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Supporting Information of: Energetics and *J*-coupling constants for Ala, Gly, and Val peptides demonstrated using ABEEM polarizable force field in vacuo and an aqueous solution

Chao Zhang[a], Dong-Xia Zhao*[a], Yue Feng[a], Jie Wang[a] and Zhong-Zhi Yang*[a]

[a] School of Chemistry and Chemical Engineering, Liaoning Normal University, Dalian, 116029, Liaoning, P. R. China.

* Corresponding authors: Tel: (86) 411-82158977; Fax: (86) 411-82158977

E-mail address: zhaodxchem@lnnu.edu.cn and yangzz@lnnu.edu.cn.

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from MD simulation by ABEEM polarizable force field

Table S1 The number of each amino acid and the distribution percentage in 16 regions of PES from coil library

Residue	Number	β_L-1	β_L-2	β_L-3	β_L-4	ε_L-1	ε_L-2	ε_D-1	ε_D-2	δ_L-1	δ_L-2	δ_D-1	δ_D-2	γ_L	α_D	α_L	γ_D
Ala	280950	0.17	0.00	0.00	0.00	0.23	0.00	0.00	0.00	0.03	0.00	0.00	0.00	0.08	0.02	0.45	0.00
Cys	45944	0.22	0.00	0.01	0.00	0.32	0.01	0.00	0.00	0.07	0.00	0.01	0.00	0.14	0.04	0.17	0.00
Asp	229731	0.08	0.00	0.01	0.00	0.18	0.02	0.00	0.01	0.06	0.00	0.01	0.00	0.18	0.09	0.36	0.01
Glu	278149	0.12	0.00	0.00	0.00	0.20	0.00	0.00	0.00	0.03	0.00	0.01	0.00	0.09	0.03	0.50	0.00
Phe	142724	0.26	0.00	0.00	0.00	0.30	0.00	0.00	0.00	0.05	0.00	0.01	0.00	0.13	0.01	0.23	0.00
Gly	340778	0.06	0.02	0.02	0.05	0.09	0.03	0.04	0.09	0.01	0.00	0.00	0.01	0.03	0.29	0.12	0.13
His	90335	0.20	0.00	0.01	0.00	0.22	0.00	0.00	0.00	0.06	0.00	0.02	0.00	0.16	0.05	0.27	0.01
Ile	207926	0.21	0.00	0.00	0.00	0.31	0.00	0.00	0.00	0.07	0.00	0.01	0.00	0.16	0.00	0.23	0.00
Lys	252806	0.13	0.00	0.00	0.00	0.25	0.00	0.00	0.00	0.03	0.00	0.01	0.00	0.11	0.04	0.41	0.01
Leu	300972	0.12	0.00	0.00	0.00	0.33	0.00	0.00	0.00	0.04	0.00	0.01	0.00	0.15	0.01	0.35	0.00
Met	65713	0.19	0.00	0.00	0.00	0.27	0.00	0.00	0.01	0.05	0.00	0.01	0.00	0.12	0.01	0.34	0.00
Asn	172723	0.09	0.00	0.01	0.00	0.16	0.01	0.00	0.00	0.06	0.00	0.01	0.00	0.21	0.18	0.26	0.01
Pro	153828	0.00	0.00	0.00	0.00	0.50	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.06	0.00	0.42	0.00
Gln	148167	0.15	0.00	0.00	0.00	0.23	0.00	0.00	0.00	0.04	0.00	0.01	0.00	0.11	0.04	0.42	0.00
Arg	200214	0.17	0.00	0.00	0.00	0.24	0.00	0.00	0.00	0.04	0.00	0.01	0.00	0.11	0.04	0.38	0.00
Ser	244401	0.24	0.00	0.01	0.00	0.25	0.01	0.00	0.00	0.04	0.00	0.01	0.00	0.08	0.03	0.32	0.00
Thr	230955	0.25	0.00	0.01	0.00	0.31	0.01	0.00	0.00	0.04	0.00	0.02	0.00	0.10	0.00	0.26	0.00
Val	272223	0.27	0.00	0.00	0.00	0.31	0.00	0.00	0.00	0.07	0.00	0.01	0.00	0.13	0.00	0.20	0.00
Trp	46042	0.22	0.00	0.01	0.00	0.31	0.00	0.00	0.00	0.04	0.00	0.01	0.00	0.11	0.01	0.29	0.00
Tyr	123590	0.25	0.00	0.01	0.00	0.27	0.00	0.00	0.00	0.07	0.00	0.02	0.00	0.12	0.01	0.25	0.00
Total	3828171	0.16	0.00	0.01	0.00	0.25	0.01	0.00	0.01	0.04	0.00	0.01	0.00	0.11	0.06	0.32	0.02

Most researches focus on the special conformations of amino acids distributed in special regions of the classical Ramachandran map. Experimental data illustrate that the conformational structures in mammal prefer locating in β_L-1, ε_L-1, γ_L and α_L, which consist well with their distribution in Ramachandran map, but there are also various configurations of amion acids found in other regions which close to and far away from the empirical regions. In Table S2, taking Gly, which is characterized by its most flexible backbone torsions, as an example, its distribution covers all 16 regions.

Equation S1 Hydrogen bonding fitting function

For hydrogen-bond regions, the k_{ij} is replaced by a $k_{\mathrm{HB}}(R_{H,lp})$ (Eq. S1) function to

depict the electrostatic interaction between the hydrogen atom and the lone-pair electron, and its form is as follows:

$$k_{HB}(R_{H,lp}) = 0.570 - \frac{B}{1+\exp(\frac{R_{H,lp}-C}{D})} \quad \text{(S1)}$$

In Eq. S1, $R_{H,lp}$ means the distance between H atom and lone-pair, and B, C and D means the span, balance distance and gradient of this function respectively (Table S2).

Table S2 Parameters in the function $k_{HB}(R_{H,lp})$ for different H, *lp* pairs

H, *lp* pairs	*B*	*C*	*D*
lp of Alcohol O in Ser and Thr and Amide H	0.0435	1.6032	0.0150
lp of Alcohol O in Ser and Thr and Alcohol H in Ser and Thr	1.1054	1.4843	0.5308
lp of Amide O and Amide H	0.0496	1.3978	0.1034
lp of Amide O and Thiol H in Cys	0.1206	1.3998	0.1758
lp of Amide O and Alcohol H in Ser and Thr	0.0127	1.9482	0.0434
lp of Amide O and Phenol H in Tyr	0.0920	1.0988	0.0190
lp of Amide O and H in $H_2NC{=}O$ of Asn and Gln	0.0792	2.0874	0.3202
lp of Amide O and H in NH^{3+} of Lys	0.0487	1.3008	0.0794
lp of Amide O and H in guanidinium ions of Arg	0.0427	1.5642	0.0420
lp of Amide O and HN in His(+)	0.0470	1.0970	0.0560
lp of O in Asp and Glu and Amide H	0.0130	1.5875	0.0230
lp of Thiol and Thioether S and Amide H	0.0043	1.5201	0.0033

Table S3 *J*-coupling constants and their Karplus parameterizations used in this study

J-Coupling	Parameterization
$^3J(H_N,H_\alpha)$	$7.09\cos^2(\varphi\text{-}60°)\text{-}1.42\cos(\varphi\text{-}60°)\text{+}1.55$
$^3J(H_N,C')$	$4.29\cos^2(\varphi\text{+}180°)\text{-}1.01\cos(\varphi\text{-}60°)$
$^3J(H_\alpha,C')$	$3.72\cos^2(\varphi\text{+}120°)\text{-}2.18\cos(\varphi\text{+}120°)\text{+}1.28$
$^3J(C',C')$	$1.36\cos^2(\varphi)\text{-}0.93\cos(\varphi)\text{+}0.60$
$^3J(H_N,C_\beta)$	$3.06\cos^2(\varphi\text{+}60°)\text{-}0.74\cos(\varphi\text{+}60°)\text{+}0.13$
$^1J(N,C_\alpha)$	$1.70\cos^2(\psi)\text{-}0.98\cos(\psi)\text{+}9.51$
$^2J(N,C_\alpha)$	$-0.66\cos^2(\psi_{i-1})\text{-}1.52\cos(\psi_{i-1})\text{+}7.85$
$^3J(H_N,C_\alpha)$	$-0.23\cos(\varphi)\text{-}0.20\cos(\psi_{i-1})\text{+}0.07\sin(\varphi)\text{+}0.08\sin(\psi_{i-1})\text{+}0.07\cos(\varphi)\cos(\psi_{i-1})\text{+}0.12\cos(\varphi)\sin(\psi_{i-1})\text{-}0.08\sin(\varphi)\cos(\psi_{i-1})\text{-}0.14\sin(\varphi)\sin(\psi_{i-1})\text{+}0.54$

In Table S3, all parameterizations are original without any modified to be consistent

with most studies.

Table S4 The details of transfer by crossing φ=0° of Ala-, Gly- and Val-dipeptide and tripeptide obtained by different methods

		B3LYP/6-311++G(d,p)[a]	ABEEM[b]	OPLS/AA	AMBER99sb	CHARMM27	AMOEBA
Dipeptide		None	None	Val:7($\alpha_D \rightarrow \gamma_L$)[c]	None	None	None
Tripeptide	N-terminal	None	None	Ala:1($\alpha_D \rightarrow \varepsilon_L$) Val:1($\alpha_D \rightarrow \varepsilon_L$) Val:1($\alpha_D \rightarrow \gamma_L$)	None	None	None
	C-terminal	None	None	Val:1($\alpha_D \rightarrow \gamma_L$)	None	None	None

[a]: All minima selected from scan by B3LYP/6-311++G(d,p) were optimized by the same level, and none Ala, Gly and Val dipeptide and tripeptide crossed φ=0°. [b]: All minima selected from scan by B3LYP/6-311++G(d,p) were minimized by force field, and ABEEM, AMBER99sb, CHARMM27 and AMOEBA captured none crossing of φ=0°. [c]: Val:7($\alpha_D \rightarrow \gamma_L$) means that in Val-dipeptides, total 7 times of the transformation from α_D to γ_L. Only OPLS/AA obtained a few times, and the torsions were from (56.08°,41.09°) to (-78.64°,78.39°), from (51.07°,41.09°) to (-78.69°,78.30°), from (51.06°,41.11°) to (-78.67°,78.29°), from (51.08°,41.10°) to (-78.65°,78.61°), from (51.08°,41.11°) to (-78.72°,78.51°), from (51.08°,41.09°) to (-78.65°,78.69°), from (51.08°,41.10°) to (-78.71°,78.38°), from (62.3°,29.7°) to (-64.0°,128.5°), from (48.1°,42.8°) to (-64.8°,136.4°), from (54.0°,36.7°) to (-79.5°,74.4°), and from (52.1°,41.3°) to (-78.5°,72.4°). Though these transfers, there are still stable conformations that locate in α_D successfully, such as a05.

Table S5. The backbone torsions (°) of all Gly- and Val-dipeptides conformations obtained by B3LYP/6-311++G(d,p), ABEEM, OPLS/AA, AMBER99sb, CHARMM27, and AMOEBA and MAD values (°) obtained by each FF compared with those of B3LYP/6-311++G(d,p)

Model	B3LYP/6-311++G(d,p)	ABEEM	OPLS/AA	AMBER99sb	CHARMM27	AMOEBA

		φ	ψ	φ	ψ	φ	ψ	φ	ψ	φ	ψ	φ	ψ
Gly	g01	82.4	-70.4	86.1	-70.5	79.93	-69.64	74.71	-62.51	83.08	-68.02	81.9	-74.1
	g02	112.7	-17.0	111.3	-20.1	79.97	-69.59	74.70	-62.63	82.99	-67.95	105.6	-11.8
	g03	-112.9	17.0	-121.4	18.8	-79.94	69.63	-74.72	62.46	-82.93	67.89	-105.6	11.8
	g04	-82.4	70.4	-86.1	70.5	-79.94	69.64	-74.71	62.45	-83.04	68.03	-81.8	74.2
	g05	179.5	179.5	178.1	177.8	-179.92	179.98	-179.91	-179.98	-179.91	179.92	-170.2	-179.7
	MAD	--		2.6		17.8		20.0		16.8		4.5	
Val	v01	63.3	-40.3	77.4	-47.7	55.5	-52.1	54.6	-42.7	58.5	-56.2	66.5	-40.0
	v02	-116.9	8.7	-112.0	12.5	-78.6	78.6	-78.8	69.6	-78.4	-27.2	-80.7	-15.0
	v03	-157.1	-42.5	-154.3	-40.9	-151.0	-64.5	-78.7	69.7	-149.8	-60.5	-163.0	-36.1
	v04	51.1	41.1	47.7	31.3	-78.7	78.3	54.6	-42.7	58.4	-56.2	58.5	29.2
	v05	-84.7	76.4	-83.2	76.8	-78.6	78.6	-78.7	70.0	-82.2	82.5	-82.2	72.4
	v06	-150.1	154.1	-153.2	148.2	-145.7	159.1	-147.8	151.6	-142.3	150.5	-146.1	155.7
	MAD	--		4.9		28.4		33.8		20.4		8.9	

Table S6 The number of conformation and mean absolute deviation (MAD/°) of dihedral angles at the backbones of Gly and Val dipeptides and tripeptides and Ala tripeptides and tetrapeptides in details obtained by the OPLS/AA, AMBER99sb, CHARMM27, AMOEBA, and ABEEM methods compared with B3LYP/6-311++G(d,p)

Mode		Type	B3LYP/6-311++G(d,p)	ABEEM[d]	OPLS/AA	AMBER99sb	CHARMM27	AMOEBA
Dipeptide	Gly	Number/MAD of all conformations	5/--	5/2.6	5/17.8	5/20.0	5/16.8	5/4.5
		Number/MAD of stable conformations			3/1.3	3/5.4	3/1.2	
	Val	Number/MAD of all conformations	6/--	6/4.9	6/28.4	6/33.8	6/20.4	6/8.9
		Number/MAD of stable conformations			4/8.2	3/4.7	4/8.3	5/4.7
Tripeptide	Ala	Number/MAD[e] of all conformations	30/--	30 / (5.5 / 3.9 / 4.7)	30 / (25.5 / 24.6 / 25.1)	30 / (24.8 / 24.7 / 24.7)	30 / (25.8 / 22.1 / 23.9)	30 / (9.5 / 7.6 / 8.5)
		Number/MAD[e] of stable conformations			14 / (11.4 / 9.4 / 10.4)	14 / (10.9 / 9.9 / 9.9)	12 / (10.6 / 10.3 / 10.4)	24 / (5.5 / 4.1 / 4.8)
	Gly	Number/MAD of all conformations	25/--	25 / (8.0 / 6.6 / 7.3)	25 / (17.7 / 25.8 / 21.8)	25 / (19.5 / 27.5 / 23.5)	25 / (18.1 / 19.8 / 19.0)	25 / (7.3 / 10.8 / 9.0)
		Number/MAD of stable conformations			7 / (2.3 / 2.9 / 2.6)	9 / (6.6 / 10.7 / 8.6)	9 / (3.1 / 3.9 / 3.5)	21 / (6.3 / 6.9 / 6.6)
	Val	Number/MAD of all conformations	28/--	28 / (6.7 / 6.6 / 6.7)	28 / (25.6 / 33.8 / 29.7)	28 / (13.0 / 23.3 / 18.1)	28 / (25.3 / 25.7 / 25.5)	28 / (12.5 / 15.3 / 13.9)
		Number/MAD of stable conformations			13 / (10.8 / 10.6 / 10.7)	13 / (6.1 / 8.2 / 7.1)	11 / (7.9 / 15.6 / 11.7)	19 / (8.2 / 7.2 / 7.7)
Tetrapeptide	Ala	Number/MAD[e] of all conformations	169/--	169 / (4.5 / 4.8 / 3.8 / 4.4)	169 / (31.8 / 21.5 / 25.2 / 26.2)	169 / (30.2 / 24.3 / 29.4 / 27.9)	169 / (30.2 / 24.2 / 27.4 / 27.3)	169 / (10.8 / 9.6 / 10.4 / 10.3)
		Number/MAD[e] of stable conformations			61 / (11.8 / 12.6 / 12.1 / 12.2)	53 / (10.5 / 10.4 / 11.4 / 10.8)	50 / (11.7 / 11.8 / 14.6 / 12.7)	128 / (7.8 / 6.9 / 6.3 / 7.0)

[a]: for B3LYP/6-311++G(d,p), all conformations equal to stable conformations, and the conformations are standard conformations, while for each FF, it donates the results from further optimization of every conformation processed by each FF, and MAD means the mean absolutely deviation value of φ and ψ compared with the standard conformations; [b]: for each FF, stable conformations mean the conformation locate around the standard conformation succefully by each FF, and the MAD

donates the corresponding deviation value of dihedral angles between stable conformations successfully located by each FF and their standard conformations; [c]: the MAD includes three values, which are the averge deviation of φ and ψ at N-terminal, C-terminal (above te line) and all two pairs compared with the standard conformations (below the line); [d]: the FF succefully locates all stable conformations, so the number and MAD are not listed repeatedly; [e]: values above the line donate MAD of three pairs of φ and ψ belong to N-terminal, central and C-terminal residue in turn respectively, and the value below donate the average of all φ and ψ compared with the standard conformations.

Table S7 The backbone torsions (°) of Ala stable conformations obtained by B3LYP/6-311++G(d,p), ABEEM, OPLS/AA, AMBER99sb, CHARMM27, and AMOEBA, the number of conformations that located by each force field and the MAD with B3LYP/6-311++G(d,p)

Model		B3LYP/6-311++(d,p)		ABEEM		OPLS/AA		AMBER99sb		CHARMM27		AMOEBA	
		φ	ψ	φ	ψ	φ	ψ	φ	ψ	φ	ψ	φ	ψ
Ala	a01	73.1	-57.3	78.2	-58.8	67.7	-61.2	59.8	-55.4	69.7	-67.6	72.1	-53.1
	a02	-164.5	-44.8	-158.5	-45.7	--	--	-149.7	-57.0	--	--	-167.4	-35.5
	a03	-115.2	13.7	-81.2	17.0	--	--	--	--	--	--	-116.2	10.6
	a04	-83.5	76.0	-83.8	76.1	-79.3	76.9	-76.4	69.0	-81.4	70.6	-83.2	76.3
	a05	72.1	19.6	80.9	15.2	49.3	39.2	--	--	--	--	66.1	30.1
	a06	-154.6	160.2	-154.5	158.2	-147.3	165.2	-147.2	163.3	-151.3	170.6	-155.7	162.0
	Number	6		6		4		4		3		6	
	MAD	--		5.2		8.6		8.3		5.8		3.5	
Gly	g01	82.4	-70.4	86.0	-70.6	79.9	-69.6	74.7	-62.5	83.1	-68.0	81.9	-74.1
	g02	112.7	-17.0	111.3	-20.1	--	--	--	--	--	--	105.6	-11.8
	g03	-112.9	17.0	-121.4	18.8	--	--	--	--	--	--	-105.6	11.8
	g04	-82.4	70.4	-86.1	70.5	-79.9	69.6	-74.7	62.5	-83.0	68.0	-81.8	74.2
	g05	179.5	179.5	178.1	177.8	-179.9	180.0	-179.9	-180.0	-179.9	179.9	-170.2	-179.7
	Number	5		5		3		3		3		5	
	MAD	--		2.6		1.3		5.4		1.2		4.5	
Val	v01	63.3	-40.3	77.4	-47.7	55.5	-52.1	54.6	-42.7	58.5	-56.2	66.5	-40.0
	v02	-116.9	8.7	-112.0	12.5	--	--	--	--	--	--	--	--
	v03	-157.1	-42.5	-154.3	-40.9	-151.0	-64.5	--	--	-149.8	-60.5	-163.0	-36.1
	v04	51.1	41.1	47.7	31.3	--	--	--	--	--	--	58.5	29.2
	v05	-84.7	76.4	-83.2	76.8	-78.6	78.6	-78.7	70.0	-82.2	82.5	-82.2	72.4
	v06	-150.1	154.1	-153.2	148.2	-145.7	159.1	-147.8	151.6	-142.3	150.5	-146.1	155.7
	Number	6		6		4		3		4		5	
	MAD	--		4.9		8.2		4.7		8.3		4.7	

In Table S7, lower deviation values are obtained from the results after classification, because the deviation values of the missed conformation contribute none to them, and only the conformations successfully obtained take part in the compare.

Table S8 The number, value (°) and mean absolute deviation (MAD/°) of dihedral angles at backbone of the Ala-tripeptide's stable conformations by B3LYP/6-311++G(d,p), OPLS/AA, AMBER99sb, CHARMM27, AMOEBA, and ABEEM methods

Tripeptide	Method	φ_1	ψ_1	φ_2	ψ_2	MAD
Ala-Ala-001	B3LYP/6-311++G(d,p)	-162.9	-45.2	-156.2	159.7	--
	ABEEM	-162.7	-47.0	-154.6	160.1	1.0
	OPLS/AA	--	--	--	--	--
	AMBER99sb	-147.9	-36.7	-140.2	166.3	11.5

	CHARMM27	--	--	--	--	--
	AMOEBA	-167.4	-35.1	-149.4	168.1	7.4
Ala-Ala-002	B3LYP/6-311++G(d,p)	-165.9	-46.4	-84.7	78.5	--
	ABEEM	-168.4	-48.6	-81.5	77.7	2.2
	OPLS/AA	-150.4	-66.6	-75.5	84.7	12.7
	AMBER99sb	-147.0	-44.9	-73.9	81.7	8.6
	CHARMM27	--	--	--	--	--
	AMOEBA	-167.2	-37.9	-80.7	83.9	4.8
Ala-Ala-003	B3LYP/6-311++G(d,p)	-167.1	-48.8	72.3	14.9	--
	ABEEM	-156.0	-55.2	78.5	12.0	6.6
	OPLS/AA	--	--	--	--	--
	AMBER99sb	--	--	--	--	--
	CHARMM27	--	--	--	--	--
	AMOEBA	--	--	--	--	--
Ala-Ala-004	B3LYP/6-311++G(d,p)	-165.4	-44.8	72.1	-56.4	--
	ABEEM	-168.1	-51.2	78.2	-57.8	4.1
	OPLS/AA	--	--	--	--	--
	AMBER99sb	--	--	--	--	--
	CHARMM27	--	--	--	--	--
	AMOEBA	-167.9	-35.7	75.6	-57.1	4.0
Ala-Ala-005	B3LYP/6-311++G(d,p)	-153.1	159.0	-162.1	-49.1	--
	ABEEM	-155.1	156.8	-162.8	-51.6	1.9
	OPLS/AA	--	--	--	--	--
	AMBER99sb	-146.8	163.6	-148.0	-41.9	8.0
	CHARMM27	--	--	--	--	--
	AMOEBA	-154.7	163.1	-166.6	-35.7	5.9
Ala-Ala-006	B3LYP/6-311++G(d,p)	-155.4	161.1	-155.8	160.5	--
	ABEEM	-155.0	159.3	-153.7	158.1	1.7
	OPLS/AA	-148.7	167.1	-144.7	164.4	6.9
	AMBER99sb	-147.2	163.7	-146.7	162.4	5.4
	CHARMM27	-150.6	173.1	-150.2	172.8	8.6
	AMOEBA	-155.8	168.0	-152.0	164.9	3.9
Ala-Ala-007	B3LYP/6-311++G(d,p)	-155.1	163.8	-112.1	10.0	--
	ABEEM	-153.8	139.0	-83.0	11.0	14.0
	OPLS/AA	--	--	--	--	--
	AMBER99sb	--	--	--	--	--
	CHARMM27	--	--	--	--	--
	AMOEBA	-156.7	171.3	-109.4	10.5	3.1
Ala-Ala-008	B3LYP/6-311++G(d,p)	-154.7	156.8	-83.5	77.0	--
	ABEEM	-153.3	155.2	-82.1	77.1	1.1
	OPLS/AA	-146.6	162.6	-80.0	71.8	5.7
	AMBER99sb	-146.8	160.3	-77.2	58.8	9.0
	CHARMM27	-148.3	169.1	-81.7	73.7	6.0
	AMOEBA	-155.8	162.2	-83.6	79.9	2.4

Ala-Ala-009	B3LYP/6-311++G(d,p)	-153.6	156.6	72.9	18.6	--
	ABEEM	-158.0	148.9	77.7	16.5	4.7
	OPLS/AA	-142.8	168.0	53.3	37.5	15.2
	AMBER99sb	--	--	--	--	--
	CHARMM27	--	--	--	--	--
	AMOEBA	-152.8	160.0	64.9	33.1	6.7
Ala-Ala-010	B3LYP/6-311++G(d,p)	-153.8	155.4	74.2	-55.6	--
	ABEEM	-155.2	150.2	78.5	-57.3	3.2
	OPLS/AA	-146.4	167.9	67.9	-57.7	7.1
	AMBER99sb	-146.1	165.1	60.2	-47.7	9.8
	CHARMM27	-150.3	171.1	70.3	-68.6	9.0
	AMOEBA	-152.7	163.7	73.7	-55.6	2.5
Ala-Ala-011	B3LYP/6-311++G(d,p)	-116.1	10.2	-165.0	-42.5	--
	ABEEM	-87.4	1.2	-158.6	-45.3	11.8
	OPLS/AA	--	--	--	--	--
	AMBER99sb	--	--	--	--	--
	CHARMM27	--	--	--	--	--
	AMOEBA	--	--	--	--	--
Ala-Ala-012	B3LYP/6-311++G(d,p)	-108.9	4.7	-155.2	157.4	--
	ABEEM	-90.8	8.5	-159.1	152.6	7.7
	OPLS/AA	-70.1	-26.9	-130.8	159.1	24.1
	AMBER99sb	-71.0	-9.9	-147.0	159.4	15.7
	CHARMM27	-79.5	-31.9	-152.4	168.0	19.8
	AMOEBA	-82.1	-15.4	-156.1	158.6	12.2
Ala-Ala-013	B3LYP/6-311++G(d,p)	-74.8	-11.1	-97.8	4.9	--
	ABEEM	-68.4	-22.7	-85.1	5.2	7.7
	OPLS/AA	--	--	--	--	--
	AMBER99sb	-60.6	-19.9	-76.9	-1.3	12.5
	CHARMM27	-64.3	-18.9	-84.7	-5.7	10.4
	AMOEBA	-74.2	-11.8	-91.0	-2.1	3.8
Ala-Ala-014	B3LYP/6-311++G(d,p)	-112.5	6.0	-83.5	73.7	--
	ABEEM	-108.2	9.9	-83.6	74.2	2.2
	OPLS/AA	--	--	--	--	--
	AMBER99sb	--	--	--	--	--
	CHARMM27	--	--	--	--	--
	AMOEBA	-129.4	9.4	-85.3	77.8	6.5
Ala-Ala-015	B3LYP/6-311++G(d,p)	-111.0	10.7	74.1	-57.3	--
	ABEEM	-101.8	8.0	79.4	-60.5	5.1
	OPLS/AA	--	--	--	--	--
	AMBER99sb	--	--	--	--	--
	CHARMM27	--	--	--	--	--
	AMOEBA	-120.4	11.7	73.0	-68.4	5.6
Ala-Ala-016	B3LYP/6-311++G(d,p)	-79.8	74.7	-174.8	-34.7	--
	ABEEM	-79.2	75.1	-174.5	-33.2	0.7

	OPLS/AA	-74.7	75.8	-158.8	-48.6	9.0
	AMBER99sb	--	--	--	--	--
	CHARMM27	-77.8	70.6	-142.8	-63.1	16.6
	AMOEBA	-78.2	69.8	-168.6	-31.4	4.0
Ala-Ala-017	B3LYP/6-311++G(d,p)	-84.0	74.9	-116.9	7.6	--
	ABEEM	-83.6	73.2	-112.7	11.2	2.5
	OPLS/AA	--	--	--	--	--
	AMBER99sb	--	--	--	--	--
	CHARMM27	--	--	--	--	--
	AMOEBA	--	--	--	--	--
Ala-Ala-018	B3LYP/6-311++G(d,p)	-84.3	72.2	-84.6	72.2	--
	ABEEM	-84.5	72.8	-83.2	72.0	0.6
	OPLS/AA	-80.0	73.4	-77.5	67.6	4.3
	AMBER99sb	-77.2	62.5	-76.4	54.0	10.8
	CHARMM27	-80.5	73.1	-80.0	68.2	3.3
	AMOEBA	-82.5	69.5	-82.0	77.1	3.0
Ala-Ala-019	B3LYP/6-311++G(d,p)	-85.7	67.4	70.6	19.4	--
	ABEEM	-83.0	69.3	71.7	13.5	2.9
	OPLS/AA	--	--	--	--	--
	AMBER99sb	--	--	--	--	--
	CHARMM27	--	--	--	--	--
	AMOEBA	--	--	--	--	--
Ala-Ala-020	B3LYP/6-311++G(d,p)	-83.7	72.2	70.8	-55.5	--
	ABEEM	-84.0	71.2	74.7	-56.2	1.5
	OPLS/AA	-79.5	70.7	66.3	-60.4	3.8
	AMBER99sb	-77.8	60.2	58.9	-56.9	7.8
	CHARMM27	-81.3	66.5	69.1	-67.2	5.4
	AMOEBA	-80.2	79.8	75.5	-52.1	4.8
Ala-Ala-021	B3LYP/6-311++G(d,p)	55.7	-127.6	-100.7	12.6	--
	ABEEM	75.8	-122.2	-104.2	17.3	8.4
	OPLS/AA	59.9	-151.0	-82.6	62.8	24.0
	AMBER99sb	48.4	-134.5	-77.1	7.3	10.8
	CHARMM27	--	--	--	--	--
	AMOEBA	52.2	-124.5	-103.8	12.4	2.4
Ala-Ala-022	B3LYP/6-311++G(d,p)	69.8	22.4	-158.9	157.0	--
	ABEEM	79.4	14.5	-153.4	160.2	6.6
	OPLS/AA	--	--	--	--	--
	AMBER99sb	--	--	--	--	--
	CHARMM27	--	--	--	--	--
	AMOEBA	66.5	29.4	-156.5	164.8	5.1
Ala-Ala-023	B3LYP/6-311++G(d,p)	68.2	27.0	-117.6	11.6	--
	ABEEM	79.4	-3.7	-83.6	16.2	20.1
	OPLS/AA	--	--	--	--	--
	AMBER99sb	--	--	--	--	--

	CHARMM27	--	--	--	--	--
	AMOEBA	64.6	31.9	-111.9	12.9	3.9
Ala-Ala-024	B3LYP/6-311++G(d,p)	71.7	19.4	-86.0	75.2	--
	ABEEM	67.4	16.9	-82.0	75.0	2.7
	OPLS/AA	51.7	40.0	-79.7	72.1	12.5
	AMBER99sb	--	--	--	--	--
	CHARMM27	--	--	--	--	--
	AMOEBA	65.3	31.6	-84.5	79.6	6.1
Ala-Ala-025	B3LYP/6-311++G(d,p)	62.3	29.7	68.1	16.3	--
	ABEEM	64.3	25.2	73.6	11.1	4.3
	OPLS/AA	--	--	--	--	--
	AMBER99sb	48.4	33.5	55.6	12.8	8.4
	CHARMM27	57.7	17.5	70.2	13.4	5.4
	AMOEBA	59.6	31.5	70.1	8.2	3.6
Ala-Ala-026	B3LYP/6-311++G(d,p)	69.1	29.1	72.7	-58.1	--
	ABEEM	68.6	21.6	79.6	-58.3	3.8
	OPLS/AA	47.6	54.5	69.3	-55.8	13.2
	AMBER99sb	--	--	--	--	--
	CHARMM27	--	--	--	--	--
	AMOEBA	--	--	--	--	--
Ala-Ala-027	B3LYP/6-311++G(d,p)	75.1	-49.9	-107.9	6.6	--
	ABEEM	79.0	-57.3	-102.4	10.4	5.1
	OPLS/AA	--	--	--	--	--
	AMBER99sb	--	--	--	--	--
	CHARMM27	62.6	-86.6	-86.6	-24.3	25.4
	AMOEBA	--	--	--	--	--
Ala-Ala-028	B3LYP/6-311++G(d,p)	73.2	-57.3	-82.7	74.5	--
	ABEEM	75.3	-58.3	-81.8	73.8	1.2
	OPLS/AA	68.7	-57.2	-75.5	74.3	3.0
	AMBER99sb	60.6	-43.9	-74.9	67.3	10.3
	CHARMM27	69.8	-64.9	-80.4	66.7	5.3
	AMOEBA	71.8	-66.5	-83.4	77.4	3.6
Ala-Ala-029	B3LYP/6-311++G(d,p)	73.6	-60.2	70.7	23.3	--
	ABEEM	78.6	-61.2	71.6	18.4	3.0
	OPLS/AA	--	--	--	--	--
	AMBER99sb	--	--	--	--	--
	CHARMM27	--	--	--	--	--
	AMOEBA	70.5	-50.2	69.7	30.0	5.2
Ala-Ala-030	B3LYP/6-311++G(d,p)	73.6	-55.6	72.9	-51.8	--
	ABEEM	78.4	-61.4	77.8	-53.3	4.2
	OPLS/AA	68.4	-58.6	66.3	-54.7	4.4
	AMBER99sb	60.7	-52.1	59.5	-39.2	10.6
	CHARMM27	68.9	-69.6	67.9	-66.8	9.7
	AMOEBA	70.5	-45.2	75.8	-53.1	4.4

Geometry information of all Ala-tripeptides after classified are list in Table S8, with the same benchmark, the deviation values of the missed conformation contribute none to them, and only the conformations successfully obtained take part in the compare. The deviation of holistic conformations before classified are listed in the manuscript.

Table S9 The number, value(°) and mean absolute deviation (MAD/°) of dihedral angles at backbone of the Gly-tripeptide's stable conformations by B3LYP/6-311++G(d,p), OPLS/AA, AMBER99sb, CHARMM27, AMOEBA, and ABEEM methods

Tripeptide	Method	φ_1	ψ_1	φ_2	ψ_2	MAD
Gly-Gly-001	B3LYP/6-311++G(d,p)	-179.9	179.8	179.8	179.4	--
	ABEEM	-179.8	180.0	179.2	178.6	0.4
	OPLS/AA	-179.4	179.7	179.1	-179.8	0.5
	AMBER99sb	-179.8	179.7	179.7	-179.8	0.3
	CHARMM27	-179.8	179.6	179.4	-179.4	1.2
	AMOEBA	-171.1	-179.6	-167.1	-178.1	6.3
Gly-Gly-002	B3LYP/6-311++G(d,p)	173.2	-174.2	-112.3	14.8	--
	ABEEM	172.4	-175.7	-111.3	18.6	1.8
	OPLS/AA	--	--	--	--	--
	AMBER99sb	--	--	--	--	--
	CHARMM27	--	--	--	--	--
	AMOEBA	163.4	-175.6	-106.2	8.3	5.9
Gly-Gly-003	B3LYP/6-311++G(d,p)	174.7	-175.2	-83.7	71.7	--
	ABEEM	174.7	-174.4	-84.7	71.6	0.5
	OPLS/AA	179.4	178.0	-80.6	66.6	4.9
	AMBER99sb	-179.6	177.4	-74.9	56.1	9.4
	CHARMM27	-179.5	178.2	-83.8	69.6	3.6
	AMOEBA	164.4	178.7	-81.9	78.9	6.3
Gly-Gly-004	B3LYP/6-311++G(d,p)	-174.7	175.3	83.7	-71.7	--
	ABEEM	-174.7	174.5	84.7	-71.6	0.5
	OPLS/AA	-179.3	-178.1	80.7	-66.6	4.8
	AMBER99sb	179.7	-177.3	74.9	-56.1	9.4
	CHARMM27	179.7	-178.5	83.8	-69.5	3.5
	AMOEBA	-164.5	-178.7	82.0	-78.7	6.3
Gly-Gly-005	B3LYP/6-311++G(d,p)	-173.2	174.1	112.3	-14.8	--
	ABEEM	-172.4	175.7	111.3	-18.6	1.8
	OPLS/AA	--	--	--	--	--
	AMBER99sb	--	--	--	--	--
	CHARMM27	--	--	--	--	--
	AMOEBA	-163.2	175.3	106.8	-9.1	5.6
Gly-Gly-006	B3LYP/6-311++G(d,p)	-109.8	11.6	172.1	-178.8	--

	ABEEM	-115.0	24.6	156.9	171.8	10.6
	OPLS/AA	--	--	--	--	--
	AMBER99sb	--	--	--	--	--
	CHARMM27	--	--	--	--	--
	AMOEBA	-117.3	12.2	153.0	172.2	9.0
Gly-Gly-007	B3LYP/6-311++G(d,p)	-74.2	-11.4	-100.0	10.0	--
	ABEEM	-82.9	0.9	-110.4	14.5	9.0
	OPLS/AA	--	--	--	--	--
	AMBER99sb	-62.3	-11.1	-81.0	-1.9	10.8
	CHARMM27	--	--	--	--	--
	AMOEBA	-69.0	-12.8	-98.5	3.1	3.7
Gly-Gly-008	B3LYP/6-311++G(d,p)	-115.1	12.7	-82.1	67.8	--
	ABEEM	-121.4	38.9	-106.9	69.0	14.6
	OPLS/AA	--	--	--	--	--
	AMBER99sb	--	--	--	--	--
	CHARMM27	--	--	--	--	--
	AMOEBA	-113.0	7.0	-83.6	76.7	4.5
Gly-Gly-009	B3LYP/6-311++G(d,p)	-113.8	16.5	83.1	-70.6	--
	ABEEM	-111.9	-5.2	108.6	-73.6	13.0
	OPLS/AA	--	--	--	--	--
	AMBER99sb	--	--	--	--	--
	CHARMM27	--	--	--	--	--
	AMOEBA	-115.6	13.6	80.6	-82.6	4.8
Gly-Gly-010	B3LYP/6-311++G(d,p)	-108.6	13.1	114.7	-16.9	--
	ABEEM	-106.8	16.4	113.4	-20.5	2.5
	OPLS/AA	--	--	--	--	--
	AMBER99sb	--	--	--	--	--
	CHARMM27	--	--	--	--	--
	AMOEBA	-99.3	4.4	105.8	-14.5	7.3
Gly-Gly-011	B3LYP/6-311++G(d,p)	-86.3	77.7	-161.1	166.7	--
	ABEEM	-118.2	49.2	-126.5	179.2	26.9
	OPLS/AA	--	--	--	--	--
	AMBER99sb	--	--	--	--	--
	CHARMM27	-89.9	65.5	174.9	176.0	12.3
	AMOEBA	--	--	--	--	--
Gly-Gly-012	B3LYP/6-311++G(d,p)	-82.5	71.0	-112.3	10.1	--
	ABEEM	-87.2	70.9	-111.7	12.5	2.0
	OPLS/AA	--	--	--	--	--
	AMBER99sb	--	--	--	--	--
	CHARMM27	--	--	--	--	--
	AMOEBA	--	--	--	--	--
Gly-Gly-013	B3LYP/6-311++G(d,p)	-82.0	65.9	-82.6	66.5	--
	ABEEM	-86.2	69.3	-86.0	66.5	2.7
	OPLS/AA	-80.9	67.5	-78.0	64.0	2.4

	AMBER99sb	-74.7	59.0	-73.4	48.9	10.3
	CHARMM27	-82.0	68.5	-81.4	65.9	1.1
	AMOEBA	-82.9	67.2	-80.9	76.1	3.4
Gly-Gly-014	B3LYP/6-311++G(d,p)	-81.9	66.6	80.5	-68.6	--
	ABEEM	-85.8	65.3	83.9	-68.6	2.1
	OPLS/AA	-80.4	66.0	76.4	-68.2	1.6
	AMBER99sb	-74.8	54.5	73.3	-61.7	8.3
	CHARMM27	-82.4	65.4	81.3	-66.3	1.2
	AMOEBA	-80.6	76.2	81.9	-75.7	4.9
Gly-Gly-015	B3LYP/6-311++G(d,p)	-83.8	60.4	106.8	-10.1	--
	ABEEM	-110.1	56.8	117.4	-17.4	12.0
	OPLS/AA	--	--	--	--	--
	AMBER99sb	--	--	--	--	--
	CHARMM27	--	--	--	--	--
	AMOEBA	-64.3	119.1	97.4	-1.4	24.0
Gly-Gly-016	B3LYP/6-311++G(d,p)	87.3	-72.5	171.8	-170.1	--
	ABEEM	109.7	-59.6	155.1	-177.0	14.7
	OPLS/AA	--	--	--	--	--
	AMBER99sb	--	--	--	--	--
	CHARMM27	89.5	-68.8	-177.7	-178.1	6.1
	AMOEBA	--	--	--	--	--
Gly-Gly-017	B3LYP/6-311++G(d,p)	83.8	-60.4	-106.8	10.1	--
	ABEEM	110.1	-56.8	-117.4	17.4	12.0
	OPLS/AA	--	--	--	--	--
	AMBER99sb	--	--	--	--	--
	CHARMM27	--	--	--	--	--
	AMOEBA	--	--	--	--	--
Gly-Gly-018	B3LYP/6-311++G(d,p)	81.9	-66.6	-80.5	68.6	--
	ABEEM	85.8	-65.3	-83.9	68.6	2.1
	OPLS/AA	80.5	-66.1	-76.5	68.3	1.6
	AMBER99sb	74.8	-54.5	-73.3	62.1	8.2
	CHARMM27	82.4	-65.3	-81.3	66.4	1.2
	AMOEBA	80.6	-76.2	-81.9	75.7	4.9
Gly-Gly-019	B3LYP/6-311++G(d,p)	82.0	-65.9	82.6	-66.5	--
	ABEEM	86.2	-69.3	86.0	-66.5	2.7
	OPLS/AA	80.9	-67.5	77.9	-64.1	2.4
	AMBER99sb	74.6	-58.8	73.4	-49.1	10.3
	CHARMM27	82.0	-68.5	81.5	-65.9	1.1
	AMOEBA	82.9	-67.3	80.9	-76.1	3.4
Gly-Gly-020	B3LYP/6-311++G(d,p)	82.5	-71.0	112.3	-10.1	--
	ABEEM	87.2	-70.9	111.7	-12.5	2.0
	OPLS/AA	--	--	--	--	--
	AMBER99sb	--	--	--	--	--
	CHARMM27	--	--	--	--	--

	AMOEBA	80.7	-67.4	137.5	-6.3	8.6
Gly-Gly-021	B3LYP/6-311++G(d,p)	109.5	-11.4	-172.2	178.0	--
	ABEEM	115.4	-25.3	-157.6	-176.3	10.0
	OPLS/AA	--	--	--	--	--
	AMBER99sb	--	--	--	--	--
	CHARMM27	--	--	--	--	--
	AMOEBA	117.4	-12.2	-152.6	-172.2	9.5
Gly-Gly-022	B3LYP/6-311++G(d,p)	108.6	-13.1	-114.7	16.9	--
	ABEEM	106.8	-16.4	-113.4	20.5	2.5
	OPLS/AA	--	--	--	--	--
	AMBER99sb	--	--	--	--	--
	CHARMM27	--	--	--	--	--
	AMOEBA	98.9	-4.1	-106.1	14.5	7.4
Gly-Gly-023	B3LYP/6-311++G(d,p)	113.9	-16.5	-83.1	70.6	--
	ABEEM	111.7	4.9	-108.2	73.7	12.9
	OPLS/AA	--	--	--	--	--
	AMBER99sb	--	--	--	--	--
	CHARMM27	--	--	--	--	--
	AMOEBA	115.3	-13.3	-80.6	82.7	4.8
Gly-Gly-024	B3LYP/6-311++G(d,p)	115.1	-12.7	82.1	-67.8	--
	ABEEM	121.5	-38.7	106.5	-69.3	14.6
	OPLS/AA	--	--	--	--	--
	AMBER99sb	--	--	--	--	--
	CHARMM27	--	--	--	--	--
	AMOEBA	112.5	-6.7	83.7	-76.6	4.7
Gly-Gly-025	B3LYP/6-311++G(d,p)	74.1	11.4	100.0	-10.0	--
	ABEEM	82.9	-0.9	110.4	-14.5	9.0
	OPLS/AA	--	--	--	--	--
	AMBER99sb	62.3	11.1	81.0	1.9	10.8
	CHARMM27	--	--	--	--	--
	AMOEBA	69.0	13.0	98.5	-3.3	3.7

Ab initio method obtains 25 Gly-tripeptide stable structures, and ABEEM, OPLS/AA, AMBER99sb, CHARMM27 and AMOEBA obtain 25, 7, 9, 9 and 21 stable structures, respectively. And the MAD values from each force field are 7.3°, 2.6°, 8.6°, 3.5° and 6.6°. But if considering all 25 structures, the MAD values increase obviously except ABEEM. And the values are 7.3°, 21.8°, 23.5°, 19.0° and 9.0°. This increase demonstrates the missing of stable conformations, and the torsions show the preference of each method.

Table S10 The number, value(°) and mean absolute deviation (MAD/°) of dihedral angles at backbone of the Val-tripeptide's stable conformations by B3LYP/6-311++G(d,p), OPLS/AA, AMBER99sb, CHARMM27, AMOEBA, and ABEEM methods

Tripeptide	Method	φ_1	ψ_1	φ_2	ψ_2	MAD
Val-Val-001	B3LYP/6-311++G(d,p)	-156.8	-51.1	-155.2	-48.7	--
	ABEEM	-154.2	-51.6	-158.4	-45.1	2.5
	OPLS/AA	--	--	--	--	--
	AMBER99sb	-152.6	-49.7	-155.5	-42.8	3.0
	CHARMM27	-152.3	-64.4	-148.8	-68.9	11.1
	AMOEBA	-163.5	-39.5	-153.4	-41.7	6.8
Val-Val-002	B3LYP/6-311++G(d,p)	-153.3	-45.8	-146.7	156.4	--
	ABEEM	-156.1	-43.0	-150.4	151.2	3.6
	OPLS/AA	--	--	--	--	--
	AMBER99sb	-147.1	-28.9	-144.7	154.1	6.9
	CHARMM27	--	--	--	--	--
	AMOEBA	--	--	--	--	--
Val-Val-003	B3LYP/6-311++G(d,p)	-153.4	-39.0	-107.1	6.2	--
	ABEEM	-152.6	-48.1	-97.1	11.4	6.3
	OPLS/AA	--	--	--	--	--
	AMBER99sb	--	--	--	--	--
	CHARMM27	--	--	--	--	--
	AMOEBA	--	--	--	--	--
Val-Val-004	B3LYP/6-311++G(d,p)	-155.8	-49.1	-85.0	80.3	--
	ABEEM	-156.5	-50.8	-82.8	79.6	1.4
	OPLS/AA	--	--	--	--	--
	AMBER99sb	--	--	--	--	--
	CHARMM27	--	--	--	--	--
	AMOEBA	-155.8	-44.5	-80.2	76.9	3.2
Val-Val-005	B3LYP/6-311++G(d,p)	-155.4	-47.7	63.0	-41.0	--
	ABEEM	-155.3	-58.5	78.2	-48.8	8.5
	OPLS/AA	-150.5	-60.3	55.4	-49.2	8.3
	AMBER99sb	-149.7	-37.6	55.0	-41.2	6.0
	CHARMM27	--	--	--	--	--
	AMOEBA	-163.7	-37.1	68.4	-39.7	6.4
Val-Val-006	B3LYP/6-311++G(d,p)	-147.8	151.9	-157.0	-45.2	--
	ABEEM	-152.5	145.4	-154.4	-45.7	3.6
	OPLS/AA	-145.6	162.3	-148.7	-56.9	8.2
	AMBER99sb	--	--	--	--	--
	CHARMM27	--	--	--	--	--
	AMOEBA	-145.1	157.8	-161.1	-36.7	5.3
Val-Val-007	B3LYP/6-311++G(d,p)	-150.6	158.6	-112.6	3.9	--
	ABEEM	-151.4	134.6	-85.5	7.4	13.8
	OPLS/AA	--	--	--	--	--

	AMBER99sb	--	--	--	--	--
	CHARMM27	-145.8	157.4	-75.4	-28.6	18.9
	AMOEBA	-147.7	160.0	-80.1	-18.9	14.9
Val-Val-008	B3LYP/6-311++G(d,p)	-149.4	152.2	-85.0	77.4	--
	ABEEM	-149.4	149.1	-82.8	77.4	1.3
	OPLS/AA	-146.4	159.7	-78.6	72.5	5.5
	AMBER99sb	-147.8	152.5	-77.8	63.1	5.9
	CHARMM27	--	--	--	--	--
	AMOEBA	-145.6	160.0	-81.8	74.4	4.5
Val-Val-009	B3LYP/6-311++G(d,p)	-149.2	152.9	54.1	36.4	--
	ABEEM	-153.2	138.1	76.0	17.0	15.0
	OPLS/AA	--	--	--	--	--
	AMBER99sb	--	--	--	--	--
	CHARMM27	--	--	--	--	--
	AMOEBA	--	--	--	--	--
Val-Val-010	B3LYP/6-311++G(d,p)	-149.6	153.0	64.9	-39.3	--
	ABEEM	-152.7	142.1	79.8	-47.1	9.2
	OPLS/AA	-144.4	160.1	55.5	-49.7	8.0
	AMBER99sb	-147.2	151.6	55.4	-40.0	3.5
	CHARMM27	-140.4	150.6	59.6	-57.0	8.7
	AMOEBA	-140.0	159.1	66.0	-39.4	4.2
Val-Val-011	B3LYP/6-311++G(d,p)	-118.3	6.7	-155.5	-40.1	--
	ABEEM	-113.1	11.3	-159.3	-47.1	5.1
	OPLS/AA	--	--	--	--	--
	AMBER99sb	--	--	--	--	--
	CHARMM27	--	--	--	--	--
	AMOEBA	-80.4	-15.7	-162.1	-35.7	17.8
Val-Val-012	B3LYP/6-311++G(d,p)	-74.2	-13.5	-95.0	1.3	--
	ABEEM	-70.2	-14.2	-94.2	4.9	2.3
	OPLS/AA	--	--	--	--	--
	AMBER99sb	-60.5	-18.3	-75.6	-9.4	12.1
	CHARMM27	-62.0	-21.8	-75.2	-18.4	15.0
	AMOEBA	-73.5	-12.1	-80.6	-11.8	7.4
Val-Val-013	B3LYP/6-311++G(d,p)	-107.3	-4.3	-85.1	74.7	--
	ABEEM	-103.0	-1.1	-84.9	74.7	1.9
	OPLS/AA	-62.1	-41.0	-81.0	72.4	22.0
	AMBER99sb	--	--	--	--	--
	CHARMM27	--	--	--	--	--
	AMOEBA	--	--	--	--	--
Val-Val-014	B3LYP/6-311++G(d,p)	-102.0	-2.4	63.8	-41.4	--
	ABEEM	-91.4	-10.3	80.4	-50.4	11.0
	OPLS/AA	--	--	--	--	--
	AMBER99sb	--	--	--	--	--
	CHARMM27	-74.5	-28.6	57.3	-58.9	19.4

	AMOEBA	-79.2	-19.5	68.0	-41.3	11.0
Val-Val-015	B3LYP/6-311++G(d,p)	-82.5	69.4	-159.5	-33.3	--
	ABEEM	-82.3	70.8	-159.7	-34.5	0.7
	OPLS/AA	-74.6	73.5	-155.9	-43.8	6.5
	AMBER99sb	-75.8	56.5	-148.8	-21.0	10.7
	CHARMM27	-77.6	72.1	-149.8	-44.5	7.1
	AMOEBA	-77.0	65.4	-163.9	-31.4	3.9
Val-Val-016	B3LYP/6-311++G(d,p)	-150.8	155.2	-151.9	153.5	--
	ABEEM	-152.3	152.3	-150.6	148.9	2.6
	OPLS/AA	-147.2	161.5	-142.1	157.9	6.0
	AMBER99sb	-148.2	153.5	-145.8	151.1	3.2
	CHARMM27	-141.9	153.3	-135.4	151.3	7.4
	AMOEBA	--	--	--	--	--
Val-Val-017	B3LYP/6-311++G(d,p)	-85.7	74.5	-114.4	-1.2	--
	ABEEM	-84.6	72.7	-110.5	2.7	2.7
	OPLS/AA	-78.9	71.5	-71.6	-27.8	19.8
	AMBER99sb	--	--	--	--	--
	CHARMM27	-80.5	70.1	-85.2	-32.2	17.4
	AMOEBA	-79.0	66.5	-129.2	0.8	7.9
Val-Val-018	B3LYP/6-311++G(d,p)	-85.9	71.5	-86.9	74.6	--
	ABEEM	-81.7	70.2	-80.6	73.9	3.2
	OPLS/AA	-79.4	74.9	-77.4	68.4	6.4
	AMBER99sb	-78.3	67.1	-78.5	55.4	9.9
	CHARMM27	--	--	--	--	--
	AMOEBA	-80.3	53.6	-85.0	72.6	6.9
Val-Val-019	B3LYP/6-311++G(d,p)	-86.7	69.2	48.3	41.5	--
	ABEEM	-84.0	68.7	51.8	34.3	3.5
	OPLS/AA	--	--	--	--	--
	AMBER99sb	--	--	--	--	--
	CHARMM27	--	--	--	--	--
	AMOEBA	--	--	--	--	--
Val-Val-020	B3LYP/6-311++G(d,p)	-85.3	73.1	59.5	-41.0	--
	ABEEM	-83.8	66.4	74.5	-48.5	7.7
	OPLS/AA	-79.0	73.2	55.3	-51.2	5.2
	AMBER99sb	-79.6	64.4	54.8	-42.5	5.2
	CHARMM27	-81.7	75.1	59.4	-55.8	5.2
	AMOEBA	-79.3	77.5	70.6	-36.9	6.4
Val-Val-021	B3LYP/6-311++G(d,p)	55.1	32.8	-157.8	154.7	--
	ABEEM	72.5	22.0	-154.7	146.7	9.8
	OPLS/AA	38.9	51.6	-147.1	157.0	12.0
	AMBER99sb	--	--	--	--	--
	CHARMM27	--	--	--	--	--
	AMOEBA	--	--	--	--	--
Val-Val-022	B3LYP/6-311++G(d,p)	54.0	36.7	-89.3	75.2	--

	ABEEM	50.1	34.1	-84.4	74.8	2.9
	OPLS/AA	--	--	--	--	--
	AMBER99sb	--	--	--	--	--
	CHARMM27	--	--	--	--	--
	AMOEBA	57.7	32.3	-85.0	75.2	3.1
Val-Val-023	B3LYP/6-311++G(d,p)	48.1	42.8	46.5	37.6	--
	ABEEM	61.4	27.0	65.6	25.4	15.1
	OPLS/AA	--	--	--	--	--
	AMBER99sb	46.9	32.5	52.1	17.0	9.4
	CHARMM27	--	--	--	--	--
	AMOEBA	52.4	31.9	56.6	25.0	9.5
Val-Val-024	B3LYP/6-311++G(d,p)	53.0	42.6	63.6	-40.1	--
	ABEEM	78.1	11.1	88.9	-24.3	24.4
	OPLS/AA	--	--	--	--	--
	AMBER99sb	--	--	--	--	--
	CHARMM27	--	--	--	--	--
	AMOEBA	--	--	--	--	--
Val-Val-025	B3LYP/6-311++G(d,p)	56.4	-61.1	-117.5	-13.5	--
	ABEEM	69.5	-65.3	-117.7	-12.6	4.6
	OPLS/AA	41.6	-92.9	-75.2	-24.6	25.1
	AMBER99sb	51.8	-52.3	-138.3	-14.7	8.9
	CHARMM27	52.1	-71.5	-89.0	-28.1	14.4
	AMOEBA	62.0	-47.2	-143.8	-9.1	12.5
Val-Val-026	B3LYP/6-311++G(d,p)	64.3	-45.0	-84.2	75.6	--
	ABEEM	76.8	-50.6	-81.7	75.0	5.3
	OPLS/AA	56.9	-55.0	-79.3	73.8	6.0
	AMBER99sb	55.6	-40.2	-79.5	61.3	8.2
	CHARMM27	59.4	-54.9	-81.8	75.3	4.4
	AMOEBA	64.6	-44.5	-81.3	74.4	1.2
Val-Val-027	B3LYP/6-311++G(d,p)	65.7	-36.7	-95.3	-8.5	--
	ABEEM	78.0	-48.6	-88.7	-6.3	8.3
	OPLS/AA	--	--	--	--	--
	AMBER99sb	--	--	--	--	--
	CHARMM27	--	--	--	--	--
	AMOEBA	--	--	--	--	--
Val-Val-028	B3LYP/6-311++G(d,p)	63.5	-46.6	50.6	42.9	--
	ABEEM	78.2	-56.6	58.4	34.8	10.1
	OPLS/AA	--	--	--	--	--
	AMBER99sb	--	--	--	--	--
	CHARMM27	--	--	--	--	--
	AMOEBA	67.7	-27.1	64.4	30.6	12.5

Ab initio method obtains 28 Val-tripeptide stable structures, and ABEEM, OPLS/AA,

AMBER99sb, CHARMM27 and AMOEBA obtain 28, 13, 13, 11 and 19 stable structures, respectively. And the MAD values from each force field are 6.7°, 10.7°, 7.1°, 11.7° and 7.7°. But if considering all 28 structures, the MAD values increase obviously except ABEEM. And the values are 6.7°, 29.7°, 18.1°, 25.5° and 13.9°. These increases demonstrate the missing of stable conformations, and the torsions show the preference of each method.

Table S11 The MAD (°) of χ_1 at side chain of all Val conformations by force fields

		ABEEM	OPLS/AA	AMBER99sb	CHARMM27	AMOEBA
Dipeptide		7.0	8.7	4.4	4.8	8.0
Tripeptide	N-terminal	2.5	6.2	3.5	4.5	8.0
	C-terminal	2.8	6.6	4.4	5.4	8.5
	Total	2.6	6.4	3.9	5.0	8.3

Val contains one dihedral angle at side chain as χ_1 and χ_1 and backbone torsions limit each other in torsion rotation. Because of the distributions of χ_1 are concentrated in a narrow range, so all force fields reproduce it with deviation value less than 10°.

Table S12 The energy ΔE values (kcal/mol) of all Ala conformations obtained by MP2/6-311++G(d,p), ABEEM, OPLS/AA, AMBER99sb, CHARMM27 and AMOEBA and RMSD values (kcal/mol) by each FF compared with those of MP2/6-311++G(d,p)

Structure		MP2/6-311++G(d,p)	ABEEM	OPLS/AA	AMBER99sb	CHARMM27	AMOEBA
Gly	g01	0.0000	0.0000	1.7864	0.6944	0.2633	0.0001
	g02	2.6703	2.6523	1.7864	0.6944	0.0001	2.1626
	g03	2.6760	2.6556	1.7864	0.6944	0.0000	2.1626
	g04	0.0000	0.0000	1.7864	0.6944	0.2632	0.0000
	g05	2.1592	2.1387	0.0000	0.0000	0.9376	1.1400
	RMSD	--	0.0152	1.5885	1.6406	1.7845	0.5586
Val	v01	4.1589	4.8537	5.4141	4.0159	3.9461	3.6558
	v02	2.9508	4.6465	1.9105	3.2877	3.0938	1.9579
	v03	4.8726	5.9602	8.2644	3.2877	4.7530	6.1293
	v04	6.3364	6.4039	1.9105	4.0158	3.9461	6.3855
	v05	0.5799	0.8088	1.9104	3.2878	0.8684	0.0000
	v06	0.0000	0.0000	0.0000	0.0000	0.0000	1.7678
	RMSD	--	0.8754	2.4331	1.6002	0.9897	1.0232

Table S13 The energy ΔE (kcal/mol) of Ala stable conformations obtained by MP2/6-311++G(d,p), ABEEM, OPLS/AA, AMBER99sb, CHARMM27, and AMOEBA

Structure		ΔE					
		MP2/6-311++G(d,p)	ABEEM	OPLS/AA	AMBER99sb	CHARMM27	AMOEBA
Ala	a01	2.1994	2.0834	3.3527	2.9429	2.0539	2.4737
	a02	6.0117	5.6330	--	9.2027	--	5.5573
	a03	3.0867	2.8260	--	--	--	2.7775
	a04	0.0000	0.0000	0.6968	1.6274	0.0000	0.0000
	a05	4.5334	4.3949	9.2528	--	--	4.4133
	a06	1.6670	1.9619	0.0000	0.0000	0.9164	1.1977
Gly	g01	0.0000	0.0000	1.7864	0.6944	0.2633	0.0001
	g02	2.6703	2.6523	--	--	0.0001	2.1626
	g03	2.6760	2.6556	--	--	0.0000	2.1626
	g04	0.0000	0.0000	1.7864	0.6944	0.2632	0.0000
	g05	2.1592	2.1387	0.0000	0.0000	0.9376	1.1400
Val	v01	4.1589	4.8537	5.4141	4.0159	3.9461	3.6558
	v02	2.9508	4.6465	--	--	--	--
	v03	4.8726	5.9602	8.2644	--	4.7530	6.1293
	v04	6.3364	6.4039	--	--	--	6.3855
	v05	0.5799	0.8088	1.9104	3.2878	0.8684	0.0000
	v06	0.0000	0.0000	0.0000	0.0000	0.0000	1.7678

Table S14 The backbone distribution of Gly-dipeptide and tripeptide in Ramachandran map from B3LYP/6-311++G(d,p) and each force field after and before classified (after classified / before classified)

	B3LYP/6-311++G(d,p)		ABEEM		OPLS/AA		AMBER99sb		CHARMM27		AMOEBA	
	Di	Tri	Di	Tri	Di	Tri	Di	Tri	Di	Tri	Di	Tri
β_L-1	0	5	0	4	1/1	1/1	0/0	2/3	1/1	2/3	0/0	1/1
β_L-2	1	1	1	2	0/0	1/2	0/0	0/0	0/0	1/2	0/0	2/2
β_L-3	0	0	0	1	0/0	1/2	1/1	0/1	0/0	1/2	1/1	4/4
β_L-4	0	4	0	3	0/0	1/1	0/0	2/3	0/0	2/3	0/0	1/1
ε_L-1	0	0	0	0	0/0	0/2	0/0	0/3	0/0	0/0	0/0	0/1
ε_D-2	0	0	0	0	0/0	0/2	0/0	0/1	0/0	0/0	0/0	0/1
δ_L-1	0	0	0	1	0/0	0/0	0/0	0/0	0/0	0/1	0/0	0/1
δ_D-2	0	0	0	1	0/0	0/0	0/0	0/0	0/0	0/1	0/0	1/1
γ_L	2	19	2	18	1/2	5/19	1/2	5/17	1/2	6/19	2/2	15/18
α_D	0	1	0	1	0/0	0/1	0/0	2/2	0/0	0/0	0/0	1/1
α_L	0	1	0	1	0/0	0/1	0/0	2/2	0/0	0/0	0/0	1/1
γ_D	2	19	2	18	1/2	5/19	1/2	5/18	1/2	6/19	2/2	16/18

Table S15 The backbone distribution of Val-dipeptide and tripeptide in Ramachandran map from B3LYP/6-311++G(d,p) and each force field after and before

classified (after classified / before classified)

	B3LYP/6-311++G(d,p)		ABEEM		OPLS/AA		AMBER99sb		CHARMM27		AMOEBA	
	Di	Tri	Di	Tri	Di	Tri	Di	Tri	Di	Tri	Di	Tri
β_L-1	1	9	1	9	1/1	6/12	1/1	5/8	1/1	4/6	1/1	4/5
ε_L-1	0	0	0	0	0/0	0/6	0/0	0/3	0/0	0/8	0/0	0/5
δ_L-1	0	0	0	0	0/0	0/0	0/0	0/0	0/0	0/0	0/0	1/1
δ_D-1	1	9	1	9	1/1	3/8	0/0	6/9	1/1	3/6	1/1	8/11
γ_L	2	15	2	16	1/3	8/13	1/3	6/15	1/1	4/7	1/1	9/11
α_D	1	8	1	8	0/0	1/2	0/0	2/2	0/0	0/0	1/1	4/6
α_L	0	6	0	5	0/0	3/6	0/0	2/4	0/1	6/13	0/1	5/6
γ_D	1	9	1	9	1/1	5/9	1/2	5/15	1/2	5/16	1/1	7/11

In Table S14 and S15, the distribution of Gly and Val-dipeptide and tripeptide are obvious, and the preference of different methods in various regions is depicted.

Table S16 The $^3J(H_N,H_\alpha)$ (Hz) of the central residue of Ala tetrapeptide under different temperature (K)

Temperautre	ABEEM
280	5.61
300	6.01
311	6.43
320	6.85
345	7.15
360	7.28

Table S17 The *J*-coupling constants (Hz) of residues in $(Ala)_4$ obtained by dynamic and NMR

Residue	*J*-coupling type	ABEEM	Exp.
Ala-2	$^3J(H_N,H_\alpha)$	6.06	5.62
Ala-2	$^3J(H_N,C')$	1.02	1.15
Ala-2	$^3J(H_\alpha,C')$	1.59	1.87
Ala-2	$^3J(C',C')$	0.46	0.19
Ala-2	$^3J(H_N,C_\beta)$	2.26	2.36
Ala-2	$^1J(N,C_\alpha)$	10.78	11.39
Ala-2	$^2J(N,C_\alpha)$	8.17	9.17
Ala-2	$^3J(H_N,C_\alpha)$	0.67	0.68
Ala-3	$^3J(H_N,H_\alpha)$	6.16	5.89
Ala-3	$^3J(H_N,C')$	1.01	1.11
Ala-3	$^3J(H_\alpha,C')$	1.62	1.95
Ala-3	$^3J(H_N,C_\beta)$	2.25	2.24
Ala-3	$^2J(N,C_\alpha)$	8.52	8.56

Ala-3	$^{3}J(H_N,C_\alpha)$	0.67	0.60
Ala-4	$^{3}J(H_N,H_\alpha)$	7.40	6.56
Ala-4	$^{3}J(H_N,C_\beta)$	1.97	2.24
Ala-4	$^{1}J(N,C_\alpha)$	11.85	11.53
Ala-4	$^{2}J(N,C_\alpha)$	7.98	8.37
Ala-4	$^{3}J(H_N,C_\alpha)$	0.77	0.60
MAD	--	0.30	--
RMSD	--	0.27	--

Table S18 The *J*-coupling constants (Hz) of residues in $(Ala)_6$ obtained by dynamic and NMR

Residue	*J*-coupling type	ABEEM	Exp.
Ala-2	$^{3}J(H_N,H_\alpha)$	6.20	5.60
Ala-2	$^{3}J(H_N,C')$	1.00	1.13
Ala-2	$^{3}J(H_\alpha,C')$	1.63	1.81
Ala-2	$^{3}J(H_N,C_\beta)$	2.24	2.33
Ala-2	$^{3}J(H_N,C_\alpha)$	0.47	0.66
Ala-3	$^{3}J(H_N,H_\alpha)$	5.29	5.67
Ala-3	$^{3}J(H_N,C')$	1.19	1.20
Ala-3	$^{3}J(H_\alpha,C')$	1.40	1.79
Ala-3	$^{3}J(H_N,C_\beta)$	2.37	2.23
Ala-3	$^{1}J(N,C_\alpha)$	10.04	11.26
Ala-3	$^{3}J(H_N,C_\alpha)$	0.67	0.59
Ala-4	$^{3}J(H_N,H_\alpha)$	6.32	5.80
Ala-4	$^{3}J(H_N,C')$	0.98	1.22
Ala-4	$^{3}J(H_\alpha,C')$	1.66	1.73
Ala-4	$^{3}J(H_N,C_\beta)$	2.22	2.18
Ala-4	$^{1}J(N,C_\alpha)$	10.22	11.27
Ala-4	$^{3}J(H_N,C_\alpha)$	0.23	0.54
Ala-5	$^{3}J(H_N,H_\alpha)$	6.29	6.02
Ala-5	$^{3}J(H_N,C')$	0.98	1.05
Ala-5	$^{3}J(H_\alpha,C')$	1.65	1.99
Ala-5	$^{3}J(H_N,C_\beta)$	2.23	2.20
Ala-5	$^{3}J(H_N,C_\alpha)$	0.31	0.53
Ala-6	$^{3}J(H_N,H_\alpha)$	6.36	6.59
Ala-6	$^{3}J(H_N,C')$	0.98	1.29
Ala-6	$^{3}J(H_N,C_\beta)$	1.68	2.23
Ala-6	$^{1}J(N,C_\alpha)$	2.21	1.94
Ala-6	$^{2}J(N,C_\alpha)$	7.79	8.18
Ala-6	$^{3}J(H_N,C_\alpha)$	0.66	0.62
MAD	--	0.30	--
RMSD	--	0.27	--

Table S19 The *J*-coupling constants (Hz) of residues in $(Ala)_7$ obtained by dynamic and NMR

Residue	*J*-coupling type	ABEEM	Exp.
Ala-2	$^3J(H_N,H_\alpha)$	6.64	5.61
Ala-2	$^3J(H_N,C')$	0.94	1.15
Ala-2	$^3J(H_\alpha,C')$	1.75	1.89
Ala-2	$^3J(H_N,C_\beta)$	2.16	2.31
Ala-2	$^1J(N,C_\alpha)$	9.54	11.37
Ala-2	$^2J(N,C_\alpha)$	8.57	9.17
Ala-2	$^3J(H_N,C_\alpha)$	0.67	0.71
Ala-3	$^3J(H_N,H_\alpha)$	7.03	5.66
Ala-3	$^3J(H_N,C')$	0.90	1.20
Ala-3	$^3J(H_\alpha,C')$	1.86	1.85
Ala-3	$^3J(H_N,C_\beta)$	2.07	2.20
Ala-3	$^1J(N,C_\alpha)$	10.23	11.27
Ala-3	$^2J(N,C_\alpha)$	7.84	8.52
Ala-3	$^3J(H_N,C_\alpha)$	0.67	0.66
Ala-4	$^3J(H_N,H_\alpha)$	6.42	5.77
Ala-4	$^3J(H_N,C_\beta)$	2.20	2.23
Ala-4	$^1J(N,C_\alpha)$	11.61	11.22
Ala-4	$^2J(N,C_\alpha)$	8.35	8.29
Ala-4	$^3J(H_N,C_\alpha)$	0.68	0.56
Ala-5	$^3J(H_N,H_\alpha)$	6.46	5.92
Ala-5	$^3J(H_N,C')$	0.96	1.19
Ala-5	$^3J(H_\alpha,C')$	1.70	1.56
Ala-5	$^3J(H_N,C_\beta)$	2.19	2.23
Ala-5	$^1J(N,C_\alpha)$	11.07	11.29
Ala-5	$^2J(N,C_\alpha)$	8.67	8.22
Ala-6	$^3J(H_N,C')$	0.88	1.10
Ala-6	$^3J(H_\alpha,C')$	2.12	1.67
Ala-6	$^3J(H_N,C_\beta)$	1.84	2.21
Ala-6	$^2J(N,C_\alpha)$	8.60	8.24
Ala-7	$^3J(H_N,H_\alpha)$	6.78	6.60
Ala-7	$^3J(H_N,C')$	0.92	1.25
Ala-7	$^3J(H_N,C_\beta)$	1.79	2.03
Ala-7	$^1J(N,C_\alpha)$	2.13	1.99
Ala-7	$^2J(N,C_\alpha)$	10.56	11.51
Ala-7	$^3J(H_N,C_\alpha)$	0.48	0.59
MAD	--	0.39	--
RMSD	--	0.41	--

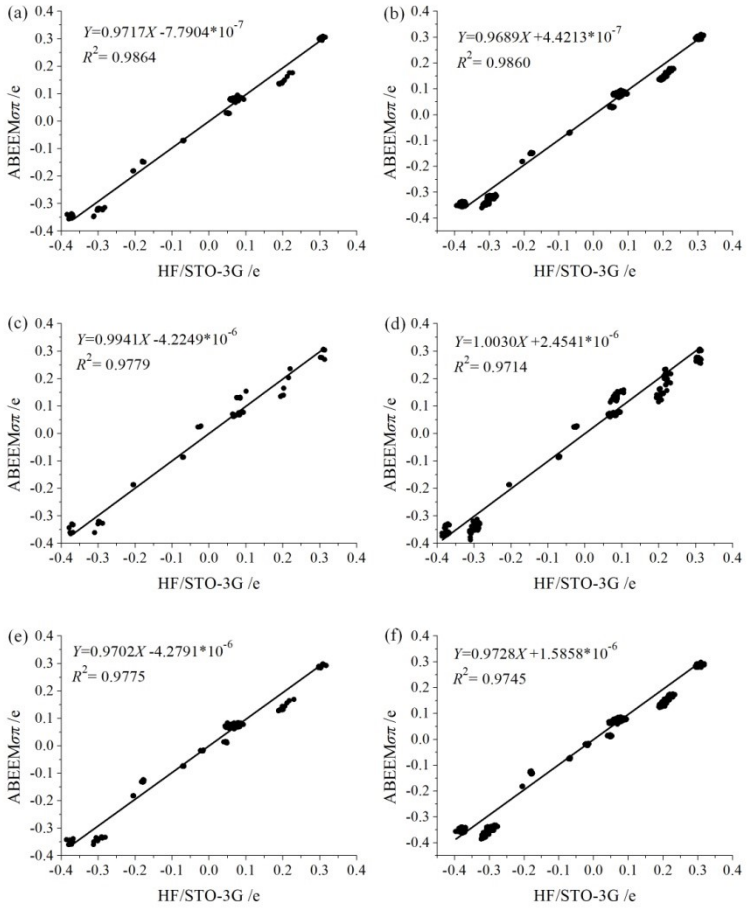

Fig. S1 A comparison of charge distributions obtained from the ABEEM method and the *ab initio* HF/STO-3G method. (a) Ala-dipeptides; (b)Ala-tripeptides; (c)Gly-dipeptides; (d) Gly-tripeptides; (e) Val-dipeptides; (f) Val-tripeptides

The partial charge of each atom in Ala, Gly, Val dipeptides and tripeptides obtained from ABEEM method is consistent with the results from HF/STO-3G based on the good transferability of parameters among different kinds peptides.

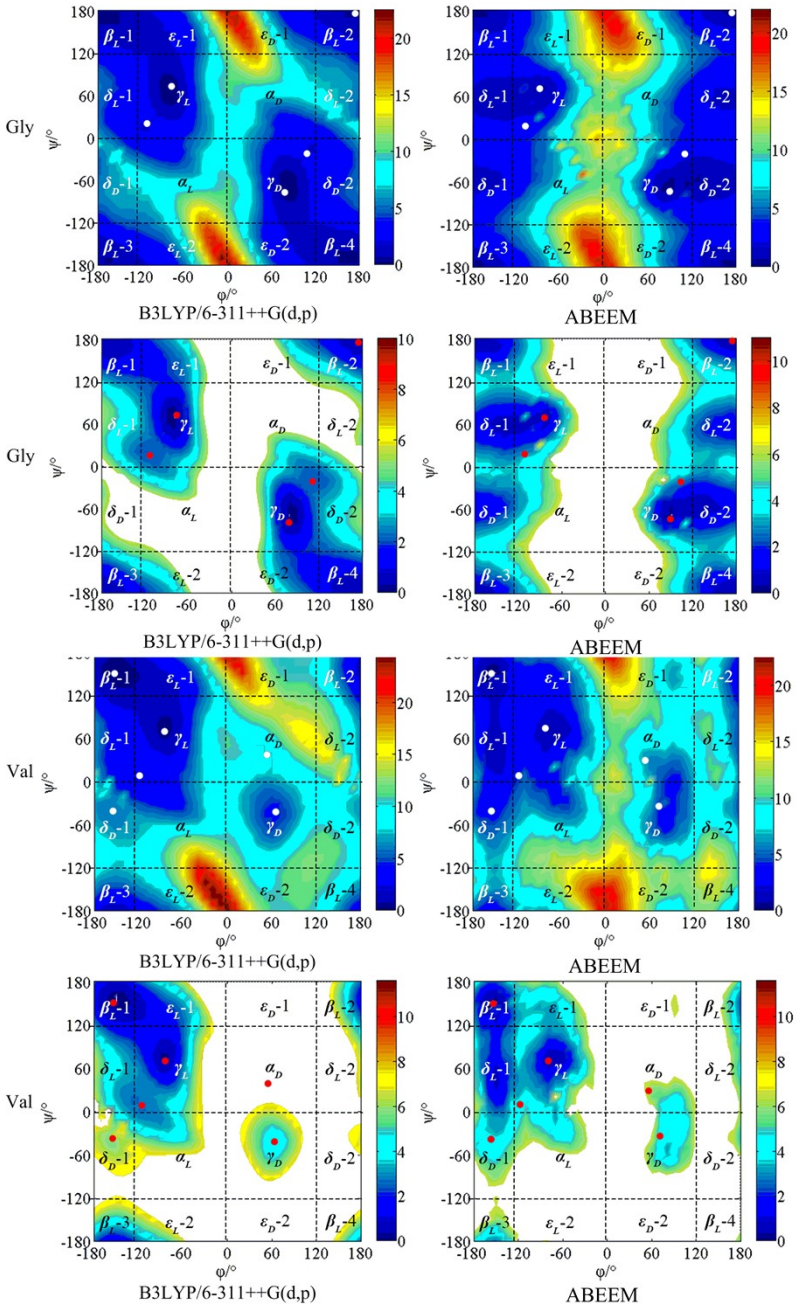

Fig. S2 Lower energy areas and stable conformations by B3LYP/6-311++G(d,p) and ABEEM polarizable force field

Figure S2 shows the lower energy area in PES of Gly and Val-dipeptide from B3LYP/6-311++G(d,p) and ABEEM polarizable force field. The distribution is similar with the favorable regions in Ramachandran map. Note that all local minima locate in the lower energy domain in the PES by ABEEM polarizable force field. The widespread area in Gly means the flexibility of its conformation, which consists well with the data from coil library.

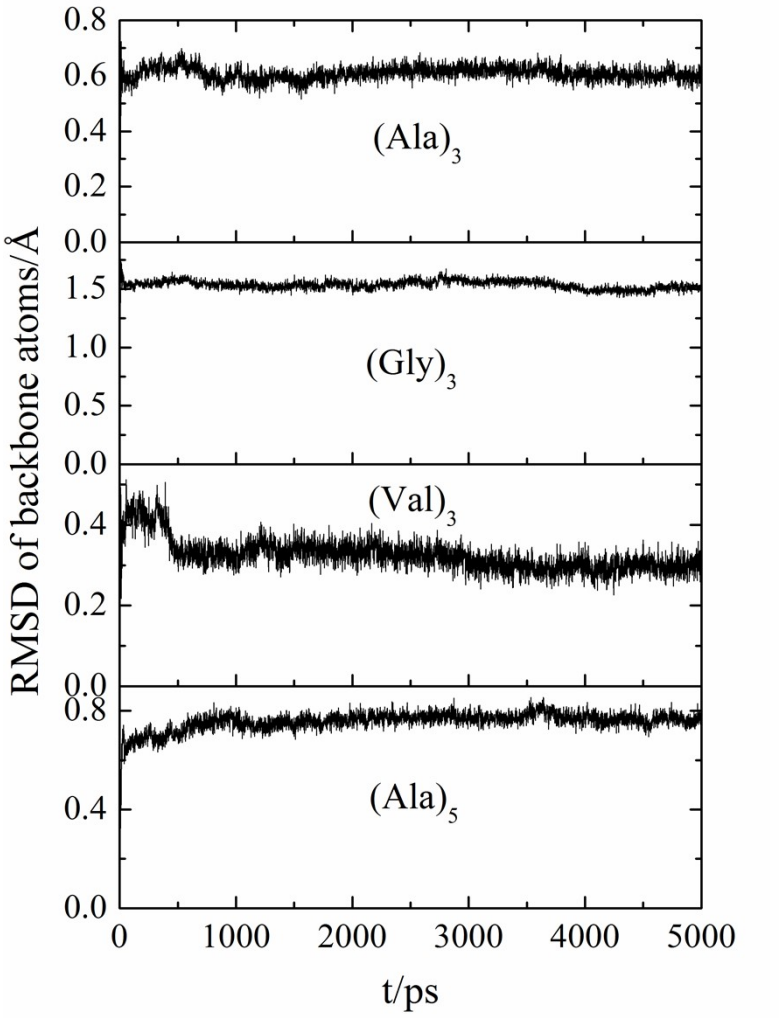

Fig. S3 RMSD of backbone atoms from dynamic simulations of $(Ala)_3$, $(Gly)_3$, $(Val)_3$ and $(Ala)_5$

For each simulation, a dynamic equilibrium of 1000 ps was carried out, followed by a dynamic simulation of 4000 ps. For $(Ala)_3$, $(Val)_3$ and $(Ala)_5$, the system achieve dynamic equilibrium after 750ps, 500ps and 800ps, so a dynamic equilibrium of 1000 ps is enough, and the results from followed dynamic are credible.

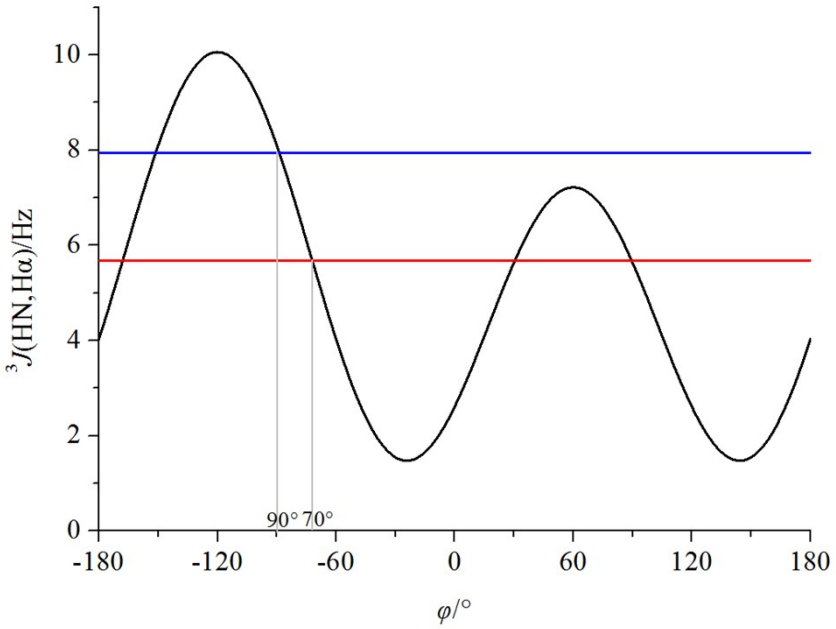

Fig. S4 Karplus curve (black line) of the measured *J*-coupling constant $^3J(H_N,H_\alpha)$ for center residue of $(Ala)_3$ (red line) and $(Val)_3$ (blue line) from conformations derived from MD simulation by ABEEM polarizable force field

$^3J(H_N,H_\alpha)$ is the most sensitive value measured by φ. $R2_{A3}$ and $R2_{V3}$ differs with more than 2 Hz with only 20° difference of φ.