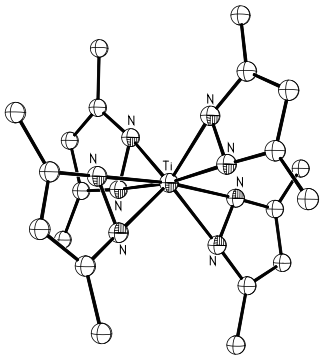


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STRUCTURAL REPORT ON Gellman124a

OCTOBER 27, 2009

Crystallographic Experimental Section

Data Collection

A colorless crystal with approximate dimensions 0.43 x 0.28 x 0.11 mm^3 was selected under oil under ambient conditions and attached to the tip of a MiTeGen MicroMount©. The crystal was mounted in a stream of cold nitrogen at 100(1) K and centered in the X-ray beam by using a video camera.

The crystal evaluation and data collection were performed on a Bruker SMART APEXII diffractometer with Cu K_α (λ = 1.54178 Å) radiation and the diffractometer to crystal distance of 4.03 cm.

The initial cell constants were obtained from three series of ω scans at different starting angles. Each series consisted of 41 frames collected at intervals of 0.6º in a 25º range about ω with the exposure time of 10 seconds per frame. The reflections were successfully indexed by an automated indexing routine built in the APEXII program. The final cell constants were calculated from a set of 9700 strong reflections from the actual data collection.

The data were collected by using the full sphere data collection routine to survey the reciprocal space to the extent of a full sphere to a resolution of 0.82 Å. A total of 125656 data were harvested by collecting 19 sets of frames with 0.5º scans in ω with an exposure time 30-60 sec per frame. These highly redundant datasets were corrected for Lorentz and polarization effects. The absorption correction was based on fitting a function to the empirical transmission surface as sampled by multiple equivalent measurements. [1]

Structure Solution and Refinement

The systematic absences in the diffraction data were uniquely consistent for the space group $P2_12_12_1$ that yielded chemically reasonable and computationally stable results of refinement [2,3].

A successful solution by the direct methods provided most non-hydrogen atoms from the *E*-map. The remaining non-hydrogen atoms were located in an alternating series of least-squares cycles and difference Fourier maps. All non-hydrogen atoms were refined with anisotropic

displacement coefficients. All hydrogen atoms were included in the structure factor calculation at idealized positions and were allowed to ride on the neighboring atoms with relative isotropic displacement coefficients.

There is also one molecule of solvate water per two molecules of the foldamer in the asymmetric unit. The water molecule was refined with an idealized geometry.

One phenyl group is disordered over two positions with the major component being occupied 62.3(4)% of the time. Restraints and constraints were used for the refinement of the disordered phenyl groups.

The final least-squares refinement of 911 parameters against 15507 data resulted in residuals *R* (based on F^2 for $I \geq 2\sigma$) and *wR* (based on F^2 for all data) of 0.0405 and 0.1000, respectively. The final difference Fourier map was featureless.

The molecular diagram is drawn with 40% probability ellipsoids.

References

[1] Bruker-AXS. (2007) APEX2, SADABS, and SAINT Software Reference Manuals. Bruker-AXS, Madison, Wisconsin, USA.

[2] Sheldrick, G. M. (2008) SHELXL. *Acta Cryst.* **A64**, 112-122.

[3] Dolomanov, O.V.; Bourhis, L.J.; Gildea, R.J.; Howard, J.A.K.; Puschmann, H. "OLEX2: a complete structure solution, refinement and analysis program". *J. Appl. Cryst.* (2009) **42**, *339-341*.

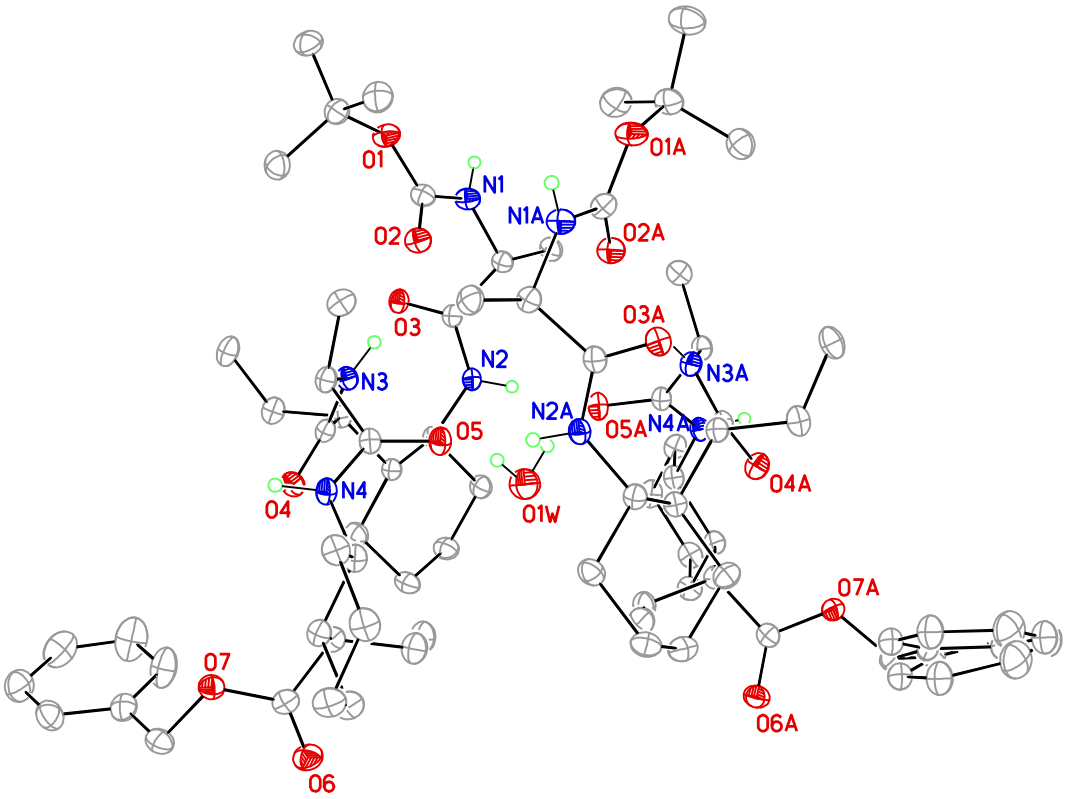


Figure 1. A molecular drawing of the unit cell content (note the water molecule and disorder). All H atoms connected to C atoms are omitted. The molecular diagram is drawn with 30% probability ellipsoids.

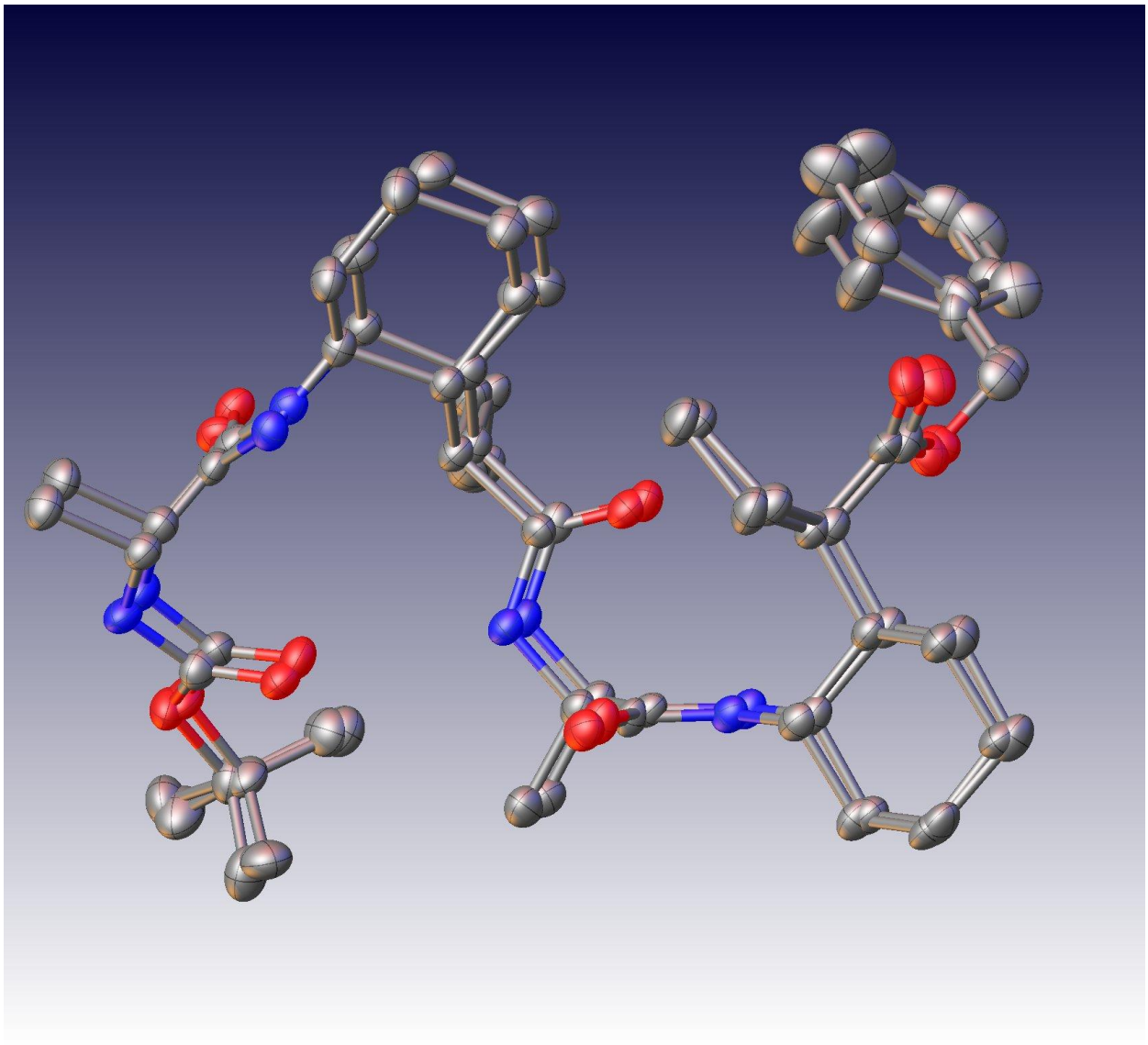


Figure 2. A molecular drawing of the two foldamer molecules overlapped. All H atoms and connected to C atoms are omitted. The molecular diagram is drawn with 50% probability ellipsoids.

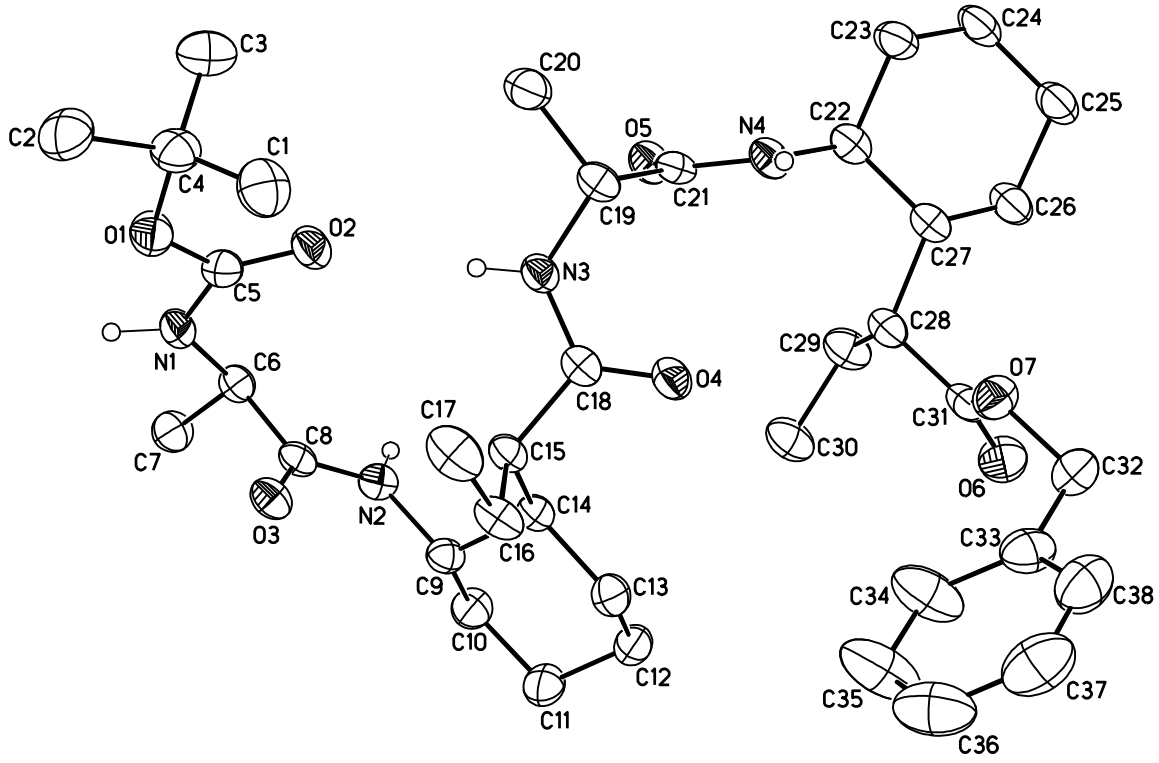


Figure 3. A molecular drawing of the first foldamer molecule. All H atoms connected to C atoms are omitted. The molecular diagram is drawn with 50% probability ellipsoids.

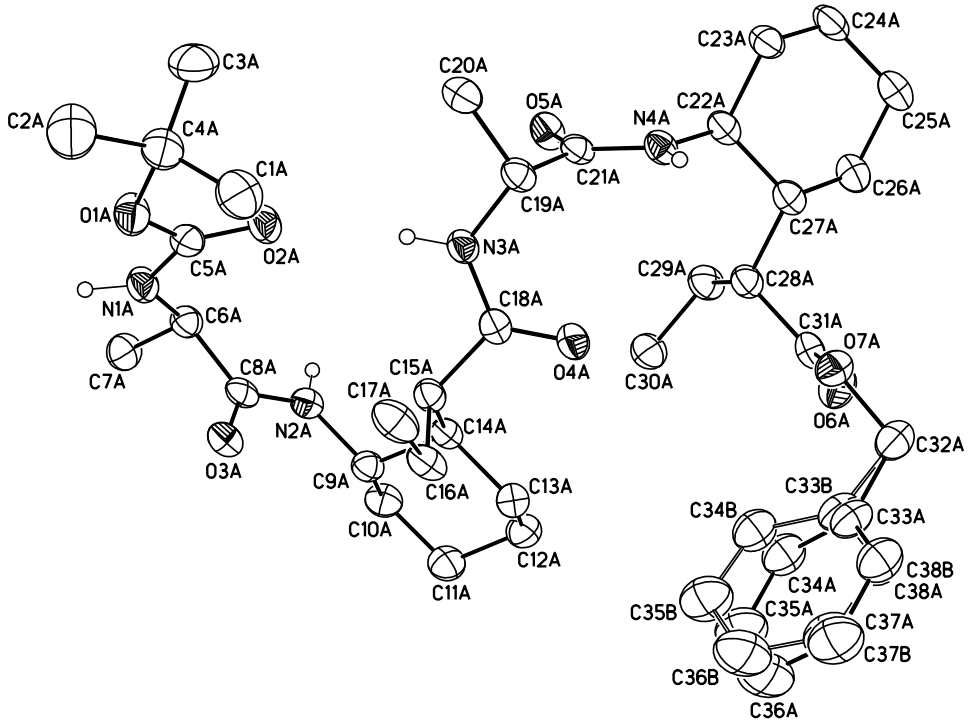


Figure 4. A molecular drawing of the second foldamer molecule. All H atoms connected to C atoms and the minor components of the disordered atoms are omitted. The molecular diagram is drawn with 50% probability ellipsoids.

Table 1. Crystal data and structure refinement for gellman124a.

Identification code	gellman124a	
Empirical formula	$C_{38}\ H_{60}\ N_4\ O_7$. 1/2 H_2O	
Formula weight	693.91	
Temperature	100(1) K	
Wavelength	1.54178 Å	
Crystal system	Orthorhombic	
Space group	$P2_12_12_1$	
Unit cell dimensions	a = 16.5265(5) Å	α= 90°.
	b = 17.3446(5) Å	β= 90°.
	c = 28.1866(9) Å	γ = 90°.
Volume	8079.6(4) $Å^3$	
Z	8	
Density (calculated)	1.141 Mg/m^3	
Absorption coefficient	0.636 mm^{-1}	
F(000)	3016	
Crystal size	0.43 x 0.28 x 0.11 mm^3	
Theta range for data collection	2.99 to 71.68°.	
Index ranges	-17<=h<=19, -21<=k<=21, -34<=l<=33	
Reflections collected	125656	
Independent reflections	15507 [R(int) = 0.0523]	
Completeness to theta = 67.00°	99.5 %	
Absorption correction	Empirical with SADABS	
Max. and min. transmission	0.9316 and 0.7714	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	15507 / 1 / 911	
Goodness-of-fit on F^2	1.039	
Final R indices [I>2sigma(I)]	R1 = 0.0405, wR2 = 0.0917	
R indices (all data)	R1 = 0.0540, wR2 = 0.1000	
Absolute structure parameter (Flack x)	-0.06(11)	
Absolute structure parameter (Hooft y)	-0.09(04)	
Largest diff. peak and hole	0.211 and -0.185 e.$Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for gellman124a. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	-780(1)	-9264(1)	-1540(1)	38(1)
O(2)	-1355(1)	-9658(1)	-843(1)	36(1)
O(3)	-210(1)	-8247(1)	-336(1)	31(1)
O(4)	-379(1)	-11035(1)	689(1)	32(1)
O(5)	-2558(1)	-11469(1)	326(1)	34(1)
O(6)	-946(1)	-11926(1)	2371(1)	44(1)
O(7)	-208(1)	-12582(1)	1837(1)	36(1)
N(1)	-1314(1)	-8395(1)	-1061(1)	32(1)
N(2)	-1205(1)	-8329(1)	212(1)	28(1)
N(3)	-1021(1)	-10797(1)	-2(1)	28(1)
N(4)	-1718(1)	-12433(1)	559(1)	28(1)
C(1)	-73(2)	-10486(1)	-1398(1)	46(1)
C(2)	-182(2)	-9862(1)	-2190(1)	48(1)
C(3)	-1414(2)	-10451(1)	-1820(1)	50(1)
C(4)	-620(1)	-10040(1)	-1729(1)	38(1)
C(5)	-1160(1)	-9158(1)	-1124(1)	32(1)
C(6)	-1586(1)	-8121(1)	-605(1)	29(1)
C(7)	-1793(1)	-7261(1)	-642(1)	36(1)
C(8)	-935(1)	-8243(1)	-231(1)	27(1)
C(9)	-678(1)	-8420(1)	624(1)	28(1)
C(10)	-1024(1)	-7929(1)	1027(1)	35(1)
C(11)	-535(2)	-8001(1)	1482(1)	39(1)
C(12)	-466(2)	-8845(1)	1629(1)	38(1)
C(13)	-101(1)	-9325(1)	1229(1)	34(1)
C(14)	-599(1)	-9272(1)	769(1)	27(1)
C(15)	-254(1)	-9758(1)	355(1)	28(1)
C(16)	671(1)	-9767(1)	325(1)	35(1)
C(17)	972(1)	-10172(1)	-122(1)	43(1)
C(18)	-559(1)	-10586(1)	371(1)	27(1)
C(19)	-1263(1)	-11597(1)	-64(1)	29(1)
C(20)	-1588(1)	-11719(1)	-565(1)	38(1)
C(21)	-1908(1)	-11824(1)	300(1)	26(1)
C(22)	-2233(1)	-12765(1)	925(1)	31(1)
C(23)	-2520(1)	-13565(1)	771(1)	35(1)
C(24)	-3043(1)	-13945(1)	1150(1)	39(1)
C(25)	-2606(2)	-13983(1)	1623(1)	40(1)
C(26)	-2318(1)	-13187(1)	1775(1)	38(1)
C(27)	-1774(1)	-12818(1)	1398(1)	30(1)
C(28)	-1426(1)	-12029(1)	1560(1)	31(1)
C(29)	-2066(1)	-11421(1)	1683(1)	41(1)
C(30)	-1697(2)	-10615(1)	1735(1)	44(1)
C(31)	-857(1)	-12154(1)	1971(1)	32(1)
C(32)	409(1)	-12736(1)	2194(1)	41(1)
C(33)	1173(2)	-12324(1)	2066(1)	41(1)
C(34)	1157(2)	-11568(1)	1909(1)	62(1)
C(35)	1864(2)	-11197(2)	1790(1)	77(1)
C(36)	2597(2)	-11575(2)	1834(1)	68(1)
C(37)	2614(2)	-12319(2)	1979(1)	62(1)
C(38)	1909(2)	-12691(2)	2095(1)	52(1)
O(1A)	-4557(1)	-10615(1)	-1535(1)	39(1)
O(2A)	-4096(1)	-10286(1)	-798(1)	35(1)

O(3A)	-5297(1)	-11748(1)	-338(1)	31(1)
O(4A)	-5109(1)	-8939(1)	704(1)	34(1)
O(5A)	-2938(1)	-8465(1)	374(1)	34(1)
O(6A)	-4612(1)	-8060(1)	2408(1)	45(1)
O(7A)	-5380(1)	-7506(1)	1848(1)	35(1)
N(1A)	-4155(1)	-11531(1)	-1046(1)	32(1)
N(2A)	-4324(1)	-11665(1)	223(1)	28(1)
N(3A)	-4445(1)	-9131(1)	17(1)	28(1)
N(4A)	-3776(1)	-7505(1)	614(1)	28(1)
C(1A)	-5255(2)	-9386(1)	-1419(1)	46(1)
C(2A)	-4936(2)	-9935(1)	-2212(1)	56(1)
C(3A)	-3811(2)	-9429(1)	-1711(1)	49(1)
C(4A)	-4631(2)	-9816(1)	-1711(1)	38(1)
C(5A)	-4265(1)	-10762(1)	-1100(1)	31(1)
C(6A)	-3909(1)	-11842(1)	-593(1)	30(1)
C(7A)	-3710(1)	-12699(1)	-648(1)	37(1)
C(8A)	-4577(1)	-11742(1)	-226(1)	27(1)
C(9A)	-4868(1)	-11554(1)	625(1)	29(1)
C(10A)	-4584(1)	-12059(1)	1036(1)	36(1)
C(11A)	-5110(2)	-11957(1)	1476(1)	39(1)
C(12A)	-5121(1)	-11108(1)	1623(1)	39(1)
C(13A)	-5432(1)	-10609(1)	1216(1)	35(1)
C(14A)	-4914(1)	-10696(1)	767(1)	28(1)
C(15A)	-5210(1)	-10200(1)	343(1)	28(1)
C(16A)	-6133(1)	-10184(1)	275(1)	34(1)
C(17A)	-6378(1)	-9778(1)	-183(1)	40(1)
C(18A)	-4912(1)	-9373(1)	378(1)	27(1)
C(19A)	-4220(1)	-8325(1)	-25(1)	29(1)
C(20A)	-3900(1)	-8158(1)	-522(1)	35(1)
C(21A)	-3583(1)	-8108(1)	347(1)	26(1)
C(22A)	-3272(1)	-7205(1)	996(1)	30(1)
C(23A)	-2937(1)	-6413(1)	858(1)	35(1)
C(24A)	-2416(1)	-6076(1)	1254(1)	39(1)
C(25A)	-2898(1)	-6019(1)	1712(1)	39(1)
C(26A)	-3233(1)	-6802(1)	1853(1)	38(1)
C(27A)	-3754(1)	-7159(1)	1461(1)	31(1)
C(28A)	-4099(1)	-7958(1)	1602(1)	31(1)
C(29A)	-3461(1)	-8561(1)	1735(1)	37(1)
C(30A)	-3812(2)	-9374(1)	1724(1)	40(1)
C(31A)	-4701(1)	-7860(1)	2004(1)	31(1)
C(32A)	-6042(1)	-7406(1)	2184(1)	39(1)
C(33A)	-6750(1)	-7917(1)	2072(1)	37(1)
C(34A)	-6622(1)	-8708(2)	2093(1)	43(1)
C(35A)	-7257(2)	-9214(1)	2007(1)	56(1)
C(36A)	-8021(1)	-8929(2)	1899(1)	66(1)
C(37A)	-8150(1)	-8138(2)	1877(1)	56(1)
C(38A)	-7514(2)	-7632(1)	1963(2)	43(1)
C(33B)	-6687(1)	-7962(2)	2012(2)	37(1)
C(34B)	-6528(1)	-8711(2)	1864(1)	43(1)
C(35B)	-7158(1)	-9183(2)	1714(2)	56(1)
C(36B)	-7947(1)	-8905(3)	1711(2)	66(1)
C(37B)	-8106(1)	-8156(3)	1859(2)	56(1)
C(38B)	-7476(2)	-7684(2)	2010(2)	43(1)
O(1W)	-2746(1)	-9987(1)	755(1)	56(1)

Table 3. Bond lengths [Å] and angles [°] for gellman124a.

O(1)-C(5)	1.344(3)	C(14)-C(15)	1.547(3)
O(1)-C(4)	1.472(2)	C(14)-H(14A)	1.0000
O(2)-C(5)	1.219(2)	C(15)-C(18)	1.523(2)
O(3)-C(8)	1.233(2)	C(15)-C(16)	1.531(3)
O(4)-C(18)	1.223(2)	C(15)-H(15A)	1.0000
O(5)-C(21)	1.239(2)	C(16)-C(17)	1.525(3)
O(6)-C(31)	1.202(2)	C(16)-H(16C)	0.9900
O(7)-C(31)	1.359(3)	C(16)-H(16D)	0.9900
O(7)-C(32)	1.457(3)	C(17)-H(17D)	0.9800
N(1)-C(5)	1.357(3)	C(17)-H(17F)	0.9800
N(1)-C(6)	1.443(3)	C(17)-H(17E)	0.9800
N(1)-H(1)	0.82(2)	C(19)-C(20)	1.525(3)
N(2)-C(8)	1.335(3)	C(19)-C(21)	1.533(3)
N(2)-C(9)	1.460(2)	C(19)-H(19A)	1.0000
N(2)-H(2)	0.85(2)	C(20)-H(20D)	0.9800
N(3)-C(18)	1.350(3)	C(20)-H(20F)	0.9800
N(3)-C(19)	1.454(2)	C(20)-H(20E)	0.9800
N(3)-H(3)	0.83(2)	C(22)-C(23)	1.529(3)
N(4)-C(21)	1.321(2)	C(22)-C(27)	1.537(3)
N(4)-C(22)	1.457(3)	C(22)-H(22A)	1.0000
N(4)-H(4)	0.90(2)	C(23)-C(24)	1.523(3)
C(1)-C(4)	1.514(3)	C(23)-H(23C)	0.9900
C(1)-H(1B)	0.9800	C(23)-H(23D)	0.9900
C(1)-H(1D)	0.9800	C(24)-C(25)	1.519(3)
C(1)-H(1C)	0.9800	C(24)-H(24C)	0.9900
C(2)-C(4)	1.518(3)	C(24)-H(24D)	0.9900
C(2)-H(2C)	0.9800	C(25)-C(26)	1.522(3)
C(2)-H(2D)	0.9800	C(25)-H(25C)	0.9900
C(2)-H(2B)	0.9800	C(25)-H(25D)	0.9900
C(3)-C(4)	1.514(3)	C(26)-C(27)	1.532(3)
C(3)-H(3C)	0.9800	C(26)-H(26D)	0.9900
C(3)-H(3D)	0.9800	C(26)-H(26C)	0.9900
C(3)-H(3B)	0.9800	C(27)-C(28)	1.553(3)
C(6)-C(8)	1.522(3)	C(27)-H(27A)	1.0000
C(6)-C(7)	1.534(3)	C(28)-C(31)	1.508(3)
C(6)-H(6)	1.0000	C(28)-C(29)	1.534(3)
C(7)-H(7B)	0.9800	C(28)-H(28A)	1.0000
C(7)-H(7C)	0.9800	C(29)-C(30)	1.532(3)
C(7)-H(7A)	0.9800	C(29)-H(29C)	0.9900
C(9)-C(10)	1.530(3)	C(29)-H(29D)	0.9900
C(9)-C(14)	1.539(3)	C(30)-H(30D)	0.9800
C(9)-H(9)	1.0000	C(30)-H(30F)	0.9800
C(10)-C(11)	1.522(3)	C(30)-H(30E)	0.9800
C(10)-H(10C)	0.9900	C(32)-C(33)	1.495(3)
C(10)-H(10D)	0.9900	C(32)-H(32F)	0.9900
C(11)-C(12)	1.526(3)	C(32)-H(32E)	0.9900
C(11)-H(11D)	0.9900	C(33)-C(38)	1.375(3)
C(11)-H(11C)	0.9900	C(33)-C(34)	1.384(4)
C(12)-C(13)	1.528(3)	C(34)-C(35)	1.375(4)
C(12)-H(12D)	0.9900	C(34)-H(34B)	0.9500
C(12)-H(12C)	0.9900	C(35)-C(36)	1.383(4)
C(13)-C(14)	1.539(3)	C(35)-H(35B)	0.9500
C(13)-H(13D)	0.9900	C(36)-C(37)	1.355(4)
C(13)-H(13C)	0.9900	C(36)-H(36B)	0.9500

C(37)-C(38)	1.371(4)	C(13A)-H(13B)	0.9900
C(37)-H(37B)	0.9500	C(14A)-C(15A)	1.552(3)
C(38)-H(38B)	0.9500	C(14A)-H(14)	1.0000
O(1A)-C(5A)	1.343(2)	C(15A)-C(18A)	1.520(3)
O(1A)-C(4A)	1.475(2)	C(15A)-C(16A)	1.538(3)
O(2A)-C(5A)	1.218(2)	C(15A)-H(15)	1.0000
O(3A)-C(8A)	1.232(2)	C(16A)-C(17A)	1.524(3)
O(4A)-C(18A)	1.229(2)	C(16A)-H(16B)	0.9900
O(5A)-C(21A)	1.235(2)	C(16A)-H(16A)	0.9900
O(6A)-C(31A)	1.202(2)	C(17A)-H(17B)	0.9800
O(7A)-C(31A)	1.353(3)	C(17A)-H(17A)	0.9800
O(7A)-C(32A)	1.457(2)	C(17A)-H(17C)	0.9800
N(1A)-C(5A)	1.355(3)	C(19A)-C(20A)	1.525(3)
N(1A)-C(6A)	1.445(3)	C(19A)-C(21A)	1.532(3)
N(1A)-H(1A)	0.82(2)	C(19A)-H(19)	1.0000
N(2A)-C(8A)	1.338(3)	C(20A)-H(20A)	0.9800
N(2A)-C(9A)	1.460(2)	C(20A)-H(20C)	0.9800
N(2A)-H(2A)	0.83(2)	C(20A)-H(20B)	0.9800
N(3A)-C(18A)	1.346(3)	C(22A)-C(23A)	1.532(3)
N(3A)-C(19A)	1.452(2)	C(22A)-C(27A)	1.535(3)
N(3A)-H(3A)	0.84(2)	C(22A)-H(22)	1.0000
N(4A)-C(21A)	1.329(2)	C(23A)-C(24A)	1.525(3)
N(4A)-C(22A)	1.458(3)	C(23A)-H(23A)	0.9900
N(4A)-H(4A)	0.88(2)	C(23A)-H(23B)	0.9900
C(1A)-C(4A)	1.517(3)	C(24A)-C(25A)	1.521(3)
C(1A)-H(1AB)	0.9800	C(24A)-H(24B)	0.9900
C(1A)-H(1AC)	0.9800	C(24A)-H(24A)	0.9900
C(1A)-H(1AA)	0.9800	C(25A)-C(26A)	1.519(3)
C(2A)-C(4A)	1.513(3)	C(25A)-H(25B)	0.9900
C(2A)-H(2AA)	0.9800	C(25A)-H(25A)	0.9900
C(2A)-H(2AC)	0.9800	C(26A)-C(27A)	1.533(3)
C(2A)-H(2AB)	0.9800	C(26A)-H(26B)	0.9900
C(3A)-C(4A)	1.512(3)	C(26A)-H(26A)	0.9900
C(3A)-H(3AA)	0.9800	C(27A)-C(28A)	1.551(3)
C(3A)-H(3AC)	0.9800	C(27A)-H(27)	1.0000
C(3A)-H(3AB)	0.9800	C(28A)-C(31A)	1.515(3)
C(6A)-C(8A)	1.523(3)	C(28A)-C(29A)	1.531(3)
C(6A)-C(7A)	1.530(3)	C(28A)-H(28)	1.0000
C(6A)-H(6A)	1.0000	C(29A)-C(30A)	1.526(3)
C(7A)-H(7AC)	0.9800	C(29A)-H(29A)	0.9900
C(7A)-H(7AB)	0.9800	C(29A)-H(29B)	0.9900
C(7A)-H(7AA)	0.9800	C(30A)-H(30A)	0.9800
C(9A)-C(10A)	1.526(3)	C(30A)-H(30C)	0.9800
C(9A)-C(14A)	1.542(3)	C(30A)-H(30B)	0.9800
C(9A)-H(9A)	1.0000	C(32A)-C(33A)	1.502(3)
C(10A)-C(11A)	1.524(3)	C(32A)-C(33B)	1.517(4)
C(10A)-H(10B)	0.9900	C(32A)-H(32A)	0.9900
C(10A)-H(10A)	0.9900	C(32A)-H(32B)	0.9900
C(11A)-C(12A)	1.530(3)	C(32A)-H(32C)	0.9900
C(11A)-H(11A)	0.9900	C(32A)-H(32D)	0.9900
C(11A)-H(11B)	0.9900	C(33A)-C(34A)	1.3900
C(12A)-C(13A)	1.527(3)	C(33A)-C(38A)	1.3900
C(12A)-H(12A)	0.9900	C(34A)-C(35A)	1.3900
C(12A)-H(12B)	0.9900	C(34A)-H(34)	0.9500
C(13A)-C(14A)	1.535(3)	C(35A)-C(36A)	1.3900
C(13A)-H(13A)	0.9900	C(35A)-H(35)	0.9500

C(36A)-C(37A)	1.3900	C(35B)-C(36B)	1.3900
C(36A)-H(36)	0.9500	C(35B)-H(35A)	0.9500
C(37A)-C(38A)	1.3900	C(36B)-C(37B)	1.3900
C(37A)-H(37)	0.9500	C(36B)-H(36A)	0.9500
C(38A)-H(38)	0.9500	C(37B)-C(38B)	1.3900
C(33B)-C(34B)	1.3900	C(37B)-H(37A)	0.9500
C(33B)-C(38B)	1.3900	C(38B)-H(38A)	0.9500
C(34B)-C(35B)	1.3900	O(1W)-H(1W)	0.9584
C(34B)-H(34A)	0.9500	O(1W)-H(2W)	0.9584

C(5)-O(1)-C(4)	121.74(16)	C(8)-C(6)-H(6)	109.0
C(31)-O(7)-C(32)	117.34(16)	C(7)-C(6)-H(6)	109.0
C(5)-N(1)-C(6)	119.65(17)	C(6)-C(7)-H(7B)	109.5
C(5)-N(1)-H(1)	113.3(17)	C(6)-C(7)-H(7C)	109.5
C(6)-N(1)-H(1)	118.6(16)	H(7B)-C(7)-H(7C)	109.5
C(8)-N(2)-C(9)	123.80(17)	C(6)-C(7)-H(7A)	109.5
C(8)-N(2)-H(2)	119.7(15)	H(7B)-C(7)-H(7A)	109.5
C(9)-N(2)-H(2)	116.4(15)	H(7C)-C(7)-H(7A)	109.5
C(18)-N(3)-C(19)	120.56(17)	O(3)-C(8)-N(2)	123.26(18)
C(18)-N(3)-H(3)	122.7(16)	O(3)-C(8)-C(6)	121.40(17)
C(19)-N(3)-H(3)	116.6(16)	N(2)-C(8)-C(6)	115.34(17)
C(21)-N(4)-C(22)	124.64(17)	N(2)-C(9)-C(10)	107.91(16)
C(21)-N(4)-H(4)	118.3(14)	N(2)-C(9)-C(14)	111.35(15)
C(22)-N(4)-H(4)	117.0(14)	C(10)-C(9)-C(14)	111.66(16)
C(4)-C(1)-H(1B)	109.5	N(2)-C(9)-H(9)	108.6
C(4)-C(1)-H(1D)	109.5	C(10)-C(9)-H(9)	108.6
H(1B)-C(1)-H(1D)	109.5	C(14)-C(9)-H(9)	108.6
C(4)-C(1)-H(1C)	109.5	C(11)-C(10)-C(9)	112.46(17)
H(1B)-C(1)-H(1C)	109.5	C(11)-C(10)-H(10C)	109.1
H(1D)-C(1)-H(1C)	109.5	C(9)-C(10)-H(10C)	109.1
C(4)-C(2)-H(2C)	109.5	C(11)-C(10)-H(10D)	109.1
C(4)-C(2)-H(2D)	109.5	C(9)-C(10)-H(10D)	109.1
H(2C)-C(2)-H(2D)	109.5	H(10C)-C(10)-H(10D)	107.8
C(4)-C(2)-H(2B)	109.5	C(10)-C(11)-C(12)	110.31(17)
H(2C)-C(2)-H(2B)	109.5	C(10)-C(11)-H(11D)	109.6
H(2D)-C(2)-H(2B)	109.5	C(12)-C(11)-H(11D)	109.6
C(4)-C(3)-H(3C)	109.5	C(10)-C(11)-H(11C)	109.6
C(4)-C(3)-H(3D)	109.5	C(12)-C(11)-H(11C)	109.6
H(3C)-C(3)-H(3D)	109.5	H(11D)-C(11)-H(11C)	108.1
C(4)-C(3)-H(3B)	109.5	C(11)-C(12)-C(13)	110.59(17)
H(3C)-C(3)-H(3B)	109.5	C(11)-C(12)-H(12D)	109.5
H(3D)-C(3)-H(3B)	109.5	C(13)-C(12)-H(12D)	109.5
O(1)-C(4)-C(1)	110.57(17)	C(11)-C(12)-H(12C)	109.5
O(1)-C(4)-C(3)	109.72(18)	C(13)-C(12)-H(12C)	109.5
C(1)-C(4)-C(3)	112.4(2)	H(12D)-C(12)-H(12C)	108.1
O(1)-C(4)-C(2)	102.10(17)	C(12)-C(13)-C(14)	112.22(17)
C(1)-C(4)-C(2)	110.2(2)	C(12)-C(13)-H(13D)	109.2
C(3)-C(4)-C(2)	111.4(2)	C(14)-C(13)-H(13D)	109.2
O(2)-C(5)-O(1)	126.35(18)	C(12)-C(13)-H(13C)	109.2
O(2)-C(5)-N(1)	124.1(2)	C(14)-C(13)-H(13C)	109.2
O(1)-C(5)-N(1)	109.52(17)	H(13D)-C(13)-H(13C)	107.9
N(1)-C(6)-C(8)	110.60(16)	C(9)-C(14)-C(13)	109.05(15)
N(1)-C(6)-C(7)	109.25(16)	C(9)-C(14)-C(15)	110.80(15)
C(8)-C(6)-C(7)	109.86(16)	C(13)-C(14)-C(15)	113.87(16)
N(1)-C(6)-H(6)	109.0	C(9)-C(14)-H(14A)	107.6

C(13)-C(14)-H(14A)	107.6	C(24)-C(25)-C(26)	110.97(18)
C(15)-C(14)-H(14A)	107.6	C(24)-C(25)-H(25C)	109.4
C(18)-C(15)-C(16)	108.80(15)	C(26)-C(25)-H(25C)	109.4
C(18)-C(15)-C(14)	111.72(16)	C(24)-C(25)-H(25D)	109.4
C(16)-C(15)-C(14)	114.52(16)	C(26)-C(25)-H(25D)	109.4
C(18)-C(15)-H(15A)	107.1	H(25C)-C(25)-H(25D)	108.0
C(16)-C(15)-H(15A)	107.1	C(25)-C(26)-C(27)	111.47(18)
C(14)-C(15)-H(15A)	107.1	C(25)-C(26)-H(26D)	109.3
C(17)-C(16)-C(15)	112.08(18)	C(27)-C(26)-H(26D)	109.3
C(17)-C(16)-H(16C)	109.2	C(25)-C(26)-H(26C)	109.3
C(15)-C(16)-H(16C)	109.2	C(27)-C(26)-H(26C)	109.3
C(17)-C(16)-H(16D)	109.2	H(26D)-C(26)-H(26C)	108.0
C(15)-C(16)-H(16D)	109.2	C(26)-C(27)-C(22)	109.66(17)
H(16C)-C(16)-H(16D)	107.9	C(26)-C(27)-C(28)	112.42(17)
C(16)-C(17)-H(17D)	109.5	C(22)-C(27)-C(28)	112.60(16)
C(16)-C(17)-H(17F)	109.5	C(26)-C(27)-H(27A)	107.3
H(17D)-C(17)-H(17F)	109.5	C(22)-C(27)-H(27A)	107.3
C(16)-C(17)-H(17E)	109.5	C(28)-C(27)-H(27A)	107.3
H(17D)-C(17)-H(17E)	109.5	C(31)-C(28)-C(29)	110.83(17)
H(17F)-C(17)-H(17E)	109.5	C(31)-C(28)-C(27)	109.25(15)
O(4)-C(18)-N(3)	122.32(17)	C(29)-C(28)-C(27)	114.70(17)
O(4)-C(18)-C(15)	122.77(18)	C(31)-C(28)-H(28A)	107.2
N(3)-C(18)-C(15)	114.87(17)	C(29)-C(28)-H(28A)	107.2
N(3)-C(19)-C(20)	109.93(16)	C(27)-C(28)-H(28A)	107.2
N(3)-C(19)-C(21)	110.78(15)	C(30)-C(29)-C(28)	112.03(18)
C(20)-C(19)-C(21)	109.84(16)	C(30)-C(29)-H(29C)	109.2
N(3)-C(19)-H(19A)	108.7	C(28)-C(29)-H(29C)	109.2
C(20)-C(19)-H(19A)	108.7	C(30)-C(29)-H(29D)	109.2
C(21)-C(19)-H(19A)	108.7	C(28)-C(29)-H(29D)	109.2
C(19)-C(20)-H(20D)	109.5	H(29C)-C(29)-H(29D)	107.9
C(19)-C(20)-H(20F)	109.5	C(29)-C(30)-H(30D)	109.5
H(20D)-C(20)-H(20F)	109.5	C(29)-C(30)-H(30F)	109.5
C(19)-C(20)-H(20E)	109.5	H(30D)-C(30)-H(30F)	109.5
H(20D)-C(20)-H(20E)	109.5	C(29)-C(30)-H(30E)	109.5
H(20F)-C(20)-H(20E)	109.5	H(30D)-C(30)-H(30E)	109.5
O(5)-C(21)-N(4)	124.77(18)	H(30F)-C(30)-H(30E)	109.5
O(5)-C(21)-C(19)	121.00(17)	O(6)-C(31)-O(7)	122.5(2)
N(4)-C(21)-C(19)	114.17(17)	O(6)-C(31)-C(28)	126.6(2)
N(4)-C(22)-C(23)	109.81(17)	O(7)-C(31)-C(28)	110.88(17)
N(4)-C(22)-C(27)	110.51(16)	O(7)-C(32)-C(33)	109.72(18)
C(23)-C(22)-C(27)	110.18(16)	O(7)-C(32)-H(32F)	109.7
N(4)-C(22)-H(22A)	108.8	C(33)-C(32)-H(32F)	109.7
C(23)-C(22)-H(22A)	108.8	O(7)-C(32)-H(32E)	109.7
C(27)-C(22)-H(22A)	108.8	C(33)-C(32)-H(32E)	109.7
C(24)-C(23)-C(22)	111.74(17)	H(32F)-C(32)-H(32E)	108.2
C(24)-C(23)-H(23C)	109.3	C(38)-C(33)-C(34)	118.3(2)
C(22)-C(23)-H(23C)	109.3	C(38)-C(33)-C(32)	120.9(2)
C(24)-C(23)-H(23D)	109.3	C(34)-C(33)-C(32)	120.8(2)
C(22)-C(23)-H(23D)	109.3	C(35)-C(34)-C(33)	120.3(3)
H(23C)-C(23)-H(23D)	107.9	C(35)-C(34)-H(34B)	119.8
C(25)-C(24)-C(23)	111.31(18)	C(33)-C(34)-H(34B)	119.8
C(25)-C(24)-H(24C)	109.4	C(34)-C(35)-C(36)	120.1(3)
C(23)-C(24)-H(24C)	109.4	C(34)-C(35)-H(35B)	120.0
C(25)-C(24)-H(24D)	109.4	C(36)-C(35)-H(35B)	120.0
C(23)-C(24)-H(24D)	109.4	C(37)-C(36)-C(35)	119.7(3)
H(24C)-C(24)-H(24D)	108.0	C(37)-C(36)-H(36B)	120.2

C(35)-C(36)-H(36B)	120.2	H(7AC)-C(7A)-H(7AB)	109.5
C(36)-C(37)-C(38)	120.2(3)	C(6A)-C(7A)-H(7AA)	109.5
C(36)-C(37)-H(37B)	119.9	H(7AC)-C(7A)-H(7AA)	109.5
C(38)-C(37)-H(37B)	119.9	H(7AB)-C(7A)-H(7AA)	109.5
C(37)-C(38)-C(33)	121.3(3)	O(3A)-C(8A)-N(2A)	123.08(18)
C(37)-C(38)-H(38B)	119.3	O(3A)-C(8A)-C(6A)	121.61(18)
C(33)-C(38)-H(38B)	119.3	N(2A)-C(8A)-C(6A)	115.29(17)
C(5A)-O(1A)-C(4A)	120.96(16)	N(2A)-C(9A)-C(10A)	108.90(16)
C(31A)-O(7A)-C(32A)	117.87(16)	N(2A)-C(9A)-C(14A)	111.10(15)
C(5A)-N(1A)-C(6A)	120.37(17)	C(10A)-C(9A)-C(14A)	111.91(16)
C(5A)-N(1A)-H(1A)	115.1(17)	N(2A)-C(9A)-H(9A)	108.3
C(6A)-N(1A)-H(1A)	120.5(16)	C(10A)-C(9A)-H(9A)	108.3
C(8A)-N(2A)-C(9A)	123.69(17)	C(14A)-C(9A)-H(9A)	108.3
C(8A)-N(2A)-H(2A)	119.8(15)	C(11A)-C(10A)-C(9A)	112.02(18)
C(9A)-N(2A)-H(2A)	115.8(15)	C(11A)-C(10A)-H(10B)	109.2
C(18A)-N(3A)-C(19A)	120.52(17)	C(9A)-C(10A)-H(10B)	109.2
C(18A)-N(3A)-H(3A)	121.8(15)	C(11A)-C(10A)-H(10A)	109.2
C(19A)-N(3A)-H(3A)	117.7(15)	C(9A)-C(10A)-H(10A)	109.2
C(21A)-N(4A)-C(22A)	124.22(17)	H(10B)-C(10A)-H(10A)	107.9
C(21A)-N(4A)-H(4A)	116.4(14)	C(10A)-C(11A)-C(12A)	109.85(18)
C(22A)-N(4A)-H(4A)	119.4(14)	C(10A)-C(11A)-H(11A)	109.7
C(4A)-C(1A)-H(1AB)	109.5	C(12A)-C(11A)-H(11A)	109.7
C(4A)-C(1A)-H(1AC)	109.5	C(10A)-C(11A)-H(11B)	109.7
H(1AB)-C(1A)-H(1AC)	109.5	C(12A)-C(11A)-H(11B)	109.7
C(4A)-C(1A)-H(1AA)	109.5	H(11A)-C(11A)-H(11B)	108.2
H(1AB)-C(1A)-H(1AA)	109.5	C(13A)-C(12A)-C(11A)	110.19(18)
H(1AC)-C(1A)-H(1AA)	109.5	C(13A)-C(12A)-H(12A)	109.6
C(4A)-C(2A)-H(2AA)	109.5	C(11A)-C(12A)-H(12A)	109.6
C(4A)-C(2A)-H(2AC)	109.5	C(13A)-C(12A)-H(12B)	109.6
H(2AA)-C(2A)-H(2AC)	109.5	C(11A)-C(12A)-H(12B)	109.6
C(4A)-C(2A)-H(2AB)	109.5	H(12A)-C(12A)-H(12B)	108.1
H(2AA)-C(2A)-H(2AB)	109.5	C(12A)-C(13A)-C(14A)	112.08(18)
H(2AC)-C(2A)-H(2AB)	109.5	C(12A)-C(13A)-H(13A)	109.2
C(4A)-C(3A)-H(3AA)	109.5	C(14A)-C(13A)-H(13A)	109.2
C(4A)-C(3A)-H(3AC)	109.5	C(12A)-C(13A)-H(13B)	109.2
H(3AA)-C(3A)-H(3AC)	109.5	C(14A)-C(13A)-H(13B)	109.2
C(4A)-C(3A)-H(3AB)	109.5	H(13A)-C(13A)-H(13B)	107.9
H(3AA)-C(3A)-H(3AB)	109.5	C(13A)-C(14A)-C(9A)	109.63(16)
H(3AC)-C(3A)-H(3AB)	109.5	C(13A)-C(14A)-C(15A)	113.84(16)
O(1A)-C(4A)-C(3A)	110.09(19)	C(9A)-C(14A)-C(15A)	110.54(15)
O(1A)-C(4A)-C(2A)	102.29(17)	C(13A)-C(14A)-H(14)	107.5
C(3A)-C(4A)-C(2A)	111.0(2)	C(9A)-C(14A)-H(14)	107.5
O(1A)-C(4A)-C(1A)	109.66(18)	C(15A)-C(14A)-H(14)	107.5
C(3A)-C(4A)-C(1A)	113.00(19)	C(18A)-C(15A)-C(16A)	108.19(15)
C(2A)-C(4A)-C(1A)	110.3(2)	C(18A)-C(15A)-C(14A)	111.75(16)
O(2A)-C(5A)-O(1A)	126.32(18)	C(16A)-C(15A)-C(14A)	114.77(16)
O(2A)-C(5A)-N(1A)	123.9(2)	C(18A)-C(15A)-H(15)	107.3
O(1A)-C(5A)-N(1A)	109.79(17)	C(16A)-C(15A)-H(15)	107.3
N(1A)-C(6A)-C(8A)	110.75(17)	C(14A)-C(15A)-H(15)	107.3
N(1A)-C(6A)-C(7A)	109.50(16)	C(17A)-C(16A)-C(15A)	112.21(18)
C(8A)-C(6A)-C(7A)	109.65(16)	C(17A)-C(16A)-H(16B)	109.2
N(1A)-C(6A)-H(6A)	109.0	C(15A)-C(16A)-H(16B)	109.2
C(8A)-C(6A)-H(6A)	109.0	C(17A)-C(16A)-H(16A)	109.2
C(7A)-C(6A)-H(6A)	109.0	C(15A)-C(16A)-H(16A)	109.2
C(6A)-C(7A)-H(7AC)	109.5	H(16B)-C(16A)-H(16A)	107.9
C(6A)-C(7A)-H(7AB)	109.5	C(16A)-C(17A)-H(17B)	109.5

C(16A)-C(17A)-H(17A)	109.5	C(26A)-C(27A)-H(27)	107.6
H(17B)-C(17A)-H(17A)	109.5	C(22A)-C(27A)-H(27)	107.6
C(16A)-C(17A)-H(17C)	109.5	C(28A)-C(27A)-H(27)	107.6
H(17B)-C(17A)-H(17C)	109.5	C(31A)-C(28A)-C(29A)	110.31(17)
H(17A)-C(17A)-H(17C)	109.5	C(31A)-C(28A)-C(27A)	109.41(16)
O(4A)-C(18A)-N(3A)	121.73(17)	C(29A)-C(28A)-C(27A)	114.83(17)
O(4A)-C(18A)-C(15A)	122.78(18)	C(31A)-C(28A)-H(28)	107.3
N(3A)-C(18A)-C(15A)	115.42(17)	C(29A)-C(28A)-H(28)	107.3
N(3A)-C(19A)-C(20A)	110.24(16)	C(27A)-C(28A)-H(28)	107.3
N(3A)-C(19A)-C(21A)	110.85(15)	C(30A)-C(29A)-C(28A)	111.41(18)
C(20A)-C(19A)-C(21A)	110.02(16)	C(30A)-C(29A)-H(29A)	109.3
N(3A)-C(19A)-H(19)	108.6	C(28A)-C(29A)-H(29A)	109.3
C(20A)-C(19A)-H(19)	108.6	C(30A)-C(29A)-H(29B)	109.3
C(21A)-C(19A)-H(19)	108.6	C(28A)-C(29A)-H(29B)	109.3
C(19A)-C(20A)-H(20A)	109.5	H(29A)-C(29A)-H(29B)	108.0
C(19A)-C(20A)-H(20C)	109.5	C(29A)-C(30A)-H(30A)	109.5
H(20A)-C(20A)-H(20C)	109.5	C(29A)-C(30A)-H(30C)	109.5
C(19A)-C(20A)-H(20B)	109.5	H(30A)-C(30A)-H(30C)	109.5
H(20A)-C(20A)-H(20B)	109.5	C(29A)-C(30A)-H(30B)	109.5
H(20C)-C(20A)-H(20B)	109.5	H(30A)-C(30A)-H(30B)	109.5
O(5A)-C(21A)-N(4A)	124.52(18)	H(30C)-C(30A)-H(30B)	109.5
O(5A)-C(21A)-C(19A)	120.93(17)	O(6A)-C(31A)-O(7A)	122.7(2)
N(4A)-C(21A)-C(19A)	114.51(16)	O(6A)-C(31A)-C(28A)	126.54(19)
N(4A)-C(22A)-C(23A)	109.79(16)	O(7A)-C(31A)-C(28A)	110.76(17)
N(4A)-C(22A)-C(27A)	110.60(16)	O(7A)-C(32A)-C(33A)	112.17(19)
C(23A)-C(22A)-C(27A)	110.95(16)	O(7A)-C(32A)-C(33B)	104.14(19)
N(4A)-C(22A)-H(22)	108.5	C(33A)-C(32A)-C(33B)	8.03(19)
C(23A)-C(22A)-H(22)	108.5	O(7A)-C(32A)-H(32A)	109.2
C(27A)-C(22A)-H(22)	108.5	C(33A)-C(32A)-H(32A)	109.2
C(24A)-C(23A)-C(22A)	111.22(18)	C(33B)-C(32A)-H(32A)	113.1
C(24A)-C(23A)-H(23A)	109.4	O(7A)-C(32A)-H(32B)	109.2
C(22A)-C(23A)-H(23A)	109.4	C(33A)-C(32A)-H(32B)	109.2
C(24A)-C(23A)-H(23B)	109.4	C(33B)-C(32A)-H(32B)	113.2
C(22A)-C(23A)-H(23B)	109.4	H(32A)-C(32A)-H(32B)	107.9
H(23A)-C(23A)-H(23B)	108.0	O(7A)-C(32A)-H(32C)	110.9
C(25A)-C(24A)-C(23A)	110.54(18)	C(33A)-C(32A)-H(32C)	106.9
C(25A)-C(24A)-H(24B)	109.5	C(33B)-C(32A)-H(32C)	110.9
C(23A)-C(24A)-H(24B)	109.5	H(32A)-C(32A)-H(32C)	2.4
C(25A)-C(24A)-H(24A)	109.5	H(32B)-C(32A)-H(32C)	108.4
C(23A)-C(24A)-H(24A)	109.5	O(7A)-C(32A)-H(32D)	110.9
H(24B)-C(24A)-H(24A)	108.1	C(33A)-C(32A)-H(32D)	106.8
C(26A)-C(25A)-C(24A)	110.82(17)	C(33B)-C(32A)-H(32D)	110.9
C(26A)-C(25A)-H(25B)	109.5	H(32A)-C(32A)-H(32D)	108.5
C(24A)-C(25A)-H(25B)	109.5	H(32B)-C(32A)-H(32D)	2.4
C(26A)-C(25A)-H(25A)	109.5	H(32C)-C(32A)-H(32D)	108.9
C(24A)-C(25A)-H(25A)	109.5	C(34A)-C(33A)-C(38A)	120.0
H(25B)-C(25A)-H(25A)	108.1	C(34A)-C(33A)-C(32A)	117.1(2)
C(25A)-C(26A)-C(27A)	112.18(18)	C(38A)-C(33A)-C(32A)	122.9(2)
C(25A)-C(26A)-H(26B)	109.2	C(35A)-C(34A)-C(33A)	120.0
C(27A)-C(26A)-H(26B)	109.2	C(35A)-C(34A)-H(34)	120.0
C(25A)-C(26A)-H(26A)	109.2	C(33A)-C(34A)-H(34)	120.0
C(27A)-C(26A)-H(26A)	109.2	C(36A)-C(35A)-C(34A)	120.0
H(26B)-C(26A)-H(26A)	107.9	C(36A)-C(35A)-H(35)	120.0
C(26A)-C(27A)-C(22A)	110.16(17)	C(34A)-C(35A)-H(35)	120.0
C(26A)-C(27A)-C(28A)	112.42(17)	C(37A)-C(36A)-C(35A)	120.0
C(22A)-C(27A)-C(28A)	111.36(15)	C(37A)-C(36A)-H(36)	120.0

C(35A)-C(36A)-H(36)	120.0	C(36B)-C(35B)-C(34B)	120.0
C(36A)-C(37A)-C(38A)	120.0	C(36B)-C(35B)-H(35A)	120.0
C(36A)-C(37A)-H(37)	120.0	C(34B)-C(35B)-H(35A)	120.0
C(38A)-C(37A)-H(37)	120.0	C(37B)-C(36B)-C(35B)	120.0
C(37A)-C(38A)-C(33A)	120.0	C(37B)-C(36B)-H(36A)	120.0
C(37A)-C(38A)-H(38)	120.0	C(35B)-C(36B)-H(36A)	120.0
C(33A)-C(38A)-H(38)	120.0	C(36B)-C(37B)-C(38B)	120.0
C(34B)-C(33B)-C(38B)	120.0	C(36B)-C(37B)-H(37A)	120.0
C(34B)-C(33B)-C(32A)	123.89(19)	C(38B)-C(37B)-H(37A)	120.0
C(38B)-C(33B)-C(32A)	116.11(19)	C(37B)-C(38B)-C(33B)	120.0
C(33B)-C(34B)-C(35B)	120.0	C(37B)-C(38B)-H(38A)	120.0
C(33B)-C(34B)-H(34A)	120.0	C(33B)-C(38B)-H(38A)	120.0
C(35B)-C(34B)-H(34A)	120.0	H(1W)-O(1W)-H(2W)	104.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for gellman124a. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	56(1)	26(1)	32(1)	-3(1)	4(1)	0(1)
O(2)	46(1)	24(1)	38(1)	2(1)	2(1)	-3(1)
O(3)	25(1)	27(1)	40(1)	1(1)	4(1)	-2(1)
O(4)	36(1)	23(1)	38(1)	3(1)	-2(1)	-1(1)
O(5)	30(1)	28(1)	43(1)	1(1)	3(1)	4(1)
O(6)	58(1)	41(1)	35(1)	-8(1)	3(1)	2(1)
O(7)	38(1)	38(1)	32(1)	-2(1)	-2(1)	1(1)
N(1)	43(1)	23(1)	30(1)	2(1)	1(1)	-4(1)
N(2)	24(1)	26(1)	33(1)	-2(1)	-1(1)	2(1)
N(3)	30(1)	21(1)	32(1)	1(1)	0(1)	0(1)
N(4)	24(1)	23(1)	38(1)	1(1)	3(1)	1(1)
C(1)	48(2)	40(1)	52(2)	3(1)	3(1)	7(1)
C(2)	62(2)	43(1)	38(1)	-8(1)	2(1)	4(1)
C(3)	53(2)	43(1)	54(2)	-13(1)	-4(1)	-2(1)
C(4)	45(1)	29(1)	39(1)	-7(1)	-2(1)	3(1)
C(5)	38(1)	28(1)	31(1)	-2(1)	-4(1)	-3(1)
C(6)	32(1)	24(1)	31(1)	1(1)	-1(1)	0(1)
C(7)	42(1)	27(1)	40(1)	0(1)	-3(1)	4(1)
C(8)	30(1)	16(1)	33(1)	-2(1)	0(1)	-1(1)
C(9)	28(1)	23(1)	31(1)	-2(1)	-2(1)	1(1)
C(10)	43(1)	27(1)	36(1)	-4(1)	-2(1)	6(1)
C(11)	53(1)	33(1)	33(1)	-5(1)	-3(1)	2(1)
C(12)	49(1)	33(1)	31(1)	1(1)	-8(1)	0(1)
C(13)	40(1)	27(1)	36(1)	2(1)	-3(1)	2(1)
C(14)	26(1)	23(1)	30(1)	0(1)	0(1)	-1(1)
C(15)	29(1)	21(1)	34(1)	1(1)	0(1)	-2(1)
C(16)	33(1)	26(1)	47(1)	-3(1)	5(1)	-5(1)
C(17)	34(1)	37(1)	58(2)	-3(1)	14(1)	0(1)
C(18)	25(1)	24(1)	32(1)	-1(1)	6(1)	0(1)
C(19)	27(1)	23(1)	37(1)	-2(1)	3(1)	0(1)
C(20)	42(1)	32(1)	39(1)	-5(1)	4(1)	-7(1)
C(21)	24(1)	21(1)	33(1)	-4(1)	-3(1)	-2(1)
C(22)	27(1)	25(1)	40(1)	0(1)	2(1)	-1(1)
C(23)	34(1)	27(1)	44(1)	-2(1)	-4(1)	-6(1)
C(24)	39(1)	24(1)	54(1)	3(1)	-2(1)	-10(1)
C(25)	50(1)	27(1)	43(1)	2(1)	4(1)	-10(1)
C(26)	47(1)	26(1)	42(1)	0(1)	5(1)	-6(1)
C(27)	32(1)	22(1)	38(1)	-1(1)	3(1)	-2(1)
C(28)	35(1)	22(1)	36(1)	0(1)	3(1)	-3(1)
C(29)	42(1)	28(1)	53(1)	-7(1)	2(1)	0(1)
C(30)	46(1)	26(1)	60(2)	-6(1)	2(1)	2(1)
C(31)	38(1)	21(1)	35(1)	-1(1)	5(1)	-8(1)
C(32)	46(1)	44(1)	34(1)	1(1)	-8(1)	0(1)
C(33)	44(1)	40(1)	39(1)	-12(1)	-3(1)	0(1)
C(34)	46(2)	37(1)	102(2)	-14(1)	12(2)	-3(1)
C(35)	57(2)	46(2)	126(3)	-13(2)	13(2)	-16(1)
C(36)	47(2)	78(2)	77(2)	-22(2)	5(1)	-19(2)
C(37)	37(2)	89(2)	59(2)	-6(2)	-7(1)	5(1)
C(38)	48(2)	58(2)	51(2)	0(1)	-10(1)	8(1)
O(1A)	63(1)	24(1)	29(1)	2(1)	-1(1)	0(1)
O(2A)	47(1)	23(1)	36(1)	-3(1)	-1(1)	-1(1)

O(3A)	30(1)	26(1)	39(1)	-1(1)	-4(1)	-2(1)
O(4A)	36(1)	25(1)	40(1)	-5(1)	4(1)	-1(1)
O(5A)	26(1)	29(1)	47(1)	-5(1)	-3(1)	3(1)
O(6A)	54(1)	49(1)	31(1)	1(1)	-2(1)	12(1)
O(7A)	34(1)	37(1)	33(1)	3(1)	3(1)	2(1)
N(1A)	44(1)	23(1)	30(1)	-1(1)	-1(1)	-2(1)
N(2A)	25(1)	25(1)	34(1)	1(1)	0(1)	1(1)
N(3A)	29(1)	21(1)	34(1)	-3(1)	1(1)	0(1)
N(4A)	25(1)	22(1)	36(1)	0(1)	-2(1)	2(1)
C(1A)	49(2)	37(1)	52(2)	0(1)	-2(1)	4(1)
C(2A)	84(2)	39(1)	44(1)	8(1)	-7(1)	5(1)
C(3A)	57(2)	40(1)	50(2)	12(1)	9(1)	-5(1)
C(4A)	52(1)	25(1)	37(1)	6(1)	0(1)	2(1)
C(5A)	35(1)	25(1)	34(1)	-1(1)	6(1)	-3(1)
C(6A)	31(1)	25(1)	33(1)	-1(1)	2(1)	-1(1)
C(7A)	43(1)	28(1)	41(1)	0(1)	4(1)	6(1)
C(8A)	30(1)	14(1)	36(1)	3(1)	0(1)	-1(1)
C(9A)	29(1)	25(1)	33(1)	1(1)	1(1)	0(1)
C(10A)	36(1)	34(1)	38(1)	7(1)	-3(1)	0(1)
C(11A)	47(1)	36(1)	33(1)	8(1)	-1(1)	-3(1)
C(12A)	42(1)	44(1)	31(1)	0(1)	2(1)	-7(1)
C(13A)	37(1)	34(1)	34(1)	-5(1)	4(1)	-4(1)
C(14A)	27(1)	23(1)	33(1)	-1(1)	-1(1)	-3(1)
C(15A)	28(1)	24(1)	31(1)	-2(1)	0(1)	0(1)
C(16A)	28(1)	24(1)	49(1)	0(1)	-4(1)	-3(1)
C(17A)	33(1)	32(1)	56(1)	2(1)	-11(1)	-2(1)
C(18A)	23(1)	26(1)	33(1)	-3(1)	-4(1)	3(1)
C(19A)	28(1)	22(1)	36(1)	0(1)	0(1)	1(1)
C(20A)	37(1)	29(1)	39(1)	2(1)	-2(1)	-5(1)
C(21A)	25(1)	19(1)	35(1)	2(1)	1(1)	-1(1)
C(22A)	28(1)	23(1)	40(1)	-2(1)	-2(1)	-1(1)
C(23A)	35(1)	25(1)	45(1)	0(1)	6(1)	-4(1)
C(24A)	34(1)	24(1)	58(2)	-5(1)	1(1)	-8(1)
C(25A)	43(1)	28(1)	48(1)	-5(1)	-6(1)	-4(1)
C(26A)	43(1)	31(1)	39(1)	-4(1)	-4(1)	-2(1)
C(27A)	32(1)	24(1)	37(1)	-1(1)	-2(1)	0(1)
C(28A)	33(1)	24(1)	34(1)	0(1)	0(1)	0(1)
C(29A)	36(1)	28(1)	47(1)	3(1)	1(1)	3(1)
C(30A)	47(1)	28(1)	47(1)	4(1)	4(1)	2(1)
C(31A)	38(1)	21(1)	36(1)	-3(1)	-3(1)	1(1)
C(32A)	40(1)	41(1)	36(1)	2(1)	7(1)	6(1)
C(33A)	32(1)	43(1)	37(2)	6(1)	8(1)	8(1)
C(34A)	38(1)	48(1)	43(1)	4(1)	2(1)	7(1)
C(35A)	36(1)	70(1)	63(2)	2(1)	-2(1)	1(1)
C(36A)	44(2)	76(2)	77(4)	-5(3)	-4(2)	-16(2)
C(37A)	36(1)	70(1)	63(2)	2(1)	-2(1)	1(1)
C(38A)	38(1)	48(1)	43(1)	4(1)	2(1)	7(1)
C(33B)	32(1)	43(1)	37(2)	6(1)	8(1)	8(1)
C(34B)	38(1)	48(1)	43(1)	4(1)	2(1)	7(1)
C(35B)	36(1)	70(1)	63(2)	2(1)	-2(1)	1(1)
C(36B)	44(2)	76(2)	77(4)	-5(3)	-4(2)	-16(2)
C(37B)	36(1)	70(1)	63(2)	2(1)	-2(1)	1(1)
C(38B)	38(1)	48(1)	43(1)	4(1)	2(1)	7(1)
O(1W)	75(1)	39(1)	55(1)	0(1)	4(1)	13(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for gellman124a.

	x	y	z	U(eq)
H(1)	-1024(15)	-8116(14)	-1222(8)	39
H(2)	-1713(15)	-8355(12)	264(8)	33
H(3)	-1152(14)	-10494(13)	-215(8)	33
H(4)	-1226(15)	-12650(13)	516(8)	34
H(1B)	436	-10205	-1356	70
H(1D)	40	-10995	-1534	70
H(1C)	-340	-10548	-1090	70
H(2C)	-537	-9561	-2397	71
H(2D)	-34	-10346	-2347	71
H(2B)	309	-9565	-2121	71
H(3C)	-1693	-10539	-1518	75
H(3D)	-1307	-10948	-1974	75
H(3B)	-1754	-10134	-2027	75
H(6)	-2083	-8412	-511	35
H(7B)	-2017	-7082	-340	54
H(7C)	-2193	-7183	-895	54
H(7A)	-1301	-6968	-716	54
H(9)	-128	-8219	541	33
H(10C)	-1033	-7382	927	42
H(10D)	-1588	-8090	1090	42
H(11D)	-801	-7703	1738	47
H(11C)	13	-7784	1433	47
H(12D)	-1010	-9047	1709	45
H(12C)	-122	-8887	1916	45
H(13D)	-70	-9871	1330	41
H(13C)	457	-9144	1166	41
H(14A)	-1155	-9468	840	32
H(15A)	-459	-9524	54	33
H(16C)	875	-9230	328	42
H(16D)	892	-10033	608	42
H(17D)	746	-9916	-402	65
H(17F)	799	-10712	-117	65
H(17E)	1564	-10147	-133	65
H(19A)	-778	-11934	-18	35
H(20D)	-2036	-11361	-623	56
H(20F)	-1782	-12250	-598	56
H(20E)	-1156	-11624	-796	56
H(22A)	-2716	-12426	970	37
H(23C)	-2835	-13519	474	42
H(23D)	-2044	-13895	706	42
H(24C)	-3551	-13649	1187	47
H(24D)	-3187	-14474	1047	47
H(25C)	-2135	-14333	1596	48
H(25D)	-2975	-14195	1867	48
H(26D)	-2016	-13231	2077	46
H(26C)	-2793	-12851	1831	46
H(27A)	-1304	-13173	1348	36
H(28A)	-1098	-11821	1291	37
H(29C)	-2482	-11411	1430	49
H(29D)	-2336	-11566	1984	49

H(30D)	-1421	-10473	1440	65
H(30F)	-1307	-10615	1997	65
H(30E)	-2127	-10241	1801	65
H(32F)	511	-13297	2213	50
H(32E)	217	-12558	2508	50
H(34B)	655	-11305	1883	74
H(35B)	1848	-10681	1679	92
H(36B)	3087	-11313	1762	81
H(37B)	3115	-12585	2000	74
H(38B)	1930	-13213	2197	63
H(1A)	-4395(15)	-11802(14)	-1239(8)	39
H(2A)	-3837(15)	-11610(13)	279(8)	33
H(3A)	-4289(14)	-9434(13)	-198(8)	34
H(4A)	-4248(15)	-7291(13)	558(8)	34
H(1AB)	-5061	-9333	-1092	69
H(1AC)	-5766	-9672	-1421	69
H(1AA)	-5342	-8873	-1556	69
H(2AA)	-5011	-9433	-2365	84
H(2AC)	-5454	-10210	-2203	84
H(2AB)	-4541	-10238	-2392	84
H(3AA)	-3855	-8921	-1862	74
H(3AC)	-3425	-9747	-1889	74
H(3AB)	-3622	-9368	-1384	74
H(6A)	-3414	-11564	-482	36
H(7AC)	-4198	-12980	-742	56
H(7AB)	-3511	-12903	-345	56
H(7AA)	-3292	-12763	-892	56
H(9A)	-5421	-11726	529	35
H(10B)	-4598	-12607	936	43
H(10A)	-4017	-11928	1115	43
H(11A)	-4893	-12275	1738	46
H(11B)	-5668	-12132	1407	46
H(12A)	-5475	-11042	1903	47
H(12B)	-4568	-10943	1711	47
H(13A)	-5432	-10062	1316	42
H(13B)	-5997	-10757	1142	42
H(14)	-4353	-10524	847	33
H(15)	-4970	-10426	48	33
H(16B)	-6340	-10719	269	40
H(16A)	-6385	-9916	547	40
H(17B)	-6124	-10037	-454	61
H(17A)	-6201	-9239	-172	61
H(17C)	-6968	-9798	-218	61
H(19)	-4713	-8002	29	34
H(20A)	-3707	-7624	-538	53
H(20C)	-4334	-8234	-754	53
H(20B)	-3452	-8510	-593	53
H(22)	-2806	-7565	1044	36
H(23A)	-2609	-6462	566	42
H(23B)	-3392	-6058	790	42
H(24B)	-1936	-6407	1304	47
H(24A)	-2225	-5557	1160	47
H(25B)	-2544	-5822	1968	47
H(25A)	-3349	-5650	1670	47
H(26B)	-3564	-6745	2144	45
H(26A)	-2779	-7154	1927	45

H(27)	-4224	-6806	1405	37
H(28)	-4404	-8162	1323	37
H(29A)	-3003	-8528	1510	44
H(29B)	-3252	-8449	2057	44
H(30A)	-3940	-9517	1396	61
H(30C)	-4306	-9391	1916	61
H(30B)	-3415	-9738	1853	61
H(32A)	-6221	-6861	2178	47
H(32B)	-5846	-7522	2508	47
H(32C)	-6245	-6868	2179	47
H(32D)	-5868	-7535	2510	47
H(34)	-6100	-8903	2167	52
H(35)	-7170	-9755	2022	68
H(36)	-8456	-9275	1840	79
H(37)	-8672	-7943	1803	68
H(38)	-7602	-7091	1948	52
H(34A)	-5989	-8901	1866	52
H(35A)	-7049	-9695	1613	68
H(36A)	-8377	-9227	1609	79
H(37A)	-8645	-7966	1857	68
H(38A)	-7585	-7172	2111	52
H(1W)	-2830	-9566	541	84
H(2W)	-2654	-10423	553	84

Table 6. Torsion angles [°] for gellman124a.

C(5)-O(1)-C(4)-C(1)	-62.0(3)	C(24)-C(25)-C(26)-C(27)	-56.6(3)
C(5)-O(1)-C(4)-C(3)	62.5(3)	C(25)-C(26)-C(27)-C(22)	57.7(2)
C(5)-O(1)-C(4)-C(2)	-179.26(19)	C(25)-C(26)-C(27)-C(28)	-176.19(18)
C(4)-O(1)-C(5)-O(2)	6.1(3)	N(4)-C(22)-C(27)-C(26)	-178.65(16)
C(4)-O(1)-C(5)-N(1)	-172.75(18)	C(23)-C(22)-C(27)-C(26)	-57.1(2)
C(6)-N(1)-C(5)-O(2)	12.2(3)	N(4)-C(22)-C(27)-C(28)	55.4(2)
C(6)-N(1)-C(5)-O(1)	-168.94(18)	C(23)-C(22)-C(27)-C(28)	176.93(17)
C(5)-N(1)-C(6)-C(8)	64.3(2)	C(26)-C(27)-C(28)-C(31)	66.2(2)
C(5)-N(1)-C(6)-C(7)	-174.62(19)	C(22)-C(27)-C(28)-C(31)	-169.32(16)
C(9)-N(2)-C(8)-O(3)	1.6(3)	C(26)-C(27)-C(28)-C(29)	-58.9(2)
C(9)-N(2)-C(8)-C(6)	-177.30(16)	C(22)-C(27)-C(28)-C(29)	65.6(2)
N(1)-C(6)-C(8)-O(3)	28.6(2)	C(31)-C(28)-C(29)-C(30)	68.0(2)
C(7)-C(6)-C(8)-O(3)	-92.0(2)	C(27)-C(28)-C(29)-C(30)	-167.67(19)
N(1)-C(6)-C(8)-N(2)	-152.47(16)	C(32)-O(7)-C(31)-O(6)	-2.4(3)
C(7)-C(6)-C(8)-N(2)	86.9(2)	C(32)-O(7)-C(31)-C(28)	178.49(16)
C(8)-N(2)-C(9)-C(10)	137.80(18)	C(29)-C(28)-C(31)-O(6)	12.1(3)
C(8)-N(2)-C(9)-C(14)	-99.3(2)	C(27)-C(28)-C(31)-O(6)	-115.2(2)
N(2)-C(9)-C(10)-C(11)	178.03(17)	C(29)-C(28)-C(31)-O(7)	-168.84(16)
C(14)-C(9)-C(10)-C(11)	55.4(2)	C(27)-C(28)-C(31)-O(7)	63.8(2)
C(9)-C(10)-C(11)-C(12)	-55.4(3)	C(31)-O(7)-C(32)-C(33)	-112.5(2)
C(10)-C(11)-C(12)-C(13)	56.0(3)	O(7)-C(32)-C(33)-C(38)	-134.9(2)
C(11)-C(12)-C(13)-C(14)	-58.0(2)	O(7)-C(32)-C(33)-C(34)	44.1(3)
N(2)-C(9)-C(14)-C(13)	-175.02(16)	C(38)-C(33)-C(34)-C(35)	-0.7(4)
C(10)-C(9)-C(14)-C(13)	-54.3(2)	C(32)-C(33)-C(34)-C(35)	-179.7(3)
N(2)-C(9)-C(14)-C(15)	58.9(2)	C(33)-C(34)-C(35)-C(36)	-0.8(5)
C(10)-C(9)-C(14)-C(15)	179.58(16)	C(34)-C(35)-C(36)-C(37)	2.1(5)
C(12)-C(13)-C(14)-C(9)	56.4(2)	C(35)-C(36)-C(37)-C(38)	-1.8(5)
C(12)-C(13)-C(14)-C(15)	-179.30(16)	C(36)-C(37)-C(38)-C(33)	0.2(4)
C(9)-C(14)-C(15)-C(18)	-150.29(16)	C(34)-C(33)-C(38)-C(37)	1.0(4)
C(13)-C(14)-C(15)-C(18)	86.3(2)	C(32)-C(33)-C(38)-C(37)	-179.9(2)
C(9)-C(14)-C(15)-C(16)	85.5(2)	C(5A)-O(1A)-C(4A)-C(3A)	59.1(3)
C(13)-C(14)-C(15)-C(16)	-37.9(2)	C(5A)-O(1A)-C(4A)-C(2A)	177.1(2)
C(18)-C(15)-C(16)-C(17)	61.2(2)	C(5A)-O(1A)-C(4A)-C(1A)	-65.9(3)
C(14)-C(15)-C(16)-C(17)	-173.04(17)	C(4A)-O(1A)-C(5A)-O(2A)	6.1(3)
C(19)-N(3)-C(18)-O(4)	-5.8(3)	C(4A)-O(1A)-C(5A)-N(1A)	-171.81(18)
C(19)-N(3)-C(18)-C(15)	171.79(16)	C(6A)-N(1A)-C(5A)-O(2A)	7.3(3)
C(16)-C(15)-C(18)-O(4)	61.1(2)	C(6A)-N(1A)-C(5A)-O(1A)	-174.76(18)
C(14)-C(15)-C(18)-O(4)	-66.3(2)	C(5A)-N(1A)-C(6A)-C(8A)	67.3(2)
C(16)-C(15)-C(18)-N(3)	-116.49(19)	C(5A)-N(1A)-C(6A)-C(7A)	-171.71(19)
C(14)-C(15)-C(18)-N(3)	116.10(19)	C(9A)-N(2A)-C(8A)-O(3A)	-2.2(3)
C(18)-N(3)-C(19)-C(20)	-165.70(18)	C(9A)-N(2A)-C(8A)-C(6A)	179.21(16)
C(18)-N(3)-C(19)-C(21)	72.7(2)	N(1A)-C(6A)-C(8A)-O(3A)	31.1(2)
C(22)-N(4)-C(21)-O(5)	-2.1(3)	C(7A)-C(6A)-C(8A)-O(3A)	-89.8(2)
C(22)-N(4)-C(21)-C(19)	-179.41(17)	N(1A)-C(6A)-C(8A)-N(2A)	-150.28(16)
N(3)-C(19)-C(21)-O(5)	57.9(2)	C(7A)-C(6A)-C(8A)-N(2A)	88.8(2)
C(20)-C(19)-C(21)-O(5)	-63.7(2)	C(8A)-N(2A)-C(9A)-C(10A)	136.98(18)
N(3)-C(19)-C(21)-N(4)	-124.68(18)	C(8A)-N(2A)-C(9A)-C(14A)	-99.3(2)
C(20)-C(19)-C(21)-N(4)	113.68(19)	N(2A)-C(9A)-C(10A)-C(11A)	178.37(17)
C(21)-N(4)-C(22)-C(23)	113.0(2)	C(14A)-C(9A)-C(10A)-C(11A)	55.2(2)
C(21)-N(4)-C(22)-C(27)	-125.29(19)	C(9A)-C(10A)-C(11A)-C(12A)	-56.7(2)
N(4)-C(22)-C(23)-C(24)	178.48(17)	C(10A)-C(11A)-C(12A)-C(13A)	57.8(2)
C(27)-C(22)-C(23)-C(24)	56.5(2)	C(11A)-C(12A)-C(13A)-C(14A)	-58.5(2)
C(22)-C(23)-C(24)-C(25)	-55.3(2)	C(12A)-C(13A)-C(14A)-C(9A)	55.5(2)
C(23)-C(24)-C(25)-C(26)	54.7(3)	C(12A)-C(13A)-C(14A)-C(15A)	179.86(16)

N(2A)-C(9A)-C(14A)-C(13A)	-175.24(16)	C(22A)-C(27A)-C(28A)-C(31A)	-168.94(17)
C(10A)-C(9A)-C(14A)-C(13A)	-53.3(2)	C(26A)-C(27A)-C(28A)-C(29A)	-57.8(2)
N(2A)-C(9A)-C(14A)-C(15A)	58.5(2)	C(22A)-C(27A)-C(28A)-C(29A)	66.4(2)
C(10A)-C(9A)-C(14A)-C(15A)	-179.57(17)	C(31A)-C(28A)-C(29A)-C(30A)	72.9(2)
C(13A)-C(14A)-C(15A)-C(18A)	82.1(2)	C(27A)-C(28A)-C(29A)-C(30A)	-162.91(18)
C(9A)-C(14A)-C(15A)-C(18A)	-153.96(16)	C(32A)-O(7A)-C(31A)-O(6A)	-3.3(3)
C(13A)-C(14A)-C(15A)-C(16A)	-41.5(2)	C(32A)-O(7A)-C(31A)-C(28A)	176.56(16)
C(9A)-C(14A)-C(15A)-C(16A)	82.4(2)	C(29A)-C(28A)-C(31A)-O(6A)	17.1(3)
C(18A)-C(15A)-C(16A)-C(17A)	62.1(2)	C(27A)-C(28A)-C(31A)-O(6A)	-110.2(2)
C(14A)-C(15A)-C(16A)-C(17A)	-172.38(17)	C(29A)-C(28A)-C(31A)-O(7A)	-162.73(16)
C(19A)-N(3A)-C(18A)-O(4A)	-6.0(3)	C(27A)-C(28A)-C(31A)-O(7A)	70.0(2)
C(19A)-N(3A)-C(18A)-C(15A)	171.07(16)	C(31A)-O(7A)-C(32A)-C(33A)	-109.3(2)
C(16A)-C(15A)-C(18A)-O(4A)	64.1(2)	C(31A)-O(7A)-C(32A)-C(33B)	-109.4(3)
C(14A)-C(15A)-C(18A)-O(4A)	-63.2(2)	O(7A)-C(32A)-C(33A)-C(34A)	62.9(3)
C(16A)-C(15A)-C(18A)-N(3A)	-113.01(19)	C(33B)-C(32A)-C(33A)-C(34A)	63(2)
C(14A)-C(15A)-C(18A)-N(3A)	119.70(18)	O(7A)-C(32A)-C(33A)-C(38A)	-119.0(2)
C(18A)-N(3A)-C(19A)-C(20A)	-164.34(17)	C(33B)-C(32A)-C(33A)-C(38A)	-119(2)
C(18A)-N(3A)-C(19A)-C(21A)	73.6(2)	C(38A)-C(33A)-C(34A)-C(35A)	0.0
C(22A)-N(4A)-C(21A)-O(5A)	-3.6(3)	C(32A)-C(33A)-C(34A)-C(35A)	178.2(3)
C(22A)-N(4A)-C(21A)-C(19A)	178.63(17)	C(33A)-C(34A)-C(35A)-C(36A)	0.0
N(3A)-C(19A)-C(21A)-O(5A)	55.8(2)	C(34A)-C(35A)-C(36A)-C(37A)	0.0
C(20A)-C(19A)-C(21A)-O(5A)	-66.4(2)	C(35A)-C(36A)-C(37A)-C(38A)	0.0
N(3A)-C(19A)-C(21A)-N(4A)	-126.34(18)	C(36A)-C(37A)-C(38A)-C(33A)	0.0
C(20A)-C(19A)-C(21A)-N(4A)	111.47(19)	C(34A)-C(33A)-C(38A)-C(37A)	0.0
C(21A)-N(4A)-C(22A)-C(23A)	111.5(2)	C(32A)-C(33A)-C(38A)-C(37A)	-178.1(3)
C(21A)-N(4A)-C(22A)-C(27A)	-125.69(19)	O(7A)-C(32A)-C(33B)-C(34B)	43.4(4)
N(4A)-C(22A)-C(23A)-C(24A)	179.13(17)	C(33A)-C(32A)-C(33B)-C(34B)	-136(3)
C(27A)-C(22A)-C(23A)-C(24A)	56.6(2)	O(7A)-C(32A)-C(33B)-C(38B)	-136.83(13)
C(22A)-C(23A)-C(24A)-C(25A)	-57.1(2)	C(33A)-C(32A)-C(33B)-C(38B)	44(2)
C(23A)-C(24A)-C(25A)-C(26A)	56.6(2)	C(38B)-C(33B)-C(34B)-C(35B)	0.0
C(24A)-C(25A)-C(26A)-C(27A)	-56.3(3)	C(32A)-C(33B)-C(34B)-C(35B)	179.8(5)
C(25A)-C(26A)-C(27A)-C(22A)	55.2(2)	C(33B)-C(34B)-C(35B)-C(36B)	0.0
C(25A)-C(26A)-C(27A)-C(28A)	-179.99(18)	C(34B)-C(35B)-C(36B)-C(37B)	0.0
N(4A)-C(22A)-C(27A)-C(26A)	-176.89(15)	C(35B)-C(36B)-C(37B)-C(38B)	0.0
C(23A)-C(22A)-C(27A)-C(26A)	-54.8(2)	C(36B)-C(37B)-C(38B)-C(33B)	0.0
N(4A)-C(22A)-C(27A)-C(28A)	57.7(2)	C(34B)-C(33B)-C(38B)-C(37B)	0.0
C(23A)-C(22A)-C(27A)-C(28A)	179.77(17)	C(32A)-C(33B)-C(38B)-C(37B)	-179.8(5)
C(26A)-C(27A)-C(28A)-C(31A)	66.9(2)		

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for gellman124a [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(2)-H(2)...O(5A)	0.85(2)	2.06(2)	2.909(2)	177(2)
N(4)-H(4)...O(3A)#1	0.90(2)	1.92(2)	2.814(2)	168(2)
N(2A)-H(2A)...O(5)	0.83(2)	2.13(2)	2.952(2)	172(2)
N(4A)-H(4A)...O(3)#2	0.88(2)	1.95(2)	2.816(2)	170(2)
O(1W)-H(2W)...O(5)	0.96	1.93	2.858(2)	162
N(1)-H(1)...O(7A)#3	0.82(2)	2.33(2)	3.121(2)	164(2)
N(3)-H(3)...O(2)	0.83(2)	2.31(2)	3.135(2)	173(2)
N(3A)-H(3A)...O(2A)	0.84(2)	2.27(2)	3.102(2)	170(2)
O(1W)-H(1W)...O(5A)	0.96	1.97	2.867(2)	154
N(1A)-H(1A)...O(7)#4	0.82(2)	2.41(2)	3.219(2)	171(2)

Symmetry transformations used to generate equivalent atoms:
#1 x+1/2,-y-5/2,-z #2 x-1/2,-y-3/2,-z #3 x+1/2,-y-3/2,-z
#4 x-1/2,-y-5/2,-z