Supporting Information

Synthesis, crystal structure, *in silico* studies of novel 2,4-dimethoxy-tetrahydropyrimido[4,5-b]quinolin-6(7H)-ones

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Table S1. Comparisons of computed geometrical parameters of **4a** using various basis sets in the gaseous phase with the corresponding experimental ones.

Structural Parameter	B3LYP							
	6-31G	6-31G(d)	6-31G (d, p)	6-311G	6-311G+ (2d, p)	6-311G++ (d, p)	6-311G++ (d, 2p)	X-ray data
Bond length(Å)								
C3-C20	1.544	1.538	1.538	1.542	1.532	1.537	1.538	1.532
C3-C21	1.548	1.543	1.542	1.546	1.539	1.541	1.542	1.539
C3-C4	1.548	1.542	1.542	1.548	1.539	1.541	1.541	1.528
C4-C5	1.523	1.527	1.527	1.519	1.522	1.525	1.525	1.5
C5-O1	1.257	1.229	1.229	1.256	1.225	1.225	1.226	1.197
C5-C6	1.459	1.465	1.465	1.457	1.461	1.463	1.463	1.488
C6-C7	1.53	1.526	1.526	1.53	1.524	1.526	1.527	1.509
C6-C1	1.367	1.362	1.362	1.364	1.356	1.36	1.359	1.318
C7-C12	1.541	1.537	1.537	1.541	1.535	1.535	1.536	1.537
C7-C8	1.517	1.516	1.516	1.516	1.514	1.514	1.514	1.517
C8-C9	1.403	1.402	1.402	1.4	1.398	1.401	1.401	1.386
C8-C11	1.402	1.396	1.396	1.398	1.391	1.393	1.393	1.392
C9-O2	1.362	1.341	1.342	1.362	1.339	1.339	1.338	1.325
O2-C18	1.466	1.433	1.433	1.466	1.435	1.436	1.437	1.443
C9-N2	1.347	1.336	1.336	1.347	1.332	1.334	1.333	1.351
N2-C10	1.349	1.337	1.338	1.348	1.333	1.335	1.335	1.315
C10-O3	1.361	1.342	1.343	1.361	1.34	1.341	1.342	1.365
O3-C19	1.464	1.43	1.43	1.464	1.432	1.433	1.434	1.427
C10-N3	1.34	1.331	1.331	1.34	1.326	1.327	1.327	1.32
N3-C11	1.352	1.341	1.34	1.353	1.336	1.337	1.337	1.356
C11-N1	1.387	1.386	1.387	1.387	1.385	1.387	1.387	1.361
N1-C1	1.386	1.38	1.38	1.387	1.379	1.38	1.38	1.389
C1-C2	1.51	1.508	1.508	1.509	1.504	1.506	1.506	1.505
C2-C3	1.551	1.545	1.545	1.551	1.542	1.543	1.543	1.536
C12-C13	1.404	1.4	1.4	1.401	1.395	1.398	1.398	1.378
C12-C17	1.405	1.4	1.401	1.403	1.395	1.398	1.398	1.384
C13-C14	1.399	1.395	1.394	1.398	1.391	1.394	1.393	1.388
C14-C15	1.392	1.393	1.393	1.388	1.387	1.39	1.39	1.374
C15-Cl1	1.833	1.763	1.763	1.835	1.761	1.762	1.762	1.731
C15-C16	1.392	1.393	1.393	1.389	1.387	1.391	1.391	1.348
C16-C17	1.4	1.396	1.394	1.397	1.391	1.393	1.394	1.395
R^2 value	0.9513	**0.9715**	0.9711	0.9507	**0.9734**	0.972	0.9724	1
Bond angle (°)								
C20-C3-C21	109.05	109.02	109.02	109.1	109.01	109.02	108.96	108.9
C21-C3-C4	110.48	110.49	110.5	110.41	110.43	110.44	110.46	110.5
C3-C4-C5	114.2	114.64	114.7	114.28	114.97	114.92	114.87	114.65
C4-C5-O1	120.08	120.35	120.32	120.07	120.2	120.23	120.31	121.02
C4-C5-C6	118.41	117.84	117.8	118.49	118.07	117.91	117.89	116.92
C5-C6-C7	117.93	118.07	118.1	118.23	118.53	118.54	118.51	115.53
C5-C6-C1	119.99	119.95	119.97	119.94	119.76	119.85	119.87	120.68
C7-C6-C1	122.08	121.98	121.92	121.84	121.7	121.6	121.62	123.78

C6-C7-C12	111.12	111.07	111.08	111.13	111.15	111.03	110.98	110.15
C6-C7-C8	109.87	109.57	109.55	109.9	109.56	109.49	109.51	109.61
C7-C8-C9	123.91	124.28	124.32	123.99	124.52	124.51	124.52	121.91
C7-C8-C11	122.04	122.21	122.18	121.72	121.86	121.9	121.9	122.21
C9-C8-C11	114.02	113.49	113.48	114.26	113.6	113.56	113.56	115.72
C8-C9-N2	123.33	123.6	123.62	123.12	123.42	123.38	123.41	122.95
C8-C9-O2	117.55	117.07	117.1	117.56	117.16	117.23	117.22	118.28
C9-O2-C18	118.46	117.9	117.89	118.73	118.19	118.38	118.4	118.18
C9-N2-C10	116.61	115.94	115.9	116.77	116.18	116.21	116.19	114.23
C10-O3-C19	118.06	117.66	117.64	118.34	117.95	118.16	118.1	116.53
N2-C10-N3	126.06	127.29	127.29	125.97	126.95	126.98	127	130.38
C10-N3-C11	115.49	114.6	114.62	115.42	114.9	114.88	114.85	113.68
N3-C11-C8	124.46	125.06	125.07	124.42	124.89	124.95	124.95	123.01
C8-C11-N1	119.4	119.01	118.99	119.4	118.98	118.94	118.94	120.79
C11-N1-C1	122.14	121.91	121.88	122.01	121.64	121.65	121.69	120.58
N1-C1-C6	120.59	120.64	120.66	120.44	120.59	120.56	120.61	122.21
C6-C1-C2	123.62	123.77	123.76	123.74	123.96	123.87	123.89	123.6
C1-C2-C3	113.16	113.45	113.45	113.3	113.72	113.64	113.57	113.1
C2-C3-C4	107.71	107.65	107.62	107.74	107.71	107.69	107.73	108
C7-C12-C13	120.09	120.21	120.18	119.99	120.1	120.04	120.09	121.96
C12-C13-C14	120.96	121.15	121.21	120.97	121.21	121.18	121.18	120.32
C13-C14-C15	118.77	119.19	119.14	118.74	119.18	119.19	119.19	119.69
C14-C15-Cl1	119.13	119.59	119.54	119.09	119.59	119.58	119.59	119.22
C14-C15-C16	121.91	120.96	120.98	122	120.96	120.58	120.97	120.57
C15-C16-C17	118.58	119.05	119.07	118.53	119.07	119.03	119.05	120.46
C16-C17-C12	121.09	121.27	121.28	121.15	121.31	121.34	121.27	119.7
C17-C12-C13	118.69	118.38	118.31	118.61	118.28	118.29	118.34	119.2
R^2 value	0.9149	**0.9279**	**0.927**	0.908	0.9165	0.9156	0.9174	1

Table S2. Comparisons of computed geometrical parameters of **4b**, **4c** and **4d** using B3LYP/6-31G(d) basis sets in the gaseous phase with the corresponding experimental ones.

Structural Parameter	B3LYP/ 6-31G(d)	X-ray data of **4b**	Structural Parameter	B3LYP/ 6-31G(d)	X-ray data of **4c**	Structural Parameter	B3LYP/ 6-31G(d)	X-ray data of **4d**
Bond length(Å)								
C3-C13	1.542	1.519	C1-C2	1.547	1.532	C3-C12	1.542	1.523
C3-C12	1.537	1.528	C2-C12	1.542	1.526	C3-C13	1.538	1.527
C3-C4	1.543	1.528	C2-C13	1.537	1.522	C3-C4	1.542	1.525
C4-C5	1.528	1.5	C2-C3	1.544	1.525	C4-C5	1.528	1.503
C5-O1	1.23	1.231	C3-C4	1.527	1.502	C5-O1	1.229	1.233
C5-C6	1.465	1.447	C4-O1	1.229	1.234	C5-C6	1.464	1.446
C6-C7	1.525	1.52	C4-C5	1.466	1.445	C6-C7	1.525	1.519
C6-C1	1.361	1.351	C5-C11	1.362	1.357	C6-C1	1.362	1.357
C7-C14	1.537	1.532	C5-C6	1.527	1.523	C7-C14	1.537	1.529
C7-C8	1.517	1.513	C6-C14	1.538	1.529	C7-C8	1.517	1.512
C8-C9	1.403	1.395	C6-C7	1.516	1.515	C8-C9	1.403	1.392
C8-C11	1.396	1.375	C7-C10	1.39	1.379	C8-C11	1.396	1.378
C9-O2	1.342	1.347	C7-C8	1.408	1.392	C9-O2	1.341	1.347
O2-C20	1.432	1.436	C8-O2	1.34	1.35	O2-C20	1.432	1.438
C9-N2	1.336	1.326	O2-C20	1.434	1.434	C9-N2	1.336	1.329
N2-C10	1.337	1.338	C8-N3	1.331	1.326	N2-C10	1.338	1.339
C10-O3	1.343	1.345	N3-C9	1.339	1.336	C10-O3	1.343	1.348
O3-C21	1.429	1.433	C9-O1	1.344	1.347	O3-C21	1.43	1.434
C10-N3	1.331	1.313	O1-C21	1.429	1.442	C10-N3	1.331	1.313
N3-C11	1.341	1.352	C9-N2	1.329	1.32	N3-C11	1.34	1.351
C11-N1	1.387	1.373	N2-C10	1.348	1.35	C11-N1	1.386	1.373
N1-C1	1.382	1.367	C10-N1	1.387	1.376	N1-C1	1.381	1.371
C1-C2	1.508	1.497	N1-C11	1.382	1.368	C1-C2	1.509	1.496
C2-C3	1.545	1.521	C11-C1	1.509	1.501	C2-C3	1.545	1.528
C14-C15	1.401	1.379	C14-C15	1.394	1.383	C14-C15	1.4	1.386
C14-C19	1.401	1.381	C15-C16	1.401	1.387	C15-C16	1.393	1.38
C15-C16	1.395	1.39	C16-O3	1.369	1.374	C16-Cl1	1.763	1.745
C16-C17	1.396	1.368	O3-C22	1.417	1.418	C16-C17	1.394	1.367
C17-C18	1.396	1.364	C16-C17	1.4	1.378	C17-C18	1.395	1.372
C18-C19	1.396	1.384	C17-C18	1.398	1.383	C18-C19	1.395	1.382
-	-	-	C18-C19	1.391	1.377	C19-C14	1.4	1.385
-	-	-	C19-C14	1.404	1.392	-	-	-
R^2 value	**0.9827**			**0.9881**			**0.9916**	
Bond angle (°)								
C12-C3-C13	109.04	109.27	C1-C2-C3	107.79	107.23	C12-C3-C13	108.98	108.99
C13-C3-C4	110.45	110.42	C1-C2-C12	110.79	110.31	C12-C3-C4	110.51	110.44
C3-C4-C5	114.65	116.2	C12-C2-C13	109.08	108.47	C3-C4-C5	114.63	115.79
C4-C5-O1	120.25	119.65	C2-C3-C4	114.44	115.97	C4-C5-O1	120.4	119.94
C4-C5-C6	117.87	118.94	C3-C4-O4	120.46	119.89	C4-C5-C6	117.81	118.73
C5-C6-C7	118.11	118.84	C3-C4-C5	117.66	118.45	C5-C6-C7	117.94	118.48
C5-C6-C1	119.91	118.89	C4-C5-C6	117.96	118.3	C5-C6-C1	120.04	119.37
C7-C6-C1	121.98	122.27	C4-C5-C11	119.92	119.63	C7-C6-C1	122.02	122.14
C6-C7-C14	111.16	111.19	C11-C5-C6	122.11	122.05	C6-C7-C14	111.12	111.08
C6-C7-C8	109.57	109.51	C5-C6-C14	110.85	112.33	C6-C7-C8	109.71	109.42
C7-C8-C9	124.34	124.26	C5-C6-C7	109.75	109.44	C7-C8-C9	124.24	124.13
C7-C8-C11	122.2	121.79	C6-C7-C8	124.25	123.63	C7-C8-C11	122.23	121.65
C9-C8-C11	113.43	113.86	C6-C7-C10	122.24	122.17	C9-C8-C11	113.5	114.09
C8-C9-O2	117.08	116.45	C10-C7-C8	113.49	113.98	C8-C9-O2	117.05	116.39
C9-O2-C20	117.87	117.67	C7-C8-O2	116.79	115.93	C9-O2-C20	117.95	117.19
C8-C9-N2	123.64	124.48	C8-O2-C20	117.58	117.56	C8-C9-N2	123.59	124.47
C9-N2-C10	115.92	114.39	C7-C8-N3	123.95	124.66	C9-N2-C10	115.9	114.16
C10-O3-C21	117.57	116.47	C8-N3-C9	115.66	114.3	C10-O3-C21	117.62	116.78
N2-C10-N3	127.32	128.49	C9-O1-C21	117.33	116.44	N2-C10-N3	127.34	128.72

C10-N3-C11	114.55	114.2	N3-C9-N2	127.39	128.5	C10-N3-C11	114.59	114.24
N3-C11-C8	125.11	124.5	C9-N2-C10	114.74	114.22	N3-C11-C8	125.05	124.24
C8-C11-N1	119	120.5	N2-C10-C7	124.75	124.26	C8-C11-N1	119.02	120.33
C11-N1-C1	121.84	121.46	C-C10-N1	119.4	120.36	C11-N1-C1	121.92	121.48
N1-C1-C6	120.67	121.09	C10-N1-C11	121.75	121.26	N1-C1-C6	120.69	120.69
C6-C1-C2	123.85	123.82	N1-C11-C5	120.63	121.53	C6-C1-C2	123.71	123.61
C1-C2-C3	113.42	114.01	C5-C11-C1	123.75	123.26	C1-C2-C3	113.45	113.8
C2-C3-C4	107.63	107.22	C11-C1-C2	113.38	113.61	C2-C3-C4	107.67	107.76
C14-C15-C16	120.69	120.61	C14-C15-C16	120.94	121.2	C14-C15-C16	119.66	119.87
C15-C16-C17	120.3	120.32	C15-C16-O3	115.44	115.33	C15-C16-Cl1	119.16	119.39
C16-C17-C18	119.48	119.68	C16-O3-C22	118.06	118.04	C15-C16-C17	121.72	121.51
C17-C18-C19	120.11	120.21	C15-C16-C17	119.95	120.42	C16-C17-C18	118.39	118.91
C18-C19-C14	120.84	121.01	C16-C17-C18	118.89	118.34	C17-C18-C19	120.6	120.53
C19-C14-C15	118.58	118.15	C17-C18-C19	121.25	121.67	C18-C19-C14	120.63	120.67
-	-	-	C18-C19-C14	119.91	120.13	C19-C14-C15	119	118.49
-	-	-	C19-14-C15	119.05	118.22	-	-	-
R^2 value	**0.9802**			**0.9795**			**0.9813**	

Crystal X-ray report of compound **4a [CCDC: 2133239]**.

checkCIF (basic structural check) running

Checking for embedded fcf data in CIF ...
Found embedded fcf data in CIF. Extracting fcf data from uploaded CIF, please wait . .

checkCIF/PLATON (basic structural check)

Structure factors have been supplied for datablock(s) 101

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary
Please wait while processing .... Interpreting this report

Structure factor report

Datablock: 101

Bond precision: C-C = 0.0082 A Wavelength=0.71073

Cell: a=6.1119(17) b=12.856(3) c=13.503(2)
alpha=74.018(10) beta=83.479(15) gamma=76.619(15)

Temperature: 296 K

	Calculated	Reported
Volume	990.9(4)	990.8(4)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C21 H22 Cl N3 O3	?
Sum formula	C21 H22 Cl N3 O3	C21 H22 Cl N3 O3
Mr	399.87	399.86
Dx,g cm-3	1.340	1.340
Z	2	2
Mu (mm-1)	0.220	0.220
F000	420.0	420.0
F000'	420.47	
h,k,lmax	7,15,16	7,15,16
Nref	3503	2395
Tmin,Tmax	0.944,0.965	0.941,0.966
Tmin'	0.940	

Correction method= # Reported T Limits: Tmin=0.941 Tmax=0.966 AbsCorr = MULTI-SCAN

Data completeness= 0.684 Theta(max)= 24.997

R(reflections)= 0.0636(1393) wR2(reflections)= 0.2058(2395)

S = 1.083 Npar= 261

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level A

PLAT029_ALERT_3_A _diffrn_measured_fraction_theta_full value Low . 0.684 Why?

Author Response: Even though crystal data was attempted to collected up to 0.78 \%A resolution, the crystal (the largest available) still diffracted quite weakly at high angle.

Alert level B

PLAT911_ALERT_3_B Missing FCF Refl Between Thmin & STh/L= 0.595 1109 Report

Author Response: These reflections were probably affected by unexpected deviations in their

intensities for symmetry equivalent measurements and omitted during initial data reduction.

Alert level C

PLAT088_ALERT_3_C Poor Data / Parameter Ratio ..... 9.18 Note
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.00816 Ang.
PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ... -2.303 Report
PLAT934_ALERT_3_C Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers .. 1 Check

Alert level G

PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical ? Check
PLAT793_ALERT_4_G Model has Chirality at C7 (Centro SPGR) S Verify
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF .... 1 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ..... 2.0 Low
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged Please Check
PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res .. 50.0 Degree
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 0 Info

1 **ALERT level A** = Most likely a serious problem - resolve or explain
1 **ALERT level B** = A potentially serious problem, consider carefully
4 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
8 **ALERT level G** = General information/check it is not something unexpected

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
2 ALERT type 2 Indicator that the structure model may be wrong or deficient
8 ALERT type 3 Indicator that the structure quality may be low
1 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

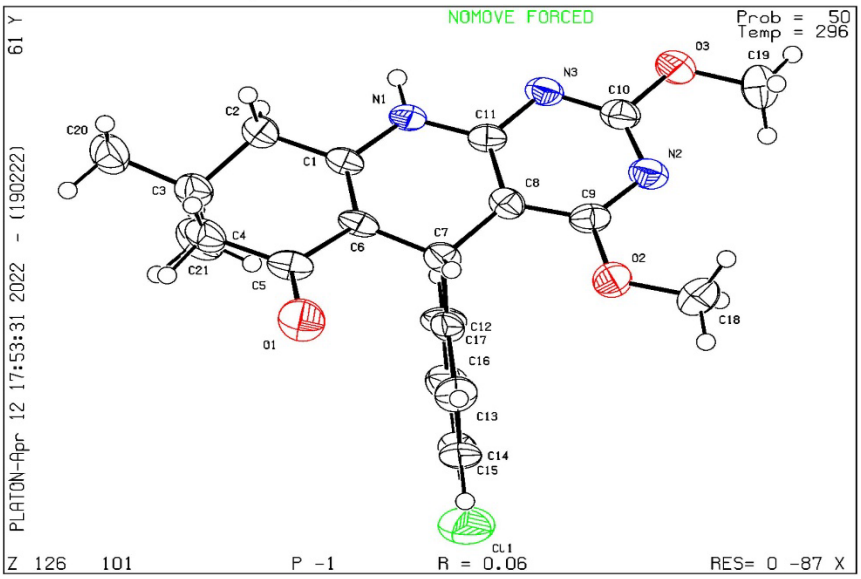
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 19/02/2022; check.def file version of 19/02/2022

Datablock 101 - ellipsoid plot



Crystal X-ray report of compound **4b [CCDC: 2149722]**.

checkCIF (basic structural check) running

Checking for embedded fcf data in CIF ...
Found embedded fcf data in CIF. Extracting fcf data from uploaded CIF, please wait ...

checkCIF/PLATON (basic structural check)

Structure factors have been supplied for datablock(s) 102

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary
Please wait while processing .... Interpreting this report

Structure factor report

Datablock: 102

Bond precision: C-C = 0.0023 A Wavelength=0.71073

Cell: a=11.3367(6) b=13.5799(7) c=13.0546(6)
alpha=90 beta=108.872(2) gamma=90

Temperature: 296 K

	Calculated	Reported
Volume	1901.73(17)	1901.73(17)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C21 H23 N3 O3	?
Sum formula	C21 H23 N3 O3	C21 H23 N3 O3
Mr	365.42	365.42
Dx,g cm-3	1.276	1.276
Z	4	4
Mu (mm-1)	0.087	0.087
F000	776.0	776.0
F000'	776.33	
h,k,lmax	13,16,15	13,16,15
Nref	3353	3353
Tmin,Tmax	0.977,0.986	0.976,0.986
Tmin'	0.976	

Correction method= # Reported T Limits: Tmin=0.976 Tmax=0.986 AbsCorr = MULTI-SCAN

Data completeness= 1.000 Theta(max)= 25.000

R(reflections)= 0.0389(2604) wR2(reflections)= 0.1134(3353)

S = 1.556 Npar= 253

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level B

PLAT230_ALERT_2_B Hirshfeld Test Diff for C3 --C4 . 8.3 s.u.

Author Response: This alarm is due to the elongated ADPs of carbon atoms which suggest that these are probably disordered.

Alert level C

PLAT230_ALERT_2_C Hirshfeld Test Diff for C3 --C13 . 6.5 s.u.

Author Response: This alarm is due to the elongated ADPs of carbon atoms which suggest that

these are probably disordered.

PLAT230_ALERT_2_C Hirshfeld Test Diff for C17 --C18 . 5.5 s.u.

Author Response: This alarm is due to the elongated ADPs of carbon atoms which suggest that these are probably disordered.

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C3 Check
PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ... -0.299 Report

Alert level G

PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical ? Check
PLAT793_ALERT_4_G Model has Chirality at C7 (Centro SPGR) S Verify
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still 50% Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ..... 4.7 Low
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged Please Check
PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res .. 50.0 Degree
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 3 Info

0 **ALERT level A** = Most likely a serious problem - resolve or explain
1 **ALERT level B** = A potentially serious problem, consider carefully
4 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
8 **ALERT level G** = General information/check it is not something unexpected

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
6 ALERT type 2 Indicator that the structure model may be wrong or deficient
3 ALERT type 3 Indicator that the structure quality may be low
1 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

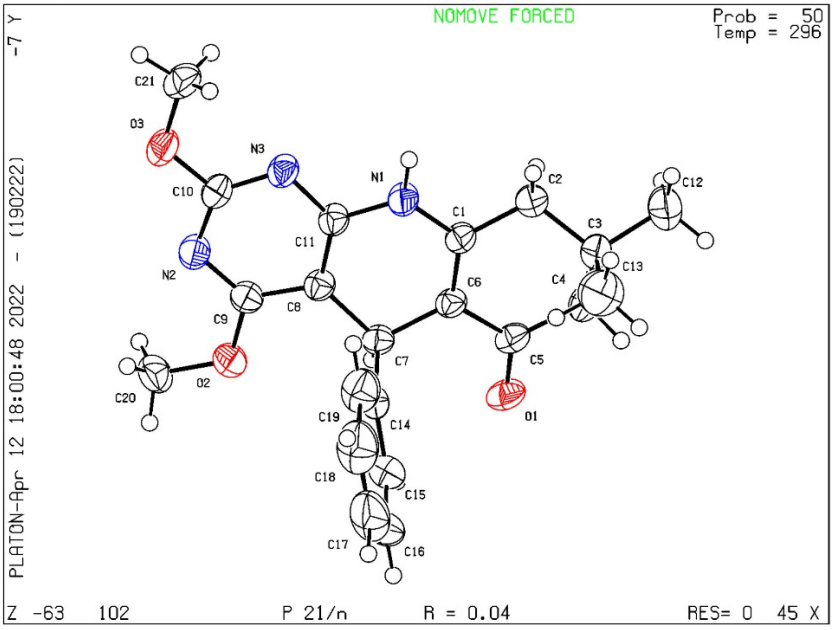
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 19/02/2022; check.def file version of 19/02/2022

Datablock 102 - ellipsoid plot



Crystal X-ray report of compound **4c [CCDC: 2157100]**.

checkCIF (basic structural check) running

Checking for embedded fcf data in CIF ...
Found embedded fcf data in CIF. Extracting fcf data from uploaded CIF, please wait . . .

checkCIF/PLATON (basic structural check)

Structure factors have been supplied for datablock(s) 105

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary
Please wait while processing .... Interpreting this report

Structure factor report

Datablock: 105

Bond precision: C-C = 0.0028 A Wavelength=0.71073

Cell: a=12.5837(13) b=13.0752(17) c=13.0356(16)
alpha=90 beta=110.844(5) gamma=90

Temperature: 296 K

	Calculated	Reported
Volume	2004.4(4)	2004.4(4)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C22 H25 N3 O4	?
Sum formula	C22 H25 N3 O4	C22 H25 N3 O4
Mr	395.45	395.45
Dx,g cm-3	1.311	1.310
Z	4	4
Mu (mm-1)	0.091	0.091
F000	840.0	840.0
F000'	840.38	
h,k,lmax	14,15,15	14,15,15
Nref	3527	3528
Tmin,Tmax	0.978,0.991	0.978,0.991
Tmin'	0.978	

Correction method= # Reported T Limits: Tmin=0.978 Tmax=0.991 AbsCorr = MULTI-SCAN

Data completeness= 1.000 Theta(max)= 24.999

R(reflections)= 0.0429(2344) wR2(reflections)= 0.1160(3528)

S = 1.029 Npar= 268

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

PLAT230_ALERT_2_C Hirshfeld Test Diff for C2 --C13 . 5.7 s.u.
PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ... -0.721 Report

Alert level G

PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..... 1 Report
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical ? Check
PLAT793_ALERT_4_G Model has Chirality at C6 (Centro SPGR) S Verify
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still 32% Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ..... 3.5 Low

PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res .. 50.0 Degree
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 4 Info

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
2 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
8 **ALERT level G** = General information/check it is not something unexpected

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
2 ALERT type 2 Indicator that the structure model may be wrong or deficient
3 ALERT type 3 Indicator that the structure quality may be low
1 ALERT type 4 Improvement, methodology, query or suggestion
2 ALERT type 5 Informative message, check

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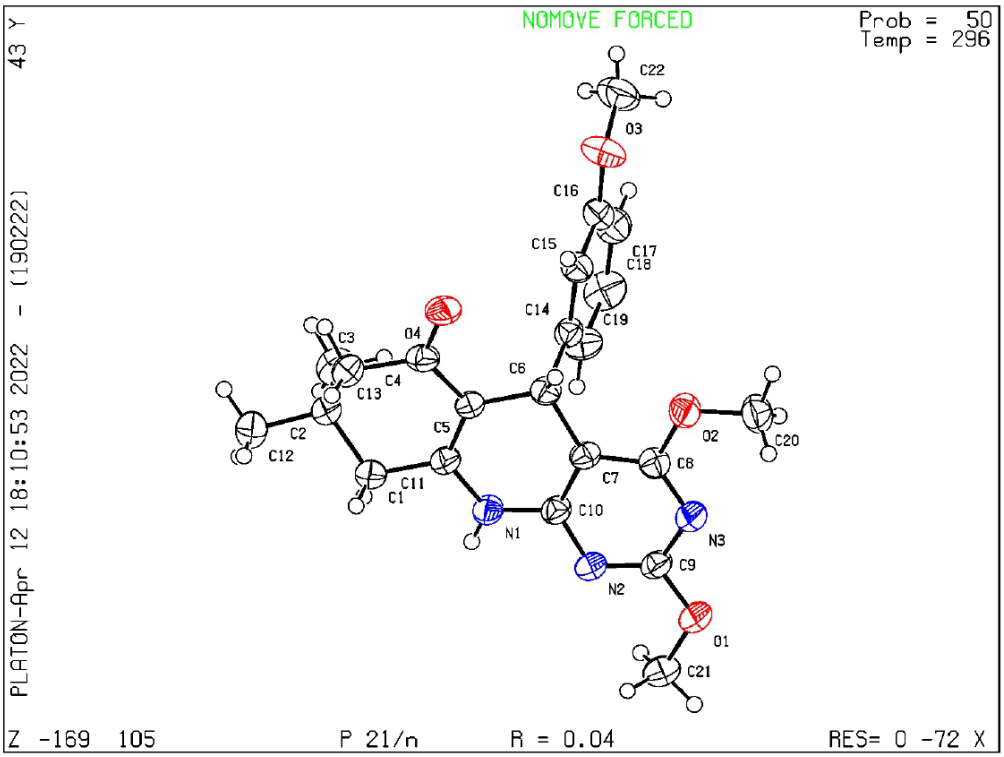
PLATON version of 19/02/2022; check.def file version of 19/02/2022

Datablock 105 - ellipsoid plot



Crystal X-ray report of compound **4d [CCDC: 2157099]**.

checkCIF (basic structural check) running

Checking for embedded fcf data in CIF ...
Found embedded fcf data in CIF. Extracting fcf data from uploaded CIF, please wait . .

checkCIF/PLATON (basic structural check)

Structure factors have been supplied for datablock(s) 104

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No syntax errors found. CIF dictionary
Please wait while processing .... Interpreting this report

Structure factor report

Datablock: 104

Bond precision: C-C = 0.0031 A Wavelength=0.71073

Cell: a=12.2403(6) b=13.3075(7) c=12.8408(7)
alpha=90 beta=109.168(2) gamma=90

Temperature: 296 K

	Calculated	Reported
Volume	1975.65(18)	1975.65(18)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C21 H22 Cl N3 O3	?
Sum formula	C21 H22 Cl N3 O3	C21 H22 Cl N3 O3
Mr	399.87	399.86
Dx,g cm-3	1.344	1.344
Z	4	4
Mu (mm-1)	0.221	0.221
F000	840.0	840.0
F000'	840.93	
h,k,lmax	14,15,15	14,15,15
Nref	3473	3472
Tmin,Tmax	0.969,0.978	0.947,0.978
Tmin'	0.946	

Correction method= # Reported T Limits: Tmin=0.947 Tmax=0.978 AbsCorr = MULTI-SCAN

Data completeness= 1.000 Theta(max)= 25.000

R(reflections)= 0.0409(2579) wR2(reflections)= 0.1089(3472)

S = 1.015 Npar= 257

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level G

PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..... 1 Report
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical ? Check
PLAT793_ALERT_4_G Model has Chirality at C7 (Centro SPGR) S Verify
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still 53% Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ..... 4.0 Low
PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res .. 50.0 Degree
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 9 Info

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2 ALERT type 3 Indicator that the structure quality may be low
1 ALERT type 4 Improvement, methodology, query or suggestion
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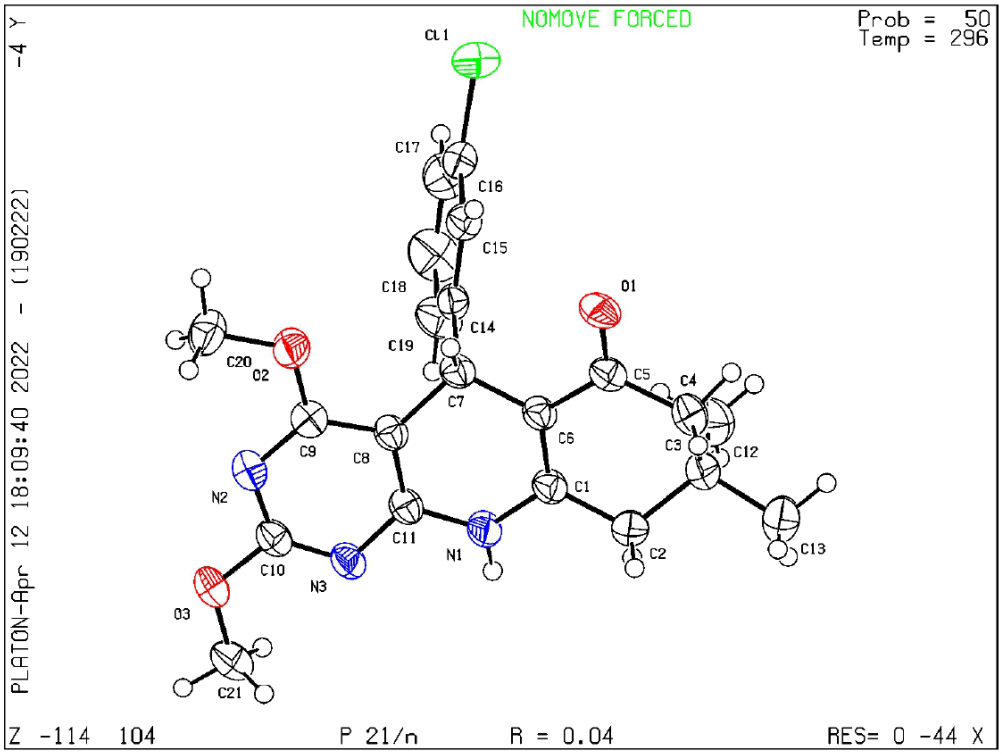
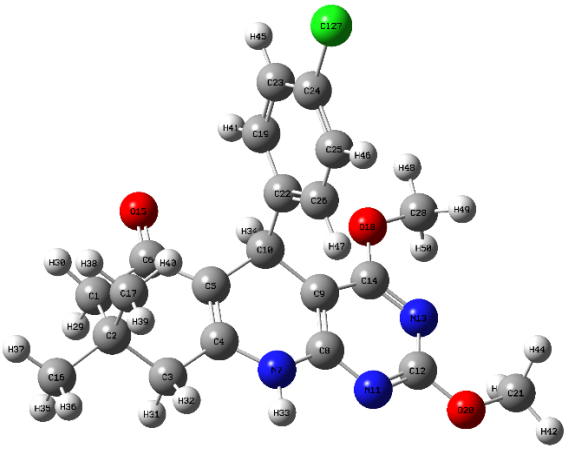
PLATON version of 19/02/2022; check.def file version of 19/02/2022

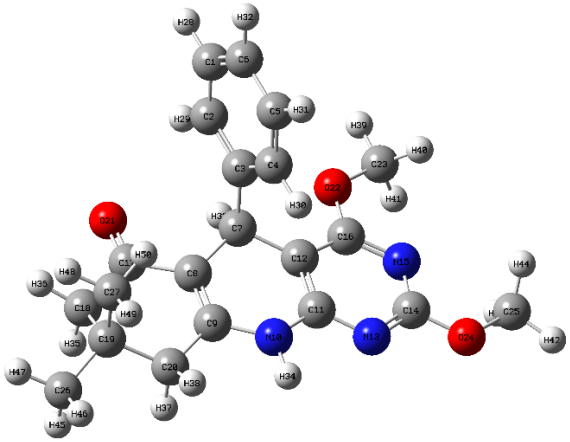
Datablock 104 - ellipsoid plot



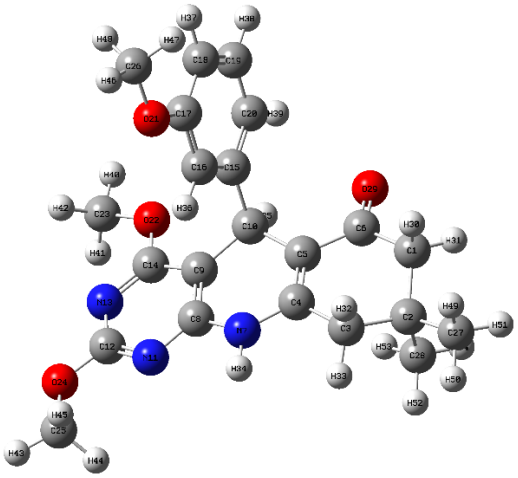
Optimised structure of Molecule **4(a-d)** using B3LYP/6-31G(d) basis sets in gaseous state.



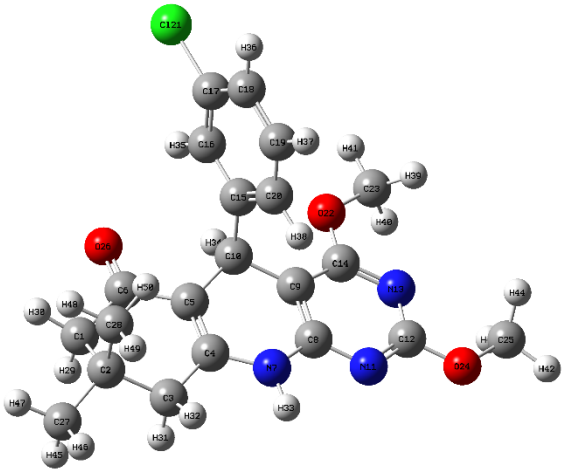
(4a)



(4b)



(4c)



(4d)