Supporting Information

Proline/Sidechain C–H/O Interactions Stabilize *cis*-Proline

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Contents

Bioinformatics analysis of conformations at X-Pro sequences in the PDB

Structure data set collection, refinement, and analysis

Structures with a resolution better than 2.5 Å and a sequence similarity of less than 30% were downloaded from the RCSB Protein Data Bank using the PISCES protein server (15,599 structures).[1] Perl scripts were written to generate separate text files containing the PDB codes and residue numbers of Glu-Pro, Gln-Pro, Asp-Pro, Asn-Pro, Ser-Pro, and Thr-Pro sequences from the culled PDB data. Perl scripts were then written to generate text files containing the resolution, chain, residue number, secondary structures, dihedral angles, Ramachandran regions, specified interatomic distances, and neighboring residue identities of each X-Pro structure. In order to avoid counting symmetry-related structures in crystal structures included as extra chains, data were only retrieved from the first chain containing an X-Pro sequence in each structure. The resultant data sets for each X-Pro sequence were manually refined on Microsoft Excel to remove structures with broken pre-proline ϕ angles, structures with a positive Pro ϕ, and structures with broken Pro ψ angles. The data search after refinement yielded 4452 structures with EP sequences, 3519 structures with QP sequences, 5322 structures with DP sequences, 4648 structures with NP sequences, 5188 structures with SP sequences, and 5392 structures with TP sequences.

Estimation of C–H$_\alpha$ hydrogen positions for bioinformatics analysis

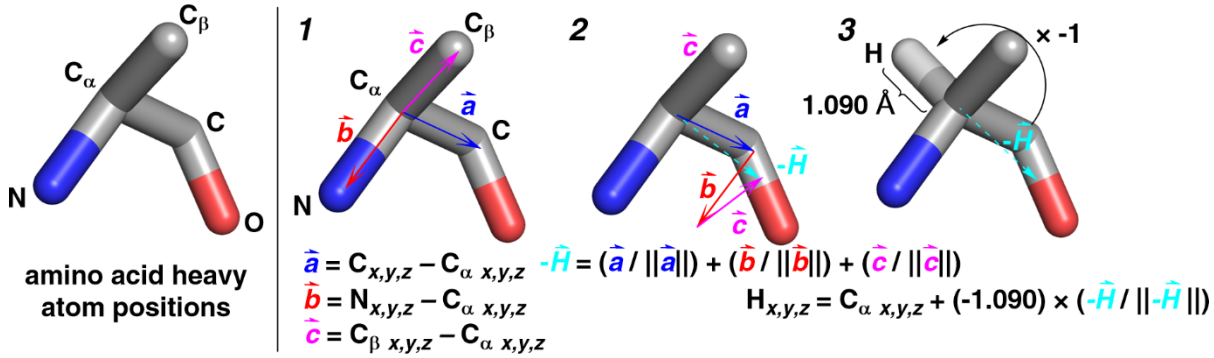

Figure S1. General formula for estimating H$_\alpha$ hydrogen positions from pdb files. H$_\alpha$ hydrogen positions were estimated by (1) generating three vectors from the position of C$_\alpha$ to the neighboring carbonyl C, N, and C$_\beta$; (2) summing the standardized vectors to generate a new vector in the opposite direction of the C–H$_\alpha$ bond; and (3) inverting the new vector, scaling it to a standard C–H bond length of 1.090 Å, and adding it to the position of C$_\alpha$ to generate an estimated position for H$_\alpha$.

Definition and analysis of Ramachandran space

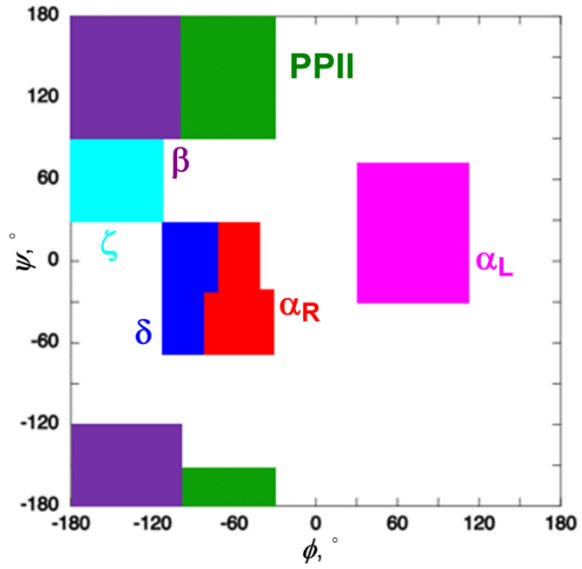

Figure S2. Definition of secondary structures by their position in the Ramachandran plot. Nomenclature and definitions of the regions occupied by residues in the Ramachandran plot. The ϕ, ψ ranges corresponding to the designated regions are indicated in Table S1. The regions outlined have been previously defined.[2]

Table S1. Definitions of conformations as employed in bioinformatics analysis. 10 nonoverlapping rectangular regions were used to define secondary structures via ranges of combinations of ϕ and ψ torsion angles of the Ramachandran plot. The values in parentheses represent the maximum range of the ϕ and ψ values of each region of the Ramachandran plot.

conformation	ϕ, ψ range
α_L	+70° (±40°), +15° (±45°)
α_R	–55° (±15°), +5° (±25°)
α_R	–55° (±25°), –40° (±20°)
β	–140° (±40°), –150° (±30°)
β	–140° (±40°), +135° (±45°)
δ	–90° (±20°), +5° (±25°)
δ	–95° (±15°), –40° (±20°)
PPII	–65° (±35°), +135° (±45°)
PPII	–65° (±35°), –165° (±15°)
ζ	–145° (±35°), +60° (±30°)

Analysis of C_α–H/O interaction frequencies and distances at X-Pro sequences in the PDB

Table S2. Frequencies of C_α–H/O interactions at X-*cis*-Pro sequences in the PDB. C–H/O interactions were defined in structures as C_α–H•••O distances below 2.72 Å. The percent of total X-Pro structures containing the X-*cis*-Pro conformation are reported alongside the percent of X-*cis*-Pro structures containing C–H/O interactions.

X-*cis*-Pro	$\%_{total}$	% C_α–H/O
Glu	7.1	36.5
Ser	5.7	29.7
Gln	4.7	25.5
Asn	4.5	34.1
Thr	3.8	15.7
Asp	3.1	36.5

Table S3. C_α–H•••O interaction distances at X-*trans*-Pro sequences in the PDB. H_α•••O distances at X-*trans*-Pro sequences were analyzed. Distances on intervals of 3.00–4.50 Å, 4.51–6.00 Å, 6.01–7.00 Å , and ≥ 7.00 Å are reported.

		H_α•••O distance, % of structures			
X-*trans*-Pro	$\%_{total}$	3.00–4.50 Å	4.51–6.00 Å	6.01–7.00 Å	≥ 7.00 Å
Glu	92.9	1.2	9.4	45.5	43.7
Ser	94.3	1.2	75.9	22.9	0.0
Gln	95.3	1.1	4.0	36.9	58.0
Asn	95.5	0.5	62.1	19.3	18.1
Thr	96.2	0.3	60.0	39.6	0.0
Asp	96.9	1.0	79.6	16.8	2.7

Analysis of side-chain rotamers at X-Pro structures in the PDB

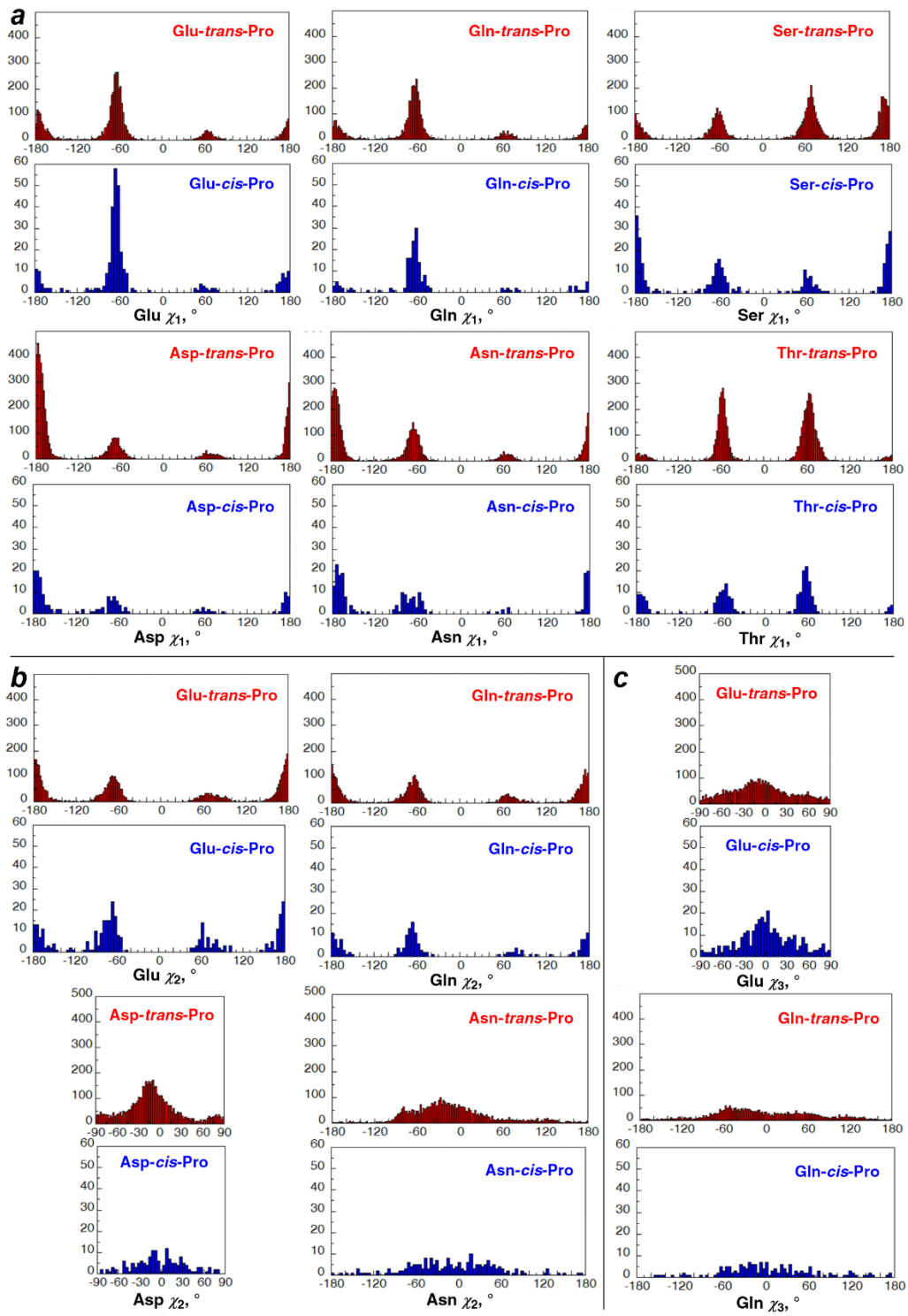

Figure S3. Pre-proline side-chain χ rotamers at X-Pro sequences in the PDB. Histograms of side-chain χ angles [(a) χ_1, (b) χ_2, (c) χ_3] of pre-proline residues in the PDB. Structures were separated by Pro amide conformation.

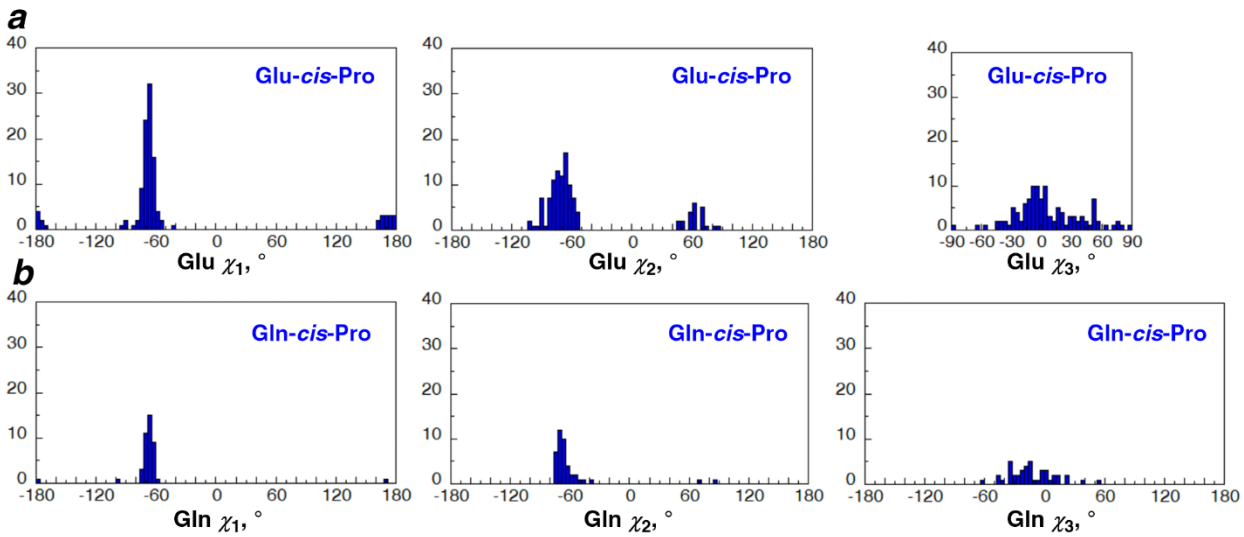

Figure S4. Pre-proline side-chain χ rotamers at Glu-Pro and Gln-Pro sequences in the PDB exhibiting C–H/O interactions with Pro C–H$_\alpha$. (a) Glu-*cis*-Pro and (b) Gln-*cis*-Pro structures stabilized via C–H/O interactions (C$_\alpha$–H•••O distances ≤ 2.72 Å) were analyzed to determine side-chain χ dihedral angles. C–H/O interactions at Glu-*cis*-Pro can be mediated by either the g^- χ_1 rotamer and the g^- χ_2 rotamer (82%) or via the t χ_1 rotamer and the g^+ χ_2 rotamer (18%). In contrast, C–H/O interactions at Gln-*cis*-Pro are mediated almost exclusively via the g^- χ_1 rotamer and the g^- χ_2 rotamer. A small percentage of C–H/O interactions at Gln-*cis*-Pro sequences can be mediated by the t χ_1 rotamer and the g^+ χ_2 rotamer (5%). Glu residues engaged in C–H/O interactions with Pro C–H$_\alpha$ also appear to have more rotational freedom of the χ_3 dihedral angle compared to preproline Gln residues engaged in C–H/O interactions. The Glu χ_3 dihedral was standardized to a range of -90° to +90° in order to normalize for the symmetrical side-chain carboxylate oxygens.

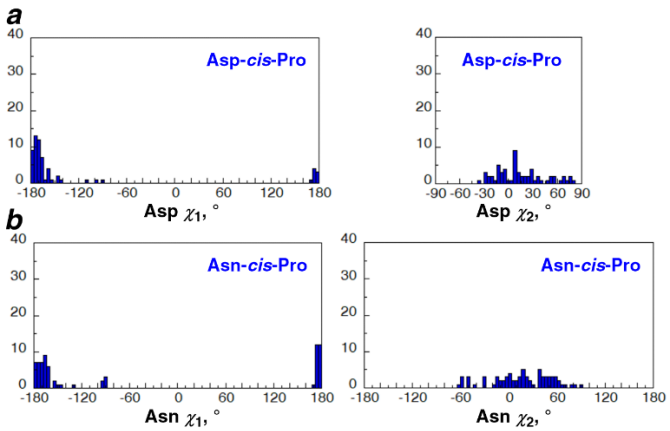

Figure S5. Pre-proline side-chain χ rotamers at Asp-Pro and Asn-Pro sequences in the PDB exhibiting C–H/O interactions with Pro C–H$_\alpha$. (a) Asp-*cis*-Pro and (b) Asn-*cis*-Pro structures stabilized via C–H/O interactions (C$_\alpha$–H•••O distances ≤ 2.72 Å) were analyzed to determine side-chain χ dihedral angles. C–H/O interactions at Asp-*cis*-Pro and Asn-*cis*-Pro are mediated almost exclusively via the *t* χ_1 rotamer. A small percentage of C–H/O interactions can alternatively be mediated by a χ_1 dihedral angle around –90° (7% and 5%, respectively).

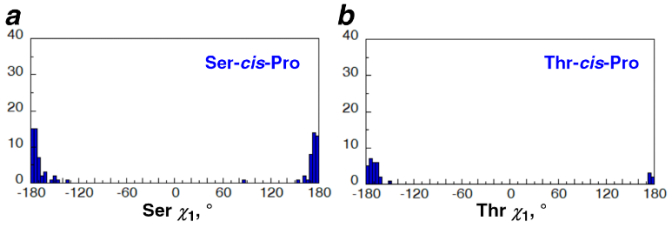

Figure S6. Pre-proline side-chain χ rotamers at Ser-Pro and Thr-Pro sequences in the PDB exhibiting C–H/O interactions with Pro C–H$_\alpha$. (a) Ser-*cis*-Pro and (b) Thr-*cis*-Pro structures stabilized via C–H/O interactions (C$_\alpha$–H•••O distances ≤ 2.72 Å) were analyzed to determine side-chain χ dihedral angles. C–H/O interactions at Ser-*cis*-Pro and Thr-*cis*-Pro are mediated almost exclusively via the *t* χ_1 rotamer.

Table S4. Frequency of the Pro *endo* ring pucker at X-*cis*-Pro sequences with C–H/O interactions.

X-*cis*-Pro with C$_\alpha$–H/O	% Pro$_{endo}$
Glu	87.8
Ser	96.6
Gln	92.9
Asn	87.3
Thr	87.5
Asp	86.9

Table S5. Frequency of type VIa1 (PcisD) β-turns at X-*cis*-Pro sequences in the PDB.

X-*cis*-Pro	% VIa1 (PcisD)
Glu	17.1
Ser	17.7
Gln	13.9
Asn	9.1
Thr	9.3
Asp	12.6

Table S6. Frequency of X-*cis*-Pro type VIa1 β-turns in the PDB with C–H/O interactions with Pro C–H$_\alpha$. C–H/O interactions were defined in structures as C$_\alpha$–H•••O distances ≤ 2.72 Å.

X-*cis*-Pro VIa1 (PcisD)	% C$_\alpha$–H/O
Glu	62
Ser	58
Gln	52
Asn	44
Thr	15
Asp	53

Table S7. Frequency of C–H/O interactions and C–H/π interactions at X-*cis*-Pro sequences. Glu, Gln, Asn, and Asp each have side-chain carboxylates or carboxamides whose π systems are capable of donating electrons to Pro C–H$_\alpha$ σ*, a stereoelectronic interaction capable of stabilizing the *cis*-amide conformation at proline, which is a mode of C–H/O interactions additional or alternative to interaction with the oxygen lone pairs. C–H/O interactions at X-*cis*-Pro sequences were defined in structures as C$_\alpha$–H•••O$_\delta$ distances (Asp and Asn) or C$_\alpha$–H•••O$_\varepsilon$ distances (Glu and Gln) ≤ 2.72 Å. C–H/π interactions at X-*cis*-Pro sequences were defined in structures as C$_\alpha$–H•••C$_\gamma$ distances (Asp and Asn) or C$_\alpha$–H•••C$_\delta$ distances (Glu and Gln) ≤ 2.90 Å.

X-*cis*-Pro	%$_{total}$	% C$_\alpha$–H/O only	% C$_\alpha$–H/π only	% either	% both	% any
Glu	7.1	31.4	1.6	33.0	4.4	37.5
Gln	4.7	24.2	1.8	26.1	1.2	27.3
Asn	4.5	28.4	1.0	29.3	5.3	34.6
Asp	3.1	32.3	0.6	32.9	4.2	37.1

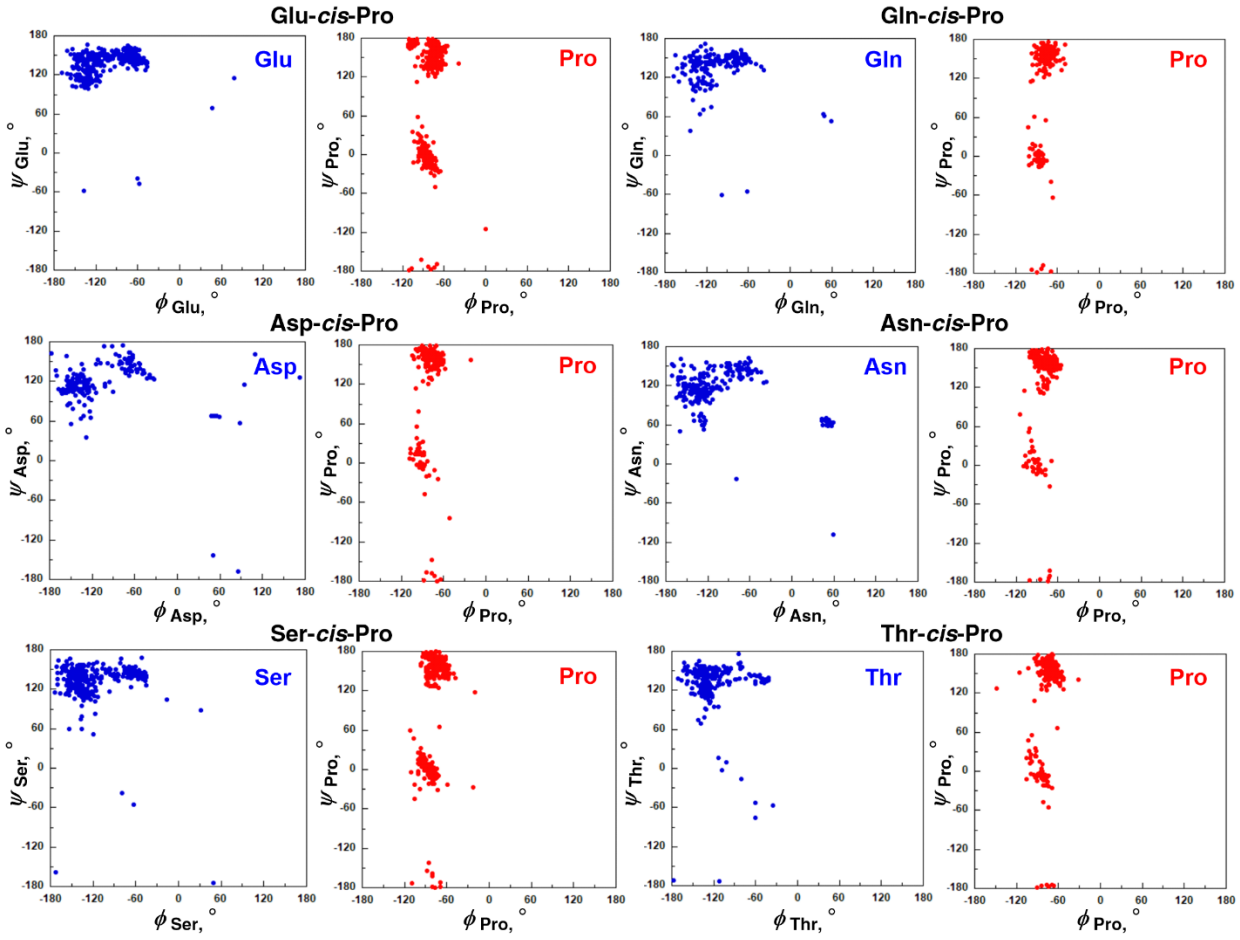

Figure S7. Ramachandran plots of X-*cis*-Pro sequences in the PDB. The backbone dihedral angles of the residues at X-*cis*-Pro sequences in the PDB are represented on Ramachandran plots. The dihedral angles of preproline residues are indicated in blue, while the dihedral angles of proline at each sequence are indicated in red.

Table S8. Frequencies of backbone conformations at proline and pre-proline residues in X-*cis*-Pro sequences in the PDB. The frequencies of backbone conformations at individual proline and pre-proline residues at X-*cis*-Pro sequences in the PDB are tabulated. Conformations that are significantly populated by each X-*cis*-Pro structure (> 5% of structures) are in bold. Conformations that are unoccupied by any structures are omitted for clarity.

	% **X**-*cis*-Pro						% **Pro**					
conformation	Glu	Gln	Asp	Asn	Ser	Thr	at EP	at QP	at DP	at NP	at SP	at TP
α_R	0.6	0.6	0.0	0.5	0.7	1.0	3.2	0.6	0.6	1.0	1.0	2.0
δ	0.0	0.0	0.0	0.0	0.0	1.5	**27.6**	**23.0**	**18.6**	**15.9**	**27.6**	**17.6**
β	**58.4**	**61.8**	**52.1**	**61.5**	**65.5**	**76.0**	**6.7**	0.0	1.8	2.4	0.3	1.5
PPII	**40.0**	**32.1**	**33.5**	**23.6**	**31.0**	**19.1**	**60.3**	**72.1**	**70.7**	**74.5**	**67.6**	**76.0**
ζ	0.0	3.0	**7.8**	**6.7**	2.0	1.5	0.6	1.8	4.2	4.8	1.3	0.0
α_L	0.0	0.6	1.8	1.4	0.0	0.0	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
undefined	1.0	1.8	4.8	**6.3**	0.7	1.0	1.6	2.4	4.2	1.4	2.0	2.9

Table S9. Frequencies of combinations of backbone conformations at X-*cis*-Pro sequences in the PDB. The frequencies of combinations of backbone conformations at X-*cis*-Pro sequences in the PDB are tabulated. Conformation pairs that are significantly populated in each X-*cis*-Pro structure (> 5% of structures) are in bold. Combinations of conformations that are unoccupied by any structures are omitted for clarity.

conformation		% of X-*cis*-Pro structures					
X	**P**	**EP**	**QP**	**DP**	**NP**	**SP**	**TP**
α_R	β	0.3	0.0	0.0	0.0	0.0	0.0
α_R	PPII	0.3	0.6	0.0	0.0	0.7	1.0
α_R	undefined	0.0	0.0	0.0	0.5	0.0	0.0
α_L	PPII	0.0	0.6	1.8	1.4	0.0	0.0
β	α_R	2.5	0.0	0.0	0.0	0.3	2.0
β	β	0.0	0.0	0.0	0.5	0.0	1.0
β	δ	**9.8**	**7.9**	3.6	**6.3**	**9.2**	**5.9**
β	PPII	**45.7**	**52.7**	**47.3**	**54.3**	**55.3**	**66.2**
β	ζ	0.0	0.0	0.0	0.5	0.0	0.0
β	undefined	0.3	1.2	1.2	0.0	0.7	1.0
δ	δ	0.0	0.0	0.0	0.0	0.0	1.5
PPII	α_R	0.6	0.6	0.0	0.5	0.7	0.0
PPII	β	**6.3**	0.0	0.6	0.0	0.3	0.0
PPII	δ	**17.5**	**13.9**	**13.8**	**8.7**	**17.7**	**9.8**
PPII	PPII	**14.3**	**16.4**	**16.2**	**13.5**	**10.2**	**7.4**
PPII	ζ	0.0	0.0	0.0	0.0	0.6	0.0
PPII	undefined	1.3	1.2	3.0	1.0	1.4	2.0
ζ	β	0.0	0.0	1.2	0.5	0.0	0.0
ζ	δ	0.0	1.2	1.2	1.0	0.7	0.0
ζ	PPII	0.0	1.8	**5.4**	**5.3**	1.4	1.5
undefined	α_R	0.0	0.0	0.6	0.5	0.0	0.0
undefined	β	0.0	0.0	0.0	1.4	0.0	0.5
undefined	δ	0.3	0.0	0.0	0.0	0.0	0.5
undefined	ζ	0.6	1.8	4.2	4.3	0.7	0.0

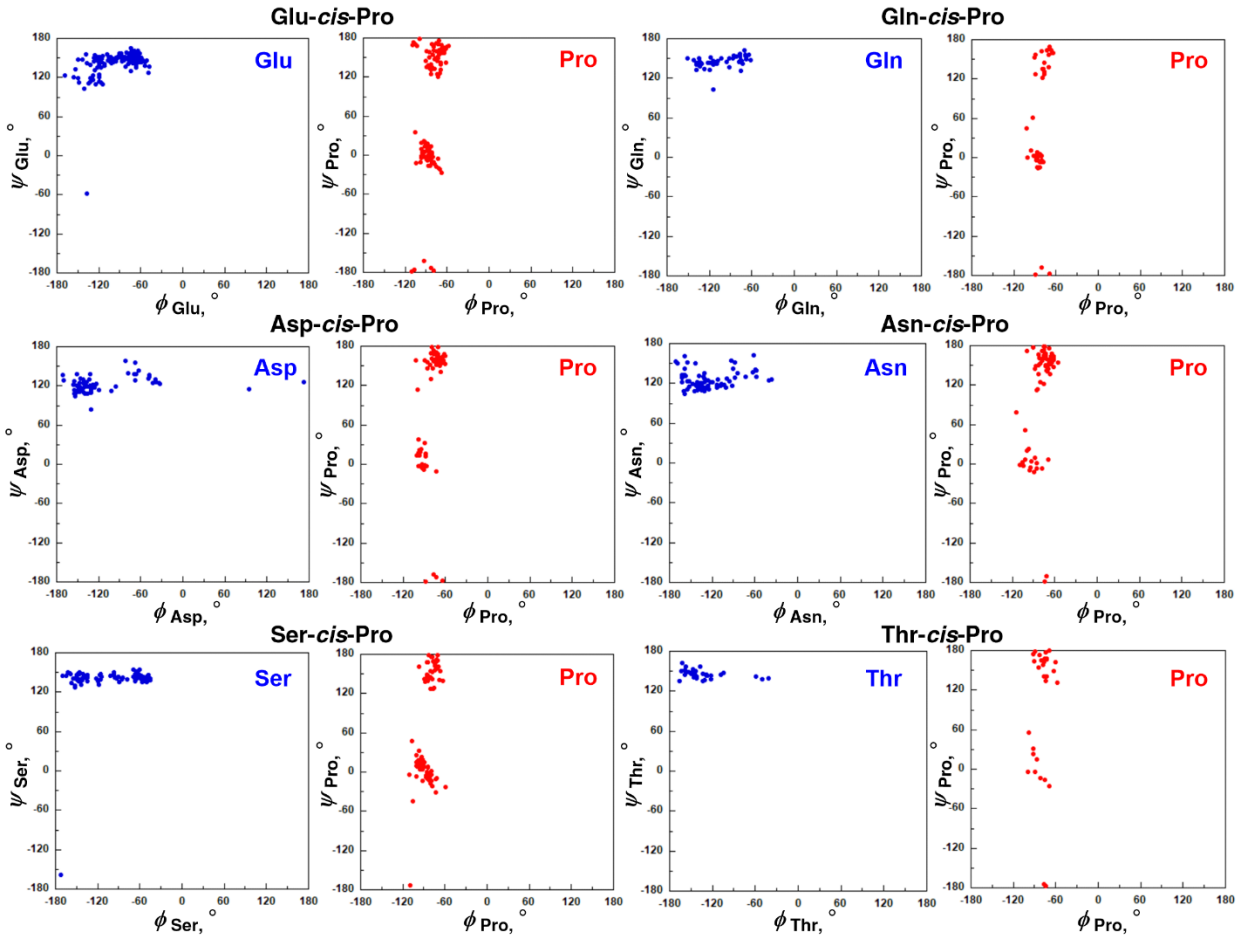

Figure S8. Ramachandran plots of X-*cis*-Pro sequences with C_α–H/O interactions in the PDB. The backbone dihedral angles of the residues at X-*cis*-Pro sequences in the PDB containing C–H/O interactions are represented on Ramachandran plots. C–H/O interactions were defined in structures as C_α–H•••O distances below 2.72 Å. The dihedral angles of preproline residues are indicated in blue, while the dihedral angles of proline at each sequence are indicated in red.

Table S10. Frequencies of backbone conformations at pre-proline and proline residues in X-*cis*-Pro sequences with C_α–H/O interactions in the PDB. The frequencies of backbone conformations at individual pre-proline and proline residues at X-*cis*-Pro sequences with C_α–H/O interactions in the PDB are tabulated. Conformations that are significantly populated by each X-*cis*-Pro structure (> 5% of structures) are in bold. Conformations that are unoccupied by any structures are omitted for clarity.

	% **X-*cis*-Pro**						% **Pro**					
conformation	Glu	Gln	Asp	Asn	Ser	Thr	at EP	at QP	at DP	at NP	at SP	at TP
α_R	0	0	0	0	0	0	3	0	0	1	3	3
δ	0	0	0	0	0	0	**44**	**48**	**25**	**24**	**49**	**19**
β	**47**	**52**	**72**	**77**	**47**	**88**	**6**	0	2	0	1	0
PPII	**53**	**48**	**26**	**23**	**53**	**13**	**45**	**48**	**67**	**72**	**43**	**72**
ζ	0	0	2	0	0	0	0	0	0	1	0	0
α_L	0	0	0	0	0	0	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
undefined	0	0	0	0	0	0	2	**5**	**7**	1	3	**6**

Table S11. Frequencies of combinations of backbone conformations at X-*cis*-Pro sequences with C_α–H/O interactions in the PDB. The frequencies of combinations of backbone conformations at X-*cis*-Pro sequences with C_α–H/O interactions in the PDB are tabulated. Conformations that are significantly populated by each X-*cis*-Pro structure (> 5% of structures) are in bold. Combinations of conformations that are unoccupied by any structures are omitted for clarity.

conformation		**% of X-*cis*-Pro structures with C_α–H/O interations**					
X	**P**	**EP**	**QP**	**DP**	**NP**	**SP**	**TP**
β	α_R	3	0	0	0	1	3
β	δ	**15**	**19**	**8**	**13**	**15**	**9**
β	PPII	**29**	**31**	**61**	**63**	**30**	**72**
β	ζ	0	0	0	1	0	0
β	undefined	1	2	3	0	1	3
PPII	α_R	0	0	0	1	2	0
PPII	β	**6**	0	0	0	1	0
PPII	δ	**30**	**29**	**16**	**11**	**34**	**9**
PPII	PPII	**17**	**17**	**7**	**8**	**13**	0
PPII	undefined	1	2	3	1	2	3
ζ	β	0	0	2	0	0	0

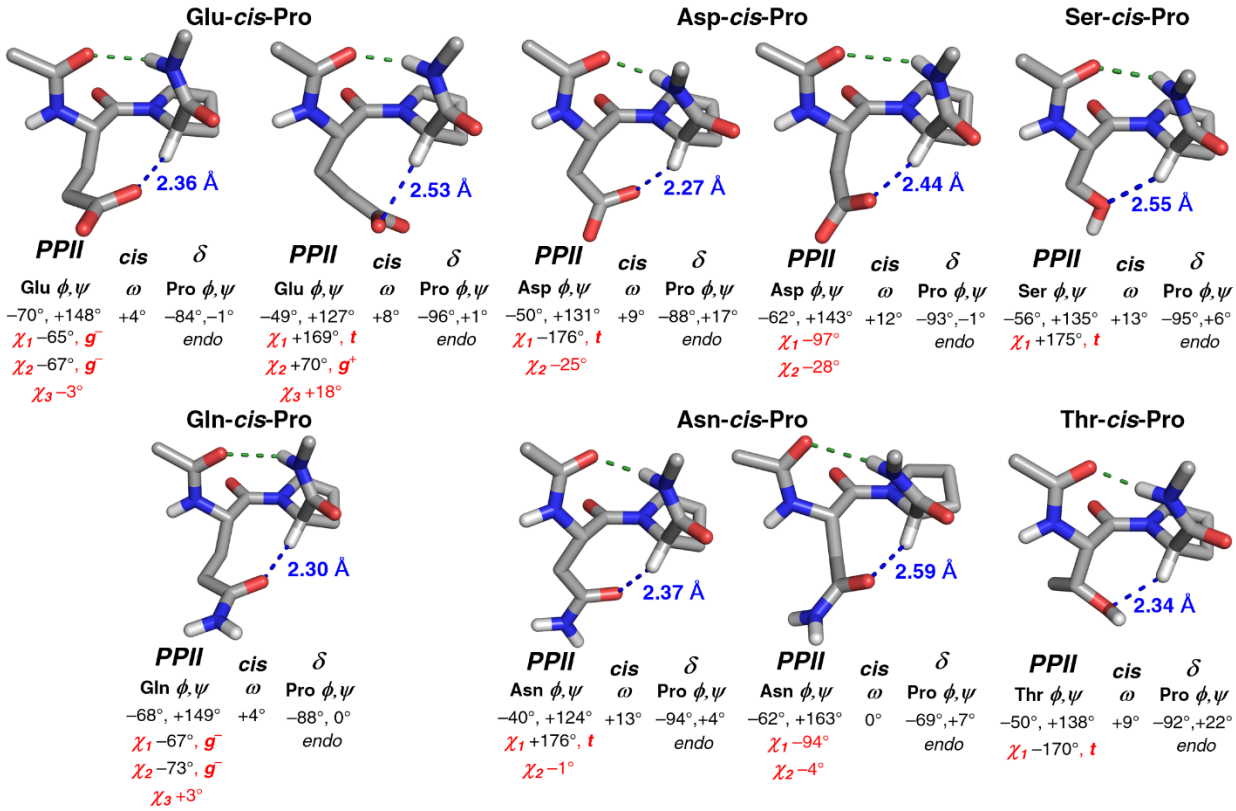

Figure S9. Interaction modes of C–H/O interactions in type VIa1 β-turns in the PDB. Type VIa1 β-turns (PPII-*cis*-δ, PcisD) were analyzed at Glu-*cis*-Pro [pdb 7f82 (left) and 4yzo (right)], Asp-*cis*-Pro [pdb 4y7s (left) and 3ksx (right)], Ser-*cis*-Pro (pdb 4d0q), Gln-*cis*-Pro (pdb 3l8a), Asn-*cis*-Pro [pdb 4i79 (left) and 3oyv (right)], and Thr-*cis*-Pro (pdb 7u9u) sequences in the PDB. A structure of Gln in the type VIa1 β-turn conformation with the combination of $\chi_1 = t$, $\chi_2 = g^+$ was not observed, although interactions with this rotamer pair were observed in other type VI β-turn subtypes (VIb [BcisP] pdb 2jks, VIb [PcisP] pdb 3oyv).

Computational methods and analysis

Calculations

All calculations were conducted using Gaussian09. NBO calculations were conducted using NBO6 as implemented within Gaussian09. Orbital analysis was conducted in GaussView5 using isovalues of 0.02. Visualization of structures was conducted with PyMOL.

Full geometry optimization of minimal model peptides

Structures of all minimal Ac-X-*cis*-Pro-NHMe peptides (X = Glu, Gln, Asp, Asn, Ser, Thr) were generated via truncation of structures from the Protein Data Bank. Structures were subjected to iterative geometry optimization, with the final geometry optimization calculations conducted using the M06-2X DFT functional, the 6-311++G(d,p) basis set, and implicit water solvation (IEFPCM continuum polarization model). Frequency calculations were conducted with the same combination of functional, basis set, and solvent model, and indicated no negative (imaginary) frequencies.

Structures of Ac-X-*cis*-Pro-NHMe (X = pSer or pThr) were either generated via modification of Glu to pSer or pThr, or via structures of Ac-pSer-*trans*-Pro-NHMe or Ac-pThr-*trans*-Pro-NHMe described previously, with appropriate rotation of torsion angles prior to full geometry optimization as described above. Ionization state was modified within GaussView, prior to full geometry optimization in each ionization state and conformation.

Structures of Ac-X-*cis*-Ala-NHMe peptides were initially generated via modification of the proline residue of Ac-X-*cis*-Pro-NHMe peptides to Ala within GaussView, followed by full geometry optimization. Structures of Ac-Glu-*cis*-[Gly/Ala/fluorinated versions thereof]-NHMe peptides were generated via structure modification in an analogous manner in GaussView, followed by full geometry optimization.

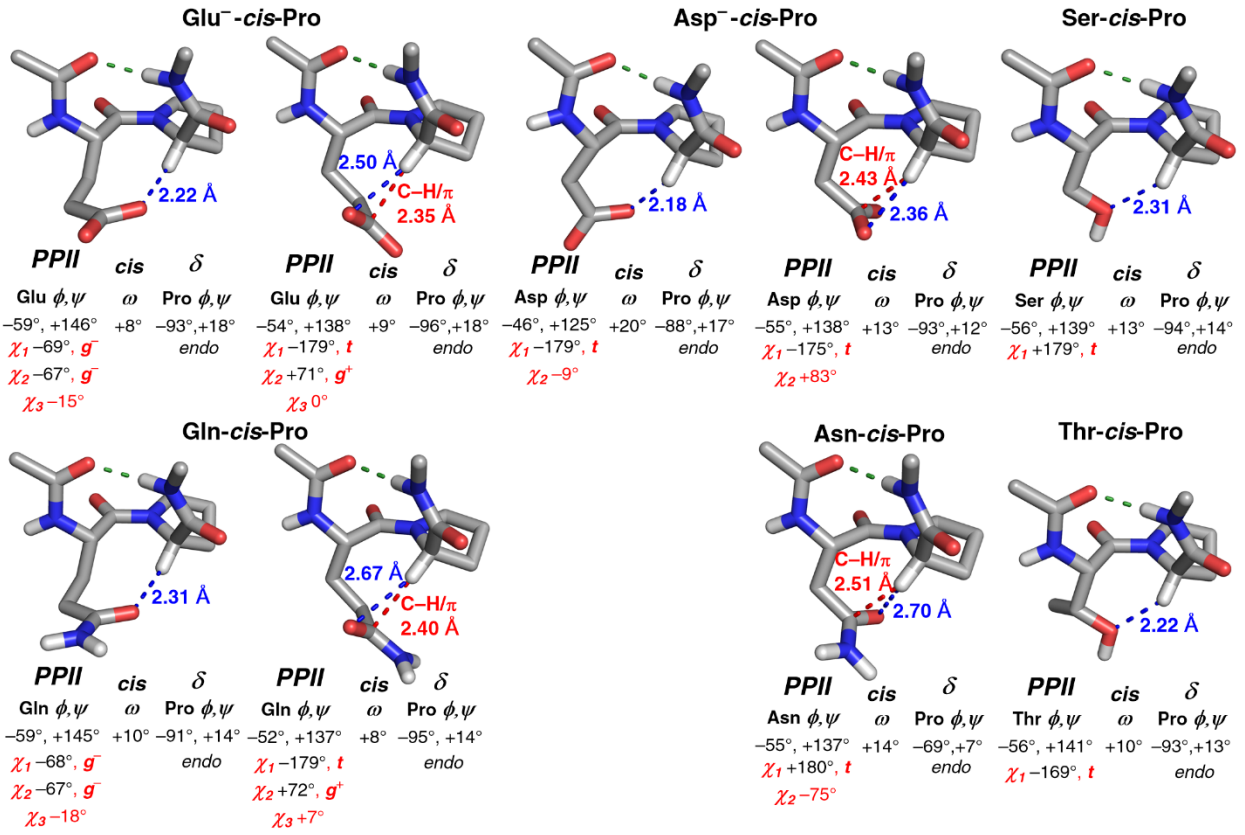

Figure S10. C–H/O interactions with Pro C–H$_\alpha$ in geometry-optimized structures with X-*cis*-Pro amide bonds in type VIa1 β-turns. Structures from the PDB (Figure 4) were modified to Ac-X-*cis*-Pro-NHMe and then subjected to geometry optimization to examine the conformations at pre-proline residues which can stabilize the *cis*-Pro conformation via C–H/O interactions (H$_\alpha$•••O distances, blue). Glu, Gln, Asp, and Asn all have one interaction mode where the nearest interaction is a C–H/π interaction between the amide or carboxylate π orbitals and Pro C–H$_\alpha$ (red). C–H/π interactions were defined as C$_{C=O}$••H distances at or below the sum of the van der Waals radii of C and H (≤ 2.90 Å). Conformations at Asp-Pro with Asp $\chi_1 = -100°$, $\chi_2 = -30°$ and Asn-Pro with Asn $\chi_1 = -90°$, $\chi_2 = -30°$ were observed with C–H/O interactions with Pro C–H$_\alpha$ in the PDB but optimized to alternative structures with intraresidue C–H/O interactions, and thus were not included.

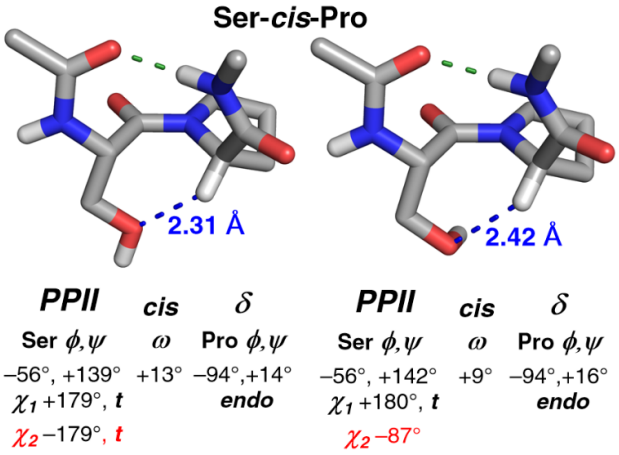

Figure S11. Effects of Ser χ_2 rotamer on C–H/O interaction distance in Ser-*cis*-Pro. Structures of Ac-Ser-*cis*-Pro-NHMe in a type VIa1 β-turn conformation were geometry-optimized as a function of the χ_2 dihedral angle of Ser. The side-chain hydroxyl of both Ser and Thr residues does not have a reliably determined hydrogen position in structures in the PDB. When Ser χ_2 adopts the *t* rotamer, the C–H/O interaction with Pro C–H_α is significantly closer than when it adopts a χ_2 of –87°.

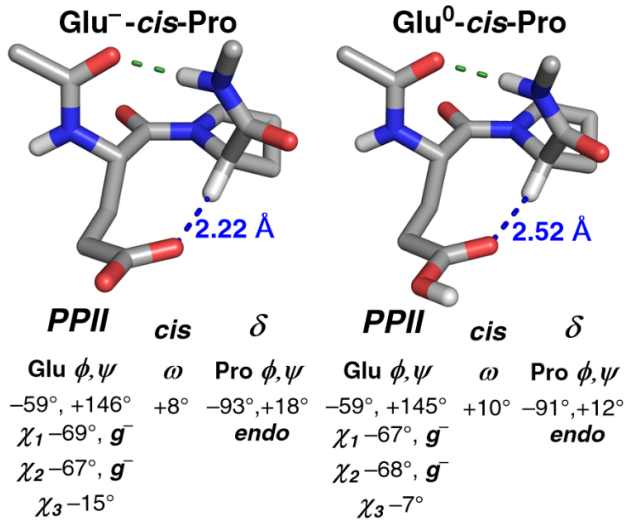

Figure S12. Effect of Glu ionization state on C–H/O interactions in geometry-optimized structures of Glu-*cis*-Pro in a type VIa1 β-turn conformation. Structures of Ac-Glu-*cis*-Pro-NHMe in a type VIa1 β-turn conformation were geometry optimized, in either the (left) anionic or (right) neutral side-chain ionization state to identify the effects of charge and electron density on the donor oxygen on H_α•••O distance (blue) and the strength of C–H/O interactions with Pro C–H_α. The anionic side chain exhibited a significantly closer C–H/O interaction than the neutral side chain.

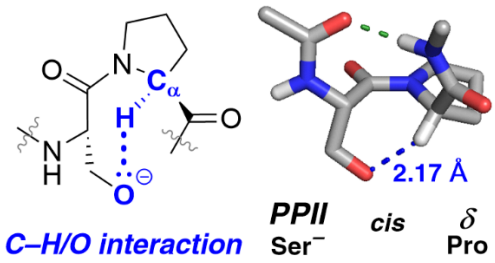

Figure S13. Geometry-optimized structure of Ac-Ser⁻-*cis*-Pro-NHMe (anionic Ser) in a type VIa1 β-turn with a C–H/O interaction. Ac-Ser⁻-*cis*-Pro-NHMe in a type VIa1 β-turn structure with an oxyanion at the Ser side chain was subjected to full geometry optimization to analyze the effect of a full negative charge on the ability of Ser to stabilize a C–H/O interaction.

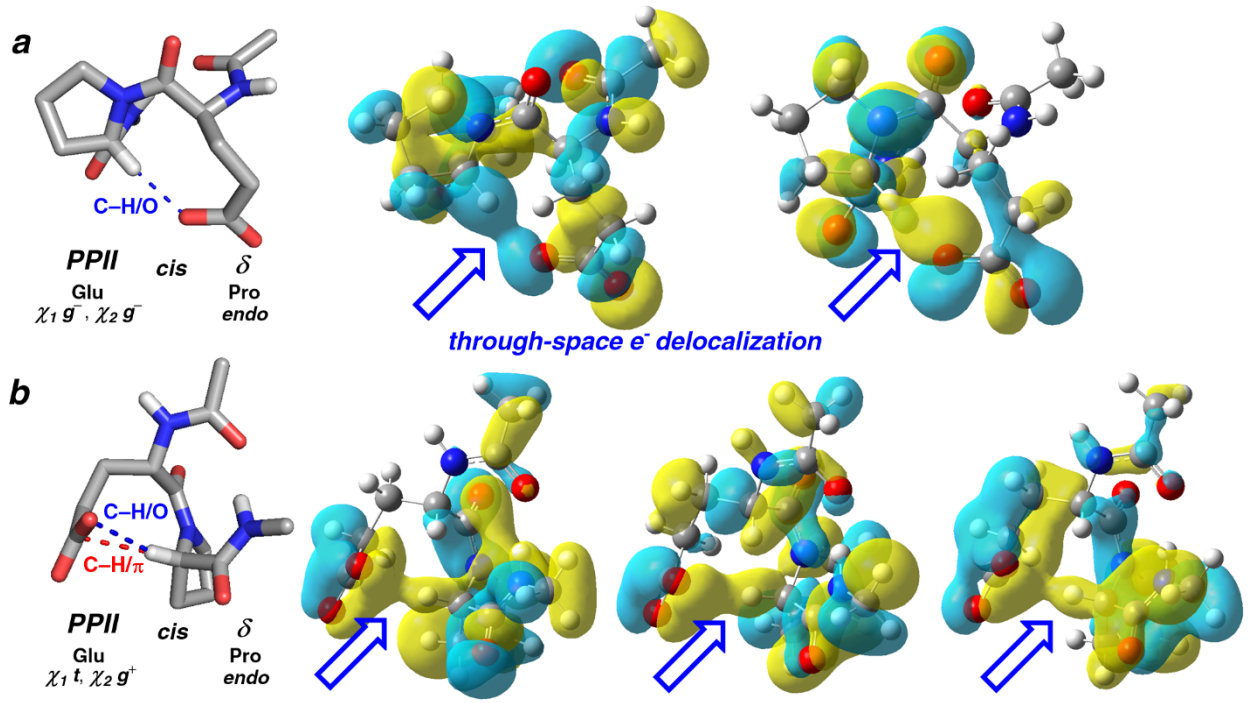

Figure S14. Molecular orbitals contributing to the stabilization of Glu-*cis*-Pro via C–H/O and C–H/π interactions. Full molecular orbital calculations were conducted on Glu-*cis*-Pro in a type VIa1 β-turn conformation with Glu (a) $\chi_1 = g^-$, $\chi_2 = g^-$ and (b) $\chi_1 = t$, $\chi_2 = g^+$, in order to assess the global contribution of molecular orbitals to stabilization of the *cis*-amide conformation via C–H/O and C–H/π interactions**.** Both conformations exhibit extensive through-space electron delocalization between the Glu carboxylate and Pro C–H_α, as observed by orbital lobes (arrows, single color = same sign of wave function) that extend between Glu and Pro.

Table S12. Calculated electronic interaction energies of C–H/O and C–H/π interactions stabilizing Glu-*cis*-Pro and Gln-*cis*-Pro in water. The interaction energies of C–H/O and C–H/π interactions stabilizing Glu-*cis*-Pro and Gln-*cis*-Pro structures were examined by comparing the calculated electronic energies of geometry-optimized structures containing the interactions of interest to the corresponding structures with side chains rotated to the non-interacting *t* rotamer and subsequent geometry optimization. Direct comparisons could only be made in the absence of confounding hydrogen bonding between the Glx carboxylate or carboxamide and the peptide backbone; the *t* rotamer for all other residues exhibited alternative interactions.

X-*cis*-Pro	χ_1	χ_2	ΔE, kcal mol^{-1}
Glu$^-$	g^-	g^-	–3.0
	t	g^+	–1.8
Gln	g^-	g^-	–2.4
	t	g^+	–1.4
Glu^0	g^-	g^-	–2.0

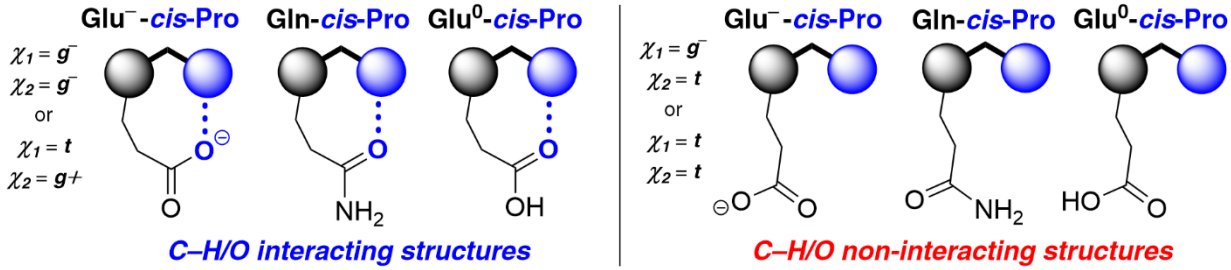

Figure S15. Glu-*cis*-Pro and Gln-*cis*-Pro interaction modes optimized to determine C–H/O and C–H/π interaction energies. Graphical depictions of identified C–H/O interaction modes and non-interacting structures obtained via side-chain rotation to be used as a reference for calculating interaction energies.

Table S13. Calculated electronic interaction energies of C–H/O and C–H/π interactions stabilizing Glu-*cis*-Pro and Gln-*cis*-Pro as a function of solvent polarity. The interaction energies of C–H/O and C–H/π interactions stabilizing Glu-*cis*-Pro and Gln-*cis*-Pro structures were examined by comparing the calculated electronic energies of full geometry-optimized structures containing the interactions of interest with the corresponding Glu-*cis*-Pro and Gln-*cis*-Pro energies with the side chain rotated away from the C–H/O or C–H/π interaction after full geometry optimization in the indicated solvents. Non-interacting structures were obtained by rotating the Glu or Gln χ_2 to the *trans* rotamer and subsequent geometry optimization to yield non-interacting (χ_1 g^-, χ_2 t) and (χ_1 t, χ_2 t) structures, respectively. Solvent dielectric constants were varied in order to understand the electrostatics component of C–H/O interactions.

		ΔE, kcal mol^{-1}				
		χ_1 g^-, χ_2 g^-			χ_1 t, χ_2 g^+	
solvent	**ε**	**Glu$^-$**	**Gln**	**Glu^0**	**Glu$^-$**	**Gln**
vacuum	1	–5.74	–5.37	–2.09	–2.50	–1.83
hexane	1.9	–3.86	–3.22	–1.90	–2.21	–1.66
$CHCl_3$	4.7	–2.78	–1.98	–1.83	–2.14	–1.50
CH_2Cl_2	8.9	–2.70	–1.78	–1.85	–2.22	–1.46
acetone	20.5	–2.83	–1.76	–1.92	–2.30	–1.41
MeCN	36	–2.92	–1.79	–1.94	–2.35	–1.39
DMSO	47	–2.95	–1.81	–1.95	–2.37	–1.38
H_2O	78	–3.00	–1.83	–1.96	–2.39	–1.37
ε = 1000	1000	–3.07	–1.87	–1.97	–2.42	–1.35
ε = 10000	10000	–3.08	–1.87	–1.97	–2.42	–1.35
ε = 100000	100000	–3.08	–1.87	–1.97	–2.42	–1.35
ε = 1000000	1000000	–3.08	–1.87	–1.97	–2.42	–1.35

Table S14. C–H/O interaction distances calculated for Glu-*cis*-Pro and Gln-*cis*-Pro structures with Glx χ_1 g^-, χ_2 g^-. The calculated C–H/O interaction distances of Glu-*cis*-Pro and Gln-*cis*-Pro with Glx χ_1 g^-, χ_2 g^- were determined as a function of solvent polarity from the structures analyzed in Table S13.

		C_α–H/O distance, Å		
solvent	**ε**	**Glu⁻**	**Gln**	**Glu⁰**
vacuum	1	2.048	2.313	2.382
hexane	1.9	2.137	2.299	2.371
$CHCl_3$	4.7	2.197	2.297	2.364
CH_2Cl_2	8.9	2.218	2.301	2.368
acetone	20.5	2.226	2.302	2.380
MeCN	35.7	2.217	2.307	2.381
DMSO	46.8	2.216	2.309	2.383
H_2O	78.3	2.218	2.311	2.384
ε = 1000	1000	2.221	2.315	2.386
ε = 10000	10000	2.221	2.315	2.387
ε = 100000	100000	2.222	2.315	2.387
ε = 1000000	1000000	2.222	2.315	2.387

Table S15. C–H/O and C–H/π interaction distances calculated for Glu⁻-*cis*-Pro and Gln-*cis*-Pro structures with Glx χ_1 t, χ_2 g^+. The calculated C–H/O and C–H/π interaction distances of Glu-*cis*-Pro and Gln-*cis*-Pro with Glx χ_1 t, χ_2 g^+ were determined as a function of solvent polarity from the structures analyzed in Table S13.

		C_α–H/O distance, Å		C_α–H/π distance, Å	
solvent	**ε**	**Glu⁻**	**Gln**	**Glu⁻**	**Gln**
vacuum	1	2.304	2.677	2.352	2.404
hexane	1.9	2.316	2.658	2.374	2.405
$CHCl_3$	4.7	2.379	2.645	2.372	2.407
CH_2Cl_2	8.9	2.396	2.639	2.392	2.404
acetone	20.5	2.468	2.670	2.362	2.401
MeCN	35.7	2.484	2.669	2.356	2.398
DMSO	46.8	2.489	2.669	2.355	2.398
H_2O	78.3	2.498	2.668	2.352	2.396
ε = 1000	1000	2.508	2.670	2.348	2.395
ε = 10000	10000	2.508	2.670	2.348	2.395
ε = 100000	100000	2.508	2.669	2.348	2.394
ε = 1000000	1000000	2.508	2.669	2.348	2.394

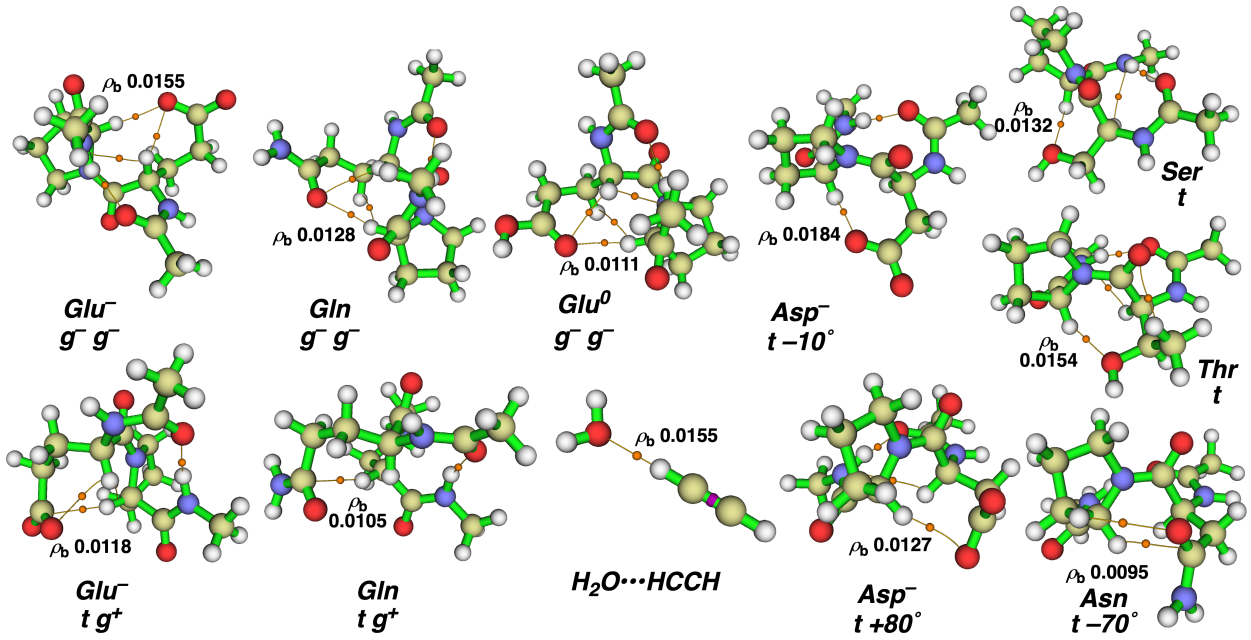

Figure S16. Atoms in Molecules (AIM) analysis of C–H/O interactions in geometry-optimized structures. Structures are shown with the indicated combination of sidechain conformations at χ_1 and χ_2 for Glu, Gln, Asp, and Asn, or with the indicated sidechain conformations at χ_1 for Ser and Thr. The calculated structures (as formatted checkpoint files) were used as input files for AIM analysis within Multiwfn. Calculated Bond Critical Points (BCPs) are indicated by orange spheres. Calculated pathways from bond critical points are indicated by yellow lines. Electron densities (ρ_b) at the key BCPs between the side chain atom and Pro Hα are indicated. The structure of acetylene•OH_2 was determined in implicit water via the same methods used for structures on peptides. The calculated H•••O distance in acetylene•OH_2 is 2.13 Å.

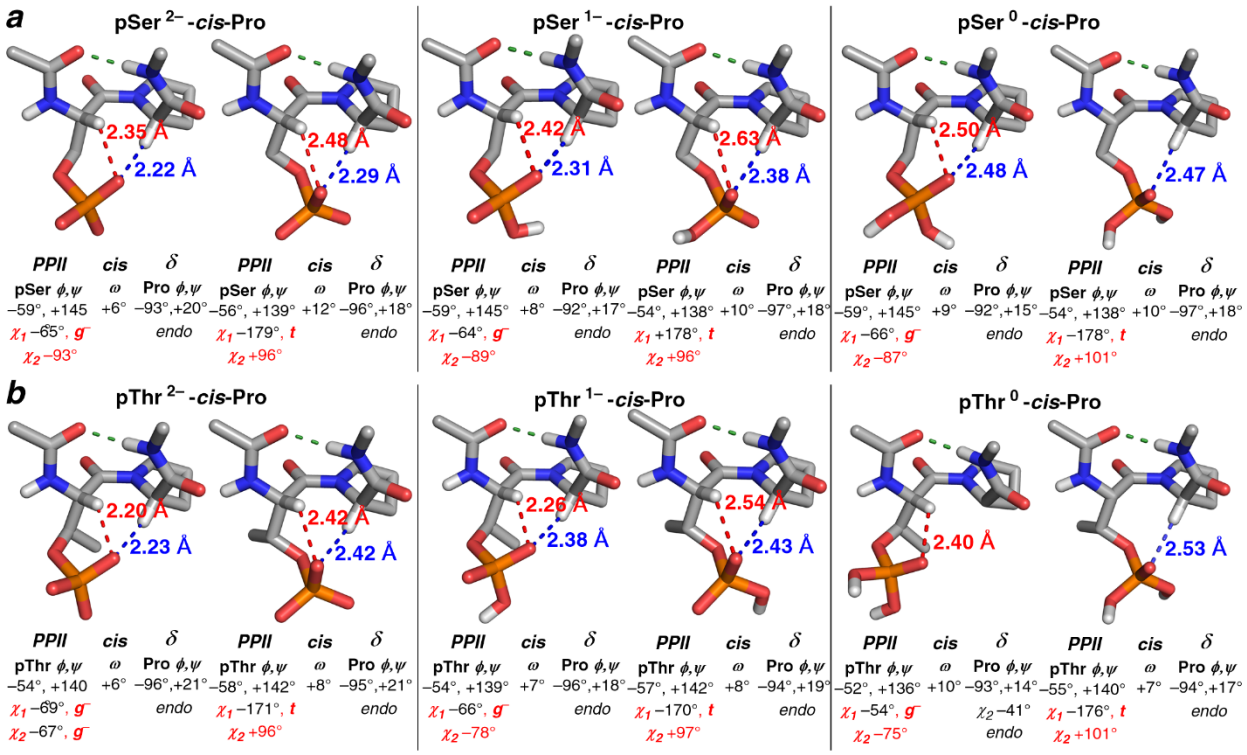

Figure S17. C–H/O interactions in pSer-*cis*-Pro and pThr-*cis*-Pro as a function of phosphate ionization state. Geometry-optimized structures of (a) Ac-pSer-*cis*-Pro-NHMe and (b) Ac-pThr-*cis*-Pro-NHMe in a type VIa1 β-turn conformation. Different ionization states were examined to understand the effect of electron density at oxygen on C–H/O interaction distances and strength. pSer-*cis*-Pro tends to optimize to include a C–H/O interaction with Pro C–H_α (blue). Longer bidentate interactions with both Pro C–H_α (blue) and Ser C–H_α (red) are also observed in some structures. Conversely, pThr-*cis*-Pro tends to include bidentate C–H/O interactions with both Thr C–H_α (red) and Pro C–H_α (blue) that have similar H_α•••O distances. Globally, pSer-*cis*-Pro tends to form closer C–H/O interactions with Pro C–H_α than pThr-*cis*-Pro.

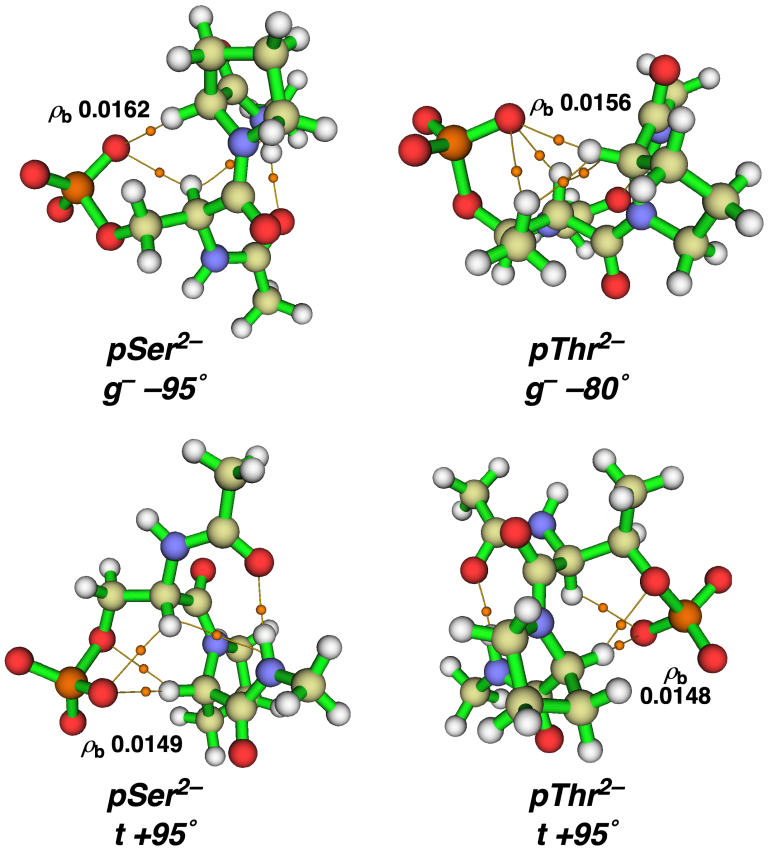

Figure S18. Atoms in Molecules (AIM) analysis of BCPs of C–H/O interactions for dianionic phosphoserine and dianionic phosphoserine. Structures are shown with the indicated sidechain combination of conformations at χ_1 and χ_2. Calculated Bond Critical Points (BCPs) are indicated by orange spheres. Calculated pathways from bond critical points are indicated by yellow lines. Electron densities (ρ_b) at key BCPs between the side-chain atom and Pro Hα are indicated. For interactions with phosphate oxygens, multiple BCPs were observed with the *t* rotamer, including with both a terminal phosphate oxygen and with Oγ; only the highest electron density is indicated. For structures with monoanionic and neutral phosphates, similar BCPs were observed, but with smaller values of ρ_b: pSer$^-$ *g*$^-$ 0.0133, *t* 0.0124; pSer^0 *g*$^-$ 0.0093, *t* 0.0103; pThr$^-$ *g*$^-$ 0.0115, *t* 0.0138; pThr^0 *t* 0.0115. For pThr^0, no BCP was observed between a phosphate oxygen and Pro Hα. For all structures, BCPs were also observed with the pSer or pThr Hα.

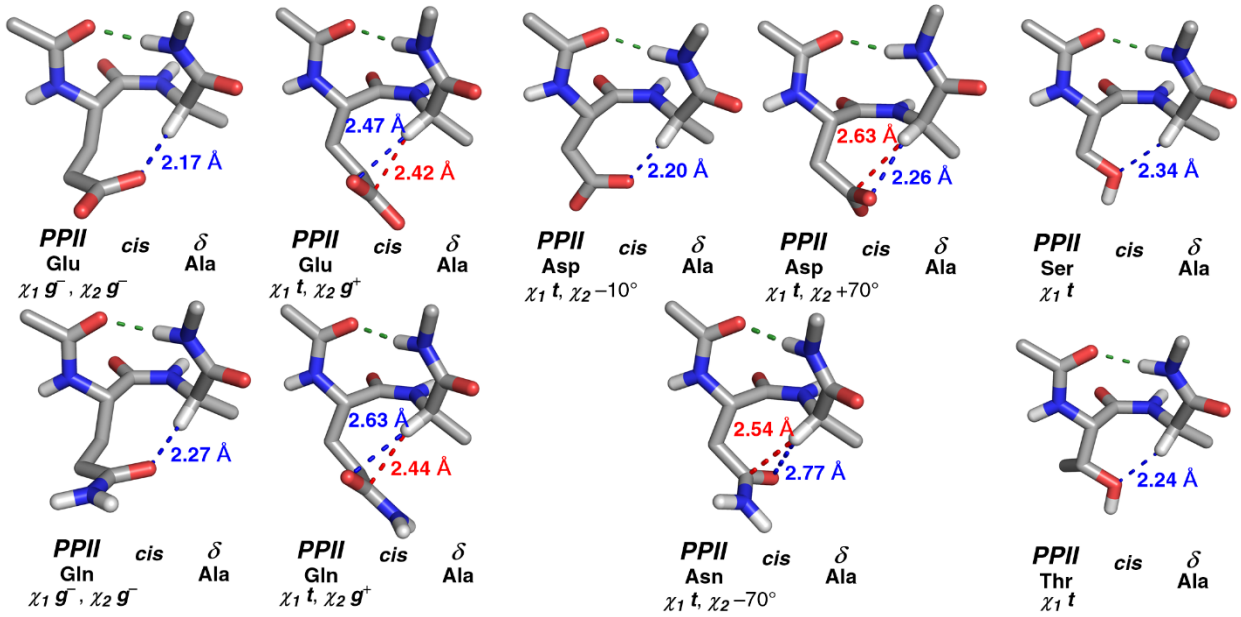

Figure S19. Geometry-optimized structures of Ac-X-*cis*-Ala-NHMe type VIa1 β-turns stabilized via C–H/O interactions. Ac-X-*cis*-Ala-NHMe in a type VIa1 β-turn conformation were subjected to full geometry optimization, with X = Glu, Gln, Asp, Asn, Ser, and Thr in order to analyze the ability of C–H/O interactions to stabilize the *cis*-nonPro conformation. Initial structures were derived from Ac-X-*cis*-Pro-NHMe structures in conformations previously shown to exhibit C–H/O interactions. C–H/O interactions (H_α•••O distances) are indicated in blue and C–H/π interactions (H_α•••$C_{C=O}$ distances) are indicated in red.

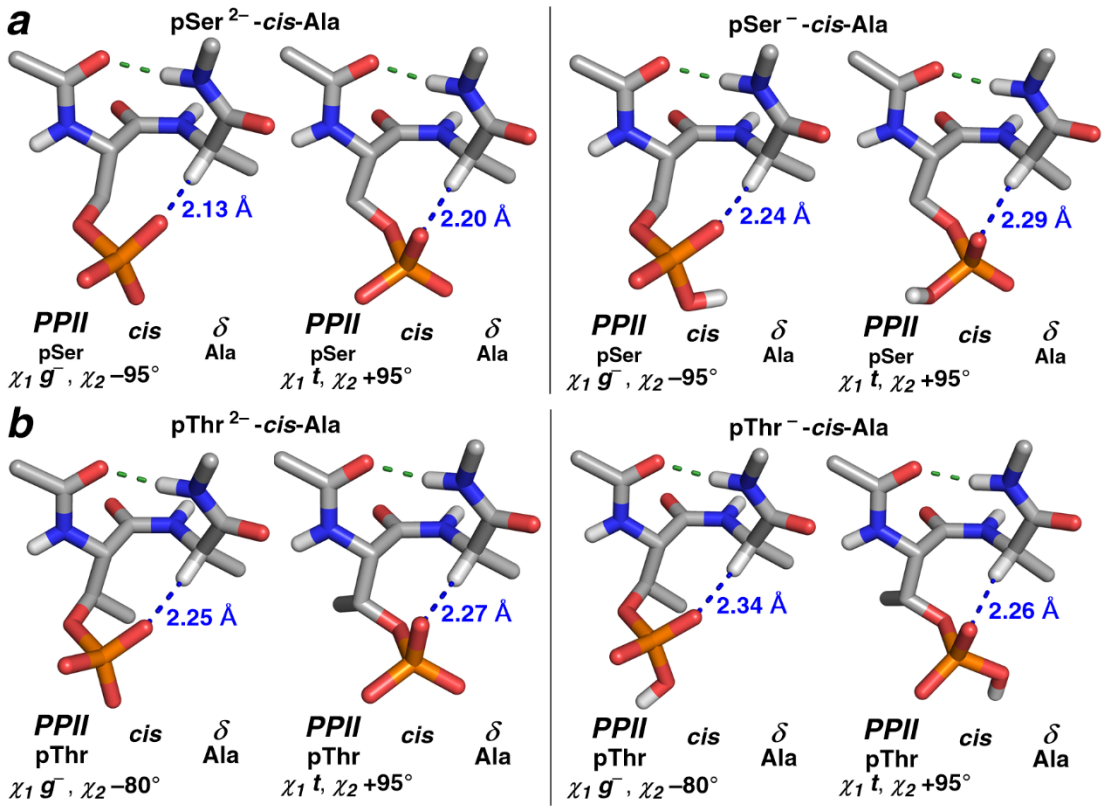

Figure S20. Geometry-optimized structures of Ac-pSer-*cis*-Ala-NHMe and Ac-pThr-*cis*-Ala-NHMe in a type VIa1 β-turn conformation stabilized via C–H/O interactions. (a) Ac-pSer-*cis*-Ala-NHMe and (b) Ac-pThr-*cis*-Ala-NHMe in a type VIa1 β-turn conformation were subjected to full geometry optimization in order to analyze the ability of C–H/O interactions (blue) mediated by post-translational modifications to stabilize the *cis*-nonPro conformation. Initial structures were derived from Ac-pSer-*cis*-Pro-NHMe and Ac-pThr-*cis*-Pro-NHMe structures determined computationally herein that exhibtied C–H/O interactions.

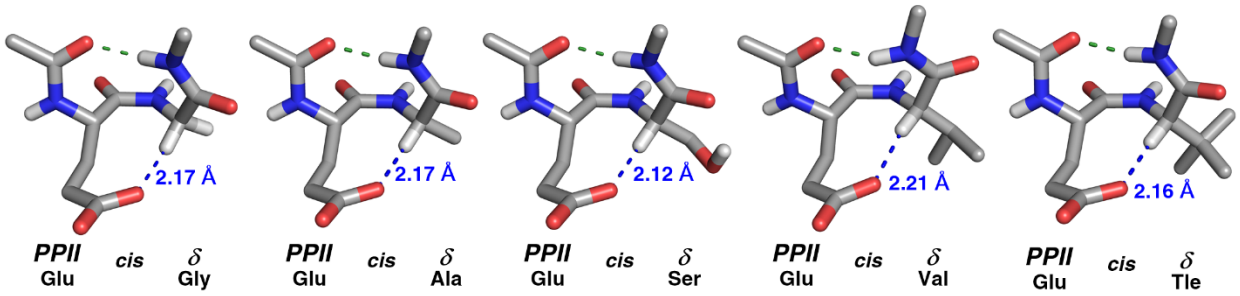

Figure S21. Geometry-optimized structures of Ac-Glu-*cis*-Z-NHMe in a type VIa1 β-turn conformation stabilized via C–H/O interactions. Structures of Ac-Glu-*cis*-Z-NHMe (Z = Gly, Ala, Ser, Val, Tle [*tert*-leucine]) in a type VIa1 β-turn conformation were subjected to full geometry optimization in order to examine the effects of the identity of the post-Glu residue on C–H/O interaction distances. All interactions were examined using the χ_1 g^-, χ_2 g^- rotamer of Glu.

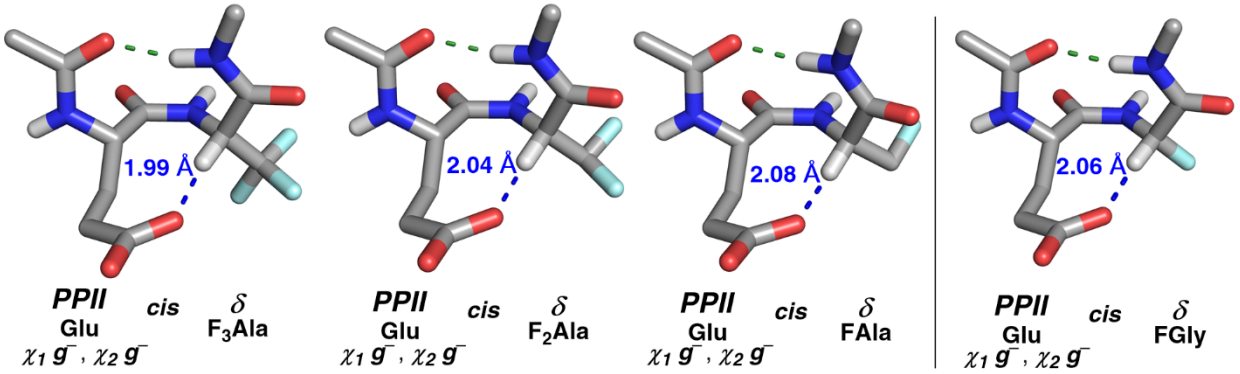

Figure S22. Geometry-optimized structures of Ac-Glu-*cis*-F_nZ-NHMe in a type VIa1 β-turn conformation stabilized via C–H/O interactions. Ac-Glu-*cis*-F_nZ-NHMe in a type VIa1 β-turn conformation were subjected to full geometry optimization, with F_nZ = β-fluorinated Ala (left) or α-fluorinated Gly (right) derivatives, in order to analyze the contribution of inductive effects on stabilization of the *cis*-amide conformation via C–H/O interactions with Glu.

Table S16. C–H/O interaction distances in geometry-optimized structures of Ac-Glu-*cis*-Z-NHMe. Geometry optimization was performed on Ac-Glu-*cis*-Z-NHMe structures where Z = Gly, Ala, Val, Tle and Ser to probe the effect of the identity of the post-Glu residue on C–H/O interactions.

Glu-*cis*-Z	C_α–H/O distance, Å
Gly	2.17
Ala	2.17
Val	2.21
Tle	2.16
Ser, $\chi_2 = g^+$	2.14
Ser, $\chi_2 = g^-$	2.13
Ser, $\chi_2 = t$	2.12

Table S17. C–H/O interaction distances in geometry-optimized structures of Ac-Glu-*cis*-F_nZ-NHMe. Geometry optimization was performed on Ac-Glu-*cis*-F_nZ-NHMe structures containing fluorinated Ala and Gly derivatives to probe the effect of electron-withdrawing groups *ipso* or *alpha* to C–H_α on C–H/O interactions.

Glu-*cis*-Z	C_α–H/O distance, Å
Ala	2.17
FAla	2.08
F_2Ala	2.04
F_3Ala	1.99
Gly	2.17
FGly	2.06

References

(1) Wang, G.; Dunbrack Jr., R. L. PISCES: a protein culling server. *Bioinformatics* **2003**, *19,* 1589–1591.

(2) Oven, H. C.; Yap, G. P. A.; Zondlo, N. J. Helical twists and β-turns in structures at serine–proline sequences: Stabilization of *cis*-proline and type VI β-turns via C–H/O interactions. *Proteins* **2024**, *92*, 1190–1205.

Coordinates of structures obtained via geometry optimization calculations

Geometry optimized structures of type VIa1 β-turns in the PDB stabilized via C–H/O interactions

Geometry-optimized structure of Ac-Glu^{1-}-*cis*-Pro-NHMe in a type VIa1 (PcisD) β-turn with a C–H/O interaction (Glu χ_1 *g*$^-$, χ_2 *g*$^-$, χ_3 *t*) (Pro χ_2 *endo*)
optimized M06-2X/6-311++G(d,p)/H2O

-1 1

C	3.03161600	-3.15939200	0.76064900
C	1.92225000	-2.15996200	0.56244900
O	0.84494700	-2.26704300	1.14998800
H	3.94921500	-2.88350000	0.24355500
H	3.22834800	-3.25515800	1.82856400
H	2.68798400	-4.12790200	0.39351500
N	2.15984600	-1.14137200	-0.28694200
C	1.10692800	-0.20415900	-0.62856000
C	-0.06433900	-0.96075600	-1.26726700
O	0.12920700	-1.93182100	-1.99072100
C	1.62677500	0.85264500	-1.60743300
C	2.63383000	1.80002000	-0.96640500
C	2.04433200	2.71490600	0.13008900
O	0.79486800	2.81269700	0.19487700
O	2.87725400	3.30592900	0.85597500
H	3.00141300	-1.15292900	-0.84451300
H	0.77729500	0.29038200	0.28749800
H	2.06580900	0.33850600	-2.46928300
H	0.77432200	1.42856800	-1.97417000
H	3.47977900	1.25570500	-0.53814000
H	3.05436200	2.45814100	-1.73326400
N	-1.30359900	-0.49434200	-1.01374900
C	-1.66792400	0.74827200	-0.32044200
C	-1.89303000	0.58398900	1.19047400
O	-2.47971600	1.46552000	1.81512100
C	-2.97433500	1.13740400	-1.02074600
C	-3.63446900	-0.22296000	-1.26078900
C	-2.46170400	-1.10639700	-1.68813200
H	-0.89086300	1.51132900	-0.42473700
H	-3.56836600	1.81662600	-0.41305900
H	-2.73916800	1.62062200	-1.97193100
H	-4.06585000	-0.59509700	-0.32734600
H	-4.42124500	-0.19428600	-2.01332700
H	-2.56793700	-2.14937000	-1.38690000
H	-2.30069400	-1.07749300	-2.76926100
N	-1.40231700	-0.51721500	1.77367900
C	-1.46023400	-0.68170100	3.21547900
H	-0.97136900	0.15271900	3.72340700
H	-2.49601300	-0.73283800	3.55507700
H	-0.95171300	-1.60829000	3.47321800

H -0.81347000 -1.15893700 1.25206500

1 2 1.0 4 1.0 5 1.0 6 1.0
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37 38 1.0 39 1.0 40 1.0
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Geometry-optimized structure of Ac-Glu^{0}-*cis*-Pro-NHMe in a type VIa1 (PcisD) β-turn with a C–H/O interaction (Glu χ_1 *g*$^-$, χ_2 *g*$^-$, χ_3 *t*) (Pro χ_2 *endo*)
optimized M06-2X/6-311++G(d,p)/H2O

0 1
C -1.66452300 2.32004800 0.68158500

O	-0.59663400	2.26364900	1.28834300
N	-2.00248700	1.38242900	-0.23138200
C	-1.03861200	0.37409500	-0.62716800
C	0.20647000	1.05860000	-1.21430800
O	0.10501800	2.08952900	-1.86713400
C	-1.65167600	-0.56897200	-1.66616200
C	-2.77293100	-1.43027600	-1.09717600
C	-2.27507100	-2.45014500	-0.10540300
O	-1.11637400	-2.68625800	0.13393800
O	-3.28159100	-3.09750200	0.49208500
H	-3.27446000	-1.98380900	-1.89602000
H	-2.79739900	1.55695000	-0.82949800
H	-0.75831600	-0.19093400	0.26417300
H	-0.86672200	-1.21331800	-2.06859700
H	-3.54842800	-0.83438000	-0.60917400
H	-2.03050600	0.02793000	-2.50015700
N	1.39836600	0.47317100	-0.97898700
C	1.64781900	-0.85003100	-0.39337600
C	1.79872500	-0.86064100	1.13585700
O	2.21702100	-1.87501800	1.68848300
C	2.96330600	-1.26224600	-1.06609800
C	3.71287700	0.06798600	-1.16591800
C	2.61631800	1.04934100	-1.57697100
H	2.77278900	2.06276300	-1.20612300
H	0.83850000	-1.54730600	-0.61833200
H	2.74685100	-1.65232700	-2.06318700
H	4.53271300	0.04620300	-1.88222500
H	2.49449900	1.09524000	-2.66268000
H	3.48366800	-2.02561000	-0.49158100
H	4.11787500	0.34336400	-0.18835900
N	1.44416500	0.24316200	1.80502100
C	1.44687300	0.26066300	3.25758200
H	0.97535900	1.00564600	1.32720800
H	2.45313800	0.08171700	3.63887000
C	-2.65333900	3.43160800	0.91250700
H	-2.79459800	3.55775500	1.98555300
H	-2.22600900	4.35504300	0.51690500
H	-3.61431000	3.24875200	0.43437600
H	0.78320600	-0.50895800	3.65849000
H	1.10510600	1.23893200	3.58840400
H	-2.91021400	-3.75036400	1.10396200

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3 4 1.0 13 1.0
4 5 1.0 7 1.0 14 1.0
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7 8 1.0 15 1.0 17 1.0
8 9 1.0 12 1.0 16 1.0
9 10 2.0 11 1.5

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11 42 1.0
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18 19 1.0 24 1.0
19 20 1.0 22 1.0 26 1.0
20 21 2.0 32 1.5
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22 23 1.0 27 1.0 30 1.0
23 24 1.0 28 1.0 31 1.0
24 25 1.0 29 1.0
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32 33 1.0 34 1.0
33 35 1.0 40 1.0 41 1.0
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36 37 1.0 38 1.0 39 1.0
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Geometry-optimized structure of Ac-Glu^{1-}-*cis*-Pro-NHMe in a type VIa1 (PcisD) β-turn with a C–H/O interaction (Glu χ_1 *t*, χ_2 g^+, χ_3 *t*) (Pro χ_2 *endo*)
optimized M06-2X/6-311++G(d,p)/H2O

-1 1

C	-4.65983800	0.32083100	-0.25318300
C	-3.16886900	0.11512100	-0.18218700
O	-2.67831800	-1.01383400	-0.13025200
H	-5.09907100	-0.04041500	0.67829200
H	-4.93869300	1.36277700	-0.40197800
H	-5.05562600	-0.28401900	-1.06898400
N	-2.40323100	1.22094700	-0.16851200
C	-0.95631800	1.17332900	-0.02630300
C	-0.59917200	0.36045300	1.22629500
O	-1.21826000	0.53278700	2.27005500
C	-0.44982600	2.61321800	0.13477100

C	1.06190500	2.75396200	0.26481400
C	1.86936900	2.47638900	-1.02167900
O	1.23205000	2.16998300	-2.05620000
O	3.11452000	2.57285100	-0.91131700
H	-0.52528300	0.72528500	-0.92358100
H	-0.93726000	3.03154400	1.02156300
H	-0.78714300	3.18016900	-0.73645400
H	-2.85235900	2.12432900	-0.14293800
H	1.45911600	2.11037000	1.05898500
H	1.30055600	3.77538000	0.57368100
N	0.42516300	-0.51755700	1.15120800
C	1.39416600	-0.69789200	0.06389400
C	1.04016500	-1.82333600	-0.92091100
O	1.90470300	-2.26567900	-1.67468300
C	2.68122400	-1.02908900	0.82436300
C	2.16037400	-1.90353300	1.96770100
C	0.87004200	-1.19521500	2.38382700
H	3.11054900	-0.10302600	1.21517500
H	3.41067700	-1.52011800	0.18405100
H	2.86155100	-1.99366500	2.79599800
H	1.93910000	-2.90772400	1.59559400
H	0.09596500	-1.87370000	2.74465700
H	1.04852300	-0.44052500	3.15441600
H	1.49689600	0.20561400	-0.53650300
N	-0.22714400	-2.24880900	-0.92995100
C	-0.67705700	-3.21893300	-1.91217000
H	-0.16063600	-4.17080400	-1.77777100
H	-1.74627900	-3.36912100	-1.77801200
H	-0.48561200	-2.86258800	-2.92676800
H	-0.93302200	-1.77252200	-0.37485700

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36 37 1.0 41 1.0
37 38 1.0 39 1.0 40 1.0
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Geometry-optimized structure of Ac-Gln-*cis*-Pro-NHMe in a type VIa1 (PcisD) β-turn with a C–H/O interaction (Gln χ_1 *g*$^-$, χ_2 *g*$^-$, χ_3 *t*) (Pro χ_2 *endo*)
optimized M06-2X/6-311++G(d,p)/H2O

0 1

C	2.78316300	-3.32239600	0.92108800
C	1.75285500	-2.25015300	0.68425500
O	0.69428700	-2.21723800	1.30956200
H	2.38040900	-4.26850300	0.55425900
H	3.72850000	-3.11827800	0.42085200
H	2.94821100	-3.41908200	1.99379200
N	2.04224900	-1.32149700	-0.25331800
C	1.04075800	-0.35076300	-0.64899400
C	-0.19346900	-1.08238300	-1.19916700
O	-0.07476200	-2.12300900	-1.83420900
C	1.60514400	0.59302500	-1.71459300
C	2.70294800	1.50202400	-1.17364300
C	2.17342000	2.49887100	-0.15344600
N	3.10874600	3.08636900	0.61885400
O	0.98077400	2.76041600	-0.05337500
H	0.76053200	0.22385200	0.23644700
H	0.79238200	1.20631300	-2.10907600
H	1.98903600	-0.00508700	-2.54574400
H	3.13827500	2.08236500	-1.99264700
H	3.52071200	0.92738400	-0.73103000
H	2.83506800	-1.47686100	-0.85926300
H	2.83250300	3.80316500	1.27278500
H	4.08888700	2.87796000	0.51776900

N	-1.39693800	-0.52542100	-0.95423500
C	-1.67155100	0.80097000	-0.38687500
C	-1.80985200	0.82828800	1.14322900
O	-2.26340100	1.83268400	1.68671100
C	-3.00209700	1.17153900	-1.05363400
C	-3.72258200	-0.17681500	-1.12127400
C	-2.60834000	-1.14179700	-1.52411600
H	-2.80439900	1.54820400	-2.05980700
H	-3.53416000	1.93309000	-0.48754300
H	-4.54952700	-0.18795100	-1.82966100
H	-4.11238100	-0.44194300	-0.13470000
H	-2.73817700	-2.15014900	-1.12971300
H	-2.49825300	-1.20884400	-2.61001700
H	-0.87829300	1.51255600	-0.62675900
N	-1.40182400	-0.24950300	1.82475700
C	-1.38517400	-0.24440200	3.27721700
H	-0.75150400	0.56021200	3.65732000
H	-2.39313700	-0.10429900	3.67007000
H	-0.99592600	-1.20127200	3.61824400
H	-0.91090000	-1.00135400	1.35221500

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Geometry-optimized structure of Ac-Gln-*cis*-Pro-NHMe in a type VIa1 (PcisD) β-turn with a C–H/O interaction (Gln χ_1 *t*, χ_2 g^+, χ_3 *t*) (Pro χ_2 *endo*)
optimized M06-2X/6-311++G(d,p)/H2O

0 1

C	4.63041800	-0.66317600	-0.28189700
C	3.16015200	-0.34736800	-0.19898100
O	2.75374700	0.81278300	-0.13898800
H	4.83006400	-1.72078300	-0.44539600
H	5.06618900	-0.07881700	-1.09214300
H	5.09981500	-0.34790000	0.65154200
N	2.31325700	-1.39442900	-0.18478800
C	0.87745500	-1.23690500	-0.02375200
C	0.59818500	-0.38019500	1.22196900
O	1.21120600	-0.59430600	2.25983600
C	0.27755200	-2.63615200	0.17341100
C	-1.23527800	-2.66902300	0.34225600
C	-1.98640900	-2.36877900	-0.94597400
N	-3.32164600	-2.22481600	-0.80959600
O	-1.41945600	-2.25153900	-2.02372100
H	0.46871100	-0.76900500	-0.92239500
H	0.74235800	-3.07073300	1.06240200
H	0.55468800	-3.24706500	-0.68863600
H	2.69449600	-2.32881700	-0.16621200
H	-1.57151200	-1.98196300	1.12689500
H	-1.53985700	-3.66741000	0.66898300
H	-3.88876400	-2.07388000	-1.63026800
H	-3.78365900	-2.36823700	0.07437700
N	-0.35278600	0.57721800	1.14616700
C	-1.31416600	0.83984500	0.06884400
C	-0.86691500	1.90237700	-0.94857400
O	-1.69300000	2.37883800	-1.72349000
C	-2.54743300	1.32106200	0.84038100
C	-1.91906400	2.15423000	1.95909500
C	-0.70480100	1.32069300	2.37225400
H	-3.07051700	0.45517700	1.25446600

H	-3.22865500	1.87637600	0.19922800
H	-2.59494700	2.33238400	2.79395200
H	-1.59797800	3.12238500	1.56542200
H	0.14320500	1.92011300	2.70564800
H	-0.94805100	0.60341200	3.16052300
H	-1.53093600	-0.05715300	-0.50963900
N	0.42567300	2.23979200	-0.95143800
C	0.95078800	3.15585800	-1.94871700
H	0.75312900	2.78788800	-2.95788300
H	0.49192700	4.14033800	-1.84370500
H	2.02496700	3.24271600	-1.79985800
H	1.09096000	1.72559000	-0.38072100

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28 29 1.0 31 1.0 32 1.0
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39 40 1.0 41 1.0 42 1.0
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Geometry-optimized structure of Ac-Asp^{1-}-*cis*-Pro-NHMe in a type VIa1 (PcisD) β-turn with a C–H/O interaction (Asp χ_1 *t*, χ_2 *t*) (Pro χ_2 *endo*)
optimized M06-2X/6-311++G(d,p)/H2O

-1 1

C	2.31847500	3.77291600	0.32336800
C	1.45520900	2.54229600	0.20192900
O	0.27256200	2.55997400	0.54274800
H	2.41712800	4.01637800	1.38255900
H	3.30957500	3.64492000	-0.10896400
H	1.80982900	4.60284100	-0.16715400
N	2.05187700	1.43824500	-0.28253400
C	1.42586600	0.11972000	-0.39613700
C	0.68830400	-0.19774100	0.91498100
O	1.29687500	-0.11526500	1.97638900
C	2.56942300	-0.87060200	-0.63549100
C	2.19221000	-2.35226700	-0.81754300
O	1.00706900	-2.68329800	-0.58814600
O	3.13149400	-3.10089600	-1.16753200
H	3.03626200	1.49318200	-0.49833800
H	0.73319100	0.12225500	-1.24041100
H	3.13076200	-0.55458100	-1.51906900
H	3.25485400	-0.80969500	0.21624000
N	-0.62569000	-0.51318100	0.87527500
C	-1.39655100	-0.98730400	-0.28200300
C	-2.22122400	0.08862400	-0.99264700
O	-3.04137500	-0.24283600	-1.84931700
C	-2.31681800	-2.04210200	0.34385800
C	-2.63867100	-1.42794500	1.70723700
C	-1.28836200	-0.86379600	2.14455000
H	-0.73052400	-1.44305100	-1.01248100
H	-3.18957900	-2.23534400	-0.27691100
H	-1.74888100	-2.96709100	0.46674800
H	-3.36962600	-0.62258900	1.59231700
H	-3.03250800	-2.14717000	2.42444500
H	-1.36406900	0.01393200	2.78839200
H	-0.68741200	-1.61596000	2.66388100
N	-1.99210700	1.36101400	-0.65414900
C	-2.65932700	2.44809100	-1.34664500
H	-2.47054400	2.40061200	-2.42149700
H	-3.73798000	2.40303900	-1.18585200
H	-2.27776200	3.38904600	-0.95525900
H	-1.22546700	1.58595800	-0.02466700

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Geometry-optimized structure of Ac-Asp^{1-}-*cis*-Pro-NHMe in a type VIa1 (PcisD) β-turn with a C–H/O interaction (Asp χ_1 *t*, χ_2 *+80°*) (Pro χ_2 *endo*)
optimized M06-2X/6-311++G(d,p)/H2O

-1 1

C	-4.43027200	-1.01333600	0.28112900
C	-2.95365300	-0.76296600	0.11923100
O	-2.12276400	-1.63836400	0.36275100
H	-4.62685800	-1.23083600	1.33211500
H	-5.04227600	-0.16946700	-0.03307900
H	-4.69875800	-1.89542900	-0.30072500

N	-2.58605000	0.46086300	-0.30518100
C	-1.19065700	0.85653700	-0.41095100
C	-0.50192500	0.63004000	0.94596400
O	-1.08079400	0.93168700	1.98278800
C	-1.12826700	2.34114900	-0.78831100
C	0.32811400	2.78226700	-1.03752500
O	0.93447200	3.30118700	-0.07473900
O	0.78985200	2.53560900	-2.17690300
H	-0.71334800	0.25465700	-1.18907100
H	-1.56932300	2.92288400	0.02402700
H	-1.71030400	2.48379000	-1.70115200
H	-3.29172900	1.17544400	-0.40503300
N	0.73402600	0.08767000	0.95668300
C	1.65658800	-0.09693300	-0.17195500
C	1.56641500	-1.46791000	-0.85647800
O	2.42938200	-1.79285400	-1.67029500
C	3.03024500	0.07740500	0.49111500
C	2.81325100	-0.55527900	1.86733100
C	1.42274900	-0.05578000	2.25156000
H	3.24132200	1.14426600	0.59125300
H	3.81841600	-0.38962800	-0.09578900
H	3.56810500	-0.26743300	2.59780500
H	1.49686700	0.65359300	-0.94777600
H	2.81435400	-1.64549100	1.78201800
H	0.87109900	-0.73939600	2.89788000
H	1.46435800	0.92098700	2.74256400
N	0.52625500	-2.24826000	-0.54358700
C	0.31018400	-3.50798600	-1.23297600
H	-0.61629600	-3.94342800	-0.86448100
H	0.23371300	-3.35415500	-2.31176400
H	1.13382600	-4.19744000	-1.04090500
H	-0.23060300	-1.88619700	0.02908700

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Geometry-optimized structure of Ac-Asn-*cis*-Pro-NHMe in a type VIa1 (PcisD) β-turn with a C–H/O interaction (Asn χ_1 *t*, χ_2 *–80°*) (Pro χ_2 *endo*)
optimized M06-2X/6-311++G(d,p)/H2O

0 1

C	-4.45908100	-0.97770500	0.23224300
C	-2.98046700	-0.74544900	0.07165300
O	-2.15957200	-1.64102500	0.26004900
H	-4.74037700	-1.84874700	-0.35956700
H	-4.65578400	-1.20477900	1.28137700
H	-5.05923200	-0.12071200	-0.06887800
N	-2.59443800	0.49717200	-0.28687800
C	-1.19125900	0.85790700	-0.36964200
C	-0.50903600	0.55465100	0.97834300
O	-1.08477500	0.82803400	2.02235600
C	-1.11028700	2.36112100	-0.68199200
C	0.32664100	2.84204500	-0.78512900
N	0.79083900	3.04637600	-2.03359100
O	1.01834800	2.99280300	0.21221900
H	-0.73069800	0.27676100	-1.17284900
H	-1.57959900	2.90872700	0.13877000
H	-1.66189900	2.55949000	-1.60259100
H	1.74071100	3.36389600	-2.16042100
H	-3.28801300	1.22862100	-0.33595600
H	0.20699100	2.94001100	-2.84716500
N	0.71029900	-0.02067700	0.95976400
C	1.62390400	-0.16123000	-0.18045700
C	1.55110100	-1.52239000	-0.88968700
O	2.42844600	-1.83280100	-1.69222100

C	2.99780000	0.04109300	0.46886900
C	2.81837100	-0.64276700	1.82541000
C	1.41519200	-0.20432300	2.24204900
H	3.16397700	1.11258200	0.60083400
H	3.79438400	-0.37813000	-0.14198000
H	3.57063900	-0.35117400	2.55686800
H	2.85779000	-1.72895100	1.70560600
H	0.89137400	-0.93432400	2.85998400
H	1.42903000	0.75088700	2.77441100
H	1.44094000	0.59572600	-0.94406500
N	0.50301300	-2.30289500	-0.60756000
C	0.29588400	-3.55463300	-1.31445800
H	-0.63597200	-3.99371300	-0.96453800
H	0.23549100	-3.38800700	-2.39218600
H	1.11638100	-4.24638300	-1.11763400
H	-0.25627900	-1.94762600	-0.03460100

1 2 1.0 4 1.0 5 1.0 6 1.0
2 3 2.0 7 1.5
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7 8 1.0 19 1.0
8 9 1.0 11 1.0 15 1.0
9 10 2.0 21 1.5
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11 12 1.0 16 1.0 17 1.0
12 13 1.5 14 2.0
13 18 1.0 20 1.0
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21 22 1.0 27 1.0
22 23 1.0 25 1.0 34 1.0
23 24 2.0 35 1.5
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25 26 1.0 28 1.0 29 1.0
26 27 1.0 30 1.0 31 1.0
27 32 1.0 33 1.0
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35 36 1.0 40 1.0
36 37 1.0 38 1.0 39 1.0
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Geometry-optimized structure of Ac-Ser-*cis*-Pro-NHMe in a type VIa1 (PcisD) β-turn with a C–H/O interaction (Ser χ_1 *t*, χ_2 *t*) (Pro χ_2 *endo*)
optimized M06-2X/6-311++G(d,p)/H2O

0 1

O	2.19256000	-1.48490900	-0.53633000
C	2.49918500	-0.11034900	-0.49751900
C	1.19588900	0.65574400	-0.28408800
H	2.95746000	0.22756500	-1.43377400
N	1.50046100	2.06956900	-0.20496100
C	0.53994700	0.19196300	1.02823900
H	0.52613300	0.48329100	-1.12994500
C	0.53706500	2.97566000	0.06089600
N	-0.49601800	-0.66817000	0.95204400
O	0.95812300	0.61100100	2.10039200
O	-0.64204400	2.64232600	0.16597700
C	-1.08684500	-1.17896800	2.20297000
C	-0.92772100	-1.45259100	-0.21241300
C	-2.07387100	-2.24385800	1.72670100
H	-0.29333600	-1.60726500	2.82162700
H	-1.55368800	-0.36558500	2.75986100
C	-1.43113100	-2.74939900	0.43354300
C	-2.03935600	-0.79890000	-1.04485700
H	-0.08777600	-1.64436300	-0.88025000
H	-2.22015600	-3.02616200	2.47013700
H	-0.57374300	-3.38774500	0.65994300
H	-2.11167200	-3.28621200	-0.22405500
N	-2.30339500	0.49197800	-0.81432200
O	-2.62677500	-1.46278600	-1.89672600
C	-3.26432600	1.21093100	-1.63183800
H	-3.27171400	2.25162800	-1.31464000
H	-2.99406100	1.15618300	-2.68865600
H	-4.26346800	0.78957800	-1.50946400
H	-1.71278400	1.03126200	-0.18913100
H	2.46653100	2.36277700	-0.18470900
C	0.97383300	4.40672200	0.22685900
H	0.34724500	5.03694300	-0.40402000
H	0.80560600	4.69577500	1.26578000
H	2.02143900	4.56315100	-0.02433700
H	-3.04510900	-1.79039600	1.51020600
H	3.01455900	-1.96879900	-0.72530800
H	3.17990500	0.12208600	0.33159600
O	4.62448100	-2.69730400	-1.09254200

H 5.40672500 -2.41193600 -0.61048400
H 4.90779100 -2.79375900 -2.00682400

1 2 1.0 36 1.0
2 3 1.0 4 1.0 37 1.0
3 5 1.0 6 1.0 7 1.0
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5 8 1.5 30 1.0
6 9 1.5 10 2.0
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8 11 2.0 31 1.0
9 12 1.0 13 1.0
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12 14 1.0 15 1.0 16 1.0
13 17 1.0 18 1.0 19 1.0
14 17 1.0 20 1.0 35 1.0
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17 21 1.0 22 1.0
18 23 1.5 24 2.0
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31 32 1.0 33 1.0 34 1.0
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38 39 1.0 40 1.0
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Geometry-optimized structure of Ac-Ser-*cis*-Pro-NHMe in a type VIa1 (PcisD) β-turn with a C–H/O interaction (Ser χ_1 *t*, χ_2 *–90°*) (Pro χ_2 *endo*)
optimized M06-2X/6-311++G(d,p)/H2O

0 1
O 0.14144900 -2.67698800 -1.73638700

C	1.40522800	-2.11199900	-1.45291900
C	1.27508000	-0.76855700	-0.72140400
H	1.90773900	-1.94491100	-2.40684600
N	2.60449200	-0.25636400	-0.46652900
C	0.53525500	-0.98476700	0.60811000
H	0.73506700	-0.05968900	-1.35337800
C	2.78752600	0.87524000	0.24669200
N	-0.77882100	-0.68683600	0.65839100
O	1.13522500	-1.43929600	1.57443300
O	1.83314700	1.55298800	0.62257800
C	-1.52766800	-0.98471200	1.89437600
C	-1.67910100	-0.34442300	-0.45146400
C	-2.97801900	-0.67665400	1.52246400
H	-1.38505400	-2.03865900	2.14736100
H	-1.14916500	-0.38056500	2.71961700
C	-3.01175400	-0.94120800	0.01570600
C	-1.82478900	1.16257100	-0.71187800
H	-1.34358400	-0.80395000	-1.38215000
H	-3.68145000	-1.29024000	2.08323300
H	-3.00804700	-2.01543300	-0.18395100
H	-3.85524200	-0.48511300	-0.49803500
N	-0.91382600	1.97420700	-0.16386100
O	-2.74281700	1.56536500	-1.42241700
C	-0.92127600	3.39804100	-0.45089800
H	-0.05220900	3.84678200	0.02540300
H	-0.87832800	3.57657800	-1.52727800
H	-1.82738400	3.86391000	-0.05992500
H	-0.10447400	1.59206600	0.31506900
H	3.40299800	-0.84241900	-0.66296700
C	4.20867800	1.25453000	0.56625500
H	4.34275600	2.31581500	0.36048600
H	4.37192400	1.09254000	1.63350500
H	4.93756100	0.67494700	0.00211300
H	-3.20535000	0.37408900	1.72206100
H	-0.15862400	-3.18865100	-0.97843400
H	2.01696600	-2.78906200	-0.84779500

1 2 1.0 36 1.0
2 3 1.0 4 1.0 37 1.0
3 5 1.0 6 1.0 7 1.0
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31 32 1.0 33 1.0 34 1.0
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Geometry-optimized structure of Ac-Ser-*cis*-Pro-NHMe in a type VIa1 (PcisD) β-turn with a C–H/O interaction (Ser χ_1 *t*) (Pro χ_2 *endo*)
optimized M06-2X/6-311++G(d,p)/H2O

-1 1

O	-0.00403600	-2.48884600	-1.94772600
C	1.23280300	-2.04023500	-1.63298800
C	1.21110400	-0.75890800	-0.74587700
H	1.85861600	-1.75499400	-2.51023900
N	2.56518000	-0.32385800	-0.47013500
C	0.49463200	-1.06339400	0.56833100
H	0.69440600	0.03511500	-1.28908900
C	2.82336600	0.74926800	0.29710100
N	-0.80424400	-0.70701300	0.67466900
O	1.08621000	-1.60666200	1.49786500
O	1.91876500	1.46253300	0.73822300
C	-1.55627200	-1.06121200	1.88846800
C	-1.69099600	-0.32578900	-0.43079000
C	-2.99147600	-0.66198000	1.54755300
H	-1.46720700	-2.13715000	2.06665300
H	-1.14999500	-0.53844400	2.75552300
C	-3.04911300	-0.86819100	0.03156800
C	-1.76670300	1.18296700	-0.68725200
H	-1.35360600	-0.81778200	-1.34805000
H	-3.72356100	-1.25586600	2.09341000
H	-3.10214200	-1.93427100	-0.20338200

H	-3.87498400	-0.35545100	-0.45787200
N	-0.84452000	1.95785300	-0.10047100
O	-2.63906800	1.63256900	-1.43018400
C	-0.77257500	3.37729400	-0.39622500
H	0.08063100	3.79441700	0.13458700
H	-0.64938200	3.54730600	-1.46838300
H	-1.68217100	3.88468600	-0.07055400
H	-0.06115600	1.53676600	0.39032700
H	3.32517300	-0.93413600	-0.73667000
C	4.27087700	1.04210800	0.59990700
H	4.46700300	2.09347000	0.38994000
H	4.43939400	0.87388600	1.66515800
H	4.95711000	0.42047300	0.02681000
H	-3.15750000	0.39216400	1.78734800
H	1.85562100	-2.76738000	-1.05816100

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2 3 1.0 4 1.0 36 1.0
3 5 1.0 6 1.0 7 1.0
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8 11 2.0 31 1.0
9 12 1.0 13 1.0
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13 17 1.0 18 1.0 19 1.0
14 17 1.0 20 1.0 35 1.0
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17 21 1.0 22 1.0
18 23 1.5 24 2.0
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31 32 1.0 33 1.0 34 1.0
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Geometry-optimized structure of Ac-Thr-*cis*-Pro-NHMe in a type VIa1 (PcisD) β-turn with a C–H/O interaction (Thr χ_1 *t*, χ_2 *t*) (Pro χ_2 *endo*)
optimized M06-2X/6-311++G(d,p)/H2O

0 1

C	3.61810900	2.39768000	0.53583200
C	2.34152900	1.64484800	0.27031500
O	1.24489500	2.09261600	0.60118000
H	3.50631000	3.41463800	0.16032000
H	3.76488100	2.45024700	1.61592800
H	4.48917900	1.93228700	0.07755800
N	2.45569500	0.44936100	-0.34341900
C	1.29700700	-0.38425800	-0.58804700
C	0.57151000	-0.65857500	0.74281100
O	1.21556600	-0.85403200	1.76608200
C	1.75011200	-1.68503500	-1.27353900
C	2.57794000	-2.60981300	-0.39426300
O	0.55540800	-2.32308400	-1.70231800
H	3.37635500	0.09171800	-0.54961400
H	0.62880700	0.13857300	-1.27783500
H	2.33844900	-1.38332100	-2.14918300
H	0.78025000	-3.18046800	-2.07722800
H	2.90381400	-3.46999600	-0.98338200
H	3.47033200	-2.11356600	-0.00821800
H	1.98637600	-2.96076800	0.45190600
N	-0.77764600	-0.66067000	0.74346300
C	-1.69755900	-0.62409100	-0.40046000
C	-2.15040900	0.78442800	-0.81080900
O	-3.08598800	0.91015300	-1.59832100
C	-2.89061700	-1.43680300	0.11721900
C	-2.95465300	-1.02140000	1.58856500
C	-1.48295400	-0.97947900	1.99916500
H	-1.24619200	-1.09035800	-1.27557600
H	-3.79616100	-1.22112500	-0.44599700
H	-2.65882400	-2.50091500	0.03004100
H	-3.39993800	-0.02653700	1.67575000
H	-3.53167100	-1.70836100	2.20589000
H	-1.26190600	-0.22685600	2.75721200
H	-1.13187300	-1.94743900	2.36633700
N	-1.48161200	1.82356300	-0.29881100
C	-1.78381600	3.18059100	-0.71876400
H	-0.63620500	1.67313500	0.24276300
H	-1.68960600	3.28354400	-1.80207800
H	-2.80154700	3.45271100	-0.43414000
H	-1.08213100	3.85328900	-0.23020300

1 2 1.0 4 1.0 5 1.0 6 1.0
2 3 2.0 7 1.5

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7 8 1.0 14 1.0
8 9 1.0 11 1.0 15 1.0
9 10 2.0 21 1.5
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11 12 1.0 13 1.0 16 1.0
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22 23 1.0 25 1.0 28 1.0
23 24 2.0 35 1.5
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26 27 1.0 31 1.0 32 1.0
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Geometry optimized structures of pSer-*cis*-Pro and pThr-*cis*-Pro in type VIa1 β-turns stabilized via C–H/O interactions derived from Glu-*cis*-Pro structures in the PDB

Geometry-optimized structure of Ac-pSer^{2-}-*cis*-Pro-NHMe in a type VIa1 (PcisD) β-turn with a C–H/O interaction (pSer χ_1 *g*$^-$, χ_2 *–90°*) (Pro χ_2 *endo*)
optimized M06-2X/6-311++G(d,p)/H2O

-2 1

P	-3.13009700	-1.12066500	0.32897600
O	-2.81458900	0.25961800	-0.62979600

O	-1.78752900	-1.41697800	1.00798100
O	-4.23585000	-0.61588200	1.24805200
O	-3.55963900	-2.19686400	-0.66891800
C	-1.63028300	0.23642600	-1.37965300
C	-0.48207100	0.88724900	-0.60143000
H	-1.78708500	0.79542600	-2.30902300
N	-0.76580600	2.29335100	-0.40186100
C	0.80631800	0.70774000	-1.40209000
H	-0.41999800	0.38836300	0.36745000
C	0.10130700	3.09530400	0.23816200
N	1.56749400	-0.35863600	-1.08305000
O	1.10378600	1.46844900	-2.31734200
O	1.18180300	2.67188400	0.65627100
C	2.74191800	-0.68491500	-1.90941700
C	1.25335700	-1.43246600	-0.13107700
C	3.22221100	-2.02334000	-1.34401400
H	2.42812600	-0.76983200	-2.95336100
H	3.48730200	0.10890300	-1.84132300
C	1.94291200	-2.64073300	-0.77119900
C	1.79756200	-1.18384000	1.28423200
H	0.17291300	-1.57322300	-0.01150600
H	3.69683900	-2.64106400	-2.10517100
H	1.31124600	-3.02598300	-1.57512400
H	2.12012700	-3.43216600	-0.04611800
N	2.09878600	0.07850300	1.61626800
O	1.91075000	-2.12339700	2.06936100
C	2.50344900	0.41041000	2.97072500
H	2.62322000	1.48985800	3.03645400
H	1.75225700	0.08396500	3.69333800
H	3.45055300	-0.07251500	3.21801400
H	-1.33972600	-0.78691700	-1.64678800
H	1.88278200	0.84641700	0.98767300
H	-1.66452000	2.64943200	-0.69228300
C	-0.30111700	4.53615900	0.41645200
H	-0.28871900	4.77005700	1.48158400
H	0.44178000	5.16579300	-0.07481900
H	-1.28669400	4.75424900	0.00816800
H	3.94450700	-1.85591600	-0.54032800

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6 7 1.0 8 1.0 33 1.0
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9 12 1.5 35 1.0
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Geometry-optimized structure of Ac-pSer^{2-}-*cis*-Pro-NHMe in a type VIa1 (PcisD) β-turn with a C–H/O interaction (pSer χ_1 *t*, χ_2 *+90°*) (Pro χ_2 *endo*)
optimized M06-2X/6-311++G(d,p)/H2O

-2 1

P	-3.08850400	-0.66858200	-0.50964900
O	-2.04843700	-0.97526500	0.81233600
O	-3.89101500	-1.95773400	-0.67907200

O	-3.88240000	0.53061200	-0.00447200
O	-2.13007900	-0.37401000	-1.66825400
C	-1.07685800	-1.96809000	0.62973600
C	0.26773100	-1.35782100	0.20942300
H	-1.38438400	-2.69456700	-0.13227700
N	1.21485200	-2.43979400	0.01305300
C	0.76776200	-0.43402800	1.32707400
H	0.12235800	-0.81555200	-0.72656500
C	2.51343500	-2.21171500	-0.25677200
N	0.63481900	0.89729500	1.16163700
O	1.27012100	-0.91068400	2.34062500
O	2.94923100	-1.07132500	-0.41893200
C	1.01332000	1.79367000	2.26859200
C	-0.14341200	1.60371000	0.13597800
C	0.52971700	3.16828400	1.80481200
H	0.50120700	1.46885400	3.17854500
H	2.08846300	1.74470700	2.44723000
C	-0.65825400	2.82583000	0.90201500
C	0.67050700	2.03737200	-1.08888700
H	-0.95422000	0.98120100	-0.24659300
H	0.26593300	3.81199000	2.64297900
H	-1.52104500	2.53044900	1.50401700
H	-0.95088500	3.62860200	0.22839500
N	1.85472600	1.44413200	-1.28407900
O	0.20848000	2.87517000	-1.86257700
C	2.62399900	1.70308500	-2.48752800
H	3.51496500	1.07880500	-2.46464700
H	2.04163400	1.46887300	-3.38157400
H	2.92142700	2.75206300	-2.53608900
H	-0.93021300	-2.50056800	1.57662800
H	2.14777400	0.67323400	-0.69075200
H	0.92093900	-3.38340500	0.21968100
C	3.41315200	-3.41638300	-0.35285900
H	3.91065000	-3.40076200	-1.32298300
H	4.17955200	-3.33288700	0.41913800
H	2.87999300	-4.35795700	-0.23250200
H	1.30884600	3.66663100	1.22110900

1 2 1.0 3 2.0 4 2.0 5 2.0
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Geometry-optimized structure of Ac-pSer^{1-}-*cis*-Pro-NHMe in a type VIa1 (PcisD) β-turn with a C–H/O interaction (pSer χ_1 *g*$^-$, χ_2 *–90°*) (Pro χ_2 *endo*)
optimized M06-2X/6-311++G(d,p)/H2O

-1 1

P	-3.12187700	-0.96103700	0.35131900
O	-2.78436700	0.30015800	-0.65462200
O	-4.28898100	-0.52431200	1.16814100
O	-3.64825200	-2.09355600	-0.71003900

O	-1.83413100	-1.44993200	0.94963800
C	-1.57753600	0.26313700	-1.39579500
C	-0.43826500	0.89463900	-0.59806000
H	-1.73872600	0.82902900	-2.31631300
N	-0.71274200	2.29912000	-0.38336900
C	0.86275000	0.71993700	-1.38980600
H	-0.37454800	0.38827100	0.36717800
C	0.16670100	3.08222400	0.26828000
N	1.62312800	-0.34687200	-1.07194600
O	1.16846300	1.49869900	-2.28403500
O	1.22777300	2.62962300	0.70055900
C	2.82572400	-0.64057200	-1.87124200
C	1.28787700	-1.45056700	-0.16215900
C	3.31972800	-1.97127900	-1.30238500
H	2.54084300	-0.72605000	-2.92339900
H	3.54929300	0.17016400	-1.77769200
C	2.03418000	-2.63009100	-0.79516600
C	1.74819300	-1.23497300	1.28803300
H	0.20923900	-1.62188800	-0.10829400
H	3.84294400	-2.56542200	-2.05010700
H	1.44711300	-3.01528900	-1.63208600
H	2.19849000	-3.42984300	-0.07633400
N	2.06944800	0.01110100	1.65717600
O	1.78290400	-2.19120500	2.05918300
C	2.40306000	0.30942400	3.03895700
H	2.57505700	1.38018600	3.12541600
H	1.59027300	0.01745100	3.70756000
H	3.30527500	-0.22626100	3.33863200
H	-1.30604600	-0.76184600	-1.66926200
H	1.91375200	0.79398100	1.02967900
H	-1.58468700	2.68470700	-0.71444400
C	-0.20200000	4.53240200	0.43655800
H	-0.17905300	4.77490000	1.49942400
H	0.55378600	5.13916300	-0.06394200
H	-1.18356800	4.77010800	0.02988900
H	4.00216400	-1.79408400	-0.46662000
H	-2.96201600	-2.73664700	-0.91600400

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10 13 1.5 14 2.0
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Geometry-optimized structure of Ac-pSer^{1-}-*cis*-Pro-NHMe in a type VIa1 (PcisD) β-turn with a C–H/O interaction (pSer χ_1 *t*, χ_2 *+90°*) (Pro χ_2 *endo*)
optimized M06-2X/6-311++G(d,p)/H2O

-1 1

P	-3.08956400	-0.33837000	-0.48564900
O	-2.10614900	-0.83835800	0.73687700
O	-4.09120600	-1.62461900	-0.63644400
O	-3.86368600	0.80644700	0.07257100

O	-2.27008800	-0.22868700	-1.73834000
C	-1.21228200	-1.90908900	0.49770900
C	0.17746400	-1.38394200	0.12669900
H	-1.57474300	-2.56480900	-0.30063400
N	1.04944800	-2.52840600	-0.05357900
C	0.69245100	-0.51264000	1.28288000
H	0.11383900	-0.81862400	-0.80551200
C	2.37957600	-2.38659200	-0.22688000
N	0.66942200	0.82667200	1.13523600
O	1.09665200	-1.04474300	2.31029300
O	2.89953900	-1.27667200	-0.32568900
C	1.04149000	1.67245700	2.28529200
C	0.02763600	1.61488000	0.07605900
C	0.66764200	3.08635400	1.83630300
H	0.46277200	1.35488000	3.15654000
H	2.10069800	1.55286800	2.51714700
C	-0.47022900	2.84365000	0.84143000
C	0.97289300	2.02996700	-1.06142600
H	-0.79028000	1.06760600	-0.39277800
H	0.37941800	3.71642300	2.67654600
H	-1.39093400	2.58180200	1.36808000
H	-0.66421200	3.68086500	0.17439200
N	2.11957800	1.35218700	-1.17954900
O	0.64098700	2.93061900	-1.82955500
C	3.02056100	1.59837500	-2.29125500
H	3.84290300	0.88892800	-2.22684500
H	2.50582500	1.47024800	-3.24588900
H	3.41786400	2.61398000	-2.24729900
H	-1.13546300	-2.48720200	1.42198000
H	2.29866000	0.54352600	-0.59192100
H	0.67963600	-3.45403500	0.10897500
C	3.19352100	-3.65284600	-0.27190900
H	3.95917900	-3.55061400	-1.03941300
H	3.69080800	-3.77229300	0.69304900
H	2.58705700	-4.53571800	-0.46876000
H	1.51196400	3.55955400	1.32751800
H	-3.91339400	-2.12035000	-1.44230700

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Geometry-optimized structure of Ac-pSer^0-*cis*-Pro-NHMe in a type VIa1 (PcisD) β-turn with a C–H/O interaction (pSer χ_1 *g*$^-$, χ_2 *–90°*) (Pro χ_2 *endo*)
optimized M06-2X/6-311++G(d,p)/H2O

0 1

P	-3.02471600	-0.96617100	0.21911400
O	-2.73541700	0.28813400	-0.72108000
O	-1.89451400	-1.41507900	1.04992200
O	-4.26453400	-0.48843200	1.07787000
O	-3.55291300	-2.03260500	-0.84247100
C	-1.50320600	0.31273900	-1.46046000
C	-0.39533500	0.92163200	-0.61042300
H	-1.68840800	0.91940000	-2.34668400
N	-0.67326600	2.31764900	-0.35894600
C	0.93474400	0.76683300	-1.36682700
H	-0.35047700	0.39107700	0.34389000
C	0.19807600	3.06892600	0.34603100
N	1.68318400	-0.31091900	-1.06046300
O	1.26952200	1.58309100	-2.21332600

O	1.22029500	2.57679800	0.82118000
C	2.92416900	-0.56172400	-1.81676300
C	1.31791500	-1.45606600	-0.21535100
C	3.41065400	-1.90457700	-1.27235100
H	2.68580200	-0.61408800	-2.88241000
H	3.63006200	0.25494200	-1.66270900
C	2.11191000	-2.59996800	-0.85756800
C	1.69531400	-1.30318700	1.26729300
H	0.24288400	-1.64894200	-0.23264700
H	3.97945900	-2.46336100	-2.01385200
H	1.57275300	-2.95738100	-1.73767700
H	2.25095700	-3.42566100	-0.16339100
N	2.01304300	-0.07857700	1.70241100
O	1.67329900	-2.29105400	1.99668000
C	2.27986000	0.16115200	3.11022800
H	2.46245600	1.22484200	3.24665500
H	1.42924900	-0.14225500	3.72427200
H	3.15800700	-0.40007800	3.43358300
H	-1.23003100	-0.69580400	-1.78311100
H	1.90755900	0.72985400	1.09796600
H	-1.48173700	2.74984300	-0.78089600
C	-0.13561000	4.52686500	0.51145200
H	-0.06523500	4.78136100	1.56887100
H	0.61199100	5.11120800	-0.02748700
H	-1.12675100	4.77943100	0.13874600
H	4.04696100	-1.74868700	-0.39691900
H	-5.06726500	-0.26158600	0.58980900
H	-3.51509500	-2.95120000	-0.54550900

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4 41 1.0
5 42 1.0
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Geometry-optimized structure of Ac-pSer^0-*cis*-Pro-NHMe in a type VIa1 (PcisD) β-turn with a C–H/O interaction (pSer χ_1 *t*, χ_2 *+90°*) (Pro χ_2 *endo*)
optimized M06-2X/6-311++G(d,p)/H2O

0 1

P	3.07204200	0.41098200	-0.53946300
O	2.07025700	0.84839700	0.62048500
O	4.06479200	1.65547100	-0.57939500
O	3.83651800	-0.80882800	0.11814200
O	2.44839200	0.04944500	-1.82259500
C	1.17136500	1.94440400	0.40039900
C	-0.22143300	1.40571000	0.07843000
H	1.52938200	2.58618300	-0.40873800
N	-1.10167800	2.54489400	-0.07900200
C	-0.68976000	0.53864000	1.26201200

H	-0.19415100	0.83193400	-0.85154700
C	-2.43673900	2.38780600	-0.21108000
N	-0.66810800	-0.80137700	1.12629200
O	-1.05043600	1.08392500	2.29661600
O	-2.94396900	1.27080500	-0.27474500
C	-0.99958500	-1.63205300	2.30120500
C	-0.07221000	-1.60811800	0.05400900
C	-0.63968300	-3.05182300	1.86021900
H	-0.39230300	-1.30005100	3.14692300
H	-2.05050400	-1.50925100	2.56583200
C	0.45847400	-2.82392500	0.81845600
C	-1.06341700	-2.04407400	-1.03748300
H	0.72796700	-1.07449900	-0.45832800
H	-0.31747400	-3.66778800	2.69834300
H	1.39882000	-2.55370900	1.30478200
H	0.62679700	-3.67060900	0.15667800
N	-2.21520900	-1.37088800	-1.11789200
O	-0.75917500	-2.95672000	-1.80159100
C	-3.16229800	-1.63858200	-2.18603900
H	-3.97588600	-0.92065300	-2.10728300
H	-2.68396300	-1.53885700	-3.16251700
H	-3.56495900	-2.64926400	-2.09967700
H	1.14049900	2.51424800	1.32928600
H	-2.37344700	-0.55520500	-0.53443800
H	-0.73289700	3.47536000	0.05407000
C	-3.26636700	3.64203900	-0.27212900
H	-3.89688100	3.59806600	-1.16016700
H	-3.91718300	3.66178000	0.60343100
H	-2.66591500	4.54981100	-0.29521900
H	-1.50166500	-3.53491700	1.39232900
H	4.56179500	1.75646800	-1.40134900
H	4.29518800	-0.63228900	0.95041400

1 2 1.5 3 1.5 4 1.5 5 2.0
2 6 1.0
3 41 1.0
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6 7 1.0 8 1.0 33 1.0
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9 12 1.5 35 1.0
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12 15 2.0 36 1.0
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Geometry-optimized structure of Ac-pThr^{2-}-*cis*-Pro-NHMe in a type VIa1 (PcisD) β-turn with a C–H/O interaction (pThr χ_1 *g*$^-$, χ_2 *–90°*) (Pro χ_2 *endo*)
optimized M06-2X/6-311++G(d,p)/H2O

-2 1

P	-3.06460800	-0.97763400	0.68309600
O	-2.82042200	0.17328600	-0.56203600
O	-1.65957300	-1.30189900	1.20624100
O	-3.94518100	-0.19378500	1.65275900
O	-3.76524000	-2.15613800	0.00932900
C	-1.68019300	0.14574900	-1.39182000
C	-0.49656800	0.79117300	-0.63009400

H	-1.90319400	0.82077900	-2.22795700
N	-0.79530100	2.20336500	-0.46543200
C	0.79239800	0.60802100	-1.42113400
H	-0.43366100	0.31548900	0.34877500
C	0.08245900	3.07099200	0.06197700
N	1.62590300	-0.36996400	-1.00724100
O	1.03177400	1.28267100	-2.41833100
O	1.21056800	2.72048400	0.41816700
C	2.78345900	-0.72743600	-1.84560400
C	1.39516600	-1.36747100	0.04800600
C	3.33028600	-1.99843900	-1.19131400
H	2.43469100	-0.91099600	-2.86613600
H	3.50294400	0.09212300	-1.87497100
C	2.09386000	-2.60405900	-0.52138200
C	1.99348500	-0.98051200	1.40807900
H	0.32918600	-1.53086700	0.23298200
H	3.79855300	-2.66208300	-1.91697700
H	1.44258200	-3.06647400	-1.26774300
H	2.32269100	-3.33135800	0.25464900
N	2.25051600	0.31642400	1.61619300
O	2.18135000	-1.84544800	2.26227800
C	2.69914800	0.78501400	2.91507700
H	2.79521700	1.86804100	2.87291800
H	1.98546300	0.51542700	3.69688300
H	3.66672100	0.34784200	3.16792500
H	1.97000600	1.01319000	0.93142900
H	-1.73000400	2.51300900	-0.68913600
C	-0.36510500	4.50524700	0.18261000
H	-0.21461800	4.83114800	1.21196300
H	0.26874200	5.11807700	-0.46034000
H	-1.40722600	4.65032000	-0.09763200
H	4.07399800	-1.74294000	-0.43128400
C	-1.36968500	-1.22389600	-1.98829200
H	-0.53528400	-1.15529400	-2.69107400
H	-1.13706300	-1.95560800	-1.21575800
H	-2.24691900	-1.57374200	-2.53352000

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9 12 1.5 34 1.0
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Geometry-optimized structure of Ac-pThr^{2-}-*cis*-Pro-NHMe in a type VIa1 (PcisD) β-turn with a C–H/O interaction (pThr χ_1 *t*, χ_2 *+90°*) (Pro χ_2 *endo*)
optimized M06-2X/6-311++G(d,p)/H2O

-2 1
P 3.01782100 0.03373200 -0.75107000
O 2.09974200 0.51509100 0.60576300

O	3.60933600	-1.28542500	-0.26546500
O	1.98224400	-0.09819100	-1.87268600
O	4.02592600	1.16323900	-0.96029800
C	1.32876200	1.68552600	0.47981800
C	-0.11949200	1.29840500	0.09896400
H	1.70637000	2.29476300	-0.35255400
N	-0.86768800	2.49533000	-0.23737000
C	-0.82579900	0.55942100	1.24337600
H	-0.04440900	0.66228200	-0.78573300
C	-2.15938000	2.43797300	-0.60973800
N	-0.83838900	-0.78910400	1.21315100
O	-1.36666100	1.18246300	2.15267000
O	-2.74568900	1.36277900	-0.74356700
C	-1.41440100	-1.52248400	2.35426500
C	-0.13249800	-1.69055700	0.29595200
C	-1.06341500	-2.98465600	2.06705400
H	-0.94912600	-1.16308400	3.27583200
H	-2.48783700	-1.33843000	2.42323200
C	0.19688000	-2.87733800	1.20433500
C	-0.96980500	-2.14044200	-0.90815100
H	0.76244800	-1.21935300	-0.10949100
H	-0.91404600	-3.55503400	2.98292800
H	1.06192800	-2.61733700	1.81979700
H	0.42115600	-3.77534900	0.63268700
N	-2.02766500	-1.38789900	-1.23783900
O	-0.63714200	-3.13680500	-1.54855900
C	-2.79347200	-1.67208500	-2.43795800
H	-3.55357900	-0.90128700	-2.54866300
H	-2.15011800	-1.67513900	-3.32068100
H	-3.27846700	-2.64710700	-2.36330900
H	-2.20643700	-0.50896600	-0.76073800
H	-0.44832000	3.39885700	-0.07526300
C	-2.85938900	3.75047700	-0.84950800
H	-3.35306900	3.71010000	-1.82036400
H	-3.62868600	3.87260600	-0.08496400
H	-2.18440300	4.60424200	-0.81743000
H	-1.86405000	-3.46145800	1.49479300
C	1.44339000	2.47917800	1.77310300
H	0.80176100	3.36373000	1.78032800
H	1.16909000	1.85289900	2.62357600
H	2.47832200	2.80308900	1.89453500

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35 36 1.0 37 1.0 38 1.0
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40 41 1.0 42 1.0 43 1.0
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Geometry-optimized structure of Ac-pThr^{1-}-*cis*-Pro-NHMe in a type VIa1 (PcisD) β-turn with a C–H/O interaction (pThr χ_1 *g*$^-$, χ_2 *–90°*) (Pro χ_2 *endo*)

optimized M06-2X/6-311++G(d,p)/H2O

-1 1

P	-3.05232300	-0.80759000	0.70966000
O	-2.80150100	0.21647900	-0.55814300
O	-1.73319100	-1.24190800	1.27319300
O	-4.10638800	-0.15214100	1.54231100
O	-3.68073900	-2.12745000	-0.02759400
C	-1.63995700	0.14229800	-1.38583300
C	-0.45952000	0.78404000	-0.62812600
H	-1.86205100	0.79871900	-2.23278700
N	-0.74769700	2.19830500	-0.47217500
C	0.82689300	0.58482300	-1.42783800
H	-0.38043500	0.32137900	0.35596900
C	0.14687700	3.05899900	0.04471500
N	1.66267500	-0.38728300	-1.00613700
O	1.05621300	1.25059600	-2.43077000
O	1.26988000	2.69171700	0.39397400
C	2.82974800	-0.73457800	-1.83772300
C	1.43695600	-1.38555200	0.04952800
C	3.39161000	-1.99168300	-1.17083500
H	2.48799100	-0.93093600	-2.85800600
H	3.53527800	0.09667200	-1.86858800
C	2.15894200	-2.61408000	-0.51026100
C	2.01143000	-0.99399400	1.41933900
H	0.37393700	-1.57004000	0.21769800
H	3.87668300	-2.65179300	-1.88835900
H	1.52174500	-3.08827000	-1.26110700
H	2.38999900	-3.33540900	0.27054800
N	2.29634500	0.29776800	1.61799200
O	2.15971200	-1.85582400	2.28328300
C	2.73253700	0.76867700	2.92077300
H	2.88593000	1.84415600	2.86197300
H	1.98452300	0.55169900	3.68679000
H	3.66833900	0.28624900	3.20723500
H	2.04104800	0.99309800	0.92250800
H	-1.67560500	2.52249400	-0.70303700
C	-0.28194100	4.49840000	0.16145300
H	-0.12290100	4.82503400	1.18928200
H	0.35712600	5.10083300	-0.48594300
H	-1.32335900	4.65545400	-0.11456700
H	4.12405900	-1.71942300	-0.40588100
C	-1.37488100	-1.25323800	-1.93394600
H	-0.54068200	-1.22728600	-2.63856900

H	-1.15796800	-1.97150600	-1.14386300
H	-2.26319500	-1.59463800	-2.46634800
H	-4.59894200	-1.99057700	-0.28512300

1 2 1.0 3 2.0 4 2.0 5 1.0
2 6 1.0
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5 44 1.0
6 7 1.0 8 1.0 40 1.0
7 9 1.0 10 1.0 11 1.0
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9 12 1.5 34 1.0
10 13 1.5 14 2.0
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12 15 2.0 35 1.0
13 16 1.0 17 1.0
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16 18 1.0 19 1.0 20 1.0
17 21 1.0 22 1.0 23 1.0
18 21 1.0 24 1.0 39 1.0
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Geometry-optimized structure of Ac-pThr^{1-}-*cis*-Pro-NHMe in a type VIa1 (PcisD) β-turn with a C–H/O interaction (pThr χ_1 *t*, χ_2 *+90°*) (Pro χ_2 *endo*)
optimized M06-2X/6-311++G(d,p)/H2O

-1 1

P	2.98037600	0.17256200	-0.77134600
O	2.08169800	0.59042700	0.55173300
O	3.58173000	-1.22627100	-0.19610000
O	2.04304500	-0.17059300	-1.88802400
O	4.06894100	1.18412200	-0.95450300
C	1.26449800	1.75042500	0.44099200
C	-0.16888300	1.31058200	0.07354300
H	1.61936100	2.37510800	-0.38889700
N	-0.94943600	2.48590600	-0.26067800
C	-0.84553200	0.55947000	1.23311200
H	-0.09587600	0.66926700	-0.80845000
C	-2.24902200	2.38930300	-0.60495600
N	-0.83602200	-0.78896300	1.21149700
O	-1.38225100	1.18240900	2.14248700
O	-2.80420200	1.29688200	-0.71596300
C	-1.39810700	-1.51958200	2.36292500
C	-0.13045900	-1.69270100	0.29627000
C	-1.04377800	-2.98116700	2.07962100
H	-0.92500700	-1.15283000	3.27737000
H	-2.47120200	-1.33812400	2.43969700
C	0.21081300	-2.87337900	1.20915400
C	-0.96541400	-2.15756700	-0.90519500
H	0.76051100	-1.22375200	-0.11575600
H	-0.88544300	-3.54654600	2.99688000
H	1.07869000	-2.60779800	1.81776900
H	0.43474700	-3.77242900	0.63920000
N	-2.04773500	-1.43554400	-1.21945000
O	-0.60630700	-3.13965200	-1.55192700
C	-2.82082300	-1.73877100	-2.41075500
H	-3.59171600	-0.97864900	-2.51988000
H	-2.18424500	-1.73917300	-3.29804900
H	-3.29210800	-2.71957900	-2.32493200
H	-2.24941500	-0.56681800	-0.73349000
H	-0.55509000	3.40206500	-0.10595400

C	-2.98830900	3.67945700	-0.84247500
H	-3.50085900	3.61474800	-1.80212100
H	-3.74426500	3.78883500	-0.06289600
H	-2.33611400	4.55116600	-0.83396600
H	-1.84631800	-3.46358200	1.51502700
C	1.38093700	2.52374100	1.74214500
H	0.70913800	3.38399800	1.76826200
H	1.13924600	1.87568800	2.58541200
H	2.40595300	2.88024400	1.85013300
H	4.31996600	-1.08750500	0.40735200

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2 6 1.0
3 44 1.0
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6 7 1.0 8 1.0 40 1.0
7 9 1.0 10 1.0 11 1.0
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9 12 1.5 34 1.0
10 13 1.5 14 2.0
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12 15 2.0 35 1.0
13 16 1.0 17 1.0
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Geometry-optimized structure of Ac-pThr^0-*cis*-Pro-NHMe in a type VIa1 (PcisD) β-turn with a C–H/O interaction (pThr χ_1 *g*$^-$, χ_2 *–90°*) (Pro χ_2 *endo*)
optimized M06-2X/6-311++G(d,p)/H2O

0 1

P	-3.15869800	-0.82723700	0.58255500
O	-2.77727100	-0.10867700	-0.78708800
O	-2.05691200	-1.04710600	1.53425200
O	-4.32667900	0.15886500	1.01849600
O	-3.83942700	-2.21685300	0.20010400
C	-1.49174700	-0.28717400	-1.43108300
C	-0.43548800	0.51197600	-0.65225100
H	-1.62390100	0.19990200	-2.39853500
N	-0.89914100	1.88384100	-0.55919600
C	0.88003800	0.45279300	-1.44324000
H	-0.31693900	0.09666100	0.35071600
C	-0.10985600	2.88732600	-0.12761100
N	1.86814600	-0.33180700	-0.96497400
O	0.99358000	1.08367400	-2.48470300
O	1.05355400	2.68967700	0.21973500
C	3.10046600	-0.47612000	-1.76423500
C	1.81165400	-1.31838000	0.12282800
C	3.90182400	-1.53295700	-1.00518600
H	2.83175800	-0.81255400	-2.76933000
H	3.60780900	0.48542400	-1.84845200
C	2.81184600	-2.38120900	-0.34715800
C	2.20717200	-0.77885400	1.50618700
H	0.81163500	-1.73798200	0.23407000
H	4.55107100	-2.10541600	-1.66574100
H	2.32813000	-3.02279300	-1.08762800
H	3.15992500	-2.99338000	0.48191500
N	2.28768100	0.54693500	1.64865400

O	2.40895600	-1.57213900	2.42237700
C	2.55540500	1.13882800	2.94777600
H	2.47485700	2.21967400	2.85307500
H	1.83654300	0.78380700	3.68894200
H	3.55928900	0.88051500	3.28927700
H	2.00403700	1.16418900	0.89333000
H	-1.85778700	2.07880600	-0.81012400
C	-0.71672300	4.26517400	-0.10769400
H	-0.58737400	4.68677200	0.88924200
H	-0.16502400	4.88995800	-0.81182300
H	-1.77264900	4.26990100	-0.37281100
H	4.52151000	-1.06068100	-0.23816000
C	-1.16082700	-1.75373800	-1.63492300
H	-0.22139900	-1.85211600	-2.18343600
H	-1.07318500	-2.28445900	-0.68478700
H	-1.94912700	-2.22425600	-2.22290000
H	-4.56865900	-2.16813100	-0.43211600
H	-4.73584100	-0.04358600	1.86972200

1 2 1.5 3 2.0 4 1.5 5 1.5
2 6 1.0
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4 45 1.0
5 44 1.0
6 7 1.0 8 1.0 40 1.0
7 9 1.0 10 1.0 11 1.0
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9 12 1.5 34 1.0
10 13 1.5 14 2.0
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12 15 2.0 35 1.0
13 16 1.0 17 1.0
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16 18 1.0 19 1.0 20 1.0
17 21 1.0 22 1.0 23 1.0
18 21 1.0 24 1.0 39 1.0
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Geometry-optimized structure of Ac-pThr^0-*cis*-Pro-NHMe in a type VIa1 (PcisD) β-turn with a C–H/O interaction (pThr χ_1 *t*, χ_2 *+90°*) (Pro χ_2 *endo*)
optimized M06-2X/6-311++G(d,p)/H2O

0 1

P	2.97972600	-0.13827400	-0.72348400
O	2.09383700	0.45277000	0.45957700
O	3.60763700	-1.43059300	-0.05649200
O	2.26628500	-0.45442900	-1.97161500
O	4.12564100	0.96237800	-0.84558400
C	1.36592000	1.68840700	0.27631000
C	-0.10460800	1.32114400	0.00004600
H	1.74505900	2.20081900	-0.61448300
N	-0.83250600	2.53962700	-0.28761700
C	-0.73373200	0.60952700	1.21249500
H	-0.13145700	0.67334900	-0.88121900
C	-2.16489800	2.52981900	-0.50413200
N	-0.83862100	-0.73494500	1.18261300
O	-1.11726000	1.26540300	2.17209400
O	-2.80557600	1.48143600	-0.50103500
C	-1.33556800	-1.42651200	2.38867300
C	-0.31745600	-1.68981200	0.19819300
C	-1.14292900	-2.90985500	2.06783300

H	-0.73531000	-1.11011100	3.24526300
H	-2.37400000	-1.15323700	2.58065400
C	0.01685100	-2.90456300	1.06936400
C	-1.31203700	-2.07705200	-0.90830600
H	0.56277200	-1.30312600	-0.31000400
H	-0.93725700	-3.49579700	2.96234400
H	0.96517500	-2.72287900	1.58075500
H	0.09693400	-3.81284900	0.47606100
N	-2.38041200	-1.29165100	-1.07453300
O	-1.08126500	-3.06102300	-1.60709300
C	-3.30743200	-1.52078900	-2.16918400
H	-4.05367500	-0.72933300	-2.15590200
H	-2.78528300	-1.51141100	-3.12830600
H	-3.80323500	-2.48620500	-2.05548000
H	-2.46181100	-0.42202000	-0.55712900
H	-0.35290700	3.42636000	-0.24918600
C	-2.82428700	3.86061400	-0.74919500
H	-3.35190400	3.81271400	-1.70213400
H	-3.56273600	4.02601600	0.03647400
H	-2.12001900	4.69045200	-0.76457500
H	-2.04026600	-3.31457300	1.59221200
C	1.61866900	2.53117600	1.50946800
H	1.04304600	3.45748800	1.48557400
H	1.34331900	1.97778200	2.40675900
H	2.67865900	2.78368700	1.55032600
H	4.10029900	-1.29229600	0.76340900
H	4.57412600	0.98790700	-1.70061700

1 2 1.5 3 1.5 4 2.0 5 1.5
2 6 1.0
3 44 1.0
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5 45 1.0
6 7 1.0 8 1.0 40 1.0
7 9 1.0 10 1.0 11 1.0
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9 12 1.5 34 1.0
10 13 1.5 14 2.0
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12 15 2.0 35 1.0
13 16 1.0 17 1.0
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16 18 1.0 19 1.0 20 1.0

17 21 1.0 22 1.0 23 1.0
18 21 1.0 24 1.0 39 1.0
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21 25 1.0 26 1.0
22 27 1.5 28 2.0
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Geometry optimized structures of Ac-X-cis-Ala-NHMe type VIa1 β-turns stabilized via C–H/O interactions derived from calculated X-*cis*-Pro structures

Geometry-optimized structure of Ac-Asn-*cis*-Ala-NHMe in a type VIa1 (PcisD) β-turn with a C–H/O interaction (Asn χ_1 *t*, χ_2 *–70°*)
optimized M06-2X/6-311++G(d,p)/H2O

0 1

C	4.38252500	0.40650500	-0.23964500
C	2.87998400	0.37142800	-0.16597500
O	2.22015100	1.36129100	0.14485500
H	4.68094400	1.26801000	-0.83665200
H	4.77077100	0.54460800	0.77097700
H	4.80660600	-0.50088700	-0.66622600

N	2.28172500	-0.80375800	-0.45345600
C	0.84573100	-0.95793000	-0.32539500
C	0.43132500	-0.61774700	1.12105900
O	1.11883600	-0.99619900	2.05546700
C	0.48740200	-2.41266400	-0.66563900
C	-1.01033900	-2.64972700	-0.58502600
N	-1.67130300	-2.63875000	-1.75939200
O	-1.57095800	-2.79181500	0.49211300
H	0.36622200	-0.27335800	-1.03004600
H	0.96437000	-3.07038300	0.06423700
H	0.87385300	-2.64347600	-1.65964100
H	-2.66999600	-2.78653900	-1.76463600
H	2.85109000	-1.62347400	-0.60381100
H	-1.19357700	-2.55550500	-2.64225900
N	-0.68114400	0.12797300	1.30482400
C	-1.74531000	0.45803300	0.36364000
C	-1.64184500	1.88343400	-0.20620600
O	-2.62459800	2.41469300	-0.71679300
C	-3.09961900	0.23046100	1.02641300
H	-3.18089400	-0.81588000	1.32110400
H	-3.89878900	0.47862000	0.33090900
H	-1.68100300	-0.20639600	-0.50124300
N	-0.43806400	2.46483900	-0.15886900
C	-0.21300400	3.76012000	-0.77522100
H	0.84425000	4.00130400	-0.68648700
H	-0.49300400	3.74137400	-1.83052300
H	-0.80076800	4.53270300	-0.27622500
H	0.36671800	1.95608200	0.19368300
H	-0.89087900	0.30054500	2.28160600
H	-3.20295700	0.86528800	1.91033100

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12 13 1.5 14 2.0
13 18 1.0 20 1.0

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21 22 1.0 35 1.0
22 23 1.0 25 1.0 28 1.0
23 24 2.0 29 1.5
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29 30 1.0 34 1.0
30 31 1.0 32 1.0 33 1.0
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Geometry-optimized structure of Ac-Asp-*cis*-Ala-NHMe in a type VIa1 (PcisD) β-turn with a C–H/O interaction (Asp χ_1 *t*, χ_2 *–10°*)
optimized M06-2X/6-311++G(d,p)/H2O

-1 1

C	0.48576400	4.26760600	-0.19622000
C	0.21605900	2.78701000	-0.11123500
O	-0.87340300	2.35577200	0.26584200
H	0.50755300	4.66883400	0.81862200
H	1.42604900	4.50147700	-0.69296700
H	-0.33827200	4.74172000	-0.72876300
N	1.22851800	1.97012900	-0.45165400
C	1.17574500	0.51334400	-0.35739600
C	0.66710400	0.12438300	1.04128700
O	1.19787200	0.61719300	2.02892700
C	2.60550400	0.00869400	-0.56243700
C	2.79523900	-1.51924700	-0.58964700
O	1.76429000	-2.22761400	-0.61720400
O	3.98352500	-1.91065800	-0.59802900
H	2.11559200	2.38607000	-0.69329800

H	0.51330400	0.12649200	-1.13316200
H	2.97916800	0.39773600	-1.51516100
H	3.24054100	0.42478100	0.22434300
N	-0.37719800	-0.72781800	1.16364000
C	-1.00194600	-1.61530200	0.18941700
C	-2.38483300	-1.13855000	-0.27379000
O	-3.18141800	-1.93152700	-0.77448800
C	-1.07380400	-3.02667800	0.76236300
H	-0.36059900	-1.65277500	-0.69077000
H	-1.54036900	-3.69807000	0.04360200
H	-0.06177600	-3.36951000	0.97426000
N	-2.64223800	0.16827900	-0.14794300
C	-3.87029300	0.73995900	-0.66794300
H	-3.95605800	0.57488800	-1.74457900
H	-4.73847500	0.29108000	-0.18239200
H	-3.86248000	1.80967900	-0.46848500
H	-1.91507200	0.79820400	0.17996800
H	-1.66608100	-3.04269700	1.68177300
H	-0.62076000	-0.90467900	2.13193900

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9 10 2.0 19 1.5
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11 12 1.0 17 1.0 18 1.0
12 13 2.0 14 2.0
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19 20 1.0 34 1.0
20 21 1.0 23 1.0 24 1.0
21 22 2.0 27 1.5
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23 25 1.0 26 1.0 33 1.0
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27 28 1.0 32 1.0
28 29 1.0 30 1.0 31 1.0
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Geometry-optimized structure of Ac-Asp-*cis*-Ala-NHMe in a type VIa1 (PcisD) β-turn with a C–H/O interaction (Asp χ_1 *t*, χ_2 +90°)
optimized M06-2X/6-311++G(d,p)/H2O

-1 1

C	4.19425700	1.32573600	-0.23245600
C	2.73740200	0.94805600	-0.18915600
O	1.86086000	1.77971700	0.05053700
H	4.48517400	1.68779900	0.75470400
H	4.83817300	0.49527700	-0.51688700
H	4.31967100	2.14382400	-0.94206700
N	2.43164300	-0.34106500	-0.42791800
C	1.06274000	-0.81679300	-0.34185200
C	0.52588100	-0.53794900	1.07203800
O	1.24335000	-0.71549700	2.04703100
C	1.02465000	-2.32318500	-0.61303400
C	-0.42705100	-2.84845900	-0.67988800
O	-0.80787300	-3.59141200	0.24980700
O	-1.10034700	-2.46144300	-1.66490700
H	0.47079000	-0.28935800	-1.09234100
H	1.57971500	-2.83879600	0.17313600
H	1.50761500	-2.50503100	-1.57655800
H	3.17439400	-1.01672500	-0.52903600
N	-0.74978800	-0.11248100	1.20470900
C	-1.80421200	0.05072700	0.21002700
C	-2.05370900	1.52528600	-0.14621800
O	-3.16588800	1.90824100	-0.50072700
C	-3.07673300	-0.63506500	0.69096700
H	-2.87165500	-1.69667700	0.83353900
H	-3.86668100	-0.51537200	-0.04845500
H	-1.49532200	-0.44509200	-0.71281600
N	-0.98675400	2.33491500	-0.10125200
C	-1.08555300	3.71873600	-0.52814900
H	-0.10353800	4.17784100	-0.43295600

H	-1.41638900	3.78549300	-1.56696500
H	-1.79727700	4.26366400	0.09459500
H	-0.06646900	1.96614200	0.12132800
H	-3.42074800	-0.20169500	1.63405700
H	-1.03000200	0.01974500	2.17034100

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2 3 2.0 7 1.5
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7 8 1.0 18 1.0
8 9 1.0 11 1.0 15 1.0
9 10 2.0 19 1.5
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11 12 1.0 16 1.0 17 1.0
12 13 2.0 14 2.0
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19 20 1.0 34 1.0
20 21 1.0 23 1.0 26 1.0
21 22 2.0 27 1.5
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23 24 1.0 25 1.0 33 1.0
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27 28 1.0 32 1.0
28 29 1.0 30 1.0 31 1.0
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Geometry-optimized structure of Ac-Gln-*cis*-Ala-NHMe in a type VIa1 (PcisD) β-turn with a C–H/O interaction (Gln χ_1 g^-, χ_2 g^-, χ_3 –10°)

optimized M06-2X/6-311++G(d,p)/H2O

0 1

C	3.10484700	-2.82069800	0.87376100
C	1.89662400	-1.98634200	0.54261600
O	0.76268800	-2.31933100	0.88356400
H	3.04325500	-3.75186000	0.30764700
H	4.04196400	-2.31888900	0.63858000
H	3.07772100	-3.06864500	1.93465100
N	2.11092300	-0.84653100	-0.15056100
C	0.98481200	-0.06430300	-0.61763500
C	0.12975300	-0.91545200	-1.56933000
O	0.64111400	-1.75462000	-2.29474800
C	1.46470000	1.19727800	-1.34123500
C	2.15033300	2.18756500	-0.40749900
C	1.18653700	2.79332600	0.60205100
N	1.76316300	3.42615000	1.64269900
O	-0.02968900	2.72382400	0.46891800
H	0.39047300	0.21740900	0.25448600
H	0.60670900	1.68006100	-1.81403000
H	2.14873300	0.90322700	-2.14226500
H	2.56806100	3.01434400	-0.98960800
H	2.98794100	1.72522500	0.12114600
H	3.02085200	-0.68808900	-0.55934900
H	1.18201200	3.90276100	2.31557000
H	2.76375400	3.49789400	1.73409400
N	-1.20246400	-0.68273500	-1.56841200
C	-1.95218100	0.35360400	-0.86706200
C	-2.50142900	-0.09002600	0.49956700
O	-3.41078500	0.54344900	1.02977200
C	-3.08097500	0.85217400	-1.76357100
H	-2.66547600	1.25476600	-2.68791200
H	-3.64339000	1.63079800	-1.25280100
H	-1.28528200	1.19303700	-0.64844900
N	-1.91612500	-1.14329100	1.08494100
C	-2.29550400	-1.54795800	2.42720900
H	-2.14281100	-0.73370200	3.13891100
H	-3.34710600	-1.83788800	2.45615100
H	-1.68058300	-2.39841900	2.71397500
H	-1.09685700	-1.58018600	0.67651000
H	-3.76587300	0.03632900	-2.00897400
H	-1.72431300	-1.25491200	-2.22229300

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32 33 1.0 37 1.0
33 34 1.0 35 1.0 36 1.0
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Geometry-optimized structure of Ac-Gln-*cis*-Ala-NHMe in a type VIa1 (PcisD) β-turn with a C–H/O interaction (Gln χ_1 *t*, χ_2 g^+, χ_3 *+30°*)
optimized M06-2X/6-311++G(d,p)/H2O

0 1

C	4.35827300	-1.17037900	-0.61872500
C	2.95897800	-0.67534600	-0.36780800
O	2.71990000	0.51474700	-0.16278100
H	4.38541400	-2.20110300	-0.96837900
H	4.83173000	-0.51957800	-1.35303500
H	4.91947700	-1.09360100	0.31441800
N	1.97694800	-1.59677200	-0.36480800
C	0.60397600	-1.24209000	-0.05569800
C	0.56244100	-0.55532300	1.31960500
O	1.23005200	-0.99277400	2.24419800
C	-0.22851600	-2.53004000	-0.01920800
C	-1.71314500	-2.32005800	0.24744500
C	-2.44229800	-1.67211700	-0.92023600
N	-3.72758400	-1.33928500	-0.67909600
O	-1.89744800	-1.45497000	-1.99421700
H	0.23574100	-0.57433000	-0.83672700
H	0.18593300	-3.17386600	0.76120600
H	-0.10433000	-3.03658200	-0.97878400
H	2.21634000	-2.57331000	-0.45473500
H	-1.88234100	-1.72668400	1.15267800
H	-2.18778400	-3.28797700	0.43138600
H	-4.28491700	-0.95121800	-1.42529200
H	-4.18386600	-1.57552300	0.18761000
N	-0.24470400	0.52043400	1.48095200
C	-1.21122000	1.13228500	0.57653300
C	-0.68629200	2.41165600	-0.10302500
O	-1.47109000	3.26934800	-0.49782500
C	-2.51110900	1.40840100	1.32380300
H	-2.90360800	0.48019400	1.74117100
H	-3.24683800	1.83719600	0.64660200
H	-1.41908800	0.44108400	-0.24264800
N	0.63712600	2.49303900	-0.27754400
C	1.22215000	3.60175200	-1.01046000
H	0.80198000	3.66791000	-2.01624200
H	1.03391300	4.54568800	-0.49598900
H	2.29565300	3.43826200	-1.07759600
H	1.24366700	1.72257500	-0.01088300
H	-2.33828900	2.11521900	2.13935400
H	-0.22203600	0.90048500	2.42100600

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Geometry-optimized structure of Ac-Gln-*cis*-Ala-NHMe in a type VIa1 (PcisD) β-turn with a C–H/O interaction (Gln χ_1 *g*$^-$, χ_2 *t*, χ_3 *–30°*)
optimized M06-2X/6-311++G(d,p)/H2O

0 1

C	-0.80186200	4.30770400	-0.30337000
C	-0.30176600	2.90220000	-0.10238600
O	0.86674700	2.66561000	0.19986000

H	-0.30597400	4.72438700	-1.18174200
H	-1.88062600	4.35696000	-0.44232700
H	-0.51603100	4.90663300	0.56123300
N	-1.19787100	1.90495600	-0.26896600
C	-0.76667300	0.52149100	-0.23348700
C	0.29882200	0.28898900	-1.31651500
O	0.23003100	0.86622400	-2.39344000
C	-1.95045200	-0.41484700	-0.48269100
C	-2.95869300	-0.39079800	0.65835600
C	-4.13783300	-1.31193400	0.39230600
N	-5.01680000	-1.42283300	1.41135400
O	-4.28209900	-1.90546600	-0.66680900
H	-0.33852200	0.33028000	0.75456600
H	-1.57692900	-1.43291700	-0.61769100
H	-2.43021300	-0.13630600	-1.42511700
H	-3.35070600	0.61792700	0.82125000
H	-2.48213900	-0.69288400	1.59621400
H	-2.09676200	2.12412200	-0.67355000
H	-5.83513500	-2.00159200	1.30002100
H	-4.89167800	-0.92610800	2.27841500
N	1.28872900	-0.58351100	-1.03390000
C	1.40151400	-1.47463700	0.12562800
C	2.15148700	-0.87360400	1.32669800
O	2.50599200	-1.61086200	2.24290500
C	2.17822700	-2.66611400	-0.44965300
C	3.14665500	-1.98591700	-1.41969200
C	2.28050300	-0.91103400	-2.07482600
H	1.48602300	-3.31268900	-0.99340800
H	2.66343600	-3.24198200	0.33537600
H	3.57110300	-2.67125100	-2.15178400
H	3.96807900	-1.52396200	-0.86528900
H	2.83484400	-0.01653700	-2.36045600
H	1.75768500	-1.28813500	-2.95787000
H	0.41987200	-1.78235300	0.49187700
N	2.36539600	0.44668200	1.32372200
C	2.96854600	1.10271600	2.47109100
H	2.40911600	0.88074200	3.38225500
H	3.99800200	0.76754700	2.60779600
H	2.95997700	2.17570300	2.29301000
H	1.94418400	1.03602100	0.61285700

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38 39 1.0 43 1.0
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Geometry-optimized structure of Ac-Gln-*cis*-Ala-NHMe in a type VIa1 (PcisD) β-turn with a C–H/O interaction (Gln χ_1 *t*, χ_2 *t*, χ_3 *+30°*)
optimized M06-2X/6-311++G(d,p)/H2O

0 1

C	-1.44668600	4.40446700	0.11627000
C	-1.18561600	2.92483800	0.01469400
O	-2.07972700	2.09841300	0.19247400
H	-0.59128300	5.00810600	-0.18241000
H	-2.30557600	4.65074100	-0.50784300
H	-1.70490500	4.63397200	1.15159600
N	0.07630600	2.54927100	-0.27150700
C	0.48510700	1.15529700	-0.30876300
C	0.06380500	0.46952800	1.00235200
O	0.24303800	1.03754700	2.07148000
C	2.01202200	1.12081200	-0.43788600
C	2.59328100	-0.28238300	-0.53505200
C	4.11485800	-0.26249900	-0.51365800
N	4.70278300	-1.43735900	-0.82421500
O	4.75610800	0.73787100	-0.22837500
H	0.00868400	0.67173100	-1.16601700
H	2.43499600	1.62855200	0.43245100
H	2.29594400	1.69494900	-1.32362300
H	0.79220300	3.25795200	-0.33667700
H	2.26915700	-0.78275700	-1.45169100
H	2.26857500	-0.90622600	0.30673500
H	5.70774900	-1.51347700	-0.78453800
H	4.16608200	-2.26190200	-1.04027500
N	-0.47704800	-0.76710300	0.93852200
C	-0.57331300	-1.67341400	-0.21228800
C	-1.88642000	-1.57396500	-1.00555600
O	-2.15364600	-2.44172400	-1.83357500
C	-0.45341500	-3.05276400	0.44808600
C	-1.23402000	-2.85472000	1.74814900
C	-0.79851900	-1.46130700	2.20100600
H	0.59888500	-3.25604500	0.66150000
H	-0.84570400	-3.83783800	-0.19450900
H	-1.01991100	-3.61362100	2.49910900
H	-2.30797700	-2.86800900	1.54376800
H	-1.57132200	-0.91556300	2.74351000
H	0.09919800	-1.49564600	2.82393100
H	0.23180200	-1.50463900	-0.92699200
N	-2.67175400	-0.52183700	-0.76047200
C	-3.88149100	-0.30068500	-1.53337700
H	-3.65778000	-0.25108600	-2.60116900
H	-4.59583300	-1.10877000	-1.36785000
H	-4.32292500	0.64042900	-1.21250100

H -2.34580200 0.23227000 -0.16271300

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Geometry-optimized structure of Ac-Glu-*cis*-Ala-NHMe in a type VIa1 (PcisD) β-turn with a C–H/O interaction (Glu χ_1 g^-, χ_2 g^-, χ_3 *–10°*)
optimized M06-2X/6-311++G(d,p)/H2O

-1 1

C	-3.26149800	-2.66968300	-0.79555700
C	-2.01603000	-1.88609500	-0.47585100
O	-0.89525500	-2.30295900	-0.77154800
H	-4.17515600	-2.12244300	-0.56935900
H	-3.24544900	-2.93318200	-1.85322900
H	-3.24269300	-3.59486000	-0.21716400
N	-2.17910100	-0.70293300	0.14853700
C	-1.02410700	0.05798600	0.58152600
C	-0.22285700	-0.76590900	1.59735200
O	-0.77689700	-1.53450600	2.37088600
C	-1.45084000	1.38691900	1.21224200
C	-2.04229800	2.35241700	0.19215200
C	-1.03869800	2.86696300	-0.86370300
O	0.18114900	2.64926500	-0.66190200
O	-1.53494200	3.48329600	-1.83430000
H	-3.09285200	-0.45021100	0.49530100
H	-0.40959300	0.26583500	-0.29657800
H	-2.16670100	1.17748600	2.01434000
H	-0.57255400	1.84387400	1.67386300
H	-2.88982300	1.90511300	-0.33422600
H	-2.43766400	3.23243800	0.70857400
N	1.11741400	-0.58632700	1.60770600
C	1.92357600	0.35039000	0.83276400
C	2.51201300	-0.26366700	-0.44860800
O	3.52001900	0.21819700	-0.96064800
C	3.02553600	0.92230900	1.71751300
H	1.28682800	1.17401800	0.49035100
H	3.63146600	1.62532500	1.14972900
H	2.57996200	1.43682900	2.56975300
N	1.84559200	-1.29106800	-0.99353600
C	2.25672700	-1.84967200	-2.26909700
H	2.30672100	-1.07296400	-3.03503100
H	3.24001500	-2.31712100	-2.18810900
H	1.52669900	-2.60099200	-2.56338800
H	0.96807000	-1.61594100	-0.60025400
H	3.67855600	0.12691400	2.08634600
H	1.60510200	-1.13592100	2.30582700

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Geometry-optimized structure of Ac-Glu-*cis*-Ala-NHMe in a type VIa1 (PcisD) β-turn with a C–H/O interaction (Glu χ_1 *t*, χ_2 g^+, χ_3 *+30°*)
optimized M06-2X/6-311++G(d,p)/H2O

-1 1

C	4.37115400	-1.04026200	-0.61244400
C	2.95651200	-0.58945300	-0.35918100
O	2.68515500	0.59296600	-0.14413200
H	4.93264700	-0.94292400	0.31855600
H	4.43113100	-2.07029100	-0.96022600
H	4.82137900	-0.37633400	-1.34981300
N	2.00307800	-1.53793300	-0.36725800
C	0.61486100	-1.23144500	-0.06656600
C	0.53987900	-0.56131500	1.31316000
O	1.21340600	-0.98212300	2.24347900
C	-0.18368300	-2.54043000	-0.05484000
C	-1.67614000	-2.37225500	0.20361400
C	-2.48336600	-1.70996300	-0.93475300
O	-1.86198200	-1.36419600	-1.96743700
O	-3.70942600	-1.56826900	-0.71791600
H	0.22822100	-0.57139900	-0.84370300
H	0.25472400	-3.18619200	0.71336600
H	-0.03733900	-3.02214100	-1.02473900
H	2.27078400	-2.50585600	-0.46874100
H	-1.85942200	-1.80360400	1.12232800
H	-2.12221900	-3.35534900	0.37662600
N	-0.30045800	0.48811000	1.47412800
C	-1.27953000	1.06626300	0.56090500
C	-0.79309700	2.37091300	-0.09573700
O	-1.59960200	3.20894000	-0.49124800
C	-2.60156500	1.27933000	1.28932000
H	-2.97045400	0.32440000	1.66516600
H	-3.33736200	1.70224000	0.60819900
H	-1.44662500	0.37194100	-0.26537300
N	0.52960800	2.49987900	-0.25408900
C	1.08542900	3.63490000	-0.96822900
H	0.87188400	4.56600300	-0.44007400
H	2.16319600	3.50132500	-1.03598200
H	0.66547000	3.70577000	-1.97378800
H	1.15809300	1.74637600	0.01038200
H	-2.47104000	1.96828600	2.12785800
H	-0.30179300	0.86111200	2.41702400

1 2 1.0 4 1.0 5 1.0 6 1.0
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7 8 1.0 19 1.0
8 9 1.0 11 1.0 16 1.0
9 10 2.0 22 1.5
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11 12 1.0 17 1.0 18 1.0
12 13 1.0 20 1.0 21 1.0
13 14 2.0 15 2.0
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22 23 1.0 37 1.0
23 24 1.0 26 1.0 29 1.0
24 25 2.0 30 1.5
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26 27 1.0 28 1.0 36 1.0
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30 31 1.0 35 1.0
31 32 1.0 33 1.0 34 1.0
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Geometry-optimized structure of Ac-Glu-*cis*-Ala-NHMe in a type VIa1 (PcisD) β-turn with a C–H/O interaction (Glu χ_1 *g*$^-$, χ_2 *t*, χ_3 +30°)
optimized M06-2X/6-311++G(d,p)/H2O

-1 1

C	-0.94383700	4.27227000	-0.33965500
C	-0.40020200	2.88027100	-0.15341800
O	0.78526100	2.67892000	0.11203200
H	-2.02350200	4.29054500	-0.47934200
H	-0.67826700	4.86870100	0.53341800
H	-0.45947600	4.71610100	-1.21087800
N	-1.27126600	1.86039800	-0.28729600

C	-0.81610700	0.48465400	-0.23089100
C	0.24133900	0.25448900	-1.31936000
O	0.14754100	0.79895200	-2.41216100
C	-1.98721500	-0.47843600	-0.44432000
C	-3.00471400	-0.43313300	0.68783100
C	-4.17521700	-1.42711800	0.53280400
O	-4.11826700	-2.25342600	-0.40581500
O	-5.09121000	-1.32220000	1.38378700
H	-2.20302100	2.05176900	-0.62488000
H	-0.37490400	0.31918500	0.75620500
H	-2.46197800	-0.24375700	-1.40233700
H	-1.59695200	-1.49452800	-0.54083900
H	-2.51154100	-0.65741600	1.64035600
H	-3.43385500	0.56645800	0.79963000
N	1.25834100	-0.58463700	-1.02692200
C	1.40211000	-1.44668500	0.15059000
C	2.14226800	-0.80041700	1.33398400
O	2.51892100	-1.50785900	2.26514900
C	2.20660700	-2.62980500	-0.40351000
C	3.14788500	-1.94695000	-1.39802300
C	2.24575400	-0.91341500	-2.07080300
H	0.43069100	-1.77150000	0.52904400
H	2.71349000	-3.17417600	0.39028400
H	1.52783400	-3.30746200	-0.92602900
H	3.96038300	-1.44855600	-0.86229400
H	3.58547800	-2.63764900	-2.11733200
H	2.77243800	-0.01260700	-2.38756100
H	1.72394000	-1.32889700	-2.93723200
N	2.32415900	0.52441800	1.30051500
C	2.91409900	1.21981000	2.43133600
H	2.36006200	1.00860300	3.34841000
H	3.95042500	0.90962000	2.57514200
H	2.88349400	2.28795700	2.22788600
H	1.88202500	1.08805000	0.58095300

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8 9 1.0 11 1.0 17 1.0
9 10 2.0 22 1.5

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11 12 1.0 18 1.0 19 1.0
12 13 1.0 20 1.0 21 1.0
13 14 2.0 15 2.0
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23 24 1.0 26 1.0 29 1.0
24 25 2.0 36 1.5
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26 27 1.0 30 1.0 31 1.0
27 28 1.0 32 1.0 33 1.0
28 34 1.0 35 1.0
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36 37 1.0 41 1.0
37 38 1.0 39 1.0 40 1.0
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Geometry-optimized structure of Ac-Glu-*cis*-Ala-NHMe in a type VIa1 (PcisD) β-turn with a C–H/O interaction (Glu χ_1 *t*, χ_2 *t*, χ_3 *+30°*)
optimized M06-2X/6-311++G(d,p)/H2O

-1 1

C	-1.26608000	4.44001700	0.15319300
C	-1.05536800	2.95276200	0.04104500
O	-1.98177500	2.15770000	0.20247100
H	-1.52704700	4.67003000	1.18773900
H	-0.38722000	5.01627400	-0.13145200
H	-2.10951500	4.72100300	-0.47732800

N	0.19384200	2.53519200	-0.23519300
C	0.55717100	1.12802000	-0.28318800
C	0.10409300	0.44847600	1.01914300
O	0.29223300	1.00202000	2.09526500
C	2.08270800	1.03513100	-0.41162600
C	2.61759000	-0.38305300	-0.54754700
C	4.15977200	-0.47799300	-0.57321900
O	4.81319900	0.57868500	-0.42576900
O	4.62456900	-1.63097200	-0.74089800
H	0.06554200	0.66906400	-1.14564100
H	2.52352200	1.51066100	0.46864900
H	2.38639500	1.62375700	-1.28153300
H	0.93554700	3.21762000	-0.28926200
H	2.25581200	-0.84790200	-1.46986500
H	2.27470800	-1.01728700	0.27863000
N	-0.48350300	-0.76652000	0.94310700
C	-0.58941500	-1.66252200	-0.21445500
C	-1.88754100	-1.51717400	-1.02397900
O	-2.17853500	-2.37495000	-1.85494100
C	-0.51805200	-3.04881000	0.43717400
C	-1.30762700	-2.83718100	1.72978400
C	-0.83702400	-1.45987500	2.19677800
H	0.52570000	-3.28238100	0.66145000
H	-0.92480700	-3.81830100	-0.21528600
H	-1.12437700	-3.60677700	2.47816000
H	-2.37924100	-2.81822300	1.51330000
H	-1.59934600	-0.89694400	2.73680900
H	0.05299800	-1.52460300	2.82842600
H	0.23265400	-1.51135000	-0.91339600
N	-2.63575800	-0.43512300	-0.79075100
C	-3.82598800	-0.16993400	-1.57949400
H	-4.56744400	-0.95669900	-1.43132700
H	-4.24276200	0.78188100	-1.25697300
H	-3.58582300	-0.11858400	-2.64375100
H	-2.29032900	0.30688700	-0.18815900

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9 10 2.0 22 1.5
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22 23 1.0 28 1.0
23 24 1.0 26 1.0 35 1.0
24 25 2.0 36 1.5
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26 27 1.0 29 1.0 30 1.0
27 28 1.0 31 1.0 32 1.0
28 33 1.0 34 1.0
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36 37 1.0 41 1.0
37 38 1.0 39 1.0 40 1.0
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Geometry-optimized structure of Ac-Glu^0-*cis*-Ala-NHMe in a type VIa1 (PcisD) β-turn with a C–H/O interaction (Glu χ_1 *g*$^-$, χ_2 *t*, χ_3 +30°)
optimized M06-2X/6-311++G(d,p)/H2O

0 1

C	-0.32205600	2.89743600	-0.11466600
O	0.84644100	2.66787000	0.19157100
N	-1.21265700	1.89415400	-0.27968100
C	-0.77169800	0.51406400	-0.23776100
C	0.29576600	0.28285600	-1.31982200
O	0.22230600	0.85524800	-2.39883300

C	-1.94932100	-0.43107900	-0.48036500
C	-2.96048900	-0.39355200	0.65754100
C	-4.11413600	-1.32978900	0.41787200
O	-4.23545000	-2.06105800	-0.53125000
O	-5.01916400	-1.26552200	1.40397700
H	-3.37316000	0.60733500	0.81053500
H	-2.10871800	2.10684400	-0.69395100
H	-0.34274700	0.33037400	0.75136800
H	-1.57156100	-1.44950500	-0.59847800
H	-2.49574200	-0.67986600	1.60637300
H	-2.42709100	-0.16687000	-1.42849600
N	1.29216700	-0.58033300	-1.03270200
C	1.41097800	-1.46741600	0.12952900
C	2.15456700	-0.85787400	1.33027900
O	2.51184100	-1.59042200	2.24910400
C	2.19784500	-2.65407000	-0.44194600
C	3.16192800	-1.96862700	-1.41257300
C	2.28773900	-0.90286100	-2.07178600
H	2.83473200	-0.00453400	-2.35948500
H	0.43167900	-1.78240300	0.49573700
H	1.51147800	-3.30752200	-0.98487500
H	3.59267800	-2.65249000	-2.14234700
H	1.76880100	-1.28694800	-2.95407400
H	2.68660500	-3.22399400	0.34519000
H	3.97891400	-1.49840700	-0.85860900
N	2.35954400	0.46375900	1.32425200
C	2.95548000	1.12702800	2.47125700
H	1.93714000	1.04818300	0.61018400
H	3.98706300	0.79975900	2.61104900
C	-0.82969000	4.29918100	-0.32196600
H	-0.54724600	4.90309700	0.54026200
H	-0.33573300	4.71477900	-1.20193700
H	-1.90866600	4.34198200	-0.46135200
H	2.39556000	0.90321900	3.38164400
H	2.93943900	2.19948100	2.29052300
H	-5.73607400	-1.88628700	1.20755700

1 2 2.0 3 1.5 36 1.0
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3 4 1.0 13 1.0
4 5 1.0 7 1.0 14 1.0
5 6 2.0 18 1.5
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7 8 1.0 15 1.0 17 1.0
8 9 1.0 12 1.0 16 1.0
9 10 2.0 11 1.5
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11 42 1.0
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18 19 1.0 24 1.0
19 20 1.0 22 1.0 26 1.0
20 21 2.0 32 1.5
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22 23 1.0 27 1.0 30 1.0
23 24 1.0 28 1.0 31 1.0
24 25 1.0 29 1.0
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32 33 1.0 34 1.0
33 35 1.0 40 1.0 41 1.0
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36 37 1.0 38 1.0 39 1.0
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Geometry-optimized structure of Ac-pSer^{1-}-*cis*-Ala-NHMe in a type VIa1 (PcisD) β-turn with a C–H/O interaction (pSer χ_1 *g*$^-$, χ_2 *–95°*)
optimized M06-2X/6-311++G(d,p)/H2O

-1 1

P	2.96084900	-0.22586400	-0.61240000
O	2.41507800	1.05370600	0.27085600
O	3.82189400	0.35739600	-1.67869700
O	3.93242000	-0.97563300	0.47369100
O	1.80103700	-1.13656100	-0.89887500
C	1.40060200	0.81956400	1.23125500
C	0.01783300	0.95188800	0.59434600
H	1.51524300	1.56552900	2.02101200
N	-0.20438100	2.31599300	0.16939300
C	-1.04124200	0.54069400	1.62451100
H	-0.02040800	0.29593300	-0.27763900
C	-1.36642000	2.66810100	-0.41239500
N	-1.43772000	-0.75198200	1.59760700
O	-1.48030000	1.34103400	2.43575700
O	-2.25910200	1.84078900	-0.60186100
C	-0.92361500	-1.85379900	0.78931800
C	-0.90166000	-3.12676500	1.62894000
C	-1.69684900	-2.07841000	-0.52037100
H	0.09929500	-1.62594800	0.47097600
H	-0.26631100	-2.97913500	2.50288200
H	-0.51357000	-3.95333300	1.03757000
N	-2.41246600	-1.05041300	-0.99519200
O	-1.60265100	-3.15203700	-1.11049600
C	-3.05714800	-1.13576800	-2.29378600
H	-3.55522900	-0.18868000	-2.49034900
H	-2.32479900	-1.32972400	-3.08069000
H	-3.79474200	-1.93972800	-2.30337200
H	1.49960100	-0.17234400	1.68476100
H	-2.38603600	-0.14234900	-0.54261200
H	0.51473900	3.00666800	0.32493400
C	-1.52263000	4.11037200	-0.81442500
H	-1.72991200	4.15095600	-1.88424400
H	-2.38436400	4.52309000	-0.28836700
H	-0.64132700	4.70976900	-0.59188100
H	3.51271800	-1.75747500	0.84695400
H	-2.12643000	-0.98887300	2.30251600
H	-1.90946600	-3.38640300	1.96352800

1 2 1.0 3 2.0 4 1.0 5 2.0

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9 12 1.5 30 1.0
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13 16 1.0 36 1.0
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31 32 1.0 33 1.0 34 1.0
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Geometry-optimized structure of Ac-pSer^{1-}-*cis*-Ala-NHMe in a type VIa1 (PcisD) β-turn with a C–H/O interaction (pSer $\chi_1 t$, χ_2 +95°)
optimized M06-2X/6-311++G(d,p)/H2O

-1 1

P	-2.94981000	-0.24469200	-0.50711200
O	-2.03471300	-0.93221900	0.67646700

O	-3.82120000	-1.53247600	-1.02294400
O	-3.86585400	0.69822400	0.19382300
O	-2.04125700	0.18220000	-1.62380900
C	-1.07258900	-1.90635600	0.31977800
C	0.30199300	-1.26562400	0.11206100
H	-1.36071400	-2.44148900	-0.59077300
N	1.24589600	-2.31195400	-0.22180100
C	0.73616900	-0.57852900	1.41700800
H	0.24677000	-0.55588900	-0.71459300
C	2.55280100	-2.03081000	-0.39833200
N	0.61461000	0.76271000	1.50765100
O	1.17701900	-1.24926700	2.34013700
O	2.96673500	-0.87328100	-0.35210000
C	-0.01075600	1.71457900	0.59685800
C	-0.97090600	2.61415700	1.36445700
C	1.02041100	2.53618100	-0.19587800
H	-0.58460100	1.16409100	-0.15223300
H	-1.75166600	2.00261400	1.81695400
H	-1.42910900	3.33207000	0.68640600
N	2.16802600	1.91324000	-0.49523300
O	0.76261400	3.67645300	-0.57299600
C	3.16043500	2.54642500	-1.34464500
H	3.96984900	1.83839700	-1.51048900
H	2.72553700	2.82977400	-2.30548500
H	3.56117900	3.44461400	-0.87081100
H	-1.01126600	-2.62340600	1.14231400
H	2.31808200	0.94639900	-0.22242500
H	0.95633900	-3.27727900	-0.15795100
C	3.47494300	-3.19301200	-0.65144300
H	4.05247200	-2.98701300	-1.55265000
H	4.17073600	-3.26583900	0.18594500
H	2.94604600	-4.13785500	-0.76403100
H	-3.53608200	-1.82872700	-1.89339900
H	0.91569000	1.13567200	2.40146900
H	-0.44359300	3.16714200	2.14630900

1 2 1.0 3 1.0 4 2.0 5 2.0
2 6 1.0
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9 12 1.5 30 1.0
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Geometry-optimized structure of Ac-pSer^{2-}-*cis*-Ala-NHMe in a type VIa1 (PcisD) β-turn with a C–H/O interaction (pSer χ_1 *g*$^-$, χ_2 *–95°*)
optimized M06-2X/6-311++G(d,p)/H2O

-2 1

P	3.03608500	-0.27720900	-0.56523000
O	2.41779400	1.11423300	0.21325300
O	1.78609300	-1.09176600	-0.92117600
O	3.78092900	0.32872800	-1.74740500
O	3.92056500	-0.94659100	0.48654600
C	1.43776500	0.88708500	1.18978800
C	0.03419100	0.97474400	0.57983500
H	1.53165400	1.64746500	1.97319400
N	-0.23772200	2.33149900	0.15589600

C	-0.99123600	0.53327600	1.62413800
H	0.01605400	0.31597600	-0.29038200
C	-1.40868100	2.65178000	-0.42034300
N	-1.33770300	-0.77419500	1.61154200
O	-1.44740000	1.31674900	2.44577300
O	-2.28894500	1.80597500	-0.59598800
C	-0.81495900	-1.85094200	0.77574800
C	-0.66245500	-3.11635800	1.61165700
C	-1.66485200	-2.11723000	-0.47604000
H	0.17127600	-1.56640400	0.38586200
H	0.02324200	-2.92779500	2.43869500
H	-0.26732400	-3.92170100	0.99585600
N	-2.39757400	-1.09667600	-0.94395800
O	-1.61667800	-3.20952000	-1.03847500
C	-3.12196100	-1.21851800	-2.19626900
H	-3.60325900	-0.26541900	-2.40583300
H	-2.44576200	-1.47050900	-3.01620400
H	-3.88319600	-1.99753800	-2.12608600
H	1.55790300	-0.09646200	1.66013600
H	-2.34256900	-0.17537100	-0.52039200
H	0.47776500	3.03318900	0.27467400
C	-1.59888100	4.08655400	-0.83759000
H	-1.79289100	4.11254400	-1.91047800
H	-2.47806800	4.48111000	-0.32686500
H	-0.73676100	4.71140100	-0.60962900
H	-1.62635400	-3.43644500	2.01685800
H	-2.00444900	-1.03510700	2.32892000

1 2 1.0 3 2.0 4 2.0 5 2.0
2 6 1.0
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6 7 1.0 8 1.0 28 1.0
7 9 1.0 10 1.0 11 1.0
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9 12 1.5 30 1.0
10 13 1.5 14 2.0
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12 15 2.0 31 1.0
13 16 1.0 36 1.0
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16 17 1.0 18 1.0 19 1.0

17 20 1.0 21 1.0 35 1.0
18 22 1.5 23 2.0
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22 24 1.0 29 1.0
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24 25 1.0 26 1.0 27 1.0
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31 32 1.0 33 1.0 34 1.0
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Geometry-optimized structure of Ac-pSer^{2-}-*cis*-Ala-NHMe in a type VIa1 (PcisD) β-turn with a C–H/O interaction (pSer $\chi_1 t$, χ_2 +95°)
optimized M06-2X/6-311++G(d,p)/H2O

-2 1

P	-2.96361400	-0.56686800	-0.59994700
O	-1.96471800	-1.10349600	0.67991900
O	-3.55105300	-1.84562000	-1.19607900
O	-3.95800400	0.32339400	0.13540900
O	-1.99682300	0.16801700	-1.53530900
C	-0.91432400	-1.96491100	0.33865800
C	0.40027800	-1.19788100	0.13765700
H	-1.13620900	-2.51983900	-0.58062500
N	1.42451500	-2.15025200	-0.24608100
C	0.80288900	-0.52112700	1.45438600
H	0.25839400	-0.46480500	-0.65850800
C	2.70981600	-1.78299100	-0.40379300
N	0.57318700	0.80370900	1.58561600
O	1.32558600	-1.17280800	2.35000900
O	3.05978500	-0.60684100	-0.30136100
C	-0.19085300	1.70149500	0.72625800
C	-1.05497600	2.61391700	1.59020900

C	0.68275500	2.52431400	-0.23021200
H	-0.84677500	1.10735200	0.08123300
H	-1.72041300	2.00822200	2.20642300
H	-1.65151700	3.26937500	0.95843300
N	1.88538400	2.02032100	-0.53640800
O	0.25533800	3.56846600	-0.72063500
C	2.73291300	2.66182400	-1.52435900
H	3.63278500	2.06159800	-1.64344200
H	2.22208900	2.74170100	-2.48648000
H	3.01256200	3.66584300	-1.19992500
H	-0.76758500	-2.68733400	1.15004500
H	2.17160600	1.11228500	-0.18311800
H	1.19390000	-3.13342900	-0.25150900
C	3.70067100	-2.87621500	-0.70645600
H	4.27163400	-2.59410900	-1.59111300
H	4.39435100	-2.95008200	0.13274300
H	3.22929200	-3.84411800	-0.86918500
H	0.86733400	1.17933000	2.48018200
H	-0.43474000	3.23513000	2.24243300

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7 9 1.0 10 1.0 11 1.0
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9 12 1.5 30 1.0
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12 15 2.0 31 1.0
13 16 1.0 35 1.0
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17 20 1.0 21 1.0 36 1.0
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24 25 1.0 26 1.0 27 1.0

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31 32 1.0 33 1.0 34 1.0
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Geometry-optimized structure of Ac-pThr^{1-}-*cis*-Ala-NHMe in a type VIa1 (PcisD) β-turn with a C–H/O interaction (pThr χ_1 *g*$^-$, χ_2 *–95°*)
optimized M06-2X/6-311++G(d,p)/H2O

-1 1

P	2.80115600	-0.49771900	-0.93830400
O	2.56025800	0.67316500	0.19704700
O	1.51320200	-1.22000500	-1.19618800
O	3.58381900	0.16435700	-2.02577400
O	3.75936400	-1.56201700	-0.14521600
C	1.57343700	0.55808600	1.22218200
C	0.19327400	0.86298100	0.60681800
H	1.79785300	1.37338300	1.91688000
N	0.16652400	2.25859100	0.21295300
C	-0.91289500	0.58684300	1.62697200
H	0.06338400	0.24430100	-0.28041400
C	-0.93645100	2.81811100	-0.31407100
N	-1.57810500	-0.58555900	1.50895300
O	-1.15853500	1.38395100	2.52048900
O	-1.97005400	2.16723200	-0.47901100
C	-1.34248600	-1.71023300	0.60670300
C	-1.39487900	-3.01590100	1.39146500
C	-2.31403900	-1.73851100	-0.58556700
H	-0.34864700	-1.61123200	0.15956200
H	-0.63741000	-3.00223900	2.17629000
H	-1.20954300	-3.85759400	0.72708300
N	-2.77467200	-0.55371100	-1.00586200
O	-2.58989400	-2.79880100	-1.14141300
C	-3.59373900	-0.45380700	-2.20029100
H	-3.76534600	0.60039900	-2.40835900
H	-3.09197000	-0.91470100	-3.05344700

H	-4.55494900	-0.95107900	-2.05600900
H	-2.46927700	0.30941500	-0.56505400
H	1.00637200	2.80834600	0.32016700
C	-0.85686400	4.27689500	-0.67838100
H	-1.17393900	4.39354800	-1.71477300
H	-1.55764300	4.82623600	-0.04777700
H	0.14158400	4.69205900	-0.55218300
C	1.65591600	-0.75191400	1.99356900
H	0.95735900	-0.73896800	2.83247700
H	1.44348000	-1.61261600	1.35892100
H	2.66546100	-0.86374400	2.38975000
H	4.66551900	-1.24273000	-0.07302700
H	-2.28169700	-0.72915900	2.22483500
H	-2.37705700	-3.15144800	1.85146200

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5 38 1.0
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9 12 1.5 29 1.0
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Geometry-optimized structure of Ac-pThr^{1-}-*cis*-Ala-NHMe in a type VIa1 (PcisD) β-turn with a C–H/O interaction (pThr $\chi_1 t$, χ_2 +95°)
optimized M06-2X/6-311++G(d,p)/H2O

-1 1

P	-2.82613800	-0.07118600	-0.83394800
O	-1.98308200	-0.67083900	0.45345100
O	-3.65079900	1.08843200	-0.04744100
O	-1.86204400	0.61229300	-1.75583600
O	-3.75206100	-1.13513600	-1.33817600
C	-1.10088400	-1.76082400	0.20666700
C	0.32312800	-1.19281200	0.03779200
H	-1.36354600	-2.24413200	-0.74278700
N	1.22061800	-2.23898100	-0.40361600
C	0.83726100	-0.59622000	1.35755000
H	0.27646100	-0.42559900	-0.73789500
C	2.51944400	-1.97126800	-0.64465700
N	0.67747600	0.72944900	1.56106800
O	1.36676900	-1.31222200	2.19667200
O	2.96581600	-0.82968900	-0.53441800
C	0.06193500	1.75158100	0.72335300
C	-0.88949900	2.60206100	1.55395100
C	1.10565000	2.61395200	-0.00642700
H	-0.51814200	1.26719900	-0.06458000
H	-1.67117200	1.96209700	1.96337400
H	-1.34729700	3.36656200	0.92866500
N	2.23764600	1.99289800	-0.36742800
O	0.87381700	3.78811000	-0.28360600
C	3.23981500	2.67463400	-1.16625700
H	4.05093700	1.97727000	-1.36554200
H	2.81811100	3.01817500	-2.11343600
H	3.63487100	3.54071300	-0.63206400

H	2.36292500	1.00092800	-0.18991900
H	0.89800800	-3.19431900	-0.44037900
C	3.39336500	-3.12863100	-1.04818200
H	3.92283700	-2.86168700	-1.96274000
H	4.13518300	-3.28707600	-0.26369500
H	2.83359900	-4.04914100	-1.20532600
C	-1.25915000	-2.75631400	1.34181000
H	-0.54229300	-3.57642100	1.26740900
H	-1.11219100	-2.25918900	2.30153400
H	-2.26670800	-3.17234900	1.30805200
H	-4.40129900	0.73479100	0.44250300
H	1.03675500	1.04436400	2.45571400
H	-0.35888400	3.09747800	2.37139500

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Geometry-optimized structure of Ac-pThr^{2-}-*cis*-Ala-NHMe in a type VIa1 (PcisD) β-turn with a C–H/O interaction (pThr χ_1 *g*$^-$, χ_2 *–95°*)
optimized M06-2X/6-311++G(d,p)/H2O

-2 1

P	2.83142000	-0.65417800	-0.92095500
O	2.60231500	0.57657200	0.24933800
O	1.43627200	-1.24968100	-1.15288600
O	3.39054000	0.14760300	-2.09275000
O	3.82619400	-1.62690900	-0.29009600
C	1.61978100	0.47720100	1.25538800
C	0.24732700	0.83495600	0.63845800
H	1.84550600	1.27332600	1.97658000
N	0.27891100	2.23346700	0.25184700
C	-0.87562300	0.59543400	1.64121100
H	0.11919400	0.22401800	-0.25406200
C	-0.78491900	2.83739900	-0.29964500
N	-1.57375300	-0.55717400	1.51059100
O	-1.11287400	1.39290500	2.53955200
O	-1.85268100	2.24105100	-0.46585000
C	-1.35862600	-1.67523600	0.59579200
C	-1.43905800	-2.98992300	1.36244400
C	-2.33027100	-1.66356400	-0.59501000
H	-0.36142600	-1.58993800	0.14873400
H	-0.68193100	-3.00101400	2.14772700
H	-1.26783400	-3.82649200	0.68756600
N	-2.74503000	-0.45976300	-1.01181100
O	-2.65090400	-2.70931600	-1.15606500
C	-3.56071700	-0.32613200	-2.20492600
H	-3.70916200	0.73416600	-2.39971200
H	-3.07035600	-0.78700200	-3.06494500
H	-4.53265000	-0.80402700	-2.06672300
H	-2.40276100	0.38992100	-0.57100600

H	1.16124500	2.72085800	0.31133800
C	-0.62726000	4.28418500	-0.68946500
H	-0.91673700	4.39612000	-1.73452600
H	-1.31289500	4.87966900	-0.08456600
H	0.38726700	4.65366800	-0.54960900
C	1.63864300	-0.84649700	2.01321600
H	0.91109200	-0.83465700	2.82826800
H	1.43314300	-1.68602700	1.34904900
H	2.63113100	-0.98781600	2.44264600
H	-2.28754500	-0.68761100	2.21854500
H	-2.42405000	-3.11493300	1.81991400

1 2 1.0 3 2.0 4 2.0 5 2.0
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Geometry-optimized structure of Ac-pThr^{2-}-*cis*-Ala-NHMe in a type VIa1 (PcisD) β-turn with a C–H/O interaction (pThr χ_1 *t*, χ_2 *+95°*)
optimized M06-2X/6-311++G(d,p)/H2O

-2 1

P	-2.82485900	-0.19509600	-0.84756800
O	-1.98840300	-0.80780600	0.50960800
O	-3.79389500	0.78363800	-0.19473500
O	-1.72646000	0.45292300	-1.69899000
O	-3.47121400	-1.41982700	-1.49489000
C	-1.01145000	-1.79399500	0.28060800
C	0.37178500	-1.12390900	0.10005300
H	-1.21987100	-2.31051800	-0.66619700
N	1.32047800	-2.10246900	-0.39609300
C	0.89791900	-0.53240500	1.41420500
H	0.24007500	-0.34359100	-0.65219600
C	2.59390700	-1.76482200	-0.66943600
N	0.67028300	0.77855800	1.65604100
O	1.51358100	-1.22648400	2.21399400
O	2.98780900	-0.60228000	-0.56324900
C	-0.08351500	1.75934800	0.88557200
C	-0.92939800	2.60679100	1.82776500
C	0.80030300	2.63994000	-0.00997900
H	-0.74688900	1.23090400	0.19660800
H	-1.61426500	1.96081500	2.37818000
H	-1.50427800	3.33575500	1.25980000
N	1.93432600	2.08964000	-0.46592300
O	0.43620500	3.76898600	-0.33398600
C	2.76098300	2.78762100	-1.43311500
H	3.58858900	2.13666000	-1.70797300
H	2.18636600	3.03917100	-2.32728200
H	3.15776700	3.71223100	-1.00953100
H	2.17591400	1.12786600	-0.24491400
H	1.05397000	-3.07538900	-0.42708400
C	3.51752100	-2.87174500	-1.10562200

H	4.01810000	-2.56633900	-2.02438100
H	4.27914900	-3.00502200	-0.33531300
H	3.00196500	-3.81710800	-1.26698600
C	-1.06373100	-2.79901800	1.42191300
H	-0.27013300	-3.54677300	1.35232800
H	-0.96348600	-2.28548700	2.37991700
H	-2.02644500	-3.31180000	1.39741100
H	1.05339600	1.09857500	2.53853600
H	-0.29957500	3.14635400	2.54061100

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Geometry-optimized structure of Ac-Ser-*cis*-Ala-NHMe in a type VIa1 (PcisD) β-turn with a C–H/O interaction (Ser χ_1 *t*, χ_2 *t*)
optimized M06-2X/6-311++G(d,p)/H2O

0 1

O	0.00969200	-2.87853700	-1.05323100
C	1.27110700	-2.23897000	-1.08126700
C	1.07133300	-0.82979200	-0.53232100
H	1.66372600	-2.17273200	-2.10050800
N	2.34522200	-0.14388100	-0.54432900
C	0.54317400	-0.91184700	0.91180000
H	0.37019400	-0.28355200	-1.16797200
C	2.46110000	1.10502400	-0.04551500
N	-0.77815600	-0.71410000	1.11774100
O	1.31448800	-1.13596000	1.83173000
O	1.47754400	1.72111400	0.36037400
C	-1.86943700	-0.66089100	0.15057200
C	-3.06130200	-1.44362900	0.69222100
C	-2.28608400	0.76626800	-0.23893500
H	-1.54000000	-1.14616900	-0.76995500
H	-2.77024400	-2.48119500	0.85867000
H	-3.88246300	-1.40876300	-0.02049100
N	-1.40315600	1.74400100	-0.00339700
O	-3.37071900	0.96146400	-0.78256700
C	-1.66490300	3.10221700	-0.44535800
H	-0.80724000	3.71815400	-0.18316600
H	-1.81934100	3.13788300	-1.52596500
H	-2.55634900	3.49955000	0.04272500
H	-0.47926800	1.53011200	0.35816800
H	3.18133800	-0.66003200	-0.77676700
C	3.84497000	1.69451000	-0.00255400
H	3.80430000	2.70969600	-0.39562800
H	4.16040900	1.74717700	1.04126200
H	4.57051100	1.10995100	-0.56574800
H	0.10913900	-3.78213700	-1.36629900
H	1.99610100	-2.76539300	-0.45007000
H	-1.04931600	-0.78112600	2.09234100
H	-3.40666200	-1.01555600	1.63699500

1 2 1.0 30 1.0
2 3 1.0 4 1.0 31 1.0
3 5 1.0 6 1.0 7 1.0
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Geometry-optimized structure of Ac-Thr-*cis*-Ala-NHMe in a type VIa1 (PcisD) β-turn with a C–H/O interaction (Thr χ_1 *t*, χ_2 *t*)
optimized M06-2X/6-311++G(d,p)/H2O

0 1

C	3.06077900	2.85065700	-0.06666300
C	1.90342800	1.88851700	-0.07147900
O	0.77477200	2.22821800	0.28008300
H	2.77414000	3.74230400	-0.62429100

H	3.25492500	3.14590700	0.96575300
H	3.96718300	2.42673700	-0.49566600
N	2.15827500	0.62741600	-0.47629400
C	1.11865900	-0.37813400	-0.45908600
C	0.57903700	-0.53266000	0.97465300
O	1.33300800	-0.44440500	1.93201200
C	1.67422500	-1.70364700	-1.00574300
C	2.71196300	-2.36868900	-0.11451800
O	0.53862600	-2.53871200	-1.18264300
H	3.10580000	0.36381000	-0.70146100
H	0.31534600	-0.05418000	-1.12590600
H	2.11784600	-1.47372800	-1.98250700
H	0.83554600	-3.41518400	-1.44661900
H	3.10000300	-3.25934700	-0.61375900
H	3.55695000	-1.70773000	0.08863800
H	2.26652100	-2.66089900	0.83740200
N	-0.74574400	-0.75209000	1.13498000
C	-1.79131800	-1.00116600	0.14880100
C	-2.59419700	0.25429300	-0.23054600
O	-3.70811100	0.14300400	-0.73716400
C	-2.71442500	-2.10214400	0.66048900
H	-1.32216500	-1.35628600	-0.76979900
H	-3.49870600	-2.29708200	-0.06780000
H	-2.13791700	-3.01291000	0.82496600
N	-2.00057800	1.43810100	-0.03306100
C	-2.63218500	2.66784900	-0.47725200
H	-1.04256800	1.49044300	0.29791000
H	-2.82341300	2.64199800	-1.55225000
H	-3.58258900	2.81959100	0.03712000
H	-1.96475100	3.49634700	-0.24964800
H	-1.02332400	-0.83329000	2.10681000
H	-3.18465400	-1.80459100	1.60149300

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11 12 1.0 13 1.0 16 1.0

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21 22 1.0 35 1.0
22 23 1.0 25 1.0 26 1.0
23 24 2.0 29 1.5
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25 27 1.0 28 1.0 36 1.0
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30 32 1.0 33 1.0 34 1.0
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Geometry optimized structures of Ac-Glu-cis-nonAla-NHMe type VIa1 β-turns stabilized via C–H/O interactions derived from calculated Glu-*cis*-Ala structures

Geometry-optimized structure of Ac-Glu-*cis*-F_2Ala-NHMe in a type VIa1 (PcisD) β-turn with a C–H/O interaction (Glu $\chi_1 g^-$, $\chi_2 g^-$, χ_3 *+30°*)
optimized M06-2X/6-311++G(d,p)/H2O

-1 1

C	4.21246200	-2.02694900	0.27015600
C	2.81200800	-1.48525700	0.16810700
O	1.84313700	-2.10419000	0.61139800
H	4.96229100	-1.33330900	-0.10690800
H	4.42043200	-2.25606300	1.31563900
H	4.26262000	-2.95844400	-0.29557000
N	2.65698000	-0.28551100	-0.42698700
C	1.32749700	0.25028100	-0.62728600
C	0.53923500	-0.68115800	-1.55574400

O	1.08418200	-1.32121700	-2.43773900
C	1.38024800	1.66172800	-1.21933400
C	1.88829600	2.69053600	-0.21703500
C	0.93950200	2.94786400	0.97503700
O	-0.20900300	2.43746100	0.92834500
O	1.39560000	3.66655300	1.89092900
H	3.44088300	0.14405000	-0.89616300
H	0.84169700	0.29550500	0.34922900
H	2.00850600	1.64081200	-2.11601800
H	0.37329000	1.93943600	-1.53941300
H	2.86515200	2.40502800	0.18347100
H	2.03584300	3.65126900	-0.71877400
N	-0.80418800	-0.74947800	-1.35696700
C	-1.59992800	-0.04066800	-0.37367400
C	-1.95095900	-0.88815500	0.86509900
O	-3.01091200	-0.73898400	1.45951800
C	-2.83126600	0.49544900	-1.08416900
H	-1.05765900	0.84593500	-0.01447300
H	-2.56080400	1.02168000	-2.00035900
N	-0.99543300	-1.73768000	1.26421200
C	-1.15538600	-2.50804300	2.48562300
H	-1.38164600	-1.85125600	3.32737900
H	-1.96489100	-3.23352500	2.38454500
H	-0.22366500	-3.03550600	2.67856300
H	-0.10445800	-1.80318600	0.77972000
H	-1.28334100	-1.41766900	-1.95052900
F	-3.67053200	-0.52935300	-1.42628400
F	-3.53280700	1.34526000	-0.29398800

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Geometry-optimized structure of Ac-Glu-*cis*-F_3Ala-NHMe in a type VIa1 (PcisD) β-turn with a C–H/O interaction (Glu $\chi_1 g^-$, $\chi_2 g^-$, χ_3 *+30°*)
optimized M06-2X/6-311++G(d,p)/H2O

-1 1

C	4.49565200	-1.74730600	-0.06594900
C	3.05969600	-1.30006400	-0.03264300
O	2.16675000	-2.02036700	0.41807800
H	5.17027700	-0.97638600	-0.43418200
H	4.79118100	-2.04069200	0.94165600
H	4.56549300	-2.62741800	-0.70700400
N	2.78301700	-0.07223500	-0.51517500
C	1.40774000	0.37271300	-0.58163200
C	0.63241100	-0.52136500	-1.55581700

O	1.16191700	-1.02170600	-2.53077700
C	1.30554000	1.83598300	-1.02127100
C	1.76672500	2.79889300	0.06529600
C	0.84956500	2.85098600	1.30702200
O	-0.24108400	2.22446300	1.25636600
O	1.26676900	3.53356400	2.26694000
H	3.50123700	0.45121200	-0.99429900
H	0.99119900	0.27615900	0.42188400
H	1.88790700	1.96533600	-1.93944100
H	0.26243400	2.04671000	-1.26875400
H	2.77919200	2.55910700	0.40267900
H	1.81493800	3.81429500	-0.33822500
N	-0.68887600	-0.72113200	-1.29266800
C	-1.45270600	-0.22459200	-0.17182100
C	-1.72351900	-1.30084600	0.90061600
O	-2.81832300	-1.41840300	1.43398800
C	-2.74331900	0.38575400	-0.69561400
H	-0.93134900	0.61490900	0.31157500
N	-0.65790300	-2.04633400	1.21419400
C	-0.74548900	-3.05374900	2.25819300
H	-1.07848900	-2.60592700	3.19598400
H	-1.44947400	-3.84009000	1.97936900
H	0.24246000	-3.48808600	2.39489200
H	0.23988900	-1.91727000	0.75273800
H	-1.14861800	-1.36737500	-1.92489300
F	-3.53339000	-0.52107900	-1.29356500
F	-3.45241000	0.98136500	0.26337600
F	-2.46908300	1.32355500	-1.61797600

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Geometry-optimized structure of Ac-Glu-*cis*-FAla-NHMe in a type VIa1 (PcisD) β-turn with a C–H/O interaction (Glu $\chi_1 g^-$, $\chi_2 g^-$, χ_3 *+30°*)
optimized M06-2X/6-311++G(d,p)/H2O

-1 1

C	3.57920100	-2.62864400	0.46483600
C	2.29639700	-1.85839000	0.29999000
O	1.22347700	-2.28649000	0.72777500
H	4.45879500	-2.04572000	0.19625100
H	3.65852600	-2.95796300	1.50048600
H	3.52992300	-3.51620100	-0.16887700
N	2.36911200	-0.67629600	-0.34388000
C	1.16087100	0.06907700	-0.63277400
C	0.24031200	-0.77686200	-1.52063500
O	0.68652200	-1.55484200	-2.34916700
C	1.48705000	1.39342300	-1.32991800
C	2.15782600	2.39281300	-0.39527800
C	1.25750800	2.90023700	0.75287000
O	0.02846200	2.64649700	0.68508200
O	1.83372500	3.54644800	1.65586600
H	3.23335700	-0.40857600	-0.79190500
H	0.66273900	0.28085700	0.31559600
H	2.11860500	1.18065100	-2.19901900
H	0.55603400	1.82224300	-1.70787700

H	3.06904300	1.97832600	0.04451300
H	2.47034400	3.27302800	-0.96542700
N	-1.09263400	-0.60618300	-1.34668500
C	-1.77731900	0.32999100	-0.47090800
C	-2.18553300	-0.25935600	0.89186300
O	-3.09941800	0.25281700	1.53229500
C	-2.98654600	0.88484500	-1.19016200
H	-1.12510300	1.18375100	-0.23837900
H	-3.56554600	1.53095900	-0.53452200
H	-2.68788000	1.40857000	-2.09817300
N	-1.46044600	-1.28870800	1.34366600
C	-1.67888100	-1.81885000	2.67858700
H	-1.56789200	-1.03459000	3.43026700
H	-2.68099900	-2.24192400	2.76558100
H	-0.94257900	-2.59906800	2.85912200
H	-0.64860000	-1.62184700	0.83210000
H	-1.67765000	-1.18883400	-1.93490700
F	-3.80675500	-0.18338800	-1.57579500

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30 31 1.0 35 1.0
31 32 1.0 33 1.0 34 1.0
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Geometry-optimized structure of Ac-Glu-*cis*-FGly-NHMe in a type VIa1 (PcisD) β-turn with a C–H/O interaction (Glu $\chi_1 g^-$, $\chi_2 g^-$, χ_3 *+30°*)
optimized M06-2X/6-311++G(d,p)/H2O

-1 1

C	-2.47376200	-3.37457300	-0.86303600
C	-1.50990700	-2.27240500	-0.51688600
O	-0.31229200	-2.34532500	-0.79928500
H	-3.50791200	-3.11611200	-0.64134800
H	-2.37287200	-3.60494800	-1.92362900
H	-2.19443200	-4.26439200	-0.29638500
N	-2.00830700	-1.19310800	0.11877800
C	-1.10764600	-0.14748500	0.55703800
C	-0.14521400	-0.72343600	1.60301700
O	-0.49493900	-1.58317200	2.38938800
C	-1.86873000	1.04802600	1.13463800
C	-2.60225500	1.83926200	0.05861400
C	-1.68046300	2.57913900	-0.93647600
O	-0.44325000	2.56149800	-0.71310900
O	-2.25421300	3.15319300	-1.88768200
H	-2.95933600	-1.20733000	0.45748300
H	-0.54920400	0.18124300	-0.31957200
H	-2.56232900	0.68453700	1.90008500
H	-1.15009800	1.70190300	1.63458900
H	-3.27231300	1.19547900	-0.51868700
H	-3.23893200	2.59531900	0.52667400
N	1.12891900	-0.23842400	1.60814900
C	1.68995200	0.77999000	0.77317500
C	2.67190500	0.23283300	-0.28142800
O	3.73071900	0.79562300	-0.51703100
H	0.90138400	1.34509100	0.26653200
N	2.22215100	-0.84131200	-0.94121100
C	2.97788100	-1.40060800	-2.04958300
H	3.15381200	-0.64203500	-2.81433000
H	3.94238500	-1.78063600	-1.70790600
H	2.40194100	-2.21768700	-2.47841700

H	1.33387100	-1.27560200	-0.69883200
H	1.76163900	-0.70293200	2.25067000
F	2.37714400	1.66655700	1.57893100

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Geometry-optimized structure of Ac-Glu-*cis*-Gly-NHMe in a type VIa1 (PcisD) β-turn with a C–H/O interaction (Glu $\chi_1 g^-$, $\chi_2 g^-$, χ_3 *+30°*)
optimized M06-2X/6-311++G(d,p)/H2O

-1 1

C	1.76251500	3.41341000	-1.40793400
C	0.94706500	2.29961900	-0.80653400
O	-0.28050400	2.27056200	-0.90443600
H	2.83471100	3.23496400	-1.34415800
H	1.47295300	3.53295300	-2.45187500
H	1.51914800	4.33827600	-0.88224200
N	1.61929600	1.33197200	-0.15244600
C	0.90186600	0.28118800	0.54130300
C	0.01606700	0.89912300	1.62999800
O	0.35833900	1.90273100	2.23795200
C	1.87854100	-0.71554200	1.17352600
C	2.61937000	-1.54403300	0.13104800
C	1.72388500	-2.51729800	-0.66813500
O	0.56383100	-2.72701900	-0.23621300
O	2.24671900	-3.03686000	-1.68057400
H	2.60755600	1.44687200	0.01810000
H	0.28308400	-0.24606400	-0.18759300
H	2.57948700	-0.15926800	1.80498700
H	1.31240600	-1.38207100	1.82758500
H	3.15026900	-0.90637700	-0.58080400
H	3.38561400	-2.15030200	0.62376800
N	-1.14749700	0.26259900	1.89894900
C	-1.65420200	-0.96485400	1.31219400
C	-2.55924200	-0.80491600	0.09253900
O	-3.32589200	-1.71697800	-0.21053300
H	-0.83246900	-1.62167100	1.00605300
N	-2.43811700	0.32015700	-0.62173600
C	-3.18306300	0.50388500	-1.85496700
H	-2.97947500	-0.30740300	-2.55683100
H	-4.25607800	0.52773500	-1.65692600
H	-2.87962000	1.44957800	-2.29909400
H	-1.71782600	1.00090400	-0.39933100
H	-1.69899300	0.69207000	2.63044600
H	-2.23330400	-1.49627600	2.06673900

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27 28 1.0 32 1.0
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Geometry-optimized structure of Ac-Glu-*cis*-Ser-NHMe in a type VIa1 (PcisD) β-turn with a C–H/O interaction (Glu $\chi_1 g^-$, $\chi_2 g^-$, χ_3 *+30°*) (Ser $\chi_1 g^-$)
optimized M06-2X/6-311++G(d,p)/H2O

-1 1

C	3.90930100	-2.15396900	0.09724100
C	2.52008400	-1.57590300	0.05472100
O	1.53549900	-2.22751200	0.40711700
H	4.68221600	-1.40711200	-0.07711400
H	4.06314800	-2.62211900	1.06920400
H	3.98133400	-2.93011200	-0.66702300
N	2.39477800	-0.31082000	-0.39303100
C	1.07843300	0.27019100	-0.55661900
C	0.28930400	-0.54123400	-1.59089800
O	0.84194700	-1.09882900	-2.52554600
C	1.16760000	1.73268100	-1.00155900
C	1.72238800	2.64163100	0.08822400
C	0.81150800	2.78922900	1.32760400

O	-0.36182900	2.34891700	1.24427200
O	1.32379700	3.36076300	2.31650200
H	3.19620000	0.15685800	-0.79067100
H	0.57323300	0.22541800	0.40971000
H	1.78258300	1.78289700	-1.90654800
H	0.16319900	2.06674000	-1.27259100
H	2.70497400	2.30375400	0.42840000
H	1.87205900	3.64699400	-0.31697300
N	-1.05750100	-0.58987400	-1.42894000
C	-1.86894700	0.01036200	-0.37931000
C	-2.22919900	-0.96377100	0.75114000
O	-3.28329500	-0.83782600	1.36958400
C	-3.12844100	0.61057600	-1.00053700
H	-1.31335700	0.83696300	0.07982300
H	-3.74030500	1.04610600	-0.21429600
N	-1.32082700	-1.90439100	1.04217100
C	-1.52040900	-2.80649400	2.16315900
H	-1.60073900	-2.25325100	3.10145600
H	-2.43285700	-3.38923800	2.02689000
H	-0.66809300	-3.48062700	2.21454100
H	-0.42147500	-1.93074000	0.57004600
H	-3.71423400	-0.17324300	-1.49712800
H	-1.53181900	-1.18975500	-2.09601300
O	-2.80344300	1.65167800	-1.90266400
H	-2.24235700	1.28874700	-2.59623600

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12 13 1.0 20 1.0 21 1.0
13 14 2.0 15 2.0
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22 23 1.0 36 1.0
23 24 1.0 26 1.0 27 1.0
24 25 2.0 29 1.5
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26 28 1.0 35 1.0 37 1.0
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29 30 1.0 34 1.0
30 31 1.0 32 1.0 33 1.0
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37 38 1.0
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Geometry-optimized structure of Ac-Glu-*cis*-Ser-NHMe in a type VIa1 (PcisD) β-turn with a C–H/O interaction (Glu $\chi_1 g^-$, $\chi_2 g^-$, χ_3 *+30°*) (Ser $\chi_1 g^+$)
optimized M06-2X/6-311++G(d,p)/H2O

-1 1

C	3.51666300	-2.69649000	0.45566900
C	2.24559100	-1.90734700	0.28651500
O	1.16823600	-2.31598900	0.72191900
H	4.39637300	-2.16500100	0.09651500
H	3.64031900	-2.93367300	1.51250500
H	3.41338100	-3.63556200	-0.09028100
N	2.33608800	-0.72929200	-0.36156900
C	1.14291900	0.04276700	-0.64503900
C	0.19136500	-0.78663500	-1.51562100
O	0.61337500	-1.57498700	-2.34950300
C	1.49688400	1.34837300	-1.36331300
C	2.22500000	2.33357100	-0.45720600
C	1.37292700	2.87343200	0.71302000
O	0.13185200	2.68665400	0.66171800
O	1.99787900	3.47711600	1.61390700
H	3.20420700	-0.47706300	-0.81068300
H	0.65998800	0.27987100	0.30527100
H	2.09851700	1.10552600	-2.24572400

H	0.57114300	1.80489100	-1.72080800
H	3.13788300	1.89819900	-0.04196100
H	2.54291300	3.20138900	-1.04350300
N	-1.13207100	-0.58827500	-1.32256700
C	-1.79102000	0.37634000	-0.45491000
C	-2.16776600	-0.17844100	0.93086900
O	-3.02699000	0.38280700	1.60575000
C	-3.02468400	0.90222300	-1.16746900
H	-1.12716400	1.22746500	-0.25782300
H	-2.71267500	1.43990000	-2.06770500
N	-1.47559400	-1.23811300	1.36796100
C	-1.66022900	-1.73873700	2.71879300
H	-1.51363400	-0.94214800	3.45112500
H	-2.66541400	-2.14444500	2.84675900
H	-0.93097400	-2.52734500	2.89189700
H	-0.69656100	-1.60802200	0.83239200
H	-3.56097300	1.57958300	-0.50108600
H	-1.74649100	-1.14078400	-1.91062700
O	-3.82329100	-0.22545200	-1.50719600
H	-4.58418300	0.07145800	-2.01364000

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2 3 2.0 7 1.5
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8 9 1.0 11 1.0 17 1.0
9 10 2.0 22 1.5
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11 12 1.0 18 1.0 19 1.0
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13 14 2.0 15 2.0
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23 24 1.0 26 1.0 27 1.0

24 25 2.0 29 1.5
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26 28 1.0 35 1.0 37 1.0
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30 31 1.0 32 1.0 33 1.0
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Geometry-optimized structure of Ac-Glu-*cis*-Ser-NHMe in a type VIa1 (PcisD) β-turn with a C–H/O interaction (Glu $\chi_1 g^-$, $\chi_2 g^-$, $\chi_3 +30°$) (Ser $\chi_1 t$)
optimized M06-2X/6-311++G(d,p)/H2O

-1 1

C	-4.11112400	-1.78430900	-0.53710500
C	-2.69014500	-1.34004200	-0.31555900
O	-1.73296200	-2.04392900	-0.64248200
H	-4.83923600	-1.01790000	-0.27635700
H	-4.23044600	-2.05995700	-1.58501500
H	-4.29102800	-2.67448700	0.06786600
N	-2.50487700	-0.13395600	0.25675400
C	-1.16765900	0.31035500	0.59198700
C	-0.55263300	-0.65526200	1.61325900
O	-1.23727900	-1.21743000	2.45359800
C	-1.18622500	1.73075700	1.16398000
C	-1.54241100	2.77628000	0.11390700
C	-0.49166900	2.94597700	-1.00583300
O	0.63026200	2.40706000	-0.83846300
O	-0.84775300	3.63254300	-1.98996300
H	-3.29901200	0.36484100	0.63032600
H	-0.57563600	0.30691600	-0.32491700
H	-1.89085200	1.75841700	2.00201500
H	-0.19498600	1.94928500	1.56847100
H	-2.50589700	2.55888500	-0.35511400
H	-1.65436000	3.75307700	0.59429500
N	0.78810400	-0.84061900	1.54484600
C	1.74509600	-0.18903500	0.66722400

C	2.10246600	-1.02297900	-0.57159600
O	3.21437000	-0.90504900	-1.09832700
C	3.00572000	0.15682300	1.47101100
H	1.32899400	0.75360200	0.29130000
H	3.50614600	-0.76762200	1.78891500
N	1.15481000	-1.82124600	-1.06483000
C	1.36780900	-2.56373400	-2.29578900
H	1.64105800	-1.88971600	-3.10948900
H	2.16493800	-3.29865200	-2.17109200
H	0.44238300	-3.07748800	-2.54669100
H	0.23189000	-1.86339900	-0.64014100
H	2.70094500	0.70561300	2.36333100
H	1.15494900	-1.49265600	2.22928000
O	3.88649000	0.98479800	0.74363100
H	4.06351000	0.50906300	-0.08123500

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22 23 1.0 36 1.0
23 24 1.0 26 1.0 27 1.0
24 25 2.0 29 1.5
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26 28 1.0 35 1.0 37 1.0
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29 30 1.0 34 1.0
30 31 1.0 32 1.0 33 1.0
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37 38 1.0
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Geometry-optimized structure of Ac-Glu-*cis*-Tle-NHMe in a type VIa1 (PcisD) β-turn with a C–H/O interaction (Glu $\chi_1 g^-$, $\chi_2 g^-$, χ_3 *+30°*)
optimized M06-2X/6-311++G(d,p)/H2O

-1 1

C	4.49210100	-1.78687600	-0.17544900
C	3.05106700	-1.35673500	-0.09850700
O	2.17535600	-2.10263800	0.34224300
H	5.15793400	-0.98031200	-0.47806600
H	4.79623900	-2.16551100	0.80032000
H	4.56796000	-2.60518200	-0.89349100
N	2.75823900	-0.11695300	-0.53602000
C	1.38274600	0.33949800	-0.58733300
C	0.57888400	-0.57250500	-1.52297900
O	1.08836100	-1.05807600	-2.52426800
C	1.31360200	1.78606800	-1.08395600
C	1.85635200	2.77930000	-0.06419700
C	0.99124100	2.92113900	1.20854700
O	-0.15486100	2.40841200	1.19249800
O	1.50799800	3.56221200	2.15207800
H	3.47249900	0.42332300	-1.00188600
H	0.97244400	0.28762400	0.42316000
H	1.85920300	1.85236700	-2.03123200
H	0.26939300	2.02446100	-1.29311300
H	2.87392900	2.52190700	0.24282800
H	1.91980400	3.77346500	-0.51699800
N	-0.71040100	-0.81407200	-1.19560700
C	-1.52836100	-0.21867500	-0.14212500
C	-1.64049000	-1.17067600	1.07013400
O	-2.58912900	-1.13752100	1.84923400
C	-2.89003200	0.26913500	-0.71772500
H	-1.01581900	0.67623800	0.23319100
N	-0.60093100	-1.99993000	1.26130700

C	-0.53557000	-2.83808600	2.44443700
H	-0.57158200	-2.23499000	3.35453700
H	-1.37020100	-3.54103500	2.46605800
H	0.40000900	-3.39305000	2.41673900
H	0.21841700	-1.96939100	0.66423700
H	-1.18165700	-1.43277900	-1.84515700
C	-3.61180100	1.15409100	0.31012100
H	-4.47178500	1.63043700	-0.16919600
H	-3.95941500	0.57797700	1.16420300
H	-2.94243900	1.94174100	0.66924700
C	-2.60979400	1.14139900	-1.95037100
H	-1.97908400	1.99469200	-1.68329900
H	-2.11874300	0.58832300	-2.75343000
H	-3.55386900	1.53197600	-2.33828300
C	-3.78649700	-0.90821900	-1.11724300
H	-4.72622100	-0.52961000	-1.52819800
H	-3.32888300	-1.53389000	-1.89022500
H	-4.01897500	-1.53435100	-0.25412100

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Geometry-optimized structure of Ac-Glu-*cis*-Val-NHMe in a type VIa1 (PcisD) β-turn with a C–H/O interaction (Glu $\chi_1 g^-, \chi_2 g^-, \chi_3 +30°$)
optimized M06-2X/6-311++G(d,p)/H2O

-1 1

C	-4.25738900	-1.87227000	-0.05731100
C	-2.83773700	-1.37203000	-0.08484000
O	-1.93362700	-2.02256800	-0.61230900
H	-4.95626200	-1.14050800	0.34452100
H	-4.55132300	-2.14072900	-1.07211100
H	-4.29031700	-2.77631200	0.55308900
N	-2.59528000	-0.17830700	0.49023200
C	-1.23949900	0.32075500	0.59078900
C	-0.45178800	-0.51166800	1.61291000
O	-1.01255200	-1.00257300	2.58458100
C	-1.22499800	1.79232900	1.01347700
C	-1.77187000	2.71474200	-0.06847800
C	-0.90074000	2.79999200	-1.34212500
O	0.22905800	2.25335300	-1.31467100
O	-1.40028700	3.43193600	-2.30166700
H	-3.32443300	0.26837400	1.02722600
H	-0.79067600	0.24332600	-0.39874400

H	-1.79501600	1.89418600	1.94344100
H	-0.19160800	2.06596000	1.23304700
H	-2.78119600	2.41928600	-0.36834900
H	-1.85929900	3.73153000	0.32585400
N	0.88286500	-0.62881100	1.43234400
C	1.70370500	-0.20341200	0.29993200
C	2.01211500	-1.45064400	-0.56104500
O	3.14946400	-1.88544300	-0.70846900
C	2.98400400	0.50929300	0.75966800
H	1.13112300	0.51424900	-0.29666700
N	0.94058100	-2.03961900	-1.12018600
C	1.08296000	-3.27946200	-1.86349200
H	1.75280600	-3.13985600	-2.71320500
H	1.48890700	-4.07380300	-1.23207200
H	0.10054400	-3.57564500	-2.22544100
H	-0.00366200	-1.76447700	-0.86247100
H	3.63956600	-0.23592100	1.22344800
H	1.35044100	-1.16391400	2.15618600
C	3.69695600	1.11951400	-0.45030400
H	4.60798700	1.63134600	-0.13194900
H	3.96838000	0.36174500	-1.18443300
H	3.04254700	1.85501300	-0.92805500
C	2.67209900	1.60957600	1.77397400
H	2.03302700	2.37226700	1.31839500
H	2.16954100	1.22763000	2.66405800
H	3.59839500	2.09547300	2.08884500

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