Table S4. Force Field Parameters Added to the AMBER Parameter Set (Version 1.6, 21-May-96) and Gasteiger-Marsili Charges for ACRAMTU.

Atom Types

identifier	element	connectivity
CZ	carbon	sp^2 hybridized thiourea carbon attached to sp^2 sulfur
ST	sulfur	sp^2 hybridized thiourea sulfur attached to sp^2 carbon

Bond Stretch Deformation

bond	r_0 (Å)	K_r (kcal $mol^{-1}Å^{-2}$)
NT-CA	1.3190	477.0000
NT-H	0.9100	434.0000
CT-NT	1.4630	337.0000
NT-CZ	1.3530	488.0000
CZ-ST	1.6880	222.0000

Angle Bond Deformation

Angle	θ_0 (deg)	K_θ (kcal $mol^{-1}rad^{-2}$)
CA-NA-CA	123.2000	70.0000
NA-CA-CA	119.9000	70.0000
CA-CA-NT	120.0000	70.0000
CA-NT-CT	128.7000	80.0000
CA-NT-H2	119.0000	35.0000
H2-NT-CT	118.5500	35.0000
NT-CT-CT	111.1000	80.0000
NT-CT-HC	109.0000	35.0000
CT-NT-CZ	122.9000	50.0000
NT-CZ-ST	121.2500	35.0000
NT-CZ-NT	119.3730	60.0000
CZ-NT-H2	118.5500	35.0000
CT-NT-CT	114.8000	70.0000
CT-N2-H2	118.5500	35.0000
CA-CA-N2	120.0000	70.0000

Table S4, contd.

Torsional Deformation

torsional angle	V_2	ϕ_0 (deg)
CA-CA-NT-CT	16.0000	180.0
CA-CA-CA-CA	10.0000	180.0
CA-CA-CA-HC	10.0000	180.0
CA-CA-NT-H	0.0000	180.0
CA-NT-CT-CT	0.0000	180.0
CA-NT-CT-HC	0.0000	180.0
H2-NT-CT-CT	0.0000	180.0
H2-NT-CT-HC	0.0000	180.0
CT-CT-NT-CZ	0.0000	180.0
CT-CT-NT-CT	0.0000	180.0
HC-CT-NT-CZ	0.0000	180.0
CT-NT-CZ-ST	10.0000	180.0
CT-NT-CZ-NT	10.0000	180.0
CT-NT-CT-HC	0.0000	180.0
NT-CZ-NT-H2	0.0000	180.0
ST-CZ-NT-H2	10.0000	180.0
NT-CA-CA-CA	10.0000	180.0

Improper Torsional Deformation

improper angle	χ_0 (deg)	n	K_χ (kcal mol^{-1})
H-NT-**-**[a]	3.0000	2	180.0000
-NT--**	4.0000	2	180.0000
CA-CA-CA-CA	4.0000	2	180.0000
H-NT-CZ-CT	0.0000	2	180.0000
HC-CA-CA-CA	0.0000	2	180.0000
CZ-NT-CT-CT	0.0000	2	180.0000
CA-CA-CA-N2	0.0000	2	180.0000
ST-CZ-NT-NT	7.0000	2	180.0000
-CZ--**	0.0000	2	180.0000
--CA-HC	4.0000	2	180.0000

[a] ** Denotes any atom type.

Nonbond Interaction

atom type	r_j* (Å)	ε* (kcal/mol)
CZ	3.2000	0.10000
ST	4.0000	0.20000

Table S4, contd.

Partial Charges for ACRAMTU

atom no. in pdb file	atom type	charge (e)
C1	CT	0.082
H11	HC	0.065
H12	HC	0.066
H13	HC	0.065
C1	CZ	0.460
S2	ST	-0.807
N3	NT	-0.399
H3	H2	0.278
C1	CT	0.120
H11	HC	0.073
H12	HC	0.073
C2	CT	0.130
H21	HC	0.076
H22	HC	0.073
C1	CA	-0.048
C2	CA	-0.027
C3	CA	-0.073
C4	CA	-0.020
C4A	CA	0.057
C9A	CA	0.234
C10	CA	0.324
C10A	CA	0.058
C8A	CA	0.236
N9	NA	-0.344
C5	CA	-0.021
C6	CA	-0.076
C7	CA	-0.026
C8	CA	-0.051
H1	HC	0.055
H2	HC	0.051
H3	HC	0.044
H4	HC	0.055
H5	HC	0.060
H6	HC	0.044
H7	HC	0.051
H8	HC	0.055
H9	HC	0.260
N1	N2	-0.426
H1	H2	0.274
N1	NT	-0.371
C1	CT	0.079
H11	HC	0.066
H12	HC	0.065
H13	HC	0.065