80920100	0.20787300
H	-4.24995500	0.50665300	-0.20385500
H	-3.65024400	0.65043300	1.44447200
C	3.68351600	-0.16134900	0.46998900
H	4.45814100	-0.74408700	-0.03004100
H	3.78491900	0.88575300	0.19387100
H	3.81365300	-0.24902900	1.55204400

AcGlyNHMe optimized at *d* = 2.424 Å

C	-2.29277800	-0.19612900	0.06446500
O	-2.46919300	-1.39933500	0.18946300
N	-1.09748300	0.33019600	-0.32076000
H	-0.97285700	1.32985500	-0.36576100
C	0.05817200	-0.50208700	-0.55639700
H	0.14380700	-0.77201100	-1.61713000
H	-0.07852600	-1.43256300	-0.00306100
C	1.35061700	0.21032800	-0.15893700
O	1.43471100	1.42768000	-0.09957600
N	2.40326100	-0.61800900	0.05777100
H	2.23344700	-1.61041300	0.08923200
C	-3.39928400	0.80638500	0.32523800
H	-3.08957100	1.84347900	0.18929900
H	-4.23100600	0.59068300	-0.34707900
H	-3.75832200	0.67032800	1.34622700
C	3.72987500	-0.12656300	0.39414800
H	4.48467100	-0.78651900	-0.03413200
H	3.84526500	0.87163700	-0.02270600
H	3.87889700	-0.06814400	1.47582700

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AcGlyNHMe optimized at *d* = 2.374 Å

C	-2.32731700	-0.18735200	0.04244200
O	-2.54128000	-1.39030500	0.09103800
N	-1.08388700	0.31837600	-0.17651100
H	-0.93166300	1.31460800	-0.21502000
C	0.05705100	-0.54662000	-0.35807800
H	0.08995800	-0.94907700	-1.37895000
H	-0.04168800	-1.40434800	0.31056500
C	1.36597400	0.20116000	-0.10874500
O	1.43821000	1.42064600	-0.11837100
N	2.43889000	-0.60961200	0.07656400
H	2.28372300	-1.60434400	0.11733600
C	-3.43323400	0.83289400	0.22610300
H	-3.08792000	1.86592900	0.16621400
H	-4.19363100	0.66477300	-0.53795000
H	-3.90154300	0.66781300	1.19741800
C	3.79122500	-0.10846600	0.25764200
H	4.47277500	-0.57567000	-0.45592900
H	3.77581500	0.96537000	0.08693200
H	4.15151400	-0.29882600	1.27149300

AcGlyNHMe optimized at *d* = 2.324 Å

C	-2.34124400	-0.18174500	0.02339800
O	-2.57457400	-1.38221100	0.03704900
N	-1.07661400	0.30452100	-0.08356500
H	-0.89936500	1.29739500	-0.10584500
C	0.05643300	-0.58187300	-0.19066400
H	0.05389700	-1.10422400	-1.15518000
H	-0.00979700	-1.35597800	0.57866400
C	1.36932800	0.18921000	-0.06184000
O	1.42206900	1.40950700	-0.08724700
N	2.46484600	-0.60385400	0.05389300
H	2.32919600	-1.60154400	0.09587300
C	-3.44346000	0.85350900	0.12849200
H	-3.07919900	1.88147600	0.10360600
H	-4.14440600	0.70184200	-0.69357900
H	-3.98837300	0.68942800	1.05923100
C	3.81865600	-0.08209400	0.14110000
H	4.44908400	-0.51067700	-0.64068900
H	3.77032300	0.99614200	0.00881400
H	4.26278600	-0.29894500	1.11547800

AcGlyNHMe optimized at *d* = 2.274 Å

C	-2.34454600	-0.17858400	-0.00000700
O	-2.59191000	-1.37648300	-0.00002900
N	-1.07001800	0.29134600	0.00002500
H	-0.87110300	1.28082900	0.00003300
C	0.05714200	-0.60743500	0.00002700
H	0.02338700	-1.26324700	-0.87649400
H	0.02340000	-1.26323600	0.87655700
C	1.36757600	0.17865700	0.00001100
O	1.39998200	1.40006800	-0.00000600
N	2.47923900	-0.59950300	0.00003700
H	2.36035000	-1.60032100	-0.00002000
C	-3.43917600	0.86998000	-0.00000800
H	-3.06127600	1.89330100	-0.00002000
H	-4.06630100	0.71974000	-0.87991800
H	-4.06628400	0.71975900	0.87991800
C	3.82895900	-0.06011800	-0.00003500
H	4.37706200	-0.37872700	-0.88949200
H	3.75454500	1.02469400	0.00036000
H	4.37736800	-0.37937200	0.88899700

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AcGlyNHMe optimized at *d* = 2.224 Å

C	-2.34145800	-0.17606200	-0.00002100
O	-2.60299700	-1.37108500	-0.00012700
N	-1.06199900	0.27864200	0.00011700
H	-0.84233600	1.26444800	0.00020800
C	0.05840400	-0.62725200	0.00012400
H	0.02502600	-1.28241900	-0.87691800
H	0.02511900	-1.28233800	0.87723400
C	1.36320900	0.16755900	0.00003800
O	1.37835100	1.38963600	-0.00003000
N	2.48365200	-0.59654500	0.00018100
H	2.37632800	-1.59869100	-0.00029900
C	-3.42351100	0.88546500	-0.00004200
H	-3.03304600	1.90401600	0.00007100
H	-4.05233400	0.74285200	-0.88002700
H	-4.05251700	0.74271400	0.87978900
C	3.82699400	-0.04118900	-0.00015800
H	4.37776700	-0.35119100	-0.89099200
H	3.73981700	1.04265800	0.00295200
H	4.37995000	-0.35625000	0.88750800

AcGlyNHMe optimized at *d* = 2.174 Å

C	-2.33825300	-0.17346800	-0.00004000
O	-2.61392200	-1.36546200	0.00001000
N	-1.05407800	0.26603100	0.00002100
H	-0.81330800	1.24778000	0.00005200
C	0.05960100	-0.64688100	0.00022500
H	0.02673800	-1.30151000	-0.87726100
H	0.02673400	-1.30115700	0.87797900
C	1.35889700	0.15652600	0.00011400
O	1.35693900	1.37905200	0.00023600
N	2.48784000	-0.59354500	0.00001900
H	2.39195700	-1.59687400	-0.00052300
C	-3.40765400	0.90079200	-0.00019900
H	-3.00479300	1.91446100	-0.00028800
H	-4.03822300	0.76553800	-0.88011400
H	-4.03830700	0.76571400	0.87968100
C	3.82469800	-0.02247900	-0.00026200
H	4.37894600	-0.32613600	-0.89109200
H	3.72492000	1.06027200	0.00285400
H	4.38114000	-0.33115100	0.88744000

AcGlyNHMe optimized at *d* = 2.124 Å

C	-2.33492400	-0.17079500	-0.00004800
O	-2.62465700	-1.35961200	-0.00008900
N	-1.04626300	0.25354700	0.00008800
H	-0.78396900	1.23083700	0.00016600
C	0.06071700	-0.66632800	0.00022200
H	0.02836200	-1.32021100	-0.87785900
H	0.02839500	-1.31997900	0.87847900
C	1.35462600	0.14554300	0.00012100
O	1.33579100	1.36831300	0.00015100
N	2.49178000	-0.59051400	0.00016900
H	2.40723500	-1.59488500	-0.00048000
C	-3.39162000	0.91595300	-0.00015500
H	-2.97653300	1.92463500	-0.00018400
H	-4.02378100	0.78820000	-0.88006600
H	-4.02388000	0.78828600	0.87969900
C	3.82204900	-0.00397500	-0.00030800
H	4.37926000	-0.30067700	-0.89160500
H	3.70988900	1.07755000	0.00362100
H	4.38224300	-0.30698100	0.88694400

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AcGlyNHMe optimized at *d* = 2.074 Å

C	-2.33148200	-0.16806400	-0.00003900
O	-2.63521300	-1.35356000	-0.00004000
N	-1.03856400	0.24118900	0.00000100
H	-0.75433800	1.21362600	0.00008000
C	0.06175700	-0.68557500	0.00011600
H	0.03002600	-1.33873500	-0.87854600
H	0.02998400	-1.33859700	0.87887700
C	1.35041600	0.13464400	0.00009600
O	1.31488100	1.35747700	0.00013500
N	2.49549100	-0.58744100	0.00022900
H	2.42212300	-1.59271300	-0.00057000
C	-3.37542900	0.93093200	-0.00009800
H	-2.94828000	1.93452200	-0.00015500
H	-4.00914100	0.81058900	-0.87995900
H	-4.00913600	0.81069300	0.87978300
C	3.81909600	0.01427400	-0.00025400
H	4.37912000	-0.27525000	-0.89211900
H	3.69472500	1.09444700	0.00485900
H	4.38292500	-0.28341700	0.88645400

AcGlyNHMe optimized at *d* = 2.024 Å

C	-2.32793800	-0.16529000	0.00004800
O	-2.64567400	-1.34729700	0.00037100
N	-1.03097800	0.22890400	-0.00081100
H	-0.72439900	1.19608100	-0.00047300
C	0.06271700	-0.70467600	-0.00086100
H	0.03196000	-1.35669400	-0.88043200
H	0.03131200	-1.35748000	0.87807800
C	1.34625600	0.12379600	-0.00014000
O	1.29421600	1.34652400	-0.00020300
N	2.49896400	-0.58433500	0.00084100
H	2.43666900	-1.59038000	-0.00068100
C	-3.35899900	0.94581900	0.00050400
H	-2.91983100	1.94416700	-0.00001800
H	-3.99472200	0.83276000	-0.87889300
H	-3.99355000	0.83316200	0.88080500
C	3.81582300	0.03231700	0.00028500
H	4.37742200	-0.24744600	-0.89369100
H	3.67951100	1.11100100	0.00987000
H	4.38425000	-0.26276900	0.88485500

AcGlyNHMe optimized at *d* = 1.974 Å

C	-2.32427500	-0.16249700	0.00013600
O	-2.65595900	-1.34087500	0.00134800
N	-1.02351400	0.21677700	-0.00204400
H	-0.69424100	1.17833400	-0.00133800
C	0.06360400	-0.72354300	-0.00152800
H	0.03392900	-1.37505700	-0.88151800
H	0.03255900	-1.37550500	0.87807600
C	1.34217200	0.11306400	-0.00040100
O	1.27370200	1.33553700	0.00002400
N	2.50222900	-0.58114800	0.00002700
H	2.45080200	-1.58783500	-0.00026500
C	-3.34242800	0.96048200	0.00075000
H	-2.89139400	1.95349300	-0.00026200
H	-3.97989000	0.85460600	-0.87830700
H	-3.97785800	0.85547500	0.88138200
C	3.81231800	0.05004200	0.00119700
H	4.38112800	-0.23149100	-0.88754900
H	3.66420200	1.12719400	0.00089300
H	4.37946900	-0.23120400	0.89110300

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Energies of AcGlyNHMe optimized at *d* = 2.974–1.974 Å. Values are corrected for the zero-point vibrational energy.

d (Å)	Energy (Hartree)
2.974	–456.533758
2.924	–456.533586
2.874	–456.533458
2.824	–456.533614
2.774	–456.533817
2.724	–456.533977
2.674	–456.534115
2.624	–456.534316
2.574	–456.534519
2.524	–456.534791
2.474	–456.535157
2.424	–456.535401
2.374	–456.535690
2.324	–456.536146
2.274	–456.536401
2.224	–456.536491
2.174	–456.536475
2.124	–456.536346
2.074	–456.536090
2.024	–456.535714
1.974	–456.535143

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