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Supporting information for article:

Conformational polymorphism of 3-(azidomethyl)benzoic acid

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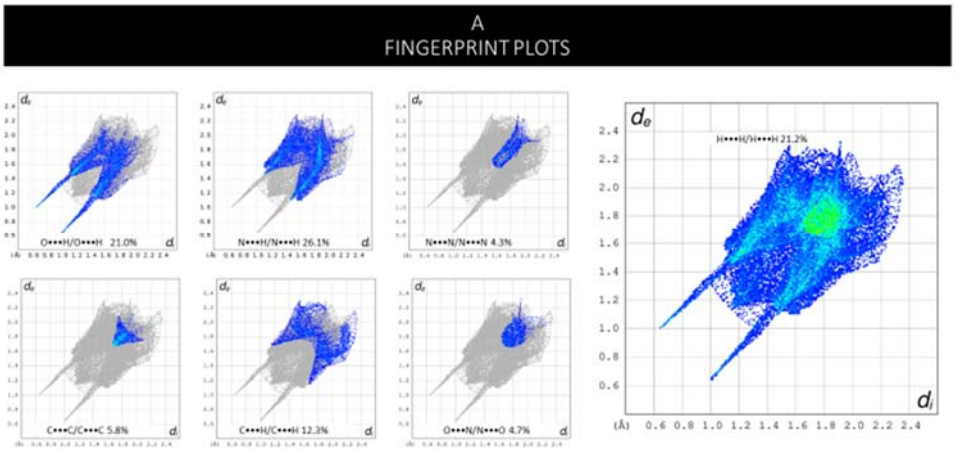


Figure S1 Element-to-element breakdown of Fingerprint Plots of A

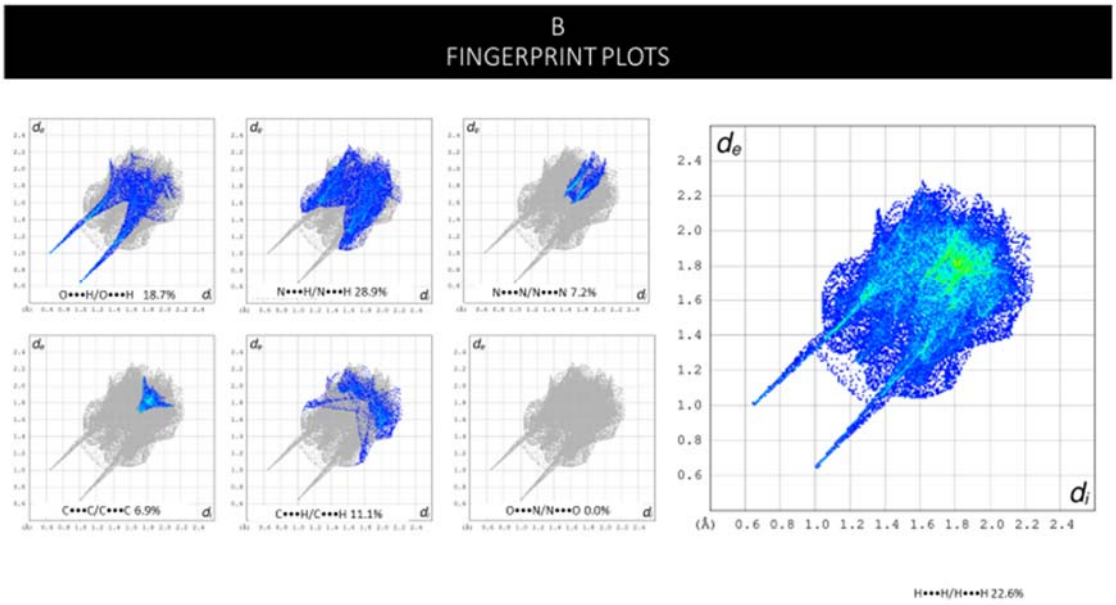


Figure S2 Element-to-element breakdown of Fingerprint Plots of B

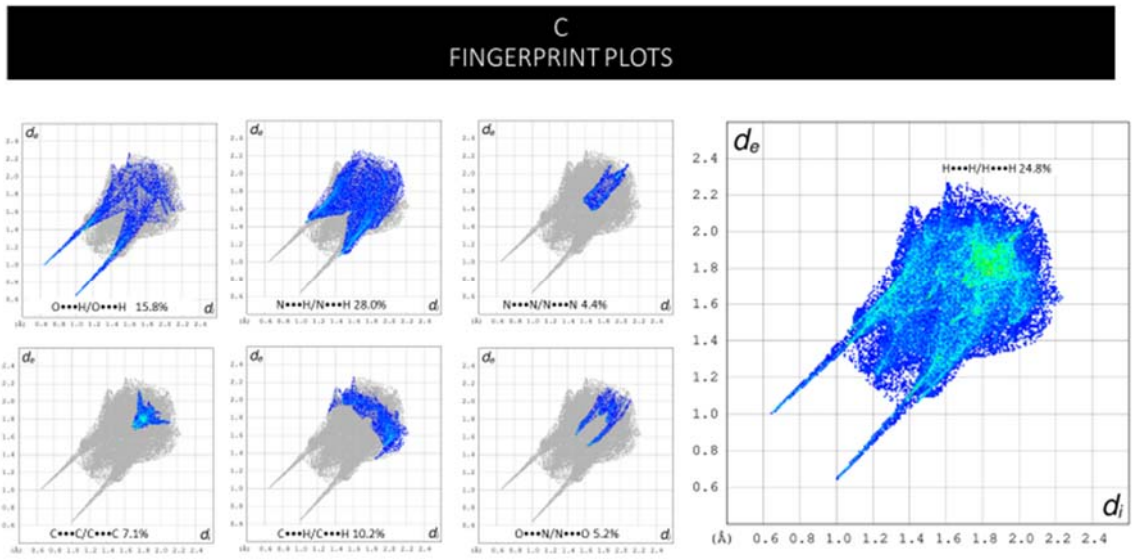


Figure S3 Element-to-element breakdown of Fingerprint Plots of C

Polymorph A Selected geometric parameters (Å, º)

O1—C7	1.244 (2)	C2—C3	1.388 (2)
O2—H2	0.90 (4)	C3—C4	1.403 (2)
O2—C7	1.305 (2)	C3—C8	1.506 (2)
N1—N2	1.234 (2)	C4—H4	0.9500
N1—C8	1.495 (2)	C4—C5	1.388 (3)
N2—N3	1.131 (2)	C5—H5	0.9500
C1—C2	1.402 (2)	C5—C6	1.387 (3)
C1—C6	1.395 (2)	C6—H6	0.9500
C1—C7	1.480 (2)	C8—H8A	0.9900
C2—H2A	0.9500	C8—H8B	0.9900
C7—O2—H2	111 (2)	C4—C5—H5	119.8
N2—N1—C8	114.61 (16)	C6—C5—C4	120.50 (16)
N3—N2—N1	173.0 (2)	C6—C5—H5	119.8
C2—C1—C7	118.71 (15)	C1—C6—H6	120.2
C6—C1—C2	120.07 (16)	C5—C6—C1	119.52 (16)
C6—C1—C7	121.11 (16)	C5—C6—H6	120.2
C1—C2—H2A	119.8	O1—C7—O2	122.73 (17)
C3—C2—C1	120.36 (16)	O1—C7—C1	121.24 (16)
C3—C2—H2A	119.8	O2—C7—C1	116.02 (15)
C2—C3—C4	119.06 (16)	N1—C8—C3	112.99 (15)
C2—C3—C8	120.40 (15)	N1—C8—H8A	109.0
C4—C3—C8	120.53 (16)	N1—C8—H8B	109.0
C3—C4—H4	119.8	C3—C8—H8A	109.0
C5—C4—C3	120.47 (16)	C3—C8—H8B	109.0
C5—C4—H4	119.8	H8A—C8—H8B	107.8
N2—N1—C8—C3	60.0 (2)	C4—C3—C8—N1	85.1 (2)
C1—C2—C3—C4	−0.4 (3)	C4—C5—C6—C1	−0.4 (3)
C1—C2—C3—C8	−179.44 (16)	C6—C1—C2—C3	−0.2 (3)
C2—C1—C6—C5	0.6 (3)	C6—C1—C7—O1	179.23 (17)
C2—C1—C7—O1	2.9 (3)	C6—C1—C7—O2	0.8 (2)

C2—C1—C7—O2	−175.46 (16)	C7—C1—C2—C3	176.12 (16)
C2—C3—C4—C5	0.6 (3)	C7—C1—C6—C5	−175.65 (16)
C2—C3—C8—N1	−95.81 (19)	C8—C3—C4—C5	179.65 (16)
C3—C4—C5—C6	−0.2 (3)		

Polymorph B Selected geometric parameters (Å, º)

O1—C7	1.230 (3)	C2—C3	1.391 (3)
O2—H2	0.81 (4)	C3—C4	1.389 (4)
O2—C7	1.309 (3)	C3—C8	1.509 (3)
N1—N2	1.233 (3)	C4—H4	0.9500
N1—C8	1.489 (3)	C4—C5	1.391 (4)
N2—N3	1.131 (3)	C5—H5	0.9500
C1—C2	1.392 (3)	C5—C6	1.384 (4)
C1—C6	1.394 (4)	C6—H6	0.9500
C1—C7	1.487 (3)	C8—H8A	0.9900
C2—H2A	0.9500	C8—H8B	0.9900
C7—O2—H2	110 (3)	C4—C5—H5	120.0
N2—N1—C8	116.2 (2)	C6—C5—C4	119.9 (2)
N3—N2—N1	171.3 (3)	C6—C5—H5	120.0
C2—C1—C6	119.9 (2)	C1—C6—H6	120.0
C2—C1—C7	119.0 (2)	C5—C6—C1	119.9 (2)
C6—C1—C7	121.0 (2)	C5—C6—H6	120.0
C1—C2—H2A	119.8	O1—C7—O2	123.5 (2)
C3—C2—C1	120.3 (2)	O1—C7—C1	121.8 (2)
C3—C2—H2A	119.8	O2—C7—C1	114.7 (2)
C2—C3—C8	120.1 (2)	N1—C8—C3	109.4 (2)
C4—C3—C2	119.2 (2)	N1—C8—H8A	109.8
C4—C3—C8	120.6 (2)	N1—C8—H8B	109.8
C3—C4—H4	119.7	C3—C8—H8A	109.8

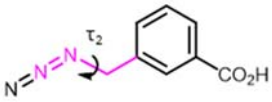
C3—C4—C5	120.7 (2)	C3—C8—H8B	109.8
C5—C4—H4	119.7	H8A—C8—H8B	108.2
N2—N1—C8—C3	−147.0 (2)	C4—C3—C8—N1	−129.8 (3)
C1—C2—C3—C4	−0.7 (4)	C4—C5—C6—C1	0.4 (4)
C1—C2—C3—C8	177.6 (2)	C6—C1—C2—C3	−0.1 (4)
C2—C1—C6—C5	0.3 (4)	C6—C1—C7—O1	−172.7 (3)
C2—C1—C7—O1	6.4 (4)	C6—C1—C7—O2	7.3 (4)
C2—C1—C7—O2	−173.6 (2)	C7—C1—C2—C3	−179.3 (2)
C2—C3—C4—C5	1.3 (4)	C7—C1—C6—C5	179.4 (2)
C2—C3—C8—N1	51.9 (3)	C8—C3—C4—C5	−176.9 (3)
C3—C4—C5—C6	−1.2 (4)		

Polymorph C Selected geometric parameters (Å, º)

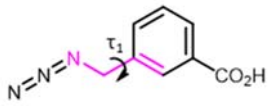
O1—C7	1.233 (2)	C2—C3	1.390 (2)
O2—H2	0.88 (3)	C3—C4	1.397 (2)
O2—C7	1.315 (2)	C3—C8	1.507 (2)
N1—N2	1.234 (2)	C4—H4	0.9500
N1—C8	1.484 (2)	C4—C5	1.374 (3)
N2—N3	1.133 (2)	C5—H5	0.9500
C1—C2	1.391 (2)	C5—C6	1.390 (2)
C1—C6	1.395 (2)	C6—H6	0.9500
C1—C7	1.483 (2)	C8—H8A	0.9900
C2—H2A	0.9500	C8—H8B	0.9900
C7—O2—H2	110.1 (16)	C4—C5—H5	119.8
N2—N1—C8	115.30 (14)	C4—C5—C6	120.45 (16)
N3—N2—N1	172.91 (18)	C6—C5—H5	119.8
C2—C1—C6	120.06 (15)	C1—C6—H6	120.4
C2—C1—C7	118.88 (14)	C5—C6—C1	119.20 (16)

C6—C1—C7	121.05 (15)	C5—C6—H6	120.4
C1—C2—H2A	119.7	O1—C7—O2	123.07 (15)
C3—C2—C1	120.69 (15)	O1—C7—C1	122.25 (15)
C3—C2—H2A	119.7	O2—C7—C1	114.67 (14)
C2—C3—C4	118.52 (16)	N1—C8—C3	111.70 (14)
C2—C3—C8	120.36 (15)	N1—C8—H8A	109.3
C4—C3—C8	121.12 (15)	N1—C8—H8B	109.3
C3—C4—H4	119.5	C3—C8—H8A	109.3
C5—C4—C3	121.08 (16)	C3—C8—H8B	109.3
C5—C4—H4	119.5	H8A—C8—H8B	107.9
N2—N1—C8—C3	−108.16 (17)	C4—C3—C8—N1	49.2 (2)
C1—C2—C3—C4	0.1 (2)	C4—C5—C6—C1	0.6 (2)
C1—C2—C3—C8	−179.07 (15)	C6—C1—C2—C3	0.0 (2)
C2—C1—C6—C5	−0.4 (2)	C6—C1—C7—O1	−173.71 (15)
C2—C1—C7—O1	5.0 (2)	C6—C1—C7—O2	5.6 (2)
C2—C1—C7—O2	−175.66 (14)	C7—C1—C2—C3	−178.72 (14)
C2—C3—C4—C5	0.1 (2)	C7—C1—C6—C5	178.31 (14)
C2—C3—C8—N1	−131.58 (15)	C8—C3—C4—C5	179.32 (15)
C3—C4—C5—C6	−0.5 (3)		

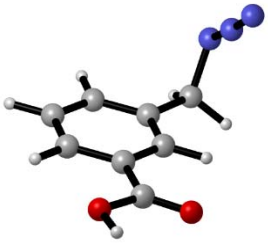
Computational Coordinates



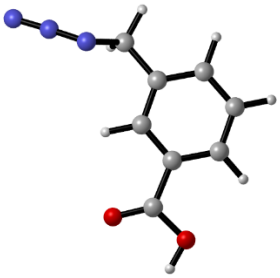
X_{cryst} (where X = A, B, or C) is the restricted optimization where the dihedrals τ_1 and τ_2 (image) were frozen to the values observed in the crystal structure, and all other parameters optimized. X_{gas} (where X = A, B, or C) is an unrestricted optimization from the crystal structure coordinates to a minimum.



A_{cryst}

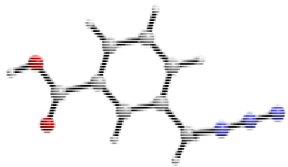


O	2.35262	-1.93923	0.67333
O	3.62267	-0.42616	-0.42959
H	4.25316	-1.15704	-0.32034
N	-3.22476	-0.14681	0.02556
N	-2.84013	-1.13328	-0.60006
N	-2.59061	-2.03652	-1.25130
C	1.36909	0.16914	0.07090
C	0.11779	-0.17076	0.60874
H	-0.00661	-1.15271	1.05700
C	-0.94335	0.73525	0.57524
C	-0.74807	1.99492	-0.01102
H	-1.57558	2.70006	-0.04706
C	0.49257	2.34193	-0.54715
H	0.63613	3.32192	-0.99434
C	1.55242	1.43353	-0.51004
H	2.51795	1.70090	-0.92523
C	2.45862	-0.84754	0.15216
C	-2.30182	0.33830	1.10274
H	-2.20227	-0.43851	1.87344
H	-2.82011	1.19603	1.53781



B_{cryst}

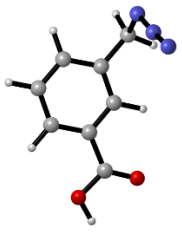
O	-1.93981	-2.38782	0.16000
O	-3.71689	-1.02058	-0.13979
H	-4.14808	-1.89085	-0.12287
N	2.70654	-0.15961	-0.58823
N	3.65836	-0.82700	-0.19197
N	4.54007	-1.50862	0.05613
C	-1.56004	-0.01720	0.02539
C	-0.17274	-0.15070	0.17054
H	0.25046	-1.14624	0.26385
C	0.65445	0.97466	0.17962
C	0.08026	2.24325	0.03507
H	0.72140	3.12243	0.02952
C	-1.30333	2.38667	-0.10607
H	-1.73686	3.37669	-0.21921
C	-2.12643	1.26216	-0.11233
H	-3.19965	1.36762	-0.22657
C	-2.38055	-1.26426	0.02665
C	2.14715	0.83075	0.37475
H	2.63929	1.79971	0.21394
H	2.35940	0.51239	1.40635



C_{cryst}

O	-3.25078	-1.73074	-0.00403

O	-4.08110	0.36879	-0.14552
H	-4.89579	-0.15919	-0.17881
N	2.97043	-0.76882	-0.63604
N	3.98287	-0.23783	-0.18994
N	4.97298	0.25519	0.09622
C	-1.71620	0.11909	0.02334
C	-0.59054	-0.71404	0.12611
H	-0.74058	-1.79002	0.15125
C	0.69377	-0.17541	0.19032
C	0.85242	1.21756	0.14036
H	1.85046	1.64730	0.17569
C	-0.25990	2.05315	0.03395
H	-0.12539	3.13074	-0.00614
C	-1.54538	1.51103	-0.02307
H	-2.41093	2.15891	-0.10728
C	-3.05704	-0.53207	-0.04047
C	1.89281	-1.09037	0.34188
H	2.28333	-1.04110	1.36855
H	1.59044	-2.12454	0.14692



A_{gas}

Max. Force 0.000001

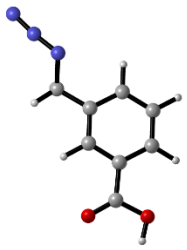
RMS Force 0.000000

Max. Displacement 0.000010

RMS Displacement 0.000003

O	2.42866	-1.93062	0.65032
O	3.65519	-0.38892	-0.46207
H	4.30143	-1.10732	-0.36242
N	-3.24432	-0.10634	0.08961
N	-2.92812	-1.06371	-0.61529

N	-2.74507	-1.93045	-1.33445
C	1.39605	0.15932	0.06623
C	0.15916	-0.20566	0.62184
H	0.06029	-1.18991	1.07144
C	-0.92016	0.67802	0.60286
C	-0.75925	1.94138	0.01317
H	-1.60169	2.62900	-0.01201
C	0.46570	2.31246	-0.54166
H	0.58260	3.29437	-0.99239
C	1.54494	1.42616	-0.51840
H	2.49857	1.71278	-0.94802
C	2.50663	-0.83530	0.13159
C	-2.26121	0.25998	1.15952
H	-2.14204	-0.58270	1.85425
H	-2.73854	1.08553	1.69330



B_{gas}

Max. Force 0.000001

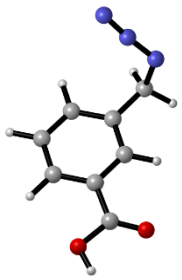
RMS Force 0.000000

Max. Displacement 0.000054

RMS Displacement 0.000010

O	-3.00351	-1.99704	-0.01534
O	-4.14128	-0.04953	-0.18684
H	-4.86518	-0.69607	-0.22571
N	3.03627	0.04046	-0.40622
N	4.17320	-0.38007	-0.20869
N	5.26943	-0.68582	-0.11857
C	-1.76863	0.06515	0.01474
C	-0.53146	-0.58606	0.14145
H	-0.51809	-1.67217	0.17543
C	0.65545	0.14195	0.21824
C	0.60242	1.54213	0.15539

H	1.52697	2.11140	0.19576
C	-0.62298	2.19704	0.02165
H	-0.65244	3.28211	-0.03143
C	-1.81045	1.46666	-0.04566
H	-2.76292	1.97465	-0.14969
C	-2.99336	-0.78298	-0.06023
C	1.96466	-0.58639	0.41636
H	2.25457	-0.55143	1.47882
H	1.84919	-1.64288	0.13694



C_{gas}

Max. Force 0.000001

RMS Force 0.000000

Max. Displacement 0.000014

RMS Displacement 0.000004

O	2.90379	-1.81236	-0.13217
O	3.78042	0.21518	-0.62065
H	4.54335	-0.36380	-0.78308
N	-2.81424	-1.28491	-0.06356
N	-3.29059	-0.39940	-0.76991
N	-3.77594	0.33155	-1.50046
C	1.49914	0.12834	0.06653
C	0.38185	-0.62173	0.45960
H	0.47476	-1.70204	0.52697
C	-0.82935	0.00569	0.75910
C	-0.91918	1.40142	0.65615
H	-1.85919	1.89642	0.89046
C	0.18767	2.15654	0.26029
H	0.10809	3.23761	0.18499
C	1.39617	1.52621	-0.03474
H	2.25854	2.10928	-0.33869

C	2.76324	-0.60981	-0.22587
C	-2.04208	-0.81347	1.13255
H	-1.74962	-1.73112	1.64734
H	-2.70911	-0.23876	1.79046