

***Supporting Information For***  
**Solubility, crystallization process optimization,  
thermal property of Afoxolaner and the single crystal  
structure for its hydrate**

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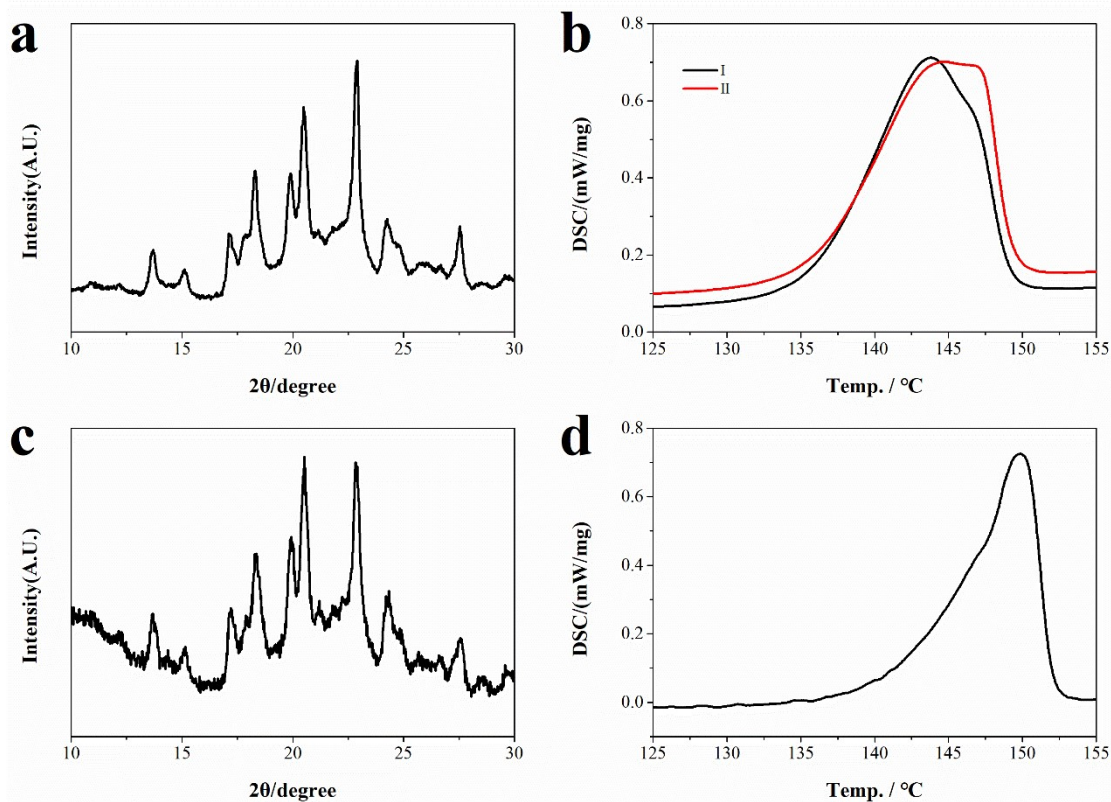


Fig. S1 (a, c) The XRD of starting material (a) and products after crystallization (c). (b, d) The DSC curves of starting material (b) and products after crystallization (d).

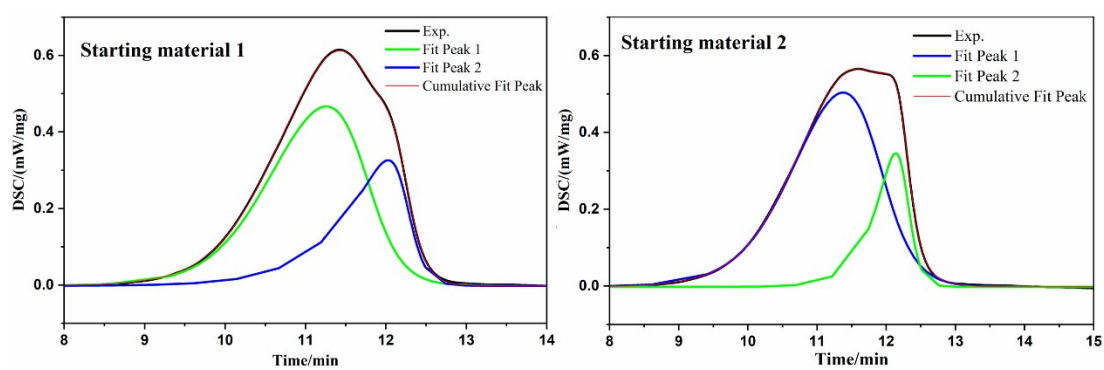


Fig. S2 The DSC curves of starting material was fitted by Asym2sig function. Black lines represent the raw data, colorful lines represent the peak fitting by the Asym2sig function.

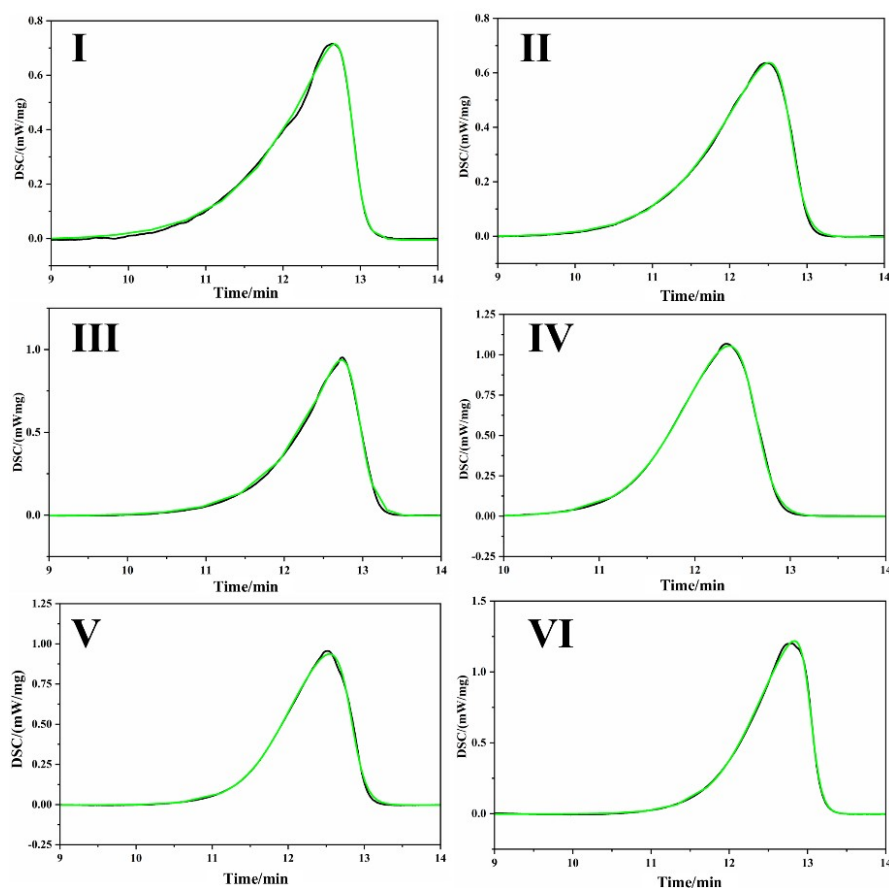


Fig. S3 The DSC curves of the crystal products obtained in the six parallel experiments. Black lines represent the raw data, green lines represent the peak fitting by the Asym2sig function.

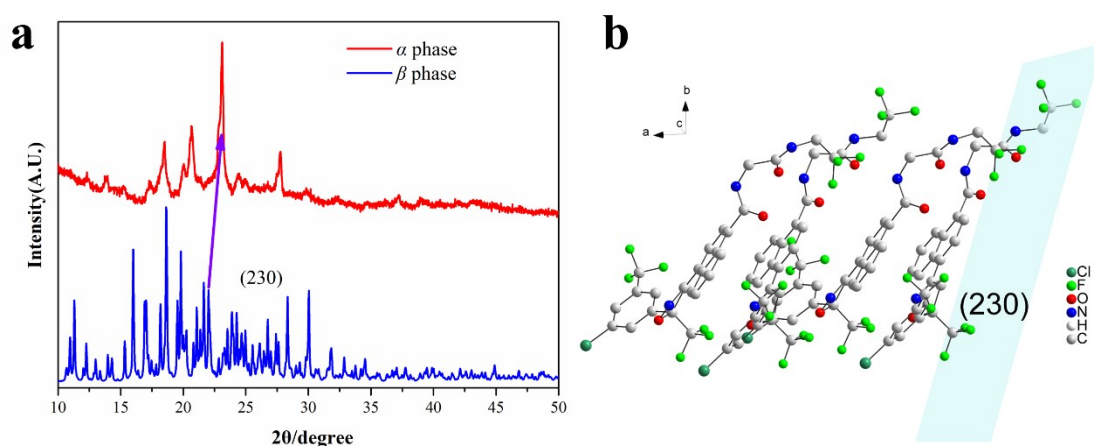


Fig. S4 (a) PXRD patterns of spherical solid ( $\alpha$  phase) and crystal ( $\beta$  phase). (b) The molecular arrangement of (2 3 0) in the  $\beta$  phase. Color scheme is listed in the corner of figure.

Table S1. The solubility (S) of Afoxolaner starting material at 22 °C

<b>Solvent</b>	<b>m<sub>1</sub> / g</b>	<b>m<sub>2</sub> / g</b>	<b><math>\bar{S}</math> / mg·g<sup>-1</sup></b>
<b>Ethanol</b>	4.0781	4.4143	<b>82.8(4)</b>
	4.0785	4.4150	
	4.0748	4.4145	
<b>Methanol</b>	4.0844	4.7282	<b>157.5(4)</b>
	4.0855	4.7309	
	4.0863	4.7274	
<b>Dichloro-methane</b>	6.8361	6.9671	<b>19.2(1)</b>
	6.8337	6.9661	
	6.8359	6.9660	
<b>Acetone</b>	4.0748	5.0864	<b>248(1)</b>
	4.0744	5.0891	
	4.0781	5.0822	
<b>Water</b>	5.1731	5.1624	<b>0</b>
	5.1738	5.1631	
	5.1749	5.1703	

Table S2. Summary of the endothermic peak data of the starting materials (Raw 1 and Raw 2) and six parallel crystallization solids in the ethanol solution experiments (I ~ VI).

	<b>Raw 1</b>	<b>Raw 2</b>	<b>I</b>	<b>II</b>	<b>III</b>	<b>IV</b>	<b>V</b>	<b>VI</b>
<b>Initial Tem. / °C</b>	128.5	128.6	134.1	131.8	135.1	137.3	136.8	139.3
<b>Peak Tem. / °C</b>	143.8	144.7	149.9	149.1	150.4	148.3	149.3	150.7
<b>Final Temp. / °C</b>	155.4	156.2	153.7	154.0	153.8	152.3	153.3	153.8
<b>Integral area / mW·mg<sup>-1</sup></b>	1.063	1.057	0.8362	0.8275	0.9337	1.046	0.9936	1.107
<b>Total enthalpy / J·g<sup>-1</sup></b>	63.78	63.42	50.17	49.65	56.02	62.76	59.62	66.42
<b>Temp. of Fit Peak 1 / °C</b>	143.0	143.6	150.0	149.2	150.3	148.5	149.4	150.8
<b>Temp. of Fit Peak 2 / °C</b>	146.8	147.4	/	/	/	/	/	/
<b>Area of Fit peak 1 / mW·mg<sup>-1</sup></b>	0.7237	0.8391	0.8698	0.8153	0.9539	1.081	1.000	1.120
<b>Enthalpy of Fit peak 1 / J·g<sup>-1</sup></b>	43.42	50.35	52.19	48.92	57.23	64.86	60.00	67.20
<b>Area of Fit peak 2 / mW·mg<sup>-1</sup></b>	0.3503	0.2293	/	/	/	/	/	/
<b>Enthalpy of Fit peak 2 / J·g<sup>-1</sup></b>	21.02	13.76	/	/	/	/	/	/
<b>R<sup>2</sup></b>	0.9999	0.9999	0.9982	0.9995	0.9996	0.9997	0.9992	0.9994

Table S3. Comparison of the 2 $\theta$ /° in the XRD diffraction peaks of  $\alpha$  phase and Form B in literature (Patent: WO2011149749A1).

<b><math>\alpha</math> phase</b>	<b>Form B</b>
13.88	
15.37	
17.40	17.43
18.11	
18.53	18.59
20.13	20.21
20.74	20.79
21.40	21.41
	22.11
23.05	23.18
24.39	
24.55	24.57
26.78	
27.79	27.84
29.80	

Table S4. The Miller index of peaks in PXRD of the  $\beta$  phase.

<b>2<math>\theta</math>(deg)</b>	<b>(<i>h, k, l</i>)</b>	<b>2<math>\theta</math>(deg)</b>	<b>(<i>h, k, l</i>)</b>	<b>2<math>\theta</math>(deg)</b>	<b>(<i>h, k, l</i>)</b>
5.846	(0,1,1)	17.049	(1,3,2)	23.538	(0,4,4)
8.892	(0,3,1)	17.599	(0,3,3)	23.913	(2,4,1)
9.472	(0,4,0)	18.178	(1,4,2)	24.662	(2,2,2)
10.961	(0,1,2)	18.643	(-1,1,3)	24.751	(1,1,4)
11.401	(1,2,0)	19.538	(1,5,2)	25.668	(1,3,4)
12.259	(1,1,1)	19.828	(-1,3,3)	26.754	(2,7,0)
12.931	(1,2,1)	20.398	(1,2,3)	27.416	(1,5,4)
13.36	(1,3,-1)	20.819	(2,0,0)	27.62	(2,7,1)
15.331	(1,4,1)	21.087	(1,3,3)	28.174	(2,6,2)
15.662	(1,1,2)	21.362	(2,2,0)	28.337	(2,8,0)
15.991	(0,5,2)	21.642	(2,2,-1)	30.04	(2,9,0)
16.018	(-1,3,2)	22.017	(1,4,3)	31.345	(2,1,4)
16.772	(0,2,3)	22.023	(2,3,0)	31.6	(3,1,-1)
16.914	(1,5,1)	22.423	(2,2,1)	36.91	(2,4,5)

Table S5. Fractional Atomic Coordinates ( $\times 10^4$ ) and Equivalent Isotropic

Displacement Parameters ( $\text{\AA}^2 \times 10^3$ ).  $U_{\text{eq}}$  is defined as 1/3 of of the trace of the orthogonalised  $U_{ij}$  tensor.

Atom	x	y	z	$U_{\text{eq}}$
Cl01	-2741.7(19)	64.8(5)	11911.5(11)	76.3(5)
F301	804(8)	938(2)	13886(3)	141(2)
F302	1867(11)	1296(3)	13092(4)	205(5)
F303	-492(9)	1324.3(18)	13210(4)	141(2)
F304	2956(17)	76(5)	10856(11)	97(5)
F305	4291(18)	405(5)	10092(11)	95(5)
F306	4150(20)	498(5)	11402(9)	91(5)
F307	9479(10)	3235(2)	8176(4)	90(2)
F308	11721(10)	3236(4)	7672(7)	157(6)
F309	9690(8)	3483(2)	7024(5)	94(2)
F351	3977(16)	364(3)	11118(6)	64(3)
F352	3857(15)	301(3)	9831(7)	64(3)
F353	2413(12)	-18(2)	10528(6)	61(2)
F354	9980(20)	2436(6)	6944(14)	174(6)
F355	11702(16)	2823(7)	6772(13)	179(6)
F356	9674(19)	2746(6)	5848(11)	160(5)
O301	1090(20)	500(6)	9821(12)	67(5)
O302	5669(12)	2086(4)	6954(9)	68(3)
O303	7475(12)	2713(6)	8267(7)	97(5)
O351	686(18)	506(4)	9650(9)	51(3)
O352	6101(10)	1889(2)	6747(4)	54.0(17)
O353	7939(10)	2510(2)	8075(4)	53.1(19)
N301	1440(30)	727(10)	9127(15)	60(6)
N302	4488(13)	2444(4)	7723(8)	54(3)
N303	7803(18)	2906(6)	6957(11)	90(5)
N351	1090(20)	703(5)	8981(13)	50(4)

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N352	4983(16)	2297(4)	7484(6)	47(3)
N353	8357(13)	2789(3)	6903(7)	50(3)
C023	9781(14)	2855(5)	7091(7)	70(3)
C301	-1234(7)	364.0(18)	11887(4)	64.7(16)
C302	-358(7)	374.9(18)	11196(4)	67.7(16)
C303	825(7)	615.1(19)	11167(4)	69.2(17)
C304	1183(8)	839(2)	11800(4)	78(2)
C305	298(8)	839(2)	12488(4)	78.2(19)
C306	-919(8)	589(2)	12529(4)	74.9(19)
C307	578(12)	1095(3)	13189(5)	102(3)
C308	2020(30)	652(9)	10558(16)	64(6)
C309	2270(30)	977(11)	10180(20)	56(5)
C310	2310(30)	974(9)	9348(16)	57(6)
C311	2910(30)	1263(9)	8821(17)	62(6)
C312	2820(30)	1230(8)	7966(19)	66(6)
C313	3310(20)	1513(5)	7481(13)	54(4)
C314	4084(15)	1815(5)	7926(10)	53(3)
C315	4225(17)	1851(5)	8775(12)	61(4)
C316	3550(20)	1550(6)	9203(14)	64(5)
C317	2130(30)	938(10)	7390(20)	65(6)
C318	2020(30)	967(8)	6600(20)	75(7)
C319	2520(40)	1229(8)	6190(20)	66(7)
C320	3220(30)	1505(6)	6641(16)	65(6)
C321	4820(20)	2111(10)	7476(13)	61(4)
C322	5134(15)	2770(5)	7396(10)	65(3)
C323	6887(15)	2803(6)	7591(9)	70(4)
C325	10109(14)	3215(4)	7514(9)	87(4)
C326	3330(30)	403(7)	10733(19)	76(5)
C351	1700(20)	603(6)	10369(11)	50(4)

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C352	2640(30)	974(8)	10180(20)	59(5)
C353	2080(30)	953(6)	9219(13)	48(4)
C354	2957(18)	309(4)	10451(8)	51(3)
C355	2860(30)	1198(6)	8670(12)	49(4)
C356	2650(30)	1169(5)	7811(11)	48(4)
C357	1740(20)	894(5)	7455(11)	39(3)
C358	1617(19)	879(4)	6592(10)	40(3)
C359	2360(30)	1127(5)	6122(14)	47(4)
C360	3360(20)	1387(4)	6498(9)	45(3)
C361	3593(17)	1419(3)	7334(8)	45(3)
C362	4450(16)	1696(3)	7740(6)	49(2)
C363	4522(17)	1719(3)	8582(7)	52(3)
C364	3802(19)	1466(4)	9039(9)	51(3)
C365	5270(20)	1961(4)	7284(8)	52(3)
C366	5730(12)	2598(3)	7124(5)	44.3(19)
C367	7400(13)	2627(3)	7422(5)	44(2)
C368	9430(20)	3043(8)	7116(18)	122(6)
C369	10200(30)	2732(8)	6700(20)	136(5)
C110	-3128(12)	4975(4)	411(7)	78(3)
F101	440(20)	4284(5)	-1509(10)	123(5)
F102	340(20)	3768(6)	-745(12)	117(5)
F103	2280(20)	4031(5)	-771(9)	108(4)
F104	4011(16)	4748(6)	1603(13)	57(3)
F105	2316(15)	5087(5)	2158(11)	46(2)
F106	3895(13)	4749(4)	2906(7)	44(2)
F107	10518(11)	2516(2)	5385(7)	97(3)
F108	10643(11)	2163(3)	6415(7)	110(3)
F109	12285(12)	2136(3)	5538(9)	122(3)
O101	860(12)	4490(4)	2773(10)	47(3)

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O102	6525(9)	2851(3)	5284(5)	60(2)
O103	7837(12)	2249(5)	4042(8)	109(4)
N101	1340(13)	4238(4)	3366(9)	42(2)
N102	4889(15)	2507(4)	4497(7)	68(3)
N103	8160(12)	1959(3)	5238(7)	81(3)
C101	590(30)	4069(5)	-801(15)	69(4)
C102	270(30)	4307(6)	-105(15)	64(4)
C103	-950(20)	4510(5)	-199(10)	56(4)
C104	-1470(20)	4719(4)	461(12)	47(3)
C105	-490(20)	4690(5)	1232(14)	48(3)
C106	830(20)	4478(6)	1296(16)	51(4)
C107	1280(30)	4285(6)	630(15)	57(4)
C108	1852(14)	4456(5)	2112(10)	44(3)
C109	3063(16)	4764(5)	2198(13)	43(3)
C110	2722(14)	4101(5)	2286(10)	47(3)
C111	2366(13)	4034(4)	3139(10)	41(3)
C112	3141(12)	3732(4)	3571(9)	43(3)
C113	3880(15)	3483(4)	3137(10)	49(3)
C114	4706(16)	3202(4)	3505(9)	55(3)
C115	4648(15)	3141(4)	4342(8)	55(3)
C116	3910(13)	3399(4)	4811(8)	51(2)
C117	3081(12)	3702(4)	4439(9)	45(3)
C118	2361(12)	3939(4)	4944(8)	47(3)
C119	2289(13)	3898(5)	5755(8)	47(2)
C120	3083(13)	3602(4)	6138(7)	50(3)
C121	3864(14)	3366(4)	5681(7)	57(3)
C122	5495(17)	2819(5)	4735(7)	64(3)
C123	5641(17)	2183(5)	4811(8)	76(3)
C124	7319(17)	2123(4)	4653(7)	79(3)

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C125	9891(14)	1926(5)	5206(11)	98(4)
C126	10813(18)	2153(5)	5569(10)	103(4)
C120	-3336(17)	5061(5)	472(7)	81(4)
F201	1790(20)	4116(5)	-915(12)	88(4)
F202	-265(19)	4215(4)	-1529(10)	84(4)
F203	-329(17)	3804(6)	-770(14)	86(4)
F204	3590(20)	4800(6)	1500(15)	52(3)
F205	1890(20)	5134(7)	2083(15)	62(5)
F206	3520(20)	4788(6)	2768(11)	63(4)
F207	11476(17)	2561(3)	5010(9)	145(5)
F208	13030(17)	2128(4)	5089(9)	145(5)
F209	11310(17)	2164(4)	5934(7)	111(4)
O201	394(16)	4558(4)	2702(9)	45(3)
O202	6258(18)	3025(3)	5422(7)	74(4)
O203	7924(17)	2458(2)	3736(5)	80(3)
N201	884(18)	4332(5)	3333(10)	46(3)
N202	5220(20)	2645(4)	4464(10)	73(3)
N203	8786(19)	2055(4)	4748(6)	94(3)
C201	340(40)	4167(8)	-840(20)	89(5)
C202	-50(30)	4381(7)	-147(17)	54(4)
C203	-1410(20)	4607(5)	-170(14)	52(4)
C204	-1720(30)	4811(6)	534(16)	57(4)
C205	-810(30)	4770(7)	1198(19)	54(4)
C206	520(30)	4539(7)	1248(17)	45(4)
C207	890(20)	4345(7)	563(17)	49(4)
C208	1430(20)	4506(6)	2031(12)	46(3)
C209	2610(20)	4806(7)	2125(15)	49(4)
C210	2187(18)	4139(5)	2200(10)	43(3)
C211	1890(20)	4095(6)	3085(13)	45(3)

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C212	2647(19)	3819(4)	3609(11)	46(3)
C213	3440(20)	3573(5)	3208(13)	47(3)
C214	4270(20)	3296(5)	3609(11)	52(3)
C215	4290(20)	3264(5)	4447(11)	54(3)
C216	3390(20)	3516(4)	4879(11)	56(3)
C217	2620(20)	3796(5)	4487(12)	51(3)
C218	1800(20)	4041(4)	4938(10)	54(3)
C219	1730(20)	4011(5)	5752(10)	58(3)
C220	2510(20)	3728(5)	6110(12)	57(3)
C221	3290(20)	3485(5)	5751(13)	59(3)
C222	5320(20)	2978(5)	4852(10)	65(3)
C223	6130(20)	2338(5)	4731(9)	71(3)
C224	7470(30)	2294(5)	4403(8)	78(3)
C225	10490(19)	2017(4)	4624(8)	104(4)
C226	11500(20)	2210(4)	5165(10)	119(4)
O1	6892(16)	1607(4)	6028(9)	104(4)
O2	8226(14)	1661(6)	6103(9)	170(8)

Table S6. Anisotropic Displacement Parameters ( $\text{\AA}^2 \times 10^3$ ). The Anisotropic displacement factor exponent takes the form:  $-2\pi^2[h^2a^2U_{11}+2hka*b*U_{12}+\dots]$ .

Atom	$U_{11}$	$U_{22}$	$U_{33}$	$U_{12}$	$U_{13}$	$U_{23}$
Cl01	75.0(10)	73.8(11)	83.2(11)	29.4(8)	25.9(8)	16.6(8)
F301	146(4)	213(7)	60(3)	17(3)	-15(3)	58(5)
F302	195(7)	331(13)	92(4)	-56(6)	26(4)	-115(8)
F303	189(6)	126(5)	98(4)	-14(3)	-62(4)	17(5)
F304	90(10)	91(11)	117(12)	35(10)	43(8)	24(8)
F305	84(9)	86(11)	123(13)	58(9)	62(9)	37(7)
F306	87(8)	119(13)	69(9)	43(7)	20(7)	55(9)
F307	121(6)	85(5)	62(4)	-15(3)	1(4)	-65(5)

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F308	72(5)	212(11)	178(9)	131(9)	-42(5)	-92(6)
F309	64(4)	96(5)	121(6)	42(5)	3(4)	-33(4)
F351	86(5)	60(6)	45(5)	14(4)	-5(5)	23(5)
F352	80(6)	45(5)	68(5)	20(4)	4(4)	9(4)
F353	80(6)	37(4)	67(5)	27(3)	13(4)	12(3)
F354	159(11)	171(14)	192(14)	87(12)	13(11)	-14(11)
F355	82(7)	255(16)	201(14)	90(13)	14(8)	-16(9)
F356	129(9)	185(13)	171(13)	59(11)	31(9)	28(10)
O301	58(9)	85(8)	60(10)	51(8)	16(8)	18(7)
O302	56(6)	84(9)	65(7)	12(7)	7(5)	17(6)
O303	45(6)	195(16)	50(6)	29(8)	-8(4)	-17(8)
O351	66(7)	38(4)	46(5)	15(4)	-13(4)	9(4)
O352	80(5)	48(4)	32(3)	7(3)	-5(3)	-12(4)
O353	61(5)	67(5)	30(3)	9(3)	-5(3)	8(3)
N301	60(11)	79(12)	44(9)	31(9)	15(9)	25(8)
N302	45(5)	63(8)	54(6)	35(6)	0(4)	-6(5)
N303	56(8)	148(13)	61(8)	35(9)	-37(6)	-44(8)
N351	63(9)	33(5)	53(8)	10(5)	-7(5)	-3(5)
N352	72(7)	41(6)	28(4)	-5(4)	6(4)	-6(5)
N353	51(6)	68(6)	33(4)	7(4)	4(4)	13(4)
C023	63(6)	112(9)	37(5)	17(6)	23(4)	20(6)
C301	59(3)	67(4)	70(4)	36(3)	18(3)	22(3)
C302	73(4)	60(3)	72(4)	33(3)	20(3)	24(3)
C303	59(3)	72(4)	78(4)	42(3)	13(3)	23(3)
C304	71(4)	90(5)	72(4)	42(4)	-2(3)	11(3)
C305	73(4)	101(5)	59(3)	28(3)	-6(3)	19(4)
C306	80(4)	87(5)	58(3)	31(3)	13(3)	29(4)
C307	103(6)	139(8)	62(4)	11(5)	-11(4)	17(6)
C308	43(9)	84(11)	68(11)	38(9)	14(8)	16(7)

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C309	30(8)	87(11)	53(9)	37(7)	11(7)	26(7)
C310	45(8)	80(11)	48(9)	33(8)	22(8)	12(7)
C311	57(9)	67(12)	65(11)	34(9)	26(8)	27(9)
C312	45(9)	67(11)	87(12)	26(9)	22(9)	22(8)
C313	35(6)	64(10)	67(8)	31(7)	29(5)	37(6)
C314	33(5)	65(9)	62(8)	21(6)	13(5)	20(5)
C315	44(6)	72(10)	72(9)	36(7)	24(6)	31(6)
C316	51(7)	76(12)	69(10)	36(8)	35(7)	29(7)
C317	56(11)	53(10)	92(12)	35(8)	42(9)	11(8)
C318	67(12)	72(13)	89(12)	20(11)	24(10)	17(9)
C319	48(10)	67(15)	87(13)	22(11)	25(9)	14(11)
C320	41(7)	74(12)	80(12)	21(9)	6(7)	28(8)
C321	48(7)	83(12)	50(8)	21(10)	0(6)	18(8)
C322	45(6)	82(9)	67(7)	35(7)	-15(5)	-28(6)
C323	36(6)	125(11)	48(6)	19(8)	-2(5)	-1(7)
C325	56(6)	114(9)	87(8)	41(7)	-9(5)	-47(6)
C326	65(11)	90(13)	76(13)	33(10)	28(9)	21(9)
C351	49(8)	54(6)	43(7)	19(5)	-10(5)	9(5)
C352	62(11)	56(8)	59(8)	23(6)	-4(9)	3(9)
C353	66(8)	26(5)	49(7)	12(5)	-13(5)	1(5)
C354	64(7)	49(7)	40(6)	14(5)	-5(5)	-3(5)
C355	65(7)	39(7)	40(7)	4(5)	-18(5)	-3(5)
C356	60(7)	38(7)	44(6)	16(5)	-12(5)	-1(5)
C357	46(8)	33(6)	39(5)	10(4)	18(5)	0(5)
C358	47(7)	35(6)	40(5)	10(4)	13(4)	3(4)
C359	49(7)	41(8)	49(6)	6(6)	4(5)	-4(6)
C360	54(7)	41(7)	39(5)	7(5)	7(5)	2(6)
C361	59(7)	33(6)	42(6)	6(4)	-1(5)	15(5)
C362	68(7)	43(6)	35(5)	7(4)	7(4)	6(5)

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C363	78(8)	38(6)	38(5)	7(4)	-11(5)	-10(5)
C364	62(7)	46(6)	43(6)	5(4)	-10(5)	-2(5)
C365	82(8)	41(6)	30(5)	6(5)	-10(5)	-10(6)
C366	62(5)	35(5)	36(4)	6(3)	2(4)	0(4)
C367	60(5)	39(5)	31(4)	5(3)	1(4)	-3(4)
C368	108(8)	138(9)	121(9)	44(8)	8(7)	-13(7)
C369	106(8)	159(10)	143(9)	74(9)	8(8)	-15(8)
C110	60(3)	93(5)	82(4)	8(3)	13(2)	-23(4)
F101	176(13)	153(11)	43(5)	-4(6)	19(8)	-24(9)
F102	185(13)	85(8)	79(6)	-18(5)	5(10)	-15(10)
F103	173(12)	101(8)	51(6)	-6(5)	20(7)	35(7)
F104	40(7)	71(7)	61(7)	12(5)	6(5)	-10(5)
F105	45(5)	45(6)	49(5)	1(4)	-4(4)	-1(4)
F106	42(5)	52(5)	34(5)	2(4)	-18(4)	-17(4)
F107	79(5)	78(5)	130(7)	-2(5)	-22(5)	19(4)
F108	80(5)	136(8)	114(7)	14(6)	4(5)	-4(5)
F109	94(6)	134(9)	140(9)	25(7)	30(7)	22(6)
O101	37(4)	59(5)	44(5)	2(4)	1(4)	-4(4)
O102	49(4)	87(7)	41(4)	-3(5)	-18(3)	12(4)
O103	79(6)	166(12)	88(8)	-7(8)	39(5)	-27(7)
N101	33(5)	55(6)	35(4)	4(4)	-11(4)	-4(4)
N102	77(6)	81(7)	43(4)	21(5)	-8(4)	-13(5)
N103	83(6)	72(6)	87(6)	0(5)	8(5)	-5(5)
C101	92(8)	64(8)	50(6)	-8(6)	3(6)	-6(6)
C102	96(8)	59(7)	37(5)	1(5)	10(6)	-19(6)
C103	79(8)	59(8)	33(5)	1(5)	13(6)	-26(6)
C104	53(6)	46(7)	44(5)	-7(5)	15(4)	-19(5)
C105	54(7)	52(7)	39(5)	-6(6)	9(6)	-23(6)
C106	54(7)	57(7)	42(5)	4(5)	6(5)	-19(5)

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C107	80(8)	54(7)	38(6)	3(5)	10(6)	-15(6)
C108	39(5)	53(5)	40(5)	5(4)	4(4)	-8(4)
C109	39(6)	49(6)	43(6)	3(5)	4(5)	-12(5)
C110	39(5)	55(5)	45(6)	2(4)	-3(5)	-3(5)
C111	28(4)	55(6)	38(5)	2(4)	-7(4)	-12(4)
C112	29(4)	62(6)	36(4)	4(4)	-6(4)	-4(4)
C113	43(5)	67(7)	37(5)	6(5)	-4(4)	4(4)
C114	56(5)	73(7)	35(5)	-3(5)	-4(4)	19(5)
C115	55(5)	73(6)	36(5)	-2(5)	-9(4)	12(4)
C116	45(4)	72(6)	34(4)	-2(5)	-6(4)	5(4)
C117	30(4)	66(6)	38(4)	-2(5)	-7(4)	0(4)
C118	33(4)	64(7)	43(5)	-6(5)	-6(4)	-8(4)
C119	36(4)	69(7)	35(4)	-2(5)	-3(4)	-3(4)
C120	48(5)	77(7)	26(4)	-2(5)	-6(4)	9(5)
C121	56(5)	82(7)	33(4)	-9(5)	-3(4)	11(5)
C122	79(5)	77(6)	34(4)	2(5)	-13(4)	6(5)
C123	88(6)	87(7)	50(5)	21(5)	-20(5)	-21(6)
C124	102(6)	89(7)	47(5)	4(5)	11(5)	-28(6)
C125	77(7)	109(10)	110(9)	5(8)	22(7)	16(7)
C126	75(7)	120(9)	114(9)	22(8)	-4(7)	-10(7)
C120	92(6)	104(8)	50(3)	14(4)	16(3)	-6(4)
F201	99(9)	109(10)	56(7)	-6(7)	-1(6)	6(7)
F202	133(9)	85(7)	33(4)	-16(4)	-7(6)	-1(7)
F203	97(8)	79(8)	80(7)	-31(5)	-12(7)	-8(7)
F204	44(8)	57(7)	52(6)	6(5)	-5(6)	-13(6)
F205	73(11)	50(8)	60(6)	-10(5)	-22(7)	-2(7)
F206	68(9)	68(7)	46(6)	20(4)	-49(5)	-25(6)
F207	133(9)	137(10)	173(11)	80(9)	78(9)	60(8)
F208	185(12)	138(10)	118(9)	72(8)	53(9)	66(9)

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F209	127(10)	120(9)	91(8)	44(7)	53(8)	50(8)
O201	57(7)	55(6)	21(4)	3(4)	-5(5)	-9(5)
O202	121(9)	52(6)	41(5)	-8(5)	-39(6)	0(6)
O203	167(9)	31(4)	39(4)	26(4)	-8(5)	-16(5)
N201	48(7)	59(7)	28(5)	5(5)	-9(5)	-9(5)
N202	100(7)	59(7)	51(5)	32(5)	-40(5)	-32(6)
N203	175(9)	76(6)	33(4)	36(5)	23(6)	48(6)
C201	133(10)	86(9)	48(7)	-10(8)	10(7)	-8(8)
C202	66(7)	58(8)	39(6)	-13(6)	4(6)	-20(6)
C203	61(7)	56(8)	39(6)	-8(6)	2(6)	-22(6)
C204	65(8)	66(9)	42(6)	0(7)	15(6)	-21(7)
C205	60(8)	64(9)	38(6)	4(6)	11(6)	-11(6)
C206	55(7)	48(7)	31(5)	-7(5)	1(6)	-22(6)
C207	56(7)	55(8)	37(6)	-10(6)	3(6)	-23(6)
C208	55(6)	50(6)	30(5)	-3(4)	-8(5)	-17(5)
C209	60(8)	51(7)	33(6)	0(5)	-20(6)	-15(7)
C210	49(7)	50(6)	26(4)	8(4)	-15(5)	-22(6)
C211	48(7)	50(6)	35(5)	2(5)	-15(6)	-18(6)
C212	48(6)	49(6)	39(5)	-5(5)	-10(5)	-19(5)
C213	55(7)	49(7)	36(6)	-8(5)	-6(6)	-17(6)
C214	63(7)	52(7)	41(6)	-11(5)	-1(6)	-11(6)
C215	71(7)	47(6)	41(5)	-6(5)	-4(5)	-17(5)
C216	66(6)	46(6)	53(6)	-11(5)	-9(5)	-22(5)
C217	59(6)	51(6)	40(5)	-11(5)	-7(6)	-14(5)
C218	63(7)	50(6)	47(5)	-13(5)	-11(6)	-15(6)
C219	68(7)	55(7)	48(6)	-14(5)	-12(6)	-6(6)
C220	68(7)	51(7)	51(6)	-11(6)	-11(6)	-6(6)
C221	70(7)	50(7)	55(7)	-5(6)	-6(7)	-10(6)
C222	96(7)	50(6)	47(6)	10(5)	-17(5)	-20(6)

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C223	103(7)	67(6)	39(5)	26(5)	-17(5)	-8(6)
C224	146(8)	59(6)	29(5)	28(5)	3(6)	15(7)
C225	174(9)	88(7)	55(6)	37(6)	44(7)	75(7)
C226	157(9)	111(8)	97(8)	46(7)	56(8)	71(8)
O1	85(8)	95(9)	131(11)	37(8)	0(7)	23(7)
O2	65(7)	310(30)	134(11)	73(13)	23(7)	11(9)

Table S7. Bond Lengths.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C101	C301	1.708(7)	F106	C109	1.326(19)
F301	C307	1.296(10)	F107	C126	1.410(17)
F302	C307	1.352(13)	F108	C126	1.422(15)
F303	C307	1.255(11)	F109	C126	1.265(15)
F304	C326	1.28(3)	O101	N101	1.398(15)
F305	C326	1.39(3)	O101	C108	1.442(19)
F306	C326	1.32(3)	O102	C122	1.223(13)
F307	C325	1.261(17)	O103	C124	1.227(13)
F308	C325	1.386(14)	N101	C111	1.240(18)
F309	C325	1.322(16)	N102	C122	1.32(2)
F351	C354	1.371(15)	N102	C123	1.45(2)
F352	C354	1.33(2)	N103	C124	1.314(15)
F353	C354	1.317(18)	N103	C125	1.490(14)
F354	C369	1.20(3)	C101	C102	1.50(3)
F355	C369	1.32(3)	C102	C103	1.29(3)
F356	C369	1.44(3)	C102	C107	1.44(3)
O301	N301	1.48(3)	C103	C104	1.44(2)
O301	C308	1.51(3)	C104	C105	1.48(3)
O302	C321	1.17(2)	C105	C106	1.38(2)
O303	C323	1.239(17)	C106	C107	1.40(3)

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O351	N351	1.40(3)	C106	C108	1.55(2)
O351	C351	1.462(16)	C108	C110	1.536(19)
O352	C365	1.21(2)	C108	C109	1.55(2)
O353	C367	1.225(11)	C110	C111	1.49(2)
N301	C310	1.22(4)	C111	C112	1.467(18)
N302	C321	1.34(3)	C112	C113	1.359(18)
N302	C322	1.459(17)	C112	C117	1.446(19)
N303	C323	1.41(2)	C113	C114	1.382(18)
N303	C368	1.485(18)	C114	C115	1.409(18)
N351	C353	1.30(3)	C115	C116	1.414(17)
N352	C365	1.326(18)	C115	C122	1.53(2)
N352	C366	1.443(15)	C116	C121	1.450(16)
N353	C023	1.259(18)	C116	C117	1.447(18)
N353	C367	1.371(15)	C117	C118	1.393(17)
C023	C325	1.53(2)	C118	C119	1.358(17)
C301	C306	1.365(11)	C119	C120	1.421(18)
C301	C302	1.416(8)	C120	C121	1.367(17)
C302	C303	1.356(10)	C123	C124	1.49(2)
C303	C304	1.358(11)	C125	C126	1.27(2)
C303	C308	1.49(3)	C120	C204	1.67(3)
C303	C351	1.57(2)	F201	C201	1.27(4)
C304	C305	1.415(10)	F202	C201	1.23(4)
C305	C306	1.403(11)	F203	C201	1.48(4)
C305	C307	1.510(13)	F204	C209	1.38(4)
C308	C309	1.39(5)	F205	C209	1.37(3)
C308	C326	1.47(4)	F206	C209	1.27(2)
C309	C310	1.38(5)	F207	C226	1.334(15)
C310	C311	1.50(4)	F208	C226	1.359(16)
C311	C316	1.34(4)	F209	C226	1.308(16)

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C311	C312	1.42(4)	O201	N201	1.383(18)
C312	C313	1.41(4)	O201	C208	1.49(2)
C312	C317	1.53(4)	O202	C222	1.207(14)
C313	C320	1.39(3)	O203	C224	1.348(15)
C313	C314	1.47(3)	N201	C211	1.32(3)
C314	C315	1.41(2)	N202	C222	1.40(2)
C314	C321	1.50(3)	N202	C223	1.44(2)
C315	C316	1.47(3)	N203	C225	1.494(16)
C317	C318	1.31(5)	N203	C224	1.52(2)
C318	C319	1.29(4)	C201	C202	1.46(4)
C319	C320	1.39(4)	C202	C207	1.38(3)
C322	C323	1.514(17)	C202	C203	1.44(3)
C351	C354	1.53(2)	C203	C204	1.43(3)
C351	C352	1.64(4)	C204	C205	1.31(3)
C352	C353	1.63(4)	C205	C206	1.42(3)
C353	C355	1.48(3)	C206	C207	1.40(3)
C355	C364	1.40(2)	C206	C208	1.47(3)
C355	C356	1.42(2)	C208	C209	1.51(3)
C356	C357	1.39(2)	C208	C210	1.53(2)
C356	C361	1.50(3)	C210	C211	1.51(3)
C357	C358	1.43(2)	C211	C212	1.47(2)
C358	C359	1.39(2)	C212	C213	1.34(2)
C359	C360	1.41(2)	C212	C217	1.46(2)
C360	C361	1.390(19)	C213	C214	1.40(2)
C361	C362	1.409(19)	C214	C215	1.39(2)
C362	C363	1.394(15)	C215	C216	1.44(2)
C362	C365	1.46(2)	C215	C222	1.51(2)
C363	C364	1.38(2)	C216	C217	1.37(2)
C366	C367	1.479(15)	C216	C221	1.46(3)

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C368	C369	1.53(2)	C217	C218	1.40(2)
C110	C104	1.71(2)	C218	C219	1.36(2)
F101	C101	1.42(3)	C219	C220	1.36(2)
F102	C101	1.15(3)	C220	C221	1.29(3)
F103	C101	1.45(3)	C223	C224	1.32(3)
F104	C109	1.32(3)	C225	C226	1.396(18)
F105	C109	1.36(2)			

Table S8. Bond Angles.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N301	O301	C308	107(2)	F101	C101	C102	107.0(16)
N351	O351	C351	110.5(14)	F103	C101	C102	105.9(17)
C310	N301	O301	111(2)	C103	C102	C107	124.4(19)
C321	N302	C322	124.3(17)	C103	C102	C101	116.7(18)
C323	N303	C368	121.7(17)	C107	C102	C101	118.9(16)
C353	N351	O351	109.4(16)	C102	C103	C104	121.1(17)
C365	N352	C366	122.4(12)	C103	C104	C105	115.6(14)
C023	N353	C367	122.9(10)	C103	C104	C110	124.5(15)
N353	C023	C325	115.3(13)	C105	C104	C110	119.8(12)
C306	C301	C302	121.8(7)	C106	C105	C104	121.1(16)
C306	C301	C101	119.2(5)	C105	C106	C107	120.6(17)
C302	C301	C101	119.0(6)	C105	C106	C108	120.1(18)
C303	C302	C301	119.3(7)	C107	C106	C108	119.4(14)
C302	C303	C304	120.3(7)	C106	C107	C102	117.0(16)
C302	C303	C308	129.4(13)	O101	C108	C110	103.7(11)
C304	C303	C308	109.8(12)	O101	C108	C109	107.0(12)
C302	C303	C351	114.4(9)	C110	C108	C109	108.2(10)
C304	C303	C351	125.2(9)	O101	C108	C106	109.5(11)
C303	C304	C305	121.3(7)	C110	C108	C106	116.2(13)

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C306	C305	C304	118.9(8)	C109	C108	C106	111.6(13)
C306	C305	C307	117.3(7)	F104	C109	F106	109.8(12)
C304	C305	C307	123.8(8)	F104	C109	F105	108.5(16)
C301	C306	C305	118.3(6)	F106	C109	F105	107.5(16)
F303	C307	F301	110.1(8)	F104	C109	C108	109.8(17)
F303	C307	F302	103.2(11)	F106	C109	C108	111.1(14)
F301	C307	F302	106.8(8)	F105	C109	C108	110.1(11)
F303	C307	C305	112.3(7)	C111	C110	C108	101.0(11)
F301	C307	C305	113.8(10)	N101	C111	C112	128.8(14)
F302	C307	C305	110.0(8)	N101	C111	C110	112.7(12)
C309	C308	C326	120(2)	C112	C111	C110	118.3(11)
C309	C308	C303	122(2)	C113	C112	C117	121.7(12)
C326	C308	C303	111.0(19)	C113	C112	C111	118.5(12)
C309	C308	O301	93(2)	C117	C112	C111	119.7(13)
C326	C308	O301	105(2)	C112	C113	C114	122.0(13)
C303	C308	O301	99.8(15)	C113	C114	C115	120.0(12)
C310	C309	C308	117(4)	C114	C115	C116	118.9(11)
N301	C310	C309	104(3)	C114	C115	C122	119.7(11)
N301	C310	C311	126(3)	C116	C115	C122	121.3(11)
C309	C310	C311	128(3)	C115	C116	C121	122.4(12)
C316	C311	C312	122(2)	C115	C116	C117	121.4(11)
C316	C311	C310	116(2)	C121	C116	C117	116.1(13)
C312	C311	C310	122(3)	C118	C117	C112	126.8(12)
C313	C312	C311	120(3)	C118	C117	C116	117.7(12)
C313	C312	C317	107(2)	C112	C117	C116	115.5(11)
C311	C312	C317	132(3)	C119	C118	C117	125.4(13)
C320	C313	C312	124(2)	C118	C119	C120	118.2(12)
C320	C313	C314	120.6(18)	C121	C120	C119	119.3(10)
C312	C313	C314	115.4(19)	C120	C121	C116	123.3(12)

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C315	C314	C313	125.0(15)	O102	C122	N102	123.5(15)
C315	C314	C321	114.8(19)	O102	C122	C115	122.2(16)
C313	C314	C321	120.2(18)	N102	C122	C115	113.8(11)
C314	C315	C316	114(2)	N102	C123	C124	117.8(13)
C311	C316	C315	123(2)	O103	C124	N103	125.0(15)
C318	C317	C312	123(3)	O103	C124	C123	120.0(13)
C319	C318	C317	127(3)	N103	C124	C123	114.8(11)
C318	C319	C320	115(3)	C126	C125	N103	120.7(15)
C319	C320	C313	124(2)	F109	C126	C125	122.1(16)
O302	C321	N302	117(3)	F109	C126	F107	101.5(14)
O302	C321	C314	128(3)	C125	C126	F107	116.2(14)
N302	C321	C314	115.1(16)	F109	C126	F108	102.6(13)
N302	C322	C323	112.6(13)	C125	C126	F108	112.2(15)
O303	C323	N303	122.5(12)	F107	C126	F108	99.0(13)
O303	C323	C322	120.0(12)	N201	O201	C208	108.7(12)
N303	C323	C322	117.3(11)	C211	N201	O201	109.9(14)
F307	C325	F309	112.0(15)	C222	N202	C223	123.6(14)
F307	C325	F308	108.4(12)	C225	N203	C224	135.1(12)
F309	C325	F308	107.0(9)	F202	C201	F201	106(3)
F307	C325	C023	112.1(9)	F202	C201	C202	123(3)
F309	C325	C023	110.6(12)	F201	C201	C202	116(3)
F308	C325	C023	106.3(15)	F202	C201	F203	94(2)
F304	C326	F306	104(2)	F201	C201	F203	105(2)
F304	C326	F305	107(2)	C202	C201	F203	109(2)
F306	C326	F305	109(2)	C207	C202	C203	120(2)
F304	C326	C308	116(2)	C207	C202	C201	118(2)
F306	C326	C308	110(2)	C203	C202	C201	122(2)
F305	C326	C308	110(2)	C204	C203	C202	119.2(19)
O351	C351	C354	105.3(14)	C205	C204	C203	119(2)

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O351	C351	C303	113.9(14)	C205	C204	Cl20	123.8(19)
C354	C351	C303	108.8(12)	C203	C204	Cl20	116.7(18)
O351	C351	C352	108.8(18)	C204	C205	C206	123(2)
C354	C351	C352	105.6(15)	C207	C206	C205	119.5(19)
C303	C351	C352	113.8(17)	C207	C206	C208	122.4(19)
C353	C352	C351	91.9(19)	C205	C206	C208	118(2)
N351	C353	C355	124.5(17)	C202	C207	C206	119.2(19)
N351	C353	C352	118(2)	C206	C208	O201	110.0(15)
C355	C353	C352	117.5(18)	C206	C208	C209	109.6(16)
F353	C354	F352	106.4(12)	O201	C208	C209	104.9(15)
F353	C354	F351	105.6(11)	C206	C208	C210	115.2(15)
F352	C354	F351	104.8(13)	O201	C208	C210	104.3(13)
F353	C354	C351	114.8(13)	C209	C208	C210	112.1(14)
F352	C354	C351	113.1(12)	F206	C209	F205	110(2)
F351	C354	C351	111.4(12)	F206	C209	F204	105.1(18)
C364	C355	C356	121.2(19)	F205	C209	F204	106(2)
C364	C355	C353	116.3(15)	F206	C209	C208	114(2)
C356	C355	C353	122.6(15)	F205	C209	C208	111.4(17)
C357	C356	C355	120.3(18)	F204	C209	C208	110(2)
C357	C356	C361	122.8(16)	C211	C210	C208	100.2(15)
C355	C356	C361	116.5(15)	N201	C211	C212	123.6(18)
C356	C357	C358	116.9(14)	N201	C211	C210	112.8(14)
C359	C358	C357	122.2(13)	C212	C211	C210	123.6(19)
C358	C359	C360	119.7(17)	C213	C212	C217	119.9(16)
C361	C360	C359	122.6(15)	C213	C212	C211	113.7(16)
C360	C361	C362	124.7(13)	C217	C212	C211	126.4(17)
C360	C361	C356	115.4(13)	C212	C213	C214	121.9(17)
C362	C361	C356	119.2(11)	C215	C214	C213	120.2(16)
C363	C362	C361	120.3(11)	C214	C215	C216	118.4(15)

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C363	C362	C365	119.3(11)	C214	C215	C222	117.7(18)
C361	C362	C365	120.3(10)	C216	C215	C222	123.8(16)
C364	C363	C362	121.2(11)	C217	C216	C215	121.1(16)
C363	C364	C355	121.0(14)	C217	C216	C221	117.8(16)
O352	C365	N352	121.6(14)	C215	C216	C221	121.1(16)
O352	C365	C362	124.4(12)	C216	C217	C218	119.1(16)
N352	C365	C362	114.0(17)	C216	C217	C212	118.3(16)
N352	C366	C367	111.5(9)	C218	C217	C212	122.5(15)
O353	C367	N353	120.6(10)	C219	C218	C217	122.3(16)
O353	C367	C366	123.9(9)	C218	C219	C220	116.1(17)
N353	C367	C366	115.5(8)	C221	C220	C219	126.6(19)
N303	C368	C369	95(2)	C220	C221	C216	118.1(17)
F354	C369	F355	112(2)	O202	C222	N202	120.3(16)
F354	C369	F356	109(3)	O202	C222	C215	125.1(15)
F355	C369	F356	108(2)	N202	C222	C215	114.3(12)
F354	C369	C368	117(3)	C224	C223	N202	116.1(15)
F355	C369	C368	102(2)	C223	C224	O203	126.8(15)
F356	C369	C368	107(2)	C223	C224	N203	124.3(13)
N101	O101	C108	108.5(10)	O203	C224	N203	108.9(16)
C111	N101	O101	112.1(13)	C226	C225	N203	115.2(12)
C122	N102	C123	118.3(12)	F209	C226	F207	108.4(16)
C124	N103	C125	120.1(13)	F209	C226	F208	104.5(16)
F102	C101	F101	128(2)	F207	C226	F208	101.8(13)
F102	C101	F103	95.2(17)	F209	C226	C225	116.1(13)
F101	C101	F103	96.4(17)	F207	C226	C225	112.6(14)
F102	C101	C102	118(2)	F208	C226	C225	112.2(14)

Table S9. Torsion Angles.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
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C308	O301	N301	C310	-2(3)	F101	C101	C102	C107	-135.8(19)
C351	O351	N351	C353	-10(2)	F103	C101	C102	C107	-34(2)
C367	N353	C023	C325	-87.2(15)	C107	C102	C103	C104	-4(3)
C306	C301	C302	C303	-0.1(8)	C101	C102	C103	C104	172.9(16)
C101	C301	C302	C303	179.0(4)	C102	C103	C104	C105	2(2)
C301	C302	C303	C304	1.1(8)	C102	C103	C104	C110	-176.1(15)
C301	C302	C303	C308	172.5(14)	C103	C104	C105	C106	0(2)
C301	C302	C303	C351	-179.6(9)	C110	C104	C105	C106	178.2(15)
C302	C303	C304	C305	-2.7(9)	C104	C105	C106	C107	0(2)
C308	C303	C304	C305	-175.6(13)	C104	C105	C106	C108	179.4(15)
C351	C303	C304	C305	178.0(10)	C105	C106	C107	C102	-3(3)
C303	C304	C305	C306	3.3(9)	C108	C106	C107	C102	178.3(17)
C303	C304	C305	C307	-176.4(7)	C103	C102	C107	C106	5(3)
C302	C301	C306	C305	0.7(9)	C101	C102	C107	C106	-172.4(19)
C101	C301	C306	C305	-178.4(4)	N101	O101	C108	C110	12.6(13)
C304	C305	C306	C301	-2.3(9)	N101	O101	C108	C109	-101.7(12)
C307	C305	C306	C301	177.5(6)	N101	O101	C108	C106	137.2(13)
C306	C305	C307	F303	-71.0(11)	C105	C106	C108	O101	33(2)
C304	C305	C307	F303	108.7(10)	C107	C106	C108	O101	-147.9(16)
C306	C305	C307	F301	54.9(10)	C105	C106	C108	C110	150.0(15)
C304	C305	C307	F301	-125.4(9)	C107	C106	C108	C110	-31(2)
C306	C305	C307	F302	174.6(8)	C105	C106	C108	C109	-85.3(18)
C304	C305	C307	F302	-5.7(12)	C107	C106	C108	C109	93.8(18)
C302	C303	C308	C309	128(3)	O101	C108	C109	F104	-179.9(12)
C304	C303	C308	C309	-60(3)	C110	C108	C109	F104	68.9(16)
C351	C303	C308	C309	101(7)	C106	C108	C109	F104	-60.2(16)
C302	C303	C308	C326	-83(2)	O101	C108	C109	F106	58.4(14)
C304	C303	C308	C326	89(2)	C110	C108	C109	F106	-52.8(16)
C351	C303	C308	C326	-109(8)	C106	C108	C109	F106	178.2(14)

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C302	C303	C308	O301	28(2)	O101	C108	C109	F105	-60.5(17)
C304	C303	C308	O301	-159.7(13)	C110	C108	C109	F105	-171.8(15)
C351	C303	C308	O301	1(5)	C106	C108	C109	F105	59.2(19)
N301	O301	C308	C309	17(2)	O101	C108	C110	C111	-13.6(12)
N301	O301	C308	C326	-105(2)	C109	C108	C110	C111	99.9(13)
N301	O301	C308	C303	139.5(18)	C106	C108	C110	C111	-133.7(13)
C326	C308	C309	C310	81(4)	O101	N101	C111	C112	-178.4(13)
C303	C308	C309	C310	-132(2)	O101	N101	C111	C110	-3.6(14)
O301	C308	C309	C310	-28(3)	C108	C110	C111	N101	11.1(13)
O301	N301	C310	C309	-14(3)	C108	C110	C111	C112	-173.5(11)
O301	N301	C310	C311	-179(2)	N101	C111	C112	C113	161.0(14)
C308	C309	C310	N301	30(4)	C110	C111	C112	C113	-13.6(17)
C308	C309	C310	C311	-165(3)	N101	C111	C112	C117	-18.0(19)
N301	C310	C311	C316	165(3)	C110	C111	C112	C117	167.4(11)
C309	C310	C311	C316	3(4)	C117	C112	C113	C114	-4.6(19)
N301	C310	C311	C312	-15(4)	C111	C112	C113	C114	176.5(12)
C309	C310	C311	C312	-177(3)	C112	C113	C114	C115	8(2)
C316	C311	C312	C313	-4(4)	C113	C114	C115	C116	-8(2)
C310	C311	C312	C313	177(2)	C113	C114	C115	C122	176.9(14)
C316	C311	C312	C317	-179(3)	C114	C115	C116	C121	-177.0(12)
C310	C311	C312	C317	2(4)	C122	C115	C116	C121	-2(2)
C311	C312	C313	C320	-178.3(19)	C114	C115	C116	C117	6.5(19)
C317	C312	C313	C320	-2(3)	C122	C115	C116	C117	-178.8(13)
C311	C312	C313	C314	7(3)	C113	C112	C117	C118	-179.9(12)
C317	C312	C313	C314	-177.1(16)	C111	C112	C117	C118	-1.1(17)
C320	C313	C314	C315	179.1(13)	C113	C112	C117	C116	2.5(16)
C312	C313	C314	C315	-6(2)	C111	C112	C117	C116	-178.7(11)
C320	C313	C314	C321	-2(2)	C115	C116	C117	C118	178.7(11)
C312	C313	C314	C321	173.2(17)	C121	C116	C117	C118	2.0(15)

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C313	C314	C315	C316	1.3(18)	C115	C116	C117	C112	-3.5(17)
C321	C314	C315	C316	-177.7(13)	C121	C116	C117	C112	179.8(11)
C312	C311	C316	C315	-1(3)	C112	C117	C118	C119	178.1(11)
C310	C311	C316	C315	178.4(18)	C116	C117	C118	C119	-4.3(16)
C314	C315	C316	C311	2(2)	C117	C118	C119	C120	3.9(16)
C313	C312	C317	C318	-2(3)	C118	C119	C120	C121	-1.2(16)
C311	C312	C317	C318	174(3)	C119	C120	C121	C116	-0.9(18)
C312	C317	C318	C319	4(5)	C115	C116	C121	C120	-176.3(12)
C317	C318	C319	C320	-1(4)	C117	C116	C121	C120	0.4(18)
C318	C319	C320	C313	-3(3)	C123	N102	C122	O102	-10(2)
C312	C313	C320	C319	5(3)	C123	N102	C122	C115	177.8(12)
C314	C313	C320	C319	179.4(19)	C114	C115	C122	O102	120.7(15)
C322	N302	C321	O302	-1(2)	C116	C115	C122	O102	-54(2)
C322	N302	C321	C314	177.1(12)	C114	C115	C122	N102	-67.0(17)
C315	C314	C321	O302	131(2)	C116	C115	C122	N102	118.4(15)
C313	C314	C321	O302	-48(2)	C122	N102	C123	C124	-59.2(18)
C315	C314	C321	N302	-46.5(17)	C125	N103	C124	O103	3(2)
C313	C314	C321	N302	134.4(16)	C125	N103	C124	C123	-171.9(13)
C321	N302	C322	C323	-67(2)	N102	C123	C124	O103	-29(2)
C368	N303	C323	O303	-23(4)	N102	C123	C124	N103	145.6(13)
C368	N303	C323	C322	163(2)	C124	N103	C125	C126	95(2)
N302	C322	C323	O303	-40(3)	N103	C125	C126	F109	-178.4(16)
N302	C322	C323	N303	135(2)	N103	C125	C126	F107	-54(2)
N353	C023	C325	F307	61.3(16)	N103	C125	C126	F108	59(2)
N353	C023	C325	F309	-64.5(14)	C208	O201	N201	C211	-12.4(16)
N353	C023	C325	F308	179.7(10)	F202	C201	C202	C207	-169(3)
C309	C308	C326	F304	-160(3)	F201	C201	C202	C207	-36(3)
C303	C308	C326	F304	50(3)	F203	C201	C202	C207	83(3)
O301	C308	C326	F304	-57(3)	F202	C201	C202	C203	15(4)

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C309	C308	C326	F306	82(3)	F201	C201	C202	C203	148(2)
C303	C308	C326	F306	-68(2)	F203	C201	C202	C203	-93(3)
O301	C308	C326	F306	-175.6(18)	C207	C202	C203	C204	4(3)
C309	C308	C326	F305	-39(4)	C201	C202	C203	C204	-180(2)
C303	C308	C326	F305	171(2)	C202	C203	C204	C205	-4(3)
O301	C308	C326	F305	64(3)	C202	C203	C204	Cl20	-178.7(18)
N351	O351	C351	C354	-98.9(16)	C203	C204	C205	C206	2(3)
N351	O351	C351	C303	142.0(15)	Cl20	C204	C205	C206	176(2)
N351	O351	C351	C352	14(2)	C204	C205	C206	C207	0(3)
C302	C303	C351	O351	32.9(17)	C204	C205	C206	C208	-178(2)
C304	C303	C351	O351	-147.8(11)	C203	C202	C207	C206	-2(3)
C308	C303	C351	O351	-170(8)	C201	C202	C207	C206	-178(2)
C302	C303	C351	C354	-84.2(12)	C205	C206	C207	C202	0(3)
C304	C303	C351	C354	95.1(13)	C208	C206	C207	C202	178(2)
C308	C303	C351	C354	73(6)	C207	C206	C208	O201	-148(2)
C302	C303	C351	C352	158.4(14)	C205	C206	C208	O201	30(2)
C304	C303	C351	C352	-22(2)	C207	C206	C208	C209	97(2)
C308	C303	C351	C352	-44(6)	C205	C206	C208	C209	-85(2)
O351	C351	C352	C353	-11(2)	C207	C206	C208	C210	-30(3)
C354	C351	C352	C353	101.5(16)	C205	C206	C208	C210	147.9(19)
C303	C351	C352	C353	-139.3(15)	N201	O201	C208	C206	144.0(16)
O351	N351	C353	C355	175(2)	N201	O201	C208	C209	-98.2(15)
O351	N351	C353	C352	1(3)	N201	O201	C208	C210	19.9(14)
C351	C352	C353	N351	6(2)	C206	C208	C209	F206	-176(2)
C351	C352	C353	C355	-168.4(19)	O201	C208	C209	F206	66(2)
O351	C351	C354	F353	-58.9(16)	C210	C208	C209	F206	-47(3)
C303	C351	C354	F353	63.5(15)	C206	C208	C209	F205	59(2)
C352	C351	C354	F353	-174.0(17)	O201	C208	C209	F205	-59(2)
O351	C351	C354	F352	63.4(17)	C210	C208	C209	F205	-171.6(19)

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C303	C351	C354	F352	-174.1(11)	C206	C208	C209	F204	-58(2)
C352	C351	C354	F352	-51.6(19)	O201	C208	C209	F204	-176.1(15)
O351	C351	C354	F351	-178.8(14)	C210	C208	C209	F204	71.2(18)
C303	C351	C354	F351	-56.4(16)	C206	C208	C210	C211	-139.2(17)
C352	C351	C354	F351	66.1(19)	O201	C208	C210	C211	-18.4(13)
N351	C353	C355	C364	175(2)	C209	C208	C210	C211	94.6(16)
C352	C353	C355	C364	-10(3)	O201	N201	C211	C212	179.4(14)
N351	C353	C355	C356	-4(3)	O201	N201	C211	C210	-0.7(17)
C352	C353	C355	C356	171(2)	C208	C210	C211	N201	12.6(16)
C364	C355	C356	C357	178(2)	C208	C210	C211	C212	-167.5(14)
C353	C355	C356	C357	-3(3)	N201	C211	C212	C213	170.3(15)
C364	C355	C356	C361	5(3)	C210	C211	C212	C213	-10(2)
C353	C355	C356	C361	-175.8(19)	N201	C211	C212	C217	-11(2)
C355	C356	C357	C358	-178.7(19)	C210	C211	C212	C217	169.2(14)
C361	C356	C357	C358	-6(3)	C217	C212	C213	C214	-1(2)
C356	C357	C358	C359	0(3)	C211	C212	C213	C214	177.9(14)
C357	C358	C359	C360	4(3)	C212	C213	C214	C215	1(2)
C358	C359	C360	C361	-2(3)	C213	C214	C215	C216	2(2)
C359	C360	C361	C362	-173.4(17)	C213	C214	C215	C222	-175.2(13)
C359	C360	C361	C356	-3(2)	C214	C215	C216	C217	-5(2)
C357	C356	C361	C360	8(3)	C222	C215	C216	C217	172.4(14)
C355	C356	C361	C360	-179.5(17)	C214	C215	C216	C221	176.3(14)
C357	C356	C361	C362	178.5(17)	C222	C215	C216	C221	-7(2)
C355	C356	C361	C362	-9(3)	C215	C216	C217	C218	-178.1(13)
C360	C361	C362	C363	175.1(14)	C221	C216	C217	C218	1(2)
C356	C361	C362	C363	5(2)	C215	C216	C217	C212	4(2)
C360	C361	C362	C365	-5(2)	C221	C216	C217	C212	-176.5(13)
C356	C361	C362	C365	-174.8(16)	C213	C212	C217	C216	-2(2)
C361	C362	C363	C364	2(2)	C211	C212	C217	C216	179.6(15)

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C365	C362	C363	C364	-177.8(15)	C213	C212	C217	C218	-179.0(14)
C362	C363	C364	C355	-6(2)	C211	C212	C217	C218	2(2)
C356	C355	C364	C363	2(3)	C216	C217	C218	C219	0(2)
C353	C355	C364	C363	-177.1(17)	C212	C217	C218	C219	177.5(15)
C366	N352	C365	O352	-5.1(19)	C217	C218	C219	C220	0(2)
C366	N352	C365	C362	177.6(11)	C218	C219	C220	C221	-1(2)
C363	C362	C365	O352	132.9(13)	C219	C220	C221	C216	2(2)
C361	C362	C365	O352	-47(2)	C217	C216	C221	C220	-2(2)
C363	C362	C365	N352	-49.9(18)	C215	C216	C221	C220	177.2(14)
C361	C362	C365	N352	130.3(13)	C223	N202	C222	O202	4(3)
C365	N352	C366	C367	-72.5(13)	C223	N202	C222	C215	178.0(17)
C023	N353	C367	O353	-6.9(18)	C214	C215	C222	O202	129(2)
C023	N353	C367	C366	175.0(12)	C216	C215	C222	O202	-48(3)
N352	C366	C367	O353	-25.2(15)	C214	C215	C222	N202	-45(2)
N352	C366	C367	N353	152.9(10)	C216	C215	C222	N202	138.1(17)
C323	N303	C368	C369	116(2)	C222	N202	C223	C224	-92(2)
N303	C368	C369	F354	-58(3)	N202	C223	C224	O203	-15(3)
N303	C368	C369	F355	178(2)	N202	C223	C224	N203	162.8(16)
N303	C368	C369	F356	65(2)	C225	N203	C224	C223	-163.6(19)
C108	O101	N101	C111	-6.3(14)	C225	N203	C224	O203	14(3)
F102	C101	C102	C103	-106(2)	C224	N203	C225	C226	93.8(19)
F101	C101	C102	C103	47(2)	N203	C225	C226	F209	51.8(17)
F103	C101	C102	C103	148.9(18)	N203	C225	C226	F207	-74.1(15)
F102	C101	C102	C107	71(3)	N203	C225	C226	F208	171.9(11)

Table S10. Hydrogen Atom Coordinates ( $\text{\AA}\times 10^4$ ) and Isotropic Displacement Parameters ( $\text{\AA}^2\times 10^3$ ).

Atom	x	y	z	U(eq)
H30A	3840	2466	8108	65

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H303	7401	2888	6453	109
H352	4312	2339	7850	57
H353	7958	2848	6416	61
H02A	10350	2849	6593	84
H02B	10215	2662	7451	84
H302	-597	215	10757	81
H304	2044	999	11780	94
H306	-1509	577	12991	90
H30B	1433	1145	10315	68
H30C	3277	1076	10413	68
H315	4711	2051	9046	74
H316	3564	1559	9777	77
H317	1763	723	7625	78
H318	1515	776	6307	90
H319	2419	1232	5611	80
H320	3651	1699	6363	78
H32A	4607	2980	7618	78
H32B	4909	2772	6801	78
H35A	2222	1187	10453	71
H35B	3785	955	10298	71
H357	1233	724	7771	46
H358	1005	695	6330	48
H359	2198	1119	5548	56
H360	3887	1548	6168	54
H363	5075	1912	8846	63
H364	3952	1475	9613	61
H36A	5177	2821	7254	53
H36B	5652	2570	6528	53
H36C	9757	3058	7701	146

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H36D	9590	3277	6851	146
H102	4049	2497	4156	81
H103	7700	1868	5649	97
H10A	-1521	4522	-713	68
H105	-773	4821	1690	57
H107	2214	4145	659	69
H11A	2306	3908	1921	56
H11B	3863	4127	2237	56
H113	3826	3504	2564	59
H114	5314	3049	3193	66
H118	1881	4146	4702	57
H119	1722	4063	6058	56
H120	3073	3568	6706	61
H121	4403	3172	5946	69
H12A	5027	1976	4586	92
H12B	5568	2180	5405	92
H12C	10193	1686	5419	117
H12D	10110	1928	4628	117
H202	4558	2622	4032	87
H20A	8473	1902	5106	113
H203	-2100	4622	-646	63
H205	-1044	4899	1667	65
H207	1773	4190	588	59
H21A	1664	3949	1861	51
H21B	3321	4142	2118	51
H213	3430	3589	2635	57
H214	4832	3128	3309	63
H218	1269	4235	4664	65
H219	1179	4179	6055	69

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H220	2486	3706	6680	69
H221	3771	3291	6047	71
H22A	6344	2355	5325	85
H22B	5480	2121	4619	85
H22C	10773	1760	4667	124
H22D	10663	2096	4067	124

Table S11. Atomic Occupancy.

Atom	Occupancy	Atom	Occupancy	Atom	Occupancy
F304	0.45	F305	0.45	F306	0.45
F307	0.55	F308	0.55	F309	0.55
F351	0.55	F352	0.55	F353	0.55
F354	0.45	F355	0.45	F356	0.45
O301	0.45	O302	0.45	O303	0.45
O351	0.55	O352	0.55	O353	0.55
N301	0.45	N302	0.45	H30A	0.45
N303	0.45	H303	0.45	N351	0.55
N352	0.55	H352	0.55	N353	0.55
H353	0.55	C023	0.55	H02A	0.55
H02B	0.55	C308	0.45	C309	0.45
H30B	0.45	H30C	0.45	C310	0.45
C311	0.45	C312	0.45	C313	0.45
C314	0.45	C315	0.45	H315	0.45
C316	0.45	H316	0.45	C317	0.45
H317	0.45	C318	0.45	H318	0.45
C319	0.45	H319	0.45	C320	0.45
H320	0.45	C321	0.45	C322	0.45
H32A	0.45	H32B	0.45	C323	0.45
C325	0.55	C326	0.45	C351	0.55

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C352	0.55	H35A	0.55	H35B	0.55
C353	0.55	C354	0.55	C355	0.55
C356	0.55	C357	0.55	H357	0.55
C358	0.55	H358	0.55	C359	0.55
H359	0.55	C360	0.55	H360	0.55
C361	0.55	C362	0.55	C363	0.55
H363	0.55	C364	0.55	H364	0.55
C365	0.55	C366	0.55	H36A	0.55
H36B	0.55	C367	0.55	C368	0.45
H36C	0.45	H36D	0.45	C369	0.45
C110	0.55	F101	0.55	F102	0.55
F103	0.55	F104	0.55	F105	0.55
F106	0.55	F107	0.55	F108	0.55
F109	0.55	O101	0.55	O102	0.55
O103	0.55	N101	0.55	N102	0.55
H102	0.55	N103	0.55	H103	0.55
C101	0.55	C102	0.55	C103	0.55
H10A	0.55	C104	0.55	C105	0.55
H105	0.55	C106	0.55	C107	0.55
H107	0.55	C108	0.55	C109	0.55
C110	0.55	H11A	0.55	H11B	0.55
C111	0.55	C112	0.55	C113	0.55
H113	0.55	C114	0.55	H114	0.55
C115	0.55	C116	0.55	C117	0.55
C118	0.55	H118	0.55	C119	0.55
H119	0.55	C120	0.55	H120	0.55
C121	0.55	H121	0.55	C122	0.55
C123	0.55	H12A	0.55	H12B	0.55
C124	0.55	C125	0.55	H12C	0.55

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H12D	0.55	C126	0.55	C120	0.45
F201	0.45	F202	0.45	F203	0.45
F204	0.45	F205	0.45	F206	0.45
F207	0.45	F208	0.45	F209	0.45
O201	0.45	O202	0.45	O203	0.45
N201	0.45	N202	0.45	H202	0.45
N203	0.45	H20A	0.45	C201	0.45
C202	0.45	C203	0.45	H203	0.45
C204	0.45	C205	0.45	H205	0.45
C206	0.45	C207	0.45	H207	0.45
C208	0.45	C209	0.45	C210	0.45
H21A	0.45	H21B	0.45	C211	0.45
C212	0.45	C213	0.45	H213	0.45
C214	0.45	H214	0.45	C215	0.45
C216	0.45	C217	0.45	C218	0.45
H218	0.45	C219	0.45	H219	0.45
C220	0.45	H220	0.45	C221	0.45
H221	0.45	C222	0.45	C223	0.45
H22A	0.45	H22B	0.45	C224	0.45
C225	0.45	H22C	0.45	H22D	0.45
C226	0.45	O1	0.45	O2	0.55

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