Supporting Information (X-ray data)

X-ray Crystallography: Crystals of **4f** were removed from the mother liquor and transferred to a glass slide covered in Paraton™ oil where it was evaluated and mounted with the assistance of an optical microscope. X-ray reflection intensity data were collected on a Bruker D8 Quest with a Photon II CPAD detector employing graphite-monochromated Mo-Kα radiation (λ = 0.71073 Å) at a temperature of 173(1) K. Rotation frames were integrated using SAINT,[1] producing a listing of unaveraged F^2 and $\sigma(F^2)$ values which were then passed to the SHELXT[2] program package for further processing and structure solution. The intensity data were corrected for Lorentz and polarization effects and for absorption using SADABS.[3] The structures were solved by direct methods (SHELXT).[2] Refinement was by full-matrix least squares based on F^2 using SHELXL.[4] All reflections were used during refinements. Non-hydrogen atoms were refined anisotropically and hydrogen atoms were refined using a riding model.

Table S1. Crystal data and structure refinement for **4f.**

Identification code	MX20220725_0m
Empirical formula	$C_{32}H_{22}N_6O_4$
Formula weight	554.55
Temperature/K	173.0
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	11.0961(4)
b/Å	9.9627(3)
c/Å	22.3275(6)
α/°	90
β/°	94.4300(10)
γ/°	90
Volume/Å^3	2460.87(13)
Z	4
ρ_{calc}g/cm^3	1.497
μ/mm^{-1}	0.102
F(000)	1152.0
Crystal size/mm^3	0.16 × 0.16 × 0.06
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.48 to 55.104
Index ranges	$-14 \le h \le 14$, $-12 \le k \le 12$, $-29 \le l \le 28$
Reflections collected	62503
Independent reflections	5678 [R_{int} = 0.0327, R_{sigma} = 0.0150]
Data/restraints/parameters	5678/0/379
Goodness-of-fit on F^2	1.031
Final R indexes [I>=2σ (I)]	R_1 = 0.0387, wR_2 = 0.0984
Final R indexes [all data]	R_1 = 0.0446, wR_2 = 0.1027
Largest diff. peak/hole / e Å^{-3}	0.39/-0.43
CCDC Deposit #	2193153

Table S2. Bond distances for **4f.**

Atom	Atom	Length (Å)	Atom	Atom	Length (Å)
O1	C1	1.2192(15)	O3	C17	1.2160(15)
O2	C1	1.3764(14)	O4	C17	1.3833(15)
O2	C9	1.3713(14)	O4	C25	1.3733(14)
N1	N2	1.3828(14)	N4	N5	1.3750(14)
N1	C3	1.3647(16)	N4	C19	1.3614(15)
N2	C11	1.2868(16)	N5	C27	1.2873(16)
N3	C12	1.3437(16)	N6	C28	1.3381(16)
N3	C16	1.3438(16)	N6	C32	1.3358(16)
C1	C2	1.4295(17)	C17	C18	1.4304(16)
C2	C3	1.3643(16)	C18	C19	1.3656(16)
C2	C10	1.4983(16)	C18	C26	1.5003(16)
C3	C4	1.4534(16)	C19	C20	1.4528(16)
C4	C5	1.4061(17)	C20	C21	1.4054(17)
C4	C9	1.3970(17)	C20	C25	1.3950(16)
C5	C6	1.3832(18)	C21	C22	1.3818(17)
C6	C7	1.393(2)	C22	C23	1.3925(18)
C7	C8	1.3840(19)	C23	C24	1.3813(18)
C8	C9	1.3908(17)	C24	C25	1.3880(17)
C10	C11	1.5070(16)	C26	C27	1.5098(16)
C11	C12	1.4840(16)	C27	C28	1.4785(16)
C12	C13	1.3982(17)	C28	C29	1.3962(17)
C13	C14	1.3848(18)	C29	C30	1.3824(18)
C14	C15	1.388(2)	C30	C31	1.3821(19)
C15	C16	1.3825(19)	C31	C32	1.3814(19)

Table S3. Bond angles for **4f.**

Atom	Atom	Atom	Angle (°)	Atom	Atom	Atom	Angle (°)
C9	O2	C1	121.19(9)	C25	O4	C17	121.27(9)
C3	N1	N2	122.57(10)	C19	N4	N5	123.64(10)
C11	N2	N1	118.03(10)	C27	N5	N4	118.26(10)
C16	N3	C12	117.69(11)	C32	N6	C28	117.15(11)
O1	C1	O2	116.31(11)	O3	C17	O4	116.29(11)
O1	C1	C2	125.28(11)	O3	C17	C18	125.61(11)
O2	C1	C2	118.41(10)	O4	C17	C18	118.10(10)
C1	C2	C10	118.13(10)	C17	C18	C26	117.52(10)
C3	C2	C1	121.23(11)	C19	C18	C17	121.25(11)
C3	C2	C10	120.63(11)	C19	C18	C26	121.19(10)
N1	C3	C4	120.09(10)	N4	C19	C18	120.38(11)
C2	C3	N1	120.00(11)	N4	C19	C20	119.57(10)
C2	C3	C4	119.90(11)	C18	C19	C20	120.05(10)
C5	C4	C3	124.82(11)	C21	C20	C19	124.81(11)
C9	C4	C3	116.97(11)	C25	C20	C19	117.06(11)
C9	C4	C5	118.20(11)	C25	C20	C21	118.10(11)

Atom	Atom	Atom	Angle (°)	Atom	Atom	Atom	Angle (°)
C6	C5	C4	120.48(12)	C22	C21	C20	120.53(11)
C5	C6	C7	119.98(12)	C21	C22	C23	120.04(12)
C8	C7	C6	120.77(12)	C24	C23	C22	120.53(11)
C7	C8	C9	118.87(12)	C23	C24	C25	119.14(11)
O2	C9	C4	122.29(11)	O4	C25	C20	122.19(11)
O2	C9	C8	116.03(11)	O4	C25	C24	116.16(10)
C8	C9	C4	121.68(11)	C24	C25	C20	121.65(11)
C2	C10	C11	110.05(10)	C18	C26	C27	110.13(10)
N2	C11	C10	125.52(11)	N5	C27	C26	126.36(11)
N2	C11	C12	116.74(11)	N5	C27	C28	116.23(10)
C12	C11	C10	117.65(10)	C28	C27	C26	117.41(10)
N3	C12	C11	114.85(10)	N6	C28	C27	115.21(10)
N3	C12	C13	122.55(11)	N6	C28	C29	122.63(11)
C13	C12	C11	122.50(11)	C29	C28	C27	122.15(11)
C14	C13	C12	118.49(12)	C30	C29	C28	118.93(12)
C13	C14	C15	119.35(12)	C31	C30	C29	118.82(12)
C16	C15	C14	118.24(12)	C32	C31	C30	118.17(12)
N3	C16	C15	123.55(12)	N6	C32	C31	124.24(13)

Table S4. Torsion angles for **4f.**

A	B	C	D	Angle (°)	A	B	C	D	Angle (°)
O1	C1	C2	C3	178.74(12)	O3	C17	C18	C19	178.90(12)
O1	C1	C2	C10	-0.77(19)	O3	C17	C18	C26	1.10(19)
O2	C1	C2	C3	-0.09(17)	O4	C17	C18	C19	-0.21(18)
O2	C1	C2	C10	-179.60(10)	O4	C17	C18	C26	-178.01(10)
N1	N2	C11	C10	1.50(18)	N4	N5	C27	C26	0.45(18)
N1	N2	C11	C12	-174.89(10)	N4	N5	C27	C28	-179.17(10)
N1	C3	C4	C5	-1.41(18)	N4	C19	C20	C21	-2.38(18)
N1	C3	C4	C9	179.54(11)	N4	C19	C20	C25	179.57(11)
N2	N1	C3	C2	-15.09(17)	N5	N4	C19	C18	-0.86(18)
N2	N1	C3	C4	164.65(11)	N5	N4	C19	C20	178.82(11)
N2	C11	C12	N3	-177.74(11)	N5	C27	C28	N6	-171.36(11)
N2	C11	C12	C13	5.81(17)	N5	C27	C28	C29	9.86(17)
N3	C12	C13	C14	-3.97(18)	N6	C28	C29	C30	-2.49(19)
C1	O2	C9	C4	0.08(17)	C17	O4	C25	C20	3.53(17)
C1	O2	C9	C8	-179.25(11)	C17	O4	C25	C24	-176.07(11)
C1	C2	C3	N1	-179.69(11)	C17	C18	C19	N4	-178.56(11)
C1	C2	C3	C4	0.58(18)	C17	C18	C19	C20	1.77(17)
C1	C2	C10	C11	-167.24(10)	C17	C18	C26	C27	179.79(10)
C2	C3	C4	C5	178.33(11)	C18	C19	C20	C21	177.30(11)
C2	C3	C4	C9	-0.72(17)	C18	C19	C20	C25	-0.76(17)
C2	C10	C11	N2	-14.41(17)	C18	C26	C27	N5	-1.87(17)
C2	C10	C11	C12	161.95(10)	C18	C26	C27	C28	177.75(10)

A	B	C	D	Angle (°)	A	B	C	D	Angle (°)
C3	N1	N2	C11	14.46(17)	C19	N4	N5	C27	1.07(18)
C3	C2	C10	C11	13.25(16)	C19	C18	C26	C27	1.98(15)
C3	C4	C5	C6	-178.39(12)	C19	C20	C21	C22	-177.95(11)
C3	C4	C9	O2	0.40(17)	C19	C20	C25	O4	-1.87(17)
C3	C4	C9	C8	179.70(11)	C19	C20	C25	C24	177.71(11)
C4	C5	C6	C7	-1.3(2)	C20	C21	C22	C23	0.64(19)
C5	C4	C9	O2	-178.71(11)	C21	C20	C25	O4	179.94(11)
C5	C4	C9	C8	0.58(18)	C21	C20	C25	C24	-0.48(18)
C5	C6	C7	C8	0.7(2)	C21	C22	C23	C24	-1.00(19)
C6	C7	C8	C9	0.5(2)	C22	C23	C24	C25	0.61(19)
C7	C8	C9	O2	178.16(11)	C23	C24	C25	O4	179.74(11)
C7	C8	C9	C4	-1.17(19)	C23	C24	C25	C20	0.14(18)
C9	O2	C1	O1	-179.18(11)	C25	O4	C17	O3	178.38(11)
C9	O2	C1	C2	-0.25(17)	C25	O4	C17	C18	-2.43(17)
C9	C4	C5	C6	0.65(18)	C25	C20	C21	C22	0.09(18)
C10	C2	C3	N1	-0.19(17)	C26	C18	C19	N4	-0.84(17)
C10	C2	C3	C4	-179.93(10)	C26	C18	C19	C20	179.49(10)
C10	C11	C12	N3	5.57(15)	C26	C27	C28	N6	8.98(16)
C10	C11	C12	C13	-170.88(11)	C26	C27	C28	C29	-169.79(11)
C11	C12	C13	C14	172.21(11)	C27	C28	C29	C30	176.19(11)
C12	N3	C16	C15	0.58(19)	C28	N6	C32	C31	1.5(2)
C12	C13	C14	C15	1.64(18)	C28	C29	C30	C31	1.44(19)
C13	C14	C15	C16	1.51(18)	C29	C30	C31	C32	0.9(2)
C14	C15	C16	N3	-2.75(19)	C30	C31	C32	N6	-2.5(2)
C16	N3	C12	C11	-173.60(11)	C32	N6	C28	C27	-177.73(11)
C16	N3	C12	C13	2.84(18)	C32	N6	C28	C29	1.04(19)

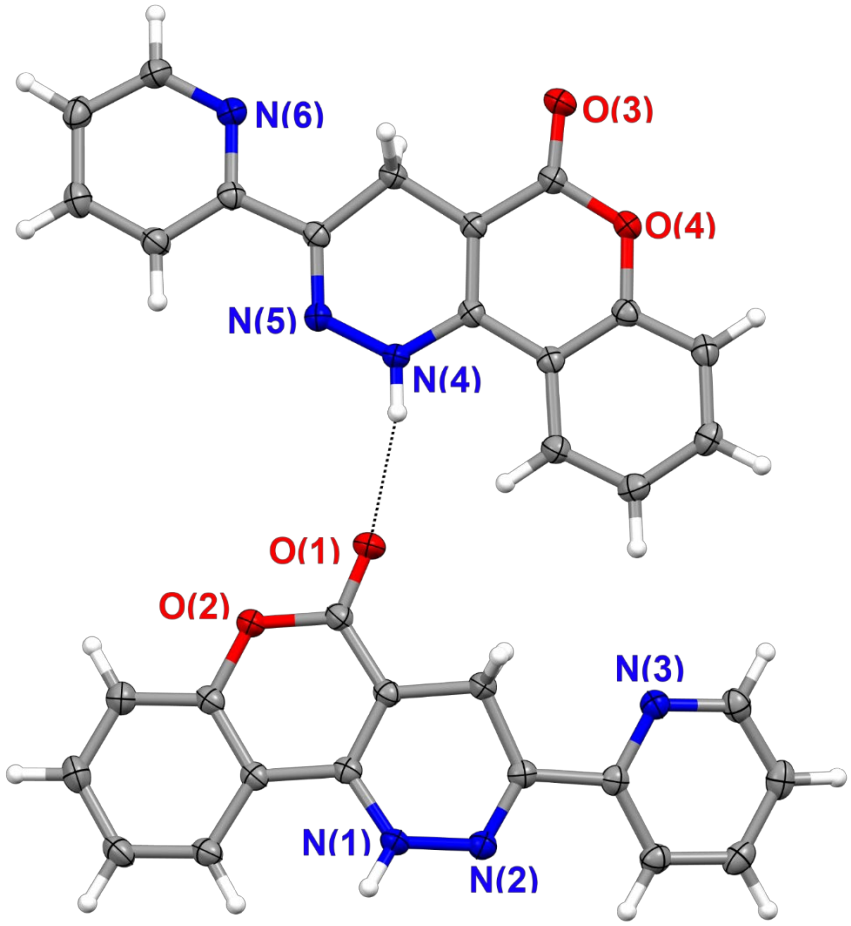

Figure S1. Thermal ellipsoid plot (50% probability) of **4f**. N(1) –H···O(4): 2.257(1) Å N(4) –H···O(1): 2.124(1) Å. N(2)–C(11)–C(12)–N(3): 177.8°. N(5)–C(27)–C(28)–N(6): 171.4°.

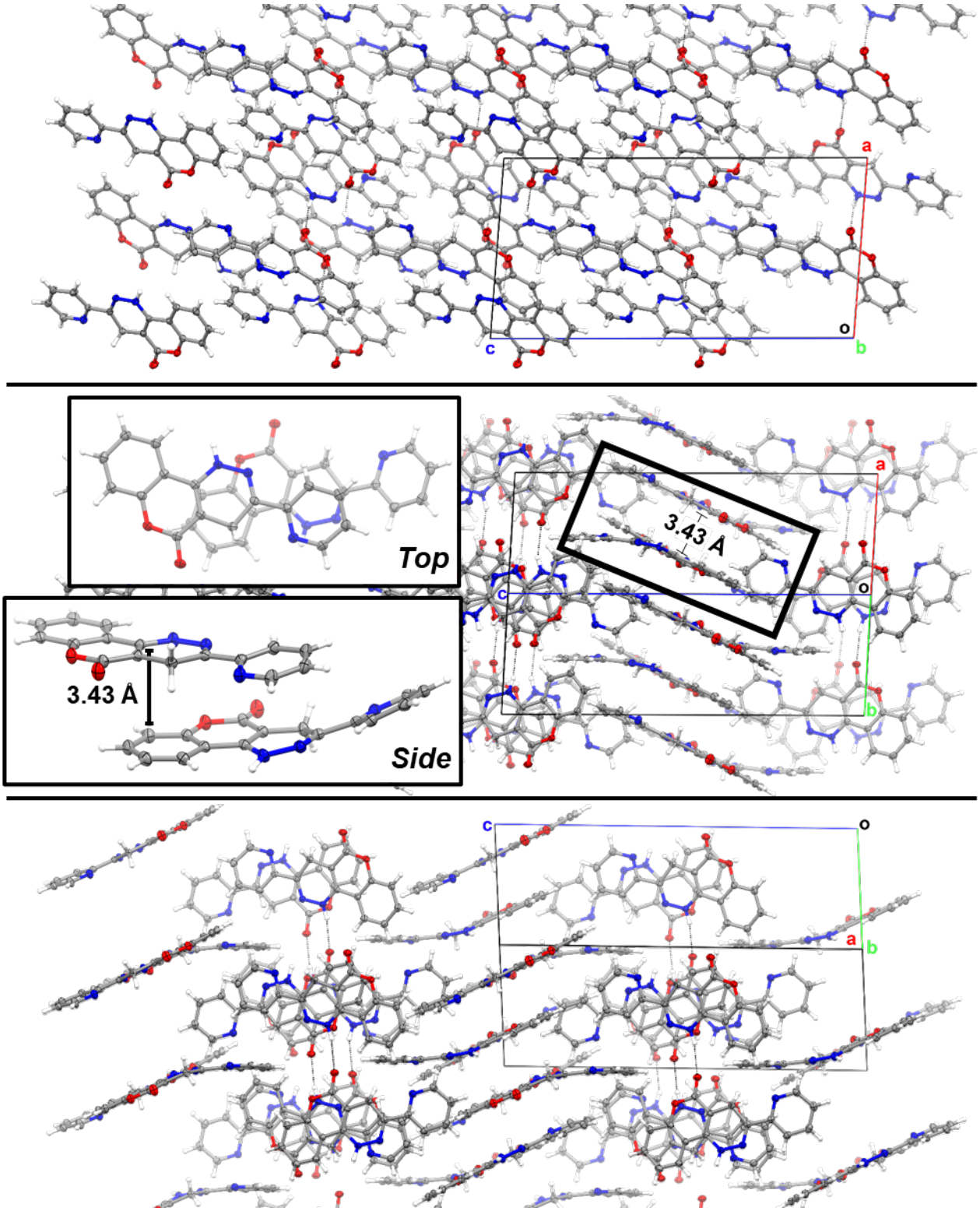

Figure S2. Thermal ellipsoid plot (50% probability) of **4f** with a 3 x 3 packing highlighting the orthogonal H-bonding (N(1) –H···O(4) and N(4) –H···O(1)) and pi-stacking layers (~3.43 Å) with varied rotations about the *c* axis (*Top*, *Mid*, *Bottom*).

References

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2. Sheldrick, G. SHELXT - Integrated space-group and crystal-structure determination. *Acta Crystallogr., Sect. A: Found. Adv.* **2015**, *71*(1), 3−8.
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