

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) BW27

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: BW27

Bond precision:	C-C = 0.0069 A	Wavelength=0.71073
Cell:	a=11.569(2)	b=10.294(2) c=15.764(3)
	alpha=90	beta=94.14(3) gamma=90
Temperature:	170 K	
	Calculated	Reported
Volume	1872.5(6)	1872.5(7)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C14 H17 N5 O2, C H Cl3	C14 H17 N5 O2, C H Cl3
Sum formula	C15 H18 Cl3 N5 O2	C15 H18 Cl3 N5 O2
Mr	406.69	406.69
Dx,g cm-3	1.443	1.443
Z	4	4
Mu (mm-1)	0.509	0.509
F000	840.0	840.0
F000'	842.03	
h,k,lmax	13,12,18	13,12,18
Nref	3308	3306
Tmin,Tmax	0.777,0.910	0.797,0.977
Tmin'	0.777	

Correction method= # Reported T Limits: Tmin=0.797 Tmax=0.977
AbsCorr = NUMERICAL

Data completeness= 0.999 Theta(max)= 25.023

R(reflections)= 0.0929(1910) wR2(reflections)= 0.2815(3306)

S = 0.987 Npar= 288

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

PLAT084_ALERT_3_C	High wR2 Value (i.e. > 0.25)	0.28	Report
PLAT245_ALERT_2_C	U(iso) H1N5 Smaller than U(eq) N5 by	0.014	Ang**2
PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor	2.3	Note
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including C11	0.108	Check
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including C11'	0.140	Check
PLAT340_ALERT_3_C	Low Bond Precision on C-C Bonds	0.00689	Ang.
PLAT351_ALERT_3_C	Long C-H (X0.96,N1.08A) C7 - H4C7 .	1.15	Ang.
PLAT351_ALERT_3_C	Long C-H (X0.96,N1.08A) C9 - H6C9 .	1.11	Ang.
PLAT420_ALERT_2_C	D-H Without Acceptor N5 --H2N5 .		Please Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	4.944	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.595		3 Report



Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	8	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	8	Report
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records	2	Report
PLAT177_ALERT_4_G	The CIF-Embedded .res File Contains DELU Records	1	Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records	1	Report
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 3)	100%	Note
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in (Resd 2)	3.08	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in (Resd 3)	1.92	Check
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	6	Note
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	96	Note
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF	1	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	4.0	Low
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	0	Info

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- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
11 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
14 **ALERT level G** = General information/check it is not something unexpected
- 0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
8 ALERT type 2 Indicator that the structure model may be wrong or deficient
9 ALERT type 3 Indicator that the structure quality may be low
8 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check
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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.

