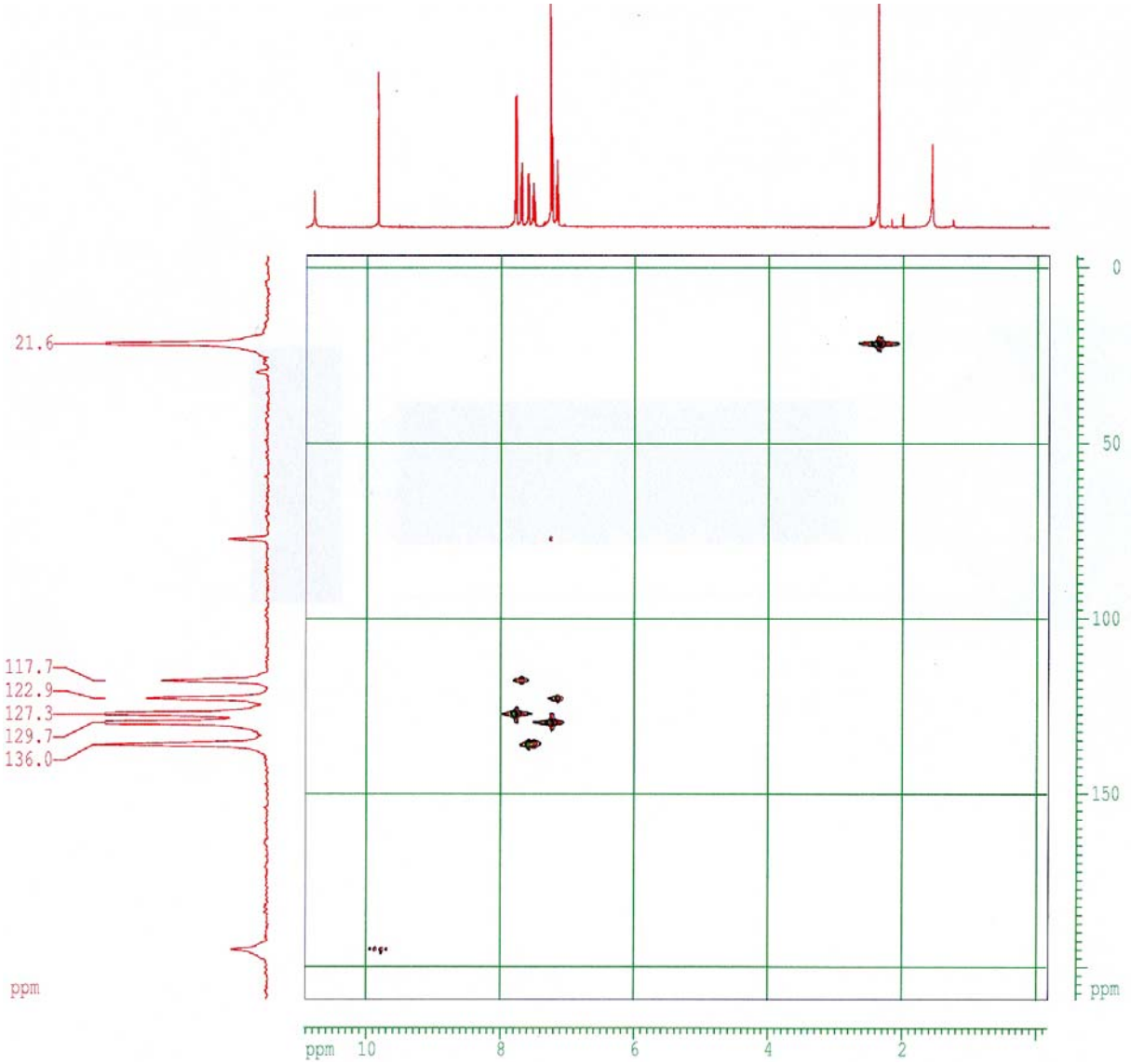

Figure S1 HMQC spectrum of **B** in $CDCl_3$

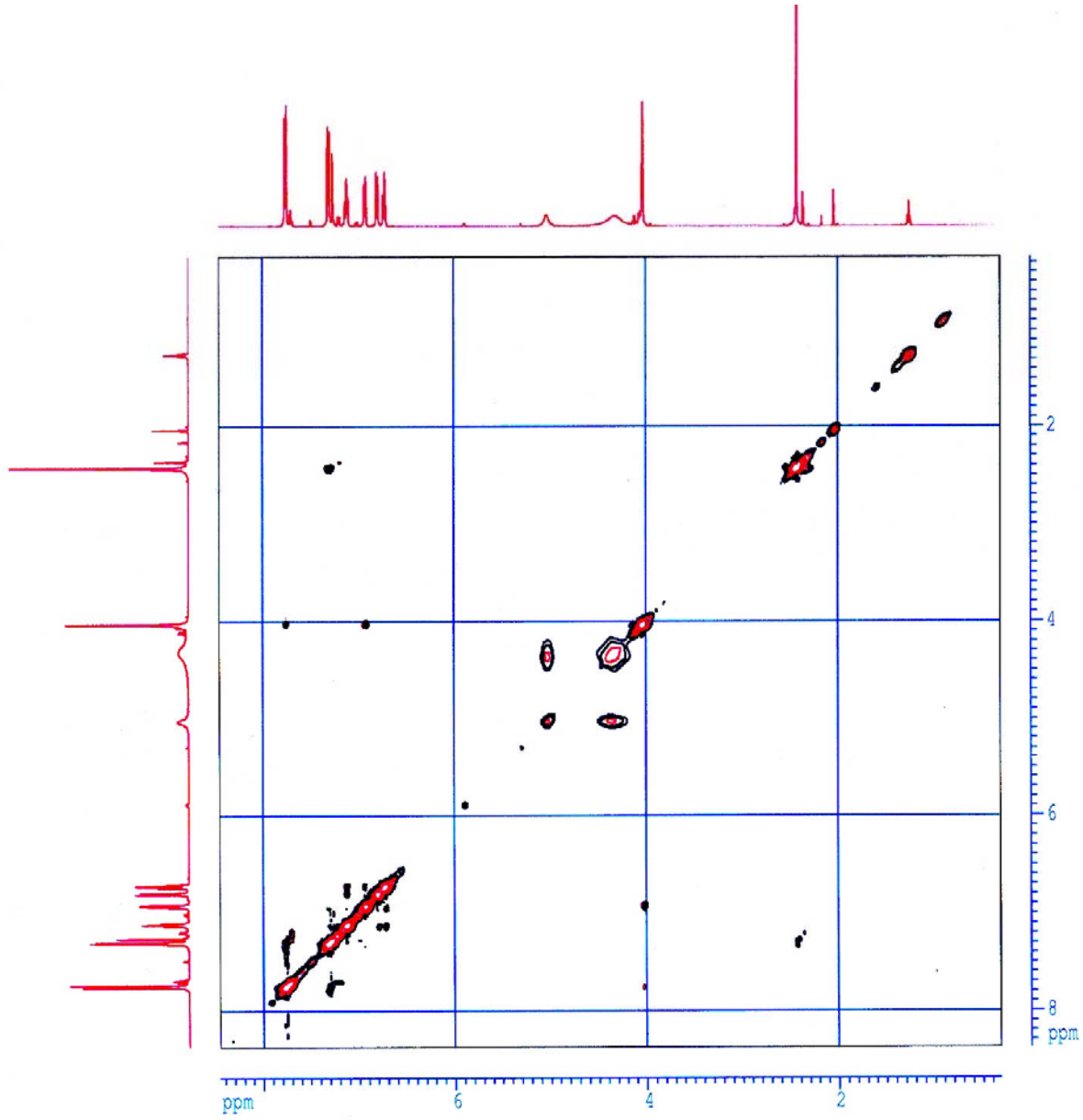

Figure S2 Representation of a NOESY spectrum of **A** in $CDCl_3$

Packing schemes

Table S1. A

```
=============================================================================================================================
  6-Membered Ring ( 1)   C(1)   -->   C(2)   -->   C(3)   -->   C(4)   -->   C(5)   -->   C(6)   -->
=============================================================================================================================
  6-Membered Ring ( 2)   C(8)   -->   C(9)   -->   C(10)  -->   C(11)  -->   C(12)  -->   C(13)  -->
=============================================================================================================================
Analysis of Short Ring-Interactions with Cg-Cg Distances <   6.0 Angstrom and Beta < 60.0 Deg.
=============================================================================================================================
- Cg(I)    = Plane number I (= ring number in () above)
- Alpha    = Dihedral Angle between Planes I and J (Deg)
- Beta     = Angle Cg(I)-->Cg(J) or Cg(I)-->Me vector and normal to plane I (Deg)
- Gamma    = Angle Cg(I)-->Cg(J) vector and normal to plane J (Deg)
- Cg-Cg    = Distance between ring Centroids (Ang.)
- CgI_Perp = Perpendicular distance of Cg(I) on ring J (Ang.)
- CgJ_Perp = Perpendicular distance of Cg(J) on ring I (Ang.)
- Slippage = Distance between Cg(I) and Perpendicular Projection of Cg(J) on Ring I (Ang).
- P,Q,R,S  = J-Plane Parameters for Carth. Coord. (Xo, Yo, Zo)

Cg(I) Res(I)   Cg(J)  [   ARU(J)]       Cg-Cg   Transformed J-Plane P, Q, R, S   Alpha    Beta   Gamma CgI_Perp CgJ_Perp Slippage

Cg(1)  [ 1] -> Cg(1)  [  3756.01]    5.686(3)  -0.6865-0.7212 0.0928   -8.6720    0.00   53.78   53.78   3.359   3.359   4.587
Cg(1)  [ 1] -> Cg(2)  [  2656.01]    5.982(3)  -0.1687 0.5192-0.8378  -13.7130   70.34   53.58   67.98   2.243   3.552
Cg(2)  [ 1] -> Cg(1)  [  2656.01]    5.402(3)  -0.6865 0.7212 0.0928   -0.0086   70.34   14.10   83.52   0.609   5.239
Cg(2)  [ 1] -> Cg(1)  [  3656.01]    5.510(3)  -0.6865-0.7212 0.0928    0.3781   65.63   38.80   77.78   1.166   4.294
                                      -------                                    ------------------------------------
                           Min or Max  5.402                                      0.00   14.10   83.52   0.609   3.359
[  3756] = 2-X,-Y,1-Z
[  2656] = 3/2-X,1/2+Y,3/2-Z
[  3656] = 1-X,-Y,1-Z
=============================================================================================================================
Analysis of Y-X...Cg(Pi-Ring) Interactions (X..Cg < 4.0 Ang. - Gamma <  30.0 Deg)
=============================================================================================================================

   Y--X(I)    Res(I)   Cg(J)  [   ARU(J)]       X..Cg  Transformed J-Plane P, Q, R, S  X-Perp Gamma      Y-X..Cg        Y..Cg Y-X,Pi

S(1)   -O(1)   [ 1] -> Cg(1)  [  1565.01]    3.571(4)   0.6865 0.7212-0.0928   9.4743  3.418  16.82   112.06(16)     4.314(3)  34.39
                                           -------                                 ------------------------------------------
                                  Min or Max  3.571                                  3.418  16.82       112.06        4.314  34.39
[  1565] = X,1+Y,Z
```

The Cg(I) refer to the Ring Centre-of-Gravity numbers given in () in the Ring-Analysis above

Cg(I)	x	y	z	Xo	Yo	Zo
Cg(1)	0.90667(14)	-0.0789(4)	0.62308(11)	9.7641(19)	-0.455(2)	11.442(2)
Cg(2)	0.36770(15)	0.0204(4)	0.63780(11)	2.607(2)	0.118(2)	11.712(2)

Summary of Shortest Inter Contacts with d(I-J) < R(I) + R(J) + 0.2 of Residue # 1 to Neighbouring ARU'S

Nr	ARU	Nr.Cont.	d(min)	Del	XHn	X - At(I)		At(J) - Y	YHn	Note	Partaking ARU's in Close Contact Resd.
1	[2656.01]	5	2.0200	-0.70	0	S(1) - O(1)	...	H(1A) -N(1)	1	<<	2656.01
2	[3666.01]	9	2.2500	-0.47	2	N(2) - H(2A)	...	O(2) -S(1)	0	<<	3666.01
3	[2646.01]	5	2.0200	-0.70	1	N(1) - H(1A)	...	O(1) -S(1)	0	<<	2646.01
4	[1455.01]	3	2.4400	0.04	1	C(10) - H(10)	...	H(40C) -C(40)	3		1455.01
5	[3656.01]	2	2.9500	0.05	1	C(2) - H(2)	...	C(12) -C(11)	1		3656.01
6	[3746.01]	2	2.2800	-0.12	3	C(40) - H(40A)	...	H(3) -C(3)	1	<	3746.01
7	[1655.01]	3	2.4400	0.04	3	C(40) - H(40C)	...	H(10) -C(10)	1		1655.01

Symbols :: < denotes contacts less than the sum of the van der Waals Radii and << contacts less than this sum minus 0.2 Angstrom.
Nr.Cont. = Number of short contacts from current ARU to surrounding ARU's (from list above).

Analysis of Potential Hydrogen Bonds and Schemes with d(D...A) < R(D)+R(A)+0.50, d(H...A) < R(H)+R(A)-0.12 Ang., D-H...A > 100.0 Deg

Note: - ARU codes in [] are with reference to the Coordinates printed above (Possibly transformed, when MOVE .NE. 1.555)

Nr	Typ	Res	Donor	---	H....Acceptor	[ARU]	D - H	H...A	D...A	D - H...A	A..H..A*	A'..H..A"	Sum(XY,YZ)	Sum(XZ)
1		1	N(1)	--H(1A)	..O(1)	[2646.01]	0.99(4)	2.02(4)	2.996(5)	169(3)				
2		1	N(2)	--H(2A)	..O(2)	[3666.01]	0.87(6)	2.25(6)	3.092(6)	165(5)				
3	Intra	1	N(2)	--H(2B)	..O(2)	[ ]	0.78(5)	2.47(5)	3.238(6)	170(6)				
4	Intra	1	C(2)	--H(2)	..O(2)	[ ]	0.93	2.53	2.893(7)	104				
5	Intra	1	C(7)	--H(7B)	..O(2)	[ ]	0.97	2.57	2.994(5)	106				

Translation of ARU-code to Equivalent Position Code

[3666.] = 1-x,1-y,1-z
[2646.] = 3/2-x,-1/2+y,3/2-z

For C--H...Acceptor Interactions See: Th. Steiner, Cryst. Rev, (1996), 6, 1-57

H-Bond classification [G.A.Jeffrey, H.Maluszynska & J.Mitra., Int.J.Biol.Macromol.(1985),7,336-348]

2-Centre (linear) D-H...X most prob. angle 160 deg - also: G.A.Jeffrey & W.Saenger, Hydrogen Bonding in Biological Structures
3-Centre (bifurcated) SUM of 3 angl. about H = 360 deg Springer-Verlag, Berlin, 1991, pp 20.
4-Centre (trifurcated)

Table S2. T_a

```
==========================================================================================================================
  6-Membered Ring ( 1)   C(1)   -->   C(2)   -->   C(3)   -->   C(4)   -->   C(5)   -->   C(6)   -->
==========================================================================================================================
  6-Membered Ring ( 2)   C(8)   -->   C(9)   -->   C(10)  -->   C(11)  -->   C(12)  -->   C(13)  -->
==========================================================================================================================
  6-Membered Ring ( 3)   C(15)  -->   C(16)  -->   C(17)  -->   C(18)  -->   C(19)  -->   C(20)  -->
==========================================================================================================================
  6-Membered Ring ( 4)   C(21)  -->   C(22)  -->   C(23)  -->   C(24)  -->   C(25)  -->   C(26)  -->
==========================================================================================================================


Analysis of Short Ring-Interactions with Cg-Cg Distances <   6.0 Angstrom and Beta < 60.0 Deg.
==========================================================================================================================
Cg(I) Res(I)   Cg(J)  [   ARU(J)]       Cg-Cg   Transformed J-Plane P, Q, R, S   Alpha    Beta   Gamma CgI_Perp CgJ_Perp Slippage

Cg(1)  [ 1] -> Cg(2)  [  2755.01]    4.786(3)  -0.8033 0.4675-0.3690   -8.7594   50.68    4.02   53.13   2.872   4.774
Cg(1)  [ 1] -> Cg(4)  [  2754.01]    4.059(3)  -0.4448-0.1338-0.8856    4.5104    1.29   21.03   21.22   3.784   3.788
Cg(2)  [ 1] -> Cg(1)  [  2755.01]    4.786(3)  -0.4457-0.1114-0.8882   -8.5542   50.68   53.13    4.02   4.774   2.872
Cg(2)  [ 1] -> Cg(2)  [  2655.01]    4.691(3)  -0.8033 0.4675-0.3690   -1.6928    0.02   38.30   38.30   3.681   3.681   2.907
Cg(2)  [ 1] -> Cg(2)  [  2755.01]    5.023(3)  -0.8033 0.4675-0.3690   -8.7594    0.02   47.62   47.62   3.386   3.386   3.711
Cg(2)  [ 1] -> Cg(3)  [  2765.01]    4.871(3)  -0.8315 0.5490 0.0850   -1.7673   26.72   44.14   46.88   3.330   3.495
Cg(3)  [ 1] -> Cg(2)  [  2765.01]    4.871(3)  -0.8033 0.4675-0.3690   -2.2571   26.72   46.88   44.14   3.495   3.330
Cg(3)  [ 1] -> Cg(3)  [  2765.01]    4.973(3)  -0.8315 0.5490 0.0850   -1.7673    0.00   42.40   42.40   3.672   3.672   3.353
Cg(3)  [ 1] -> Cg(3)  [  2865.01]    4.004(3)  -0.8315 0.5490 0.0850   -9.0816    0.00   24.56   24.56   3.642   3.642   1.664
Cg(4)  [ 1] -> Cg(1)  [  2754.01]    4.059(3)  -0.4457-0.1114-0.8882    2.2141    1.29   21.22   21.03   3.789   3.784
Cg(4)  [ 1] -> Cg(3)  [  1555.01]    5.322(3)   0.8315-0.5490-0.0850    5.4396   77.23   42.35   64.82   2.264   3.933
Cg(4)  [ 1] -> Cg(3)  [  2865.01]    5.031(3)  -0.8315 0.5490 0.0850   -9.0816   77.23    3.17   74.11   1.378   5.023
                                      -------                                  ---------------------------------------
                           Min or Max  4.004                                     0.00    3.17   74.11   1.378   2.872
[  2755] = 2-X,-Y,-Z
[  2754] = 2-X,-Y,-1-Z
[  2655] = 1-X,-Y,-Z
[  2765] = 2-X,1-Y,-Z
[  2865] = 3-X,1-Y,-Z
[  1555] = X,Y,Z

The Cg(I) refer to the Ring Centre-of-Gravity numbers given in () in the Ring-Analysis above

Cg(I)          x              y              z                Xo              Yo              Zo
Cg(1)      0.87898(13)    -0.20205(9)    -0.38002(7)       9.2534(12)     -0.9022(10)    -5.3321(10)
Cg(2)      0.77542(11)     0.06055(9)     0.06681(7)       6.5060(10)      0.4243(10)     0.9374(10)
Cg(3)      1.29368(11)     0.53630(9)     0.02266(7)      10.2854(10)      5.6195(10)     0.3180(10)
Cg(4)      1.28888(14)    0.31640(14)    -0.33278(8)      11.7250(13)      4.4475(15)    -4.6693(11)
```

Summary of Shortest Inter Contacts with d(I-J) < R(I) + R(J) + 0.2 of Residue # 1 to Neighbouring ARU'S

Nr	ARU	Nr.Cont.	d(min)	Del	XHn	X - At(I)		At(J) - Y	YHn	Note	Partaking ARU's in Close Contact Resd.
1	[1455.01]	3	2.5500	-0.17	0	S(1) - O(2)	...	H(25) -C(25)	1	<	1455.01
2	[1565.01]	2	2.6400	-0.08	0	S(2) - O(4)	...	H(5) -C(5)	1	<	1565.01
3	[2765.01]	8	2.7500	0.03	1	C(14) - H(14)	...	O(4) -S(2)	0		2765.01
4	[1545.01]	2	2.6400	-0.08	1	C(5) - H(5)	...	O(4) -S(2)	0	<	1545.01
5	[2755.01]	11	2.8000	-0.10	2	C(7) - H(7B)	...	C(13) -N(2)	0	<	2755.01
6	[1445.01]	4	2.3500	-0.05	1	C(9) - H(9)	...	H(18) -C(18)	1	<	1445.01
7	[2754.01]	3	2.4300	0.03	1	C(3) - H(3)	...	H(3) -C(3)	1		2754.01
8	[2865.01]	4	2.9400	0.04	1	C(17) - H(17)	...	C(25) -C(24)	0		2865.01
9	[2854.01]	2	3.5800	0.18	0	C(24) - C(240)	...	C(40) -C(4)	0		2854.01
10	[1665.01]	4	2.3500	-0.05	1	C(18) - H(18)	...	H(9) -C(9)	1	<	1665.01
11	[1655.01]	3	2.5500	-0.17	1	C(25) - H(25)	...	O(2) -S(1)	0	<	1655.01

Symbols :: < denotes contacts less than the sum of the van der Waals Radii and << contacts less than this sum minus 0.2 Angstrom.
Nr.Cont. = Number of short contacts from current ARU to surrounding ARU's (from list above).

Analysis of Potential Hydrogen Bonds and Schemes with d(D...A) < R(D)+R(A)+0.50, d(H...A) < R(H)+R(A)-0.12 Ang., D-H...A > 100.0 Deg

Note: - ARU codes in [] are with reference to the Coordinates printed above (Possibly transformed, when MOVE .NE. 1.555)

Nr	Typ	Res	Donor	---	H....Acceptor	[ARU]	D - H	H...A	D...A	D - H...A	A..H..A*	A'..H..A"	Sum(XY,YZ)	Sum(XZ)
1	Intra	1	N(1)	--H(1A)	..O(3)	[ ]	0.82(3)	2.38(3)	3.137(3)	154(3)				
2	Intra	1	N(3)	--H(3A)	..N(2)	[ ]	0.82(3)	1.93(3)	2.634(3)	143(3)				
3	Intra	1	C(6)	--H(6)	..O(1)	[ ]	0.93	2.50	2.879(4)	104				
4	Intra	1	C(7)	--H(7A)	..N(2)	[ ]	0.97	2.46	2.867(3)	105				
5	Intra	1	C(22)	--H(22)	..O(4)	[ ]	0.93	2.49	2.868(4)	104				
6		1	C(25)	--H(25)	..O(2)	[1655.01]	0.93	2.55	3.465(5)	167				

Translation of ARU-code to Equivalent Position Code

[1655.] = 1+x,y,z

Table S3. T_c

6-Membered Ring (1) C(1) --> C(2) --> C(3) --> C(4) --> C(5) --> C(6) -->

6-Membered Ring (2) C(8) --> C(9) --> C(10) --> C(11) --> C(12) --> C(13) -->

6-Membered Ring (3) C(15) --> C(16) --> C(17) --> C(18) --> C(19) --> C(20) -->

6-Membered Ring (4) C(21) --> C(22) --> C(23) --> C(24) --> C(25) --> C(26) -->

Analysis of Short Ring-Interactions with Cg-Cg Distances < 6.0 Angstrom and Beta < 60.0 Deg.

Cg(I)	Res(I)	Cg(J)	ARU(J)]	Cg-Cg	Transformed J-Plane P, Q, R, S	Alpha	Beta	Gamma	CgI_Perp	CgJ_Perp	Slippage
Cg(1)	[1] ->	Cg(2)	[1555.01]	5.5425(15)	-0.0169 0.7273-0.6861 -1.9467	46.11	31.74	64.26	2.407	4.713	
Cg(1)	[1] ->	Cg(2)	[2766.01]	5.3704(15)	0.0169-0.7273 0.6861 1.2461	46.11	40.38	54.64	3.108	4.091	
Cg(1)	[1] ->	Cg(3)	[2656.01]	4.3304(14)	0.3646 0.6265-0.6890 -6.9438	23.59	37.07	20.70	4.051	3.455	
Cg(2)	[1] ->	Cg(1)	[2766.01]	5.3703(15)	-0.6784-0.3702 0.6346 -7.2056	46.11	54.64	40.38	4.091	3.108	
Cg(2)	[1] ->	Cg(3)	[2655.01]	5.1442(14)	0.3646 0.6265-0.6890 3.6213	22.76	42.20	57.30	2.779	3.811	
Cg(2)	[1] ->	Cg(4)	[2656.01]	5.8982(14)	-0.7934 0.6081 0.0277 -6.5943	64.11	30.79	75.35	1.492	5.067	
Cg(3)	[1] ->	Cg(1)	[2656.01]	4.3304(14)	-0.6784-0.3702 0.6346 1.1481	23.59	20.70	37.07	3.455	4.051	
Cg(3)	[1] ->	Cg(2)	[2655.01]	5.1443(14)	0.0169-0.7273 0.6861 -1.7741	22.76	57.30	42.20	3.811	2.779	
Cg(3)	[1] ->	Cg(3)	[2655.01]	5.1320(12)	0.3646 0.6265-0.6890 3.6213	0.00	46.66	46.66	3.522	3.522	3.733
Cg(3)	[1] ->	Cg(4)	[1555.01]	5.1954(15)	0.7934-0.6081-0.0277 1.5915	85.84	52.30	41.91	3.867	3.177	
Cg(4)	[1] ->	Cg(1)	[2656.01]	4.8704(16)	-0.6784-0.3702 0.6346 1.1481	70.69	16.69	77.11	1.086	4.665	
Cg(4)	[1] ->	Cg(2)	[1455.01]	4.9205(15)	-0.0169 0.7273-0.6861 -1.7741	64.11	21.24	69.96	1.686	4.586	
Cg(4)	[1] ->	Cg(3)	[1555.01]	5.1953(15)	-0.3646-0.6265 0.6890 -0.0993	85.84	41.91	52.30	3.177	3.867	
				Min or Max 4.330		0.00	16.69	77.11	1.086	2.779	

Analysis of X-H...Cg(Pi-Ring) Interactions (H..Cg < 3.0 Ang. - Gamma < 30.0 Deg)

X--H(I)	Res(I)	Cg(J)	ARU(J)]	H..Cg	Transformed J-Plane P, Q, R, S	H-Perp	Gamma	X-H..Cg	X..Cg	X-H,Pi
C(5) -H(5)	[1] ->	Cg(4)	[2656.01]	2.78	-0.7934 0.6081 0.0277 -6.5943	2.764	5.49	147	3.593(3)	56
C(12) -H(12)	[1] ->	Cg(4)	[1655.01]	3.00	0.7934-0.6081-0.0277 9.6886	2.938	11.20	135	3.715(2)	45
			Min or Max	2.780		2.764	5.49	147.00	3.593	56.00

[1555] = X,Y,Z
[2766] = 2-X,1-Y,1-Z
[2656] = 1-X,-Y,1-Z
[2655] = 1-X,-Y,-Z
[1455] = -1+X,Y,Z
[1655] = 1+X,Y,Z

The Cg(I) refer to the Ring Centre-of-Gravity numbers given in () in the Ring-Analysis above

Cg(I)	x	y	z	Xo	Yo	Zo
Cg(1)	0.65170(12)	0.38244(9)	0.68848(8)	4.5069(12)	2.3118(9)	8.6858(10)
Cg(2)	0.87465(10)	0.22548(10)	0.33748(8)	7.7447(11)	1.5198(10)	4.2575(10)
Cg(3)	0.39993(10)	-0.24893(8)	0.01092(8)	4.9251(11)	-2.5561(8)	0.1377(9)
Cg(4)	0.01592(10)	-0.16192(10)	0.21850(7)	0.4568(11)	-2.1468(10)	2.7566(9)

Summary of Shortest Inter Contacts with d(I-J) < R(I) + R(J) + 0.2 of Residue # 1 to Neighbouring ARU'S

Nr	ARU	Nr.Cont.	d(min)	Del	XHn X - At(I)		At(J) - Y	YHn	Note	Partaking ARU's in Close Contact Resd.
1	[2656.01]	16	1.9900	-0.73	1 N(1) - H(1)	...	O(2) -S(1)	0	<<	2656.01
2	[1455.01]	5	2.5800	0.18	1 C(25) - H(25)	...	H(16) -C(16)	1		1455.01
3	[2556.01]	2	2.7100	-0.01	3 C(240) - H(24A)	...	O(1) -S(1)	0	<	2556.01
4	[2666.01]	4	2.5300	-0.19	1 C(3) - H(3A)	...	O(3) -S(2)	0	<	2666.01
5	[2655.01]	10	2.6900	-0.03	1 C(12) - H(12)	...	O(4) -S(2)	0	<	2655.01
6	[2555.01]	4	2.8800	0.16	1 C(26) - H(26)	...	O(4) -S(2)	0		2555.01
7	[1655.01]	5	2.5800	0.18	1 C(16) - H(16)	...	H(25) -C(25)	1		1655.01
8	[2766.01]	4	2.4500	0.05	1 C(10) - H(10)	...	H(9) -C(9)	1		2766.01
9	[1666.01]	2	2.5200	0.12	3 C(40) - H(40B)	...	H(26) -C(26)	1		1666.01

Analysis of Potential Hydrogen Bonds and Schemes with d(D...A) < R(D)+R(A)+0.50, d(H...A) < R(H)+R(A)-0.12 Ang., D-H...A > 100.0 Deg

Note: - ARU codes in [] are with reference to the Coordinates printed above (Possibly transformed, when MOVE .NE. 1.555)

Nr	Typ	Res	Donor	---	H....Acceptor	[ARU]	D - H	H...A	D...A	D - H...A	A..H..A*	A'..H..A"	Sum(XY,YZ)	Sum(XZ)
1		1	N(1)	--H(1)	..O(2)	[2656.01]	0.99	1.99	2.977(3)	175				
2	Intra	1	N(3)	--H(3)	..N(2)	[ ]	0.92	1.91	2.665(3)	138				
3	Intra	1	C(2)	--H(2)	..O(1)	[ ]	0.93	2.51	2.889(3)	105				
4		1	C(3)	--H(3A)	..O(3)	[2666.01]	0.93	2.53	3.419(3)	161				
5	Intra	1	C(19)	--H(19)	..O(4)	[ ]	0.93	2.45	3.069(3)	124				
6	Intra	1	C(26)	--H(26)	..O(4)	[ ]	0.93	2.54	2.903(3)	104				

Translation of ARU-code to Equivalent Position Code

[2656.] = 1-x,-y,1-z
[2666.] = 1-x,1-y,1-z

Table S4. M

6-Membered Ring (1) C(1) --> C(2) --> C(3) --> C(4) --> C(5) --> C(6) -->

6-Membered Ring (2) C(8) --> C(9) --> C(10) --> C(11) --> C(12) --> C(13) -->

6-Membered Ring (3) C(15) --> C(16) --> C(17) --> C(18) --> C(19) --> C(20) -->

6-Membered Ring (4) C(21) --> C(22) --> C(23) --> C(24) --> C(25) --> C(26) -->

Analysis of Short Ring-Interactions with Cg-Cg Distances < 6.0 Angstrom and Beta < 60.0 Deg.

Cg(I)	Res(I)	Cg(J)	[ARU(J)]	Cg-Cg	Transformed J-Plane P, Q, R, S	Alpha	Beta	Gamma	CgI_Perp	CgJ_Perp	Slippage
Cg(1)	[1] ->	Cg(2)	[1555.01]	5.193(2)	-0.1303 0.9012 0.4133	2.7573	38.78	29.39	61.26	2.497	4.525
Cg(1)	[1] ->	Cg(3)	[3655.01]	4.1133(17)	-0.4287-0.8773-0.2157	1.7658	5.32	30.84	28.84	3.603	3.532
Cg(1)	[1] ->	Cg(4)	[3555.01]	5.7694(19)	-0.9503 0.1993 0.2394	1.7808	75.01	42.31	47.33	3.911	4.266
Cg(2)	[1] ->	Cg(1)	[1655.01]	5.931(2)	0.5057 0.8297 0.2364	6.4179	38.78	51.70	89.52	0.050	3.675
Cg(2)	[1] ->	Cg(3)	[4454.01]	4.4402(17)	0.4287-0.8773 0.2157	-5.3510	40.77	52.86	20.03	4.172	2.681
Cg(2)	[1] ->	Cg(4)	[3655.01]	5.9871(19)	-0.9503 0.1993 0.2394	-6.8149	66.27	28.11	72.34	1.816	5.281
Cg(3)	[1] ->	Cg(1)	[3655.01]	4.1133(17)	-0.5057-0.8297-0.2364	-2.7309	5.32	28.84	30.84	3.531	3.603
Cg(3)	[1] ->	Cg(2)	[4555.01]	4.4403(17)	-0.1303-0.9012 0.4133	-2.8645	40.77	20.03	52.86	2.681	4.172
Cg(3)	[1] ->	Cg(4)	[1555.01]	4.8652(18)	0.9503-0.1993-0.2394	1.7808	79.58	42.50	37.12	3.879	3.587
Cg(4)	[1] ->	Cg(1)	[3555.01]	5.7694(19)	-0.5057-0.8297-0.2364	1.8435	75.01	47.33	42.31	4.266	3.911
Cg(4)	[1] ->	Cg(1)	[3655.01]	4.9156(18)	-0.5057-0.8297-0.2364	-2.7309	75.01	17.62	86.41	0.308	4.685
Cg(4)	[1] ->	Cg(3)	[1455.01]	4.9583(18)	0.4287 0.8773 0.2157	1.7658	79.58	17.97	86.64	0.290	4.716
Cg(4)	[1] ->	Cg(3)	[1555.01]	4.8652(18)	0.4287 0.8773 0.2157	5.6434	79.58	37.12	42.50	3.587	3.879
				Min or Max 4.113		5.32	17.62	89.52	0.050	2.681	

Analysis of X-H...Cg(Pi-Ring) Interactions (H..Cg < 3.0 Ang. - Gamma < 30.0 Deg)

X--H(I)	Res(I)	Cg(J)	[ARU(J)]	H..Cg	Transformed J-Plane P, Q, R, S	H-Perp	Gamma	X-H..Cg	X..Cg	X-H,Pi
C(5) -H(5)	[1] ->	Cg(4)	[3655.01]	2.75	-0.9503 0.1993 0.2394 -6.8149	2.722	8.43	155	3.614(3)	59
C(10) -H(10)	[1] ->	Cg(3)	[4454.01]	2.95	0.4287-0.8773 0.2157 -5.3510	2.818	17.01	115	3.448(3)	36
C(17) -H(17)	[1] ->	Cg(4)	[1655.01]	2.76	0.9503-0.1993-0.2394 10.3765	2.733	7.24	156	3.624(3)	59
			Min or Max	2.750		2.722	7.24	156.00	3.448	59.00

[1555] = X,Y,Z [3655] = 1-X,-Y,-Z [3555] = -X,-Y,-Z [1655] = 1+X,Y,Z
[4454] = -1/2+X,1/2-Y,-1/2+Z [4555] = 1/2+X,1/2-Y,1/2+Z [1455] = -1+X,Y,Z [1655] = 1+X,Y,Z

Analysis of Y-X...Cg(Pi-Ring) Interactions (X..Cg < 4.0 Ang. - Gamma < 30.0 Deg)

Y--X(I)	Res(I)	Cg(J)	[ARU(J)]	X..Cg	Transformed J-Plane P, Q, R, S	X-Perp	Gamma	Y-X..Cg	Y..Cg	Y-X,Pi
S(1)	-O(1)	[1] ->	Cg(2) [3655.01]	3.651(2)	0.1303-0.9012-0.4133 3.9360	3.199	28.82	166.62(10)	5.0582(15)	64.11
			Min or Max	3.651		3.199	28.82	166.62	5.058	64.11

[3655] = 1-X,-Y,-Z

The Cg(I) refer to the Ring Centre-of-Gravity numbers given in () in the Ring-Analysis above

Cg(I)	x	y	z	Xo	Yo	Zo
Cg(1)	0.13282(12)	0.09617(6)	-0.17540(7)	1.9372(12)	1.8158(11)	-2.7186(10)
Cg(2)	0.64913(15)	0.22013(5)	-0.03215(7)	6.0067(14)	4.1565(10)	-0.4983(11)
Cg(3)	0.99005(11)	0.07794(6)	0.33219(6)	7.5622(10)	1.4716(11)	5.1487(10)
Cg(4)	0.49700(12)	-0.02347(7)	0.33514(7)	3.0899(11)	-0.4432(13)	5.1945(11)

Summary of Shortest Inter Contacts with d(I-J) < R(I) + R(J) + 0.2 of Residue # 1 to Neighbouring ARU'S

Nr	ARU	Nr.Cont.	d(min)	Del	XHn	X	- At(I)		At(J)	- Y	YHn	Note	Partaking ARU's in Close Contact Resd.
1	[3655.01]	20	2.2400	-0.48	1	N(1)	- H(1A)	...	O(1)	-S(1)	0	<<	3655.01
2	[1455.01]	8	2.7500	0.03	0	S(1)	- O(2)	...	H(16)	-C(16)	1		1455.01
3	[4455.01]	1	2.6200	-0.10	0	S(2)	- O(4)	...	H(11)	-C(11)	1	<	4455.01
4	[4555.01]	9	2.3400	-0.06	2	C(7)	- H(7A)	...	*H(40E)	-C(40)	3	<	4555.01
5	[4454.01]	9	2.3400	-0.06	3	C(40)	-*H(40E)	...	H(7A)	-C(7)	2	<	4454.01
6	[1655.01]	8	2.7500	0.03	1	C(16)	- H(16)	...	O(2)	-S(1)	0		1655.01
7	[3656.01]	5	3.0200	0.12	1	C(22)	- H(22)	...	C(23)	-C(22)	1		3656.01
8	[3555.01]	2	2.3800	-0.02	3	C(240)	- H(24B)	...	H(3)	-C(3)	1	<	3555.01
9	[4554.01]	1	2.6200	-0.10	1	C(11)	- H(11)	...	O(4)	-S(2)	0	<	4554.01

Analysis of Potential Hydrogen Bonds and Schemes with d(D...A) < R(D)+R(A)+0.50, d(H...A) < R(H)+R(A)-0.12 Ang., D-H...A > 100.0 Deg

Nr	Typ	Res	Donor	---	H....Acceptor	[ARU]	D - H	H...A	D...A	D - H...A	A..H..A*	A'..H..A"	Sum(XY,YZ)	Sum(XZ)
1		1	N(1)	--H(1A)	..O(1)	[3655.01]	0.80(3)	2.24(3)	3.038(3)	176(2)				
2	Intra	1	N(3)	--H(3A)	..N(2)	[ ]	0.85(2)	1.95(3)	2.660(3)	141(3)				
3	Intra	1	C(2)	--H(2)	..O(2)	[ ]	0.93	2.53	2.901(3)	104				
4	Intra	1	C(19)	--H(19)	..O(3)	[ ]	0.93	2.47	3.122(3)	127				
5	Intra	1	C(22)	--H(22)	..O(3)	[ ]	0.93	2.57	2.921(4)	103				

Translation of ARU-code to Equivalent Position Code

[3655.] = 1-x,-y,-z

For C--H...Acceptor Interactions See: Th. Steiner, Cryst. Rev, (1996), 6, 1-57

H-Bond classification [G.A.Jeffrey, H.Maluszynska & J.Mitra., Int.J.Biol.Macromol.(1985),7,336-348]

2-Centre (linear) D-H...X most prob. angle 160 deg - also: G.A.Jeffrey & W.Saenger, Hydrogen Bonding in Biological Structures
3-Centre (bifurcated) SUM of 3 angl. about H = 360 deg Springer-Verlag, Berlin, 1991, pp 20.
4-Centre (trifurcated)