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Supporting information for article:

Crystal structure and energetic features of the cocrystal of carbamazepine with 3,5-dinitrobenzoic acid

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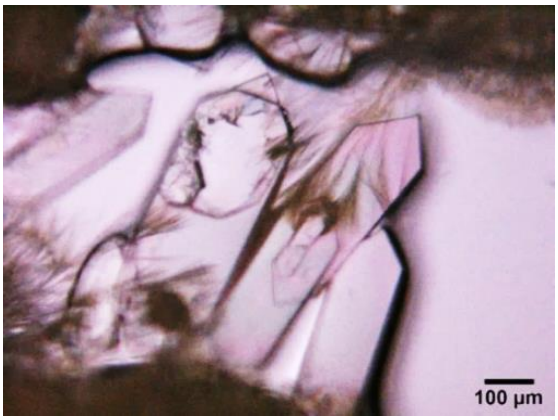

Figure S1 General view on the crystals of investigated system.

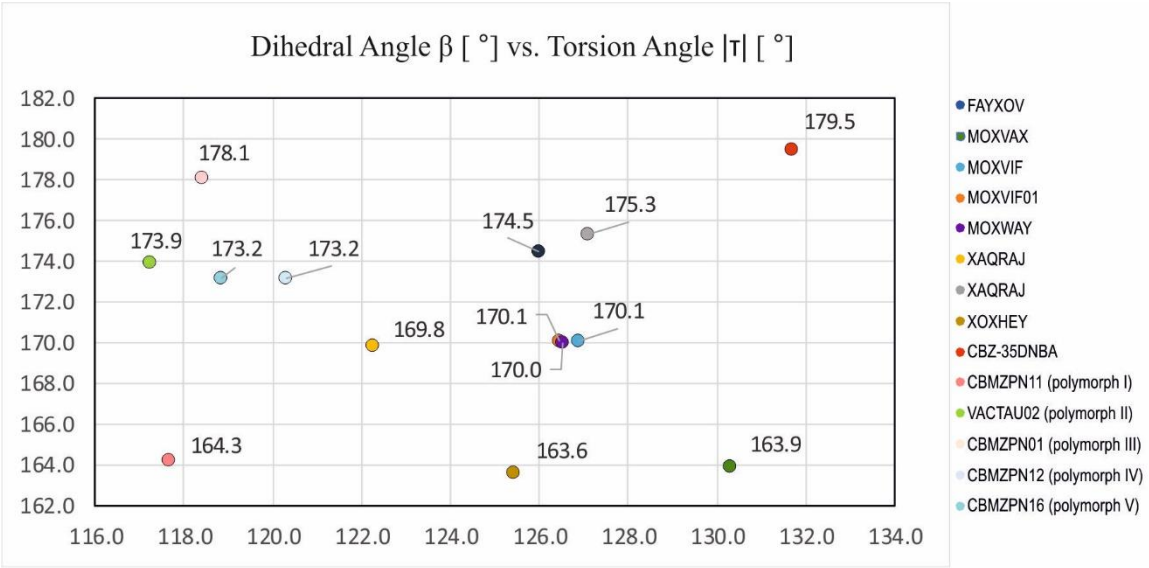

Figure S2 Values of dihedral (β) vs. value of modulus of torsion (τ) angles in analysed **CBZ** cocrystals and pure **CBZ** polymorphs deposited in the Cambridge Structural Database (CSD, v. 2.0.1).

Table S1 Values of geometric parameters of **CBZ · 35DNBA** (Å, º).

Atoms	Length/Å	Atoms	Length/Å
O17–C16	1.2560(11)	C13–C14	1.3948(16)
N1–C2	1.4359(12)	C14–C15	1.3908(16)
N1–C15	1.4330(12)	O26–N25	1.2273(14)

N1–C16	1.3619(12)	O27–N25	1.2282(15)
N18–C16	1.3424(12)	O29–N28	1.2277(12)
C2–C3	1.3890(14)	O30–N28	1.2253(12)
C2–C7	1.4004(13)	O32–C31	1.2261(12)
C3–C4	1.3917(13)	O33–C31	1.3025(11)
C4–C5	1.3915(15)	N25–C19	1.4687(14)
C5–C6	1.3848(15)	N28–C23	1.4747(12)
C6–C7	1.4060(14)	C19–C20	1.3864(14)
C7–C8	1.4612(15)	C19–C24	1.3845(14)
C8–C9	1.3472(17)	C20–C21	1.3928(14)
C9–C10	1.4599(18)	C21–C22	1.3937(13)
C10–C11	1.4074(15)	C21–C31	1.4986(13)
C10–C15	1.4004(16)	C22–C23	1.3829(14)
C11–C12	1.378(2)	C23–C24	1.3814(15)
C12–C13	1.386(2)		

C15–N1–C2	117.77(7)	O17–C16–N1	119.72(8)
C16–N1–C2	119.67(8)	O17–C16–N18	122.17(9)
C16–N1–C15	121.18(8)	N18–C16–N1	118.07(8)
C3–C2–N1	119.83(8)	O26–N25–O27	124.24(11)
C3–C2–C7	121.81(9)	O26–N25–C19	118.36(11)
C7–C2–N1	118.31(9)	O27–N25–C19	117.40(10)
C2–C3–C4	119.51(9)	O29–N28–C23	117.62(9)
C5–C4–C3	119.85(9)	O30– N28–O29	124.99(9)
C6–C5–C4	120.19(9)	O30–N28–C23	117.39(9)
C5–C6–C7	121.20(9)	C20–C19–N24	118.18(9)
C2–C7–C6	117.39(9)	C24–C19–N25	118.16(10)
C2–C7–C8	123.32(9)	C24–C19–C20	123.66(10)
C6–C7–C8	119.29(9)	C19–C20–C21	117.99(9)
C9–C8–C7	128.13(11)	C20–C21–C22	120.25(9)

C8–C9–C10	127.42(10)	C20–C21–C31	121.50(8)
C11–C10–C9	120.03(11)	C22–C21–C31	118.24(9)
C15–C10–C9	122.79(10)	C23–C22–C21	118.97(9)
C15–C10–C11	117.18(12)	C22–C23–N28	118.56(9)
C12–C11–C10	121.30(13)	C24–C23–N28	118.54(9)
C11–C12–C13	120.45(11)	C24–C23–C22	122.89(9)
C12–C13–C14	119.91(13)	C23–C24–C19	116.24(9)
C15–C14–C13	119.16(12)	O32–C31–O33	125.55(9)
C10–C15–N1	119.10(10)	O32–C31–C21	120.28(8)
C14–C15–N1	118.93(10)	O33–C31–C21	114.17(8)
C14–C15–C10	121.91(10)		

N1–C2–C3–C4	-175.76(9)	C15–N1–C16–O17	-179.52(9)
N1–C2–C7–C6	174.50(9)	C15–N1–C16–N18	2.83(14)
N1–C2–C7–C8	-4.88(14)	C15–C10–C11–C12	-1.97(16)
C2–N1–C15–C10	-69.20(12)	C16–N1–C2–C3	77.77(12)
C2–N1–C15–C14	113.56(11)	C16–N1–C2–C7	-99.54(11)
C2–N1–C16–O17	-13.22(14)	C16–N1–C15–C10	97.36(11)
C2–N1–C16–N18	169.14(9)	C16–N1–C15–C14	-79.89(13)
C2–C3–C4–C5	0.58(15)	O26–N25–C19–C20	-160.53(12)
C2–C7–C8–C9	-29.72(17)	O26–N25–C19–C24	19.74(18)
C3–C2–C7–C6	-2.75(14)	O27–N25–C19–C20	20.14(18)
C3–C2–C7–C8	177.87(10)	O27–N25–C19–C24	-159.60(12)
C3–C4–C5–C6	-1.21(15)	O29–N28–C23–C22	-179.10(9)
C4–C5–C6–C7	-0.17(15)	O29–N28–C23–C24	0.13(14)
C5–C6–C7–C2	2.10(15)	O30–N28–C23–C22	-0.14(13)
C5–C6–C7–C8	-178.49(10)	O30–N28–C23–C24	179.09(9)
C6–C7–C8–C9	150.91(12)	N25–C19–C20–C21	179.86(10)
C7–C2–C3–C4	1.45(15)	N25–C19–C24–C23	179.31(10)
C7–C8–C9–C10	-0.5(2)	N28–C23–C24–C19	-178.36(9)

C8–C9–C10–C11	-149.86(12)	C19–C20–C21–C22	0.86(15)
C8–C9–C10–C15	29.08(18)	C19–C20–C21–C31	-179.13(10)
C9–C10–C11–C12	177.04(11)	C20–C19–C24–C23	-0.41(17)
C9–C10–C15–N1	7.26(15)	C20–C21–C22–C23	-0.47(14)
C9–C10–C15–C14	-175.58(10)	C20–C21–C31–O32	-172.63(9)
C10–C11–C12–C13	-0.30(18)	C20–C21–C31–O33	7.65(13)
C11–C10–C15–N1	-173.77(9)	C21–C22–C23–N28	178.78(8)
C11–C10–C15–C14	3.39(15)	C21–C22–C23–C24	-0.42(15)
C11–C12–C13–C14	1.25(18)	C22–C21–C31–O32	7.38(14)
C12–C13–C14–C15	0.13(17)	C22–C21–C31–O33	-172.34(9)
C13–C14–C15–N1	174.64(9)	C22–C23–C24–C19	0.84(16)
C13–C14–C15–C10	-2.52(16)	C24–C19–C20–C21	-0.42(17)
C15–N1–C2–C3	-115.47(10)	C31–C21–C22–C23	179.52(9)
C15–N1–C2–C7	67.22(12)		

Figure S3 The values of dihedral (β) and modulus of torsion (τ) angles in analysed **CBZ** cocrystals and pure **CBZ** polymorphs deposited in the Cambridge Structural Database (CSD, v. 2.0.1).

Refcode	β /°	|τ|/°
FAYXOV	126.0	174.5
MOXVAX	130.3	163.9
MOXVIF	126.9	170.1
MOXVIF01	126.4	170.1
MOXWAY	126.5	170.0
XAQRAJ	122.3	169.8
XAQRAJ	127.1	175.3
XOXHEY	125.4	163.6
CBZ-35DNBA	131.7	179.5
CBMZPN11 (polymorph I)	117.7	164.3
VACTAU02 (polymorph II)	117.2	173.9

CBMZPN01 (polymorph III)	118.4	178.1
CBMZPN12 (polymorph IV)	120.3	173.2
CBMZPN16 (polymorph V)	118.8	173.2