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C9-C14	1.530 (6)
C9-C15	1.534 (6)
C10-H101	0.96 (4)
C10-H102	1.11 (4)
C11-C13	1.498 (7)
C11-C12	1.526 (8)
C12-H121	1.0380
C12-H122	1.0380
C12-H123	1.0380
C13-H131	0.9425
C13-H132	0.9425
C13-H133	0.9425
C14-H141	0.99 (5)
C14-H142	0.97 (5)
C16-C21	1.527 (6)
C16-C22	1.528 (5)
C16-C17	1.538 (6)
C17-H171	0.85 (5)
C17-H172	1.03 (4)
C18-C20	1.502 (7)
C18-C19	1.519 (7)
C19-H191	0.9881
C19-H192	0.9881
C19-H193	0.9881
C20-H201	0.9776
C20-H202	0.9776
C20-H203	0.9776
C21-H211	1.05 (5)
C21-H212	0.98 (4)
C23-C29	1.513 (6)
C23-C28	1.528 (6)
C23-C24	1.535 (6)
C24-H241	1.07 (6)
C24-H242	0.99 (6)
C25-C27	1.491 (11)
C25-C26	1.510 (11)
C26-H261	0.8072
C26-H262	0.8072
C26-H263	0.8072
C27-H271	0.9308
C27-H272	0.9308
C27-H273	0.9308
C28-H281	0.99 (5)
C28-H282	0.98 (5)
C30-C31	1.525 (5)
C30-C36	1.529 (5)
C30-C35	1.533 (6)
C31-H311	0.95 (5)
C31-H312	1.04 (5)
C32-C33	1.505 (7)
C32-C34	1.522 (7)
C33-H331	0.9928
C33-H332	0.9928
C33-H333	0.9928
C34-H341	0.9322
C34-H342	0.9322
C34-H343	0.9322
C35-H351	1.05 (4)
C35-H352	0.95 (4)
C37-C43	1.518 (6)
C37-C38	1.524 (6)
C37-C42	1.541 (5)
C38-H381	0.97 (4)

C39-C41	1.507(7)
C39-C40	1.510(7)
C40-H401	0.9706
C40-H402	0.9706
C40-H403	0.9706
C41-H411	1.0114
C41-H412	1.0114
C41-H413	1.0114
C42-H421	1.05(5)
C42-H422	0.98(4)
C44-H441	0.8837
C44-H442	0.8837
C44-H443	0.8837

C8-N1-C9	120.1(4)
C8-N1-H1	118(3)
C9-N1-H1	122(3)
C15-N2-C16	121.5(3)
C15-N2-H2	119(3)
C16-N2-H2	117(3)
C22-N3-C23	122.1(4)
C22-N3-H3	120(4)
C23-N3-H3	117(4)
C29-N4-C30	121.2(3)
C29-N4-H4	117(4)
C30-N4-H4	121(4)
C36-N5-C37	122.3(4)
C36-N5-H5	115(3)
C37-N5-H5	123(3)
C8-O1-C7	117.8(4)
C10-O3-C11	114.3(3)
C11-O4-C14	114.8(4)
C18-O6-C17	114.3(4)
C21-O7-C18	114.5(3)
C24-O9-C25	114.6(5)
C25-O10-C28	114.7(4)
C32-O12-C31	114.6(3)
C35-O13-C32	113.7(3)
C38-O15-C39	114.9(3)
C42-O16-C39	115.8(3)
C43-O18-C44	115.8(4)
C7-C1-C2	119.0(6)
C7-C1-C6	125.2(6)
C2-C1-C6	115.6(7)
C1-C2-C3	120.1(7)
C1-C2-H21	119.9
C3-C2-H21	120.0
C4-C3-C2	116.3(7)
C4-C3-H31	121.8
C2-C3-H31	121.8
C5-C4-C3	126.2(8)
C5-C4-H41	116.9
C3-C4-H41	116.9
C4-C5-C6	116.2(8)
C4-C5-H51	121.9
C6-C5-H51	121.9
C1-C6-C5	123.2(7)
C1-C6-H61	118.4
C5-C6-H61	118.4
C1-C7-O1	105.5(6)
C1-C7-H71	110.5
O1-C7-H71	110.5
C1-C7-H72	110.8

H71-C7-H72	108.7
O2-C8-O1	124.7(4)
O2-C8-N1	124.5(4)
O1-C8-N1	110.6(4)
N1-C9-C10	109.6(3)
N1-C9-C14	111.2(4)
C10-C9-C14	107.0(4)
N1-C9-C15	111.4(3)
C10-C9-C15	107.4(3)
C14-C9-C15	110.1(3)
O3-C10-C9	110.6(3)
O3-C10-H101	107(2)
C9-C10-H101	114(2)
O3-C10-H102	109(2)
C9-C10-H102	111(2)
H101-C10-H102	105(3)
O4-C11-O3	110.0(4)
O4-C11-C13	106.4(4)
O3-C11-C13	104.3(4)
O4-C11-C12	112.4(4)
O3-C11-C12	111.1(4)
C13-C11-C12	112.2(5)
C11-C12-H121	109.5
C11-C12-H122	109.5
H121-C12-H122	109.5
C11-C12-H123	109.5
H121-C12-H123	109.5
H122-C12-H123	109.5
C11-C13-H131	109.5
C11-C13-H132	109.5
H131-C13-H132	109.5
C11-C13-H133	109.5
H131-C13-H133	109.5
H132-C13-H133	109.5
O4-C14-C9	108.4(3)
O4-C14-H141	104(3)
C9-C14-H141	108(3)
O4-C14-H142	113(3)
C9-C14-H142	107(3)
H141-C14-H142	117(4)
O5-C15-N2	121.6(4)
O5-C15-C9	122.2(4)
N2-C15-C9	116.1(3)
N2-C16-C21	109.0(3)
N2-C16-C22	111.3(3)
C21-C16-C22	106.8(3)
N2-C16-C17	111.5(4)
C21-C16-C17	106.7(4)
C22-C16-C17	111.3(3)
O6-C17-C16	109.4(4)
O6-C17-H171	104(3)
C16-C17-H171	112(3)
O6-C17-H172	114(2)
C16-C17-H172	105(2)
H171-C17-H172	112(4)
O6-C18-O7	109.3(3)
O6-C18-C20	106.3(4)
O7-C18-C20	105.5(4)
O6-C18-C19	111.9(4)
O7-C18-C19	111.8(4)
C20-C18-C19	111.6(4)
C18-C19-H191	109.5
C18-C19-H192	109.5

C18-C19-H193	109.5
H191-C19-H193	109.5
H192-C19-H193	109.5
C18-C20-H201	109.5
C18-C20-H202	109.5
H201-C20-H202	109.5
C18-C20-H203	109.5
H201-C20-H203	109.5
H202-C20-H203	109.5
O7-C21-C16	110.3 (4)
O7-C21-H211	109 (2)
C16-C21-H211	100 (3)
O7-C21-H212	113 (2)
C16-C21-H212	105 (2)
H211-C21-H212	118 (3)
O8-C22-N3	122.6 (4)
O8-C22-C16	121.3 (4)
N3-C22-C16	115.9 (3)
N3-C23-C29	112.1 (3)
N3-C23-C28	108.0 (4)
C29-C23-C28	107.6 (4)
N3-C23-C24	110.0 (4)
C29-C23-C24	110.9 (4)
C28-C23-C24	107.9 (4)
O9-C24-C23	109.6 (4)
O9-C24-H241	107 (3)
C23-C24-H241	108 (3)
O9-C24-H242	110 (3)
C23-C24-H242	104 (3)
H241-C24-H242	116 (4)
O10-C25-O9	109.0 (5)
O10-C25-C27	112.4 (7)
O9-C25-C27	113.2 (7)
O10-C25-C26	105.0 (7)
O9-C25-C26	105.9 (9)
C27-C25-C26	110.9 (9)
C25-C26-H261	109.5
C25-C26-H262	109.5
H261-C26-H262	109.5
C25-C26-H263	109.4
H261-C26-H263	109.5
H262-C26-H263	109.5
C25-C27-H271	109.5
C25-C27-H272	109.5
H271-C27-H272	109.5
C25-C27-H273	109.5
H271-C27-H273	109.5
H272-C27-H273	109.5
O10-C28-C23	110.7 (4)
O10-C28-H281	114 (3)
C23-C28-H281	102 (3)
O10-C28-H282	110 (3)
C23-C28-H282	106 (3)
H281-C28-H282	114 (4)
O11-C29-N4	122.0 (4)
O11-C29-C23	121.1 (4)
N4-C29-C23	116.8 (4)
N4-C30-C31	111.7 (3)
N4-C30-C36	111.4 (3)
C31-C30-C36	111.5 (3)
N4-C30-C35	108.1 (3)
C31-C30-C35	108.7 (3)
C36-C30-C35	105.1 (3)

O12-C31-H311	101(3)
C30-C31-H311	112(3)
O12-C31-H312	108(3)
C30-C31-H312	111(3)
H311-C31-H312	113(4)
O12-C32-O13	109.9(3)
O12-C32-C33	106.3(4)
O13-C32-C33	104.5(4)
O12-C32-C34	111.9(4)
O13-C32-C34	110.9(4)
C33-C32-C34	112.8(4)
C32-C33-H331	109.5
C32-C33-H332	109.5
H331-C33-H332	109.5
C32-C33-H333	109.5
H331-C33-H333	109.5
H332-C33-H333	109.5
C32-C34-H341	109.5
C32-C34-H342	109.5
H341-C34-H342	109.5
C32-C34-H343	109.5
H341-C34-H343	109.5
H342-C34-H343	109.5
O13-C35-C30	111.4(3)
O13-C35-H351	107(2)
C30-C35-H351	113(2)
O13-C35-H352	104(3)
C30-C35-H352	112(3)
H351-C35-H352	109(3)
O14-C36-N5	122.0(4)
O14-C36-C30	121.6(3)
N5-C36-C30	115.9(3)
N5-C37-C43	111.9(3)
N5-C37-C38	110.2(3)
C43-C37-C38	111.5(3)
N5-C37-C42	107.9(3)
C43-C37-C42	109.0(3)
C38-C37-C42	106.2(4)
O15-C38-C37	110.0(4)
O15-C38-H381	105(2)
C37-C38-H381	111(3)
O15-C38-H382	106(2)
C37-C38-H382	110(2)
H381-C38-H382	114(4)
O15-C39-O16	109.9(3)
O15-C39-C41	111.2(4)
O16-C39-C41	112.0(4)
O15-C39-C40	105.1(4)
O16-C39-C40	105.3(4)
C41-C39-C40	112.9(4)
C39-C40-H401	109.5
C39-C40-H402	109.5
H401-C40-H402	109.5
C39-C40-H403	109.5
H401-C40-H403	109.5
H402-C40-H403	109.5
C39-C41-H411	109.5
C39-C41-H412	109.5
H411-C41-H412	109.5
C39-C41-H413	109.5
H411-C41-H413	109.5
H412-C41-H413	109.5
O16-C42-C37	110.8(3)

C37-C42-H421	117 (3)
O16-C42-H422	115 (2)
C37-C42-H422	106 (2)
H421-C42-H422	102 (3)
O17-C43-O18	124.9 (4)
O17-C43-C37	123.6 (4)
O18-C43-C37	111.3 (4)
O18-C44-H441	109.5
O18-C44-H442	109.5
H441-C44-H442	109.5
O18-C44-H443	109.5
H441-C44-H443	109.5
H442-C44-H443	109.5

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

	U11	U22	U33	U23	U13	U12
N1	52(2)	41(2)	48(2)	8(2)	5(2)	11(2)
N2	49(2)	37(2)	55(2)	16(2)	16(2)	7(2)
N3	53(2)	41(2)	47(2)	9(2)	11(2)	7(2)
N4	45(2)	39(2)	44(2)	7(2)	11(1)	6(1)
N5	40(2)	40(2)	62(2)	19(2)	16(2)	10(1)
O1	151(4)	62(2)	65(2)	9(2)	-32(2)	38(2)
O2	66(2)	50(2)	60(2)	-1(2)	3(2)	9(1)
O3	59(2)	51(2)	61(2)	-1(1)	14(2)	7(1)
O4	45(2)	69(2)	63(2)	-1(2)	14(1)	7(1)
O5	64(2)	40(2)	60(2)	18(1)	20(2)	7(1)
O6	52(2)	58(2)	61(2)	12(2)	4(1)	4(1)
O7	53(2)	46(2)	64(2)	18(1)	20(1)	7(1)
O8	58(2)	41(2)	72(2)	18(2)	15(2)	18(1)
O9	130(3)	87(3)	69(2)	25(2)	51(2)	21(2)
O10	117(3)	79(2)	57(2)	26(2)	11(2)	33(2)
O11	98(3)	43(2)	56(2)	1(2)	24(2)	6(2)
O12	37(2)	65(2)	78(2)	17(2)	7(1)	10(1)
O13	44(2)	55(2)	62(2)	9(1)	18(1)	13(1)
O14	53(2)	42(2)	82(2)	19(2)	18(2)	5(1)
O15	61(2)	59(2)	57(2)	13(2)	26(2)	8(1)
O16	59(2)	53(2)	51(2)	12(1)	17(1)	-1(1)
O17	82(2)	45(2)	86(2)	23(2)	34(2)	24(2)
O18	88(2)	59(2)	61(2)	11(2)	18(2)	25(2)
C1	112(4)	64(3)	66(3)	6(3)	15(3)	6(3)
C2	116(5)	82(4)	90(4)	-4(4)	14(4)	15(4)
C3	79(4)	159(7)	118(6)	-43(5)	33(4)	-8(4)
C4	92(4)	113(5)	93(5)	28(4)	43(4)	37(4)
C5	119(6)	174(9)	157(9)	-71(7)	53(6)	21(5)
C6	129(5)	86(4)	102(5)	-2(4)	18(4)	25(4)
C7	108(4)	96(4)	98(4)	-20(4)	-44(4)	56(4)
C8	58(3)	57(3)	49(2)	7(2)	11(2)	21(2)
C9	47(2)	42(2)	43(2)	10(2)	7(2)	7(2)
C10	47(2)	47(2)	48(2)	6(2)	10(2)	2(2)
C11	57(3)	67(3)	57(3)	-2(2)	16(2)	5(2)
C12	90(4)	105(4)	58(3)	18(3)	24(3)	6(4)
C13	82(4)	93(4)	100(5)	-20(4)	24(4)	31(3)
C14	50(2)	52(2)	59(3)	6(2)	20(2)	2(2)
C15	47(2)	40(2)	46(2)	10(2)	10(2)	3(2)
C16	43(2)	40(2)	51(2)	12(2)	10(2)	6(2)
C17	51(2)	55(3)	59(3)	20(2)	10(2)	7(2)
C18	46(2)	58(3)	61(3)	12(2)	11(2)	5(2)
C19	49(3)	83(4)	103(4)	18(3)	19(3)	16(3)
C20	73(4)	63(3)	90(4)	11(3)	14(3)	-6(3)
C21	50(2)	47(2)	62(3)	16(2)	22(2)	9(2)
C22	47(2)	45(2)	53(2)	18(2)	17(2)	9(2)
C23	65(3)	45(2)	41(2)	8(2)	11(2)	11(2)
C24	94(4)	58(3)	56(3)	14(2)	33(3)	17(3)
C25	156(6)	112(5)	62(4)	39(3)	35(4)	51(5)
C26	268(16)	184(9)	132(9)	113(9)	93(10)	79(10)
C27	198(9)	163(8)	56(4)	-2(5)	5(5)	71(7)
C28	69(3)	59(3)	48(3)	13(2)	2(2)	11(2)
C29	58(2)	44(2)	44(2)	7(2)	10(2)	7(2)
C30	37(2)	41(2)	45(2)	10(2)	11(2)	7(2)

C32	44 (2)	70 (3)	75 (3)	20 (2)	24 (2)	16 (2)
C33	60 (3)	96 (4)	115 (5)	22 (4)	33 (3)	34 (3)
C34	53 (3)	97 (4)	101 (5)	35 (4)	36 (3)	7 (3)
C35	43 (2)	49 (2)	43 (2)	11 (2)	10 (2)	13 (2)
C36	41 (2)	43 (2)	48 (2)	10 (2)	14 (2)	5 (2)
C37	43 (2)	43 (2)	53 (2)	18 (2)	17 (2)	11 (2)
C38	51 (3)	57 (3)	60 (3)	22 (2)	19 (2)	12 (2)
C39	62 (3)	61 (3)	49 (2)	13 (2)	17 (2)	4 (2)
C40	93 (4)	68 (3)	65 (3)	4 (3)	23 (3)	2 (3)
C41	68 (3)	97 (4)	61 (3)	16 (3)	8 (3)	14 (3)
C42	39 (2)	52 (2)	57 (3)	17 (2)	16 (2)	9 (2)
C43	43 (2)	50 (2)	65 (3)	16 (2)	20 (2)	13 (2)
C44	112 (5)	81 (4)	75 (4)	-8 (3)	25 (4)	24 (4)

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

	x	y	z	U(eq)
H1	2110(5)	-230(5)	2240(3)	88(17)
H2	170(4)	1190(4)	2440(2)	43(12)
H3	1720(5)	3100(5)	3460(3)	100(2)
H4	2270(5)	4720(5)	2710(3)	75(17)
H5	640(4)	5980(4)	2390(3)	56(14)
H21	5896	2201	4921	150(3)
H31	7852	1653	5154	190(4)
H41	8117	285	4275	150(3)
H51	6637	-1171	3682	220(5)
H61	4686	-755	3466	198
H71	3866(6)	1870(5)	4356(9)	196
H72	3510(2)	470(2)	4610(2)	210
H101	300(4)	-20(3)	1200(2)	41(10)
H102	590(3)	900(3)	680(2)	30(9)
H121	1730(2)	1287(19)	35(4)	140(3)
H122	1900(16)	100(2)	-520(16)	87(17)
H123	3080(3)	1201(16)	-146(5)	180(3)
H131	4040(2)	-511(11)	335(6)	110(2)
H132	2831(17)	-1350(2)	49(14)	84(17)
H133	3490(8)	-1139(13)	864(14)	130(3)
H141	3490(4)	2240(4)	1970(3)	61(13)
H142	2560(5)	2300(4)	1180(3)	75(16)
H171	-1200(4)	2850(4)	1650(3)	51(13)
H172	-1900(4)	3280(3)	2220(2)	43(11)
H191	-3939(10)	1441(11)	2861(13)	140(3)
H192	-4340(2)	1689(5)	2043(14)	72(15)
H193	-3275(12)	2570(3)	2647(7)	130(3)
H201	-2703(18)	-553(13)	1741(5)	90(19)
H202	-3939(19)	-147(5)	1441(13)	110(2)
H203	-3666(12)	-524(13)	2220(10)	77(16)
H211	-290(4)	1900(4)	3560(3)	63(13)
H212	-1460(3)	2650(3)	3390(2)	35(9)
H241	500(5)	5330(5)	4280(3)	89(18)
H242	1920(5)	5990(5)	4840(3)	92(19)
H261	1610(3)	2660(3)	5430(2)	140(4)
H262	1720(3)	3363(19)	6050(2)	210(5)
H263	2650(4)	2943(18)	5915(15)	230(7)
H271	3810(3)	4950(14)	6216(13)	200(5)
H272	2690(2)	5425(15)	6288(17)	180(4)
H273	3366(15)	5780(3)	5737(11)	170(4)
H281	3540(4)	4200(4)	3990(3)	71(15)
H282	3710(4)	5270(4)	4680(3)	58(13)
H311	4270(4)	7130(4)	3250(3)	55(13)
H312	4250(4)	7550(4)	2460(3)	60(13)
H331	5283(9)	4117(18)	2269(10)	110(2)
H332	6380(3)	5044(12)	2182(8)	120(2)
H333	5458(5)	4229(15)	1462(16)	71(16)
H341	4999(5)	5975(13)	969(14)	120(3)
H342	5800(2)	6825(15)	1634(7)	88(18)
H343	4469(18)	6875(16)	1386(4)	65(14)
H351	1820(4)	5020(3)	1450(2)	50(11)
H352	2760(4)	6080(4)	1330(2)	49(12)
H381	490(4)	7720(4)	1180(2)	51(12)
H382	-940(4)	7660(3)	1040(2)	45(11)

H402	-2110 (2)	3743 (18)	335 (4)	84 (17)
H403	-710 (2)	4054 (9)	696 (9)	100 (2)
H411	-2658 (5)	6650 (2)	612 (8)	96 (19)
H412	-3360 (2)	5301 (17)	347 (3)	120 (2)
H413	-2571 (5)	5889 (5)	-165 (16)	78 (16)
H421	-1500 (4)	6160 (4)	2480 (3)	64 (13)
H422	-2030 (4)	6860 (3)	1880 (2)	48 (11)
H441	740 (3)	9820 (2)	3673 (4)	130 (3)
H442	313 (10)	9147 (8)	4160 (2)	190 (4)
H443	-530 (3)	9533 (13)	3615 (6)	160 (4)

Table 6. Selected torsion angles [deg] for 4.

C7-C1-C2-C3	169.5(7)
C6-C1-C2-C3	-5.9(10)
C1-C2-C3-C4	12.4(12)
C2-C3-C4-C5	-18.6(14)
C3-C4-C5-C6	17(2)
C7-C1-C6-C5	-171.0(9)
C2-C1-C6-C5	4.1(12)
C4-C5-C6-C1	-9(2)
C2-C1-C7-O1	149.3(6)
C6-C1-C7-O1	-35.8(10)
C8-O1-C7-C1	-104.3(6)
C7-O1-C8-O2	-6.0(8)
C7-O1-C8-N1	178.3(5)
C9-N1-C8-O2	5.6(7)
C9-N1-C8-O1	-178.6(4)
C8-N1-C9-C10	-173.0(4)
C8-N1-C9-C14	68.9(5)
C8-N1-C9-C15	-54.3(5)
C11-O3-C10-C9	-55.9(5)
N1-C9-C10-O3	-65.0(4)
C14-C9-C10-O3	55.7(5)
C15-C9-C10-O3	173.9(3)
C14-O4-C11-O3	-56.6(5)
C14-O4-C11-C13	-169.0(5)
C14-O4-C11-C12	67.7(5)
C10-O3-C11-O4	54.2(5)
C10-O3-C11-C13	168.0(4)
C10-O3-C11-C12	-70.9(5)
C11-O4-C14-C9	59.7(5)
N1-C9-C14-O4	63.3(5)
C10-C9-C14-O4	-56.4(5)
C15-C9-C14-O4	-172.7(3)
C16-N2-C15-O5	4.0(6)
C16-N2-C15-C9	-176.0(3)
N1-C9-C15-O5	140.2(4)
C10-C9-C15-O5	-99.8(4)
C14-C9-C15-O5	16.3(5)
N1-C9-C15-N2	-39.8(5)
C10-C9-C15-N2	80.2(4)
C14-C9-C15-N2	-163.6(4)
C15-N2-C16-C21	-170.7(4)
C15-N2-C16-C22	-53.2(5)
C15-N2-C16-C17	71.7(5)
C18-O6-C17-C16	58.8(5)
N2-C16-C17-O6	63.7(5)
C21-C16-C17-O6	-55.2(5)
C22-C16-C17-O6	-171.4(4)
C17-O6-C18-O7	-57.2(5)
C17-O6-C18-C20	-170.6(4)
C17-O6-C18-C19	67.3(5)
C21-O7-C18-O6	56.5(5)
C21-O7-C18-C20	170.4(4)
C21-O7-C18-C19	-68.1(5)
C18-O7-C21-C16	-57.9(5)
N2-C16-C21-O7	-65.5(4)
C22-C16-C21-O7	174.2(3)
C17-C16-C21-O7	55.1(4)
C23-N3-C22-O8	2.7(6)
C22-N3-C22-C16	-172.3(3)

C21-C16-C22-O8	-94.9 (4)
C17-C16-C22-O8	21.3 (6)
N2-C16-C22-N3	-38.7 (5)
C21-C16-C22-N3	80.2 (4)
C17-C16-C22-N3	-163.7 (4)
C22-N3-C23-C29	-59.9 (5)
C22-N3-C23-C28	-178.3 (4)
C22-N3-C23-C24	64.1 (5)
C25-O9-C24-C23	58.1 (6)
N3-C23-C24-O9	64.3 (6)
C29-C23-C24-O9	-171.0 (4)
C28-C23-C24-O9	-53.4 (6)
C28-O10-C25-O9	56.5 (7)
C28-O10-C25-C27	-69.7 (7)
C28-O10-C25-C26	169.6 (8)
C24-O9-C25-O10	-57.9 (7)
C24-O9-C25-C27	67.9 (8)
C24-O9-C25-C26	-170.4 (7)
C25-O10-C28-C23	-56.6 (6)
N3-C23-C28-O10	-66.3 (5)
C29-C23-C28-O10	172.4 (4)
C24-C23-C28-O10	52.7 (5)
C30-N4-C29-O11	-2.2 (6)
C30-N4-C29-C23	-179.4 (3)
N3-C23-C29-O11	153.6 (4)
C28-C23-C29-O11	-87.7 (5)
C24-C23-C29-O11	30.1 (6)
N3-C23-C29-N4	-29.1 (5)
C28-C23-C29-N4	89.5 (5)
C24-C23-C29-N4	-152.6 (4)
C29-N4-C30-C31	68.4 (5)
C29-N4-C30-C36	-57.1 (5)
C29-N4-C30-C35	-172.1 (4)
C32-O12-C31-C30	56.3 (5)
N4-C30-C31-O12	68.7 (5)
C36-C30-C31-O12	-165.9 (4)
C35-C30-C31-O12	-50.5 (5)
C31-O12-C32-O13	-58.1 (5)
C31-O12-C32-C33	-170.7 (4)
C31-O12-C32-C34	65.7 (5)
C35-O13-C32-O12	57.4 (5)
C35-O13-C32-C33	171.2 (4)
C35-O13-C32-C34	-67.0 (5)
C32-O13-C35-C30	-55.6 (5)
N4-C30-C35-O13	-70.4 (4)
C31-C30-C35-O13	51.0 (5)
C36-C30-C35-O13	170.5 (3)
C37-N5-C36-O14	8.2 (6)
C37-N5-C36-C30	-164.3 (4)
N4-C30-C36-O14	149.9 (4)
C31-C30-C36-O14	24.4 (6)
C35-C30-C36-O14	-93.2 (4)
N4-C30-C36-N5	-37.6 (5)
C31-C30-C36-N5	-163.1 (4)
C35-C30-C36-N5	79.3 (4)
C36-N5-C37-C43	-61.2 (5)
C36-N5-C37-C38	63.5 (5)
C36-N5-C37-C42	179.0 (4)
C39-O15-C38-C37	59.1 (5)
N5-C37-C38-O15	60.1 (5)
C43-C37-C38-O15	-175.0 (3)
C42-C37-C38-O15	-56.5 (4)
C28-O15-C38-O16	-54.0 (5)

C38-O15-C39-C40	-166.9(4)
C42-O16-C39-O15	52.1(5)
C42-O16-C39-C41	-72.1(5)
C42-O16-C39-C40	164.8(4)
C39-O16-C42-C37	-55.0(5)
N5-C37-C42-O16	-63.4(4)
C43-C37-C42-O16	174.9(3)
C38-C37-C42-O16	54.7(4)
C44-O18-C43-O17	-3.2(7)
C44-O18-C43-C37	-178.6(5)
N5-C37-C43-O17	137.3(4)
C38-C37-C43-O17	13.4(6)
C42-C37-C43-O17	-103.5(5)
N5-C37-C43-O18	-47.3(5)
C38-C37-C43-O18	-171.3(4)
C42-C37-C43-O18	71.9(4)
