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Table 1) Influence of truncation on crystal minimizations of N-methylamide and the alanine dipeptide.[a]

Cutoffs	Unit Cell Parameters				Energies		
	A	B	C	Vol	Total	Image	GRMS
NMA							
Experiment	9.61	6.52	7.24	454			
10-9-7	9.49	6.45	7.08	433	-41.9	-18.1	0.00023
13-12-10	9.45	6.28	7.11	422	-46.4	-19.7	0.00016
16-15-13	9.58	6.27	7.17	431	-47.1	-19.1	0.00011
19-18-16	9.51	6.25	7.06	420	-47.7	-18.9	0.00026
22-21-19	9.41	6.25	7.04	414	-48.2	-19.0	0.00019
25-24-22	9.57	6.23	7.09	423	-48.4	-18.9	0.00011
Alanine Dipeptide							
Experiment	13.87	6.98	16.29	1577			
10-9-7	14.46	6.82	15.65	1543	-84.3	-44.3	0.00073
13-12-10	14.03	6.85	15.89	1527	-89.5	-46.2	0.00048
16-15-13	14.24	6.82	15.67	1523	-91.4	-46.1	0.00057
19-18-16	14.18	6.77	15.77	1515	-92.7	-46.6	0.00058
22-21-19	14.13	6.81	15.78	1519	-93.0	-46.3	0.00053
25-24-22	14.14	6.80	15.81	1519	-93.3	-46.2	0.00064

[a]Lengths in Å, volumes in $Å^3$, energies in kcal/mole and forces in kcal/mole/Å. The three values in the cutoff column represent the truncation distances in Å for the non-bond interaction list (first term); the truncation distance for the electrostatic shift and van der Waals switch functions (second term) and the inner distance for the van der Waals the VDW switch function (third term). For the energies, Total represents the total energy of the system, including image contributions and Image represents the interaction energy of the images with the primary atoms.

Table 2) N-methylacetamide and alanine dipeptide crystal non-bonded interaction distances.[a]

Interaction	X-ray	Min	Diff	NVT	Diff	NPT	Diff
NMA							
Primary to Image[b]							
N7-C036 O6	2.82	2.82	0.01	2.84±0.09	0.02	2.84±0.12	0.02
C4-C002 C9	3.51	3.43	-0.08	3.57±0.08	0.06	3.50±0.08	-0.01
C4-C025 O6	3.77	3.54	-0.23	3.83±0.20	0.05	3.69±0.18	-0.09
Cl-C036 O6	3.51	3.41	-0.10	3.54±0.12	0.03	3.49±0.11	-0.03
C5-C036 O6	3.63	3.60	-0.04	3.66±0.04	0.03	3.64±0.07	0.00
O6-C025 C9	3.86	3.70	-0.17	3.81±0.23	-0.05	3.74±0.18	-0.13
N7-C015 C9	3.66	3.49	-0.17	3.74±0.19	0.08	3.60±0.16	-0.05
N7-C036 C5	3.86	3.75	-0.11	3.88±0.07	0.02	3.83±0.09	-0.03
C9-C015 C9	3.76	3.67	-0.09	3.84±0.20	0.09	3.75±0.17	-0.01
C9-C036 O6	3.77	3.80	0.03	3.74±0.16	-0.03	3.77±0.18	0.00
Alanine Dipeptide							
Primary to Primary							
1 N17 -2 O6	2.73	2.80	0.07	2.90±0.16	0.17	2.99±0.21	0.26
1 O6-2 N17	2.80	2.81	0.00	3.00±0.21	0.19	2.98±0.22	0.17
1 O6-2 C9	3.34	3.36	0.02	3.46±0.17	0.12	3.49±0.21	0.15
1 C9-2 O6	3.32	3.42	0.10	3.60±0.21	0.28	3.55±0.23	0.24
1 C12-2 O6	3.45	3.57	0.12	3.72±0.16	0.26	3.73±0.18	0.28
1 C12-2 N17	3.35	3.52	0.16	3.70±0.25	0.35	3.69±0.26	0.34
1 N17-2 C12	3.46	3.52	0.07	3.62±0.19	0.16	3.71±0.24	0.25
1 N17-2 N17	3.27	3.54	0.27	3.58±0.22	0.32	3.67±0.25	0.40
Primary to Image[b]							
2 N7-C004 1 N17	3.47	3.44	-0.02	3.57±0.19	0.10	3.58±0.22	0.11
2 N7-C004 1 O13	2.93	2.82	-0.10	2.98±0.15	0.05	2.95±0.16	0.03
2 O6-C023 1 C11	3.32	3.27	-0.05	3.25±0.15	-0.07	3.79±0.31	0.47
2 O13-C004 1 N7	2.73	2.77	0.05	2.88±0.13	0.16	2.91±0.16	0.18
2 O6-C001 1 C19	3.47	3.50	0.03	3.59±0.25	0.13	4.10±0.54	0.63

[a]Distance in Å. All nonbonded distances less than 4.0 Å in the N-methylacetamide experimental structure and less than 3.5 Å in the alanine dipeptide experimental structure are included. The variations in the NVT and NPT simulation results indicate the rms fluctuations. See Figure 5 for atom designations.

[b]Image atoms are represented by the CHARMM identifier for the specific image and the atom name.

Table 3) Influence of truncation length on crystal minimizations of the tripeptides.[a]

Cutoffs	Unitcell Parameters					Energies		
	A	B	C	β	Vol	Total	Image	GRMS
Gly-Ala-Val, $3H_2O$								
experiment	8.052	6.032	15.779	98.52	757.9			
10-9-7	8.013	6.063	15.783	103.69	745.0	-165.0	-173.6	0.00072
13-12-10	7.821	5.914	16.034	103.04	722.5	-167.3	-170.6	0.00487
16-15-13	7.792	6.000	15.954	100.08	734.4	-169.2	-166.0	0.00063
19-18-16	7.900	5.979	15.955	104.18	730.7	-170.3	-164.2	0.00071
22-21-19	7.889	6.029	15.948	104.35	734.9	-169.9	-161.9	0.00088
25-24-22	7.955	5.938	15.665	104.28	717.1	-169.9	-161.0	0.00170
Gly-Ala-Leu, $3H_2O$								
Experiment	6.024	8.171	32.791		1614.0			
10-9-7	6.005	7.996	32.687		1569.5	-176.6	-172.3	0.00087
13-12-10	5.897	7.829	32.697		1509.5	-181.9	-171.7	0.00299
16-15-13	5.981	7.983	32.573		1555.2	-183.5	-170.3	0.01062
19-18-16	5.947	7.893	32.914		1545.0	-185.1	-164.9	0.00070
22-21-19	5.920	7.964	32.411		1528.1	-185.4	-162.7	0.00549
25-24-22	5.949	7.864	32.574		1523.9	-185.5	-161.4	0.00262
Ala-Ala-Ala								
Experiment	11.849	10.004	9.862	101.30	1146.4			
10-9-7	11.828	9.895	9.695	101.15	1113.3	-233.1	-290.7	0.00037
13-12-10	11.774	9.961	9.705	100.97	1117.4	-238.5	-279.3	0.00032
16-15-13	11.775	9.931	9.700	100.85	1114.0	-241.3	-267.4	0.00025
19-18-16	11.823	9.898	9.764	100.99	1121.7	-243.5	-261.6	0.00032
22-21-19	11.818	9.928	9.727	101.23	1119.4	-243.6	-256.8	0.00026
25-24-22	11.766	9.910	9.729	100.56	1115.2	-242.8	-254.3	0.00035

[a]Lengths in Å, volumes in $Å^3$, energies in kcal/mole and GRMS represents the rms forces in kcal/mole/Å. The three values in the cutoff scheme represent the truncation distance for the non-bond interaction list, the truncation distance for the electrostatic shift and VDW switch smoothing functions and the smallest is the where the VDW switch smoothing function is turned on.

Table 4) Tripeptide intramolecular dihedral angles.[a]

	X-ray	Minimized		NVT		NPT	
		Calc	Diff	Calc	Diff	Calc	Diff
Gly-Ala-Leu, $3H_20$							
1N-1CA-1C-2N	-150	-146	5	-76±13	75	-86±14	64
1CA-1C-2N-2CA	-172	-176	-4	-180±8	-8	-176±7	-5
1C-2N-2CA-2C	-68	-69	-1	-78±14	-10	-70±10	-3
2N-2CA-2C-3N	-39	-43	-4	-58±10	-19	-48±10	-9
2CA-2C-3N-3CA	-173	-174	-1	-162±10	11	-173±6	0
2C-3N-3CA-3C	-72	-74	-1	-77±11	-5	-74±10	-2
3N-3CA-3CB-3CG	-69	-63	5	-66±9	3	-63±8	5
3CA-3CB-3CG-3CD1	159	154	-5	109±26	-50	155±13	-4
3N-3CA-3C-3OT2	138	123	-15	135±10	-3	115±8	-22
Gly-Ala-Val, $3H_20$							
1N-1CA-1C-2N	-151	-144	7	-89±14	62		
1CA-1C-2N-2CA	-171	-175	-4	-173±7	-1		
1C-2N-2CA-2C	-69	-69	0	-68±10	1		
2N-2CA-2C-3N	-38	-45	-7	-48±9	-10		
2CA-2C-3N-3CA	-172	-173	-1	-173±6	0		
2C-3N-3CA-3C	-75	-73	2	-73±9	2		
3N-3CA-3CB-3CG1	-62	-51	11	-53±7	9		
3N-3CA-3C-3OT2	136	125	-11	119±7	-17		
Ala-Ala-Ala							
Molecule 1							
1N-1CA-1C-2N	177	173	-4	174±7	-3		
1CA-1C-2N-2CA	178	179	1	178±6	0		
1C-2N-2CA-2C	-143	-139	4	-141±8	3		
2N-2CA-2C-3N	160	166	5	166±8	6		
2CA-2C-3N-3CA	178	179	1	179±6	1		
2C-3N-3CA-3C	-149	-154	-5	-152±9	-3		
3N-3CA-3C-3OT2	-13	-9	4	-9±8	4		
Molecule 2							
4N-4CA-4C-5N	148	143	-5	142±7	-5		
4CA-4C-5N-5CA	-178	180	-2	-180±6	-2		
4C-5N-5CA-5C	-164	-158	6	-157±7	7		
5N-5CA-5C-6N	149	149	0	150±7	1		
5CA-5C-6N-6CA	173	178	4	177±6	4		
5C-6N-6CA-6C	-163	-161	2	-161±7	2		
6N-6CA-6C-6OT2	-41	-54	-13	-54±8	-14		

[a]Dihedral angles in degrees. Errors from the NVT and NPT simulations represent the rms fluctuations.

Table 5) Tripeptide interaction distances involving nitrogen or oxygen atoms.[a]

Interaction	X-ray	Minimized		NVT		NPT	
		Calc	Diff	Calc	Diff	Calc	Diff
Gly-Ala-Leu, $3H_20$							
Primary to Primary							
GAL 1O-GAL 3N	3.48	3.68	0.20	4.13±0.24	0.65	4.13±0.24	0.65
WAT 1OH2-GAL 1N	2.81	2.88	0.07	3.35±0.37	0.54	3.35±0.37	0.54
WAT 2OH2-GAL 1N	2.75	2.78	0.03	3.45±0.33	0.70	3.45±0.33	0.70
WAT 3OH2-GAL 1N	2.93	2.84	-0.09	3.06±0.23	0.13	3.06±0.23	0.13
Primary to Image							
GAL 1N-C002 2OH2	3.40	3.21	-0.19	2.88±0.27	-0.52	2.75±0.27	-0.66
GAL 1N-C017 2OH2	3.00	2.89	-0.11	3.66±0.48	0.66	6.07±0.67	3.07
GAL 1O-C002 2OH2	2.85	2.68	-0.16	3.44±0.29	0.60	3.41±0.30	0.56
GAL 2O-C002 2N	2.87	2.77	-0.10	2.91±0.13	0.04	2.76±0.14	-0.11
GAL 2O-C018 3OH2	2.90	2.78	-0.12	3.74±0.57	0.84	6.65±0.73	3.75
GAL 3OT1-C002 1OH2	3.45	3.53	0.08	3.37±0.36	-0.08	3.25±0.35	-0.20
GAL 3OT1-C002 2OH2	3.41	3.59	0.18	2.66±0.10	-0.75	2.76±0.12	-0.65
GAL 3OT1-C017 3OH2	2.73	2.57	-0.15	2.69±0.12	-0.04	4.72±0.57	1.99
GAL 3OT2-C002 2N	3.33	3.05	-0.28	2.90±0.15	-0.43	2.87±0.16	-0.46
GAL 3OT2-C002 3N	3.27	3.14	-0.13	3.16±0.16	-0.11	3.03±0.16	-0.24
GAL 3OT2-C002 1OH2	2.73	2.64	-0.09	2.93±0.52	0.20	2.88±0.55	0.15
WAT 1OH2-C002 2OH2	3.44	3.11	-0.33	3.04±0.19	-0.40	2.97±0.20	-0.47
WAT 1OH2-C017 2OH2	3.03	2.92	-0.11	2.88±0.26	-0.15	5.91±0.52	2.88
WAT 3OH2-C002 2OH2	2.80	2.69	-0.12	3.42±0.56	0.62	3.36±0.57	0.56
WAT 3OH2-C017 1OH2	3.49	3.85	0.36	3.44±0.42	-0.06	4.41±0.61	0.92
WAT 3OH2-C018 2N	3.43	3.33	-0.10	4.17±0.58	0.74	5.11±0.89	1.68
Gly-Ala-Val, $3H_20$							
primary to primary							
WAT 1OH2-GAV 1N	2.81	2.90	0.09	2.95±0.15	0.14		
WAT 2OH2 - GAV 1N	2.76	2.79	0.04	2.79±0.09	0.03		
WAT 3OH2 - GAV 1N	2.91	2.84	-0.06	3.71±0.63	0.80		
primary to image							
GAV 1N-C007 2OH2	3.40	3.31	-0.10	4.57±0.34	1.17		
GAV 1N-C030 2OH2	2.99	2.91	-0.08	3.39±0.50	0.40		
GAV 1O-C007 2OH2	2.86	2.70	-0.17	3.65±0.37	0.79		
GAV 2O-C007 2N	2.88	2.82	-0.06	2.87±0.10	0.00		
GAV 2O- C026 3OH2	2.87	2.79	-0.09	3.41±0.87	0.54		
GAV 3OT1-C007 1OH2	3.48	3.61	0.13	3.58±0.13	0.10		
GAV 3OT1-C007 2OH2	3.48	3.56	0.09	3.94±0.45	0.46		
GAV 3OT1-C030 3OH2	2.72	2.57	-0.14	2.67±0.10	-0.04		
GAV 3OT2-C007 2N	3.23	3.01	-0.22	3.01±0.16	-0.22		
GAV 3OT2-C007 3N	3.22	3.21	-0.01	3.20±0.16	-0.01		
GAV 3OT2-C007 1OH2	2.76	2.65	-0.11	2.66±0.10	-0.10		
WAT 1OH2-C007 2OH2	3.44	3.12	-0.32	3.87±0.55	0.43		
WAT 1OH2-C030 2OH2	2.99	2.93	-0.06	2.75±0.14	-0.24		
WAT 3OH2-C007 2OH2	2.78	2.71	-0.08	2.82±0.15	0.04		
WAT 3OH2-C026 2N	3.39	3.39	0.00	3.86±0.72	0.47		
WAT 3OH2-C030 1OH2	3.48	3.94	0.46	4.01±0.47	0.54		
Ala-Ala-Ala							
Primary to Image							
ALA1 1N-C006 3OT1	2.74	2.64	-0.10	2.66±0.07	-0.08		
ALA1 1N-C017 3OT1	3.14	2.97	-0.16	3.02±0.11	-0.12		
ALA1 1N-C017 3OT2	2.86	2.70	-0.16	2.73±0.09	-0.13		
ALA1 1N-C027 3OT2	2.84	2.67	-0.17	2.72±0.09	-0.12		

Table 5, continued

ALA1 1O-C026 2N	3.36	3.28	-0.08	3.39±0.12	0.02
ALA1 2N-C019 1O	3.20	3.08	-0.13	3.16±0.11	-0.04
ALA1 2O-C019 3N	3.35	3.31	-0.04	3.43±0.16	0.08
ALA1 3N-C026 2O	3.20	3.19	-0.01	3.28±0.16	0.08
ALA1 3OT1-C029 1N	3.12	3.08	-0.04	3.14±0.15	0.02
ALA1 3OT2-C029 1N	2.87	2.67	-0.20	2.75±0.10	-0.12
ALA2 1N-C015 3OT1	2.73	2.67	-0.07	2.71±0.08	-0.03
ALA2 1N-C019 3OT2	2.92	2.66	-0.25	2.71±0.09	-0.21

[a]Distances in Å. All interactions involving nitrogen or oxygen atoms less than 3.5 Å in the crystal structure are included. Errors from the simulation represent the rms fluctuations. See Figure 6 for atom names. [b]Image atoms are represented by the CHARMM identifier for the specific image and the atom name.

Table 6) Influence of truncation length on crystal minimizations of the cyclic peptides.[a]

Cutoffs	Unitcell Parameters					Energetics		
	A	B	C	Beta	Vol	Total	Image	GRMS
CP1								
Experiment	12.312	4.959	15.876	99.07	957.2			
10-12-10	12.098	4.933	16.360	97.28	968.5	-16.7	-82.1	0.00058
13-12-10	12.171	4.914	16.174	98.14	957.6	-14.1	-82.9	0.00033
16-15-13	12.109	4.892	16.348	97.60	960.0	-12.9	-83.6	0.00049
19-18-16	12.106	4.938	16.402	97.46	972.2	-12.3	-83.3	0.00034
22-21-19	11.978	4.909	16.613	96.83	969.9	-11.1	-82.9	0.00046
25-24-22	12.062	4.931	16.253	97.56	958.2	-11.2	-83.3	0.00043
CP2								
Experiment	9.274	24.357	9.168		2070.9			
10-9-7	8.976	25.357	8.948		2036.6	-25.7	-74.1	0.00096
13-12-10	8.759	24.475	9.344		2003.1	-22.2	-75.2	0.00054
16-15-13	8.772	24.612	9.342		2016.9	-20.3	-74.2	0.00232
19-18-16	8.881	24.540	9.266		2019.4	-19.3	-74.2	0.00090
22-21-19	8.929	24.712	9.261		2043.5	-18.6	-73.1	0.00063
25-24-22	8.869	24.673	9.268		2028.1	-17.8	-73.2	0.00083
CP3								
Experiment	12.662	18.102	8.678		1989.1			
10-9-7	13.057	18.413	8.507		2045.3	-44.6	-69.1	0.00060
13-12-10	12.694	17.857	8.630		1956.2	-42.2	-70.4	0.00034
16-15-13	12.586	18.072	8.538		1941.9	-41.3	-71.7	0.00048
19-18-16	12.865	17.809	8.591		1968.2	-41.3	-72.1	0.00039
22-21-19	12.726	18.010	8.525		1953.9	-39.7	-71.4	0.00052
25-24-22	12.760	18.004	8.566		1967.8	-39.9	-71.4	0.00042
CP4								
Experiment	7.619	21.071	7.702	108.90	1169.8			
10-9-7	7.553	21.176	7.864	110.83	1175.6	-18.3	-103.7	0.00059
13-12-10	7.413	21.331	7.646	108.72	1145.1	-12.5	-102.7	0.00037
16-15-13	7.395	21.167	7.725	108.93	1143.8	-11.9	-103.6	0.00039
19-18-16	7.517	21.155	7.721	110.82	1147.6	-8.9	-102.0	0.00050
22-21-19	7.468	21.185	7.715	110.47	1143.4	-8.1	-101.6	0.00034
25-24-22	7.402	21.226	7.716	109.40	1143.4	-7.3	-100.8	0.00071
CP5								
Experiment	10.254	21.320	8.565		1872.4			
10-9-7	10.216	21.369	8.603		1878.0	62.1	-45.0	0.00039
13-12-10	10.153	21.297	8.674		1875.6	64.9	-47.4	0.00033
16-15-13	10.169	21.359	8.608		1869.6	66.4	-48.1	0.00042
19-18-16	10.095	21.503	8.589		1864.6	67.1	-48.8	0.00049
22-21-19	10.087	21.316	8.754		1882.2	68.0	-48.4	0.00041
25-24-22	10.131	21.508	8.582		1869.8	68.4	-48.6	0.00047
CP6								
Experiment	10.164	13.610	15.702	101.12	2131.3			
10-9-7	10.860	13.478	15.043	101.27	2159.4	25.6	-115.7	0.00059
13-12-10	10.384	13.642	15.401	101.21	2140.2	28.5	-117.8	0.00055
16-15-13	10.515	13.573	15.108	100.71	2118.6	30.0	-120.5	0.00071
19-18-16	10.497	13.558	15.292	100.82	2137.7	30.2	-120.9	0.00038
22-21-19	10.381	13.564	15.407	100.74	2131.3	31.4	-120.2	0.00043
25-24-22	10.603	13.572	15.171	100.90	2143.6	32.6	-120.3	0.00052

[a]Distances in Å, angles in degrees, volumes in $Å^3$, energies in kcal/mole and GRMS represents the rms forces in kcal/mole/Å. The three values in the cutoff scheme represent the truncation distance for the non-bond interaction list, the truncation distance for the electrostatic shift and VDW switch smoothing functions and the smallest is the where the VDW switch smoothing function is turned on.

Table 7) Cyclic Peptide dihedral angles.[a]

Interaction	X-ray	Minimized		NVT	
		Calc	Diff	Calc	Diff
CP1					
1N-1CA-1C-2N	-43	-46	-3	-49±5	-6
1CA-1C-2N-2CA	-175	-178	-3	180±4	-5
1C-2N -2CA-2C	-84	-82	2	-80±4	5
2N-2CA-2C-3N	0	-12	-12	-10±6	-10
2CA-2C-3N-3CA	176	176	1	170±5	-5
2C-3N-3CA-3C	139	165	25	157±8	18
3N-3CA-3C-4N	158	132	-26	149±7	-9
3CA-3C-4N-4CA	-177	179	-4	179±5	-5
3C-4N-4CA-4C	84	101	16	94±6	10
4N-4CA-4C-5N	-113	-112	0	-113±5	0
4CA-4C-5N-5CA	169	170	1	167±4	-2
4C-5N-5CA-5C	-106	-103	3	-102±6	4
5N-5CA-5C -6N	-9	-32	-22	-23±7	-13
5CA-5C-6N-6CA	179	172	-7	176±4	-3
5C-6N-6CA-6C	-96	-75	22	-85±7	12
6N-6CA-6C-1N	173	154	-19	164±6	-9
6CA-6C-1N-1CA	-176	-172	3	-175±5	1
6C-1N-1CA-1C	-53	-43	11	-47±7	6
CP2					
1N-1CA-1C-2N	-33	-44	-11	-46±7	-13
1CA-1C-2N-2CA	-178	-175	3	-177±5	1
1C-2N-2CA-2C	-95	-89	6	-84±8	11
2N-2CA-2C-3N	14	-29	-42	-19±12	-33
2CA-2C-3N-3CA	-174	-179	-5	-176±7	-2
2C-3N-3CA-3C	106	170	64	155±16	49
3N-3CA-3C-4N	179	-177	3	-177±7	4
3CA-3C-4N-4CA	178	173	-5	175±5	-3
3C-4N-4CA-4C	54	41	-12	41±7	-12
4N-4CA-4C-5N	38	42	4	43±7	5
4CA-4C-5N-5CA	174	179	5	178±4	4
4C-5N-5CA-5C	91	87	-4	90±7	-1
5N-5CA-5C-6N	-6	42	48	22±16	28
5CA-5C-6N-6CA	173	177	4	176±5	2
5C-6N-6CA-6C	-119	-162	-43	-145±16	-26
6N-6CA-6C-1N	-167	-157	11	-156±7	12
6CA-6C-1N-1CA	-174	-178	-3	-177±4	-3
6C-1N-1CA-1C	-62	-75	-13	-73±7	-11
CP3					
1N-1CA-1C-2N	17	21	4	2±17	-15
1CA-1C-2N-CA	-179	176	-6	178±9	-3
1C-2N-2C-2C	101	105	4	125±16	24
2N-2CA-2C-3N	175	173	-2	175±10	0
2CA-2C-3N-3CA	177	175	-3	173±8	-4
2C-3N-3C-3C	66	70	4	67±10	1
3N-3CA-3C-4N	14	18	4	23±12	9
3CA-3C-4N-4CA	-176	-172	5	-173±7	4

Table 7, continued

3C-4N-4C-4C	131	122	-9	117±12	-14
4N-4CA-4C-5N	-35	-28	7	-26±12	9
4CA-4C-5N-5CA	-172	-176	-4	-176±7	-4
4C-5N-5C-5C	-105	-104	1	-108±14	-3
5N-5CA-5C-6N	-168	-166	2	-164±11	4
5CA-5C-6N-6CA	-177	-175	2	-173±7	4
5C-6N-6C-6C	-70	-83	-13	-81±12	-11
6N-6CA-6C-1N	-16	-6	10	-11±13	5
6CA-6C-1N-1CA	173	169	-4	170±8	-2
6C-1N-1C-1C	-106	-119	-13	-111±13	-5
CP4					
1N -1CA-1C-2N	-173	-171	2	-170±6	3
1CA-1C -2N-2CA	-177	-175	2	-175±6	2
1C -2N -2CA-2C	-66	-73	-8	-71±7	-5
2N -2CA-2C-3N	-36	-17	19	-20±10	15
2CA-2C -3N-3CA	-173	-173	0	-172±6	1
2N -2CA-2CB-2CG	-27	-25	1	-27±6	0
2CA-2CB-2CG-2CD	38	36	-2	36±6	-2
2C -3N -3CA-3C	-115	-126	-11	-125±11	-11
3N -3CA-3C-4N	-7	-21	-14	-15±11	-8
3CA-3C -4N-4CA	-177	179	-4	180±7	-3
3C -4N -4CA-4C	-150	-140	11	-144±11	7
4N -4CA-4C-5N	178	-172	10	-172±7	10
4CA-4C -5N-5CA	-180	-179	0	179±6	-1
4C -5N -5CA-5C	-53	-61	-7	-60±6	-7
5N -5CA-5C-6N	126	120	-6	118±8	-8
5CA-5C -6N-6CA	179	180	1	179±5	0
5N -5CA-5CB-5CG	-31	-30	1	-29±6	2
5CA-5CB-5CG-5CD	42	36	-6	36±5	-6
5C -6N -6CA-6C	83	91	9	95±10	12
6N -6CA-6C-1N	-3	-8	-5	-9±9	-7
6CA-6C -1N-1CA	-175	-176	-1	-176±7	-1
6C -1N -1CA-1C	-142	-137	5	-139±9	4
CP5					
1N -1CA-1C -2N	-134	-127	7	-128±8	7
1CA-1C -2N -2CA	174	173	-1	173±7	-1
1C -2N -2CA-2C	-52	-60	-7	-60±7	-8
2N -2CA-2C -3N	126	106	-19	108±9	-18
2CA-2C -3N -3CA	-179	-177	2	-177±6	2
2N -2CA-2CB-2CG	-27	-31	-4	-29±6	-3
2CA-2CB-2CG-2CD	39	38	-2	37±6	-2
2C -3N -3CA-3C	74	83	9	85±10	11
3N -3CA-3C -4N	12	31	19	25±8	13
3CA-3C -4N -4CA	177	174	-2	176±6	0
3C -4N -4CA-4C	134	124	-10	127±9	-7
4N -4CA-4C -5N	-69	-79	-10	-77±8	-9
4CA-4C -5N -5CA	178	168	-10	169±7	-9
4C -5N -5CA-5C	-86	-75	11	-76±7	10
5N -5CA-5CB-5CG	28	34	6	32±6	4
5CA-5CB-5CG-5CD	-23	-31	-8	-27±9	-4
5N -5CA-5C -1N	70	66	-4	65±9	-5

Table 7, continued

5CA-5C -1N -1CA	-160	-168	-8	-167±6	-7
5C -1N -1CA-1C	83	92	9	93±11	10
CP6					
1N -1CA -1C -2N	11	3	-8	-3±10	-14
1CA -1C -2N -2CA	165	165	0	163±6	-2
1N -1CA -1CB -1SG	59	55	-4	57±6	-2
1C -2N -2CA -2C	102	106	4	117±11	15
2N -2CA -2C -3N	173	176	3	175±6	3
2CA -2C -3N -3CA	-168	-164	4	-166±7	2
2C -3N -3CA -3C	-63	-73	-10	-68±7	-5
3N -3CA -3C -4N	-23	-8	14	-15±8	7
3CA -3C -4N -4CA	-179	176	-4	179±5	-1
3N -3CA -3CB -3CG	1	26	25	5±24	4
3CA -3CB -3CG -3CD	-5	-36	-31	-11±30	-6
3C -4N -4CA -4C	-96	-101	-5	-100±8	-4
4N -4CA -4C -5N	1	-19	-20	-13±10	-13
4CA -4C -5N -5CA	-163	-171	-8	-169±6	-6
4N -4CA -4CB -4CG	-54	-57	-3	-56±6	-1
4CA -4CB -4CG -4CD1	104	108	4	106±11	2
4CB -4CG -4CD1-4CE1	-177	-177	0	-178±7	-1
4CB -4CG -4CD2-4CE2	177	177	0	178±7	1
4CG -4CD1-4CE1-4CZ	0	0	1	0±6	0
4C -5N -5CA -5C	-126	-102	24	-108±12	18
5N -5CA -5C -6N	-60	-64	-4	-66±8	-6
5CA -5C -6N -6CA	-174	-169	5	-169±7	5
5N -5CA -5CB -5SG	177	-180	3	180±5	2
5C -6N -6CA -6C	157	154	-3	159±10	2
6N -6CA -6C -7N	171	177	6	175±8	4
6CA -6C -7N -7CA	177	-179	4	179±7	2
6C -7N -7CA -7C	-53	-60	-7	-62±7	-8
7N -7CA -7C -8N	137	131	-6	139±7	2
7CA -7C -8N -8CA	178	-179	3	-178±6	4
7N -7CA -7CB -7CG	-25	-34	-9	-18±21	7
7CA -7CB -7CG -7CD	36	38	2	22±26	-14
7C -8N -8CA -8C	74	76	2	72±8	-2
8N -8CA -8CB -8CG	-61	-66	-6	-64±6	-4
8CA -8CB -8CG -8CD1	-88	-96	-8	-96±9	-8
8CB -8CG -8CD1-8CE1	175	177	1	177±7	2
8CB -8CG -8CD2-8CE2	-173	-175	-2	-176±7	-2
8CG -8CD1-8CE1-8CZ	-2	0	2	0±7	2
1CA -1CB -1SG -5SG	117	123	5	119±7	2
1CB -1SG -5SG -5CB	-89	-84	5	-88±6	1
1SG -5SG -5CB -5CA	-99	-109	-11	-107±7	-9
8N -8CA -8C -1N	1	6	6	2±12	2
8CA -8C -1N -1CA	172	171	-1	172±6	1
8C -1N -1CA -1C	-134	-137	-3	-133±13	1

[a]Dihedral angles in degrees. Errors from the NVT simulation represent the rms fluctuations. Atom names correspond to the nomenclature used for the amino acid residues as presented in Figure 1 of the appendix.

Table 8) Interaction distances for the cyclic peptide structures from the crystal, minimized and dynamics averages.[a]

Interaction[b]	X-ray	Min.	Diff	Dynamics	Diff
CP1					
CP1 1 C -CP1 3 N	3.22	3.37	0.14	3.29±0.07	0.07
CP1 1 C -CP1 6 O	2.79	2.92	0.13	2.95±0.07	0.16
CP1 1 O -CP1 2 C	3.36	3.36	0.00	3.33±0.08	-0.02
CP1 1 O -CP1 3 N	3.44	3.59	0.15	3.50±0.11	0.06
CP1 1 O -CP1 6 O	3.38	3.55	0.16	3.49±0.09	0.11
CP1 2 N -CP1 6 C	3.22	3.37	0.15	3.41±0.07	0.19
CP1 2 N -CP1 6 O	3.14	3.15	0.01	3.29±0.10	0.15
CP1 3 N -CP1 6 O	2.92	2.94	0.02	2.94±0.10	0.02
CP1 3 O -CP1 4 C	3.36	3.61	0.25	3.50±0.08	0.13
CP1 3 O -CP1 5 N	3.45	3.79	0.34	3.64±0.11	0.19
CP1 3 O -CP1 6 N	3.35	4.05	0.70	3.61±0.15	0.25
CP1 3 O -CP1 6 O	3.45	3.49	0.05	3.31±0.15	-0.14
CP1 5 C -CP1 6 O	3.48	3.32	-0.16	3.40±0.08	-0.08
CP1 1 N -C018 5 O	2.89	2.83	-0.06	2.80±0.07	-0.09
CP1 2 N -C005 1 O	2.93	2.84	-0.10	2.89±0.05	-0.04
CP1 2 O -C028 4 N	3.04	3.65	0.61	3.20±0.15	0.17
CP1 3 O -C005 4 N	3.25	2.93	-0.32	3.12±0.12	-0.13
CP1 5 N -C005 4 O	2.77	2.76	-0.01	2.80±0.03	0.04
CP1 6 N -C005 4 O	3.16	2.90	-0.26	3.04±0.13	-0.12
CP1 2 CB -C005 1 O	3.32	3.32	0.00	3.28±0.11	-0.04
CP1 2 CB -C005 2 O	3.47	3.47	-0.01	3.43±0.12	-0.05
CP1 2 O -C028 4 CA	3.30	3.97	0.67	3.49±0.14	0.18
CP1 3 O -C005 3 CA	3.45	3.57	0.12	3.59±0.10	0.14
CP1 4 CA -C028 2 O	3.47	3.82	0.34	3.47±0.12	0.00
CP1 5 CA -C005 4 O	3.37	3.41	0.04	3.43±0.08	0.06
CP1 5 CB -C005 4 O	3.47	3.47	0.00	3.46±0.12	0.00
CP1 6 CA -C005 6 O	3.29	3.56	0.27	3.47±0.12	0.18
CP1 5 O -C018 1 CA	3.34	3.59	0.24	3.56±0.14	0.22
WAT 1 OH2 -C003 4 CA	3.29	3.51	0.22	3.44±0.12	0.15
WAT 1 OH2 -C024 1 OH2	2.78	2.69	-0.10	2.74±0.05	-0.05
CP2					
CP2 1 C -CP2 3 N	3.29	3.54	0.25	3.41±0.13	0.11
CP2 1 C -CP2 6 O	2.93	3.24	0.31	3.20±0.11	0.27
CP2 2 N -CP2 6 C	3.22	3.62	0.40	3.62±0.11	0.40
CP2 2 N -CP2 6 O	3.23	3.85	0.62	3.82±0.16	0.59
CP2 3 N -CP2 6 O	3.10	4.21	1.11	3.95±0.34	0.85
CP2 3 C -CP2 5 N	3.08	3.32	0.24	3.31±0.07	0.23
CP2 3 O -CP2 4 CB	3.21	3.54	0.33	3.54±0.14	0.32
CP2 3 O -CP2 4 C	2.77	2.96	0.19	2.95±0.06	0.18
CP2 3 O -CP2 4 O	3.40	3.68	0.28	3.63±0.12	0.22
CP2 3 O -CP2 5 N	3.03	3.10	0.07	3.11±0.11	0.08
CP2 3 O -CP2 6 N	2.99	3.15	0.16	3.05±0.14	0.06
CP2 4 C -CP2 6 N	3.33	3.63	0.30	3.52±0.16	0.19
CP2 4 O -CP2 5 C	3.48	3.36	-0.13	3.43±0.11	-0.05
CP2 1 N -WAT 1 OH2	3.33	3.19	-0.13	3.26±0.12	-0.06
CP2 2 N -WAT 1 OH2	2.87	2.95	0.08	2.99±0.10	0.12
CP2 2 CA -WAT 1 OH2	3.43	3.61	0.18	3.62±0.11	0.19

Table 8, continued

CP2 2 CB -WAT 1 OH2	3.48	3.63	0.14	3.61±0.14	0.12
CP2 3 N -WAT 1 OH2	3.46	3.01	-0.44	3.16±0.16	-0.29
CP2 3 O -WAT 1 OH2	2.80	2.68	-0.12	2.73±0.09	-0.07
CP2 5 N -WAT 2 OH2	2.96	2.98	0.03	3.09±0.14	0.13
CP2 5 CA -WAT 2 OH2	3.24	3.41	0.17	3.41±0.11	0.17
CP2 5 C -WAT 2 OH2	3.37	3.62	0.25	3.54±0.13	0.17
CP2 6 N -WAT 2 OH2	3.32	2.90	-0.42	3.07±0.16	-0.25
CP2 6 CA -WAT 1 OH2	3.30	3.41	0.11	3.47±0.13	0.17
CP2 6 C -WAT 1 OH2	3.18	3.37	0.19	3.41±0.13	0.23
CP2 6 O -WAT 2 OH2	2.83	2.70	-0.13	2.72±0.07	-0.11
CP2 1 N -C024 4 O	2.85	2.82	-0.03	2.82±0.07	-0.03
CP2 1 O -C011 3 CA	3.18	3.67	0.49	3.66±0.28	0.49
CP2 1 O -C011 2 OH2	2.86	2.64	-0.22	2.67±0.07	-0.19
CP2 2 CB -C002 2 OH2	3.48	3.62	0.14	3.52±0.12	0.04
CP2 2 O -C012 3 CA	3.38	3.60	0.22	3.66±0.18	0.28
CP2 2 O -C012 4 N	2.81	2.85	0.04	2.84±0.08	0.02
CP2 5 CA -C027 4 O	3.27	3.19	-0.08	3.28±0.11	0.01
CP2 5 O -C024 1 OH2	2.78	2.64	-0.14	2.67±0.07	-0.11
CP2 5 O -C027 4 C	3.25	4.10	0.85	3.69±0.29	0.44
CP2 5 O -C027 5 N	3.33	4.43	1.10	3.92±0.41	0.59
CP2 6 CA -C024 4 O	3.37	3.42	0.06	3.42±0.12	0.05
CP3					
CP3 1 N -CP3 5 C	3.18	3.29	0.11	3.34±0.15	0.16
CP3 1 N -CP3 5 O	3.25	3.46	0.21	3.47±0.29	0.23
CP3 1 C -CP3 2 O	3.49	3.59	0.10	3.76±0.17	0.27
CP3 2 N -CP3 5 O	3.04	3.23	0.18	3.31±0.34	0.27
CP3 2 N -CP3 6 C	3.43	3.45	0.03	3.51±0.13	0.08
CP3 2 C -CP3 4 N	3.09	3.25	0.16	3.28±0.09	0.19
CP3 2 O -CP3 3 C	3.12	3.23	0.11	3.15±0.13	0.04
CP3 2 O -CP3 4 N	3.13	3.32	0.18	3.29±0.15	0.16
CP3 2 O -CP3 5 N	3.16	3.08	-0.08	3.08±0.20	-0.08
CP3 5 O -CP3 6 C	3.12	3.35	0.23	3.34±0.18	0.22
WAT 1 OH2 -CP3 1 N	2.81	2.90	0.08	2.94±0.12	0.12
WAT 1 OH2 -CP3 1 CA	3.29	3.42	0.14	3.53±0.16	0.24
WAT 1 OH2 -CP3 1 C	3.35	3.34	-0.01	3.71±0.26	0.36
WAT 1 OH2 -CP3 2 N	3.31	3.24	-0.07	3.43±0.26	0.12
WAT 1 OH2 -CP3 2 O	2.83	2.80	-0.03	3.14±0.30	0.31
WAT 1 OH2 -CP3 5 CA	3.32	3.34	0.02	3.49±0.17	0.17
WAT 1 OH2 -CP3 5 C	3.25	3.33	0.07	3.42±0.19	0.17
WAT 1 OH2 -CP3 6 N	3.40	3.34	-0.06	3.30±0.23	-0.10
WAT 2 OH2 -CP3 2 CA	3.35	3.34	-0.01	3.57±0.22	0.22
WAT 2 OH2 -CP3 2 C	3.33	3.29	-0.04	3.47±0.21	0.14
WAT 2 OH2 -CP3 3 N	3.46	3.34	-0.12	3.50±0.25	0.04
WAT 2 OH2 -CP3 4 N	2.89	2.90	0.01	3.01±0.18	0.12
WAT 2 OH2 -CP3 4 CA	3.39	3.44	0.05	3.51±0.16	0.12
WAT 2 OH2 -CP3 4 C	3.20	3.31	0.11	3.42±0.21	0.22
WAT 2 OH2 -CP3 5 N	3.30	3.28	-0.02	3.42±0.21	0.12
WAT 2 OH2 -CP3 5 O	2.87	2.77	-0.10	2.93±0.28	0.06
WAT 3 OH2 -CP3 2 CA	3.22	3.17	-0.05	3.35±0.21	0.14
WAT 3 OH2 -CP3 3 N	2.86	2.85	-0.01	2.93±0.15	0.07
CP3 1 CA -C023 3 O	3.28	3.16	-0.12	3.35±0.26	0.07

Table 8, continued

CP3 1 O -C023 5 N	3.20	3.21	0.02	3.37±0.25	0.17
CP3 1 O -C023 5 CA	3.31	3.32	0.01	3.49±0.23	0.17
CP3 2 CA -C021 4 O	3.45	3.35	-0.11	3.52±0.26	0.07
CP3 2 CA -C023 1 OH2	3.33	3.52	0.19	3.52±0.22	0.18
CP3 3 CB -C006 1 O	3.45	3.45	0.00	3.72±0.25	0.28
CP3 4 CB -C001 2 O	3.41	3.19	-0.22	3.33±0.19	-0.07
CP3 4 O -C001 1 OH2	2.85	2.73	-0.12	2.77±0.15	-0.08
CP3 6 N -C005 6 C	3.38	3.45	0.07	3.50±0.14	0.12
CP3 6 N -C005 6 O	3.34	3.35	0.01	3.45±0.25	0.11
CP3 6 N -C013 3 O	2.92	3.01	0.09	3.41±0.35	0.49
CP3 6 CA -C005 1 N	3.37	3.38	0.01	3.50±0.16	0.13
CP3 6 CA -C013 3 O	3.49	3.54	0.06	3.77±0.35	0.28
CP3 6 O -C011 3 OH2	2.73	2.67	-0.06	2.82±0.20	0.09
WAT 2 OH2 -C001 1 O	2.82	2.69	-0.14	2.90±0.24	0.07
WAT 2 OH2 -C021 4 C	3.29	3.32	0.03	3.37±0.16	0.07
WAT 2 OH2 -C021 5 N	3.49	3.52	0.03	3.37±0.20	-0.12
WAT 3 OH2 -C021 4 O	2.95	2.96	0.01	3.36±0.40	0.41
CP4					
CP4 1 N -CP4 4 O	2.91	3.09	0.19	3.19±0.18	0.29
CP4 1 N -CP4 5 C	3.25	3.31	0.06	3.37±0.11	0.12
CP4 1 N -CP4 5 O	3.40	3.56	0.16	3.63±0.19	0.24
CP4 1 CA -WAT 1 OH2	3.25	3.33	0.08	3.37±0.14	0.12
CP4 1 C -CP4 3 N	3.31	3.28	-0.03	3.30±0.11	-0.01
CP4 1 C -CP4 4 O	3.49	3.58	0.08	3.67±0.15	0.18
CP4 1 C -WAT 1 OH2	3.40	3.30	-0.10	3.36±0.15	-0.04
CP4 1 O -CP4 2 C	2.96	3.16	0.20	3.12±0.09	0.16
CP4 1 O -CP4 3 N	3.37	3.36	-0.01	3.35±0.16	-0.02
CP4 1 O -CP4 4 O	3.04	3.04	0.00	3.09±0.17	0.05
CP4 1 O -WAT 2 OH2	2.81	2.74	-0.07	2.78±0.14	-0.04
CP4 2 N -WAT 1 OH2	3.44	3.31	-0.13	3.43±0.17	-0.02
CP4 3 N -WAT 1 OH2	3.35	3.00	-0.35	3.15±0.22	-0.19
CP4 3 N -WAT 4 OH2	3.12	3.36	0.23	3.31±0.17	0.18
CP4 3 CA -WAT 4 OH2	3.38	3.44	0.06	3.49±0.14	0.11
CP4 4 N -WAT 1 OH2	3.16	2.91	-0.25	3.01±0.16	-0.14
CP4 4 C -CP4 5 O	3.35	3.55	0.20	3.59±0.13	0.23
CP4 4 O -CP4 5 C	2.80	2.97	0.17	2.98±0.08	0.19
CP4 4 O -CP4 5 O	3.32	3.62	0.30	3.67±0.16	0.35
CP4 4 O -CP4 6 N	3.14	3.22	0.08	3.21±0.13	0.06
CP4 4 O -WAT 2 OH2	3.45	3.51	0.05	3.45±0.25	0.00
CP4 5 O -CP4 6 C	3.34	3.51	0.17	3.57±0.14	0.22
CP4 6 N -WAT 3 OH2	2.99	3.04	0.06	3.05±0.14	0.06
WAT 1 OH2 -WAT 4 OH2	2.85	2.69	-0.16	2.73±0.08	-0.11
WAT 2 OH2 -WAT 3 OH2	2.84	2.76	-0.08	2.82±0.12	-0.02
CP4 1 O -C003 5 CD	3.47	3.33	-0.14	3.46±0.19	-0.01
CP4 2 CA -C003 3 O	3.37	3.44	0.06	3.54±0.17	0.17
CP4 2 CB -C003 3 O	3.37	3.48	0.11	3.48±0.21	0.11
CP4 2 CG -C005 2 O	3.37	3.64	0.27	3.66±0.22	0.29
CP4 2 O -C004 4 OH2	2.82	2.72	-0.10	2.82±0.14	0.00
CP4 5 CB -C025 3 O	3.42	3.36	-0.07	3.40±0.14	-0.02
CP4 6 N -C017 2 O	3.25	3.21	-0.04	3.27±0.19	0.03
CP4 6 CA -C017 2 O	3.22	3.35	0.13	3.40±0.20	0.19

Table 8, continued

CP4 6 O -C005 5 CA	3.39	3.44	0.05	3.50±0.17	0.11
CP4 6 O -C005 3 OH2	2.76	2.68	-0.07	2.78±0.13	0.02
CP4 6 O -C015 2 CB	3.38	3.43	0.05	3.41±0.11	0.03
WAT 2 OH2 -C004 4 CA	3.49	3.67	0.18	3.70±0.19	0.21
WAT 2 OH2 -C004 1 OH2	2.84	2.72	-0.11	2.80±0.13	-0.04
WAT 3 OH2 -C004 5 O	2.79	2.80	0.01	2.83±0.12	0.04
WAT 4 OH2 -C005 3 O	2.85	2.72	-0.13	2.79±0.13	-0.06
CP5					
CP5 1 N -CP5 4 C	3.14	3.12	-0.03	3.14±0.10	-0.01
CP5 1 N -CP5 4 O	2.92	2.86	-0.06	2.90±0.12	-0.02
CP5 1 C -CP5 2 O	3.34	3.74	0.40	3.72±0.14	0.38
CP5 1 C -CP5 5 O	3.40	3.55	0.15	3.56±0.16	0.17
CP5 1 O -CP5 2 C	2.82	3.02	0.20	3.02±0.09	0.20
CP5 1 O -CP5 2 O	3.37	3.87	0.51	3.85±0.16	0.48
CP5 1 O -CP5 3 N	3.15	3.04	-0.11	3.08±0.14	-0.08
CP5 1 O -CP5 4 N	2.87	3.12	0.25	3.13±0.16	0.26
CP5 1 O -CP5 4 C	3.31	3.69	0.37	3.67±0.18	0.36
CP5 1 O -CP5 4 O	3.46	3.68	0.22	3.68±0.21	0.22
CP5 2 C -CP5 4 N	3.23	3.55	0.32	3.52±0.14	0.29
CP5 2 O -CP5 3 C	3.21	3.43	0.22	3.45±0.14	0.24
CP5 2 O -CP5 4 N	3.38	3.93	0.55	3.88±0.21	0.51
CP5 3 C -CP5 5 CD	3.41	3.60	0.19	3.63±0.15	0.22
CP5 3 O -CP5 5 CD	3.48	3.38	-0.09	3.50±0.20	0.02
CP5 4 N -CP5 5 CD	3.11	3.37	0.26	3.35±0.12	0.24
CP5 4 O -CP5 5 C	3.36	3.25	-0.10	3.27±0.09	-0.08
CP5 5 CG -CP5 5 O	3.27	3.21	-0.06	3.27±0.17	0.00
CP5 2 O -C010 2 CG	3.46	3.79	0.34	3.76±0.30	0.31
CP5 3 O -C003 2 CD	3.13	3.26	0.13	3.33±0.16	0.19
CP5 3 O -C009 2 CA	3.44	3.37	-0.07	3.36±0.12	-0.08
CP5 3 O -C009 3 N	2.90	2.80	-0.10	2.83±0.12	-0.06
CP6					
CP6 1 N -CP6 6 O	2.94	3.11	0.17	3.22±0.16	0.28
CP6 1 N -CP6 7 C	3.13	3.22	0.09	3.18±0.09	0.05
CP6 1 N -CP6 7 O	3.22	3.41	0.19	3.27±0.18	0.05
CP6 1 SG -CP6 6 N	3.44	3.56	0.11	3.54±0.18	0.10
CP6 1 SG -CP6 6 O	3.47	3.35	-0.12	3.39±0.19	-0.08
CP6 1 C -CP6 2 O	3.48	3.56	0.09	3.69±0.13	0.21
CP6 1 O -CP6 5 CB	3.31	3.44	0.13	3.57±0.25	0.26
CP6 2 N -CP6 6 O	3.14	3.04	-0.10	3.05±0.15	-0.08
CP6 2 C -CP6 4 N	3.19	3.21	0.01	3.21±0.08	0.02
CP6 2 O -CP6 3 C	2.96	3.12	0.15	3.04±0.10	0.08
CP6 2 O -CP6 4 N	3.05	3.08	0.03	3.08±0.13	0.03
CP6 2 O -CP6 5 N	2.99	3.01	0.02	3.02±0.15	0.03
CP6 2 O -CP6 6 N	3.11	2.92	-0.18	3.04±0.15	-0.07
CP6 2 O -CP6 6 O	3.32	3.18	-0.14	3.14±0.15	-0.18
CP6 3 C -CP6 5 N	3.38	3.51	0.13	3.48±0.10	0.10
CP6 4 N -CP6 4 CD1	3.31	3.37	0.05	3.37±0.16	0.06
CP6 6 C -CP6 7 O	3.15	3.39	0.25	3.29±0.13	0.14
CP6 6 O -CP6 7 C	2.74	2.94	0.20	2.95±0.10	0.21
CP6 6 O -CP6 7 O	3.15	3.42	0.26	3.33±0.16	0.18
CP6 6 O -CP6 8 N	3.24	3.39	0.15	3.51±0.14	0.27

Table 8, continued

CP6 7 C -CP6 8 CD2	3.43	3.52	0.09	3.55±0.13	0.12
CP6 7 O -CP6 8 CB	3.02	3.10	0.09	3.12±0.11	0.11
CP6 7 O -CP6 8 C	3.25	3.38	0.13	3.30±0.12	0.05
CP6 8 N -CP6 8 CD2	3.22	3.23	0.00	3.22±0.11	0.00
WAT 1 OH2 -CP6 5 O	2.82	2.65	-0.18	2.77±0.12	-0.06
WAT 2 OH2 -CP6 8 O	2.80	2.70	-0.10	2.76±0.12	-0.04
WAT 3 OH2 -CP6 4 O	2.84	2.72	-0.12	2.76±0.14	-0.08
WAT 3 OH2 -CP6 5 O	3.44	3.06	-0.37	3.10±0.18	-0.34
WAT 4 OH2 -CP6 7 O	2.77	2.65	-0.12	2.73±0.11	-0.04
CP6 1 O -C016 2 OH2	2.97	2.89	-0.09	3.11±0.25	0.14
CP6 2 N -C004 3 OH2	2.89	3.05	0.17	3.06±0.16	0.17
CP6 2 CA -C004 4 O	3.39	3.60	0.21	3.61±0.19	0.22
CP6 2 CA -C004 3 OH2	3.21	3.44	0.23	3.35±0.13	0.14
CP6 2 CA -C016 2 OH2	3.25	3.31	0.06	3.34±0.15	0.09
CP6 2 C -C016 2 OH2	3.07	3.12	0.05	3.23±0.16	0.17
CP6 2 O -C016 2 OH2	3.43	3.41	-0.02	3.59±0.20	0.16
CP6 3 N -C016 2 OH2	3.33	3.45	0.13	3.53±0.18	0.20
CP6 3 CA -C025 1 OH2	3.28	3.29	0.00	3.33±0.14	0.05
CP6 3 C -C025 1 OH2	3.50	3.86	0.36	3.54±0.13	0.05
CP6 3 O -C025 7 CD	3.27	3.14	-0.13	3.26±0.14	0.00
CP6 3 O -C025 1 OH2	2.86	3.49	0.63	2.91±0.16	0.05
CP6 4 N -C016 2 OH2	3.05	3.17	0.11	3.28±0.21	0.23
CP6 6 N -C023 8 CE2	3.38	3.47	0.09	3.52±0.18	0.14
CP6 6 CA -C023 8 CE2	3.32	3.42	0.10	3.49±0.14	0.17
CP6 6 CA -C023 8 CZ	3.49	3.69	0.20	3.65±0.15	0.17
CP6 6 O -C004 3 OH2	3.14	3.32	0.18	3.24±0.19	0.09
CP6 8 N -C004 5 O	3.00	3.20	0.20	3.05±0.14	0.05
CP6 8 N -C004 3 OH2	3.30	3.02	-0.28	3.14±0.18	-0.16
CP6 8 CA -C004 5 O	3.27	3.38	0.11	3.41±0.16	0.15
WAT 1 OH2 -C025 4 OH2	2.79	2.71	-0.07	2.77±0.10	-0.02
WAT 3 OH2 -C025 4 OH2	2.80	2.79	-0.02	2.80±0.12	-0.01
RMS difference			0.23		0.19
Average difference			0.05±0.14		0.04±0.07

[a]All non-hydrogen to non-hydrogen nonbonded interactions less than 3.5 Å in the X-ray structures are included. Distances in Å.

[b]Image atoms are represented by the CHARMM identifier for the specific image and the atom name.

Appendix Table I. Atom Types

Atom type	Mass	Description
H	1.00800	polar H
HC	1.00800	N-ter H
HA	1.00800	nonpolar H
HT	1.00800	TIPS3P WATER HYDROGEN
HP	1.00800	aromatic H
HB	1.00800	backbone H
HR1	1.00800	his he1, (+) his HG,HD2
HR2	1.00800	(+) his HE1
HR3	1.00800	neutral his HG, HD2
HS	1.00800	thiol hydrogen
HA1	1.00800	for alkene; RHC=CR
HA2	1.00800	for alkene; H2C=CR
C	12.01100	polar C
CA	12.01100	aromatic C
CT1	12.01100	aliphatic sp3 C for CH
CT2	12.01100	aliphatic sp3 C for CH2
CT3	12.01100	aliphatic sp3 C for CH3
CPH1	12.01100	his CG and CD2 carbons
CPH2	12.01100	his CE1 carbon
CPT	12.01100	trp C between rings
CY	12.01100	TRP C in pyrrole ring
CP1	12.01100	tetrahedral C (proline CA)
CP2	12.01100	tetrahedral C (proline CB/CG)
CP3	12.01100	tetrahedral C (proline CD)
CC	12.01100	carbonyl C for sidechains asn,asp,gln,glu
CD	12.01100	carbonyl C for none amides, asp,glu,cter
CPA	12.01100	heme alpha-C
CPB	12.01100	heme beta-C
CPM	12.01100	heme meso-C
CM	12.01100	heme CO carbon
CS	12.01100	thiolate carbon
CE1	12.01100	for alkene; RHC=CR
CE2	12.01100	for alkene; H2C=CR
N	14.00700	proline N
NR1	14.00700	neutral his protonated ring nitrogen
NR2	14.00700	neutral his unprotonated ring nitrogen
NR3	14.00700	charged his ring nitrogen
NH1	14.00700	peptide nitrogen
NH2	14.00700	amide nitrogen
NH3	14.00700	ammonium nitrogen
NC2	14.00700	guanidinium nitroogen
NY	14.00700	TRP N in pyrrole ring
NP	14.00700	Proline ring NH2+ (N-terminal)
NPH	14.00700	heme pyrrole N
O	15.99900	carbonyl oxygen
OB	15.99900	carbonyl oxygen in acetic acid
OC	15.99900	carboxylate oxygen
OH1	15.99900	hydroxyl oxygen
OS	15.99940	ester oxygen
OT	15.99940	TIPS3P WATER OXYGEN
OM	15.99900	heme CO/O2 oxygen
S	32.06000	sulphur
SM	32.06000	sulfur C-S-S-C type
SS	32.06000	thiolate sulfur
FE	55.84700	heme iron

Appendix Table II. Bond parameters

Atom types		K_b	b_o
C	C	600.00	1.3350
CA	CA	305.00	1.3750
CP1	C	250.00	1.4900
CP1	CC	250.00	1.4900
CP1	CD	200.00	1.4900
CP2	CP1	222.50	1.5270
CP2	CP2	222.50	1.5370
CP3	CP2	222.50	1.5370
CPB	C	450.00	1.3800
CPB	CPA	299.80	1.4432
CPB	CPB	340.70	1.3464
CPH1	CPH1	410.00	1.3600
CPM	CPA	360.00	1.3716
CPT	CA	305.00	1.3680
CPT	CPT	360.00	1.4000
CT1	C	250.00	1.4900
CT1	CC	200.00	1.5220
CT1	CD	200.00	1.5220
CT1	CT1	222.50	1.5000
CT2	C	250.00	1.4900
CT2	CA	230.00	1.4900
CT2	CC	200.00	1.5220
CT2	CD	200.00	1.5220
CT2	CPB	230.00	1.4900
CT2	CPH1	229.63	1.5000
CT2	CT1	222.50	1.5380
CT2	CT2	222.50	1.5300
CT3	C	250.00	1.4900
CT3	CA	230.00	1.4900
CT3	CC	200.00	1.5220
CT3	CD	200.00	1.5220
CT3	CPB	230.00	1.4900
CT3	CPH1	229.63	1.5000
CT3	CS	190.00	1.5310
CT3	CT1	222.50	1.5380
CT3	CT2	222.50	1.5280
CT3	CT3	222.50	1.5300
CY	CA	350.00	1.3650
CY	CPT	350.00	1.4400
CY	CT2	230.00	1.5100
FE	CM	258.00	1.9000
FE	CPM	0.00	3.3814
H	CD	330.00	1.1100
HA	C	330.00	1.1000
HA	CA	340.00	1.0830
HA	CC	317.13	1.1000
HA	CP2	309.00	1.1110
HA	CP3	309.00	1.1110
HA	CPM	367.60	1.0900
HA	CS	300.00	1.1110
HA	CT1	309.00	1.1110
HA	CT2	309.00	1.1110
HA	CT3	322.00	1.1110

Appendix Table II continued

HA	CY	330.00	1.0800
HB	CP1	330.00	1.0800
HB	CT1	330.00	1.0800
HB	CT2	330.00	1.0800
HB	CT3	330.00	1.0800
HP	CA	340.00	1.0800
HP	CY	350.00	1.0800
HR1	CPH1	375.00	1.0830
HR1	CPH2	340.00	1.0900
HR2	CPH2	333.00	1.0700
HR3	CPH1	365.00	1.0830
HT	HT	0.00	1.5139
N	C	260.00	1.3000
N	CP1	320.00	1.4340
N	CP3	320.00	1.4550
NC2	C	463.00	1.3650
NC2	CT2	261.00	1.4900
NC2	CT3	261.00	1.4900
NC2	HC	455.00	1.0000
NH1	C	370.00	1.3450
NH1	CT1	320.00	1.4300
NH1	CT2	320.00	1.4300
NH1	CT3	320.00	1.4300
NH1	H	440.00	0.9970
NH1	HC	405.00	0.9800
NH2	CC	430.00	1.3600
NH2	CT3	240.00	1.4550
NH2	H	480.00	1.0000
NH2	HC	460.00	1.0000
NH3	CT1	200.00	1.4800
NH3	CT2	200.00	1.4800
NH3	CT3	200.00	1.4800
NH3	HC	403.00	1.0400
NP	CP1	320.00	1.4850
NP	CP3	320.00	1.5020
NP	HC	460.00	1.0060
NPH	CPA	377.20	1.3757
NPH	FE	270.20	1.9580
NR1	CPH1	400.00	1.3800
NR1	CPH2	400.00	1.3600
NR1	H	466.00	1.0000
NR2	CPH1	400.00	1.3800
NR2	CPH2	400.00	1.3200
NR2	FE	65.00	2.2000
NR3	CPH1	380.00	1.3700
NR3	CPH2	380.00	1.3200
NR3	H	453.00	1.0000
NY	CA	270.00	1.3700
NY	CPT	270.00	1.3750
NY	H	465.00	0.9760
O	C	620.00	1.2300
O	CC	650.00	1.2300
OB	CC	750.00	1.2200
OB	CD	750.00	1.2200
OC	CA	525.00	1.2600

Appendix Table II continued

OC	CC	525.00	1.2600
OC	CT2	450.00	1.3300
OC	CT3	450.00	1.3300
OH1	CA	334.30	1.4110
OH1	CD	230.00	1.4000
OH1	CT1	428.00	1.4200
OH1	CT2	428.00	1.4200
OH1	CT3	428.00	1.4200
OH1	H	545.00	0.9600
OM	CM	1115.00	1.1280
OM	FE	250.00	1.8000
OM	OM	600.00	1.2300
OS	CD	150.00	1.3340
OS	CT3	340.00	1.4300
OT	HT	450.00	0.9572
S	CT2	198.00	1.8180
S	CT3	240.00	1.8160
S	HS	275.00	1.3250
SM	CT2	214.00	1.8160
SM	CT3	214.00	1.8160
SM	SM	173.00	2.0290
SS	CS	205.00	1.8360

K_b in kcal/mole/Å^2 and b_o in Å.

Appendix Table III. Bond Angle Parameters

Atom types			K_θ	θ_o	K_{UB}	S_o
CA	CA	CA	40.00	120.00	35.00	2.4162
CP1	N	C	60.00	117.00		
CP2	CP1	C	52.00	112.30		
CP2	CP1	CC	52.00	112.30		
CP2	CP1	CD	50.00	112.30		
CP2	CP2	CP1	70.00	108.50		
CP3	CP2	CP2	70.00	108.50		
CP3	N	C	60.00	117.00		
CP3	N	CP1	100.00	114.20		
CP3	NP	CP1	100.00	111.00		
CPA	CPB	C	70.00	126.74		
CPA	CPM	CPA	94.20	125.12		
CPA	NPH	CPA	139.30	103.90		
CPB	C	C	70.00	121.50		
CPB	CPB	C	70.00	126.75		
CPB	CPB	CPA	30.80	106.51		
CPH2	NR1	CPH1	130.00	107.50		
CPH2	NR2	CPH1	130.00	104.00		
CPH2	NR3	CPH1	145.00	108.00		
CPM	CPA	CPB	61.60	124.07		
CPT	CA	CA	60.00	118.00		
CPT	CPT	CA	60.00	122.00		
CPT	CY	CA	120.00	107.40	25.00	2.2610
CPT	NY	CA	110.00	108.00		
CT1	CT1	C	52.00	108.00		
CT1	CT1	CC	52.00	108.00		
CT1	CT1	CT1	53.35	111.00	8.00	2.5610
CT1	CT2	CA	51.80	107.50		
CT1	CT2	CC	52.00	108.00		
CT1	CT2	CD	52.00	108.00		
CT1	CT2	CPH1	58.35	113.00		
CT1	CT2	CT1	58.35	113.50	11.16	2.5610
CT1	NH1	C	50.00	120.00		
CT2	CA	CA	45.80	122.30		
CT2	CPB	CPA	65.00	126.74		
CT2	CPB	CPB	65.00	126.75		
CT2	CPH1	CPH1	45.80	130.00		
CT2	CT1	C	52.00	108.00		
CT2	CT1	CC	52.00	108.00		
CT2	CT1	CD	52.00	108.00		
CT2	CT1	CT1	53.35	111.00	8.00	2.5610
CT2	CT2	C	52.00	108.00		
CT2	CT2	CC	52.00	108.00		
CT2	CT2	CD	52.00	108.00		
CT2	CT2	CPB	70.00	113.00		
CT2	CT2	CT1	58.35	113.50	11.16	2.5610
CT2	CT2	CT2	58.35	113.60	11.16	2.5610
CT2	CT3	CT1	58.35	113.50	11.16	2.5610
CT2	CY	CA	45.80	129.40		
CT2	CY	CPT	45.80	124.00		
CT2	NC2	C	62.30	120.00		
CT2	NH1	C	50.00	120.00		
CT2	OS	CD	40.00	109.60	30.00	2.2651
CT3	CA	CA	45.80	122.30		

Appendix Table III continued

CT3	CPB	CPA	65.00	126.74		
CT3	CPB	CPB	65.00	126.75		
CT3	CPH1	CPH1	45.80	130.00		
CT3	CT1	C	52.00	108.00		
CT3	CT1	CC	52.00	108.00		
CT3	CT1	CT1	53.35	108.50	8.00	2.5610
CT3	CT1	CT2	53.35	114.00	8.00	2.5610
CT3	CT1	CT3	53.35	114.00	8.00	2.5610
CT3	CT2	CA	51.80	107.50		
CT3	CT2	CPH1	58.35	113.00		
CT3	CT2	CT1	58.35	113.50	11.16	2.5610
CT3	CT2	CT2	58.00	115.00	8.00	2.5610
CT3	CT2	CT3	53.35	114.00	8.00	2.5610
CT3	NC2	C	62.30	120.00		
CT3	NH1	C	50.00	120.00		
CT3	OS	CD	40.00	109.60	30.00	2.2651
CT3	S	CT2	34.00	95.00		
CY	CPT	CA	160.00	130.60		
CY	CPT	CPT	110.00	107.40		
CY	CT2	CT1	58.35	114.00		
CY	CT2	CT3	58.35	114.00		
FE	NPH	CPA	96.15	128.05		
FE	NR2	CPH1	30.00	133.00		
FE	NR2	CPH2	30.00	123.00		
H	NH1	C	34.00	123.00		
H	NH1	CT1	35.00	117.00		
H	NH1	CT2	35.00	117.00		
H	NH1	CT3	35.00	117.00		
H	NH2	CC	50.00	120.00		
H	NH2	H	23.00	120.00		
H	NR1	CPH1	30.00	125.50	20.00	2.1500
H	NR1	CPH2	30.00	127.00	20.00	2.1400
H	NR3	CPH1	25.00	126.00	15.00	2.1300
H	NR3	CPH2	25.00	126.00	15.00	2.0900
H	NY	CA	28.00	126.00		
H	NY	CPT	28.00	126.00		
H	OH1	CA	65.00	108.00		
H	OH1	CD	55.00	115.00		
H	OH1	CT1	57.50	106.00		
H	OH1	CT2	57.50	106.00		
H	OH1	CT3	57.50	106.00		
HA	C	C	50.00	120.50		
HA	C	CPB	50.00	120.00		
HA	C	HA	50.00	118.00		
HA	CA	CA	29.00	120.00	25.00	2.1525
HA	CA	CPT	41.00	122.00		
HA	CA	CY	32.00	125.00	25.00	2.1730
HA	CP2	CP1	33.43	110.10	22.53	2.1790
HA	CP2	CP2	26.50	110.10	22.53	2.1790
HA	CP2	CP3	26.50	110.10	22.53	2.1790
HA	CP2	HA	35.50	109.00	5.40	1.8020
HA	CP3	CP2	26.50	110.10	22.53	2.1790
HA	CP3	HA	35.50	109.00	5.40	1.8020
HA	CPM	CPA	12.70	117.44		
HA	CPM	FE	0.00	180.00		

Appendix Table III continued

HA	CS	CT3	34.60	110.10	22.53	2.1790
HA	CS	HA	35.50	108.40	14.00	1.7750
HA	CT1	C	33.00	109.50	30.00	2.1630
HA	CT1	CD	33.00	109.50	30.00	2.1630
HA	CT1	CT1	34.50	110.10	22.53	2.1790
HA	CT1	CT2	34.50	110.10	22.53	2.1790
HA	CT1	CT3	34.50	110.10	22.53	2.1790
HA	CT1	HA	35.50	109.00	5.40	1.8020
HA	CT2	C	33.00	109.50	30.00	2.1630
HA	CT2	CA	49.30	107.50		
HA	CT2	CC	33.00	109.50	30.00	2.1630
HA	CT2	CD	33.00	109.50	30.00	2.1630
HA	CT2	CPB	50.00	109.50		
HA	CT2	CPH1	33.43	109.50		
HA	CT2	CT1	33.43	110.10	22.53	2.1790
HA	CT2	CT2	26.50	110.10	22.53	2.1790
HA	CT2	CT3	34.60	110.10	22.53	2.1790
HA	CT2	CY	33.43	109.50		
HA	CT2	HA	35.50	109.00	5.40	1.8020
HA	CT3	C	33.00	109.50	30.00	2.1630
HA	CT3	CA	49.30	107.50		
HA	CT3	CC	33.00	109.50	30.00	2.1630
HA	CT3	CD	33.00	109.50	30.00	2.1630
HA	CT3	CPB	50.00	109.50		
HA	CT3	CPH1	33.43	109.50		
HA	CT3	CS	34.60	110.10	22.53	2.1790
HA	CT3	CT1	33.43	110.10	22.53	2.1790
HA	CT3	CT2	34.60	110.10	22.53	2.1790
HA	CT3	CT3	37.50	110.10	22.53	2.1790
HA	CT3	HA	35.50	108.40	5.40	1.8020
HA	CY	CA	20.00	126.40	25.00	2.1860
HA	CY	CPT	32.00	126.40	25.00	2.2550
HB	CP1	C	50.00	112.00		
HB	CP1	CC	50.00	112.00		
HB	CP1	CD	50.00	112.00		
HB	CP1	CP2	35.00	118.00		
HB	CT1	C	50.00	109.50		
HB	CT1	CC	50.00	109.50		
HB	CT1	CD	50.00	109.50		
HB	CT1	CT1	35.00	111.00		
HB	CT1	CT2	35.00	111.00		
HB	CT1	CT3	35.00	111.00		
HB	CT2	C	50.00	109.50		
HB	CT2	CC	50.00	109.50		
HB	CT2	CD	50.00	109.50		
HB	CT2	HB	36.00	115.00		
HB	CT3	C	50.00	109.50		
HC	NC2	C	49.00	120.00		
HC	NC2	CT2	40.40	120.00		
HC	NC2	CT3	40.40	120.00		
HC	NC2	HC	25.00	120.00		
HC	NH2	CT3	50.00	111.00		
HC	NH2	HC	39.00	106.50		
HC	NH3	CT1	30.00	109.50	20.00	2.0740
HC	NH3	CT2	30.00	109.50	20.00	2.0740
HC	NH3	CT3	30.00	109.50	20.00	2.0740

Appendix Table III continued

HC	NH3	HC	44.00	109.50		
HC	NP	CP1	33.00	109.50	4.00	2.0560
HC	NP	CP3	33.00	109.50	4.00	2.0560
HC	NP	HC	51.00	107.50		
HP	CA	CA	30.00	120.00	22.00	2.1525
HP	CA	CPT	30.00	122.00	22.00	2.1460
HP	CA	CY	32.00	125.00	25.00	2.1730
HP	CY	CA	32.00	126.40	25.00	2.1860
HP	CY	CPT	32.00	126.40	25.00	2.2550
HR1	CPH1	CPH1	22.00	130.00	15.00	2.2150
HR3	CPH1	CPH1	25.00	130.00	20.00	2.2000
HS	S	CT2	38.80	95.00		
HS	S	CT3	43.00	95.00		
HT	OT	HT	55.00	104.52		
N	C	CP1	20.00	112.50		
N	C	CT1	20.00	112.50		
N	C	CT2	20.00	112.50		
N	C	CT3	20.00	112.50		
N	CP1	C	50.00	108.20		
N	CP1	CC	50.00	108.20		
N	CP1	CD	50.00	108.20		
N	CP1	CP2	70.00	110.80		
N	CP1	HB	48.00	112.00		
N	CP3	CP2	70.00	110.50		
N	CP3	HA	48.00	108.00		
NC2	C	NC2	52.00	120.00	90.00	2.3642
NC2	CT2	CT2	67.70	107.50		
NC2	CT2	HA	51.50	107.50		
NC2	CT3	HA	51.50	107.50		
NH1	C	CP1	80.00	116.50		
NH1	C	CT1	80.00	116.50		
NH1	C	CT2	80.00	116.50		
NH1	C	CT3	80.00	116.50		
NH1	CT1	C	50.00	107.00		
NH1	CT1	CC	50.00	107.00		
NH1	CT1	CD	50.00	107.00		
NH1	CT1	CT1	70.00	113.50		
NH1	CT1	CT2	70.00	113.50		
NH1	CT1	CT3	70.00	113.50		
NH1	CT1	HB	48.00	108.00		
NH1	CT2	C	50.00	107.00		
NH1	CT2	CC	50.00	107.00		
NH1	CT2	CD	50.00	107.00		
NH1	CT2	CT2	70.00	113.50		
NH1	CT2	HA	51.50	109.50		
NH1	CT2	HB	48.00	108.00		
NH1	CT3	HA	51.50	109.50		
NH2	CC	CP1	80.00	112.50		
NH2	CC	CT1	50.00	116.50	50.00	2.4500
NH2	CC	CT2	50.00	116.50	50.00	2.4500
NH2	CC	CT3	50.00	116.50	50.00	2.4500
NH2	CC	HA	44.00	111.00	50.00	1.9800
NH2	CT3	HA	38.00	109.50	50.00	2.1400
NH3	CT1	C	43.70	110.00		
NH3	CT1	CC	43.70	110.00		

Appendix Table III continued

NH3	CT1	CT1	67.70	110.00		
NH3	CT1	CT2	67.70	110.00		
NH3	CT1	CT3	67.70	110.00		
NH3	CT1	HB	51.50	107.50		
NH3	CT2	C	43.70	110.00		
NH3	CT2	CC	43.70	110.00		
NH3	CT2	CD	43.70	110.00		
NH3	CT2	CT2	67.70	110.00		
NH3	CT2	HA	45.00	107.50	35.00	2.1010
NH3	CT2	HB	51.50	107.50		
NH3	CT3	HA	45.00	107.50	35.00	2.1010
NP	CP1	C	50.00	106.00		
NP	CP1	CC	50.00	106.00		
NP	CP1	CD	50.00	106.00		
NP	CP1	CP2	70.00	108.50		
NP	CP1	HB	51.50	107.50		
NP	CP3	CP2	70.00	108.50		
NP	CP3	HA	51.50	109.15		
NPH	CPA	CPB	122.00	111.54		
NPH	CPA	CPM	88.00	124.39		
NPH	FE	CM	50.00	90.00		
NPH	FE	CPM	0.00	45.00		
NPH	FE	NPH	14.39	90.00		
NR1	CPH1	CPH1	130.00	106.00		
NR1	CPH1	CT2	45.80	124.00		
NR1	CPH1	CT3	45.80	124.00		
NR1	CPH1	HR3	25.00	124.00	20.00	2.1400
NR1	CPH2	HR1	25.00	122.50	20.00	2.1400
NR2	CPH1	CPH1	130.00	110.00		
NR2	CPH1	CT2	45.80	120.00		
NR2	CPH1	HR3	25.00	120.00	20.00	2.1400
NR2	CPH2	HR1	25.00	125.00	20.00	2.1200
NR2	CPH2	NR1	130.00	112.50		
NR2	FE	CM	50.00	180.00		
NR2	FE	NPH	50.00	90.00		
NR3	CPH1	CPH1	145.00	108.00		
NR3	CPH1	CT2	45.80	122.00		
NR3	CPH1	HR1	22.00	122.00	15.00	2.1800
NR3	CPH2	HR2	32.00	126.00	25.00	2.1400
NR3	CPH2	NR3	145.00	108.00		
NY	CA	CY	120.00	110.00	25.00	2.2400
NY	CA	HA	32.00	125.00	25.00	2.1770
NY	CA	HP	32.00	125.00	25.00	2.1770
NY	CPT	CA	160.00	130.60		
NY	CPT	CPT	110.00	107.40		
O	C	CP1	80.00	118.00		
O	C	CT1	80.00	121.00		
O	C	CT2	80.00	121.00		
O	C	CT3	80.00	121.00		
O	C	H	50.00	121.70		
O	C	N	80.00	122.50		
O	C	NH1	80.00	122.50		
O	CC	CP1	80.00	118.00		
O	CC	CT1	15.00	121.00	50.00	2.4400
O	CC	CT2	15.00	121.00	50.00	2.4400
O	CC	CT3	15.00	121.00	50.00	2.4400

Appendix Table III continued

O	CC	HA	44.00	122.00		
O	CC	NH2	75.00	122.50	50.00	2.3700
OB	CD	CP1	70.00	125.00	20.00	2.4420
OB	CD	CT1	70.00	125.00	20.00	2.4420
OB	CD	CT2	70.00	125.00	20.00	2.4420
OB	CD	CT3	70.00	125.00	20.00	2.4420
OC	CA	CA	40.00	120.00		
OC	CC	CP1	40.00	118.00	50.00	2.3880
OC	CC	CT1	40.00	118.00	50.00	2.3880
OC	CC	CT2	40.00	118.00	50.00	2.3880
OC	CC	CT3	40.00	118.00	50.00	2.3880
OC	CC	OC	100.00	124.00	70.00	2.2250
OC	CT2	CT3	65.00	122.00		
OC	CT2	HA	65.00	118.30		
OC	CT3	HA	65.00	118.30		
OH1	CA	CA	45.20	120.00		
OH1	CD	CT2	55.00	110.50		
OH1	CD	CT3	55.00	110.50		
OH1	CD	OB	50.00	123.00	10.00	2.2620
OH1	CT1	CT1	75.70	110.10		
OH1	CT1	CT3	75.70	110.10		
OH1	CT1	HA	45.90	108.89		
OH1	CT2	CT1	75.70	110.10		
OH1	CT2	CT2	75.70	110.10		
OH1	CT2	CT3	75.70	110.10		
OH1	CT2	HA	45.90	108.89		
OH1	CT3	HA	45.90	108.89		
OM	CM	FE	35.00	180.00		
OM	FE	NPH	5.00	90.00		
OM	OM	FE	0.00	180.00		
OS	CD	CP1	55.00	109.00	20.00	2.3260
OS	CD	CT1	55.00	109.00	20.00	2.3260
OS	CD	CT2	55.00	109.00	20.00	2.3260
OS	CD	CT3	55.00	109.00	20.00	2.3260
OS	CD	OB	90.00	125.90	160.00	2.2576
OS	CT2	HA	60.00	109.50		
OS	CT3	HA	60.00	109.50		
S	CT2	CT1	58.00	112.50		
S	CT2	CT2	58.00	114.50		
S	CT2	CT3	58.00	114.50		
S	CT2	HA	46.10	111.30		
S	CT3	HA	46.10	111.30		
SM	CT2	CT1	58.00	112.50		
SM	CT2	HA	38.00	111.00		
SM	CT3	HA	38.00	111.00		
SM	SM	CT2	72.50	103.30		
SM	SM	CT3	72.50	103.30		
SS	CS	CT3	55.00	118.00		
SS	CS	HA	40.00	112.30		

K_θ in kcal/mole/rad^2, θ_o in degrees, K_{UB} in kcal/mole/Å^2 and S_o in Å.

Appendix Table IV. Dihedral Angle Parameters

Atom types				K_δ	n	δ
C	CT1	NH1	C	0.200	1	180.0
C	CT2	NH1	C	0.200	1	180.0
C	N	CP1	C	0.800	3	0.0
CA	CA	CA	CA	3.100	2	180.0
CA	CPT	CPT	CA	3.100	2	180.0
CA	CT2	CT1	C	0.040	3	0.0
CA	CY	CPT	CA	3.000	2	180.0
CA	NY	CPT	CA	3.000	2	180.0
CC	CP1	N	C	0.800	3	0.0
CC	CT1	CT2	CA	0.040	3	0.0
CC	CT1	NH1	C	0.200	1	180.0
CC	CT2	NH1	C	0.200	1	180.0
CD	CP1	N	C	0.000	1	180.0
CD	CT1	NH1	C	0.200	1	180.0
CD	CT2	NH1	C	0.200	1	180.0
CP1	C	N	CP1	2.750	2	180.0
CP1	C	N	CP1	0.300	4	0.0
CP2	CP1	N	C	0.800	3	0.0
CP2	CP3	N	C	0.000	3	180.0
CP2	CP3	N	CP1	0.100	3	0.0
CP2	CP3	NP	CP1	0.080	3	0.0
CP3	N	C	CP1	2.750	2	180.0
CP3	N	C	CP1	0.300	4	0.0
CP3	N	CP1	C	0.100	3	0.0
CP3	N	CP1	CC	0.100	3	0.0
CP3	N	CP1	CP2	0.100	3	0.0
CP3	NP	CP1	C	0.080	3	0.0
CP3	NP	CP1	CC	0.080	3	0.0
CP3	NP	CP1	CD	0.080	3	0.0
CP3	NP	CP1	CP2	0.080	3	0.0
CPH2	NR1	CPH1	CPH1	14.000	2	180.0
CPH2	NR2	CPH1	CPH1	14.000	2	180.0
CPH2	NR3	CPH1	CPH1	12.000	2	180.0
CPT	CA	CA	CA	3.100	2	180.0
CPT	CPT	CA	CA	3.100	2	180.0
CPT	CPT	CY	CA	4.000	2	180.0
CPT	CPT	NY	CA	5.000	2	180.0
CT1	C	N	CP1	2.750	2	180.0
CT1	C	N	CP1	0.300	4	0.0
CT1	C	N	CP3	2.750	2	180.0
CT1	C	N	CP3	0.300	4	0.0
CT1	C	NH1	CT1	1.600	1	0.0
CT1	C	NH1	CT1	2.500	2	180.0
CT1	CT1	NH1	C	1.800	1	0.0
CT1	CT2	CA	CA	0.230	2	180.0
CT1	CT2	CPH1	CPH1	0.200	1	0.0
CT1	CT2	CPH1	CPH1	0.270	2	0.0
CT1	CT2	CPH1	CPH1	0.000	3	0.0
CT1	CT2	CY	CA	0.230	2	180.0
CT1	CT2	CY	CPT	0.230	2	180.0
CT1	NH1	C	CP1	1.600	1	0.0
CT1	NH1	C	CP1	2.500	2	180.0
CT2	C	N	CP1	2.750	2	180.0
CT2	C	N	CP1	0.300	4	0.0

Appendix Table IV continued

CT2	C	N	CP3	2.750	2	180.0
CT2	C	N	CP3	0.300	4	0.0
CT2	C	NH1	CT1	1.600	1	0.0
CT2	C	NH1	CT1	2.500	2	180.0
CT2	C	NH1	CT2	1.600	1	0.0
CT2	C	NH1	CT2	2.500	2	180.0
CT2	CA	CA	CA	3.100	2	180.0
CT2	CPH1	NR1	CPH2	3.000	2	180.0
CT2	CPH1	NR2	CPH2	3.000	2	180.0
CT2	CPH1	NR3	CPH2	2.500	2	180.0
CT2	CT1	NH1	C	1.800	1	0.0
CT2	CT2	CPH1	CPH1	0.400	1	0.0
CT2	CT2	CT2	CT2	0.150	1	0.0
CT2	CT2	NH1	C	1.800	1	0.0
CT2	CY	CPT	CA	3.000	2	180.0
CT2	CY	CPT	CPT	3.000	2	180.0
CT2	NH1	C	CP1	1.600	1	0.0
CT2	NH1	C	CP1	2.500	2	180.0
CT2	NH1	C	CT1	1.600	1	0.0
CT2	NH1	C	CT1	2.500	2	180.0
CT2	SM	SM	CT2	1.000	1	0.0
CT2	SM	SM	CT2	4.100	2	0.0
CT2	SM	SM	CT2	0.900	3	0.0
CT3	C	N	CP1	2.750	2	180.0
CT3	C	N	CP1	0.300	4	0.0
CT3	C	N	CP3	2.750	2	180.0
CT3	C	N	CP3	0.300	4	0.0
CT3	C	NH1	CT1	1.600	1	0.0
CT3	C	NH1	CT1	2.500	2	180.0
CT3	C	NH1	CT2	1.600	1	0.0
CT3	C	NH1	CT2	2.500	2	180.0
CT3	C	NH1	CT3	1.600	1	0.0
CT3	C	NH1	CT3	2.500	2	180.0
CT3	CA	CA	CA	3.100	2	180.0
CT3	CPH1	NR1	CPH2	3.000	2	180.0
CT3	CT1	NH1	C	1.800	1	0.0
CT3	CT2	CA	CA	0.230	2	180.0
CT3	CT2	CPH1	CPH1	0.200	1	0.0
CT3	CT2	CPH1	CPH1	0.270	2	0.0
CT3	CT2	CPH1	CPH1	0.000	3	0.0
CT3	CT2	CT2	CT2	0.150	1	0.0
CT3	CT2	CT2	CT3	0.150	1	0.0
CT3	CT2	CY	CA	0.230	2	180.0
CT3	CT2	CY	CPT	0.230	2	180.0
CT3	CT2	S	CT3	0.240	1	180.0
CT3	CT2	S	CT3	0.370	3	0.0
CT3	NH1	C	CP1	1.600	1	0.0
CT3	NH1	C	CP1	2.500	2	180.0
CT3	NH1	C	CT1	1.600	1	0.0
CT3	NH1	C	CT1	2.500	2	180.0
CT3	S	CT2	CT2	0.240	1	180.0
CT3	S	CT2	CT2	0.370	3	0.0
CT3	SM	SM	CT3	1.000	1	0.0
CT3	SM	SM	CT3	4.100	2	0.0
CT3	SM	SM	CT3	0.900	3	0.0
CY	CA	NY	CPT	5.000	2	180.0

Appendix Table IV continued

CY	CPT	CA	CA	3.000	2	180.0
CY	CPT	CPT	CA	10.000	2	180.0
H	NH1	C	CP1	2.500	2	180.0
H	NH1	C	CT1	2.500	2	180.0
H	NH1	C	CT2	2.500	2	180.0
H	NH1	C	CT3	2.500	2	180.0
H	NH1	CT1	C	0.000	1	0.0
H	NH1	CT1	CC	0.000	1	0.0
H	NH1	CT1	CD	0.000	1	0.0
H	NH1	CT1	CT1	0.000	1	0.0
H	NH1	CT1	CT2	0.000	1	0.0
H	NH1	CT1	CT3	0.000	1	0.0
H	NH1	CT2	C	0.000	1	0.0
H	NH1	CT2	CC	0.000	1	0.0
H	NH1	CT2	CD	0.000	1	0.0
H	NH1	CT2	CT2	0.000	1	0.0
H	NH1	CT2	CT3	0.000	1	0.0
H	NH2	CC	CT1	1.400	2	180.0
H	NH2	CC	CT2	1.400	2	180.0
H	NH2	CC	CT3	1.400	2	180.0
H	NH2	CC	CP1	2.500	2	180.0
H	NR1	CPH1	CPH1	1.000	2	180.0
H	NR1	CPH1	CT2	1.000	2	180.0
H	NR1	CPH1	CT3	1.000	2	180.0
H	NR3	CPH1	CPH1	1.400	2	180.0
H	NR3	CPH1	CT2	3.000	2	180.0
H	NR3	CPH1	CT3	3.000	2	180.0
H	NY	CA	CY	0.800	2	180.0
H	NY	CPT	CA	0.800	2	180.0
H	NY	CPT	CPT	0.800	2	180.0
H	OH1	CA	CA	0.990	2	180.0
H	OH1	CT1	CT1	1.330	1	0.0
H	OH1	CT1	CT1	0.180	2	0.0
H	OH1	CT1	CT1	0.320	3	0.0
H	OH1	CT1	CT3	1.330	1	0.0
H	OH1	CT1	CT3	0.180	2	0.0
H	OH1	CT1	CT3	0.320	3	0.0
H	OH1	CT2	CT1	1.300	1	0.0
H	OH1	CT2	CT1	0.300	2	0.0
H	OH1	CT2	CT1	0.420	3	0.0
H	OH1	CT2	CT2	1.300	1	0.0
H	OH1	CT2	CT2	0.300	2	0.0
H	OH1	CT2	CT2	0.420	3	0.0
H	OH1	CT2	CT3	1.300	1	0.0
H	OH1	CT2	CT3	0.300	2	0.0
H	OH1	CT2	CT3	0.420	3	0.0
HA	CA	CA	CA	3.500	2	180.0
HA	CA	CA	CPT	3.500	2	180.0
HA	CA	CA	HA	2.500	2	180.0
HA	CA	CPT	CPT	3.000	2	180.0
HA	CA	CPT	CY	4.000	2	180.0
HA	CA	CY	CPT	1.200	2	180.0
HA	CA	CY	CT2	1.200	2	180.0
HA	CA	NY	CPT	3.000	2	180.0
HA	CA	NY	H	1.000	2	180.0
HA	CC	NH2	H	1.400	2	180.0

Appendix Table IV continued

HA	CP3	N	C	0.000	3	180.0
HA	CP3	N	CP1	0.100	3	0.0
HA	CP3	NP	CP1	0.080	3	0.0
HA	CT1	CT2	CA	0.040	3	0.0
HA	CT2	CPH1	CPH1	0.000	3	0.0
HA	CT2	CY	CA	0.250	2	180.0
HA	CT2	CY	CPT	0.250	2	180.0
HA	CT2	NH1	C	0.000	3	0.0
HA	CT2	NH1	H	0.000	3	0.0
HA	CT2	S	CT3	0.280	3	0.0
HA	CT3	CPH1	CPH1	0.000	3	0.0
HA	CT3	CS	HA	0.160	3	0.0
HA	CT3	CT2	CA	0.040	3	0.0
HA	CT3	NH1	C	0.000	3	0.0
HA	CT3	NH1	H	0.000	3	0.0
HA	CT3	S	CT2	0.280	3	0.0
HA	CY	CA	CPT	1.200	2	180.0
HA	CY	CA	HA	1.200	2	180.0
HA	CY	CPT	CA	3.000	2	180.0
HA	CY	CPT	CPT	3.000	2	180.0
HB	CP1	N	C	0.800	3	0.0
HB	CP1	N	CP3	0.100	3	0.0
HB	CP1	NP	CP3	0.080	3	0.0
HB	CT1	NH1	C	0.000	1	0.0
HB	CT1	NH1	H	0.000	1	0.0
HB	CT2	NH1	C	0.000	1	0.0
HB	CT2	NH1	H	0.000	1	0.0
HB	CT3	NH1	C	0.000	1	0.0
HB	CT3	NH1	H	0.000	1	0.0
HC	NP	CP1	C	0.080	3	0.0
HC	NP	CP1	CC	0.080	3	0.0
HC	NP	CP1	CD	0.080	3	0.0
HC	NP	CP1	CP2	0.080	3	0.0
HC	NP	CP1	HB	0.080	3	0.0
HC	NP	CP3	CP2	0.080	3	0.0
HC	NP	CP3	HA	0.080	3	0.0
HP	CA	CA	CA	4.200	2	180.0
HP	CA	CA	CPT	3.000	2	180.0
HP	CA	CA	CT2	4.200	2	180.0
HP	CA	CA	CT3	4.200	2	180.0
HP	CA	CA	HP	2.400	2	180.0
HP	CA	CPT	CPT	3.000	2	180.0
HP	CA	CPT	CY	3.000	2	180.0
HP	CA	CY	CPT	2.000	2	180.0
HP	CA	CY	CT2	1.200	2	180.0
HP	CA	NY	CPT	2.000	2	180.0
HP	CA	NY	H	0.400	2	180.0
HP	CY	CA	HP	1.000	2	180.0
HP	CY	CPT	CA	2.800	2	180.0
HP	CY	CPT	CPT	2.800	2	180.0
HR1	CPH1	CPH1	CT2	1.000	2	180.0
HR1	CPH1	CPH1	CT3	1.000	2	180.0
HR1	CPH1	CPH1	HR1	1.000	2	180.0
HR1	CPH1	NR3	CPH2	2.500	2	180.0
HR1	CPH1	NR3	H	3.000	2	180.0
HR1	CPH2	NR1	CPH1	3.000	2	180.0

Appendix Table IV continued

HR1	CPH2	NR1	H	1.000	2	180.0
HR1	CPH2	NR2	CPH1	3.000	2	180.0
HR2	CPH2	NR3	CPH1	3.000	2	180.0
HR2	CPH2	NR3	H	0.000	2	180.0
HR3	CPH1	CPH1	CT2	2.000	2	180.0
HR3	CPH1	CPH1	CT3	2.000	2	180.0
HR3	CPH1	CPH1	HR3	2.000	2	180.0
HR3	CPH1	NR1	CPH2	3.000	2	180.0
HR3	CPH1	NR1	H	1.000	2	180.0
HR3	CPH1	NR2	CPH2	3.000	2	180.0
HS	S	CT2	CT1	0.240	1	0.0
HS	S	CT2	CT1	0.150	2	0.0
HS	S	CT2	CT1	0.270	3	0.0
HS	S	CT2	CT3	0.240	1	0.0
HS	S	CT2	CT3	0.150	2	0.0
HS	S	CT2	CT3	0.270	3	0.0
HS	S	CT2	HA	0.200	3	0.0
HS	S	CT3	HA	0.200	3	0.0
N	C	CP1	CP2	0.400	1	0.0
N	C	CP1	CP2	0.600	2	0.0
N	C	CP1	HB	0.400	1	180.0
N	C	CP1	HB	0.600	2	0.0
N	C	CP1	N	0.300	1	0.0
N	C	CP1	N	-0.300	4	0.0
N	C	CT1	CT1	0.000	1	0.0
N	C	CT1	CT2	0.000	1	0.0
N	C	CT1	CT3	0.000	1	0.0
N	C	CT1	HB	0.000	1	0.0
N	C	CT2	HB	0.000	1	0.0
N	C	CT3	HA	0.000	1	0.0
N	CT1	CT2	CA	0.040	3	0.0
NH1	C	CP1	CP2	0.400	1	0.0
NH1	C	CP1	CP2	0.600	2	0.0
NH1	C	CP1	HB	0.400	1	180.0
NH1	C	CP1	HB	0.600	2	0.0
NH1	C	CP1	N	0.300	1	0.0
NH1	C	CP1	N	-0.300	4	0.0
NH1	C	CT1	CT1	0.000	1	0.0
NH1	C	CT1	CT2	0.000	1	0.0
NH1	C	CT1	CT3	0.000	1	0.0
NH1	C	CT1	HB	0.000	1	0.0
NH1	C	CT1	NH1	0.600	1	0.0
NH1	C	CT2	CT2	0.000	1	0.0
NH1	C	CT2	HA	0.000	3	0.0
NH1	C	CT2	HB	0.000	1	0.0
NH1	C	CT2	NH1	0.600	1	0.0
NH1	C	CT3	HA	0.000	3	0.0
NH1	CT1	C	N	0.400	1	0.0
NH1	CT2	C	N	0.400	1	0.0
NH2	CC	CP1	CP2	0.400	1	0.0
NH2	CC	CP1	CP2	0.600	2	0.0
NH2	CC	CP1	HB	0.400	1	180.0
NH2	CC	CP1	HB	0.600	2	0.0
NH2	CC	CP1	N	0.300	1	0.0
NH2	CC	CP1	N	-0.300	4	0.0
NH2	CC	CT2	HA	0.000	3	180.0

Appendix Table IV continued

NH3	CT1	C	N	0.400	1	0.0
NH3	CT1	C	NH1	0.600	1	0.0
NH3	CT1	CC	NH2	0.400	1	0.0
NH3	CT2	C	N	0.400	1	0.0
NH3	CT2	C	NH1	0.400	1	0.0
NH3	CT2	CC	NH2	0.400	1	0.0
NP	CP1	C	N	0.300	1	0.0
NP	CP1	C	NH1	0.300	1	0.0
NP	CP1	CC	NH2	0.300	1	0.0
NR1	CPH1	CPH1	CT2	3.000	2	180.0
NR1	CPH1	CPH1	CT3	3.000	2	180.0
NR1	CPH1	CPH1	HR3	3.000	2	180.0
NR1	CPH1	CT2	CT1	0.190	3	0.0
NR1	CPH1	CT2	CT2	0.190	3	0.0
NR1	CPH1	CT2	CT3	0.190	3	0.0
NR1	CPH1	CT2	HA	0.190	3	0.0
NR1	CPH1	CT3	HA	0.190	3	0.0
NR1	CPH2	NR2	CPH1	14.000	2	180.0
NR2	CPH1	CPH1	CT2	3.000	2	180.0
NR2	CPH1	CPH1	CT3	3.000	2	180.0
NR2	CPH1	CPH1	HR3	3.000	2	180.0
NR2	CPH1	CPH1	NR1	14.000	2	180.0
NR2	CPH1	CT2	CT1	0.190	3	0.0
NR2	CPH1	CT2	CT2	0.190	3	0.0
NR2	CPH1	CT2	CT3	0.190	3	0.0
NR2	CPH1	CT2	HA	0.190	3	0.0
NR2	CPH1	CT3	HA	0.190	3	0.0
NR2	CPH2	NR1	CPH1	14.000	2	180.0
NR2	CPH2	NR1	H	1.000	2	180.0
NR3	CPH1	CPH1	CT2	2.500	2	180.0
NR3	CPH1	CPH1	CT3	2.500	2	180.0
NR3	CPH1	CPH1	HR1	2.500	2	180.0
NR3	CPH1	CPH1	NR3	12.000	2	180.0
NR3	CPH1	CT2	CT1	0.190	3	0.0
NR3	CPH1	CT2	CT2	0.190	3	0.0
NR3	CPH1	CT2	CT3	0.190	3	0.0
NR3	CPH1	CT2	HA	0.190	3	0.0
NR3	CPH1	CT3	HA	0.190	3	0.0
NR3	CPH2	NR3	CPH1	12.000	2	180.0
NR3	CPH2	NR3	H	1.400	2	180.0
NY	CA	CY	CPT	4.000	2	180.0
NY	CA	CY	CT2	3.500	2	180.0
NY	CA	CY	HA	3.500	2	180.0
NY	CA	CY	HP	3.500	2	180.0
NY	CPT	CA	CA	2.800	2	180.0
NY	CPT	CA	HA	4.000	2	180.0
NY	CPT	CA	HP	3.000	2	180.0
NY	CPT	CPT	CA	10.000	2	180.0
NY	CPT	CPT	CY	5.000	2	180.0
O	C	CP1	CP2	0.400	1	180.0
O	C	CP1	CP2	0.600	2	0.0
O	C	CP1	HB	0.400	1	0.0
O	C	CP1	HB	0.600	2	0.0
O	C	CP1	N	-0.300	4	0.0
O	C	CT1	CT1	1.400	1	0.0
O	C	CT1	CT2	1.400	1	0.0

Appendix Table IV continued

O	C	CT1	CT3	1.400	1	0.0
O	C	CT1	HB	0.000	1	0.0
O	C	CT1	NH1	0.000	1	0.0
O	C	CT1	NH3	0.000	1	0.0
O	C	CT2	CT2	1.400	1	0.0
O	C	CT2	HA	0.000	3	180.0
O	C	CT2	HB	0.000	1	0.0
O	C	CT2	NH1	0.000	1	0.0
O	C	CT2	NH3	0.000	1	0.0
O	C	CT3	HA	0.000	3	180.0
O	C	N	CP1	2.750	2	180.0
O	C	N	CP1	0.300	4	0.0
O	C	N	CP3	2.750	2	180.0
O	C	N	CP3	0.300	4	0.0
O	C	NH1	CT1	2.500	2	180.0
O	C	NH1	CT2	2.500	2	180.0
O	C	NH1	CT3	2.500	2	180.0
O	C	NH1	H	2.500	2	180.0
O	CC	CP1	CP2	0.400	1	180.0
O	CC	CP1	CP2	0.600	2	0.0
O	CC	CP1	HB	0.400	1	0.0
O	CC	CP1	HB	0.600	2	0.0
O	CC	CP1	N	-0.300	4	0.0
O	CC	CT2	HA	0.000	3	180.0
O	CC	NH2	H	1.400	2	180.0
OB	CD	OS	CT2	0.965	1	180.0
OB	CD	OS	CT2	3.850	2	180.0
OB	CD	OS	CT3	0.965	1	180.0
OB	CD	OS	CT3	3.850	2	180.0
OC	CA	CA	CA	3.100	2	180.0
OC	CA	CA	HP	4.200	2	180.0
OC	CC	CP1	CP2	0.160	3	0.0
OC	CC	CP1	HB	0.160	3	0.0
OC	CC	CP1	N	0.160	3	0.0
OC	CC	CP1	NP	0.160	3	0.0
OC	CC	CT1	NH3	3.200	2	180.0
OC	CC	CT2	NH3	3.200	2	180.0
OH1	CA	CA	CA	3.100	2	180.0
OH1	CA	CA	HP	4.200	2	180.0
S	CT2	CT2	HA	0.010	3	0.0
SM	CT2	CT2	HA	0.010	3	0.0
SM	SM	CT2	CT1	0.310	3	0.0
SM	SM	CT2	CT2	0.310	3	0.0
SM	SM	CT2	HA	0.158	3	0.0
SM	SM	CT3	HA	0.158	3	0.0
SS	CS	CT3	HA	0.150	3	0.0
X	C	C	X	4.000	2	180.0
X	C	NC2	X	2.250	2	180.0
X	CD	OH1	X	2.050	2	180.0
X	CD	OS	X	2.050	2	180.0
X	CP1	C	X	0.000	6	180.0
X	CP1	CC	X	0.000	6	180.0
X	CP1	CD	X	0.000	6	180.0
X	CP1	CP2	X	0.140	3	0.0
X	CP2	CP2	X	0.160	3	0.0
X	CP3	CP2	X	0.140	3	0.0

Appendix Table IV continued

X	CPA	CPB	X	0.000	2	0.0
X	CPA	CPM	X	0.000	2	0.0
X	CPB	C	X	3.000	2	180.0
X	CPB	CPB	X	0.000	2	0.0
X	CPB	CT2	X	0.000	6	0.0
X	CPB	CT3	X	0.000	6	0.0
X	CPT	CPT	X	0.000	2	180.0
X	CT1	CC	X	0.050	6	180.0
X	CT1	CD	X	0.000	6	180.0
X	CT1	CT1	X	0.200	3	0.0
X	CT1	CT2	X	0.200	3	0.0
X	CT1	CT3	X	0.200	3	0.0
X	CT1	NH3	X	0.100	3	0.0
X	CT1	OH1	X	0.140	3	0.0
X	CT1	OS	X	-0.100	3	0.0
X	CT2	CA	X	0.000	6	0.0
X	CT2	CC	X	0.050	6	180.0
X	CT2	CD	X	0.000	6	180.0
X	CT2	CT2	X	0.195	3	0.0
X	CT2	CT3	X	0.160	3	0.0
X	CT2	NC2	X	0.000	6	180.0
X	CT2	NH3	X	0.100	3	0.0
X	CT2	OH1	X	0.140	3	0.0
X	CT2	OS	X	-0.100	3	0.0
X	CT3	CA	X	0.000	6	0.0
X	CT3	CC	X	0.050	6	180.0
X	CT3	CD	X	0.000	6	180.0
X	CT3	CT3	X	0.155	3	0.0
X	CT3	NC2	X	0.000	6	180.0
X	CT3	NH2	X	0.110	3	0.0
X	CT3	NH3	X	0.090	3	0.0
X	CT3	OH1	X	0.140	3	0.0
X	CT3	OS	X	-0.100	3	0.0
X	FE	CM	X	0.050	4	0.0
X	FE	NPH	X	0.000	2	0.0
X	FE	OM	X	0.000	4	0.0
X	NPH	CPA	X	0.000	2	0.0

K_δ in kcal/mole, δ in degrees. X indicates a wild card.

Appendix Table IVb. Alternate dihedral parameters used for the computations in Tables 5 and 6.

Atom types				K_δ	n	δ
Set 1						
C	CT1	NH1	C	0.5000	1	0.00
NH1	C	CT1	NH1	0.5000	1	0.00
O	C	CT1	CT3	0.2000	1	0.00
CT3	CT1	NH1	C	0.5000	1	0.00
Set 2						
C	CT1	NH1	C	0.1000	1	0.00
O	C	CT1	CT3	0.6000	1	0.00
CT3	CT1	NH1	C	1.1000	1	0.00
Set 3						
O	C	CT1	CT3	1.0000	1	0.00
CT3	CT1	NH1	C	1.4000	1	0.00
Set 4						
see Appendix Table IV						
Set 5						
C	CT1	NH1	C	0.6000	1	180.00
NH1	C	CT1	NH1	0.8000	1	0.00
O	C	CT1	CT3	1.8000	1	0.00
CT3	CT1	NH1	C	2.3000	1	0.00
Set 6						
C	CT1	NH1	C	0.6000	1	0.00
NH1	C	CT1	NH1	1.0000	1	0.00
O	C	CT1	CT3	1.7000	1	0.00
CT3	CT1	NH1	C	2.5000	1	0.00
O	C	CT1	NH1	1.0000	1	0.00
NH1	C	CT1	CT3	0.3000	1	180.00

K_δ in kcal/mole, δ in degrees.
Substitute the listed dihedral parameters for the identical terms above in Appendix Table IV to obtain the parameters sets used in Tables 5 and 6.

Appendix Table V. Improper Dihedral Angle Parameters.

Atom Types				K_φ	φ_o
CPB	CPA	NPH	CPA	20.80	0.0
CPB	X	X	C	90.00	0.0
CT2	X	X	CPB	90.00	0.0
CT3	X	X	CPB	90.00	0.0
HA	C	C	HA	20.00	0.0
HA	CPA	CPA	CPM	29.40	0.0
HA	CPB	C	C	20.00	0.0
HA	HA	C	C	20.00	180.0
HR1	NR1	NR2	CPH2	0.50	0.0
HR1	NR2	NR1	CPH2	0.50	0.0
HR3	CPH1	NR1	CPH1	0.50	0.0
HR3	CPH1	NR2	CPH1	0.50	0.0
HR3	CPH1	NR3	CPH1	1.00	0.0
HR3	NR1	CPH1	CPH1	0.50	0.0
HR3	NR2	CPH1	CPH1	0.50	0.0
N	C	CP1	CP3	0.00	0.0
NC2	X	X	C	40.00	0.0
NH1	X	X	H	20.00	0.0
NH2	X	X	H	4.00	0.0
NPH	CPA	CPA	FE	137.40	0.0
NPH	CPA	CPB	CPB	40.60	0.0
NPH	CPA	CPM	CPA	18.30	0.0
NPH	CPM	CPB	CPA	32.70	0.0
NR1	CPH1	CPH2	H	0.45	0.0
NR1	CPH2	CPH1	H	0.45	0.0
NR3	CPH1	CPH2	H	1.20	0.0
NR3	CPH2	CPH1	H	1.20	0.0
NY	CA	CY	CPT	100.00	0.0
O	CP1	NH2	CC	45.00	0.0
O	CT1	NH2	CC	45.00	0.0
O	CT2	NH2	CC	45.00	0.0
O	CT3	NH2	CC	45.00	0.0
O	HA	NH2	CC	45.00	0.0
O	N	CT2	CC	120.00	0.0
O	NH2	CP1	CC	45.00	0.0
O	NH2	CT1	CC	45.00	0.0
O	NH2	CT2	CC	45.00	0.0
O	NH2	CT3	CC	45.00	0.0
O	NH2	HA	CC	45.00	0.0
O	X	X	C	120.00	0.0
OB	X	X	CD	100.00	0.0
OC	X	X	CC	96.00	0.0

K_φ in kcal/mole/rad^2, φ_o in degrees. X indicates a wildcard

Appendix Table VI. Lennard-Jones Parameters

Atom type	ε	$R_{min/2}$	$\varepsilon_{1,4}$	$R_{min,1,4/2}$
C	-0.1100	2.0000		
CA	-0.0700	1.9924		
CC	-0.0700	2.0000		
CD	-0.0700	2.0000		
CM	-0.1100	2.1000		
CP1	-0.0200	2.2750	-0.0100	1.9000
CP2	-0.0550	2.1750	-0.0100	1.9000
CP3	-0.0550	2.1750	-0.0100	1.9000
CPA	-0.0900	1.8000		
CPB	-0.0900	1.8000		
CPH1	-0.0500	1.8000		
CPH2	-0.0500	1.8000		
CPM	-0.0900	1.8000		
CPT	-0.0900	1.8000	-0.0900	1.9000
CS	-0.1100	2.2000		
CT1	-0.0200	2.2750	-0.0100	1.9000
CT2	-0.0550	2.1750	-0.0100	1.9000
CT3	-0.0800	2.0600	-0.0100	1.9000
CY	-0.0700	1.9924		
H	-0.0460	0.2245		
HA	-0.0220	1.3200		
HB	-0.0220	1.3200		
HC	-0.0460	0.2245		
HP	-0.0300	1.3582	-0.0300	1.3582
HR1	-0.0460	0.9000		
HR2	-0.0460	0.7000		
HR3	-0.0078	1.4680		
HS	-0.1000	0.4500		
HT	-0.0460	0.2245		
N	-0.2000	1.8500	-0.0001	1.8500
NC2	-0.2000	1.8500		
NH1	-0.2000	1.8500	-0.2000	1.5500
NH2	-0.2000	1.8500		
NH3	-0.2000	1.8500		
NP	-0.2000	1.8500		
NPH	-0.2000	1.8500		
NR1	-0.2000	1.8500		
NR2	-0.2000	1.8500		
NR3	-0.2000	1.8500		
NY	-0.2000	1.8500		
O	-0.1200	1.7000	-0.1200	1.4000
OB	-0.1200	1.7000	-0.1200	1.4000
OC	-0.1200	1.7000		
OH1	-0.1521	1.7700		
OM	-0.1200	1.7000		
OS	-0.1521	1.7700		
OT	-0.1521	1.7682		
FE	0.0000	0.6500		
S	-0.4500	2.0000		
SM	-0.3800	1.9750		
SS	-0.4700	2.2000		

ε in kcal/mole, $R_{min/2}$ in Å, $\varepsilon_{1,4}$ in kcal/mole and $R_{min,1,4/2}$ in Å.