

Supplementary Information For

Synthesis, crystal structures and phase transformation of the new

solid-state forms of tetrandrine

Zhengzheng Zhou,^a Henry H.Y. Tong,^{b*} Liang Li,^c Fanny L.Y. Shek,^d Yang Lv^e,
Ying Zheng,^{a*}

^a State Key Laboratory of Quality Research in Chinese Medicine, Institute of Chinese Medical Sciences, University of Macau, Macao SAR, China

^b School of Health Sciences, Macao Polytechnic Institute, Macao SAR, China

^c Department of Forensic Medicine, Zhongshan School of Medicine, Sun Yat-sen University, Guangzhou, China

^d Material Characterization and Preparation Facility, Hong Kong University of Science and Technology, Hong Kong SAR, China

^e Beijing Key Laboratory of Polymorphic Drugs, Institute of Materia Medica, Chinese Academy of Medical Sciences and Peking Union Medical College, Beijing, China

Crystalline data for form I

Table S1. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for form I. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	$U(\text{eq})$
N(1)	9343(2)	718(1)	8901(1)	20(1)
N(2)	2628(2)	7837(1)	8643(1)	21(1)
O(1)	3705(2)	4995(1)	7218(1)	27(1)
O(2)	4530(2)	3670(1)	7772(1)	22(1)
O(3)	4223(2)	4509(1)	8450(1)	17(1)
O(4)	7454(2)	5272(1)	8090(1)	22(1)
O(5)	2356(2)	4726(1)	9926(1)	24(1)
O(6)	-37(2)	6069(1)	10217(1)	22(1)
C(2)	7883(2)	1530(1)	9002(1)	18(1)
C(3)	6071(2)	3063(1)	8692(1)	15(1)
C(4)	5945(2)	3956(1)	8462(1)	15(1)
C(5)	7542(2)	4290(1)	8276(1)	16(1)
C(6)	9151(2)	3646(1)	8299(1)	17(1)
C(7)	11046(2)	2023(1)	8525(1)	20(1)
C(8)	11162(2)	1267(1)	8845(1)	22(1)
C(9)	9271(2)	2718(1)	8520(1)	17(1)
C(10)	7741(2)	2449(1)	8728(1)	16(1)
C(11)	9503(3)	-211(2)	9147(1)	29(1)
C(12)	8212(2)	2044(2)	9369(1)	22(1)
C(13)	6641(2)	2760(1)	9504(1)	18(1)
C(14)	4909(2)	2287(1)	9591(1)	20(1)
C(15)	3463(2)	2945(1)	9722(1)	20(1)
C(16)	3775(2)	4076(1)	9775(1)	19(1)
C(17)	5477(2)	4564(1)	9693(1)	22(1)
C(18)	6892(2)	3909(1)	9553(1)	21(1)
C(19)	1386(2)	5425(1)	9703(1)	17(1)
C(20)	78(2)	6144(1)	9862(1)	18(1)
C(21)	-978(2)	6849(1)	9652(1)	19(1)
C(22)	-745(2)	6836(1)	9289(1)	20(1)
C(23)	556(2)	6136(1)	9131(1)	17(1)
C(24)	1616(2)	5423(1)	9345(1)	18(1)
C(25)	-1422(3)	6740(2)	10385(1)	29(1)
C(26)	833(2)	6068(1)	8742(1)	18(1)
C(27)	2666(2)	6606(1)	8605(1)	17(1)
C(28)	1381(3)	8348(1)	8384(1)	24(1)
C(29)	1947(3)	8118(1)	8005(1)	24(1)

C(30)	2574(2)	6916(1)	7948(1)	19(1)
C(31)	3010(2)	6232(1)	8230(1)	16(1)
C(32)	3717(2)	5157(1)	8161(1)	16(1)
C(33)	3848(2)	4736(1)	7825(1)	17(1)
C(34)	3422(2)	5448(1)	7544(1)	19(1)
C(35)	2802(2)	6529(1)	7606(1)	20(1)
C(36)	4528(3)	8298(2)	8624(1)	28(1)
C(37)	3087(3)	5657(2)	6929(1)	39(1)
C(38)	3234(3)	2912(2)	7614(1)	26(1)
C(39)	8506(3)	5309(2)	7776(1)	31(1)

Table S2. Bond lengths [Å] and angles [deg] for form I.

N(1)-C(11)	1.460(2)	N(1)-C(8)-H(8A)	109.8
N(1)-C(8)	1.467(2)	C(7)-C(8)-H(8A)	109.8
N(1)-C(2)	1.472(2)	N(1)-C(8)-H(8B)	109.8
N(2)-C(36)	1.463(2)	C(7)-C(8)-H(8B)	109.8
N(2)-C(28)	1.465(2)	H(8A)-C(8)-H(8B)	108.2
N(2)-C(27)	1.475(2)	C(10)-C(9)-C(6)	118.91(15)
O(1)-C(34)	1.3730(19)	C(10)-C(9)-C(7)	121.53(14)
O(1)-C(37)	1.430(2)	C(6)-C(9)-C(7)	119.55(15)
O(2)-C(33)	1.375(2)	C(9)-C(10)-C(3)	119.22(14)
O(2)-C(38)	1.427(2)	C(9)-C(10)-C(2)	120.64(14)
O(3)-C(4)	1.3931(19)	C(3)-C(10)-C(2)	120.10(14)
O(3)-C(32)	1.3951(19)	N(1)-C(11)-H(11A)	109.5
O(4)-C(5)	1.3717(19)	N(1)-C(11)-H(11B)	109.5
O(4)-C(39)	1.417(2)	H(11A)-C(11)-H(11B)	109.5
O(5)-C(19)	1.3806(19)	N(1)-C(11)-H(11C)	109.5
O(5)-C(16)	1.399(2)	H(11A)-C(11)-H(11C)	109.5
O(6)-C(20)	1.368(2)	H(11B)-C(11)-H(11C)	109.5
O(6)-C(25)	1.423(2)	C(13)-C(12)-C(2)	115.16(14)
C(2)-C(10)	1.519(2)	C(13)-C(12)-H(12A)	108.5
C(2)-C(12)	1.552(2)	C(2)-C(12)-H(12A)	108.5
C(2)-H(2A)	0.9800	C(13)-C(12)-H(12B)	108.5
C(3)-C(4)	1.385(2)	C(2)-C(12)-H(12B)	108.5
C(3)-C(10)	1.403(2)	H(12A)-C(12)-H(12B)	107.5
C(3)-H(3A)	0.9300	C(18)-C(13)-C(14)	118.56(15)
C(4)-C(5)	1.400(2)	C(18)-C(13)-C(12)	120.69(15)
C(5)-C(6)	1.382(2)	C(14)-C(13)-C(12)	120.74(15)
C(6)-C(9)	1.397(2)	C(15)-C(14)-C(13)	120.85(16)
C(6)-H(6A)	0.9300	C(15)-C(14)-H(14A)	119.6
C(7)-C(9)	1.512(2)	C(13)-C(14)-H(14A)	119.6
C(7)-C(8)	1.521(2)	C(16)-C(15)-C(14)	119.04(16)
C(7)-H(7A)	0.9700	C(16)-C(15)-H(15A)	120.5

C(7)-H(7B)	0.9700	C(14)-C(15)-H(15A)	120.5
C(8)-H(8A)	0.9700	C(17)-C(16)-C(15)	121.25(15)
C(8)-H(8B)	0.9700	C(17)-C(16)-O(5)	119.68(14)
C(9)-C(10)	1.388(2)	C(15)-C(16)-O(5)	119.03(15)
C(11)-H(11A)	0.9600	C(16)-C(17)-C(18)	119.33(15)
C(11)-H(11B)	0.9600	C(16)-C(17)-H(17A)	120.3
C(11)-H(11C)	0.9600	C(18)-C(17)-H(17A)	120.3
C(12)-C(13)	1.500(2)	C(17)-C(18)-C(13)	120.93(16)
C(12)-H(12A)	0.9700	C(17)-C(18)-H(18A)	119.5
C(12)-H(12B)	0.9700	C(13)-C(18)-H(18A)	119.5
C(13)-C(18)	1.393(2)	O(5)-C(19)-C(24)	123.73(14)
C(13)-C(14)	1.397(2)	O(5)-C(19)-C(20)	115.61(14)
C(14)-C(15)	1.388(2)	C(24)-C(19)-C(20)	120.65(15)
C(14)-H(14A)	0.9300	O(6)-C(20)-C(21)	125.73(15)
C(15)-C(16)	1.382(2)	O(6)-C(20)-C(19)	115.54(14)
C(15)-H(15A)	0.9300	C(21)-C(20)-C(19)	118.73(15)
C(16)-C(17)	1.381(2)	C(20)-C(21)-C(22)	120.24(15)
C(17)-C(18)	1.383(2)	C(20)-C(21)-H(21A)	119.9
C(17)-H(17A)	0.9300	C(22)-C(21)-H(21A)	119.9
C(18)-H(18A)	0.9300	C(23)-C(22)-C(21)	121.31(15)
C(19)-C(24)	1.381(2)	C(23)-C(22)-H(22A)	119.3
C(19)-C(20)	1.405(2)	C(21)-C(22)-H(22A)	119.3
C(20)-C(21)	1.383(2)	C(22)-C(23)-C(24)	118.10(15)
C(21)-C(22)	1.401(2)	C(22)-C(23)-C(26)	123.51(15)
C(21)-H(21A)	0.9300	C(24)-C(23)-C(26)	118.35(14)
C(22)-C(23)	1.386(2)	C(19)-C(24)-C(23)	120.96(15)
C(22)-H(22A)	0.9300	C(19)-C(24)-H(24A)	119.5
C(23)-C(24)	1.400(2)	C(23)-C(24)-H(24A)	119.5
C(23)-C(26)	1.507(2)	O(6)-C(25)-H(25A)	109.5
C(24)-H(24A)	0.9300	O(6)-C(25)-H(25B)	109.5
C(25)-H(25A)	0.9600	H(25A)-C(25)-H(25B)	109.5
C(25)-H(25B)	0.9600	O(6)-C(25)-H(25C)	109.5
C(25)-H(25C)	0.9600	H(25A)-C(25)-H(25C)	109.5
C(26)-C(27)	1.545(2)	H(25B)-C(25)-H(25C)	109.5
C(26)-H(26A)	0.9700	C(23)-C(26)-C(27)	115.02(13)
C(26)-H(26B)	0.9700	C(23)-C(26)-H(26A)	108.5
C(27)-C(31)	1.527(2)	C(27)-C(26)-H(26A)	108.5
C(27)-H(27A)	0.9800	C(23)-C(26)-H(26B)	108.5
C(28)-C(29)	1.532(2)	C(27)-C(26)-H(26B)	108.5
C(28)-H(28A)	0.9700	H(26A)-C(26)-H(26B)	107.5
C(28)-H(28B)	0.9700	N(2)-C(27)-C(31)	112.69(13)
C(29)-C(30)	1.516(2)	N(2)-C(27)-C(26)	111.38(14)
C(29)-H(29A)	0.9700	C(31)-C(27)-C(26)	109.45(13)
C(29)-H(29B)	0.9700	N(2)-C(27)-H(27A)	107.7

C(30)-C(31)	1.387(2)	C(31)-C(27)-H(27A)	107.7
C(30)-C(35)	1.399(2)	C(26)-C(27)-H(27A)	107.7
C(31)-C(32)	1.401(2)	N(2)-C(28)-C(29)	114.12(14)
C(32)-C(33)	1.385(2)	N(2)-C(28)-H(28A)	108.7
C(33)-C(34)	1.405(2)	C(29)-C(28)-H(28A)	108.7
C(34)-C(35)	1.384(2)	N(2)-C(28)-H(28B)	108.7
C(35)-H(35A)	0.9300	C(29)-C(28)-H(28B)	108.7
C(36)-H(36A)	0.9600	H(28A)-C(28)-H(28B)	107.6
C(36)-H(36B)	0.9600	C(30)-C(29)-C(28)	112.44(14)
C(36)-H(36C)	0.9600	C(30)-C(29)-H(29A)	109.1
C(37)-H(37A)	0.9600	C(28)-C(29)-H(29A)	109.1
C(37)-H(37B)	0.9600	C(30)-C(29)-H(29B)	109.1
C(37)-H(37C)	0.9600	C(28)-C(29)-H(29B)	109.1
C(38)-H(38A)	0.9600	H(29A)-C(29)-H(29B)	107.8
C(38)-H(38B)	0.9600	C(31)-C(30)-C(35)	120.56(15)
C(38)-H(38C)	0.9600	C(31)-C(30)-C(29)	120.75(15)
C(39)-H(39A)	0.9600	C(35)-C(30)-C(29)	118.61(14)
C(39)-H(39B)	0.9600	C(30)-C(31)-C(32)	118.23(15)
C(39)-H(39C)	0.9600	C(30)-C(31)-C(27)	121.65(14)
C(11)-N(1)-C(8)	111.35(14)	C(32)-C(31)-C(27)	120.07(14)
C(11)-N(1)-C(2)	112.58(13)	C(33)-C(32)-O(3)	121.21(14)
C(8)-N(1)-C(2)	111.69(13)	C(33)-C(32)-C(31)	121.94(14)
C(36)-N(2)-C(28)	111.75(14)	O(3)-C(32)-C(31)	116.81(14)
C(36)-N(2)-C(27)	110.62(14)	O(2)-C(33)-C(32)	119.71(14)
C(28)-N(2)-C(27)	111.00(13)	O(2)-C(33)-C(34)	121.41(14)
C(34)-O(1)-C(37)	116.25(13)	C(32)-C(33)-C(34)	118.68(14)
C(33)-O(2)-C(38)	114.79(13)	O(1)-C(34)-C(35)	124.71(15)
C(4)-O(3)-C(32)	121.03(12)	O(1)-C(34)-C(33)	115.31(14)
C(5)-O(4)-C(39)	116.26(13)	C(35)-C(34)-C(33)	119.97(15)
C(19)-O(5)-C(16)	116.05(12)	C(34)-C(35)-C(30)	120.38(15)
C(20)-O(6)-C(25)	117.02(13)	C(34)-C(35)-H(35A)	119.8
N(1)-C(2)-C(10)	109.92(13)	C(30)-C(35)-H(35A)	119.8
N(1)-C(2)-C(12)	113.01(13)	N(2)-C(36)-H(36A)	109.5
C(10)-C(2)-C(12)	110.44(13)	N(2)-C(36)-H(36B)	109.5
N(1)-C(2)-H(2A)	107.8	H(36A)-C(36)-H(36B)	109.5
C(10)-C(2)-H(2A)	107.8	N(2)-C(36)-H(36C)	109.5
C(12)-C(2)-H(2A)	107.8	H(36A)-C(36)-H(36C)	109.5
C(4)-C(3)-C(10)	121.28(15)	H(36B)-C(36)-H(36C)	109.5
C(4)-C(3)-H(3A)	119.4	O(1)-C(37)-H(37A)	109.5
C(10)-C(3)-H(3A)	119.4	O(1)-C(37)-H(37B)	109.5
C(3)-C(4)-O(3)	116.23(14)	H(37A)-C(37)-H(37B)	109.5
C(3)-C(4)-C(5)	119.28(14)	O(1)-C(37)-H(37C)	109.5
O(3)-C(4)-C(5)	124.36(13)	H(37A)-C(37)-H(37C)	109.5
O(4)-C(5)-C(6)	123.00(15)	H(37B)-C(37)-H(37C)	109.5

O(4)-C(5)-C(4)	117.99(14)	O(2)-C(38)-H(38A)	109.5
C(6)-C(5)-C(4)	118.95(14)	O(2)-C(38)-H(38B)	109.5
C(5)-C(6)-C(9)	121.94(15)	H(38A)-C(38)-H(38B)	109.5
C(5)-C(6)-H(6A)	119.0	O(2)-C(38)-H(38C)	109.5
C(9)-C(6)-H(6A)	119.0	H(38A)-C(38)-H(38C)	109.5
C(9)-C(7)-C(8)	112.34(14)	H(38B)-C(38)-H(38C)	109.5
C(9)-C(7)-H(7A)	109.1	O(4)-C(39)-H(39A)	109.5
C(8)-C(7)-H(7A)	109.1	O(4)-C(39)-H(39B)	109.5
C(9)-C(7)-H(7B)	109.1	H(39A)-C(39)-H(39B)	109.5
C(8)-C(7)-H(7B)	109.1	O(4)-C(39)-H(39C)	109.5
H(7A)-C(7)-H(7B)	107.9	H(39A)-C(39)-H(39C)	109.5
N(1)-C(8)-C(7)	109.51(13)	H(39B)-C(39)-H(39C)	109.5

Table S3. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for form I.

	x	y	z	U(eq)
H(2A)	6680	1131	9007	21
H(3A)	5030	2867	8825	18
H(6A)	10184	3836	8162	21
H(7A)	12125	2519	8522	24
H(7B)	11093	1564	8316	24
H(8A)	12128	704	8810	26
H(8B)	11492	1708	9048	26
H(11A)	10472	-715	9071	44
H(11B)	8330	-605	9159	44
H(11C)	9814	76	9374	44
H(12A)	8425	1438	9533	27
H(12B)	9346	2494	9361	27
H(14A)	4722	1521	9560	23
H(15A)	2302	2629	9773	23
H(17A)	5670	5325	9732	26
H(18A)	8027	4239	9492	25
H(21A)	-1846	7333	9753	23
H(22A)	-1478	7306	9152	23
H(24A)	2488	4941	9244	21
H(25A)	-1370	6618	10633	44
H(25B)	-2643	6538	10300	44
H(25C)	-1188	7517	10336	44
H(26A)	-222	6432	8628	22
H(26B)	818	5285	8673	22
H(27A)	3702	6321	8748	20
H(28A)	1358	9153	8421	29
H(28B)	117	8068	8421	29

H(29A)	888	8275	7853	29
H(29B)	2960	8620	7940	29
H(35A)	2535	7002	7419	23
H(36A)	4478	9098	8650	42
H(36B)	5072	8116	8401	42
H(36C)	5282	7982	8807	42
H(37A)	3354	5267	6715	58
H(37B)	3733	6363	6930	58
H(37C)	1760	5784	6947	58
H(38A)	3815	2190	7587	39
H(38B)	2874	3193	7389	39
H(38C)	2141	2843	7759	39
H(39A)	8349	6028	7668	47
H(39B)	8072	4732	7621	47
H(39C)	9810	5190	7828	47

Table S4. Torsion angles [deg] for form I.

C(11)-N(1)-C(2)-C(10)	-177.94(14)
C(8)-N(1)-C(2)-C(10)	55.92(17)
C(11)-N(1)-C(2)-C(12)	58.18(19)
C(8)-N(1)-C(2)-C(12)	-67.96(17)
C(10)-C(3)-C(4)-O(3)	-179.47(13)
C(10)-C(3)-C(4)-C(5)	-3.5(2)
C(32)-O(3)-C(4)-C(3)	-159.15(14)
C(32)-O(3)-C(4)-C(5)	25.1(2)
C(39)-O(4)-C(5)-C(6)	35.9(2)
C(39)-O(4)-C(5)-C(4)	-146.73(16)
C(3)-C(4)-C(5)-O(4)	-170.55(14)
O(3)-C(4)-C(5)-O(4)	5.0(2)
C(3)-C(4)-C(5)-C(6)	6.9(2)
O(3)-C(4)-C(5)-C(6)	-177.51(14)
O(4)-C(5)-C(6)-C(9)	172.71(14)
C(4)-C(5)-C(6)-C(9)	-4.6(2)
C(11)-N(1)-C(8)-C(7)	166.02(14)
C(2)-N(1)-C(8)-C(7)	-67.17(17)
C(9)-C(7)-C(8)-N(1)	44.76(18)
C(5)-C(6)-C(9)-C(10)	-1.2(2)
C(5)-C(6)-C(9)-C(7)	177.98(15)
C(8)-C(7)-C(9)-C(10)	-16.8(2)
C(8)-C(7)-C(9)-C(6)	163.97(15)
C(6)-C(9)-C(10)-C(3)	4.7(2)
C(7)-C(9)-C(10)-C(3)	-174.53(14)
C(6)-C(9)-C(10)-C(2)	-173.19(14)

C(7)-C(9)-C(10)-C(2)	7.6(2)
C(4)-C(3)-C(10)-C(9)	-2.3(2)
C(4)-C(3)-C(10)-C(2)	175.55(14)
N(1)-C(2)-C(10)-C(9)	-25.9(2)
C(12)-C(2)-C(10)-C(9)	99.47(17)
N(1)-C(2)-C(10)-C(3)	156.26(14)
C(12)-C(2)-C(10)-C(3)	-78.37(18)
N(1)-C(2)-C(12)-C(13)	-172.38(14)
C(10)-C(2)-C(12)-C(13)	64.03(19)
C(2)-C(12)-C(13)-C(18)	-113.78(17)
C(2)-C(12)-C(13)-C(14)	67.8(2)
C(18)-C(13)-C(14)-C(15)	0.4(2)
C(12)-C(13)-C(14)-C(15)	178.85(15)
C(13)-C(14)-C(15)-C(16)	-1.8(2)
C(14)-C(15)-C(16)-C(17)	1.4(2)
C(14)-C(15)-C(16)-O(5)	-176.24(14)
C(19)-O(5)-C(16)-C(17)	77.20(19)
C(19)-O(5)-C(16)-C(15)	-105.11(17)
C(15)-C(16)-C(17)-C(18)	0.4(2)
O(5)-C(16)-C(17)-C(18)	178.05(14)
C(16)-C(17)-C(18)-C(13)	-1.9(2)
C(14)-C(13)-C(18)-C(17)	1.5(2)
C(12)-C(13)-C(18)-C(17)	-176.98(15)
C(16)-O(5)-C(19)-C(24)	6.8(2)
C(16)-O(5)-C(19)-C(20)	-174.67(14)
C(25)-O(6)-C(20)-C(21)	2.9(2)
C(25)-O(6)-C(20)-C(19)	-176.55(15)
O(5)-C(19)-C(20)-O(6)	1.1(2)
C(24)-C(19)-C(20)-O(6)	179.61(15)
O(5)-C(19)-C(20)-C(21)	-178.42(14)
C(24)-C(19)-C(20)-C(21)	0.1(2)
O(6)-C(20)-C(21)-C(22)	-179.10(16)
C(19)-C(20)-C(21)-C(22)	0.3(2)
C(20)-C(21)-C(22)-C(23)	-1.0(3)
C(21)-C(22)-C(23)-C(24)	1.1(2)
C(21)-C(22)-C(23)-C(26)	178.55(16)
O(5)-C(19)-C(24)-C(23)	178.45(15)
C(20)-C(19)-C(24)-C(23)	0.0(3)
C(22)-C(23)-C(24)-C(19)	-0.6(2)
C(26)-C(23)-C(24)-C(19)	-178.22(15)
C(22)-C(23)-C(26)-C(27)	107.65(18)
C(24)-C(23)-C(26)-C(27)	-74.91(19)
C(36)-N(2)-C(27)-C(31)	-75.07(18)
C(28)-N(2)-C(27)-C(31)	49.57(19)

C(36)-N(2)-C(27)-C(26)	161.48(14)
C(28)-N(2)-C(27)-C(26)	-73.88(17)
C(23)-C(26)-C(27)-N(2)	-68.71(18)
C(23)-C(26)-C(27)-C(31)	166.00(13)
C(36)-N(2)-C(28)-C(29)	63.68(19)
C(27)-N(2)-C(28)-C(29)	-60.32(19)
N(2)-C(28)-C(29)-C(30)	41.6(2)
C(28)-C(29)-C(30)-C(31)	-14.9(2)
C(28)-C(29)-C(30)-C(35)	168.46(16)
C(35)-C(30)-C(31)-C(32)	1.3(2)
C(29)-C(30)-C(31)-C(32)	-175.26(16)
C(35)-C(30)-C(31)-C(27)	-176.31(15)
C(29)-C(30)-C(31)-C(27)	7.1(2)
N(2)-C(27)-C(31)-C(30)	-24.3(2)
C(26)-C(27)-C(31)-C(30)	100.25(17)
N(2)-C(27)-C(31)-C(32)	158.18(15)
C(26)-C(27)-C(31)-C(32)	-77.30(18)
C(4)-O(3)-C(32)-C(33)	50.4(2)
C(4)-O(3)-C(32)-C(31)	-131.89(15)
C(30)-C(31)-C(32)-C(33)	-5.2(2)
C(27)-C(31)-C(32)-C(33)	172.47(15)
C(30)-C(31)-C(32)-O(3)	177.10(15)
C(27)-C(31)-C(32)-O(3)	-5.3(2)
C(38)-O(2)-C(33)-C(32)	118.22(17)
C(38)-O(2)-C(33)-C(34)	-67.1(2)
O(3)-C(32)-C(33)-O(2)	-1.5(2)
C(31)-C(32)-C(33)-O(2)	-179.17(15)
O(3)-C(32)-C(33)-C(34)	-176.39(15)
C(31)-C(32)-C(33)-C(34)	6.0(2)
C(37)-O(1)-C(34)-C(35)	-8.0(3)
C(37)-O(1)-C(34)-C(33)	173.34(16)
O(2)-C(33)-C(34)-O(1)	1.0(2)
C(32)-C(33)-C(34)-O(1)	175.78(15)
O(2)-C(33)-C(34)-C(35)	-177.68(15)
C(32)-C(33)-C(34)-C(35)	-2.9(2)
O(1)-C(34)-C(35)-C(30)	-179.36(16)
C(33)-C(34)-C(35)-C(30)	-0.8(3)
C(31)-C(30)-C(35)-C(34)	1.6(3)
C(29)-C(30)-C(35)-C(34)	178.23(16)

Crystalline data for acetonitrile solvate

Table S5. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for acetonitrile solvate. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
N(1)	-6019(1)	-6379(1)	-5332(1)	25(1)
N(2)	-4403(1)	-237(1)	-6668(1)	25(1)
N(3)	-1442(3)	-3530(2)	-8739(2)	114(1)
N(4)	-10547(3)	-1644(2)	-7675(1)	79(1)
O(1)	-7603(1)	-3311(1)	-7933(1)	31(1)
O(2)	-7077(1)	-3896(1)	-6994(1)	28(1)
O(3)	-5979(1)	-2726(1)	-6255(1)	24(1)
O(4)	-3492(1)	-3215(1)	-6647(1)	33(1)
O(5)	-5295(2)	-1458(1)	-4313(1)	37(1)
O(6)	-4888(1)	193(1)	-4078(1)	33(1)
C(2)	-6287(2)	-5430(1)	-5232(1)	22(1)
C(3)	-6081(2)	-4067(1)	-5784(1)	21(1)
C(4)	-5399(2)	-3546(1)	-6131(1)	21(1)
C(5)	-4110(2)	-3802(1)	-6321(1)	23(1)
C(6)	-3573(2)	-4610(1)	-6169(1)	24(1)
C(7)	-3748(2)	-6082(1)	-5722(1)	31(1)
C(8)	-4544(2)	-6582(1)	-5317(1)	29(1)
C(9)	-4286(2)	-5159(1)	-5830(1)	22(1)
C(10)	-5528(2)	-4877(1)	-5623(1)	20(1)
C(11)	-6776(2)	-6961(1)	-4989(1)	37(1)
C(12)	-5968(2)	-5154(1)	-4669(1)	31(1)
C(13)	-5810(2)	-4171(1)	-4583(1)	23(1)
C(14)	-6945(2)	-3632(1)	-4487(1)	29(1)
C(15)	-6790(2)	-2723(1)	-4408(1)	30(1)
C(16)	-5494(2)	-2358(1)	-4425(1)	26(1)
C(17)	-4346(2)	-2876(1)	-4525(1)	30(1)
C(18)	-4521(2)	-3779(1)	-4605(1)	29(1)
C(19)	-5420(2)	-861(1)	-4711(1)	23(1)
C(20)	-5179(2)	31(1)	-4581(1)	24(1)
C(21)	-5274(2)	665(1)	-4960(1)	29(1)
C(22)	-5628(2)	433(1)	-5458(1)	28(1)
C(23)	-5888(2)	-441(1)	-5587(1)	22(1)
C(24)	-5758(2)	-1088(1)	-5206(1)	22(1)
C(25)	-4532(2)	1085(1)	-3949(1)	38(1)
C(26)	-6342(2)	-714(1)	-6114(1)	23(1)
C(27)	-5155(2)	-1008(1)	-6470(1)	22(1)
C(28)	-5161(2)	193(1)	-7087(1)	29(1)
C(29)	-5396(2)	-413(1)	-7545(1)	32(1)
C(30)	-5905(2)	-1325(1)	-7390(1)	25(1)
C(31)	-5720(2)	-1611(1)	-6889(1)	21(1)
C(32)	-6118(2)	-2480(1)	-6765(1)	22(1)
C(33)	-6729(2)	-3038(1)	-7119(1)	22(1)
C(34)	-6953(2)	-2724(1)	-7616(1)	24(1)

C(35)	-6526(2)	-1878(1)	-7748(1)	26(1)
C(36)	-3013(2)	-493(1)	-6828(1)	35(1)
C(37)	-7854(3)	-3044(1)	-8444(1)	48(1)
C(38)	-8499(2)	-3996(2)	-6859(1)	49(1)
C(39)	-2171(2)	-3452(1)	-6846(1)	38(1)
C(40)	-2250(3)	-3061(2)	-8586(1)	70(1)
C(41)	-3286(3)	-2448(2)	-8403(1)	77(1)
C(42)	-10059(2)	-1388(2)	-7314(1)	58(1)
C(43)	-9459(3)	-1105(3)	-6851(1)	114(2)

Table S6. Bond lengths [Å] and angles [deg] for acetonitrile solvate.

N(1)-C(11)	1.454(2)	N(1)-C(8)-H(8B)	109.2
N(1)-C(8)	1.464(2)	C(7)-C(8)-H(8B)	109.2
N(1)-C(2)	1.4766(18)	H(8A)-C(8)-H(8B)	107.9
N(2)-C(36)	1.464(2)	C(10)-C(9)-C(6)	119.83(14)
N(2)-C(27)	1.466(2)	C(10)-C(9)-C(7)	120.52(14)
N(2)-C(28)	1.470(2)	C(6)-C(9)-C(7)	119.50(14)
N(3)-C(40)	1.130(4)	C(9)-C(10)-C(3)	118.87(14)
N(4)-C(42)	1.125(3)	C(9)-C(10)-C(2)	121.27(13)
O(1)-C(34)	1.3668(19)	C(3)-C(10)-C(2)	119.86(13)
O(1)-C(37)	1.417(2)	N(1)-C(11)-H(11A)	109.5
O(2)-C(33)	1.3762(19)	N(1)-C(11)-H(11B)	109.5
O(2)-C(38)	1.432(2)	H(11A)-C(11)-H(11B)	109.5
O(3)-C(32)	1.3925(17)	N(1)-C(11)-H(11C)	109.5
O(3)-C(4)	1.3949(18)	H(11A)-C(11)-H(11C)	109.5
O(4)-C(5)	1.3678(18)	H(11B)-C(11)-H(11C)	109.5
O(4)-C(39)	1.428(2)	C(13)-C(12)-C(2)	114.99(12)
O(5)-C(19)	1.3821(19)	C(13)-C(12)-H(12A)	108.5
O(5)-C(16)	1.3996(19)	C(2)-C(12)-H(12A)	108.5
O(6)-C(20)	1.3660(19)	C(13)-C(12)-H(12B)	108.5
O(6)-C(25)	1.427(2)	C(2)-C(12)-H(12B)	108.5
C(2)-C(10)	1.510(2)	H(12A)-C(12)-H(12B)	107.5
C(2)-C(12)	1.562(2)	C(18)-C(13)-C(14)	118.27(15)
C(2)-H(2)	0.9800	C(18)-C(13)-C(12)	120.33(16)
C(3)-C(4)	1.372(2)	C(14)-C(13)-C(12)	121.40(16)
C(3)-C(10)	1.398(2)	C(13)-C(14)-C(15)	121.06(16)
C(3)-H(3)	0.9300	C(13)-C(14)-H(14)	119.5
C(4)-C(5)	1.400(2)	C(15)-C(14)-H(14)	119.5
C(5)-C(6)	1.383(2)	C(16)-C(15)-C(14)	119.12(15)
C(6)-C(9)	1.396(2)	C(16)-C(15)-H(15)	120.4
C(6)-H(6)	0.9300	C(14)-C(15)-H(15)	120.4
C(7)-C(9)	1.512(2)	C(15)-C(16)-C(17)	121.14(14)
C(7)-C(8)	1.512(2)	C(15)-C(16)-O(5)	120.41(15)

C(7)-H(7A)	0.9700	C(17)-C(16)-O(5)	118.35(15)
C(7)-H(7B)	0.9700	C(16)-C(17)-C(18)	118.92(16)
C(8)-H(8A)	0.9700	C(16)-C(17)-H(17)	120.5
C(8)-H(8B)	0.9700	C(18)-C(17)-H(17)	120.5
C(9)-C(10)	1.388(2)	C(13)-C(18)-C(17)	121.48(16)
C(11)-H(11A)	0.9600	C(13)-C(18)-H(18)	119.3
C(11)-H(11B)	0.9600	C(17)-C(18)-H(18)	119.3
C(11)-H(11C)	0.9600	C(24)-C(19)-O(5)	124.49(14)
C(12)-C(13)	1.506(2)	C(24)-C(19)-C(20)	120.38(14)
C(12)-H(12A)	0.9700	O(5)-C(19)-C(20)	115.13(13)
C(12)-H(12B)	0.9700	O(6)-C(20)-C(21)	125.62(14)
C(13)-C(18)	1.385(2)	O(6)-C(20)-C(19)	116.05(14)
C(13)-C(14)	1.391(2)	C(21)-C(20)-C(19)	118.32(14)
C(14)-C(15)	1.393(2)	C(20)-C(21)-C(22)	121.12(15)
C(14)-H(14)	0.9300	C(20)-C(21)-H(21)	119.4
C(15)-C(16)	1.374(2)	C(22)-C(21)-H(21)	119.4
C(15)-H(15)	0.9300	C(23)-C(22)-C(21)	120.82(15)
C(16)-C(17)	1.385(2)	C(23)-C(22)-H(22)	119.6
C(17)-C(18)	1.386(2)	C(21)-C(22)-H(22)	119.6
C(17)-H(17)	0.9300	C(22)-C(23)-C(24)	118.17(14)
C(18)-H(18)	0.9300	C(22)-C(23)-C(26)	122.56(14)
C(19)-C(24)	1.377(2)	C(24)-C(23)-C(26)	119.24(13)
C(19)-C(20)	1.406(2)	C(19)-C(24)-C(23)	121.15(14)
C(20)-C(21)	1.380(2)	C(19)-C(24)-H(24)	119.4
C(21)-C(22)	1.392(2)	C(23)-C(24)-H(24)	119.4
C(21)-H(21)	0.9300	O(6)-C(25)-H(25A)	109.5
C(22)-C(23)	1.383(2)	O(6)-C(25)-H(25B)	109.5
C(22)-H(22)	0.9300	H(25A)-C(25)-H(25B)	109.5
C(23)-C(24)	1.401(2)	O(6)-C(25)-H(25C)	109.5
C(23)-C(26)	1.503(2)	H(25A)-C(25)-H(25C)	109.5
C(24)-H(24)	0.9300	H(25B)-C(25)-H(25C)	109.5
C(25)-H(25A)	0.9600	C(23)-C(26)-C(27)	114.39(13)
C(25)-H(25B)	0.9600	C(23)-C(26)-H(26A)	108.7
C(25)-H(25C)	0.9600	C(27)-C(26)-H(26A)	108.7
C(26)-C(27)	1.547(2)	C(23)-C(26)-H(26B)	108.7
C(26)-H(26A)	0.9700	C(27)-C(26)-H(26B)	108.7
C(26)-H(26B)	0.9700	H(26A)-C(26)-H(26B)	107.6
C(27)-C(31)	1.526(2)	N(2)-C(27)-C(31)	113.42(12)
C(27)-H(27)	0.9800	N(2)-C(27)-C(26)	110.92(13)
C(28)-C(29)	1.524(2)	C(31)-C(27)-C(26)	109.63(13)
C(28)-H(28A)	0.9700	N(2)-C(27)-H(27)	107.5
C(28)-H(28B)	0.9700	C(31)-C(27)-H(27)	107.5
C(29)-C(30)	1.516(2)	C(26)-C(27)-H(27)	107.5
C(29)-H(29A)	0.9700	N(2)-C(28)-C(29)	113.47(13)

C(29)-H(29B)	0.9700	N(2)-C(28)-H(28A)	108.9
C(30)-C(31)	1.390(2)	C(29)-C(28)-H(28A)	108.9
C(30)-C(35)	1.392(2)	N(2)-C(28)-H(28B)	108.9
C(31)-C(32)	1.402(2)	C(29)-C(28)-H(28B)	108.9
C(32)-C(33)	1.383(2)	H(28A)-C(28)-H(28B)	107.7
C(33)-C(34)	1.403(2)	C(30)-C(29)-C(28)	112.30(13)
C(34)-C(35)	1.383(2)	C(30)-C(29)-H(29A)	109.1
C(35)-H(35)	0.9300	C(28)-C(29)-H(29A)	109.1
C(36)-H(36A)	0.9600	C(30)-C(29)-H(29B)	109.1
C(36)-H(36B)	0.9600	C(28)-C(29)-H(29B)	109.1
C(36)-H(36C)	0.9600	H(29A)-C(29)-H(29B)	107.9
C(37)-H(37A)	0.9600	C(31)-C(30)-C(35)	120.32(14)
C(37)-H(37B)	0.9600	C(31)-C(30)-C(29)	119.50(14)
C(37)-H(37C)	0.9600	C(35)-C(30)-C(29)	120.17(14)
C(38)-H(38A)	0.9600	C(30)-C(31)-C(32)	118.16(14)
C(38)-H(38B)	0.9600	C(30)-C(31)-C(27)	122.53(13)
C(38)-H(38C)	0.9600	C(32)-C(31)-C(27)	119.26(13)
C(39)-H(39A)	0.9600	C(33)-C(32)-O(3)	121.33(13)
C(39)-H(39B)	0.9600	C(33)-C(32)-C(31)	122.07(13)
C(39)-H(39C)	0.9600	O(3)-C(32)-C(31)	116.36(13)
C(40)-C(41)	1.446(4)	O(2)-C(33)-C(32)	121.21(13)
C(41)-H(41A)	0.9600	O(2)-C(33)-C(34)	119.96(14)
C(41)-H(41B)	0.9600	C(32)-C(33)-C(34)	118.80(14)
C(41)-H(41C)	0.9600	O(1)-C(34)-C(35)	125.66(14)
C(42)-C(43)	1.411(4)	O(1)-C(34)-C(33)	114.62(14)
C(43)-H(43A)	0.9600	C(35)-C(34)-C(33)	119.72(14)
C(43)-H(43B)	0.9600	C(34)-C(35)-C(30)	120.86(14)
C(43)-H(43C)	0.9600	C(34)-C(35)-H(35)	119.6
C(11)-N(1)-C(8)	110.61(13)	C(30)-C(35)-H(35)	119.6
C(11)-N(1)-C(2)	112.72(13)	N(2)-C(36)-H(36A)	109.5
C(8)-N(1)-C(2)	111.72(12)	N(2)-C(36)-H(36B)	109.5
C(36)-N(2)-C(27)	110.53(13)	H(36A)-C(36)-H(36B)	109.5
C(36)-N(2)-C(28)	111.31(13)	N(2)-C(36)-H(36C)	109.5
C(27)-N(2)-C(28)	111.25(13)	H(36A)-C(36)-H(36C)	109.5
C(34)-O(1)-C(37)	117.90(13)	H(36B)-C(36)-H(36C)	109.5
C(33)-O(2)-C(38)	113.17(13)	O(1)-C(37)-H(37A)	109.5
C(32)-O(3)-C(4)	119.84(11)	O(1)-C(37)-H(37B)	109.5
C(5)-O(4)-C(39)	117.28(13)	H(37A)-C(37)-H(37B)	109.5
C(19)-O(5)-C(16)	117.51(12)	O(1)-C(37)-H(37C)	109.5
C(20)-O(6)-C(25)	116.49(13)	H(37A)-C(37)-H(37C)	109.5
N(1)-C(2)-C(10)	109.20(12)	H(37B)-C(37)-H(37C)	109.5
N(1)-C(2)-C(12)	112.89(12)	O(2)-C(38)-H(38A)	109.5
C(10)-C(2)-C(12)	113.30(13)	O(2)-C(38)-H(38B)	109.5
N(1)-C(2)-H(2)	107.0	H(38A)-C(38)-H(38B)	109.5

C(10)-C(2)-H(2)	107.0	O(2)-C(38)-H(38C)	109.5
C(12)-C(2)-H(2)	107.0	H(38A)-C(38)-H(38C)	109.5
C(4)-C(3)-C(10)	120.92(14)	H(38B)-C(38)-H(38C)	109.5
C(4)-C(3)-H(3)	119.5	O(4)-C(39)-H(39A)	109.5
C(10)-C(3)-H(3)	119.5	O(4)-C(39)-H(39B)	109.5
C(3)-C(4)-O(3)	117.75(14)	H(39A)-C(39)-H(39B)	109.5
C(3)-C(4)-C(5)	120.53(14)	O(4)-C(39)-H(39C)	109.5
O(3)-C(4)-C(5)	121.51(13)	H(39A)-C(39)-H(39C)	109.5
O(4)-C(5)-C(6)	125.72(14)	H(39B)-C(39)-H(39C)	109.5
O(4)-C(5)-C(4)	115.73(13)	N(3)-C(40)-C(41)	178.3(4)
C(6)-C(5)-C(4)	118.56(14)	C(40)-C(41)-H(41A)	109.5
C(5)-C(6)-C(9)	121.15(15)	C(40)-C(41)-H(41B)	109.5
C(5)-C(6)-H(6)	119.4	H(41A)-C(41)-H(41B)	109.5
C(9)-C(6)-H(6)	119.4	C(40)-C(41)-H(41C)	109.5
C(9)-C(7)-C(8)	114.41(14)	H(41A)-C(41)-H(41C)	109.5
C(9)-C(7)-H(7A)	108.7	H(41B)-C(41)-H(41C)	109.5
C(8)-C(7)-H(7A)	108.7	N(4)-C(42)-C(43)	177.4(4)
C(9)-C(7)-H(7B)	108.7	C(42)-C(43)-H(43A)	109.5
C(8)-C(7)-H(7B)	108.7	C(42)-C(43)-H(43B)	109.5
H(7A)-C(7)-H(7B)	107.6	H(43A)-C(43)-H(43B)	109.5
N(1)-C(8)-C(7)	112.13(13)	C(42)-C(43)-H(43C)	109.5
N(1)-C(8)-H(8A)	109.2	H(43A)-C(43)-H(43C)	109.5
C(7)-C(8)-H(8A)	109.2	H(43B)-C(43)-H(43C)	109.5

Table S7. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for acetonitrile solvate.

	x	y	z	U(eq)
H(2)	-7274	-5331	-5288	26
H(3)	-6923	-3879	-5653	25
H(6)	-2722	-4792	-6295	29
H(7A)	-2794	-6038	-5615	38
H(7B)	-3771	-6422	-6037	38
H(8A)	-4414	-7215	-5367	35
H(8B)	-4181	-6430	-4983	35
H(11A)	-6564	-7568	-5068	55
H(11B)	-7747	-6862	-5030	55
H(11C)	-6516	-6837	-4642	55
H(12A)	-6705	-5370	-4452	38
H(12B)	-5125	-5446	-4562	38
H(14)	-7820	-3882	-4475	35
H(15)	-7555	-2368	-4344	36
H(17)	-3473	-2623	-4537	36
H(18)	-3755	-4129	-4676	35
H(21)	-5098	1256	-4882	34

H(22)	-5691	872	-5707	34
H(24)	-5902	-1682	-5287	27
H(25A)	-4343	1122	-3590	57
H(25B)	-5285	1472	-4033	57
H(25C)	-3729	1260	-4138	57
H(26A)	-6821	-220	-6271	27
H(26B)	-6992	-1200	-6082	27
H(27)	-4508	-1359	-6265	27
H(28A)	-4653	712	-7198	35
H(28B)	-6047	392	-6959	35
H(29A)	-6065	-141	-7772	38
H(29B)	-4539	-475	-7733	38
H(35)	-6657	-1676	-8080	31
H(36A)	-2545	-773	-6548	52
H(36B)	-2512	26	-6932	52
H(36C)	-3072	-900	-7110	52
H(37A)	-8306	-3515	-8625	72
H(37B)	-6995	-2908	-8608	72
H(37C)	-8432	-2526	-8445	72
H(38A)	-8680	-4606	-6776	73
H(38B)	-9066	-3821	-7142	73
H(38C)	-8703	-3629	-6569	73
H(39A)	-1846	-2990	-7067	57
H(39B)	-2245	-3997	-7034	57
H(39C)	-1534	-3529	-6568	57
H(41A)	-3643	-2112	-8686	92
H(41B)	-2882	-2052	-8158	92
H(41C)	-4022	-2774	-8245	92
H(43A)	-9346	-472	-6857	136
H(43B)	-8576	-1383	-6809	136
H(43C)	-10047	-1267	-6571	136

Table S8. Torsion angles [deg] for acetonitrile solvate.

C(11)-N(1)-C(2)-C(10)	-176.76(14)
C(8)-N(1)-C(2)-C(10)	57.96(16)
C(11)-N(1)-C(2)-C(12)	56.25(19)
C(8)-N(1)-C(2)-C(12)	-69.03(17)
C(10)-C(3)-C(4)-O(3)	-176.91(13)
C(10)-C(3)-C(4)-C(5)	-2.0(2)
C(32)-O(3)-C(4)-C(3)	-131.65(15)
C(32)-O(3)-C(4)-C(5)	53.52(19)
C(39)-O(4)-C(5)-C(6)	-0.5(2)
C(39)-O(4)-C(5)-C(4)	179.59(14)

C(3)-C(4)-C(5)-O(4)	-177.06(14)
O(3)-C(4)-C(5)-O(4)	-2.4(2)
C(3)-C(4)-C(5)-C(6)	3.1(2)
O(3)-C(4)-C(5)-C(6)	177.73(13)
O(4)-C(5)-C(6)-C(9)	179.46(14)
C(4)-C(5)-C(6)-C(9)	-0.7(2)
C(11)-N(1)-C(8)-C(7)	171.93(14)
C(2)-N(1)-C(8)-C(7)	-61.63(18)
C(9)-C(7)-C(8)-N(1)	35.1(2)
C(5)-C(6)-C(9)-C(10)	-2.7(2)
C(5)-C(6)-C(9)-C(7)	172.74(15)
C(8)-C(7)-C(9)-C(10)	-9.2(2)
C(8)-C(7)-C(9)-C(6)	175.31(15)
C(6)-C(9)-C(10)-C(3)	3.8(2)
C(7)-C(9)-C(10)-C(3)	-171.68(14)
C(6)-C(9)-C(10)-C(2)	-176.47(14)
C(7)-C(9)-C(10)-C(2)	8.1(2)
C(4)-C(3)-C(10)-C(9)	-1.4(2)
C(4)-C(3)-C(10)-C(2)	178.82(14)
N(1)-C(2)-C(10)-C(9)	-31.51(19)
C(12)-C(2)-C(10)-C(9)	95.24(17)
N(1)-C(2)-C(10)-C(3)	148.26(14)
C(12)-C(2)-C(10)-C(3)	-84.99(18)
N(1)-C(2)-C(12)-C(13)	162.57(14)
C(10)-C(2)-C(12)-C(13)	37.8(2)
C(2)-C(12)-C(13)-C(18)	-92.9(2)
C(2)-C(12)-C(13)-C(14)	86.3(2)
C(18)-C(13)-C(14)-C(15)	-0.9(2)
C(12)-C(13)-C(14)-C(15)	179.94(15)
C(13)-C(14)-C(15)-C(16)	-0.1(3)
C(14)-C(15)-C(16)-C(17)	0.7(2)
C(14)-C(15)-C(16)-O(5)	-175.78(14)
C(19)-O(5)-C(16)-C(15)	-87.86(19)
C(19)-O(5)-C(16)-C(17)	95.58(18)
C(15)-C(16)-C(17)-C(18)	-0.4(2)
O(5)-C(16)-C(17)-C(18)	176.18(14)
C(14)-C(13)-C(18)-C(17)	1.2(2)
C(12)-C(13)-C(18)-C(17)	-179.58(15)
C(16)-C(17)-C(18)-C(13)	-0.6(2)
C(16)-O(5)-C(19)-C(24)	1.7(2)
C(16)-O(5)-C(19)-C(20)	-178.57(15)
C(25)-O(6)-C(20)-C(21)	-6.0(2)
C(25)-O(6)-C(20)-C(19)	175.08(16)
C(24)-C(19)-C(20)-O(6)	178.23(15)

O(5)-C(19)-C(20)-O(6)	-1.5(2)
C(24)-C(19)-C(20)-C(21)	-0.8(2)
O(5)-C(19)-C(20)-C(21)	179.46(15)
O(6)-C(20)-C(21)-C(22)	-177.50(17)
C(19)-C(20)-C(21)-C(22)	1.4(3)
C(20)-C(21)-C(22)-C(23)	-0.4(3)
C(21)-C(22)-C(23)-C(24)	-1.3(2)
C(21)-C(22)-C(23)-C(26)	176.91(16)
O(5)-C(19)-C(24)-C(23)	178.86(15)
C(20)-C(19)-C(24)-C(23)	-0.9(2)
C(22)-C(23)-C(24)-C(19)	1.9(2)
C(26)-C(23)-C(24)-C(19)	-176.36(15)
C(22)-C(23)-C(26)-C(27)	94.58(18)
C(24)-C(23)-C(26)-C(27)	-87.25(17)
C(36)-N(2)-C(27)-C(31)	-78.51(16)
C(28)-N(2)-C(27)-C(31)	45.69(17)
C(36)-N(2)-C(27)-C(26)	157.61(13)
C(28)-N(2)-C(27)-C(26)	-78.20(15)
C(23)-C(26)-C(27)-N(2)	-77.30(16)
C(23)-C(26)-C(27)-C(31)	156.67(13)
C(36)-N(2)-C(28)-C(29)	62.80(18)
C(27)-N(2)-C(28)-C(29)	-60.94(18)
N(2)-C(28)-C(29)-C(30)	46.2(2)
C(28)-C(29)-C(30)-C(31)	-19.0(2)
C(28)-C(29)-C(30)-C(35)	162.44(16)
C(35)-C(30)-C(31)-C(32)	2.8(2)
C(29)-C(30)-C(31)-C(32)	-175.78(14)
C(35)-C(30)-C(31)-C(27)	-174.83(15)
C(29)-C(30)-C(31)-C(27)	6.6(2)
N(2)-C(27)-C(31)-C(30)	-19.8(2)
C(26)-C(27)-C(31)-C(30)	104.76(17)
N(2)-C(27)-C(31)-C(32)	162.56(13)
C(26)-C(27)-C(31)-C(32)	-72.86(17)
C(4)-O(3)-C(32)-C(33)	50.7(2)
C(4)-O(3)-C(32)-C(31)	-134.78(14)
C(30)-C(31)-C(32)-C(33)	-2.5(2)
C(27)-C(31)-C(32)-C(33)	175.23(15)
C(30)-C(31)-C(32)-O(3)	-176.92(14)
C(27)-C(31)-C(32)-O(3)	0.8(2)
C(38)-O(2)-C(33)-C(32)	97.95(19)
C(38)-O(2)-C(33)-C(34)	-84.13(19)
O(3)-C(32)-C(33)-O(2)	-7.7(2)
C(31)-C(32)-C(33)-O(2)	178.14(14)
O(3)-C(32)-C(33)-C(34)	174.35(14)

C(31)-C(32)-C(33)-C(34)	0.2(2)
C(37)-O(1)-C(34)-C(35)	0.8(3)
C(37)-O(1)-C(34)-C(33)	-179.50(17)
O(2)-C(33)-C(34)-O(1)	4.1(2)
C(32)-C(33)-C(34)-O(1)	-177.94(14)
O(2)-C(33)-C(34)-C(35)	-176.17(14)
C(32)-C(33)-C(34)-C(35)	1.8(2)
O(1)-C(34)-C(35)-C(30)	178.24(16)
C(33)-C(34)-C(35)-C(30)	-1.5(2)
C(31)-C(30)-C(35)-C(34)	-0.9(2)
C(29)-C(30)-C(35)-C(34)	177.69(15)

Crystalline data for acetone solvate

Table S9. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for acetone solvate. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
N(1)	9671(1)	-3795(2)	-7973(1)	34(1)
N(2)	7721(1)	-1720(2)	-3309(1)	21(1)
N(3)	5810(1)	-9022(2)	3024(1)	25(1)
N(4)	7218(1)	-7006(2)	-1789(1)	27(1)
O(1)	5887(1)	-4649(2)	-5839(1)	25(1)
O(2)	7269(1)	-4656(2)	-6113(1)	22(1)
O(3)	8295(1)	-3492(2)	-5175(1)	20(1)
O(4)	7803(1)	-1020(2)	-5624(1)	25(1)
O(5)	10857(1)	-2371(2)	-4098(1)	32(1)
O(6)	11345(1)	-2647(2)	-2827(1)	29(1)
O(7)	9197(1)	-9750(2)	710(1)	31(1)
O(8)	7825(1)	-9959(2)	1000(1)	22(1)
O(9)	6746(1)	-8853(2)	104(1)	19(1)
O(10)	7132(1)	-6255(2)	415(1)	24(1)
O(11)	4139(1)	-7798(2)	-722(1)	28(1)
O(12)	3590(1)	-7820(2)	-1974(1)	26(1)
O(13)	8554(2)	-3322(4)	-653(2)	100(1)
O(14)	6350(1)	-7993(3)	-4587(2)	68(1)
C(2)	9705(1)	-4016(3)	-7217(1)	26(1)
C(3)	8929(1)	-3725(3)	-6202(1)	21(1)
C(4)	8474(1)	-2980(2)	-5820(1)	18(1)
C(5)	8228(1)	-1712(2)	-6054(1)	19(1)
C(6)	8428(1)	-1267(2)	-6693(1)	22(1)
C(7)	9060(2)	-1608(3)	-7808(1)	32(1)
C(8A)	9119(3)	-2873(5)	-8257(2)	30(1)
C(8B)	9671(4)	-2278(7)	-8075(3)	32(2)

C(9)	8878(1)	-2026(2)	-7094(1)	21(1)
C(10)	9147(1)	-3248(3)	-6838(1)	21(1)
C(11A)	9568(3)	-5102(5)	-8361(2)	38(2)
C(11B)	9153(4)	-4412(10)	-8294(4)	50(3)
C(12)	10476(1)	-3635(4)	-6955(2)	43(1)
C(13)	10584(1)	-3337(3)	-6193(1)	29(1)
C(14)	10666(1)	-4349(3)	-5702(2)	31(1)
C(15)	10742(1)	-4055(3)	-4998(1)	28(1)
C(16)	10733(1)	-2721(3)	-4795(1)	24(1)
C(17)	10651(1)	-1687(3)	-5273(1)	25(1)
C(18)	10575(1)	-2012(3)	-5969(1)	28(1)
C(19)	10370(1)	-2811(2)	-3638(1)	21(1)
C(20)	10634(1)	-2939(2)	-2947(1)	22(1)
C(21)	10166(1)	-3343(3)	-2460(1)	24(1)
C(22)	9449(1)	-3602(3)	-2653(1)	22(1)
C(23)	9186(1)	-3466(2)	-3333(1)	18(1)
C(24)	9658(1)	-3068(2)	-3826(1)	21(1)
C(25)	11664(1)	-2926(3)	-2152(1)	34(1)
C(26)	8418(1)	-3787(2)	-3566(1)	19(1)
C(27)	7984(1)	-2571(2)	-3870(1)	17(1)
C(28)	7073(1)	-2311(3)	-3036(1)	24(1)
C(29)	6449(1)	-2439(3)	-3568(1)	23(1)
C(30)	6673(1)	-3034(2)	-4242(1)	18(1)
C(31)	7393(1)	-3044(2)	-4385(1)	17(1)
C(32)	7575(1)	-3529(2)	-5034(1)	18(1)
C(33)	7074(1)	-4097(2)	-5497(1)	18(1)
C(34)	6346(1)	-4091(3)	-5345(1)	20(1)
C(35)	6154(1)	-3536(3)	-4726(1)	22(1)
C(36)	7587(1)	-345(2)	-3557(1)	26(1)
C(37)	5161(1)	-4797(4)	-5669(2)	40(1)
C(38)	7605(1)	-5955(3)	-6016(1)	29(1)
C(39)	7498(1)	220(3)	-5881(2)	31(1)
C(40)	5589(1)	-9329(3)	2296(1)	22(1)
C(41)	6209(1)	-9039(3)	1188(1)	20(1)
C(42)	6590(1)	-8280(2)	742(1)	18(1)
C(43)	6786(1)	-6949(2)	905(1)	18(1)
C(44)	6629(1)	-6440(2)	1549(1)	20(1)
C(45)	6175(2)	-6699(3)	2738(1)	32(1)
C(46)	5738(1)	-7600(3)	3183(1)	30(1)
C(47)	6267(1)	-7224(2)	2015(1)	19(1)
C(48)	6038(1)	-8513(2)	1828(1)	19(1)
C(49)	5458(1)	-9858(3)	3517(1)	31(1)
C(50)	4768(1)	-9134(3)	2114(1)	31(1)
C(51)	4578(1)	-8789(3)	1361(1)	23(1)

C(52)	4485(1)	-9803(3)	865(1)	25(1)
C(53)	4349(1)	-9490(3)	167(1)	25(1)
C(54)	4316(1)	-8154(3)	-32(1)	23(1)
C(55)	4402(1)	-7131(3)	448(1)	23(1)
C(56)	4532(1)	-7458(3)	1146(1)	24(1)
C(57)	4603(1)	-8145(2)	-1220(1)	21(1)
C(58)	4304(1)	-8116(2)	-1906(1)	22(1)
C(59)	4740(1)	-8386(3)	-2443(1)	24(1)
C(60)	5468(1)	-8690(3)	-2300(1)	24(1)
C(61)	5763(1)	-8715(2)	-1630(1)	21(1)
C(62)	5317(1)	-8440(2)	-1088(1)	21(1)
C(63)	3267(1)	-7766(3)	-2666(1)	31(1)
C(64)	6542(1)	-9035(3)	-1459(1)	21(1)
C(65)	6993(1)	-7806(2)	-1196(1)	20(1)
C(66)	7882(1)	-7533(3)	-2051(1)	30(1)
C(67)	8517(1)	-7497(3)	-1525(1)	26(1)
C(68)	8326(1)	-8129(2)	-851(1)	21(1)
C(69)	7614(1)	-8241(2)	-700(1)	19(1)
C(70)	7462(1)	-8800(2)	-58(1)	18(1)
C(71)	7990(1)	-9330(2)	391(1)	19(1)
C(72)	8709(1)	-9212(3)	229(1)	22(1)
C(73)	8870(1)	-8590(3)	-382(1)	22(1)
C(74)	7291(2)	-5583(3)	-1604(2)	36(1)
C(75)	9926(2)	-9703(6)	549(2)	72(1)
C(76)	7538(1)	-11295(3)	888(1)	30(1)
C(77)	7453(1)	-4996(3)	623(2)	31(1)
C(78)	8493(2)	-1564(4)	-1493(2)	66(1)
C(79)	8180(2)	-2500(4)	-1011(2)	59(1)
C(80)	7390(2)	-2411(4)	-936(2)	53(1)
C(81)	7482(1)	-7112(3)	-4229(1)	32(1)
C(82)	6703(2)	-7309(3)	-4168(2)	36(1)
C(83)	6383(2)	-6603(4)	-3574(2)	50(1)

Table S10. Bond lengths [Å] and angles [deg] for acetone solvate.

N(1)-C(11B)	1.277(8)	C(13)-C(12)-H(12A)	108.3
N(1)-C(8A)	1.463(5)	C(2)-C(12)-H(12A)	108.3
N(1)-C(2)	1.477(3)	C(13)-C(12)-H(12B)	108.3
N(1)-C(11A)	1.504(6)	C(2)-C(12)-H(12B)	108.3
N(1)-C(8B)	1.517(7)	H(12A)-C(12)-H(12B)	107.4
N(2)-C(36)	1.463(3)	C(18)-C(13)-C(14)	118.3(2)
N(2)-C(28)	1.474(3)	C(18)-C(13)-C(12)	119.3(3)
N(2)-C(27)	1.480(3)	C(14)-C(13)-C(12)	122.3(3)
N(3)-C(46)	1.451(3)	C(13)-C(14)-C(15)	121.4(3)

N(3)-C(49)	1.451(3)	C(13)-C(14)-H(14A)	119.3
N(3)-C(40)	1.476(3)	C(15)-C(14)-H(14A)	119.3
N(4)-C(74)	1.460(4)	C(16)-C(15)-C(14)	118.5(2)
N(4)-C(66)	1.466(3)	C(16)-C(15)-H(15A)	120.7
N(4)-C(65)	1.476(3)	C(14)-C(15)-H(15A)	120.7
O(1)-C(34)	1.367(3)	C(15)-C(16)-C(17)	121.5(2)
O(1)-C(37)	1.425(3)	C(15)-C(16)-O(5)	120.6(2)
O(2)-C(33)	1.381(3)	C(17)-C(16)-O(5)	117.8(2)
O(2)-C(38)	1.441(3)	C(18)-C(17)-C(16)	118.7(3)
O(3)-C(32)	1.393(2)	C(18)-C(17)-H(17A)	120.7
O(3)-C(4)	1.405(3)	C(16)-C(17)-H(17A)	120.7
O(4)-C(5)	1.368(3)	C(17)-C(18)-C(13)	121.6(3)
O(4)-C(39)	1.433(3)	C(17)-C(18)-H(18A)	119.2
O(5)-C(19)	1.382(3)	C(13)-C(18)-H(18A)	119.2
O(5)-C(16)	1.399(3)	O(5)-C(19)-C(24)	123.4(2)
O(6)-C(20)	1.371(3)	O(5)-C(19)-C(20)	115.5(2)
O(6)-C(25)	1.431(3)	C(24)-C(19)-C(20)	121.0(2)
O(7)-C(72)	1.373(3)	O(6)-C(20)-C(21)	126.4(2)
O(7)-C(75)	1.419(3)	O(6)-C(20)-C(19)	115.4(2)
O(8)-C(71)	1.384(3)	C(21)-C(20)-C(19)	118.2(2)
O(8)-C(76)	1.441(3)	C(20)-C(21)-C(22)	120.6(2)
O(9)-C(70)	1.397(2)	C(20)-C(21)-H(21A)	119.7
O(9)-C(42)	1.405(3)	C(22)-C(21)-H(21A)	119.7
O(10)-C(43)	1.366(3)	C(23)-C(22)-C(21)	121.3(2)
O(10)-C(77)	1.433(3)	C(23)-C(22)-H(22A)	119.3
O(11)-C(57)	1.378(3)	C(21)-C(22)-H(22A)	119.3
O(11)-C(54)	1.400(3)	C(22)-C(23)-C(24)	118.2(2)
O(12)-C(58)	1.369(3)	C(22)-C(23)-C(26)	122.8(2)
O(12)-C(63)	1.437(3)	C(24)-C(23)-C(26)	119.0(2)
O(13)-C(79)	1.255(5)	C(19)-C(24)-C(23)	120.7(2)
O(14)-C(82)	1.223(4)	C(19)-C(24)-H(24A)	119.7
C(2)-C(10)	1.516(3)	C(23)-C(24)-H(24A)	119.7
C(2)-C(12)	1.549(4)	O(6)-C(25)-H(25A)	109.5
C(2)-H(2A)	0.9800	O(6)-C(25)-H(25B)	109.5
C(3)-C(4)	1.375(3)	H(25A)-C(25)-H(25B)	109.5
C(3)-C(10)	1.399(3)	O(6)-C(25)-H(25C)	109.5
C(3)-H(3A)	0.9300	H(25A)-C(25)-H(25C)	109.5
C(4)-C(5)	1.404(3)	H(25B)-C(25)-H(25C)	109.5
C(5)-C(6)	1.386(3)	C(23)-C(26)-C(27)	114.68(19)
C(6)-C(9)	1.398(3)	C(23)-C(26)-H(26A)	108.6
C(6)-H(6A)	0.9300	C(27)-C(26)-H(26A)	108.6
C(7)-C(8B)	1.443(7)	C(23)-C(26)-H(26B)	108.6
C(7)-C(9)	1.502(3)	C(27)-C(26)-H(26B)	108.6
C(7)-C(8A)	1.533(5)	H(26A)-C(26)-H(26B)	107.6

C(7)-H(7A)	0.7624	N(2)-C(27)-C(31)	113.27(17)
C(8A)-H(8AA)	0.9700	N(2)-C(27)-C(26)	110.72(18)
C(8A)-H(8AB)	0.9700	C(31)-C(27)-C(26)	110.79(18)
C(8B)-H(8BA)	0.9700	N(2)-C(27)-H(27A)	107.2
C(8B)-H(8BB)	0.9700	C(31)-C(27)-H(27A)	107.2
C(9)-C(10)	1.392(3)	C(26)-C(27)-H(27A)	107.2
C(11A)-H(11A)	0.9600	N(2)-C(28)-C(29)	114.1(2)
C(11A)-H(11B)	0.9600	N(2)-C(28)-H(28A)	108.7
C(11A)-H(11C)	0.9600	C(29)-C(28)-H(28A)	108.7
C(11B)-H(11D)	0.9600	N(2)-C(28)-H(28B)	108.7
C(11B)-H(11E)	0.9600	C(29)-C(28)-H(28B)	108.7
C(11B)-H(11F)	0.9600	H(28A)-C(28)-H(28B)	107.6
C(12)-C(13)	1.505(4)	C(30)-C(29)-C(28)	112.06(18)
C(12)-H(12A)	0.9700	C(30)-C(29)-H(29A)	109.2
C(12)-H(12B)	0.9700	C(28)-C(29)-H(29A)	109.2
C(13)-C(18)	1.384(4)	C(30)-C(29)-H(29B)	109.2
C(13)-C(14)	1.385(4)	C(28)-C(29)-H(29B)	109.2
C(14)-C(15)	1.390(4)	H(29A)-C(29)-H(29B)	107.9
C(14)-H(14A)	0.9300	C(31)-C(30)-C(35)	120.4(2)
C(15)-C(16)	1.380(4)	C(31)-C(30)-C(29)	119.7(2)
C(15)-H(15A)	0.9300	C(35)-C(30)-C(29)	119.93(19)
C(16)-C(17)	1.383(4)	C(30)-C(31)-C(32)	118.0(2)
C(17)-C(18)	1.383(4)	C(30)-C(31)-C(27)	122.97(19)
C(17)-H(17A)	0.9300	C(32)-C(31)-C(27)	119.06(18)
C(18)-H(18A)	0.9300	C(33)-C(32)-O(3)	120.99(19)
C(19)-C(24)	1.387(3)	C(33)-C(32)-C(31)	121.87(19)
C(19)-C(20)	1.403(3)	O(3)-C(32)-C(31)	117.01(19)
C(20)-C(21)	1.382(3)	C(32)-C(33)-O(2)	121.32(19)
C(21)-C(22)	1.398(3)	C(32)-C(33)-C(34)	119.5(2)
C(21)-H(21A)	0.9300	O(2)-C(33)-C(34)	119.1(2)
C(22)-C(23)	1.384(3)	O(1)-C(34)-C(35)	125.51(19)
C(22)-H(22A)	0.9300	O(1)-C(34)-C(33)	115.5(2)
C(23)-C(24)	1.394(3)	C(35)-C(34)-C(33)	119.0(2)
C(23)-C(26)	1.517(3)	C(34)-C(35)-C(30)	120.98(19)
C(24)-H(24A)	0.9300	C(34)-C(35)-H(35A)	119.5
C(25)-H(25A)	0.9600	C(30)-C(35)-H(35A)	119.5
C(25)-H(25B)	0.9600	N(2)-C(36)-H(36A)	109.5
C(25)-H(25C)	0.9600	N(2)-C(36)-H(36B)	109.5
C(26)-C(27)	1.551(3)	H(36A)-C(36)-H(36B)	109.5
C(26)-H(26A)	0.9700	N(2)-C(36)-H(36C)	109.5
C(26)-H(26B)	0.9700	H(36A)-C(36)-H(36C)	109.5
C(27)-C(31)	1.522(3)	H(36B)-C(36)-H(36C)	109.5
C(27)-H(27A)	0.9800	O(1)-C(37)-H(37A)	109.5
C(28)-C(29)	1.519(3)	O(1)-C(37)-H(37B)	109.5

C(28)-H(28A)	0.9700	H(37A)-C(37)-H(37B)	109.5
C(28)-H(28B)	0.9700	O(1)-C(37)-H(37C)	109.5
C(29)-C(30)	1.511(3)	H(37A)-C(37)-H(37C)	109.5
C(29)-H(29A)	0.9700	H(37B)-C(37)-H(37C)	109.5
C(29)-H(29B)	0.9700	O(2)-C(38)-H(38A)	109.5
C(30)-C(31)	1.394(3)	O(2)-C(38)-H(38B)	109.5
C(30)-C(35)	1.402(3)	H(38A)-C(38)-H(38B)	109.5
C(31)-C(32)	1.404(3)	O(2)-C(38)-H(38C)	109.5
C(32)-C(33)	1.379(3)	H(38A)-C(38)-H(38C)	109.5
C(33)-C(34)	1.412(3)	H(38B)-C(38)-H(38C)	109.5
C(34)-C(35)	1.383(3)	O(4)-C(39)-H(39A)	109.5
C(35)-H(35A)	0.9300	O(4)-C(39)-H(39B)	109.5
C(36)-H(36A)	0.9600	H(39A)-C(39)-H(39B)	109.5
C(36)-H(36B)	0.9600	O(4)-C(39)-H(39C)	109.5
C(36)-H(36C)	0.9600	H(39A)-C(39)-H(39C)	109.5
C(37)-H(37A)	0.9600	H(39B)-C(39)-H(39C)	109.5
C(37)-H(37B)	0.9600	N(3)-C(40)-C(48)	109.00(19)
C(37)-H(37C)	0.9600	N(3)-C(40)-C(50)	113.98(18)
C(38)-H(38A)	0.9600	C(48)-C(40)-C(50)	111.9(2)
C(38)-H(38B)	0.9600	N(3)-C(40)-H(40A)	107.2
C(38)-H(38C)	0.9600	C(48)-C(40)-H(40A)	107.2
C(39)-H(39A)	0.9600	C(50)-C(40)-H(40A)	107.2
C(39)-H(39B)	0.9600	C(42)-C(41)-C(48)	120.4(2)
C(39)-H(39C)	0.9600	C(42)-C(41)-H(41A)	119.8
C(40)-C(48)	1.505(3)	C(48)-C(41)-H(41A)	119.8
C(40)-C(50)	1.571(3)	C(41)-C(42)-C(43)	120.9(2)
C(40)-H(40A)	0.9800	C(41)-C(42)-O(9)	118.1(2)
C(41)-C(42)	1.374(3)	C(43)-C(42)-O(9)	120.90(19)
C(41)-C(48)	1.398(3)	O(10)-C(43)-C(44)	124.9(2)
C(41)-H(41A)	0.9300	O(10)-C(43)-C(42)	116.6(2)
C(42)-C(43)	1.400(3)	C(44)-C(43)-C(42)	118.5(2)
C(43)-C(44)	1.391(3)	C(43)-C(44)-C(47)	120.8(2)
C(44)-C(47)	1.396(3)	C(43)-C(44)-H(44A)	119.6
C(44)-H(44A)	0.9300	C(47)-C(44)-H(44A)	119.6
C(45)-C(47)	1.511(3)	C(47)-C(45)-C(46)	114.7(2)
C(45)-C(46)	1.513(4)	C(47)-C(45)-H(45A)	108.6
C(45)-H(45A)	0.9700	C(46)-C(45)-H(45A)	108.6
C(45)-H(45B)	0.9700	C(47)-C(45)-H(45B)	108.6
C(46)-H(46A)	0.9700	C(46)-C(45)-H(45B)	108.6
C(46)-H(46B)	0.9700	H(45A)-C(45)-H(45B)	107.6
C(47)-C(48)	1.389(3)	N(3)-C(46)-C(45)	113.1(2)
C(49)-H(49A)	0.9600	N(3)-C(46)-H(46A)	109.0
C(49)-H(49B)	0.9600	C(45)-C(46)-H(46A)	109.0
C(49)-H(49C)	0.9600	N(3)-C(46)-H(46B)	109.0

C(50)-C(51)	1.518(3)	C(45)-C(46)-H(46B)	109.0
C(50)-H(50A)	0.9700	H(46A)-C(46)-H(46B)	107.8
C(50)-H(50B)	0.9700	C(48)-C(47)-C(44)	120.0(2)
C(51)-C(56)	1.384(4)	C(48)-C(47)-C(45)	120.5(2)
C(51)-C(52)	1.394(4)	C(44)-C(47)-C(45)	119.4(2)
C(52)-C(53)	1.394(4)	C(47)-C(48)-C(41)	119.3(2)
C(52)-H(52A)	0.9300	C(47)-C(48)-C(40)	120.9(2)
C(53)-C(54)	1.380(4)	C(41)-C(48)-C(40)	119.8(2)
C(53)-H(53A)	0.9300	N(3)-C(49)-H(49A)	109.5
C(54)-C(55)	1.379(3)	N(3)-C(49)-H(49B)	109.5
C(55)-C(56)	1.394(4)	H(49A)-C(49)-H(49B)	109.5
C(55)-H(55A)	0.9300	N(3)-C(49)-H(49C)	109.5
C(56)-H(56A)	0.9300	H(49A)-C(49)-H(49C)	109.5
C(57)-C(62)	1.379(3)	H(49B)-C(49)-H(49C)	109.5
C(57)-C(58)	1.411(3)	C(51)-C(50)-C(40)	114.53(19)
C(58)-C(59)	1.384(3)	C(51)-C(50)-H(50A)	108.6
C(59)-C(60)	1.409(3)	C(40)-C(50)-H(50A)	108.6
C(59)-H(59A)	0.9300	C(51)-C(50)-H(50B)	108.6
C(60)-C(61)	1.380(3)	C(40)-C(50)-H(50B)	108.6
C(60)-H(60A)	0.9300	H(50A)-C(50)-H(50B)	107.6
C(61)-C(62)	1.405(3)	C(56)-C(51)-C(52)	118.5(2)
C(61)-C(64)	1.512(3)	C(56)-C(51)-C(50)	120.7(2)
C(62)-H(62A)	0.9300	C(52)-C(51)-C(50)	120.7(2)
C(63)-H(63A)	0.9600	C(53)-C(52)-C(51)	121.0(2)
C(63)-H(63B)	0.9600	C(53)-C(52)-H(52A)	119.5
C(63)-H(63C)	0.9600	C(51)-C(52)-H(52A)	119.5
C(64)-C(65)	1.552(3)	C(54)-C(53)-C(52)	119.1(2)
C(64)-H(64A)	0.9700	C(54)-C(53)-H(53A)	120.4
C(64)-H(64B)	0.9700	C(52)-C(53)-H(53A)	120.5
C(65)-C(69)	1.527(3)	C(55)-C(54)-C(53)	121.1(2)
C(65)-H(65A)	0.9800	C(55)-C(54)-O(11)	118.0(2)
C(66)-C(67)	1.522(4)	C(53)-C(54)-O(11)	120.8(2)
C(66)-H(66A)	0.9700	C(54)-C(55)-C(56)	119.2(2)
C(66)-H(66B)	0.9700	C(54)-C(55)-H(55A)	120.4
C(67)-C(68)	1.508(3)	C(56)-C(55)-H(55A)	120.4
C(67)-H(67A)	0.9700	C(51)-C(56)-C(55)	121.1(2)
C(67)-H(67B)	0.9700	C(51)-C(56)-H(56A)	119.4
C(68)-C(69)	1.387(3)	C(55)-C(56)-H(56A)	119.4
C(68)-C(73)	1.401(3)	O(11)-C(57)-C(62)	124.6(2)
C(69)-C(70)	1.403(3)	O(11)-C(57)-C(58)	114.90(19)
C(70)-C(71)	1.381(3)	C(62)-C(57)-C(58)	120.4(2)
C(71)-C(72)	1.407(3)	O(12)-C(58)-C(59)	125.9(2)
C(72)-C(73)	1.383(3)	O(12)-C(58)-C(57)	115.3(2)
C(73)-H(73A)	0.9300	C(59)-C(58)-C(57)	118.8(2)

C(74)-H(74A)	0.9600	C(58)-C(59)-C(60)	120.1(2)
C(74)-H(74B)	0.9600	C(58)-C(59)-H(59A)	119.9
C(74)-H(74C)	0.9600	C(60)-C(59)-H(59A)	119.9
C(75)-H(75A)	0.9600	C(61)-C(60)-C(59)	121.3(2)
C(75)-H(75B)	0.9600	C(61)-C(60)-H(60A)	119.4
C(75)-H(75C)	0.9600	C(59)-C(60)-H(60A)	119.4
C(76)-H(76A)	0.9600	C(60)-C(61)-C(62)	118.2(2)
C(76)-H(76B)	0.9600	C(60)-C(61)-C(64)	122.6(2)
C(76)-H(76C)	0.9600	C(62)-C(61)-C(64)	119.2(2)
C(77)-H(77A)	0.9600	C(57)-C(62)-C(61)	121.1(2)
C(77)-H(77B)	0.9600	C(57)-C(62)-H(62A)	119.4
C(77)-H(77C)	0.9600	C(61)-C(62)-H(62A)	119.4
C(78)-C(79)	1.462(6)	O(12)-C(63)-H(63A)	109.5
C(78)-H(78A)	0.9600	O(12)-C(63)-H(63B)	109.5
C(78)-H(78B)	0.9600	H(63A)-C(63)-H(63B)	109.5
C(78)-H(78C)	0.9600	O(12)-C(63)-H(63C)	109.5
C(79)-C(80)	1.498(5)	H(63A)-C(63)-H(63C)	109.5
C(80)-H(80A)	0.9600	H(63B)-C(63)-H(63C)	109.5
C(80)-H(80B)	0.9600	C(61)-C(64)-C(65)	114.0(2)
C(80)-H(80C)	0.9600	C(61)-C(64)-H(64A)	108.7
C(81)-C(82)	1.484(4)	C(65)-C(64)-H(64A)	108.7
C(81)-H(81A)	0.9600	C(61)-C(64)-H(64B)	108.7
C(81)-H(81B)	0.9600	C(65)-C(64)-H(64B)	108.7
C(81)-H(81C)	0.9600	H(64A)-C(64)-H(64B)	107.6
C(82)-C(83)	1.499(4)	N(4)-C(65)-C(69)	113.49(18)
C(83)-H(83A)	0.9600	N(4)-C(65)-C(64)	109.95(19)
C(83)-H(83B)	0.9600	C(69)-C(65)-C(64)	111.40(19)
C(83)-H(83C)	0.9600	N(4)-C(65)-H(65A)	107.2
C(11B)-N(1)-C(8A)	67.4(5)	C(69)-C(65)-H(65A)	107.2
C(11B)-N(1)-C(2)	113.5(4)	C(64)-C(65)-H(65A)	107.2
C(8A)-N(1)-C(2)	117.0(2)	N(4)-C(66)-C(67)	114.0(2)
C(11B)-N(1)-C(11A)	43.4(5)	N(4)-C(66)-H(66A)	108.7
C(8A)-N(1)-C(11A)	106.4(3)	C(67)-C(66)-H(66A)	108.7
C(2)-N(1)-C(11A)	111.4(3)	N(4)-C(66)-H(66B)	108.7
C(11B)-N(1)-C(8B)	114.6(6)	C(67)-C(66)-H(66B)	108.7
C(8A)-N(1)-C(8B)	48.4(3)	H(66A)-C(66)-H(66B)	107.6
C(2)-N(1)-C(8B)	106.0(3)	C(68)-C(67)-C(66)	110.69(19)
C(11A)-N(1)-C(8B)	142.2(4)	C(68)-C(67)-H(67A)	109.5
C(36)-N(2)-C(28)	110.99(18)	C(66)-C(67)-H(67A)	109.5
C(36)-N(2)-C(27)	110.36(18)	C(68)-C(67)-H(67B)	109.5
C(28)-N(2)-C(27)	110.65(18)	C(66)-C(67)-H(67B)	109.5
C(46)-N(3)-C(49)	111.3(2)	H(67A)-C(67)-H(67B)	108.1
C(46)-N(3)-C(40)	112.3(2)	C(69)-C(68)-C(73)	120.7(2)
C(49)-N(3)-C(40)	113.4(2)	C(69)-C(68)-C(67)	119.6(2)

C(74)-N(4)-C(66)	111.1(2)	C(73)-C(68)-C(67)	119.6(2)
C(74)-N(4)-C(65)	110.8(2)	C(68)-C(69)-C(70)	117.7(2)
C(66)-N(4)-C(65)	111.3(2)	C(68)-C(69)-C(65)	123.6(2)
C(34)-O(1)-C(37)	116.84(19)	C(70)-C(69)-C(65)	118.77(19)
C(33)-O(2)-C(38)	112.48(18)	C(71)-C(70)-O(9)	120.45(19)
C(32)-O(3)-C(4)	117.84(16)	C(71)-C(70)-C(69)	122.09(19)
C(5)-O(4)-C(39)	117.0(2)	O(9)-C(70)-C(69)	117.41(19)
C(19)-O(5)-C(16)	117.57(18)	C(70)-C(71)-O(8)	121.31(19)
C(20)-O(6)-C(25)	117.66(19)	C(70)-C(71)-C(72)	119.4(2)
C(72)-O(7)-C(75)	116.8(2)	O(8)-C(71)-C(72)	119.3(2)
C(71)-O(8)-C(76)	112.68(18)	O(7)-C(72)-C(73)	125.6(2)
C(70)-O(9)-C(42)	115.70(16)	O(7)-C(72)-C(71)	115.3(2)
C(43)-O(10)-C(77)	116.90(19)	C(73)-C(72)-C(71)	119.1(2)
C(57)-O(11)-C(54)	118.63(18)	C(72)-C(73)-C(68)	120.8(2)
C(58)-O(12)-C(63)	117.04(18)	C(72)-C(73)-H(73A)	119.6
N(1)-C(2)-C(10)	114.4(2)	C(68)-C(73)-H(73A)	119.6
N(1)-C(2)-C(12)	105.9(2)	N(4)-C(74)-H(74A)	109.5
C(10)-C(2)-C(12)	112.1(2)	N(4)-C(74)-H(74B)	109.5
N(1)-C(2)-H(2A)	108.1	H(74A)-C(74)-H(74B)	109.5
C(10)-C(2)-H(2A)	108.1	N(4)-C(74)-H(74C)	109.5
C(12)-C(2)-H(2A)	108.1	H(74A)-C(74)-H(74C)	109.5
C(4)-C(3)-C(10)	120.9(2)	H(74B)-C(74)-H(74C)	109.5
C(4)-C(3)-H(3A)	119.6	O(7)-C(75)-H(75A)	109.5
C(10)-C(3)-H(3A)	119.6	O(7)-C(75)-H(75B)	109.5
C(3)-C(4)-O(3)	118.1(2)	H(75A)-C(75)-H(75B)	109.5
C(3)-C(4)-C(5)	120.6(2)	O(7)-C(75)-H(75C)	109.5
O(3)-C(4)-C(5)	121.20(19)	H(75A)-C(75)-H(75C)	109.5
O(4)-C(5)-C(6)	125.4(2)	H(75B)-C(75)-H(75C)	109.5
O(4)-C(5)-C(4)	116.4(2)	O(8)-C(76)-H(76A)	109.5
C(6)-C(5)-C(4)	118.1(2)	O(8)-C(76)-H(76B)	109.5
C(5)-C(6)-C(9)	121.7(2)	H(76A)-C(76)-H(76B)	109.5
C(5)-C(6)-H(6A)	119.1	O(8)-C(76)-H(76C)	109.5
C(9)-C(6)-H(6A)	119.1	H(76A)-C(76)-H(76C)	109.5
C(8B)-C(7)-C(9)	115.4(3)	H(76B)-C(76)-H(76C)	109.5
C(8B)-C(7)-C(8A)	48.4(4)	O(10)-C(77)-H(77A)	109.5
C(9)-C(7)-C(8A)	108.9(3)	O(10)-C(77)-H(77B)	109.5
C(8B)-C(7)-H(7A)	130.7	H(77A)-C(77)-H(77B)	109.5
C(9)-C(7)-H(7A)	106.0	O(10)-C(77)-H(77C)	109.5
C(8A)-C(7)-H(7A)	94.3	H(77A)-C(77)-H(77C)	109.5
N(1)-C(8A)-C(7)	111.8(3)	H(77B)-C(77)-H(77C)	109.5
N(1)-C(8A)-H(8AA)	109.3	C(79)-C(78)-H(78A)	109.5
C(7)-C(8A)-H(8AA)	109.3	C(79)-C(78)-H(78B)	109.5
N(1)-C(8A)-H(8AB)	109.3	H(78A)-C(78)-H(78B)	109.5
C(7)-C(8A)-H(8AB)	109.3	C(79)-C(78)-H(78C)	109.5

H(8AA)-C(8A)-H(8AB)	107.9	H(78A)-C(78)-H(78C)	109.5
C(7)-C(8B)-N(1)	113.8(4)	H(78B)-C(78)-H(78C)	109.5
C(7)-C(8B)-H(8BA)	108.8	O(13)-C(79)-C(78)	122.2(4)
N(1)-C(8B)-H(8BA)	108.8	O(13)-C(79)-C(80)	120.5(4)
C(7)-C(8B)-H(8BB)	108.8	C(78)-C(79)-C(80)	117.3(4)
N(1)-C(8B)-H(8BB)	108.8	C(79)-C(80)-H(80A)	109.5
H(8BA)-C(8B)-H(8BB)	107.7	C(79)-C(80)-H(80B)	109.5
C(10)-C(9)-C(6)	119.3(2)	H(80A)-C(80)-H(80B)	109.5
C(10)-C(9)-C(7)	118.1(2)	C(79)-C(80)-H(80C)	109.5
C(6)-C(9)-C(7)	122.5(2)	H(80A)-C(80)-H(80C)	109.5
C(9)-C(10)-C(3)	119.2(2)	H(80B)-C(80)-H(80C)	109.5
C(9)-C(10)-C(2)	120.7(2)	C(82)-C(81)-H(81A)	109.5
C(3)-C(10)-C(2)	120.0(2)	C(82)-C(81)-H(81B)	109.5
N(1)-C(11A)-H(11A)	109.5	H(81A)-C(81)-H(81B)	109.5
N(1)-C(11A)-H(11B)	109.5	C(82)-C(81)-H(81C)	109.5
H(11A)-C(11A)-H(11B)	109.5	H(81A)-C(81)-H(81C)	109.5
N(1)-C(11A)-H(11C)	109.5	H(81B)-C(81)-H(81C)	109.5
H(11A)-C(11A)-H(11C)	109.5	O(14)-C(82)-C(81)	121.1(3)
H(11B)-C(11A)-H(11C)	109.5	O(14)-C(82)-C(83)	122.9(3)
N(1)-C(11B)-H(11D)	109.5	C(81)-C(82)-C(83)	116.0(3)
N(1)-C(11B)-H(11E)	109.5	C(82)-C(83)-H(83A)	109.5
H(11D)-C(11B)-H(11E)	109.5	C(82)-C(83)-H(83B)	109.5
N(1)-C(11B)-H(11F)	109.5	H(83A)-C(83)-H(83B)	109.5
H(11D)-C(11B)-H(11F)	109.5	C(82)-C(83)-H(83C)	109.5
H(11E)-C(11B)-H(11F)	109.5	H(83A)-C(83)-H(83C)	109.5
C(13)-C(12)-C(2)	115.9(2)	H(83B)-C(83)-H(83C)	109.5

Table S11. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for acetone solvate.

	x	y	z	U(eq)
H(2A)	9638	-4981	-7132	31
H(3A)	9093	-4556	-6037	25
H(6A)	8259	-440	-6860	26
H(7A)	8711	-1374	-7991	38
H(8AA)	8663	-3336	-8288	36
H(8AB)	9232	-2609	-8722	36
H(8BA)	10102	-1908	-7849	38
H(8BB)	9682	-2086	-8566	38
H(11A)	9620	-5843	-8043	58
H(11B)	9919	-5175	-8702	58
H(11C)	9098	-5122	-8587	58
H(11D)	9189	-5361	-8199	75
H(11E)	9172	-4261	-8783	75
H(11F)	8709	-4076	-8140	75

H(12A)	10792	-4370	-7066	52
H(12B)	10622	-2849	-7210	52
H(14A)	10671	-5244	-5845	37
H(15A)	10797	-4742	-4672	34
H(17A)	10648	-792	-5130	30
H(18A)	10516	-1323	-6294	34
H(21A)	10331	-3443	-2000	28
H(22A)	9143	-3870	-2318	27
H(24A)	9493	-2975	-4287	25
H(25A)	12159	-2672	-2134	51
H(25B)	11625	-3872	-2056	51
H(25C)	11421	-2421	-1813	51
H(26A)	8178	-4138	-3173	23
H(26B)	8418	-4493	-3913	23
H(27A)	8313	-2017	-4126	20
H(28A)	6927	-1756	-2656	28
H(28B)	7189	-3200	-2851	28
H(29A)	6084	-3006	-3383	28
H(29B)	6242	-1554	-3657	28
H(35A)	5674	-3496	-4630	26
H(36A)	7415	193	-3190	39
H(36B)	7235	-362	-3938	39
H(36C)	8023	36	-3708	39
H(37A)	4890	-5196	-6052	61
H(37B)	4966	-3927	-5570	61
H(37C)	5139	-5367	-5269	61
H(38A)	7732	-6301	-6457	43
H(38B)	7280	-6566	-5813	43
H(38C)	8028	-5863	-5716	43
H(39A)	7216	615	-5535	46
H(39B)	7201	45	-6292	46
H(39C)	7874	831	-5988	46
H(40A)	5698	-10282	2218	26
H(41A)	6065	-9908	1064	23
H(44A)	6767	-5566	1671	24
H(45A)	5947	-5821	2703	38
H(45B)	6644	-6576	2968	38
H(46A)	5887	-7454	3666	36
H(46B)	5239	-7347	3119	36
H(49A)	5619	-9605	3979	46
H(49B)	5572	-10788	3441	46
H(49C)	4950	-9733	3459	46
H(50A)	4521	-9957	2228	37
H(50B)	4593	-8420	2402	37

H(52A)	4514	-10702	1001	30
H(53A)	4281	-10173	-160	30
H(55A)	4375	-6234	309	28
H(56A)	4588	-6771	1471	29
H(59A)	4553	-8367	-2899	29
H(60A)	5755	-8877	-2665	28
H(62A)	5506	-8458	-633	25
H(63A)	2769	-7549	-2648	46
H(63B)	3316	-8627	-2885	46
H(63C)	3500	-7086	-2925	46
H(64A)	6748	-9392	-1870	26
H(64B)	6574	-9734	-1108	26
H(65A)	6680	-7230	-934	24
H(66A)	7998	-7011	-2454	36
H(66B)	7803	-8458	-2200	36
H(67A)	8915	-7981	-1707	32
H(67B)	8664	-6569	-1444	32
H(73A)	9345	-8475	-484	27
H(74A)	7438	-5082	-1997	53
H(74B)	7643	-5486	-1227	53
H(74C)	6840	-5244	-1468	53
H(75A)	10215	-10106	919	107
H(75B)	10068	-8781	491	107
H(75C)	9987	-10190	127	107
H(76A)	7433	-11686	1325	45
H(76B)	7883	-11845	671	45
H(76C)	7109	-11244	595	45
H(77A)	7680	-4603	239	47
H(77B)	7803	-5148	997	47
H(77C)	7092	-4393	773	47
H(78A)	8999	-1720	-1496	100
H(78B)	8408	-653	-1350	100
H(78C)	8278	-1704	-1950	100
H(80A)	7249	-3079	-612	79
H(80B)	7144	-2566	-1378	79
H(80C)	7272	-1530	-771	79
H(81A)	7634	-7608	-4621	49
H(81B)	7736	-7432	-3816	49
H(81C)	7580	-6171	-4289	49
H(83A)	5881	-6795	-3580	75
H(83B)	6454	-5648	-3615	75
H(83C)	6611	-6916	-3146	75

Table S12. Torsion angles [deg] for acetone solvate.

C(11B)-N(1)-C(2)-C(10)	-75.0(6)
C(8A)-N(1)-C(2)-C(10)	0.6(4)
C(11A)-N(1)-C(2)-C(10)	-122.1(3)
C(8B)-N(1)-C(2)-C(10)	51.7(4)
C(11B)-N(1)-C(2)-C(12)	161.0(5)
C(8A)-N(1)-C(2)-C(12)	-123.4(3)
C(11A)-N(1)-C(2)-C(12)	114.0(3)
C(8B)-N(1)-C(2)-C(12)	-72.3(4)
C(10)-C(3)-C(4)-O(3)	-177.8(2)
C(10)-C(3)-C(4)-C(5)	-1.0(3)
C(32)-O(3)-C(4)-C(3)	-130.7(2)
C(32)-O(3)-C(4)-C(5)	52.5(3)
C(39)-O(4)-C(5)-C(6)	5.0(3)
C(39)-O(4)-C(5)-C(4)	-174.8(2)
C(3)-C(4)-C(5)-O(4)	-177.2(2)
O(3)-C(4)-C(5)-O(4)	-0.5(3)
C(3)-C(4)-C(5)-C(6)	3.0(3)
O(3)-C(4)-C(5)-C(6)	179.67(19)
O(4)-C(5)-C(6)-C(9)	178.5(2)
C(4)-C(5)-C(6)-C(9)	-1.7(3)
C(11B)-N(1)-C(8A)-C(7)	148.6(5)
C(2)-N(1)-C(8A)-C(7)	42.7(4)
C(11A)-N(1)-C(8A)-C(7)	167.9(3)
C(8B)-N(1)-C(8A)-C(7)	-45.1(4)
C(8B)-C(7)-C(8A)-N(1)	48.1(4)
C(9)-C(7)-C(8A)-N(1)	-59.6(4)
C(9)-C(7)-C(8B)-N(1)	46.5(6)
C(8A)-C(7)-C(8B)-N(1)	-46.8(4)
C(11B)-N(1)-C(8B)-C(7)	63.6(7)
C(8A)-N(1)-C(8B)-C(7)	49.7(4)
C(2)-N(1)-C(8B)-C(7)	-62.4(5)
C(11A)-N(1)-C(8B)-C(7)	108.0(6)
C(5)-C(6)-C(9)-C(10)	-1.6(3)
C(5)-C(6)-C(9)-C(7)	175.6(2)
C(8B)-C(7)-C(9)-C(10)	-19.0(5)
C(8A)-C(7)-C(9)-C(10)	33.1(4)
C(8B)-C(7)-C(9)-C(6)	163.8(4)
C(8A)-C(7)-C(9)-C(6)	-144.1(3)
C(6)-C(9)-C(10)-C(3)	3.5(3)
C(7)-C(9)-C(10)-C(3)	-173.7(2)
C(6)-C(9)-C(10)-C(2)	-172.6(2)
C(7)-C(9)-C(10)-C(2)	10.1(3)
C(4)-C(3)-C(10)-C(9)	-2.3(3)
C(4)-C(3)-C(10)-C(2)	173.8(2)

N(1)-C(2)-C(10)-C(9)	-28.9(3)
C(12)-C(2)-C(10)-C(9)	91.7(3)
N(1)-C(2)-C(10)-C(3)	155.0(2)
C(12)-C(2)-C(10)-C(3)	-84.4(3)
N(1)-C(2)-C(12)-C(13)	160.8(3)
C(10)-C(2)-C(12)-C(13)	35.4(4)
C(2)-C(12)-C(13)-C(18)	-96.7(3)
C(2)-C(12)-C(13)-C(14)	80.9(3)
C(18)-C(13)-C(14)-C(15)	-0.3(3)
C(12)-C(13)-C(14)-C(15)	-177.9(2)
C(13)-C(14)-C(15)-C(16)	0.0(4)
C(14)-C(15)-C(16)-C(17)	0.1(3)
C(14)-C(15)-C(16)-O(5)	-175.51(19)
C(19)-O(5)-C(16)-C(15)	-63.9(3)
C(19)-O(5)-C(16)-C(17)	120.4(2)
C(15)-C(16)-C(17)-C(18)	0.1(3)
O(5)-C(16)-C(17)-C(18)	175.83(19)
C(16)-C(17)-C(18)-C(13)	-0.4(3)
C(14)-C(13)-C(18)-C(17)	0.5(3)
C(12)-C(13)-C(18)-C(17)	178.2(2)
C(16)-O(5)-C(19)-C(24)	-27.2(4)
C(16)-O(5)-C(19)-C(20)	155.1(2)
C(25)-O(6)-C(20)-C(21)	7.7(4)
C(25)-O(6)-C(20)-C(19)	-172.2(2)
O(5)-C(19)-C(20)-O(6)	-1.8(3)
C(24)-C(19)-C(20)-O(6)	-179.5(2)
O(5)-C(19)-C(20)-C(21)	178.4(2)
C(24)-C(19)-C(20)-C(21)	0.6(4)
O(6)-C(20)-C(21)-C(22)	179.6(2)
C(19)-C(20)-C(21)-C(22)	-0.6(4)
C(20)-C(21)-C(22)-C(23)	0.1(4)
C(21)-C(22)-C(23)-C(24)	0.3(4)
C(21)-C(22)-C(23)-C(26)	177.7(2)
O(5)-C(19)-C(24)-C(23)	-177.8(2)
C(20)-C(19)-C(24)-C(23)	-0.2(4)
C(22)-C(23)-C(24)-C(19)	-0.3(4)
C(26)-C(23)-C(24)-C(19)	-177.8(2)
C(22)-C(23)-C(26)-C(27)	118.1(2)
C(24)-C(23)-C(26)-C(27)	-64.5(3)
C(36)-N(2)-C(27)-C(31)	-78.6(2)
C(28)-N(2)-C(27)-C(31)	44.7(3)
C(36)-N(2)-C(27)-C(26)	156.25(18)
C(28)-N(2)-C(27)-C(26)	-80.5(2)
C(23)-C(26)-C(27)-N(2)	-80.9(2)

C(23)-C(26)-C(27)-C(31)	152.51(19)
C(36)-N(2)-C(28)-C(29)	61.8(3)
C(27)-N(2)-C(28)-C(29)	-61.1(3)
N(2)-C(28)-C(29)-C(30)	46.5(3)
C(28)-C(29)-C(30)-C(31)	-17.8(3)
C(28)-C(29)-C(30)-C(35)	164.2(2)
C(35)-C(30)-C(31)-C(32)	2.0(3)
C(29)-C(30)-C(31)-C(32)	-176.1(2)
C(35)-C(30)-C(31)-C(27)	-177.3(2)
C(29)-C(30)-C(31)-C(27)	4.6(3)
N(2)-C(27)-C(31)-C(30)	-18.1(3)
C(26)-C(27)-C(31)-C(30)	107.0(2)
N(2)-C(27)-C(31)-C(32)	162.6(2)
C(26)-C(27)-C(31)-C(32)	-72.3(3)
C(4)-O(3)-C(32)-C(33)	50.7(3)
C(4)-O(3)-C(32)-C(31)	-133.3(2)
C(30)-C(31)-C(32)-C(33)	-6.0(3)
C(27)-C(31)-C(32)-C(33)	173.4(2)
C(30)-C(31)-C(32)-O(3)	178.1(2)
C(27)-C(31)-C(32)-O(3)	-2.5(3)
O(3)-C(32)-C(33)-O(2)	0.4(3)
C(31)-C(32)-C(33)-O(2)	-175.4(2)
O(3)-C(32)-C(33)-C(34)	-178.6(2)
C(31)-C(32)-C(33)-C(34)	5.7(3)
C(38)-O(2)-C(33)-C(32)	75.8(3)
C(38)-O(2)-C(33)-C(34)	-105.2(2)
C(37)-O(1)-C(34)-C(35)	-7.0(4)
C(37)-O(1)-C(34)-C(33)	173.1(2)
C(32)-C(33)-C(34)-O(1)	178.6(2)
O(2)-C(33)-C(34)-O(1)	-0.4(3)
C(32)-C(33)-C(34)-C(35)	-1.4(3)
O(2)-C(33)-C(34)-C(35)	179.7(2)
O(1)-C(34)-C(35)-C(30)	177.5(2)
C(33)-C(34)-C(35)-C(30)	-2.5(4)
C(31)-C(30)-C(35)-C(34)	2.1(4)
C(29)-C(30)-C(35)-C(34)	-179.8(2)
C(46)-N(3)-C(40)-C(48)	58.6(2)
C(49)-N(3)-C(40)-C(48)	-174.2(2)
C(46)-N(3)-C(40)-C(50)	-67.2(3)
C(49)-N(3)-C(40)-C(50)	60.0(3)
C(48)-C(41)-C(42)-C(43)	-2.8(3)
C(48)-C(41)-C(42)-O(9)	-179.75(19)
C(70)-O(9)-C(42)-C(41)	-128.7(2)
C(70)-O(9)-C(42)-C(43)	54.3(3)

C(77)-O(10)-C(43)-C(44)	10.3(3)
C(77)-O(10)-C(43)-C(42)	-168.5(2)
C(41)-C(42)-C(43)-O(10)	-176.8(2)
O(9)-C(42)-C(43)-O(10)	0.0(3)
C(41)-C(42)-C(43)-C(44)	4.3(3)
O(9)-C(42)-C(43)-C(44)	-178.85(19)
O(10)-C(43)-C(44)-C(47)	179.5(2)
C(42)-C(43)-C(44)-C(47)	-1.8(3)
C(49)-N(3)-C(46)-C(45)	172.7(2)
C(40)-N(3)-C(46)-C(45)	-59.0(3)
C(47)-C(45)-C(46)-N(3)	31.5(3)
C(43)-C(44)-C(47)-C(48)	-2.2(3)
C(43)-C(44)-C(47)-C(45)	173.5(2)
C(46)-C(45)-C(47)-C(48)	-7.6(4)
C(46)-C(45)-C(47)-C(44)	176.7(2)
C(44)-C(47)-C(48)-C(41)	3.7(3)
C(45)-C(47)-C(48)-C(41)	-172.0(2)
C(44)-C(47)-C(48)-C(40)	-174.4(2)
C(45)-C(47)-C(48)-C(40)	9.9(3)
C(42)-C(41)-C(48)-C(47)	-1.2(3)
C(42)-C(41)-C(48)-C(40)	176.9(2)
N(3)-C(40)-C(48)-C(47)	-34.3(3)
C(50)-C(40)-C(48)-C(47)	92.8(3)
N(3)-C(40)-C(48)-C(41)	147.7(2)
C(50)-C(40)-C(48)-C(41)	-85.3(3)
N(3)-C(40)-C(50)-C(51)	152.4(2)
C(48)-C(40)-C(50)-C(51)	28.2(3)
C(40)-C(50)-C(51)-C(56)	-91.2(3)
C(40)-C(50)-C(51)-C(52)	85.3(3)
C(56)-C(51)-C(52)-C(53)	0.1(3)
C(50)-C(51)-C(52)-C(53)	-176.5(2)
C(51)-C(52)-C(53)-C(54)	0.9(3)
C(52)-C(53)-C(54)-C(55)	-1.2(3)
C(52)-C(53)-C(54)-O(11)	-176.23(19)
C(57)-O(11)-C(54)-C(55)	119.0(2)
C(57)-O(11)-C(54)-C(53)	-65.8(3)
C(53)-C(54)-C(55)-C(56)	0.7(3)
O(11)-C(54)-C(55)-C(56)	175.80(19)
C(52)-C(51)-C(56)-C(55)	-0.7(3)
C(50)-C(51)-C(56)-C(55)	175.9(2)
C(54)-C(55)-C(56)-C(51)	0.3(3)
C(54)-O(11)-C(57)-C(62)	-20.8(4)
C(54)-O(11)-C(57)-C(58)	162.3(2)
C(63)-O(12)-C(58)-C(59)	-0.9(4)

C(63)-O(12)-C(58)-C(57)	179.4(2)
O(11)-C(57)-C(58)-O(12)	-3.4(3)
C(62)-C(57)-C(58)-O(12)	179.6(2)
O(11)-C(57)-C(58)-C(59)	176.9(2)
C(62)-C(57)-C(58)-C(59)	-0.1(4)
O(12)-C(58)-C(59)-C(60)	-179.4(2)
C(57)-C(58)-C(59)-C(60)	0.3(4)
C(58)-C(59)-C(60)-C(61)	-0.5(4)
C(59)-C(60)-C(61)-C(62)	0.6(4)
C(59)-C(60)-C(61)-C(64)	-179.9(2)
O(11)-C(57)-C(62)-C(61)	-176.5(2)
C(58)-C(57)-C(62)-C(61)	0.1(4)
C(60)-C(61)-C(62)-C(57)	-0.4(4)
C(64)-C(61)-C(62)-C(57)	-179.9(2)
C(60)-C(61)-C(64)-C(65)	109.4(3)
C(62)-C(61)-C(64)-C(65)	-71.1(3)
C(74)-N(4)-C(65)-C(69)	-84.7(3)
C(66)-N(4)-C(65)-C(69)	39.5(3)
C(74)-N(4)-C(65)-C(64)	149.8(2)
C(66)-N(4)-C(65)-C(64)	-86.0(2)
C(61)-C(64)-C(65)-N(4)	-82.9(2)
C(61)-C(64)-C(65)-C(69)	150.4(2)
C(74)-N(4)-C(66)-C(67)	62.6(3)
C(65)-N(4)-C(66)-C(67)	-61.4(3)
N(4)-C(66)-C(67)-C(68)	50.6(3)
C(66)-C(67)-C(68)-C(69)	-20.7(3)
C(66)-C(67)-C(68)-C(73)	159.7(2)
C(73)-C(68)-C(69)-C(70)	1.5(3)
C(67)-C(68)-C(69)-C(70)	-178.2(2)
C(73)-C(68)-C(69)-C(65)	-177.8(2)
C(67)-C(68)-C(69)-C(65)	2.5(4)
N(4)-C(65)-C(69)-C(68)	-11.6(3)
C(64)-C(65)-C(69)-C(68)	113.1(2)
N(4)-C(65)-C(69)-C(70)	169.1(2)
C(64)-C(65)-C(69)-C(70)	-66.2(3)
C(42)-O(9)-C(70)-C(71)	55.5(3)
C(42)-O(9)-C(70)-C(69)	-127.0(2)
C(68)-C(69)-C(70)-C(71)	-5.4(3)
C(65)-C(69)-C(70)-C(71)	173.9(2)
C(68)-C(69)-C(70)-O(9)	177.1(2)
C(65)-C(69)-C(70)-O(9)	-3.5(3)
O(9)-C(70)-C(71)-O(8)	1.8(3)
C(69)-C(70)-C(71)-O(8)	-175.5(2)
O(9)-C(70)-C(71)-C(72)	-177.3(2)

C(69)-C(70)-C(71)-C(72)	5.3(4)
C(76)-O(8)-C(71)-C(70)	75.9(3)
C(76)-O(8)-C(71)-C(72)	-105.0(2)
C(75)-O(7)-C(72)-C(73)	-2.5(4)
C(75)-O(7)-C(72)-C(71)	177.3(3)
C(70)-C(71)-C(72)-O(7)	179.1(2)
O(8)-C(71)-C(72)-O(7)	-0.1(3)
C(70)-C(71)-C(72)-C(73)	-1.2(4)
O(8)-C(71)-C(72)-C(73)	179.6(2)
O(7)-C(72)-C(73)-C(68)	177.1(2)
C(71)-C(72)-C(73)-C(68)	-2.6(4)
C(69)-C(68)-C(73)-C(72)	2.4(4)
C(67)-C(68)-C(73)-C(72)	-177.9(2)
