Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supplementary Information

for

Molecular Docking and Molecular Dynamics Simulation Studies on Adsorption/Desorption Behavior of Bone Morphogenetic Protein-7 on β-tricalcium Phosphate Surface

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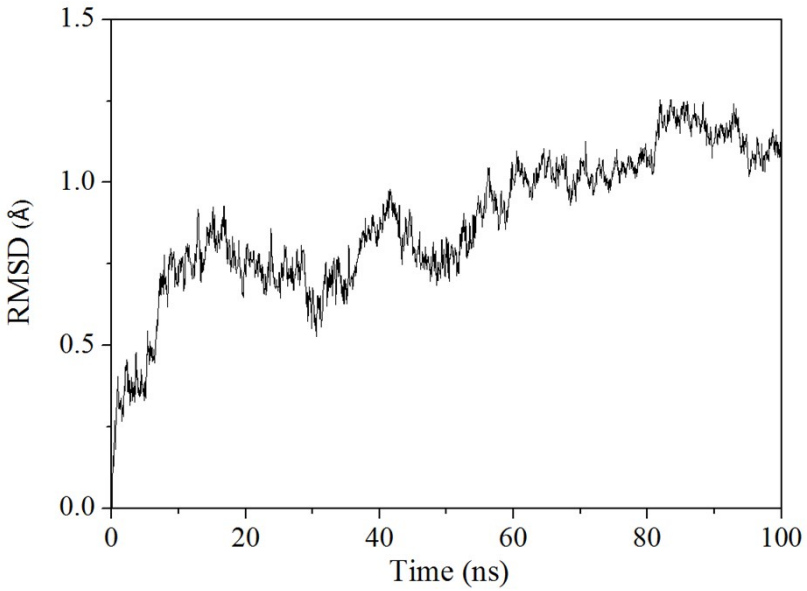

Fig. S1 RMSD values of BMP-7 backbone during 100ns dynamic simulation.

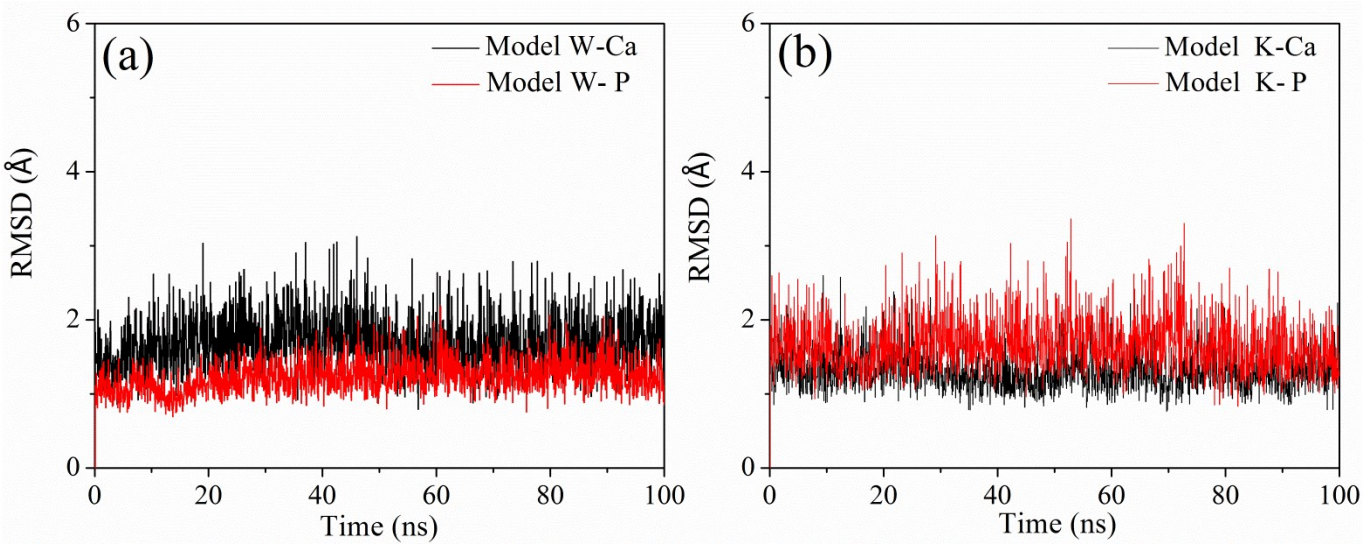

Fig. S2 RMSD values of BMP-7 backbone in four target models. (a) Model **W-Ca** and **W-P**, (b) Model **K-Ca** and **K-P**.

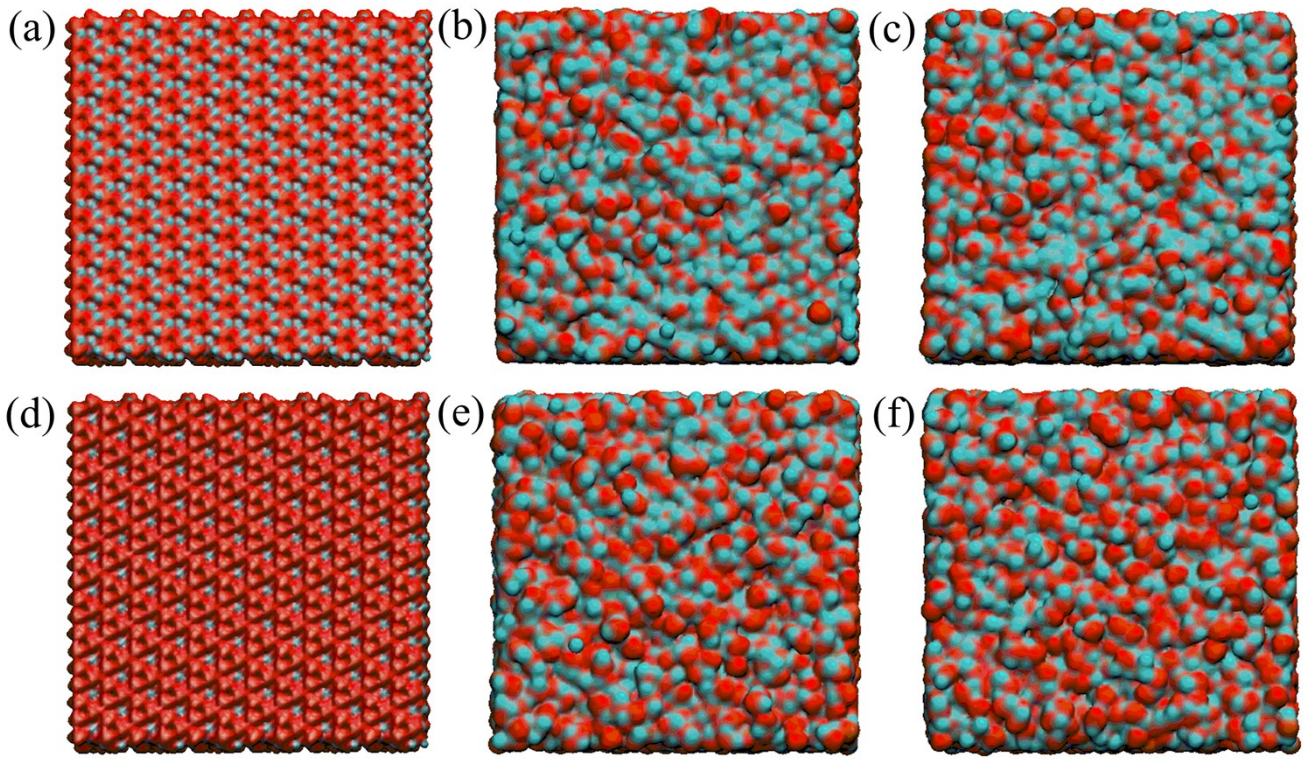

Fig. S3 Top view of β-TCP (001) Ca-rich and P-rich surfaces by VMD quicksurf module. Surfaces before molecular dynamics (a) Ca-rich initial surface, (d) P-rich initial surface. Surfaces after molecular dynamics: (b) Model **W-Ca**, (c) Model **K-Ca**, (e) Model **W-P**, and (f) Model **K-P**. Color codes: Ca^{2+}, cyan; PO_4^{3-}, red.

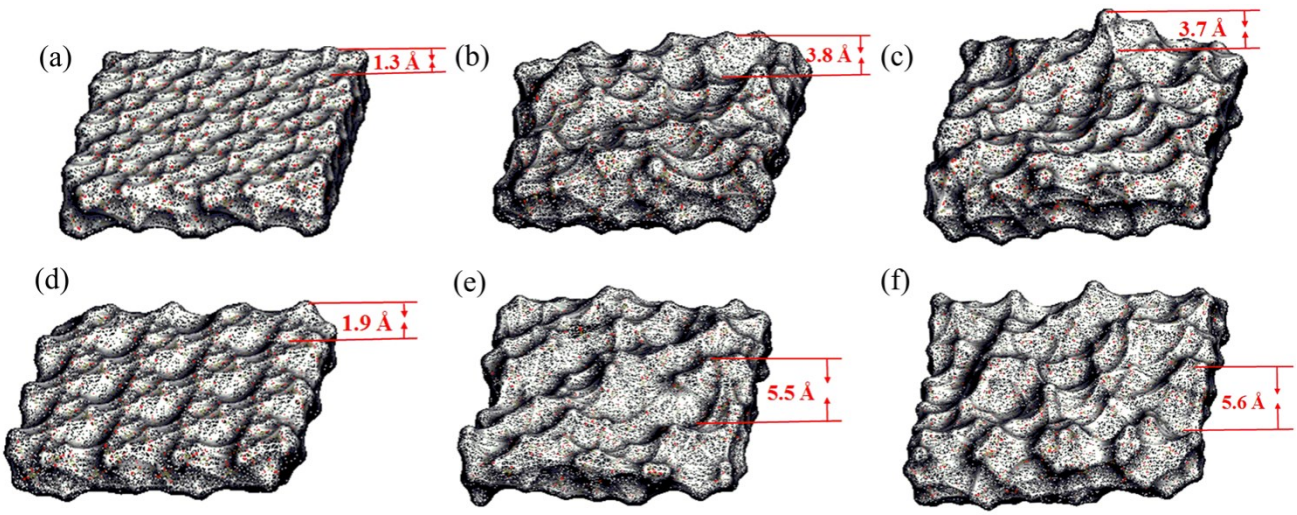

Fig. S4 Morphology of the β-TCP surfaces in the four target models. (a) and (b) show the grooves on the Ca-rich and P-rich surfaces before MD, respectively. (b)(c)(e)(f) are surfaces after MD: (b) Model **W-Ca**, (c) Model **K-Ca**, (e) Model **W-P**, and (f) Model **K-P**.

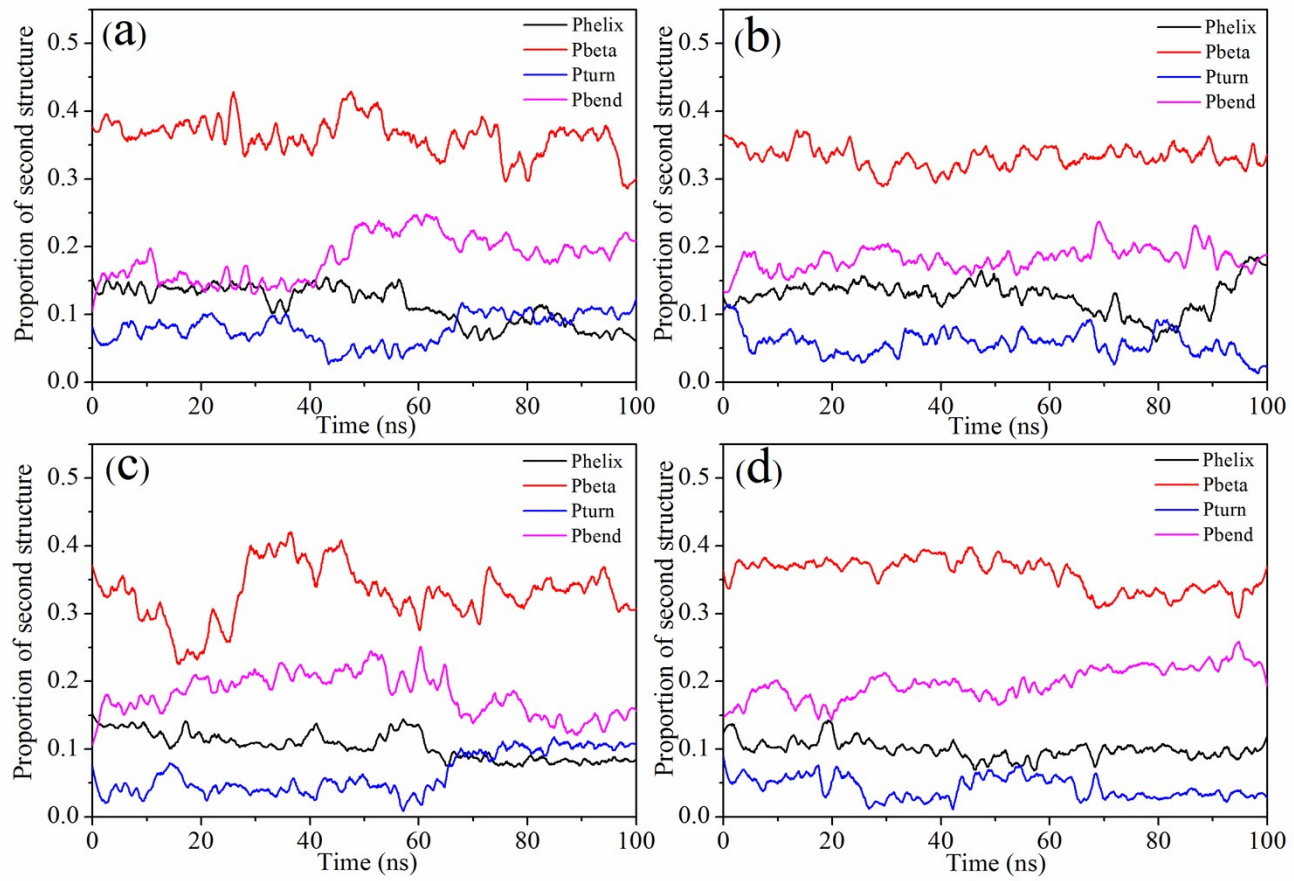

Fig. S5 The proportion of second structure for BMP-7 during the MD simulation. (a) Model **W-Ca**, (b) Model **K-Ca**, (c) Model **W-P**, and (d) Model **K-P**.

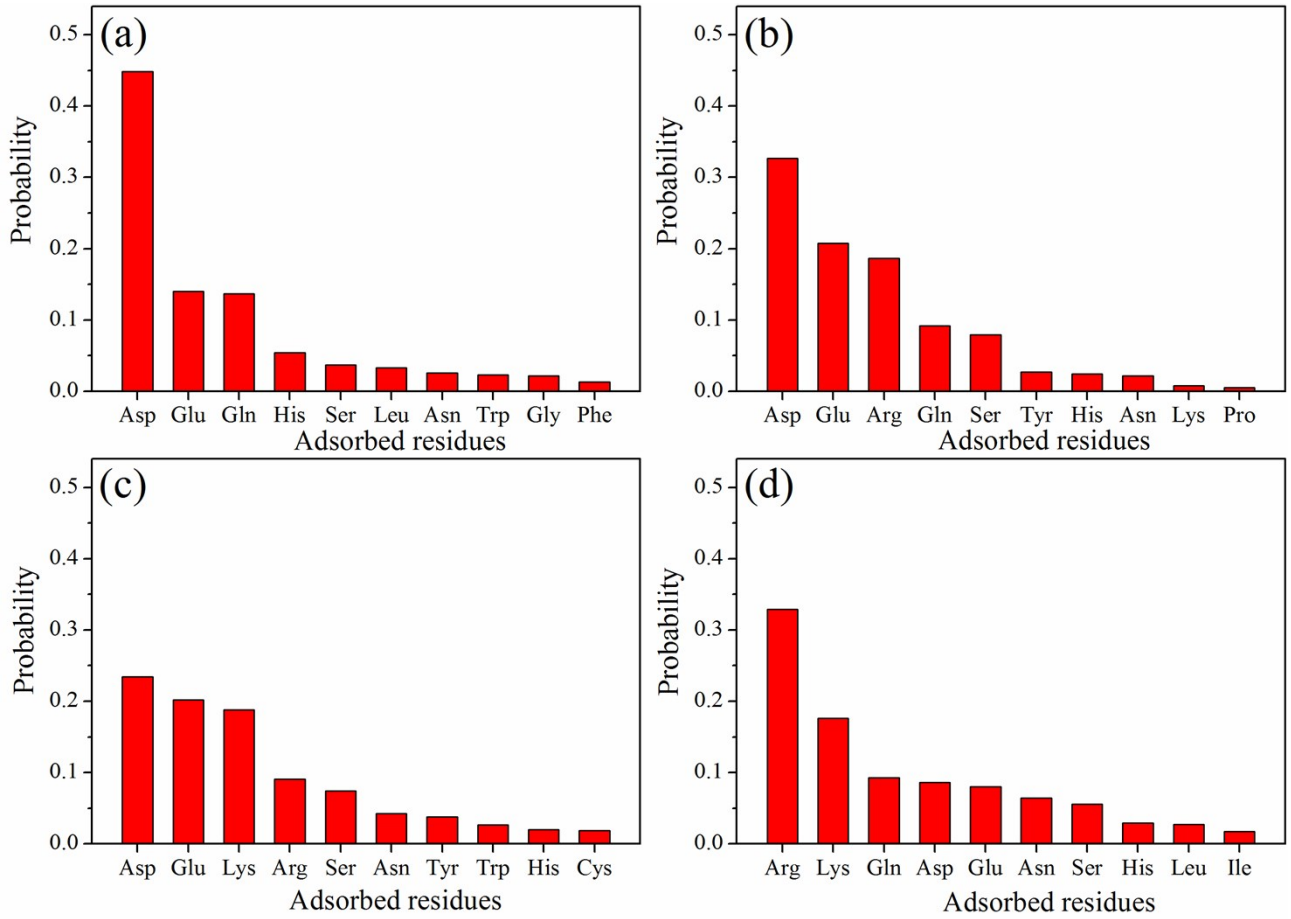

Fig. S6 Proportion of adsorbed residues of BMP-7 on the β-TCP surfaces. (a) Model **W-Ca**, (b) Model **K-Ca**, (c) Model **W-P**, and (d) Model **K-P**.

Table S1 The total number of atoms in BMP-7, β-TCP, water and ions (Na^+ and Cl^-) for each model in the dynamic simulations

Models	BMP-7	β-TCP	Water	Ions (Na^+ and Cl^-)
W-Ca	1741	22880	110802	148
K-Ca	1741	22880	110856	148
W-P	1741	21840	111018	148
K-P	1741	21840	110889	148

Table S2 Ten models with the lowest scoring energy among the 1000 docking structures on β-TCP (001) Ca-rich surface

Docking Structures		**Scoring Energy**
Model **Ws-Ca**	1	-161.2
	2	-155.6
	3	-155.5
	4	-155.0
	5	-154.4
	6	-153.6
Model **Ks-Ca**	1	-156.2
	2	-155.8
Model **Others-Ca**	1	-158.1
	2	-157.2

Table S3 Ten models with the lowest scoring energy among the 1000 docking structures on β-TCP (001) P-rich surface

Docking Structures		**Scoring Energy**
Model **Ws-P**	1	-158.2
	2	-158.1
Model **Ks-P**	1	-158.4
	2	-158.0
	3	-157.8
	4	-157.7
	5	-157.1
Model **Others-P**	1	-165.6
	2	-163.6
	3	-161.7

The INTERFACE potential is in the 12-6 Lennard-Jones formula, and the specific function form of IFF is as follows:[1]

$$E_{total} = \sum_{bonds} k_{r,ij}(r_{ij} - r_{0,ij})^2 + \sum_{angles} k_{\Theta,ijk}(\Theta_{ijk} - \Theta_{0,ijk})^2 + \sum_{ijnonbonded} \frac{q_i q_j}{4\pi\varepsilon_0 r_{ij}} + \sum_{ijnonbonded} \varepsilon_{ij}\left[\left(\frac{\sigma_{ij}}{r_{ij}}\right)^{12} - 2\left(\frac{\sigma_{ij}}{r_{ij}}\right)^{6}\right] \quad \ldots(1)$$

The interaction strength between BMP-7 and β-TCP surfaces was evaluated by the calculated interaction energies. The formulas for calculating the interaction energy (E_{int}) are as follows:

$$E_{int} = E_{total(\beta\text{-TCP+ BMP-7})} - E_{total(\beta\text{-TCP})} - E_{total(BMP\text{-7})} \quad ...(2)$$

$$E_{total} = E_{vdw} + E_{Coulomb} \quad ...(3)$$

$$E_{vdw}(i,j) = \varepsilon_{i,j}[(\frac{\sigma_{i,j}}{d_{i,j}})^{12} - 2(\frac{\sigma_{i,j}}{d_{i,j}})^{6}] \quad ...(4)$$

$$E_{Coulomb}(i,j) = \frac{C_0 q_i q_j}{\varepsilon} \frac{1}{d_{i,j}} \quad ...(5)$$

The formula 3 to 5 were referenced from Rosetta.[2, 3] In these formulas, E_{vdw} and $E_{Coulomb}$ represent the energy of Van der Waals and coulomb, respectively. E_{total} is the sum energy of Van der Waals and coulomb. The $E_{total(\beta\text{-TCP+BMP-7})}$, $E_{total(\beta\text{-TCP})}$, and $E_{total(BMP\text{-7})}$ represent the intramolecular and intermolecular interactions of the (β-TCP and protein), β-TCP, and BMP-7, respectively. Then we calculated the interaction energy by formula 2.

The force filed parameters we used were as follows:

Lammps Data File:

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Pair Coeffs

1	0.046	0.4000135	0.046	0.4000135	# H
2	0.046	0.4000135	0.046	0.4000135	# HC
3	0.022	2.351973	0.022	2.351973	# HA
4	0.046	0.4000135	0.046	0.4000135	# HT
5	0.03	2.420037	0.03	2.420037	# HP
6	0.022	2.351973	0.022	2.351973	# HB
7	0.046	1.603618	0.046	1.603618	# HR1
8	0.0078	2.615679	0.0078	2.615679	# HR3
9	0.1	0.8018088	0.1	0.8018088	# HS
10	0.11	3.563595	0.11	3.563595	# C
11	0.07	3.550053	0.07	3.550053	# CA
12	0.02	4.053589	0.01	3.385415	# CT1
13	0.055	3.875409	0.01	3.385415	# CT2
14	0.08	3.670503	0.01	3.385415	# CT3
15	0.05	3.207235	0.05	3.207235	# CPH1
16	0.05	3.207235	0.05	3.207235	# CPH2
17	0.09	3.207235	0.09	3.385415	# CPT
18	0.07	3.550053	0.07	3.550053	# CY
19	0.02	4.053589	0.01	3.385415	# CP1
20	0.055	3.875409	0.01	3.385415	# CP2
21	0.055	3.875409	0.01	3.385415	# CP3
22	0.07	3.563595	0.07	3.563595	# CC
23	0.2	3.296325	0.0001	3.296325	# N
24	0.2	3.296325	0.2	3.296325	# NR1
25	0.2	3.296325	0.2	3.296325	# NR2
26	0.2	3.296325	0.2	2.761786	# NH1
27	0.2	3.296325	0.2	3.296325	# NH2
28	0.2	3.296325	0.2	3.296325	# NH3
29	0.2	3.296325	0.2	3.296325	# NC2
30	0.2	3.296325	0.2	3.296325	# NY
31	0.12	3.029056	0.12	2.494516	# O
32	0.12	3.029056	0.12	3.029056	# OC
33	0.1521	3.153781	0.1521	3.153781	# OH1
34	0.1521	3.150574	0.1521	3.150574	# OT
35	0.45	3.563595	0.45	3.563595	# S
36	**0.28**	**4.300000**	**0.28**	**4.300000**	**# P8**
37	**0.07**	**3.400000**	**0.07**	**3.400000**	**# OP8**
38	**0.13**	**3.300000**	**0.13**	**3.300000**	**# CA8**

39	0.15	4.04468	0.15	4.04468	# CL
40	0.0469	2.429926	0.0469	2.429926	# NA

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Bond Coeffs

1	250	1.49	# C	CP1
2	250	1.49	# C	CT1
3	250	1.49	# C	CT2
4	260	1.3	# C	N
5	463	1.365	# C	NC2
6	370	1.345	# C	NH1
7	620	1.23	# C	O
8	305	1.375	# CA	CA
9	305	1.368	# CA	CPT
10	230	1.49	# CA	CT2
11	350	1.365	# CA	CY
12	340	1.08	# CA	HP
13	270	1.37	# CA	NY
14	334.3	1.411	# CA	OH1
15	200	1.522	# CC	CT1
16	200	1.522	# CC	CT2
17	430	1.36	# CC	NH2
18	650	1.23	# CC	O
19	525	1.26	# CC	OC
20	222.5	1.527	# CP1	CP2
21	330	1.08	# CP1	HB
22	320	1.434	# CP1	N
23	222.5	1.537	# CP2	CP2
24	222.5	1.537	# CP2	CP3
25	309	1.111	# CP2	HA
26	309	1.111	# CP3	HA
27	320	1.455	# CP3	N
28	410	1.36	# CPH1	CPH1
29	229.63	1.5	# CPH1	CT2
30	365	1.083	# CPH1	HR3
31	400	1.38	# CPH1	NR1
32	400	1.38	# CPH1	NR2
33	340	1.09	# CPH2	HR1
34	400	1.36	# CPH2	NR1
35	400	1.32	# CPH2	NR2
36	360	1.4	# CPT	CPT
37	350	1.44	# CPT	CY
38	270	1.375	# CPT	NY
39	222.5	1.5	# CT1	CT1

40	222.5	1.538	# CT1	CT2
41	222.5	1.538	# CT1	CT3
42	309	1.111	# CT1	HA
43	330	1.08	# CT1	HB
44	320	1.43	# CT1	NH1
45	200	1.48	# CT1	NH3
46	428	1.42	# CT1	OH1
47	222.5	1.53	# CT2	CT2
48	222.5	1.528	# CT2	CT3
49	230	1.51	# CT2	CY
50	309	1.111	# CT2	HA
51	330	1.08	# CT2	HB
52	261	1.49	# CT2	NC2
53	320	1.43	# CT2	NH1
54	200	1.48	# CT2	NH3
55	428	1.42	# CT2	OH1
56	198	1.818	# CT2	S
57	322	1.111	# CT3	HA
58	240	1.816	# CT3	S
59	440	0.997	# H	NH1
60	480	1	# H	NH2
61	466	1	# H	NR1
62	465	0.976	# H	NY
63	545	0.96	# H	OH1
64	455	1	# HC	NC2
65	403	1.04	# HC	NH3
66	275	1.325	# HS	S
67	412.2848	1	# HT	OT
68	**430**	**1.57**	**# OP8**	**P8**

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Angle Coeffs

1	52	112.3	0	0	# C	CP1	CP2
2	50	112	0	0	# C	CP1	HB
3	50	108.2	0	0	# C	CP1	N
4	52	108	0	0	# C	CT1	CT1
5	52	108	0	0	# C	CT1	CT2
6	52	108	0	0	# C	CT1	CT3
7	50	109.5	0	0	# C	CT1	HB
8	50	107	0	0	# C	CT1	NH1
9	43.7	110	0	0	# C	CT1	NH3
10	50	109.5	0	0	# C	CT2	HB
11	50	107	0	0	# C	CT2	NH1
12	60	117	0	0	# C	N	CP1

13	60	117	0	0	# C	N	CP3
14	62.3	120	0	0	# C	NC2	CT2
15	49	120	0	0	# C	NC2	HC
16	50	120	0	0	# C	NH1	CT1
17	50	120	0	0	# C	NH1	CT2
18	34	123	0	0	# C	NH1	H
19	40	120	35	2.4162	# CA	CA	CA
20	60	118	0	0	# CA	CA	CPT
21	45.8	122.3	0	0	# CA	CA	CT2
22	30	120	22	2.1525	# CA	CA	HP
23	45.2	120	0	0	# CA	CA	OH1
24	60	122	0	0	# CA	CPT	CPT
25	160	130.6	0	0	# CA	CPT	CY
26	160	130.6	0	0	# CA	CPT	NY
27	51.8	107.5	0	0	# CA	CT2	CT1
28	49.3	107.5	0	0	# CA	CT2	HA
29	120	107.4	25	2.261	# CA	CY	CPT
30	45.8	129.4	0	0	# CA	CY	CT2
31	110	108	0	0	# CA	NY	CPT
32	28	126	0	0	# CA	NY	H
33	65	108	0	0	# CA	OH1	H
34	52	108	0	0	# CC	CT1	CT2
35	50	109.5	0	0	# CC	CT1	HB
36	50	107	0	0	# CC	CT1	NH1
37	52	108	0	0	# CC	CT2	CT1
38	52	108	0	0	# CC	CT2	CT2
39	33	109.5	30	2.163	# CC	CT2	HA
40	50	120	0	0	# CC	NH2	H
41	80	116.5	0	0	# CP1	C	NH1
42	80	118	0	0	# CP1	C	O
43	70	108.5	0	0	# CP1	CP2	CP2
44	33.43	110.1	22.53	2.179	# CP1	CP2	HA
45	100	114.2	0	0	# CP1	N	CP3
46	35	118	0	0	# CP2	CP1	HB
47	70	110.8	0	0	# CP2	CP1	N
48	70	108.5	0	0	# CP2	CP2	CP3
49	26.5	110.1	22.53	2.179	# CP2	CP2	HA
50	26.5	110.1	22.53	2.179	# CP2	CP3	HA
51	70	110.5	0	0	# CP2	CP3	N
52	26.5	110.1	22.53	2.179	# CP3	CP2	HA
53	45.8	130	0	0	# CPH1	CPH1	CT2
54	25	130	20	2.2	# CPH1	CPH1	HR3
55	130	106	0	0	# CPH1	CPH1	NR1
56	130	110	0	0	# CPH1	CPH1	NR2

57	58.35	113	0	0	#	CPH1	CT2	CT1
58	33.43	109.5	0	0	#	CPH1	CT2	HA
59	130	107.5	0	0	#	CPH1	NR1	CPH2
60	30	125.5	20	2.15	#	CPH1	NR1	H
61	130	104	0	0	#	CPH1	NR2	CPH2
62	30	127	20	2.14	#	CPH2	NR1	H
63	30	122	22	2.146	#	CPT	CA	HP
64	110	107.4	0	0	#	CPT	CPT	CY
65	110	107.4	0	0	#	CPT	CPT	NY
66	45.8	124	0	0	#	CPT	CY	CT2
67	28	126	0	0	#	CPT	NY	H
68	20	112.5	0	0	#	CT1	C	N
69	80	116.5	0	0	#	CT1	C	NH1
70	80	121	0	0	#	CT1	C	O
71	40	118	50	2.388	#	CT1	CC	OC
72	53.35	111	8	2.561	#	CT1	CT1	CT2
73	53.35	108.5	8	2.561	#	CT1	CT1	CT3
74	34.5	110.1	22.53	2.179	#	CT1	CT1	HA
75	35	111	0	0	#	CT1	CT1	HB
76	70	113.5	0	0	#	CT1	CT1	NH1
77	75.7	110.1	0	0	#	CT1	CT1	OH1
78	58.35	113.5	11.16	2.561	#	CT1	CT2	CT1
79	58.35	113.5	11.16	2.561	#	CT1	CT2	CT2
80	58.35	113.5	11.16	2.561	#	CT1	CT2	CT3
81	58.35	114	0	0	#	CT1	CT2	CY
82	33.43	110.1	22.53	2.179	#	CT1	CT2	HA
83	75.7	110.1	0	0	#	CT1	CT2	OH1
84	58	112.5	0	0	#	CT1	CT2	S
85	33.43	110.1	22.53	2.179	#	CT1	CT3	HA
86	35	117	0	0	#	CT1	NH1	H
87	30	109.5	20	2.074	#	CT1	NH3	HC
88	57.5	106	0	0	#	CT1	OH1	H
89	80	116.5	0	0	#	CT2	C	NH1
90	80	121	0	0	#	CT2	C	O
91	50	116.5	50	2.45	#	CT2	CC	NH2
92	15	121	50	2.44	#	CT2	CC	O
93	40	118	50	2.388	#	CT2	CC	OC
94	45.8	120	0	0	#	CT2	CPH1	NR2
95	53.35	114	8	2.561	#	CT2	CT1	CT3
96	34.5	110.1	22.53	2.179	#	CT2	CT1	HA
97	35	111	0	0	#	CT2	CT1	HB
98	70	113.5	0	0	#	CT2	CT1	NH1
99	67.7	110	0	0	#	CT2	CT1	NH3
100	58.35	113.6	11.16	2.561	#	CT2	CT2	CT2

101	26.5	110.1	22.53	2.179	#	CT2	CT2	HA
102	67.7	107.5	0	0	#	CT2	CT2	NC2
103	67.7	110	0	0	#	CT2	CT2	NH3
104	58	114.5	0	0	#	CT2	CT2	S
105	34.6	110.1	22.53	2.179	#	CT2	CT3	HA
106	40.4	120	0	0	#	CT2	NC2	HC
107	35	117	0	0	#	CT2	NH1	H
108	30	109.5	20	2.074	#	CT2	NH3	HC
109	57.5	106	0	0	#	CT2	OH1	H
110	34	95	0	0	#	CT2	S	CT3
111	38.8	95	0	0	#	CT2	S	HS
112	53.35	114	8	2.561	#	CT3	CT1	CT3
113	34.5	110.1	22.53	2.179	#	CT3	CT1	HA
114	35	111	0	0	#	CT3	CT1	HB
115	70	113.5	0	0	#	CT3	CT1	NH1
116	75.7	110.1	0	0	#	CT3	CT1	OH1
117	34.6	110.1	22.53	2.179	#	CT3	CT2	HA
118	32	125	25	2.173	#	CY	CA	HP
119	120	110	25	2.24	#	CY	CA	NY
120	33.43	109.5	0	0	#	CY	CT2	HA
121	23	120	0	0	#	H	NH2	H
122	35.5	109	5.4	1.802	#	HA	CP2	HA
123	35.5	109	5.4	1.802	#	HA	CP3	HA
124	48	108	0	0	#	HA	CP3	N
125	45.9	108.89	0	0	#	HA	CT1	OH1
126	35.5	109	5.4	1.802	#	HA	CT2	HA
127	51.5	107.5	0	0	#	HA	CT2	NC2
128	45	107.5	35	2.101	#	HA	CT2	NH3
129	45.9	108.89	0	0	#	HA	CT2	OH1
130	46.1	111.3	0	0	#	HA	CT2	S
131	35.5	108.4	5.4	1.802	#	HA	CT3	HA
132	46.1	111.3	0	0	#	HA	CT3	S
133	48	112	0	0	#	HB	CP1	N
134	48	108	0	0	#	HB	CT1	NH1
135	51.5	107.5	0	0	#	HB	CT1	NH3
136	36	115	0	0	#	HB	CT2	HB
137	48	108	0	0	#	HB	CT2	NH1
138	25	120	0	0	#	HC	NC2	HC
139	44	109.5	0	0	#	HC	NH3	HC
140	32	125	25	2.177	#	HP	CA	NY
141	25	122.5	20	2.14	#	HR1	CPH2	NR1
142	25	125	20	2.12	#	HR1	CPH2	NR2
143	25	124	20	2.14	#	HR3	CPH1	NR1
144	45.94	109.47	0	0	#	HT	OT	HT

145	80	122.5	0	0	# N	C	O	
146	52	120	90	2.3642	# NC2	C	NC2	
147	80	122.5	0	0	# NH1	C	O	
148	75	122.5	50	2.37	# NH2	CC	O	
149	130	112.5	0	0	# NR1	CPH2	NR2	
150	100	124	70	2.225	# OC	CC	OC	
151	**125**	**109.47**	**0**	**0**	**# OP8**	**P8**	**OP8**	

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Dihedral Coeffs

1	0.14	3	0	1	# C	CP1	CP2	CP2
2	0.14	3	0	1	# C	CP1	CP2	HA
3	0.8	3	0	1	# C	CP1	N	C
4	0.1	3	0	1	# C	CP1	N	CP3
5	0.2	3	0	1	# C	CT1	CT1	CT2
6	0.2	3	0	1	# C	CT1	CT1	CT3
7	0.2	3	0	1	# C	CT1	CT1	HA
8	0.2	3	0	1	# C	CT1	CT1	OH1
9	0.04	3	0	1	# C	CT1	CT2	CA
10	0.2	3	0	1	# C	CT1	CT2	CC
11	0.2	3	0	1	# C	CT1	CT2	CPH1
12	0.2	3	0	1	# C	CT1	CT2	CT1
13	0.2	3	0	1	# C	CT1	CT2	CT2
14	0.2	3	0	1	# C	CT1	CT2	CY
15	0.2	3	0	1	# C	CT1	CT2	HA
16	0.2	3	0	1	# C	CT1	CT2	OH1
17	0.2	3	0	1	# C	CT1	CT2	S
18	0.2	3	0	1	# C	CT1	CT3	HA
19	0.2	1	180	1	# C	CT1	NH1	C
20	0	1	0	1	# C	CT1	NH1	H
21	0.1	3	0	1	# C	CT1	NH3	HC
22	0.2	1	180	1	# C	CT2	NH1	C
23	0	1	0	1	# C	CT2	NH1	H
24	0.8	3	0	1	# C	N	CP1	CP2
25	0.8	3	0	1	# C	N	CP1	HB
26	0	3	180	1	# C	N	CP3	CP2
27	0	3	180	1	# C	N	CP3	HA
28	0	6	180	1	# C	NC2	CT2	CT2
29	0	6	180	1	# C	NC2	CT2	HA
30	0.2	1	180	1	# C	NH1	CT1	CC
31	1.8	1	0	1	# C	NH1	CT1	CT1
32	1.8	1	0	1	# C	NH1	CT1	CT2
33	1.8	1	0	1	# C	NH1	CT1	CT3
34	0	1	0	1	# C	NH1	CT1	HB

35	0	1	0	1	# C	NH1	CT2	HB
36	3.1	2	180	0.5	# CA	CA	CA	CA
37	3.1	2	180	0.5	# CA	CA	CA	CPT
38	3.1	2	180	1	# CA	CA	CA	CT2
39	4.2	2	180	1	# CA	CA	CA	HP
40	3.1	2	180	1	# CA	CA	CA	OH1
41	3.1	2	180	0.5	# CA	CA	CPT	CPT
42	3	2	180	1	# CA	CA	CPT	CY
43	2.8	2	180	1	# CA	CA	CPT	NY
44	0.23	2	180	1	# CA	CA	CT2	CT1
45	0	6	0	1	# CA	CA	CT2	HA
46	0.99	2	180	1	# CA	CA	OH1	H
47	3.1	2	180	0.5	# CA	CPT	CPT	CA
48	10	2	180	1	# CA	CPT	CPT	CY
49	10	3	180	1	# CA	CPT	CPT	NY
50	3	3	180	1	# CA	CPT	CY	CA
51	3	3	180	1	# CA	CPT	CY	CT2
52	3	3	180	1	# CA	CPT	NY	CA
53	0.8	3	180	1	# CA	CPT	NY	H
54	0.2	3	0	1	# CA	CT2	CT1	HB
55	0.2	3	0	1	# CA	CT2	CT1	NH1
56	4	3	180	0	# CA	CY	CPT	CPT
57	0.23	3	180	1	# CA	CY	CT2	CT1
58	0.25	3	180	1	# CA	CY	CT2	HA
59	5	3	180	0	# CA	NY	CPT	CPT
60	0.2	3	0	1	# CC	CT1	CT2	CPH1
61	0.2	3	0	1	# CC	CT1	CT2	HA
62	0	3	0	1	# CC	CT1	NH1	H
63	0.2	3	0	1	# CC	CT2	CT1	HB
64	0.2	3	0	1	# CC	CT2	CT1	NH1
65	0.195	3	0	1	# CC	CT2	CT2	CT1
66	0.195	3	0	1	# CC	CT2	CT2	HA
67	1.6	1	0	1	# CP1	C	NH1	CT1
68	2.5	1	180	0	# CP1	C	NH1	CT1
69	2.5	3	180	1	# CP1	C	NH1	H
70	0.16	1	0	0	# CP1	CP2	CP2	CP3
71	0.16	1	0	1	# CP1	CP2	CP2	HA
72	2.75	3	180	1	# CP1	N	C	CT1
73	0.3	3	0	0	# CP1	N	C	CT1
74	2.75	3	180	1	# CP1	N	C	O
75	0.3	3	0	0	# CP1	N	C	O
76	0.1	6	0	0	# CP1	N	CP3	CP2
77	0.1	6	0	1	# CP1	N	CP3	HA
78	0.4	1	0	1	# CP2	CP1	C	NH1

79	0.6	1	0	0	# CP2 CP1 C NH1
80	0.4	1	180	1	# CP2 CP1 C O
81	0.6	1	0	0	# CP2 CP1 C O
82	0.1	1	0	0	# CP2 CP1 N CP3
83	0.14	1	0	1	# CP2 CP2 CP1 HB
84	0.14	2	0	0	# CP2 CP2 CP1 N
85	0.14	2	0	1	# CP2 CP2 CP3 HA
86	0.14	2	0	0	# CP2 CP2 CP3 N
87	0.16	2	0	1	# CP3 CP2 CP2 HA
88	2.75	2	180	1	# CP3 N C CT1
89	0.3	2	0	0	# CP3 N C CT1
90	2.75	2	180	1	# CP3 N C O
91	0.3	2	0	0	# CP3 N C O
92	0.1	2	0	1	# CP3 N CP1 HB
93	0.2	6	0	1	# CPH1 CPH1 CT2 CT1
94	0.27	2	0	0	# CPH1 CPH1 CT2 CT1
95	0	2	0	0	# CPH1 CPH1 CT2 CT1
96	0	2	0	1	# CPH1 CPH1 CT2 HA
97	14	3	180	0	# CPH1 CPH1 NR1 CPH2
98	1	3	180	1	# CPH1 CPH1 NR1 H
99	14	3	180	0	# CPH1 CPH1 NR2 CPH2
100	0.2	3	0	1	# CPH1 CT2 CT1 HB
101	0.2	3	0	1	# CPH1 CT2 CT1 NH1
102	3	3	180	1	# CPH1 NR1 CPH2 HR1
103	14	3	180	0	# CPH1 NR1 CPH2 NR2
104	3	3	180	1	# CPH1 NR2 CPH2 HR1
105	14	3	180	0	# CPH1 NR2 CPH2 NR1
106	3	3	180	1	# CPH2 NR1 CPH1 HR3
107	3	3	180	1	# CPH2 NR2 CPH1 CT2
108	3	3	180	1	# CPT CA CA HP
109	3	3	180	1	# CPT CPT CA HP
110	3	3	180	1	# CPT CPT CY CT2
111	0.8	3	180	1	# CPT CPT NY H
112	2	3	180	1	# CPT CY CA HP
113	4	3	180	0	# CPT CY CA NY
114	0.23	3	180	1	# CPT CY CT2 CT1
115	0.25	1	180	1	# CPT CY CT2 HA
116	5	1	180	0	# CPT NY CA CY
117	2	3	180	1	# CPT NY CA HP
118	1.6	1	0	1	# CT1 C NH1 CT1
119	2.5	1	180	0	# CT1 C NH1 CT1
120	1.6	3	0	1	# CT1 C NH1 CT2
121	2.5	3	180	0	# CT1 C NH1 CT2
122	2.5	3	180	1	# CT1 C NH1 H

123	0	3	0	1	# CT1	CT1	C	N
124	0	6	0	1	# CT1	CT1	C	NH1
125	1.4	6	0	1	# CT1	CT1	C	O
126	0.2	1	0	1	# CT1	CT1	CT2	CT3
127	0.2	1	0	1	# CT1	CT1	CT2	HA
128	0.2	1	0	1	# CT1	CT1	CT3	HA
129	0	1	0	1	# CT1	CT1	NH1	H
130	1.33	1	0	1	# CT1	CT1	OH1	H
131	0.18	1	0	0	# CT1	CT1	OH1	H
132	0.32	2	0	0	# CT1	CT1	OH1	H
133	0.05	2	180	1	# CT1	CT2	CC	NH2
134	0.05	2	180	1	# CT1	CT2	CC	O
135	0.05	2	180	1	# CT1	CT2	CC	OC
136	0.19	2	0	1	# CT1	CT2	CPH1	NR2
137	0.2	2	0	1	# CT1	CT2	CT1	CT3
138	0.2	2	0	1	# CT1	CT2	CT1	HA
139	0.2	2	0	1	# CT1	CT2	CT1	HB
140	0.2	2	0	1	# CT1	CT2	CT1	NH1
141	0.195	6	0	1	# CT1	CT2	CT2	CT2
142	0.195	2	0	1	# CT1	CT2	CT2	HA
143	0.195	2	0	1	# CT1	CT2	CT2	S
144	0.16	2	0	1	# CT1	CT2	CT3	HA
145	1.3	3	0	1	# CT1	CT2	OH1	H
146	0.3	3	0	0	# CT1	CT2	OH1	H
147	0.42	3	0	0	# CT1	CT2	OH1	H
148	0.24	3	0	1	# CT1	CT2	S	HS
149	0.15	3	0	0	# CT1	CT2	S	HS
150	0.27	3	0	0	# CT1	CT2	S	HS
151	1.6	3	0	1	# CT1	NH1	C	CT2
152	2.5	3	180	0	# CT1	NH1	C	CT2
153	2.5	3	180	1	# CT1	NH1	C	O
154	2.5	3	180	1	# CT2	C	NH1	H
155	4.2	3	180	1	# CT2	CA	CA	HP
156	1.4	3	180	1	# CT2	CC	NH2	H
157	2	3	180	1	# CT2	CPH1	CPH1	HR3
158	3	3	180	1	# CT2	CPH1	CPH1	NR1
159	0	3	0	1	# CT2	CT1	C	N
160	0	3	0	1	# CT2	CT1	C	NH1
161	1.4	3	0	1	# CT2	CT1	C	O
162	0.05	3	180	1	# CT2	CT1	CC	OC
163	0.2	1	0	1	# CT2	CT1	CT1	HB
164	0.2	1	0	1	# CT2	CT1	CT1	NH1
165	0.2	3	0	1	# CT2	CT1	CT3	HA
166	0	1	0	1	# CT2	CT1	NH1	H

167	0.1	1	0	1	#	CT2	CT1	NH3	HC
168	0.05	3	180	1	#	CT2	CT2	CC	NH2
169	0.05	3	180	1	#	CT2	CT2	CC	O
170	0.05	3	180	1	#	CT2	CT2	CC	OC
171	0.2	3	0	1	#	CT2	CT2	CT1	HB
172	0.2	6	0	1	#	CT2	CT2	CT1	NH1
173	0.2	6	0	1	#	CT2	CT2	CT1	NH3
174	0.15	1	0	1	#	CT2	CT2	CT2	CT2
175	0.195	1	0	1	#	CT2	CT2	CT2	HA
176	0.195	1	0	1	#	CT2	CT2	CT2	NC2
177	0.195	1	0	1	#	CT2	CT2	CT2	NH3
178	0	1	180	1	#	CT2	CT2	NC2	HC
179	0.1	1	0	1	#	CT2	CT2	NH3	HC
180	0.24	2	180	1	#	CT2	CT2	S	CT3
181	0.37	2	0	0	#	CT2	CT2	S	CT3
182	1.2	2	180	1	#	CT2	CY	CA	HP
183	3.5	2	180	1	#	CT2	CY	CA	NY
184	2.25	2	180	1	#	CT2	NC2	C	NC2
185	2.5	2	180	1	#	CT2	NH1	C	O
186	0.28	2	0	1	#	CT2	S	CT3	HA
187	0	2	0	1	#	CT3	CT1	C	N
188	0	2	0	1	#	CT3	CT1	C	NH1
189	1.4	6	0	1	#	CT3	CT1	C	O
190	0.2	2	0	1	#	CT3	CT1	CT1	HB
191	0.2	2	0	1	#	CT3	CT1	CT1	NH1
192	0.2	2	0	1	#	CT3	CT1	CT2	CT3
193	0.2	3	0	1	#	CT3	CT1	CT2	HA
194	0.2	3	0	1	#	CT3	CT1	CT3	HA
195	0	3	0	1	#	CT3	CT1	NH1	H
196	1.33	3	0	1	#	CT3	CT1	OH1	H
197	0.18	3	0	0	#	CT3	CT1	OH1	H
198	0.32	3	0	0	#	CT3	CT1	OH1	H
199	0.2	3	0	1	#	CT3	CT2	CT1	HA
200	0.28	3	0	1	#	CT3	S	CT2	HA
201	0.8	3	180	1	#	CY	CA	NY	H
202	3	3	180	1	#	CY	CPT	CA	HP
203	5	3	180	0	#	CY	CPT	CPT	NY
204	0.2	3	0	1	#	CY	CT2	CT1	HB
205	0.2	3	0	1	#	CY	CT2	CT1	NH1
206	2.5	3	180	1	#	H	NH1	C	O
207	0	3	0	1	#	H	NH1	CT1	HB
208	0	3	0	1	#	H	NH1	CT2	HB
209	1.4	3	180	1	#	H	NH2	CC	O
210	1	3	180	1	#	H	NR1	CPH1	HR3

211	1	1	180	1	# H	NR1	CPH2	HR1
212	1	1	180	1	# H	NR1	CPH2	NR2
213	0.4	3	180	1	# H	NY	CA	HP
214	0.14	1	0	1	# H	OH1	CT1	HA
215	0.14	1	0	1	# H	OH1	CT2	HA
216	0.14	3	0	1	# HA	CP2	CP1	HB
217	0.14	3	0	1	# HA	CP2	CP1	N
218	0.16	3	0	1	# HA	CP2	CP2	HA
219	0.14	3	0	1	# HA	CP2	CP3	HA
220	0.14	6	0	1	# HA	CP2	CP3	N
221	0.2	6	0	1	# HA	CT1	CT1	HB
222	0.2	1	0	1	# HA	CT1	CT1	NH1
223	0.2	1	0	1	# HA	CT1	CT2	HA
224	0.2	1	0	1	# HA	CT1	CT3	HA
225	0	1	180	1	# HA	CT2	CC	NH2
226	0	1	180	1	# HA	CT2	CC	O
227	0.05	1	180	1	# HA	CT2	CC	OC
228	0.19	2	0	1	# HA	CT2	CPH1	NR2
229	0.2	2	0	1	# HA	CT2	CT1	HB
230	0.2	2	0	1	# HA	CT2	CT1	NH1
231	0.2	2	0	1	# HA	CT2	CT1	NH3
232	0.195	2	0	1	# HA	CT2	CT2	HA
233	0.195	2	0	1	# HA	CT2	CT2	NC2
234	0.195	2	0	1	# HA	CT2	CT2	NH3
235	0.01	2	0	1	# HA	CT2	CT2	S
236	0.16	2	0	1	# HA	CT2	CT3	HA
237	0	6	180	1	# HA	CT2	NC2	HC
238	0.1	2	0	1	# HA	CT2	NH3	HC
239	0.2	2	0	1	# HA	CT2	S	HS
240	0.2	2	0	1	# HA	CT3	CT1	HB
241	0.2	3	0	1	# HA	CT3	CT1	NH1
242	0.2	3	0	1	# HA	CT3	CT1	OH1
243	0.4	3	180	1	# HB	CP1	C	NH1
244	0.6	3	0	0	# HB	CP1	C	NH1
245	0.4	3	0	1	# HB	CP1	C	O
246	0.6	3	0	0	# HB	CP1	C	O
247	0	3	0	1	# HB	CT1	C	N
248	0	3	0	1	# HB	CT1	C	NH1
249	0	3	0	1	# HB	CT1	C	O
250	0.05	3	180	1	# HB	CT1	CC	OC
251	0.2	3	0	1	# HB	CT1	CT1	OH1
252	0.2	3	0	1	# HB	CT1	CT2	OH1
253	0.2	3	0	1	# HB	CT1	CT2	S
254	0.1	3	0	1	# HB	CT1	NH3	HC

255	0	3	0	1	# HB	CT2	C	NH1
256	0	3	0	1	# HB	CT2	C	O
257	2.25	3	180	1	# HC	NC2	C	NC2
258	2.4	3	180	1	# HP	CA	CA	HP
259	4.2	1	180	1	# HP	CA	CA	OH1
260	3	1	180	1	# HP	CA	CPT	NY
261	3	3	180	1	# HR3	CPH1	CPH1	NR2
262	0.4	1	0	1	# N	C	CT1	NH1
263	0.3	1	0	1	# N	CP1	C	NH1
264	-0.3	3	0	0	# N	CP1	C	NH1
265	-0.3	3	0	1	# N	CP1	C	O
266	0.6	3	0	1	# NH1	C	CT1	NH1
267	0.6	3	0	1	# NH1	C	CT1	NH3
268	0.6	6	0	1	# NH1	C	CT2	NH1
269	0	6	0	1	# NH1	CT1	C	O
270	0.05	1	180	1	# NH1	CT1	CC	OC
271	0.2	1	0	1	# NH1	CT1	CT1	OH1
272	0.2	1	0	1	# NH1	CT1	CT2	OH1
273	0.2	1	0	1	# NH1	CT1	CT2	S
274	0	1	0	1	# NH1	CT2	C	O
275	0	1	0	1	# NH3	CT1	C	O
276	14	2	180	0	# NR1	CPH1	CPH1	NR2

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Improper Coeffs

1	120	0	# C	CP1	NH1	O	
2	120	0	# C	CT1	N	O	
3	120	0	# C	CT1	NH1	O	
4	120	0	# C	CT2	NH1	O	
5	40	0	# C	NC2	NC2	NC2	
6	96	0	# CC	CT1	OC	OC	
7	45	0	# CC	CT2	NH2	O	
8	96	0	# CC	CT2	OC	OC	
9	45	0	# CC	NH2	CT2	O	
10	0	0	# CP3	CP1	C	N	
11	0.5	0	# CPH1	CPH1	NR1	HR3	
12	0.5	0	# CPH1	NR1	CPH1	HR3	
13	0.5	0	# CPH2	NR1	NR2	HR1	
14	0.5	0	# CPH2	NR2	NR1	HR1	
15	0.45	0	# H	CPH1	CPH2	NR1	
16	0.45	0	# H	CPH2	CPH1	NR1	
17	20	0	# H	CT1	C	NH1	
18	20	0	# H	CT2	C	NH1	
19	4	0	# H	H	CC	NH2	

Lammps script:

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```
bond_style          harmonic
angle_style         charmm
dihedral_style    charmm
improper_style    harmonic
pair_style          lj/charmm/coul/long 10 12
```

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