Polypeptides Folding: Rules for the Calculation of the Backbone Dihedral Angles φ starting from the Amino Acid Sequence

Michele Larocca

Submitted date: 19/03/2020 • Posted date: 20/03/2020

Licence: CC BY 4.0

Citation information: Larocca, Michele (2020): Polypeptides Folding: Rules for the Calculation of the Backbone Dihedral Angles φ starting from the Amino Acid Sequence. ChemRxiv. Preprint.

<https://doi.org/10.26434/chemrxiv.12000132.v2>

Protein folding is strictly related to the determination of the backbone dihedral angles and depends on the information contained in the amino acid sequence as well as on the hydrophobic effect. To date, the type of information embedded in the amino acid sequence has not yet been revealed. The present study deals with these problematics and aims to furnish a possible explanation of the information contained in the amino acid sequence, showing and reporting rules to calculate the backbone dihedral angles φ . The study is based on the development of mechanical forces once specific chemical interactions are established among the side chain of the residues in a polypeptide chain. It aims to furnish a theoretical approach to predict backbone dihedral angles which, in the future, may be applied to computational developments focused on the prediction of polypeptide structures.

File list (2)

Polypeptides Folding Rules for the Calculation of the Ba... (611.00 KiB)	view on ChemRxiv • download file
--	--

Supporting Information_Polypeptide Folding.pdf (1.01 MiB)	view on ChemRxiv • download file
---	--

Polypeptides Folding: Rules for the Calculation of the Backbone Dihedral Angles ϕ starting from the Amino Acid Sequence

Michele Larocca

Planetario Osservatorio Astronomico di Anzi-Basilicata, via Salita Rosario s.n.c. 85010, Anzi (PZ), Italy.

michele.larocca@studio.unibo.it

<https://orcid.org/0000-0003-0613-5187>

Abstract

The DNA binding domain of the γ^δ resolvase (PDB code: 1res) is a peptide of 43 amino acids that was used in this study in order to describe a theoretical method useful to calculate the backbone dihedral angles ϕ starting from the amino acid sequence. The

method is based on the development of mechanical forces due to the chemical interactions among the side chains of the residues, with the latter supposed to be the information required to fold the peptide. This study reports rules concerning the threshold distances related to the chemical interactions that occur and the univocal definition of the degrees of freedom (from now ahead twisting constants). With the rules described, the calculated backbone dihedral angles ϕ of the DNA binding domain of the γ^δ resolvase, show a good agreement with the values experimentally determined, hence the methodology proposed, reveals to be a tool to calculate and predict at least the backbone dihedral angles ϕ .

Introduction

The prediction of a protein structure, starting from the amino acid sequence, turns to be very challenging and was deeply investigated over the years. Concerning this, in the past were reported very significant outcomes, as the thermodynamic hypothesis^[1] and the driving forces of the folding process^[2-5]. In 2019 it was described a survey which focuses on the

amino acid sequence to calculate the structure of two peptides (Leu-enkephalin and calcitonin)^[6] and is based on the development of the main mechanical forces (MMFs) arising from the chemical interactions among the residues side chains. Anyway, concerning the calculations, the latter study showed some limits on the definition of the degrees of freedom^[6] (now twisting constant) so that, this problem was further investigated in order to enunciate rules to define univocally the twisting constants and the threshold distances for the chemical interactions to occur. In this context, the present study realized on the DNA binding domain of the γ^δ resolvase (PDB code: 1res)^[7], aims to establish rules that allow to predict and calculate the backbone dihedral angles φ , so that, combined with the previous study^[6], could furnish a theoretical method to predict the structure of peptides and proteins starting from the amino acid sequence. This study is focused on the chemical interactions developed amongst the side chains of the residues and these were considered to be the informations required to fold the polypeptide. The survey shows a good agreement between the calculated and the experimentally determined values, thus the method presented, combined to the previous^[6], reveals to be an efficient approach to predict at least the backbone dihedral angles φ starting from the amino acid sequence.

Methods

Measurement of distances

The interatomic distances related to the chemical interactions were measured from a dedicated PDB file of the fully unfolded peptide (Figure 1). It was realized with Molefacture^[8] in VMD^[9].

Figure 1. Fully unfolded peptide: the unfolded DNA binding domain of the γ^δ resolvase.

Rules for threshold distances and twisting constants (η) for the calculation of the angles φ

For the calculations of the dihedral angles φ , is necessary to consider all the possible chemical interactions occurring among the side chains of the residues, according to the following rules, moreover the partial charges for the calculations were taken from the literature^[10] :

1) *Electrostatic interaction between the terminal charges*

The electrostatic interaction between the terminal charges occurs to define a partial twisting, which is needed to calculate all the dihedral angles φ of the peptide. For the polar residues, on the twisting constant it was found $\eta = 2$, whereas η have the specific values listed in Table 1 for the apolar residues.

Residue (Apolar)	η
Isoleucine	0.1
Alanine	15
Valine	2
Leucine	1.5
Methionine	0.1
Glycine	-0.4

Table 1. Twisting constants for the apolar residues used to calculate the folding factors.

2) *Intrachain electrostatic interactions between charges (attraction and repulsion)*

With the exception of the two terminal charges, the intrachain electrostatic interactions may occur up to a distance of 16 Å for the attraction and 14.5 Å for the repulsion. For the electrostatic attraction, it was found $\eta = 3$, whereas $\eta = 2$ in the case of the repulsion. For both attraction and repulsion, the final equilibrium distance is $r_f = 2.9$ Å.

3) *Hydrophobic Interactions*

For the polar residues, the hydrophobic interactions may occur up to a distance of 12 Å, whereas for the apolar residues, the threshold distances for the hydrophobic interactions are listed in table 2.

Residue (Apolar)	Distance
Isoleucine	11.5 Å
Alanine	11 Å
Valine	13.5 Å
Leucine	14 Å
Methionine	12 Å
Glycine	12 Å

Table 2. Threshold distances required to establish hydrophobic interactions concerning apolar residues.

4) *H-bonds*

H-bonds may occur up to a distance of 14.6 Å and the twisting constant for this type of interaction is $\eta = 2$ for the calculation of ϕ . The final equilibrium distance is $r_f = 2.9$ Å.

5) *C-H... π cloud interactions*

C-H... π cloud interactions occur up to a distance of 14 Å and the twisting constant is $\eta = 1.5$ for the calculation of ϕ .

6) *Pile stacking (π - π interactions)*

In the molecule studied there are not π - π interactions.

Results and Discussion

In this study, on the DNA binding domain of the γ^{δ} resolvase, has been reported a physical-chemical method to calculate the backbone dihedral angles ϕ of a given polypeptide chain starting from the amino acid sequence. Calculations are based on the MMF method^[6] which focuses on the development of mechanical forces after the establishment of precise chemical interactions among the side chains of the residues. To define the occurring chemical interactions it was necessary, in turn, to define rules in order to calculate the partial twistings for each interaction occurred; then, for a given residue, all the partial twistings were added up in order to calculate the dihedral angle ϕ . The rules reported in the section Methods concern the twisting constants (former degrees of freedom^[6]) and the distances for the chemical interactions to occur. Twisting constants have been reported to be fundamental for the determination of the folding factors^[6] and the latter to be, in turn, a fundamental physical measure for the calculation of dihedral angles. Anyway, in the previous study, the definition of the twisting constants was described as the main limit of the whole work^[6]. At this purpose, this work has been realized with the aim to define univocally the twisting constants in order to allow, in the end, the precise calculation of the backbone dihedral angles, specifically the backbone dihedral angles ϕ . With the rules proposed on the twisting constants, as well as on the threshold distances for the chemical interactions, the backbone dihedral angles ϕ of 1res have been calculated and then compared to the values experimentally obtained by NMR^[7]. A comparison between the two sets of data is shown in Figure 2 and can be seen that 38 calculated values, out of 42, show a good agreement with the experimental data^[7], whereas only 2 values have a weak agreement (ϕ_{18} and ϕ_{25}) and just 2 calculated values (ϕ_{21} and ϕ_{42}) do not match the experimental data. This results make the method proposed a good tool to determine and predict at least the backbone dihedral

angles ϕ of polypeptides, even if, further improvements will be realized studying other polypeptides.

Figure 2. Histogram showing the comparison between calculated (black) and experimentally determined (green) backbone dihedral angles ϕ .

Conclusions

The present study deals with the problem of the structural prediction of polypeptides starting from the amino acid sequence. To date it is still a problem in the field of protein folding and still needs to be solved, although it has been deeply investigated over the years. To predict the structure of a protein, is necessary to determine the backbone dihedral angles ϕ and ψ and, as reported from previous studies, the informations to fold a polypeptide chain in its three dimensional structure are contained in the amino acid sequence. To date, the type of informations contained in the sequence still need to be revealed. In this regard, the present study aims to furnish a theoretical method that allows the calculation of backbone dihedral angles, specifically the dihedral angles ϕ , starting from the amino acid sequence, attempting to furnish a possible explanation of the informations to fold a polypeptide, according to the amino acid sequence. The chemical interactions among the side chains of the amino acid residues were supposed to be the informations required to fold the polypeptide: these allow the development of mechanical forces which induce the twistings necessary to fold the polypeptide. This approach, already reported in literature^[6] and deepen in this study, showed that it is possible to calculate the backbone dihedral angles ϕ starting from the amino acid sequence. Results report that 38 values out of 42 (90%) show a good agreement with the experimental data, 2 values show a weak agreement with the experimental data and only 2

are wrong. The method thus, aims to be a useful tool to investigate partially the structure of a polypeptide chain (since concerns only ϕ), predicting it starting from the amino acid sequence. It may represent a good starting point for future computational developments that focus on the prediction of protein structures starting from the amino acid sequence.

Bibliography

- [1] Anfinsen, C. B. (1973) Principles that govern the folding of protein chains. *Science* 181, 223-230.
- [2] Dill, K. A. (1990) Dominant forces in protein folding. *Biochemistry* 29, 7133-7155.
- [3] Camilloni, C., Bonetti, D., Morrone, A., Giri, R., Dobson, C. M., Brunori, M., Gianni, S. and Vendruscolo, M. (2016) Towards a structural biology of the hydrophobic effect in protein folding. *Sci. Rep.* 6, 28285.
- [4] Baldwin, R. L., and Rose, G. D. (2016) How the hydrophobic factor drives protein folding. *Proc. Natl. Acad. Sci. USA* 113, 12462-12466.
- [5] Kauzmann, W. (1964) The three dimensional structures of proteins. *Biophys. J.* 4, 43-54.
- [6] Larocca M., Foglia F. and Cilibrizzi A. (2019) Dihedral angle calculations to elucidate the folding of peptides through its main mechanical forces. *Biochemistry* 58, 8, 1032-1037.
- [7] Liu T., DeRose E. F., and Mullen G. P. (1994) Determination of the structure of the DNA binding domain of γ^{δ} resolvase in solution. *Protein Science*, 3:1286-1295.
- [8] Mayne, C. G., Saam, J., Schulten, K., Tajkhorshid, E. and Gumbart, J. C. (2013) Rapid parameterization of small molecules using the Force Field Toolkit. *J. Comput. Chem.* 34, 2757-2770.
- [9] Humphrey, W., Dalke, A. and Schulten, K. (1996) VMD: Visual molecular dynamics. *J. Molec. Graphics* 14, 33-38.
- [10] Cornell, W. D., Cieplak, P., Bayly, C. I., Gould, I. R., Merz, K. M. Jr., Ferguson, D. M., Spellmeyer, D. C., Fox, T., Caldwell, J. W. and Kollman, P. A. (1995) A Second Generation Force Field for the Simulation of Proteins, Nucleic Acids, and Organic Molecules. *J. Am. Chem. Soc.* 117, 5179-5197.

Polypeptides Folding Rules for the Calculation of the Ba... (611.00 KiB)

[view on ChemRxiv](#) • [download file](#)

Supporting Information for

**Polypeptides Folding: Rules for the Calculation of the Backbone
Dihedral Angles φ Starting from the Amino Acid Sequence**

Michele Larocca

Planetario Osservatorio Astronomico di Anzi-Basilicata, via Salita Rosario s.n.c. 85010, Anzi (PZ), Italy.

michele.larocca@studio.unibo.it

<https://orcid.org/0000-0003-0613-5187>

K(NÅ ² /c ²)	1.12E+28			Note
e (C)	1.60E-19			q stands for a charge
SIN(109.50°)	0.94			or a partial charge
GLY1				
	φ°			
CALCULATED	0			
EXPERIMENTAL	0			

[illegible][illegible][illegible]

[illegible]

LEU12													
	ϕ°												
CALCULATED	-93		ϕ°										
EXPERIMENTAL	-63		Electrostatic Interaction	Hydrophobic interaction	Hydrophobic interaction	Hydrophobic interaction	Hydrophobic interaction	Hydrophobic interaction	Hydrophobic interaction	Hydrophobic interaction	CH- π cloud interaction		
			between terminal charges										
			qGLY-N 1	qVAL11:CG2 -0.3192	qLEU12:CD1 -0.4121	qLEU12:CD2 -0.4121	qLEU12:CD2 -0.4121	qLEU12:CD2 -0.4121	qLEU12:CD2 -0.4121	qLEU12:CD2 -0.4121	qLEU12:HD21 0.1		
			qASN43-O -1	qLEU12:HD21 0.1	qALA10:HB2 0.0603	qASN13:HB1 0.0797	qMET14:HE2 0.0684	qGLN16:HB2 0.0171	qTRP15:CD2 -0.1415				
			ri 154.93	ri 9.79	ri 9.08	ri 6.81	ri 9.21	ri 13.04	ri 13.19				
			F -1.19E-14	F -9.55E-14	F -8.64E-14	F -2.03E-13	F -9.53E-14	F -1.19E-14	F -2.33E-14				
			U -1.85E-12	U -9.35E-13	U -7.85E-13	U -1.38E-12	U -8.78E-13	U -1.55E-13	U -3.08E-13				
			rf 2.9	rf 2.9	rf 2.9	rf 2.9	rf 2.9	rf 2.9	rf 2.9				
			θ 12.84	θ 11.01	θ 25.68	θ 19.26	θ 11.01	θ 12.84	θ 12.84				
			rf + θ 15.74	rf + θ 13.91	rf + θ 28.58	rf + θ 22.16	rf + θ 13.91	rf + θ 15.74	rf + θ 15.74				
			τ -1.88E-13	τ -1.33E-12	τ -2.47E-12	τ -4.50E-12	τ -1.32E-12	τ -1.87E-13	τ -3.67E-13				
			tg 9.84	tg 0.70	tg 0.32	tg 0.31	tg 0.66	tg 0.83	tg 0.84				
			arctg 1.47	arctg 0.61	arctg 0.31	arctg 0.30	arctg 0.59	arctg 0.69	arctg 0.70				
			degrees° 84.24	degrees° 35.17	degrees° 17.63	degrees° 17.09	degrees° 33.54	degrees° 39.66	degrees° 39.98				

ASN13																		
	ϕ°																	
Calculated	-51		ϕ°															
EXPERIMENTAL	-72		Electrostatic interaction	Hydrophobic interaction	Hydrophobic interaction	Hydrophobic interaction	H-bond		H-bond		H-bond		H-bond					
			between terminal charges															
			qGLY-N	1	qLEU12:CD2	-0.4121	qVAL11:CG1	-0.3192	qASN13:HB1	0.0797	qMET14:SD	0.2737	qTRP15:HE1	0.3412	qGLN16:HE22	0.4251	qGLN17:HE22	0.4251
			qASN43:O	-1	qASN13:HB1	0.0797	qASN13:HB1	0.0797	qALA10:CB	0.0603	qASN13:HD22	0.4196	qASN13:ND2	-0.9191	qASN13:ND2	-0.9191	qASN13:ND2	-0.9191
			ri	154.93	ri	6.81	ri	5.04	ri	10.81	ri	9.59	ri	6.3	ri	13.16	ri	13.89
			F	-1.19E-14	F	-2.03E-13	F	-2.87E-13	F	1.18E-14	F	3.58E-13	F	-2.27E-12	F	-6.47E-13	F	-5.81E-13
			U	-1.85E-12	U	-1.38E-12	U	-1.45E-12	U	1.27E-13	U	3.43E-12	U	-1.43E-11	U	-8.51E-12	U	-8.07E-12
			rf	2.9	rf	2.9	rf	2.9	rf	2.9	rf	2.9	rf	2.9	rf	2.9	rf	2.9
			θ	17.12	θ	3.80	θ	4.89	θ	11.41	θ	17.12	θ	17.12	θ	17.12	θ	17.12
			rf + θ	20.02	rf + θ	6.70	rf + θ	7.79	rf + θ	14.31	rf + θ	20.02	rf + θ	20.02	rf + θ	20.02	rf + θ	20.02
			τ	-2.39E-13	τ	-1.36E-12	τ	-2.24E-12	τ	1.69E-13	τ	7.17E-12	τ	-4.54E-11	τ	-1.29E-11	τ	-1.16E-11
			tg	7.74	tg	1.02	tg	0.65	tg	0.76	tg	0.48	tg	0.31	tg	0.66	tg	0.69
			arctg	1.44	arctg	0.79	arctg	0.57	arctg	0.65	arctg	0.45	arctg	0.30	arctg	0.58	arctg	0.61
			degrees°	82.68	degrees°	45.47	degrees°	32.91	degrees°	37.08	degrees°	25.61	degrees°	17.48	degrees°	33.34	degrees°	34.77

MET14																
	ϕ°															
Calculated	-87		ϕ°													
EXPERIMENTAL	-69		Electrostatic interaction	H-bond		Hydrophobic interaction	Hydrophobic interaction	H-bond		H-bond		H-bond		H-bond		
			between terminal charges													
			qGLY-N	1	qMET14:SD	0.2737	qLEU12:CD2	-0.4121	qVAL11:CG2	-0.3192	qMET14:SD	0.2737	qMET14:SD	0.2737	qMET14:SD	0.2737
			qASN43:O	-1	qASN13:HD22	0.4196	qMET14:HE2	0.0684	qMET14:HB1	0.0241	qGLN16:HE22	0.4251	qTRP15:HE1	0.3412	qGLN17:HE21	0.4251
			ri	154.93	ri	9.59	ri	9.21	ri	10.52	ri	6.32	ri	9.08	ri	11.48
			F	-1.19E-14	F	3.58E-13	F	-9.53E-14	F	-1.99E-14	F	8.35E-13	F	3.25E-13	F	2.53E-13
			U	-1.85E-12	U	3.43E-12	U	-8.78E-13	U	-2.10E-13	U	5.28E-12	U	2.95E-12	U	2.91E-12
			rf	2.9	rf	2.9	rf	2.9	rf	2.9	rf	2.9	rf	2.9	rf	2.9
			θ	0.86	θ	17.12	θ	6.66	θ	8.56	θ	17.12	θ	17.12	θ	17.12
			rf + θ	3.76	rf + θ	20.02	rf + θ	9.56	rf + θ	11.46	rf + θ	20.02	rf + θ	20.02	rf + θ	20.02
			τ	-4.49E-14	τ	7.17E-12	τ	-9.11E-13	τ	-2.28E-13	τ	1.67E-11	τ	6.50E-12	τ	5.07E-12
			tg	41.25	tg	0.48	tg	0.96	tg	0.92	tg	0.32	tg	0.45	tg	0.57
			arctg	1.55	arctg	0.45	arctg	0.77	arctg	0.74	arctg	0.31	arctg	0.43	arctg	0.52
			degrees°	88.66	degrees°	25.61	degrees°	43.96	degrees°	42.57	degrees°	17.53	degrees°	24.41	degrees°	29.85

TRP15																		
	ϕ°																	
CALCULATED	-64		ϕ°															
EXPERIMENTAL	-72		Electrostatic interaction	H-bond		H-bond		CH- π cloud interaction		Hydrophobic interaction		H-bond		H-bond		CH- π cloud interaction		
			between terminal charges															
			qGLY-N	1	qMET14:SD	0.2737	qTRP15:HE1	0.3412	qLEU12:HD21	0.1	qVAL11:CG2	-0.3192	qTRP15:NE1	-0.3418	qTRP15:NE1	-0.3418	qGLY18:HA1	0.0698
			qASN43:O	-1	qTRP15:HE1	0.3412	qASN13:ND2	-0.9191	qTRP15:CD2	-0.1415	qTRP15:HB1	0.0339	qGLN16:HE21	0.4251	qGLN17:HE22	0.4251	qTRP15:CD2	-0.1415
			ri	154.93	ri	9.08	ri	6.3	ri	13.19	ri	12.26	ri	10.79	ri	9.14	ri	10.7
			F	-1.19E-14	F	3.25E-13	F	-2.27E-12	F	-2.33E-14	F	-2.06E-14	F	-3.58E-13	F	-4.99E-13	F	-2.47E-14
			U	-1.85E-12	U	2.95E-12	U	-1.43E-11	U	-3.08E-13	U	-2.53E-13	U	-3.86E-12	U	-4.56E-12	U	-2.65E-13
			rf	2.9	rf	2.9	rf	2.9	rf	2.9	rf	2.9	rf	2.9	rf	2.9	rf	2.9
			θ	17.12	θ	17.12	θ	17.12	θ	12.84	θ	9.78	θ	17.12	θ	17.12	θ	12.84
			rf + θ	20.02	rf + θ	20.02	rf + θ	20.02	rf + θ	15.74	rf + θ	12.68	rf + θ	20.02	rf + θ	20.02	rf + θ	15.74
			τ	-2.39E-13	τ	6.50E-12	τ	-4.54E-11	τ	-3.67E-13	τ	-2.62E-13	τ	-7.16E-12	τ	-9.98E-12	τ	-3.89E-13
			tg	7.74	tg	0.45	tg	0.31	tg	0.84	tg	0.97	tg	0.54	tg	0.46	tg	0.68
			arctg	1.44	arctg	0.43	arctg	0.30	arctg	0.70	arctg	0.77	arctg	0.49	arctg	0.43	arctg	0.60
			degrees°	82.68	degrees°	24.41	degrees°	17.48	degrees°	39.98	degrees°	44.05	degrees°	28.34	degrees°	24.55	degrees°	34.23

GLN16																		
	ϕ°																	
CALCULATED	-48		ϕ°															
EXPERIMENTAL	-69		Electrostatic interaction	H-bond		H-bond		H-bond		Hydrophobic interaction	H-bond		Hydrophobic interaction		Hydrophobic interaction			
			between terminal charges															
			qGLY-N	1	qTRP15:NE1	-0.3418	qMET14:SD	0.2737	qGLN16:HE22	0.4251	qLEU12:CD2	-0.4121	qGLN17:HE21	0.4251	qGLY18:HA1	0.0698	qLEU19:HD12	0.1
			qASN43:O	-1	qGLN16:HE21	0.4251	qGLN16:HE22	0.4251	qASN13:ND2	-0.9191	qGLN16:HB2	0.0171	qGLN16:NE2	-0.9407	qGLN16:CB	-0.0036	qGLN16:CB	-0.0036
			r	154.93	r	10.79	r	6.32	r	13.16	r	13.04	r	11.92	r	7.26	r	12.11
			F	-1.19E-14	F	-3.58E-13	F	8.35E-13	F	-6.47E-13	F	-1.19E-14	F	-8.07E-13	F	-1.37E-15	F	-7.04E-16
			U	-1.85E-12	U	-3.86E-12	U	5.28E-12	U	-8.51E-12	U	-1.55E-13	U	-9.62E-12	U	-9.92E-15	U	-8.52E-15
			rf	2.9	rf	2.9	rf	2.9	rf	2.9	rf	2.9	rf	2.9	rf	2.9	rf	2.9
			θ	17.12	θ	17.12	θ	17.12	θ	17.12	θ	5.71	θ	17.12	θ	51.36	θ	5.71
			rf + θ	20.02	rf + θ	20.02	rf + θ	20.02	rf + θ	20.02	rf + θ	8.61	rf + θ	20.02	rf + θ	54.26	rf + θ	8.61
			τ	-2.39E-13	τ	-7.16E-12	τ	1.67E-11	τ	-1.29E-11	τ	-1.02E-13	τ	-1.62E-11	τ	-7.42E-14	τ	-6.06E-15
			tg	7.74	tg	0.54	tg	0.32	tg	0.66	tg	1.52	tg	0.60	tg	0.13	tg	1.41
			arctg	1.44	arctg	0.49	arctg	0.31	arctg	0.58	arctg	0.99	arctg	0.54	arctg	0.13	arctg	0.95
			degrees°	82.68	degrees°	28.34	degrees°	17.53	degrees°	33.34	degrees°	56.60	degrees°	30.79	degrees°	7.63	degrees°	54.63

GLY20												
	ϕ°											
CALCULATED	-132		ϕ°									
EXPERIMENTAL	-159		Electrostatic interaction	Hydrophobic interaction	Hydrophobic interaction	Hydrophobic interaction	Hydrophobic interaction	Hydrophobic interaction	Hydrophobic interaction	Hydrophobic interaction	Hydrophobic interaction	
			between terminal charges									
			qGLY-N 1	qGLY20:HA1 0.0698	qGLY18:HA1 0.0698	qGLY20:HA1 0.0698	qGLY20:HA1 0.0698	qGLY20:HA1 0.0698	qGLY20:HA1 0.0698	qGLY20:HA1 0.0698	qGLY20:CA -0.0252	
			qASN43:O -1	qLEU19:CD1 -0.4121	qGLY20:CA -0.0252	qGLN17:CB -0.0036	qALA21:CB -0.1825	qHIS23:CB -0.0074	qSER22:HB2 0.035			
			ri 154.93	ri 6.1	ri 7.31	ri 11.35	ri 4.89	ri 11.36	ri 6.97			
			F -1.19E-14	F -2.22E-13	F -9.44E-15	F -5.59E-16	F -1.53E-13	F -1.15E-15	F -5.21E-15			
			U -1.85E-12	U -1.35E-12	U -6.90E-14	U -6.30E-15	U -7.47E-13	U -1.30E-14	U -3.63E-14			
			rf 2.9	rf 2.9	rf 2.9	rf 2.9	rf 2.9	rf 2.9	rf 2.9			
			θ -3.42	θ 0.95	θ 8.56	θ 1.43	θ 2.85	θ 1.71	θ 2.85			
			rf + θ -0.52	rf + θ 3.85	rf + θ 11.46	rf + θ 4.33	rf + θ 5.75	rf + θ 4.61	rf + θ 5.75			
			τ 6.26E-15	τ -8.54E-13	τ -1.08E-13	τ -2.42E-15	τ -8.79E-13	τ -5.29E-15	τ -2.99E-14			
			tg -295.75	tg 1.58	tg 0.64	tg 2.62	tg 0.85	tg 2.46	tg 1.21			
			arctg -1.57	arctg 1.01	arctg 0.57	arctg 1.21	arctg 0.70	arctg 1.19	arctg 0.88			
			degrees° -89.85	degrees° 57.76	degrees° 32.55	degrees° 69.17	degrees° 40.38	degrees° 67.94	degrees° 50.49			

[illegible]

[illegible]

[illegible]

[illegible]

[illegible]

ASN43															
		ϕ^*													
CALCULATED		-79													
EXPERIMENTAL		-79													
		ϕ^*													
		Electrostatic interaction	H-bond		H-bond		H-bond		Electrostatic Repulsion		H-bond		H-bond		Hydrophobic interaction
		between terminal charges													
qGLY:N	1	qASN43:ND2	-0.9191	qASN43:O	-1	qGLU41:OE2	-1	qGLU41:OE2	-1	qASN40:ND2	-0.9191	qASN40:HD22	0.4196	qILE39:CG2	-0.066
qASN43:O	-1	qSER42:HG1	0.4275	qSER42:HG1	0.4275	qASN43:HD22	0.4196	qASN43:O	-1	qASN43:HD22	0.4196	qASN43:O	-1	qASN43:HB1	0.0797
ri	154.93	ri	8.39	ri	6.21	ri	8.55	ri	11.91	ri	9.79	ri	11.25	ri	13.57
F	-1.19E-14	F	-1.60E-12	F	-3.18E-12	F	-1.65E-12	F	2.02E-12	F	-1.15E-12	F	-9.51E-13	F	-8.19E-15
U	-1.85E-12	U	-1.34E-11	U	-1.97E-11	U	-1.41E-11	U	2.41E-11	U	-1.13E-11	U	-1.07E-11	U	-1.11E-13
rf	2.9	rf	2.9	rf	2.9	rf	2.9	rf	2.9	rf	2.9	rf	2.9	rf	2.9
θ	17.12	θ	17.12	θ	17.12	θ	25.68	θ	25.68	θ	17.12	θ	17.12	θ	3.80
$rf + \theta$	20.02	$rf + \theta$	20.02	$rf + \theta$	20.02	$rf + \theta$	28.58	$rf + \theta$	28.58	$rf + \theta$	20.02	$rf + \theta$	20.02	$rf + \theta$	6.70
τ	-2.39E-13	τ	-3.20E-11	τ	-6.36E-11	τ	-4.70E-11	τ	5.78E-11	τ	-2.31E-11	τ	-1.90E-11	τ	-5.49E-14
tg	7.74	tg	0.42	tg	0.31	tg	0.30	tg	0.42	tg	0.49	tg	0.56	tg	2.02
arctg	1.44	arctg	0.40	arctg	0.30	arctg	0.29	arctg	0.39	arctg	0.45	arctg	0.51	arctg	1.11
degrees°	82.68	degrees°	22.75	degrees°	17.24	degrees°	16.66	degrees°	22.63	degrees°	26.07	degrees°	29.35	degrees°	63.74

Supporting Information_Polypeptide Folding.pdf (1.01 MiB)

[view on ChemRxiv](#) • [download file](#)