Journal of
Medicinal Chemistry
J. Med. Chem., 1997, 40(12), 1835-1844, DOI:10.1021/jm960868t

Table 1. Crystal data and structure refinement for 1.

Identification code	pete02
Empirical formula	$C_{24}H_{33}FN_3O_4ReS_2$
Formula weight	696.85
Temperature	293(2) K
Wavelength	1.54178 Å
Crystal system	Orthorhombic
Space group	$P2_12_12_1$
Unit cell dimensions	a = 7.4147(5) Å α = 90° b = 15.9123(11) Å β = 90° c = 22.2645(14) Å γ = 90°
Volume	2626.9(3) Å^3
Z	4
Density (calculated)	1.762 Mg/m^3
Absorption coefficient	10.895 mm^{-1}
F(000)	1384
Crystal size	0.40 x 0.38 x 0.14 mm
θ range for data collection	3.41 to 57.51°
Index ranges	$-1 \le h \le 8$, $-1 \le k \le 17$, $-24 \le \ell \le 5$
Reflections collected	2723
Independent reflections	2512 (R_{int} = 0.0232)
Absorption correction	Face
Max. and min. transmission	0.296 and 0.034
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2512 / 0 / 317
Goodness-of-fit on F^2	1.006
Final R indices [I>2σ(I)]	R1 = 0.0322, wR2 = 0.0836
R indices (all data)	R1 = 0.0335, wR2 = 0.0851
Absolute structure parameter	-0.01(2)

Extinction coefficient	0.00128(8)
Largest diff. peak and hole	1.330 and -1.206 $eÅ^{-3}$

Table 2. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for 1. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Re(1)	-3262(1)	6718(1)	8124(1)	31(1)
O(1)	-4570(9)	6854(4)	8734(2)	40(2)
O(2)	144(13)	8631(5)	7678(3)	74(3)
O(3)	-4852(11)	5963(5)	10254(4)	64(2)
O(4)	-3920(10)	4699(4)	9978(3)	51(2)
F(1')	-6616(11)	1594(4)	10983(4)	92(2)
C(1')	-3154(14)	3628(6)	10989(3)	35(2)
C(2')	-2870(15)	2939(6)	10628(4)	49(3)
C(3')	-3993(19)	2244(6)	10643(5)	61(3)
C(4')	-5490(18)	2255(7)	10988(5)	60(3)
C(5')	-5881(18)	2942(8)	11348(5)	65(3)
C(6')	-4691(15)	3604(7)	11340(4)	50(3)
C(1)	-1472(13)	5944(6)	10909(3)	36(2)
C(2)	-2827(13)	5233(5)	10916(3)	34(2)
C(3)	-1924(14)	4383(5)	11004(4)	35(2)
C(4)	-260(14)	4313(5)	10590(4)	35(2)
C(5)	848(13)	5115(6)	10613(4)	39(2)
C(6)	1383(14)	5368(6)	11255(4)	46(3)
C(7)	-194(17)	5912(6)	11468(4)	48(3)
N(8)	-311(11)	5800(4)	10385(3)	31(2)
C(9)	722(13)	6547(5)	10198(4)	38(2)
C(10)	1059(13)	6538(6)	9533(4)	36(2)
C(11)	-723(14)	6576(6)	9184(3)	37(2)
N(12)	-522(11)	6717(5)	8515(3)	34(2)
C(13)	304(16)	7547(6)	8405(4)	43(2)
C(14)	-560(15)	8022(6)	7902(4)	42(3)
N(15)	-2233(12)	7726(5)	7733(3)	39(2)
C(16)	-3053(15)	8159(6)	7213(4)	51(3)
C(17)	-4991(16)	7870(6)	7127(4)	49(3)
S(18)	-5125(4)	6754(2)	7308(1)	47(1)
S(19)	-2634(4)	5357(1)	7896(1)	50(1)
C(20)	-439(17)	5202(7)	8238(4)	58(3)
C(21)	543(15)	6030(6)	8219(4)	44(2)
C(22)	-3992(13)	5353(6)	10358(4)	38(2)
C(23)	-4905(16)	4774(8)	9419(4)	62(3)

Table 3. Bond lengths [Å] and angles [°] for 1.

Re(1)-O(1)	1.682(5)	Re(1)-N(15)	1.978(7)
Re(1)-N(12)	2.210(8)	Re(1)-S(19)	2.273(2)
Re(1)-S(18)	2.283(2)	O(2)-C(14)	1.208(11)
O(3)-C(22)	1.183(11)	O(4)-C(22)	1.342(11)
O(4)-C(23)	1.449(11)	F(1')-C(4')	1.343(13)
C(1')-C(2')	1.375(13)	C(1')-C(6')	1.383(14)
C(1')-C(3)	1.509(13)	C(2')-C(3')	1.38(2)
C(3')-C(4')	1.35(2)	C(4')-C(5')	1.39(2)
C(5')-C(6')	1.37(2)	C(1)-N(8)	1.467(10)
C(1)-C(2)	1.514(13)	C(1)-C(7)	1.565(13)
C(2)-C(3)	1.521(12)	C(2)-C(22)	1.525(13)
C(3)-C(4)	1.544(12)	C(4)-C(5)	1.519(12)
C(5)-N(8)	1.477(11)	C(5)-C(6)	1.538(12)
C(6)-C(7)	1.529(14)	N(8)-C(9)	1.474(11)
C(9)-C(10)	1.501(11)	C(10)-C(11)	1.534(13)
C(11)-N(12)	1.514(10)	N(12)-C(13)	1.477(12)
N(12)-C(21)	1.500(11)	C(13)-C(14)	1.496(13)
C(14)-N(15)	1.379(13)	N(15)-C(16)	1.479(11)
C(16)-C(17)	1.52(2)	C(17)-S(18)	1.823(10)
S(19)-C(20)	1.814(12)	C(20)-C(21)	1.51(2)

O(1)-Re(1)-N(15)	118.2(3)	O(1)-Re(1)-N(12)	102.3(3)
N(15)-Re(1)-N(12)	79.6(3)	O(1)-Re(1)-S(19)	114.9(2)
N(15)-Re(1)-S(19)	126.6(2)	N(12)-Re(1)-S(19)	84.2(2)
O(1)-Re(1)-S(18)	106.9(2)	N(15)-Re(1)-S(18)	82.1(2)
N(12)-Re(1)-S(18)	150.4(2)	S(19)-Re(1)-S(18)	88.29(10)
C(22)-O(4)-C(23)	117.3(8)	C(2')-C(1')-C(6')	115.8(9)
C(2')-C(1')-C(3)	123.7(9)	C(6')-C(1')-C(3)	120.5(8)
C(1')-C(2')-C(3')	122.1(10)	C(4')-C(3')-C(2')	119.9(10)
F(1')-C(4')-C(3')	119.8(12)	F(1')-C(4')-C(5')	119.6(12)
C(3')-C(4')-C(5')	120.7(11)	C(6')-C(5')-C(4')	117.6(11)
C(5')-C(6')-C(1')	123.9(10)	N(8)-C(1)-C(2)	106.3(7)
N(8)-C(1)-C(7)	105.8(7)	C(2)-C(1)-C(7)	111.6(7)
C(1)-C(2)-C(3)	112.0(7)	C(1)-C(2)-C(22)	105.9(7)
C(3)-C(2)-C(22)	117.8(7)	C(1')-C(3)-C(2)	116.0(8)
C(1')-C(3)-C(4)	114.3(7)	C(2)-C(3)-C(4)	109.8(7)
C(5)-C(4)-C(3)	110.6(7)	N(8)-C(5)-C(4)	107.1(7)
N(8)-C(5)-C(6)	106.0(7)	C(4)-C(5)-C(6)	113.0(7)
C(7)-C(6)-C(5)	103.8(7)	C(6)-C(7)-C(1)	103.6(7)
C(1)-N(8)-C(9)	113.8(7)	C(1)-N(8)-C(5)	100.6(6)
C(9)-N(8)-C(5)	112.9(7)	N(8)-C(9)-C(10)	110.9(7)
C(9)-C(10)-C(11)	110.9(8)	N(12)-C(11)-C(10)	114.8(8)
C(13)-N(12)-C(21)	111.1(7)	C(13)-N(12)-C(11)	109.6(7)
C(21)-N(12)-C(11)	112.2(7)	C(13)-N(12)-Re(1)	108.3(6)
C(21)-N(12)-Re(1)	108.1(5)	C(11)-N(12)-Re(1)	107.3(6)
N(12)-C(13)-C(14)	113.5(8)	O(2)-C(14)-N(15)	123.4(10)
O(2)-C(14)-C(13)	121.9(10)	N(15)-C(14)-C(13)	114.7(8)
C(14)-N(15)-C(16)	115.1(8)	C(14)-N(15)-Re(1)	120.3(6)
C(16)-N(15)-Re(1)	124.3(6)	N(15)-C(16)-C(17)	110.3(8)
C(16)-C(17)-S(18)	108.6(7)	C(17)-S(18)-Re(1)	99.7(3)
C(20)-S(19)-Re(1)	102.7(3)	C(21)-C(20)-S(19)	107.7(7)
N(12)-C(21)-C(20)	111.7(8)	O(3)-C(22)-O(4)	122.2(9)
O(3)-C(22)-C(2)	124.6(9)	O(4)-C(22)-C(2)	113.2(8)

Table 4. Anisotropic displacement parameters [$Å^2$ x 10^3] for 1.

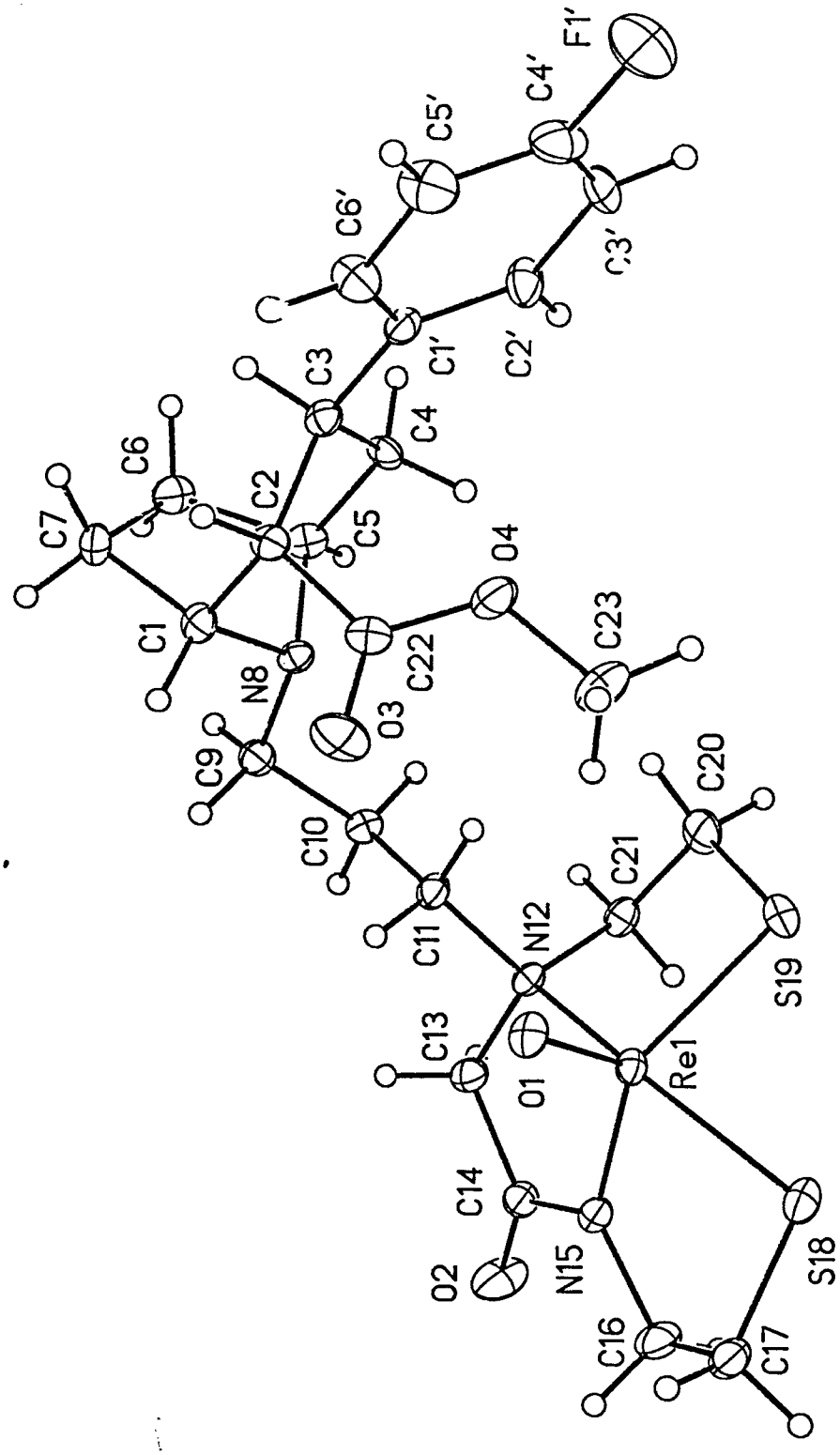
The anisotropic displacement factor exponent takes the form:

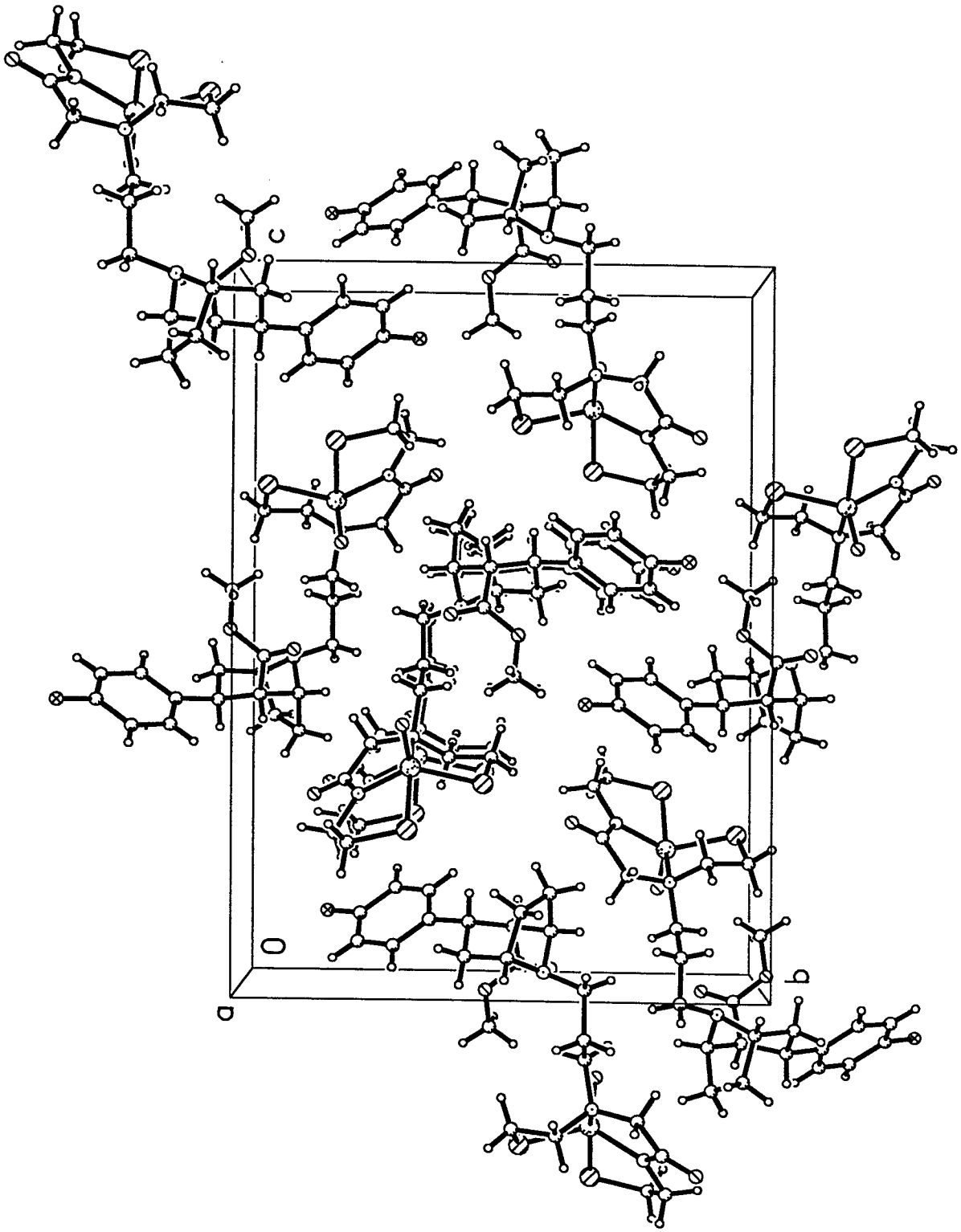
$-2\pi^2 [(ha^*)^2 U_{11} + ... + 2hka^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
Re(1)	33(1)	33(1)	25(1)	-3(1)	2(1)	-5(1)
O(1)	38(3)	53(4)	29(3)	-1(3)	15(3)	-9(4)
O(2)	71(6)	77(5)	72(5)	39(4)	-16(5)	-45(6)
O(3)	46(5)	51(4)	96(6)	5(4)	-10(5)	22(5)
O(4)	55(4)	61(4)	38(3)	6(3)	-6(3)	10(4)
F(1')	82(6)	78(5)	117(6)	1(4)	-4(5)	-52(5)
C(1')	37(5)	42(4)	27(4)	4(4)	-5(4)	-4(5)
C(2')	50(6)	55(5)	42(5)	-11(4)	4(5)	-20(6)
C(3')	89(9)	40(6)	53(6)	-12(5)	-4(7)	-29(7)
C(4')	56(8)	55(7)	71(7)	20(6)	-16(7)	-22(7)
C(5')	57(7)	63(7)	75(7)	6(6)	25(7)	7(7)
C(6')	44(6)	47(5)	59(6)	0(5)	25(5)	-5(6)
C(1)	37(6)	41(5)	30(4)	-4(3)	13(4)	2(5)
C(2)	37(6)	34(4)	31(4)	3(3)	15(4)	1(5)
C(3)	34(5)	39(5)	31(4)	1(3)	5(4)	3(5)
C(4)	40(5)	25(4)	41(4)	-1(4)	8(5)	8(4)
C(5)	28(5)	45(5)	44(5)	8(5)	2(4)	3(5)
C(6)	42(6)	48(5)	48(5)	6(4)	-18(5)	-15(5)
C(7)	72(8)	42(5)	31(4)	-10(4)	-5(5)	-9(6)
N(8)	28(4)	35(4)	30(3)	4(3)	1(3)	4(4)
C(9)	37(5)	38(5)	40(4)	-1(4)	-5(4)	0(5)
C(10)	28(5)	41(5)	38(4)	7(4)	0(4)	-5(5)
C(11)	45(6)	41(5)	26(4)	1(4)	0(4)	-9(5)
N(12)	45(4)	37(4)	21(3)	3(3)	4(3)	-1(4)
C(13)	52(6)	41(5)	36(4)	8(4)	-2(5)	-4(6)
C(14)	54(7)	35(5)	38(5)	5(4)	-6(5)	-17(5)
N(15)	48(5)	38(4)	30(3)	1(3)	-6(4)	-3(4)
C(16)	62(7)	54(5)	36(4)	16(4)	-2(5)	-2(7)
C(17)	57(7)	53(6)	38(5)	7(4)	-12(5)	-7(6)
S(18)	49(1)	56(1)	36(1)	-6(1)	-10(1)	-6(2)
S(19)	62(2)	35(1)	52(1)	-12(1)	-6(1)	-4(1)
C(20)	71(8)	50(6)	53(6)	-19(5)	-5(6)	31(7)
C(21)	50(6)	55(6)	27(4)	-2(4)	7(4)	1(6)
C(22)	26(5)	40(5)	47(5)	10(4)	10(4)	0(5)
C(23)	52(7)	89(8)	45(5)	13(5)	-15(6)	0(7)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for 1.

	x	y	z	U(eq)
H(2'A)	-1894(15)	2940(6)	10366(4)	59
H(3'A)	-3716(19)	1771(6)	10415(5)	73
H(5'A)	-6911(18)	2954(8)	11586(5)	78
H(6'A)	-4934(15)	4064(7)	11585(4)	60
H(1A)	-2079(13)	6490(6)	10881(3)	43
H(2A)	-3610(13)	5324(5)	11264(3)	41
H(3A)	-1437(14)	4397(5)	11413(4)	41
H(4A)	479(14)	3842(5)	10716(4)	42
H(4B)	-650(14)	4210(5)	10180(4)	42
H(5A)	1926(13)	5060(6)	10361(4)	47
H(6A)	1524(14)	4877(6)	11509(4)	55
H(6B)	2500(14)	5685(6)	11256(4)	55
H(7A)	212(17)	6470(6)	11578(4)	58
H(7B)	-796(17)	5658(6)	11809(4)	58
H(9A)	1866(13)	6559(5)	10410(4)	46
H(9B)	58(13)	7050(5)	10305(4)	46
H(10A)	1704(13)	6029(6)	9426(4)	43
H(10B)	1805(13)	7015(6)	9425(4)	43
H(11A)	-1370(14)	6054(6)	9248(3)	45
H(11B)	-1453(14)	7026(6)	9349(3)	45
H(13A)	1573(16)	7470(6)	8315(4)	51
H(13B)	221(16)	7880(6)	8770(4)	51
H(16A)	-2361(15)	8037(6)	6853(4)	61
H(16B)	-3029(15)	8761(6)	7278(4)	61
H(17A)	-5363(16)	7962(6)	6714(4)	59
H(17B)	-5787(16)	8187(6)	7387(4)	59
H(20A)	-575(17)	5016(7)	8650(4)	69
H(20B)	234(17)	4779(7)	8019(4)	69
H(21A)	1697(15)	5973(6)	8420(4)	53
H(21B)	772(15)	6182(6)	7804(4)	53
H(23A)	-4750(16)	4270(8)	9187(4)	93
H(23B)	-4453(16)	5246(8)	9196(4)	93
H(23C)	-6162(16)	4856(8)	9502(4)	93




c
O
a
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