

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 1, 2

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: 1

Bond precision: C-C = 0.0019 Å Wavelength=0.71073

Cell: a=8.9372(4) b=8.7877(5) c=16.8366(8)
 alpha=90 beta=97.888(2) gamma=90

Temperature: 173 K

	Calculated	Reported
Volume	1309.79(11)	1309.79(11)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C14 H18 N6	C14 H18 N6
Sum formula	C14 H18 N6	C14 H18 N6
Mr	270.34	270.34
Dx,g cm-3	1.371	1.371
Z	4	4
Mu (mm-1)	0.089	0.089
F000	576.0	576.0
F000'	576.15	
h,k,lmax	11,11,21	11,10,21
Nref	2686	2656
Tmin,Tmax	0.977,0.982	0.920,0.963
Tmin'	0.976	

Correction method= # Reported T Limits: Tmin=0.920 Tmax=0.963
AbsCorr = EMPIRICAL

Data completeness= 0.989 Theta(max)= 26.415

R(reflections)= 0.0388(2056) wR2(reflections)= 0.1032(2656)

S = 1.058 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 C

PLAT480_ALERT_4_C	Long H...A H-Bond Reported H2	..N4	.	2.71 Ang.
PLAT480_ALERT_4_C	Long H...A H-Bond Reported H4	..N5	.	2.71 Ang.
PLAT480_ALERT_4_C	Long H...A H-Bond Reported H11B	..N1	.	2.78 Ang.
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600		6 Report

Alert level G

PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600	25 Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	3.6 Low
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.		9 Info

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

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

Datablock: 2

Bond precision: C-C = 0.0033 A Wavelength=0.71073

Cell: a=9.6759(10) b=16.3052(8) c=10.0229(11)
alpha=90 beta=90 gamma=90
Temperature: 173 K

	Calculated	Reported
Volume	1581.3(3)	1581.3(3)
Space group	P n m a	P n m a
Hall group	-P 2ac 2n	-P 2ac 2n
Moiety formula	C14 H18 N6, 3(H2 O)	C14 H18 N6, 3(H2 O)
Sum formula	C14 H24 N6 O3	C14 H24 N6 O3
Mr	324.39	324.39
Dx,g cm-3	1.363	1.363
Z	4	4
Mu (mm-1)	0.099	0.099
F000	696.0	696.0
F000'	696.27	
h,k,lmax	12,20,12	11,19,12
Nref	1684	1656
Tmin,Tmax	0.981,0.987	0.912,0.957
Tmin'	0.968	

Correction method= # Reported T Limits: Tmin=0.912 Tmax=0.957
AbsCorr = EMPIRICAL

Data completeness= 0.983

Theta(max)= 26.405

R(reflections)= 0.0493(857)

wR2(reflections)= 0.1043(1656)

S = 0.977

Npar= 164

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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 C3	--C9	.	5.8 s.u.
PLAT245_ALERT_2_C	U(iso) H8	Smaller than U(eq) C8	by	0.026 Ang**2
PLAT245_ALERT_2_C	U(iso) H3W	Smaller than U(eq) O2	by	0.016 Ang**2
PLAT351_ALERT_3_C	Long C-H (X0.96,N1.08A) C6	- H6	.	1.12 Ang.
PLAT480_ALERT_4_C	Long H...A H-Bond Reported H1	..O1	.	2.62 Ang.
PLAT480_ALERT_4_C	Long H...A H-Bond Reported H4A	..O2	.	2.69 Ang.
PLAT480_ALERT_4_C	Long H...A H-Bond Reported H8	..O2	.	2.80 Ang.
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance		10.582 Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance		2.301 Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600		7 Report



Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite			5 Note
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records			1 Report
PLAT860_ALERT_3_G	Number of Least-Squares Restraints		3 Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600		10 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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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.



