

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 231123_bn_2ph_0m_sq

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 Interpreting this report

Datablock: 231123_bn_2ph_0m_sq

Bond precision: C-C = 0.0037 Å Wavelength=1.34139

Cell: a=42.767(3) b=17.7275(12) c=17.8667(12)
 alpha=90 beta=109.868(2) gamma=90

Temperature: 170 K

	Calculated	Reported
Volume	12739.4(15)	12739.3(15)
Space group	C 2/c	C 2/c
Hall group	-C 2yc	-C 2yc
Moiety formula	C39 H28 B N [+ solvent]	?
Sum formula	C39 H28 B N [+ solvent]	C39 H28 B N O0
Mr	521.43	521.43
Dx, g cm ⁻³	1.087	1.087
Z	16	16
Mu (mm ⁻¹)	0.299	0.299
F000	4384.0	4384.0
F000'	4392.42	
h, k, lmax		53, 22, 22
Nref		13028
Tmin, Tmax	0.986, 0.994	
Tmin'	0.982	

Correction method= Not given

Data completeness= Theta(max)= 57.345

R(reflections)= 0.0711(7408)

wR2(reflections)=
0.2014(13028)

S = 1.131

Npar= 739

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

PLAT052_ALERT_1_C	Info on Absorption Correction Method	Not Given	Please Do !
PLAT085_ALERT_2_C	SHELXL Default Weighting Scheme is not Optimized		Please Check
PLAT220_ALERT_2_C	NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range	4.2 Ratio	
PLAT222_ALERT_3_C	NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range	4.1 Ratio	
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C26 Check	
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C27 Check	
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C25 Check	
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C28 Check	
PLAT905_ALERT_3_C	Negative K value in the Analysis of Variance ...	-2.507 Report	
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	64 Report	

42	0	0,	-28	14	1,	-10	18	1,	8	18	1,	15	17	1,	40	4	1,
41	9	1,	-10	2	2,	-10	18	2,	-1	9	2,	6	18	2,	-5	1	3,
0	4	3,	4	18	3,	32	10	3,	-44	2	4,	-6	18	4,	-4	0	4,
-4	18	4,	-2	18	4,	0	18	4,	-42	6	5,	28	14	5,	32	8	5,
-42	6	6,	-17	19	6,	-42	6	7,	-41	7	7,	-28	14	7,	-11	17	7,
-7	5	7,	-1	17	7,	-44	2	8,	-23	15	8,	-29	13	9,	-21	15	9,
-12	16	9,	-37	9	10,	-17	15	10,	-2	18	10,	-40	6	11,	-34	10	11,
-29	15	11,	-41	3	12,	-36	8	12,	-30	10	13,	-27	11	13,	18	4	13,
-39	1	14,	-32	8	14,	-16	12	14,	-8	12	14,	-37	1	15,	-31	5	16,
-24	8	16,	-19	9	16,	-7	9	16,	-4	6	17,	3	1	17,	-25	1	18,
-24	2	18,	-4	0	18,	-10	4	20,	-7	3	20,						



Alert level G

ABSMU01_ALERT_1_G	Calculation of _exptl_absorpt_correction_mu		
	not performed for this radiation type.		
CELLZ01_ALERT_1_G	Difference between formula and atom_site contents detected.		
CELLZ01_ALERT_1_G	ALERT: Large difference may be due to a		
	symmetry error - see SYMMG tests		
	From the CIF: _cell_formula_units_Z 16		
	From the CIF: _chemical_formula_sum C39 H28 B N O0		
	TEST: Compare cell contents of formula and atom_site data		

atom	Z*formula	cif sites	diff
C	624.00	624.00	0.00
H	448.00	448.00	0.00
B	16.00	16.00	0.00
N	16.00	16.00	0.00
O	16.00	0.00	16.00

PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	1 Report	
PLAT041_ALERT_1_G	Calc. and Reported SumFormula Strings Differ	Please Check	
	Calc: C39 H28 B N		
	Rep.: C39 H28 B N O0		
PLAT128_ALERT_4_G	Alternate Setting for Input Space Group C2/c	I2/a Note	
PLAT186_ALERT_4_G	The CIF-Embedded .res File Contains ISOR Records	1 Report	
PLAT606_ALERT_4_G	Solvent Accessible VOID(S) in Structure	! Info	
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	6 Note	
	C01F H01F C01H H01H C00T H00T		
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	6 Note	
PLAT869_ALERT_4_G	ALERTS Related to the Use of SQUEEZE Suppressed	! Info	

PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .	Please Do !
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min). 1 1 0, 2 0 0,	2 Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	116 Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File -10 2 2, -4 0 4, 0 4 3, 1 1 0, -1 9 2, -7 5 7, -5 1 3,	7 Note
PLAT965_ALERT_2_G	The SHELXL WEIGHT Optimisation has not Converged	Please Check
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	0 Info
PLAT992_ALERT_5_G	Repd & Actual _reflns_number_gt Values Differ by	2 Check

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

6 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
10 ALERT type 2 Indicator that the structure model may be wrong or deficient
5 ALERT type 3 Indicator that the structure quality may be low
6 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 14/11/2023; check.def file version of 14/09/2023

Datablock 231123_bn_2ph_0m_sq - ellipsoid plot

