Supporting Information for: "Optimization of the additive CHARMM all-atom protein force field targeting improved sampling of the backbone ϕ, ψ and sidechain χ_1 and χ_2 dihedral angles."

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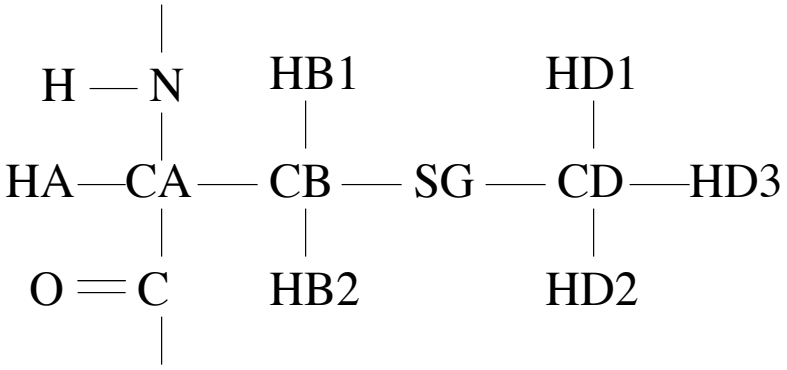

Figure S1) Covalent structure of the modified CME residue (see SI TableS1 for the parameters).

Figure S2) RMS difference of the individual helicies of the dimeric coiled-coil 1u0i as a function of simulation time. Results are for the backbone (N, Ca, C, O) atoms following least squares alignment of the backbone atoms of the individual helicies, with results presented for the helix being aligned to itself (ie. Helix A vs Helix A) or for the second helix based on alignment to the first (ie. Helix B vs Helix A). Results are presented for alignment to helix A (A) or helix B (B). The N- and C-terminal residues were excluded from the analysis.

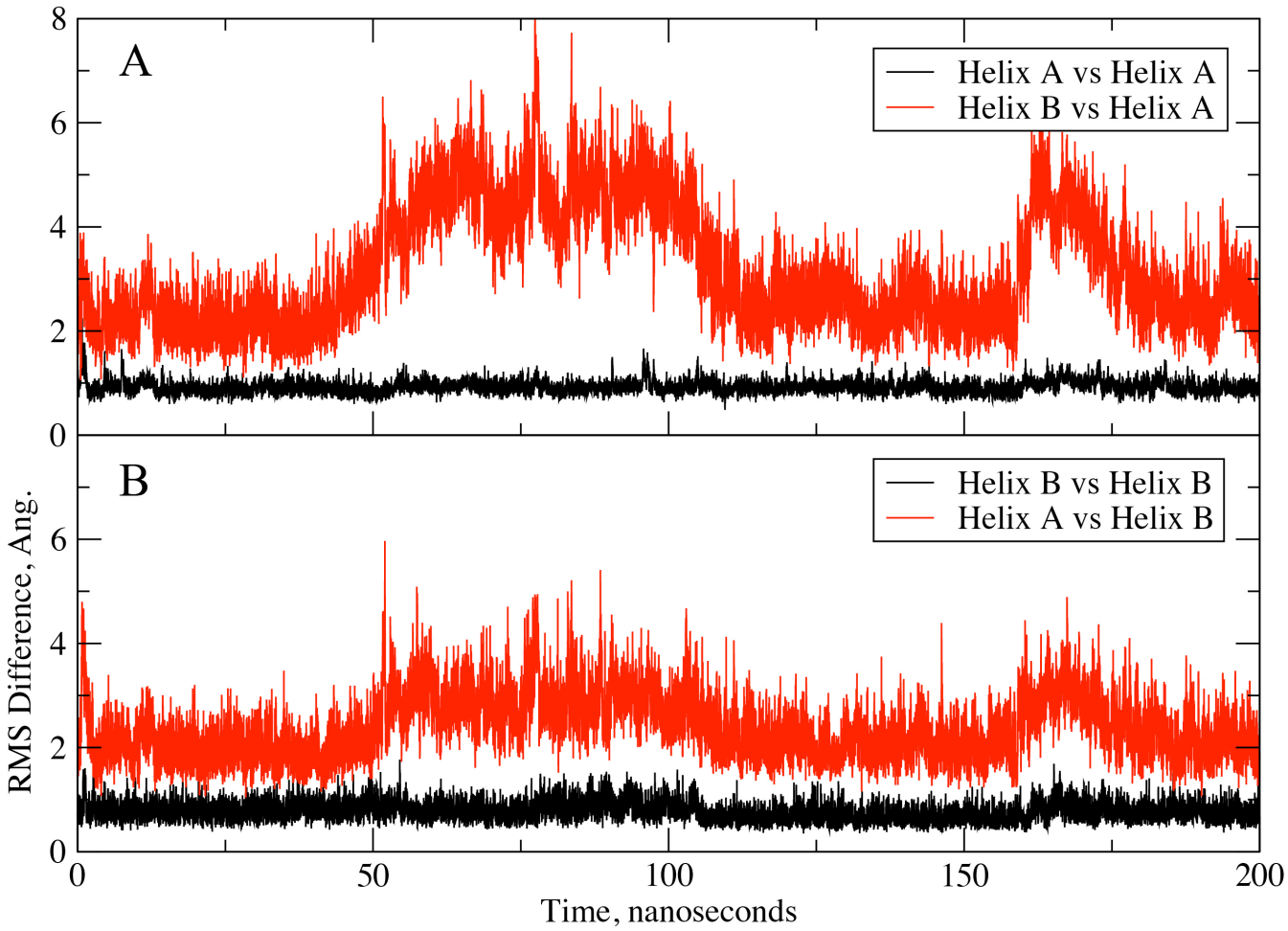

Table S1) Additional parameters for the S-methylated cysteine (CME) residue in HEWL19. Atom types and charges are given in upper part and torsion angle parameters are given in the lower part. The torsion potential has the form: $V_n(\chi) = k_n(1 + \cos[n\chi - \delta_n])$ where k_n is a force constant, δ_n is a phase shift, and n the multiplicity. All other parameter values were taken from the standard C36 force-fields. Figure S1 shows the structure of the residue.

Atom	CHARMM Atom Type	Charge (e)
N	NH1	-0.47
H	H	0.31
CA	CT1	-0.07
HA	HB1	0.09
CB	CT2	-0.11
HB1	HA2	0.09
HB2	HA2	0.09
SG	S	-0.23
CD	CT3	-0.11
HD1	HA3	0.09
HD2	HA3	0.09
HD3	HA3	0.09
C	C	0.51
O	O	-0.51

ATOM 1	ATOM 2	ATOM 3	ATOM 4	n	k_n [kcal/mol]	δ_n
CT3	S	CT2	CT1	1	0.24	180.0°
CT3	S	CT2	CT1	3	0.37	0.0°

Table S2) Distances used for water deletion, simulation temperatures, experimental protein crystal lattice distances and average percent changes for the lattice distances for the full unit-cell crystal simulations.

PDB	Water	T(K)	Crystallographic			C22/CMAP			C36		
ID	del (Å)[1]		A	B	C	ΔA (%)	ΔB	ΔC	ΔA	ΔB	ΔC
135L	2.82	298	38.59	32.89	48.37	1.46	0.39	3.58	1.55	1.51	2.47
3EBX	4.00	298	52.19	47.49	21.49	5.10	1.09	0.91	6.00	3.62	-0.70
1EJG	3.20	100	40.83	18.51	22.34	-0.75	0.30	0.17	0.05	-0.19	0.14
1I27	3.50	282	29.42	44.34	49.20	1.72	3.83	1.70	2.82	2.13	1.17
5PTI	3.50	298	71.88	25.14	28.89	-2.05	3.94	-0.19	-0.43	3.41	-0.79
3ICB	2.78	298	53.32	43.94	29.95	-4.15	0.87	2.60	-1.27	0.80	0.43
1BYI	2.85	100	72.53	47.73	61.58	-0.57	0.34	2.40	0.00	0.02	0.77
1BZP	3.10	298	36.68	30.60	68.22	2.54	0.20	7.63	4.13	-1.74	10.58

Lattice parameters (Å) were calculated by averaging over all snapshots at 5ps intervals within the last 35ns of the 40ns crystal simulations. 1) Water O to protein non-hydrogen distance used for the deletion of water molecules during preparation of the crystal for MD simulations.

Table S3) Estimated uncertainty for predictions of scalar couplings from various Karplus equation parametrizations and for predictions of chemical shifts by SPARTA+. In most cases, the RMSD between experimental and predicted observables reported by the original authors was used (since the same data were often used in the parameter fitting, this value of σ should be considered a lower bound). Deviations reported by Hu and Bax were absolute deviations, and have therefore been increased by 30% to approximate mean-square deviations.[1] Deviations from the data of Ding and Gronenborn[2] and Hennig *et al*.[3] were computed directly from the experimental and predicted couplings in those papers. The value of σ for prediction of C' chemical shifts is one case in which the data used in the test were not included in the optimization of the method.[4]

Parameter	**σ**	**Source**
Backbone J-Couplings		
$^3J_{HNHA}$	0.91 Hz	Hu and Bax[1]
$^3J_{HNC}$	0.59 Hz	Hu and Bax[1]
$^3J_{HAC}$	0.38 Hz	Hu and Bax[1]
$^3J_{CC}$	0.22 Hz	Hu and Bax[1]
$^3J_{HNCB}$	0.39 Hz	Hu and Bax[1]
$^1J_{NCA}$	0.59 Hz	Ding and Gronenborn[2]
$^2J_{NCA}$	0.50 Hz	Ding and Gronenborn[2]
$^3J_{NCA}$	0.10 Hz	Hennig *et al*.[3]
Side-chain J-Couplings		
$^3J_{NCG}$ (Thr)	0.21 Hz	Chou and Bax[5]
$^3J_{CCG}$ (Thr)	0.21 Hz	Chou and Bax[5]
$^3J_{NCG}$ (Ile,Val)	0.25 Hz	Chou and Bax[5]
$^3J_{CCG}$ (Ile,Val)	0.25 Hz	Chou and Bax[5]
$^3J_{HAHB}$	0.31 Hz	Perez *et al*.[6]
$^3J_{NHB}$	0.41 Hz	Perez *et al*.[6]
$^3J_{CHB}$	0.47 Hz	Perez *et al*.[6]
$^3J_{HACG}$	0.33 Hz	Perez *et al*.[6]
$^3J_{NCG}$	0.18 Hz	Perez *et al*.[6]
$^3J_{CCG}$	0.36 Hz	Perez *et al*.[6]
Chemical Shifts		
C' Shifts	1.09 p.p.m.	Shen and Bax[4]

Table S4) Sidechain dihedral parameter definitions.

Residue	χ^1				$\chi^{1'}$				χ^2				$\chi^{2'}$			
Ile	NH1/C	CT1	CT1	CT2	NH1/C	CT1	CT1	CT3	CT1	CT1	CT2	CT3				
Val	NH1/C	CT1	CT1	CT3												
Thr	NH1/C	CT1	CT1	OH1	NH1/C	CT1	CT1	CT3	CT1	CT1	OH1	H				
Leu	NH1/C	CT1	CT2	CT1					CT1	CT2	CT1	CT3				
Lys	NH1/C	CT1	CT2	CT2					CT1	CT2	CT2	CT2				
Arg	NH1/C	CT1	CT2	CT2					CT1	CT2	CT2	CT2				
Gln	NH1/C	CT1	CT2	CT2					CT1	CT2	CT2	CC				
Met	NH1/C	CT1	CT2	CT2					CT1	CT2	CT2	S				
Phe	NH1/C	CT1	CT2	CA					CT1	CT2	CA	CA				
Tyr	NH1/C	CT1	CT2	CA					CT1	CT2	CA	CA				
Asn	NH1/C	CT1	CT2	CC					CT1	CT2	CC	NH2	CT1	CT2	CC	O
Asp	NH1/C	CT1	CT2A	CC					CT1	CT2A	CC	OC				
Trp	NH1/C	CT1	CT2	CY					CT1	CT2	CY	CA	CT1	CT2	CY	CPT
Hsd/Hse	NH1/C	CT1	CT2	CPH1					CT1	CT2	CPH1	CPH1	CT1	CT2	CPH1	NR
Hsp	NH1/C	CT1	CT2A	CPH1					CT1	CT2A	CPH1	CPH1	CT1	CT2A	CPH1	NR
Ser	NH1/C	CT1	CT2	OH1					CT1	CT2	OH1	H				
Glu	NH1/C	CT1	CT2A	CT2					CT1	CT2A	CT2	CC				
Cys	NH1/C	CT1	CT2	S					CT1	CT2	S	HS				
Ala/Gly	-	-	-	-												
Pro	-	-	-	-												

*Boxed parameters are shared by two or more residues; NR1 (HSD), NR2 (HSE) Atom type CT2A created for Cb atom of Glu and Hsp to differentiate those parameters from Lys/Arg/Gln/Met and Hsd/Hse sets, respectively

Table S5) Differences in relative energy of local minima between C22/CMAP and QM calculations.

Residue \ Rotamer	tt	tm	tp	mt	mm	mp	pt	pm	pp	RMSD
					Alpha					
Arg	2.94	5.12	1.65	2.77	1.54	6.40	5.57	10.70	7.74	5.72
Asn	3.68	1.75	-0.03	2.29	-2.07	1.64	-0.93	3.01	-0.53	2.08
Asp	2.29	2.58	0.84	2.07	-2.66	0.42	0.40	-1.12	-3.40	2.03
Cys	1.23	1.15	0.53	-0.16	0.97	0.19	-2.23	-0.53	0.43	1.03
Gln	1.70	4.27	0.86	-0.04	0.40	2.12	-0.24	4.20	0.92	2.24
Glu	-1.42	12.93	7.33	-2.04	4.51	2.03	-3.11	-1.31	4.51	5.61
Hsd	2.93	2.00	3.26	0.15	1.72	1.87	1.87	0.18	-0.68	1.93
Hse	7.33	5.06	3.81	5.30	1.28	4.09	1.11	2.74	1.06	4.08
Hsp	8.99	2.42	4.46	6.20	4.28	5.61	16.15	10.68	7.43	8.33
Ile	0.80	2.51	1.32	0.79	1.13	1.01	-0.53	-0.72	-0.87	1.21
Leu	3.43	3.14	1.98	0.91	0.28	0.56	0.78	0.12	0.36	1.75
Lys	3.97	6.00	1.71	3.54	1.96	7.35	6.03	11.95	9.38	6.60
Met	0.88	4.03	1.52	-0.51	1.60	1.38	0.24	1.59	-2.68	1.94
Phe	1.96	2.78	1.44	0.17	0.34	-0.01	-1.42	-0.28	0.19	1.33
Ser	1.37	2.16	1.46	-0.33	0.01	0.56	-2.99	-1.45	1.27	1.55
Thr	0.94	1.63	0.94	0.67	1.07	1.13	-3.76	-1.97	0.05	1.68
Trp	1.11	0.83	0.63	1.00	-0.55	-1.16	-1.60	-1.82	-1.79	1.25
Tyr	1.73	3.12	1.80	0.45	0.95	0.06	-0.79	-0.25	0.67	1.42
Val	0.98				-0.08				1.13	0.86
AVG	2.47	3.53	1.97	1.29	0.88	1.96	0.81	1.98	1.33	
RMSD	3.39	4.42	2.61	2.40	1.90	3.02	4.58	4.84	3.65	
AVG(Alpha)					1.80					
RMSD(Alpha)					3.55					
					Beta					
Arg	0.95	2.36	1.75	1.15	1.58	3.08	1.39	3.71	2.00	2.17
Asn	0.26	-0.23	-0.37	-0.07	-2.93	-0.73	-0.76	0.45	-2.49	1.35
Asp	4.78	4.49	2.55	4.46	1.08	2.96	2.86	4.29	-0.98	3.45
Cys	-1.79	-0.19	0.56	-1.93	-1.22	-1.23	-2.48	-1.82	-1.38	1.55
Gln	-1.03	1.95	0.56	-1.08	-0.53	2.32	-1.10	1.62	0.23	1.33
Glu	0.33	11.96	3.56	-0.37	3.81	8.45	-0.76	7.62	9.33	6.56
Hsd	0.60	-0.28	0.33	0.55	-0.20	0.06	-0.11	0.56	-1.40	0.59
Hse	3.21	2.53	3.54	4.73	1.85	2.30	3.92	3.19	1.26	3.12
Hsp	6.42	1.42	2.33	5.52	1.22	1.32	5.55	3.03	-0.45	3.69
Ile	-0.25	0.86	-0.92	-0.24	0.00	1.42	-0.63	-0.05	0.42	0.69
Leu	1.39	0.56	-0.38	0.22	0.71	1.10	0.27	0.53	0.46	0.72
Lys	1.43	3.65	2.91	2.13	2.47	4.49	2.18	4.83	2.98	3.19
Met	-1.05	2.16	-0.34	-0.89	0.29	-1.14	-0.79	0.48	-3.12	1.44
Phe	-0.27	0.94	-0.10	0.16	-1.24	0.09	-1.32	0.11	-0.57	0.72
Ser	-2.81	-1.37	-0.18	-2.54	-1.18	-0.85	-2.03	0.20	-0.06	1.58
Thr	-2.40	-1.30	0.05	-2.59	-0.94	-1.11	-1.82	0.21	-0.17	1.48
Trp	-1.50	-1.26	-0.79	0.51	-1.80	-1.23	-0.44	-1.30	-2.39	1.38
Tyr	-0.14	1.09	-0.22	0.05	-1.04	0.16	-1.45	-0.12	-0.20	0.71
Val	0.00				1.91				-0.20	1.11
AVG	0.43	1.63	0.82	0.54	0.20	1.19	0.14	1.53	0.17	
RMSD	2.31	3.39	1.69	2.34	1.65	2.71	2.14	2.81	2.61	
AVG(Beta)					0.74					
RMSD(Beta)					2.46					
					AlphaL					
Arg	3.04	4.07	4.42	2.18	4.49	3.72	1.00	4.02	0.00	3.35
Asn	3.77	1.50	5.01	0.79	2.50	0.83	7.06	1.02	1.06	3.35
Asp	8.59	6.46	7.91	5.22	2.10	4.82	15.93	13.53	12.02	9.51

Cys	0.75	0.80	1.62	0.29	2.83	2.02	3.65	1.23	2.42	2.02
Gln	2.56	5.68	4.94	0.67	3.22	3.13	3.78	8.31	3.35	4.45
Glu	6.70		6.82	5.20	3.68	8.23	8.46	14.48		8.29
Hsd	2.73	1.67	3.16	0.62	1.04	1.51	2.24	4.65	3.48	2.64
Hse	5.46	4.00	7.68	4.52	6.24	4.09	11.58	6.43	6.14	6.62
Hsp	4.71	-1.40	2.20	3.67	1.41	1.66	0.68	-4.79	-5.02	3.26
Ile	5.80	7.78	5.47	4.24	3.44	4.69	3.20	5.51	4.42	5.12
Leu	5.88	5.32	3.76	2.56	2.58	3.28	7.05	6.78	5.10	4.97
Lys	3.70	4.94	5.25	2.59	6.10	5.94	2.24	5.72	0.00	4.50
Met	3.11	9.44	4.18	2.17	2.87	2.92	3.73	7.75	4.51	5.08
Phe	3.30	4.76	3.31	2.02	1.90	2.61	5.29	5.19	5.19	3.96
Ser	-0.28	1.36	3.64	-2.05	1.48	-0.33	4.71	2.47	3.86	2.68
Thr	1.44	2.83	4.81	0.52	4.21	1.71	3.45	1.77	2.54	2.90
Trp	3.29	2.21	1.98	2.97	1.66	0.89	4.14	2.39	5.69	3.11
Tyr	2.79	5.16	2.55	2.29	1.61	2.48	4.68	4.82	5.58	3.82
Val	0.23				1.91				-1.76	1.51
AVG	3.56	3.92	4.37	2.25	2.91	3.01	5.16	5.07	3.25	
RMSD	4.18	4.73	4.72	2.92	3.25	3.61	6.34	6.67	4.82	
AVG(AlphaL)					3.72					
RMSD(AlphaL)					4.73					
AVG(all)						2.09				
RMSD(all)						3.69				

Energy differences in kcal/mol. See Methods for rotamer and secondary structure definitions. Some values were not successfully calculated due to structural clash.

Table S6) Differences in relative energy of local minima between C22/CMAP with MCSA-fitted sidechain parameters and QM calculations.

Residue \ Rotamer	tt	tm	tp	mt	mm	mp	pt	pm	pp	RMSD
					Alpha					
Arg	2.31	3.90	0.14	1.26	-0.48	2.93	4.07	6.88	5.64	3.75
Asn	2.56	4.26	1.44	2.53	-0.64	3.39	0.23	4.40	3.06	2.86
Asp	-2.53	0.53	-0.96	-0.19	-1.97	1.29	-0.31	1.32	-0.73	1.31
Cys	1.89	1.24	0.44	1.75	2.00	0.99	0.54	1.00	2.04	1.45
Gln	2.97	3.85	-0.20	2.41	0.78	2.08	1.65	3.70	1.42	2.42
Glu	0.67	8.14	1.41	1.28	0.76	0.83	1.25	-1.23	3.62	3.12
Hsd	2.30	0.56	1.15	-0.80	0.72	0.56	3.61	0.14	-0.64	1.56
Hse	4.09	4.10	2.40	3.24	-0.31	2.04	0.35	1.39	1.28	2.53
Hsp	5.04	3.83	5.42	1.66	4.00	5.58	9.60	8.23	4.99	5.81
Ile	1.42	3.18	1.62	0.97	1.13	0.86	0.56	0.22	0.32	1.42
Leu	3.46	3.48	1.80	1.23	0.96	0.78	1.45	1.77	1.60	2.06
Lys	1.92	3.87	-0.47	0.63	-0.93	2.39	3.09	6.32	6.00	3.52
Met	1.43	3.99	1.26	0.84	1.76	2.21	0.92	1.56	-2.87	2.10
Phe	1.43	2.15	0.64	0.86	1.26	1.32	-0.47	0.91	1.47	1.26
Ser	2.20	1.64	0.65	1.79	0.45	-0.08	-1.04	-1.87	1.58	1.43
Thr	2.07	1.08	0.31	2.61	1.08	0.28	-1.28	-2.13	0.56	1.49
Trp	2.79	2.72	1.89	2.27	1.32	2.34	-0.08	1.95	1.33	2.02
Tyr	1.18	2.32	0.85	1.02	1.73	1.42	-0.04	0.93	1.85	1.41
Val	0.92				0.28				1.18	0.88
AVG	2.01	3.05	1.10	1.41	0.73	1.73	1.34	1.97	1.77	
RMSD	2.51	3.52	1.74	1.71	1.46	2.17	2.81	3.44	2.78	
AVG(Alpha)					1.68					
RMSD(Alpha)					2.55					
					Beta					
Arg	-0.06	0.32	-0.56	1.07	0.99	2.05	0.66	1.52	1.28	1.11
Asn	0.21	0.78	0.33	-0.38	-0.64	0.97	-0.20	2.39	0.83	0.98
Asp	0.59	3.08	0.84	0.22	0.14	2.06	-1.14	3.34	-1.73	1.83
Cys	-0.67	-0.15	0.51	-0.25	-0.62	-0.62	0.10	-0.53	0.06	0.45
Gln	0.60	2.03	-0.05	1.18	-0.67	2.61	0.28	1.12	0.39	1.27
Glu	1.26	7.36	-1.46	0.99	-0.91	5.09	1.45	4.54	5.77	3.97
Hsd	-0.80	-2.13	-1.66	-0.38	-1.49	-1.61	0.02	-0.44	-1.10	1.26
Hse	0.80	0.55	1.34	1.99	0.08	0.52	2.20	2.40	1.68	1.51
Hsp	1.03	1.71	2.33	2.48	3.09	2.99	-0.14	1.88	-1.01	2.07
Ile	0.21	1.37	-0.49	-0.22	0.00	1.44	0.12	0.56	1.72	0.92
Leu	1.42	1.07	-0.38	0.34	1.35	1.24	0.57	1.84	1.53	1.19
Lys	-0.64	0.57	-0.67	0.76	1.00	2.63	0.24	1.40	1.65	1.27
Met	-0.49	1.87	-0.34	0.23	0.70	-0.66	-0.38	0.10	-3.24	1.31
Phe	-0.69	0.66	-0.39	0.79	-0.74	0.62	-0.55	0.50	0.28	0.60
Ser	-1.21	-1.70	-0.67	-0.76	-1.29	-0.93	-0.63	-0.24	-0.35	0.97
Thr	-0.77	-1.80	-0.70	-0.84	-1.37	-1.50	-0.02	-0.14	-0.31	1.01
Trp	-0.56	0.25	0.81	1.52	-0.40	0.89	0.79	1.51	0.38	0.90
Tyr	-0.70	0.75	-0.49	0.64	-0.71	0.62	-0.72	0.25	0.45	0.61
Val	0.00				0.47				-1.44	0.87
AVG	-0.02	0.92	-0.09	0.52	-0.05	1.02	0.15	1.22	0.36	
RMSD	0.77	2.24	0.96	1.04	1.10	1.97	0.79	1.81	1.85	
AVG(Beta)					0.45					
RMSD(Beta)					1.49					
					AlphaL					
Arg	2.63	3.71	2.45	1.77	2.14	1.69	1.21	4.44	0.00	2.55
Asn	3.10	3.48	5.56	1.54	3.32	1.39	8.14	2.73	4.04	4.19

Asp	1.12	1.54	2.85	2.53	2.48	5.20	14.25	14.23	11.90	8.15
Cys	1.08	0.68	0.98	2.34	3.41	2.48	5.82	1.91	3.69	2.92
Gln	3.49	5.59	3.26	3.18	3.27	3.85	4.35	7.88	2.97	4.47
Glu	5.76		0.54	6.40	0.28	7.60	9.19	17.63		8.68
Hsd	1.12	0.65	1.31	-0.82	-0.13	0.21	2.87	4.39	2.77	2.09
Hse	2.93	3.86	5.99	2.96	3.93	1.88	10.19	5.44	6.24	5.37
Hsp	1.47	1.01	4.39	-0.56	2.70	3.03	-2.50	-3.23	-3.08	2.70
Ile	5.82	7.63	5.00	4.10	3.16	4.57	3.58	6.97	5.10	5.29
Leu	5.28	5.17	3.13	2.54	3.33	3.50	8.43	8.64	5.43	5.47
Lys	2.37	4.30	2.22	1.33	2.18	2.60	1.40	5.39	0.00	2.85
Met	3.20	8.33	3.48	3.02	2.87	3.84	3.42	8.14	3.56	4.88
Phe	2.07	4.06	2.00	2.40	2.55	3.37	6.58	6.25	6.41	4.37
Ser	0.31	0.70	1.84	0.24	1.21	-0.72	5.85	1.13	3.99	2.53
Thr	2.37	2.29	3.27	2.59	3.44	0.94	5.40	0.74	3.17	3.00
Trp	3.44	4.01	3.42	3.18	3.25	2.90	6.64	4.98	7.08	4.57
Tyr	1.57	4.22	1.27	2.52	2.24	3.24	5.91	5.90	6.48	4.16
Val	5.44				3.91				6.15	5.25
AVG	2.87	3.60	2.94	2.29	2.61	2.87	5.60	5.75	4.22	
RMSD	3.31	4.24	3.31	2.80	2.83	3.41	6.71	7.40	5.28	
AVG(AlphaL)					3.64					
RMSD(AlphaL)					4.64					
AVG(all)						1.92				
RMSD(all)						3.17				

Energy differences in kcal/mol. See Methods for rotamer and secondary structure definitions. Some values were not successfully calculated due to structural clash.

Table S7) Differences in relative energy of local minima between C36 and QM calculations.

C36 Residue \ Rotamer	tt	tm	tp	mt	mm	mp	pt	pm	pp	RMSD
					Alpha					
Arg	3.49	5.28	1.71	1.20	-0.60	2.71	3.94	6.84	4.66	3.89
Asn	1.36	1.58	-0.53	2.12	-0.81	1.68	-0.42	3.54	1.05	1.71
Asp	-1.77	1.23	-0.48	0.80	-0.83	2.21	-0.73	0.61	-1.15	1.22
Cys	1.27	0.74	0.03	1.25	1.76	0.60	0.08	0.79	2.06	1.16
Gln	1.62	3.08	-1.06	-0.61	-2.02	-0.31	-0.87	1.73	-1.94	1.68
Glu	-3.85	8.92	2.91	-5.06	0.38	0.52	-4.63	-1.04	3.13	4.23
Hsd	1.76	0.40	1.56	-1.23	0.41	0.89	1.05	0.45	-0.71	1.05
Hse	5.06	4.54	3.22	3.69	1.29	2.78	0.58	2.26	1.96	3.14
Hsp	4.32	1.99	3.99	1.52	2.81	4.52	9.02	6.85	3.11	4.80
Ile	1.46	2.72	1.37	1.31	0.97	0.84	0.69	-0.01	-0.23	1.30
Leu	3.44	3.19	1.88	0.76	0.28	0.46	0.98	0.60	0.69	1.77
Lys	3.34	5.60	1.36	0.79	-0.84	2.45	3.18	6.45	4.95	3.77
Met	1.57	3.69	0.80	-0.73	-0.36	-0.02	-0.29	0.06	-4.55	2.06
Phe	0.94	1.66	0.14	0.06	0.59	0.22	-1.57	-0.09	0.45	0.87
Ser	1.95	1.13	0.30	2.09	0.47	0.29	-1.05	-2.14	1.16	1.37
Thr	0.80	0.65	-0.21	2.55	1.69	1.07	-1.98	-2.08	0.52	1.50
Trp	1.40	1.74	1.33	2.81	2.50	3.30	-1.20	1.86	0.88	2.04
Tyr	0.88	1.96	0.51	0.37	1.20	0.42	-1.00	0.10	0.97	0.98
Val	0.78				4.44				1.15	2.68
AVG	1.57	2.78	1.05	0.76	0.70	1.37	0.32	1.49	0.96	
RMSD	2.51	3.50	1.70	2.03	1.64	1.89	2.82	3.08	2.37	
AVG(Alpha)					1.22					
RMSD(Alpha)					2.46					
					Beta					
Arg	1.83	2.19	1.36	0.96	0.87	1.94	1.27	2.13	1.19	1.60
Asn	-0.36	-0.08	-0.47	-0.50	-2.20	-0.11	-0.98	0.84	-1.31	0.99
Asp	1.37	3.83	1.56	1.25	1.02	2.97	-1.53	2.49	-2.44	2.23
Cys	-0.94	-0.10	0.58	-0.52	-0.54	-0.59	-0.43	-0.56	0.08	0.54
Gln	-0.24	1.35	-0.61	-1.58	-3.18	0.02	-1.83	-0.85	-2.27	1.64
Glu	-3.05	9.04	0.12	-5.25	-1.19	4.81	-4.31	4.71	5.21	4.84
Hsd	-0.54	-0.66	0.20	-0.78	-1.63	-1.28	-0.77	-0.07	-2.13	1.10
Hse	2.13	2.22	2.87	2.74	0.97	1.40	2.70	2.67	1.32	2.22
Hsp	0.86	0.13	1.19	3.01	2.24	2.28	-0.24	0.92	-2.59	1.80
Ile	0.62	1.34	-0.57	0.32	0.00	1.48	0.44	0.42	1.00	0.83
Leu	1.69	0.99	-0.14	0.00	0.67	0.95	0.28	0.91	0.77	0.86
Lys	1.44	2.64	1.45	0.86	1.08	2.71	1.02	2.24	1.43	1.78
Met	0.04	1.85	-0.34	-1.16	-1.19	-2.55	-1.15	-1.14	-4.90	2.09
Phe	-1.02	0.56	-0.58	0.22	-1.10	0.28	-1.69	-0.16	-0.55	0.83
Ser	-1.13	-1.94	-0.89	-0.21	-1.04	-0.77	-0.59	-0.59	-0.49	0.97
Thr	-1.43	-1.81	-0.65	-0.63	-0.47	-0.63	-0.63	-0.09	-0.08	0.89
Trp	-1.53	0.05	0.92	2.20	0.91	2.03	-0.32	0.97	-0.59	1.26
Tyr	-0.83	0.79	-0.54	0.26	-0.92	0.43	-1.69	-0.24	-0.22	0.79
Val	0.00				4.44				-0.09	2.56
AVG	-0.06	1.24	0.30	0.07	-0.07	0.85	-0.58	0.81	-0.35	
RMSD	1.34	2.68	1.06	1.79	1.69	1.93	1.57	1.69	2.09	
AVG(Beta)					0.25					
RMSD(Beta)					1.81					
					AlphaL					
Arg	4.08	5.50	3.90	1.67	1.96	1.62	1.26	3.25	0.00	3.05
Asn	2.27	1.21	3.07	1.19	2.80	1.17	6.57	1.38	2.44	2.94

Asp	1.33	2.01	2.99	2.89	2.72	5.65	11.24	11.28	10.30	6.85
Cys	0.59	0.16	0.46	1.66	3.13	2.34	4.97	1.81	3.32	2.53
Gln	2.24	4.11	2.15	0.09	0.43	0.41	1.58	3.73	-0.63	2.20
Glu	0.33		1.67	-0.65	-0.48	4.70	2.41	9.53		4.18
Hsd	1.00	-0.12	1.77	-1.38	0.23	0.63	0.90	3.49	1.66	1.57
Hse	4.10	3.46	5.63	3.12	4.76	2.80	9.05	4.96	5.99	5.20
Hsp	1.21	-1.21	2.56	-0.34	2.12	2.03	-3.53	-4.34	-5.06	2.89
Ile	5.30	6.94	4.48	4.31	2.89	4.04	3.52	5.75	4.37	4.76
Leu	5.37	4.92	3.11	1.99	2.21	2.73	6.72	6.44	4.55	4.55
Lys	4.03	6.34	3.83	1.40	2.20	2.73	1.63	4.33	0.00	3.44
Met	3.19	8.34	2.98	1.28	0.61	1.12	1.93	3.62	1.36	3.50
Phe	1.53	2.97	1.42	1.44	1.82	2.52	4.25	4.19	4.41	2.98
Ser	0.34	0.25	1.53	0.51	1.19	-0.56	5.44	0.92	2.93	2.20
Thr	0.92	1.42	2.23	2.40	3.92	1.66	4.04	0.83	2.25	2.44
Trp	2.08	2.25	2.15	3.55	4.41	3.88	4.34	4.16	6.22	3.89
Tyr	1.21	3.33	0.88	1.72	1.69	2.54	3.96	3.97	4.70	2.97
Val	5.10				4.44				5.99	5.21
AVG	2.43	3.05	2.60	1.49	2.27	2.33	3.90	3.85	3.04	
RMSD	2.96	4.02	2.89	2.07	2.69	2.78	5.06	5.07	4.47	
AVG(AlphaL)					2.77					
RMSD(AlphaL)					3.70					
AVG(all)						1.41				
RMSD(all)						2.77				

Energy differences in kcal/mol. See Methods for rotamer and secondary structure definitions. Some values were not successfully calculated due to structural clash.

Table S8) RMS Difference between the QM and MM potential energy surfaces based on regions with relative energies below 2 kcal/mol (Low) and from 2 – 12 kcal/mol (high) above the local minima on each of the three $\chi 1/\chi 2$ surfaces for each amino acid.

	LOW (0-2 kcal/mol)			HIGH (2-12 kcal/mol)		
Residue	**C22**	**C36**	**DIFF**	**C22**	**C36**	**DIFF**

Arg	1.16	1.06	-0.10	2.50	2.49	-0.02
Asn	1.11	1.27	0.16	1.99	1.68	-0.31
Asp	1.07	1.10	0.03	2.71	1.93	-0.78
Cys	0.96	0.63	-0.33	1.70	1.34	-0.37
Gln	1.38	1.49	0.11	1.84	1.68	-0.16
Glu	1.05	1.37	0.32	3.16	2.88	-0.28
Hsd	1.12	1.20	0.08	1.41	1.28	-0.13
Hse	1.45	1.35	-0.10	2.19	1.82	-0.37
Hsp	0.72	0.85	0.13	3.57	2.39	-1.17
Ile	0.72	0.51	-0.21	1.32	1.12	-0.20
Leu	0.61	0.64	0.03	1.57	1.46	-0.11
Lys	1.20	1.07	-0.12	2.39	2.23	-0.16
Met	0.68	0.90	0.22	1.29	1.60	0.31
Phe	0.67	0.48	-0.18	1.51	1.09	-0.42
Ser	1.23	0.94	-0.28	2.44	1.71	-0.73
Thr	1.55	1.51	-0.04	2.45	1.80	-0.65
Trp	1.36	0.71	-0.66	1.71	1.16	-0.55
Tyr	0.71	1.11	0.40	1.51	1.26	-0.24
Val	0.61	0.48	-0.13	1.09	0.75	-0.34
Mean signed error			**-0.04**			**-0.35**
Mean unsigned error			**0.19**			**0.38**

Table S9) NMR J-coupling constants for Ala_3, Ala_5, Ala_7, Val_3, and Gly_3 peptides from experiment[7] and simulation with new force field. Results with flavodoxin-based[8] and DFT-based Karplus parameters (in parentheses)[9] for alanine- and valine-peptides. For Gly_3, only DFT-based parameters were used[10].

		Ala_3		**Ala_5**		**Ala_7**		**Val_3**		**Gly_3**	
		Exp	*Sim*	*Exp*	*Sim*	*Exp*	*Sim*	*Exp*	*Sim*	*Exp*	*Sim*
$^2J(N,C_\alpha)$	ψ_1	9.14	8.60	9.20	8.60	9.17	8.60	8.35	8.58	10.45	8.58
$^3J(H_N,C_\alpha)$	ϕ_2,ψ_1	0.70	0.56	0.67	0.57	0.71	0.57	0.77	0.62	0.78	0.61
$^3J(H_N,H_\alpha)$	ϕ_2	5.68	5.26 (6.19)	5.59	5.40 (6.23)	5.61	5.37 (6.30)	7.94	5.52 (6.64)	5.89	5.82
$^3J(H_N,C')$	ϕ_2	1.13	1.61 (1.05)	1.13	1.62 (1.13)	1.15	1.59 (1.04)	0.58	1.31 (0.66)	1.10	1.10
$^3J(H_\alpha,C')$	ϕ_2	1.84	1.73 (1.74)	1.85	1.97 (2.02)	1.89	1.77 (1.78)	2.42	1.80 (1.84)	4.01	3.73
$^3J(C',C')$	ϕ_2	-	0.79 (0.84)	0.19	0.78 (0.83)	-	0.81 (0.86)	0.34	0.62 (0.57)	0.26	0.48
$^3J(H_N,C_\beta)$	ϕ_2	2.39	1.87 (2.71)	2.30	1.82 (2.61)	2.31	1.84 (2.66)	1.38	1.98 (2.92)	-	-
$^1J(N,C_a)$	ψ_2	11.34	11.29	11.36	11.27	11.37	11.29	10.80	10.80	12.17	11.74
$^2J(N,C_\alpha)$	ψ_2	8.45	8.36	8.55	8.33	8.52	8.35	7.80	8.13	9.05	8.50
$^3J(H_N,C_\alpha)$	ϕ_3,ψ_2	0.65	0.60	0.68	0.61	0.66	0.62	0.75	0.56 (0.58)	0.61	0.62
$^3J(H_N,H_\alpha)$	ϕ_3	6.52	5.76 (7.07)	5.74	5.30 (6.19)	5.66	5.38 (6.24)	7.91	5.76 (7.07)	5.87	5.77
$^3J(H_N,C')$	ϕ_3	1.29	1.01 (0.28)	-	1.57 (1.01)	1.20	1.58 (1.05)	1.01	1.03 (0.30)	0.99	1.18
$^3J(H_\alpha,C')$	ϕ_3	2.14	1.79 (1.86)	1.86	1.88 (1.92)	1.85	1.97 (2.01)	2.45	1.79 (1.86)	3.90	3.92
$^3J(C',C')$	ϕ_3	-	0.51 (0.38)	-	0.72 (0.74)	-	0.73 (0.76)	-	0.52 (0.39)	-	-
$^3J(H_N,C_\beta)$	ϕ_3	2.02	2.08 (3.09)	2.24	1.90 (2.75)	2.20	1.87 (2.69)	1.40	2.07 (3.07)	-	-
$^1J(N,C_a)$	ψ_3			11.26	11.13	11.27	11.18				
$^2J(N,C_\alpha)$	ψ_3			8.40	8.16	8.29	8.22				
$^3J(H_N,C_\alpha)$	ϕ_4,ψ_3			0.69	0.60	0.56	0.61				
$^3J(H_N,H_\alpha)$	ϕ_4			5.98	5.41 (6.31)	5.77	5.38 (6.25)				
$^3J(H_N,C')$	ϕ_4			1.15	1.57 (1.04)	1.20	1.59 (1.06)				
$^3J(H_\alpha,C')$	ϕ_4			1.89	1.90 (1.94)	1.80	1.95 (1.99)				
$^3J(C',C')$	ϕ_4			-	0.77 (0.80)	-	0.75 (0.78)				
$^3J(H_N,C_\beta)$	ϕ_4			2.14	1.85 (2.66)	2.23	1.86 (2.67)				
$^1J(N,C_a)$	ψ_4			11.25	11.14	11.22	11.19				
$^2J(N,C_\alpha)$	ψ_4			8.27	8.15	8.22	8.27				
$^3J(H_N,C_\alpha)$	ϕ_5,ψ_4			0.73	0.59	-	0.62				
$^3J(H_N,H_\alpha)$	ϕ_5			6.54	5.82 (7.13)	5.92	5.45 (6.36)				
$^3J(H_N,C')$	ϕ_5			1.16	1.00 (0.28)	1.19	1.52 (0.98)				
$^3J(H_\alpha,C')$	ϕ_5			2.19	1.81 (1.88)	1.56	1.95 (2.00)				
$^3J(C',C')$	ϕ_5			-	0.52 (0.39)	-	0.72 (0.74)				
$^3J(H_N,C_\beta)$	ϕ_5			1.96	2.06 (3.06)	2.23	1.88 (2.70)				
$^1J(N,C_a)$	ψ_5					11.29	11.01				
$^2J(N,C_\alpha)$	ψ_5					8.24	7.96				
$^3J(H_N,C_\alpha)$	ϕ_6,ψ_5					-	0.58				
$^3J(H_N,H_\alpha)$	ϕ_6					6.04	5.53 (6.36)				
$^3J(H_N,C')$	ϕ_6					1.10	1.58 (1.11)				
$^3J(H_\alpha,C')$	ϕ_6					1.67	2.06 (2.13)				
$^3J(C',C')$	ϕ_6					-	0.78 (0.82)				
$^3J(H_N,C_\beta)$	ϕ_6					2.21	1.80 (2.56)				
$^1J(N,C_a)$	ψ_6					11.29	11.13				
$^2J(N,C_\alpha)$	ψ_6					8.18	8.14				
$^3J(H_N,C_\alpha)$	ϕ_7,ψ_6					0.59	0.59				
$^3J(H_N,H_\alpha)$	ϕ_7					6.60	5.79 (7.11)				
$^3J(H_N,C')$	ϕ_7					1.25	1.01 (0.28)				
$^3J(H_\alpha,C')$	ϕ_7					2.03	1.80 (1.87)				
$^3J(C',C')$	ϕ_7					-	0.52 (0.39)				
$^3J(H_N,C_\beta)$	ϕ_7					1.99	2.07 (3.07)				

Table S10: NMR J-coupling constants for Ala_5 from experiment[7] and simulations with different force fields. Flavodoxin-based Karplus parameters[8] were used in all cases.

		NMR	***C36***	***C22/CMAP***	***C22/MP2***	***Amber 99SB***	***OPLS***	***Gromos 53A6***
$^2J(N,C_\alpha)$	ψ_1	9.20	8.60	8.59	8.60	8.54	8.64	8.61
$^3J(H_N,C_\alpha)$	ϕ_2,ψ_1	0.67	0.57	0.61	0.49	0.70	0.68	0.71
$^3J(H_N,H_\alpha)$	ϕ_2	5.59	5.40	5.85	3.79	6.26	7.07	6.90
$^3J(H_N,C')$	ϕ_2	1.13	1.62	1.60	2.30	1.35	0.90	1.17
$^3J(H_\alpha,C')$	ϕ_2	1.85	1.97	1.96	1.72	1.97	2.21	2.23
$^3J(C',C')$	ϕ_2	0.19	0.78	1.04	0.52	1.01	0.91	1.00
$^3J(H_N,C_\beta)$	ϕ_2	2.30	1.82	1.60	2.12	1.58	1.56	1.46
$^1J(N,C_\alpha)$	ψ_2	11.36	11.27	11.10	11.18	11.40	11.33	10.74
$^2J(N,C_\alpha)$	ψ_2	8.55	8.33	7.95	8.21	8.28	8.33	8.21
$^3J(H_N,C_\alpha)$	ϕ_3,ψ_2	0.68	0.61	0.58	0.55	0.64	0.64	0.65
$^3J(H_N,H_\alpha)$	ϕ_3	5.74	5.30	5.97	3.91	6.41	7.12	6.81
$^3J(H_N,C')$	ϕ_3	-	1.57	1.51	2.21	1.39	0.88	1.17
$^3J(H_\alpha,C')$	ϕ_3	1.86	1.88	2.23	1.74	2.37	2.23	2.26
$^3J(C',C')$	ϕ_3	-	0.72	0.90	0.52	0.90	0.90	0.94
$^3J(H_N,C_\beta)$	ϕ_3	2.24	1.90	1.65	2.12	1.56	1.56	1.51
$^1J(N,C_\alpha)$	ψ_3	11.26	11.13	10.74	11.03	11.05	11.17	10.59
$^2J(N,C_\alpha)$	ψ_3	8.40	8.16	7.42	8.06	7.75	8.20	8.11
$^3J(H_N,C_\alpha)$	ϕ_4,ψ_3	0.69	0.60	0.52	0.54	0.59	0.63	0.65
$^3J(H_N,H_\alpha)$	ϕ_4	5.98	5.41	6.20	4.35	6.62	7.14	6.98
$^3J(H_N,C')$	ϕ_4	1.15	1.57	1.46	2.13	1.23	0.89	1.15
$^3J(H_\alpha,C')$	ϕ_4	1.89	1.90	2.11	2.08	2.07	2.23	2.32
$^3J(C',C')$	ϕ_4	-	0.77	1.03	0.55	1.04	0.91	0.99
$^3J(H_N,C_\beta)$	ϕ_4	2.14	1.85	1.55	2.01	1.51	1.54	1.44
$^1J(N,C_\alpha)$	ψ_4	11.25	11.14	10.88	10.89	11.20	11.06	10.58
$^2J(N,C_\alpha)$	ψ_4	8.27	8.15	7.58	7.82	7.98	8.10	8.12
$^3J(H_N,C_\alpha)$	ϕ_5,ψ_4	0.73	0.59	0.49	0.55	0.58	0.63	0.68
$^3J(H_N,H_\alpha)$	ϕ_5	6.54	5.82	5.83	5.82	6.06	7.52	7.66
$^3J(H_N,C')$	ϕ_5	1.16	1.00	0.99	1.00	1.75	0.90	1.04
$^3J(H_\alpha,C')$	ϕ_5	2.19	1.81	1.81	1.81	2.52	2.40	2.47
$^3J(C',C')$	ϕ_5	-	0.52	0.52	0.52	0.84	1.03	1.19
$^3J(H_N,C_\beta)$	ϕ_5	1.96	2.06	2.06	2.06	1.52	1.37	1.20

Table S11. Old and new dihedral parameters for Glycine termini. Torsion potentials are of the form $V_n(\theta) = k_n(1+\cos[n\theta - \theta_0])$, where θ is the torsion angle as defined, θ_0 is a phase offset and k_n is the force constant, which was optimized, and the multiplicity n=1.

Atom types	Backbone torsion	Old k_θ [kcal/mol]	Old θ_0	New k_θ [kcal/mol]	New θ_0
NH3-CT2-C-NH1	N-ter, ψ	0.4	0°	1.0	0°
CC-CT2-NH1-C	C-ter, ϕ	0.2	180°	2.0	180°

Table S12. Scalar couplings of GPGG

Residue	***J*-coupling type**	**Torsion probed**	***J* (expt)**	***J* (ff99SB)**	***J* (C22/CMAP)**	***J* (C36)**
Pro 2	$^3J_{H\alpha C}$	ϕ_2	1.3	1.22	1.12	1.00
Gly 3	$^3J_{H\alpha C}$	ϕ_3	4.1	4.27	5.01	3.96
Gly 4	$^3J_{H\alpha C}$	ϕ_4	3.7	2.49	1.04	2.43
Gly 4	$^3J_{HNC}$	ϕ_4	1.1	1.68	2.55	1.59
Gly 3	$^3J_{HNH\alpha}$	ϕ_3	6.3	5.92	6.58	6.32
Gly 4	$^3J_{HNH\alpha}$	ϕ_4	6.0	4.49	2.03	4.18

Table S13) Scalar couplings of central Ala residues in the HEWL19 peptide.

		Expt		Amber ff99SB	Amber ff99SB*	C22/CMAP	C36
A9	$^{1}J_{NC\alpha}$ (ψ_9)	10.54	0.59	10.84	10.53	9.90	10.40
A10	$^{1}J_{NC\alpha}$ (ψ_{10})	10.58	0.59	10.84	10.27	9.79	10.35
A11	$^{1}J_{NC\alpha}$ (ψ_{11})	10.57	0.59	10.64	10.21	9.78	10.40
A10	$^{2}J_{NC\alpha}$ (ψ_9)	7.24	0.50	7.50	7.06	6.49	7.02
A11	$^{2}J_{NC\alpha}$ (ψ_{10})	7.02	0.50	7.54	6.64	6.37	6.91
M12	$^{2}J_{NC\alpha}$ (ψ_{11})	7.17	0.50	7.01	6.57	6.33	7.06
A9	$^{3}J_{H\alpha C}(\phi_9)$	2.06	0.38	2.47	1.76	1.15	1.93
A10	$^{3}J_{H\alpha C}(\phi_{10})$	1.72	0.38	2.55	1.82	1.18	2.10
A11	$^{3}J_{H\alpha C}(\phi_{11})$	2.20	0.38	2.87	2.16	1.09	2.32
A9	$^{3}J_{HNC}(\phi_9)$	1.39	0.59	1.05	0.65	0.76	1.03
A10	$^{3}J_{HNC}(\phi_{10})$	1.33	0.59	1.10	0.65	0.77	0.88
A11	$^{3}J_{HNC}(\phi_{11})$	1.09	0.59	1.22	0.77	0.85	0.97
A9	$^{3}J_{HNC\beta}$ (ϕ_9)	2.26	0.39	2.03	2.74	3.68	2.77
A10	$^{3}J_{HNC\beta}$ (ϕ_{10})	2.19	0.39	2.23	3.01	3.73	2.86
A11	$^{3}J_{HNC\beta}$ (ϕ_{11})	2.21	0.39	2.31	2.37	3.75	2.73
A9	$^{3}J_{HNH\alpha}$ (ϕ_9)	5.18	0.91	7.49	6.22	4.94	6.15
A10	$^{3}J_{HNH\alpha}$ (ϕ_{10})	5.10	0.91	7.08	6.46	4.83	6.19
A11	$^{3}J_{HNH\alpha}$ (ϕ_{11})	5.67	0.91	6.67	7.45	4.78	6.23
A10	$^{3}J_{HNC\alpha}$ (ϕ_{10}, ψ_9)	0.46	0.10	0.52	0.39	0.19	0.37
A11	$^{3}J_{HNC\alpha}$ (ϕ_{11}, ψ_{10})	0.43	0.10	0.49	0.38	0.16	0.38
M12	$^{3}J_{HNC\alpha}$ (ϕ_{12}, ψ_{11})	0.43	0.10	0.49	0.38	0.16	0.41
$\chi 2$(J)				1.2	1.0	4.7	0.6

Table S14) New atom types and parameters in the C36 force field.

```
MASS    51 CT2A  12.01100

BONDS
CT2A CT1   222.500     1.5380
CT2  CT2A  222.500     1.5300
CT2A HA2   309.000     1.1110
CT2A CPH1  229.630     1.5000
CT2A CC    200.000     1.5220

ANGLES
CT2A CT1  CC     52.000   108.0000
CT2A CT2  CD     52.000   108.0000
NH1  CT1  CT2A   70.000   113.5000
HB1  CT1  CT2A   35.000   111.0000
CT2A CT1  C      52.000   108.0000
CT1  CT2A HA2    26.500   110.1000  22.53   2.17900
CT1  CT2A CT2    58.350   113.5000  11.16   2.56100
HA2  CT2A HA2    35.500   109.0000   5.40   1.80200
HA2  CT2A CT2    26.500   110.1000  22.53   2.17900
CT2A CT2  HA2    26.500   110.1000  22.53   2.17900
CT2A CT2  CC     52.000   108.0000
CT1  CT2A CPH1   58.350   113.0000
HA2  CT2A CPH1   33.430   109.5000
CT2A CPH1 CPH1   45.800   130.0000
CT2A CPH1 NR3    45.800   122.0000
CT1  CT2A CC     52.000   108.0000
HA2  CT2A CC     33.000   109.5000  30.00   2.16300
OC   CC   CT2A   40.000   118.0000  50.00   2.38800
NH3  CT1  CT2A   67.700   110.0000
CT2A CT1  CD     52.000   108.0000
DIHEDRALS
!Glu/Hsp, CT2A terms
NH1  CT1  CT2A HA2      0.2000  3     0.00
CT1  CT2A CT2  HA2      0.1900  3     0.00
HB1  CT1  CT2A HA2      0.2000  3     0.00
HB1  CT1  CT2A CT2      0.2000  3     0.00
HA2  CT2A CT1  C        0.2000  3     0.00
HA2  CT2A CT1  CC       0.2000  3     0.00
HA2  CT2A CT2  HA2      0.1900  3     0.00
HA2  CT2A CT2  CC       0.1900  3     0.00
HB1  CT1  CT2A CPH1     0.2000  3     0.00
C    NH1  CT1  CT2A     1.8000  1     0.00
H    NH1  CT1  CT2A     0.0000  1     0.00
CT2A CT1  C    O        1.4000  1     0.00
CT2A CT1  C    NH1      0.0000  1     0.00
CT2A CT1  C    N        0.0000  1     0.00
! Glup
CT1  CT2A CT2  CD       0.1900  3     0.00
HA2  CT2A CT2  CD       0.1900  3     0.00
CT2A CPH1 CPH1 HR1      1.0000  2   180.00
CT2A CPH1 CPH1 NR3      2.5000  2   180.00
CT2A CPH1 NR3  H        3.0000  2   180.00
CT2A CPH1 NR3  CPH2     2.5000  2   180.00
HA2  CT2A CPH1 CPH1     0.0000  3     0.00
HA2  CT2A CPH1 NR3      0.1900  3     0.00
! Fit dihedrals
```

```
! Group-fitted for Lys/Arg/Gln/Met
C    CT1  CT2  CT2       0.3500  1   180.00
C    CT1  CT2  CT2       0.4200  2   180.00
C    CT1  CT2  CT2       1.9100  3   180.00
CT2  CT2  CT1  NH1       0.8800  1   180.00
CT2  CT2  CT1  NH1       0.0000  2   180.00
CT2  CT2  CT1  NH1       1.9000  3     0.00
CC   CT2  CT2  CT1       1.8400  1   180.00
CC   CT2  CT2  CT1       0.8400  2   180.00
CC   CT2  CT2  CT1       0.3900  3   180.00
CT1  CT2  CT2  CT2       0.6300  1   180.00
CT1  CT2  CT2  CT2       0.0100  2     0.00
CT1  CT2  CT2  CT2       0.1500  3     0.00
CT1  CT2  CT2  S         0.1400  1   180.00
CT1  CT2  CT2  S         0.5400  2     0.00
CT1  CT2  CT2  S         0.6900  3     0.00
! Fitted Asn
C    CT1  CT2  CC        1.4100  1   180.00
C    CT1  CT2  CC        1.2900  2   180.00
C    CT1  CT2  CC        0.5900  3   180.00
CC   CT2  CT1  NH1       0.2800  1   180.00
CC   CT2  CT1  NH1       0.5000  2   180.00
CC   CT2  CT1  NH1       0.3800  3     0.00
CT1  CT2  CC   NH2       0.6200  1   180.00
CT1  CT2  CC   NH2       0.6600  2   180.00
CT1  CT2  CC   NH2       0.7200  3   180.00
CT1  CT2  CC   O         0.4200  1   180.00
CT1  CT2  CC   O         0.1500  2   180.00
CT1  CT2  CC   O         0.9500  3   180.00
! Fitted Asp
C    CT1  CT2A CC        1.6100  1   180.00
C    CT1  CT2A CC        1.2900  2   180.00
C    CT1  CT2A CC        0.5900  3   180.00
CC   CT2A CT1  NH1       0.6800  1   180.00
CC   CT2A CT1  NH1       0.1000  2   180.00
CC   CT2A CT1  NH1       0.3800  3     0.00
CT1  CT2A CC   OC        0.8400  1     0.00
CT1  CT2A CC   OC        0.9800  2   180.00
CT1  CT2A CC   OC        1.4600  3     0.00
! Fitted Cys
CT1  CT2  S    HS        0.2000  1     0.00
CT1  CT2  S    HS        0.6500  2     0.00
CT1  CT2  S    HS        0.2200  3     0.00
C    CT1  CT2  S         0.2400  1   180.00
C    CT1  CT2  S         0.7500  2   180.00
C    CT1  CT2  S         1.3500  3   180.00
NH1  CT1  CT2  S         0.3400  1     0.00
NH1  CT1  CT2  S         0.5000  2   180.00
NH1  CT1  CT2  S         1.4300  3     0.00
! Fitted Glu
CC   CT2  CT2A CT1       0.0000  1   180.00
CC   CT2  CT2A CT1       0.3800  2   180.00
CC   CT2  CT2A CT1       0.5900  3   180.00
C    CT1  CT2A CT2       0.1100  1     0.00
C    CT1  CT2A CT2       0.9800  2   180.00
C    CT1  CT2A CT2       1.6000  3   180.00
CC   CT1  CT2A CT2       1.6000  3   180.00
CT2  CT2A CT1  NH1       0.3000  1     0.00
CT2  CT2A CT1  NH1       0.3500  2     0.00
CT2  CT2A CT1  NH1       1.7600  3     0.00
! Group-fitted for Hsd/Hse
```

```
CPH1 CPH1 CT2  CT1      1.7400  1     0.00
CPH1 CPH1 CT2  CT1      0.1500  2     0.00
CPH1 CPH1 CT2  CT1      0.7700  3   180.00
CT1  CT2  CPH1 NR1      1.4900  1     0.00
CT1  CT2  CPH1 NR1      0.0900  2   180.00
CT1  CT2  CPH1 NR1      0.7900  3   180.00
CT1  CT2  CPH1 NR2      1.0900  1     0.00
CT1  CT2  CPH1 NR2      0.0900  2     0.00
CT1  CT2  CPH1 NR2      0.6700  3   180.00
C    CT1  CT2  CPH1     0.1800  1   180.00
C    CT1  CT2  CPH1     0.6400  2   180.00
C    CT1  CT2  CPH1     0.8700  3   180.00
CPH1 CT2  CT1  NH1      0.0000  1     0.00
CPH1 CT2  CT1  NH1      0.0000  2   180.00
CPH1 CT2  CT1  NH1      0.9000  3     0.00
! Group-fitted for Hsp
CPH1 CPH1 CT2A CT1      2.0400  1     0.00
CPH1 CPH1 CT2A CT1      0.4400  2     0.00
CPH1 CPH1 CT2A CT1      0.1300  3   180.00
CT1  CT2A CPH1 NR3      0.5300  1   180.00
CT1  CT2A CPH1 NR3      0.4200  2   180.00
CT1  CT2A CPH1 NR3      0.3000  3   180.00
C    CT1  CT2A CPH1     1.7500  1   180.00
C    CT1  CT2A CPH1     0.1300  2     0.00
C    CT1  CT2A CPH1     1.8600  3   180.00
CPH1 CT2A CT1  NH1      1.0900  1   180.00
CPH1 CT2A CT1  NH1      0.2200  2   180.00
CPH1 CT2A CT1  NH1      2.3200  3     0.00
! Group-fitted for Ile/Thr
CT1  CT1  CT2  CT3      0.3800  1   180.00
CT1  CT1  CT2  CT3      0.1300  2   180.00
CT1  CT1  CT2  CT3      0.2900  3   180.00
C    CT1  CT1  CT2      0.1000  1   180.00
C    CT1  CT1  CT2      0.5200  2   180.00
C    CT1  CT1  CT2      0.2900  3   180.00
CT2  CT1  CT1  NH1      0.1200  1   180.00
CT2  CT1  CT1  NH1      0.3600  2   180.00
CT2  CT1  CT1  NH1      0.4100  3     0.00
! Fitted Leu
CT1  CT2  CT1  CT3      0.0500  1     0.00
CT1  CT2  CT1  CT3      0.1000  2   180.00
CT1  CT2  CT1  CT3      0.0100  3   180.00
C    CT1  CT2  CT1      0.3200  1   180.00
C    CT1  CT2  CT1      0.6100  2   180.00
C    CT1  CT2  CT1      0.7200  3   180.00
CT1  CT2  CT1  NH1      0.4800  1   180.00
CT1  CT2  CT1  NH1      0.4200  2   180.00
CT1  CT2  CT1  NH1      0.6500  3     0.00
! Group-fitted for Phe/Tyr
CA   CA   CT2  CT1      1.0700  1     0.00
CA   CA   CT2  CT1      0.2400  2   180.00
CA   CA   CT2  CT1      0.1700  3   180.00
C    CT1  CT2  CA       1.2800  1   180.00
C    CT1  CT2  CA       0.9400  2   180.00
C    CT1  CT2  CA       1.5700  3   180.00
CA   CT2  CT1  NH1      0.5200  1   180.00
CA   CT2  CT1  NH1      0.6200  2   180.00
CA   CT2  CT1  NH1      1.5800  3     0.00
! Fitted Ser
CT1  CT2  OH1  H        0.0200  1     0.00
CT1  CT2  OH1  H        0.5600  2     0.00
```

```
CT1  CT2  OH1  H        0.4900  3     0.00
C    CT1  CT2  OH1      0.6500  1   180.00
C    CT1  CT2  OH1      0.2500  2   180.00
C    CT1  CT2  OH1      1.1700  3   180.00
NH1  CT1  CT2  OH1      0.1800  1   180.00
NH1  CT1  CT2  OH1      0.1900  2   180.00
NH1  CT1  CT2  OH1      1.4600  3     0.00
! Group-fitted for Ile/Thr
CT1  CT1  OH1  H        0.1800  1     0.00
CT1  CT1  OH1  H        0.0600  2     0.00
CT1  CT1  OH1  H        0.2500  3     0.00
C    CT1  CT1  OH1      0.7900  1   180.00
C    CT1  CT1  OH1      0.3900  2   180.00
C    CT1  CT1  OH1      0.9900  3   180.00
NH1  CT1  CT1  OH1      0.0900  1     0.00
NH1  CT1  CT1  OH1      0.1900  2   180.00
NH1  CT1  CT1  OH1      0.1700  3     0.00
! Fitted Trp side-chain
CA   CY   CT2  CT1      0.0300  1     0.00
CA   CY   CT2  CT1      0.5500  2     0.00
CA   CY   CT2  CT1      0.3900  3   180.00
CPT  CY   CT2  CT1      0.3600  1   180.00
CPT  CY   CT2  CT1      0.0500  2     0.00
CPT  CY   CT2  CT1      0.1900  3   180.00
C    CT1  CT2  CY       1.0900  1   180.00
C    CT1  CT2  CY       0.5000  2   180.00
C    CT1  CT2  CY       1.1700  3   180.00
CY   CT2  CT1  NH1      0.2900  1   180.00
CY   CT2  CT1  NH1      0.6600  2   180.00
CY   CT2  CT1  NH1      1.1700  3     0.00
! Fitted Val
C    CT1  CT1  CT3      0.1400  1   180.00
C    CT1  CT1  CT3      0.2600  2   180.00
C    CT1  CT1  CT3      0.3300  3   180.00
CT3  CT1  CT1  NH1      0.1800  1     0.00
CT3  CT1  CT1  NH1      0.0600  2     0.00
CT3  CT1  CT1  NH1      0.5900  3     0.00

Lennard-Jones parameters
CT1      0.0       -0.0320    2.000 0.0 -0.01 1.9
CT2      0.0       -0.0560    2.010 0.0 -0.01 1.9
CT2A     0.0       -0.0560    2.010 0.0 -0.01 1.9
CT3      0.0       -0.0780    2.040 0.0 -0.01 1.9
HA1      0.0       -0.045     1.3400
HA2      0.0       -0.034     1.3400
HA3      0.0       -0.024     1.3400

CMAP
! 2D grid correction data.
! alanine map
C    NH1  CT1  C    NH1  CT1  C    NH1   24

! phi = -180.0
     0.126790      0.768700      0.971260      1.250970      2.121010
     2.720430      2.089440      1.789790      0.780870     -0.688474
     1.001130     -2.200520     -4.827670     -4.821447     -4.913223
    -3.591106     -2.766446     -2.784200     -2.454589     -2.346991
    -2.335350     -1.522656     -0.951542     -0.036650

! phi = -165.0
    -0.127133      1.377090      1.577020      1.872290      2.398990
```

```
     2.486630      2.436754      1.929070      1.086456      0.643400
     0.258676     -2.800440     -4.009477     -4.135306     -3.420090
    -2.602140     -2.299128     -1.501241     -1.101780     -0.861434
    -0.640168     -0.207701     -1.076344     -1.122030

! phi = -150.0
     0.084069      1.420317      1.624350      2.047200      2.653910
     2.716410      2.321416      1.985454      1.557466      2.463293
    -0.225720     -1.815886     -2.583256     -3.006154     -2.551995
    -1.890683     -1.354215     -0.727243      0.068512     -0.225016
    -0.765479     -1.283444     -1.293226     -0.816303

! phi = -135.0
     0.927992      1.521370      2.242218      2.546305      3.111384
     2.918410      2.460813      2.187970      2.058314      1.852278
     0.115935     -1.183897     -1.995479     -2.278329     -1.959136
    -1.340467     -0.932949      0.021790      0.313725     -0.517358
    -1.152891     -0.983285     -0.566518     -0.442565

! phi = -120.0
     1.357468      1.959160      2.698894      3.037857      3.698960
     3.558453      2.639296      2.773853      2.719664      1.627997
     0.705667     -0.785637     -2.118268     -2.628489     -1.803113
    -0.425969     -0.062320      0.439040      0.910952     -0.546994
    -0.968118     -0.856791     -0.250116      0.449309

! phi = -105.0
     2.045006      2.544424      2.818030      3.088582      3.370620
     3.551568      3.073520      2.903794      2.956634      2.124759
     0.906487     -0.823628     -2.090819     -2.241579     -1.456524
     0.206160      0.082195      0.771710      1.040241     -0.124647
    -0.316550     -0.164333      0.314474      0.733747

! phi = -90.0
     1.451735      2.748481      2.738185      3.156796      3.450028
     3.344157      3.180200      3.898724      3.335030      2.440579
     0.912671     -0.606502     -1.511772     -1.620864     -0.962798
    -0.020653      0.415153      0.908250      0.459433      0.145910
    -0.071054      0.017622      0.280839      0.748823

! phi = -75.0
     1.378160      3.345958      2.352424      3.063543      3.814070
     3.700796      3.580310      4.212293      3.536425      1.693809
     0.095172     -0.682452     -0.123614     -0.427765     -0.598368
     0.226352      0.423308      0.301999      0.551890      0.191719
    -0.253585     -0.190548     -0.253412      0.468922

! phi = -60.0
     0.237754      1.229980      1.716960      3.168570      4.208190
     4.391860      4.276080      3.673107      2.272295     -0.482789
    -0.406695     -0.038919     -0.357600     -0.823341     -0.173146
     0.139806      0.267796      0.322420      0.309664     -0.666399
    -0.948631     -1.534365     -1.479968     -0.204264

! phi = -45.0
    -1.184837      0.078060      2.347410      4.211350      5.376000
     5.389940      4.380200      2.461506      1.123713      0.107016
     0.007574     -0.149443     -0.797230     -0.582210      0.082910
     0.271580     -0.045570      0.379430      0.247770     -0.890956
    -1.582430     -1.954532     -1.980965     -2.000433
```

```
! phi = -30.0
    -1.174720      1.067030      4.180460      6.741610      6.070770
     4.806470      2.783340      1.320806      0.765978     -0.008448
     0.276860     -0.707140      1.314360      1.522590      1.915550
     2.223490      0.194290      0.534000      0.331780     -1.595147
    -2.849141     -3.550465     -3.277369     -2.655135

! phi = -15.0
     0.293590      5.588070      3.732620      3.217620      3.272450
     2.517320      1.588700      1.381760      0.856410      0.655170
     1.616970      0.846920      0.511070      0.740760      1.021020
     1.616580     -0.342400      0.181770     -0.613920     -2.558037
    -3.786839     -3.807325     -3.155346     -1.749204

! phi =   0.0
     2.832310      0.787990      0.323280      0.479230      0.628600
     0.976330      1.238750      1.671950      1.645480      2.520340
     1.606970      0.776350      0.119780      0.070390      0.121170
    -1.569230     -1.213010     -1.846360     -2.744510     -3.792530
    -3.934880     -3.615930     -2.675750     -0.924170

! phi =  15.0
    -0.778340     -1.912680     -2.052140     -1.846280     -1.047430
     0.183400      1.682950      2.223500      1.358370      2.448660
     1.436920      0.678570     -0.237060     -0.535320     -0.790380
    -2.182580     -3.251140     -4.195110     -4.269270     -3.908210
    -3.455620     -2.773970      1.755370      0.313410

! phi =  30.0
    -2.963810     -3.483730     -3.441809     -2.400349     -1.125083
     0.336200      1.428450      1.394630      0.970370      2.462720
     1.522430      0.553620     -0.407380     -1.482950     -3.613920
    -4.159810     -4.709721     -4.496271     -3.764540     -2.959140
    -1.963850     -1.071260     -1.599580     -2.445320

! phi =  45.0
    -4.021496     -3.836549     -3.365327     -2.334377     -0.984725
     0.362000      0.814380      0.754110      0.502370      1.903420
     0.770220     -0.416420     -3.286310     -3.875270     -4.611550
    -5.287977     -5.146239     -4.038627     -2.865450     -2.368170
    -2.860490     -3.416560     -3.666490     -3.595217

! phi =  60.0
    -3.353683     -2.984416     -2.317412     -1.240143     -0.257890
     0.722610      0.668070      0.438130      2.395330      1.632470
    -2.041450     -3.218100     -3.915080     -4.568574     -5.096776
    -5.526955     -5.005312     -3.777879     -2.840678     -3.508820
    -3.756430     -3.640810     -3.451845     -3.342810

! phi =  75.0
    -2.248733     -1.641080     -1.010583      0.039656      0.636063
     0.823710      0.517140     -0.013120     -0.370910     -1.192809
    -2.305650     -3.420580     -4.484960     -5.597237     -5.601264
    -5.727739     -4.740525     -3.819378     -3.685150     -4.151360
    -4.170739     -3.725589     -3.736732     -2.620673

! phi =  90.0
    -1.720840     -1.177830     -0.428430      0.277730      0.807900
     0.803260      0.482510     -0.336900     -0.786270     -1.774070
    -2.793220     -3.828560     -5.211800     -6.294328     -6.617221
    -5.763953     -5.072995     -3.911450     -4.158306     -4.473413
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    -4.099325     -3.769822     -3.157300     -2.651694

! phi = 105.0
    -1.850640     -1.092420     -0.445020      0.128490      1.005520
     0.884820      0.485850     -0.218470     -0.857670     -1.682330
    -3.014400     -4.481110     -6.053510     -6.865400     -6.871130
    -5.728240     -3.912230     -4.802110     -5.034640     -4.715990
    -4.600554     -4.086721     -3.274630     -2.410940

! phi = 120.0
    -1.969230     -1.116650     -0.540250     -0.150330      0.763520
     1.038890      0.758480      0.313530     -0.333050     -1.872770
    -3.366270     -5.008260     -6.124810     -7.034830     -6.724320
    -3.700200     -4.510620     -5.185650     -5.361620     -4.847490
    -4.444320     -4.004260     -3.415720     -2.751230

! phi = 135.0
    -2.111250     -1.168960     -0.322790     -0.006920      0.316660
     1.086270      0.939170      0.625340     -0.166360     -1.830310
    -3.469470     -4.946030     -6.112560     -1.915580     -4.047310
    -4.996740     -4.996730     -4.842690     -4.886620     -4.300540
    -4.494620     -4.442210     -4.163570     -3.183510

! phi = 150.0
    -1.757590     -0.403620      0.023920      0.362390      0.634520
     1.264920      1.361360      0.948420     -0.073680     -1.483560
    -3.152820      1.835120     -1.762860     -5.093660     -5.744830
    -5.390070     -4.783930     -4.190630     -4.115420     -4.042280
    -4.125570     -4.028550     -4.026100     -2.937910

! phi = 165.0
    -0.810590     -0.071500      0.378890      0.543310      1.277880
     1.641310      1.698840      1.519950      0.631950     -1.088670
    -2.736530     -0.735240     -4.563830     -6.408350     -5.889450
    -5.141750     -4.194970     -3.666490     -3.843450     -3.555000
    -3.548722     -3.246995     -2.751289     -1.814368


! alanine before proline map

C    NH1  CT1  C    NH1  CT1  C    N     24

! phi = -180.0
     0.126790      0.768700      0.971260      1.250970      2.121010
     2.720430      2.089440      1.789790      0.780870     -0.688474
     1.001130     -2.200520     -4.827670     -4.821447     -4.913223
    -3.591106     -2.766446     -2.784200     -2.454589     -2.346991
    -2.335350     -1.522656     -0.951542     -0.036650

! phi = -165.0
    -0.127133      1.377090      1.577020      1.872290      2.398990
     2.486630      2.436754      1.929070      1.086456      0.643400
     0.258676     -2.800440     -4.009477     -4.135306     -3.420090
    -2.602140     -2.299128     -1.501241     -1.101780     -0.861434
    -0.640168     -0.207701     -1.076344     -1.122030

! phi = -150.0
     0.084069      1.420317      1.624350      2.047200      2.653910
     2.716410      2.321416      1.985454      1.557466      2.463293
    -0.225720     -1.815886     -2.583256     -3.006154     -2.551995
    -1.890683     -1.354215     -0.727243      0.068512     -0.225016
```

```
    -0.765479     -1.283444     -1.293226     -0.816303

! phi = -135.0
     0.927992      1.521370      2.242218      2.546305      3.111384
     2.918410      2.460813      2.187970      2.058314      1.852278
     0.115935     -1.183897     -1.995479     -2.278329     -1.959136
    -1.340467     -0.932949      0.021790      0.313725     -0.517358
    -1.152891     -0.983285     -0.566518     -0.442565

! phi = -120.0
     1.357468      1.959160      2.698894      3.037857      3.698960
     3.558453      2.639296      2.773853      2.719664      1.627997
     0.705667     -0.785637     -2.118268     -2.628489     -1.803113
    -0.425969     -0.062320      0.439040      0.910952     -0.546994
    -0.968118     -0.856791     -0.250116      0.449309

! phi = -105.0
     2.045006      2.544424      2.818030      3.088582      3.370620
     3.551568      3.073520      2.903794      2.956634      2.124759
     0.906487     -0.823628     -2.090819     -2.241579     -1.456524
     0.206160      0.082195      0.771710      1.040241     -0.124647
    -0.316550     -0.164333      0.314474      0.733747

! phi = -90.0
     1.451735      2.748481      2.738185      3.156796      3.450028
     3.344157      3.180200      3.898724      3.335030      2.440579
     0.912671     -0.606502     -1.511772     -1.620864     -0.962798
    -0.020653      0.415153      0.908250      0.459433      0.145910
    -0.071054      0.017622      0.280839      0.748823

! phi = -75.0
     1.378160      3.345958      2.352424      3.063543      3.814070
     3.700796      3.580310      4.212293      3.536425      1.693809
     0.095172     -0.682452     -0.123614     -0.427765     -0.598368
     0.226352      0.423308      0.301999      0.551890      0.191719
    -0.253585     -0.190548     -0.253412      0.468922

! phi = -60.0
     0.237754      1.229980      1.716960      3.168570      4.208190
     4.391860      4.276080      3.673107      2.272295     -0.482789
    -0.406695     -0.038919     -0.357600     -0.823341     -0.173146
     0.139806      0.267796      0.322420      0.309664     -0.666399
    -0.948631     -1.534365     -1.479968     -0.204264

! phi = -45.0
    -1.184837      0.078060      2.347410      4.211350      5.376000
     5.389940      4.380200      2.461506      1.123713      0.107016
     0.007574     -0.149443     -0.797230     -0.582210      0.082910
     0.271580     -0.045570      0.379430      0.247770     -0.890956
    -1.582430     -1.954532     -1.980965     -2.000433

! phi = -30.0
    -1.174720      1.067030      4.180460      6.741610      6.070770
     4.806470      2.783340      1.320806      0.765978     -0.008448
     0.276860     -0.707140      1.314360      1.522590      1.915550
     2.223490      0.194290      0.534000      0.331780     -1.595147
    -2.849141     -3.550465     -3.277369     -2.655135

! phi = -15.0
     0.293590      5.588070      3.732620      3.217620      3.272450
     2.517320      1.588700      1.381760      0.856410      0.655170
```

```
     1.616970      0.846920      0.511070      0.740760      1.021020
     1.616580     -0.342400      0.181770     -0.613920     -2.558037
    -3.786839     -3.807325     -3.155346     -1.749204

! phi =   0.0
     2.832310      0.787990      0.323280      0.479230      0.628600
     0.976330      1.238750      1.671950      1.645480      2.520340
     1.606970      0.776350      0.119780      0.070390      0.121170
    -1.569230     -1.213010     -1.846360     -2.744510     -3.792530
    -3.934880     -3.615930     -2.675750     -0.924170

! phi =  15.0
    -0.778340     -1.912680     -2.052140     -1.846280     -1.047430
     0.183400      1.682950      2.223500      1.358370      2.448660
     1.436920      0.678570     -0.237060     -0.535320     -0.790380
    -2.182580     -3.251140     -4.195110     -4.269270     -3.908210
    -3.455620     -2.773970      1.755370      0.313410

! phi =  30.0
    -2.963810     -3.483730     -3.441809     -2.400349     -1.125083
     0.336200      1.428450      1.394630      0.970370      2.462720
     1.522430      0.553620     -0.407380     -1.482950     -3.613920
    -4.159810     -4.709721     -4.496271     -3.764540     -2.959140
    -1.963850     -1.071260     -1.599580     -2.445320

! phi =  45.0
    -4.021496     -3.836549     -3.365327     -2.334377     -0.984725
     0.362000      0.814380      0.754110      0.502370      1.903420
     0.770220     -0.416420     -3.286310     -3.875270     -4.611550
    -5.287977     -5.146239     -4.038627     -2.865450     -2.368170
    -2.860490     -3.416560     -3.666490     -3.595217

! phi =  60.0
    -3.353683     -2.984416     -2.317412     -1.240143     -0.257890
     0.722610      0.668070      0.438130      2.395330      1.632470
    -2.041450     -3.218100     -3.915080     -4.568574     -5.096776
    -5.526955     -5.005312     -3.777879     -2.840678     -3.508820
    -3.756430     -3.640810     -3.451845     -3.342810

! phi =  75.0
    -2.248733     -1.641080     -1.010583      0.039656      0.636063
     0.823710      0.517140     -0.013120     -0.370910     -1.192809
    -2.305650     -3.420580     -4.484960     -5.597237     -5.601264
    -5.727739     -4.740525     -3.819378     -3.685150     -4.151360
    -4.170739     -3.725589     -3.736732     -2.620673

! phi =  90.0
    -1.720840     -1.177830     -0.428430      0.277730      0.807900
     0.803260      0.482510     -0.336900     -0.786270     -1.774070
    -2.793220     -3.828560     -5.211800     -6.294328     -6.617221
    -5.763953     -5.072995     -3.911450     -4.158306     -4.473413
    -4.099325     -3.769822     -3.157300     -2.651694

! phi = 105.0
    -1.850640     -1.092420     -0.445020      0.128490      1.005520
     0.884820      0.485850     -0.218470     -0.857670     -1.682330
    -3.014400     -4.481110     -6.053510     -6.865400     -6.871130
    -5.728240     -3.912230     -4.802110     -5.034640     -4.715990
    -4.600554     -4.086721     -3.274630     -2.410940

! phi = 120.0
```

```
    -1.969230     -1.116650     -0.540250     -0.150330      0.763520
     1.038890      0.758480      0.313530     -0.333050     -1.872770
    -3.366270     -5.008260     -6.124810     -7.034830     -6.724320
    -3.700200     -4.510620     -5.185650     -5.361620     -4.847490
    -4.444320     -4.004260     -3.415720     -2.751230

! phi = 135.0
    -2.111250     -1.168960     -0.322790     -0.006920      0.316660
     1.086270      0.939170      0.625340     -0.166360     -1.830310
    -3.469470     -4.946030     -6.112560     -1.915580     -4.047310
    -4.996740     -4.996730     -4.842690     -4.886620     -4.300540
    -4.494620     -4.442210     -4.163570     -3.183510

! phi = 150.0
    -1.757590     -0.403620      0.023920      0.362390      0.634520
     1.264920      1.361360      0.948420     -0.073680     -1.483560
    -3.152820      1.835120     -1.762860     -5.093660     -5.744830
    -5.390070     -4.783930     -4.190630     -4.115420     -4.042280
    -4.125570     -4.028550     -4.026100     -2.937910

! phi = 165.0
    -0.810590     -0.071500      0.378890      0.543310      1.277880
     1.641310      1.698840      1.519950      0.631950     -1.088670
    -2.736530     -0.735240     -4.563830     -6.408350     -5.889450
    -5.141750     -4.194970     -3.666490     -3.843450     -3.555000
    -3.548722     -3.246995     -2.751289     -1.814368


! proline
! VTZ CBS map
C    N    CP1  C    N    CP1    C    NH1 24

! phi = -180
     2.973500      3.348200      3.062900      2.113400      1.040500
     0.770600      0.785200      0.263300     -0.479000     -0.583000
    -0.463800     -0.292600      0.000000      0.259100      0.177100
    -0.151200     -0.173500      0.211700      0.348900     -0.135600
    -0.950000     -1.256600     -0.292800      1.560000

! phi = -165
     5.674100      6.011400      5.562700      4.467300      3.390800
     3.008800      2.848600      2.311200      1.661400      1.468400
     1.142700      1.437400      2.113200      2.799500      2.989100
     2.869000      3.016100      3.328500      3.232900      2.547600
     1.647200      1.422700      2.517100      4.339800

! phi = -150
     6.752800      6.973200      6.444300      5.389800      4.438600
     4.046000      3.832800      3.442400      3.303500      3.010000
     2.838100      3.162200      3.778300      4.362800      4.603600
     4.546200      4.702100      4.837200      4.549500      3.849600
     3.099200      3.031800      4.060200      5.624800

! phi = -135
     7.627800      8.153400      7.342500      5.893500      4.799200
     4.433400      4.551500      4.442800      2.222200      0.776300
     0.790000      2.152300      3.932900      5.274900      5.830800
     5.988600      5.588500      5.211000      4.918000      4.292100
     3.495500      3.449800      4.617700      6.311700

! phi = -120
```

```
     8.115600      8.477200      7.754300      6.585000      5.537900
     4.964300      4.929000      4.421200      2.336100      1.257800
     1.769300      3.359900      5.018000      6.055500      6.217600
     5.726100      5.512200      5.820200      5.716700      4.872300
     4.066800      4.094600      5.284900      6.931500

! phi = -105
     9.249700      9.483000      8.668500      7.525300      7.003200
     6.834600      6.822100      5.287600      3.320600      2.640300
     3.464800      5.100300      6.537600      6.885600      5.842000
     5.248700      5.540200      6.652400      7.196700      6.625400
     5.710100      5.581700      6.651500      8.192800

! phi = -90
     9.335600      9.208000      8.564600      8.010200      7.885100
     8.212200      8.737100      8.429100      7.306500      6.474200
     6.651300      7.484700      8.195300      8.295000      7.407200
     6.529900      6.242000      6.227500      6.347300      6.449700
     6.404700      6.579300      7.391700      8.570700

! phi = -75
    10.955200     11.455400     11.173300     10.428700     10.062400
    10.044500      9.279600      6.965100      5.361500      5.102700
     6.267600      7.871600      8.009800      7.104500      6.616400
     6.733700      7.504000      8.664700      9.282800      8.795900
     7.872500      7.612400      8.498100      9.894000

! phi = -60
     8.422900      8.529200      8.608500      9.306400     10.239400
    11.025900     11.510800      9.283500      7.566000      6.624600
     7.038700      8.222400      8.786400      8.512000      8.103500
     7.988200      8.192900      8.291000      8.055600      7.436800
     6.651800      6.317000      6.802500      7.746300

! phi = -45
     6.913200      7.937400      8.610800      9.316600      9.388500
     9.408400      8.828800      7.297900      5.456400      4.742700
     5.793100      7.118800      7.565400      7.598500      7.438700
     7.512500      7.878100      8.082200      7.642700      6.320500
     4.680400      3.830500      4.215800      5.435200

! phi = -30
     5.466700      7.116000      8.908800      8.347200      7.413500
     7.047000      6.031600      4.193100      2.674800      3.023700
     4.485300      5.451700      6.214900      6.422600      6.229300
     6.191100      6.488900      6.646400      5.833400      3.751300
     1.719800      1.064900      1.955800      3.860800

! phi = -15
     3.061500      5.603800     12.179500      6.295200      5.323400
     4.826500      3.705600      2.461500      2.291600      3.145900
     3.562100      4.443600      5.337500      5.728800      5.694800
     5.641600      5.943300      6.169000      4.759500      2.569400
     1.357100      1.669800      3.212300      5.031900

! phi = 0
     8.085900      8.051100      5.023600      3.450800      2.836100
     2.192500      1.566200      1.456300      2.039300      1.945200
     2.188400      2.921300      3.467500      3.543500      3.374500
     3.472300      4.069900      3.615600      2.082200      0.958600
     0.792600      1.494200      2.794900      4.853100
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```
! phi = 15
     6.639500      5.177400      3.252300      1.952700      1.078400
     0.888300      1.505400      2.442300      2.178600      1.578600
     1.777400      2.395400      2.820200      2.795200      2.662400
     2.917100      2.562100      1.557900      1.322300      1.631400
     2.051200      2.555600      3.039100      4.915000

! phi = 30
     7.548800      5.095500      2.747000      0.955200      0.444500
     1.318700      2.733300      3.223200      2.565500      2.150900
     2.394400      2.939300      3.266000      3.210000      3.113400
     2.491300      0.978300      0.815300      1.522700      2.055600
     2.199900      2.327600      3.474200      7.977800

! phi = 45
     0.000000      0.000000      0.000000      0.000000      0.000000
     0.000000      0.000000      0.000000      0.000000      0.000000
     0.000000      0.000000      0.000000      0.000000      0.000000
     0.000000      0.000000      0.000000      0.000000      0.000000
     0.000000      0.000000      0.000000      0.000000

! phi = 60
     0.000000      0.000000      0.000000      0.000000      0.000000
     0.000000      0.000000      0.000000      0.000000      0.000000
     0.000000      0.000000      0.000000      0.000000      0.000000
     0.000000      0.000000      0.000000      0.000000      0.000000
     0.000000      0.000000      0.000000      0.000000

! phi = 75
     0.000000      0.000000      0.000000      0.000000      0.000000
     0.000000      0.000000      0.000000      0.000000      0.000000
     0.000000      0.000000      0.000000      0.000000      0.000000
     0.000000      0.000000      0.000000      0.000000      0.000000
     0.000000      0.000000      0.000000      0.000000

! phi = 90
     0.000000      0.000000      0.000000      0.000000      0.000000
     0.000000      0.000000      0.000000      0.000000      0.000000
     0.000000      0.000000      0.000000      0.000000      0.000000
     0.000000      0.000000      0.000000      0.000000      0.000000
     0.000000      0.000000      0.000000      0.000000

! phi = 105
     0.000000      0.000000      0.000000      0.000000      0.000000
     0.000000      0.000000      0.000000      0.000000      0.000000
     0.000000      0.000000      0.000000      0.000000      0.000000
     0.000000      0.000000      0.000000      0.000000      0.000000
     0.000000      0.000000      0.000000      0.000000

! phi = 120
     0.000000      0.000000      0.000000      0.000000      0.000000
     0.000000      0.000000      0.000000      0.000000      0.000000
     0.000000      0.000000      0.000000      0.000000      0.000000
     0.000000      0.000000      0.000000      0.000000      0.000000
     0.000000      0.000000      0.000000      0.000000

! phi = 135
     0.000000      0.000000      0.000000      0.000000      0.000000
     0.000000      0.000000      0.000000      0.000000      0.000000
     0.000000      0.000000      0.000000      0.000000      0.000000
```

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     0.000000      0.000000      0.000000      0.000000      0.000000
     0.000000      0.000000      0.000000      0.000000

! phi = 150
     0.000000      0.000000      0.000000      0.000000      0.000000
     0.000000      0.000000      0.000000      0.000000      0.000000
     0.000000      0.000000      0.000000      0.000000      0.000000
     0.000000      0.000000      0.000000      0.000000      0.000000
     0.000000      0.000000      0.000000      0.000000

! phi = 165
     0.000000      0.000000      0.000000      0.000000      0.000000
     0.000000      0.000000      0.000000      0.000000      0.000000
     0.000000      0.000000      0.000000      0.000000      0.000000
     0.000000      0.000000      0.000000      0.000000      0.000000
     0.000000      0.000000      0.000000      0.000000



!2 adjacent prolines
! VTZ CBS map
C    N    CP1  C    N    CP1    C    N 24

! phi = -180
     2.973500      3.348200      3.062900      2.113400      1.040500
     0.770600      0.785200      0.263300     -0.479000     -0.583000
    -0.463800     -0.292600      0.000000      0.259100      0.177100
    -0.151200     -0.173500      0.211700      0.348900     -0.135600
    -0.950000     -1.256600     -0.292800      1.560000

! phi = -165
     5.674100      6.011400      5.562700      4.467300      3.390800
     3.008800      2.848600      2.311200      1.661400      1.468400
     1.142700      1.437400      2.113200      2.799500      2.989100
     2.869000      3.016100      3.328500      3.232900      2.547600
     1.647200      1.422700      2.517100      4.339800

! phi = -150
     6.752800      6.973200      6.444300      5.389800      4.438600
     4.046000      3.832800      3.442400      3.303500      3.010000
     2.838100      3.162200      3.778300      4.362800      4.603600
     4.546200      4.702100      4.837200      4.549500      3.849600
     3.099200      3.031800      4.060200      5.624800

! phi = -135
     7.627800      8.153400      7.342500      5.893500      4.799200
     4.433400      4.551500      4.442800      2.222200      0.776300
     0.790000      2.152300      3.932900      5.274900      5.830800
     5.988600      5.588500      5.211000      4.918000      4.292100
     3.495500      3.449800      4.617700      6.311700

! phi = -120
     8.115600      8.477200      7.754300      6.585000      5.537900
     4.964300      4.929000      4.421200      2.336100      1.257800
     1.769300      3.359900      5.018000      6.055500      6.217600
     5.726100      5.512200      5.820200      5.716700      4.872300
     4.066800      4.094600      5.284900      6.931500

! phi = -105
     9.249700      9.483000      8.668500      7.525300      7.003200
     6.834600      6.822100      5.287600      3.320600      2.640300
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     3.464800      5.100300      6.537600      6.885600      5.842000
     5.248700      5.540200      6.652400      7.196700      6.625400
     5.710100      5.581700      6.651500      8.192800

! phi = -90
     9.335600      9.208000      8.564600      8.010200      7.885100
     8.212200      8.737100      8.429100      7.306500      6.474200
     6.651300      7.484700      8.195300      8.295000      7.407200
     6.529900      6.242000      6.227500      6.347300      6.449700
     6.404700      6.579300      7.391700      8.570700

! phi = -75
    10.955200     11.455400     11.173300     10.428700     10.062400
    10.044500      9.279600      6.965100      5.361500      5.102700
     6.267600      7.871600      8.009800      7.104500      6.616400
     6.733700      7.504000      8.664700      9.282800      8.795900
     7.872500      7.612400      8.498100      9.894000

! phi = -60
     8.422900      8.529200      8.608500      9.306400     10.239400
    11.025900     11.510800      9.283500      7.566000      6.624600
     7.038700      8.222400      8.786400      8.512000      8.103500
     7.988200      8.192900      8.291000      8.055600      7.436800
     6.651800      6.317000      6.802500      7.746300

! phi = -45
     6.913200      7.937400      8.610800      9.316600      9.388500
     9.408400      8.828800      7.297900      5.456400      4.742700
     5.793100      7.118800      7.565400      7.598500      7.438700
     7.512500      7.878100      8.082200      7.642700      6.320500
     4.680400      3.830500      4.215800      5.435200

! phi = -30
     5.466700      7.116000      8.908800      8.347200      7.413500
     7.047000      6.031600      4.193100      2.674800      3.023700
     4.485300      5.451700      6.214900      6.422600      6.229300
     6.191100      6.488900      6.646400      5.833400      3.751300
     1.719800      1.064900      1.955800      3.860800

! phi = -15
     3.061500      5.603800     12.179500      6.295200      5.323400
     4.826500      3.705600      2.461500      2.291600      3.145900
     3.562100      4.443600      5.337500      5.728800      5.694800
     5.641600      5.943300      6.169000      4.759500      2.569400
     1.357100      1.669800      3.212300      5.031900

! phi = 0
     8.085900      8.051100      5.023600      3.450800      2.836100
     2.192500      1.566200      1.456300      2.039300      1.945200
     2.188400      2.921300      3.467500      3.543500      3.374500
     3.472300      4.069900      3.615600      2.082200      0.958600
     0.792600      1.494200      2.794900      4.853100

! phi = 15
     6.639500      5.177400      3.252300      1.952700      1.078400
     0.888300      1.505400      2.442300      2.178600      1.578600
     1.777400      2.395400      2.820200      2.795200      2.662400
     2.917100      2.562100      1.557900      1.322300      1.631400
     2.051200      2.555600      3.039100      4.915000

! phi = 30
```

```
     7.548800      5.095500      2.747000      0.955200      0.444500
     1.318700      2.733300      3.223200      2.565500      2.150900
     2.394400      2.939300      3.266000      3.210000      3.113400
     2.491300      0.978300      0.815300      1.522700      2.055600
     2.199900      2.327600      3.474200      7.977800

! phi = 45
     0.000000      0.000000      0.000000      0.000000      0.000000
     0.000000      0.000000      0.000000      0.000000      0.000000
     0.000000      0.000000      0.000000      0.000000      0.000000
     0.000000      0.000000      0.000000      0.000000      0.000000
     0.000000      0.000000      0.000000      0.000000

! phi = 60
     0.000000      0.000000      0.000000      0.000000      0.000000
     0.000000      0.000000      0.000000      0.000000      0.000000
     0.000000      0.000000      0.000000      0.000000      0.000000
     0.000000      0.000000      0.000000      0.000000      0.000000
     0.000000      0.000000      0.000000      0.000000

! phi = 75
     0.000000      0.000000      0.000000      0.000000      0.000000
     0.000000      0.000000      0.000000      0.000000      0.000000
     0.000000      0.000000      0.000000      0.000000      0.000000
     0.000000      0.000000      0.000000      0.000000      0.000000
     0.000000      0.000000      0.000000      0.000000

! phi = 90
     0.000000      0.000000      0.000000      0.000000      0.000000
     0.000000      0.000000      0.000000      0.000000      0.000000
     0.000000      0.000000      0.000000      0.000000      0.000000
     0.000000      0.000000      0.000000      0.000000      0.000000
     0.000000      0.000000      0.000000      0.000000

! phi = 105
     0.000000      0.000000      0.000000      0.000000      0.000000
     0.000000      0.000000      0.000000      0.000000      0.000000
     0.000000      0.000000      0.000000      0.000000      0.000000
     0.000000      0.000000      0.000000      0.000000      0.000000
     0.000000      0.000000      0.000000      0.000000

! phi = 120
     0.000000      0.000000      0.000000      0.000000      0.000000
     0.000000      0.000000      0.000000      0.000000      0.000000
     0.000000      0.000000      0.000000      0.000000      0.000000
     0.000000      0.000000      0.000000      0.000000      0.000000
     0.000000      0.000000      0.000000      0.000000

! phi = 135
     0.000000      0.000000      0.000000      0.000000      0.000000
     0.000000      0.000000      0.000000      0.000000      0.000000
     0.000000      0.000000      0.000000      0.000000      0.000000
     0.000000      0.000000      0.000000      0.000000      0.000000
     0.000000      0.000000      0.000000      0.000000

! phi = 150
     0.000000      0.000000      0.000000      0.000000      0.000000
     0.000000      0.000000      0.000000      0.000000      0.000000
     0.000000      0.000000      0.000000      0.000000      0.000000
     0.000000      0.000000      0.000000      0.000000      0.000000
     0.000000      0.000000      0.000000      0.000000
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```
! phi = 165
     0.000000      0.000000      0.000000      0.000000      0.000000
     0.000000      0.000000      0.000000      0.000000      0.000000
     0.000000      0.000000      0.000000      0.000000      0.000000
     0.000000      0.000000      0.000000      0.000000      0.000000
     0.000000      0.000000      0.000000      0.000000



! glycine map
! VTZ CBS map
C    NH1  CT2  C    NH1  CT2  C    NH1   24

! phi = -180
     0.235350      0.182300      0.177200      0.396800      0.859400
     1.489700      2.092500      2.297700      1.808600      0.696200
    -0.563300     -1.432700     -1.015100      1.426300     -0.564300
     0.696200      1.808200      2.301700      2.092600      1.489100
     0.859500      0.396900      0.176900      0.182400

! phi = -165
     0.020100     -0.203800     -0.269700      0.014200      0.620800
     1.392400      2.046200      2.188200      1.683900      0.688500
    -0.373700     -0.703500      0.837800      3.704000     -0.730100
     0.594100      1.713100      2.205800      2.026400      1.529800
     1.027400      0.623800      0.348400      0.182800

! phi = -150
    -0.533600     -0.807400     -0.804600     -0.379800      0.365300
     1.168000      1.641000      1.618100      1.302200      0.615100
     0.065700      0.738500      2.959500     -2.036600     -0.934600
     0.407900      1.517000      1.984800      1.833100      1.435200
     0.995600      0.562200      0.150600     -0.209000

! phi = -135
    -1.208500     -1.429400     -1.319200     -0.817500     -0.112400
     0.454400      0.737600      0.879300      0.850100      0.670300
     0.943500     -2.651200     -2.829400     -2.199100     -1.065700
     0.279600      1.322000      1.668300      1.521300      1.193900
     0.765300      0.246000     -0.315500     -0.823200

! phi = -120
    -1.789100     -1.965500     -1.860700     -1.447900     -0.896500
    -0.401000     -0.015100      0.321300      0.634600      0.976300
    -1.977500     -2.883200     -2.848500     -2.137900     -0.960300
     0.308700      1.098100      1.245300      1.133600      0.881800
     0.448200     -0.153900     -0.823700     -1.404300

! phi = -105
    -2.246700     -2.487000     -2.473700     -2.135600     -1.577700
    -0.980600     -0.429100      0.144700      0.734000     -0.918300
    -2.299200     -2.882200     -2.668600     -1.847100     -0.719800
     0.107000      0.496000      0.553500      0.584300      0.494000
     0.098300     -0.529800     -1.237900     -1.840100

! phi = -90
    -2.851100     -3.181100     -3.199500     -2.785300     -2.054300
    -1.242900     -0.476500      0.288100     -0.045300     -1.470600
    -2.558800     -2.869400     -2.450300     -1.582200     -0.930800
    -0.426400     -0.022700      0.000000     -0.097400     -0.136100
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    -0.439600     -1.038600     -1.741000     -2.373200

! phi = -75
    -3.961800     -4.268200     -4.109000     -3.364700     -2.252200
    -1.140400     -0.209800      0.487300     -0.746200     -2.127700
    -2.932100     -2.898500     -2.247900     -1.730400     -1.177200
    -0.448200      0.034900     -0.073300     -0.531600     -0.933300
    -1.360700     -2.009200     -2.745700     -3.424900

! phi = -60
    -5.408000     -5.355100     -4.640100     -3.283200     -1.710200
    -0.423800      0.354400     -0.103700     -1.577700     -2.828300
    -3.151200     -2.649200     -2.183000     -1.761200     -0.981700
    -0.174700      0.262600      0.039200     -0.663000     -1.530700
    -2.478200     -3.465600     -4.334200     -5.011200

! phi = -45
    -6.093200     -5.298400     -3.816620     -1.922530     -0.196160
     0.768200      0.568500     -0.831300     -2.343900     -3.037100
    -2.663700     -2.191100     -2.022900     -1.438500     -0.649000
     0.077000      0.441500      0.257500     -0.491100     -1.820600
    -3.473100     -4.895200     -5.790700     -6.205900

! phi = -30
    -5.258225     -3.675795     -1.631110      0.430085      1.496470
     0.318200     -0.555100     -1.695500     -2.434200     -2.192600
    -1.691300     -1.890000     -1.708500     -1.206300     -0.567400
     0.054300      0.497200      0.599600     -0.171000     -2.137600
    -4.237000     -5.584100     -6.135100     -6.067000

! phi = -15
    -3.161820     -0.902080      1.432450     -1.452885     -1.560780
    -1.665600     -1.783100     -1.755100     -1.329300     -0.731100
    -1.317000     -1.662800     -1.601200     -1.294900     -0.817300
    -0.197100      0.549500      0.850400     -0.689700     -2.819900
    -4.393000     -5.111500     -5.205690     -4.654785

! phi = 0
     0.034035     -2.349860     -3.412065     -3.620070     -3.450950
    -2.875650     -1.787800     -0.541250      0.410450     -0.372500
    -1.126850     -1.498450     -1.608700     -1.498450     -1.126850
    -0.372500      0.410450     -0.541250     -1.787800     -2.875650
    -3.450950     -3.620070     -3.412065     -2.349860

! phi = 15
    -3.162345     -4.654785     -5.205690     -5.111500     -4.393000
    -2.819900     -0.689700      0.850400      0.549500     -0.197100
    -0.817300     -1.294900     -1.601200     -1.662800     -1.317000
    -0.731100     -1.329300     -1.755100     -1.783100     -1.665600
    -1.560780     -1.452885      1.432450     -0.902080

! phi = 30
    -5.258220     -6.067000     -6.135100     -5.584100     -4.237000
    -2.137600     -0.171000      0.599600      0.497200      0.054300
    -0.567400     -1.206300     -1.708500     -1.890000     -1.691300
    -2.192600     -2.434200     -1.695500     -0.555100      0.318200
     1.496470      0.430085     -1.631110     -3.675795

! phi = 45
    -6.093300     -6.205900     -5.790700     -4.895200     -3.473100
    -1.820600     -0.491100      0.257500      0.441500      0.077000
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    -0.649000     -1.438500     -2.022900     -2.191100     -2.663700
    -3.037100     -2.343900     -0.831300      0.568500      0.768200
    -0.196160     -1.922530     -3.816620     -5.298400

! phi = 60
    -5.407500     -5.011200     -4.334200     -3.465600     -2.478200
    -1.530700     -0.663000      0.039200      0.262600     -0.174700
    -0.981700     -1.761200     -2.183000     -2.649200     -3.151200
    -2.828300     -1.577700     -0.103700      0.354400     -0.423800
    -1.710200     -3.283200     -4.640100     -5.355100

! phi = 75
    -3.961900     -3.424900     -2.745700     -2.009200     -1.360700
    -0.933300     -0.531600     -0.073300      0.034900     -0.448200
    -1.177200     -1.730400     -2.247900     -2.898500     -2.932100
    -2.127700     -0.746200      0.487300     -0.209800     -1.140400
    -2.252200     -3.364700     -4.109000     -4.268200

! phi = 90
    -2.854500     -2.373200     -1.741000     -1.038600     -0.439600
    -0.136100     -0.097400      0.000000     -0.022700     -0.426400
    -0.930800     -1.582200     -2.450300     -2.869400     -2.558800
    -1.470600     -0.045300      0.288100     -0.476500     -1.242900
    -2.054300     -2.785300     -3.199500     -3.181100

! phi = 105
    -2.246400     -1.840100     -1.237900     -0.529800      0.098300
     0.494000      0.584300      0.553500      0.496000      0.107000
    -0.719800     -1.847100     -2.668600     -2.882200     -2.299200
    -0.918300      0.734000      0.144700     -0.429100     -0.980600
    -1.577700     -2.135600     -2.473700     -2.487000

! phi = 120
    -1.788800     -1.404300     -0.823700     -0.153900      0.448200
     0.881800      1.133600      1.245300      1.098100      0.308700
    -0.960300     -2.137900     -2.848500     -2.883200     -1.977500
     0.976300      0.634600      0.321300     -0.015100     -0.401000
    -0.896500     -1.447900     -1.860700     -1.965500

! phi = 135
    -1.208900     -0.823200     -0.315500      0.246000      0.765300
     1.193900      1.521300      1.668300      1.322000      0.279600
    -1.065700     -2.199100     -2.829400     -2.651200      0.943500
     0.670300      0.850100      0.879300      0.737600      0.454400
    -0.112400     -0.817500     -1.319200     -1.429400

! phi = 150
    -0.533400     -0.209000      0.150600      0.562200      0.995600
     1.435200      1.833100      1.984800      1.517000      0.407900
    -0.934600     -2.036600      2.959500      0.738500      0.065700
     0.615100      1.302200      1.618100      1.641000      1.168000
     0.365300     -0.379800     -0.804600     -0.807400

! phi = 165
     0.019900      0.182800      0.348400      0.623800      1.027400
     1.529800      2.026400      2.205800      1.713100      0.594100
    -0.730100      3.704000      0.837800     -0.703500     -0.373700
     0.688500      1.683900      2.188200      2.046200      1.392400
     0.620800      0.014200     -0.269700     -0.203800

! glycine before proline map: use glycine map
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```
! VTZ CBS map
C    NH1  CT2  C    NH1  CT2  C    N    24

! phi = -180
     0.235350      0.182300      0.177200      0.396800      0.859400
     1.489700      2.092500      2.297700      1.808600      0.696200
    -0.563300     -1.432700     -1.015100      1.426300     -0.564300
     0.696200      1.808200      2.301700      2.092600      1.489100
     0.859500      0.396900      0.176900      0.182400

! phi = -165
     0.020100     -0.203800     -0.269700      0.014200      0.620800
     1.392400      2.046200      2.188200      1.683900      0.688500
    -0.373700     -0.703500      0.837800      3.704000     -0.730100
     0.594100      1.713100      2.205800      2.026400      1.529800
     1.027400      0.623800      0.348400      0.182800

! phi = -150
    -0.533600     -0.807400     -0.804600     -0.379800      0.365300
     1.168000      1.641000      1.618100      1.302200      0.615100
     0.065700      0.738500      2.959500     -2.036600     -0.934600
     0.407900      1.517000      1.984800      1.833100      1.435200
     0.995600      0.562200      0.150600     -0.209000

! phi = -135
    -1.208500     -1.429400     -1.319200     -0.817500     -0.112400
     0.454400      0.737600      0.879300      0.850100      0.670300
     0.943500     -2.651200     -2.829400     -2.199100     -1.065700
     0.279600      1.322000      1.668300      1.521300      1.193900
     0.765300      0.246000     -0.315500     -0.823200

! phi = -120
    -1.789100     -1.965500     -1.860700     -1.447900     -0.896500
    -0.401000     -0.015100      0.321300      0.634600      0.976300
    -1.977500     -2.883200     -2.848500     -2.137900     -0.960300
     0.308700      1.098100      1.245300      1.133600      0.881800
     0.448200     -0.153900     -0.823700     -1.404300

! phi = -105
    -2.246700     -2.487000     -2.473700     -2.135600     -1.577700
    -0.980600     -0.429100      0.144700      0.734000     -0.918300
    -2.299200     -2.882200     -2.668600     -1.847100     -0.719800
     0.107000      0.496000      0.553500      0.584300      0.494000
     0.098300     -0.529800     -1.237900     -1.840100

! phi = -90
    -2.851100     -3.181100     -3.199500     -2.785300     -2.054300
    -1.242900     -0.476500      0.288100     -0.045300     -1.470600
    -2.558800     -2.869400     -2.450300     -1.582200     -0.930800
    -0.426400     -0.022700      0.000000     -0.097400     -0.136100
    -0.439600     -1.038600     -1.741000     -2.373200

! phi = -75
    -3.961800     -4.268200     -4.109000     -3.364700     -2.252200
    -1.140400     -0.209800      0.487300     -0.746200     -2.127700
    -2.932100     -2.898500     -2.247900     -1.730400     -1.177200
    -0.448200      0.034900     -0.073300     -0.531600     -0.933300
    -1.360700     -2.009200     -2.745700     -3.424900

! phi = -60
    -5.408000     -5.355100     -4.640100     -3.283200     -1.710200
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    -0.423800     0.354400    -0.103700    -1.577700    -2.828300
    -3.151200    -2.649200    -2.183000    -1.761200    -0.981700
    -0.174700     0.262600     0.039200    -0.663000    -1.530700
    -2.478200    -3.465600    -4.334200    -5.011200

! phi = -45
    -6.093200    -5.298400    -3.816620    -1.922530    -0.196160
     0.768200     0.568500    -0.831300    -2.343900    -3.037100
    -2.663700    -2.191100    -2.022900    -1.438500    -0.649000
     0.077000     0.441500     0.257500    -0.491100    -1.820600
    -3.473100    -4.895200    -5.790700    -6.205900

! phi = -30
    -5.258225    -3.675795    -1.631110     0.430085     1.496470
     0.318200    -0.555100    -1.695500    -2.434200    -2.192600
    -1.691300    -1.890000    -1.708500    -1.206300    -0.567400
     0.054300     0.497200     0.599600    -0.171000    -2.137600
    -4.237000    -5.584100    -6.135100    -6.067000

! phi = -15
    -3.161820    -0.902080     1.432450    -1.452885    -1.560780
    -1.665600    -1.783100    -1.755100    -1.329300    -0.731100
    -1.317000    -1.662800    -1.601200    -1.294900    -0.817300
    -0.197100     0.549500     0.850400    -0.689700    -2.819900
    -4.393000    -5.111500    -5.205690    -4.654785

! phi = 0
     0.034035    -2.349860    -3.412065    -3.620070    -3.450950
    -2.875650    -1.787800    -0.541250     0.410450    -0.372500
    -1.126850    -1.498450    -1.608700    -1.498450    -1.126850
    -0.372500     0.410450    -0.541250    -1.787800    -2.875650
    -3.450950    -3.620070    -3.412065    -2.349860

! phi = 15
    -3.162345    -4.654785    -5.205690    -5.111500    -4.393000
    -2.819900    -0.689700     0.850400     0.549500    -0.197100
    -0.817300    -1.294900    -1.601200    -1.662800    -1.317000
    -0.731100    -1.329300    -1.755100    -1.783100    -1.665600
    -1.560780    -1.452885     1.432450    -0.902080

! phi = 30
    -5.258220    -6.067000    -6.135100    -5.584100    -4.237000
    -2.137600    -0.171000     0.599600     0.497200     0.054300
    -0.567400    -1.206300    -1.708500    -1.890000    -1.691300
    -2.192600    -2.434200    -1.695500    -0.555100     0.318200
     1.496470     0.430085    -1.631110    -3.675795

! phi = 45
    -6.093300    -6.205900    -5.790700    -4.895200    -3.473100
    -1.820600    -0.491100     0.257500     0.441500     0.077000
    -0.649000    -1.438500    -2.022900    -2.191100    -2.663700
    -3.037100    -2.343900    -0.831300     0.568500     0.768200
    -0.196160    -1.922530    -3.816620    -5.298400

! phi = 60
    -5.407500    -5.011200    -4.334200    -3.465600    -2.478200
    -1.530700    -0.663000     0.039200     0.262600    -0.174700
    -0.981700    -1.761200    -2.183000    -2.649200    -3.151200
    -2.828300    -1.577700    -0.103700     0.354400    -0.423800
    -1.710200    -3.283200    -4.640100    -5.355100
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! phi = 75
    -3.961900     -3.424900     -2.745700     -2.009200     -1.360700
    -0.933300     -0.531600     -0.073300      0.034900     -0.448200
    -1.177200     -1.730400     -2.247900     -2.898500     -2.932100
    -2.127700     -0.746200      0.487300     -0.209800     -1.140400
    -2.252200     -3.364700     -4.109000     -4.268200

! phi = 90
    -2.854500     -2.373200     -1.741000     -1.038600     -0.439600
    -0.136100     -0.097400      0.000000     -0.022700     -0.426400
    -0.930800     -1.582200     -2.450300     -2.869400     -2.558800
    -1.470600     -0.045300      0.288100     -0.476500     -1.242900
    -2.054300     -2.785300     -3.199500     -3.181100

! phi = 105
    -2.246400     -1.840100     -1.237900     -0.529800      0.098300
     0.494000      0.584300      0.553500      0.496000      0.107000
    -0.719800     -1.847100     -2.668600     -2.882200     -2.299200
    -0.918300      0.734000      0.144700     -0.429100     -0.980600
    -1.577700     -2.135600     -2.473700     -2.487000

! phi = 120
    -1.788800     -1.404300     -0.823700     -0.153900      0.448200
     0.881800      1.133600      1.245300      1.098100      0.308700
    -0.960300     -2.137900     -2.848500     -2.883200     -1.977500
     0.976300      0.634600      0.321300     -0.015100     -0.401000
    -0.896500     -1.447900     -1.860700     -1.965500

! phi = 135
    -1.208900     -0.823200     -0.315500      0.246000      0.765300
     1.193900      1.521300      1.668300      1.322000      0.279600
    -1.065700     -2.199100     -2.829400     -2.651200      0.943500
     0.670300      0.850100      0.879300      0.737600      0.454400
    -0.112400     -0.817500     -1.319200     -1.429400

! phi = 150
    -0.533400     -0.209000      0.150600      0.562200      0.995600
     1.435200      1.833100      1.984800      1.517000      0.407900
    -0.934600     -2.036600      2.959500      0.738500      0.065700
     0.615100      1.302200      1.618100      1.641000      1.168000
     0.365300     -0.379800     -0.804600     -0.807400

! phi = 165
     0.019900      0.182800      0.348400      0.623800      1.027400
     1.529800      2.026400      2.205800      1.713100      0.594100
    -0.730100      3.704000      0.837800     -0.703500     -0.373700
     0.688500      1.683900      2.188200      2.046200      1.392400
     0.620800      0.014200     -0.269700     -0.203800
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