

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 2BEX-LIG

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: 2BEX-LIG

Bond precision: C-C = 0.0030 A Wavelength=1.54178

Cell: a=49.28(2) b=8.517(3) c=11.787(4)
 alpha=90 beta=100.410(5) gamma=90

Temperature: 566 K

	Calculated	Reported
Volume	4866(3)	4866(3)
Space group	C 2/c	C 1 2/c 1
Hall group	-C 2yc	-C 2yc
Moiety formula	C24 H28 O2, 0.5(C8 H12 N2)	C24 H28 O2, C4 H6 N
Sum formula	C28 H34 N O2	C28 H34 N O2
Mr	416.56	416.56
Dx,g cm-3	1.137	1.137
Z	8	8
Mu (mm-1)	0.546	0.546
F000	1800.0	1800.0
F000'	1804.85	
h,k,lmax	60,10,14	60,10,14
Nref	4842	4729
Tmin,Tmax	0.897,0.897	
Tmin'	0.897	

Correction method= Not given

Data completeness= 0.977 Theta(max)= 72.679

R(reflections)= 0.0621(2886) wR2(reflections)= 0.1887(4729)

S = 0.961 Npar= 296

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	C18	--C19	.	6.0	s.u.
PLAT230_ALERT_2_C	Hirshfeld Test Diff for	C19	--C21	.	6.0	s.u.
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of				C18	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of				C16	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of				C19	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance			5.214	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600			17	Report

● **Alert level G**

PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...				3	Report
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms				1	Report
PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings Differ				Please	Check
PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT Unusually Large				0.11	Report
PLAT128_ALERT_4_G	Alternate Setting for Input Space Group	C2/c			I2/a	Note
PLAT177_ALERT_4_G	The CIF-Embedded .res File Contains DELU Records				2	Report
PLAT432_ALERT_2_G	Short Inter X...Y Contact	O1	..C27		3.02	Ang.
		x,-y,-1/2+z =			6_555	Check
PLAT860_ALERT_3_G	Number of Least-Squares Restraints				2	Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).				2	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600			95	Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...				8	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity				3.8	Low
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.				1	Info

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

1 **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
3 **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 10/08/2020; check.def file version of 06/08/2020

