Crystal Structure Report for LewClark_brucine

A colorless plate-like specimen of $C_{31}H_{37}N_2O_6PS$, approximate dimensions 0.080 mm x 0.300 mm x 0.400 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured on a Bruker SMART X2S benchtop diffractometer system equipped with a doubly curved silicon crystal monochromator and a MoK_α microfocus source (λ = 0.71073 Å).

Table 1: Data collection details for LewClark_brucine.

Axis	dx/mm	2θ/°	ω/°	φ/°	χ/°	Width/°	Frames	Time/s	Wavelength/Å	Voltage/kV	Current/mA	Temperature/K
Omega	40.164	-20.00	340.00	0.00	35.13	0.50	360	60.00	0.71073	50	1.0	198.00
Omega	40.164	-20.00	340.00	60.00	35.13	0.50	360	60.00	0.71073	50	1.0	198.00
Omega	40.164	-20.00	340.00	120.00	35.13	0.50	360	60.00	0.71073	50	1.0	198.00
Omega	40.164	-20.00	340.00	180.00	35.13	0.50	360	60.00	0.71073	50	1.0	198.00
Omega	40.164	-20.00	340.00	240.00	35.13	0.50	360	60.00	0.71073	50	1.0	198.00
Omega	40.164	-20.00	340.00	300.00	35.13	0.50	360	60.00	0.71073	50	1.0	198.00

A total of 2160 frames were collected. The total exposure time was 36.00 hours. The frames were integrated with the Bruker SAINT software package using a SAINT v7.68 (Bruker, 2009) algorithm. The integration of the data using a monoclinic unit cell yielded a total of 23505 reflections to a maximum θ angle of 25.02° (0.84 Å resolution), of which 5180 were independent (average redundancy 4.538, completeness = 99.4%, R_{int} = 7.06%, R_{sig} = 5.69%) and 4240 (81.85%) were greater than $2\sigma(F^2)$. The final cell constants of a = 8.608(2) Å, b = 14.461(3) Å, c = 12.669(4) Å, β = 109.748(9)°, volume = 1484.3(7) $Å^3$, are based upon the refinement of the XYZ-centroids of 7888 reflections above 20 σ(I) with 4.429° < 2θ < 44.58°. Data were corrected for absorption effects using the multi-scan method (SADABS). The ratio of minimum to maximum apparent transmission was 0.707. The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.9208 and 0.9834.

The structure was solved and refined using the Bruker SHELXTL Software Package, using the space group P 1 21 1, with Z = 2 for the formula unit, $C_{31}H_{37}N_2O_6PS$. The final anisotropic full-matrix least-squares refinement on F^2 with 377 variables converged at R1 = 4.28%, for the observed data and wR2 = 10.98% for all data. The goodness-of-fit was 1.024. The largest peak in the final difference electron density synthesis was 0.350 $e^-/Å^3$ and the largest hole was -0.261 $e^-/Å^3$ with an RMS deviation of 0.039 $e^-/Å^3$. On the basis of the final model, the calculated density was 1.335 g/cm^3 and F(000), 632 e^-.

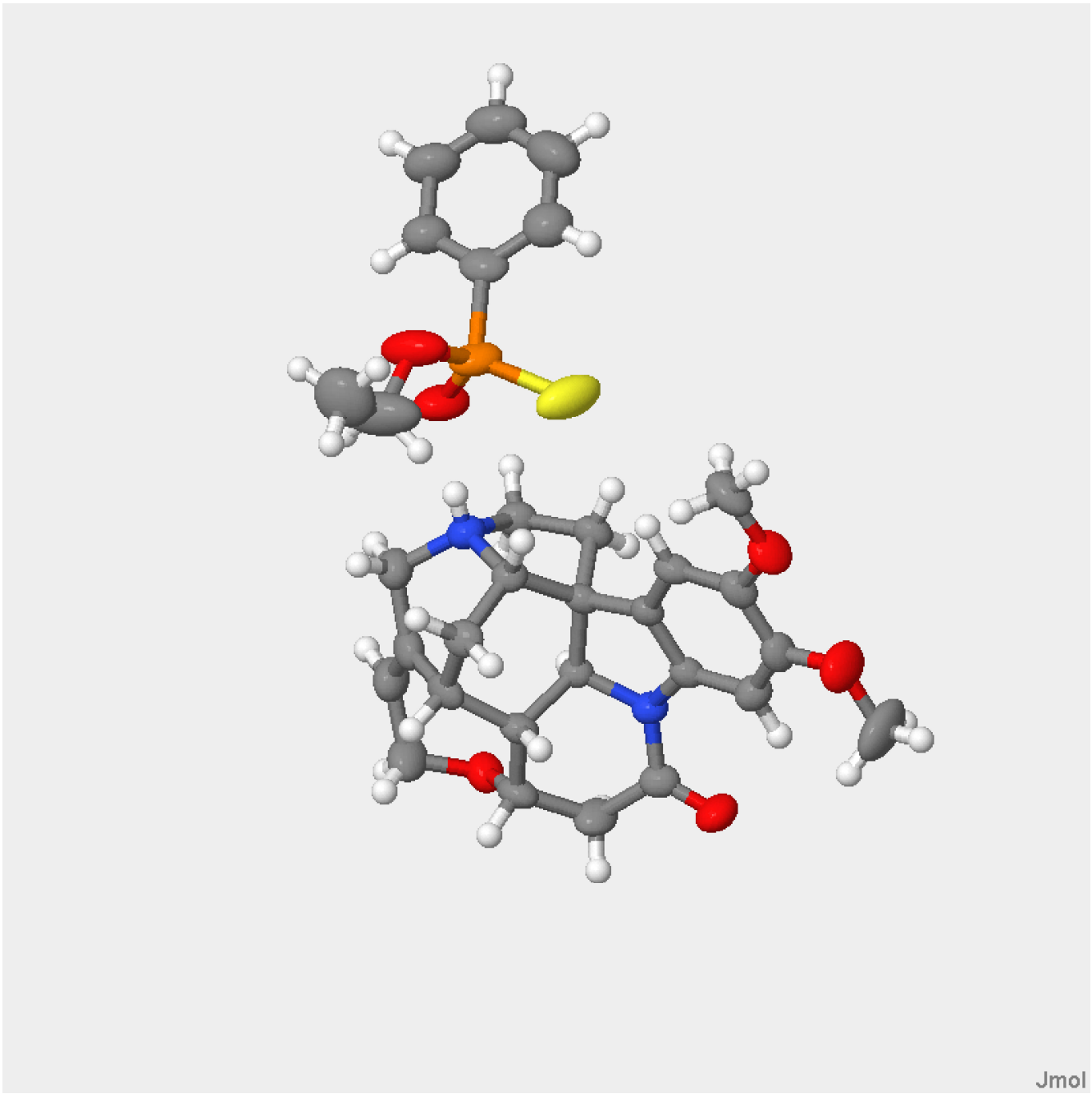

Table 2. Sample and crystal data for LewClark_brucine.

Identification code	LewClark_brucine	
Chemical formula	$C_{31}H_{37}N_2O_6PS$	
Formula weight	596.66	
Temperature	199(2) K	
Wavelength	0.71073 Å	
Crystal size	0.080 x 0.300 x 0.400 mm	
Crystal habit	colorless plate	
Crystal system	monoclinic	
Space group	P 1 21 1	
Unit cell dimensions	a = 8.608(2) Å	α = 90°
	b = 14.461(3) Å	β = 109.748(9)°

	c = 12.669(4) Å	γ = 90°
Volume	1484.3(7) $Å^3$	
Z	2	
Density (calculated)	1.335 Mg/cm^3	
Absorption coefficient	0.210 mm^{-1}	
F(000)	632	

Table 3. Data collection and structure refinement for LewClark_brucine.

Diffractometer	Bruker SMART X2S benchtop diffractometer
Radiation source	microfocus source, MoK_α
Theta range for data collection	2.52 to 25.02°
Index ranges	-10<=h<=10, -17<=k<=17, -15<=l<=15
Reflections collected	23505
Independent reflections	5180 [R(int) = 0.0706]
Coverage of independent reflections	99.4%
Absorption correction	multi-scan
Max. and min. transmission	0.9834 and 0.9208
Structure solution technique	direct methods
Structure solution program	SHELXS-97 (Sheldrick, 2008)
Refinement method	Full-matrix least-squares on F^2
Refinement program	SHELXL-97 (Sheldrick, 2008)
Function minimized	$\Sigma\ w(F_o^2 - F_c^2)^2$
Data / restraints / parameters	5180 / 1 / 377
Goodness-of-fit on F^2	1.024
Final R indices	4240 data; I>2σ(I) R1 = 0.0428, wR2 = 0.1023 all data R1 = 0.0581, wR2 = 0.1098
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0508P)^2+0.2209P]$ where $P=(F_o^2+2F_c^2)/3$
Absolute structure parameter	0.1(1)
Largest diff. peak and hole	0.350 and -0.261 $eÅ^{-3}$
R.M.S. deviation from mean	0.039 $eÅ^{-3}$

Table 4. Atomic coordinates and equivalent isotropic atomic displacement parameters ($Å^2$) for LewClark_brucine.

U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x/a	y/b	z/c	U(eq)
N1	0.3247(3)	0.37055(17)	0.6653(2)	0.0388(6)
N2	0.4028(3)	0.50761(14)	0.00892(18)	0.0328(5)
O1	0.0708(3)	0.35363(18)	0.2090(2)	0.0643(7)
O2	0.9540(3)	0.24372(15)	0.04016(19)	0.0506(6)
O3	0.7410(2)	0.58468(14)	0.90184(18)	0.0439(5)
O4	0.5059(3)	0.56997(16)	0.18291(18)	0.0514(6)
C1	0.1275(4)	0.3693(2)	0.1214(2)	0.0399(7)
C2	0.0658(3)	0.3074(2)	0.0296(2)	0.0385(7)
C3	0.1158(3)	0.31632(18)	0.9372(2)	0.0337(6)
C4	0.2292(3)	0.38578(18)	0.9363(2)	0.0304(6)

	x/a	y/b	z/c	U(eq)
C5	0.2932(3)	0.41338(18)	0.8437(2)	0.0304(6)
C6	0.1605(3)	0.4612(2)	0.7448(2)	0.0364(6)
C7	0.2359(4)	0.46143(19)	0.6525(2)	0.0396(7)
C8	0.4853(4)	0.3782(2)	0.6427(3)	0.0471(8)
C9	0.6131(4)	0.4243(2)	0.7406(3)	0.0417(7)
C10	0.6941(4)	0.4990(3)	0.7292(3)	0.0531(8)
C11	0.8167(4)	0.5477(3)	0.8267(3)	0.0585(9)
C12	0.7311(3)	0.5229(2)	0.9872(3)	0.0408(7)
C13	0.6741(4)	0.5833(2)	0.0657(3)	0.0506(8)
C14	0.5222(4)	0.55230(19)	0.0936(2)	0.0385(7)
C15	0.2867(3)	0.44500(19)	0.0264(2)	0.0302(6)
C16	0.2379(4)	0.4390(2)	0.1202(2)	0.0392(7)
C17	0.4367(3)	0.48093(18)	0.9048(2)	0.0304(6)
C18	0.6110(3)	0.44146(19)	0.9423(2)	0.0342(6)
C19	0.6399(3)	0.37826(19)	0.8534(2)	0.0384(7)
C20	0.5192(3)	0.2974(2)	0.8379(3)	0.0406(7)
C21	0.3452(3)	0.33246(18)	0.7818(2)	0.0333(6)
C22	0.1328(6)	0.4101(3)	0.3051(3)	0.0857(14)
C23	0.9004(4)	0.1757(2)	0.9551(3)	0.0523(9)
P1	0.99506(12)	0.19490(6)	0.52723(7)	0.0534(2)
S1	0.94002(17)	0.19250(10)	0.66540(8)	0.0904(4)
O5	0.0542(3)	0.09466(17)	0.5014(2)	0.0779(9)
O6	0.1206(3)	0.26474(18)	0.5210(2)	0.0631(7)
C24	0.8128(4)	0.2094(2)	0.4031(3)	0.0491(8)
C25	0.8333(4)	0.2235(2)	0.3003(3)	0.0527(8)
C26	0.7002(5)	0.2406(3)	0.2048(3)	0.0668(10)
C27	0.5436(5)	0.2437(3)	0.2112(3)	0.0713(12)
C28	0.5206(5)	0.2290(3)	0.3114(4)	0.0782(13)
C29	0.6540(5)	0.2114(3)	0.4087(3)	0.0651(10)
C30	0.2136(6)	0.0630(3)	0.5700(5)	0.112(2)
C31	0.2299(6)	0.9643(3)	0.5592(4)	0.0941(15)

Table 5. Bond lengths (Å) for LewClark_brucine.

N1-C7	1.502(4)	N1-C8	1.507(4)
N1-C21	1.529(4)	N1-H1N	0.80(3)
N2-C14	1.371(4)	N2-C15	1.420(3)
N2-C17	1.494(3)	O1-C1	1.373(4)
O1-C22	1.413(5)	O2-C2	1.370(3)
O2-C23	1.416(4)	O3-C11	1.427(4)
O3-C12	1.428(4)	O4-C14	1.214(4)
C1-C16	1.389(4)	C1-C2	1.422(4)
C2-C3	1.383(4)	C3-C4	1.403(4)
C3-H3	0.95	C4-C15	1.378(4)
C4-C5	1.508(4)	C5-C6	1.545(4)
C5-C21	1.556(4)	C5-C17	1.560(4)
C6-C7	1.517(4)	C6-H6A	0.99
C6-H6B	0.99	C7-H7A	0.99
C7-H7B	0.99	C8-C9	1.507(4)
C8-H8A	0.99	C8-H8B	0.99
C9-C10	1.320(5)	C9-C19	1.522(4)
C10-C11	1.502(5)	C10-H10	0.95

C11-H11A	0.99	C11-H11B	0.99
C12-C13	1.524(4)	C12-C18	1.543(4)
C12-H12	1.0	C13-C14	1.532(4)
C13-H13A	0.99	C13-H13B	0.99
C15-C16	1.390(4)	C16-H16	0.95
C17-C18	1.523(4)	C17-H17	1.0
C18-C19	1.535(4)	C18-H18	1.0
C19-C20	1.531(4)	C19-H19	1.0
C20-C21	1.512(4)	C20-H20A	0.99
C20-H20B	0.99	C21-H21	1.0
C22-H22A	0.98	C22-H22B	0.98
C22-H22C	0.98	C23-H23A	0.98
C23-H23B	0.98	C23-H23C	0.98
P1-O6	1.501(3)	P1-O5	1.607(3)
P1-C24	1.820(3)	P1-S1	1.9621(15)
O5-C30	1.429(5)	C24-C25	1.387(5)
C24-C29	1.393(5)	C25-C26	1.379(5)
C25-H25	0.95	C26-C27	1.379(6)
C26-H26	0.95	C27-C28	1.366(6)
C27-H27	0.95	C28-C29	1.395(5)
C28-H28	0.95	C29-H29	0.95
C30-C31	1.446(6)	C30-H30A	0.99
C30-H30B	0.99	C31-H31A	0.98
C31-H31B	0.98	C31-H31C	0.98

Table 6. Bond angles (°) for LewClark_brucine.

C7-N1-C8	112.4(2)	C7-N1-C21	107.9(2)
C8-N1-C21	113.3(2)	C7-N1-H1N	110.(2)
C8-N1-H1N	107.(2)	C21-N1-H1N	106.(2)
C14-N2-C15	124.0(2)	C14-N2-C17	119.6(2)
C15-N2-C17	109.3(2)	C1-O1-C22	117.8(3)
C2-O2-C23	116.8(2)	C11-O3-C12	115.4(2)
O1-C1-C16	124.1(3)	O1-C1-C2	114.8(3)
C16-C1-C2	121.1(3)	O2-C2-C3	125.1(3)
O2-C2-C1	115.1(3)	C3-C2-C1	119.7(3)
C2-C3-C4	119.4(3)	C2-C3-H3	120.3
C4-C3-H3	120.3	C15-C4-C3	119.6(3)
C15-C4-C5	110.9(2)	C3-C4-C5	129.3(2)
C4-C5-C6	112.6(2)	C4-C5-C21	115.8(2)
C6-C5-C21	100.8(2)	C4-C5-C17	102.4(2)
C6-C5-C17	111.5(2)	C21-C5-C17	114.0(2)
C7-C6-C5	103.5(2)	C7-C6-H6A	111.1
C5-C6-H6A	111.1	C7-C6-H6B	111.1
C5-C6-H6B	111.1	H6A-C6-H6B	109.0
N1-C7-C6	104.5(2)	N1-C7-H7A	110.9
C6-C7-H7A	110.9	N1-C7-H7B	110.9
C6-C7-H7B	110.9	H7A-C7-H7B	108.9
C9-C8-N1	109.7(2)	C9-C8-H8A	109.7
N1-C8-H8A	109.7	C9-C8-H8B	109.7
N1-C8-H8B	109.7	H8A-C8-H8B	108.2
C10-C9-C8	122.6(3)	C10-C9-C19	122.8(3)
C8-C9-C19	114.6(3)	C9-C10-C11	123.0(3)

C9-C10-H10	118.5	C11-C10-H10	118.5
O3-C11-C10	111.8(3)	O3-C11-H11A	109.3
C10-C11-H11A	109.3	O3-C11-H11B	109.3
C10-C11-H11B	109.3	H11A-C11-H11B	107.9
O3-C12-C13	104.5(2)	O3-C12-C18	113.7(2)
C13-C12-C18	110.8(2)	O3-C12-H12	109.2
C13-C12-H12	109.2	C18-C12-H12	109.2
C12-C13-C14	118.1(3)	C12-C13-H13A	107.8
C14-C13-H13A	107.8	C12-C13-H13B	107.8
C14-C13-H13B	107.8	H13A-C13-H13B	107.1
O4-C14-N2	122.5(3)	O4-C14-C13	122.0(3)
N2-C14-C13	115.5(3)	C4-C15-C16	122.8(2)
C4-C15-N2	110.0(2)	C16-C15-N2	127.2(2)
C1-C16-C15	117.4(3)	C1-C16-H16	121.3
C15-C16-H16	121.3	N2-C17-C18	106.7(2)
N2-C17-C5	104.0(2)	C18-C17-C5	116.8(2)
N2-C17-H17	109.7	C18-C17-H17	109.7
C5-C17-H17	109.7	C17-C18-C19	112.4(2)
C17-C18-C12	107.2(2)	C19-C18-C12	118.1(2)
C17-C18-H18	106.1	C19-C18-H18	106.1
C12-C18-H18	106.1	C9-C19-C20	109.4(2)
C9-C19-C18	114.7(2)	C20-C19-C18	106.1(2)
C9-C19-H19	108.8	C20-C19-H19	108.8
C18-C19-H19	108.8	C21-C20-C19	109.0(2)
C21-C20-H20A	109.9	C19-C20-H20A	109.9
C21-C20-H20B	109.9	C19-C20-H20B	109.9
H20A-C20-H20B	108.3	C20-C21-N1	110.3(2)
C20-C21-C5	115.0(2)	N1-C21-C5	104.9(2)
C20-C21-H21	108.8	N1-C21-H21	108.8
C5-C21-H21	108.8	O1-C22-H22A	109.5
O1-C22-H22B	109.5	H22A-C22-H22B	109.5
O1-C22-H22C	109.5	H22A-C22-H22C	109.5
H22B-C22-H22C	109.5	O2-C23-H23A	109.5
O2-C23-H23B	109.5	H23A-C23-H23B	109.5
O2-C23-H23C	109.5	H23A-C23-H23C	109.5
H23B-C23-H23C	109.5	O6-P1-O5	108.23(16)
O6-P1-C24	107.63(15)	O5-P1-C24	99.64(13)
O6-P1-S1	117.03(11)	O5-P1-S1	110.78(13)
C24-P1-S1	112.05(13)	C30-O5-P1	118.0(2)
C25-C24-C29	118.9(3)	C25-C24-P1	118.8(2)
C29-C24-P1	122.2(3)	C26-C25-C24	121.3(4)
C26-C25-H25	119.4	C24-C25-H25	119.4
C25-C26-C27	119.6(4)	C25-C26-H26	120.2
C27-C26-H26	120.2	C28-C27-C26	120.1(4)
C28-C27-H27	120.0	C26-C27-H27	120.0
C27-C28-C29	121.0(4)	C27-C28-H28	119.5
C29-C28-H28	119.5	C24-C29-C28	119.2(4)
C24-C29-H29	120.4	C28-C29-H29	120.4
O5-C30-C31	111.3(4)	O5-C30-H30A	109.4
C31-C30-H30A	109.4	O5-C30-H30B	109.4
C31-C30-H30B	109.4	H30A-C30-H30B	108.0
C30-C31-H31A	109.5	C30-C31-H31B	109.5
H31A-C31-H31B	109.5	C30-C31-H31C	109.5
H31A-C31-H31C	109.5	H31B-C31-H31C	109.5

Table 7. Anisotropic atomic displacement parameters ($Å^2$) for LewClark_brucine.

The anisotropic atomic 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}
N1	0.0417(14)	0.0345(14)	0.0369(13)	-0.0069(11)	0.0091(11)	-0.0047(11)
N2	0.0342(13)	0.0277(12)	0.0342(12)	-0.0033(10)	0.0084(10)	-0.0034(10)
O1	0.0810(17)	0.0662(16)	0.0591(15)	-0.0044(12)	0.0413(14)	-0.0189(14)
O2	0.0484(12)	0.0429(12)	0.0647(14)	0.0027(11)	0.0248(11)	-0.0129(11)
O3	0.0413(11)	0.0373(11)	0.0569(13)	-0.0072(10)	0.0216(10)	-0.0068(9)
O4	0.0576(14)	0.0522(14)	0.0434(12)	-0.0165(10)	0.0157(10)	-0.0114(11)
C1	0.0402(16)	0.0435(17)	0.0395(16)	0.0065(13)	0.0183(13)	0.0026(14)
C2	0.0334(15)	0.0345(16)	0.0469(16)	0.0083(13)	0.0128(13)	0.0028(13)
C3	0.0299(14)	0.0254(14)	0.0406(14)	-0.0012(12)	0.0048(12)	-0.0021(11)
C4	0.0247(13)	0.0319(15)	0.0322(13)	0.0013(11)	0.0065(11)	0.0019(11)
C5	0.0249(13)	0.0266(14)	0.0351(14)	0.0015(11)	0.0043(11)	0.0009(11)
C6	0.0298(14)	0.0327(16)	0.0419(15)	0.0032(12)	0.0059(12)	0.0013(12)
C7	0.0413(16)	0.0337(16)	0.0377(15)	0.0025(12)	0.0055(12)	0.0015(13)
C8	0.0477(18)	0.0457(19)	0.0528(18)	-0.0107(15)	0.0235(15)	-0.0032(14)
C9	0.0380(16)	0.0384(18)	0.0547(18)	-0.0116(14)	0.0233(14)	0.0004(14)
C10	0.055(2)	0.058(2)	0.056(2)	-0.0097(16)	0.0315(17)	-0.0089(17)
C11	0.057(2)	0.058(2)	0.069(2)	-0.0169(18)	0.0337(19)	-0.0193(18)
C12	0.0268(15)	0.0367(16)	0.0515(18)	-0.0073(13)	0.0035(13)	-0.0035(12)
C13	0.0498(19)	0.0488(19)	0.0531(19)	-0.0138(15)	0.0174(15)	-0.0192(16)
C14	0.0396(16)	0.0293(15)	0.0417(17)	-0.0028(13)	0.0072(13)	-0.0019(12)
C15	0.0272(13)	0.0264(13)	0.0346(14)	0.0025(11)	0.0073(11)	0.0011(11)
C16	0.0450(17)	0.0358(15)	0.0360(15)	-0.0023(12)	0.0127(13)	-0.0001(14)
C17	0.0302(14)	0.0242(13)	0.0341(14)	-0.0020(11)	0.0074(11)	-0.0023(11)
C18	0.0278(14)	0.0300(14)	0.0398(15)	-0.0010(12)	0.0050(12)	-0.0037(12)
C19	0.0269(14)	0.0294(15)	0.0557(18)	-0.0044(13)	0.0096(13)	0.0052(12)
C20	0.0415(16)	0.0243(14)	0.0516(17)	-0.0051(13)	0.0099(14)	0.0045(13)
C21	0.0348(15)	0.0266(14)	0.0368(14)	-0.0026(11)	0.0098(12)	-0.0047(12)
C22	0.132(4)	0.087(3)	0.061(2)	-0.016(2)	0.063(3)	-0.025(3)
C23	0.0336(16)	0.0364(19)	0.085(2)	0.0039(16)	0.0176(16)	-0.0042(14)
P1	0.0618(6)	0.0405(5)	0.0441(4)	-0.0050(4)	0.0000(4)	-0.0148(4)
S1	0.1097(9)	0.1076(9)	0.0454(5)	-0.0050(6)	0.0151(5)	-0.0428(8)
O5	0.0734(18)	0.0479(15)	0.0767(17)	-0.0100(13)	-0.0216(14)	0.0044(13)
O6	0.0640(15)	0.0594(15)	0.0527(14)	-0.0055(11)	0.0025(11)	-0.0227(12)
C24	0.0488(19)	0.0292(16)	0.0574(19)	-0.0071(14)	0.0024(15)	-0.0060(14)
C25	0.0537(19)	0.045(2)	0.0506(18)	-0.0022(14)	0.0057(15)	-0.0031(15)
C26	0.072(3)	0.058(2)	0.054(2)	0.0018(18)	-0.0007(19)	0.002(2)
C27	0.072(3)	0.053(2)	0.064(2)	-0.0044(19)	-0.010(2)	0.005(2)
C28	0.052(2)	0.071(3)	0.100(3)	-0.015(2)	0.011(2)	0.004(2)
C29	0.070(2)	0.056(2)	0.066(2)	-0.0088(18)	0.0168(19)	-0.0062(19)
C30	0.094(3)	0.073(3)	0.118(4)	-0.013(3)	-0.033(3)	0.016(3)
C31	0.088(3)	0.079(4)	0.107(4)	0.021(3)	0.023(3)	0.024(3)

Table 8. Hydrogen atomic coordinates and isotropic atomic

displacement parameters (Å^2) for LewClark_brucine.

	x/a	y/b	z/c	U(eq)
H1N	0.269(4)	0.334(2)	0.622(3)	0.047
H3	0.0738	0.2758	0.8750	0.04
H6A	0.0556	0.4261	0.7218	0.044
H6B	0.1394	0.5250	0.7648	0.044
H7A	0.1492	0.4662	0.5778	0.047
H7B	0.3137	0.5137	0.6620	0.047
H8A	0.5239	0.3157	0.6311	0.056
H8B	0.4686	0.4148	0.5738	0.056
H10	0.6740	0.5230	0.6560	0.064
H11A	0.9044	0.5037	0.8678	0.07
H11B	0.8691	0.5985	0.7984	0.07
H12	0.8436	0.4980	1.0289	0.049
H13A	0.6515	0.6458	1.0324	0.061
H13B	0.7673	0.5891	1.1372	0.061
H16	0.2785	0.4810	1.1810	0.047
H17	0.4306	0.5369	0.8573	0.036
H18	0.6211	0.4011	1.0085	0.041
H19	0.7552	0.3538	0.8830	0.046
H20A	0.5446	0.2489	0.7910	0.049
H20B	0.5301	0.2701	0.9117	0.049
H21	0.2665	0.2799	0.7738	0.04
H22A	0.2537	0.4106	1.3301	0.129
H22B	0.0965	0.3857	1.3651	0.129
H22C	0.0912	0.4733	1.2867	0.129
H23A	-0.1571	0.2057	0.8831	0.078
H23B	-0.1749	0.1328	0.9732	0.078
H23C	-0.0039	0.1417	0.9501	0.078
H25	-0.0589	0.2213	0.2956	0.063
H26	-0.2836	0.2502	0.1350	0.08
H27	-0.5485	0.2561	0.1458	0.086
H28	-0.5879	0.2307	0.3149	0.094
H29	-0.3633	0.2009	0.4780	0.078
H30A	0.2312	0.0784	0.6493	0.135
H30B	0.2994	0.0952	0.5479	0.135
H31A	0.1338	-0.0670	0.5676	0.141
H31B	0.3304	-0.0573	0.6176	0.141
H31C	0.2367	-0.0497	0.4852	0.141

Table 9. Hydrogen bond distances (Å) and angles (°) for LewClark_brucine.

	Donor-H	Acceptor-H	Donor-Acceptor	Angle
N1-H1N···O6	0.80(3)	1.78(4)	2.569(3)	172.0