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Supporting information for article:

Experimental and theoretical charge-density analysis of hippuric acid: insight into its binding with human serum albumin

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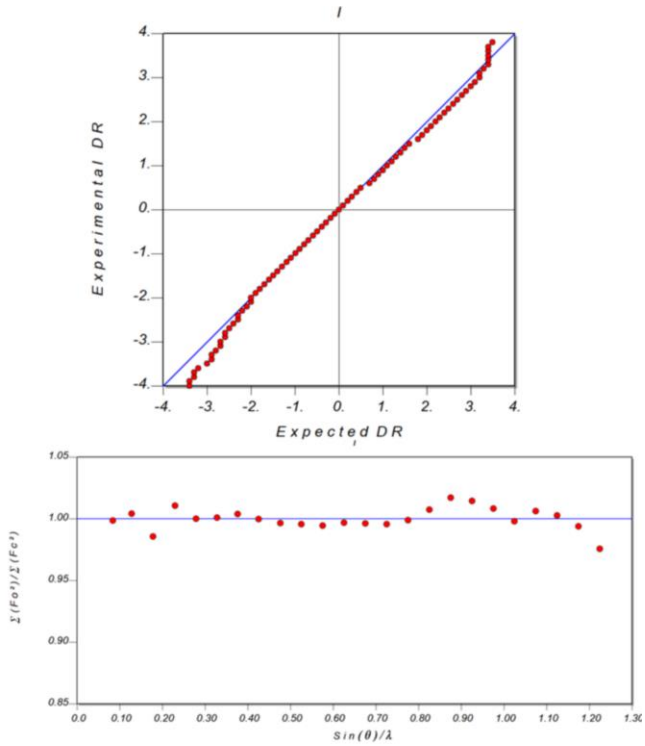

Figure S1: Normal probability plot showing the quality of the data used.

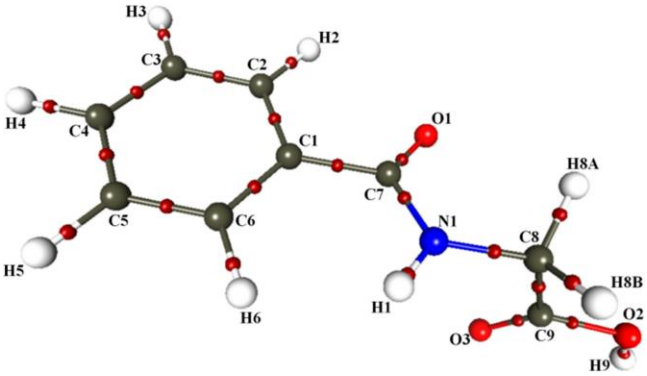

Figure S2: A view of the molecule showing the covalent bond critical points.

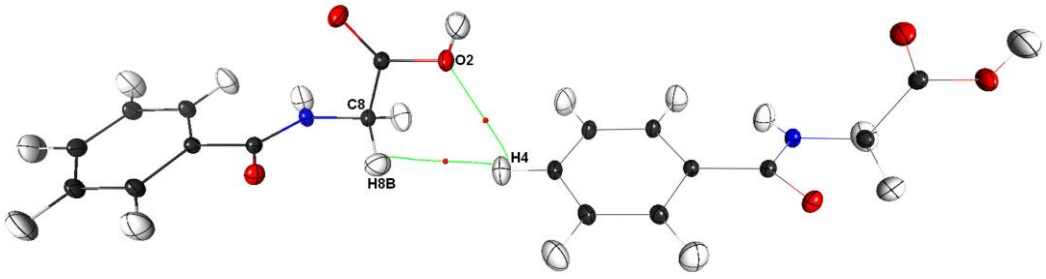

Figure S3: A molecular dimer showing the intermolecular H···H interactions.

Table S1: The optimized bond lengths for H atoms

No.	Bond	d (Å)
1	C2-H2	1.08750

2	C3-H3	1.08859
3	C4-H4	1.08565
4	C5-H5	1.08738
5	C6-H6	1.08829
6	C8-H8A	1.09516
7	C8-H8B	1.09825
8	N1-H1	1.02319
9	O2-H9	1.00417

Table S2. *Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2) for (Multipolar)*

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.39576 (2)	0.63963 (2)	0.584744 (17)	0.011131 (13)
C2	0.46751 (3)	0.52380 (2)	0.519658 (18)	0.013730 (15)
H2	0.53553	0.43665	0.57409	0.03054
C3	0.45602 (3)	0.51496 (3)	0.388750 (19)	0.016250 (18)
H3	0.51437	0.42070	0.33567	0.03547
C4	0.37191 (3)	0.62075 (3)	0.322268 (19)	0.016216 (17)
H4	0.36206	0.61298	0.21560	0.03314
C5	0.29882 (3)	0.73531 (3)	0.38671 (2)	0.016159 (17)
H5	0.23002	0.82251	0.33300	0.03444
C6	0.31026 (3)	0.74437 (2)	0.517426 (19)	0.014109 (15)
H6	0.24997	0.83723	0.57031	0.03204
C7	0.40741 (2)	0.65980 (2)	0.724016 (17)	0.010806 (12)
C8	0.46951 (3)	0.55966 (2)	0.929769 (17)	0.013106 (14)
H8A	0.45802	0.44344	0.97261	0.03131
H8B	0.36605	0.62821	0.96551	0.02953
C9	0.61678 (2)	0.62936 (2)	0.978623 (17)	0.012381 (14)
N1	0.46290 (2)	0.54945 (2)	0.793974 (15)	0.012666 (13)
O1	0.36586 (2)	0.778866 (18)	0.773453 (15)	0.014240 (12)
O2	0.62223 (2)	0.61871 (2)	1.103186 (15)	0.018008 (15)
O3	0.71466 (2)	0.68682 (3)	0.913917 (17)	0.019846 (17)
H1	0.49780	0.46317	0.75554	0.02774
H9	0.70258	0.65963	1.13162	0.03066

Table S3. *Atomic displacement parameters (Å^2) for (Multipolar)*

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.01219 (6)	0.01149 (6)	0.00973 (5)	0.00055 (5)	-0.00049 (4)	-0.00014 (4)
C2	0.01638 (7)	0.01408 (7)	0.01080 (6)	0.00271 (6)	-0.00068 (5)	-0.00122 (5)
H2	0.03913	0.02807	0.02440	0.01306	-0.00441	0.00051
C3	0.01831 (8)	0.01947 (8)	0.01101 (6)	0.00269 (7)	0.00025 (5)	-0.00236 (5)
H3	0.04435	0.03732	0.02474	0.01410	0.00064	-0.00931
C4	0.01623 (7)	0.02233 (9)	0.01009 (6)	0.00002 (7)	-0.00024 (5)	0.00074 (6)
H4	0.03875	0.04484	0.01582	0.00277	-0.00218	-0.00011
C5	0.01695 (8)	0.01929 (8)	0.01225 (6)	0.00203 (6)	-0.00206 (5)	0.00269 (6)
H5	0.03977	0.03600	0.02755	0.01124	-0.00611	0.00789
C6	0.01552 (7)	0.01447 (7)	0.01239 (6)	0.00276 (5)	-0.00135 (5)	0.00071 (5)
H6	0.03932	0.02887	0.02794	0.01382	0.00045	-0.00289
C7	0.01198 (6)	0.01051 (5)	0.00995 (5)	-0.00011 (4)	0.00017 (4)	-0.00050 (4)
C8	0.01361 (6)	0.01551 (7)	0.01019 (5)	-0.00168 (5)	-0.00039 (5)	0.00110 (5)
H8A	0.04273	0.02366	0.02755	-0.00666	-0.00481	0.00656
H8B	0.02528	0.03588	0.02744	0.00354	0.00212	-0.00590
C9	0.01291 (6)	0.01396 (6)	0.01031 (5)	-0.00123 (5)	0.00060 (4)	0.00001 (4)
N1	0.01635 (6)	0.01195 (5)	0.00971 (5)	0.00077 (5)	-0.00094 (4)	0.00005 (4)
O1	0.01777 (6)	0.01220 (5)	0.01275 (5)	0.00163 (4)	0.00193 (4)	-0.00177 (4)
O2	0.01797 (7)	0.02607 (8)	0.01012 (5)	-0.00639 (6)	-0.00107 (4)	0.00000 (5)
O3	0.01776 (7)	0.02801 (9)	0.01389 (6)	-0.00815 (6)	0.00234 (5)	0.00120 (5)
H1	0.04033	0.02052	0.02237	0.00710	-0.00097	-0.00324
H9	0.02667	0.04373	0.02158	-0.01118	-0.00289	-0.00006
	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.01218 (6)	0.01147 (6)	0.00974 (5)	0.00056 (5)	-0.00048 (4)	-0.00014 (4)
C2	0.01637 (7)	0.01404 (7)	0.01078 (6)	0.00271 (6)	-0.00066 (5)	-0.00120 (5)
H2	0.03913	0.02807	0.02440	0.01306	-0.00441	0.00051
C3	0.01832 (8)	0.01945 (8)	0.01098 (6)	0.00273 (7)	0.00025 (5)	-0.00240 (5)
H3	0.04435	0.03732	0.02474	0.01410	0.00064	-0.00931
C4	0.01624 (7)	0.02237 (9)	0.01005 (6)	0.00001 (7)	-0.00025 (5)	0.00075 (6)
H4	0.03875	0.04484	0.01582	0.00277	-0.00218	-0.00011
C5	0.01693 (8)	0.01929 (8)	0.01226 (6)	0.00203 (6)	-0.00209 (5)	0.00275 (5)
H5	0.03977	0.03600	0.02755	0.01124	-0.00611	0.00789
C6	0.01553 (7)	0.01441 (7)	0.01239 (6)	0.00281 (5)	-0.00137 (5)	0.00068 (5)
H6	0.03932	0.02887	0.02794	0.01382	0.00045	-0.00289
C7	0.01194 (6)	0.01051 (5)	0.00997 (5)	-0.00010 (4)	0.00018 (4)	-0.00050 (4)

C8	0.01361 (6)	0.01549 (7)	0.01022 (5)	-0.00168 (5)	-0.00036 (5)	0.00109 (5)
H8A	0.04273	0.02366	0.02755	-0.00666	-0.00481	0.00656
H8B	0.02528	0.03588	0.02744	0.00354	0.00212	-0.00590
C9	0.01288 (6)	0.01400 (6)	0.01026 (5)	-0.00128 (5)	0.00059 (4)	0.00001 (4)
N1	0.01633 (6)	0.01196 (5)	0.00970 (5)	0.00077 (5)	-0.00096 (4)	0.00007 (4)
O1	0.01779 (6)	0.01218 (5)	0.01274 (5)	0.00164 (4)	0.00192 (4)	-0.00174 (4)
O2	0.01794 (7)	0.02597 (8)	0.01012 (5)	-0.00631 (6)	-0.00100 (4)	0.00012 (5)
O3	0.01774 (7)	0.02796 (9)	0.01384 (6)	-0.00819 (6)	0.00231 (5)	0.00117 (5)
H1	0.04033	0.02052	0.02237	0.00710	-0.00097	-0.00324
H9	0.02667	0.04373	0.02158	-0.01118	-0.00289	-0.00006

Table S4. *Geometric parameters (Å, º) for (Multipolar)*

C1—C7	1.4921 (3)	C6—H6	1.09
C1—C6	1.4011 (3)	C7—O1	1.2536 (3)
C1—C2	1.4026 (3)	C7—N1	1.3358 (3)
C2—C3	1.3947 (3)	C8—N1	1.4448 (3)
C2—H2	1.09	C8—C9	1.5172 (3)
C3—C4	1.3966 (4)	C8—H8A	1.10
C3—H3	1.09	C8—H8B	1.10
C4—C5	1.3963 (4)	C9—O2	1.3261 (2)
C4—H4	1.09	C9—O3	1.2099 (3)
C5—C6	1.3929 (3)	N1—H1	1.02
C5—H5	1.09	O2—H9	1.00
C7—C1—C6	117.216 (15)	C5—C6—H6	120.1
C7—C1—C2	123.307 (15)	O1—C7—N1	121.104 (17)
C6—C1—C2	119.469 (17)	O1—C7—C1	120.026 (15)
C1—C2—C3	120.112 (17)	N1—C7—C1	118.869 (15)
C1—C2—H2	120	N1—C8—C9	113.602 (15)
C3—C2—H2	120.0	N1—C8—H8A	109.3
C2—C3—C4	120.042 (18)	N1—C8—H8B	109.3
C2—C3—H3	120.2	C9—C8—H8A	109
C4—C3—H3	120	C9—C8—H8B	109
C5—C4—C3	120.08 (2)	H8A—C8—H8B	107
C5—C4—H4	120	O2—C9—O3	124.871 (17)
C3—C4—H4	120	O2—C9—C8	109.868 (16)
C6—C5—C4	119.950 (18)	O3—C9—C8	125.260 (18)

C6—C5—H5	119.5	C7—N1—C8	121.351 (15)
C4—C5—H5	121	C7—N1—H1	120
C1—C6—C5	120.334 (17)	C8—N1—H1	118.8
C1—C6—H6	120	C9—O2—H9	110.7
C1—C7—N1—C8	-176.76 (3)	H4—C4—C5—C6	180 (1)
C1—C7—N1—H1	2 (2)	H4—C4—C5—H5	-1 (4)
C1—C6—C5—C4	0.46 (3)	C5—C6—C1—C7	177.82 (3)
C1—C6—C5—H5	-179 (4)	H5—C5—C6—H6	1 (6)
C1—C2—C3—C4	-0.56 (3)	C6—C1—C7—O1	-12.34 (3)
C1—C2—C3—H3	-180 (4)	C6—C1—C7—N1	167.85 (3)
C2—C1—C7—O1	166.63 (3)	H6—C6—C1—C7	-2 (5)
C2—C1—C7—N1	-13.19 (3)	C7—N1—C8—C9	-88.04 (3)
C2—C1—C6—C5	-1.18 (3)	C7—N1—C8—H8A	150 (2)
C2—C1—C6—H6	179 (4)	C7—N1—C8—H8B	33 (5)
C2—C3—C4—C5	-0.17 (4)	C8—N1—C7—O1	3.43 (3)
C2—C3—C4—H4	-179.6 (8)	C8—C9—O2—H9	-178 (3)
H2—C2—C1—C7	2 (5)	H8A—C8—N1—H1	-28 (1)
H2—C2—C1—C6	-179 (5)	H8A—C8—C9—O2	-51 (3)
H2—C2—C3—C4	179 (5)	H8A—C8—C9—O3	130 (4)
H2—C2—C3—H3	0 (6)	H8B—C8—N1—H1	-145 (7)
C3—C2—C1—C7	-177.71 (4)	H8B—C8—C9—O2	65.6 (7)
C3—C2—C1—C6	1.23 (4)	H8B—C8—C9—O3	-114.1 (8)
C3—C4—C5—C6	0.22 (4)	C9—C8—N1—H1	93 (6)
C3—C4—C5—H5	180 (4)	N1—C8—C9—O2	-172.56 (3)
H3—C3—C4—C5	179 (5)	N1—C8—C9—O3	7.76 (4)
H3—C3—C4—H4	0 (5)	O1—C7—N1—H1	-178 (3)
C4—C5—C6—H6	-180 (4)	O3—C9—O2—H9	2 (3)

Table S5*. Hydrogen-bond geometry (Å, º) for (Multipolar)*

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C8—H8*B*···O3^{i}	1.10	2.54	3.5953 (3)	161
C4—H4···O2^{ii}	1.09	2.57	3.1810 (3)	114
N1—H1···C2	1.02	2.55	2.9197 (3)	101
O2—H9···O1^{iii}	1.00	1.67	2.6544 (3)	165
C2—H2···O1^{iv}	1.09	2.38	3.4411 (3)	166
C8—H8*A*···C6^{iv}	1.10	2.74	3.4842 (4)	125

N1—H1···O1^{iv}	1.02	1.99	2.9561 (3)	156

Symmetry codes: (i) *x*-1/2, -*y*+3/2, -*z*+2; (ii) *x*, *y*, *z*-1; (iii) *x*+1/2, -*y*+3/2, -*z*+2; (iv) -*x*+1, *y*-1/2, -*z*+3/2.

Table S6. *Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2) for (IAM_MoPro)*

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.39580 (4)	0.63965 (4)	0.58472 (3)	0.01133 (2)
C2	0.46753 (5)	0.52385 (4)	0.51962 (3)	0.01392 (2)
H2	0.532 (2)	0.441 (11)	0.5714 (14)	0.03054
C3	0.45598 (5)	0.51498 (5)	0.38867 (4)	0.01642 (3)
H3	0.5116 (19)	0.425 (11)	0.3381 (16)	0.03547
C4	0.37199 (5)	0.62074 (5)	0.32223 (3)	0.01637 (3)
H4	0.363 (2)	0.613 (2)	0.220 (11)	0.03314
C5	0.29887 (5)	0.73527 (5)	0.38667 (4)	0.01632 (3)
H5	0.2334 (17)	0.818 (11)	0.3356 (14)	0.03444
C6	0.31017 (5)	0.74441 (4)	0.51749 (3)	0.01430 (2)
H6	0.253 (2)	0.833 (11)	0.5680 (13)	0.03204
C7	0.40745 (4)	0.65973 (4)	0.72401 (3)	0.01103 (2)
C8	0.46941 (4)	0.55963 (4)	0.92983 (3)	0.01333 (2)
H8A	0.459 (2)	0.449 (11)	0.9705 (15)	0.03131
H8B	0.371 (11)	0.6248 (18)	0.9638 (16)	0.02953
C9	0.61687 (4)	0.62933 (4)	0.97854 (3)	0.01254 (2)
N1	0.46286 (4)	0.54933 (3)	0.79392 (3)	0.01290 (2)
O1	0.36575 (4)	0.77897 (3)	0.77352 (3)	0.01449 (2)
O2	0.62203 (4)	0.61883 (5)	1.10332 (3)	0.01833 (3)
O3	0.71468 (4)	0.68671 (5)	0.91385 (3)	0.01999 (3)
H1	0.501 (2)	0.458 (11)	0.7466 (16)	0.02774
H9	0.720 (11)	0.664 (2)	1.1343 (15)	0.03066

Table S7. *Atomic displacement parameters (Å^2) for (IAM_MoPro)*

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.01234 (9)	0.01171 (9)	0.00995 (8)	0.00029 (7)	-0.00047 (7)	-0.00004 (6)
C2	0.01636 (11)	0.01423 (10)	0.01116 (9)	0.00241 (9)	-0.00062 (8)	-0.00107 (8)

H2	0.03913	0.02807	0.02440	0.01306	-0.00441	0.00051
C3	0.01812 (13)	0.01968 (13)	0.01146 (10)	0.00240 (10)	0.00024 (9)	-0.00227 (9)
H3	0.04435	0.03732	0.02474	0.01410	0.00064	-0.00931
C4	0.01600 (12)	0.02257 (14)	0.01055 (9)	-0.00048 (11)	-0.00019 (8)	0.00068 (9)
H4	0.03875	0.04484	0.01582	0.00277	-0.00218	-0.00011
C5	0.01667 (12)	0.01957 (13)	0.01271 (10)	0.00166 (10)	-0.00196 (9)	0.00281 (9)
H5	0.03977	0.03600	0.02755	0.01124	-0.00611	0.00789
C6	0.01543 (11)	0.01471 (11)	0.01277 (10)	0.00256 (8)	-0.00140 (8)	0.00075 (8)
H6	0.03932	0.02887	0.02794	0.01382	0.00045	-0.00289
C7	0.01175 (9)	0.01102 (8)	0.01032 (8)	-0.00038 (7)	0.00020 (7)	-0.00036 (7)
C8	0.01387 (10)	0.01577 (11)	0.01034 (9)	-0.00180 (8)	-0.00049 (7)	0.00119 (8)
H8A	0.04273	0.02366	0.02755	-0.00666	-0.00481	0.00656
H8B	0.02528	0.03588	0.02744	0.00354	0.00212	-0.00590
C9	0.01331 (10)	0.01364 (10)	0.01067 (9)	-0.00083 (8)	0.00047 (7)	-0.00012 (7)
N1	0.01653 (10)	0.01217 (8)	0.01001 (7)	0.00068 (7)	-0.00100 (7)	0.00003 (6)
O1	0.01801 (10)	0.01222 (8)	0.01324 (8)	0.00145 (7)	0.00206 (7)	-0.00197 (6)
O2	0.01860 (11)	0.02648 (14)	0.00991 (8)	-0.00617 (10)	-0.00103 (7)	-0.00012 (8)
O3	0.01795 (11)	0.02761 (15)	0.01439 (10)	-0.00763 (10)	0.00246 (8)	0.00123 (9)
H1	0.04033	0.02052	0.02237	0.00710	-0.00097	-0.00324
H9	0.02667	0.04373	0.02158	-0.01118	-0.00289	-0.00006

Table S8. *Geometric parameters (Å, º) for (IAM_MoPro)*

C1—C7	1.4923 (4)	C6—H6	1.09
C1—C6	1.4012 (5)	C7—O1	1.2553 (4)
C1—C2	1.4025 (5)	C7—N1	1.3355 (4)
C2—C3	1.3951 (5)	C8—N1	1.4459 (4)
C2—H2	1.09	C8—C9	1.5181 (5)
C3—C4	1.3956 (6)	C8—H8A	1.10
C3—H3	1.09	C8—H8B	1.10
C4—C5	1.3959 (6)	C9—O2	1.3279 (4)
C4—H4	1.09	C9—O3	1.2092 (5)
C5—C6	1.3937 (5)	N1—H1	1.02
C5—H5	1.09	O2—H9	1.00
C7—C1—C6	117.21 (3)	C5—C6—H6	120.1

C7—C1—C2	123.29 (3)	O1—C7—N1	121.14 (3)
C6—C1—C2	119.49 (3)	O1—C7—C1	119.99 (3)
C1—C2—C3	120.11 (3)	N1—C7—C1	118.87 (3)
C1—C2—H2	120	N1—C8—C9	113.54 (3)
C3—C2—H2	120.0	N1—C8—H8A	109.3
C2—C3—C4	120.05 (3)	N1—C8—H8B	109.4
C2—C3—H3	120.1	C9—C8—H8A	109
C4—C3—H3	120	C9—C8—H8B	109
C3—C4—C5	120.08 (3)	H8A—C8—H8B	107
C3—C4—H4	120	O2—C9—O3	124.95 (3)
C5—C4—H4	120	O2—C9—C8	109.75 (3)
C6—C5—C4	120.00 (3)	O3—C9—C8	125.30 (3)
C6—C5—H5	119.5	C7—N1—C8	121.30 (3)
C4—C5—H5	121	C7—N1—H1	117
C1—C6—C5	120.25 (3)	C8—N1—H1	122
C1—C6—H6	120	C9—O2—H9	109.0
C1—C7—N1—C8	-176.78 (4)	H4—C4—C5—C6	180 (2)
C1—C7—N1—H1	4 (3)	H4—C4—C5—H5	-1 (4)
C1—C6—C5—C4	0.52 (5)	C5—C6—C1—C7	177.81 (5)
C1—C6—C5—H5	-179 (4)	H5—C5—C6—H6	1 (6)
C1—C2—C3—C4	-0.50 (5)	C6—C1—C7—O1	-12.37 (5)
C1—C2—C3—H3	180 (4)	C6—C1—C7—N1	167.76 (5)
C2—C1—C7—O1	166.66 (5)	H6—C6—C1—C7	-2 (5)
C2—C1—C7—N1	-13.21 (5)	C7—N1—C8—C9	-88.03 (5)
C2—C1—C6—C5	-1.26 (5)	C7—N1—C8—H8A	151 (3)
C2—C1—C6—H6	179 (4)	C7—N1—C8—H8B	33 (5)
C2—C3—C4—C5	-0.24 (6)	C8—N1—C7—O1	3.35 (5)
C2—C3—C4—H4	-180 (1)	C8—C9—O2—H9	179 (3)
H2—C2—C1—C7	2 (5)	H8A—C8—N1—H1	-30 (2)
H2—C2—C1—C6	-179 (5)	H8A—C8—C9—O2	-51 (3)
H2—C2—C3—C4	179 (5)	H8A—C8—C9—O3	130 (4)
H2—C2—C3—H3	0 (6)	H8B—C8—N1—H1	-147 (7)
C3—C2—C1—C7	-177.76 (6)	H8B—C8—C9—O2	65 (2)
C3—C2—C1—C6	1.25 (6)	H8B—C8—C9—O3	-114 (2)
C3—C4—C5—C6	0.23 (6)	C9—C8—N1—H1	92 (6)
C3—C4—C5—H5	180 (4)	N1—C8—C9—O2	-172.64 (5)

H3—C3—C4—C5	179 (5)	N1—C8—C9—O3	7.80 (6)
H3—C3—C4—H4	0 (5)	O1—C7—N1—H1	-176 (3)
C4—C5—C6—H6	-180 (4)	O3—C9—O2—H9	-1 (3)

Table S9. *Hydrogen-bond geometry (Å, º) for (IAM_MoPro)*

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C8—H8*B*···O3^{i}	1.10	2.54	3.5956 (6)	161
C4—H4···O2^{ii}	1.09	2.57	3.1786 (5)	114
N1—H1···C2	1.02	2.50	2.9193 (5)	104
O2—H9···O1^{iii}	1.00	1.68	2.6534 (5)	163
C2—H2···O1^{iv}	1.09	2.38	3.4409 (5)	166
C8—H8*A*···C6^{iv}	1.10	2.74	3.4845 (6)	125
N1—H1···O1^{iv}	1.02	2.01	2.9553 (5)	153

Symmetry codes: (i) *x*-1/2, -*y*+3/2, -*z*+2; (ii) *x*, *y*, *z*-1; (iii) *x*+1/2, -*y*+3/2, -*z*+2; (iv) -*x*+1, *y*-1/2, -*z*+3/2.

Table S10. *Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2) for (IAM_shelx)*

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.39576 (5)	0.63962 (4)	0.58464 (4)	0.01144 (5)
C2	0.46749 (6)	0.52386 (5)	0.51968 (4)	0.01397 (6)
H2	0.524053	0.451396	0.564858	0.017*
C3	0.45590 (6)	0.51492 (6)	0.38867 (5)	0.01645 (7)
H3	0.505176	0.436769	0.344712	0.020*
C4	0.37198 (6)	0.62069 (6)	0.32222 (4)	0.01646 (7)
H4	0.364544	0.614726	0.233023	0.020*
C5	0.29893 (6)	0.73527 (6)	0.38669 (5)	0.01636 (7)
H5	0.241555	0.807039	0.341378	0.020*
C6	0.31018 (6)	0.74439 (5)	0.51747 (4)	0.01434 (6)
H6	0.259629	0.821934	0.561238	0.017*
C7	0.40743 (5)	0.65975 (4)	0.72403 (4)	0.01117 (5)
C8	0.46938 (5)	0.55963 (5)	0.92978 (4)	0.01334 (5)
H8A	0.459587	0.459377	0.965858	0.016*
H8B	0.380515	0.618466	0.959681	0.016*
C9	0.61684 (5)	0.62938 (5)	0.97856 (4)	0.01261 (5)
N1	0.46273 (5)	0.54938 (4)	0.79395 (3)	0.01294 (5)
O1	0.36571 (5)	0.77896 (4)	0.77349 (3)	0.01455 (5)
O2	0.62201 (5)	0.61874 (6)	1.10332 (4)	0.01829 (6)
O3	0.71455 (5)	0.68679 (6)	0.91376 (4)	0.02006 (7)
H1	0.493 (2)	0.4700 (19)	0.7538 (19)	0.036 (4)*
H9	0.7006 (18)	0.6563 (18)	1.1289 (15)	0.029 (4)*

Table S11. *Atomic displacement parameters (Å^2) for (IAM_shelx)*

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.01241 (12)	0.01172 (11)	0.01018 (10)	0.00024 (9)	-0.00041 (8)	-0.00002 (8)
C2	0.01644 (14)	0.01424 (13)	0.01121 (11)	0.00236 (11)	-0.00072 (10)	-0.00111 (10)
C3	0.01823 (16)	0.01959 (17)	0.01153 (12)	0.00228 (13)	0.00043 (11)	-0.00225 (11)
C4	0.01601 (15)	0.02277 (18)	0.01060 (11)	-0.00047 (13)	-0.00019 (10)	0.00071 (12)
C5	0.01673 (15)	0.01956 (17)	0.01278 (13)	0.00167 (13)	-0.00205 (11)	0.00284 (12)

C6	0.01542 (14)	0.01484 (13)	0.01276 (12)	0.00258 (11)	-0.00143 (10)	0.00070 (10)
C7	0.01197 (11)	0.01117 (10)	0.01036 (10)	-0.00033 (8)	0.00022 (9)	-0.00026 (8)
C8	0.01390 (12)	0.01584 (13)	0.01029 (11)	-0.00165 (10)	-0.00045 (9)	0.00108 (10)
C9	0.01320 (12)	0.01387 (12)	0.01076 (11)	-0.00083 (10)	0.00046 (9)	0.00000 (9)
N1	0.01657 (12)	0.01214 (10)	0.01010 (9)	0.00067 (9)	-0.00099 (8)	0.00007 (8)
O1	0.01802 (12)	0.01238 (10)	0.01326 (10)	0.00146 (9)	0.00195 (9)	-0.00198 (8)
O2	0.01851 (14)	0.02632 (17)	0.01005 (9)	-0.00604 (12)	-0.00098 (9)	-0.00018 (10)
O3	0.01811 (14)	0.02761 (18)	0.01445 (12)	-0.00767 (13)	0.00250 (10)	0.00125 (12)

Table S12. *Geometric parameters (Å, º) for (IAM_shelx)*

C1—C6	1.4007 (6)	C6—H6	0.9500
C1—C2	1.4015 (6)	C7—O1	1.2549 (5)
C1—C7	1.4933 (5)	C7—N1	1.3349 (5)
C2—C3	1.3958 (6)	C8—N1	1.4451 (5)
C2—H2	0.9500	C8—C9	1.5185 (6)
C3—C4	1.3955 (8)	C8—H8A	0.9900
C3—H3	0.9500	C8—H8B	0.9900
C4—C5	1.3961 (8)	C9—O3	1.2095 (6)
C4—H4	0.9500	C9—O2	1.3278 (5)
C5—C6	1.3933 (6)	N1—H1	0.876 (18)
C5—H5	0.9500	O2—H9	0.809 (16)
C6—C1—C2	119.56 (4)	C1—C6—H6	119.9
C6—C1—C7	117.18 (4)	O1—C7—N1	121.14 (4)
C2—C1—C7	123.25 (4)	O1—C7—C1	119.98 (4)
C3—C2—C1	120.08 (4)	N1—C7—C1	118.88 (3)
C3—C2—H2	120.0	N1—C8—C9	113.60 (4)
C1—C2—H2	120.0	N1—C8—H8A	108.8
C4—C3—C2	120.04 (4)	C9—C8—H8A	108.8
C4—C3—H3	120.0	N1—C8—H8B	108.8
C2—C3—H3	120.0	C9—C8—H8B	108.8
C3—C4—C5	120.07 (4)	H8A—C8—H8B	107.7
C3—C4—H4	120.0	O3—C9—O2	125.04 (4)

C5—C4—H4	120.0	O3—C9—C8	125.21 (4)
C6—C5—C4	120.01 (4)	O2—C9—C8	109.75 (4)
C6—C5—H5	120.0	C7—N1—C8	121.35 (4)
C4—C5—H5	120.0	C7—N1—H1	116.9 (13)
C5—C6—C1	120.23 (4)	C8—N1—H1	121.7 (13)
C5—C6—H6	119.9	C9—O2—H9	109.4 (11)

Table S13. *Hydrogen-bond geometry (Å, º) for (IAM_shelx)*

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C8—H8*B*···O3^{i}	0.99	2.64	3.5963 (7)	161
N1—H1···O1^{ii}	0.876 (18)	2.143 (19)	2.9566 (6)	154.2 (19)
O2—H9···O1^{iii}	0.809 (16)	1.863 (16)	2.6537 (6)	165.3 (16)

Symmetry codes: (i) *x*-1/2, -*y*+3/2, -*z*+2; (ii) -*x*+1, *y*-1/2, -*z*+3/2; (iii) *x*+1/2, -*y*+3/2, -*z*+2.

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