

Supporting Information for
Improved Modeling of Cation- π and Anion-Ring Interactions Using the Drude
Polarizable Empirical Force Field for Proteins

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Table S1. QM and MM rigid scan interactions computed by approach 1 with the original Drude-2013 force field without NBFIX parameters. The protein aromatic and charged model compound complexes are labeled as Ar_Mol⁺ for cation and Ar_Mol⁻ for anion. The QM single point interaction energies calculated at RIMP2/cc-PVQZ and SAPT2+/aug-cc-PVDZ model chemistries are in the columns "MP2 Energy" and "SAPT2+ Energy", and the differences between MM and QM are in the "Diff. MM-MP2" and "Diff. MM-SAPT2+" columns. Distance (Dist.) at which the energies are minimum are shown in Å, and the energies are shown in kcal/mol. Statistical analysis reported includes average differences (AVG), standard errors (SE), absolute unsigned error (AUE), and root-mean-square differences (RMS). The final letter in the Ar_Mol^(+,-) column corresponds to the interaction orientation shown in Figure 2 of the main text.

#	Ar_Mol ⁺	MM Dist.	MM Energy	MP2 Dist.	MP2 Energy	Diff. MM-MP2	SAPT2+ Dist.	SAPT2+ Energy	Diff. MM-SAPT2+
1	BENZ_MAM1a	1.9	-18.59	2.0	-18.32	-0.27	2.0	-16.51	-2.08
2	BENZ_MAM1b	2.8	-10.08	2.8	-10.98	0.90	2.9	-9.79	-0.29
3	TOLU_MAM1a	1.9	-17.40	1.9	-19.54	2.14	2.0	-17.67	0.27
4	TOLU_MAM1b	2.8	-11.03	2.8	-12.37	1.34	2.9	-11.09	0.06
5	TOLU_MAM1b	2.8	-10.69	2.8	-12.13	1.44	2.9	-10.94	0.25
6	TOLU_MAM1b	2.8	-10.01	2.8	-11.72	1.71	2.9	-10.41	0.40
7	PHEN_MAM1a	1.9	-16.68	1.9	-18.45	1.77	2.0	-16.67	-0.01
8	PHEN_MAM1b	2.8	-9.63	2.8	-10.47	0.84	2.9	-9.37	-0.26
9	PHEN_MAM1b	2.8	-10.18	2.8	-13.31	3.13	2.9	-11.96	1.78
10	PHEN_MAM1b	2.6	-12.01	2.8	-12.02	0.01	2.8	-11.95	-0.06
11	CRES_MAM1a	1.9	-14.35	1.9	-19.59	5.24	2.0	-17.75	3.40
12	CRES_MAM1b	2.8	-9.45	2.8	-11.40	1.95	2.8	-10.19	0.74
13	CRES_MAM1b	2.8	-10.70	2.8	-14.33	3.63	2.9	-13.09	2.39
14	CRES_MAM1b	2.6	-14.38	2.7	-13.05	-1.33	2.8	-13.00	-1.38
15	INDO_MAM1a	1.8	-22.73	1.9	-23.62	0.89	2.0	-21.33	-1.40
16	INDO_MAM1b	2.8	-15.80	2.8	-16.67	0.87	2.8	-15.41	-0.39
17	INDO_MAM1b	2.8	-13.90	2.8	-16.30	2.40	2.9	-14.76	0.86
18	INDO_MAM1b	2.8	-11.50	2.8	-15.14	3.64	2.8	-13.80	2.30
19	INDO_MAM1b	2.8	-10.20	2.8	-12.19	1.99	2.8	-10.76	0.56
20	INDO_MAM1b	2.8	-18.62	2.9	-18.88	0.26	2.9	-17.49	-1.13
21	MIND_MAM1a	1.8	-24.36	1.9	-24.14	-0.22	1.9	-22.06	-2.30
22	MIND_MAM1b	2.8	-14.64	2.8	-17.00	2.36	2.8	-15.76	1.12
23	MIND_MAM1b	2.8	-15.03	2.8	-16.83	1.80	2.8	-15.25	0.22
24	MIND_MAM1b	2.7	-14.67	2.8	-15.84	1.17	2.8	-14.51	-0.16
25	MIND_MAM1b	2.7	-11.86	2.8	-13.03	1.17	2.8	-11.59	-0.27
26	IMID_MAM1a	1.9	-16.87	2.0	-14.94	-1.93	2.1	-13.47	-3.40
27	IMID_MAM1a	2.7	-5.35	2.8	-5.74	0.39	2.9	-4.62	-0.73
28	IMID_MAM1b	2.6	0.27	2.8	-0.29	0.56	2.9	0.50	-0.23
29	IMID_MAM1b	2.7	-11.95	2.7	-12.52	0.57	2.8	-11.43	-0.52
30	IMID_MAM1b	2.7	-7.30	2.8	-7.49	0.19	2.9	-6.72	-0.58
31	IMID_MAM1b	2.5	-21.42	2.6	-21.95	0.53	2.6	-21.05	-0.37
32	IMID_MAM1b	1.8	-25.64	1.7	-30.52	4.88	1.7	-30.19	4.55
33	4MIE_MAM1a	1.9	-16.19	2.0	-16.42	0.23	2.0	-14.95	-1.24
34	4MIE_MAM1b	2.5	-29.24	2.5	-22.94	-6.30	2.5	-21.92	-7.32
35	4MIE_MAM1b	2.8	-0.37	2.8	-6.99	6.62	2.8	-5.79	5.42
36	4MIE_MAM1b	2.6	-12.46	2.8	-8.69	-3.77	2.8	-7.94	-4.52
37	4MIE_MAM1b	1.8	-34.72	1.7	-31.03	-3.69	1.7	-30.88	-3.84
38	4MIM_MAM1a	1.9	-15.23	2.0	-16.56	1.33	2.0	-15.10	-0.13
39	4MIM_MAM1b	2.7	-10.23	2.7	-13.61	3.38	2.7	-12.43	2.20
40	4MIM_MAM1b	2.6	-12.21	2.8	-9.24	-2.97	2.8	-8.45	-3.76
41	4MIM_MAM1b	2.5	-22.83	2.5	-23.85	1.02	2.6	-22.93	0.10
42	4MIM_MAM1b	1.8	-28.53	1.7	-32.47	3.94	1.7	-32.23	3.70
43	BENZ_MGUANc	2.0	-13.23	2.2	-13.59	0.36	2.2	-12.11	-1.12
44	BENZ_MGUANd	2.9	-7.29	3.0	-8.27	0.98	3.0	-7.47	0.18
45	BENZ_MGUANe	3.5	-6.86	3.5	-8.21	1.35	3.5	-7.34	0.48

46	TOLU_MGUANc	2.0	-12.78	2.1	-14.68	1.90	2.2	-13.40	0.62
47	TOLU_MGUANd	2.9	-7.69	2.9	-9.13	1.44	3.0	-8.29	0.60
48	TOLU_MGUANd	2.9	-7.51	2.9	-9.00	1.49	3.0	-8.23	0.72
49	TOLU_MGUANd	2.9	-7.06	2.9	-8.98	1.92	3.0	-8.09	1.03
50	TOLU_MGUANe	3.5	-4.76	3.5	-5.32	0.56	3.4	-4.85	0.09
51	PHEN_MGUANc	2.0	-11.37	2.1	-13.22	1.85	2.2	-11.80	0.43
52	PHEN_MGUANd	2.8	-8.50	2.9	-8.69	0.19	3.0	-7.79	-0.71
53	PHEN_MGUANd	2.9	-7.11	2.9	-9.38	2.27	3.0	-8.51	1.40
54	PHEN_MGUANd	3.0	-6.63	3.0	-9.11	2.48	3.1	-8.96	2.33
55	PHEN_MGUANe	3.5	-6.88	3.4	-8.46	1.58	3.5	-7.60	0.72
56	CRES_MGUANc	2.0	-9.72	2.1	-14.30	4.58	2.2	-12.84	3.12
57	CRES_MGUANd	2.9	-7.05	2.9	-10.03	2.98	3.0	-9.18	2.13
58	CRES_MGUANd	3.0	-7.08	3.0	-9.80	2.72	3.1	-9.62	2.54
59	CRES_MGUANe	3.5	-6.87	3.4	-9.27	2.40	3.5	-8.38	1.51
60	INDO_MGUANc	1.9	-15.09	2.1	-16.65	1.56	2.2	-15.00	-0.09
61	INDO_MGUANd	2.8	-10.65	2.9	-12.31	1.66	2.9	-11.39	0.74
62	INDO_MGUANd	2.8	-9.72	2.9	-12.24	2.52	2.9	-11.13	1.41
63	INDO_MGUANd	2.8	-8.16	2.9	-11.59	3.43	2.9	-10.65	2.49
64	INDO_MGUANd	2.8	-7.59	2.9	-9.86	2.27	2.9	-8.87	1.28
65	INDO_MGUANe	3.4	-9.76	3.3	-12.57	2.81	3.4	-11.53	1.77
66	MIND_MGUANc	2.9	-9.97	2.9	-12.69	2.72	2.9	-11.80	1.83
67	MIND_MGUANd	2.8	-10.61	2.9	-12.62	2.01	3.0	-11.50	0.89
68	MIND_MGUANd	2.8	-10.38	2.9	-12.06	1.68	2.9	-11.16	0.78
69	MIND_MGUANd	2.8	-8.61	2.9	-10.39	1.78	2.9	-9.40	0.79
70	MIND_MGUANe	3.4	-10.56	3.3	-13.04	2.48	3.4	-11.95	1.39
71	IMID_MGUANc	2.0	-10.99	2.2	-10.40	-0.59	2.3	-9.39	-1.60
72	IMID_MGUANc	3.4	-6.20	3.4	-6.80	0.60	3.4	-6.30	0.10
73	IMID_MGUANd	2.8	-4.60	2.9	-4.96	0.36	3.0	-4.15	-0.45
74	IMID_MGUANd	2.6	-1.07	2.9	-1.63	0.56	2.9	-1.10	0.03
75	IMID_MGUANd	2.8	-8.16	2.9	-8.69	0.53	2.9	-7.97	-0.19
76	IMID_MGUANd	2.7	-5.33	2.9	-5.68	0.35	3.0	-5.21	-0.12
77	IMID_MGUANd	2.6	-14.94	2.7	-15.51	0.57	2.7	-14.90	-0.04
78	IMID_MGUANe	1.9	-19.96	1.8	-23.52	3.56	1.8	-23.36	3.40
79	4MIE_MGUANc	2.0	-12.66	2.2	-11.55	-1.11	2.2	-10.55	-2.11
80	4MIE_MGUANd	3.4	-6.91	3.4	-7.40	0.49	3.4	-7.02	0.11
81	4MIE_MGUANd	2.5	-19.59	2.6	-16.31	-3.28	2.7	-15.60	-3.99
82	4MIE_MGUANd	2.9	-1.38	2.8	-5.94	4.56	2.9	-5.08	3.70
83	4MIE_MGUANd	2.7	-8.60	2.9	-6.46	-2.14	2.9	-6.00	-2.60
84	4MIE_MGUANe	2.8	1.95	2.9	-2.56	4.51	2.9	-2.05	4.00
85	4MIM_MGUANc	2.0	-11.94	2.2	-11.82	-0.12	2.2	-10.81	-1.13
86	4MIM_MGUANd	3.4	-6.88	3.4	-7.81	0.93	3.4	-7.38	0.50
87	4MIM_MGUANd	2.7	-1.17	2.8	-2.50	1.33	2.9	-1.93	0.76
88	4MIM_MGUANd	2.8	-7.04	2.8	-9.64	2.60	2.9	-8.84	1.80
89	4MIM_MGUANd	2.7	-8.34	2.9	-6.82	-1.52	2.9	-6.32	-2.02
90	4MIM_MGUANd	2.6	-15.50	2.6	-16.76	1.26	2.7	-16.15	0.65
91	4MIM_MGUANe	1.9	-21.94	1.8	-25.03	3.09	1.8	-24.95	3.01
92	BENZ_IMIMf	1.9	-14.48	2.0	-15.50	1.02	2.1	-13.54	-0.94
93	BENZ_IMIMg	2.7	-7.77	2.9	-9.41	1.64	3.0	-8.03	0.26
94	BENZ_IMIMh	3.5	-6.73	3.5	-8.93	2.20	3.6	-7.50	0.77
95	TOLU_IMIMf	1.9	-13.30	1.9	-16.69	3.39	2.0	-14.69	1.39
96	TOLU_IMIMg	2.7	-8.41	2.9	-10.50	2.09	2.9	-9.07	0.66
97	TOLU_IMIMg	2.7	-8.16	2.8	-10.32	2.16	2.9	-9.01	0.85
98	TOLU_IMIMg	2.7	-7.58	2.8	-10.27	2.69	2.9	-8.81	1.23
99	TOLU_IMIMh	3.5	-7.06	3.5	-9.69	2.63	3.6	-8.18	1.12
100	PHEN_IMIMf	1.9	-12.56	2.0	-15.42	2.86	2.1	-13.49	0.93
101	PHEN_IMIMg	2.7	-9.73	2.9	-10.00	0.27	2.9	-8.49	-1.24
102	PHEN_IMIMg	3.0	-6.51	3.1	-10.15	3.64	3.1	-9.80	3.29
103	PHEN_IMIMg	2.8	-2.84	2.9	-7.47	4.63	2.9	-6.02	3.18
104	PHEN_IMIMg	2.7	-7.62	2.9	-8.96	1.34	2.9	-7.73	0.11
105	PHEN_IMIMg	2.7	-9.47	2.9	-9.98	0.51	2.9	-8.49	-0.98
106	PHEN_IMIMh	3.5	-7.24	3.4	-9.67	2.43	3.6	-8.20	0.96
107	CRES_IMIMf	2.0	-10.34	1.9	-16.53	6.19	2.0	-14.58	4.24
108	CRES_IMIMg	3.1	-6.35	3.0	-9.80	3.45	3.1	-9.22	2.87
109	CRES_IMIMg	3.0	-7.74	3.1	-11.17	3.43	3.1	-10.84	3.10
110	CRES_IMIMg	2.8	-3.39	2.8	-8.38	4.99	2.9	-6.94	3.55

111	CRES_IMIMg	2.7	-7.08	2.8	-9.83	2.75	2.9	-8.48	1.40
112	CRES_IMIMg	3.7	-4.41	3.6	-5.53	1.12	3.4	-4.11	-0.30
113	CRES_IMIMh	3.5	-7.13	3.4	-10.42	3.29	3.5	-8.83	1.70
114	INDO_IMIMf	1.8	-18.11	1.9	-20.37	2.26	2.0	-18.15	0.04
115	INDO_IMIMg	2.7	-10.89	2.8	-13.78	2.89	2.9	-12.14	1.25
116	INDO_IMIMg	2.7	-8.75	2.8	-12.87	4.12	2.9	-11.37	2.62
117	INDO_IMIMg	2.7	-12.26	2.9	-13.86	1.60	2.9	-12.52	0.26
118	INDO_IMIMh	3.3	-10.44	3.3	-14.17	3.73	3.4	-12.23	1.79
119	MIND_IMIMf	1.7	-19.54	1.9	-21.05	1.51	2.0	-18.78	-0.76
120	MIND_IMIMg	2.7	-9.31	2.8	-11.29	1.98	2.9	-9.68	0.37
121	MIND_IMIMg	2.7	-11.86	2.8	-11.29	-0.57	2.9	-12.53	0.67
122	MIND_IMIMg	2.7	-11.60	2.8	-13.43	1.83	2.9	-11.93	0.33
123	MIND_IMIMg	2.7	-11.21	2.8	-11.29	0.08	2.9	-13.01	1.80
124	MIND_IMIMh	3.3	-11.16	3.3	-14.60	3.44	3.4	-12.62	1.46
125	IMID_IMIMf	2.7	-4.14	2.8	-5.19	1.05	2.9	-3.94	-0.20
126	IMID_IMIMh	3.5	-4.87	3.5	-6.47	1.60	3.6	-5.45	0.58
127	4MIE_IMIMh	3.4	-8.35	3.3	-9.63	1.28	3.4	-8.37	0.02
128	4MIM_IMIMh	3.5	-5.31	3.4	-7.48	2.17	3.5	-6.34	1.03
AVG					-12.48	1.59		-11.40	0.52
SE						0.02			0.01
AUE						2.06			1.41
RMS						2.49			1.94

#	Ar_Mol-	MM Dist.	MM Energy	MP2 Dist.	MP2 Energy	Diff. MM-MP2	SAPT2+ Dist.	SAPT2+ Energy	Diff. MM-SAPT2+
1	BENZ_ACETi	4.4	1.33	3.2	1.23	0.10	3.0	0.10	1.23
2	BENZ_ACETj	4.3	-1.28	3.9	-1.72	0.44	3.8	-2.61	1.33
3	TOLU_ACETi	3.7	0.59	3.2	0.72	-0.13	3.0	-0.53	1.12
4	TOLU_ACETj	4.3	-1.01	3.9	-1.30	0.29	3.8	-2.14	1.13
5	PHEN_ACETi	4.0	0.23	3.8	-0.43	0.66	3.7	-1.44	1.67
6	PHEN_ACETj	4.4	0.41	3.9	-1.29	1.70	3.8	-2.29	2.70
7	CRES_ACETi	3.8	-4.04	3.8	-0.24	-3.80	3.7	-1.27	-2.77
8	CRES_ACETj	2.8	-13.89	2.4	-19.99	6.10	2.3	-21.76	7.87
9	INDO_ACETi	4.4	2.41	3.2	2.66	-0.25	3.0	1.45	0.96
10	INDO_ACETj	4.3	-1.16	4.0	-0.33	-0.83	3.8	-1.04	-0.12
11	INDO_ACETj	4.3	-1.16	4.0	-0.33	-0.83	3.8	-1.34	0.18
12	INDO_ACETj	1.8	-27.17	1.7	-27.71	0.54	1.7	-29.77	2.60
13	MIND_ACETi	4.4	2.47	3.2	2.43	0.04	2.9	0.94	1.53
14	MIND_ACETj	4.4	-0.07	4.0	-0.14	0.07	3.8	-1.14	1.07
15	MIND_ACETj	4.4	-0.61	4.5	-1.24	0.63	4.3	-3.52	2.91
16	IMID_ACETi	3.9	0.82	3.2	0.77	0.05	3.0	-0.49	1.31
17	IMID_ACETj	4.4	-6.91	4.3	-6.44	-0.47	4.1	-8.69	1.78
18	IMID_ACETj	4.4	1.66	4.8	1.69	-0.03	4.3	0.23	1.43
19	IMID_ACETj	4.4	-4.52	4.4	-3.15	-1.37	4.1	-5.31	0.79
20	IMID_ACETj	4.4	6.97	5.5	5.98	0.99	4.2	5.51	1.46
21	IMID_ACETj	4.3	-12.68	4.2	-11.10	-1.58	4.0	-13.76	1.08
22	4MIE_ACETi	3.7	0.22	3.1	0.23	-0.01	3.0	-1.15	1.37
23	4MIE_ACETj	4.4	-12.37	4.2	-7.83	-4.54	4.1	-10.44	-1.93
24	4MIE_ACETj	4.4	-0.44	4.4	-2.83	2.39	4.1	-4.97	4.53
25	4MIE_ACETj	4.4	11.48	5.5	5.31	6.17	4.1	3.91	7.57
26	4MIM_ACETi	3.6	-0.09	3.1	0.26	-0.35	3.0	-1.10	1.01
27	4MIM_ACETj	4.4	-1.09	4.5	0.19	-1.28	4.2	-1.79	0.70
28	4MIM_ACETj	4.4	-0.56	4.4	-2.37	1.81	4.2	-4.44	3.88
29	BENZ_ACETi	4.3	-12.86	4.2	-11.95	-0.91	4.0	-14.96	2.10
AVG					-2.72	0.19		-4.27	1.74
SE						0.07			0.08
AUE						1.32			2.07
RMS						2.14			2.76

Table S2. QM and MM rigid scan interactions computed by approach 1 with the optimized NBFIX parameters (Drude-2013-CP FF). The protein aromatic and charged model compound complexes are labeled as Ar_Mol⁺ for cation and Ar_Mol⁻ for anion. The QM single point interaction energies calculated at RIMP2/cc-PVQZ and SAPT2+/aug-cc-PVDZ model chemistries are in the columns "MP2 Energy" and "SAPT2+ Energy", and the differences between MM and QM are in the "Diff. MM-MP2" and "Diff. MM-SAPT2+" columns. Distance (Dist.) at which the energies are minimum are shown in Å, and the energies are shown in kcal/mol. Statistical analysis reported includes average differences (AVG), standard errors (SE), absolute unsigned error (AUE), and root-mean-square differences (RMS). The final letter in the Ar_Mol^(+,-) column corresponds to the interaction orientation shown in Figure 2 of the main text.

#	Ar_Mol ⁺	MM Dist.	MM Energy	MP2 Dist.	MP2 Energy	Diff. MM-MP2	SAPT2+ Dist.	SAPT2+ Energy	Diff. MM-SAPT2+
1	BENZ_MAM1a	1.9	-17.82	2.0	-18.32	0.50	2.0	-16.51	-1.31
2	BENZ_MAM1b	2.7	-11.35	2.8	-10.98	-0.37	2.9	-9.79	-1.56
3	TOLU_MAM1a	1.9	-16.64	1.9	-19.54	2.90	2.0	-17.67	1.03
4	TOLU_MAM1b	2.7	-12.37	2.8	-12.37	0.00	2.9	-11.09	-1.28
5	TOLU_MAM1b	2.7	-12.02	2.8	-12.13	0.11	2.9	-10.94	-1.08
6	TOLU_MAM1b	2.7	-11.25	2.8	-11.72	0.47	2.9	-10.41	-0.84
7	PHEN_MAM1a	1.9	-16.08	1.9	-18.45	2.37	2.0	-16.67	0.59
8	PHEN_MAM1b	2.7	-10.87	2.8	-10.47	-0.40	2.9	-9.37	-1.50
9	PHEN_MAM1b	2.7	-11.18	2.8	-13.31	2.13	2.9	-11.96	0.78
10	PHEN_MAM1b	2.6	-11.87	2.8	-12.02	0.15	2.8	-11.95	0.08
11	CRES_MAM1a	1.9	-13.76	1.9	-19.59	5.83	2.0	-17.75	3.99
12	CRES_MAM1b	2.6	-10.60	2.8	-11.40	0.80	2.8	-10.19	-0.41
13	CRES_MAM1b	2.7	-11.79	2.8	-14.33	2.54	2.9	-13.09	1.30
14	CRES_MAM1b	2.6	-14.24	2.7	-13.05	-1.19	2.8	-13.00	-1.24
15	INDO_MAM1a	1.8	-22.19	1.9	-23.62	1.43	2.0	-21.33	-0.86
16	INDO_MAM1b	2.6	-17.45	2.8	-16.67	-0.78	2.8	-15.41	-2.04
17	INDO_MAM1b	2.6	-15.53	2.8	-16.30	0.77	2.9	-14.76	-0.77
18	INDO_MAM1b	2.6	-12.96	2.8	-15.14	2.18	2.8	-13.80	0.84
19	INDO_MAM1b	2.6	-11.57	2.8	-12.19	0.62	2.8	-10.76	-0.81
20	INDO_MAM1b	2.8	-17.77	2.9	-18.88	1.11	2.9	-17.49	-0.28
21	MIND_MAM1a	1.8	-23.82	1.9	-24.14	0.32	1.9	-22.06	-1.76
22	MIND_MAM1b	2.6	-16.16	2.8	-17.00	0.84	2.8	-15.76	-0.40
23	MIND_MAM1b	2.6	-16.90	2.8	-16.83	-0.07	2.8	-15.25	-1.65
24	MIND_MAM1b	2.6	-16.55	2.8	-15.84	-0.71	2.8	-14.51	-2.04
25	MIND_MAM1b	2.6	-13.43	2.8	-13.03	-0.40	2.8	-11.59	-1.84
26	IMID_MAM1a	2.0	-15.24	2.0	-14.94	-0.30	2.1	-13.47	-1.77
27	IMID_MAM1a	2.6	-6.74	2.8	-5.74	-1.00	2.9	-4.62	-2.12
28	IMID_MAM1b	2.7	1.11	2.8	-0.29	1.40	2.9	0.50	0.61
29	IMID_MAM1b	2.6	-13.22	2.7	-12.52	-0.70	2.8	-11.43	-1.79
30	IMID_MAM1b	2.6	-7.77	2.8	-7.49	-0.28	2.9	-6.72	-1.05
31	IMID_MAM1b	2.5	-22.61	2.6	-21.95	-0.66	2.6	-21.05	-1.56
32	IMID_MAM1b	1.8	-26.73	1.7	-30.52	3.79	1.7	-30.19	3.46
33	4MIE_MAM1a	2.0	-14.76	2.0	-16.42	1.66	2.0	-14.95	0.19
34	4MIE_MAM1b	2.4	-30.80	2.5	-22.94	-7.86	2.5	-21.92	-8.88
35	4MIE_MAM1b	2.7	-1.14	2.8	-6.99	5.85	2.8	-5.79	4.65
36	4MIE_MAM1b	2.6	-12.97	2.8	-8.69	-4.28	2.8	-7.94	-5.03
37	4MIE_MAM1b	1.7	-35.88	1.7	-31.03	-4.85	1.7	-30.88	-5.00
38	4MIM_MAM1a	2.0	-13.88	2.0	-16.56	2.68	2.0	-15.10	1.22
39	4MIM_MAM1b	2.6	-11.34	2.7	-13.61	2.27	2.7	-12.43	1.09
40	4MIM_MAM1b	2.6	-12.72	2.8	-9.24	-3.48	2.8	-8.45	-4.27
41	4MIM_MAM1b	2.5	-24.00	2.5	-23.85	-0.15	2.6	-22.93	-1.07
42	4MIM_MAM1b	1.8	-29.62	1.7	-32.47	2.85	1.7	-32.23	2.61
43	BENZ_MGUANc	2.3	-13.71	2.2	-13.59	-0.12	2.2	-12.11	-1.60
44	BENZ_MGUANd	3.1	-7.60	3.0	-8.27	0.67	3.0	-7.47	-0.13
45	BENZ_MGUANe	3.6	-10.14	3.5	-8.21	-1.93	3.5	-7.34	-2.80
46	TOLU_MGUANc	2.3	-13.45	2.1	-14.68	1.23	2.2	-13.40	-0.05
47	TOLU_MGUANd	3.1	-7.98	2.9	-9.13	1.15	3.0	-8.29	0.31

48	TOLU_MGUANd	3.1	-7.81	2.9	-9.00	1.19	3.0	-8.23	0.42
49	TOLU_MGUANd	3.1	-7.44	2.9	-8.98	1.54	3.0	-8.09	0.65
50	TOLU_MGUANe	3.5	-6.06	3.5	-5.32	-0.74	3.4	-4.85	-1.21
51	PHEN_MGUANc	2.5	-12.02	2.1	-13.22	1.20	2.2	-11.80	-0.22
52	PHEN_MGUANd	3.0	-10.12	2.9	-8.69	-1.43	3.0	-7.79	-2.33
53	PHEN_MGUANd	3.1	-9.12	2.9	-9.38	0.26	3.0	-8.51	-0.61
54	PHEN_MGUANd	3.1	-8.92	3.0	-9.11	0.19	3.1	-8.96	0.04
55	PHEN_MGUANe	3.7	-12.47	3.4	-8.46	-4.01	3.5	-7.60	-4.87
56	CRES_MGUANc	2.5	-10.92	2.1	-14.30	3.38	2.2	-12.84	1.92
57	CRES_MGUANd	3.1	-9.08	2.9	-10.03	0.95	3.0	-9.18	0.10
58	CRES_MGUANd	3.1	-9.36	3.0	-9.80	0.44	3.1	-9.62	0.26
59	CRES_MGUANe	3.6	-12.42	3.4	-9.27	-3.15	3.5	-8.38	-4.04
60	INDO_MGUANc	2.2	-16.50	2.1	-16.65	0.15	2.2	-15.00	-1.50
61	INDO_MGUANd	3.0	-11.40	2.9	-12.31	0.91	2.9	-11.39	-0.01
62	INDO_MGUANd	3.0	-10.36	2.9	-12.24	1.88	2.9	-11.13	0.77
63	INDO_MGUANd	3.0	-8.93	2.9	-11.59	2.66	2.9	-10.65	1.72
64	INDO_MGUANd	3.0	-8.46	2.9	-9.86	1.40	2.9	-8.87	0.41
65	INDO_MGUANe	3.6	-14.25	3.3	-12.57	-1.68	3.4	-11.53	-2.72
66	MIND_MGUANc	3.1	-10.81	2.9	-12.69	1.88	2.9	-11.80	0.99
67	MIND_MGUANd	3.0	-11.10	2.9	-12.62	1.52	3.0	-11.50	0.40
68	MIND_MGUANd	3.0	-10.83	2.9	-12.06	1.23	2.9	-11.16	0.33
69	MIND_MGUANd	3.0	-9.37	2.9	-10.39	1.02	2.9	-9.40	0.03
70	MIND_MGUANe	3.6	-14.97	3.3	-13.04	-1.93	3.4	-11.95	-3.02
71	IMID_MGUANc	2.3	-10.10	2.2	-10.40	0.30	2.3	-9.39	-0.71
72	IMID_MGUANc	3.7	-7.55	3.4	-6.80	-0.75	3.4	-6.30	-1.25
73	IMID_MGUANd	3.0	-4.14	2.9	-4.96	0.82	3.0	-4.15	0.01
74	IMID_MGUANd	2.8	-1.77	2.9	-1.63	-0.14	2.9	-1.10	-0.67
75	IMID_MGUANd	3.0	-7.92	2.9	-8.69	0.77	2.9	-7.97	0.05
76	IMID_MGUANd	3.1	-4.87	2.9	-5.68	0.81	3.0	-5.21	0.34
77	IMID_MGUANd	2.7	-15.21	2.7	-15.51	0.30	2.7	-14.90	-0.31
78	IMID_MGUANe	1.9	-20.26	1.8	-23.52	3.26	1.8	-23.36	3.10
79	4MIE_MGUANc	2.3	-11.59	2.2	-11.55	-0.04	2.2	-10.55	-1.04
80	4MIE_MGUANd	3.7	-8.09	3.4	-7.40	-0.69	3.4	-7.02	-1.07
81	4MIE_MGUANd	2.6	-19.75	2.6	-16.31	-3.44	2.7	-15.60	-4.15
82	4MIE_MGUANd	3.1	-1.50	2.8	-5.94	4.44	2.9	-5.08	3.58
83	4MIE_MGUANd	3.0	-7.87	2.9	-6.46	-1.41	2.9	-6.00	-1.87
84	4MIE_MGUANe	2.9	1.02	2.9	-2.56	3.58	2.9	-2.05	3.07
85	4MIM_MGUANc	2.3	-11.06	2.2	-11.82	0.76	2.2	-10.81	-0.25
86	4MIM_MGUANd	3.7	-8.12	3.4	-7.81	-0.31	3.4	-7.38	-0.74
87	4MIM_MGUANd	2.8	-1.93	2.8	-2.50	0.57	2.9	-1.93	0.00
88	4MIM_MGUANd	3.0	-6.95	2.8	-9.64	2.69	2.9	-8.84	1.89
89	4MIM_MGUANd	3.0	-7.68	2.9	-6.82	-0.86	2.9	-6.32	-1.36
90	4MIM_MGUANd	2.7	-15.80	2.6	-16.76	0.96	2.7	-16.15	0.35
91	4MIM_MGUANe	1.9	-22.23	1.8	-25.03	2.80	1.8	-24.95	2.72
92	BENZ_IMIMf	2.3	-14.23	2.0	-15.50	1.27	2.1	-13.54	-0.69
93	BENZ_IMIMg	3.0	-8.01	2.9	-9.41	1.40	3.0	-8.03	0.02
94	BENZ_IMIMh	3.5	-11.37	3.5	-8.93	-2.44	3.6	-7.50	-3.87
95	TOLU_IMIMf	2.3	-13.51	1.9	-16.69	3.18	2.0	-14.69	1.18
96	TOLU_IMIMg	3.0	-8.64	2.9	-10.50	1.86	2.9	-9.07	0.43
97	TOLU_IMIMg	3.0	-8.42	2.8	-10.32	1.90	2.9	-9.01	0.59
98	TOLU_IMIMg	3.0	-7.99	2.8	-10.27	2.28	2.9	-8.81	0.82
99	TOLU_IMIMh	3.5	-11.70	3.5	-9.69	-2.01	3.6	-8.18	-3.52
100	PHEN_IMIMf	2.2	-14.77	2.0	-15.42	0.65	2.1	-13.49	-1.28
101	PHEN_IMIMg	3.0	-9.91	2.9	-10.00	0.09	2.9	-8.49	-1.42
102	PHEN_IMIMg	3.1	-8.21	3.1	-10.15	1.94	3.1	-9.80	1.59
103	PHEN_IMIMg	3.1	-4.04	2.9	-7.47	3.43	2.9	-6.02	1.98
104	PHEN_IMIMg	3.0	-8.04	2.9	-8.96	0.92	2.9	-7.73	-0.31
105	PHEN_IMIMg	3.0	-9.75	2.9	-9.98	0.23	2.9	-8.49	-1.26
106	PHEN_IMIMh	3.5	-12.87	3.4	-9.67	-3.20	3.6	-8.20	-4.67
107	CRES_IMIMf	2.2	-13.08	1.9	-16.53	3.45	2.0	-14.58	1.50
108	CRES_IMIMg	3.2	-8.14	3.0	-9.80	1.66	3.1	-9.22	1.08
109	CRES_IMIMg	3.1	-9.39	3.1	-11.17	1.78	3.1	-10.84	1.45
110	CRES_IMIMg	3.1	-4.55	2.8	-8.38	3.83	2.9	-6.94	2.39
111	CRES_IMIMg	3.0	-7.70	2.8	-9.83	2.13	2.9	-8.48	0.78
112	CRES_IMIMg	3.6	-6.08	3.6	-5.53	-0.55	3.4	-4.11	-1.97

113	CRES_IMIMh	3.5	-12.76	3.4	-10.42	-2.34	3.5	-8.83	-3.93
114	INDO_IMIMf	2.1	-17.80	1.9	-20.37	2.57	2.0	-18.15	0.35
115	INDO_IMIMg	3.0	-10.54	2.8	-13.78	3.24	2.9	-12.14	1.60
116	INDO_IMIMg	3.0	-8.67	2.8	-12.87	4.20	2.9	-11.37	2.70
117	INDO_IMIMg	3.0	-11.61	2.9	-13.86	2.25	2.9	-12.52	0.91
118	INDO_IMIMh	3.4	-14.45	3.3	-14.17	-0.28	3.4	-12.23	-2.22
119	MIND_IMIMf	2.1	-18.95	1.9	-21.05	2.10	2.0	-18.78	-0.17
120	MIND_IMIMg	3.0	-8.91	2.8	-11.29	2.38	2.9	-9.68	0.77
121	MIND_IMIMg	3.0	-11.27	2.8	-11.29	0.02	2.9	-12.53	1.26
122	MIND_IMIMg	3.0	-10.89	2.8	-13.43	2.54	2.9	-11.93	1.04
123	MIND_IMIMg	3.1	-10.76	2.8	-11.29	0.53	2.9	-13.01	2.25
124	MIND_IMIMh	3.4	-15.14	3.3	-14.60	-0.54	3.4	-12.62	-2.52
125	IMID_IMIMf	2.8	-5.18	2.8	-5.19	0.01	2.9	-3.94	-1.24
126	IMID_IMIMh	3.6	-7.90	3.5	-6.47	-1.43	3.6	-5.45	-2.45
127	4MIE_IMIMh	3.5	-11.11	3.3	-9.63	-1.48	3.4	-8.37	-2.74
128	4MIM_IMIMh	3.6	-8.30	3.4	-7.48	-0.82	3.5	-6.34	-1.96
AVG						0.62			-0.46
SE						0.02			0.02
AUE						1.64			1.56
RMS						2.15			2.09
#	Ar_Mol-	MM Dist.	MM Energy	MP2 Dist.	MP2 Energy	Diff. MM-MP2	SAPT2+ Dist.	SAPT2+ Energy	Diff. MM-SAPT2+
1	BENZ_ACETi	3.4	-1.55	3.2	1.23	-2.78	3.0	0.10	-1.65
2	BENZ_ACETj	4.2	-3.25	3.9	-1.72	-1.53	3.8	-2.61	-0.64
3	TOLU_ACETi	3.3	-2.74	3.2	0.72	-3.46	3.0	-0.53	-2.21
4	TOLU_ACETj	4.2	-2.99	3.9	-1.30	-1.69	3.8	-2.14	-0.85
5	PHEN_ACETi	4.0	-2.58	3.8	-0.43	-2.15	3.7	-1.44	-1.14
6	PHEN_ACETj	4.2	-2.04	3.9	-1.29	-0.75	3.8	-2.29	0.25
7	CRES_ACETi	3.8	-4.04	3.8	-0.24	-3.80	3.7	-1.27	-2.77
8	CRES_ACETj	2.8	-16.56	2.4	-19.99	3.43	2.3	-21.76	5.20
9	INDO_ACETi	3.8	-0.11	3.2	2.66	-2.77	3.0	1.45	-1.56
10	INDO_ACETj	4.1	-3.87	4.0	-0.33	-3.54	3.8	-1.04	-2.83
11	INDO_ACETj	4.1	-3.87	4.0	-0.33	-3.54	3.8	-1.34	-2.53
12	INDO_ACETj	1.7	-31.61	1.7	-27.71	-3.90	1.7	-29.77	-1.84
13	MIND_ACETi	3.8	-0.06	3.2	2.43	-2.49	2.9	0.94	-1.00
14	MIND_ACETj	4.2	-2.65	4.0	-0.14	-2.51	3.8	-1.14	-1.51
15	MIND_ACETj	4.4	-5.80	4.5	-1.24	-4.56	4.3	-3.52	-2.28
16	IMID_ACETi	4.4	1.11	3.2	0.77	0.34	3.0	-0.49	1.60
17	IMID_ACETj	4.3	-7.20	4.3	-6.44	-0.76	4.1	-8.69	1.49
18	IMID_ACETj	4.4	1.56	4.8	1.69	-0.13	4.3	0.23	1.33
19	IMID_ACETj	4.3	-4.37	4.4	-3.15	-1.22	4.1	-5.31	0.94
20	IMID_ACETj	4.4	6.98	5.5	5.98	1.00	4.2	5.51	1.47
21	IMID_ACETj	4.1	-12.96	4.2	-11.10	-1.86	4.0	-13.76	0.80
22	4MIE_ACETi	3.5	0.58	3.1	0.23	0.35	3.0	-1.15	1.73
23	4MIE_ACETj	4.2	-13.00	4.2	-7.83	-5.17	4.1	-10.44	-2.56
24	4MIE_ACETj	4.4	-0.24	4.4	-2.83	2.59	4.1	-4.97	4.73
25	4MIE_ACETj	4.4	11.53	5.5	5.31	6.22	4.1	3.91	7.62
26	4MIM_ACETi	3.4	0.23	3.1	0.26	-0.03	3.0	-1.10	1.33
27	4MIM_ACETj	4.4	-1.19	4.5	0.19	-1.38	4.2	-1.79	0.60
28	4MIM_ACETj	4.4	-0.35	4.4	-2.37	2.02	4.2	-4.44	4.09
29	BENZ_ACETi	4.2	-12.88	4.2	-11.95	-0.93	4.0	-14.96	2.08
AVG						-1.21			0.34
SE						0.09			0.09
AUE						2.31			2.09
RMS						2.77			2.61

Table S3. QM and MM optimized interactions computed by approach 2 with the original Drude-2013 force field without NBFIX parameters. The protein aromatic and charged model compound complexes are labeled as Ar_Mol⁺ for cation and Ar_Mol⁻ for anion. Distance differences in the ion-pi distance between the MM and QM optimized interaction geometries are shown in Å. The QM single point interaction energies calculated at RIMP2/cc-PVQZ and SAPT2+/aug-cc-PVDZ model chemistries are in the columns "QM MP2" and "QM SAPT2+", and the differences between MM and QM are in the "Diff. MM-MP2" and "Diff. MM-SAPT2+" columns. The differences between the QM interaction energies obtained at the two model chemistries are in "Diff. SAPT2+-MP2" column. Statistical analysis reported includes average differences (AVG), standard errors (SE), absolute unsigned error (AUE), and root-mean-square differences (RMS). Energies are in kcal/mol. The final letter in the Ar_Mol^(+,-) column corresponds to the interaction orientation shown in Figure 2 of the main text. Cartesian coordinates for the QM optimized interaction orientations are included in Table S7.

#	Ar_Mol ⁺	Dist Diff	MM	QM MP2	Diff. MM- MP2	QM SAPT2+	Diff. MM- SAPT2+	Diff. SAPT2+- MP2
1	BENZ_MAM1a	0.01	-19.07	-18.92	-0.15	-17.06	-2.01	1.86
2	BENZ_MAM1b	0.01	-19.07	-18.94	-0.13	-17.09	-1.98	1.85
3	TOLU_MAM1a	0.04	-17.86	-20.65	2.79	-18.72	0.86	1.93
4	TOLU_MAM1b	0.04	-17.86	-20.65	2.79	-18.74	0.88	1.91
5	TOLU_MAM1b	0.04	-17.84	-20.47	2.63	-18.61	0.77	1.86
6	TOLU_MAM1b	0.04	-17.86	-20.65	2.79	-18.74	0.88	1.91
7	PHEN_MAM1a	0.02	-18.32	-20.61	2.29	-18.72	0.40	1.89
8	PHEN_MAM1b	0.02	-18.02	-20.04	2.02	-18.23	0.21	1.81
9	PHEN_MAM1b	0.02	-16.84	-21.99	5.15	-20.68	3.84	1.31
10	PHEN_MAM1b	0.02	-16.87	-21.96	5.09	-20.33	3.46	1.63
11	CRES_MAM1a	0.05	-15.43	-22.17	6.74	-20.28	4.85	1.89
12	CRES_MAM1b	0.05	-15.11	-21.50	6.39	-19.61	4.50	1.89
13	CRES_MAM1b	0.02	-18.82	-23.41	4.59	-22.09	3.27	1.32
14	CRES_MAM1b	0.02	-18.75	-23.41	4.66	-21.72	2.97	1.69
15	INDO_MAM1a	0.04	-25.73	-25.21	-0.52	-23.64	-2.09	1.57
16	INDO_MAM1b	0.04	-25.91	-25.59	-0.32	-23.64	-2.27	1.95
17	INDO_MAM1b	0.04	-25.81	-25.18	-0.63	-23.00	-2.81	2.18
18	INDO_MAM1b	0.03	-25.94	-25.86	-0.08	-23.63	-2.31	2.23
19	INDO_MAM1b	0.04	-25.93	-25.59	-0.34	-23.42	-2.51	2.17
20	INDO_MAM1b	0.03	-25.71	-25.08	-0.63	-22.99	-2.72	2.09
21	MIND_MAM1a	0.06	-26.00	-26.89	0.89	-24.60	-1.40	2.29
22	MIND_MAM1b	0.04	-26.01	-26.89	0.88	-24.60	-1.41	2.29
23	MIND_MAM1b	0.04	-25.87	-26.06	0.19	-23.85	-2.02	2.21
24	MIND_MAM1b	0.06	-25.87	-27.00	1.13	-24.69	-1.18	2.31
25	MIND_MAM1b	0.06	-26.66	-26.49	-0.17	-24.27	-2.39	2.22
26	IMID_MAM1a	0.02	-25.94	-36.49	10.55	-36.27	10.33	0.22
27	IMID_MAM1a	0.02	-25.91	-36.45	10.54	-36.22	10.31	0.23
28	IMID_MAM1b	0.02	-25.85	-36.44	10.59	-36.22	10.37	0.22
29	IMID_MAM1b	0.02	-25.93	-36.53	10.60	-36.32	10.39	0.21
30	IMID_MAM1b	0.02	-25.95	-36.45	10.50	-36.23	10.28	0.22
31	IMID_MAM1b	0.02	-25.94	-36.53	10.59	-36.32	10.38	0.21
32	IMID_MAM1b	0.02	-25.96	-36.51	10.55	-36.29	10.33	0.22
33	4MIE_MAM1a	0.04	-36.03	-38.43	2.40	-38.45	2.42	-0.02
34	4MIE_MAM1b	0.04	-36.11	-38.61	2.50	-38.64	2.53	-0.03
35	4MIE_MAM1b	0.04	-36.12	-38.47	2.35	-38.47	2.35	0.00

36	4MIE_MAM1b	0.03	-36.12	-38.52	2.40	-38.54	2.42	-0.02
37	4MIE_MAM1b	0.04	-36.11	-38.52	2.41	-38.61	2.50	-0.09
38	4MIM_MAM1a	0.03	-30.31	-39.64	9.33	-39.67	9.36	-0.03
39	4MIM_MAM1b	0.03	-30.26	-39.58	9.32	-39.60	9.34	-0.02
40	4MIM_MAM1b	0.02	-30.28	-39.57	9.29	-39.59	9.31	-0.02
41	4MIM_MAM1b	0.02	-30.25	-39.66	9.41	-39.69	9.44	-0.03
42	4MIM_MAM1b	0.02	-30.27	-39.58	9.31	-39.58	9.31	0.00
43	BENZ_MGUANc	0.01	-13.76	-14.74	0.98	-12.94	-0.82	1.80
44	BENZ_MGUANd	0.01	-13.67	-14.74	1.07	-12.94	-0.73	1.80
45	BENZ_MGUANe	0.01	-14.67	-15.46	0.79	-13.45	-1.22	2.01
46	TOLU_MGUANc	0.01	-13.79	-16.13	2.34	-14.26	0.47	1.87
47	TOLU_MGUANd	0.03	-13.11	-16.04	2.93	-14.19	1.08	1.85
48	TOLU_MGUANd	0.02	-12.68	-16.09	3.41	-14.26	1.58	1.83
49	TOLU_MGUANd	0.01	-13.79	-16.14	2.35	-14.26	0.47	1.88
50	TOLU_MGUANe	0.01	-13.81	-16.11	2.30	-14.25	0.44	1.86
51	PHEN_MGUANc	0.02	-13.60	-15.75	2.15	-13.95	0.35	1.80
52	PHEN_MGUANd	0.02	-15.85	-18.53	2.68	-17.14	1.29	1.39
53	PHEN_MGUANd	0.02	-15.87	-18.54	2.67	-17.39	1.52	1.15
54	PHEN_MGUANd	0.02	-15.87	-18.55	2.68	-17.14	1.27	1.41
55	PHEN_MGUANe	0.02	-10.74	-16.19	5.45	-15.08	4.34	1.11
56	CRES_MGUANc	0.04	-15.53	-18.18	2.65	-16.64	1.11	1.54
57	CRES_MGUANd	0.04	-15.52	-20.01	4.49	-18.66	3.14	1.35
58	CRES_MGUANd	0.04	-15.56	-19.81	4.25	-18.42	2.86	1.39
59	CRES_MGUANe	0.04	-9.89	-17.60	7.71	-16.46	6.57	1.14
60	INDO_MGUANc	0.04	-19.31	-19.53	0.22	-19.68	0.37	-0.15
61	INDO_MGUANd	0.06	-20.29	-21.82	1.53	-19.77	-0.52	2.05
62	INDO_MGUANd	0.06	-20.29	-21.83	1.54	-19.78	-0.51	2.05
63	INDO_MGUANd	0.05	-20.29	-21.59	1.30	-19.54	-0.75	2.05
64	INDO_MGUANd	0.05	-20.29	-21.60	1.31	-19.54	-0.75	2.06
65	INDO_MGUANe	0.03	-19.03	-19.25	0.22	-17.43	-1.60	1.82
66	MIND_MGUANc	0.05	-21.10	-22.72	1.62	-20.61	-0.49	2.11
67	MIND_MGUANd	0.04	-21.11	-22.71	1.60	-20.61	-0.50	2.10
68	MIND_MGUANd	0.04	-21.11	-22.54	1.43	-20.42	-0.69	2.12
69	MIND_MGUANd	0.04	-21.11	-22.54	1.43	-20.43	-0.68	2.11
70	MIND_MGUANe	0.04	-22.36	-22.92	0.56	-20.89	-1.47	2.03
71	IMID_MGUANc	0.01	-23.05	-27.53	4.48	-27.37	4.32	0.16
72	IMID_MGUANc	0.01	-21.17	-25.01	3.84	-24.77	3.60	0.24
73	IMID_MGUANd	0.02	-23.00	-26.86	3.86	-26.57	3.57	0.29
74	IMID_MGUANd	0.02	-22.99	-26.22	3.23	-25.67	2.68	0.55
75	IMID_MGUANd	0.01	-23.04	-27.52	4.48	-27.38	4.34	0.14
76	IMID_MGUANd	0.01	-23.04	-27.50	4.46	-27.36	4.32	0.14
77	IMID_MGUANd	0.01	-23.05	-27.45	4.40	-27.32	4.27	0.13
78	IMID_MGUANe	0.01	-23.04	-27.51	4.47	-27.38	4.34	0.13
79	4MIE_MGUANc	0.13	-31.79	-28.44	-3.35	-28.36	-3.43	0.08
80	4MIE_MGUANd	0.07	-31.74	-16.77	-14.97	-17.71	-14.03	-0.94
81	4MIE_MGUANd	0.17	-31.82	-28.53	-3.29	-28.43	-3.39	0.10
82	4MIE_MGUANd	0.05	-31.73	-27.85	-3.88	-27.57	-4.16	0.28
83	4MIE_MGUANd	0.18	-31.83	-28.53	-3.30	-28.43	-3.40	0.10
84	4MIE_MGUANe	0.19	-31.82	-27.67	-4.15	-27.44	-4.38	0.23
85	4MIM_MGUANc	0.02	-26.43	-29.26	2.83	-29.21	2.78	0.05
86	4MIM_MGUANd	0.02	-24.22	-27.03	2.81	-26.63	2.41	0.40
87	4MIM_MGUANd	0.35	-26.34	-28.80	2.46	-28.60	2.26	0.20
88	4MIM_MGUANd	0.02	-26.42	-29.28	2.86	-29.22	2.80	0.06
89	4MIM_MGUANd	0.02	-26.40	-29.28	2.88	-29.22	2.82	0.06
90	4MIM_MGUANd	0.02	-26.43	-29.27	2.84	-29.21	2.78	0.06
91	4MIM_MGUANe	0.02	-26.39	-29.26	2.87	-29.21	2.82	0.05

92	BENZ_IMIMf	0.01	-14.83	-15.60	0.77	-13.55	-1.28	2.05
93	BENZ_IMIMg	0.01	-14.84	-15.79	0.95	-13.69	-1.15	2.10
94	BENZ_IMIMh	0.01	-14.84	-15.79	0.95	-13.69	-1.15	2.10
95	TOLU_IMIMf	0.03	-13.65	-17.10	3.45	-14.94	1.29	2.16
96	TOLU_IMIMg	0.03	-13.64	-17.09	3.45	-14.97	1.33	2.12
97	TOLU_IMIMg	0.03	-13.65	-17.11	3.46	-14.98	1.33	2.13
98	TOLU_IMIMg	0.01	-13.79	-17.17	3.38	-15.01	1.22	2.16
99	TOLU_IMIMh	0.03	-13.66	-17.10	3.44	-14.98	1.32	2.12
100	PHEN_IMIMf	0.02	-15.01	-17.70	2.69	-15.65	0.64	2.05
101	PHEN_IMIMg	0.02	-15.19	-18.32	3.13	-16.41	1.22	1.91
102	PHEN_IMIMg	0.02	-15.01	-17.70	2.69	-15.64	0.63	2.06
103	PHEN_IMIMg	0.02	-15.19	-18.32	3.13	-16.42	1.23	1.90
104	PHEN_IMIMg	0.02	-15.19	-18.33	3.14	-16.41	1.22	1.92
105	PHEN_IMIMg	0.02	-15.19	-18.32	3.13	-16.42	1.23	1.90
106	PHEN_IMIMh	0.02	-15.23	-19.37	4.14	-17.93	2.70	1.44
107	CRES_IMIMf	0.04	-12.29	-18.82	6.53	-16.75	4.46	2.07
108	CRES_IMIMg	0.04	-12.17	-18.57	6.40	-16.85	4.68	1.72
109	CRES_IMIMg	0.04	-12.31	-18.88	6.57	-16.82	4.51	2.06
110	CRES_IMIMg	0.04	-12.56	-19.68	7.12	-17.78	5.22	1.90
111	CRES_IMIMg	0.04	-12.57	-19.69	7.12	-17.79	5.22	1.90
112	CRES_IMIMg	0.10	-12.49	-19.36	6.87	-17.44	4.95	1.92
113	CRES_IMIMh	0.02	-12.27	-18.70	6.43	-16.64	4.37	2.06
114	INDO_IMIMf	0.04	-21.13	-22.98	1.85	-20.53	-0.60	2.45
115	INDO_IMIMg	0.07	-20.65	-20.27	-0.38	-18.11	-2.54	2.16
116	INDO_IMIMg	0.05	-21.13	-22.98	1.85	-20.53	-0.60	2.45
117	INDO_IMIMg	0.04	-21.22	-22.98	1.76	-20.53	-0.69	2.45
118	INDO_IMIMh	0.03	-19.34	-20.12	0.78	-17.84	-1.50	2.28
119	MIND_IMIMf	0.04	-21.07	-23.94	2.87	-21.46	0.39	2.48
120	MIND_IMIMg	0.04	-20.51	-23.32	2.81	-20.66	0.15	2.66
121	MIND_IMIMg	0.04	-20.49	-23.32	2.83	-20.66	0.17	2.66
122	MIND_IMIMg	0.04	-21.06	-23.94	2.88	-21.47	0.41	2.47
123	MIND_IMIMg	0.04	-20.51	-23.32	2.81	-20.66	0.15	2.66
124	MIND_IMIMh	0.04	-20.85	-21.02	0.17	-18.63	-2.22	2.39
125	IMID_IMIMf	0.01	-24.57	-25.16	0.59	-24.40	-0.17	0.76
126	IMID_IMIMh	0.01	-17.45	-15.67	-1.78	-15.85	-1.60	-0.18
127	4MIE_IMIMh	0.31	-28.22	-15.95	-12.27	-16.44	-11.78	-0.49
128	4MIM_IMIMh	0.14	-28.60	-24.97	-3.63	-23.65	-4.95	1.32
AVG				-23.87	2.78	-22.52	1.44	1.34
SE					3.81		3.99	0.08
AUE					3.63		3.02	1.37
RMS					4.71		4.22	1.63
#	Ar_Mol-	Dist	MM	QM	Diff.	QM	Diff.	Diff.
		Diff		MP2	MM-	SAPT2+	MM-	SAPT2+-
					MP2		SAPT2+	MP2
1	BENZ_ACETi	0.02	-5.90	-7.81	1.91	-7.02	1.12	0.79
2	BENZ_ACETj	0.01	-5.16	-7.94	2.78	-8.89	3.73	-0.95
3	TOLU_ACETi	0.02	-8.51	-10.55	2.04	-12.05	3.54	-1.50
4	TOLU_ACETj	0.03	-7.15	-10.35	3.20	-11.90	4.75	-1.55
5	PHEN_ACETi	0.02	-6.84	-10.42	3.58	-12.21	5.37	-1.79
6	PHEN_ACETj	0.02	-6.16	-10.95	4.79	-12.54	6.38	-1.59
7	CRES_ACETi	0.02	-6.94	-11.41	4.47	-12.95	6.01	-1.54
8	CRES_ACETj	0.03	-21.11	-31.64	10.53	-33.04	11.93	-1.40
9	INDO_ACETi	0.04	-28.74	-31.97	3.23	-33.36	4.62	-1.39
10	INDO_ACETj	0.05	-27.63	-31.50	3.87	-32.89	5.26	-1.39
11	INDO_ACETj	0.05	-27.63	-31.46	3.83	-32.86	5.23	-1.40
12	INDO_ACETj	0.04	-28.69	-32.01	3.32	-33.41	4.72	-1.40

13	MIND_ACETi	0.04	-25.39	-31.36	5.97	-32.77	7.38	-1.41
14	MIND_ACETj	0.12	-24.70	-30.79	6.09	-27.80	3.10	2.99
15	MIND_ACETj	0.05	-24.81	-30.87	6.06	-32.18	7.37	-1.31
16	IMID_ACETi	0.02	-26.18	-32.97	6.79	-34.21	8.03	-1.24
17	IMID_ACETj	0.02	-26.18	-32.96	6.78	-34.22	8.04	-1.26
18	IMID_ACETj	0.02	-26.18	-32.96	6.78	-34.24	8.06	-1.28
19	IMID_ACETj	0.02	-26.38	-32.49	6.11	-33.63	7.25	-1.14
20	IMID_ACETj	0.02	-26.37	-32.73	6.36	-33.72	7.35	-0.99
21	IMID_ACETj	0.02	-26.32	-32.32	6.00	-33.48	7.16	-1.16
22	4MIE_ACETi	0.06	-33.64	-31.68	-1.96	-32.76	-0.88	-1.08
23	4MIE_ACETj	0.14	-33.65	-31.75	-1.90	-33.30	-0.35	-1.55
24	4MIE_ACETj	0.05	-33.63	-31.66	-1.97	-32.76	-0.87	-1.10
25	4MIE_ACETj	0.09	-33.67	-31.77	-1.90	-33.11	-0.56	-1.34
26	4MIM_ACETi	0.03	-29.13	-31.92	2.79	-33.15	4.02	-1.23
27	4MIM_ACETj	0.24	-12.31	-10.49	-1.82	-12.02	-0.29	-1.53
28	4MIM_ACETj	0.03	-29.13	-31.92	2.79	-33.15	4.02	-1.23
29	BENZ_ACETi	0.20	-29.06	-32.74	3.68	-34.07	5.01	-1.33
AVG				-25.91	3.59	-27.02	4.71	-1.11
SE					3.15		3.19	0.17
AUE					4.25		4.91	1.37
RMS					4.74		5.65	1.42

Table S4. QM and MM optimized interactions computed by approach 2 with optimized NBFIX parameters (Drude-2013-CP FF). The protein aromatic and charged model compound complexes are labeled as Ar_Mol⁺ for cation and Ar_Mol⁻ for anion. Distance differences in the ion-pi distance between the MM and QM optimized interaction geometries are shown in Å. The QM single point interaction energies calculated at RIMP2/cc-PVQZ and SAPT2+/aug-cc-PVDZ model chemistries are in the column of "QM MP2" and "QM SAPT2+", and the differences between MM and QM are in the "Diff. MM-MP2" and "Diff. MM-SAPT2+" columns. Statistical analysis reported includes average differences (AVG), standard errors (SE), absolute unsigned error (AUE), and root-mean-square differences (RMS). Energies in kcal/mol and distances in Å. The final letter in the Ar_Mol^(+,-) column corresponds to the interaction orientation shown in Figure 2 of the main text. Cartesian coordinates for the QM optimized interaction orientations are included in Table S7.

#	Ar_Mol ^(+,-)	Dist Diff	MM	QM MP2	Diff. MM-MP2	QM SAPT2+	Diff. MM-SAPT2+
1	BENZ_MAM1a	0.03	-19.04	-18.92	-0.12	-17.06	-1.98
2	BENZ_MAM1b	0.03	-19.04	-18.94	-0.10	-17.09	-1.95
3	TOLU_MAM1a	0.07	-17.98	-20.65	2.67	-18.72	0.74
4	TOLU_MAM1b	0.07	-18.00	-20.65	2.65	-18.74	0.74
5	TOLU_MAM1b	0.08	-17.87	-20.47	2.60	-18.61	0.74
6	TOLU_MAM1b	0.07	-17.96	-20.65	2.69	-18.74	0.78
7	PHEN_MAM1a	0.02	-19.39	-20.61	1.22	-18.72	-0.67
8	PHEN_MAM1b	0.02	-18.92	-20.04	1.12	-18.23	-0.69
9	PHEN_MAM1b	0.02	-16.98	-21.99	5.01	-20.68	3.70
10	PHEN_MAM1b	0.02	-16.98	-21.96	4.98	-20.33	3.35
11	CRES_MAM1a	0.06	-15.86	-22.17	6.31	-20.28	4.42
12	CRES_MAM1b	0.02	-16.71	-21.50	4.79	-19.61	2.90
13	CRES_MAM1b	0.02	-18.73	-23.41	4.68	-22.09	3.36
14	CRES_MAM1b	0.02	-18.72	-23.41	4.69	-21.72	3.00
15	INDO_MAM1a	0.04	-24.41	-25.21	0.80	-23.64	-0.77
16	INDO_MAM1b	0.06	-24.36	-25.59	1.23	-23.64	-0.72
17	INDO_MAM1b	0.04	-24.40	-25.18	0.78	-23.00	-1.40
18	INDO_MAM1b	0.04	-24.51	-25.86	1.35	-23.63	-0.88
19	INDO_MAM1b	0.05	-24.39	-25.59	1.20	-23.42	-0.97
20	INDO_MAM1b	0.04	-23.99	-25.08	1.09	-22.99	-1.00
21	MIND_MAM1a	0.06	-26.14	-26.89	0.75	-24.60	-1.54
22	MIND_MAM1b	0.05	-26.20	-26.89	0.69	-24.60	-1.60
23	MIND_MAM1b	0.05	-26.22	-26.06	-0.16	-23.85	-2.37
24	MIND_MAM1b	0.05	-26.22	-27.00	0.78	-24.69	-1.53
25	MIND_MAM1b	0.06	-26.23	-26.49	0.26	-24.27	-1.96
26	IMID_MAM1a	0.01	-30.24	-36.49	6.25	-36.27	6.03
27	IMID_MAM1a	0.01	-30.23	-36.45	6.22	-36.22	5.99
28	IMID_MAM1b	0.01	-30.25	-36.44	6.19	-36.22	5.97
29	IMID_MAM1b	0.01	-30.25	-36.53	6.28	-36.32	6.07
30	IMID_MAM1b	0.01	-30.23	-36.45	6.22	-36.23	6.00
31	IMID_MAM1b	0.01	-30.25	-36.53	6.28	-36.32	6.07
32	IMID_MAM1b	0.01	-30.20	-36.51	6.31	-36.29	6.09
33	4MIE_MAM1a	0.07	-42.72	-38.43	-4.29	-38.45	-4.27
34	4MIE_MAM1b	0.05	-42.81	-38.61	-4.20	-38.64	-4.17
35	4MIE_MAM1b	0.05	-42.81	-38.47	-4.34	-38.47	-4.34
36	4MIE_MAM1b	0.05	-42.80	-38.52	-4.28	-38.54	-4.26
37	4MIE_MAM1b	0.05	-42.81	-38.52	-4.29	-38.61	-4.20
38	4MIM_MAM1a	0.03	-35.11	-39.64	4.53	-39.67	4.56
39	4MIM_MAM1b	0.03	-35.09	-39.58	4.49	-39.60	4.51

40	4MIM_MAM1b	0.03	-35.05	-39.57	4.52	-39.59	4.54
41	4MIM_MAM1b	0.03	-35.09	-39.66	4.57	-39.69	4.60
42	4MIM_MAM1b	0.03	-35.14	-39.58	4.44	-39.58	4.44
43	BENZ_MGUANc	0.01	-14.27	-14.74	0.47	-12.94	-1.33
44	BENZ_MGUANd	0.01	-14.24	-14.74	0.50	-12.94	-1.30
45	BENZ_MGUANe	0.01	-15.08	-15.46	0.38	-13.45	-1.63
46	TOLU_MGUANc	0.01	-14.33	-16.13	1.80	-14.26	-0.07
47	TOLU_MGUANd	0.02	-14.13	-16.04	1.91	-14.19	0.06
48	TOLU_MGUANd	0.03	-13.50	-16.09	2.59	-14.26	0.76
49	TOLU_MGUANd	0.01	-14.35	-16.14	1.79	-14.26	-0.09
50	TOLU_MGUANe	0.01	-14.33	-16.11	1.78	-14.25	-0.08
51	PHEN_MGUANc	0.02	-15.38	-15.75	0.37	-13.95	-1.43
52	PHEN_MGUANd	0.02	-17.41	-18.53	1.12	-17.14	-0.27
53	PHEN_MGUANd	0.02	-17.52	-18.54	1.02	-17.39	-0.13
54	PHEN_MGUANd	0.02	-17.51	-18.55	1.04	-17.14	-0.37
55	PHEN_MGUANe	0.02	-13.46	-16.19	2.73	-15.08	1.62
56	CRES_MGUANc	0.05	-18.11	-18.18	0.07	-16.64	-1.47
57	CRES_MGUANd	0.04	-18.17	-20.01	1.84	-18.66	0.49
58	CRES_MGUANd	0.04	-18.25	-19.81	1.56	-18.42	0.17
59	CRES_MGUANe	0.05	-13.91	-17.60	3.69	-16.46	2.55
60	INDO_MGUANc	0.04	-19.33	-19.53	0.20	-19.68	0.35
61	INDO_MGUANd	0.03	-20.91	-21.82	0.91	-19.77	-1.14
62	INDO_MGUANd	0.03	-20.92	-21.83	0.91	-19.78	-1.14
63	INDO_MGUANd	0.04	-20.97	-21.59	0.62	-19.54	-1.43
64	INDO_MGUANd	0.04	-20.98	-21.60	0.62	-19.54	-1.44
65	INDO_MGUANe	0.04	-15.45	-19.25	3.80	-17.43	1.98
66	MIND_MGUANc	0.04	-21.60	-22.72	1.12	-20.61	-0.99
67	MIND_MGUANd	0.04	-21.57	-22.71	1.14	-20.61	-0.96
68	MIND_MGUANd	0.04	-21.57	-22.54	0.97	-20.42	-1.15
69	MIND_MGUANd	0.04	-21.58	-22.54	0.96	-20.43	-1.15
70	MIND_MGUANe	0.04	-22.58	-22.92	0.34	-20.89	-1.69
71	IMID_MGUANc	0.01	-22.92	-27.53	4.61	-27.37	4.45
72	IMID_MGUANc	0.01	-21.27	-25.01	3.74	-24.77	3.50
73	IMID_MGUANd	0.02	-22.88	-26.86	3.98	-26.57	3.69
74	IMID_MGUANd	0.02	-22.88	-26.22	3.34	-25.67	2.79
75	IMID_MGUANd	0.01	-22.92	-27.52	4.60	-27.38	4.46
76	IMID_MGUANd	0.01	-22.91	-27.50	4.59	-27.36	4.45
77	IMID_MGUANd	0.01	-22.92	-27.45	4.53	-27.32	4.40
78	IMID_MGUANe	0.01	-22.92	-27.51	4.59	-27.38	4.46
79	4MIE_MGUANc	0.17	-31.31	-28.44	-2.87	-28.36	-2.95
80	4MIE_MGUANd	0.24	-20.91	-16.77	-4.14	-17.71	-3.20
81	4MIE_MGUANd	0.18	-31.34	-28.53	-2.81	-28.43	-2.91
82	4MIE_MGUANd	0.07	-31.27	-27.85	-3.42	-27.57	-3.70
83	4MIE_MGUANd	0.18	-31.34	-28.53	-2.81	-28.43	-2.91
84	4MIE_MGUANe	0.18	-31.33	-27.67	-3.66	-27.44	-3.89
85	4MIM_MGUANc	0.02	-26.25	-29.26	3.01	-29.21	2.96
86	4MIM_MGUANd	0.02	-24.21	-27.03	2.82	-26.63	2.42
87	4MIM_MGUANd	0.33	-26.23	-28.80	2.57	-28.60	2.37
88	4MIM_MGUANd	0.02	-26.25	-29.28	3.03	-29.22	2.97
89	4MIM_MGUANd	0.02	-26.25	-29.28	3.03	-29.22	2.97
90	4MIM_MGUANd	0.02	-26.25	-29.27	3.02	-29.21	2.96
91	4MIM_MGUANe	0.02	-26.25	-29.26	3.01	-29.21	2.96
92	BENZ_IMIMf	0.01	-15.32	-15.60	0.28	-13.55	-1.77
93	BENZ_IMIMg	0.02	-14.72	-15.79	1.07	-13.69	-1.03
94	BENZ_IMIMh	0.02	-14.71	-15.79	1.08	-13.69	-1.02
95	TOLU_IMIMf	0.04	-14.00	-17.10	3.10	-14.94	0.94

96	TOLU_IMIMg	0.04	-14.05	-17.09	3.04	-14.97	0.92
97	TOLU_IMIMg	0.03	-14.00	-17.11	3.11	-14.98	0.98
98	TOLU_IMIMg	0.04	-14.02	-17.17	3.15	-15.01	0.99
99	TOLU_IMIMh	0.04	-14.04	-17.10	3.06	-14.98	0.94
100	PHEN_IMIMf	0.02	-16.46	-17.70	1.24	-15.65	-0.81
101	PHEN_IMIMg	0.02	-17.24	-18.32	1.08	-16.41	-0.83
102	PHEN_IMIMg	0.02	-16.46	-17.70	1.24	-15.64	-0.82
103	PHEN_IMIMg	0.02	-17.23	-18.32	1.09	-16.42	-0.81
104	PHEN_IMIMg	0.02	-17.24	-18.33	1.09	-16.41	-0.83
105	PHEN_IMIMg	0.02	-17.24	-18.32	1.08	-16.42	-0.82
106	PHEN_IMIMh	0.02	-16.70	-19.37	2.67	-17.93	1.23
107	CRES_IMIMf	0.04	-14.70	-18.82	4.12	-16.75	2.05
108	CRES_IMIMg	0.03	-14.61	-18.57	3.96	-16.85	2.24
109	CRES_IMIMg	0.04	-14.68	-18.88	4.20	-16.82	2.14
110	CRES_IMIMg	0.04	-15.99	-19.68	3.69	-17.78	1.79
111	CRES_IMIMg	0.04	-16.01	-19.69	3.68	-17.79	1.78
112	CRES_IMIMg	0.04	-15.97	-19.36	3.39	-17.44	1.47
113	CRES_IMIMh	0.02	-14.67	-18.70	4.03	-16.64	1.97
114	INDO_IMIMf	0.05	-21.54	-22.98	1.44	-20.53	-1.01
115	INDO_IMIMg	0.07	-19.06	-20.27	1.21	-18.11	-0.95
116	INDO_IMIMg	0.03	-21.54	-22.98	1.44	-20.53	-1.01
117	INDO_IMIMg	0.03	-21.55	-22.98	1.43	-20.53	-1.02
118	INDO_IMIMh	0.04	-20.98	-20.12	-0.86	-17.84	-3.14
119	MIND_IMIMf	0.05	-22.35	-23.94	1.59	-21.46	-0.89
120	MIND_IMIMg	0.05	-20.01	-23.32	3.31	-20.66	0.65
121	MIND_IMIMg	0.04	-20.02	-23.32	3.30	-20.66	0.64
122	MIND_IMIMg	0.05	-22.35	-23.94	1.59	-21.47	-0.88
123	MIND_IMIMg	0.05	-20.00	-23.32	3.32	-20.66	0.66
124	MIND_IMIMh	0.04	-21.39	-21.02	-0.37	-18.63	-2.76
125	IMID_IMIMf	0.01	-21.80	-25.16	3.36	-24.40	2.60
126	IMID_IMIMh	0.02	-13.57	-15.67	2.10	-15.85	2.28
127	4MIE_IMIMh	0.15	-18.49	-15.95	-2.54	-16.44	-2.05
128	4MIM_IMIMh	0.18	-25.32	-24.97	-0.35	-23.65	-1.67
AVG					1.89		0.55
SE					0.22		0.23
AUE					2.61		2.18
RMS					3.12		2.70
#	Ar_Mol-	Dist Diff	MM	QM MP2	Diff. MM-MP2	QM SAPT2+	Diff. MM-SAPT2+
1	BENZ_ACETi	0.02	-7.76	-7.81	1.34	-7.02	-0.74
2	BENZ_ACETj	0.01	-6.60	-7.94	1.34	-8.89	2.29
3	TOLU_ACETi	0.02	-11.22	-10.55	-0.67	-12.05	0.83
4	TOLU_ACETj	0.02	-10.04	-10.35	0.31	-11.90	1.86
5	PHEN_ACETi	0.02	-10.49	-10.42	-0.07	-12.21	1.72
6	PHEN_ACETj	0.02	-9.74	-10.95	1.21	-12.54	2.80
7	CRES_ACETi	0.02	-10.27	-11.41	1.14	-12.95	2.68
8	CRES_ACETj	0.04	-24.80	-31.64	6.84	-33.04	8.24
9	INDO_ACETi	0.04	-33.42	-31.97	-1.45	-33.36	-0.06
10	INDO_ACETj	0.05	-33.22	-31.50	-1.72	-32.89	-0.33
11	INDO_ACETj	0.05	-33.21	-31.46	-1.75	-32.86	-0.35
12	INDO_ACETj	0.03	-33.37	-32.01	-1.36	-33.41	0.04
13	MIND_ACETi	0.04	-29.73	-31.36	1.63	-32.77	3.04
14	MIND_ACETj	0.11	-29.78	-30.79	1.01	-27.80	-1.98
15	MIND_ACETj	0.06	-29.93	-30.87	0.94	-32.18	2.25
16	IMID_ACETi	0.02	-27.90	-32.97	5.07	-34.21	6.31
17	IMID_ACETj	0.02	-27.90	-32.96	5.06	-34.22	6.32

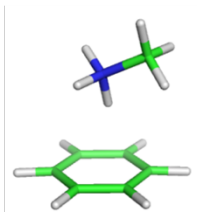
18	IMID_ACETj	0.02	-27.89	-32.96	5.07	-34.24	6.35
19	IMID_ACETj	0.02	-28.00	-32.49	4.49	-33.63	5.63
20	IMID_ACETj	0.02	-28.00	-32.73	4.73	-33.72	5.72
21	IMID_ACETj	0.02	-27.94	-32.32	4.38	-33.48	5.54
22	4MIE_ACETi	0.07	-36.01	-31.68	-4.33	-32.76	-3.25
23	4MIE_ACETj	0.19	-36.05	-31.75	-4.30	-33.30	-2.75
24	4MIE_ACETj	0.06	-36.01	-31.66	-4.35	-32.76	-3.25
25	4MIE_ACETj	0.10	-36.04	-31.77	-4.27	-33.11	-2.93
26	4MIM_ACETi	0.03	-30.85	-31.92	1.07	-33.15	2.30
27	4MIM_ACETj	0.23	-11.86	-10.49	-1.37	-12.02	0.16
28	4MIM_ACETj	0.03	-30.85	-31.92	1.07	-33.15	2.30
29	4MIM_ACETj	0.18	-30.79	-32.74	1.95	-34.07	3.28
AVG					0.79		1.86
SE					0.55		0.57
AUE					2.56		2.94
RMS					3.16		3.66

Table S5. Cation- π and Anion-ring pairs measured in all the protein systems and shown in Figures S1-S8, and their residue identifiers (Id) used in simulations. The residue Ids assigned in the PDB structures are indicated in the parenthesis; otherwise they are same in the simulations.

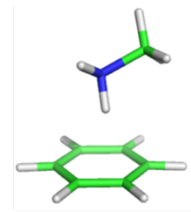
PDB	#	Residue1	Id1	Residue2	Id2	Figure	Interaction Type
2IGD	1	LYS	31 (36)	TRP	43 (48)	S1b	Cation- π
	2	ASP	47 (52)	TYR	45 (50)	S1c	Anion-ring
2QMT	1	LYS	31	TRP	43	S2b	Cation- π
	2	ASP	47	TYR	45	S2c	Anion-ring
1BFG	1	ARG	26 (44)	PHE	12 (30)	S3b	Cation- π
	2	ARG	91 (109)	PHE	75 (93)	S3c	Cation- π
	3	ARG	89 (107)	TYR	97 (115)	S3d	Cation- π
	4	LYS	8 (26)	TYR	85 (103)	S3e	Cation- π
	5	ARG	4 (22)	PHE	13 (31)	S3f	Cation- π
	6	ARG	15 (32)	HIS	17 (35)	S3g	Cation- π
	7	GLU	40 (58)	PHE	75 (93)	S3h	Anion-ring
	8	ASP	23 (41)	HIS	17 (35)	S3j	Anion-ring
1F4I	1	LYS	28	PHE	24	S4b	Cation- π
	2	GLU	2	TYR	23	S4c	Anion-ring
6LYT	1	ARG	114	PHE	34	S5b	Cation- π
	2	ARG	61	TRP	62	S5c	Cation- π
	3	LYS	1	PHE	3	S5d	Cation- π
	4	LYS	96	TYR	20	S5e	Cation- π
	5	LYS	116	TRP	111	S5f	Cation- π
	6	ARG	14	HIS	15	S5g	Cation- π
	7	ASP	66	TYR	53	S5h	Anion-ring
	8	GLU	7	PHE	3	S5i	Anion-ring
4IEJ	1	ARG	45 (177)	PHE	35 (167)	S6b	Cation- π
	2	ARG	54 (186)	TRP	20 (152)	S6c	Cation- π
	3	ARG	62 (194)	TRP	20 (152)	S6d	Cation- π
	4	LYS	22 (154)	TYR	11 (143)	S6e	Cation- π
	5	ASP	26 (158)	TYR	6 (138)	S6f	Anion-ring
	6	GLU	24 (156)	TYR	46 (178)	S6g	Anion-ring
	7	ASP	47 (179)	PHE	51 (183)	S6h	Anion-ring
	8	ASP	47 (179)	HIS	27 (159)	S6i	Anion-ring
	9	GLU	24 (156)	PHE	51 (183)	S6j	Anion-ring
	10	GLU	24 (156)	TRP	20 (152)	S6k	Anion-ring
135L	1	LYS	33	PHE	34	S7b	Cation- π
	2	LYS	1	TYR	3	S7c	Cation- π
	3	LYS	116	TRP	111	S7d	Cation- π
	4	GLU	7	TYR	3	S7e	Anion-ring
	5	ASP	66	TYR	53	S7f	Anion-ring
2EVQ	1	LYS	1	TRP	10	2	Cation- π

Figure S1. Structures of the fully optimized interactions methylammonium in **a-e** or acetate in **f-i** with benzene and phenol with the optimized Drude 2013-FF-CP force field. The assigned number for the geometries correspond to the numbers labeled in Table S4.

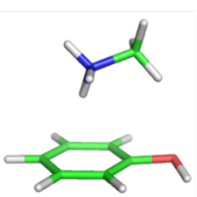
a) No. 1



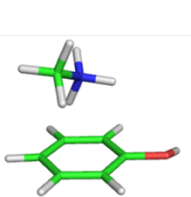
b) No. 2



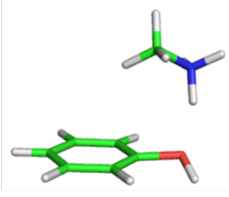
c) No. 7



d) No. 8



e) No. 9



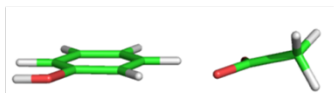
f) No. 1



g) No. 2



h) No. 5



i) No. 6

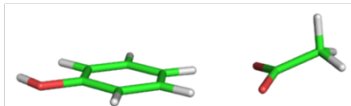


Figure S2. Analysis of cation- π interaction distances for protein GB3 domain (PDB:2IGD) based on the original Drude model (Drude-2013) and Drude-2013 model with NBFIX parameters (Drude-2013-CP). **a)** Structure of the protein and the analyzed cation- and Anion-ring pairs (Table S5), where oxygen is in red, nitrogen in blue, and carbon in white. **b)** Comparison of the normalized distributions of the distances between the aromatic ring center (cyan point) and the cation computed from simulations using the Drude-2013 (black) and Drude-2013-CP (red) FFs with respect to that in the crystal structure (Exp, blue).

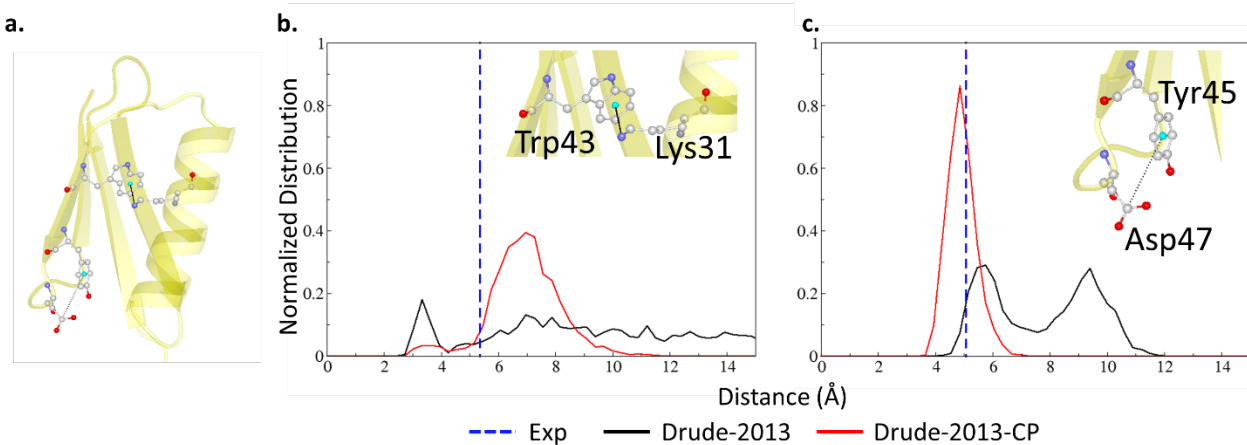


Figure S3. Analysis of cation- π interaction distances for protein GB1 domain (PDB:2QMT) based on the original Drude model (Drude-2013) and Drude-2013 model with NBFIX parameters (Drude-2013-CP). **a)** Structure of the protein and the analyzed cation- and Anion-ring pair (Table S5), where oxygen is in red, nitrogen in blue, and carbon in white. **b-c)** Comparison of the normalized distributions of the distances between the aromatic ring center (cyan point) and the cation computed from simulations using the Drude-2013 (black) and Drude-2013-CP (red) FFs with respect to that in the crystal structure (Exp, blue).

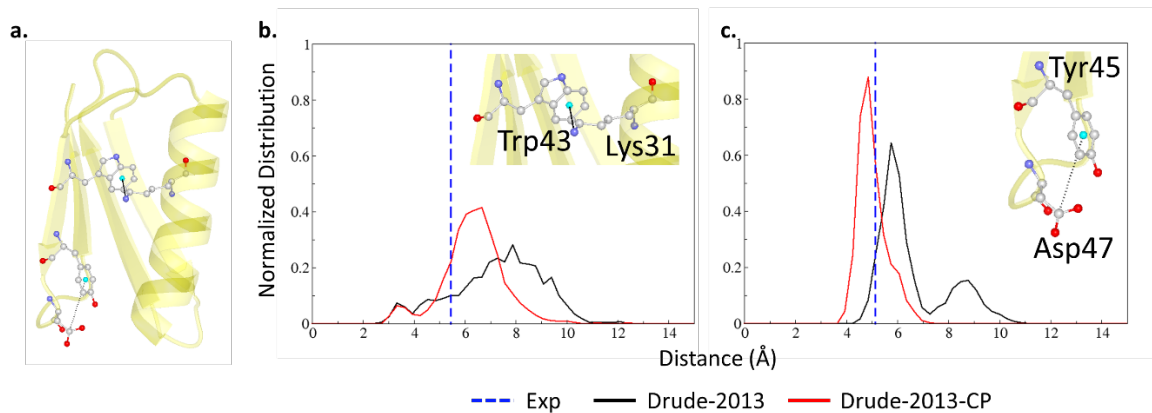


Figure S4. Analysis of cation- π interaction distances for basic fibroblast growth factor (PDB:1BFG) based on the original Drude model (Drude-2013) and Drude-2013 model with NBFIX parameters (Drude-2013-CP). **a)** Structure of the protein and the analyzed cation- and Anion-ring pairs (Table S5), where oxygen is in red, nitrogen in blue, and carbon in white. **b-i)** Comparison of the normalized distributions of the distances between the aromatic ring center (cyan point) and the cation computed from simulations using the Drude-2013 (black) and Drude- with respect to that in the crystal structure (Exp, blue).

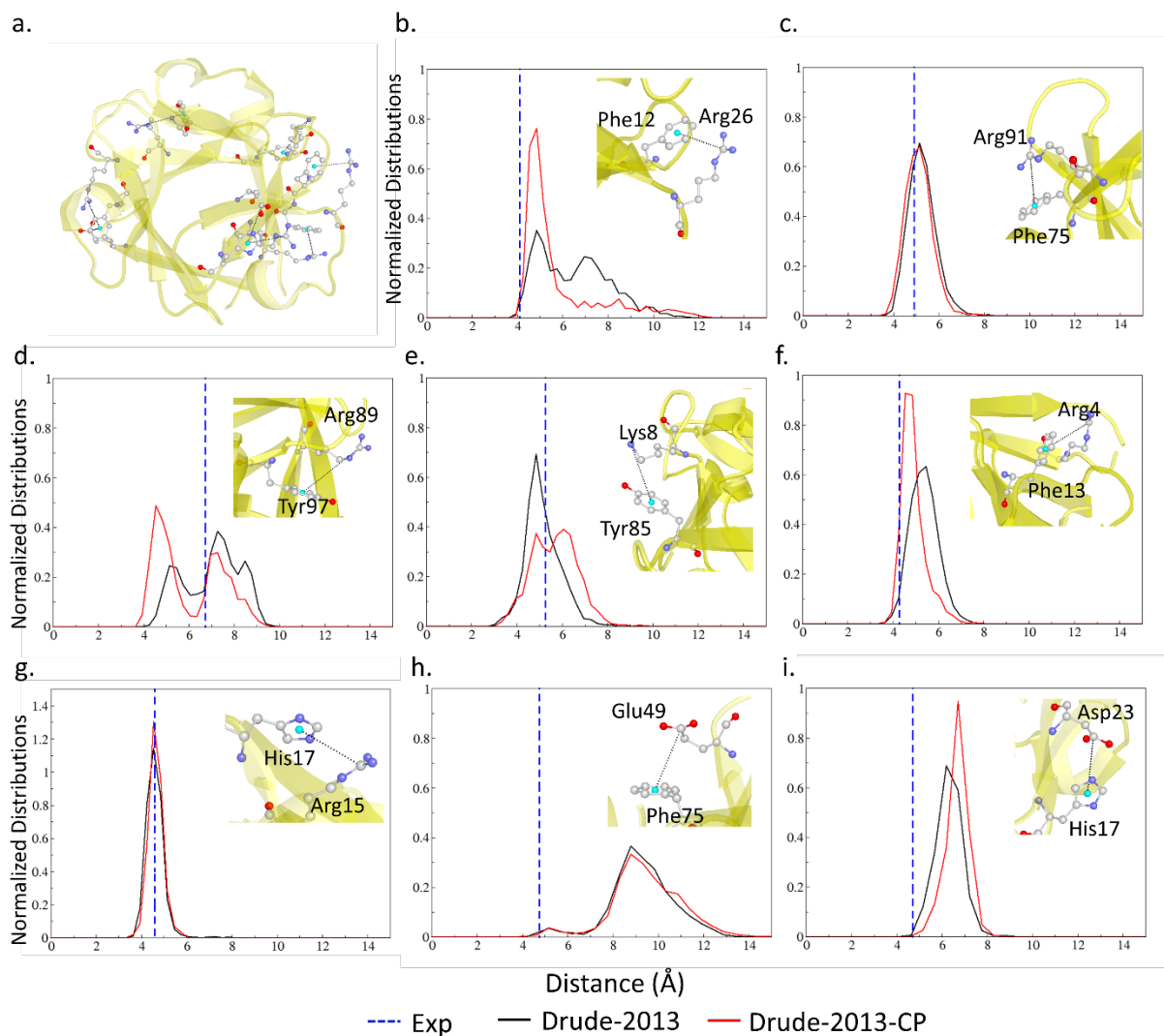


Figure S5. Analysis of cation- and Anion-ring interaction distances for DNA repair protein (PDB:1F4I) based on the original Drude model (Drude-2013) and Drude-2013 model with NBFIX parameters (Drude-2013-CP). **a)** Structure of the protein and the analyzed cation- and Anion-ring pairs (Table S5), where oxygen is in red, nitrogen in blue, and carbon in white. **b-c)** Comparison of the normalized distributions of the distances between the aromatic ring center (cyan point) and the cation computed from simulations using the Drude-2013 (black) and Drude-2013-CP (red) FFs with respect to that in the NMR structure (Exp, blue).

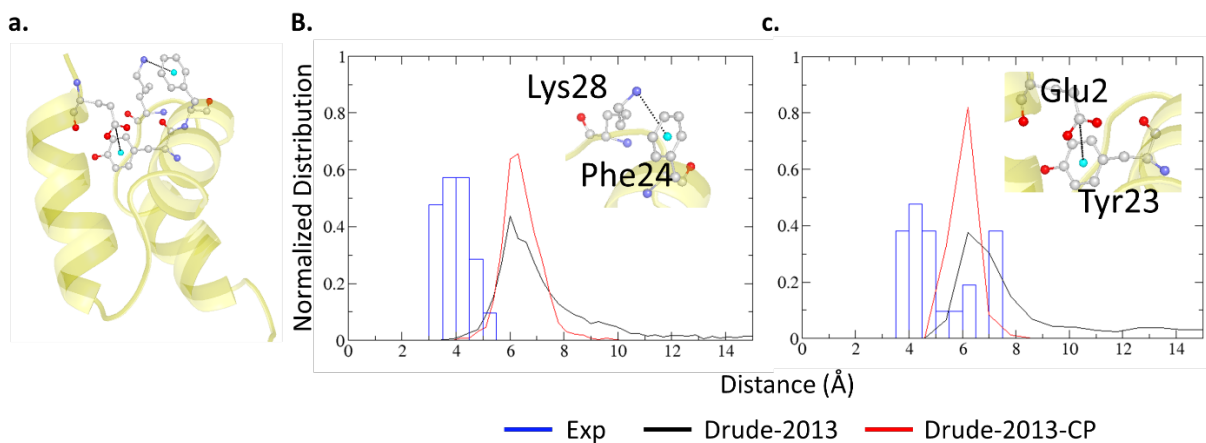


Figure S6. Analysis of cation- and Anion-ring interaction distances for the hen egg white lysozyme (PDB:6LYT) based on the original Drude model (Drude-2013) and Drude-2013 model with NBFIX parameters (Drude-2013-CP). **a)** Structure of the protein and the analyzed cation- and Anion-ring pairs (Table S5), where oxygen is in red, nitrogen in blue, and carbon in white. **b-i)** Comparison of the normalized distributions of the distances between the aromatic ring center (cyan point) and the cation computed from simulations using the Drude-2013 (black) and Drude-2013-CP (red) FFs with respect to that in the crystal structure (Exp, blue).

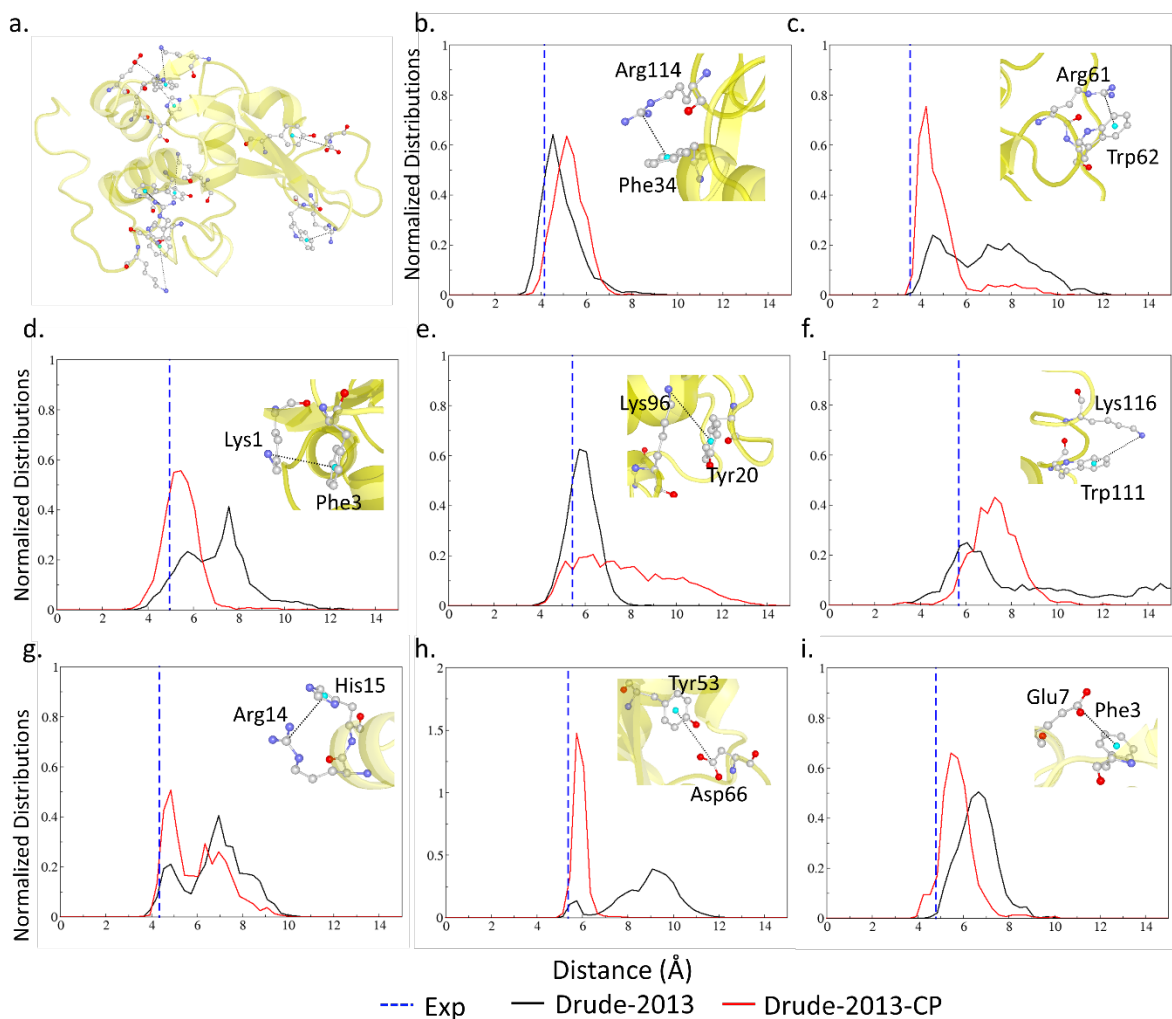


Figure S7. Analysis of cation- and Anion-ring interaction distances for DNA methyltransferase associated protein (PDB:4IEJ) based on the original Drude model (Drude-2013) and Drude-2013 model with NBFIX parameters (Drude-2013-CP). **a)** Structure of the protein and the analyzed cation- and Anion-ring pairs (Table S5), where oxygen is in red, nitrogen in blue, and carbon in white. **b-k)** Comparison of the normalized distributions of the distances between the aromatic ring center (cyan point) and the cation computed from simulations using the Drude-2013 (black) and Drude-2013-CP (red) FFs with respect to that in the crystal structure (Exp, blue).

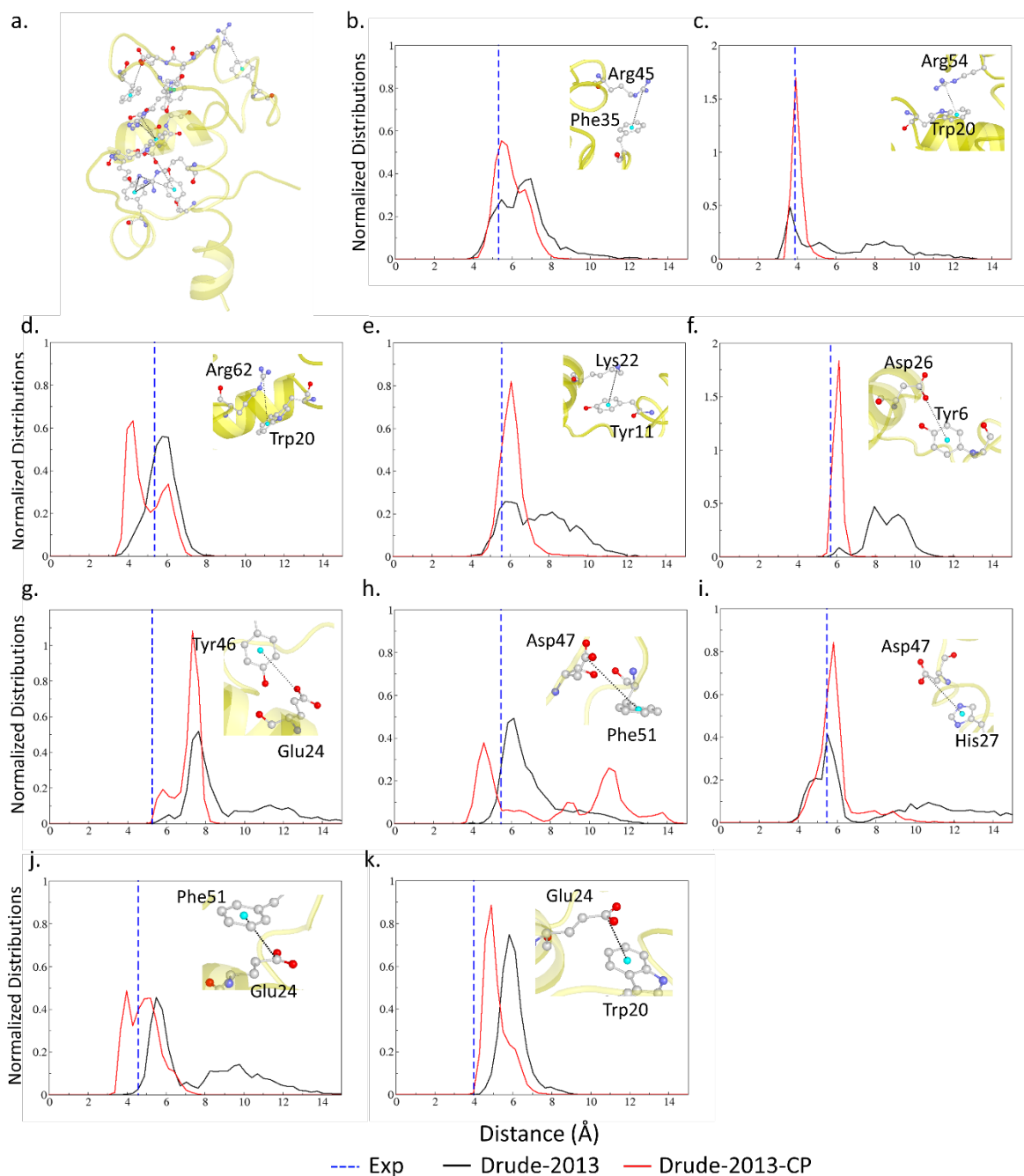


Figure S8. Analysis of cation- and Anion-ring interaction distances for turkey egg lysozyme (PDB: 135L) based on the original Drude model (Drude-2013) and Drude-2013 model with NBFIX parameters (Drude-2013-CP). **a)** Structure of the protein and the analyzed cation- and Anion-ring pairs (Table S5), where oxygen is in red, nitrogen in blue, and carbon in white. **b-f)** Comparison of the normalized distributions of the distances between the aromatic ring center (cyan point) and the cation computed from simulations using the Drude-2013 (black) and Drude-2013-CP (red) FFs with respect to that in the crystal structure (Exp, blue).

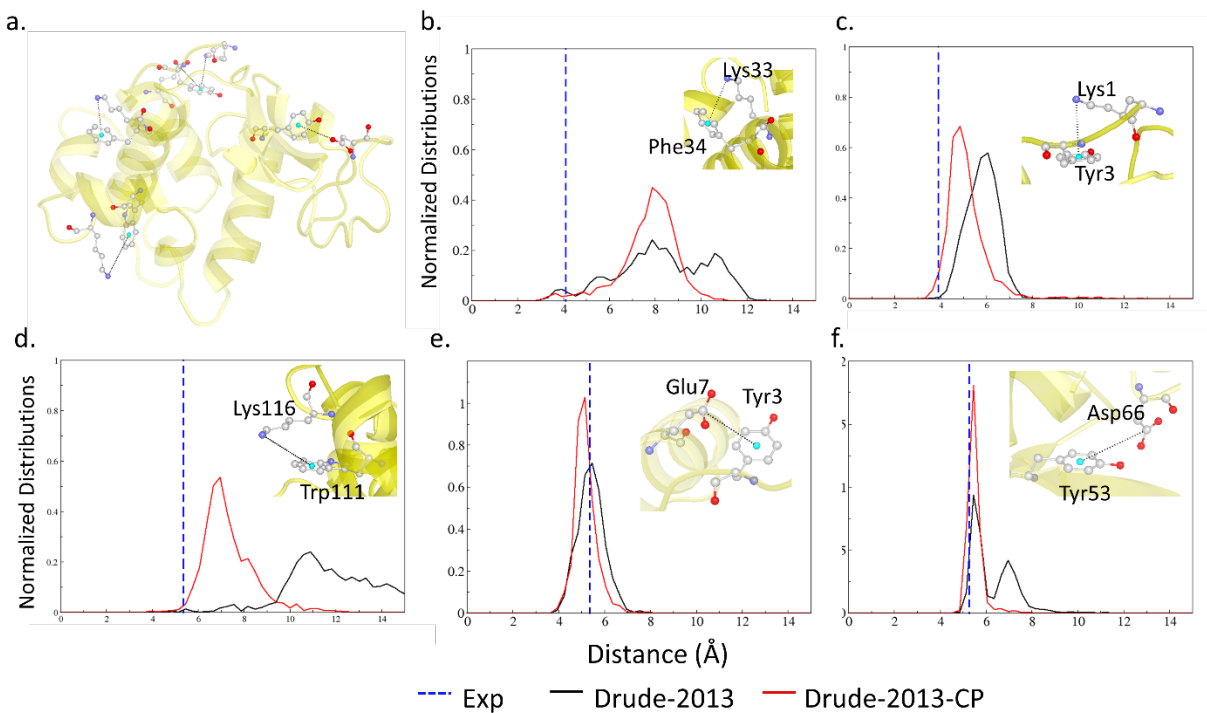


Figure S9. Comparison of the side-chain non-hydrogen atom root-mean-square fluctuations (RMSF), between Drude-2013 (black) and Drude-2013-CP (red) FFs with respect to the experimental RMSF values (Exp) from crystal structures (blue). The Exp RMSF values were computed based on the B-factors (B), where $B = [(8\pi^2)/3] \times (\text{RMSF})^2$, and data collected temperatures are indicated as T_{exp} . The NMR structures from PDB:1F4I and 2EVQ do not have B-factors, thus the Exp RMSF values are not shown. The dots correspond to the RMSF of the cation- and Anion-ring pairs labeled in Table S5.

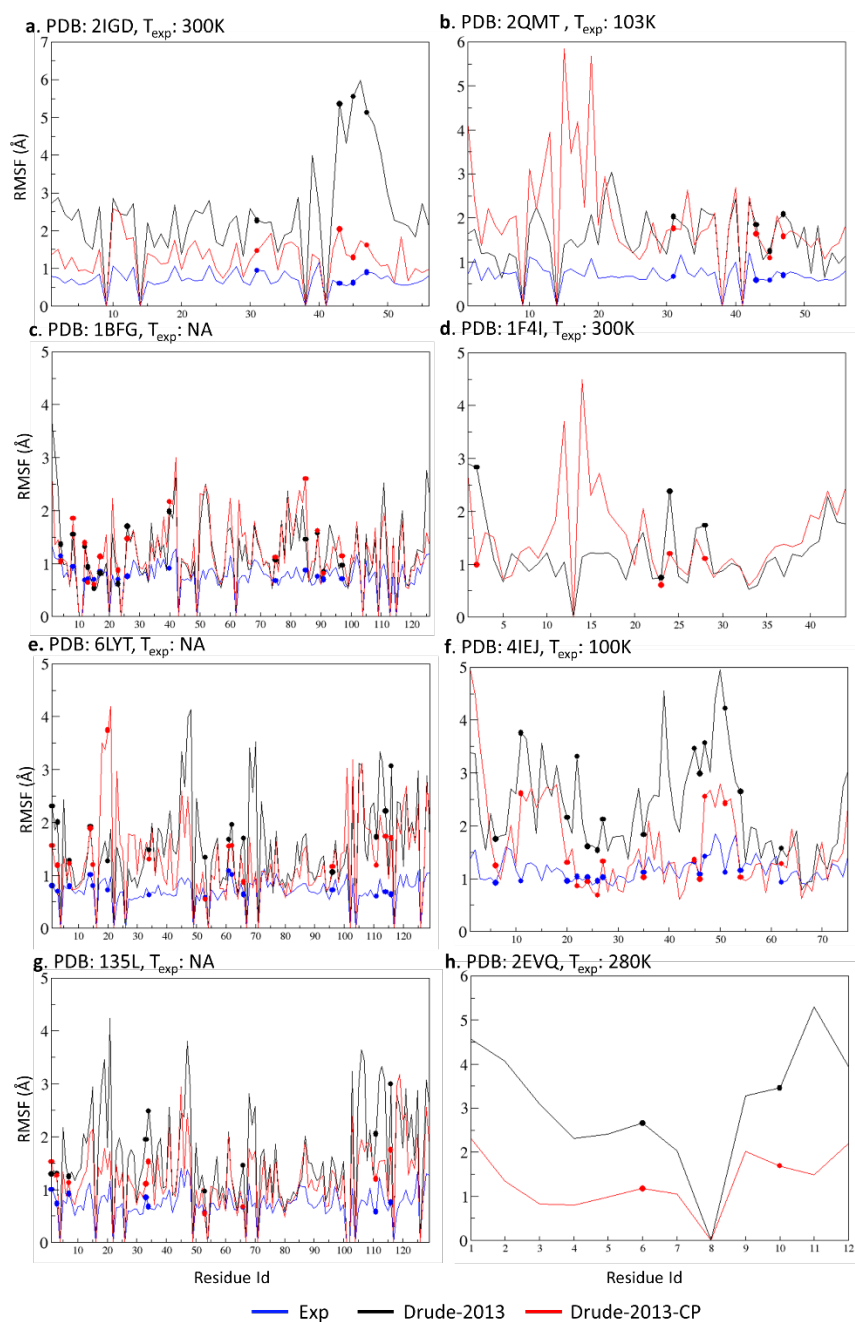


Table S6. Parameters involved in the optimized Drude-2013-CP FF for proteins. The full Drude-2013-CP FF for proteins will be available in MacKerell lab website:

http://mackerell.umaryland.edu/charmm_drude_ff.shtml

```
MASS  -1 LPA1      0.00000 H ! lone pair on aromatic benz/tolu, for improving cation-pi interaction
MASS  -1 LPA2      0.00000 H ! lone pair on aromatic phen/cres, for improving cation-pi interaction
MASS  -1 LPA3      0.00000 H ! lone pair on aromatic mind/cres, for improving cation-pi interaction
MASS  -1 LP5N      0.00000 H ! lone pair on histidine
```

```
RESI PHE          0.000 ! phenylalanine
```

```
!
!      |          HD1 HE1
! HN-N  |          |
!      |  HB1  CD1--CE1
!      |  |  //      \
! HA-CA--CB--CG LP  CZ--HZ
!      |  |  \  _  /
!      |  HB2 CD2--CE2
!      |  |  |  |
!      |  |  HD2 HE2
!
```

```
GROUP
```

```
ATOM N   ND2A2  -0.382  ALPHA -1.942  THOLE 0.250
ATOM HN  HDP1A   0.272
ATOM CA  CD31C   0.169  ALPHA -0.960  THOLE 1.078
ATOM HA  HDA1A  -0.017
ATOM C   CD2O1A  0.497  ALPHA -0.675  THOLE 0.295
ATOM O   OD2C1A  0.000  ALPHA -0.651  THOLE 0.310
ATOM LPOA LPD01 -0.312
ATOM LPOB LPD01 -0.227
```

```
GROUP
```

```
ATOM CB  CD32A  -0.150  ALPHA -1.608  THOLE 0.438
ATOM HB1 HDA2A   0.079
ATOM HB2 HDA2A   0.079
ATOM CG  CD2R6A  0.037  ALPHA -1.550  THOLE 1.262
ATOM CD1 CD2R6A -0.087  ALPHA -1.604  THOLE 1.262
ATOM HD1 HDR6A   0.099
ATOM CD2 CD2R6A -0.087  ALPHA -1.604  THOLE 1.262
ATOM HD2 HDR6A   0.099
ATOM CE1 CD2R6A -0.114  ALPHA -1.606  THOLE 1.262
ATOM HE1 HDR6A   0.096
ATOM CE2 CD2R6A -0.114  ALPHA -1.606  THOLE 1.262
ATOM HE2 HDR6A   0.096
ATOM CZ  CD2R6A -0.133  ALPHA -1.610  THOLE 1.262
ATOM HZ  HDR6A   0.100
ATOM LP  LPA1    0.000  ! pi fylin
```

```
BOND N   CA      CA  C      C  +N      CA  HA
BOND N   HN      C   O
BOND CA  CB      CB  HB1     CB  HB2
BOND CB  CG      CG  CD1     CD1 CE1     CE1  CZ
BOND CG  CD2     CD2 CE2     CE2  CZ
BOND CD1 HD1     CD2 HD2     CE1 HE1
BOND CE2 HE2     CZ   HZ
BOND O   LPOA    O    LPOB
```

```
IMPR C   CA  +N  O   N  -C  CA  HN
CMAP -C   N   CA  C   N  CA  C  +N
```

```
LONEPAIR bisector LP CG CD1 CD2 distance 1.419 angle 0.0 dihe 0.0 ! fylin
LONEPAIR relative LPOA O C CA distance 0.30 angle 91.0 dihe 0.0
```

LONEPAIR relative LPOB O C CA distance 0.30 angle 91.0 dihe 180.0
 ANISOTROPY O C LPOA LPOB A11 0.82322 A22 1.14332

DONOR HN N

ACCEPTOR O C

!C22 IC Table

IC -C	CA	*N	HN	1.3476	123.8900	180.0000	114.4700	0.9987
IC -C	N	CA	C	1.3476	123.8900	180.0000	106.3800	1.5229
IC N	CA	C	+N	1.4504	106.3800	180.0000	117.6500	1.3483
IC +N	CA	*C	O	1.3483	117.6500	180.0000	120.4900	1.2287
IC CA	C	+N	+CA	1.5229	117.6500	180.0000	124.1000	1.4523
IC N	C	*CA	CB	1.4504	106.3800	122.4900	112.4500	1.5594
IC N	C	*CA	HA	1.4504	106.3800	-115.6300	107.0500	1.0832
IC N	CA	CB	CG	1.4504	111.6300	180.0000	112.7600	1.5109
IC CG	CA	*CB	HB1	1.5109	112.7600	118.2700	109.1000	1.1119
IC CG	CA	*CB	HB2	1.5109	112.7600	-123.8300	111.1100	1.1113
IC CA	CB	CG	CD1	1.5594	112.7600	90.0000	120.3200	1.4059
IC CD1	CB	*CG	CD2	1.4059	120.3200	-177.9600	120.7600	1.4062
IC CB	CG	CD1	CE1	1.5109	120.3200	-177.3700	120.6300	1.4006
IC CE1	CG	*CD1	HD1	1.4006	120.6300	179.7000	119.6500	1.0814
IC CB	CG	CD2	CE2	1.5109	120.7600	177.2000	120.6200	1.4002
IC CE2	CG	*CD2	HD2	1.4002	120.6200	-178.6900	119.9900	1.0811
IC CG	CD1	CE1	CZ	1.4059	120.6300	-0.1200	119.9300	1.4004
IC CZ	CD1	*CE1	HE1	1.4004	119.9300	-179.6900	120.0100	1.0808
IC CZ	CD2	*CE2	HE2	1.4000	119.9600	-179.9300	119.8700	1.0811
IC CE1	CE2	*CZ	HZ	1.4004	119.9800	179.5100	119.9700	1.0807

RESI TYR 0.000 ! tyrosine

!

```

!      |      HD1 HE1
! HN-N |      |      |
!      | HB1  CD1--CE1
!      | | //  \ \
! HA-CA--CB--CG LP CZ--OH
!      | | \  _ /  \
!      | HB2 CD2--CE2   HH
! O=C   |      |
!      |      HD2 HE2
!
```

GROUP

ATOM N	ND2A2	-0.382	ALPHA	-1.942	THOLE	0.250
ATOM HN	HDP1A	0.272				
ATOM CA	CD31C	0.169	ALPHA	-0.960	THOLE	1.078
ATOM HA	HDA1A	-0.017				
ATOM C	CD201A	0.497	ALPHA	-0.675	THOLE	0.295
ATOM O	OD2C1A	0.000	ALPHA	-0.651	THOLE	0.310
ATOM LPOA	LPD01	-0.312				
ATOM LPOB	LPD01	-0.227				

GROUP

ATOM CB	CD32A	-0.192	ALPHA	-1.802	THOLE	0.148
ATOM HB1	HDA2A	0.075				
ATOM HB2	HDA2A	0.075				
ATOM CG	CD2R6A	0.086	ALPHA	-1.418	THOLE	1.270
ATOM CD1	CD2R6A	-0.202	ALPHA	-1.427	THOLE	1.270
ATOM HD1	HDR6A	0.118				
ATOM CD2	CD2R6A	-0.202	ALPHA	-1.427	THOLE	1.270
ATOM HD2	HDR6A	0.118				
ATOM CE1	CD2R6A	-0.136	ALPHA	-1.444	THOLE	1.270
ATOM HE1	HDR6A	0.123				
ATOM CE2	CD2R6A	-0.136	ALPHA	-1.444	THOLE	1.270
ATOM HE2	HDR6A	0.123				
ATOM CZ	CD2R6A	0.297	ALPHA	-1.174	THOLE	1.270


```

!      |      HD1   NE1   CZ2
!      |      |      |
!      |      HE1   HZ2
!

```

GROUP

```

ATOM N   ND2A2  -0.382  ALPHA -1.942  THOLE 0.250
ATOM HN  HDP1A   0.272
ATOM CA  CD31C   0.169  ALPHA -0.960  THOLE 1.078
ATOM HA  HDA1A  -0.017
ATOM C   CD201A  0.497  ALPHA -0.675  THOLE 0.295
ATOM O   OD2C1A  0.000  ALPHA -0.651  THOLE 0.310
ATOM LPOA LPD01  -0.312
ATOM LPOB LPD01  -0.227

```

GROUP

```

ATOM CB  CD32A  -0.046  ALPHA -2.044  THOLE 1.346 !adjusted to neutralize group
ATOM HB1 HDA2A   0.045
ATOM HB2 HDA2A   0.045
ATOM CG  CD2R5C -0.098  ALPHA -1.269  THOLE 1.346
ATOM CD1 CD2R5A  0.059  ALPHA -1.612  THOLE 1.265
ATOM HD1 HDR5A   0.083
ATOM NE1 ND2R5A -0.276  ALPHA -1.380  THOLE 1.146
ATOM HE1 HDP1A   0.294
ATOM CE2 CD2R6D  0.053  ALPHA -1.267  THOLE 1.009
ATOM CD2 CD2R6D -0.099  ALPHA -1.266  THOLE 1.344
ATOM CE3 CD2R6A -0.034  ALPHA -1.622  THOLE 1.300
ATOM HE3 HDR6A   0.094
ATOM CZ3 CD2R6A -0.154  ALPHA -1.617  THOLE 1.300
ATOM HZ3 HDR6A   0.087
ATOM CZ2 CD2R6A -0.115  ALPHA -1.611  THOLE 1.300
ATOM HZ2 HDR6A   0.110
ATOM CH2 CD2R6A -0.188  ALPHA -1.621  THOLE 1.300
ATOM HH2 HDR6A   0.140
ATOM LP  LPA3    0.000  ! pi fylin

```

```

BOND N   CA      CA  C      C  +N      CA  HA
BOND N   HN      C   0
BOND CA  CB      CB  HB1    CB  HB2
BOND CB  CG      CG  CD1    CD1  NE1    NE1  CE2
BOND CE2 CD2     CD2  CG     CD2  CE3    CE3  CZ3
BOND CZ3 CH2     CH2  CZ2    CZ2  CE2
BOND CD1 HD1     NE1  HE1    CE3  HE3    CZ3  HZ3
BOND CH2 HH2     CZ2  HZ2
BOND O   LPOA    0    LPOB

```

```

IMPR C   CA  +N  0   N  -C  CA  HN
CMAP -C  N   CA  C   N  CA  C  +N

```

```

LONEPAIR bisector LP CZ2 CE2 CH2 distance 1.410 angle 0.0 dihe 0.0 ! fylin
LONEPAIR relative LPOA O C CA distance 0.30 angle 91.0 dihe 0.0
LONEPAIR relative LPOB O C CA distance 0.30 angle 91.0 dihe 180.0
ANISOTROPY O C LPOA LPOB A11 0.82322 A22 1.14332

```

DONOR HN N

DONOR HE1 NE1

ACCEPTOR O C

!C22 IC Table

```

IC -C  CA  *N  HN  1.3482 123.5100 180.0000 115.0200 0.9972
IC -C  N   CA  C   1.3482 123.5100 180.0000 107.6900 1.5202
IC N   CA  C   +N  1.4507 107.6900 180.0000 117.5700 1.3505
IC +N  CA  *C  O   1.3505 117.5700 180.0000 121.0800 1.2304
IC CA  C   +N  +CA 1.5202 117.5700 180.0000 124.8800 1.4526
IC N   C   *CA  CB  1.4507 107.6900 122.6800 111.2300 1.5560

```

IC N	C	*CA	HA	1.4507	107.6900	-117.0200	106.9200	1.0835
IC N	CA	CB	CG	1.4507	111.6800	180.0000	115.1400	1.5233
IC CG	CA	*CB	HB1	1.5233	115.1400	119.1700	107.8400	1.1127
IC CG	CA	*CB	HB2	1.5233	115.1400	-124.7300	109.8700	1.1118
IC CA	CB	CG	CD2	1.5560	115.1400	90.0000	123.9500	1.4407
IC CD2	CB	*CG	CD1	1.4407	123.9500	-172.8100	129.1800	1.3679
IC CD1	CG	CD2	CE2	1.3679	106.5700	-0.0800	106.6500	1.4126
IC CG	CD2	CE2	NE1	1.4407	106.6500	0.1400	107.8700	1.3746
IC CE2	CG	*CD2	CE3	1.4126	106.6500	179.2100	132.5400	1.4011
IC CE2	CD2	CE3	CZ3	1.4126	120.8000	-0.2000	118.1600	1.4017
IC CD2	CE3	CZ3	CH2	1.4011	118.1600	0.1000	120.9700	1.4019
IC CE3	CZ3	CH2	CZ2	1.4017	120.9700	0.0100	120.8700	1.4030
IC CZ3	CD2	*CE3	HE3	1.4017	118.1600	-179.6200	121.8400	1.0815
IC CH2	CE3	*CZ3	HZ3	1.4019	120.9700	-179.8200	119.4500	1.0811
IC CZ2	CZ3	*CH2	HH2	1.4030	120.8700	-179.9200	119.5700	1.0811
IC CE2	CH2	*CZ2	HZ2	1.3939	118.4200	179.8700	120.0800	1.0790
IC CD1	CE2	*NE1	HE1	1.3752	108.8100	177.7800	124.6800	0.9767
IC CG	NE1	*CD1	HD1	1.3679	110.1000	178.1000	125.4300	1.0820

RESI HSD 0.000 ! neutral HIS, proton on ND1

```

!
!      |      HD1  HE1
! HN-N      |      /
!      |      HB1  ND1--CE1
!      |      |      /      ||
! HA-CA--CB--CG LP  ||
!      |      |      \\      ||
!      |      HB2  CD2--NE2
! O=C      |
!      |      HD2
!

```

GROUP

ATOM N	ND2A2	-0.382	ALPHA	-1.942	THOLE	0.250
ATOM HN	HDP1A	0.272				
ATOM CA	CD31C	0.169	ALPHA	-0.960	THOLE	1.078
ATOM HA	HDA1A	-0.017				
ATOM C	CD201A	0.497	ALPHA	-0.675	THOLE	0.295
ATOM O	OD2C1A	0.000	ALPHA	-0.651	THOLE	0.310
ATOM LPOA	LPDO1	-0.312				
ATOM LPOB	LPDO1	-0.227				

GROUP

ATOM CB	CD32A	0.017	ALPHA	-1.739	THOLE	0.399 !charge adjusted
ATOM HB1	HDA2A	0.078				
ATOM HB2	HDA2A	0.078				
ATOM ND1	ND2R5A	-0.040	ALPHA	-1.522	THOLE	1.114
ATOM HD1	HDP1A	0.256				
ATOM CG	CD2R5A	-0.252	ALPHA	-1.272	THOLE	1.190
ATOM CE1	CD2R5B	0.064	ALPHA	-1.493	THOLE	1.297
ATOM HE1	HDR5B	-0.018				
ATOM NE2	ND2R5B	0.000	ALPHA	-1.146	THOLE	0.816
ATOM LPE2	LPD	-0.365				
ATOM CD2	CD2R5A	0.141	ALPHA	-1.515	THOLE	1.190
ATOM HD2	HDR5A	0.041				
ATOM LPA	LP5N	0.000				

BOND N	CA	CA	C	C	+N	CA	HA
BOND N	HN	C	O				
BOND CA	CB	CB	HB1	CB	HB2		
BOND CB	CG	CG	ND1	ND1	CE1	CE1	NE2
BOND NE2	CD2	CD2	CG				
BOND ND1	HD1	CE1	HE1	CD2	HD2		
BOND O	LPOA	O	LPOB				

```

BOND NE2 LPE2
IMPR ND1 CG CE1 HD1 CD2 CG NE2 HD2 CE1 ND1 NE2 HE1
IMPR C CA +N O N -C CA HN
CMAP -C N CA C N CA C +N

```

```

LONEPAIR bisector LPA ND1 CG CE1 distance 1.173 angle 0.0 dihe 0.0 ! fylin
LONEPAIR relative LPOA O C CA distance 0.30 angle 91.0 dihe 0.0
LONEPAIR relative LPOB O C CA distance 0.30 angle 91.0 dihe 180.0
ANISOTROPY O C LPOA LPOB A11 0.82322 A22 1.14332

```

```

LONEPAIR bisector LPE2 NE2 CE1 CD2 distance 0.35 angle 179.99 dihe 179.99
ANISOTROPY NE2 LPE2 CE1 CD2 A11 0.808 A22 1.384

```

```

DONOR HN N
DONOR HD1 ND1
ACCEPTOR NE2
ACCEPTOR O C
!C22 IC table

```

IC -C	CA	*N	HN	1.3475	123.2700	180.0000	115.2100	0.9988
IC -C	N	CA	C	1.3475	123.2700	180.0000	107.7000	1.5166
IC N	CA	C	+N	1.4521	107.7000	180.0000	117.5700	1.3509
IC +N	CA	*C	O	1.3509	117.5700	180.0000	120.2400	1.2273
IC CA	C	+N	+CA	1.5166	117.5700	180.0000	123.7200	1.4545
IC N	C	*CA	CB	1.4521	107.7000	122.4600	109.9900	1.5519
IC N	C	*CA	HA	1.4521	107.7000	-117.4900	107.3700	1.0830
IC N	CA	CB	CG	1.4521	112.1200	180.0000	114.0500	1.5041
IC CG	CA	*CB	HB1	1.5041	114.0500	121.1700	109.0100	1.1118
IC CG	CA	*CB	HB2	1.5041	114.0500	-122.3600	109.5300	1.1121
IC CA	CB	CG	ND1	1.5519	114.0500	90.0000	124.1000	1.3783
IC ND1	CB	*CG	CD2	1.3783	124.1000	-171.2900	129.6000	1.3597
IC CB	CG	ND1	CE1	1.5041	124.1000	-173.2100	107.0300	1.3549
IC CB	CG	CD2	NE2	1.5041	129.6000	171.9900	110.0300	1.3817
IC NE2	ND1	*CE1	HE1	1.3166	111.6300	-179.6300	123.8900	1.0932
IC CE1	CG	*ND1	HD1	1.3549	107.0300	-174.6500	126.2600	1.0005
IC NE2	CG	*CD2	HD2	1.3817	110.0300	-177.8500	129.6300	1.0834

```

RESI HSE 0.000 ! neutral HIS, proton on NE2, see patch HS2 below

```

```

!
! | HE1
! HN-N /
! | HB1 ND1--CE1
! | | / ||
! HA-CA--CB--CG LP ||
! | | \\ ||
! | HB2 CD2--NE2
! O=C | \
! | HD2 HE2
!

```

```

GROUP
ATOM N ND2A2 -0.382 ALPHA -1.942 THOLE 0.250
ATOM HN HDP1A 0.272
ATOM CA CD31C 0.169 ALPHA -0.960 THOLE 1.078
ATOM HA HDA1A -0.017
ATOM C CD2O1A 0.497 ALPHA -0.675 THOLE 0.295
ATOM O OD2C1A 0.000 ALPHA -0.651 THOLE 0.310
ATOM LPOA LPD01 -0.312
ATOM LPOB LPD01 -0.227
GROUP
ATOM CB CD32A 0.017 ALPHA -1.739 THOLE 0.399 !charge adjusted
ATOM HB1 HDA2A 0.078
ATOM HB2 HDA2A 0.078
ATOM ND1 ND2R5B 0.000 ALPHA -1.146 THOLE 0.816

```

ATOM LPD1 LPD -0.365
 ATOM NE2 ND2R5A -0.040 ALPHA -1.522 THOLE 1.114
 ATOM HE2 HDP1A 0.256
 ATOM CG CD2R5A -0.252 ALPHA -1.272 THOLE 1.190
 ATOM CE1 CD2R5B 0.064 ALPHA -1.493 THOLE 1.297
 ATOM HE1 HDR5B -0.018
 ATOM CD2 CD2R5A 0.141 ALPHA -1.515 THOLE 1.190
 ATOM HD2 HDR5A 0.041
 ATOM LPA LP5N 0.000

BOND N CA CA C C +N CA HA
 BOND N HN C O
 BOND CA CB CB HB1 CB HB2
 BOND CB CG CG ND1 ND1 CE1 CE1 NE2
 BOND NE2 CD2 CD2 CG
 BOND NE2 HE2 CE1 HE1 CD2 HD2
 BOND O LPOA O LPOB
 BOND ND1 LPD1

IMPR NE2 CD2 CE1 HE2 CD2 CG NE2 HD2 CE1 ND1 NE2 HE1
 IMPR C CA +N O N -C CA HN
 CMAP -C N CA C N CA C +N

LONEPAIR bisector LPA ND1 CG CE1 distance 1.173 angle 0.0 dihe 0.0 ! fylin

LONEPAIR relative LPOA O C CA distance 0.30 angle 91.0 dihe 0.0
 LONEPAIR relative LPOB O C CA distance 0.30 angle 91.0 dihe 180.0
 ANISOTROPY O C LPOA LPOB A11 0.82322 A22 1.14332

LONEPAIR bisector LPD1 ND1 CE1 CG distance 0.35 angle 179.99 dihe 179.99
 ANISOTROPY ND1 LPD1 CE1 CG A11 0.808 A22 1.384

DONOR HN N
 DONOR HE2 NE2
 ACCEPTOR ND1
 ACCEPTOR O C

!C22 IC table

IC -C	CA	*N	HN	1.3472	124.1600	180.0000	114.3600	0.9991
IC -C	N	CA	C	1.3472	124.1600	180.0000	106.4300	1.5166
IC N	CA	C	+N	1.4532	106.4300	180.0000	116.9700	1.3446
IC +N	CA	*C	O	1.3446	116.9700	180.0000	120.6800	1.2290
IC CA	C	+N	+CA	1.5166	116.9700	180.0000	124.9500	1.4505
IC N	C	*CA	CB	1.4532	106.4300	123.5200	111.6700	1.5578
IC N	C	*CA	HA	1.4532	106.4300	-116.4900	107.0800	1.0833
IC N	CA	CB	CG	1.4532	112.8200	180.0000	116.9400	1.5109
IC CG	CA	*CB	HB1	1.5109	116.9400	119.8000	107.9100	1.1114
IC CG	CA	*CB	HB2	1.5109	116.9400	-124.0400	109.5000	1.1101
IC CA	CB	CG	ND1	1.5578	116.9400	90.0000	120.1700	1.3859
IC ND1	CB	*CG	CD2	1.3859	120.1700	-178.2600	129.7100	1.3596
IC CB	CG	ND1	CE1	1.5109	120.1700	-179.2000	105.2000	1.3170
IC CB	CG	CD2	NE2	1.5109	129.7100	178.6600	105.8000	1.3782
IC NE2	ND1	*CE1	HE1	1.3539	111.7600	179.6900	124.5800	1.0929
IC CE1	CD2	*NE2	HE2	1.3539	107.1500	-178.6900	125.8600	0.9996
IC NE2	CG	*CD2	HD2	1.3782	105.8000	-179.3500	129.8900	1.0809

! Nonbonded parameters

LPA1 0.0 -0.0000 0.0000 ! lone pair on aromatic benz/tolu, for improving cation-pi interaction
 LPA2 0.0 -0.0000 0.0000 ! lone pair on aromatic phen/cres, for improving cation-pi interaction
 LPA3 0.0 -0.0000 0.0000 ! lone pair on aromatic mind/cres, for improving cation-pi interaction
 LP5N 0.0 -0.0000 0.0000 ! lone pair on aromatic, for improving cation-pi interaction

!! NBFIX for Cation-Pi interactions, fylin April 9, 2019

! MAM1

! =====

! benz/tolu/cres/phen/indo/mind...mam1

! -----

CD2R6A	ND3P3A	-0.020	3.85
CD2R6D	ND3P3A	-0.090	3.85
LPA1	ND3P3A	-0.110	3.85
LPA2	ND3P3A	-0.100	3.85
LPA3	ND3P3A	-0.040	3.85

! With MGUAN

! =====

! benz/tolu/cres/phen/indo/mind...mguan

! -----

CD2R6A	ND2P1A	-0.300	3.90
CD2R6D	ND2P1A	-0.400	3.80
LPA1	CD2N1A	-0.050	3.80
LPA2	ND2P1A	-0.850	4.00
LPA3	CD2N1A	-0.850	3.85

! With IMIM, LPA3 is not necessary

! =====

! benz/tolu/cres/phen/indo/mind...imim

! -----

CD2R6A	ND2R5C	-0.520	3.80
CD2R6D	ND2R5C	-0.200	3.90
LPA1	ND2R5C	-0.180	4.00
LPA2	ND2R5C	-0.890	3.20

!!! With ACET

! =====

! benz/tolu/cres/phen/indo/mind...acet

! -----

CD2R6A	OD2C2A	-0.600	3.65
CD2R6D	OD2C2A	-0.600	3.65
LPA1	OD2C2A	-0.050	3.60
LPA2	OD2C2A	-0.580	4.10
LPA3	OD2C2A	-0.580	4.10

! =====

!! IMID/4MIM/4MIE

! =====

! imid/4mim/4mie...nc1

! -----

CD2R5A	ND3P3A	-0.010	3.60
CD2R5B	ND3P3A	-0.010	4.25
ND2R5A	ND3P3A	-0.100	3.80
ND2R5B	ND3P3A	-0.035	3.70
LP5N	ND3P3A	-0.200	3.80

! imid/4mim/4mie...mguan

! -----

CD2R5A	ND2P1A	-0.250	4.00
CD2R5B	ND2P1A	-0.350	3.90
ND2R5A	ND2P1A	-0.090	3.80
ND2R5B	ND2P1A	-0.045	4.04
LP5N	CD2N1A	-0.400	4.00

! imid/4mim/4mie...imim

```
! -----
CD2R5A    ND2R5C  -0.600  3.65
CD2R5B    ND2R5C  -0.100  4.05
ND2R5A    ND2R5C  -0.450  3.90
ND2R5B    ND2R5C  -0.130  3.95
LP5N      ND2R5C  -0.300  3.95
ND2R5B    CD2R5E  -0.300  3.95

! indo/mind/4mim/4mie ..acet
! -----
CD2R5B    OD2C2A  -0.080  3.85
ND2R5B    OD2C2A  -0.005  3.95
! -----
! shared among indo/mind/4mim/4mie/imid..acet
CD2R5A    OD2C2A  -0.080  3.85
ND2R5A    OD2C2A  -0.065  3.80
```

Table S7. Cartesian coordinates for the QM optimized interaction orientations with ID and residue names as indicated in Table S3 and S4.

REMARK	1_BENZ_MAM1									
ATOM	1	CG	BENZ	1	1.271	-1.171	0.320	1.00	0.00	BENZ
ATOM	2	HG	BENZ	1	1.547	-2.184	0.589	1.00	0.00	BENZ
ATOM	3	CD1	BENZ	1	1.362	-0.751	-1.014	1.00	0.00	BENZ
ATOM	4	HD1	BENZ	1	1.706	-1.440	-1.777	1.00	0.00	BENZ
ATOM	5	CD2	BENZ	1	0.873	-0.267	1.315	1.00	0.00	BENZ
ATOM	6	HD2	BENZ	1	0.842	-0.581	2.351	1.00	0.00	BENZ
ATOM	7	CE1	BENZ	1	1.053	0.573	-1.356	1.00	0.00	BENZ
ATOM	8	HE1	BENZ	1	1.157	0.908	-2.381	1.00	0.00	BENZ
ATOM	9	CE2	BENZ	1	0.563	1.058	0.975	1.00	0.00	BENZ
ATOM	10	HE2	BENZ	1	0.291	1.767	1.749	1.00	0.00	BENZ
ATOM	11	CZ	BENZ	1	0.652	1.479	-0.360	1.00	0.00	BENZ
ATOM	12	HZ	BENZ	1	0.449	2.511	-0.618	1.00	0.00	BENZ
ATOM	13	N	MAM1	1	-1.904	-0.553	-0.460	1.00	0.00	MAM1
ATOM	14	C1	MAM1	1	-2.863	-0.173	0.627	1.00	0.00	MAM1
ATOM	15	HN2	MAM1	1	-1.048	0.022	-0.421	1.00	0.00	MAM1
ATOM	16	HN3	MAM1	1	-2.317	-0.432	-1.386	1.00	0.00	MAM1
ATOM	17	HN4	MAM1	1	-1.605	-1.527	-0.377	1.00	0.00	MAM1
ATOM	18	H11	MAM1	1	-3.749	-0.794	0.545	1.00	0.00	MAM1
ATOM	19	H12	MAM1	1	-3.116	0.874	0.501	1.00	0.00	MAM1
ATOM	20	H13	MAM1	1	-2.367	-0.332	1.578	1.00	0.00	MAM1
END										
REMARK	2_BENZ_MAM1									
ATOM	1	CG	BENZ	1	0.683	-0.074	-1.661	1.00	0.00	BENZ
ATOM	2	HG	BENZ	1	0.531	-0.200	-2.726	1.00	0.00	BENZ
ATOM	3	CD1	BENZ	1	0.853	1.210	-1.122	1.00	0.00	BENZ
ATOM	4	HD1	BENZ	1	0.831	2.076	-1.772	1.00	0.00	BENZ
ATOM	5	CD2	BENZ	1	0.757	-1.201	-0.826	1.00	0.00	BENZ
ATOM	6	HD2	BENZ	1	0.663	-2.194	-1.248	1.00	0.00	BENZ
ATOM	7	CE1	BENZ	1	1.096	1.368	0.249	1.00	0.00	BENZ
ATOM	8	HE1	BENZ	1	1.266	2.357	0.658	1.00	0.00	BENZ
ATOM	9	CE2	BENZ	1	1.004	-1.041	0.547	1.00	0.00	BENZ
ATOM	10	HE2	BENZ	1	1.102	-1.912	1.183	1.00	0.00	BENZ
ATOM	11	CZ	BENZ	1	1.173	0.244	1.083	1.00	0.00	BENZ
ATOM	12	HZ	BENZ	1	1.402	0.364	2.135	1.00	0.00	BENZ
ATOM	13	N	MAM1	1	-2.018	0.195	0.187	1.00	0.00	MAM1
ATOM	14	C1	MAM1	1	-2.553	-0.661	1.294	1.00	0.00	MAM1
ATOM	15	HN2	MAM1	1	-1.118	-0.167	-0.165	1.00	0.00	MAM1
ATOM	16	HN3	MAM1	1	-1.843	1.152	0.500	1.00	0.00	MAM1
ATOM	17	HN4	MAM1	1	-2.665	0.239	-0.602	1.00	0.00	MAM1
ATOM	18	H11	MAM1	1	-3.500	-0.250	1.628	1.00	0.00	MAM1
ATOM	19	H12	MAM1	1	-1.826	-0.658	2.098	1.00	0.00	MAM1
ATOM	20	H13	MAM1	1	-2.688	-1.666	0.908	1.00	0.00	MAM1
END										
REMARK	3_TOLU_MAM1									
ATOM	1	CB	TOLU	1	1.881	-1.472	0.990	1.00	0.00	TOLU
ATOM	2	HB1	TOLU	1	1.431	-1.801	1.926	1.00	0.00	TOLU
ATOM	3	HB2	TOLU	1	2.907	-1.170	1.207	1.00	0.00	TOLU
ATOM	4	HB3	TOLU	1	1.927	-2.321	0.307	1.00	0.00	TOLU
ATOM	5	CG	TOLU	1	1.118	-0.322	0.387	1.00	0.00	TOLU
ATOM	6	CD1	TOLU	1	1.100	-0.115	-1.004	1.00	0.00	TOLU
ATOM	7	HD1	TOLU	1	1.608	-0.820	-1.653	1.00	0.00	TOLU
ATOM	8	CD2	TOLU	1	0.486	0.631	1.208	1.00	0.00	TOLU
ATOM	9	HD2	TOLU	1	0.514	0.509	2.286	1.00	0.00	TOLU
ATOM	10	CE1	TOLU	1	0.474	1.008	-1.561	1.00	0.00	TOLU
ATOM	11	HE1	TOLU	1	0.505	1.165	-2.633	1.00	0.00	TOLU
ATOM	12	CE2	TOLU	1	-0.139	1.761	0.657	1.00	0.00	TOLU
ATOM	13	HE2	TOLU	1	-0.588	2.500	1.311	1.00	0.00	TOLU
ATOM	14	CZ	TOLU	1	-0.144	1.954	-0.732	1.00	0.00	TOLU
ATOM	15	HZ	TOLU	1	-0.596	2.842	-1.158	1.00	0.00	TOLU
ATOM	16	N	MAM1	1	-2.074	-0.673	-0.291	1.00	0.00	MAM1
ATOM	17	C1	MAM1	1	-1.983	-2.058	0.270	1.00	0.00	MAM1
ATOM	18	HN2	MAM1	1	-1.345	-0.059	0.111	1.00	0.00	MAM1
ATOM	19	HN3	MAM1	1	-2.982	-0.246	-0.098	1.00	0.00	MAM1
ATOM	20	HN4	MAM1	1	-1.934	-0.664	-1.303	1.00	0.00	MAM1
ATOM	21	H11	MAM1	1	-2.773	-2.665	-0.161	1.00	0.00	MAM1
ATOM	22	H12	MAM1	1	-2.096	-1.993	1.347	1.00	0.00	MAM1

ATOM	23	H13	MAM1	1	-1.007	-2.456	0.015	1.00	0.00	MAM1
END										
REMARK	4_TOLU_MAM1									
ATOM	1	CB	TOLU	1	1.907	1.746	0.011	1.00	0.00	TOLU
ATOM	2	HB1	TOLU	1	1.698	2.346	0.897	1.00	0.00	TOLU
ATOM	3	HB2	TOLU	1	1.668	2.336	-0.874	1.00	0.00	TOLU
ATOM	4	HB3	TOLU	1	2.979	1.547	-0.006	1.00	0.00	TOLU
ATOM	5	CG	TOLU	1	1.140	0.450	0.032	1.00	0.00	TOLU
ATOM	6	CD1	TOLU	1	0.827	-0.221	-1.166	1.00	0.00	TOLU
ATOM	7	HD1	TOLU	1	1.105	0.226	-2.115	1.00	0.00	TOLU
ATOM	8	CD2	TOLU	1	0.805	-0.173	1.247	1.00	0.00	TOLU
ATOM	9	HD2	TOLU	1	1.066	0.311	2.182	1.00	0.00	TOLU
ATOM	10	CE1	TOLU	1	0.204	-1.479	-1.150	1.00	0.00	TOLU
ATOM	11	HE1	TOLU	1	0.005	-1.992	-2.084	1.00	0.00	TOLU
ATOM	12	CE2	TOLU	1	0.179	-1.427	1.270	1.00	0.00	TOLU
ATOM	13	HE2	TOLU	1	-0.037	-1.903	2.220	1.00	0.00	TOLU
ATOM	14	CZ	TOLU	1	-0.119	-2.088	0.071	1.00	0.00	TOLU
ATOM	15	HZ	TOLU	1	-0.570	-3.072	0.087	1.00	0.00	TOLU
ATOM	16	N	MAM1	1	-2.139	0.506	-0.082	1.00	0.00	MAM1
ATOM	17	C1	MAM1	1	-2.056	1.997	-0.180	1.00	0.00	MAM1
ATOM	18	HN2	MAM1	1	-1.277	0.061	-0.439	1.00	0.00	MAM1
ATOM	19	HN3	MAM1	1	-2.926	0.136	-0.619	1.00	0.00	MAM1
ATOM	20	HN4	MAM1	1	-2.248	0.195	0.885	1.00	0.00	MAM1
ATOM	21	H11	MAM1	1	-2.983	2.426	0.187	1.00	0.00	MAM1
ATOM	22	H12	MAM1	1	-1.900	2.259	-1.221	1.00	0.00	MAM1
ATOM	23	H13	MAM1	1	-1.216	2.323	0.423	1.00	0.00	MAM1
END										
REMARK	5_TOLU_MAM1									
ATOM	1	CB	TOLU	1	2.026	-2.005	0.088	1.00	0.00	TOLU
ATOM	2	HB1	TOLU	1	1.924	-2.455	-0.899	1.00	0.00	TOLU
ATOM	3	HB2	TOLU	1	1.699	-2.728	0.835	1.00	0.00	TOLU
ATOM	4	HB3	TOLU	1	3.087	-1.814	0.256	1.00	0.00	TOLU
ATOM	5	CG	TOLU	1	1.247	-0.719	0.190	1.00	0.00	TOLU
ATOM	6	CD1	TOLU	1	0.764	-0.267	1.431	1.00	0.00	TOLU
ATOM	7	HD1	TOLU	1	0.911	-0.878	2.315	1.00	0.00	TOLU
ATOM	8	CD2	TOLU	1	1.083	0.115	-0.931	1.00	0.00	TOLU
ATOM	9	HD2	TOLU	1	1.482	-0.199	-1.890	1.00	0.00	TOLU
ATOM	10	CE1	TOLU	1	0.129	0.978	1.551	1.00	0.00	TOLU
ATOM	11	HE1	TOLU	1	-0.206	1.322	2.523	1.00	0.00	TOLU
ATOM	12	CE2	TOLU	1	0.450	1.360	-0.821	1.00	0.00	TOLU
ATOM	13	HE2	TOLU	1	0.367	2.002	-1.690	1.00	0.00	TOLU
ATOM	14	CZ	TOLU	1	-0.029	1.798	0.423	1.00	0.00	TOLU
ATOM	15	HZ	TOLU	1	-0.484	2.777	0.519	1.00	0.00	TOLU
ATOM	16	N	MAM1	1	-2.058	-0.647	-0.224	1.00	0.00	MAM1
ATOM	17	C1	MAM1	1	-2.792	-0.140	-1.427	1.00	0.00	MAM1
ATOM	18	HN2	MAM1	1	-1.392	0.058	0.134	1.00	0.00	MAM1
ATOM	19	HN3	MAM1	1	-1.507	-1.480	-0.439	1.00	0.00	MAM1
ATOM	20	HN4	MAM1	1	-2.698	-0.884	0.536	1.00	0.00	MAM1
ATOM	21	H11	MAM1	1	-3.482	-0.906	-1.766	1.00	0.00	MAM1
ATOM	22	H12	MAM1	1	-2.058	0.084	-2.193	1.00	0.00	MAM1
ATOM	23	H13	MAM1	1	-3.328	0.758	-1.142	1.00	0.00	MAM1
END										
REMARK	6_TOLU_MAM1									
ATOM	1	CB	TOLU	1	-0.481	2.532	-0.205	1.00	0.00	TOLU
ATOM	2	HB1	TOLU	1	-0.292	2.743	-1.257	1.00	0.00	TOLU
ATOM	3	HB2	TOLU	1	0.328	2.957	0.389	1.00	0.00	TOLU
ATOM	4	HB3	TOLU	1	-1.400	3.051	0.073	1.00	0.00	TOLU
ATOM	5	CG	TOLU	1	-0.626	1.053	0.042	1.00	0.00	TOLU
ATOM	6	CD1	TOLU	1	-0.350	0.505	1.309	1.00	0.00	TOLU
ATOM	7	HD1	TOLU	1	0.012	1.152	2.102	1.00	0.00	TOLU
ATOM	8	CD2	TOLU	1	-1.135	0.199	-0.953	1.00	0.00	TOLU
ATOM	9	HD2	TOLU	1	-1.385	0.608	-1.926	1.00	0.00	TOLU
ATOM	10	CE1	TOLU	1	-0.580	-0.854	1.577	1.00	0.00	TOLU
ATOM	11	HE1	TOLU	1	-0.394	-1.246	2.570	1.00	0.00	TOLU
ATOM	12	CE2	TOLU	1	-1.363	-1.159	-0.694	1.00	0.00	TOLU
ATOM	13	HE2	TOLU	1	-1.789	-1.789	-1.466	1.00	0.00	TOLU
ATOM	14	CZ	TOLU	1	-1.092	-1.690	0.574	1.00	0.00	TOLU
ATOM	15	HZ	TOLU	1	-1.301	-2.731	0.787	1.00	0.00	TOLU
ATOM	16	N	MAM1	1	1.931	-0.935	-0.487	1.00	0.00	MAM1
ATOM	17	C1	MAM1	1	2.729	0.277	-0.854	1.00	0.00	MAM1
ATOM	18	HN2	MAM1	1	1.152	-0.690	0.147	1.00	0.00	MAM1
ATOM	19	HN3	MAM1	1	2.507	-1.637	-0.018	1.00	0.00	MAM1

ATOM	20	HN4	MAM1	1	1.509	-1.374	-1.307	1.00	0.00	MAM1
ATOM	21	H11	MAM1	1	3.544	-0.022	-1.505	1.00	0.00	MAM1
ATOM	22	H12	MAM1	1	3.112	0.719	0.059	1.00	0.00	MAM1
ATOM	23	H13	MAM1	1	2.065	0.970	-1.360	1.00	0.00	MAM1

END

REMARK 7_PHEN_MAM1

ATOM	1	CG	PHEN	1	0.477	2.074	0.069	1.00	0.00	PHEN
ATOM	2	HG	PHEN	1	0.335	3.146	0.034	1.00	0.00	PHEN
ATOM	3	CD1	PHEN	1	0.207	1.363	1.249	1.00	0.00	PHEN
ATOM	4	HD1	PHEN	1	-0.143	1.887	2.131	1.00	0.00	PHEN
ATOM	5	CD2	PHEN	1	0.989	1.393	-1.043	1.00	0.00	PHEN
ATOM	6	HD2	PHEN	1	1.234	1.937	-1.947	1.00	0.00	PHEN
ATOM	7	CE1	PHEN	1	0.426	-0.019	1.312	1.00	0.00	PHEN
ATOM	8	HE1	PHEN	1	0.261	-0.577	2.226	1.00	0.00	PHEN
ATOM	9	CE2	PHEN	1	1.197	0.008	-0.996	1.00	0.00	PHEN
ATOM	10	HE2	PHEN	1	1.607	-0.512	-1.856	1.00	0.00	PHEN
ATOM	11	CZ	PHEN	1	0.922	-0.693	0.187	1.00	0.00	PHEN
ATOM	12	OH	PHEN	1	1.044	-2.057	0.293	1.00	0.00	PHEN
ATOM	13	HH	PHEN	1	1.677	-2.394	-0.359	1.00	0.00	PHEN
ATOM	14	N	MAM1	1	-2.103	0.018	-0.668	1.00	0.00	MAM1
ATOM	15	C1	MAM1	1	-2.434	-1.366	-0.192	1.00	0.00	MAM1
ATOM	16	HN2	MAM1	1	-1.376	0.448	-0.074	1.00	0.00	MAM1
ATOM	17	HN3	MAM1	1	-2.923	0.627	-0.656	1.00	0.00	MAM1
ATOM	18	HN4	MAM1	1	-1.733	0.011	-1.621	1.00	0.00	MAM1
ATOM	19	H11	MAM1	1	-3.187	-1.787	-0.848	1.00	0.00	MAM1
ATOM	20	H12	MAM1	1	-2.811	-1.288	0.822	1.00	0.00	MAM1
ATOM	21	H13	MAM1	1	-1.523	-1.955	-0.211	1.00	0.00	MAM1

END

REMARK 8_PHEN_MAM1

ATOM	1	CG	PHEN	1	0.115	1.832	0.449	1.00	0.00	PHEN
ATOM	2	HG	PHEN	1	-0.255	2.844	0.558	1.00	0.00	PHEN
ATOM	3	CD1	PHEN	1	0.522	1.357	-0.808	1.00	0.00	PHEN
ATOM	4	HD1	PHEN	1	0.466	2.004	-1.675	1.00	0.00	PHEN
ATOM	5	CD2	PHEN	1	0.258	1.008	1.575	1.00	0.00	PHEN
ATOM	6	HD2	PHEN	1	-0.014	1.378	2.556	1.00	0.00	PHEN
ATOM	7	CE1	PHEN	1	1.043	0.067	-0.946	1.00	0.00	PHEN
ATOM	8	HE1	PHEN	1	1.398	-0.301	-1.901	1.00	0.00	PHEN
ATOM	9	CE2	PHEN	1	0.773	-0.290	1.446	1.00	0.00	PHEN
ATOM	10	HE2	PHEN	1	0.896	-0.916	2.323	1.00	0.00	PHEN
ATOM	11	CZ	PHEN	1	1.167	-0.756	0.184	1.00	0.00	PHEN
ATOM	12	OH	PHEN	1	1.634	-2.026	-0.034	1.00	0.00	PHEN
ATOM	13	HH	PHEN	1	1.953	-2.419	0.793	1.00	0.00	PHEN
ATOM	14	N	MAM1	1	-2.072	-0.526	-0.218	1.00	0.00	MAM1
ATOM	15	C1	MAM1	1	-2.793	0.009	-1.418	1.00	0.00	MAM1
ATOM	16	HN2	MAM1	1	-1.368	0.146	0.124	1.00	0.00	MAM1
ATOM	17	HN3	MAM1	1	-1.573	-1.391	-0.435	1.00	0.00	MAM1
ATOM	18	HN4	MAM1	1	-2.715	-0.723	0.551	1.00	0.00	MAM1
ATOM	19	H11	MAM1	1	-3.529	-0.720	-1.738	1.00	0.00	MAM1
ATOM	20	H12	MAM1	1	-2.058	0.183	-2.196	1.00	0.00	MAM1
ATOM	21	H13	MAM1	1	-3.273	0.940	-1.135	1.00	0.00	MAM1

END

REMARK 9_PHEN_MAM1

ATOM	1	CG	PHEN	1	1.943	-1.576	0.144	1.00	0.00	PHEN
ATOM	2	HG	PHEN	1	2.540	-2.468	0.281	1.00	0.00	PHEN
ATOM	3	CD1	PHEN	1	1.259	-1.370	-1.058	1.00	0.00	PHEN
ATOM	4	HD1	PHEN	1	1.319	-2.104	-1.852	1.00	0.00	PHEN
ATOM	5	CD2	PHEN	1	1.897	-0.604	1.150	1.00	0.00	PHEN
ATOM	6	HD2	PHEN	1	2.440	-0.752	2.074	1.00	0.00	PHEN
ATOM	7	CE1	PHEN	1	0.496	-0.212	-1.246	1.00	0.00	PHEN
ATOM	8	HE1	PHEN	1	0.007	-0.007	-2.191	1.00	0.00	PHEN
ATOM	9	CE2	PHEN	1	1.122	0.549	0.985	1.00	0.00	PHEN
ATOM	10	HE2	PHEN	1	1.072	1.299	1.767	1.00	0.00	PHEN
ATOM	11	CZ	PHEN	1	0.449	0.734	-0.222	1.00	0.00	PHEN
ATOM	12	OH	PHEN	1	-0.411	1.834	-0.423	1.00	0.00	PHEN
ATOM	13	HH	PHEN	1	-0.035	2.635	-0.024	1.00	0.00	PHEN
ATOM	14	N	MAM1	1	-2.807	0.520	-0.214	1.00	0.00	MAM1
ATOM	15	C1	MAM1	1	-2.600	-0.472	0.892	1.00	0.00	MAM1
ATOM	16	HN2	MAM1	1	-2.909	0.050	-1.115	1.00	0.00	MAM1
ATOM	17	HN3	MAM1	1	-1.991	1.170	-0.289	1.00	0.00	MAM1
ATOM	18	HN4	MAM1	1	-3.651	1.075	-0.065	1.00	0.00	MAM1
ATOM	19	H11	MAM1	1	-2.475	0.078	1.818	1.00	0.00	MAM1
ATOM	20	H12	MAM1	1	-1.703	-1.040	0.667	1.00	0.00	MAM1

ATOM	21	H13	MAM1	1	-3.467	-1.121	0.949	1.00	0.00	MAM1
END										
REMARK	10_PHEN_MAM1									
ATOM	1	CG	PHEN	1	2.114	0.877	-1.019	1.00	0.00	PHEN
ATOM	2	HG	PHEN	1	2.810	1.398	-1.663	1.00	0.00	PHEN
ATOM	3	CD1	PHEN	1	1.456	1.567	0.004	1.00	0.00	PHEN
ATOM	4	HD1	PHEN	1	1.635	2.624	0.151	1.00	0.00	PHEN
ATOM	5	CD2	PHEN	1	1.912	-0.499	-1.177	1.00	0.00	PHEN
ATOM	6	HD2	PHEN	1	2.434	-1.039	-1.957	1.00	0.00	PHEN
ATOM	7	CE1	PHEN	1	0.564	0.894	0.847	1.00	0.00	PHEN
ATOM	8	HE1	PHEN	1	0.090	1.398	1.682	1.00	0.00	PHEN
ATOM	9	CE2	PHEN	1	1.009	-1.181	-0.355	1.00	0.00	PHEN
ATOM	10	HE2	PHEN	1	0.839	-2.244	-0.482	1.00	0.00	PHEN
ATOM	11	CZ	PHEN	1	0.363	-0.473	0.659	1.00	0.00	PHEN
ATOM	12	OH	PHEN	1	-0.615	-1.082	1.471	1.00	0.00	PHEN
ATOM	13	HH	PHEN	1	-0.359	-1.993	1.685	1.00	0.00	PHEN
ATOM	14	N	MAM1	1	-2.839	0.077	0.362	1.00	0.00	MAM1
ATOM	15	C1	MAM1	1	-2.554	0.109	-1.112	1.00	0.00	MAM1
ATOM	16	HN2	MAM1	1	-2.847	1.020	0.755	1.00	0.00	MAM1
ATOM	17	HN3	MAM1	1	-2.107	-0.469	0.870	1.00	0.00	MAM1
ATOM	18	HN4	MAM1	1	-3.750	-0.341	0.557	1.00	0.00	MAM1
ATOM	19	H11	MAM1	1	-2.534	-0.914	-1.472	1.00	0.00	MAM1
ATOM	20	H12	MAM1	1	-1.587	0.578	-1.254	1.00	0.00	MAM1
ATOM	21	H13	MAM1	1	-3.337	0.672	-1.609	1.00	0.00	MAM1
END										
REMARK	11_CRES_MAM1									
ATOM	1	CB	CRES	1	3.063	-1.062	-0.074	1.00	0.00	CRES
ATOM	2	HB1	CRES	1	3.311	-2.070	0.260	1.00	0.00	CRES
ATOM	3	HB2	CRES	1	3.606	-0.360	0.558	1.00	0.00	CRES
ATOM	4	HB3	CRES	1	3.422	-0.953	-1.097	1.00	0.00	CRES
ATOM	5	CG	CRES	1	1.576	-0.837	0.009	1.00	0.00	CRES
ATOM	6	CD1	CRES	1	0.975	-0.397	1.205	1.00	0.00	CRES
ATOM	7	HD1	CRES	1	1.598	-0.170	2.064	1.00	0.00	CRES
ATOM	8	CD2	CRES	1	0.729	-1.177	-1.059	1.00	0.00	CRES
ATOM	9	HD2	CRES	1	1.158	-1.549	-1.983	1.00	0.00	CRES
ATOM	10	CE1	CRES	1	-0.416	-0.274	1.324	1.00	0.00	CRES
ATOM	11	HE1	CRES	1	-0.876	0.029	2.258	1.00	0.00	CRES
ATOM	12	CE2	CRES	1	-0.662	-1.039	-0.965	1.00	0.00	CRES
ATOM	13	HE2	CRES	1	-1.294	-1.318	-1.802	1.00	0.00	CRES
ATOM	14	CZ	CRES	1	-1.236	-0.607	0.238	1.00	0.00	CRES
ATOM	15	OZ	CRES	1	-2.586	-0.392	0.392	1.00	0.00	CRES
ATOM	16	HZ	CRES	1	-3.089	-0.945	-0.225	1.00	0.00	CRES
ATOM	17	N	MAM1	1	0.125	2.142	-0.676	1.00	0.00	MAM1
ATOM	18	C1	MAM1	1	-1.137	2.794	-0.194	1.00	0.00	MAM1
ATOM	19	HN2	MAM1	1	0.394	1.360	-0.056	1.00	0.00	MAM1
ATOM	20	HN3	MAM1	1	0.902	2.804	-0.711	1.00	0.00	MAM1
ATOM	21	HN4	MAM1	1	0.011	1.743	-1.610	1.00	0.00	MAM1
ATOM	22	H11	MAM1	1	-1.395	3.597	-0.877	1.00	0.00	MAM1
ATOM	23	H12	MAM1	1	-0.953	3.184	0.801	1.00	0.00	MAM1
ATOM	24	H13	MAM1	1	-1.916	2.039	-0.165	1.00	0.00	MAM1
END										
REMARK	12_CRES_MAM1									
ATOM	1	CB	CRES	1	0.756	2.910	-0.246	1.00	0.00	CRES
ATOM	2	HB1	CRES	1	1.305	3.090	0.677	1.00	0.00	CRES
ATOM	3	HB2	CRES	1	0.009	3.699	-0.347	1.00	0.00	CRES
ATOM	4	HB3	CRES	1	1.447	3.000	-1.084	1.00	0.00	CRES
ATOM	5	CG	CRES	1	0.086	1.560	-0.231	1.00	0.00	CRES
ATOM	6	CD1	CRES	1	-0.406	1.004	0.967	1.00	0.00	CRES
ATOM	7	HD1	CRES	1	-0.262	1.539	1.899	1.00	0.00	CRES
ATOM	8	CD2	CRES	1	-0.172	0.862	-1.426	1.00	0.00	CRES
ATOM	9	HD2	CRES	1	0.163	1.278	-2.370	1.00	0.00	CRES
ATOM	10	CE1	CRES	1	-1.110	-0.204	0.980	1.00	0.00	CRES
ATOM	11	HE1	CRES	1	-1.517	-0.608	1.899	1.00	0.00	CRES
ATOM	12	CE2	CRES	1	-0.870	-0.354	-1.430	1.00	0.00	CRES
ATOM	13	HE2	CRES	1	-1.064	-0.865	-2.367	1.00	0.00	CRES
ATOM	14	CZ	CRES	1	-1.345	-0.885	-0.222	1.00	0.00	CRES
ATOM	15	OZ	CRES	1	-1.986	-2.095	-0.132	1.00	0.00	CRES
ATOM	16	HZ	CRES	1	-2.369	-2.341	-0.987	1.00	0.00	CRES
ATOM	17	N	MAM1	1	1.854	-1.183	0.163	1.00	0.00	MAM1
ATOM	18	C1	MAM1	1	2.617	-0.928	1.426	1.00	0.00	MAM1
ATOM	19	HN2	MAM1	1	1.263	-0.372	-0.086	1.00	0.00	MAM1
ATOM	20	HN3	MAM1	1	1.225	-1.984	0.258	1.00	0.00	MAM1

ATOM	21	HN4	MAM1	1	2.478	-1.369	-0.624	1.00	0.00	MAM1
ATOM	22	H11	MAM1	1	3.227	-1.797	1.649	1.00	0.00	MAM1
ATOM	23	H12	MAM1	1	1.897	-0.750	2.217	1.00	0.00	MAM1
ATOM	24	H13	MAM1	1	3.239	-0.053	1.274	1.00	0.00	MAM1

END

REMARK 13_CRES_MAM1

ATOM	1	CB	CRES	1	3.206	-1.558	0.163	1.00	0.00	CRES
ATOM	2	HB1	CRES	1	4.098	-1.032	-0.181	1.00	0.00	CRES
ATOM	3	HB2	CRES	1	3.097	-2.460	-0.438	1.00	0.00	CRES
ATOM	4	HB3	CRES	1	3.371	-1.854	1.198	1.00	0.00	CRES
ATOM	5	CG	CRES	1	1.991	-0.677	0.041	1.00	0.00	CRES
ATOM	6	CD1	CRES	1	1.240	-0.644	-1.145	1.00	0.00	CRES
ATOM	7	HD1	CRES	1	1.521	-1.284	-1.974	1.00	0.00	CRES
ATOM	8	CD2	CRES	1	1.622	0.189	1.082	1.00	0.00	CRES
ATOM	9	HD2	CRES	1	2.192	0.190	2.004	1.00	0.00	CRES
ATOM	10	CE1	CRES	1	0.137	0.206	-1.284	1.00	0.00	CRES
ATOM	11	HE1	CRES	1	-0.405	0.272	-2.221	1.00	0.00	CRES
ATOM	12	CE2	CRES	1	0.511	1.032	0.972	1.00	0.00	CRES
ATOM	13	HE2	CRES	1	0.230	1.684	1.792	1.00	0.00	CRES
ATOM	14	CZ	CRES	1	-0.206	1.042	-0.224	1.00	0.00	CRES
ATOM	15	OZ	CRES	1	-1.387	1.800	-0.370	1.00	0.00	CRES
ATOM	16	HZ	CRES	1	-1.285	2.670	0.047	1.00	0.00	CRES
ATOM	17	N	MAM1	1	-3.166	-0.265	-0.162	1.00	0.00	MAM1
ATOM	18	C1	MAM1	1	-2.584	-1.172	0.882	1.00	0.00	MAM1
ATOM	19	HN2	MAM1	1	-3.136	-0.700	-1.085	1.00	0.00	MAM1
ATOM	20	HN3	MAM1	1	-2.631	0.632	-0.220	1.00	0.00	MAM1
ATOM	21	HN4	MAM1	1	-4.144	-0.046	0.038	1.00	0.00	MAM1
ATOM	22	H11	MAM1	1	-2.610	-0.652	1.833	1.00	0.00	MAM1
ATOM	23	H12	MAM1	1	-1.559	-1.389	0.600	1.00	0.00	MAM1
ATOM	24	H13	MAM1	1	-3.176	-2.080	0.928	1.00	0.00	MAM1

END

REMARK 14_CRES_MAM1

ATOM	1	CB	CRES	1	3.233	-0.368	1.471	1.00	0.00	CRES
ATOM	2	HB1	CRES	1	4.132	-0.318	0.855	1.00	0.00	CRES
ATOM	3	HB2	CRES	1	3.201	-1.352	1.937	1.00	0.00	CRES
ATOM	4	HB3	CRES	1	3.325	0.380	2.257	1.00	0.00	CRES
ATOM	5	CG	CRES	1	2.004	-0.124	0.636	1.00	0.00	CRES
ATOM	6	CD1	CRES	1	1.369	-1.180	-0.036	1.00	0.00	CRES
ATOM	7	HD1	CRES	1	1.751	-2.189	0.071	1.00	0.00	CRES
ATOM	8	CD2	CRES	1	1.505	1.175	0.449	1.00	0.00	CRES
ATOM	9	HD2	CRES	1	1.984	2.008	0.949	1.00	0.00	CRES
ATOM	10	CE1	CRES	1	0.254	-0.958	-0.852	1.00	0.00	CRES
ATOM	11	HE1	CRES	1	-0.198	-1.766	-1.415	1.00	0.00	CRES
ATOM	12	CE2	CRES	1	0.379	1.417	-0.345	1.00	0.00	CRES
ATOM	13	HE2	CRES	1	-0.003	2.425	-0.467	1.00	0.00	CRES
ATOM	14	CZ	CRES	1	-0.220	0.344	-1.002	1.00	0.00	CRES
ATOM	15	OZ	CRES	1	-1.409	0.505	-1.747	1.00	0.00	CRES
ATOM	16	HZ	CRES	1	-1.378	1.326	-2.262	1.00	0.00	CRES
ATOM	17	N	MAM1	1	-3.124	-0.605	0.069	1.00	0.00	MAM1
ATOM	18	C1	MAM1	1	-2.628	-0.129	1.403	1.00	0.00	MAM1
ATOM	19	HN2	MAM1	1	-4.125	-0.439	-0.039	1.00	0.00	MAM1
ATOM	20	HN3	MAM1	1	-2.969	-1.608	-0.044	1.00	0.00	MAM1
ATOM	21	HN4	MAM1	1	-2.621	-0.121	-0.711	1.00	0.00	MAM1
ATOM	22	H11	MAM1	1	-1.569	-0.358	1.465	1.00	0.00	MAM1
ATOM	23	H12	MAM1	1	-3.183	-0.636	2.185	1.00	0.00	MAM1
ATOM	24	H13	MAM1	1	-2.785	0.943	1.457	1.00	0.00	MAM1

END

REMARK 15_INDO_MAM1

ATOM	1	CD2	INDO	1	-0.478	0.056	0.921	1.00	0.00	INDO
ATOM	2	CE2	INDO	1	-0.853	0.312	-0.435	1.00	0.00	INDO
ATOM	3	CZ2	INDO	1	-0.236	1.307	-1.212	1.00	0.00	INDO
ATOM	4	CH2	INDO	1	0.722	2.105	-0.588	1.00	0.00	INDO
ATOM	5	CZ3	INDO	1	1.077	1.903	0.770	1.00	0.00	INDO
ATOM	6	CE3	INDO	1	0.478	0.900	1.533	1.00	0.00	INDO
ATOM	7	CG	INDO	1	-1.283	-1.035	1.381	1.00	0.00	INDO
ATOM	8	CD1	INDO	1	-2.089	-1.409	0.326	1.00	0.00	INDO
ATOM	9	NE1	INDO	1	-1.808	-0.620	-0.773	1.00	0.00	INDO
ATOM	10	HZ2	INDO	1	-0.532	1.493	-2.238	1.00	0.00	INDO
ATOM	11	HH2	INDO	1	1.187	2.910	-1.143	1.00	0.00	INDO
ATOM	12	HZ3	INDO	1	1.794	2.570	1.233	1.00	0.00	INDO
ATOM	13	HE3	INDO	1	0.736	0.774	2.579	1.00	0.00	INDO
ATOM	14	HG	INDO	1	-1.294	-1.472	2.367	1.00	0.00	INDO

ATOM	15	HD1	INDO	1	-2.853	-2.170	0.273	1.00	0.00	INDO
ATOM	16	HE1	INDO	1	-2.353	-0.611	-1.623	1.00	0.00	INDO
ATOM	17	N	MAM1	1	2.277	-0.901	-0.400	1.00	0.00	MAM1
ATOM	18	C1	MAM1	1	1.450	-1.948	-1.083	1.00	0.00	MAM1
ATOM	19	HN2	MAM1	1	1.684	-0.180	0.047	1.00	0.00	MAM1
ATOM	20	HN3	MAM1	1	2.901	-0.425	-1.053	1.00	0.00	MAM1
ATOM	21	HN4	MAM1	1	2.854	-1.307	0.339	1.00	0.00	MAM1
ATOM	22	H11	MAM1	1	2.108	-2.733	-1.440	1.00	0.00	MAM1
ATOM	23	H12	MAM1	1	0.929	-1.474	-1.906	1.00	0.00	MAM1
ATOM	24	H13	MAM1	1	0.737	-2.331	-0.360	1.00	0.00	MAM1

END

REMARK 16_INDO_MAM1

ATOM	1	CD2	INDO	1	0.638	-0.490	-0.655	1.00	0.00	INDO
ATOM	2	CE2	INDO	1	1.052	0.357	0.422	1.00	0.00	INDO
ATOM	3	CZ2	INDO	1	0.523	1.645	0.612	1.00	0.00	INDO
ATOM	4	CH2	INDO	1	-0.366	2.120	-0.354	1.00	0.00	INDO
ATOM	5	CZ3	INDO	1	-0.732	1.326	-1.473	1.00	0.00	INDO
ATOM	6	CE3	INDO	1	-0.213	0.045	-1.648	1.00	0.00	INDO
ATOM	7	CG	INDO	1	1.343	-1.726	-0.511	1.00	0.00	INDO
ATOM	8	CD1	INDO	1	2.116	-1.617	0.627	1.00	0.00	INDO
ATOM	9	NE1	INDO	1	1.925	-0.373	1.196	1.00	0.00	INDO
ATOM	10	HZ2	INDO	1	0.840	2.276	1.435	1.00	0.00	INDO
ATOM	11	HH2	INDO	1	-0.757	3.127	-0.266	1.00	0.00	INDO
ATOM	12	HZ3	INDO	1	-1.376	1.753	-2.232	1.00	0.00	INDO
ATOM	13	HE3	INDO	1	-0.475	-0.541	-2.523	1.00	0.00	INDO
ATOM	14	HG	INDO	1	1.309	-2.582	-1.167	1.00	0.00	INDO
ATOM	15	HD1	INDO	1	2.804	-2.320	1.069	1.00	0.00	INDO
ATOM	16	HE1	INDO	1	2.442	-0.018	1.987	1.00	0.00	INDO
ATOM	17	N	MAM1	1	-2.015	-0.381	0.960	1.00	0.00	MAM1
ATOM	18	C1	MAM1	1	-3.324	-0.662	0.290	1.00	0.00	MAM1
ATOM	19	HN2	MAM1	1	-1.313	-1.093	0.735	1.00	0.00	MAM1
ATOM	20	HN3	MAM1	1	-2.111	-0.338	1.976	1.00	0.00	MAM1
ATOM	21	HN4	MAM1	1	-1.609	0.513	0.638	1.00	0.00	MAM1
ATOM	22	H11	MAM1	1	-4.009	0.144	0.530	1.00	0.00	MAM1
ATOM	23	H12	MAM1	1	-3.707	-1.609	0.654	1.00	0.00	MAM1
ATOM	24	H13	MAM1	1	-3.144	-0.703	-0.778	1.00	0.00	MAM1

END

REMARK 17_INDO_MAM1

ATOM	1	CD2	INDO	1	-0.654	-0.380	0.729	1.00	0.00	INDO
ATOM	2	CE2	INDO	1	-0.782	0.436	-0.438	1.00	0.00	INDO
ATOM	3	CZ2	INDO	1	-0.161	1.691	-0.552	1.00	0.00	INDO
ATOM	4	CH2	INDO	1	0.546	2.159	0.556	1.00	0.00	INDO
ATOM	5	CZ3	INDO	1	0.647	1.389	1.743	1.00	0.00	INDO
ATOM	6	CE3	INDO	1	0.046	0.134	1.844	1.00	0.00	INDO
ATOM	7	CG	INDO	1	-1.378	-1.589	0.478	1.00	0.00	INDO
ATOM	8	CD1	INDO	1	-1.905	-1.484	-0.793	1.00	0.00	INDO
ATOM	9	NE1	INDO	1	-1.520	-0.280	-1.353	1.00	0.00	INDO
ATOM	10	HZ2	INDO	1	-0.270	2.302	-1.442	1.00	0.00	INDO
ATOM	11	HH2	INDO	1	1.003	3.140	0.519	1.00	0.00	INDO
ATOM	12	HZ3	INDO	1	1.169	1.803	2.597	1.00	0.00	INDO
ATOM	13	HE3	INDO	1	0.107	-0.433	2.766	1.00	0.00	INDO
ATOM	14	HG	INDO	1	-1.527	-2.416	1.153	1.00	0.00	INDO
ATOM	15	HD1	INDO	1	-2.533	-2.167	-1.342	1.00	0.00	INDO
ATOM	16	HE1	INDO	1	-1.881	0.085	-2.223	1.00	0.00	INDO
ATOM	17	N	MAM1	1	2.404	-0.530	-0.231	1.00	0.00	MAM1
ATOM	18	C1	MAM1	1	1.863	-1.180	-1.469	1.00	0.00	MAM1
ATOM	19	HN2	MAM1	1	1.689	0.043	0.245	1.00	0.00	MAM1
ATOM	20	HN3	MAM1	1	3.199	0.078	-0.440	1.00	0.00	MAM1
ATOM	21	HN4	MAM1	1	2.718	-1.227	0.447	1.00	0.00	MAM1
ATOM	22	H11	MAM1	1	2.636	-1.812	-1.895	1.00	0.00	MAM1
ATOM	23	H12	MAM1	1	1.582	-0.394	-2.161	1.00	0.00	MAM1
ATOM	24	H13	MAM1	1	0.992	-1.761	-1.184	1.00	0.00	MAM1

END

REMARK 18_INDO_MAM1

ATOM	1	CD2	INDO	1	0.730	0.496	-0.482	1.00	0.00	INDO
ATOM	2	CE2	INDO	1	0.696	-0.363	0.660	1.00	0.00	INDO
ATOM	3	CZ2	INDO	1	0.003	-0.028	1.836	1.00	0.00	INDO
ATOM	4	CH2	INDO	1	-0.600	1.228	1.889	1.00	0.00	INDO
ATOM	5	CZ3	INDO	1	-0.558	2.111	0.780	1.00	0.00	INDO
ATOM	6	CE3	INDO	1	0.117	1.768	-0.393	1.00	0.00	INDO
ATOM	7	CG	INDO	1	1.521	-0.158	-1.478	1.00	0.00	INDO
ATOM	8	CD1	INDO	1	1.911	-1.370	-0.948	1.00	0.00	INDO

ATOM	9	NE1	INDO	1	1.385	-1.507	0.324	1.00	0.00	INDO
ATOM	10	HZ2	INDO	1	0.006	-0.681	2.703	1.00	0.00	INDO
ATOM	11	HH2	INDO	1	-1.101	1.540	2.796	1.00	0.00	INDO
ATOM	12	HZ3	INDO	1	-1.008	3.092	0.869	1.00	0.00	INDO
ATOM	13	HE3	INDO	1	0.180	2.469	-1.218	1.00	0.00	INDO
ATOM	14	HG	INDO	1	1.788	0.216	-2.454	1.00	0.00	INDO
ATOM	15	HD1	INDO	1	2.530	-2.146	-1.370	1.00	0.00	INDO
ATOM	16	HE1	INDO	1	1.635	-2.246	0.967	1.00	0.00	INDO
ATOM	17	N	MAM1	1	-2.348	-0.288	-0.465	1.00	0.00	MAM1
ATOM	18	C1	MAM1	1	-1.952	-1.368	-1.424	1.00	0.00	MAM1
ATOM	19	HN2	MAM1	1	-1.647	0.475	-0.447	1.00	0.00	MAM1
ATOM	20	HN3	MAM1	1	-2.404	-0.635	0.495	1.00	0.00	MAM1
ATOM	21	HN4	MAM1	1	-3.254	0.120	-0.705	1.00	0.00	MAM1
ATOM	22	H11	MAM1	1	-2.709	-2.146	-1.405	1.00	0.00	MAM1
ATOM	23	H12	MAM1	1	-0.987	-1.752	-1.112	1.00	0.00	MAM1
ATOM	24	H13	MAM1	1	-1.878	-0.930	-2.413	1.00	0.00	MAM1

END

REMARK 19_INDO_MAM1

ATOM	1	CD2	INDO	1	-0.913	-0.106	0.479	1.00	0.00	INDO
ATOM	2	CE2	INDO	1	-0.699	-0.252	-0.929	1.00	0.00	INDO
ATOM	3	CZ2	INDO	1	-0.014	0.712	-1.688	1.00	0.00	INDO
ATOM	4	CH2	INDO	1	0.379	1.882	-1.033	1.00	0.00	INDO
ATOM	5	CZ3	INDO	1	0.108	2.080	0.346	1.00	0.00	INDO
ATOM	6	CE3	INDO	1	-0.561	1.116	1.096	1.00	0.00	INDO
ATOM	7	CG	INDO	1	-1.596	-1.283	0.922	1.00	0.00	INDO
ATOM	8	CD1	INDO	1	-1.747	-2.098	-0.181	1.00	0.00	INDO
ATOM	9	NE1	INDO	1	-1.190	-1.486	-1.286	1.00	0.00	INDO
ATOM	10	HZ2	INDO	1	0.148	0.590	-2.753	1.00	0.00	INDO
ATOM	11	HH2	INDO	1	0.867	2.667	-1.598	1.00	0.00	INDO
ATOM	12	HZ3	INDO	1	0.374	3.026	0.802	1.00	0.00	INDO
ATOM	13	HE3	INDO	1	-0.791	1.291	2.141	1.00	0.00	INDO
ATOM	14	HG	INDO	1	-1.953	-1.499	1.917	1.00	0.00	INDO
ATOM	15	HD1	INDO	1	-2.224	-3.061	-0.271	1.00	0.00	INDO
ATOM	16	HE1	INDO	1	-1.250	-1.841	-2.229	1.00	0.00	INDO
ATOM	17	N	MAM1	1	2.180	-0.403	0.463	1.00	0.00	MAM1
ATOM	18	C1	MAM1	1	2.998	0.125	1.600	1.00	0.00	MAM1
ATOM	19	HN2	MAM1	1	1.764	0.363	-0.091	1.00	0.00	MAM1
ATOM	20	HN3	MAM1	1	1.385	-0.960	0.793	1.00	0.00	MAM1
ATOM	21	HN4	MAM1	1	2.737	-0.984	-0.166	1.00	0.00	MAM1
ATOM	22	H11	MAM1	1	3.408	-0.712	2.155	1.00	0.00	MAM1
ATOM	23	H12	MAM1	1	2.343	0.720	2.227	1.00	0.00	MAM1
ATOM	24	H13	MAM1	1	3.793	0.739	1.192	1.00	0.00	MAM1

END

REMARK 20_INDO_MAM1

ATOM	1	CD2	INDO	1	0.418	0.820	0.727	1.00	0.00	INDO
ATOM	2	CE2	INDO	1	0.514	0.670	-0.693	1.00	0.00	INDO
ATOM	3	CZ2	INDO	1	0.917	-0.533	-1.298	1.00	0.00	INDO
ATOM	4	CH2	INDO	1	1.310	-1.573	-0.457	1.00	0.00	INDO
ATOM	5	CZ3	INDO	1	1.266	-1.435	0.955	1.00	0.00	INDO
ATOM	6	CE3	INDO	1	0.853	-0.242	1.552	1.00	0.00	INDO
ATOM	7	CG	INDO	1	-0.034	2.154	0.979	1.00	0.00	INDO
ATOM	8	CD1	INDO	1	-0.227	2.750	-0.249	1.00	0.00	INDO
ATOM	9	NE1	INDO	1	0.074	1.848	-1.252	1.00	0.00	INDO
ATOM	10	HZ2	INDO	1	0.996	-0.628	-2.375	1.00	0.00	INDO
ATOM	11	HH2	INDO	1	1.672	-2.498	-0.888	1.00	0.00	INDO
ATOM	12	HZ3	INDO	1	1.622	-2.248	1.576	1.00	0.00	INDO
ATOM	13	HE3	INDO	1	0.861	-0.135	2.631	1.00	0.00	INDO
ATOM	14	HG	INDO	1	-0.188	2.624	1.937	1.00	0.00	INDO
ATOM	15	HD1	INDO	1	-0.546	3.751	-0.492	1.00	0.00	INDO
ATOM	16	HE1	INDO	1	0.126	2.082	-2.234	1.00	0.00	INDO
ATOM	17	N	MAM1	1	-1.877	-1.295	0.313	1.00	0.00	MAM1
ATOM	18	C1	MAM1	1	-2.260	-2.546	-0.412	1.00	0.00	MAM1
ATOM	19	HN2	MAM1	1	-0.900	-1.336	0.658	1.00	0.00	MAM1
ATOM	20	HN3	MAM1	1	-2.481	-1.122	1.119	1.00	0.00	MAM1
ATOM	21	HN4	MAM1	1	-1.924	-0.471	-0.291	1.00	0.00	MAM1
ATOM	22	H11	MAM1	1	-3.286	-2.457	-0.751	1.00	0.00	MAM1
ATOM	23	H12	MAM1	1	-2.156	-3.380	0.273	1.00	0.00	MAM1
ATOM	24	H13	MAM1	1	-1.583	-2.661	-1.252	1.00	0.00	MAM1

END

REMARK 21_MIND_MAM1

ATOM	1	CG	MIND	1	1.706	0.617	0.298	1.00	0.00	MIND
ATOM	2	CB	MIND	1	2.375	1.676	1.116	1.00	0.00	MIND

ATOM	3	HB1	MIND	1	3.293	2.012	0.636	1.00	0.00	MIND
ATOM	4	HB2	MIND	1	2.633	1.299	2.107	1.00	0.00	MIND
ATOM	5	HB3	MIND	1	1.730	2.547	1.252	1.00	0.00	MIND
ATOM	6	CD2	MIND	1	0.464	-0.038	0.589	1.00	0.00	MIND
ATOM	7	CD1	MIND	1	2.167	0.053	-0.877	1.00	0.00	MIND
ATOM	8	HD1	MIND	1	3.075	0.252	-1.424	1.00	0.00	MIND
ATOM	9	NE1	MIND	1	1.272	-0.904	-1.330	1.00	0.00	MIND
ATOM	10	HE1	MIND	1	1.462	-1.551	-2.082	1.00	0.00	MIND
ATOM	11	CE2	MIND	1	0.242	-1.024	-0.424	1.00	0.00	MIND
ATOM	12	CE3	MIND	1	-0.439	0.035	1.675	1.00	0.00	MIND
ATOM	13	HE3	MIND	1	-0.264	0.726	2.493	1.00	0.00	MIND
ATOM	14	CZ2	MIND	1	-0.887	-1.859	-0.427	1.00	0.00	MIND
ATOM	15	HZ2	MIND	1	-1.030	-2.617	-1.189	1.00	0.00	MIND
ATOM	16	CZ3	MIND	1	-1.556	-0.804	1.682	1.00	0.00	MIND
ATOM	17	HZ3	MIND	1	-2.242	-0.774	2.520	1.00	0.00	MIND
ATOM	18	CH2	MIND	1	-1.767	-1.752	0.651	1.00	0.00	MIND
ATOM	19	HH2	MIND	1	-2.623	-2.413	0.705	1.00	0.00	MIND
ATOM	20	N	MAM1	1	-2.073	1.183	-0.831	1.00	0.00	MAM1
ATOM	21	C1	MAM1	1	-1.080	2.016	-1.581	1.00	0.00	MAM1
ATOM	22	HN2	MAM1	1	-1.674	0.841	0.063	1.00	0.00	MAM1
ATOM	23	HN3	MAM1	1	-2.337	0.345	-1.353	1.00	0.00	MAM1
ATOM	24	HN4	MAM1	1	-2.925	1.705	-0.620	1.00	0.00	MAM1
ATOM	25	H11	MAM1	1	-1.538	2.357	-2.505	1.00	0.00	MAM1
ATOM	26	H12	MAM1	1	-0.209	1.400	-1.779	1.00	0.00	MAM1
ATOM	27	H13	MAM1	1	-0.808	2.859	-0.956	1.00	0.00	MAM1

END

REMARK 22_MIND_MAM1										
ATOM	1	CG	MIND	1	0.998	-1.529	-0.215	1.00	0.00	MIND
ATOM	2	CB	MIND	1	0.972	-2.760	-1.066	1.00	0.00	MIND
ATOM	3	HB1	MIND	1	1.434	-3.598	-0.546	1.00	0.00	MIND
ATOM	4	HB2	MIND	1	1.517	-2.602	-1.997	1.00	0.00	MIND
ATOM	5	HB3	MIND	1	-0.049	-3.048	-1.325	1.00	0.00	MIND
ATOM	6	CD2	MIND	1	0.455	-0.244	-0.546	1.00	0.00	MIND
ATOM	7	CD1	MIND	1	1.568	-1.390	1.036	1.00	0.00	MIND
ATOM	8	HD1	MIND	1	2.096	-2.116	1.635	1.00	0.00	MIND
ATOM	9	NE1	MIND	1	1.394	-0.095	1.499	1.00	0.00	MIND
ATOM	10	HE1	MIND	1	1.854	0.284	2.314	1.00	0.00	MIND
ATOM	11	CE2	MIND	1	0.764	0.650	0.528	1.00	0.00	MIND
ATOM	12	CE3	MIND	1	-0.174	0.274	-1.701	1.00	0.00	MIND
ATOM	13	HE3	MIND	1	-0.363	-0.362	-2.560	1.00	0.00	MIND
ATOM	14	CZ2	MIND	1	0.385	2.002	0.513	1.00	0.00	MIND
ATOM	15	HZ2	MIND	1	0.646	2.674	1.324	1.00	0.00	MIND
ATOM	16	CZ3	MIND	1	-0.540	1.622	-1.725	1.00	0.00	MIND
ATOM	17	HZ3	MIND	1	-1.001	2.036	-2.614	1.00	0.00	MIND
ATOM	18	CH2	MIND	1	-0.247	2.480	-0.636	1.00	0.00	MIND
ATOM	19	HH2	MIND	1	-0.511	3.528	-0.700	1.00	0.00	MIND
ATOM	20	N	MAM1	1	-2.442	0.325	0.561	1.00	0.00	MAM1
ATOM	21	C1	MAM1	1	-2.252	-0.954	1.317	1.00	0.00	MAM1
ATOM	22	HN2	MAM1	1	-1.816	0.368	-0.263	1.00	0.00	MAM1
ATOM	23	HN3	MAM1	1	-2.206	1.141	1.130	1.00	0.00	MAM1
ATOM	24	HN4	MAM1	1	-3.404	0.435	0.236	1.00	0.00	MAM1
ATOM	25	H11	MAM1	1	-2.927	-0.961	2.166	1.00	0.00	MAM1
ATOM	26	H12	MAM1	1	-1.217	-1.001	1.638	1.00	0.00	MAM1
ATOM	27	H13	MAM1	1	-2.474	-1.777	0.646	1.00	0.00	MAM1

END

REMARK 23_MIND_MAM1										
ATOM	1	CG	MIND	1	1.509	-1.094	0.156	1.00	0.00	MIND
ATOM	2	CB	MIND	1	2.023	-2.400	-0.367	1.00	0.00	MIND
ATOM	3	HB1	MIND	1	2.682	-2.873	0.360	1.00	0.00	MIND
ATOM	4	HB2	MIND	1	2.590	-2.254	-1.288	1.00	0.00	MIND
ATOM	5	HB3	MIND	1	1.211	-3.095	-0.584	1.00	0.00	MIND
ATOM	6	CD2	MIND	1	0.581	-0.213	-0.492	1.00	0.00	MIND
ATOM	7	CD1	MIND	1	1.866	-0.468	1.336	1.00	0.00	MIND
ATOM	8	HD1	MIND	1	2.560	-0.786	2.099	1.00	0.00	MIND
ATOM	9	NE1	MIND	1	1.199	0.740	1.455	1.00	0.00	MIND
ATOM	10	HE1	MIND	1	1.404	1.438	2.156	1.00	0.00	MIND
ATOM	11	CE2	MIND	1	0.435	0.948	0.330	1.00	0.00	MIND
ATOM	12	CE3	MIND	1	-0.076	-0.247	-1.743	1.00	0.00	MIND
ATOM	13	HE3	MIND	1	0.069	-1.082	-2.421	1.00	0.00	MIND
ATOM	14	CZ2	MIND	1	-0.423	2.006	-0.009	1.00	0.00	MIND
ATOM	15	HZ2	MIND	1	-0.525	2.881	0.623	1.00	0.00	MIND
ATOM	16	CZ3	MIND	1	-0.916	0.811	-2.093	1.00	0.00	MIND

ATOM	17	HZ3	MIND	1	-1.414	0.805	-3.056	1.00	0.00	MIND
ATOM	18	CH2	MIND	1	-1.087	1.926	-1.234	1.00	0.00	MIND
ATOM	19	HH2	MIND	1	-1.725	2.744	-1.547	1.00	0.00	MIND
ATOM	20	N	MAM1	1	-2.461	-0.672	0.373	1.00	0.00	MAM1
ATOM	21	C1	MAM1	1	-1.913	-0.793	1.763	1.00	0.00	MAM1
ATOM	22	HN2	MAM1	1	-1.823	-0.144	-0.244	1.00	0.00	MAM1
ATOM	23	HN3	MAM1	1	-3.365	-0.197	0.363	1.00	0.00	MAM1
ATOM	24	HN4	MAM1	1	-2.589	-1.590	-0.058	1.00	0.00	MAM1
ATOM	25	H11	MAM1	1	-2.586	-1.412	2.348	1.00	0.00	MAM1
ATOM	26	H12	MAM1	1	-1.844	0.205	2.181	1.00	0.00	MAM1
ATOM	27	H13	MAM1	1	-0.926	-1.240	1.692	1.00	0.00	MAM1

END

REMARK 24_MIND_MAM1

ATOM	1	CG	MIND	1	1.597	-0.331	0.899	1.00	0.00	MIND
ATOM	2	CB	MIND	1	2.261	-1.422	1.680	1.00	0.00	MIND
ATOM	3	HB1	MIND	1	2.953	-1.005	2.411	1.00	0.00	MIND
ATOM	4	HB2	MIND	1	2.828	-2.082	1.022	1.00	0.00	MIND
ATOM	5	HB3	MIND	1	1.535	-2.034	2.218	1.00	0.00	MIND
ATOM	6	CD2	MIND	1	0.602	-0.488	-0.122	1.00	0.00	MIND
ATOM	7	CD1	MIND	1	1.843	1.026	0.985	1.00	0.00	MIND
ATOM	8	HD1	MIND	1	2.539	1.559	1.616	1.00	0.00	MIND
ATOM	9	NE1	MIND	1	1.051	1.713	0.080	1.00	0.00	MIND
ATOM	10	HE1	MIND	1	1.151	2.694	-0.138	1.00	0.00	MIND
ATOM	11	CE2	MIND	1	0.312	0.810	-0.649	1.00	0.00	MIND
ATOM	12	CE3	MIND	1	0.022	-1.618	-0.743	1.00	0.00	MIND
ATOM	13	HE3	MIND	1	0.285	-2.620	-0.420	1.00	0.00	MIND
ATOM	14	CZ2	MIND	1	-0.628	1.011	-1.674	1.00	0.00	MIND
ATOM	15	HZ2	MIND	1	-0.838	1.999	-2.069	1.00	0.00	MIND
ATOM	16	CZ3	MIND	1	-0.904	-1.426	-1.766	1.00	0.00	MIND
ATOM	17	HZ3	MIND	1	-1.344	-2.283	-2.261	1.00	0.00	MIND
ATOM	18	CH2	MIND	1	-1.221	-0.125	-2.233	1.00	0.00	MIND
ATOM	19	HH2	MIND	1	-1.916	-0.009	-3.055	1.00	0.00	MIND
ATOM	20	N	MAM1	1	-2.361	-0.091	0.832	1.00	0.00	MAM1
ATOM	21	C1	MAM1	1	-1.890	0.812	1.930	1.00	0.00	MAM1
ATOM	22	HN2	MAM1	1	-2.027	0.234	-0.092	1.00	0.00	MAM1
ATOM	23	HN3	MAM1	1	-3.380	-0.154	0.799	1.00	0.00	MAM1
ATOM	24	HN4	MAM1	1	-1.985	-1.037	0.935	1.00	0.00	MAM1
ATOM	25	H11	MAM1	1	-2.278	0.443	2.874	1.00	0.00	MAM1
ATOM	26	H12	MAM1	1	-2.264	1.811	1.730	1.00	0.00	MAM1
ATOM	27	H13	MAM1	1	-0.805	0.800	1.925	1.00	0.00	MAM1

END

REMARK 25_MIND_MAM1

ATOM	1	CG	MIND	1	-1.718	-0.884	0.303	1.00	0.00	MIND
ATOM	2	CB	MIND	1	-2.585	-1.070	1.510	1.00	0.00	MIND
ATOM	3	HB1	MIND	1	-3.152	-1.998	1.437	1.00	0.00	MIND
ATOM	4	HB2	MIND	1	-3.296	-0.249	1.609	1.00	0.00	MIND
ATOM	5	HB3	MIND	1	-1.995	-1.110	2.427	1.00	0.00	MIND
ATOM	6	CD2	MIND	1	-0.748	0.152	0.093	1.00	0.00	MIND
ATOM	7	CD1	MIND	1	-1.719	-1.644	-0.852	1.00	0.00	MIND
ATOM	8	HD1	MIND	1	-2.317	-2.506	-1.106	1.00	0.00	MIND
ATOM	9	NE1	MIND	1	-0.812	-1.130	-1.761	1.00	0.00	MIND
ATOM	10	HE1	MIND	1	-0.705	-1.454	-2.711	1.00	0.00	MIND
ATOM	11	CE2	MIND	1	-0.226	-0.005	-1.232	1.00	0.00	MIND
ATOM	12	CE3	MIND	1	-0.361	1.284	0.844	1.00	0.00	MIND
ATOM	13	HE3	MIND	1	-0.807	1.482	1.813	1.00	0.00	MIND
ATOM	14	CZ2	MIND	1	0.770	0.839	-1.750	1.00	0.00	MIND
ATOM	15	HZ2	MIND	1	1.162	0.709	-2.752	1.00	0.00	MIND
ATOM	16	CZ3	MIND	1	0.619	2.132	0.332	1.00	0.00	MIND
ATOM	17	HZ3	MIND	1	0.918	3.009	0.892	1.00	0.00	MIND
ATOM	18	CH2	MIND	1	1.179	1.912	-0.954	1.00	0.00	MIND
ATOM	19	HH2	MIND	1	1.911	2.611	-1.341	1.00	0.00	MIND
ATOM	20	N	MAM1	1	2.151	-0.685	0.768	1.00	0.00	MAM1
ATOM	21	C1	MAM1	1	2.705	-0.374	2.123	1.00	0.00	MAM1
ATOM	22	HN2	MAM1	1	2.043	0.169	0.196	1.00	0.00	MAM1
ATOM	23	HN3	MAM1	1	1.209	-1.087	0.824	1.00	0.00	MAM1
ATOM	24	HN4	MAM1	1	2.747	-1.337	0.255	1.00	0.00	MAM1
ATOM	25	H11	MAM1	1	2.789	-1.297	2.687	1.00	0.00	MAM1
ATOM	26	H12	MAM1	1	2.020	0.313	2.607	1.00	0.00	MAM1
ATOM	27	H13	MAM1	1	3.679	0.087	1.997	1.00	0.00	MAM1

END

REMARK 26_IMID_MAM1

ATOM	1	CG	IMID	1	2.297	-0.203	-0.223	1.00	0.00	IMID
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ATOM	2	HG	IMID	1	3.274	-0.422	-0.616	1.00	0.00	IMID
ATOM	3	CD2	IMID	1	1.039	-0.622	-0.594	1.00	0.00	IMID
ATOM	4	HD2	IMID	1	0.769	-1.291	-1.393	1.00	0.00	IMID
ATOM	5	ND1	IMID	1	2.101	0.635	0.848	1.00	0.00	IMID
ATOM	6	HD1	IMID	1	2.826	1.115	1.363	1.00	0.00	IMID
ATOM	7	CE1	IMID	1	0.773	0.710	1.104	1.00	0.00	IMID
ATOM	8	HE1	IMID	1	0.354	1.304	1.899	1.00	0.00	IMID
ATOM	9	NE2	IMID	1	0.096	-0.048	0.237	1.00	0.00	IMID
ATOM	10	N	MAM1	1	-2.534	-0.446	0.016	1.00	0.00	MAM1
ATOM	11	C1	MAM1	1	-2.951	0.003	-1.345	1.00	0.00	MAM1
ATOM	12	HN2	MAM1	1	-1.443	-0.287	0.155	1.00	0.00	MAM1
ATOM	13	HN3	MAM1	1	-2.742	-1.434	0.160	1.00	0.00	MAM1
ATOM	14	HN4	MAM1	1	-3.035	0.070	0.739	1.00	0.00	MAM1
ATOM	15	H11	MAM1	1	-4.022	-0.122	-1.467	1.00	0.00	MAM1
ATOM	16	H12	MAM1	1	-2.420	-0.594	-2.079	1.00	0.00	MAM1
ATOM	17	H13	MAM1	1	-2.679	1.047	-1.455	1.00	0.00	MAM1

END

REMARK 27 IMID_MAM1

ATOM	1	CG	IMID	1	-2.054	0.500	-0.948	1.00	0.00	IMID
ATOM	2	HG	IMID	1	-2.875	1.030	-1.397	1.00	0.00	IMID
ATOM	3	CD2	IMID	1	-0.726	0.822	-0.785	1.00	0.00	IMID
ATOM	4	HD2	IMID	1	-0.216	1.719	-1.094	1.00	0.00	IMID
ATOM	5	ND1	IMID	1	-2.197	-0.747	-0.387	1.00	0.00	IMID
ATOM	6	HD1	IMID	1	-3.055	-1.279	-0.340	1.00	0.00	IMID
ATOM	7	CE1	IMID	1	-0.995	-1.150	0.090	1.00	0.00	IMID
ATOM	8	HE1	IMID	1	-0.837	-2.096	0.578	1.00	0.00	IMID
ATOM	9	NE2	IMID	1	-0.073	-0.209	-0.138	1.00	0.00	IMID
ATOM	10	N	MAM1	1	2.518	-0.177	0.499	1.00	0.00	MAM1
ATOM	11	C1	MAM1	1	2.753	0.997	1.390	1.00	0.00	MAM1
ATOM	12	HN2	MAM1	1	1.446	-0.236	0.218	1.00	0.00	MAM1
ATOM	13	HN3	MAM1	1	2.784	-1.045	0.963	1.00	0.00	MAM1
ATOM	14	HN4	MAM1	1	3.077	-0.114	-0.352	1.00	0.00	MAM1
ATOM	15	H11	MAM1	1	3.795	1.034	1.693	1.00	0.00	MAM1
ATOM	16	H12	MAM1	1	2.112	0.894	2.259	1.00	0.00	MAM1
ATOM	17	H13	MAM1	1	2.490	1.898	0.845	1.00	0.00	MAM1

END

REMARK 28 IMID_MAM1

ATOM	1	CG	IMID	1	2.252	0.537	-0.041	1.00	0.00	IMID
ATOM	2	HG	IMID	1	3.221	0.913	0.233	1.00	0.00	IMID
ATOM	3	CD2	IMID	1	1.112	0.302	0.693	1.00	0.00	IMID
ATOM	4	HD2	IMID	1	0.956	0.455	1.748	1.00	0.00	IMID
ATOM	5	ND1	IMID	1	1.935	0.179	-1.329	1.00	0.00	IMID
ATOM	6	HD1	IMID	1	2.555	0.227	-2.127	1.00	0.00	IMID
ATOM	7	CE1	IMID	1	0.652	-0.254	-1.358	1.00	0.00	IMID
ATOM	8	HE1	IMID	1	0.159	-0.595	-2.253	1.00	0.00	IMID
ATOM	9	NE2	IMID	1	0.120	-0.190	-0.133	1.00	0.00	IMID
ATOM	10	N	MAM1	1	-2.342	-0.816	0.687	1.00	0.00	MAM1
ATOM	11	C1	MAM1	1	-2.938	0.401	1.313	1.00	0.00	MAM1
ATOM	12	HN2	MAM1	1	-1.317	-0.597	0.321	1.00	0.00	MAM1
ATOM	13	HN3	MAM1	1	-2.909	-1.134	-0.100	1.00	0.00	MAM1
ATOM	14	HN4	MAM1	1	-2.295	-1.590	1.350	1.00	0.00	MAM1
ATOM	15	H11	MAM1	1	-3.953	0.195	1.636	1.00	0.00	MAM1
ATOM	16	H12	MAM1	1	-2.930	1.198	0.577	1.00	0.00	MAM1
ATOM	17	H13	MAM1	1	-2.325	0.681	2.164	1.00	0.00	MAM1

END

REMARK 29 IMID_MAM1

ATOM	1	CG	IMID	1	-2.181	-0.100	-0.774	1.00	0.00	IMID
ATOM	2	HG	IMID	1	-3.072	-0.404	-1.293	1.00	0.00	IMID
ATOM	3	CD2	IMID	1	-0.854	-0.415	-0.958	1.00	0.00	IMID
ATOM	4	HD2	IMID	1	-0.420	-1.063	-1.699	1.00	0.00	IMID
ATOM	5	ND1	IMID	1	-2.206	0.764	0.294	1.00	0.00	IMID
ATOM	6	HD1	IMID	1	-3.032	1.190	0.692	1.00	0.00	IMID
ATOM	7	CE1	IMID	1	-0.937	0.955	0.729	1.00	0.00	IMID
ATOM	8	HE1	IMID	1	-0.683	1.593	1.559	1.00	0.00	IMID
ATOM	9	NE2	IMID	1	-0.086	0.246	-0.018	1.00	0.00	IMID
ATOM	10	N	MAM1	1	2.566	0.026	0.175	1.00	0.00	MAM1
ATOM	11	C1	MAM1	1	2.891	-1.414	0.396	1.00	0.00	MAM1
ATOM	12	HN2	MAM1	1	1.466	0.165	0.099	1.00	0.00	MAM1
ATOM	13	HN3	MAM1	1	3.002	0.378	-0.678	1.00	0.00	MAM1
ATOM	14	HN4	MAM1	1	2.915	0.599	0.943	1.00	0.00	MAM1
ATOM	15	H11	MAM1	1	3.963	-1.542	0.506	1.00	0.00	MAM1
ATOM	16	H12	MAM1	1	2.534	-1.979	-0.459	1.00	0.00	MAM1

ATOM	17	H13	MAM1	1	2.378	-1.742	1.293	1.00	0.00	MAM1
END										
REMARK 30_IMID_MAM1										
ATOM	1	CG	IMID	1	-2.194	0.411	0.621	1.00	0.00	IMID
ATOM	2	HG	IMID	1	-3.098	0.503	1.198	1.00	0.00	IMID
ATOM	3	CD2	IMID	1	-0.874	0.288	0.989	1.00	0.00	IMID
ATOM	4	HD2	IMID	1	-0.460	0.259	1.983	1.00	0.00	IMID
ATOM	5	ND1	IMID	1	-2.192	0.400	-0.752	1.00	0.00	IMID
ATOM	6	HD1	IMID	1	-3.007	0.474	-1.346	1.00	0.00	IMID
ATOM	7	CE1	IMID	1	-0.915	0.274	-1.185	1.00	0.00	IMID
ATOM	8	HE1	IMID	1	-0.640	0.241	-2.225	1.00	0.00	IMID
ATOM	9	NE2	IMID	1	-0.084	0.203	-0.141	1.00	0.00	IMID
ATOM	10	N	MAM1	1	2.570	-0.082	-0.097	1.00	0.00	MAM1
ATOM	11	C1	MAM1	1	2.881	-1.348	0.630	1.00	0.00	MAM1
ATOM	12	HN2	MAM1	1	1.471	0.071	-0.148	1.00	0.00	MAM1
ATOM	13	HN3	MAM1	1	2.941	-0.106	-1.046	1.00	0.00	MAM1
ATOM	14	HN4	MAM1	1	2.992	0.724	0.365	1.00	0.00	MAM1
ATOM	15	H11	MAM1	1	3.953	-1.513	0.649	1.00	0.00	MAM1
ATOM	16	H12	MAM1	1	2.383	-2.163	0.115	1.00	0.00	MAM1
ATOM	17	H13	MAM1	1	2.498	-1.264	1.641	1.00	0.00	MAM1
END										
REMARK 31_IMID_MAM1										
ATOM	1	CG	IMID	1	2.150	0.622	0.578	1.00	0.00	IMID
ATOM	2	HG	IMID	1	2.984	1.142	1.017	1.00	0.00	IMID
ATOM	3	CD2	IMID	1	0.822	0.957	0.443	1.00	0.00	IMID
ATOM	4	HD2	IMID	1	0.326	1.856	0.767	1.00	0.00	IMID
ATOM	5	ND1	IMID	1	2.274	-0.619	0.002	1.00	0.00	IMID
ATOM	6	HD1	IMID	1	3.128	-1.156	-0.069	1.00	0.00	IMID
ATOM	7	CE1	IMID	1	1.061	-1.007	-0.459	1.00	0.00	IMID
ATOM	8	HE1	IMID	1	0.887	-1.946	-0.956	1.00	0.00	IMID
ATOM	9	NE2	IMID	1	0.151	-0.063	-0.203	1.00	0.00	IMID
ATOM	10	N	MAM1	1	-2.462	-0.045	-0.742	1.00	0.00	MAM1
ATOM	11	C1	MAM1	1	-3.191	0.236	0.530	1.00	0.00	MAM1
ATOM	12	HN2	MAM1	1	-1.365	-0.064	-0.563	1.00	0.00	MAM1
ATOM	13	HN3	MAM1	1	-2.667	0.660	-1.451	1.00	0.00	MAM1
ATOM	14	HN4	MAM1	1	-2.744	-0.945	-1.131	1.00	0.00	MAM1
ATOM	15	H11	MAM1	1	-4.262	0.213	0.359	1.00	0.00	MAM1
ATOM	16	H12	MAM1	1	-2.891	1.217	0.885	1.00	0.00	MAM1
ATOM	17	H13	MAM1	1	-2.908	-0.520	1.254	1.00	0.00	MAM1
END										
REMARK 32_IMID_MAM1										
ATOM	1	CG	IMID	1	-1.992	-0.593	1.048	1.00	0.00	IMID
ATOM	2	HG	IMID	1	-2.862	-0.592	1.680	1.00	0.00	IMID
ATOM	3	CD2	IMID	1	-1.132	0.410	0.662	1.00	0.00	IMID
ATOM	4	HD2	IMID	1	-1.162	1.452	0.930	1.00	0.00	IMID
ATOM	5	ND1	IMID	1	-1.524	-1.730	0.436	1.00	0.00	IMID
ATOM	6	HD1	IMID	1	-1.931	-2.653	0.511	1.00	0.00	IMID
ATOM	7	CE1	IMID	1	-0.425	-1.413	-0.290	1.00	0.00	IMID
ATOM	8	HE1	IMID	1	0.132	-2.129	-0.869	1.00	0.00	IMID
ATOM	9	NE2	IMID	1	-0.158	-0.109	-0.168	1.00	0.00	IMID
ATOM	10	N	MAM1	1	1.823	1.327	-1.237	1.00	0.00	MAM1
ATOM	11	C1	MAM1	1	2.734	1.754	-0.135	1.00	0.00	MAM1
ATOM	12	HN2	MAM1	1	0.989	0.713	-0.832	1.00	0.00	MAM1
ATOM	13	HN3	MAM1	1	2.324	0.776	-1.933	1.00	0.00	MAM1
ATOM	14	HN4	MAM1	1	1.430	2.131	-1.725	1.00	0.00	MAM1
ATOM	15	H11	MAM1	1	3.561	2.330	-0.537	1.00	0.00	MAM1
ATOM	16	H12	MAM1	1	3.103	0.863	0.363	1.00	0.00	MAM1
ATOM	17	H13	MAM1	1	2.164	2.355	0.565	1.00	0.00	MAM1
END										
REMARK 33_4MIE_MAM1										
ATOM	1	CB	4MIE	1	-1.464	-1.644	-0.072	1.00	0.00	4MIE
ATOM	2	HB1	4MIE	1	-0.942	-2.054	-0.937	1.00	0.00	4MIE
ATOM	3	HB2	4MIE	1	-1.174	-2.208	0.815	1.00	0.00	4MIE
ATOM	4	HB3	4MIE	1	-2.530	-1.800	-0.228	1.00	0.00	4MIE
ATOM	5	CG	4MIE	1	-1.174	-0.189	0.093	1.00	0.00	4MIE
ATOM	6	ND1	4MIE	1	0.116	0.293	0.249	1.00	0.00	4MIE
ATOM	7	CD2	4MIE	1	-2.049	0.876	0.137	1.00	0.00	4MIE
ATOM	8	HD2	4MIE	1	-3.121	0.925	0.055	1.00	0.00	4MIE
ATOM	9	CE1	4MIE	1	0.024	1.619	0.384	1.00	0.00	4MIE
ATOM	10	HE1	4MIE	1	0.839	2.308	0.524	1.00	0.00	4MIE
ATOM	11	NE2	4MIE	1	-1.274	1.998	0.319	1.00	0.00	4MIE
ATOM	12	HE2	4MIE	1	-1.613	2.947	0.394	1.00	0.00	4MIE

ATOM	13	N	MAM1	1	2.274	-1.251	0.181	1.00	0.00	MAM1
ATOM	14	C1	MAM1	1	2.807	-1.259	-1.212	1.00	0.00	MAM1
ATOM	15	HN2	MAM1	1	1.374	-0.586	0.250	1.00	0.00	MAM1
ATOM	16	HN3	MAM1	1	2.979	-0.926	0.844	1.00	0.00	MAM1
ATOM	17	HN4	MAM1	1	2.005	-2.190	0.476	1.00	0.00	MAM1
ATOM	18	H11	MAM1	1	3.673	-1.910	-1.280	1.00	0.00	MAM1
ATOM	19	H12	MAM1	1	3.080	-0.243	-1.477	1.00	0.00	MAM1
ATOM	20	H13	MAM1	1	2.021	-1.610	-1.873	1.00	0.00	MAM1

END

REMARK 34_4MIE_MAM1

ATOM	1	CB	4MIE	1	0.506	2.000	0.487	1.00	0.00	4MIE
ATOM	2	HB1	4MIE	1	0.002	2.441	-0.375	1.00	0.00	4MIE
ATOM	3	HB2	4MIE	1	-0.167	2.033	1.344	1.00	0.00	4MIE
ATOM	4	HB3	4MIE	1	1.367	2.624	0.718	1.00	0.00	4MIE
ATOM	5	CG	4MIE	1	0.945	0.603	0.198	1.00	0.00	4MIE
ATOM	6	ND1	4MIE	1	0.062	-0.380	-0.220	1.00	0.00	4MIE
ATOM	7	CD2	4MIE	1	2.203	0.046	0.305	1.00	0.00	4MIE
ATOM	8	HD2	4MIE	1	3.149	0.469	0.597	1.00	0.00	4MIE
ATOM	9	CE1	4MIE	1	0.772	-1.504	-0.370	1.00	0.00	4MIE
ATOM	10	HE1	4MIE	1	0.396	-2.462	-0.688	1.00	0.00	4MIE
ATOM	11	NE2	4MIE	1	2.068	-1.273	-0.057	1.00	0.00	4MIE
ATOM	12	HE2	4MIE	1	2.810	-1.959	-0.087	1.00	0.00	4MIE
ATOM	13	N	MAM1	1	-2.513	-0.009	-0.748	1.00	0.00	MAM1
ATOM	14	C1	MAM1	1	-3.188	0.427	0.509	1.00	0.00	MAM1
ATOM	15	HN2	MAM1	1	-1.417	-0.175	-0.561	1.00	0.00	MAM1
ATOM	16	HN3	MAM1	1	-2.622	0.687	-1.486	1.00	0.00	MAM1
ATOM	17	HN4	MAM1	1	-2.920	-0.876	-1.097	1.00	0.00	MAM1
ATOM	18	H11	MAM1	1	-4.254	0.544	0.341	1.00	0.00	MAM1
ATOM	19	H12	MAM1	1	-2.753	1.371	0.820	1.00	0.00	MAM1
ATOM	20	H13	MAM1	1	-3.008	-0.328	1.268	1.00	0.00	MAM1

END

REMARK 35_4MIE_MAM1

ATOM	1	CB	4MIE	1	0.559	2.025	0.255	1.00	0.00	4MIE
ATOM	2	HB1	4MIE	1	-0.328	2.303	0.826	1.00	0.00	4MIE
ATOM	3	HB2	4MIE	1	1.385	2.638	0.612	1.00	0.00	4MIE
ATOM	4	HB3	4MIE	1	0.394	2.270	-0.795	1.00	0.00	4MIE
ATOM	5	CG	4MIE	1	0.880	0.577	0.428	1.00	0.00	4MIE
ATOM	6	ND1	4MIE	1	-0.035	-0.424	0.144	1.00	0.00	4MIE
ATOM	7	CD2	4MIE	1	2.056	-0.008	0.849	1.00	0.00	4MIE
ATOM	8	HD2	4MIE	1	2.995	0.419	1.155	1.00	0.00	4MIE
ATOM	9	CE1	4MIE	1	0.574	-1.589	0.392	1.00	0.00	4MIE
ATOM	10	HE1	4MIE	1	0.148	-2.572	0.279	1.00	0.00	4MIE
ATOM	11	NE2	4MIE	1	1.838	-1.365	0.818	1.00	0.00	4MIE
ATOM	12	HE2	4MIE	1	2.507	-2.079	1.072	1.00	0.00	4MIE
ATOM	13	N	MAM1	1	-2.545	-0.038	-0.636	1.00	0.00	MAM1
ATOM	14	C1	MAM1	1	-2.529	0.710	-1.927	1.00	0.00	MAM1
ATOM	15	HN2	MAM1	1	-1.498	-0.221	-0.280	1.00	0.00	MAM1
ATOM	16	HN3	MAM1	1	-3.016	-0.937	-0.744	1.00	0.00	MAM1
ATOM	17	HN4	MAM1	1	-3.054	0.476	0.083	1.00	0.00	MAM1
ATOM	18	H11	MAM1	1	-3.542	0.847	-2.293	1.00	0.00	MAM1
ATOM	19	H12	MAM1	1	-1.945	0.140	-2.641	1.00	0.00	MAM1
ATOM	20	H13	MAM1	1	-2.061	1.674	-1.755	1.00	0.00	MAM1

END

REMARK 36_4MIE_MAM1

ATOM	1	CB	4MIE	1	-1.316	1.659	0.009	1.00	0.00	4MIE
ATOM	2	HB1	4MIE	1	-0.988	2.053	-0.954	1.00	0.00	4MIE
ATOM	3	HB2	4MIE	1	-2.370	1.904	0.122	1.00	0.00	4MIE
ATOM	4	HB3	4MIE	1	-0.770	2.169	0.804	1.00	0.00	4MIE
ATOM	5	CG	4MIE	1	-1.120	0.181	0.082	1.00	0.00	4MIE
ATOM	6	ND1	4MIE	1	0.115	-0.415	-0.122	1.00	0.00	4MIE
ATOM	7	CD2	4MIE	1	-2.042	-0.806	0.363	1.00	0.00	4MIE
ATOM	8	HD2	4MIE	1	-3.095	-0.758	0.580	1.00	0.00	4MIE
ATOM	9	CE1	4MIE	1	-0.058	-1.732	0.027	1.00	0.00	4MIE
ATOM	10	HE1	4MIE	1	0.698	-2.493	-0.066	1.00	0.00	4MIE
ATOM	11	NE2	4MIE	1	-1.352	-1.995	0.322	1.00	0.00	4MIE
ATOM	12	HE2	4MIE	1	-1.743	-2.913	0.483	1.00	0.00	4MIE
ATOM	13	N	MAM1	1	2.344	0.860	-0.802	1.00	0.00	MAM1
ATOM	14	C1	MAM1	1	2.680	1.838	0.273	1.00	0.00	MAM1
ATOM	15	HN2	MAM1	1	1.406	0.301	-0.542	1.00	0.00	MAM1
ATOM	16	HN3	MAM1	1	3.100	0.187	-0.930	1.00	0.00	MAM1
ATOM	17	HN4	MAM1	1	2.212	1.327	-1.699	1.00	0.00	MAM1
ATOM	18	H11	MAM1	1	3.611	2.345	0.041	1.00	0.00	MAM1

ATOM	19	H12	MAM1	1	2.771	1.294	1.207	1.00	0.00	MAM1
ATOM	20	H13	MAM1	1	1.872	2.557	0.343	1.00	0.00	MAM1
END										
REMARK 37_4MIE_MAM1										
ATOM	1	CB	4MIE	1	-2.068	-0.342	0.356	1.00	0.00	4MIE
ATOM	2	HB1	4MIE	1	-1.985	-1.424	0.458	1.00	0.00	4MIE
ATOM	3	HB2	4MIE	1	-2.032	0.110	1.348	1.00	0.00	4MIE
ATOM	4	HB3	4MIE	1	-3.047	-0.126	-0.068	1.00	0.00	4MIE
ATOM	5	CG	4MIE	1	-0.993	0.200	-0.526	1.00	0.00	4MIE
ATOM	6	ND1	4MIE	1	0.352	-0.026	-0.281	1.00	0.00	4MIE
ATOM	7	CD2	4MIE	1	-1.108	0.979	-1.659	1.00	0.00	4MIE
ATOM	8	HD2	4MIE	1	-1.969	1.369	-2.174	1.00	0.00	4MIE
ATOM	9	CE1	4MIE	1	1.035	0.600	-1.245	1.00	0.00	4MIE
ATOM	10	HE1	4MIE	1	2.105	0.626	-1.360	1.00	0.00	4MIE
ATOM	11	NE2	4MIE	1	0.176	1.216	-2.090	1.00	0.00	4MIE
ATOM	12	HE2	4MIE	1	0.439	1.756	-2.903	1.00	0.00	4MIE
ATOM	13	N	MAM1	1	1.333	-1.443	1.740	1.00	0.00	MAM1
ATOM	14	C1	MAM1	1	0.938	-0.781	3.016	1.00	0.00	MAM1
ATOM	15	HN2	MAM1	1	0.929	-0.871	0.862	1.00	0.00	MAM1
ATOM	16	HN3	MAM1	1	0.984	-2.401	1.697	1.00	0.00	MAM1
ATOM	17	HN4	MAM1	1	2.348	-1.496	1.657	1.00	0.00	MAM1
ATOM	18	H11	MAM1	1	1.368	-1.308	3.862	1.00	0.00	MAM1
ATOM	19	H12	MAM1	1	-0.145	-0.788	3.084	1.00	0.00	MAM1
ATOM	20	H13	MAM1	1	1.297	0.243	2.991	1.00	0.00	MAM1
END										
REMARK 38_4MIM_MAM1										
ATOM	1	CB	4MIM	1	3.239	-0.145	-0.570	1.00	0.00	4MIM
ATOM	2	HB1	4MIM	1	3.828	-0.892	-0.036	1.00	0.00	4MIM
ATOM	3	HB2	4MIM	1	3.215	-0.423	-1.621	1.00	0.00	4MIM
ATOM	4	HB3	4MIM	1	3.742	0.818	-0.486	1.00	0.00	4MIM
ATOM	5	CG	4MIM	1	1.846	-0.078	-0.044	1.00	0.00	4MIM
ATOM	6	ND1	4MIM	1	1.547	0.253	1.262	1.00	0.00	4MIM
ATOM	7	HD1	4MIM	1	2.222	0.483	1.979	1.00	0.00	4MIM
ATOM	8	CD2	4MIM	1	0.618	-0.303	-0.631	1.00	0.00	4MIM
ATOM	9	HD2	4MIM	1	0.418	-0.588	-1.651	1.00	0.00	4MIM
ATOM	10	CE1	4MIM	1	0.203	0.225	1.436	1.00	0.00	4MIM
ATOM	11	HE1	4MIM	1	-0.283	0.447	2.371	1.00	0.00	4MIM
ATOM	12	NE2	4MIM	1	-0.395	-0.113	0.290	1.00	0.00	4MIM
ATOM	13	N	MAM1	1	-2.977	-0.372	-0.238	1.00	0.00	MAM1
ATOM	14	C1	MAM1	1	-3.308	0.541	-1.370	1.00	0.00	MAM1
ATOM	15	HN2	MAM1	1	-1.886	-0.287	0.024	1.00	0.00	MAM1
ATOM	16	HN3	MAM1	1	-3.185	-1.343	-0.473	1.00	0.00	MAM1
ATOM	17	HN4	MAM1	1	-3.531	-0.143	0.587	1.00	0.00	MAM1
ATOM	18	H11	MAM1	1	-4.367	0.486	-1.600	1.00	0.00	MAM1
ATOM	19	H12	MAM1	1	-2.723	0.241	-2.233	1.00	0.00	MAM1
ATOM	20	H13	MAM1	1	-3.038	1.551	-1.079	1.00	0.00	MAM1
END										
REMARK 39_4MIM_MAM1										
ATOM	1	CB	4MIM	1	-2.845	1.216	-1.127	1.00	0.00	4MIM
ATOM	2	HB1	4MIM	1	-3.178	2.187	-0.762	1.00	0.00	4MIM
ATOM	3	HB2	4MIM	1	-2.581	1.322	-2.177	1.00	0.00	4MIM
ATOM	4	HB3	4MIM	1	-3.675	0.514	-1.057	1.00	0.00	4MIM
ATOM	5	CG	4MIM	1	-1.659	0.729	-0.366	1.00	0.00	4MIM
ATOM	6	ND1	4MIM	1	-1.678	0.494	0.993	1.00	0.00	4MIM
ATOM	7	HD1	4MIM	1	-2.477	0.622	1.600	1.00	0.00	4MIM
ATOM	8	CD2	4MIM	1	-0.371	0.418	-0.750	1.00	0.00	4MIM
ATOM	9	HD2	4MIM	1	0.053	0.471	-1.740	1.00	0.00	4MIM
ATOM	10	CE1	4MIM	1	-0.456	0.064	1.392	1.00	0.00	4MIM
ATOM	11	HE1	4MIM	1	-0.214	-0.187	2.411	1.00	0.00	4MIM
ATOM	12	NE2	4MIM	1	0.369	0.007	0.343	1.00	0.00	4MIM
ATOM	13	N	MAM1	1	2.903	-0.757	0.245	1.00	0.00	MAM1
ATOM	14	C1	MAM1	1	3.005	-1.882	-0.729	1.00	0.00	MAM1
ATOM	15	HN2	MAM1	1	1.838	-0.406	0.323	1.00	0.00	MAM1
ATOM	16	HN3	MAM1	1	3.489	0.029	-0.036	1.00	0.00	MAM1
ATOM	17	HN4	MAM1	1	3.221	-1.047	1.170	1.00	0.00	MAM1
ATOM	18	H11	MAM1	1	4.026	-2.245	-0.779	1.00	0.00	MAM1
ATOM	19	H12	MAM1	1	2.689	-1.521	-1.702	1.00	0.00	MAM1
ATOM	20	H13	MAM1	1	2.340	-2.675	-0.400	1.00	0.00	MAM1
END										
REMARK 40_4MIM_MAM1										
ATOM	1	CB	4MIM	1	3.188	0.752	-0.328	1.00	0.00	4MIM
ATOM	2	HB1	4MIM	1	3.507	1.587	0.295	1.00	0.00	4MIM

ATOM	3	HB2	4MIM	1	3.922	-0.049	-0.239	1.00	0.00	4MIM
ATOM	4	HB3	4MIM	1	3.178	1.087	-1.362	1.00	0.00	4MIM
ATOM	5	CG	4MIM	1	1.826	0.281	0.053	1.00	0.00	4MIM
ATOM	6	ND1	4MIM	1	1.517	-0.202	1.307	1.00	0.00	4MIM
ATOM	7	HD1	4MIM	1	2.163	-0.284	2.081	1.00	0.00	4MIM
ATOM	8	CD2	4MIM	1	0.641	0.198	-0.649	1.00	0.00	4MIM
ATOM	9	HD2	4MIM	1	0.461	0.478	-1.674	1.00	0.00	4MIM
ATOM	10	CE1	4MIM	1	0.208	-0.554	1.343	1.00	0.00	4MIM
ATOM	11	HE1	4MIM	1	-0.277	-0.961	2.214	1.00	0.00	4MIM
ATOM	12	NE2	4MIM	1	-0.357	-0.319	0.156	1.00	0.00	4MIM
ATOM	13	N	MAM1	1	-2.865	-0.695	-0.608	1.00	0.00	MAM1
ATOM	14	C1	MAM1	1	-3.395	0.609	-1.100	1.00	0.00	MAM1
ATOM	15	HN2	MAM1	1	-1.801	-0.577	-0.266	1.00	0.00	MAM1
ATOM	16	HN3	MAM1	1	-2.901	-1.408	-1.337	1.00	0.00	MAM1
ATOM	17	HN4	MAM1	1	-3.422	-1.042	0.172	1.00	0.00	MAM1
ATOM	18	H11	MAM1	1	-4.435	0.506	-1.394	1.00	0.00	MAM1
ATOM	19	H12	MAM1	1	-2.797	0.923	-1.949	1.00	0.00	MAM1
ATOM	20	H13	MAM1	1	-3.302	1.335	-0.299	1.00	0.00	MAM1

END

REMARK 41_4MIM_MAM1

ATOM	1	CB	4MIM	1	-3.117	1.043	0.155	1.00	0.00	4MIM
ATOM	2	HB1	4MIM	1	-3.572	1.203	-0.822	1.00	0.00	4MIM
ATOM	3	HB2	4MIM	1	-3.821	0.494	0.781	1.00	0.00	4MIM
ATOM	4	HB3	4MIM	1	-2.949	2.016	0.612	1.00	0.00	4MIM
ATOM	5	CG	4MIM	1	-1.819	0.321	0.038	1.00	0.00	4MIM
ATOM	6	ND1	4MIM	1	-1.703	-0.942	-0.505	1.00	0.00	4MIM
ATOM	7	HD1	4MIM	1	-2.466	-1.496	-0.872	1.00	0.00	4MIM
ATOM	8	CD2	4MIM	1	-0.530	0.660	0.396	1.00	0.00	4MIM
ATOM	9	HD2	4MIM	1	-0.193	1.572	0.859	1.00	0.00	4MIM
ATOM	10	CE1	4MIM	1	-0.405	-1.330	-0.469	1.00	0.00	4MIM
ATOM	11	HE1	4MIM	1	-0.056	-2.281	-0.834	1.00	0.00	4MIM
ATOM	12	NE2	4MIM	1	0.340	-0.367	0.079	1.00	0.00	4MIM
ATOM	13	N	MAM1	1	2.958	-0.305	0.467	1.00	0.00	MAM1
ATOM	14	C1	MAM1	1	3.492	0.913	-0.209	1.00	0.00	MAM1
ATOM	15	HN2	MAM1	1	1.844	-0.371	0.325	1.00	0.00	MAM1
ATOM	16	HN3	MAM1	1	3.165	-0.295	1.465	1.00	0.00	MAM1
ATOM	17	HN4	MAM1	1	3.387	-1.148	0.085	1.00	0.00	MAM1
ATOM	18	H11	MAM1	1	4.572	0.957	-0.106	1.00	0.00	MAM1
ATOM	19	H12	MAM1	1	3.039	1.785	0.252	1.00	0.00	MAM1
ATOM	20	H13	MAM1	1	3.216	0.867	-1.257	1.00	0.00	MAM1

END

REMARK 42_4MIM_MAM1

ATOM	1	CB	4MIM	1	0.052	3.272	0.360	1.00	0.00	4MIM
ATOM	2	HB1	4MIM	1	0.184	3.891	-0.527	1.00	0.00	4MIM
ATOM	3	HB2	4MIM	1	-0.789	3.660	0.935	1.00	0.00	4MIM
ATOM	4	HB3	4MIM	1	0.948	3.362	0.971	1.00	0.00	4MIM
ATOM	5	CG	4MIM	1	-0.156	1.842	-0.005	1.00	0.00	4MIM
ATOM	6	ND1	4MIM	1	-1.214	1.405	-0.775	1.00	0.00	4MIM
ATOM	7	HD1	4MIM	1	-1.941	1.992	-1.163	1.00	0.00	4MIM
ATOM	8	CD2	4MIM	1	0.556	0.695	0.282	1.00	0.00	4MIM
ATOM	9	HD2	4MIM	1	1.459	0.609	0.863	1.00	0.00	4MIM
ATOM	10	CE1	4MIM	1	-1.129	0.062	-0.936	1.00	0.00	4MIM
ATOM	11	HE1	4MIM	1	-1.839	-0.518	-1.501	1.00	0.00	4MIM
ATOM	12	NE2	4MIM	1	-0.051	-0.403	-0.297	1.00	0.00	4MIM
ATOM	13	N	MAM1	1	0.822	-2.894	-0.085	1.00	0.00	MAM1
ATOM	14	C1	MAM1	1	0.924	-3.223	1.366	1.00	0.00	MAM1
ATOM	15	HN2	MAM1	1	0.446	-1.844	-0.220	1.00	0.00	MAM1
ATOM	16	HN3	MAM1	1	0.184	-3.534	-0.558	1.00	0.00	MAM1
ATOM	17	HN4	MAM1	1	1.726	-2.984	-0.549	1.00	0.00	MAM1
ATOM	18	H11	MAM1	1	1.252	-4.249	1.497	1.00	0.00	MAM1
ATOM	19	H12	MAM1	1	-0.054	-3.080	1.814	1.00	0.00	MAM1
ATOM	20	H13	MAM1	1	1.637	-2.543	1.821	1.00	0.00	MAM1

END

REMARK 43_BENZ_MGUAN

ATOM	1	CG	BENZ	1	1.834	1.434	-0.444	1.00	0.00	BENZ
ATOM	2	HG	BENZ	1	1.664	2.504	-0.477	1.00	0.00	BENZ
ATOM	3	CD1	BENZ	1	2.096	0.800	0.779	1.00	0.00	BENZ
ATOM	4	HD1	BENZ	1	2.129	1.378	1.696	1.00	0.00	BENZ
ATOM	5	CD2	BENZ	1	1.847	0.694	-1.634	1.00	0.00	BENZ
ATOM	6	HD2	BENZ	1	1.665	1.187	-2.581	1.00	0.00	BENZ
ATOM	7	CE1	BENZ	1	2.378	-0.573	0.812	1.00	0.00	BENZ
ATOM	8	HE1	BENZ	1	2.607	-1.057	1.754	1.00	0.00	BENZ

ATOM	9	CE2	BENZ	1	2.135	-0.676	-1.602	1.00	0.00	BENZ
ATOM	10	HE2	BENZ	1	2.180	-1.242	-2.525	1.00	0.00	BENZ
ATOM	11	CZ	BENZ	1	2.402	-1.309	-0.379	1.00	0.00	BENZ
ATOM	12	HZ	BENZ	1	2.655	-2.363	-0.358	1.00	0.00	BENZ
ATOM	13	C	MGUA	1	-1.785	-0.212	0.322	1.00	0.00	MGUA
ATOM	14	N1	MGUA	1	-0.954	-1.118	-0.210	1.00	0.00	MGUA
ATOM	15	H11	MGUA	1	0.044	-0.947	-0.256	1.00	0.00	MGUA
ATOM	16	H12	MGUA	1	-1.316	-1.863	-0.784	1.00	0.00	MGUA
ATOM	17	N2	MGUA	1	-1.303	0.968	0.726	1.00	0.00	MGUA
ATOM	18	H21	MGUA	1	-1.826	1.551	1.360	1.00	0.00	MGUA
ATOM	19	H22	MGUA	1	-0.320	1.172	0.590	1.00	0.00	MGUA
ATOM	20	N3	MGUA	1	-3.091	-0.478	0.429	1.00	0.00	MGUA
ATOM	21	H31	MGUA	1	-3.382	-1.434	0.291	1.00	0.00	MGUA
ATOM	22	C2	MGUA	1	-4.084	0.488	0.898	1.00	0.00	MGUA
ATOM	23	HC1	MGUA	1	-5.067	0.066	0.717	1.00	0.00	MGUA
ATOM	24	HC2	MGUA	1	-3.979	0.682	1.966	1.00	0.00	MGUA
ATOM	25	HC3	MGUA	1	-3.996	1.413	0.332	1.00	0.00	MGUA

END

REMARK 44_BENZ_MGUA

ATOM	1	CG	BENZ	1	-2.029	-1.306	-0.314	1.00	0.00	BENZ
ATOM	2	HG	BENZ	1	-2.014	-2.373	-0.507	1.00	0.00	BENZ
ATOM	3	CD1	BENZ	1	-2.068	-0.830	1.004	1.00	0.00	BENZ
ATOM	4	HD1	BENZ	1	-2.082	-1.527	1.835	1.00	0.00	BENZ
ATOM	5	CD2	BENZ	1	-2.071	-0.406	-1.388	1.00	0.00	BENZ
ATOM	6	HD2	BENZ	1	-2.067	-0.775	-2.406	1.00	0.00	BENZ
ATOM	7	CE1	BENZ	1	-2.146	0.548	1.250	1.00	0.00	BENZ
ATOM	8	HE1	BENZ	1	-2.198	0.914	2.268	1.00	0.00	BENZ
ATOM	9	CE2	BENZ	1	-2.160	0.971	-1.141	1.00	0.00	BENZ
ATOM	10	HE2	BENZ	1	-2.228	1.665	-1.970	1.00	0.00	BENZ
ATOM	11	CZ	BENZ	1	-2.197	1.447	0.178	1.00	0.00	BENZ
ATOM	12	HZ	BENZ	1	-2.292	2.509	0.367	1.00	0.00	BENZ
ATOM	13	C	MGUA	1	1.832	-0.331	0.172	1.00	0.00	MGUA
ATOM	14	N1	MGUA	1	1.252	-1.466	0.592	1.00	0.00	MGUA
ATOM	15	H11	MGUA	1	0.242	-1.534	0.585	1.00	0.00	MGUA
ATOM	16	H12	MGUA	1	1.783	-2.320	0.650	1.00	0.00	MGUA
ATOM	17	N2	MGUA	1	1.073	0.659	-0.305	1.00	0.00	MGUA
ATOM	18	H21	MGUA	1	1.438	1.595	-0.372	1.00	0.00	MGUA
ATOM	19	H22	MGUA	1	0.071	0.549	-0.404	1.00	0.00	MGUA
ATOM	20	N3	MGUA	1	3.161	-0.200	0.220	1.00	0.00	MGUA
ATOM	21	H31	MGUA	1	3.675	-0.882	0.758	1.00	0.00	MGUA
ATOM	22	C2	MGUA	1	3.885	0.955	-0.308	1.00	0.00	MGUA
ATOM	23	HC1	MGUA	1	4.944	0.718	-0.290	1.00	0.00	MGUA
ATOM	24	HC2	MGUA	1	3.589	1.137	-1.339	1.00	0.00	MGUA
ATOM	25	HC3	MGUA	1	3.717	1.844	0.300	1.00	0.00	MGUA

END

REMARK 45_BENZ_MGUA

ATOM	1	CG	BENZ	1	1.848	1.509	0.292	1.00	0.00	BENZ
ATOM	2	HG	BENZ	1	1.921	2.429	0.858	1.00	0.00	BENZ
ATOM	3	CD1	BENZ	1	2.124	0.283	0.914	1.00	0.00	BENZ
ATOM	4	HD1	BENZ	1	2.406	0.256	1.959	1.00	0.00	BENZ
ATOM	5	CD2	BENZ	1	1.516	1.546	-1.070	1.00	0.00	BENZ
ATOM	6	HD2	BENZ	1	1.331	2.496	-1.556	1.00	0.00	BENZ
ATOM	7	CE1	BENZ	1	2.081	-0.904	0.167	1.00	0.00	BENZ
ATOM	8	HE1	BENZ	1	2.350	-1.844	0.637	1.00	0.00	BENZ
ATOM	9	CE2	BENZ	1	1.466	0.360	-1.813	1.00	0.00	BENZ
ATOM	10	HE2	BENZ	1	1.234	0.392	-2.871	1.00	0.00	BENZ
ATOM	11	CZ	BENZ	1	1.752	-0.865	-1.195	1.00	0.00	BENZ
ATOM	12	HZ	BENZ	1	1.764	-1.775	-1.784	1.00	0.00	BENZ
ATOM	13	C	MGUA	1	-1.873	-0.817	0.467	1.00	0.00	MGUA
ATOM	14	N1	MGUA	1	-1.193	-1.941	0.186	1.00	0.00	MGUA
ATOM	15	H11	MGUA	1	-1.534	-2.833	0.511	1.00	0.00	MGUA
ATOM	16	H12	MGUA	1	-0.212	-1.869	-0.051	1.00	0.00	MGUA
ATOM	17	N2	MGUA	1	-3.186	-0.903	0.740	1.00	0.00	MGUA
ATOM	18	H21	MGUA	1	-3.718	-0.087	0.995	1.00	0.00	MGUA
ATOM	19	H22	MGUA	1	-3.705	-1.727	0.480	1.00	0.00	MGUA
ATOM	20	N3	MGUA	1	-1.257	0.357	0.456	1.00	0.00	MGUA
ATOM	21	H31	MGUA	1	-0.243	0.365	0.403	1.00	0.00	MGUA
ATOM	22	C2	MGUA	1	-1.944	1.645	0.527	1.00	0.00	MGUA
ATOM	23	HC1	MGUA	1	-1.205	2.415	0.334	1.00	0.00	MGUA
ATOM	24	HC2	MGUA	1	-2.717	1.704	-0.238	1.00	0.00	MGUA
ATOM	25	HC3	MGUA	1	-2.372	1.812	1.515	1.00	0.00	MGUA

END

REMARK 46_TOLU_MGUA

ATOM	1	CB	TOLU	1	-2.500	-1.872	-0.836	1.00	0.00	TOLU
ATOM	2	HB1	TOLU	1	-2.694	-2.227	0.177	1.00	0.00	TOLU
ATOM	3	HB2	TOLU	1	-1.819	-2.569	-1.323	1.00	0.00	TOLU
ATOM	4	HB3	TOLU	1	-3.447	-1.901	-1.376	1.00	0.00	TOLU
ATOM	5	CG	TOLU	1	-1.942	-0.471	-0.833	1.00	0.00	TOLU
ATOM	6	CD1	TOLU	1	-1.249	0.025	-1.952	1.00	0.00	TOLU
ATOM	7	HD1	TOLU	1	-1.070	-0.628	-2.799	1.00	0.00	TOLU
ATOM	8	CD2	TOLU	1	-2.180	0.402	0.244	1.00	0.00	TOLU
ATOM	9	HD2	TOLU	1	-2.746	0.052	1.101	1.00	0.00	TOLU
ATOM	10	CE1	TOLU	1	-0.825	1.357	-2.003	1.00	0.00	TOLU
ATOM	11	HE1	TOLU	1	-0.322	1.727	-2.889	1.00	0.00	TOLU
ATOM	12	CE2	TOLU	1	-1.752	1.737	0.201	1.00	0.00	TOLU
ATOM	13	HE2	TOLU	1	-1.969	2.399	1.030	1.00	0.00	TOLU
ATOM	14	CZ	TOLU	1	-1.077	2.220	-0.927	1.00	0.00	TOLU
ATOM	15	HZ	TOLU	1	-0.775	3.259	-0.977	1.00	0.00	TOLU
ATOM	16	C	MGUA	1	1.597	-0.634	1.027	1.00	0.00	MGUA
ATOM	17	N1	MGUA	1	0.498	-1.361	1.281	1.00	0.00	MGUA
ATOM	18	H11	MGUA	1	-0.390	-1.049	0.905	1.00	0.00	MGUA
ATOM	19	H12	MGUA	1	0.482	-2.004	2.057	1.00	0.00	MGUA
ATOM	20	N2	MGUA	1	1.492	0.492	0.317	1.00	0.00	MGUA
ATOM	21	H21	MGUA	1	2.306	0.911	-0.103	1.00	0.00	MGUA
ATOM	22	H22	MGUA	1	0.587	0.835	0.011	1.00	0.00	MGUA
ATOM	23	N3	MGUA	1	2.786	-1.032	1.490	1.00	0.00	MGUA
ATOM	24	H31	MGUA	1	2.852	-1.973	1.849	1.00	0.00	MGUA
ATOM	25	C2	MGUA	1	4.019	-0.260	1.340	1.00	0.00	MGUA
ATOM	26	HC1	MGUA	1	4.783	-0.735	1.945	1.00	0.00	MGUA
ATOM	27	HC2	MGUA	1	4.356	-0.243	0.303	1.00	0.00	MGUA
ATOM	28	HC3	MGUA	1	3.868	0.753	1.707	1.00	0.00	MGUA

END

REMARK 47_TOLU_MGUA

ATOM	1	CB	TOLU	1	2.637	2.230	-0.266	1.00	0.00	TOLU
ATOM	2	HB1	TOLU	1	2.324	2.865	0.562	1.00	0.00	TOLU
ATOM	3	HB2	TOLU	1	2.244	2.647	-1.192	1.00	0.00	TOLU
ATOM	4	HB3	TOLU	1	3.726	2.271	-0.319	1.00	0.00	TOLU
ATOM	5	CG	TOLU	1	2.178	0.809	-0.069	1.00	0.00	TOLU
ATOM	6	CD1	TOLU	1	1.990	-0.045	-1.169	1.00	0.00	TOLU
ATOM	7	HD1	TOLU	1	2.134	0.339	-2.172	1.00	0.00	TOLU
ATOM	8	CD2	TOLU	1	2.011	0.277	1.223	1.00	0.00	TOLU
ATOM	9	HD2	TOLU	1	2.180	0.912	2.086	1.00	0.00	TOLU
ATOM	10	CE1	TOLU	1	1.647	-1.390	-0.987	1.00	0.00	TOLU
ATOM	11	HE1	TOLU	1	1.552	-2.041	-1.850	1.00	0.00	TOLU
ATOM	12	CE2	TOLU	1	1.661	-1.066	1.413	1.00	0.00	TOLU
ATOM	13	HE2	TOLU	1	1.558	-1.460	2.418	1.00	0.00	TOLU
ATOM	14	CZ	TOLU	1	1.480	-1.906	0.306	1.00	0.00	TOLU
ATOM	15	HZ	TOLU	1	1.259	-2.957	0.453	1.00	0.00	TOLU
ATOM	16	C	MGUA	1	-2.091	-0.180	-0.180	1.00	0.00	MGUA
ATOM	17	N1	MGUA	1	-1.723	-1.373	-0.671	1.00	0.00	MGUA
ATOM	18	H11	MGUA	1	-0.746	-1.637	-0.635	1.00	0.00	MGUA
ATOM	19	H12	MGUA	1	-2.406	-2.102	-0.803	1.00	0.00	MGUA
ATOM	20	N2	MGUA	1	-1.177	0.606	0.394	1.00	0.00	MGUA
ATOM	21	H21	MGUA	1	-1.363	1.584	0.548	1.00	0.00	MGUA
ATOM	22	H22	MGUA	1	-0.228	0.284	0.549	1.00	0.00	MGUA
ATOM	23	N3	MGUA	1	-3.367	0.213	-0.261	1.00	0.00	MGUA
ATOM	24	H31	MGUA	1	-3.973	-0.308	-0.877	1.00	0.00	MGUA
ATOM	25	C2	MGUA	1	-3.880	1.445	0.337	1.00	0.00	MGUA
ATOM	26	HC1	MGUA	1	-4.962	1.422	0.265	1.00	0.00	MGUA
ATOM	27	HC2	MGUA	1	-3.604	1.488	1.389	1.00	0.00	MGUA
ATOM	28	HC3	MGUA	1	-3.514	2.327	-0.190	1.00	0.00	MGUA

END

REMARK 48_TOLU_MGUA

ATOM	1	CB	TOLU	1	2.493	2.166	-0.480	1.00	0.00	TOLU
ATOM	2	HB1	TOLU	1	2.152	2.870	0.279	1.00	0.00	TOLU
ATOM	3	HB2	TOLU	1	2.067	2.461	-1.438	1.00	0.00	TOLU
ATOM	4	HB3	TOLU	1	3.578	2.258	-0.555	1.00	0.00	TOLU
ATOM	5	CG	TOLU	1	2.109	0.755	-0.124	1.00	0.00	TOLU
ATOM	6	CD1	TOLU	1	1.905	-0.211	-1.126	1.00	0.00	TOLU
ATOM	7	HD1	TOLU	1	2.006	0.078	-2.168	1.00	0.00	TOLU
ATOM	8	CD2	TOLU	1	2.037	0.342	1.217	1.00	0.00	TOLU
ATOM	9	HD2	TOLU	1	2.224	1.063	2.005	1.00	0.00	TOLU
ATOM	10	CE1	TOLU	1	1.618	-1.544	-0.799	1.00	0.00	TOLU
ATOM	11	HE1	TOLU	1	1.504	-2.282	-1.586	1.00	0.00	TOLU

ATOM	12	CE2	TOLU	1	1.758	-0.991	1.552	1.00	0.00	TOLU
ATOM	13	HE2	TOLU	1	1.733	-1.291	2.592	1.00	0.00	TOLU
ATOM	14	CZ	TOLU	1	1.542	-1.939	0.543	1.00	0.00	TOLU
ATOM	15	HZ	TOLU	1	1.346	-2.973	0.798	1.00	0.00	TOLU
ATOM	16	C	MGUA	1	-2.017	0.075	-0.380	1.00	0.00	MGUA
ATOM	17	N1	MGUA	1	-1.445	-0.277	-1.543	1.00	0.00	MGUA
ATOM	18	H11	MGUA	1	-0.459	-0.511	-1.550	1.00	0.00	MGUA
ATOM	19	H12	MGUA	1	-2.012	-0.604	-2.309	1.00	0.00	MGUA
ATOM	20	N2	MGUA	1	-1.284	0.088	0.735	1.00	0.00	MGUA
ATOM	21	H21	MGUA	1	-1.612	0.562	1.561	1.00	0.00	MGUA
ATOM	22	H22	MGUA	1	-0.324	-0.240	0.740	1.00	0.00	MGUA
ATOM	23	N3	MGUA	1	-3.311	0.410	-0.345	1.00	0.00	MGUA
ATOM	24	H31	MGUA	1	-3.770	0.577	-1.228	1.00	0.00	MGUA
ATOM	25	C2	MGUA	1	-4.038	0.723	0.885	1.00	0.00	MGUA
ATOM	26	HC1	MGUA	1	-5.091	0.799	0.636	1.00	0.00	MGUA
ATOM	27	HC2	MGUA	1	-3.911	-0.083	1.605	1.00	0.00	MGUA
ATOM	28	HC3	MGUA	1	-3.711	1.671	1.312	1.00	0.00	MGUA

END

REMARK 49_TOLU_MGUAN

ATOM	1	CB	TOLU	1	2.057	2.495	0.026	1.00	0.00	TOLU
ATOM	2	HB1	TOLU	1	1.524	2.949	-0.809	1.00	0.00	TOLU
ATOM	3	HB2	TOLU	1	3.107	2.783	-0.057	1.00	0.00	TOLU
ATOM	4	HB3	TOLU	1	1.677	2.920	0.955	1.00	0.00	TOLU
ATOM	5	CG	TOLU	1	1.925	0.993	0.010	1.00	0.00	TOLU
ATOM	6	CD1	TOLU	1	1.859	0.258	1.208	1.00	0.00	TOLU
ATOM	7	HD1	TOLU	1	1.870	0.783	2.158	1.00	0.00	TOLU
ATOM	8	CD2	TOLU	1	1.959	0.284	-1.204	1.00	0.00	TOLU
ATOM	9	HD2	TOLU	1	2.026	0.832	-2.138	1.00	0.00	TOLU
ATOM	10	CE1	TOLU	1	1.842	-1.144	1.197	1.00	0.00	TOLU
ATOM	11	HE1	TOLU	1	1.817	-1.690	2.133	1.00	0.00	TOLU
ATOM	12	CE2	TOLU	1	1.949	-1.115	-1.221	1.00	0.00	TOLU
ATOM	13	HE2	TOLU	1	2.009	-1.641	-2.166	1.00	0.00	TOLU
ATOM	14	CZ	TOLU	1	1.892	-1.835	-0.019	1.00	0.00	TOLU
ATOM	15	HZ	TOLU	1	1.913	-2.918	-0.030	1.00	0.00	TOLU
ATOM	16	C	MGUA	1	-1.991	0.169	0.136	1.00	0.00	MGUA
ATOM	17	N1	MGUA	1	-1.343	1.191	0.718	1.00	0.00	MGUA
ATOM	18	H11	MGUA	1	-0.335	1.138	0.812	1.00	0.00	MGUA
ATOM	19	H12	MGUA	1	-1.839	1.829	1.320	1.00	0.00	MGUA
ATOM	20	N2	MGUA	1	-1.301	-0.896	-0.279	1.00	0.00	MGUA
ATOM	21	H21	MGUA	1	-1.706	-1.545	-0.934	1.00	0.00	MGUA
ATOM	22	H22	MGUA	1	-0.303	-0.969	-0.117	1.00	0.00	MGUA
ATOM	23	N3	MGUA	1	-3.318	0.217	-0.017	1.00	0.00	MGUA
ATOM	24	H31	MGUA	1	-3.769	1.108	0.131	1.00	0.00	MGUA
ATOM	25	C2	MGUA	1	-4.115	-0.882	-0.558	1.00	0.00	MGUA
ATOM	26	HC1	MGUA	1	-5.162	-0.633	-0.416	1.00	0.00	MGUA
ATOM	27	HC2	MGUA	1	-3.932	-1.022	-1.624	1.00	0.00	MGUA
ATOM	28	HC3	MGUA	1	-3.901	-1.799	-0.012	1.00	0.00	MGUA

END

REMARK 50_TOLU_MGUAN

ATOM	1	CB	TOLU	1	1.872	2.603	0.311	1.00	0.00	TOLU
ATOM	2	HB1	TOLU	1	1.304	2.912	1.188	1.00	0.00	TOLU
ATOM	3	HB2	TOLU	1	1.467	3.110	-0.566	1.00	0.00	TOLU
ATOM	4	HB3	TOLU	1	2.897	2.955	0.441	1.00	0.00	TOLU
ATOM	5	CG	TOLU	1	1.851	1.105	0.142	1.00	0.00	TOLU
ATOM	6	CD1	TOLU	1	1.882	0.520	-1.137	1.00	0.00	TOLU
ATOM	7	HD1	TOLU	1	1.883	1.158	-2.016	1.00	0.00	TOLU
ATOM	8	CD2	TOLU	1	1.895	0.257	1.263	1.00	0.00	TOLU
ATOM	9	HD2	TOLU	1	1.890	0.688	2.258	1.00	0.00	TOLU
ATOM	10	CE1	TOLU	1	1.964	-0.869	-1.295	1.00	0.00	TOLU
ATOM	11	HE1	TOLU	1	2.008	-1.297	-2.290	1.00	0.00	TOLU
ATOM	12	CE2	TOLU	1	1.986	-1.132	1.112	1.00	0.00	TOLU
ATOM	13	HE2	TOLU	1	2.052	-1.765	1.989	1.00	0.00	TOLU
ATOM	14	CZ	TOLU	1	2.021	-1.700	-0.170	1.00	0.00	TOLU
ATOM	15	HZ	TOLU	1	2.119	-2.772	-0.289	1.00	0.00	TOLU
ATOM	16	C	MGUA	1	-1.995	0.050	-0.162	1.00	0.00	MGUA
ATOM	17	N1	MGUA	1	-1.397	1.173	-0.586	1.00	0.00	MGUA
ATOM	18	H11	MGUA	1	-0.386	1.202	-0.642	1.00	0.00	MGUA
ATOM	19	H12	MGUA	1	-1.900	2.047	-0.599	1.00	0.00	MGUA
ATOM	20	N2	MGUA	1	-1.249	-0.976	0.254	1.00	0.00	MGUA
ATOM	21	H21	MGUA	1	-1.643	-1.901	0.325	1.00	0.00	MGUA
ATOM	22	H22	MGUA	1	-0.240	-0.899	0.318	1.00	0.00	MGUA
ATOM	23	N3	MGUA	1	-3.329	-0.032	-0.141	1.00	0.00	MGUA

ATOM	24	H31	MGUA	1	-3.844	0.670	-0.651	1.00	0.00	MGUA
ATOM	25	C2	MGUA	1	-4.067	-1.174	0.399	1.00	0.00	MGUA
ATOM	26	HC1	MGUA	1	-5.115	-0.899	0.445	1.00	0.00	MGUA
ATOM	27	HC2	MGUA	1	-3.965	-2.053	-0.237	1.00	0.00	MGUA
ATOM	28	HC3	MGUA	1	-3.722	-1.392	1.408	1.00	0.00	MGUA

END

REMARK 51_PHEN_MGUAN

ATOM	1	CG	PHEN	1	1.705	-1.769	0.873	1.00	0.00	PHEN
ATOM	2	HG	PHEN	1	1.651	-2.817	1.137	1.00	0.00	PHEN
ATOM	3	CD1	PHEN	1	1.901	-1.385	-0.460	1.00	0.00	PHEN
ATOM	4	HD1	PHEN	1	1.997	-2.138	-1.233	1.00	0.00	PHEN
ATOM	5	CD2	PHEN	1	1.646	-0.786	1.868	1.00	0.00	PHEN
ATOM	6	HD2	PHEN	1	1.523	-1.069	2.907	1.00	0.00	PHEN
ATOM	7	CE1	PHEN	1	2.007	-0.031	-0.800	1.00	0.00	PHEN
ATOM	8	HE1	PHEN	1	2.235	0.281	-1.814	1.00	0.00	PHEN
ATOM	9	CE2	PHEN	1	1.746	0.572	1.538	1.00	0.00	PHEN
ATOM	10	HE2	PHEN	1	1.714	1.325	2.318	1.00	0.00	PHEN
ATOM	11	CZ	PHEN	1	1.934	0.948	0.202	1.00	0.00	PHEN
ATOM	12	OH	PHEN	1	2.040	2.249	-0.209	1.00	0.00	PHEN
ATOM	13	HH	PHEN	1	2.134	2.838	0.554	1.00	0.00	PHEN
ATOM	14	C	MGUA	1	-1.927	-0.126	-0.724	1.00	0.00	MGUA
ATOM	15	N1	MGUA	1	-1.116	-0.184	-1.791	1.00	0.00	MGUA
ATOM	16	H11	MGUA	1	-0.116	-0.245	-1.636	1.00	0.00	MGUA
ATOM	17	H12	MGUA	1	-1.416	0.212	-2.669	1.00	0.00	MGUA
ATOM	18	N2	MGUA	1	-1.416	-0.284	0.502	1.00	0.00	MGUA
ATOM	19	H21	MGUA	1	-2.025	-0.472	1.283	1.00	0.00	MGUA
ATOM	20	H22	MGUA	1	-0.435	-0.506	0.630	1.00	0.00	MGUA
ATOM	21	N3	MGUA	1	-3.234	0.100	-0.883	1.00	0.00	MGUA
ATOM	22	H31	MGUA	1	-3.596	0.089	-1.825	1.00	0.00	MGUA
ATOM	23	C2	MGUA	1	-4.190	0.169	0.222	1.00	0.00	MGUA
ATOM	24	HC1	MGUA	1	-5.151	0.457	-0.191	1.00	0.00	MGUA
ATOM	25	HC2	MGUA	1	-4.298	-0.797	0.715	1.00	0.00	MGUA
ATOM	26	HC3	MGUA	1	-3.882	0.931	0.936	1.00	0.00	MGUA

END

REMARK 52_PHEN_MGUAN

ATOM	1	CG	PHEN	1	2.274	-2.273	-0.142	1.00	0.00	PHEN
ATOM	2	HG	PHEN	1	2.472	-3.333	-0.229	1.00	0.00	PHEN
ATOM	3	CD1	PHEN	1	1.921	-1.529	-1.273	1.00	0.00	PHEN
ATOM	4	HD1	PHEN	1	1.849	-2.009	-2.241	1.00	0.00	PHEN
ATOM	5	CD2	PHEN	1	2.405	-1.635	1.097	1.00	0.00	PHEN
ATOM	6	HD2	PHEN	1	2.695	-2.201	1.973	1.00	0.00	PHEN
ATOM	7	CE1	PHEN	1	1.681	-0.153	-1.169	1.00	0.00	PHEN
ATOM	8	HE1	PHEN	1	1.439	0.446	-2.038	1.00	0.00	PHEN
ATOM	9	CE2	PHEN	1	2.153	-0.264	1.220	1.00	0.00	PHEN
ATOM	10	HE2	PHEN	1	2.239	0.228	2.182	1.00	0.00	PHEN
ATOM	11	CZ	PHEN	1	1.794	0.463	0.081	1.00	0.00	PHEN
ATOM	12	OH	PHEN	1	1.433	1.808	0.141	1.00	0.00	PHEN
ATOM	13	HH	PHEN	1	1.841	2.227	0.914	1.00	0.00	PHEN
ATOM	14	C	MGUA	1	-2.027	0.328	-0.015	1.00	0.00	MGUA
ATOM	15	N1	MGUA	1	-1.281	-0.765	0.200	1.00	0.00	MGUA
ATOM	16	H11	MGUA	1	-0.307	-0.787	-0.077	1.00	0.00	MGUA
ATOM	17	H12	MGUA	1	-1.698	-1.613	0.549	1.00	0.00	MGUA
ATOM	18	N2	MGUA	1	-1.433	1.504	-0.238	1.00	0.00	MGUA
ATOM	19	H21	MGUA	1	-1.967	2.283	-0.585	1.00	0.00	MGUA
ATOM	20	H22	MGUA	1	-0.435	1.646	-0.080	1.00	0.00	MGUA
ATOM	21	N3	MGUA	1	-3.362	0.244	0.025	1.00	0.00	MGUA
ATOM	22	H31	MGUA	1	-3.771	-0.676	-0.040	1.00	0.00	MGUA
ATOM	23	C2	MGUA	1	-4.256	1.401	-0.001	1.00	0.00	MGUA
ATOM	24	HC1	MGUA	1	-5.256	1.052	0.235	1.00	0.00	MGUA
ATOM	25	HC2	MGUA	1	-3.953	2.121	0.756	1.00	0.00	MGUA
ATOM	26	HC3	MGUA	1	-4.275	1.870	-0.985	1.00	0.00	MGUA

END

REMARK 53_PHEN_MGUAN

ATOM	1	CG	PHEN	1	-2.240	-2.029	-0.221	1.00	0.00	PHEN
ATOM	2	HG	PHEN	1	-2.432	-3.085	-0.361	1.00	0.00	PHEN
ATOM	3	CD1	PHEN	1	-1.887	-1.541	1.042	1.00	0.00	PHEN
ATOM	4	HD1	PHEN	1	-1.808	-2.217	1.885	1.00	0.00	PHEN
ATOM	5	CD2	PHEN	1	-2.380	-1.142	-1.294	1.00	0.00	PHEN
ATOM	6	HD2	PHEN	1	-2.672	-1.510	-2.270	1.00	0.00	PHEN
ATOM	7	CE1	PHEN	1	-1.654	-0.174	1.233	1.00	0.00	PHEN
ATOM	8	HE1	PHEN	1	-1.409	0.228	2.209	1.00	0.00	PHEN
ATOM	9	CE2	PHEN	1	-2.136	0.225	-1.122	1.00	0.00	PHEN

ATOM	10	HE2	PHEN	1	-2.229	0.910	-1.957	1.00	0.00	PHEN
ATOM	11	CZ	PHEN	1	-1.775	0.694	0.144	1.00	0.00	PHEN
ATOM	12	OH	PHEN	1	-1.420	2.022	0.371	1.00	0.00	PHEN
ATOM	13	HH	PHEN	1	-1.844	2.597	-0.284	1.00	0.00	PHEN
ATOM	14	C	MGUA	1	2.031	0.509	0.061	1.00	0.00	MGUA
ATOM	15	N1	MGUA	1	1.465	1.609	0.573	1.00	0.00	MGUA
ATOM	16	H11	MGUA	1	0.466	1.797	0.491	1.00	0.00	MGUA
ATOM	17	H12	MGUA	1	2.036	2.304	1.028	1.00	0.00	MGUA
ATOM	18	N2	MGUA	1	1.270	-0.540	-0.270	1.00	0.00	MGUA
ATOM	19	H21	MGUA	1	1.635	-1.288	-0.837	1.00	0.00	MGUA
ATOM	20	H22	MGUA	1	0.300	-0.584	0.017	1.00	0.00	MGUA
ATOM	21	N3	MGUA	1	3.359	0.446	-0.091	1.00	0.00	MGUA
ATOM	22	H31	MGUA	1	3.872	1.313	-0.048	1.00	0.00	MGUA
ATOM	23	C2	MGUA	1	4.086	-0.773	-0.442	1.00	0.00	MGUA
ATOM	24	HC1	MGUA	1	5.144	-0.582	-0.296	1.00	0.00	MGUA
ATOM	25	HC2	MGUA	1	3.785	-1.586	0.216	1.00	0.00	MGUA
ATOM	26	HC3	MGUA	1	3.924	-1.050	-1.484	1.00	0.00	MGUA

END

REMARK 54_PHEN_MGUA

ATOM	1	CG	PHEN	1	2.375	-1.884	-0.053	1.00	0.00	PHEN
ATOM	2	HG	PHEN	1	2.642	-2.929	-0.141	1.00	0.00	PHEN
ATOM	3	CD1	PHEN	1	2.078	-1.136	-1.198	1.00	0.00	PHEN
ATOM	4	HD1	PHEN	1	2.117	-1.598	-2.177	1.00	0.00	PHEN
ATOM	5	CD2	PHEN	1	2.363	-1.267	1.203	1.00	0.00	PHEN
ATOM	6	HD2	PHEN	1	2.610	-1.835	2.091	1.00	0.00	PHEN
ATOM	7	CE1	PHEN	1	1.750	0.221	-1.091	1.00	0.00	PHEN
ATOM	8	HE1	PHEN	1	1.546	0.825	-1.967	1.00	0.00	PHEN
ATOM	9	CE2	PHEN	1	2.022	0.084	1.327	1.00	0.00	PHEN
ATOM	10	HE2	PHEN	1	1.996	0.559	2.302	1.00	0.00	PHEN
ATOM	11	CZ	PHEN	1	1.719	0.815	0.175	1.00	0.00	PHEN
ATOM	12	OH	PHEN	1	1.275	2.134	0.226	1.00	0.00	PHEN
ATOM	13	HH	PHEN	1	1.602	2.565	1.031	1.00	0.00	PHEN
ATOM	14	C	MGUA	1	-2.055	0.385	-0.122	1.00	0.00	MGUA
ATOM	15	N1	MGUA	1	-1.548	1.610	-0.312	1.00	0.00	MGUA
ATOM	16	H11	MGUA	1	-0.573	1.833	-0.113	1.00	0.00	MGUA
ATOM	17	H12	MGUA	1	-2.141	2.355	-0.641	1.00	0.00	MGUA
ATOM	18	N2	MGUA	1	-1.237	-0.662	0.019	1.00	0.00	MGUA
ATOM	19	H21	MGUA	1	-1.579	-1.547	0.357	1.00	0.00	MGUA
ATOM	20	H22	MGUA	1	-0.249	-0.577	-0.188	1.00	0.00	MGUA
ATOM	21	N3	MGUA	1	-3.382	0.205	-0.101	1.00	0.00	MGUA
ATOM	22	H31	MGUA	1	-3.959	1.024	0.016	1.00	0.00	MGUA
ATOM	23	C2	MGUA	1	-4.030	-1.105	-0.103	1.00	0.00	MGUA
ATOM	24	HC1	MGUA	1	-5.088	-0.951	-0.285	1.00	0.00	MGUA
ATOM	25	HC2	MGUA	1	-3.625	-1.717	-0.907	1.00	0.00	MGUA
ATOM	26	HC3	MGUA	1	-3.913	-1.612	0.855	1.00	0.00	MGUA

END

REMARK 55_PHEN_MGUA

ATOM	1	CG	PHEN	1	-1.320	2.048	1.128	1.00	0.00	PHEN
ATOM	2	HG	PHEN	1	-1.300	3.010	1.624	1.00	0.00	PHEN
ATOM	3	CD1	PHEN	1	-1.600	1.968	-0.242	1.00	0.00	PHEN
ATOM	4	HD1	PHEN	1	-1.814	2.867	-0.807	1.00	0.00	PHEN
ATOM	5	CD2	PHEN	1	-1.116	0.875	1.863	1.00	0.00	PHEN
ATOM	6	HD2	PHEN	1	-0.942	0.927	2.931	1.00	0.00	PHEN
ATOM	7	CE1	PHEN	1	-1.662	0.723	-0.880	1.00	0.00	PHEN
ATOM	8	HE1	PHEN	1	-1.929	0.638	-1.926	1.00	0.00	PHEN
ATOM	9	CE2	PHEN	1	-1.158	-0.374	1.232	1.00	0.00	PHEN
ATOM	10	HE2	PHEN	1	-1.006	-1.285	1.801	1.00	0.00	PHEN
ATOM	11	CZ	PHEN	1	-1.426	-0.439	-0.139	1.00	0.00	PHEN
ATOM	12	OH	PHEN	1	-1.410	-1.642	-0.838	1.00	0.00	PHEN
ATOM	13	HH	PHEN	1	-1.788	-2.347	-0.290	1.00	0.00	PHEN
ATOM	14	C	MGUA	1	1.602	-0.331	-0.774	1.00	0.00	MGUA
ATOM	15	N1	MGUA	1	1.093	-0.660	-1.977	1.00	0.00	MGUA
ATOM	16	H11	MGUA	1	0.927	0.082	-2.640	1.00	0.00	MGUA
ATOM	17	H12	MGUA	1	0.441	-1.436	-2.009	1.00	0.00	MGUA
ATOM	18	N2	MGUA	1	1.778	0.956	-0.451	1.00	0.00	MGUA
ATOM	19	H21	MGUA	1	2.271	1.209	0.392	1.00	0.00	MGUA
ATOM	20	H22	MGUA	1	1.128	1.640	-0.813	1.00	0.00	MGUA
ATOM	21	N3	MGUA	1	1.984	-1.305	0.051	1.00	0.00	MGUA
ATOM	22	H31	MGUA	1	2.080	-2.226	-0.355	1.00	0.00	MGUA
ATOM	23	C2	MGUA	1	2.420	-1.095	1.430	1.00	0.00	MGUA
ATOM	24	HC1	MGUA	1	2.448	-2.062	1.921	1.00	0.00	MGUA
ATOM	25	HC2	MGUA	1	3.418	-0.657	1.469	1.00	0.00	MGUA

ATOM	26	HC3	MGUA	1	1.703	-0.460	1.947	1.00	0.00	MGUA
END										
REMARK	56_CRES_MGUAN									
ATOM	1	CB	CRES	1	-1.869	3.092	0.948	1.00	0.00	CRES
ATOM	2	HB1	CRES	1	-2.920	3.381	1.024	1.00	0.00	CRES
ATOM	3	HB2	CRES	1	-1.410	3.707	0.172	1.00	0.00	CRES
ATOM	4	HB3	CRES	1	-1.391	3.324	1.901	1.00	0.00	CRES
ATOM	5	CG	CRES	1	-1.747	1.626	0.621	1.00	0.00	CRES
ATOM	6	CD1	CRES	1	-1.795	1.171	-0.711	1.00	0.00	CRES
ATOM	7	HD1	CRES	1	-1.876	1.889	-1.522	1.00	0.00	CRES
ATOM	8	CD2	CRES	1	-1.666	0.659	1.636	1.00	0.00	CRES
ATOM	9	HD2	CRES	1	-1.632	0.933	2.681	1.00	0.00	CRES
ATOM	10	CE1	CRES	1	-1.736	-0.197	-1.020	1.00	0.00	CRES
ATOM	11	HE1	CRES	1	-1.807	-0.552	-2.044	1.00	0.00	CRES
ATOM	12	CE2	CRES	1	-1.619	-0.709	1.349	1.00	0.00	CRES
ATOM	13	HE2	CRES	1	-1.547	-1.435	2.155	1.00	0.00	CRES
ATOM	14	CZ	CRES	1	-1.647	-1.128	0.021	1.00	0.00	CRES
ATOM	15	OZ	CRES	1	-1.485	-2.467	-0.315	1.00	0.00	CRES
ATOM	16	HZ	CRES	1	-1.723	-3.024	0.444	1.00	0.00	CRES
ATOM	17	C	MGUA	1	2.051	-0.537	-0.575	1.00	0.00	MGUA
ATOM	18	N1	MGUA	1	1.424	-1.452	-1.349	1.00	0.00	MGUA
ATOM	19	H11	MGUA	1	0.426	-1.702	-1.264	1.00	0.00	MGUA
ATOM	20	H12	MGUA	1	2.000	-2.185	-1.739	1.00	0.00	MGUA
ATOM	21	N2	MGUA	1	1.389	0.223	0.299	1.00	0.00	MGUA
ATOM	22	H21	MGUA	1	1.849	0.995	0.755	1.00	0.00	MGUA
ATOM	23	H22	MGUA	1	0.407	0.078	0.509	1.00	0.00	MGUA
ATOM	24	N3	MGUA	1	3.374	-0.375	-0.722	1.00	0.00	MGUA
ATOM	25	H31	MGUA	1	3.800	-0.809	-1.528	1.00	0.00	MGUA
ATOM	26	C2	MGUA	1	4.170	0.591	0.034	1.00	0.00	MGUA
ATOM	27	HC1	MGUA	1	5.214	0.441	-0.230	1.00	0.00	MGUA
ATOM	28	HC2	MGUA	1	3.890	1.618	-0.210	1.00	0.00	MGUA
ATOM	29	HC3	MGUA	1	4.063	0.409	1.104	1.00	0.00	MGUA
END										
REMARK	57_CRES_MGUAN									
ATOM	1	CB	CRES	1	2.667	-2.839	0.418	1.00	0.00	CRES
ATOM	2	HB1	CRES	1	3.736	-2.911	0.213	1.00	0.00	CRES
ATOM	3	HB2	CRES	1	2.156	-3.551	-0.229	1.00	0.00	CRES
ATOM	4	HB3	CRES	1	2.505	-3.138	1.453	1.00	0.00	CRES
ATOM	5	CG	CRES	1	2.177	-1.436	0.175	1.00	0.00	CRES
ATOM	6	CD1	CRES	1	1.793	-1.018	-1.111	1.00	0.00	CRES
ATOM	7	HD1	CRES	1	1.805	-1.729	-1.929	1.00	0.00	CRES
ATOM	8	CD2	CRES	1	2.180	-0.481	1.204	1.00	0.00	CRES
ATOM	9	HD2	CRES	1	2.492	-0.769	2.202	1.00	0.00	CRES
ATOM	10	CE1	CRES	1	1.395	0.298	-1.364	1.00	0.00	CRES
ATOM	11	HE1	CRES	1	1.118	0.622	-2.359	1.00	0.00	CRES
ATOM	12	CE2	CRES	1	1.776	0.841	0.975	1.00	0.00	CRES
ATOM	13	HE2	CRES	1	1.775	1.563	1.785	1.00	0.00	CRES
ATOM	14	CZ	CRES	1	1.399	1.222	-0.317	1.00	0.00	CRES
ATOM	15	OZ	CRES	1	0.886	2.490	-0.595	1.00	0.00	CRES
ATOM	16	HZ	CRES	1	1.301	3.150	-0.018	1.00	0.00	CRES
ATOM	17	C	MGUA	1	-2.245	0.439	0.016	1.00	0.00	MGUA
ATOM	18	N1	MGUA	1	-1.904	1.660	-0.413	1.00	0.00	MGUA
ATOM	19	H11	MGUA	1	-0.938	1.979	-0.462	1.00	0.00	MGUA
ATOM	20	H12	MGUA	1	-2.619	2.312	-0.694	1.00	0.00	MGUA
ATOM	21	N2	MGUA	1	-1.342	-0.345	0.619	1.00	0.00	MGUA
ATOM	22	H21	MGUA	1	-1.509	-1.335	0.691	1.00	0.00	MGUA
ATOM	23	H22	MGUA	1	-0.377	-0.041	0.697	1.00	0.00	MGUA
ATOM	24	N3	MGUA	1	-3.510	0.016	-0.102	1.00	0.00	MGUA
ATOM	25	H31	MGUA	1	-4.130	0.557	-0.685	1.00	0.00	MGUA
ATOM	26	C2	MGUA	1	-4.008	-1.234	0.466	1.00	0.00	MGUA
ATOM	27	HC1	MGUA	1	-5.088	-1.238	0.362	1.00	0.00	MGUA
ATOM	28	HC2	MGUA	1	-3.607	-2.101	-0.061	1.00	0.00	MGUA
ATOM	29	HC3	MGUA	1	-3.762	-1.287	1.525	1.00	0.00	MGUA
END										
REMARK	58_CRES_MGUAN									
ATOM	1	CB	CRES	1	3.043	-2.587	-0.088	1.00	0.00	CRES
ATOM	2	HB1	CRES	1	4.124	-2.485	-0.198	1.00	0.00	CRES
ATOM	3	HB2	CRES	1	2.673	-3.148	-0.945	1.00	0.00	CRES
ATOM	4	HB3	CRES	1	2.854	-3.170	0.812	1.00	0.00	CRES
ATOM	5	CG	CRES	1	2.390	-1.232	-0.004	1.00	0.00	CRES
ATOM	6	CD1	CRES	1	1.983	-0.552	-1.163	1.00	0.00	CRES
ATOM	7	HD1	CRES	1	2.107	-1.023	-2.132	1.00	0.00	CRES

ATOM	8	CD2	CRES	1	2.246	-0.575	1.230	1.00	0.00	CRES
ATOM	9	HD2	CRES	1	2.565	-1.071	2.139	1.00	0.00	CRES
ATOM	10	CE1	CRES	1	1.433	0.733	-1.100	1.00	0.00	CRES
ATOM	11	HE1	CRES	1	1.143	1.267	-1.997	1.00	0.00	CRES
ATOM	12	CE2	CRES	1	1.682	0.701	1.317	1.00	0.00	CRES
ATOM	13	HE2	CRES	1	1.561	1.183	2.281	1.00	0.00	CRES
ATOM	14	CZ	CRES	1	1.285	1.350	0.145	1.00	0.00	CRES
ATOM	15	OZ	CRES	1	0.622	2.577	0.158	1.00	0.00	CRES
ATOM	16	HZ	CRES	1	0.880	3.085	0.942	1.00	0.00	CRES
ATOM	17	C	MGUA	1	-2.332	0.232	-0.106	1.00	0.00	MGUA
ATOM	18	N1	MGUA	1	-2.059	1.527	-0.307	1.00	0.00	MGUA
ATOM	19	H11	MGUA	1	-1.138	1.926	-0.130	1.00	0.00	MGUA
ATOM	20	H12	MGUA	1	-2.778	2.144	-0.649	1.00	0.00	MGUA
ATOM	21	N2	MGUA	1	-1.337	-0.650	0.029	1.00	0.00	MGUA
ATOM	22	H21	MGUA	1	-1.508	-1.573	0.394	1.00	0.00	MGUA
ATOM	23	H22	MGUA	1	-0.381	-0.387	-0.181	1.00	0.00	MGUA
ATOM	24	N3	MGUA	1	-3.604	-0.186	-0.068	1.00	0.00	MGUA
ATOM	25	H31	MGUA	1	-4.318	0.516	0.060	1.00	0.00	MGUA
ATOM	26	C2	MGUA	1	-4.004	-1.592	-0.056	1.00	0.00	MGUA
ATOM	27	HC1	MGUA	1	-5.074	-1.634	-0.232	1.00	0.00	MGUA
ATOM	28	HC2	MGUA	1	-3.500	-2.126	-0.859	1.00	0.00	MGUA
ATOM	29	HC3	MGUA	1	-3.792	-2.062	0.904	1.00	0.00	MGUA

END

REMARK 59_CRES_MGUAN

ATOM	1	CB	CRES	1	2.008	3.149	-0.414	1.00	0.00	CRES
ATOM	2	HB1	CRES	1	3.067	3.254	-0.654	1.00	0.00	CRES
ATOM	3	HB2	CRES	1	1.820	3.705	0.504	1.00	0.00	CRES
ATOM	4	HB3	CRES	1	1.438	3.613	-1.218	1.00	0.00	CRES
ATOM	5	CG	CRES	1	1.644	1.695	-0.256	1.00	0.00	CRES
ATOM	6	CD1	CRES	1	1.789	1.043	0.981	1.00	0.00	CRES
ATOM	7	HD1	CRES	1	2.148	1.602	1.840	1.00	0.00	CRES
ATOM	8	CD2	CRES	1	1.245	0.925	-1.361	1.00	0.00	CRES
ATOM	9	HD2	CRES	1	1.162	1.394	-2.336	1.00	0.00	CRES
ATOM	10	CE1	CRES	1	1.532	-0.326	1.119	1.00	0.00	CRES
ATOM	11	HE1	CRES	1	1.691	-0.835	2.062	1.00	0.00	CRES
ATOM	12	CE2	CRES	1	0.963	-0.440	-1.236	1.00	0.00	CRES
ATOM	13	HE2	CRES	1	0.655	-1.019	-2.101	1.00	0.00	CRES
ATOM	14	CZ	CRES	1	1.108	-1.060	0.008	1.00	0.00	CRES
ATOM	15	OZ	CRES	1	0.771	-2.396	0.213	1.00	0.00	CRES
ATOM	16	HZ	CRES	1	1.059	-2.928	-0.544	1.00	0.00	CRES
ATOM	17	C	MGUA	1	-1.856	-0.477	0.626	1.00	0.00	MGUA
ATOM	18	N1	MGUA	1	-1.546	-1.335	1.618	1.00	0.00	MGUA
ATOM	19	H11	MGUA	1	-1.261	-0.946	2.504	1.00	0.00	MGUA
ATOM	20	H12	MGUA	1	-1.093	-2.203	1.354	1.00	0.00	MGUA
ATOM	21	N2	MGUA	1	-1.693	0.841	0.806	1.00	0.00	MGUA
ATOM	22	H21	MGUA	1	-2.033	1.493	0.116	1.00	0.00	MGUA
ATOM	23	H22	MGUA	1	-0.916	1.154	1.373	1.00	0.00	MGUA
ATOM	24	N3	MGUA	1	-2.388	-0.957	-0.496	1.00	0.00	MGUA
ATOM	25	H31	MGUA	1	-2.731	-1.907	-0.462	1.00	0.00	MGUA
ATOM	26	C2	MGUA	1	-2.636	-0.163	-1.698	1.00	0.00	MGUA
ATOM	27	HC1	MGUA	1	-2.826	-0.849	-2.518	1.00	0.00	MGUA
ATOM	28	HC2	MGUA	1	-3.507	0.482	-1.576	1.00	0.00	MGUA
ATOM	29	HC3	MGUA	1	-1.752	0.427	-1.933	1.00	0.00	MGUA

END

REMARK 60_INDO_MGUAN

ATOM	1	CD2	INDO	1	1.698	-0.469	-0.375	1.00	0.00	INDO
ATOM	2	CE2	INDO	1	1.491	-0.659	1.026	1.00	0.00	INDO
ATOM	3	CZ2	INDO	1	1.336	0.418	1.917	1.00	0.00	INDO
ATOM	4	CH2	INDO	1	1.498	1.703	1.402	1.00	0.00	INDO
ATOM	5	CZ3	INDO	1	1.770	1.914	0.028	1.00	0.00	INDO
ATOM	6	CE3	INDO	1	1.910	0.842	-0.853	1.00	0.00	INDO
ATOM	7	CG	INDO	1	1.789	-1.769	-0.965	1.00	0.00	INDO
ATOM	8	CD1	INDO	1	1.602	-2.684	0.049	1.00	0.00	INDO
ATOM	9	NE1	INDO	1	1.397	-2.016	1.242	1.00	0.00	INDO
ATOM	10	HZ2	INDO	1	1.173	0.261	2.977	1.00	0.00	INDO
ATOM	11	HH2	INDO	1	1.416	2.555	2.065	1.00	0.00	INDO
ATOM	12	HZ3	INDO	1	1.954	2.924	-0.322	1.00	0.00	INDO
ATOM	13	HE3	INDO	1	2.162	1.012	-1.894	1.00	0.00	INDO
ATOM	14	HG	INDO	1	1.970	-2.007	-2.001	1.00	0.00	INDO
ATOM	15	HD1	INDO	1	1.610	-3.762	0.021	1.00	0.00	INDO
ATOM	16	HE1	INDO	1	1.363	-2.460	2.148	1.00	0.00	INDO
ATOM	17	C	MGUA	1	-2.111	0.726	-0.689	1.00	0.00	MGUA

ATOM	18	N1	MGUA	1	-1.283	1.544	-1.355	1.00	0.00	MGUA
ATOM	19	H11	MGUA	1	-0.310	1.611	-1.069	1.00	0.00	MGUA
ATOM	20	H12	MGUA	1	-1.507	1.822	-2.298	1.00	0.00	MGUA
ATOM	21	N2	MGUA	1	-1.658	0.043	0.366	1.00	0.00	MGUA
ATOM	22	H21	MGUA	1	-2.298	-0.388	1.012	1.00	0.00	MGUA
ATOM	23	H22	MGUA	1	-0.681	0.093	0.637	1.00	0.00	MGUA
ATOM	24	N3	MGUA	1	-3.383	0.592	-1.081	1.00	0.00	MGUA
ATOM	25	H31	MGUA	1	-3.732	1.257	-1.755	1.00	0.00	MGUA
ATOM	26	C2	MGUA	1	-4.337	-0.320	-0.454	1.00	0.00	MGUA
ATOM	27	HC1	MGUA	1	-5.239	-0.323	-1.057	1.00	0.00	MGUA
ATOM	28	HC2	MGUA	1	-3.930	-1.330	-0.439	1.00	0.00	MGUA
ATOM	29	HC3	MGUA	1	-4.594	0.002	0.556	1.00	0.00	MGUA

END

REMARK 61_INDO_MGUA

ATOM	1	CD2	INDO	1	-1.601	-0.340	0.679	1.00	0.00	INDO
ATOM	2	CE2	INDO	1	-1.595	0.136	-0.667	1.00	0.00	INDO
ATOM	3	CZ2	INDO	1	-1.609	1.503	-0.986	1.00	0.00	INDO
ATOM	4	CH2	INDO	1	-1.586	2.403	0.074	1.00	0.00	INDO
ATOM	5	CZ3	INDO	1	-1.582	1.958	1.420	1.00	0.00	INDO
ATOM	6	CE3	INDO	1	-1.587	0.601	1.735	1.00	0.00	INDO
ATOM	7	CG	INDO	1	-1.649	-1.772	0.619	1.00	0.00	INDO
ATOM	8	CD1	INDO	1	-1.693	-2.116	-0.720	1.00	0.00	INDO
ATOM	9	NE1	INDO	1	-1.645	-0.972	-1.487	1.00	0.00	INDO
ATOM	10	HZ2	INDO	1	-1.638	1.847	-2.014	1.00	0.00	INDO
ATOM	11	HH2	INDO	1	-1.612	3.466	-0.131	1.00	0.00	INDO
ATOM	12	HZ3	INDO	1	-1.599	2.690	2.218	1.00	0.00	INDO
ATOM	13	HE3	INDO	1	-1.617	0.273	2.768	1.00	0.00	INDO
ATOM	14	HG	INDO	1	-1.711	-2.460	1.448	1.00	0.00	INDO
ATOM	15	HD1	INDO	1	-1.773	-3.086	-1.185	1.00	0.00	INDO
ATOM	16	HE1	INDO	1	-1.725	-0.949	-2.493	1.00	0.00	INDO
ATOM	17	C	MGUA	1	2.161	-0.027	0.120	1.00	0.00	MGUA
ATOM	18	N1	MGUA	1	1.518	1.034	0.620	1.00	0.00	MGUA
ATOM	19	H11	MGUA	1	0.548	0.966	0.914	1.00	0.00	MGUA
ATOM	20	H12	MGUA	1	1.889	1.961	0.486	1.00	0.00	MGUA
ATOM	21	N2	MGUA	1	1.513	-1.184	-0.055	1.00	0.00	MGUA
ATOM	22	H21	MGUA	1	2.029	-2.041	-0.167	1.00	0.00	MGUA
ATOM	23	H22	MGUA	1	0.524	-1.266	0.169	1.00	0.00	MGUA
ATOM	24	N3	MGUA	1	3.451	0.076	-0.229	1.00	0.00	MGUA
ATOM	25	H31	MGUA	1	3.952	0.889	0.096	1.00	0.00	MGUA
ATOM	26	C2	MGUA	1	4.215	-1.002	-0.853	1.00	0.00	MGUA
ATOM	27	HC1	MGUA	1	5.172	-0.594	-1.160	1.00	0.00	MGUA
ATOM	28	HC2	MGUA	1	4.393	-1.823	-0.158	1.00	0.00	MGUA
ATOM	29	HC3	MGUA	1	3.694	-1.361	-1.738	1.00	0.00	MGUA

END

REMARK 62_INDO_MGUA

ATOM	1	CD2	INDO	1	-1.607	0.041	0.744	1.00	0.00	INDO
ATOM	2	CE2	INDO	1	-1.592	0.145	-0.680	1.00	0.00	INDO
ATOM	3	CZ2	INDO	1	-1.456	1.373	-1.347	1.00	0.00	INDO
ATOM	4	CH2	INDO	1	-1.295	2.509	-0.560	1.00	0.00	INDO
ATOM	5	CZ3	INDO	1	-1.300	2.433	0.855	1.00	0.00	INDO
ATOM	6	CE3	INDO	1	-1.452	1.216	1.515	1.00	0.00	INDO
ATOM	7	CG	INDO	1	-1.823	-1.340	1.062	1.00	0.00	INDO
ATOM	8	CD1	INDO	1	-1.950	-2.014	-0.140	1.00	0.00	INDO
ATOM	9	NE1	INDO	1	-1.794	-1.124	-1.180	1.00	0.00	INDO
ATOM	10	HZ2	INDO	1	-1.477	1.439	-2.429	1.00	0.00	INDO
ATOM	11	HH2	INDO	1	-1.205	3.477	-1.037	1.00	0.00	INDO
ATOM	12	HZ3	INDO	1	-1.206	3.345	1.433	1.00	0.00	INDO
ATOM	13	HE3	INDO	1	-1.485	1.174	2.598	1.00	0.00	INDO
ATOM	14	HG	INDO	1	-1.936	-1.777	2.042	1.00	0.00	INDO
ATOM	15	HD1	INDO	1	-2.156	-3.055	-0.333	1.00	0.00	INDO
ATOM	16	HE1	INDO	1	-1.905	-1.354	-2.157	1.00	0.00	INDO
ATOM	17	C	MGUA	1	2.147	-0.250	0.123	1.00	0.00	MGUA
ATOM	18	N1	MGUA	1	1.647	0.974	0.324	1.00	0.00	MGUA
ATOM	19	H11	MGUA	1	0.684	1.103	0.622	1.00	0.00	MGUA
ATOM	20	H12	MGUA	1	2.118	1.781	-0.052	1.00	0.00	MGUA
ATOM	21	N2	MGUA	1	1.364	-1.326	0.257	1.00	0.00	MGUA
ATOM	22	H21	MGUA	1	1.773	-2.238	0.375	1.00	0.00	MGUA
ATOM	23	H22	MGUA	1	0.379	-1.228	0.492	1.00	0.00	MGUA
ATOM	24	N3	MGUA	1	3.429	-0.397	-0.239	1.00	0.00	MGUA
ATOM	25	H31	MGUA	1	4.031	0.406	-0.136	1.00	0.00	MGUA
ATOM	26	C2	MGUA	1	4.045	-1.684	-0.552	1.00	0.00	MGUA
ATOM	27	HC1	MGUA	1	5.035	-1.489	-0.950	1.00	0.00	MGUA

ATOM	28	HC2	MGUA	1	4.145	-2.309	0.337	1.00	0.00	MGUA
ATOM	29	HC3	MGUA	1	3.462	-2.199	-1.313	1.00	0.00	MGUA

END

REMARK 63_INDO_MGUAN

ATOM	1	CD2	INDO	1	-1.621	0.199	0.658	1.00	0.00	INDO
ATOM	2	CE2	INDO	1	-1.597	0.035	-0.760	1.00	0.00	INDO
ATOM	3	CZ2	INDO	1	-1.438	1.114	-1.644	1.00	0.00	INDO
ATOM	4	CH2	INDO	1	-1.286	2.378	-1.082	1.00	0.00	INDO
ATOM	5	CZ3	INDO	1	-1.305	2.568	0.323	1.00	0.00	INDO
ATOM	6	CE3	INDO	1	-1.472	1.497	1.197	1.00	0.00	INDO
ATOM	7	CG	INDO	1	-1.849	-1.098	1.228	1.00	0.00	INDO
ATOM	8	CD1	INDO	1	-1.968	-1.984	0.172	1.00	0.00	INDO
ATOM	9	NE1	INDO	1	-1.794	-1.306	-1.016	1.00	0.00	INDO
ATOM	10	HZ2	INDO	1	-1.443	0.976	-2.719	1.00	0.00	INDO
ATOM	11	HH2	INDO	1	-1.177	3.238	-1.731	1.00	0.00	INDO
ATOM	12	HZ3	INDO	1	-1.214	3.572	0.720	1.00	0.00	INDO
ATOM	13	HE3	INDO	1	-1.513	1.658	2.268	1.00	0.00	INDO
ATOM	14	HG	INDO	1	-1.974	-1.342	2.271	1.00	0.00	INDO
ATOM	15	HD1	INDO	1	-2.183	-3.042	0.176	1.00	0.00	INDO
ATOM	16	HE1	INDO	1	-1.917	-1.711	-1.933	1.00	0.00	INDO
ATOM	17	C	MGUA	1	2.143	-0.260	0.195	1.00	0.00	MGUA
ATOM	18	N1	MGUA	1	1.640	0.977	0.108	1.00	0.00	MGUA
ATOM	19	H11	MGUA	1	0.651	1.151	0.252	1.00	0.00	MGUA
ATOM	20	H12	MGUA	1	2.254	1.775	0.154	1.00	0.00	MGUA
ATOM	21	N2	MGUA	1	1.342	-1.288	0.488	1.00	0.00	MGUA
ATOM	22	H21	MGUA	1	1.660	-2.236	0.372	1.00	0.00	MGUA
ATOM	23	H22	MGUA	1	0.362	-1.147	0.720	1.00	0.00	MGUA
ATOM	24	N3	MGUA	1	3.451	-0.466	-0.009	1.00	0.00	MGUA
ATOM	25	H31	MGUA	1	3.983	0.294	-0.403	1.00	0.00	MGUA
ATOM	26	C2	MGUA	1	4.108	-1.761	0.151	1.00	0.00	MGUA
ATOM	27	HC1	MGUA	1	5.178	-1.602	0.061	1.00	0.00	MGUA
ATOM	28	HC2	MGUA	1	3.903	-2.165	1.141	1.00	0.00	MGUA
ATOM	29	HC3	MGUA	1	3.797	-2.467	-0.619	1.00	0.00	MGUA

END

REMARK 64_INDO_MGUAN

ATOM	1	CD2	INDO	1	1.658	0.128	-0.578	1.00	0.00	INDO
ATOM	2	CE2	INDO	1	1.559	-0.388	0.749	1.00	0.00	INDO
ATOM	3	CZ2	INDO	1	1.509	0.442	1.881	1.00	0.00	INDO
ATOM	4	CH2	INDO	1	1.555	1.815	1.664	1.00	0.00	INDO
ATOM	5	CZ3	INDO	1	1.654	2.353	0.357	1.00	0.00	INDO
ATOM	6	CE3	INDO	1	1.709	1.528	-0.764	1.00	0.00	INDO
ATOM	7	CG	INDO	1	1.727	-0.999	-1.463	1.00	0.00	INDO
ATOM	8	CD1	INDO	1	1.684	-2.133	-0.673	1.00	0.00	INDO
ATOM	9	NE1	INDO	1	1.559	-1.764	0.650	1.00	0.00	INDO
ATOM	10	HZ2	INDO	1	1.454	0.034	2.884	1.00	0.00	INDO
ATOM	11	HH2	INDO	1	1.537	2.487	2.513	1.00	0.00	INDO
ATOM	12	HZ3	INDO	1	1.717	3.427	0.232	1.00	0.00	INDO
ATOM	13	HE3	INDO	1	1.812	1.950	-1.758	1.00	0.00	INDO
ATOM	14	HG	INDO	1	1.858	-0.984	-2.534	1.00	0.00	INDO
ATOM	15	HD1	INDO	1	1.751	-3.174	-0.948	1.00	0.00	INDO
ATOM	16	HE1	INDO	1	1.590	-2.403	1.431	1.00	0.00	INDO
ATOM	17	C	MGUA	1	-2.149	0.105	-0.263	1.00	0.00	MGUA
ATOM	18	N1	MGUA	1	-1.487	1.193	0.148	1.00	0.00	MGUA
ATOM	19	H11	MGUA	1	-0.478	1.256	0.055	1.00	0.00	MGUA
ATOM	20	H12	MGUA	1	-1.982	2.057	0.303	1.00	0.00	MGUA
ATOM	21	N2	MGUA	1	-1.483	-0.918	-0.803	1.00	0.00	MGUA
ATOM	22	H21	MGUA	1	-1.936	-1.805	-0.950	1.00	0.00	MGUA
ATOM	23	H22	MGUA	1	-0.485	-0.863	-0.988	1.00	0.00	MGUA
ATOM	24	N3	MGUA	1	-3.481	0.045	-0.131	1.00	0.00	MGUA
ATOM	25	H31	MGUA	1	-3.922	0.748	0.443	1.00	0.00	MGUA
ATOM	26	C2	MGUA	1	-4.301	-1.060	-0.621	1.00	0.00	MGUA
ATOM	27	HC1	MGUA	1	-5.342	-0.780	-0.499	1.00	0.00	MGUA
ATOM	28	HC2	MGUA	1	-4.112	-1.225	-1.680	1.00	0.00	MGUA
ATOM	29	HC3	MGUA	1	-4.120	-1.975	-0.056	1.00	0.00	MGUA

END

REMARK 65_INDO_MGUAN

ATOM	1	CD2	INDO	1	-0.984	0.478	-0.964	1.00	0.00	INDO
ATOM	2	CE2	INDO	1	-1.251	0.401	0.434	1.00	0.00	INDO
ATOM	3	CZ2	INDO	1	-0.759	1.344	1.349	1.00	0.00	INDO
ATOM	4	CH2	INDO	1	-0.020	2.408	0.833	1.00	0.00	INDO
ATOM	5	CZ3	INDO	1	0.222	2.528	-0.559	1.00	0.00	INDO
ATOM	6	CE3	INDO	1	-0.278	1.594	-1.461	1.00	0.00	INDO

ATOM	7	CG	INDO	1	-1.663	-0.623	-1.583	1.00	0.00	INDO
ATOM	8	CD1	INDO	1	-2.293	-1.327	-0.575	1.00	0.00	INDO
ATOM	9	NE1	INDO	1	-2.011	-0.736	0.645	1.00	0.00	INDO
ATOM	10	HZ2	INDO	1	-0.991	1.289	2.407	1.00	0.00	INDO
ATOM	11	HH2	INDO	1	0.339	3.181	1.502	1.00	0.00	INDO
ATOM	12	HZ3	INDO	1	0.751	3.399	-0.927	1.00	0.00	INDO
ATOM	13	HE3	INDO	1	-0.125	1.721	-2.527	1.00	0.00	INDO
ATOM	14	HG	INDO	1	-1.727	-0.846	-2.637	1.00	0.00	INDO
ATOM	15	HD1	INDO	1	-2.940	-2.188	-0.630	1.00	0.00	INDO
ATOM	16	HE1	INDO	1	-2.532	-0.925	1.490	1.00	0.00	INDO
ATOM	17	C	MGUA	1	1.407	-1.195	0.710	1.00	0.00	MGUA
ATOM	18	N1	MGUA	1	1.341	-1.174	2.053	1.00	0.00	MGUA
ATOM	19	H11	MGUA	1	0.596	-1.660	2.528	1.00	0.00	MGUA
ATOM	20	H12	MGUA	1	1.839	-0.467	2.570	1.00	0.00	MGUA
ATOM	21	N2	MGUA	1	0.957	-2.268	0.042	1.00	0.00	MGUA
ATOM	22	H21	MGUA	1	0.569	-2.138	-0.884	1.00	0.00	MGUA
ATOM	23	H22	MGUA	1	0.632	-3.071	0.558	1.00	0.00	MGUA
ATOM	24	N3	MGUA	1	2.020	-0.214	0.054	1.00	0.00	MGUA
ATOM	25	H31	MGUA	1	1.986	0.709	0.475	1.00	0.00	MGUA
ATOM	26	C2	MGUA	1	2.423	-0.318	-1.347	1.00	0.00	MGUA
ATOM	27	HC1	MGUA	1	3.074	0.523	-1.564	1.00	0.00	MGUA
ATOM	28	HC2	MGUA	1	2.974	-1.244	-1.492	1.00	0.00	MGUA
ATOM	29	HC3	MGUA	1	1.562	-0.275	-2.014	1.00	0.00	MGUA

END

REMARK 66_MIND_MGUA

ATOM	1	CG	MIND	1	1.535	1.640	-0.066	1.00	0.00	MIND
ATOM	2	CB	MIND	1	1.625	2.920	0.706	1.00	0.00	MIND
ATOM	3	HB1	MIND	1	1.672	3.775	0.033	1.00	0.00	MIND
ATOM	4	HB2	MIND	1	2.523	2.932	1.326	1.00	0.00	MIND
ATOM	5	HB3	MIND	1	0.767	3.056	1.367	1.00	0.00	MIND
ATOM	6	CD2	MIND	1	1.457	0.312	0.478	1.00	0.00	MIND
ATOM	7	CD1	MIND	1	1.595	1.485	-1.442	1.00	0.00	MIND
ATOM	8	HD1	MIND	1	1.696	2.234	-2.213	1.00	0.00	MIND
ATOM	9	NE1	MIND	1	1.546	0.143	-1.768	1.00	0.00	MIND
ATOM	10	HE1	MIND	1	1.649	-0.228	-2.701	1.00	0.00	MIND
ATOM	11	CE2	MIND	1	1.492	-0.607	-0.614	1.00	0.00	MIND
ATOM	12	CE3	MIND	1	1.453	-0.194	1.798	1.00	0.00	MIND
ATOM	13	HE3	MIND	1	1.476	0.478	2.649	1.00	0.00	MIND
ATOM	14	CZ2	MIND	1	1.451	-1.998	-0.429	1.00	0.00	MIND
ATOM	15	HZ2	MIND	1	1.483	-2.685	-1.268	1.00	0.00	MIND
ATOM	16	CZ3	MIND	1	1.425	-1.575	1.984	1.00	0.00	MIND
ATOM	17	HZ3	MIND	1	1.440	-1.979	2.989	1.00	0.00	MIND
ATOM	18	CH2	MIND	1	1.432	-2.466	0.882	1.00	0.00	MIND
ATOM	19	HH2	MIND	1	1.432	-3.533	1.064	1.00	0.00	MIND
ATOM	20	C	MGUA	1	-2.272	-0.119	0.018	1.00	0.00	MGUA
ATOM	21	N1	MGUA	1	-1.661	-0.911	0.908	1.00	0.00	MGUA
ATOM	22	H11	MGUA	1	-0.685	-0.766	1.146	1.00	0.00	MGUA
ATOM	23	H12	MGUA	1	-2.050	-1.816	1.124	1.00	0.00	MGUA
ATOM	24	N2	MGUA	1	-1.594	0.864	-0.582	1.00	0.00	MGUA
ATOM	25	H21	MGUA	1	-2.084	1.610	-1.047	1.00	0.00	MGUA
ATOM	26	H22	MGUA	1	-0.600	0.998	-0.407	1.00	0.00	MGUA
ATOM	27	N3	MGUA	1	-3.562	-0.322	-0.282	1.00	0.00	MGUA
ATOM	28	H31	MGUA	1	-4.086	-0.931	0.329	1.00	0.00	MGUA
ATOM	29	C2	MGUA	1	-4.297	0.445	-1.284	1.00	0.00	MGUA
ATOM	30	HC1	MGUA	1	-5.265	-0.026	-1.418	1.00	0.00	MGUA
ATOM	31	HC2	MGUA	1	-4.453	1.477	-0.966	1.00	0.00	MGUA
ATOM	32	HC3	MGUA	1	-3.767	0.418	-2.235	1.00	0.00	MGUA

END

REMARK 67_MIND_MGUA

ATOM	1	CG	MIND	1	-1.836	-1.292	0.063	1.00	0.00	MIND
ATOM	2	CB	MIND	1	-2.167	-2.473	0.924	1.00	0.00	MIND
ATOM	3	HB1	MIND	1	-2.399	-3.344	0.312	1.00	0.00	MIND
ATOM	4	HB2	MIND	1	-3.036	-2.261	1.548	1.00	0.00	MIND
ATOM	5	HB3	MIND	1	-1.341	-2.735	1.587	1.00	0.00	MIND
ATOM	6	CD2	MIND	1	-1.478	0.025	0.512	1.00	0.00	MIND
ATOM	7	CD1	MIND	1	-1.894	-1.221	-1.320	1.00	0.00	MIND
ATOM	8	HD1	MIND	1	-2.163	-1.983	-2.036	1.00	0.00	MIND
ATOM	9	NE1	MIND	1	-1.583	0.058	-1.739	1.00	0.00	MIND
ATOM	10	HE1	MIND	1	-1.628	0.379	-2.696	1.00	0.00	MIND
ATOM	11	CE2	MIND	1	-1.351	0.857	-0.641	1.00	0.00	MIND
ATOM	12	CE3	MIND	1	-1.343	0.607	1.793	1.00	0.00	MIND
ATOM	13	HE3	MIND	1	-1.483	0.012	2.689	1.00	0.00	MIND

ATOM	14	CZ2	MIND	1	-1.024	2.219	-0.555	1.00	0.00	MIND
ATOM	15	HZ2	MIND	1	-0.935	2.840	-1.438	1.00	0.00	MIND
ATOM	16	CZ3	MIND	1	-1.030	1.962	1.882	1.00	0.00	MIND
ATOM	17	HZ3	MIND	1	-0.940	2.426	2.856	1.00	0.00	MIND
ATOM	18	CH2	MIND	1	-0.881	2.760	0.720	1.00	0.00	MIND
ATOM	19	HH2	MIND	1	-0.660	3.814	0.828	1.00	0.00	MIND
ATOM	20	C	MGUA	1	2.248	-0.348	-0.011	1.00	0.00	MGUA
ATOM	21	N1	MGUA	1	1.831	0.612	0.824	1.00	0.00	MGUA
ATOM	22	H11	MGUA	1	0.853	0.681	1.089	1.00	0.00	MGUA
ATOM	23	H12	MGUA	1	2.401	1.429	0.976	1.00	0.00	MGUA
ATOM	24	N2	MGUA	1	1.371	-1.209	-0.534	1.00	0.00	MGUA
ATOM	25	H21	MGUA	1	1.689	-2.071	-0.947	1.00	0.00	MGUA
ATOM	26	H22	MGUA	1	0.375	-1.125	-0.341	1.00	0.00	MGUA
ATOM	27	N3	MGUA	1	3.546	-0.432	-0.336	1.00	0.00	MGUA
ATOM	28	H31	MGUA	1	4.196	0.096	0.227	1.00	0.00	MGUA
ATOM	29	C2	MGUA	1	4.085	-1.398	-1.290	1.00	0.00	MGUA
ATOM	30	HC1	MGUA	1	5.125	-1.143	-1.466	1.00	0.00	MGUA
ATOM	31	HC2	MGUA	1	4.037	-2.416	-0.903	1.00	0.00	MGUA
ATOM	32	HC3	MGUA	1	3.549	-1.326	-2.234	1.00	0.00	MGUA

END

REMARK 68_MIND_MGUAN

ATOM	1	CG	MIND	1	1.907	-1.081	-0.352	1.00	0.00	MIND
ATOM	2	CB	MIND	1	2.335	-1.908	-1.526	1.00	0.00	MIND
ATOM	3	HB1	MIND	1	2.607	-2.915	-1.212	1.00	0.00	MIND
ATOM	4	HB2	MIND	1	3.204	-1.462	-2.013	1.00	0.00	MIND
ATOM	5	HB3	MIND	1	1.544	-1.989	-2.274	1.00	0.00	MIND
ATOM	6	CD2	MIND	1	1.486	0.293	-0.377	1.00	0.00	MIND
ATOM	7	CD1	MIND	1	1.932	-1.448	0.984	1.00	0.00	MIND
ATOM	8	HD1	MIND	1	2.232	-2.384	1.433	1.00	0.00	MIND
ATOM	9	NE1	MIND	1	1.529	-0.387	1.772	1.00	0.00	MIND
ATOM	10	HE1	MIND	1	1.550	-0.379	2.782	1.00	0.00	MIND
ATOM	11	CE2	MIND	1	1.279	0.707	0.973	1.00	0.00	MIND
ATOM	12	CE3	MIND	1	1.342	1.243	-1.414	1.00	0.00	MIND
ATOM	13	HE3	MIND	1	1.535	0.970	-2.445	1.00	0.00	MIND
ATOM	14	CZ2	MIND	1	0.876	2.010	1.308	1.00	0.00	MIND
ATOM	15	HZ2	MIND	1	0.726	2.312	2.338	1.00	0.00	MIND
ATOM	16	CZ3	MIND	1	0.953	2.539	-1.083	1.00	0.00	MIND
ATOM	17	HZ3	MIND	1	0.856	3.284	-1.864	1.00	0.00	MIND
ATOM	18	CH2	MIND	1	0.730	2.919	0.264	1.00	0.00	MIND
ATOM	19	HH2	MIND	1	0.446	3.940	0.486	1.00	0.00	MIND
ATOM	20	C	MGUA	1	-2.218	-0.475	-0.191	1.00	0.00	MGUA
ATOM	21	N1	MGUA	1	-1.839	0.743	-0.595	1.00	0.00	MGUA
ATOM	22	H11	MGUA	1	-0.857	0.980	-0.688	1.00	0.00	MGUA
ATOM	23	H12	MGUA	1	-2.500	1.352	-1.050	1.00	0.00	MGUA
ATOM	24	N2	MGUA	1	-1.298	-1.403	0.087	1.00	0.00	MGUA
ATOM	25	H21	MGUA	1	-1.551	-2.241	0.586	1.00	0.00	MGUA
ATOM	26	H22	MGUA	1	-0.305	-1.215	-0.036	1.00	0.00	MGUA
ATOM	27	N3	MGUA	1	-3.520	-0.768	-0.074	1.00	0.00	MGUA
ATOM	28	H31	MGUA	1	-4.174	-0.001	-0.125	1.00	0.00	MGUA
ATOM	29	C2	MGUA	1	-4.031	-2.091	0.277	1.00	0.00	MGUA
ATOM	30	HC1	MGUA	1	-5.110	-2.070	0.162	1.00	0.00	MGUA
ATOM	31	HC2	MGUA	1	-3.627	-2.840	-0.402	1.00	0.00	MGUA
ATOM	32	HC3	MGUA	1	-3.798	-2.349	1.310	1.00	0.00	MGUA

END

REMARK 69_MIND_MGUAN

ATOM	1	CG	MIND	1	1.838	-1.117	-0.557	1.00	0.00	MIND
ATOM	2	CB	MIND	1	2.285	-1.612	-1.898	1.00	0.00	MIND
ATOM	3	HB1	MIND	1	2.452	-2.688	-1.877	1.00	0.00	MIND
ATOM	4	HB2	MIND	1	3.221	-1.133	-2.190	1.00	0.00	MIND
ATOM	5	HB3	MIND	1	1.548	-1.399	-2.675	1.00	0.00	MIND
ATOM	6	CD2	MIND	1	1.528	0.242	-0.202	1.00	0.00	MIND
ATOM	7	CD1	MIND	1	1.733	-1.849	0.615	1.00	0.00	MIND
ATOM	8	HD1	MIND	1	1.925	-2.898	0.788	1.00	0.00	MIND
ATOM	9	NE1	MIND	1	1.357	-1.022	1.657	1.00	0.00	MIND
ATOM	10	HE1	MIND	1	1.303	-1.304	2.625	1.00	0.00	MIND
ATOM	11	CE2	MIND	1	1.255	0.273	1.199	1.00	0.00	MIND
ATOM	12	CE3	MIND	1	1.538	1.457	-0.925	1.00	0.00	MIND
ATOM	13	HE3	MIND	1	1.785	1.471	-1.980	1.00	0.00	MIND
ATOM	14	CZ2	MIND	1	0.931	1.459	1.877	1.00	0.00	MIND
ATOM	15	HZ2	MIND	1	0.728	1.469	2.941	1.00	0.00	MIND
ATOM	16	CZ3	MIND	1	1.229	2.636	-0.251	1.00	0.00	MIND
ATOM	17	HZ3	MIND	1	1.250	3.578	-0.786	1.00	0.00	MIND

ATOM	18	CH2	MIND	1	0.936	2.637	1.135	1.00	0.00	MIND
ATOM	19	HH2	MIND	1	0.717	3.575	1.630	1.00	0.00	MIND
ATOM	20	C	MGUA	1	-2.228	-0.183	-0.430	1.00	0.00	MGUA
ATOM	21	N1	MGUA	1	-1.725	1.057	-0.448	1.00	0.00	MGUA
ATOM	22	H11	MGUA	1	-0.723	1.214	-0.419	1.00	0.00	MGUA
ATOM	23	H12	MGUA	1	-2.300	1.831	-0.739	1.00	0.00	MGUA
ATOM	24	N2	MGUA	1	-1.408	-1.237	-0.387	1.00	0.00	MGUA
ATOM	25	H21	MGUA	1	-1.764	-2.152	-0.163	1.00	0.00	MGUA
ATOM	26	H22	MGUA	1	-0.397	-1.119	-0.403	1.00	0.00	MGUA
ATOM	27	N3	MGUA	1	-3.555	-0.368	-0.467	1.00	0.00	MGUA
ATOM	28	H31	MGUA	1	-4.140	0.441	-0.323	1.00	0.00	MGUA
ATOM	29	C2	MGUA	1	-4.194	-1.680	-0.537	1.00	0.00	MGUA
ATOM	30	HC1	MGUA	1	-5.256	-1.523	-0.695	1.00	0.00	MGUA
ATOM	31	HC2	MGUA	1	-3.800	-2.243	-1.381	1.00	0.00	MGUA
ATOM	32	HC3	MGUA	1	-4.061	-2.240	0.389	1.00	0.00	MGUA

END

REMARK 70_MIND_MGUAN

ATOM	1	CG	MIND	1	-2.284	0.271	-0.130	1.00	0.00	MIND
ATOM	2	CB	MIND	1	-3.121	1.492	0.085	1.00	0.00	MIND
ATOM	3	HB1	MIND	1	-3.864	1.596	-0.704	1.00	0.00	MIND
ATOM	4	HB2	MIND	1	-2.511	2.397	0.098	1.00	0.00	MIND
ATOM	5	HB3	MIND	1	-3.650	1.436	1.038	1.00	0.00	MIND
ATOM	6	CD2	MIND	1	-1.206	-0.187	0.706	1.00	0.00	MIND
ATOM	7	CD1	MIND	1	-2.393	-0.646	-1.153	1.00	0.00	MIND
ATOM	8	HD1	MIND	1	-3.093	-0.682	-1.976	1.00	0.00	MIND
ATOM	9	NE1	MIND	1	-1.415	-1.631	-1.022	1.00	0.00	MIND
ATOM	10	HE1	MIND	1	-1.467	-2.530	-1.484	1.00	0.00	MIND
ATOM	11	CE2	MIND	1	-0.731	-1.416	0.166	1.00	0.00	MIND
ATOM	12	CE3	MIND	1	-0.688	0.262	1.938	1.00	0.00	MIND
ATOM	13	HE3	MIND	1	-1.062	1.171	2.396	1.00	0.00	MIND
ATOM	14	CZ2	MIND	1	0.293	-2.162	0.771	1.00	0.00	MIND
ATOM	15	HZ2	MIND	1	0.644	-3.098	0.351	1.00	0.00	MIND
ATOM	16	CZ3	MIND	1	0.324	-0.474	2.549	1.00	0.00	MIND
ATOM	17	HZ3	MIND	1	0.721	-0.150	3.504	1.00	0.00	MIND
ATOM	18	CH2	MIND	1	0.802	-1.678	1.979	1.00	0.00	MIND
ATOM	19	HH2	MIND	1	1.564	-2.248	2.497	1.00	0.00	MIND
ATOM	20	C	MGUA	1	1.604	1.082	-1.380	1.00	0.00	MGUA
ATOM	21	N1	MGUA	1	0.638	0.537	-2.141	1.00	0.00	MGUA
ATOM	22	H11	MGUA	1	0.159	1.128	-2.803	1.00	0.00	MGUA
ATOM	23	H12	MGUA	1	0.097	-0.244	-1.783	1.00	0.00	MGUA
ATOM	24	N2	MGUA	1	2.203	2.210	-1.810	1.00	0.00	MGUA
ATOM	25	H21	MGUA	1	2.979	2.600	-1.300	1.00	0.00	MGUA
ATOM	26	H22	MGUA	1	2.133	2.467	-2.782	1.00	0.00	MGUA
ATOM	27	N3	MGUA	1	1.973	0.516	-0.239	1.00	0.00	MGUA
ATOM	28	H31	MGUA	1	1.397	-0.239	0.126	1.00	0.00	MGUA
ATOM	29	C2	MGUA	1	3.085	0.978	0.585	1.00	0.00	MGUA
ATOM	30	HC1	MGUA	1	3.221	0.251	1.379	1.00	0.00	MGUA
ATOM	31	HC2	MGUA	1	4.002	1.026	-0.002	1.00	0.00	MGUA
ATOM	32	HC3	MGUA	1	2.867	1.948	1.033	1.00	0.00	MGUA

END

REMARK 71_IMID_MGUAN

ATOM	1	CG	IMID	1	3.155	-0.673	1.615	1.00	0.00	IMID
ATOM	2	HG	IMID	1	3.917	-1.238	2.120	1.00	0.00	IMID
ATOM	3	CD2	IMID	1	1.912	-1.018	1.131	1.00	0.00	IMID
ATOM	4	HD2	IMID	1	1.430	-1.980	1.165	1.00	0.00	IMID
ATOM	5	ND1	IMID	1	3.296	0.664	1.327	1.00	0.00	IMID
ATOM	6	HD1	IMID	1	4.100	1.236	1.547	1.00	0.00	IMID
ATOM	7	CE1	IMID	1	2.174	1.089	0.694	1.00	0.00	IMID
ATOM	8	HE1	IMID	1	2.032	2.104	0.360	1.00	0.00	IMID
ATOM	9	NE2	IMID	1	1.304	0.084	0.556	1.00	0.00	IMID
ATOM	10	C	MGUA	1	-1.724	-0.044	-1.024	1.00	0.00	MGUA
ATOM	11	N1	MGUA	1	-0.600	-0.163	-1.752	1.00	0.00	MGUA
ATOM	12	H11	MGUA	1	0.276	-0.140	-1.233	1.00	0.00	MGUA
ATOM	13	H12	MGUA	1	-0.624	-0.639	-2.640	1.00	0.00	MGUA
ATOM	14	N2	MGUA	1	-1.608	0.181	0.287	1.00	0.00	MGUA
ATOM	15	H21	MGUA	1	-2.387	0.511	0.831	1.00	0.00	MGUA
ATOM	16	H22	MGUA	1	-0.655	0.243	0.658	1.00	0.00	MGUA
ATOM	17	N3	MGUA	1	-2.926	-0.155	-1.602	1.00	0.00	MGUA
ATOM	18	H31	MGUA	1	-2.955	-0.167	-2.610	1.00	0.00	MGUA
ATOM	19	C2	MGUA	1	-4.188	-0.052	-0.873	1.00	0.00	MGUA
ATOM	20	HC1	MGUA	1	-4.989	-0.310	-1.558	1.00	0.00	MGUA
ATOM	21	HC2	MGUA	1	-4.199	-0.762	-0.048	1.00	0.00	MGUA

ATOM	22	HC3	MGUA	1	-4.355	0.960	-0.506	1.00	0.00	MGUA
END										
REMARK	72_IMID_MGUA									
ATOM	1	CG	IMID	1	3.342	0.302	-0.758	1.00	0.00	IMID
ATOM	2	HG	IMID	1	4.265	0.098	-1.272	1.00	0.00	IMID
ATOM	3	CD2	IMID	1	2.144	-0.376	-0.702	1.00	0.00	IMID
ATOM	4	HD2	IMID	1	1.877	-1.296	-1.193	1.00	0.00	IMID
ATOM	5	ND1	IMID	1	3.169	1.408	0.039	1.00	0.00	IMID
ATOM	6	HD1	IMID	1	3.862	2.120	0.222	1.00	0.00	IMID
ATOM	7	CE1	IMID	1	1.909	1.380	0.546	1.00	0.00	IMID
ATOM	8	HE1	IMID	1	1.520	2.140	1.203	1.00	0.00	IMID
ATOM	9	NE2	IMID	1	1.254	0.303	0.107	1.00	0.00	IMID
ATOM	10	C	MGUA	1	-2.261	-1.000	0.354	1.00	0.00	MGUA
ATOM	11	N1	MGUA	1	-3.139	-1.969	0.697	1.00	0.00	MGUA
ATOM	12	H11	MGUA	1	-2.807	-2.826	1.109	1.00	0.00	MGUA
ATOM	13	H12	MGUA	1	-4.075	-1.974	0.324	1.00	0.00	MGUA
ATOM	14	N2	MGUA	1	-1.106	-0.893	1.003	1.00	0.00	MGUA
ATOM	15	H21	MGUA	1	-0.273	-0.369	0.638	1.00	0.00	MGUA
ATOM	16	H22	MGUA	1	-0.963	-1.463	1.823	1.00	0.00	MGUA
ATOM	17	N3	MGUA	1	-2.587	-0.125	-0.601	1.00	0.00	MGUA
ATOM	18	H31	MGUA	1	-3.395	-0.330	-1.169	1.00	0.00	MGUA
ATOM	19	C2	MGUA	1	-1.888	1.144	-0.815	1.00	0.00	MGUA
ATOM	20	HC1	MGUA	1	-2.410	1.675	-1.604	1.00	0.00	MGUA
ATOM	21	HC2	MGUA	1	-1.910	1.738	0.097	1.00	0.00	MGUA
ATOM	22	HC3	MGUA	1	-0.857	0.973	-1.112	1.00	0.00	MGUA
END										
REMARK	73_IMID_MGUA									
ATOM	1	CG	IMID	1	3.423	-0.791	0.447	1.00	0.00	IMID
ATOM	2	HG	IMID	1	4.253	-1.376	0.797	1.00	0.00	IMID
ATOM	3	CD2	IMID	1	2.194	-0.511	1.002	1.00	0.00	IMID
ATOM	4	HD2	IMID	1	1.817	-0.810	1.966	1.00	0.00	IMID
ATOM	5	ND1	IMID	1	3.423	-0.157	-0.772	1.00	0.00	IMID
ATOM	6	HD1	IMID	1	4.187	-0.146	-1.434	1.00	0.00	IMID
ATOM	7	CE1	IMID	1	2.232	0.475	-0.928	1.00	0.00	IMID
ATOM	8	HE1	IMID	1	1.977	1.050	-1.802	1.00	0.00	IMID
ATOM	9	NE2	IMID	1	1.452	0.274	0.139	1.00	0.00	IMID
ATOM	10	C	MGUA	1	-1.940	-0.089	0.002	1.00	0.00	MGUA
ATOM	11	N1	MGUA	1	-1.210	-1.187	-0.294	1.00	0.00	MGUA
ATOM	12	H11	MGUA	1	-0.216	-1.137	-0.098	1.00	0.00	MGUA
ATOM	13	H12	MGUA	1	-1.644	-2.095	-0.230	1.00	0.00	MGUA
ATOM	14	N2	MGUA	1	-1.297	1.034	0.313	1.00	0.00	MGUA
ATOM	15	H21	MGUA	1	-1.790	1.903	0.427	1.00	0.00	MGUA
ATOM	16	H22	MGUA	1	-0.264	0.999	0.339	1.00	0.00	MGUA
ATOM	17	N3	MGUA	1	-3.275	-0.138	-0.049	1.00	0.00	MGUA
ATOM	18	H31	MGUA	1	-3.700	-0.988	-0.388	1.00	0.00	MGUA
ATOM	19	C2	MGUA	1	-4.137	1.012	0.215	1.00	0.00	MGUA
ATOM	20	HC1	MGUA	1	-5.166	0.684	0.118	1.00	0.00	MGUA
ATOM	21	HC2	MGUA	1	-3.986	1.376	1.230	1.00	0.00	MGUA
ATOM	22	HC3	MGUA	1	-3.957	1.809	-0.505	1.00	0.00	MGUA
END										
REMARK	74_IMID_MGUA									
ATOM	1	CG	IMID	1	-3.308	-0.357	0.846	1.00	0.00	IMID
ATOM	2	HG	IMID	1	-4.094	-0.605	1.538	1.00	0.00	IMID
ATOM	3	CD2	IMID	1	-2.198	0.454	0.955	1.00	0.00	IMID
ATOM	4	HD2	IMID	1	-1.887	1.050	1.796	1.00	0.00	IMID
ATOM	5	ND1	IMID	1	-3.261	-0.864	-0.430	1.00	0.00	IMID
ATOM	6	HD1	IMID	1	-3.920	-1.516	-0.829	1.00	0.00	IMID
ATOM	7	CE1	IMID	1	-2.165	-0.364	-1.056	1.00	0.00	IMID
ATOM	8	HE1	IMID	1	-1.905	-0.598	-2.075	1.00	0.00	IMID
ATOM	9	NE2	IMID	1	-1.488	0.445	-0.233	1.00	0.00	IMID
ATOM	10	C	MGUA	1	1.870	-0.028	0.103	1.00	0.00	MGUA
ATOM	11	N1	MGUA	1	1.109	-1.029	0.598	1.00	0.00	MGUA
ATOM	12	H11	MGUA	1	0.104	-0.914	0.548	1.00	0.00	MGUA
ATOM	13	H12	MGUA	1	1.469	-1.972	0.592	1.00	0.00	MGUA
ATOM	14	N2	MGUA	1	1.274	1.060	-0.375	1.00	0.00	MGUA
ATOM	15	H21	MGUA	1	1.800	1.901	-0.553	1.00	0.00	MGUA
ATOM	16	H22	MGUA	1	0.238	1.059	-0.435	1.00	0.00	MGUA
ATOM	17	N3	MGUA	1	3.204	-0.154	0.109	1.00	0.00	MGUA
ATOM	18	H31	MGUA	1	3.593	-0.881	0.693	1.00	0.00	MGUA
ATOM	19	C2	MGUA	1	4.112	0.859	-0.425	1.00	0.00	MGUA
ATOM	20	HC1	MGUA	1	5.111	0.436	-0.440	1.00	0.00	MGUA
ATOM	21	HC2	MGUA	1	3.829	1.104	-1.447	1.00	0.00	MGUA

ATOM	22	HC3	MGUA	1	4.120	1.758	0.191	1.00	0.00	MGUA
END										
REMARK	75_IMID_MGUA									
ATOM	1	CG	IMID	1	-3.544	0.594	-0.324	1.00	0.00	IMID
ATOM	2	HG	IMID	1	-4.452	1.058	-0.668	1.00	0.00	IMID
ATOM	3	CD2	IMID	1	-2.216	0.860	-0.573	1.00	0.00	IMID
ATOM	4	HD2	IMID	1	-1.799	1.630	-1.200	1.00	0.00	IMID
ATOM	5	ND1	IMID	1	-3.544	-0.482	0.531	1.00	0.00	IMID
ATOM	6	HD1	IMID	1	-4.362	-0.935	0.914	1.00	0.00	IMID
ATOM	7	CE1	IMID	1	-2.257	-0.837	0.776	1.00	0.00	IMID
ATOM	8	HE1	IMID	1	-1.982	-1.656	1.419	1.00	0.00	IMID
ATOM	9	NE2	IMID	1	-1.416	-0.034	0.115	1.00	0.00	IMID
ATOM	10	C	MGUA	1	2.000	0.098	0.116	1.00	0.00	MGUA
ATOM	11	N1	MGUA	1	1.314	0.685	1.111	1.00	0.00	MGUA
ATOM	12	H11	MGUA	1	0.298	0.635	1.048	1.00	0.00	MGUA
ATOM	13	H12	MGUA	1	1.731	1.439	1.634	1.00	0.00	MGUA
ATOM	14	N2	MGUA	1	1.315	-0.566	-0.818	1.00	0.00	MGUA
ATOM	15	H21	MGUA	1	1.772	-1.219	-1.433	1.00	0.00	MGUA
ATOM	16	H22	MGUA	1	0.297	-0.589	-0.710	1.00	0.00	MGUA
ATOM	17	N3	MGUA	1	3.334	0.189	0.060	1.00	0.00	MGUA
ATOM	18	H31	MGUA	1	3.806	0.566	0.868	1.00	0.00	MGUA
ATOM	19	C2	MGUA	1	4.142	-0.412	-0.998	1.00	0.00	MGUA
ATOM	20	HC1	MGUA	1	5.165	-0.073	-0.868	1.00	0.00	MGUA
ATOM	21	HC2	MGUA	1	4.125	-1.501	-0.945	1.00	0.00	MGUA
ATOM	22	HC3	MGUA	1	3.791	-0.074	-1.972	1.00	0.00	MGUA
END										
REMARK	76_IMID_MGUA									
ATOM	1	CG	IMID	1	3.473	0.592	0.779	1.00	0.00	IMID
ATOM	2	HG	IMID	1	4.327	1.030	1.265	1.00	0.00	IMID
ATOM	3	CD2	IMID	1	2.119	0.778	0.941	1.00	0.00	IMID
ATOM	4	HD2	IMID	1	1.616	1.439	1.628	1.00	0.00	IMID
ATOM	5	ND1	IMID	1	3.592	-0.351	-0.214	1.00	0.00	IMID
ATOM	6	HD1	IMID	1	4.459	-0.719	-0.581	1.00	0.00	IMID
ATOM	7	CE1	IMID	1	2.348	-0.707	-0.621	1.00	0.00	IMID
ATOM	8	HE1	IMID	1	2.165	-1.433	-1.395	1.00	0.00	IMID
ATOM	9	NE2	IMID	1	1.419	-0.035	0.067	1.00	0.00	IMID
ATOM	10	C	MGUA	1	-1.997	-0.184	0.035	1.00	0.00	MGUA
ATOM	11	N1	MGUA	1	-1.314	-0.920	0.928	1.00	0.00	MGUA
ATOM	12	H11	MGUA	1	-0.298	-0.892	0.857	1.00	0.00	MGUA
ATOM	13	H12	MGUA	1	-1.749	-1.715	1.367	1.00	0.00	MGUA
ATOM	14	N2	MGUA	1	-1.306	0.567	-0.826	1.00	0.00	MGUA
ATOM	15	H21	MGUA	1	-1.749	1.318	-1.329	1.00	0.00	MGUA
ATOM	16	H22	MGUA	1	-0.285	0.547	-0.733	1.00	0.00	MGUA
ATOM	17	N3	MGUA	1	-3.334	-0.218	0.004	1.00	0.00	MGUA
ATOM	18	H31	MGUA	1	-3.803	-0.671	0.774	1.00	0.00	MGUA
ATOM	19	C2	MGUA	1	-4.140	0.546	-0.944	1.00	0.00	MGUA
ATOM	20	HC1	MGUA	1	-5.172	0.232	-0.832	1.00	0.00	MGUA
ATOM	21	HC2	MGUA	1	-4.078	1.617	-0.750	1.00	0.00	MGUA
ATOM	22	HC3	MGUA	1	-3.823	0.327	-1.962	1.00	0.00	MGUA
END										
REMARK	77_IMID_MGUA									
ATOM	1	CG	IMID	1	-3.489	0.491	0.773	1.00	0.00	IMID
ATOM	2	HG	IMID	1	-4.364	0.653	1.376	1.00	0.00	IMID
ATOM	3	CD2	IMID	1	-2.168	0.271	1.096	1.00	0.00	IMID
ATOM	4	HD2	IMID	1	-1.725	0.213	2.076	1.00	0.00	IMID
ATOM	5	ND1	IMID	1	-3.532	0.472	-0.601	1.00	0.00	IMID
ATOM	6	HD1	IMID	1	-4.358	0.603	-1.170	1.00	0.00	IMID
ATOM	7	CE1	IMID	1	-2.278	0.247	-1.069	1.00	0.00	IMID
ATOM	8	HE1	IMID	1	-2.041	0.186	-2.117	1.00	0.00	IMID
ATOM	9	NE2	IMID	1	-1.416	0.119	-0.055	1.00	0.00	IMID
ATOM	10	C	MGUA	1	1.947	-0.474	-0.017	1.00	0.00	MGUA
ATOM	11	N1	MGUA	1	1.077	-1.490	-0.064	1.00	0.00	MGUA
ATOM	12	H11	MGUA	1	0.084	-1.257	-0.074	1.00	0.00	MGUA
ATOM	13	H12	MGUA	1	1.377	-2.448	-0.004	1.00	0.00	MGUA
ATOM	14	N2	MGUA	1	1.468	0.768	-0.162	1.00	0.00	MGUA
ATOM	15	H21	MGUA	1	2.039	1.566	0.061	1.00	0.00	MGUA
ATOM	16	H22	MGUA	1	0.450	0.862	-0.161	1.00	0.00	MGUA
ATOM	17	N3	MGUA	1	3.261	-0.690	0.112	1.00	0.00	MGUA
ATOM	18	H31	MGUA	1	3.571	-1.640	0.247	1.00	0.00	MGUA
ATOM	19	C2	MGUA	1	4.264	0.372	0.079	1.00	0.00	MGUA
ATOM	20	HC1	MGUA	1	5.242	-0.096	0.096	1.00	0.00	MGUA
ATOM	21	HC2	MGUA	1	4.173	0.950	-0.839	1.00	0.00	MGUA

ATOM	22	HC3	MGUA	1	4.177	1.023	0.948	1.00	0.00	MGUA
END										
REMARK	78_IMID_MGUAN									
ATOM	1	CG	IMID	1	-3.552	0.418	0.445	1.00	0.00	IMID
ATOM	2	HG	IMID	1	-4.481	0.571	0.967	1.00	0.00	IMID
ATOM	3	CD2	IMID	1	-2.252	0.300	0.883	1.00	0.00	IMID
ATOM	4	HD2	IMID	1	-1.885	0.340	1.895	1.00	0.00	IMID
ATOM	5	ND1	IMID	1	-3.485	0.299	-0.923	1.00	0.00	IMID
ATOM	6	HD1	IMID	1	-4.269	0.340	-1.560	1.00	0.00	IMID
ATOM	7	CE1	IMID	1	-2.188	0.117	-1.276	1.00	0.00	IMID
ATOM	8	HE1	IMID	1	-1.865	-0.005	-2.297	1.00	0.00	IMID
ATOM	9	NE2	IMID	1	-1.403	0.111	-0.193	1.00	0.00	IMID
ATOM	10	C	MGUA	1	1.957	-0.418	0.148	1.00	0.00	MGUA
ATOM	11	N1	MGUA	1	1.132	-1.473	0.034	1.00	0.00	MGUA
ATOM	12	H11	MGUA	1	0.138	-1.263	-0.045	1.00	0.00	MGUA
ATOM	13	H12	MGUA	1	1.410	-2.370	0.400	1.00	0.00	MGUA
ATOM	14	N2	MGUA	1	1.431	0.807	0.063	1.00	0.00	MGUA
ATOM	15	H21	MGUA	1	2.012	1.613	-0.101	1.00	0.00	MGUA
ATOM	16	H22	MGUA	1	0.420	0.862	-0.086	1.00	0.00	MGUA
ATOM	17	N3	MGUA	1	3.267	-0.595	0.349	1.00	0.00	MGUA
ATOM	18	H31	MGUA	1	3.629	-1.531	0.249	1.00	0.00	MGUA
ATOM	19	C2	MGUA	1	4.220	0.504	0.494	1.00	0.00	MGUA
ATOM	20	HC1	MGUA	1	5.178	0.078	0.775	1.00	0.00	MGUA
ATOM	21	HC2	MGUA	1	4.341	1.053	-0.440	1.00	0.00	MGUA
ATOM	22	HC3	MGUA	1	3.896	1.174	1.289	1.00	0.00	MGUA
END										
REMARK	79_4MIE_MGUAN									
ATOM	1	CB	4MIE	1	1.601	0.589	1.936	1.00	0.00	4MIE
ATOM	2	HB1	4MIE	1	2.108	1.073	1.101	1.00	0.00	4MIE
ATOM	3	HB2	4MIE	1	0.711	1.170	2.180	1.00	0.00	4MIE
ATOM	4	HB3	4MIE	1	2.268	0.620	2.796	1.00	0.00	4MIE
ATOM	5	CG	4MIE	1	1.246	-0.824	1.604	1.00	0.00	4MIE
ATOM	6	ND1	4MIE	1	0.411	-1.138	0.541	1.00	0.00	4MIE
ATOM	7	CD2	4MIE	1	1.642	-1.989	2.228	1.00	0.00	4MIE
ATOM	8	HD2	4MIE	1	2.279	-2.168	3.078	1.00	0.00	4MIE
ATOM	9	CE1	4MIE	1	0.306	-2.472	0.530	1.00	0.00	4MIE
ATOM	10	HE1	4MIE	1	-0.268	-3.060	-0.167	1.00	0.00	4MIE
ATOM	11	NE2	4MIE	1	1.037	-3.012	1.535	1.00	0.00	4MIE
ATOM	12	HE2	4MIE	1	1.122	-3.998	1.738	1.00	0.00	4MIE
ATOM	13	C	MGUA	1	-0.839	1.288	-1.491	1.00	0.00	MGUA
ATOM	14	N1	MGUA	1	0.273	0.625	-1.848	1.00	0.00	MGUA
ATOM	15	H11	MGUA	1	0.599	-0.090	-1.197	1.00	0.00	MGUA
ATOM	16	H12	MGUA	1	0.930	1.045	-2.486	1.00	0.00	MGUA
ATOM	17	N2	MGUA	1	-1.461	0.921	-0.367	1.00	0.00	MGUA
ATOM	18	H21	MGUA	1	-2.415	1.189	-0.191	1.00	0.00	MGUA
ATOM	19	H22	MGUA	1	-1.044	0.139	0.148	1.00	0.00	MGUA
ATOM	20	N3	MGUA	1	-1.301	2.299	-2.236	1.00	0.00	MGUA
ATOM	21	H31	MGUA	1	-0.889	2.429	-3.148	1.00	0.00	MGUA
ATOM	22	C2	MGUA	1	-2.493	3.074	-1.899	1.00	0.00	MGUA
ATOM	23	HC1	MGUA	1	-2.555	3.907	-2.591	1.00	0.00	MGUA
ATOM	24	HC2	MGUA	1	-3.400	2.475	-1.992	1.00	0.00	MGUA
ATOM	25	HC3	MGUA	1	-2.404	3.471	-0.890	1.00	0.00	MGUA
END										
REMARK	80_4MIE_MGUAN									
ATOM	1	CB	4MIE	1	-1.879	1.270	1.242	1.00	0.00	4MIE
ATOM	2	HB1	4MIE	1	-1.663	2.036	0.495	1.00	0.00	4MIE
ATOM	3	HB2	4MIE	1	-2.889	1.448	1.607	1.00	0.00	4MIE
ATOM	4	HB3	4MIE	1	-1.198	1.395	2.086	1.00	0.00	4MIE
ATOM	5	CG	4MIE	1	-1.765	-0.100	0.658	1.00	0.00	4MIE
ATOM	6	ND1	4MIE	1	-0.592	-0.555	0.078	1.00	0.00	4MIE
ATOM	7	CD2	4MIE	1	-2.728	-1.089	0.609	1.00	0.00	4MIE
ATOM	8	HD2	4MIE	1	-3.748	-1.120	0.950	1.00	0.00	4MIE
ATOM	9	CE1	4MIE	1	-0.849	-1.805	-0.313	1.00	0.00	4MIE
ATOM	10	HE1	4MIE	1	-0.161	-2.476	-0.800	1.00	0.00	4MIE
ATOM	11	NE2	4MIE	1	-2.127	-2.160	-0.010	1.00	0.00	4MIE
ATOM	12	HE2	4MIE	1	-2.557	-3.054	-0.200	1.00	0.00	4MIE
ATOM	13	C	MGUA	1	1.594	1.194	-0.561	1.00	0.00	MGUA
ATOM	14	N1	MGUA	1	0.835	1.782	-1.508	1.00	0.00	MGUA
ATOM	15	H11	MGUA	1	0.430	2.685	-1.315	1.00	0.00	MGUA
ATOM	16	H12	MGUA	1	0.298	1.178	-2.113	1.00	0.00	MGUA
ATOM	17	N2	MGUA	1	1.719	1.768	0.641	1.00	0.00	MGUA
ATOM	18	H21	MGUA	1	2.398	1.428	1.303	1.00	0.00	MGUA

ATOM	19	H22	MGUA	1	0.968	2.333	1.005	1.00	0.00	MGUA
ATOM	20	N3	MGUA	1	2.306	0.117	-0.871	1.00	0.00	MGUA
ATOM	21	H31	MGUA	1	2.336	-0.141	-1.847	1.00	0.00	MGUA
ATOM	22	C2	MGUA	1	2.860	-0.798	0.125	1.00	0.00	MGUA
ATOM	23	HC1	MGUA	1	3.125	-1.721	-0.381	1.00	0.00	MGUA
ATOM	24	HC2	MGUA	1	3.762	-0.390	0.580	1.00	0.00	MGUA
ATOM	25	HC3	MGUA	1	2.102	-1.007	0.879	1.00	0.00	MGUA

END

REMARK 81_4MIE_MGUAN

ATOM	1	CB	4MIE	1	-1.603	1.804	-0.964	1.00	0.00	4MIE
ATOM	2	HB1	4MIE	1	-0.954	1.724	-1.837	1.00	0.00	4MIE
ATOM	3	HB2	4MIE	1	-2.444	2.441	-1.231	1.00	0.00	4MIE
ATOM	4	HB3	4MIE	1	-1.046	2.299	-0.168	1.00	0.00	4MIE
ATOM	5	CG	4MIE	1	-2.086	0.461	-0.524	1.00	0.00	4MIE
ATOM	6	ND1	4MIE	1	-1.219	-0.504	-0.032	1.00	0.00	4MIE
ATOM	7	CD2	4MIE	1	-3.370	-0.045	-0.532	1.00	0.00	4MIE
ATOM	8	HD2	4MIE	1	-4.310	0.384	-0.834	1.00	0.00	4MIE
ATOM	9	CE1	4MIE	1	-1.971	-1.575	0.247	1.00	0.00	4MIE
ATOM	10	HE1	4MIE	1	-1.621	-2.513	0.647	1.00	0.00	4MIE
ATOM	11	NE2	4MIE	1	-3.272	-1.328	-0.043	1.00	0.00	4MIE
ATOM	12	HE2	4MIE	1	-4.037	-1.976	0.081	1.00	0.00	4MIE
ATOM	13	C	MGUA	1	2.062	0.225	0.511	1.00	0.00	MGUA
ATOM	14	N1	MGUA	1	1.162	0.559	1.453	1.00	0.00	MGUA
ATOM	15	H11	MGUA	1	0.205	0.247	1.291	1.00	0.00	MGUA
ATOM	16	H12	MGUA	1	1.464	0.710	2.403	1.00	0.00	MGUA
ATOM	17	N2	MGUA	1	1.625	-0.390	-0.590	1.00	0.00	MGUA
ATOM	18	H21	MGUA	1	2.201	-0.460	-1.412	1.00	0.00	MGUA
ATOM	19	H22	MGUA	1	0.615	-0.571	-0.643	1.00	0.00	MGUA
ATOM	20	N3	MGUA	1	3.360	0.502	0.683	1.00	0.00	MGUA
ATOM	21	H31	MGUA	1	3.605	1.108	1.451	1.00	0.00	MGUA
ATOM	22	C2	MGUA	1	4.392	0.176	-0.299	1.00	0.00	MGUA
ATOM	23	HC1	MGUA	1	5.355	0.409	0.143	1.00	0.00	MGUA
ATOM	24	HC2	MGUA	1	4.368	-0.888	-0.526	1.00	0.00	MGUA
ATOM	25	HC3	MGUA	1	4.274	0.762	-1.211	1.00	0.00	MGUA

END

REMARK 82_4MIE_MGUAN

ATOM	1	CB	4MIE	1	1.841	2.091	-0.076	1.00	0.00	4MIE
ATOM	2	HB1	4MIE	1	0.787	2.220	-0.320	1.00	0.00	4MIE
ATOM	3	HB2	4MIE	1	2.065	2.688	0.806	1.00	0.00	4MIE
ATOM	4	HB3	4MIE	1	2.423	2.487	-0.909	1.00	0.00	4MIE
ATOM	5	CG	4MIE	1	2.142	0.644	0.153	1.00	0.00	4MIE
ATOM	6	ND1	4MIE	1	1.283	-0.361	-0.267	1.00	0.00	4MIE
ATOM	7	CD2	4MIE	1	3.264	0.068	0.718	1.00	0.00	4MIE
ATOM	8	HD2	4MIE	1	4.141	0.500	1.167	1.00	0.00	4MIE
ATOM	9	CE1	4MIE	1	1.881	-1.519	0.031	1.00	0.00	4MIE
ATOM	10	HE1	4MIE	1	1.491	-2.506	-0.157	1.00	0.00	4MIE
ATOM	11	NE2	4MIE	1	3.078	-1.291	0.628	1.00	0.00	4MIE
ATOM	12	HE2	4MIE	1	3.722	-2.001	0.947	1.00	0.00	4MIE
ATOM	13	C	MGUA	1	-2.088	0.050	0.008	1.00	0.00	MGUA
ATOM	14	N1	MGUA	1	-1.383	0.099	1.160	1.00	0.00	MGUA
ATOM	15	H11	MGUA	1	-0.374	0.134	1.065	1.00	0.00	MGUA
ATOM	16	H12	MGUA	1	-1.785	0.562	1.961	1.00	0.00	MGUA
ATOM	17	N2	MGUA	1	-1.428	-0.148	-1.130	1.00	0.00	MGUA
ATOM	18	H21	MGUA	1	-1.916	-0.344	-1.988	1.00	0.00	MGUA
ATOM	19	H22	MGUA	1	-0.397	-0.246	-1.070	1.00	0.00	MGUA
ATOM	20	N3	MGUA	1	-3.419	0.180	0.030	1.00	0.00	MGUA
ATOM	21	H31	MGUA	1	-3.869	0.228	0.932	1.00	0.00	MGUA
ATOM	22	C2	MGUA	1	-4.258	0.106	-1.163	1.00	0.00	MGUA
ATOM	23	HC1	MGUA	1	-5.288	0.252	-0.855	1.00	0.00	MGUA
ATOM	24	HC2	MGUA	1	-3.992	0.895	-1.865	1.00	0.00	MGUA
ATOM	25	HC3	MGUA	1	-4.176	-0.870	-1.641	1.00	0.00	MGUA

END

REMARK 83_4MIE_MGUAN

ATOM	1	CB	4MIE	1	-1.696	1.419	1.375	1.00	0.00	4MIE
ATOM	2	HB1	4MIE	1	-0.880	1.177	2.056	1.00	0.00	4MIE
ATOM	3	HB2	4MIE	1	-1.367	2.224	0.718	1.00	0.00	4MIE
ATOM	4	HB3	4MIE	1	-2.530	1.790	1.967	1.00	0.00	4MIE
ATOM	5	CG	4MIE	1	-2.111	0.217	0.590	1.00	0.00	4MIE
ATOM	6	ND1	4MIE	1	-1.202	-0.519	-0.157	1.00	0.00	4MIE
ATOM	7	CD2	4MIE	1	-3.366	-0.340	0.452	1.00	0.00	4MIE
ATOM	8	HD2	4MIE	1	-4.322	-0.068	0.865	1.00	0.00	4MIE
ATOM	9	CE1	4MIE	1	-1.902	-1.500	-0.738	1.00	0.00	4MIE

ATOM	10	HE1	4MIE	1	-1.511	-2.260	-1.393	1.00	0.00	4MIE
ATOM	11	NE2	4MIE	1	-3.209	-1.418	-0.389	1.00	0.00	4MIE
ATOM	12	HE2	4MIE	1	-3.941	-2.044	-0.695	1.00	0.00	4MIE
ATOM	13	C	MGUA	1	2.129	0.168	-0.019	1.00	0.00	MGUA
ATOM	14	N1	MGUA	1	1.587	-0.602	0.942	1.00	0.00	MGUA
ATOM	15	H11	MGUA	1	0.606	-0.850	0.817	1.00	0.00	MGUA
ATOM	16	H12	MGUA	1	2.175	-1.218	1.481	1.00	0.00	MGUA
ATOM	17	N2	MGUA	1	1.334	0.620	-0.990	1.00	0.00	MGUA
ATOM	18	H21	MGUA	1	1.625	1.368	-1.598	1.00	0.00	MGUA
ATOM	19	H22	MGUA	1	0.347	0.341	-0.940	1.00	0.00	MGUA
ATOM	20	N3	MGUA	1	3.434	0.464	0.004	1.00	0.00	MGUA
ATOM	21	H31	MGUA	1	3.945	0.236	0.843	1.00	0.00	MGUA
ATOM	22	C2	MGUA	1	4.091	1.298	-1.000	1.00	0.00	MGUA
ATOM	23	HC1	MGUA	1	5.158	1.280	-0.801	1.00	0.00	MGUA
ATOM	24	HC2	MGUA	1	3.922	0.887	-1.994	1.00	0.00	MGUA
ATOM	25	HC3	MGUA	1	3.744	2.330	-0.952	1.00	0.00	MGUA

END

REMARK 84_4MIE_MGUAN

ATOM	1	CB	4MIE	1	1.781	1.525	-1.001	1.00	0.00	4MIE
ATOM	2	HB1	4MIE	1	0.921	1.972	-0.504	1.00	0.00	4MIE
ATOM	3	HB2	4MIE	1	2.616	2.217	-0.911	1.00	0.00	4MIE
ATOM	4	HB3	4MIE	1	1.546	1.417	-2.061	1.00	0.00	4MIE
ATOM	5	CG	4MIE	1	2.103	0.208	-0.368	1.00	0.00	4MIE
ATOM	6	ND1	4MIE	1	1.212	-0.441	0.474	1.00	0.00	4MIE
ATOM	7	CD2	4MIE	1	3.236	-0.569	-0.509	1.00	0.00	4MIE
ATOM	8	HD2	4MIE	1	4.144	-0.422	-1.067	1.00	0.00	4MIE
ATOM	9	CE1	4MIE	1	1.805	-1.581	0.846	1.00	0.00	4MIE
ATOM	10	HE1	4MIE	1	1.401	-2.322	1.515	1.00	0.00	4MIE
ATOM	11	NE2	4MIE	1	3.024	-1.687	0.264	1.00	0.00	4MIE
ATOM	12	HE2	4MIE	1	3.653	-2.471	0.358	1.00	0.00	4MIE
ATOM	13	C	MGUA	1	-2.069	0.187	-0.038	1.00	0.00	MGUA
ATOM	14	N1	MGUA	1	-1.466	-0.748	-0.790	1.00	0.00	MGUA
ATOM	15	H11	MGUA	1	-0.514	-1.004	-0.544	1.00	0.00	MGUA
ATOM	16	H12	MGUA	1	-1.869	-1.074	-1.652	1.00	0.00	MGUA
ATOM	17	N2	MGUA	1	-1.397	0.678	1.003	1.00	0.00	MGUA
ATOM	18	H21	MGUA	1	-1.804	1.368	1.612	1.00	0.00	MGUA
ATOM	19	H22	MGUA	1	-0.408	0.404	1.092	1.00	0.00	MGUA
ATOM	20	N3	MGUA	1	-3.313	0.593	-0.319	1.00	0.00	MGUA
ATOM	21	H31	MGUA	1	-3.804	0.125	-1.065	1.00	0.00	MGUA
ATOM	22	C2	MGUA	1	-4.022	1.615	0.447	1.00	0.00	MGUA
ATOM	23	HC1	MGUA	1	-4.997	1.753	-0.008	1.00	0.00	MGUA
ATOM	24	HC2	MGUA	1	-4.165	1.301	1.480	1.00	0.00	MGUA
ATOM	25	HC3	MGUA	1	-3.487	2.563	0.409	1.00	0.00	MGUA

END

REMARK 85_4MIM_MGUAN

ATOM	1	CB	4MIM	1	3.912	-0.950	-2.153	1.00	0.00	4MIM
ATOM	2	HB1	4MIM	1	3.855	-1.380	-3.153	1.00	0.00	4MIM
ATOM	3	HB2	4MIM	1	4.195	0.095	-2.251	1.00	0.00	4MIM
ATOM	4	HB3	4MIM	1	4.699	-1.463	-1.600	1.00	0.00	4MIM
ATOM	5	CG	4MIM	1	2.602	-1.043	-1.446	1.00	0.00	4MIM
ATOM	6	ND1	4MIM	1	1.975	-2.242	-1.172	1.00	0.00	4MIM
ATOM	7	HD1	4MIM	1	2.328	-3.159	-1.412	1.00	0.00	4MIM
ATOM	8	CD2	4MIM	1	1.748	-0.087	-0.935	1.00	0.00	4MIM
ATOM	9	HD2	4MIM	1	1.875	0.983	-0.950	1.00	0.00	4MIM
ATOM	10	CE1	4MIM	1	0.806	-1.994	-0.528	1.00	0.00	4MIM
ATOM	11	HE1	4MIM	1	0.131	-2.770	-0.205	1.00	0.00	4MIM
ATOM	12	NE2	4MIM	1	0.634	-0.679	-0.364	1.00	0.00	4MIM
ATOM	13	C	MGUA	1	-1.799	1.053	1.271	1.00	0.00	MGUA
ATOM	14	N1	MGUA	1	-0.791	0.513	1.976	1.00	0.00	MGUA
ATOM	15	H11	MGUA	1	-0.078	0.022	1.436	1.00	0.00	MGUA
ATOM	16	H12	MGUA	1	-0.542	0.897	2.873	1.00	0.00	MGUA
ATOM	17	N2	MGUA	1	-1.836	0.837	-0.046	1.00	0.00	MGUA
ATOM	18	H21	MGUA	1	-2.673	1.005	-0.579	1.00	0.00	MGUA
ATOM	19	H22	MGUA	1	-1.078	0.267	-0.437	1.00	0.00	MGUA
ATOM	20	N3	MGUA	1	-2.734	1.795	1.876	1.00	0.00	MGUA
ATOM	21	H31	MGUA	1	-2.747	1.789	2.885	1.00	0.00	MGUA
ATOM	22	C2	MGUA	1	-3.852	2.419	1.173	1.00	0.00	MGUA
ATOM	23	HC1	MGUA	1	-4.373	3.058	1.879	1.00	0.00	MGUA
ATOM	24	HC2	MGUA	1	-3.480	3.039	0.360	1.00	0.00	MGUA
ATOM	25	HC3	MGUA	1	-4.552	1.675	0.793	1.00	0.00	MGUA

END

REMARK 86_4MIM_MGUAN

ATOM	1	CB	4MIM	1	-3.854	0.369	-1.063	1.00	0.00	4MIM
ATOM	2	HB1	4MIM	1	-4.126	-0.087	-2.026	1.00	0.00	4MIM
ATOM	3	HB2	4MIM	1	-4.727	0.328	-0.394	1.00	0.00	4MIM
ATOM	4	HB3	4MIM	1	-3.609	1.424	-1.240	1.00	0.00	4MIM
ATOM	5	CG	4MIM	1	-2.672	-0.314	-0.455	1.00	0.00	4MIM
ATOM	6	ND1	4MIM	1	-2.663	-1.658	-0.108	1.00	0.00	4MIM
ATOM	7	HD1	4MIM	1	-3.430	-2.313	-0.246	1.00	0.00	4MIM
ATOM	8	CD2	4MIM	1	-1.419	0.146	-0.087	1.00	0.00	4MIM
ATOM	9	HD2	4MIM	1	-1.022	1.153	-0.188	1.00	0.00	4MIM
ATOM	10	CE1	4MIM	1	-1.454	-1.973	0.435	1.00	0.00	4MIM
ATOM	11	HE1	4MIM	1	-1.226	-2.978	0.773	1.00	0.00	4MIM
ATOM	12	NE2	4MIM	1	-0.667	-0.887	0.455	1.00	0.00	4MIM
ATOM	13	C	MGUA	1	2.397	1.151	0.513	1.00	0.00	MGUA
ATOM	14	N1	MGUA	1	3.109	2.250	0.935	1.00	0.00	MGUA
ATOM	15	H11	MGUA	1	2.797	2.798	1.741	1.00	0.00	MGUA
ATOM	16	H12	MGUA	1	4.015	2.487	0.519	1.00	0.00	MGUA
ATOM	17	N2	MGUA	1	1.460	0.593	1.313	1.00	0.00	MGUA
ATOM	18	H21	MGUA	1	0.625	-0.012	0.949	1.00	0.00	MGUA
ATOM	19	H22	MGUA	1	1.413	0.923	2.283	1.00	0.00	MGUA
ATOM	20	N3	MGUA	1	2.663	0.683	-0.740	1.00	0.00	MGUA
ATOM	21	H31	MGUA	1	3.270	1.269	-1.308	1.00	0.00	MGUA
ATOM	22	C2	MGUA	1	2.372	-0.686	-1.236	1.00	0.00	MGUA
ATOM	23	HC1	MGUA	1	2.033	-0.666	-2.278	1.00	0.00	MGUA
ATOM	24	HC2	MGUA	1	3.330	-1.212	-1.132	1.00	0.00	MGUA
ATOM	25	HC3	MGUA	1	1.575	-1.194	-0.689	1.00	0.00	MGUA

END

REMARK 87_4MIM_MGUAN

ATOM	1	CB	4MIM	1	-4.075	1.788	-0.543	1.00	0.00	4MIM
ATOM	2	HB1	4MIM	1	-4.798	1.886	0.266	1.00	0.00	4MIM
ATOM	3	HB2	4MIM	1	-3.697	2.781	-0.774	1.00	0.00	4MIM
ATOM	4	HB3	4MIM	1	-4.598	1.407	-1.419	1.00	0.00	4MIM
ATOM	5	CG	4MIM	1	-2.955	0.883	-0.148	1.00	0.00	4MIM
ATOM	6	ND1	4MIM	1	-3.048	-0.027	0.885	1.00	0.00	4MIM
ATOM	7	HD1	4MIM	1	-3.829	-0.123	1.517	1.00	0.00	4MIM
ATOM	8	CD2	4MIM	1	-1.694	0.674	-0.671	1.00	0.00	4MIM
ATOM	9	HD2	4MIM	1	-1.232	1.185	-1.500	1.00	0.00	4MIM
ATOM	10	CE1	4MIM	1	-1.889	-0.730	0.966	1.00	0.00	4MIM
ATOM	11	HE1	4MIM	1	-1.716	-1.506	1.693	1.00	0.00	4MIM
ATOM	12	NE2	4MIM	1	-1.032	-0.321	0.026	1.00	0.00	4MIM
ATOM	13	C	MGUA	1	2.355	-0.278	0.087	1.00	0.00	MGUA
ATOM	14	N1	MGUA	1	1.683	0.507	0.949	1.00	0.00	MGUA
ATOM	15	H11	MGUA	1	0.675	0.376	0.996	1.00	0.00	MGUA
ATOM	16	H12	MGUA	1	2.158	0.928	1.730	1.00	0.00	MGUA
ATOM	17	N2	MGUA	1	1.652	-1.075	-0.718	1.00	0.00	MGUA
ATOM	18	H21	MGUA	1	2.090	-1.568	-1.478	1.00	0.00	MGUA
ATOM	19	H22	MGUA	1	0.626	-1.030	-0.638	1.00	0.00	MGUA
ATOM	20	N3	MGUA	1	3.691	-0.247	0.038	1.00	0.00	MGUA
ATOM	21	H31	MGUA	1	4.167	0.427	0.617	1.00	0.00	MGUA
ATOM	22	C2	MGUA	1	4.487	-1.063	-0.876	1.00	0.00	MGUA
ATOM	23	HC1	MGUA	1	5.533	-0.853	-0.682	1.00	0.00	MGUA
ATOM	24	HC2	MGUA	1	4.307	-2.121	-0.698	1.00	0.00	MGUA
ATOM	25	HC3	MGUA	1	4.271	-0.811	-1.914	1.00	0.00	MGUA

END

REMARK 88_4MIM_MGUAN

ATOM	1	CB	4MIM	1	4.347	0.961	1.022	1.00	0.00	4MIM
ATOM	2	HB1	4MIM	1	4.811	1.829	0.554	1.00	0.00	4MIM
ATOM	3	HB2	4MIM	1	4.125	1.214	2.056	1.00	0.00	4MIM
ATOM	4	HB3	4MIM	1	5.067	0.142	1.023	1.00	0.00	4MIM
ATOM	5	CG	4MIM	1	3.086	0.575	0.326	1.00	0.00	4MIM
ATOM	6	ND1	4MIM	1	3.041	0.197	-1.000	1.00	0.00	4MIM
ATOM	7	HD1	4MIM	1	3.835	0.144	-1.624	1.00	0.00	4MIM
ATOM	8	CD2	4MIM	1	1.775	0.490	0.750	1.00	0.00	4MIM
ATOM	9	HD2	4MIM	1	1.388	0.702	1.733	1.00	0.00	4MIM
ATOM	10	CE1	4MIM	1	1.758	-0.095	-1.335	1.00	0.00	4MIM
ATOM	11	HE1	4MIM	1	1.461	-0.416	-2.320	1.00	0.00	4MIM
ATOM	12	NE2	4MIM	1	0.951	0.075	-0.283	1.00	0.00	4MIM
ATOM	13	C	MGUA	1	-2.437	-0.158	-0.041	1.00	0.00	MGUA
ATOM	14	N1	MGUA	1	-1.892	0.968	-0.535	1.00	0.00	MGUA
ATOM	15	H11	MGUA	1	-0.873	0.997	-0.564	1.00	0.00	MGUA
ATOM	16	H12	MGUA	1	-2.400	1.836	-0.482	1.00	0.00	MGUA
ATOM	17	N2	MGUA	1	-1.622	-1.166	0.276	1.00	0.00	MGUA
ATOM	18	H21	MGUA	1	-1.976	-2.096	0.427	1.00	0.00	MGUA

ATOM	19	H22	MGUA	1	-0.619	-1.009	0.129	1.00	0.00	MGUA
ATOM	20	N3	MGUA	1	-3.760	-0.256	0.132	1.00	0.00	MGUA
ATOM	21	H31	MGUA	1	-4.334	0.468	-0.274	1.00	0.00	MGUA
ATOM	22	C2	MGUA	1	-4.420	-1.444	0.667	1.00	0.00	MGUA
ATOM	23	HC1	MGUA	1	-5.468	-1.204	0.814	1.00	0.00	MGUA
ATOM	24	HC2	MGUA	1	-4.347	-2.286	-0.022	1.00	0.00	MGUA
ATOM	25	HC3	MGUA	1	-3.990	-1.705	1.632	1.00	0.00	MGUA

END

REMARK 89_4MIM_MGUAN

ATOM	1	CB	4MIM	1	-4.314	1.350	-0.550	1.00	0.00	4MIM
ATOM	2	HB1	4MIM	1	-4.904	0.921	-1.360	1.00	0.00	4MIM
ATOM	3	HB2	4MIM	1	-4.944	1.420	0.338	1.00	0.00	4MIM
ATOM	4	HB3	4MIM	1	-4.028	2.359	-0.840	1.00	0.00	4MIM
ATOM	5	CG	4MIM	1	-3.087	0.547	-0.284	1.00	0.00	4MIM
ATOM	6	ND1	4MIM	1	-3.120	-0.776	0.109	1.00	0.00	4MIM
ATOM	7	HD1	4MIM	1	-3.956	-1.327	0.249	1.00	0.00	4MIM
ATOM	8	CD2	4MIM	1	-1.742	0.853	-0.335	1.00	0.00	4MIM
ATOM	9	HD2	4MIM	1	-1.293	1.795	-0.605	1.00	0.00	4MIM
ATOM	10	CE1	4MIM	1	-1.848	-1.221	0.278	1.00	0.00	4MIM
ATOM	11	HE1	4MIM	1	-1.609	-2.227	0.582	1.00	0.00	4MIM
ATOM	12	NE2	4MIM	1	-0.974	-0.246	0.011	1.00	0.00	4MIM
ATOM	13	C	MGUA	1	2.428	-0.154	-0.092	1.00	0.00	MGUA
ATOM	14	N1	MGUA	1	1.739	-0.402	-1.219	1.00	0.00	MGUA
ATOM	15	H11	MGUA	1	0.728	-0.492	-1.118	1.00	0.00	MGUA
ATOM	16	H12	MGUA	1	2.193	-0.849	-1.999	1.00	0.00	MGUA
ATOM	17	N2	MGUA	1	1.742	0.029	1.039	1.00	0.00	MGUA
ATOM	18	H21	MGUA	1	2.172	0.453	1.844	1.00	0.00	MGUA
ATOM	19	H22	MGUA	1	0.721	-0.022	0.966	1.00	0.00	MGUA
ATOM	20	N3	MGUA	1	3.765	-0.104	-0.107	1.00	0.00	MGUA
ATOM	21	H31	MGUA	1	4.216	-0.083	-1.009	1.00	0.00	MGUA
ATOM	22	C2	MGUA	1	4.577	0.158	1.079	1.00	0.00	MGUA
ATOM	23	HC1	MGUA	1	5.618	0.013	0.807	1.00	0.00	MGUA
ATOM	24	HC2	MGUA	1	4.447	1.180	1.436	1.00	0.00	MGUA
ATOM	25	HC3	MGUA	1	4.327	-0.553	1.865	1.00	0.00	MGUA

END

REMARK 90_4MIM_MGUAN

ATOM	1	CB	4MIM	1	4.356	1.127	-0.762	1.00	0.00	4MIM
ATOM	2	HB1	4MIM	1	4.840	1.805	-0.059	1.00	0.00	4MIM
ATOM	3	HB2	4MIM	1	5.061	0.337	-1.024	1.00	0.00	4MIM
ATOM	4	HB3	4MIM	1	4.126	1.686	-1.666	1.00	0.00	4MIM
ATOM	5	CG	4MIM	1	3.096	0.565	-0.195	1.00	0.00	4MIM
ATOM	6	ND1	4MIM	1	3.059	-0.196	0.955	1.00	0.00	4MIM
ATOM	7	HD1	4MIM	1	3.859	-0.449	1.519	1.00	0.00	4MIM
ATOM	8	CD2	4MIM	1	1.778	0.639	-0.597	1.00	0.00	4MIM
ATOM	9	HD2	4MIM	1	1.381	1.150	-1.459	1.00	0.00	4MIM
ATOM	10	CE1	4MIM	1	1.774	-0.552	1.212	1.00	0.00	4MIM
ATOM	11	HE1	4MIM	1	1.483	-1.152	2.058	1.00	0.00	4MIM
ATOM	12	NE2	4MIM	1	0.958	-0.057	0.276	1.00	0.00	4MIM
ATOM	13	C	MGUA	1	-2.387	-0.470	-0.208	1.00	0.00	MGUA
ATOM	14	N1	MGUA	1	-1.541	-1.425	-0.630	1.00	0.00	MGUA
ATOM	15	H11	MGUA	1	-0.548	-1.245	-0.479	1.00	0.00	MGUA
ATOM	16	H12	MGUA	1	-1.814	-2.046	-1.374	1.00	0.00	MGUA
ATOM	17	N2	MGUA	1	-1.880	0.581	0.440	1.00	0.00	MGUA
ATOM	18	H21	MGUA	1	-2.468	1.194	0.979	1.00	0.00	MGUA
ATOM	19	H22	MGUA	1	-0.863	0.589	0.572	1.00	0.00	MGUA
ATOM	20	N3	MGUA	1	-3.700	-0.570	-0.443	1.00	0.00	MGUA
ATOM	21	H31	MGUA	1	-4.042	-1.454	-0.789	1.00	0.00	MGUA
ATOM	22	C2	MGUA	1	-4.676	0.432	-0.021	1.00	0.00	MGUA
ATOM	23	HC1	MGUA	1	-5.636	0.161	-0.449	1.00	0.00	MGUA
ATOM	24	HC2	MGUA	1	-4.774	0.464	1.064	1.00	0.00	MGUA
ATOM	25	HC3	MGUA	1	-4.394	1.410	-0.405	1.00	0.00	MGUA

END

REMARK 91_4MIM_MGUAN

ATOM	1	CB	4MIM	1	-4.523	0.014	0.605	1.00	0.00	4MIM
ATOM	2	HB1	4MIM	1	-4.905	0.182	1.612	1.00	0.00	4MIM
ATOM	3	HB2	4MIM	1	-5.142	0.573	-0.098	1.00	0.00	4MIM
ATOM	4	HB3	4MIM	1	-4.628	-1.044	0.377	1.00	0.00	4MIM
ATOM	5	CG	4MIM	1	-3.088	0.403	0.496	1.00	0.00	4MIM
ATOM	6	ND1	4MIM	1	-2.634	1.686	0.726	1.00	0.00	4MIM
ATOM	7	HD1	4MIM	1	-3.210	2.476	0.983	1.00	0.00	4MIM
ATOM	8	CD2	4MIM	1	-1.949	-0.311	0.182	1.00	0.00	4MIM
ATOM	9	HD2	4MIM	1	-1.877	-1.358	-0.063	1.00	0.00	4MIM

ATOM	10	CE1	4MIM	1	-1.287	1.718	0.553	1.00	0.00	4MIM
ATOM	11	HE1	4MIM	1	-0.695	2.610	0.676	1.00	0.00	4MIM
ATOM	12	NE2	4MIM	1	-0.832	0.507	0.217	1.00	0.00	4MIM
ATOM	13	C	MGUA	1	2.292	-0.531	-0.652	1.00	0.00	MGUA
ATOM	14	N1	MGUA	1	1.524	0.075	-1.574	1.00	0.00	MGUA
ATOM	15	H11	MGUA	1	0.589	0.348	-1.270	1.00	0.00	MGUA
ATOM	16	H12	MGUA	1	1.684	-0.097	-2.553	1.00	0.00	MGUA
ATOM	17	N2	MGUA	1	1.817	-0.646	0.590	1.00	0.00	MGUA
ATOM	18	H21	MGUA	1	2.423	-0.867	1.362	1.00	0.00	MGUA
ATOM	19	H22	MGUA	1	0.880	-0.262	0.758	1.00	0.00	MGUA
ATOM	20	N3	MGUA	1	3.498	-1.011	-0.979	1.00	0.00	MGUA
ATOM	21	H31	MGUA	1	3.869	-0.754	-1.881	1.00	0.00	MGUA
ATOM	22	C2	MGUA	1	4.382	-1.688	-0.034	1.00	0.00	MGUA
ATOM	23	HC1	MGUA	1	5.227	-2.080	-0.590	1.00	0.00	MGUA
ATOM	24	HC2	MGUA	1	4.753	-1.003	0.729	1.00	0.00	MGUA
ATOM	25	HC3	MGUA	1	3.861	-2.523	0.430	1.00	0.00	MGUA

END

REMARK 92_BENZ_IMIM

ATOM	1	CG	BENZ	1	1.940	0.701	-1.215	1.00	0.00	BENZ
ATOM	2	HG	BENZ	1	1.966	1.243	-2.153	1.00	0.00	BENZ
ATOM	3	CD1	BENZ	1	1.942	1.402	0.000	1.00	0.00	BENZ
ATOM	4	HD1	BENZ	1	1.977	2.485	0.000	1.00	0.00	BENZ
ATOM	5	CD2	BENZ	1	1.935	-0.700	-1.215	1.00	0.00	BENZ
ATOM	6	HD2	BENZ	1	1.959	-1.241	-2.153	1.00	0.00	BENZ
ATOM	7	CE1	BENZ	1	1.940	0.701	1.215	1.00	0.00	BENZ
ATOM	8	HE1	BENZ	1	1.966	1.242	2.153	1.00	0.00	BENZ
ATOM	9	CE2	BENZ	1	1.933	-1.401	-0.000	1.00	0.00	BENZ
ATOM	10	HE2	BENZ	1	1.965	-2.484	-0.000	1.00	0.00	BENZ
ATOM	11	CZ	BENZ	1	1.935	-0.700	1.215	1.00	0.00	BENZ
ATOM	12	HZ	BENZ	1	1.959	-1.241	2.153	1.00	0.00	BENZ
ATOM	13	CG	IMIM	1	-1.856	1.140	-0.000	1.00	0.00	IMIM
ATOM	14	HG	IMIM	1	-1.445	2.134	-0.000	1.00	0.00	IMIM
ATOM	15	CD2	IMIM	1	-3.158	0.702	-0.000	1.00	0.00	IMIM
ATOM	16	HD2	IMIM	1	-4.088	1.243	-0.000	1.00	0.00	IMIM
ATOM	17	ND1	IMIM	1	-1.064	0.019	-0.000	1.00	0.00	IMIM
ATOM	18	HD1	IMIM	1	-0.044	0.012	-0.000	1.00	0.00	IMIM
ATOM	19	NE2	IMIM	1	-3.101	-0.673	0.000	1.00	0.00	IMIM
ATOM	20	HE2	IMIM	1	-3.900	-1.296	0.000	1.00	0.00	IMIM
ATOM	21	CE1	IMIM	1	-1.821	-1.083	0.000	1.00	0.00	IMIM
ATOM	22	HE1	IMIM	1	-1.470	-2.100	0.000	1.00	0.00	IMIM

END

REMARK 93_BENZ_IMIM

ATOM	1	CG	BENZ	1	1.686	0.035	1.718	1.00	0.00	BENZ
ATOM	2	HG	BENZ	1	1.551	0.047	2.793	1.00	0.00	BENZ
ATOM	3	CD1	BENZ	1	1.789	-1.186	1.036	1.00	0.00	BENZ
ATOM	4	HD1	BENZ	1	1.744	-2.118	1.587	1.00	0.00	BENZ
ATOM	5	CD2	BENZ	1	1.788	1.243	1.011	1.00	0.00	BENZ
ATOM	6	HD2	BENZ	1	1.738	2.186	1.543	1.00	0.00	BENZ
ATOM	7	CE1	BENZ	1	1.994	-1.199	-0.351	1.00	0.00	BENZ
ATOM	8	HE1	BENZ	1	2.108	-2.141	-0.873	1.00	0.00	BENZ
ATOM	9	CE2	BENZ	1	1.993	1.228	-0.376	1.00	0.00	BENZ
ATOM	10	HE2	BENZ	1	2.101	2.160	-0.917	1.00	0.00	BENZ
ATOM	11	CZ	BENZ	1	2.099	0.008	-1.056	1.00	0.00	BENZ
ATOM	12	HZ	BENZ	1	2.281	-0.003	-2.123	1.00	0.00	BENZ
ATOM	13	CG	IMIM	1	-1.869	1.129	-0.276	1.00	0.00	IMIM
ATOM	14	HG	IMIM	1	-1.520	2.139	-0.153	1.00	0.00	IMIM
ATOM	15	CD2	IMIM	1	-3.075	0.638	-0.713	1.00	0.00	IMIM
ATOM	16	HD2	IMIM	1	-3.969	1.141	-1.037	1.00	0.00	IMIM
ATOM	17	ND1	IMIM	1	-1.081	0.041	0.010	1.00	0.00	IMIM
ATOM	18	HD1	IMIM	1	-0.122	0.078	0.363	1.00	0.00	IMIM
ATOM	19	NE2	IMIM	1	-2.969	-0.734	-0.673	1.00	0.00	IMIM
ATOM	20	HE2	IMIM	1	-3.695	-1.388	-0.938	1.00	0.00	IMIM
ATOM	21	CE1	IMIM	1	-1.750	-1.090	-0.232	1.00	0.00	IMIM
ATOM	22	HE1	IMIM	1	-1.381	-2.092	-0.101	1.00	0.00	IMIM

END

REMARK 94_BENZ_IMIM

ATOM	1	CG	BENZ	1	-1.622	0.815	-1.578	1.00	0.00	BENZ
ATOM	2	HG	BENZ	1	-1.448	1.276	-2.542	1.00	0.00	BENZ
ATOM	3	CD1	BENZ	1	-1.765	-0.577	-1.479	1.00	0.00	BENZ
ATOM	4	HD1	BENZ	1	-1.713	-1.190	-2.372	1.00	0.00	BENZ
ATOM	5	CD2	BENZ	1	-1.735	1.613	-0.429	1.00	0.00	BENZ
ATOM	6	HD2	BENZ	1	-1.653	2.690	-0.510	1.00	0.00	BENZ

ATOM	7	CE1	BENZ	1	-2.021	-1.170	-0.234	1.00	0.00	BENZ
ATOM	8	HE1	BENZ	1	-2.163	-2.241	-0.164	1.00	0.00	BENZ
ATOM	9	CE2	BENZ	1	-1.991	1.018	0.815	1.00	0.00	BENZ
ATOM	10	HE2	BENZ	1	-2.109	1.637	1.696	1.00	0.00	BENZ
ATOM	11	CZ	BENZ	1	-2.137	-0.372	0.912	1.00	0.00	BENZ
ATOM	12	HZ	BENZ	1	-2.358	-0.828	1.869	1.00	0.00	BENZ
ATOM	13	CG	IMIM	1	3.052	0.107	1.040	1.00	0.00	IMIM
ATOM	14	HG	IMIM	1	3.938	0.337	1.605	1.00	0.00	IMIM
ATOM	15	CD2	IMIM	1	1.866	0.786	0.900	1.00	0.00	IMIM
ATOM	16	HD2	IMIM	1	1.530	1.714	1.326	1.00	0.00	IMIM
ATOM	17	ND1	IMIM	1	2.938	-1.031	0.273	1.00	0.00	IMIM
ATOM	18	HD1	IMIM	1	3.649	-1.743	0.166	1.00	0.00	IMIM
ATOM	19	NE2	IMIM	1	1.081	0.036	0.059	1.00	0.00	IMIM
ATOM	20	HE2	IMIM	1	0.136	0.279	-0.246	1.00	0.00	IMIM
ATOM	21	CE1	IMIM	1	1.733	-1.067	-0.322	1.00	0.00	IMIM
ATOM	22	HE1	IMIM	1	1.360	-1.836	-0.975	1.00	0.00	IMIM

END

REMARK 95_TOLU_IMIM

ATOM	1	CB	TOLU	1	2.248	2.336	0.023	1.00	0.00	TOLU
ATOM	2	HB1	TOLU	1	1.843	2.845	-0.851	1.00	0.00	TOLU
ATOM	3	HB2	TOLU	1	3.330	2.476	0.017	1.00	0.00	TOLU
ATOM	4	HB3	TOLU	1	1.857	2.819	0.918	1.00	0.00	TOLU
ATOM	5	CG	TOLU	1	1.915	0.867	0.004	1.00	0.00	TOLU
ATOM	6	CD1	TOLU	1	1.817	0.133	1.201	1.00	0.00	TOLU
ATOM	7	HD1	TOLU	1	1.950	0.644	2.149	1.00	0.00	TOLU
ATOM	8	CD2	TOLU	1	1.766	0.174	-1.211	1.00	0.00	TOLU
ATOM	9	HD2	TOLU	1	1.865	0.716	-2.146	1.00	0.00	TOLU
ATOM	10	CE1	TOLU	1	1.581	-1.249	1.186	1.00	0.00	TOLU
ATOM	11	HE1	TOLU	1	1.534	-1.797	2.120	1.00	0.00	TOLU
ATOM	12	CE2	TOLU	1	1.529	-1.207	-1.232	1.00	0.00	TOLU
ATOM	13	HE2	TOLU	1	1.449	-1.726	-2.181	1.00	0.00	TOLU
ATOM	14	CZ	TOLU	1	1.440	-1.924	-0.033	1.00	0.00	TOLU
ATOM	15	HZ	TOLU	1	1.278	-2.995	-0.047	1.00	0.00	TOLU
ATOM	16	CG	IMIM	1	-2.099	0.099	1.172	1.00	0.00	IMIM
ATOM	17	HG	IMIM	1	-1.757	0.084	2.191	1.00	0.00	IMIM
ATOM	18	CD2	IMIM	1	-3.367	0.153	0.647	1.00	0.00	IMIM
ATOM	19	HD2	IMIM	1	-4.330	0.196	1.124	1.00	0.00	IMIM
ATOM	20	ND1	IMIM	1	-1.233	0.058	0.106	1.00	0.00	IMIM
ATOM	21	HD1	IMIM	1	-0.213	0.019	0.171	1.00	0.00	IMIM
ATOM	22	NE2	IMIM	1	-3.219	0.144	-0.721	1.00	0.00	IMIM
ATOM	23	HE2	IMIM	1	-3.973	0.174	-1.396	1.00	0.00	IMIM
ATOM	24	CE1	IMIM	1	-1.915	0.086	-1.043	1.00	0.00	IMIM
ATOM	25	HE1	IMIM	1	-1.496	0.062	-2.034	1.00	0.00	IMIM

END

REMARK 96_TOLU_IMIM

ATOM	1	CB	TOLU	1	-2.629	1.669	-0.740	1.00	0.00	TOLU
ATOM	2	HB1	TOLU	1	-2.425	2.449	-0.007	1.00	0.00	TOLU
ATOM	3	HB2	TOLU	1	-3.712	1.569	-0.827	1.00	0.00	TOLU
ATOM	4	HB3	TOLU	1	-2.247	1.995	-1.707	1.00	0.00	TOLU
ATOM	5	CG	TOLU	1	-2.015	0.357	-0.326	1.00	0.00	TOLU
ATOM	6	CD1	TOLU	1	-1.645	-0.600	-1.287	1.00	0.00	TOLU
ATOM	7	HD1	TOLU	1	-1.770	-0.373	-2.340	1.00	0.00	TOLU
ATOM	8	CD2	TOLU	1	-1.872	0.024	1.032	1.00	0.00	TOLU
ATOM	9	HD2	TOLU	1	-2.179	0.739	1.789	1.00	0.00	TOLU
ATOM	10	CE1	TOLU	1	-1.147	-1.854	-0.905	1.00	0.00	TOLU
ATOM	11	HE1	TOLU	1	-0.892	-2.587	-1.662	1.00	0.00	TOLU
ATOM	12	CE2	TOLU	1	-1.375	-1.226	1.422	1.00	0.00	TOLU
ATOM	13	HE2	TOLU	1	-1.303	-1.475	2.475	1.00	0.00	TOLU
ATOM	14	CZ	TOLU	1	-1.011	-2.172	0.454	1.00	0.00	TOLU
ATOM	15	HZ	TOLU	1	-0.647	-3.148	0.752	1.00	0.00	TOLU
ATOM	16	CG	IMIM	1	2.134	0.305	-1.041	1.00	0.00	IMIM
ATOM	17	HG	IMIM	1	1.929	-0.076	-2.026	1.00	0.00	IMIM
ATOM	18	CD2	IMIM	1	3.181	1.056	-0.565	1.00	0.00	IMIM
ATOM	19	HD2	IMIM	1	4.054	1.448	-1.056	1.00	0.00	IMIM
ATOM	20	ND1	IMIM	1	1.292	0.083	0.021	1.00	0.00	IMIM
ATOM	21	HD1	IMIM	1	0.424	-0.455	-0.012	1.00	0.00	IMIM
ATOM	22	NE2	IMIM	1	2.931	1.259	0.773	1.00	0.00	IMIM
ATOM	23	HE2	IMIM	1	3.521	1.780	1.410	1.00	0.00	IMIM
ATOM	24	CE1	IMIM	1	1.778	0.663	1.123	1.00	0.00	IMIM
ATOM	25	HE1	IMIM	1	1.328	0.653	2.100	1.00	0.00	IMIM

END

REMARK 97_TOLU_IMIM

ATOM	1	CB	TOLU	1	2.404	-2.091	-0.171	1.00	0.00	TOLU
ATOM	2	HB1	TOLU	1	1.935	-2.679	-0.958	1.00	0.00	TOLU
ATOM	3	HB2	TOLU	1	2.172	-2.551	0.789	1.00	0.00	TOLU
ATOM	4	HB3	TOLU	1	3.485	-2.147	-0.313	1.00	0.00	TOLU
ATOM	5	CG	TOLU	1	1.945	-0.657	-0.214	1.00	0.00	TOLU
ATOM	6	CD1	TOLU	1	1.913	0.126	0.952	1.00	0.00	TOLU
ATOM	7	HD1	TOLU	1	2.191	-0.322	1.900	1.00	0.00	TOLU
ATOM	8	CD2	TOLU	1	1.617	-0.043	-1.435	1.00	0.00	TOLU
ATOM	9	HD2	TOLU	1	1.660	-0.624	-2.351	1.00	0.00	TOLU
ATOM	10	CE1	TOLU	1	1.562	1.482	0.905	1.00	0.00	TOLU
ATOM	11	HE1	TOLU	1	1.574	2.076	1.811	1.00	0.00	TOLU
ATOM	12	CE2	TOLU	1	1.265	1.312	-1.493	1.00	0.00	TOLU
ATOM	13	HE2	TOLU	1	1.041	1.773	-2.448	1.00	0.00	TOLU
ATOM	14	CZ	TOLU	1	1.237	2.082	-0.321	1.00	0.00	TOLU
ATOM	15	HZ	TOLU	1	0.986	3.134	-0.364	1.00	0.00	TOLU
ATOM	16	CG	IMIM	1	-2.182	-0.353	-0.847	1.00	0.00	IMIM
ATOM	17	HG	IMIM	1	-1.977	-0.296	-1.901	1.00	0.00	IMIM
ATOM	18	CD2	IMIM	1	-3.269	-0.842	-0.164	1.00	0.00	IMIM
ATOM	19	HD2	IMIM	1	-4.184	-1.286	-0.514	1.00	0.00	IMIM
ATOM	20	ND1	IMIM	1	-1.293	0.098	0.098	1.00	0.00	IMIM
ATOM	21	HD1	IMIM	1	-0.386	0.530	-0.096	1.00	0.00	IMIM
ATOM	22	NE2	IMIM	1	-2.995	-0.664	1.173	1.00	0.00	IMIM
ATOM	23	HE2	IMIM	1	-3.605	-0.925	1.939	1.00	0.00	IMIM
ATOM	24	CE1	IMIM	1	-1.789	-0.091	1.325	1.00	0.00	IMIM
ATOM	25	HE1	IMIM	1	-1.310	0.166	2.253	1.00	0.00	IMIM

END

REMARK 98_TOLU_IMIM

ATOM	1	CB	TOLU	1	1.500	2.770	0.433	1.00	0.00	TOLU
ATOM	2	HB1	TOLU	1	0.947	3.070	1.322	1.00	0.00	TOLU
ATOM	3	HB2	TOLU	1	1.017	3.207	-0.441	1.00	0.00	TOLU
ATOM	4	HB3	TOLU	1	2.501	3.199	0.507	1.00	0.00	TOLU
ATOM	5	CG	TOLU	1	1.581	1.271	0.318	1.00	0.00	TOLU
ATOM	6	CD1	TOLU	1	1.784	0.655	-0.929	1.00	0.00	TOLU
ATOM	7	HD1	TOLU	1	1.840	1.268	-1.822	1.00	0.00	TOLU
ATOM	8	CD2	TOLU	1	1.540	0.455	1.463	1.00	0.00	TOLU
ATOM	9	HD2	TOLU	1	1.414	0.912	2.439	1.00	0.00	TOLU
ATOM	10	CE1	TOLU	1	1.934	-0.733	-1.034	1.00	0.00	TOLU
ATOM	11	HE1	TOLU	1	2.118	-1.183	-2.003	1.00	0.00	TOLU
ATOM	12	CE2	TOLU	1	1.693	-0.936	1.367	1.00	0.00	TOLU
ATOM	13	HE2	TOLU	1	1.677	-1.544	2.264	1.00	0.00	TOLU
ATOM	14	CZ	TOLU	1	1.891	-1.535	0.115	1.00	0.00	TOLU
ATOM	15	HZ	TOLU	1	2.038	-2.606	0.041	1.00	0.00	TOLU
ATOM	16	CG	IMIM	1	-2.121	0.429	0.474	1.00	0.00	IMIM
ATOM	17	HG	IMIM	1	-1.879	1.171	1.213	1.00	0.00	IMIM
ATOM	18	CD2	IMIM	1	-3.297	0.161	-0.185	1.00	0.00	IMIM
ATOM	19	HD2	IMIM	1	-4.265	0.626	-0.124	1.00	0.00	IMIM
ATOM	20	ND1	IMIM	1	-1.197	-0.475	0.013	1.00	0.00	IMIM
ATOM	21	HD1	IMIM	1	-0.220	-0.533	0.315	1.00	0.00	IMIM
ATOM	22	NE2	IMIM	1	-3.036	-0.900	-1.022	1.00	0.00	IMIM
ATOM	23	HE2	IMIM	1	-3.703	-1.335	-1.647	1.00	0.00	IMIM
ATOM	24	CE1	IMIM	1	-1.753	-1.281	-0.896	1.00	0.00	IMIM
ATOM	25	HE1	IMIM	1	-1.264	-2.079	-1.427	1.00	0.00	IMIM

END

REMARK 99_TOLU_IMIM

ATOM	1	CB	TOLU	1	2.663	-1.718	0.379	1.00	0.00	TOLU
ATOM	2	HB1	TOLU	1	2.427	-1.975	1.412	1.00	0.00	TOLU
ATOM	3	HB2	TOLU	1	3.748	-1.648	0.294	1.00	0.00	TOLU
ATOM	4	HB3	TOLU	1	2.331	-2.532	-0.264	1.00	0.00	TOLU
ATOM	5	CG	TOLU	1	2.023	-0.414	-0.018	1.00	0.00	TOLU
ATOM	6	CD1	TOLU	1	1.650	-0.169	-1.351	1.00	0.00	TOLU
ATOM	7	HD1	TOLU	1	1.798	-0.945	-2.095	1.00	0.00	TOLU
ATOM	8	CD2	TOLU	1	1.858	0.622	0.918	1.00	0.00	TOLU
ATOM	9	HD2	TOLU	1	2.161	0.461	1.947	1.00	0.00	TOLU
ATOM	10	CE1	TOLU	1	1.128	1.071	-1.741	1.00	0.00	TOLU
ATOM	11	HE1	TOLU	1	0.875	1.249	-2.780	1.00	0.00	TOLU
ATOM	12	CE2	TOLU	1	1.336	1.866	0.537	1.00	0.00	TOLU
ATOM	13	HE2	TOLU	1	1.243	2.659	1.269	1.00	0.00	TOLU
ATOM	14	CZ	TOLU	1	0.969	2.096	-0.797	1.00	0.00	TOLU
ATOM	15	HZ	TOLU	1	0.585	3.063	-1.098	1.00	0.00	TOLU
ATOM	16	CG	IMIM	1	-1.963	0.024	1.361	1.00	0.00	IMIM
ATOM	17	HG	IMIM	1	-1.620	0.613	2.192	1.00	0.00	IMIM
ATOM	18	CD2	IMIM	1	-3.060	-0.793	1.226	1.00	0.00	IMIM

ATOM	19	HD2	IMIM	1	-3.846	-1.043	1.915	1.00	0.00	IMIM
ATOM	20	ND1	IMIM	1	-1.289	-0.020	0.165	1.00	0.00	IMIM
ATOM	21	HD1	IMIM	1	-0.432	0.492	-0.054	1.00	0.00	IMIM
ATOM	22	NE2	IMIM	1	-3.006	-1.301	-0.053	1.00	0.00	IMIM
ATOM	23	HE2	IMIM	1	-3.677	-1.940	-0.462	1.00	0.00	IMIM
ATOM	24	CE1	IMIM	1	-1.924	-0.825	-0.693	1.00	0.00	IMIM
ATOM	25	HE1	IMIM	1	-1.622	-1.048	-1.701	1.00	0.00	IMIM

END

REMARK 100_PHEN_IMIM

ATOM	1	CG	PHEN	1	1.750	-1.821	0.548	1.00	0.00	PHEN
ATOM	2	HG	PHEN	1	1.801	-2.847	0.888	1.00	0.00	PHEN
ATOM	3	CD1	PHEN	1	1.666	-1.535	-0.824	1.00	0.00	PHEN
ATOM	4	HD1	PHEN	1	1.650	-2.340	-1.548	1.00	0.00	PHEN
ATOM	5	CD2	PHEN	1	1.824	-0.768	1.469	1.00	0.00	PHEN
ATOM	6	HD2	PHEN	1	1.921	-0.978	2.527	1.00	0.00	PHEN
ATOM	7	CE1	PHEN	1	1.631	-0.208	-1.270	1.00	0.00	PHEN
ATOM	8	HE1	PHEN	1	1.588	0.032	-2.325	1.00	0.00	PHEN
ATOM	9	CE2	PHEN	1	1.781	0.562	1.034	1.00	0.00	PHEN
ATOM	10	HE2	PHEN	1	1.830	1.374	1.752	1.00	0.00	PHEN
ATOM	11	CZ	PHEN	1	1.678	0.835	-0.336	1.00	0.00	PHEN
ATOM	12	OH	PHEN	1	1.538	2.111	-0.834	1.00	0.00	PHEN
ATOM	13	HH	PHEN	1	1.883	2.759	-0.201	1.00	0.00	PHEN
ATOM	14	CG	IMIM	1	-1.608	0.854	-0.466	1.00	0.00	IMIM
ATOM	15	HG	IMIM	1	-0.885	1.510	-0.921	1.00	0.00	IMIM
ATOM	16	CD2	IMIM	1	-2.954	1.006	-0.234	1.00	0.00	IMIM
ATOM	17	HD2	IMIM	1	-3.624	1.815	-0.465	1.00	0.00	IMIM
ATOM	18	ND1	IMIM	1	-1.264	-0.379	0.039	1.00	0.00	IMIM
ATOM	19	HD1	IMIM	1	-0.326	-0.786	0.005	1.00	0.00	IMIM
ATOM	20	NE2	IMIM	1	-3.373	-0.143	0.398	1.00	0.00	IMIM
ATOM	21	HE2	IMIM	1	-4.319	-0.338	0.700	1.00	0.00	IMIM
ATOM	22	CE1	IMIM	1	-2.336	-0.983	0.560	1.00	0.00	IMIM
ATOM	23	HE1	IMIM	1	-2.365	-1.955	1.022	1.00	0.00	IMIM

END

REMARK 101_PHEN_IMIM

ATOM	1	CG	PHEN	1	1.385	0.486	2.192	1.00	0.00	PHEN
ATOM	2	HG	PHEN	1	1.250	0.800	3.219	1.00	0.00	PHEN
ATOM	3	CD1	PHEN	1	1.311	-0.873	1.854	1.00	0.00	PHEN
ATOM	4	HD1	PHEN	1	1.117	-1.614	2.619	1.00	0.00	PHEN
ATOM	5	CD2	PHEN	1	1.688	1.430	1.201	1.00	0.00	PHEN
ATOM	6	HD2	PHEN	1	1.777	2.478	1.458	1.00	0.00	PHEN
ATOM	7	CE1	PHEN	1	1.507	-1.285	0.530	1.00	0.00	PHEN
ATOM	8	HE1	PHEN	1	1.474	-2.332	0.254	1.00	0.00	PHEN
ATOM	9	CE2	PHEN	1	1.877	1.030	-0.126	1.00	0.00	PHEN
ATOM	10	HE2	PHEN	1	2.099	1.764	-0.893	1.00	0.00	PHEN
ATOM	11	CZ	PHEN	1	1.777	-0.328	-0.455	1.00	0.00	PHEN
ATOM	12	OH	PHEN	1	1.836	-0.785	-1.758	1.00	0.00	PHEN
ATOM	13	HH	PHEN	1	2.366	-0.182	-2.301	1.00	0.00	PHEN
ATOM	14	CG	IMIM	1	-2.578	0.571	0.472	1.00	0.00	IMIM
ATOM	15	HG	IMIM	1	-2.788	0.991	1.440	1.00	0.00	IMIM
ATOM	16	CD2	IMIM	1	-3.385	0.392	-0.625	1.00	0.00	IMIM
ATOM	17	HD2	IMIM	1	-4.423	0.625	-0.786	1.00	0.00	IMIM
ATOM	18	ND1	IMIM	1	-1.337	0.092	0.129	1.00	0.00	IMIM
ATOM	19	HD1	IMIM	1	-0.514	0.064	0.733	1.00	0.00	IMIM
ATOM	20	NE2	IMIM	1	-2.597	-0.191	-1.590	1.00	0.00	IMIM
ATOM	21	HE2	IMIM	1	-2.901	-0.452	-2.521	1.00	0.00	IMIM
ATOM	22	CE1	IMIM	1	-1.349	-0.375	-1.126	1.00	0.00	IMIM
ATOM	23	HE1	IMIM	1	-0.511	-0.793	-1.662	1.00	0.00	IMIM

END

REMARK 102_PHEN_IMIM

ATOM	1	CG	PHEN	1	2.265	-1.248	0.021	1.00	0.00	PHEN
ATOM	2	HG	PHEN	1	2.658	-2.256	-0.008	1.00	0.00	PHEN
ATOM	3	CD1	PHEN	1	2.037	-0.543	-1.171	1.00	0.00	PHEN
ATOM	4	HD1	PHEN	1	2.251	-1.007	-2.126	1.00	0.00	PHEN
ATOM	5	CD2	PHEN	1	2.034	-0.617	1.251	1.00	0.00	PHEN
ATOM	6	HD2	PHEN	1	2.236	-1.141	2.177	1.00	0.00	PHEN
ATOM	7	CE1	PHEN	1	1.558	0.772	-1.136	1.00	0.00	PHEN
ATOM	8	HE1	PHEN	1	1.396	1.338	-2.045	1.00	0.00	PHEN
ATOM	9	CE2	PHEN	1	1.546	0.694	1.296	1.00	0.00	PHEN
ATOM	10	HE2	PHEN	1	1.361	1.176	2.250	1.00	0.00	PHEN
ATOM	11	CZ	PHEN	1	1.305	1.381	0.100	1.00	0.00	PHEN
ATOM	12	OH	PHEN	1	0.741	2.637	0.060	1.00	0.00	PHEN
ATOM	13	HH	PHEN	1	0.885	3.096	0.901	1.00	0.00	PHEN

ATOM	14	CG	IMIM	1	-1.816	0.412	-0.264	1.00	0.00	IMIM
ATOM	15	HG	IMIM	1	-1.362	1.378	-0.408	1.00	0.00	IMIM
ATOM	16	CD2	IMIM	1	-3.128	0.041	-0.098	1.00	0.00	IMIM
ATOM	17	HD2	IMIM	1	-4.032	0.624	-0.087	1.00	0.00	IMIM
ATOM	18	ND1	IMIM	1	-1.072	-0.743	-0.189	1.00	0.00	IMIM
ATOM	19	HD1	IMIM	1	-0.056	-0.795	-0.291	1.00	0.00	IMIM
ATOM	20	NE2	IMIM	1	-3.128	-1.326	0.065	1.00	0.00	IMIM
ATOM	21	HE2	IMIM	1	-3.948	-1.903	0.209	1.00	0.00	IMIM
ATOM	22	CE1	IMIM	1	-1.871	-1.797	0.008	1.00	0.00	IMIM
ATOM	23	HE1	IMIM	1	-1.566	-2.825	0.103	1.00	0.00	IMIM

END

REMARK 103 PHEN_IMIM

ATOM	1	CG	PHEN	1	-1.981	-1.458	0.950	1.00	0.00	PHEN
ATOM	2	HG	PHEN	1	-2.175	-2.427	1.392	1.00	0.00	PHEN
ATOM	3	CD1	PHEN	1	-2.005	-1.302	-0.444	1.00	0.00	PHEN
ATOM	4	HD1	PHEN	1	-2.217	-2.150	-1.083	1.00	0.00	PHEN
ATOM	5	CD2	PHEN	1	-1.760	-0.342	1.768	1.00	0.00	PHEN
ATOM	6	HD2	PHEN	1	-1.770	-0.447	2.845	1.00	0.00	PHEN
ATOM	7	CE1	PHEN	1	-1.779	-0.046	-1.019	1.00	0.00	PHEN
ATOM	8	HE1	PHEN	1	-1.813	0.098	-2.092	1.00	0.00	PHEN
ATOM	9	CE2	PHEN	1	-1.522	0.916	1.203	1.00	0.00	PHEN
ATOM	10	HE2	PHEN	1	-1.338	1.776	1.838	1.00	0.00	PHEN
ATOM	11	CZ	PHEN	1	-1.526	1.054	-0.191	1.00	0.00	PHEN
ATOM	12	OH	PHEN	1	-1.186	2.236	-0.823	1.00	0.00	PHEN
ATOM	13	HH	PHEN	1	-1.387	2.991	-0.250	1.00	0.00	PHEN
ATOM	14	CG	IMIM	1	2.294	-1.349	0.342	1.00	0.00	IMIM
ATOM	15	HG	IMIM	1	2.207	-2.282	0.868	1.00	0.00	IMIM
ATOM	16	CD2	IMIM	1	3.402	-0.654	-0.079	1.00	0.00	IMIM
ATOM	17	HD2	IMIM	1	4.451	-0.870	0.013	1.00	0.00	IMIM
ATOM	18	ND1	IMIM	1	1.199	-0.612	-0.042	1.00	0.00	IMIM
ATOM	19	HD1	IMIM	1	0.222	-0.865	0.108	1.00	0.00	IMIM
ATOM	20	NE2	IMIM	1	2.930	0.479	-0.704	1.00	0.00	IMIM
ATOM	21	HE2	IMIM	1	3.502	1.200	-1.126	1.00	0.00	IMIM
ATOM	22	CE1	IMIM	1	1.587	0.499	-0.681	1.00	0.00	IMIM
ATOM	23	HE1	IMIM	1	0.941	1.268	-1.077	1.00	0.00	IMIM

END

REMARK 104 PHEN_IMIM

ATOM	1	CG	PHEN	1	-1.530	1.997	-0.764	1.00	0.00	PHEN
ATOM	2	HG	PHEN	1	-1.462	3.015	-1.126	1.00	0.00	PHEN
ATOM	3	CD1	PHEN	1	-1.565	1.738	0.614	1.00	0.00	PHEN
ATOM	4	HD1	PHEN	1	-1.519	2.556	1.322	1.00	0.00	PHEN
ATOM	5	CD2	PHEN	1	-1.635	0.934	-1.671	1.00	0.00	PHEN
ATOM	6	HD2	PHEN	1	-1.641	1.126	-2.737	1.00	0.00	PHEN
ATOM	7	CE1	PHEN	1	-1.674	0.427	1.085	1.00	0.00	PHEN
ATOM	8	HE1	PHEN	1	-1.719	0.209	2.145	1.00	0.00	PHEN
ATOM	9	CE2	PHEN	1	-1.737	-0.385	-1.209	1.00	0.00	PHEN
ATOM	10	HE2	PHEN	1	-1.808	-1.208	-1.913	1.00	0.00	PHEN
ATOM	11	CZ	PHEN	1	-1.750	-0.630	0.170	1.00	0.00	PHEN
ATOM	12	OH	PHEN	1	-1.727	-1.908	0.697	1.00	0.00	PHEN
ATOM	13	HH	PHEN	1	-2.165	-2.528	0.094	1.00	0.00	PHEN
ATOM	14	CG	IMIM	1	2.560	0.682	-0.406	1.00	0.00	IMIM
ATOM	15	HG	IMIM	1	2.714	1.597	-0.950	1.00	0.00	IMIM
ATOM	16	CD2	IMIM	1	3.454	-0.161	0.208	1.00	0.00	IMIM
ATOM	17	HD2	IMIM	1	4.526	-0.117	0.292	1.00	0.00	IMIM
ATOM	18	ND1	IMIM	1	1.312	0.146	-0.202	1.00	0.00	IMIM
ATOM	19	HD1	IMIM	1	0.429	0.538	-0.531	1.00	0.00	IMIM
ATOM	20	NE2	IMIM	1	2.708	-1.179	0.757	1.00	0.00	IMIM
ATOM	21	HE2	IMIM	1	3.077	-1.963	1.282	1.00	0.00	IMIM
ATOM	22	CE1	IMIM	1	1.402	-0.988	0.507	1.00	0.00	IMIM
ATOM	23	HE1	IMIM	1	0.581	-1.620	0.809	1.00	0.00	IMIM

END

REMARK 105 PHEN_IMIM

ATOM	1	CG	PHEN	1	1.436	-2.207	-0.163	1.00	0.00	PHEN
ATOM	2	HG	PHEN	1	1.323	-3.282	-0.219	1.00	0.00	PHEN
ATOM	3	CD1	PHEN	1	1.440	-1.436	-1.335	1.00	0.00	PHEN
ATOM	4	HD1	PHEN	1	1.327	-1.913	-2.301	1.00	0.00	PHEN
ATOM	5	CD2	PHEN	1	1.636	-1.584	1.076	1.00	0.00	PHEN
ATOM	6	HD2	PHEN	1	1.665	-2.175	1.983	1.00	0.00	PHEN
ATOM	7	CE1	PHEN	1	1.610	-0.048	-1.268	1.00	0.00	PHEN
ATOM	8	HE1	PHEN	1	1.635	0.562	-2.163	1.00	0.00	PHEN
ATOM	9	CE2	PHEN	1	1.797	-0.196	1.155	1.00	0.00	PHEN
ATOM	10	HE2	PHEN	1	1.939	0.286	2.116	1.00	0.00	PHEN

ATOM	11	CZ	PHEN	1	1.776	0.565	-0.021	1.00	0.00	PHEN
ATOM	12	OH	PHEN	1	1.812	1.947	-0.013	1.00	0.00	PHEN
ATOM	13	HH	PHEN	1	2.280	2.266	0.773	1.00	0.00	PHEN
ATOM	14	CG	IMIM	1	-2.592	-0.675	0.183	1.00	0.00	IMIM
ATOM	15	HG	IMIM	1	-2.791	-1.730	0.241	1.00	0.00	IMIM
ATOM	16	CD2	IMIM	1	-3.427	0.407	0.312	1.00	0.00	IMIM
ATOM	17	HD2	IMIM	1	-4.484	0.467	0.501	1.00	0.00	IMIM
ATOM	18	ND1	IMIM	1	-1.334	-0.174	-0.056	1.00	0.00	IMIM
ATOM	19	HD1	IMIM	1	-0.489	-0.723	-0.215	1.00	0.00	IMIM
ATOM	20	NE2	IMIM	1	-2.639	1.524	0.145	1.00	0.00	IMIM
ATOM	21	HE2	IMIM	1	-2.961	2.483	0.182	1.00	0.00	IMIM
ATOM	22	CE1	IMIM	1	-1.364	1.165	-0.082	1.00	0.00	IMIM
ATOM	23	HE1	IMIM	1	-0.521	1.821	-0.232	1.00	0.00	IMIM

END

REMARK 106_PHEN_IMIM

ATOM	1	CG	PHEN	1	-2.186	1.858	1.324	1.00	0.00	PHEN
ATOM	2	HG	PHEN	1	-2.416	2.697	1.967	1.00	0.00	PHEN
ATOM	3	CD1	PHEN	1	-1.800	2.078	-0.003	1.00	0.00	PHEN
ATOM	4	HD1	PHEN	1	-1.725	3.087	-0.388	1.00	0.00	PHEN
ATOM	5	CD2	PHEN	1	-2.314	0.551	1.806	1.00	0.00	PHEN
ATOM	6	HD2	PHEN	1	-2.630	0.376	2.827	1.00	0.00	PHEN
ATOM	7	CE1	PHEN	1	-1.515	0.997	-0.844	1.00	0.00	PHEN
ATOM	8	HE1	PHEN	1	-1.243	1.143	-1.882	1.00	0.00	PHEN
ATOM	9	CE2	PHEN	1	-2.016	-0.540	0.982	1.00	0.00	PHEN
ATOM	10	HE2	PHEN	1	-2.103	-1.554	1.354	1.00	0.00	PHEN
ATOM	11	CZ	PHEN	1	-1.635	-0.297	-0.339	1.00	0.00	PHEN
ATOM	12	OH	PHEN	1	-1.227	-1.343	-1.188	1.00	0.00	PHEN
ATOM	13	HH	PHEN	1	-1.761	-2.135	-1.018	1.00	0.00	PHEN
ATOM	14	CG	IMIM	1	1.647	-0.040	0.439	1.00	0.00	IMIM
ATOM	15	HG	IMIM	1	0.839	0.366	1.023	1.00	0.00	IMIM
ATOM	16	CD2	IMIM	1	3.006	0.138	0.529	1.00	0.00	IMIM
ATOM	17	HD2	IMIM	1	3.600	0.728	1.204	1.00	0.00	IMIM
ATOM	18	ND1	IMIM	1	1.429	-0.902	-0.611	1.00	0.00	IMIM
ATOM	19	HD1	IMIM	1	0.497	-1.224	-0.930	1.00	0.00	IMIM
ATOM	20	NE2	IMIM	1	3.562	-0.621	-0.475	1.00	0.00	IMIM
ATOM	21	HE2	IMIM	1	4.551	-0.700	-0.676	1.00	0.00	IMIM
ATOM	22	CE1	IMIM	1	2.595	-1.251	-1.165	1.00	0.00	IMIM
ATOM	23	HE1	IMIM	1	2.736	-1.909	-2.005	1.00	0.00	IMIM

END

REMARK 107_CRES_IMIM

ATOM	1	CB	CRES	1	2.063	2.884	-0.520	1.00	0.00	CRES
ATOM	2	HB1	CRES	1	3.133	3.080	-0.439	1.00	0.00	CRES
ATOM	3	HB2	CRES	1	1.553	3.534	0.191	1.00	0.00	CRES
ATOM	4	HB3	CRES	1	1.751	3.161	-1.527	1.00	0.00	CRES
ATOM	5	CG	CRES	1	1.773	1.433	-0.238	1.00	0.00	CRES
ATOM	6	CD1	CRES	1	1.592	0.972	1.080	1.00	0.00	CRES
ATOM	7	HD1	CRES	1	1.612	1.680	1.901	1.00	0.00	CRES
ATOM	8	CD2	CRES	1	1.775	0.478	-1.270	1.00	0.00	CRES
ATOM	9	HD2	CRES	1	1.936	0.798	-2.294	1.00	0.00	CRES
ATOM	10	CE1	CRES	1	1.399	-0.384	1.359	1.00	0.00	CRES
ATOM	11	HE1	CRES	1	1.273	-0.736	2.376	1.00	0.00	CRES
ATOM	12	CE2	CRES	1	1.576	-0.884	-1.009	1.00	0.00	CRES
ATOM	13	HE2	CRES	1	1.570	-1.600	-1.824	1.00	0.00	CRES
ATOM	14	CZ	CRES	1	1.388	-1.312	0.311	1.00	0.00	CRES
ATOM	15	OZ	CRES	1	1.091	-2.618	0.642	1.00	0.00	CRES
ATOM	16	HZ	CRES	1	1.417	-3.219	-0.043	1.00	0.00	CRES
ATOM	17	CG	IMIM	1	-1.866	-0.985	0.340	1.00	0.00	IMIM
ATOM	18	HG	IMIM	1	-1.222	-1.777	0.684	1.00	0.00	IMIM
ATOM	19	CD2	IMIM	1	-3.235	-0.902	0.250	1.00	0.00	IMIM
ATOM	20	HD2	IMIM	1	-4.004	-1.606	0.513	1.00	0.00	IMIM
ATOM	21	ND1	IMIM	1	-1.372	0.207	-0.137	1.00	0.00	IMIM
ATOM	22	HD1	IMIM	1	-0.382	0.455	-0.191	1.00	0.00	IMIM
ATOM	23	NE2	IMIM	1	-3.516	0.339	-0.275	1.00	0.00	IMIM
ATOM	24	HE2	IMIM	1	-4.442	0.705	-0.460	1.00	0.00	IMIM
ATOM	25	CE1	IMIM	1	-2.375	1.010	-0.508	1.00	0.00	IMIM
ATOM	26	HE1	IMIM	1	-2.286	2.002	-0.915	1.00	0.00	IMIM

END

REMARK 108_CRES_IMIM

ATOM	1	CB	CRES	1	-3.044	-0.023	-1.870	1.00	0.00	CRES
ATOM	2	HB1	CRES	1	-3.698	0.846	-1.907	1.00	0.00	CRES
ATOM	3	HB2	CRES	1	-3.664	-0.917	-1.925	1.00	0.00	CRES
ATOM	4	HB3	CRES	1	-2.413	-0.002	-2.761	1.00	0.00	CRES

ATOM	5	CG	CRES	1	-2.224	-0.020	-0.604	1.00	0.00	CRES
ATOM	6	CD1	CRES	1	-1.798	-1.224	-0.011	1.00	0.00	CRES
ATOM	7	HD1	CRES	1	-2.073	-2.170	-0.465	1.00	0.00	CRES
ATOM	8	CD2	CRES	1	-1.893	1.181	0.046	1.00	0.00	CRES
ATOM	9	HD2	CRES	1	-2.231	2.124	-0.370	1.00	0.00	CRES
ATOM	10	CE1	CRES	1	-1.053	-1.231	1.175	1.00	0.00	CRES
ATOM	11	HE1	CRES	1	-0.751	-2.160	1.643	1.00	0.00	CRES
ATOM	12	CE2	CRES	1	-1.136	1.193	1.222	1.00	0.00	CRES
ATOM	13	HE2	CRES	1	-0.890	2.135	1.702	1.00	0.00	CRES
ATOM	14	CZ	CRES	1	-0.717	-0.018	1.786	1.00	0.00	CRES
ATOM	15	OZ	CRES	1	0.101	-0.087	2.895	1.00	0.00	CRES
ATOM	16	HZ	CRES	1	0.007	0.715	3.430	1.00	0.00	CRES
ATOM	17	CG	IMIM	1	2.142	-0.173	0.202	1.00	0.00	IMIM
ATOM	18	HG	IMIM	1	1.910	-0.361	1.237	1.00	0.00	IMIM
ATOM	19	CD2	IMIM	1	3.334	0.085	-0.430	1.00	0.00	IMIM
ATOM	20	HD2	IMIM	1	4.338	0.149	-0.049	1.00	0.00	IMIM
ATOM	21	ND1	IMIM	1	1.169	-0.134	-0.770	1.00	0.00	IMIM
ATOM	22	HD1	IMIM	1	0.174	-0.306	-0.606	1.00	0.00	IMIM
ATOM	23	NE2	IMIM	1	3.037	0.265	-1.762	1.00	0.00	IMIM
ATOM	24	HE2	IMIM	1	3.707	0.472	-2.493	1.00	0.00	IMIM
ATOM	25	CE1	IMIM	1	1.715	0.130	-1.962	1.00	0.00	IMIM
ATOM	26	HE1	IMIM	1	1.197	0.218	-2.901	1.00	0.00	IMIM

END

REMARK 109_CRES_IMIM

ATOM	1	CB	CRES	1	3.054	-1.858	-0.108	1.00	0.00	CRES
ATOM	2	HB1	CRES	1	4.105	-1.587	-0.217	1.00	0.00	CRES
ATOM	3	HB2	CRES	1	2.782	-2.481	-0.959	1.00	0.00	CRES
ATOM	4	HB3	CRES	1	2.958	-2.452	0.801	1.00	0.00	CRES
ATOM	5	CG	CRES	1	2.198	-0.620	-0.043	1.00	0.00	CRES
ATOM	6	CD1	CRES	1	1.765	0.025	-1.217	1.00	0.00	CRES
ATOM	7	HD1	CRES	1	2.009	-0.405	-2.182	1.00	0.00	CRES
ATOM	8	CD2	CRES	1	1.893	-0.012	1.187	1.00	0.00	CRES
ATOM	9	HD2	CRES	1	2.237	-0.467	2.110	1.00	0.00	CRES
ATOM	10	CE1	CRES	1	1.033	1.214	-1.170	1.00	0.00	CRES
ATOM	11	HE1	CRES	1	0.713	1.712	-2.076	1.00	0.00	CRES
ATOM	12	CE2	CRES	1	1.155	1.180	1.253	1.00	0.00	CRES
ATOM	13	HE2	CRES	1	0.923	1.624	2.215	1.00	0.00	CRES
ATOM	14	CZ	CRES	1	0.729	1.792	0.068	1.00	0.00	CRES
ATOM	15	OZ	CRES	1	-0.083	2.907	0.051	1.00	0.00	CRES
ATOM	16	HZ	CRES	1	0.047	3.428	0.858	1.00	0.00	CRES
ATOM	17	CG	IMIM	1	-2.133	0.217	-0.110	1.00	0.00	IMIM
ATOM	18	HG	IMIM	1	-1.897	1.267	-0.170	1.00	0.00	IMIM
ATOM	19	CD2	IMIM	1	-3.310	-0.463	-0.304	1.00	0.00	IMIM
ATOM	20	HD2	IMIM	1	-4.294	-0.114	-0.564	1.00	0.00	IMIM
ATOM	21	ND1	IMIM	1	-1.184	-0.728	0.204	1.00	0.00	IMIM
ATOM	22	HD1	IMIM	1	-0.201	-0.530	0.408	1.00	0.00	IMIM
ATOM	23	NE2	IMIM	1	-3.029	-1.795	-0.098	1.00	0.00	IMIM
ATOM	24	HE2	IMIM	1	-3.693	-2.556	-0.171	1.00	0.00	IMIM
ATOM	25	CE1	IMIM	1	-1.730	-1.949	0.211	1.00	0.00	IMIM
ATOM	26	HE1	IMIM	1	-1.227	-2.876	0.421	1.00	0.00	IMIM

END

REMARK 110_CRES_IMIM

ATOM	1	CB	CRES	1	2.703	-2.296	-0.779	1.00	0.00	CRES
ATOM	2	HB1	CRES	1	2.451	-3.047	-0.031	1.00	0.00	CRES
ATOM	3	HB2	CRES	1	3.789	-2.204	-0.804	1.00	0.00	CRES
ATOM	4	HB3	CRES	1	2.378	-2.658	-1.754	1.00	0.00	CRES
ATOM	5	CG	CRES	1	2.071	-0.968	-0.452	1.00	0.00	CRES
ATOM	6	CD1	CRES	1	1.906	-0.553	0.882	1.00	0.00	CRES
ATOM	7	HD1	CRES	1	2.195	-1.219	1.688	1.00	0.00	CRES
ATOM	8	CD2	CRES	1	1.720	-0.063	-1.468	1.00	0.00	CRES
ATOM	9	HD2	CRES	1	1.863	-0.342	-2.507	1.00	0.00	CRES
ATOM	10	CE1	CRES	1	1.382	0.703	1.196	1.00	0.00	CRES
ATOM	11	HE1	CRES	1	1.268	1.024	2.225	1.00	0.00	CRES
ATOM	12	CE2	CRES	1	1.188	1.200	-1.172	1.00	0.00	CRES
ATOM	13	HE2	CRES	1	0.911	1.877	-1.973	1.00	0.00	CRES
ATOM	14	CZ	CRES	1	1.021	1.578	0.166	1.00	0.00	CRES
ATOM	15	OZ	CRES	1	0.389	2.753	0.536	1.00	0.00	CRES
ATOM	16	HZ	CRES	1	0.549	3.441	-0.127	1.00	0.00	CRES
ATOM	17	CG	IMIM	1	-2.174	-1.584	-0.285	1.00	0.00	IMIM
ATOM	18	HG	IMIM	1	-1.869	-2.505	-0.748	1.00	0.00	IMIM
ATOM	19	CD2	IMIM	1	-3.368	-1.217	0.288	1.00	0.00	IMIM
ATOM	20	HD2	IMIM	1	-4.289	-1.757	0.412	1.00	0.00	IMIM

ATOM	21	ND1	IMIM	1	-1.334	-0.502	-0.169	1.00	0.00	IMIM
ATOM	22	HD1	IMIM	1	-0.367	-0.451	-0.496	1.00	0.00	IMIM
ATOM	23	NE2	IMIM	1	-3.202	0.077	0.726	1.00	0.00	IMIM
ATOM	24	HE2	IMIM	1	-3.904	0.634	1.198	1.00	0.00	IMIM
ATOM	25	CE1	IMIM	1	-1.960	0.509	0.447	1.00	0.00	IMIM
ATOM	26	HE1	IMIM	1	-1.542	1.479	0.669	1.00	0.00	IMIM

END

REMARK 111_CRES_IMIM

ATOM	1	CB	CRES	1	-1.235	3.335	-0.735	1.00	0.00	CRES
ATOM	2	HB1	CRES	1	-0.634	3.857	0.009	1.00	0.00	CRES
ATOM	3	HB2	CRES	1	-2.227	3.790	-0.738	1.00	0.00	CRES
ATOM	4	HB3	CRES	1	-0.791	3.500	-1.716	1.00	0.00	CRES
ATOM	5	CG	CRES	1	-1.333	1.865	-0.421	1.00	0.00	CRES
ATOM	6	CD1	CRES	1	-1.381	1.409	0.909	1.00	0.00	CRES
ATOM	7	HD1	CRES	1	-1.299	2.123	1.720	1.00	0.00	CRES
ATOM	8	CD2	CRES	1	-1.481	0.914	-1.446	1.00	0.00	CRES
ATOM	9	HD2	CRES	1	-1.478	1.238	-2.482	1.00	0.00	CRES
ATOM	10	CE1	CRES	1	-1.538	0.054	1.210	1.00	0.00	CRES
ATOM	11	HE1	CRES	1	-1.586	-0.292	2.236	1.00	0.00	CRES
ATOM	12	CE2	CRES	1	-1.634	-0.451	-1.162	1.00	0.00	CRES
ATOM	13	HE2	CRES	1	-1.732	-1.169	-1.969	1.00	0.00	CRES
ATOM	14	CZ	CRES	1	-1.662	-0.875	0.172	1.00	0.00	CRES
ATOM	15	OZ	CRES	1	-1.683	-2.213	0.528	1.00	0.00	CRES
ATOM	16	HZ	CRES	1	-2.169	-2.728	-0.134	1.00	0.00	CRES
ATOM	17	CG	IMIM	1	2.668	0.315	-0.305	1.00	0.00	IMIM
ATOM	18	HG	IMIM	1	2.850	1.272	-0.761	1.00	0.00	IMIM
ATOM	19	CD2	IMIM	1	3.533	-0.592	0.255	1.00	0.00	IMIM
ATOM	20	HD2	IMIM	1	4.602	-0.572	0.374	1.00	0.00	IMIM
ATOM	21	ND1	IMIM	1	1.408	-0.219	-0.187	1.00	0.00	IMIM
ATOM	22	HD1	IMIM	1	0.537	0.211	-0.507	1.00	0.00	IMIM
ATOM	23	NE2	IMIM	1	2.758	-1.644	0.688	1.00	0.00	IMIM
ATOM	24	HE2	IMIM	1	3.101	-2.477	1.151	1.00	0.00	IMIM
ATOM	25	CE1	IMIM	1	1.463	-1.412	0.418	1.00	0.00	IMIM
ATOM	26	HE1	IMIM	1	0.625	-2.055	0.640	1.00	0.00	IMIM

END

REMARK 112_CRES_IMIM

ATOM	1	CB	CRES	1	-0.946	3.501	-0.116	1.00	0.00	CRES
ATOM	2	HB1	CRES	1	-1.511	3.959	-0.928	1.00	0.00	CRES
ATOM	3	HB2	CRES	1	0.110	3.720	-0.286	1.00	0.00	CRES
ATOM	4	HB3	CRES	1	-1.242	3.982	0.814	1.00	0.00	CRES
ATOM	5	CG	CRES	1	-1.205	2.017	-0.060	1.00	0.00	CRES
ATOM	6	CD1	CRES	1	-1.299	1.256	-1.240	1.00	0.00	CRES
ATOM	7	HD1	CRES	1	-1.192	1.745	-2.202	1.00	0.00	CRES
ATOM	8	CD2	CRES	1	-1.404	1.356	1.164	1.00	0.00	CRES
ATOM	9	HD2	CRES	1	-1.366	1.921	2.089	1.00	0.00	CRES
ATOM	10	CE1	CRES	1	-1.556	-0.120	-1.202	1.00	0.00	CRES
ATOM	11	HE1	CRES	1	-1.653	-0.699	-2.113	1.00	0.00	CRES
ATOM	12	CE2	CRES	1	-1.646	-0.021	1.221	1.00	0.00	CRES
ATOM	13	HE2	CRES	1	-1.785	-0.511	2.179	1.00	0.00	CRES
ATOM	14	CZ	CRES	1	-1.720	-0.756	0.033	1.00	0.00	CRES
ATOM	15	OZ	CRES	1	-1.846	-2.135	0.012	1.00	0.00	CRES
ATOM	16	HZ	CRES	1	-2.332	-2.436	0.795	1.00	0.00	CRES
ATOM	17	CG	IMIM	1	2.698	0.183	0.079	1.00	0.00	IMIM
ATOM	18	HG	IMIM	1	2.966	1.224	0.109	1.00	0.00	IMIM
ATOM	19	CD2	IMIM	1	3.466	-0.947	0.220	1.00	0.00	IMIM
ATOM	20	HD2	IMIM	1	4.520	-1.069	0.393	1.00	0.00	IMIM
ATOM	21	ND1	IMIM	1	1.407	-0.242	-0.124	1.00	0.00	IMIM
ATOM	22	HD1	IMIM	1	0.591	0.351	-0.285	1.00	0.00	IMIM
ATOM	23	NE2	IMIM	1	2.606	-2.014	0.093	1.00	0.00	IMIM
ATOM	24	HE2	IMIM	1	2.868	-2.991	0.148	1.00	0.00	IMIM
ATOM	25	CE1	IMIM	1	1.352	-1.580	-0.119	1.00	0.00	IMIM
ATOM	26	HE1	IMIM	1	0.466	-2.184	-0.239	1.00	0.00	IMIM

END

REMARK 113_CRES_IMIM

ATOM	1	CB	CRES	1	-1.747	3.078	-0.285	1.00	0.00	CRES
ATOM	2	HB1	CRES	1	-2.674	3.288	-0.817	1.00	0.00	CRES
ATOM	3	HB2	CRES	1	-0.924	3.439	-0.905	1.00	0.00	CRES
ATOM	4	HB3	CRES	1	-1.751	3.652	0.640	1.00	0.00	CRES
ATOM	5	CG	CRES	1	-1.623	1.602	-0.005	1.00	0.00	CRES
ATOM	6	CD1	CRES	1	-1.749	0.660	-1.044	1.00	0.00	CRES
ATOM	7	HD1	CRES	1	-1.924	1.004	-2.057	1.00	0.00	CRES
ATOM	8	CD2	CRES	1	-1.440	1.115	1.300	1.00	0.00	CRES

ATOM	9	HD2	CRES	1	-1.374	1.812	2.129	1.00	0.00	CRES
ATOM	10	CE1	CRES	1	-1.667	-0.712	-0.800	1.00	0.00	CRES
ATOM	11	HE1	CRES	1	-1.782	-1.434	-1.599	1.00	0.00	CRES
ATOM	12	CE2	CRES	1	-1.350	-0.262	1.563	1.00	0.00	CRES
ATOM	13	HE2	CRES	1	-1.204	-0.613	2.579	1.00	0.00	CRES
ATOM	14	CZ	CRES	1	-1.466	-1.173	0.508	1.00	0.00	CRES
ATOM	15	OZ	CRES	1	-1.297	-2.533	0.669	1.00	0.00	CRES
ATOM	16	HZ	CRES	1	-1.521	-2.793	1.575	1.00	0.00	CRES
ATOM	17	CG	IMIM	1	3.037	-1.270	-0.638	1.00	0.00	IMIM
ATOM	18	HG	IMIM	1	3.686	-2.091	-0.885	1.00	0.00	IMIM
ATOM	19	CD2	IMIM	1	1.732	-1.246	-0.209	1.00	0.00	IMIM
ATOM	20	HD2	IMIM	1	1.030	-2.040	-0.016	1.00	0.00	IMIM
ATOM	21	ND1	IMIM	1	3.445	0.043	-0.718	1.00	0.00	IMIM
ATOM	22	HD1	IMIM	1	4.361	0.359	-1.010	1.00	0.00	IMIM
ATOM	23	NE2	IMIM	1	1.400	0.079	-0.046	1.00	0.00	IMIM
ATOM	24	HE2	IMIM	1	0.488	0.421	0.267	1.00	0.00	IMIM
ATOM	25	CE1	IMIM	1	2.441	0.860	-0.355	1.00	0.00	IMIM
ATOM	26	HE1	IMIM	1	2.469	1.935	-0.324	1.00	0.00	IMIM

END

REMARK 114_INDO_IMIM

ATOM	1	CD2	INDO	1	-1.516	-0.016	0.751	1.00	0.00	INDO
ATOM	2	CE2	INDO	1	-1.484	-0.017	-0.677	1.00	0.00	INDO
ATOM	3	CZ2	INDO	1	-1.195	1.133	-1.428	1.00	0.00	INDO
ATOM	4	CH2	INDO	1	-0.931	2.304	-0.723	1.00	0.00	INDO
ATOM	5	CZ3	INDO	1	-0.953	2.333	0.695	1.00	0.00	INDO
ATOM	6	CE3	INDO	1	-1.249	1.189	1.437	1.00	0.00	INDO
ATOM	7	CG	INDO	1	-1.833	-1.350	1.167	1.00	0.00	INDO
ATOM	8	CD1	INDO	1	-1.983	-2.103	0.019	1.00	0.00	INDO
ATOM	9	NE1	INDO	1	-1.739	-1.309	-1.086	1.00	0.00	INDO
ATOM	10	HZ2	INDO	1	-1.193	1.119	-2.512	1.00	0.00	INDO
ATOM	11	HH2	INDO	1	-0.725	3.217	-1.268	1.00	0.00	INDO
ATOM	12	HZ3	INDO	1	-0.768	3.269	1.207	1.00	0.00	INDO
ATOM	13	HE3	INDO	1	-1.287	1.229	2.520	1.00	0.00	INDO
ATOM	14	HG	INDO	1	-1.975	-1.705	2.175	1.00	0.00	INDO
ATOM	15	HD1	INDO	1	-2.258	-3.139	-0.101	1.00	0.00	INDO
ATOM	16	HE1	INDO	1	-1.911	-1.590	-2.041	1.00	0.00	INDO
ATOM	17	CG	IMIM	1	2.868	0.736	-0.027	1.00	0.00	IMIM
ATOM	18	HG	IMIM	1	3.153	1.773	-0.034	1.00	0.00	IMIM
ATOM	19	CD2	IMIM	1	3.605	-0.402	-0.247	1.00	0.00	IMIM
ATOM	20	HD2	IMIM	1	4.647	-0.538	-0.477	1.00	0.00	IMIM
ATOM	21	ND1	IMIM	1	1.581	0.328	0.227	1.00	0.00	IMIM
ATOM	22	HD1	IMIM	1	0.783	0.937	0.435	1.00	0.00	IMIM
ATOM	23	NE2	IMIM	1	2.730	-1.457	-0.117	1.00	0.00	IMIM
ATOM	24	HE2	IMIM	1	2.970	-2.436	-0.216	1.00	0.00	IMIM
ATOM	25	CE1	IMIM	1	1.497	-1.006	0.171	1.00	0.00	IMIM
ATOM	26	HE1	IMIM	1	0.608	-1.594	0.340	1.00	0.00	IMIM

END

REMARK 115_INDO_IMIM

ATOM	1	CD2	INDO	1	-1.578	-0.268	0.790	1.00	0.00	INDO
ATOM	2	CE2	INDO	1	-1.726	0.259	-0.534	1.00	0.00	INDO
ATOM	3	CZ2	INDO	1	-1.209	1.505	-0.919	1.00	0.00	INDO
ATOM	4	CH2	INDO	1	-0.623	2.286	0.074	1.00	0.00	INDO
ATOM	5	CZ3	INDO	1	-0.505	1.805	1.412	1.00	0.00	INDO
ATOM	6	CE3	INDO	1	-0.981	0.542	1.783	1.00	0.00	INDO
ATOM	7	CG	INDO	1	-2.304	-1.507	0.817	1.00	0.00	INDO
ATOM	8	CD1	INDO	1	-2.824	-1.696	-0.442	1.00	0.00	INDO
ATOM	9	NE1	INDO	1	-2.456	-0.648	-1.260	1.00	0.00	INDO
ATOM	10	HZ2	INDO	1	-1.346	1.860	-1.934	1.00	0.00	INDO
ATOM	11	HH2	INDO	1	-0.281	3.279	-0.184	1.00	0.00	INDO
ATOM	12	HZ3	INDO	1	-0.086	2.480	2.146	1.00	0.00	INDO
ATOM	13	HE3	INDO	1	-0.932	0.209	2.821	1.00	0.00	INDO
ATOM	14	HG	INDO	1	-2.420	-2.203	1.626	1.00	0.00	INDO
ATOM	15	HD1	INDO	1	-3.469	-2.490	-0.794	1.00	0.00	INDO
ATOM	16	HE1	INDO	1	-2.837	-0.447	-2.169	1.00	0.00	INDO
ATOM	17	CG	IMIM	1	3.051	0.084	0.737	1.00	0.00	IMIM
ATOM	18	HG	IMIM	1	3.261	0.585	1.665	1.00	0.00	IMIM
ATOM	19	CD2	IMIM	1	3.811	-0.781	-0.013	1.00	0.00	IMIM
ATOM	20	HD2	IMIM	1	4.803	-1.167	0.139	1.00	0.00	IMIM
ATOM	21	ND1	IMIM	1	1.859	0.238	0.074	1.00	0.00	IMIM
ATOM	22	HD1	IMIM	1	1.067	0.814	0.387	1.00	0.00	IMIM
ATOM	23	NE2	IMIM	1	3.043	-1.120	-1.104	1.00	0.00	IMIM
ATOM	24	HE2	IMIM	1	3.322	-1.749	-1.847	1.00	0.00	IMIM

ATOM	25	CE1	IMIM	1	1.854	-0.496	-1.042	1.00	0.00	IMIM
ATOM	26	HE1	IMIM	1	1.047	-0.572	-1.749	1.00	0.00	IMIM

END

REMARK 116_INDO_IMIM

ATOM	1	CD2	INDO	1	1.501	0.507	-0.596	1.00	0.00	INDO
ATOM	2	CE2	INDO	1	1.473	-0.126	0.684	1.00	0.00	INDO
ATOM	3	CZ2	INDO	1	1.033	0.531	1.844	1.00	0.00	INDO
ATOM	4	CH2	INDO	1	0.606	1.849	1.706	1.00	0.00	INDO
ATOM	5	CZ3	INDO	1	0.617	2.500	0.446	1.00	0.00	INDO
ATOM	6	CE3	INDO	1	1.066	1.847	-0.703	1.00	0.00	INDO
ATOM	7	CG	INDO	1	1.997	-0.456	-1.533	1.00	0.00	INDO
ATOM	8	CD1	INDO	1	2.255	-1.612	-0.821	1.00	0.00	INDO
ATOM	9	NE1	INDO	1	1.907	-1.422	0.503	1.00	0.00	INDO
ATOM	10	HZ2	INDO	1	1.037	0.042	2.811	1.00	0.00	INDO
ATOM	11	HH2	INDO	1	0.279	2.396	2.581	1.00	0.00	INDO
ATOM	12	HZ3	INDO	1	0.303	3.535	0.383	1.00	0.00	INDO
ATOM	13	HE3	INDO	1	1.094	2.363	-1.656	1.00	0.00	INDO
ATOM	14	HG	INDO	1	2.184	-0.311	-2.585	1.00	0.00	INDO
ATOM	15	HD1	INDO	1	2.671	-2.551	-1.149	1.00	0.00	INDO
ATOM	16	HE1	INDO	1	2.122	-2.069	1.249	1.00	0.00	INDO
ATOM	17	CG	IMIM	1	-2.940	0.281	0.184	1.00	0.00	IMIM
ATOM	18	HG	IMIM	1	-3.365	1.165	0.625	1.00	0.00	IMIM
ATOM	19	CD2	IMIM	1	-3.513	-0.921	-0.154	1.00	0.00	IMIM
ATOM	20	HD2	IMIM	1	-4.524	-1.274	-0.063	1.00	0.00	IMIM
ATOM	21	ND1	IMIM	1	-1.611	0.192	-0.152	1.00	0.00	IMIM
ATOM	22	HD1	IMIM	1	-0.905	0.925	-0.030	1.00	0.00	IMIM
ATOM	23	NE2	IMIM	1	-2.502	-1.693	-0.683	1.00	0.00	IMIM
ATOM	24	HE2	IMIM	1	-2.605	-2.637	-1.033	1.00	0.00	IMIM
ATOM	25	CE1	IMIM	1	-1.344	-1.009	-0.677	1.00	0.00	IMIM
ATOM	26	HE1	IMIM	1	-0.384	-1.347	-1.037	1.00	0.00	IMIM

END

REMARK 117_INDO_IMIM

ATOM	1	CD2	INDO	1	1.415	-0.446	-0.815	1.00	0.00	INDO
ATOM	2	CE2	INDO	1	1.542	0.067	0.512	1.00	0.00	INDO
ATOM	3	CZ2	INDO	1	1.430	1.434	0.809	1.00	0.00	INDO
ATOM	4	CH2	INDO	1	1.166	2.297	-0.252	1.00	0.00	INDO
ATOM	5	CZ3	INDO	1	1.025	1.813	-1.578	1.00	0.00	INDO
ATOM	6	CE3	INDO	1	1.153	0.455	-1.871	1.00	0.00	INDO
ATOM	7	CG	INDO	1	1.587	-1.866	-0.736	1.00	0.00	INDO
ATOM	8	CD1	INDO	1	1.816	-2.170	0.591	1.00	0.00	INDO
ATOM	9	NE1	INDO	1	1.756	-1.012	1.344	1.00	0.00	INDO
ATOM	10	HZ2	INDO	1	1.552	1.810	1.819	1.00	0.00	INDO
ATOM	11	HH2	INDO	1	1.091	3.361	-0.066	1.00	0.00	INDO
ATOM	12	HZ3	INDO	1	0.848	2.518	-2.381	1.00	0.00	INDO
ATOM	13	HE3	INDO	1	1.069	0.101	-2.892	1.00	0.00	INDO
ATOM	14	HG	INDO	1	1.589	-2.572	-1.552	1.00	0.00	INDO
ATOM	15	HD1	INDO	1	2.030	-3.118	1.060	1.00	0.00	INDO
ATOM	16	HE1	INDO	1	2.015	-0.949	2.318	1.00	0.00	INDO
ATOM	17	CG	IMIM	1	-2.784	1.001	-0.007	1.00	0.00	IMIM
ATOM	18	HG	IMIM	1	-2.993	1.996	-0.356	1.00	0.00	IMIM
ATOM	19	CD2	IMIM	1	-3.569	0.104	0.676	1.00	0.00	IMIM
ATOM	20	HD2	IMIM	1	-4.582	0.174	1.029	1.00	0.00	IMIM
ATOM	21	ND1	IMIM	1	-1.569	0.391	-0.203	1.00	0.00	IMIM
ATOM	22	HD1	IMIM	1	-0.760	0.794	-0.687	1.00	0.00	IMIM
ATOM	23	NE2	IMIM	1	-2.793	-1.017	0.868	1.00	0.00	IMIM
ATOM	24	HE2	IMIM	1	-3.088	-1.864	1.338	1.00	0.00	IMIM
ATOM	25	CE1	IMIM	1	-1.573	-0.836	0.331	1.00	0.00	IMIM
ATOM	26	HE1	IMIM	1	-0.755	-1.539	0.314	1.00	0.00	IMIM

END

REMARK 118_INDO_IMIM

ATOM	1	CD2	INDO	1	-1.150	0.402	0.867	1.00	0.00	INDO
ATOM	2	CE2	INDO	1	-1.048	0.460	-0.556	1.00	0.00	INDO
ATOM	3	CZ2	INDO	1	-0.355	1.482	-1.223	1.00	0.00	INDO
ATOM	4	CH2	INDO	1	0.233	2.470	-0.438	1.00	0.00	INDO
ATOM	5	CZ3	INDO	1	0.142	2.438	0.977	1.00	0.00	INDO
ATOM	6	CE3	INDO	1	-0.567	1.436	1.633	1.00	0.00	INDO
ATOM	7	CG	INDO	1	-1.950	-0.742	1.185	1.00	0.00	INDO
ATOM	8	CD1	INDO	1	-2.289	-1.342	-0.011	1.00	0.00	INDO
ATOM	9	NE1	INDO	1	-1.721	-0.636	-1.056	1.00	0.00	INDO
ATOM	10	HZ2	INDO	1	-0.317	1.531	-2.306	1.00	0.00	INDO
ATOM	11	HH2	INDO	1	0.742	3.298	-0.918	1.00	0.00	INDO
ATOM	12	HZ3	INDO	1	0.568	3.254	1.549	1.00	0.00	INDO

ATOM	13	HE3	INDO	1	-0.676	1.452	2.712	1.00	0.00	INDO
ATOM	14	HG	INDO	1	-2.275	-1.065	2.163	1.00	0.00	INDO
ATOM	15	HD1	INDO	1	-2.920	-2.195	-0.206	1.00	0.00	INDO
ATOM	16	HE1	INDO	1	-1.956	-0.773	-2.029	1.00	0.00	INDO
ATOM	17	CG	IMIM	1	2.233	-0.524	-1.097	1.00	0.00	IMIM
ATOM	18	HG	IMIM	1	2.767	0.076	-1.812	1.00	0.00	IMIM
ATOM	19	CD2	IMIM	1	1.600	-1.735	-1.231	1.00	0.00	IMIM
ATOM	20	HD2	IMIM	1	1.493	-2.386	-2.080	1.00	0.00	IMIM
ATOM	21	ND1	IMIM	1	2.082	-0.148	0.217	1.00	0.00	IMIM
ATOM	22	HD1	IMIM	1	2.332	0.755	0.607	1.00	0.00	IMIM
ATOM	23	NE2	IMIM	1	1.079	-2.038	0.007	1.00	0.00	IMIM
ATOM	24	HE2	IMIM	1	0.509	-2.845	0.233	1.00	0.00	IMIM
ATOM	25	CE1	IMIM	1	1.358	-1.059	0.878	1.00	0.00	IMIM
ATOM	26	HE1	IMIM	1	1.080	-1.027	1.916	1.00	0.00	IMIM

END

REMARK 119_MIND_IMIM

ATOM	1	CG	MIND	1	1.952	-1.132	-0.393	1.00	0.00	MIND
ATOM	2	CB	MIND	1	2.427	-1.928	-1.569	1.00	0.00	MIND
ATOM	3	HB1	MIND	1	2.771	-2.913	-1.256	1.00	0.00	MIND
ATOM	4	HB2	MIND	1	3.259	-1.425	-2.065	1.00	0.00	MIND
ATOM	5	HB3	MIND	1	1.636	-2.065	-2.307	1.00	0.00	MIND
ATOM	6	CD2	MIND	1	1.396	0.191	-0.421	1.00	0.00	MIND
ATOM	7	CD1	MIND	1	2.020	-1.488	0.942	1.00	0.00	MIND
ATOM	8	HD1	MIND	1	2.410	-2.388	1.395	1.00	0.00	MIND
ATOM	9	NE1	MIND	1	1.510	-0.470	1.732	1.00	0.00	MIND
ATOM	10	HE1	MIND	1	1.586	-0.434	2.738	1.00	0.00	MIND
ATOM	11	CE2	MIND	1	1.161	0.595	0.928	1.00	0.00	MIND
ATOM	12	CE3	MIND	1	1.095	1.093	-1.465	1.00	0.00	MIND
ATOM	13	HE3	MIND	1	1.292	0.830	-2.499	1.00	0.00	MIND
ATOM	14	CZ2	MIND	1	0.602	1.839	1.258	1.00	0.00	MIND
ATOM	15	HZ2	MIND	1	0.436	2.134	2.287	1.00	0.00	MIND
ATOM	16	CZ3	MIND	1	0.537	2.331	-1.143	1.00	0.00	MIND
ATOM	17	HZ3	MIND	1	0.316	3.040	-1.931	1.00	0.00	MIND
ATOM	18	CH2	MIND	1	0.303	2.702	0.206	1.00	0.00	MIND
ATOM	19	HH2	MIND	1	-0.106	3.682	0.422	1.00	0.00	MIND
ATOM	20	CG	IMIM	1	-3.090	0.315	-0.411	1.00	0.00	IMIM
ATOM	21	HG	IMIM	1	-3.521	1.226	-0.787	1.00	0.00	IMIM
ATOM	22	CD2	IMIM	1	-3.680	-0.818	0.095	1.00	0.00	IMIM
ATOM	23	HD2	IMIM	1	-4.714	-1.075	0.237	1.00	0.00	IMIM
ATOM	24	ND1	IMIM	1	-1.733	0.107	-0.362	1.00	0.00	IMIM
ATOM	25	HD1	IMIM	1	-1.008	0.763	-0.672	1.00	0.00	IMIM
ATOM	26	NE2	IMIM	1	-2.651	-1.669	0.430	1.00	0.00	IMIM
ATOM	27	HE2	IMIM	1	-2.758	-2.594	0.828	1.00	0.00	IMIM
ATOM	28	CE1	IMIM	1	-1.465	-1.099	0.151	1.00	0.00	IMIM
ATOM	29	HE1	IMIM	1	-0.484	-1.526	0.295	1.00	0.00	IMIM

END

REMARK 120_MIND_IMIM

ATOM	1	CG	MIND	1	1.962	-1.251	0.079	1.00	0.00	MIND
ATOM	2	CB	MIND	1	2.721	-1.820	1.238	1.00	0.00	MIND
ATOM	3	HB1	MIND	1	2.942	-2.874	1.075	1.00	0.00	MIND
ATOM	4	HB2	MIND	1	2.156	-1.735	2.168	1.00	0.00	MIND
ATOM	5	HB3	MIND	1	3.668	-1.296	1.377	1.00	0.00	MIND
ATOM	6	CD2	MIND	1	1.478	0.092	-0.053	1.00	0.00	MIND
ATOM	7	CD1	MIND	1	1.624	-1.895	-1.097	1.00	0.00	MIND
ATOM	8	HD1	MIND	1	1.830	-2.908	-1.409	1.00	0.00	MIND
ATOM	9	NE1	MIND	1	0.943	-1.027	-1.934	1.00	0.00	MIND
ATOM	10	HE1	MIND	1	0.705	-1.227	-2.895	1.00	0.00	MIND
ATOM	11	CE2	MIND	1	0.875	0.214	-1.342	1.00	0.00	MIND
ATOM	12	CE3	MIND	1	1.534	1.230	0.783	1.00	0.00	MIND
ATOM	13	HE3	MIND	1	2.021	1.182	1.751	1.00	0.00	MIND
ATOM	14	CZ2	MIND	1	0.281	1.404	-1.788	1.00	0.00	MIND
ATOM	15	HZ2	MIND	1	-0.170	1.482	-2.770	1.00	0.00	MIND
ATOM	16	CZ3	MIND	1	0.948	2.418	0.342	1.00	0.00	MIND
ATOM	17	HZ3	MIND	1	1.000	3.303	0.965	1.00	0.00	MIND
ATOM	18	CH2	MIND	1	0.337	2.506	-0.935	1.00	0.00	MIND
ATOM	19	HH2	MIND	1	-0.083	3.450	-1.258	1.00	0.00	MIND
ATOM	20	CG	IMIM	1	-1.560	-1.001	0.525	1.00	0.00	IMIM
ATOM	21	HG	IMIM	1	-0.688	-1.548	0.205	1.00	0.00	IMIM
ATOM	22	CD2	IMIM	1	-2.857	-1.397	0.748	1.00	0.00	IMIM
ATOM	23	HD2	IMIM	1	-3.330	-2.357	0.655	1.00	0.00	IMIM
ATOM	24	ND1	IMIM	1	-1.508	0.344	0.804	1.00	0.00	IMIM
ATOM	25	HD1	IMIM	1	-0.666	0.927	0.735	1.00	0.00	IMIM

ATOM	26	NE2	IMIM	1	-3.541	-0.272	1.153	1.00	0.00	IMIM
ATOM	27	HE2	IMIM	1	-4.524	-0.234	1.393	1.00	0.00	IMIM
ATOM	28	CE1	IMIM	1	-2.711	0.786	1.184	1.00	0.00	IMIM
ATOM	29	HE1	IMIM	1	-2.968	1.794	1.459	1.00	0.00	IMIM

END

REMARK 121_MIND_IMIM

ATOM	1	CG	MIND	1	1.963	-1.251	0.080	1.00	0.00	MIND
ATOM	2	CB	MIND	1	2.721	-1.819	1.239	1.00	0.00	MIND
ATOM	3	HB1	MIND	1	2.950	-2.871	1.073	1.00	0.00	MIND
ATOM	4	HB2	MIND	1	2.152	-1.741	2.168	1.00	0.00	MIND
ATOM	5	HB3	MIND	1	3.664	-1.289	1.383	1.00	0.00	MIND
ATOM	6	CD2	MIND	1	1.478	0.093	-0.053	1.00	0.00	MIND
ATOM	7	CD1	MIND	1	1.625	-1.895	-1.096	1.00	0.00	MIND
ATOM	8	HD1	MIND	1	1.831	-2.908	-1.408	1.00	0.00	MIND
ATOM	9	NE1	MIND	1	0.942	-1.028	-1.934	1.00	0.00	MIND
ATOM	10	HE1	MIND	1	0.707	-1.228	-2.895	1.00	0.00	MIND
ATOM	11	CE2	MIND	1	0.875	0.213	-1.343	1.00	0.00	MIND
ATOM	12	CE3	MIND	1	1.534	1.231	0.782	1.00	0.00	MIND
ATOM	13	HE3	MIND	1	2.021	1.184	1.750	1.00	0.00	MIND
ATOM	14	CZ2	MIND	1	0.280	1.403	-1.788	1.00	0.00	MIND
ATOM	15	HZ2	MIND	1	-0.172	1.480	-2.771	1.00	0.00	MIND
ATOM	16	CZ3	MIND	1	0.948	2.418	0.340	1.00	0.00	MIND
ATOM	17	HZ3	MIND	1	0.999	3.304	0.963	1.00	0.00	MIND
ATOM	18	CH2	MIND	1	0.336	2.505	-0.937	1.00	0.00	MIND
ATOM	19	HH2	MIND	1	-0.084	3.449	-1.260	1.00	0.00	MIND
ATOM	20	CG	IMIM	1	-1.559	-1.001	0.526	1.00	0.00	IMIM
ATOM	21	HG	IMIM	1	-0.687	-1.548	0.208	1.00	0.00	IMIM
ATOM	22	CD2	IMIM	1	-2.856	-1.397	0.751	1.00	0.00	IMIM
ATOM	23	HD2	IMIM	1	-3.329	-2.358	0.660	1.00	0.00	IMIM
ATOM	24	ND1	IMIM	1	-1.508	0.345	0.803	1.00	0.00	IMIM
ATOM	25	HD1	IMIM	1	-0.666	0.928	0.733	1.00	0.00	IMIM
ATOM	26	NE2	IMIM	1	-3.541	-0.272	1.153	1.00	0.00	IMIM
ATOM	27	HE2	IMIM	1	-4.524	-0.235	1.394	1.00	0.00	IMIM
ATOM	28	CE1	IMIM	1	-2.712	0.786	1.182	1.00	0.00	IMIM
ATOM	29	HE1	IMIM	1	-2.969	1.795	1.456	1.00	0.00	IMIM

END

REMARK 122_MIND_IMIM

ATOM	1	CG	MIND	1	-2.059	-0.039	1.004	1.00	0.00	MIND
ATOM	2	CB	MIND	1	-2.623	0.730	2.158	1.00	0.00	MIND
ATOM	3	HB1	MIND	1	-3.058	0.057	2.896	1.00	0.00	MIND
ATOM	4	HB2	MIND	1	-3.406	1.412	1.822	1.00	0.00	MIND
ATOM	5	HB3	MIND	1	-1.857	1.328	2.656	1.00	0.00	MIND
ATOM	6	CD2	MIND	1	-1.376	0.504	-0.136	1.00	0.00	MIND
ATOM	7	CD1	MIND	1	-2.147	-1.402	0.782	1.00	0.00	MIND
ATOM	8	HD1	MIND	1	-2.619	-2.166	1.381	1.00	0.00	MIND
ATOM	9	NE1	MIND	1	-1.531	-1.728	-0.416	1.00	0.00	MIND
ATOM	10	HE1	MIND	1	-1.593	-2.633	-0.862	1.00	0.00	MIND
ATOM	11	CE2	MIND	1	-1.088	-0.575	-1.026	1.00	0.00	MIND
ATOM	12	CE3	MIND	1	-0.996	1.813	-0.505	1.00	0.00	MIND
ATOM	13	HE3	MIND	1	-1.228	2.658	0.133	1.00	0.00	MIND
ATOM	14	CZ2	MIND	1	-0.406	-0.391	-2.239	1.00	0.00	MIND
ATOM	15	HZ2	MIND	1	-0.200	-1.219	-2.908	1.00	0.00	MIND
ATOM	16	CZ3	MIND	1	-0.315	2.000	-1.709	1.00	0.00	MIND
ATOM	17	HZ3	MIND	1	-0.032	3.001	-2.014	1.00	0.00	MIND
ATOM	18	CH2	MIND	1	-0.032	0.909	-2.570	1.00	0.00	MIND
ATOM	19	HH2	MIND	1	0.473	1.094	-3.510	1.00	0.00	MIND
ATOM	20	CG	IMIM	1	3.102	0.411	0.171	1.00	0.00	IMIM
ATOM	21	HG	IMIM	1	3.616	1.109	-0.465	1.00	0.00	IMIM
ATOM	22	CD2	IMIM	1	3.582	-0.524	1.055	1.00	0.00	IMIM
ATOM	23	HD2	IMIM	1	4.588	-0.788	1.331	1.00	0.00	IMIM
ATOM	24	ND1	IMIM	1	1.731	0.322	0.211	1.00	0.00	IMIM
ATOM	25	HD1	IMIM	1	1.072	0.890	-0.331	1.00	0.00	IMIM
ATOM	26	NE2	IMIM	1	2.478	-1.144	1.597	1.00	0.00	IMIM
ATOM	27	HE2	IMIM	1	2.498	-1.883	2.289	1.00	0.00	IMIM
ATOM	28	CE1	IMIM	1	1.351	-0.625	1.077	1.00	0.00	IMIM
ATOM	29	HE1	IMIM	1	0.335	-0.900	1.313	1.00	0.00	IMIM

END

REMARK 123_MIND_IMIM

ATOM	1	CG	MIND	1	1.963	-1.251	0.079	1.00	0.00	MIND
ATOM	2	CB	MIND	1	2.722	-1.818	1.238	1.00	0.00	MIND
ATOM	3	HB1	MIND	1	2.943	-2.872	1.076	1.00	0.00	MIND
ATOM	4	HB2	MIND	1	2.158	-1.731	2.168	1.00	0.00	MIND

ATOM	5	HB3	MIND	1	3.670	-1.295	1.374	1.00	0.00	MIND
ATOM	6	CD2	MIND	1	1.477	0.093	-0.055	1.00	0.00	MIND
ATOM	7	CD1	MIND	1	1.624	-1.896	-1.097	1.00	0.00	MIND
ATOM	8	HD1	MIND	1	1.831	-2.909	-1.409	1.00	0.00	MIND
ATOM	9	NE1	MIND	1	0.942	-1.029	-1.935	1.00	0.00	MIND
ATOM	10	HE1	MIND	1	0.704	-1.229	-2.895	1.00	0.00	MIND
ATOM	11	CE2	MIND	1	0.874	0.213	-1.344	1.00	0.00	MIND
ATOM	12	CE3	MIND	1	1.534	1.231	0.780	1.00	0.00	MIND
ATOM	13	HE3	MIND	1	2.021	1.184	1.748	1.00	0.00	MIND
ATOM	14	CZ2	MIND	1	0.280	1.403	-1.790	1.00	0.00	MIND
ATOM	15	HZ2	MIND	1	-0.172	1.480	-2.772	1.00	0.00	MIND
ATOM	16	CZ3	MIND	1	0.948	2.419	0.338	1.00	0.00	MIND
ATOM	17	HZ3	MIND	1	0.999	3.304	0.961	1.00	0.00	MIND
ATOM	18	CH2	MIND	1	0.336	2.505	-0.938	1.00	0.00	MIND
ATOM	19	HH2	MIND	1	-0.084	3.449	-1.262	1.00	0.00	MIND
ATOM	20	CG	IMIM	1	-1.560	-1.001	0.527	1.00	0.00	IMIM
ATOM	21	HG	IMIM	1	-0.688	-1.548	0.207	1.00	0.00	IMIM
ATOM	22	CD2	IMIM	1	-2.856	-1.397	0.754	1.00	0.00	IMIM
ATOM	23	HD2	IMIM	1	-3.329	-2.358	0.664	1.00	0.00	IMIM
ATOM	24	ND1	IMIM	1	-1.508	0.345	0.804	1.00	0.00	IMIM
ATOM	25	HD1	IMIM	1	-0.666	0.928	0.732	1.00	0.00	IMIM
ATOM	26	NE2	IMIM	1	-3.540	-0.272	1.158	1.00	0.00	IMIM
ATOM	27	HE2	IMIM	1	-4.522	-0.234	1.401	1.00	0.00	IMIM
ATOM	28	CE1	IMIM	1	-2.711	0.786	1.185	1.00	0.00	IMIM
ATOM	29	HE1	IMIM	1	-2.967	1.795	1.459	1.00	0.00	IMIM

END

REMARK 124_MIND_IMIM

ATOM	1	CG	MIND	1	-2.035	-0.607	0.266	1.00	0.00	MIND
ATOM	2	CB	MIND	1	-2.858	-1.479	1.163	1.00	0.00	MIND
ATOM	3	HB1	MIND	1	-3.532	-2.108	0.582	1.00	0.00	MIND
ATOM	4	HB2	MIND	1	-3.464	-0.874	1.839	1.00	0.00	MIND
ATOM	5	HB3	MIND	1	-2.239	-2.134	1.780	1.00	0.00	MIND
ATOM	6	CD2	MIND	1	-1.034	0.339	0.672	1.00	0.00	MIND
ATOM	7	CD1	MIND	1	-2.139	-0.487	-1.108	1.00	0.00	MIND
ATOM	8	HD1	MIND	1	-2.814	-0.982	-1.792	1.00	0.00	MIND
ATOM	9	NE1	MIND	1	-1.240	0.460	-1.572	1.00	0.00	MIND
ATOM	10	HE1	MIND	1	-1.261	0.854	-2.502	1.00	0.00	MIND
ATOM	11	CE2	MIND	1	-0.578	1.017	-0.498	1.00	0.00	MIND
ATOM	12	CE3	MIND	1	-0.530	0.733	1.930	1.00	0.00	MIND
ATOM	13	HE3	MIND	1	-0.898	0.277	2.843	1.00	0.00	MIND
ATOM	14	CZ2	MIND	1	0.392	2.029	-0.452	1.00	0.00	MIND
ATOM	15	HZ2	MIND	1	0.707	2.558	-1.345	1.00	0.00	MIND
ATOM	16	CZ3	MIND	1	0.449	1.724	1.978	1.00	0.00	MIND
ATOM	17	HZ3	MIND	1	0.825	2.058	2.939	1.00	0.00	MIND
ATOM	18	CH2	MIND	1	0.893	2.377	0.802	1.00	0.00	MIND
ATOM	19	HH2	MIND	1	1.613	3.183	0.882	1.00	0.00	MIND
ATOM	20	CG	IMIM	1	2.564	-0.362	-0.922	1.00	0.00	IMIM
ATOM	21	HG	IMIM	1	3.346	0.349	-1.122	1.00	0.00	IMIM
ATOM	22	CD2	IMIM	1	1.828	-1.153	-1.769	1.00	0.00	IMIM
ATOM	23	HD2	IMIM	1	1.863	-1.267	-2.838	1.00	0.00	IMIM
ATOM	24	ND1	IMIM	1	2.119	-0.633	0.350	1.00	0.00	IMIM
ATOM	25	HD1	IMIM	1	2.376	-0.121	1.188	1.00	0.00	IMIM
ATOM	26	NE2	IMIM	1	0.959	-1.867	-0.976	1.00	0.00	IMIM
ATOM	27	HE2	IMIM	1	0.240	-2.502	-1.301	1.00	0.00	IMIM
ATOM	28	CE1	IMIM	1	1.124	-1.529	0.311	1.00	0.00	IMIM
ATOM	29	HE1	IMIM	1	0.589	-1.929	1.152	1.00	0.00	IMIM

END

REMARK 125_IMID_IMIM

ATOM	1	CG	IMID	1	-3.086	-1.236	0.277	1.00	0.00	IMID
ATOM	2	HG	IMID	1	-3.747	-2.049	0.475	1.00	0.00	IMID
ATOM	3	CD2	IMID	1	-1.980	-0.785	0.952	1.00	0.00	IMID
ATOM	4	HD2	IMID	1	-1.593	-1.125	1.898	1.00	0.00	IMID
ATOM	5	ND1	IMID	1	-3.162	-0.467	-0.858	1.00	0.00	IMID
ATOM	6	HD1	IMID	1	-3.878	-0.527	-1.569	1.00	0.00	IMID
ATOM	7	CE1	IMID	1	-2.127	0.411	-0.848	1.00	0.00	IMID
ATOM	8	HE1	IMID	1	-1.952	1.129	-1.632	1.00	0.00	IMID
ATOM	9	NE2	IMID	1	-1.380	0.237	0.244	1.00	0.00	IMID
ATOM	10	CG	IMIM	1	2.304	-0.822	0.007	1.00	0.00	IMIM
ATOM	11	HG	IMIM	1	2.164	-1.886	-0.045	1.00	0.00	IMIM
ATOM	12	CD2	IMIM	1	3.443	-0.059	-0.084	1.00	0.00	IMIM
ATOM	13	HD2	IMIM	1	4.473	-0.334	-0.223	1.00	0.00	IMIM
ATOM	14	ND1	IMIM	1	1.248	0.049	0.138	1.00	0.00	IMIM

ATOM	15	HD1	IMIM	1	0.213	-0.130	0.216	1.00	0.00	IMIM
ATOM	16	NE2	IMIM	1	3.040	1.250	0.060	1.00	0.00	IMIM
ATOM	17	HE2	IMIM	1	3.650	2.058	0.054	1.00	0.00	IMIM
ATOM	18	CE1	IMIM	1	1.705	1.300	0.221	1.00	0.00	IMIM
ATOM	19	HE1	IMIM	1	1.107	2.182	0.364	1.00	0.00	IMIM

END

REMARK 126_IMID_IMIM

ATOM	1	CG	IMID	1	2.937	0.551	0.089	1.00	0.00	IMID
ATOM	2	HG	IMID	1	3.842	1.073	-0.171	1.00	0.00	IMID
ATOM	3	CD2	IMID	1	1.623	0.716	-0.296	1.00	0.00	IMID
ATOM	4	HD2	IMID	1	1.230	1.453	-0.976	1.00	0.00	IMID
ATOM	5	ND1	IMID	1	2.922	-0.511	0.960	1.00	0.00	IMID
ATOM	6	HD1	IMID	1	3.724	-0.902	1.434	1.00	0.00	IMID
ATOM	7	CE1	IMID	1	1.636	-0.945	1.075	1.00	0.00	IMID
ATOM	8	HE1	IMID	1	1.359	-1.774	1.705	1.00	0.00	IMID
ATOM	9	NE2	IMID	1	0.811	-0.217	0.320	1.00	0.00	IMID
ATOM	10	CG	IMIM	1	-1.760	0.442	-1.556	1.00	0.00	IMIM
ATOM	11	HG	IMIM	1	-1.563	0.650	-2.593	1.00	0.00	IMIM
ATOM	12	CD2	IMIM	1	-1.955	1.283	-0.490	1.00	0.00	IMIM
ATOM	13	HD2	IMIM	1	-1.958	2.357	-0.429	1.00	0.00	IMIM
ATOM	14	ND1	IMIM	1	-1.883	-0.836	-1.069	1.00	0.00	IMIM
ATOM	15	HD1	IMIM	1	-1.744	-1.685	-1.603	1.00	0.00	IMIM
ATOM	16	NE2	IMIM	1	-2.188	0.480	0.600	1.00	0.00	IMIM
ATOM	17	HE2	IMIM	1	-2.320	0.802	1.550	1.00	0.00	IMIM
ATOM	18	CE1	IMIM	1	-2.116	-0.809	0.248	1.00	0.00	IMIM
ATOM	19	HE1	IMIM	1	-2.232	-1.658	0.897	1.00	0.00	IMIM

END

REMARK 127_4MIE_IMIM

ATOM	1	CB	4MIE	1	-1.892	1.825	0.046	1.00	0.00	4MIE
ATOM	2	HB1	4MIE	1	-1.648	2.089	-0.985	1.00	0.00	4MIE
ATOM	3	HB2	4MIE	1	-2.891	2.203	0.254	1.00	0.00	4MIE
ATOM	4	HB3	4MIE	1	-1.199	2.345	0.712	1.00	0.00	4MIE
ATOM	5	CG	4MIE	1	-1.834	0.347	0.254	1.00	0.00	4MIE
ATOM	6	ND1	4MIE	1	-0.658	-0.370	0.099	1.00	0.00	4MIE
ATOM	7	CD2	4MIE	1	-2.863	-0.506	0.601	1.00	0.00	4MIE
ATOM	8	HD2	4MIE	1	-3.906	-0.334	0.804	1.00	0.00	4MIE
ATOM	9	CE1	4MIE	1	-0.981	-1.639	0.351	1.00	0.00	4MIE
ATOM	10	HE1	4MIE	1	-0.312	-2.484	0.327	1.00	0.00	4MIE
ATOM	11	NE2	4MIE	1	-2.301	-1.760	0.656	1.00	0.00	4MIE
ATOM	12	HE2	4MIE	1	-2.783	-2.618	0.886	1.00	0.00	4MIE
ATOM	13	CG	IMIM	1	2.494	-0.662	-0.739	1.00	0.00	IMIM
ATOM	14	HG	IMIM	1	2.826	-1.600	-1.148	1.00	0.00	IMIM
ATOM	15	CD2	IMIM	1	2.550	-0.168	0.540	1.00	0.00	IMIM
ATOM	16	HD2	IMIM	1	2.935	-0.599	1.447	1.00	0.00	IMIM
ATOM	17	ND1	IMIM	1	1.916	0.318	-1.508	1.00	0.00	IMIM
ATOM	18	HD1	IMIM	1	1.692	0.240	-2.492	1.00	0.00	IMIM
ATOM	19	NE2	IMIM	1	2.006	1.092	0.492	1.00	0.00	IMIM
ATOM	20	HE2	IMIM	1	1.858	1.699	1.288	1.00	0.00	IMIM
ATOM	21	CE1	IMIM	1	1.596	1.372	-0.750	1.00	0.00	IMIM
ATOM	22	HE1	IMIM	1	1.113	2.275	-1.078	1.00	0.00	IMIM

END

REMARK 128_4MIM_IMIM

ATOM	1	CB	4MIM	1	-3.255	1.449	0.192	1.00	0.00	4MIM
ATOM	2	HB1	4MIM	1	-4.208	1.471	-0.335	1.00	0.00	4MIM
ATOM	3	HB2	4MIM	1	-3.463	1.363	1.257	1.00	0.00	4MIM
ATOM	4	HB3	4MIM	1	-2.737	2.396	0.024	1.00	0.00	4MIM
ATOM	5	CG	4MIM	1	-2.403	0.305	-0.243	1.00	0.00	4MIM
ATOM	6	ND1	4MIM	1	-2.194	-0.031	-1.565	1.00	0.00	4MIM
ATOM	7	HD1	4MIM	1	-2.690	0.356	-2.357	1.00	0.00	4MIM
ATOM	8	CD2	4MIM	1	-1.567	-0.539	0.460	1.00	0.00	4MIM
ATOM	9	HD2	4MIM	1	-1.446	-0.604	1.530	1.00	0.00	4MIM
ATOM	10	CE1	4MIM	1	-1.274	-1.035	-1.625	1.00	0.00	4MIM
ATOM	11	HE1	4MIM	1	-0.955	-1.493	-2.546	1.00	0.00	4MIM
ATOM	12	NE2	4MIM	1	-0.861	-1.362	-0.399	1.00	0.00	4MIM
ATOM	13	CG	IMIM	1	2.845	-0.831	0.922	1.00	0.00	IMIM
ATOM	14	HG	IMIM	1	3.234	-1.812	1.133	1.00	0.00	IMIM
ATOM	15	CD2	IMIM	1	3.389	0.412	1.145	1.00	0.00	IMIM
ATOM	16	HD2	IMIM	1	4.326	0.709	1.582	1.00	0.00	IMIM
ATOM	17	ND1	IMIM	1	1.621	-0.632	0.331	1.00	0.00	IMIM
ATOM	18	HD1	IMIM	1	0.862	-1.306	0.069	1.00	0.00	IMIM
ATOM	19	NE2	IMIM	1	2.466	1.324	0.680	1.00	0.00	IMIM
ATOM	20	HE2	IMIM	1	2.550	2.332	0.704	1.00	0.00	IMIM

ATOM	21	CE1	IMIM	1	1.397	0.677	0.189	1.00	0.00	IMIM
ATOM	22	HE1	IMIM	1	0.509	1.122	-0.225	1.00	0.00	IMIM

END

REMARK 1_BENZ_ACET

ATOM	1	CG	BENZ	1	-1.489	0.930	-1.147	1.00	0.00	BENZ
ATOM	2	HG	BENZ	1	-0.763	1.194	-1.907	1.00	0.00	BENZ
ATOM	3	CD1	BENZ	1	-1.071	0.201	-0.027	1.00	0.00	BENZ
ATOM	4	HD1	BENZ	1	-0.024	-0.060	0.105	1.00	0.00	BENZ
ATOM	5	CD2	BENZ	1	-2.839	1.256	-1.326	1.00	0.00	BENZ
ATOM	6	HD2	BENZ	1	-3.153	1.817	-2.201	1.00	0.00	BENZ
ATOM	7	CE1	BENZ	1	-2.015	-0.130	0.954	1.00	0.00	BENZ
ATOM	8	HE1	BENZ	1	-1.694	-0.689	1.825	1.00	0.00	BENZ
ATOM	9	CE2	BENZ	1	-3.775	0.920	-0.341	1.00	0.00	BENZ
ATOM	10	HE2	BENZ	1	-4.821	1.176	-0.472	1.00	0.00	BENZ
ATOM	11	CZ	BENZ	1	-3.366	0.193	0.783	1.00	0.00	BENZ
ATOM	12	HZ	BENZ	1	-4.090	-0.073	1.546	1.00	0.00	BENZ
ATOM	13	C1	ACET	1	3.875	-0.159	-0.885	1.00	0.00	ACET
ATOM	14	H1	ACET	1	4.947	-0.354	-0.864	1.00	0.00	ACET
ATOM	15	H2	ACET	1	3.444	-0.561	-1.804	1.00	0.00	ACET
ATOM	16	H3	ACET	1	3.697	0.919	-0.885	1.00	0.00	ACET
ATOM	17	C2	ACET	1	3.165	-0.793	0.335	1.00	0.00	ACET
ATOM	18	O1	ACET	1	1.900	-0.625	0.362	1.00	0.00	ACET
ATOM	19	O2	ACET	1	3.893	-1.401	1.173	1.00	0.00	ACET

END

REMARK 2_BENZ_ACET

ATOM	1	CG	BENZ	1	-0.895	-0.001	0.305	1.00	0.00	BENZ
ATOM	2	HG	BENZ	1	0.165	-0.001	0.569	1.00	0.00	BENZ
ATOM	3	CD1	BENZ	1	-1.585	-1.207	0.129	1.00	0.00	BENZ
ATOM	4	HD1	BENZ	1	-1.057	-2.143	0.268	1.00	0.00	BENZ
ATOM	5	CD2	BENZ	1	-1.585	1.205	0.127	1.00	0.00	BENZ
ATOM	6	HD2	BENZ	1	-1.057	2.141	0.265	1.00	0.00	BENZ
ATOM	7	CE1	BENZ	1	-2.946	-1.212	-0.200	1.00	0.00	BENZ
ATOM	8	HE1	BENZ	1	-3.470	-2.151	-0.339	1.00	0.00	BENZ
ATOM	9	CE2	BENZ	1	-2.946	1.209	-0.202	1.00	0.00	BENZ
ATOM	10	HE2	BENZ	1	-3.470	2.149	-0.342	1.00	0.00	BENZ
ATOM	11	CZ	BENZ	1	-3.624	-0.001	-0.388	1.00	0.00	BENZ
ATOM	12	HZ	BENZ	1	-4.678	-0.002	-0.644	1.00	0.00	BENZ
ATOM	13	C1	ACET	1	2.494	0.003	-1.296	1.00	0.00	ACET
ATOM	14	H1	ACET	1	3.306	0.006	-2.023	1.00	0.00	ACET
ATOM	15	H2	ACET	1	1.866	-0.876	-1.452	1.00	0.00	ACET
ATOM	16	H3	ACET	1	1.863	0.882	-1.449	1.00	0.00	ACET
ATOM	17	C2	ACET	1	3.042	0.002	0.153	1.00	0.00	ACET
ATOM	18	O1	ACET	1	2.147	-0.001	1.065	1.00	0.00	ACET
ATOM	19	O2	ACET	1	4.300	0.002	0.289	1.00	0.00	ACET

END

REMARK 3_TOLU_ACET

ATOM	1	CB	TOLU	1	0.192	1.085	1.253	1.00	0.00	TOLU
ATOM	2	HB1	TOLU	1	0.435	1.439	2.258	1.00	0.00	TOLU
ATOM	3	HB2	TOLU	1	-0.812	0.664	1.232	1.00	0.00	TOLU
ATOM	4	HB3	TOLU	1	0.173	1.937	0.571	1.00	0.00	TOLU
ATOM	5	CG	TOLU	1	1.190	0.055	0.795	1.00	0.00	TOLU
ATOM	6	CD1	TOLU	1	0.837	-0.858	-0.212	1.00	0.00	TOLU
ATOM	7	HD1	TOLU	1	-0.168	-0.796	-0.625	1.00	0.00	TOLU
ATOM	8	CD2	TOLU	1	2.474	-0.016	1.354	1.00	0.00	TOLU
ATOM	9	HD2	TOLU	1	2.751	0.689	2.134	1.00	0.00	TOLU
ATOM	10	CE1	TOLU	1	1.773	-1.793	-0.667	1.00	0.00	TOLU
ATOM	11	HE1	TOLU	1	1.491	-2.495	-1.445	1.00	0.00	TOLU
ATOM	12	CE2	TOLU	1	3.413	-0.946	0.895	1.00	0.00	TOLU
ATOM	13	HE2	TOLU	1	4.405	-0.979	1.334	1.00	0.00	TOLU
ATOM	14	CZ	TOLU	1	3.056	-1.854	-0.108	1.00	0.00	TOLU
ATOM	15	HZ	TOLU	1	3.777	-2.581	-0.466	1.00	0.00	TOLU
ATOM	16	C1	ACET	1	-4.223	1.143	-0.464	1.00	0.00	ACET
ATOM	17	H1	ACET	1	-4.591	2.050	-0.945	1.00	0.00	ACET
ATOM	18	H2	ACET	1	-4.819	0.283	-0.774	1.00	0.00	ACET
ATOM	19	H3	ACET	1	-4.333	1.245	0.619	1.00	0.00	ACET
ATOM	20	C2	ACET	1	-2.733	0.902	-0.794	1.00	0.00	ACET
ATOM	21	O1	ACET	1	-2.285	-0.248	-0.472	1.00	0.00	ACET
ATOM	22	O2	ACET	1	-2.095	1.868	-1.312	1.00	0.00	ACET

END

REMARK 4_TOLU_ACET

ATOM	1	CB	TOLU	1	4.180	1.382	0.187	1.00	0.00	TOLU
ATOM	2	HB1	TOLU	1	4.216	1.745	1.216	1.00	0.00	TOLU

ATOM	3	HB2	TOLU	1	4.272	2.249	-0.472	1.00	0.00	TOLU
ATOM	4	HB3	TOLU	1	5.052	0.747	0.023	1.00	0.00	TOLU
ATOM	5	CG	TOLU	1	2.901	0.623	-0.071	1.00	0.00	TOLU
ATOM	6	CD1	TOLU	1	2.870	-0.445	-0.979	1.00	0.00	TOLU
ATOM	7	HD1	TOLU	1	3.779	-0.725	-1.504	1.00	0.00	TOLU
ATOM	8	CD2	TOLU	1	1.715	0.961	0.601	1.00	0.00	TOLU
ATOM	9	HD2	TOLU	1	1.727	1.781	1.314	1.00	0.00	TOLU
ATOM	10	CE1	TOLU	1	1.672	-1.119	-1.248	1.00	0.00	TOLU
ATOM	11	HE1	TOLU	1	1.669	-1.945	-1.952	1.00	0.00	TOLU
ATOM	12	CE2	TOLU	1	0.514	0.294	0.338	1.00	0.00	TOLU
ATOM	13	HE2	TOLU	1	-0.414	0.540	0.850	1.00	0.00	TOLU
ATOM	14	CZ	TOLU	1	0.498	-0.774	-0.569	1.00	0.00	TOLU
ATOM	15	HZ	TOLU	1	-0.451	-1.273	-0.738	1.00	0.00	TOLU
ATOM	16	C1	ACET	1	-4.625	0.095	0.104	1.00	0.00	ACET
ATOM	17	H1	ACET	1	-5.111	0.489	0.996	1.00	0.00	ACET
ATOM	18	H2	ACET	1	-4.635	0.876	-0.660	1.00	0.00	ACET
ATOM	19	H3	ACET	1	-5.170	-0.767	-0.280	1.00	0.00	ACET
ATOM	20	C2	ACET	1	-3.156	-0.276	0.405	1.00	0.00	ACET
ATOM	21	O1	ACET	1	-2.669	-1.235	-0.275	1.00	0.00	ACET
ATOM	22	O2	ACET	1	-2.569	0.444	1.275	1.00	0.00	ACET

END

REMARK 5_PHEN_ACET

ATOM	1	CG	PHEN	1	1.692	-1.549	-0.636	1.00	0.00	PHEN
ATOM	2	HG	PHEN	1	1.547	-2.598	-0.865	1.00	0.00	PHEN
ATOM	3	CD1	PHEN	1	0.587	-0.742	-0.330	1.00	0.00	PHEN
ATOM	4	HD1	PHEN	1	-0.432	-1.124	-0.358	1.00	0.00	PHEN
ATOM	5	CD2	PHEN	1	2.984	-1.018	-0.577	1.00	0.00	PHEN
ATOM	6	HD2	PHEN	1	3.845	-1.635	-0.811	1.00	0.00	PHEN
ATOM	7	CE1	PHEN	1	0.767	0.614	-0.041	1.00	0.00	PHEN
ATOM	8	HE1	PHEN	1	-0.108	1.212	0.186	1.00	0.00	PHEN
ATOM	9	CE2	PHEN	1	3.171	0.339	-0.284	1.00	0.00	PHEN
ATOM	10	HE2	PHEN	1	4.173	0.757	-0.233	1.00	0.00	PHEN
ATOM	11	CZ	PHEN	1	2.062	1.133	0.027	1.00	0.00	PHEN
ATOM	12	OH	PHEN	1	2.204	2.478	0.355	1.00	0.00	PHEN
ATOM	13	HH	PHEN	1	3.143	2.698	0.304	1.00	0.00	PHEN
ATOM	14	C1	ACET	1	-4.442	-0.444	0.803	1.00	0.00	ACET
ATOM	15	H1	ACET	1	-4.745	-1.462	1.047	1.00	0.00	ACET
ATOM	16	H2	ACET	1	-4.546	0.205	1.673	1.00	0.00	ACET
ATOM	17	H3	ACET	1	-5.103	-0.063	0.021	1.00	0.00	ACET
ATOM	18	C2	ACET	1	-2.990	-0.412	0.280	1.00	0.00	ACET
ATOM	19	O1	ACET	1	-2.393	0.707	0.367	1.00	0.00	ACET
ATOM	20	O2	ACET	1	-2.545	-1.498	-0.214	1.00	0.00	ACET

END

REMARK 6_PHEN_ACET

ATOM	1	CG	PHEN	1	0.358	0.417	-0.619	1.00	0.00	PHEN
ATOM	2	HG	PHEN	1	-0.644	0.786	-0.828	1.00	0.00	PHEN
ATOM	3	CD1	PHEN	1	0.575	-0.270	0.584	1.00	0.00	PHEN
ATOM	4	HD1	PHEN	1	-0.267	-0.362	1.262	1.00	0.00	PHEN
ATOM	5	CD2	PHEN	1	1.412	0.547	-1.527	1.00	0.00	PHEN
ATOM	6	HD2	PHEN	1	1.260	1.072	-2.464	1.00	0.00	PHEN
ATOM	7	CE1	PHEN	1	1.845	-0.757	0.906	1.00	0.00	PHEN
ATOM	8	HE1	PHEN	1	2.029	-1.288	1.833	1.00	0.00	PHEN
ATOM	9	CE2	PHEN	1	2.692	0.066	-1.213	1.00	0.00	PHEN
ATOM	10	HE2	PHEN	1	3.511	0.171	-1.920	1.00	0.00	PHEN
ATOM	11	CZ	PHEN	1	2.888	-0.622	-0.014	1.00	0.00	PHEN
ATOM	12	OH	PHEN	1	4.132	-1.143	0.343	1.00	0.00	PHEN
ATOM	13	HH	PHEN	1	4.738	-0.985	-0.392	1.00	0.00	PHEN
ATOM	14	C1	ACET	1	-4.672	0.068	0.333	1.00	0.00	ACET
ATOM	15	H1	ACET	1	-5.273	0.796	-0.212	1.00	0.00	ACET
ATOM	16	H2	ACET	1	-4.759	-0.894	-0.179	1.00	0.00	ACET
ATOM	17	H3	ACET	1	-5.045	-0.052	1.350	1.00	0.00	ACET
ATOM	18	C2	ACET	1	-3.186	0.486	0.340	1.00	0.00	ACET
ATOM	19	O1	ACET	1	-2.504	0.120	1.350	1.00	0.00	ACET
ATOM	20	O2	ACET	1	-2.782	1.120	-0.688	1.00	0.00	ACET

END

REMARK 7_CRES_ACET

ATOM	1	CB	CRES	1	0.747	-1.924	-0.713	1.00	0.00	CRES
ATOM	2	HB1	CRES	1	0.421	-2.074	-1.746	1.00	0.00	CRES
ATOM	3	HB2	CRES	1	-0.101	-2.149	-0.061	1.00	0.00	CRES
ATOM	4	HB3	CRES	1	1.557	-2.631	-0.515	1.00	0.00	CRES
ATOM	5	CG	CRES	1	1.215	-0.506	-0.504	1.00	0.00	CRES
ATOM	6	CD1	CRES	1	0.309	0.476	-0.062	1.00	0.00	CRES

ATOM	7	HD1	CRES	1	-0.731	0.208	0.126	1.00	0.00	CRES
ATOM	8	CD2	CRES	1	2.551	-0.137	-0.708	1.00	0.00	CRES
ATOM	9	HD2	CRES	1	3.270	-0.883	-1.036	1.00	0.00	CRES
ATOM	10	CE1	CRES	1	0.723	1.801	0.098	1.00	0.00	CRES
ATOM	11	HE1	CRES	1	0.026	2.557	0.440	1.00	0.00	CRES
ATOM	12	CE2	CRES	1	2.974	1.189	-0.548	1.00	0.00	CRES
ATOM	13	HE2	CRES	1	4.016	1.457	-0.704	1.00	0.00	CRES
ATOM	14	CZ	CRES	1	2.060	2.149	-0.108	1.00	0.00	CRES
ATOM	15	OZ	CRES	1	2.422	3.480	0.090	1.00	0.00	CRES
ATOM	16	HZ	CRES	1	3.372	3.555	-0.072	1.00	0.00	CRES
ATOM	17	C1	ACET	1	-4.296	-2.127	0.259	1.00	0.00	ACET
ATOM	18	H1	ACET	1	-4.475	-3.026	0.849	1.00	0.00	ACET
ATOM	19	H2	ACET	1	-5.087	-1.395	0.428	1.00	0.00	ACET
ATOM	20	H3	ACET	1	-4.311	-2.402	-0.799	1.00	0.00	ACET
ATOM	21	C2	ACET	1	-2.916	-1.521	0.589	1.00	0.00	ACET
ATOM	22	O1	ACET	1	-2.788	-0.274	0.364	1.00	0.00	ACET
ATOM	23	O2	ACET	1	-2.031	-2.329	1.013	1.00	0.00	ACET

END

REMARK 8_CRES_ACET

ATOM	1	CB	CRES	1	-4.138	-1.589	0.381	1.00	0.00	CRES
ATOM	2	HB1	CRES	1	-5.035	-1.136	-0.045	1.00	0.00	CRES
ATOM	3	HB2	CRES	1	-4.338	-1.787	1.438	1.00	0.00	CRES
ATOM	4	HB3	CRES	1	-3.985	-2.552	-0.110	1.00	0.00	CRES
ATOM	5	CG	CRES	1	-2.938	-0.694	0.192	1.00	0.00	CRES
ATOM	6	CD1	CRES	1	-3.075	0.699	0.108	1.00	0.00	CRES
ATOM	7	HD1	CRES	1	-4.063	1.146	0.187	1.00	0.00	CRES
ATOM	8	CD2	CRES	1	-1.645	-1.225	0.074	1.00	0.00	CRES
ATOM	9	HD2	CRES	1	-1.507	-2.302	0.117	1.00	0.00	CRES
ATOM	10	CE1	CRES	1	-1.959	1.531	-0.020	1.00	0.00	CRES
ATOM	11	HE1	CRES	1	-2.070	2.607	-0.086	1.00	0.00	CRES
ATOM	12	CE2	CRES	1	-0.514	-0.414	-0.057	1.00	0.00	CRES
ATOM	13	HE2	CRES	1	0.474	-0.845	-0.189	1.00	0.00	CRES
ATOM	14	CZ	CRES	1	-0.668	0.985	-0.139	1.00	0.00	CRES
ATOM	15	OZ	CRES	1	0.370	1.832	-0.306	1.00	0.00	CRES
ATOM	16	HZ	CRES	1	1.272	1.360	-0.176	1.00	0.00	CRES
ATOM	17	C1	ACET	1	4.599	-0.525	0.419	1.00	0.00	ACET
ATOM	18	H1	ACET	1	5.059	-1.365	-0.100	1.00	0.00	ACET
ATOM	19	H2	ACET	1	5.200	0.376	0.298	1.00	0.00	ACET
ATOM	20	H3	ACET	1	4.551	-0.755	1.485	1.00	0.00	ACET
ATOM	21	C2	ACET	1	3.173	-0.288	-0.096	1.00	0.00	ACET
ATOM	22	O1	ACET	1	2.698	0.879	0.162	1.00	0.00	ACET
ATOM	23	O2	ACET	1	2.587	-1.239	-0.680	1.00	0.00	ACET

END

REMARK 9_INDO_ACET

ATOM	1	CD2	INDO	1	2.196	-0.311	0.334	1.00	0.00	INDO
ATOM	2	CE2	INDO	1	1.038	0.498	0.082	1.00	0.00	INDO
ATOM	3	CZ2	INDO	1	1.111	1.899	0.013	1.00	0.00	INDO
ATOM	4	CH2	INDO	1	2.372	2.487	0.085	1.00	0.00	INDO
ATOM	5	CZ3	INDO	1	3.533	1.704	0.298	1.00	0.00	INDO
ATOM	6	CE3	INDO	1	3.459	0.316	0.384	1.00	0.00	INDO
ATOM	7	CG	INDO	1	1.736	-1.662	0.377	1.00	0.00	INDO
ATOM	8	CD1	INDO	1	0.359	-1.618	0.204	1.00	0.00	INDO
ATOM	9	NE1	INDO	1	-0.055	-0.324	0.029	1.00	0.00	INDO
ATOM	10	HZ2	INDO	1	0.217	2.490	-0.152	1.00	0.00	INDO
ATOM	11	HH2	INDO	1	2.462	3.566	0.026	1.00	0.00	INDO
ATOM	12	HZ3	INDO	1	4.501	2.193	0.344	1.00	0.00	INDO
ATOM	13	HE3	INDO	1	4.359	-0.270	0.549	1.00	0.00	INDO
ATOM	14	HG	INDO	1	2.327	-2.550	0.543	1.00	0.00	INDO
ATOM	15	HD1	INDO	1	-0.383	-2.401	0.180	1.00	0.00	INDO
ATOM	16	HE1	INDO	1	-1.067	-0.038	-0.114	1.00	0.00	INDO
ATOM	17	C1	ACET	1	-4.807	-0.470	-0.679	1.00	0.00	ACET
ATOM	18	H1	ACET	1	-5.386	-1.343	-0.381	1.00	0.00	ACET
ATOM	19	H2	ACET	1	-5.179	0.425	-0.182	1.00	0.00	ACET
ATOM	20	H3	ACET	1	-4.918	-0.325	-1.756	1.00	0.00	ACET
ATOM	21	C2	ACET	1	-3.320	-0.674	-0.361	1.00	0.00	ACET
ATOM	22	O1	ACET	1	-2.613	0.399	-0.338	1.00	0.00	ACET
ATOM	23	O2	ACET	1	-2.905	-1.853	-0.182	1.00	0.00	ACET

END

REMARK 10_INDO_ACET

ATOM	1	CD2	INDO	1	-2.249	0.496	-0.409	1.00	0.00	INDO
ATOM	2	CE2	INDO	1	-0.839	0.402	-0.173	1.00	0.00	INDO
ATOM	3	CZ2	INDO	1	-0.006	1.534	-0.112	1.00	0.00	INDO

ATOM	4	CH2	INDO	1	-0.589	2.764	-0.402	1.00	0.00	INDO
ATOM	5	CZ3	INDO	1	-1.976	2.882	-0.672	1.00	0.00	INDO
ATOM	6	CE3	INDO	1	-2.800	1.760	-0.713	1.00	0.00	INDO
ATOM	7	CG	INDO	1	-2.755	-0.838	-0.357	1.00	0.00	INDO
ATOM	8	CD1	INDO	1	-1.673	-1.655	-0.057	1.00	0.00	INDO
ATOM	9	NE1	INDO	1	-0.528	-0.913	0.056	1.00	0.00	INDO
ATOM	10	HZ2	INDO	1	1.050	1.410	0.102	1.00	0.00	INDO
ATOM	11	HH2	INDO	1	0.022	3.660	-0.375	1.00	0.00	INDO
ATOM	12	HZ3	INDO	1	-2.391	3.859	-0.897	1.00	0.00	INDO
ATOM	13	HE3	INDO	1	-3.861	1.866	-0.918	1.00	0.00	INDO
ATOM	14	HG	INDO	1	-3.777	-1.161	-0.493	1.00	0.00	INDO
ATOM	15	HD1	INDO	1	-1.633	-2.726	0.075	1.00	0.00	INDO
ATOM	16	HE1	INDO	1	0.433	-1.311	0.271	1.00	0.00	INDO
ATOM	17	C1	ACET	1	4.202	-2.012	0.640	1.00	0.00	ACET
ATOM	18	H1	ACET	1	4.155	-2.920	1.241	1.00	0.00	ACET
ATOM	19	H2	ACET	1	4.460	-2.300	-0.381	1.00	0.00	ACET
ATOM	20	H3	ACET	1	4.971	-1.341	1.020	1.00	0.00	ACET
ATOM	21	C2	ACET	1	2.835	-1.314	0.623	1.00	0.00	ACET
ATOM	22	O1	ACET	1	2.812	-0.053	0.651	1.00	0.00	ACET
ATOM	23	O2	ACET	1	1.822	-2.102	0.545	1.00	0.00	ACET

END

REMARK 11_INDO_ACET

ATOM	1	CD2	INDO	1	-2.247	0.498	-0.412	1.00	0.00	INDO
ATOM	2	CE2	INDO	1	-0.838	0.403	-0.175	1.00	0.00	INDO
ATOM	3	CZ2	INDO	1	-0.003	1.533	-0.120	1.00	0.00	INDO
ATOM	4	CH2	INDO	1	-0.583	2.762	-0.419	1.00	0.00	INDO
ATOM	5	CZ3	INDO	1	-1.969	2.881	-0.691	1.00	0.00	INDO
ATOM	6	CE3	INDO	1	-2.795	1.761	-0.726	1.00	0.00	INDO
ATOM	7	CG	INDO	1	-2.757	-0.835	-0.353	1.00	0.00	INDO
ATOM	8	CD1	INDO	1	-1.676	-1.652	-0.046	1.00	0.00	INDO
ATOM	9	NE1	INDO	1	-0.530	-0.912	0.064	1.00	0.00	INDO
ATOM	10	HZ2	INDO	1	1.052	1.409	0.097	1.00	0.00	INDO
ATOM	11	HH2	INDO	1	0.030	3.657	-0.397	1.00	0.00	INDO
ATOM	12	HZ3	INDO	1	-2.382	3.857	-0.924	1.00	0.00	INDO
ATOM	13	HE3	INDO	1	-3.856	1.867	-0.933	1.00	0.00	INDO
ATOM	14	HG	INDO	1	-3.779	-1.156	-0.488	1.00	0.00	INDO
ATOM	15	HD1	INDO	1	-1.640	-2.723	0.093	1.00	0.00	INDO
ATOM	16	HE1	INDO	1	0.429	-1.311	0.282	1.00	0.00	INDO
ATOM	17	C1	ACET	1	4.199	-2.013	0.638	1.00	0.00	ACET
ATOM	18	H1	ACET	1	4.156	-2.923	1.236	1.00	0.00	ACET
ATOM	19	H2	ACET	1	4.450	-2.298	-0.386	1.00	0.00	ACET
ATOM	20	H3	ACET	1	4.970	-1.343	1.015	1.00	0.00	ACET
ATOM	21	C2	ACET	1	2.832	-1.316	0.632	1.00	0.00	ACET
ATOM	22	O1	ACET	1	2.808	-0.055	0.666	1.00	0.00	ACET
ATOM	23	O2	ACET	1	1.818	-2.103	0.557	1.00	0.00	ACET

END

REMARK 12_INDO_ACET

ATOM	1	CD2	INDO	1	-2.236	-0.183	0.000	1.00	0.00	INDO
ATOM	2	CE2	INDO	1	-0.904	-0.716	0.000	1.00	0.00	INDO
ATOM	3	CZ2	INDO	1	-0.655	-2.099	0.000	1.00	0.00	INDO
ATOM	4	CH2	INDO	1	-1.753	-2.955	0.000	1.00	0.00	INDO
ATOM	5	CZ3	INDO	1	-3.077	-2.451	0.000	1.00	0.00	INDO
ATOM	6	CE3	INDO	1	-3.325	-1.081	0.000	1.00	0.00	INDO
ATOM	7	CG	INDO	1	-2.097	1.238	0.000	1.00	0.00	INDO
ATOM	8	CD1	INDO	1	-0.733	1.503	0.000	1.00	0.00	INDO
ATOM	9	NE1	INDO	1	-0.024	0.332	0.000	1.00	0.00	INDO
ATOM	10	HZ2	INDO	1	0.361	-2.476	0.000	1.00	0.00	INDO
ATOM	11	HH2	INDO	1	-1.593	-4.028	0.000	1.00	0.00	INDO
ATOM	12	HZ3	INDO	1	-3.909	-3.147	0.000	1.00	0.00	INDO
ATOM	13	HE3	INDO	1	-4.345	-0.709	0.000	1.00	0.00	INDO
ATOM	14	HG	INDO	1	-2.887	1.974	0.000	1.00	0.00	INDO
ATOM	15	HD1	INDO	1	-0.188	2.434	0.000	1.00	0.00	INDO
ATOM	16	HE1	INDO	1	1.036	0.278	0.000	1.00	0.00	INDO
ATOM	17	C1	ACET	1	4.638	1.510	0.000	1.00	0.00	ACET
ATOM	18	H1	ACET	1	4.950	2.553	0.000	1.00	0.00	ACET
ATOM	19	H2	ACET	1	5.037	1.003	0.880	1.00	0.00	ACET
ATOM	20	H3	ACET	1	5.037	1.003	-0.880	1.00	0.00	ACET
ATOM	21	C2	ACET	1	3.108	1.399	0.000	1.00	0.00	ACET
ATOM	22	O1	ACET	1	2.652	0.196	0.000	1.00	0.00	ACET
ATOM	23	O2	ACET	1	2.426	2.461	0.000	1.00	0.00	ACET

END

REMARK 13_MIND_ACET

ATOM	1	CG	MIND	1	-1.499	-1.463	-0.390	1.00	0.00	MIND
ATOM	2	CB	MIND	1	-2.302	-2.700	-0.644	1.00	0.00	MIND
ATOM	3	HB1	MIND	1	-1.655	-3.579	-0.651	1.00	0.00	MIND
ATOM	4	HB2	MIND	1	-2.815	-2.656	-1.609	1.00	0.00	MIND
ATOM	5	HB3	MIND	1	-3.066	-2.856	0.124	1.00	0.00	MIND
ATOM	6	CD2	MIND	1	-1.978	-0.117	-0.374	1.00	0.00	MIND
ATOM	7	CD1	MIND	1	-0.130	-1.383	-0.164	1.00	0.00	MIND
ATOM	8	HD1	MIND	1	0.624	-2.155	-0.107	1.00	0.00	MIND
ATOM	9	NE1	MIND	1	0.255	-0.080	0.021	1.00	0.00	MIND
ATOM	10	HE1	MIND	1	1.254	0.220	0.213	1.00	0.00	MIND
ATOM	11	CE2	MIND	1	-0.850	0.719	-0.078	1.00	0.00	MIND
ATOM	12	CE3	MIND	1	-3.254	0.476	-0.482	1.00	0.00	MIND
ATOM	13	HE3	MIND	1	-4.131	-0.133	-0.682	1.00	0.00	MIND
ATOM	14	CZ2	MIND	1	-0.964	2.117	-0.008	1.00	0.00	MIND
ATOM	15	HZ2	MIND	1	-0.095	2.732	0.195	1.00	0.00	MIND
ATOM	16	CZ3	MIND	1	-3.368	1.861	-0.397	1.00	0.00	MIND
ATOM	17	HZ3	MIND	1	-4.344	2.327	-0.485	1.00	0.00	MIND
ATOM	18	CH2	MIND	1	-2.236	2.672	-0.135	1.00	0.00	MIND
ATOM	19	HH2	MIND	1	-2.356	3.749	-0.077	1.00	0.00	MIND
ATOM	20	C1	ACET	1	4.973	-0.200	0.942	1.00	0.00	ACET
ATOM	21	H1	ACET	1	5.573	-1.062	0.653	1.00	0.00	ACET
ATOM	22	H2	ACET	1	5.358	0.708	0.480	1.00	0.00	ACET
ATOM	23	H3	ACET	1	5.035	-0.076	2.025	1.00	0.00	ACET
ATOM	24	C2	ACET	1	3.503	-0.411	0.555	1.00	0.00	ACET
ATOM	25	O1	ACET	1	2.789	0.657	0.515	1.00	0.00	ACET
ATOM	26	O2	ACET	1	3.106	-1.591	0.344	1.00	0.00	ACET

END

REMARK 14_MIND_ACET

ATOM	1	CG	MIND	1	-2.620	0.398	0.508	1.00	0.00	MIND
ATOM	2	CB	MIND	1	-4.061	0.476	0.902	1.00	0.00	MIND
ATOM	3	HB1	MIND	1	-4.353	1.513	1.083	1.00	0.00	MIND
ATOM	4	HB2	MIND	1	-4.258	-0.090	1.817	1.00	0.00	MIND
ATOM	5	HB3	MIND	1	-4.720	0.078	0.126	1.00	0.00	MIND
ATOM	6	CD2	MIND	1	-1.872	-0.781	0.225	1.00	0.00	MIND
ATOM	7	CD1	MIND	1	-1.716	1.440	0.387	1.00	0.00	MIND
ATOM	8	HD1	MIND	1	-1.869	2.493	0.579	1.00	0.00	MIND
ATOM	9	NE1	MIND	1	-0.475	0.999	-0.003	1.00	0.00	MIND
ATOM	10	HE1	MIND	1	0.428	1.566	0.065	1.00	0.00	MIND
ATOM	11	CE2	MIND	1	-0.535	-0.364	-0.102	1.00	0.00	MIND
ATOM	12	CE3	MIND	1	-2.220	-2.124	0.219	1.00	0.00	MIND
ATOM	13	HE3	MIND	1	-3.205	-2.506	0.338	1.00	0.00	MIND
ATOM	14	CZ2	MIND	1	0.473	-1.231	-0.542	1.00	0.00	MIND
ATOM	15	HZ2	MIND	1	1.479	-0.877	-0.804	1.00	0.00	MIND
ATOM	16	CZ3	MIND	1	-1.186	-3.008	-0.103	1.00	0.00	MIND
ATOM	17	HZ3	MIND	1	-1.412	-4.059	-0.182	1.00	0.00	MIND
ATOM	18	CH2	MIND	1	0.102	-2.578	-0.549	1.00	0.00	MIND
ATOM	19	HH2	MIND	1	0.857	-3.245	-1.025	1.00	0.00	MIND
ATOM	20	C1	ACET	1	4.193	1.895	0.655	1.00	0.00	ACET
ATOM	21	H1	ACET	1	3.825	2.686	1.296	1.00	0.00	ACET
ATOM	22	H2	ACET	1	4.560	1.069	1.262	1.00	0.00	ACET
ATOM	23	H3	ACET	1	5.031	2.256	0.059	1.00	0.00	ACET
ATOM	24	C2	ACET	1	3.101	1.378	-0.288	1.00	0.00	ACET
ATOM	25	O1	ACET	1	3.438	0.510	-1.116	1.00	0.00	ACET
ATOM	26	O2	ACET	1	1.962	1.936	-0.157	1.00	0.00	ACET

END

REMARK 15_MIND_ACET

ATOM	1	CG	MIND	1	2.560	0.266	-0.119	1.00	0.00	MIND
ATOM	2	CB	MIND	1	4.048	0.420	-0.163	1.00	0.00	MIND
ATOM	3	HB1	MIND	1	4.320	1.437	-0.452	1.00	0.00	MIND
ATOM	4	HB2	MIND	1	4.507	-0.264	-0.884	1.00	0.00	MIND
ATOM	5	HB3	MIND	1	4.503	0.218	0.811	1.00	0.00	MIND
ATOM	6	CD2	MIND	1	1.825	-0.898	0.265	1.00	0.00	MIND
ATOM	7	CD1	MIND	1	1.606	1.238	-0.397	1.00	0.00	MIND
ATOM	8	HD1	MIND	1	1.749	2.262	-0.712	1.00	0.00	MIND
ATOM	9	NE1	MIND	1	0.337	0.741	-0.240	1.00	0.00	MIND
ATOM	10	HE1	MIND	1	-0.555	1.290	-0.405	1.00	0.00	MIND
ATOM	11	CE2	MIND	1	0.436	-0.571	0.142	1.00	0.00	MIND
ATOM	12	CE3	MIND	1	2.184	-2.219	0.608	1.00	0.00	MIND
ATOM	13	HE3	MIND	1	3.228	-2.508	0.687	1.00	0.00	MIND
ATOM	14	CZ2	MIND	1	-0.583	-1.483	0.464	1.00	0.00	MIND
ATOM	15	HZ2	MIND	1	-1.621	-1.182	0.373	1.00	0.00	MIND
ATOM	16	CZ3	MIND	1	1.177	-3.131	0.915	1.00	0.00	MIND

ATOM	17	HZ3	MIND	1	1.440	-4.149	1.187	1.00	0.00	MIND
ATOM	18	CH2	MIND	1	-0.191	-2.772	0.816	1.00	0.00	MIND
ATOM	19	HH2	MIND	1	-0.951	-3.507	1.061	1.00	0.00	MIND
ATOM	20	C1	ACET	1	-4.161	2.659	-0.558	1.00	0.00	ACET
ATOM	21	H1	ACET	1	-5.079	2.092	-0.702	1.00	0.00	ACET
ATOM	22	H2	ACET	1	-4.231	3.210	0.382	1.00	0.00	ACET
ATOM	23	H3	ACET	1	-4.029	3.385	-1.361	1.00	0.00	ACET
ATOM	24	C2	ACET	1	-2.949	1.720	-0.488	1.00	0.00	ACET
ATOM	25	O1	ACET	1	-1.810	2.285	-0.673	1.00	0.00	ACET
ATOM	26	O2	ACET	1	-3.156	0.502	-0.229	1.00	0.00	ACET

END

REMARK 16_IMID_ACET

ATOM	1	CG	IMID	1	1.260	-1.174	-0.337	1.00	0.00	IMID
ATOM	2	HG	IMID	1	0.446	-1.880	-0.349	1.00	0.00	IMID
ATOM	3	CD2	IMID	1	2.627	-1.280	-0.539	1.00	0.00	IMID
ATOM	4	HD2	IMID	1	3.201	-2.166	-0.766	1.00	0.00	IMID
ATOM	5	ND1	IMID	1	1.023	0.150	-0.081	1.00	0.00	IMID
ATOM	6	HD1	IMID	1	0.068	0.575	0.118	1.00	0.00	IMID
ATOM	7	CE1	IMID	1	2.223	0.784	-0.134	1.00	0.00	IMID
ATOM	8	HE1	IMID	1	2.322	1.845	0.033	1.00	0.00	IMID
ATOM	9	NE2	IMID	1	3.236	-0.049	-0.411	1.00	0.00	IMID
ATOM	10	C1	ACET	1	-3.717	0.771	0.491	1.00	0.00	ACET
ATOM	11	H1	ACET	1	-4.381	-0.073	0.672	1.00	0.00	ACET
ATOM	12	H2	ACET	1	-3.788	1.493	1.304	1.00	0.00	ACET
ATOM	13	H3	ACET	1	-4.024	1.274	-0.427	1.00	0.00	ACET
ATOM	14	C2	ACET	1	-2.266	0.297	0.335	1.00	0.00	ACET
ATOM	15	O1	ACET	1	-1.380	1.226	0.406	1.00	0.00	ACET
ATOM	16	O2	ACET	1	-2.056	-0.930	0.126	1.00	0.00	ACET

END

REMARK 17_IMID_ACET

ATOM	1	CG	IMID	1	1.337	1.090	0.310	1.00	0.00	IMID
ATOM	2	HG	IMID	1	0.560	1.817	0.477	1.00	0.00	IMID
ATOM	3	CD2	IMID	1	2.721	1.132	0.370	1.00	0.00	IMID
ATOM	4	HD2	IMID	1	3.352	1.972	0.616	1.00	0.00	IMID
ATOM	5	ND1	IMID	1	1.018	-0.194	-0.044	1.00	0.00	IMID
ATOM	6	HD1	IMID	1	0.031	-0.564	-0.180	1.00	0.00	IMID
ATOM	7	CE1	IMID	1	2.189	-0.868	-0.183	1.00	0.00	IMID
ATOM	8	HE1	IMID	1	2.224	-1.909	-0.459	1.00	0.00	IMID
ATOM	9	NE2	IMID	1	3.260	-0.100	0.061	1.00	0.00	IMID
ATOM	10	C1	ACET	1	-3.778	-0.592	-0.153	1.00	0.00	ACET
ATOM	11	H1	ACET	1	-3.966	-1.246	-1.003	1.00	0.00	ACET
ATOM	12	H2	ACET	1	-4.011	-1.151	0.756	1.00	0.00	ACET
ATOM	13	H3	ACET	1	-4.417	0.288	-0.199	1.00	0.00	ACET
ATOM	14	C2	ACET	1	-2.299	-0.185	-0.115	1.00	0.00	ACET
ATOM	15	O1	ACET	1	-2.013	1.005	0.191	1.00	0.00	ACET
ATOM	16	O2	ACET	1	-1.467	-1.131	-0.378	1.00	0.00	ACET

END

REMARK 18_IMID_ACET

ATOM	1	CG	IMID	1	1.094	-1.297	0.433	1.00	0.00	IMID
ATOM	2	HG	IMID	1	0.189	-1.861	0.582	1.00	0.00	IMID
ATOM	3	CD2	IMID	1	2.443	-1.588	0.574	1.00	0.00	IMID
ATOM	4	HD2	IMID	1	2.894	-2.517	0.888	1.00	0.00	IMID
ATOM	5	ND1	IMID	1	1.037	0.004	0.013	1.00	0.00	IMID
ATOM	6	HD1	IMID	1	0.143	0.542	-0.196	1.00	0.00	IMID
ATOM	7	CE1	IMID	1	2.317	0.446	-0.085	1.00	0.00	IMID
ATOM	8	HE1	IMID	1	2.559	1.448	-0.399	1.00	0.00	IMID
ATOM	9	NE2	IMID	1	3.215	-0.493	0.249	1.00	0.00	IMID
ATOM	10	C1	ACET	1	-3.591	1.256	-0.410	1.00	0.00	ACET
ATOM	11	H1	ACET	1	-4.379	0.505	-0.439	1.00	0.00	ACET
ATOM	12	H2	ACET	1	-3.760	1.917	0.443	1.00	0.00	ACET
ATOM	13	H3	ACET	1	-3.614	1.868	-1.312	1.00	0.00	ACET
ATOM	14	C2	ACET	1	-2.216	0.594	-0.258	1.00	0.00	ACET
ATOM	15	O1	ACET	1	-1.213	1.360	-0.506	1.00	0.00	ACET
ATOM	16	O2	ACET	1	-2.169	-0.611	0.114	1.00	0.00	ACET

END

REMARK 19_IMID_ACET

ATOM	1	CG	IMID	1	2.205	0.857	-0.216	1.00	0.00	IMID
ATOM	2	HG	IMID	1	2.228	1.913	-0.430	1.00	0.00	IMID
ATOM	3	CD2	IMID	1	3.213	-0.079	-0.038	1.00	0.00	IMID
ATOM	4	HD2	IMID	1	4.281	0.075	-0.079	1.00	0.00	IMID
ATOM	5	ND1	IMID	1	1.027	0.174	-0.066	1.00	0.00	IMID
ATOM	6	HD1	IMID	1	0.042	0.566	-0.141	1.00	0.00	IMID

ATOM	7	CE1	IMID	1	1.350	-1.119	0.191	1.00	0.00	IMID
ATOM	8	HE1	IMID	1	0.586	-1.862	0.350	1.00	0.00	IMID
ATOM	9	NE2	IMID	1	2.675	-1.322	0.219	1.00	0.00	IMID
ATOM	10	C1	ACET	1	-3.752	0.738	-0.001	1.00	0.00	ACET
ATOM	11	H1	ACET	1	-4.421	-0.118	-0.074	1.00	0.00	ACET
ATOM	12	H2	ACET	1	-3.944	1.257	0.940	1.00	0.00	ACET
ATOM	13	H3	ACET	1	-3.941	1.441	-0.812	1.00	0.00	ACET
ATOM	14	C2	ACET	1	-2.287	0.285	-0.025	1.00	0.00	ACET
ATOM	15	O1	ACET	1	-1.431	1.216	-0.261	1.00	0.00	ACET
ATOM	16	O2	ACET	1	-2.032	-0.928	0.210	1.00	0.00	ACET

END

REMARK 20_IMID_ACET

ATOM	1	CG	IMID	1	-1.946	1.301	-0.192	1.00	0.00	IMID
ATOM	2	HG	IMID	1	-1.747	2.213	-0.730	1.00	0.00	IMID
ATOM	3	CD2	IMID	1	-3.084	0.821	0.437	1.00	0.00	IMID
ATOM	4	HD2	IMID	1	-4.054	1.289	0.513	1.00	0.00	IMID
ATOM	5	ND1	IMID	1	-0.984	0.342	-0.017	1.00	0.00	IMID
ATOM	6	HD1	IMID	1	0.028	0.387	-0.358	1.00	0.00	IMID
ATOM	7	CE1	IMID	1	-1.554	-0.662	0.696	1.00	0.00	IMID
ATOM	8	HE1	IMID	1	-0.994	-1.539	0.975	1.00	0.00	IMID
ATOM	9	NE2	IMID	1	-2.838	-0.415	0.997	1.00	0.00	IMID
ATOM	10	C1	ACET	1	3.766	-0.178	-0.682	1.00	0.00	ACET
ATOM	11	H1	ACET	1	3.928	0.066	-1.732	1.00	0.00	ACET
ATOM	12	H2	ACET	1	4.140	0.657	-0.088	1.00	0.00	ACET
ATOM	13	H3	ACET	1	4.312	-1.082	-0.415	1.00	0.00	ACET
ATOM	14	C2	ACET	1	2.266	-0.349	-0.410	1.00	0.00	ACET
ATOM	15	O1	ACET	1	1.885	-1.347	0.258	1.00	0.00	ACET
ATOM	16	O2	ACET	1	1.521	0.587	-0.887	1.00	0.00	ACET

END

REMARK 21_IMID_ACET

ATOM	1	CG	IMID	1	-1.984	1.312	0.023	1.00	0.00	IMID
ATOM	2	HG	IMID	1	-1.790	2.371	0.066	1.00	0.00	IMID
ATOM	3	CD2	IMID	1	-3.163	0.582	-0.018	1.00	0.00	IMID
ATOM	4	HD2	IMID	1	-4.176	0.952	-0.015	1.00	0.00	IMID
ATOM	5	ND1	IMID	1	-0.971	0.391	-0.001	1.00	0.00	IMID
ATOM	6	HD1	IMID	1	0.074	0.582	0.018	1.00	0.00	IMID
ATOM	7	CE1	IMID	1	-1.552	-0.835	-0.056	1.00	0.00	IMID
ATOM	8	HE1	IMID	1	-0.955	-1.732	-0.084	1.00	0.00	IMID
ATOM	9	NE2	IMID	1	-2.891	-0.768	-0.068	1.00	0.00	IMID
ATOM	10	C1	ACET	1	3.828	-0.078	0.064	1.00	0.00	ACET
ATOM	11	H1	ACET	1	4.156	0.959	0.117	1.00	0.00	ACET
ATOM	12	H2	ACET	1	4.199	-0.629	0.929	1.00	0.00	ACET
ATOM	13	H3	ACET	1	4.240	-0.552	-0.828	1.00	0.00	ACET
ATOM	14	C2	ACET	1	2.297	-0.176	0.024	1.00	0.00	ACET
ATOM	15	O1	ACET	1	1.795	-1.333	-0.033	1.00	0.00	ACET
ATOM	16	O2	ACET	1	1.654	0.937	0.052	1.00	0.00	ACET

END

REMARK 22_4MIE_ACET

ATOM	1	CB	4MIE	1	3.785	1.758	-0.663	1.00	0.00	4MIE
ATOM	2	HB1	4MIE	1	4.488	1.132	-1.217	1.00	0.00	4MIE
ATOM	3	HB2	4MIE	1	3.565	2.640	-1.268	1.00	0.00	4MIE
ATOM	4	HB3	4MIE	1	4.286	2.088	0.250	1.00	0.00	4MIE
ATOM	5	CG	4MIE	1	2.528	1.011	-0.350	1.00	0.00	4MIE
ATOM	6	ND1	4MIE	1	2.545	-0.145	0.401	1.00	0.00	4MIE
ATOM	7	CD2	4MIE	1	1.225	1.313	-0.718	1.00	0.00	4MIE
ATOM	8	HD2	4MIE	1	0.812	2.123	-1.299	1.00	0.00	4MIE
ATOM	9	CE1	4MIE	1	1.259	-0.522	0.474	1.00	0.00	4MIE
ATOM	10	HE1	4MIE	1	0.874	-1.389	0.983	1.00	0.00	4MIE
ATOM	11	NE2	4MIE	1	0.434	0.328	-0.186	1.00	0.00	4MIE
ATOM	12	HE2	4MIE	1	-0.621	0.233	-0.266	1.00	0.00	4MIE
ATOM	13	C1	ACET	1	-4.145	-1.079	0.318	1.00	0.00	ACET
ATOM	14	H1	ACET	1	-4.391	-2.092	0.633	1.00	0.00	ACET
ATOM	15	H2	ACET	1	-4.554	-0.373	1.043	1.00	0.00	ACET
ATOM	16	H3	ACET	1	-4.595	-0.859	-0.650	1.00	0.00	ACET
ATOM	17	C2	ACET	1	-2.624	-0.889	0.249	1.00	0.00	ACET
ATOM	18	O1	ACET	1	-2.232	0.144	-0.410	1.00	0.00	ACET
ATOM	19	O2	ACET	1	-1.889	-1.719	0.852	1.00	0.00	ACET

END

REMARK 23_4MIE_ACET

ATOM	1	CB	4MIE	1	3.041	2.297	-0.118	1.00	0.00	4MIE
ATOM	2	HB1	4MIE	1	3.737	2.300	-0.960	1.00	0.00	4MIE
ATOM	3	HB2	4MIE	1	2.349	3.132	-0.242	1.00	0.00	4MIE

ATOM	4	HB3	4MIE	1	3.621	2.464	0.792	1.00	0.00	4MIE
ATOM	5	CG	4MIE	1	2.276	1.015	-0.053	1.00	0.00	4MIE
ATOM	6	ND1	4MIE	1	2.907	-0.209	0.047	1.00	0.00	4MIE
ATOM	7	CD2	4MIE	1	0.900	0.843	-0.079	1.00	0.00	4MIE
ATOM	8	HD2	4MIE	1	0.065	1.521	-0.136	1.00	0.00	4MIE
ATOM	9	CE1	4MIE	1	1.902	-1.098	0.082	1.00	0.00	4MIE
ATOM	10	HE1	4MIE	1	2.024	-2.167	0.155	1.00	0.00	4MIE
ATOM	11	NE2	4MIE	1	0.683	-0.506	0.008	1.00	0.00	4MIE
ATOM	12	HE2	4MIE	1	-0.276	-0.954	0.024	1.00	0.00	4MIE
ATOM	13	C1	ACET	1	-4.105	-0.844	0.102	1.00	0.00	ACET
ATOM	14	H1	ACET	1	-4.284	-1.917	0.147	1.00	0.00	ACET
ATOM	15	H2	ACET	1	-4.521	-0.363	0.989	1.00	0.00	ACET
ATOM	16	H3	ACET	1	-4.608	-0.419	-0.767	1.00	0.00	ACET
ATOM	17	C2	ACET	1	-2.604	-0.533	0.020	1.00	0.00	ACET
ATOM	18	O1	ACET	1	-2.272	0.682	-0.068	1.00	0.00	ACET
ATOM	19	O2	ACET	1	-1.810	-1.544	0.054	1.00	0.00	ACET

END

REMARK 24_4MIE_ACET

ATOM	1	CB	4MIE	1	-4.222	-0.161	0.035	1.00	0.00	4MIE
ATOM	2	HB1	4MIE	1	-4.632	-0.836	0.789	1.00	0.00	4MIE
ATOM	3	HB2	4MIE	1	-4.523	0.857	0.289	1.00	0.00	4MIE
ATOM	4	HB3	4MIE	1	-4.676	-0.422	-0.923	1.00	0.00	4MIE
ATOM	5	CG	4MIE	1	-2.731	-0.266	-0.027	1.00	0.00	4MIE
ATOM	6	ND1	4MIE	1	-2.103	-1.458	-0.319	1.00	0.00	4MIE
ATOM	7	CD2	4MIE	1	-1.782	0.727	0.178	1.00	0.00	4MIE
ATOM	8	HD2	4MIE	1	-1.879	1.772	0.423	1.00	0.00	4MIE
ATOM	9	CE1	4MIE	1	-0.793	-1.170	-0.286	1.00	0.00	4MIE
ATOM	10	HE1	4MIE	1	0.018	-1.855	-0.466	1.00	0.00	4MIE
ATOM	11	NE2	4MIE	1	-0.558	0.133	0.009	1.00	0.00	4MIE
ATOM	12	HE2	4MIE	1	0.397	0.590	0.089	1.00	0.00	4MIE
ATOM	13	C1	ACET	1	4.179	0.934	0.297	1.00	0.00	ACET
ATOM	14	H1	ACET	1	4.315	1.922	-0.143	1.00	0.00	ACET
ATOM	15	H2	ACET	1	4.350	1.023	1.372	1.00	0.00	ACET
ATOM	16	H3	ACET	1	4.897	0.230	-0.119	1.00	0.00	ACET
ATOM	17	C2	ACET	1	2.743	0.446	0.064	1.00	0.00	ACET
ATOM	18	O1	ACET	1	2.565	-0.764	-0.248	1.00	0.00	ACET
ATOM	19	O2	ACET	1	1.829	1.334	0.240	1.00	0.00	ACET

END

REMARK 25_4MIE_ACET

ATOM	1	CB	4MIE	1	2.894	2.336	-0.814	1.00	0.00	4MIE
ATOM	2	HB1	4MIE	1	2.756	2.623	-1.858	1.00	0.00	4MIE
ATOM	3	HB2	4MIE	1	2.491	3.136	-0.190	1.00	0.00	4MIE
ATOM	4	HB3	4MIE	1	3.964	2.248	-0.622	1.00	0.00	4MIE
ATOM	5	CG	4MIE	1	2.194	1.046	-0.530	1.00	0.00	4MIE
ATOM	6	ND1	4MIE	1	2.713	-0.164	-0.947	1.00	0.00	4MIE
ATOM	7	CD2	4MIE	1	0.952	0.855	0.055	1.00	0.00	4MIE
ATOM	8	HD2	4MIE	1	0.211	1.520	0.467	1.00	0.00	4MIE
ATOM	9	CE1	4MIE	1	1.778	-1.063	-0.603	1.00	0.00	4MIE
ATOM	10	HE1	4MIE	1	1.853	-2.126	-0.765	1.00	0.00	4MIE
ATOM	11	NE2	4MIE	1	0.709	-0.493	0.007	1.00	0.00	4MIE
ATOM	12	HE2	4MIE	1	-0.203	-0.944	0.313	1.00	0.00	4MIE
ATOM	13	C1	ACET	1	-3.977	-0.957	0.565	1.00	0.00	ACET
ATOM	14	H1	ACET	1	-4.621	-0.087	0.676	1.00	0.00	ACET
ATOM	15	H2	ACET	1	-4.155	-1.420	-0.407	1.00	0.00	ACET
ATOM	16	H3	ACET	1	-4.210	-1.699	1.329	1.00	0.00	ACET
ATOM	17	C2	ACET	1	-2.499	-0.558	0.665	1.00	0.00	ACET
ATOM	18	O1	ACET	1	-1.673	-1.545	0.680	1.00	0.00	ACET
ATOM	19	O2	ACET	1	-2.208	0.669	0.705	1.00	0.00	ACET

END

REMARK 26_4MIM_ACET

ATOM	1	CB	4MIM	1	1.389	1.620	1.959	1.00	0.00	4MIM
ATOM	2	HB1	4MIM	1	0.907	2.490	1.508	1.00	0.00	4MIM
ATOM	3	HB2	4MIM	1	0.701	1.215	2.703	1.00	0.00	4MIM
ATOM	4	HB3	4MIM	1	2.293	1.955	2.471	1.00	0.00	4MIM
ATOM	5	CG	4MIM	1	1.746	0.598	0.931	1.00	0.00	4MIM
ATOM	6	ND1	4MIM	1	0.805	-0.014	0.142	1.00	0.00	4MIM
ATOM	7	HD1	4MIM	1	-0.242	0.156	0.167	1.00	0.00	4MIM
ATOM	8	CD2	4MIM	1	2.961	0.054	0.540	1.00	0.00	4MIM
ATOM	9	HD2	4MIM	1	3.942	0.284	0.930	1.00	0.00	4MIM
ATOM	10	CE1	4MIM	1	1.461	-0.880	-0.674	1.00	0.00	4MIM
ATOM	11	HE1	4MIM	1	0.930	-1.483	-1.391	1.00	0.00	4MIM
ATOM	12	NE2	4MIM	1	2.785	-0.873	-0.467	1.00	0.00	4MIM

ATOM	13	C1	ACET	1	-3.945	0.088	-0.702	1.00	0.00	ACET
ATOM	14	H1	ACET	1	-4.442	-0.712	-1.250	1.00	0.00	ACET
ATOM	15	H2	ACET	1	-4.381	0.200	0.290	1.00	0.00	ACET
ATOM	16	H3	ACET	1	-4.092	1.028	-1.239	1.00	0.00	ACET
ATOM	17	C2	ACET	1	-2.440	-0.186	-0.590	1.00	0.00	ACET
ATOM	18	O1	ACET	1	-1.821	0.513	0.296	1.00	0.00	ACET
ATOM	19	O2	ACET	1	-1.925	-1.031	-1.373	1.00	0.00	ACET

END

REMARK 27_4MIM_ACET

ATOM	1	CB	4MIM	1	1.042	1.530	0.153	1.00	0.00	4MIM
ATOM	2	HB1	4MIM	1	1.245	2.174	-0.707	1.00	0.00	4MIM
ATOM	3	HB2	4MIM	1	-0.038	1.508	0.306	1.00	0.00	4MIM
ATOM	4	HB3	4MIM	1	1.509	1.981	1.033	1.00	0.00	4MIM
ATOM	5	CG	4MIM	1	1.558	0.151	-0.079	1.00	0.00	4MIM
ATOM	6	ND1	4MIM	1	2.849	-0.108	-0.507	1.00	0.00	4MIM
ATOM	7	HD1	4MIM	1	3.537	0.591	-0.743	1.00	0.00	4MIM
ATOM	8	CD2	4MIM	1	0.996	-1.102	0.089	1.00	0.00	4MIM
ATOM	9	HD2	4MIM	1	-0.013	-1.293	0.422	1.00	0.00	4MIM
ATOM	10	CE1	4MIM	1	3.009	-1.466	-0.591	1.00	0.00	4MIM
ATOM	11	HE1	4MIM	1	3.931	-1.925	-0.913	1.00	0.00	4MIM
ATOM	12	NE2	4MIM	1	1.899	-2.102	-0.233	1.00	0.00	4MIM
ATOM	13	C1	ACET	1	-3.868	0.155	-0.290	1.00	0.00	ACET
ATOM	14	H1	ACET	1	-4.310	-0.606	0.353	1.00	0.00	ACET
ATOM	15	H2	ACET	1	-4.574	0.966	-0.465	1.00	0.00	ACET
ATOM	16	H3	ACET	1	-3.633	-0.308	-1.252	1.00	0.00	ACET
ATOM	17	C2	ACET	1	-2.560	0.695	0.326	1.00	0.00	ACET
ATOM	18	O1	ACET	1	-2.242	1.888	0.016	1.00	0.00	ACET
ATOM	19	O2	ACET	1	-1.900	-0.119	1.048	1.00	0.00	ACET

END

REMARK 28_4MIM_ACET

ATOM	1	CB	4MIM	1	-2.363	-1.667	-0.197	1.00	0.00	4MIM
ATOM	2	HB1	4MIM	1	-1.943	-2.269	0.611	1.00	0.00	4MIM
ATOM	3	HB2	4MIM	1	-3.444	-1.813	-0.209	1.00	0.00	4MIM
ATOM	4	HB3	4MIM	1	-1.954	-2.047	-1.135	1.00	0.00	4MIM
ATOM	5	CG	4MIM	1	-2.056	-0.217	-0.016	1.00	0.00	4MIM
ATOM	6	ND1	4MIM	1	-0.773	0.265	0.026	1.00	0.00	4MIM
ATOM	7	HD1	4MIM	1	0.117	-0.305	-0.069	1.00	0.00	4MIM
ATOM	8	CD2	4MIM	1	-2.871	0.896	0.144	1.00	0.00	4MIM
ATOM	9	HD2	4MIM	1	-3.951	0.924	0.167	1.00	0.00	4MIM
ATOM	10	CE1	4MIM	1	-0.851	1.611	0.202	1.00	0.00	4MIM
ATOM	11	HE1	4MIM	1	0.037	2.218	0.265	1.00	0.00	4MIM
ATOM	12	NE2	4MIM	1	-2.116	2.043	0.280	1.00	0.00	4MIM
ATOM	13	C1	ACET	1	3.784	-1.319	-0.110	1.00	0.00	ACET
ATOM	14	H1	ACET	1	4.619	-0.636	-0.259	1.00	0.00	ACET
ATOM	15	H2	ACET	1	3.906	-1.827	0.849	1.00	0.00	ACET
ATOM	16	H3	ACET	1	3.770	-2.081	-0.889	1.00	0.00	ACET
ATOM	17	C2	ACET	1	2.453	-0.555	-0.099	1.00	0.00	ACET
ATOM	18	O1	ACET	1	1.402	-1.287	-0.218	1.00	0.00	ACET
ATOM	19	O2	ACET	1	2.482	0.698	0.049	1.00	0.00	ACET

END