

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for bt179. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor. meso-5

	x	y	z	$U(\text{eq})$
Ca(1)	10441(1)	7475(1)	882(1)	39(1)
O(1)	10832(2)	5609(2)	900(1)	76(1)
O(2)	11273(2)	6929(3)	87(1)	81(1)
C(1)	8733(2)	7587(3)	1090(2)	50(1)
C(2)	8814(2)	6992(3)	604(2)	59(1)
C(3)	9072(2)	7677(3)	190(2)	60(1)
C(4)	9145(2)	8714(3)	415(1)	49(1)
C(5)	8928(2)	8669(2)	976(1)	41(1)
C(6)	8906(2)	9667(2)	1353(1)	41(1)
C(7)	9928(2)	10079(2)	1395(1)	34(1)
C(8)	10646(2)	9227(2)	1447(1)	34(1)
C(12)	11376(2)	9155(2)	1085(1)	43(1)
C(11)	11945(2)	8321(2)	1256(2)	50(1)
C(10)	11557(2)	7862(3)	1721(1)	50(1)
C(9)	10767(2)	8416(2)	1840(1)	41(1)
C(13)	10198(2)	11098(2)	1732(1)	44(1)
C(14)	10246(2)	10899(3)	2355(1)	56(1)
C(15)	11149(2)	11432(3)	1566(2)	59(1)
C(16)	9601(2)	12055(3)	1587(2)	60(1)
C(17)	8227(2)	9545(2)	1837(1)	42(1)
C(18)	7965(2)	10599(3)	2104(2)	61(1)
C(19)	7342(2)	9079(3)	1626(1)	56(1)
C(20)	8560(2)	8815(3)	2312(1)	57(1)
C(21)	10404(5)	4810(4)	1214(2)	142(3)
C(22)	11348(4)	5218(4)	458(2)	106(2)
C(23)	11812(3)	6055(5)	187(3)	114(2)
C(24)	11638(3)	7748(5)	-255(2)	112(2)

Table 3. Bond lengths [Å] and angles [°] for bt179. meso-5

Ca(1)-O(2)	2.399(3)	C(17)-C(18)	1.524(4)
Ca(1)-O(1)	2.410(3)	C(17)-C(19)	1.534(4)
Ca(1)-C(12)	2.575(3)	C(17)-C(20)	1.557(5)
Ca(1)-C(2)	2.595(3)	C(22)-C(23)	1.419(7)
Ca(1)-C(1)	2.606(3)		
Ca(1)-C(8)	2.610(3)	O(2)-Ca(1)-O(1)	67.24(11)
Ca(1)-C(11)	2.647(3)	O(2)-Ca(1)-C(12)	96.14(11)
Ca(1)-C(9)	2.660(3)	O(1)-Ca(1)-C(12)	131.14(10)
Ca(1)-C(3)	2.663(3)	O(2)-Ca(1)-C(2)	102.04(10)
Ca(1)-C(10)	2.681(3)	O(1)-Ca(1)-C(2)	90.35(11)
Ca(1)-C(5)	2.721(3)	C(12)-Ca(1)-C(2)	138.50(11)
Ca(1)-C(4)	2.730(3)	O(2)-Ca(1)-C(1)	132.83(10)
O(1)-C(21)	1.412(6)	O(1)-Ca(1)-C(1)	106.62(11)
O(1)-C(22)	1.413(5)	C(12)-Ca(1)-C(1)	116.74(10)
O(2)-C(23)	1.380(6)	C(2)-Ca(1)-C(1)	31.34(10)
O(2)-C(24)	1.430(5)	O(2)-Ca(1)-C(8)	127.22(10)
C(1)-C(2)	1.405(5)	O(1)-Ca(1)-C(8)	141.03(9)
C(1)-C(5)	1.415(4)	C(12)-Ca(1)-C(8)	31.48(9)
C(2)-C(3)	1.379(5)	C(2)-Ca(1)-C(8)	116.32(10)
C(3)-C(4)	1.414(5)	C(1)-Ca(1)-C(8)	88.09(9)
C(4)-C(5)	1.406(4)	O(2)-Ca(1)-C(11)	87.25(10)
C(5)-C(6)	1.552(4)	O(1)-Ca(1)-C(11)	100.14(10)
C(6)-C(17)	1.562(4)	C(12)-Ca(1)-C(11)	31.30(9)
C(6)-C(7)	1.615(4)	C(2)-Ca(1)-C(11)	168.13(10)
C(7)-C(8)	1.518(4)	C(1)-Ca(1)-C(11)	137.98(10)
C(7)-C(13)	1.571(4)	C(8)-Ca(1)-C(11)	51.81(9)
C(8)-C(12)	1.407(4)	O(2)-Ca(1)-C(9)	137.67(10)
C(8)-C(9)	1.408(4)	O(1)-Ca(1)-C(9)	111.63(9)
C(12)-C(11)	1.410(4)	C(12)-Ca(1)-C(9)	50.94(10)
C(11)-C(10)	1.396(5)	C(2)-Ca(1)-C(9)	120.23(10)
C(10)-C(9)	1.399(4)	C(1)-Ca(1)-C(9)	89.10(10)
C(13)-C(16)	1.535(4)	C(8)-Ca(1)-C(9)	30.98(9)
C(13)-C(15)	1.536(4)	C(11)-Ca(1)-C(9)	50.58(10)
C(13)-C(14)	1.538(5)	O(2)-Ca(1)-C(3)	85.12(10)

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O(1)-Ca(1)-C(3)	106.90(11)	C(5)-Ca(1)-C(4)	29.89(9)
C(12)-Ca(1)-C(3)	117.44(11)	C(21)-O(1)-C(22)	114.5(4)
C(2)-Ca(1)-C(3)	30.37(12)	C(21)-O(1)-Ca(1)	126.0(3)
C(1)-Ca(1)-C(3)	50.63(11)	C(22)-O(1)-Ca(1)	117.0(3)
C(8)-Ca(1)-C(3)	110.13(10)	C(23)-O(2)-C(24)	116.7(4)
C(11)-Ca(1)-C(3)	146.33(12)	C(23)-O(2)-Ca(1)	112.7(3)
C(9)-Ca(1)-C(3)	130.84(10)	C(24)-O(2)-Ca(1)	117.6(3)
O(2)-Ca(1)-C(10)	110.13(10)	C(2)-C(1)-C(5)	109.0(3)
O(1)-Ca(1)-C(10)	90.59(10)	C(2)-C(1)-Ca(1)	73.88(17)
C(12)-Ca(1)-C(10)	50.82(10)	C(5)-C(1)-Ca(1)	79.15(16)
C(2)-Ca(1)-C(10)	145.42(12)	C(3)-C(2)-C(1)	108.1(3)
C(1)-Ca(1)-C(10)	116.78(11)	C(3)-C(2)-Ca(1)	77.54(19)
C(8)-Ca(1)-C(10)	51.14(9)	C(1)-C(2)-Ca(1)	74.79(17)
C(11)-Ca(1)-C(10)	30.37(10)	C(2)-C(3)-C(4)	108.0(3)
C(9)-Ca(1)-C(10)	30.37(9)	C(2)-C(3)-Ca(1)	72.08(19)
C(3)-Ca(1)-C(10)	160.52(10)	C(4)-C(3)-Ca(1)	77.47(18)
O(2)-Ca(1)-C(5)	130.95(10)	C(5)-C(4)-C(3)	108.8(3)
O(1)-Ca(1)-C(5)	137.17(10)	C(5)-C(4)-Ca(1)	74.69(17)
C(12)-Ca(1)-C(5)	89.14(9)	C(3)-C(4)-Ca(1)	72.16(19)
C(2)-Ca(1)-C(5)	51.08(10)	C(4)-C(5)-C(1)	106.1(3)
C(1)-Ca(1)-C(5)	30.70(10)	C(4)-C(5)-C(6)	123.3(3)
C(8)-Ca(1)-C(5)	65.80(8)	C(1)-C(5)-C(6)	130.7(3)
C(11)-Ca(1)-C(5)	117.13(9)	C(4)-C(5)-Ca(1)	75.42(17)
C(9)-Ca(1)-C(5)	80.46(9)	C(1)-C(5)-Ca(1)	70.15(16)
C(3)-Ca(1)-C(5)	50.41(10)	C(6)-C(5)-Ca(1)	120.70(17)
C(10)-Ca(1)-C(5)	110.65(10)	C(5)-C(6)-C(17)	112.4(2)
O(2)-Ca(1)-C(4)	101.18(10)	C(5)-C(6)-C(7)	105.9(2)
O(1)-Ca(1)-C(4)	137.01(10)	C(17)-C(6)-C(7)	126.8(2)
C(12)-Ca(1)-C(4)	90.00(10)	C(8)-C(7)-C(13)	110.3(2)
C(2)-Ca(1)-C(4)	50.15(12)	C(8)-C(7)-C(6)	116.7(2)
C(1)-Ca(1)-C(4)	49.89(11)	C(13)-C(7)-C(6)	122.3(2)
C(8)-Ca(1)-C(4)	79.90(9)	C(12)-C(8)-C(9)	106.3(3)
C(11)-Ca(1)-C(4)	121.20(10)	C(12)-C(8)-C(7)	122.7(3)
C(9)-Ca(1)-C(4)	104.09(9)	C(9)-C(8)-C(7)	130.9(3)
C(3)-Ca(1)-C(4)	30.37(10)	C(12)-C(8)-Ca(1)	72.89(16)
C(10)-Ca(1)-C(4)	130.96(10)	C(9)-C(8)-Ca(1)	76.49(17)

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C(7)-C(8)-Ca(1)	117.66(17)	C(16)-C(13)-C(14)	112.4(3)
C(8)-C(12)-C(11)	109.3(3)	C(15)-C(13)-C(14)	105.1(3)
C(8)-C(12)-Ca(1)	75.63(16)	C(16)-C(13)-C(7)	111.4(2)
C(11)-C(12)-Ca(1)	77.17(17)	C(15)-C(13)-C(7)	108.7(2)
C(10)-C(11)-C(12)	107.1(3)	C(14)-C(13)-C(7)	113.3(3)
C(10)-C(11)-Ca(1)	76.18(17)	C(18)-C(17)-C(19)	104.5(2)
C(12)-C(11)-Ca(1)	71.53(16)	C(18)-C(17)-C(20)	105.9(3)
C(11)-C(10)-C(9)	108.4(3)	C(19)-C(17)-C(20)	107.5(3)
C(11)-C(10)-Ca(1)	73.45(18)	C(18)-C(17)-C(6)	113.8(3)
C(9)-C(10)-Ca(1)	73.97(17)	C(19)-C(17)-C(6)	110.2(2)
C(10)-C(9)-C(8)	108.9(3)	C(20)-C(17)-C(6)	114.2(2)
C(10)-C(9)-Ca(1)	75.66(18)	O(1)-C(22)-C(23)	111.4(4)
C(8)-C(9)-Ca(1)	72.54(17)	O(2)-C(23)-C(22)	112.5(4)
C(16)-C(13)-C(15)	105.4(3)		

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for bt179. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$ meso-5

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ca(1)	33(1)	40(1)	44(1)	-5(1)	4(1)	1(1)
O(1)	101(2)	46(2)	82(2)	-11(1)	-14(2)	10(1)
O(2)	56(2)	123(2)	63(2)	-1(2)	15(1)	27(2)
C(1)	33(2)	56(2)	61(2)	-17(2)	11(1)	-7(2)
C(2)	38(2)	62(2)	78(3)	-34(2)	1(2)	-3(2)
C(3)	45(2)	81(3)	54(2)	-33(2)	-11(2)	10(2)
C(4)	36(2)	66(2)	45(2)	-7(2)	-5(1)	5(2)
C(5)	25(1)	46(2)	53(2)	-10(2)	-1(1)	-2(1)
C(6)	33(2)	42(2)	46(2)	-6(2)	1(1)	0(1)
C(7)	31(1)	33(2)	39(2)	0(1)	-3(1)	0(1)
C(8)	29(1)	32(2)	42(2)	-1(1)	-2(1)	-5(1)
C(12)	32(2)	40(2)	58(2)	7(2)	5(1)	-3(1)
C(11)	26(1)	47(2)	76(3)	-5(2)	-2(2)	0(1)
C(10)	46(2)	40(2)	63(2)	4(2)	-18(2)	4(1)
C(9)	41(2)	38(2)	42(2)	4(1)	-6(1)	-3(1)
C(13)	39(2)	38(2)	54(2)	-6(2)	-1(1)	-4(1)
C(14)	54(2)	54(2)	59(2)	-16(2)	-4(2)	-6(2)
C(15)	50(2)	49(2)	76(3)	-11(2)	1(2)	-17(2)
C(16)	66(2)	33(2)	82(3)	-8(2)	-2(2)	2(2)
C(17)	34(2)	43(2)	48(2)	-8(2)	8(1)	1(1)
C(18)	44(2)	64(2)	74(3)	-23(2)	13(2)	3(2)
C(19)	32(2)	72(2)	62(2)	-18(2)	7(2)	-3(2)
C(20)	55(2)	66(2)	51(2)	3(2)	10(2)	-4(2)
C(21)	278(9)	61(3)	85(4)	21(3)	-5(5)	-6(4)
C(22)	121(4)	95(4)	102(4)	-36(3)	-21(3)	62(4)
C(23)	62(3)	117(5)	163(6)	-66(4)	23(3)	15(3)
C(24)	76(3)	197(6)	64(3)	8(3)	25(2)	-29(3)

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Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for bt179.

	x	y	z	U(eq)
H(1)	8575	7310	1436	60
H(2)	8711	6255	567	71
H(3)	9180	7488	-178	72
H(4)	9311	9332	221	59
H(6)	8530(20)	10270(20)	1131(14)	74(11)
H(7)	10003(19)	10350(20)	977(10)	41(8)
H(12)	11470	9594	777	52
H(11)	12484	8113	1088	60
H(10)	11787	7281	1920	60
H(9)	10380	8269	2135	49
H(14A)	10628	10289	2426	84
H(14B)	9650	10757	2495	84
H(14C)	10490	11524	2535	84
H(15A)	11176	11524	1171	88
H(15B)	11569	10882	1677	88
H(15C)	11302	12099	1745	88
H(16A)	9768	12663	1812	90
H(16B)	8980	11873	1656	90
H(16C)	9677	12233	1202	90
H(18A)	7697	11064	1831	91
H(18B)	8493	10939	2256	91
H(18C)	7537	10466	2396	91
H(19A)	6904	9084	1920	83
H(19B)	7438	8352	1503	83
H(19C)	7124	9508	1322	83
H(20A)	9099	9117	2471	86
H(20B)	8689	8109	2169	86
H(20C)	8100	8765	2592	86
H(21A)	10068	4344	972	212
H(21B)	10000	5141	1475	212

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H(21C)	10850	4397	1410	212
H(22A)	10955	4856	195	127
H(22B)	11781	4694	595	127
H(23A)	12321	6277	413	137
H(23B)	12048	5789	-163	137
H(24A)	12144	8076	-71	169
H(24B)	11184	8284	-326	169
H(24C)	11833	7439	-600	169

Table 6. Torsion angles [°] for bt179. meso-5

O(2)-Ca(1)-O(1)-C(21)	-158.9(4)	C(12)-Ca(1)-O(2)-C(24)	-33.9(3)
C(12)-Ca(1)-O(1)-C(21)	123.3(4)	C(2)-Ca(1)-O(2)-C(24)	108.6(3)
C(2)-Ca(1)-O(1)-C(21)	-56.0(4)	C(1)-Ca(1)-O(2)-C(24)	101.9(3)
C(1)-Ca(1)-O(1)-C(21)	-28.8(4)	C(8)-Ca(1)-O(2)-C(24)	-28.4(3)
C(8)-Ca(1)-O(1)-C(21)	79.5(4)	C(11)-Ca(1)-O(2)-C(24)	-64.0(3)
C(11)-Ca(1)-O(1)-C(21)	118.4(4)	C(9)-Ca(1)-O(2)-C(24)	-68.5(3)
C(9)-Ca(1)-O(1)-C(21)	67.0(4)	C(3)-Ca(1)-O(2)-C(24)	83.2(3)
C(3)-Ca(1)-O(1)-C(21)	-81.9(4)	C(10)-Ca(1)-O(2)-C(24)	-84.3(3)
C(10)-Ca(1)-O(1)-C(21)	89.4(4)	C(5)-Ca(1)-O(2)-C(24)	60.3(3)
C(5)-Ca(1)-O(1)-C(21)	-32.6(4)	C(4)-Ca(1)-O(2)-C(24)	57.3(3)
C(4)-Ca(1)-O(1)-C(21)	-77.1(4)	O(2)-Ca(1)-C(1)-C(2)	12.7(3)
O(2)-Ca(1)-O(1)-C(22)	2.0(3)	O(1)-Ca(1)-C(1)-C(2)	-61.4(2)
C(12)-Ca(1)-O(1)-C(22)	-75.8(3)	C(12)-Ca(1)-C(1)-C(2)	141.7(2)
C(2)-Ca(1)-O(1)-C(22)	104.9(3)	C(8)-Ca(1)-C(1)-C(2)	155.2(2)
C(1)-Ca(1)-O(1)-C(22)	132.1(3)	C(11)-Ca(1)-C(1)-C(2)	171.3(2)
C(8)-Ca(1)-O(1)-C(22)	-119.7(3)	C(9)-Ca(1)-C(1)-C(2)	-173.8(2)
C(11)-Ca(1)-O(1)-C(22)	-80.7(3)	C(3)-Ca(1)-C(1)-C(2)	37.0(2)
C(9)-Ca(1)-O(1)-C(22)	-132.2(3)	C(10)-Ca(1)-C(1)-C(2)	-160.8(2)
C(3)-Ca(1)-O(1)-C(22)	79.0(3)	C(5)-Ca(1)-C(1)-C(2)	113.6(3)
C(10)-Ca(1)-O(1)-C(22)	-109.7(3)	C(4)-Ca(1)-C(1)-C(2)	76.9(2)
C(5)-Ca(1)-O(1)-C(22)	128.3(3)	O(2)-Ca(1)-C(1)-C(5)	-100.9(2)
C(4)-Ca(1)-O(1)-C(22)	83.8(3)	O(1)-Ca(1)-C(1)-C(5)	-175.02(18)
O(1)-Ca(1)-O(2)-C(23)	-26.0(3)	C(12)-Ca(1)-C(1)-C(5)	28.2(2)
C(12)-Ca(1)-O(2)-C(23)	106.2(3)	C(2)-Ca(1)-C(1)-C(5)	-113.6(3)
C(2)-Ca(1)-O(2)-C(23)	-111.3(3)	C(8)-Ca(1)-C(1)-C(5)	41.67(19)
C(1)-Ca(1)-O(2)-C(23)	-118.0(3)	C(11)-Ca(1)-C(1)-C(5)	57.7(3)
C(8)-Ca(1)-O(2)-C(23)	111.7(3)	C(9)-Ca(1)-C(1)-C(5)	72.64(19)
C(11)-Ca(1)-O(2)-C(23)	76.2(3)	C(3)-Ca(1)-C(1)-C(5)	-76.5(2)
C(9)-Ca(1)-O(2)-C(23)	71.6(3)	C(10)-Ca(1)-C(1)-C(5)	85.6(2)
C(3)-Ca(1)-O(2)-C(23)	-136.7(3)	C(4)-Ca(1)-C(1)-C(5)	-36.72(18)
C(10)-Ca(1)-O(2)-C(23)	55.8(3)	C(5)-C(1)-C(2)-C(3)	1.1(4)
C(5)-Ca(1)-O(2)-C(23)	-159.6(3)	Ca(1)-C(1)-C(2)-C(3)	-71.1(2)
C(4)-Ca(1)-O(2)-C(23)	-162.6(3)	C(5)-C(1)-C(2)-Ca(1)	72.1(2)
O(1)-Ca(1)-O(2)-C(24)	-166.2(3)	O(2)-Ca(1)-C(2)-C(3)	-57.6(2)

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O(1)-Ca(1)-C(2)-C(3)	-124.4(2)	C(1)-Ca(1)-C(3)-C(4)	75.6(2)
C(12)-Ca(1)-C(2)-C(3)	56.4(3)	C(8)-Ca(1)-C(3)-C(4)	5.9(2)
C(1)-Ca(1)-C(2)-C(3)	113.0(3)	C(11)-Ca(1)-C(3)-C(4)	-44.5(3)
C(8)-Ca(1)-C(2)-C(3)	85.1(2)	C(9)-Ca(1)-C(3)-C(4)	33.0(3)
C(11)-Ca(1)-C(2)-C(3)	83.3(6)	C(10)-Ca(1)-C(3)-C(4)	20.5(5)
C(9)-Ca(1)-C(2)-C(3)	120.2(2)	C(5)-Ca(1)-C(3)-C(4)	35.52(19)
C(10)-Ca(1)-C(2)-C(3)	144.1(2)	C(2)-C(3)-C(4)-C(5)	-0.1(4)
C(5)-Ca(1)-C(2)-C(3)	76.0(2)	Ca(1)-C(3)-C(4)-C(5)	-66.3(2)
C(4)-Ca(1)-C(2)-C(3)	37.02(19)	C(2)-C(3)-C(4)-Ca(1)	66.2(2)
O(2)-Ca(1)-C(2)-C(1)	-170.5(2)	O(2)-Ca(1)-C(4)-C(5)	175.48(19)
O(1)-Ca(1)-C(2)-C(1)	122.7(2)	O(1)-Ca(1)-C(4)-C(5)	107.0(2)
C(12)-Ca(1)-C(2)-C(1)	-56.6(3)	C(12)-Ca(1)-C(4)-C(5)	-88.26(19)
C(8)-Ca(1)-C(2)-C(1)	-27.8(3)	C(2)-Ca(1)-C(4)-C(5)	79.0(2)
C(11)-Ca(1)-C(2)-C(1)	-29.6(7)	C(1)-Ca(1)-C(4)-C(5)	37.77(17)
C(9)-Ca(1)-C(2)-C(1)	7.2(3)	C(8)-Ca(1)-C(4)-C(5)	-58.29(18)
C(3)-Ca(1)-C(2)-C(1)	-113.0(3)	C(11)-Ca(1)-C(4)-C(5)	-90.9(2)
C(10)-Ca(1)-C(2)-C(1)	31.1(3)	C(9)-Ca(1)-C(4)-C(5)	-38.8(2)
C(5)-Ca(1)-C(2)-C(1)	-37.0(2)	C(3)-Ca(1)-C(4)-C(5)	116.1(3)
C(4)-Ca(1)-C(2)-C(1)	-75.9(2)	C(10)-Ca(1)-C(4)-C(5)	-55.0(2)
C(1)-C(2)-C(3)-C(4)	-0.6(4)	O(2)-Ca(1)-C(4)-C(3)	59.4(2)
Ca(1)-C(2)-C(3)-C(4)	-69.8(2)	O(1)-Ca(1)-C(4)-C(3)	-9.1(3)
C(1)-C(2)-C(3)-Ca(1)	69.2(2)	C(12)-Ca(1)-C(4)-C(3)	155.7(2)
O(2)-Ca(1)-C(3)-C(2)	124.0(2)	C(2)-Ca(1)-C(4)-C(3)	-37.0(2)
O(1)-Ca(1)-C(3)-C(2)	59.6(2)	C(1)-Ca(1)-C(4)-C(3)	-78.3(2)
C(12)-Ca(1)-C(3)-C(2)	-141.6(2)	C(8)-Ca(1)-C(4)-C(3)	-174.4(2)
C(1)-Ca(1)-C(3)-C(2)	-38.3(2)	C(11)-Ca(1)-C(4)-C(3)	153.0(2)
C(8)-Ca(1)-C(3)-C(2)	-108.0(2)	C(9)-Ca(1)-C(4)-C(3)	-154.8(2)
C(11)-Ca(1)-C(3)-C(2)	-158.4(2)	C(10)-Ca(1)-C(4)-C(3)	-171.1(2)
C(9)-Ca(1)-C(3)-C(2)	-80.9(2)	C(5)-Ca(1)-C(4)-C(3)	-116.1(3)
C(10)-Ca(1)-C(3)-C(2)	-93.4(4)	C(3)-C(4)-C(5)-C(1)	0.7(3)
C(5)-Ca(1)-C(3)-C(2)	-78.4(2)	Ca(1)-C(4)-C(5)-C(1)	-63.9(2)
C(4)-Ca(1)-C(3)-C(2)	-113.9(3)	C(3)-C(4)-C(5)-C(6)	-178.0(3)
O(2)-Ca(1)-C(3)-C(4)	-122.0(2)	Ca(1)-C(4)-C(5)-C(6)	117.4(2)
O(1)-Ca(1)-C(3)-C(4)	173.5(2)	C(3)-C(4)-C(5)-Ca(1)	64.6(2)
C(12)-Ca(1)-C(3)-C(4)	-27.7(2)	C(2)-C(1)-C(5)-C(4)	-1.1(3)
C(2)-Ca(1)-C(3)-C(4)	113.9(3)	Ca(1)-C(1)-C(5)-C(4)	67.5(2)

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C(2)-C(1)-C(5)-C(6)	177.5(3)	Ca(1)-C(5)-C(6)-C(17)	-116.6(2)
Ca(1)-C(1)-C(5)-C(6)	-113.9(3)	C(4)-C(5)-C(6)-C(7)	-66.5(3)
C(2)-C(1)-C(5)-Ca(1)	-68.6(2)	C(1)-C(5)-C(6)-C(7)	115.1(3)
O(2)-Ca(1)-C(5)-C(4)	-5.9(2)	Ca(1)-C(5)-C(6)-C(7)	25.7(3)
O(1)-Ca(1)-C(5)-C(4)	-106.4(2)	C(5)-C(6)-C(7)-C(8)	-40.4(3)
C(12)-Ca(1)-C(5)-C(4)	91.51(19)	C(17)-C(6)-C(7)-C(8)	94.7(3)
C(2)-Ca(1)-C(5)-C(4)	-75.6(2)	C(5)-C(6)-C(7)-C(13)	178.7(3)
C(1)-Ca(1)-C(5)-C(4)	-113.4(3)	C(17)-C(6)-C(7)-C(13)	-46.3(4)
C(8)-Ca(1)-C(5)-C(4)	113.3(2)	C(13)-C(7)-C(8)-C(12)	-89.6(3)
C(11)-Ca(1)-C(5)-C(4)	106.0(2)	C(6)-C(7)-C(8)-C(12)	125.0(3)
C(9)-Ca(1)-C(5)-C(4)	142.0(2)	C(13)-C(7)-C(8)-C(9)	87.7(4)
C(3)-Ca(1)-C(5)-C(4)	-36.1(2)	C(6)-C(7)-C(8)-C(9)	-57.7(4)
C(10)-Ca(1)-C(5)-C(4)	138.60(19)	C(13)-C(7)-C(8)-Ca(1)	-176.24(18)
O(2)-Ca(1)-C(5)-C(1)	107.6(2)	C(6)-C(7)-C(8)-Ca(1)	38.3(3)
O(1)-Ca(1)-C(5)-C(1)	7.0(3)	O(2)-Ca(1)-C(8)-C(12)	-10.5(2)
C(12)-Ca(1)-C(5)-C(1)	-155.1(2)	O(1)-Ca(1)-C(8)-C(12)	89.1(2)
C(2)-Ca(1)-C(5)-C(1)	37.8(2)	C(2)-Ca(1)-C(8)-C(12)	-142.40(19)
C(8)-Ca(1)-C(5)-C(1)	-133.2(2)	C(1)-Ca(1)-C(8)-C(12)	-156.47(19)
C(11)-Ca(1)-C(5)-C(1)	-140.5(2)	C(11)-Ca(1)-C(8)-C(12)	37.13(18)
C(9)-Ca(1)-C(5)-C(1)	-104.6(2)	C(9)-Ca(1)-C(8)-C(12)	112.1(2)
C(3)-Ca(1)-C(5)-C(1)	77.3(2)	C(3)-Ca(1)-C(8)-C(12)	-109.95(19)
C(10)-Ca(1)-C(5)-C(1)	-108.0(2)	C(10)-Ca(1)-C(8)-C(12)	76.24(19)
C(4)-Ca(1)-C(5)-C(1)	113.4(3)	C(5)-Ca(1)-C(8)-C(12)	-134.6(2)
O(2)-Ca(1)-C(5)-C(6)	-126.2(2)	C(4)-Ca(1)-C(8)-C(12)	-106.92(19)
O(1)-Ca(1)-C(5)-C(6)	133.3(2)	O(2)-Ca(1)-C(8)-C(9)	-122.58(17)
C(12)-Ca(1)-C(5)-C(6)	-28.8(2)	O(1)-Ca(1)-C(8)-C(9)	-23.0(2)
C(2)-Ca(1)-C(5)-C(6)	164.0(3)	C(12)-Ca(1)-C(8)-C(9)	-112.1(2)
C(1)-Ca(1)-C(5)-C(6)	126.3(3)	C(2)-Ca(1)-C(8)-C(9)	105.50(19)
C(8)-Ca(1)-C(5)-C(6)	-7.0(2)	C(1)-Ca(1)-C(8)-C(9)	91.44(18)
C(11)-Ca(1)-C(5)-C(6)	-14.3(3)	C(11)-Ca(1)-C(8)-C(9)	-74.96(18)
C(9)-Ca(1)-C(5)-C(6)	21.7(2)	C(3)-Ca(1)-C(8)-C(9)	137.95(18)
C(3)-Ca(1)-C(5)-C(6)	-156.4(3)	C(10)-Ca(1)-C(8)-C(9)	-35.85(17)
C(10)-Ca(1)-C(5)-C(6)	18.3(3)	C(5)-Ca(1)-C(8)-C(9)	113.29(18)
C(4)-Ca(1)-C(5)-C(6)	-120.3(3)	C(4)-Ca(1)-C(8)-C(9)	140.99(18)
C(4)-C(5)-C(6)-C(17)	151.2(3)	O(2)-Ca(1)-C(8)-C(7)	108.0(2)
C(1)-C(5)-C(6)-C(17)	-27.2(4)	O(1)-Ca(1)-C(8)-C(7)	-152.4(2)

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C(12)-Ca(1)-C(8)-C(7)	118.5(3)	C(8)-C(12)-C(11)-Ca(1)	69.6(2)
C(2)-Ca(1)-C(8)-C(7)	-23.9(2)	O(2)-Ca(1)-C(11)-C(10)	-139.76(19)
C(1)-Ca(1)-C(8)-C(7)	-38.0(2)	O(1)-Ca(1)-C(11)-C(10)	-73.5(2)
C(11)-Ca(1)-C(8)-C(7)	155.6(3)	C(12)-Ca(1)-C(11)-C(10)	113.7(3)
C(9)-Ca(1)-C(8)-C(7)	-129.4(3)	C(2)-Ca(1)-C(11)-C(10)	78.4(6)
C(3)-Ca(1)-C(8)-C(7)	8.5(2)	C(1)-Ca(1)-C(11)-C(10)	55.8(3)
C(10)-Ca(1)-C(8)-C(7)	-165.3(3)	C(8)-Ca(1)-C(11)-C(10)	76.3(2)
C(5)-Ca(1)-C(8)-C(7)	-16.13(19)	C(9)-Ca(1)-C(11)-C(10)	36.27(17)
C(4)-Ca(1)-C(8)-C(7)	11.6(2)	C(3)-Ca(1)-C(11)-C(10)	143.3(2)
C(9)-C(8)-C(12)-C(11)	-0.8(3)	C(5)-Ca(1)-C(11)-C(10)	84.8(2)
C(7)-C(8)-C(12)-C(11)	177.1(3)	C(4)-Ca(1)-C(11)-C(10)	118.83(19)
Ca(1)-C(8)-C(12)-C(11)	-70.6(2)	O(2)-Ca(1)-C(11)-C(12)	106.6(2)
C(9)-C(8)-C(12)-Ca(1)	69.8(2)	O(1)-Ca(1)-C(11)-C(12)	172.86(19)
C(7)-C(8)-C(12)-Ca(1)	-112.3(2)	C(2)-Ca(1)-C(11)-C(12)	-35.3(7)
O(2)-Ca(1)-C(12)-C(8)	171.61(17)	C(1)-Ca(1)-C(11)-C(12)	-57.9(3)
O(1)-Ca(1)-C(12)-C(8)	-123.39(18)	C(8)-Ca(1)-C(11)-C(12)	-37.35(18)
C(2)-Ca(1)-C(12)-C(8)	55.6(3)	C(9)-Ca(1)-C(11)-C(12)	-77.4(2)
C(1)-Ca(1)-C(12)-C(8)	26.5(2)	C(3)-Ca(1)-C(11)-C(12)	29.6(3)
C(11)-Ca(1)-C(12)-C(8)	-114.0(3)	C(10)-Ca(1)-C(11)-C(12)	-113.7(3)
C(9)-Ca(1)-C(12)-C(8)	-37.89(16)	C(5)-Ca(1)-C(11)-C(12)	-28.9(2)
C(3)-Ca(1)-C(12)-C(8)	83.9(2)	C(4)-Ca(1)-C(11)-C(12)	5.2(2)
C(10)-Ca(1)-C(12)-C(8)	-77.36(19)	C(12)-C(11)-C(10)-C(9)	-0.9(4)
C(5)-Ca(1)-C(12)-C(8)	40.49(18)	Ca(1)-C(11)-C(10)-C(9)	-66.3(2)
C(4)-Ca(1)-C(12)-C(8)	70.37(18)	C(12)-C(11)-C(10)-Ca(1)	65.4(2)
O(2)-Ca(1)-C(12)-C(11)	-74.3(2)	O(2)-Ca(1)-C(10)-C(11)	43.4(2)
O(1)-Ca(1)-C(12)-C(11)	-9.4(3)	O(1)-Ca(1)-C(10)-C(11)	109.31(19)
C(2)-Ca(1)-C(12)-C(11)	169.7(2)	C(12)-Ca(1)-C(10)-C(11)	-37.86(18)
C(1)-Ca(1)-C(12)-C(11)	140.6(2)	C(2)-Ca(1)-C(10)-C(11)	-159.2(2)
C(8)-Ca(1)-C(12)-C(11)	114.0(3)	C(1)-Ca(1)-C(10)-C(11)	-141.68(18)
C(9)-Ca(1)-C(12)-C(11)	76.1(2)	C(8)-Ca(1)-C(10)-C(11)	-78.7(2)
C(3)-Ca(1)-C(12)-C(11)	-162.0(2)	C(9)-Ca(1)-C(10)-C(11)	-115.3(3)
C(10)-Ca(1)-C(12)-C(11)	36.68(19)	C(3)-Ca(1)-C(10)-C(11)	-96.4(4)
C(5)-Ca(1)-C(12)-C(11)	154.5(2)	C(5)-Ca(1)-C(10)-C(11)	-108.72(19)
C(4)-Ca(1)-C(12)-C(11)	-175.6(2)	C(4)-Ca(1)-C(10)-C(11)	-82.8(2)
C(8)-C(12)-C(11)-C(10)	1.1(4)	O(2)-Ca(1)-C(10)-C(9)	158.74(18)
Ca(1)-C(12)-C(11)-C(10)	-68.5(2)	O(1)-Ca(1)-C(10)-C(9)	-135.36(19)

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C(12)-Ca(1)-C(10)-C(9)	77.46(19)	O(1)-Ca(1)-C(9)-C(8)	164.67(16)
C(2)-Ca(1)-C(10)-C(9)	-43.9(3)	C(12)-Ca(1)-C(9)-C(8)	38.54(16)
C(1)-Ca(1)-C(10)-C(9)	-26.4(2)	C(2)-Ca(1)-C(9)-C(8)	-91.51(19)
C(8)-Ca(1)-C(10)-C(9)	36.60(17)	C(1)-Ca(1)-C(9)-C(8)	-87.78(17)
C(11)-Ca(1)-C(10)-C(9)	115.3(3)	C(11)-Ca(1)-C(9)-C(8)	79.30(18)
C(3)-Ca(1)-C(10)-C(9)	18.9(5)	C(3)-Ca(1)-C(9)-C(8)	-56.2(2)
C(5)-Ca(1)-C(10)-C(9)	6.6(2)	C(10)-Ca(1)-C(9)-C(8)	115.6(3)
C(4)-Ca(1)-C(10)-C(9)	32.5(2)	C(5)-Ca(1)-C(9)-C(8)	-58.16(16)
C(11)-C(10)-C(9)-C(8)	0.5(3)	C(4)-Ca(1)-C(9)-C(8)	-39.71(18)
Ca(1)-C(10)-C(9)-C(8)	-65.5(2)	C(8)-C(7)-C(13)-C(16)	167.3(3)
C(11)-C(10)-C(9)-Ca(1)	65.9(2)	C(6)-C(7)-C(13)-C(16)	-49.6(4)
C(12)-C(8)-C(9)-C(10)	0.2(3)	C(8)-C(7)-C(13)-C(15)	51.6(3)
C(7)-C(8)-C(9)-C(10)	-177.4(3)	C(6)-C(7)-C(13)-C(15)	-165.2(3)
Ca(1)-C(8)-C(9)-C(10)	67.5(2)	C(8)-C(7)-C(13)-C(14)	-64.8(3)
C(12)-C(8)-C(9)-Ca(1)	-67.3(2)	C(6)-C(7)-C(13)-C(14)	78.3(3)
C(7)-C(8)-C(9)-Ca(1)	115.1(3)	C(5)-C(6)-C(17)-C(18)	-161.7(3)
O(2)-Ca(1)-C(9)-C(10)	-30.4(3)	C(7)-C(6)-C(17)-C(18)	65.6(4)
O(1)-Ca(1)-C(9)-C(10)	49.1(2)	C(5)-C(6)-C(17)-C(19)	-44.6(3)
C(12)-Ca(1)-C(9)-C(10)	-77.0(2)	C(7)-C(6)-C(17)-C(19)	-177.3(3)
C(2)-Ca(1)-C(9)-C(10)	152.9(2)	C(5)-C(6)-C(17)-C(20)	76.6(3)
C(1)-Ca(1)-C(9)-C(10)	156.7(2)	C(7)-C(6)-C(17)-C(20)	-56.2(4)
C(8)-Ca(1)-C(9)-C(10)	-115.6(3)	C(21)-O(1)-C(22)-C(23)	-175.6(5)
C(11)-Ca(1)-C(9)-C(10)	-36.27(18)	Ca(1)-O(1)-C(22)-C(23)	21.4(6)
C(3)-Ca(1)-C(9)-C(10)	-171.8(2)	C(24)-O(2)-C(23)-C(22)	-171.0(4)
C(5)-Ca(1)-C(9)-C(10)	-173.7(2)	Ca(1)-O(2)-C(23)-C(22)	48.5(5)
C(4)-Ca(1)-C(9)-C(10)	-155.28(19)	O(1)-C(22)-C(23)-O(2)	-45.9(6)
O(2)-Ca(1)-C(9)-C(8)	85.2(2)		