

CrystEngComm

Supporting Information

Crystallographic studies towards solid state behavior of *syn*- and *anti*- conformers of terphenyl based perfluorinated halogen bond donors.

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A.) General Information

A.1.) Experimental setup for crystal growth

Single crystals of all the halogen bond donors were obtained by dissolving 5 mg of each one in pentane and letting the solvent slowly evaporate.

Co-crystallization experiments were set up as follows:

A 34,4 mM stock solution of the designated halogen bond donors and halide salts were set up in DCM. After that 0.1 mL of the Host and 0.1 mL of the guest solutions were transferred into a GC-vial and the solvent was slowly evaporated leading to crystal formation.

A.2.) Crystal structure determination

Crystal structure determination was carried out on a *Rigaku* XtaLAB mini, equipped with a 600 W Mo micro-fine focus glass sealed tube, graphite monochromator (Mo K_{α}) and Mercury375R CCD detector or a *Rigaku* Synergy dual source device, with Cu and Mo micro focus sealed tubes (Cu & Mo K_{α}) using mirror monochromators and a HyPix-6000HE: Hybrid photon counting X-ray detector, Rigaku Supernova with a Cu micro focus sealed tubes, mirror monochromator and an Atlas detector, and an Agilent XCalibur with a Mo fine focus glass sealed tube, graphite monochromator, and Sapphire2 detector. Crystals were mounted in *Hampton* CryoLoops using *GE/Bayer* silicone grease or were glued on the tip of glass fibers. (Caveat: Our perfluorinated compounds have a tendency to dissolve in common cryoprotectants such as Parabar/Paratone). Data on all systems was recorded and reduced using the CrysAlisPro¹ Software. Structures were solved using WinGX² in combination with ShelXT³ and refined with shelXle⁴ and ShelXL. Tables for the publication were generated using a modified version of CifTab. Pictures of the structures were generated with Diamond 4⁵.

A.3) Crystal Data

All ellipsoids are depicted at 50% probability. The TDA and TEA cations are generally shown only as sticks. Fluorine and hydrogen substituents are left out for clarity, if necessary. All atoms involved in non-covalent interactions are labelled and connected via dashed bonds.

Atoms colours:

Atom	Colour	RGB
H	White	0/0/0
C	Black	255/255/255
N	Dark blue	0/53/96
F	Light green	153/204/0
Cl	Dark green	0/139/41
Br	Orange	218/87/0
I	Purple	128/0/128

A.2.1.) Crystal structures mentioned in the article

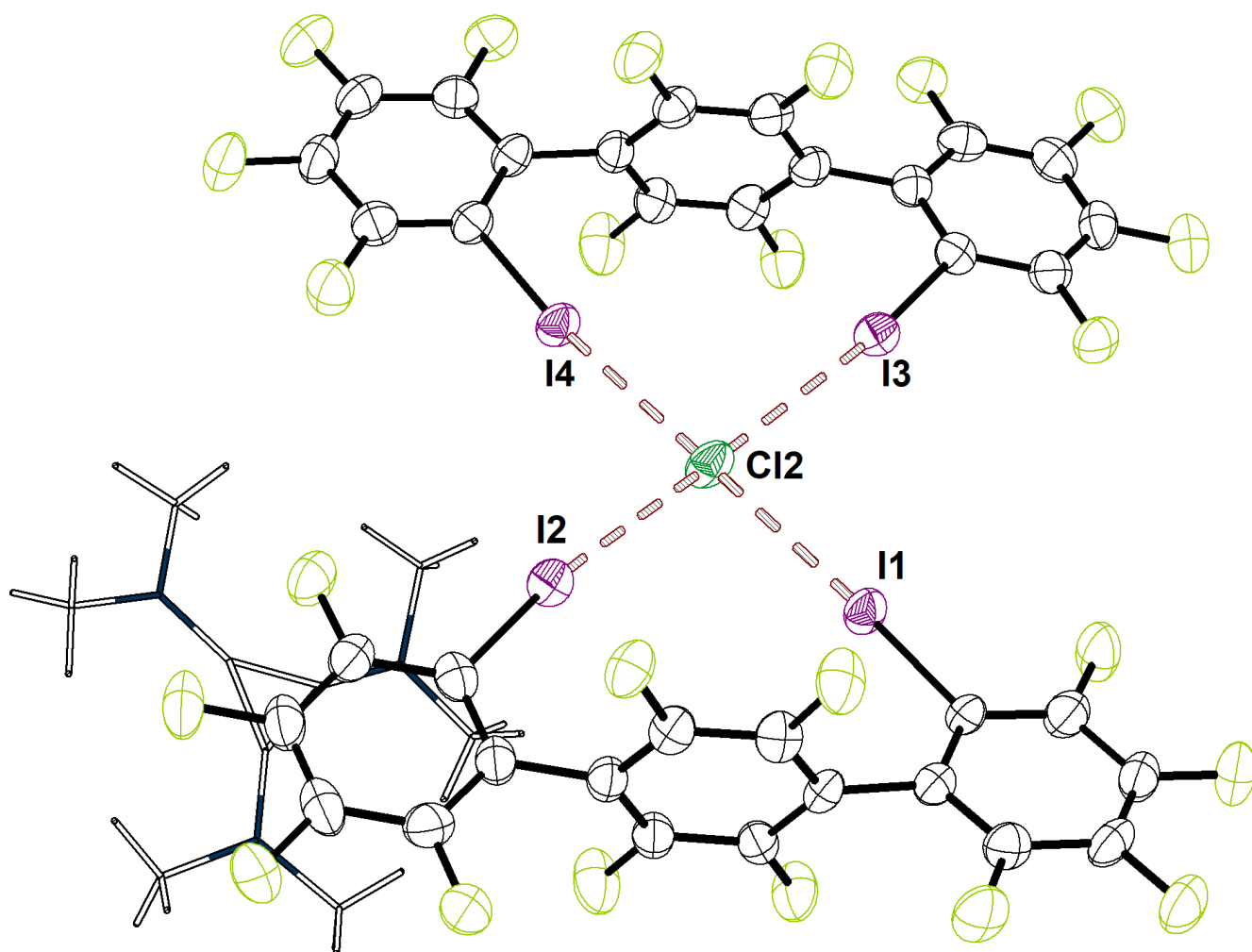


Figure S1: Cocystal structure of *syn-p-1* and TDA-Cl.

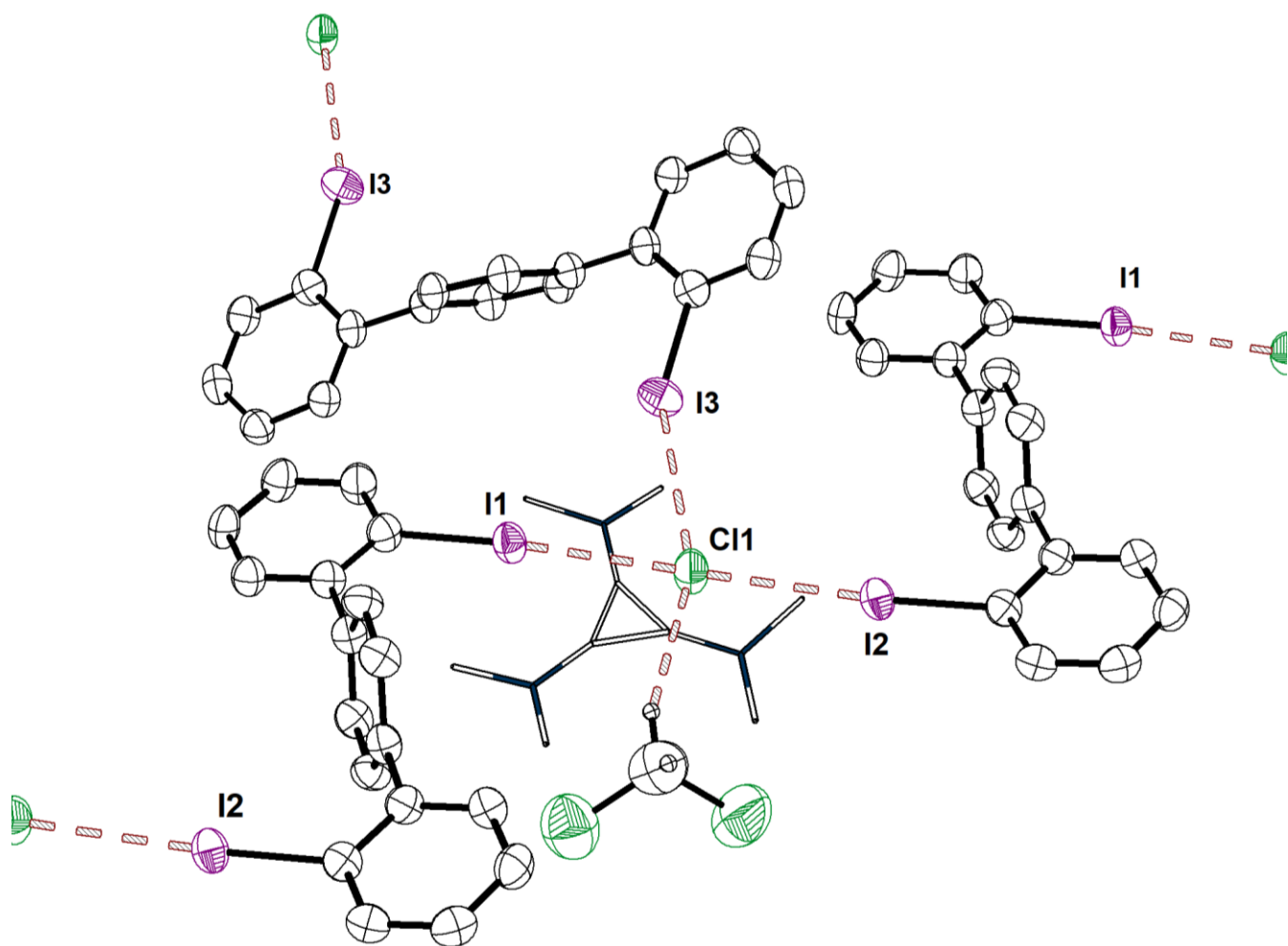


Figure S2: Cocrystal structure of *anti-p-1* and TDA-Cl.

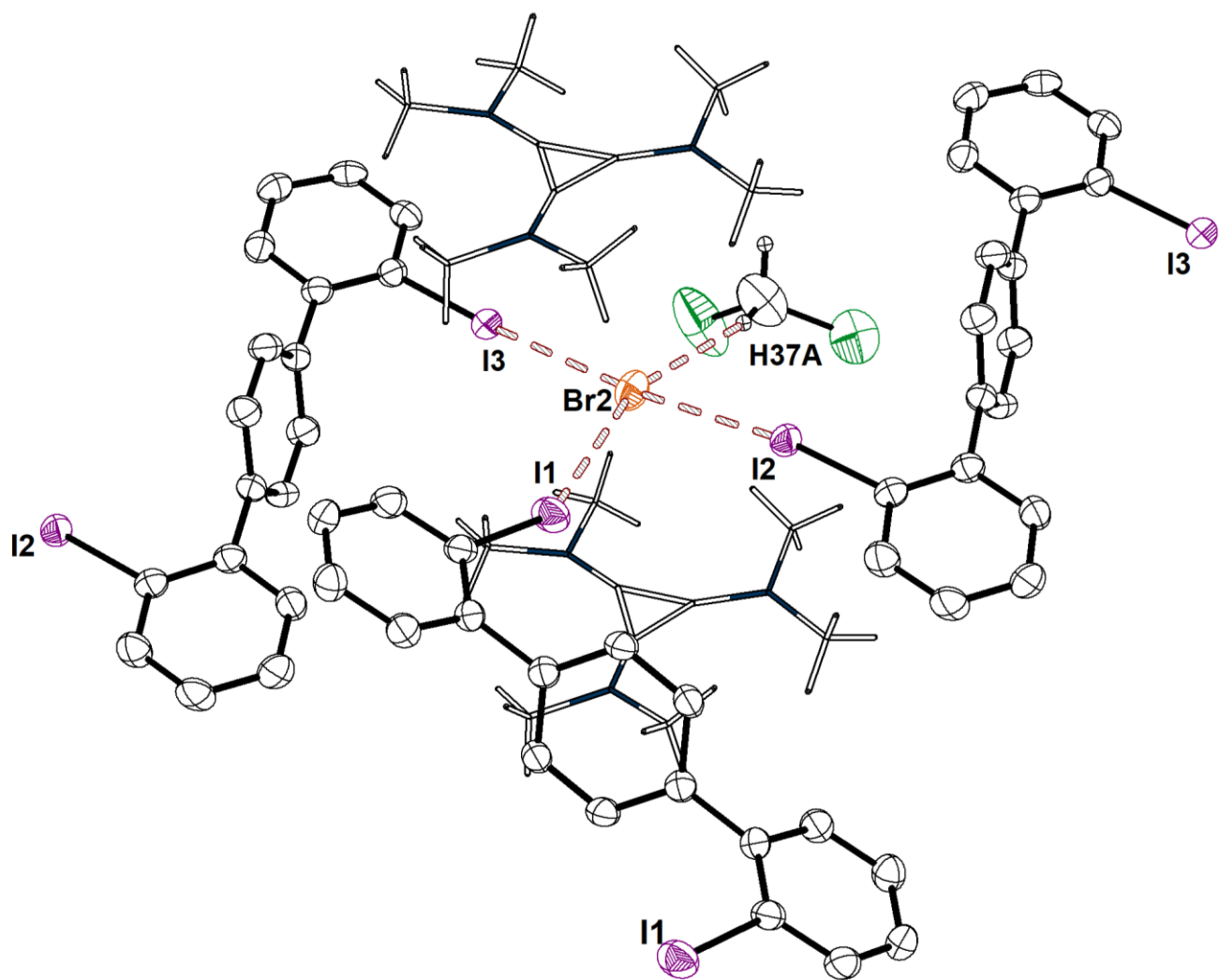


Figure S3: Cocrystal structure of *anti-p-1* and TDA-Br.

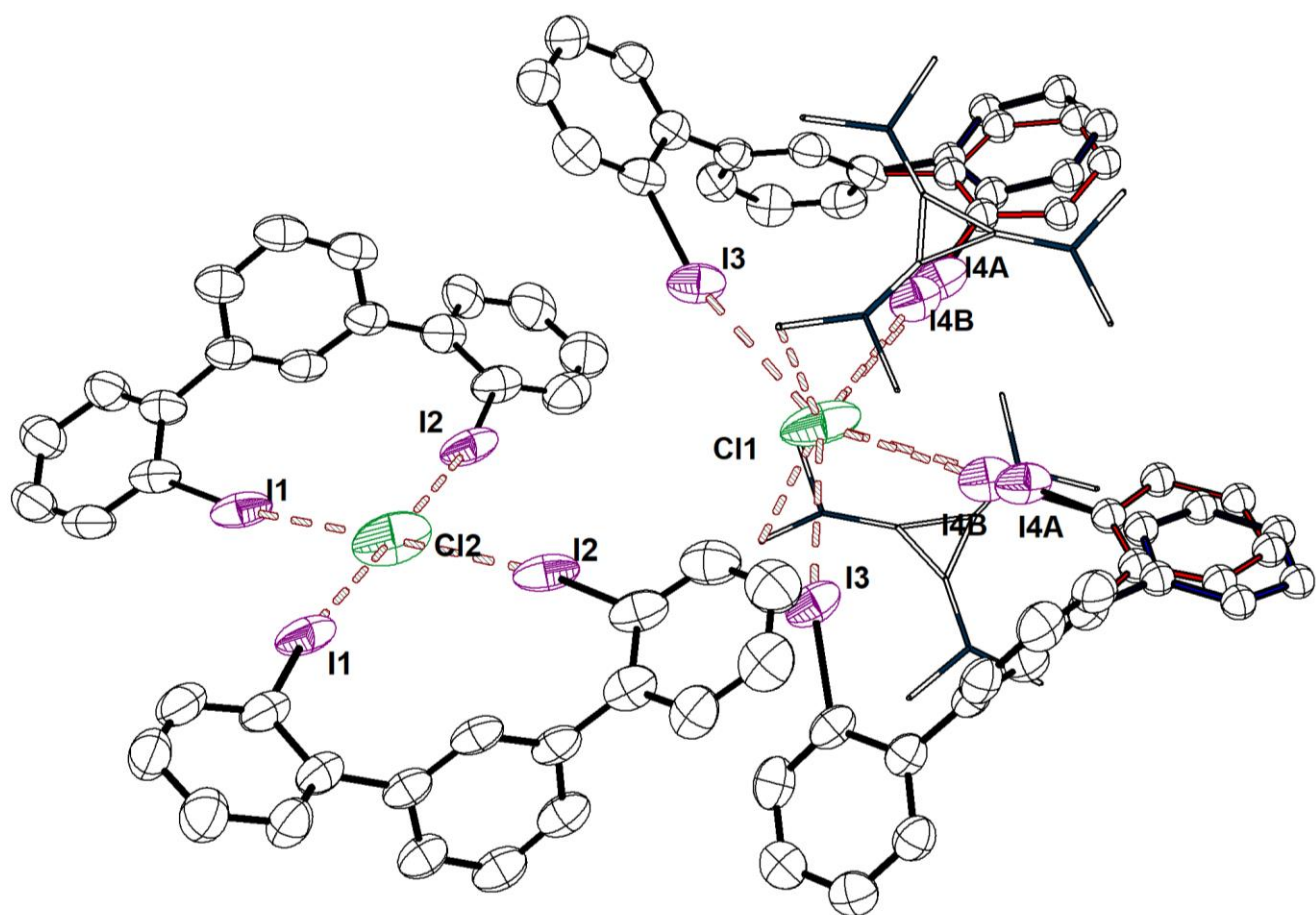


Figure S4: Cocrystal structure of *syn-m-1* and TDA-Cl. The disordered atoms on the right-hand side of the picture are shown as balls and sticks with red and blue bonds connecting the separate parts. Both chlorides are located on one of the twofold axes of the crystal. Attempts of solving the disorders of the chlorides resulted in non-positive defined ellipsoids and/or unstable refinements.

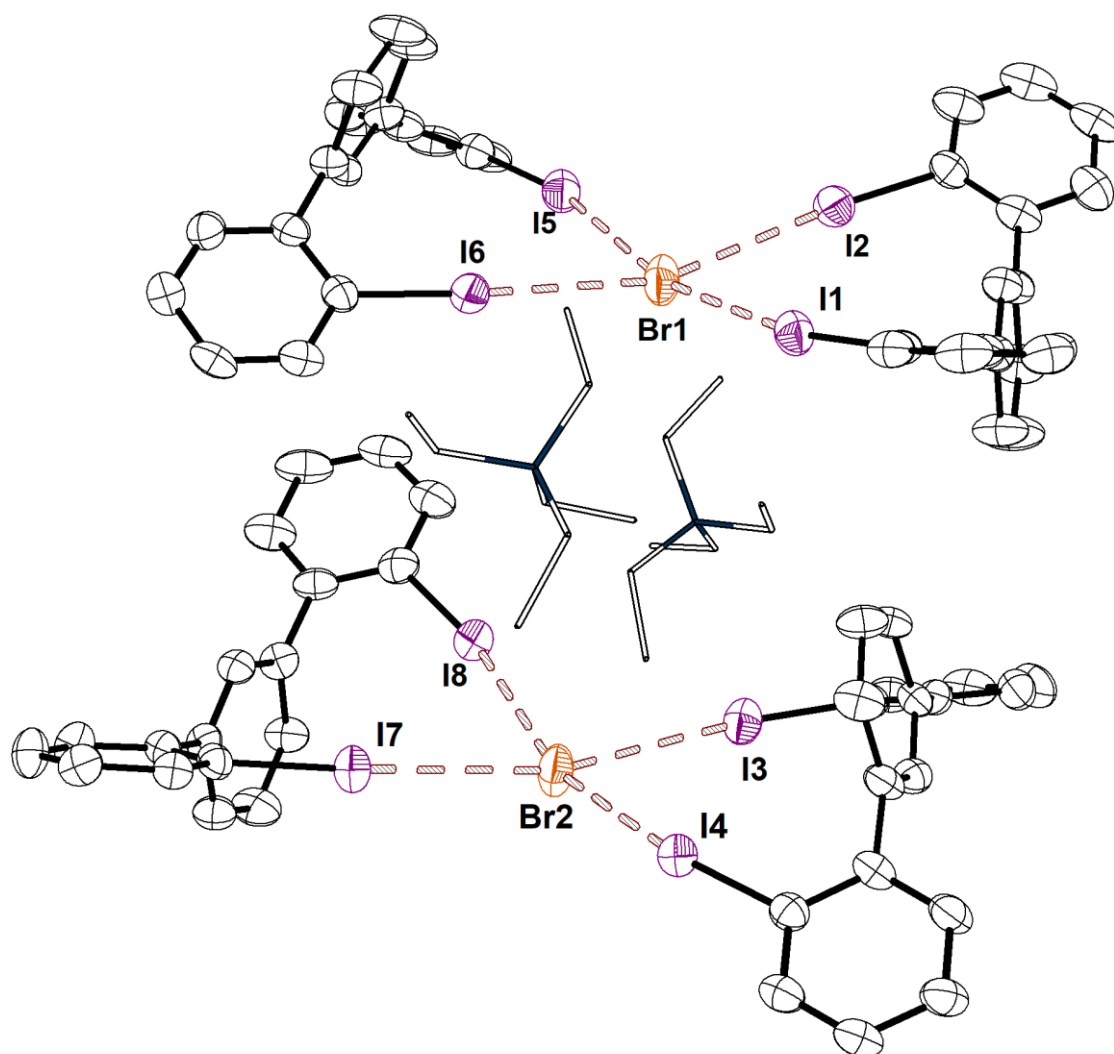


Figure S5: Cocrystal structure of *syn-m-1* and TEA-Br.

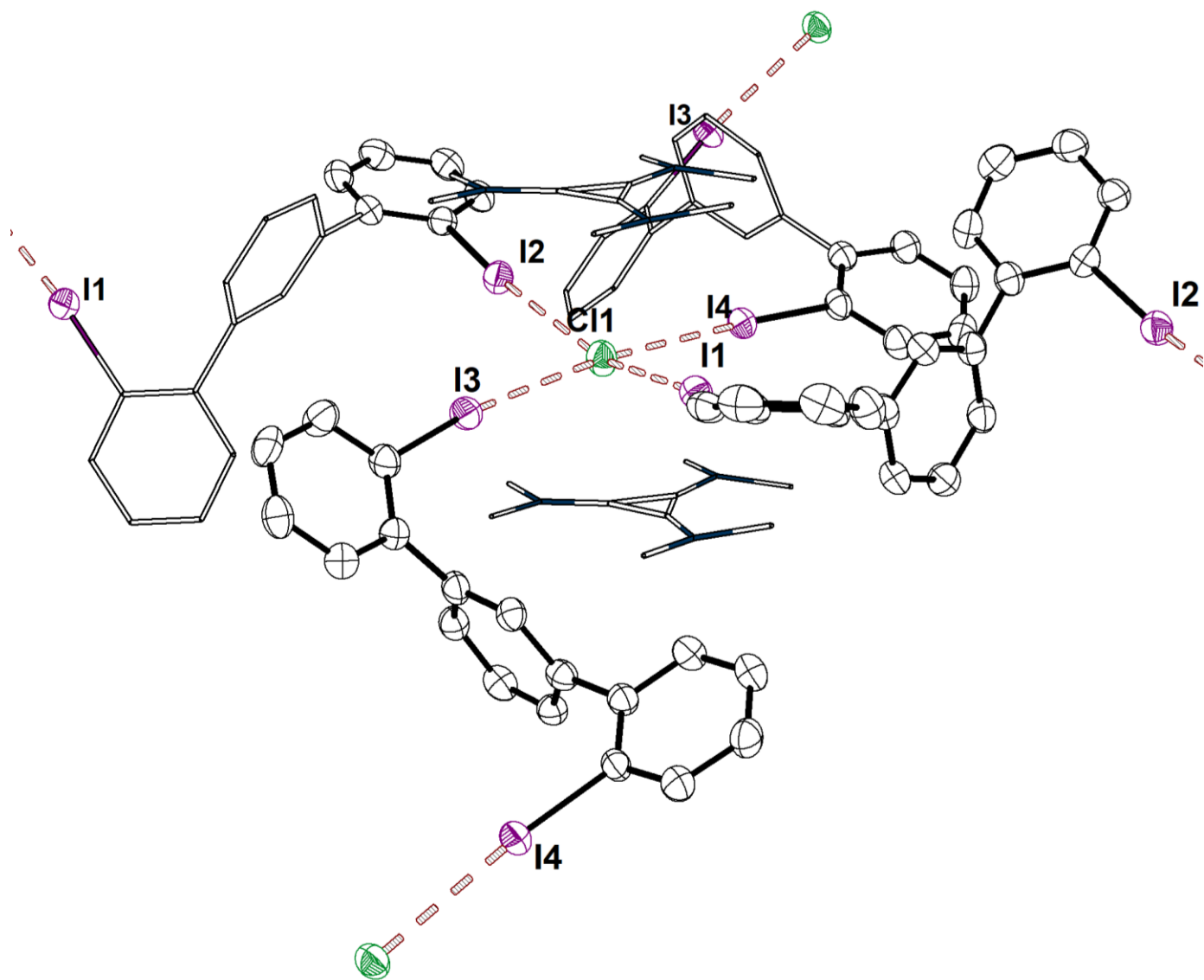


Figure S6: Cocrystal structure of *anti-m-1* and TDA-Cl.

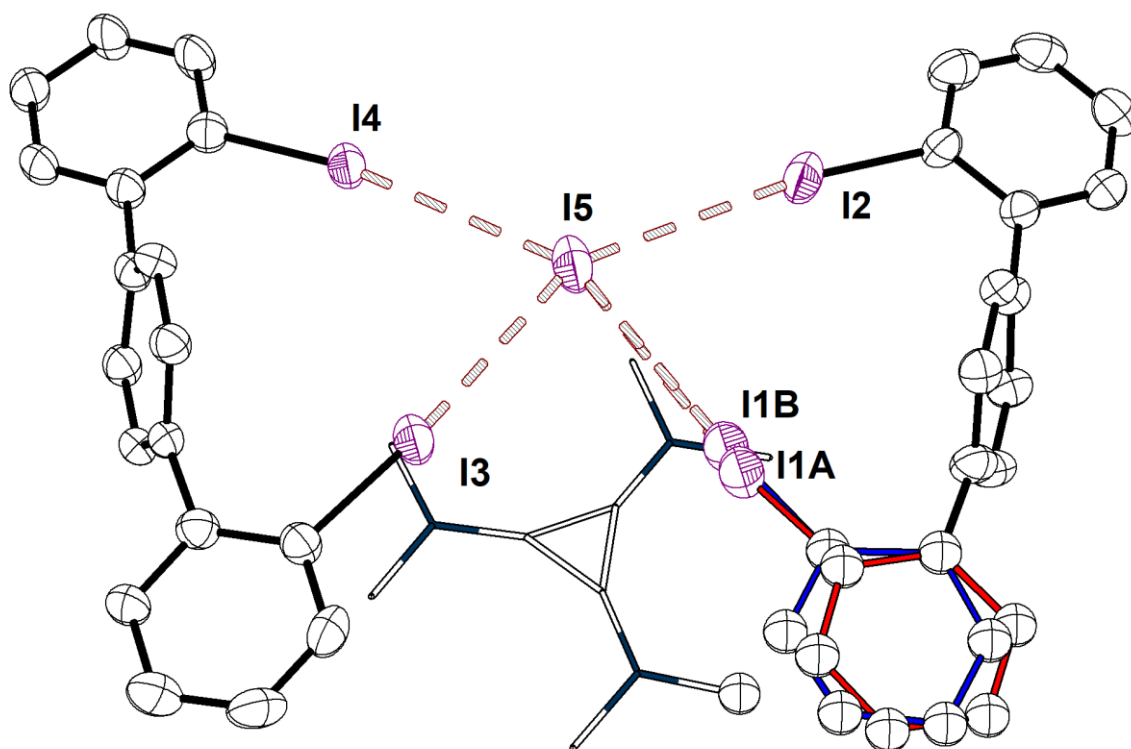


Figure S7: Cocrystal structure of **syn-p-1** and TDA-I. The disordered atoms are shown as balls and sticks, with bonds in red and blue, separating the two parts.

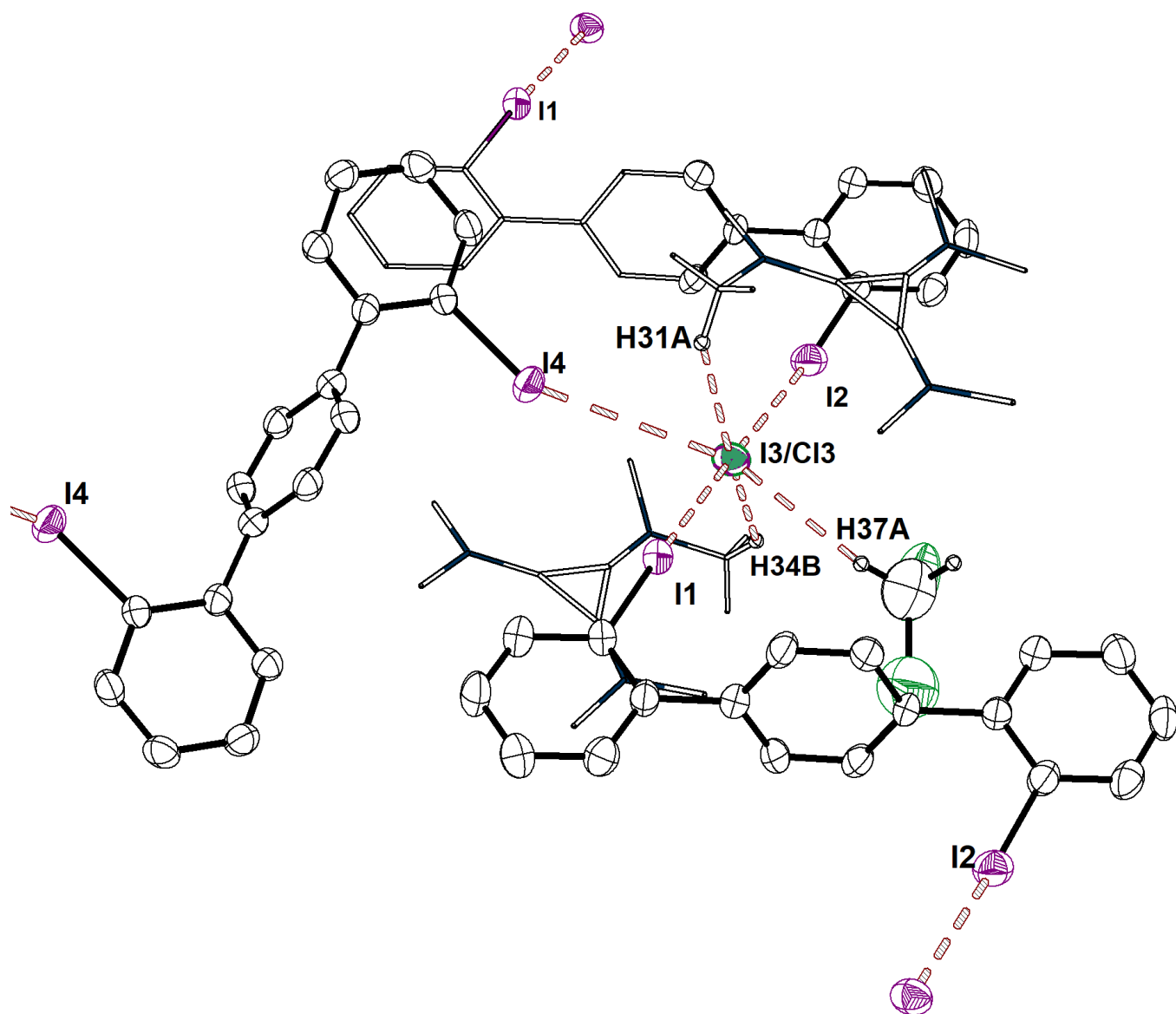


Figure S8: Cocrystal structure of *anti-p-1* and TDA-I. Iodide is replaced by chloride in about 40%. A solution with only iodide has a much larger R_{int} . We speculate that HCl contained in methylene chloride is the cause of the enrichment with chloride.

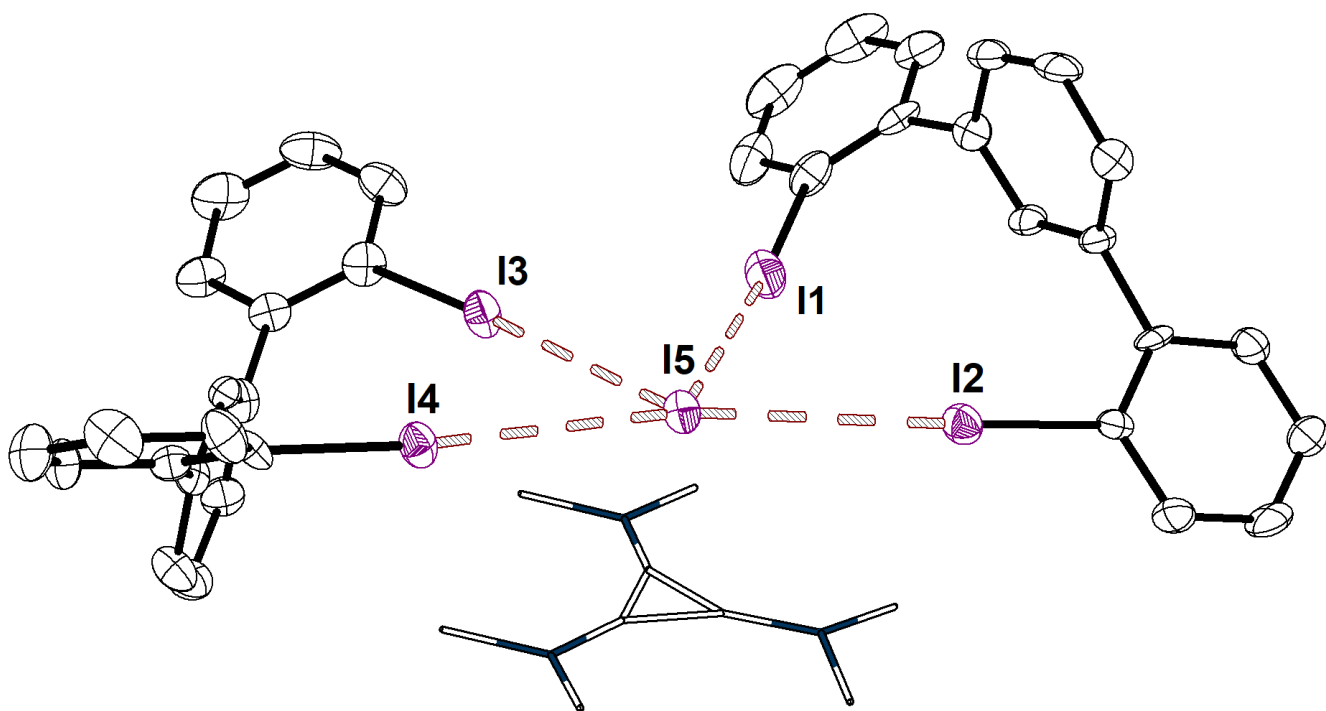


Figure S9: Cocrystal structure of *syn-m-1* and TDA-I.

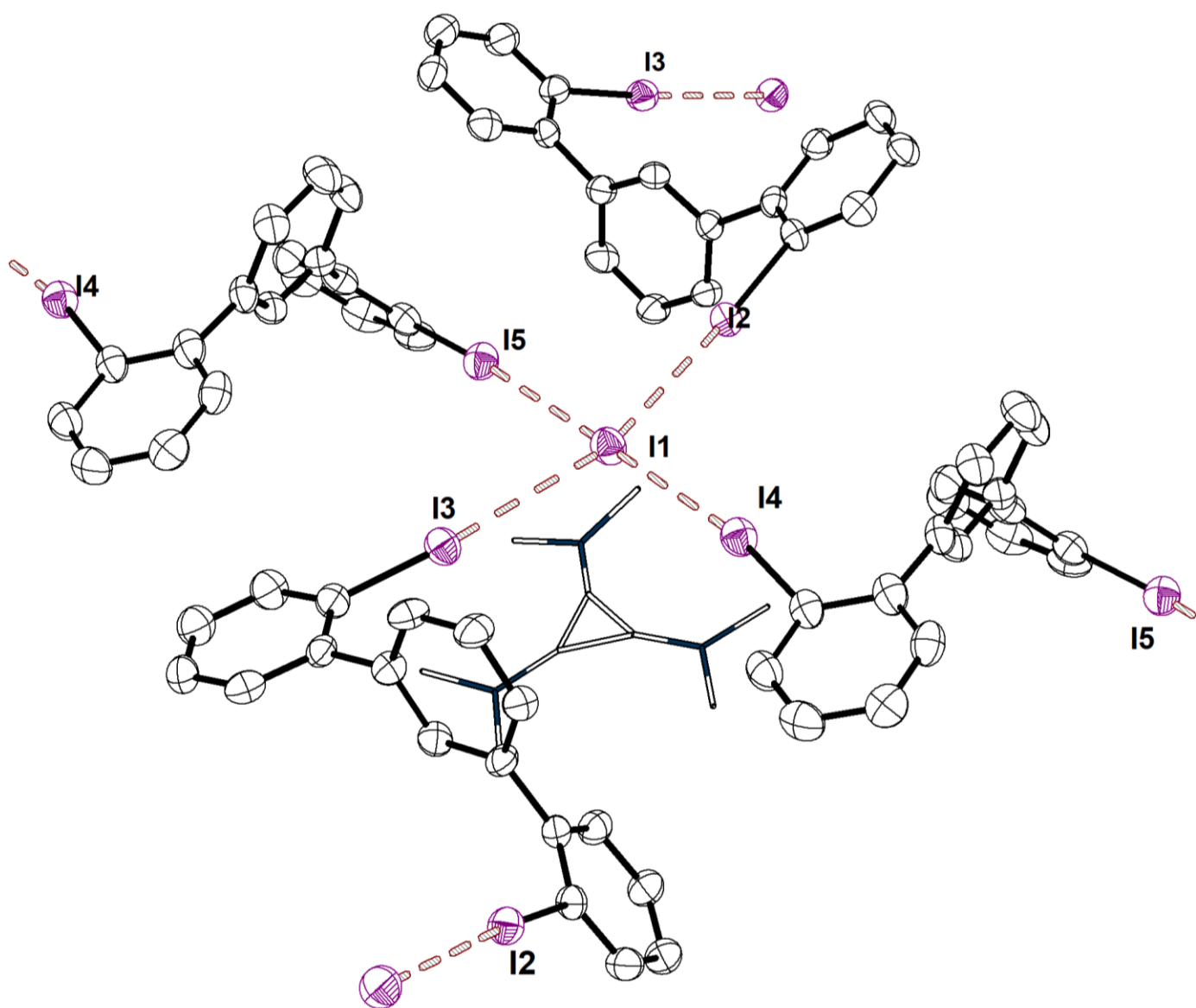


Figure S10: Cocrystal structure of *anti-m-1* and TDA-I.

B Crystal data

Table S1: Crystal data and structure refinement

CCDC No	2167349	2167339	2167342	2167336	2167343	2167344	2167347	2167338	2167348	2167340	2167345	2167341	2167337	2167346	
Compound	syn-p-1	anti-p-1	syn-m-1	anti-m-1	syn-p-1-TDACl	syn-p-1-TDAI	anti-p-1-TDACl	anti-p-1-TDABr	anti-p-1-TDAI	syn-m-1-TDACl	syn-m-1-TEABr	syn-m-1-TDAI	anti-m-1-TDACl	anti-m-1-TDAI	
Empirical formula	C18 F12 I2	C18 F12 I2	C18 F12 I2	C18 F12 I2	C45 H18 Cl F24 I4 N3	C8.18 H3.27 F4.36 I0.91 N0.55 O0	C74 H40 Cl6 F36 I6 N6	C74 H40 Br2 Cl4 F36 I6 N6	C74 H40 Cl4.79 F36 I7.21 N6	C45 H18 Cl F24 I4 N3	C44 H20 Br F24 I4 N	C45 H18 F24 I5 N3	C45 H18 Cl F24 I4 N3	C45 H18 F24 I5 N3	
Formula weight [g/mol]	697.98	697.98	697.98	697.98	1599.67	307.48	2671.05	2760.14	2781.49	1599.67	1606.12	1691.12	1599.67	1691.12	
Crystal system	Triclinic	Monoclinic	Triclinic	Monoclinic	Triclinic	Monoclinic	Triclinic	Triclinic	Triclinic	Orthorhombic	Triclinic	Orthorhombic	Monoclinic	Monoclinic	
Space group	P-1 (2)	P21/n (14)	P-1 (2)	P21/c (14)	P-1 (2)	P21/n (14)	P-1 (2)	P-1 (2)	P-1 (2)	Pbcn (60)	P-1 (2)	Pbcn (60)	Ia (9)	Pc (7)	
Lattice parameters [Å]															
a	7.7774(4)	7.6232(9)	8.2040(4)	11.8867(10)	9.0859(9)	7.3349(2)	7.867	7.82960(10)	7.84560(10)	15.6729(2)	10.2153(4)	20.5688(18)	25.56024(12)	12.59520(10)	
b	10.5846(6)	8.0459(7)	10.2959(5)	10.7984(11)	10.7062(10)	33.8687(19)	12.37760(10)	12.4477(2)	12.5041(3)	20.0722(4)	14.8333(6)	7.5520(4)	8.05461(4)	7.87140(10)	
c	13.0896(5)	15.3895(17)	12.6309(6)	14.7513(11)	25.696(3)	20.5960(8)	22.96440(10)	23.1195(2)	23.2075(4)	32.1725(3)	33.3212(9)	65.850(11)	24.62605(10)	26.3715(2)	
α	106.273(4)	90	77.925(4)	90	82.495(8)	90	75.6600(10)	76.3010(10)	76.694(2)	90	80.102(3)	90	90	90	
β	98.342(4)	101.119(11)	86.254(4)	91.235(7)	89.647(8)	91.808(3)	82.4300(10)	81.9550(10)	81.5980(10)	90	89.936(3)	90	91.1507(4)	97.1660(10)	
γ	110.384(5)	90	68.455(5)	90	86.629(8)	90	88.6400(10)	88.1070(10)	88.0240(10)	90	85.987(3)	90	90	90	
Density [g/cm ³]	2.483	2.503	2.389	2.449	2.147	2.196	2.066	2.114	2.107	2.1	2.15	2.196	2.096	2.165	
Crystal size [mm ³]	0.5 x 0.2 x 0.2	0.42 x 0.21 x 0.2	0.401 x 0.272 x 0.174	0.5 x 0.43 x 0.41	0.241 x 0.170 x 0.170	1.004 x 0.054 x 0.035	0.310 x 0.165 x 0.089	0.215 x 0.091 x 0.049	0.096 x 0.050 x 0.041	0.246 x 0.171 x 0.102	0.221 x 0.155 x 0.065	0.084 x 0.052 x 0.032	0.336 x 0.154 x 0.118	0.177 x 0.096 x 0.093	
Volume [Å ³]	933.67(9)	926.21(18)	970.32(9)	1893.0(3)	2473.9(4)	5114.0(4)	2147.50(2)	2167.60(5)	2191.81(7)	10121.1(3)	4961.4(3)	10228.8(19)	5068.93(4)	2594.10(4)	
Z	2	2	2	4	2	22	1	1	1	8	4	8	4	2	
Temperature [K]	170(2)	170(2)	170(2)	170(2)	170(2)	170.0(7)	169.99(10)	169.99(10)	169.99(10)	170.00(14)	170.00(14)	170.00(14)	170.00(10)	170.02(14)	
Diffraction Device	Xcalibur, Sapphire2, large Be window				SuperNova, Single source at offset/far, Atlas			XtaLAB Synergy, Dualflex, HyPix			SuperNova, Single source at offset/far, Atlas			XtaLAB Synergy, Dualflex, HyPix	
Radiation Type	0.7107 Å (Mo K α / fine-focus sealed X-ray tube)						1.54184 Å (Cu K α / micro-focus sealed X-ray tube)								
F(000)	644	644	644	1288	1508	3160	1270	1306	1313	6032	3016	6320	3016	1580	
Absorption coefficient [mm ⁻¹]	3.488	3.516	3.357	3.441	21.47	25.032	19.897	20.225	22.491	20.991	21.824	25.03	20.957	24.674	
Absorption correction	Semi-empirical from equivalents	Semi-empirical from equivalents	Analytical	Semi-empirical from equivalents	Sphere	Sphere	Gaussian	Gaussian	Gaussian	Gaussian	Gaussian	Semi-empirical from equivalents	Gaussian	Gaussian	
Measurement range	3.2 - 27.5	3.3 - 25.0	3.4 - 25.0	2.9 - 26.6	3.5 - 74.4	3.4 - 66.5	3.7 - 66.5	3.7 - 66.5	3.6 - 66.5	3.6 - 66.5	3.5 - 66.5	3.4 - 66.5	3.5 - 66.5	3.4 - 66.5	
Index range	-10 < h < 10	-8 < h < 8	-9 < h < 9	-14 < h < 14	-11 < h < 7	-8 < h < 8	-9 < h < 9	-9 < h < 9	-9 < h < 8	-18 < h < 14	-12 < h < 12	-24 < h < 23	-29 < h < 30	-14 < h < 14	
	-13 < k < 13	-8 < k < 9	-12 < k < 12	-13 < k < 13	-11 < k < 13	-40 < k < 40	-14 < k < 14	-14 < k < 11	-14 < k < 14	-23 < k < 23	-17 < k < 17	-6 < k < 8	-9 < k < 9	-9 < k < 8	
	-16 < l < 16	-17 < l < 18	-14 < l < 14	-18 < l < 18	-31 < l < 32	-23 < l < 24	-27 < l < 27	-27 < l < 27	-27 < l < 23	-37 < l < 38	-39 < l < 39	-77 < l < 78	-29 < l < 28	-31 < l < 31	
Measured reflexes	16217	6649	18900	15844	15445	29426	56202	24385	24971	54556	77496	56470	34691	26783	
Independent	4251	1589	3401	3893	9624	8988	7555	7603	7727	8895	17224	8956	7403	8240	
Observed	3498	1293	2936	3200	7353	7186	7249	6984	7110	7291	14454	7859	7357	8140	
R(int)	0.0363	0.0402	0.0232	0.0751	0.0482	0.0502	0.0479	0.0445	0.0437	0.0499	0.0605	0.072	0.0424	0.0401	
Completeness (%) / theta (°)	99.8 / 25.242	97.7 / 24.986	99.6 / 24.985	99.4 / 25.242	99.0 / 67.684	99.7 / 66.500	99.7 / 66.494	99.4 / 66.496	99.9 / 66.500	99.6 / 66.499	98.5 / 66.497	99.5 / 66.500	100.0 / 66.499	100.0 / 66.482	
Transmission (min / max)	0.66631 / 1.00000	0.70796 / 1.00000	0.457 / 0.667	0.46411 / 1.00000	0.12796 / 0.22666	0.20281 / 0.29134	0.019 / 0.674	0.113 / 0.839	0.182 / 0.579	0.238 / 0.590	0.038 / 0.536	0.17745 / 1.00000	0.012 / 0.390	0.164 / 0.451	
R1 (observed/all)	0.0263 / 0.0377	0.0400 / 0.0537	0.0329 / 0.0389	0.0448 / 0.0551	0.0516 / 0.0694	0.0337 / 0.0475	0.0322 / 0.0332	0.0329 / 0.0355	0.0444 / 0.0476	0.0469 / 0.0612	0.0480 / 0.0581	0.0541 / 0.0631	0.0323 / 0.0324	0.0408 / 0.0411	
wR2 (observed/all)	0.0545 / 0.0592	0.1024 / 0.1135	0.0780 / 0.0816	0.1107 / 0.1208	0.1288 / 0.1432	0.0726 / 0.0802	0.0847 / 0.0855	0.0855 / 0.0870	0.1020 / 0.1035	0.1064 / 0.1189	0.1230 / 0.1286	0.1011 / 0.1046	0.0798 / 0.0798	0.1034 / 0.1039	
Goof = S	1.039	1.111	1.065	1.035	1.004	1.032	1.033	1.014	1.133	1.175	1.085	1.207	1.034	1.019	
Rest electron density max./min. [e-Å ⁻³]	-0.382 / 0.628	-0.819 / 1.051	-0.758 / 1.234	-0.91 / 1.626	-1.296 / 1.395	-0.773 / 0.961	-0.943 / 1.496	-0.81 / 0.867	-1.352 / 1.344	-1.16 / 1.04	-0.944 / 1.6	-1.192 / 1.149	-0.903 / 1.233	-2.11 / 1.071	

Table S2. Atomic coordinates and equivalent isotropic displacement parameters [Å²] for **syn-p1**

	x	y	z	U(eq)
I(1)	1.14930(3)	0.92541(2)	0.92068(2)	0.03622(8)
I(2)	0.43172(3)	0.65519(2)	0.95802(2)	0.03687(8)
F(1)	0.9212(3)	0.6135(2)	0.48327(14)	0.0372(5)
F(2)	1.2413(3)	0.7745(2)	0.44545(15)	0.0430(5)
F(3)	1.5203(2)	1.0003(2)	0.61468(16)	0.0370(5)
F(4)	1.4798(2)	1.0635(2)	0.82038(15)	0.0396(5)
F(5)	0.6853(2)	0.7937(2)	0.64389(18)	0.0400(5)
F(6)	0.3717(2)	0.62914(19)	0.68118(17)	0.0351(4)
F(7)	0.6818(2)	0.34896(19)	0.77175(16)	0.0326(4)
F(8)	0.9975(2)	0.5169(2)	0.73659(16)	0.0347(4)
F(9)	0.2891(3)	0.20084(18)	0.58922(15)	0.0352(4)
F(10)	-0.0217(3)	0.02966(19)	0.62705(17)	0.0436(5)
F(11)	-0.1241(3)	0.1262(2)	0.81424(18)	0.0469(5)
F(12)	0.0760(3)	0.3962(2)	0.95678(17)	0.0479(5)
C(1)	1.0300(4)	0.7539(3)	0.6730(2)	0.0217(6)
C(2)	1.0565(4)	0.7256(3)	0.5686(2)	0.0247(6)
C(3)	1.2194(4)	0.8062(3)	0.5478(2)	0.0260(6)
C(4)	1.3620(4)	0.9210(3)	0.6338(3)	0.0268(7)
C(5)	1.3381(4)	0.9514(3)	0.7387(3)	0.0258(6)
C(6)	1.1740(4)	0.8701(3)	0.7598(2)	0.0229(6)
C(7)	0.8512(4)	0.6603(3)	0.6902(2)	0.0215(6)
C(8)	0.6872(4)	0.6848(3)	0.6762(3)	0.0247(6)
C(9)	0.5244(4)	0.5984(3)	0.6948(3)	0.0250(6)
C(10)	0.5180(4)	0.4853(3)	0.7287(2)	0.0210(6)
C(11)	0.6811(4)	0.4587(3)	0.7405(2)	0.0223(6)
C(12)	0.8432(4)	0.5455(3)	0.7219(2)	0.0220(6)
C(13)	0.3460(4)	0.3946(3)	0.7532(2)	0.0206(6)
C(14)	0.2397(4)	0.2535(3)	0.6814(2)	0.0250(6)
C(15)	0.0813(4)	0.1637(3)	0.7004(3)	0.0291(7)
C(16)	0.0274(4)	0.2135(3)	0.7947(3)	0.0310(7)
C(17)	0.1306(4)	0.3523(4)	0.8662(3)	0.0290(7)
C(18)	0.2878(4)	0.4443(3)	0.8465(2)	0.0226(6)

Table S3. Anisotropic displacement parameters [Å²] for **syn-p-1**

	U11	U22	U33	U23	U13	U12
I(1)	0.03648(13)	0.03559(13)	0.02640(12)	0.00274(9)	0.01348(9)	0.00776(10)
I(2)	0.04432(14)	0.02716(12)	0.03012(13)	0.00049(9)	0.00216(10)	0.01517(10)
F(1)	0.0319(10)	0.0329(10)	0.0250(10)	0.0032(8)	0.0013(8)	-0.0033(8)
F(2)	0.0466(12)	0.0469(12)	0.0251(10)	0.0109(9)	0.0172(9)	0.0058(10)
F(3)	0.0270(10)	0.0350(11)	0.0440(12)	0.0177(9)	0.0167(8)	0.0013(8)
F(4)	0.0268(10)	0.0304(10)	0.0343(11)	-0.0014(8)	0.0054(8)	-0.0080(8)
F(5)	0.0271(10)	0.0328(11)	0.0732(15)	0.0371(10)	0.0163(10)	0.0116(8)
F(6)	0.0182(9)	0.0330(10)	0.0623(13)	0.0280(10)	0.0107(8)	0.0111(8)
F(7)	0.0318(10)	0.0286(10)	0.0509(12)	0.0266(9)	0.0174(9)	0.0156(8)
F(8)	0.0227(9)	0.0386(11)	0.0565(13)	0.0277(10)	0.0171(9)	0.0172(8)
F(9)	0.0400(11)	0.0229(9)	0.0316(10)	0.0020(8)	0.0149(8)	0.0041(8)
F(10)	0.0352(11)	0.0216(10)	0.0531(13)	0.0075(9)	0.0048(9)	-0.0047(8)
F(11)	0.0277(10)	0.0506(13)	0.0682(15)	0.0364(12)	0.0233(10)	0.0066(9)
F(12)	0.0492(12)	0.0583(14)	0.0476(13)	0.0211(11)	0.0329(10)	0.0256(11)
C(1)	0.0176(14)	0.0194(14)	0.0292(16)	0.0108(12)	0.0083(12)	0.0064(12)
C(2)	0.0224(15)	0.0205(15)	0.0238(15)	0.0055(12)	0.0023(12)	0.0037(12)
C(3)	0.0269(16)	0.0292(17)	0.0222(15)	0.0109(13)	0.0096(12)	0.0092(13)
C(4)	0.0199(15)	0.0238(16)	0.0362(18)	0.0136(13)	0.0115(13)	0.0044(12)
C(5)	0.0200(15)	0.0191(15)	0.0292(16)	0.0045(12)	0.0037(12)	0.0022(12)
C(6)	0.0222(15)	0.0211(15)	0.0244(15)	0.0079(12)	0.0081(12)	0.0074(12)
C(7)	0.0188(14)	0.0165(14)	0.0232(15)	0.0055(11)	0.0051(11)	0.0019(11)
C(8)	0.0229(15)	0.0165(14)	0.0352(17)	0.0133(13)	0.0061(13)	0.0060(12)
C(9)	0.0162(14)	0.0231(15)	0.0338(17)	0.0111(13)	0.0036(12)	0.0064(12)
C(10)	0.0191(14)	0.0161(14)	0.0238(15)	0.0053(11)	0.0044(11)	0.0046(11)
C(11)	0.0237(15)	0.0163(14)	0.0281(16)	0.0109(12)	0.0083(12)	0.0066(12)
C(12)	0.0172(14)	0.0243(15)	0.0233(15)	0.0076(12)	0.0062(11)	0.0076(12)
C(13)	0.0183(14)	0.0176(14)	0.0263(15)	0.0107(12)	0.0052(11)	0.0058(11)
C(14)	0.0261(16)	0.0233(15)	0.0238(15)	0.0081(12)	0.0062(12)	0.0085(13)
C(15)	0.0217(15)	0.0192(15)	0.0373(18)	0.0100(13)	0.0014(13)	0.0008(12)
C(16)	0.0161(15)	0.0303(17)	0.049(2)	0.0257(16)	0.0079(14)	0.0033(13)
C(17)	0.0270(16)	0.0390(19)	0.0323(17)	0.0192(15)	0.0157(14)	0.0182(15)
C(18)	0.0189(14)	0.0190(14)	0.0283(16)	0.0090(12)	0.0029(12)	0.0068(12)

Table S4. Atomic coordinates and equivalent isotropic displacement parameters [Å²] for **anti-p-1**

	x	y	z	U(eq)
I(001)	0.09777(6)	0.98643(5)	0.27621(3)	0.0486(2)
F(1)	-0.1154(5)	0.6512(5)	0.2416(3)	0.0575(11)
F(2)	-0.0967(6)	0.3624(5)	0.3283(3)	0.0627(12)
F(3)	0.1498(6)	0.3189(5)	0.4791(3)	0.0631(12)
F(4)	0.3709(6)	0.5685(5)	0.5442(3)	0.0543(10)
F(5)	0.5675(5)	0.8093(5)	0.3656(2)	0.0521(10)
F(6)	0.1967(6)	0.9574(5)	0.5636(3)	0.0523(10)
C(1)	0.1201(8)	0.7652(7)	0.3477(4)	0.0333(13)
C(2)	0.0061(8)	0.6364(8)	0.3159(4)	0.0384(15)
C(3)	0.0158(9)	0.4861(7)	0.3602(5)	0.0407(16)
C(4)	0.1416(10)	0.4650(7)	0.4365(5)	0.0417(16)
C(5)	0.2539(9)	0.5938(8)	0.4693(4)	0.0402(15)
C(6)	0.2470(8)	0.7444(7)	0.4255(4)	0.0343(14)
C(7)	0.3770(8)	0.8757(7)	0.4634(4)	0.0349(14)
C(8)	0.5326(8)	0.9035(8)	0.4323(4)	0.0358(14)
C(9)	0.3476(9)	0.9776(7)	0.5314(4)	0.0349(14)

Table S5. Anisotropic displacement parameters [Å²] for **anti-p-1**

	U11	U22	U33	U23	U13	U12
I(001)	0.0538(4)	0.0410(3)	0.0475(3)	0.01032(18)	0.0012(2)	-0.00020(19)
F(1)	0.051(3)	0.051(2)	0.059(3)	-0.0037(19)	-0.020(2)	-0.0067(18)
F(2)	0.063(3)	0.037(2)	0.083(3)	-0.012(2)	0.002(2)	-0.0168(19)
F(3)	0.078(3)	0.032(2)	0.079(3)	0.0131(19)	0.015(2)	0.0015(19)
F(4)	0.062(3)	0.052(2)	0.041(2)	0.0104(18)	-0.007(2)	0.005(2)
F(5)	0.053(3)	0.060(2)	0.046(2)	-0.0228(19)	0.0161(19)	-0.0120(19)
F(6)	0.044(3)	0.063(2)	0.055(2)	-0.014(2)	0.019(2)	-0.0148(19)
C(1)	0.037(4)	0.032(3)	0.032(3)	-0.001(2)	0.009(3)	0.000(3)
C(2)	0.034(4)	0.037(3)	0.040(4)	-0.003(3)	-0.001(3)	0.001(3)
C(3)	0.039(4)	0.030(3)	0.054(4)	-0.011(3)	0.010(3)	-0.003(3)
C(4)	0.048(4)	0.028(3)	0.050(4)	0.004(3)	0.012(3)	0.002(3)
C(5)	0.042(4)	0.046(4)	0.029(3)	0.002(3)	-0.001(3)	0.004(3)
C(6)	0.035(4)	0.032(3)	0.036(3)	-0.002(2)	0.008(3)	-0.001(3)
C(7)	0.035(4)	0.037(3)	0.028(3)	-0.001(2)	-0.004(3)	-0.005(3)
C(8)	0.033(4)	0.041(3)	0.033(3)	-0.008(3)	0.006(3)	-0.002(3)
C(9)	0.029(3)	0.040(3)	0.036(3)	0.005(3)	0.005(3)	-0.002(3)

Table S6. Atomic coordinates and equivalent isotropic displacement parameters
[Å²] **syn-m-1**

	x	y	z	U(eq)
I(1)	-0.20537(5)	0.82579(4)	0.32762(4)	0.08125(15)
I(2)	0.22466(4)	0.87369(3)	-0.01023(3)	0.06117(13)
F(1)	-0.2705(4)	0.9358(3)	0.5456(3)	0.0895(10)
F(2)	-0.0573(5)	0.9194(3)	0.7037(2)	0.0953(12)
F(3)	0.2933(5)	0.7764(3)	0.6941(3)	0.0949(12)
F(4)	0.4255(4)	0.6517(3)	0.5267(2)	0.0764(9)
F(5)	0.1054(4)	0.4742(3)	0.4137(2)	0.0633(7)
F(6)	0.2634(4)	0.3325(3)	0.2574(2)	0.0660(7)
F(7)	0.4758(4)	0.4287(3)	0.1175(2)	0.0591(7)
F(8)	0.3711(3)	0.8118(2)	0.2909(2)	0.0529(6)
F(9)	0.7943(3)	0.5016(3)	0.2262(2)	0.0650(7)
F(10)	1.0190(3)	0.5758(4)	0.0866(3)	0.0746(8)
F(11)	0.8994(4)	0.7826(3)	-0.0910(2)	0.0702(8)
F(12)	0.5538(4)	0.9186(3)	-0.1291(2)	0.0639(7)
C(1)	-0.0326(6)	0.7997(4)	0.4500(3)	0.0481(10)
C(2)	-0.0985(7)	0.8629(5)	0.5385(4)	0.0593(13)
C(3)	0.0089(8)	0.8558(5)	0.6206(4)	0.0634(14)
C(4)	0.1851(8)	0.7841(5)	0.6160(4)	0.0644(14)
C(5)	0.2544(6)	0.7196(4)	0.5294(3)	0.0540(11)
C(6)	0.1481(5)	0.7244(4)	0.4456(3)	0.0424(9)
C(7)	0.2315(5)	0.6495(4)	0.3556(3)	0.0389(8)
C(8)	0.2083(5)	0.5253(4)	0.3445(3)	0.0445(9)
C(9)	0.2896(6)	0.4519(4)	0.2655(3)	0.0438(9)
C(10)	0.3984(5)	0.5005(4)	0.1952(3)	0.0409(9)
C(11)	0.4282(5)	0.6229(4)	0.2010(3)	0.0369(8)
C(12)	0.3438(5)	0.6933(4)	0.2826(3)	0.0398(9)
C(13)	0.5490(5)	0.6723(4)	0.1236(3)	0.0373(8)
C(14)	0.7287(5)	0.6063(5)	0.1408(3)	0.0461(10)
C(15)	0.8457(5)	0.6439(5)	0.0690(4)	0.0501(10)
C(16)	0.7851(5)	0.7486(5)	-0.0211(3)	0.0466(10)
C(17)	0.6076(5)	0.8168(4)	-0.0396(3)	0.0432(9)
C(18)	0.4892(5)	0.7793(4)	0.0312(3)	0.0383(8)

Table S7. Anisotropic displacement parameters [\AA^2] for **syn-m-1**

	U11	U22	U33	U23	U13	U12
I(1)	0.0550(2)	0.0795(3)	0.1049(3)	-0.0235(2)	-0.01573(19)	-0.01385(18)
I(2)	0.03645(17)	0.0617(2)	0.0749(2)	-0.00622(16)	-0.00598(13)	-0.00865(13)
F(1)	0.0670(19)	0.076(2)	0.117(3)	-0.0348(19)	0.0440(19)	-0.0153(16)
F(2)	0.152(3)	0.0659(19)	0.0558(18)	-0.0278(15)	0.0445(19)	-0.023(2)
F(3)	0.139(3)	0.073(2)	0.0576(19)	-0.0252(16)	-0.0309(19)	-0.009(2)
F(4)	0.0627(18)	0.083(2)	0.0730(19)	-0.0323(16)	-0.0209(14)	-0.0020(15)
F(5)	0.0812(19)	0.0565(15)	0.0610(16)	-0.0124(12)	0.0306(14)	-0.0397(14)
F(6)	0.095(2)	0.0533(15)	0.0692(17)	-0.0238(13)	0.0217(15)	-0.0469(15)
F(7)	0.0795(18)	0.0597(15)	0.0511(15)	-0.0301(12)	0.0221(13)	-0.0335(14)
F(8)	0.0592(15)	0.0481(13)	0.0642(16)	-0.0270(12)	0.0201(12)	-0.0288(12)
F(9)	0.0493(15)	0.0635(16)	0.0669(17)	0.0112(13)	-0.0161(12)	-0.0131(13)
F(10)	0.0317(13)	0.100(2)	0.085(2)	-0.0163(17)	-0.0011(13)	-0.0163(14)
F(11)	0.0578(16)	0.104(2)	0.0629(17)	-0.0151(15)	0.0187(13)	-0.0488(16)
F(12)	0.0657(17)	0.0666(17)	0.0535(15)	0.0096(13)	-0.0021(12)	-0.0282(14)
C(1)	0.051(2)	0.041(2)	0.050(2)	-0.0062(19)	0.0119(19)	-0.0170(19)
C(2)	0.064(3)	0.041(2)	0.065(3)	-0.010(2)	0.032(3)	-0.016(2)
C(3)	0.097(4)	0.040(2)	0.041(3)	-0.0083(19)	0.023(3)	-0.015(3)
C(4)	0.104(4)	0.043(2)	0.035(2)	-0.0056(19)	-0.006(2)	-0.015(3)
C(5)	0.069(3)	0.040(2)	0.043(2)	-0.0113(19)	-0.001(2)	-0.006(2)
C(6)	0.050(2)	0.037(2)	0.039(2)	-0.0065(17)	0.0070(17)	-0.0149(18)
C(7)	0.043(2)	0.040(2)	0.032(2)	-0.0089(16)	0.0052(16)	-0.0127(17)
C(8)	0.044(2)	0.046(2)	0.042(2)	-0.0083(18)	0.0035(18)	-0.0159(19)
C(9)	0.053(2)	0.041(2)	0.043(2)	-0.0090(18)	0.0031(18)	-0.0244(19)
C(10)	0.049(2)	0.043(2)	0.033(2)	-0.0140(17)	0.0044(17)	-0.0170(18)
C(11)	0.038(2)	0.038(2)	0.035(2)	-0.0087(16)	0.0052(15)	-0.0143(16)
C(12)	0.041(2)	0.0360(19)	0.045(2)	-0.0109(17)	0.0015(17)	-0.0160(16)
C(13)	0.037(2)	0.039(2)	0.040(2)	-0.0152(16)	0.0058(16)	-0.0155(16)
C(14)	0.043(2)	0.052(2)	0.045(2)	-0.0098(19)	0.0009(18)	-0.0189(19)
C(15)	0.033(2)	0.067(3)	0.054(3)	-0.020(2)	-0.0012(18)	-0.0171(19)
C(16)	0.044(2)	0.060(3)	0.047(2)	-0.017(2)	0.0100(18)	-0.030(2)
C(17)	0.050(2)	0.046(2)	0.039(2)	-0.0112(18)	0.0022(17)	-0.0219(19)
C(18)	0.0336(19)	0.040(2)	0.044(2)	-0.0146(17)	0.0034(16)	-0.0137(16)

Table S8. Atomic coordinates and equivalent isotropic displacement parameters [Å²] for **anti-m-1**

	x	y	z	U(eq)
I(1)	0.41865(3)	0.40165(4)	0.88496(2)	0.06158(16)
F(1)	0.6804(3)	0.4477(3)	0.9161(2)	0.0644(9)
C(1)	0.5142(4)	0.4984(4)	0.7101(3)	0.0346(9)
I(2)	0.22010(4)	0.71726(4)	0.42860(2)	0.06040(16)
F(2)	0.8390(2)	0.5328(3)	0.8085(2)	0.0668(9)
C(2)	0.5412(4)	0.4666(4)	0.7995(3)	0.0361(9)
F(003)	0.3464(2)	0.6833(3)	0.6990(2)	0.0496(7)
F(3)	0.7871(3)	0.6038(4)	0.6360(2)	0.0688(10)
C(3)	0.6506(4)	0.4802(4)	0.8313(3)	0.0427(11)
F(004)	0.4456(3)	0.2739(3)	0.6333(2)	0.0548(8)
F(4)	0.5764(3)	0.5753(3)	0.57083(19)	0.0591(8)
C(4)	0.7333(4)	0.5232(5)	0.7769(3)	0.0451(11)
F(005)	0.0915(2)	0.4221(3)	0.5457(2)	0.0533(7)
F(5)	0.0045(3)	0.8788(3)	0.4576(2)	0.0584(8)
C(5)	0.7073(4)	0.5593(5)	0.6898(3)	0.0479(12)
F(6)	-0.1272(3)	0.9128(3)	0.6002(3)	0.0657(9)
C(6)	0.5985(4)	0.5449(5)	0.6564(3)	0.0409(10)
C(7)	0.3208(4)	0.5723(4)	0.6629(3)	0.0350(9)
F(7)	-0.0902(3)	0.7840(3)	0.7551(2)	0.0720(10)
C(8)	0.3997(4)	0.4811(4)	0.6687(3)	0.0347(9)
F(8)	0.0723(3)	0.6090(3)	0.7629(2)	0.0609(8)
C(9)	0.3709(4)	0.3666(4)	0.6304(3)	0.0379(10)
F(00B)	0.2429(3)	0.2365(3)	0.5534(2)	0.0606(8)
C(10)	0.2678(4)	0.3467(4)	0.5900(3)	0.0395(10)
C(11)	0.1925(4)	0.4424(4)	0.5858(3)	0.0378(10)
C(12)	0.2158(4)	0.5577(4)	0.6212(3)	0.0348(9)
C(13)	0.0606(4)	0.6791(5)	0.6870(3)	0.0448(11)
C(14)	0.1309(4)	0.6598(4)	0.6153(3)	0.0357(9)
C(15)	0.1138(4)	0.7309(4)	0.5381(3)	0.0374(10)
C(16)	0.0263(4)	0.8158(4)	0.5333(3)	0.0429(11)
C(17)	-0.0416(4)	0.8332(5)	0.6059(4)	0.0484(12)
C(18)	-0.0234(4)	0.7673(5)	0.6842(3)	0.0484(12)

Table S9. Anisotropic displacement parameters [\AA^2] for **anti-m-1**

	U11	U22	U33	U23	U13	U12
I(1)	0.0576(3)	0.0859(3)	0.0415(2)	0.00717(16)	0.00796(16)	-0.0189(2)
F(1)	0.059(2)	0.086(2)	0.0473(16)	0.0122(15)	-0.0197(15)	-0.0019(18)
C(1)	0.031(2)	0.036(2)	0.036(2)	-0.0011(17)	0.0000(17)	-0.0020(18)
I(2)	0.0702(3)	0.0660(3)	0.0458(2)	0.00389(15)	0.01923(18)	0.01474(19)
F(2)	0.0293(15)	0.088(2)	0.083(2)	-0.0103(19)	-0.0154(15)	-0.0008(16)
C(2)	0.034(2)	0.038(2)	0.036(2)	-0.0009(17)	0.0027(17)	-0.0036(19)
F(003)	0.0370(15)	0.0471(15)	0.0640(18)	-0.0159(13)	-0.0108(13)	-0.0003(13)
F(3)	0.0442(18)	0.102(3)	0.0608(19)	-0.0082(17)	0.0179(15)	-0.0313(18)
C(3)	0.041(3)	0.046(3)	0.041(2)	0.0011(19)	-0.010(2)	0.003(2)
F(004)	0.0493(18)	0.0451(16)	0.0695(19)	-0.0084(13)	-0.0098(15)	0.0063(13)
F(4)	0.0548(19)	0.087(2)	0.0358(14)	0.0068(14)	-0.0006(13)	-0.0217(16)
C(4)	0.027(2)	0.054(3)	0.054(3)	-0.012(2)	-0.004(2)	0.003(2)
F(005)	0.0356(15)	0.0602(17)	0.0634(18)	-0.0108(14)	-0.0156(13)	-0.0094(13)
F(5)	0.063(2)	0.0535(17)	0.0584(18)	0.0046(14)	-0.0019(15)	0.0128(15)
C(5)	0.037(3)	0.059(3)	0.048(3)	-0.011(2)	0.009(2)	-0.009(2)
F(6)	0.0460(19)	0.0545(18)	0.097(3)	-0.0149(17)	0.0099(17)	0.0156(15)
C(6)	0.037(2)	0.048(3)	0.037(2)	-0.0018(19)	0.0022(19)	-0.009(2)
C(7)	0.031(2)	0.038(2)	0.036(2)	-0.0023(17)	-0.0021(17)	-0.0076(19)
F(7)	0.067(2)	0.079(2)	0.071(2)	-0.0181(17)	0.0378(18)	0.0030(18)
C(8)	0.029(2)	0.045(2)	0.0296(19)	-0.0008(17)	-0.0002(16)	-0.0103(19)
F(8)	0.063(2)	0.081(2)	0.0399(15)	0.0067(14)	0.0129(14)	0.0004(17)
C(9)	0.036(2)	0.042(2)	0.036(2)	0.0021(18)	0.0004(18)	0.000(2)
F(00B)	0.061(2)	0.0421(16)	0.078(2)	-0.0168(14)	-0.0141(17)	-0.0070(15)
C(10)	0.042(3)	0.035(2)	0.042(2)	-0.0050(18)	0.0014(19)	-0.008(2)
C(11)	0.030(2)	0.049(2)	0.035(2)	-0.0006(18)	-0.0017(17)	-0.010(2)
C(12)	0.027(2)	0.044(2)	0.033(2)	0.0009(17)	0.0012(17)	-0.0017(18)
C(13)	0.039(3)	0.053(3)	0.042(2)	-0.003(2)	0.002(2)	-0.008(2)
C(14)	0.027(2)	0.045(2)	0.035(2)	-0.0064(18)	-0.0013(17)	-0.0020(19)
C(15)	0.031(2)	0.044(2)	0.037(2)	-0.0083(18)	0.0025(17)	-0.0053(19)
C(16)	0.039(3)	0.040(2)	0.049(3)	-0.009(2)	-0.003(2)	-0.003(2)
C(17)	0.032(2)	0.048(3)	0.066(3)	-0.017(2)	0.006(2)	-0.001(2)
C(18)	0.036(3)	0.061(3)	0.048(3)	-0.017(2)	0.016(2)	-0.006(2)

Table S10. Atomic coordinates and equivalent isotropic displacement parameters [Å²] for **syn-p1-TDACI**

	x	y	z	U(eq)
I(1)	-0.05136(5)	0.62723(4)	0.13469(2)	0.03972(13)
I(2)	0.29522(5)	0.40474(4)	0.22152(2)	0.03835(13)
F(1)	-0.2969(5)	0.7902(5)	0.0605(2)	0.0586(14)
F(2)	-0.2797(6)	0.9319(5)	-0.0333(2)	0.0587(13)
F(3)	-0.0191(6)	0.9511(5)	-0.0845(2)	0.0565(13)
F(4)	0.2235(6)	0.8177(5)	-0.0432(2)	0.0537(12)
F(5)	0.3139(6)	0.8228(4)	0.0880(2)	0.0532(13)
F(6)	0.5274(5)	0.6749(4)	0.14040(18)	0.0446(10)
F(7)	0.3508(6)	0.3223(4)	0.0737(2)	0.0642(16)
F(8)	0.1380(6)	0.4702(4)	0.0219(2)	0.0546(13)
F(9)	0.7293(6)	0.4226(5)	0.0765(2)	0.0536(12)
F(10)	0.9243(6)	0.2756(5)	0.1401(2)	0.0640(15)
F(11)	0.8463(6)	0.1890(5)	0.2397(2)	0.0603(14)
F(12)	0.5798(6)	0.2501(4)	0.2764(2)	0.0505(12)
C(1)	-0.0429(8)	0.7249(6)	0.0585(3)	0.0341(14)
C(2)	-0.1653(9)	0.7932(8)	0.0356(3)	0.0434(17)
C(3)	-0.1587(9)	0.8679(7)	-0.0127(3)	0.0408(17)
C(4)	-0.0270(10)	0.8767(7)	-0.0386(3)	0.0412(17)
C(5)	0.0963(9)	0.8065(7)	-0.0166(3)	0.0384(16)
C(6)	0.0899(8)	0.7300(6)	0.0305(3)	0.0326(14)
C(7)	0.2215(8)	0.6524(6)	0.0525(3)	0.0334(14)
C(8)	0.3250(8)	0.6997(6)	0.0822(3)	0.0371(16)
C(9)	0.4352(8)	0.6244(7)	0.1094(3)	0.0356(15)
C(10)	0.4457(8)	0.4945(7)	0.1078(3)	0.0346(15)
C(11)	0.3453(9)	0.4463(7)	0.0767(3)	0.0378(16)
C(12)	0.2360(8)	0.5234(7)	0.0489(3)	0.0367(15)
C(13)	0.5490(8)	0.4107(6)	0.1425(3)	0.0372(16)
C(14)	0.6889(9)	0.3799(8)	0.1254(3)	0.0441(18)
C(15)	0.7899(9)	0.3064(7)	0.1577(4)	0.048(2)
C(16)	0.7505(10)	0.2617(7)	0.2082(4)	0.047(2)
C(17)	0.6115(9)	0.2924(6)	0.2264(3)	0.0404(17)
C(18)	0.5089(8)	0.3652(6)	0.1936(3)	0.0370(16)
N(1)	0.2536(7)	0.0441(6)	0.2416(3)	0.0424(15)
N(2)	0.5764(7)	-0.0450(6)	0.3253(3)	0.0409(14)
N(3)	0.6140(8)	-0.0112(6)	0.1810(3)	0.0445(15)
C(37)	0.5331(8)	-0.0072(7)	0.2241(3)	0.0376(16)
C(38)	0.3986(8)	0.0144(6)	0.2465(3)	0.0347(15)
C(39)	0.5205(8)	-0.0201(7)	0.2777(3)	0.0370(15)
C(40)	0.7358(9)	-0.0574(9)	0.3335(4)	0.056(2)
C(41)	0.4785(10)	-0.0399(8)	0.3704(3)	0.0461(18)
C(42)	0.1676(10)	0.0761(8)	0.2864(4)	0.051(2)
C(43)	0.1841(9)	0.0598(8)	0.1901(4)	0.050(2)
C(44)	0.5486(11)	0.0260(9)	0.1291(3)	0.054(2)
C(45)	0.7613(10)	-0.0680(9)	0.1839(4)	0.057(2)
Cl(2)	-0.0350(2)	0.48628(18)	0.24890(7)	0.0447(4)
I(3)	0.63880(5)	0.60659(4)	0.27823(2)	0.03782(12)
I(4)	0.98260(5)	0.34096(5)	0.36239(2)	0.04013(13)

F(13)	0.3485(5)	0.7548(4)	0.22468(18)	0.0448(10)
F(14)	0.0737(6)	0.7898(4)	0.2591(2)	0.0548(13)
F(15)	-0.0033(5)	0.6890(5)	0.3574(2)	0.0575(13)
F(16)	0.1999(5)	0.5528(5)	0.42097(19)	0.0498(11)
F(17)	0.6065(6)	0.6859(4)	0.4152(2)	0.0566(13)
F(18)	0.8214(6)	0.5410(4)	0.4676(2)	0.0517(12)
F(19)	0.3947(5)	0.3233(4)	0.3707(2)	0.0554(13)
F(20)	0.6078(6)	0.1777(4)	0.4248(2)	0.0611(15)
F(21)	0.7176(6)	0.2189(5)	0.54983(19)	0.0504(11)
F(22)	0.9519(7)	0.0757(5)	0.5926(2)	0.0601(14)
F(23)	1.2024(6)	0.0530(5)	0.5364(2)	0.0608(14)
F(24)	1.2153(6)	0.1634(5)	0.4374(2)	0.0603(14)
C(19)	0.4256(8)	0.6408(6)	0.3062(3)	0.0346(15)
C(20)	0.3175(9)	0.7076(7)	0.2739(3)	0.0408(17)
C(21)	0.1744(9)	0.7234(7)	0.2906(4)	0.0433(18)
C(22)	0.1365(9)	0.6723(7)	0.3404(4)	0.0447(18)
C(23)	0.2409(9)	0.6036(7)	0.3728(3)	0.0419(17)
C(24)	0.3848(8)	0.5878(6)	0.3568(3)	0.0359(15)
C(25)	0.4939(9)	0.5083(7)	0.3923(3)	0.0370(15)
C(26)	0.6032(9)	0.5593(7)	0.4183(3)	0.0394(16)
C(27)	0.7130(9)	0.4849(7)	0.4454(3)	0.0381(16)
C(28)	0.7180(8)	0.3549(7)	0.4483(3)	0.0356(15)
C(29)	0.6067(9)	0.3033(7)	0.4239(3)	0.0393(16)
C(30)	0.4972(9)	0.3770(7)	0.3969(3)	0.0419(17)
C(31)	0.8475(8)	0.2735(7)	0.4714(3)	0.0358(15)
C(32)	0.8419(9)	0.2111(7)	0.5211(3)	0.0408(17)
C(33)	0.9614(10)	0.1374(7)	0.5442(3)	0.0440(18)
C(34)	1.0865(10)	0.1248(8)	0.5155(3)	0.0465(19)
C(35)	1.0931(9)	0.1841(7)	0.4638(3)	0.0441(18)
C(36)	0.9763(8)	0.2587(7)	0.4410(3)	0.0367(15)
H(40A)	0.785449	-0.063569	0.299927	0.083
H(40B)	0.761158	-0.133716	0.357985	0.083
H(40C)	0.767592	0.016581	0.348208	0.083
H(41A)	0.441942	0.047579	0.371811	0.069
H(41B)	0.532923	-0.071547	0.402744	0.069
H(41C)	0.395107	-0.092236	0.36699	0.069
H(42A)	0.079849	0.026642	0.290018	0.077
H(42B)	0.137371	0.166263	0.281086	0.077
H(42C)	0.227521	0.056986	0.318355	0.077
H(43A)	0.239443	0.007687	0.167199	0.074
H(43B)	0.183427	0.148634	0.174866	0.074
H(43C)	0.082572	0.03361	0.193642	0.074
H(44A)	0.623777	0.061214	0.104802	0.081
H(44B)	0.467757	0.089763	0.131381	0.081
H(44C)	0.510478	-0.048012	0.116155	0.081
H(45A)	0.826409	-0.014148	0.16164	0.086
H(45B)	0.761846	-0.151097	0.171732	0.086
H(45C)	0.796051	-0.077736	0.220308	0.086

Table S11. Anisotropic displacement parameters [\AA^2] for **syn-p1-TDACI**

	U11	U22	U33	U23	U13	U12
I(1)	0.0374(2)	0.0470(2)	0.0313(2)	0.00657(18)	0.00442(18)	0.00042(18)
I(2)	0.0378(2)	0.0386(2)	0.0381(3)	-0.00036(18)	0.00086(19)	-0.00753(17)
F(1)	0.037(3)	0.077(3)	0.054(3)	0.014(3)	0.007(2)	0.014(2)
F(2)	0.058(3)	0.054(3)	0.058(3)	0.011(2)	-0.015(3)	0.011(2)
F(3)	0.066(3)	0.058(3)	0.040(3)	0.015(2)	-0.003(2)	0.004(2)
F(4)	0.049(3)	0.066(3)	0.042(3)	0.011(2)	0.011(2)	-0.008(2)
F(5)	0.060(3)	0.031(2)	0.068(3)	-0.002(2)	-0.020(3)	-0.006(2)
F(6)	0.045(2)	0.043(2)	0.045(3)	-0.0010(19)	-0.015(2)	-0.0118(19)
F(7)	0.070(4)	0.038(2)	0.087(4)	-0.024(2)	-0.034(3)	0.010(2)
F(8)	0.055(3)	0.045(2)	0.066(3)	-0.018(2)	-0.030(3)	0.003(2)
F(9)	0.044(3)	0.070(3)	0.045(3)	-0.006(2)	0.006(2)	0.010(2)
F(10)	0.044(3)	0.077(4)	0.069(4)	-0.015(3)	-0.002(3)	0.019(3)
F(11)	0.055(3)	0.050(3)	0.072(4)	0.002(2)	-0.023(3)	0.012(2)
F(12)	0.064(3)	0.041(2)	0.044(3)	0.0035(19)	-0.010(2)	-0.002(2)
C(1)	0.044(4)	0.033(3)	0.024(3)	0.002(3)	0.001(3)	0.002(3)
C(2)	0.043(4)	0.051(4)	0.035(4)	-0.002(3)	-0.004(3)	0.000(3)
C(3)	0.045(4)	0.038(4)	0.037(4)	0.003(3)	-0.007(3)	0.002(3)
C(4)	0.060(5)	0.035(3)	0.027(4)	0.005(3)	-0.008(3)	-0.008(3)
C(5)	0.046(4)	0.033(3)	0.036(4)	0.000(3)	0.004(3)	-0.006(3)
C(6)	0.036(4)	0.033(3)	0.029(4)	-0.002(3)	-0.002(3)	-0.003(3)
C(7)	0.036(4)	0.037(3)	0.025(3)	0.002(3)	-0.004(3)	-0.002(3)
C(8)	0.037(4)	0.032(3)	0.042(4)	0.002(3)	0.002(3)	-0.009(3)
C(9)	0.028(3)	0.043(4)	0.036(4)	0.000(3)	0.001(3)	-0.007(3)
C(10)	0.031(3)	0.038(3)	0.033(4)	-0.001(3)	-0.001(3)	0.001(3)
C(11)	0.042(4)	0.033(3)	0.040(4)	-0.010(3)	-0.010(3)	0.003(3)
C(12)	0.037(4)	0.036(3)	0.037(4)	-0.009(3)	-0.005(3)	0.005(3)
C(13)	0.036(4)	0.033(3)	0.042(4)	-0.005(3)	-0.007(3)	0.003(3)
C(14)	0.045(4)	0.051(4)	0.037(4)	-0.012(3)	-0.001(3)	-0.001(3)
C(15)	0.038(4)	0.040(4)	0.066(6)	-0.012(4)	-0.006(4)	0.009(3)
C(16)	0.047(5)	0.036(4)	0.058(6)	-0.009(3)	-0.015(4)	0.010(3)
C(17)	0.054(5)	0.030(3)	0.038(4)	-0.004(3)	-0.010(3)	-0.003(3)
C(18)	0.034(4)	0.028(3)	0.050(5)	-0.010(3)	-0.005(3)	-0.003(3)
N(1)	0.030(3)	0.048(3)	0.050(4)	-0.011(3)	-0.001(3)	0.000(3)
N(2)	0.037(3)	0.050(4)	0.035(4)	0.002(3)	-0.005(3)	-0.010(3)
N(3)	0.040(4)	0.051(4)	0.042(4)	-0.003(3)	0.010(3)	-0.007(3)
C(37)	0.033(4)	0.035(3)	0.045(4)	-0.002(3)	0.000(3)	-0.008(3)
C(38)	0.037(4)	0.028(3)	0.039(4)	-0.004(3)	0.003(3)	-0.007(3)
C(39)	0.032(4)	0.039(4)	0.039(4)	-0.002(3)	0.005(3)	-0.005(3)
C(40)	0.038(4)	0.075(6)	0.051(5)	0.005(4)	-0.011(4)	-0.007(4)
C(41)	0.052(5)	0.048(4)	0.039(4)	-0.006(3)	0.000(4)	-0.005(4)
C(42)	0.044(5)	0.055(5)	0.057(6)	-0.010(4)	0.006(4)	-0.005(4)
C(43)	0.037(4)	0.058(5)	0.051(5)	0.003(4)	-0.008(4)	-0.001(4)
C(44)	0.056(5)	0.068(5)	0.038(5)	-0.008(4)	0.005(4)	-0.018(4)
C(45)	0.044(5)	0.062(5)	0.068(6)	-0.017(5)	0.022(4)	-0.011(4)
Cl(2)	0.0389(9)	0.0633(11)	0.0289(9)	0.0065(8)	0.0057(7)	-0.0073(8)
I(3)	0.0364(2)	0.0414(2)	0.0355(3)	-0.00224(17)	0.00434(18)	-0.00775(17)
I(4)	0.0404(3)	0.0490(3)	0.0289(2)	0.00291(18)	0.00506(19)	-0.00329(19)

F(13)	0.058(3)	0.037(2)	0.038(3)	0.0017(18)	-0.001(2)	-0.0056(19)
F(14)	0.046(3)	0.045(2)	0.070(4)	0.002(2)	-0.010(2)	0.004(2)
F(15)	0.038(3)	0.058(3)	0.075(4)	-0.008(3)	0.011(2)	0.004(2)
F(16)	0.045(3)	0.059(3)	0.044(3)	-0.003(2)	0.012(2)	-0.006(2)
F(17)	0.069(3)	0.035(2)	0.067(4)	-0.008(2)	-0.020(3)	-0.005(2)
F(18)	0.061(3)	0.045(2)	0.050(3)	-0.007(2)	-0.020(2)	-0.009(2)
F(19)	0.045(3)	0.043(2)	0.078(4)	-0.005(2)	-0.020(3)	-0.008(2)
F(20)	0.061(3)	0.033(2)	0.088(4)	-0.001(2)	-0.022(3)	-0.010(2)
F(21)	0.053(3)	0.061(3)	0.036(3)	0.001(2)	0.014(2)	-0.011(2)
F(22)	0.076(4)	0.065(3)	0.035(3)	0.009(2)	-0.007(3)	-0.011(3)
F(23)	0.060(3)	0.067(3)	0.051(3)	0.008(2)	-0.017(3)	0.006(3)
F(24)	0.045(3)	0.080(4)	0.051(3)	0.005(3)	0.007(2)	0.010(2)
C(19)	0.036(4)	0.029(3)	0.038(4)	-0.003(3)	0.003(3)	-0.005(3)
C(20)	0.051(5)	0.032(3)	0.039(4)	-0.002(3)	0.002(3)	-0.002(3)
C(21)	0.044(4)	0.032(3)	0.053(5)	-0.003(3)	-0.008(4)	0.001(3)
C(22)	0.037(4)	0.045(4)	0.054(5)	-0.011(4)	0.005(4)	0.000(3)
C(23)	0.046(4)	0.042(4)	0.039(4)	-0.008(3)	0.011(3)	-0.010(3)
C(24)	0.036(4)	0.034(3)	0.038(4)	-0.005(3)	-0.001(3)	-0.003(3)
C(25)	0.040(4)	0.041(4)	0.029(4)	0.000(3)	0.003(3)	-0.003(3)
C(26)	0.049(4)	0.034(3)	0.036(4)	-0.003(3)	0.002(3)	-0.007(3)
C(27)	0.042(4)	0.037(4)	0.036(4)	-0.005(3)	-0.003(3)	-0.006(3)
C(28)	0.032(4)	0.039(3)	0.034(4)	-0.002(3)	-0.002(3)	0.001(3)
C(29)	0.042(4)	0.034(3)	0.041(4)	0.001(3)	0.000(3)	-0.006(3)
C(30)	0.041(4)	0.043(4)	0.041(4)	0.000(3)	-0.001(3)	-0.007(3)
C(31)	0.036(4)	0.040(3)	0.030(4)	0.003(3)	-0.001(3)	-0.007(3)
C(32)	0.040(4)	0.044(4)	0.038(4)	-0.004(3)	0.007(3)	-0.006(3)
C(33)	0.058(5)	0.043(4)	0.030(4)	0.003(3)	-0.004(4)	-0.009(3)
C(34)	0.051(5)	0.046(4)	0.039(5)	0.005(3)	-0.009(4)	0.003(4)
C(35)	0.047(5)	0.047(4)	0.037(4)	-0.001(3)	0.005(3)	-0.002(3)
C(36)	0.039(4)	0.037(3)	0.033(4)	0.000(3)	0.000(3)	-0.005(3)

Table 12. Atomic coordinates and equivalent isotropic displacement parameters [\AA^2] for **syn-p1-TDAI**

	x	y	z	U(eq)	S.O.F.
I(2)	0.85027(5)	0.66558(2)	0.27581(2)	0.04721(9)	1
F(5)	1.2004(4)	0.58883(13)	0.06038(17)	0.0603(10)	1
F(6)	1.2113(4)	0.56958(11)	0.18715(16)	0.0518(8)	1
F(7)	0.5697(4)	0.61135(10)	0.06981(15)	0.0432(7)	1
F(8)	0.5820(4)	0.59347(9)	0.19676(14)	0.0384(6)	1
F(9)	0.9636(5)	0.50765(9)	0.25242(16)	0.0520(8)	1
F(10)	0.9825(6)	0.49531(11)	0.38162(19)	0.0622(9)	1
F(11)	0.9282(6)	0.55595(14)	0.46358(18)	0.0704(11)	1
F(12)	0.8616(6)	0.62917(13)	0.41776(18)	0.0727(11)	1
I(1A^a)	0.8511(5)	0.69398(10)	0.04637(18)	0.0455(3)	0.320(6)
F(1A^a)	0.840(5)	0.7176(7)	-0.0850(13)	0.064(5)	0.320(6)
F(2A^a)	0.858(4)	0.6700(8)	-0.1870(13)	0.070(5)	0.320(6)
F(3A^a)	0.893(5)	0.5919(7)	-0.1741(12)	0.078(6)	0.320(6)
F(4A^a)	0.917(5)	0.5606(8)	-0.0575(12)	0.061(5)	0.320(6)
C(10A^a)	0.858(5)	0.6610(12)	-0.0091(12)	0.0564(10)	0.320(6)
C(11A^a)	0.856(3)	0.6786(9)	-0.0686(11)	0.0564(10)	0.320(6)
C(12A^a)	0.875(3)	0.6583(9)	-0.1222(12)	0.0564(10)	0.320(6)
C(13A^a)	0.883(3)	0.6180(9)	-0.1278(10)	0.0564(10)	0.320(6)
C(14A^a)	0.894(4)	0.5986(10)	-0.0659(13)	0.0564(10)	0.320(6)
C(15A^a)	0.8808(8)	0.6165(2)	-0.0051(3)	0.0564(10)	0.320(6)
I(1B^b)	0.8453(2)	0.70003(6)	0.06402(13)	0.0455(3)	0.680(6)
F(1B^b)	0.842(2)	0.7025(4)	-0.1011(8)	0.098(4)	0.680(6)
F(2B^b)	0.874(2)	0.6499(6)	-0.1960(6)	0.125(7)	0.680(6)
F(3B^b)	0.914(2)	0.5716(5)	-0.1662(6)	0.111(5)	0.680(6)
F(4B^b)	0.916(2)	0.5484(4)	-0.0415(5)	0.069(3)	0.680(6)
C(10B^b)	0.862(2)	0.6556(6)	-0.0200(5)	0.0564(10)	0.680(6)
C(11B^b)	0.8598(14)	0.6666(4)	-0.0847(5)	0.0564(10)	0.680(6)
C(12B^b)	0.8737(14)	0.6404(5)	-0.1342(5)	0.0564(10)	0.680(6)
C(13B^b)	0.8965(14)	0.6011(4)	-0.1188(5)	0.0564(10)	0.680(6)
C(14B^b)	0.8989(17)	0.5884(5)	-0.0537(6)	0.0564(10)	0.680(6)
C(15B^b)	0.8808(8)	0.6165(2)	-0.0051(3)	0.0564(10)	0.680(6)
C(16)	0.8856(7)	0.60116(16)	0.0621(2)	0.0378(11)	1
C(17)	1.0456(7)	0.58913(17)	0.0934(3)	0.0399(11)	1
C(18)	1.0514(7)	0.57959(16)	0.1582(2)	0.0369(11)	1
C(19)	0.8987(6)	0.58155(14)	0.1955(2)	0.0327(10)	1
C(20)	0.7361(6)	0.59142(14)	0.1634(2)	0.0322(10)	1
C(21)	0.7302(6)	0.60098(14)	0.0983(2)	0.0344(10)	1
C(22)	0.9057(6)	0.57537(14)	0.2662(2)	0.0328(10)	1
C(23)	0.8810(7)	0.60697(15)	0.3098(3)	0.0377(11)	1
C(24)	0.8867(8)	0.59989(19)	0.3753(3)	0.0488(14)	1
C(25)	0.9201(8)	0.5623(2)	0.4000(3)	0.0477(13)	1
C(26)	0.9473(8)	0.53143(17)	0.3579(3)	0.0458(13)	1
C(27)	0.9392(7)	0.53799(15)	0.2919(3)	0.0384(11)	1
N(1)	0.1724(6)	0.21585(14)	0.3274(2)	0.0440(10)	1
N(2)	0.1846(6)	0.31569(12)	0.3978(2)	0.0380(9)	1

N(3)	0.1653(8)	0.23078(15)	0.5057(2)	0.0528(12)	1
C(1)	0.1730(6)	0.23926(15)	0.3794(3)	0.0345(10)	1
C(2)	0.1771(6)	0.27681(14)	0.4047(2)	0.0321(10)	1
C(3)	0.1701(7)	0.24500(15)	0.4454(3)	0.0366(10)	1
C(4)	0.1542(9)	0.17374(17)	0.3348(3)	0.0562(15)	1
C(5)	0.1749(8)	0.23138(18)	0.2626(3)	0.0476(13)	1
C(6)	0.1749(9)	0.33329(17)	0.3333(3)	0.0482(13)	1
C(7)	0.1919(7)	0.34036(15)	0.4553(3)	0.0384(11)	1
C(8)	0.1530(14)	0.2575(2)	0.5603(3)	0.082(3)	1
C(9)	0.1525(8)	0.18903(17)	0.5185(3)	0.0515(14)	1
I(3)	0.67667(4)	0.32323(2)	0.43797(2)	0.04083(9)	1
I(4)	0.62993(5)	0.35249(2)	0.21501(2)	0.03951(8)	1
F(13)	0.6849(5)	0.31638(10)	0.59191(19)	0.0622(9)	1
F(14)	0.6435(6)	0.36916(13)	0.68707(17)	0.0666(10)	1
F(15)	0.5917(6)	0.44649(12)	0.65954(17)	0.0678(10)	1
F(16)	0.5867(6)	0.47107(9)	0.53566(16)	0.0571(9)	1
F(17)	0.9349(4)	0.40731(9)	0.41566(14)	0.0418(6)	1
F(18)	0.9108(4)	0.42227(9)	0.28913(14)	0.0407(6)	1
F(19)	0.3139(4)	0.43826(9)	0.43463(14)	0.0417(7)	1
F(20)	0.2900(4)	0.45390(10)	0.30747(15)	0.0451(7)	1
F(21)	0.5370(5)	0.51107(9)	0.23616(14)	0.0484(8)	1
F(22)	0.4989(6)	0.52204(10)	0.10728(16)	0.0603(10)	1
F(23)	0.5253(7)	0.45976(11)	0.02531(16)	0.0719(12)	1
F(24)	0.5875(6)	0.38729(10)	0.07200(16)	0.0648(10)	1
C(28)	0.6578(6)	0.36629(14)	0.5118(2)	0.0339(10)	1
C(29)	0.6605(8)	0.35472(15)	0.5753(3)	0.0433(12)	1
C(30)	0.6383(8)	0.38121(19)	0.6258(3)	0.0478(13)	1
C(31)	0.6121(8)	0.42053(19)	0.6115(3)	0.0468(13)	1
C(32)	0.6098(8)	0.43245(15)	0.5480(2)	0.0392(11)	1
C(33)	0.6309(6)	0.40660(15)	0.4965(2)	0.0329(10)	1
C(34)	0.6232(6)	0.42085(13)	0.4287(2)	0.0301(9)	1
C(35)	0.4621(7)	0.43457(13)	0.3992(2)	0.0321(10)	1
C(36)	0.4511(7)	0.44268(14)	0.3339(2)	0.0330(10)	1
C(37)	0.5987(7)	0.43786(14)	0.2942(2)	0.0322(10)	1
C(38)	0.7622(6)	0.42633(14)	0.3243(2)	0.0319(10)	1
C(39)	0.7737(6)	0.41854(14)	0.3900(2)	0.0316(10)	1
C(40)	0.5801(7)	0.44300(14)	0.2236(2)	0.0335(10)	1
C(41)	0.5485(7)	0.47962(15)	0.1971(2)	0.0372(11)	1
C(42)	0.5292(8)	0.48613(15)	0.1311(3)	0.0435(12)	1
C(43)	0.5433(9)	0.45433(16)	0.0893(3)	0.0469(13)	1
C(44)	0.5779(8)	0.41729(16)	0.1147(3)	0.0443(12)	1
C(45)	0.5940(7)	0.41044(15)	0.1801(2)	0.0368(10)	1
H(4A)	0.172018	0.166668	0.380664	0.084	1
H(4AB)	0.246102	0.160356	0.309148	0.084	1
H(4AC)	0.032102	0.165542	0.31948	0.084	1
H(5A)	0.215614	0.258931	0.26405	0.071	1
H(5AB)	0.051978	0.230002	0.242675	0.071	1

H(5AC)	0.258893	0.215797	0.236808	0.071	1
H(6A)	0.285174	0.326556	0.309993	0.072	1
H(6AB)	0.165433	0.362052	0.337173	0.072	1
H(6AC)	0.067511	0.323119	0.309171	0.072	1
H(7A)	0.275892	0.328673	0.48789	0.058	1
H(7AB)	0.069865	0.342308	0.473066	0.058	1
H(7AC)	0.234953	0.366776	0.443851	0.058	1
H(8A)	0.275013	0.267161	0.572674	0.123	1
H(8AB)	0.1012	0.243473	0.597032	0.123	1
H(8AC)	0.074351	0.279811	0.547992	0.123	1
H(9A)	0.02698	0.18238	0.529256	0.077	1
H(9AB)	0.234984	0.182108	0.555158	0.077	1
H(9AC)	0.187005	0.174232	0.479933	0.077	1

Table 13. Anisotropic displacement parameters [Å²] for **syn-p-1-TDAI**

	U11	U22	U33	U23	U13	U12
I(2)	0.05336(19)	0.03311(17)	0.0552(2)	-0.01186(14)	0.00163(15)	-0.00008(14)
F(5)	0.0392(16)	0.101(3)	0.0409(18)	-0.0034(18)	0.0132(14)	0.0027(17)
F(6)	0.0355(15)	0.076(2)	0.0439(17)	0.0012(16)	0.0010(13)	0.0094(14)
F(7)	0.0366(14)	0.0547(19)	0.0384(15)	0.0030(13)	0.0007(12)	0.0026(13)
F(8)	0.0368(14)	0.0412(16)	0.0378(15)	0.0006(12)	0.0101(12)	0.0025(12)
F(9)	0.075(2)	0.0351(16)	0.0448(18)	-0.0034(13)	-0.0058(16)	0.0091(15)
F(10)	0.082(2)	0.051(2)	0.053(2)	0.0142(16)	-0.0080(18)	-0.0078(18)
F(11)	0.086(3)	0.095(3)	0.0298(17)	0.0051(18)	0.0037(17)	-0.010(2)
F(12)	0.103(3)	0.076(3)	0.0394(19)	-0.0281(18)	0.0081(19)	0.006(2)
I(1A^a)	0.0510(2)	0.0384(5)	0.0470(9)	0.0029(5)	-0.0001(5)	-0.0038(3)
F(1A^a)	0.093(11)	0.056(11)	0.042(9)	0.015(7)	-0.008(7)	0.010(10)
F(2A^a)	0.065(11)	0.110(14)	0.034(8)	0.003(8)	0.006(7)	0.001(10)
F(3A^a)	0.107(15)	0.101(15)	0.026(8)	-0.014(9)	0.011(8)	0.023(12)
F(4A^a)	0.090(10)	0.068(15)	0.027(10)	0.014(7)	0.014(8)	0.001(10)
C(10A^a)	0.0488(13)	0.096(4)	0.0250(19)	0.0058(17)	0.0055(12)	-0.0051(18)
C(11A^a)	0.0488(13)	0.096(4)	0.0250(19)	0.0058(17)	0.0055(12)	-0.0051(18)
C(12A^a)	0.0488(13)	0.096(4)	0.0250(19)	0.0058(17)	0.0055(12)	-0.0051(18)
C(13A^a)	0.0488(13)	0.096(4)	0.0250(19)	0.0058(17)	0.0055(12)	-0.0051(18)
C(14A^a)	0.0488(13)	0.096(4)	0.0250(19)	0.0058(17)	0.0055(12)	-0.0051(18)
C(15A^a)	0.0488(13)	0.096(4)	0.0250(19)	0.0058(17)	0.0055(12)	-0.0051(18)
I(1B^b)	0.0510(2)	0.0384(5)	0.0470(9)	0.0029(5)	-0.0001(5)	-0.0038(3)
F(1B^b)	0.088(6)	0.119(12)	0.088(11)	0.064(8)	0.000(7)	-0.006(9)
F(2B^b)	0.072(5)	0.27(2)	0.033(5)	0.045(9)	0.006(4)	0.025(11)
F(3B^b)	0.089(6)	0.207(16)	0.037(5)	-0.034(9)	0.007(4)	0.019(11)
F(4B^b)	0.095(5)	0.076(8)	0.035(6)	-0.015(4)	0.015(5)	-0.001(6)
C(10B^b)	0.0488(13)	0.096(4)	0.0250(19)	0.0058(17)	0.0055(12)	-0.0051(18)
C(11B^b)	0.0488(13)	0.096(4)	0.0250(19)	0.0058(17)	0.0055(12)	-0.0051(18)
C(12B^b)	0.0488(13)	0.096(4)	0.0250(19)	0.0058(17)	0.0055(12)	-0.0051(18)
C(13B^b)	0.0488(13)	0.096(4)	0.0250(19)	0.0058(17)	0.0055(12)	-0.0051(18)
C(14B^b)	0.0488(13)	0.096(4)	0.0250(19)	0.0058(17)	0.0055(12)	-0.0051(18)
C(15B^b)	0.0488(13)	0.096(4)	0.0250(19)	0.0058(17)	0.0055(12)	-0.0051(18)
C(16)	0.042(3)	0.045(3)	0.027(2)	-0.007(2)	0.003(2)	-0.005(2)
C(17)	0.036(2)	0.050(3)	0.035(3)	-0.008(2)	0.010(2)	-0.004(2)
C(18)	0.036(2)	0.043(3)	0.031(3)	-0.005(2)	0.002(2)	0.001(2)
C(19)	0.038(2)	0.030(2)	0.030(2)	-0.0054(18)	0.0039(19)	0.0006(19)
C(20)	0.036(2)	0.028(2)	0.033(2)	-0.0051(18)	0.0095(19)	-0.0007(18)
C(21)	0.035(2)	0.035(3)	0.033(2)	-0.0006(19)	-0.0037(19)	-0.0013(19)
C(22)	0.032(2)	0.033(2)	0.034(3)	-0.0023(19)	0.0041(19)	-0.0004(18)
C(23)	0.043(3)	0.035(3)	0.035(3)	-0.010(2)	0.006(2)	-0.001(2)
C(24)	0.050(3)	0.060(4)	0.036(3)	-0.016(3)	0.004(2)	-0.007(3)
C(25)	0.050(3)	0.069(4)	0.025(3)	0.001(2)	0.002(2)	-0.012(3)
C(26)	0.050(3)	0.045(3)	0.042(3)	0.009(2)	-0.002(2)	-0.009(2)
C(27)	0.045(3)	0.037(3)	0.033(3)	-0.005(2)	0.003(2)	-0.002(2)
N(1)	0.055(3)	0.040(2)	0.037(2)	-0.0101(19)	0.002(2)	0.000(2)
N(2)	0.053(2)	0.033(2)	0.029(2)	0.0015(16)	0.0029(18)	-0.0018(18)

N(3)	0.086(4)	0.042(3)	0.031(2)	0.0045(19)	0.006(2)	-0.007(2)
C(1)	0.035(2)	0.034(2)	0.034(3)	-0.005(2)	0.0022(19)	-0.0022(19)
C(2)	0.036(2)	0.033(2)	0.027(2)	-0.0039(18)	0.0013(18)	0.0002(19)
C(3)	0.042(3)	0.029(2)	0.039(3)	0.000(2)	-0.001(2)	-0.0014(19)
C(4)	0.076(4)	0.038(3)	0.055(4)	-0.013(3)	0.004(3)	-0.008(3)
C(5)	0.051(3)	0.056(4)	0.036(3)	-0.010(2)	-0.001(2)	0.001(3)
C(6)	0.069(4)	0.039(3)	0.037(3)	0.010(2)	0.006(3)	0.004(3)
C(7)	0.045(3)	0.034(3)	0.036(3)	-0.006(2)	0.000(2)	0.005(2)
C(8)	0.155(8)	0.059(4)	0.032(3)	0.005(3)	0.018(4)	-0.007(5)
C(9)	0.058(3)	0.042(3)	0.054(3)	0.019(3)	0.002(3)	-0.002(3)
I(3)	0.03904(16)	0.03042(16)	0.05317(19)	-0.00658(13)	0.00367(13)	0.00039(12)
I(4)	0.05278(18)	0.02852(15)	0.03725(16)	-0.00189(12)	0.00172(13)	0.00163(13)
F(13)	0.083(2)	0.044(2)	0.059(2)	0.0206(16)	-0.0032(19)	0.0049(17)
F(14)	0.091(3)	0.079(3)	0.0304(17)	0.0198(17)	0.0056(17)	0.007(2)
F(15)	0.097(3)	0.075(3)	0.0316(17)	-0.0123(16)	0.0045(17)	0.019(2)
F(16)	0.098(3)	0.0330(17)	0.0400(17)	-0.0048(13)	0.0005(17)	0.0150(16)
F(17)	0.0353(14)	0.0535(18)	0.0363(15)	0.0028(13)	-0.0013(12)	0.0051(12)
F(18)	0.0377(14)	0.0516(18)	0.0333(15)	-0.0002(12)	0.0081(12)	0.0017(12)
F(19)	0.0424(15)	0.0461(17)	0.0373(15)	0.0029(12)	0.0113(12)	0.0069(13)
F(20)	0.0392(15)	0.0593(19)	0.0364(15)	0.0053(13)	-0.0034(12)	0.0108(13)
F(21)	0.083(2)	0.0320(15)	0.0299(14)	-0.0070(12)	0.0005(14)	0.0064(15)
F(22)	0.113(3)	0.0339(17)	0.0343(16)	0.0028(13)	0.0002(18)	0.0089(18)
F(23)	0.141(4)	0.051(2)	0.0232(16)	0.0010(14)	0.0014(19)	0.011(2)
F(24)	0.123(3)	0.0389(18)	0.0320(16)	-0.0112(13)	-0.0016(19)	0.0111(19)
C(28)	0.035(2)	0.032(2)	0.034(2)	-0.0043(19)	0.0030(19)	-0.0012(19)
C(29)	0.050(3)	0.031(3)	0.048(3)	0.011(2)	0.002(2)	-0.001(2)
C(30)	0.050(3)	0.063(4)	0.031(3)	0.012(2)	0.009(2)	0.007(3)
C(31)	0.053(3)	0.056(3)	0.032(3)	-0.006(2)	0.004(2)	0.003(3)
C(32)	0.056(3)	0.036(3)	0.026(2)	-0.0035(19)	0.004(2)	0.001(2)
C(33)	0.035(2)	0.035(2)	0.029(2)	0.0003(19)	0.0015(18)	0.0019(19)
C(34)	0.040(2)	0.024(2)	0.026(2)	-0.0025(17)	0.0045(19)	-0.0021(18)
C(35)	0.040(2)	0.027(2)	0.029(2)	-0.0041(18)	0.0062(19)	-0.0002(19)
C(36)	0.039(2)	0.030(2)	0.030(2)	-0.0019(18)	-0.0011(19)	0.0023(19)
C(37)	0.045(3)	0.026(2)	0.026(2)	-0.0022(17)	0.0018(19)	0.0010(19)
C(38)	0.035(2)	0.034(2)	0.026(2)	-0.0040(18)	0.0062(19)	0.0013(19)
C(39)	0.034(2)	0.032(2)	0.029(2)	-0.0027(18)	0.0004(18)	0.0001(19)
C(40)	0.043(3)	0.031(2)	0.027(2)	-0.0019(18)	-0.0002(19)	0.001(2)
C(41)	0.054(3)	0.032(3)	0.026(2)	-0.0080(19)	0.002(2)	-0.001(2)
C(42)	0.070(3)	0.032(3)	0.029(3)	0.002(2)	0.003(2)	0.002(2)
C(43)	0.079(4)	0.038(3)	0.023(2)	-0.004(2)	0.000(2)	0.005(3)
C(44)	0.069(4)	0.036(3)	0.027(3)	-0.008(2)	-0.001(2)	0.006(2)
C(45)	0.046(3)	0.034(3)	0.031(3)	-0.0001(19)	0.002(2)	0.000(2)
I(5)	0.04917(18)	0.03127(17)	0.0704(2)	-0.00877(15)	0.00191(16)	0.00168(14)

Table S14. Atomic coordinates and equivalent isotropic displacement parameters [\AA^2] for **anti-p-1-TDACI**

	x	y	z	U(eq)	S.O.F.
I(1)	0.51402(3)	0.84424(2)	0.28855(2)	0.04085(8)	1
I(2)	0.83268(3)	0.30002(2)	0.14595(2)	0.03982(8)	1
F(1)	1.1196(3)	0.35373(19)	0.03187(10)	0.0472(5)	1
F(2)	1.3400(3)	0.5246(2)	-0.01405(10)	0.0523(6)	1
F(3)	1.3226(3)	0.7053(2)	0.03306(11)	0.0561(6)	1
F(4)	1.0701(3)	0.72006(19)	0.12171(11)	0.0528(6)	1
F(5)	0.6167(3)	0.5774(2)	0.10605(10)	0.0510(5)	1
F(6)	0.3653(3)	0.6049(2)	0.19098(10)	0.0522(6)	1
F(7)	0.7613(3)	0.5644(2)	0.33117(10)	0.0552(6)	1
F(8)	1.0133(3)	0.5368(2)	0.24640(10)	0.0531(6)	1
F(9)	0.3286(3)	0.41135(18)	0.31776(11)	0.0517(5)	1
F(10)	0.0765(3)	0.4159(2)	0.40820(12)	0.0613(7)	1
F(11)	0.0265(3)	0.6017(2)	0.45063(12)	0.0621(7)	1
F(12)	0.2212(3)	0.7847(2)	0.39952(12)	0.0592(7)	1
C(1)	0.3831(5)	0.6929(3)	0.33173(16)	0.0380(7)	1
C(2)	0.2527(5)	0.6932(3)	0.37861(17)	0.0443(8)	1
C(3)	0.1499(5)	0.5998(3)	0.40519(17)	0.0446(8)	1
C(4)	0.1763(5)	0.5057(3)	0.38406(18)	0.0447(9)	1
C(5)	0.3073(5)	0.5051(3)	0.33749(16)	0.0395(8)	1
C(6)	0.4131(4)	0.5957(3)	0.31176(15)	0.0358(7)	1
C(7)	0.5548(4)	0.5859(3)	0.26357(16)	0.0362(7)	1
C(8)	0.5250(4)	0.5877(3)	0.20534(17)	0.0387(8)	1
C(9)	0.6554(5)	0.5736(3)	0.16131(16)	0.0395(8)	1
C(10)	0.8233(4)	0.5555(3)	0.17364(16)	0.0357(7)	1
C(11)	0.8528(4)	0.5543(3)	0.23170(17)	0.0391(8)	1
C(12)	0.7231(5)	0.5685(3)	0.27639(16)	0.0397(8)	1
C(13)	0.9630(4)	0.5419(3)	0.12557(15)	0.0360(7)	1
C(14)	1.0797(5)	0.6274(3)	0.10088(16)	0.0397(8)	1
C(15)	1.2097(5)	0.6216(3)	0.05500(17)	0.0431(8)	1
C(16)	1.2188(4)	0.5294(3)	0.03179(16)	0.0408(8)	1
C(17)	1.1043(5)	0.4425(3)	0.05603(16)	0.0376(7)	1
C(18)	0.9780(4)	0.4455(3)	0.10363(15)	0.0355(7)	1
N(1)	0.0178(4)	0.1274(3)	0.29485(14)	0.0446(7)	1
N(2)	0.1590(5)	-0.0486(3)	0.19037(16)	0.0503(8)	1
N(3)	0.3034(4)	0.2433(3)	0.15341(14)	0.0423(7)	1
C(29)	0.1077(5)	0.1154(3)	0.24376(16)	0.0391(8)	1
C(30)	0.1615(5)	0.0488(3)	0.20505(17)	0.0408(8)	1
C(31)	0.2174(4)	0.1575(3)	0.19136(16)	0.0389(8)	1
C(32)	-0.0086(6)	0.2353(4)	0.3073(2)	0.0561(10)	1
C(33)	-0.0660(6)	0.0305(4)	0.33747(18)	0.0535(10)	1
C(34)	0.0486(6)	-0.1393(4)	0.2284(2)	0.0589(11)	1
C(35)	0.2838(6)	-0.0703(4)	0.1420(2)	0.0587(11)	1
C(36)	0.4072(5)	0.2240(4)	0.09928(18)	0.0478(9)	1
C(37)	0.3447(5)	0.3380(3)	0.17639(19)	0.0486(9)	1
Cl(1)	0.65210(14)	0.07546(8)	0.21791(4)	0.0533(2)	1
Cl(2A)	0.2130(6)	-0.0736(2)	0.96744(13)	0.1238(13)	0.700(4)
Cl(3A)	0.3050(4)	0.1568(2)	0.92796(16)	0.1032(8)	0.700(4)
C(28A)	0.1874(15)	0.0502(6)	0.9126(5)	0.082(3)	0.700(4)
Cl(2B)	0.053(2)	-0.0949(8)	0.9575(5)	0.1238(13)	0.198(3)
Cl(3B)	0.3114(13)	0.0737(9)	0.9542(5)	0.1032(8)	0.198(3)
C(28B)	0.189(5)	0.011(3)	0.9131(13)	0.082(3)	0.198(3)
Cl(2C)	0.366(4)	-0.0211(15)	0.9756(8)	0.1238(13)	0.101(3)
Cl(3C)	0.274(3)	0.1607(15)	0.8896(10)	0.1032(8)	0.101(3)
C(28C)	0.237(10)	0.017(2)	0.918(3)	0.082(3)	0.101(3)
I(3)	0.42807(3)	0.12129(2)	0.35804(2)	0.04968(9)	1

F(13)	0.6392(3)	0.3106(2)	0.38212(11)	0.0563(6)	1
F(14)	0.6282(3)	0.4097(2)	0.47355(12)	0.0573(6)	1
F(15)	0.3797(3)	0.3537(2)	0.56997(11)	0.0544(6)	1
F(16)	0.1493(3)	0.19405(19)	0.57558(10)	0.0479(5)	1
F(17)	-0.0838(3)	0.21832(16)	0.47676(10)	0.0435(5)	1
F(18)	-0.3309(3)	0.06491(18)	0.49898(11)	0.0484(5)	1
C(19)	0.3966(5)	0.1976(3)	0.43048(16)	0.0391(8)	1
C(20)	0.5138(5)	0.2796(3)	0.42908(17)	0.0411(8)	1
C(21)	0.5102(5)	0.3326(3)	0.47548(18)	0.0431(8)	1
C(22)	0.3855(5)	0.3038(3)	0.52452(17)	0.0420(8)	1
C(23)	0.2669(5)	0.2223(3)	0.52654(16)	0.0380(7)	1
C(24)	0.2682(4)	0.1680(3)	0.48001(16)	0.0357(7)	1
C(25)	0.1324(5)	0.0821(3)	0.48784(16)	0.0355(7)	1
C(26)	-0.0398(5)	0.1105(3)	0.48888(16)	0.0369(7)	1
C(27)	-0.1673(4)	0.0313(3)	0.50065(16)	0.0375(7)	1
H(32A)	-0.074496	0.226907	0.347458	0.084	0.5
H(32B)	-0.071892	0.282345	0.276552	0.084	0.5
H(32C)	0.102694	0.270127	0.306275	0.084	0.5
H(32D)	0.045367	0.292679	0.272732	0.084	0.5
H(32E)	0.042762	0.237241	0.343638	0.084	0.5
H(32F)	-0.131823	0.249459	0.313915	0.084	0.5
H(33A)	-0.130557	0.053491	0.37183	0.08	0.5
H(33B)	0.020696	-0.024062	0.352127	0.08	0.5
H(33C)	-0.144694	-0.003317	0.317155	0.08	0.5
H(33D)	-0.039146	-0.036083	0.322245	0.08	0.5
H(33E)	-0.1904	0.04147	0.341947	0.08	0.5
H(33F)	-0.025009	0.020725	0.376919	0.08	0.5
H(34A)	0.005706	-0.182516	0.202792	0.088	0.5
H(34B)	-0.04844	-0.108196	0.250076	0.088	0.5
H(34C)	0.114406	-0.188019	0.257644	0.088	0.5
H(34D)	0.042076	-0.136637	0.270882	0.088	0.5
H(34E)	0.096222	-0.210958	0.223599	0.088	0.5
H(34F)	-0.066625	-0.131135	0.216031	0.088	0.5
H(35A)	0.28205	-0.149971	0.143115	0.088	0.5
H(35B)	0.398538	-0.048813	0.14759	0.088	0.5
H(35C)	0.254979	-0.026909	0.102785	0.088	0.5
H(35D)	0.341662	-0.000491	0.119212	0.088	0.5
H(35E)	0.225174	-0.101649	0.114737	0.088	0.5
H(35F)	0.368732	-0.123553	0.159542	0.088	0.5
H(36A)	0.489083	0.285726	0.082366	0.072	0.5
H(36B)	0.332271	0.219361	0.069081	0.072	0.5
H(36C)	0.469685	0.153952	0.110117	0.072	0.5
H(36D)	0.371609	0.153633	0.09201	0.072	0.5
H(36E)	0.528422	0.219998	0.105296	0.072	0.5
H(36F)	0.391007	0.285408	0.064259	0.072	0.5
H(37A)	0.384564	0.400714	0.142292	0.073	0.5
H(37B)	0.435126	0.31697	0.202524	0.073	0.5
H(37C)	0.242115	0.35981	0.199781	0.073	0.5
H(37D)	0.323306	0.317615	0.220773	0.073	0.5
H(37E)	0.272744	0.40136	0.160541	0.073	0.5
H(37F)	0.465755	0.358519	0.163284	0.073	0.5
H(28A)	0.064509	0.070094	0.913811	0.099	0.700(4)
H(28B)	0.22941	0.04036	0.871668	0.099	0.700(4)
H(28C)	0.119639	0.069344	0.889342	0.099	0.198(3)
H(28D)	0.267741	-0.019641	0.884077	0.099	0.198(3)
H(28E)	0.114924	0.000436	0.933492	0.099	0.101(3)
H(28F)	0.271478	-0.023479	0.885664	0.099	0.101(3)

Table S15. Anisotropic displacement parameters [Å²] for **anti-p-1-TDACI**

	U11	U22	U33	U23	U13	U12
I(1)	0.03744(13)	0.03616(13)	0.04811(14)	-0.01337(10)	0.00428(9)	-0.00613(9)
I(2)	0.03303(13)	0.03523(13)	0.05143(14)	-0.01078(10)	-0.00576(9)	-0.00188(9)
F(1)	0.0447(12)	0.0512(13)	0.0520(12)	-0.0256(10)	-0.0053(9)	0.0068(10)
F(2)	0.0377(11)	0.0723(16)	0.0449(11)	-0.0167(11)	0.0053(9)	0.0014(11)
F(3)	0.0432(12)	0.0554(14)	0.0634(14)	-0.0080(11)	0.0059(10)	-0.0166(11)
F(4)	0.0515(13)	0.0416(12)	0.0679(14)	-0.0230(11)	0.0042(11)	-0.0118(10)
F(5)	0.0396(12)	0.0756(16)	0.0431(11)	-0.0239(11)	-0.0075(9)	0.0065(11)
F(6)	0.0318(11)	0.0772(16)	0.0517(12)	-0.0231(11)	-0.0081(9)	0.0080(11)
F(7)	0.0427(12)	0.0849(18)	0.0427(11)	-0.0247(11)	-0.0067(9)	0.0072(12)
F(8)	0.0294(11)	0.0838(17)	0.0506(12)	-0.0245(12)	-0.0068(9)	0.0038(11)
F(9)	0.0545(14)	0.0364(11)	0.0632(13)	-0.0171(10)	0.0061(11)	-0.0053(10)
F(10)	0.0587(15)	0.0404(12)	0.0733(16)	-0.0062(11)	0.0203(12)	-0.0124(11)
F(11)	0.0591(15)	0.0514(14)	0.0634(14)	-0.0094(11)	0.0285(12)	-0.0022(12)
F(12)	0.0653(16)	0.0426(13)	0.0654(14)	-0.0223(11)	0.0258(12)	-0.0056(11)
C(1)	0.0328(17)	0.0382(19)	0.0420(18)	-0.0108(15)	0.0012(14)	-0.0024(15)
C(2)	0.046(2)	0.039(2)	0.047(2)	-0.0142(16)	0.0077(16)	-0.0017(17)
C(3)	0.041(2)	0.040(2)	0.0465(19)	-0.0068(16)	0.0096(16)	0.0008(16)
C(4)	0.041(2)	0.0361(19)	0.049(2)	-0.0020(16)	0.0062(16)	-0.0096(16)
C(5)	0.0404(19)	0.0323(18)	0.0447(18)	-0.0089(14)	-0.0027(15)	0.0014(15)
C(6)	0.0298(17)	0.0379(18)	0.0389(17)	-0.0090(14)	-0.0018(13)	-0.0002(14)
C(7)	0.0317(17)	0.0343(17)	0.0423(17)	-0.0117(14)	0.0007(14)	0.0005(14)
C(8)	0.0279(17)	0.043(2)	0.0468(19)	-0.0143(15)	-0.0035(14)	-0.0018(15)
C(9)	0.0375(19)	0.045(2)	0.0383(17)	-0.0165(15)	-0.0016(14)	-0.0012(16)
C(10)	0.0308(17)	0.0324(17)	0.0441(18)	-0.0125(14)	-0.0004(14)	0.0006(14)
C(11)	0.0266(16)	0.047(2)	0.0460(19)	-0.0157(16)	-0.0041(14)	0.0009(15)
C(12)	0.0379(19)	0.047(2)	0.0369(17)	-0.0161(15)	-0.0032(14)	-0.0007(16)
C(13)	0.0297(17)	0.0403(19)	0.0377(17)	-0.0106(14)	-0.0007(13)	-0.0014(14)
C(14)	0.0384(19)	0.0376(19)	0.0440(18)	-0.0116(15)	-0.0053(15)	-0.0015(15)
C(15)	0.0329(18)	0.046(2)	0.0453(19)	-0.0044(16)	-0.0007(15)	-0.0075(16)
C(16)	0.0296(17)	0.054(2)	0.0373(17)	-0.0104(16)	-0.0022(14)	0.0034(16)
C(17)	0.0322(17)	0.0434(19)	0.0402(17)	-0.0162(15)	-0.0056(14)	0.0072(15)
C(18)	0.0279(16)	0.0395(18)	0.0397(17)	-0.0103(14)	-0.0056(13)	0.0006(14)
N(1)	0.0382(16)	0.0511(19)	0.0428(16)	-0.0107(14)	0.0009(13)	-0.0057(14)
N(2)	0.0472(19)	0.0421(18)	0.063(2)	-0.0191(15)	0.0016(15)	-0.0078(15)
N(3)	0.0354(16)	0.0411(17)	0.0483(16)	-0.0095(13)	0.0002(13)	-0.0056(13)
C(29)	0.0319(17)	0.0412(19)	0.0434(18)	-0.0080(15)	-0.0057(14)	-0.0036(15)
C(30)	0.0335(18)	0.0405(19)	0.0464(19)	-0.0076(15)	-0.0030(15)	-0.0027(15)
C(31)	0.0306(17)	0.0405(19)	0.0447(18)	-0.0088(15)	-0.0046(14)	0.0008(15)
C(32)	0.055(3)	0.055(3)	0.056(2)	-0.016(2)	0.0034(19)	0.005(2)
C(33)	0.048(2)	0.065(3)	0.043(2)	-0.0081(18)	0.0032(17)	-0.014(2)
C(34)	0.059(3)	0.048(2)	0.069(3)	-0.017(2)	0.002(2)	-0.016(2)
C(35)	0.056(3)	0.056(3)	0.068(3)	-0.027(2)	0.002(2)	-0.006(2)
C(36)	0.040(2)	0.053(2)	0.048(2)	-0.0093(17)	0.0018(16)	-0.0049(18)
C(37)	0.042(2)	0.045(2)	0.057(2)	-0.0106(18)	-0.0049(17)	-0.0059(17)
Cl(1)	0.0592(6)	0.0407(5)	0.0567(5)	-0.0041(4)	-0.0084(4)	-0.0126(4)

CI(2A)	0.201(4)	0.0653(13)	0.0933(15)	-0.0154(11)	0.011(2)	0.0214(19)
CI(3A)	0.0995(16)	0.0910(16)	0.121(2)	-0.0334(16)	-0.0061(15)	0.0020(14)
C(28A)	0.101(6)	0.070(7)	0.077(4)	-0.021(5)	-0.010(4)	0.033(6)
CI(2B)	0.201(4)	0.0653(13)	0.0933(15)	-0.0154(11)	0.011(2)	0.0214(19)
CI(3B)	0.0995(16)	0.0910(16)	0.121(2)	-0.0334(16)	-0.0061(15)	0.0020(14)
C(28B)	0.101(6)	0.070(7)	0.077(4)	-0.021(5)	-0.010(4)	0.033(6)
CI(2C)	0.201(4)	0.0653(13)	0.0933(15)	-0.0154(11)	0.011(2)	0.0214(19)
CI(3C)	0.0995(16)	0.0910(16)	0.121(2)	-0.0334(16)	-0.0061(15)	0.0020(14)
C(28C)	0.101(6)	0.070(7)	0.077(4)	-0.021(5)	-0.010(4)	0.033(6)
I(3)	0.04569(15)	0.05637(16)	0.05325(15)	-0.02590(12)	-0.00649(11)	0.00731(12)
F(13)	0.0424(12)	0.0628(15)	0.0598(13)	-0.0164(11)	0.0116(10)	-0.0122(11)
F(14)	0.0477(13)	0.0474(13)	0.0777(16)	-0.0188(12)	-0.0023(11)	-0.0169(11)
F(15)	0.0659(15)	0.0480(13)	0.0543(13)	-0.0216(10)	-0.0071(11)	-0.0080(11)
F(16)	0.0512(13)	0.0443(12)	0.0449(11)	-0.0115(9)	0.0078(9)	-0.0073(10)
F(17)	0.0386(11)	0.0287(10)	0.0607(12)	-0.0094(9)	-0.0012(9)	0.0028(8)
F(18)	0.0298(10)	0.0374(11)	0.0762(15)	-0.0104(10)	-0.0086(10)	0.0041(9)
C(19)	0.0370(18)	0.0368(18)	0.0446(18)	-0.0129(15)	-0.0042(15)	0.0055(15)
C(20)	0.0307(17)	0.0401(19)	0.0485(19)	-0.0062(15)	0.0008(14)	-0.0010(15)
C(21)	0.0399(19)	0.0311(17)	0.057(2)	-0.0076(15)	-0.0078(16)	-0.0050(15)
C(22)	0.048(2)	0.0353(18)	0.0456(19)	-0.0126(15)	-0.0108(16)	0.0022(16)
C(23)	0.0374(18)	0.0347(18)	0.0406(17)	-0.0082(14)	-0.0027(14)	0.0005(15)
C(24)	0.0317(17)	0.0287(16)	0.0456(18)	-0.0080(14)	-0.0034(14)	0.0005(14)
C(25)	0.0341(17)	0.0305(17)	0.0421(17)	-0.0098(14)	-0.0041(14)	0.0001(14)
C(26)	0.0376(18)	0.0306(17)	0.0424(17)	-0.0096(14)	-0.0036(14)	0.0011(14)
C(27)	0.0298(17)	0.0344(18)	0.0477(18)	-0.0096(14)	-0.0043(14)	0.0014(14)

Table S16. Atomic coordinates and equivalent isotropic displacement parameters [\AA^2] for **anti-p-1-TDABr**

	x	y	z	U(eq)	S.O.F.
I(1)	0.43198(3)	0.11959(2)	0.35969(2)	0.04006(9)	1
F(1)	-0.3334(3)	0.06396(19)	0.49815(12)	0.0389(5)	1
N(1)	0.1739(5)	-0.0527(3)	0.19085(18)	0.0428(8)	1
C(1)	-0.1696(5)	0.0304(3)	0.50020(17)	0.0289(7)	1
I(2)	0.51986(3)	0.83267(2)	0.29180(2)	0.03396(8)	1
Br(2)	0.66220(6)	0.06982(3)	0.21780(2)	0.04245(12)	1
F(2)	-0.0882(3)	0.21644(17)	0.47653(11)	0.0347(5)	1
C(2)	-0.0420(5)	0.1097(3)	0.48873(16)	0.0287(7)	1
N(2)	0.0266(5)	0.1232(3)	0.29527(15)	0.0364(7)	1
N(3)	0.3059(4)	0.2388(3)	0.15350(15)	0.0371(7)	1
F(3)	0.1421(3)	0.1949(2)	0.57563(10)	0.0399(5)	1
I(3)	0.84456(3)	0.30045(2)	0.14214(2)	0.03284(8)	1
C(3)	0.1311(5)	0.0814(3)	0.48805(16)	0.0276(7)	1
C(27)	1.0823(5)	0.6263(3)	0.10121(18)	0.0336(8)	1
C(28)	0.2239(5)	0.1536(3)	0.19143(18)	0.0325(8)	1
C(29)	0.1714(5)	0.0448(3)	0.20501(17)	0.0320(8)	1
C(30)	0.1151(5)	0.1117(3)	0.24426(17)	0.0319(8)	1
C(31)	0.2992(7)	-0.0738(4)	0.1421(2)	0.0531(12)	1
C(32)	0.0644(7)	-0.1426(4)	0.2282(2)	0.0497(11)	1
C(33)	-0.0522(6)	0.0267(4)	0.33830(19)	0.0438(10)	1
C(34)	-0.0096(7)	0.2309(4)	0.3074(2)	0.0508(11)	1
C(35)	0.3475(6)	0.3323(4)	0.1769(2)	0.0409(9)	1
C(36)	0.4079(6)	0.2212(4)	0.09871(19)	0.0421(10)	1
C(37A)	0.8175(10)	0.9459(5)	0.0834(3)	0.0824(19)	0.888(3)
Cl(1A)	0.7833(5)	1.06687(19)	0.03084(11)	0.1167(11)	0.888(3)
Cl(2A)	0.7073(3)	0.8336(2)	0.06788(12)	0.0973(7)	0.888(3)
C(37B)	0.8175(10)	0.9459(5)	0.0834(3)	0.0824(19)	0.112(3)
Cl(1B)	0.922(3)	1.0799(12)	0.0510(9)	0.1167(11)	0.112(3)
Cl(2B)	0.683(2)	0.9188(16)	0.0362(9)	0.0973(7)	0.112(3)
C(26)	1.2121(5)	0.6234(3)	0.05437(18)	0.0352(8)	1
C(25)	1.2250(5)	0.5326(4)	0.02990(16)	0.0325(8)	1
C(24)	1.1122(5)	0.4453(3)	0.05329(16)	0.0305(8)	1
C(23)	0.9863(5)	0.4465(3)	0.10148(16)	0.0281(7)	1
C(22)	0.9669(5)	0.5393(3)	0.12521(16)	0.0289(7)	1
C(21)	0.7270(5)	0.5598(3)	0.27627(17)	0.0319(8)	1
C(20)	0.8579(5)	0.5478(3)	0.23156(18)	0.0323(8)	1
C(9)	0.3955(5)	0.1967(3)	0.43183(16)	0.0283(7)	1
F(9)	0.0738(4)	0.4132(2)	0.40849(13)	0.0541(7)	1
C(8)	0.5111(5)	0.2795(3)	0.43033(18)	0.0336(8)	1
F(8)	0.0273(4)	0.5978(2)	0.45231(13)	0.0555(7)	1
C(7)	0.5037(5)	0.3323(3)	0.47649(19)	0.0348(8)	1
F(7)	0.2276(4)	0.7768(2)	0.40270(12)	0.0524(7)	1
C(6)	0.3771(5)	0.3046(3)	0.52515(18)	0.0340(8)	1
F(6)	0.6375(3)	0.3088(2)	0.38426(12)	0.0457(6)	1
C(5)	0.2611(5)	0.2225(3)	0.52684(16)	0.0301(8)	1

F(5)	0.6204(3)	0.4095(2)	0.47467(13)	0.0495(6)	1
C(4)	0.2650(5)	0.1672(3)	0.48112(16)	0.0275(7)	1
F(4)	0.3684(4)	0.3551(2)	0.57025(11)	0.0467(6)	1
C(11)	0.2565(6)	0.6856(3)	0.38086(18)	0.0367(9)	1
F(11)	0.3652(3)	0.5984(2)	0.19332(11)	0.0458(6)	1
C(10)	0.3860(5)	0.6838(3)	0.33422(17)	0.0303(8)	1
F(10)	0.3268(3)	0.4060(2)	0.31796(12)	0.0453(6)	1
C(12)	0.1516(6)	0.5952(4)	0.40677(18)	0.0382(9)	1
F(12)	0.6178(3)	0.5740(2)	0.10748(10)	0.0442(6)	1
C(14)	0.3062(5)	0.4986(3)	0.33864(18)	0.0328(8)	1
F(14)	1.0187(3)	0.5304(3)	0.24544(11)	0.0466(6)	1
C(13)	0.1749(6)	0.5009(3)	0.38505(19)	0.0374(9)	1
F(13)	0.7648(3)	0.5550(3)	0.33123(11)	0.0476(6)	1
F(15)	1.0706(3)	0.7168(2)	0.12351(12)	0.0469(6)	1
C(15)	0.4154(5)	0.5883(3)	0.31316(16)	0.0286(7)	1
F(16)	1.3227(4)	0.7071(2)	0.03321(13)	0.0515(7)	1
C(16)	0.5572(5)	0.5780(3)	0.26483(16)	0.0281(7)	1
C(19)	0.8262(5)	0.5513(3)	0.17348(16)	0.0282(7)	1
C(18)	0.6577(5)	0.5686(3)	0.16249(17)	0.0318(8)	1
F(18)	1.1305(3)	0.3586(2)	0.02756(11)	0.0411(5)	1
C(17)	0.5268(5)	0.5816(3)	0.20696(18)	0.0307(8)	1
F(17)	1.3457(3)	0.5306(2)	-0.01681(11)	0.0453(6)	1
H(31A)	0.246319	-0.05939	0.105051	0.08	1
H(31B)	0.336665	-0.15108	0.152121	0.08	1
H(31C)	0.399045	-0.025092	0.136417	0.08	1
H(32A)	-0.047141	-0.112641	0.242029	0.075	1
H(32B)	0.120436	-0.179337	0.262991	0.075	1
H(32C)	0.046356	-0.196106	0.204629	0.075	1
H(33A)	-0.171886	0.019645	0.331709	0.066	1
H(33B)	-0.050148	0.035332	0.379236	0.066	1
H(33C)	0.012402	-0.039798	0.332872	0.066	1
H(34A)	0.051073	0.287598	0.274854	0.076	1
H(34B)	0.029702	0.233275	0.345504	0.076	1
H(34C)	-0.134013	0.24488	0.310061	0.076	1
H(35A)	0.410175	0.38829	0.14452	0.061	1
H(35B)	0.419467	0.307027	0.208982	0.061	1
H(35C)	0.240654	0.364544	0.193078	0.061	1
H(36A)	0.34139	0.17689	0.079894	0.063	1
H(36B)	0.514548	0.182086	0.10861	0.063	1
H(36C)	0.436335	0.292774	0.070802	0.063	1
H(37A)	0.773701	0.954616	0.124282	0.099	0.888(3)
H(37B)	0.942539	0.929843	0.081466	0.099	0.888(3)
H(37C)	0.905899	0.887069	0.089504	0.099	0.112(3)
H(37D)	0.750548	0.94649	0.12292	0.099	0.112(3)

Table S17. Anisotropic displacement parameters [Å²] for **anti-p-1-TDABr**

	U11	U22	U33	U23	U13	U12
I(1)	0.03698(16)	0.04769(16)	0.03985(15)	-0.02111(11)	-0.00252(11)	0.00502(11)
F(1)	0.0217(11)	0.0327(11)	0.0604(14)	-0.0078(10)	-0.0051(10)	0.0035(9)
N(1)	0.038(2)	0.0387(19)	0.052(2)	-0.0175(16)	0.0045(16)	-0.0063(16)
C(1)	0.0219(18)	0.0295(19)	0.0343(18)	-0.0062(14)	-0.0040(14)	0.0038(15)
I(2)	0.03199(15)	0.03107(14)	0.03730(14)	-0.01074(10)	0.00669(10)	-0.00635(10)
Br(2)	0.0458(3)	0.0353(2)	0.0432(2)	-0.00250(18)	-0.00515(19)	-0.01001(19)
F(2)	0.0314(12)	0.0224(10)	0.0481(12)	-0.0067(9)	-0.0010(10)	0.0029(9)
C(2)	0.030(2)	0.0231(17)	0.0321(18)	-0.0076(14)	0.0002(15)	0.0019(15)
N(2)	0.0332(18)	0.0427(19)	0.0319(16)	-0.0092(14)	0.0031(14)	-0.0063(15)
N(3)	0.0287(17)	0.0417(19)	0.0374(17)	-0.0068(14)	0.0042(14)	-0.0064(15)
F(3)	0.0462(14)	0.0385(12)	0.0321(11)	-0.0096(9)	0.0095(10)	-0.0104(10)
I(3)	0.02832(14)	0.02966(13)	0.04040(14)	-0.00840(10)	-0.00348(10)	-0.00172(9)
C(3)	0.0271(19)	0.0256(17)	0.0291(17)	-0.0064(14)	-0.0005(14)	-0.0004(14)
C(27)	0.033(2)	0.033(2)	0.0358(19)	-0.0119(16)	-0.0020(16)	-0.0035(16)
C(28)	0.0227(19)	0.037(2)	0.0375(19)	-0.0108(16)	-0.0003(15)	-0.0002(16)
C(29)	0.0259(19)	0.035(2)	0.0338(18)	-0.0077(15)	-0.0010(15)	-0.0021(16)
C(30)	0.030(2)	0.0335(19)	0.0314(18)	-0.0059(15)	-0.0036(15)	-0.0033(16)
C(31)	0.050(3)	0.054(3)	0.059(3)	-0.028(2)	0.006(2)	-0.006(2)
C(32)	0.049(3)	0.041(2)	0.058(3)	-0.015(2)	0.002(2)	-0.010(2)
C(33)	0.041(2)	0.052(3)	0.033(2)	-0.0025(18)	0.0026(18)	-0.010(2)
C(34)	0.054(3)	0.051(3)	0.045(2)	-0.015(2)	0.005(2)	0.004(2)
C(35)	0.033(2)	0.039(2)	0.049(2)	-0.0084(18)	0.0001(18)	-0.0060(18)
C(36)	0.036(2)	0.052(3)	0.035(2)	-0.0063(18)	0.0027(17)	-0.0016(19)
C(37A)	0.096(5)	0.075(4)	0.073(4)	-0.018(3)	-0.004(4)	0.021(4)
Cl(1A)	0.177(3)	0.0723(12)	0.0803(13)	-0.0054(10)	0.0208(15)	0.0423(16)
Cl(2A)	0.0978(15)	0.0833(14)	0.1139(17)	-0.0326(12)	-0.0097(13)	0.0017(12)
C(37B)	0.096(5)	0.075(4)	0.073(4)	-0.018(3)	-0.004(4)	0.021(4)
Cl(1B)	0.177(3)	0.0723(12)	0.0803(13)	-0.0054(10)	0.0208(15)	0.0423(16)
Cl(2B)	0.0978(15)	0.0833(14)	0.1139(17)	-0.0326(12)	-0.0097(13)	0.0017(12)
C(26)	0.029(2)	0.038(2)	0.0351(19)	-0.0022(16)	-0.0013(16)	-0.0062(17)
C(25)	0.0219(19)	0.050(2)	0.0240(17)	-0.0075(16)	0.0013(14)	0.0014(17)
C(24)	0.030(2)	0.036(2)	0.0284(17)	-0.0122(15)	-0.0066(15)	0.0074(16)
C(23)	0.0257(19)	0.0295(18)	0.0290(17)	-0.0073(14)	-0.0029(14)	-0.0014(15)
C(22)	0.0237(18)	0.0329(19)	0.0298(17)	-0.0081(15)	-0.0011(14)	-0.0003(15)
C(21)	0.030(2)	0.039(2)	0.0271(17)	-0.0110(15)	-0.0001(15)	-0.0011(16)
C(20)	0.0232(19)	0.039(2)	0.0364(19)	-0.0125(16)	-0.0032(15)	0.0002(16)
C(9)	0.0226(18)	0.0323(18)	0.0315(18)	-0.0112(15)	-0.0033(14)	0.0027(15)
F(9)	0.0512(16)	0.0346(13)	0.0642(17)	-0.0020(12)	0.0202(13)	-0.0123(12)
C(8)	0.028(2)	0.0317(19)	0.037(2)	-0.0034(16)	0.0018(16)	-0.0007(16)
F(8)	0.0548(17)	0.0466(14)	0.0509(15)	-0.0059(12)	0.0316(13)	-0.0017(13)
C(7)	0.031(2)	0.0276(18)	0.046(2)	-0.0080(16)	-0.0042(17)	-0.0048(16)
F(7)	0.0602(17)	0.0410(14)	0.0528(15)	-0.0225(12)	0.0246(13)	-0.0064(12)
C(6)	0.038(2)	0.0326(19)	0.0329(19)	-0.0115(15)	-0.0045(16)	-0.0014(17)
F(6)	0.0330(13)	0.0510(15)	0.0484(13)	-0.0127(11)	0.0148(11)	-0.0131(11)
C(5)	0.032(2)	0.0286(18)	0.0278(17)	-0.0046(14)	0.0002(15)	-0.0001(15)

F(5)	0.0440(15)	0.0403(14)	0.0656(16)	-0.0167(12)	-0.0013(12)	-0.0177(11)
C(4)	0.0260(19)	0.0225(17)	0.0329(18)	-0.0049(14)	-0.0028(14)	0.0004(14)
F(4)	0.0630(17)	0.0406(13)	0.0411(13)	-0.0189(11)	-0.0052(12)	-0.0085(12)
C(11)	0.039(2)	0.034(2)	0.0334(19)	-0.0078(16)	0.0072(17)	0.0003(17)
F(11)	0.0249(12)	0.0743(18)	0.0401(12)	-0.0179(12)	-0.0048(10)	0.0057(11)
C(10)	0.0256(19)	0.0317(19)	0.0315(18)	-0.0058(15)	0.0018(15)	-0.0034(15)
F(10)	0.0514(15)	0.0294(12)	0.0532(14)	-0.0135(10)	0.0074(12)	-0.0075(11)
C(12)	0.035(2)	0.039(2)	0.0342(19)	-0.0049(16)	0.0133(17)	0.0013(17)
F(12)	0.0341(13)	0.0706(17)	0.0310(11)	-0.0189(11)	-0.0039(10)	0.0016(12)
C(14)	0.034(2)	0.0269(19)	0.0366(19)	-0.0087(15)	0.0015(16)	0.0006(16)
F(14)	0.0241(12)	0.0776(18)	0.0415(13)	-0.0211(12)	-0.0050(10)	0.0066(12)
C(13)	0.035(2)	0.031(2)	0.038(2)	0.0028(16)	0.0075(17)	-0.0079(17)
F(13)	0.0348(13)	0.0802(19)	0.0314(12)	-0.0206(12)	-0.0056(10)	0.0052(13)
F(15)	0.0489(15)	0.0366(13)	0.0570(15)	-0.0210(11)	0.0071(12)	-0.0127(11)
C(15)	0.0256(19)	0.0325(19)	0.0261(16)	-0.0063(14)	0.0014(14)	-0.0018(15)
F(16)	0.0424(15)	0.0509(15)	0.0540(15)	-0.0047(12)	0.0091(12)	-0.0191(12)
C(16)	0.0252(19)	0.0288(18)	0.0304(17)	-0.0106(14)	0.0024(14)	-0.0007(15)
C(19)	0.0252(19)	0.0283(18)	0.0308(18)	-0.0092(14)	0.0015(15)	-0.0019(14)
C(18)	0.031(2)	0.040(2)	0.0264(17)	-0.0123(15)	-0.0009(15)	-0.0015(16)
F(18)	0.0432(14)	0.0446(13)	0.0400(12)	-0.0223(11)	-0.0017(10)	0.0085(11)
C(17)	0.0199(18)	0.036(2)	0.0358(19)	-0.0091(15)	-0.0017(15)	-0.0004(15)
F(17)	0.0312(13)	0.0668(17)	0.0337(12)	-0.0111(11)	0.0076(10)	0.0015(12)

Table S18. Atomic coordinates and equivalent isotropic displacement parameters [\AA^2] for **anti-p-1-TDAI**

	x	y	z	U(eq)	S.O.F.
I(1)	0.52266(5)	0.82597(4)	0.29325(2)	0.04305(12)	1
I(2)	0.85142(5)	0.30194(4)	0.13967(2)	0.04273(12)	1
F(1)	0.2308(6)	0.7718(4)	0.4039(2)	0.0605(12)	1
F(2)	0.0288(6)	0.5949(4)	0.4524(2)	0.0639(12)	1
F(3)	0.0736(6)	0.4112(4)	0.4087(2)	0.0631(12)	1
F(4)	0.3266(5)	0.4031(3)	0.31828(18)	0.0510(10)	1
F(5)	0.7659(5)	0.5501(4)	0.33127(16)	0.0541(11)	1
F(6)	1.0191(4)	0.5288(4)	0.24458(17)	0.0511(10)	1
F(7)	0.6188(5)	0.5713(4)	0.10831(16)	0.0516(10)	1
F(8)	0.3662(5)	0.5933(4)	0.19473(18)	0.0535(11)	1
F(9)	1.0673(5)	0.7160(3)	0.12482(19)	0.0540(10)	1
F(10)	1.3201(5)	0.7110(4)	0.0336(2)	0.0619(12)	1
F(11)	1.3493(5)	0.5366(4)	-0.01781(17)	0.0605(12)	1
F(12)	1.1375(5)	0.3628(4)	0.02578(19)	0.0563(11)	1
C(1)	0.3883(8)	0.6784(5)	0.3354(3)	0.0368(14)	1
C(2)	0.2567(9)	0.6808(6)	0.3821(3)	0.0435(15)	1
C(3)	0.1519(9)	0.5922(6)	0.4074(3)	0.0438(16)	1
C(4)	0.1770(9)	0.4987(6)	0.3852(3)	0.0439(15)	1
C(5)	0.3079(8)	0.4953(5)	0.3395(3)	0.0381(14)	1
C(6)	0.4163(8)	0.5821(6)	0.3142(3)	0.0360(14)	1
C(7)	0.5584(8)	0.5725(5)	0.2656(3)	0.0345(13)	1
C(8)	0.7267(8)	0.5558(6)	0.2764(3)	0.0376(14)	1
C(9)	0.8586(8)	0.5449(6)	0.2314(3)	0.0365(14)	1
C(10)	0.8280(7)	0.5497(5)	0.1736(3)	0.0323(13)	1
C(11)	0.6582(8)	0.5653(5)	0.1633(3)	0.0353(13)	1
C(12)	0.5285(7)	0.5773(5)	0.2080(3)	0.0362(14)	1
C(13)	0.9691(7)	0.5407(6)	0.1244(3)	0.0348(13)	1
C(14)	1.0813(8)	0.6269(6)	0.1015(3)	0.0395(14)	1
C(15)	1.2119(8)	0.6255(6)	0.0543(3)	0.0452(16)	1
C(16)	1.2266(8)	0.5370(7)	0.0290(3)	0.0431(16)	1
C(17)	1.1174(8)	0.4494(6)	0.0513(3)	0.0416(16)	1
C(18)	0.9900(8)	0.4483(5)	0.0998(3)	0.0353(13)	1
C(37A)	0.8154(17)	0.9411(10)	0.0797(6)	0.099(4)	0.874(6)
Cl(1A)	0.7090(5)	0.8282(3)	0.06593(19)	0.1260(12)	0.874(6)
Cl(2A)	0.7758(7)	1.0609(3)	0.03014(17)	0.1210(17)	0.874(6)
C(37B)	0.8154(17)	0.9411(10)	0.0797(6)	0.099(4)	0.126(6)
Cl(1B)	0.7090(5)	0.8282(3)	0.06593(19)	0.1260(12)	0.126(6)
Cl(2B)	0.942(5)	1.081(2)	0.0500(12)	0.1210(17)	0.126(6)
N(1)	0.0312(7)	0.1217(5)	0.2959(2)	0.0408(12)	1
N(2)	0.3080(6)	0.2354(5)	0.1538(2)	0.0392(12)	1
N(3)	0.1805(8)	-0.0560(5)	0.1920(3)	0.0485(14)	1
C(28)	0.1767(8)	0.0417(6)	0.2055(3)	0.0394(14)	1
C(29)	0.1202(8)	0.1085(5)	0.2446(3)	0.0360(13)	1
C(30)	0.2258(7)	0.1506(6)	0.1916(3)	0.0363(14)	1
C(31)	-0.0442(10)	0.0259(7)	0.3390(3)	0.0532(18)	1

C(32)	-0.0063(10)	0.2287(6)	0.3069(3)	0.0489(17)	1
C(33)	0.3470(9)	0.3300(6)	0.1760(3)	0.0448(16)	1
C(34)	0.4062(9)	0.2178(7)	0.0980(3)	0.0491(17)	1
C(35)	0.3012(10)	-0.0759(7)	0.1421(4)	0.059(2)	1
C(36)	0.0726(10)	-0.1451(6)	0.2292(4)	0.0549(19)	1
I(3)	0.67222(7)	0.06571(5)	0.21635(2)	0.0385(2)	0.603(3)
CI(3)	0.67222(7)	0.06571(5)	0.21635(2)	0.0385(2)	0.397(3)
I(4)	0.43388(5)	0.11762(4)	0.36124(2)	0.04277(12)	1
F(13)	0.6384(5)	0.3063(3)	0.38588(18)	0.0496(10)	1
F(14)	0.6166(5)	0.4089(3)	0.4756(2)	0.0526(10)	1
F(15)	0.3630(5)	0.3560(3)	0.57037(17)	0.0486(9)	1
F(16)	0.1379(5)	0.1963(3)	0.57581(15)	0.0414(8)	1
F(17)	-0.0890(4)	0.2159(3)	0.47684(16)	0.0377(8)	1
F(18)	-0.3330(4)	0.0626(3)	0.49779(18)	0.0421(8)	1
C(19)	0.3937(7)	0.1953(5)	0.4330(3)	0.0310(12)	1
C(20)	0.5097(8)	0.2777(5)	0.4316(3)	0.0360(13)	1
C(21)	0.5012(8)	0.3315(5)	0.4777(3)	0.0371(14)	1
C(22)	0.3734(8)	0.3045(5)	0.5259(3)	0.0368(14)	1
C(23)	0.2592(8)	0.2225(5)	0.5272(3)	0.0327(13)	1
C(24)	0.2641(7)	0.1670(5)	0.4822(3)	0.0299(12)	1
C(25)	0.1308(7)	0.0814(5)	0.4887(3)	0.0299(12)	1
C(26)	-0.0422(7)	0.1084(5)	0.4892(3)	0.0304(12)	1
C(27)	-0.1682(7)	0.0302(5)	0.4996(3)	0.0309(12)	1
H(37A)	0.775016	0.948665	0.121052	0.119	0.874(6)
H(37B)	0.941001	0.926952	0.076101	0.119	0.874(6)
H(37C)	0.897417	0.89999	0.105358	0.119	0.126(6)
H(37D)	0.723512	0.96416	0.108417	0.119	0.126(6)
H(31A)	-0.148299	0.003977	0.325904	0.08	1
H(31B)	-0.07424	0.04379	0.378178	0.08	1
H(31C)	0.039052	-0.034689	0.341951	0.08	1
H(32A)	0.068575	0.283059	0.277971	0.073	1
H(32B)	0.013813	0.229267	0.34754	0.073	1
H(32C)	-0.127081	0.247042	0.302811	0.073	1
H(33A)	0.406723	0.385604	0.143045	0.067	1
H(33B)	0.421011	0.307248	0.207235	0.067	1
H(33C)	0.239675	0.361038	0.192643	0.067	1
H(34A)	0.335906	0.176173	0.079166	0.074	1
H(34B)	0.511405	0.176497	0.106654	0.074	1
H(34C)	0.436823	0.289008	0.070785	0.074	1
H(35A)	0.245451	-0.060133	0.105882	0.088	1
H(35B)	0.3382	-0.152889	0.150622	0.088	1
H(35C)	0.401764	-0.028032	0.135863	0.088	1
H(36A)	-0.045362	-0.118291	0.237177	0.082	1
H(36B)	0.11785	-0.17204	0.267153	0.082	1
H(36C)	0.072623	-0.205063	0.208474	0.082	1

Table S19. Anisotropic displacement parameters [\AA^2] for **anti-p-1-TDAI**

	U11	U22	U33	U23	U13	U12
I(1)	0.0360(2)	0.0516(3)	0.0440(2)	-0.02269(19)	0.00675(17)	-0.00776(18)
I(2)	0.0372(2)	0.0446(2)	0.0533(3)	-0.02196(19)	-0.01308(18)	0.00537(17)
F(1)	0.065(3)	0.059(3)	0.058(3)	-0.034(2)	0.026(2)	-0.008(2)
F(2)	0.061(3)	0.057(3)	0.058(3)	-0.008(2)	0.033(2)	0.005(2)
F(3)	0.066(3)	0.048(2)	0.062(3)	-0.002(2)	0.023(2)	-0.011(2)
F(4)	0.059(2)	0.042(2)	0.052(2)	-0.0183(18)	0.0056(19)	-0.0027(18)
F(5)	0.041(2)	0.095(3)	0.0332(19)	-0.028(2)	-0.0063(16)	0.010(2)
F(6)	0.0240(17)	0.092(3)	0.044(2)	-0.028(2)	-0.0055(15)	0.0053(18)
F(7)	0.040(2)	0.088(3)	0.0332(19)	-0.027(2)	-0.0077(16)	0.006(2)
F(8)	0.0282(18)	0.093(3)	0.046(2)	-0.030(2)	-0.0068(16)	0.0087(19)
F(9)	0.056(2)	0.049(2)	0.061(3)	-0.027(2)	0.004(2)	-0.0134(19)
F(10)	0.049(2)	0.074(3)	0.055(3)	-0.007(2)	0.007(2)	-0.019(2)
F(11)	0.039(2)	0.104(4)	0.036(2)	-0.020(2)	0.0049(17)	0.016(2)
F(12)	0.055(2)	0.072(3)	0.053(2)	-0.042(2)	-0.0083(19)	0.022(2)
C(1)	0.030(3)	0.046(4)	0.034(3)	-0.014(3)	0.005(2)	-0.003(3)
C(2)	0.039(3)	0.052(4)	0.040(3)	-0.018(3)	0.006(3)	0.002(3)
C(3)	0.047(4)	0.046(4)	0.033(3)	-0.007(3)	0.011(3)	0.000(3)
C(4)	0.039(3)	0.047(4)	0.039(3)	-0.003(3)	0.003(3)	0.000(3)
C(5)	0.041(3)	0.036(3)	0.037(3)	-0.009(3)	-0.004(3)	0.005(3)
C(6)	0.029(3)	0.050(4)	0.031(3)	-0.015(3)	-0.001(2)	0.003(3)
C(7)	0.032(3)	0.040(3)	0.032(3)	-0.014(3)	0.001(2)	-0.001(3)
C(8)	0.037(3)	0.051(4)	0.028(3)	-0.018(3)	-0.003(2)	0.004(3)
C(9)	0.029(3)	0.047(4)	0.036(3)	-0.015(3)	-0.006(2)	0.001(3)
C(10)	0.029(3)	0.037(3)	0.033(3)	-0.018(3)	0.003(2)	0.001(2)
C(11)	0.035(3)	0.048(4)	0.028(3)	-0.018(3)	-0.005(2)	0.002(3)
C(12)	0.023(3)	0.047(4)	0.040(3)	-0.017(3)	-0.001(2)	0.002(3)
C(13)	0.026(3)	0.049(4)	0.033(3)	-0.019(3)	-0.003(2)	0.001(3)
C(14)	0.033(3)	0.048(4)	0.040(3)	-0.020(3)	-0.001(3)	0.000(3)
C(15)	0.034(3)	0.062(5)	0.037(3)	-0.010(3)	0.001(3)	-0.005(3)
C(16)	0.029(3)	0.074(5)	0.025(3)	-0.013(3)	-0.001(2)	0.010(3)
C(17)	0.036(3)	0.061(4)	0.034(3)	-0.022(3)	-0.012(3)	0.014(3)
C(18)	0.033(3)	0.045(4)	0.032(3)	-0.017(3)	-0.007(2)	0.007(3)
C(37A)	0.105(9)	0.092(8)	0.095(8)	-0.015(7)	-0.016(7)	0.020(7)
CI(1A)	0.116(3)	0.124(3)	0.142(3)	-0.040(2)	-0.015(2)	0.001(2)
CI(2A)	0.165(4)	0.091(2)	0.085(2)	-0.0076(18)	0.022(2)	0.045(3)
C(37B)	0.105(9)	0.092(8)	0.095(8)	-0.015(7)	-0.016(7)	0.020(7)
CI(1B)	0.116(3)	0.124(3)	0.142(3)	-0.040(2)	-0.015(2)	0.001(2)
CI(2B)	0.165(4)	0.091(2)	0.085(2)	-0.0076(18)	0.022(2)	0.045(3)
N(1)	0.038(3)	0.056(3)	0.028(3)	-0.013(2)	0.003(2)	-0.012(3)
N(2)	0.028(3)	0.050(3)	0.036(3)	-0.008(2)	0.004(2)	-0.005(2)
N(3)	0.050(3)	0.048(3)	0.049(3)	-0.021(3)	0.006(3)	-0.012(3)
C(28)	0.031(3)	0.050(4)	0.039(3)	-0.017(3)	-0.004(3)	0.000(3)
C(29)	0.032(3)	0.044(4)	0.034(3)	-0.011(3)	-0.007(2)	0.000(3)
C(30)	0.027(3)	0.049(4)	0.034(3)	-0.011(3)	-0.003(2)	0.001(3)
C(31)	0.058(4)	0.063(5)	0.034(4)	-0.007(3)	0.005(3)	-0.011(4)

C(32)	0.051(4)	0.053(4)	0.040(4)	-0.015(3)	0.009(3)	-0.004(3)
C(33)	0.036(3)	0.044(4)	0.054(4)	-0.010(3)	-0.003(3)	-0.007(3)
C(34)	0.036(3)	0.069(5)	0.036(4)	-0.007(3)	0.007(3)	-0.005(3)
C(35)	0.054(4)	0.068(5)	0.061(5)	-0.037(4)	0.005(4)	-0.007(4)
C(36)	0.058(4)	0.049(4)	0.059(5)	-0.022(4)	0.005(4)	-0.014(4)
I(3)	0.0420(4)	0.0344(3)	0.0376(3)	-0.0040(2)	-0.0057(2)	-0.0091(2)
CI(3)	0.0420(4)	0.0344(3)	0.0376(3)	-0.0040(2)	-0.0057(2)	-0.0091(2)
I(4)	0.0396(2)	0.0532(3)	0.0406(2)	-0.02463(19)	-0.00145(17)	0.00556(18)
F(13)	0.039(2)	0.056(2)	0.050(2)	-0.0151(19)	0.0153(17)	-0.0129(18)
F(14)	0.050(2)	0.043(2)	0.066(3)	-0.018(2)	-0.0024(19)	-0.0167(18)
F(15)	0.064(2)	0.043(2)	0.044(2)	-0.0233(17)	-0.0006(18)	-0.0121(18)
F(16)	0.048(2)	0.041(2)	0.0330(18)	-0.0124(15)	0.0098(15)	-0.0103(16)
F(17)	0.0366(18)	0.0269(17)	0.049(2)	-0.0114(15)	0.0010(15)	0.0023(14)
F(18)	0.0253(16)	0.040(2)	0.060(2)	-0.0112(17)	-0.0048(15)	0.0033(15)
C(19)	0.024(3)	0.035(3)	0.034(3)	-0.012(3)	0.000(2)	0.000(2)
C(20)	0.030(3)	0.034(3)	0.040(3)	-0.007(3)	0.007(2)	-0.005(2)
C(21)	0.037(3)	0.029(3)	0.044(4)	-0.007(3)	-0.003(3)	-0.008(3)
C(22)	0.045(4)	0.034(3)	0.033(3)	-0.012(3)	-0.003(3)	-0.005(3)
C(23)	0.034(3)	0.030(3)	0.033(3)	-0.008(2)	0.002(2)	-0.005(2)
C(24)	0.029(3)	0.030(3)	0.031(3)	-0.011(2)	0.001(2)	0.000(2)
C(25)	0.030(3)	0.031(3)	0.031(3)	-0.013(2)	-0.002(2)	-0.001(2)
C(26)	0.032(3)	0.028(3)	0.032(3)	-0.012(2)	0.000(2)	0.003(2)
C(27)	0.024(3)	0.035(3)	0.034(3)	-0.010(2)	0.000(2)	0.000(2)

Table S20. Atomic coordinates and equivalent isotropic displacement parameters [Å²] for **anti-m-1-TDACI**

	x	y	z	U(eq)
I(1)	0.73278(2)	0.05400(5)	0.48321(2)	0.03569(13)
Cl(1)	0.33087(7)	0.1010(2)	0.42129(7)	0.0407(4)
F(1)	0.7402(2)	0.3011(6)	0.5820(2)	0.0502(11)
N(1)	0.3901(3)	0.5587(10)	0.4432(4)	0.0528(18)
C(1)	0.3005(3)	0.6146(9)	0.3943(4)	0.0420(17)
I(2)	0.43586(2)	0.11135(6)	0.35604(2)	0.03637(13)
F(2)	0.6716(3)	0.5139(7)	0.6243(2)	0.0599(15)
N(2)	0.2858(3)	0.6835(9)	0.3469(3)	0.0479(16)
C(2)	0.3397(3)	0.5650(9)	0.4295(4)	0.0419(17)
I(3)	0.39094(2)	0.50431(6)	0.03083(2)	0.03768(14)
F(3)	0.5690(3)	0.5011(8)	0.5942(3)	0.0691(16)
N(3)	0.2546(3)	0.4663(9)	0.4737(3)	0.0455(15)
C(3)	0.2891(3)	0.5291(10)	0.4400(4)	0.0427(17)
C(4)	0.4076(4)	0.4714(13)	0.4913(5)	0.062(3)
I(4)	0.25932(2)	0.22257(5)	0.32236(2)	0.03317(13)
F(4)	0.5359(2)	0.2753(9)	0.5200(3)	0.0635(15)
F(5)	0.5948(2)	0.2707(5)	0.4045(2)	0.0458(11)
C(5)	0.4303(4)	0.6347(16)	0.4104(6)	0.069(3)
F(6)	0.6063(2)	-0.1725(7)	0.5276(2)	0.0492(11)
C(6)	0.3242(4)	0.7687(11)	0.3143(4)	0.055(2)
F(7)	0.5638(2)	-0.3778(6)	0.4531(2)	0.0535(12)
C(7)	0.2309(5)	0.7126(12)	0.3349(5)	0.062(3)
F(8)	0.53476(19)	-0.2596(6)	0.3543(2)	0.0434(10)
C(8)	0.2002(3)	0.4366(11)	0.4550(4)	0.0458(18)
F(9)	0.64044(19)	0.0525(8)	0.3005(2)	0.0541(12)
C(9)	0.2737(4)	0.3816(11)	0.5233(4)	0.0474(18)
F(10)	0.6235(2)	0.1865(9)	0.2018(2)	0.0612(14)
C(10)	0.6744(3)	0.1817(9)	0.5250(3)	0.0351(14)
C(12)	0.6551(4)	0.4010(10)	0.5878(3)	0.0458(18)
F(12)	0.4446(2)	0.2186(7)	0.2349(2)	0.0518(12)
C(11)	0.6905(3)	0.2919(9)	0.5652(3)	0.0394(16)
F(11)	0.5248(2)	0.2650(8)	0.1681(2)	0.0590(14)
F(14)	0.5144(3)	0.8547(8)	0.1686(2)	0.0660(16)
C(14)	0.5870(3)	0.2810(11)	0.5346(4)	0.0450(18)
C(13)	0.6037(4)	0.3942(11)	0.5725(4)	0.0481(19)
F(13)	0.4828(2)	0.7468(8)	0.0699(2)	0.0565(13)
F(15)	0.4677(2)	0.7414(7)	0.2590(2)	0.0548(13)
C(15)	0.6216(3)	0.1729(9)	0.5105(3)	0.0352(14)
F(16)	0.39312(19)	0.5089(6)	0.25113(19)	0.0425(10)
C(16)	0.6004(3)	0.0564(10)	0.4683(3)	0.0362(15)
C(17)	0.5928(3)	-0.1112(10)	0.4789(3)	0.0379(16)
F(17)	0.29342(17)	0.5511(5)	0.1860(2)	0.0407(10)
F(18)	0.41765(17)	0.1677(6)	0.1250(2)	0.0421(10)
C(18)	0.5704(3)	-0.2172(10)	0.4410(4)	0.0396(17)
C(19)	0.5562(3)	-0.1563(9)	0.3905(3)	0.0352(14)
F(19)	0.3524(2)	-0.0821(6)	0.1469(3)	0.0509(12)
C(21)	0.5861(3)	0.1081(9)	0.4164(3)	0.0350(15)
F(21)	0.19421(19)	0.3753(7)	0.11629(19)	0.0461(11)
C(22)	0.5513(3)	0.0753(9)	0.3219(3)	0.0337(14)
F(22)	0.0965(2)	0.4517(8)	0.1462(2)	0.0583(14)
C(23)	0.5916(3)	0.0953(11)	0.2853(3)	0.0401(16)
F(23)	0.07016(19)	0.4329(8)	0.2522(2)	0.0582(14)
C(24)	0.5834(3)	0.1608(11)	0.2339(3)	0.0438(16)
F(24)	0.14102(18)	0.3353(7)	0.3277(2)	0.0488(11)
C(25)	0.5333(3)	0.2027(10)	0.2173(3)	0.0416(17)

C(26)	0.4923(3)	0.1797(9)	0.2529(3)	0.0361(14)
C(27)	0.5003(3)	0.1206(9)	0.3051(3)	0.0323(14)
C(28)	0.4198(3)	0.5677(9)	0.1083(3)	0.0345(14)
C(29)	0.4598(3)	0.6845(11)	0.1135(3)	0.0426(16)
C(30)	0.4760(3)	0.7410(11)	0.1644(4)	0.0444(18)
C(31)	0.4529(3)	0.6846(11)	0.2097(3)	0.0414(17)
C(32)	0.4142(3)	0.5652(9)	0.2051(3)	0.0350(14)
C(33)	0.3978(3)	0.5045(8)	0.1550(3)	0.0326(14)
C(34)	0.3580(3)	0.3694(9)	0.1562(3)	0.0328(14)
C(35)	0.3711(3)	0.2051(10)	0.1453(3)	0.0341(14)
C(36)	0.3375(3)	0.0748(9)	0.1566(3)	0.0362(15)
C(37)	0.2894(3)	0.1068(9)	0.1783(3)	0.0326(14)
C(38)	0.2724(3)	0.2695(8)	0.1872(3)	0.0310(13)
C(39)	0.3084(3)	0.3950(8)	0.1759(3)	0.0308(13)
C(40)	0.2194(3)	0.3079(8)	0.2066(3)	0.0319(13)
C(41)	0.1824(3)	0.3613(10)	0.1679(3)	0.0381(15)
C(42)	0.1321(3)	0.4014(11)	0.1836(4)	0.0417(17)
C(43)	0.1183(3)	0.3908(10)	0.2374(4)	0.0417(17)
C(44)	0.1554(3)	0.3413(10)	0.2757(3)	0.0384(15)
C(45)	0.2056(3)	0.2989(8)	0.2613(3)	0.0315(13)
C(20)	0.5640(3)	0.0098(9)	0.3770(3)	0.0327(14)
F(20)	0.25868(19)	-0.0191(6)	0.1909(2)	0.0439(10)
H(4A)	0.387651	0.368095	0.494825	0.092
H(4B)	0.402043	0.541194	0.523314	0.092
H(4C)	0.444887	0.445477	0.488623	0.092
H(5A)	0.452398	0.547812	0.39499	0.103
H(5B)	0.45191	0.708555	0.433173	0.103
H(5C)	0.413761	0.698838	0.38094	0.103
H(6A)	0.359482	0.734065	0.325805	0.082
H(6B)	0.320661	0.888921	0.319099	0.082
H(6C)	0.318454	0.740529	0.2759	0.082
H(7A)	0.225169	0.715563	0.295434	0.092
H(7B)	0.220406	0.818906	0.350617	0.092
H(7C)	0.210085	0.622938	0.350439	0.092
H(8A)	0.185998	0.538202	0.438496	0.069
H(8B)	0.178894	0.40508	0.486024	0.069
H(8C)	0.199541	0.346975	0.42812	0.069
H(9A)	0.296752	0.289824	0.513322	0.071
H(9B)	0.243876	0.338086	0.543252	0.071
H(9C)	0.293132	0.460632	0.546228	0.071

Table S21. Anisotropic displacement parameters [\AA^2] for **anti-m-1-TDACI**

	U11	U22	U33	U23	U13	U12
I(1)	0.0359(2)	0.0349(2)	0.0362(2)	0.00002(17)	-0.00114(16)	0.00188(17)
Cl(1)	0.0367(8)	0.0554(10)	0.0297(8)	0.0043(7)	-0.0017(6)	0.0025(7)
F(1)	0.053(3)	0.051(3)	0.046(3)	-0.004(2)	-0.013(2)	-0.010(2)
N(1)	0.040(4)	0.053(4)	0.065(5)	0.016(4)	-0.006(3)	-0.007(3)
C(1)	0.044(4)	0.033(4)	0.049(5)	-0.004(3)	-0.006(3)	0.001(3)
I(2)	0.0321(2)	0.0419(2)	0.0351(2)	0.00182(17)	0.00067(16)	0.00187(17)
F(2)	0.086(4)	0.053(3)	0.040(3)	-0.019(2)	-0.005(3)	-0.011(3)
N(2)	0.056(4)	0.038(3)	0.049(4)	0.003(3)	-0.007(3)	-0.001(3)
C(2)	0.046(4)	0.028(3)	0.051(5)	0.003(3)	-0.004(3)	-0.002(3)
I(3)	0.0419(2)	0.0423(3)	0.0287(2)	-0.00054(17)	-0.00337(16)	-0.00616(17)
F(3)	0.077(4)	0.066(4)	0.065(4)	-0.022(3)	0.015(3)	0.020(3)
N(3)	0.040(3)	0.048(4)	0.048(4)	0.001(3)	0.000(3)	-0.003(3)
C(3)	0.044(4)	0.036(4)	0.047(5)	-0.003(3)	-0.006(3)	0.003(3)
C(4)	0.052(5)	0.049(5)	0.083(7)	0.017(5)	-0.018(5)	-0.005(4)
I(4)	0.0336(2)	0.0367(2)	0.0290(2)	0.00053(16)	-0.00392(15)	0.00102(16)
F(4)	0.042(3)	0.083(4)	0.065(4)	-0.019(3)	-0.003(2)	0.018(2)
F(5)	0.063(3)	0.034(2)	0.040(2)	0.0006(18)	-0.012(2)	-0.0051(19)
C(5)	0.052(5)	0.069(6)	0.086(8)	0.026(6)	-0.002(5)	-0.014(5)
F(6)	0.061(3)	0.051(3)	0.035(2)	0.008(2)	-0.014(2)	-0.003(2)
C(6)	0.075(6)	0.040(4)	0.049(5)	0.004(4)	0.008(4)	0.009(4)
F(7)	0.062(3)	0.042(3)	0.055(3)	0.010(2)	-0.012(2)	-0.012(2)
C(7)	0.070(6)	0.047(5)	0.066(6)	0.003(4)	-0.028(5)	0.002(4)
F(8)	0.045(2)	0.043(2)	0.042(2)	-0.0057(19)	-0.0074(18)	-0.0086(18)
C(8)	0.038(4)	0.047(5)	0.053(5)	-0.010(4)	0.001(3)	-0.002(3)
F(9)	0.034(2)	0.080(4)	0.048(3)	0.004(3)	-0.002(2)	0.002(2)
C(9)	0.053(5)	0.045(4)	0.045(5)	0.004(3)	0.004(4)	-0.001(3)
F(10)	0.049(3)	0.093(4)	0.042(3)	0.007(3)	0.013(2)	-0.015(3)
C(10)	0.044(4)	0.036(3)	0.026(3)	0.000(3)	0.002(3)	0.005(3)
C(12)	0.069(6)	0.037(4)	0.031(4)	-0.006(3)	0.001(4)	-0.003(4)
F(12)	0.044(2)	0.071(3)	0.040(3)	0.011(2)	-0.009(2)	0.008(2)
C(11)	0.051(4)	0.038(4)	0.029(4)	0.005(3)	-0.004(3)	-0.003(3)
F(11)	0.068(3)	0.075(4)	0.033(3)	0.016(2)	-0.002(2)	-0.010(3)
F(14)	0.068(3)	0.071(4)	0.059(3)	-0.011(3)	-0.002(3)	-0.042(3)
C(14)	0.040(4)	0.056(5)	0.040(4)	-0.005(3)	0.000(3)	0.009(3)
C(13)	0.060(5)	0.044(4)	0.040(4)	-0.005(3)	0.006(4)	0.011(4)
F(13)	0.058(3)	0.066(3)	0.045(3)	0.004(2)	0.003(2)	-0.025(2)
F(15)	0.059(3)	0.062(3)	0.043(3)	-0.019(2)	-0.009(2)	-0.015(2)
C(15)	0.042(4)	0.035(3)	0.028(3)	-0.001(3)	-0.004(3)	0.005(3)
F(16)	0.049(2)	0.048(2)	0.030(2)	-0.0052(17)	0.0024(19)	-0.0054(18)
C(16)	0.031(3)	0.045(4)	0.033(4)	-0.001(3)	-0.002(3)	0.003(3)
C(17)	0.034(4)	0.042(4)	0.037(4)	0.005(3)	-0.007(3)	0.004(3)
F(17)	0.039(2)	0.030(2)	0.053(3)	-0.0038(18)	0.0059(19)	0.0005(16)
F(18)	0.035(2)	0.045(2)	0.047(3)	-0.0071(19)	0.0022(18)	0.0039(18)
C(18)	0.040(4)	0.036(4)	0.043(4)	0.003(3)	-0.005(3)	-0.005(3)
C(19)	0.030(3)	0.037(4)	0.039(4)	-0.002(3)	-0.006(3)	-0.001(3)

F(19)	0.050(3)	0.030(2)	0.072(3)	-0.008(2)	0.005(2)	0.0045(19)
C(21)	0.035(3)	0.036(4)	0.034(4)	0.002(3)	-0.002(3)	0.002(3)
F(21)	0.048(3)	0.059(3)	0.031(2)	0.0072(19)	-0.0038(19)	0.006(2)
C(22)	0.033(3)	0.037(3)	0.031(4)	-0.003(3)	-0.005(3)	0.000(3)
F(22)	0.042(3)	0.081(4)	0.052(3)	0.010(3)	-0.013(2)	0.018(2)
C(23)	0.029(3)	0.050(4)	0.042(4)	-0.007(3)	-0.001(3)	-0.004(3)
F(23)	0.031(2)	0.080(4)	0.063(3)	0.010(3)	0.002(2)	0.012(2)
C(24)	0.047(4)	0.048(4)	0.038(4)	-0.006(3)	0.006(3)	-0.010(3)
F(24)	0.039(2)	0.069(3)	0.038(2)	0.006(2)	0.0074(18)	0.005(2)
C(25)	0.049(4)	0.041(4)	0.034(4)	0.001(3)	-0.004(3)	-0.006(3)
C(26)	0.039(4)	0.039(4)	0.031(4)	0.001(3)	-0.004(3)	-0.003(3)
C(27)	0.030(3)	0.034(3)	0.033(4)	-0.003(3)	0.003(3)	-0.003(2)
C(28)	0.039(4)	0.035(3)	0.030(4)	-0.004(3)	-0.005(3)	-0.003(3)
C(29)	0.043(4)	0.048(4)	0.038(4)	-0.004(3)	0.006(3)	-0.011(3)
C(30)	0.036(4)	0.041(4)	0.056(5)	-0.006(3)	-0.004(3)	-0.012(3)
C(31)	0.039(4)	0.046(4)	0.039(4)	-0.013(3)	-0.009(3)	0.000(3)
C(32)	0.035(3)	0.034(3)	0.036(4)	-0.005(3)	0.002(3)	0.003(3)
C(33)	0.031(3)	0.033(4)	0.033(4)	0.000(3)	-0.002(3)	-0.002(3)
C(34)	0.031(3)	0.034(3)	0.033(3)	-0.001(3)	-0.008(3)	-0.002(3)
C(35)	0.031(3)	0.042(4)	0.030(3)	-0.002(3)	-0.001(3)	0.002(3)
C(36)	0.044(4)	0.028(3)	0.036(4)	-0.005(3)	-0.006(3)	0.007(3)
C(37)	0.035(3)	0.031(3)	0.032(4)	0.002(3)	-0.004(3)	-0.003(3)
C(38)	0.037(4)	0.028(3)	0.028(3)	-0.001(2)	-0.004(3)	0.000(2)
C(39)	0.031(3)	0.029(3)	0.032(3)	-0.004(2)	-0.003(3)	0.000(2)
C(40)	0.034(3)	0.028(3)	0.033(3)	0.001(3)	-0.004(3)	-0.001(3)
C(41)	0.039(4)	0.041(4)	0.034(4)	0.003(3)	-0.004(3)	0.001(3)
C(42)	0.036(4)	0.048(4)	0.041(4)	0.006(3)	-0.008(3)	0.004(3)
C(43)	0.029(3)	0.045(4)	0.051(5)	0.002(3)	0.000(3)	0.003(3)
C(44)	0.036(4)	0.045(4)	0.035(4)	0.002(3)	-0.002(3)	-0.002(3)
C(45)	0.032(3)	0.029(3)	0.034(3)	0.003(2)	-0.007(3)	0.000(2)
C(20)	0.027(3)	0.037(4)	0.034(4)	-0.002(3)	0.000(3)	0.002(3)
F(20)	0.046(2)	0.032(2)	0.054(3)	-0.0001(18)	-0.001(2)	-0.0051(17)

Table S22. Atomic coordinates and equivalent isotropic displacement parameters [Å²] for **syn-m-1-TEABr**

	x	y	z	U(eq)
I(1)	0.16685(6)	-0.13001(4)	0.67593(2)	0.04710(14)
I(2)	0.13857(6)	0.14244(4)	0.68883(2)	0.04931(15)
F(1)	0.0422(5)	-0.3005(3)	0.64695(18)	0.0598(15)
F(2)	-0.0326(5)	-0.3309(4)	0.5737(2)	0.0640(16)
F(3)	0.0035(6)	-0.2049(4)	0.50631(18)	0.0660(16)
F(4)	0.1224(6)	-0.0515(4)	0.51217(15)	0.0544(13)
F(5)	0.4123(5)	-0.0883(4)	0.5739(3)	0.084(2)
F(6)	0.5443(6)	0.0614(5)	0.5757(3)	0.120(4)
F(7)	0.4150(6)	0.2190(4)	0.5875(3)	0.082(2)
F(8)	0.1655(6)	0.3063(4)	0.53120(16)	0.0596(14)
F(9)	0.0400(7)	0.4643(4)	0.5440(2)	0.080(2)
F(10)	-0.0414(6)	0.4817(4)	0.6203(2)	0.0753(18)
F(11)	-0.0015(6)	0.3419(4)	0.68217(19)	0.0678(16)
F(48)	0.0206(4)	0.0756(3)	0.59585(18)	0.0512(13)
C(1)	0.1210(8)	-0.1577(6)	0.6181(2)	0.0368(18)
C(2)	0.0624(8)	-0.2368(5)	0.6145(3)	0.0406(19)
C(3)	0.0231(8)	-0.2539(6)	0.5771(3)	0.047(2)
C(4)	0.0421(8)	-0.1897(6)	0.5430(3)	0.046(2)
C(5)	0.1019(8)	-0.1111(6)	0.5466(3)	0.0396(19)
C(6)	0.1438(8)	-0.0945(5)	0.5832(2)	0.0360(17)
C(7)	0.2118(7)	-0.0094(5)	0.5846(2)	0.0339(17)
C(8)	0.1511(8)	0.0714(5)	0.5908(2)	0.0349(17)
C(9)	0.2125(8)	0.1526(5)	0.5920(2)	0.0354(17)
C(10)	0.3474(9)	0.1448(6)	0.5864(3)	0.050(2)
C(11)	0.4136(9)	0.0664(7)	0.5812(4)	0.063(3)
C(12)	0.3471(9)	-0.0107(6)	0.5802(3)	0.051(2)
C(13)	0.1440(8)	0.2382(6)	0.5998(3)	0.0406(19)
C(14)	0.1209(9)	0.3125(6)	0.5685(3)	0.050(2)
C(15)	0.0570(9)	0.3932(6)	0.5754(4)	0.056(3)
C(16)	0.0175(9)	0.4027(7)	0.6136(4)	0.058(3)
C(17)	0.0392(9)	0.3309(7)	0.6440(3)	0.052(2)
C(18)	0.1008(8)	0.2483(6)	0.6391(3)	0.0400(19)
N(1)	0.8130(7)	0.5122(5)	0.2440(2)	0.0457(17)
C(72)	0.9309(11)	0.4558(8)	0.2634(4)	0.076(3)
C(73)	0.9834(14)	0.3808(10)	0.2409(6)	0.122(7)
C(74)	0.6996(11)	0.4536(8)	0.2397(4)	0.068(3)
C(75)	0.6581(12)	0.3964(10)	0.2778(5)	0.096(5)
C(76)	0.8411(13)	0.5621(9)	0.2021(4)	0.081(4)
C(77)	0.9517(13)	0.6273(9)	0.2001(4)	0.092(4)
C(78)	0.7757(13)	0.5801(10)	0.2712(4)	0.086(4)
C(79)	0.6577(13)	0.6472(10)	0.2560(5)	0.095(4)
Br(1)	0.79197(11)	0.03902(8)	0.24139(3)	0.0569(3)
N(2)	0.3121(7)	0.0009(5)	0.2560(2)	0.0442(17)
C(80)	0.4926(12)	-0.1267(8)	0.2520(4)	0.077(3)
C(81)	0.2645(13)	0.0929(8)	0.2321(4)	0.078(3)
C(82)	0.1455(12)	0.1398(9)	0.2478(4)	0.084(4)
C(83)	0.3433(12)	0.0075(11)	0.2996(3)	0.085(4)
C(84)	0.4505(13)	0.0753(14)	0.3020(6)	0.137(8)
C(85)	0.2050(11)	-0.0658(9)	0.2588(4)	0.079(4)
C(86)	0.1567(14)	-0.0850(12)	0.2191(6)	0.122(7)
C(88)	0.4309(10)	-0.0329(8)	0.2341(3)	0.063(3)
Br(2)	0.30125(11)	0.54070(7)	0.25784(3)	0.0548(3)
I(3)	0.30681(6)	0.36014(4)	0.33036(2)	0.04581(14)
I(4)	0.33411(6)	0.64951(4)	0.33626(2)	0.04573(14)
F(12)	0.1960(5)	0.1608(4)	0.35220(18)	0.0601(15)

F(13)	0.1921(6)	0.0407(4)	0.4217(2)	0.0734(19)
F(14)	0.3092(7)	0.0744(4)	0.4901(2)	0.087(2)
F(15)	0.4268(6)	0.2313(4)	0.48846(16)	0.0631(15)
F(16)	0.2628(4)	0.4450(3)	0.43946(15)	0.0433(11)
F(17)	0.6350(5)	0.2905(3)	0.39512(17)	0.0498(12)
F(18)	0.7626(5)	0.4451(4)	0.3856(2)	0.0696(18)
F(19)	0.6383(5)	0.6004(3)	0.4015(2)	0.0624(16)
F(20)	0.2264(6)	0.8275(4)	0.37168(16)	0.0582(14)
F(21)	0.2063(5)	0.8606(3)	0.44805(17)	0.0542(13)
F(22)	0.2915(6)	0.7327(4)	0.51180(16)	0.0627(15)
F(23)	0.4040(6)	0.5717(4)	0.49895(15)	0.0646(16)
C(19)	0.3138(8)	0.2618(6)	0.3833(3)	0.0376(18)
C(20)	0.2558(8)	0.1805(6)	0.3858(3)	0.044(2)
C(21)	0.2516(9)	0.1186(6)	0.4211(3)	0.051(2)
C(22)	0.3081(10)	0.1366(6)	0.4558(3)	0.055(3)
C(23)	0.3703(8)	0.2167(6)	0.4543(3)	0.042(2)
C(24)	0.3741(7)	0.2795(5)	0.4189(2)	0.0332(17)
C(25)	0.4452(7)	0.3640(5)	0.4180(2)	0.0299(16)
C(26)	0.5740(8)	0.3668(5)	0.4044(2)	0.0356(17)
C(27)	0.6380(8)	0.4461(6)	0.3993(3)	0.043(2)
C(28)	0.5743(8)	0.5230(6)	0.4078(3)	0.0413(19)
C(29)	0.4463(8)	0.5261(5)	0.4215(2)	0.0348(17)
C(30)	0.3873(7)	0.4453(5)	0.4267(2)	0.0335(17)
C(31)	0.3777(8)	0.6147(5)	0.4280(2)	0.0348(17)
C(32)	0.3614(9)	0.6325(6)	0.4667(3)	0.043(2)
C(33)	0.3034(8)	0.7156(6)	0.4737(3)	0.0419(19)
C(34)	0.2590(8)	0.7810(6)	0.4415(3)	0.0421(19)
C(35)	0.2724(8)	0.7622(5)	0.4027(3)	0.0386(18)
C(36)	0.3297(7)	0.6806(5)	0.3954(2)	0.0335(17)
I(5)	0.80935(6)	-0.08530(4)	0.16675(2)	0.05054(15)
I(6)	0.81825(6)	0.20675(4)	0.16160(2)	0.04554(14)
F(24)	0.6918(5)	-0.2592(4)	0.13809(19)	0.0637(16)
F(25)	0.6626(5)	-0.3039(4)	0.0644(2)	0.0697(18)
F(26)	0.7626(6)	-0.2007(5)	-0.0026(2)	0.0759(19)
F(27)	0.8949(6)	-0.0556(4)	0.00561(16)	0.0661(16)
F(28)	0.7638(5)	0.1061(3)	0.06047(16)	0.0483(12)
F(29)	1.1249(5)	-0.0995(4)	0.1037(2)	0.0716(19)
F(30)	1.2653(5)	0.0408(4)	0.1149(3)	0.088(2)
F(31)	1.1569(5)	0.2134(4)	0.0981(2)	0.0640(16)
F(32)	0.9678(5)	0.2885(4)	0.00457(15)	0.0560(13)
F(33)	0.8550(7)	0.4610(4)	-0.00612(17)	0.0700(17)
F(34)	0.7189(6)	0.5206(4)	0.05528(18)	0.0634(15)
F(35)	0.7053(6)	0.4129(4)	0.12814(17)	0.0599(14)
C(37)	0.8085(8)	-0.1304(6)	0.1102(3)	0.0401(19)
C(38)	0.7444(8)	-0.2070(6)	0.1056(3)	0.046(2)
C(39)	0.7289(8)	-0.2311(6)	0.0683(4)	0.054(3)
C(40)	0.7783(9)	-0.1787(7)	0.0351(3)	0.055(2)
C(41)	0.8453(9)	-0.1030(6)	0.0392(3)	0.048(2)
C(42)	0.8950(8)	0.2593(6)	0.0725(2)	0.0367(18)
C(43)	0.9401(8)	0.0007(5)	0.0800(2)	0.0362(18)
C(44)	1.0696(9)	-0.0140(6)	0.0940(3)	0.049(2)
C(45)	1.1415(8)	0.0572(7)	0.0998(3)	0.052(2)
C(46)	1.0869(8)	0.1449(6)	0.0916(3)	0.046(2)
C(47)	0.9578(8)	0.1647(5)	0.0780(2)	0.0345(17)
C(48)	0.8894(7)	0.0903(6)	0.0727(2)	0.0345(17)
C(49)	0.9029(8)	0.3179(6)	0.0365(2)	0.042(2)
C(50)	0.8442(9)	0.4043(6)	0.0297(3)	0.047(2)
C(51)	0.7757(9)	0.4361(6)	0.0610(3)	0.045(2)

C(52)	0.7701(8)	0.3792(6)	0.0983(3)	0.043(2)
C(53)	0.8285(7)	0.2914(5)	0.1047(2)	0.0345(17)
C(87)	0.8636(8)	-0.0794(6)	0.0766(3)	0.0398(19)
I(7)	0.34952(6)	0.68723(4)	0.17540(2)	0.04165(13)
I(8)	0.35284(6)	0.40085(4)	0.19217(2)	0.04957(15)
F(36)	0.4690(5)	0.8810(3)	0.14504(14)	0.0452(11)
F(37)	0.5004(5)	0.9783(3)	0.07068(15)	0.0520(13)
F(38)	0.4129(6)	0.9191(4)	0.00406(15)	0.0663(17)
F(39)	0.3020(6)	0.7562(4)	0.01198(14)	0.0594(15)
F(40)	0.4662(4)	0.5586(3)	0.08694(17)	0.0493(12)
F(41)	0.0568(5)	0.7219(3)	0.08789(18)	0.0510(13)
F(42)	-0.0615(5)	0.5633(4)	0.1013(2)	0.0696(18)
F(43)	0.0827(5)	0.4029(3)	0.1076(2)	0.0609(15)
F(44)	0.3593(6)	0.3876(4)	0.03167(16)	0.0663(16)
F(45)	0.4810(6)	0.2193(5)	0.0416(2)	0.078(2)
F(46)	0.5378(5)	0.1258(4)	0.1176(2)	0.0720(18)
F(47)	0.4842(6)	0.2040(4)	0.18247(19)	0.0678(17)
C(54)	0.3727(7)	0.7654(5)	0.1174(2)	0.0324(16)
C(55)	0.4271(7)	0.8479(5)	0.1124(2)	0.0314(16)
C(56)	0.4437(8)	0.8996(5)	0.0747(2)	0.0369(18)
C(57)	0.3999(9)	0.8687(6)	0.0406(2)	0.043(2)
C(58)	0.3431(9)	0.7855(6)	0.0454(2)	0.0403(19)
C(59)	0.3306(7)	0.7339(5)	0.0828(2)	0.0303(16)
C(60)	0.2651(7)	0.6445(5)	0.0866(2)	0.0314(16)
C(61)	0.1304(8)	0.6433(6)	0.0897(3)	0.0378(18)
C(62)	0.0716(8)	0.5614(6)	0.0967(3)	0.049(2)
C(63)	0.1437(8)	0.4811(5)	0.1001(3)	0.0385(19)
C(64)	0.2783(8)	0.4751(5)	0.0966(2)	0.0357(17)
C(65)	0.3351(7)	0.5603(5)	0.0896(2)	0.0316(16)
C(66)	0.3558(8)	0.3855(6)	0.1020(3)	0.0391(18)
C(67)	0.3901(9)	0.3456(6)	0.0694(3)	0.049(2)
C(68)	0.4521(9)	0.2586(7)	0.0739(3)	0.054(3)
C(69)	0.4812(8)	0.2114(6)	0.1123(3)	0.050(2)
C(70)	0.4514(8)	0.2517(6)	0.1456(3)	0.048(2)
C(71)	0.3907(8)	0.3391(6)	0.1409(3)	0.0397(19)
H(72A)	0.907972	0.427418	0.291362	0.091
H(72B)	1.001566	0.4971	0.265593	0.091
H(73A)	0.930192	0.327852	0.24741	0.182
H(73B)	1.074642	0.362408	0.249282	0.182
H(73C)	0.979297	0.403631	0.211514	0.182
H(74A)	0.623295	0.494527	0.228056	0.082
H(74B)	0.724442	0.412772	0.219964	0.082
H(75A)	0.604707	0.34853	0.271089	0.144
H(75B)	0.606218	0.434947	0.293933	0.144
H(75C)	0.735782	0.367945	0.293453	0.144
H(76A)	0.75995	0.597789	0.190789	0.098
H(76B)	0.864148	0.516205	0.184394	0.098
H(77A)	0.941523	0.673449	0.175228	0.138
H(77B)	1.036603	0.592321	0.199793	0.138
H(77C)	0.947668	0.657847	0.223939	0.138
H(78A)	0.852155	0.615879	0.274271	0.103
H(78B)	0.755349	0.546132	0.298442	0.103
H(79A)	0.688957	0.703534	0.240281	0.143
H(79B)	0.607444	0.661971	0.279342	0.143
H(79C)	0.601441	0.618875	0.238583	0.143
H(80A)	0.428711	-0.172765	0.251278	0.116
H(80B)	0.519593	-0.127319	0.280243	0.116
H(80C)	0.569539	-0.141019	0.236007	0.116

H(81A)	0.336967	0.134222	0.230857	0.094
H(81B)	0.245501	0.084935	0.203815	0.094
H(82A)	0.102295	0.183242	0.225407	0.126
H(82B)	0.171727	0.172936	0.269146	0.126
H(82C)	0.084638	0.093972	0.258979	0.126
H(83A)	0.37377	-0.053915	0.314494	0.102
H(83B)	0.262648	0.028399	0.312843	0.102
H(84A)	0.532518	0.052224	0.290858	0.206
H(84B)	0.464801	0.080991	0.330556	0.206
H(84C)	0.42216	0.135509	0.286293	0.206
H(85A)	0.238451	-0.124563	0.27554	0.095
H(85B)	0.129605	-0.041156	0.273257	0.095
H(86A)	0.225584	-0.120388	0.206746	0.182
H(86B)	0.133871	-0.026976	0.200717	0.182
H(86C)	0.078841	-0.120347	0.223614	0.182
H(88A)	0.405029	-0.033578	0.205555	0.075
H(88B)	0.498466	0.011982	0.233525	0.075

Table S23. Anisotropic displacement parameters [Å²] for **syn-m-1-TEABr**

	U11	U22	U33	U23	U13	U12
I(1)	0.0485(3)	0.0464(3)	0.0441(3)	0.0001(2)	-0.0024(2)	-0.0063(3)
I(2)	0.0462(3)	0.0547(4)	0.0473(3)	-0.0099(2)	-0.0027(2)	-0.0025(3)
F(1)	0.056(3)	0.038(3)	0.080(4)	0.009(3)	0.007(3)	-0.011(3)
F(2)	0.052(3)	0.045(3)	0.104(5)	-0.029(3)	0.013(3)	-0.026(3)
F(3)	0.066(4)	0.075(4)	0.068(4)	-0.033(3)	-0.001(3)	-0.030(3)
F(4)	0.068(4)	0.053(3)	0.046(3)	-0.012(2)	-0.001(2)	-0.020(3)
F(5)	0.037(3)	0.042(3)	0.183(8)	-0.041(4)	0.022(4)	-0.005(3)
F(6)	0.032(3)	0.061(4)	0.278(12)	-0.058(6)	0.039(5)	-0.016(3)
F(7)	0.044(3)	0.047(3)	0.163(7)	-0.034(4)	0.011(4)	-0.020(3)
F(8)	0.074(4)	0.050(3)	0.054(3)	-0.006(2)	-0.009(3)	-0.005(3)
F(9)	0.094(5)	0.038(3)	0.100(5)	0.009(3)	-0.019(4)	0.009(3)
F(10)	0.059(4)	0.044(3)	0.123(6)	-0.023(3)	-0.005(4)	0.014(3)
F(11)	0.053(3)	0.079(4)	0.080(4)	-0.044(3)	-0.005(3)	0.007(3)
F(48)	0.027(2)	0.042(3)	0.090(4)	-0.026(3)	-0.001(2)	-0.004(2)
C(1)	0.030(4)	0.035(4)	0.046(4)	-0.009(3)	0.003(3)	-0.002(3)
C(2)	0.033(4)	0.028(4)	0.060(5)	-0.003(4)	0.009(4)	-0.005(4)
C(3)	0.033(5)	0.034(5)	0.080(6)	-0.019(4)	0.009(4)	-0.012(4)
C(4)	0.032(5)	0.049(5)	0.061(5)	-0.026(4)	0.001(4)	-0.009(4)
C(5)	0.040(5)	0.036(4)	0.047(5)	-0.015(4)	0.009(4)	-0.012(4)
C(6)	0.027(4)	0.033(4)	0.048(4)	-0.006(3)	0.003(3)	-0.006(3)
C(7)	0.029(4)	0.033(4)	0.039(4)	-0.003(3)	0.000(3)	-0.007(3)
C(8)	0.030(4)	0.034(4)	0.043(4)	-0.010(3)	-0.003(3)	-0.005(3)
C(9)	0.034(4)	0.028(4)	0.045(4)	-0.008(3)	-0.003(3)	-0.002(3)
C(10)	0.037(5)	0.033(5)	0.083(7)	-0.016(4)	0.002(4)	-0.013(4)
C(11)	0.028(5)	0.044(6)	0.121(9)	-0.022(6)	0.014(5)	-0.011(4)
C(12)	0.033(5)	0.034(5)	0.087(7)	-0.016(4)	0.012(5)	-0.001(4)
C(13)	0.033(4)	0.032(4)	0.060(5)	-0.015(4)	-0.013(4)	-0.005(4)
C(14)	0.046(5)	0.046(5)	0.057(6)	-0.006(4)	-0.015(4)	-0.011(4)
C(15)	0.042(5)	0.034(5)	0.089(8)	-0.006(5)	-0.020(5)	0.006(4)
C(16)	0.040(5)	0.041(6)	0.097(8)	-0.026(5)	-0.016(5)	0.002(4)
C(17)	0.038(5)	0.045(6)	0.077(7)	-0.024(5)	-0.015(5)	0.002(4)
C(18)	0.037(5)	0.039(5)	0.044(4)	-0.009(4)	-0.010(4)	-0.003(4)
N(1)	0.035(4)	0.052(5)	0.048(4)	-0.003(3)	-0.008(3)	-0.005(3)
C(72)	0.051(6)	0.075(8)	0.092(9)	0.012(7)	-0.014(6)	0.001(6)
C(73)	0.059(8)	0.076(10)	0.23(2)	-0.050(12)	0.014(11)	0.021(7)
C(74)	0.055(6)	0.062(7)	0.088(8)	-0.012(6)	-0.009(6)	-0.016(5)
C(75)	0.055(7)	0.094(10)	0.122(11)	0.033(8)	-0.003(7)	-0.019(7)
C(76)	0.079(9)	0.097(10)	0.064(7)	0.002(6)	0.000(6)	-0.020(7)
C(77)	0.075(9)	0.089(9)	0.099(10)	0.029(8)	0.007(7)	-0.022(7)
C(78)	0.081(9)	0.111(11)	0.072(8)	-0.029(7)	-0.001(7)	-0.015(8)
C(79)	0.061(8)	0.087(10)	0.139(13)	-0.026(9)	0.002(8)	0.007(7)
Br(1)	0.0645(6)	0.0704(7)	0.0338(4)	-0.0011(4)	-0.0038(4)	-0.0113(5)
N(2)	0.036(4)	0.050(4)	0.047(4)	-0.008(3)	0.007(3)	-0.006(3)
C(80)	0.062(7)	0.075(8)	0.098(9)	-0.025(7)	0.003(6)	0.001(6)
C(81)	0.084(9)	0.062(7)	0.080(8)	0.004(6)	0.015(7)	0.007(6)
C(82)	0.063(8)	0.071(8)	0.117(11)	-0.018(7)	-0.001(7)	0.015(6)
C(83)	0.068(8)	0.139(13)	0.050(6)	-0.025(7)	-0.012(5)	0.010(8)
C(84)	0.055(8)	0.24(2)	0.161(16)	-0.143(16)	0.012(9)	-0.030(11)
C(85)	0.048(6)	0.069(8)	0.126(11)	-0.030(7)	0.012(7)	-0.010(6)
C(86)	0.071(9)	0.156(16)	0.169(16)	-0.110(14)	-0.012(10)	-0.016(10)
C(88)	0.048(6)	0.079(8)	0.063(6)	-0.014(5)	0.015(5)	-0.012(5)
Br(2)	0.0735(7)	0.0588(6)	0.0301(4)	-0.0016(4)	0.0026(4)	-0.0063(5)
I(3)	0.0463(3)	0.0542(3)	0.0376(3)	-0.0062(2)	0.0002(2)	-0.0123(3)
I(4)	0.0460(3)	0.0516(3)	0.0371(3)	-0.0037(2)	0.0007(2)	0.0040(3)
F(12)	0.049(3)	0.060(3)	0.081(4)	-0.036(3)	0.005(3)	-0.016(3)
F(13)	0.050(3)	0.035(3)	0.134(6)	-0.005(3)	0.005(3)	-0.018(3)

F(14)	0.081(5)	0.066(4)	0.097(5)	0.044(4)	-0.006(4)	-0.023(4)
F(15)	0.068(4)	0.069(4)	0.047(3)	0.010(3)	-0.007(3)	-0.016(3)
F(16)	0.036(3)	0.034(2)	0.060(3)	-0.009(2)	0.014(2)	0.000(2)
F(17)	0.037(3)	0.034(3)	0.082(4)	-0.021(2)	0.009(2)	0.001(2)
F(18)	0.029(3)	0.051(3)	0.135(6)	-0.031(3)	0.021(3)	-0.008(2)
F(19)	0.039(3)	0.037(3)	0.115(5)	-0.020(3)	0.005(3)	-0.010(2)
F(20)	0.064(4)	0.042(3)	0.060(3)	0.009(2)	0.005(3)	0.017(3)
F(21)	0.053(3)	0.037(3)	0.073(3)	-0.016(2)	-0.001(3)	0.012(2)
F(22)	0.069(4)	0.073(4)	0.049(3)	-0.028(3)	-0.013(3)	0.022(3)
F(23)	0.083(4)	0.065(4)	0.041(3)	-0.013(2)	-0.017(3)	0.036(3)
C(19)	0.026(4)	0.037(4)	0.049(5)	-0.001(3)	0.005(3)	-0.005(3)
C(20)	0.030(4)	0.043(5)	0.061(5)	-0.015(4)	0.000(4)	-0.003(4)
C(21)	0.032(5)	0.030(5)	0.090(7)	-0.005(4)	0.008(5)	-0.008(4)
C(22)	0.048(5)	0.037(5)	0.069(6)	0.020(4)	0.008(5)	-0.005(4)
C(23)	0.033(4)	0.048(5)	0.042(4)	0.005(4)	0.002(4)	-0.006(4)
C(24)	0.031(4)	0.031(4)	0.037(4)	-0.001(3)	0.006(3)	-0.004(3)
C(25)	0.027(4)	0.027(4)	0.034(4)	0.000(3)	-0.004(3)	0.000(3)
C(26)	0.032(4)	0.027(4)	0.048(4)	-0.010(3)	-0.001(3)	0.007(3)
C(27)	0.022(4)	0.050(5)	0.061(5)	-0.017(4)	0.005(4)	-0.002(4)
C(28)	0.030(4)	0.035(5)	0.061(5)	-0.012(4)	-0.003(4)	-0.009(4)
C(29)	0.034(4)	0.031(4)	0.039(4)	-0.008(3)	-0.009(3)	0.007(3)
C(30)	0.026(4)	0.040(5)	0.036(4)	-0.010(3)	-0.002(3)	-0.002(3)
C(31)	0.032(4)	0.028(4)	0.044(4)	-0.005(3)	-0.009(3)	0.001(3)
C(32)	0.045(5)	0.040(5)	0.042(4)	-0.012(4)	-0.014(4)	0.013(4)
C(33)	0.039(5)	0.041(5)	0.048(5)	-0.018(4)	-0.008(4)	0.008(4)
C(34)	0.036(5)	0.035(5)	0.055(5)	-0.010(4)	-0.006(4)	0.007(4)
C(35)	0.033(4)	0.031(4)	0.050(5)	-0.003(3)	-0.001(4)	0.002(4)
C(36)	0.029(4)	0.034(4)	0.037(4)	-0.005(3)	-0.002(3)	-0.003(3)
I(5)	0.0421(3)	0.0621(4)	0.0456(3)	-0.0009(3)	-0.0033(2)	-0.0122(3)
I(6)	0.0425(3)	0.0525(3)	0.0408(3)	-0.0064(2)	0.0011(2)	-0.0013(3)
F(24)	0.048(3)	0.041(3)	0.095(4)	0.013(3)	-0.003(3)	-0.012(3)
F(25)	0.042(3)	0.044(3)	0.130(6)	-0.031(3)	0.002(3)	-0.013(3)
F(26)	0.057(4)	0.103(5)	0.085(4)	-0.059(4)	0.009(3)	-0.026(4)
F(27)	0.067(4)	0.089(4)	0.052(3)	-0.026(3)	0.014(3)	-0.036(3)
F(28)	0.033(3)	0.037(3)	0.072(3)	-0.002(2)	-0.019(2)	-0.004(2)
F(29)	0.035(3)	0.036(3)	0.146(6)	-0.023(3)	-0.013(3)	0.005(2)
F(30)	0.028(3)	0.054(4)	0.186(8)	-0.035(4)	-0.032(4)	0.005(3)
F(31)	0.034(3)	0.040(3)	0.125(5)	-0.031(3)	-0.010(3)	-0.009(2)
F(32)	0.061(3)	0.055(3)	0.049(3)	-0.005(2)	0.009(2)	0.008(3)
F(33)	0.089(5)	0.054(3)	0.056(3)	0.014(3)	-0.002(3)	0.011(3)
F(34)	0.062(4)	0.044(3)	0.080(4)	-0.007(3)	-0.010(3)	0.017(3)
F(35)	0.060(3)	0.056(3)	0.064(3)	-0.017(3)	0.003(3)	0.014(3)
C(37)	0.034(4)	0.034(4)	0.052(5)	-0.003(4)	0.002(4)	-0.008(4)
C(38)	0.026(4)	0.036(5)	0.074(6)	-0.005(4)	-0.001(4)	-0.003(4)
C(39)	0.024(4)	0.041(5)	0.101(8)	-0.028(5)	-0.003(5)	-0.005(4)
C(40)	0.035(5)	0.060(6)	0.078(7)	-0.036(5)	0.007(5)	-0.004(5)
C(41)	0.038(5)	0.049(5)	0.059(5)	-0.012(4)	-0.002(4)	-0.012(4)
C(42)	0.028(4)	0.037(4)	0.044(4)	-0.005(3)	-0.004(3)	0.001(3)
C(43)	0.029(4)	0.034(4)	0.048(4)	-0.012(3)	0.004(3)	-0.009(3)
C(44)	0.035(5)	0.028(4)	0.087(7)	-0.018(4)	-0.001(4)	0.004(4)
C(45)	0.018(4)	0.050(6)	0.092(7)	-0.021(5)	-0.010(4)	-0.001(4)
C(46)	0.029(4)	0.039(5)	0.072(6)	-0.017(4)	-0.001(4)	-0.008(4)
C(47)	0.029(4)	0.034(4)	0.041(4)	-0.009(3)	0.001(3)	-0.002(3)
C(48)	0.022(4)	0.043(5)	0.036(4)	0.000(3)	-0.003(3)	-0.004(3)
C(49)	0.037(5)	0.051(5)	0.039(4)	-0.006(4)	0.001(4)	-0.003(4)
C(50)	0.050(5)	0.047(5)	0.041(5)	0.000(4)	-0.002(4)	0.000(4)
C(51)	0.042(5)	0.030(4)	0.061(5)	-0.009(4)	-0.011(4)	0.010(4)
C(52)	0.036(5)	0.044(5)	0.051(5)	-0.014(4)	-0.004(4)	0.004(4)

C(53)	0.029(4)	0.035(4)	0.039(4)	-0.002(3)	-0.004(3)	-0.006(3)
C(87)	0.025(4)	0.037(5)	0.059(5)	-0.011(4)	-0.002(4)	-0.005(4)
I(7)	0.0498(3)	0.0414(3)	0.0334(2)	-0.0031(2)	-0.0021(2)	-0.0089(2)
I(8)	0.0480(3)	0.0562(4)	0.0421(3)	-0.0036(2)	0.0053(2)	0.0010(3)
F(36)	0.047(3)	0.045(3)	0.048(3)	-0.016(2)	-0.007(2)	-0.010(2)
F(37)	0.062(3)	0.040(3)	0.056(3)	-0.007(2)	0.006(2)	-0.026(3)
F(38)	0.100(5)	0.062(4)	0.040(3)	0.000(2)	0.007(3)	-0.046(3)
F(39)	0.088(4)	0.058(3)	0.036(3)	-0.008(2)	-0.003(3)	-0.038(3)
F(40)	0.026(2)	0.042(3)	0.079(4)	-0.006(2)	0.007(2)	-0.005(2)
F(41)	0.033(3)	0.031(3)	0.089(4)	-0.014(2)	-0.001(2)	0.004(2)
F(42)	0.025(3)	0.050(3)	0.138(6)	-0.026(3)	0.009(3)	-0.010(2)
F(43)	0.040(3)	0.034(3)	0.111(5)	-0.015(3)	0.004(3)	-0.016(2)
F(44)	0.069(4)	0.081(4)	0.050(3)	-0.024(3)	-0.009(3)	0.018(3)
F(45)	0.066(4)	0.082(4)	0.100(5)	-0.061(4)	-0.015(3)	0.018(3)
F(46)	0.045(3)	0.041(3)	0.132(6)	-0.024(3)	-0.004(3)	0.007(3)
F(47)	0.059(4)	0.052(3)	0.079(4)	0.019(3)	0.016(3)	0.010(3)
C(54)	0.028(4)	0.034(4)	0.034(4)	-0.001(3)	-0.002(3)	-0.002(3)
C(55)	0.029(4)	0.031(4)	0.036(4)	-0.009(3)	-0.002(3)	-0.005(3)
C(56)	0.039(5)	0.027(4)	0.048(4)	-0.010(3)	0.006(4)	-0.011(4)
C(57)	0.049(5)	0.042(5)	0.037(4)	0.001(4)	0.001(4)	-0.017(4)
C(58)	0.047(5)	0.042(5)	0.036(4)	-0.012(3)	0.002(4)	-0.015(4)
C(59)	0.027(4)	0.024(4)	0.039(4)	-0.002(3)	0.001(3)	-0.006(3)
C(60)	0.032(4)	0.028(4)	0.035(4)	-0.005(3)	0.004(3)	-0.008(3)
C(61)	0.030(4)	0.036(5)	0.049(5)	-0.012(4)	0.000(3)	-0.002(4)
C(62)	0.024(4)	0.051(6)	0.072(6)	-0.010(4)	-0.005(4)	-0.007(4)
C(63)	0.030(4)	0.028(4)	0.060(5)	-0.009(4)	0.005(4)	-0.009(4)
C(64)	0.034(4)	0.034(4)	0.041(4)	-0.010(3)	0.002(3)	-0.008(4)
C(65)	0.023(4)	0.033(4)	0.039(4)	-0.006(3)	0.000(3)	-0.007(3)
C(66)	0.025(4)	0.040(5)	0.055(5)	-0.016(4)	0.002(3)	-0.003(4)
C(67)	0.036(5)	0.047(5)	0.069(6)	-0.025(5)	-0.009(4)	-0.001(4)
C(68)	0.038(5)	0.048(6)	0.086(7)	-0.041(5)	-0.004(5)	0.001(4)
C(69)	0.029(5)	0.037(5)	0.087(7)	-0.016(5)	0.000(4)	0.000(4)
C(70)	0.032(5)	0.037(5)	0.073(6)	0.001(4)	0.000(4)	-0.006(4)
C(71)	0.033(4)	0.036(5)	0.050(5)	-0.007(4)	0.007(4)	-0.008(4)

Table S24. Atomic coordinates and equivalent isotropic displacement parameters [Å²] for **syn-m-1-TDAI**

	x	y	z	U(eq)
I(1)	0.46498(3)	0.26964(9)	0.40633(2)	0.04048(15)
I(2)	0.64588(2)	0.32230(7)	0.42846(2)	0.02835(12)
F(1)	0.3161(3)	0.3610(9)	0.39828(10)	0.0633(18)
F(2)	0.2079(3)	0.2986(10)	0.41944(12)	0.074(2)
F(3)	0.2140(3)	0.1442(10)	0.45648(12)	0.075(2)
F(4)	0.3291(3)	0.0454(8)	0.47214(9)	0.0500(15)
F(5)	0.4255(3)	-0.1995(6)	0.44948(8)	0.0376(12)
F(6)	0.5414(3)	-0.2889(6)	0.46582(9)	0.0414(13)
F(7)	0.6255(3)	-0.0374(7)	0.47721(9)	0.0402(13)
F(8)	0.4784(2)	0.4010(6)	0.45653(8)	0.0343(12)
F(9)	0.5595(3)	0.3266(8)	0.50614(7)	0.0497(16)
F(10)	0.6449(3)	0.5764(8)	0.51817(8)	0.0551(17)
F(11)	0.7339(3)	0.7054(8)	0.49161(9)	0.0531(15)
F(12)	0.7345(3)	0.5919(8)	0.45288(9)	0.0524(16)
C(10)	0.3819(4)	0.2360(12)	0.42420(14)	0.033(2)
C(11)	0.3218(5)	0.2834(14)	0.41670(15)	0.045(2)
C(12)	0.2654(5)	0.2516(14)	0.42744(19)	0.050(3)
C(13)	0.2691(4)	0.1720(14)	0.44587(19)	0.049(3)
C(14)	0.3289(5)	0.1237(13)	0.45383(15)	0.038(2)
C(15)	0.3859(4)	0.1547(11)	0.44332(13)	0.0273(18)
C(16)	0.4490(4)	0.1044(11)	0.45274(12)	0.0257(17)
C(17)	0.4661(4)	-0.0728(11)	0.45558(12)	0.0271(18)
C(18)	0.5248(4)	-0.1188(11)	0.46387(13)	0.0308(19)
C(19)	0.5678(4)	0.0110(11)	0.46950(12)	0.0271(18)
C(20)	0.5540(4)	0.1894(10)	0.46712(11)	0.0231(17)
C(21)	0.4938(4)	0.2303(10)	0.45894(11)	0.0221(16)
C(22)	0.6017(4)	0.3275(9)	0.47284(12)	0.0202(16)
C(23)	0.6026(4)	0.3891(11)	0.49272(12)	0.0275(18)
C(24)	0.6469(5)	0.5180(12)	0.49905(13)	0.033(2)
C(25)	0.6905(5)	0.5819(11)	0.48543(14)	0.034(2)
C(26)	0.6910(4)	0.5229(12)	0.46581(13)	0.0301(19)
C(27)	0.6467(4)	0.3966(10)	0.45930(11)	0.0213(16)
N(1)	0.4594(4)	0.7251(13)	0.37212(18)	0.061(3)
N(2)	0.6158(4)	0.7473(10)	0.39913(12)	0.0412(19)
N(3)	0.6130(4)	0.6609(11)	0.34454(12)	0.0405(19)
C(1)	0.4221(6)	0.6942(17)	0.3537(3)	0.092(6)
C(2)	0.4241(6)	0.7676(16)	0.3903(3)	0.085(5)
C(3)	0.5835(7)	0.8007(15)	0.41751(16)	0.058(3)
C(4)	0.6857(5)	0.7590(14)	0.39830(18)	0.056(3)
C(5)	0.6828(5)	0.6375(17)	0.34481(18)	0.058(3)
C(6)	0.5768(7)	0.6282(15)	0.32581(16)	0.059(3)
C(7)	0.5239(4)	0.7174(12)	0.37186(15)	0.036(2)
C(8)	0.5821(4)	0.7276(12)	0.38204(14)	0.0315(19)
C(9)	0.5808(4)	0.6916(11)	0.36144(14)	0.0315(19)
I(3)	0.47410(2)	0.19940(8)	0.34760(2)	0.03158(13)
I(4)	0.64475(2)	0.10802(7)	0.32265(2)	0.02728(12)
F(13)	0.3292(3)	0.0915(9)	0.35826(9)	0.0538(16)
F(14)	0.2188(3)	0.0868(10)	0.33690(12)	0.069(2)
F(15)	0.2179(3)	0.1915(11)	0.29742(12)	0.079(2)
F(16)	0.3279(3)	0.3023(9)	0.27959(8)	0.0517(15)
F(17)	0.4909(2)	0.0239(6)	0.29961(7)	0.0290(10)
F(18)	0.4101(3)	0.6040(7)	0.29595(9)	0.0444(14)
F(19)	0.5153(3)	0.7029(7)	0.27409(9)	0.0519(16)
F(20)	0.6093(3)	0.4664(7)	0.26568(8)	0.0416(13)
F(21)	0.5679(3)	0.1191(8)	0.24374(8)	0.0461(14)

F(22)	0.6569(3)	-0.1202(9)	0.23189(9)	0.0612(18)
F(23)	0.7405(3)	-0.2588(9)	0.25940(9)	0.0635(19)
F(24)	0.7360(3)	-0.1568(9)	0.29839(9)	0.0596(19)
C(28)	0.3885(4)	0.1983(12)	0.32986(13)	0.0288(18)
C(29)	0.3317(4)	0.1443(13)	0.33868(14)	0.037(2)
C(30)	0.2741(5)	0.1418(13)	0.32778(17)	0.043(2)
C(31)	0.2737(4)	0.1945(15)	0.30795(17)	0.047(3)
C(32)	0.3306(4)	0.2510(12)	0.29919(14)	0.032(2)
C(33)	0.3885(4)	0.2525(11)	0.30955(12)	0.0264(18)
C(34)	0.4478(4)	0.3110(11)	0.29875(12)	0.0255(17)
C(35)	0.4981(4)	0.1934(10)	0.29396(11)	0.0211(16)
C(36)	0.5536(4)	0.2389(10)	0.28312(11)	0.0210(16)
C(37)	0.5569(4)	0.4116(12)	0.27649(13)	0.032(2)
C(38)	0.5092(5)	0.5352(12)	0.28058(14)	0.033(2)
C(39)	0.4565(4)	0.4830(12)	0.29163(13)	0.0287(18)
C(40)	0.6046(4)	0.1075(10)	0.27775(12)	0.0214(16)
C(41)	0.6088(4)	0.0519(12)	0.25772(12)	0.0299(19)
C(42)	0.6539(5)	-0.0681(12)	0.25145(13)	0.036(2)
C(43)	0.6964(5)	-0.1391(12)	0.26543(15)	0.040(2)
C(44)	0.6922(4)	-0.0864(13)	0.28537(13)	0.036(2)
C(45)	0.6477(4)	0.0370(11)	0.29176(11)	0.0221(16)
I(5)	0.61764(3)	0.21830(8)	0.37560(2)	0.03090(13)
H(1A)	0.37739	0.735475	0.355707	0.138
H(1AB)	0.421835	0.567256	0.350637	0.138
H(1AC)	0.441957	0.759	0.342419	0.138
H(2A)	0.395561	0.868985	0.387726	0.128
H(2AB)	0.454848	0.797363	0.40115	0.128
H(2AC)	0.397909	0.665389	0.394426	0.128
H(3A)	0.564588	0.918694	0.41565	0.087
H(3AB)	0.615005	0.804059	0.42868	0.087
H(3AC)	0.548996	0.715866	0.42073	0.087
H(4A)	0.702947	0.659142	0.390467	0.083
H(4AB)	0.703409	0.755518	0.412111	0.083
H(4AC)	0.698328	0.870381	0.39175	0.083
H(5A)	0.699052	0.63039	0.330838	0.086
H(5AB)	0.69359	0.527963	0.352045	0.086
H(5AC)	0.703101	0.738263	0.351718	0.086
H(6A)	0.542457	0.717324	0.324357	0.088
H(6AB)	0.557208	0.509973	0.326333	0.088
H(6AC)	0.606383	0.635403	0.314177	0.088

Table S25. Anisotropic displacement parameters [\AA^2] for syn-m-1-TDAI

	U11	U22	U33	U23	U13	U12
I(1)	0.0433(3)	0.0489(4)	0.0292(3)	0.0063(3)	-0.0028(2)	-0.0027(3)
I(2)	0.0271(3)	0.0327(3)	0.0253(2)	0.0018(2)	0.00310(19)	-0.0015(2)
F(1)	0.057(4)	0.068(4)	0.065(4)	0.005(3)	-0.027(3)	0.013(3)
F(2)	0.033(3)	0.072(5)	0.118(6)	-0.025(4)	-0.029(4)	0.018(3)
F(3)	0.029(3)	0.088(5)	0.108(6)	-0.019(5)	0.020(3)	-0.004(3)
F(4)	0.040(3)	0.055(4)	0.055(4)	-0.001(3)	0.019(3)	-0.012(3)
F(5)	0.044(3)	0.016(3)	0.052(3)	-0.004(2)	-0.001(2)	-0.012(2)
F(6)	0.042(3)	0.016(3)	0.066(4)	0.005(2)	-0.004(3)	-0.004(2)
F(7)	0.037(3)	0.025(3)	0.058(3)	0.007(2)	-0.011(2)	0.002(2)
F(8)	0.039(3)	0.013(2)	0.050(3)	-0.003(2)	-0.007(2)	-0.002(2)
F(9)	0.064(4)	0.061(4)	0.024(3)	-0.006(2)	0.014(2)	-0.030(3)
F(10)	0.070(4)	0.062(4)	0.034(3)	-0.022(3)	-0.002(3)	-0.020(3)
F(11)	0.048(3)	0.050(4)	0.061(4)	-0.012(3)	-0.010(3)	-0.027(3)
F(12)	0.039(3)	0.065(4)	0.053(3)	0.004(3)	0.004(3)	-0.032(3)
C(10)	0.021(4)	0.038(5)	0.041(5)	-0.010(4)	-0.006(3)	0.001(4)
C(11)	0.048(6)	0.041(6)	0.045(6)	-0.009(5)	-0.017(5)	0.006(5)
C(12)	0.027(5)	0.044(6)	0.080(8)	-0.019(6)	-0.015(5)	0.009(4)
C(13)	0.021(5)	0.043(6)	0.083(8)	-0.021(6)	0.006(5)	0.002(4)
C(14)	0.036(5)	0.031(5)	0.046(6)	-0.011(4)	0.006(4)	-0.009(4)
C(15)	0.025(4)	0.019(4)	0.038(5)	-0.011(3)	-0.003(3)	-0.006(3)
C(16)	0.027(4)	0.024(5)	0.025(4)	-0.003(3)	0.004(3)	0.003(3)
C(17)	0.036(5)	0.018(4)	0.027(4)	-0.003(3)	0.009(3)	-0.007(4)
C(18)	0.043(5)	0.013(4)	0.036(5)	0.004(3)	0.007(4)	-0.004(4)
C(19)	0.022(4)	0.029(5)	0.030(4)	0.002(3)	0.001(3)	0.004(3)
C(20)	0.028(4)	0.018(4)	0.023(4)	-0.002(3)	0.002(3)	-0.008(3)
C(21)	0.026(4)	0.014(4)	0.026(4)	-0.003(3)	0.002(3)	-0.002(3)
C(22)	0.021(4)	0.008(4)	0.031(4)	-0.003(3)	-0.004(3)	-0.004(3)
C(23)	0.035(5)	0.026(5)	0.022(4)	0.000(3)	0.004(3)	-0.004(4)
C(24)	0.045(5)	0.026(5)	0.028(4)	-0.006(4)	-0.002(4)	-0.006(4)
C(25)	0.040(5)	0.014(4)	0.047(5)	-0.003(4)	-0.009(4)	-0.007(4)
C(26)	0.023(4)	0.034(5)	0.034(5)	0.006(4)	-0.001(3)	-0.009(4)
C(27)	0.025(4)	0.018(4)	0.022(4)	0.003(3)	0.002(3)	-0.004(3)
N(1)	0.021(4)	0.045(6)	0.118(9)	-0.002(6)	0.006(5)	0.001(4)
N(2)	0.053(5)	0.029(5)	0.041(4)	0.003(3)	-0.005(4)	-0.003(4)
N(3)	0.044(5)	0.038(5)	0.039(4)	0.008(4)	0.001(4)	-0.001(4)
C(1)	0.052(8)	0.046(8)	0.178(17)	-0.017(9)	-0.057(9)	0.008(6)
C(2)	0.050(7)	0.038(7)	0.168(16)	0.008(8)	0.052(9)	0.006(6)
C(3)	0.096(9)	0.031(6)	0.046(6)	-0.002(5)	0.002(6)	0.003(6)
C(4)	0.043(6)	0.040(6)	0.083(8)	0.012(6)	-0.035(6)	0.000(5)
C(5)	0.045(6)	0.068(8)	0.060(7)	0.005(6)	0.020(5)	0.005(6)
C(6)	0.092(9)	0.039(7)	0.045(6)	0.002(5)	-0.003(6)	-0.019(6)
C(7)	0.029(5)	0.021(5)	0.059(6)	0.006(4)	-0.001(4)	0.003(4)
C(8)	0.028(4)	0.024(5)	0.043(5)	0.006(4)	-0.002(4)	0.004(4)
C(9)	0.027(4)	0.022(5)	0.045(5)	0.007(4)	-0.005(4)	-0.004(4)
I(3)	0.0285(3)	0.0432(3)	0.0230(2)	0.0025(2)	0.00068(19)	0.0026(2)

I(4)	0.0209(2)	0.0378(3)	0.0231(2)	0.0039(2)	-0.00219(18)	0.0026(2)
F(13)	0.043(3)	0.070(4)	0.048(3)	0.016(3)	0.020(3)	0.003(3)
F(14)	0.018(3)	0.087(5)	0.102(5)	0.022(4)	0.018(3)	-0.008(3)
F(15)	0.024(3)	0.116(6)	0.097(5)	0.025(5)	-0.017(3)	-0.014(4)
F(16)	0.031(3)	0.081(4)	0.043(3)	0.012(3)	-0.016(2)	-0.002(3)
F(17)	0.028(2)	0.024(3)	0.034(3)	0.001(2)	0.0045(19)	0.001(2)
F(18)	0.034(3)	0.036(3)	0.063(4)	0.007(3)	0.008(3)	0.021(2)
F(19)	0.063(4)	0.024(3)	0.069(4)	0.016(3)	0.019(3)	0.011(3)
F(20)	0.037(3)	0.034(3)	0.053(3)	0.009(2)	0.021(2)	0.000(2)
F(21)	0.039(3)	0.073(4)	0.027(3)	-0.004(3)	-0.007(2)	0.021(3)
F(22)	0.068(4)	0.080(5)	0.036(3)	-0.024(3)	0.004(3)	0.018(4)
F(23)	0.067(4)	0.066(4)	0.058(4)	-0.001(3)	0.018(3)	0.044(4)
F(24)	0.050(4)	0.081(5)	0.047(3)	0.016(3)	0.005(3)	0.047(3)
C(28)	0.016(4)	0.035(5)	0.036(4)	0.000(4)	-0.001(3)	0.007(4)
C(29)	0.032(5)	0.041(6)	0.037(5)	0.008(4)	0.011(4)	0.002(4)
C(30)	0.027(5)	0.034(6)	0.069(7)	0.011(5)	0.008(4)	-0.001(4)
C(31)	0.020(4)	0.052(6)	0.068(7)	0.008(5)	-0.011(4)	-0.001(4)
C(32)	0.017(4)	0.032(5)	0.048(5)	0.002(4)	-0.005(3)	0.002(3)
C(33)	0.022(4)	0.024(5)	0.033(4)	-0.001(3)	0.001(3)	0.004(3)
C(34)	0.021(4)	0.032(5)	0.024(4)	0.002(3)	-0.006(3)	0.007(3)
C(35)	0.019(4)	0.024(4)	0.020(4)	0.002(3)	-0.005(3)	-0.005(3)
C(36)	0.023(4)	0.020(4)	0.021(4)	0.002(3)	-0.005(3)	0.006(3)
C(37)	0.036(5)	0.033(5)	0.028(4)	0.006(4)	0.008(4)	0.006(4)
C(38)	0.039(5)	0.023(5)	0.037(5)	0.009(4)	-0.005(4)	0.003(4)
C(39)	0.022(4)	0.030(5)	0.035(5)	0.000(4)	0.000(3)	0.000(3)
C(40)	0.021(4)	0.016(4)	0.027(4)	-0.001(3)	0.001(3)	0.002(3)
C(41)	0.030(4)	0.037(5)	0.023(4)	-0.001(4)	-0.004(3)	0.005(4)
C(42)	0.042(5)	0.035(5)	0.030(5)	-0.013(4)	0.005(4)	0.010(4)
C(43)	0.047(6)	0.030(5)	0.044(5)	-0.002(4)	0.018(4)	0.019(4)
C(44)	0.034(5)	0.045(6)	0.029(5)	0.011(4)	-0.001(4)	0.009(4)
C(45)	0.021(4)	0.027(4)	0.019(4)	0.009(3)	0.005(3)	0.004(3)
I(5)	0.0345(3)	0.0346(3)	0.0236(2)	0.0030(2)	-0.0040(2)	-0.0021(2)

Table S26. Atomic coordinates and equivalent isotropic displacement parameters [\AA^2] for syn-m-1-TDACl

	x	y	z	U(eq)	S.O.F.
I(3)	0.56824(3)	0.64127(3)	0.33980(2)	0.06596(15)	1
F(00A)	0.4671(3)	0.6625(2)	0.47127(13)	0.0672(11)	1
F(00C)	0.3861(3)	0.8772(2)	0.43224(16)	0.0806(13)	1
F(00M)	0.3516(3)	0.7623(3)	0.47166(16)	0.0866(15)	1
F(008)	0.6531(2)	0.7930(2)	0.39219(13)	0.0624(10)	1
F(13)	0.6970(3)	0.5287(2)	0.36824(15)	0.0830(14)	1
F(14)	0.7748(3)	0.5016(2)	0.43976(17)	0.0812(13)	1
F(15)	0.7592(3)	0.5857(2)	0.50543(14)	0.0796(13)	1
F(16)	0.6588(3)	0.6936(2)	0.49948(12)	0.0692(11)	1
F(17A)	0.5208(9)	0.9474(7)	0.4674(4)	0.065(3)	0.472(13)
F(18A)	0.5683(8)	1.0698(6)	0.4433(5)	0.079(4)	0.472(13)
F(19A)	0.6018(8)	1.0940(6)	0.3617(5)	0.092(4)	0.472(13)
F(20A)	0.5890(8)	0.9972(8)	0.3060(5)	0.088(5)	0.472(13)
C(40A)	0.5350(15)	0.9075(14)	0.3986(6)	0.050(5)	0.472(13)
C(41A)	0.5365(17)	0.9596(13)	0.4275(8)	0.047(5)	0.472(13)
C(42A)	0.5607(10)	1.0216(10)	0.4153(7)	0.063(4)	0.472(13)
C(43A)	0.576(2)	1.0337(16)	0.3746(13)	0.070(6)	0.472(13)
C(44A)	0.5736(16)	0.9833(17)	0.3450(9)	0.075(5)	0.472(13)
C(45A)	0.5509(14)	0.9211(13)	0.3573(7)	0.055(4)	0.472(13)
I(4A)	0.53819(19)	0.8449(4)	0.31131(9)	0.0652(9)	0.472(13)
F(17B)	0.5438(10)	0.9597(6)	0.4469(6)	0.072(4)	0.528(13)
F(18B)	0.5809(7)	1.0740(5)	0.4082(7)	0.113(7)	0.528(13)
F(19B)	0.5993(8)	1.0769(6)	0.3235(7)	0.128(7)	0.528(13)
F(20B)	0.5793(8)	0.9649(8)	0.2788(5)	0.106(5)	0.528(13)
C(40B)	0.5434(15)	0.8989(11)	0.3833(9)	0.060(5)	0.528(13)
C(41B)	0.5500(12)	0.9583(10)	0.4060(9)	0.065(5)	0.528(13)
C(42B)	0.572(2)	1.0180(13)	0.3857(13)	0.079(7)	0.528(13)
C(43B)	0.5775(13)	1.0180(12)	0.3455(11)	0.077(6)	0.528(13)
C(44B)	0.5702(13)	0.9617(11)	0.3202(10)	0.081(5)	0.528(13)
C(45B)	0.5544(12)	0.9024(8)	0.3417(7)	0.055(4)	0.528(13)
I(4B)	0.53631(14)	0.8176(3)	0.30270(15)	0.0633(8)	0.528(13)
C(28)	0.6323(4)	0.6248(4)	0.39612(18)	0.0493(15)	1
C(29)	0.6858(5)	0.5708(4)	0.4001(2)	0.0580(18)	1
C(30)	0.7278(5)	0.5572(4)	0.4367(2)	0.0591(18)	1
C(31)	0.7195(5)	0.5993(4)	0.4696(2)	0.0573(17)	1
C(32)	0.6672(4)	0.6541(3)	0.4659(2)	0.0519(16)	1
C(33)	0.6223(4)	0.6685(3)	0.43035(18)	0.0455(14)	1
C(34)	0.5620(4)	0.7249(3)	0.43003(17)	0.0418(13)	1
C(35)	0.4846(4)	0.7195(3)	0.45092(18)	0.0496(15)	1
C(36)	0.4258(5)	0.7692(4)	0.4514(2)	0.0590(17)	1
C(37)	0.4443(4)	0.8281(4)	0.4318(2)	0.0588(18)	1
C(38)	0.5205(4)	0.8379(3)	0.4109(2)	0.0558(17)	1
C(39)	0.5774(4)	0.7851(3)	0.4113(2)	0.0491(15)	1
I(1)	0.44924(3)	0.22400(3)	0.31990(2)	0.06722(16)	1
I(2)	0.45077(3)	0.42440(3)	0.32111(2)	0.06846(16)	1

F(1)	0.3665(3)	0.0801(3)	0.33215(16)	0.0904(16)	1
F(2)	0.3259(3)	0.0091(2)	0.39981(19)	0.0889(16)	1
F(3)	0.3544(4)	0.0586(3)	0.47640(18)	0.0953(16)	1
F(4)	0.4299(3)	0.1782(2)	0.48549(12)	0.0782(13)	1
F(5)	0.3561(2)	0.3202(2)	0.40624(11)	0.0567(9)	1
F(6)	0.6099(3)	0.2048(2)	0.43367(15)	0.0754(12)	1
F(7)	0.6933(3)	0.3209(3)	0.44244(17)	0.0810(13)	1
F(8)	0.6087(3)	0.4372(2)	0.43194(15)	0.0787(13)	1
F(9)	0.4284(3)	0.4554(2)	0.48775(12)	0.0735(12)	1
F(10)	0.3441(3)	0.5715(3)	0.48307(17)	0.0891(15)	1
F(11)	0.3156(3)	0.6290(3)	0.4078(2)	0.0946(16)	1
F(12)	0.3571(3)	0.5635(3)	0.33759(16)	0.0886(15)	1
C(10)	0.4190(4)	0.1691(4)	0.3732(2)	0.0553(17)	1
C(11)	0.3821(5)	0.1064(4)	0.3703(3)	0.065(2)	1
C(12)	0.3616(5)	0.0695(4)	0.4040(3)	0.068(2)	1
C(13)	0.3759(5)	0.0940(4)	0.4432(3)	0.068(2)	1
C(14)	0.4137(5)	0.1566(4)	0.4467(2)	0.0598(18)	1
C(15)	0.4363(4)	0.1942(4)	0.4133(2)	0.0518(16)	1
C(16)	0.4802(4)	0.2592(4)	0.41964(17)	0.0491(15)	1
C(17)	0.5663(4)	0.2619(4)	0.4293(2)	0.0556(17)	1
C(18)	0.6094(4)	0.3210(4)	0.4338(2)	0.0588(18)	1
C(19)	0.5663(4)	0.3792(4)	0.42847(19)	0.0564(17)	1
C(20)	0.4792(4)	0.3815(3)	0.41922(17)	0.0483(15)	1
C(21)	0.4400(4)	0.3201(4)	0.41531(17)	0.0499(16)	1
C(22)	0.4349(4)	0.4463(4)	0.4147(2)	0.0557(17)	1
C(23)	0.4108(5)	0.4806(4)	0.4499(2)	0.0610(18)	1
C(24)	0.3699(5)	0.5416(4)	0.4483(3)	0.072(2)	1
C(25)	0.3532(5)	0.5693(5)	0.4103(3)	0.075(2)	1
C(26)	0.3766(5)	0.5363(5)	0.3749(3)	0.069(2)	1
C(27)	0.4167(4)	0.4747(4)	0.3761(2)	0.0596(19)	1
N(1A)	0.7457(5)	1.2095(4)	0.2667(2)	0.0670(12)	0.813(4)
N(2A)	0.7225(5)	1.3876(4)	0.2856(2)	0.0670(12)	0.813(4)
N(3A)	0.7897(5)	1.3232(4)	0.1816(2)	0.0670(12)	0.813(4)
C(1A)	0.7493(5)	1.2708(4)	0.2524(3)	0.0454(11)	0.813(4)
C(2A)	0.7403(5)	1.3375(5)	0.2591(3)	0.0454(11)	0.813(4)
C(3A)	0.7667(5)	1.3141(5)	0.2209(3)	0.0454(11)	0.813(4)
C(4A)	0.7010(8)	1.3736(6)	0.3280(3)	0.0773(12)	0.813(4)
C(5A)	0.7120(7)	1.4545(5)	0.2714(3)	0.0773(12)	0.813(4)
C(6A)	0.8002(8)	1.3887(5)	0.1653(4)	0.0773(12)	0.813(4)
C(7A)	0.8081(7)	1.2681(5)	0.1551(3)	0.0773(12)	0.813(4)
C(8A)	0.7696(8)	1.1535(5)	0.2421(4)	0.0773(12)	0.813(4)
C(9A)	0.7067(7)	1.1952(6)	0.3058(3)	0.0773(12)	0.813(4)
N(1B)	0.719(2)	1.2983(15)	0.3115(10)	0.0670(12)	0.187(4)
N(2B)	0.770(2)	1.4024(16)	0.2193(9)	0.0670(12)	0.187(4)
N(3B)	0.776(2)	1.2201(17)	0.2147(9)	0.0670(12)	0.187(4)
C(1B)	0.738(2)	1.303(2)	0.2682(12)	0.0454(11)	0.187(4)
C(2B)	0.759(2)	1.348(2)	0.2389(13)	0.0454(11)	0.187(4)

C(3B)	0.765(2)	1.279(2)	0.2346(13)	0.0454(11)	0.187(4)
C(4B)	0.754(3)	1.4623(19)	0.2417(14)	0.0773(12)	0.187(4)
C(5B)	0.807(3)	1.411(3)	0.1790(11)	0.0773(12)	0.187(4)
C(6B)	0.806(3)	1.223(3)	0.1727(10)	0.0773(12)	0.187(4)
C(7B)	0.795(3)	1.156(2)	0.2307(16)	0.0773(12)	0.187(4)
C(8B)	0.705(3)	1.2332(18)	0.3279(15)	0.0773(12)	0.187(4)
C(9B)	0.679(3)	1.352(2)	0.3328(16)	0.0773(12)	0.187(4)
Cl(1)	0.5	0.7006(3)	0.25	0.1128(15)	1
Cl(2)	0.5	0.3255(2)	0.25	0.1065(13)	1
H(4A1)	0.690232	1.414658	0.34245	0.116	0.407(2)
H(4A2)	0.650858	1.346186	0.328977	0.116	0.407(2)
H(4A3)	0.747545	1.350683	0.34114	0.116	0.407(2)
H(4A4)	0.702191	1.32636	0.332595	0.116	0.407(2)
H(4A5)	0.741565	1.394832	0.346068	0.116	0.407(2)
H(4A6)	0.644878	1.390335	0.333905	0.116	0.407(2)
H(5A1)	0.699657	1.482889	0.294715	0.116	0.407(2)
H(5A2)	0.763594	1.469229	0.258224	0.116	0.407(2)
H(5A3)	0.665754	1.456514	0.251927	0.116	0.407(2)
H(5A4)	0.719679	1.456199	0.241863	0.116	0.407(2)
H(5A5)	0.655743	1.469859	0.278353	0.116	0.407(2)
H(5A6)	0.753582	1.482574	0.28465	0.116	0.407(2)
H(6A1)	0.81688	1.385929	0.13659	0.116	0.407(2)
H(6A2)	0.747344	1.412565	0.167423	0.116	0.407(2)
H(6A3)	0.843566	1.41167	0.18072	0.116	0.407(2)
H(6A4)	0.788314	1.420847	0.186565	0.116	0.407(2)
H(6A5)	0.857849	1.394211	0.155732	0.116	0.407(2)
H(6A6)	0.761628	1.395105	0.142436	0.116	0.407(2)
H(7A1)	0.82353	1.284275	0.128008	0.116	0.407(2)
H(7A2)	0.854648	1.242927	0.166466	0.116	0.407(2)
H(7A3)	0.758659	1.240165	0.152874	0.116	0.407(2)
H(7A4)	0.801028	1.227303	0.170224	0.116	0.407(2)
H(7A5)	0.76991	1.268651	0.131765	0.116	0.407(2)
H(7A6)	0.865899	1.271413	0.145358	0.116	0.407(2)
H(8A1)	0.762543	1.113436	0.257979	0.116	0.407(2)
H(8A2)	0.734134	1.151544	0.217761	0.116	0.407(2)
H(8A3)	0.828221	1.157834	0.233827	0.116	0.407(2)
H(8A4)	0.787389	1.168441	0.215065	0.116	0.407(2)
H(8A5)	0.815798	1.130332	0.255284	0.116	0.407(2)
H(8A6)	0.721711	1.124042	0.239217	0.116	0.407(2)
H(9A1)	0.710023	1.148179	0.311116	0.116	0.407(2)
H(9A2)	0.735969	1.218957	0.327385	0.116	0.407(2)
H(9A3)	0.648012	1.208693	0.305083	0.116	0.407(2)
H(9A4)	0.685979	1.235707	0.31794	0.116	0.407(2)
H(9A5)	0.660034	1.164929	0.301671	0.116	0.407(2)
H(9A6)	0.74799	1.175193	0.323972	0.116	0.407(2)
H(4B1)	0.764763	1.499917	0.224013	0.116	0.093(2)
H(4B2)	0.695621	1.462988	0.250639	0.116	0.093(2)

H(4B3)	0.790858	1.464405	0.265508	0.116	0.093(2)
H(4B4)	0.736065	1.451623	0.269427	0.116	0.093(2)
H(4B5)	0.805207	1.488552	0.2428	0.116	0.093(2)
H(4B6)	0.70997	1.487136	0.227932	0.116	0.093(2)
H(5B1)	0.807796	1.457551	0.172062	0.116	0.093(2)
H(5B2)	0.864432	1.394165	0.179077	0.116	0.093(2)
H(5B3)	0.773888	1.387201	0.158831	0.116	0.093(2)
H(5B4)	0.822948	1.368394	0.167918	0.116	0.093(2)
H(5B5)	0.766312	1.43178	0.160904	0.116	0.093(2)
H(5B6)	0.856856	1.438744	0.181149	0.116	0.093(2)
H(6B1)	0.810753	1.179226	0.161639	0.116	0.093(2)
H(6B2)	0.765945	1.248508	0.156209	0.116	0.093(2)
H(6B3)	0.860403	1.244929	0.172081	0.116	0.093(2)
H(6B4)	0.813981	1.269216	0.16498	0.116	0.093(2)
H(6B5)	0.858789	1.199934	0.17041	0.116	0.093(2)
H(6B6)	0.764331	1.203513	0.154538	0.116	0.093(2)
H(7B1)	0.797772	1.124232	0.208205	0.116	0.093(2)
H(7B2)	0.848377	1.156729	0.245022	0.116	0.093(2)
H(7B3)	0.75056	1.142212	0.249673	0.116	0.093(2)
H(7B4)	0.800034	1.157883	0.260395	0.116	0.093(2)
H(7B5)	0.749429	1.125386	0.223578	0.116	0.093(2)
H(7B6)	0.847246	1.139903	0.218927	0.116	0.093(2)
H(8B1)	0.73467	1.201204	0.31104	0.116	0.093(2)
H(8B2)	0.726141	1.231205	0.355836	0.116	0.093(2)
H(8B3)	0.645081	1.223403	0.327706	0.116	0.093(2)
H(8B4)	0.669258	1.236004	0.352015	0.116	0.093(2)
H(8B5)	0.677787	1.206003	0.307218	0.116	0.093(2)
H(8B6)	0.758847	1.213805	0.335349	0.116	0.093(2)
H(9B1)	0.692563	1.392769	0.319153	0.116	0.093(2)
H(9B2)	0.61838	1.345176	0.332818	0.116	0.093(2)
H(9B3)	0.69944	1.352979	0.360949	0.116	0.093(2)
H(9B4)	0.647693	1.334514	0.356127	0.116	0.093(2)
H(9B5)	0.721875	1.382106	0.342462	0.116	0.093(2)
H(9B6)	0.640815	1.374304	0.314332	0.116	0.093(2)

Table S27. Anisotropic displacement parameters [Å²] for syn-m-1-TDACI

	U11	U22	U33	U23	U13	U12
I(3)	0.0621(3)	0.1026(4)	0.0333(2)	-0.0150(2)	0.00260(18)	-0.0074(3)
F(00A)	0.071(3)	0.077(3)	0.053(2)	0.007(2)	0.021(2)	-0.015(2)
F(00C)	0.066(3)	0.079(3)	0.097(4)	-0.010(3)	-0.001(2)	0.020(2)
F(00M)	0.067(3)	0.112(4)	0.081(3)	0.001(3)	0.034(2)	0.011(3)
F(008)	0.040(2)	0.070(3)	0.077(3)	0.019(2)	0.0009(18)	-0.0065(18)
F(13)	0.094(3)	0.082(3)	0.073(3)	-0.028(2)	0.019(3)	0.012(3)
F(14)	0.067(3)	0.068(3)	0.109(4)	0.006(3)	0.014(3)	0.015(2)
F(15)	0.084(3)	0.087(3)	0.068(3)	0.017(2)	-0.024(2)	0.004(3)
F(16)	0.091(3)	0.078(3)	0.0386(19)	-0.0134(19)	-0.013(2)	0.005(2)
F(17A)	0.084(8)	0.072(7)	0.041(6)	-0.009(5)	0.011(5)	0.004(6)
F(18A)	0.070(7)	0.062(6)	0.105(9)	-0.013(7)	-0.005(7)	0.007(5)
F(19A)	0.078(7)	0.075(7)	0.123(12)	0.044(8)	0.030(7)	0.011(6)
F(20A)	0.083(8)	0.097(10)	0.085(10)	0.045(9)	0.028(7)	0.013(7)
C(40A)	0.040(9)	0.064(10)	0.046(8)	-0.014(7)	-0.012(7)	0.020(7)
C(41A)	0.042(10)	0.059(8)	0.040(11)	-0.006(8)	-0.016(10)	0.010(6)
C(42A)	0.040(8)	0.066(9)	0.083(10)	0.004(8)	-0.002(8)	0.008(6)
C(43A)	0.053(13)	0.064(12)	0.092(13)	0.018(9)	0.010(10)	0.011(11)
C(44A)	0.054(11)	0.078(12)	0.093(12)	0.006(10)	0.010(10)	0.014(11)
C(45A)	0.046(9)	0.069(10)	0.051(9)	-0.017(8)	0.005(8)	0.017(8)
I(4A)	0.0544(7)	0.106(3)	0.0350(8)	-0.0015(11)	0.0065(6)	0.0148(11)
F(17B)	0.073(8)	0.058(6)	0.084(14)	-0.017(9)	-0.009(10)	0.001(5)
F(18B)	0.066(7)	0.038(5)	0.23(2)	-0.013(9)	-0.040(10)	0.006(5)
F(19B)	0.090(8)	0.085(8)	0.208(19)	0.085(11)	-0.006(10)	-0.013(6)
F(20B)	0.093(8)	0.130(11)	0.095(9)	0.059(9)	0.006(7)	-0.015(7)
C(40B)	0.052(10)	0.047(8)	0.082(12)	-0.001(8)	-0.002(10)	-0.014(7)
C(41B)	0.048(9)	0.054(9)	0.092(13)	-0.012(9)	-0.010(10)	0.003(7)
C(42B)	0.048(12)	0.052(9)	0.136(18)	0.008(10)	-0.026(13)	0.005(8)
C(43B)	0.042(9)	0.050(9)	0.138(17)	0.022(10)	-0.012(10)	0.003(8)
C(44B)	0.067(11)	0.065(9)	0.112(14)	0.025(9)	-0.007(11)	-0.011(8)
C(45B)	0.040(8)	0.042(8)	0.084(11)	0.000(7)	-0.002(8)	0.004(6)
I(4B)	0.0511(6)	0.0933(19)	0.0455(11)	0.0100(11)	0.0103(6)	-0.0047(8)
C(28)	0.048(4)	0.068(4)	0.032(3)	-0.007(3)	0.007(2)	-0.011(3)
C(29)	0.061(4)	0.062(4)	0.051(4)	-0.015(3)	0.020(3)	-0.002(3)
C(30)	0.050(4)	0.059(4)	0.068(5)	0.007(4)	0.007(3)	-0.002(3)
C(31)	0.057(4)	0.063(4)	0.052(4)	0.009(3)	0.002(3)	-0.007(3)
C(32)	0.058(4)	0.055(4)	0.042(3)	-0.003(3)	0.003(3)	-0.006(3)
C(33)	0.051(4)	0.052(4)	0.033(3)	0.000(2)	0.007(2)	-0.007(3)
C(34)	0.047(3)	0.048(3)	0.030(3)	-0.005(2)	-0.002(2)	-0.005(3)
C(35)	0.063(4)	0.053(4)	0.033(3)	-0.004(3)	0.006(3)	-0.007(3)
C(36)	0.055(4)	0.073(5)	0.049(4)	-0.011(3)	0.010(3)	0.002(4)
C(37)	0.050(4)	0.067(5)	0.060(4)	-0.013(3)	-0.009(3)	0.009(3)
C(38)	0.052(4)	0.049(4)	0.066(4)	-0.006(3)	-0.013(3)	-0.009(3)
C(39)	0.043(3)	0.057(4)	0.048(3)	0.001(3)	-0.005(3)	-0.009(3)
I(1)	0.0543(3)	0.1123(4)	0.0350(2)	-0.0181(2)	-0.00921(17)	0.0107(3)
I(2)	0.0520(3)	0.1199(4)	0.0335(2)	0.0185(2)	-0.00636(17)	-0.0057(3)
F(1)	0.093(3)	0.100(4)	0.079(3)	-0.044(3)	-0.041(3)	0.013(3)
F(2)	0.073(3)	0.067(3)	0.127(4)	-0.025(3)	-0.028(3)	-0.004(2)
F(3)	0.115(4)	0.076(3)	0.094(4)	0.004(3)	0.003(3)	-0.032(3)
F(4)	0.120(4)	0.074(3)	0.041(2)	-0.0050(19)	-0.001(2)	-0.029(3)
F(5)	0.052(2)	0.068(2)	0.050(2)	0.0017(18)	-0.0108(17)	-0.0111(18)
F(6)	0.060(3)	0.083(3)	0.084(3)	-0.017(2)	-0.011(2)	0.004(2)
F(7)	0.048(2)	0.098(3)	0.098(4)	-0.009(3)	-0.007(2)	-0.013(2)
F(8)	0.072(3)	0.084(3)	0.081(3)	0.009(2)	-0.007(2)	-0.034(2)
F(9)	0.110(4)	0.070(3)	0.040(2)	0.0063(18)	0.009(2)	-0.025(3)
F(10)	0.099(4)	0.081(3)	0.088(3)	-0.008(3)	0.031(3)	-0.017(3)
F(11)	0.071(3)	0.086(4)	0.127(5)	0.014(3)	-0.003(3)	0.005(3)

F(12)	0.071(3)	0.113(4)	0.082(3)	0.038(3)	-0.024(2)	0.003(3)
C(10)	0.043(4)	0.077(5)	0.046(3)	-0.018(3)	-0.009(3)	0.007(3)
C(11)	0.050(4)	0.078(5)	0.068(5)	-0.030(4)	-0.022(3)	0.014(4)
C(12)	0.054(4)	0.053(4)	0.097(6)	-0.023(4)	-0.019(4)	0.005(3)
C(13)	0.063(5)	0.062(5)	0.078(5)	-0.007(4)	-0.004(4)	-0.007(4)
C(14)	0.068(5)	0.060(4)	0.051(4)	-0.011(3)	-0.005(3)	-0.007(4)
C(15)	0.048(4)	0.066(4)	0.041(3)	-0.012(3)	-0.005(3)	-0.001(3)
C(16)	0.050(4)	0.069(4)	0.028(3)	-0.004(3)	-0.002(2)	-0.007(3)
C(17)	0.056(4)	0.072(5)	0.039(3)	-0.008(3)	-0.001(3)	-0.004(4)
C(18)	0.041(4)	0.087(5)	0.048(4)	-0.005(4)	0.000(3)	-0.013(4)
C(19)	0.055(4)	0.078(5)	0.036(3)	0.003(3)	0.001(3)	-0.021(4)
C(20)	0.054(4)	0.066(4)	0.025(3)	0.006(3)	-0.003(2)	-0.016(3)
C(21)	0.047(4)	0.076(5)	0.027(3)	0.003(3)	-0.004(2)	-0.013(3)
C(22)	0.054(4)	0.072(5)	0.041(3)	0.010(3)	0.002(3)	-0.020(3)
C(23)	0.074(5)	0.059(4)	0.050(4)	0.007(3)	0.007(3)	-0.022(4)
C(24)	0.068(5)	0.078(6)	0.071(5)	0.008(4)	0.014(4)	-0.023(4)
C(25)	0.052(4)	0.079(6)	0.094(7)	0.006(5)	0.000(4)	-0.005(4)
C(26)	0.052(4)	0.089(6)	0.066(5)	0.021(4)	-0.006(4)	-0.011(4)
C(27)	0.047(4)	0.092(6)	0.040(3)	0.012(3)	-0.001(3)	-0.016(4)
N(1A)	0.063(3)	0.078(3)	0.060(3)	0.004(2)	0.003(2)	0.003(2)
N(2A)	0.063(3)	0.078(3)	0.060(3)	0.004(2)	0.003(2)	0.003(2)
N(3A)	0.063(3)	0.078(3)	0.060(3)	0.004(2)	0.003(2)	0.003(2)
C(1A)	0.040(2)	0.053(3)	0.043(3)	0.001(3)	0.0002(19)	-0.005(2)
C(2A)	0.040(2)	0.053(3)	0.043(3)	0.001(3)	0.0002(19)	-0.005(2)
C(3A)	0.040(2)	0.053(3)	0.043(3)	0.001(3)	0.0002(19)	-0.005(2)
C(4A)	0.074(3)	0.086(3)	0.072(3)	0.000(2)	-0.001(2)	0.005(2)
C(5A)	0.074(3)	0.086(3)	0.072(3)	0.000(2)	-0.001(2)	0.005(2)
C(6A)	0.074(3)	0.086(3)	0.072(3)	0.000(2)	-0.001(2)	0.005(2)
C(7A)	0.074(3)	0.086(3)	0.072(3)	0.000(2)	-0.001(2)	0.005(2)
C(8A)	0.074(3)	0.086(3)	0.072(3)	0.000(2)	-0.001(2)	0.005(2)
C(9A)	0.074(3)	0.086(3)	0.072(3)	0.000(2)	-0.001(2)	0.005(2)
N(1B)	0.063(3)	0.078(3)	0.060(3)	0.004(2)	0.003(2)	0.003(2)
N(2B)	0.063(3)	0.078(3)	0.060(3)	0.004(2)	0.003(2)	0.003(2)
N(3B)	0.063(3)	0.078(3)	0.060(3)	0.004(2)	0.003(2)	0.003(2)
C(1B)	0.040(2)	0.053(3)	0.043(3)	0.001(3)	0.0002(19)	-0.005(2)
C(2B)	0.040(2)	0.053(3)	0.043(3)	0.001(3)	0.0002(19)	-0.005(2)
C(3B)	0.040(2)	0.053(3)	0.043(3)	0.001(3)	0.0002(19)	-0.005(2)
C(4B)	0.074(3)	0.086(3)	0.072(3)	0.000(2)	-0.001(2)	0.005(2)
C(5B)	0.074(3)	0.086(3)	0.072(3)	0.000(2)	-0.001(2)	0.005(2)
C(6B)	0.074(3)	0.086(3)	0.072(3)	0.000(2)	-0.001(2)	0.005(2)
C(7B)	0.074(3)	0.086(3)	0.072(3)	0.000(2)	-0.001(2)	0.005(2)
C(8B)	0.074(3)	0.086(3)	0.072(3)	0.000(2)	-0.001(2)	0.005(2)
C(9B)	0.074(3)	0.086(3)	0.072(3)	0.000(2)	-0.001(2)	0.005(2)
Cl(1)	0.082(2)	0.213(5)	0.0435(14)	0	-0.0109(14)	0
Cl(2)	0.104(2)	0.191(4)	0.0251(11)	0	0.0127(13)	0

Table S28. Atomic coordinates and equivalent isotropic displacement parameters [Å²] for anti-m-1-TDAI

	x	y	z	U(eq)
I(1)	0.72214(5)	-0.04639(10)	0.65623(2)	0.04135(17)
I(2)	0.81934(4)	0.17716(7)	0.27687(2)	0.03442(16)
I(3)	0.55376(5)	0.07403(8)	0.54730(3)	0.03872(16)
F(1)	1.0060(6)	0.4348(9)	0.3094(2)	0.0461(15)
F(2)	1.0715(6)	0.5979(8)	0.3969(3)	0.0481(15)
F(3)	0.9756(6)	0.5429(9)	0.4816(3)	0.0511(16)
F(4)	0.8167(5)	0.3167(8)	0.4796(2)	0.0434(14)
F(5)	0.6222(5)	0.3472(7)	0.4137(3)	0.0420(13)
F(6)	0.8437(5)	-0.1079(7)	0.3785(2)	0.0396(12)
F(7)	0.6910(6)	-0.3271(7)	0.3964(3)	0.0554(18)
F(8)	0.5043(6)	-0.2146(8)	0.4243(3)	0.0509(16)
F(9)	0.3201(6)	0.2171(11)	0.5461(3)	0.0566(17)
F(10)	0.1713(6)	0.3252(11)	0.4717(3)	0.0605(19)
F(11)	0.2056(6)	0.3043(10)	0.3724(3)	0.0564(17)
F(12)	0.3931(6)	0.1844(9)	0.3482(2)	0.0485(15)
C(1)	0.8745(7)	0.2853(12)	0.3486(3)	0.0295(18)
C(2)	0.9570(9)	0.4019(12)	0.3507(4)	0.036(2)
C(3)	0.9934(9)	0.4888(11)	0.3955(4)	0.037(2)
C(4)	0.9429(9)	0.4599(12)	0.4382(4)	0.037(2)
C(5)	0.8614(8)	0.3423(12)	0.4363(4)	0.0337(19)
C(6)	0.8252(7)	0.2532(11)	0.3921(3)	0.0288(17)
C(7)	0.7377(8)	0.1290(12)	0.3951(4)	0.0304(18)
C(8)	0.7516(8)	-0.0461(12)	0.3910(4)	0.0309(18)
C(9)	0.6740(9)	-0.1596(11)	0.3999(4)	0.037(2)
C(10)	0.5786(9)	-0.1002(12)	0.4144(4)	0.037(2)
C(11)	0.5600(8)	0.0708(12)	0.4193(4)	0.0317(19)
C(12)	0.6393(8)	0.1800(11)	0.4090(4)	0.033(2)
C(13)	0.4572(7)	0.1383(11)	0.4353(4)	0.0296(17)
C(14)	0.4392(8)	0.1469(12)	0.4862(4)	0.0342(19)
C(15)	0.3418(10)	0.2111(14)	0.4975(4)	0.043(2)
C(16)	0.2646(9)	0.2646(14)	0.4591(5)	0.045(2)
C(17)	0.2820(8)	0.2564(13)	0.4093(4)	0.041(2)
C(18)	0.3778(9)	0.1918(12)	0.3973(4)	0.039(2)
N(1)	0.6401(10)	0.5326(14)	0.5884(5)	0.059(3)
N(2)	0.6805(11)	0.4251(13)	0.7247(5)	0.059(3)
N(3)	0.9035(9)	0.3784(15)	0.6479(5)	0.055(2)
C(37)	0.6799(18)	0.5829(19)	0.5429(7)	0.076(5)
C(38)	0.5286(15)	0.567(2)	0.5936(9)	0.081(5)
C(39)	0.5794(15)	0.5015(17)	0.7310(8)	0.071(4)
C(40)	0.7384(15)	0.3350(18)	0.7680(6)	0.064(4)
C(41)	0.9740(13)	0.330(3)	0.6928(6)	0.076(5)
C(42)	0.9474(14)	0.3875(16)	0.5985(6)	0.061(3)
C(43)	0.7055(11)	0.4793(13)	0.6299(5)	0.051(3)
C(44)	0.7198(11)	0.4352(14)	0.6803(5)	0.047(3)
C(45)	0.8039(11)	0.4207(12)	0.6511(5)	0.045(3)
I(4)	-0.05987(5)	0.90079(8)	0.59193(3)	0.03913(17)
I(5)	0.49812(5)	1.00628(8)	0.71819(3)	0.04133(17)
F(13)	-0.0664(7)	1.0131(10)	0.4782(3)	0.0566(18)
F(14)	0.0730(7)	0.9905(10)	0.4088(3)	0.0593(19)
F(15)	0.2642(6)	0.8440(11)	0.4334(3)	0.0556(17)
F(16)	0.3243(5)	0.7322(11)	0.5290(3)	0.0561(17)
F(17)	0.1948(6)	1.0428(7)	0.6371(2)	0.0419(14)
F(18)	0.2059(7)	0.4732(8)	0.5852(3)	0.0549(18)
F(19)	0.2822(9)	0.3811(8)	0.6815(3)	0.072(3)
F(20)	0.3098(8)	0.6177(9)	0.7560(3)	0.063(2)

F(21)	0.0815(7)	0.9353(12)	0.7468(4)	0.066(2)
F(22)	0.0873(9)	1.1885(13)	0.8152(4)	0.076(3)
F(23)	0.2749(9)	1.3542(10)	0.8445(3)	0.069(2)
F(24)	0.4541(7)	1.2648(9)	0.8060(3)	0.0589(18)
C(19)	0.0586(9)	0.8863(11)	0.5414(4)	0.0340(19)
C(20)	0.0302(9)	0.9438(13)	0.4926(4)	0.040(2)
C(21)	0.0982(11)	0.9329(14)	0.4565(4)	0.045(3)
C(22)	0.1975(10)	0.8553(14)	0.4688(4)	0.043(2)
C(23)	0.2254(9)	0.8008(13)	0.5177(4)	0.040(2)
C(24)	0.1592(9)	0.8148(12)	0.5558(4)	0.038(2)
C(25)	0.1991(8)	0.7625(12)	0.6083(4)	0.0343(19)
C(26)	0.2163(8)	0.8780(11)	0.6484(4)	0.0332(19)
C(27)	0.2536(8)	0.8382(12)	0.6985(4)	0.0338(19)
C(28)	0.2745(9)	0.6658(13)	0.7090(4)	0.041(2)
C(29)	0.2592(10)	0.5457(13)	0.6705(5)	0.045(2)
C(30)	0.2215(9)	0.5925(13)	0.6210(5)	0.041(2)
C(31)	0.2648(9)	0.9698(13)	0.7386(4)	0.036(2)
C(32)	0.3610(9)	1.0561(13)	0.7537(4)	0.036(2)
C(33)	0.3629(11)	1.1825(12)	0.7899(4)	0.043(3)
C(34)	0.2713(12)	1.2268(16)	0.8111(4)	0.050(3)
C(35)	0.1760(11)	1.1440(17)	0.7960(5)	0.050(3)
C(36)	0.1760(10)	1.0160(15)	0.7606(5)	0.044(2)
H(37A)	0.636631	0.533684	0.514059	0.115
H(37B)	0.752444	0.544658	0.543567	0.115
H(37C)	0.677623	0.70448	0.540114	0.115
H(38A)	0.485816	0.550243	0.561262	0.121
H(38B)	0.521366	0.68202	0.604646	0.121
H(38C)	0.505027	0.490828	0.61841	0.121
H(39A)	0.571349	0.605536	0.711858	0.107
H(39B)	0.576652	0.525107	0.766499	0.107
H(39C)	0.522523	0.425035	0.718736	0.107
H(40A)	0.694519	0.244904	0.778392	0.097
H(40B)	0.755652	0.412522	0.795871	0.097
H(40C)	0.803156	0.288163	0.75809	0.097
H(41A)	0.942172	0.23847	0.709854	0.114
H(41B)	0.98553	0.425072	0.715516	0.114
H(41C)	1.041216	0.292799	0.683075	0.114
H(42A)	0.89477	0.347448	0.571672	0.092
H(42B)	1.010314	0.318006	0.599971	0.092
H(42C)	0.965542	0.503105	0.591714	0.092

Table S29. Anisotropic displacement parameters [\AA^2] for **anti-m-1-TDAI**

	U11	U22	U33	U23	U13	U12
I(1)	0.0415(4)	0.0484(3)	0.0337(3)	0.0014(2)	0.0032(2)	0.0045(3)
I(2)	0.0338(3)	0.0349(3)	0.0340(3)	-0.0009(2)	0.0021(2)	-0.0027(2)
I(3)	0.0409(3)	0.0370(3)	0.0375(3)	-0.0014(2)	0.0022(2)	0.0036(2)
F(1)	0.047(4)	0.056(4)	0.036(3)	0.004(3)	0.007(3)	-0.019(3)
F(2)	0.046(4)	0.045(3)	0.053(4)	-0.002(3)	0.007(3)	-0.023(3)
F(3)	0.058(4)	0.051(3)	0.044(3)	-0.017(3)	0.006(3)	-0.021(3)
F(4)	0.049(4)	0.046(3)	0.038(3)	-0.005(2)	0.015(3)	-0.010(3)
F(5)	0.038(3)	0.022(2)	0.068(4)	-0.003(2)	0.012(3)	0.000(2)
F(6)	0.038(3)	0.033(3)	0.050(3)	-0.001(2)	0.013(3)	0.006(2)
F(7)	0.061(4)	0.019(3)	0.092(5)	-0.003(3)	0.028(4)	-0.001(3)
F(8)	0.045(4)	0.033(3)	0.080(5)	0.000(3)	0.027(3)	-0.012(3)
F(9)	0.051(4)	0.075(5)	0.047(4)	-0.003(3)	0.019(3)	0.018(4)
F(10)	0.040(4)	0.074(5)	0.069(5)	0.004(4)	0.016(3)	0.022(3)
F(11)	0.038(4)	0.069(4)	0.060(4)	0.008(3)	-0.007(3)	0.008(3)
F(12)	0.053(4)	0.056(4)	0.036(3)	0.002(3)	0.005(3)	0.005(3)
C(1)	0.029(5)	0.032(4)	0.026(4)	-0.001(3)	-0.003(3)	-0.004(4)
C(2)	0.039(5)	0.033(5)	0.037(5)	0.006(4)	0.007(4)	-0.001(4)
C(3)	0.037(5)	0.028(4)	0.044(5)	-0.002(4)	0.001(4)	-0.008(4)
C(4)	0.036(5)	0.032(4)	0.041(5)	-0.004(4)	0.001(4)	-0.008(4)
C(5)	0.031(5)	0.032(4)	0.040(5)	0.000(4)	0.009(4)	0.000(4)
C(6)	0.024(4)	0.029(4)	0.032(4)	0.003(3)	0.000(3)	0.001(3)
C(7)	0.026(5)	0.025(4)	0.039(5)	0.000(4)	0.004(4)	-0.004(4)
C(8)	0.032(5)	0.029(4)	0.033(4)	-0.002(3)	0.008(4)	0.002(4)
C(9)	0.038(6)	0.023(4)	0.052(6)	0.000(4)	0.011(4)	-0.002(4)
C(10)	0.042(5)	0.027(4)	0.044(5)	0.001(4)	0.011(4)	-0.009(4)
C(11)	0.032(5)	0.030(4)	0.033(4)	-0.002(3)	0.006(4)	-0.001(4)
C(12)	0.034(5)	0.021(4)	0.041(5)	-0.002(3)	0.002(4)	0.002(3)
C(13)	0.025(5)	0.028(4)	0.036(4)	-0.001(3)	0.003(3)	-0.004(3)
C(14)	0.033(5)	0.029(4)	0.041(5)	-0.001(4)	0.005(4)	0.002(4)
C(15)	0.043(6)	0.042(5)	0.045(6)	-0.002(4)	0.007(4)	0.005(5)
C(16)	0.040(6)	0.042(5)	0.053(6)	0.000(5)	0.009(5)	0.005(4)
C(17)	0.030(5)	0.040(5)	0.051(6)	0.005(4)	0.000(4)	0.003(4)
C(18)	0.042(6)	0.032(4)	0.043(5)	0.000(4)	0.011(4)	-0.007(4)
N(1)	0.059(7)	0.041(5)	0.072(7)	-0.001(5)	-0.017(6)	0.004(5)
N(2)	0.065(7)	0.042(5)	0.071(7)	0.006(5)	0.013(6)	-0.005(5)
N(3)	0.046(6)	0.060(6)	0.057(6)	0.000(5)	-0.005(5)	0.001(5)
C(37)	0.104(14)	0.048(7)	0.069(10)	-0.007(6)	-0.024(9)	0.024(8)
C(38)	0.061(10)	0.057(8)	0.115(15)	0.005(8)	-0.023(9)	0.011(7)
C(39)	0.070(10)	0.042(6)	0.107(13)	0.006(7)	0.033(9)	-0.001(6)
C(40)	0.079(10)	0.048(7)	0.067(8)	-0.001(6)	0.012(7)	-0.013(6)
C(41)	0.050(8)	0.112(13)	0.064(9)	-0.001(8)	-0.004(7)	0.026(8)
C(42)	0.073(9)	0.038(6)	0.075(9)	0.001(6)	0.020(7)	0.005(6)
C(43)	0.056(7)	0.025(4)	0.066(8)	-0.007(5)	-0.013(6)	-0.001(5)
C(44)	0.049(7)	0.033(5)	0.057(7)	-0.006(4)	0.001(5)	-0.005(4)
C(45)	0.051(7)	0.030(5)	0.050(6)	0.002(4)	-0.004(5)	0.000(4)
I(4)	0.0406(4)	0.0336(3)	0.0424(3)	-0.0034(2)	0.0021(2)	0.0039(2)
I(5)	0.0390(3)	0.0365(3)	0.0478(3)	-0.0061(2)	0.0031(3)	-0.0014(2)

F(13)	0.053(4)	0.063(4)	0.050(4)	0.009(3)	-0.011(3)	0.018(3)
F(14)	0.069(5)	0.069(5)	0.038(3)	0.009(3)	-0.001(3)	-0.012(4)
F(15)	0.047(4)	0.073(4)	0.048(4)	-0.011(3)	0.012(3)	-0.011(3)
F(16)	0.037(4)	0.074(5)	0.056(4)	-0.010(3)	0.001(3)	0.010(3)
F(17)	0.060(4)	0.024(2)	0.039(3)	0.001(2)	-0.006(3)	-0.002(3)
F(18)	0.069(5)	0.036(3)	0.057(4)	-0.018(3)	-0.006(3)	0.007(3)
F(19)	0.115(7)	0.026(3)	0.069(5)	-0.001(3)	-0.011(5)	0.022(4)
F(20)	0.096(6)	0.042(3)	0.046(4)	0.008(3)	-0.010(4)	0.009(4)
F(21)	0.046(4)	0.083(5)	0.071(5)	-0.017(4)	0.017(4)	-0.004(4)
F(22)	0.082(6)	0.090(6)	0.062(5)	-0.016(4)	0.036(4)	0.020(5)
F(23)	0.118(7)	0.050(4)	0.043(4)	-0.016(3)	0.024(4)	0.000(4)
F(24)	0.078(5)	0.049(4)	0.049(4)	-0.016(3)	0.007(3)	-0.012(4)
C(19)	0.035(5)	0.030(4)	0.034(5)	-0.007(4)	-0.004(4)	0.001(4)
C(20)	0.041(6)	0.039(5)	0.037(5)	0.000(4)	-0.005(4)	0.002(4)
C(21)	0.060(7)	0.043(5)	0.029(5)	-0.001(4)	-0.009(5)	-0.009(5)
C(22)	0.046(6)	0.041(5)	0.040(5)	-0.011(4)	0.004(4)	-0.005(4)
C(23)	0.031(5)	0.041(5)	0.046(5)	-0.012(4)	0.000(4)	0.000(4)
C(24)	0.038(6)	0.030(4)	0.043(5)	-0.008(4)	-0.009(4)	0.000(4)
C(25)	0.028(4)	0.032(4)	0.041(5)	-0.004(4)	-0.002(4)	0.006(4)
C(26)	0.036(5)	0.024(4)	0.038(5)	-0.002(4)	0.001(4)	0.002(4)
C(27)	0.032(5)	0.029(4)	0.040(5)	0.003(4)	0.002(4)	-0.002(3)
C(28)	0.043(6)	0.035(5)	0.041(5)	0.001(4)	-0.003(4)	0.010(4)
C(29)	0.052(7)	0.029(5)	0.053(6)	0.000(4)	-0.002(5)	0.010(4)
C(30)	0.042(6)	0.033(5)	0.046(6)	-0.009(4)	-0.002(4)	0.004(4)
C(31)	0.046(6)	0.036(5)	0.028(5)	0.005(4)	0.008(4)	0.006(4)
C(32)	0.041(6)	0.035(5)	0.030(5)	0.002(4)	0.000(4)	0.003(4)
C(33)	0.067(8)	0.029(4)	0.033(5)	-0.001(4)	0.002(5)	-0.005(4)
C(34)	0.075(9)	0.045(6)	0.031(5)	-0.002(4)	0.018(5)	0.009(6)
C(35)	0.060(8)	0.054(6)	0.040(6)	-0.002(5)	0.016(5)	0.012(6)
C(36)	0.041(6)	0.048(6)	0.044(6)	0.001(5)	0.010(4)	0.006(5)

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